

Supporting Information

Cycloaddition Reactions of Azomethine Ylides and 1,3-Dienes on C_{2v} -Symmetrical Pentakisadduct of C_{60}

Radoslav Z. Pavlović[†], Aleksandra Mitrović[†], William H. Coldren[‡], Mira S. Bjelaković[§], Christopher M. Hadad[‡], Veselin R. Maslak[†], Dragana R. Milić^{†*}

[†]Faculty of Chemistry, University of Belgrade, Studentski trg 16, P.O. Box 51, 11158 Belgrade, Serbia

[‡]Department of Chemistry and Biochemistry, The Ohio State University, 100 West 18th Avenue, Columbus, Ohio 43210, United States

[§]Center for Chemistry, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia

Radoslav Pavlovic present address: Department of Chemistry and Biochemistry, The Ohio State University, 100 West 18th Avenue, Columbus, Ohio 43210, United States

Contents

▪ General information	S3
▪ Optimization of reaction conditions of the Prato reaction of sarcosine to the pentakisadduct 1 (Table S1 and Figures S1-S8)	S3
▪ Characterization of hexaadducts 8-15 (Figures S9-S14)	S8
▪ Figure S15: DFT optimized geometries of possible regio- and stereoisomers and the corresponding transition states for DA reaction (1 and cyclopentadiene)	S16
▪ Figure S16: ¹ H NMR spectrum of the mixture of regioisomers 8	S17
▪ Spectral characterization of hexaadduct 8a	S18
▪ Spectral characterization of hexaadduct 8b	S24
▪ Spectral characterization of hexaadducts 8c/8d	S30
▪ Figure S17: ¹ H NMR spectrum of the mixture of regioisomers 9	S36
▪ Spectral characterization of hexaadduct 9a	S37
▪ Spectral characterization of hexaadduct 9b	S43
▪ Figure S18: ¹ H NMR spectrum of the mixture of regioisomers 10	S49
▪ Spectral characterization of hexaadduct 10a	S50
▪ Spectral characterization of hexaadduct 10b	S56
▪ Figure S19: ¹ H NMR spectrum of the mixture of regioisomers 11	S63
▪ Spectral characterization of hexaadduct 11a	S64
▪ Spectral characterization of hexaadduct 11b	S70
▪ Figure S20: ¹ H NMR spectrum of the mixture of regioisomers 12	S76
▪ Spectral characterization of hexaadduct 12a	S77
▪ Spectral characterization of hexaadduct 12b	S83
▪ Spectral characterization of hexaadduct 13a	S89
▪ Spectral characterization of hexaadduct 14a	S95
▪ Spectral characterization of hexaadduct 15a	S101
▪ Computational data	S107

▪ General information

N-methylglycine **2**, dicyclopentadiene and Danishefsky's diene were purchased from Sigma Aldrich and used without further purification. Glycine derivatives **3**,¹ **4**,² **5**,³ **6**,³ **7**,⁴ isoxazolinofullerene monoadduct,⁵ the protected fullerene [5:1]-hexaadduct,⁶ the symmetrical pentakisadduct **1**⁶ and 2,3,5,6-tetramethylenebicyclo[2.2.2]oct-7-ene⁷ were synthesized according to the literature procedures. Flash column chromatography (FCC) and dry-column flash chromatography (DCFC) were carried out with Merck silica gel 0.04–0.063 mm and 0.015–0.04 mm, respectively. Thin layer chromatography (TLC) was carried out on precoated silica gel 60 F₂₅₄ plates. IR spectra (ATR) were recorded with a Perkin–Elmer-FT-IR 1725X spectrophotometer; ν values are given in cm⁻¹. ¹H and ¹³C NMR spectra were recorded with Bruker Avance (¹H at 500 MHz, ¹³C at 125 MHz) and Bruker Ascend 400 (¹H at 400 MHz, ¹³C at 100 MHz) spectrometers. Chemical shifts (δ) are expressed in ppm and coupling constants (*J*) in Hz. TMS was used as an internal reference. The following abbreviations were used for signal multiplicities (s = singlet, br s = broad singlet, br t = broad triplet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet, dd = doublet of doublets, etc.). The homonuclear 2D (DQF-COSY and ROESY) and the heteronuclear 2D ¹H-¹³C spectra (HSQC, HMBC) were recorded with the usual settings. UV spectra were recorded with a GBC-Cintra 40 UV/Vis spectrophotometer. The high-resolution MS spectra were taken with Agilent 6210 LC ESI-MS TOF spectrometer. Reactions induced by microwave irradiation were performed in a Milestone MultiSynth microwave multimode oven by using a MonoPREP kit containing a sealed reaction vessel and a fiber-optic internal probe for the reaction temperature monitoring.

▪ Optimization of reaction conditions of the Prato cycloaddition reaction of sarcosine to the symmetrical pentakisadduct **1** under conventional thermal and Microwave-assisted conditions in different solvents (PhMe, ODCB, EtOAc and MeCN).

A mixture of **1** (5 mg, 0.0033 mmol), paraformaldehyde (0.5 mg, 0.016 mmol, 5 mol equiv.), and sarcosine **2** (0.88 mg, 0.099 mmol, 3 mol equiv) was heated in *solvent* (0.5mL) to reflux, except for ODCB (110 °C), during 1 h (MeCN), 2 h (ODCB and PhMe) and 2.5 h (EtOAc). The resulting mixture was cooled and the solvent was then evaporated to dryness. The residue was purified by DCFC on SiO₂ to give unconsumed pentakisadduct (2.1 mg in PhMe; 0.7 mg in ODCB; 2.1 mg in EtOAc; 0 mg in MeCN) and the mixture of regioisomers (1.6 mg PhMe; 3.2 mg ODCB; 1.7 mg EtOAc; 2.2 mg MeCN), which were analyzed by ¹H NMR spectra (Table S1, Figs S1, S3, S5, S7, respectively).

A mixture of **1** (5 mg, 0.0033 mmol), paraformaldehyde (0.5 mg, 0.016 mmol, 5 mol equiv.), and sarcosine **2** (0.88 mg, 0.099 mmol, 3 mol equiv) was heated in *solvent* (0.5mL) under microwave irradiation for 90 min, with applied pulse of 500W and inner temperature set to reflux. The resulting mixture was cooled and the solvent was then evaporated to dryness. The residue was purified by FCC on SiO₂ to give unconsumed pentakisadduct (2.7 mg in PhMe; 1.1 mg in ODCB; 1 mg in EtOAc; 0 mg in MeCN) and mixture of regioisomers **10** (1.4 mg in PhMe; 2.6 mg in ODCB; 2.8mg in EtOAc; 1.3 mg in MeCN). Relative ratio of regioisomers in the isolated mixtures was calculated by integration of signals corresponding to the pyrrolidine protons in ¹H NMR spectra (Table S1, Figs S2, S4, S6, S8, respectively).

Table S1. Screening of the reaction conditions of Prato cycloaddition reaction of sarcosine to the symmetrical pentakisadduct **1** under conventional heating (CH) and MW-assisted conditions in different solvents.

Heating	Solvent	t ^a (h)	T (°C)	Yield ^b	Recovered 1	Regioisomeric ratio ^c (a:b:c)
CH	ODCB	2	110	62%	15%	57:37:6
MW ^c	ODCB	1.5	Reflux	51%	22%	47:43:10
CH	PhMe	2 h	Reflux	31%	42%	58:42:0
MW	PhMe	1.5	Reflux	27%	54%	53:47:0
CH	EtOAc	3 h	Reflux	34%	43%	59:41:0
MW	EtOAc	1.5	Reflux	54%	20%	54:46:0
CH ^d	MeCN	1	Reflux	42	0%	60:40:0
MW ^e	MeCN	1.5	Reflux	26	0%	48:44:8

^aReactions were monitored by TLC. ^bIsolated yield of mixtures of regioisomers. ^cDetermined by ¹H NMR spectrum of the isolated mixture of regioisomers **8** (Figs S1-S8); ^eMW irradiation with applied pulse of 500 W and inner temperature set to reflux

- Expanded ¹H NMR spectra of the Prato reactions of **1** with sarcosine in different solvents and heating

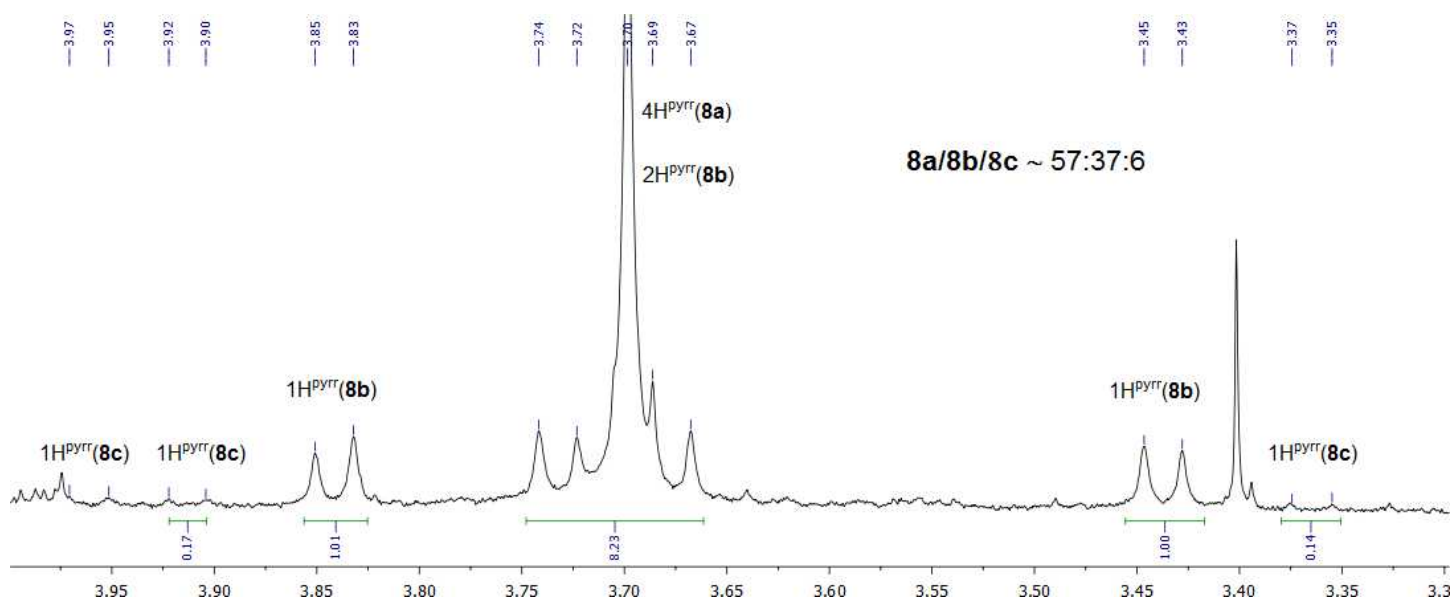


Figure S1. ODCB/CH

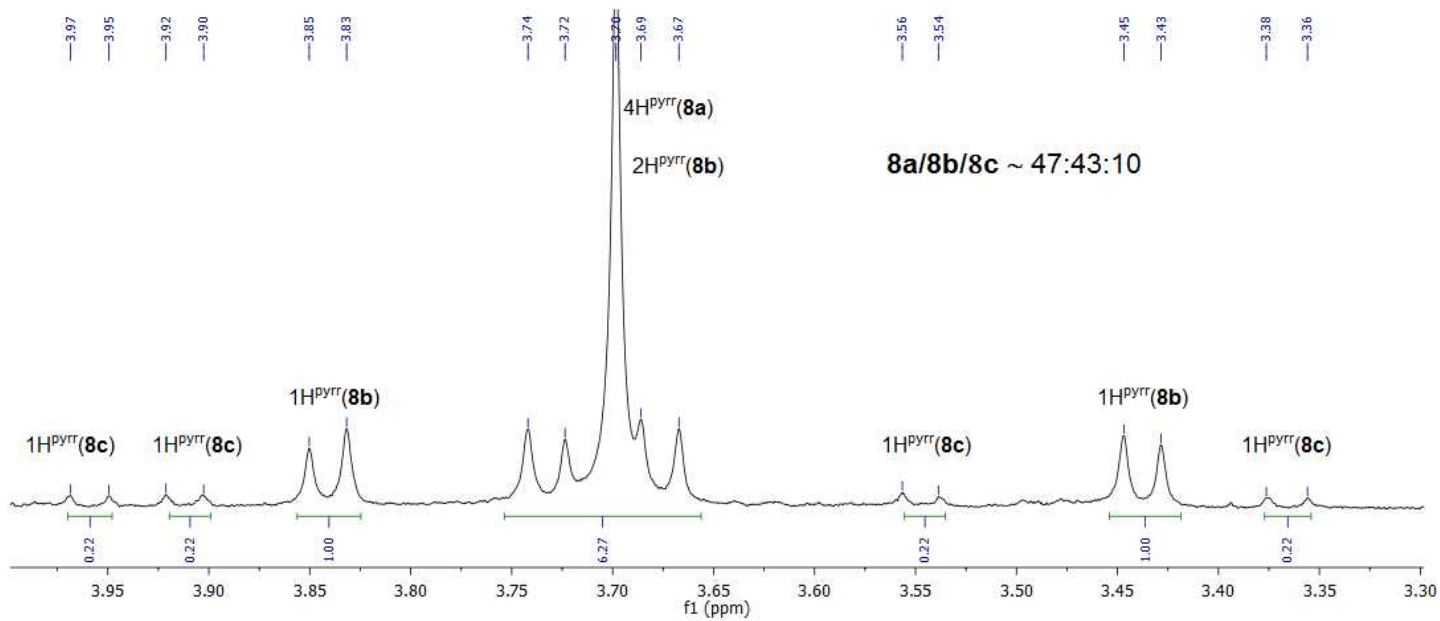


Figure S2. ODCB/MW

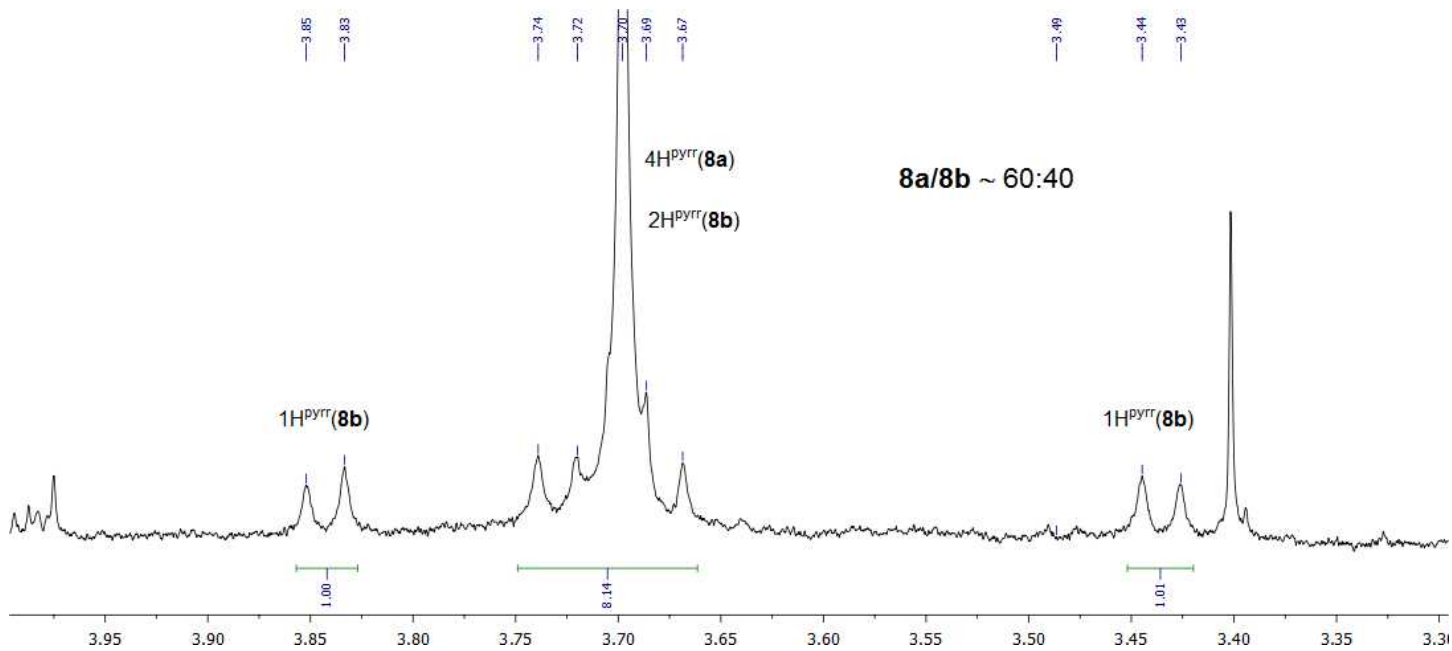


Figure S3. MeCN/CH

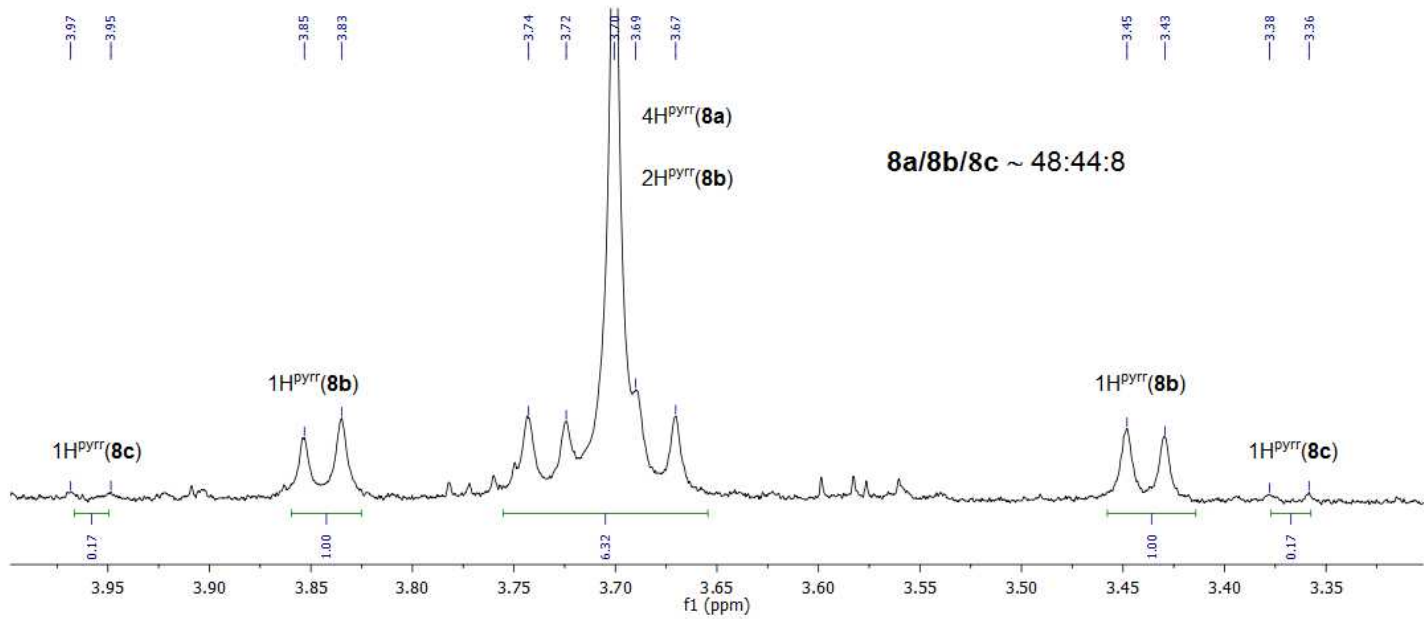


Figure S4. MeCN/MW

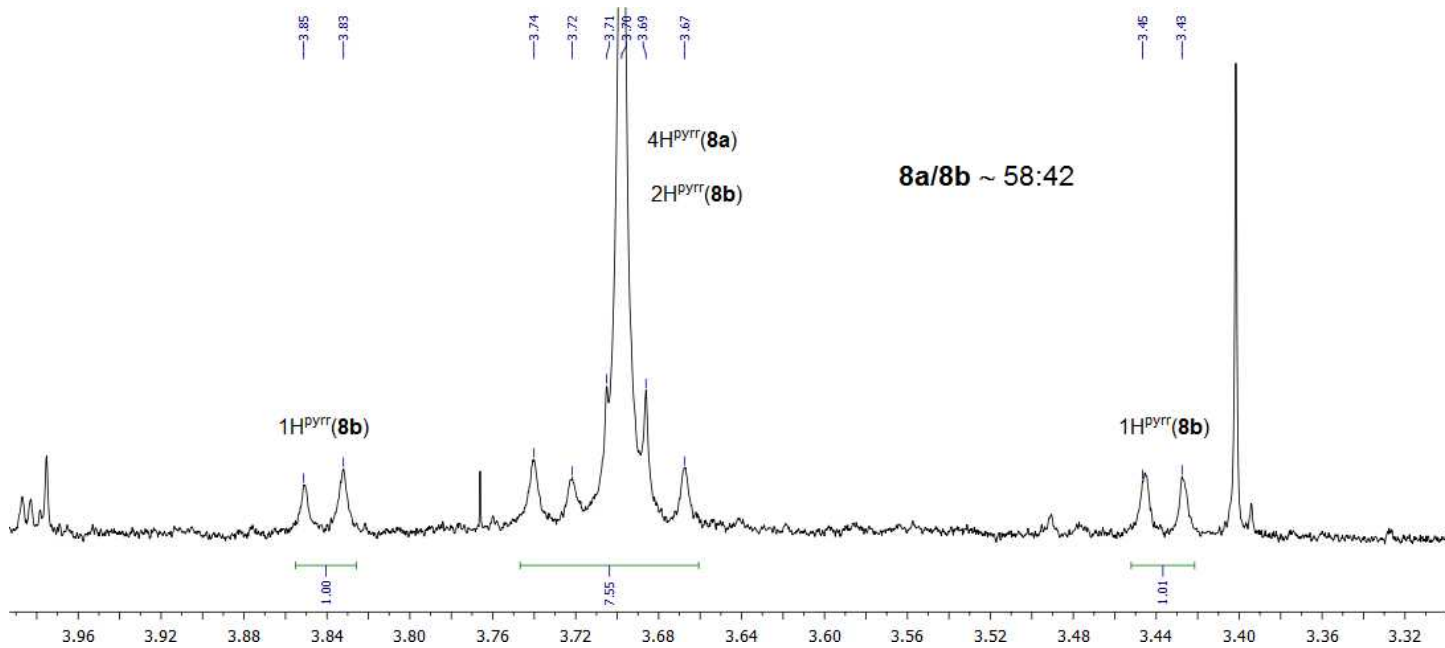


Figure S5. PhMe/CH

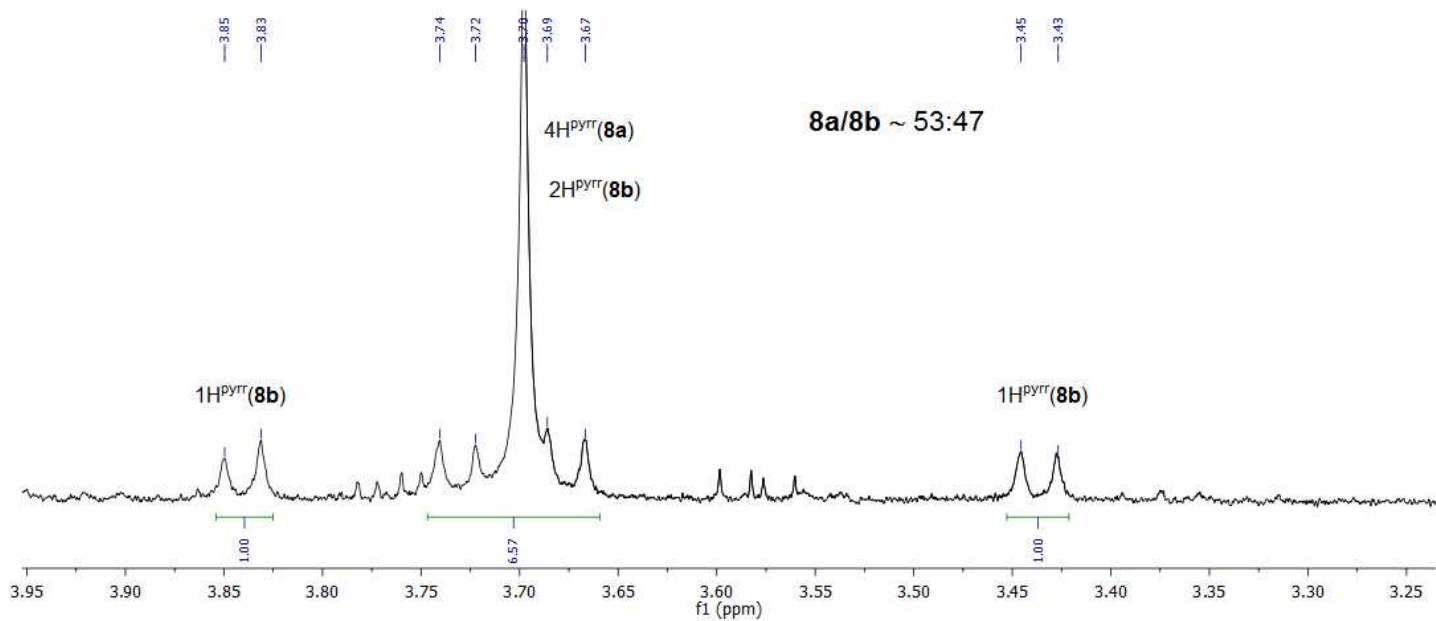


Figure S6. PhMe/MW

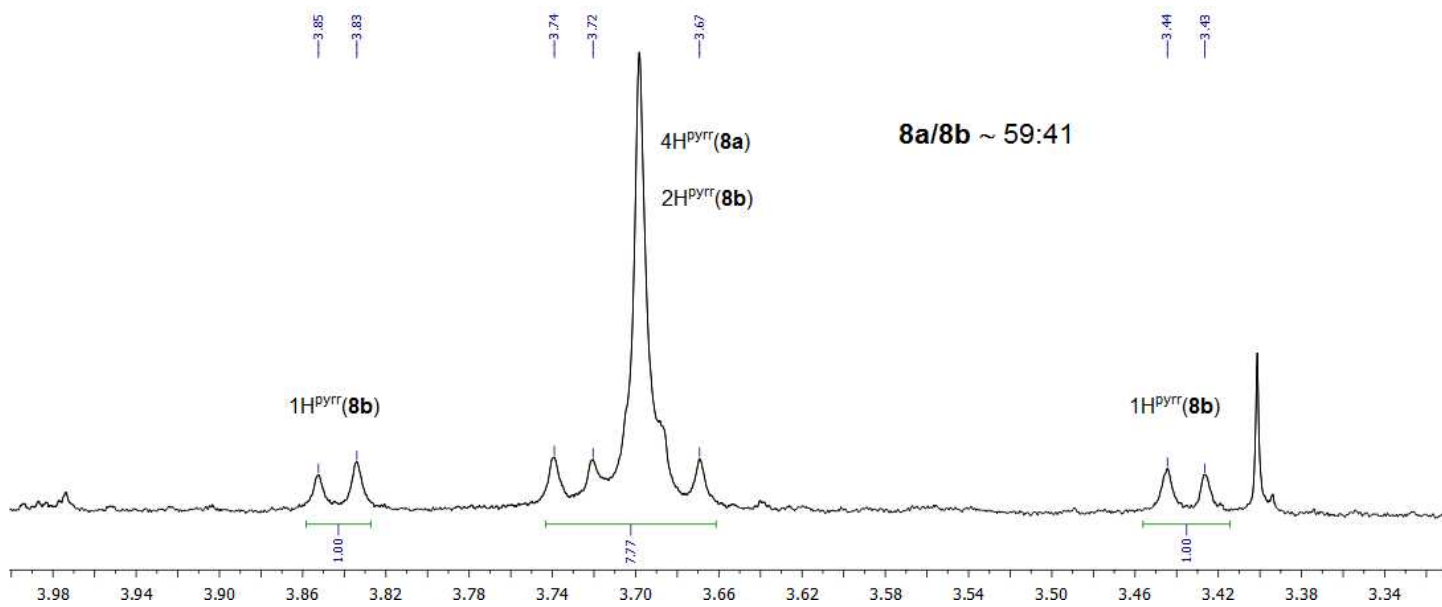


Figure S7. EtOAc/CH

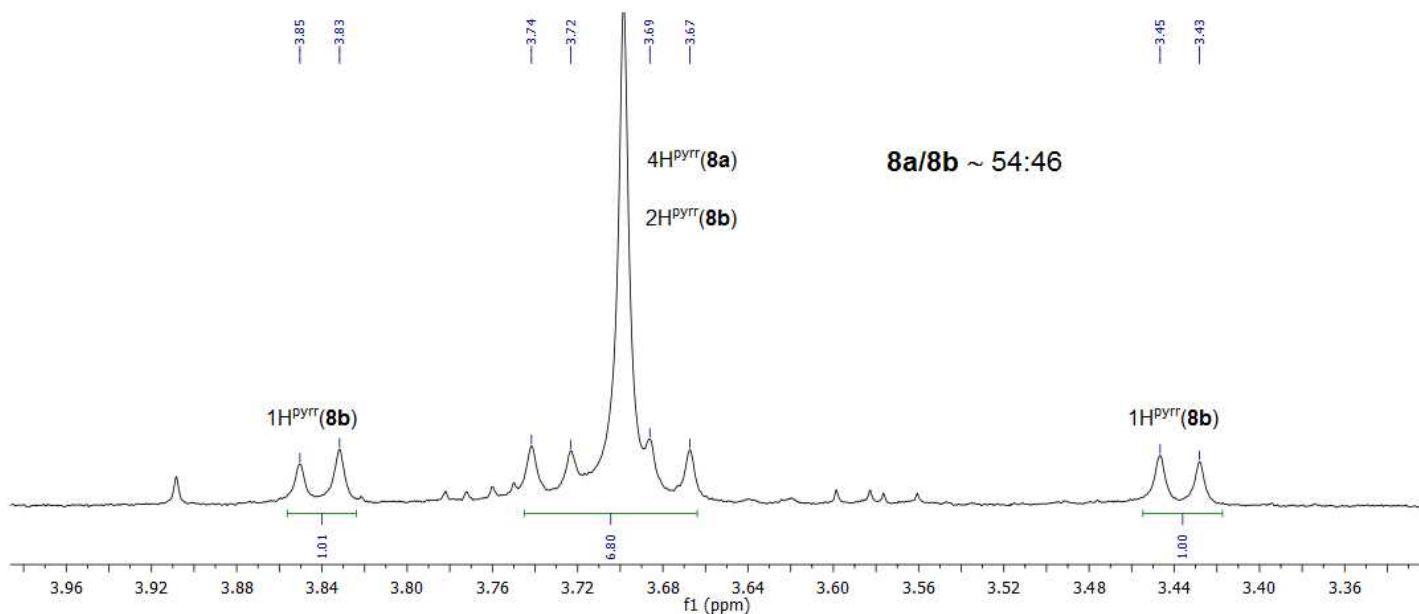


Figure S8. EtOAc/MW

▪ Characterization of hexaadducts 8-15

New mixed C_{60} hexaadducts **8-15** were fully characterized using FTIR, UV/Vis, 1D (^1H and ^{13}C), 2D (COSY, HSQC and HMBC) NMR spectroscopy, and HR (ESI-TOF) mass spectrometry (see Experimental part). The expanded parts of ^1H and ^{13}C NMR spectra of representatives of the Bingel-Prato regioisomers (**8a**, **8b**, and a mixture of **8c/8d**) are presented in Figure S9, as well as the Bingel-Diels-Alder hexaadduct regioisomer **13a** (Figure S10). In addition, the characteristic part of ^1H spectra of the Bingel-Prato **8a,b-12a,b** are given in Figure S11. Unambiguous evidence for the addition pattern of the obtained regioisomers was provided by detailed analysis of their UV and NMR spectra, and by spectral data comparison. Similar trends and a great similarity of the chemical shifts for characteristic signals of the fullerene core, cyclopropane and pyrrolidine moieties in the same type of hexaaddition pattern were observed.

As shown in Figure S9 the C_{2v} -symmetry of **8a** was clearly revealed by the ^1H NMR spectrum which displayed a characteristic singlet at δ 3.7 ppm corresponding to its four symmetry-equivalent pyrrolidine methylene protons. Symmetric regioisomers **9a** and **10a** showed a pyrrolidine protons singlet at almost the same chemical shift compared to **8a**, while a deshielded singlet at δ 4.4 ppm (**12a**) and δ 4.6 ppm (**11a**) (Figure S11) was observed in the ^1H NMR spectra of hexaadducts containing *p*-substituted aromatic ring. The ^1H NMR spectra of all the isolated isomers showed two characteristic groups of signals in the ranges of δ 4.2-4.5 ppm (overlapped quartets, 20H) and 1.2-1.4 ppm (overlapped triplets, 30H) for the CH_2O and CH_3 groups, respectively, of the five diethyl malonates, including the separated signals which belong to the diethyl malonate

unit in *trans*-1 position in regard to the pyrrolidine ring. Also, the ^{13}C NMR spectra of fullerene hexaadduct **8a** (Figure S9), as well as adducts **9a-12a** are in full agreement with their C_{2v} -symmetrical structure and show the three sets of expected fullerene resonances (11 signals, with 1 signal showing of double intensity, or 12 signals, respectively, in the range of 138-153 ppm for the 48 sp^2 -C atoms, 6 signals in the range of 67.0-70.0 ppm for the 12 fullerene sp^3 -C atoms and 2 pyrrolidine methylene carbons, from which 4 signals corresponding to the C-atoms connected to the malonate bridges (1 - *trans*-1, 1 - *e*-edge, and 2 - *e*-face), and 2 signals of double intensity which belong to the fullerene sp^3 -C atoms and pyrrolidine methylene carbons. In addition, the expected signals for the five ethyl malonate addends are located in the range of 41-46 ppm (three signals with the intensity ratio of 2/2/1) for the bridging C-atoms of the malonate esters, at $\delta \sim 164$ ppm (three or four signals with the intensity ratios of 1/2/2 or 1/1/1/2) for the carbonyl groups, and multiple signals at $\delta \sim 14$ ppm and 63 ppm for the $\text{CH}_3\text{CH}_2\text{O}$ group.

In contrast to the symmetric hexaadducts of C_{60} whose pyrrolidine protons appeared as a singlet in the ^1H NMR spectra, the structures of red regioisomer **8b**, as well as **8c/8d** mixture seems to be asymmetric based on the ^1H NMR spectra (Figure S9), which exhibited two doublets pairs corresponding to the nonequivalent pyrrolidinic methylene protons in the δ range of 3.0-4.4 ppm with geminal coupling constants of about 10 Hz and significant chemical shifts difference ($\Delta\delta$ 0.11 and 0.25 ppm (**8b**), 0.36 and 0.60 ppm (**8c**) and 0.63 and 0.92 ppm (**8d**)). With the exception of regioisomer **11b**, all the other red hexaadducts gave the two pairs of doublets in the range of δ 3.3–4.80 ppm belonging to the germinal protons of pyrrolidine ring. The ^1H NMR spectrum of compound **11b** displayed two doublets at δ 4.4 and 4.6 ppm and a singlet at δ 4.74 ppm for the CH_2 protons, whereas the other signals showed no major changes. It was observed that the chemical shifts difference of a one methylene group of hexaadducts with aromatic rings is reduced in *p*-methoxybenzene derivative **12b** ($\Delta\delta=0.07$ ppm) and completely disappears in *p*-nitrobenzene adduct **11b**. The ^{13}C NMR spectra of the obtained red regioisomers (**8b-12b**) and the **8c/8d** mixture of regioisomers display a total of 41-47 (red) and 38 (brown) out of 48 fullerene sp^2 resonances in a wider NMR region (125-152 ppm), thereby reflecting a C_1 symmetrical hexaaddition pattern with a clear difference in the distribution and intensities of the fullerene sp^2 - and sp^3 -C signals. Twelve fullerene sp^3 -C-atom resonances are observed in ^{13}C NMR spectrum of **8b**, two at $\delta=65.7$ and 63.1 ppm for the C-atoms carrying the pyrrolidine ring and ten between δ 66 and 71 ppm for the C-atoms connected to the malonate bridges. The malonate bridge carbon atoms give five signals between δ 41 and 58 ppm, whereas the carbonyl carbon atoms give up to ten signals between δ 163 and 165 ppm. Finally, the ^1H and ^{13}C NMR spectra of all the regioisomers show the presence of all the expected signals of the pyrrolidine *N*-addends.

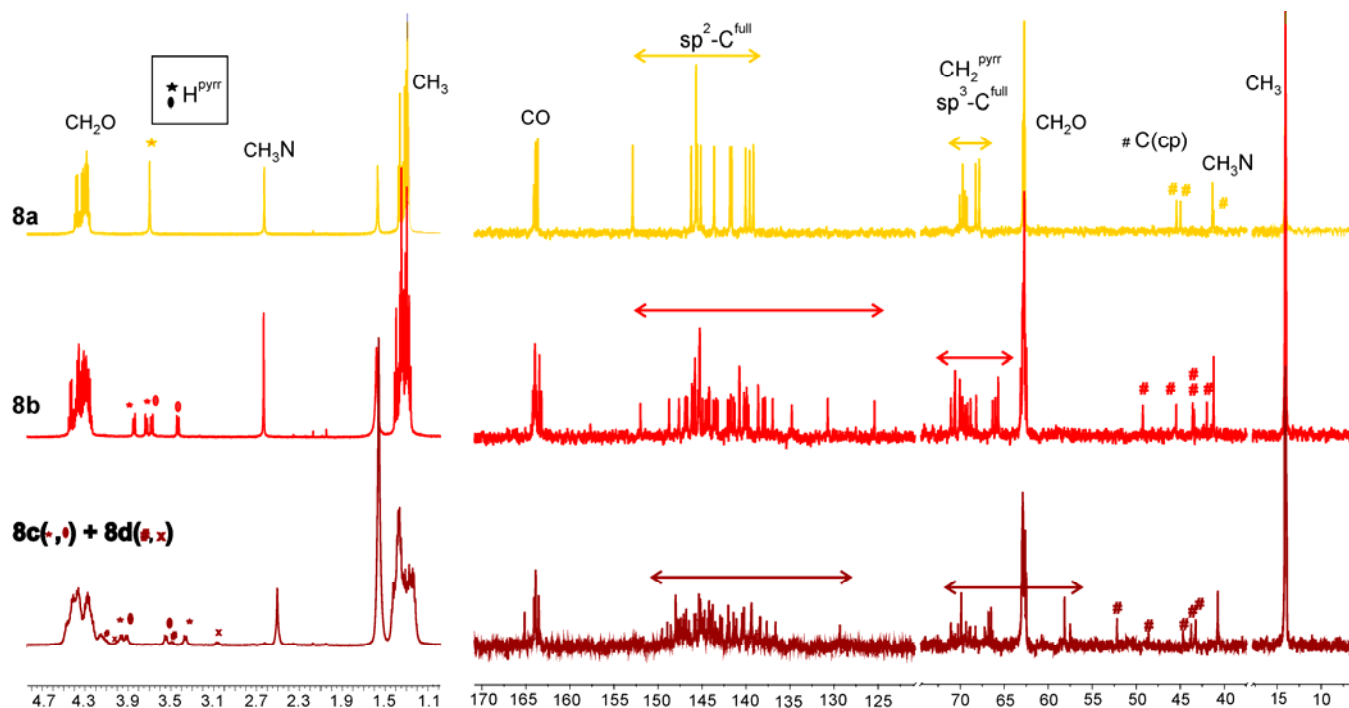


Figure S9. Comparison of the expanded regions of ^1H and ^{13}C NMR spectra of representatives of mixed Bingel-Prato [5:1]-hexaadduct regioisomers **8a**, **8b**, and the **8c/8d** mixture.

Mixed Bingel-Diels-Alder [5:1]-hexaadducts **13a** and **15a** were confirmed to be C_s symmetric, while **14a** was asymmetric. For example, the ^1H -NMR spectrum of **13a** showed single resonances at 6.57 ppm (HC=) and at 3.89 ppm (HC), as well as two doublets at 2.0 and 2.58 ppm (CH_2), indicating that the mirror plane in which lie two *e*-face cyclopropane rings bisects the Diels-Alder addend and the cyclopropane ring in *trans*-1 position (Figure S10). Furthermore, in the ^{13}C NMR spectrum of **13a**, 20 signals (from which 4 signals with double intensity) for the sp^2 carbons of the fullerene skeleton were observed in the region between 138 and 155 ppm clearly indicating a C_s -symmetrical structure. This was further confirmed by the presence of three signals at 164.1, 163.9 and 163.8 ppm corresponding to the carbonyl carbons, one signal at 72.3 ppm corresponding to the sp^3 - C_{60} (Diels-Alder), seven distinct peaks with three of double intensity in the range of 67-71 ppm characteristic for the fullerene sp^3 carbons (cyclopropane), and four signals at δ 45.4 (*e*-face), 45.3 (*e*-face), 45.1 (*e*-edge) and 41.2 ppm (*trans*-1) with the intensity ratio of 1/1/2/1, respectively, attributed to the malonate bridge carbon atoms (for detailed spectroscopic data see SI). In addition, the ^{13}C NMR spectrum **13a** consists of three signals at δ = 137.2, 56.5 and 45.4 ppm for the carbon atoms of the DA addend.

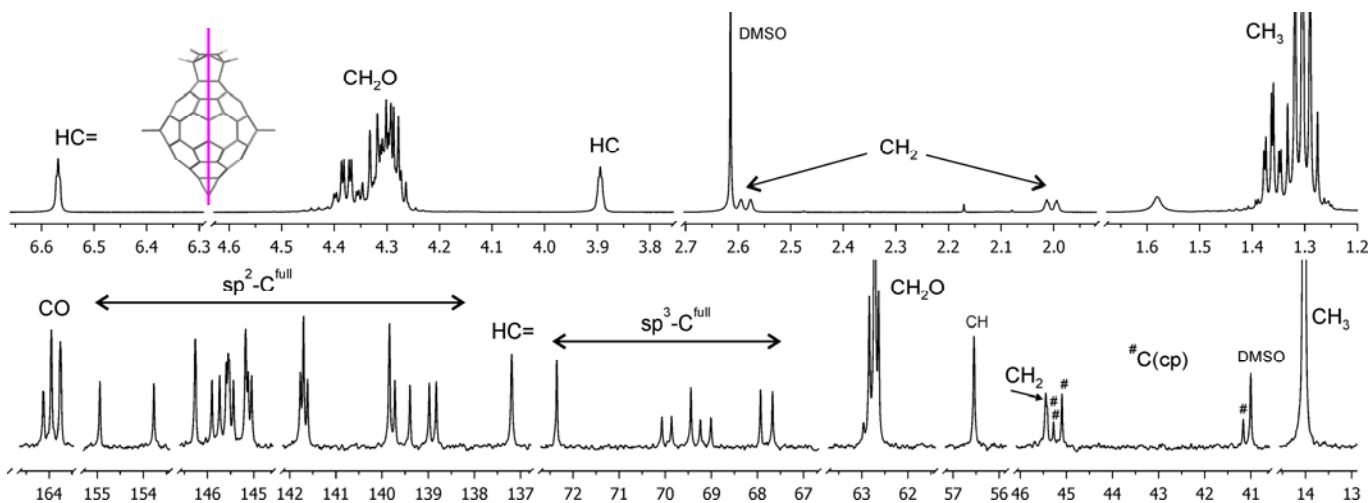


Figure S10. Expanded parts of ^1H and ^{13}C NMR spectra of C_s symmetric Bingel-Diels-Alder [5:1]-hexaadduct **13a**.

The second C_s symmetrical Bingel-Diels-Alder regioisomer (**15a**) gave in addition to the characteristic signals of the DA addend in the NMR spectra very similar spectral regions for fullerene sp^2 - and sp^3 -C and cyclopropane C atoms with the additional signals of fullerene sp^3 -C belonging to the DA addend. Regioisomer **14a** is confirmed to be asymmetric on the basis of the NMR analyses (see Experimental and S95).

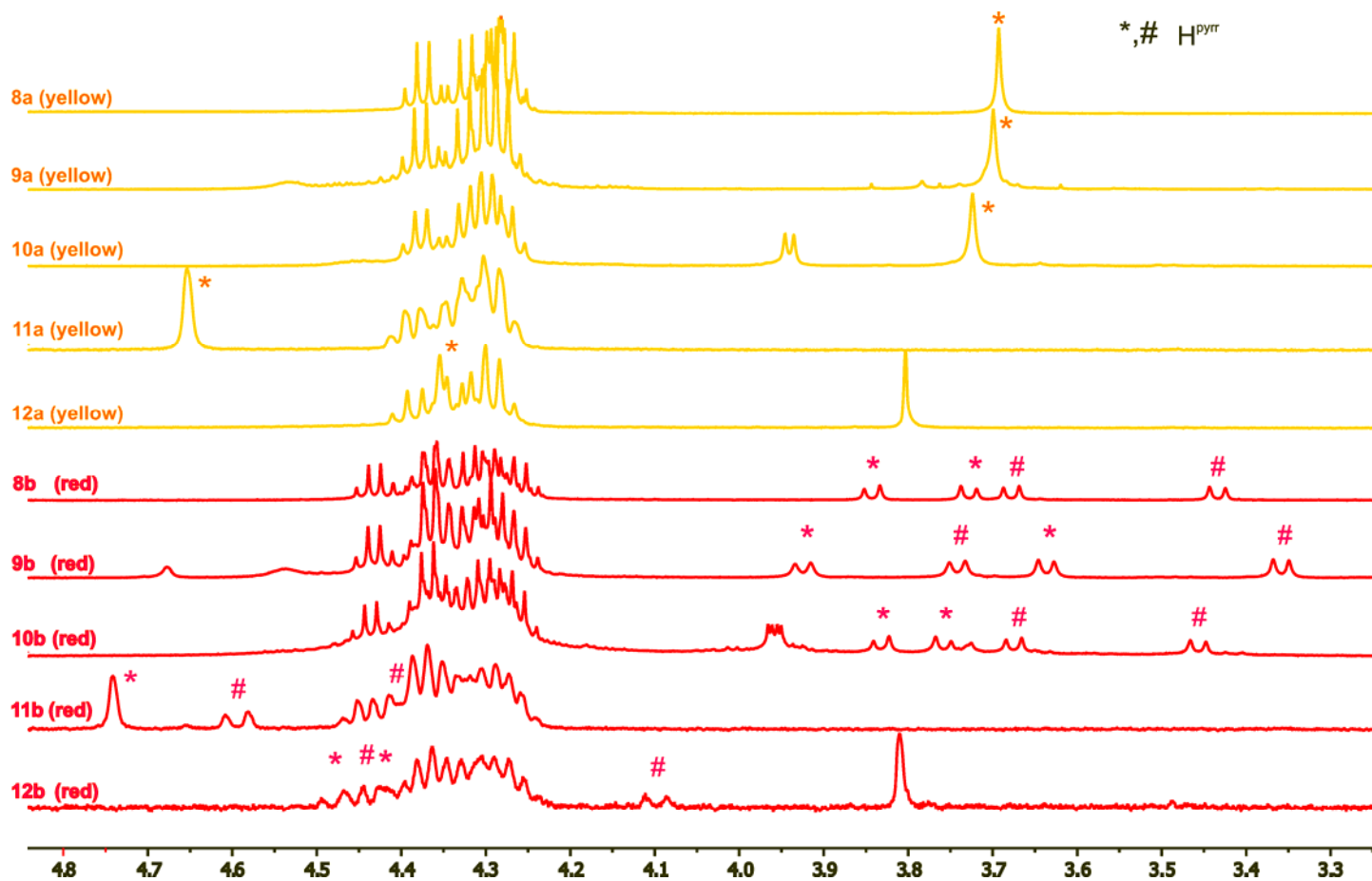


Figure S11. Comparison of the pyrrolidinic ^1H NMR region of of symmetrical **8a-12a** (yellow) and unsymmetrical **8b-12b** (red) regioisomers.

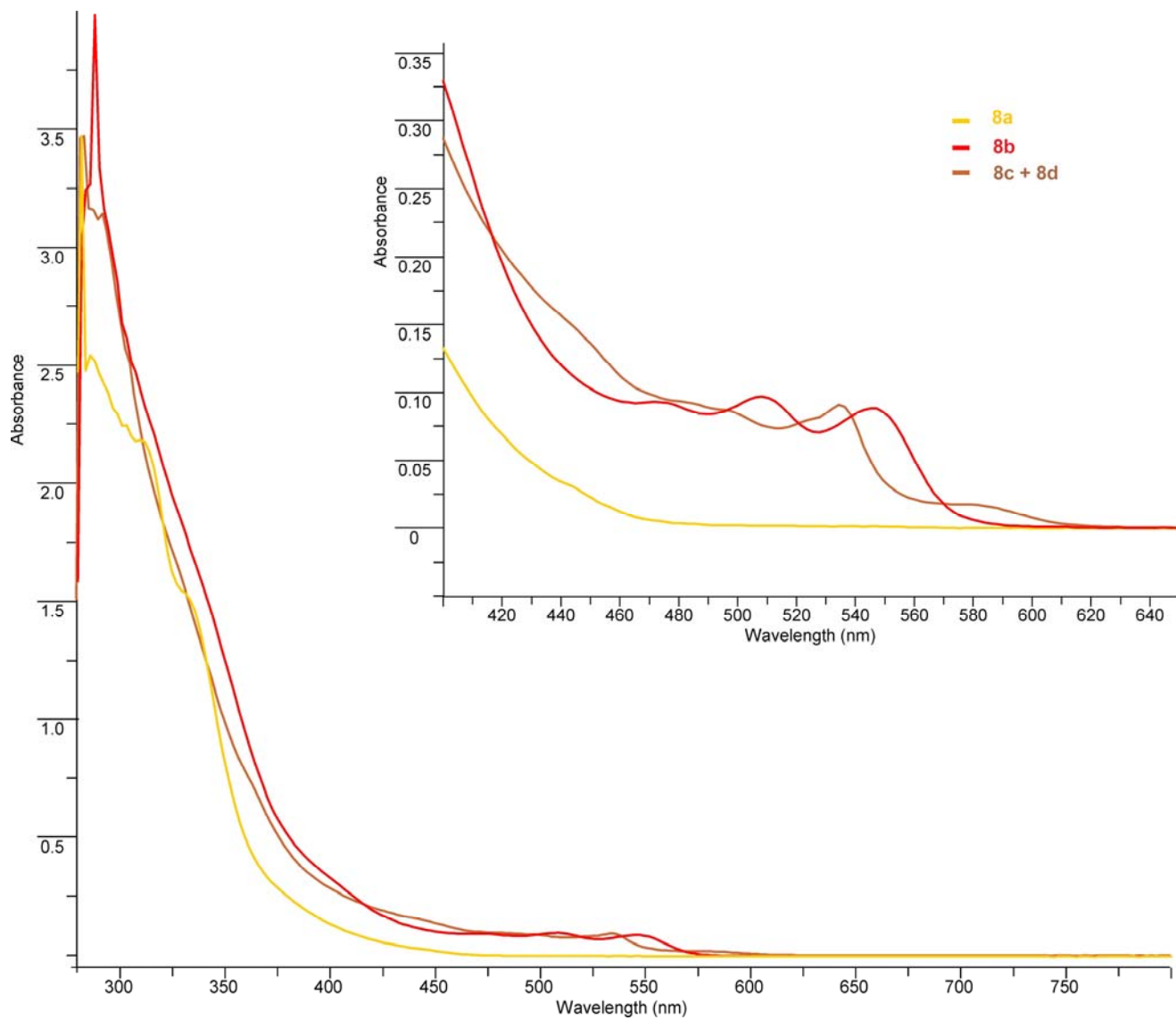


Figure S12. Comparison of UV-Vis spectra of representatives of Bingel-Prato [5:1]-hexaadduct regioisomers **8a**, **8b**, and the **8c/8d** mixture in PhMe.

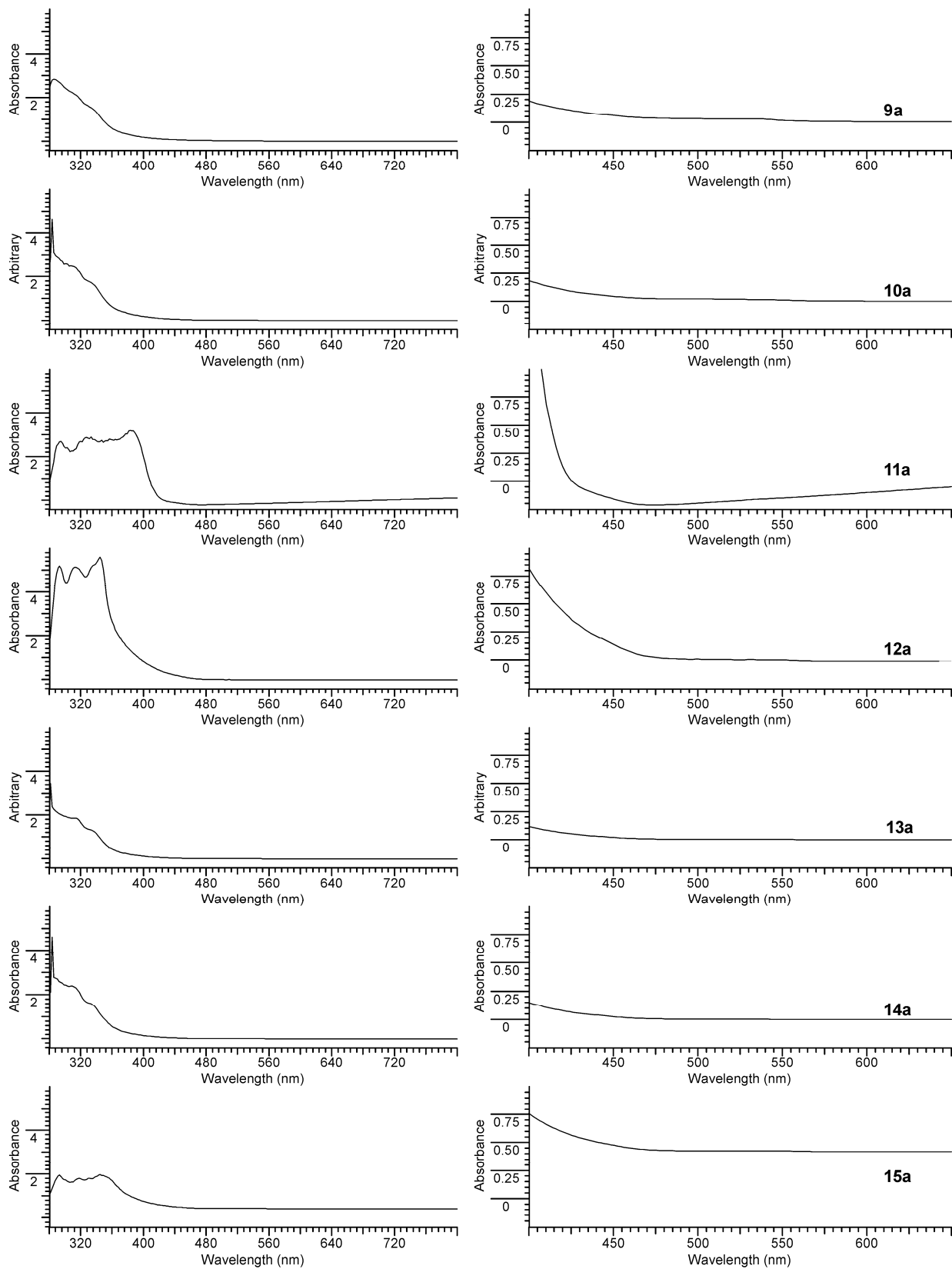


Figure S13. Comparison of UV-Vis spectra of yellow symmetric [5:1]-hexaadduct regioisomers **9a-15a** in PhMe.

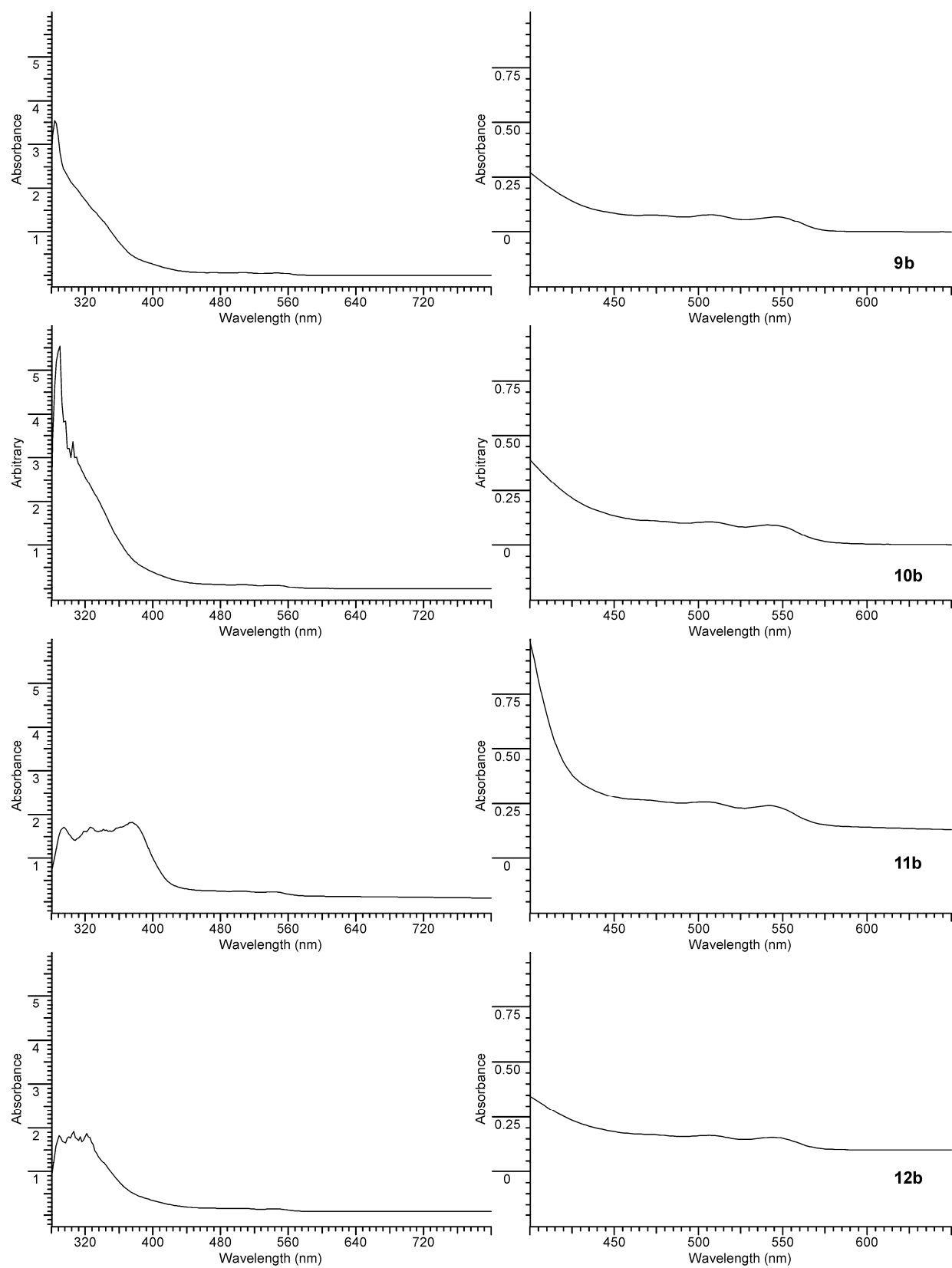


Figure S14. Comparison of UV-Vis spectra of red asymmetric [5:1]-hexaadduct regioisomers **9b-12b** in PhMe.

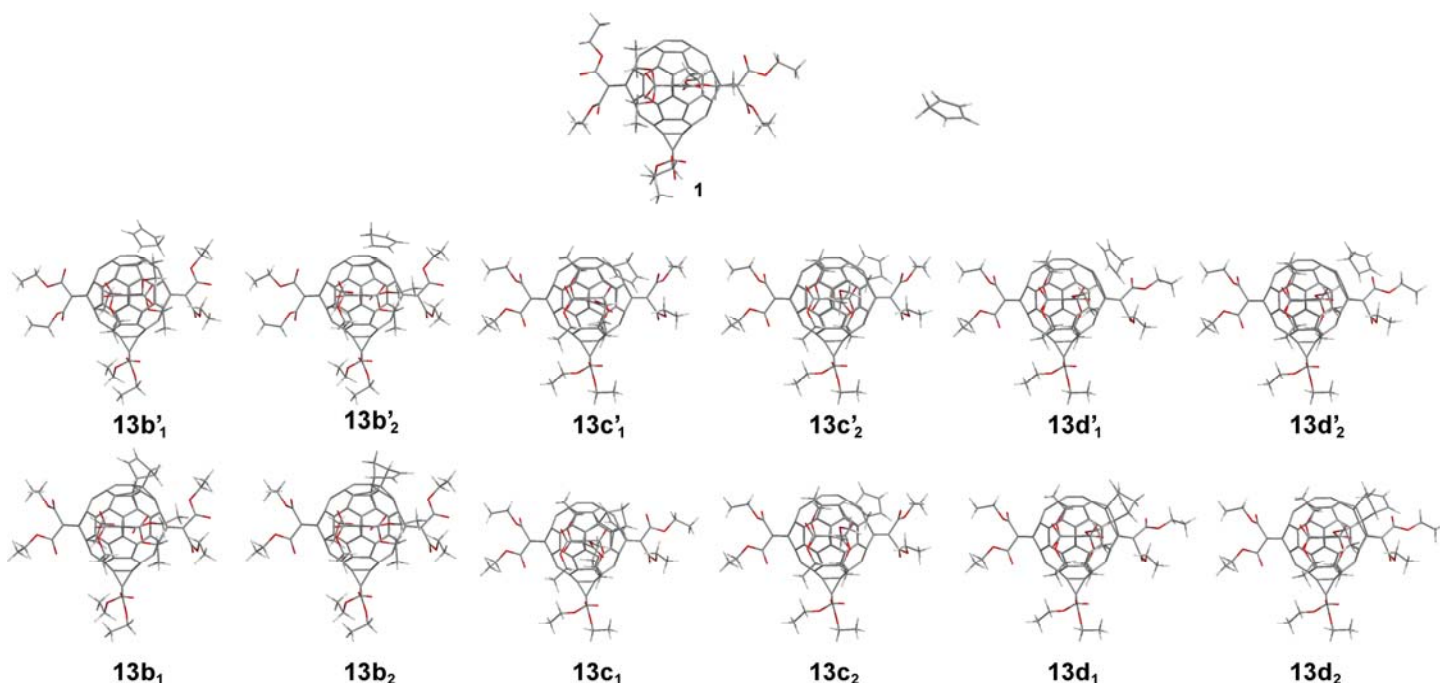


Figure S15. DFT optimized geometries of starting materials for DA reaction (**1** and cyclopentadiene), the corresponding transition states and products (**b₁/b₂**, **c₁/c₂** and **d₁/d₂** correspond to two possible stereoisomers obtained by reaction of C=C bond-**b**, **c** and **d**, respectively)

References

1. Mitrović, A.; Todorović, N.; Žekić, A.; Stanković, D.; Milić, D.; Maslak, V. *Eur. J. Org. Chem.* **2013**, 2188.
2. Bjelaković, M.; Todorović, N.; Milić, M. *Eur. J. Org. Chem.*, **2012**, 5291.
3. Specklin, S.; Decuypere, E.; Plougastel, L.; Aliani, S.; Taran, F. *J. Org. Chem.* **2014**, *79*, 7772.
4. Barlos, K.; Papaioannou, D.; Theodoropoulos, D. *J. Org. Chem.* **1982**, *47*, 1324.
5. Langa, F.; de la Cruz, P.; Espíldora, E.; González-Cortés, A.; de la Hoz, A.; López-Arza V. *J. Org. Chem.* **2000**, *65*, 8675.
6. Hörmann, F.; Donaubaue, W.; Hampel, F.; Hirsch, A. *Chem. Eur. J.* **2012**, *18*, 3329.
7. Uno, H.; Watanabe, H.; Yamashita, Y.; Ono, N. *Org. Biomol. Chem.*, **2005**, *3*, 448.

Regioisomeric Bingel-Prato [5:1]-hexaadducts **8**

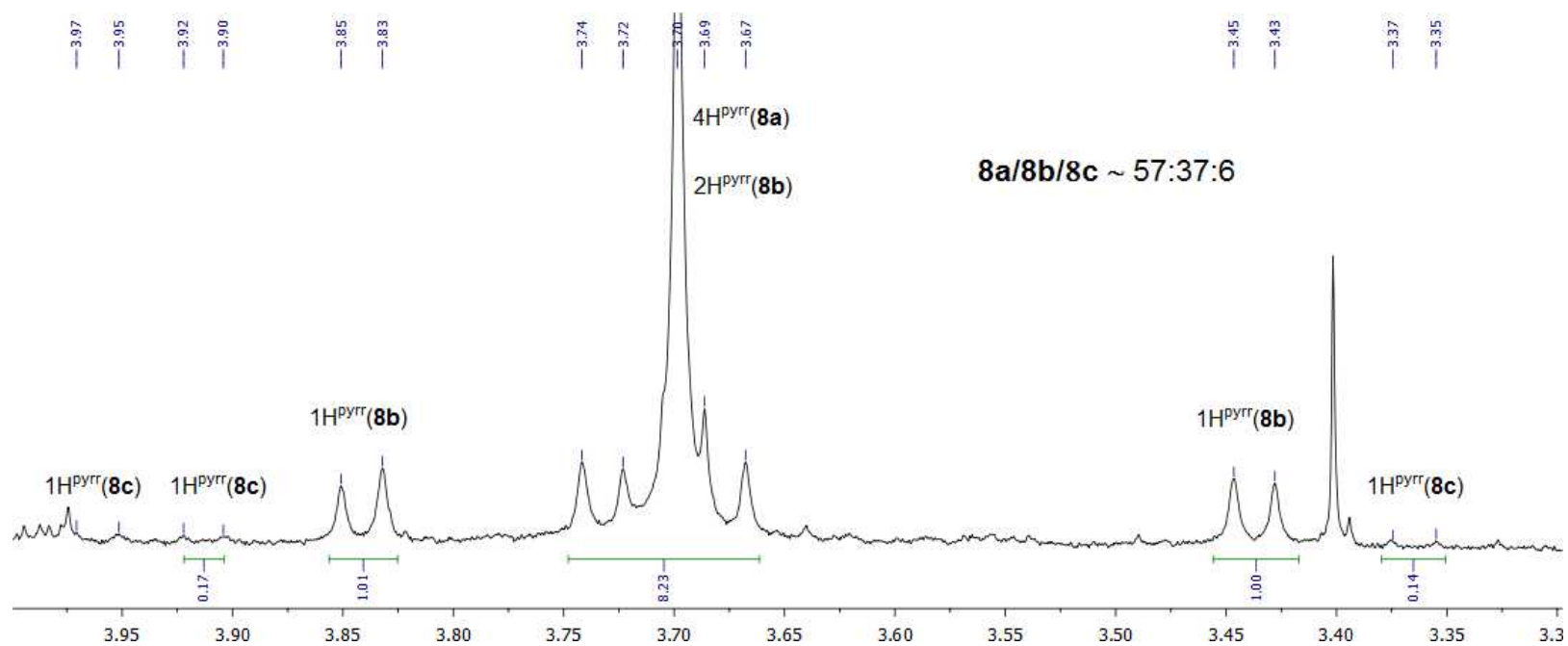
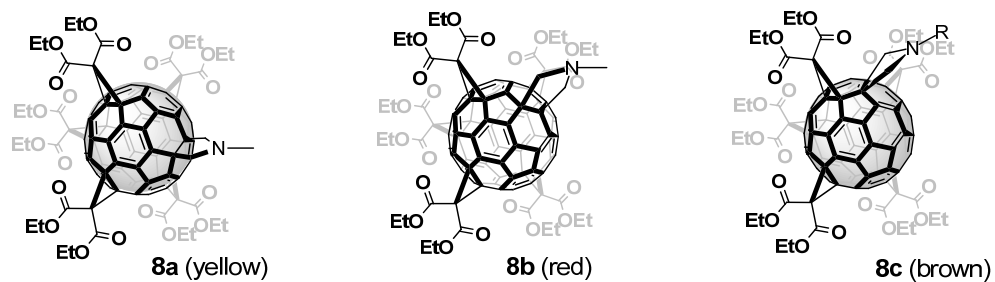
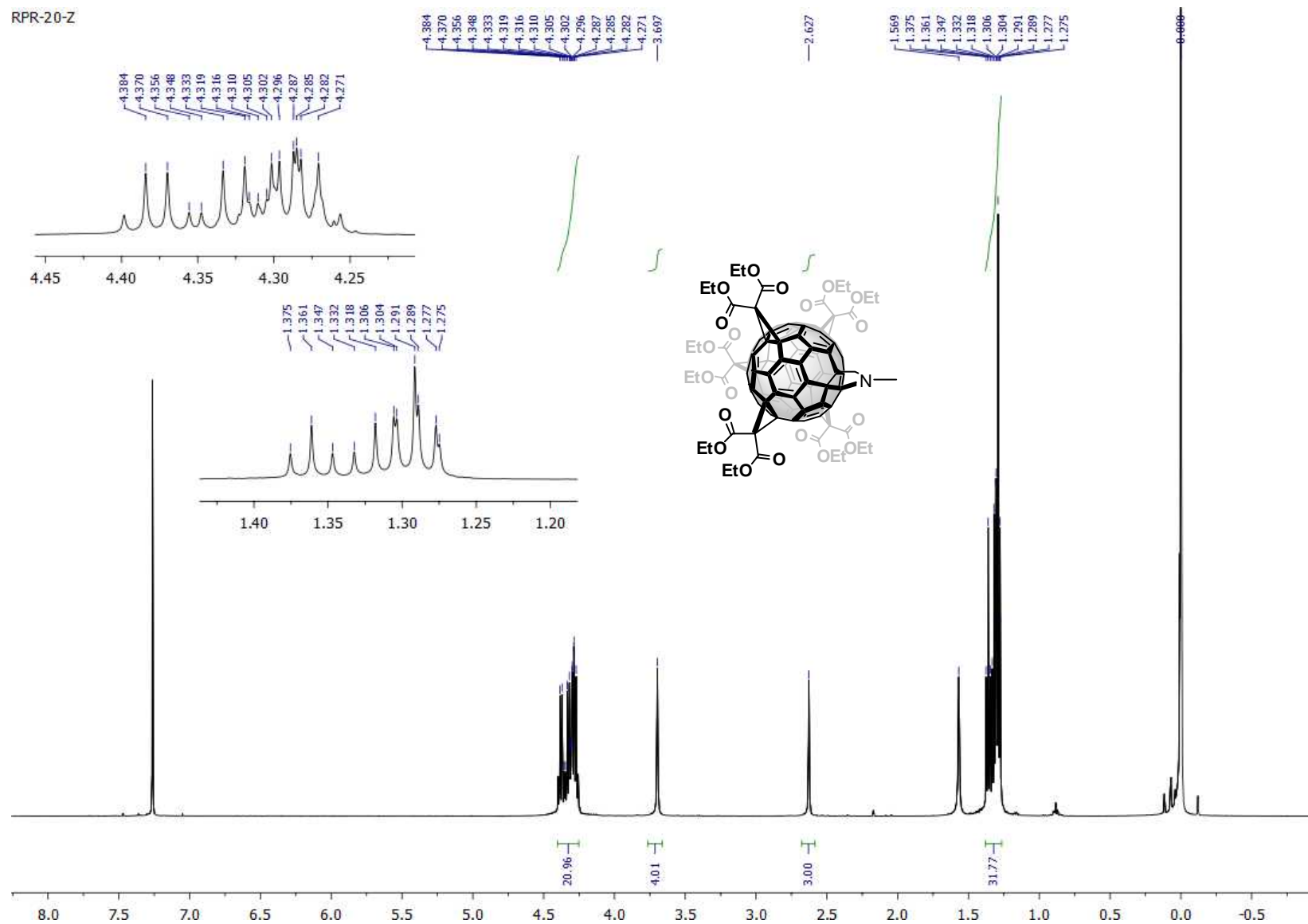


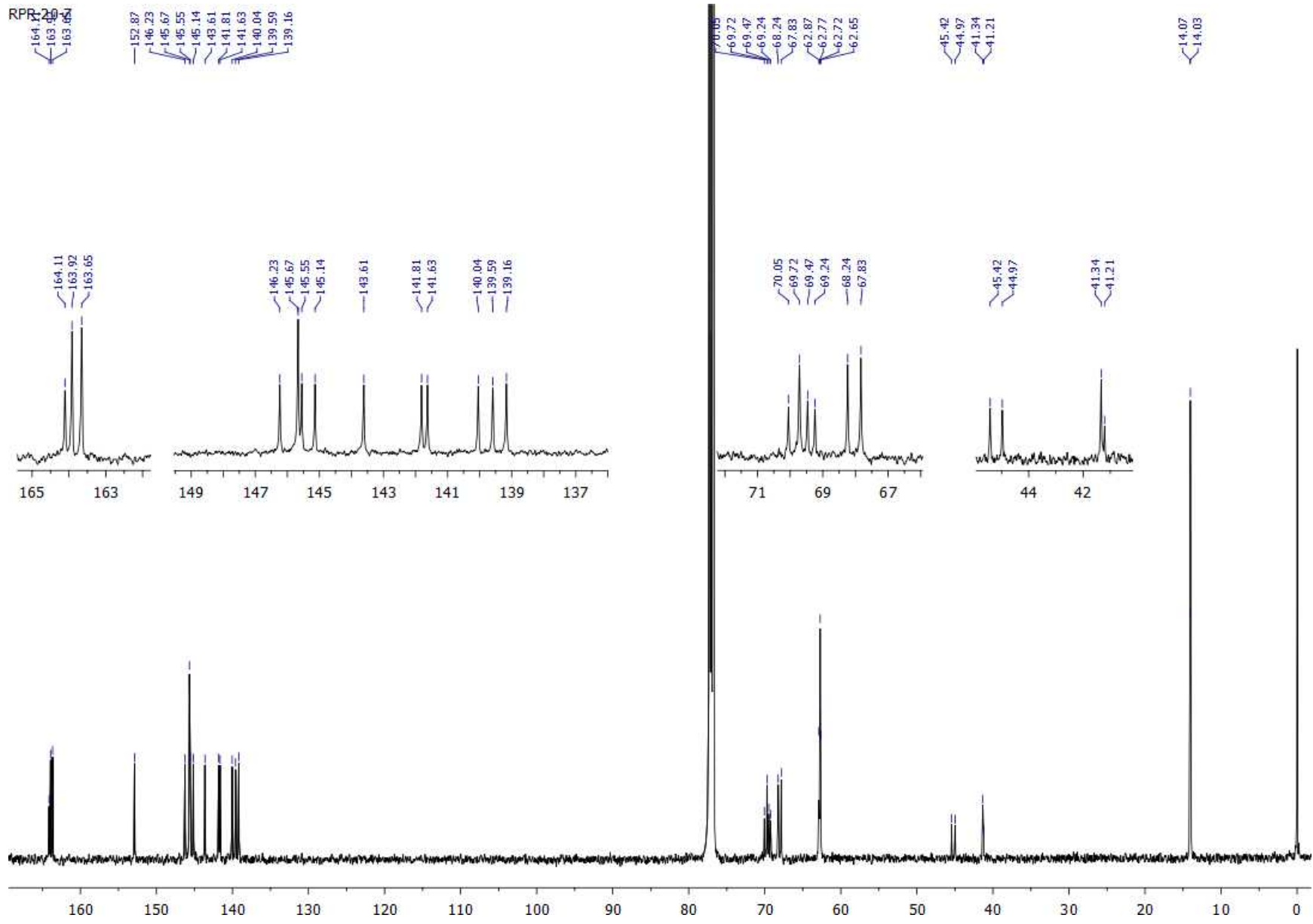
Figure S16. The expanded 1H NMR pyrrolidine region of the isolated mixture of regioisomers **8a-c**

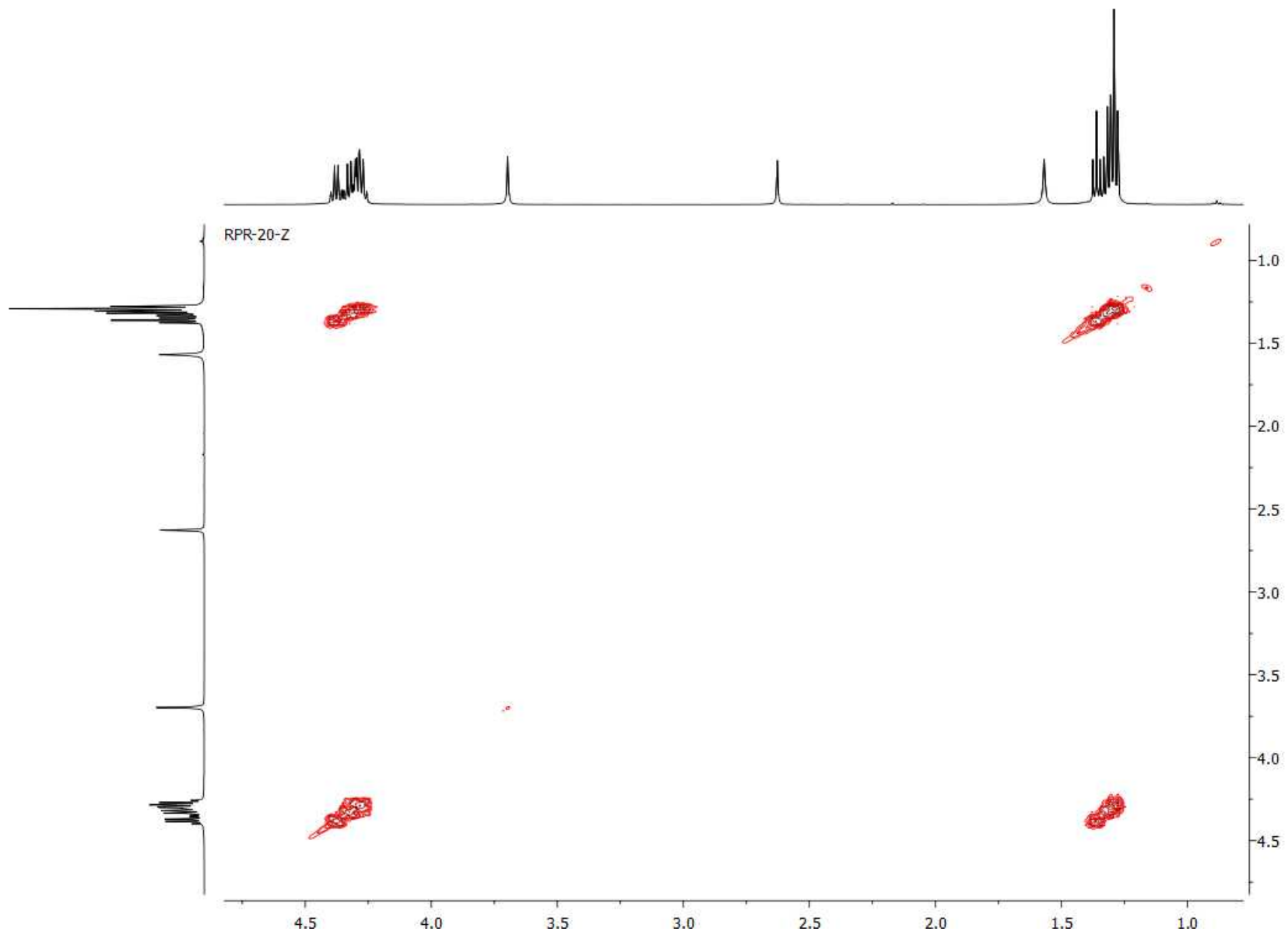
Hexaadduct 8a

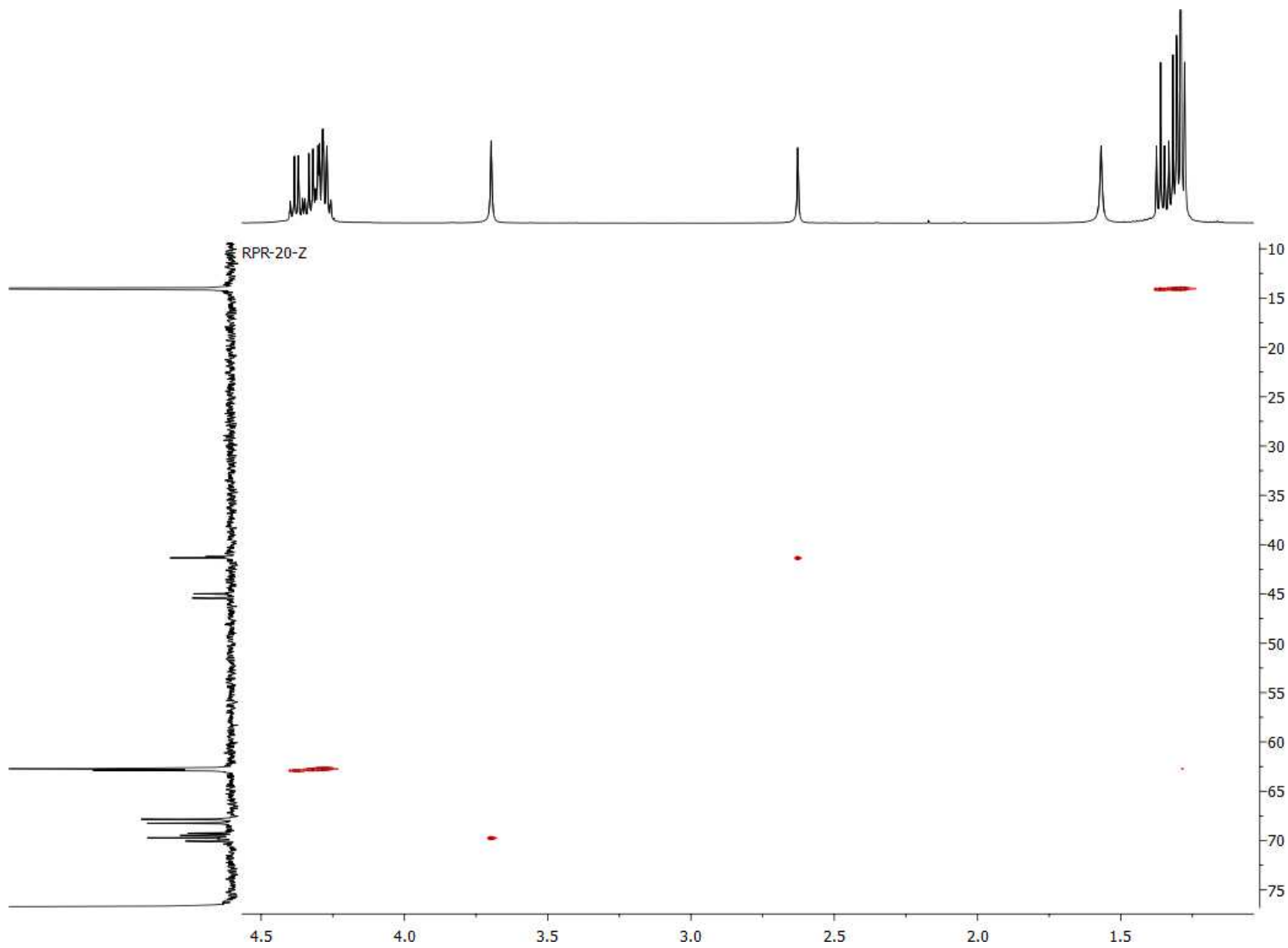
RPR-20-Z

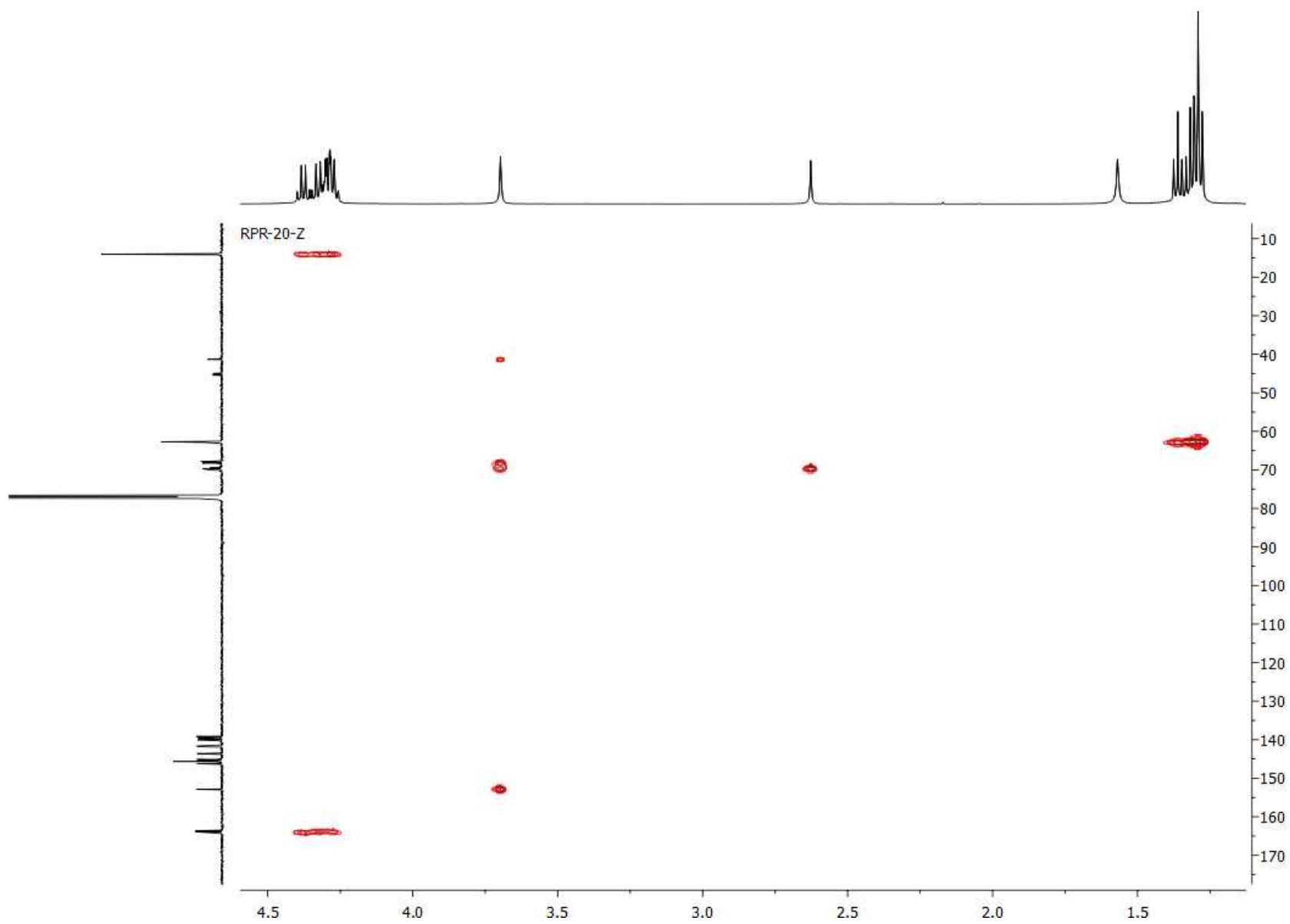


RPR-20

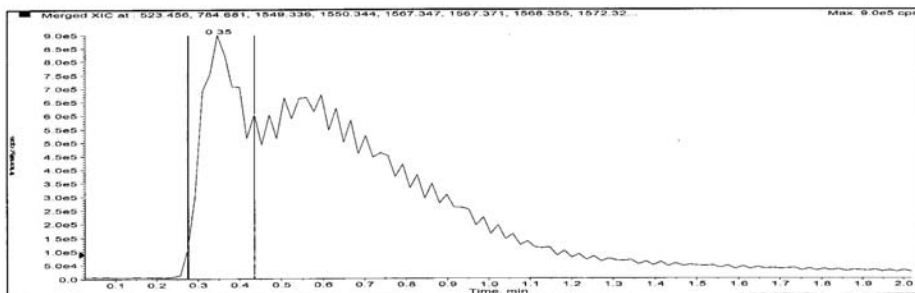




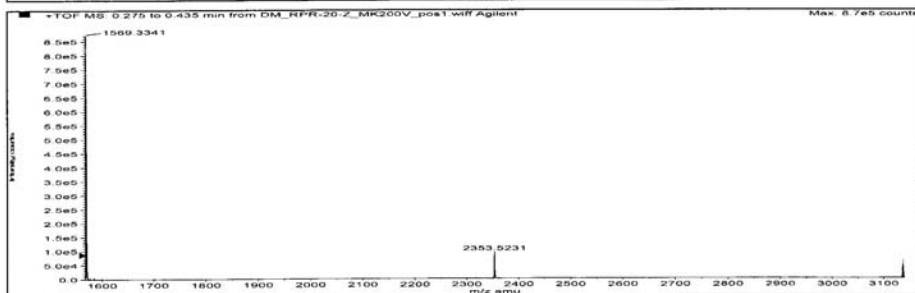
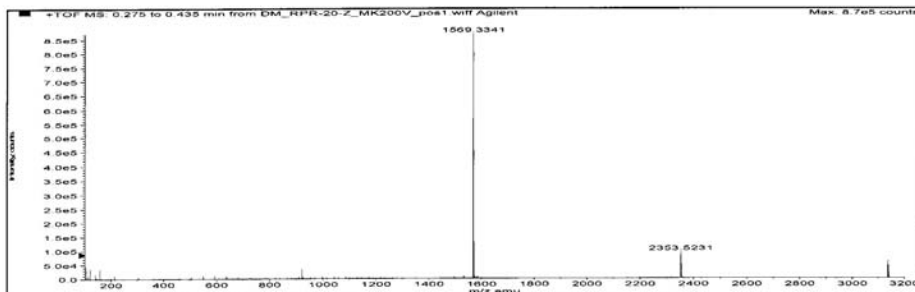




Sample Name: RPR-20-Z Sample Location: P1-D3 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciecx Data\Projects\ID_Milic\Data\DM_RPR-20-Z_MK200V_pos1.wiff Acq Time: September 28 2015, 01:04:49 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml



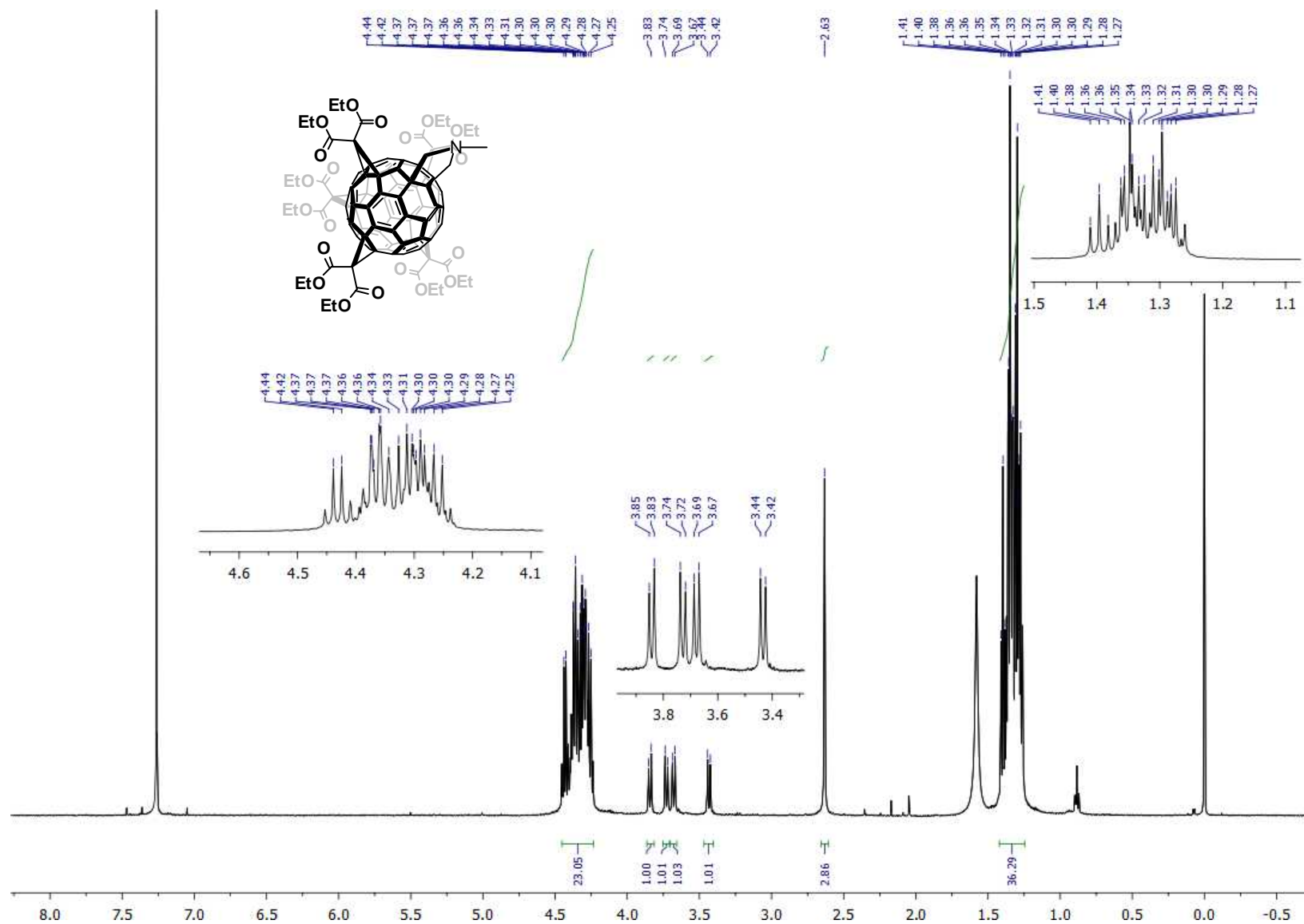
Merged XIC, Period# : 1 Experiment# : 1

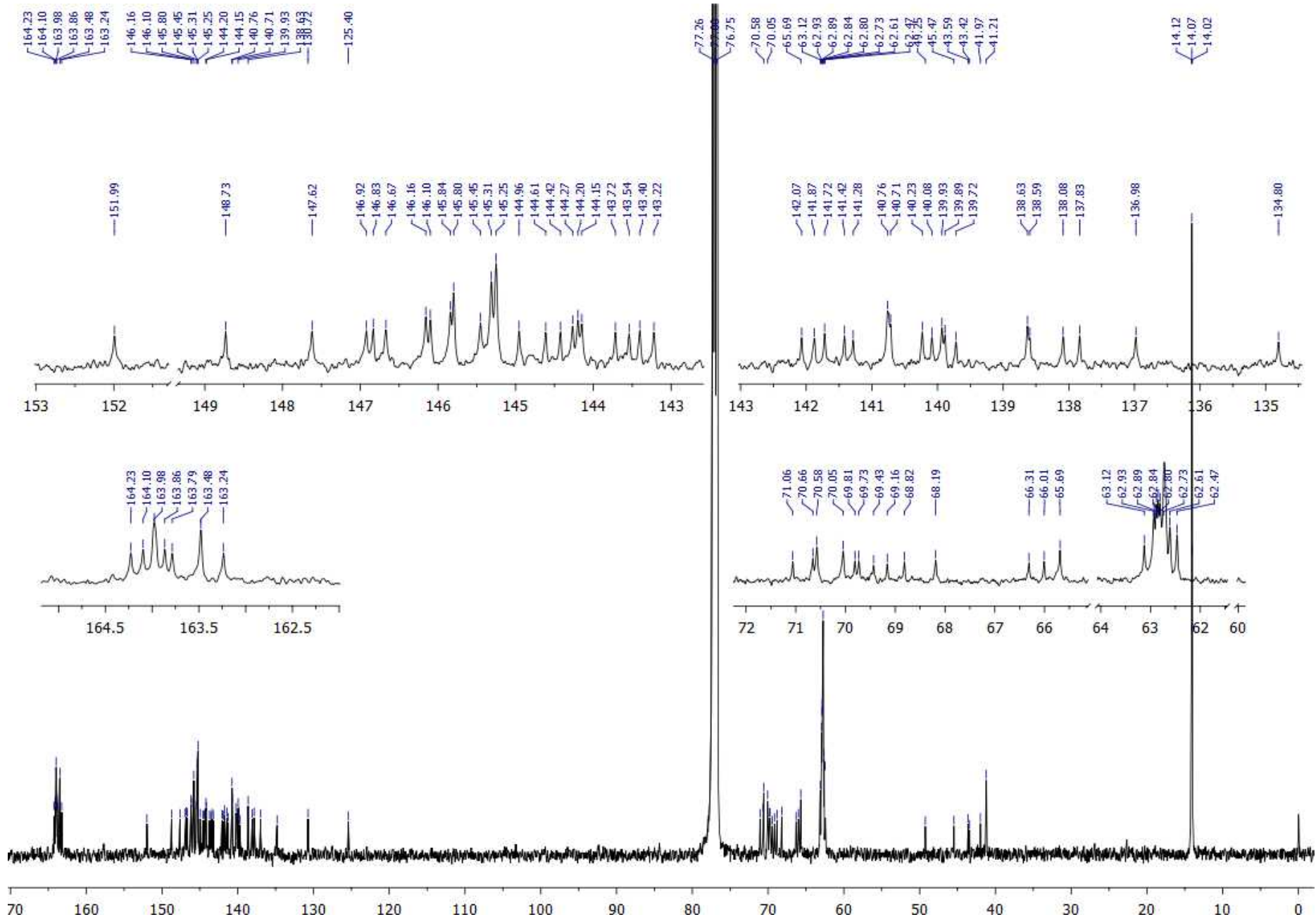


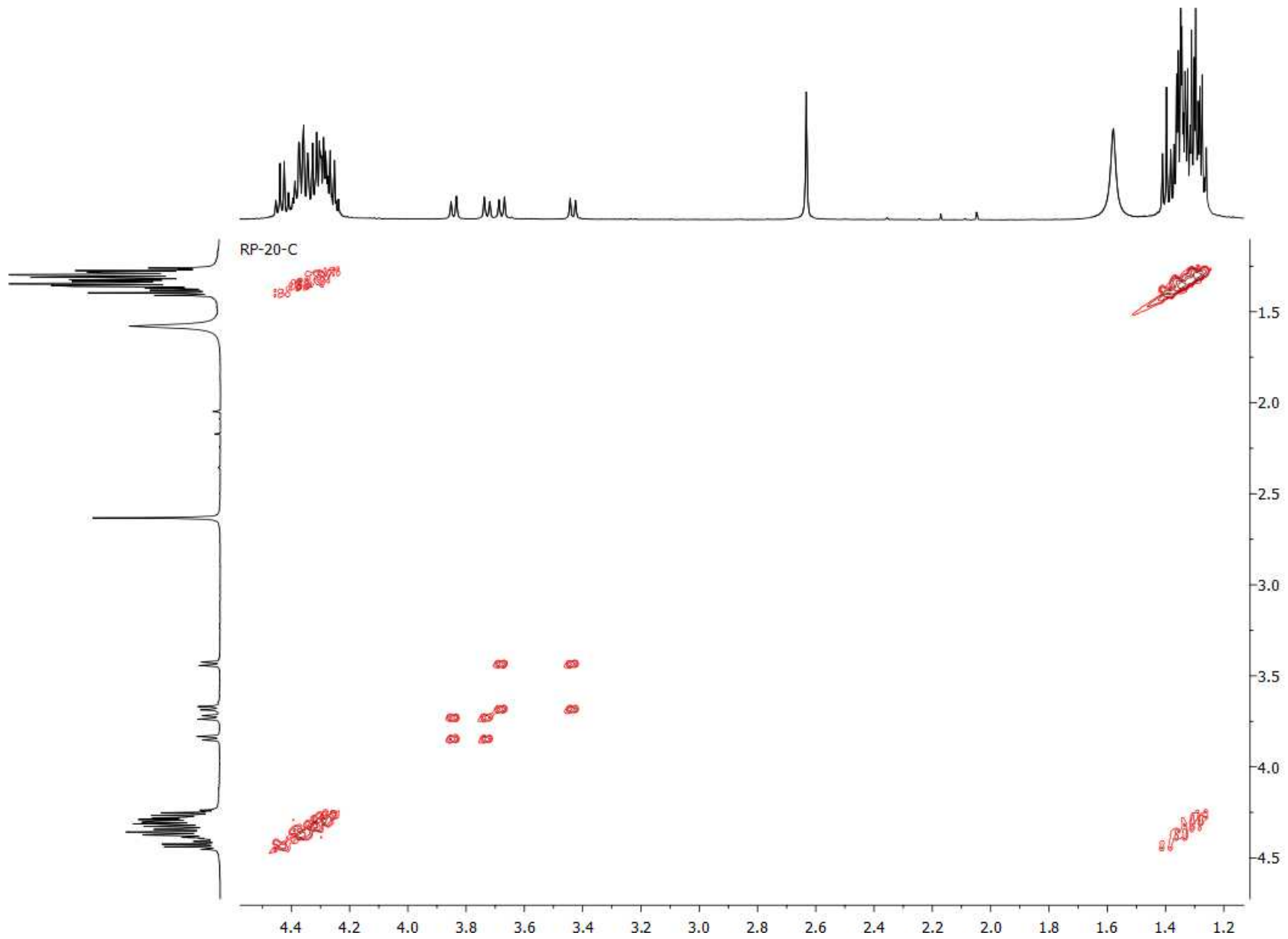
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C98H57NO20	--	1567.34739	0.35	6.67339 E6	--

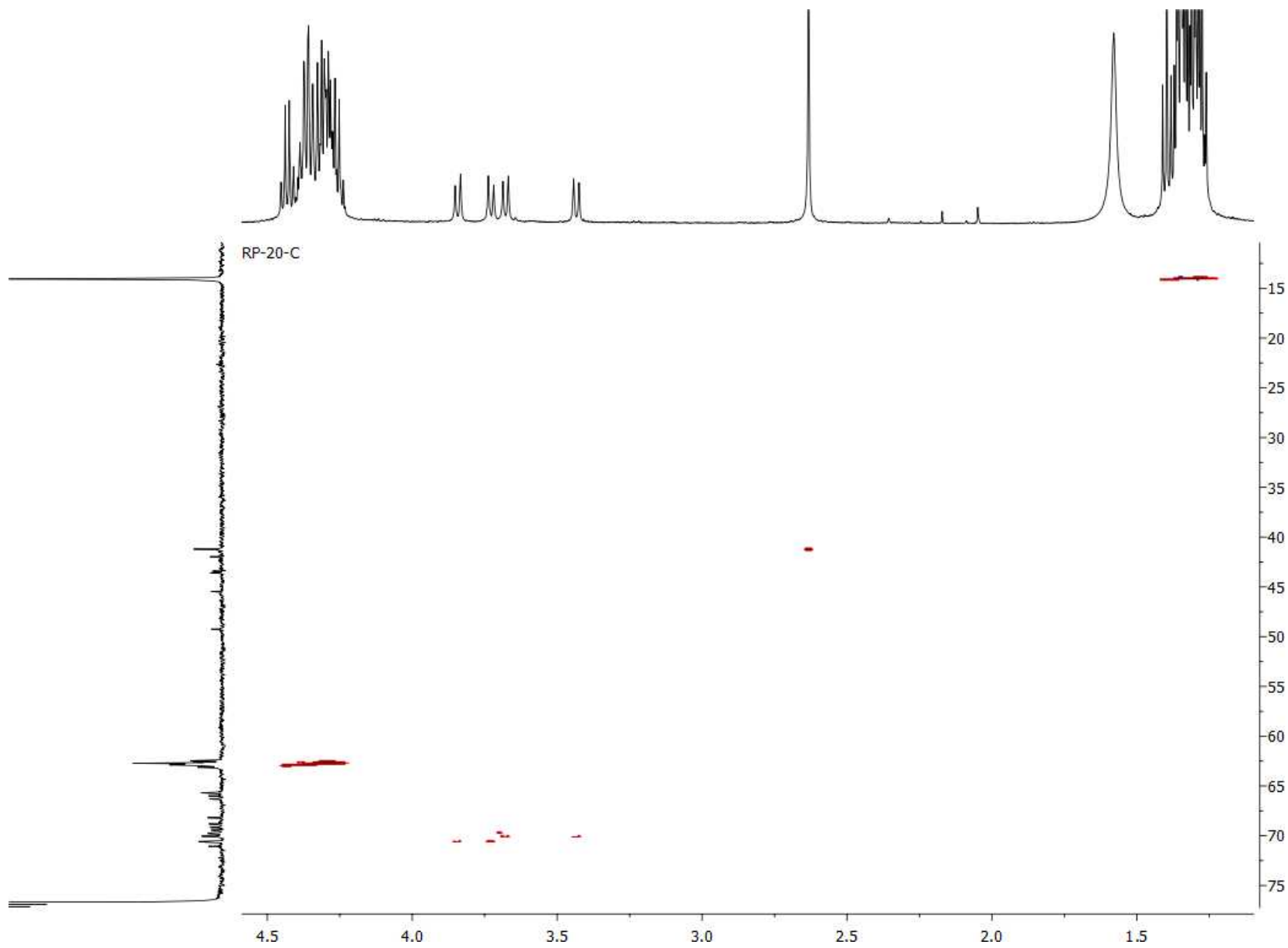
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	580669.42	1568.35467	1568.35012	-4.55245	-2.90	--
[M+Na-H2O] ⁺	30051.87	1572.32605	1572.36230	36.25376	23.06	--
[2M+H] ⁺	14761.49	3135.70206	3135.70107	-0.98813	-0.32	--

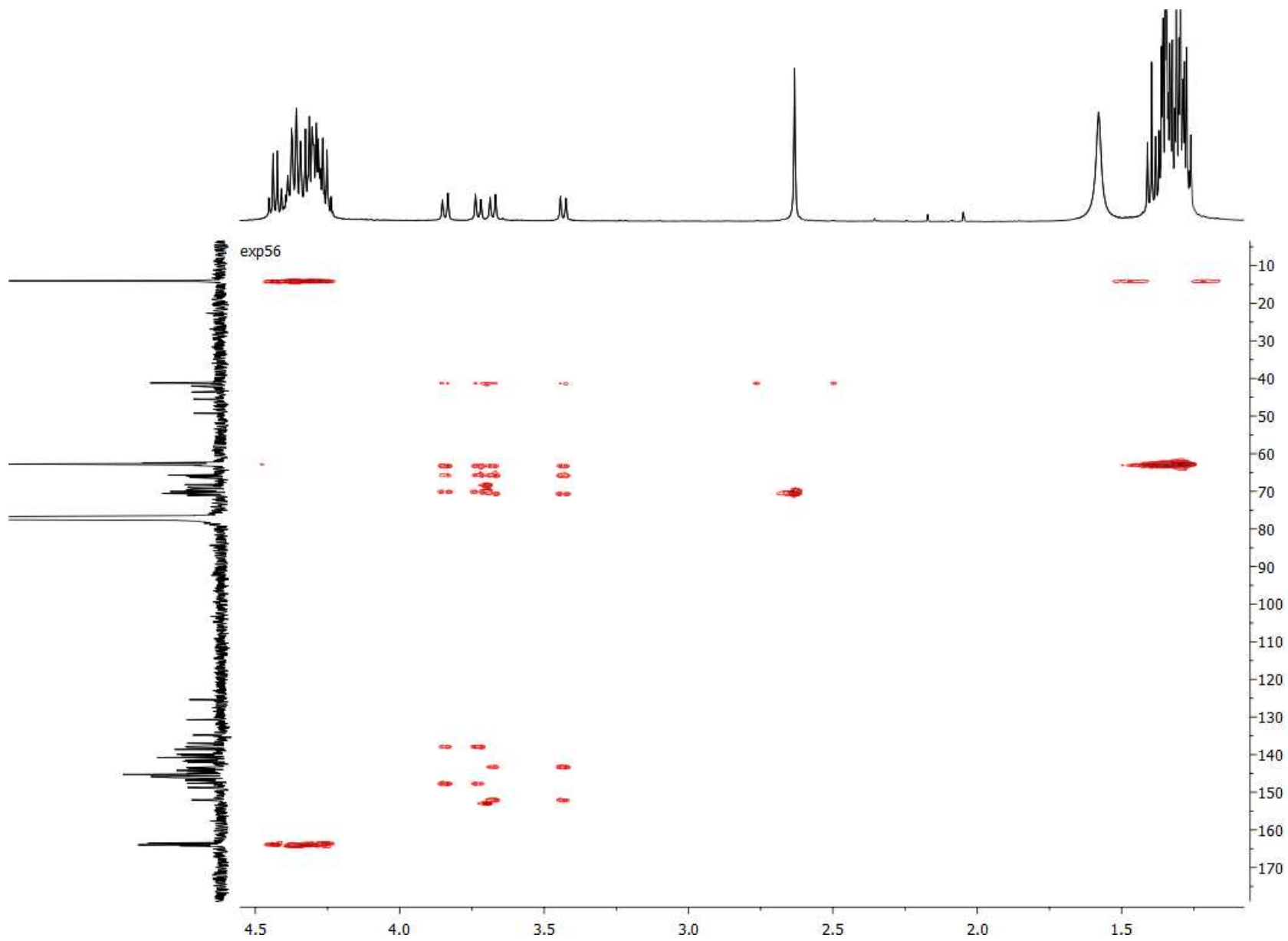
Hexaadduct 8b



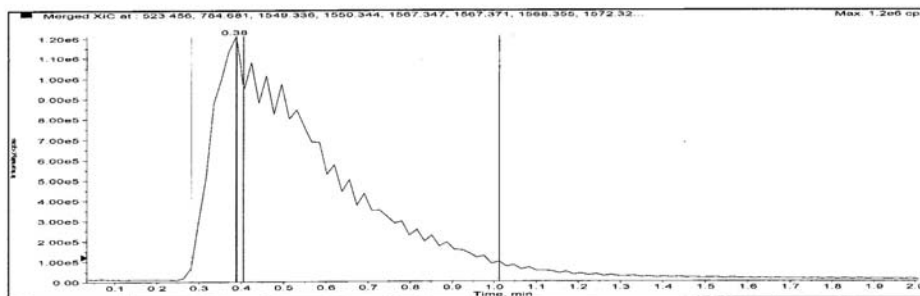




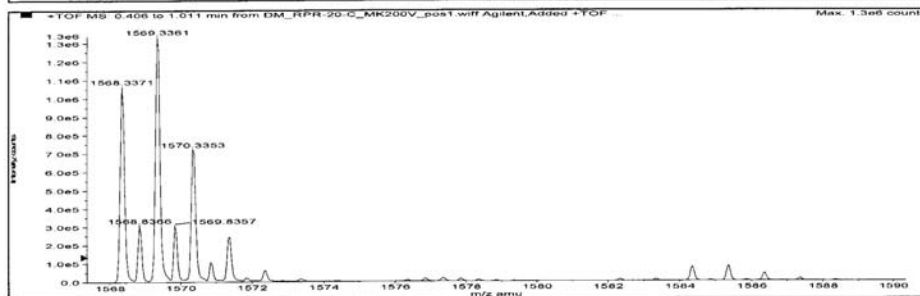
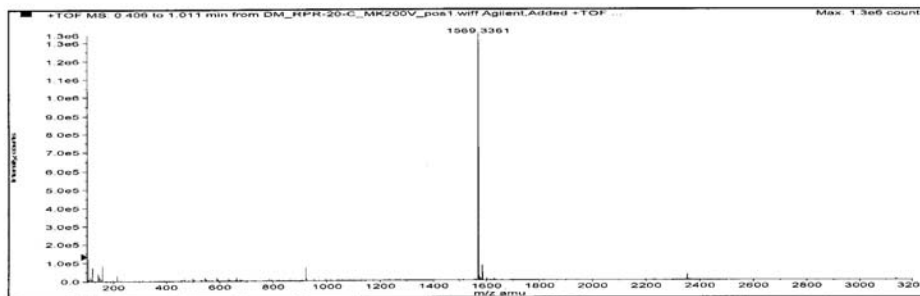




Sample Name: RPR-20-C Sample Location: P1-D2 Sample Id: Operator: Milka
 Data File Name: D:\PE Scielex Data\Projects\ID_Milica\Data\DM_RPR-20-C_MK200V_pos1.wiff Acq Time: September 28 2015, 01:01:37 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml



Merged XIC, Period# : 1 Experiment# : 1

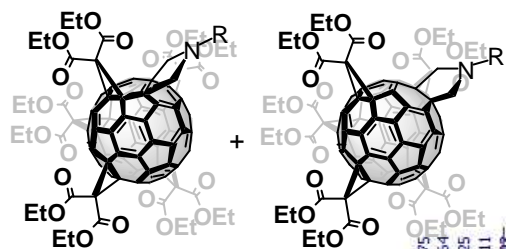


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C98H57NO20	--	1567.34739	0.38	2.24115 E7	--

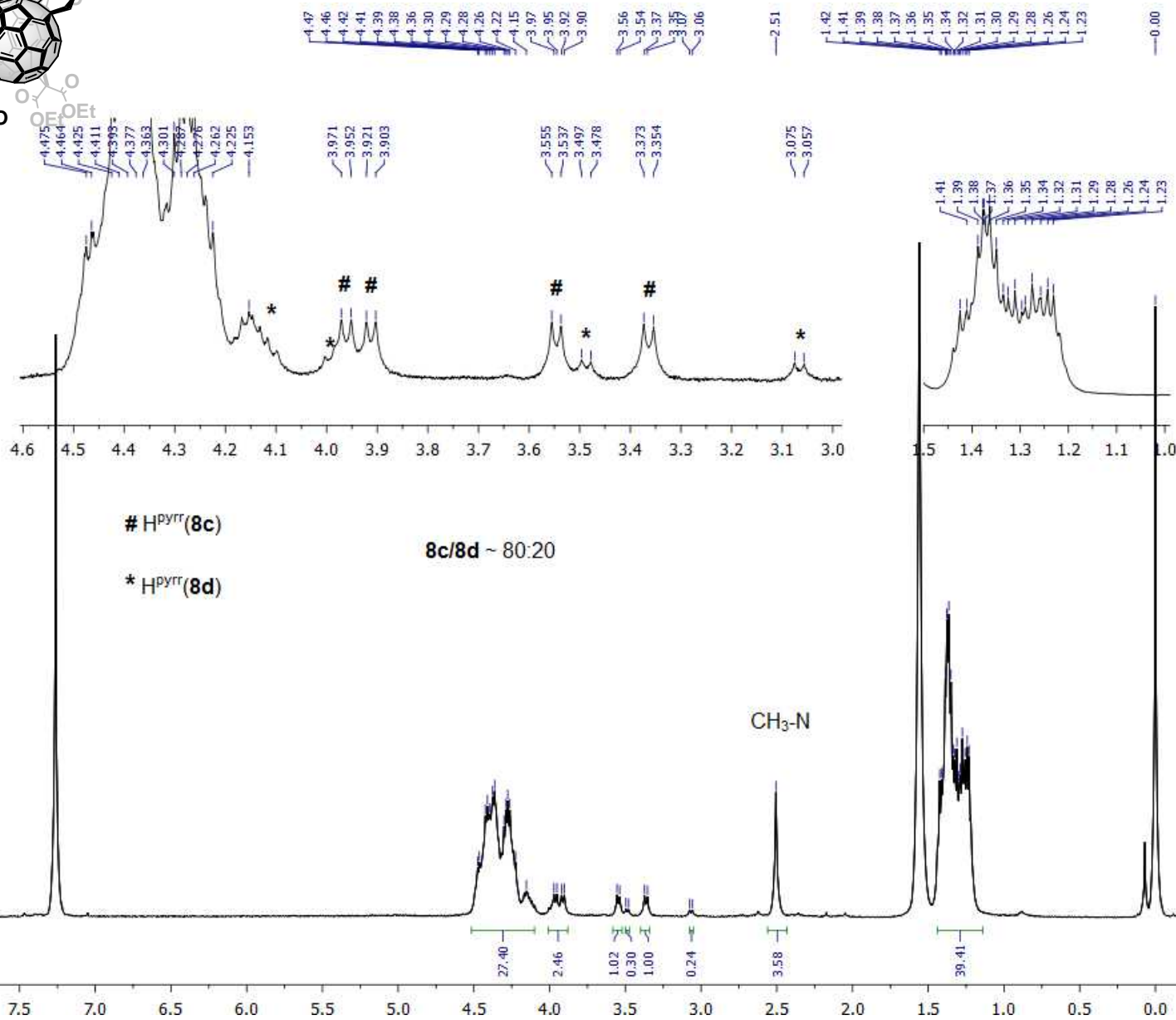
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1095438.79	1568.35467	1568.35241	-2.25511	-1.44	--
[M+Na-H2O] ⁺	63382.39	1572.32605	1572.36439	38.34368	24.39	--
[M+NH4] ⁺	83575.03	1585.38122	1585.35092	-30.30218	-19.11	--

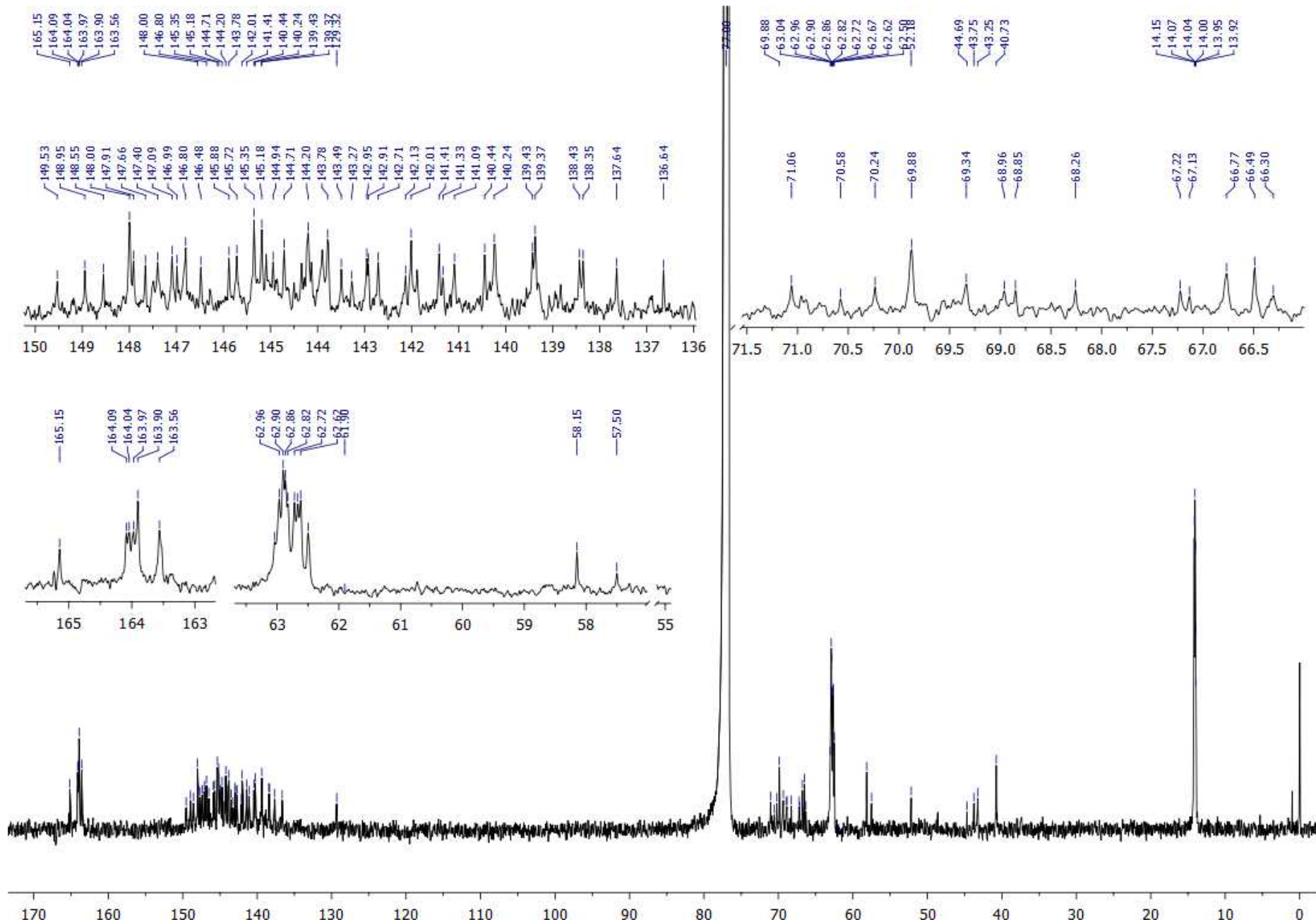
check MS

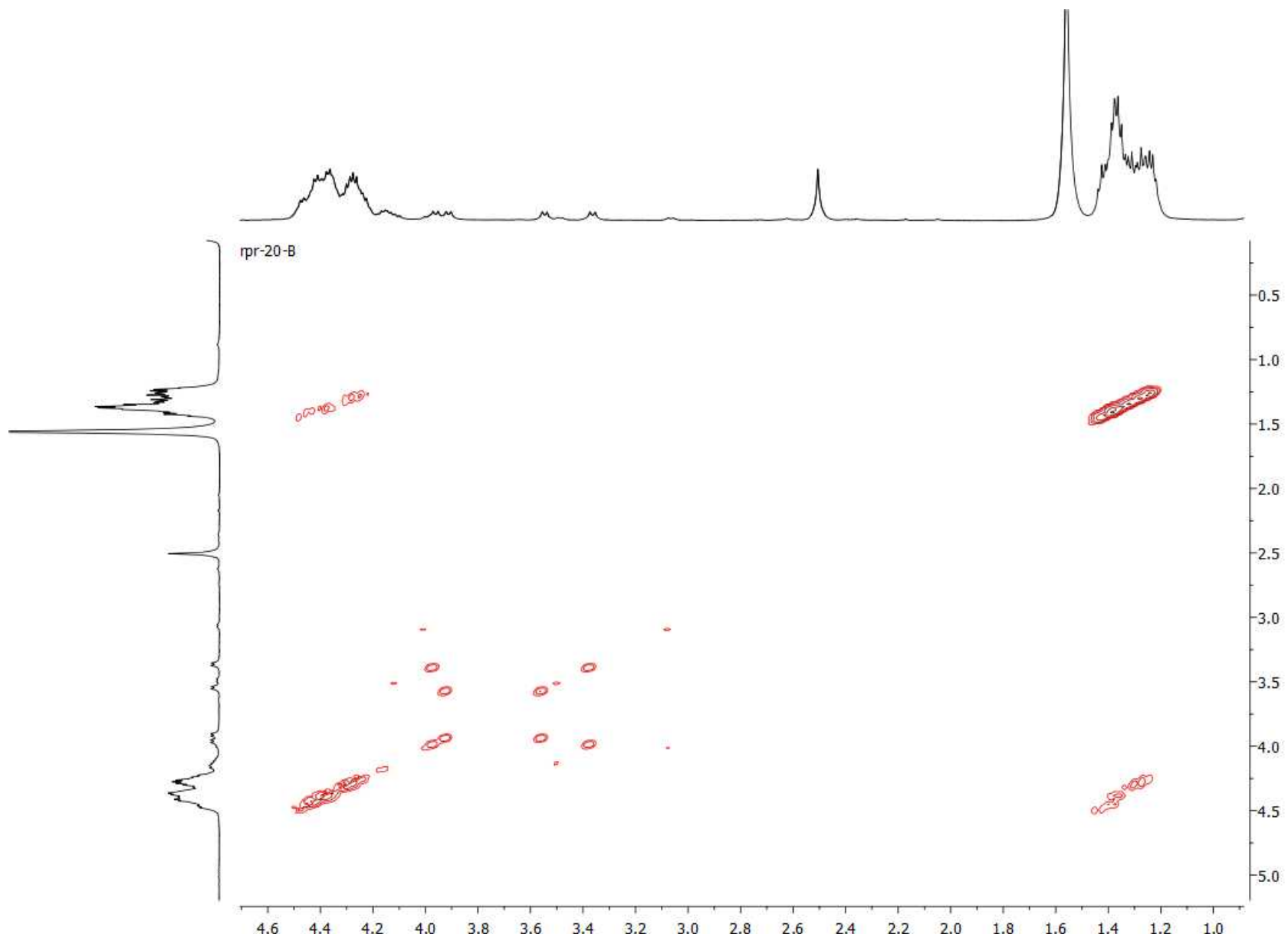
Hexaadducts 8c+8d

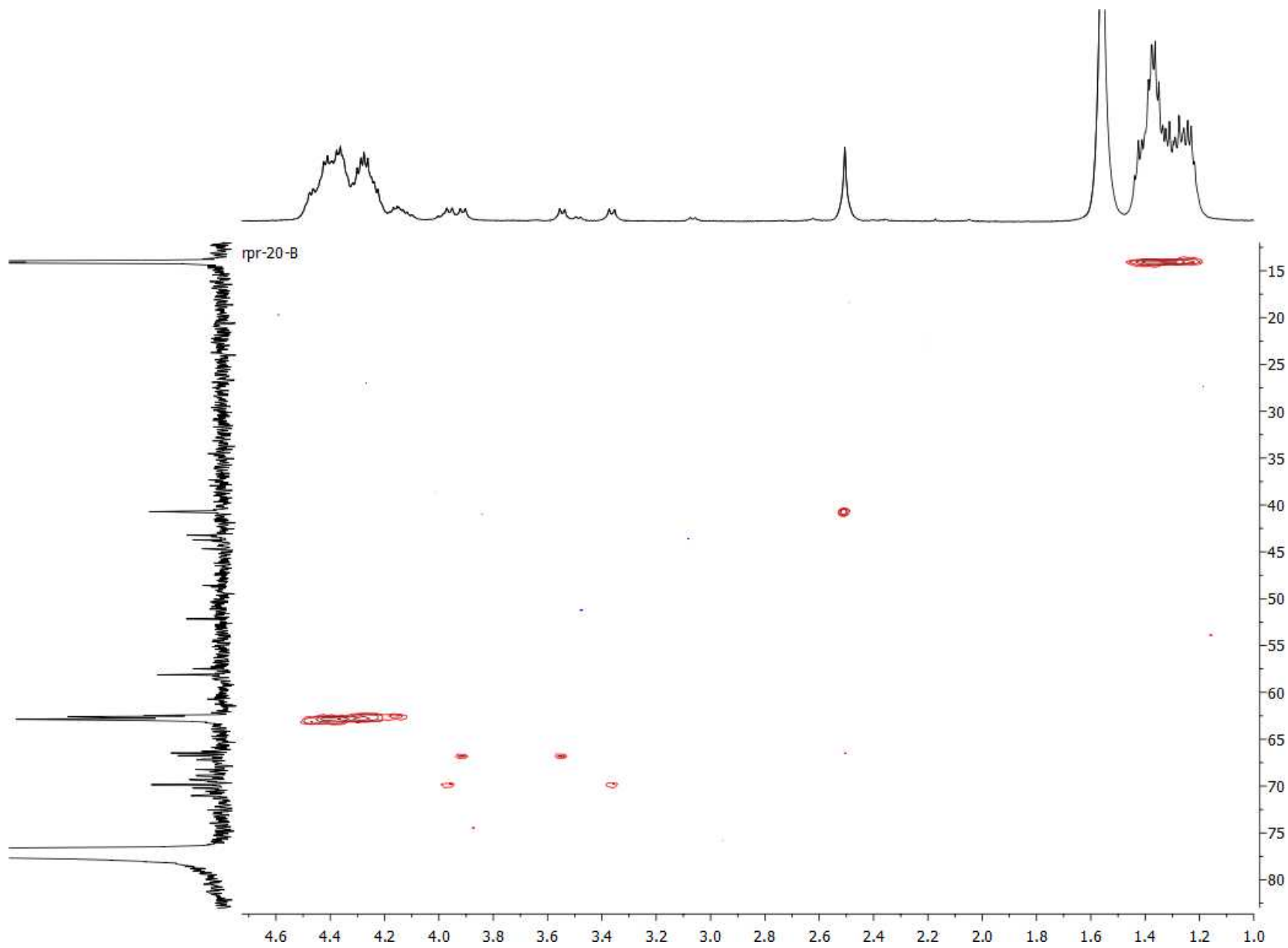


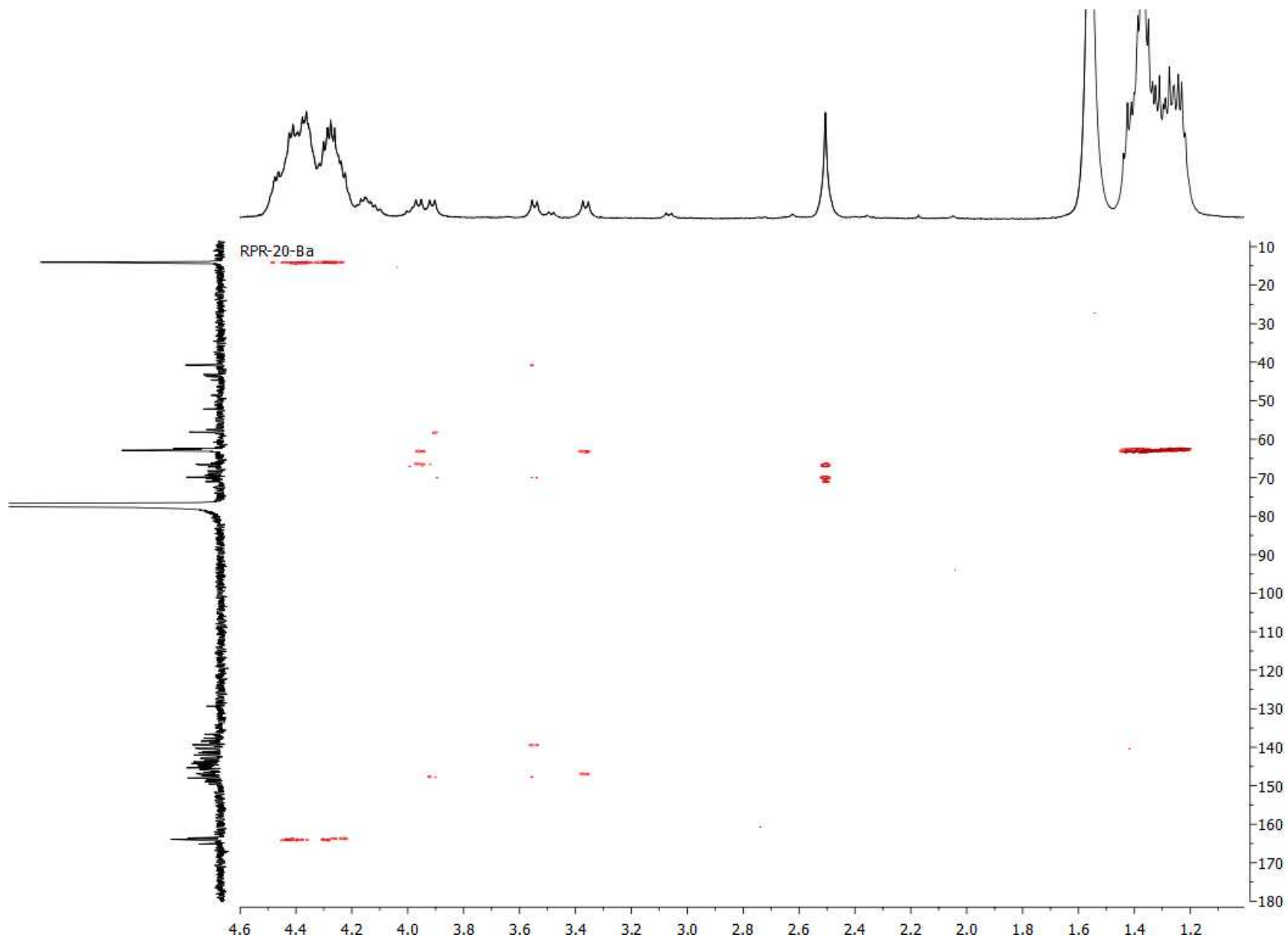
8c + 8d





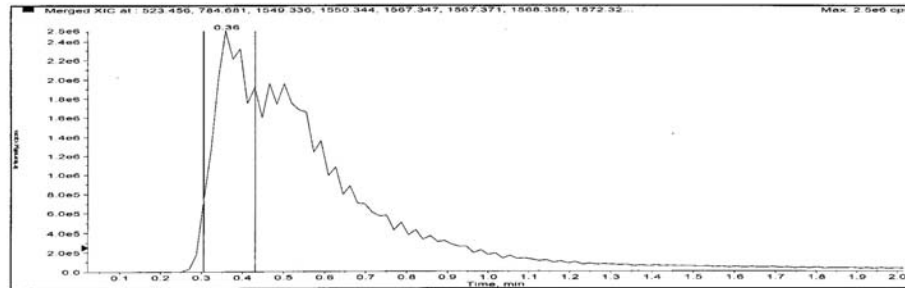




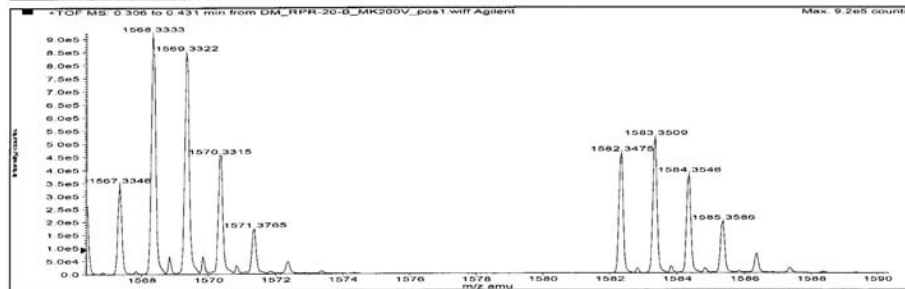
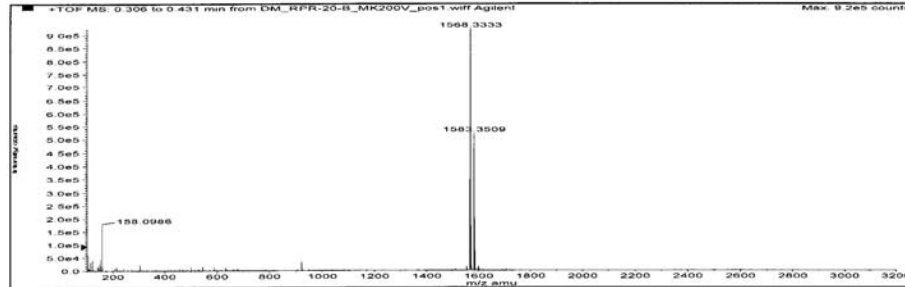


Sarosine
 2016-01-18

Sample Name: RPR-20-B Sample Location: P1-D1 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\DM_Milic\Data\DM_RPR-20-B_MK200V_pos1.wiff Acq Time: September 28 2015, 12:58:25 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.anmlfc.xml



Merged XIC, Period#: 1 Experiment#: 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C98H57NO20	--	1567.34739	0.36	8.14129 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
M+	347724.11	1567.34684	1567.33787	-8.97804	-5.73	--
[M+H] ⁺	945754.65	1568.35467	1568.34883	-5.84429	-3.73	--
[M+Na-H2O] ⁺	47590.02	1572.32605	1572.36259	36.54291	23.24	--
[M+NH4] ⁺	205818.15	1585.38122	1585.34346	-37.76334	-23.82	--

← OK! Jig

Regioisomeric Bingel-Prato [5:1]-hexaadducts **9**

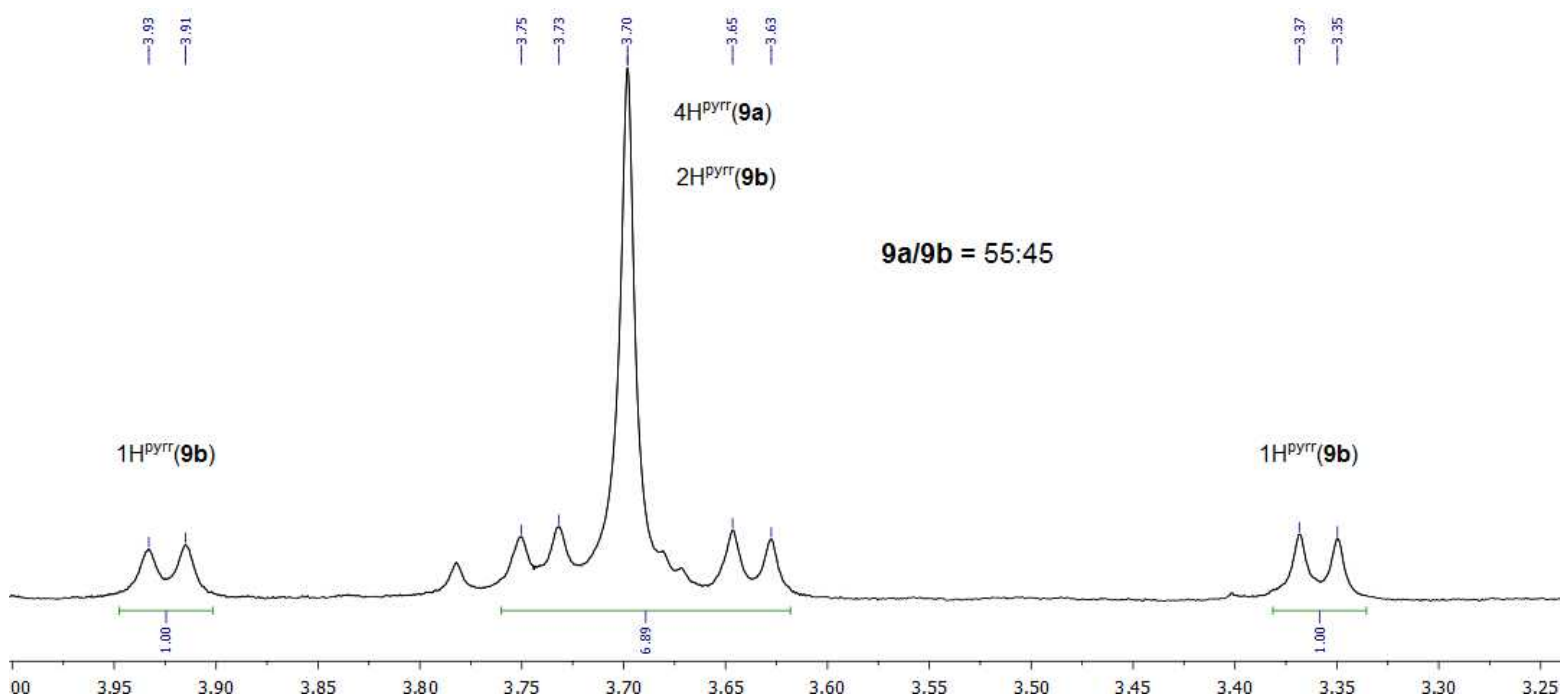
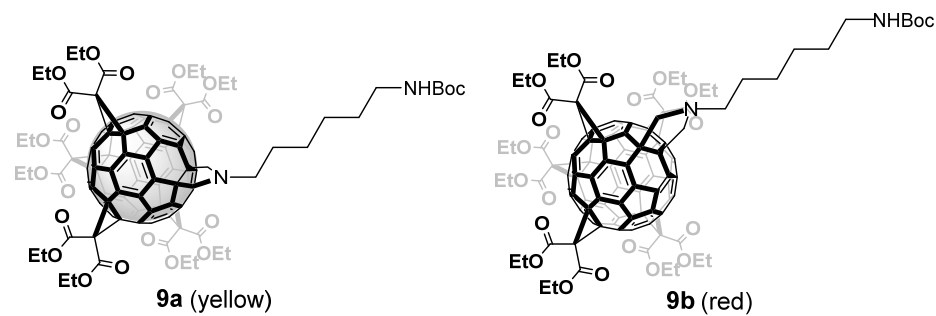
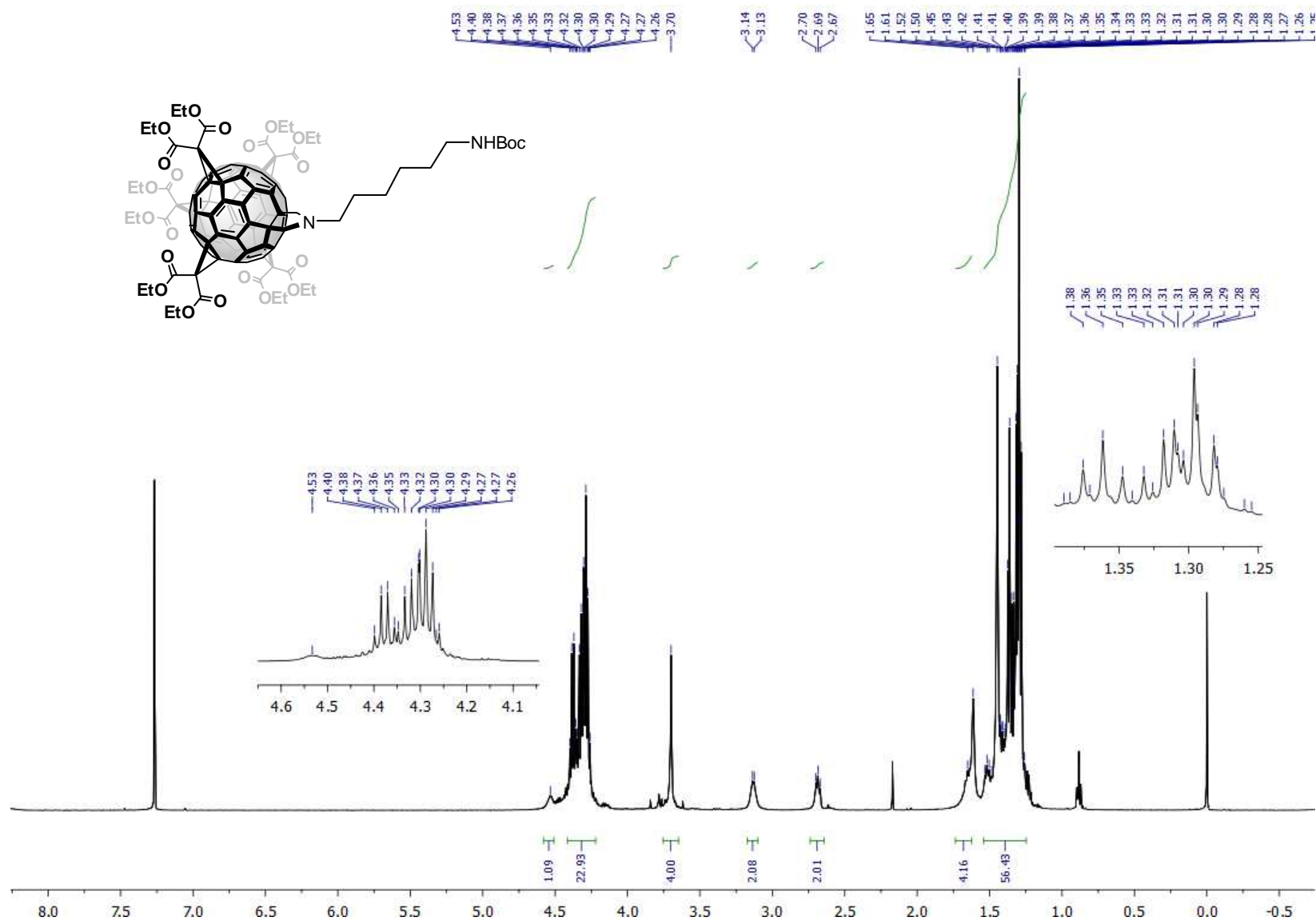
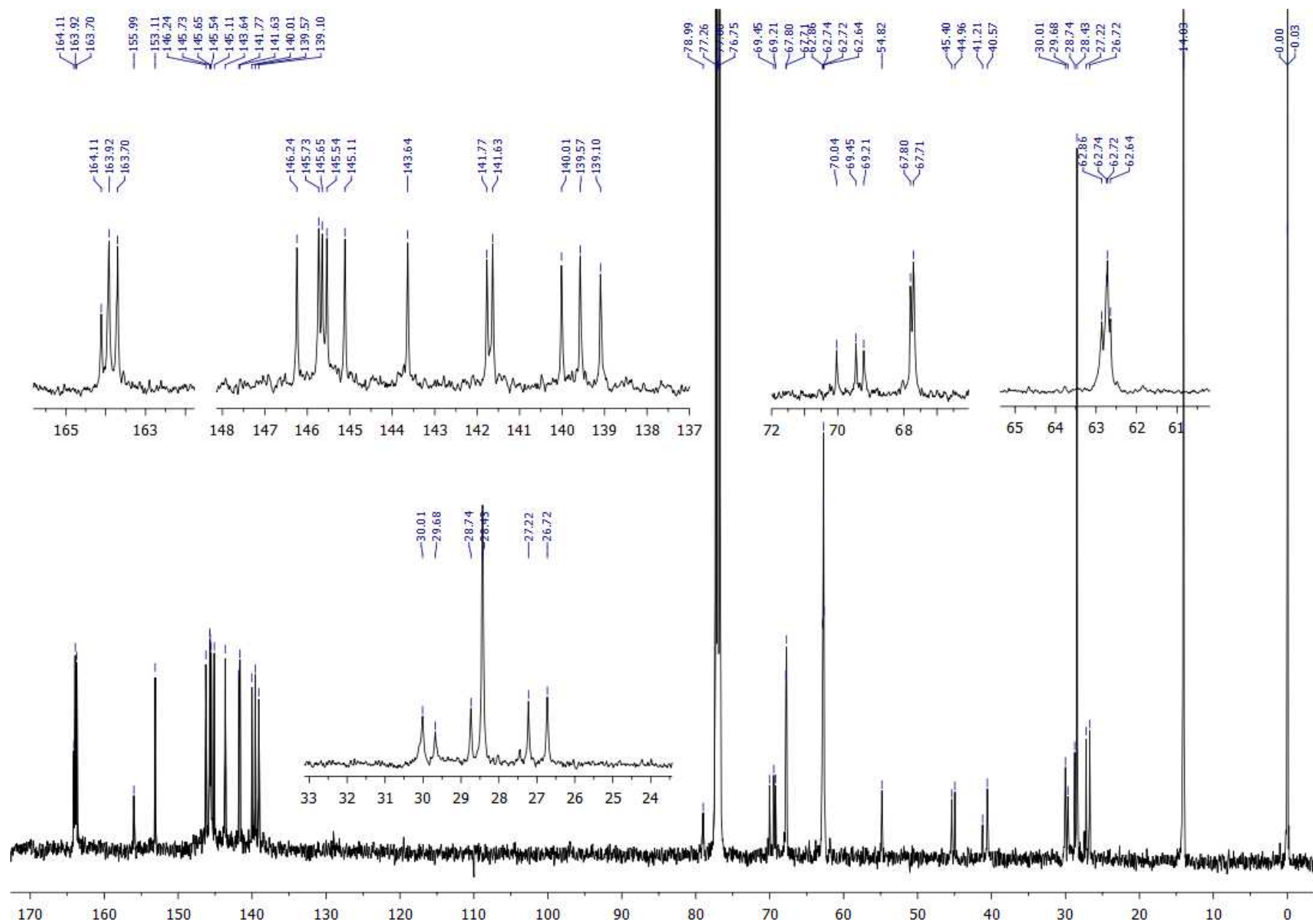
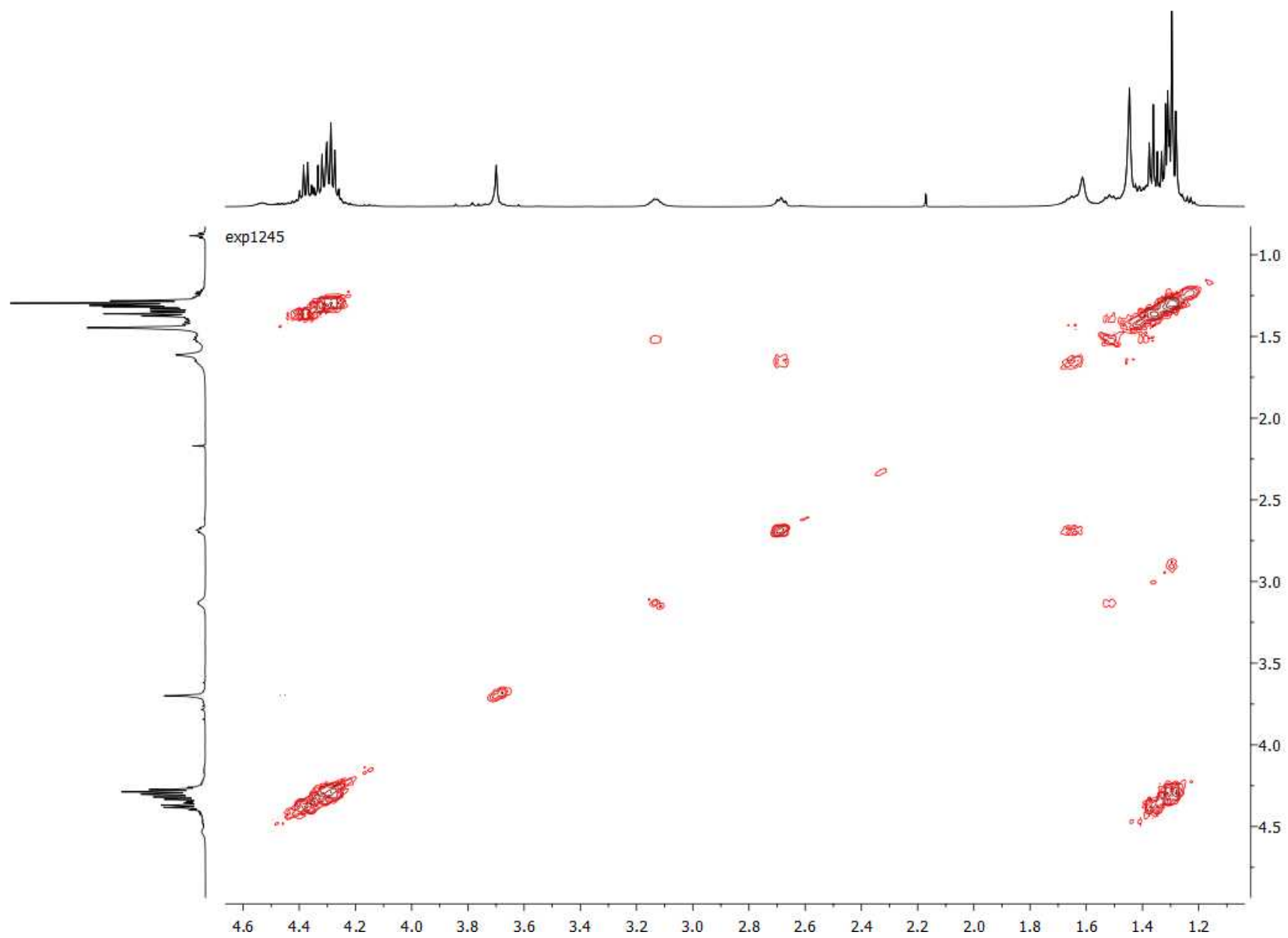


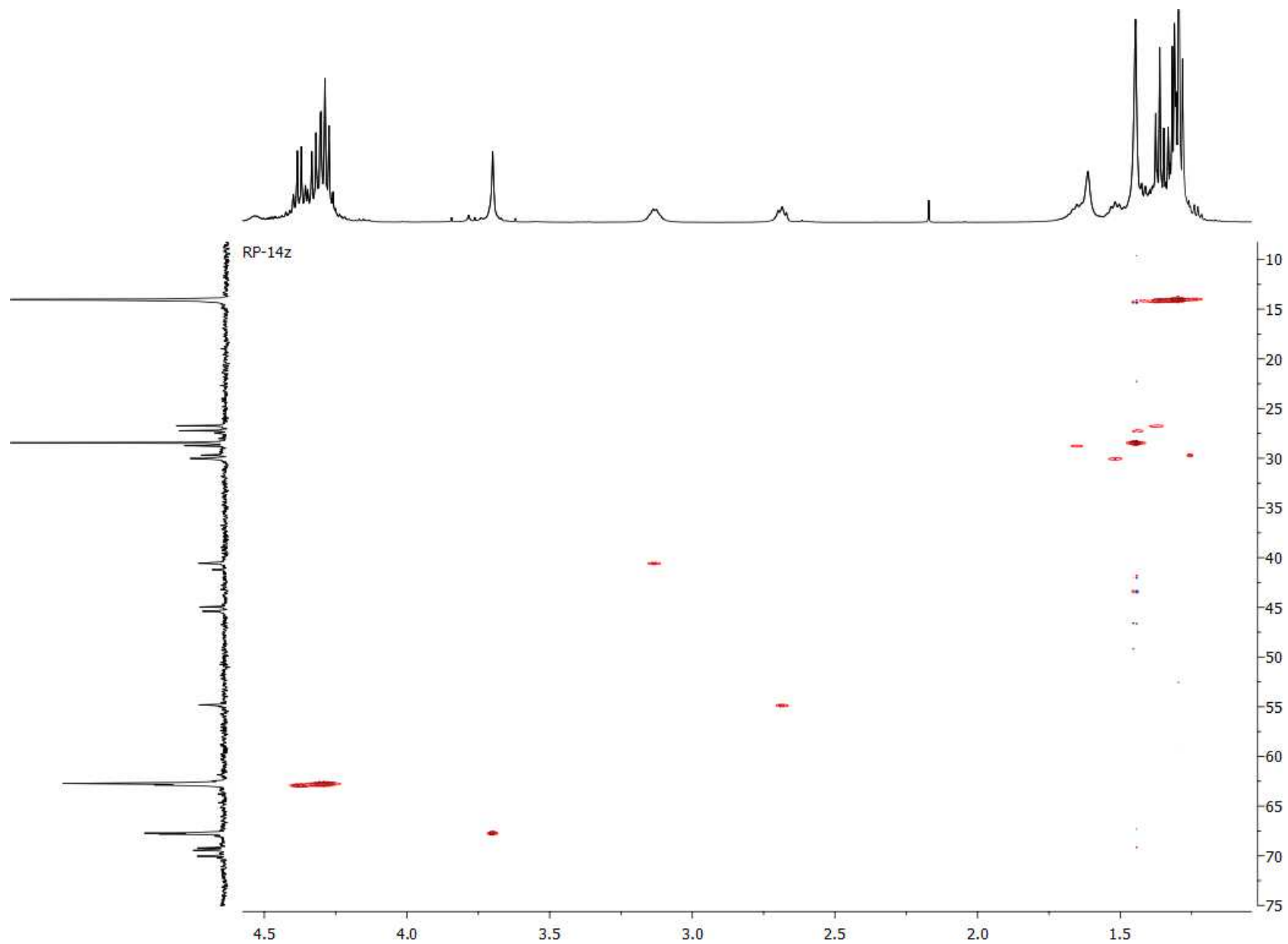
Figure S17. The expanded ¹H NMR pyrrolidine region of the isolated mixture of regioisomers **9**.

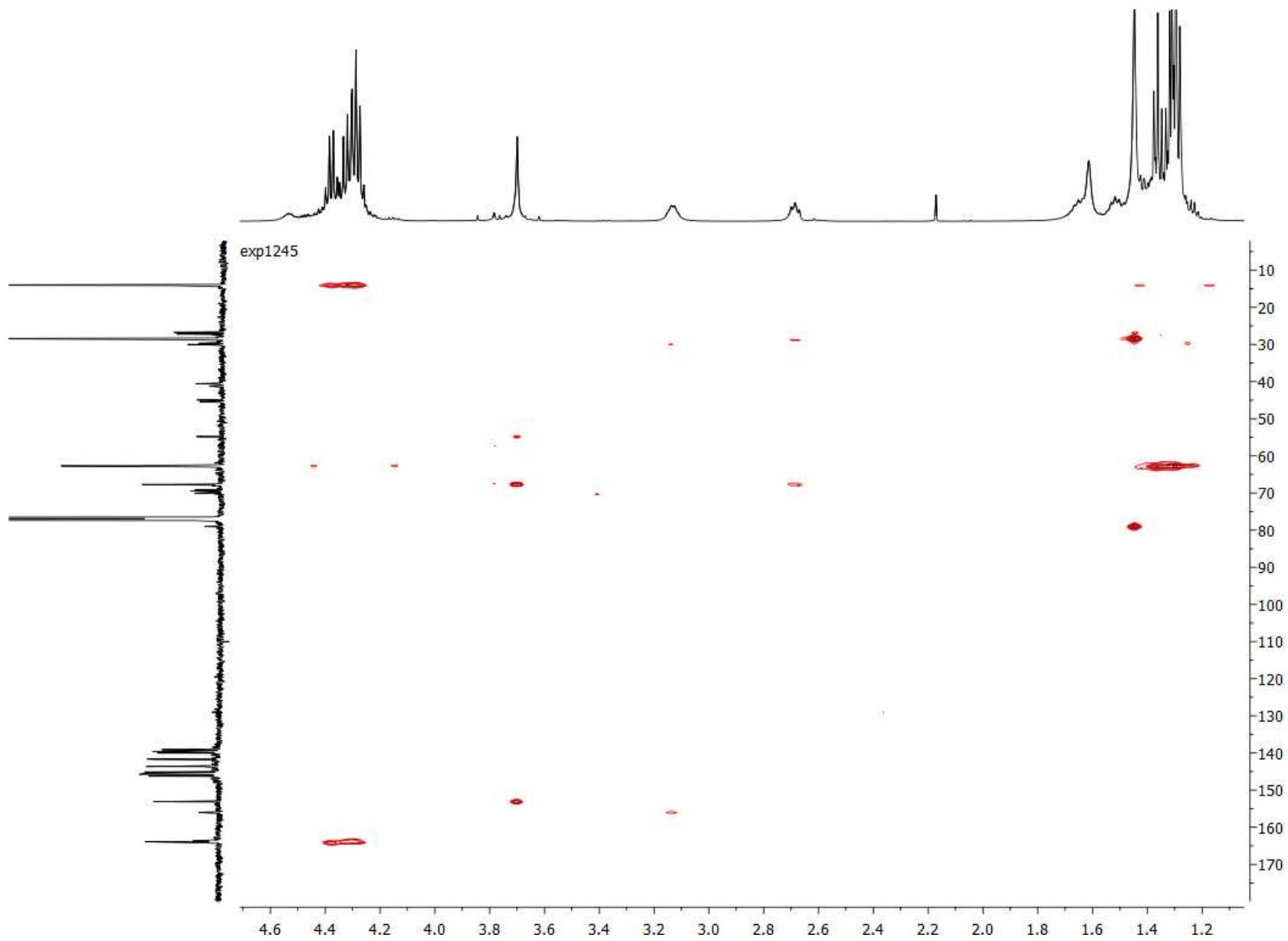
Hexaadduct 9a



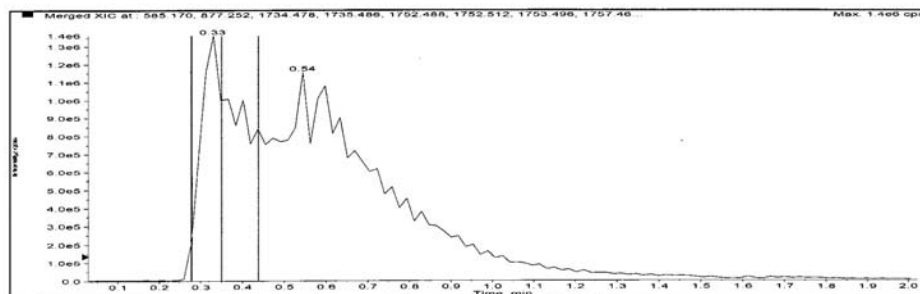




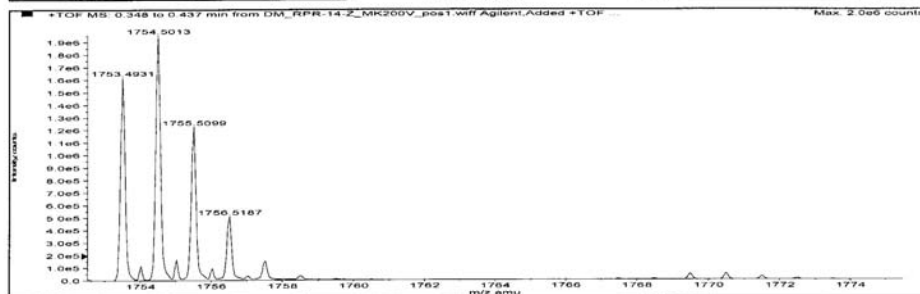
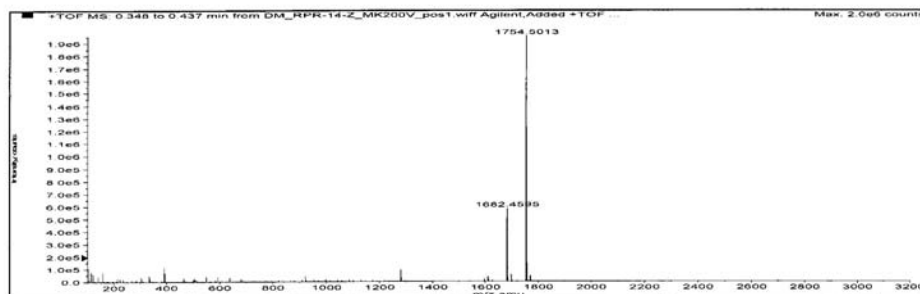




Sample Name: RPR-14-Z Sample Location: P1-D5 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\DM_MilicData\DM_RPR-14-Z_MK200V_pos1.wiff Acq Time: September 02 2015, 12:41:58 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anml\efc.xml



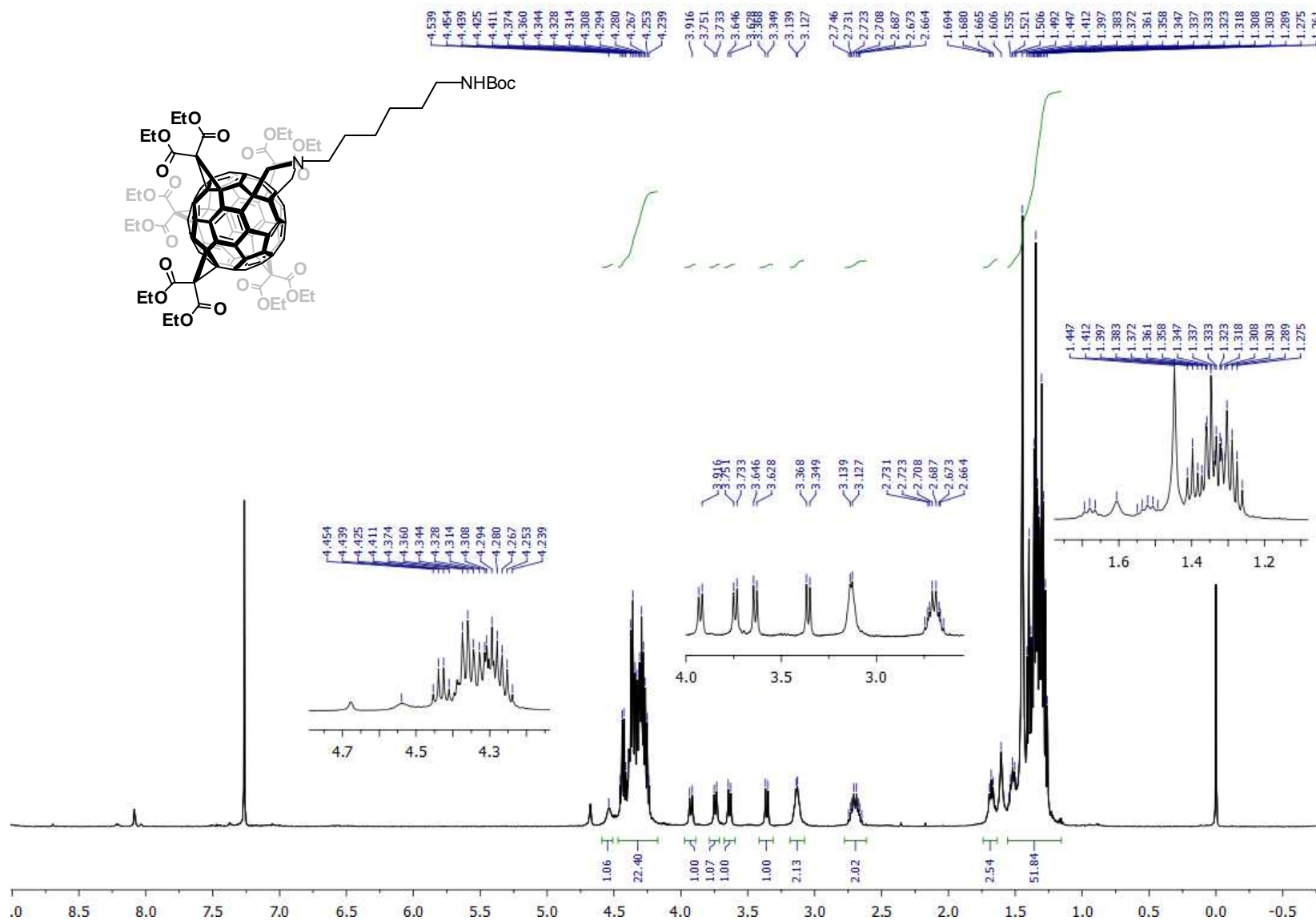
Merged XIC, Period#: 1 Experiment#: 1

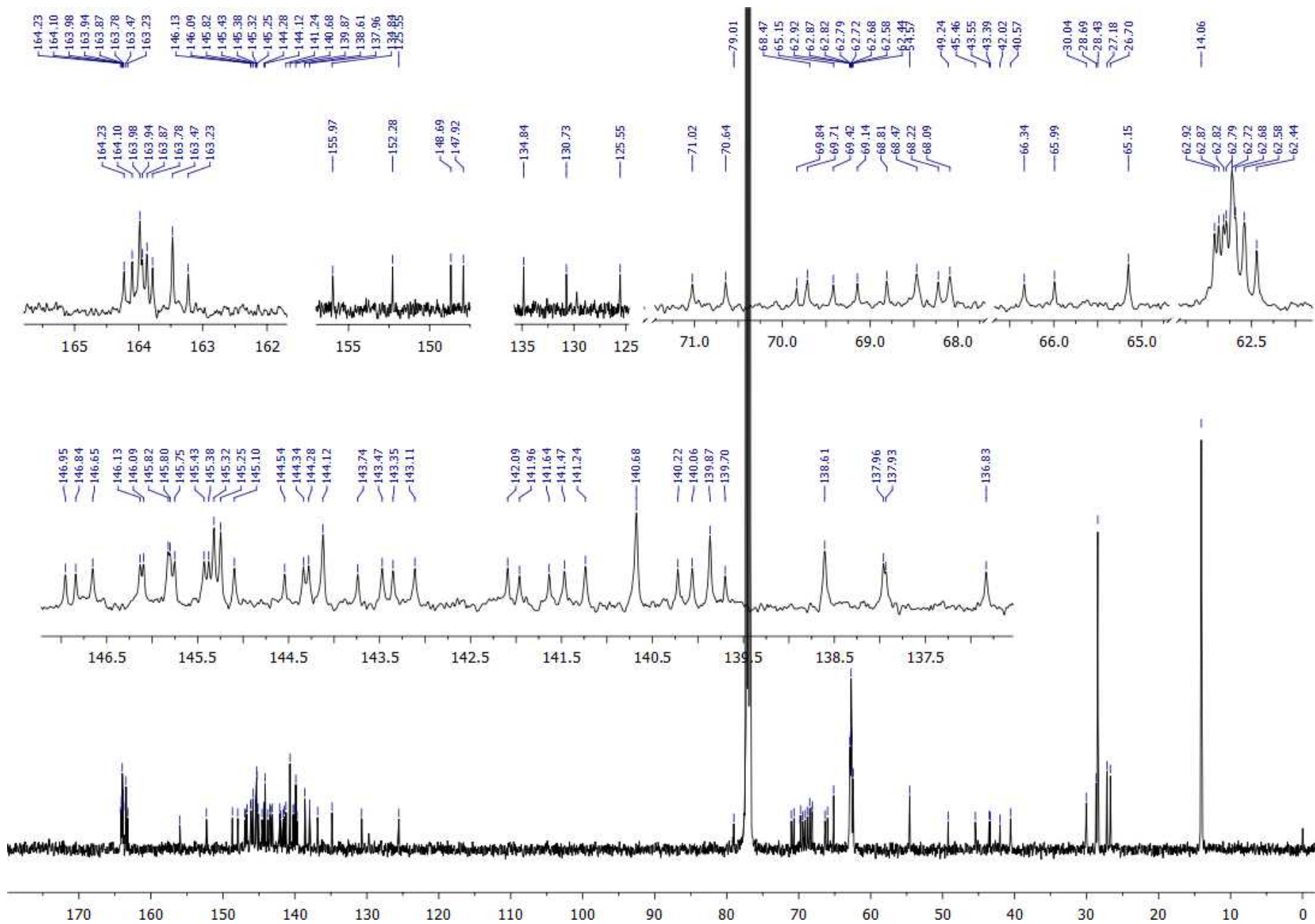


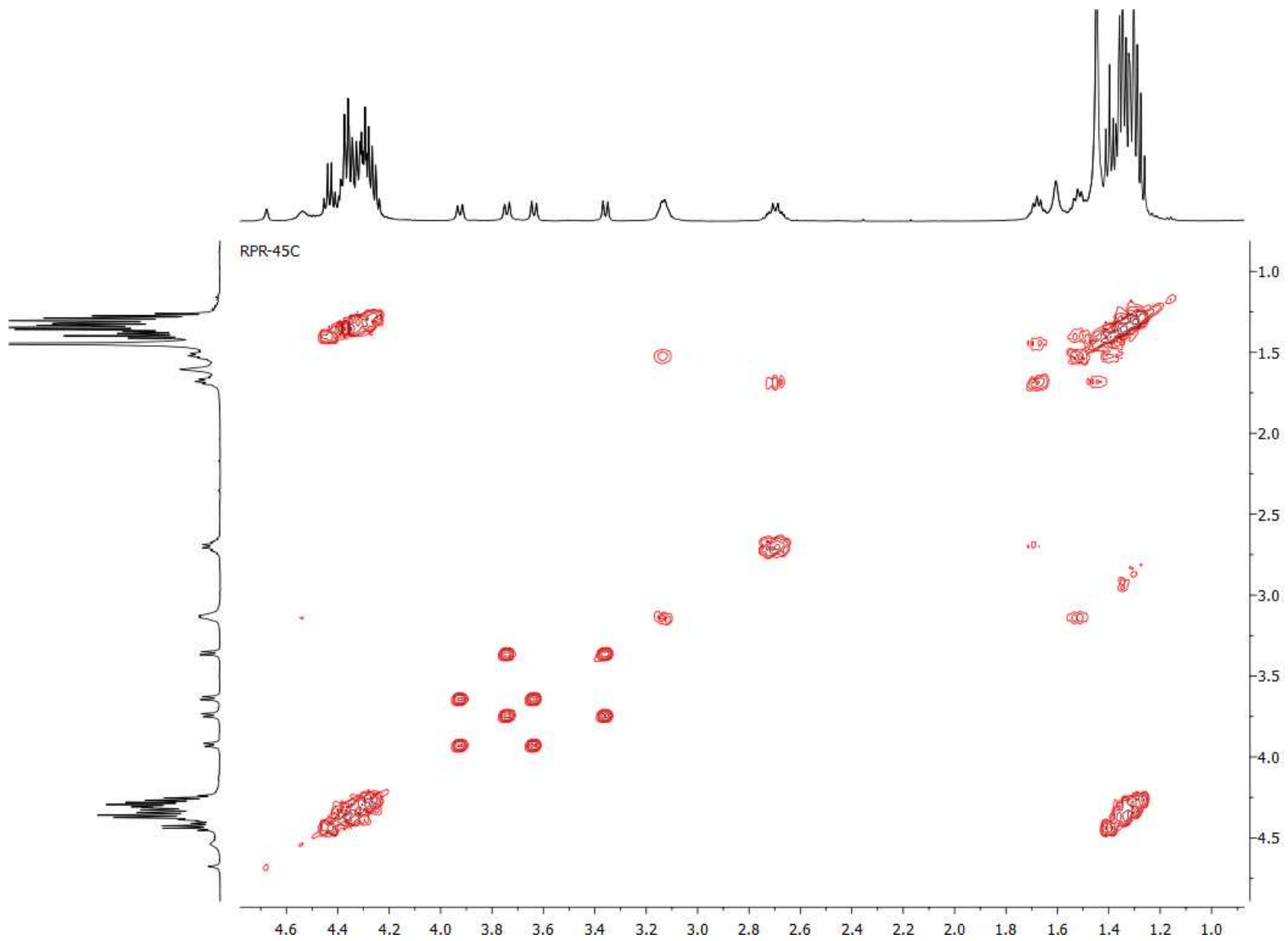
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C108H76N2O22	--	1752.48897	0.33	5.40672 E6	--

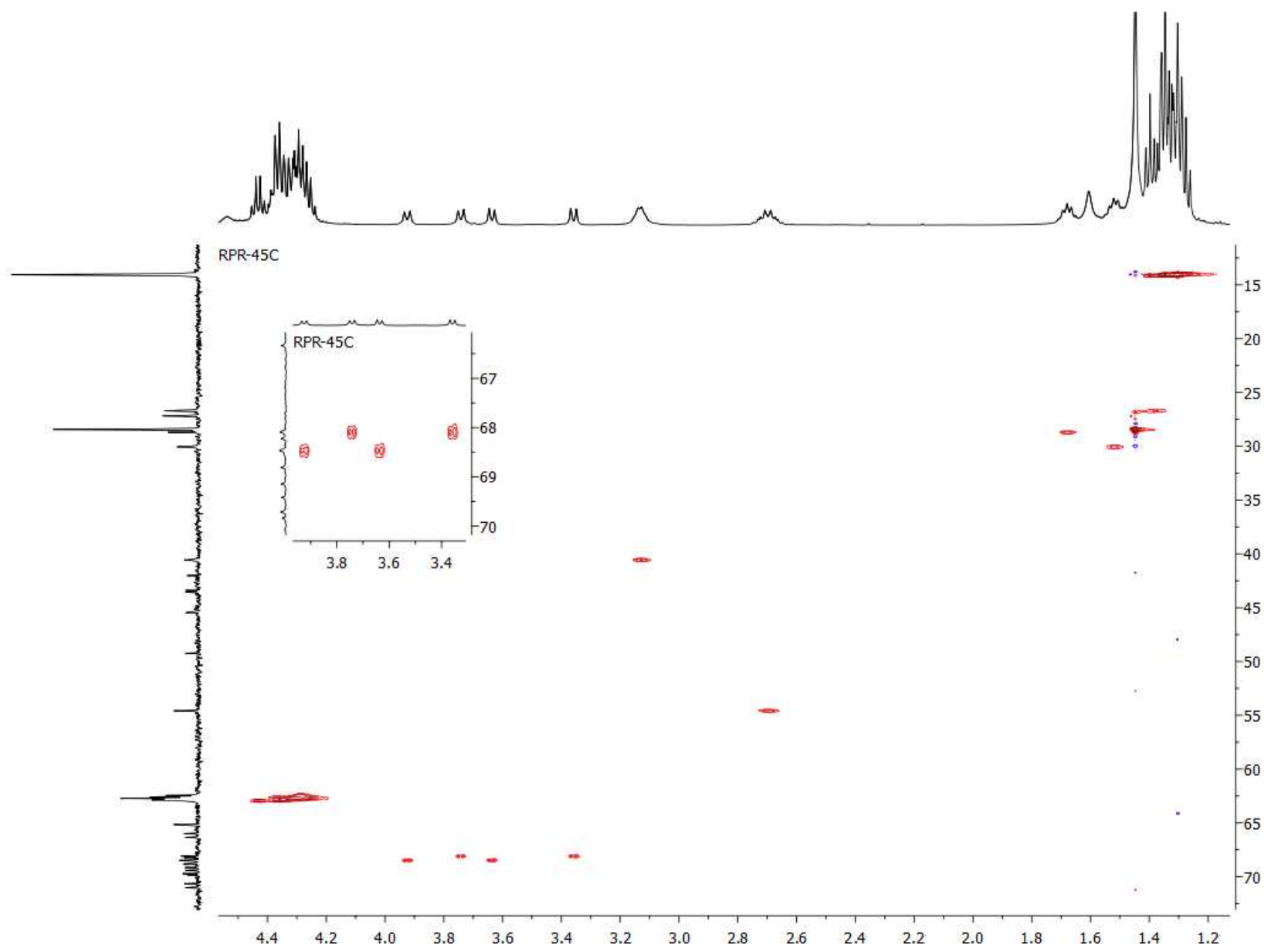
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1622319.55	1753.49625	1753.49393	-2.31724	-1.32	--
[M+Na-H2O] ⁺	155158.84	1767.46763	1757.51028	42.65557	24.27	--
[M+NH4] ⁺	50372.91	1770.52280	1770.49354	-29.15811	-16.47	--

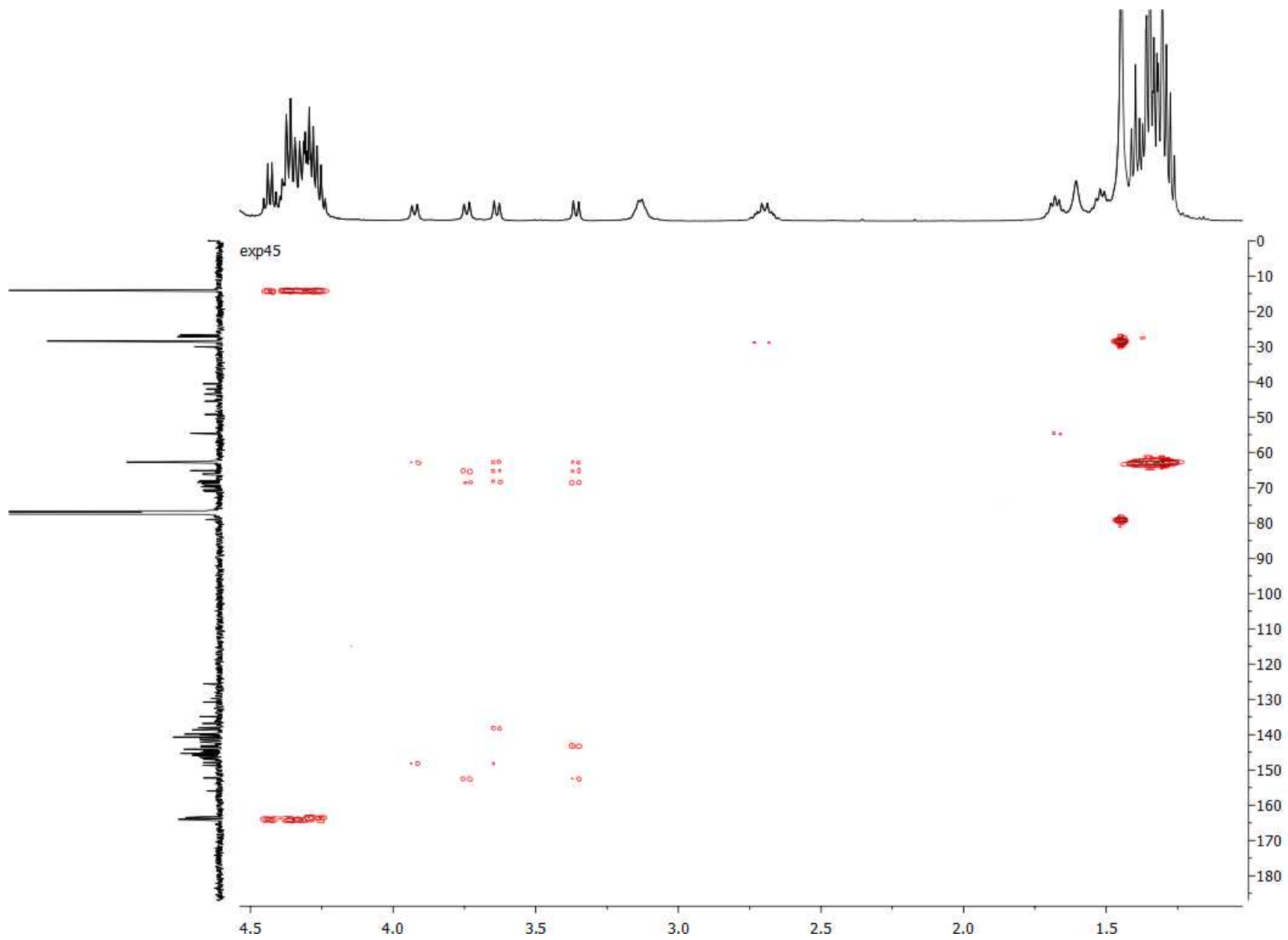
Hexaadduct 9b



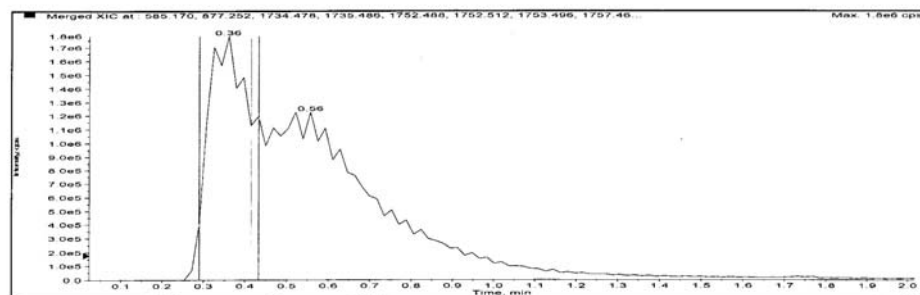




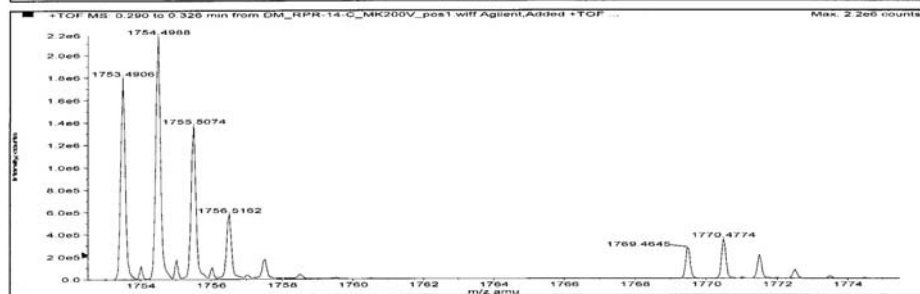
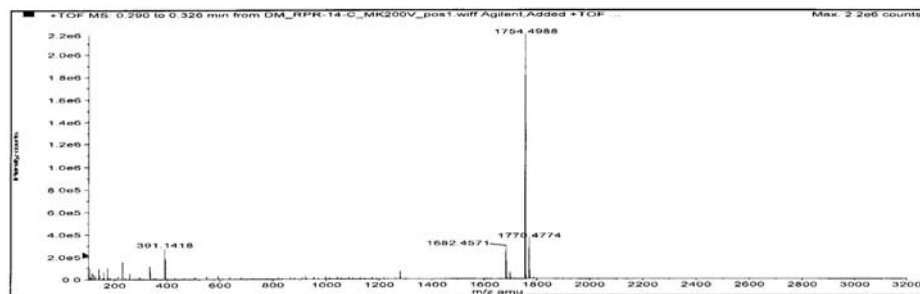




Sample Name: RPR-14-C Sample Location: P1-D4 Sample Id: Operator: Milka
 Data File Name: D:\PE Sclex Data\Projects\ID_Milic\Data\DM_RPR-14-C_MK200V_pos1.wiff Acq Time: September 02 2015, 12:38:44 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlfc.xml



Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C108H76N2O22	--	1752.48897	0.36	1.31658 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1802622.00	1753.49625	1753.49159	-4.66023	-2.66	--
[M+Na-H ₂ O] ⁺	183078.80	1767.46763	1757.50713	99.66328	22.48	--
[M+NH ₄] ⁺	360529.08	1770.52280	1770.49082	-31.98251	-18.06	--

Regioisomeric Bingel-Prato [5:1]-hexaadducts **10**

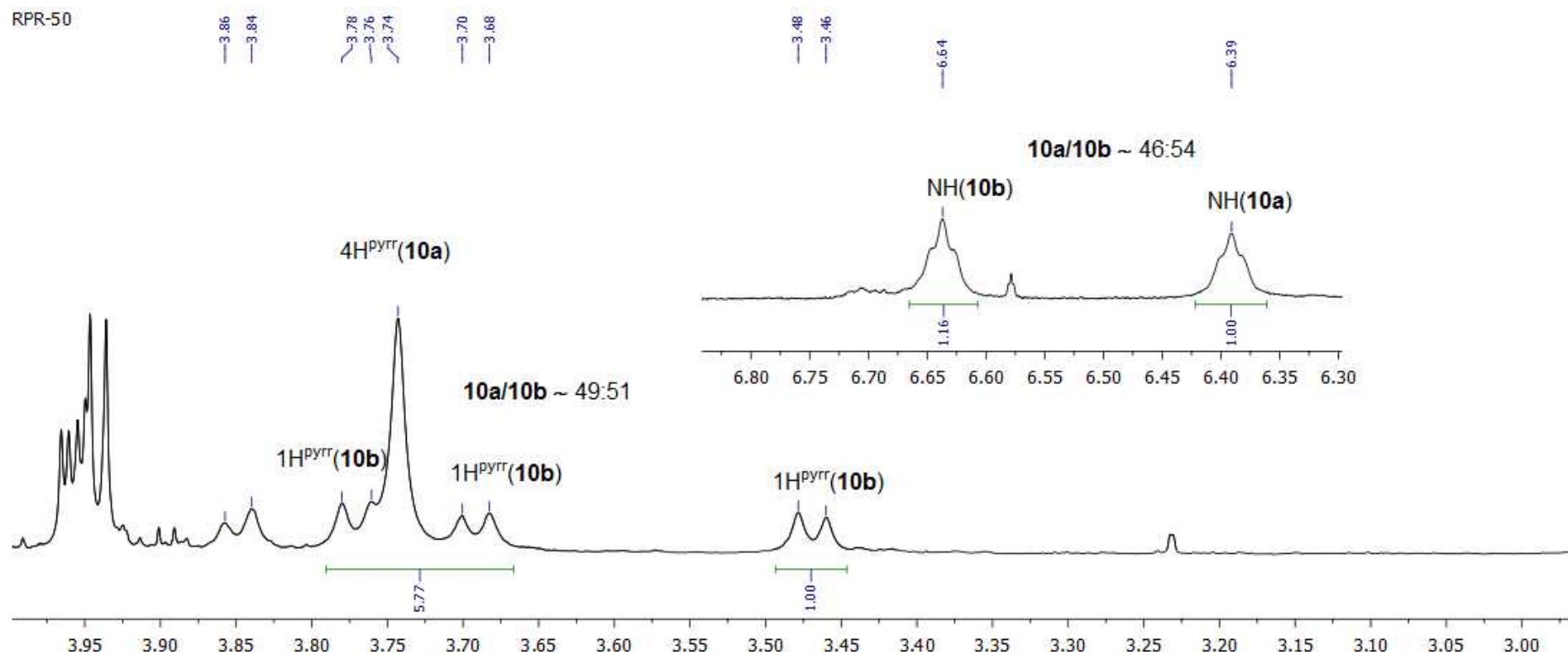
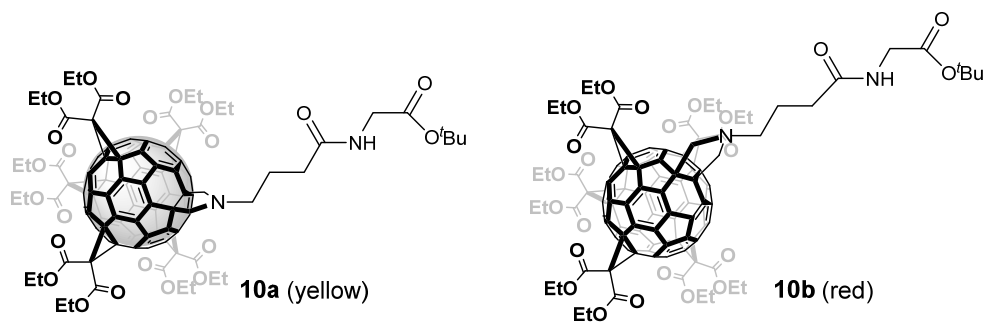
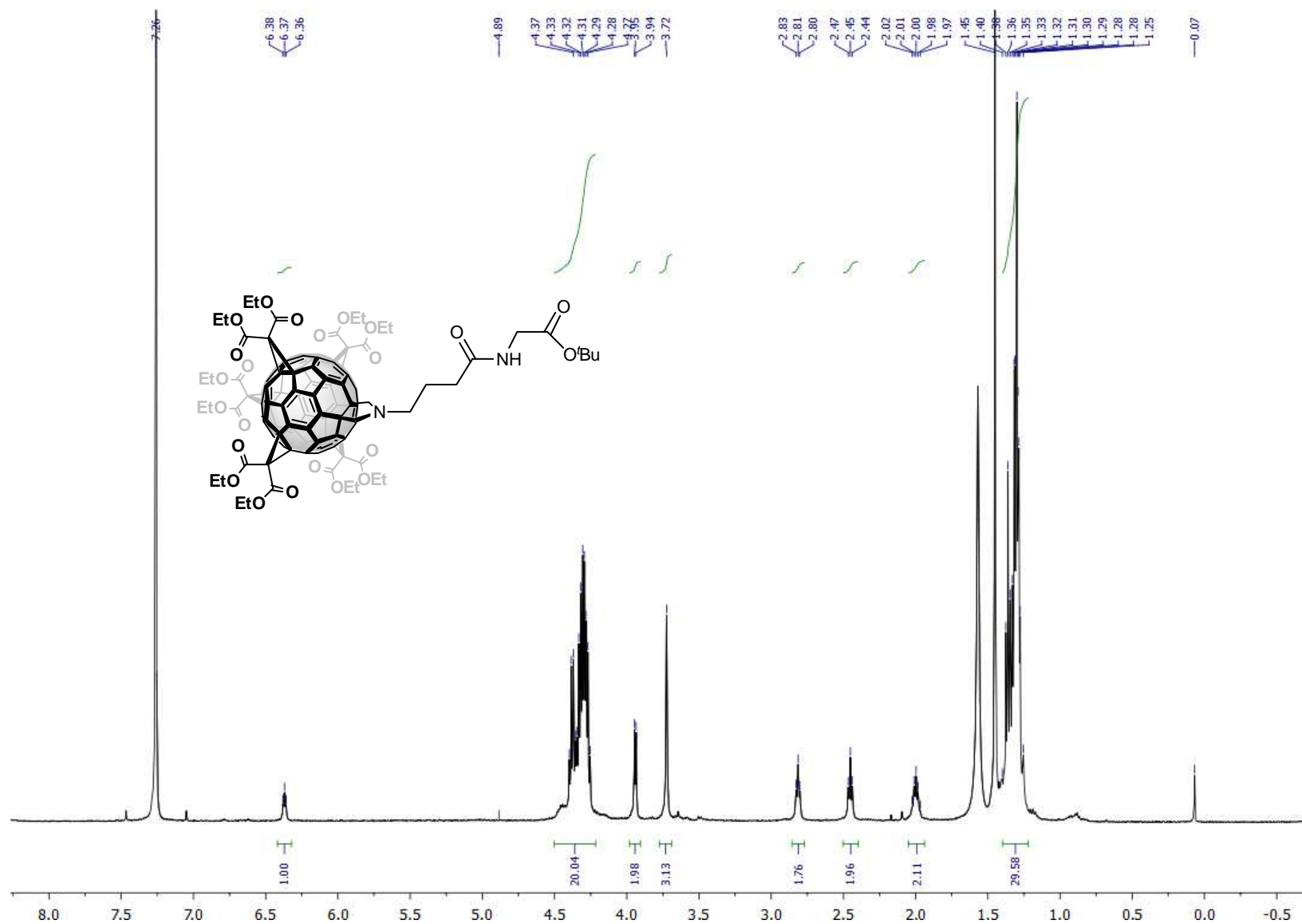
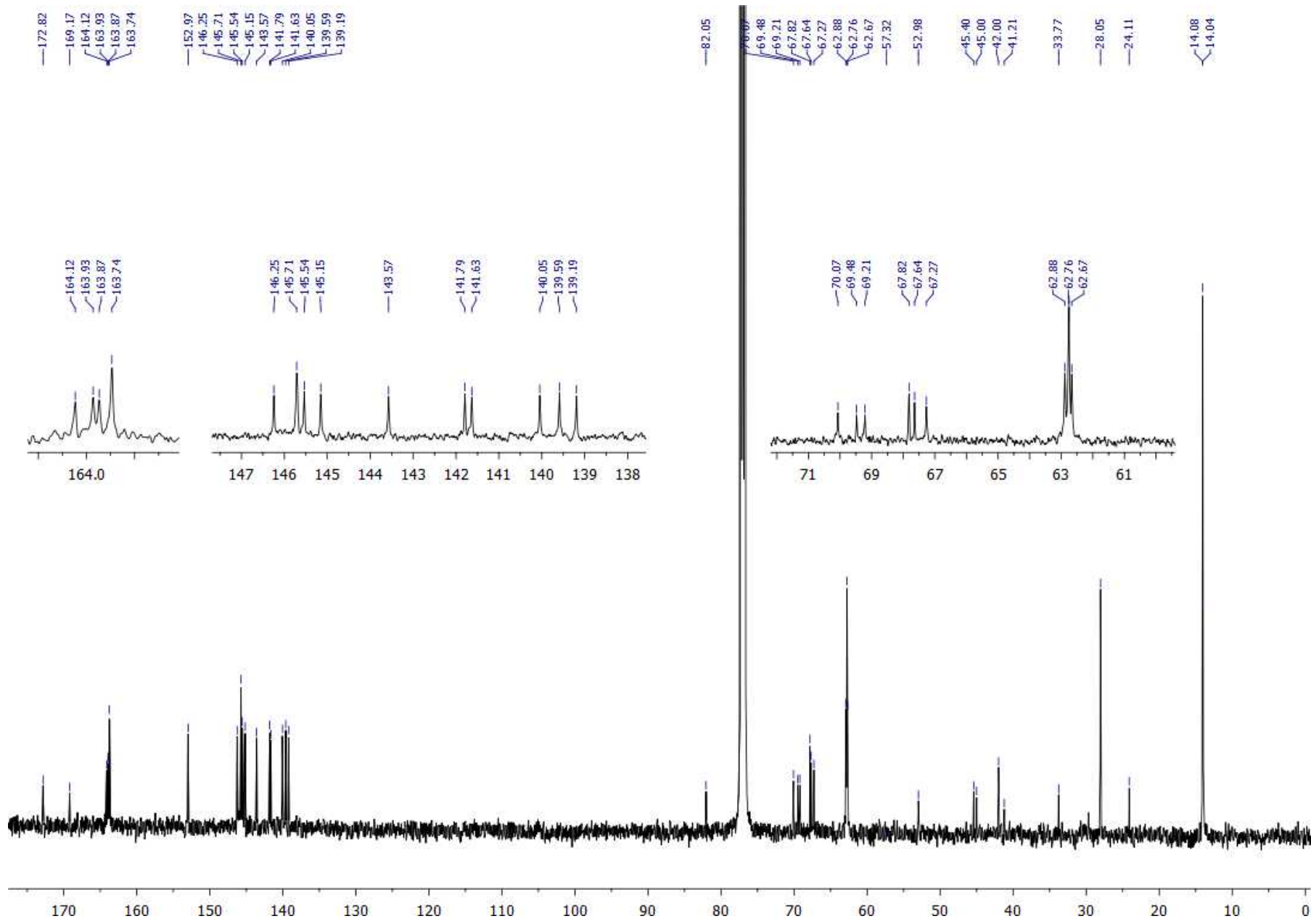
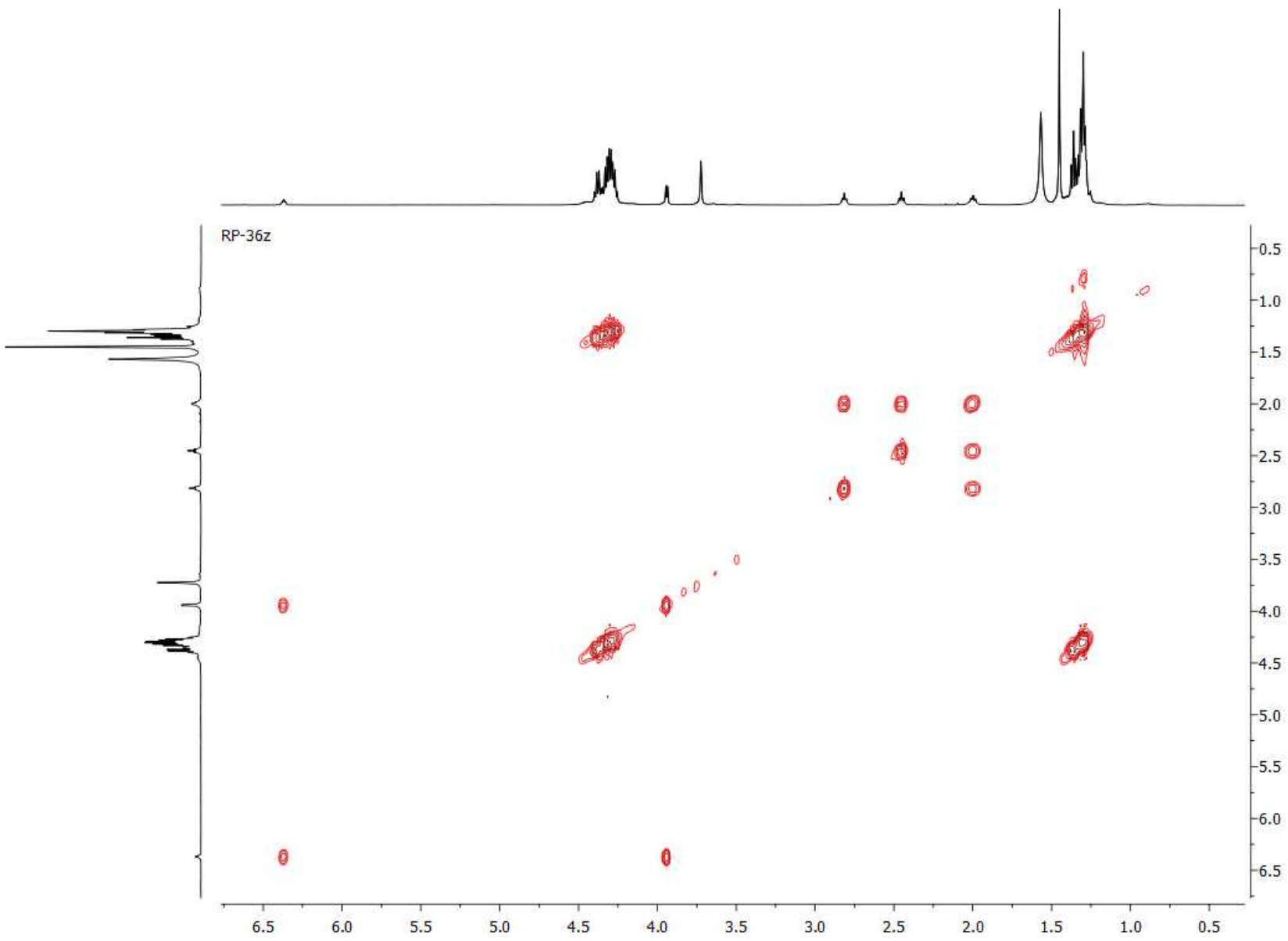


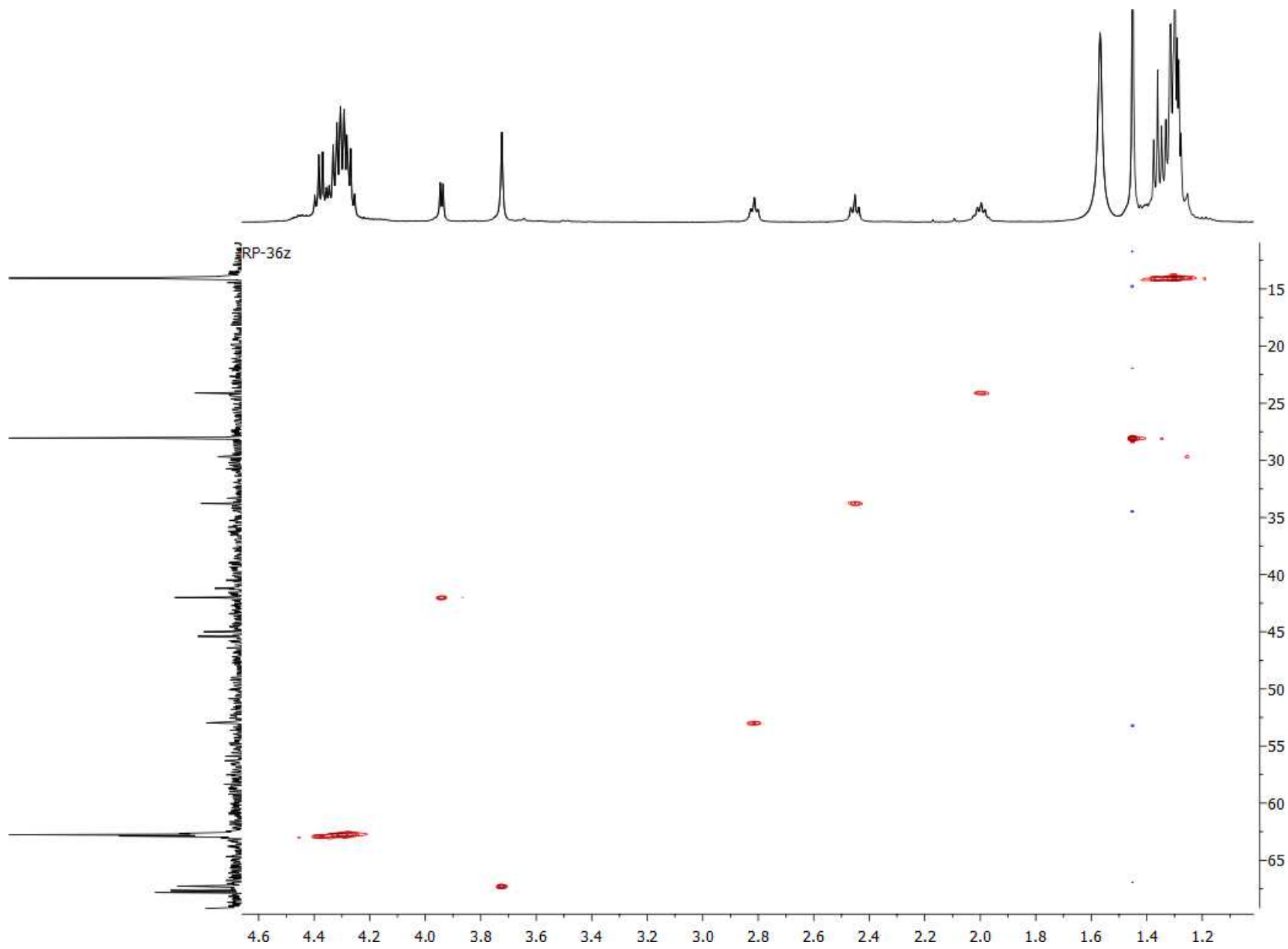
Figure S18. The expanded ¹H NMR pyrrolidine and amide regions of the isolated mixture of regioisomers **10**.

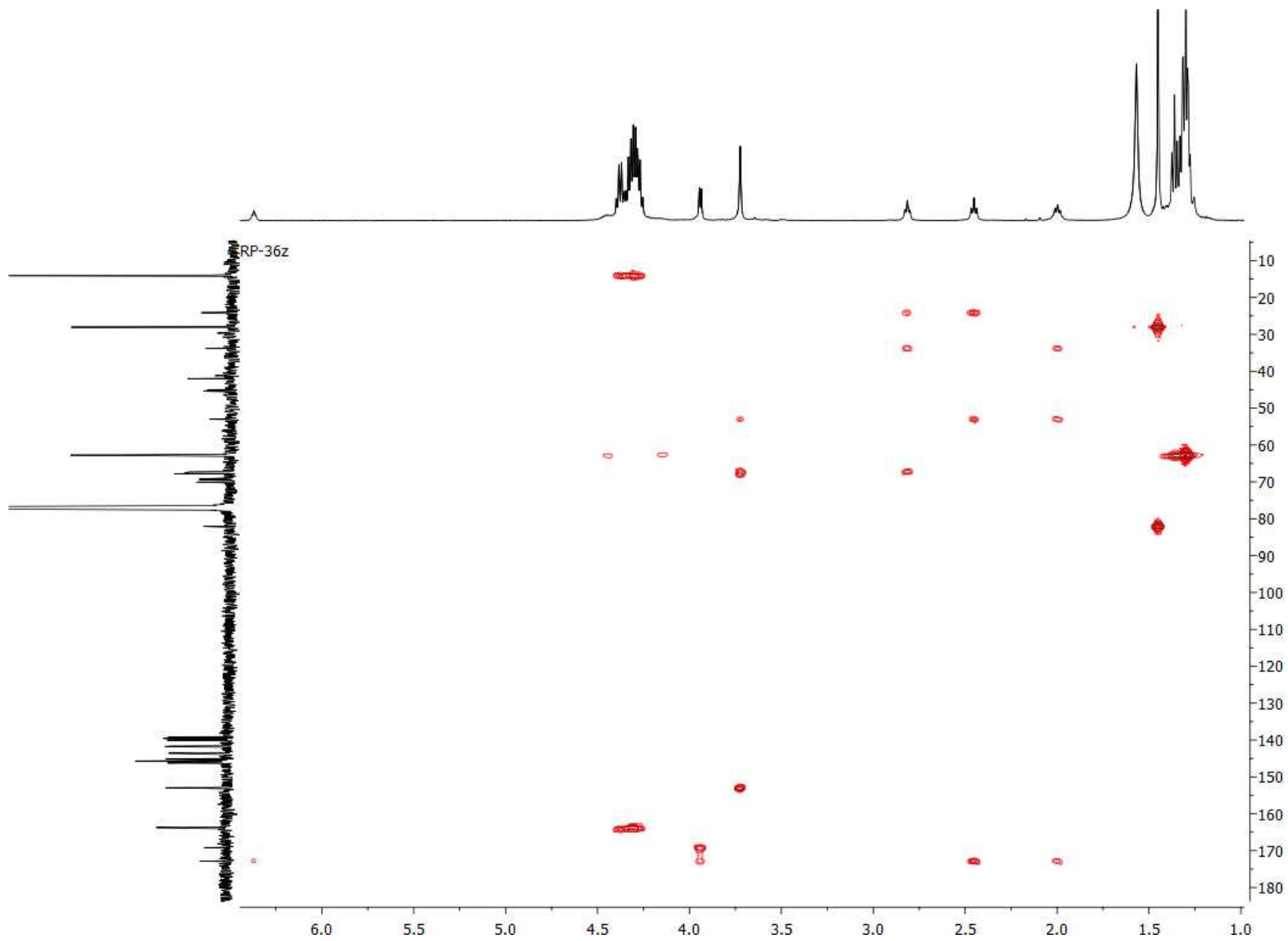
Hexaadduct 10a



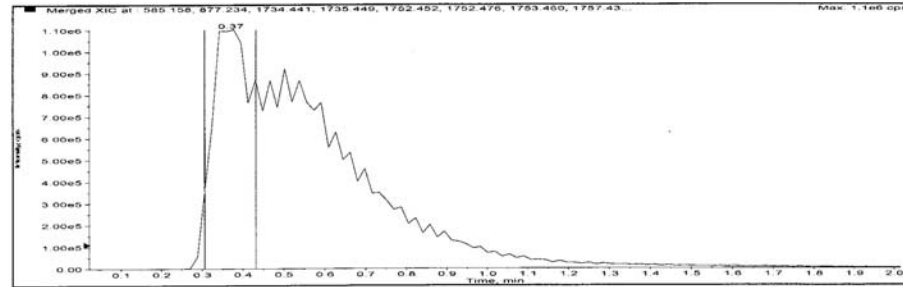




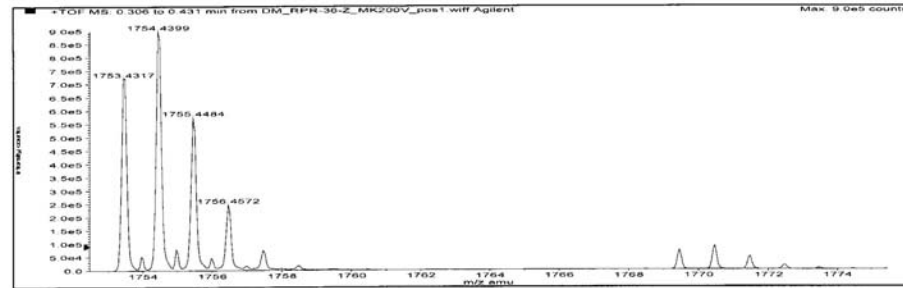
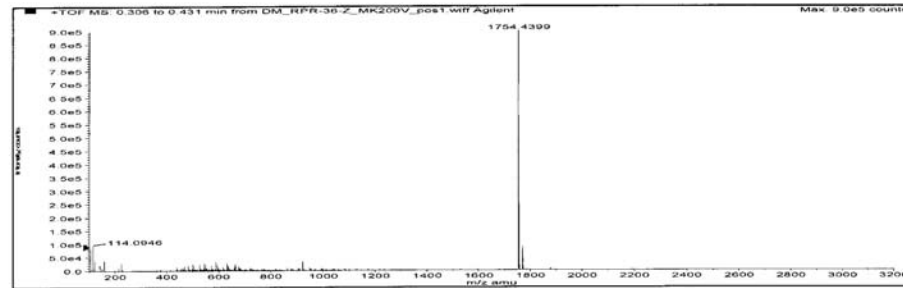




Sample Name: RPR-36-Z Sample Location: P1-E2 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\DM_Milic\Data\DM_RPR-36-Z_MK200V_pos1.wiff Acq Time: October 19 2015, 01:43:29 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.anml\efc.xml



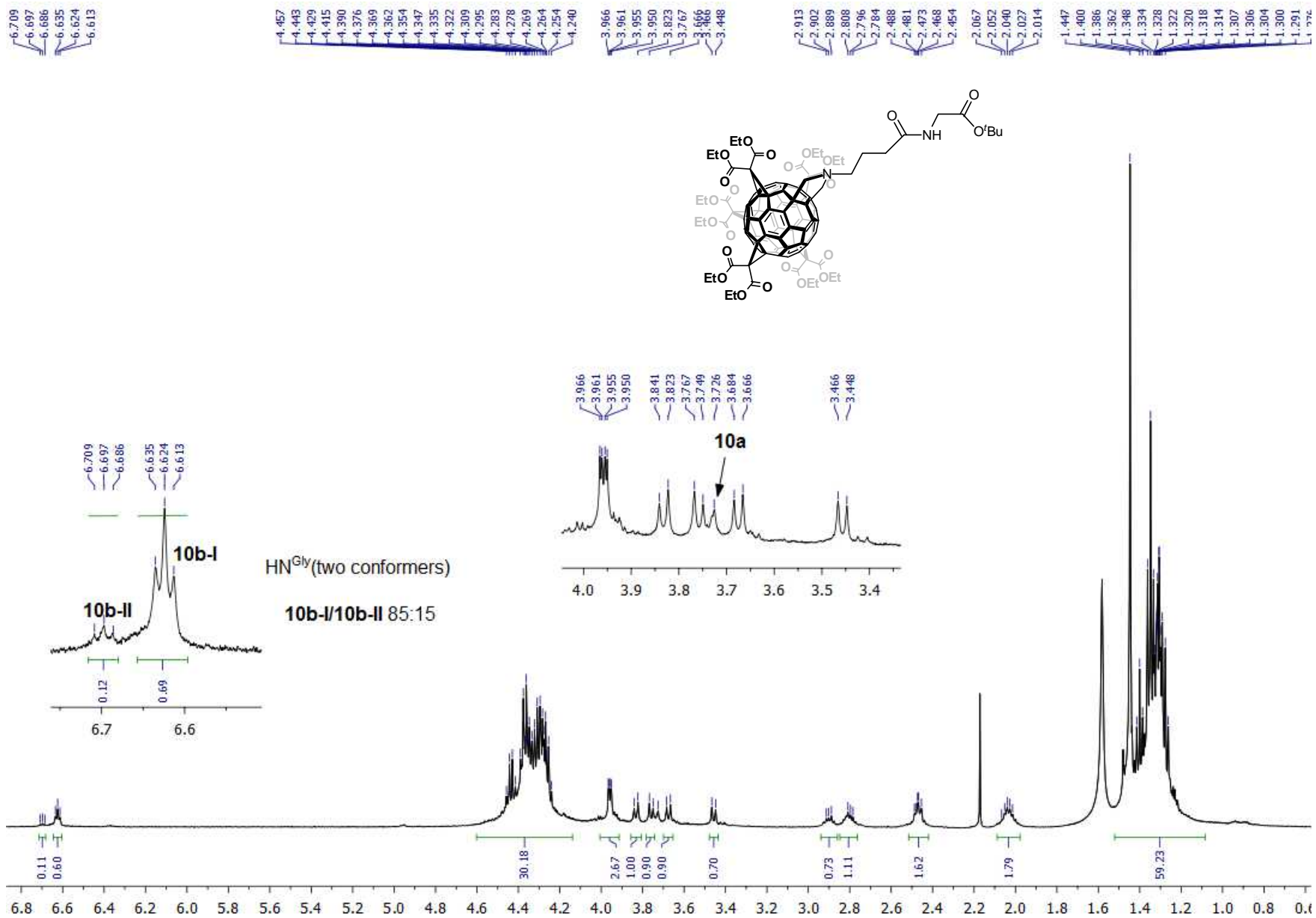
Merged XIC, Period# : 1 Experiment# : 1

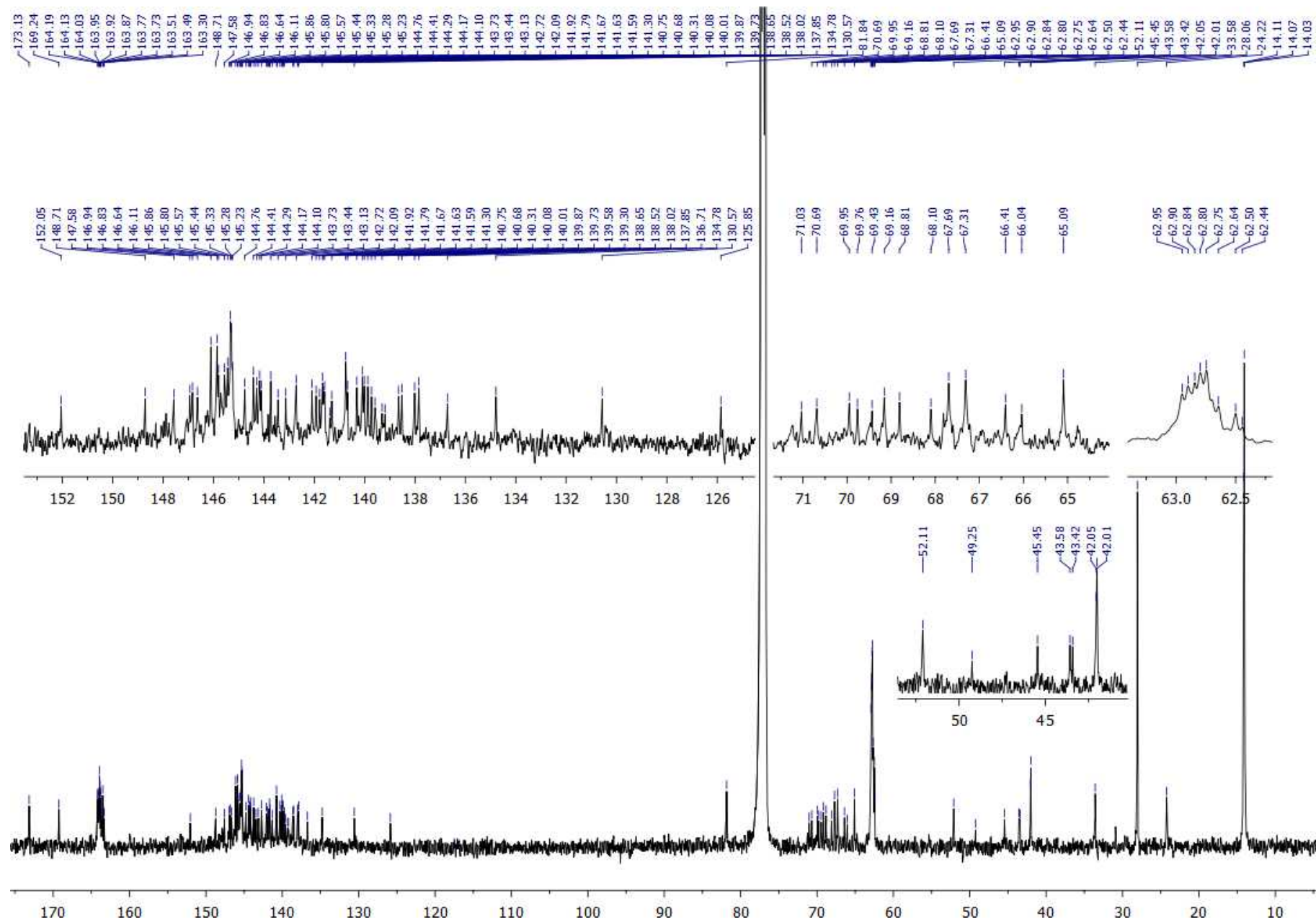


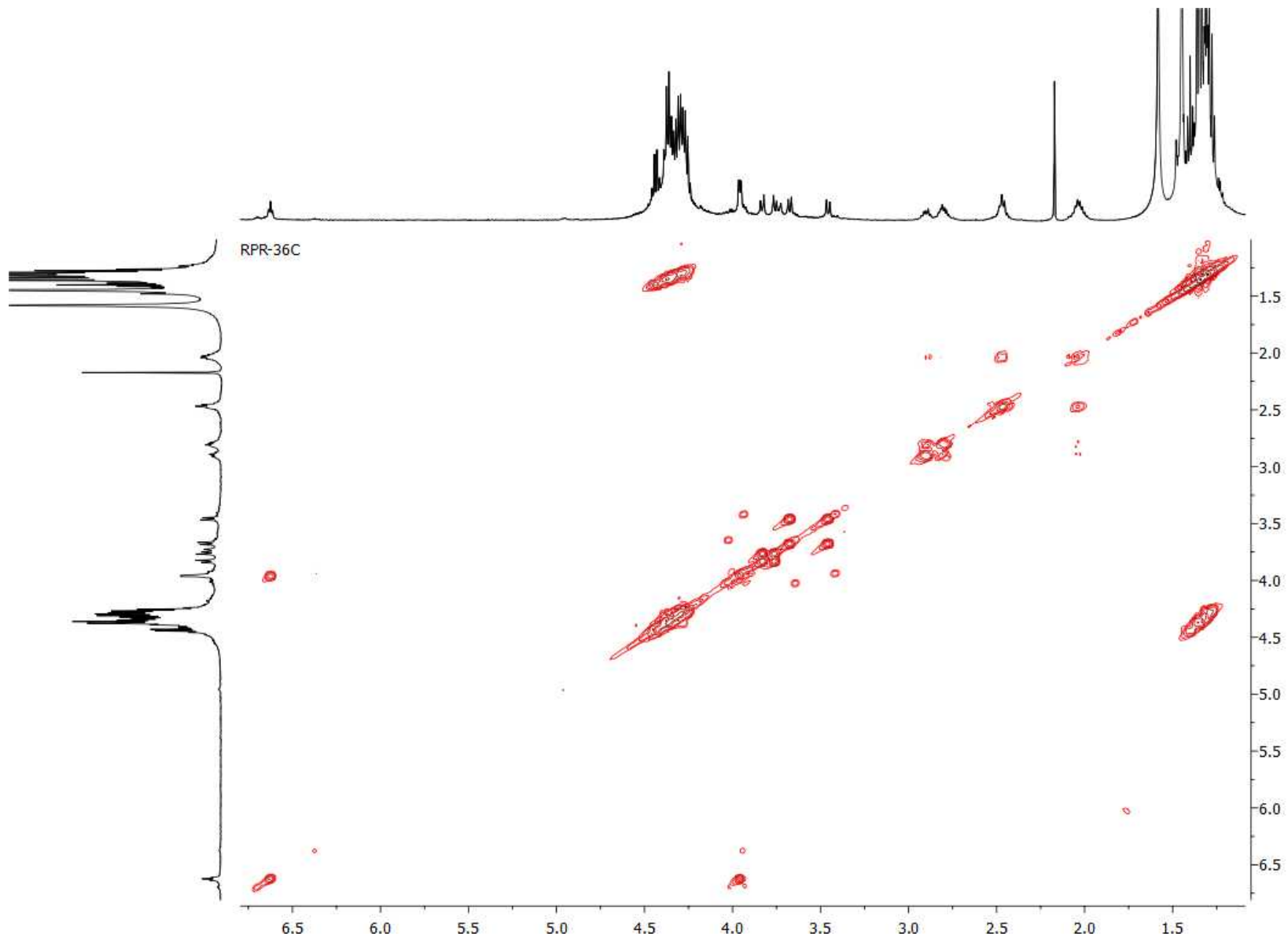
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C10H7N2O23	--	1752.45259	0.37	4.11680 E6	--

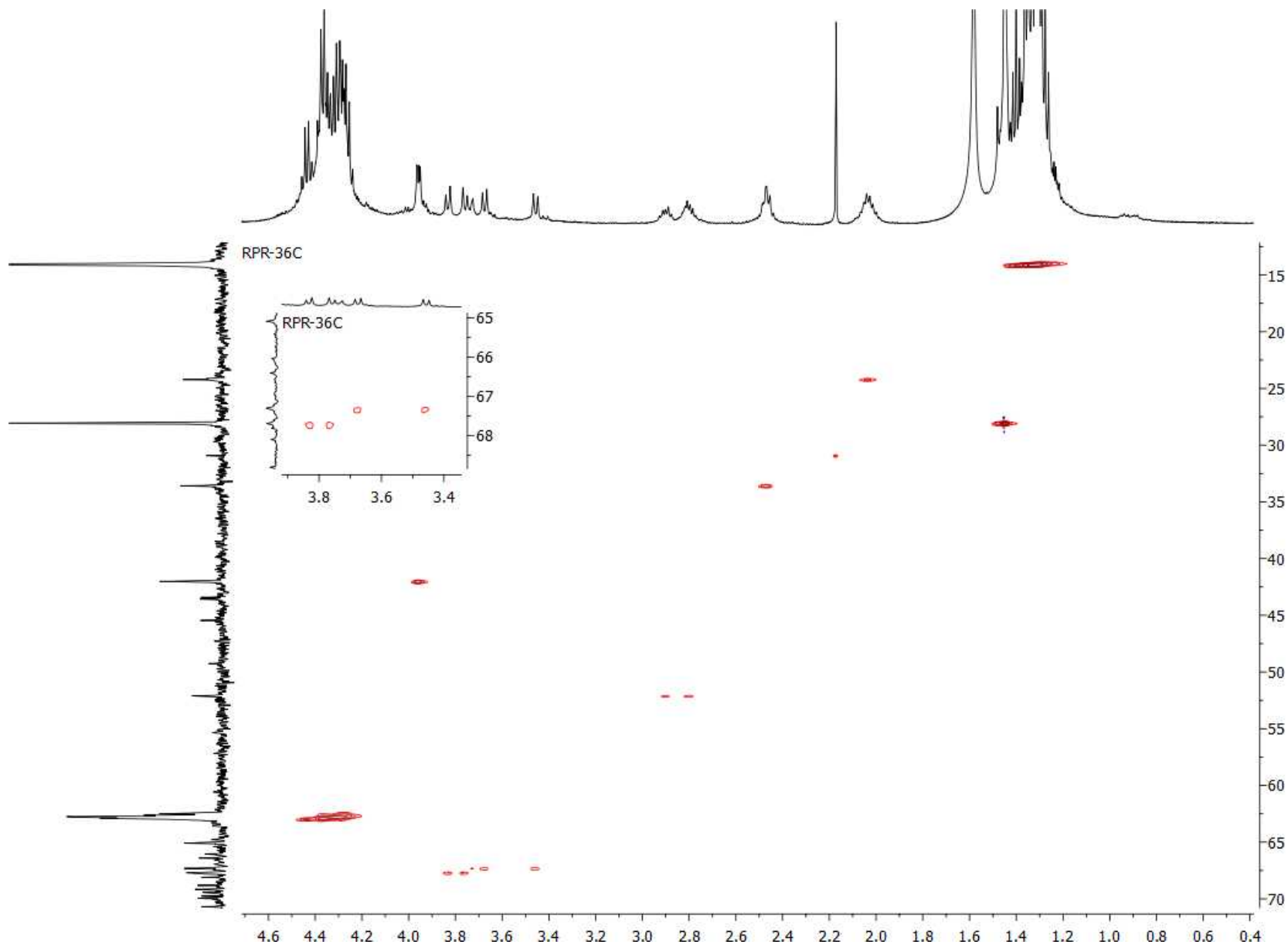
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	760924.58	1753.45986	1753.45613	-3.73650	-2.13	--
[M+Na-H2O] ⁺	75140.76	1757.43124	1757.47274	41.49414	23.61	--
[M+NH4] ⁺	90640.30	1770.48641	1770.45679	-29.62512	-16.73	--

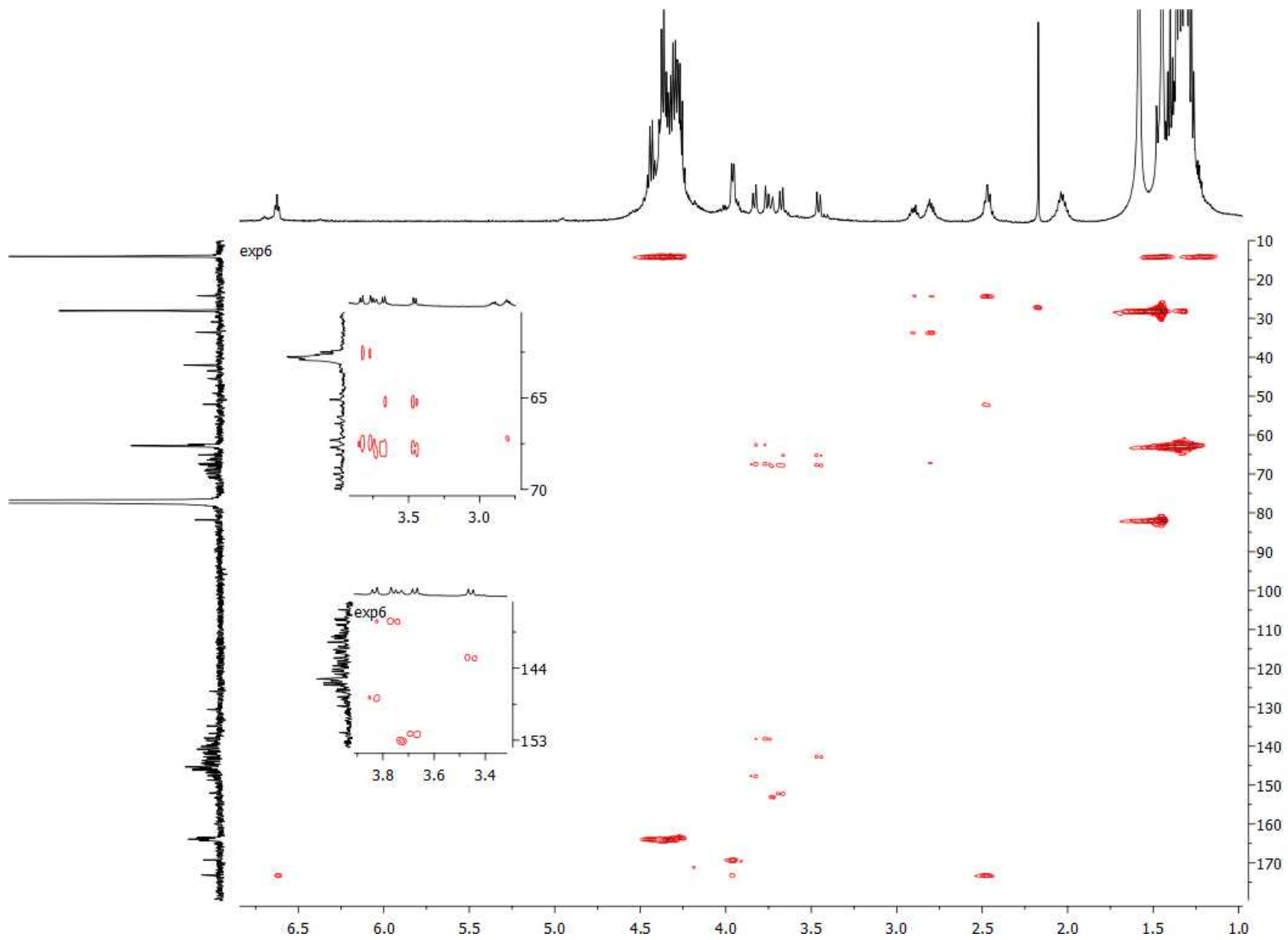
Hexaadduct 10b

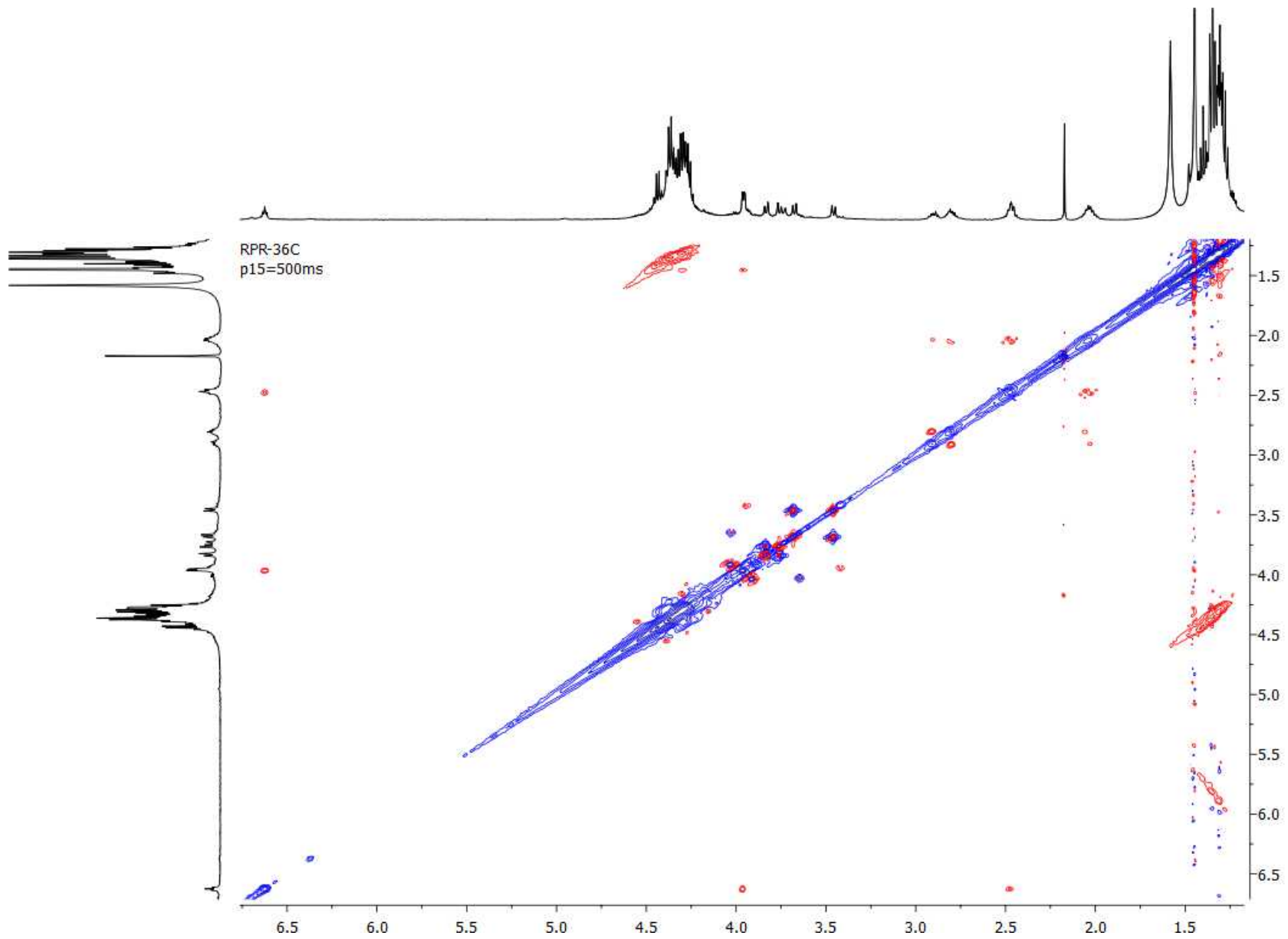




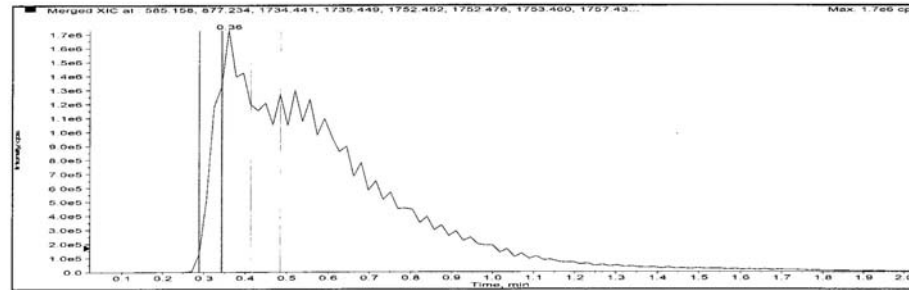




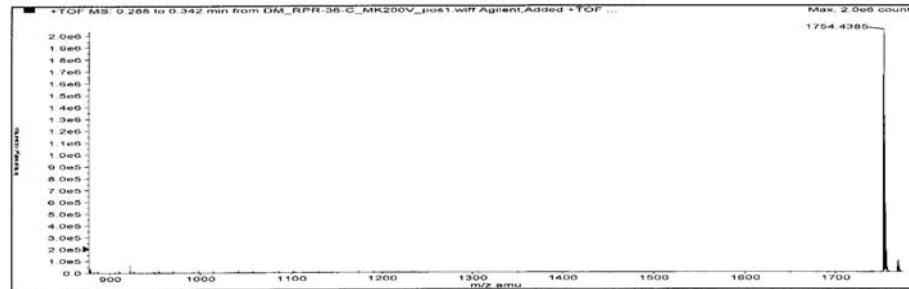
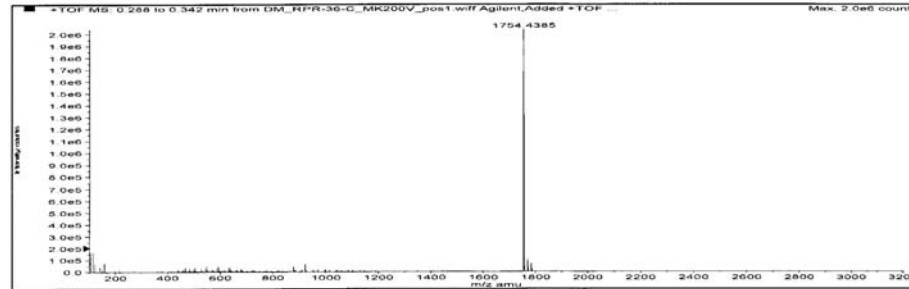




Sample Name: RPR-36-C Sample Location: P1-E1 Sample Id: Operator: Milka
 Data File Name: D:\PE ScieX Data\Projects\DM_MilicData\DM_RPR-36-C_MK200V_pos1.wiff Acq Time: October 19 2015, 01:40:16 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml



Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C107H72N2O23	--	1752.45259	0.36	1.49891 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H]2+	36120.04	877.23357	877.23238	-1.18606	-1.35	--
[M+H]+	1752998.75	1753.45986	1753.45424	-5.62193	-3.21	--
[M+Na-H2O]+	187427.45	1757.43124	1757.46997	38.72200	22.03	--
[M+NH4]+	105491.04	1770.48641	1770.45499	-31.42268	-17.75	--

Regioisomeric Bingel-Prato [5:1]-hexaadducts **11**

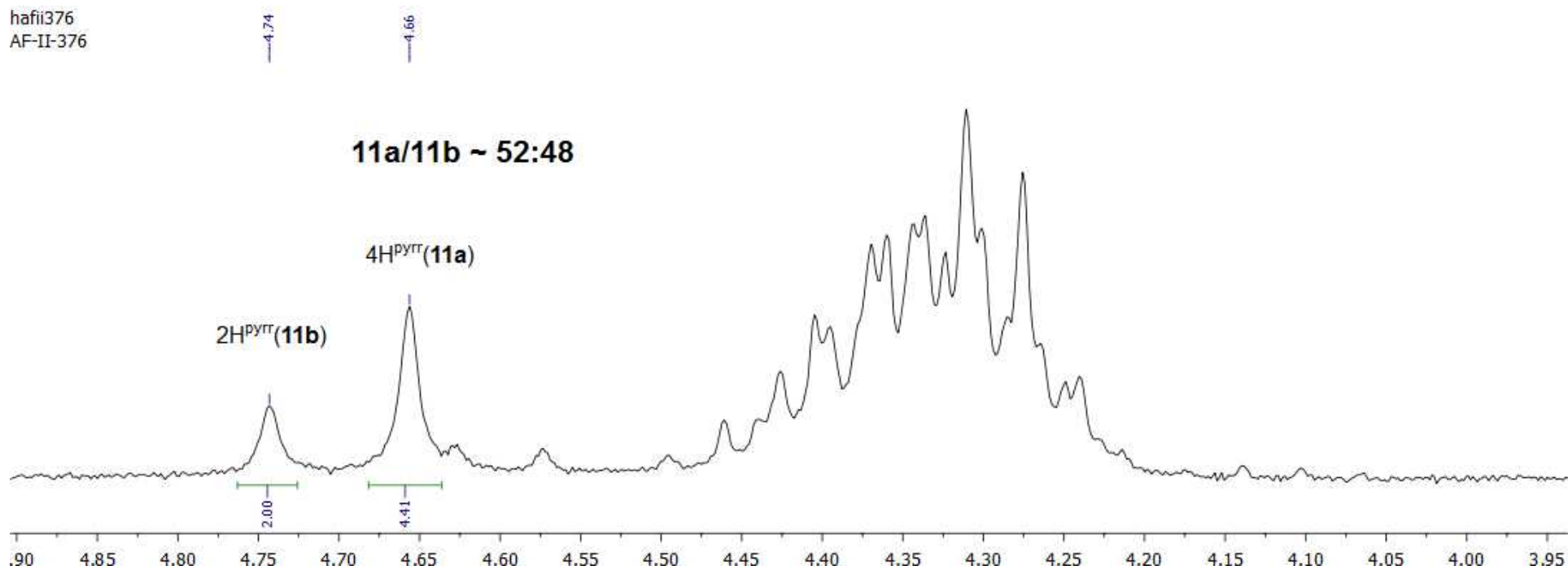
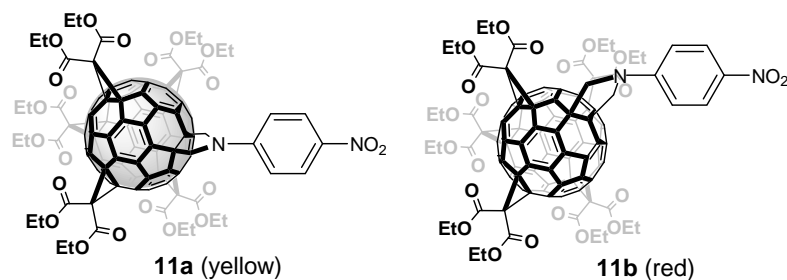
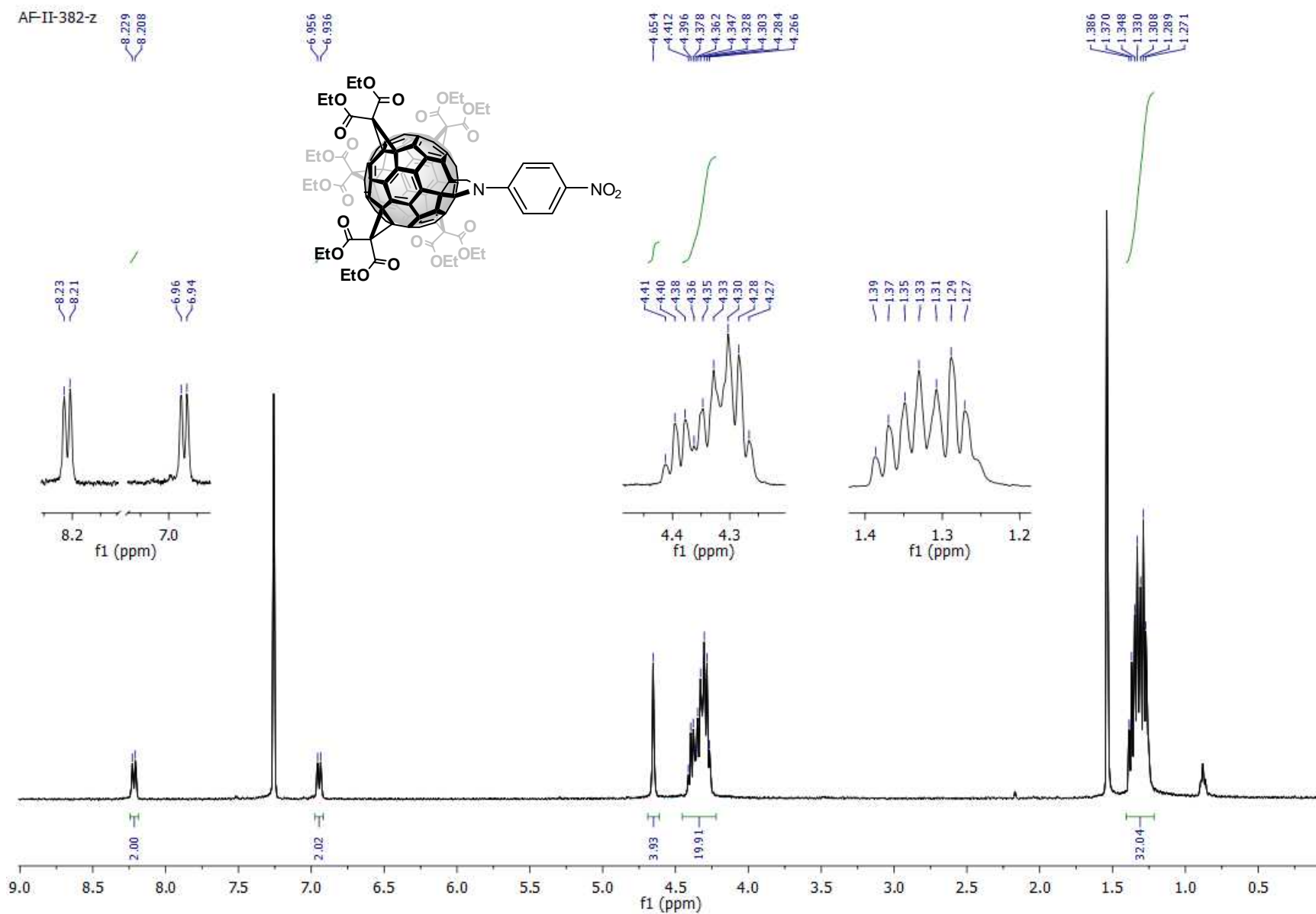
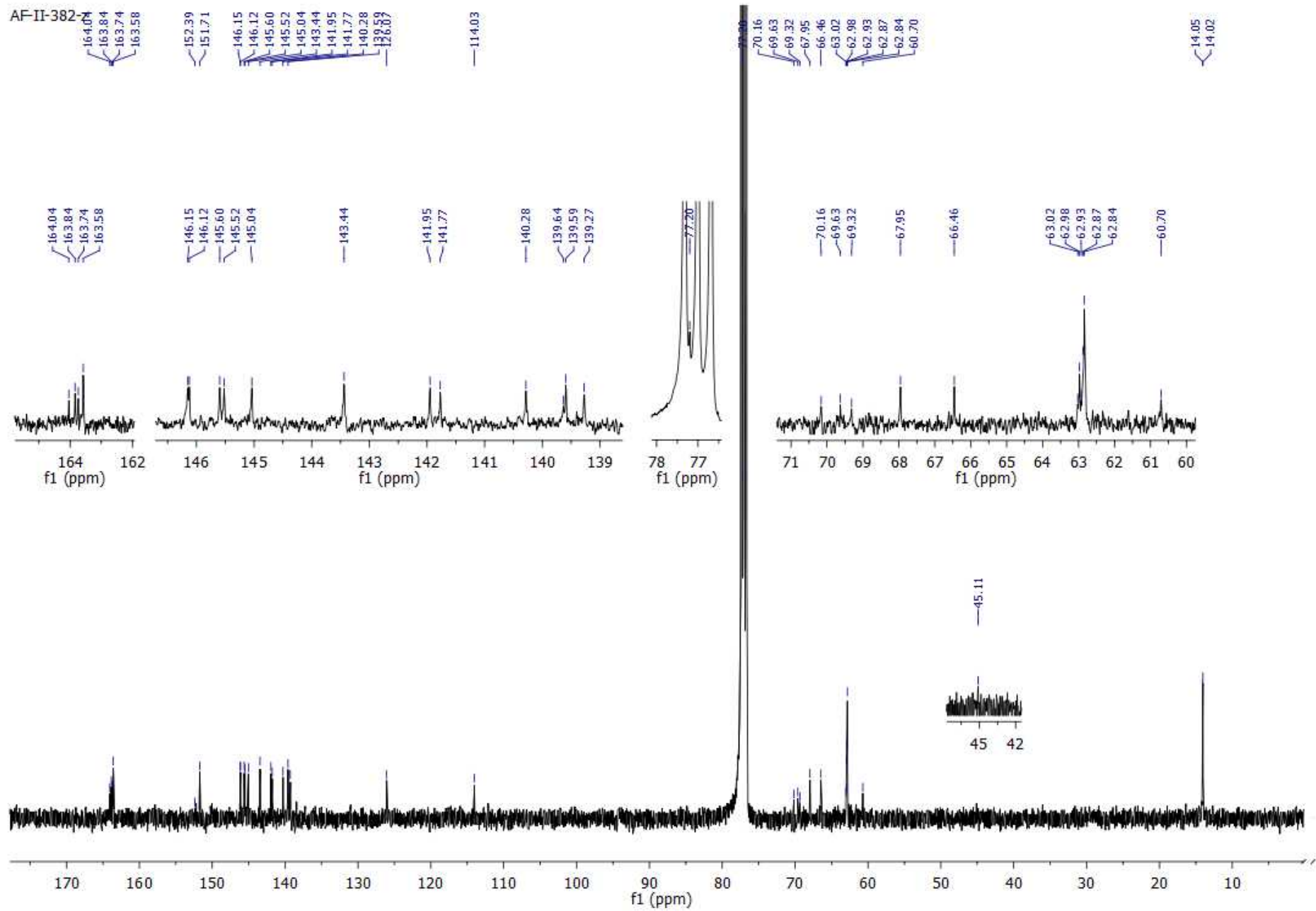
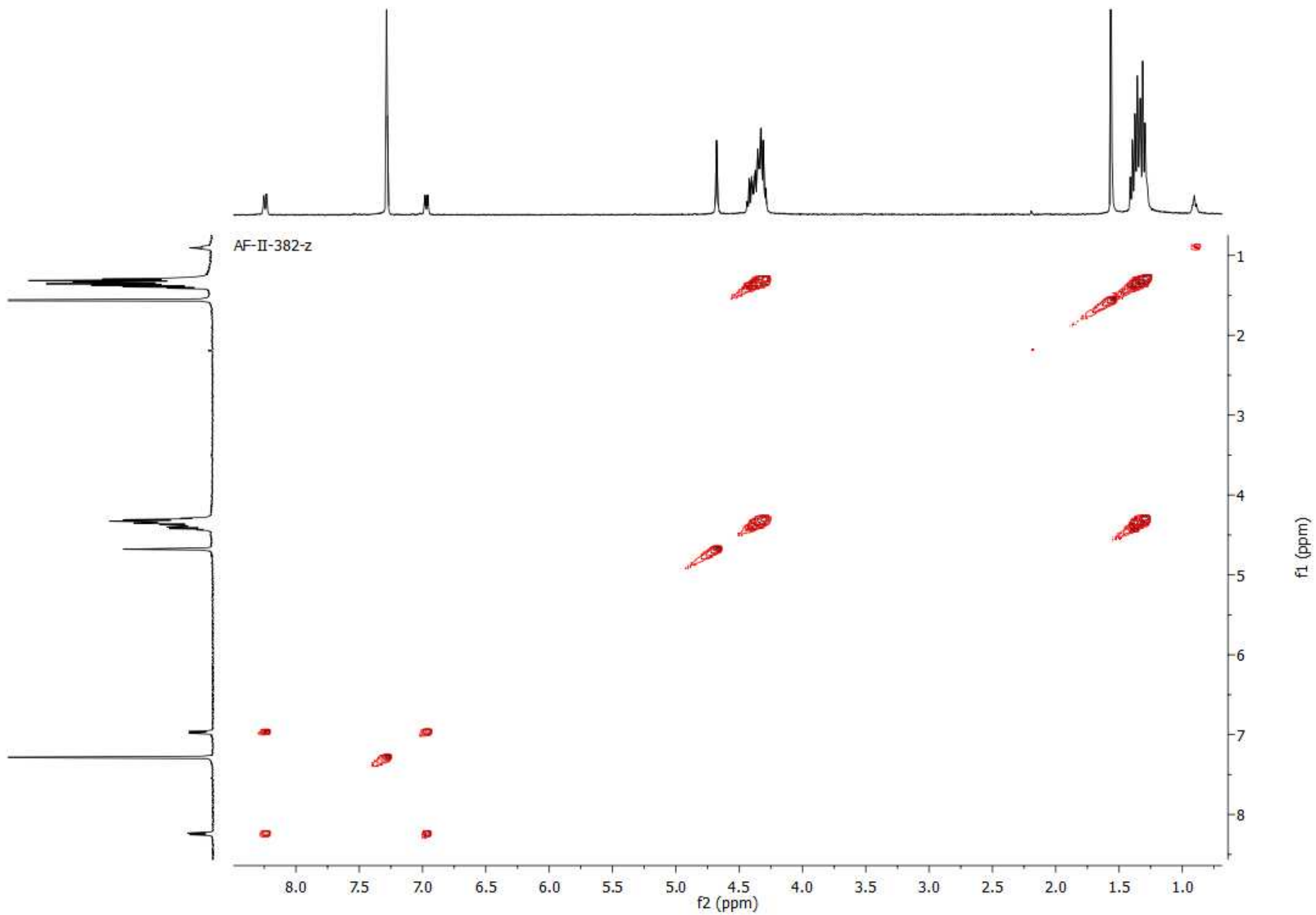


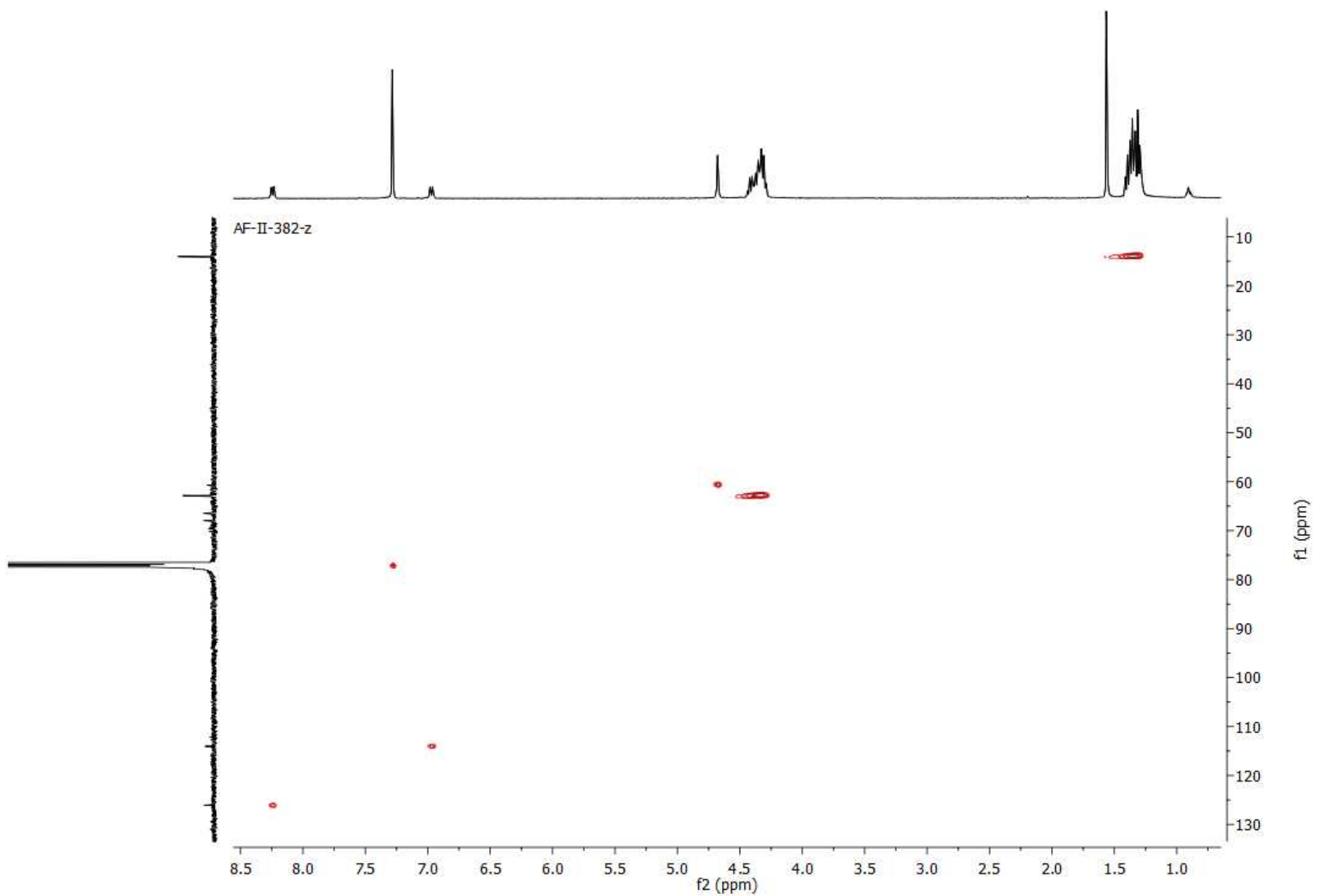
Figure S19. The expanded ¹H NMR pyrrolidine region of the isolated mixture of regioisomers **11**.

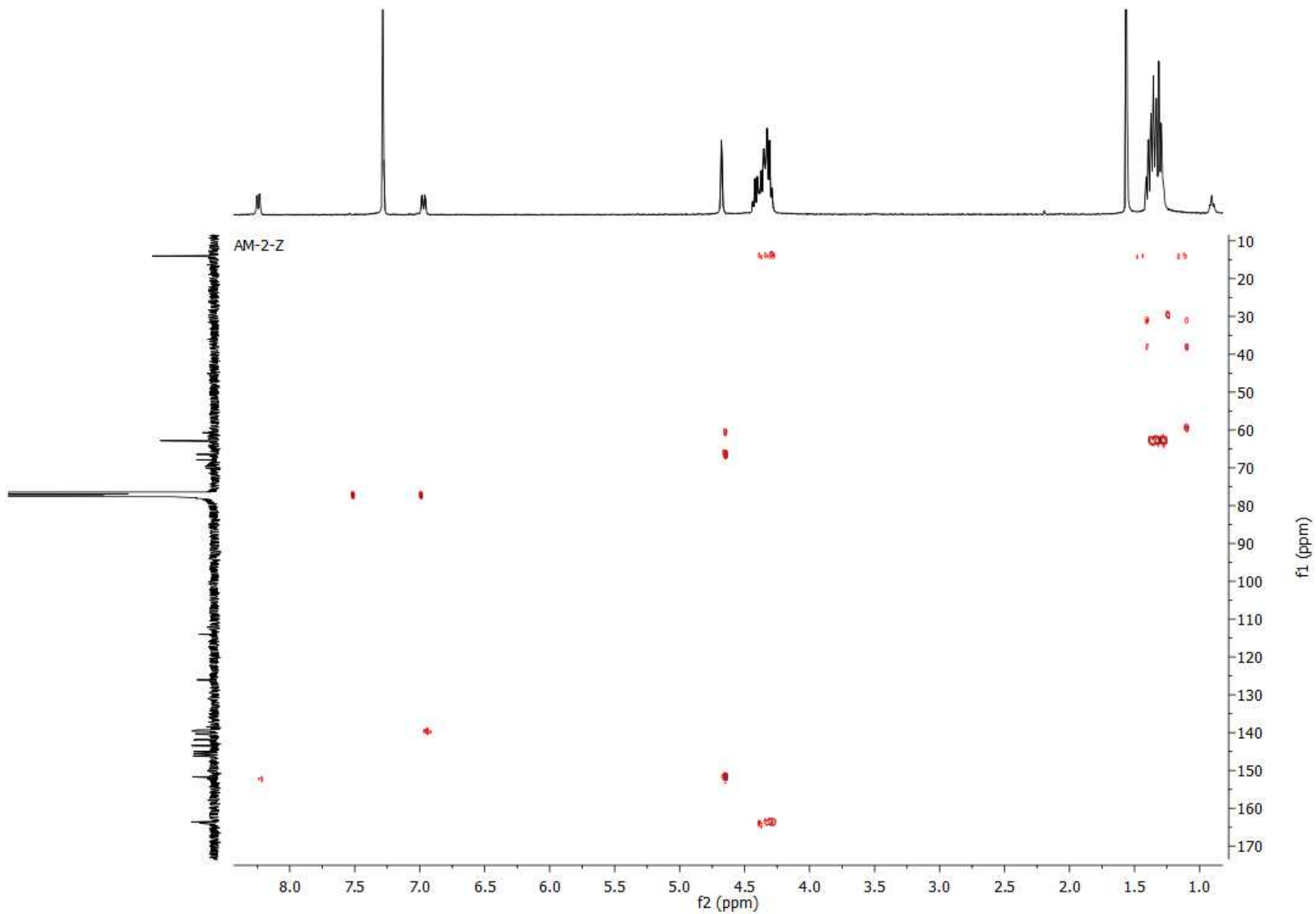
Hexaadduct 11a



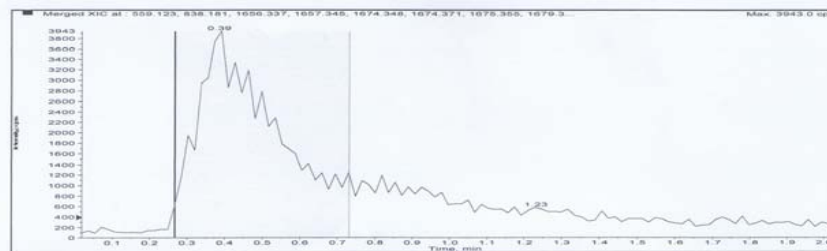




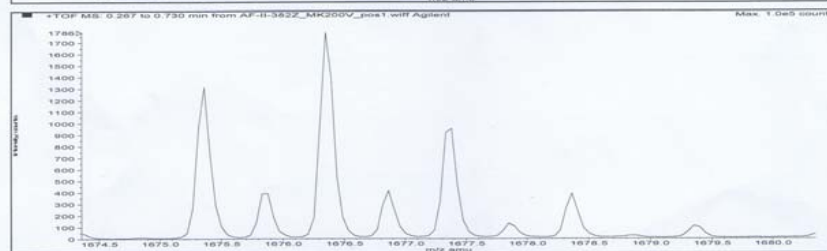




Sample Name: AF-II-382Z Sample Location: P1-E6 Sample Id: Operator: Milka
 Data File Name: D:\PE_Sciex_Data\Projects\Maslak\Data\AF-II-382Z_MK200V_pos1.wiff Acq Time: April 22 2016, 02:11:49 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.anml\efc.xml



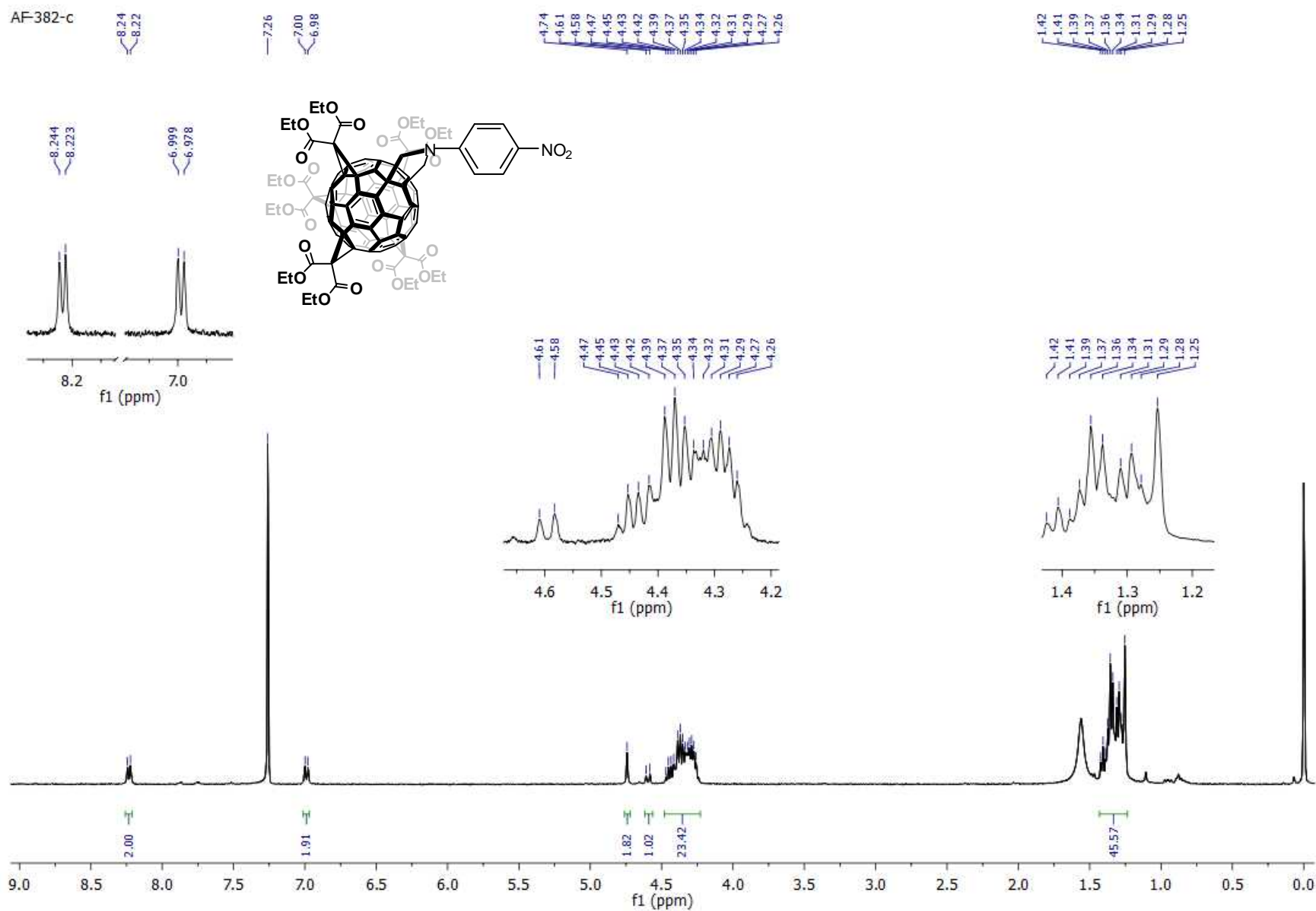
Merged XIC, Period# : 1 Experiment# : 1

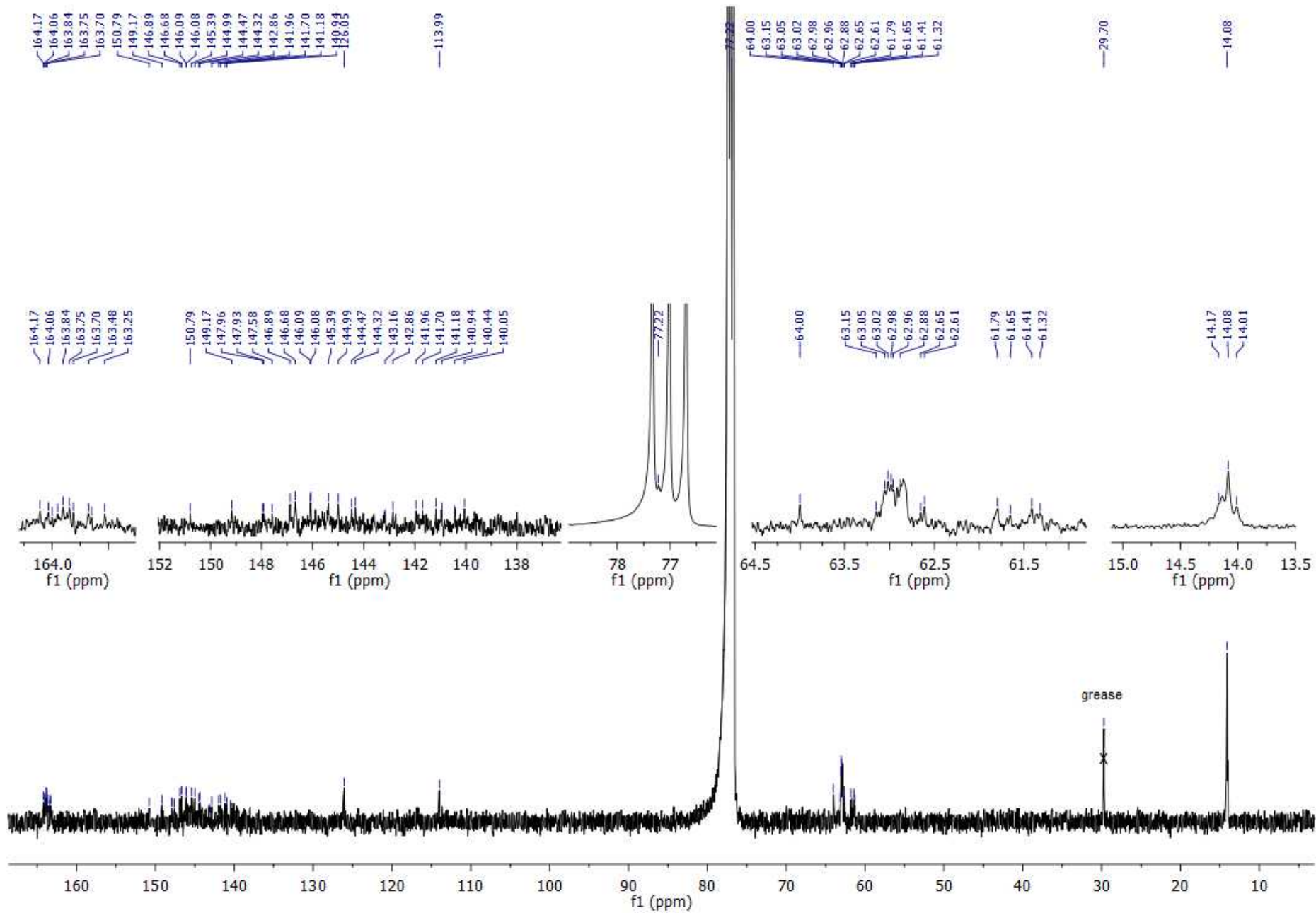


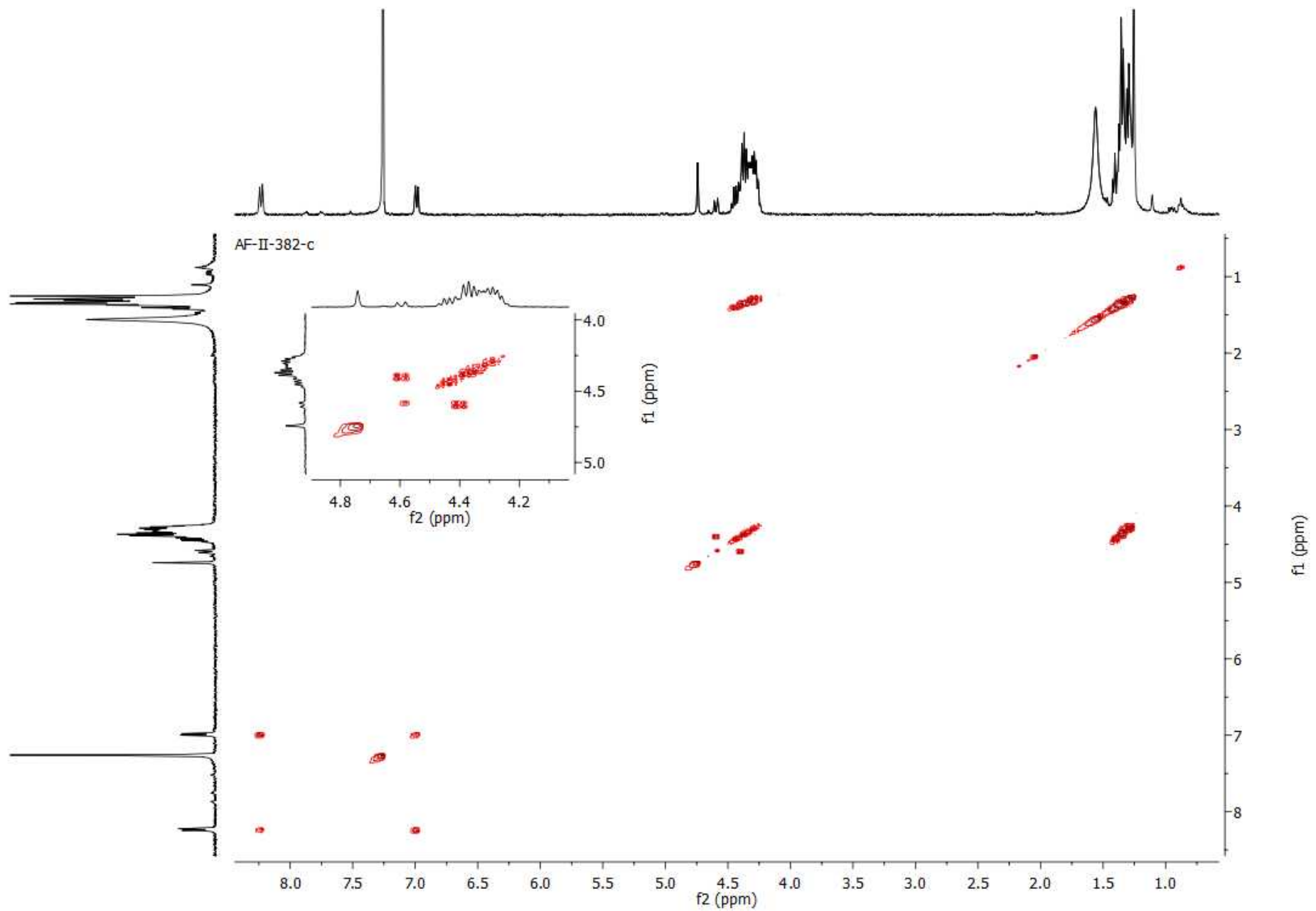
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C103H58N2O22	--	1674.34812	0.39	4.51552 E4	--

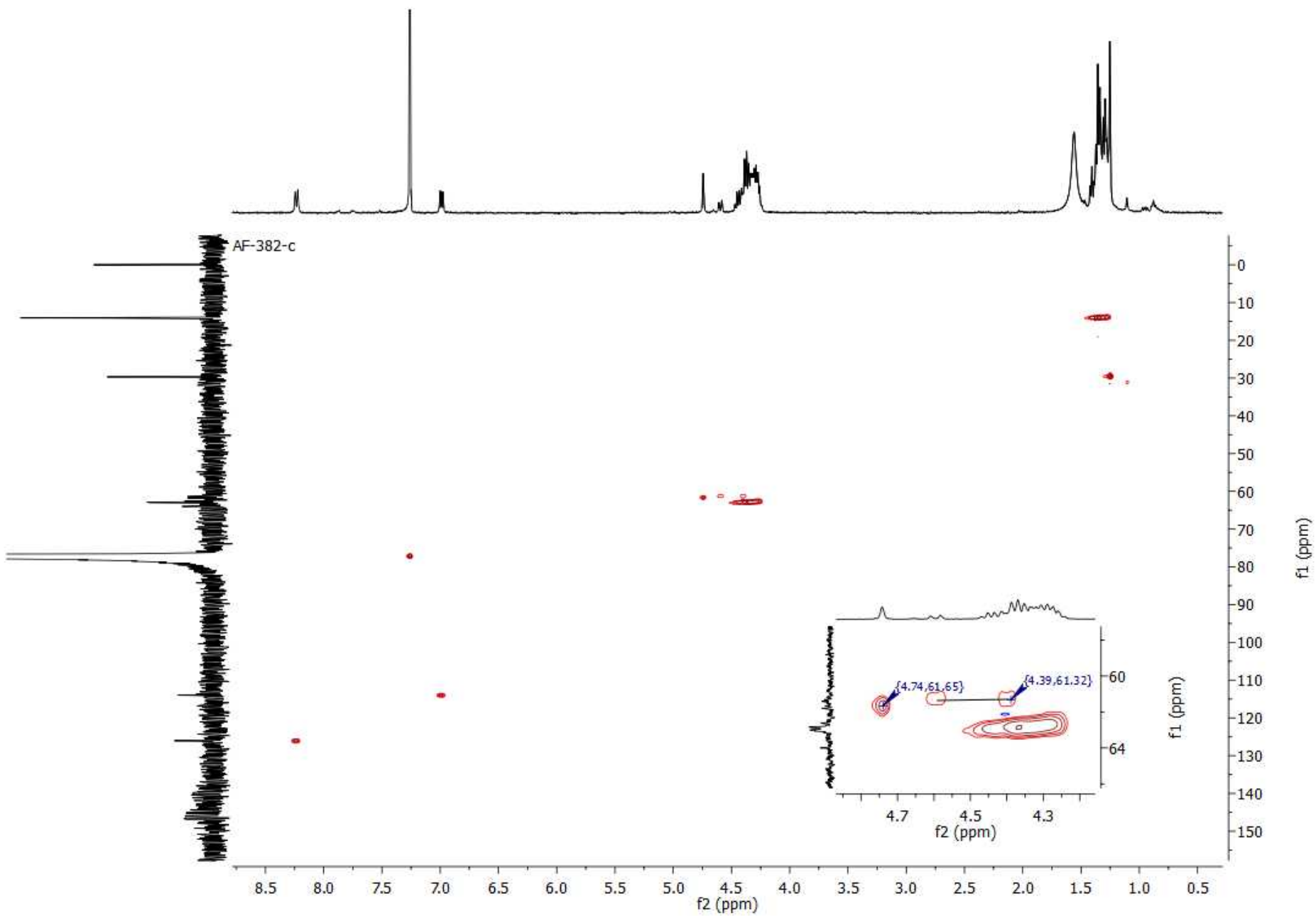
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1323.00	1675.35540	1675.35408	-1.31392	-0.78	--

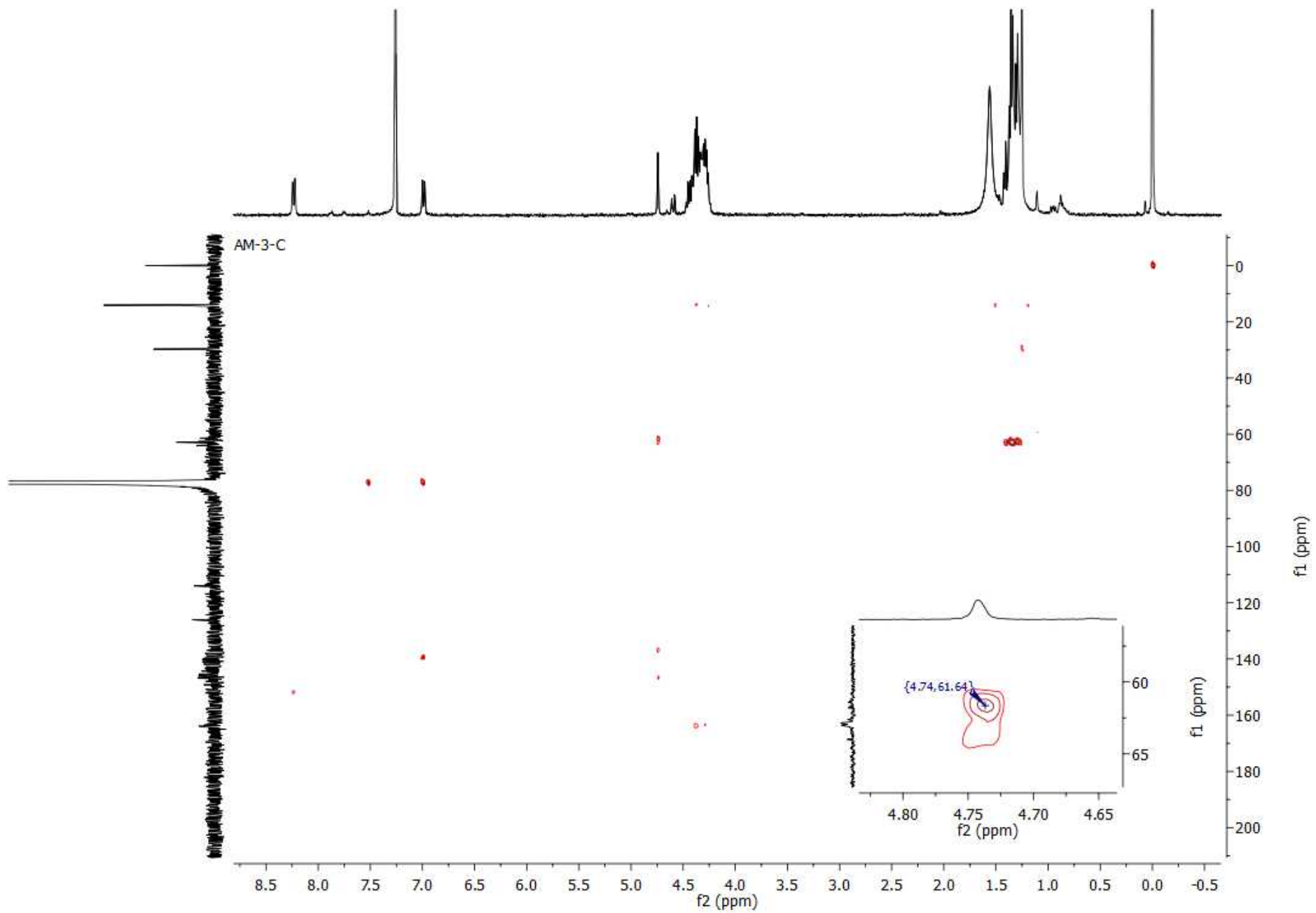
Hexaadduct 11b



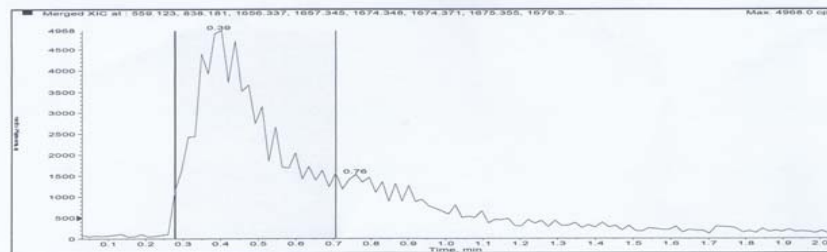




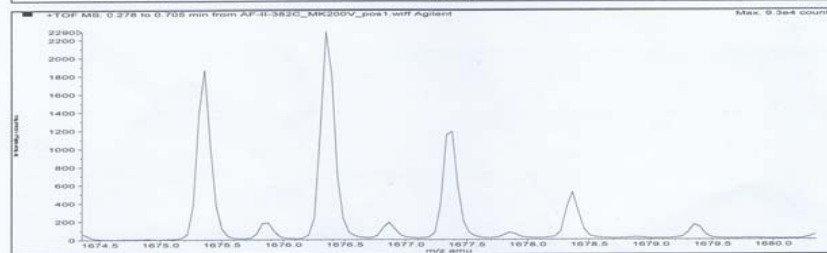
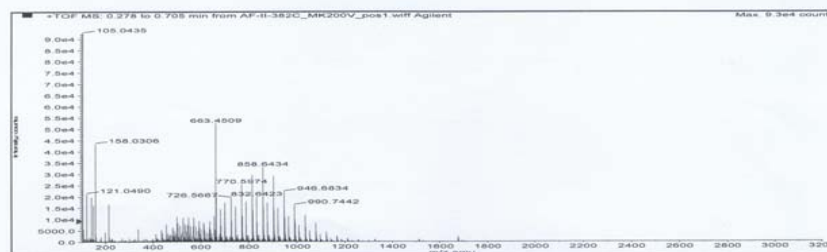




Sample Name: AF-II-382C Sample Location: P1-E5 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Maslak\Data\AF-II-382C_MK200V_pos1.wiff Acq Time: April 22 2016, 02:08:50 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.anmlcfc.xml



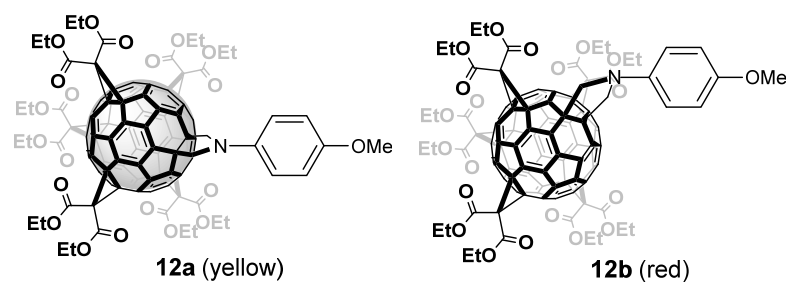
Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C103H58N2O22	--	1674.34812	0.39	5.37338 E4	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1878.75	1675.35540	1675.35396	-1.43398	-0.86	--

Regioisomeric Bingel-Prato [5:1]-hexaadducts **12**



hafii375zc
AF-II-375-zc

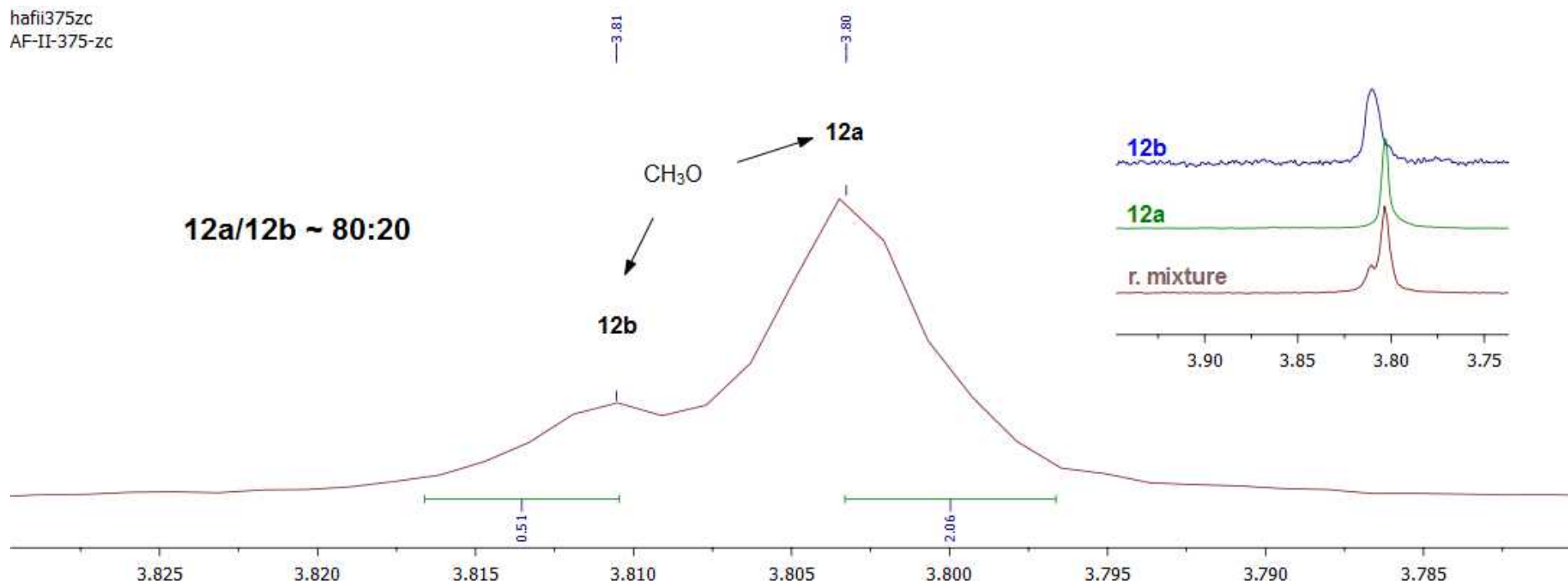
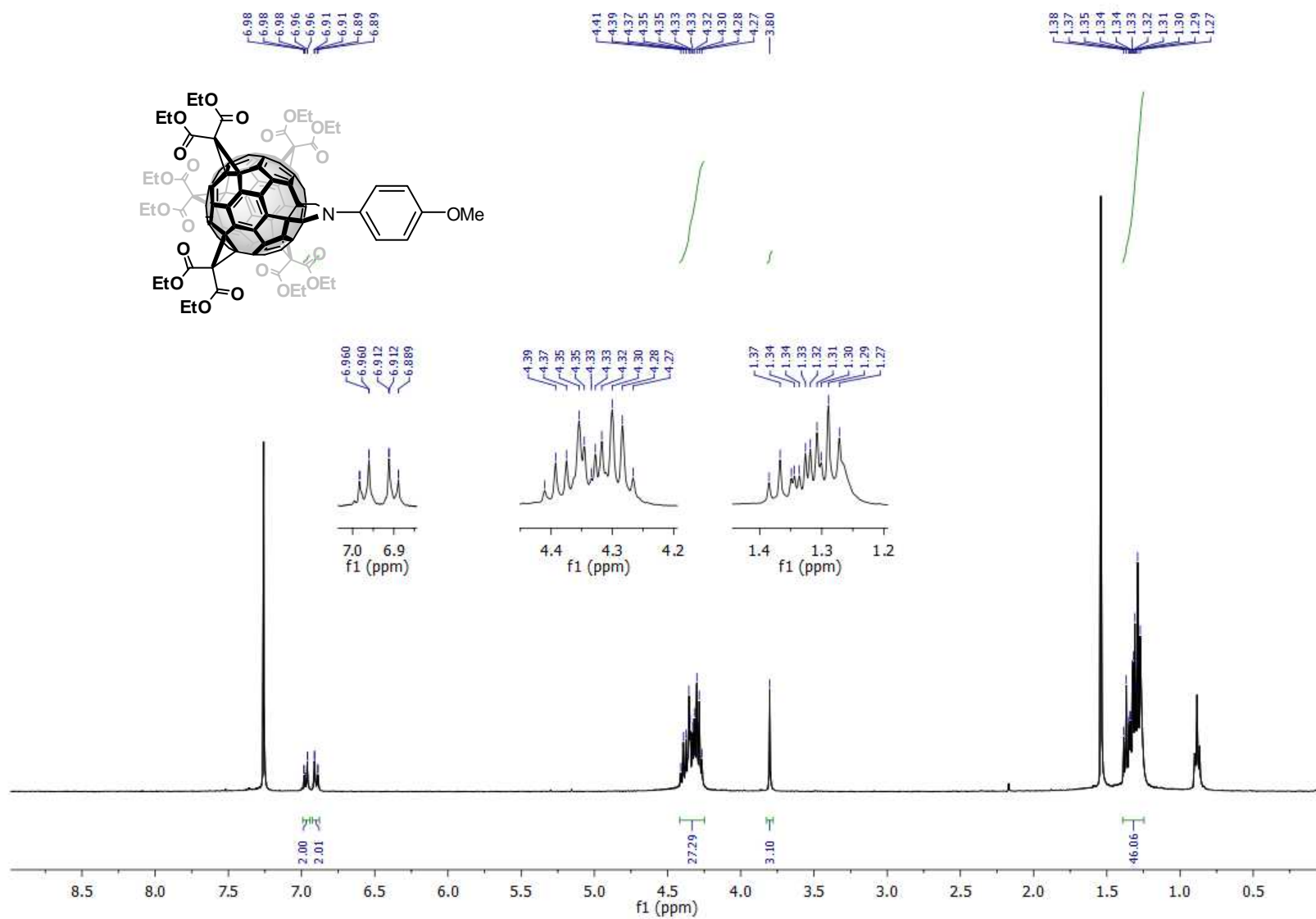
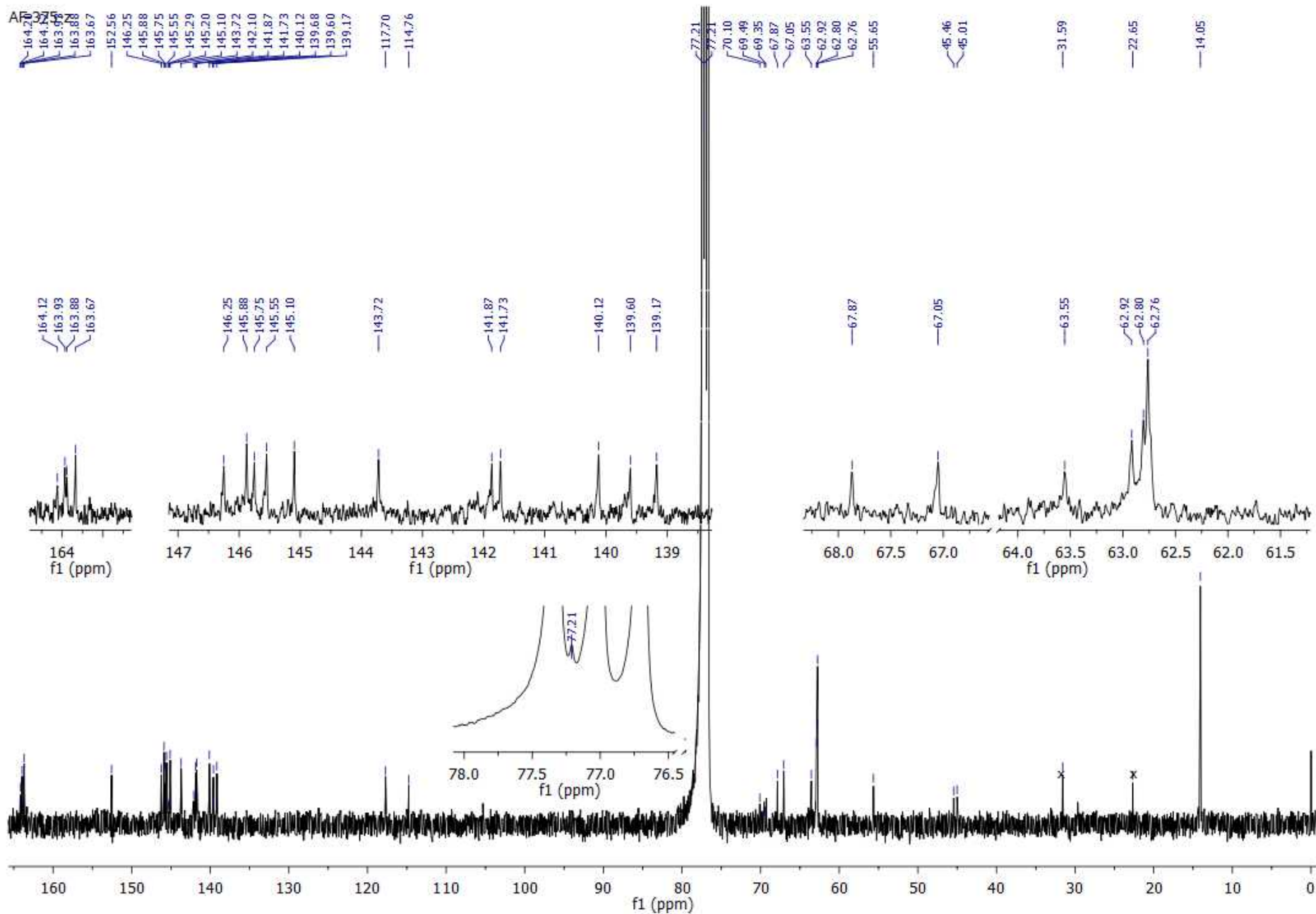
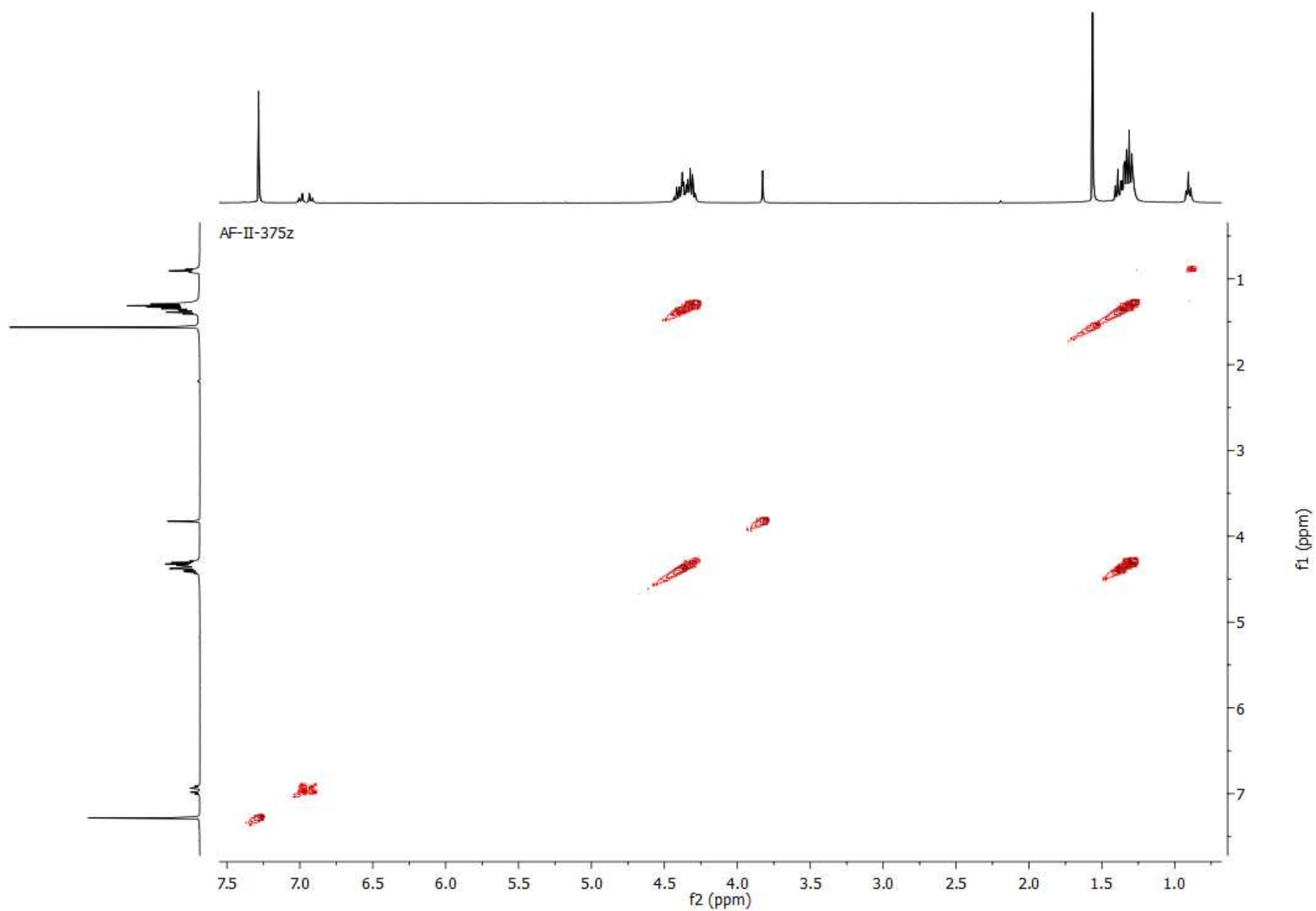


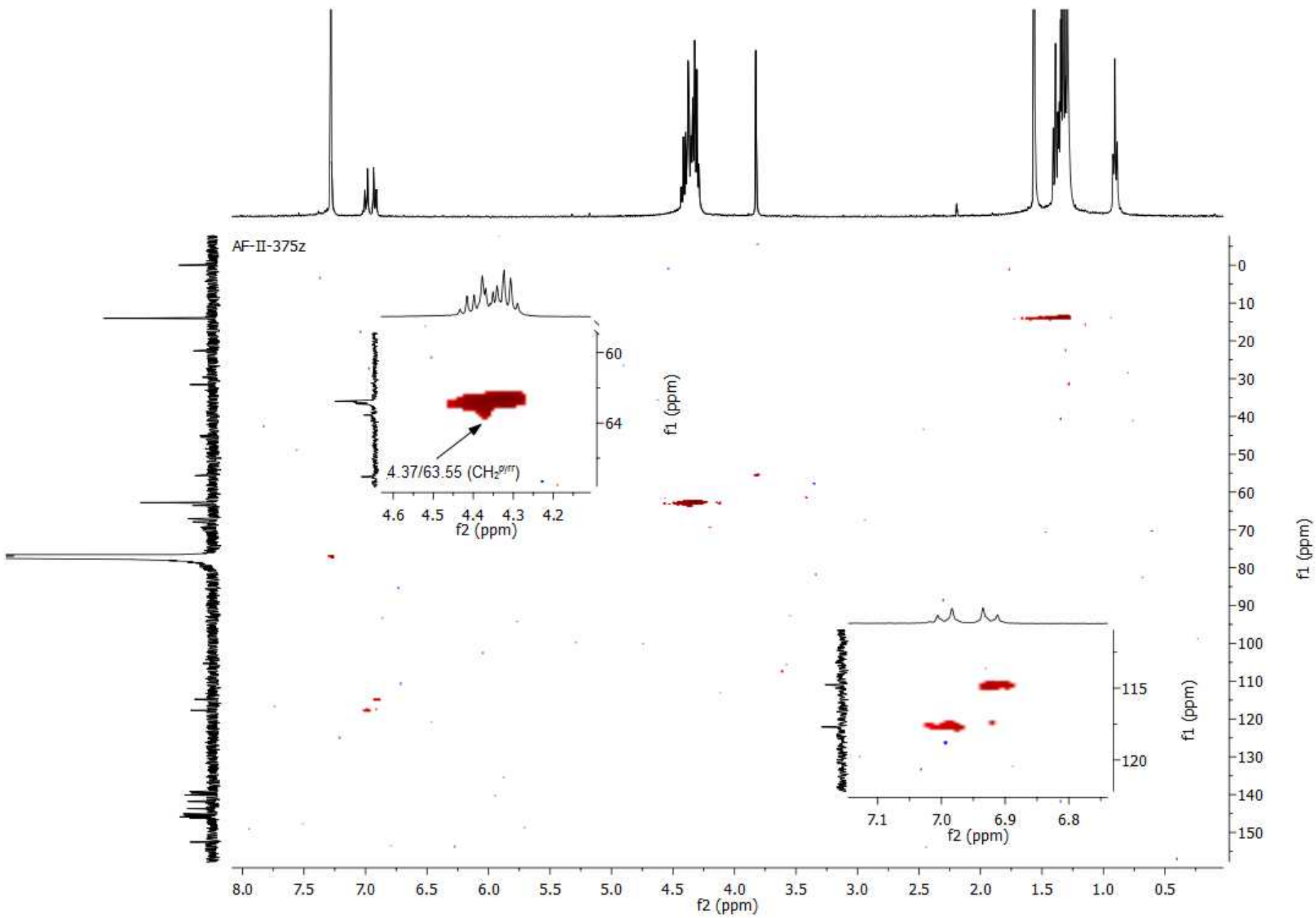
Figure S20. The expanded part of ¹H NMR spectrum of the mixture of regioisomers **12**.

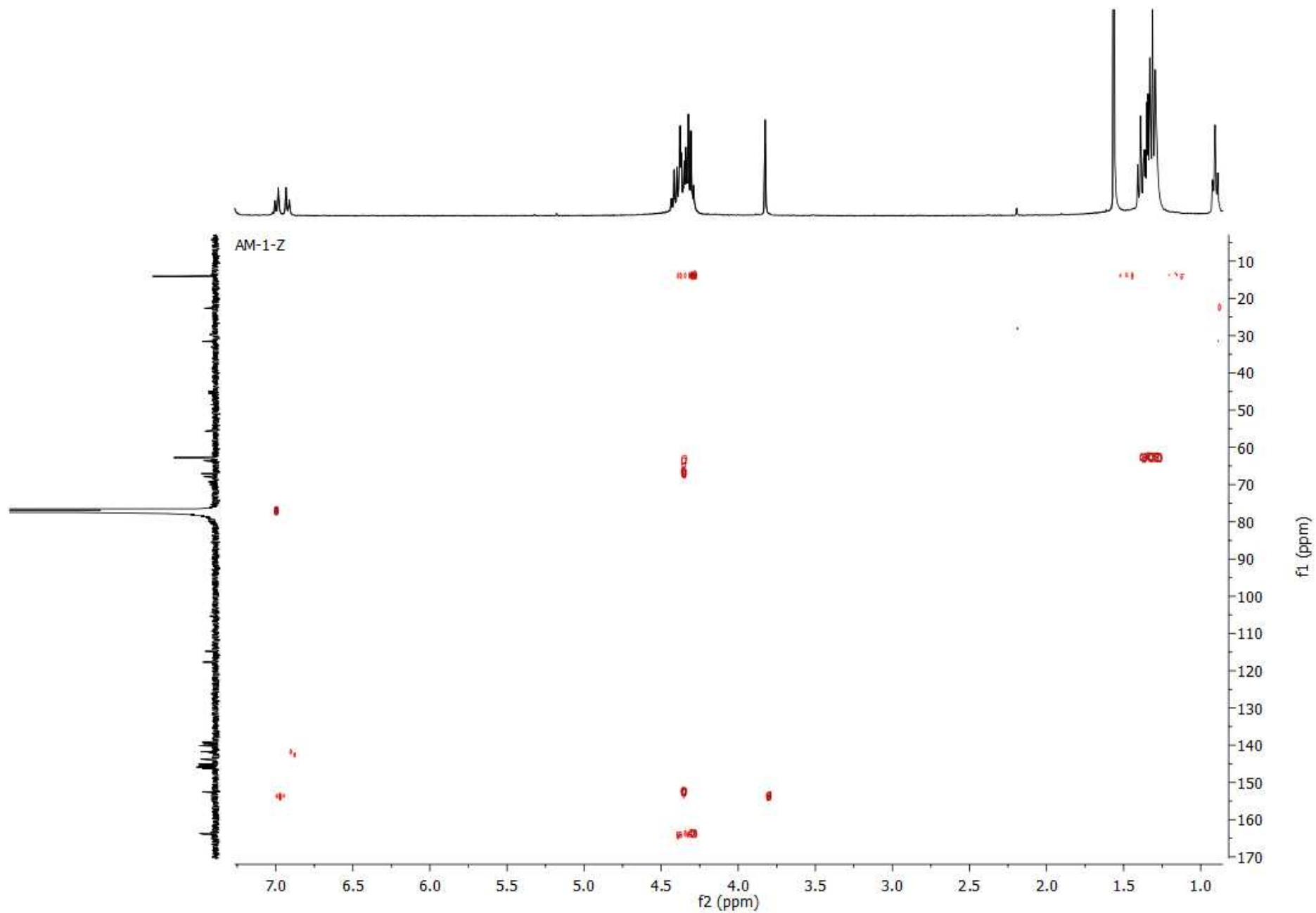
Hexaadduct 12a



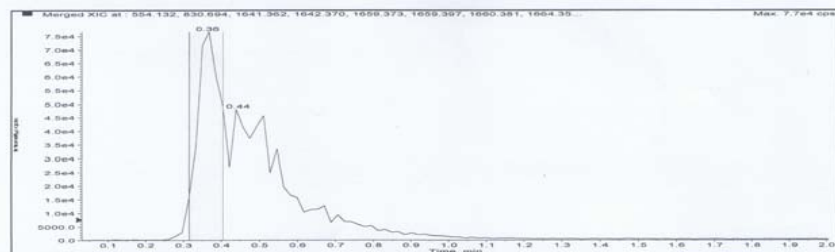




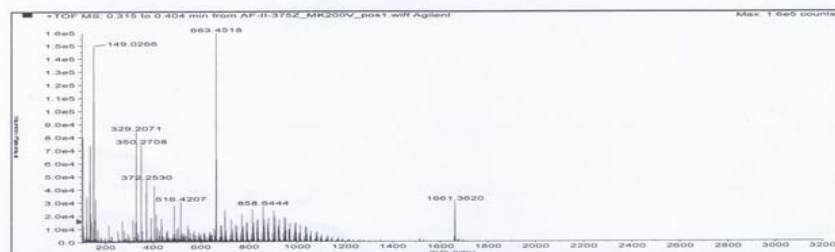




Sample Name: AF-II-375Z Sample Location: P1-E4 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Maslak\Data\AF-II-375Z_MK200V_pos1.wiff Acq Time: April 22 2016, 02:05:50 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlcfc.xml



Merged XIC, Period#: 1 Experiment#: 1

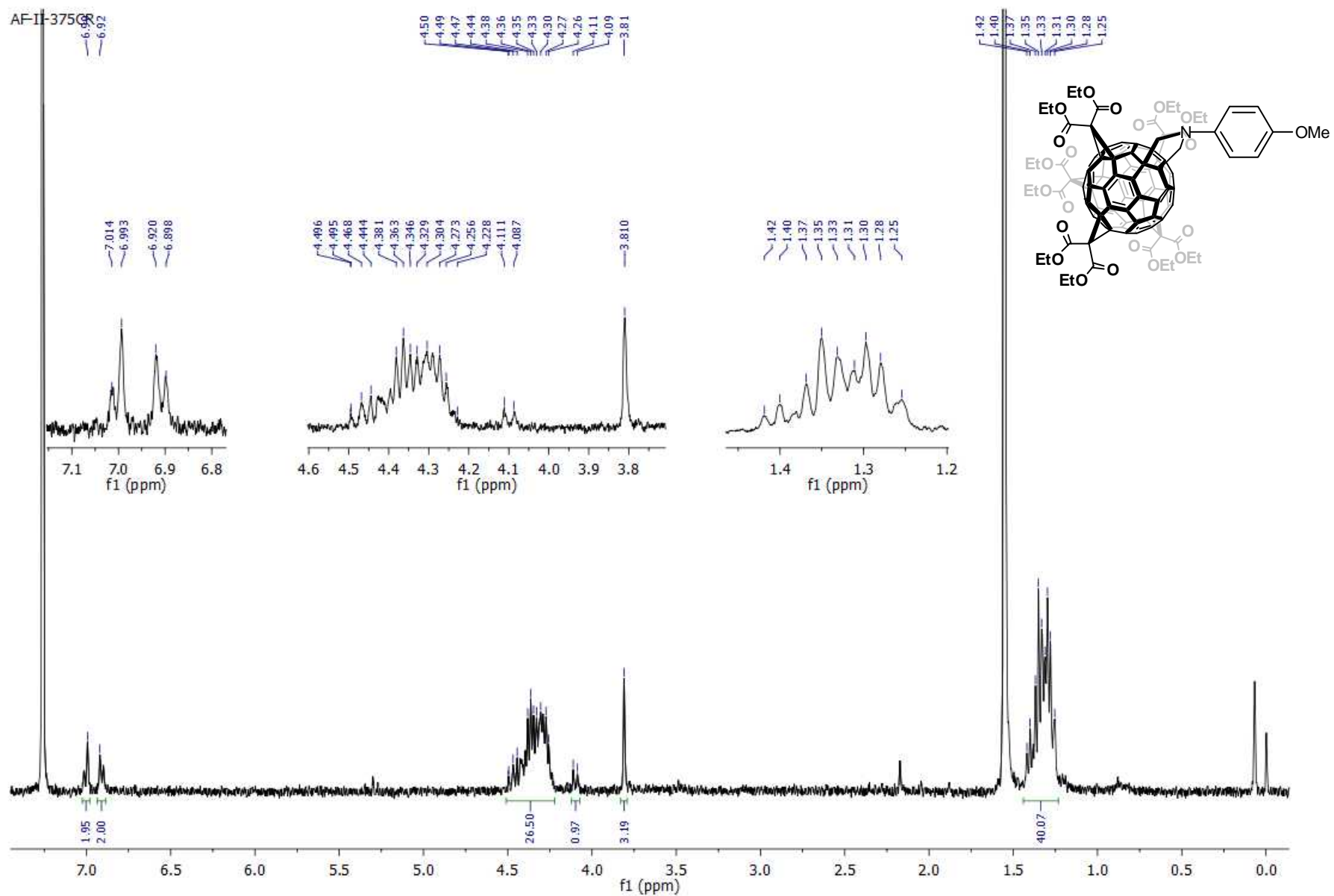


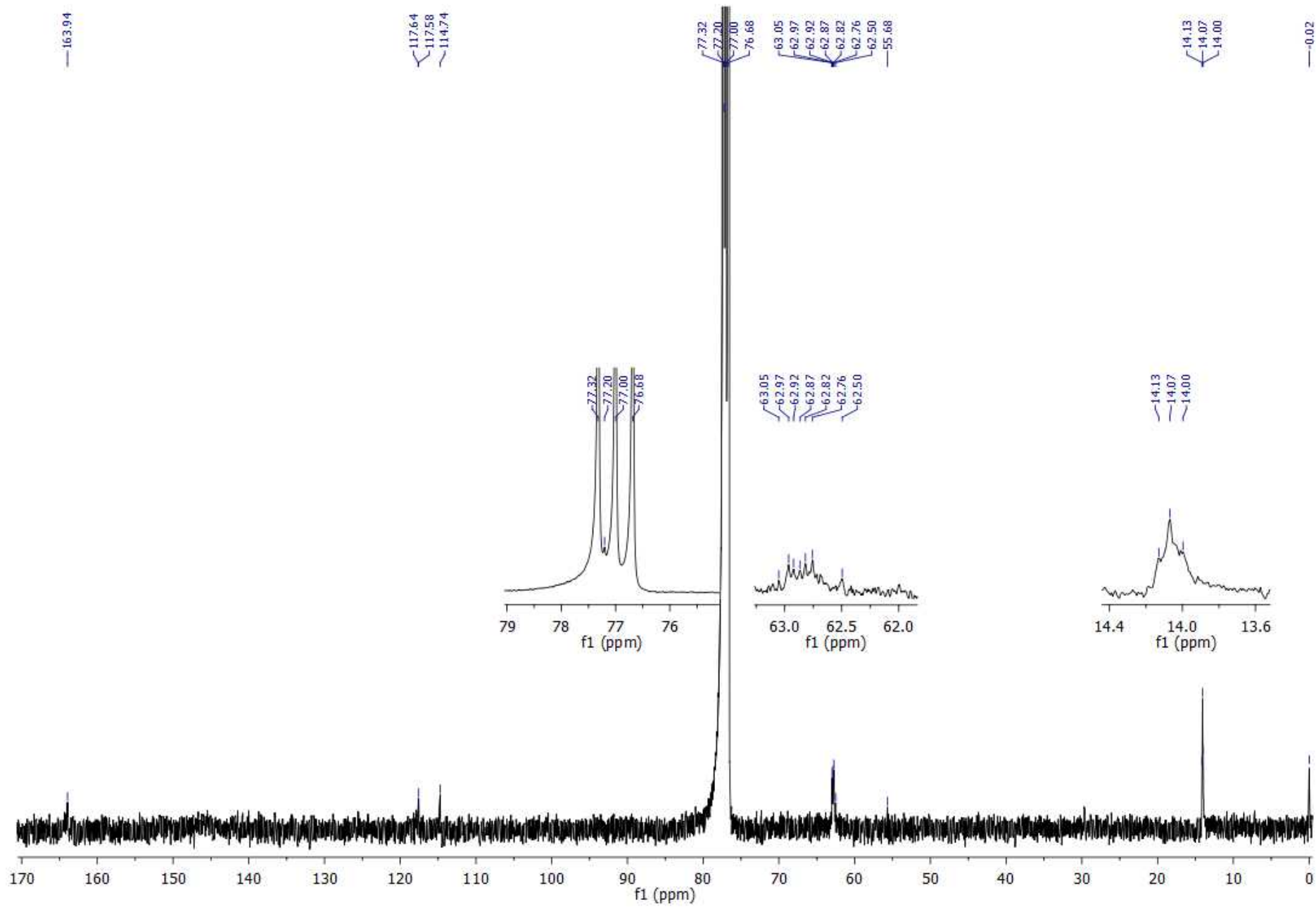
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C104H61NO21	--	1659.37361	0.36	3.46405 E5	--

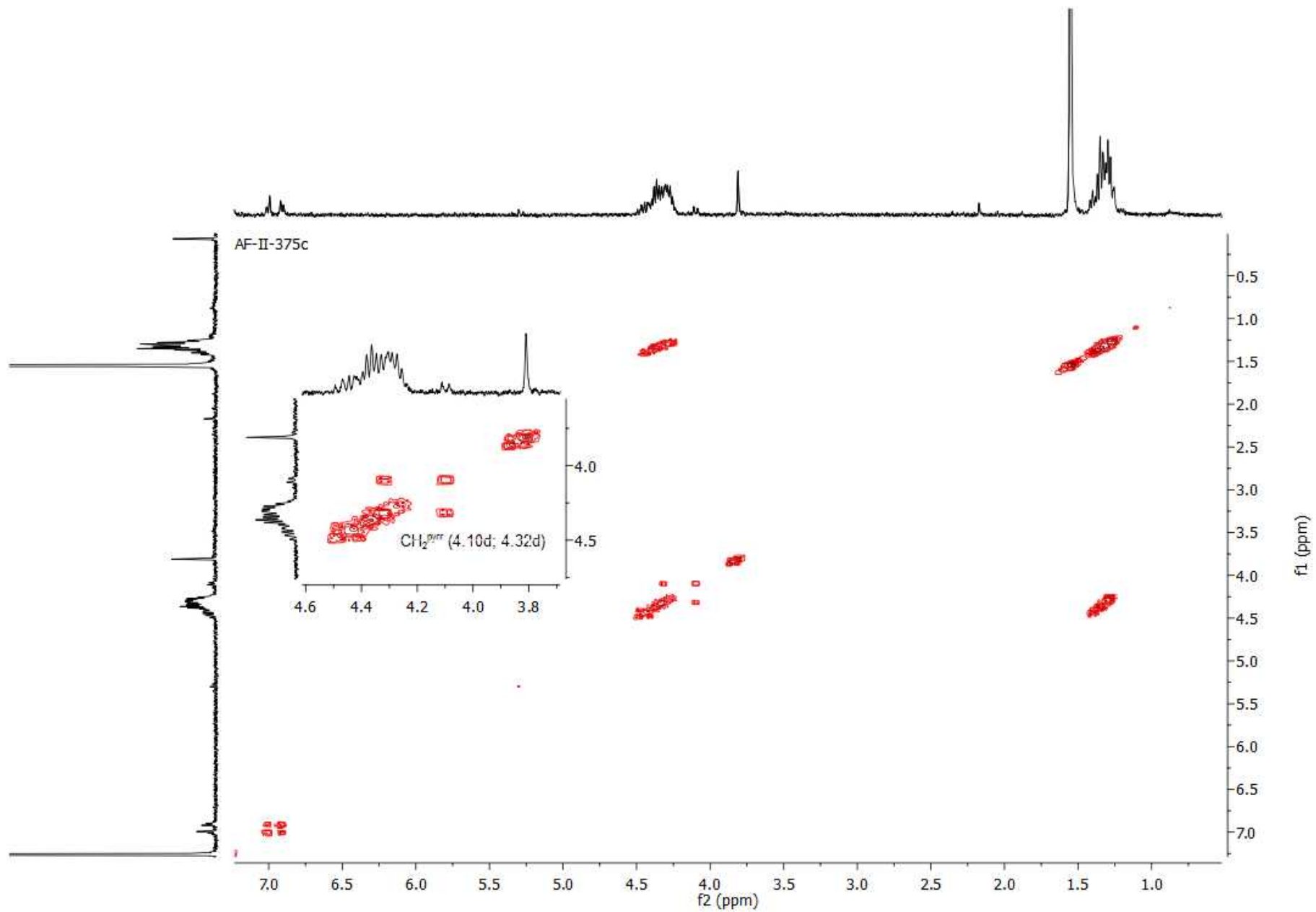
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
M+	4363.55	1659.37306	1659.36750	-5.55773	-3.35	--
[M+H] ⁺	23485.70	1660.38088	1660.37766	-3.22316	-1.94	--
[M+NH4] ⁺	1605.37	1677.40743	1677.37964	-27.79463	-16.57	--

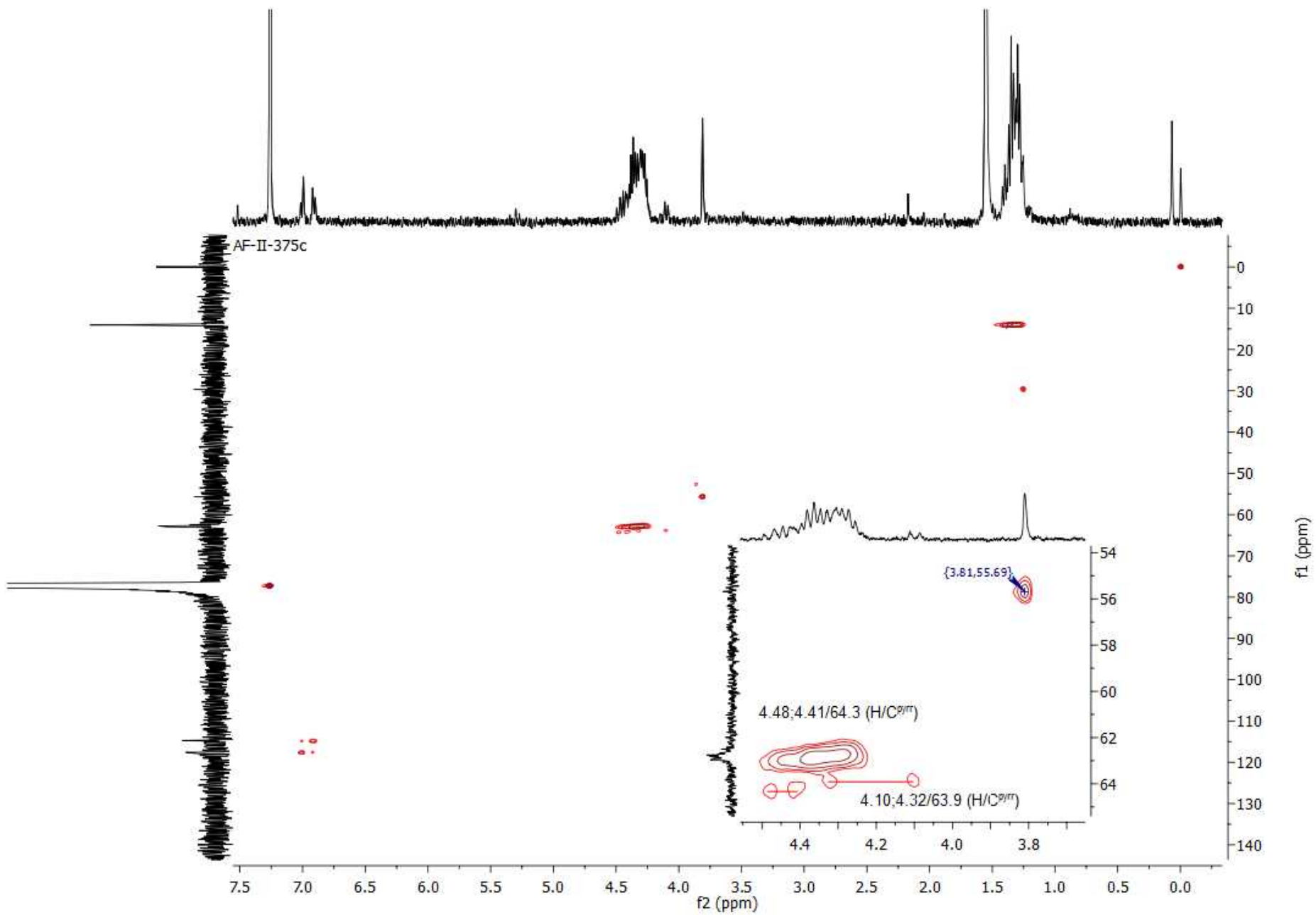
3 w OK!

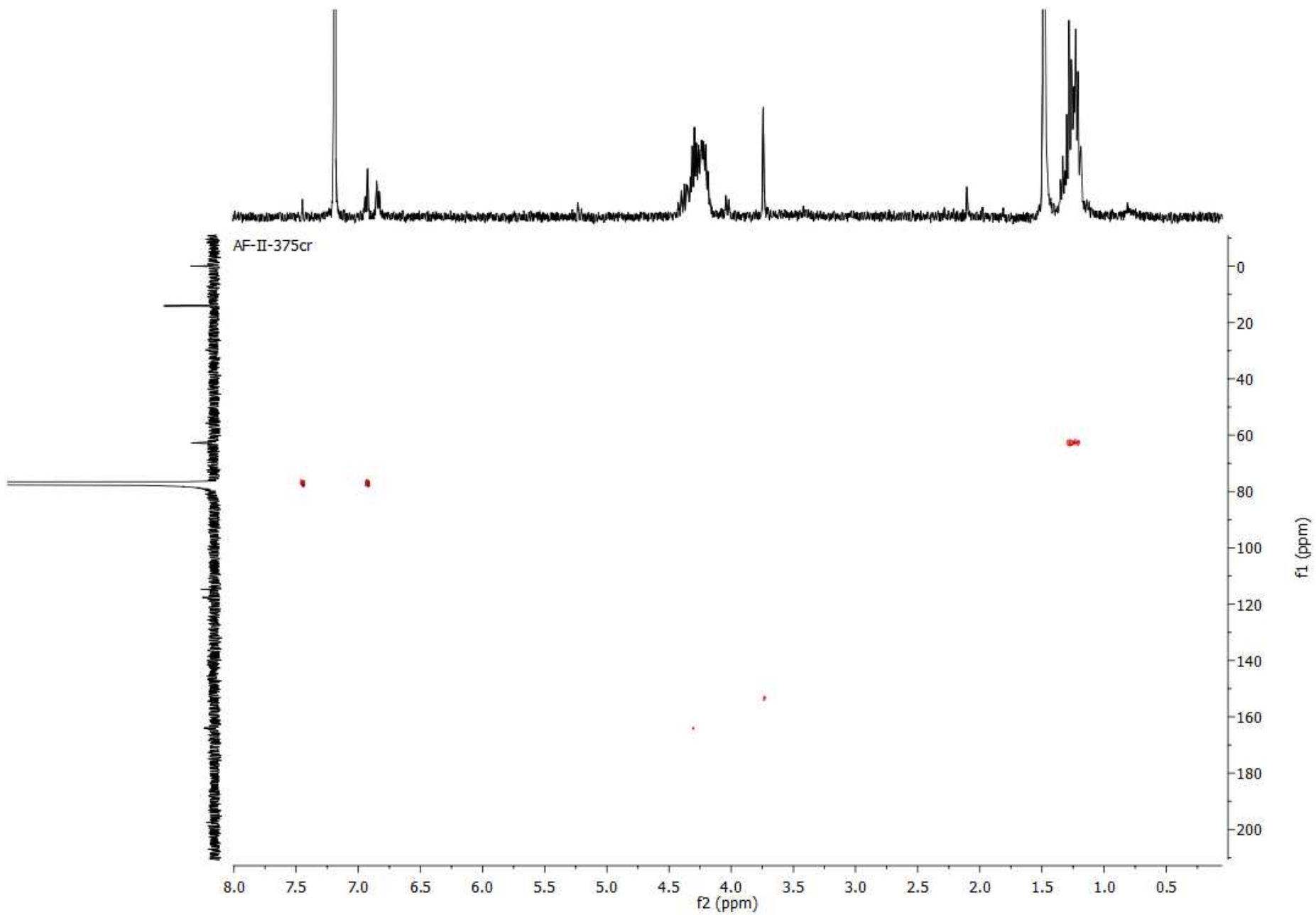
Hexaadduct 12b



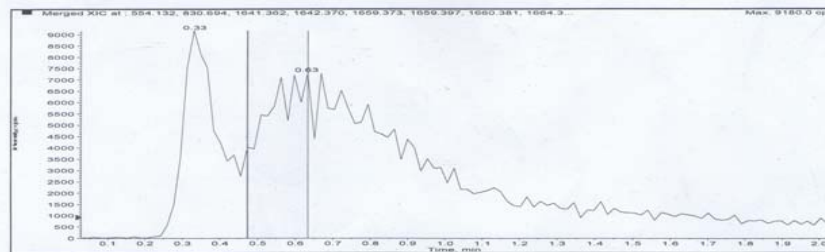




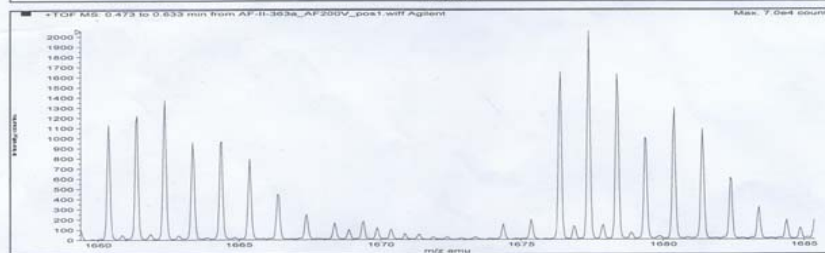
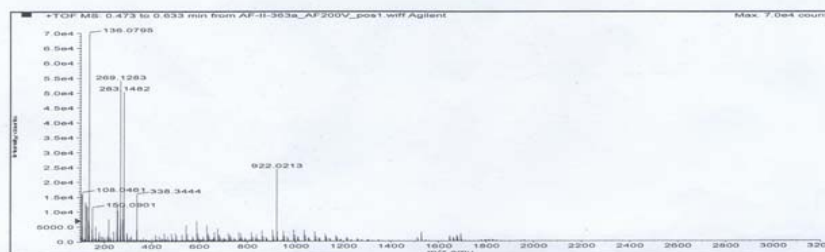




Sample Name: AF-II-363a Sample Location: P1-C3 Sample Id: Operator: Milka
 Data File Name: D:\PE_Sciex_Data\Projects\Maslak\Data\AF-II-363a_AF200V_pos1.wiff Acq Time: December 28 2015, 09:50:12 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.anmiefc.xml



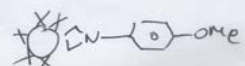
Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C104H61NO21	--	1659.37361	0.63	2.56740 E4	--

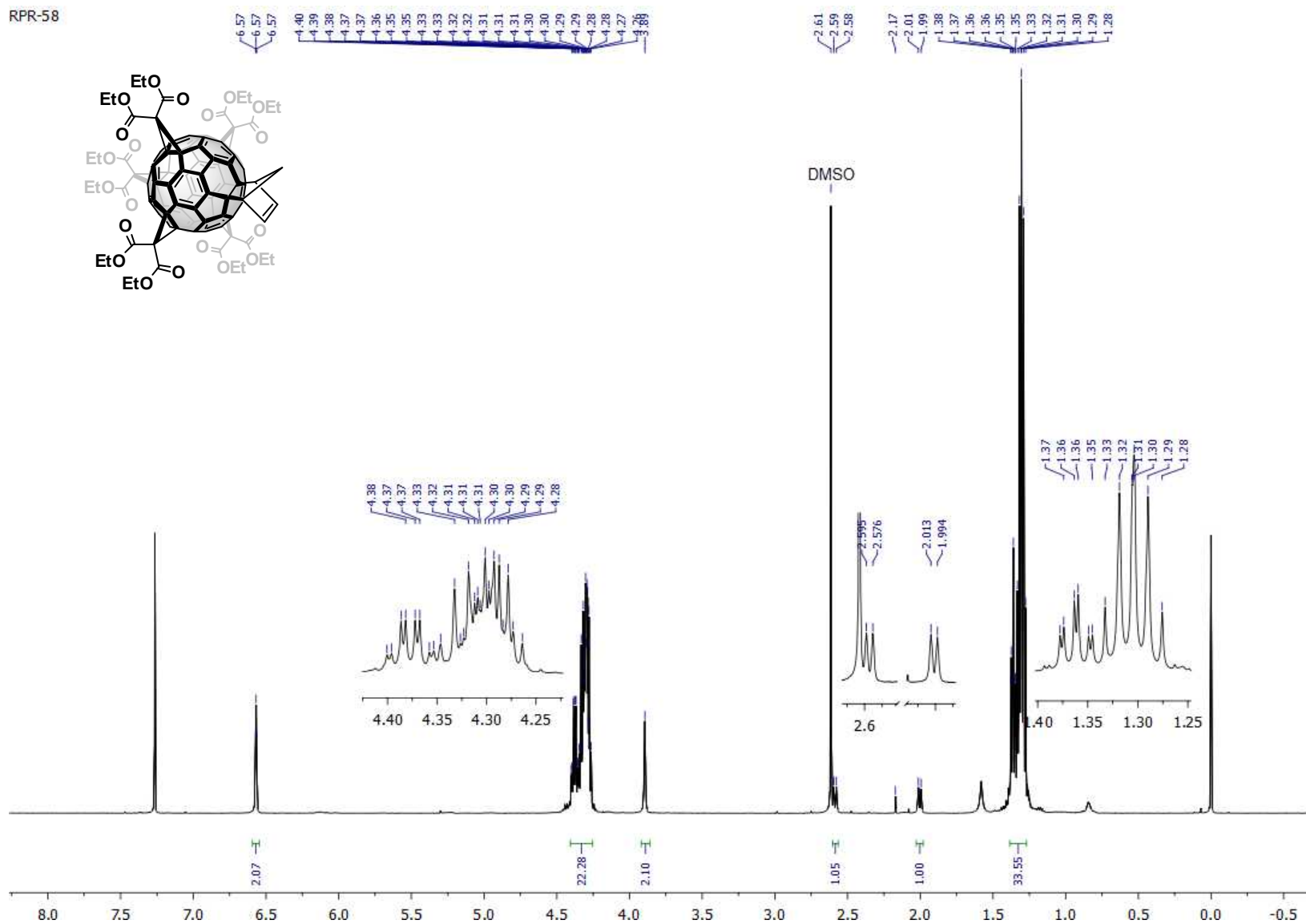
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1138.36	1660.38088	1660.37661	-4.27694	-2.58	--
[M+Na-H2O] ⁺	1026.74	1664.35226	1664.36912	16.85481	10.13	--
[M+NH4] ⁺	2054.06	1677.40743	1677.37489	-32.53997	-19.40	--
[M+K-H2O] ⁺	1310.65	1680.32620	1680.36722	41.02207	24.41	--

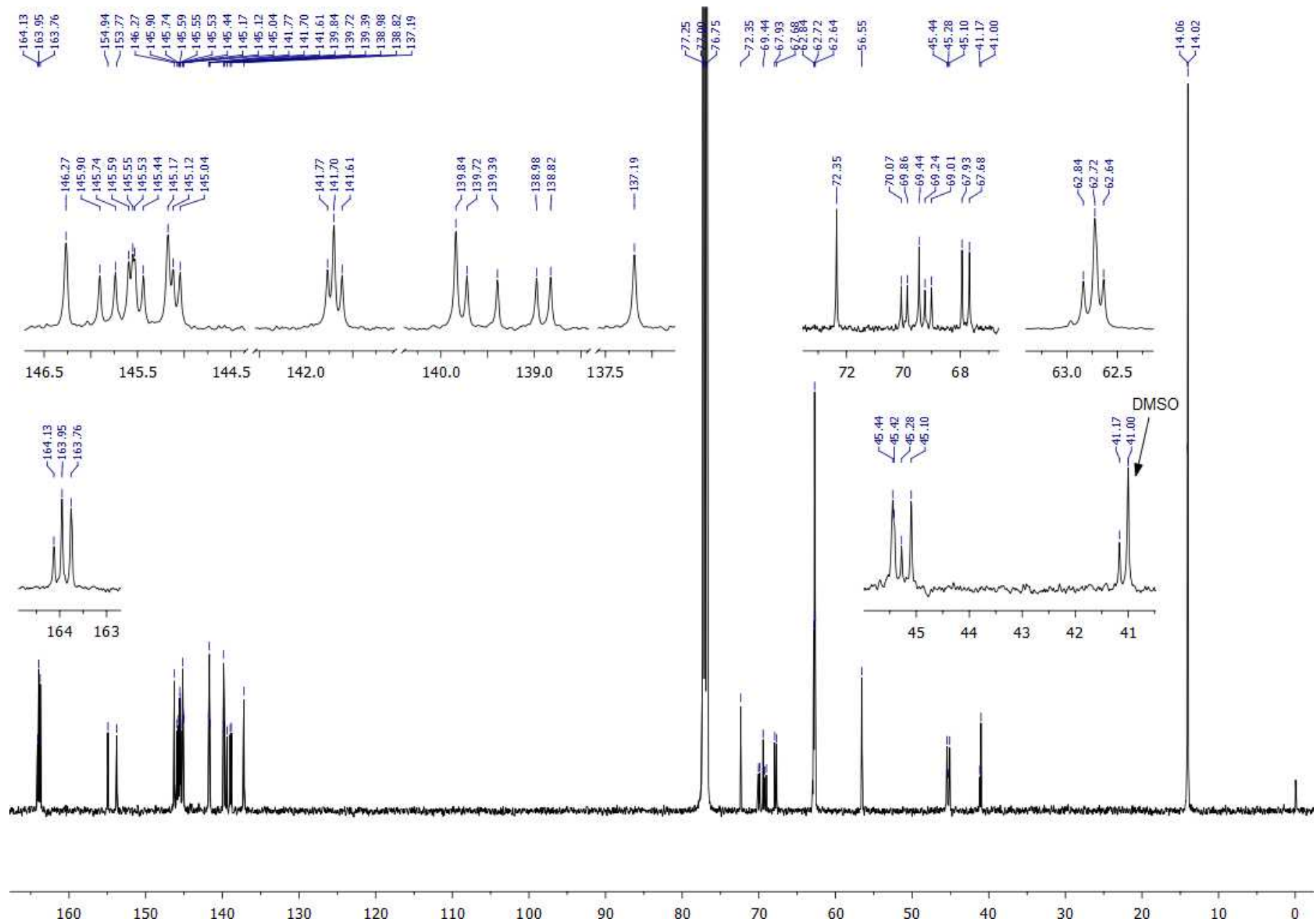
OK! JH

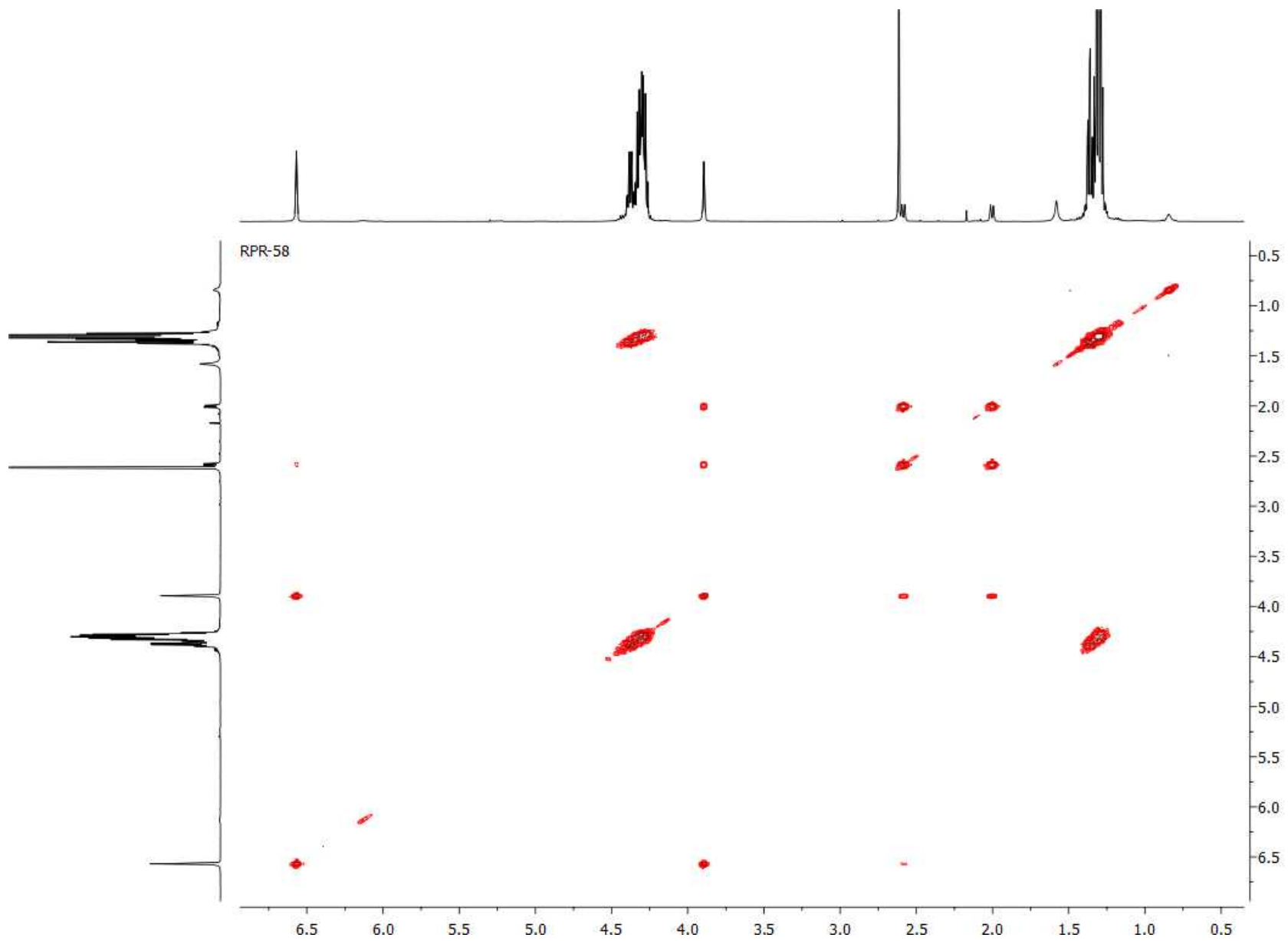


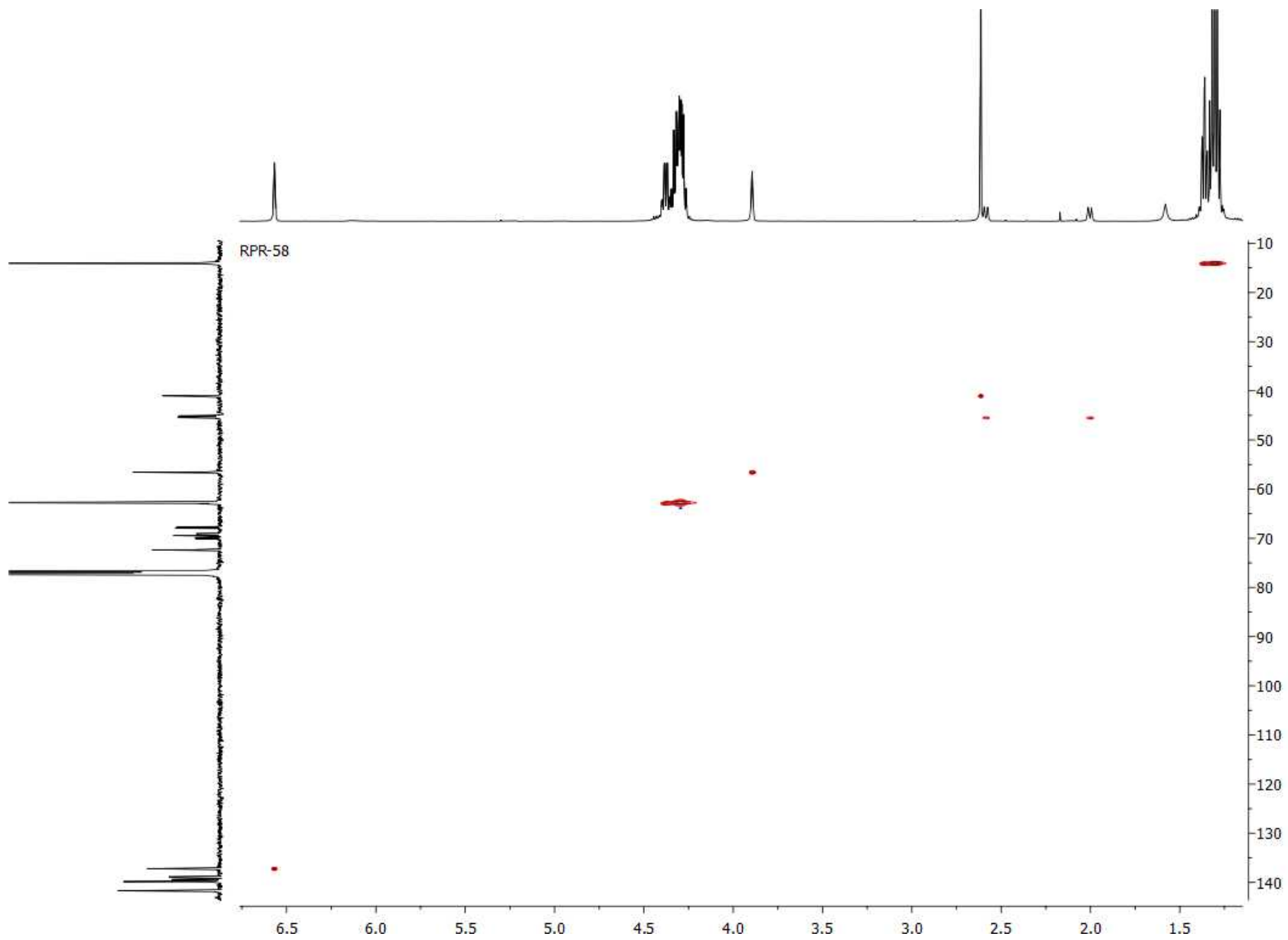
Bingel-Diels-Alder [5:1]-hexaadduct 13a

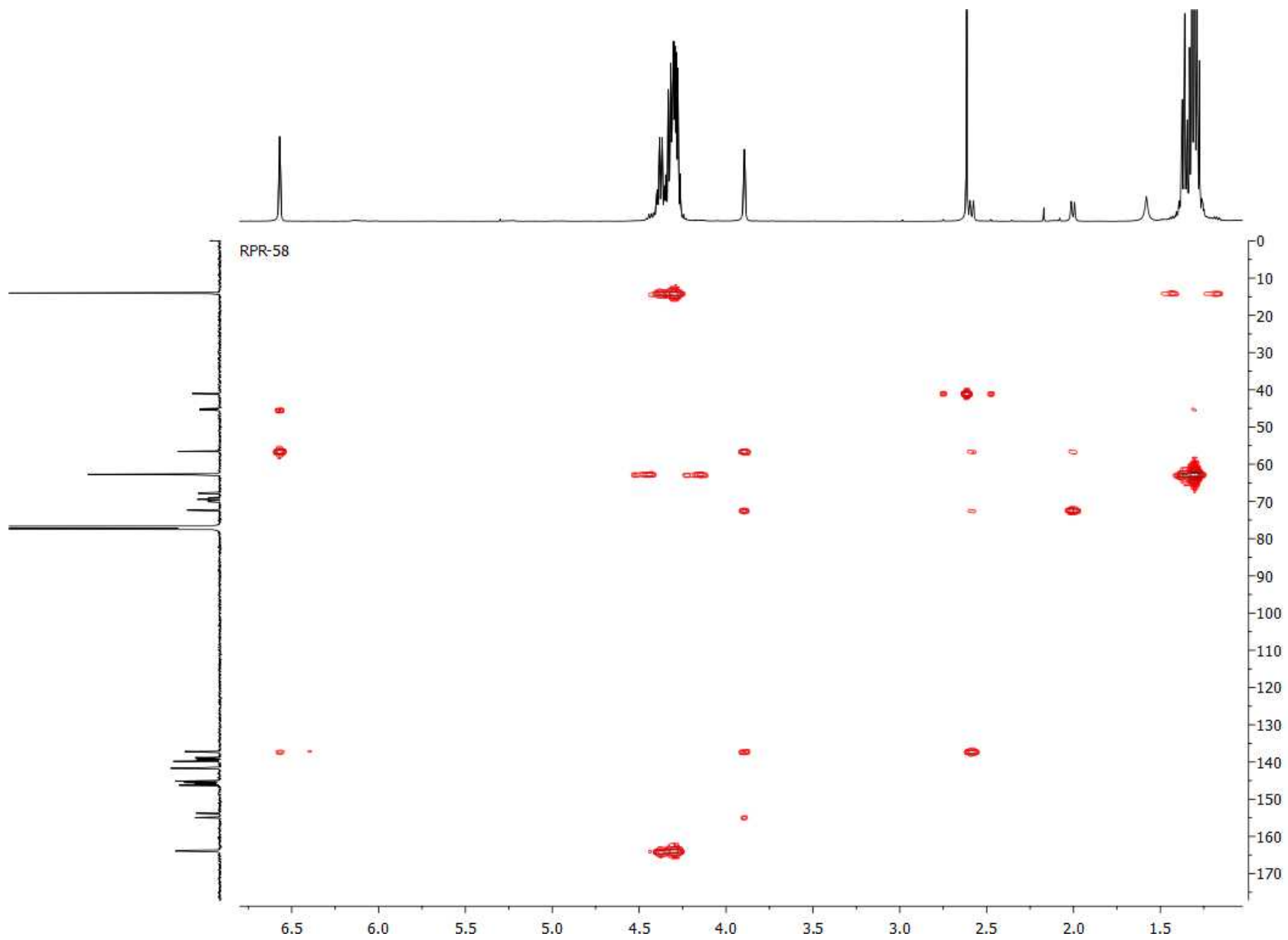
RPR-58



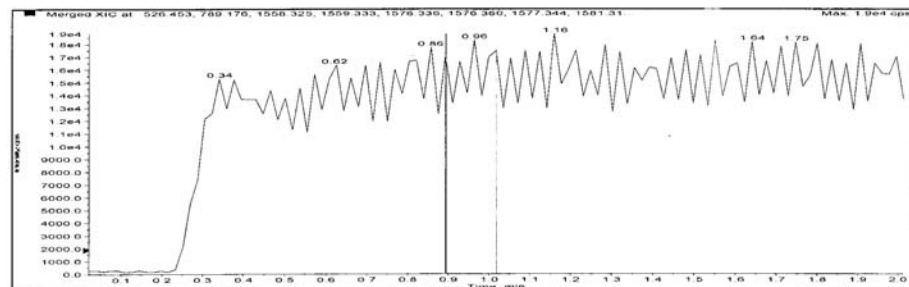




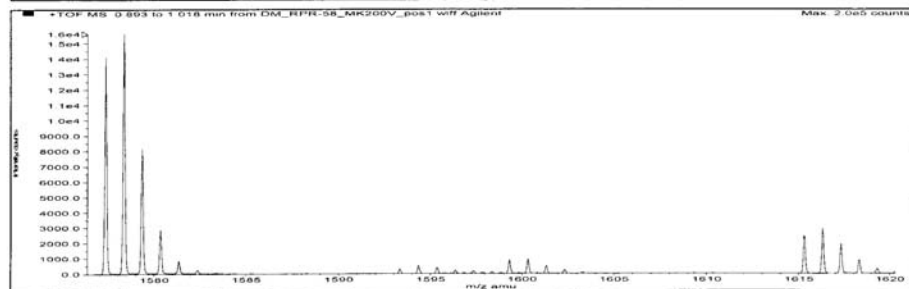
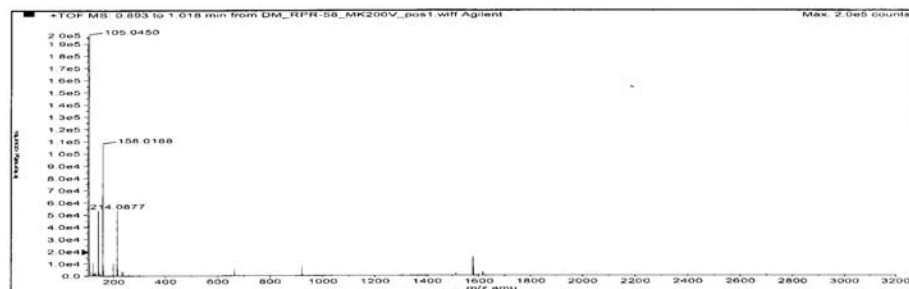




Sample Name: RPR-58 Sample Location: P1-D6 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\ID_MilicData\DM_RPR-58_MK200V_pos1.wiff Acq Time: March 25 2016, 01:14:29 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.anml\efc.xml



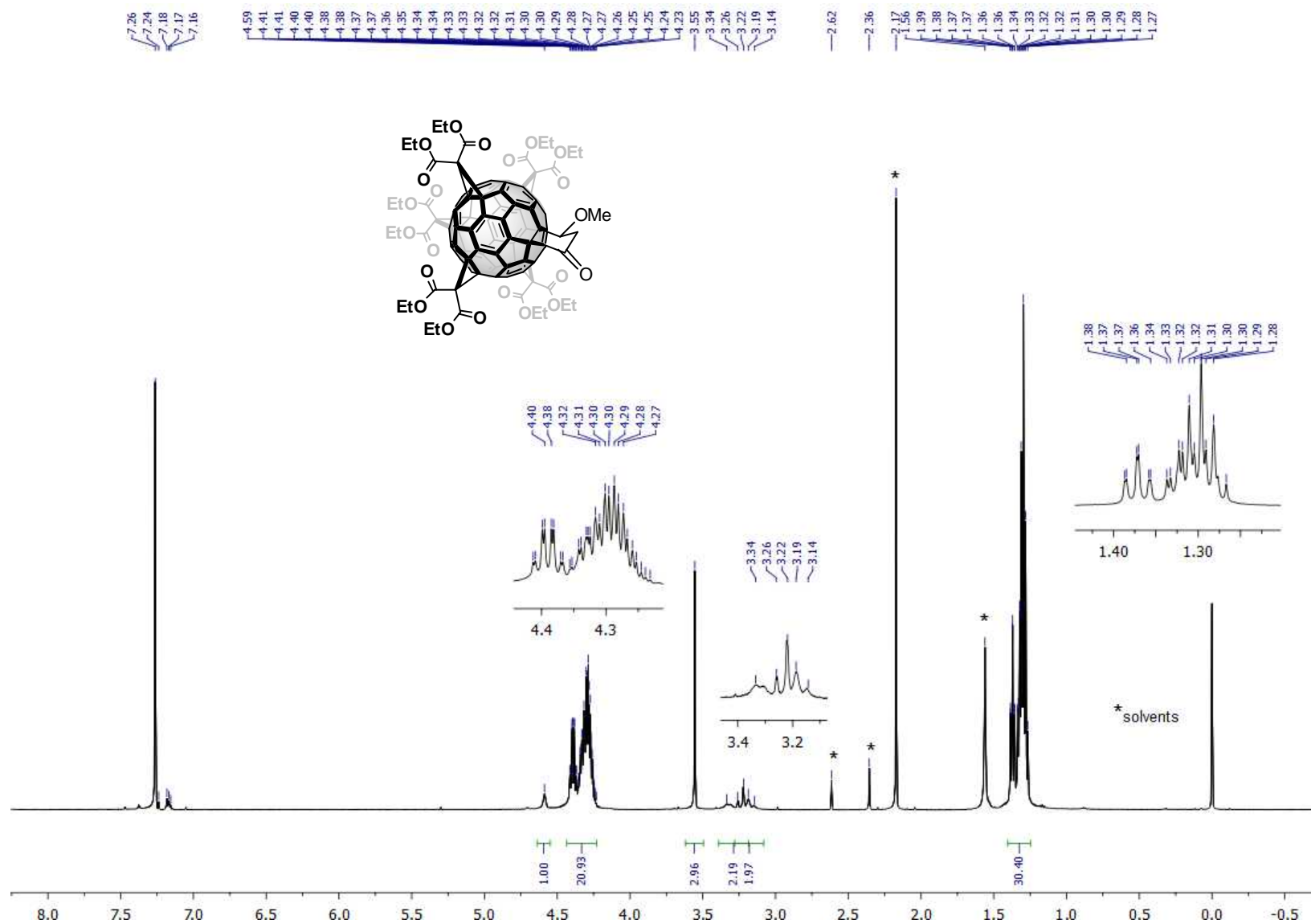
Merged XIC, Period# : 1 Experiment# : 1

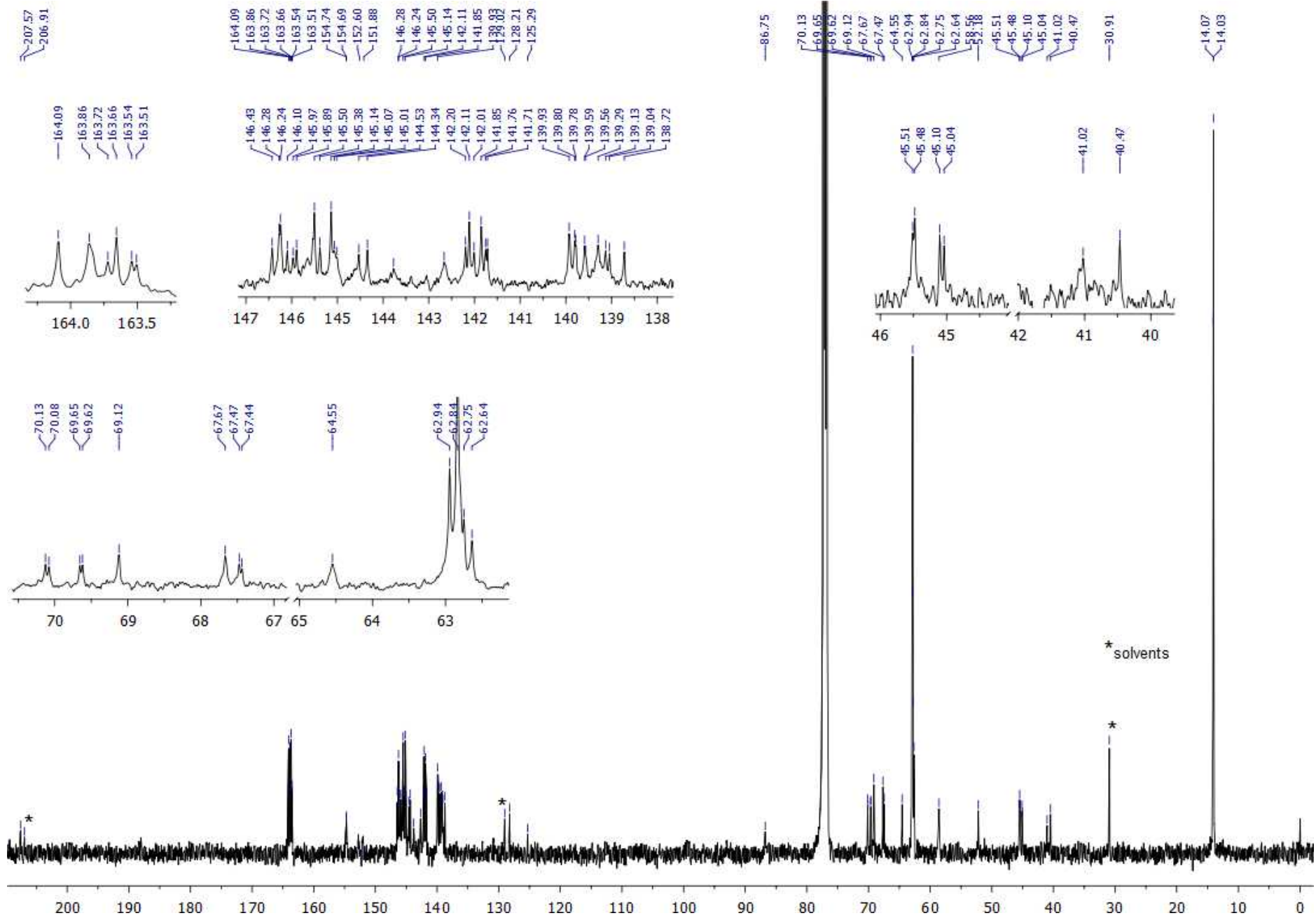


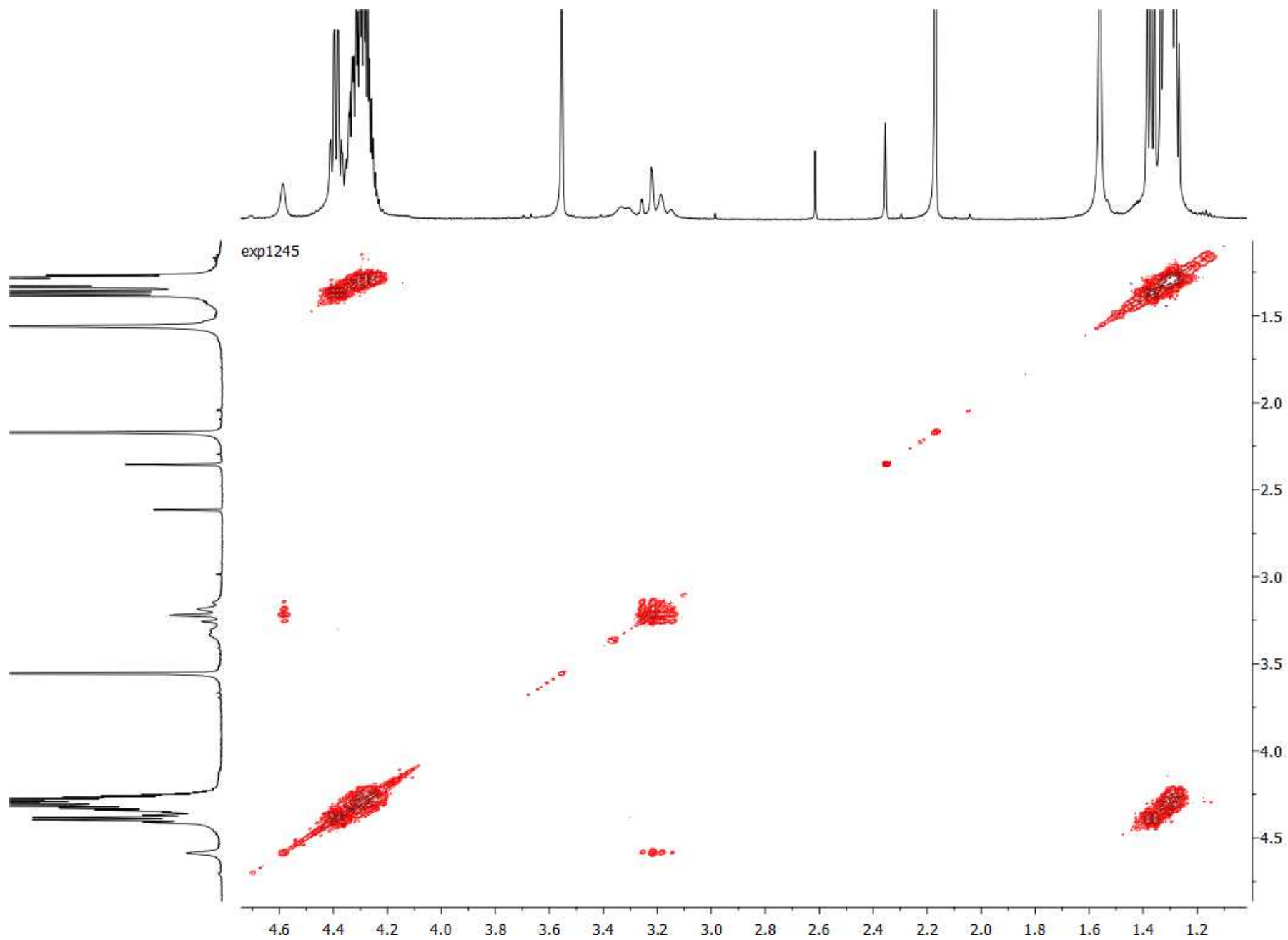
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C100H56O20	--	1576.33649	0.96	3.75623 E4	--

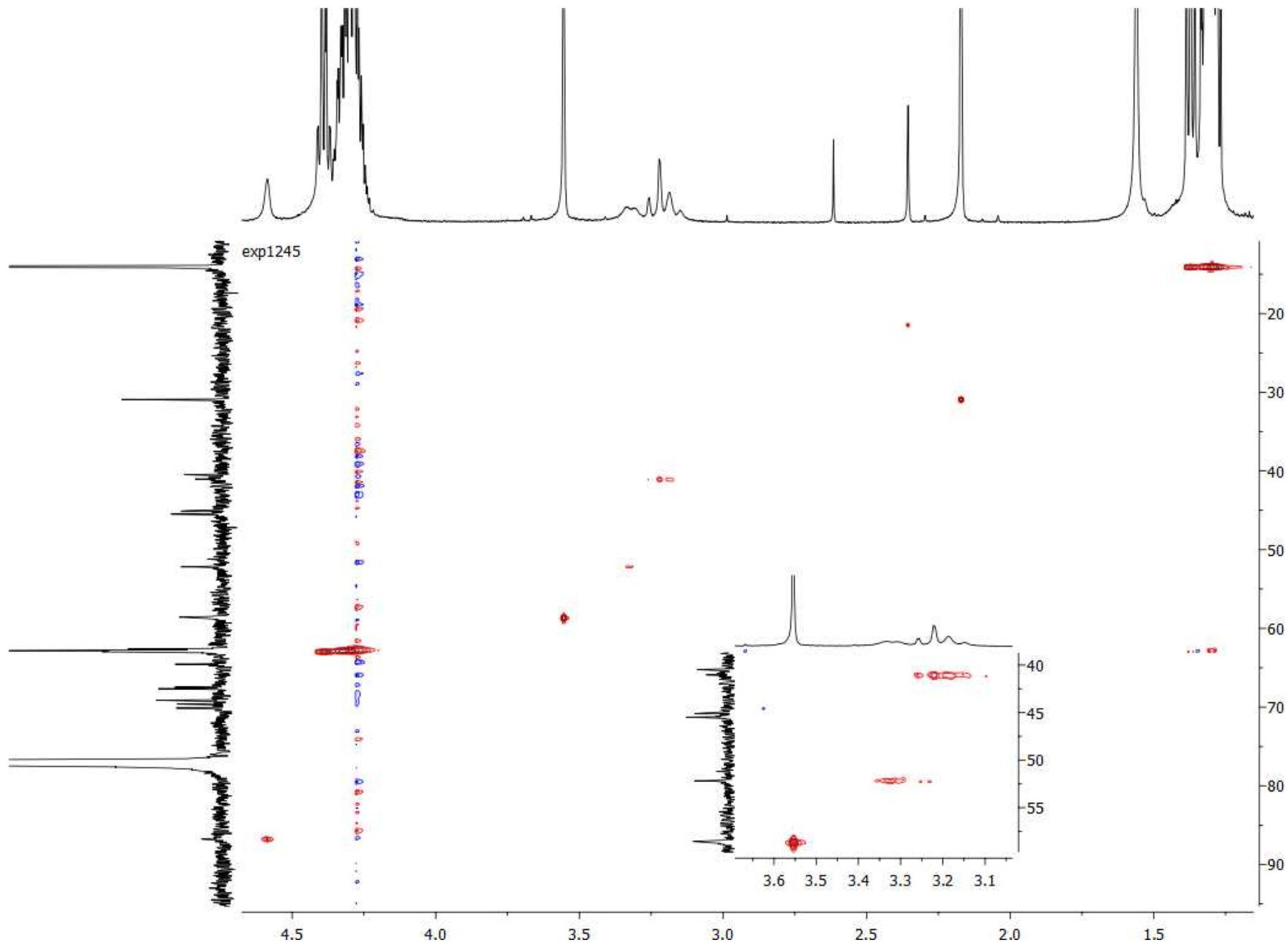
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	14187.02	1577.34377	1577.34242	-1.35253	-0.86	--
[M+K] ⁺	2588.65	1615.29965	1615.29781	-1.84483	-1.14	--

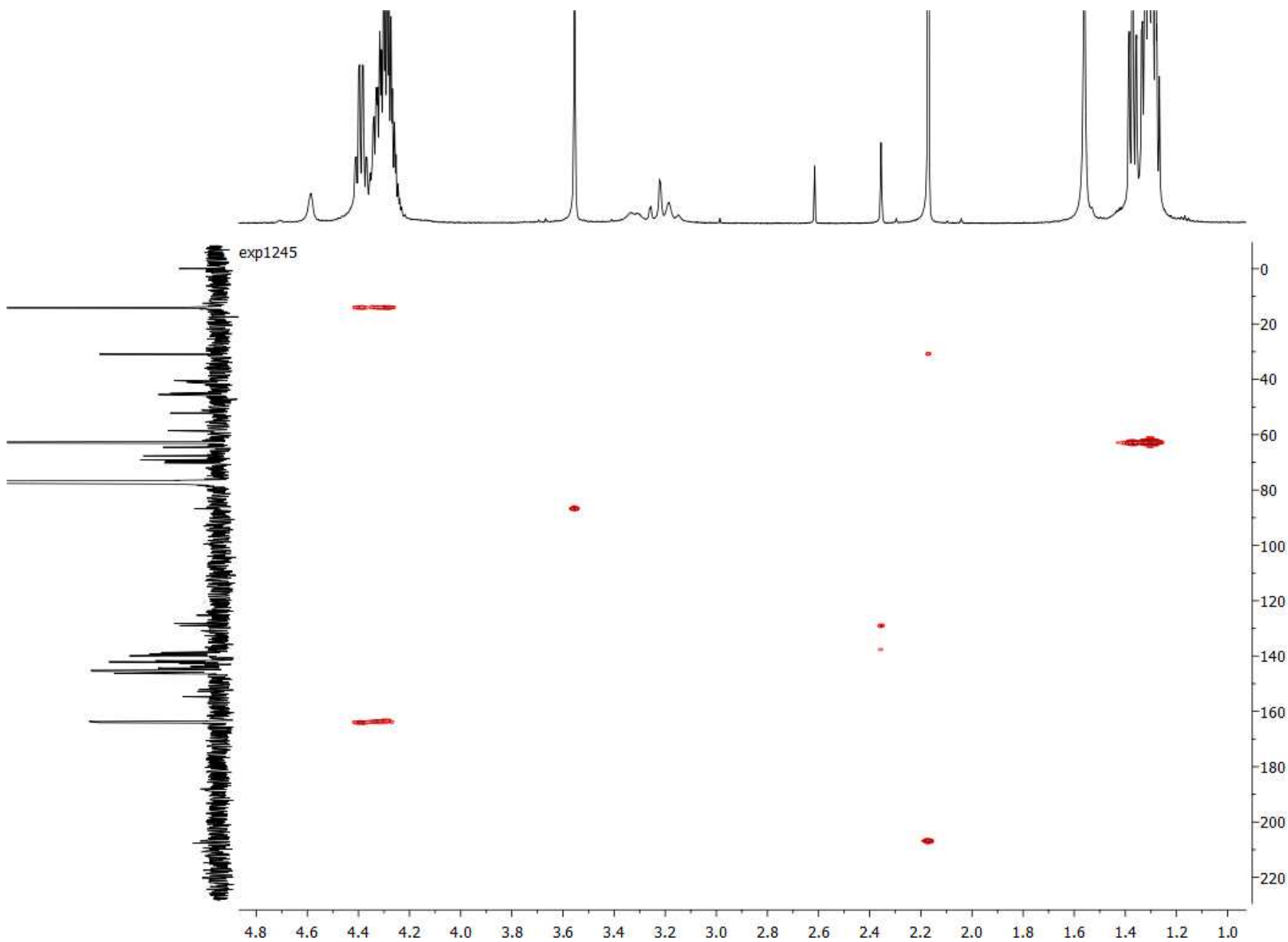
Bingel-Diels-Alder [5:1]-hexaadduct 14a



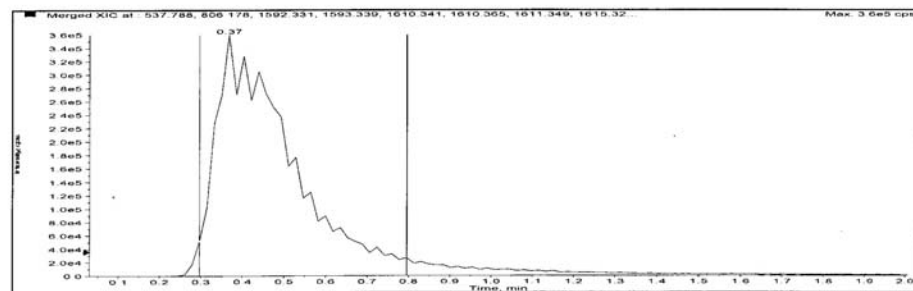




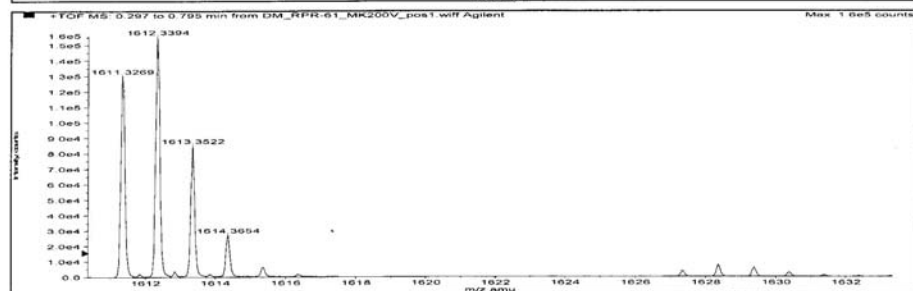
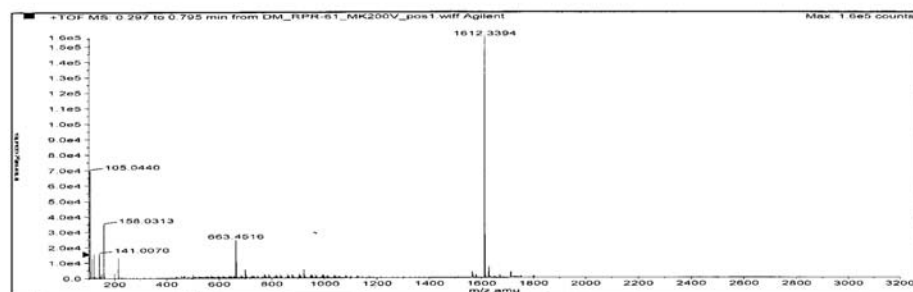




Sample Name: RPR-61 Sample Location: P1-E2 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\DM_MilicaData\DM_RPR-61_MK200V_pos1.wiff Acq Time: April 22 2016, 01:59:43 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.anmlfc.xml



Merged XIC, Period#: 1 Experiment#: 1



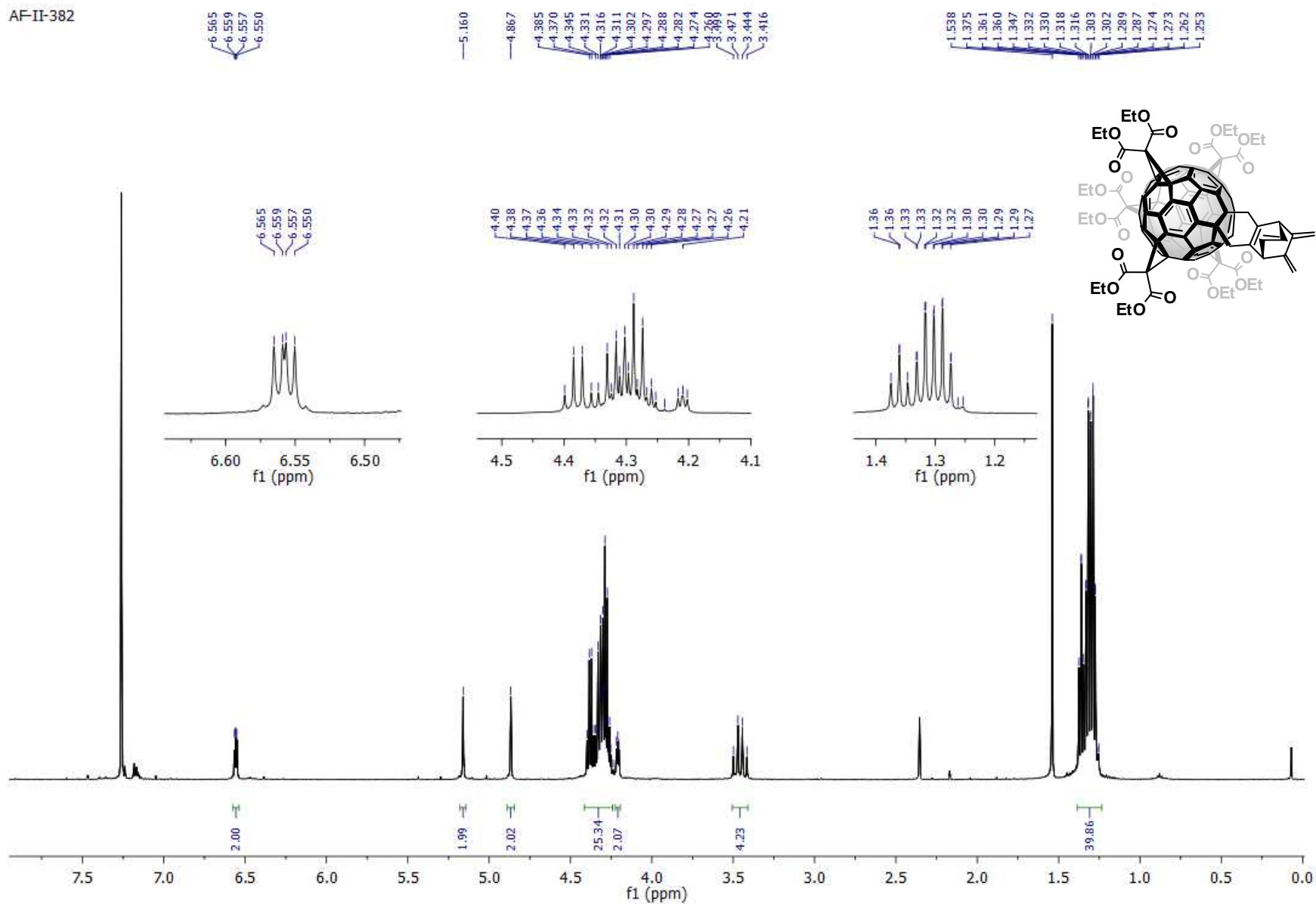
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C100H58O22	--	1610.34197	0.37	4.44028 E6	--

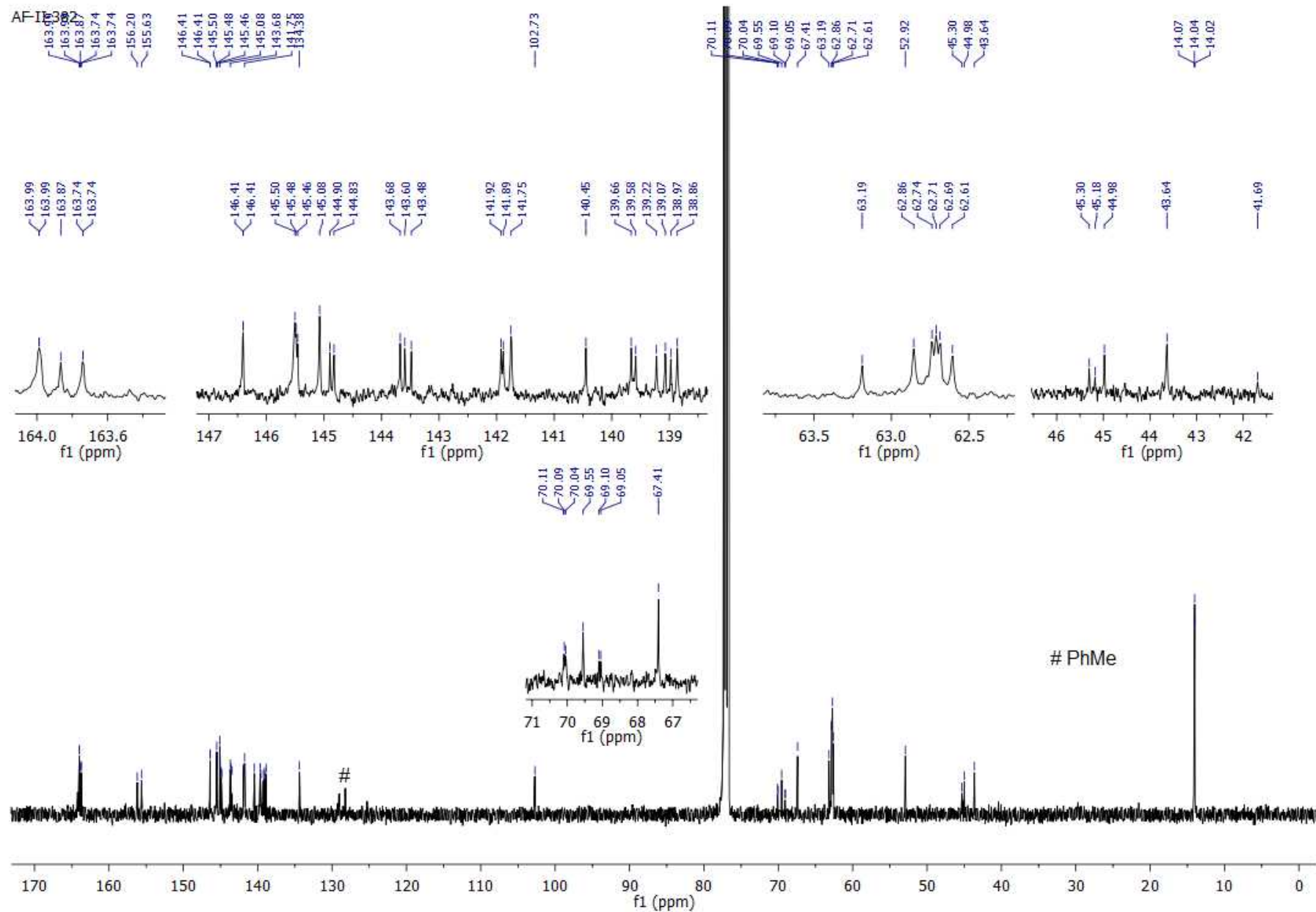
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	136490.98	1611.34925	1611.34716	-2.09372	-1.30	--
[M+Na-H2O] ⁺	6675.81	1615.32063	1615.36199	41.35944	25.60	--
[M+NH4] ⁺	7745.00	1628.37580	1628.35884	-16.96053	-10.42	--

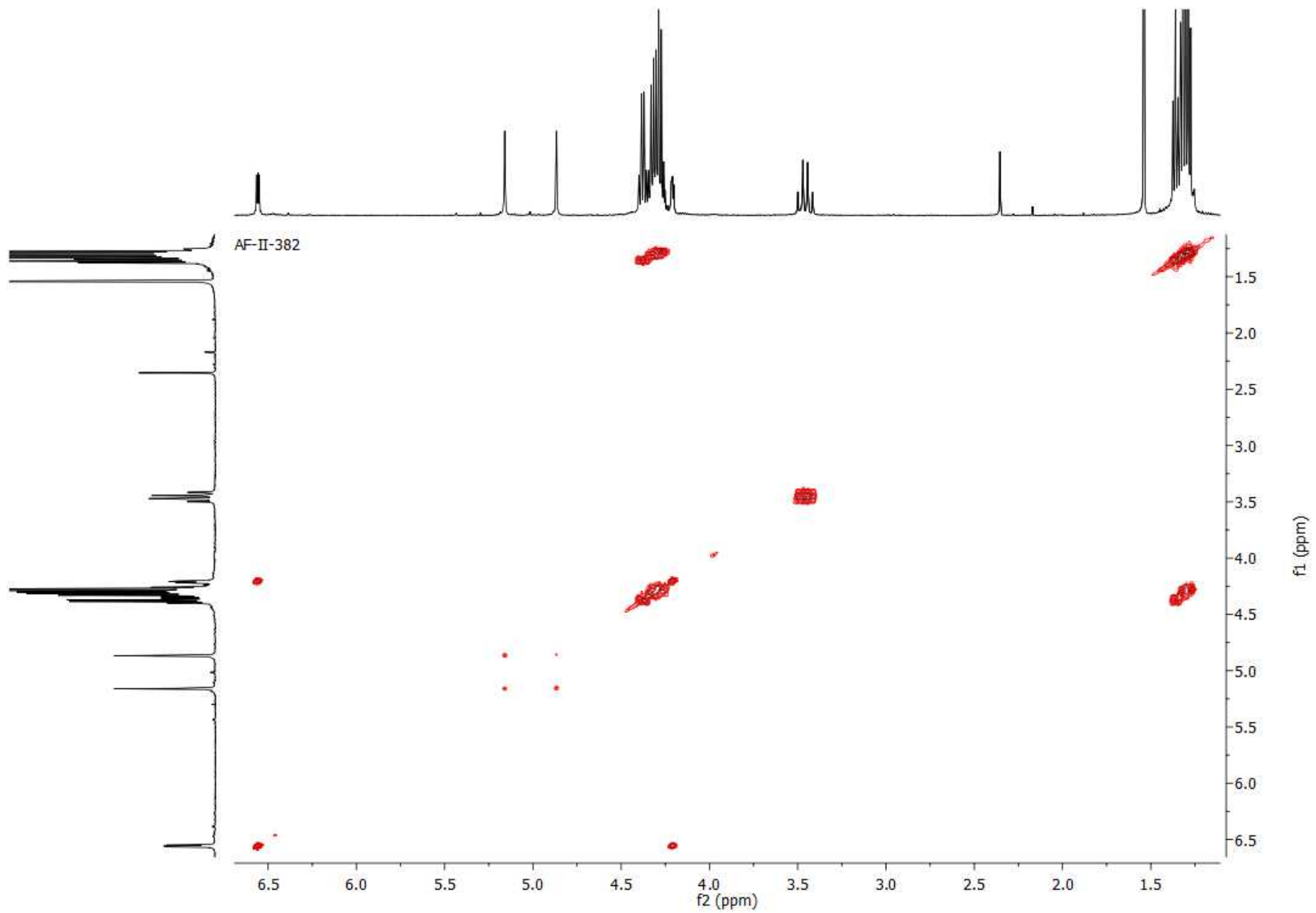
OK!

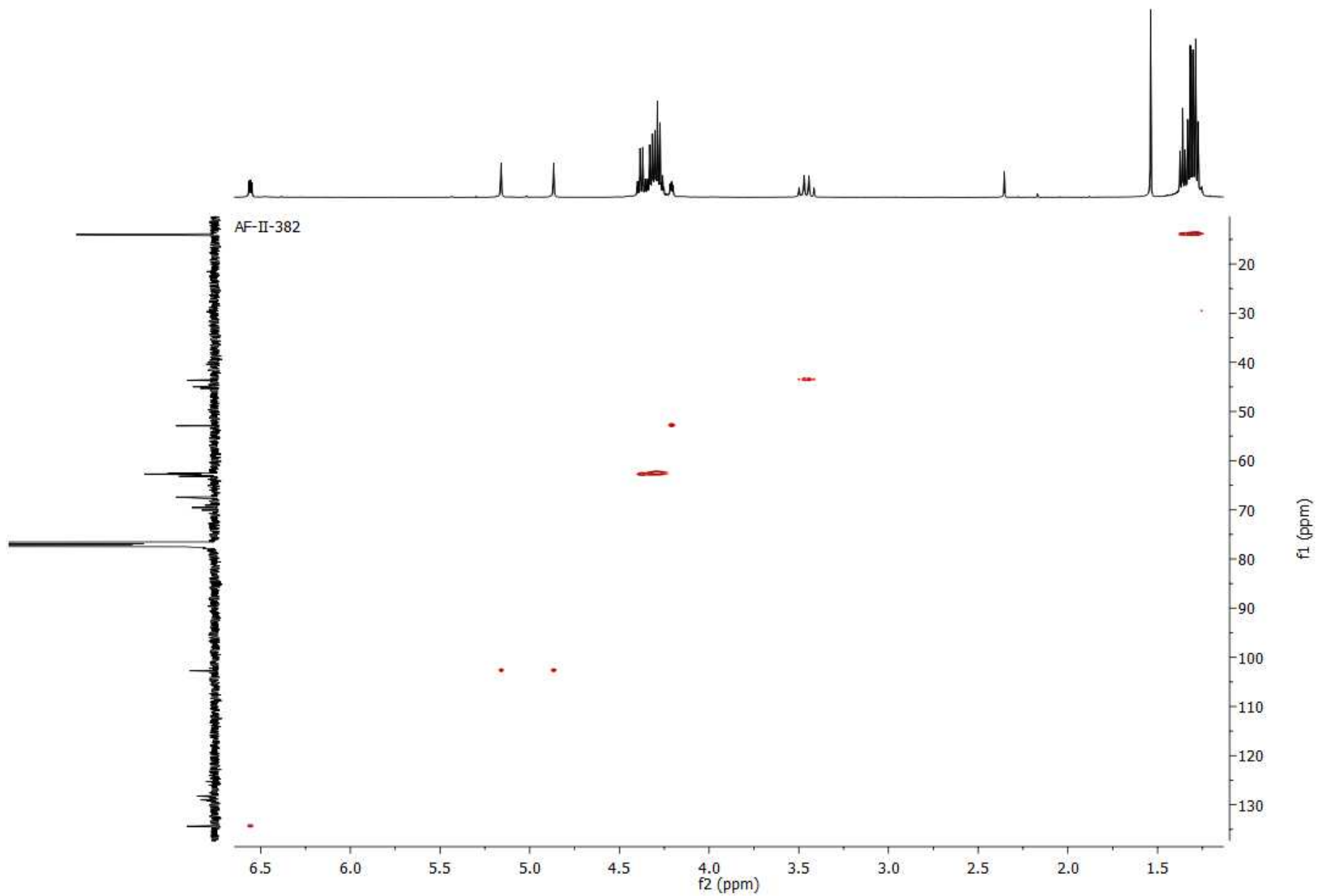
Bingel-Diels-Alder [5:1]-hexaadduct 15a

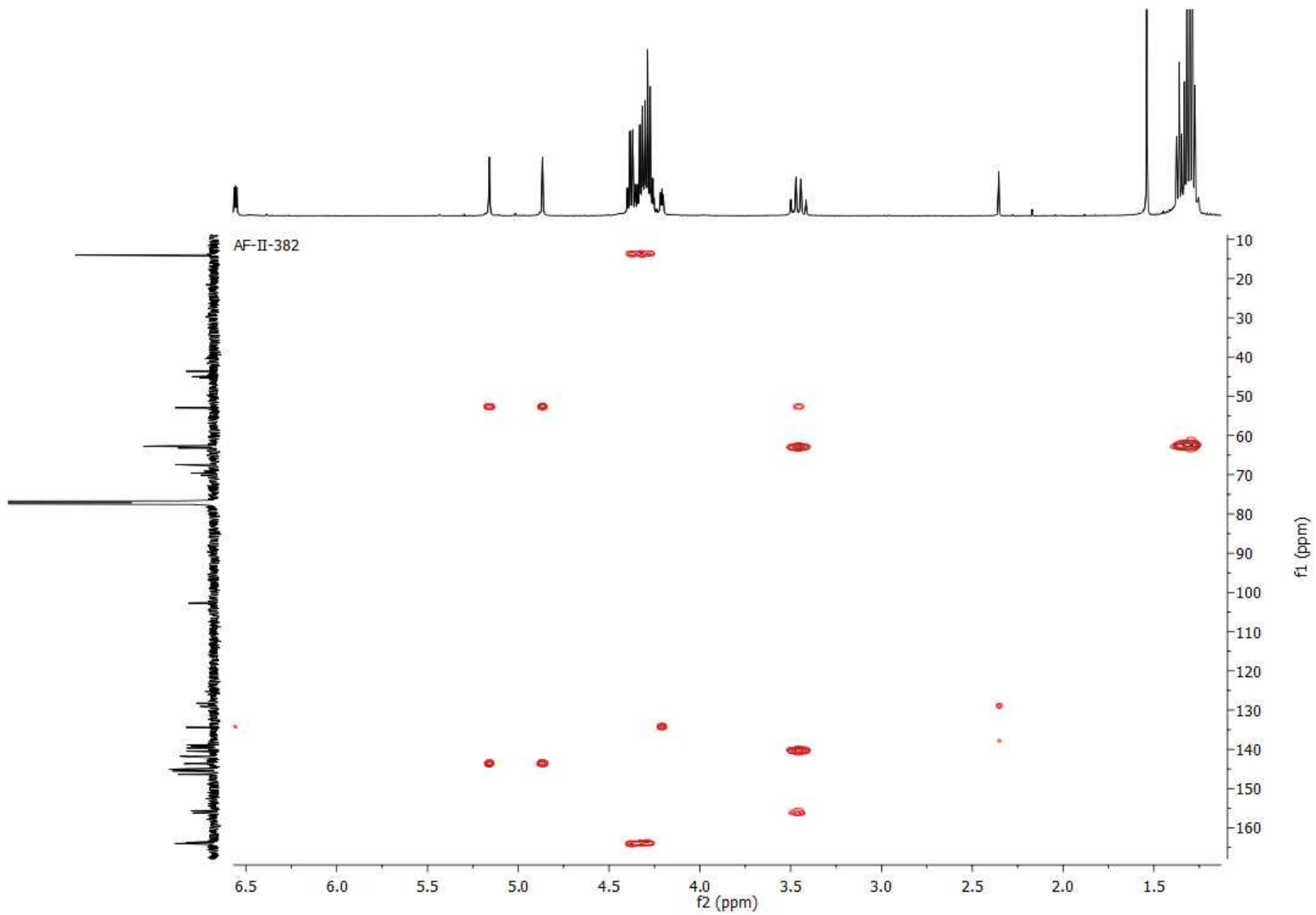
AF-II-382



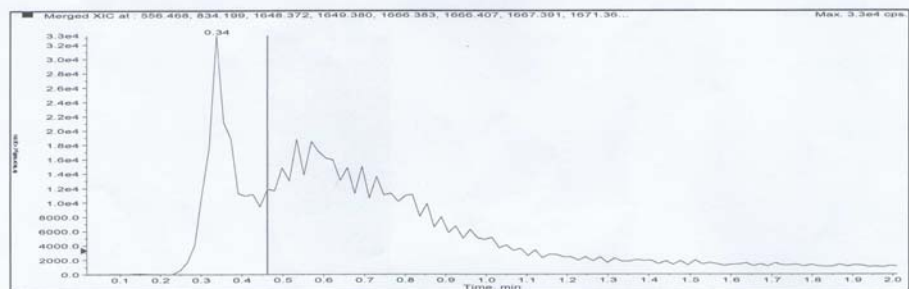




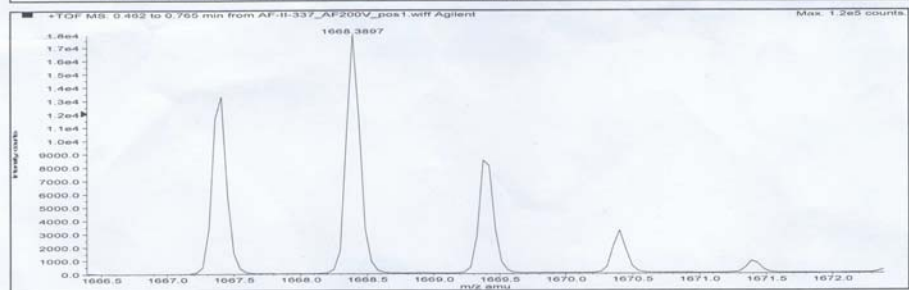
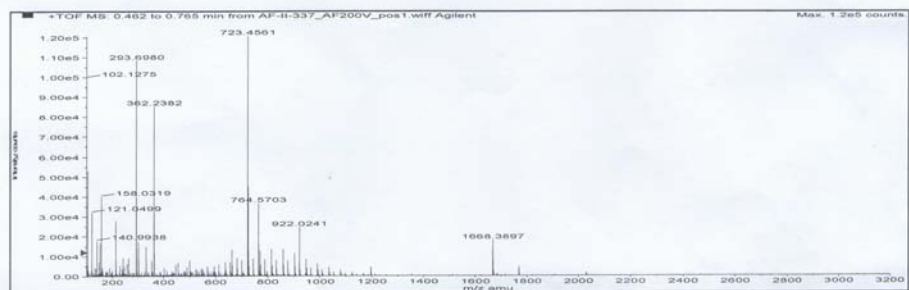




Sample Name: AF-II-337 Sample Location: P1-D2 Sample Id: Operator: Milka
 Data File Name: D:\PE_Sciex_Data\Projects\MaslakData\AF-II-337_AF200V_pos1.wiff Acq Time: November 24 2015, 01:48:41 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlfc.xml



Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C107H62O20	-	1666.38344	0.53	1.37363 E5	-

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	13755.44	1667.39072	1667.39006	-0.66177	-0.40	-

Summary of Calculations

Methods:

Density functional theory (DFT) calculations were performed using the Gaussian 09 suite of programs.¹ All geometries were optimized at the B3LYP/6-31G(d) level of theory.²⁻⁴ Vibrational frequency analyses at the B3LYP/6-31G(d) level of theory were utilized in order to verify that computed stationary points corresponded to either local minima or saddle points on the respective potential energy surface. Intrinsic reaction coordinate calculations were performed in order to confirm that the transition states connected to the appropriate local minima as reactants and products.

¹ Gaussian 09, Revision **A.1**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

² Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648-5652.

³ Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* 1988, *37*, 785–789.

⁴ Frisch, M. J.; Pople, J. A.; Binkley, J. S. *J. Chem. Phys.* **1984**, *80*, 3265-3269

Computational data

Optimized XYZ coordinates, bottom of the well energies, and unscaled vibrational frequencies supplied for all species calculated at the B3LYP/6-31G* level of theory.

Coordinates for the symmetrical pentakisadduct of C₆₀ 1

Energy = -5154.50332366 Hartrees

C	-1.08843700	-2.64716900	-2.96256000
C	-1.14915800	-3.38920900	-1.74174500
C	-2.21434900	-1.72772400	-3.00761700
C	-2.42797400	-3.04491700	-1.04290400
C	-2.98171400	-1.88581500	-1.81330800
C	1.30921300	-3.29500200	-1.61931300
C	0.03400700	-3.64439300	-1.05662200
C	1.36705600	-2.58982400	-2.81602400
C	0.14741100	-2.26498000	-3.50383200

C	-3.43200200	-0.58254300	0.26021900
C	-3.51595200	-0.75629500	-1.19869300
C	-2.81851200	-1.54013600	1.06266600
C	-2.34622800	-2.85109400	0.52539200
C	0.10882100	-3.47232300	0.40190000
C	-0.99558100	-3.04433100	1.14004500
C	-2.06470100	-0.46324200	-3.59291500
C	-2.66222800	0.69011500	-2.97748600
C	-0.78270500	-0.07421700	-4.15001600
C	-3.40186800	0.54027200	-1.81109100
C	0.29575800	-0.95190800	-4.10436900
C	-0.80989700	-2.06032800	2.15757000
C	-1.94613400	-1.12571400	2.11188200
C	-3.26634400	0.80603700	0.53705200
C	-3.40647700	1.57910100	-0.73567000
C	-1.73626500	1.82305600	-3.15400800
C	-0.58958700	1.33739600	-3.87383900
C	1.62489500	-0.46430700	-3.78322700
C	2.29409500	-1.45835300	-2.99128100
C	2.26730400	-3.04281000	-0.49906500
C	1.41772300	-3.01661500	0.72893600
C	1.58514300	-2.06455100	1.73068100
C	0.46603900	-1.60956600	2.48312300
C	0.72913600	-0.21570300	2.95452600
C	-0.48872300	0.78651000	2.90238500
C	-1.77948000	0.22790300	2.39311800
C	-2.41445900	1.20287200	1.56630500
C	-1.48332200	2.32901200	1.39236900
C	-1.43244700	3.03286800	0.19237000

C	-2.40558100	2.79886800	-0.91705000
C	-1.56823300	2.78026900	-2.15789500
C	-0.24539900	3.22957500	-1.82224100
C	0.86244800	2.80090500	-2.54415300
C	0.69098800	1.81312000	-3.55894200
C	1.82052900	0.89719200	-3.51282300
C	2.71042600	1.31199100	-2.47235900
C	3.30753800	0.33789100	-1.67541900
C	3.14443400	-1.05978300	-1.96786700
C	3.26407100	-1.83053300	-0.69144200
C	3.24972600	-0.79122000	0.38328700
C	2.51489600	-0.93694300	1.55882500
C	1.96237600	0.20551200	2.21559300
C	-0.28833400	2.04318200	2.11789200
C	-0.16840100	3.38662700	-0.36129200
C	2.20969700	2.61277900	-1.92216400
C	3.37326500	0.49517700	-0.21528700
C	1.00660400	3.10790200	0.33576700
C	0.94246400	2.38630700	1.56367000
C	2.08115700	1.45633600	1.61100500
C	2.84236700	1.61865400	0.41401600
C	2.28906400	2.77424500	-0.35441500
C	-3.25627900	-3.90298800	-0.09444700
C	3.03001200	3.72637900	-1.28191800
C	0.14293800	0.37916800	4.22959900
C	-3.90814400	3.01572300	-0.79684300
C	3.77720300	-3.25107800	-0.49710700
C	-3.03182500	-5.38127100	0.13516200
C	-4.75931500	-3.63247200	-0.05928600

C	4.53531000	3.64773300	-1.38175300
C	2.48928500	5.14639100	-1.38967000
C	0.92717700	1.32369500	5.11169000
C	-0.66409900	-0.55840600	5.12698400
C	-4.42035300	3.61761200	0.51172900
C	-4.72510400	3.59200900	-1.93255100
C	4.40637000	-3.97899000	-1.66286000
C	4.42834100	-3.58432800	0.83991700
O	3.98515600	-4.36512500	1.64930200
O	5.57158300	-2.89473800	0.98160300
O	5.28152100	-4.90273000	-1.22185100
O	4.15578800	-3.78695800	-2.83099900
C	5.94322900	-5.69123400	-2.24307300
C	6.87627700	-6.65534800	-1.53670200
C	6.31620000	-3.15039800	2.19827300
C	7.54925200	-2.26815600	2.16852300
O	-5.48048000	4.52652800	-1.76056100
O	-4.52288800	2.99520800	-3.11155500
C	-5.25341700	3.55076300	-4.23721500
C	-4.85429500	2.76684500	-5.47201900
O	-3.87599900	4.50023500	1.13138300
O	-5.56905600	3.02199500	0.86233700
C	-6.21721200	3.54686900	2.04779400
C	-7.48069000	2.73832900	2.26883700
O	0.95193700	1.19934000	6.31928300
O	1.58370000	2.27052500	4.43143100
C	2.37978400	3.20735000	5.20490000
C	1.53093600	4.36653000	5.70136600
O	-0.34673000	-1.69302300	5.39408500

O	-1.76021500	0.07339500	5.57387000
C	-2.58176200	-0.65006400	6.52759000
C	-2.05921700	-0.46698800	7.94368100
O	-3.93712700	-6.11763200	0.46962000
O	-1.76687500	-5.77430000	-0.04249800
C	-1.49201900	-7.17547800	0.22616500
C	-0.00873200	-7.40053300	0.00769100
O	-5.35571400	-3.13998800	0.86868900
O	-5.31908000	-4.03208400	-1.21090800
C	-6.76183300	-3.91956000	-1.28232900
C	-7.19095300	-4.44953300	-2.63667100
O	1.94708300	5.61626400	-2.36200900
O	2.70862100	5.80491000	-0.23865600
C	2.27001000	7.18619200	-0.20957500
C	2.56227600	7.72572700	1.17705100
O	5.20930900	2.68012600	-1.10909300
O	5.03411800	4.80633000	-1.85286900
C	6.47215800	4.85367600	-2.03295900
C	6.81790900	6.23256600	-2.56025500
H	6.47745900	-5.01197000	-2.91439100
H	5.17891700	-6.20893800	-2.83073900
H	7.62751700	-6.11535900	-0.95170900
H	7.39519700	-7.27481000	-2.27619200
H	6.32067500	-7.31442200	-0.86232400
H	6.56745800	-4.21527600	2.23383400
H	5.67007100	-2.93066100	3.05363400
H	7.27103700	-1.21079700	2.11965500
H	8.17619200	-2.50013600	1.30170600
H	8.14082700	-2.42928400	3.07629600

H	-5.00393300	4.61269800	-4.32003800
H	-6.32371800	3.47422900	-4.02311400
H	-5.39443900	3.15494800	-6.34242900
H	-5.09720100	1.70583400	-5.35884900
H	-3.78062100	2.85688100	-5.66251800
H	-6.42630000	4.60845600	1.88376800
H	-5.52109300	3.46610400	2.88845100
H	-7.24655000	1.67918700	2.41538100
H	-8.15674700	2.82868500	1.41279300
H	-8.00174000	3.10393300	3.16042000
H	3.14819600	3.53875200	4.50317000
H	2.84646700	2.66702800	6.03149200
H	1.02920600	4.86579500	4.86636000
H	2.16840700	5.09869500	6.21024800
H	0.77599800	4.01676900	6.41094800
H	-2.60472700	-1.70344300	6.23919700
H	-3.57700600	-0.21741400	6.40247400
H	-1.06209700	-0.90308100	8.04725800
H	-2.73197700	-0.96443300	8.65193000
H	-2.00358600	0.59473700	8.20291100
H	-2.10888500	-7.78060500	-0.44507200
H	-1.79937000	-7.39496200	1.25285700
H	0.23259700	-8.45211300	0.19768800
H	0.58696800	-6.78163100	0.68537500
H	0.27650300	-7.16131900	-1.02155300
H	-7.03578600	-2.86903000	-1.14248200
H	-7.19369600	-4.49316500	-0.45664200
H	-6.89952900	-5.49782100	-2.75505600
H	-6.73555300	-3.86990800	-3.44600000

H	-8.28003100	-4.38046800	-2.73277100
H	1.20286100	7.21754500	-0.44887500
H	2.80483400	7.73642300	-0.99040800
H	2.24518100	8.77221600	1.24127700
H	3.63281800	7.67510300	1.40049500
H	2.02177300	7.15498800	1.93874100
H	6.75998400	4.05939200	-2.72843200
H	6.94974600	4.64469500	-1.07072800
H	7.89970500	6.30719100	-2.71520900
H	6.51720700	7.01013600	-1.85091400
H	6.31812300	6.42327300	-3.51501800

Vibrational frequencies for 1

10.04	14.02	16.40	18.11	18.29	23.92
27.07	28.08	29.75	31.60	32.82	34.16
34.63	35.92	37.09	40.65	45.44	47.93
48.44	50.98	54.52	59.48	60.32	62.51
65.46	68.40	68.93	69.37	69.72	72.55
73.54	74.93	75.06	77.49	90.20	92.78
94.08	97.43	99.93	110.13	110.99	117.74
121.67	124.93	132.12	135.34	141.36	143.01
144.39	150.11	153.29	156.05	157.77	158.83
161.93	167.91	177.16	182.26	191.71	193.79
208.92	209.41	216.75	224.47	226.46	236.04
237.13	245.45	250.19	250.65	259.49	262.69
264.37	265.68	266.96	268.57	271.18	274.04
276.72	277.24	279.93	281.38	299.87	308.21
310.27	312.69	320.49	321.31	324.34	329.75
341.20	342.24	345.98	352.05	354.26	356.25

358.10	367.69	369.90	379.65	382.63	385.27
389.42	392.90	395.79	397.82	398.42	405.01
414.92	422.54	426.44	428.78	431.32	432.24
435.53	437.17	440.63	446.11	450.19	455.87
470.80	471.56	475.96	480.45	481.80	492.94
521.04	522.89	531.64	536.55	538.26	540.60
545.43	547.96	550.09	555.16	556.88	560.83
561.95	566.61	570.11	574.30	577.96	579.89
581.61	582.49	585.66	592.55	626.80	631.13
637.89	644.63	646.79	650.84	658.97	662.87
666.54	672.85	679.00	681.54	684.42	690.66
697.85	704.78	707.66	709.60	710.04	719.06
727.04	729.51	730.03	731.64	734.44	736.93
737.18	740.17	743.70	744.28	744.59	748.02
751.11	751.22	753.20	754.76	756.71	758.46
759.61	763.53	765.41	767.96	769.90	780.69
787.71	790.17	794.24	798.82	801.57	803.00
810.86	813.92	815.88	816.80	817.65	818.45
818.94	819.23	819.79	820.64	821.38	822.60
823.74	825.74	826.65	829.29	831.42	832.44
835.08	838.34	842.75	844.67	845.91	847.17
867.98	872.51	877.83	880.91	881.47	885.65
887.24	888.77	894.44	895.76	900.01	907.41
911.33	924.88	927.44	930.00	940.82	942.38
954.07	955.81	963.10	978.75	984.04	991.49
1016.34	1017.67	1023.38	1032.42	1035.48	1037.04
1040.20	1042.61	1044.82	1052.04	1055.32	1055.76

1063.67	1064.70	1086.86	1089.78	1094.36	1107.87
1108.39	1112.49	1121.72	1125.68	1127.45	1129.00
1130.27	1133.71	1136.26	1141.35	1141.53	1146.95
1147.35	1147.69	1148.23	1148.68	1148.71	1152.51
1154.46	1155.51	1176.56	1186.53	1187.61	1189.99
1191.14	1191.35	1191.68	1191.77	1191.90	1192.09
1192.13	1192.31	1196.85	1207.55	1211.23	1216.68
1225.84	1231.88	1235.53	1242.19	1243.17	1248.06
1254.81	1255.82	1263.63	1266.69	1270.73	1273.10
1278.96	1281.44	1285.50	1287.53	1288.23	1291.22
1296.47	1307.19	1307.25	1307.60	1307.90	1307.99
1308.14	1308.18	1308.66	1310.31	1313.17	1315.50
1317.38	1320.05	1325.72	1339.64	1340.76	1341.73
1342.21	1343.68	1353.27	1354.96	1366.93	1367.84
1369.24	1370.68	1377.67	1389.64	1392.82	1396.48
1397.58	1397.86	1401.29	1405.63	1408.65	1410.82
1412.08	1414.87	1415.33	1415.95	1416.49	1417.23
1417.67	1417.78	1418.37	1419.79	1420.54	1421.64
1423.01	1433.81	1444.42	1444.68	1445.23	1447.22
1450.54	1450.70	1450.84	1451.49	1451.67	1451.94
1452.09	1452.38	1452.52	1473.36	1495.47	1513.88
1515.55	1515.90	1515.93	1515.97	1516.21	1516.35
1516.39	1516.41	1516.78	1518.43	1518.95	1525.55
1525.86	1525.94	1525.98	1526.29	1526.43	1526.66
1526.87	1532.31	1536.75	1541.51	1542.97	1543.24
1543.33	1543.74	1543.92	1544.04	1544.86	1545.09
1566.76	1572.12	1573.99	1576.81	1577.18	1579.10

1598.14	1599.38	1600.43	1611.23	1612.99	1623.54
1624.05	1625.85	1627.73	1793.37	1795.28	1796.49
1815.81	1816.63	1828.26	1829.87	1830.61	1831.17
1831.70	3062.36	3062.47	3062.64	3062.72	3062.74
3063.24	3063.76	3063.83	3064.15	3065.28	3077.41
3077.56	3077.90	3078.36	3079.48	3079.91	3081.62
3081.72	3098.00	3100.26	3117.45	3117.74	3118.31
3118.64	3118.98	3119.38	3122.11	3122.23	3130.70
3131.17	3133.13	3133.33	3133.77	3134.20	3134.57
3134.64	3134.65	3135.76	3141.80	3142.51	3144.07
3145.29	3145.31	3145.78	3146.12	3146.20	3149.36
3149.47	3162.69	3163.48			

Coordinates for N-methyl azomethine ylide

Energy = -173.19528031 Hartrees

C	-0.71172300	1.20649600	-0.00609400
H	-1.78930100	1.26718000	0.04652300
H	-0.08827200	2.08543100	0.00030300
C	-0.70803100	-1.20841400	-0.00055800
H	-0.08275800	-2.08581900	-0.02102100
H	-1.78549900	-1.27253700	0.04941800
N	-0.13289300	-0.00019000	-0.01925000
C	1.34615800	0.00196300	0.00995700
H	1.68997800	-0.00133200	1.04689400
H	1.71520500	-0.88493500	-0.50633400
H	1.71247900	0.89306800	-0.50086200

Vibrational frequencies for 1,3 dipole

108.1631	128.5051	418.0156	484.7116	490.8449	510.297
512.9345	715.3652	897.5332	1087.0756	1139.5661	1146.1822
1157.7898	1394.2749	1458.9014	1477.5845	1502.9683	1529.4395
1553.9941	1623.0005	3090.5612	3171.9537	3182.9883	3216.8404
3225.3686	3336.2461	3339.2589			

Coordinates for TS (8a')

Energy = -5327.68863731 Hartrees

C 2.19323300 2.31407600 -2.09179300
C 2.29392000 2.84474800 -0.76957300
C 2.95671700 1.07380600 -2.15842800
C 3.26102600 2.00362700 0.00461900
C 3.52905700 0.82026400 -0.87555200
C -0.04474100 3.59178600 -0.94041700
C 1.16515300 3.41602400 -0.18849900
C -0.13511500 3.08582700 -2.23330300
C 1.00507100 2.44283900 -2.82577600
C 3.18682600 -0.78408400 0.99887700
C 3.55954100 -0.48749200 -0.39388200
C 2.79876100 0.22831600 1.87145000
C 2.87079800 1.67302200 1.50097100
C 0.80552200 3.11444100 1.20482500
C 1.57654700 2.24994600 1.98348900
C 2.49347900 0.01508500 -2.95479300
C 2.57374500 -1.33521700 -2.46749100

C	1.26953200	0.15830600	-3.72968600
C	3.12892800	-1.58515200	-1.21653900
C	0.53942000	1.34980700	-3.66620100
C	0.91978900	1.28187200	2.80152900
C	1.68152900	0.02421300	2.73381900
C	2.53349400	-2.05079800	1.02914700
C	2.61140800	-2.67428600	-0.32883200
C	1.37096000	-2.04870600	-2.92663700
C	0.58012600	-1.12009000	-3.68446900
C	-0.91093600	1.30954700	-3.55719400
C	-1.33739800	2.37290500	-2.69289100
C	-1.20096900	3.55869600	0.00827600
C	-0.61517400	3.10268300	1.30402400
C	-1.24194100	2.16033500	2.11395800
C	-0.46819700	1.26436800	2.90410700
C	-1.24346600	0.00358400	3.11313200
C	-0.42559100	-1.34587500	3.03854700
C	1.03986100	-1.21148700	2.77445100
C	1.44575800	-2.24395400	1.87776900
C	0.24233500	-2.95521700	1.42105300
C	0.16183300	-3.45678100	0.12512600
C	1.32596400	-3.44540000	-0.81516000
C	0.74581800	-2.99818800	-2.12323100
C	-0.68388000	-3.00279900	-2.01697600
C	-1.45920500	-2.13433000	-2.78000700

C	-0.81781700	-1.16077200	-3.59816100
C	-1.58149700	0.07923900	-3.53358900
C	-2.71022800	-0.11867300	-2.67955500
C	-3.08095600	0.90433300	-1.80832600
C	-2.42635800	2.18052000	-1.85028100
C	-2.49121000	2.79489700	-0.48785000
C	-2.98998700	1.70019500	0.39969100
C	-2.44755300	1.44926600	1.65868000
C	-2.41087900	0.11973600	2.18184900
C	-0.89446100	-2.35829500	2.04386000
C	-1.04129100	-3.28723400	-0.61825700
C	-2.75375100	-1.56578100	-2.29166800
C	-3.42695900	0.61257400	-0.40966000
C	-2.15679400	-2.69942300	-0.02272600
C	-2.06204200	-2.18884600	1.30446700
C	-2.82991800	-0.93582800	1.37247800
C	-3.40012600	-0.68893200	0.08630500
C	-3.13204300	-1.86869000	-0.79103400
C	1.95843000	0.32229400	-6.88839100
N	1.92616600	1.61859800	-6.56187000
C	0.86872200	2.43610000	-6.54586900
C	4.16118700	2.41100400	1.16636200
C	-3.98141500	-2.39857700	-1.93883000
C	-1.09532900	-0.89807800	4.33283300
C	2.63546000	-4.19032800	-0.55982300

C	-2.54131600	4.27437800	-0.12538900
C	4.38927600	3.83846300	1.60834800
C	5.47060100	1.64053300	1.31581000
C	-5.34541900	-1.80176500	-2.18839400
C	-3.91331400	-3.89475900	-2.21870600
C	-2.27785800	-1.60356300	4.95650000
C	-0.18205500	-0.40661500	5.45525900
C	2.65031500	-5.10782600	0.67706100
C	3.41673100	-4.84430900	-1.67312600
C	-2.70274700	5.30167800	-1.22090000
C	-3.25256600	4.65898900	1.16697100
O	-2.71000000	5.15288400	2.12802000
O	-4.56285900	4.37650400	1.07305000
O	-3.32482700	6.39953900	-0.74418400
O	-2.31925800	5.17638800	-2.36221400
C	-3.53044800	7.49036700	-1.67887800
C	-2.30792600	8.39182100	-1.74943600
C	-5.38535300	4.73097000	2.21434200
C	-5.82723700	6.18444000	2.14412300
O	4.01965200	-5.88719200	-1.50212600
O	3.37043500	-4.18175900	-2.83256200
C	4.07266200	-4.76840300	-3.96076200
C	5.53675300	-4.35955600	-3.96944900
O	1.70378800	-5.80173400	0.95512300
O	3.73122800	-5.10078100	1.47798700

C	4.99660000	-4.49568200	1.12996000
C	5.83071800	-4.45734800	2.39770500
O	-2.47017900	-1.59087500	6.15542000
O	-3.07231300	-2.20764000	4.06529400
C	-4.24499900	-2.89017300	4.58323200
C	-3.90672400	-4.30838100	5.01383100
O	-0.14109000	0.73144500	5.85874700
O	0.54960000	-1.42978300	5.92197600
C	1.39367800	-1.15422600	7.07036800
C	0.61171100	-1.30509700	8.36568100
O	5.41141400	4.17490700	2.17111100
O	3.36186100	4.65191400	1.34287400
C	3.47264700	6.02688000	1.79945100
C	4.20135800	6.88541600	0.77846700
O	5.71833100	0.84372500	2.18940700
O	6.31328900	1.98571700	0.32894200
C	7.63728200	1.40373900	0.40062500
C	8.43753500	1.95265000	-0.76466300
O	-3.43513200	-4.39660300	-3.20865200
O	-4.46822100	-4.57721400	-1.20269400
C	-4.49163100	-6.01887200	-1.35082900
C	-5.11137000	-6.59394200	-0.09206500
O	-5.68671000	-0.68169200	-1.88073000
O	-6.13019900	-2.68657300	-2.83571000
C	-7.47146700	-2.24646200	-3.17186900

C	-8.43027900	-2.46273200	-2.01164200
C	3.16009900	2.14615300	-5.93687300
H	1.06030600	-0.14468500	-7.26623900
H	2.90126500	-0.19887700	-6.85522700
H	1.00523200	3.46310700	-6.24988400
H	-0.07940000	2.07005700	-6.91289300
H	-4.39961900	8.01895100	-1.28094100
H	-3.77539800	7.06937800	-2.65665600
H	-2.04641600	8.77144700	-0.75651900
H	-2.51707100	9.24713300	-2.40218500
H	-1.45154600	7.84894000	-2.15917800
H	-4.82086100	4.52823400	3.12749200
H	-6.23467800	4.04695800	2.15167200
H	-6.35501000	6.38508700	1.20617000
H	-4.96538800	6.85353300	2.21601200
H	-6.50562900	6.40469400	2.97641000
H	3.53822400	-4.37946800	-4.82994300
H	3.95770100	-5.85342700	-3.91511500
H	6.02045400	-4.74107700	-4.87588800
H	6.05956100	-4.77364200	-3.10276800
H	5.63509300	-3.26935500	-3.95787800
H	4.84086200	-3.48594000	0.73952100
H	5.46578100	-5.10885500	0.35605300
H	5.96628400	-5.46544100	2.80105500
H	5.34832300	-3.83826700	3.16003000

H	6.81686900	-4.03274400	2.17995200
H	-4.94622600	-2.87677800	3.74600500
H	-4.65054700	-2.30384400	5.41078100
H	-3.45668100	-4.86839300	4.18795000
H	-4.82070300	-4.82649000	5.32634400
H	-3.21090500	-4.30070400	5.85735300
H	1.80924600	-0.14946400	6.96431100
H	2.19710300	-1.89031800	6.99244300
H	-0.19245800	-0.56629400	8.42019600
H	1.28141400	-1.15488900	9.22045200
H	0.17178100	-2.30444700	8.43929500
H	3.98206900	6.03090400	2.76548300
H	2.43580500	6.34316500	1.93061600
H	4.20038400	7.93058500	1.10853900
H	3.70786700	6.83162400	-0.19722700
H	5.23979900	6.56004500	0.67055700
H	7.54163500	0.31389600	0.36004300
H	8.07870500	1.66671800	1.36667300
H	8.51264100	3.04295300	-0.70594100
H	7.97074500	1.68849300	-1.71909200
H	9.45016800	1.53506100	-0.74814400
H	-3.46647000	-6.36910700	-1.50365900
H	-5.06785800	-6.26633000	-2.24814300
H	-5.14666600	-7.68642200	-0.16292900
H	-6.13226900	-6.22379500	0.04730400

H	-4.52132300	-6.32515700	0.78973800
H	-7.73955400	-2.85641500	-4.03739600
H	-7.42917000	-1.19510800	-3.46536700
H	-9.44797400	-2.19634000	-2.31927800
H	-8.15376800	-1.83524200	-1.15981200
H	-8.42924900	-3.51094600	-1.69577100
H	4.03106000	1.70154700	-6.41973700
H	3.10384000	1.84908900	-4.89057700
H	3.19112600	3.23065800	-6.03818700

Vibrational frequencies for TS (8a')

48.23i	9.71	12.81	14.10	15.08	15.33
25.42	28.74	28.81	29.83	30.64	31.22
32.01	32.54	33.01	33.28	34.05	35.08
36.14	37.29	39.83	42.68	43.45	45.48
48.16	50.45	55.45	60.82	66.88	67.77
70.25	72.84	80.41	83.42	85.70	88.87
89.74	92.23	94.25	98.16	104.16	105.06
107.35	108.54	111.65	112.42	113.02	115.80
118.14	120.53	124.31	128.33	131.73	133.30
143.88	146.27	148.69	149.39	156.35	160.54
175.16	177.02	179.41	185.37	192.30	198.22
202.96	207.12	213.89	217.08	219.93	222.87
232.37	233.74	238.71	244.87	250.62	260.25

261.67	262.43	267.45	268.99	270.60	276.30
280.71	292.19	293.76	302.53	305.00	305.83
316.30	319.07	320.04	325.92	334.73	335.27
336.70	341.51	342.12	345.04	346.97	352.83
355.55	358.90	361.46	376.76	381.15	383.33
386.16	394.03	394.43	399.66	401.82	403.31
420.26	425.59	428.60	432.11	435.06	440.41
447.09	450.65	452.08	453.23	454.16	456.63
457.76	463.18	470.20	472.54	475.47	476.81
486.55	492.52	495.21	496.38	499.87	520.92
523.60	525.63	530.13	534.83	537.71	541.07
548.60	550.41	551.28	554.85	556.18	559.13
560.62	564.51	567.39	569.37	576.43	578.10
579.34	582.67	583.61	589.44	596.56	623.85
632.39	637.95	639.31	645.36	647.94	652.60
657.96	664.45	666.99	672.64	679.01	680.46
685.23	691.81	695.84	704.14	706.44	707.16
709.42	710.94	718.83	723.15	728.77	729.69
731.40	734.73	735.40	736.74	739.24	741.45
743.36	743.59	748.51	749.41	751.71	752.38
753.46	755.90	757.74	758.44	762.17	763.86
765.00	767.27	778.67	780.17	781.97	786.73
787.25	788.73	792.77	795.18	797.99	802.99
808.10	813.40	817.98	818.60	819.04	819.93

823.88	824.40	826.59	829.19	830.93	832.40
835.01	835.55	837.45	840.72	842.17	845.50
846.91	849.31	859.32	869.14	871.59	872.88
874.86	878.50	882.96	885.50	891.68	893.56
894.62	895.76	906.83	918.71	921.80	925.86
928.73	935.71	938.81	950.81	954.16	957.37
975.52	979.51	987.00	1011.83	1015.46	1017.77
1020.14	1025.18	1027.00	1030.40	1039.06	1041.50
1050.76	1052.95	1055.01	1061.41	1062.01	1084.32
1087.12	1087.81	1093.15	1103.55	1104.40	1112.07
1118.09	1125.07	1126.65	1128.54	1129.01	1129.29
1129.60	1130.04	1130.66	1131.08	1132.75	1134.64
1141.64	1141.74	1142.57	1146.70	1147.28	1148.34
1150.35	1153.29	1167.99	1175.24	1182.49	1183.59
1186.00	1187.01	1191.71	1192.51	1194.86	1206.93
1207.29	1209.55	1209.76	1210.98	1211.21	1212.51
1216.98	1225.44	1231.13	1235.50	1239.99	1240.39
1244.65	1252.24	1253.67	1258.70	1264.73	1267.27
1269.86	1275.31	1277.65	1281.69	1285.36	1287.86
1288.82	1294.53	1305.74	1305.94	1310.47	1311.86
1312.36	1312.70	1317.17	1320.64	1324.32	1336.68
1339.99	1341.21	1341.91	1342.85	1343.10	1343.62
1343.86	1345.64	1346.67	1352.43	1354.00	1359.38
1367.21	1368.20	1369.39	1379.07	1385.56	1391.98

1395.21	1395.74	1396.69	1398.10	1402.09	1405.22
1407.78	1409.53	1411.22	1415.27	1416.41	1416.94
1417.65	1418.64	1418.96	1419.88	1420.29	1420.42
1421.89	1422.09	1422.36	1427.93	1441.12	1443.31
1443.48	1444.02	1444.13	1444.36	1444.62	1445.50
1445.53	1447.20	1447.99	1450.38	1451.69	1455.37
1468.84	1477.95	1487.77	1498.27	1513.91	1514.57
1514.65	1515.28	1515.42	1515.94	1516.00	1516.31
1516.66	1516.87	1518.10	1518.50	1518.87	1519.00
1519.08	1519.23	1519.98	1526.30	1526.61	1527.56
1530.06	1532.08	1534.56	1536.19	1536.21	1536.68
1536.97	1536.99	1542.51	1543.20	1544.40	1548.66
1559.64	1565.27	1570.92	1573.03	1575.50	1575.90
1579.05	1591.69	1597.25	1599.26	1600.49	1606.17
1610.39	1622.03	1622.47	1624.46	1628.17	1780.56
1792.81	1794.32	1813.17	1813.56	1825.50	1828.80
1830.00	1830.77	1836.66	3061.45	3062.00	3062.15
3062.22	3062.24	3062.32	3062.39	3062.43	3062.63
3064.45	3076.43	3078.26	3085.22	3097.65	3097.91
3098.40	3099.04	3099.66	3102.94	3102.97	3104.21
3117.04	3118.21	3128.33	3129.29	3129.55	3130.06
3130.24	3130.61	3131.00	3131.12	3133.08	3133.98
3135.52	3140.64	3140.74	3140.94	3141.66	3141.75
3141.77	3142.44	3144.26	3144.45	3152.97	3161.26

3161.81	3162.07	3162.15	3163.12	3165.32	3165.68
3190.89	3209.99	3220.58	3229.37	3341.81	3345.48

Coordinates for TS (8b')

Energy = -5327.68311587 Hartrees

C -1.86775200 -1.67463700 -2.97077800
C -1.90802200 -2.62482400 -1.91191600
C -2.82140300 -0.59115900 -2.70047400
C -2.96829100 -2.21635200 -0.94386200
C -3.37020000 -0.84365700 -1.38510600
C 0.48690400 -3.04839600 -2.21618900
C -0.73742700 -3.26363800 -1.51328700
C 0.53188400 -2.12687200 -3.25642400
C -0.66436800 -1.43583300 -3.64647100
C -3.22124300 0.03326300 0.93046500
C -3.54423200 0.19431500 -0.49102000
C -2.74735500 -1.17537600 1.43612600
C -2.63694300 -2.39215300 0.57750200
C -0.42423500 -3.43487400 -0.08615100
C -1.29055800 -2.96286200 0.89916600
C -2.46390900 0.74598800 -3.07177700
C -2.64765000 1.81366300 -2.09646200
C -1.16066700 0.97548700 -3.69619500
C -3.22169900 1.55293100 -0.86871100
C -0.30755100 -0.07240300 -4.01592900

C	-0.76256400	-2.28025900	2.03377900
C	-1.66296800	-1.16489200	2.36472600
C	-2.72043600	1.27329300	1.42959600
C	-2.85889600	2.31117200	0.36136400
C	-1.52018300	2.75282800	-2.21365600
C	-0.61882700	2.22298800	-3.20118200
C	1.12514300	0.07059300	-3.84714200
C	1.65705400	-1.18343900	-3.38053800
C	1.62577400	-3.23786000	-1.26996700
C	0.99027200	-3.33160800	0.08290100
C	1.49135600	-2.65479500	1.19548200
C	0.61298000	-2.17259500	2.21257600
C	1.23622100	-0.98099600	2.86386700
C	0.27879800	0.22067300	3.21403400
C	-1.16484100	0.03708400	2.86634000
C	-1.66912600	1.27058400	2.34712300
C	-0.54784900	2.21614000	2.22094700
C	-0.50227100	3.14646200	1.18524600
C	-1.63545800	3.34309500	0.23757400
C	-1.00268900	3.42521000	-1.10936900
C	0.41962200	3.53564700	-0.94007300
C	1.29343500	3.07196800	-1.91445600
C	0.76690200	2.37321600	-3.04235900
C	1.66003300	1.27628200	-3.37113400
C	2.75332600	1.27938400	-2.44737300

C	3.22036600	0.06171100	-1.96011100
C	2.70412000	-1.18002700	-2.46526700
C	2.83268000	-2.22115800	-1.39879000
C	3.20179100	-1.46030300	-0.16776900
C	2.60989600	-1.70971700	1.06786200
C	2.41348800	-0.65242600	2.00212800
C	0.64008100	1.55389900	2.64704700
C	0.72501600	3.36083100	0.48842400
C	2.63643600	2.50247000	-1.58920300
C	3.51960100	-0.11920400	-0.53261900
C	1.89187900	2.71793500	0.90057000
C	1.83341600	1.77249400	1.96596400
C	2.73373900	0.65476700	1.63829200
C	3.34445300	0.92358700	0.37561000
C	2.96188600	2.30154500	-0.05670000
C	-3.77044100	-3.19028200	-0.07254300
C	3.76454200	3.27267000	-0.91242600
C	1.06843500	-0.50509500	4.30035200
C	-3.03292200	3.79174000	0.58880600
C	3.02005400	-3.70678600	-1.66949800
C	-3.55343400	-4.68303700	-0.34951200
C	-5.20254000	-2.83061300	0.22704800
C	5.18457000	2.92886500	-1.29500100
C	3.55057000	4.75852500	-0.65028300
C	2.25336900	0.22012300	4.92505800

C	0.29764500	-1.35112700	5.28623500
C	-3.26935700	4.32810500	2.00677100
C	-3.76086300	4.62302800	-0.45981600
C	3.24270300	-4.12221100	-3.11824200
C	3.78920100	-4.55490700	-0.68309200
O	3.97240900	-4.28554400	0.48279600
O	4.21187000	-5.68836100	-1.27792500
O	4.46605800	-3.72301900	-3.51374200
O	2.45080500	-4.72495200	-3.80326200
C	4.86069700	-4.08464800	-4.86170000
C	4.38098100	-3.05381800	-5.87158900
C	4.94060600	-6.62899200	-0.44801400
C	6.41992300	-6.28182200	-0.38988100
O	-4.64909600	4.22664500	-1.18613900
O	-3.28596600	5.87624500	-0.44232200
C	-3.86141400	6.81869500	-1.38581900
C	-3.12840200	6.76685800	-2.71669400
O	-2.42659400	4.93323400	2.61977000
O	-4.49669700	4.15879100	2.54138100
C	-5.49965700	3.26732000	1.98850200
C	-6.79971800	3.57276400	2.71006700
O	2.30306000	1.40366500	5.16490000
O	3.23673000	-0.66427500	5.17319600
C	4.43455800	-0.14293800	5.80370200
C	5.40387200	0.41098600	4.77100600

O	-0.51657100	-2.20057600	5.00007700
O	0.61382700	-0.99427200	6.54711900
C	-0.06435400	-1.70021000	7.61740100
C	0.65181600	-2.99679000	7.96166300
O	-3.43988400	-5.11722300	-1.46898500
O	-3.49348600	-5.52863900	0.70068200
C	-3.68287800	-5.11468600	2.07117800
C	-3.64375400	-6.37431200	2.91829000
O	-5.60868600	-1.73723700	0.55385600
O	-5.99685800	-3.91369200	0.06456400
C	-7.41878700	-3.72255900	0.27513400
C	-8.09566300	-3.19819200	-0.98155400
O	2.98898500	5.52465100	-1.39818900
O	4.08994900	5.08525100	0.53694800
C	3.99979200	6.47890500	0.93313300
C	2.69374400	6.76004200	1.65920700
O	5.64592700	1.81080800	-1.34658400
O	5.86508900	4.04856200	-1.61321100
C	7.24559400	3.87785600	-2.02510300
C	8.17532400	3.80689500	-0.82374500
C	-4.80558800	-0.93946400	-4.30570400
N	-4.96111800	0.38767600	-4.41723700
C	-4.03823100	1.20564100	-4.95268300
C	-6.03032200	1.03704600	-3.63037600
H	4.46629900	-5.07860300	-5.08621500

H	5.95168700	-4.12703500	-4.81724600
H	3.28858800	-3.02930400	-5.90856900
H	4.75492400	-3.31203600	-6.86920500
H	4.74724400	-2.05552700	-5.61226900
H	4.76996300	-7.59381500	-0.93084800
H	4.49114100	-6.63482300	0.54762400
H	6.57147300	-5.31765200	0.10326800
H	6.84891200	-6.23653000	-1.39603400
H	6.95703400	-7.04861900	0.18019900
H	-3.74339400	7.78777300	-0.89630800
H	-4.92437000	6.59392700	-1.50078500
H	-2.05948700	6.95654800	-2.57972600
H	-3.53265500	7.53109200	-3.39042600
H	-3.25229000	5.78878400	-3.19041100
H	-5.18074900	2.23551100	2.16658700
H	-5.59964800	3.42170000	0.91198600
H	-6.68662700	3.43172200	3.78926700
H	-7.58732400	2.90098400	2.35157900
H	-7.11348300	4.60543800	2.52732100
H	4.85476800	-1.00433300	6.32836600
H	4.14354100	0.61985600	6.52994700
H	6.33169000	0.72218000	5.26506600
H	4.97419300	1.27987000	4.26534700
H	5.64818100	-0.34784000	4.02119900
H	-1.09820500	-1.88141400	7.31465300

H	-0.04687700	-0.99484400	8.45121700
H	1.69853300	-2.80620800	8.21928100
H	0.61626900	-3.69357500	7.11956200
H	0.16536500	-3.47077000	8.82200500
H	-4.64795800	-4.60853500	2.17244600
H	-2.88592300	-4.42460900	2.36166000
H	-2.68168900	-6.88321100	2.80593600
H	-4.43810700	-7.06652300	2.62244500
H	-3.77848700	-6.11534400	3.97412000
H	-7.55946200	-3.04278800	1.11899000
H	-7.78267300	-4.71718300	0.54175900
H	-7.90356300	-3.86143200	-1.83086200
H	-7.73363300	-2.19443000	-1.22257100
H	-9.17883900	-3.14357100	-0.82340700
H	4.10723500	7.10205600	0.04214200
H	4.86328800	6.62545100	1.58653200
H	2.68471300	7.79751100	2.01310600
H	2.57720000	6.09938000	2.52366700
H	1.83949300	6.61722000	0.99198700
H	7.44717100	4.75698800	-2.64121600
H	7.31659700	2.97739600	-2.63962700
H	8.06081100	4.69249900	-0.19055100
H	9.21597600	3.75800800	-1.16444300
H	7.96682000	2.91485500	-0.22677500
H	-5.58859000	-1.51279800	-3.83263400

H -4.10099600 -1.42786300 -4.96374200
H -3.33447200 0.78506400 -5.65695100
H -4.25679700 2.26381700 -4.97731200
H -6.62194600 0.27711900 -3.12145700
H -6.67053200 1.61128900 -4.30470200
H -5.58112500 1.70635900 -2.89292200

Vibrational frequencies for TS (8b')

136.31i	11.41	14.31	16.38	18.78	24.86
29.37	30.18	31.79	32.21	32.58	34.18
35.43	37.06	37.51	38.19	38.24	40.22
40.67	42.56	45.21	48.58	52.25	62.95
63.75	66.43	67.38	69.00	70.22	70.58
73.99	75.87	77.12	83.74	87.14	89.51
90.14	94.01	94.72	97.49	100.91	103.41
105.90	108.43	109.42	110.84	114.02	116.43
120.00	123.14	125.42	128.09	130.14	132.02
138.95	140.92	144.48	149.01	159.44	172.05
174.70	184.93	188.08	194.76	199.92	200.59
205.50	208.88	213.97	215.85	220.57	223.15
225.49	227.40	228.36	232.01	237.20	249.13
256.01	259.90	261.16	264.07	266.79	267.84
271.75	280.64	284.96	293.57	313.17	317.10
324.99	325.25	325.87	329.24	334.37	335.69

342.47	343.37	344.64	346.34	357.18	368.44
371.99	378.20	383.52	386.20	388.11	392.29
394.25	398.76	402.44	412.15	417.72	421.25
425.08	429.60	432.20	439.61	440.47	443.65
447.88	453.23	453.96	455.96	458.65	460.92
467.74	471.04	472.32	473.78	479.55	481.61
486.13	498.27	503.14	510.07	514.63	520.03
529.48	533.33	535.17	536.91	541.77	546.83
550.49	554.39	557.77	559.61	560.29	564.89
566.35	571.63	575.00	577.07	578.91	579.50
586.69	591.61	603.70	614.72	631.24	634.03
635.40	638.77	644.60	651.06	656.94	657.52
663.47	666.64	672.69	677.56	677.96	681.41
686.11	694.52	697.11	700.23	707.61	709.55
716.41	718.63	721.83	723.22	726.08	727.96
730.94	733.32	737.00	738.74	740.10	741.49
742.51	743.63	745.48	748.32	749.79	753.08
754.37	755.84	758.82	762.23	764.13	765.42
768.23	769.32	771.48	777.66	784.26	784.45
787.55	789.56	789.92	791.25	795.88	797.73
799.78	803.09	813.79	817.10	820.32	821.15
822.61	823.57	828.81	829.99	833.44	834.64
834.99	835.27	835.65	837.34	837.72	843.32
845.93	847.70	856.83	865.24	868.83	870.08

870.36	872.32	876.82	882.04	893.09	895.00
896.68	897.85	914.03	920.40	925.30	928.07
931.68	934.26	949.27	953.32	954.32	959.12
971.10	976.15	984.56	1011.87	1016.52	1025.09
1026.91	1028.85	1030.82	1033.46	1035.48	1043.06
1050.18	1053.80	1058.43	1061.60	1066.85	1080.96
1088.83	1093.06	1094.34	1099.30	1104.40	1110.06
1116.55	1123.32	1127.91	1128.80	1129.09	1129.31
1129.50	1129.71	1130.65	1130.80	1131.28	1134.61
1138.53	1140.61	1142.43	1144.58	1146.84	1148.50
1151.28	1151.61	1159.14	1178.67	1183.16	1183.95
1185.58	1187.20	1192.40	1195.21	1206.43	1206.87
1207.79	1209.04	1209.81	1211.63	1211.99	1213.31
1221.49	1222.34	1230.47	1232.07	1235.27	1238.69
1240.09	1243.50	1245.48	1254.50	1255.16	1257.04
1261.47	1264.13	1266.17	1268.15	1276.21	1278.29
1281.58	1288.53	1290.88	1292.03	1299.95	1311.49
1314.39	1318.00	1326.21	1332.85	1333.28	1337.14
1341.09	1341.79	1342.02	1342.14	1342.48	1342.54
1342.73	1343.18	1343.92	1350.68	1351.93	1363.10
1366.32	1368.07	1370.63	1375.61	1385.21	1390.79
1394.63	1397.54	1397.79	1402.04	1403.98	1407.40
1408.13	1410.10	1413.62	1417.12	1417.64	1418.37
1418.50	1419.68	1420.09	1420.70	1421.18	1421.65

1421.98	1422.10	1427.88	1433.30	1439.37	1441.15
1442.76	1443.08	1443.67	1443.94	1444.42	1445.23
1445.35	1445.47	1448.17	1449.86	1453.15	1467.65
1469.11	1477.49	1495.57	1513.04	1514.97	1515.16
1515.23	1515.45	1515.68	1515.82	1515.91	1516.01
1516.04	1516.11	1518.12	1518.22	1518.24	1518.79
1519.28	1519.39	1519.76	1520.56	1523.88	1527.48
1529.89	1533.20	1534.41	1534.45	1535.25	1535.86
1535.97	1536.20	1536.25	1537.78	1541.83	1552.45
1564.72	1565.34	1567.99	1571.71	1573.73	1576.01
1578.62	1587.33	1590.55	1597.42	1602.40	1605.01
1613.13	1623.33	1623.75	1626.06	1630.66	1794.23
1808.80	1812.00	1812.74	1814.13	1826.99	1828.27
1829.86	1837.14	1838.86	3061.57	3061.75	3061.98
3062.07	3062.18	3062.51	3062.90	3063.19	3063.76
3064.34	3076.09	3082.73	3086.65	3093.76	3094.38
3094.69	3097.69	3097.93	3098.67	3098.90	3099.20
3123.74	3129.14	3129.44	3129.57	3129.65	3130.62
3131.29	3132.20	3132.35	3133.55	3134.26	3136.14
3136.74	3139.60	3139.97	3140.38	3140.56	3140.81
3140.83	3141.31	3149.77	3155.34	3160.13	3160.38
3161.13	3161.31	3161.82	3161.86	3161.94	3162.46
3163.28	3193.61	3207.82	3220.19	3320.38	3330.42

Coordinates for TS (8c')

Energy = -5327.65127510 Hartrees

C	-0.73898300	-1.78944900	-3.30861700
C	-0.66464800	-2.78143000	-2.28628100
C	-1.95050800	-1.02764700	-3.12507900
C	-1.94699800	-2.77414400	-1.50751000
C	1.77543400	-2.45686600	-2.21997900
C	0.57399800	-3.06399200	-1.71964200
C	1.70976400	-1.51163700	-3.23527500
C	0.42743700	-1.17474700	-3.79882500
C	-3.10590200	-0.77964400	0.32711400
C	-2.37254200	-1.82058100	0.89090800
C	-1.77436300	-2.90258900	0.04802800
C	0.71744800	-3.21229100	-0.26639100
C	-0.38468000	-3.06013900	0.57097700
C	-1.95724100	0.33515900	-3.41834500
C	-2.65106600	1.26457000	-2.54395800
C	-0.75417000	0.97508000	-3.90014400
C	-3.28308900	0.76547500	-1.42105400
C	0.41376100	0.23664000	-4.09972600
C	-0.25802600	-2.32285400	1.78212100
C	-1.48913100	-1.54396900	1.97866300
C	-3.06455400	0.52079300	0.91580300
C	-3.34437100	1.53077500	-0.14453000
C	-1.84630400	2.49393700	-2.48265400

C	-0.69311000	2.30481400	-3.32502400
C	1.69782500	0.78781600	-3.71045300
C	2.50794800	-0.27387700	-3.17771100
C	2.76771500	-2.36358200	-1.10481800
C	1.99432700	-2.71126000	0.12510200
C	2.10256800	-1.98178200	1.30713500
C	0.98281100	-1.83400200	2.17941400
C	1.12086000	-0.54946200	2.92990400
C	-0.18491400	0.29474500	3.13670700
C	-1.44560600	-0.28132900	2.56920700
C	-2.20880700	0.77646700	1.98702900
C	-1.41307200	2.01463900	2.04319600
C	-1.49287400	2.97339700	1.03565600
C	-2.48258600	2.88394500	-0.07576000
C	-1.71487500	3.22863500	-1.30598100
C	-0.43058000	3.73696500	-0.91643300
C	0.67419200	3.60544000	-1.74989200
C	0.54661200	2.84163400	-2.94968200
C	1.76480500	2.06856500	-3.14555000
C	2.65508100	2.33769900	-2.05945900
C	3.39717600	1.29079900	-1.51602800
C	3.35658800	-0.01540700	-2.10850200
C	3.62758100	-1.03268300	-1.04989300
C	3.57268700	-0.27109500	0.23683300
C	2.90295900	-0.75072800	1.36213000

C	2.26402700	0.15232600	2.26514900
C	-0.15908700	1.70465700	2.64435400
C	-0.29716400	3.57648800	0.54077100
C	2.06207600	3.43087700	-1.22549100
C	3.52496000	1.12593600	-0.05851100
C	0.93375600	3.28178100	1.12644200
C	1.00012800	2.29913900	2.15971400
C	2.22679900	1.51141800	1.96627700
C	2.90837900	2.01553900	0.81892700
C	2.21223000	3.24878800	0.35035700
C	-2.48394200	-3.99273300	-0.74832000
C	2.83693300	4.41492500	-0.37982400
C	0.61764300	-0.22043000	4.33494800
C	-3.98303200	2.88261700	0.06212300
C	4.27629400	-2.38901400	-1.29794900
C	-1.76116100	-5.32475600	-0.99298200
C	-3.97205300	-4.16341300	-0.57783100
C	4.36589300	4.43304100	-0.51520400
C	2.24443000	5.81949100	-0.18887200
C	1.38427000	0.82963400	5.14807600
C	-0.02765000	-1.29687300	5.17329600
C	-4.55204700	3.28150400	1.43431900
C	-4.78605200	3.49367600	-1.08016300
C	4.78755300	-2.68032500	-2.70421800
C	5.15728900	-2.96248300	-0.21179000

O	4.85995000	-3.05054300	0.95868300
O	6.34675300	-3.33101400	-0.72573700
O	4.52539000	-3.96087600	-3.01860800
O	5.34229200	-1.88237100	-3.42248700
C	4.98615100	-4.41868800	-4.31594700
C	6.43945600	-4.86276700	-4.25897400
C	7.32041200	-3.87825000	0.20136400
C	7.11556200	-5.37228400	0.39576500
O	-5.49342600	2.87802900	-1.85385600
O	-4.62773300	4.81932200	-1.09047500
C	-5.34827600	5.55531700	-2.11475000
C	-5.00448900	7.02118400	-1.94032500
O	-4.01893700	4.10842200	2.12947600
O	-5.71598100	2.72667700	1.82909300
C	-6.34378900	1.60566600	1.15838000
C	-7.70069000	1.41354700	1.81159300
O	0.94415400	1.93253300	5.35798600
O	2.59519100	0.49271700	5.63923700
C	3.19902000	-0.80650900	5.45736500
C	4.49555400	-0.80144900	6.24760000
O	-0.56046200	-2.29906100	4.75034000
O	0.05237100	-0.97220000	6.48052500
C	-0.59508700	-1.86746000	7.42302500
C	-2.07014600	-1.53027100	7.57003300
O	-1.33151100	-5.63935200	-2.07430600

O	-1.63474600	-6.17875800	0.04599500
C	-2.06806800	-5.87957800	1.39098200
C	-1.95819200	-7.16917300	2.18467300
O	-4.72027700	-3.38303800	-0.02699500
O	-4.37144600	-5.32639700	-1.13313700
C	-5.77646600	-5.67736900	-1.02366000
C	-6.06974400	-6.38459200	0.28996700
O	1.69152800	6.40295500	-1.09355100
O	2.40916200	6.42793800	0.99303800
C	2.93899200	5.78876800	2.19088500
C	3.42085400	6.90071600	3.10375400
O	5.09055000	4.03099900	0.36744400
O	4.90808000	4.92809100	-1.63634500
C	4.18027000	5.46665500	-2.77336600
C	4.84052000	4.93762600	-4.03373400
H	4.84233200	-3.61396400	-5.04073300
H	4.31831400	-5.24878300	-4.55646400
H	6.57833800	-5.64175100	-3.50222500
H	7.09230000	-4.01835800	-4.02169500
H	6.73985900	-5.26929900	-5.23152900
H	7.24317400	-3.33623500	1.14650100
H	8.28236800	-3.65885000	-0.26700300
H	6.15275300	-5.57242200	0.87414900
H	7.90889100	-5.77318800	1.03701600
H	7.15000100	-5.89780100	-0.56400600

H	-6.41825600	5.35927700	-1.99274200
H	-5.04351500	5.16923900	-3.09214500
H	-5.71280500	0.72076200	1.28764100
H	-6.44258200	1.81424900	0.09091300
H	-8.21302600	0.55826600	1.35720800
H	-8.32546700	2.30264200	1.68082300
H	-7.59084600	1.22304500	2.88342200
H	3.39047600	-0.97683000	4.39397200
H	2.52315800	-1.58422900	5.82666500
H	4.30176100	-0.62571500	7.31020300
H	5.16502700	-0.01641700	5.88337700
H	5.00027500	-1.76744900	6.13788700
H	-0.04898200	-1.70798400	8.35521700
H	-0.44874600	-2.89569700	7.08385800
H	-3.10035200	-5.51486000	1.38905100
H	-1.42500000	-5.10147200	1.81197900
H	-2.60358300	-7.94446900	1.75975100
H	-2.25872400	-6.99252600	3.22306800
H	-0.92781700	-7.53709200	2.17893400
H	-5.94941300	-6.33153100	-1.88054300
H	-6.37524800	-4.77002200	-1.13105800
H	-7.11411900	-6.71635400	0.30396100
H	-5.91521800	-5.71164800	1.13847100
H	-5.42905600	-7.26422000	0.40828500
H	3.74970800	5.10694500	1.93168900

H	2.12434800	5.22140200	2.65054000
H	2.60779300	7.59557700	3.33505600
H	4.23752300	7.46111200	2.63785900
H	3.78673000	6.46915600	4.04161300
H	4.25773500	6.55623600	-2.70413800
H	3.12493700	5.20448200	-2.72382100
H	4.73877900	3.84998200	-4.09725500
H	5.90523900	5.18979900	-4.05104400
H	4.36291800	5.38333100	-4.91347500
H	-3.92881500	7.18508600	-2.05477900
H	-5.30516400	7.37817300	-0.95062400
H	-5.52860600	7.61434500	-2.69753500
H	-2.51902400	-2.16821200	8.34000700
H	-2.20173900	-0.48520900	7.86692000
H	-2.60163500	-1.70109900	6.62960500
C	-2.73680300	-1.58546500	-2.03302700
C	-3.30997200	-0.65134500	-1.12652700
C	-4.72513900	-2.32217200	-3.33100200
H	-4.85483500	-3.21288100	-2.73751900
H	-4.41364600	-2.42634100	-4.36056800
N	-5.47614900	-1.24147500	-3.01959000
C	-5.62540200	-0.19213200	-4.05251000
H	-6.51576400	-0.40357600	-4.65159500
H	-5.71704800	0.78094400	-3.56996900
H	-4.74270200	-0.19260000	-4.69176400

C -5.93888200 -0.97108500 -1.79824200
H -5.92276400 -1.74752300 -1.04871300
H -6.48055300 -0.04868600 -1.65400800

Vibrational frequencies for TS (8c')

129.64i	17.56	18.70	20.14	20.96	23.09
25.07	29.11	31.94	32.21	35.13	36.56
37.75	38.63	38.90	41.95	42.75	44.54
47.25	49.36	50.05	52.70	55.80	56.88
59.43	63.23	64.72	65.90	68.36	72.34
74.34	78.33	80.91	85.72	90.00	90.56
95.64	96.16	97.24	102.01	107.78	109.12
110.45	112.24	113.48	118.33	120.56	123.01
126.07	129.30	129.43	130.49	132.84	138.13
142.64	147.22	148.69	153.50	157.21	160.78
161.31	168.39	175.92	181.44	186.37	192.68
195.94	201.71	208.16	214.56	215.58	224.13
232.52	235.49	238.55	242.21	245.25	254.69
258.40	262.03	263.05	264.45	265.51	266.44
271.81	272.90	278.18	284.47	287.46	291.17
295.77	310.24	314.52	330.03	333.44	334.26
336.53	339.58	341.13	344.57	346.56	351.84
357.04	371.79	373.79	379.02	385.15	387.89
389.38	393.68	399.19	408.26	414.12	416.47

420.75	423.05	431.12	432.28	441.17	446.75
448.51	450.26	456.14	456.92	464.63	468.32
472.23	478.64	482.23	484.23	486.43	488.95
496.32	502.24	511.94	518.85	521.11	525.55
530.48	531.28	536.79	540.13	546.41	547.63
551.56	552.22	554.45	558.39	563.87	565.13
565.91	568.53	571.55	574.15	581.23	584.30
589.22	592.21	598.39	611.90	612.66	624.06
626.62	633.30	635.53	643.51	645.88	650.22
657.35	659.01	662.21	666.29	670.14	672.54
679.24	682.43	684.96	692.31	696.06	699.16
705.91	709.73	710.65	718.20	722.99	723.75
725.11	727.42	730.05	733.07	734.34	737.69
739.34	742.11	743.52	745.09	747.67	748.18
748.55	751.05	752.47	755.37	757.45	758.50
761.58	763.28	767.05	769.27	773.77	777.41
784.27	787.00	787.91	794.33	797.94	799.78
802.42	809.21	812.54	817.25	819.70	823.43
823.75	825.12	826.69	828.20	829.46	831.78
832.63	833.58	835.06	836.94	838.75	842.57
846.13	850.01	853.14	859.50	867.29	868.53
873.08	884.77	888.82	891.16	894.57	903.25
905.37	911.49	915.51	927.12	928.57	942.20
946.22	953.17	953.86	955.52	958.74	964.72

975.29	976.21	988.26	1011.03	1016.13	1025.52
1027.46	1032.83	1034.13	1037.26	1045.50	1045.77
1051.35	1053.39	1061.35	1062.88	1065.09	1081.84
1087.21	1098.84	1099.60	1101.04	1102.22	1108.03
1119.05	1122.48	1126.96	1127.97	1128.83	1129.74
1130.45	1134.94	1136.44	1139.73	1140.19	1141.52
1143.82	1144.76	1145.28	1146.29	1148.44	1150.20
1151.47	1157.82	1165.24	1169.87	1173.46	1181.19
1182.71	1184.26	1186.56	1187.86	1191.15	1191.40
1193.28	1197.56	1207.13	1208.23	1210.73	1212.07
1221.72	1223.89	1229.82	1231.29	1235.65	1239.01
1242.60	1245.95	1248.09	1252.41	1255.56	1258.43
1261.23	1265.06	1268.10	1273.09	1275.54	1281.62
1283.95	1287.09	1290.73	1296.04	1301.84	1307.91
1309.54	1312.74	1323.84	1325.31	1325.54	1330.87
1333.84	1335.99	1336.96	1339.90	1340.25	1341.46
1341.54	1342.38	1343.80	1347.80	1354.87	1359.91
1365.20	1369.12	1373.75	1375.87	1385.11	1389.97
1396.26	1397.47	1399.39	1401.46	1403.87	1405.60
1410.42	1411.25	1412.32	1418.14	1418.21	1418.90
1419.20	1420.15	1421.04	1421.35	1422.09	1422.22
1424.96	1427.14	1429.97	1433.30	1441.61	1441.98
1442.76	1444.42	1444.46	1444.97	1449.25	1449.45
1450.00	1451.74	1452.14	1453.16	1454.67	1469.55

1474.22	1479.84	1484.29	1512.49	1513.57	1513.82
1514.38	1514.66	1514.93	1515.14	1515.54	1516.29
1516.58	1517.05	1517.74	1519.16	1519.37	1520.06
1521.57	1525.23	1525.44	1525.80	1526.70	1529.06
1529.23	1530.46	1533.46	1535.84	1536.28	1536.47
1538.84	1541.22	1543.12	1543.44	1549.41	1551.50
1556.48	1559.33	1566.79	1571.83	1574.35	1576.02
1577.73	1591.09	1593.59	1597.62	1598.65	1605.69
1612.34	1618.18	1623.18	1625.27	1627.62	1786.00
1797.62	1806.52	1809.74	1812.65	1813.34	1828.80
1837.46	1839.08	1839.80	3061.16	3062.25	3062.47
3062.96	3062.99	3063.59	3063.84	3064.20	3064.78
3066.36	3073.07	3073.98	3077.87	3081.47	3085.65
3089.82	3090.44	3098.64	3098.88	3100.47	3100.51
3120.11	3120.31	3121.23	3127.55	3129.85	3131.98
3132.54	3133.12	3133.50	3133.51	3136.31	3136.60
3136.70	3137.19	3137.77	3138.32	3140.71	3141.30
3141.39	3142.32	3147.95	3149.44	3150.76	3154.63
3161.94	3162.64	3162.94	3162.97	3170.48	3170.84
3186.11	3198.99	3223.76	3231.75	3339.04	3351.20

Coordinates for TS (8d')

Energy = -5327.64823989 Hartrees

C -0.15952100 -1.97177500 -3.36222900

C 0.11752300 -2.91305300 -2.32396600

C	-1.52202000	-1.50309300	-3.21418900
C	-1.14506300	-3.17424500	-1.56371900
C	-2.11683500	-2.15295100	-2.06915800
C	2.41102800	-2.03983500	-2.19010500
C	1.36754100	-2.90768000	-1.71963500
C	2.15414800	-1.13351200	-3.21060900
C	0.84754300	-1.10324100	-3.81818400
C	-2.79292300	-1.51518800	0.21716800
C	-2.92849100	-1.40965500	-1.23439300
C	-1.85953200	-2.37024800	0.80614600
C	-1.01478800	-3.29300200	-0.00792100
C	1.49352000	-3.02291100	-0.25980000
C	0.36419100	-3.14069800	0.55229500
C	-1.83675600	-0.17314900	-3.49608600
C	-2.79466800	0.56667100	-2.69524600
C	-0.79747800	0.72136300	-3.94951200
C	-3.40018500	-0.07158300	-1.58213500
C	0.51294100	0.27003400	-4.11552000
C	0.28710900	-2.38959700	1.76092400
C	-1.09316800	-1.90716900	1.91748200
C	-3.07509100	-0.24318700	0.79152300
C	-3.57429100	0.68625700	-0.27932400
C	-2.25728800	1.93826900	-2.57929200
C	-1.06297500	2.02437300	-3.37832700
C	1.62448000	1.10299300	-3.69537600

C	2.64232700	0.25590400	-3.13608400
C	3.31916200	-1.72109500	-1.04638500
C	2.60925400	-2.23982300	0.16243400
C	2.51522600	-1.50583700	1.34281500
C	1.36849900	-1.62159200	2.18248200
C	1.18796400	-0.34124700	2.93136200
C	-0.27933500	0.18087400	3.10121900
C	-1.35744900	-0.66759200	2.49618000
C	-2.32577600	0.18913800	1.88792600
C	-1.83123700	1.57012500	1.96521700
C	-2.09607500	2.47045500	0.94180700
C	-3.02005400	2.14742200	-0.18157300
C	-2.33594900	2.68197900	-1.40459600
C	-1.21179600	3.47353000	-0.98240900
C	-0.07975200	3.60479900	-1.78061800
C	0.00799500	2.83456700	-2.97679600
C	1.37676100	2.36290600	-3.13524200
C	2.15061600	2.82920800	-2.02706800
C	3.09842100	1.98080600	-1.45902500
C	3.37844400	0.70131900	-2.04562800
C	3.84730100	-0.22708700	-0.97447800
C	3.58252100	0.49952100	0.30548400
C	3.01036300	-0.12323500	1.41444100
C	2.15779700	0.60780600	2.29557300
C	-0.56158500	1.55951700	2.60497400

C	-1.07273000	3.34246800	0.47718800
C	1.29647600	3.75455900	-1.21528700
C	3.22299600	1.84855900	0.00199900
C	0.17503500	3.34596100	1.10299900
C	0.43968400	2.40755300	2.14613800
C	1.81941900	1.92387700	1.99056100
C	2.39713600	2.57267700	0.85820300
C	1.44683200	3.61167200	0.36337400
C	-1.46813100	-4.49113200	-0.85180100
C	1.80031700	4.89203600	-0.35702900
C	0.58655400	-0.14287100	4.32237200
C	-4.51215200	1.86450200	0.03014600
C	4.79828100	-1.39764100	-1.19413100
C	-0.48038100	-5.64346400	-1.07583500
C	-2.91182200	-4.92137600	-0.83274000
C	3.28467400	5.26748000	-0.46111700
C	0.89225700	6.11841200	-0.18380800
C	1.07323300	1.05212000	5.15125600
C	0.18033300	-1.34064600	5.14600800
C	-5.03505000	2.02278000	1.46626900
C	-5.44057400	2.45784100	-0.99533600
C	5.40638500	-1.56013100	-2.58266700
C	5.75394900	-1.75208000	-0.07837300
O	5.45112400	-1.89599800	1.08531700
O	7.00933200	-1.85083000	-0.55643000

O	5.45022100	-2.86503700	-2.90342200
O	5.78916400	-0.65344000	-3.28397500
C	6.04099100	-3.19888100	-4.18573000
C	7.55352000	-3.31587700	-4.08071100
C	8.05382500	-2.15884900	0.40335300
C	8.17511300	-3.65837300	0.62414100
O	-5.24704400	2.51166600	-2.19175800
O	-6.52889800	2.98040100	-0.39741000
C	-7.45521400	3.70203700	-1.25147000
C	-8.52519000	4.29649200	-0.35694800
O	-4.68435500	2.92757300	2.18108100
O	-5.91633500	1.11234400	1.93449300
C	-6.49261200	0.07058000	1.12136400
C	-7.44705500	-0.70361500	2.01370900
O	0.38747600	2.02408500	5.34850700
O	2.31948200	1.00166500	5.66636300
C	3.20064300	-0.13367100	5.52206700
C	4.47457200	0.20289500	6.27665100
O	-0.11127400	-2.43264700	4.71069500
O	0.16451400	-1.01509000	6.45519900
C	-0.28441400	-2.03784200	7.38370200
C	-1.80004300	-2.04080400	7.50193100
O	-0.00083800	-5.86858900	-2.15971200
O	-0.15149500	-6.42734700	-0.02872600
C	-0.69712000	-6.26609400	1.29863100

C	-0.29199100	-7.49586600	2.09197700
O	-3.86944100	-4.19039400	-0.69315500
O	-3.00454300	-6.25545300	-1.02575100
C	-4.33848100	-6.82079800	-1.09911000
C	-4.88201400	-7.14984300	0.28241600
O	0.23215900	6.55476000	-1.09897700
O	0.89370700	6.75135400	0.99774400
C	1.53381100	6.24988600	2.20691100
C	1.68734900	7.43391200	3.14299700
O	4.07041500	5.03343100	0.42967700
O	3.71316800	5.88906300	-1.56964600
C	2.88309800	6.26695700	-2.70117400
C	3.77732600	6.25665900	-3.92704100
C	-4.83493600	0.31380000	-4.45515700
N	-5.22897400	-0.75398400	-3.75829000
C	-5.66381500	-0.71171200	-2.47900900
C	-5.00705200	-2.09249100	-4.34376300
H	5.74852500	-2.43785900	-4.91288900
H	5.57853200	-4.15221200	-4.45079000
H	7.83468300	-4.05633100	-3.32479800
H	7.99759300	-2.35264500	-3.81503600
H	7.96748700	-3.63307800	-5.04476100
H	7.83523100	-1.63226300	1.33506600
H	8.95673300	-1.74172200	-0.04782600
H	7.26707500	-4.05693300	1.08497700

H	9.01962700	-3.86571300	1.29131500
H	8.34903200	-4.17857900	-0.32327300
H	-7.86762500	3.00306200	-1.98639200
H	-6.89463500	4.46795900	-1.79485900
H	-5.70418200	-0.58145400	0.73490600
H	-7.02679600	0.52306800	0.27940000
H	-7.92225300	-1.50836200	1.44198400
H	-8.22779100	-0.04655200	2.40887800
H	-6.90959100	-1.14745200	2.85710900
H	3.41020100	-0.30810300	4.46290200
H	2.72316200	-1.02406600	5.94329800
H	4.26232600	0.38539600	7.33455200
H	4.94414500	1.09809600	5.85809900
H	5.18225600	-0.62965000	6.19919100
H	0.19382000	-1.76473200	8.32673400
H	0.09556700	-3.00518600	7.04665400
H	-1.78600300	-6.17969700	1.24737800
H	-0.28920700	-5.35665500	1.74913300
H	-0.70157400	-8.40365900	1.63803000
H	-0.66737500	-7.41576800	3.11802100
H	0.79760100	-7.58935500	2.12766900
H	-4.21041000	-7.71899200	-1.70694300
H	-4.98597800	-6.11448700	-1.62382000
H	-5.86117700	-7.63316200	0.18787100
H	-5.00517700	-6.24056600	0.87766300

H	-4.21312700	-7.83606600	0.81201900
H	2.49945100	5.80176500	1.96873200
H	0.87949800	5.48585500	2.63713600
H	0.71642100	7.89219800	3.35425200
H	2.34450700	8.19321900	2.70741400
H	2.12556100	7.09658700	4.08845600
H	2.48042600	7.26375100	-2.50007400
H	2.04374900	5.58074500	-2.80875800
H	4.15856500	5.24913000	-4.11984400
H	4.62871300	6.93109600	-3.79377000
H	3.20567300	6.58630900	-4.80156200
H	-4.46347300	0.16230700	-5.45781800
H	-5.08258400	1.29589300	-4.08471300
H	-6.10216300	0.21260700	-2.14179800
H	-5.95915200	-1.64836100	-2.02768400
H	-4.69259100	-2.77844000	-3.55700800
H	-4.22533200	-2.03459800	-5.10086400
H	-8.08365900	4.97587200	0.37816700
H	-9.07033700	3.51378000	0.17996300
H	-9.24058700	4.86016000	-0.96542500
H	-2.10830100	-2.76466100	8.26503800
H	-2.16866600	-1.05261100	7.79380500
H	-2.26200100	-2.32523000	6.55235700
H	-5.93767300	-2.44715800	-4.79606300

Vibrational frequencies for TS (8d')

126.74i	13.54	18.90	19.82	21.66	23.82
32.18	33.19	34.48	35.44	35.77	36.87
38.36	38.70	38.89	40.78	42.09	42.65
46.16	47.01	49.62	53.93	56.67	59.07
60.08	63.33	64.95	67.99	73.05	73.86
76.32	84.01	88.09	93.12	95.23	97.02
99.01	99.72	102.94	106.37	109.66	110.42
113.39	114.99	115.72	118.79	121.98	123.57
126.17	128.70	129.11	131.58	133.63	136.25
137.54	147.12	148.61	152.21	155.81	160.80
162.50	169.04	174.92	179.22	186.60	192.70
198.80	201.15	209.71	212.90	215.63	222.96
230.21	237.41	240.86	242.13	256.36	256.79
258.73	262.00	265.27	265.49	265.70	267.00
267.74	274.12	276.76	284.17	288.39	292.68
296.56	304.87	315.32	320.99	332.58	333.66
334.11	339.31	340.53	343.57	344.35	353.86
359.30	370.64	377.39	381.91	384.11	388.67
392.28	395.69	398.98	409.93	415.76	417.45
422.55	423.59	427.94	433.45	439.06	447.00
447.84	451.57	456.10	458.45	463.17	466.56
474.06	477.65	481.71	483.66	484.24	487.28
488.27	501.43	514.81	516.32	522.33	526.20

528.88	532.77	535.81	538.52	542.57	547.76
549.18	553.31	556.91	560.05	563.60	565.55
567.38	570.27	572.22	574.52	582.21	586.12
592.12	592.32	599.59	609.77	624.98	632.38
632.57	636.92	640.67	643.85	647.30	648.41
655.74	661.02	662.13	663.83	666.16	672.49
676.69	680.75	685.54	689.18	694.08	701.13
704.26	707.62	709.11	712.73	715.14	721.39
726.92	729.31	730.73	733.63	739.01	739.41
741.66	742.35	743.63	744.56	746.30	747.38
750.96	751.75	753.38	756.69	758.25	759.79
760.49	762.24	766.78	769.32	773.90	776.72
785.33	786.84	788.96	791.03	797.41	799.52
801.63	814.14	817.04	818.12	819.38	822.81
825.09	825.81	828.05	830.80	832.95	833.58
834.01	834.55	834.79	835.73	837.76	843.42
845.82	850.68	853.17	858.85	863.53	867.63
870.82	884.80	887.72	892.89	898.21	900.01
904.00	906.75	914.35	926.19	928.67	939.68
943.36	949.39	951.86	953.76	959.12	964.55
973.77	980.43	987.75	1011.61	1014.41	1023.25
1026.42	1028.84	1033.65	1036.30	1039.04	1043.88
1051.02	1054.28	1063.02	1064.53	1065.97	1082.28
1084.41	1099.90	1102.64	1103.02	1104.74	1107.93

1117.46	1124.17	1125.06	1128.59	1129.28	1129.80
1130.40	1131.30	1137.76	1138.91	1139.86	1140.97
1142.14	1145.50	1146.19	1146.92	1147.85	1148.76
1150.58	1158.01	1165.11	1170.69	1175.16	1182.07
1183.33	1183.91	1184.03	1185.92	1187.06	1189.73
1191.60	1196.63	1206.42	1208.45	1209.16	1211.77
1213.05	1221.78	1226.58	1230.69	1237.03	1238.87
1241.13	1244.57	1249.33	1253.01	1254.76	1258.41
1261.66	1262.76	1267.15	1271.62	1275.45	1278.07
1280.78	1285.45	1290.33	1293.03	1298.60	1306.95
1308.98	1311.07	1320.74	1323.97	1324.24	1329.93
1332.38	1333.04	1335.27	1336.15	1338.92	1341.39
1341.54	1342.60	1342.84	1349.28	1351.22	1358.02
1361.12	1364.16	1367.51	1374.02	1382.56	1383.68
1394.46	1396.55	1400.09	1401.61	1405.62	1406.55
1409.68	1410.77	1414.72	1415.47	1418.30	1418.75
1418.97	1419.11	1420.62	1420.81	1421.37	1421.56
1421.76	1423.88	1429.62	1433.16	1441.83	1442.27
1443.53	1443.65	1444.48	1445.55	1448.00	1448.61
1449.74	1451.00	1451.88	1452.59	1454.46	1469.65
1471.17	1478.11	1483.51	1510.01	1513.77	1513.82
1514.26	1514.81	1514.94	1515.11	1515.60	1516.23
1516.32	1516.69	1517.76	1518.48	1518.48	1519.10
1519.38	1523.86	1524.72	1527.64	1527.74	1527.98

1529.10	1529.72	1533.91	1535.64	1535.96	1536.10
1538.06	1542.00	1542.83	1543.14	1543.58	1550.02
1551.88	1556.18	1567.65	1572.27	1574.24	1575.17
1578.24	1590.39	1591.22	1596.21	1602.28	1605.42
1610.31	1621.55	1623.82	1624.82	1630.56	1799.95
1800.45	1807.66	1810.20	1811.79	1814.21	1828.37
1835.33	1837.94	1839.71	3061.26	3061.53	3062.21
3063.50	3063.56	3063.60	3063.68	3064.02	3065.07
3065.33	3070.53	3074.39	3077.52	3081.67	3084.96
3088.93	3097.38	3098.43	3098.94	3099.30	3100.03
3120.15	3121.39	3122.45	3125.18	3127.77	3128.58
3129.67	3133.18	3134.73	3135.14	3135.41	3136.34
3136.65	3136.88	3136.92	3139.69	3140.41	3140.82
3141.22	3141.47	3148.91	3149.59	3149.86	3150.10
3161.79	3161.99	3162.78	3162.81	3166.82	3168.01
3178.14	3195.08	3222.52	3231.83	3347.33	3355.12

Coordinates for product (8a)

Energy = -5327.76880753 Hartrees

C 2.00033900 2.41767500 -2.16971200
C 2.09182200 2.95926900 -0.85230600
C 2.84227500 1.20930800 -2.23179800
C 3.12113400 2.19455800 -0.08522600
C 3.44060300 1.01758800 -0.95037700
C -0.27401700 3.57308800 -0.97902400

C	0.94829800	3.47966400	-0.24986000
C	-0.34130200	3.03154500	-2.26265100
C	0.81373500	2.47919500	-2.88210300
C	3.25012200	-0.57120000	0.96217800
C	3.57496800	-0.27389900	-0.44234000
C	2.81077300	0.42925300	1.82432100
C	2.78521600	1.86828000	1.42992000
C	0.63422000	3.18235600	1.15537100
C	1.46879700	2.37446100	1.92969700
C	2.46132300	0.12542700	-3.00464300
C	2.61086700	-1.18914800	-2.47996700
C	1.33547700	0.16387700	-4.04108500
C	3.20741700	-1.40274900	-1.23807000
C	0.41226500	1.48259300	-3.97285100
C	0.88542100	1.37924100	2.77010900
C	1.72182400	0.16944400	2.70688300
C	2.67670600	-1.87521800	1.02041800
C	2.77117700	-2.51003900	-0.33035200
C	1.44892600	-1.98331300	-2.91157200
C	0.61477100	-1.13692300	-3.69224100
C	-1.03974700	1.22513000	-3.57091900
C	-1.50488300	2.24137500	-2.69360900
C	-1.41293000	3.48304300	-0.01444400
C	-0.78197100	3.08546100	1.27900700
C	-1.33724300	2.11637100	2.10964000

C	-0.49792200	1.27920600	2.89710600
C	-1.19151300	-0.02204600	3.13298200
C	-0.29005100	-1.32572800	3.06299800
C	1.15907300	-1.10421000	2.77585300
C	1.61556700	-2.12313300	1.88815000
C	0.45162500	-2.91321800	1.45840700
C	0.38367700	-3.43659900	0.17009400
C	1.53150400	-3.36375200	-0.78647100
C	0.90558500	-2.97051300	-2.08961100
C	-0.51220300	-3.05531100	-1.96321100
C	-1.33864000	-2.23446800	-2.72640900
C	-0.76258900	-1.24269200	-3.57073400
C	-1.61152200	-0.03744200	-3.51092000
C	-2.70624900	-0.30341400	-2.63293300
C	-3.14250200	0.69989400	-1.76716200
C	-2.57516100	2.00701900	-1.83298800
C	-2.65854200	2.63608400	-0.47997600
C	-3.07908300	1.52655300	0.42803800
C	-2.50333700	1.32593800	1.68124800
C	-2.37595700	0.00796500	2.21863600
C	-0.71070700	-2.37620300	2.08826600
C	-0.83754900	-3.35018300	-0.55877800
C	-2.65768600	-1.74294600	-2.23083800
C	-3.45831900	0.40358900	-0.36241900
C	-1.97820700	-2.82021100	0.04373000

C	-1.89692700	-2.28750100	1.36286100
C	-2.73928800	-1.08279300	1.42722000
C	-3.33991600	-0.88742800	0.14655100
C	-3.00888400	-2.05700500	-0.72178300
C	1.86979000	0.19974400	-5.50484300
N	1.86396100	1.61159900	-5.85066700
C	0.55835000	2.07469300	-5.40722600
C	4.01839700	2.67672100	1.04856900
C	-3.83003700	-2.64489700	-1.86030000
C	-0.96930900	-0.89860200	4.35773400
C	2.88860600	-4.02405900	-0.54574600
C	-2.79459400	4.11616600	-0.14165900
C	4.16851400	4.12350500	1.46298200
C	5.37714600	1.99249600	1.18047900
C	-5.22900700	-2.13388500	-2.11052900
C	-3.67533600	-4.13733600	-2.12647100
C	-2.10091900	-1.66277200	5.00699200
C	-0.07305300	-0.33769500	5.46166800
C	2.98021400	-4.92738100	0.69793000
C	3.68984300	-4.63422300	-1.66840400
C	-3.02518800	5.10729300	-1.25684100
C	-3.51354200	4.48297600	1.15090700
O	-2.99141600	5.02818200	2.09538100
O	-4.80576100	4.12118200	1.07834500
O	-3.70976200	6.17590300	-0.80146400

O	-2.64010200	4.97916400	-2.39784700
C	-3.98449400	7.23154300	-1.75875600
C	-2.81643800	8.19971700	-1.85992000
C	-5.63665600	4.45526900	2.21965500
C	-6.16264000	5.87857100	2.11814400
O	4.35907500	-5.63692000	-1.50472100
O	3.58464700	-3.98047200	-2.83024300
C	4.30938600	-4.52651600	-3.96471500
C	5.74170400	-4.01840000	-3.99718700
O	2.08071400	-5.67238800	0.99953300
O	4.07360900	-4.85167900	1.47761700
C	5.29066100	-4.16569100	1.10722900
C	6.15225200	-4.09272300	2.35495000
O	-2.28929400	-1.62865700	6.20598200
O	-2.85713100	-2.34196100	4.13728900
C	-3.98199300	-3.08322700	4.68020900
C	-3.55097100	-4.46065900	5.15767500
O	-0.08898300	0.80821200	5.84383300
O	0.71619100	-1.31160200	5.93946400
C	1.55666400	-0.96873300	7.07244500
C	0.79762200	-1.13298700	8.37961300
O	5.17325700	4.52538300	2.01376100
O	3.09749900	4.87483800	1.18768800
C	3.13791700	6.26354200	1.61375400
C	3.81278600	7.13646700	0.56825700

O	5.69264400	1.22239600	2.05625400
O	6.17554600	2.38191900	0.17416800
C	7.53733600	1.89195300	0.22381100
C	8.27468200	2.48249900	-0.96241600
O	-3.16019400	-4.62101200	-3.10683700
O	-4.20143300	-4.84025400	-1.10902700
C	-4.14479500	-6.28233000	-1.24464400
C	-4.75373600	-6.88002300	0.00880800
O	-5.64593500	-1.04411200	-1.78797300
O	-5.94757700	-3.05650200	-2.78133700
C	-7.31111100	-2.69863300	-3.12597800
C	-8.26612600	-2.99255300	-1.97978800
C	2.15330100	1.88632000	-7.24711200
H	1.19506600	-0.39107900	-6.15659300
H	2.87534000	-0.22556900	-5.58699000
H	0.50081400	3.16758700	-5.40917800
H	-0.25849800	1.68869700	-6.04927600
H	-4.87976300	7.71817000	-1.36531200
H	-4.21210700	6.77490500	-2.72464300
H	-2.57100200	8.61724100	-0.87822800
H	-3.07858500	9.02581300	-2.53088500
H	-1.93282200	7.69728000	-2.26324100
H	-5.05274800	4.30875800	3.13130300
H	-6.44522600	3.72181200	2.18296900
H	-6.70879700	6.02454900	1.18064400

H	-5.34018000	6.59758100	2.16459100
H	-6.84546300	6.08066000	2.95138700
H	3.73755500	-4.18252200	-4.82920500
H	4.26950900	-5.61639700	-3.90992000
H	6.23831500	-4.37374500	-4.90725900
H	6.30321200	-4.38844900	-3.13479900
H	5.76591800	-2.92396700	-3.99498500
H	5.06307700	-3.16233300	0.73608000
H	5.77776500	-4.73864700	0.31384700
H	6.36044900	-5.09577000	2.73951800
H	5.65154100	-3.51566400	3.13815400
H	7.10421300	-3.60413800	2.11996500
H	-4.68207400	-3.14452700	3.84426700
H	-4.42588800	-2.49752700	5.48826700
H	-3.06118800	-5.01560700	4.35130400
H	-4.42950000	-5.02850100	5.48509400
H	-2.86076900	-4.37920500	6.00184600
H	1.91783600	0.05383500	6.94112300
H	2.39653600	-1.66340700	7.00001700
H	-0.04331500	-0.43604000	8.42876900
H	1.46784800	-0.93016200	9.22302500
H	0.41155000	-2.15210300	8.47899100
H	3.65302100	6.31586700	2.57531700
H	2.08656100	6.52695800	1.74638900
H	3.75956200	8.18710400	0.87597300

H	3.31575500	7.03554200	-0.40183000
H	4.86600700	6.86349600	0.45822900
H	7.51560600	0.79777000	0.19455200
H	7.97856700	2.19407100	1.17847700
H	8.27722300	3.57586000	-0.91390700
H	7.80709000	2.17895600	-1.90456200
H	9.31332900	2.13412700	-0.96377200
H	-3.09978000	-6.57785400	-1.37749200
H	-4.69163500	-6.56749800	-2.14907600
H	-4.72972200	-7.97332400	-0.05351000
H	-5.79503400	-6.56379700	0.12858300
H	-4.19358000	-6.57362000	0.89778200
H	-7.53043100	-3.31213200	-4.00264200
H	-7.33336900	-1.64263700	-3.40466300
H	-9.29570900	-2.78995400	-2.29635400
H	-8.04144200	-2.35932300	-1.11704400
H	-8.19928700	-4.04245600	-1.67690200
H	1.42853900	1.41503300	-7.93976300
H	3.15393300	1.51665400	-7.49568900
H	2.13837700	2.96758900	-7.42046800

Vibrational frequencies for product (8a)

14.41	14.93	15.92	17.03	21.32	28.68
30.06	30.72	31.31	31.89	32.02	33.00

34.18	34.74	36.30	38.36	38.65	41.55
43.30	45.17	46.42	50.05	53.86	59.53
66.62	67.01	69.58	70.20	74.30	78.60
81.14	84.20	89.26	89.54	94.59	98.05
104.11	105.37	107.00	108.66	110.23	112.11
114.22	114.94	118.37	120.23	127.05	130.15
130.68	135.89	142.73	146.14	148.76	156.02
158.47	172.89	175.92	176.76	178.97	187.49
191.89	195.36	201.70	206.44	214.07	218.67
222.28	222.73	231.55	232.97	235.46	238.16
244.22	249.60	253.94	260.73	263.23	263.74
264.75	266.17	269.17	273.97	275.95	279.37
291.23	294.81	302.62	310.89	315.26	318.77
325.56	327.15	331.61	334.61	335.99	338.46
343.59	345.89	347.64	349.78	351.20	356.46
360.59	366.58	377.36	380.65	383.01	384.18
386.07	391.35	399.29	403.33	409.52	424.41
425.68	428.99	432.35	434.64	436.22	443.86
447.83	451.28	452.94	454.33	455.08	457.77
458.69	463.03	469.91	474.63	480.43	482.34
493.98	511.15	519.16	522.67	529.31	533.33
541.62	544.14	546.85	548.46	549.52	553.41
555.82	559.76	566.87	570.71	572.89	574.49
578.69	583.61	586.83	598.34	600.16	603.03

622.49	632.54	636.90	641.26	644.11	648.15
650.52	655.23	660.87	665.88	669.76	671.38
677.77	684.23	688.63	691.05	701.01	703.81
705.52	708.29	711.27	724.94	727.52	727.85
730.71	734.46	735.85	737.26	739.64	741.05
741.61	744.31	745.68	747.02	752.23	755.34
755.74	757.04	760.09	761.05	764.36	765.80
767.63	772.27	778.24	780.01	781.27	784.80
786.73	788.63	792.51	796.57	799.44	801.24
807.67	811.86	818.56	818.85	819.54	821.05
822.62	823.85	826.26	828.78	831.52	832.78
834.49	836.21	837.57	839.52	841.73	843.40
844.87	850.28	859.71	865.38	870.09	872.52
873.92	876.99	878.04	882.61	884.89	892.40
895.30	898.72	900.12	914.85	917.67	921.43
928.36	929.22	935.83	942.25	947.50	957.96
965.40	971.70	973.38	989.94	1009.28	1013.00
1015.45	1019.14	1021.72	1024.20	1029.04	1032.44
1033.70	1042.10	1043.78	1051.18	1053.02	1054.49
1060.24	1062.10	1068.27	1072.48	1081.78	1088.63
1093.00	1098.70	1105.26	1105.94	1113.41	1123.86
1125.59	1127.00	1128.75	1129.31	1129.69	1130.10
1130.67	1130.85	1131.19	1131.92	1136.57	1142.56
1142.66	1147.01	1148.44	1151.02	1159.10	1161.76

1170.87	1175.92	1177.91	1181.34	1183.82	1186.91
1191.73	1192.15	1204.16	1206.83	1207.66	1208.88
1209.21	1209.74	1211.64	1211.70	1213.78	1223.53
1225.18	1232.45	1235.52	1236.20	1242.09	1246.71
1251.47	1255.48	1260.15	1265.90	1266.45	1272.08
1273.48	1275.71	1276.59	1280.19	1281.68	1285.83
1290.40	1293.15	1306.51	1307.41	1309.15	1310.22
1312.44	1313.16	1315.28	1324.42	1326.45	1336.78
1337.87	1341.44	1342.34	1342.94	1343.25	1343.54
1343.83	1344.52	1346.44	1347.34	1354.11	1359.04
1359.81	1362.76	1364.23	1367.43	1383.31	1388.86
1391.67	1392.75	1394.29	1395.52	1396.83	1398.59
1399.73	1400.44	1410.22	1411.59	1412.13	1416.41
1416.85	1418.37	1419.50	1419.91	1420.05	1420.22
1420.44	1420.73	1420.95	1421.78	1422.29	1425.25
1443.00	1443.08	1443.27	1443.55	1444.11	1444.99
1445.07	1445.37	1446.14	1448.86	1449.59	1451.01
1451.31	1468.18	1479.54	1513.84	1514.63	1515.17
1515.22	1515.73	1515.78	1515.94	1516.10	1516.41
1516.61	1517.19	1517.68	1518.33	1518.51	1518.56
1519.03	1519.33	1519.72	1526.32	1526.35	1527.79
1529.82	1532.23	1534.92	1535.10	1536.01	1536.13
1536.53	1536.55	1536.76	1543.26	1543.92	1548.78
1551.57	1568.29	1570.50	1571.15	1576.63	1579.74

1581.96	1585.39	1589.97	1604.42	1606.52	1607.88
1623.78	1625.43	1625.90	1631.90	1634.47	1781.17
1793.73	1794.90	1811.32	1814.05	1825.36	1828.94
1830.35	1830.79	1835.78	2920.34	2927.42	2945.76
3061.66	3062.08	3062.29	3062.36	3062.50	3062.55
3062.57	3062.68	3062.86	3064.61	3076.31	3078.36
3081.45	3085.92	3094.56	3098.38	3098.68	3098.69
3099.04	3100.20	3102.10	3102.69	3102.76	3117.04
3118.17	3124.44	3128.70	3129.44	3129.85	3130.31
3130.64	3130.88	3130.90	3131.40	3133.00	3134.11
3135.59	3140.83	3141.08	3141.16	3141.58	3142.51
3142.57	3142.73	3144.43	3144.92	3153.10	3161.71
3162.04	3162.21	3163.02	3163.96	3164.59	3165.65

Coordinates for product (8b)

Energy = -5327.74694853 Hartrees

C -1.71343900 -2.03345400 -2.89060000
C -1.65555600 -2.88528000 -1.76811900
C -2.95040700 -1.13848900 -2.84698800
C -2.77266500 -2.55588400 -0.83186400
C -3.30934900 -1.26418700 -1.36830900
C 0.76368800 -3.10034900 -2.04709800
C -0.42773300 -3.38883900 -1.33062300
C 0.71336000 -2.23800500 -3.13947100
C -0.54328900 -1.70217100 -3.56554100

C	-3.21928100	-0.23178700	0.86974400
C	-3.53905700	-0.19927900	-0.56455300
C	-2.64490100	-1.35299500	1.46840200
C	-2.41143200	-2.60716100	0.69839600
C	-0.10300400	-3.45258400	0.10151100
C	-1.01636200	-3.01183300	1.05570300
C	-2.69249000	0.37618100	-3.34177500
C	-2.83677900	1.44211900	-2.25026100
C	-1.26349500	0.65210400	-3.80684100
C	-3.36942200	1.19290200	-1.02563700
C	-0.32026800	-0.32423900	-4.03208300
C	-0.56620600	-2.21202200	2.14471000
C	-1.57605400	-1.17395500	2.39962100
C	-2.84319900	1.07715500	1.28405200
C	-3.07628200	2.04326300	0.16739000
C	-1.79617600	2.45531000	-2.41013600
C	-0.84300600	1.95036400	-3.35722200
C	1.09151900	-0.03800200	-3.86876600
C	1.74072100	-1.20075800	-3.32686900
C	1.91684500	-3.12190600	-1.09942500
C	1.29331100	-3.19931400	0.26002400
C	1.71881900	-2.40657300	1.32644300
C	0.79152900	-1.95264700	2.31285600
C	1.28886600	-0.66611900	2.88548600
C	0.21076600	0.45524700	3.16015400

C	-1.20140900	0.10270300	2.81906300
C	-1.81741400	1.24018300	2.21484100
C	-0.80228000	2.28918400	2.03782300
C	-0.84652800	3.15537600	0.94802200
C	-1.99605500	3.18569200	-0.00763800
C	-1.36222800	3.25555500	-1.35575100
C	0.04193300	3.50999900	-1.19149000
C	0.96652600	3.07553300	-2.13409100
C	0.52107400	2.25654900	-3.21125200
C	1.51362400	1.23909200	-3.47483800
C	2.60139000	1.40808900	-2.55887500
C	3.17777100	0.27376000	-1.99630100
C	2.78269700	-1.04135500	-2.42139900
C	3.01347300	-1.99850500	-1.29502300
C	3.30306700	-1.13159000	-0.11491000
C	2.73619500	-1.36322500	1.13593000
C	2.42957600	-0.27387100	2.00229800
C	0.44077700	1.77904900	2.50838400
C	0.35632600	3.45321700	0.24364300
C	2.35880600	2.66412600	-1.77802900
C	3.48830800	0.21076700	-0.56282600
C	1.57825900	2.95189700	0.69391800
C	1.61030100	2.07364900	1.81485700
C	2.61936300	1.03374400	1.55761300
C	3.20755700	1.28546100	0.28022200

C	2.69083200	2.58918000	-0.23418800
C	-3.44891200	-3.56094200	0.08902500
C	3.39453100	3.58562400	-1.14682800
C	1.06403600	-0.11725800	4.28711300
C	-3.42924900	3.52019600	0.39307300
C	3.34960000	-3.47028900	-1.48305800
C	-3.06127100	-5.03353500	-0.14550300
C	-4.90813000	-3.49270500	0.47490600
C	4.84896600	3.36847600	-1.48851600
C	3.01633800	5.05413500	-0.98853700
C	2.16758200	0.76178700	4.86219500
C	0.37643200	-0.97334900	5.32601000
C	-3.60641500	4.01766900	1.84049200
C	-4.37260900	4.27975600	-0.50654000
C	3.60281800	-3.93979200	-2.91029100
C	4.20588200	-4.17574400	-0.45720600
O	4.32945800	-3.84239600	0.70003100
O	4.78755600	-5.26012700	-1.00523700
O	4.76075400	-3.42378700	-3.35760600
O	2.87831500	-4.66663900	-3.54742500
C	5.14700300	-3.81305800	-4.69839400
C	6.46230600	-3.12511900	-5.00882700
C	5.61942200	-6.06784600	-0.13196900
C	7.03530900	-5.51871100	-0.05491500
O	-5.24569400	4.99735000	-0.05412900

O	-4.15700100	4.08967300	-1.81117800
C	-5.04529300	4.77397200	-2.73455400
C	-6.32144800	3.97782300	-2.95787100
O	-2.83698800	4.80919200	2.32556900
O	-4.61696300	3.53071900	2.58491900
C	-5.73967300	2.79612500	2.05339700
C	-6.46282400	2.18117900	3.23866700
O	2.09590600	1.95690800	5.02664200
O	3.23277600	-0.00244900	5.16268400
C	4.36838900	0.67152200	5.76354700
C	5.29485300	1.24125600	4.70070600
O	-0.36630600	-1.90051500	5.09100300
O	0.67340000	-0.52936200	6.56215700
C	0.06512000	-1.23470400	7.67552800
C	0.87851800	-2.45952700	8.06319900
O	-3.07092500	-5.48820800	-1.26419700
O	-2.70717200	-5.80819800	0.88971000
C	-2.83738600	-5.44817900	2.28475900
C	-3.57806700	-6.56943200	2.99236200
O	-5.48057300	-4.43744500	0.98494000
O	-5.49996000	-2.32617900	0.20179900
C	-6.91012800	-2.23371900	0.53350400
C	-7.39912300	-0.88052100	0.05477400
O	2.44966800	5.71740100	-1.82531300
O	3.40766100	5.50118400	0.21463200

C	3.12111600	6.89430400	0.49725100
C	3.59233000	7.17566700	1.91062900
O	5.39728300	2.29072300	-1.55215500
O	5.45253500	4.54698300	-1.73834800
C	6.86051800	4.49869900	-2.08754900
C	7.73457000	4.46419200	-0.84362700
C	-4.09586900	-1.61364200	-3.78771800
N	-4.80699800	-0.39026100	-4.13157800
C	-3.74766000	0.54548900	-4.47741500
C	-5.80650900	-0.56073700	-5.17309500
H	4.35129500	-3.51576700	-5.38843600
H	5.22994900	-4.90396200	-4.73399200
H	6.35621900	-2.03720300	-4.95313000
H	6.78891300	-3.38994800	-6.02037300
H	7.24095700	-3.43223300	-4.30327700
H	5.59407400	-7.05960400	-0.58871200
H	5.15111300	-6.10825000	0.85410200
H	7.04278700	-4.53244300	0.41723500
H	7.47614000	-5.43727800	-1.05365400
H	7.65960900	-6.19186700	0.54379300
H	-4.45425500	4.85892100	-3.64895800
H	-5.25544600	5.77098000	-2.34172600
H	-6.09157600	2.95555000	-3.27576200
H	-6.92472200	4.45806500	-3.73666500
H	-6.91640500	3.93617000	-2.04124100

H	-5.39519800	2.01982400	1.36346100
H	-6.37774000	3.49587100	1.50818800
H	-5.81032700	1.48240100	3.77126100
H	-7.34959200	1.63788500	2.89305900
H	-6.78372400	2.95798100	3.93916400
H	4.86030900	-0.10816700	6.34994200
H	3.99798200	1.45178800	6.43273200
H	6.18109500	1.67535800	5.17801400
H	4.79164100	2.02638700	4.12986000
H	5.62218400	0.45806900	4.00985700
H	-0.95736100	-1.50295700	7.39994100
H	0.04410200	-0.49245100	8.47640100
H	1.91227100	-2.18322200	8.29403200
H	0.88060800	-3.19463200	7.25372800
H	0.43967900	-2.92716800	8.95204800
H	-3.37085500	-4.50487800	2.39495500
H	-1.82133300	-5.32434700	2.67132700
H	-3.06379100	-7.52479200	2.84906200
H	-4.59557000	-6.65284700	2.60079500
H	-3.62899000	-6.35944900	4.06699900
H	-7.02151300	-2.35943000	1.61489600
H	-7.43385800	-3.06071800	0.04550700
H	-7.22964600	-0.76176000	-1.01984900
H	-6.87992400	-0.06953200	0.57492100
H	-8.47257900	-0.78666900	0.25198500

H	2.04554200	7.05703500	0.38020700
H	3.63727300	7.51139900	-0.24519100
H	3.38927900	8.22127900	2.16630200
H	4.66841800	6.99923500	2.00818800
H	3.06974400	6.53718200	2.62950500
H	7.01889500	5.40974800	-2.66872800
H	7.03220000	3.62625800	-2.72204800
H	7.51920700	5.31802800	-0.19335600
H	8.79075300	4.50819600	-1.13311200
H	7.57038200	3.54034300	-0.28214300
H	-4.75755700	-2.33586500	-3.29949200
H	-3.65690000	-2.10424200	-4.67903400
H	-3.27844800	0.29941400	-5.45072300
H	-4.12773200	1.57067100	-4.53876600
H	-5.37867100	-0.93001400	-6.12537900
H	-6.30272800	0.39587200	-5.37001700
H	-6.56654200	-1.27577800	-4.84086800

Vibrational frequencies for product (8b)

13.54	14.19	15.43	17.18	19.88	27.27
29.43	30.13	31.52	32.97	34.23	36.13
36.50	37.99	40.57	41.19	42.31	46.87
48.12	52.66	54.72	59.12	60.30	63.67
65.88	68.93	74.09	75.41	76.58	80.76

83.42	85.22	87.55	89.52	93.14	94.49
100.04	103.02	105.06	106.19	109.45	109.94
112.15	115.20	118.27	123.76	124.96	132.02
134.80	141.02	143.78	148.81	150.77	158.80
159.97	170.42	173.22	180.56	182.94	184.04
191.34	193.35	200.02	208.41	211.07	216.61
217.94	223.85	227.47	228.50	234.38	234.40
239.72	244.33	249.96	257.40	258.89	259.53
261.86	265.97	269.00	271.41	273.99	280.53
291.59	294.47	302.19	303.18	313.75	315.47
322.41	323.77	325.43	329.61	335.23	336.00
342.86	343.83	344.51	356.13	358.20	359.95
367.24	375.01	380.61	383.09	385.89	389.10
391.23	396.05	398.19	399.31	404.55	408.99
415.27	423.75	426.29	428.12	430.51	440.35
442.64	449.11	451.79	453.76	454.80	456.14
461.88	466.62	471.00	473.33	476.18	488.47
491.69	505.70	518.54	525.94	529.80	531.49
538.77	543.09	547.70	552.21	552.41	558.09
560.79	564.24	565.81	569.20	572.84	576.00
577.17	580.52	584.50	593.07	597.90	603.42
617.54	626.94	631.30	636.68	641.47	642.32
649.51	654.10	661.76	662.49	667.75	671.35
674.33	680.66	684.39	689.43	695.13	698.54

704.56	708.80	709.70	713.04	718.72	726.63
727.78	730.75	732.82	736.69	738.24	739.59
740.85	742.68	743.89	746.23	748.41	750.69
751.64	753.75	758.14	759.27	760.96	763.41
767.91	769.40	772.07	781.43	784.81	787.18
788.19	790.08	793.56	795.73	800.67	808.57
810.29	815.24	816.09	818.12	818.79	819.97
823.04	823.59	824.61	825.63	826.90	829.42
830.26	832.83	834.98	836.82	836.90	841.58
846.31	848.08	858.55	864.02	869.05	872.19
873.06	874.73	879.61	882.17	890.91	895.45
898.11	903.79	906.90	912.81	919.93	925.97
932.25	933.86	938.60	942.46	949.84	955.65
960.29	972.65	975.07	982.70	993.71	1010.40
1015.89	1019.79	1023.75	1026.19	1032.55	1036.45
1039.97	1042.30	1048.71	1051.44	1053.60	1054.56
1056.29	1062.09	1064.28	1074.81	1082.02	1089.96
1091.34	1095.57	1106.32	1108.24	1112.27	1120.44
1123.86	1128.71	1129.43	1129.69	1129.98	1130.18
1132.97	1134.13	1138.01	1141.78	1143.04	1146.07
1147.09	1148.09	1148.88	1150.30	1153.58	1161.12
1168.02	1176.23	1179.40	1182.32	1185.66	1187.59
1190.71	1191.44	1191.66	1192.37	1192.57	1200.79
1207.29	1208.69	1209.48	1209.96	1211.76	1215.72

1220.46	1230.68	1234.74	1236.44	1239.58	1244.14
1248.23	1252.08	1256.98	1257.59	1263.52	1266.20
1269.41	1273.18	1276.46	1277.41	1284.46	1288.75
1289.74	1290.56	1293.05	1301.62	1306.55	1307.58
1308.05	1308.72	1309.94	1312.72	1315.18	1317.00
1319.68	1326.62	1334.82	1342.12	1342.28	1342.39
1342.56	1343.24	1343.76	1346.95	1351.52	1352.71
1359.18	1362.55	1365.01	1369.85	1376.19	1377.59
1383.57	1389.67	1393.22	1395.24	1397.36	1398.84
1404.22	1405.68	1408.71	1413.10	1413.79	1416.50
1416.97	1417.42	1417.87	1419.22	1419.52	1419.62
1420.18	1421.25	1422.10	1423.74	1428.08	1432.99
1443.81	1443.99	1444.59	1444.64	1445.00	1445.57
1446.67	1447.15	1448.87	1451.51	1452.15	1452.18
1469.91	1479.97	1501.77	1512.61	1513.83	1514.42
1514.89	1515.23	1515.30	1515.75	1515.90	1516.31
1516.87	1517.14	1518.12	1518.57	1518.61	1519.17
1520.00	1524.06	1524.38	1526.21	1526.71	1527.01
1529.42	1533.58	1534.13	1535.88	1536.27	1536.36
1537.91	1540.92	1543.39	1543.64	1544.24	1547.49
1549.23	1567.40	1569.18	1571.30	1575.96	1578.84
1584.15	1590.20	1598.18	1607.18	1610.29	1621.99
1623.91	1624.46	1626.98	1635.66	1679.69	1778.10
1781.38	1811.57	1812.53	1814.01	1826.77	1827.74

1828.83	1831.88	1837.17	2924.57	2933.11	2950.34
3061.66	3061.83	3062.15	3062.17	3062.47	3062.72
3062.75	3062.89	3063.16	3064.03	3077.12	3077.78
3080.20	3081.72	3082.89	3091.46	3091.48	3095.07
3099.59	3099.70	3099.88	3102.38	3102.57	3116.57
3118.44	3121.63	3122.97	3128.73	3129.55	3130.23
3130.30	3130.44	3130.53	3130.54	3133.56	3133.58
3134.04	3135.50	3140.33	3140.99	3141.68	3141.78
3141.87	3144.42	3146.10	3147.59	3149.82	3152.62
3160.77	3162.87	3162.93	3162.99	3163.98	3175.45

Coordinates for product (8c)

Energy = -5327.71720910 Hartrees

C -0.34680000 -1.96567800 -3.29527700
C -0.23285600 -2.90189200 -2.22932200
C -1.63337900 -1.34253500 -3.22425600
C -1.55762800 -3.03295500 -1.53530000
C 2.15981100 -2.31917500 -2.05891600
C 1.00007900 -3.02456500 -1.59296200
C 2.05819800 -1.43134200 -3.12138200
C 0.78091400 -1.25596500 -3.75935700
C -3.01235600 -1.04235500 0.12538000
C -2.19732100 -1.96867700 0.75977500
C -1.44513500 -3.03361500 0.01491300

C	1.07980500	-3.09686800	-0.13264100
C	-0.08236400	-3.01113700	0.62477500
C	-1.75591100	-0.01247100	-3.55535500
C	-2.59286900	0.88834000	-2.74623800
C	-0.61040900	0.73686300	-4.00596600
C	-3.29108700	0.40989900	-1.68887000
C	0.63824600	0.12627000	-4.12560300
C	-0.10333800	-2.21993200	1.80346700
C	-1.41414300	-1.56562400	1.88828800
C	-3.10557300	0.27470500	0.64753800
C	-3.45675000	1.22599800	-0.44655700
C	-1.92334900	2.19830700	-2.72180500
C	-0.71960900	2.08929400	-3.49237200
C	1.83510500	0.83071100	-3.70473200
C	2.72044600	-0.11505900	-3.08235200
C	3.07590000	-2.07754700	-0.90177800
C	2.27531400	-2.45158700	0.30221800
C	2.23738700	-1.66261900	1.44996500
C	1.05706700	-1.59423300	2.24927900
C	1.02268400	-0.27494400	2.94746300
C	-0.37324300	0.43768000	3.04544000
C	-1.52941500	-0.28676700	2.42704500
C	-2.35322800	0.66028500	1.75788400
C	-1.69873200	1.97565600	1.81119900
C	-1.82214100	2.87685300	0.75960700

C	-2.74461500	2.63345600	-0.39012300
C	-1.95004200	3.01111600	-1.59489300
C	-0.74497700	3.66799900	-1.16806500
C	0.41406900	3.60714400	-1.93510200
C	0.43446200	2.77917700	-3.09773600
C	1.73591800	2.13385600	-3.19922000
C	2.53134600	2.54346000	-2.08502300
C	3.34540500	1.60410300	-1.45361400
C	3.47542600	0.27743500	-1.98340800
C	3.79063900	-0.65933500	-0.86447500
C	3.58259500	0.14563700	0.37892700
C	2.90213200	-0.35313700	1.48881100
C	2.12344500	0.51566200	2.31299700
C	-0.45968000	1.82337900	2.49428900
C	-0.67279500	3.58433700	0.30012900
C	1.78202400	3.60274100	-1.33594100
C	3.40715900	1.51642300	0.01412000
C	0.54859600	3.44130000	0.96152300
C	0.65817000	2.51549700	2.04281500
C	1.96630300	1.85041900	1.94934600
C	2.65612900	2.37397400	0.81519500
C	1.86438800	3.50717700	0.25437200
C	-1.95726900	-4.26820700	-0.71954400
C	2.40436300	4.69798800	-0.50185000
C	0.40469200	0.05203600	4.30514800

C	-4.26353600	2.51404100	-0.25621200
C	4.58727800	-1.94844800	-1.01721100
C	-1.04617900	-5.49936500	-0.85220400
C	-3.40485900	-4.67272200	-0.53452600
C	3.92850500	4.87091800	-0.56378300
C	1.66098400	6.03971200	-0.41253600
C	1.01424100	1.20516400	5.11194300
C	-0.17930000	-1.05393700	5.15125500
C	-4.83219500	2.85359400	1.12962200
C	-5.09698600	3.04520100	-1.39928700
C	5.20554500	-2.23463000	-2.38169500
C	5.45797100	-2.38615200	0.13863600
O	5.11584200	-2.41343700	1.29998200
O	6.68763700	-2.71176200	-0.30205900
O	5.05926100	-3.53717000	-2.67731000
O	5.74433600	-1.41187700	-3.08396800
C	5.62850500	-3.98733100	-3.93410300
C	7.10034700	-4.33559400	-3.77748500
C	7.65410500	-3.12779700	0.69873600
C	7.52999300	-4.61272800	1.00065400
O	-4.90884100	2.82652900	-2.57487900
O	-6.08844300	3.82700000	-0.92751000
C	-6.92452800	4.47496700	-1.92145900
C	-7.91072000	5.35434900	-1.17814700
O	-4.38795100	3.75053100	1.80073600

O	-5.87096300	2.12942300	1.59895400
C	-6.48931700	1.05337700	0.86823300
C	-7.75704900	0.68216200	1.61787600
O	0.45801700	2.26675900	5.24388700
O	2.22126000	1.01082800	5.68267900
C	2.95018200	-0.23434500	5.61296200
C	4.22430800	-0.04031000	6.41573600
O	-0.58211400	-2.11976000	4.74041000
O	-0.21303400	-0.67429200	6.44463000
C	-0.82515400	-1.59528200	7.38715100
C	-2.33361800	-1.41174500	7.42902300
O	-0.51881000	-5.80024500	-1.89355900
O	-0.86914000	-6.28442300	0.23190500
C	-1.40522800	-5.99010900	1.54212500
C	-1.07832800	-7.18142400	2.42465500
O	-4.22577200	-4.07666800	0.13030500
O	-3.65296000	-5.82181900	-1.19069200
C	-5.00835500	-6.34647800	-1.12549600
C	-5.23030300	-7.17103200	0.13208200
O	1.09376100	6.51460100	-1.36986800
O	1.70900000	6.72055300	0.73994100
C	2.23595000	6.19835800	1.99444700
C	2.57710200	7.39788700	2.85875300
O	4.64317300	4.58204600	0.36975300
O	4.47409800	5.37271300	-1.68013200

C	3.74840700	5.79905300	-2.86545200
C	4.59280800	5.42562700	-4.06985900
H	5.47954100	-3.20619700	-4.68320100
H	5.03099300	-4.86294400	-4.19709800
H	7.23994500	-5.09284300	-2.99915800
H	7.68196600	-3.44740400	-3.51581500
H	7.48728600	-4.73610500	-4.72150600
H	7.50731700	-2.52180300	1.59557500
H	8.61907000	-2.88505200	0.24860700
H	6.56232600	-4.83572100	1.45859100
H	8.31915800	-4.91384200	1.69907400
H	7.63450100	-5.20603700	0.08661700
H	-7.42121400	3.70143900	-2.51591300
H	-6.27845500	5.04872300	-2.59225200
H	-5.79871400	0.20561800	0.82271400
H	-6.72488100	1.37664900	-0.15094500
H	-8.26090600	-0.14828700	1.11128500
H	-8.44287500	1.53365800	1.66224500
H	-7.52221000	0.37419400	2.64111200
H	3.17907200	-0.47174400	4.57013500
H	2.34247800	-1.03967800	6.03763600
H	3.99311700	0.20591500	7.45658400
H	4.82540200	0.77034900	5.99320300
H	4.81853000	-0.96033600	6.39641000
H	-0.36031900	-1.34079400	8.34194900

H	-0.55068100	-2.61473000	7.10594400
H	-2.48741800	-5.83616200	1.48610600
H	-0.94270700	-5.07697900	1.92694500
H	-1.54128200	-8.09353900	2.03528800
H	-1.45170500	-7.00420500	3.43899600
H	0.00347000	-7.33721300	2.47444300
H	-5.09106000	-6.95735600	-2.02649300
H	-5.70593500	-5.50822700	-1.18881400
H	-6.22656200	-7.62655400	0.09939100
H	-5.17225900	-6.54433600	1.02644300
H	-4.48951000	-7.97364400	0.20664200
H	3.11358600	5.57730300	1.81112800
H	1.45201400	5.58805900	2.45271800
H	1.69733300	8.02997400	3.01279000
H	3.36398300	8.00094500	2.39493900
H	2.93364600	7.05379300	3.83556600
H	3.61257500	6.88190700	-2.78562200
H	2.76154600	5.34061700	-2.90334600
H	4.70561900	4.33950400	-4.14206600
H	5.58811200	5.87544300	-4.00290400
H	4.10850200	5.78667400	-4.98391000
H	-7.38788400	6.10827200	-0.58204500
H	-8.53986600	4.76033000	-0.50770300
H	-8.55928700	5.86788500	-1.89609800
H	-2.76140100	-2.05892900	8.20325300

H	-2.59215900	-0.37465100	7.66391600
H	-2.78385300	-1.68110400	6.46946000
C	-2.56874400	-2.07750200	-2.27899800
C	-3.42918400	-1.08097500	-1.34800400
C	-3.68008500	-2.85044100	-3.10848600
H	-3.73029000	-3.88866700	-2.76929600
H	-3.42127200	-2.88345000	-4.16997300
N	-4.96246200	-2.18844200	-2.91470600
C	-5.37966100	-1.28842700	-3.99334700
H	-6.40535200	-0.95708200	-3.79968700
H	-4.75223200	-0.39374500	-4.11862400
H	-5.38683200	-1.84375400	-4.93652000
C	-4.91073800	-1.58347300	-1.59284900
H	-5.15264700	-2.32507900	-0.82903600
H	-5.62913400	-0.76290800	-1.51813700

Vibrational frequencies for product (8c)

14.59	15.90	17.00	25.64	28.00	31.44
32.13	32.89	34.16	34.62	34.95	36.67
38.40	40.36	41.63	42.61	45.20	49.91
50.64	52.11	57.82	58.55	60.96	63.34
67.16	69.59	70.17	73.32	75.44	76.93
81.82	87.22	93.94	95.33	97.73	99.23
101.36	102.81	107.16	110.32	112.87	115.72

119.72	121.23	122.92	124.27	127.82	130.27
131.09	132.37	136.81	144.85	147.69	150.99
153.45	159.14	160.43	164.24	176.38	181.01
183.55	189.87	193.58	195.32	201.26	207.44
212.52	215.06	220.45	228.13	232.08	234.57
236.03	238.28	246.82	250.83	256.33	260.50
262.07	264.94	266.47	266.77	269.78	271.31
276.66	281.37	283.71	289.79	298.81	307.56
312.78	325.60	329.83	331.93	333.80	335.63
339.22	342.56	343.41	355.38	361.97	366.87
374.55	375.60	383.14	383.72	388.57	392.69
396.89	402.36	410.99	414.34	415.28	421.43
424.59	428.18	435.11	438.17	440.01	446.94
449.80	451.71	452.70	456.02	462.12	466.55
470.99	475.29	481.23	485.37	488.03	490.93
508.53	512.69	519.24	522.07	530.81	534.51
537.87	544.17	549.32	551.83	553.99	560.45
560.83	565.41	567.21	569.56	571.18	576.58
580.13	583.61	586.78	589.25	595.27	612.63
619.30	620.77	624.04	632.47	636.22	639.65
642.87	647.26	651.50	654.93	659.41	661.32
666.98	671.97	677.65	680.12	685.27	689.56
697.37	699.39	703.22	710.09	713.06	715.35
716.00	723.27	726.37	729.83	731.10	732.12

736.36	738.92	742.09	743.97	745.10	748.03
748.43	749.17	751.34	753.34	755.64	757.30
761.58	762.32	764.62	768.75	770.04	776.01
782.42	787.15	787.59	789.52	791.91	798.17
801.10	809.33	811.67	815.57	816.91	817.88
819.53	822.96	826.70	830.30	831.29	831.93
833.39	835.48	835.56	836.03	837.59	842.73
844.72	849.80	853.88	857.95	859.33	861.43
866.96	870.08	880.65	884.28	890.75	897.20
902.30	904.24	914.53	917.65	921.69	929.22
935.68	939.87	944.05	950.52	955.08	959.44
960.79	966.31	970.71	978.75	988.12	995.43
1003.10	1014.09	1022.16	1025.60	1028.38	1033.13
1034.73	1039.00	1040.15	1046.26	1049.78	1052.32
1061.94	1062.97	1063.37	1065.73	1067.06	1076.89
1085.22	1093.88	1101.00	1102.42	1105.11	1107.36
1120.92	1122.93	1127.37	1128.17	1129.02	1129.49
1131.97	1136.15	1139.44	1140.55	1141.04	1144.23
1144.62	1146.39	1149.22	1149.52	1152.59	1154.94
1163.18	1166.11	1172.19	1177.44	1180.06	1181.42
1183.74	1183.74	1186.56	1189.29	1191.66	1191.88
1199.39	1206.93	1208.54	1209.14	1211.89	1219.38
1220.29	1227.34	1229.67	1233.71	1240.54	1243.25
1245.32	1247.72	1248.89	1252.23	1258.69	1259.86

1262.15	1266.10	1272.65	1273.09	1274.63	1279.55
1284.21	1289.34	1291.15	1298.33	1302.20	1306.86
1306.91	1311.01	1322.31	1326.67	1326.84	1329.42
1332.40	1335.99	1338.12	1341.14	1341.44	1341.68
1342.08	1342.38	1343.54	1350.01	1352.02	1356.34
1358.36	1364.82	1366.66	1373.08	1375.14	1379.21
1382.31	1384.51	1390.96	1398.10	1398.75	1404.96
1407.91	1409.17	1410.49	1414.69	1416.86	1418.46
1418.55	1419.48	1419.68	1420.36	1420.69	1422.50
1424.09	1424.77	1425.68	1426.52	1428.13	1441.25
1441.69	1442.55	1443.84	1444.18	1446.60	1447.63
1449.17	1449.96	1451.49	1452.08	1452.32	1455.25
1469.96	1483.98	1488.04	1513.24	1514.13	1514.28
1514.37	1514.89	1514.95	1515.03	1515.50	1515.95
1516.23	1518.01	1518.52	1519.51	1520.14	1521.14
1523.56	1525.43	1525.88	1527.05	1527.29	1528.52
1530.21	1531.43	1533.63	1535.54	1536.50	1536.67
1537.05	1538.66	1541.61	1542.90	1543.69	1544.56
1545.59	1550.49	1568.62	1572.81	1577.38	1581.01
1584.06	1592.52	1598.98	1602.52	1608.19	1618.11
1621.27	1624.84	1628.49	1630.78	1667.70	1798.56
1807.76	1810.70	1812.40	1813.78	1814.66	1828.47
1837.57	1838.33	1839.91	3023.98	3061.30	3062.47
3062.58	3063.48	3063.60	3064.32	3064.65	3064.72

3064.75	3064.98	3067.47	3074.09	3078.27	3078.64
3088.91	3091.72	3092.55	3094.16	3098.76	3098.93
3099.48	3100.81	3102.92	3114.58	3120.27	3122.26
3123.46	3124.43	3127.94	3130.24	3130.80	3131.15
3133.20	3134.72	3136.00	3136.17	3136.67	3136.82
3137.27	3138.13	3140.62	3140.76	3140.93	3141.32
3141.86	3148.40	3148.89	3149.63	3149.85	3150.19
3161.78	3163.00	3163.52	3164.99	3169.07	3184.41

Coordinates for product (8d)

Energy = -5327.71753475 Hartrees

C -0.10318100 -1.95619000 -3.36913400
C 0.14120900 -2.89701000 -2.32479700
C -1.46200600 -1.46960900 -3.26314400
C -1.13708800 -3.15213200 -1.59550200
C -2.09493000 -2.12560800 -2.11359500
C 2.44191300 -2.05366000 -2.14732200
C 1.38030800 -2.91018400 -1.69771600
C 2.22155200 -1.15003000 -3.17829400
C 0.92581500 -1.10651800 -3.80924000
C -2.79375000 -1.49142300 0.13869500
C -2.91856200 -1.40064800 -1.30554100
C -1.88407300 -2.35577800 0.75624800
C -1.03529100 -3.28875000 -0.03374100

C	1.47897300	-3.03353700	-0.23690600
C	0.33412100	-3.14766500	0.55317400
C	-1.76636700	-0.16602000	-3.58581400
C	-2.91649600	0.63237900	-2.96892700
C	-0.70346400	0.71283000	-3.97913800
C	-3.60703200	-0.09767800	-1.71321900
C	0.61186800	0.26112400	-4.12205500
C	0.23753600	-2.39332300	1.75908000
C	-1.14129900	-1.89886300	1.88186400
C	-3.07939800	-0.21943500	0.69768500
C	-3.59329200	0.70779300	-0.36315500
C	-2.18600000	1.94493000	-2.65410700
C	-0.97082500	2.01499900	-3.40537300
C	1.71930200	1.08759900	-3.67825000
C	2.71938500	0.23519500	-3.09618700
C	3.33011400	-1.74515400	-0.98678800
C	2.59139200	-2.25738900	0.20730600
C	2.47787700	-1.52090300	1.38462100
C	1.31351400	-1.62895300	2.20083100
C	1.12486600	-0.34567500	2.94353100
C	-0.34389000	0.18724300	3.08235600
C	-1.41050600	-0.65510200	2.45042700
C	-2.35620100	0.20431800	1.81698300
C	-1.85977200	1.58023200	1.90611200
C	-2.09386700	2.46641800	0.86558700

C	-3.00865000	2.14585800	-0.26866500
C	-2.28461600	2.66826000	-1.48110500
C	-1.16622100	3.46236300	-1.03336500
C	-0.01660000	3.59357000	-1.80221700
C	0.09634700	2.82277700	-2.99284400
C	1.46660600	2.34815800	-3.12473100
C	2.21674200	2.81268700	-2.00047100
C	3.14662500	1.95891200	-1.40934900
C	3.43228300	0.67755200	-1.98807900
C	3.86967000	-0.25250400	-0.90544500
C	3.57997400	0.47656600	0.36747900
C	2.97951700	-0.14115700	1.46413200
C	2.11242900	0.59649700	2.32597500
C	-0.60630100	1.56660000	2.57748600
C	-1.06010300	3.33593200	0.42637100
C	1.34788500	3.74247700	-1.20922200
C	3.23551600	1.82771700	0.05408300
C	0.17173700	3.34213100	1.08387500
C	0.40912900	2.40640000	2.13629700
C	1.78829600	1.91382200	2.01119900
C	2.39437300	2.55768200	0.89031700
C	1.46146900	3.60146500	0.37433700
C	-1.48610500	-4.46752100	-0.89487100
C	1.83635200	4.87784100	-0.34014600
C	0.49445800	-0.14102200	4.32039000

C	-4.49803800	1.91209100	-0.03749200
C	4.81347500	-1.43117600	-1.10425100
C	-0.50752900	-5.62873900	-1.10822100
C	-2.93693700	-4.88128000	-0.89982500
C	3.32565500	5.24571300	-0.40725200
C	0.93015500	6.10985300	-0.19114700
C	0.97032800	1.05307800	5.15753900
C	0.06256600	-1.33536500	5.13701800
C	-5.00042200	2.14736300	1.40057800
C	-5.44219400	2.54733800	-1.03791400
C	5.45033300	-1.59783500	-2.47987300
C	5.74293700	-1.79337500	0.03191700
O	5.41365200	-1.93334200	1.18883800
O	7.00626600	-1.90337700	-0.42005400
O	5.48493800	-2.90178800	-2.80362700
O	5.85978000	-0.69317600	-3.16851600
C	6.10155900	-3.23962900	-4.07333700
C	7.60956400	-3.37544400	-3.93337500
C	8.02909700	-2.21928700	0.56098400
C	8.13502600	-3.71970700	0.78286200
O	-5.12758400	3.04192300	-2.09690900
O	-6.70572900	2.54056100	-0.56756600
C	-7.69739300	3.22320800	-1.38304400
C	-9.01059300	3.18664300	-0.62682500
O	-4.73222300	3.17231600	1.97805600

O	-5.75191700	1.21702900	2.01933900
C	-6.30255800	0.04787600	1.37455600
C	-7.34511200	-0.52194600	2.32091000
O	0.28445100	2.02825400	5.33792900
O	2.20543500	0.99853400	5.69713600
C	3.08222700	-0.14354500	5.57982400
C	4.34821100	0.19644200	6.34607100
O	-0.23584300	-2.42273600	4.69485500
O	0.03235900	-1.01180900	6.44583300
C	-0.44088100	-2.03110900	7.36691500
C	-1.95780500	-2.01694900	7.46478700
O	0.03624400	-5.82705700	-2.16613500
O	-0.26173900	-6.45337700	-0.06884100
C	-0.86694400	-6.29993800	1.23330900
C	-0.47529800	-7.52149200	2.04562500
O	-3.87702300	-4.17094300	-0.61610800
O	-3.05041600	-6.16434800	-1.30229300
C	-4.39380400	-6.69892800	-1.43147200
C	-4.90617200	-7.24384400	-0.10766600
O	0.29659900	6.54687100	-1.12455300
O	0.90422400	6.74433700	0.98830800
C	1.50918700	6.24284400	2.21567600
C	1.65000600	7.42980200	3.14997200
O	4.08376600	5.01224200	0.50739600
O	3.78690400	5.86118100	-1.50431200

C	3.00224300	6.22452300	-2.67307100
C	3.84453500	5.92405400	-3.89939600
C	-4.12183500	0.79418800	-3.98507800
N	-5.08810500	-0.25397300	-3.69277500
C	-5.06869200	-0.41907300	-2.24991600
C	-4.95193600	-1.48043400	-4.47969700
H	5.83528000	-2.47297400	-4.80458700
H	5.63352300	-4.18638300	-4.35160800
H	7.86411200	-4.12198400	-3.17404600
H	8.05920200	-2.41863300	-3.65418000
H	8.04169300	-3.69445500	-4.88877500
H	7.79494900	-1.69153400	1.48820700
H	8.94370100	-1.80810700	0.12841200
H	7.21484200	-4.11233000	1.22433400
H	8.96388800	-3.93332100	1.46740700
H	8.32528600	-4.24050200	-0.16106000
H	-7.75732200	2.71379000	-2.34962200
H	-7.34864600	4.24428500	-1.56046400
H	-5.50259600	-0.67582700	1.19332700
H	-6.75377200	0.33475500	0.42230900
H	-7.78599800	-1.42608000	1.88655400
H	-8.14304400	0.20468900	2.50210200
H	-6.89239400	-0.78419100	3.28198900
H	3.30450600	-0.33405900	4.52605100
H	2.59346900	-1.02469200	6.00738300

H	4.12326300	0.39544300	7.39832100
H	4.82880000	1.08258800	5.92086000
H	5.05156600	-0.64144200	6.28992700
H	0.02787400	-1.76458200	8.31649800
H	-0.06726100	-3.00205000	7.03326300
H	-1.95479800	-6.23359900	1.13514200
H	-0.49694500	-5.38268200	1.70068600
H	-0.84414800	-8.43695200	1.57272600
H	-0.90128900	-7.45002100	3.05226700
H	0.61300600	-7.59247200	2.13328500
H	-4.29142800	-7.48731500	-2.18006300
H	-5.04424100	-5.91080600	-1.81749800
H	-5.89099400	-7.70190200	-0.25425700
H	-5.00867900	-6.44147900	0.62859100
H	-4.22963500	-8.00859400	0.28759900
H	2.47626200	5.78472100	2.00385000
H	0.83666100	5.48722500	2.63247600
H	0.67840200	7.89810500	3.33424500
H	2.32531900	8.18072800	2.72793400
H	2.06072000	7.09272900	4.10778500
H	2.78277300	7.29298500	-2.58481200
H	2.05419000	5.68983600	-2.68808200
H	4.04025500	4.85054300	-3.98189700
H	4.80287000	6.45028400	-3.85262700
H	3.31189200	6.25055400	-4.79951400

H	-3.78102300	0.73597000	-5.02190800
H	-4.57521800	1.77327900	-3.82389000
H	-5.77817800	0.27635400	-1.78970600
H	-5.37765500	-1.42947200	-1.96901500
H	-3.98899900	-2.00045100	-4.36860500
H	-5.08717900	-1.23609900	-5.53836500
H	-8.91602900	3.68306100	0.34375800
H	-9.34289100	2.15683800	-0.46031500
H	-9.78129700	3.70536400	-1.20701200
H	-2.28409500	-2.73802000	8.22297300
H	-2.31920000	-1.02502800	7.75299600
H	-2.41040600	-2.29561700	6.50900700
H	-5.75074300	-2.17386700	-4.19718100

Vibrational Frequencies for product (8d)

12.10	18.90	19.70	20.25	22.95	32.83
33.92	35.10	35.37	36.49	37.97	38.36
39.63	41.82	42.14	43.61	45.48	46.69
51.37	51.90	56.12	58.99	62.75	65.08
67.51	70.44	74.31	74.72	82.49	84.99
90.86	92.08	94.24	94.89	97.22	99.14
99.91	105.14	109.13	111.01	111.36	114.98
118.32	120.21	123.71	126.54	127.79	128.82
129.95	133.15	137.37	143.59	145.97	154.77

155.37	159.70	167.20	169.78	174.97	180.13
185.70	191.11	196.65	199.36	201.38	207.69
208.93	216.31	221.81	227.26	230.35	236.14
238.47	239.84	245.99	252.28	257.91	260.80
262.66	265.26	266.04	266.87	272.23	274.76
278.04	284.22	286.95	294.11	297.91	308.25
314.94	327.52	330.68	333.48	334.86	337.08
342.40	343.08	344.34	350.41	354.07	367.99
374.69	379.19	383.15	386.54	389.18	393.12
395.64	397.43	405.78	410.57	415.06	420.32
425.38	429.28	432.33	439.04	440.39	443.06
448.47	451.47	456.54	459.95	465.15	470.93
473.21	476.03	481.36	487.28	487.86	491.52
509.51	514.41	518.17	528.48	530.14	533.66
537.09	543.40	544.78	548.40	555.60	561.15
562.53	564.58	569.26	569.81	571.83	575.00
580.19	584.30	588.74	594.85	600.45	609.76
615.14	625.37	625.55	632.16	635.80	640.06
646.27	649.54	653.47	656.08	658.43	665.87
666.91	673.82	677.40	682.02	685.06	689.02
696.73	700.98	702.29	706.81	712.77	716.38
718.49	723.35	730.11	730.84	732.50	733.17
738.73	741.34	741.98	743.69	744.17	748.28
748.41	749.74	751.76	752.89	756.92	758.24

759.37	762.69	764.85	767.56	769.77	776.46
783.19	785.96	786.82	787.93	793.63	797.48
802.81	808.71	811.96	812.62	815.49	821.07
821.25	823.67	826.65	828.52	831.06	833.57
834.42	835.37	835.58	836.65	837.30	840.08
842.93	851.33	852.07	856.98	862.36	864.93
869.72	876.62	883.25	885.42	892.42	895.97
902.39	903.71	913.93	917.33	923.71	926.72
934.03	940.50	942.43	948.91	956.87	958.44
963.35	963.61	970.65	980.86	991.10	992.35
1001.04	1007.09	1024.06	1026.00	1028.65	1032.07
1034.07	1037.06	1039.22	1048.98	1049.19	1054.36
1060.32	1062.27	1064.59	1065.59	1069.32	1077.43
1084.50	1092.90	1100.92	1102.17	1107.07	1108.65
1118.75	1121.77	1128.51	1128.71	1129.40	1130.37
1131.80	1135.61	1139.18	1139.97	1141.42	1145.74
1146.53	1146.81	1146.97	1147.45	1149.98	1157.12
1164.84	1170.43	1171.72	1176.38	1181.17	1183.35
1183.61	1184.04	1186.23	1187.93	1192.07	1192.87
1200.35	1206.38	1208.96	1209.42	1211.82	1212.94
1222.06	1224.23	1233.14	1238.94	1239.56	1242.44
1245.22	1247.02	1249.55	1253.96	1260.97	1261.73
1265.17	1266.29	1273.30	1274.93	1277.10	1280.97
1283.48	1287.62	1294.09	1299.40	1300.20	1307.64

1310.06	1313.83	1321.86	1323.27	1325.30	1329.78
1335.18	1335.77	1335.93	1340.80	1341.24	1341.70
1342.24	1343.30	1343.57	1348.94	1352.24	1356.85
1362.11	1362.27	1366.01	1372.71	1375.64	1376.23
1382.67	1386.59	1390.38	1396.86	1400.49	1402.51
1407.14	1407.57	1410.85	1414.86	1415.27	1418.61
1418.81	1418.95	1420.40	1420.70	1421.83	1422.08
1422.96	1425.86	1426.96	1427.54	1430.01	1442.35
1442.65	1443.67	1444.60	1444.81	1447.15	1448.83
1449.68	1449.82	1451.49	1452.17	1454.50	1456.65
1468.71	1483.64	1484.66	1513.94	1514.23	1514.81
1514.87	1514.87	1515.49	1515.65	1516.00	1516.37
1516.66	1517.72	1518.45	1518.47	1519.26	1520.82
1524.28	1525.20	1526.53	1527.00	1527.75	1529.71
1530.09	1534.00	1535.40	1535.63	1535.73	1535.95
1538.43	1538.84	1540.31	1542.01	1542.51	1543.27
1546.00	1551.66	1562.27	1571.61	1572.59	1576.00
1581.04	1587.74	1598.37	1604.01	1605.55	1616.21
1618.70	1624.51	1627.51	1632.85	1648.86	1805.75
1807.09	1809.82	1810.42	1812.16	1814.55	1828.54
1830.18	1838.18	1838.40	3023.29	3061.31	3061.60
3062.48	3063.26	3063.29	3063.80	3063.89	3064.29
3064.32	3065.40	3070.78	3074.79	3076.62	3084.03
3084.27	3088.86	3092.04	3093.69	3099.08	3099.56

3100.54	3100.91	3102.74	3120.87	3121.69	3122.80
3124.16	3127.25	3128.20	3129.23	3130.09	3131.99
3133.50	3134.30	3134.77	3135.86	3136.35	3136.57
3137.22	3137.45	3139.01	3141.08	3141.48	3141.57
3141.69	3148.76	3149.08	3150.50	3154.43	3157.66
3162.32	3162.96	3163.18	3163.24	3167.09	3187.67

Coordinates for cyclopentadiene

Energy = -194.10105798 Hartrees

```

C      0.00007500 -1.21734300  0.00036100
H      0.00012200 -1.88229400 -0.87737200
H      0.00011000 -1.88154900  0.87868400
C      1.18117200 -0.28161400 -0.00035400
H      2.21409700 -0.61065600 -0.00056400
C      0.73492200  0.99130300  0.00011200
H      1.34729400  1.88739600  0.00022200
C     -1.18113800 -0.28175900 -0.00037700
H     -2.21402200 -0.61092700 -0.00060400
C     -0.73504400  0.99121300  0.00015000
H     -1.34752400  1.88723200  0.00028000

```

Vibrational frequencies for cyclopentadiene

349.72	521.38	688.21	711.04	813.01	813.65
--------	--------	--------	--------	--------	--------

930.88	931.47	949.85	956.26	979.11	1022.12
1124.63	1133.67	1140.45	1283.70	1331.85	1419.22
1447.76	1575.22	1662.11	3026.86	3050.45	3209.41
3219.96	3238.72	3244.74			

Coordinates for TS (13a')

Energy = -5348.56125701 Hartrees

```

C      2.93358900  1.00299900 -2.11528000
C      3.34896500  1.32698700 -0.78755900
C      2.94483700 -0.45319900 -2.26479700
C      3.78137500  0.06835600 -0.10393600
C      3.36263900 -1.03193600 -1.02952000
C      1.72124900  3.15925800 -0.77153100
C      2.70416100  2.35934400 -0.11020000
C      1.32853800  2.84326500 -2.06961400
C      1.95179800  1.75570200 -2.76310400
C      2.34137000 -2.34377600  0.82686500
C      2.74848500 -2.20023700 -0.58046400
C      2.56507300 -1.32434300  1.74748000
C      3.34891300 -0.09938900  1.40894600
C      2.30487700  2.21072500  1.29717000
C      2.55828900  1.02878500  1.99611400
C      1.97759900 -1.07806100 -3.05320800
C      1.37721600 -2.29570500 -2.59733100

```

C	1.00514600	-0.30644400	-3.85436300
C	1.78223600	-2.87406500	-1.39746800
C	0.99019500	1.14370400	-3.70420300
C	1.53527100	0.48511200	2.82875900
C	1.54105500	-0.97902300	2.67752400
C	1.13355100	-3.10056800	0.86901700
C	0.81925500	-3.59644700	-0.50670100
C	-0.03761000	-2.26898300	-2.99256000
C	-0.26846600	-1.03739000	-3.67930300
C	-0.29749400	1.80029900	-3.38937100
C	-0.08719000	2.86889700	-2.46614700
C	0.75771900	3.67796600	0.24760400
C	1.08612800	2.92542000	1.49598300
C	0.09875200	2.38045900	2.31278200
C	0.33961100	1.17184200	3.02273000
C	-0.96086600	0.47340400	3.25018400
C	-0.95492100	-1.09891200	3.08667200
C	0.35923700	-1.71555300	2.73022700
C	0.13896900	-2.75855700	1.78256700
C	-1.27769500	-2.72991800	1.38816600
C	-1.66157700	-3.04747700	0.08849000
C	-0.69759200	-3.57689900	-0.92645300
C	-1.02554200	-2.82276900	-2.18016500
C	-2.24537100	-2.10562500	-1.98005200
C	-2.49192100	-0.91993800	-2.66839600

C	-1.47909900	-0.36876800	-3.50339600
C	-1.49745500	1.09016000	-3.35495400
C	-2.52757300	1.44060100	-2.43028900
C	-2.29183900	2.45902400	-1.50635200
C	-1.08153900	3.21359000	-1.55629000
C	-0.76113300	3.70992200	-0.18487400
C	-1.71504200	2.98625000	0.71323700
C	-1.31762800	2.41233200	1.92074100
C	-1.94255100	1.22134000	2.40195400
C	-1.91891400	-1.67244100	2.09957000
C	-2.63934900	-2.24667500	-0.56910400
C	-3.28973500	0.20003600	-2.08141300
C	-2.67869000	2.31269200	-0.09583100
C	-3.26695900	-1.20463800	0.11334700
C	-2.86597100	-0.88942100	1.44386000
C	-2.87886000	0.57382300	1.59591800
C	-3.29728200	1.15019600	0.35904400
C	-3.70776900	0.05028800	-0.56697300
C	1.65798100	-0.51142900	-5.93944100
C	1.63496700	1.78572600	-5.70212700
C	4.81736200	-0.10785300	1.00164100
C	-4.75481200	0.09345500	-1.67226300
C	-1.24361900	-0.44410100	4.43264200
C	0.05556800	-4.89855100	-0.78118100
C	0.00273900	4.99408200	0.11943300

C	5.76974800	0.97463000	1.45467200
C	5.55056200	-1.44639500	1.04495000
C	-5.62752800	1.31651200	-1.82173300
C	-5.47634900	-1.20905700	-1.99507200
C	-2.59286600	-0.47427400	5.11377900
C	-0.16118500	-0.55919000	5.50515200
C	-0.34784800	-5.76817100	0.42389100
C	0.35124200	-5.79014100	-1.96099100
C	0.38386400	5.89215300	-1.04920200
C	-0.37467800	5.76337600	1.36449900
O	-0.47270500	5.29460200	2.47567500
O	-0.63068800	7.05006800	1.05426100
O	1.59654100	6.43274900	-0.82018900
O	-0.29380400	6.09724100	-2.02859300
C	2.08820900	7.36334900	-1.81730700
C	2.79169200	6.63673800	-2.95338000
C	-1.03818900	7.91499900	2.14667600
C	0.16617700	8.46927200	2.89118100
O	0.35318000	-7.00264500	-1.86102200
O	0.59884300	-5.12815900	-3.09606800
C	0.87328300	-5.92344600	-4.27955200
C	2.34523500	-6.29473800	-4.36172600
O	-1.50317200	-5.89855200	0.74483600
O	0.61754400	-6.35935400	1.15083200
C	1.99640900	-6.47368800	0.73575500

C	2.80533200	-6.81958100	1.97300500
O	-2.69974900	-0.41101800	6.32167400
O	-3.62165900	-0.55535200	4.26259200
C	-4.95477900	-0.56120000	4.83903100
C	-5.36824500	-1.96569700	5.24830000
O	0.49664000	0.36375300	5.92335000
O	-0.06554500	-1.83514400	5.90998300
C	0.83825400	-2.10078700	7.01408000
C	0.14615500	-1.86890400	8.34809700
O	6.85081000	0.71024100	1.94048300
O	5.29172000	2.21293100	1.28950700
C	6.11795700	3.30820200	1.76551100
C	7.11994100	3.73909300	0.70660500
O	5.40627200	-2.29558000	1.89193200
O	6.38990400	-1.53718200	0.00071900
C	7.22635100	-2.71866600	-0.03228100
C	8.11316600	-2.61274900	-1.25781000
O	-5.36168200	-1.83246300	-3.02419900
O	-6.26618200	-1.56295000	-0.96709600
C	-7.03163700	-2.77973200	-1.15122800
C	-7.81781900	-3.01866200	0.12312800
O	-5.33403000	2.43497100	-1.46379900
O	-6.77860300	0.99393400	-2.44571500
C	-7.71235900	2.07710200	-2.69278200
C	-8.59860600	2.33102600	-1.48349100

H	1.97724100	-1.54675500	-5.99157200
H	1.93226300	2.81595900	-5.53913100
H	2.77702500	8.00689700	-1.26469800
H	1.24909700	7.95934500	-2.18419800
H	3.60152900	6.00757500	-2.57051000
H	3.21977400	7.36652600	-3.65038700
H	2.08604900	6.00746900	-3.50235200
H	-1.69402100	7.34882600	2.81190800
H	-1.61035300	8.70570000	1.65629600
H	0.83992000	8.99389100	2.20599800
H	0.71800800	7.66536300	3.38595600
H	-0.16801700	9.17869400	3.65689600
H	0.57239700	-5.27472900	-5.10498200
H	0.23513000	-6.80938700	-4.25937200
H	2.54245800	-6.81617000	-5.30533200
H	2.62264000	-6.95976000	-3.53908000
H	2.97412700	-5.39947200	-4.32314000
H	2.34409800	-5.53412500	0.29736000
H	2.05581400	-7.26047000	-0.02115200
H	2.43813900	-7.74474800	2.42751800
H	2.74158500	-6.01696600	2.71381400
H	3.85780700	-6.95772300	1.70191600
H	-5.58693300	-0.16902900	4.03953700
H	-4.96899400	0.12600500	5.68788600
H	-5.30135600	-2.65357700	4.39947700

H	-6.40473400	-1.95527000	5.60478500
H	-4.73106300	-2.33631900	6.05591500
H	1.72135300	-1.46745500	6.90261500
H	1.12168500	-3.14714500	6.87976600
H	-0.13755400	-0.81889900	8.45867700
H	0.82484800	-2.13470900	9.16691800
H	-0.75556400	-2.48349900	8.42937500
H	6.61561300	2.99336900	2.68529000
H	5.39944300	4.09929800	1.99012700
H	7.67352800	4.61712500	1.05872900
H	6.61028300	4.00353400	-0.22549000
H	7.83756300	2.93903200	0.50449400
H	6.58070300	-3.60216600	-0.06403500
H	7.80491200	-2.75879300	0.89563900
H	8.74425800	-1.72002600	-1.20615600
H	7.51283700	-2.55989100	-2.17179700
H	8.76323000	-3.49218900	-1.32167800
H	-6.33711400	-3.59712200	-1.36721600
H	-7.68165200	-2.65253000	-2.02284600
H	-8.41139800	-3.93402800	0.02526600
H	-8.49866600	-2.18574100	0.32648500
H	-7.14564500	-3.13426900	0.97912500
H	-8.29114300	1.73401500	-3.55326200
H	-7.14489600	2.96937700	-2.96703900
H	-9.34427100	3.09642300	-1.72735300

H	-8.00517200	2.68752700	-0.63708700
H	-9.12602500	1.41813200	-1.18851400
C	2.61803700	0.64106300	-5.76375300
H	3.31478000	0.56251600	-4.92749200
H	3.21274300	0.74249900	-6.68693800
C	0.52821600	0.00296400	-6.59960200
H	-0.27422700	-0.59096800	-7.02316700
C	0.51411700	1.39501200	-6.45516900
H	-0.30021900	2.04794000	-6.74921500

Vibrational frequencies for TS (13a')

430.33i	11.62	14.72	18.27	20.00	23.73
27.46	28.42	31.31	31.68	32.62	33.30
34.17	35.01	36.26	37.15	38.45	39.26
40.69	44.59	46.52	54.20	55.49	58.93
61.45	63.30	67.22	69.62	71.22	75.96
76.45	80.10	85.21	85.41	86.82	88.67
90.52	94.81	97.27	101.94	105.52	107.47
108.45	110.99	112.26	113.55	116.88	119.43
122.85	126.61	128.72	132.64	136.83	143.84
146.26	153.76	157.68	160.29	174.33	178.12
179.98	184.70	189.09	196.05	198.66	209.86
214.60	217.36	219.21	220.90	224.45	228.51
233.26	241.21	243.75	250.14	258.00	259.79

264.34	265.72	268.46	270.58	273.63	278.38
285.29	295.63	298.70	303.61	315.37	317.09
319.97	324.60	326.82	332.40	335.11	337.21
342.68	344.50	346.87	349.17	353.35	356.51
360.53	367.25	381.13	385.34	386.48	388.44
392.20	398.38	403.20	410.92	422.15	424.87
426.97	428.52	433.54	434.89	444.56	446.74
450.79	452.14	453.29	455.91	456.76	460.22
463.73	471.90	474.16	475.13	484.48	494.51
495.97	515.33	522.63	523.68	528.30	536.27
544.84	546.25	549.05	550.45	551.17	555.07
556.95	560.87	568.30	570.22	571.46	573.99
577.45	580.66	584.15	584.36	592.96	600.72
623.80	632.23	637.31	639.91	642.40	647.08
653.20	660.47	662.28	666.87	673.61	677.03
681.03	683.09	690.45	694.41	699.07	701.76
705.84	708.73	710.20	719.20	727.67	730.37
733.41	735.04	735.85	736.67	739.60	740.36
741.60	742.36	747.55	748.19	751.66	753.12
754.84	757.68	759.23	760.78	763.95	765.63
766.62	770.24	777.23	780.86	781.52	782.14
786.83	788.60	789.37	792.82	795.45	798.87
801.07	807.93	812.11	813.41	817.05	817.80
819.37	819.55	822.62	823.52	824.38	826.84

828.32	830.77	832.32	833.84	835.63	837.65
840.16	841.18	845.22	847.30	849.31	860.11
868.77	869.13	870.05	871.49	874.57	878.73
883.18	886.12	891.10	895.06	896.93	903.65
915.73	918.59	921.13	925.48	930.04	936.31
938.09	948.22	954.00	957.67	964.11	969.26
979.59	980.29	982.50	983.82	990.99	1010.12
1015.89	1020.40	1021.27	1024.99	1028.71	1034.30
1040.00	1042.67	1051.16	1053.60	1055.34	1061.95
1063.08	1084.20	1088.09	1092.63	1095.20	1099.64
1104.25	1105.19	1111.85	1116.00	1120.89	1125.64
1127.05	1128.22	1128.95	1129.60	1129.90	1130.24
1130.85	1131.29	1131.84	1133.19	1136.08	1142.02
1143.10	1146.63	1148.21	1150.49	1156.78	1176.88
1178.82	1182.04	1183.57	1186.94	1187.83	1191.47
1191.56	1206.82	1207.70	1209.07	1209.17	1210.40
1211.63	1212.21	1224.10	1228.14	1230.40	1232.97
1234.81	1236.75	1246.02	1246.28	1251.44	1258.73
1263.19	1264.89	1268.46	1273.13	1274.43	1278.31
1281.73	1283.33	1288.27	1289.67	1296.13	1305.96
1307.15	1307.32	1310.11	1312.53	1314.19	1315.49
1321.98	1322.12	1323.17	1339.03	1341.68	1341.84
1342.54	1342.77	1342.94	1343.83	1344.51	1345.69
1346.63	1352.59	1355.18	1360.27	1361.74	1363.46

1365.43	1387.23	1389.10	1392.98	1395.20	1396.07
1397.71	1397.81	1398.92	1403.78	1405.06	1408.89
1410.94	1415.26	1415.64	1418.00	1418.71	1418.88
1419.07	1419.37	1420.12	1420.59	1420.60	1420.74
1421.71	1422.72	1422.99	1442.69	1442.98	1443.25
1443.57	1443.79	1444.73	1444.91	1445.69	1446.09
1446.35	1449.18	1450.30	1450.48	1467.76	1485.33
1504.82	1509.18	1514.75	1514.82	1515.07	1515.13
1515.20	1515.21	1515.75	1515.95	1515.99	1516.45
1517.48	1517.75	1518.40	1519.08	1519.20	1519.37
1520.12	1526.35	1526.54	1529.19	1532.68	1533.45
1536.35	1536.52	1536.57	1536.62	1536.76	1543.24
1543.28	1548.08	1561.27	1566.83	1569.68	1574.85
1575.88	1577.45	1579.84	1580.68	1599.49	1600.65
1603.09	1620.67	1622.77	1624.20	1625.78	1626.83
1781.16	1793.29	1794.40	1814.11	1815.61	1828.20
1829.39	1830.44	1831.49	1836.12	3014.81	3061.20
3061.69	3061.96	3062.07	3062.09	3062.32	3062.47
3062.53	3062.69	3064.60	3076.65	3077.69	3085.05
3094.04	3098.36	3098.46	3099.36	3100.69	3101.59
3101.69	3116.83	3117.66	3128.33	3129.00	3129.08
3129.22	3129.63	3130.17	3130.64	3131.54	3132.85
3133.89	3135.28	3139.38	3141.09	3141.49	3141.76
3142.13	3142.51	3142.57	3144.19	3144.33	3144.87

3152.88	3159.25	3162.03	3162.77	3162.84	3163.87
3164.06	3164.35	3218.26	3224.76	3234.09	3246.17

Coordinates for TS (13b₁)'

Energy = -5348.54733367 Hartrees

C -2.00156300 -1.92517500 -2.66687800
C -1.88462800 -2.77517100 -1.53970300
C -3.05947300 -0.90368400 -2.44703900
C -2.87877000 -2.34895400 -0.51861300
C -3.40149400 -1.04436900 -1.02460100
C 0.49150800 -3.10468500 -2.04063200
C -0.64567500 -3.32147700 -1.20523500
C 0.37920500 -2.26256300 -3.14415500
C -0.88716900 -1.67659500 -3.46707400
C -3.09169200 0.03209900 1.18840200
C -3.55445800 0.05026100 -0.20791200
C -2.49453100 -1.09672200 1.74468700
C -2.40013400 -2.38139800 0.99949300
C -0.19833100 -3.35017000 0.19672500
C -0.99695000 -2.85029000 1.22596700
C -2.80315700 0.45297600 -2.95178900
C -2.91642900 1.57823700 -2.01060300
C -1.53757200 0.69071300 -3.67577600
C -3.36932700 1.40323200 -0.72230400
C -0.65522700 -0.32860900 -3.98555200

C	-0.40481000	-2.03953600	2.24097500
C	-1.33645300	-0.94842400	2.56392600
C	-2.62156000	1.33342100	1.52759600
C	-2.92201700	2.27783900	0.40619400
C	-1.86283400	2.55774400	-2.30622400
C	-1.02741900	1.99548300	-3.32665900
C	0.77557400	-0.09726100	-3.96544500
C	1.42533800	-1.27554300	-3.45544500
C	1.72070200	-3.14172600	-1.19239900
C	1.21402500	-3.14491300	0.21610900
C	1.77897800	-2.35534800	1.21731600
C	0.97146600	-1.83830100	2.27583100
C	1.57660600	-0.56230100	2.76436200
C	0.57994600	0.61435400	3.10789800
C	-0.87270700	0.31884800	2.91381800
C	-1.49942300	1.46959600	2.34460800
C	-0.45940400	2.46270800	2.03677800
C	-0.57254700	3.29886900	0.92997200
C	-1.80792700	3.35253200	0.08853300
C	-1.30098700	3.35882800	-1.31763800
C	0.12148300	3.56096000	-1.29549600
C	0.93281600	3.06209800	-2.30834400
C	0.35384000	2.24068600	-3.31979000
C	1.27842400	1.17221600	-3.64613500
C	2.45054000	1.31464700	-2.83851600

C	3.03245400	0.16914500	-2.30312100
C	2.55650200	-1.14153400	-2.65739600
C	2.84289900	-2.07223900	-1.52022300
C	3.26681500	-1.18342300	-0.40030400
C	2.82071100	-1.36361500	0.90526400
C	2.64562400	-0.24212400	1.76815000
C	0.80189600	1.90999100	2.40104600
C	0.56809000	3.52611200	0.10558300
C	2.33468400	2.59861500	-2.07242100
C	3.46983300	0.13412900	-0.90180000
C	1.80623500	2.98524200	0.45243600
C	1.90988000	2.13467200	1.59088600
C	2.84518500	1.04460700	1.26912100
C	3.31687400	1.23892500	-0.06600000
C	2.80770300	2.55084500	-0.56684500
C	-3.55057500	-3.22833500	0.50629100
C	3.46248500	3.49208400	-1.57079300
C	1.50907100	0.02639800	4.16500000
C	-3.17810900	3.77702500	0.61264100
C	3.12361500	-3.56876400	-1.59253800
C	-3.38569600	-4.74617600	0.36181100
C	-4.97062900	-2.84644900	0.89428200
C	4.86804500	3.20279700	-2.03903200
C	3.16024500	4.97909600	-1.42417900
C	2.70273800	0.86007100	4.61226700

C	0.88396100	-0.77069700	5.28716800
C	-3.19285700	4.32830500	2.05248100
C	-4.14672700	4.57271000	-0.22794600
C	3.36175900	-4.17889300	-2.95524100
C	3.99135000	-4.18067000	-0.50033100
O	4.95362300	-3.65475200	0.00791000
O	3.51558500	-5.39943200	-0.18420700
O	4.53446900	-4.84221900	-2.96998000
O	2.63393300	-4.06847000	-3.91492700
C	4.90434800	-5.44670800	-4.23499300
C	6.25382300	-6.11114600	-4.04346800
C	4.24486500	-6.13944000	0.82689500
C	5.40340500	-6.91264900	0.21660600
O	-4.92385600	5.36591300	0.27054700
O	-4.05962900	4.33321800	-1.54033900
C	-4.93104700	5.10434300	-2.40945900
C	-6.30669900	4.46707000	-2.52370200
O	-2.34386000	5.09629700	2.43190400
O	-4.15823800	3.93043500	2.90061900
C	-5.31639900	3.15980000	2.50841500
C	-6.19704900	3.04346200	3.73993400
O	2.72077200	2.06371300	4.71567300
O	3.73727000	0.04100900	4.87742200
C	4.95832700	0.66688900	5.34946100
C	5.82748700	1.12305800	4.18810500

O	0.14428500	-1.71957100	5.15060000
O	1.23400400	-0.24217500	6.47575600
C	0.68909400	-0.87713400	7.66144900
C	1.53995500	-2.06089800	8.09384900
O	-3.31959100	-5.28743500	-0.71360300
O	-3.38435000	-5.48547400	1.48862300
C	-3.26684800	-4.92205400	2.82257100
C	-3.61577200	-6.03138600	3.79775000
O	-5.30284100	-2.29909900	1.92297200
O	-5.82407500	-3.22617000	-0.07201500
C	-7.22980200	-2.96971900	0.18257800
C	-8.01430600	-3.53628600	-0.98449700
O	2.55918100	5.64573600	-2.23399900
O	3.66064900	5.43881300	-0.26692600
C	3.44929800	6.84801700	-0.00014100
C	4.03280100	7.14226600	1.36806300
O	5.35446800	2.09911900	-2.14524100
O	5.50567600	4.34937200	-2.34740800
C	6.86755800	4.22666800	-2.83416100
C	7.85857900	4.11707600	-1.68606700
C	-4.79527400	-1.45943900	-3.52118000
C	-4.47500600	0.66383700	-4.37031700
H	4.93271000	-4.66311000	-4.99809400
H	4.12576900	-6.16152300	-4.51885200
H	7.01192600	-5.37859200	-3.74929000

H	6.57075800	-6.57891800	-4.98191800
H	6.20346000	-6.88607800	-3.27202700
H	3.49666200	-6.80813400	1.25862800
H	4.59021000	-5.43847700	1.59048700
H	6.14272000	-6.22840600	-0.20875200
H	5.04879500	-7.58574300	-0.57076600
H	5.89443200	-7.51491300	0.98972200
H	-4.40533700	5.10817600	-3.36666500
H	-4.99309100	6.12376200	-2.02267300
H	-6.22771200	3.42767200	-2.85903600
H	-6.90934200	5.02001600	-3.25323600
H	-6.82583800	4.49179400	-1.56174300
H	-5.00082900	2.17074200	2.16290700
H	-5.83460300	3.68205200	1.70128200
H	-5.66331800	2.53890700	4.55111800
H	-7.09427800	2.46180800	3.50082900
H	-6.50490400	4.03355500	4.08940400
H	5.44778200	-0.11473300	5.93543400
H	4.69302000	1.50060300	6.00404000
H	6.77629000	1.51731400	4.57023000
H	5.32986900	1.91361300	3.62005400
H	6.04561100	0.28892800	3.51391500
H	-0.34012900	-1.17796900	7.45282900
H	0.69178400	-0.08202600	8.41020000
H	2.57853600	-1.75523100	8.25581000

H	1.51703600	-2.85047000	7.33766200
H	1.15082900	-2.47163400	9.03260400
H	-3.93677100	-4.06760800	2.93927200
H	-2.23624000	-4.58110500	2.96224900
H	-2.95104200	-6.89004200	3.66276900
H	-4.64783200	-6.36671500	3.65403800
H	-3.50879900	-5.66558700	4.82466000
H	-7.36880200	-1.88971200	0.29316000
H	-7.50211200	-3.44042600	1.13213000
H	-7.83984800	-4.61166800	-1.08696300
H	-7.73072200	-3.04973800	-1.92326900
H	-9.08522800	-3.37269400	-0.82230400
H	2.37504500	7.05100000	-0.04334100
H	3.93297600	7.42735000	-0.79321100
H	3.88931000	8.20073000	1.61097400
H	5.10552300	6.92479200	1.39238800
H	3.53978200	6.54164300	2.13858900
H	7.02120900	5.13809900	-3.41606100
H	6.92302400	3.35837400	-3.49493800
H	7.76199400	4.96903500	-1.00533000
H	8.88076300	4.10571900	-2.08151700
H	7.69744100	3.19322000	-1.12406100
H	-5.16844900	-2.30385500	-2.95072500
H	-4.52846400	1.73360300	-4.54193300
C	-5.37482800	-0.06623900	-3.40276000

H -6.39815500 -0.07646200 -3.81309600
H -5.42227800 0.34632200 -2.39292900
C -4.28039200 -1.56145100 -4.83152400
H -3.95054900 -2.48096500 -5.30228300
C -4.08088700 -0.27528400 -5.34070400
H -3.57083900 -0.04072700 -6.26858000

Vibrational frequencies for TS (13b₁')

458.46i	6.93	14.66	15.14	22.37	26.90
28.58	28.80	30.40	31.59	33.31	33.58
36.26	36.68	38.98	39.79	40.79	41.66
47.51	51.23	54.63	56.54	56.88	59.90
63.30	65.11	68.22	70.20	72.70	75.74
77.13	78.98	81.66	86.11	87.46	90.48
91.11	91.95	94.89	99.69	102.31	106.74
109.44	109.97	114.07	115.79	116.78	119.86
128.66	130.71	133.19	134.50	141.54	143.04
149.93	152.61	156.69	164.55	169.38	172.36
177.14	181.78	182.20	191.94	198.03	203.11
206.92	212.32	215.59	219.24	221.57	227.85
234.45	240.18	245.16	248.91	256.71	260.75
264.11	266.26	266.85	268.17	273.45	274.28
276.92	280.53	289.53	292.71	299.13	305.81
311.08	315.10	324.54	325.34	328.91	333.33

342.80	344.41	345.24	353.22	354.39	359.01
367.19	375.61	380.30	384.44	388.06	391.73
395.16	396.83	398.70	403.63	413.02	418.77
425.67	428.38	433.82	434.09	439.90	441.93
445.98	449.84	451.69	452.71	455.41	465.36
469.69	472.60	474.47	481.44	484.96	491.14
502.23	512.59	522.44	526.44	533.13	533.95
541.66	542.01	549.08	551.56	553.72	556.75
560.64	561.46	565.26	568.04	571.37	573.19
575.54	579.18	584.56	587.55	591.62	601.04
615.15	628.26	633.40	637.35	639.97	642.12
651.31	655.80	658.93	664.95	667.65	675.17
677.57	681.55	686.44	688.86	696.43	698.37
704.79	709.88	713.32	719.16	722.70	724.60
727.42	729.06	734.18	735.34	738.61	739.18
740.19	743.45	744.44	745.69	746.94	750.28
753.53	755.91	757.56	759.76	762.27	766.38
766.78	768.98	773.07	778.43	782.68	786.66
787.09	789.77	791.41	795.44	796.45	800.50
808.66	812.50	814.60	816.98	818.46	818.72
819.34	821.45	822.41	823.60	825.25	827.90
829.15	830.40	831.33	833.31	834.58	835.95
837.50	838.48	843.72	846.27	848.53	858.31
863.38	869.85	873.66	874.24	878.01	881.27

883.84	888.22	893.90	895.88	904.65	909.68
919.74	922.15	925.30	929.27	934.04	938.36
950.58	953.25	956.80	959.61	963.73	968.95
977.75	981.14	982.67	988.18	999.30	1012.18
1017.77	1026.43	1028.42	1030.66	1036.17	1038.12
1041.68	1044.44	1053.99	1055.77	1060.37	1063.92
1064.17	1084.02	1087.59	1093.50	1094.39	1100.12
1102.97	1103.66	1111.15	1112.09	1123.53	1125.72
1128.65	1129.29	1129.63	1129.92	1130.36	1130.92
1133.49	1138.14	1140.22	1141.63	1142.79	1143.18
1147.29	1147.84	1149.73	1150.59	1154.52	1177.54
1182.01	1183.07	1185.41	1188.11	1191.40	1191.57
1192.00	1192.95	1194.59	1206.95	1207.66	1209.49
1211.27	1211.60	1216.35	1224.29	1228.95	1231.98
1235.45	1238.08	1242.65	1243.84	1247.78	1254.66
1256.98	1258.24	1262.95	1263.89	1270.81	1271.44
1274.74	1280.04	1285.81	1290.84	1291.28	1296.01
1296.64	1303.18	1307.70	1308.02	1308.72	1309.09
1310.53	1317.31	1321.20	1326.17	1326.99	1331.83
1336.78	1342.10	1342.20	1342.45	1343.15	1344.38
1346.00	1351.18	1353.04	1356.95	1365.66	1367.61
1370.42	1375.90	1381.97	1385.77	1392.37	1392.82
1398.20	1400.30	1401.33	1405.50	1408.16	1409.18
1413.87	1415.16	1415.94	1417.22	1418.90	1419.61

1420.03	1421.03	1421.16	1421.53	1421.98	1422.49
1425.48	1428.24	1435.98	1443.22	1443.29	1443.35
1444.16	1444.90	1445.62	1448.07	1448.74	1451.52
1451.69	1451.94	1452.68	1468.81	1486.90	1500.95
1502.96	1507.90	1513.95	1514.10	1514.62	1514.80
1515.01	1515.31	1515.73	1516.17	1516.67	1517.78
1518.19	1518.63	1518.70	1519.30	1520.22	1525.13
1526.01	1526.64	1529.19	1530.27	1534.57	1536.03
1536.15	1536.55	1536.59	1543.63	1544.06	1544.79
1545.66	1546.19	1551.96	1566.94	1569.25	1573.65
1577.35	1578.63	1582.14	1592.27	1600.04	1605.21
1607.17	1620.52	1623.15	1624.24	1627.97	1636.30
1777.74	1805.27	1812.67	1813.00	1817.59	1827.29
1829.31	1830.30	1835.80	1836.24	3015.83	3060.78
3061.98	3062.30	3062.33	3062.51	3063.02	3063.34
3063.50	3063.58	3063.95	3077.28	3078.40	3079.97
3083.13	3083.94	3094.72	3097.16	3098.49	3099.52
3101.97	3118.00	3118.17	3119.58	3127.06	3128.43
3129.18	3130.00	3130.34	3132.02	3132.75	3133.82
3134.30	3134.54	3135.70	3135.93	3137.11	3139.88
3140.35	3140.87	3142.26	3143.05	3146.05	3146.19
3146.71	3156.15	3156.19	3160.20	3160.77	3162.50
3162.51	3164.49	3216.70	3221.88	3232.26	3245.45

Coordinates for TS (13b₂)'

Energy = -5348.54208382 Hartrees

C	-1.48121400	-2.13603200	-2.91233900
C	-1.27173800	-3.01429000	-1.81997000
C	-2.71682300	-1.33943500	-2.71087200
C	-2.38656900	-2.84273700	-0.83914200
C	-3.10832000	-1.62401700	-1.32236800
C	1.15100000	-2.88533600	-2.19294500
C	0.02755100	-3.34552800	-1.43997500
C	0.94714900	-2.01650900	-3.25986000
C	-0.38711000	-1.64853000	-3.63052000
C	-3.11529500	-0.63696400	0.94473600
C	-3.49396200	-0.61869300	-0.47498300
C	-2.35888400	-1.67700500	1.48820000
C	-1.97609400	-2.87073600	0.67736400
C	0.40269400	-3.37636100	-0.01845700
C	-0.52679400	-3.08175900	0.97624900
C	-2.69169100	0.06679100	-3.14404800
C	-3.05393700	1.10337000	-2.15841300
C	-1.44860900	0.56823400	-3.76933700
C	-3.52987700	0.77526800	-0.91320800
C	-0.37687000	-0.25583900	-4.06779100
C	-0.15233000	-2.24748200	2.06799800
C	-1.28771600	-1.36676100	2.38363100

C	-2.90869500	0.70693800	1.37613600
C	-3.31197300	1.64837300	0.28217200
C	-2.18192700	2.26867400	-2.34020200
C	-1.20463600	1.92367500	-3.33152700
C	0.98509200	0.22746400	-3.95158000
C	1.81123100	-0.84225100	-3.45851000
C	2.32110600	-2.75317300	-1.27332700
C	1.75016000	-2.92614600	0.09901600
C	2.10657900	-2.10858700	1.17137500
C	1.16122300	-1.80595300	2.19842100
C	1.49786000	-0.47479000	2.78498000
C	0.28387800	0.48136400	3.11900700
C	-1.07901800	-0.05872000	2.81933000
C	-1.87144000	0.99282300	2.26358700
C	-1.01382500	2.17168000	2.07131300
C	-1.21599500	3.03704900	1.00051800
C	-2.39280600	2.91923400	0.08817000
C	-1.82635700	3.10012300	-1.28172900
C	-0.46720200	3.54919700	-1.16084700
C	0.47330800	3.26279800	-2.14290300
C	0.10745000	2.40988800	-3.22555900
C	1.22867600	1.54550500	-3.54245600
C	2.31075100	1.84950000	-2.65696600
C	3.06492400	0.79900400	-2.14120800
C	2.85556700	-0.55344900	-2.58616600

C	3.24614000	-1.48148500	-1.47826900
C	3.44002800	-0.59777000	-0.29269800
C	2.96460900	-0.92966100	0.97221400
C	2.54218600	0.08999400	1.87469800
C	0.30462800	1.83381700	2.48841300
C	-0.09487100	3.51301600	0.26161200
C	1.92139700	3.04552700	-1.84082000
C	3.42643500	0.76151100	-0.71784400
C	1.20055800	3.18397400	0.66080700
C	1.39542300	2.30085400	1.76189700
C	2.53034300	1.41804500	1.44975000
C	3.03001400	1.77055700	0.15778600
C	2.31859700	2.99693400	-0.31200200
C	-2.88831700	-3.95115800	0.07912900
C	2.84091100	4.09487000	-1.22811500
C	1.24473400	0.00830600	4.20420700
C	-3.84260400	3.06470800	0.54762400
C	3.79677900	-2.89640400	-1.60550800
C	-2.30667300	-5.34903300	-0.20949500
C	-4.32534200	-4.10718000	0.51048600
C	4.29537900	4.09141300	-1.63401200
C	2.26854600	5.49272200	-1.02353200
C	2.24254200	1.01152600	4.76769700
C	0.70953200	-0.94963200	5.24444200
C	-4.02670800	3.50993600	2.01102200

C	-4.87307300	3.76021100	-0.30557700
C	4.21584300	-3.36956600	-2.97964500
C	4.70337200	-3.40882800	-0.49368600
O	5.51300300	-2.74741400	0.11281100
O	4.45807700	-4.71605100	-0.28872300
O	5.50092700	-3.77333300	-2.95970400
O	3.52416400	-3.35875400	-3.97167700
C	6.04581400	-4.21524700	-4.22892000
C	7.50074100	-4.57461700	-3.99849100
C	5.26664800	-5.37934400	0.71583300
C	6.58260700	-5.86611400	0.12930100
O	-5.71501400	4.49036400	0.18454200
O	-4.75943500	3.52109500	-1.61586800
C	-5.65489900	4.25481700	-2.49422600
C	-7.02303400	3.59839600	-2.58654000
O	-3.31590500	4.34402300	2.51245600
O	-4.98548600	2.92111700	2.75315400
C	-6.03638500	2.10082000	2.20467400
C	-6.73860100	1.44487600	3.38083100
O	2.05248600	2.19746200	4.89871300
O	3.37624500	0.36459600	5.09595800
C	4.44006700	1.16698700	5.67113600
C	5.31650000	1.77229300	4.58607900
O	0.19105400	-2.02007200	5.01789600
O	0.84715300	-0.41371900	6.47250300

C	0.34732000	-1.19443200	7.58901100
C	1.38369100	-2.19843600	8.06867900
O	-2.29126200	-5.77807900	-1.33781900
O	-1.80516800	-6.08518400	0.79367100
C	-1.95294400	-5.78464500	2.19999700
C	-2.56883600	-6.99342400	2.88355600
O	-4.75505800	-5.17019900	0.91864500
O	-5.06854400	-2.99903900	0.41451700
C	-6.44989100	-3.13398100	0.84064200
C	-7.12032600	-1.78815300	0.64880500
O	1.56182200	6.07729100	-1.81087500
O	2.66757500	5.97957900	0.16220600
C	2.20443300	7.31446400	0.48695700
C	2.71903600	7.64722300	1.87382700
O	5.00065000	3.10965800	-1.69905200
O	4.69450200	5.33975500	-1.94831100
C	6.06852400	5.49462300	-2.38934800
C	7.01388100	5.64913800	-1.20853300
H	5.92884500	-3.40630500	-4.95624400
H	5.45750600	-5.06854500	-4.58041000
H	8.06446100	-3.70923000	-3.63623800
H	7.95032200	-4.91101400	-4.93905000
H	7.59447600	-5.38092400	-3.26419400
H	4.64302200	-6.21022100	1.05337400
H	5.43060400	-4.68684200	1.54479800

H	7.19068500	-5.02142700	-0.20611800
H	6.40575500	-6.53488600	-0.71928200
H	7.14614600	-6.41704100	0.89110700
H	-5.13617000	4.24640500	-3.45503400
H	-5.73084700	5.28188800	-2.12996000
H	-6.93348200	2.55192000	-2.89572800
H	-7.63252100	4.12447500	-3.33009900
H	-7.54034200	3.64239800	-1.62484600
H	-5.61666200	1.34753200	1.53039100
H	-6.71709900	2.74340000	1.63970700
H	-6.04668400	0.80518500	3.93756200
H	-7.57311800	0.83116800	3.02358700
H	-7.13358400	2.20312500	4.06351600
H	4.99779400	0.46297500	6.29342900
H	3.99333100	1.93786700	6.30341200
H	6.15626100	2.30676300	5.04522100
H	4.74694200	2.48205400	3.97986700
H	5.71866700	0.99349600	3.93071400
H	-0.57716800	-1.68847700	7.28146300
H	0.12433600	-0.44692300	8.35346100
H	2.32099000	-1.69605100	8.32818400
H	1.58483100	-2.94649100	7.29678700
H	1.01093800	-2.71533100	8.96040100
H	-2.57086400	-4.89914700	2.34707400
H	-0.94832200	-5.57208800	2.57771500

H	-1.96337400	-7.88789300	2.70714900
H	-3.57790900	-7.16807900	2.50064300
H	-2.62516000	-6.81952200	3.96442400
H	-6.46094400	-3.45732300	1.88579100
H	-6.92006100	-3.92118800	0.24396700
H	-7.07620100	-1.47251100	-0.39826200
H	-6.63594300	-1.02115300	1.26051000
H	-8.17238200	-1.85640300	0.94629200
H	1.11141500	7.32267200	0.43850900
H	2.57998400	8.00594300	-0.27419800
H	2.38717000	8.65116100	2.16005300
H	3.81323100	7.62416200	1.90226800
H	2.33812600	6.93455600	2.61178300
H	6.04578800	6.39338100	-3.00969500
H	6.33480100	4.63271700	-3.00538000
H	6.70901800	6.48640700	-0.57250200
H	8.02914300	5.84450600	-1.57244900
H	7.03502700	4.73618400	-0.60689600
C	-3.63370600	-1.33058200	-5.19090700
H	-4.15937600	-1.62531900	-6.11375200
H	-2.56205800	-1.38794100	-5.38721400
C	-4.14845500	-2.18577000	-4.05554100
H	-3.95212100	-3.25037500	-3.98256100
C	-4.15827300	0.01579600	-4.75127000
H	-3.96396000	0.93306100	-5.29700300

C -5.33523300 -1.56912700 -3.60682700
H -6.04992900 -2.01614500 -2.92429300
C -5.33900900 -0.23742800 -4.02490400
H -6.05903200 0.51340200 -3.71848500

Vibrational frequencies for TS (13b₂')

464.96i	10.65	15.73	17.08	21.11	28.81
29.28	29.82	32.80	33.41	34.44	36.05
37.91	39.16	40.20	43.14	45.77	48.50
50.39	53.51	55.42	58.57	61.51	62.90
63.67	64.45	69.02	71.45	71.65	76.23
77.39	79.33	83.95	85.46	87.52	88.18
89.75	92.89	96.66	99.93	104.04	106.29
106.78	109.68	112.10	115.21	119.95	120.49
127.66	129.41	132.33	134.33	141.10	144.05
147.85	150.18	160.13	164.66	171.65	176.50
181.08	182.83	191.55	192.64	198.15	201.52
209.10	210.38	214.21	217.25	222.10	228.74
232.31	241.48	245.74	248.06	256.29	260.23
261.30	265.55	266.77	272.15	273.07	276.09
280.90	284.13	291.62	294.26	302.90	312.38
319.71	324.46	326.39	328.81	335.95	341.98
344.72	345.09	348.28	354.29	359.05	362.45
367.57	375.81	380.91	386.18	390.10	392.49

394.76	398.78	401.41	405.16	411.78	422.15
425.93	427.08	430.10	433.62	438.24	441.01
445.36	450.24	451.32	452.64	454.76	463.60
464.38	472.77	473.79	475.62	486.15	489.32
499.05	513.70	523.98	525.99	533.02	534.84
540.62	543.05	548.95	552.20	555.14	556.41
560.32	562.20	566.68	567.37	572.06	574.98
576.58	579.70	583.30	587.13	592.66	599.13
620.88	631.24	631.73	637.17	639.76	642.11
648.83	652.21	658.32	666.49	667.73	670.05
677.42	680.57	684.12	689.88	696.48	697.87
701.41	708.70	711.46	717.70	721.32	725.36
728.37	729.33	733.15	737.79	740.21	740.35
741.31	741.96	744.15	746.40	748.21	752.31
753.63	756.64	757.23	760.21	763.11	765.72
767.05	768.55	774.10	778.36	783.22	784.85
787.56	790.51	792.41	794.27	796.28	799.69
808.34	812.50	813.87	814.17	817.15	818.75
818.98	820.07	820.58	822.75	824.24	824.92
827.44	830.13	832.51	833.93	834.06	835.72
835.87	837.58	844.37	846.77	849.05	856.77
863.33	869.63	873.60	875.38	877.07	879.17
880.76	882.72	895.08	895.55	900.18	908.96
916.89	921.23	924.38	929.93	932.38	936.08

938.72	952.22	955.35	957.96	959.71	969.67
974.67	979.64	982.28	987.01	994.41	1011.81
1018.46	1023.55	1027.26	1029.14	1032.68	1035.42
1037.66	1042.45	1054.61	1055.94	1057.58	1061.87
1064.10	1084.98	1089.08	1090.56	1092.30	1098.33
1103.02	1104.60	1110.37	1112.64	1120.92	1123.17
1126.74	1128.60	1129.15	1129.47	1130.04	1130.29
1132.74	1136.18	1137.49	1137.52	1141.35	1142.13
1147.09	1148.24	1149.83	1150.07	1152.27	1175.84
1178.73	1180.63	1184.53	1186.66	1189.85	1191.72
1191.81	1191.83	1193.50	1206.73	1206.98	1209.29
1211.09	1211.94	1215.69	1220.90	1228.07	1231.15
1233.86	1237.65	1242.45	1245.11	1250.44	1256.29
1259.39	1261.27	1261.59	1268.38	1269.63	1275.97
1277.05	1285.61	1286.84	1290.08	1294.57	1296.02
1301.84	1305.93	1307.00	1307.58	1307.88	1309.50
1314.10	1316.48	1320.43	1321.40	1323.87	1335.06
1340.61	1341.00	1342.71	1343.15	1343.37	1344.56
1346.80	1350.17	1352.41	1354.07	1362.17	1363.99
1368.35	1370.23	1380.02	1383.89	1389.76	1391.95
1393.25	1398.59	1402.16	1404.00	1404.45	1409.64
1413.21	1414.53	1415.34	1416.04	1416.49	1416.99
1417.92	1418.83	1419.44	1421.04	1421.23	1421.54
1422.02	1425.04	1436.70	1443.19	1443.40	1443.70

1443.91	1444.45	1444.63	1445.77	1446.53	1448.41
1450.32	1451.02	1451.15	1468.47	1490.82	1498.90
1503.01	1509.59	1511.55	1512.71	1514.48	1515.23
1515.32	1515.43	1515.66	1515.82	1516.61	1517.01
1517.49	1519.04	1519.06	1519.69	1520.38	1523.89
1525.19	1525.84	1526.22	1530.41	1534.55	1534.81
1536.00	1536.07	1537.16	1542.38	1542.98	1543.37
1544.43	1549.37	1551.05	1567.70	1568.65	1572.24
1576.42	1577.80	1582.98	1591.22	1599.13	1606.64
1607.16	1618.32	1624.12	1624.93	1627.57	1642.06
1776.31	1778.58	1813.15	1813.88	1818.18	1828.18
1828.83	1829.81	1830.72	1839.90	3022.76	3061.17
3061.89	3062.18	3062.36	3062.52	3062.58	3062.85
3063.42	3064.54	3064.87	3077.20	3078.01	3079.96
3082.21	3091.08	3095.26	3097.70	3099.10	3099.51
3101.18	3117.99	3119.53	3121.91	3124.97	3127.83
3129.43	3129.57	3130.01	3130.44	3130.84	3133.18
3133.75	3134.37	3135.54	3139.91	3140.21	3140.96
3141.11	3145.84	3145.96	3146.14	3148.69	3150.00
3150.21	3150.40	3160.42	3160.85	3162.06	3162.52
3165.83	3170.88	3214.27	3221.41	3230.14	3242.66

Coordinates for TS (13c₁)

Energy = -5348.50378773 Hartrees

C	-0.90187700	-1.76160400	-3.25607200
C	-0.88919300	-2.74486400	-2.22505700
C	-2.05422100	-0.93285600	-3.09110700
C	-2.17767800	-2.67702100	-1.45037700
C	1.57506800	-2.57974100	-2.19331200
C	0.33894500	-3.09551400	-1.66994100
C	1.56318500	-1.65044700	-3.22290400
C	0.29928800	-1.23938600	-3.77740000
C	-3.15348800	-0.55719200	0.36278300
C	-2.48976100	-1.64049200	0.94040200
C	-1.96121400	-2.77104600	0.10965500
C	0.49806600	-3.23440200	-0.21885300
C	-0.57940600	-2.98719300	0.62253100
C	-1.97469000	0.41789500	-3.39147500
C	-2.61250000	1.41740700	-2.53908800
C	-0.74262300	0.97483400	-3.89790000
C	-3.24577300	0.97429800	-1.39420400
C	0.37323900	0.16027700	-4.09884600
C	-0.39748100	-2.25103100	1.82258000
C	-1.57882600	-1.39871400	2.01805500
C	-3.02270500	0.74910800	0.93897600
C	-3.24561600	1.76008400	-0.13096300

C	-1.72499300	2.58695800	-2.50126100
C	-0.59286100	2.30691400	-3.34760600
C	1.69536700	0.63549500	-3.73545900
C	2.44165000	-0.46768700	-3.19434000
C	2.58690700	-2.53733100	-1.09210300
C	1.80918300	-2.81436000	0.15176700
C	1.97577000	-2.07529500	1.32128200
C	0.87717100	-1.84108800	2.20192700
C	1.10633000	-0.55921100	2.93176800
C	-0.14498100	0.37006200	3.13501500
C	-1.44541400	-0.13267500	2.58778300
C	-2.14446000	0.96545400	1.99689600
C	-1.26985800	2.15067800	2.02760200
C	-1.29702900	3.09746000	1.00634900
C	-2.30238300	3.05769000	-0.09241200
C	-1.53009500	3.33239700	-1.33733500
C	-0.21178900	3.76079800	-0.96981600
C	0.87417200	3.54524300	-1.81231400
C	0.68311300	2.76984100	-2.99481000
C	1.84704200	1.91683000	-3.19072600
C	2.76488100	2.14660200	-2.11863000
C	3.44523700	1.06288600	-1.56620800
C	3.31642600	-0.24686500	-2.13728600
C	3.53320100	-1.26245400	-1.06553700
C	3.54081200	-0.48014700	0.20951800

C	2.85432500	-0.89802500	1.34904800
C	2.28408200	0.05818000	2.24445500
C	-0.03268100	1.76728600	2.62009000
C	-0.07131600	3.61371300	0.48883800
C	2.25425200	3.29200200	-1.29998700
C	3.57913400	0.91289600	-0.10782800
C	1.14345300	3.24617400	1.06630200
C	1.15762300	2.27819300	2.11515200
C	2.33012000	1.41151700	1.92354800
C	3.03005900	1.85344200	0.76071600
C	2.40859900	3.12068600	0.27946700
C	-2.70215200	-3.86006000	-0.64063600
C	3.09788600	4.23335400	-0.47380500
C	0.63566300	-0.17715800	4.33309500
C	-3.79533500	3.15379500	0.06140800
C	4.08774100	-2.66183300	-1.30032600
C	-2.00640200	-5.21312200	-0.90453000
C	-4.15531900	-4.14005600	-0.30266300
C	4.62666200	4.16392700	-0.61426200
C	2.59543900	5.67461300	-0.28655500
C	1.47354000	0.83474200	5.12422200
C	-0.07011600	-1.19767700	5.19299000
C	-4.32255500	3.60808900	1.43346700
C	-4.57563800	3.79958200	-1.07868600
C	4.56712100	-3.00311100	-2.70666100

C	4.94242600	-3.27561900	-0.21463000
O	4.64798500	-3.33784900	0.95823400
O	6.10620700	-3.71313400	-0.73267400
O	4.22024900	-4.26789900	-3.00234100
O	5.16781300	-2.25196600	-3.43819800
C	4.64595600	-4.77301000	-4.29428700
C	6.06365000	-5.31923500	-4.23023700
C	7.05554600	-4.30392300	0.19323200
C	6.77454700	-5.78393000	0.39904500
O	-5.37312000	3.22766800	-1.79409400
O	-4.28278200	5.10037700	-1.15264600
C	-4.97026000	5.86452200	-2.17932300
C	-4.50587400	7.30208900	-2.05636300
O	-3.73090700	4.41383500	2.10586100
O	-5.51371400	3.13463300	1.85089700
C	-6.21502600	2.03643300	1.21619000
C	-7.60700700	2.00199200	1.82143500
O	1.11023200	1.96880000	5.31353500
O	2.66084600	0.42542700	5.61798300
C	3.17342000	-0.91560600	5.46095300
C	4.48642100	-0.97390500	6.22120300
O	-0.65128200	-2.18079400	4.78974200
O	0.01733000	-0.84359000	6.49145800
C	-0.68310800	-1.67875200	7.45179100
C	-2.13990800	-1.26263600	7.57625900

O	-1.65943300	-5.54719800	-2.00925000
O	-1.83284500	-6.05999500	0.12953800
C	-2.21787700	-5.80770200	1.50417800
C	-1.15943200	-6.43040200	2.39641300
O	-4.70421800	-3.81396200	0.72826200
O	-4.72195600	-4.88692700	-1.26836800
C	-6.06390000	-5.39167100	-1.02581500
C	-6.02235200	-6.72161300	-0.29071100
O	2.07909900	6.28822900	-1.19438000
O	2.79116700	6.27683500	0.89180100
C	3.28650700	5.62205300	2.09692700
C	3.83203500	6.71620900	2.99521600
O	5.33198600	3.78543600	0.29413700
O	5.18823000	4.58846000	-1.75400800
C	4.45882400	4.93566900	-2.96589000
C	5.37525200	5.82248600	-3.78834400
H	4.56042300	-3.96867000	-5.02852800
H	3.92012800	-5.55571400	-4.52548100
H	6.14506100	-6.10078000	-3.46780300
H	6.77425100	-4.52163900	-3.99674000
H	6.33683200	-5.75282800	-5.19909100
H	7.01145500	-3.75214600	1.13481000
H	8.02494600	-4.13779600	-0.28163300
H	5.80513700	-5.93070100	0.88344700
H	7.54927900	-6.22099900	1.03938800

H	6.77706500	-6.31704600	-0.55712800
H	-6.04867500	5.75868800	-2.02532900
H	-4.72383400	5.42845800	-3.15219500
H	-5.66922000	1.11064900	1.42603000
H	-6.25404200	2.18721200	0.13548200
H	-8.17607100	1.16651000	1.39836400
H	-8.14628300	2.93065000	1.61010400
H	-7.55476900	1.87148000	2.90650100
H	3.32732500	-1.12888200	4.39923300
H	2.45668400	-1.63557500	5.86880300
H	4.33092400	-0.75323400	7.28169000
H	5.19740300	-0.24712900	5.81698300
H	4.92295400	-1.97455700	6.13135900
H	-0.13656300	-1.52203800	8.38415200
H	-0.58723900	-2.72193400	7.14152700
H	-3.19576700	-6.27643900	1.66018500
H	-2.31659900	-4.73976000	1.69493900
H	-1.04976100	-7.49798800	2.18244500
H	-1.44536900	-6.31038000	3.44704600
H	-0.19301200	-5.94153100	2.24253400
H	-6.48898700	-5.49907800	-2.02600100
H	-6.62600000	-4.64070700	-0.46691800
H	-7.03642100	-7.12969700	-0.21252000
H	-5.62912800	-6.59556200	0.72250600
H	-5.39952700	-7.44377300	-0.82737000

H	4.05625800	4.89255200	1.84358900
H	2.44074600	5.10901900	2.56399300
H	3.06064500	7.46008700	3.21651800
H	4.68025600	7.22185300	2.52312100
H	4.17166700	6.27627600	3.93904500
H	3.52740500	5.44533500	-2.71791700
H	4.23130100	4.00243900	-3.49030300
H	6.31882600	5.31343700	-4.00766900
H	5.59633900	6.75290700	-3.25616000
H	4.88657900	6.07413100	-4.73596700
H	-3.42382300	7.37629700	-2.20059900
H	-4.75198800	7.70890500	-1.07083700
H	-5.00039200	7.91445500	-2.81818000
H	-2.62642900	-1.85553900	8.35922000
H	-2.22007600	-0.20453000	7.84389100
H	-2.67274700	-1.43227000	6.63638900
C	-2.98141400	-1.46703300	-2.03864600
C	-3.37657900	-0.42372400	-1.08149300
C	-5.99158000	-0.46110800	-1.91344800
H	-6.56681800	0.07945200	-1.17257000
C	-4.54946500	-2.02238600	-2.89655600
H	-4.27799600	-3.00610900	-3.27439700
C	-4.88870400	-0.97508500	-3.82537400
H	-4.46278200	-0.87208600	-4.81661600
C	-5.67649000	-0.01099900	-3.18738700

H -5.92936300 0.96320500 -3.58895400
 C -5.63463200 -1.90596800 -1.81799600
 H -5.37531700 -2.22230000 -0.81295400
 H -6.48777800 -2.51897300 -2.15583800

Vibrational frequencies for TS (13c₁')

313.70i	13.89	16.05	20.99	24.28	29.10
30.58	31.09	31.64	33.78	35.21	37.07
38.12	38.55	40.13	41.21	43.63	46.68
47.05	48.95	51.54	53.14	57.52	61.56
62.65	63.57	65.73	68.40	70.72	74.71
78.20	82.63	85.86	89.37	91.02	94.01
95.51	98.18	99.57	102.33	103.04	106.98
108.67	111.02	113.92	118.90	120.27	124.61
126.42	129.96	131.28	133.37	139.94	143.12
147.22	152.75	156.25	160.46	170.80	174.96
178.25	185.17	186.36	194.14	194.95	204.51
205.60	212.65	212.88	221.47	225.97	231.87
234.71	238.71	242.44	245.63	253.46	256.53
261.56	262.67	265.27	265.42	269.26	271.32
271.71	275.86	284.08	288.29	295.42	298.54
302.26	311.73	321.49	332.81	333.22	335.07
336.21	338.63	341.26	343.54	350.96	355.65
363.45	368.36	372.95	383.20	387.18	388.51

395.14	398.78	403.03	411.35	419.66	421.16
423.68	429.51	435.40	439.60	447.15	448.58
449.43	455.12	460.38	462.92	467.13	472.55
478.83	481.48	483.76	487.05	490.32	497.93
516.23	517.52	522.06	528.02	529.21	533.67
540.50	546.13	547.72	550.30	553.49	557.14
560.49	561.88	564.15	566.80	570.45	571.66
574.56	581.96	584.77	589.08	591.44	600.51
610.52	613.07	615.53	623.69	633.22	637.49
641.40	646.10	650.74	659.79	661.04	665.62
670.13	671.18	677.49	682.21	685.79	692.62
694.55	700.12	706.14	710.37	711.64	717.23
720.16	723.87	724.88	726.87	728.70	731.82
735.01	737.22	740.04	741.99	745.45	746.31
747.86	748.41	749.88	752.36	754.31	755.62
760.26	760.69	763.74	768.09	768.71	772.66
775.13	782.48	785.82	786.71	792.62	794.17
796.56	800.29	809.28	813.02	813.94	816.25
819.40	820.32	822.67	823.44	825.39	825.87
829.23	829.94	832.68	834.39	835.05	836.10
836.31	840.40	842.57	844.95	849.35	853.69
856.81	859.39	867.34	871.62	874.29	884.69
884.93	896.13	902.46	904.53	912.29	914.61
917.02	927.84	928.70	939.93	946.49	950.50

953.33	957.07	961.73	963.72	968.83	972.84
976.63	977.51	987.83	1001.33	1012.06	1015.55
1021.93	1027.78	1029.77	1033.61	1036.47	1038.40
1048.45	1050.14	1051.60	1058.12	1060.05	1064.02
1071.26	1079.35	1081.84	1084.56	1095.77	1096.41
1102.05	1105.54	1109.27	1112.70	1116.16	1126.64
1126.99	1128.93	1129.50	1129.91	1131.70	1136.14
1138.55	1138.82	1140.45	1141.76	1142.83	1143.14
1146.23	1147.69	1149.89	1153.06	1164.42	1168.33
1169.41	1180.80	1182.34	1184.72	1186.30	1186.86
1188.80	1190.96	1193.33	1199.84	1206.31	1207.93
1210.62	1210.70	1215.95	1220.92	1226.53	1228.88
1234.14	1236.35	1239.90	1243.75	1247.00	1251.38
1253.67	1255.90	1260.26	1263.59	1266.78	1271.42
1271.99	1280.74	1281.24	1286.21	1290.03	1299.47
1301.24	1306.85	1307.20	1312.01	1314.55	1320.03
1322.98	1325.44	1327.07	1331.98	1335.29	1335.79
1337.65	1338.05	1339.69	1341.31	1341.35	1342.02
1343.30	1345.20	1355.48	1356.62	1366.45	1370.11
1374.47	1376.82	1379.46	1381.91	1391.07	1395.37
1399.02	1401.04	1403.20	1408.01	1409.46	1411.16
1412.34	1417.66	1418.20	1418.62	1419.08	1420.18
1420.45	1420.99	1422.88	1423.57	1427.29	1429.87
1430.32	1431.30	1439.94	1442.14	1442.60	1443.94

1444.71	1444.73	1448.85	1449.03	1452.78	1454.30
1454.42	1455.10	1455.78	1469.84	1477.42	1482.83
1496.70	1512.82	1513.55	1514.15	1514.44	1514.50
1514.97	1515.27	1515.64	1516.11	1516.99	1518.24
1518.48	1519.17	1519.31	1519.41	1521.27	1522.90
1525.81	1526.54	1529.13	1529.40	1529.72	1532.92
1533.22	1535.46	1536.22	1539.32	1540.80	1542.70
1550.54	1550.86	1552.42	1552.71	1566.64	1570.32
1572.93	1576.40	1578.82	1590.39	1596.65	1599.05
1607.63	1614.20	1617.64	1623.04	1627.65	1628.29
1792.86	1796.38	1806.16	1808.38	1810.56	1812.93
1829.02	1834.91	1837.44	1839.04	2998.90	3061.18
3062.23	3062.31	3063.42	3063.60	3063.73	3064.41
3064.74	3065.23	3066.20	3072.76	3075.81	3076.43
3078.32	3085.12	3091.51	3098.92	3099.18	3100.60
3101.91	3120.25	3120.79	3127.77	3129.97	3131.73
3133.17	3133.71	3134.05	3134.52	3135.74	3136.52
3136.81	3137.05	3138.36	3138.49	3139.10	3140.97
3141.10	3141.31	3144.86	3149.51	3150.44	3155.32
3161.99	3162.95	3163.08	3164.35	3170.50	3172.68
3176.61	3181.41	3219.22	3236.28	3248.88	3264.01

Coordinates for TS (13c₂)'

Energy = -5348.50090129 Hartrees

C	-0.72915500	-1.65271200	-3.38458400
C	-0.76199600	-2.66896300	-2.38498800
C	-1.89375000	-0.83016900	-3.24743800
C	-2.09376900	-2.62504100	-1.66834700
C	1.70099100	-2.47686000	-2.22511100
C	0.44584500	-3.01992800	-1.78051800
C	1.73112900	-1.51541900	-3.22436100
C	0.49125200	-1.09958800	-3.82450600
C	-3.17920900	-0.56798500	0.13727500
C	-2.51616100	-1.65138300	0.71341000
C	-1.92748300	-2.74565100	-0.12103000
C	0.54004000	-3.19586700	-0.32822000
C	-0.57879100	-2.97107500	0.45896600
C	-1.80580600	0.52916200	-3.50271800
C	-2.48743900	1.49433800	-2.64787400
C	-0.55779100	1.11127600	-3.93332500
C	-3.19618200	1.01447200	-1.56821700
C	0.57099600	0.31132300	-4.10298500
C	-0.46925400	-2.27517700	1.68960000
C	-1.66736600	-1.43873100	1.84563100
C	-3.07729000	0.71868100	0.75870700
C	-3.26144900	1.76233700	-0.28350400

C	-1.61989400	2.67346800	-2.54056500
C	-0.44746000	2.42912000	-3.34016600
C	1.86982300	0.78620200	-3.66350500
C	2.59700800	-0.32678000	-3.11807500
C	2.65936200	-2.45797500	-1.07467200
C	1.82603900	-2.77778600	0.12101200
C	1.92495700	-2.07151700	1.31888800
C	0.78019000	-1.87087100	2.14830100
C	0.95837700	-0.60952000	2.92583600
C	-0.31071200	0.30267400	3.09175900
C	-1.57668900	-0.19274300	2.46210100
C	-2.25602400	0.91338800	1.86770600
C	-1.39574600	2.10433500	1.98017800
C	-1.38033500	3.08346500	0.99064100
C	-2.32942300	3.06870900	-0.15785200
C	-1.49541800	3.38680600	-1.35044100
C	-0.20025100	3.81475000	-0.90454000
C	0.92725300	3.63047600	-1.69698300
C	0.80449500	2.89147000	-2.91276000
C	1.98428100	2.05325400	-3.07555900
C	2.84537600	2.25794700	-1.95254200
C	3.50484400	1.16277100	-1.39801700
C	3.41610400	-0.13045900	-2.01306200
C	3.58977000	-1.17592300	-0.96248000
C	3.52626100	-0.43125200	0.33408200

C	2.78835100	-0.88809800	1.42553400
C	2.16390300	0.03673700	2.31800600
C	-0.18621800	1.71544800	2.62533000
C	-0.13380700	3.62562100	0.55366700
C	2.28143800	3.37103800	-1.12419300
C	3.56663100	0.97070700	0.06043500
C	1.05413700	3.25131400	1.18057500
C	1.02382900	2.25106800	2.19838300
C	2.21249700	1.39933000	2.03979700
C	2.96581900	1.88085600	0.92776600
C	2.35856300	3.15835400	0.45459000
C	-2.64940700	-3.84137100	-0.89838500
C	3.07445300	4.29757700	-0.23213700
C	0.41222300	-0.27433200	4.31200500
C	-3.83011600	3.14443600	-0.07396700
C	4.17002300	-2.56201200	-1.21301300
C	-1.93205700	-5.16744400	-1.21972500
C	-4.08588100	-4.08510900	-0.47238100
C	4.60594200	4.23241700	-0.30902900
C	2.55338800	5.73065100	-0.04372900
C	1.19853600	0.71973300	5.17527800
C	-0.32603800	-1.32727400	5.10276700
C	-4.42405500	3.55300800	1.28571500
C	-4.56599400	3.80950900	-1.23166500
C	4.71966300	-2.85584400	-2.60441600

C	4.97595600	-3.20319300	-0.10594800
O	4.62838000	-3.29565400	1.05026200
O	6.16237800	-3.62717500	-0.58176200
O	4.39511100	-4.11199800	-2.95617600
O	5.35002200	-2.07879200	-3.28195100
C	4.88545700	-4.57448100	-4.24127300
C	6.30194000	-5.11536800	-4.12591800
C	7.06931400	-4.24225600	0.37058500
C	6.77799400	-5.72612900	0.52808700
O	-5.30758800	3.23984900	-2.00666800
O	-4.30557800	5.11913800	-1.24971500
C	-4.95996100	5.89757200	-2.28761400
C	-4.52304300	7.33822800	-2.11183800
O	-3.87167400	4.34501400	2.00634300
O	-5.62388600	3.05186000	1.63956600
C	-6.29834400	1.98248700	0.92986300
C	-7.67765200	1.85363900	1.55092700
O	0.81264600	1.84315500	5.38246800
O	2.36570500	0.30768000	5.71280900
C	2.89966900	-1.02343400	5.54329400
C	4.17667300	-1.08994700	6.36205400
O	-0.88481500	-2.29689100	4.63955500
O	-0.29582200	-1.02101100	6.41601900
C	-1.03234200	-1.89315800	7.31438900
C	-2.49392900	-1.48339100	7.39650300

O	-1.65155400	-5.46986800	-2.35294000
O	-1.60351700	-6.00293900	-0.21326200
C	-2.02858300	-5.85766900	1.15850600
C	-0.92687600	-6.41162000	2.04470700
O	-4.73784400	-3.38310400	0.26787900
O	-4.51011300	-5.28332800	-0.94072600
C	-5.85143800	-5.70294500	-0.57270100
C	-5.88474300	-6.39859800	0.77854500
O	2.06603400	6.35346200	-0.95945900
O	2.71175100	6.31578300	1.15094600
C	3.15554900	5.63161900	2.35890900
C	3.65443200	6.70289800	3.31038200
O	5.27313500	3.76959100	0.58889000
O	5.21613000	4.71874100	-1.39895500
C	4.55725100	5.33762100	-2.53721700
C	5.36763700	4.98196700	-3.76995000
H	4.82973100	-3.74806400	-4.95356900
H	4.17658200	-5.35320600	-4.53105100
H	6.35169900	-5.91955800	-3.38462200
H	6.99552200	-4.32194800	-3.83426900
H	6.62387700	-5.51763000	-5.09329500
H	6.98447200	-3.71308800	1.32232200
H	8.05879900	-4.06675400	-0.05709700
H	5.78753600	-5.88243300	0.96450700
H	7.52257100	-6.17975800	1.19223100

H	6.82326300	-6.23651000	-0.43936700
H	-6.04223200	5.77292100	-2.18219800
H	-4.66647500	5.48807200	-3.25886700
H	-5.72131900	1.06059400	1.05300500
H	-6.36242300	2.22106300	-0.13382600
H	-8.22834600	1.04074700	1.06479100
H	-8.24715400	2.78022800	1.42891300
H	-7.60234600	1.63191400	2.61972000
H	3.10484300	-1.20605300	4.48451100
H	2.17270500	-1.76091700	5.89819500
H	3.96962200	-0.90051000	7.41976100
H	4.89747700	-0.34519900	6.01154500
H	4.62802400	-2.08335300	6.26526100
H	-0.52421000	-1.77217100	8.27344500
H	-0.92157200	-2.92352600	6.96832000
H	-2.95524300	-6.42889000	1.27636200
H	-2.23153900	-4.81261000	1.39993700
H	-0.71243500	-7.45368400	1.78834500
H	-1.23687500	-6.36497900	3.09432100
H	-0.01006000	-5.82695100	1.92759700
H	-6.14247900	-6.38014700	-1.37855000
H	-6.50384800	-4.82675500	-0.58008600
H	-6.90345300	-6.74779800	0.98268500
H	-5.59306300	-5.71182600	1.57778700
H	-5.21976100	-7.26814800	0.78850500

H	3.94023800	4.91197400	2.12249000
H	2.29365500	5.10088000	2.77395600
H	2.86925100	7.43609000	3.51838000
H	4.51873000	7.22627300	2.88958300
H	3.95595200	6.23883800	4.25557900
H	4.54394300	6.41680500	-2.35778500
H	3.52523900	4.99939100	-2.61965000
H	5.35732300	3.90120100	-3.94154000
H	6.40678500	5.30699300	-3.66047700
H	4.93848000	5.47806100	-4.64748500
H	-3.43719600	7.43117300	-2.20920600
H	-4.81568200	7.71817600	-1.12827700
H	-4.99486800	7.96142800	-2.87922800
H	-3.00924600	-2.10517800	8.13754400
H	-2.58717200	-0.43596000	7.69949300
H	-2.98956500	-1.61865400	6.43099800
C	-2.87457000	-1.41705800	-2.28050400
C	-3.37787200	-0.40599200	-1.31935000
C	-4.28851400	-1.90840900	-3.42474600
H	-3.78668300	-2.36409200	-4.27541600
C	-5.72405000	-0.48201300	-2.29522500
H	-6.18546600	0.42049000	-1.91403900
C	-5.24854500	-2.66872800	-2.67764600
H	-5.26226300	-3.74818900	-2.62655100
C	-6.03310700	-1.79164200	-1.92629500

H -6.70891000 -2.07767100 -1.12899500
 C -4.95952400 -0.54334000 -3.58167200
 H -4.31468200 0.30637700 -3.79153700
 H -5.67583000 -0.61978100 -4.41537600

Vibrational frequencies for TS (13c₂')

327.20i	17.66	20.27	20.80	26.72	30.32
30.93	33.16	33.58	35.04	35.88	37.19
38.45	40.54	42.21	42.80	45.77	47.83
50.59	52.19	55.84	58.64	59.60	62.85
65.51	69.74	70.92	74.44	75.93	78.21
82.40	89.99	90.69	91.17	94.12	94.74
97.47	99.06	103.97	107.69	109.40	110.42
112.42	115.70	118.45	120.62	124.10	125.14
128.46	130.97	132.40	137.06	144.75	146.67
152.33	157.01	160.44	167.11	170.18	176.01
180.42	182.63	186.86	194.29	194.46	204.83
208.74	214.24	215.53	220.82	229.04	231.26
236.71	241.85	242.91	246.61	255.20	258.34
261.14	263.81	264.38	265.66	268.45	273.44
276.26	279.72	284.26	291.33	296.76	307.72
312.26	319.79	323.94	333.95	336.10	336.55
339.50	340.73	342.75	344.17	352.36	359.23
370.66	372.49	379.90	385.51	387.73	388.85

394.91	399.90	409.91	412.48	417.99	421.37
423.59	429.74	434.47	437.89	446.43	449.08
451.47	451.97	456.19	464.96	468.11	471.36
477.62	478.96	486.08	487.17	493.97	502.78
515.02	516.36	521.75	529.63	530.03	533.94
541.71	546.09	550.51	551.20	554.03	558.36
561.95	563.75	566.29	568.50	570.50	573.10
576.75	583.91	585.86	590.59	594.29	602.00
611.73	613.41	623.63	626.15	633.19	637.83
643.27	645.98	650.34	659.31	661.16	663.18
670.06	672.16	679.13	680.07	682.68	691.38
692.31	701.59	703.46	710.35	711.29	718.58
723.59	724.46	727.22	729.03	729.74	734.89
736.12	740.06	742.18	743.91	745.35	746.30
749.03	750.76	751.50	753.12	755.53	758.03
759.75	762.28	763.13	766.70	768.80	772.84
776.27	781.79	786.25	787.65	793.01	795.22
798.09	800.84	809.73	814.08	815.46	817.75
820.07	822.05	823.09	824.07	826.12	827.27
827.78	831.25	831.80	834.95	835.96	836.63
838.24	840.21	844.83	845.79	850.10	854.58
859.21	866.54	867.40	872.69	876.12	883.18
886.39	890.32	903.97	905.67	911.24	916.08
925.74	926.80	928.57	939.04	943.61	951.75

953.46	954.32	960.18	962.19	965.75	970.11
975.93	981.59	987.13	994.94	1004.76	1015.92
1023.98	1027.25	1029.31	1033.45	1036.20	1038.77
1041.01	1051.14	1052.55	1058.41	1060.44	1064.38
1071.13	1079.35	1082.40	1091.35	1094.12	1099.65
1102.13	1104.10	1105.49	1111.95	1116.46	1124.93
1127.13	1128.25	1128.87	1129.75	1131.45	1136.70
1137.39	1138.93	1140.22	1142.31	1143.08	1143.29
1146.01	1147.35	1149.83	1150.31	1158.94	1166.32
1171.22	1174.13	1182.01	1182.59	1184.09	1186.53
1187.85	1191.21	1192.42	1199.14	1206.11	1208.06
1210.24	1210.71	1215.38	1216.96	1221.99	1227.73
1231.97	1235.15	1238.25	1242.97	1244.96	1250.16
1254.17	1256.26	1260.88	1261.99	1265.22	1271.20
1272.14	1280.36	1281.01	1285.52	1289.25	1297.25
1297.93	1299.56	1305.33	1307.51	1308.10	1315.28
1318.66	1325.91	1327.12	1328.40	1329.27	1332.59
1336.00	1338.15	1338.81	1341.82	1341.85	1343.83
1345.52	1347.02	1353.38	1356.75	1360.76	1365.49
1370.51	1375.87	1377.56	1382.80	1389.33	1393.03
1398.20	1400.42	1402.94	1407.20	1408.61	1411.86
1412.27	1417.72	1418.04	1418.78	1419.37	1419.65
1420.44	1421.09	1421.31	1423.92	1424.62	1426.30
1428.50	1430.00	1441.37	1442.22	1442.46	1444.87

1445.07	1445.26	1447.17	1449.01	1450.42	1452.64
1453.37	1453.85	1454.50	1468.61	1482.54	1485.97
1506.82	1512.90	1513.31	1513.85	1514.48	1514.87
1515.32	1515.44	1515.97	1516.17	1517.00	1517.91
1519.15	1519.19	1519.37	1520.19	1523.54	1524.30
1526.15	1526.80	1527.13	1529.40	1530.23	1533.48
1535.41	1536.11	1536.23	1537.66	1541.41	1543.11
1544.36	1551.78	1552.39	1557.44	1567.62	1571.88
1574.34	1576.96	1580.62	1592.13	1598.31	1600.64
1610.73	1615.70	1621.19	1623.87	1628.72	1630.59
1792.34	1801.01	1807.41	1810.10	1812.71	1814.04
1829.06	1833.88	1836.90	1838.76	3023.57	3061.36
3062.24	3062.39	3063.49	3063.52	3063.63	3064.53
3064.80	3065.64	3066.22	3073.42	3078.88	3080.31
3081.61	3091.09	3094.45	3098.76	3099.01	3099.31
3100.83	3120.84	3121.10	3128.02	3128.58	3130.13
3133.08	3133.32	3133.41	3134.33	3134.82	3136.58
3137.05	3137.06	3138.15	3140.46	3141.21	3141.33
3141.39	3141.52	3141.83	3149.69	3150.38	3155.60
3157.26	3162.06	3162.63	3162.66	3163.27	3170.13
3181.43	3182.66	3195.12	3237.70	3260.71	3275.71

Coordinates for TS (13d₁)

Energy = -5348.49956224 Hartrees

C	-0.21471800	-1.93259000	-3.39192800
C	0.02297200	-2.89129800	-2.35944700
C	-1.55564900	-1.41014000	-3.24450800
C	-1.24741700	-3.10485000	-1.59981000
C	-2.17551600	-2.03758300	-2.08849800
C	2.35251700	-2.12019800	-2.21868800
C	1.27234500	-2.94578300	-1.75586700
C	2.13503000	-1.19508500	-3.23171900
C	0.83173200	-1.10412100	-3.83943900
C	-2.81204200	-1.39762900	0.18670900
C	-2.96031900	-1.28553300	-1.25194200
C	-1.92338200	-2.30218900	0.77527700
C	-1.12120400	-3.25305700	-0.04455300
C	1.39551200	-3.08441500	-0.29754200
C	0.26379200	-3.16572400	0.51548200
C	-1.80366000	-0.06563000	-3.49982100
C	-2.75061000	0.70627600	-2.71792300
C	-0.73197500	0.78860800	-3.94521000
C	-3.50073400	0.06401600	-1.63305000
C	0.55731500	0.28442600	-4.12083100
C	0.21837000	-2.42260900	1.73094600
C	-1.13952300	-1.88213600	1.88924900

C	-3.04867200	-0.12347400	0.76865400
C	-3.55267100	0.83430000	-0.27731200
C	-2.14756800	2.04362500	-2.56222800
C	-0.94623200	2.09240200	-3.36004200
C	1.70114700	1.06674400	-3.69345900
C	2.68213600	0.17210900	-3.14310300
C	3.27383700	-1.85207200	-1.07306100
C	2.54345100	-2.35279100	0.13121200
C	2.48065900	-1.62714100	1.31903100
C	1.33064000	-1.70369900	2.15883800
C	1.20365900	-0.42436200	2.92052600
C	-0.24229400	0.15673300	3.09560500
C	-1.35329700	-0.63830600	2.47771700
C	-2.28254900	0.26357000	1.87305700
C	-1.73159200	1.61992700	1.97291200
C	-1.95207500	2.53233700	0.95361900
C	-2.90429200	2.26768700	-0.15798100
C	-2.19842000	2.78138800	-1.38095700
C	-1.03955600	3.52479300	-0.95693900
C	0.09825500	3.61867300	-1.75307200
C	0.15527900	2.85576100	-2.95623500
C	1.50276000	2.32907000	-3.11981600
C	2.29404500	2.75235500	-2.00666800
C	3.20680600	1.86006800	-1.44812100
C	3.43438300	0.57564400	-2.04754200

C	3.86487600	-0.38157100	-0.98597700
C	3.63037300	0.34226100	0.30113600
C	3.03253200	-0.26714300	1.40380800
C	2.21178300	0.48980500	2.29350400
C	-0.46452100	1.55098800	2.61504000
C	-0.89952900	3.37097500	0.49963700
C	1.48076900	3.70848100	-1.18840600
C	3.32704100	1.70838600	0.01126100
C	0.34558200	3.31845000	1.12713400
C	0.57046400	2.36028600	2.16239800
C	1.92869800	1.82178100	2.00185600
C	2.53263600	2.45770900	0.87509300
C	1.62660900	3.54002100	0.39155900
C	-1.62721700	-4.41484800	-0.90309600
C	2.03252000	4.81044400	-0.31501800
C	0.60903200	-0.21526400	4.31287000
C	-4.38273400	2.07034000	0.09767000
C	4.76514500	-1.58847000	-1.21904900
C	-0.69026400	-5.60505500	-1.14583800
C	-3.08864400	-4.78269200	-0.88503300
C	3.53244100	5.13460400	-0.39937600
C	1.17618200	6.07280900	-0.11976400
C	1.14096200	0.95156900	5.15455900
C	0.15464700	-1.40409000	5.12473800
C	-4.85096600	2.27790800	1.55753700

C	-5.33076400	2.87066200	-0.78251900
C	5.36585000	-1.75949300	-2.61002400
C	5.70523000	-1.99539700	-0.10762300
O	5.39886700	-2.12359800	1.05701400
O	6.95103700	-2.16236700	-0.59056700
O	5.34868500	-3.05957700	-2.95055700
O	5.79171400	-0.86065900	-3.29652300
C	5.92576600	-3.40165700	-4.23725700
C	7.43078300	-3.59170700	-4.13175700
C	7.98120200	-2.52833000	0.36484200
C	8.01495900	-4.03141900	0.59172900
O	-5.00532600	3.77778600	-1.51186800
O	-6.61308500	2.50650800	-0.56721500
C	-7.62537400	3.34043400	-1.19586500
C	-8.97991500	2.84299600	-0.73128500
O	-4.57234200	3.30088800	2.13396900
O	-5.60125500	1.35202800	2.18132000
C	-6.17966000	0.18479400	1.55458200
C	-7.24428900	-0.33658500	2.50429700
O	0.49067200	1.94527400	5.36343400
O	2.38524900	0.85089400	5.66617500
C	3.22219700	-0.31684300	5.51592500
C	4.51617900	-0.02476400	6.25471400
O	-0.18790500	-2.47639400	4.67780000
O	0.16085600	-1.09458400	6.43776400

C	-0.32716600	-2.10840300	7.35663400
C	-1.84054700	-2.04496300	7.48606800
O	-0.19795000	-5.82361300	-2.22494600
O	-0.42119400	-6.43074800	-0.11327300
C	-0.98125500	-6.26915700	1.20788900
C	-0.59023100	-7.50190200	2.00356700
O	-4.00768700	-4.02699100	-0.65088800
O	-3.24391100	-6.08628200	-1.20049400
C	-4.60272400	-6.58688800	-1.29301900
C	-5.13169900	-7.01876700	0.06570100
O	0.55374100	6.56241800	-1.03595600
O	1.17486300	6.67087600	1.07686200
C	1.77757400	6.12657600	2.28761300
C	2.00105600	7.29611600	3.22782200
O	4.28077900	4.92309300	0.52874300
O	4.00397600	5.71867500	-1.50862700
C	3.24993200	5.90437000	-2.74087800
C	3.93150600	7.02406500	-3.50541400
C	-4.66293600	0.53637500	-4.44911000
C	-5.27531500	-0.20681500	-2.33067800
H	5.67127400	-2.61652500	-4.95295500
H	5.41905900	-4.32774600	-4.51742100
H	7.67517100	-4.35789100	-3.38883100
H	7.91887400	-2.65523500	-3.84831900
H	7.83162600	-3.91079600	-5.10069100

H	7.80003200	-1.98580700	1.29545100
H	8.90425500	-2.16717400	-0.09368200
H	7.08837100	-4.37336700	1.06097300
H	8.85063600	-4.28541600	1.25385500
H	8.15087700	-4.56507700	-0.35439100
H	-7.50691000	3.26905800	-2.28111400
H	-7.44116800	4.37829000	-0.90515400
H	-5.39639000	-0.56159300	1.39670500
H	-6.61298800	0.46625600	0.59329700
H	-7.70329700	-1.23922400	2.08579400
H	-8.02641200	0.41239000	2.66268200
H	-6.80651500	-0.58864800	3.47492400
H	3.41320000	-0.50276700	4.45526500
H	2.71599400	-1.18680800	5.94620000
H	4.32275100	0.17007000	7.31399900
H	5.01389400	0.85051400	5.82670100
H	5.19159500	-0.88333500	6.17340700
H	0.16936000	-1.86928800	8.29940500
H	0.00661900	-3.08723300	7.00428600
H	-2.06960800	-6.17947300	1.14284400
H	-0.57680100	-5.36217700	1.66638700
H	-0.99398800	-8.40761700	1.54046900
H	-0.98146200	-7.42459400	3.02383800
H	0.49855300	-7.59680800	2.05571500
H	-4.52549000	-7.42993800	-1.98273300

H	-5.22932700	-5.80929700	-1.73586800
H	-6.13111100	-7.45376700	-0.04913300
H	-5.20678600	-6.16290100	0.74256900
H	-4.48029000	-7.77515700	0.51547100
H	2.71367600	5.61953000	2.05134400
H	1.07195000	5.40572400	2.71089800
H	1.06072100	7.81660400	3.43320400
H	2.71016400	8.01130700	2.79920100
H	2.40907800	6.92823200	4.17542200
H	2.21045900	6.14801200	-2.51987700
H	3.29057300	4.96128200	-3.29470600
H	4.98184600	6.78412400	-3.69726200
H	3.88485800	7.96231300	-2.94392200
H	3.42626900	7.17116500	-4.46624800
H	-4.35179500	1.17944500	-5.26344300
H	-5.88938500	-0.29762400	-1.43865700
H	-9.07079100	2.91491300	0.35699500
H	-9.14156200	1.80129100	-1.02736000
H	-9.76910600	3.45347200	-1.18302000
H	-2.17555500	-2.76318000	8.24319100
H	-2.16241600	-1.04475900	7.79198400
H	-2.32141600	-2.29752600	6.53684300
C	-5.43225400	1.00009700	-3.25633700
H	-5.11377200	1.96616500	-2.88318800
H	-6.50250800	1.06964500	-3.51667300

C -4.70718000 -0.85595900 -4.47170100
H -4.37076400 -1.48599400 -5.28777400
C -5.14900500 -1.31621300 -3.22854600
H -5.20846400 -2.35608300 -2.92907400

Vibrational frequencies for TS (13d₁')

376.66i	11.44	17.51	22.88	26.16	27.98
31.67	32.79	34.33	34.72	35.22	38.36
38.84	41.34	42.00	42.69	44.68	46.36
46.55	49.39	49.98	53.92	58.84	61.25
63.22	68.44	71.86	73.39	75.66	81.64
85.82	90.35	92.81	94.15	94.98	97.18
98.43	99.38	101.02	103.05	109.91	114.15
115.08	116.17	120.72	122.94	126.09	128.55
129.40	131.18	133.97	136.17	137.10	140.41
145.77	148.43	155.55	156.26	165.31	176.82
180.27	185.95	186.79	191.98	197.62	200.60
204.51	214.31	216.03	219.98	230.88	233.56
235.48	242.72	243.98	248.15	256.58	261.00
263.50	266.03	266.26	267.78	271.46	273.46
275.33	280.53	283.70	287.81	290.77	298.33
299.51	306.54	321.02	330.85	333.26	334.50
336.30	338.95	341.42	341.85	345.58	353.81
367.65	375.98	380.97	382.67	385.84	390.83

394.10	397.08	401.72	406.50	415.89	421.06
422.60	426.02	432.38	438.25	445.97	448.00
450.91	456.43	460.20	462.38	471.72	474.67
477.90	483.64	484.12	485.71	492.13	496.57
516.92	518.37	523.95	528.29	533.42	537.22
541.67	545.18	546.93	549.08	555.09	557.47
563.22	564.51	565.63	569.35	572.13	573.43
575.46	582.63	585.81	591.08	595.48	601.84
609.28	613.68	623.71	633.42	636.09	639.09
646.19	647.02	655.88	658.84	661.79	662.93
668.17	672.80	679.66	681.77	685.22	690.84
698.62	698.92	704.82	708.82	713.39	716.97
723.73	725.36	726.58	730.83	731.41	733.37
737.30	740.79	741.33	742.85	744.58	744.92
747.92	749.63	751.12	752.47	754.79	756.00
758.35	759.76	761.73	766.96	770.46	771.66
776.03	782.91	786.39	787.54	789.98	794.50
797.64	800.95	811.82	814.05	815.59	819.03
819.87	820.32	823.93	826.24	827.35	829.61
832.14	833.22	834.06	834.33	834.64	837.06
838.41	838.54	840.25	845.33	851.27	852.34
858.00	865.20	867.89	869.85	877.48	884.42
887.37	891.96	902.39	903.86	906.09	917.06
917.96	924.35	926.25	941.07	944.79	948.33

952.23	953.06	956.28	964.75	967.32	971.61
975.17	979.92	989.35	998.61	1009.38	1013.96
1025.38	1026.99	1028.75	1031.11	1034.29	1035.96
1044.40	1046.33	1052.87	1053.48	1058.34	1063.13
1066.22	1073.83	1083.67	1086.04	1095.08	1097.71
1100.91	1104.80	1107.72	1108.53	1117.83	1124.12
1128.40	1128.95	1129.45	1129.73	1131.12	1134.21
1135.69	1138.30	1140.04	1140.87	1145.47	1145.70
1146.63	1146.96	1147.85	1149.10	1158.81	1162.96
1176.10	1183.43	1183.71	1184.02	1184.79	1186.49
1189.55	1190.64	1192.21	1197.80	1204.73	1206.86
1208.91	1209.27	1211.53	1216.73	1220.25	1228.87
1232.66	1235.74	1238.15	1240.08	1246.31	1247.84
1254.94	1258.72	1262.02	1262.93	1265.89	1271.33
1272.43	1274.78	1281.65	1282.04	1289.45	1292.33
1295.03	1307.43	1308.79	1310.59	1316.96	1319.46
1321.14	1323.06	1323.29	1326.95	1331.52	1333.15
1335.77	1337.53	1338.58	1341.43	1341.71	1343.11
1343.28	1347.12	1352.48	1358.74	1361.47	1364.17
1370.01	1374.08	1378.44	1382.82	1388.00	1394.69
1397.42	1400.40	1401.77	1403.24	1407.26	1408.19
1412.74	1413.69	1417.34	1418.40	1418.62	1418.97
1420.40	1420.61	1422.63	1423.11	1424.15	1428.04
1428.92	1430.62	1439.11	1442.14	1443.57	1443.90

1444.29	1446.44	1448.90	1449.35	1449.54	1450.95
1452.51	1453.25	1455.29	1467.77	1482.40	1483.93
1501.42	1513.62	1513.79	1514.19	1514.41	1514.62
1514.68	1514.98	1515.96	1516.16	1516.31	1517.43
1517.68	1518.23	1518.93	1519.27	1524.53	1525.21
1527.64	1527.79	1529.40	1529.48	1531.41	1533.99
1535.10	1536.19	1536.27	1542.11	1542.44	1542.89
1549.00	1550.03	1552.33	1552.99	1568.88	1572.31
1572.83	1575.31	1579.80	1590.44	1596.31	1602.83
1605.97	1612.79	1623.55	1624.72	1629.56	1633.91
1801.18	1806.35	1807.61	1808.06	1810.56	1811.69
1828.01	1828.92	1837.02	1838.41	2998.91	3061.46
3061.63	3062.35	3062.92	3063.11	3063.49	3063.53
3063.98	3064.01	3065.06	3074.66	3079.26	3083.91
3085.61	3089.73	3089.97	3098.79	3099.16	3100.29
3100.32	3123.02	3123.64	3124.08	3127.97	3129.17
3130.01	3133.17	3133.95	3134.71	3135.47	3135.71
3135.97	3136.33	3136.90	3137.94	3138.66	3139.68
3140.65	3141.41	3141.74	3147.78	3149.50	3150.42
3159.91	3162.08	3162.79	3162.86	3163.13	3170.00
3170.87	3199.73	3227.26	3242.20	3246.29	3255.88

Coordinates for TS (13d₂)

Energy = -5348.50147408 Hartrees

C -0.06554900 1.93478200 -3.42300300

C	-0.39224100	2.87969100	-2.40401300
C	1.32394900	1.55923700	-3.28058700
C	0.85830100	3.24526100	-1.66890700
C	1.89167900	2.28117100	-2.15757000
C	-2.61669600	1.85268800	-2.21922000
C	-1.63168900	2.80276200	-1.78316800
C	-2.31329800	0.94353100	-3.22475400
C	-1.01419700	0.98937500	-3.84690700
C	2.64009700	1.74706600	0.11794100
C	2.77190900	1.62713000	-1.32770100
C	1.65490000	2.54858800	0.70247200
C	0.73928900	3.39640400	-0.11402400
C	-1.74791000	2.94592700	-0.32525500
C	-0.61950800	3.16251100	0.46750600
C	1.72989500	0.25821400	-3.54253900
C	2.82144400	-0.39334000	-2.80389100
C	0.75397200	-0.71389800	-3.95432200
C	3.43660700	0.34608900	-1.68772800
C	-0.58741400	-0.36167200	-4.11891900
C	-0.47379100	2.44647200	1.69088200
C	0.93888000	2.06371600	1.83497600
C	3.02376700	0.51389700	0.71012000
C	3.60926200	-0.39776000	-0.34115300
C	2.32911600	-1.78910800	-2.59260500
C	1.12510700	-1.97835000	-3.36023400

C	-1.63108900	-1.26044600	-3.66666000
C	-2.70014800	-0.47482300	-3.11209100
C	-3.48655900	1.49976800	-1.05673100
C	-2.80011000	2.09603300	0.12988800
C	-2.63943600	1.39818800	1.32505400
C	-1.49278000	1.61432600	2.14492000
C	-1.21239900	0.36815800	2.91979700
C	0.29111800	-0.04500200	3.08124200
C	1.29867200	0.85957500	2.43515500
C	2.31540200	0.05966100	1.82930100
C	1.91726300	-1.34661300	1.95425000
C	2.22083400	-2.23854900	0.93962000
C	3.11709400	-1.87921600	-0.18947800
C	2.46374400	-2.48661200	-1.39740500
C	1.40241300	-3.35132300	-0.94421600
C	0.27433900	-3.58722400	-1.72033600
C	0.11768100	-2.85276200	-2.93126800
C	-1.28335200	-2.48401600	-3.08098300
C	-2.00751000	-2.97811400	-1.95102500
C	-3.00860000	-2.18762400	-1.38927700
C	-3.38679200	-0.94510100	-2.00049500
C	-3.90696500	-0.02697400	-0.94407900
C	-3.57430600	-0.70192300	0.34793200
C	-3.03358800	-0.01418800	1.43376400
C	-2.11989000	-0.66183700	2.31921700

C	0.66103400	-1.41277000	2.61558200
C	1.26611500	-3.19727200	0.51199600
C	-1.08082500	-3.82544900	-1.13405000
C	-3.12485200	-2.02980700	0.06990600
C	0.03329100	-3.27994700	1.16021200
C	-0.28292000	-2.33954300	2.18794100
C	-1.69432100	-1.95764300	2.03965800
C	-2.23894400	-2.67280800	0.93031300
C	-1.22444600	-3.65308000	0.44622500
C	1.10311500	4.59568600	-0.99071600
C	-1.49356400	-4.97047600	-0.23950800
C	-0.57939000	0.24885100	4.30591600
C	4.57919400	-1.53853200	0.03756800
C	-4.94011600	1.06821300	-1.17733000
C	0.03968100	5.67516700	-1.22549600
C	2.51809200	5.11791600	-0.99701700
C	-2.94770800	-5.46269200	-0.30325000
C	-0.49646800	-6.12316600	-0.03561600
C	-0.97010200	-0.95592200	5.17104800
C	-0.24833000	1.49361800	5.09328900
C	5.07427800	-1.61875400	1.49780400
C	5.55006900	-2.31269000	-0.84174700
C	-5.57539500	1.15259000	-2.56097000
C	-5.90456100	1.38306800	-0.05670200
O	-5.59757400	1.56922900	1.09987900

O	-7.16850200	1.39265100	-0.52073300
O	-5.70395600	2.44178900	-2.91852700
O	-5.91086500	0.20295600	-3.22883100
C	-6.33232400	2.70092500	-4.20066000
C	-7.84736500	2.73028600	-4.07421100
C	-8.21987600	1.65438900	0.44583500
C	-8.43435700	3.14765300	0.63523100
O	5.25811500	-3.03253000	-1.76674300
O	6.80738900	-2.19966200	-0.35242500
C	7.80588700	-3.07757700	-0.93578100
C	9.07074000	-2.93820400	-0.11139300
O	4.85226200	-2.59525600	2.17065500
O	5.78418700	-0.60065600	2.01993400
C	6.25431300	0.53333300	1.26167500
C	7.46963100	1.08175600	1.98931000
O	-0.21504600	-1.87231400	5.38071200
O	-2.20949200	-0.97941700	5.70367600
C	-3.17195900	0.08545400	5.54183400
C	-4.40218700	-0.31180900	6.33816500
O	-0.03586400	2.59056400	4.62576500
O	-0.19787000	1.20516100	6.40987000
C	0.19050400	2.28021700	7.30656500
C	1.70357400	2.38589100	7.40839600
O	-0.50467600	5.82038800	-2.29179600
O	-0.28259200	6.48850000	-0.19814400

C	0.31536500	6.39674800	1.11304900
C	-0.15339800	7.61104100	1.89491600
O	3.51160200	4.47669400	-0.73096400
O	2.53183500	6.41331500	-1.37627200
C	3.83011800	7.04972700	-1.50386400
C	4.31266000	7.60428100	-0.17292400
O	0.17446400	-6.54898800	-0.94952300
O	-0.41954600	-6.70158500	1.16825600
C	-1.07240900	-6.21470600	2.37754000
C	-1.15898400	-7.39163700	3.33107500
O	-3.70858000	-5.32015600	0.62776200
O	-3.35827600	-6.11496200	-1.39886900
C	-2.59672700	-6.23286300	-2.63482600
C	-3.14843100	-7.43731900	-3.37477300
C	4.44288800	-0.13349000	-4.34822800
C	5.20951400	1.04799800	-2.52183900
H	-6.00483700	1.93697500	-4.90957000
H	-5.93202000	3.67181900	-4.50068700
H	-8.16110100	3.47282900	-3.33333800
H	-8.22950000	1.74988800	-3.77678100
H	-8.29330600	2.99658300	-5.03937200
H	-7.95675500	1.16395800	1.38570800
H	-9.09903200	1.16999400	0.01552200
H	-7.54769700	3.61399600	1.07362200
H	-9.28137800	3.31571400	1.31018300

H	-8.65418700	3.63374700	-0.32070300
H	7.95826900	-2.78590700	-1.98024700
H	7.41307200	-4.09784200	-0.92591900
H	5.45349100	1.27771400	1.21204200
H	6.51353600	0.22218900	0.24818600
H	7.84450800	1.97105500	1.47032700
H	8.26837300	0.33448700	2.02648000
H	7.21172100	1.36218100	3.01507500
H	-3.41581300	0.20581800	4.48241800
H	-2.75044300	1.02207100	5.92011200
H	-4.15489000	-0.43936000	7.39649200
H	-4.81589200	-1.25274200	5.96325000
H	-5.16866700	0.46555400	6.24809000
H	-0.26029500	2.00158400	8.26138900
H	-0.25580100	3.21079100	6.94809600
H	1.40615100	6.38909000	1.02847700
H	-0.00889600	5.47009400	1.59570800
H	0.17069600	8.53573400	1.40734600
H	0.26267500	7.58346600	2.90786400
H	-1.24501000	7.62366200	1.96818500
H	3.66218000	7.84340500	-2.23487400
H	4.53421000	6.32075100	-1.91148900
H	5.25773200	8.14000800	-0.31804500
H	4.48400000	6.79686800	0.54472600
H	3.58354800	8.30616000	0.24488900

H	-2.06067700	-5.81799900	2.14292300
H	-0.44911000	-5.41521600	2.78868300
H	-0.16542100	-7.80185600	3.53582200
H	-1.78618800	-8.18597200	2.91436000
H	-1.60046700	-7.06134400	4.27752700
H	-1.53437400	-6.34963100	-2.41917300
H	-2.75111500	-5.31034500	-3.20318400
H	-4.22132900	-7.32555700	-3.55913500
H	-2.98689100	-8.35416100	-2.79939600
H	-2.63786600	-7.53993400	-4.33855600
H	3.93900400	-0.41790100	-5.26512800
H	5.49233100	1.87063300	-1.87158100
H	8.88895200	-3.22158600	0.92969600
H	9.44526900	-1.90940800	-0.13162300
H	9.84827200	-3.59376500	-0.51808500
H	1.97018100	3.14949400	8.14805700
H	2.13896500	1.43256900	7.72332300
H	2.13746400	2.67332000	6.44655100
C	4.58626700	1.29282600	-3.88186800
H	5.34083300	1.79212600	-4.51036600
H	3.68955500	1.90718700	-3.90369000
C	6.00723400	-0.11144800	-2.69652900
H	6.79415800	-0.43107400	-2.02662700
C	5.50619900	-0.84701400	-3.77198000
H	5.79933500	-1.85624200	-4.03261300

Vibrational frequencies for TS (13d₂)'

436.68i	16.69	17.95	21.89	26.80	28.29
31.17	32.00	35.05	36.01	37.16	37.97
39.32	41.18	42.16	43.01	45.35	47.02
48.33	51.40	51.98	55.92	60.70	63.66
68.05	69.61	72.17	74.43	76.49	81.66
83.62	90.05	93.51	94.73	96.47	98.74
99.58	102.84	105.49	110.74	112.21	114.39
118.65	119.90	122.62	125.40	128.28	128.68
129.82	131.17	134.96	136.11	142.70	145.87
147.33	152.41	158.40	160.05	170.65	178.39
181.21	186.46	187.96	191.98	198.77	202.38
204.20	215.04	215.70	222.57	227.39	230.54
235.08	238.44	243.34	250.32	257.10	262.36
263.13	266.83	267.28	268.21	269.55	272.99
276.23	283.77	284.51	287.76	296.15	298.48
309.63	314.15	321.41	333.09	334.47	334.79
338.19	340.38	343.19	346.61	353.17	354.40
369.38	376.65	380.86	384.39	387.75	394.64
396.60	396.80	406.10	410.47	416.24	421.77
425.12	430.48	433.11	437.44	446.05	448.44
452.09	456.86	459.99	462.84	471.83	474.26
477.96	483.27	485.90	488.64	490.49	499.91

516.33	518.80	525.83	529.14	536.02	537.09
542.43	546.39	548.35	551.23	557.77	558.70
563.65	565.85	567.53	570.53	573.52	574.47
580.91	582.61	586.58	592.92	594.20	603.32
613.07	620.70	624.73	633.72	636.18	637.65
645.78	646.82	657.17	659.63	662.85	663.49
668.21	672.51	679.23	681.11	684.74	691.38
696.65	702.14	705.19	707.68	712.50	715.25
722.98	728.00	729.10	731.91	733.54	737.99
739.87	741.75	742.71	745.06	745.27	746.73
748.73	751.87	753.55	754.27	756.95	758.77
761.32	762.57	766.09	769.39	773.49	776.64
783.75	786.87	788.24	789.27	791.26	796.76
799.75	801.97	812.35	816.75	818.15	818.95
820.14	820.50	826.27	826.80	828.87	829.69
831.06	832.89	834.18	835.03	836.02	836.35
838.39	840.53	841.69	845.96	851.18	852.75
858.78	865.55	869.86	876.38	884.46	888.74
891.59	894.58	901.17	903.60	904.77	916.20
921.59	927.07	928.01	940.67	944.59	948.11
950.88	953.63	956.97	965.16	968.02	971.28
978.40	980.78	988.29	991.87	999.85	1010.50
1021.53	1026.84	1027.97	1028.31	1033.89	1036.01
1037.37	1045.41	1049.80	1052.97	1060.72	1063.30

1066.20	1076.30	1082.29	1087.26	1094.53	1099.13
1101.66	1103.79	1105.30	1111.34	1118.77	1124.43
1126.89	1128.51	1128.90	1129.90	1130.67	1134.57
1136.11	1138.11	1139.78	1140.06	1142.10	1144.92
1145.96	1146.42	1147.17	1147.67	1150.91	1164.39
1175.55	1181.60	1182.32	1183.49	1183.71	1185.06
1186.77	1191.57	1192.43	1198.06	1205.65	1207.14
1208.69	1210.22	1211.99	1215.47	1219.10	1226.80
1229.77	1233.85	1236.85	1239.81	1246.79	1248.55
1254.52	1258.74	1261.82	1262.81	1266.46	1269.48
1273.09	1274.64	1281.08	1282.55	1289.94	1292.57
1295.02	1296.36	1307.12	1307.54	1309.18	1315.60
1319.60	1322.90	1326.50	1326.90	1327.97	1331.10
1336.93	1339.33	1341.49	1341.60	1342.25	1342.67
1343.38	1344.99	1351.56	1358.74	1360.97	1364.02
1368.79	1375.38	1376.28	1381.50	1390.14	1391.62
1397.15	1399.30	1401.85	1405.33	1406.93	1408.16
1412.82	1414.06	1418.51	1418.62	1419.35	1419.75
1420.45	1420.71	1421.09	1421.65	1423.47	1428.34
1429.64	1430.70	1442.17	1442.31	1442.62	1444.02
1444.67	1445.95	1446.70	1448.14	1449.91	1450.55
1454.29	1454.69	1455.69	1468.85	1485.95	1490.29
1502.86	1513.83	1514.12	1514.49	1514.51	1515.18
1515.21	1515.60	1516.47	1516.47	1516.95	1518.08

1518.48	1519.27	1519.48	1519.63	1524.89	1526.68
1526.94	1527.69	1529.13	1529.59	1529.60	1533.83
1535.61	1535.66	1536.53	1541.42	1541.75	1542.04
1544.11	1551.19	1553.41	1553.61	1569.50	1572.32
1575.56	1577.68	1580.13	1592.49	1598.10	1604.56
1609.28	1614.92	1624.70	1625.93	1629.55	1635.15
1805.37	1806.86	1808.07	1810.47	1812.10	1814.24
1828.91	1831.53	1837.84	1838.86	3026.29	3061.33
3061.42	3061.74	3062.48	3063.08	3063.47	3063.81
3064.12	3064.14	3065.10	3074.82	3076.49	3076.78
3082.81	3084.30	3091.09	3099.00	3099.30	3100.25
3100.71	3121.55	3121.58	3122.24	3128.16	3128.91
3130.06	3132.33	3133.49	3134.53	3134.78	3135.59
3136.17	3136.44	3136.92	3138.18	3138.69	3138.92
3141.06	3141.27	3141.67	3147.35	3148.93	3150.18
3157.58	3162.17	3162.37	3163.14	3163.30	3171.50
3171.93	3191.02	3206.28	3231.63	3251.46	3266.94

Coordinates for product (13a)

Energy = -5348.61725574 Hartrees

C 1.08680100 2.70651000 -2.54906100
C 1.17238800 3.38611900 -1.29681900
C 2.21228900 1.75769300 -2.63775700
C 2.44734300 2.99645900 -0.62143100

C	2.97540800	1.86061200	-1.43735700
C	-1.27157400	3.34771700	-1.15202000
C	0.00306900	3.64925700	-0.58662200
C	-1.33088400	2.67931500	-2.37431500
C	-0.14438000	2.38458400	-3.10226400
C	3.43455800	0.48282400	0.58888100
C	3.51014200	0.70819800	-0.86319100
C	2.83586000	1.41720500	1.42919400
C	2.37846300	2.75245100	0.94292000
C	-0.06397200	3.42552800	0.86503400
C	1.03721600	2.94669800	1.57634200
C	2.05704700	0.53707800	-3.27752000
C	2.61587200	-0.63150200	-2.68658800
C	0.85768700	0.17731100	-4.15215100
C	3.37714500	-0.55261700	-1.52178400
C	-0.37566800	1.21145300	-4.05286700
C	0.84066900	1.92577100	2.55401900
C	1.96169800	0.97551400	2.46518200
C	3.24860900	-0.91301300	0.81271500
C	3.36738700	-1.63533800	-0.49077700
C	1.67338200	-1.74054500	-2.90518300
C	0.56046100	-1.22261400	-3.62615700
C	-1.65045100	0.63071800	-3.44983800
C	-2.27698900	1.57471800	-2.59150300
C	-2.23103000	3.06475400	-0.04097500

C	-1.37893700	2.97842800	1.18197600
C	-1.55730800	1.98878700	2.14478900
C	-0.44180100	1.48399700	2.87058400
C	-0.72670100	0.07814400	3.28568500
C	0.48085800	-0.94587300	3.18641000
C	1.77656800	-0.38655500	2.69546900
C	2.39423800	-1.33750400	1.82862800
C	1.44444200	-2.44097000	1.61269700
C	1.37893800	-3.09454500	0.38528400
C	2.35074000	-2.82737700	-0.71717400
C	1.50827100	-2.74641600	-1.95164200
C	0.18721600	-3.18089900	-1.63272000
C	-0.90771800	-2.68328500	-2.33418400
C	-0.71626100	-1.66800600	-3.31445500
C	-1.84768000	-0.72453400	-3.22586300
C	-2.72774700	-1.17425200	-2.19485300
C	-3.32438900	-0.23622400	-1.35120600
C	-3.14443500	1.16012900	-1.58266400
C	-3.24453300	1.88060800	-0.27653400
C	-3.24780900	0.79852700	0.75388800
C	-2.50603700	0.88347100	1.93106400
C	-1.96760100	-0.29372300	2.53612300
C	0.25617000	-2.16395700	2.35271400
C	0.10772400	-3.40290700	-0.18020800
C	-2.24845700	-2.50305200	-1.70333700

C	-3.39227300	-0.45894500	0.10008900
C	-1.06058300	-3.12909500	0.52984800
C	-0.98199000	-2.46072200	1.78606100
C	-2.10588600	-1.51589700	1.87698300
C	-2.87326900	-1.61551200	0.67735600
C	-2.33561700	-2.74108600	-0.14407200
C	1.19465300	0.23452000	-5.71327600
C	-0.52610500	1.67634600	-5.57378700
C	3.29903200	3.80891200	0.34696200
C	-3.08713300	-3.63507700	-1.11963400
C	-0.14164400	-0.57960500	4.52813400
C	3.85029800	-3.07574400	-0.61348600
C	-3.73707600	3.30147400	-0.02576700
C	3.10366900	5.28292800	0.62523800
C	4.79773200	3.51366200	0.35941000
C	-4.59069200	-3.53251300	-1.21665100
C	-2.56729500	-5.05598700	-1.29684100
C	-0.93537900	-1.54320700	5.38092900
C	0.68703700	0.30965400	5.45522100
C	4.35897000	-3.74105500	0.66467700
C	4.65569300	-3.60746300	-1.77622800
C	-4.35382400	4.07598200	-1.16553600
C	-4.37793800	3.59985300	1.32380100
O	-3.93081000	4.36706000	2.14424300
O	-5.51588700	2.90121100	1.46447100

O	-5.26974200	4.94857000	-0.70283700
O	-4.06578000	3.95549100	-2.33536700
C	-5.92514400	5.77197500	-1.69938300
C	-6.89919200	6.67654700	-0.96973200
C	-6.24594900	3.12612400	2.69550600
C	-7.47406500	2.23705100	2.66257900
O	5.42927600	-4.53398600	-1.64587800
O	4.42495900	-2.98150700	-2.93660300
C	5.15092300	-3.49388400	-4.08392000
C	4.72385600	-2.68483500	-5.29309500
O	3.81034100	-4.65087700	1.23984300
O	5.51026400	-3.16909700	1.04598400
C	6.15266400	-3.75440100	2.20535300
C	7.41999500	-2.96439700	2.46807600
O	-0.95211400	-1.46037100	6.59189800
O	-1.60902000	-2.46361800	4.68188200
C	-2.40350100	-3.39617700	5.45989100
C	-3.11756600	-4.31153400	4.48452800
O	0.39819400	1.44039500	5.76633800
O	1.77174400	-0.35491800	5.87886000
C	2.60841000	0.34901900	6.83046500
C	3.75704700	-0.57228000	7.19212800
O	4.02798800	5.99512000	0.96078600
O	1.84215700	5.70200600	0.48710400
C	1.59680800	7.09828400	0.80391600

C	0.11263600	7.35335600	0.62803700
O	5.39613600	2.98941900	1.26850400
O	5.35314700	3.93306400	-0.78779000
C	6.79269700	3.79953100	-0.87520700
C	7.21757600	4.35007200	-2.22274800
O	-2.04630100	-5.48991800	-2.29716900
O	-2.77926200	-5.76333500	-0.17322200
C	-2.35627600	-7.14884400	-0.21261800
C	-2.64184200	-7.74963200	1.15006000
O	-5.25400500	-2.56952500	-0.90438000
O	-5.10460300	-4.66534000	-1.73426700
C	-6.54295700	-4.68783600	-1.91199600
C	-6.90734200	-6.04156700	-2.48975100
H	2.18244100	-0.17493300	-5.93433800
H	-1.11774600	2.58896900	-5.66533300
H	-6.42606200	5.11561500	-2.41766900
H	-5.16012100	6.33719200	-2.24055900
H	-7.65064100	6.08964900	-0.43212100
H	-7.41526300	7.32052300	-1.69005200
H	-6.37665200	7.31325100	-0.24903400
H	-6.50314800	4.18840000	2.75748900
H	-5.58773500	2.89207500	3.53778000
H	-7.19000900	1.18283200	2.58677200
H	-8.11363900	2.48384700	1.80915900
H	-8.05470200	2.37444800	3.58126900

H	4.91934000	-4.55745900	-4.19343000
H	6.22255900	-3.40432400	-3.88183800
H	5.25997100	-3.03929900	-6.18016500
H	4.94994700	-1.62310400	-5.15304900
H	3.64945200	-2.79048200	-5.47278600
H	6.35675000	-4.80794300	1.99074200
H	5.45531900	-3.71104700	3.04779400
H	7.19110200	-1.91226800	2.66493900
H	8.09745500	-3.01677000	1.60996300
H	7.93708800	-3.37548000	3.34200200
H	-3.10029400	-2.82416200	6.07975400
H	-1.73300100	-3.94375800	6.12924000
H	-3.77912800	-3.74187000	3.82482700
H	-3.72192600	-5.03767600	5.03920100
H	-2.40136900	-4.85830000	3.86342400
H	1.99674300	0.61081200	7.69917400
H	2.95333500	1.27887800	6.36784900
H	3.38734000	-1.49835800	7.64350400
H	4.41630800	-0.07530200	7.91213000
H	4.34581700	-0.82879000	6.30568700
H	2.20759300	7.71387800	0.13653900
H	1.93180300	7.28198400	1.82897400
H	-0.10645400	8.40271600	0.85395500
H	-0.47711600	6.72445900	1.30163200
H	-0.20104600	7.14839800	-0.40029700

H	7.05182800	2.74235700	-0.75914300
H	7.24163800	4.34962000	-0.04258300
H	6.94119300	5.40485200	-2.31746300
H	6.74554200	3.79373100	-3.03891800
H	8.30451900	4.26639000	-2.33090500
H	-1.29174000	-7.18085700	-0.46332500
H	-2.90415500	-7.65663800	-1.01294900
H	-2.33514200	-8.80112300	1.16263000
H	-3.70967400	-7.69846500	1.38587100
H	-2.08836700	-7.22070400	1.93249800
H	-6.82290400	-3.86445000	-2.57624200
H	-7.01616300	-4.50929700	-0.94145800
H	-7.99042600	-6.09737100	-2.64376800
H	-6.61392300	-6.84878600	-1.81113700
H	-6.41255100	-6.20239900	-3.45261900
C	0.95368100	1.72952200	-6.00347000
H	1.56794200	2.40489700	-5.39896400
H	1.07243800	1.97372300	-7.06329900
C	0.02001100	-0.38740400	-6.44765000
H	0.00570900	-1.39331500	-6.85326200
C	-1.00510500	0.47176400	-6.36386400
H	-2.02775700	0.31200400	-6.68795300

Vibrational frequencies for product (13a)

7.05	13.52	14.39	18.87	19.32	22.21
------	-------	-------	-------	-------	-------

26.51	27.70	28.92	29.30	33.80	34.29
35.75	36.67	37.27	44.62	47.02	47.83
50.52	52.90	55.23	56.31	61.44	63.36
64.82	66.50	69.01	69.58	71.50	72.82
73.39	74.52	75.35	77.64	78.68	92.78
93.60	96.07	97.22	99.94	107.60	117.26
118.72	120.46	125.97	133.43	135.97	138.60
140.84	143.44	147.29	151.70	154.62	154.86
155.67	158.45	159.52	168.58	170.92	175.71
180.02	182.70	193.79	206.10	212.26	217.67
225.81	227.16	234.45	236.48	245.88	249.69
251.28	252.98	260.76	261.73	264.14	265.64
266.25	269.51	271.98	276.21	277.57	277.78
278.07	279.66	281.35	305.98	307.47	309.15
312.20	314.66	320.22	327.54	335.44	342.56
345.00	348.35	351.25	355.03	356.07	366.34
367.41	371.54	381.81	383.40	383.84	385.32
386.42	391.50	393.32	398.73	405.73	407.96
414.40	421.52	422.46	427.57	429.23	430.24
431.92	435.62	438.35	447.04	458.39	460.38
467.38	472.95	478.64	480.94	490.95	495.86
518.49	522.05	526.59	533.82	540.32	542.89
547.38	548.03	549.08	550.63	555.55	558.10
564.75	566.46	570.86	574.96	577.09	579.82

581.80	589.30	591.83	609.51	626.00	630.94
640.66	641.87	646.97	650.88	653.33	657.20
659.42	667.12	670.54	677.77	682.18	683.49
686.25	692.64	696.30	704.81	707.13	709.55
713.65	717.08	727.03	729.58	733.83	735.07
736.12	737.03	739.50	739.57	742.53	744.70
745.88	748.43	751.53	752.70	753.62	755.60
759.16	760.97	763.01	767.29	772.07	783.84
788.97	790.71	793.49	798.79	799.78	801.71
809.91	812.02	814.03	816.01	816.74	817.53
817.84	818.40	819.03	819.36	819.39	820.20
820.45	822.36	822.54	823.32	825.68	827.72
830.01	831.20	832.76	836.02	838.26	839.35
843.08	845.07	852.76	866.03	869.28	880.19
882.17	884.44	887.03	888.71	892.31	892.95
895.84	898.18	901.44	906.04	909.02	919.25
922.73	924.93	927.60	934.18	940.84	942.42
946.61	951.80	953.15	959.77	964.04	971.52
985.48	991.26	997.23	999.10	1021.46	1024.60
1032.57	1033.22	1033.80	1038.66	1040.95	1042.63
1045.87	1050.98	1055.95	1056.06	1058.07	1065.35
1066.91	1079.10	1087.34	1090.83	1094.08	1107.88
1109.34	1115.18	1119.43	1120.14	1121.40	1130.24
1131.58	1136.06	1140.60	1142.06	1147.22	1147.72

1148.05	1148.33	1148.47	1148.48	1148.75	1148.93
1151.82	1154.48	1157.27	1163.87	1172.10	1177.65
1178.88	1182.91	1190.84	1191.46	1191.58	1191.67
1191.82	1191.85	1192.06	1192.17	1192.34	1192.55
1193.50	1206.46	1223.53	1225.06	1229.72	1233.42
1235.44	1236.78	1249.98	1253.67	1258.61	1263.27
1270.02	1271.82	1272.55	1274.49	1276.48	1278.49
1279.78	1282.21	1284.57	1287.75	1290.85	1293.78
1299.46	1306.57	1306.82	1307.55	1307.62	1307.71
1307.81	1308.10	1308.55	1308.68	1308.82	1309.58
1315.62	1317.01	1317.07	1319.99	1327.91	1337.41
1339.45	1344.01	1347.02	1354.89	1360.15	1360.43
1366.61	1367.33	1373.00	1382.32	1388.09	1392.32
1395.23	1396.44	1397.10	1398.25	1399.70	1399.81
1409.14	1411.20	1411.35	1414.04	1415.19	1415.91
1416.22	1416.95	1417.08	1417.45	1417.97	1418.39
1418.44	1420.95	1421.77	1424.21	1443.61	1444.47
1447.67	1449.86	1449.89	1450.75	1451.19	1451.24
1451.51	1451.68	1452.56	1452.93	1453.12	1467.30
1515.65	1515.75	1515.81	1516.02	1516.13	1516.15
1516.54	1516.56	1516.57	1516.81	1525.14	1525.42
1525.68	1525.80	1525.92	1525.97	1526.34	1526.42
1526.54	1526.83	1526.93	1542.77	1543.18	1543.22
1543.88	1543.97	1543.98	1544.08	1544.38	1544.74

1544.87	1568.63	1570.35	1571.62	1576.92	1580.49
1580.80	1583.87	1588.42	1604.03	1605.44	1606.32
1623.88	1625.28	1625.79	1630.55	1630.86	1656.13
1794.31	1794.68	1796.16	1813.38	1815.82	1826.75
1829.25	1830.91	1831.51	1832.36	3061.94	3062.15
3062.44	3062.72	3063.03	3063.27	3063.46	3063.72
3064.33	3064.37	3077.05	3077.14	3077.56	3078.06
3078.68	3079.03	3079.27	3080.90	3080.97	3081.38
3081.65	3117.09	3117.11	3117.70	3118.06	3118.18
3118.36	3119.46	3120.85	3120.90	3122.05	3128.90
3131.95	3132.62	3133.26	3133.35	3133.39	3133.94
3134.30	3134.37	3134.42	3134.63	3134.70	3136.34
3143.27	3144.71	3145.05	3145.38	3145.57	3145.64
3145.79	3146.46	3148.10	3149.74	3217.31	3240.45

Coordinates for theoretical product (13b₁)

Energy = -5348.58164339 Hartrees

C -1.68911400 -2.08219700 -2.84590300
C -1.64100600 -2.91483300 -1.70809200
C -2.92355200 -1.18844400 -2.83049900
C -2.76898500 -2.56999300 -0.78993300
C -3.30103700 -1.28995700 -1.35771900
C 0.78159800 -3.13027300 -1.95668800
C -0.41724500 -3.40836600 -1.24823000

C	0.74136000	-2.28662600	-3.06398800
C	-0.51134200	-1.76035900	-3.51323200
C	-3.23625800	-0.21507700	0.86340100
C	-3.54079600	-0.20893200	-0.57453900
C	-2.66639700	-1.32467300	1.48792000
C	-2.42221800	-2.59263200	0.74376700
C	-0.10711800	-3.44484100	0.18810300
C	-1.03094900	-2.98802500	1.12409500
C	-2.66087200	0.31836600	-3.35033600
C	-2.82200300	1.40359600	-2.28526000
C	-1.23189800	0.58886000	-3.80445700
C	-3.36778800	1.17529700	-1.05933500
C	-0.28460600	-0.39032200	-4.00136300
C	-0.59429700	-2.16816500	2.20335900
C	-1.60833300	-1.12717300	2.42768400
C	-2.86649400	1.10188900	1.25817300
C	-3.08895900	2.04765600	0.12149100
C	-1.78087900	2.41748200	-2.44946000
C	-0.81623000	1.89574700	-3.37520900
C	1.12456600	-0.09943500	-3.82765600
C	1.76962200	-1.25152500	-3.25867300
C	1.92472700	-3.13252800	-0.99646800
C	1.28694100	-3.18644900	0.35738300
C	1.69976400	-2.37435700	1.41423500
C	0.76109600	-1.90398000	2.38214500

C	1.25037300	-0.60652200	2.93677400
C	0.16748900	0.51770300	3.17937400
C	-1.24040500	0.15719500	2.82873100
C	-1.85115400	1.28282700	2.19723300
C	-0.83517200	2.32974300	2.01335600
C	-0.86827600	3.17576100	0.90766700
C	-2.00722200	3.18667700	-0.06064200
C	-1.35907000	3.23433400	-1.40315700
C	0.04286300	3.49471400	-1.22786800
C	0.97811800	3.04441000	-2.15208100
C	0.54556800	2.20619600	-3.21979300
C	1.54191200	1.18517700	-3.45343400
C	2.61929900	1.37167700	-2.52881800
C	3.19129900	0.24842500	-1.94015900
C	2.80217500	-1.07463600	-2.34575300
C	3.02183000	-2.01113000	-1.20011500
C	3.29767200	-1.12287800	-0.03256000
C	2.71758200	-1.33282600	1.21601900
C	2.40021500	-0.22858000	2.05931200
C	0.40314100	1.82976400	2.50657000
C	0.34157100	3.46325800	0.21132700
C	2.36692700	2.64121900	-1.77339100
C	3.48616200	0.21155700	-0.50245800
C	1.55910900	2.97202700	0.68411000
C	1.57981700	2.11382900	1.82081500

C	2.59320900	1.07113300	1.59333100
C	3.19517600	1.30082000	0.31822700
C	2.68236500	2.59447100	-0.22504100
C	-3.45239700	-3.55969000	0.14211100
C	3.39455800	3.57552300	-1.14771000
C	1.00935500	-0.03271000	4.32587500
C	-3.44500300	3.52852300	0.31809400
C	3.36202100	-3.48567300	-1.35844900
C	-3.06306700	-5.03534900	-0.07192900
C	-4.91003700	-3.49063100	0.53003900
C	4.85273300	3.35460900	-1.47022000
C	3.01279800	5.04602800	-1.01970000
C	2.10416100	0.85996100	4.89682900
C	0.31288600	-0.87215200	5.37222400
C	-3.63812700	4.04927800	1.75583400
C	-4.36607000	4.28750400	-0.60524100
C	3.63069600	-3.98031500	-2.77432200
C	4.20836800	-4.17138400	-0.31145800
O	4.31799300	-3.81837400	0.84138500
O	4.79933500	-5.26319000	-0.83454000
O	4.79061900	-3.46770400	-3.22061800
O	2.91539300	-4.72216700	-3.40454500
C	5.19010700	-3.87946400	-4.55065000
C	6.50367800	-3.18924800	-4.86341900
C	5.62326700	-6.05365900	0.06158400

C	7.03743500	-5.50071900	0.14324500
O	-5.23319600	5.02564000	-0.17464400
O	-4.13316600	4.08153200	-1.90476900
C	-4.96509200	4.80985500	-2.84751000
C	-6.26457400	4.07024800	-3.12177800
O	-2.87226900	4.84593400	2.23787400
O	-4.66223900	3.58114200	2.49425400
C	-5.76835100	2.82409700	1.95904500
C	-6.60032300	2.36896000	3.14504000
O	2.02417400	2.05679200	5.04436900
O	3.17141600	0.10633900	5.21598200
C	4.29856900	0.79563500	5.81540700
C	5.22957000	1.35537300	4.75119300
O	-0.43286900	-1.79892100	5.14514500
O	0.60638400	-0.41474800	6.60431500
C	-0.00927100	-1.10457100	7.72329100
C	0.79866100	-2.32700000	8.12951300
O	-3.07939300	-5.50528200	-1.18421900
O	-2.69939300	-5.79464200	0.97126200
C	-2.83260000	-5.42131500	2.36246800
C	-3.57380100	-6.53605100	3.07989200
O	-5.47592700	-4.43308600	1.05172700
O	-5.50978100	-2.32661400	0.25769100
C	-6.90957000	-2.23869100	0.63415500
C	-7.43321900	-0.90315900	0.14381300

O	2.45337600	5.69334500	-1.87367900
O	3.39176600	5.51543400	0.17899700
C	3.10035200	6.91286900	0.43362800
C	3.56297400	7.22196700	1.84407400
O	5.40349800	2.27691200	-1.50815100
O	5.45702700	4.52934200	-1.73607400
C	6.86828900	4.47656700	-2.07090700
C	7.73074500	4.46285100	-0.81851100
C	-4.10012200	-1.66313900	-3.80109000
C	-3.74745000	0.44066600	-4.51916700
H	4.39824000	-3.60009600	-5.25250200
H	5.28002400	-4.97032000	-4.56515300
H	6.39044300	-2.10117100	-4.82904400
H	6.84015900	-3.47096000	-5.86714700
H	7.27842900	-3.47813300	-4.14597900
H	5.60422900	-7.05358300	-0.37734400
H	5.14490900	-6.07700300	1.04336500
H	7.03834100	-4.50567700	0.59669300
H	7.48876600	-5.43736300	-0.85210900
H	7.65640300	-6.16131700	0.76118000
H	-4.34291100	4.88161800	-3.74213700
H	-5.14830500	5.80963300	-2.44847500
H	-6.06657300	3.05140300	-3.47019400
H	-6.83147300	4.59656800	-3.89807900
H	-6.88124500	4.02391100	-2.21986000

H	-5.39705700	1.96423700	1.39265900
H	-6.34096400	3.47234600	1.29157600
H	-6.01272700	1.72602400	3.80767600
H	-7.47213200	1.80535700	2.79395200
H	-6.95301400	3.22967500	3.72106600
H	4.79063500	0.02751500	6.41674900
H	3.91855100	1.58337700	6.47028600
H	6.10912500	1.80272100	5.22865000
H	4.72551100	2.12824300	4.16459400
H	5.56753000	0.56407100	4.07487200
H	-1.03128000	-1.37307800	7.44622500
H	-0.03169500	-0.35258900	8.51500800
H	1.83228200	-2.05099300	8.36128900
H	0.80199100	-3.07200900	7.32913800
H	0.35469400	-2.78246000	9.02214200
H	-3.36653000	-4.47711800	2.46255200
H	-1.81731900	-5.29318700	2.74944600
H	-3.05851600	-7.49235900	2.94693300
H	-4.59058900	-6.62427000	2.68753600
H	-3.62663600	-6.31546400	4.15232600
H	-6.98133800	-2.33823600	1.72166900
H	-7.44218700	-3.08204800	0.18608600
H	-7.34224600	-0.82180100	-0.94386700
H	-6.88354900	-0.07397100	0.59988800
H	-8.49133600	-0.80462100	0.40965500

H	2.02503100	7.07057800	0.30758900
H	3.61910400	7.51731500	-0.31734700
H	3.35633700	8.27178600	2.07875600
H	4.63887200	7.04976200	1.95081900
H	3.03777700	6.59603600	2.57202800
H	7.03158300	5.37817000	-2.66530200
H	7.04659900	3.59406100	-2.68949300
H	7.50882300	5.32688700	-0.18409500
H	8.78954000	4.50303700	-1.09887900
H	7.56189200	3.54801100	-0.24387000
H	-4.60511800	-2.55459300	-3.42508400
H	-3.93137600	1.47942800	-4.80135700
C	-4.91669200	-0.35987200	-3.91094500
H	-5.76066500	-0.45273900	-4.60090900
H	-5.26512700	0.02595700	-2.94694000
C	-3.51974900	-1.75157000	-5.19988200
H	-3.23026200	-2.67370400	-5.69174200
C	-3.31263900	-0.49848800	-5.62947600
H	-2.81726700	-0.18875600	-6.54328800

Vibrational frequencies for theoretical product (13b₁)

13.08	13.42	16.35	18.75	26.71	29.04
29.82	31.80	31.98	33.68	34.06	34.87
36.78	37.46	40.38	41.35	43.37	47.05

47.89	53.63	58.42	59.84	60.89	64.86
66.80	68.61	74.35	76.10	80.65	83.75
84.83	87.20	88.60	91.66	93.27	98.64
100.73	104.66	106.01	106.78	109.60	110.47
113.74	115.25	122.37	125.02	129.88	131.89
134.22	140.70	144.94	149.88	150.55	158.24
160.98	164.86	172.87	179.66	181.92	185.22
192.22	195.44	199.88	209.65	215.43	217.02
218.37	223.90	227.77	228.69	232.98	234.11
243.42	248.16	258.04	258.97	259.85	264.41
266.08	270.85	273.66	279.99	285.86	290.77
301.15	303.27	309.71	316.83	322.48	324.72
326.61	333.40	335.82	341.78	343.67	344.38
346.58	353.32	357.86	361.43	369.01	376.55
380.72	385.97	387.10	387.85	394.02	397.79
399.78	405.46	408.06	410.89	417.02	423.06
427.71	431.26	437.54	443.63	446.73	451.14
452.41	454.11	456.04	459.08	462.98	466.82
470.87	473.30	480.61	485.13	497.73	500.79
517.55	522.31	530.56	531.80	537.40	541.50
546.26	550.71	552.66	554.55	558.88	563.18
564.38	569.42	573.16	575.67	576.85	582.74
589.02	593.32	597.06	604.98	618.43	627.16
630.23	635.90	639.08	641.53	647.15	650.94

655.69	662.88	666.31	669.61	673.29	675.47
684.63	685.79	691.98	692.22	696.27	705.34
708.82	709.36	716.61	720.89	727.33	728.42
731.82	733.66	736.31	738.17	740.27	741.34
741.43	744.75	745.70	749.09	751.20	751.87
754.14	755.92	758.98	761.58	766.60	767.82
770.38	771.64	780.94	782.71	787.08	788.30
792.24	794.72	795.81	799.29	801.23	806.48
811.81	815.18	815.78	818.10	819.32	820.46
820.65	823.42	825.30	826.31	827.33	829.90
831.75	832.88	835.36	835.50	837.97	841.15
845.83	846.87	850.99	858.83	865.44	870.20
873.00	873.61	875.77	880.91	882.85	890.61
893.15	898.23	901.13	906.54	916.04	919.40
925.31	926.78	930.84	934.05	935.22	939.26
947.52	949.89	951.51	956.18	964.32	966.97
975.62	982.16	992.50	999.61	1002.79	1012.91
1021.52	1025.20	1028.98	1033.94	1036.44	1040.61
1042.33	1043.79	1053.95	1054.22	1057.46	1061.15
1063.57	1070.50	1088.34	1089.41	1094.92	1099.20
1105.87	1109.23	1111.59	1115.80	1121.67	1128.86
1129.23	1129.64	1129.96	1130.20	1132.94	1135.72
1137.63	1141.27	1142.60	1145.59	1147.24	1148.23
1149.14	1150.06	1152.39	1158.36	1169.43	1175.08

1179.22	1186.11	1187.40	1189.35	1191.46	1192.05
1192.14	1192.40	1199.44	1204.58	1207.17	1208.83
1209.07	1210.69	1211.56	1213.94	1222.16	1232.26
1235.37	1236.80	1240.95	1248.47	1250.84	1256.10
1257.80	1262.63	1265.07	1269.02	1271.14	1275.64
1276.68	1277.05	1287.03	1288.50	1290.11	1290.39
1293.40	1298.09	1301.68	1306.65	1307.74	1308.26
1308.56	1310.44	1312.24	1314.88	1317.02	1324.65
1326.15	1334.57	1341.99	1342.38	1342.47	1342.57
1343.02	1345.06	1346.86	1351.42	1352.57	1359.03
1363.01	1369.16	1373.36	1376.28	1377.34	1383.65
1389.57	1393.22	1397.16	1398.63	1404.00	1405.56
1408.46	1413.03	1413.67	1416.25	1416.81	1418.12
1419.01	1419.44	1419.56	1419.77	1420.33	1421.10
1422.35	1423.53	1427.59	1433.13	1443.75	1443.80
1444.76	1444.86	1444.89	1445.54	1446.69	1447.64
1448.99	1450.81	1451.57	1452.11	1470.12	1501.87
1512.88	1514.48	1514.80	1515.02	1515.12	1515.20
1515.75	1515.79	1516.25	1516.76	1517.88	1518.63
1518.73	1519.01	1519.42	1523.62	1524.23	1524.54
1526.15	1526.73	1530.40	1534.00	1535.91	1536.26
1536.34	1536.70	1541.01	1543.45	1543.54	1544.18
1548.79	1566.66	1569.08	1570.89	1575.15	1578.74
1583.16	1589.50	1597.38	1606.59	1609.96	1619.14

1622.99	1624.31	1626.73	1630.85	1655.11	1670.27
1776.90	1780.16	1811.39	1812.48	1813.84	1826.61
1827.76	1828.68	1831.69	1837.75	3061.94	3062.09
3062.11	3062.47	3062.50	3062.73	3062.75	3062.78
3063.10	3063.98	3077.01	3077.53	3077.70	3081.37
3082.73	3092.15	3095.06	3099.50	3099.63	3099.87
3102.79	3116.47	3118.33	3122.90	3126.10	3128.69
3129.48	3129.88	3130.24	3130.26	3130.37	3130.49
3130.55	3133.50	3133.85	3134.02	3134.49	3137.87
3140.41	3141.57	3141.62	3141.81	3142.00	3144.41
3146.06	3147.55	3149.81	3152.63	3160.87	3162.81
3162.82	3162.99	3164.83	3175.34	3219.49	3242.53

Coordinates for theoretical product (13b₂)

Energy = -5348.58094573 Hartrees

C -1.58564300 -2.09179900 -2.91424100
C -1.52477300 -2.94328100 -1.79141400
C -2.85092800 -1.23745800 -2.89417800
C -2.66832000 -2.64805700 -0.87637100
C -3.23935800 -1.37878100 -1.42925600
C 0.90479000 -3.09229700 -2.02323800
C -0.29215200 -3.41223200 -1.33002900
C 0.85136600 -2.23276900 -3.11747700
C -0.41125500 -1.73263500 -3.56724000

C	-3.21539600	-0.33356000	0.80649700
C	-3.51135100	-0.31343100	-0.63355300
C	-2.62207000	-1.43779100	1.41902700
C	-2.33734300	-2.68703000	0.65677500
C	0.00606000	-3.46606400	0.10809500
C	-0.93834300	-3.05091900	1.04323200
C	-2.62657500	0.28464400	-3.38634400
C	-2.82389700	1.35037500	-2.31147200
C	-1.19711000	0.59657000	-3.82492400
C	-3.37347400	1.08387600	-1.09503100
C	-0.21898400	-0.34968800	-4.03170400
C	-0.53322600	-2.23758000	2.13935000
C	-1.57758900	-1.22802100	2.37145900
C	-2.88743600	0.98672100	1.22642700
C	-3.12726700	1.94548200	0.10239900
C	-1.80740700	2.39172700	-2.44851100
C	-0.82139600	1.90930500	-3.37397400
C	1.18043900	-0.02370700	-3.84302700
C	1.85217500	-1.16708600	-3.28699200
C	2.03902000	-3.08008100	-1.05311000
C	1.39102800	-3.17316900	0.29379200
C	1.77267100	-2.36779500	1.36727400
C	0.81307900	-1.93940400	2.33392200
C	1.26261100	-0.63927400	2.91494300
C	0.14699100	0.45192600	3.16418800

C	-1.24762100	0.05948200	2.79501600
C	-1.88350200	1.17845200	2.17644000
C	-0.89335500	2.25370900	2.01904700
C	-0.93934000	3.11585600	0.92704300
C	-2.06946700	3.11154300	-0.04927000
C	-1.41487700	3.20241600	-1.38568300
C	-0.02155800	3.49624100	-1.19432800
C	0.93259200	3.08656400	-2.11766600
C	0.53071000	2.25358400	-3.20175400
C	1.55793500	1.26521400	-3.44354400
C	2.62219900	1.46578800	-2.50676600
C	3.21999300	0.34902800	-1.93106200
C	2.87149400	-0.97735200	-2.36165500
C	3.10662700	-1.92622700	-1.22907400
C	3.34842300	-1.05005900	-0.04488200
C	2.76370400	-1.29624700	1.19509700
C	2.40980000	-0.21526500	2.05404800
C	0.35334700	1.78005300	2.51498100
C	0.26699100	3.44894000	0.24644100
C	2.32894000	2.71529800	-1.73320300
C	3.50420500	0.29649100	-0.49157300
C	1.49333200	2.98325000	0.72209000
C	1.52778000	2.10756700	1.84473300
C	2.57083300	1.09673500	1.61002300
C	3.17700300	1.36372900	0.34408600

C	2.63367200	2.65169700	-0.18308100
C	-3.32888200	-3.68024000	0.03118100
C	3.32550600	3.66691800	-1.08397500
C	0.99132400	-0.09613000	4.30943300
C	-3.51832500	3.41356900	0.32505400
C	3.48853000	-3.38808200	-1.40758000
C	-2.87807800	-5.13522500	-0.20061000
C	-4.79651500	-3.67521300	0.37632200
C	4.79166700	3.49154300	-1.39834300
C	2.90215300	5.12416500	-0.93637900
C	2.05765000	0.81215900	4.90828100
C	0.30178200	-0.96612700	5.33582300
C	-3.73133200	3.89819400	1.77272700
C	-4.41732700	4.21096300	-0.58680100
C	3.78321500	-3.85202600	-2.82857600
C	4.34507300	-4.06636400	-0.36387700
O	4.43692800	-3.72728300	0.79466500
O	4.96879600	-5.13427000	-0.89798900
O	4.93530100	-3.30486600	-3.25381600
O	3.09193000	-4.59929200	-3.47885800
C	5.35856200	-3.68545700	-4.58579900
C	6.65975600	-2.96125300	-4.87242600
C	5.80873500	-5.91418500	-0.00744000
C	7.20681600	-5.32410000	0.08982800
O	-5.19780400	5.03358900	-0.14357800

O	-4.25979500	3.95426400	-1.88917800
C	-5.01385700	4.78593600	-2.81326800
C	-6.44623800	4.30351000	-2.97653500
O	-2.96372000	4.66234600	2.30127900
O	-4.78551300	3.42903100	2.46805000
C	-5.87973700	2.69997300	1.87564100
C	-6.76499900	2.23736400	3.01974000
O	1.96415000	2.00917200	5.04506400
O	3.12162100	0.06966400	5.26408300
C	4.22655700	0.77431000	5.88681600
C	5.17833700	1.33557400	4.84192300
O	-0.36886400	-1.94435600	5.09215800
O	0.50113300	-0.46641900	6.57057500
C	-0.12359400	-1.17343700	7.67349100
C	0.75603900	-2.31187700	8.16529600
O	-2.82168400	-5.58274300	-1.32024600
O	-2.53514400	-5.90231400	0.84541900
C	-2.73964900	-5.55497000	2.23343200
C	-3.51113000	-6.68286500	2.89687700
O	-5.37593300	-4.69039300	0.71485800
O	-5.39188900	-2.48052900	0.28486300
C	-6.80658200	-2.46034300	0.61074100
C	-7.30043700	-1.04092100	0.41312900
O	2.33303500	5.76928200	-1.78565900
O	3.25674600	5.58490800	0.27300900

C	2.92534100	6.97001800	0.54567300
C	3.36424400	7.26930800	1.96577300
O	5.37207200	2.43009400	-1.44953700
O	5.36528400	4.68668800	-1.63993700
C	6.77977300	4.67825500	-1.96514700
C	7.63375700	4.66669300	-0.70697000
H	4.56845900	-3.41214900	-5.29200700
H	5.47296800	-4.77365200	-4.61710000
H	6.52195200	-1.87664500	-4.82187100
H	7.01330000	-3.21907100	-5.87668900
H	7.43287400	-3.24461400	-4.15103000
H	5.81939800	-6.90825200	-0.45976100
H	5.32565800	-5.96370800	0.97104100
H	7.17820200	-4.33572600	0.55681300
H	7.66140900	-5.23464000	-0.90202400
H	7.84039500	-5.97601500	0.70214600
H	-4.45149900	4.70784200	-3.74598100
H	-4.98123100	5.81687900	-2.45351900
H	-6.47348800	3.25524000	-3.29090000
H	-6.94865800	4.90361000	-3.74374700
H	-6.99967300	4.40936600	-2.04027900
H	-5.49918900	1.84611100	1.30598000
H	-6.41993200	3.36851200	1.20010500
H	-6.21407200	1.57250000	3.69226300
H	-7.63275500	1.69659600	2.62589100

H	-7.12377100	3.09397300	3.59810300
H	4.71070300	0.01554300	6.50615300
H	3.82229300	1.56306700	6.52577400
H	6.03998400	1.79760200	5.33768700
H	4.68041300	2.09712100	4.23562600
H	5.54292900	0.54245200	4.18173500
H	-1.10117900	-1.53416100	7.34587800
H	-0.25586300	-0.40455100	8.43790200
H	1.74790000	-1.94363000	8.44606800
H	0.86868500	-3.07672000	7.39176500
H	0.29884300	-2.77769500	9.04581900
H	-3.27726200	-4.61124300	2.32553300
H	-1.74502300	-5.42970800	2.67200800
H	-2.98460100	-7.63459800	2.77599600
H	-4.50600800	-6.77066000	2.45174800
H	-3.61894300	-6.47881400	3.96850100
H	-6.93079300	-2.80255700	1.64258000
H	-7.32108800	-3.17318200	-0.04024400
H	-7.13591600	-0.70798600	-0.61639100
H	-6.78230400	-0.35085800	1.08578100
H	-8.37377000	-0.99245100	0.62683900
H	1.84766200	7.10115800	0.40979500
H	3.43605200	7.59947500	-0.19012900
H	3.12736300	8.30958800	2.21400600
H	4.44309900	7.12382100	2.08190600

H	2.84797500	6.61859100	2.67820400
H	6.92230600	5.59402800	-2.54299100
H	6.98636600	3.81167500	-2.59730800
H	7.38415400	5.51347400	-0.05969200
H	8.69290700	4.74044900	-0.97904700
H	7.48614200	3.73797200	-0.14900500
C	-3.50903800	-1.02961200	-5.21115200
H	-4.19791100	-1.19819400	-6.04387500
H	-2.48810000	-1.26982100	-5.52396300
C	-3.95785600	-1.75063700	-3.92438300
H	-4.02248000	-2.83992100	-3.94526100
C	-3.66422900	0.37750500	-4.59854000
H	-3.46708800	1.23716200	-5.24211200
C	-5.23665000	-0.99468200	-3.61335700
H	-6.08023500	-1.40459900	-3.06848300
C	-5.06055200	0.27280500	-4.01172300
H	-5.73241700	1.11010400	-3.85860100

Vibrational frequencies for theoretical product (13b₂)

12.59	12.96	16.53	21.11	26.78	27.18
29.22	30.65	31.22	32.62	34.12	36.51
37.29	38.96	40.78	42.52	44.23	45.73
54.12	55.78	57.15	60.20	64.21	64.66
68.15	72.73	74.14	76.19	80.31	83.19

85.03	86.58	87.51	90.43	92.97	98.22
100.37	104.30	105.71	106.74	108.80	111.02
112.44	119.59	122.72	125.68	131.58	132.28
133.31	143.44	143.96	149.29	151.02	155.41
160.15	167.46	171.94	179.56	182.31	184.78
187.08	196.27	200.14	208.72	213.28	214.78
217.15	225.60	226.88	229.80	233.39	235.06
242.06	248.60	257.64	258.27	259.91	263.68
266.51	270.54	272.63	279.06	285.54	292.33
300.85	303.18	310.18	319.31	321.98	324.18
326.05	332.65	334.86	338.10	343.11	345.58
347.93	353.20	358.64	360.70	369.51	377.15
380.91	385.64	388.63	389.46	393.47	397.82
401.66	402.35	407.71	412.41	414.27	424.02
427.83	432.93	438.79	440.21	445.48	450.01
451.82	453.09	455.08	460.76	462.31	465.51
469.22	472.74	481.16	488.29	496.79	500.43
518.40	524.82	530.72	531.83	535.47	541.35
544.78	552.25	552.66	554.58	561.53	562.71
566.96	568.98	573.89	575.66	576.69	581.40
587.79	593.86	595.85	601.79	620.05	626.64
631.23	635.51	639.29	640.70	646.35	649.69
653.45	662.26	666.17	669.10	672.98	674.34
682.86	685.80	691.01	693.67	696.69	705.79

709.16	709.26	716.82	720.71	727.27	728.23
731.73	732.28	735.42	738.31	740.39	741.10
742.21	743.82	745.32	749.03	749.79	751.32
755.92	756.92	757.66	760.23	765.13	767.22
768.34	770.24	779.90	784.19	786.93	789.53
791.14	792.30	795.18	798.06	800.03	807.04
809.88	815.05	815.32	817.45	819.14	819.84
821.41	823.42	824.77	825.68	828.49	830.88
833.28	833.57	835.12	836.53	837.38	843.25
844.49	845.96	854.02	857.68	864.65	870.04
872.89	873.61	876.10	878.97	881.00	891.84
896.74	897.33	900.67	907.21	917.34	919.49
922.40	927.36	929.55	934.34	934.86	937.91
939.48	948.99	951.08	954.67	965.74	967.07
973.31	981.99	990.09	998.82	1007.55	1013.42
1019.42	1025.51	1029.35	1033.88	1035.95	1040.02
1041.30	1044.75	1053.72	1055.51	1057.42	1061.76
1064.24	1074.69	1088.61	1089.53	1089.81	1098.93
1105.51	1109.12	1110.29	1116.12	1121.07	1128.27
1128.89	1129.53	1129.93	1130.18	1133.15	1134.64
1137.51	1141.02	1142.36	1146.52	1148.37	1148.69
1149.59	1150.42	1152.05	1155.50	1169.26	1175.70
1179.41	1185.50	1186.03	1188.70	1191.40	1192.28
1192.36	1192.70	1198.86	1205.24	1206.73	1208.53

1209.15	1211.12	1212.46	1214.55	1221.58	1232.17
1234.66	1236.37	1241.28	1247.32	1250.74	1255.67
1256.88	1262.14	1265.71	1268.47	1272.59	1274.92
1276.45	1277.04	1287.88	1288.26	1289.89	1291.13
1292.58	1299.37	1301.81	1307.65	1308.16	1308.42
1308.55	1309.39	1311.83	1314.77	1317.80	1324.61
1326.23	1334.26	1341.56	1341.83	1342.22	1342.52
1343.29	1345.39	1346.87	1351.41	1352.63	1357.86
1362.58	1369.43	1373.16	1374.92	1377.56	1383.30
1389.56	1392.91	1397.14	1398.62	1404.11	1406.07
1408.53	1413.08	1413.90	1416.14	1416.78	1418.39
1418.52	1418.98	1419.60	1419.86	1420.67	1420.76
1421.42	1423.49	1427.48	1433.16	1443.20	1443.73
1444.26	1444.41	1444.73	1445.30	1446.71	1448.16
1448.65	1451.46	1451.79	1452.01	1469.81	1501.31
1511.91	1513.73	1514.62	1514.71	1515.42	1515.66
1515.79	1515.84	1516.29	1516.79	1517.61	1517.90
1518.43	1518.53	1519.03	1524.94	1525.23	1526.02
1526.69	1528.38	1530.48	1533.94	1535.49	1535.92
1536.51	1537.01	1542.24	1543.48	1543.95	1544.18
1548.59	1566.59	1568.82	1570.92	1574.85	1579.01
1583.20	1589.52	1597.05	1607.03	1609.84	1619.07
1623.04	1624.31	1626.70	1630.64	1656.49	1669.49
1775.69	1779.07	1812.64	1812.67	1814.04	1827.67

1829.29	1829.64	1831.95	1839.66	3061.93	3062.09
3062.42	3062.47	3062.74	3062.81	3062.96	3063.02
3064.79	3065.39	3077.02	3077.32	3077.62	3082.48
3086.36	3090.27	3095.07	3099.54	3099.72	3099.90
3100.97	3116.50	3118.32	3122.10	3124.72	3129.54
3130.07	3130.23	3130.47	3130.49	3130.55	3130.80
3133.63	3133.64	3133.92	3135.20	3137.03	3138.92
3140.43	3140.46	3141.51	3142.07	3144.39	3146.09
3146.96	3147.96	3148.74	3150.10	3160.89	3162.32
3162.81	3163.06	3166.72	3167.79	3216.59	3240.56

Coordinates for theoretical product (13c₁)

Energy = -5348.54023344 Hartrees

C -0.49694500 -1.91004200 -3.27137100
C -0.31065000 -2.85724600 -2.22779800
C -1.80484400 -1.33829200 -3.14587200
C -1.60156100 -3.06589400 -1.48587500
C 2.07279800 -2.21616200 -2.14328900
C 0.95070600 -2.95632200 -1.64476500
C 1.90331600 -1.31376800 -3.18351300
C 0.59501900 -1.16107100 -3.76324500
C -3.06216400 -1.14339700 0.28074100
C -2.18345800 -2.05730400 0.85580700
C -1.41381500 -3.08622100 0.06395200

C	1.09710300	-3.05446600	-0.19064500
C	-0.03256800	-3.00638100	0.61436400
C	-1.96289800	0.00566600	-3.42691700
C	-2.78302100	0.88099100	-2.56909800
C	-0.85580800	0.79605500	-3.90676600
C	-3.38878300	0.36700800	-1.47575500
C	0.40284400	0.22306200	-4.09187400
C	-0.03022200	-2.24817800	1.80901000
C	-1.35836000	-1.64154100	1.95804000
C	-3.15588400	0.16951000	0.83828900
C	-3.56239400	1.13578400	-0.22075000
C	-2.14667400	2.20838700	-2.54576000
C	-0.97345800	2.13901700	-3.36691700
C	1.59877400	0.95129400	-3.70844900
C	2.53346200	0.01762000	-3.14365300
C	3.03169100	-1.97405300	-1.02053500
C	2.29257500	-2.39059100	0.20823200
C	2.28137200	-1.62753400	1.37457300
C	1.13315100	-1.60437300	2.22166000
C	1.09391900	-0.30208900	2.94791800
C	-0.31856000	0.36699700	3.11097700
C	-1.48077900	-0.37701500	2.52617600
C	-2.35945900	0.56114500	1.91421900
C	-1.73422700	1.89484300	1.96596800
C	-1.92009600	2.82346700	0.94628300

C	-2.87647900	2.58953800	-0.17032300
C	-2.13757800	2.99366800	-1.39740000
C	-0.93480800	3.67389100	-1.00835700
C	0.18930500	3.65655800	-1.82619000
C	0.17879000	2.85091000	-3.00566800
C	1.48995200	2.24103500	-3.17270000
C	2.32201500	2.65068100	-2.08533800
C	3.18354400	1.72020100	-1.50640000
C	3.32461100	0.40846000	-2.06878500
C	3.71067400	-0.54005700	-0.98274800
C	3.53451400	0.23435100	0.28526100
C	2.91405800	-0.30280200	1.41262900
C	2.14838500	0.52885000	2.28638800
C	-0.46255400	1.75928300	2.59194900
C	-0.80382800	3.56506900	0.45421000
C	1.58000000	3.67591300	-1.28462000
C	3.30885900	1.60657600	-0.04410400
C	0.44605500	3.43644900	1.05988000
C	0.62011200	2.49060500	2.11452700
C	1.94150500	1.86475500	1.95603500
C	2.57121500	2.42854100	0.80549200
C	1.72926700	3.55143300	0.30094700
C	-1.84531700	-4.34155800	-0.67413400
C	2.20710500	4.76988100	-0.45291500
C	0.51878200	-0.01830000	4.33279000

C	-4.36424600	2.40381200	-0.03902000
C	4.53306600	-1.80448300	-1.19509200
C	-0.81975300	-5.47880900	-0.90978900
C	-3.15367200	-5.03566400	-0.33345200
C	3.72281700	4.98472700	-0.57147500
C	1.43361600	6.08994700	-0.30860000
C	1.12243200	1.13801400	5.13935500
C	0.00025200	-1.15686400	5.17866800
C	-4.98211700	2.77790000	1.32105100
C	-5.23581100	2.88575900	-1.19384500
C	5.10149300	-2.04758000	-2.58921900
C	5.46160500	-2.24139500	-0.08498900
O	5.16610900	-2.30853100	1.08749700
O	6.68329500	-2.51426400	-0.58039800
O	4.98340900	-3.34905000	-2.90159400
O	5.58376400	-1.19657000	-3.29892700
C	5.51171700	-3.75983900	-4.18934700
C	6.99936000	-4.06231800	-4.10212200
C	7.70082800	-2.92234900	0.37189700
C	7.63461200	-4.41702400	0.64244800
O	-5.90368100	2.16892600	-1.91139700
O	-5.19027600	4.21750300	-1.27835100
C	-5.99934400	4.83102300	-2.31817900
C	-5.80328900	6.33030000	-2.21441900
O	-4.54183900	3.67777700	1.99022800

O	-6.08908600	2.12478600	1.72608800
C	-6.57792000	0.90479000	1.11605000
C	-7.96475300	0.65809600	1.68210900
O	0.53962400	2.17920500	5.31292000
O	2.35554100	0.97064500	5.66063300
C	3.11512500	-0.25272700	5.54552400
C	4.43029000	-0.02001800	6.26775000
O	-0.37861800	-2.22914500	4.76244700
O	-0.00540100	-0.79871900	6.47856900
C	-0.55549600	-1.75573500	7.42380600
C	-2.06742100	-1.62667200	7.51451300
O	-0.40744300	-5.73770800	-2.01241300
O	-0.43705900	-6.24128100	0.13307500
C	-0.85882600	-6.08529500	1.51206500
C	0.33157300	-6.42173500	2.39169700
O	-3.70980600	-4.95959900	0.74242700
O	-3.53502500	-5.84293300	-1.33800100
C	-4.69394800	-6.69017600	-1.10698000
C	-4.30182500	-7.98292000	-0.40977500
O	0.81714500	6.56729500	-1.23391500
O	1.50886100	6.75029300	0.85410900
C	2.10065500	6.21967700	2.07585000
C	2.43739600	7.41144500	2.95242200
O	4.48178700	4.69518300	0.32608900
O	4.20933500	5.52661200	-1.69635600

C	3.42655500	5.95199900	-2.84489200
C	4.23762500	5.63126300	-4.08682800
H	5.30573200	-2.97181400	-4.91742700
H	4.93148100	-4.64996100	-4.44205400
H	7.19680500	-4.82793100	-3.34477100
H	7.56285300	-3.16011000	-3.84892100
H	7.35785300	-4.43352600	-5.06907900
H	7.57092300	-2.34213400	1.28819600
H	8.63934500	-2.63875900	-0.10919000
H	6.69322700	-4.68084400	1.13232200
H	8.45983200	-4.70902500	1.30198700
H	7.72070400	-4.98549400	-0.28910900
H	-7.04141900	4.53357800	-2.16507600
H	-5.67360500	4.43345400	-3.28415200
H	-5.89311500	0.09188100	1.38032400
H	-6.60583800	1.00788000	0.02940600
H	-8.37073200	-0.27459800	1.27518800
H	-8.64265500	1.47555100	1.41759700
H	-7.92989500	0.57605500	2.77260200
H	3.28618900	-0.48600600	4.49083300
H	2.55733700	-1.07373900	6.00735400
H	4.25702400	0.22298600	7.32052700
H	4.98060400	0.80596400	5.80739700
H	5.04818800	-0.92285000	6.21311900
H	-0.07024200	-1.49990700	8.36802500

H	-0.25448100	-2.76019600	7.11706000
H	-1.68732800	-6.78144800	1.67959500
H	-1.22123600	-5.07591700	1.70092200
H	0.69937900	-7.43014300	2.17835700
H	0.03647100	-6.37175200	3.44551900
H	1.14620500	-5.71063000	2.22601400
H	-5.08467200	-6.87663500	-2.10936800
H	-5.42876900	-6.12695500	-0.52724000
H	-5.17475400	-8.64194800	-0.34066800
H	-3.94411700	-7.78494400	0.60465300
H	-3.51874200	-8.50431400	-0.96883300
H	2.98941500	5.63119300	1.84492400
H	1.35496100	5.57491900	2.55044500
H	1.54469500	8.01086000	3.15504400
H	3.18535200	8.04973100	2.47164800
H	2.84360500	7.05882500	3.90652600
H	3.25775200	7.02779400	-2.73747200
H	2.45494200	5.46073300	-2.85643900
H	4.38310900	4.55118900	-4.18615100
H	5.21949700	6.11263800	-4.04634700
H	3.70849000	5.99427700	-4.97489600
H	-4.75210800	6.59743500	-2.35880500
H	-6.12233100	6.69936600	-1.23493600
H	-6.39790800	6.83258300	-2.98512700
H	-2.44801300	-2.30062200	8.29051300

H	-2.35482200	-0.60320900	7.77443000
H	-2.53734200	-1.89741100	6.56485300
C	-2.67801900	-2.11945000	-2.16461400
C	-3.51423000	-1.12118400	-1.19137700
C	-5.02974700	-1.53234100	-1.52731700
H	-5.72964800	-1.17258500	-0.77260700
C	-3.86582100	-2.92303700	-2.85907300
H	-3.52128100	-3.84690800	-3.32578100
C	-4.60366900	-1.93736300	-3.75494100
H	-4.48244200	-1.87337300	-4.83073700
C	-5.29266800	-1.10318500	-2.96347800
H	-5.84361300	-0.21433100	-3.24644700
C	-4.89906000	-3.03947100	-1.71281300
H	-4.56400300	-3.51720600	-0.79936000
H	-5.82792200	-3.50879800	-2.05036400

Vibrational frequencies for theoretical product (13c₁)

16.00	16.79	20.81	22.78	27.12	30.46
30.63	33.67	34.04	35.51	36.82	37.90
39.10	39.89	40.95	42.09	47.50	48.42
49.66	54.40	55.71	61.42	63.17	65.00
66.67	69.26	70.79	74.34	76.36	77.81
83.93	91.77	92.48	95.44	97.22	98.94
103.75	107.46	108.36	112.04	113.98	118.33

119.05	122.49	124.08	125.87	130.66	132.81
138.38	142.94	146.34	148.22	152.46	159.01
161.09	172.00	173.40	177.30	181.08	186.79
189.96	192.87	195.79	204.09	209.18	213.05
215.16	222.66	228.56	231.87	233.39	236.92
240.08	244.68	250.87	255.32	261.46	263.31
266.25	267.10	269.62	274.32	277.26	283.14
288.52	297.33	302.56	308.75	311.07	323.11
329.70	332.03	333.47	334.93	336.54	338.72
342.30	342.60	349.68	353.72	358.18	368.98
370.76	382.80	384.84	387.51	391.21	398.42
403.08	409.18	411.74	423.11	424.58	426.80
435.32	438.42	443.92	447.33	449.64	454.72
457.31	462.57	467.56	469.27	475.21	479.65
483.98	485.29	487.70	492.20	499.44	513.88
519.95	523.50	527.12	534.44	536.24	542.11
545.26	549.38	552.11	556.33	560.12	563.67
567.03	568.58	571.95	573.61	576.69	584.42
586.35	588.42	591.98	601.52	606.09	609.53
617.11	623.08	633.08	637.84	641.46	645.33
648.19	655.81	659.36	661.15	665.54	666.58
677.87	681.50	683.49	685.11	690.70	695.51
706.80	708.12	711.77	713.23	718.82	722.34
725.53	727.38	728.79	731.34	732.24	735.42

742.18	743.35	745.77	747.76	748.48	750.25
751.53	752.70	755.69	758.12	759.66	761.25
762.39	767.04	770.56	773.91	774.71	781.28
785.10	786.50	789.05	790.35	794.28	798.08
801.51	807.80	809.10	812.62	814.89	817.72
819.71	822.96	823.12	826.27	828.01	830.61
833.96	835.21	835.83	837.41	840.47	841.77
844.30	844.96	852.79	858.20	859.50	865.76
871.31	873.19	882.43	883.83	894.93	901.96
902.63	904.01	906.66	913.35	925.12	927.25
928.39	931.29	939.34	944.33	948.68	949.51
954.00	959.38	961.58	963.27	965.83	972.64
976.42	981.37	994.43	1004.38	1012.30	1018.12
1020.23	1026.60	1027.96	1033.55	1036.44	1037.78
1043.10	1047.52	1050.23	1051.26	1056.23	1060.66
1062.83	1069.00	1075.69	1081.74	1089.83	1092.87
1101.39	1101.85	1105.32	1117.24	1124.36	1128.38
1128.59	1129.00	1129.33	1132.73	1136.19	1136.64
1137.70	1139.87	1140.66	1143.10	1144.09	1146.22
1147.15	1149.67	1153.80	1156.84	1165.07	1166.28
1172.23	1172.97	1182.78	1184.01	1187.00	1189.48
1191.44	1192.06	1194.32	1206.18	1207.23	1208.48
1210.24	1212.04	1217.78	1219.50	1221.71	1227.27
1231.60	1236.74	1240.08	1243.69	1247.65	1248.55

1252.27	1256.20	1258.72	1264.26	1265.51	1269.29
1271.22	1273.43	1279.54	1281.61	1285.36	1290.48
1291.46	1294.87	1302.43	1302.73	1307.23	1308.53
1312.32	1313.55	1324.61	1326.73	1331.29	1332.83
1334.78	1336.35	1337.77	1340.44	1341.12	1341.69
1342.01	1342.23	1343.64	1348.40	1354.88	1357.83
1370.24	1370.61	1374.93	1375.99	1380.79	1382.96
1393.29	1399.26	1401.18	1404.42	1406.13	1410.69
1413.32	1413.36	1417.90	1418.41	1418.69	1419.49
1420.25	1420.95	1421.69	1422.78	1424.81	1425.72
1427.25	1428.14	1430.93	1439.27	1441.78	1443.66
1443.87	1443.95	1445.21	1447.96	1448.32	1451.35
1452.21	1452.88	1454.90	1455.16	1470.13	1481.55
1513.31	1513.39	1514.03	1514.25	1514.77	1515.32
1515.36	1515.37	1515.99	1516.12	1517.65	1517.75
1518.45	1520.06	1520.41	1520.92	1525.73	1527.40
1528.49	1529.00	1529.52	1530.48	1533.36	1534.56
1535.25	1536.77	1538.35	1538.53	1541.92	1543.41
1549.80	1556.13	1568.02	1572.30	1575.03	1579.27
1583.55	1587.41	1595.32	1600.63	1607.02	1613.71
1617.08	1624.29	1628.83	1630.66	1653.35	1679.00
1790.99	1794.06	1807.63	1811.40	1812.39	1813.71
1828.36	1831.05	1836.44	1838.98	3061.36	3062.60
3063.50	3063.72	3063.95	3063.98	3064.27	3064.49

3064.88	3066.20	3073.47	3073.75	3079.21	3080.78
3088.70	3092.48	3098.97	3099.07	3100.11	3100.82
3102.67	3120.95	3122.62	3127.88	3130.32	3133.21
3133.72	3133.77	3134.69	3134.85	3135.05	3136.83
3136.92	3137.13	3137.95	3140.23	3141.09	3141.10
3141.45	3141.97	3143.98	3145.52	3150.24	3150.36
3150.41	3155.61	3161.98	3163.19	3163.61	3163.72
3168.70	3179.92	3184.27	3225.38	3241.04	3255.34

Coordinates for theoretical product (13c₂)

Energy = -5348.53265954 Hartrees

C -0.19940000 -1.87166700 -3.37759300
C -0.08053700 -2.83259300 -2.33314800
C -1.51054600 -1.30347100 -3.32982900
C -1.43161900 -3.05135000 -1.68309100
C 2.28558000 -2.13972800 -2.08157400
C 1.14350600 -2.90373600 -1.66436300
C 2.17681100 -1.23409300 -3.12665700
C 0.90948700 -1.10038200 -3.79204800
C -3.02286500 -1.15207800 -0.01388000
C -2.16038200 -2.04477400 0.61536500
C -1.31912100 -3.04465500 -0.13111400
C 1.19785300 -2.99684900 -0.20415000
C 0.01491700 -2.95393500 0.51493000

C	-1.67517600	0.03097200	-3.62982000
C	-2.56698000	0.88276700	-2.82336900
C	-0.55461800	0.83873300	-4.03500200
C	-3.26112800	0.35420500	-1.79067700
C	0.72010900	0.28267800	-4.13259900
C	-0.07791000	-2.20922200	1.71297400
C	-1.42277400	-1.62643300	1.77406600
C	-3.16568100	0.15746800	0.53690800
C	-3.51183400	1.12703500	-0.54309700
C	-1.95988900	2.21858300	-2.75801500
C	-0.73404200	2.17545400	-3.49789800
C	1.87423200	1.02889100	-3.66573100
C	2.78221700	0.10771500	-3.04065500
C	3.16395500	-1.88448400	-0.89628500
C	2.35260400	-2.31670500	0.27861800
C	2.24872300	-1.55773500	1.44363900
C	1.04473800	-1.55477400	2.21045200
C	0.93396400	-0.25678900	2.93671800
C	-0.49764000	0.38920800	3.00573900
C	-1.60625900	-0.36938300	2.34020500
C	-2.45472000	0.55476200	1.66977600
C	-1.85365500	1.89523000	1.76731600
C	-1.98562800	2.81881900	0.73720200
C	-2.86460700	2.56301500	-0.44120000
C	-2.05428200	3.00241600	-1.61489700

C	-0.89076000	3.70001400	-1.14135900
C	0.29002400	3.70446500	-1.87791000
C	0.37770900	2.90446900	-3.05723700
C	1.70706700	2.31591200	-3.13624700
C	2.45389300	2.73428900	-1.99217300
C	3.28977100	1.81572800	-1.35859000
C	3.48955400	0.50803800	-1.91282100
C	3.81602200	-0.43895200	-0.80670000
C	3.54238100	0.32829800	0.44876800
C	2.85484500	-0.22283400	1.52938600
C	2.01720200	0.59356700	2.35076800
C	-0.62793000	1.78025200	2.48085000
C	-0.85532400	3.58503900	0.32602800
C	1.64039100	3.74446100	-1.24180300
C	3.31651700	1.69813900	0.10834000
C	0.35273800	3.47660900	1.01664900
C	0.47156000	2.53069000	2.07891600
C	1.81073400	1.92703600	2.00978500
C	2.50781500	2.50469900	0.90636800
C	1.68331200	3.61559100	0.34866400
C	-1.71934500	-4.32419900	-0.84636500
C	2.19107800	4.84540400	-0.36580600
C	0.26098200	0.01192200	4.27975800
C	-4.38008000	2.37638600	-0.35441000
C	4.67090900	-1.68883100	-0.97033700

C	-0.68055900	-5.44963000	-1.06456000
C	-3.03068400	-4.95591500	-0.39473600
C	3.70723700	5.08676000	-0.38097500
C	1.38814000	6.15198500	-0.26642200
C	0.79103900	1.17335900	5.12954700
C	-0.29533400	-1.13886500	5.08402300
C	-4.99914100	2.66684100	1.02120000
C	-5.20455000	2.89181800	-1.51082900
C	5.33631300	-1.91036000	-2.32467100
C	5.53035700	-2.11876900	0.19666800
O	5.16233900	-2.18477700	1.34853500
O	6.78150500	-2.38813300	-0.22087400
O	5.25247600	-3.20829700	-2.66188000
O	5.85986200	-1.04586500	-2.98733000
C	5.87341900	-3.59547100	-3.91526300
C	7.35517400	-3.88213500	-3.73007800
C	7.73968000	-2.78916300	0.79380500
C	7.65895000	-4.28221100	1.06935100
O	-4.96998800	2.71027400	-2.68424500
O	-6.24952000	3.61062800	-1.05364400
C	-7.08748400	4.23770600	-2.05944700
C	-8.14291900	5.04438600	-1.32872700
O	-4.61219300	3.57137700	1.71706500
O	-6.01562000	1.88972200	1.45411900
C	-6.57756700	0.80924300	0.68592100

C	-7.81217700	0.33436500	1.43245200
O	0.18473500	2.20675100	5.26409200
O	1.98628500	1.01890800	5.73647400
C	2.76983400	-0.19252600	5.66664900
C	4.01707700	0.04503700	6.49938200
O	-0.61817400	-2.21864800	4.64062600
O	-0.40679400	-0.78274300	6.37960700
C	-1.00695800	-1.75207200	7.28056300
C	-2.52388700	-1.65757600	7.25284100
O	-0.27618100	-5.72461600	-2.16644900
O	-0.22943800	-6.15243700	-0.00519500
C	-0.71725800	-6.03560600	1.35046600
C	0.44492500	-6.33089500	2.28198000
O	-3.73245900	-4.55033800	0.50420600
O	-3.21679900	-6.13834300	-1.02279000
C	-4.38580700	-6.91518100	-0.64922300
C	-4.11340800	-7.81458000	0.54588700
O	0.82979300	6.62728100	-1.22884500
O	1.37249900	6.80411300	0.90334100
C	1.88447700	6.27093600	2.15962600
C	2.10435700	7.45650200	3.08028200
O	4.40798100	4.81032000	0.56676800
O	4.25995900	5.63703400	-1.47046400
C	3.55182700	6.05286300	-2.67015700
C	4.41669100	5.68113200	-3.86064200

H	5.70833400	-2.79995000	-4.64556900
H	5.32284200	-4.48851600	-4.21887100
H	7.50998400	-4.65782900	-2.97309100
H	7.88809300	-2.97753400	-3.42472200
H	7.78399100	-4.23302000	-4.67576100
H	7.55422000	-2.20328200	1.69688000
H	8.70522200	-2.50732600	0.36840700
H	6.69050600	-4.54409200	1.50439400
H	8.44405100	-4.56891700	1.77832900
H	7.80057600	-4.85644200	0.14814400
H	-7.52212900	3.45385400	-2.68790400
H	-6.45247000	4.86197100	-2.69475500
H	-5.83987300	0.00567200	0.59826200
H	-6.84377600	1.16099900	-0.31628800
H	-8.27670800	-0.49962400	0.89484600
H	-8.54374400	1.14303100	1.52276000
H	-7.54652300	-0.00486800	2.43811600
H	3.03101700	-0.40604400	4.62627200
H	2.18828600	-1.02884600	6.06774600
H	3.75352200	0.26766000	7.53785100
H	4.59166500	0.88598200	6.09979500
H	4.65054700	-0.84847700	6.48192500
H	-0.60285400	-1.48556700	8.25940900
H	-0.66021100	-2.74942600	6.99981900
H	-1.51885100	-6.77094300	1.47558500

H	-1.12567100	-5.04222200	1.53918800
H	0.86421600	-7.32045600	2.07560200
H	0.10111300	-6.30521200	3.32173100
H	1.23508700	-5.58453900	2.15950200
H	-4.60711700	-7.50017000	-1.54474800
H	-5.21158800	-6.22877500	-0.44846900
H	-4.98313900	-8.45687700	0.72580100
H	-3.93613200	-7.22132900	1.44716500
H	-3.24655500	-8.45663100	0.35976600
H	2.81048300	5.71986400	1.99028300
H	1.12895000	5.58985800	2.56248200
H	1.17598300	8.01836800	3.22071500
H	2.86316800	8.13180700	2.67256000
H	2.44622300	7.09994300	4.05786800
H	3.41106000	7.13549000	-2.59448400
H	2.56696300	5.59187200	-2.72203700
H	4.53478000	4.59540700	-3.92991700
H	5.40904300	6.13495500	-3.77854300
H	3.94547000	6.03920700	-4.78272000
H	-7.68076600	5.80997200	-0.69834800
H	-8.76008200	4.40114400	-0.69350100
H	-8.79518700	5.54049500	-2.05552500
H	-2.94851800	-2.34201900	7.99614800
H	-2.85406200	-0.64157700	7.49024100
H	-2.91154300	-1.93622000	6.26894000

C -2.45085500 -2.10495200 -2.44135400
 C -3.37709600 -1.15033300 -1.51133700
 C -3.55022500 -2.80557700 -3.37985100
 H -3.10582000 -3.20687300 -4.29221600
 C -4.84358300 -1.57862700 -2.00533200
 H -5.60393600 -0.87066100 -1.67125900
 C -4.38125800 -3.76513100 -2.56153100
 H -4.31036100 -4.84084200 -2.63406100
 C -5.12205200 -3.03539200 -1.71360600
 H -5.75479400 -3.39530800 -0.91096200
 C -4.57785400 -1.66043000 -3.52873100
 H -4.19450700 -0.74276700 -3.97622700
 H -5.46446700 -1.98709200 -4.07893700

Vibrational frequencies for theoretical product (13c₂)

7.04	16.30	17.58	27.71	29.08	30.21
30.98	31.83	33.85	33.93	36.43	37.51
39.05	40.28	41.78	43.47	46.04	50.45
51.79	53.53	56.00	57.86	62.46	64.54
66.56	69.52	72.70	75.89	77.66	81.10
92.66	93.92	96.53	97.73	99.84	101.86
105.63	108.61	110.47	112.48	115.85	120.42
122.94	124.69	125.07	127.25	129.32	129.93
132.46	141.41	145.61	147.14	153.15	157.29

161.44	165.51	175.11	176.54	181.24	187.70
190.47	198.12	200.02	206.93	209.76	212.86
216.81	224.54	229.44	232.80	236.40	243.20
243.57	247.48	254.47	256.93	262.11	262.86
265.21	266.66	268.98	271.96	277.14	283.49
286.39	297.99	299.45	310.64	314.54	323.87
329.23	333.15	333.56	335.98	338.63	342.78
344.25	348.47	351.30	362.14	366.19	373.14
374.16	383.86	385.47	388.92	392.98	403.87
410.02	412.35	415.68	424.53	426.64	428.11
431.54	439.27	443.17	448.82	449.86	450.77
455.29	458.68	462.54	468.14	473.22	479.52
480.17	484.16	488.62	490.52	508.38	515.42
521.55	526.50	529.41	535.23	540.86	546.41
548.20	551.96	553.41	558.32	561.91	562.83
567.84	570.52	572.98	573.89	575.74	586.34
586.69	590.59	598.85	603.39	614.02	620.88
623.68	629.59	634.92	640.22	642.91	645.47
648.10	653.41	659.23	662.21	663.69	667.31
676.64	680.21	681.83	686.69	689.54	698.20
699.67	701.76	712.11	713.55	714.50	722.43
724.88	728.08	730.15	732.51	734.11	735.74
741.97	743.74	745.83	747.15	748.76	749.53
751.09	754.18	755.62	756.43	760.53	761.63

763.59	767.68	768.84	773.97	775.66	783.24
785.73	786.80	788.79	790.06	793.57	798.55
801.22	808.66	810.22	813.92	816.30	817.50
821.27	823.10	825.99	826.97	830.95	831.72
833.40	833.83	835.22	835.70	836.43	843.54
845.70	848.16	852.78	856.98	859.09	860.89
869.91	871.21	874.28	883.85	888.48	892.16
902.80	905.37	908.11	915.65	922.49	927.54
928.39	933.34	936.52	939.45	942.26	948.78
953.58	955.54	959.21	962.93	965.86	969.00
976.64	981.24	992.15	997.41	1010.69	1018.80
1020.51	1023.97	1027.45	1032.72	1035.55	1037.25
1038.90	1046.58	1051.74	1052.50	1057.04	1062.62
1065.58	1070.35	1075.02	1084.38	1090.29	1095.32
1100.61	1105.56	1106.63	1115.20	1118.75	1126.11
1128.23	1128.89	1129.45	1130.43	1135.28	1137.84
1139.79	1140.79	1141.87	1143.66	1144.56	1146.81
1149.63	1150.80	1151.65	1155.63	1159.90	1169.11
1170.68	1174.61	1181.88	1183.31	1183.45	1185.90
1187.64	1190.68	1191.08	1198.98	1204.02	1204.12
1207.55	1210.89	1211.71	1214.95	1218.43	1220.52
1227.40	1232.43	1236.98	1243.36	1246.89	1249.20
1249.63	1254.91	1259.79	1260.74	1264.39	1270.66
1272.14	1273.84	1276.90	1279.68	1283.16	1289.45

1292.82	1297.09	1301.96	1303.89	1304.93	1305.49
1309.00	1311.85	1323.17	1326.05	1326.91	1327.10
1331.14	1333.39	1335.43	1340.65	1341.43	1342.24
1342.36	1343.76	1346.24	1348.30	1355.31	1356.58
1363.07	1365.28	1373.02	1380.11	1382.20	1383.96
1390.88	1394.70	1398.06	1404.31	1407.84	1409.64
1411.02	1413.34	1414.65	1418.57	1418.61	1419.15
1419.29	1419.68	1420.78	1421.24	1421.98	1425.77
1426.21	1427.54	1428.98	1440.27	1441.58	1441.85
1444.02	1444.53	1446.42	1447.45	1448.01	1448.60
1450.75	1451.22	1453.32	1455.03	1469.46	1486.51
1513.58	1513.61	1513.77	1514.34	1514.77	1514.82
1514.89	1515.02	1515.76	1516.03	1516.72	1518.34
1519.41	1519.55	1521.76	1525.35	1526.00	1526.61
1527.20	1529.05	1530.81	1534.16	1536.25	1536.84
1536.94	1538.94	1541.18	1541.61	1541.87	1543.16
1543.63	1550.66	1567.84	1573.25	1577.32	1579.53
1585.08	1589.88	1597.86	1602.03	1608.46	1618.86
1620.07	1624.84	1630.74	1633.74	1651.24	1676.99
1801.14	1807.77	1810.96	1812.18	1813.89	1814.85
1828.03	1832.97	1838.48	1840.18	3061.38	3061.89
3062.70	3063.32	3063.76	3063.91	3064.30	3064.81
3064.84	3065.20	3066.09	3073.11	3078.64	3082.97
3088.16	3091.70	3097.25	3099.01	3099.06	3100.67

3104.24	3113.44	3120.07	3121.66	3127.93	3129.88
3130.30	3133.27	3133.65	3134.35	3134.81	3135.20
3136.04	3136.58	3136.67	3137.13	3137.70	3139.38
3141.36	3141.44	3141.55	3142.06	3143.87	3148.27
3149.01	3150.06	3161.03	3162.11	3163.35	3163.53
3165.29	3167.41	3167.77	3185.18	3236.78	3276.86

Coordinates for theoretical product (13d₁)

Energy = -5348.53892052 Hartrees

C 0.06721400 1.94621900 -3.37813800
C -0.17064300 2.89009600 -2.33672500
C 1.42477700 1.46118500 -3.27294600
C 1.11279200 3.14418200 -1.61341800
C 2.07165100 2.11540200 -2.12953600
C -2.47191000 2.04809000 -2.14956800
C -1.40784500 2.90606300 -1.70658900
C -2.25642300 1.13959200 -3.17739900
C -0.96275000 1.09299500 -3.81195300
C 2.77978500 1.49684300 0.11887500
C 2.91644900 1.40396700 -1.32511200
C 1.86814200 2.36155900 0.73598400
C 1.01562900 3.29083900 -0.05377000
C -1.50129200 3.03582400 -0.24656400
C -0.35272300 3.15284300 0.53798700

C	1.70927300	0.15251700	-3.57939200
C	2.87622400	-0.62066700	-2.99484400
C	0.66096300	-0.73059300	-3.97558500
C	3.59978300	0.09208300	-1.73216500
C	-0.65312100	-0.27684400	-4.12008300
C	-0.25210100	2.40377400	1.74618900
C	1.12723000	1.91021700	1.86518900
C	3.06340200	0.22616800	0.68053400
C	3.59260300	-0.71017200	-0.37149100
C	2.18024500	-1.95994400	-2.66914300
C	0.94616500	-2.03124300	-3.40541100
C	-1.75719200	-1.10089800	-3.67075200
C	-2.75488000	-0.24549700	-3.08852600
C	-3.35590100	1.74495400	-0.98462400
C	-2.61250400	2.26208600	0.20447500
C	-2.49483600	1.53032900	1.38419600
C	-1.32747000	1.64190900	2.19526500
C	-1.13758700	0.36238500	2.94341800
C	0.33110600	-0.16889700	3.07917900
C	1.39666300	0.66932000	2.43796500
C	2.33830800	-0.19226200	1.80241100
C	1.83726100	-1.56568800	1.90335500
C	2.06107300	-2.45247800	0.86400000
C	2.98872800	-2.14619700	-0.25678100
C	2.27324400	-2.66982600	-1.48118900

C	1.14666800	-3.45952500	-1.02755300
C	-0.00566100	-3.59593100	-1.78934900
C	-0.12226500	-2.83165100	-2.98429500
C	-1.49503000	-2.35698300	-3.11126400
C	-2.24052700	-2.81618700	-1.98225900
C	-3.17145300	-1.96169700	-1.39235900
C	-3.46161900	-0.68315800	-1.97518800
C	-3.89522100	0.25166000	-0.89530100
C	-3.60134800	-0.47170700	0.37958500
C	-2.99696900	0.15101600	1.47140900
C	-2.12781800	-0.58312100	2.33411200
C	0.58913000	-1.55049000	2.58031000
C	1.03479000	-3.32710000	0.43110300
C	-1.36939800	-3.74257500	-1.19072700
C	-3.25788900	-1.82436700	0.07069600
C	-0.19328900	-3.33386700	1.09607300
C	-0.42662400	-2.39462500	2.14642100
C	-1.80571000	-1.90231400	2.02390900
C	-2.41552000	-2.55122100	0.90760800
C	-1.48388900	-3.59707800	0.39262500
C	1.46255800	4.46542100	-0.92250600
C	-1.85771400	-4.87537400	-0.31785400
C	-0.50178900	0.16555200	4.31911200
C	4.46059200	-1.92218600	0.02112900
C	-4.83931600	1.42983900	-1.09522700

C	0.48105700	5.62331000	-1.14187500
C	2.91170000	4.88368300	-0.93530100
C	-3.34700600	-5.24391800	-0.38352100
C	-0.95184300	-6.10754900	-0.16662800
C	-0.97412400	-1.02412300	5.16442800
C	-0.06719600	1.36427300	5.12768500
C	4.91198600	-2.09236000	1.49291400
C	5.44497000	-2.75340900	-0.79073200
C	-5.48167300	1.59178300	-2.46876600
C	-5.76499900	1.79520000	0.04315100
O	-5.43029500	1.94869300	1.19674800
O	-7.03192700	1.88994200	-0.40238300
O	-5.52341400	2.89537500	-2.79350800
O	-5.88944100	0.68480200	-3.15532800
C	-6.14656800	3.22923400	-4.06102700
C	-7.65465800	3.35799600	-3.91527700
C	-8.05163500	2.20599700	0.58182400
C	-8.17162400	3.70763200	0.78769400
O	5.15501300	-3.74719600	-1.41422900
O	6.71016200	-2.31359500	-0.62250000
C	7.75206200	-3.14524300	-1.20239000
C	9.08745900	-2.54368500	-0.81154400
O	4.65405000	-3.10968900	2.08868500
O	5.63733500	-1.13693900	2.10198200
C	6.19714500	0.02864000	1.45448800

C	7.27772400	0.56283100	2.37876300
O	-0.28809200	-1.99877700	5.34669100
O	-2.20690900	-0.96622400	5.70931100
C	-3.08352300	0.17568000	5.59005400
C	-4.34789900	-0.16128900	6.36031700
O	0.22796100	2.44992900	4.67914400
O	-0.02985800	1.04687000	6.43793300
C	0.44776300	2.07069100	7.35153600
C	1.96525400	2.05819100	7.44086300
O	-0.06084700	5.81630400	-2.20178500
O	0.23075300	6.45133100	-0.10633700
C	0.83591200	6.30698300	1.19685500
C	0.44109000	7.53237300	2.00184100
O	3.85657000	4.17520200	-0.66318600
O	3.01801300	6.17006300	-1.33050300
C	4.35813800	6.71094600	-1.46396500
C	4.87655500	7.24838400	-0.13941600
O	-0.32238900	-6.54842000	-1.10091500
O	-0.92332900	-6.73793200	1.01480600
C	-1.52398000	-6.23092500	2.24197400
C	-1.65946500	-7.41335800	3.18276700
O	-4.10413200	-5.00930900	0.53162700
O	-3.80938100	-5.86127000	-1.47907900
C	-3.02555700	-6.22858800	-2.64707700
C	-3.86966100	-5.93415100	-3.87360500

C	4.05353900	-0.64131000	-4.08579000
C	5.06405500	0.32598000	-2.32526300
H	-5.87952200	2.46324800	-4.79270000
H	-5.68416600	4.17798900	-4.34190800
H	-7.90973300	4.10373500	-3.15533000
H	-8.09872900	2.39924100	-3.63383200
H	-8.09202400	3.67448500	-4.86913300
H	-7.80583000	1.69114000	1.51325900
H	-8.96475900	1.78055400	0.16003300
H	-7.25215300	4.11477100	1.21737700
H	-8.99728100	3.92038300	1.47637000
H	-8.37470700	4.21570900	-0.16048000
H	7.60978100	-3.16968700	-2.28711100
H	7.62772700	-4.16360200	-0.82390900
H	5.40569000	0.76896400	1.30835400
H	6.61166400	-0.25544300	0.48619800
H	7.72093500	1.46676800	1.94620600
H	8.06877900	-0.17956200	2.52349800
H	6.85942200	0.81627600	3.35762800
H	-3.30814100	0.36284100	4.53618000
H	-2.59350300	1.05808600	6.01359800
H	-4.12056100	-0.35705400	7.41266500
H	-4.82980700	-1.04860600	5.93906200
H	-5.05105200	0.67670500	6.30317900
H	-0.01532200	1.80822000	8.30502900

H	0.07153900	3.03984800	7.01561000
H	1.92387400	6.24264800	1.09918600
H	0.46790000	5.39162500	1.66944100
H	0.80793700	8.44593000	1.52371100
H	0.86687400	7.46778700	3.00904100
H	-0.64740800	7.60132200	2.08874600
H	4.24820900	7.50424300	-2.20628800
H	5.00972400	5.92842900	-1.85945800
H	5.85887400	7.71097600	-0.28856200
H	4.98609900	6.44115100	0.59045700
H	4.19966800	8.00789900	0.26522400
H	-2.49254800	-5.77525700	2.03142600
H	-0.85092500	-5.47232000	2.65236500
H	-0.68639300	-7.87911900	3.36567800
H	-2.33514100	-8.16749000	2.76706700
H	-2.06707600	-7.07206400	4.14041700
H	-2.80452000	-7.29636700	-2.55472200
H	-2.07815700	-5.69286800	-2.66527200
H	-4.06685200	-4.86122900	-3.96025300
H	-4.82730500	-6.46134500	-3.82353000
H	-3.33772000	-6.26371400	-4.77302300
H	3.83908800	-1.33228600	-4.90292300
H	5.80130600	0.52629600	-1.54678700
H	9.20248700	-2.52002500	0.27668500
H	9.18906100	-1.52349100	-1.19588600

H	9.89878600	-3.14929600	-1.22938500
H	2.29530000	2.78296600	8.19388700
H	2.32906900	1.06785300	7.73146200
H	2.41213900	2.33281200	6.48122900
C	5.27312100	-0.92453400	-3.21168100
H	5.19531900	-1.88807600	-2.72321900
H	6.21338800	-0.87246900	-3.76852500
C	4.33053500	0.80704800	-4.46285700
H	3.99445100	1.28865100	-5.37431400
C	4.93582700	1.38165500	-3.41396400
H	5.18529000	2.42873100	-3.28512400

Vibrational frequencies for theoretical product (13d₁)

13.99	18.81	20.12	22.21	22.80	32.90
33.92	35.13	35.44	35.83	36.88	38.45
39.10	40.03	43.23	43.56	44.18	46.45
51.30	52.68	55.21	58.71	63.23	65.72
68.55	72.61	74.25	75.09	83.21	90.29
91.97	92.99	94.25	96.58	98.38	99.95
105.14	109.83	111.25	112.36	116.28	117.64
120.63	124.07	127.20	128.87	129.23	132.20
134.79	139.03	145.22	146.84	149.55	153.77
158.48	161.45	173.68	176.07	182.53	187.08
188.59	193.00	198.26	202.05	207.45	215.23

217.02	222.77	229.34	234.61	235.74	238.75
242.32	245.34	253.73	260.25	264.36	265.68
266.83	267.39	272.86	276.32	280.21	283.96
287.15	292.38	296.08	306.42	313.47	324.52
329.75	331.17	333.55	335.16	337.72	339.96
340.88	343.84	345.11	350.64	365.93	376.60
379.27	384.57	385.22	387.12	393.93	400.07
401.92	407.50	411.31	420.34	424.64	425.34
434.90	435.54	441.37	446.67	449.45	455.58
456.85	460.00	464.77	470.62	475.22	478.37
485.75	487.26	492.67	495.97	500.39	514.46
520.94	523.94	530.83	534.05	538.96	541.64
544.74	547.78	550.76	558.27	561.00	563.97
567.65	571.35	574.30	576.45	578.03	585.82
587.57	590.89	598.02	604.40	605.84	612.11
625.86	631.60	635.68	638.72	643.62	646.56
651.08	656.10	659.71	662.30	664.12	670.56
677.56	681.11	684.56	686.25	692.22	696.10
700.13	709.32	713.20	714.27	716.28	724.12
725.56	729.05	731.26	731.71	735.78	740.05
742.15	743.54	744.44	746.30	747.65	750.29
752.37	753.95	755.36	757.67	759.96	761.30
763.69	764.70	769.52	774.64	776.47	781.82
785.82	787.72	788.04	789.87	795.69	800.77

801.07	808.65	810.49	811.84	817.56	819.58
820.47	823.12	825.79	828.69	831.18	832.99
834.41	834.75	836.41	836.60	838.35	839.19
842.33	846.87	852.29	855.09	860.21	866.72
869.92	879.69	884.13	886.19	893.20	896.56
902.04	904.02	905.62	915.44	920.63	922.53
924.43	932.69	939.00	943.19	944.20	949.44
951.55	956.15	958.62	960.68	964.40	971.39
975.00	985.02	992.13	1006.26	1008.41	1013.74
1022.20	1026.44	1027.39	1030.54	1034.02	1037.52
1038.39	1046.64	1048.65	1053.76	1057.85	1061.55
1065.08	1069.33	1071.62	1084.64	1087.16	1096.01
1100.94	1101.20	1106.19	1118.35	1121.95	1128.48
1128.68	1129.43	1130.38	1133.40	1133.95	1135.62
1137.84	1139.47	1140.96	1144.65	1145.73	1146.60
1147.09	1147.22	1153.57	1158.50	1160.54	1168.40
1174.85	1182.46	1183.30	1183.65	1184.38	1186.86
1190.15	1190.96	1193.94	1199.74	1206.30	1208.32
1209.10	1209.66	1212.21	1216.22	1220.45	1222.20
1227.90	1234.05	1240.69	1244.48	1245.71	1247.61
1253.29	1259.54	1260.52	1263.45	1264.71	1270.28
1270.90	1272.91	1275.12	1279.76	1281.84	1284.39
1287.80	1294.11	1298.70	1301.39	1308.45	1309.75
1312.22	1312.62	1323.16	1323.23	1326.18	1331.44

1334.96	1335.89	1336.19	1340.55	1340.72	1341.33
1341.86	1343.25	1343.43	1351.72	1356.95	1363.41
1364.29	1366.69	1372.91	1375.28	1376.07	1381.26
1390.82	1396.52	1400.34	1403.65	1406.73	1408.30
1409.85	1413.97	1416.80	1418.62	1418.66	1419.03
1420.12	1420.71	1421.40	1422.93	1423.59	1425.80
1426.65	1429.40	1430.92	1442.39	1442.50	1442.92
1443.77	1444.72	1446.38	1449.36	1449.61	1449.77
1450.39	1452.10	1454.61	1457.45	1468.77	1488.98
1513.94	1514.27	1514.54	1514.81	1514.87	1515.41
1515.64	1516.49	1516.69	1517.18	1517.87	1518.28
1518.47	1519.37	1520.72	1523.55	1526.04	1527.07
1527.77	1529.75	1530.87	1533.97	1534.66	1535.51
1535.77	1536.00	1538.40	1542.04	1542.49	1542.92
1547.39	1551.69	1558.71	1570.85	1572.30	1575.89
1579.96	1587.94	1597.33	1603.68	1605.47	1612.95
1617.93	1624.81	1626.84	1635.99	1646.64	1653.49
1805.04	1805.58	1807.24	1810.34	1812.32	1814.76
1828.61	1829.00	1837.89	1838.64	3061.30	3061.58
3062.48	3062.53	3062.78	3063.20	3063.72	3064.26
3064.29	3065.35	3074.64	3077.00	3083.61	3089.19
3089.70	3092.22	3098.96	3099.54	3100.46	3100.61
3102.35	3121.96	3122.72	3122.87	3128.16	3129.17
3130.06	3133.40	3133.45	3134.24	3134.94	3136.19

3136.30	3136.51	3137.15	3137.45	3137.66	3138.93
3141.00	3141.47	3141.56	3141.58	3144.46	3146.50
3149.10	3150.45	3162.30	3162.60	3162.86	3163.14
3163.21	3166.82	3187.65	3222.82	3245.85	3254.94

Coordinates for theoretical product (13d₂)

Energy = -5348.53649368 Hartrees

C -0.20191100 1.92093200 -3.42466900
C -0.53367800 2.85295800 -2.39759100
C 1.20097700 1.58998500 -3.32679100
C 0.71955400 3.26479000 -1.69560200
C 1.77854800 2.34055700 -2.20470800
C -2.72158900 1.76050700 -2.16506700
C -1.75705600 2.74149100 -1.75114500
C -2.41734100 0.86375000 -3.18100000
C -1.13316200 0.95049800 -3.83135600
C 2.58809600 1.84281500 0.04379500
C 2.69814400 1.73526100 -1.39960100
C 1.58932600 2.61052400 0.65570000
C 0.62754300 3.42466500 -0.13735700
C -1.84662100 2.88653100 -0.29214200
C -0.70908400 3.14518300 0.47453500
C 1.63844200 0.31992800 -3.61993900
C 2.89601200 -0.31613300 -3.03045500

C	0.68725000	-0.68116200	-3.98611400
C	3.53559000	0.51832400	-1.80116900
C	-0.67214300	-0.38038900	-4.11970900
C	-0.51029000	2.43441700	1.69359500
C	0.91771600	2.10135300	1.80240500
C	3.03117600	0.62427700	0.62146500
C	3.65066900	-0.26373000	-0.43367400
C	2.34558400	-1.71054500	-2.68195100
C	1.12021900	-1.93239000	-3.40008700
C	-1.67252800	-1.31438500	-3.64249500
C	-2.75411200	-0.56654500	-3.06120300
C	-3.55212000	1.38160500	-0.98302200
C	-2.85837700	2.00142800	0.18721500
C	-2.64532500	1.30951800	1.37785500
C	-1.48819200	1.56659500	2.17097400
C	-1.14562000	0.33021100	2.93729000
C	0.37551500	-0.02980300	3.06163500
C	1.33409700	0.90962000	2.39069300
C	2.36128200	0.14783800	1.75749900
C	2.01378900	-1.26884900	1.88978900
C	2.31728700	-2.13841700	0.85825200
C	3.18497700	-1.74700800	-0.28193600
C	2.52528500	-2.37889000	-1.48210900
C	1.50326700	-3.28243700	-0.99996800
C	0.36660700	-3.56412600	-1.74432800

C	0.15216700	-2.83912700	-2.95029300
C	-1.26623700	-2.52351100	-3.06644000
C	-1.94300000	-3.04278900	-1.91987800
C	-2.95738100	-2.28776000	-1.33160200
C	-3.39554100	-1.06037900	-1.93188500
C	-3.91914300	-0.16032100	-0.86167700
C	-3.52926800	-0.82192500	0.42078200
C	-2.98676300	-0.11574700	1.49389600
C	-2.02986200	-0.73114500	2.35656900
C	0.78063000	-1.38311100	2.58448000
C	1.39435000	-3.13456500	0.45680200
C	-0.96436900	-3.85079800	-1.12447300
C	-3.04046200	-2.13303600	0.13014600
C	0.18484000	-3.26964900	1.14016700
C	-0.13943200	-2.34322700	2.17784900
C	-1.56582900	-2.01104300	2.06443200
C	-2.11213100	-2.74485200	0.96786300
C	-1.07597200	-3.68900000	0.45829000
C	0.92882900	4.62744500	-1.02884200
C	-1.31307400	-5.01416200	-0.22520600
C	-0.47449300	0.23300200	4.30717800
C	4.63854100	-1.39354700	-0.03854900
C	-4.99234700	0.90041800	-1.06842700
C	-0.17962100	5.66342800	-1.25135900
C	2.32236100	5.20367000	-1.06669600

C	-2.75242300	-5.54589800	-0.26786100
C	-0.27284900	-6.13305000	-0.06315900
C	-0.79952900	-0.98517000	5.18092200
C	-0.16631900	1.48836600	5.08733900
C	5.12216500	-1.45395200	1.42890300
C	5.63320500	-2.22325900	-0.84717200
C	-5.66429200	0.96477700	-2.43578600
C	-5.93915900	1.18364600	0.07595700
O	-5.61023800	1.37507300	1.22560600
O	-7.21343100	1.15769400	-0.35778100
O	-5.84088100	2.24938600	-2.78907000
O	-5.98793500	0.00505800	-3.09489700
C	-6.51293100	2.49001000	-4.05254600
C	-8.02387400	2.47754700	-3.88160000
C	-8.24859600	1.38274000	0.63536600
C	-8.49984400	2.86775600	0.84336100
O	5.35263600	-3.10745100	-1.61897200
O	6.89850400	-1.95982600	-0.44205800
C	7.92689900	-2.85426200	-0.94200800
C	9.21722800	-2.51263000	-0.22273800
O	4.93637400	-2.44136500	2.09728900
O	5.78955500	-0.41135900	1.95858700
C	6.25290400	0.72746100	1.20186700
C	7.36956300	1.36769000	2.00849100
O	-0.00662300	-1.87360700	5.36999700

O	-2.02265300	-1.05300300	5.74608000
C	-3.02813900	-0.02535400	5.60692800
C	-4.21961000	-0.46334600	6.43992200
O	0.00080400	2.59106100	4.61499400
O	-0.07700900	1.20249900	6.40229300
C	0.30073200	2.28899200	7.28985500
C	1.81225400	2.43511200	7.35954000
O	-0.75734800	5.77339300	-2.30417300
O	-0.51025300	6.47324400	-0.22378600
C	0.15141700	6.44530800	1.05963100
C	-0.48766700	7.53245500	1.90537400
O	3.34070900	4.61552200	-0.77470800
O	2.28280800	6.47781200	-1.51053800
C	3.55488400	7.15630700	-1.68170700
C	4.02671600	7.79470700	-0.38501800
O	0.39846800	-6.51375800	-0.99456400
O	-0.16846100	-6.73919200	1.12722800
C	-0.81169800	-6.28186300	2.35222700
C	-0.83346100	-7.46469500	3.30218000
O	-3.52604500	-5.37358900	0.64722700
O	-3.15219600	-6.23245000	-1.34759400
C	-2.32731900	-6.55547600	-2.49992300
C	-3.24470700	-6.58880900	-3.70812400
C	4.04978200	-0.18686600	-4.13623100
C	4.89968800	1.06048600	-2.46442300

H	-6.18527500	1.73475500	-4.77062600
H	-6.14862200	3.47138600	-4.36408700
H	-8.33600700	3.21139900	-3.13144500
H	-8.36997900	1.48713100	-3.57343000
H	-8.50522800	2.73106700	-4.83307700
H	-7.95020500	0.89207300	1.56453400
H	-9.12385500	0.87762000	0.22129100
H	-7.61659300	3.35485700	1.26569200
H	-9.33533700	3.00610700	1.53912500
H	-8.75538200	3.35587700	-0.10261300
H	8.00808500	-2.71825000	-2.02553100
H	7.60662800	-3.88277800	-0.75566700
H	5.42003600	1.42332600	1.06248300
H	6.61479700	0.39889800	0.22596700
H	7.73889200	2.25911400	1.48925100
H	8.20160800	0.66928300	2.14096000
H	7.00937700	1.66707200	2.99743400
H	-3.30573900	0.07944700	4.55418800
H	-2.63138900	0.92847100	5.96856500
H	-3.93786700	-0.57496200	7.49142200
H	-4.60821000	-1.42139100	6.08185500
H	-5.01696300	0.28424100	6.36769900
H	-0.12225300	1.99970200	8.25418400
H	-0.17780800	3.20666500	6.93996200
H	1.22093600	6.63652200	0.92606200

H	0.01970700	5.46321000	1.52232600
H	-0.36078100	8.51371000	1.43778800
H	-0.02194500	7.55299900	2.89662800
H	-1.55833700	7.34394300	2.02879700
H	3.35067100	7.90546500	-2.44951100
H	4.28311900	6.43509200	-2.05959300
H	4.95121800	8.35496700	-0.56576000
H	4.23202700	7.03149700	0.37109000
H	3.27657100	8.49149900	0.00309700
H	-1.81932400	-5.92082800	2.14205300
H	-0.21164600	-5.46034600	2.75488600
H	0.17944000	-7.83600300	3.48508700
H	-1.43667900	-8.28172000	2.89395200
H	-1.26873200	-7.15612000	4.25874100
H	-1.86816500	-7.53033700	-2.31129800
H	-1.52739700	-5.82602700	-2.61948600
H	-3.68199600	-5.60216800	-3.88971600
H	-4.05674400	-7.30748600	-3.56121900
H	-2.67365400	-6.88539700	-4.59479600
H	3.68863500	-0.47737600	-5.12447900
H	5.29889000	1.92038100	-1.92323500
H	9.10497700	-2.64054900	0.85825500
H	9.52091000	-1.47946700	-0.42158700
H	10.01701400	-3.17657300	-0.56805900
H	2.07397500	3.20688900	8.09242400

H	2.27946100	1.49429200	7.66633300
H	2.21806000	2.73230000	6.38840700
C	4.44080000	1.29518000	-3.92182300
H	5.27596800	1.59418300	-4.56114100
H	3.62369700	2.00803200	-4.04004400
C	5.84593800	-0.09614300	-2.69923200
H	6.74403100	-0.28419800	-2.12708900
C	5.31836900	-0.85982800	-3.66800300
H	5.67076600	-1.82439800	-4.01318600

Vibrational frequencies for theoretical product (13d₂)

15.90	18.50	20.84	23.91	24.81	32.26
33.65	33.89	34.78	36.02	36.45	38.50
39.78	40.26	42.01	43.42	44.71	46.75
51.16	53.59	55.79	58.93	63.70	69.37
71.00	73.85	76.59	76.87	82.83	92.38
93.52	95.12	96.59	99.26	100.17	103.34
108.28	110.82	112.94	113.21	115.43	119.74
122.10	124.82	127.54	129.01	130.68	133.41
135.19	138.06	145.46	147.04	153.20	155.33
157.93	167.62	175.83	177.14	181.69	189.93
191.48	195.48	198.23	202.48	208.02	215.62
217.08	223.68	229.56	232.82	235.22	238.24
242.78	245.24	254.13	260.93	263.26	264.97

266.56	268.67	270.97	277.01	278.68	283.49
285.57	292.81	295.48	306.04	308.92	322.99
327.50	333.42	334.44	336.88	339.39	340.36
342.42	344.25	350.80	355.85	369.46	374.35
378.96	385.07	386.52	388.73	395.03	401.41
404.67	406.95	414.73	421.26	425.49	430.50
432.78	436.81	442.13	446.58	448.71	456.59
457.22	460.26	463.76	472.99	475.32	478.23
487.61	488.35	492.66	500.24	505.81	518.55
522.23	527.60	532.14	537.71	538.83	541.51
545.32	552.85	554.21	559.99	562.18	564.15
565.38	570.82	573.50	575.21	578.42	585.91
588.27	593.50	597.71	606.62	613.06	615.61
625.50	633.79	635.47	638.07	642.85	646.66
651.73	657.52	659.24	663.24	665.33	669.99
677.53	680.05	684.80	687.23	692.25	698.79
699.96	707.05	710.65	714.25	715.11	721.29
725.62	729.25	731.36	731.66	736.34	740.01
742.21	742.40	744.65	746.11	747.07	748.76
750.43	752.51	755.69	756.94	758.97	761.49
762.46	767.97	768.19	775.99	777.96	782.97
785.95	786.74	789.19	791.27	798.16	800.60
803.22	808.69	812.26	813.80	818.38	820.33
822.11	822.85	825.81	829.06	830.57	831.14

833.70	835.03	835.55	836.02	838.50	841.45
842.31	848.05	851.93	856.98	858.57	865.13
870.06	879.09	884.37	887.55	887.85	893.93
899.28	904.11	908.26	916.05	921.10	924.61
925.79	932.84	938.14	939.95	944.61	949.74
954.10	955.82	958.72	963.29	964.75	968.59
980.27	983.96	992.66	998.13	1006.47	1017.51
1023.86	1025.66	1026.80	1029.39	1033.60	1036.45
1044.89	1047.21	1050.45	1054.00	1058.09	1063.15
1066.10	1070.08	1075.93	1083.62	1092.29	1097.45
1101.16	1101.81	1106.67	1116.40	1121.09	1128.58
1128.74	1129.49	1129.93	1132.37	1134.58	1137.49
1139.93	1141.21	1141.63	1145.13	1146.26	1146.46
1146.74	1147.18	1153.30	1156.96	1158.67	1171.52
1175.28	1179.35	1183.02	1183.48	1183.75	1185.18
1189.29	1191.71	1193.39	1200.79	1202.95	1207.16
1207.54	1209.03	1210.94	1212.01	1212.76	1220.47
1226.86	1234.89	1240.52	1243.64	1245.75	1247.33
1253.66	1259.64	1260.23	1263.18	1265.87	1268.26
1272.66	1273.36	1278.88	1280.00	1282.69	1288.17
1294.81	1295.97	1299.91	1303.41	1308.18	1308.22
1310.55	1313.39	1321.06	1323.07	1323.65	1325.57
1329.23	1334.56	1335.86	1337.18	1340.83	1341.37
1342.54	1342.89	1343.55	1351.24	1355.30	1361.65

1363.63	1365.71	1375.06	1376.27	1379.77	1382.70
1389.01	1395.87	1400.24	1403.64	1406.51	1408.03
1409.95	1412.40	1417.02	1418.53	1418.65	1419.10
1419.50	1419.77	1420.42	1420.82	1422.02	1424.90
1426.61	1428.99	1430.44	1442.36	1443.19	1443.84
1444.60	1445.11	1445.36	1446.44	1447.91	1449.26
1450.73	1451.53	1453.92	1458.54	1469.97	1486.74
1513.73	1514.08	1514.42	1514.93	1515.21	1515.27
1516.13	1516.36	1516.45	1516.53	1518.51	1518.69
1519.44	1519.51	1519.62	1525.17	1527.26	1527.66
1528.78	1529.24	1533.65	1535.02	1535.80	1535.94
1536.33	1538.06	1541.98	1542.00	1542.08	1543.50
1544.51	1551.67	1557.72	1570.70	1572.78	1576.35
1581.80	1588.37	1599.28	1604.56	1606.72	1614.46
1617.88	1625.13	1628.25	1637.78	1647.85	1650.47
1807.11	1807.78	1810.60	1812.21	1813.77	1816.01
1829.27	1830.99	1837.78	1839.15	3061.42	3061.45
3062.35	3062.47	3062.56	3063.62	3063.75	3064.34
3064.59	3065.04	3074.09	3074.64	3077.85	3083.48
3088.68	3095.12	3099.33	3099.37	3100.46	3100.73
3102.94	3121.98	3122.05	3122.35	3128.19	3128.65
3130.02	3131.48	3132.65	3133.54	3134.17	3135.05
3135.17	3135.28	3136.55	3136.78	3136.89	3137.82
3139.28	3140.50	3140.96	3141.22	3141.80	3146.80

3149.48	3150.08	3156.67	3162.25	3162.64	3162.81
3163.23	3163.41	3168.67	3180.25	3239.16	3265.75