The Prospect of Selective Recognition of Nerve Agents with Modular Basket-like Hosts. A Structure-Activity Study of the Entrapment of a Series of Organophosphonates in Aqueous Media

Yian Ruan, Hashem A. Taha, Ryan J. Yoder, Veselin Maslak, Christopher M. Hadad* and Jovica D. Badjić*

Department of Chemistry and Biochemistry, The Ohio State University, 100 West 18th Avenue, Columbus, Ohio, USA. Fax: 614 292 1685; Tel: 614 247 8342;
E-mail: badjic@chemistry.ohio-state.edu; hadad.1@osu.edu

SUPPORTING INFORMATION

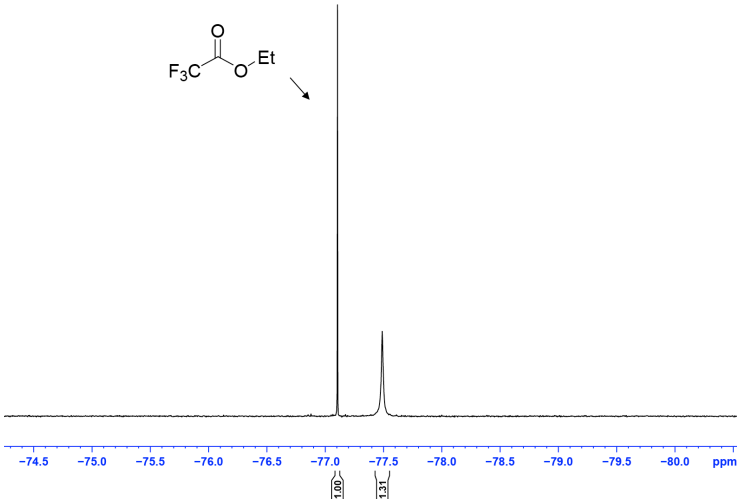
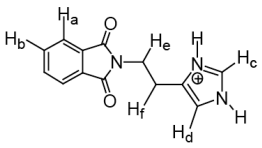


Figure S1: ^{19}F NMR spectrum (400 MHz, 298 K) of [**1**-H_3]$(CF_3CO_2)_3$ (1.0 mM) with ethyl trifluoroacetate (5.0 mM) as a calibration standard in CD_3OD; note an excess of trifluoroacetate anion (~1 mol equivalent) in solution.



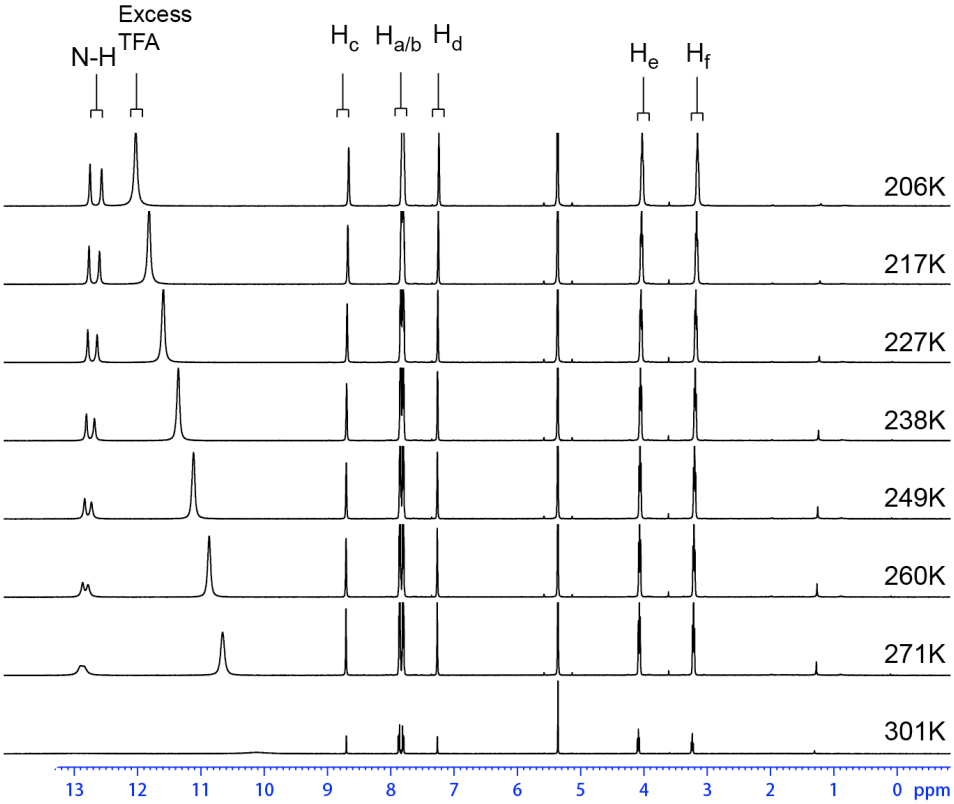
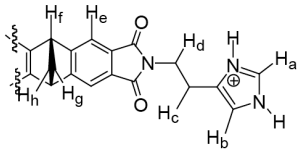


Figure S2: Variable temperature ^1H NMR (400 MHz) spectra of 14.3 mM solution of model compound [**4**-H]$^+$ in CD_2Cl_2.



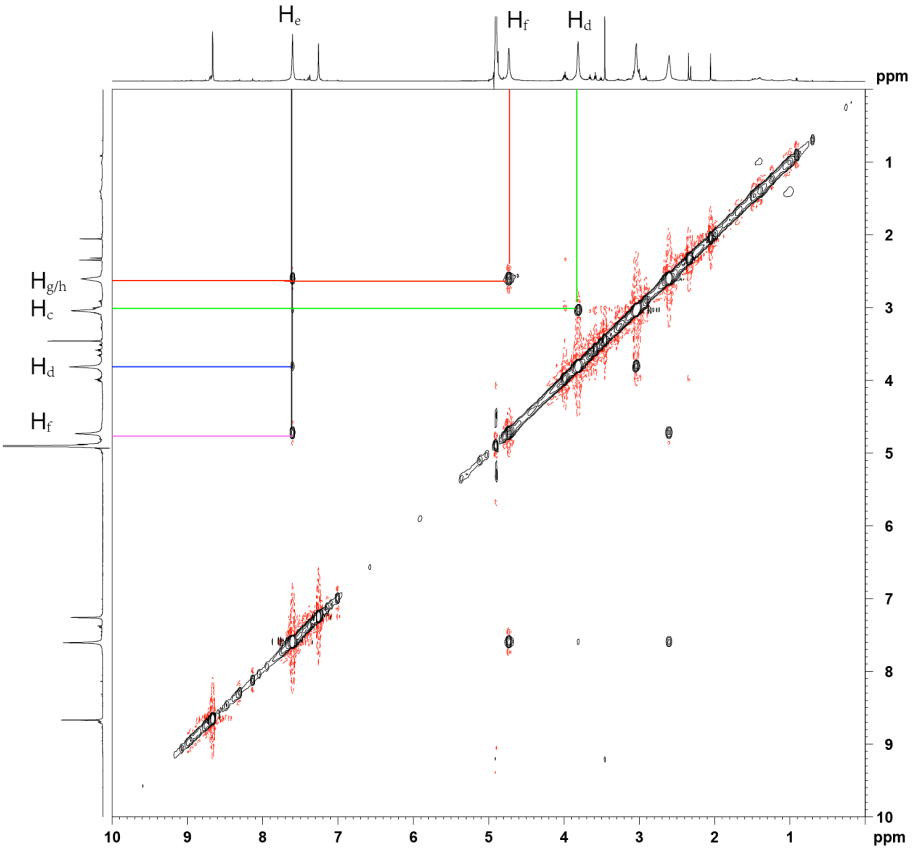


Figure S3: 2-D ^{1}H-^{1}H NOESY Spectrum (600 MHz, 298.0 K) of 1.5 mM [**1**-H_3]$^{3+}$ in D_2O; the mixing time is t_m = 200 ms.

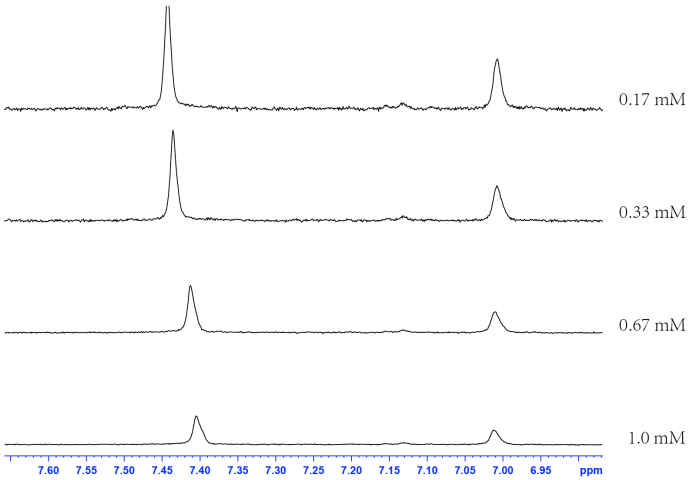


Figure S4: A segment of the ^{1}H NMR spectra (400 MHz, 298 K) of basket [**1**-H_3]$^{3+}$ obtained upon a dilution of its 1.0 mM solution (10.0 mM phosphate buffer at pH = 2.5 ± 0.1); note a downfield change in the chemical shift of H_e and H_b protons.

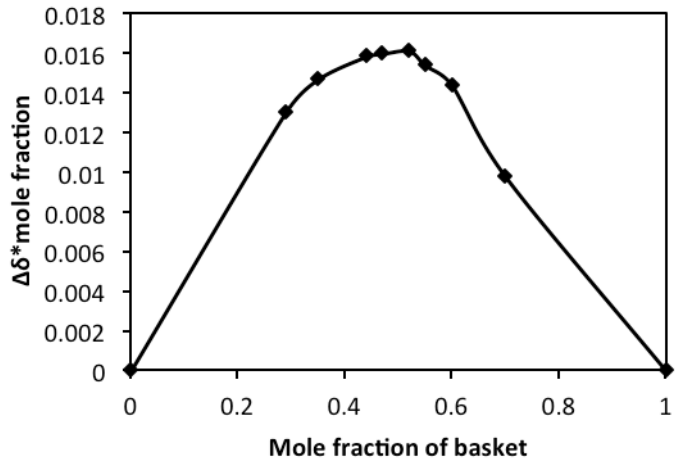


Figure S5: Job plot characterizing the binding of basket $[\mathbf{1}\text{-}H_3]^{3+}$ to dimethyl methylphosphonate (**5**) in H_2O/D_2O was obtained with ^1H NMR spectroscopy. Solid line, connecting the experimental points, is drawn to guide the eye.

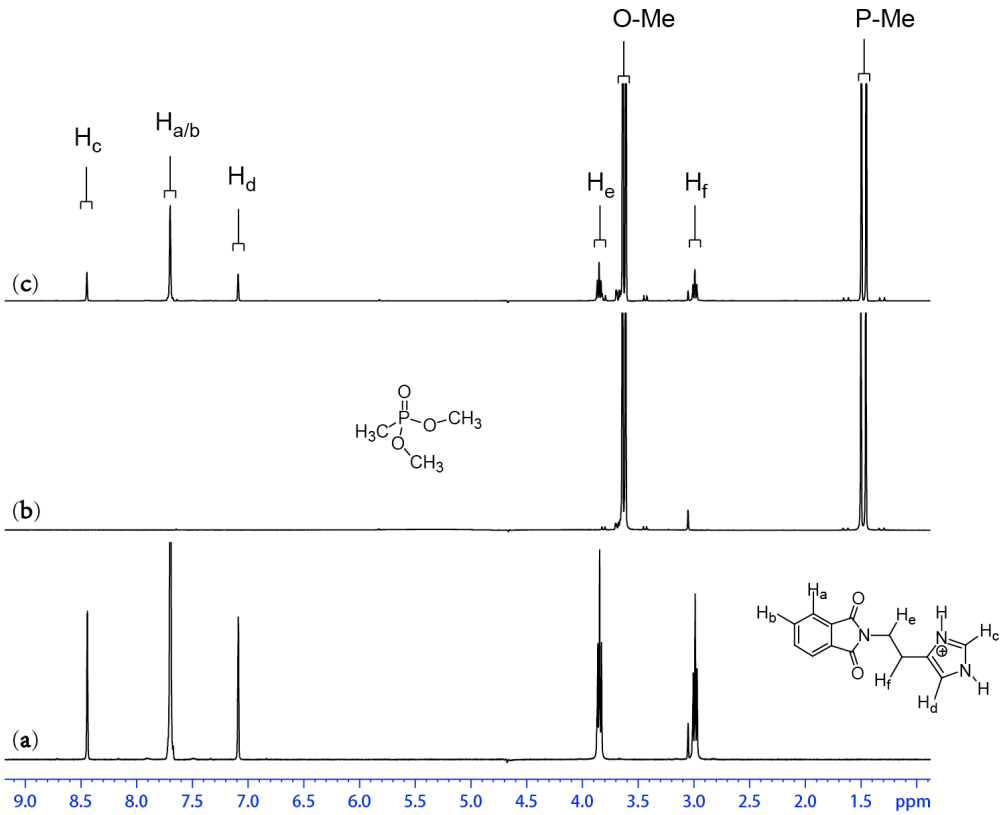


Figure S6: ^1H NMR spectra (400 MHz, 298.0 K) of (a) model compound $[\mathbf{4}\text{-}H]^+$ (14.3 mM), (b) DMMP **5** (60.0 mM) and (c) their mixture in 10.0 mM phosphate buffer at pH = 2.5 ± 0.1.

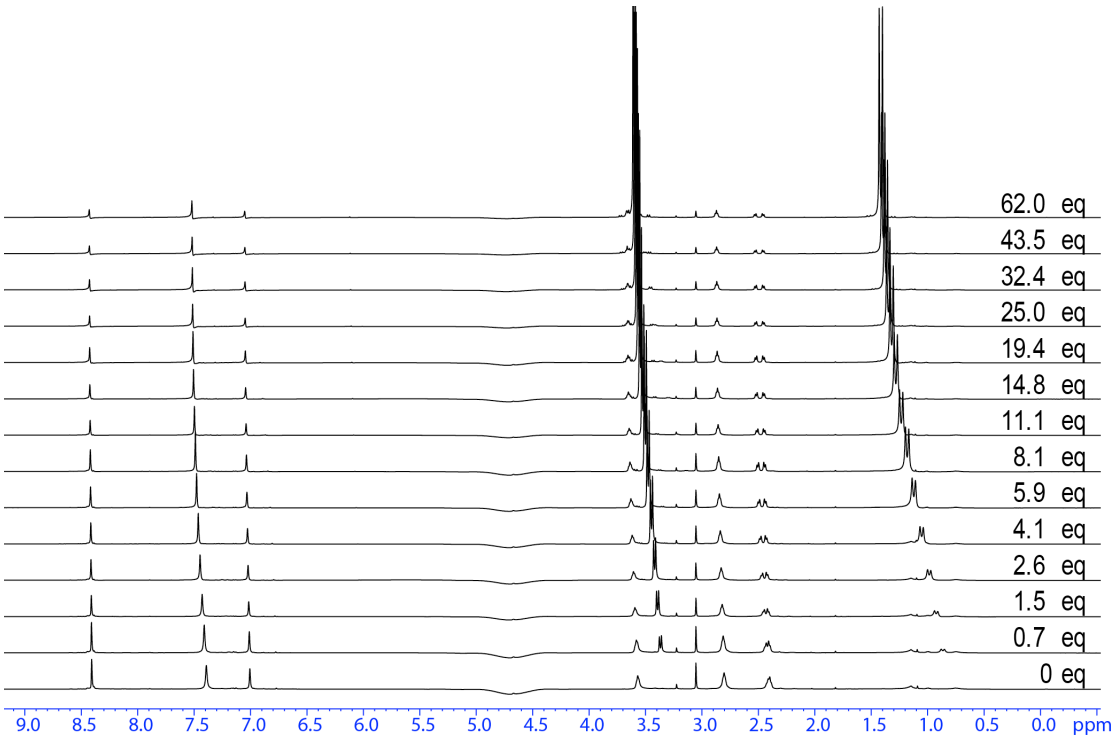


Figure S7: ^{1}H NMR spectra (600 MHz, 298.0 K) of basket $[\mathbf{1}\text{-}H_3]^{3+}$ (1.0 mM) obtained upon an incremental addition of dimethyl methylphosphonate **5** to the solution of basket (10.0 mM phosphate buffer at pH = 2.5 ± 0.1); note that the water resonance at 4.76 ppm was suppressed.

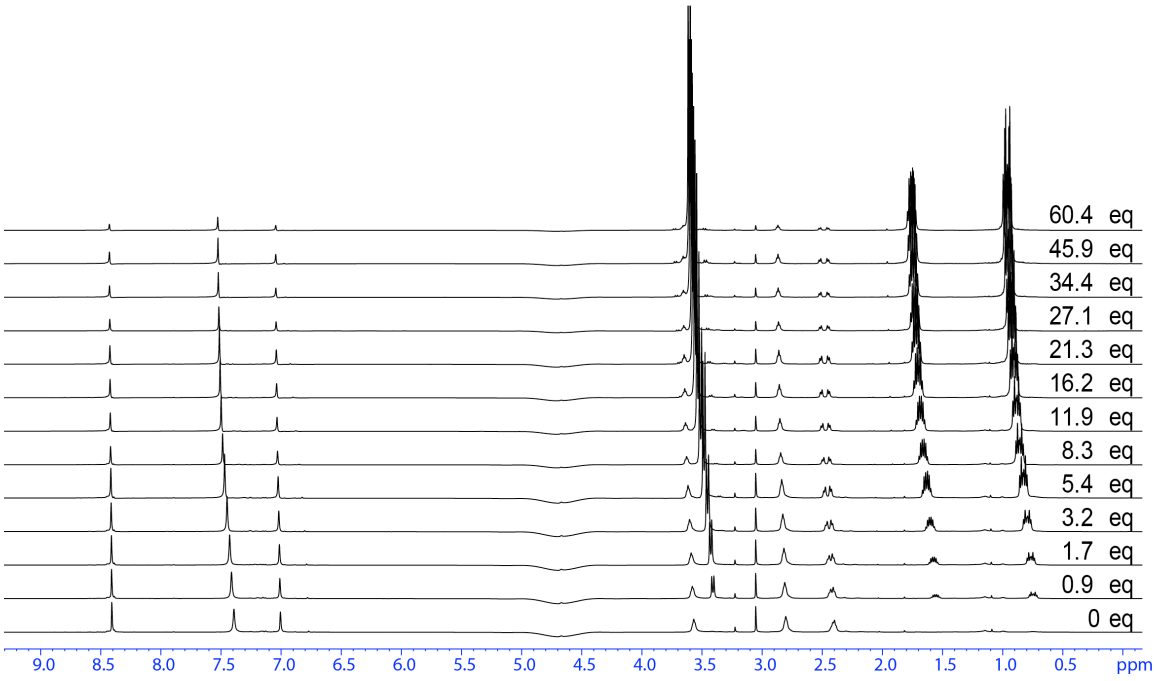


Figure S8: ^{1}H NMR spectra (600 MHz, 298.0 K) of basket $[\mathbf{1}\text{-}H_3]^{3+}$ (1.0 mM) obtained upon an incremental addition of dimethyl ethylphosphonate **6** to the solution of basket (10.0 mM phosphate buffer at pH = 2.5 ± 0.1); note that the water resonance at 4.76 ppm was suppressed.

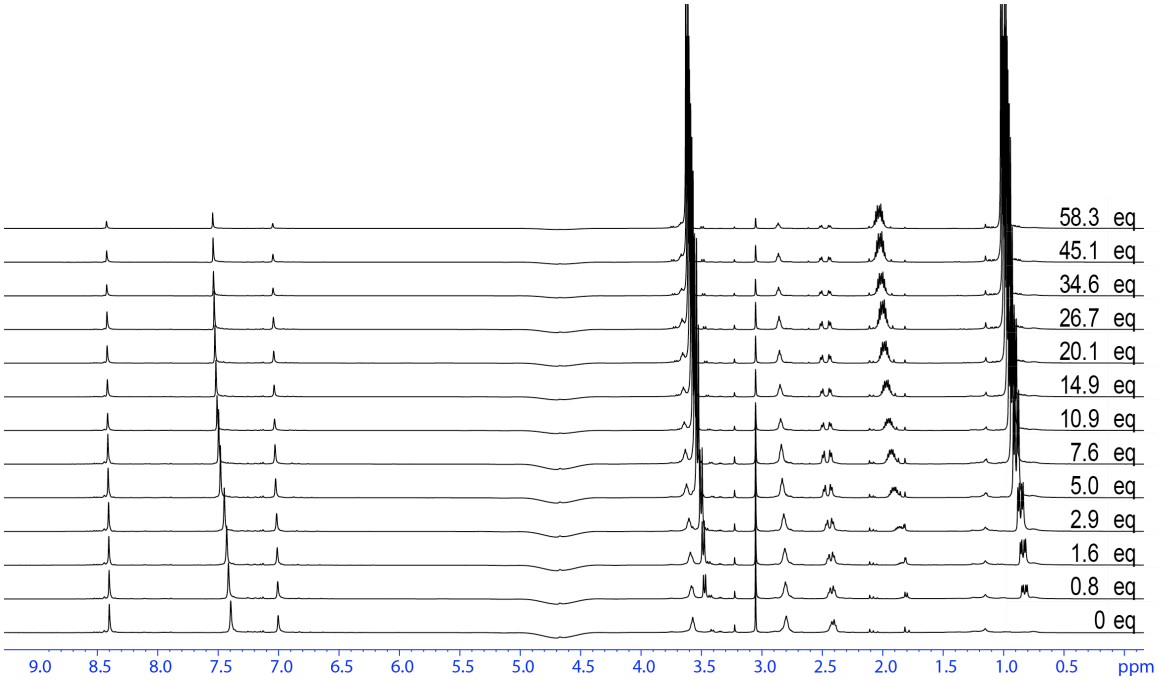


Figure S9: ^{1}H NMR spectra (600 MHz, 298.0 K) of basket $[\mathbf{1}\text{-}H_3]^{3+}$ (1.0 mM) obtained upon an incremental addition of dimethyl isopropylphosphonate **7** to the solution of basket (10.0 mM phosphate buffer at pH = 2.5 ± 0.1); note that the water resonance at 4.76 ppm was suppressed.

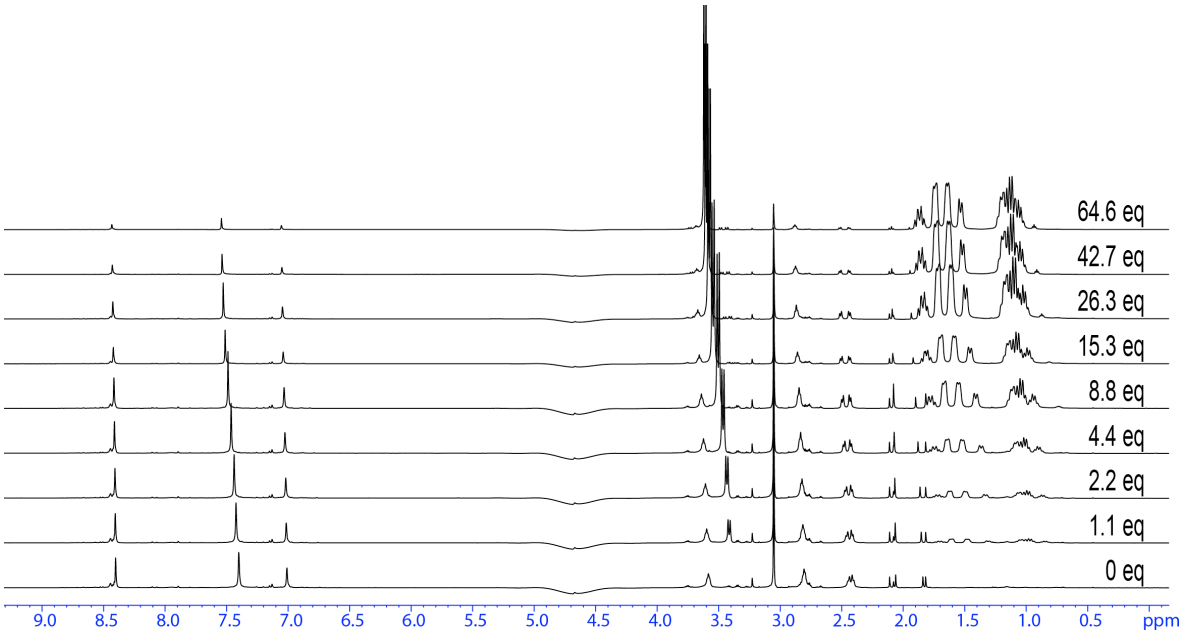
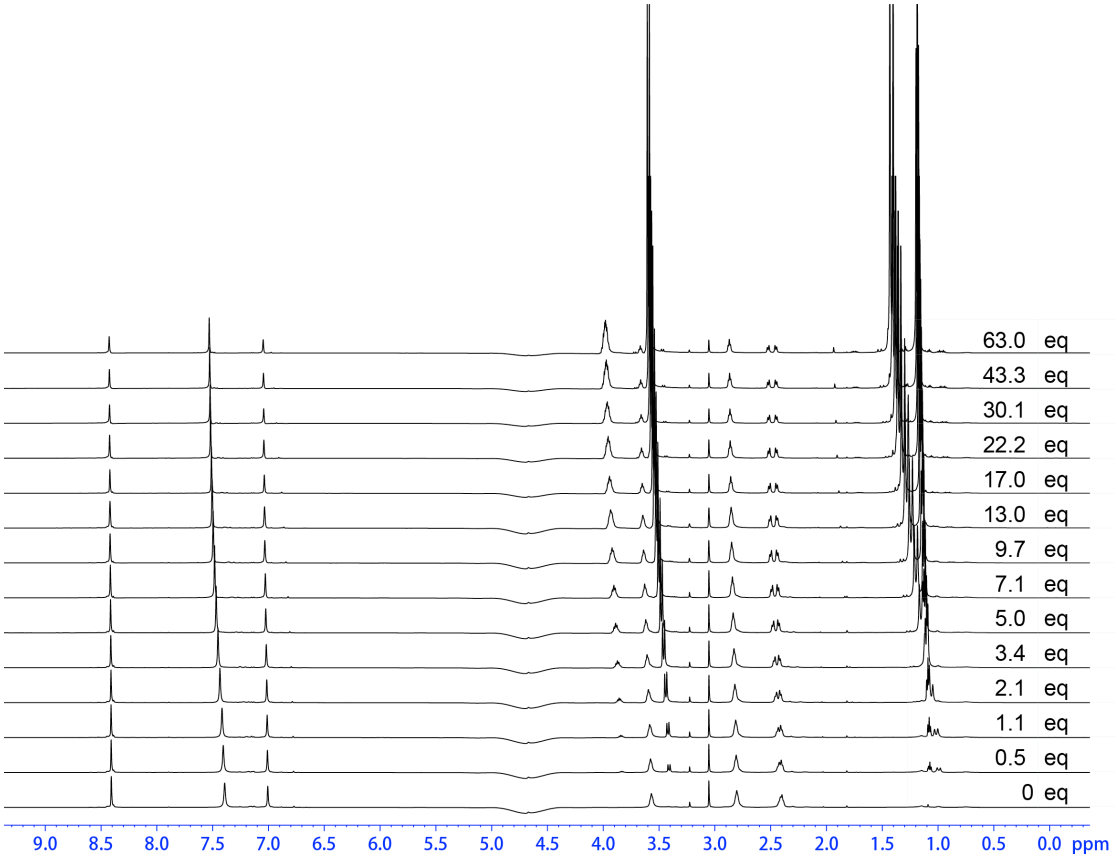


Figure S10: ^{1}H NMR spectra (600 MHz, 298.0 K) of basket $[\mathbf{1}\text{-}H_3]^{3+}$ (1.0 mM) obtained upon an incremental addition of dimethyl cyclohexylphosphonate **8** to the solution of basket (10.0 mM phosphate buffer at pH = 2.5 ± 0.1); note that the water resonance at 4.76 ppm was suppressed.



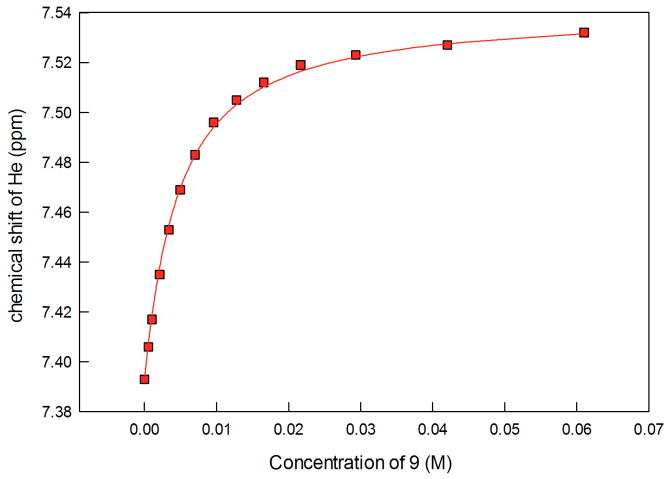
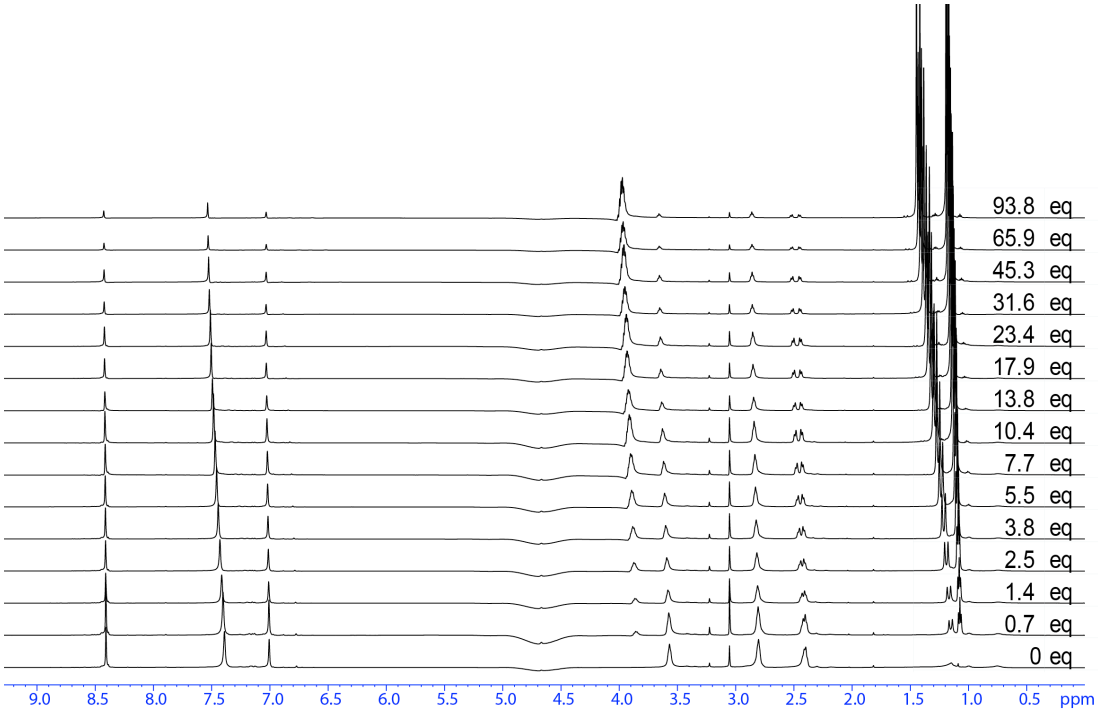


Figure S11: (Top) ^{1}H NMR spectra (600 MHz, 298.0 K) of basket [**1**-H_3]$^{3+}$ (1.0 mM) obtained upon an incremental addition of ethyl methyl methylphosphonate **9** to the solution of basket (10.0 mM phosphate buffer at pH = 2.5 ± 0.1); note that the water resonance at 4.76 ppm was suppressed. (Bottom) Nonlinear least-square analysis of the binding data (298.0 K, 1:1 binding stoichiometry) gave the apparent association constant K_{app} = 242 ± 4 M^{-1} (R^2 = 0.999, SigmaPlot).



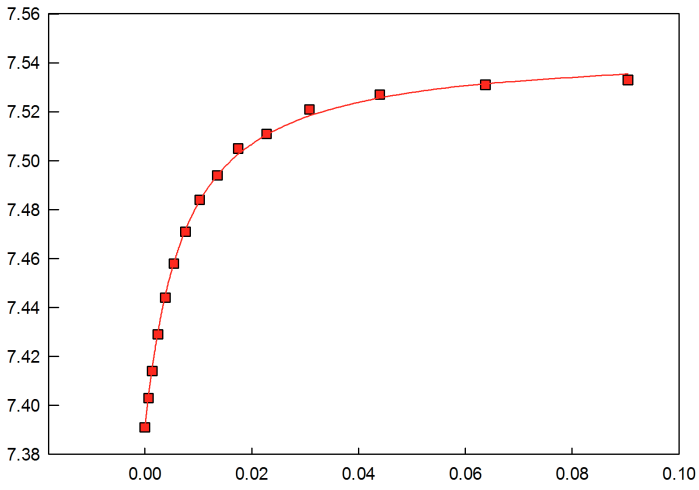
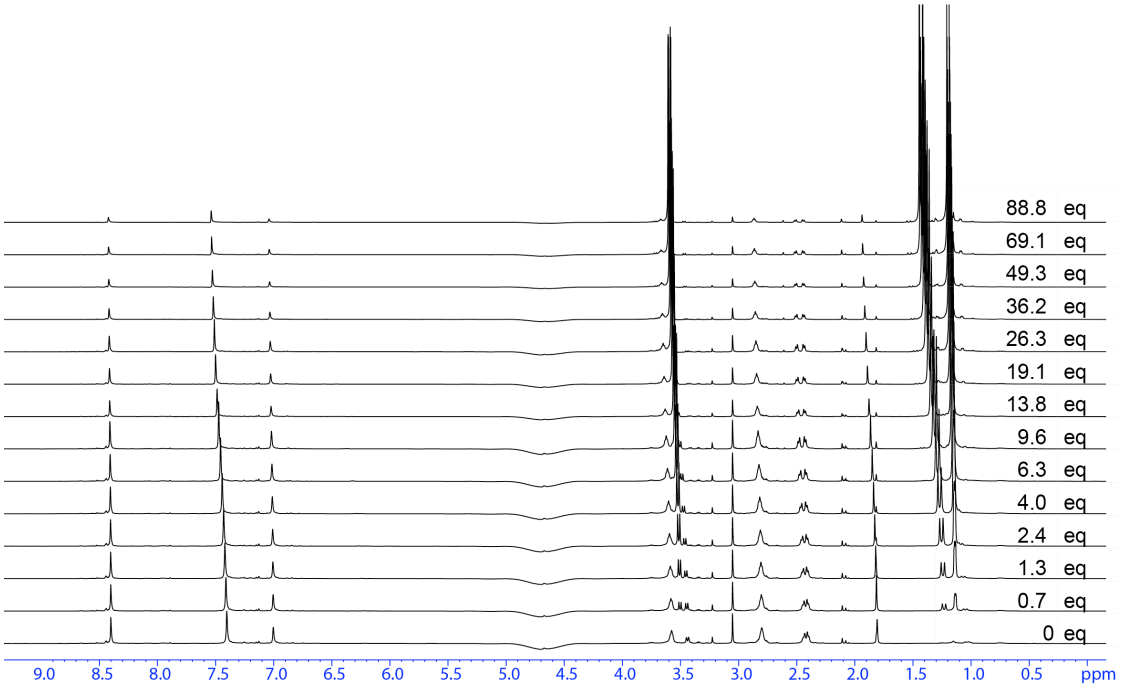


Figure S12: (Top) ^{1}H NMR spectra (600 MHz, 298.0 K) of basket [**1**-H_3]$^{3+}$ (1.0 mM) obtained upon an incremental addition of ethyl methyl methylphosphonate **10** to the solution of basket (10.0 mM phosphate buffer at pH = 2.5 ± 0.1); note that the water resonance at 4.76 ppm was suppressed. (Bottom) Nonlinear least-square analysis of the binding data (298.0 K, 1:1 binding stoichiometry) gave the apparent association constant K_{app} = 154 ± 2 M^{-1} (R^2 = 0.999, SigmaPlot).



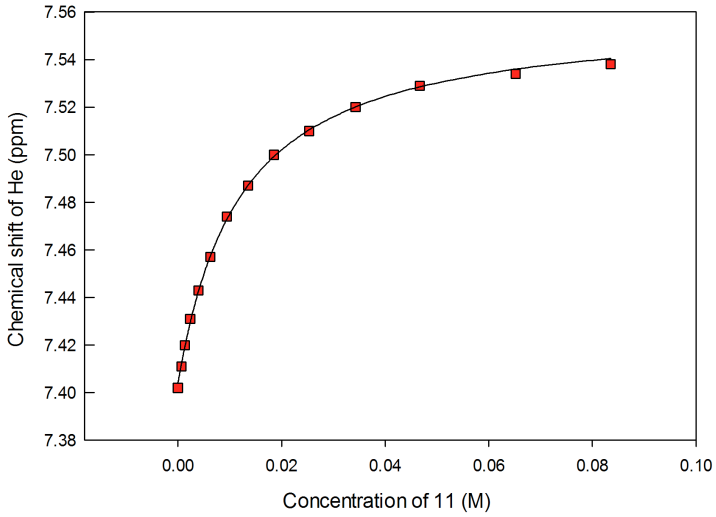
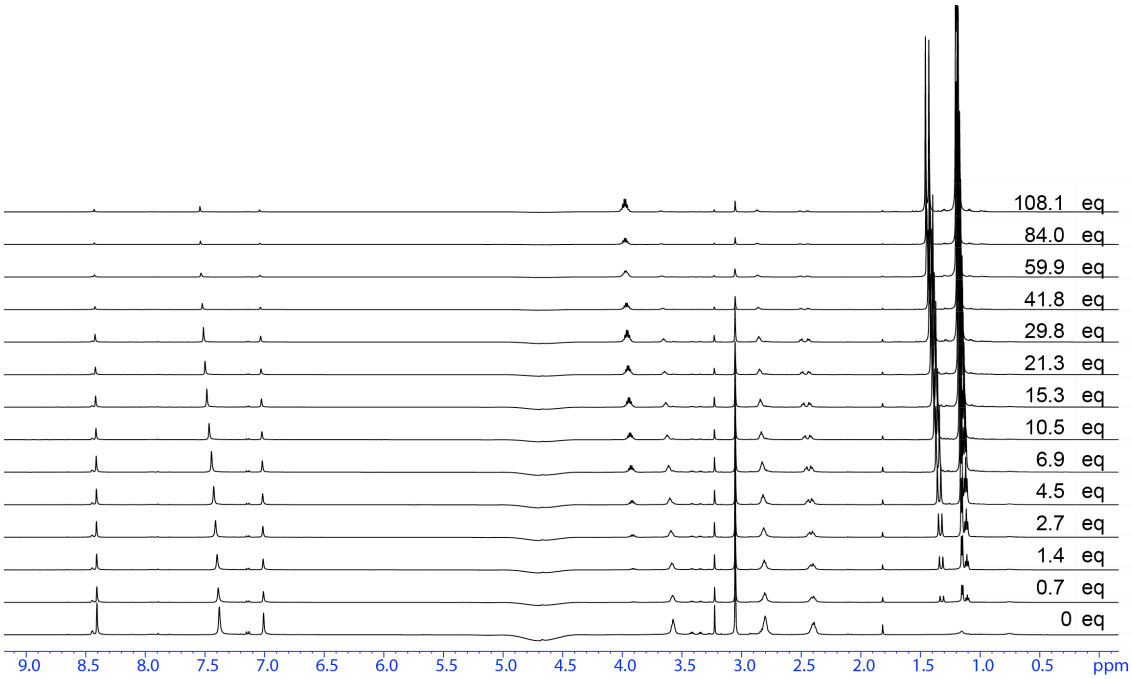


Figure S13: (Top) ^{1}H NMR spectra (600 MHz, 298.0 K) of basket [**1**-H_3]$^{3+}$ (1.0 mM) obtained upon an incremental addition of isopropyl methyl methylphosphonate **11** to the solution of basket (10.0 mM phosphate buffer at pH = 2.5 ± 0.1); note that the water resonance at 4.76 ppm was suppressed.(Bottom) Nonlinear least-square analysis of the binding data (298.0 K, 1:1 binding stoichiometry) gave the apparent association constant K_{app} = 100 ± 11 M^{-1} (R^2 = 0.999, SigmaPlot).



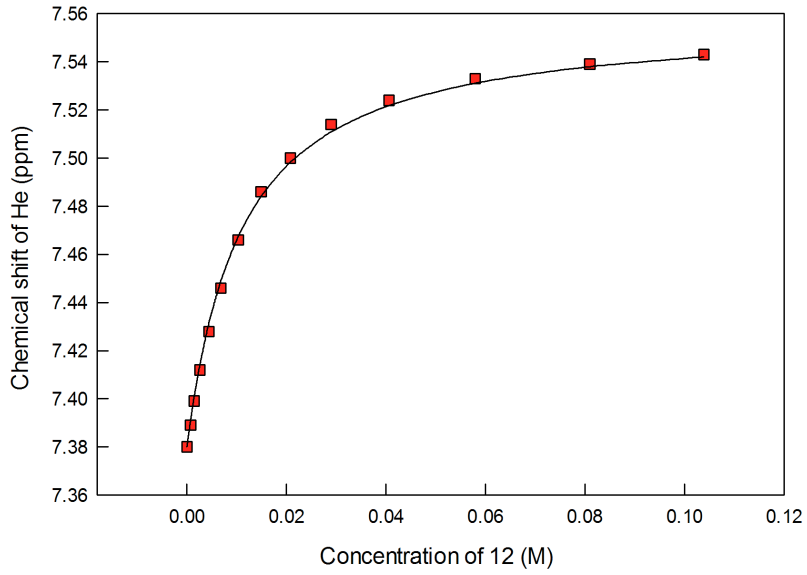
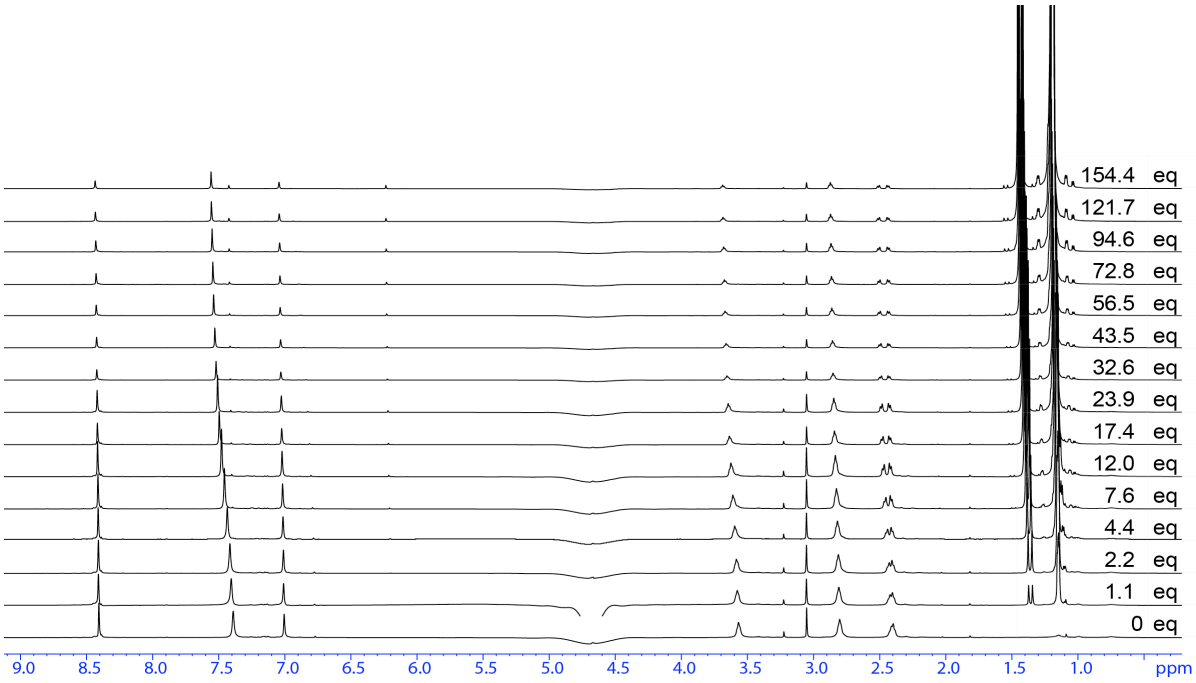


Figure S14: (Top) ^{1}H NMR spectra (600 MHz, 298.0 K) of basket [**1**-H_3]$^{3+}$ (1.0 mM) obtained upon an incremental addition of ethyl isopropyl methylphosphonate **12** to the solution of basket (10.0 mM phosphate buffer at pH = 2.5 ± 0.1); note that the water resonance at 4.76 ppm was suppressed. (Bottom) Nonlinear least-square analysis of the binding data (298.0 K, 1:1 binding stoichiometry) gave the apparent association constant K_{app} = 98 ± 2 M^{-1} (R^2 = 0.999, SigmaPlot).



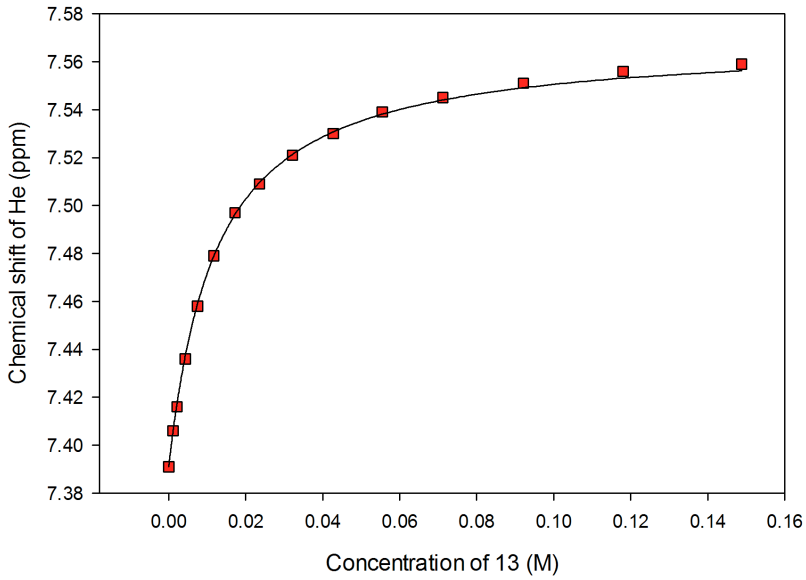


Figure S15: (Top) ^{1}H NMR spectra (600 MHz, 298.0 K) of basket [**1**-H_3]$^{3+}$ (1.0 mM) obtained upon an incremental addition of diisopropyl methylphosphonate **13** to the solution of basket (10.0 mM phosphate buffer at pH = 2.5 ± 0.1); note that the water resonance at 4.76 ppm was suppressed. (Bottom) Nonlinear least-square analysis of the binding data (298.0 K, 1:1 binding stoichiometry) gave the apparent association constant K_{app} = 87 ± 1 M^{-1} (R^2 = 0.999, SigmaPlot).

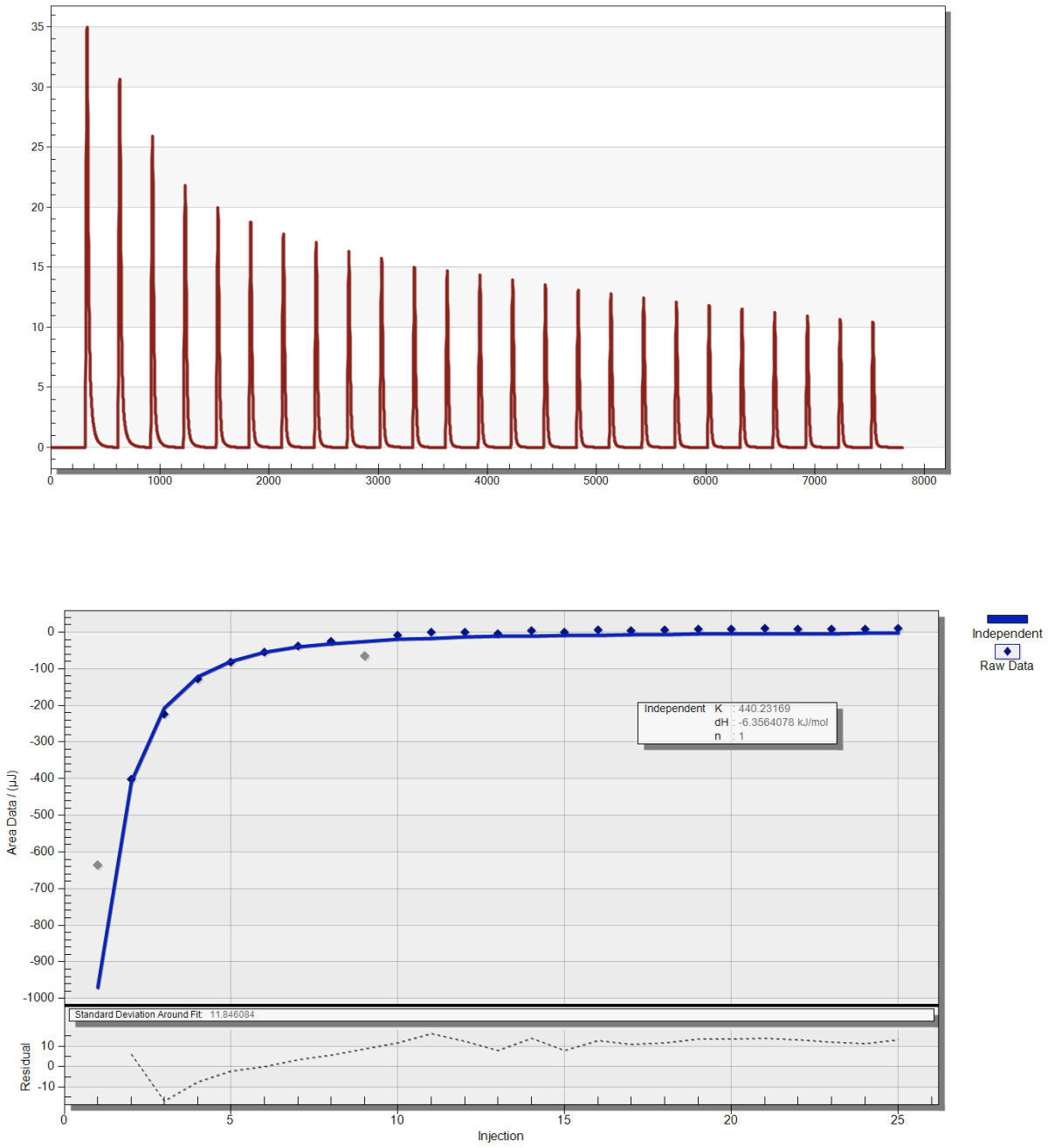


Figure S16: Exemplary raw and integrated ITC data from the titration of DMMP **5** (0.350 M) to $[\mathbf{1}\text{-}H_3]^{3+}$ (1.15 mM) at 298.0 K (top) and the fitting curve (bottom) using the single site binding model with N fixed to 1. Thermodynamic data: K = 415 ± 25 M^{-1}, ΔH^{o} = -1.60 ± 0.08 kcal/mol, ΔS^{o} = 6.3 ± 0.9 e.u; The reported data are from two measurements.

Computational Protocols

Table S1. Partial atomic charges averaged over all conformations of basket.

Atom #	Atom Type	Charge	Atom #	Atom Type	Charge
1	C	-0.0586	56	H	0.1546
2	C	-0.0729	57	H	0.1540
3	C	-0.0519	58	H	0.1570
4	C	-0.0606	59	H	0.1520
5	C	-0.0564	60	H	0.0784
6	C	-0.0598	61	H	0.1096
7	C	0.0757	62	H	0.1286
8	C	0.0839	63	H	0.0767
9	C	0.0823	64	N	-0.3433
10	C	0.0783	65	C	0.1790
11	C	0.0763	66	H	0.0529
12	C	0.0607	67	C	-0.3569
13	C	0.0557	68	H	0.1510
14	C	-0.2716	69	H	0.1616
15	C	0.0426	70	C	0.2012
16	C	0.0776	71	N	-0.1340
17	C	-0.2700	72	C	-0.1910
18	C	0.0537	73	H	0.3390
19	C	0.0658	74	C	-0.0329
20	C	-0.0720	75	N	-0.1495
21	C	-0.1960	76	H	0.2374
22	C	-0.1152	77	H	0.2376
23	C	-0.1678	78	H	0.3768
24	C	-0.0861	79	N	-0.3109
25	C	-0.1825	80	C	0.0939
26	C	-0.0927	81	H	0.0679
27	C	-0.1792	82	C	-0.2547
28	C	-0.0838	83	H	0.1309
29	C	-0.1835	84	H	0.1455
30	C	-0.0939	85	C	0.1327
31	C	-0.1850	86	N	-0.0495
32	C	0.5681	87	C	-0.1955
33	O	-0.4852	88	H	0.2966
34	C	0.5804	89	C	-0.0748
35	O	-0.5015	90	N	-0.1328
36	C	0.6042	91	H	0.2365
37	O	-0.5178	92	H	0.2356
38	C	0.5714	93	H	0.3684

39	O	-0.4722	94	N	-0.3244
40	C	0.5766	95	C	0.1511
41	O	-0.4805	96	H	0.0591
42	C	0.5707	97	C	-0.2953
43	O	-0.4952	98	H	0.1438
44	C	0.0693	99	H	0.1453
45	C	-0.2694	100	C	0.1597
46	H	0.0778	101	N	-0.0731
47	H	0.0754	102	C	-0.1965
48	H	0.0766	103	H	0.3111
49	H	0.0772	104	C	-0.0603
50	H	0.1306	105	N	-0.1416
51	H	0.1092	106	H	0.2359
52	H	0.1093	107	H	0.2407
53	H	0.1297	108	H	0.3741
54	H	0.1548	109	H	0.0624
55	H	0.1511	110	H	0.0899
			111	H	0.0651

Starting Coordinates used for MD Simulations

Conformation 1				Conformation 2			
C	1.8338	-1.8068	-3.2933	C	-1.1476	-1.4038	3.3143
C	0.6620	-1.0808	-3.6665	C	-1.8809	-0.1787	3.3052
C	-0.5799	-1.6100	-3.3882	C	-1.2134	1.0188	3.4127
C	-0.6800	-2.8465	-2.6746	C	0.2109	1.0397	3.5315
C	0.4554	-3.5229	-2.2887	C	0.9170	-0.1416	3.5358
C	1.7353	-3.0293	-2.6762	C	0.2222	-1.3862	3.4314
C	3.0263	-0.9647	-3.7389	C	-2.1892	-2.5274	3.3536
C	1.1596	0.1832	-4.3987	C	-3.3657	-0.5645	3.3477
C	2.7562	-4.1181	-2.3179	C	1.2652	-2.4842	3.6644
C	-2.1636	-3.2281	-2.6762	C	0.5959	2.4967	3.8266
C	-2.0096	-1.2459	-3.8113	C	-1.6837	2.4605	3.6260
C	-2.9353	-2.1986	-1.8560	C	0.2546	3.3383	2.5970
C	-2.8440	-0.9698	-2.5565	C	-1.1566	3.3009	2.4643
C	-2.5311	-2.6966	-4.1059	C	-0.6373	2.8888	4.7122
C	1.8392	1.0424	-3.3342	C	-3.6992	-1.2747	2.0361
C	2.9563	0.2976	-2.8737	C	-2.9614	-2.4853	2.0354
C	2.4470	-0.3952	-5.0740	C	-3.2541	-1.8287	4.2672
C	2.8412	-4.1180	-0.8034	C	2.2492	-2.4466	2.4971
C	1.5685	-4.5199	-0.3243	C	2.9433	-1.2146	2.5919
C	3.4095	1.9922	-1.2811	C	-3.9655	-3.0854	-0.0190
C	3.7293	0.7325	-1.7979	C	-3.0663	-3.4089	0.9987

C	2.4046	2.7917	-1.8430	C	-4.7118	-1.9023	-0.0079
C	1.5660	2.3235	-2.8577	C	-4.5889	-0.9560	1.0137
C	-4.4408	-1.2092	-0.3246	C	0.3709	4.8735	0.7994
C	-3.7209	-2.3403	-0.7164	C	1.0490	4.1233	1.7653
C	-4.3597	0.0034	-1.0171	C	-1.0179	4.8078	0.6486
C	-3.5461	0.1602	-2.1443	C	-1.8204	4.0147	1.4707
C	3.6154	-3.8686	1.4065	C	3.6181	-3.0715	0.6734
C	3.8965	-3.8060	0.0435	C	2.5624	-3.3951	1.5284
C	2.3455	-4.1930	1.8938	C	4.3086	-1.8583	0.7675
C	1.2884	-4.5408	1.0414	C	3.9816	-0.8909	1.7227
C	-5.4697	-1.0725	0.7428	C	0.8848	5.9027	-0.1368
O	-5.8663	-1.8867	1.5547	O	2.0502	6.2872	-0.2700
C	-5.3385	0.9527	-0.4126	C	-1.4150	5.7641	-0.4147
O	-5.6026	2.1006	-0.7193	O	-2.5080	6.0245	-0.8643
C	2.4913	4.1315	-1.2191	C	-5.6337	-1.9308	-1.1691
O	1.8699	5.1505	-1.5079	O	-6.4842	-1.0928	-1.4842
C	4.0096	2.7489	-0.1580	C	-4.3664	-3.8744	-1.2117
O	4.7792	2.3696	0.7156	O	-3.9599	-4.9378	-1.6223
C	4.5083	-3.5775	2.5571	C	4.2629	-3.8983	-0.3830
O	5.6695	-3.2162	2.5588	O	3.9973	-5.0200	-0.7712
C	2.3778	-4.0233	3.3766	C	5.4193	-1.8747	-0.2256
O	1.4543	-4.0078	4.1740	O	6.2712	-1.0371	-0.4608
C	0.7218	-4.8510	-1.5695	C	2.3828	-0.4935	3.8205
C	1.8580	-5.3862	-2.5032	C	2.1463	-1.7477	4.7309
H	3.9961	-1.4625	-3.7739	H	-1.8304	-3.5113	3.6588
H	0.4389	0.6955	-5.0374	H	-4.0611	0.2197	3.6508
H	3.7060	-4.0873	-2.8537	H	0.8783	-3.4707	3.9242
H	-2.1021	-0.5078	-4.6096	H	-2.7401	2.5957	3.8626
H	-1.9765	-3.1975	-4.9050	H	-0.7094	2.2980	5.6302
H	-3.6051	-2.7332	-4.3152	H	-0.6748	3.9571	4.9500
H	3.0770	0.3767	-5.5284	H	-4.1914	-2.3899	4.3432
H	2.2297	-1.1782	-5.8056	H	-2.8738	-1.5982	5.2668
H	4.5615	0.1532	-1.4068	H	-2.5180	-4.3467	0.9886
H	0.7652	2.9372	-3.2605	H	-5.1839	-0.0470	1.0177
H	-3.8256	-3.2845	-0.1889	H	2.1267	4.1939	1.8826
H	-3.5214	1.0981	-2.6928	H	-2.9015	4.0076	1.3639
H	4.8860	-3.5421	-0.3201	H	2.0547	-4.3531	1.4575
H	0.3174	-4.8247	1.4382	H	4.5433	0.0360	1.7991
H	-0.1395	-5.4979	-1.3982	H	3.0040	0.3092	4.2209
H	2.3324	-6.2990	-2.1293	H	3.0694	-2.2852	4.9715
H	1.5262	-5.5330	-3.5353	H	1.5995	-1.5128	5.6492
H	-2.3893	-4.2723	-2.4549	H	1.5894	2.6576	4.2477
N	3.4627	4.0534	-0.2108	N	-5.3958	-3.1142	-1.8523
C	4.0353	5.1862	0.5183	C	-6.0054	-3.5366	-3.1087

H	4.5195	5.8549	-0.2025	H	-5.3164	-4.2734	-3.5274
C	3.0352	5.9789	1.4149	C	-7.4049	-4.1990	-2.9628
H	2.1042	5.4098	1.5224	H	-7.4665	-5.0464	-3.6529
H	3.4539	6.0741	2.4212	H	-7.4917	-4.6250	-1.9551
C	2.7266	7.3643	0.9277	C	-8.5857	-3.3134	-3.2417
N	2.1436	7.6092	-0.3088	N	-8.6731	-1.9927	-2.8229
C	2.9184	8.5935	1.5010	C	-9.7660	-3.5816	-3.8853
H	1.9125	6.8416	-0.9613	H	-7.9002	-1.5027	-2.3194
C	1.9832	8.9192	-0.4926	C	-9.8454	-1.4724	-3.1848
N	2.4470	9.5347	0.6014	N	-10.5265	-2.4267	-3.8306
H	3.3411	8.8754	2.4537	H	-10.1242	-4.4806	-4.3636
H	1.5604	9.3994	-1.3633	H	-10.1841	-0.4642	-2.9975
H	2.4558	10.5405	0.7391	H	-11.4560	-2.3121	-4.2209
N	3.7152	-3.7427	3.7121	N	5.3271	-3.1189	-0.8825
C	4.2130	-3.4683	5.0516	C	6.2532	-3.5785	-1.8942
H	5.2994	-3.5626	4.9959	H	6.6728	-2.6919	-2.3785
C	3.8259	-2.0565	5.5859	C	7.3720	-4.4567	-1.2708
H	2.8253	-2.0935	6.0294	H	7.8841	-3.8875	-0.4856
H	4.5198	-1.7804	6.3860	H	6.9123	-5.3264	-0.7918
C	3.8429	-1.0135	4.5129	C	8.3726	-4.9463	-2.2689
N	2.7150	-0.7702	3.7361	N	9.4271	-4.1659	-2.7409
C	4.8291	-0.2280	3.9720	C	8.4976	-6.1475	-2.9159
H	1.8163	-1.2245	3.8757	H	9.6311	-3.2168	-2.4428
C	2.9933	0.1102	2.7685	C	10.1637	-4.8510	-3.6229
N	4.2768	0.4507	2.9002	N	9.6062	-6.0579	-3.7405
H	5.8698	-0.1256	4.2391	H	7.9021	-7.0457	-2.8507
H	2.3099	0.4730	2.0169	H	11.0463	-4.4982	-4.1365
H	4.7497	1.0955	2.2598	H	9.9588	-6.7984	-4.3392
N	-5.9652	0.2430	0.6326	N	-0.2024	6.3914	-0.8485
C	-7.0591	0.7537	1.4332	C	-0.2147	7.5561	-1.7277
H	-6.9933	1.8453	1.4155	H	0.1840	8.4186	-1.1816
C	-8.4256	0.2631	0.8812	C	0.5283	7.3699	-3.0848
H	-8.5364	0.5924	-0.1591	H	0.6930	6.3007	-3.2660
H	-8.4270	-0.8309	0.8750	H	-0.1145	7.7211	-3.8976
C	-9.6033	0.7225	1.6820	C	1.8280	8.1114	-3.1868
N	-10.1881	1.9802	1.5392	N	2.8397	7.9729	-2.2467
C	-10.3348	0.0952	2.6559	C	2.2923	9.0113	-4.1097
H	-9.8946	2.6912	0.8763	H	2.7289	7.3597	-1.4105
C	-11.2259	2.1155	2.3729	C	3.8756	8.7453	-2.5683
N	-11.3232	0.9759	3.0605	N	3.5629	9.3834	-3.7035
H	-10.2397	-0.8938	3.0787	H	1.8366	9.4122	-5.0023
H	-11.8684	2.9791	2.4662	H	4.7977	8.8461	-2.0150
H	-12.0310	0.7873	3.7641	H	4.1654	10.0463	-4.1797
H	4.8240	4.7564	1.1387	H	-6.0364	-2.6809	-3.7909

H	3.8290	-4.2265	5.7383	H	5.6942	-4.1579	-2.6346
H	-6.9269	0.4050	2.4615	H	-1.2725	7.7502	-1.9185

Conformation 3

				Conformation 4			
C	0.2210	-1.8948	3.2298	C	-0.6595	0.4806	3.4047
C	-0.8097	-0.9162	3.3822	C	0.7120	0.8847	3.3912
C	-0.4767	0.4181	3.4652	C	1.7141	-0.0567	3.3561
C	0.8955	0.8137	3.3932	C	1.3808	-1.4446	3.3420
C	1.8837	-0.1283	3.2291	C	0.0631	-1.8354	3.3610
C	1.5378	-1.5102	3.1442	C	-0.9801	-0.8585	3.3829
C	-0.4478	-3.2600	3.4049	C	-1.4788	1.7566	3.6538
C	-2.1068	-1.7002	3.6357	C	0.7179	2.3980	3.6248
C	2.8590	-2.2861	3.1505	C	-2.2887	-1.6374	3.5877
C	0.9336	2.3046	3.7365	C	2.6998	-2.2060	3.5032
C	-1.2650	1.6793	3.8517	C	3.2372	0.0188	3.5311
C	0.2072	3.0635	2.6294	C	3.5436	-1.9451	2.2560
C	-1.1588	2.6923	2.7097	C	3.8882	-0.5703	2.2789
C	-0.2065	2.3247	4.8133	C	3.4230	-1.2155	4.4801
C	-2.4420	-2.5143	2.3819	C	0.0548	3.0599	2.4194
C	-1.4044	-3.4692	2.2360	C	-1.3104	2.6783	2.4457
C	-1.5029	-2.8651	4.4959	C	-0.4857	2.4835	4.6258
C	3.6014	-1.9376	1.8608	C	-2.5261	-2.5192	2.3582
C	3.9577	-0.5688	1.9547	C	-1.4775	-3.4732	2.3416
C	-2.5546	-4.4382	0.4158	C	-1.7364	4.1244	0.6200
C	-1.4245	-4.4339	1.2334	C	-2.2359	3.2054	1.5483
C	-3.5986	-3.5216	0.5755	C	-0.3809	4.4679	0.5714
C	-3.5602	-2.5182	1.5508	C	0.5529	3.9446	1.4669
C	-0.3274	4.6510	0.9634	C	4.9023	-2.2453	0.3458
C	0.6561	4.0295	1.7339	C	4.0250	-2.8075	1.2748
C	-1.6817	4.3183	1.0686	C	5.2661	-0.8957	0.3827
C	-2.1323	3.3113	1.9292	C	4.7534	-0.0146	1.3399
C	4.7602	-2.0900	-0.1936	C	-3.5313	-3.6185	0.5160
C	3.9805	-2.7233	0.7757	C	-3.5744	-2.5701	1.4420
C	5.1348	-0.7464	-0.0899	C	-2.4765	-4.5360	0.4845
C	4.7321	0.0568	0.9811	C	-1.4157	-4.4859	1.3892
C	-0.1999	5.7924	0.0240	C	5.6715	-2.9037	-0.7405
O	0.7835	6.3875	-0.3536	O	5.6666	-4.0536	-1.1152
C	-2.4522	5.2734	0.2335	C	6.3000	-0.6710	-0.6581
O	-3.6780	5.3465	0.1057	O	6.8993	0.3779	-0.9112
C	-4.6913	-3.9095	-0.3523	C	-0.1978	5.4835	-0.4962
O	-5.8004	-3.3805	-0.4762	O	0.8070	6.0231	-0.9024
C	-2.9399	-5.4048	-0.6418	C	-2.4547	4.9594	-0.3732
O	-2.3384	-6.3532	-1.0902	O	-3.6686	5.0059	-0.5953
C	5.3807	-2.6504	-1.4215	C	-4.5414	-4.0505	-0.4831

O	5.2971	-3.7550	-1.9082	O	-5.6353	-3.5311	-0.7244
C	6.0372	-0.4333	-1.2251	C	-2.7710	-5.5495	-0.5587
O	6.6142	0.6314	-1.4648	O	-2.1323	-6.5127	-0.9149
C	3.4161	-0.0708	3.2950	C	-0.6110	-3.1942	3.5655
C	3.6639	-1.3705	4.1356	C	-1.7449	-2.7479	4.5525
H	0.2156	-4.0976	3.6254	H	-2.5041	1.6117	3.9978
H	-2.9357	-1.1359	4.0659	H	1.6670	2.8350	3.9384
H	2.7967	-3.3494	3.3863	H	-3.1490	-1.0568	3.9243
H	-2.2695	1.5177	4.2458	H	3.6392	0.9762	3.8660
H	0.0176	1.7005	5.6834	H	2.9032	-1.1027	5.4363
H	-0.4772	3.3352	5.1369	H	4.4735	-1.4712	4.6529
H	-2.2230	-3.6623	4.7079	H	-0.7834	3.5120	4.8561
H	-1.0451	-2.5169	5.4267	H	-0.3102	1.9285	5.5520
H	-0.6447	-5.1817	1.1202	H	-3.2924	2.9547	1.5840
H	-4.3857	-1.8236	1.6791	H	1.5939	4.2542	1.4395
H	1.6968	4.3346	1.6700	H	3.7842	-3.8666	1.2517
H	-3.1886	3.0723	2.0157	H	5.0582	1.0278	1.3695
H	3.7265	-3.7765	0.6943	H	-4.4084	-1.8743	1.4689
H	5.0404	1.0958	1.0562	H	-0.6271	-5.2329	1.3738
H	3.8506	0.8591	3.6650	H	0.0378	-4.0130	3.8794
H	4.7224	-1.6412	4.2077	H	-2.4753	-3.5381	4.7552
H	3.2204	-1.3248	5.1347	H	-1.3579	-2.3455	5.4935
H	1.9053	2.7093	4.0235	H	2.6232	-3.2501	3.8097
N	-4.2523	-5.0163	-1.0656	N	-1.5053	5.7444	-1.0123
C	-5.0575	-5.8796	-1.9241	C	-1.7302	6.6511	-2.1336
H	-5.9254	-6.2353	-1.3572	H	-2.4530	6.1923	-2.8156
C	-5.5028	-5.2447	-3.2752	C	-2.1553	8.0897	-1.7322
H	-4.9051	-4.3462	-3.4715	H	-1.7361	8.3189	-0.7442
H	-5.2835	-5.9408	-4.0901	H	-1.6892	8.7963	-2.4265
C	-6.9635	-4.9141	-3.3440	C	-3.6312	8.3743	-1.7357
N	-7.5895	-4.1182	-2.3945	N	-4.6008	7.4569	-1.3533
C	-7.9405	-5.2808	-4.2316	C	-4.3081	9.5224	-2.0576
H	-7.0689	-3.7289	-1.5797	H	-4.3864	6.4744	-1.0724
C	-8.8855	-3.9982	-2.6771	C	-5.8118	8.0094	-1.4313
N	-9.1181	-4.6962	-3.7962	N	-5.6529	9.2685	-1.8555
H	-7.9006	-5.8974	-5.1167	H	-3.9524	10.4817	-2.4019
H	-9.6189	-3.4467	-2.1077	H	-6.7509	7.5288	-1.2002
H	-10.0244	-4.7898	-4.2426	H	-6.4081	9.9287	-2.0080
N	6.1549	-1.5873	-1.9853	N	-4.0432	-5.1854	-1.1076
C	6.8620	-1.7305	-3.2537	C	-4.7701	-6.0803	-2.0025
H	6.6552	-0.8518	-3.8729	H	-5.6894	-6.4107	-1.5058
C	8.3895	-1.9883	-3.1228	C	-5.0824	-5.4969	-3.4130
H	8.5879	-2.4568	-2.1503	H	-4.4622	-4.6088	-3.5853
H	8.6866	-2.7245	-3.8763	H	-4.7918	-6.2246	-4.1765

C	9.2794	-0.7908	-3.2992	C	-6.5270	-5.1627	-3.6346
N	8.9903	0.4681	-2.7896	N	-7.2358	-4.3290	-2.7804
C	10.4970	-0.6740	-3.9181	C	-7.4150	-5.5539	-4.6016
H	8.1057	0.6894	-2.2816	H	-6.7949	-3.9135	-1.9324
C	9.9776	1.3170	-3.0746	C	-8.4960	-4.2099	-3.1947
N	10.9062	0.6383	-3.7589	N	-8.6238	-4.9459	-4.3062
H	11.0977	-1.4011	-4.4433	H	-7.2940	-6.2014	-5.4568
H	10.0201	2.3627	-2.8083	H	-9.2762	-3.6326	-2.7211
H	11.7730	1.0334	-4.1083	H	-9.4821	-5.0486	-4.8373
N	-1.5352	6.1148	-0.3821	N	6.4981	-1.8805	-1.3084
C	-1.8316	7.3398	-1.1184	C	7.5592	-2.1935	-2.2605
H	-0.8596	7.8140	-1.2715	H	7.5239	-3.2795	-2.3706
C	-2.5294	7.1343	-2.4965	C	7.4080	-1.5286	-3.6616
H	-2.0029	7.7181	-3.2573	H	7.5555	-2.2864	-4.4368
H	-2.4383	6.0841	-2.7995	H	6.3802	-1.1647	-3.7821
C	-3.9692	7.5516	-2.5239	C	8.3773	-0.4161	-3.9296
N	-4.9036	7.0526	-1.6268	N	8.5244	0.6671	-3.0740
C	-4.6478	8.4340	-3.3226	C	9.2624	-0.2086	-4.9547
H	-4.6355	6.3748	-0.8824	H	7.9809	0.7434	-2.1880
C	-6.0974	7.5969	-1.8556	C	9.4506	1.5014	-3.5426
N	-5.9629	8.4386	-2.8884	N	9.9095	0.9871	-4.6906
H	-4.3144	9.0488	-4.1448	H	9.4838	-0.7977	-5.8316
H	-7.0077	7.4030	-1.3076	H	9.7784	2.4216	-3.0817
H	-6.7120	9.0007	-3.2787	H	10.6305	1.4088	-5.2665
H	-4.4210	-6.7447	-2.1233	H	-0.7715	6.7123	-2.6531
H	6.4069	-2.5966	-3.7391	H	-4.1234	-6.9542	-2.1077
H	-2.4230	8.0052	-0.4791	H	8.5260	-1.9400	-1.8114

Conformation 5

C	1.1731	-3.7694	-1.7566
C	1.0015	-2.8611	-2.8470
C	-0.2695	-2.5424	-3.2771
C	-1.3939	-3.1922	-2.6857
C	-1.2217	-4.1138	-1.6828
C	0.0774	-4.3323	-1.1415
C	2.6781	-4.0273	-1.6370
C	2.4112	-2.5515	-3.3674
C	-0.1335	-5.2210	0.0908
C	-2.6377	-2.5976	-3.3429
C	-0.8447	-1.5755	-4.3301
C	-2.6519	-1.1398	-2.8703
C	-1.5715	-0.4955	-3.5272
C	-2.0913	-2.3972	-4.7921
C	3.2066	-1.8184	-2.2808

Conformation 6

C	-1.0356	-1.5901	3.3157
C	-1.5385	-0.2567	3.4051
C	-0.6602	0.8015	3.4340
C	0.7499	0.5727	3.3727
C	1.2330	-0.7135	3.2842
C	0.3196	-1.8118	3.2592
C	-2.2403	-2.5182	3.4920
C	-3.0497	-0.3826	3.6408
C	1.1684	-3.0829	3.3482
C	1.4159	1.9355	3.6141
C	-0.8416	2.2981	3.7061
C	1.0727	2.8438	2.4330
C	-0.3286	3.0547	2.4829
C	0.3915	2.5173	4.6483
C	-3.6773	-1.0001	2.3896

C	3.3748	-2.7385	-1.2157	C	-3.1658	-2.3180	2.2923
C	3.0345	-3.9785	-3.1654	C	-3.0368	-1.6671	4.5405
C	-1.0026	-4.3744	1.0495	C	1.9888	-3.1764	2.0647
C	-2.2872	-4.2975	0.4541	C	2.9107	-2.0997	2.0916
C	4.8432	-1.2285	-0.1438	C	-4.5699	-2.7166	0.4330
C	4.1811	-2.4578	-0.1178	C	-3.5842	-3.1968	1.2978
C	4.6756	-0.3130	-1.1880	C	-5.0955	-1.4251	0.5424
C	3.8385	-0.5771	-2.2780	C	-4.6483	-0.5232	1.5130
C	-3.1917	0.8963	-1.7796	C	1.2188	4.3324	0.5980
C	-3.4534	-0.4679	-1.9483	C	1.8765	3.4800	1.4905
C	-2.2010	1.5529	-2.5229	C	-0.1683	4.5124	0.6288
C	-1.3443	0.8718	-3.3902	C	-0.9813	3.8777	1.5691
C	-1.7636	-2.9234	2.7674	C	2.9631	-3.9547	0.0580
C	-0.7134	-3.6739	2.2204	C	1.9817	-4.1149	1.0365
C	-3.0405	-2.9141	2.1997	C	3.8988	-2.9153	0.0998
C	-3.3403	-3.5990	1.0261	C	3.8884	-1.9488	1.1113
C	-3.8472	1.9004	-0.9043	C	1.7744	5.2383	-0.4361
O	-4.6841	1.7433	-0.0197	O	2.9594	5.4189	-0.7337
C	-2.3044	3.0025	-2.2440	C	-0.5315	5.4965	-0.4218
O	-1.7056	3.9429	-2.7401	O	-1.6143	5.9146	-0.7658
C	5.6221	0.8187	-0.9737	C	-6.2065	-1.2946	-0.4402
O	5.8136	1.8129	-1.6470	O	-6.9558	-0.3491	-0.6471
C	5.9109	-0.7213	0.7583	C	-5.3091	-3.4359	-0.6395
O	6.3970	-1.2226	1.7553	O	-5.1763	-4.5688	-1.0500
C	-1.7767	-1.9796	3.9214	C	3.2688	-4.8080	-1.1179
O	-0.8820	-1.6492	4.6701	O	2.6994	-5.7849	-1.5485
C	-3.9145	-2.0220	2.9951	C	4.8545	-3.1168	-1.0167
O	-5.1016	-1.7733	2.8351	O	5.8593	-2.4520	-1.2898
C	-2.1892	-4.9994	-0.8847	C	2.6375	-1.3283	3.3851
C	-1.2328	-6.1673	-0.4875	C	2.2907	-2.5508	4.3037
H	2.9663	-4.9216	-1.0828	H	-2.0191	-3.5553	3.7486
H	2.4702	-2.1159	-4.3661	H	-3.5535	0.5018	4.0338
H	0.7534	-5.6798	0.5294	H	0.6457	-3.9943	3.6415
H	-0.1581	-1.2186	-5.0989	H	-1.8203	2.6076	4.0756
H	-1.8240	-3.3414	-5.2747	H	0.3337	1.9300	5.5694
H	-2.7672	-1.8254	-5.4365	H	0.5709	3.5712	4.8863
H	4.1121	-4.0091	-3.3561	H	-4.0385	-2.0604	4.7420
H	2.5281	-4.7534	-3.7490	H	-2.4932	-1.5271	5.4799
H	4.3536	-3.1728	0.6819	H	-3.2169	-4.2164	1.2199
H	3.7557	0.1247	-3.1037	H	-5.0790	0.4705	1.6006
H	-4.2550	-0.9628	-1.4072	H	2.9556	3.3571	1.4638
H	-0.5605	1.3917	-3.9339	H	-2.0523	4.0573	1.6004
H	0.2684	-3.6862	2.6857	H	1.2868	-4.9494	1.0063
H	-4.3334	-3.5680	0.5865	H	4.6264	-1.1520	1.1390

H	-3.1320	-5.2548	-1.3707	H	3.4354	-0.6610	3.7147
H	-1.6701	-6.8333	0.2631	H	3.1244	-3.2509	4.4216
H	-0.8821	-6.7490	-1.3450	H	1.9096	-2.2538	5.2852
H	-3.5714	-3.1483	-3.2215	H	2.4676	1.9149	3.9040
N	6.3289	0.5101	0.2129	N	-6.2752	-2.5134	-1.1238
C	7.5643	1.1549	0.6123	C	-7.3580	-2.8946	-2.0135
H	7.8404	1.8345	-0.1998	H	-8.3085	-2.7798	-1.4814
C	7.4371	1.9118	1.9589	C	-7.3911	-2.0912	-3.3528
H	6.7597	2.7673	1.8484	H	-6.5221	-1.4277	-3.3972
H	6.9985	1.2388	2.7008	H	-7.2905	-2.7814	-4.1978
C	8.7674	2.3612	2.4778	C	-8.6347	-1.2721	-3.5401
N	9.4900	3.4274	1.9428	N	-9.5676	-1.5231	-4.5435
C	9.5618	1.8524	3.4710	C	-9.1327	-0.2025	-2.8417
H	9.1790	4.0264	1.1846	H	-9.4959	-2.2579	-5.2401
C	10.6605	3.5690	2.5759	C	-10.5843	-0.6558	-4.4723
N	10.7164	2.6157	3.5078	N	-10.3291	0.1518	-3.4398
H	9.4012	1.0208	4.1405	H	-8.7272	0.3003	-1.9761
H	11.4154	4.3152	2.3738	H	-11.4446	-0.6173	-5.1243
H	11.4948	2.4799	4.1458	H	-10.9339	0.9105	-3.1420
N	-3.1034	-1.4560	3.9804	N	4.4407	-4.2431	-1.7129
C	-3.5604	-0.5399	5.0115	C	5.0005	-4.7621	-2.9567
H	-2.7004	-0.3791	5.6667	H	5.2622	-3.9178	-3.6024
C	-4.0495	0.8390	4.4876	C	6.1946	-5.7378	-2.7775
H	-3.9865	1.5429	5.3260	H	6.0894	-6.2514	-1.8133
H	-3.3570	1.2056	3.7216	H	6.1233	-6.5183	-3.5419
C	-5.4577	0.8634	3.9634	C	7.5671	-5.1356	-2.8855
N	-5.8000	1.0374	2.6283	N	7.8973	-3.8685	-2.4237
C	-6.6442	0.6908	4.6269	C	8.7260	-5.6631	-3.3939
H	-5.1680	1.1627	1.8336	H	7.2055	-3.2108	-1.9990
C	-7.1211	0.9380	2.4722	C	9.1918	-3.6270	-2.6320
N	-7.6513	0.7328	3.6807	N	9.7138	-4.7103	-3.2193
H	-6.8520	0.5246	5.6728	H	8.9278	-6.6196	-3.8519
H	-7.6589	1.0135	1.5395	H	9.7229	-2.7214	-2.3792
H	-8.6418	0.6176	3.8667	H	10.6849	-4.8087	-3.4963
N	-3.2973	3.1499	-1.2499	N	0.7042	5.9056	-1.0149
C	-3.8776	4.4320	-0.8706	C	0.7532	6.8217	-2.1495
H	-4.6322	4.2037	-0.1151	H	-0.2439	6.7837	-2.5934
C	-2.8459	5.4638	-0.3109	C	1.0651	8.2985	-1.7814
H	-3.1473	5.7680	0.6980	H	0.4657	8.9523	-2.4231
H	-1.8697	4.9835	-0.2052	H	0.7217	8.4868	-0.7562
C	-2.6837	6.6992	-1.1523	C	2.4974	8.7296	-1.9244
N	-3.1877	7.9429	-0.7730	N	3.5833	7.9227	-1.6120
C	-2.0854	6.9087	-2.3681	C	3.0252	9.9285	-2.3286
H	-3.6853	8.1388	0.0895	H	3.4902	6.9322	-1.2936

C	-2.9134	8.8678	-1.7005	C	4.7214	8.5882	-1.8087
N	-2.2440	8.2483	-2.6751	N	4.4013	9.8132	-2.2422
H	-1.5830	6.2100	-3.0187	H	2.5469	10.8381	-2.6591
H	-3.1808	9.9141	-1.6653	H	5.7203	8.2086	-1.6531
H	-1.9049	8.7030	-3.5175	H	5.0707	10.5394	-2.4746
H	8.3395	0.3860	0.7061	H	-7.2113	-3.9581	-2.2159
H	-4.3512	-1.0181	5.6003	H	4.1844	-5.3087	-3.4342
H	-4.3962	4.8537	-1.7396	H	1.4634	6.4318	-2.8857

Conformation 7

				Conformation 8			
C	-0.9513	-0.0058	-3.6152	C	-0.3316	-1.2835	3.4603
C	-0.3401	-1.2970	-3.5696	C	-1.0173	-0.0300	3.4813
C	1.0257	-1.4098	-3.4579	C	-0.3009	1.1433	3.4206
C	1.8393	-0.2377	-3.3993	C	1.1246	1.1059	3.3268
C	1.2517	1.0050	-3.4475	C	1.7841	-0.1008	3.3016
C	-0.1681	1.1247	-3.5620	C	1.0399	-1.3177	3.3694
C	-2.4316	-0.2456	-3.9369	C	-1.3903	-2.3594	3.7222
C	-1.4461	-2.3104	-3.8804	C	-2.4930	-0.3547	3.7471
C	-0.4547	2.6117	-3.8166	C	2.0707	-2.4462	3.4820
C	3.2938	-0.7169	-3.5050	C	1.6012	2.5574	3.4422
C	1.9876	-2.5950	-3.5838	C	-0.6809	2.6199	3.6020
C	3.6222	-1.5270	-2.2517	C	1.0979	3.3059	2.2090
C	2.8014	-2.6822	-2.2928	C	-0.3151	3.3571	2.3142
C	3.0726	-1.9167	-4.4908	C	0.5402	3.0716	4.4747
C	-2.4560	-2.2810	-2.7357	C	-3.0274	-1.1321	2.5417
C	-3.0658	-1.0020	-2.7664	C	-2.3418	-2.3724	2.5270
C	-2.2577	-1.4578	-4.9171	C	-2.2922	-1.5623	4.7259
C	-0.0605	3.3978	-2.5673	C	2.8548	-2.4824	2.1707
C	1.3446	3.2618	-2.4337	C	3.6037	-1.2801	2.1126
C	-4.5567	-1.6866	-1.0588	C	-3.6572	-3.0713	0.6908
C	-4.1179	-0.6726	-1.9162	C	-2.6323	-3.3626	1.5938
C	-3.9541	-2.9490	-1.0330	C	-4.3409	-1.8508	0.7077
C	-2.8754	-3.2757	-1.8579	C	-4.0361	-0.8425	1.6269
C	4.7052	-2.3759	-0.3272	C	0.9907	4.6202	0.2466
C	4.5885	-1.3463	-1.2659	C	1.7792	3.9213	1.1622
C	3.8736	-3.5000	-0.3510	C	-0.4010	4.6969	0.3655
C	2.8923	-3.6816	-1.3275	C	-1.0949	4.0544	1.3953
C	-0.0771	4.9081	-0.7457	C	3.8661	-3.1985	0.1575
C	-0.8019	4.2217	-1.7247	C	2.9578	-3.4602	1.1847
C	1.3032	4.7434	-0.5916	C	4.6238	-2.0236	0.1116
C	2.0521	3.9107	-1.4254	C	4.5037	-1.0242	1.0818
C	5.7114	-2.5715	0.7444	C	1.4012	5.4334	-0.9258
O	6.6442	-1.8219	1.0478	O	2.4961	5.6175	-1.4087
C	4.3095	-4.4209	0.7290	C	-0.9018	5.6005	-0.6980

O	3.8731	-5.4992	1.0612	O	-2.0634	5.9668	-0.9006
C	-4.7338	-3.8222	-0.1145	C	-5.4186	-1.9051	-0.3199
O	-4.5743	-4.9923	0.1785	O	-6.2582	-1.0750	-0.6185
C	-5.7374	-1.7128	-0.1504	C	-4.2715	-3.9400	-0.3505
O	-6.5430	-0.8393	0.1098	O	-4.0001	-5.0785	-0.6805
C	-0.5211	5.9614	0.1989	C	4.2640	-4.0511	-0.9918
O	-1.6564	6.4286	0.3274	O	3.8483	-5.1297	-1.3498
C	1.7611	5.6550	0.4865	C	5.5499	-2.1198	-1.0427
O	2.8671	5.8307	0.9453	O	6.4095	-1.3070	-1.3964
C	1.8171	2.4181	-3.6167	C	3.2649	-0.4966	3.3808
C	0.8038	2.9451	-4.6914	C	3.1328	-1.7076	4.3665
H	-2.9937	0.6167	-4.2987	H	-1.0199	-3.3345	4.0419
H	-1.1173	-3.3026	-4.1928	H	-3.1163	0.4728	4.0900
H	-1.4344	2.8496	-4.2336	H	1.6998	-3.4088	3.8369
H	1.5558	-3.5346	-3.9313	H	-1.6804	2.8173	3.9922
H	2.6813	-1.6050	-5.4638	H	0.5939	2.5518	5.4358
H	3.9678	-2.5326	-4.6267	H	0.5806	4.1548	4.6312
H	-3.2080	-1.9201	-5.2035	H	-3.2263	-2.0795	4.9684
H	-1.6790	-1.2060	-5.8112	H	-1.7676	-1.2855	5.6455
H	-4.6192	0.2909	-1.9490	H	-2.1301	-4.3261	1.5828
H	-2.4403	-4.2712	-1.8468	H	-4.5915	0.0913	1.6418
H	5.2526	-0.4867	-1.2484	H	2.8617	3.9013	1.0727
H	2.2827	-4.5805	-1.3522	H	-2.1752	4.1294	1.4826
H	-1.8714	4.3699	-1.8451	H	2.4006	-4.3921	1.2197
H	3.1300	3.8292	-1.3173	H	5.1071	-0.1216	1.0421
H	2.8807	2.4891	-3.8491	H	3.9647	0.2967	3.6478
H	0.9126	4.0146	-4.9001	H	4.0642	-2.2717	4.4821
H	0.8387	2.3758	-5.6251	H	2.7451	-1.4200	5.3483
H	4.0318	0.0357	-3.7865	H	2.6545	2.7044	3.6855
N	-5.7841	-3.0214	0.3807	N	-5.3123	-3.1760	-0.9196
C	-6.9223	-3.5666	1.0901	C	-6.2064	-3.6695	-1.9438
H	-7.1750	-4.5330	0.6412	H	-5.6333	-4.3121	-2.6181
C	-6.6478	-3.7630	2.6028	C	-7.3833	-4.4697	-1.3222
H	-5.7679	-4.4011	2.7250	H	-6.9800	-5.3337	-0.7855
H	-6.4199	-2.7967	3.0690	H	-7.8976	-3.8415	-0.5850
C	-7.7999	-4.4147	3.3010	C	-8.3680	-4.9620	-2.3346
N	-8.9836	-3.7482	3.6165	N	-9.3651	-4.1566	-2.8833
C	-7.9945	-5.7060	3.7146	C	-8.5255	-6.1850	-2.9314
H	-9.1667	-2.7646	3.4437	H	-9.5337	-3.1859	-2.6370
C	-9.8544	-4.5818	4.1972	C	-10.0994	-4.8475	-3.7627
N	-9.2645	-5.7769	4.2619	N	-9.5963	-6.0830	-3.8033
H	-7.3429	-6.5653	3.6633	H	-7.9768	-7.1058	-2.8023
H	-10.8451	-4.3342	4.5502	H	-10.9435	-4.4786	-4.3271
H	-9.6921	-6.6086	4.6579	H	-9.9607	-6.8336	-4.3821

N	0.5937	6.3623	0.9228
C	0.6861	7.5176	1.8102
H	0.3732	8.4138	1.2623
C	-0.0977	7.3894	3.1510
H	-0.3586	6.3377	3.3214
H	0.5565	7.6793	3.9787
C	-1.3300	8.2406	3.2328
N	-2.3374	8.1845	2.2797
C	-1.7270	9.1826	4.1450
H	-2.2669	7.5590	1.4485
C	-3.3068	9.0454	2.5832
N	-2.9551	9.6608	3.7195
H	-1.2503	9.5480	5.0419
H	-4.2095	9.2220	2.0170
H	-3.5043	10.3762	4.1843
N	5.4318	-3.7860	1.3551
C	6.2791	-4.4968	2.3078
H	7.2825	-4.6033	1.8804
C	6.3491	-3.8686	3.7319
H	5.5200	-3.1615	3.8583
H	6.1965	-4.6538	4.4783
C	7.6496	-3.1927	4.0506
N	8.1971	-2.2091	3.2387
C	8.5278	-3.3546	5.0898
H	7.7373	-1.9142	2.3500
C	9.3524	-1.7837	3.7462
N	9.5695	-2.4671	4.8772
H	8.5024	-4.0127	5.9450
H	10.0008	-1.0303	3.3235
H	10.3816	-2.3544	5.4746
H	-7.7551	-2.8746	0.9308
H	1.7524	7.6205	2.0229
H	5.8442	-5.4964	2.3757

Conformation 9

C	0.2321	-1.7242	3.3373
C	-0.8755	-0.8221	3.3827
C	-0.6489	0.5362	3.3731
C	0.6895	1.0352	3.3055
C	1.7529	0.1653	3.2447
C	1.5171	-1.2425	3.2608
C	-0.3383	-3.1237	3.5788
C	-2.1194	-1.6873	3.6370
C	2.8932	-1.9091	3.3568
N	5.3029	-3.3341	-1.6660
C	5.9085	-3.8240	-2.8996
H	5.9489	-3.0031	-3.6228
C	7.3003	-4.4940	-2.7203
H	7.3814	-4.8730	-1.6935
H	7.3531	-5.3736	-3.3696
C	8.4909	-3.6354	-3.0386
N	8.5904	-2.2964	-2.6857
C	9.6702	-3.9470	-3.6643
H	7.8215	-1.7743	-2.2089
C	9.7690	-1.8065	-3.0691
N	10.4422	-2.7985	-3.6644
H	10.0205	-4.8721	-4.0964
H	10.1172	-0.7936	-2.9310
H	11.3737	-2.7126	-4.0571
N	0.1976	6.0113	-1.4386
C	0.1821	6.8295	-2.6466
H	-0.6488	6.5046	-3.2810
C	0.1415	8.3628	-2.3950
H	0.5906	8.5729	-1.4159
H	0.7842	8.8555	-3.1315
C	-1.2104	9.0125	-2.4823
N	-2.3773	8.4361	-1.9988
C	-1.5758	10.2355	-2.9826
H	-2.4118	7.4813	-1.5765
C	-3.4084	9.2594	-2.1867
N	-2.9390	10.3625	-2.7820
H	-0.9915	11.0132	-3.4507
H	-4.4363	9.0708	-1.9144
H	-3.5033	11.1631	-3.0468
H	-6.5735	-2.8038	-2.5029
H	5.2116	-4.5728	-3.2824
H	1.1127	6.5916	-3.1666

C	0.5952	2.5500	3.5089
C	-1.5486	1.7568	3.6217
C	-0.1493	3.1355	2.3115
C	-1.4823	2.6589	2.3888
C	-0.5804	2.5738	4.5457
C	-2.3317	-2.5993	2.4247
C	-1.2204	-3.4785	2.3860
C	-1.4697	-2.7445	4.5962
C	3.6393	-1.6040	2.0583
C	3.8868	-0.2082	2.0509
C	-2.1976	-4.6314	0.5716
C	-1.1168	-4.4967	1.4433
C	-3.3118	-3.7880	0.6247
C	-3.4002	-2.7337	1.5408
C	-0.7378	4.4628	0.4465
C	0.2565	4.0298	1.3249
C	-2.0628	4.0244	0.5435
C	-2.4685	3.0962	1.5078
C	4.8511	-1.8210	0.0406
C	4.1023	-2.4380	1.0441
C	5.1188	-0.4483	0.0452
C	4.6323	0.4000	1.0443
C	-0.6583	5.4608	-0.6501
O	0.2927	6.0616	-1.0972
C	-2.8666	4.7777	-0.4497
O	-4.0862	4.7288	-0.6384
C	-4.3173	-4.3002	-0.3408
O	-5.4502	-3.8594	-0.5569
C	-2.4514	-5.6763	-0.4512
O	-1.7589	-6.5989	-0.8143
C	5.5358	-2.4226	-1.1324
O	5.5468	-3.5642	-1.5332
C	6.0156	-0.1524	-1.0992
O	6.5133	0.9329	-1.4128
C	3.2744	0.3475	3.3372
C	3.5989	-0.8599	4.2824
H	0.3756	-3.8914	3.8808
H	-3.0076	-1.1636	3.9939
H	2.9059	-2.9525	3.6751
H	-2.5500	1.5484	4.0011
H	-0.3381	2.0538	5.4773
H	-0.9429	3.5839	4.7639
H	-2.1363	-3.5809	4.8304
H	-1.0833	-2.3038	5.5200

H	-0.2790	-5.1876	1.4118
H	-4.2790	-2.0964	1.5852
H	1.2715	4.4113	1.2584
H	-3.5030	2.7720	1.5805
H	3.9323	-3.5111	1.0402
H	4.8575	1.4628	1.0431
H	3.6269	1.3343	3.6413
H	4.6729	-1.0399	4.3967
H	3.1274	-0.7727	5.2658
H	1.5202	3.0593	3.7832
N	-3.7602	-5.4065	-0.9668
C	-4.4500	-6.3603	-1.8299
H	-5.3345	-6.7389	-1.3053
C	-4.8323	-5.8215	-3.2408
H	-4.2741	-4.8990	-3.4425
H	-4.5149	-6.5421	-4.0003
C	-6.3003	-5.5825	-3.4301
N	-7.0405	-4.7863	-2.5667
C	-7.1843	-6.0403	-4.3713
H	-6.6075	-4.3334	-1.7339
C	-8.3153	-4.7526	-2.9512
N	-8.4221	-5.5075	-4.0521
H	-7.0425	-6.6881	-5.2231
H	-9.1194	-4.2214	-2.4639
H	-9.2845	-5.6707	-4.5610
N	6.2351	-1.3479	-1.7672
C	6.9719	-1.5315	-3.0135
H	6.7053	-0.7233	-3.7021
C	8.5130	-1.6535	-2.8482
H	8.7335	-2.0237	-1.8388
H	8.8796	-2.4221	-3.5359
C	9.3059	-0.4058	-3.1152
N	8.9094	0.8617	-2.7101
C	10.5169	-0.2393	-3.7357
H	8.0041	1.0488	-2.2252
C	9.8272	1.7634	-3.0582
N	10.8157	1.1108	-3.6813
H	11.1808	-0.9541	-4.1978
H	9.7812	2.8270	-2.8770
H	11.6509	1.5468	-4.0578
N	-1.9949	5.6119	-1.1352
C	-2.3136	6.4665	-2.2748
H	-3.0163	5.9358	-2.9249
C	-2.8346	7.8811	-1.9027

H	-2.4087	8.1704	-0.9335
H	-2.4400	8.5988	-2.6292
C	-4.3271	8.0557	-1.8736
N	-5.2148	7.0807	-1.4387
C	-5.0963	9.1399	-2.2090
H	-4.9196	6.1255	-1.1366
C	-6.4654	7.5389	-1.4980
N	-6.4126	8.7929	-1.9620
H	-4.8228	10.1121	-2.5903
H	-7.3594	6.9971	-1.2272
H	-7.2190	9.3902	-2.1120
H	-3.7522	-7.1935	-1.9378
H	6.5951	-2.4666	-3.4332
H	-1.3747	6.5826	-2.8204

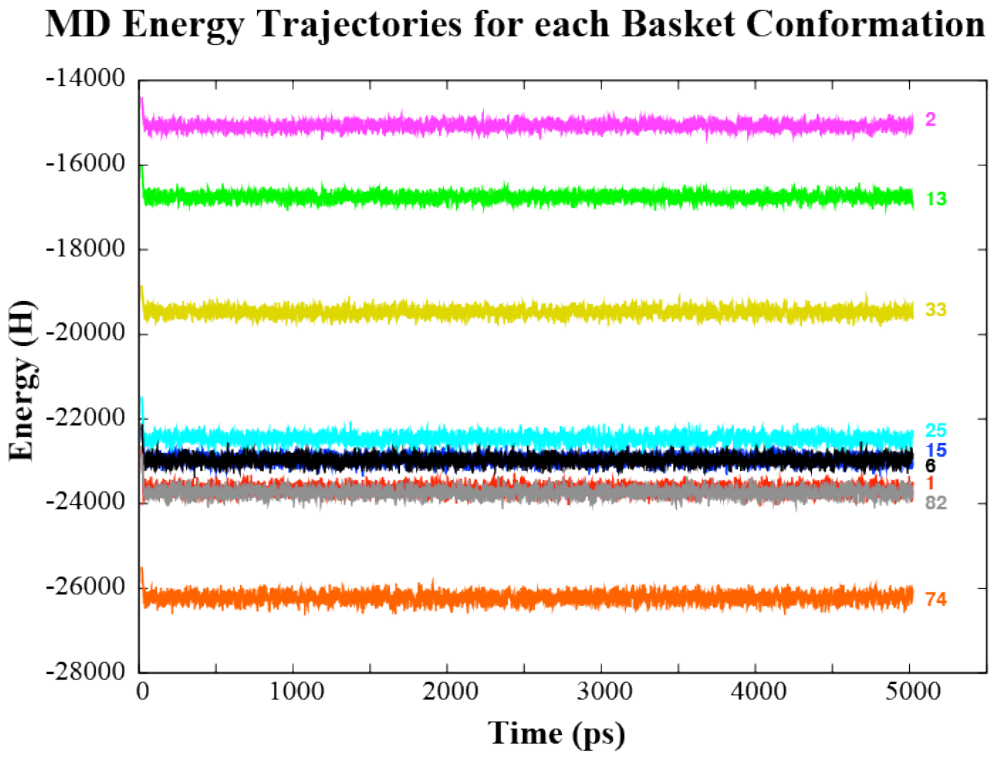


Figure S17. Total energies for each of the MD runs for different basket conformations.

Coordinates of MD Snapshots of Basket used for Docking Simulations							
Snapshot 1021				Snapshot 1099			
C	25.217	22.355	24.707	C	25.160	22.387	24.705
C	24.023	23.088	24.710	C	24.004	23.081	24.669
C	23.443	23.484	25.943	C	23.474	23.490	25.917
C	24.074	23.115	27.147	C	24.064	23.113	27.117
C	25.220	22.377	27.063	C	25.268	22.331	27.149

C	25.790	22.012	25.902	C	25.798	22.029	25.914
C	25.661	22.131	23.291	C	25.586	22.252	23.237
C	23.666	23.308	23.239	C	23.629	23.347	23.218
C	27.105	21.295	26.210	C	27.129	21.290	26.150
C	23.239	23.618	28.307	C	23.279	23.862	28.211
C	22.219	24.237	26.298	C	22.178	24.296	26.202
C	23.312	25.174	28.199	C	23.397	25.350	27.950
C	22.785	25.525	26.920	C	22.728	25.637	26.743
C	21.879	23.553	27.637	C	21.850	23.644	27.547
C	24.755	24.240	22.709	C	24.641	24.326	22.744
C	25.960	23.528	22.739	C	25.871	23.619	22.693
C	24.200	22.012	22.643	C	24.230	22.003	22.569
C	27.898	22.296	26.987	C	28.053	22.329	26.838
C	27.276	22.569	28.183	C	27.494	22.528	28.108
C	27.117	25.434	21.809	C	27.067	25.441	21.911
C	27.201	24.138	22.351	C	27.117	24.089	22.318
C	25.910	26.134	21.833	C	25.867	26.149	21.974
C	24.779	25.578	22.421	C	24.630	25.670	22.390
C	24.043	27.453	28.458	C	24.074	27.608	28.160
C	23.947	26.075	28.974	C	24.041	26.314	28.675
C	23.422	27.783	27.252	C	23.354	27.914	27.077
C	22.793	26.837	26.451	C	22.643	26.946	26.322
C	29.572	23.910	27.492	C	29.813	23.741	27.283
C	29.120	22.920	26.565	C	29.235	22.906	26.422
C	28.878	24.131	28.713	C	29.250	23.977	28.574
C	27.681	23.535	29.072	C	28.075	23.416	29.048
C	24.639	28.729	29.036	C	24.652	28.904	28.627
O	25.261	28.855	30.040	O	25.310	28.988	29.600
C	23.574	29.284	27.131	C	23.352	29.371	26.899
O	23.219	30.042	26.295	O	22.881	29.966	25.997
C	26.212	27.431	21.193	C	26.247	27.492	21.444
O	25.413	28.351	20.992	O	25.467	28.424	21.366
C	28.208	26.225	21.196	C	28.107	26.306	21.267
O	29.350	25.903	20.897	O	29.253	26.002	20.991
C	30.860	24.628	27.575	C	31.133	24.566	27.235
O	31.681	24.687	26.678	O	31.944	24.602	26.343
C	29.716	25.080	29.480	C	30.179	24.902	29.229
O	29.429	25.581	30.552	O	30.003	25.458	30.317
C	26.032	21.770	28.215	C	26.160	21.793	28.219
C	26.537	20.549	27.465	C	26.636	20.561	27.364
H	26.354	21.312	23.092	H	26.313	21.508	22.902
H	22.671	23.621	22.912	H	22.560	23.484	23.046
H	27.616	20.773	25.399	H	27.628	20.710	25.371
H	21.441	24.327	25.538	H	21.361	24.342	25.479

H	21.560	22.512	27.558	H	21.491	22.613	27.526
H	21.010	24.063	28.057	H	21.153	24.235	28.144
H	24.137	21.939	21.555	H	24.273	22.008	21.479
H	23.695	21.110	22.996	H	23.582	21.164	22.830
H	28.078	23.511	22.497	H	27.988	23.465	22.136
H	23.904	26.217	22.496	H	23.760	26.320	22.428
H	24.097	25.967	30.045	H	24.610	25.948	29.527
H	22.433	27.069	25.452	H	21.900	27.262	25.594
H	29.610	22.654	25.633	H	29.681	22.690	25.455
H	27.241	23.666	30.057	H	27.714	23.601	30.056
H	25.623	21.714	29.227	H	25.721	21.473	29.166
H	27.314	20.016	28.017	H	27.472	19.985	27.767
H	25.808	19.777	27.212	H	25.859	19.799	27.274
H	23.337	23.067	29.245	H	23.370	23.577	29.262
N	27.575	27.402	20.841	N	27.503	27.484	20.957
C	28.138	28.544	20.140	C	28.150	28.603	20.268
H	27.374	29.146	19.639	H	27.443	28.985	19.526
C	28.920	29.421	21.187	C	28.764	29.678	21.244
H	28.207	30.084	21.680	H	28.059	29.959	22.029
H	29.387	28.834	21.981	H	29.665	29.239	21.677
C	30.000	30.289	20.612	C	29.282	30.932	20.609
N	30.011	31.332	19.632	N	29.255	32.276	20.909
C	31.270	30.050	20.814	C	29.905	30.899	19.401
H	29.161	31.560	19.133	H	28.813	32.651	21.737
C	31.280	31.836	19.284	C	29.842	33.086	20.002
N	32.036	30.945	20.054	N	30.220	32.166	19.089
H	31.775	29.381	21.501	H	30.057	30.025	18.780
H	31.656	32.552	18.550	H	29.780	34.170	19.888
H	33.043	30.885	19.986	H	30.656	32.449	18.223
N	30.744	25.418	28.722	N	31.218	25.220	28.432
C	31.626	26.576	29.074	C	32.233	26.192	28.766
H	31.008	27.358	29.525	H	31.779	26.746	29.592
C	32.798	26.074	30.022	C	33.530	25.529	29.153
H	32.349	25.427	30.780	H	33.938	25.123	28.226
H	33.498	25.440	29.476	H	34.363	26.175	29.437
C	33.525	27.253	30.545	C	33.396	24.438	30.180
N	34.342	27.345	31.662	N	32.818	24.600	31.452
C	33.442	28.545	30.092	C	33.669	23.101	30.019
H	34.357	26.685	32.428	H	32.389	25.466	31.750
C	34.928	28.575	31.881	C	32.579	23.423	32.096
N	34.330	29.276	30.842	N	33.257	22.565	31.177
H	32.922	29.051	29.288	H	34.085	22.538	29.193
H	35.795	28.896	32.462	H	32.335	23.193	33.135
H	34.702	30.199	30.663	H	33.334	21.586	31.415

N	24.245	29.723	28.185	N	24.325	29.843	27.733
C	24.830	31.032	28.237	C	25.001	31.087	27.589
H	25.213	31.313	27.253	H	25.047	31.344	26.527
C	23.995	32.198	28.909	C	24.310	32.281	28.259
H	24.501	33.144	28.704	H	24.945	33.161	28.147
H	23.094	32.403	28.325	H	23.365	32.514	27.763
C	23.834	31.882	30.347	C	24.136	32.094	29.731
N	22.643	31.823	31.003	N	23.003	31.778	30.447
C	24.760	31.780	31.334	C	25.140	32.403	30.696
H	21.799	32.120	30.531	H	22.127	31.439	30.074
C	22.676	31.817	32.388	C	23.153	31.705	31.798
N	24.059	31.698	32.532	N	24.445	32.255	31.916
H	25.841	31.729	31.396	H	26.165	32.756	30.660
H	21.875	31.959	33.116	H	22.434	31.433	32.573
H	24.472	31.522	33.438	H	24.843	32.310	32.845
H	28.750	28.225	19.292	H	29.007	28.303	19.659
H	32.104	26.956	28.167	H	32.482	26.883	27.956
H	25.805	30.951	28.726	H	26.013	31.103	28.002

Snapshot 1233				**Snapshot 1356**			
C	25.179	22.326	24.645	C	25.211	22.378	24.683
C	24.030	23.102	24.700	C	24.040	23.100	24.727
C	23.476	23.489	25.943	C	23.447	23.437	25.963
C	24.030	23.107	27.142	C	24.072	23.144	27.101
C	25.249	22.359	27.144	C	25.223	22.384	27.108
C	25.804	22.046	25.899	C	25.774	21.988	25.889
C	25.496	22.009	23.184	C	25.623	22.230	23.212
C	23.673	23.337	23.139	C	23.619	23.384	23.331
C	27.079	21.168	26.193	C	27.084	21.273	26.237
C	23.135	23.554	28.303	C	23.270	23.804	28.220
C	22.208	24.170	26.319	C	22.145	24.201	26.315
C	23.096	25.046	28.232	C	23.330	25.290	27.956
C	22.486	25.447	27.053	C	22.637	25.569	26.795
C	21.832	23.266	27.507	C	21.833	23.587	27.675
C	24.823	24.095	22.531	C	24.658	24.381	22.793
C	25.936	23.285	22.597	C	25.938	23.672	22.769
C	24.063	21.904	22.641	C	24.175	22.095	22.635
C	28.116	21.949	26.968	C	27.942	22.269	26.882
C	27.516	22.285	28.175	C	27.403	22.618	28.112
C	27.310	25.060	21.818	C	27.011	25.527	21.766
C	27.211	23.761	22.295	C	27.119	24.238	22.280
C	26.170	25.841	21.693	C	25.790	26.242	21.799
C	24.906	25.385	22.077	C	24.621	25.651	22.235
C	23.352	27.283	28.910	C	23.824	27.568	28.279

C	23.498	25.935	29.242	C	24.033	26.280	28.720
C	22.847	27.716	27.652	C	23.024	27.890	27.191
C	22.408	26.805	26.686	C	22.514	26.897	26.298
C	30.104	23.079	27.648	C	29.604	23.955	27.180
C	29.444	22.290	26.735	C	29.043	22.909	26.338
C	29.508	23.485	28.810	C	29.173	24.157	28.483
C	28.205	23.034	29.100	C	28.019	23.522	28.972
C	23.776	28.559	29.626	C	24.244	28.797	28.959
O	24.238	28.625	30.771	O	24.813	28.902	30.034
C	22.954	29.237	27.642	C	23.097	29.357	27.136
O	22.554	30.024	26.782	O	22.494	30.093	26.328
C	26.576	27.122	21.110	C	26.123	27.598	21.299
O	25.952	28.124	20.867	O	25.325	28.535	21.128
C	28.437	25.898	21.278	C	28.090	26.410	21.316
O	29.571	25.587	21.208	O	29.242	26.214	21.338
C	31.493	23.574	27.726	C	30.736	24.888	26.893
O	32.368	23.458	26.946	O	31.451	24.868	25.908
C	30.444	24.193	29.620	C	29.911	25.353	28.956
O	30.229	24.555	30.766	O	29.672	26.024	29.914
C	26.108	21.661	28.230	C	26.118	21.837	28.217
C	26.475	20.373	27.418	C	26.547	20.530	27.450
H	26.162	21.182	22.929	H	26.310	21.419	22.964
H	22.657	23.523	22.787	H	22.570	23.629	23.155
H	27.333	20.452	25.408	H	27.514	20.689	25.422
H	21.472	24.223	25.514	H	21.390	24.256	25.529
H	21.756	22.186	27.375	H	21.521	22.544	27.601
H	20.988	23.611	28.108	H	20.997	24.042	28.211
H	23.983	21.679	21.574	H	24.219	22.147	21.545
H	23.595	21.065	23.158	H	23.607	21.235	22.999
H	28.083	23.136	22.471	H	27.926	23.513	22.198
H	24.025	26.018	22.007	H	23.624	26.030	22.032
H	23.729	25.581	30.244	H	24.781	26.023	29.466
H	21.998	27.083	25.718	H	21.962	27.111	25.385
H	30.038	22.166	25.833	H	29.524	22.788	25.371
H	27.727	23.360	30.020	H	27.701	23.799	29.974
H	25.562	21.557	29.169	H	25.651	21.664	29.189
H	27.233	19.834	27.988	H	27.298	19.996	28.035
H	25.554	19.840	27.171	H	25.663	19.927	27.234
H	23.242	23.180	29.323	H	23.542	23.430	29.210
N	27.872	27.030	20.851	N	27.429	27.549	21.003
C	28.684	28.062	20.192	C	28.142	28.741	20.592
H	28.036	28.780	19.682	H	27.527	29.314	19.893
C	29.567	28.916	21.058	C	28.678	29.673	21.765
H	30.165	28.337	21.764	H	29.486	29.188	22.319

H	30.260	29.444	20.399	H	29.149	30.527	21.274
C	28.762	29.906	21.908	C	27.675	30.159	22.739
N	28.156	31.043	21.471	N	26.517	30.901	22.515
C	28.355	29.697	23.248	C	27.992	30.352	24.031
H	28.236	31.396	20.527	H	25.999	30.869	21.647
C	27.362	31.620	22.391	C	26.000	31.561	23.636
N	27.527	30.744	23.470	N	27.008	31.179	24.541
H	28.568	28.898	23.949	H	28.811	29.969	24.628
H	26.682	32.465	22.271	H	25.261	32.361	23.701
H	27.003	30.942	24.312	H	26.952	31.432	25.518
N	31.586	24.241	28.873	N	30.813	25.706	27.982
C	32.821	24.920	29.270	C	31.765	26.851	27.962
H	32.444	25.717	29.916	H	31.246	27.704	28.404
C	33.810	24.044	29.970	C	33.030	26.639	28.800
H	34.195	23.258	29.315	H	32.607	26.481	29.794
H	34.697	24.635	30.206	H	33.490	25.673	28.581
C	33.255	23.531	31.302	C	33.871	27.799	28.573
N	32.979	24.187	32.472	N	34.671	28.027	27.512
C	32.943	22.189	31.497	C	34.220	28.695	29.550
H	33.053	25.192	32.557	H	34.784	27.532	26.638
C	32.371	23.366	33.412	C	35.516	29.115	27.717
N	32.400	22.122	32.763	N	35.222	29.455	29.045
H	33.019	21.337	30.833	H	33.928	28.855	30.582
H	31.914	23.526	34.390	H	36.231	29.571	27.032
H	31.921	21.329	33.168	H	35.704	30.216	29.502
N	23.406	29.582	28.858	N	23.836	29.769	28.132
C	23.770	30.995	29.200	C	24.014	31.246	28.359
H	24.107	31.423	28.253	H	24.206	31.821	27.450
C	22.683	31.859	29.762	C	22.923	31.886	29.178
H	23.080	32.877	29.770	H	23.090	32.965	29.170
H	21.811	31.942	29.110	H	21.935	31.685	28.760
C	22.397	31.290	31.113	C	23.116	31.402	30.612
N	21.493	30.348	31.505	N	22.244	30.573	31.316
C	23.084	31.670	32.187	C	24.098	31.636	31.487
H	20.859	29.937	30.834	H	21.290	30.409	31.025
C	21.381	30.102	32.835	C	22.674	30.177	32.584
N	22.500	30.892	33.194	N	23.804	30.878	32.575
H	23.865	32.398	32.368	H	24.940	32.315	31.425
H	20.814	29.305	33.319	H	22.236	29.617	33.412
H	22.799	30.855	34.158	H	24.381	30.634	33.368
H	29.371	27.625	19.464	H	29.043	28.388	20.084
H	33.201	25.357	28.343	H	32.057	27.104	26.940
H	24.602	30.973	29.909	H	24.896	31.262	29.004

Snapshot 1556				Snapshot 1807			
C	25.174	22.371	24.719	C	25.210	22.347	24.718
C	24.046	23.124	24.730	C	24.003	23.075	24.729
C	23.401	23.480	25.916	C	23.490	23.510	25.955
C	24.064	23.096	27.078	C	24.025	23.100	27.119
C	25.292	22.392	27.140	C	25.220	22.383	27.072
C	25.791	21.968	25.889	C	25.820	22.017	25.879
C	25.572	22.173	23.265	C	25.622	22.217	23.252
C	23.620	23.419	23.306	C	23.531	23.355	23.368
C	27.015	21.086	26.228	C	27.079	21.169	26.166
C	23.118	23.599	28.240	C	23.254	23.743	28.227
C	22.123	24.230	26.305	C	22.380	24.516	26.225
C	23.202	25.137	28.253	C	23.510	25.249	28.056
C	22.563	25.545	27.034	C	23.001	25.683	26.849
C	21.777	23.431	27.574	C	21.808	23.750	27.471
C	24.773	24.295	22.774	C	24.571	24.361	22.843
C	25.933	23.543	22.755	C	25.800	23.669	22.754
C	24.096	22.087	22.773	C	24.130	22.034	22.743
C	28.049	22.062	26.804	C	28.067	22.159	26.757
C	27.515	22.547	27.959	C	27.529	22.599	27.930
C	27.119	25.374	21.876	C	26.851	25.705	21.956
C	27.149	24.082	22.369	C	26.927	24.395	22.319
C	26.036	26.195	21.993	C	25.582	26.312	21.936
C	24.782	25.653	22.392	C	24.443	25.686	22.448
C	23.517	27.427	28.731	C	24.211	27.440	28.492
C	23.706	26.097	29.122	C	24.051	26.156	28.958
C	22.795	27.763	27.565	C	23.837	27.841	27.289
C	22.327	26.906	26.670	C	23.144	27.022	26.418
C	30.072	23.278	27.181	C	29.798	23.639	26.867
C	29.321	22.409	26.369	C	29.229	22.549	26.199
C	29.574	23.769	28.346	C	29.287	24.148	28.098
C	28.300	23.440	28.791	C	28.095	23.610	28.665
C	24.030	28.698	29.333	C	24.660	28.644	29.218
O	24.790	28.658	30.289	O	25.213	28.771	30.290
C	22.791	29.231	27.565	C	23.977	29.337	27.160
O	22.272	29.906	26.702	O	23.791	30.084	26.232
C	26.451	27.520	21.428	C	25.846	27.779	21.655
O	25.670	28.458	21.217	O	25.015	28.680	21.748
C	28.266	26.171	21.455	C	27.876	26.733	21.645
O	29.423	25.853	21.472	O	29.102	26.586	21.671
C	31.362	23.995	26.888	C	31.018	24.446	26.507
O	32.115	23.839	25.974	O	31.746	24.312	25.551
C	30.532	24.789	28.802	C	30.260	25.209	28.496
O	30.434	25.498	29.828	O	30.301	25.910	29.526

C	26.175	21.922	28.258	C	26.154	21.914	28.153
C	26.487	20.508	27.617	C	26.519	20.632	27.508
H	26.276	21.348	23.137	H	26.272	21.410	22.908
H	22.563	23.677	23.209	H	22.493	23.577	23.111
H	27.357	20.452	25.406	H	27.370	20.443	25.404
H	21.331	24.328	25.559	H	21.782	24.633	25.318
H	21.526	22.400	27.313	H	21.390	22.751	27.326
H	20.895	23.889	28.026	H	21.068	24.379	27.971
H	24.044	22.050	21.683	H	24.076	22.127	21.657
H	23.588	21.267	23.284	H	23.636	21.116	23.070
H	28.021	23.436	22.448	H	27.896	23.950	22.107
H	23.858	26.225	22.410	H	23.554	26.312	22.477
H	24.167	25.812	30.064	H	24.297	25.855	29.974
H	21.724	27.273	25.843	H	22.855	27.366	25.428
H	29.772	22.011	25.462	H	29.511	22.162	25.223
H	27.957	23.780	29.764	H	27.665	24.094	29.540
H	25.781	21.905	29.277	H	25.877	21.743	29.196
H	27.355	20.058	28.104	H	27.312	20.149	28.084
H	25.638	19.844	27.436	H	25.665	19.962	27.396
H	23.290	23.226	29.252	H	23.358	23.236	29.188
N	27.762	27.391	21.094	N	27.218	27.865	21.445
C	28.546	28.329	20.452	C	27.902	29.125	21.054
H	27.959	29.064	19.897	H	27.203	29.734	20.474
C	29.485	29.106	21.403	C	28.250	29.893	22.396
H	29.921	28.374	22.086	H	27.366	29.886	23.037
H	30.311	29.606	20.894	H	28.985	29.256	22.895
C	28.771	30.165	22.112	C	28.823	31.285	22.301
N	28.199	29.947	23.293	N	30.099	31.652	22.205
C	28.520	31.446	21.784	C	28.050	32.403	22.153
H	28.135	29.086	23.821	H	30.902	31.063	22.031
C	27.604	31.041	23.908	C	30.261	33.030	22.291
N	27.800	31.967	22.872	N	28.940	33.406	22.205
H	28.703	32.065	20.914	H	26.981	32.484	22.011
H	27.192	31.135	24.915	H	31.162	33.603	22.061
H	27.246	32.813	22.853	H	28.693	34.374	22.052
N	31.543	24.863	27.911	N	31.175	25.299	27.489
C	32.575	25.922	27.973	C	32.290	26.353	27.516
H	32.146	26.918	28.111	H	32.096	27.173	28.210
C	33.509	25.538	29.064	C	33.551	25.653	28.092
H	33.014	25.657	30.031	H	33.905	24.837	27.459
H	33.785	24.482	29.093	H	34.327	26.421	28.126
C	34.724	26.355	28.844	C	33.390	25.207	29.500
N	34.984	27.641	29.172	N	33.230	25.983	30.592
C	35.875	25.756	28.454	C	33.380	23.895	30.005

H	34.397	28.410	29.464	H	33.384	26.982	30.632
C	36.380	27.911	29.157	C	33.264	25.331	31.794
N	36.885	26.692	28.674	N	33.354	24.012	31.352
H	36.036	24.717	28.196	H	33.433	22.947	29.486
H	36.780	28.926	29.195	H	33.407	25.738	32.796
H	37.818	26.566	28.305	H	33.476	23.299	32.058
N	23.421	29.681	28.630	N	24.459	29.645	28.352
C	23.534	31.114	29.003	C	24.952	31.031	28.704
H	23.482	31.789	28.145	H	25.307	31.536	27.802
C	22.396	31.445	30.049	C	23.860	31.835	29.490
H	22.358	32.518	30.246	H	22.942	31.965	28.913
H	21.505	30.905	29.723	H	23.521	31.403	30.434
C	22.856	30.869	31.391	C	24.427	33.161	29.854
N	22.265	29.840	32.055	N	25.353	33.490	30.811
C	23.760	31.527	32.236	C	23.912	34.307	29.320
H	21.388	29.411	31.790	H	25.758	32.860	31.490
C	22.883	29.614	33.305	C	25.543	34.861	30.818
N	23.737	30.733	33.375	N	24.501	35.275	30.035
H	24.473	32.321	32.053	H	23.315	34.511	28.439
H	22.496	28.984	34.108	H	26.218	35.590	31.269
H	24.368	30.822	34.159	H	24.308	36.256	29.879
H	29.193	27.815	19.737	H	28.805	28.957	20.461
H	33.157	26.024	27.054	H	32.633	26.663	26.525
H	24.469	31.341	29.522	H	25.871	30.929	29.288

Snapshot 1867				**Snapshot 355**			
C	25.214	22.375	24.678	C	25.180	22.384	24.704
C	24.013	23.088	24.746	C	23.996	23.096	24.696
C	23.417	23.502	25.929	C	23.476	23.480	25.912
C	24.065	23.114	27.102	C	24.096	23.077	27.122
C	25.239	22.377	27.126	C	25.227	22.391	27.113
C	25.819	21.975	25.891	C	25.792	22.002	25.925
C	25.558	22.221	23.221	C	25.606	22.147	23.220
C	23.505	23.263	23.351	C	23.565	23.251	23.219
C	26.998	21.142	26.175	C	26.983	21.160	26.249
C	23.222	23.709	28.189	C	23.231	23.623	28.256
C	22.171	24.240	26.301	C	22.225	24.265	26.292
C	23.263	25.244	28.067	C	23.310	25.133	28.138
C	22.675	25.533	26.924	C	22.796	25.554	26.936
C	21.844	23.513	27.548	C	21.766	23.484	27.621
C	24.556	24.289	22.805	C	24.631	24.164	22.645
C	25.774	23.656	22.708	C	25.847	23.498	22.647
C	24.112	21.998	22.614	C	24.194	21.939	22.666
C	28.133	21.924	26.860	C	27.998	22.107	26.839

C	27.590	22.332	28.070	C	27.517	22.483	28.065
C	26.647	25.561	21.590	C	26.946	25.293	21.683
C	26.888	24.269	22.056	C	27.024	24.054	22.292
C	25.475	26.228	21.777	C	25.768	25.969	21.643
C	24.361	25.631	22.476	C	24.572	25.416	22.054
C	23.564	27.614	28.447	C	23.917	27.352	28.553
C	23.750	26.303	28.925	C	23.938	26.037	28.993
C	22.980	27.890	27.249	C	23.384	27.781	27.372
C	22.515	26.845	26.445	C	22.753	26.865	26.452
C	30.094	23.131	27.287	C	30.059	23.231	27.254
C	29.434	22.187	26.487	C	29.246	22.508	26.326
C	29.572	23.556	28.511	C	29.564	23.708	28.466
C	28.301	23.195	28.919	C	28.284	23.364	28.891
C	23.991	28.875	29.101	C	24.427	28.542	29.191
O	24.587	28.999	30.165	O	24.896	28.634	30.302
C	22.992	29.374	27.117	C	23.667	29.210	27.224
O	22.483	30.057	26.280	O	23.317	30.028	26.386
C	25.578	27.537	21.059	C	26.053	27.287	21.014
O	24.731	28.412	20.989	O	25.266	28.200	20.804
C	27.544	26.358	20.793	C	28.037	26.236	21.212
O	28.596	25.981	20.282	O	29.210	25.973	21.271
C	31.487	23.623	27.195	C	31.344	23.870	27.051
O	32.307	23.327	26.336	O	32.099	23.765	26.103
C	30.618	24.306	29.171	C	30.569	24.619	29.034
O	30.524	24.819	30.264	O	30.468	25.289	30.043
C	26.161	21.827	28.211	C	26.175	21.845	28.181
C	26.352	20.438	27.423	C	26.526	20.476	27.566
H	26.391	21.573	22.943	H	26.365	21.404	22.968
H	22.453	23.507	23.196	H	22.515	23.384	22.949
H	27.245	20.465	25.356	H	27.323	20.466	25.477
H	21.381	24.319	25.551	H	21.460	24.429	25.530
H	21.635	22.477	27.275	H	21.461	22.460	27.395
H	21.035	24.038	28.059	H	20.972	23.945	28.211
H	24.026	22.098	21.530	H	24.152	21.930	21.575
H	23.587	21.111	22.972	H	23.769	21.002	23.029
H	27.854	23.792	21.912	H	27.911	23.436	22.403
H	23.376	26.070	22.343	H	23.631	25.958	22.020
H	24.101	26.059	29.924	H	24.438	25.794	29.927
H	22.029	27.120	25.512	H	22.432	27.218	25.477
H	29.895	21.788	25.586	H	29.529	22.315	25.294
H	27.905	23.702	29.795	H	27.890	23.670	29.857
H	25.806	21.945	29.238	H	25.625	21.823	29.123
H	26.981	19.655	27.852	H	27.282	20.048	28.227
H	25.405	19.939	27.211	H	25.689	19.779	27.491

H	23.280	23.239	29.173	H	23.346	23.157	29.237
N	26.883	27.555	20.593	N	27.316	27.306	20.756
C	27.359	28.650	19.738	C	28.000	28.330	20.031
H	26.508	29.147	19.265	H	27.276	28.768	19.339
C	28.029	29.786	20.537	C	28.705	29.276	20.968
H	27.403	30.172	21.344	H	28.107	29.771	21.737
H	28.920	29.316	20.960	H	29.337	28.615	21.564
C	28.252	30.968	19.623	C	29.496	30.248	20.211
N	29.349	31.497	19.074	N	29.065	31.377	19.530
C	27.138	31.720	19.175	C	30.706	29.954	19.667
H	30.302	31.388	19.393	H	28.141	31.780	19.601
C	29.093	32.524	18.130	C	29.932	31.848	18.557
N	27.691	32.668	18.286	N	30.957	30.955	18.756
H	26.104	31.637	19.487	H	31.363	29.097	19.739
H	29.772	32.945	17.386	H	30.019	32.859	18.155
H	27.161	33.389	17.816	H	31.699	31.002	18.073
N	31.692	24.327	28.355	N	31.577	24.630	28.109
C	33.014	24.962	28.600	C	32.866	25.322	28.353
H	32.889	25.819	29.265	H	32.515	26.272	28.763
C	34.118	23.983	28.994	C	33.740	24.589	29.364
H	33.873	23.493	29.939	H	33.133	24.290	30.221
H	34.277	23.283	28.170	H	34.027	23.670	28.850
C	35.267	24.951	29.262	C	34.933	25.309	29.760
N	36.307	25.305	28.503	N	36.120	25.425	29.060
C	35.475	25.550	30.455	C	35.012	26.082	30.891
H	36.601	24.726	27.729	H	36.493	24.772	28.386
C	37.093	26.259	29.024	C	37.066	26.236	29.772
N	36.549	26.384	30.262	N	36.281	26.597	30.892
H	34.943	25.519	31.398	H	34.324	26.205	31.719
H	38.066	26.547	28.620	H	38.152	26.321	29.707
H	36.995	26.940	30.979	H	36.639	27.217	31.606
N	23.568	29.875	28.258	N	24.243	29.577	28.350
C	23.861	31.241	28.469	C	24.916	30.838	28.545
H	24.294	31.663	27.558	H	25.371	31.152	27.603
C	22.628	32.074	28.953	C	23.860	31.958	28.830
H	21.661	31.707	28.604	H	23.336	32.040	27.875
H	22.626	31.922	30.034	H	23.073	31.591	29.490
C	22.738	33.557	28.609	C	24.567	33.168	29.447
N	22.343	34.547	29.392	N	24.139	34.071	30.368
C	22.815	34.120	27.346	C	25.758	33.679	28.911
H	22.140	34.467	30.380	H	23.354	33.889	30.980
C	22.180	35.808	28.779	C	25.013	35.120	30.584
N	22.420	35.435	27.446	N	25.928	34.855	29.603
H	22.973	33.626	26.397	H	26.404	33.300	28.130

H	21.475	36.548	29.165	H	24.826	36.135	30.941
H	22.354	36.156	26.740	H	26.611	35.580	29.432
H	28.143	28.373	19.029	H	28.709	27.829	19.367
H	33.400	25.368	27.661	H	33.426	25.522	27.436
H	24.662	31.351	29.205	H	25.633	30.758	29.366
		Snapshot 486				**Snapshot 855**	
C	25.159	22.341	24.728	C	25.157	22.332	24.696
C	24.008	23.112	24.699	C	24.012	23.123	24.694
C	23.443	23.509	25.913	C	23.468	23.494	25.917
C	24.064	23.094	27.105	C	24.048	23.084	27.122
C	25.256	22.344	27.122	C	25.255	22.369	27.145
C	25.838	22.031	25.905	C	25.828	22.028	25.899
C	25.432	21.875	23.304	C	25.426	21.974	23.253
C	23.608	23.258	23.272	C	23.500	23.239	23.271
C	27.102	21.272	26.212	C	27.151	21.317	26.257
C	23.145	23.665	28.179	C	23.187	23.646	28.245
C	22.226	24.335	26.194	C	22.309	24.408	26.297
C	23.338	25.189	28.087	C	23.466	25.129	28.185
C	22.709	25.600	26.924	C	22.834	25.614	27.036
C	21.797	23.438	27.443	C	21.785	23.711	27.529
C	24.748	23.991	22.570	C	24.531	23.972	22.468
C	25.853	23.135	22.622	C	25.718	23.262	22.486
C	23.979	21.821	22.788	C	23.898	21.759	22.879
C	28.094	22.134	26.932	C	28.052	22.298	26.875
C	27.436	22.466	28.162	C	27.463	22.691	28.062
C	27.115	24.805	21.570	C	26.701	25.070	21.404
C	27.037	23.525	22.211	C	26.858	23.746	21.866
C	25.996	25.627	21.480	C	25.595	25.840	21.513
C	24.748	25.301	22.007	C	24.424	25.296	22.033
C	23.970	27.386	28.586	C	24.138	27.335	28.807
C	24.029	26.048	28.952	C	24.153	25.930	29.049
C	23.368	27.853	27.438	C	23.634	27.775	27.601
C	22.746	26.972	26.517	C	22.943	26.948	26.657
C	29.901	23.498	27.537	C	29.875	23.790	27.333
C	29.327	22.650	26.612	C	29.280	22.841	26.479
C	29.431	23.643	28.828	C	29.240	24.144	28.505
C	28.113	23.221	29.145	C	27.956	23.710	28.921
C	24.546	28.570	29.267	C	24.585	28.477	29.544
O	25.087	28.648	30.323	O	25.275	28.510	30.541
C	23.551	29.301	27.304	C	23.879	29.217	27.601
O	23.252	30.004	26.370	O	23.767	29.917	26.634
C	26.358	26.825	20.722	C	26.044	27.266	21.121
O	25.663	27.828	20.551	O	25.333	28.279	21.276

C	28.207	25.432	20.870	C	27.838	25.949	20.863
O	29.271	24.981	20.565	O	29.012	25.543	20.804
C	31.125	24.286	27.456	C	31.130	24.626	27.201
O	31.849	24.416	26.513	O	32.023	24.544	26.360
C	30.235	24.690	29.474	C	30.040	25.247	29.055
O	29.998	25.247	30.508	O	29.798	25.874	30.048
C	26.144	21.770	28.180	C	26.214	21.874	28.215
C	26.491	20.490	27.368	C	26.660	20.619	27.507
H	26.034	20.995	23.068	H	26.035	21.098	23.019
H	22.564	23.453	23.019	H	22.478	23.597	23.133
H	27.437	20.624	25.398	H	27.655	20.659	25.546
H	21.476	24.495	25.415	H	21.663	24.662	25.454
H	21.602	22.406	27.146	H	21.473	22.702	27.247
H	21.019	23.852	28.086	H	21.015	24.308	28.023
H	23.880	21.801	21.700	H	23.679	21.457	21.853
H	23.422	21.029	23.293	H	23.404	21.008	23.498
H	27.876	22.865	22.419	H	27.837	23.273	21.862
H	23.900	25.981	22.038	H	23.524	25.898	22.122
H	24.416	25.655	29.889	H	24.630	25.544	29.946
H	22.299	27.196	25.552	H	22.634	27.432	25.735
H	29.658	22.675	25.577	H	29.699	22.684	25.488
H	27.546	23.345	30.064	H	27.560	24.100	29.856
H	25.700	21.447	29.124	H	25.751	21.730	29.194
H	27.261	19.812	27.744	H	27.414	20.150	28.143
H	25.641	19.912	26.999	H	25.897	19.866	27.300
H	23.271	23.314	29.206	H	23.175	23.131	29.208
N	27.700	26.661	20.483	N	27.334	27.175	20.726
C	28.478	27.552	19.655	C	28.160	28.247	20.348
H	27.744	28.302	19.346	H	27.391	28.906	19.938
C	29.583	28.206	20.537	C	28.962	28.978	21.465
H	29.124	28.620	21.436	H	28.349	29.171	22.348
H	30.165	27.357	20.899	H	29.672	28.212	21.782
C	30.407	29.083	19.668	C	29.607	30.263	21.010
N	31.309	28.656	18.733	N	30.916	30.653	20.728
C	30.435	30.486	19.711	C	28.847	31.445	20.993
H	31.445	27.687	18.482	H	31.703	30.055	20.942
C	31.949	29.734	18.087	C	31.006	31.970	20.446
N	31.384	30.790	18.757	N	29.678	32.402	20.498
H	29.867	31.255	20.219	H	27.821	31.609	21.294
H	32.754	29.813	17.352	H	31.843	32.531	20.025
H	31.558	31.730	18.429	H	29.409	33.298	20.115
N	31.228	24.981	28.653	N	31.071	25.482	28.293
C	32.300	25.925	28.947	C	31.919	26.693	28.508
H	32.071	26.525	29.831	H	31.133	27.417	28.741

C	33.710	25.322	29.195	C	32.793	26.556	29.759
H	33.694	24.580	29.996	H	32.371	27.001	30.663
H	34.019	24.936	28.221	H	32.993	25.524	30.052
C	34.697	26.413	29.569	C	34.175	27.125	29.311
N	36.007	26.574	29.125	N	35.232	26.609	28.545
C	34.475	27.409	30.467	C	34.552	28.448	29.463
H	36.545	26.018	28.475	H	35.231	25.709	28.085
C	36.647	27.688	29.670	C	36.319	27.424	28.367
N	35.615	28.174	30.490	N	35.773	28.649	28.829
H	33.630	27.597	31.119	H	34.010	29.311	29.831
H	37.566	28.190	29.358	H	37.272	27.215	27.876
H	35.789	29.041	30.982	H	36.384	29.454	28.824
N	24.128	29.639	28.520	N	24.429	29.533	28.737
C	24.685	31.037	28.691	C	25.004	30.826	29.041
H	24.981	31.426	27.712	H	25.587	31.168	28.181
C	23.682	32.045	29.363	C	23.877	31.876	29.343
H	24.128	33.032	29.225	H	24.222	32.902	29.483
H	22.728	31.987	28.834	H	23.341	31.869	28.391
C	23.540	31.764	30.853	C	23.093	31.525	30.517
N	22.577	31.156	31.531	N	21.989	30.687	30.642
C	24.350	32.388	31.745	C	23.363	31.835	31.806
H	21.659	30.875	31.215	H	21.415	30.290	29.911
C	22.776	31.125	32.893	C	21.529	30.469	31.915
N	23.848	32.028	32.938	N	22.473	31.190	32.554
H	25.168	33.091	31.648	H	24.206	32.431	32.134
H	22.268	30.758	33.787	H	20.982	29.659	32.402
H	24.317	32.190	33.819	H	22.375	31.301	33.554
H	28.917	27.057	18.786	H	28.811	27.949	19.522
H	32.271	26.655	28.133	H	32.488	26.808	27.582
H	25.583	31.026	29.313	H	25.571	30.897	29.972

We performed docking simulations of a library of guests (Figure S18) into the above snapshots with a grid box centered on the basket cavity.

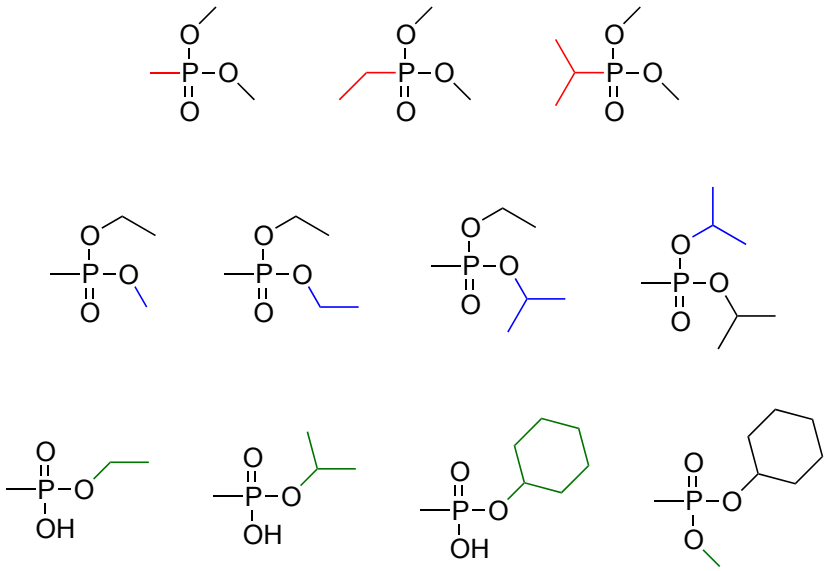


Figure S18. Library of guest molecules used for the molecular docking simulations.

Figure S19 shows the clustering analysis from one of our docking studies (DMMP in two different basket snapshots). In the majority of the docking poses, the lowest energy and most populated pose places DMMP within the basket cavity as shown in Figure S19. Other poses were less common and their populations and relative energies are presented in **Table S2**.

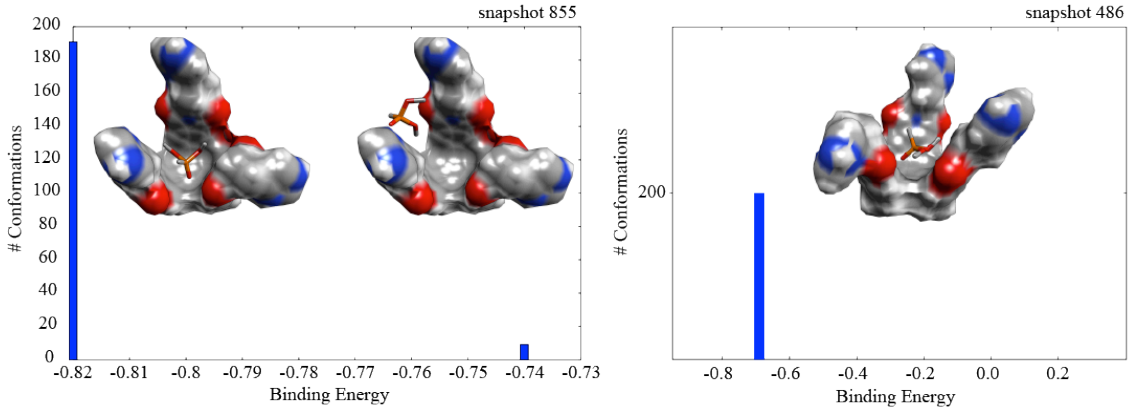


Figure S19. Clustering of docking poses for DMMP into two MD snapshots of basket.

Table S2. Summary of docking poses of DMMP in several MD snapshots of basket.

Snapshot #	# of Conformations	Absolute Energy (kcal/mol)	Overall Relative Energy (kcal/mol)
355	5	-0.82	0.92
	180	-0.75	0.99
	15	-0.71	1.03
1867	45	-0.65	1.09
	155	-0.61	1.13
486	200	-0.70	1.04

855	191 9	-0.82 -0.74	0.92 1.00
1021	194 6	-0.53 -0.49	1.21 1.25
1807	116 84	-0.87 -0.82	0.87 0.92
1099	196 3 1	-0.90 -0.82 -0.77	0.84 0.92 0.97
1233	199 1	-0.91 -0.81	0.83 0.93
1356	185 14 1	-0.91 -0.88 -0.83	0.83 0.86 0.91
1556	197 3	-1.74 -1.64	0.00 0.10

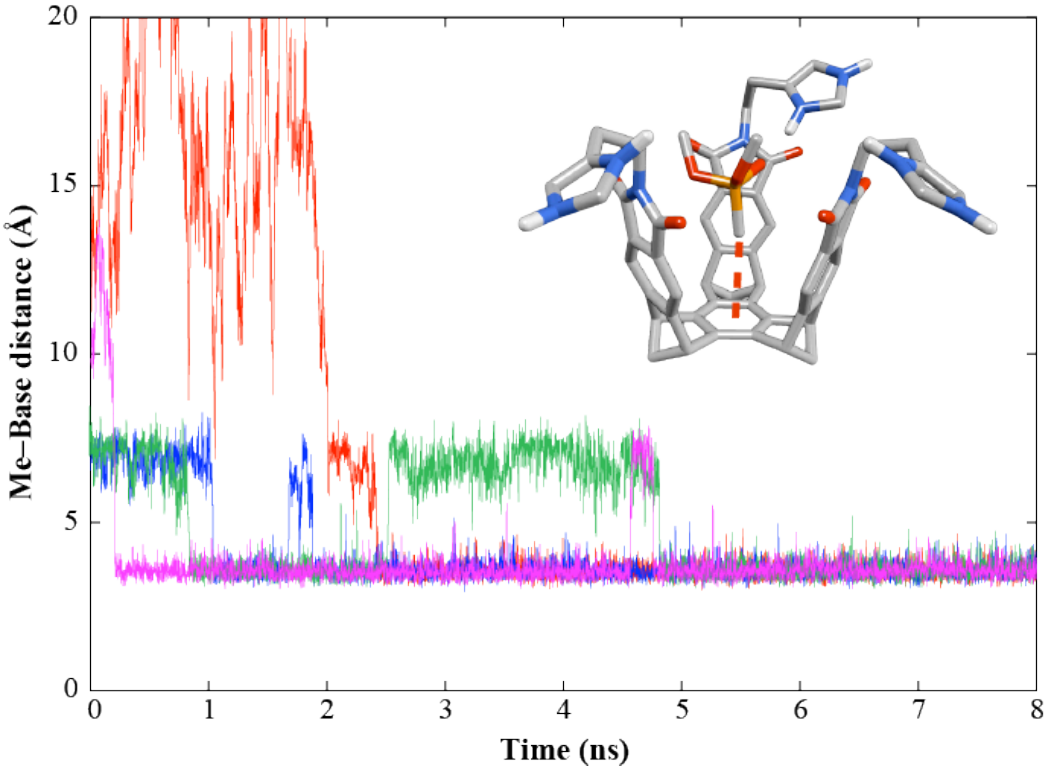


Figure S20. Plot of the distance between the basket base and methyl group carbon of DMMP as a function of simulation time for MD simulations of the solvated guest-basket complexes. Each color represents a unique host-guest complex obtained from the molecular docking protocol described above.

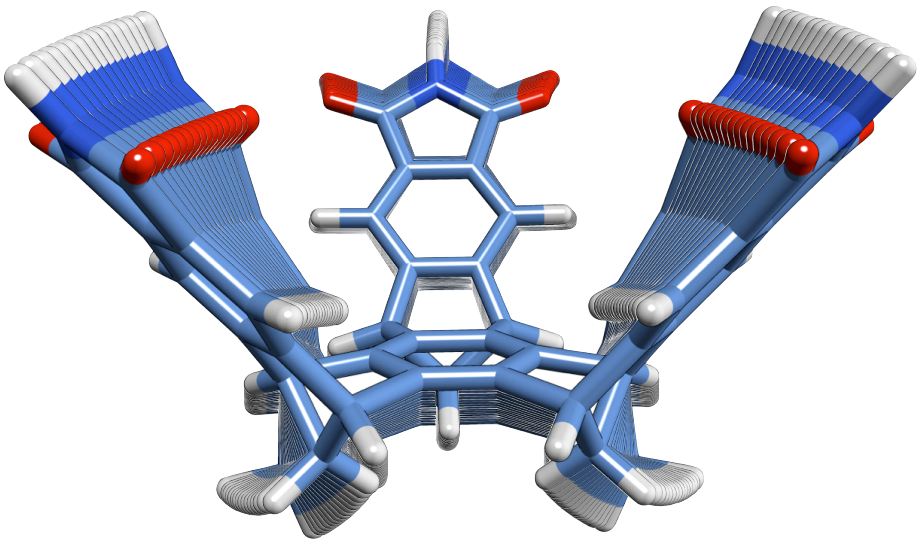


Figure S21. Expansion of the basket cavity by 2° increments (optimized coordinates are included below).

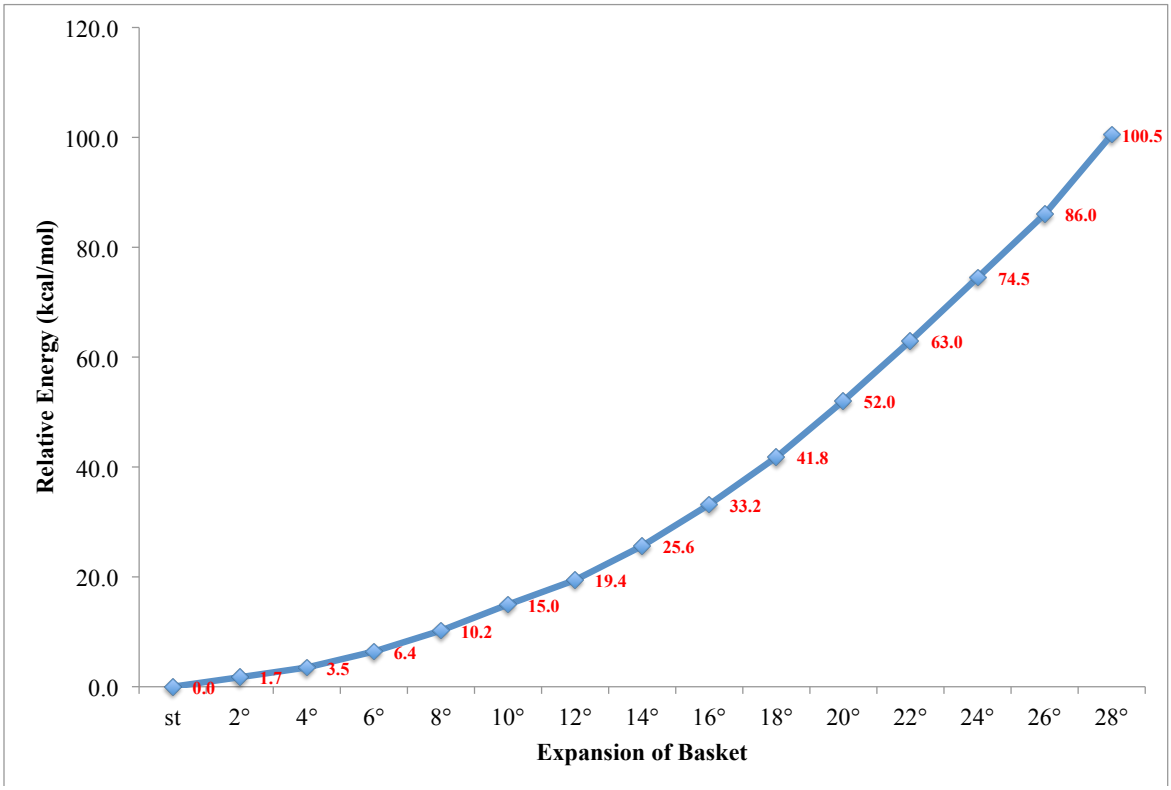


Figure S22. Relative energy profile as a function of basket cavity expansion.

Optimized Coordinates of Basket Expansions							
Start				2°			
C	-1.396	-0.015	2.507	C	-1.397	-0.016	2.450
C	1.740	2.317	2.506	C	1.744	2.320	2.461
C	2.877	0.348	2.506	C	2.882	0.351	2.461
C	1.137	-2.665	2.506	C	1.137	-2.671	2.461
C	2.439	2.223	1.156	C	2.482	2.247	1.138
C	3.145	1.001	1.156	C	3.187	1.026	1.138

C	-2.439	2.223	1.156	C	-2.482	2.247	1.138
C	-3.145	1.001	1.156	C	-3.187	1.026	1.138
C	-0.706	-3.224	1.156	C	-0.705	-3.273	1.138
C	0.706	-3.224	1.156	C	0.705	-3.273	1.138
C	2.455	3.078	0.065	C	2.529	3.120	0.063
C	-0.711	-1.202	2.507	C	-0.712	-1.202	2.450
C	3.893	0.587	0.065	C	3.966	0.630	0.063
C	-2.455	3.078	0.065	C	-2.529	3.120	0.063
C	-3.893	0.587	0.065	C	-3.966	0.630	0.063
C	-1.438	-3.665	0.065	C	-1.438	-3.750	0.063
C	1.438	-3.665	0.065	C	1.438	-3.750	0.063
C	3.218	2.661	-1.021	C	3.322	2.721	-1.008
C	3.914	1.456	-1.021	C	4.018	1.516	-1.008
C	0.695	-4.118	-1.021	C	0.696	-4.238	-1.008
C	-0.695	-4.118	-1.021	C	-0.696	-4.238	-1.008
C	-3.218	2.661	-1.021	C	-3.322	2.721	-1.008
C	0.711	-1.202	2.507	C	0.712	-1.202	2.450
C	-3.914	1.456	-1.021	C	-4.018	1.516	-1.008
C	4.631	1.327	-2.321	C	4.770	1.407	-2.289
C	3.464	3.347	-2.321	C	3.604	3.428	-2.289
C	1.166	-4.674	-2.321	C	1.166	-4.835	-2.289
C	-1.166	-4.674	-2.321	C	-1.166	-4.835	-2.289
C	-4.631	1.327	-2.321	C	-4.770	1.407	-2.289
C	-3.464	3.347	-2.321	C	-3.604	3.428	-2.289
C	1.396	-0.015	2.507	C	1.397	-0.016	2.450
C	-2.817	1.626	3.385	C	-2.763	1.595	3.386
C	0.000	-3.252	3.385	C	0.000	-3.190	3.386
C	2.817	1.626	3.385	C	2.763	1.595	3.386
C	0.685	1.216	2.507	C	0.685	1.218	2.450
C	-0.685	1.216	2.507	C	-0.685	1.218	2.450
C	-1.137	-2.665	2.506	C	-1.137	-2.671	2.461
C	-2.877	0.348	2.506	C	-2.882	0.351	2.461
C	-1.740	2.317	2.506	C	-1.744	2.320	2.461
N	-4.304	2.485	-3.027	N	-4.463	2.577	-2.985
N	4.304	2.485	-3.027	N	4.463	2.577	-2.985
N	0.000	-4.970	-3.027	N	0.000	-5.154	-2.985
O	5.347	0.435	-2.710	O	5.497	0.522	-2.673
O	3.051	4.413	-2.710	O	3.200	4.500	-2.673
O	2.297	-4.849	-2.710	O	2.297	-5.021	-2.673
O	-2.297	-4.849	-2.710	O	-2.297	-5.021	-2.673
O	-5.347	0.435	-2.710	O	-5.497	0.522	-2.673
O	-3.051	4.413	-2.710	O	-3.200	4.500	-2.673
H	-2.165	-2.873	2.802	H	-2.165	-2.871	2.764
H	1.921	4.022	0.046	H	1.994	4.064	0.044

H	-1.921	4.022	0.046	H	-1.994	4.064	0.044
H	-4.443	-0.347	0.046	H	-4.517	-0.305	0.044
H	-3.764	2.173	3.407	H	-3.707	2.140	3.490
H	-2.471	1.427	4.403	H	-2.353	1.358	4.371
H	0.000	-4.346	3.407	H	0.000	-4.280	3.490
H	0.000	-2.853	4.403	H	0.000	-2.717	4.371
H	-3.571	-0.438	2.802	H	-3.569	-0.439	2.764
H	3.764	2.173	3.407	H	3.707	2.140	3.490
H	2.471	1.427	4.403	H	2.353	1.358	4.371
H	-1.406	3.311	2.802	H	-1.404	3.310	2.764
H	1.406	3.311	2.802	H	1.404	3.310	2.764
H	3.571	-0.438	2.802	H	3.569	-0.439	2.764
H	2.165	-2.873	2.802	H	2.165	-2.871	2.764
H	-2.522	-3.675	0.046	H	-2.522	-3.759	0.044
H	2.522	-3.675	0.046	H	2.522	-3.759	0.044
H	4.443	-0.347	0.046	H	4.517	-0.305	0.044
H	-4.646	2.682	-3.955	H	-4.830	2.789	-3.901
H	4.646	2.682	-3.955	H	4.830	2.789	-3.901
H	0.000	-5.364	-3.955	H	0.000	-5.577	-3.901

	4°				**6°**		
C	-1.397	-0.016	2.425	C	-1.398	-0.017	2.393
C	1.747	2.322	2.441	C	1.749	2.323	2.417
C	2.884	0.352	2.441	C	2.887	0.353	2.417
C	1.137	-2.673	2.441	C	1.138	-2.677	2.417
C	2.500	2.256	1.130	C	2.522	2.269	1.120
C	3.204	1.037	1.130	C	3.226	1.050	1.120
C	-2.500	2.256	1.130	C	-2.522	2.269	1.120
C	-3.204	1.037	1.130	C	-3.226	1.050	1.120
C	-0.704	-3.293	1.130	C	-0.704	-3.318	1.120
C	0.704	-3.293	1.130	C	0.704	-3.318	1.120
C	2.560	3.138	0.062	C	2.597	3.159	0.060
C	-0.713	-1.202	2.425	C	-0.714	-1.202	2.393
C	3.997	0.648	0.062	C	4.035	0.670	0.060
C	-2.560	3.138	0.062	C	-2.597	3.159	0.060
C	-3.997	0.648	0.062	C	-4.035	0.670	0.060
C	-1.438	-3.785	0.062	C	-1.437	-3.829	0.060
C	1.438	-3.785	0.062	C	1.437	-3.829	0.060
C	3.366	2.747	-1.002	C	3.420	2.778	-0.994
C	4.062	1.542	-1.002	C	4.116	1.573	-0.994
C	0.696	-4.288	-1.002	C	0.696	-4.351	-0.994
C	-0.696	-4.288	-1.002	C	-0.696	-4.351	-0.994
C	-3.366	2.747	-1.002	C	-3.420	2.778	-0.994
C	0.713	-1.202	2.425	C	0.714	-1.202	2.393

C	-4.062	1.542	-1.002	C	-4.116	1.573	-0.994
C	4.830	1.442	-2.275	C	4.902	1.483	-2.256
C	3.663	3.462	-2.275	C	3.736	3.504	-2.256
C	1.166	-4.903	-2.275	C	1.166	-4.987	-2.256
C	-1.166	-4.903	-2.275	C	-1.166	-4.987	-2.256
C	-4.830	1.442	-2.275	C	-4.902	1.483	-2.256
C	-3.663	3.462	-2.275	C	-3.736	3.504	-2.256
C	1.397	-0.016	2.425	C	1.398	-0.017	2.393
C	-2.739	1.581	3.385	C	-2.709	1.564	3.382
C	0.000	-3.162	3.385	C	0.000	-3.128	3.382
C	2.739	1.581	3.385	C	2.709	1.564	3.382
C	0.684	1.218	2.425	C	0.684	1.219	2.393
C	-0.684	1.218	2.425	C	-0.684	1.219	2.393
C	-1.137	-2.673	2.441	C	-1.138	-2.677	2.417
C	-2.884	0.352	2.441	C	-2.887	0.353	2.417
C	-1.747	2.322	2.441	C	-1.749	2.323	2.417
N	-4.531	2.616	-2.966	N	-4.614	2.664	-2.942
N	4.531	2.616	-2.966	N	4.614	2.664	-2.942
N	0.000	-5.232	-2.966	N	0.000	-5.328	-2.942
O	5.560	0.558	-2.657	O	5.638	0.603	-2.635
O	3.264	4.536	-2.657	O	3.342	4.581	-2.635
O	2.297	-5.095	-2.657	O	2.297	-5.185	-2.635
O	-2.297	-5.095	-2.657	O	-2.297	-5.185	-2.635
O	-5.560	0.558	-2.657	O	-5.638	0.603	-2.635
O	-3.264	4.536	-2.657	O	-3.342	4.581	-2.635
H	-2.165	-2.870	2.747	H	-2.165	-2.869	2.727
H	2.025	4.082	0.043	H	2.063	4.104	0.042
H	-2.025	4.082	0.043	H	-2.063	4.104	0.042
H	-4.548	-0.287	0.043	H	-4.585	-0.265	0.042
H	-3.680	2.125	3.524	H	-3.646	2.105	3.562
H	-2.302	1.329	4.354	H	-2.243	1.295	4.330
H	0.000	-4.249	3.524	H	0.000	-4.210	3.562
H	0.000	-2.659	4.354	H	0.000	-2.589	4.330
H	-3.568	-0.440	2.747	H	-3.567	-0.440	2.727
H	3.680	2.125	3.524	H	3.646	2.105	3.562
H	2.302	1.329	4.354	H	2.243	1.295	4.330
H	-1.403	3.310	2.747	H	-1.402	3.309	2.727
H	1.403	3.310	2.747	H	1.402	3.309	2.727
H	3.568	-0.440	2.747	H	3.567	-0.440	2.727
H	2.165	-2.870	2.747	H	2.165	-2.869	2.727
H	-2.522	-3.795	0.043	H	-2.522	-3.838	0.042
H	2.522	-3.795	0.043	H	2.522	-3.838	0.042
H	4.548	-0.287	0.043	H	4.585	-0.265	0.042
H	-4.908	2.834	-3.876	H	-5.005	2.889	-3.844

H	4.908	2.834	-3.876	H	5.005	2.889	-3.844
H	0.000	-5.668	-3.876	H	0.000	-5.779	-3.844
		8°				**10°**	
C	-1.398	-0.018	2.358	C	-1.399	-0.019	2.323
C	1.752	2.325	2.391	C	1.755	2.327	2.364
C	2.890	0.354	2.391	C	2.893	0.356	2.364
C	1.138	-2.680	2.391	C	1.138	-2.683	2.364
C	2.544	2.281	1.110	C	2.566	2.293	1.099
C	3.247	1.063	1.110	C	3.269	1.076	1.099
C	-2.544	2.281	1.110	C	-2.566	2.293	1.099
C	-3.247	1.063	1.110	C	-3.269	1.076	1.099
C	-0.703	-3.344	1.110	C	-0.702	-3.369	1.099
C	0.703	-3.344	1.110	C	0.702	-3.369	1.099
C	2.636	3.182	0.059	C	2.674	3.204	0.058
C	-0.715	-1.202	2.358	C	-0.716	-1.202	2.323
C	4.073	0.692	0.059	C	4.111	0.714	0.058
C	-2.636	3.182	0.059	C	-2.674	3.204	0.058
C	-4.073	0.692	0.059	C	-4.111	0.714	0.058
C	-1.437	-3.874	0.059	C	-1.437	-3.917	0.058
C	1.437	-3.874	0.059	C	1.437	-3.917	0.058
C	3.474	2.810	-0.985	C	3.528	2.841	-0.977
C	4.170	1.604	-0.985	C	4.225	1.635	-0.977
C	0.696	-4.414	-0.985	C	0.696	-4.476	-0.977
C	-0.696	-4.414	-0.985	C	-0.696	-4.476	-0.977
C	-3.474	2.810	-0.985	C	-3.528	2.841	-0.977
C	0.715	-1.202	2.358	C	0.716	-1.202	2.323
C	-4.170	1.604	-0.985	C	-4.225	1.635	-0.977
C	4.976	1.526	-2.236	C	5.050	1.569	-2.216
C	3.810	3.547	-2.236	C	3.883	3.589	-2.216
C	1.166	-5.073	-2.236	C	1.167	-5.158	-2.216
C	-1.166	-5.073	-2.236	C	-1.167	-5.158	-2.216
C	-4.976	1.526	-2.236	C	-5.050	1.569	-2.216
C	-3.810	3.547	-2.236	C	-3.883	3.589	-2.216
C	1.398	-0.018	2.358	C	1.399	-0.019	2.323
C	-2.679	1.546	3.376	C	-2.647	1.528	3.368
C	0.000	-3.093	3.376	C	0.000	-3.057	3.368
C	2.679	1.546	3.376	C	2.647	1.528	3.368
C	0.684	1.220	2.358	C	0.683	1.221	2.323
C	-0.684	1.220	2.358	C	-0.683	1.221	2.323
C	-1.138	-2.680	2.391	C	-1.138	-2.683	2.364
C	-2.890	0.354	2.391	C	-2.893	0.356	2.364
C	-1.752	2.325	2.391	C	-1.755	2.327	2.364
N	-4.699	2.713	-2.915	N	-4.783	2.761	-2.888

N	4.699	2.713	-2.915	N	4.783	2.761	-2.888
N	0.000	-5.426	-2.915	N	0.000	-5.523	-2.888
O	5.718	0.649	-2.612	O	5.797	0.695	-2.587
O	3.421	4.627	-2.612	O	3.500	4.673	-2.587
O	2.297	-5.276	-2.612	O	2.297	-5.368	-2.587
O	-2.297	-5.276	-2.612	O	-2.297	-5.368	-2.587
O	-5.718	0.649	-2.612	O	-5.797	0.695	-2.587
O	-3.421	4.627	-2.612	O	-3.500	4.673	-2.587
H	-2.165	-2.868	2.705	H	-2.165	-2.867	2.682
H	2.102	4.126	0.041	H	2.140	4.148	0.040
H	-2.102	4.126	0.041	H	-2.140	4.148	0.040
H	-4.624	-0.243	0.041	H	-4.662	-0.221	0.040
H	-3.610	2.084	3.597	H	-3.572	2.062	3.630
H	-2.183	1.260	4.303	H	-2.123	1.226	4.274
H	0.000	-4.168	3.597	H	0.000	-4.124	3.630
H	0.000	-2.520	4.303	H	0.000	-2.452	4.274
H	-3.566	-0.441	2.705	H	-3.565	-0.441	2.682
H	3.610	2.084	3.597	H	3.572	2.062	3.630
H	2.183	1.260	4.303	H	2.123	1.226	4.274
H	-1.401	3.309	2.705	H	-1.401	3.308	2.682
H	1.401	3.309	2.705	H	1.401	3.308	2.682
H	3.566	-0.441	2.705	H	3.565	-0.441	2.682
H	2.165	-2.868	2.705	H	2.165	-2.867	2.682
H	-2.522	-3.883	0.041	H	-2.522	-3.927	0.040
H	2.522	-3.883	0.041	H	2.522	-3.927	0.040
H	4.624	-0.243	0.041	H	4.662	-0.221	0.040
H	-5.103	2.946	-3.809	H	-5.201	3.003	-3.773
H	5.103	2.946	-3.809	H	5.201	3.003	-3.773
H	0.000	-5.893	-3.809	H	0.000	-6.005	-3.773

	12°				**14°**		
C	-1.399	-0.020	2.294	C	-1.400	-0.021	2.261
C	1.757	2.329	2.343	C	1.760	2.331	2.317
C	2.896	0.357	2.343	C	2.899	0.358	2.317
C	1.139	-2.686	2.343	C	1.139	-2.690	2.317
C	2.584	2.302	1.090	C	2.604	2.313	1.079
C	3.286	1.086	1.090	C	3.305	1.098	1.079
C	-2.584	2.302	1.090	C	-2.604	2.313	1.079
C	-3.286	1.086	1.090	C	-3.305	1.098	1.079
C	-0.702	-3.389	1.090	C	-0.702	-3.412	1.079
C	0.702	-3.389	1.090	C	0.702	-3.412	1.079
C	2.705	3.221	0.057	C	2.739	3.241	0.055
C	-0.717	-1.202	2.294	C	-0.718	-1.202	2.261
C	4.142	0.732	0.057	C	4.177	0.752	0.055

C	-2.705	3.221	0.057	C	-2.739	3.241	0.055
C	-4.142	0.732	0.057	C	-4.177	0.752	0.055
C	-1.437	-3.953	0.057	C	-1.437	-3.993	0.055
C	1.437	-3.953	0.057	C	1.437	-3.993	0.055
C	3.572	2.866	-0.969	C	3.621	2.895	-0.960
C	4.268	1.660	-0.969	C	4.318	1.689	-0.960
C	0.696	-4.526	-0.969	C	0.696	-4.583	-0.960
C	-0.696	-4.526	-0.969	C	-0.696	-4.583	-0.960
C	-3.572	2.866	-0.969	C	-3.621	2.895	-0.960
C	0.717	-1.202	2.294	C	0.718	-1.202	2.261
C	-4.268	1.660	-0.969	C	-4.318	1.689	-0.960
C	5.109	1.603	-2.198	C	5.176	1.642	-2.177
C	3.943	3.623	-2.198	C	4.010	3.662	-2.177
C	1.167	-5.226	-2.198	C	1.167	-5.304	-2.177
C	-1.167	-5.226	-2.198	C	-1.167	-5.304	-2.177
C	-5.109	1.603	-2.198	C	-5.176	1.642	-2.177
C	-3.943	3.623	-2.198	C	-4.010	3.662	-2.177
C	1.399	-0.020	2.294	C	1.400	-0.021	2.261
C	-2.622	1.514	3.360	C	-2.592	1.496	3.350
C	0.000	-3.028	3.360	C	0.000	-2.993	3.350
C	2.622	1.514	3.360	C	2.592	1.496	3.350
C	0.683	1.222	2.294	C	0.682	1.223	2.261
C	-0.683	1.222	2.294	C	-0.682	1.223	2.261
C	-1.139	-2.686	2.343	C	-1.139	-2.690	2.317
C	-2.896	0.357	2.343	C	-2.899	0.358	2.317
C	-1.757	2.329	2.343	C	-1.760	2.331	2.317
N	-4.851	2.801	-2.865	N	-4.928	2.845	-2.837
N	4.851	2.801	-2.865	N	4.928	2.845	-2.837
N	0.000	-5.601	-2.865	N	0.000	-5.690	-2.837
O	5.861	0.732	-2.567	O	5.933	0.773	-2.543
O	3.564	4.710	-2.567	O	3.636	4.752	-2.543
O	2.297	-5.442	-2.567	O	2.297	-5.525	-2.543
O	-2.297	-5.442	-2.567	O	-2.297	-5.525	-2.543
O	-5.861	0.732	-2.567	O	-5.933	0.773	-2.543
O	-3.564	4.710	-2.567	O	-3.636	4.752	-2.543
H	-2.165	-2.866	2.663	H	-2.165	-2.866	2.641
H	2.171	4.165	0.040	H	2.205	4.185	0.039
H	-2.171	4.165	0.040	H	-2.205	4.185	0.039
H	-4.693	-0.203	0.040	H	-4.727	-0.183	0.039
H	-3.540	2.044	3.653	H	-3.501	2.022	3.679
H	-2.077	1.199	4.248	H	-2.023	1.168	4.217
H	0.000	-4.088	3.653	H	0.000	-4.043	3.679
H	0.000	-2.399	4.248	H	0.000	-2.336	4.217
H	-3.565	-0.442	2.663	H	-3.565	-0.442	2.641

H	3.540	2.044	3.653	H	3.501	2.022	3.679
H	2.077	1.199	4.248	H	2.023	1.168	4.217
H	-1.400	3.308	2.663	H	-1.400	3.308	2.641
H	1.400	3.308	2.663	H	1.400	3.308	2.641
H	3.565	-0.442	2.663	H	3.565	-0.442	2.641
H	2.165	-2.866	2.663	H	2.165	-2.866	2.641
H	-2.522	-3.962	0.040	H	-2.522	-4.003	0.039
H	2.522	-3.962	0.040	H	2.522	-4.003	0.039
H	4.693	-0.203	0.040	H	4.727	-0.183	0.039
H	-5.280	3.048	-3.743	H	-5.370	3.100	-3.708
H	5.280	3.048	-3.743	H	5.370	3.100	-3.708
H	0.000	-6.097	-3.743	H	0.000	-6.200	-3.708
		16°				**18°**	
C	-1.401	-0.022	2.226	C	-1.401	-0.023	2.190
C	1.763	2.334	2.290	C	1.767	2.337	2.262
C	2.903	0.360	2.290	C	2.907	0.362	2.262
C	1.140	-2.694	2.290	C	1.140	-2.698	2.262
C	2.624	2.325	1.068	C	2.645	2.336	1.056
C	3.325	1.110	1.068	C	3.345	1.122	1.056
C	-2.624	2.325	1.068	C	-2.645	2.336	1.056
C	-3.325	1.110	1.068	C	-3.345	1.122	1.056
C	-0.701	-3.435	1.068	C	-0.701	-3.458	1.056
C	0.701	-3.435	1.068	C	0.701	-3.458	1.056
C	2.775	3.262	0.054	C	2.810	3.282	0.053
C	-0.719	-1.202	2.226	C	-0.721	-1.202	2.190
C	4.212	0.772	0.054	C	4.248	0.793	0.053
C	-2.775	3.262	0.054	C	-2.810	3.282	0.053
C	-4.212	0.772	0.054	C	-4.248	0.793	0.053
C	-1.437	-4.034	0.054	C	-1.437	-4.075	0.053
C	1.437	-4.034	0.054	C	1.437	-4.075	0.053
C	3.672	2.924	-0.951	C	3.722	2.953	-0.941
C	4.368	1.718	-0.951	C	4.419	1.747	-0.941
C	0.697	-4.642	-0.951	C	0.697	-4.700	-0.941
C	-0.697	-4.642	-0.951	C	-0.697	-4.700	-0.941
C	-3.672	2.924	-0.951	C	-3.722	2.953	-0.941
C	0.719	-1.202	2.226	C	0.721	-1.202	2.190
C	-4.368	1.718	-0.951	C	-4.419	1.747	-0.941
C	5.245	1.681	-2.156	C	5.314	1.721	-2.133
C	4.079	3.702	-2.156	C	4.147	3.742	-2.133
C	1.167	-5.383	-2.156	C	1.167	-5.462	-2.133
C	-1.167	-5.383	-2.156	C	-1.167	-5.462	-2.133
C	-5.245	1.681	-2.156	C	-5.314	1.721	-2.133
C	-4.079	3.702	-2.156	C	-4.147	3.742	-2.133

C	1.401	-0.022	2.226	C	1.401	-0.023	2.190
C	-2.560	1.478	3.337	C	-2.528	1.459	3.323
C	0.000	-2.956	3.337	C	0.000	-2.919	3.323
C	2.560	1.478	3.337	C	2.528	1.459	3.323
C	0.681	1.224	2.226	C	0.681	1.225	2.190
C	-0.681	1.224	2.226	C	-0.681	1.225	2.190
C	-1.140	-2.694	2.290	C	-1.140	-2.698	2.262
C	-2.903	0.360	2.290	C	-2.907	0.362	2.262
C	-1.763	2.334	2.290	C	-1.767	2.337	2.262
N	-5.007	2.891	-2.808	N	-5.085	2.936	-2.778
N	5.007	2.891	-2.808	N	5.085	2.936	-2.778
N	0.000	-5.781	-2.808	N	0.000	-5.872	-2.778
O	6.007	0.816	-2.517	O	6.081	0.859	-2.490
O	3.710	4.794	-2.517	O	3.785	4.837	-2.490
O	2.297	-5.610	-2.517	O	2.297	-5.696	-2.490
O	-2.297	-5.610	-2.517	O	-2.297	-5.696	-2.490
O	-6.007	0.816	-2.517	O	-6.081	0.859	-2.490
O	-3.710	4.794	-2.517	O	-3.785	4.837	-2.490
H	-2.165	-2.866	2.618	H	-2.165	-2.866	2.595
H	2.241	4.206	0.038	H	2.276	4.226	0.037
H	-2.241	4.206	0.038	H	-2.276	4.226	0.037
H	-4.763	-0.162	0.038	H	-4.798	-0.142	0.037
H	-3.460	1.998	3.703	H	-3.417	1.973	3.725
H	-1.969	1.137	4.183	H	-1.914	1.105	4.146
H	0.000	-3.995	3.703	H	0.000	-3.946	3.725
H	0.000	-2.273	4.183	H	0.000	-2.211	4.146
H	-3.565	-0.442	2.618	H	-3.565	-0.442	2.595
H	3.460	1.998	3.703	H	3.417	1.973	3.725
H	1.969	1.137	4.183	H	1.914	1.105	4.146
H	-1.400	3.308	2.618	H	-1.400	3.308	2.595
H	1.400	3.308	2.618	H	1.400	3.308	2.595
H	3.565	-0.442	2.618	H	3.565	-0.442	2.595
H	2.165	-2.866	2.618	H	2.165	-2.866	2.595
H	-2.522	-4.044	0.038	H	-2.522	-4.085	0.037
H	2.522	-4.044	0.038	H	2.522	-4.085	0.037
H	4.763	-0.162	0.038	H	4.798	-0.142	0.037
H	-5.461	3.153	-3.670	H	-5.553	3.206	-3.630
H	5.461	3.153	-3.670	H	5.553	3.206	-3.630
H	0.000	-6.306	-3.670	H	0.000	-6.412	-3.630

20°				**22°**			
C	-1.402	-0.025	2.149	C	-1.403	-0.026	2.107
C	1.770	2.339	2.232	C	1.774	2.343	2.201
C	2.911	0.363	2.232	C	2.916	0.365	2.201

C	1.141	-2.703	2.232	C	1.142	-2.708	2.201
C	2.667	2.348	1.042	C	2.689	2.360	1.029
C	3.367	1.135	1.042	C	3.388	1.148	1.029
C	-2.667	2.348	1.042	C	-2.689	2.360	1.029
C	-3.367	1.135	1.042	C	-3.388	1.148	1.029
C	-0.700	-3.484	1.042	C	-0.700	-3.509	1.029
C	0.700	-3.484	1.042	C	0.700	-3.509	1.029
C	2.849	3.305	0.052	C	2.887	3.327	0.051
C	-0.723	-1.202	2.149	C	-0.725	-1.202	2.107
C	4.286	0.815	0.052	C	4.324	0.837	0.051
C	-2.849	3.305	0.052	C	-2.887	3.327	0.051
C	-4.286	0.815	0.052	C	-4.324	0.837	0.051
C	-1.437	-4.119	0.052	C	-1.437	-4.163	0.051
C	1.437	-4.119	0.052	C	1.437	-4.163	0.051
C	3.777	2.985	-0.930	C	3.831	3.017	-0.918
C	4.474	1.778	-0.930	C	4.528	1.810	-0.918
C	0.697	-4.764	-0.930	C	0.697	-4.827	-0.918
C	-0.697	-4.764	-0.930	C	-0.697	-4.827	-0.918
C	-3.777	2.985	-0.930	C	-3.831	3.017	-0.918
C	0.723	-1.202	2.149	C	0.725	-1.202	2.107
C	-4.474	1.778	-0.930	C	-4.528	1.810	-0.918
C	5.389	1.764	-2.107	C	5.463	1.807	-2.079
C	4.222	3.785	-2.107	C	4.296	3.828	-2.079
C	1.167	-5.549	-2.107	C	1.167	-5.634	-2.079
C	-1.167	-5.549	-2.107	C	-1.167	-5.634	-2.079
C	-5.389	1.764	-2.107	C	-5.463	1.807	-2.079
C	-4.222	3.785	-2.107	C	-4.296	3.828	-2.079
C	1.402	-0.025	2.149	C	1.403	-0.026	2.107
C	-2.492	1.439	3.304	C	-2.458	1.419	3.283
C	0.000	-2.878	3.304	C	0.000	-2.838	3.283
C	2.492	1.439	3.304	C	2.458	1.419	3.283
C	0.680	1.227	2.149	C	0.679	1.229	2.107
C	-0.680	1.227	2.149	C	-0.679	1.229	2.107
C	-1.141	-2.703	2.232	C	-1.142	-2.708	2.201
C	-2.911	0.363	2.232	C	-2.916	0.365	2.201
C	-1.770	2.339	2.232	C	-1.774	2.343	2.201
N	-5.171	2.985	-2.744	N	-5.256	3.034	-2.708
N	5.171	2.985	-2.744	N	5.256	3.034	-2.708
N	0.000	-5.971	-2.744	N	0.000	-6.069	-2.708
O	6.162	0.905	-2.460	O	6.242	0.952	-2.428
O	3.865	4.884	-2.460	O	3.945	4.930	-2.428
O	2.297	-5.789	-2.460	O	2.297	-5.881	-2.428
O	-2.297	-5.789	-2.460	O	-2.297	-5.881	-2.428
O	-6.162	0.905	-2.460	O	-6.242	0.952	-2.428

O	-3.865	4.884	-2.460	O	-3.945	4.930	-2.428
H	-2.165	-2.866	2.568	H	-2.165	-2.866	2.542
H	2.315	4.249	0.036	H	2.353	4.271	0.036
H	-2.315	4.249	0.036	H	-2.353	4.271	0.036
H	-4.837	-0.120	0.036	H	-4.875	-0.098	0.036
H	-3.370	1.945	3.744	H	-3.322	1.918	3.758
H	-1.858	1.073	4.104	H	-1.803	1.041	4.060
H	0.000	-3.891	3.744	H	0.000	-3.836	3.758
H	0.000	-2.145	4.104	H	0.000	-2.082	4.060
H	-3.565	-0.442	2.568	H	-3.565	-0.442	2.542
H	3.370	1.945	3.744	H	3.322	1.918	3.758
H	1.858	1.073	4.104	H	1.803	1.041	4.060
H	-1.400	3.308	2.568	H	-1.400	3.308	2.542
H	1.400	3.308	2.568	H	1.400	3.308	2.542
H	3.565	-0.442	2.568	H	3.565	-0.442	2.542
H	2.165	-2.866	2.568	H	2.165	-2.866	2.542
H	-2.522	-4.129	0.036	H	-2.522	-4.173	0.036
H	2.522	-4.129	0.036	H	2.522	-4.173	0.036
H	4.837	-0.120	0.036	H	4.875	-0.098	0.036
H	-5.653	3.264	-3.585	H	-5.752	3.321	-3.539
H	5.653	3.264	-3.585	H	5.752	3.321	-3.539
H	0.000	-6.527	-3.585	H	0.000	-6.641	-3.539

	24°				**26°**		
C	-1.405	-0.028	2.061	C	-1.406	-0.030	2.010
C	1.777	2.346	2.168	C	1.781	2.348	2.133
C	2.920	0.367	2.168	C	2.924	0.368	2.133
C	1.143	-2.712	2.168	C	1.143	-2.716	2.133
C	2.711	2.373	1.014	C	2.733	2.385	0.999
C	3.410	1.161	1.014	C	3.432	1.174	0.999
C	-2.711	2.373	1.014	C	-2.733	2.385	0.999
C	-3.410	1.161	1.014	C	-3.432	1.174	0.999
C	-0.699	-3.534	1.014	C	-0.699	-3.560	0.999
C	0.699	-3.534	1.014	C	0.699	-3.560	0.999
C	2.926	3.349	0.049	C	2.966	3.372	0.049
C	-0.726	-1.202	2.061	C	-0.728	-1.203	2.010
C	4.364	0.860	0.049	C	4.404	0.883	0.049
C	-2.926	3.349	0.049	C	-2.966	3.372	0.049
C	-4.364	0.860	0.049	C	-4.404	0.883	0.049
C	-1.437	-4.209	0.049	C	-1.437	-4.255	0.049
C	1.437	-4.209	0.049	C	1.437	-4.255	0.049
C	3.888	3.049	-0.906	C	3.945	3.083	-0.891
C	4.585	1.842	-0.906	C	4.642	1.875	-0.891
C	0.697	-4.892	-0.906	C	0.697	-4.958	-0.891

C	-0.697	-4.892	-0.906	C	-0.697	-4.958	-0.891
C	-3.888	3.049	-0.906	C	-3.945	3.083	-0.891
C	0.726	-1.202	2.061	C	0.728	-1.203	2.010
C	-4.585	1.842	-0.906	C	-4.642	1.875	-0.891
C	5.540	1.851	-2.050	C	5.618	1.896	-2.017
C	4.373	3.872	-2.050	C	4.452	3.917	-2.017
C	1.167	-5.723	-2.050	C	1.167	-5.814	-2.017
C	-1.167	-5.723	-2.050	C	-1.167	-5.814	-2.017
C	-5.540	1.851	-2.050	C	-5.618	1.896	-2.017
C	-4.373	3.872	-2.050	C	-4.452	3.917	-2.017
C	1.405	-0.028	2.061	C	1.406	-0.030	2.010
C	-2.423	1.399	3.258	C	-2.388	1.379	3.228
C	0.000	-2.797	3.258	C	0.000	-2.757	3.228
C	2.423	1.399	3.258	C	2.388	1.379	3.228
C	0.678	1.230	2.061	C	0.677	1.232	2.010
C	-0.678	1.230	2.061	C	-0.677	1.232	2.010
C	-1.143	-2.712	2.168	C	-1.143	-2.716	2.133
C	-2.920	0.367	2.168	C	-2.924	0.368	2.133
C	-1.777	2.346	2.168	C	-1.781	2.348	2.133
N	-5.344	3.085	-2.669	N	-5.434	3.137	-2.627
N	5.344	3.085	-2.669	N	5.434	3.137	-2.627
N	0.000	-6.170	-2.669	N	0.000	-6.274	-2.627
O	6.325	0.999	-2.393	O	6.410	1.048	-2.356
O	4.028	4.978	-2.393	O	4.113	5.027	-2.356
O	2.297	-5.977	-2.393	O	2.297	-6.075	-2.356
O	-2.297	-5.977	-2.393	O	-2.297	-6.075	-2.356
O	-6.325	0.999	-2.393	O	-6.410	1.048	-2.356
O	-4.028	4.978	-2.393	O	-4.113	5.027	-2.356
H	-2.165	-2.866	2.514	H	-2.165	-2.864	2.484
H	2.392	4.293	0.035	H	2.433	4.317	0.035
H	-2.392	4.293	0.035	H	-2.433	4.317	0.035
H	-4.914	-0.075	0.035	H	-4.955	-0.052	0.035
H	-3.274	1.890	3.767	H	-3.225	1.862	3.770
H	-1.751	1.011	4.013	H	-1.699	0.981	3.962
H	0.000	-3.781	3.767	H	0.000	-3.724	3.770
H	0.000	-2.021	4.013	H	0.000	-1.962	3.962
H	-3.564	-0.442	2.514	H	-3.563	-0.442	2.484
H	3.274	1.890	3.767	H	3.225	1.862	3.770
H	1.751	1.011	4.013	H	1.699	0.981	3.962
H	-1.399	3.308	2.514	H	-1.398	3.307	2.484
H	1.399	3.308	2.514	H	1.398	3.307	2.484
H	3.564	-0.442	2.514	H	3.563	-0.442	2.484
H	2.165	-2.866	2.514	H	2.165	-2.864	2.484
H	-2.522	-4.219	0.035	H	-2.522	-4.265	0.035

H	2.522	-4.219	0.035	H	2.522	-4.265	0.035
H	4.914	-0.075	0.035	H	4.955	-0.052	0.035
H	-5.854	3.380	-3.488	H	-5.960	3.441	-3.433
H	5.854	3.380	-3.488	H	5.960	3.441	-3.433
H	0.000	-6.760	-3.488	H	0.000	-6.881	-3.433

28°

C	-1.407	-0.031	1.948
C	1.784	2.352	2.091
C	2.929	0.369	2.091
C	1.144	-2.721	2.091
C	2.759	2.400	0.980
C	3.458	1.190	0.980
C	-2.759	2.400	0.980
C	-3.458	1.190	0.980
C	-0.699	-3.589	0.980
C	0.699	-3.589	0.980
C	3.013	3.399	0.048
C	-0.731	-1.203	1.948
C	4.450	0.910	0.048
C	-3.013	3.399	0.048
C	-4.450	0.910	0.048
C	-1.437	-4.309	0.048
C	1.437	-4.309	0.048
C	4.012	3.122	-0.874
C	4.709	1.914	-0.874
C	0.697	-5.035	-0.874
C	-0.697	-5.035	-0.874
C	-4.012	3.122	-0.874
C	0.731	-1.203	1.948
C	-4.709	1.914	-0.874
C	5.710	1.949	-1.978
C	4.543	3.970	-1.978
C	1.167	-5.919	-1.978
C	-1.167	-5.919	-1.978
C	-5.710	1.949	-1.978
C	-4.543	3.970	-1.978
C	1.407	-0.031	1.948
C	-2.347	1.355	3.190
C	0.000	-2.710	3.190
C	2.347	1.355	3.190
C	0.676	1.234	1.948
C	-0.676	1.234	1.948
C	-1.144	-2.721	2.091

C	-2.929	0.369	2.091
C	-1.784	2.352	2.091
N	-5.538	3.197	-2.576
N	5.538	3.197	-2.576
N	0.000	-6.395	-2.576
O	6.508	1.105	-2.310
O	4.211	5.084	-2.310
O	2.297	-6.189	-2.310
O	-2.297	-6.189	-2.310
O	-6.508	1.105	-2.310
O	-4.211	5.084	-2.310
H	-2.164	-2.862	2.448
H	2.479	4.343	0.034
H	-2.479	4.343	0.034
H	-5.001	-0.025	0.034
H	-3.167	1.829	3.769
H	-1.640	0.947	3.899
H	0.000	-3.657	3.769
H	0.000	-1.893	3.899
H	-3.561	-0.443	2.448
H	3.167	1.829	3.769
H	1.640	0.947	3.899
H	-1.397	3.306	2.448
H	1.397	3.306	2.448
H	3.561	-0.443	2.448
H	2.164	-2.862	2.448
H	-2.522	-4.319	0.034
H	2.522	-4.319	0.034
H	5.001	-0.025	0.034
H	-6.081	3.511	-3.366
H	6.081	3.511	-3.366
H	0.000	-7.022	-3.366

Table S3. Isotropic GIAO magnetic shielding tensors (ppm), averages and changes as a function of basket cavity size.

Hydrogen		**Arm 1**	**Arm 2**	**Arm 3**	**Average δ**	**Δδ**
HA	*st*	27.395	27.395	27.394	27.394	0.000
	2°	27.384	27.385	27.383	27.384	0.010
	4°	27.382	27.382	27.382	27.382	0.012
	6°	27.381	27.381	27.382	27.381	0.013
	8°	27.383	27.382	27.383	27.383	0.012
	10°	27.385	27.385	27.386	27.385	0.009
	12°	27.389	27.389	27.389	27.389	0.005

	14°	27.396	27.396	27.397	27.396	-0.002
	16°	27.408	27.406	27.405	27.406	-0.012
	18°	27.417	27.417	27.417	27.417	-0.022
	20°	27.434	27.433	27.433	27.433	-0.039
	22°	27.451	27.451	27.451	27.451	-0.057
	24°	27.474	27.474	27.475	27.474	-0.080
	26°	27.493	27.493	27.493	27.493	-0.099
	28°	27.518	27.518	27.516	27.517	-0.123
HB	*st*	29.187	29.187	29.185	29.187	0.000
	2°	29.088	29.088	29.090	29.089	0.098
	4°	29.040	29.040	29.039	29.039	0.147
	6°	28.976	28.976	28.976	28.976	0.210
	8°	28.908	28.908	28.905	28.907	0.280
	10°	28.830	28.830	28.831	28.830	0.357
	12°	28.769	28.769	28.767	28.768	0.419
	14°	28.684	28.684	28.684	28.684	0.503
	16°	28.592	28.592	28.592	28.592	0.595
	18°	28.495	28.495	28.494	28.495	0.692
	20°	28.383	28.383	28.383	28.383	0.804
	22°	28.272	28.272	28.272	28.272	0.914
	24°	28.161	28.161	28.162	28.161	1.025
	26°	28.056	28.056	28.056	28.056	1.130
	28°	27.928	27.928	27.929	27.929	1.258
HC	*st*	29.241	29.241	29.242	29.242	0.000
	2°	29.301	29.301	29.302	29.301	-0.059
	4°	29.320	29.320	29.319	29.319	-0.078
	6°	29.334	29.334	29.335	29.334	-0.093
	8°	29.340	29.340	29.341	29.340	-0.098
	10°	29.334	29.334	29.334	29.334	-0.092
	12°	29.320	29.320	29.321	29.320	-0.079
	14°	29.290	29.290	29.290	29.290	-0.049
	16°	29.243	29.243	29.245	29.243	-0.002
	18°	29.179	29.179	29.178	29.178	0.063
	20°	29.092	29.092	29.091	29.092	0.150
	22°	28.989	28.989	28.989	28.989	0.252
	24°	28.883	28.883	28.882	28.883	0.359
	26°	28.765	28.765	28.764	28.765	0.477
	28°	28.611	28.611	28.610	28.611	0.631
HD	*st*	27.395	27.395	27.394	27.394	0.000
	2°	27.385	27.384	27.383	27.384	0.010
	4°	27.382	27.382	27.382	27.382	0.012
	6°	27.381	27.381	27.382	27.381	0.013

8°	27.382	27.383	27.383	27.383	0.012
10°	27.385	27.385	27.386	27.385	0.009
12°	27.389	27.389	27.389	27.389	0.005
14°	27.396	27.396	27.397	27.396	-0.002
16°	27.406	27.408	27.405	27.406	-0.012
18°	27.417	27.417	27.417	27.417	-0.022
20°	27.433	27.434	27.433	27.433	-0.039
22°	27.451	27.451	27.451	27.451	-0.057
24°	27.474	27.474	27.475	27.474	-0.080
26°	27.493	27.493	27.493	27.493	-0.099
28°	27.518	27.518	27.516	27.517	-0.123

Table S4. Coupling constant data as a function of basket cavity expansion.

	J(A,B)	**J(A,C)**	**J(B,C)**	**J(B,D)**	**J(C,D)**
st	1.63	1.54	8.61	1.63	1.54
2°	1.82	1.36	8.43	1.82	1.36
4°	1.89	1.28	8.37	1.89	1.28
6°	1.98	1.19	8.29	1.98	1.19
8°	2.07	1.10	8.23	2.07	1.10
10°	2.15	1.01	8.20	2.15	1.01
12°	2.21	0.94	8.18	2.21	0.94
14°	2.29	0.86	8.20	2.29	0.86
16°	2.36	0.78	8.24	2.36	0.78
18°	2.43	0.70	8.35	2.43	0.70
20°	2.50	0.62	8.52	2.50	0.62
22°	2.57	0.55	8.76	2.57	0.55
24°	2.63	0.49	9.08	2.63	0.49
26°	2.69	0.43	9.45	2.69	0.43
28°	2.75	0.37	9.99	2.75	0.37

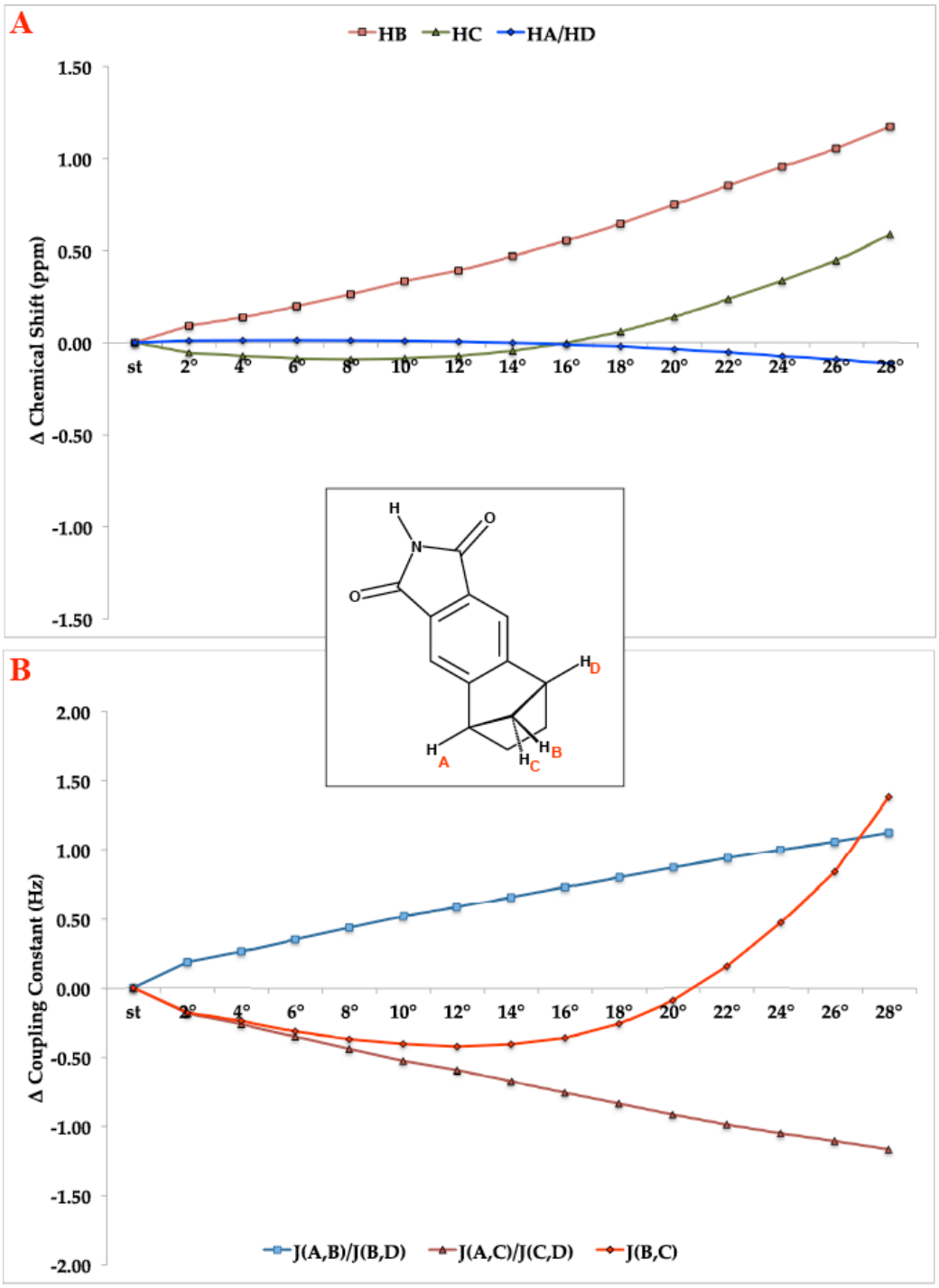


Figure S23. Change in chemical shifts (A) and coupling constants (B) as a function of increasing cavity size.