

Applied Microbiology and Biotechnology

Supporting Information

Polyhydroxyalkanoate-based 3-hydroxyoctanoic acid and it's derivatives as a platform of bioactive compounds

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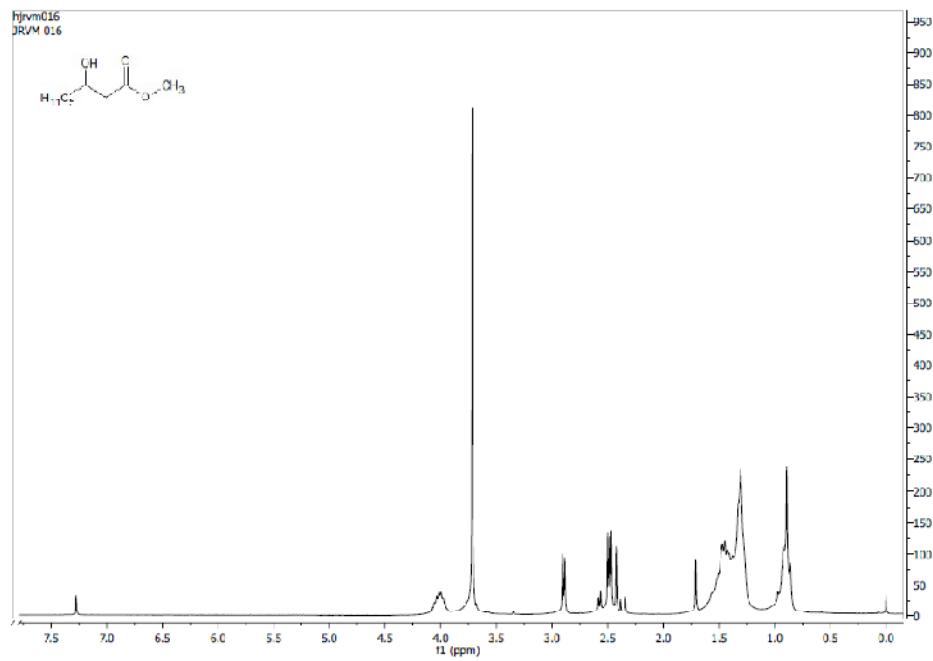
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Kevin.oconnor@ucd.ie; Tel.: + 353 1 716 1307; Fax: + 353 1 716 1183.

#Current address: Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences,
Niezapominajek 8, 30-239 Cracow, Poland

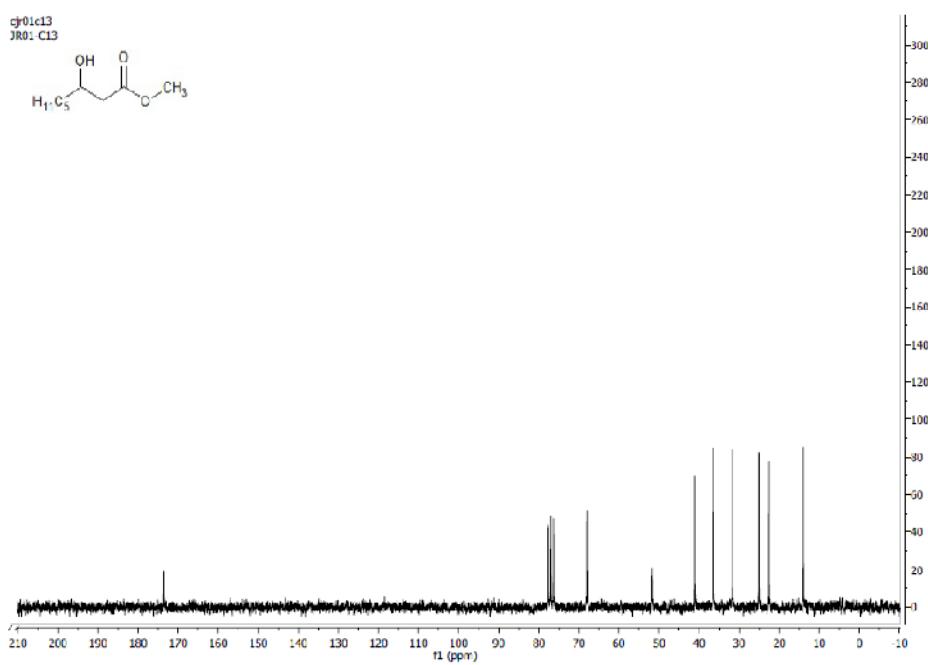
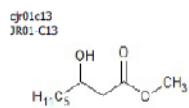
Scanned Spectra

Methyl-3-hydroxyoctanoate (1)

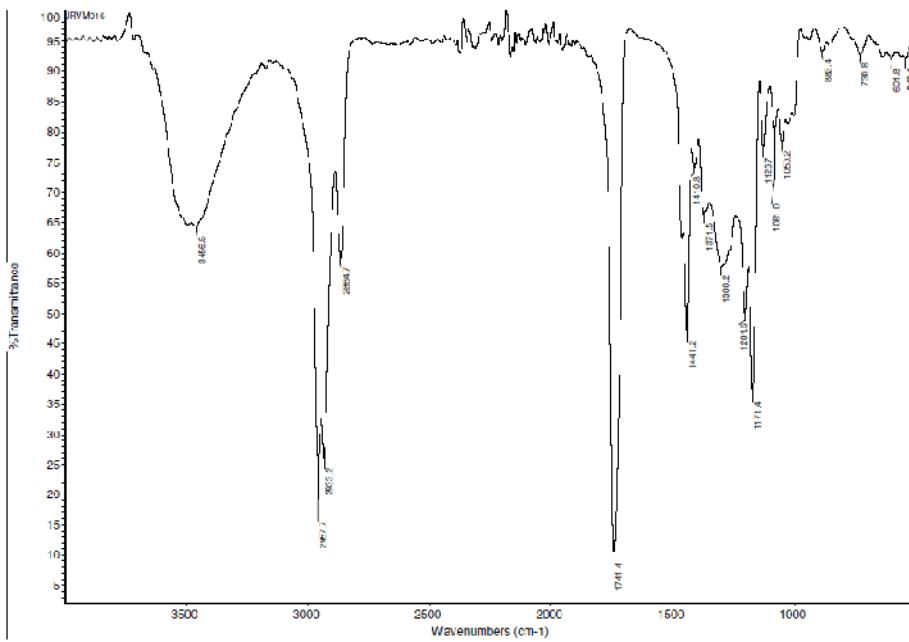
^1H NMR



¹³CNMR

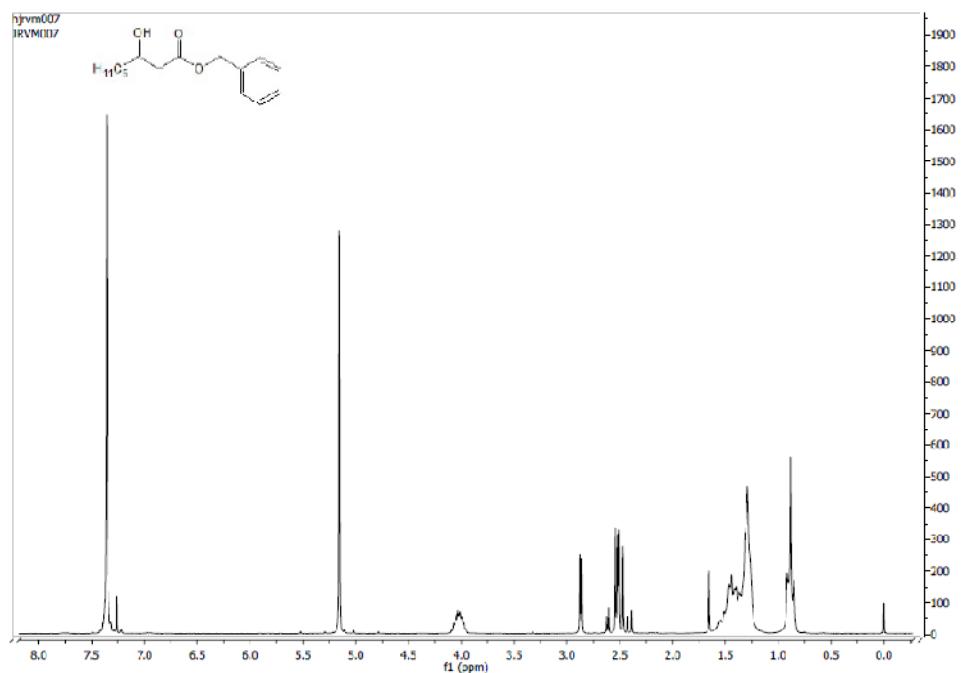


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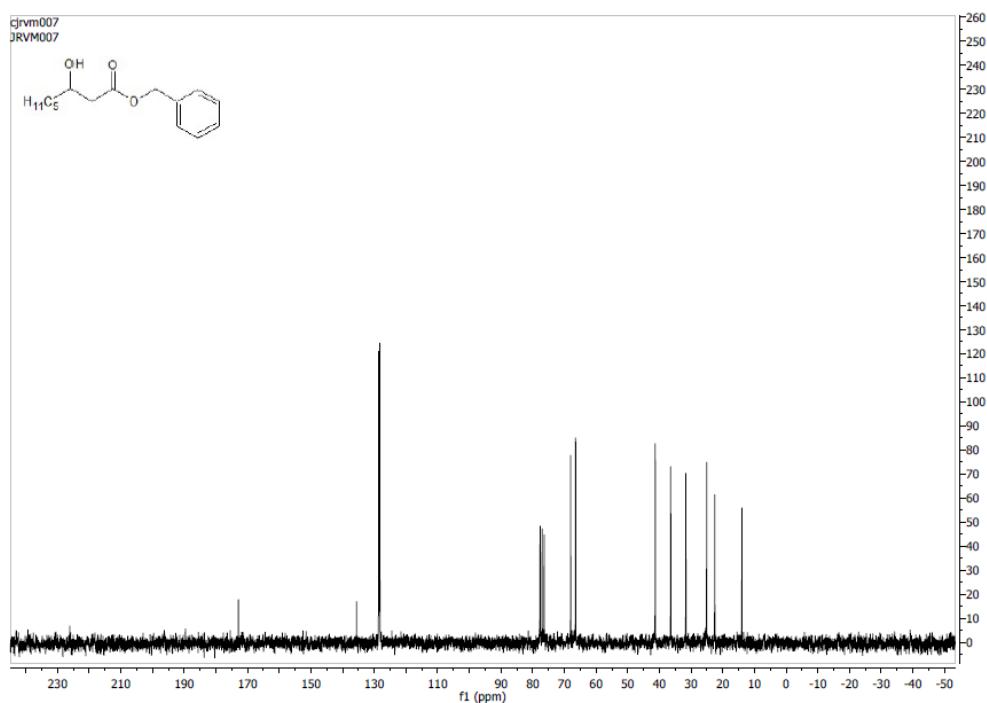


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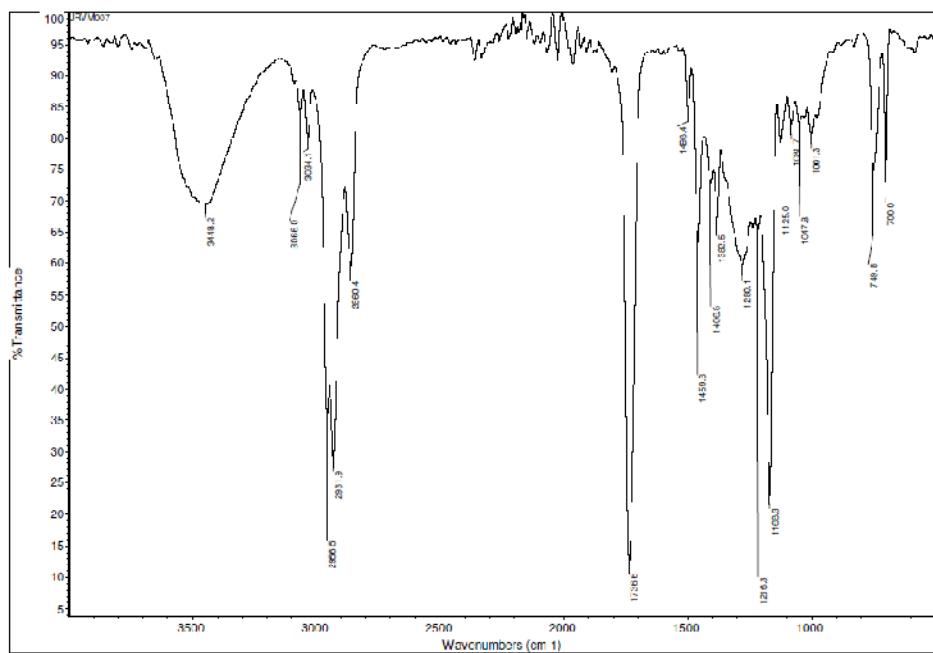
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^{13}C NMR

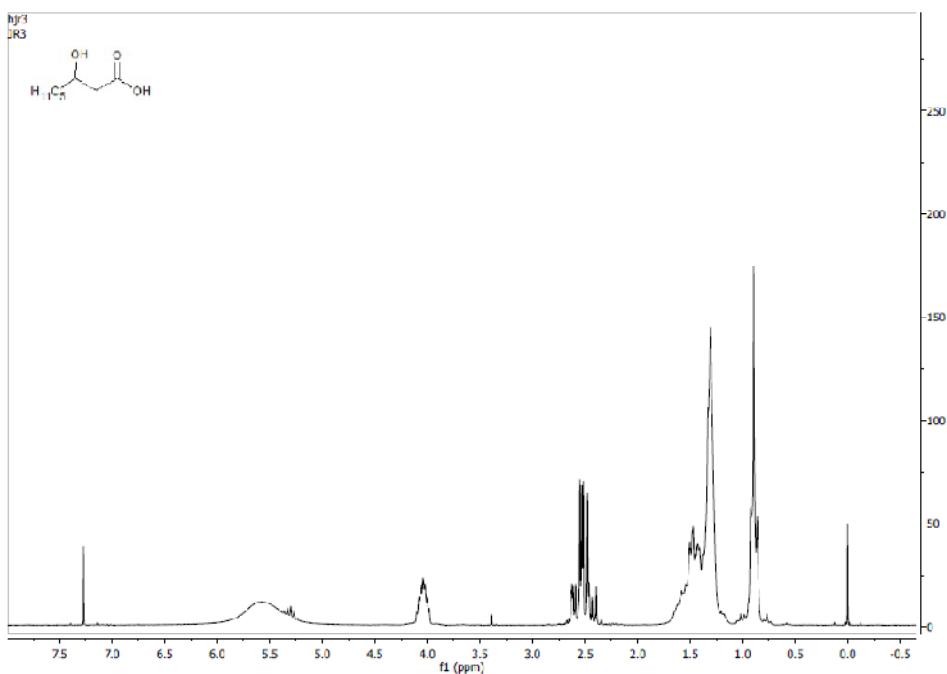


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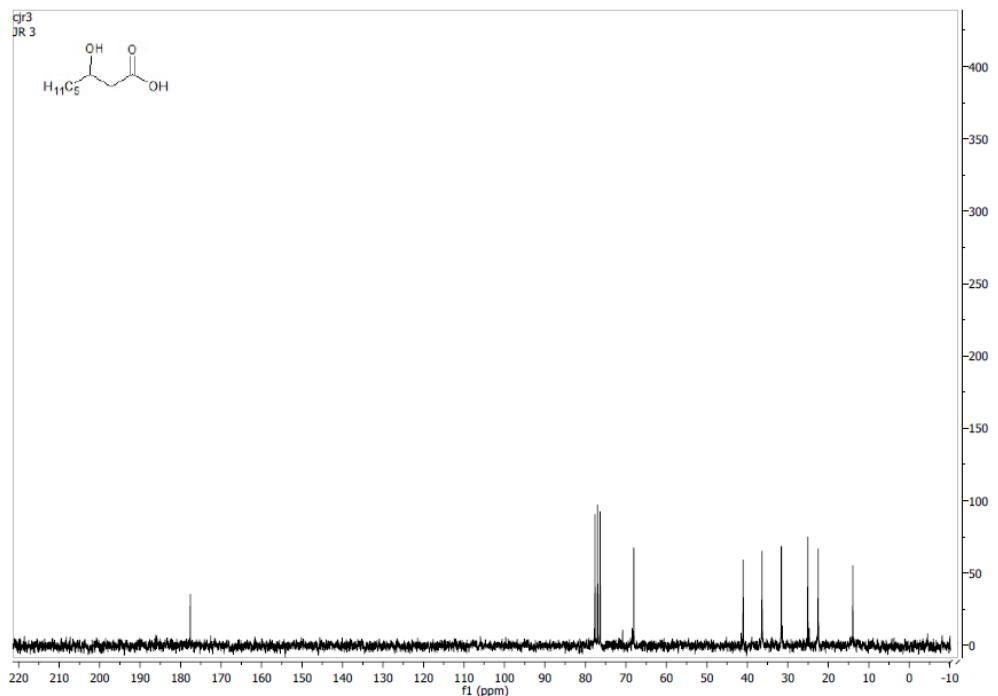


3-Hydroxyoctanoic acid (3)

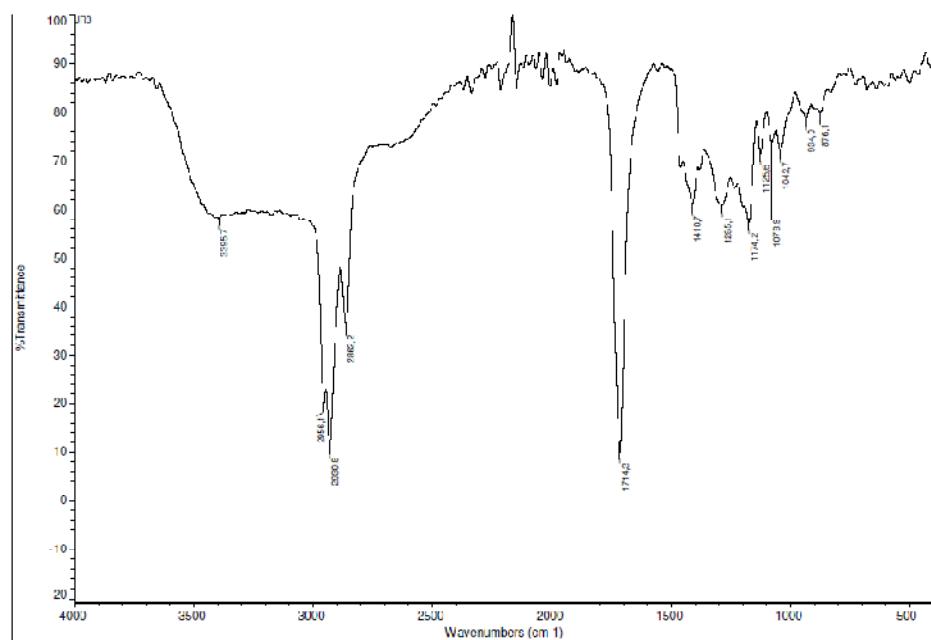
^1H NMR



¹³CNMR

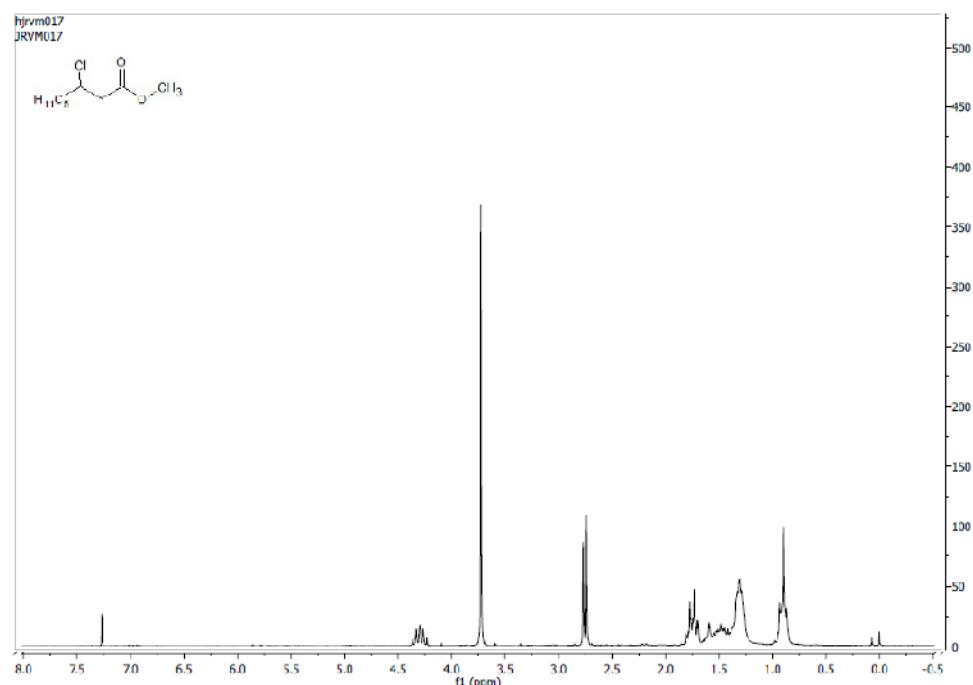


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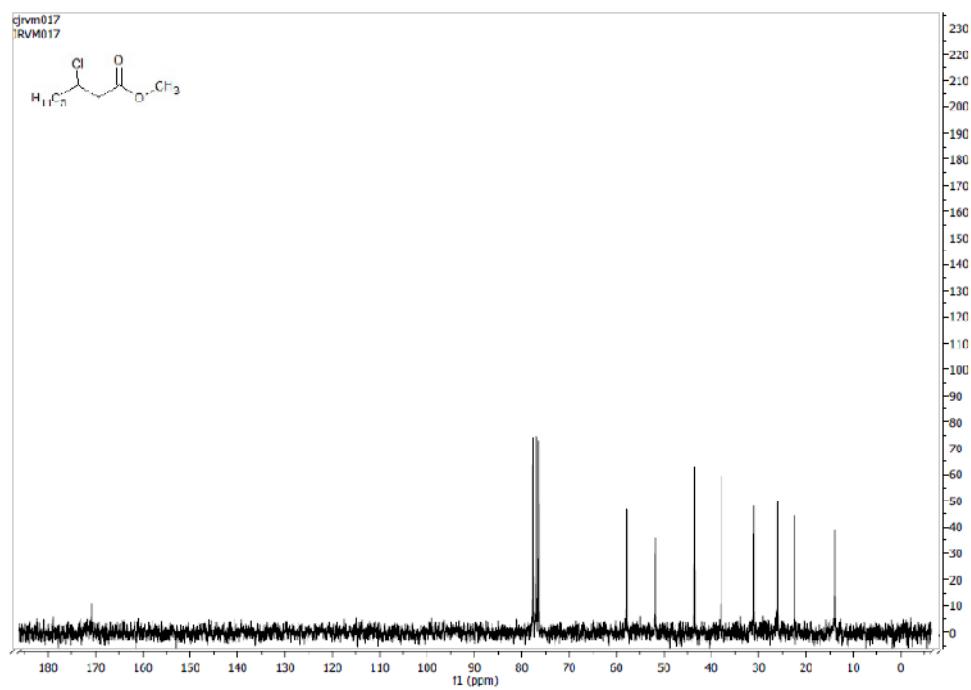


Methyl 3-chlorooctanoate (4)

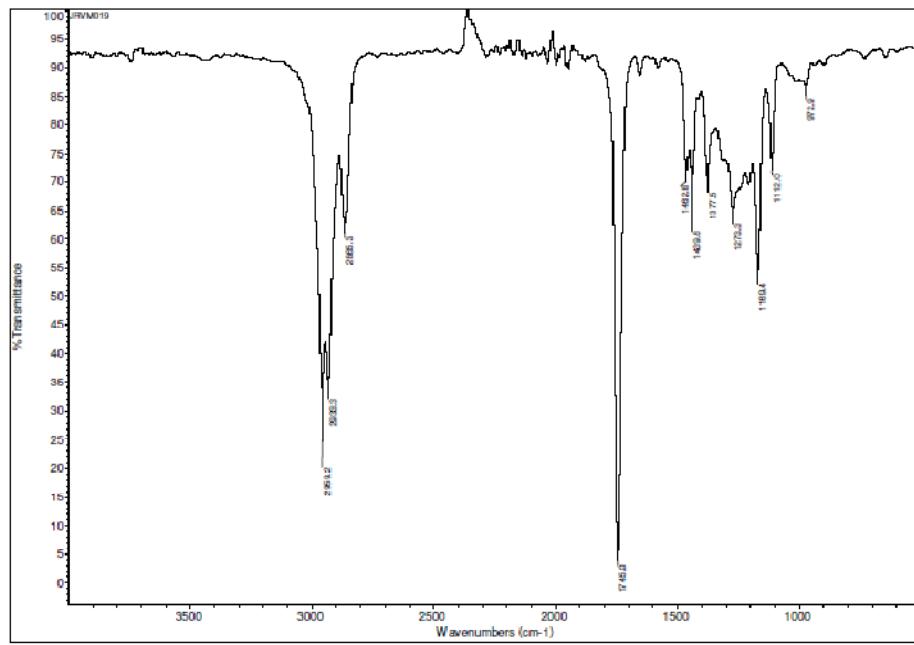
^1H NMR



¹³CNMR

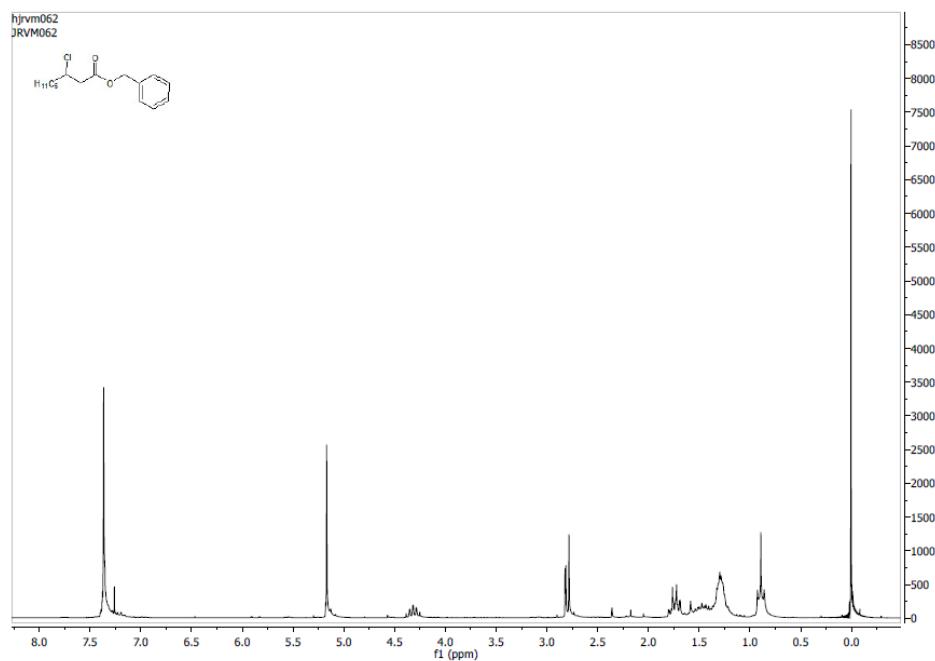


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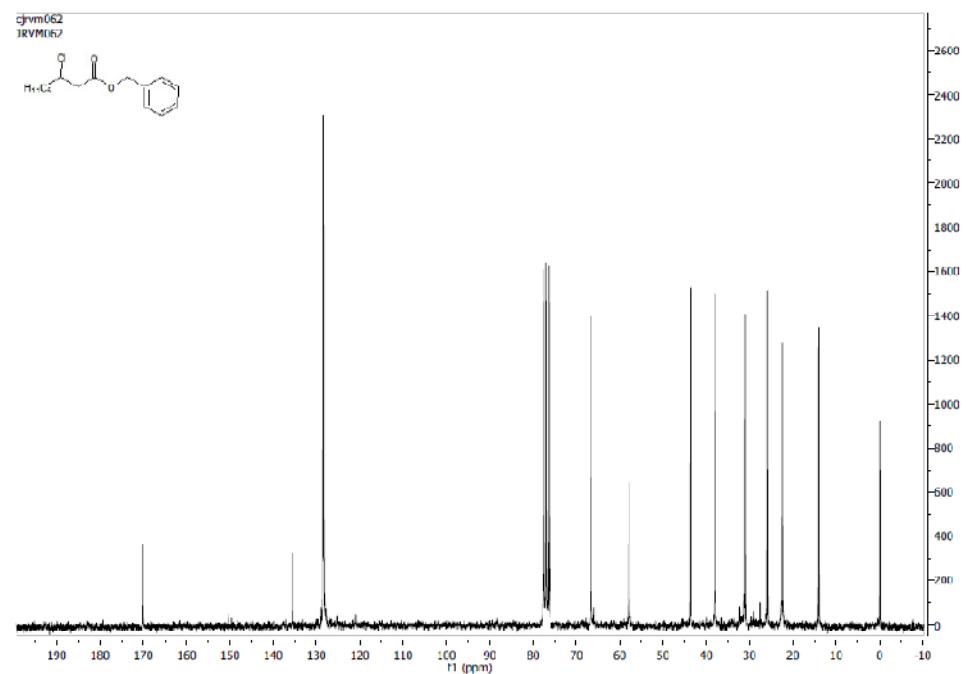


Benzyl 3-chlorooctanoate (5)

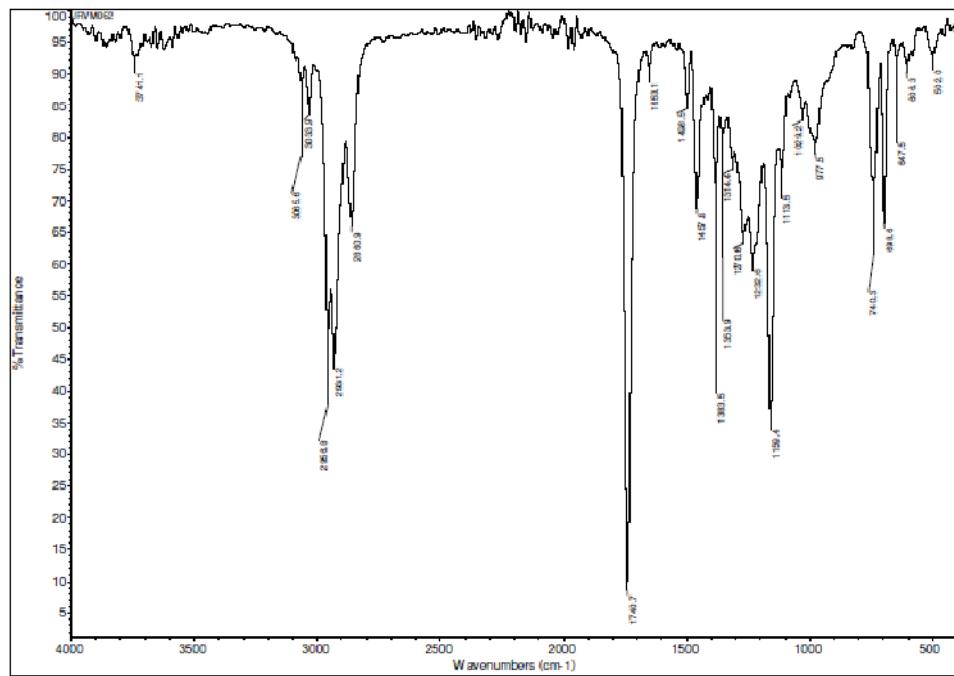
¹H NMR



¹³C NMR

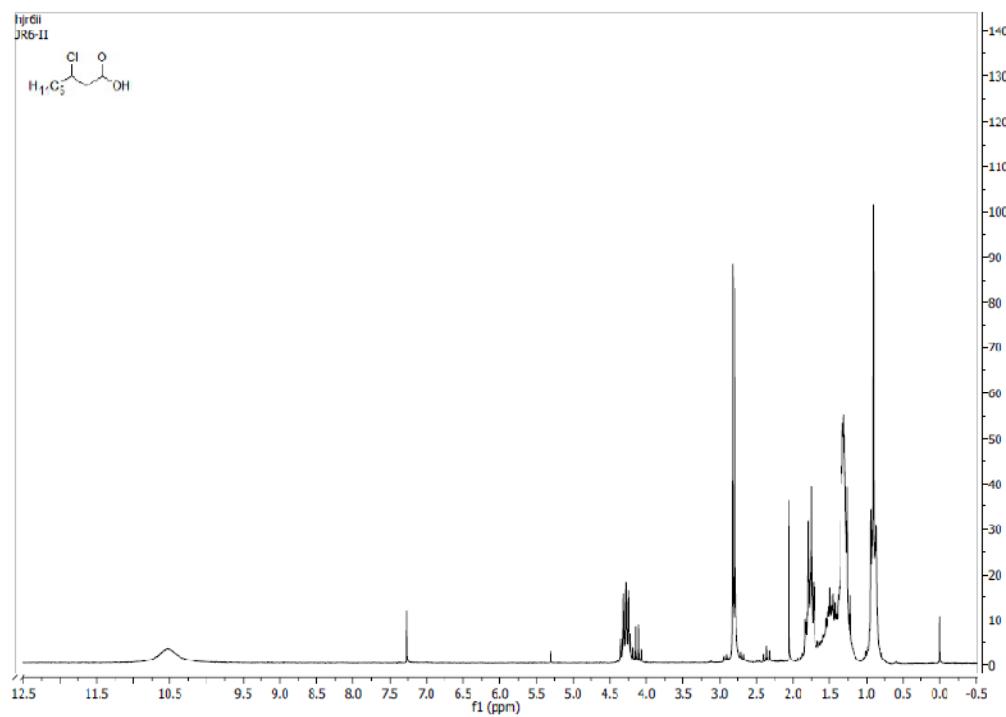


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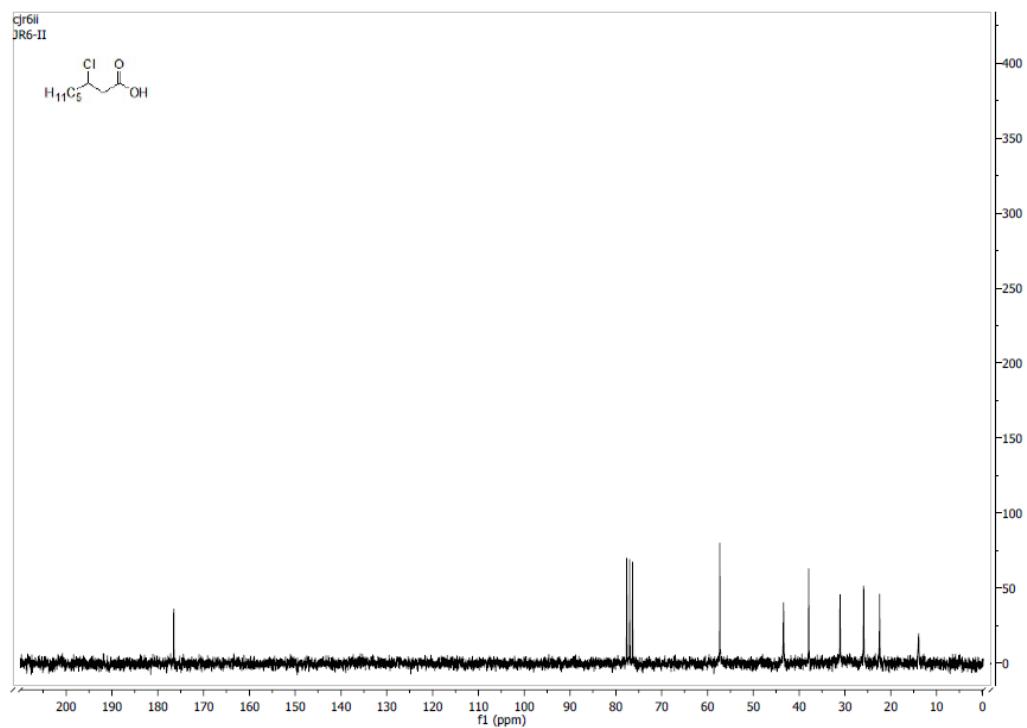


3-chlorooctanoic acid (6)

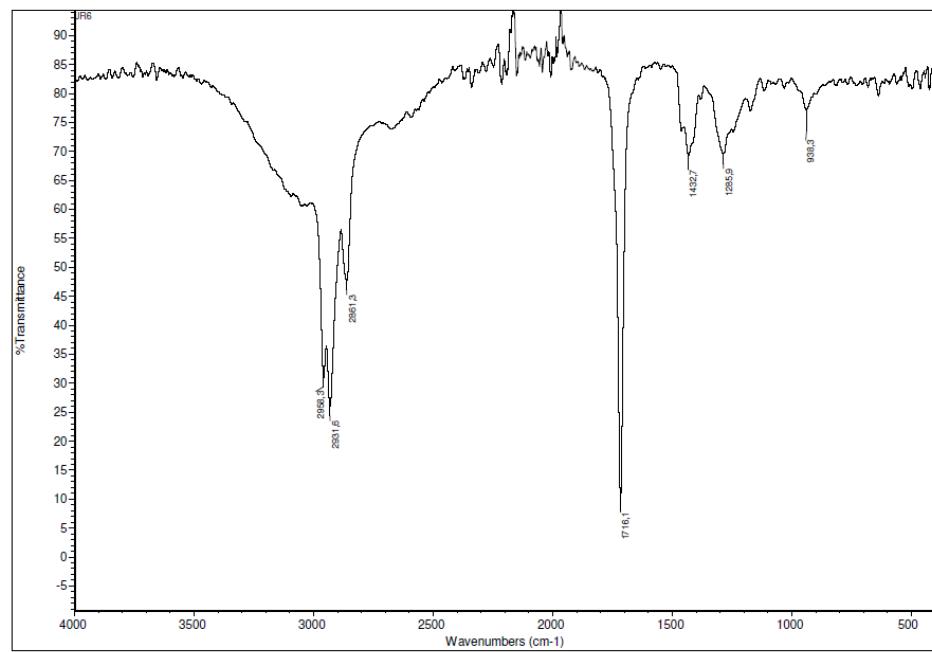
¹H NMR



¹³CNMR

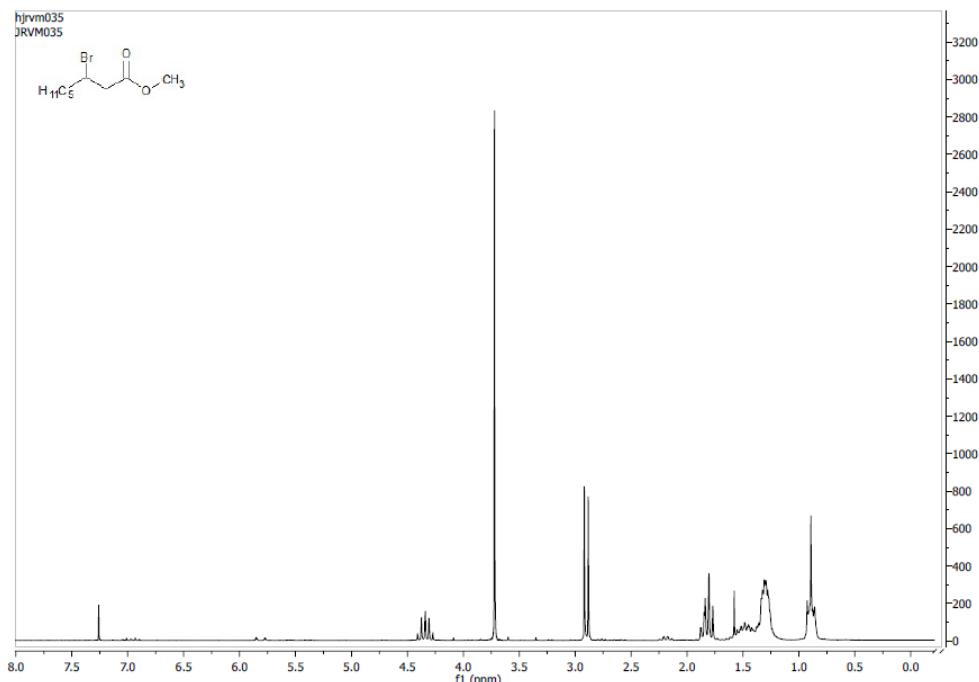


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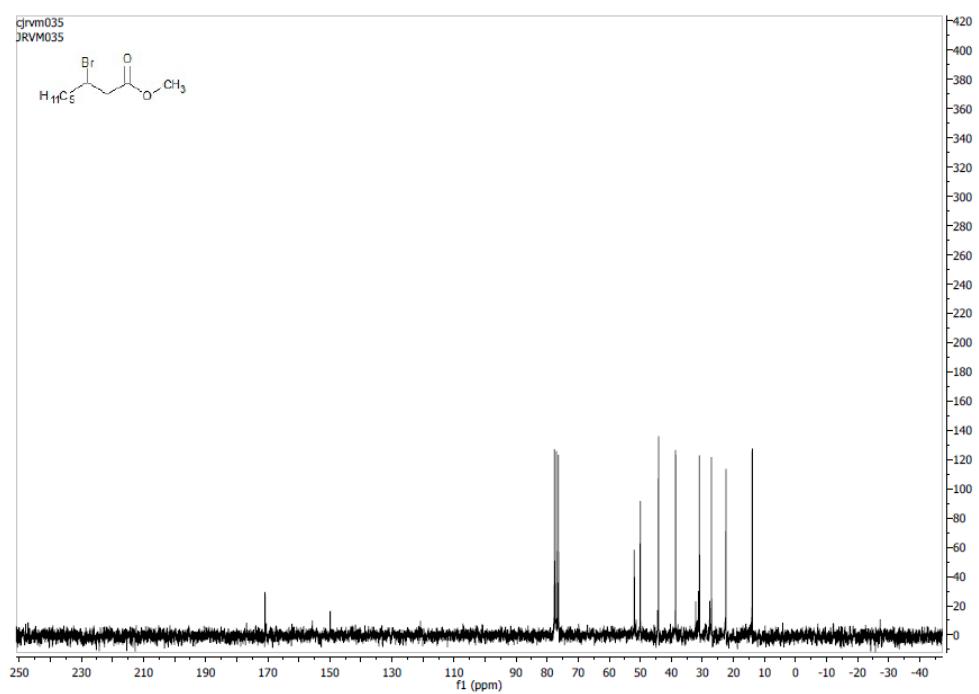


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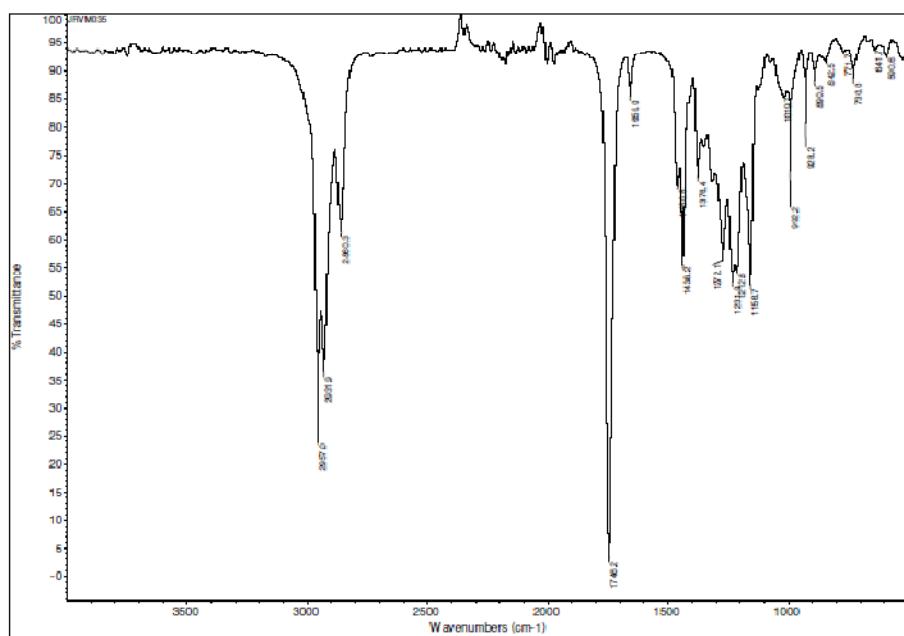
^1H NMR



^{13}C NMR

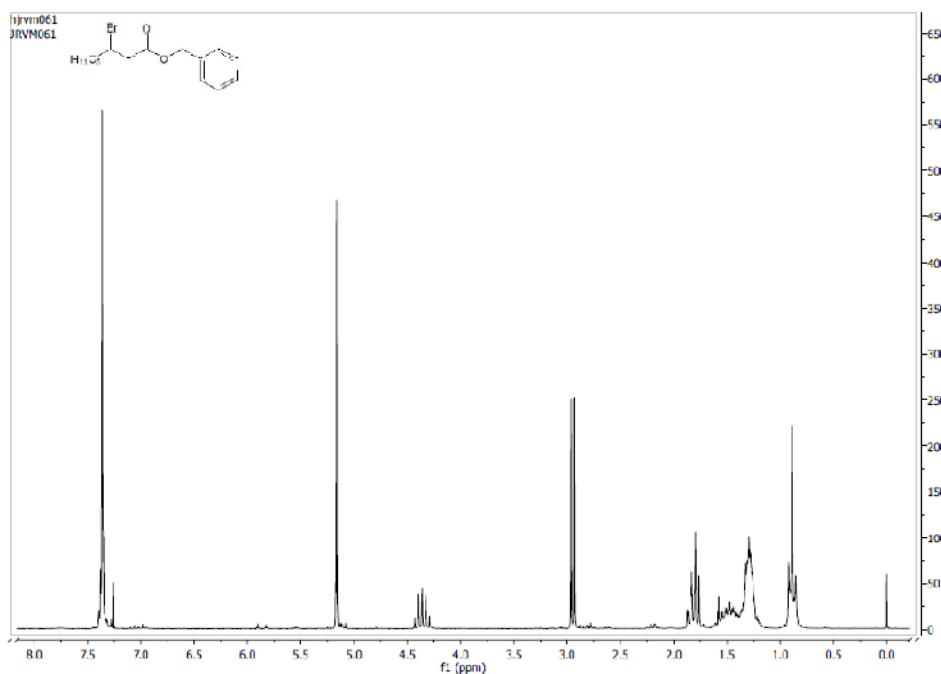


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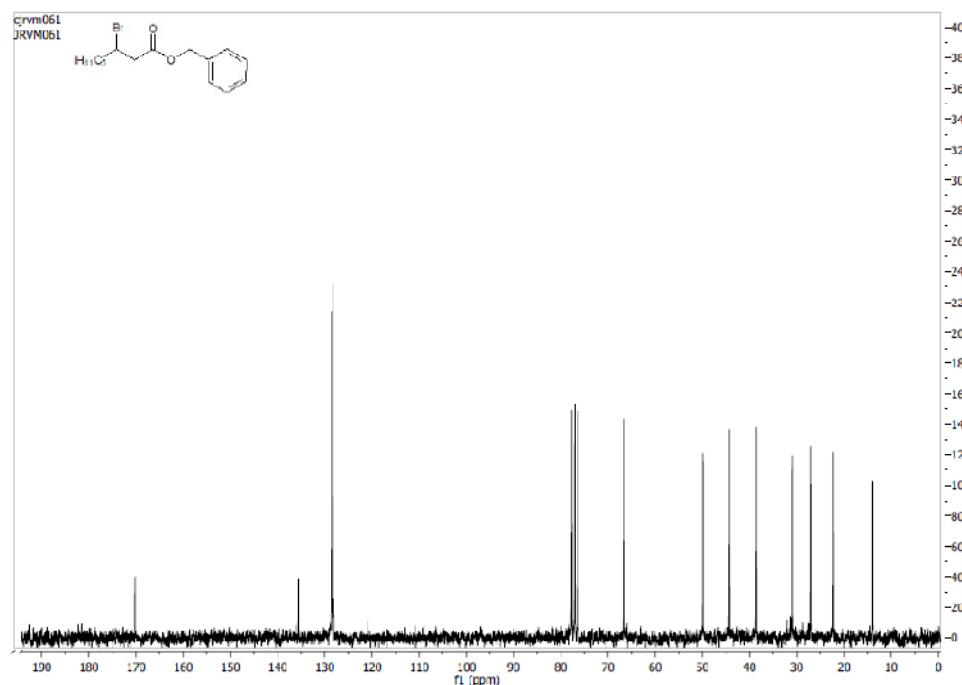


Benzyl 3-bromooctanoate (8)

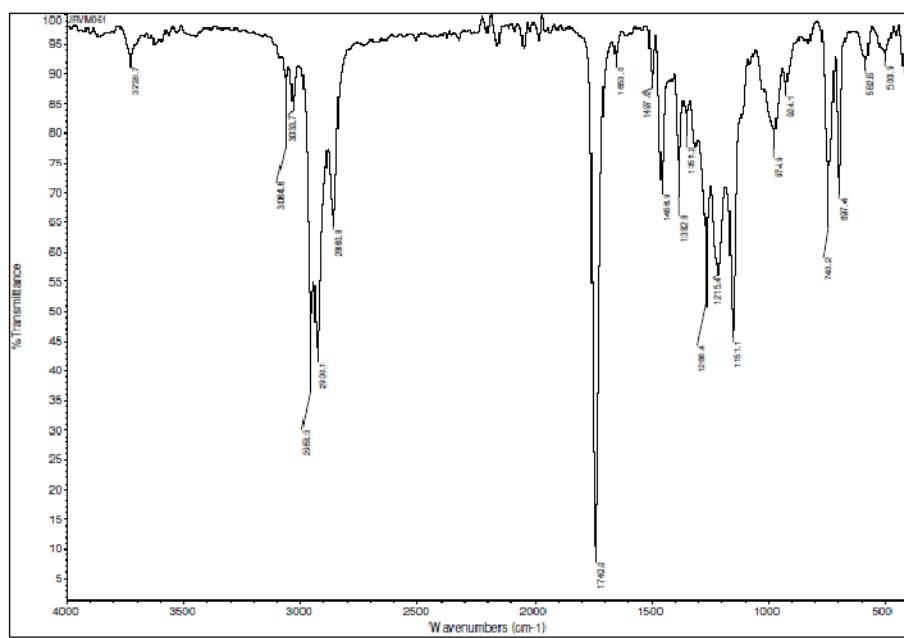
^1H NMR



¹³CNMR

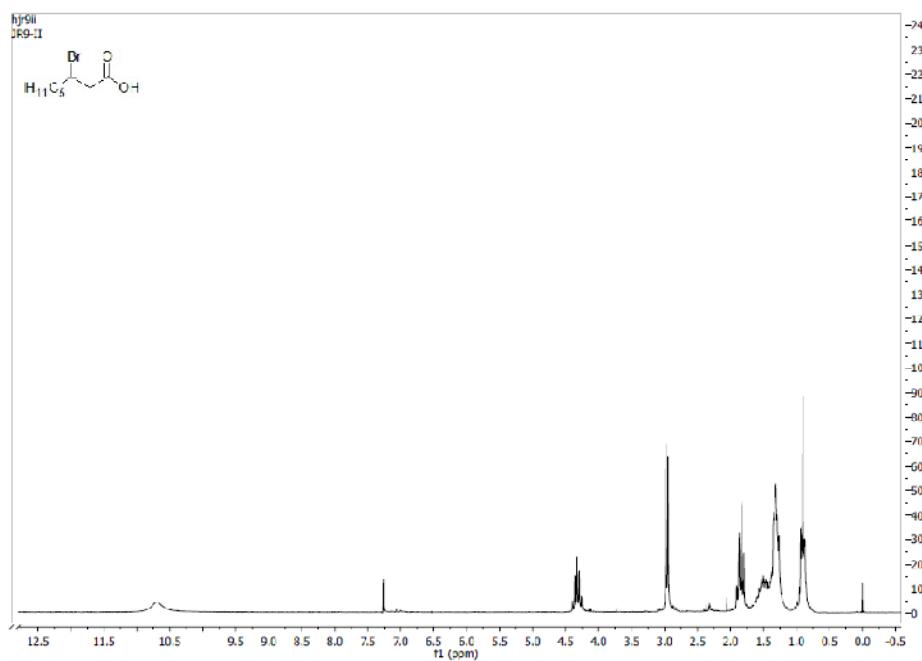


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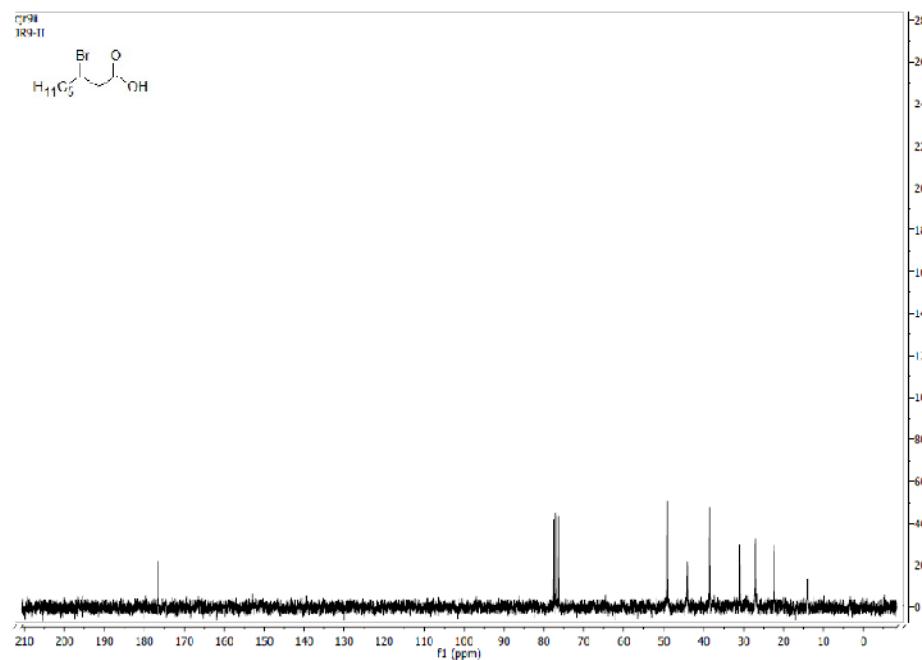


3-bromo octanoic acid (9)

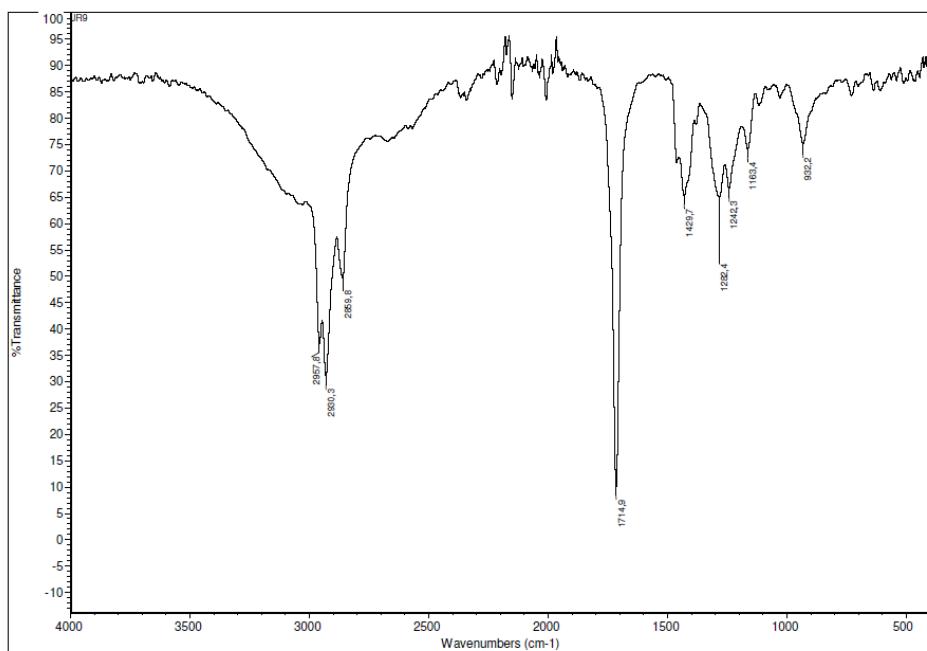
¹H NMR



¹³C NMR

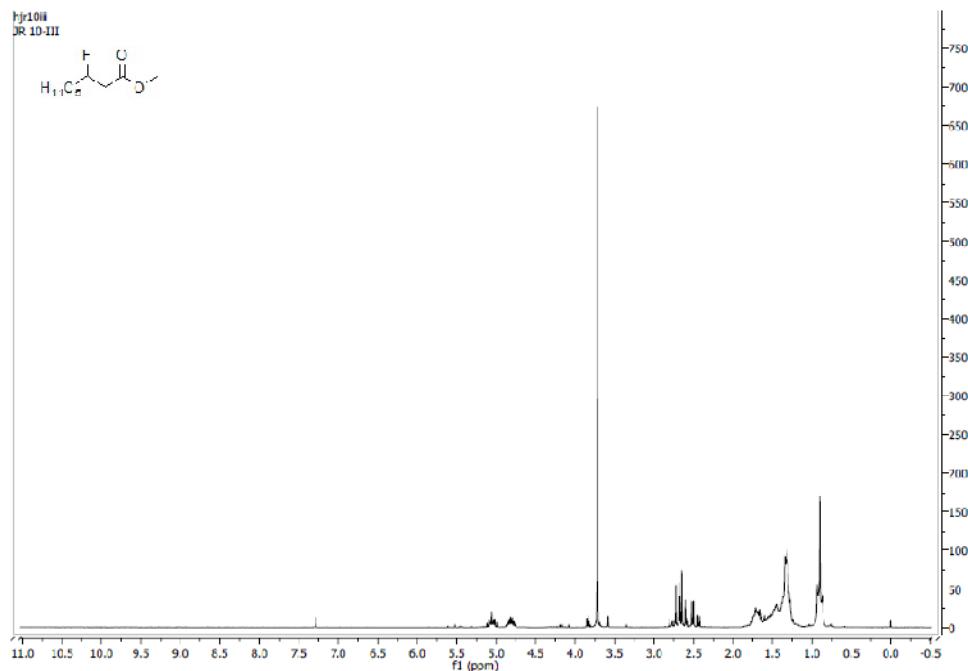


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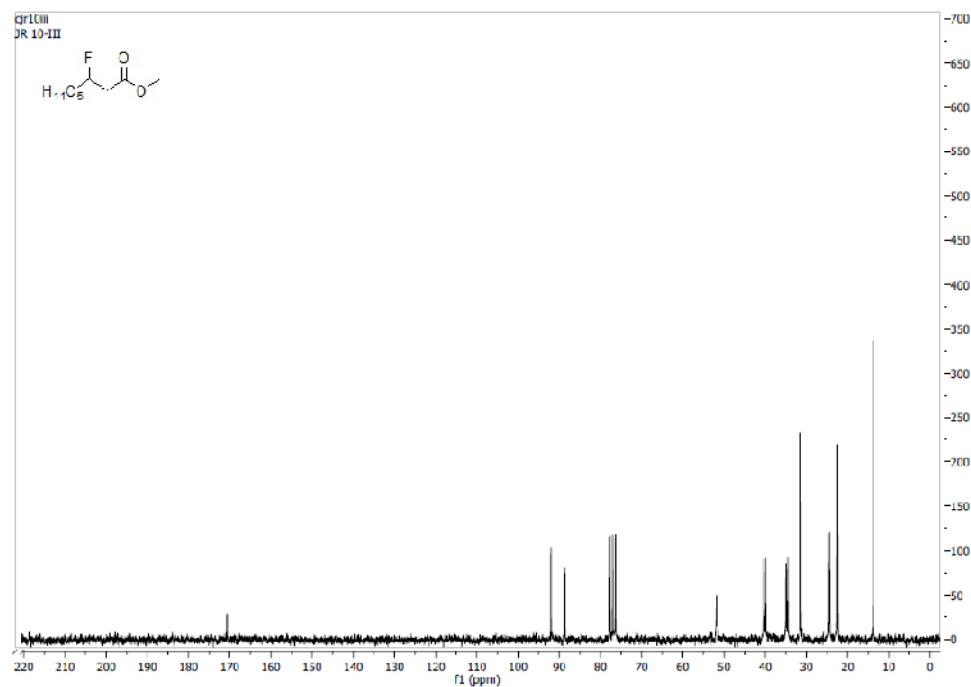


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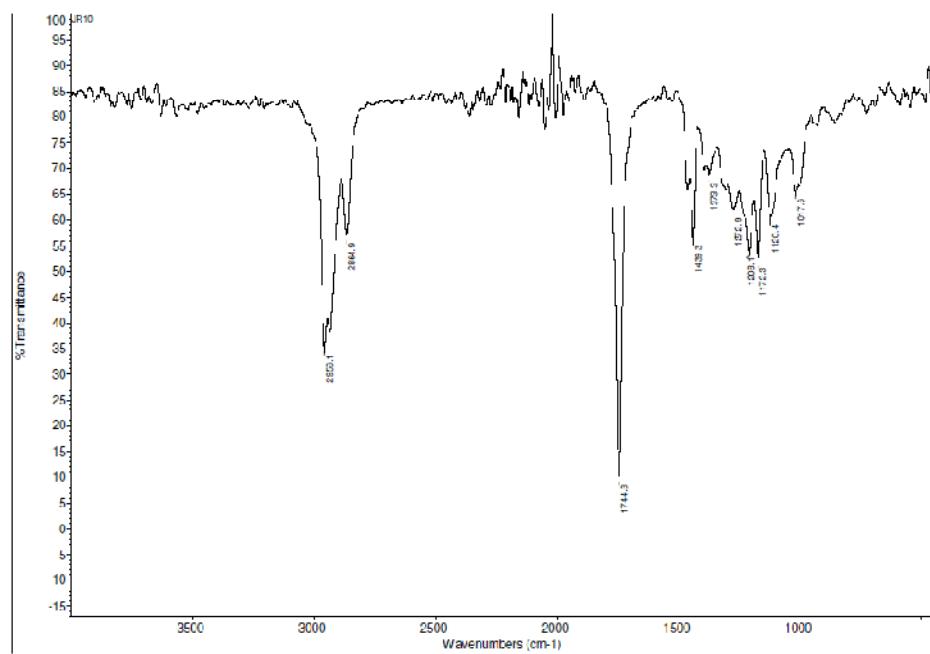
¹HNMR



¹³CNMR

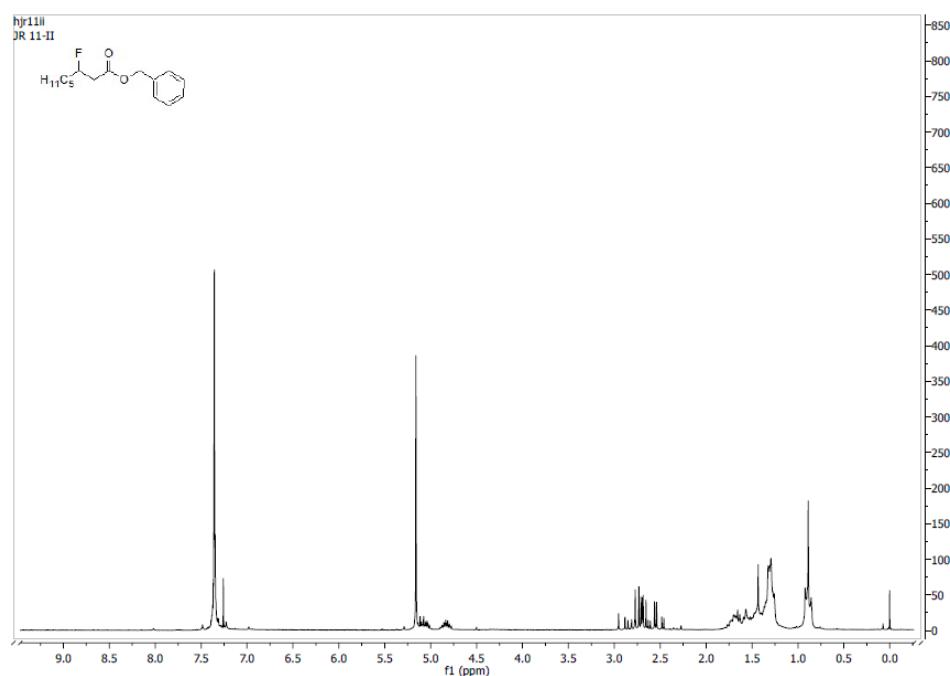


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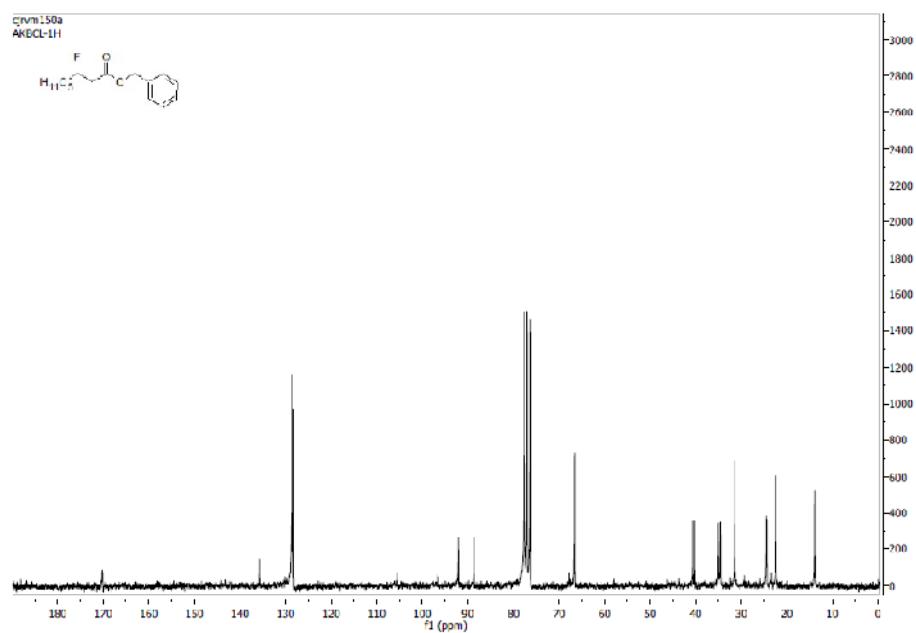


Benzyl-3-fluorooctanoate (11)

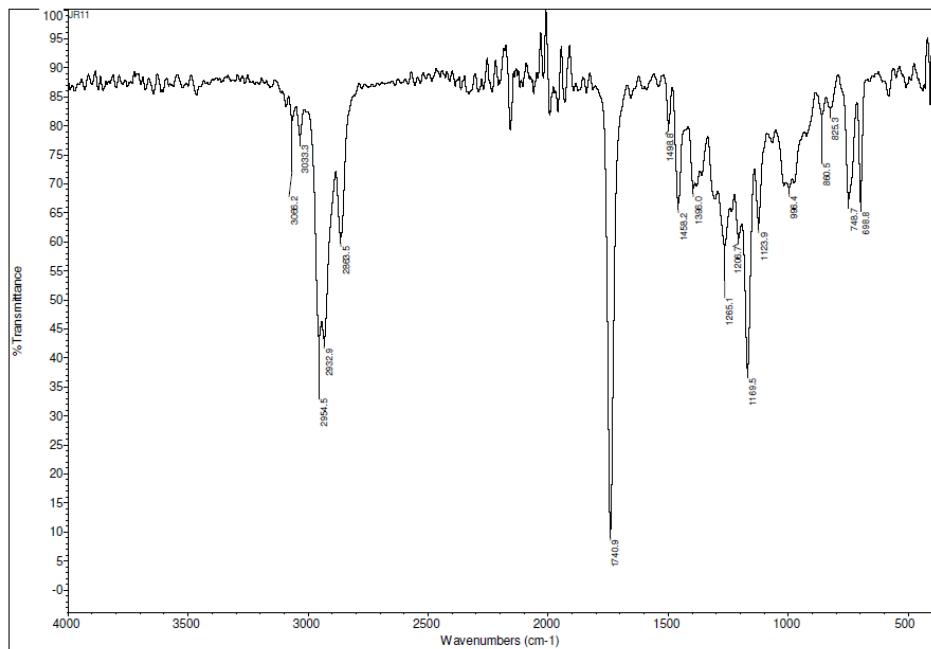
¹H NMR



¹³C NMR

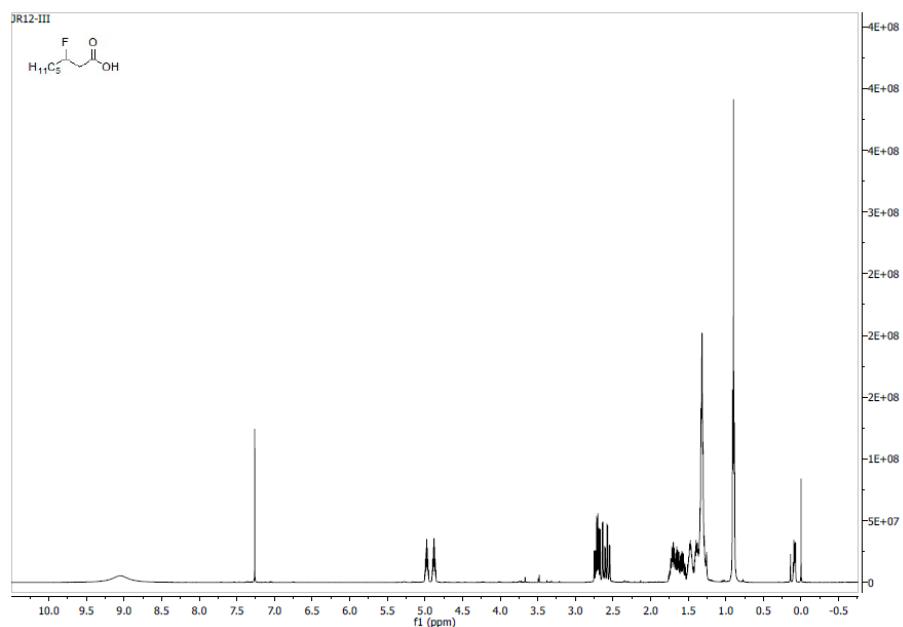


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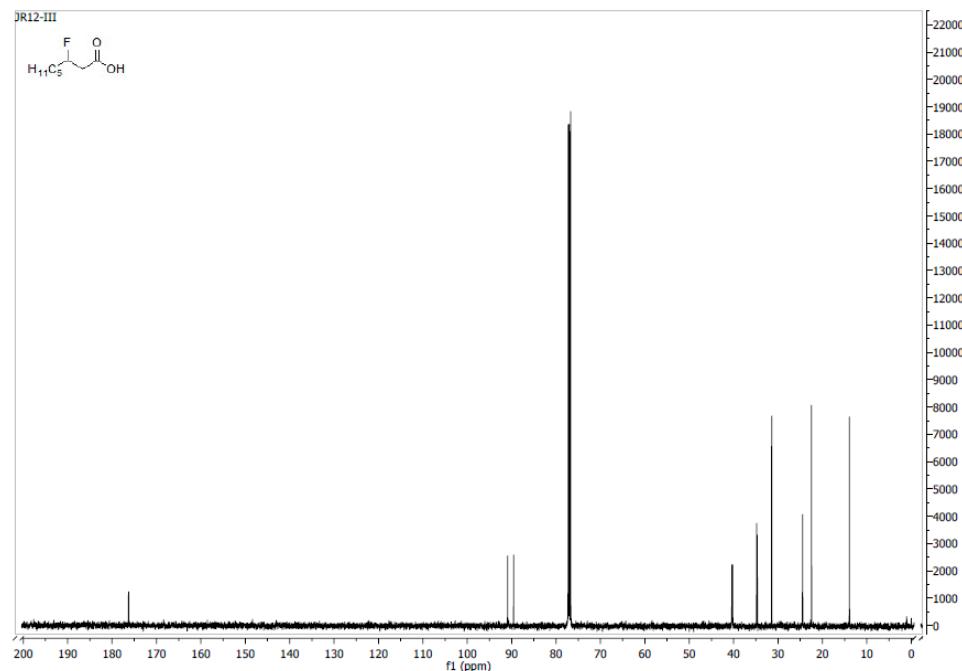


3-fluoroctanoic acid (12)

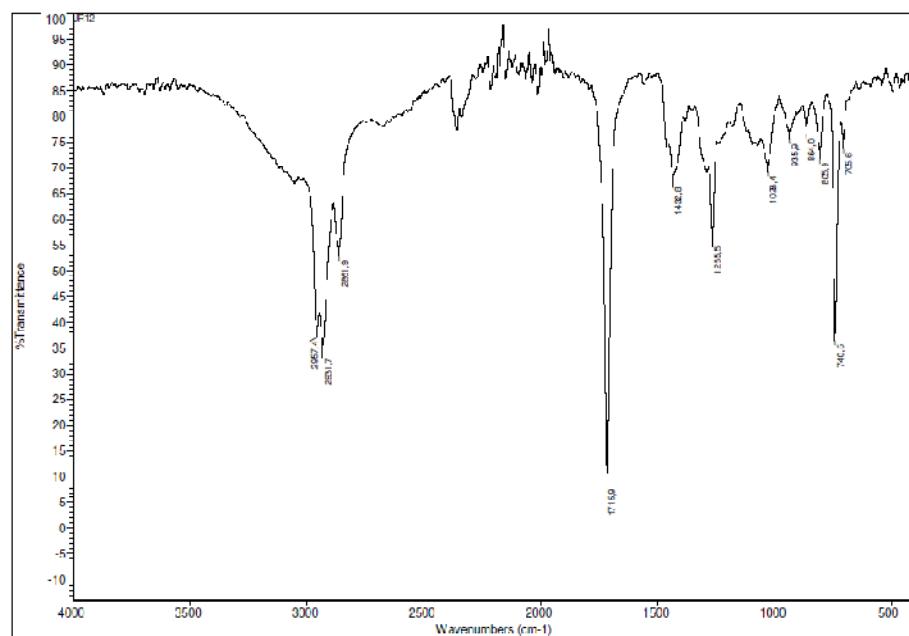
¹HNMR



¹³CNMR

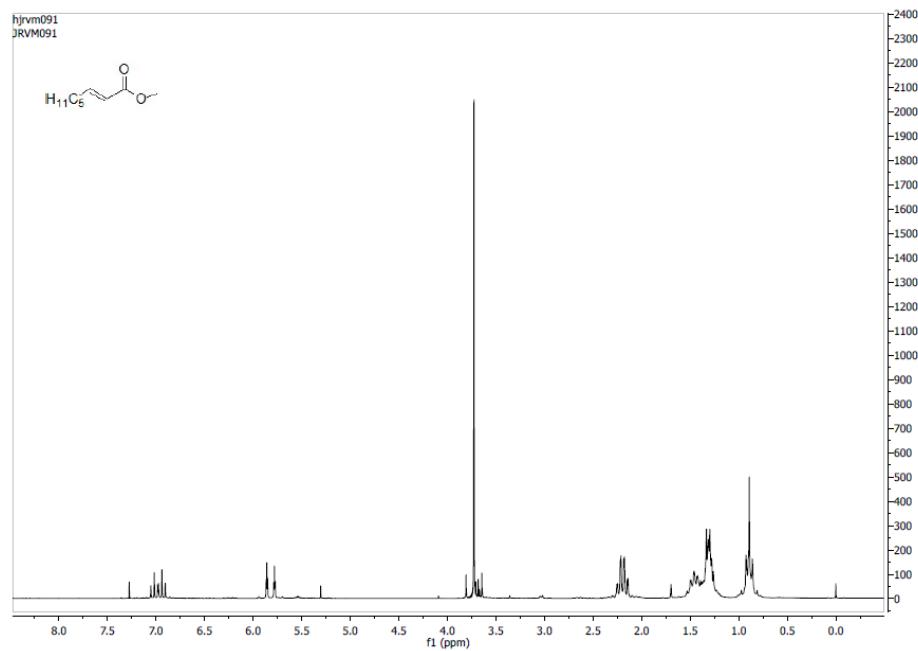


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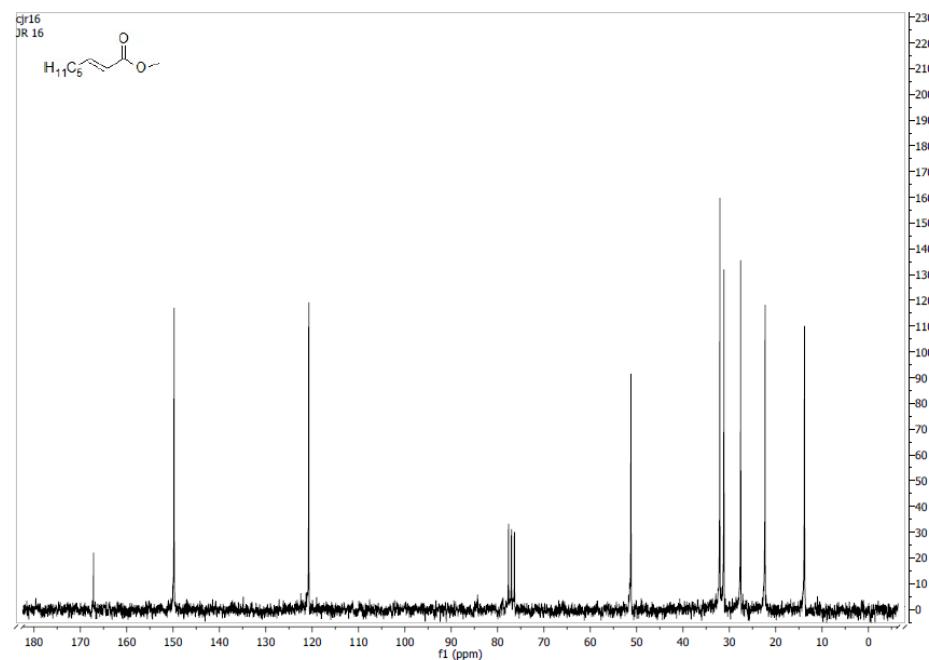


Methyl (E)-oct-2-enoate (13)

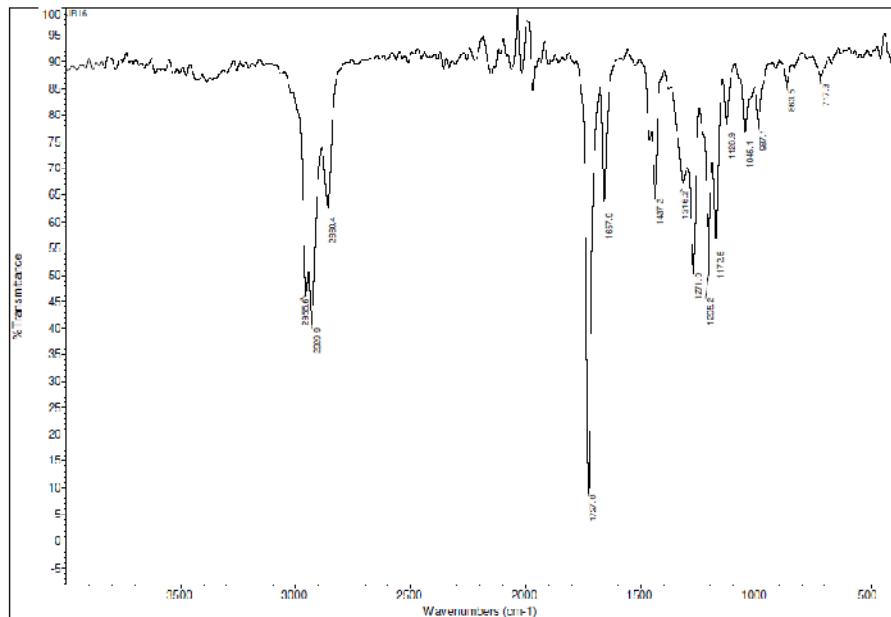
^1H NMR



^{13}C NMR

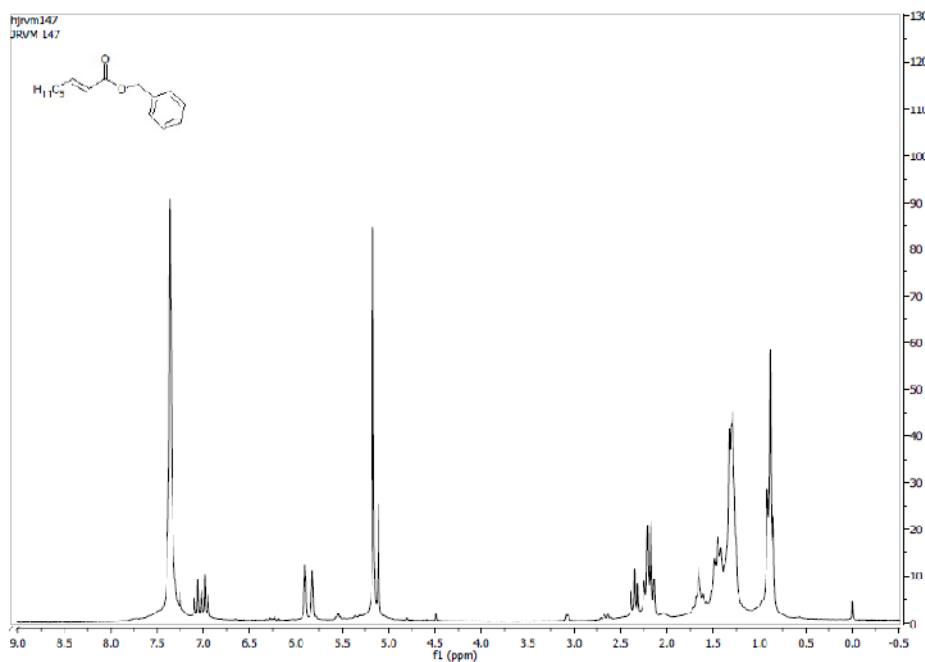


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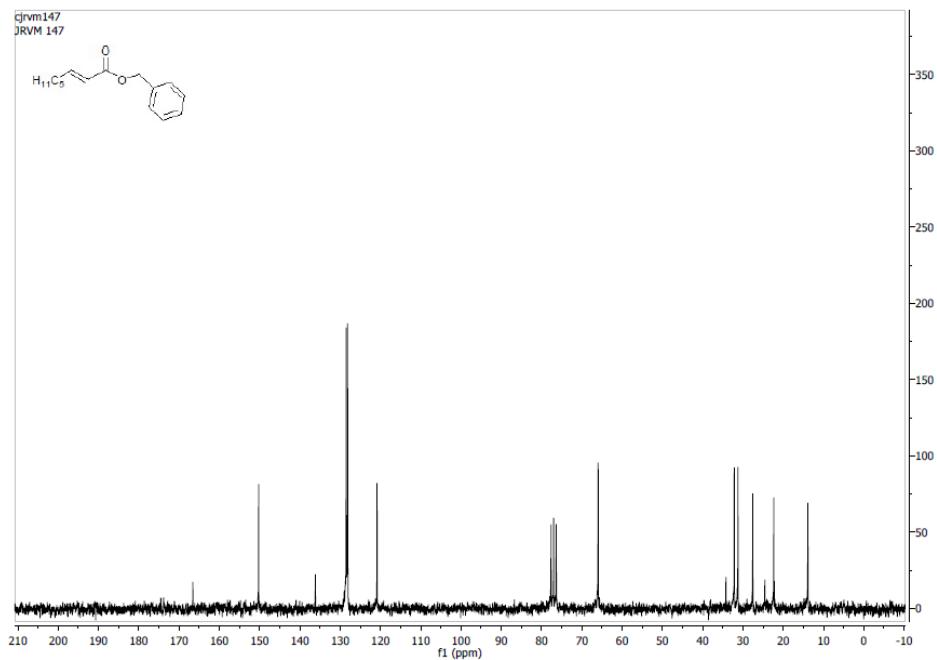


Benzyl (E)-oct-2-enoate (14)

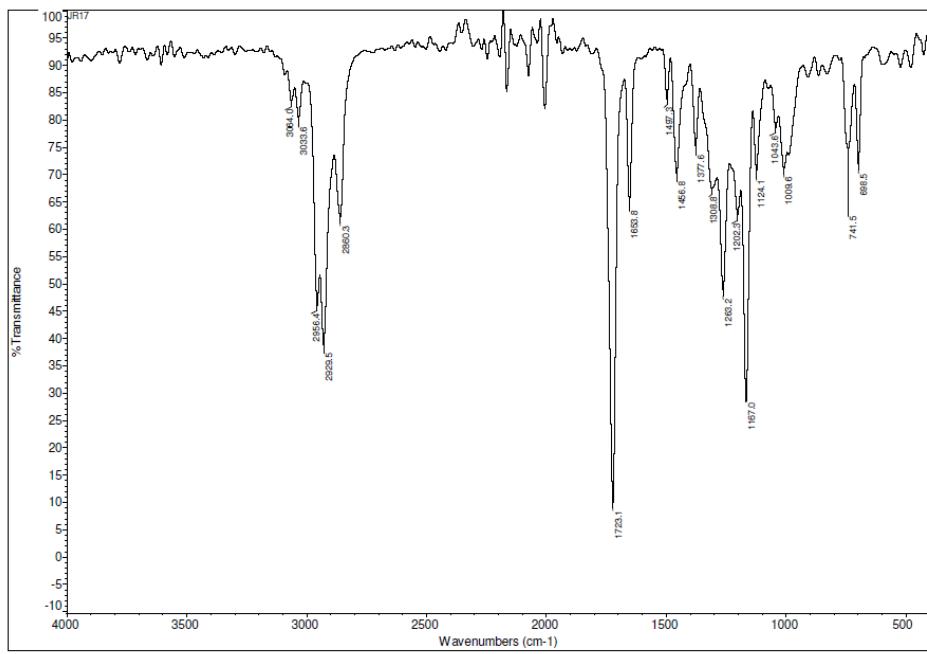
¹H NMR



¹³CNMR

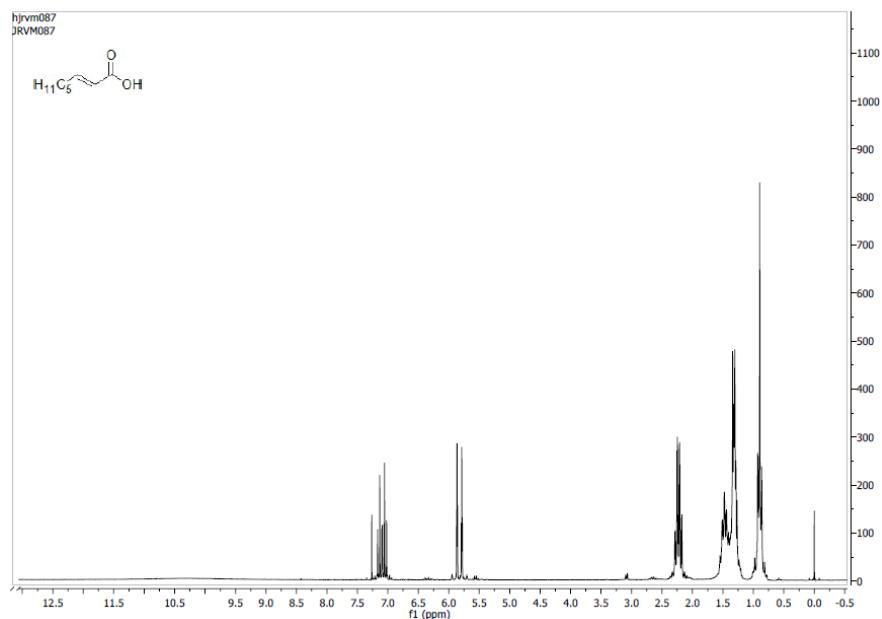


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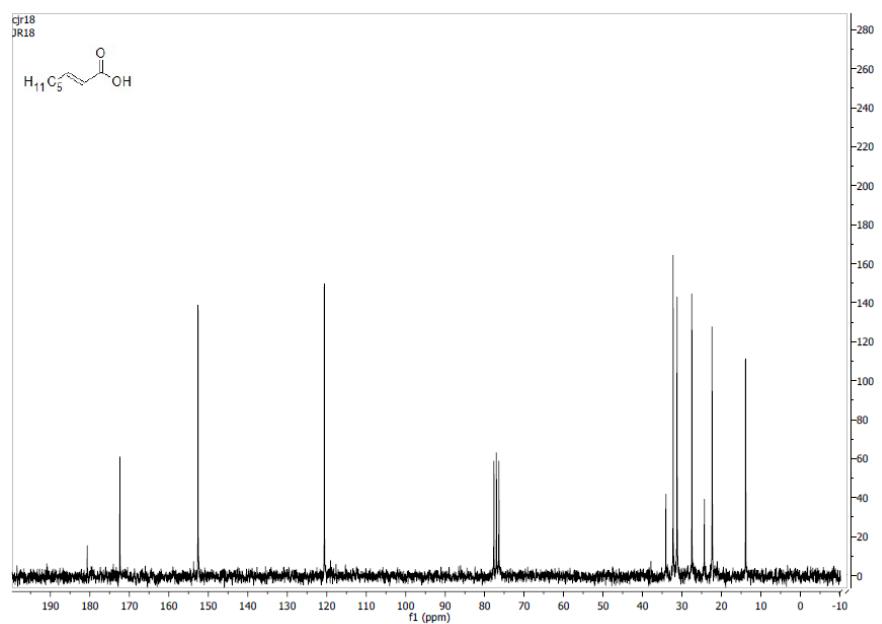


(2E)-oct-2-enoic acid (15)

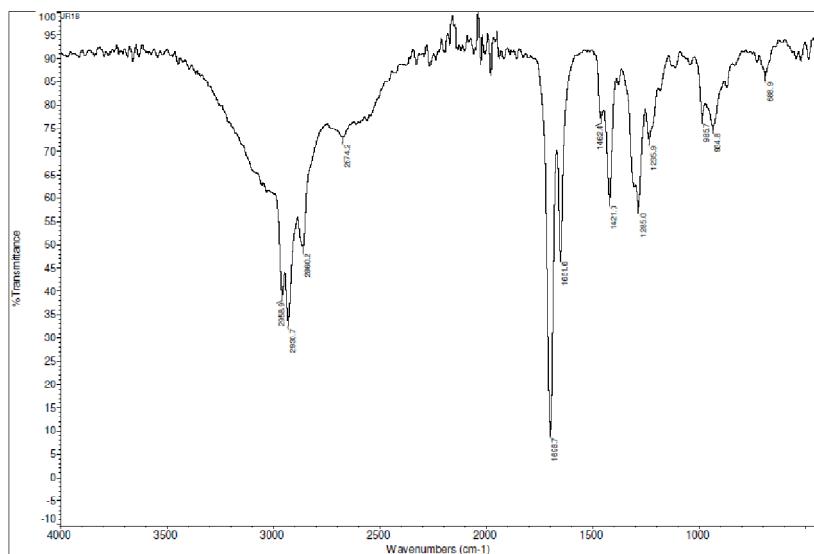
^1H NMR



^{13}C NMR

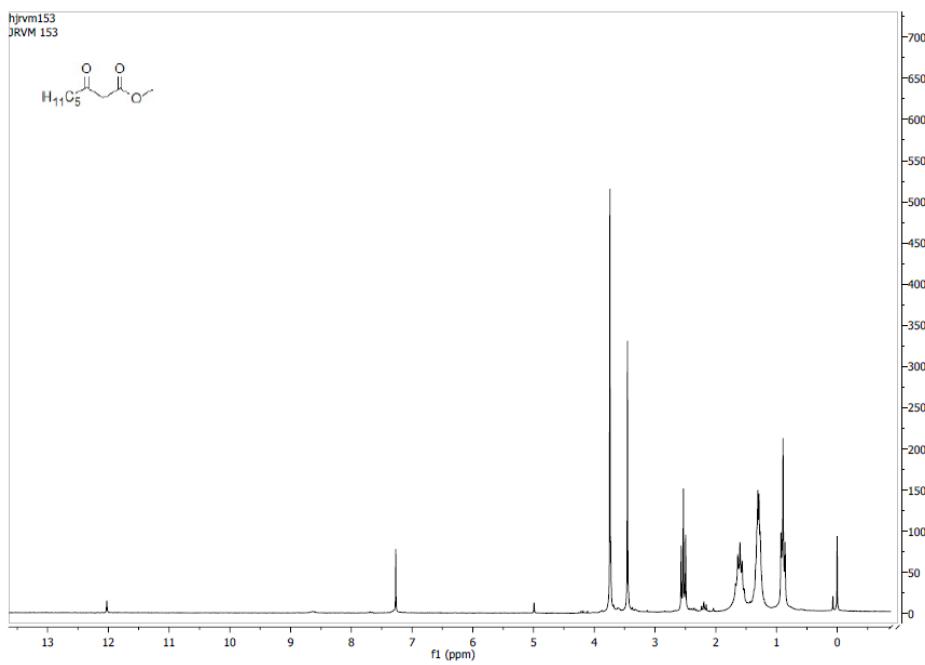


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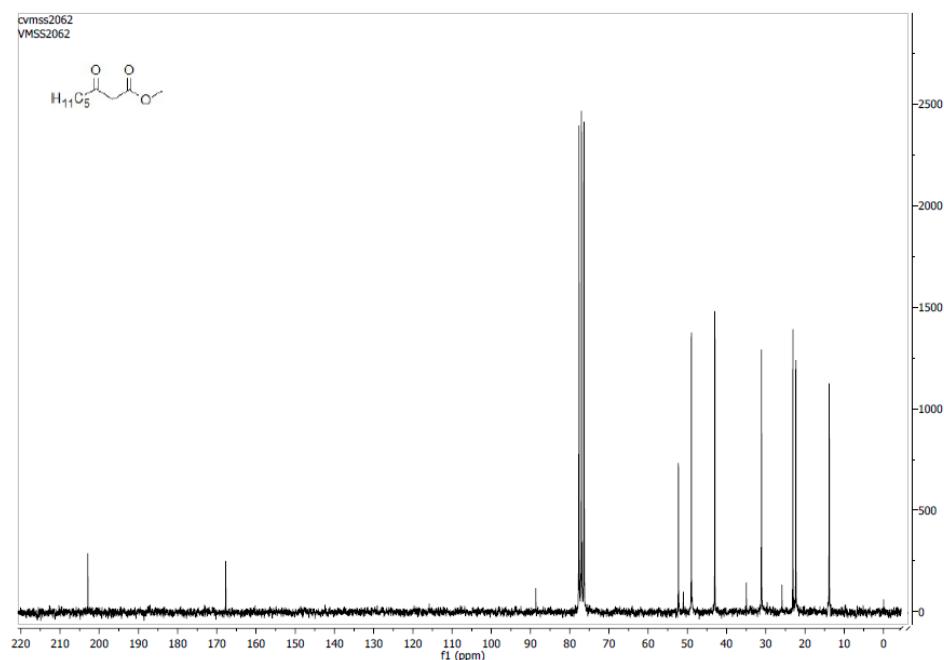


Methyl 3-oxooctanoate (16)

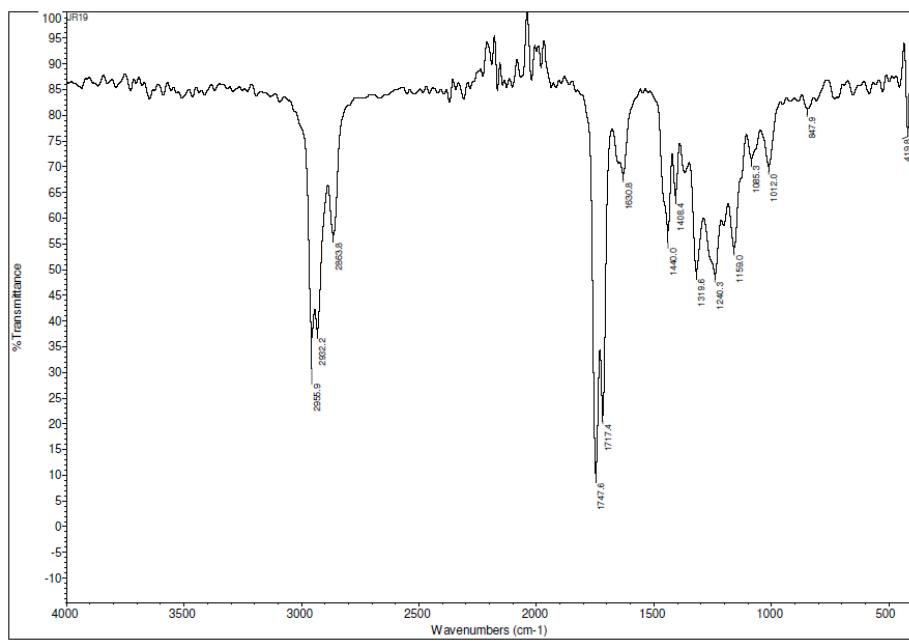
¹HNMR



¹³CNMR

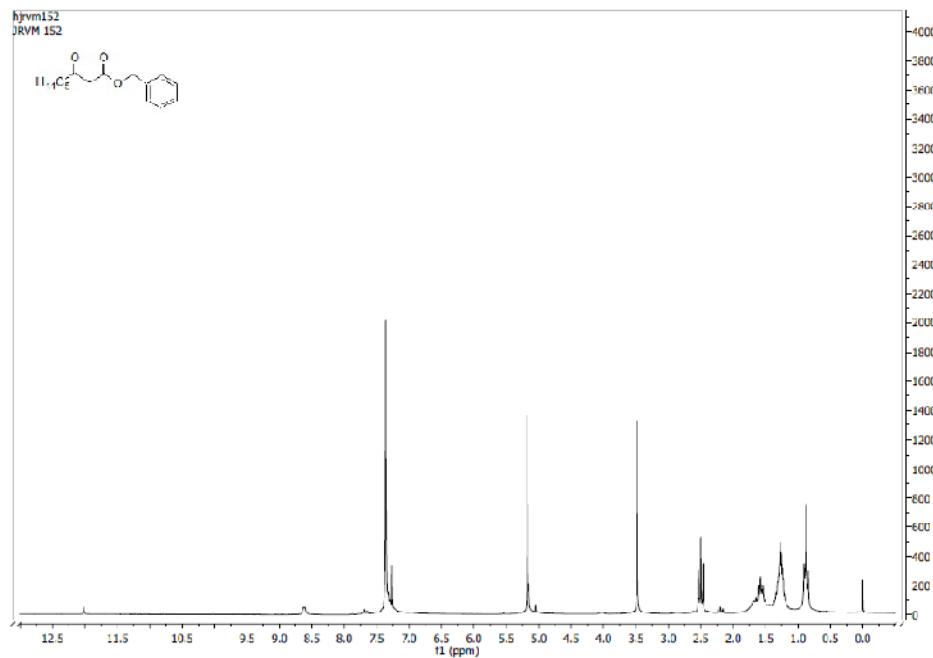


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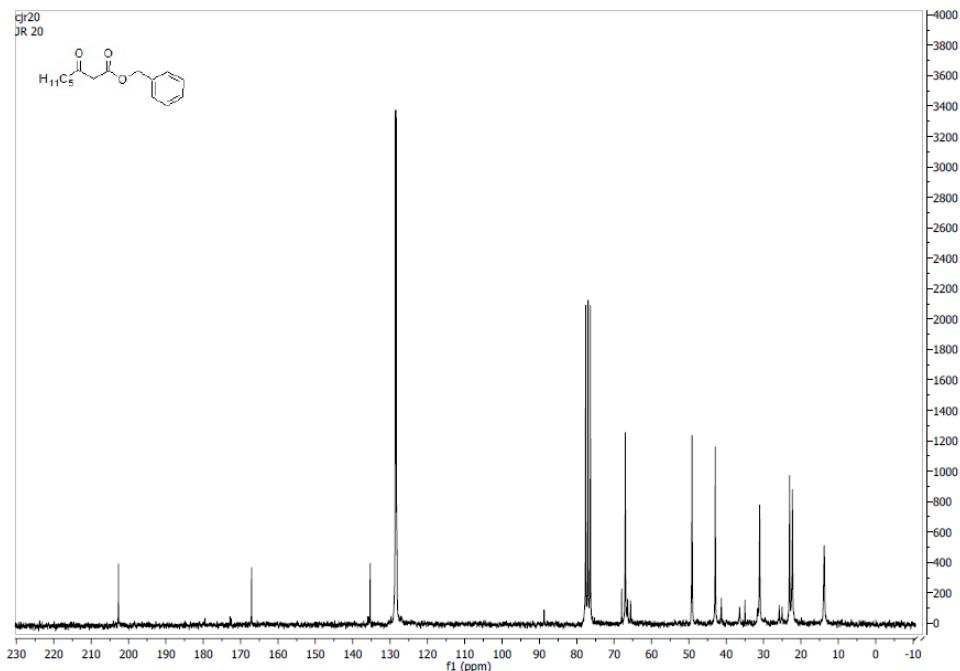


Benzyl 3-oxooctanoate (17)

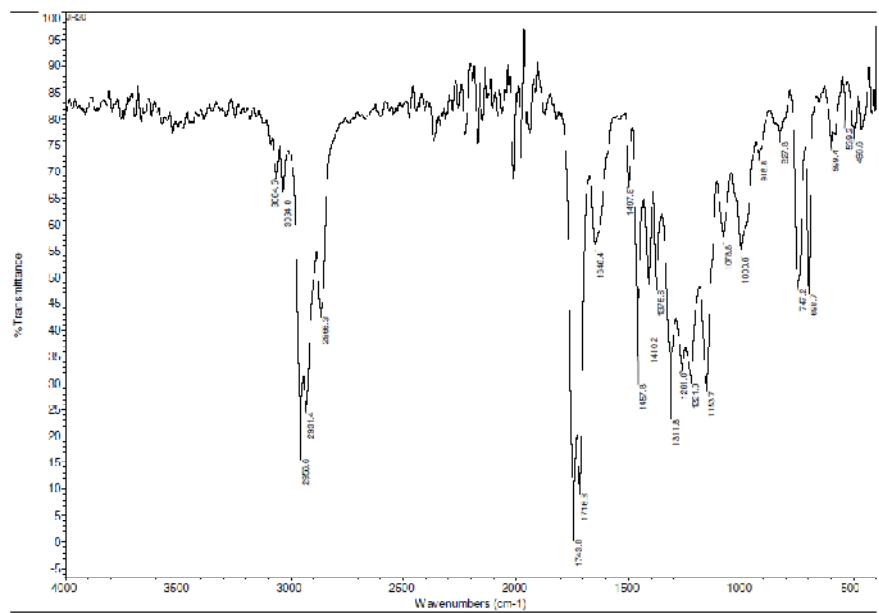
¹H NMR



¹³C NMR

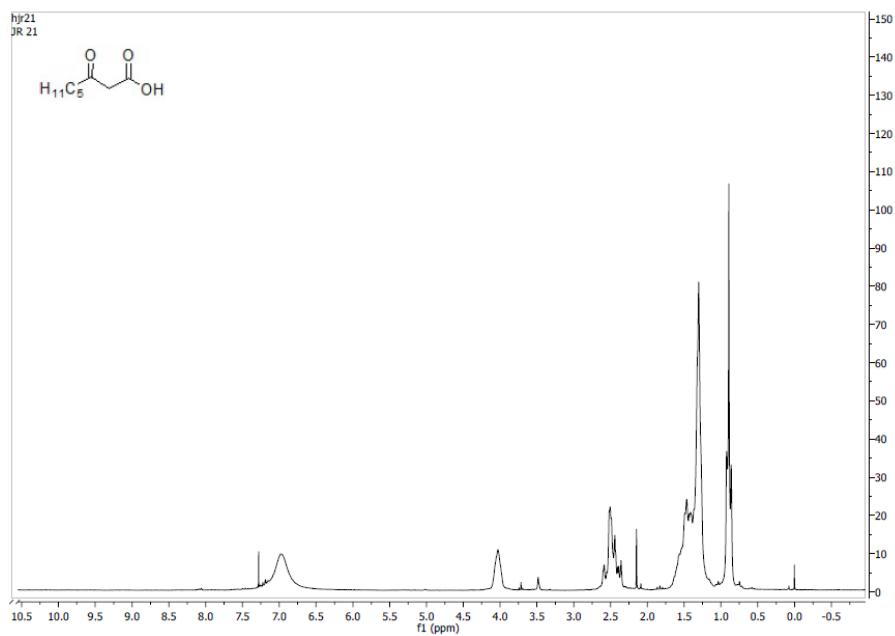


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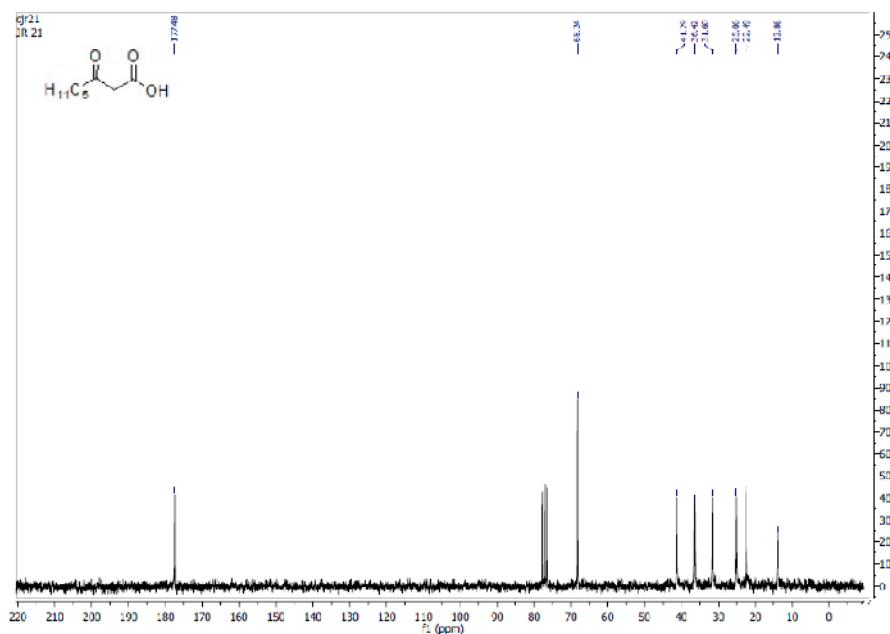


3-oxooctanoic acid (18)

¹H NMR



¹³CNMR



IR

