

Supporting Information

Regio- and Stereoselective Allylindation of Alkynes Using InBr₃ and Allylic Silanes: Synthesis, Characterization, and Application of 1,4-Dienylindiums toward Skipped Dienes

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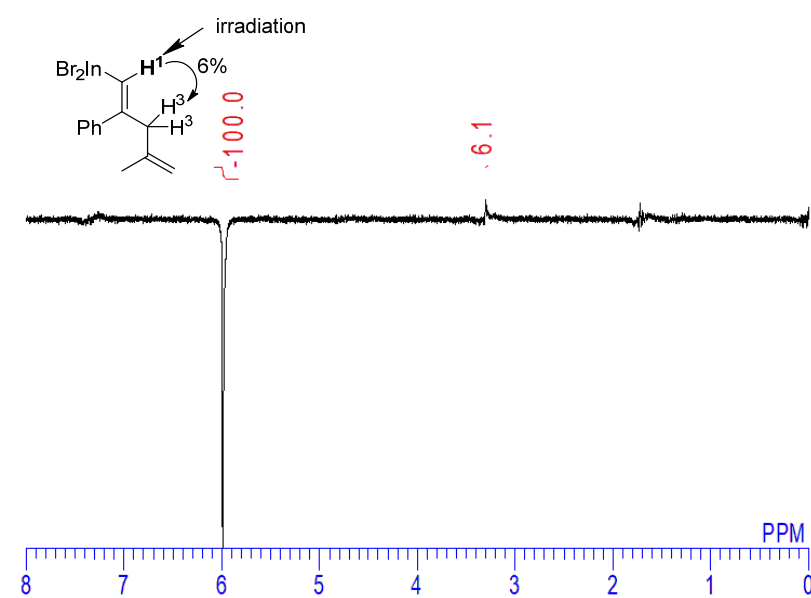
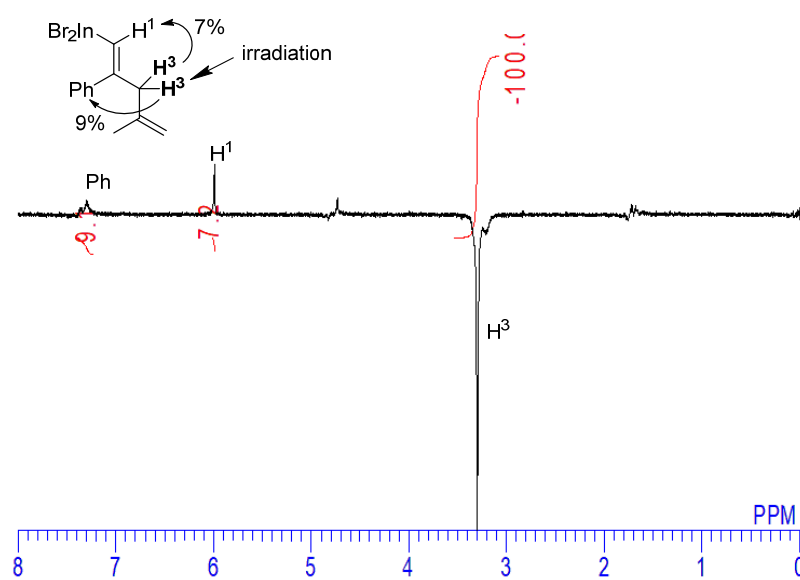
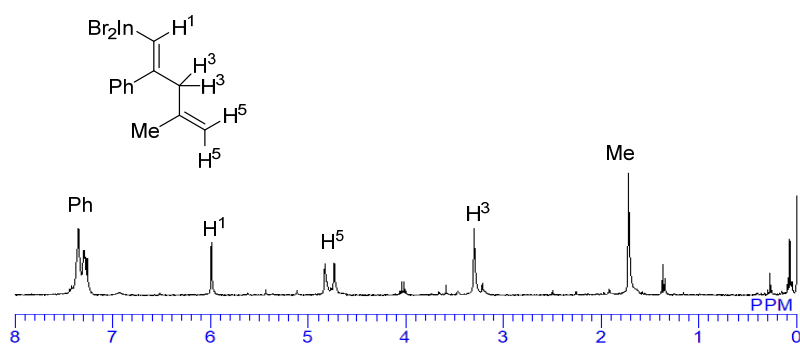
²Department of Applied Chemistry, Graduate School of Engineering, Osaka University

Contents

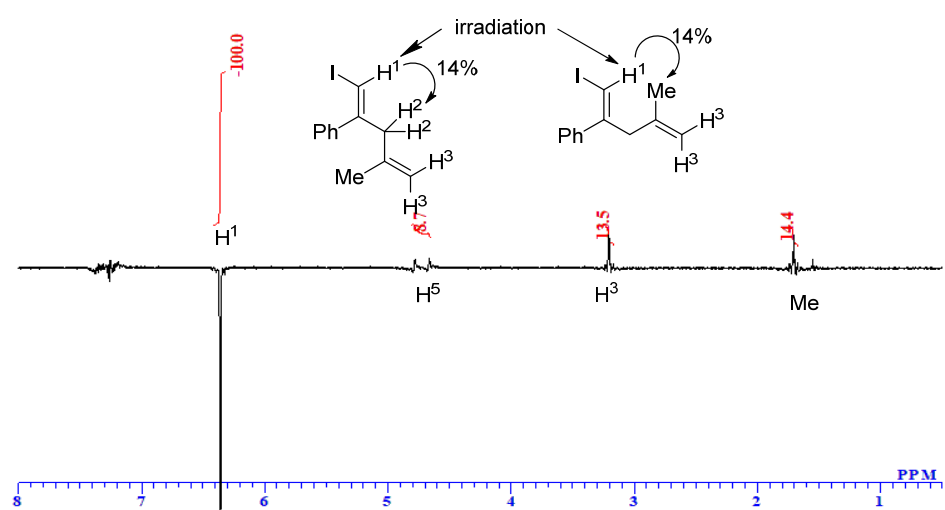
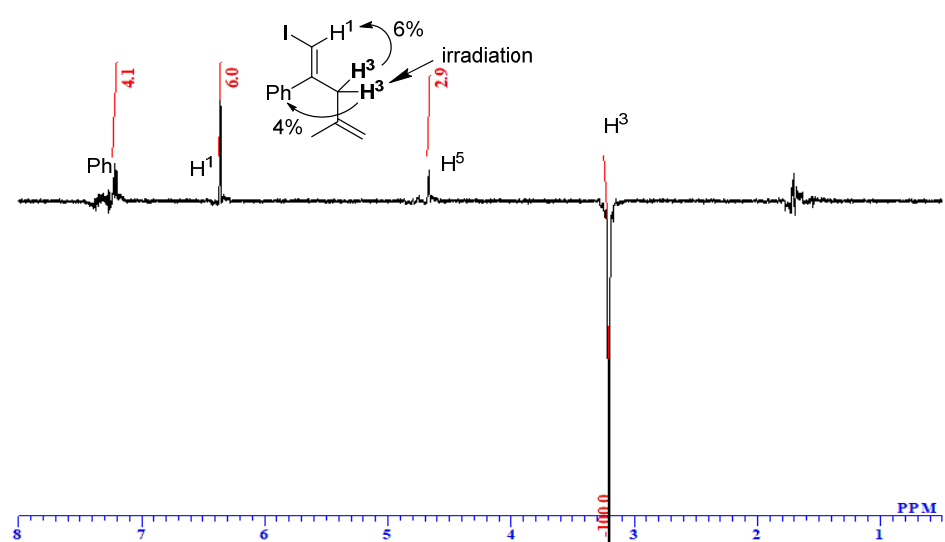
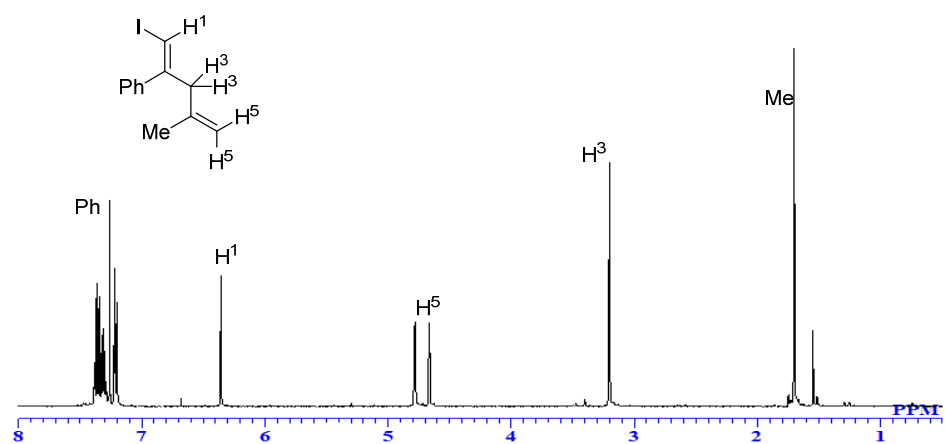
NOE Experiments	2
NMR Spectra.....	4

NOE Experiments

1,4-dienylindium 3ha

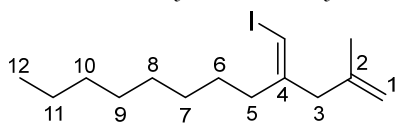


(Z)-(1-iodo-4-methylpenta-1,4-dien-2-yl)benzene (4ha)

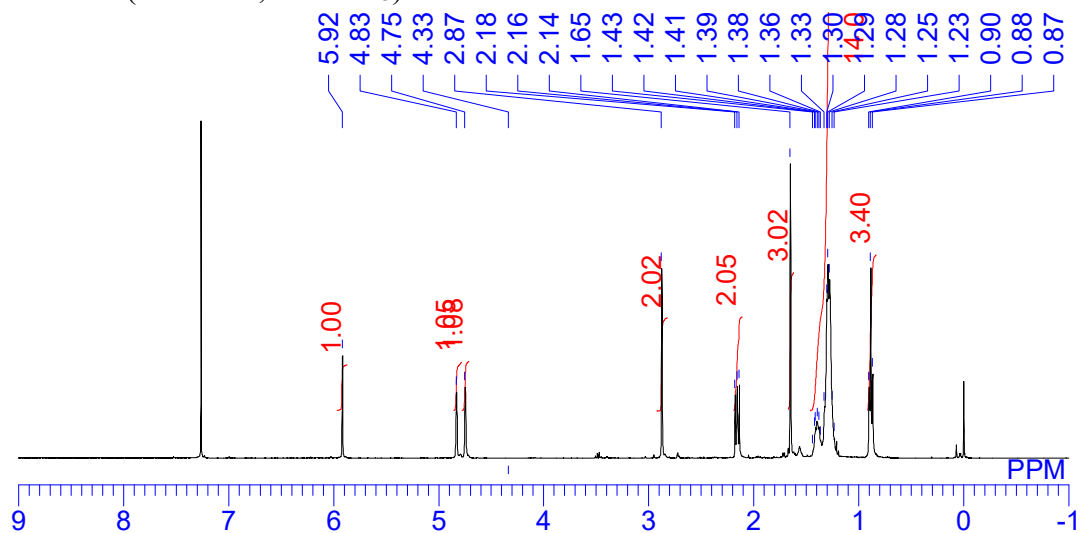


NMR Spectra

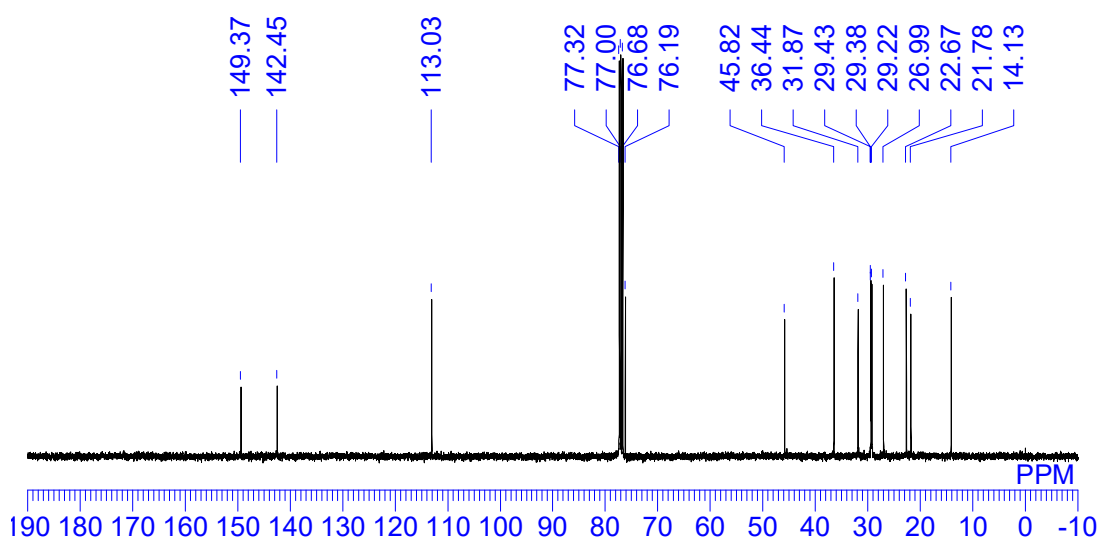
(*E*)-4-(iodomethylene)-2-methyldodec-1-ene (**4aa**)



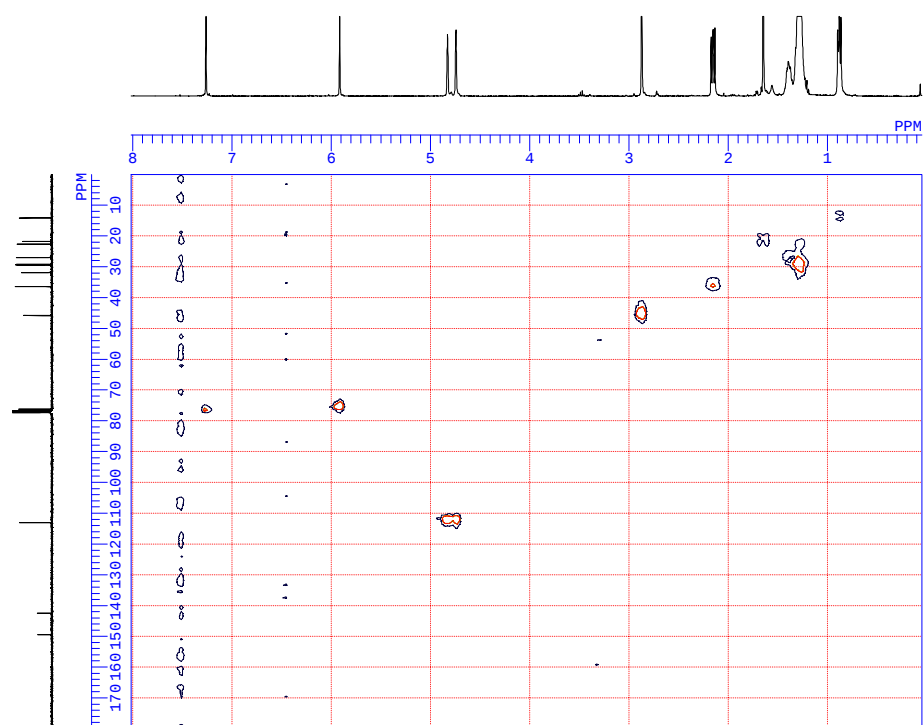
^1H NMR (400 MHz, in CDCl_3)



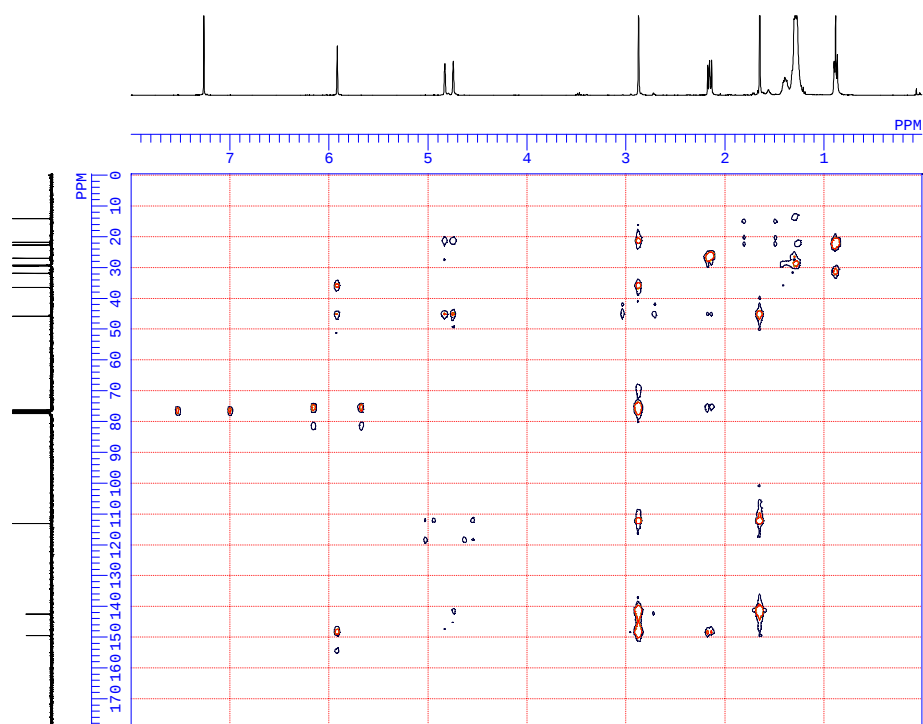
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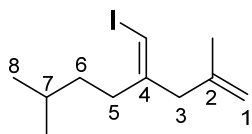
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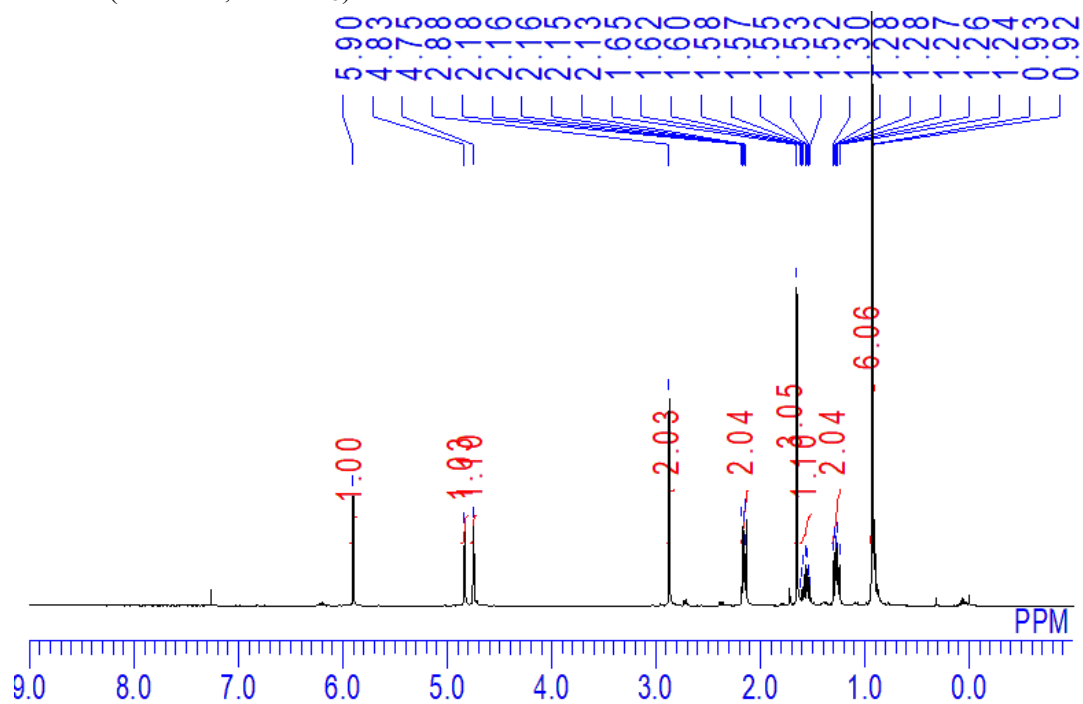
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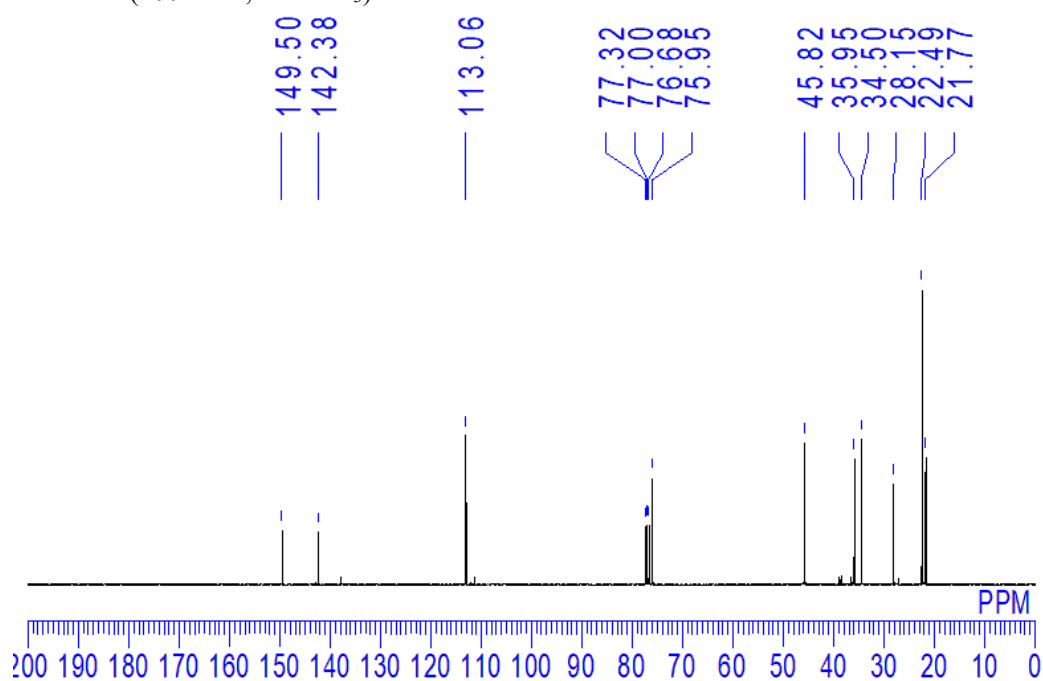
(*E*)-4-(iodomethylene)-2,7-dimethyloct-1-ene (**4ba**)



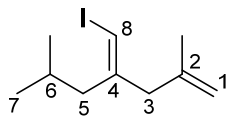
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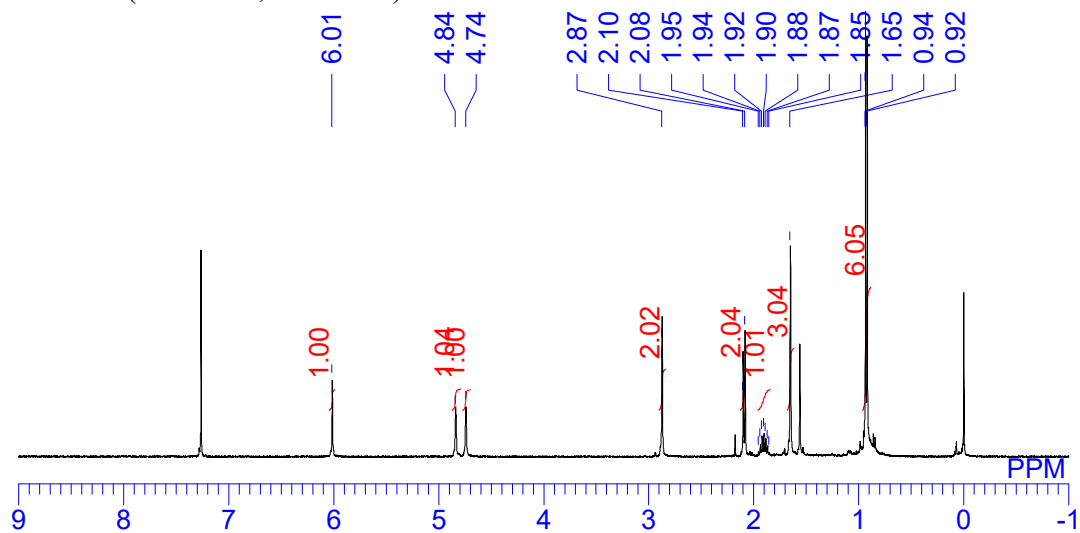
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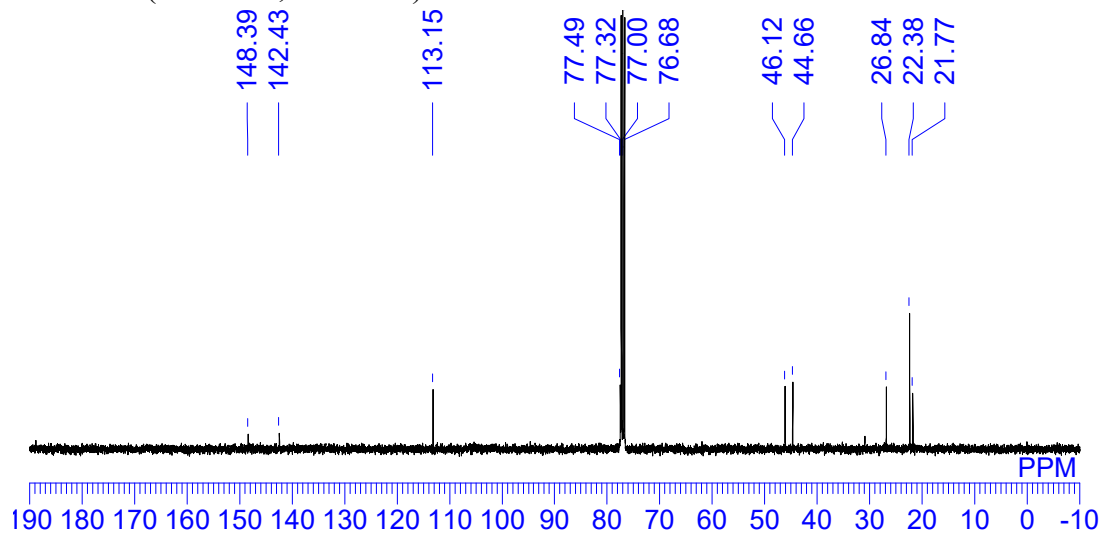
(*E*)-4-(iodomethylene)-2,6-dimethylhept-1-ene (**4ca**)



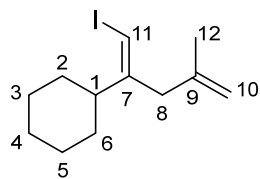
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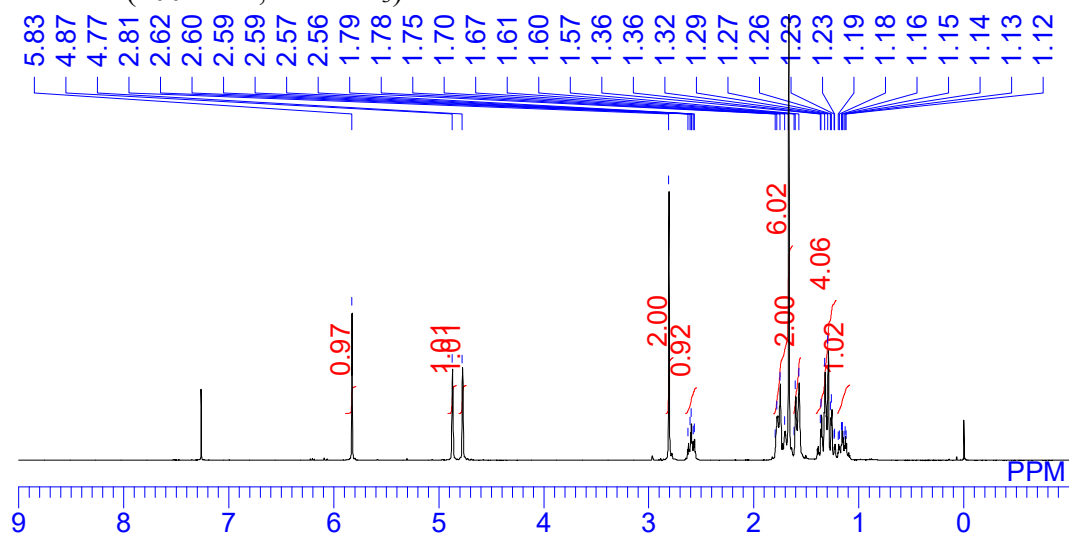
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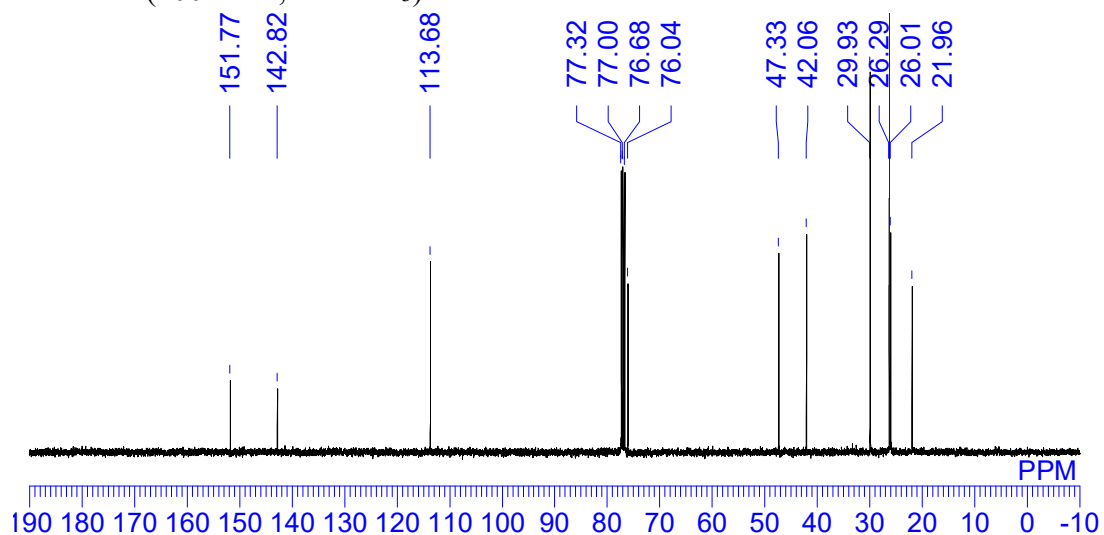
(Z)-(1-iodo-4-methylpenta-1,4-dien-2-yl)cyclohexane (**4da**)



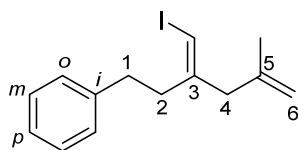
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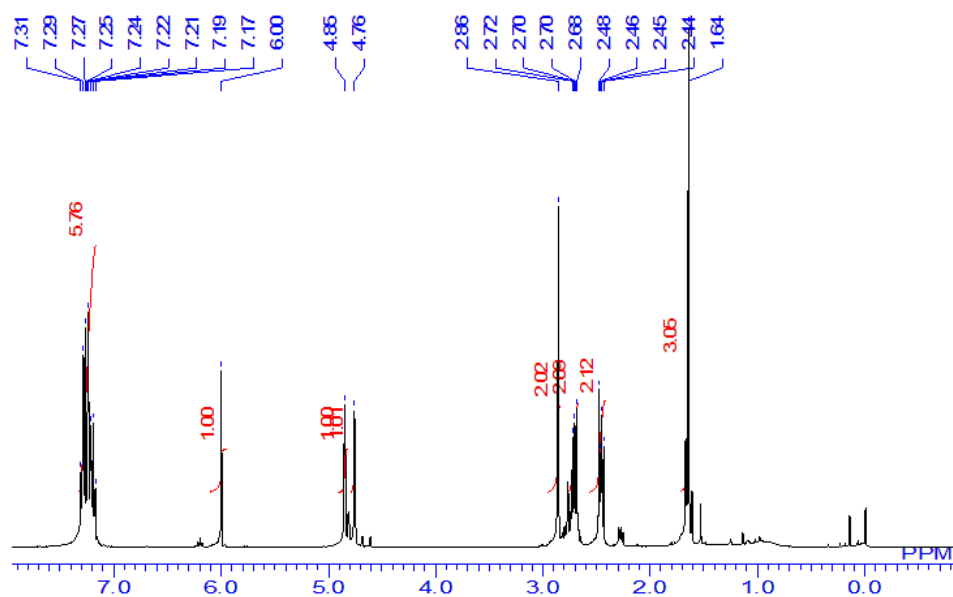
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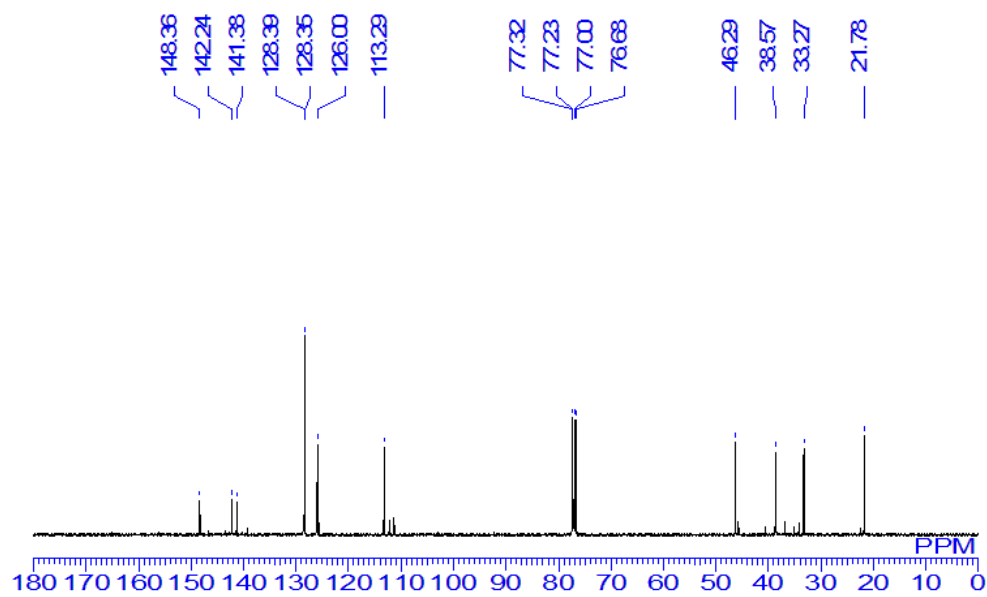
(E)-(3-(iodomethylene)-5-methylhex-5-en-1-yl)benzene (**4fa**)



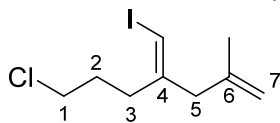
^1H NMR (400 MHz, in CDCl_3)



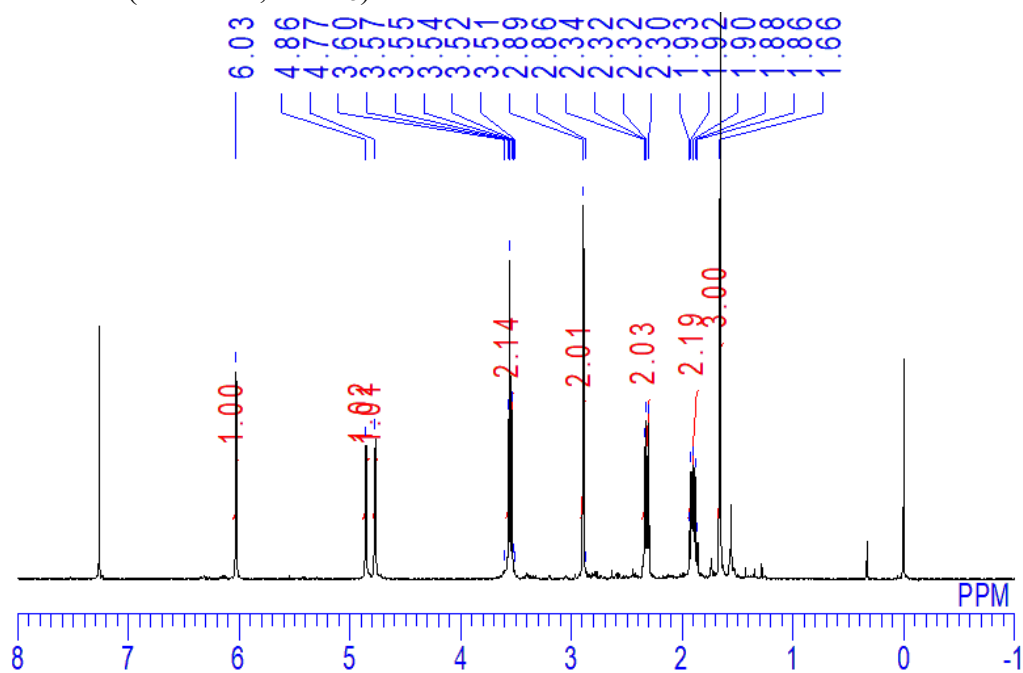
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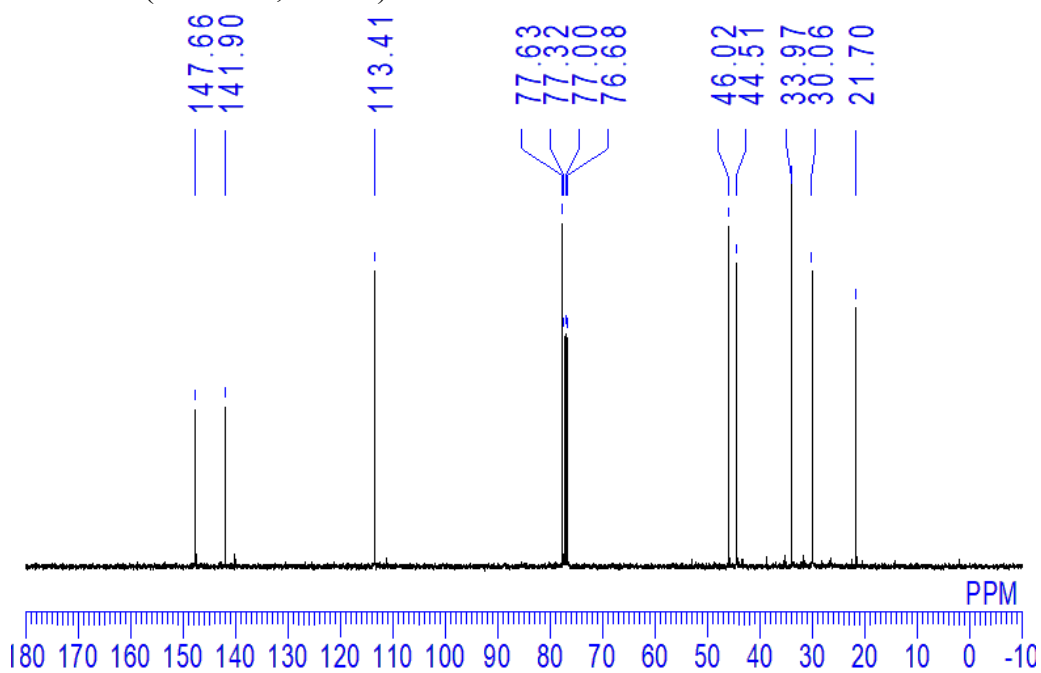
(*E*)-7-chloro-4-(iodomethylene)-2-methylhept-1-ene (**4ga**)



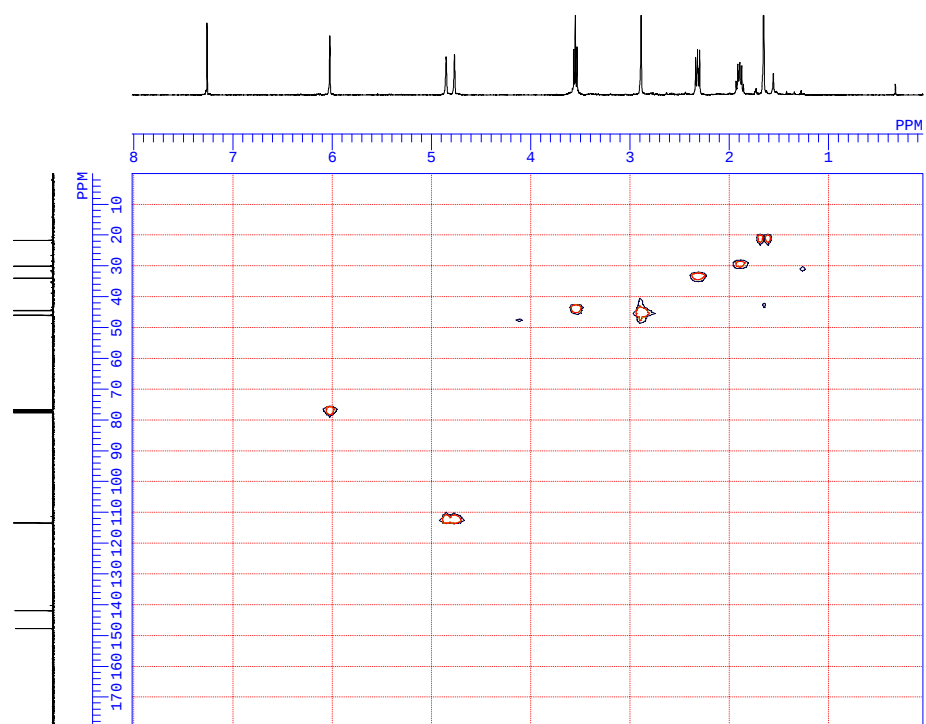
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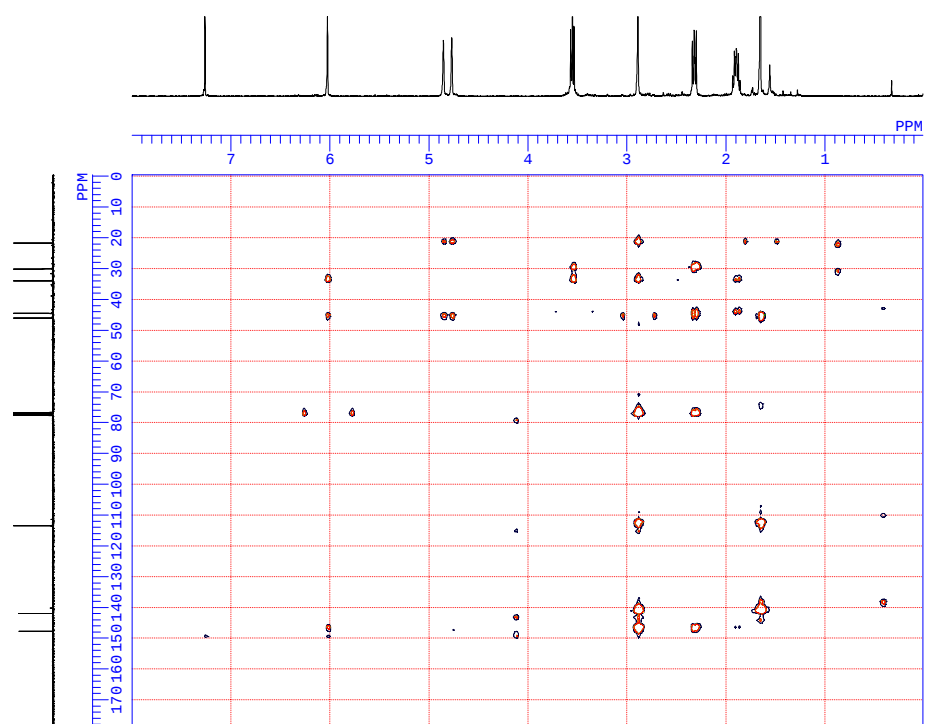
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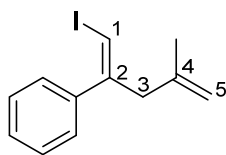
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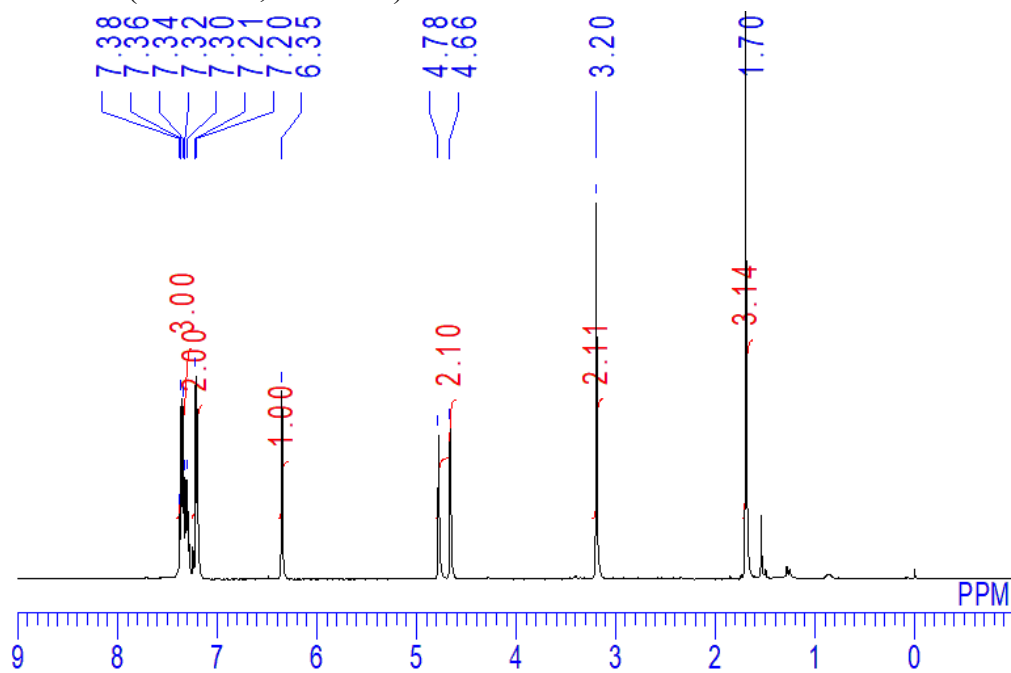
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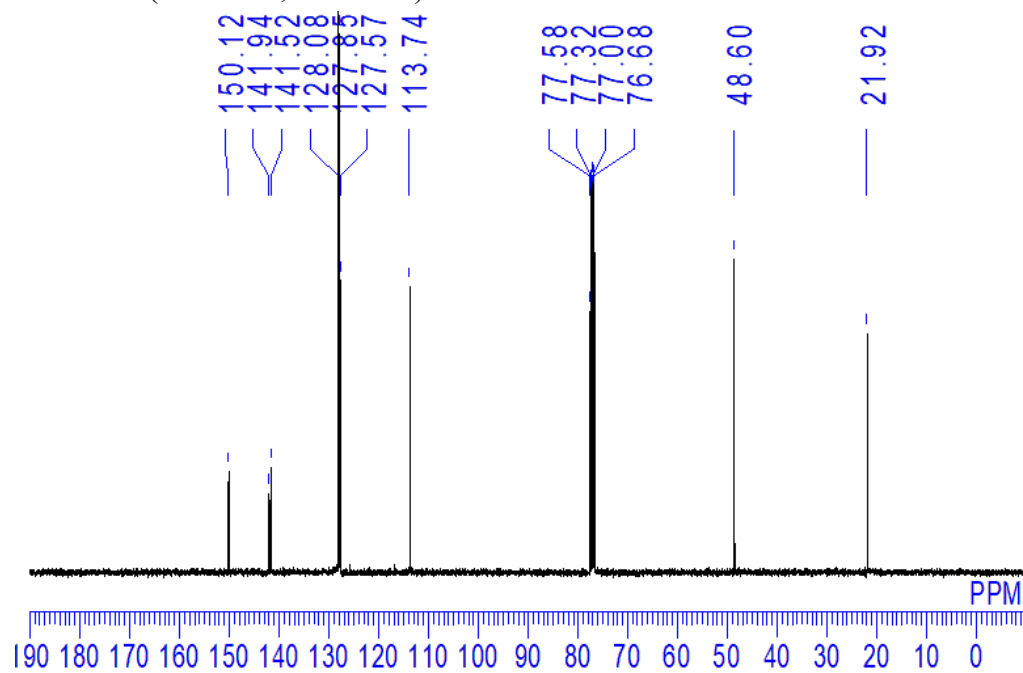
(Z)-(1-iodo-4-methylpenta-1,4-dien-2-yl)benzene (**4ha**)



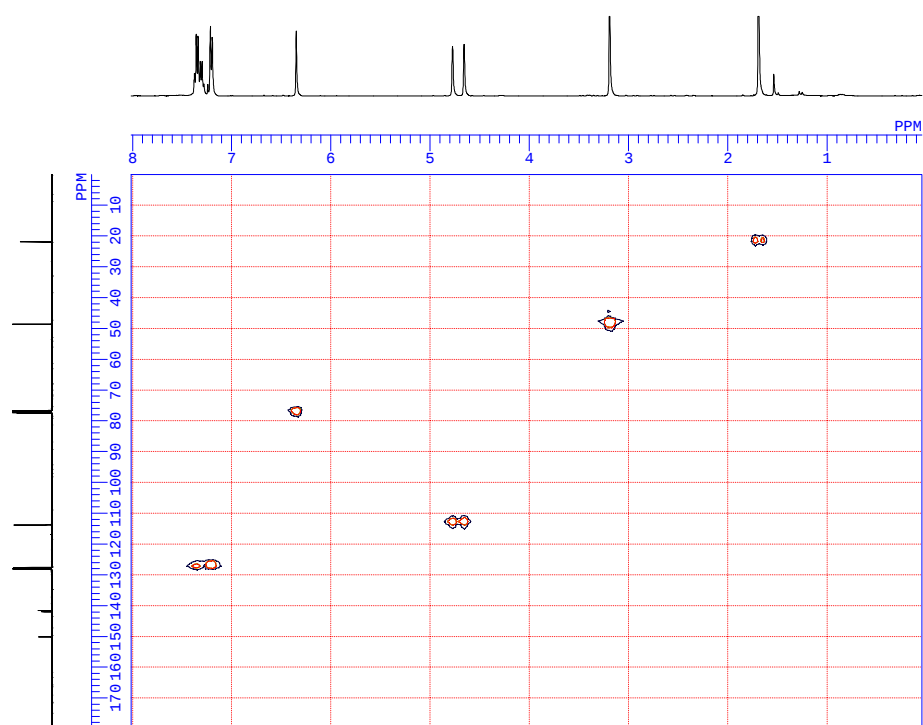
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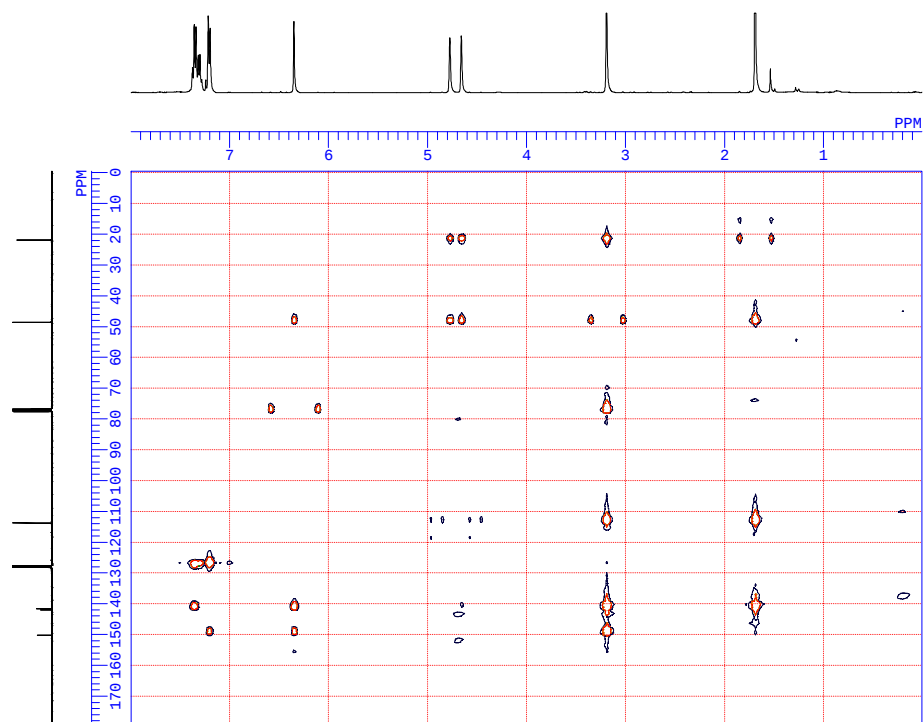
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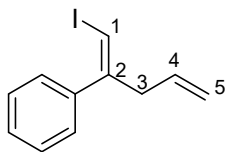
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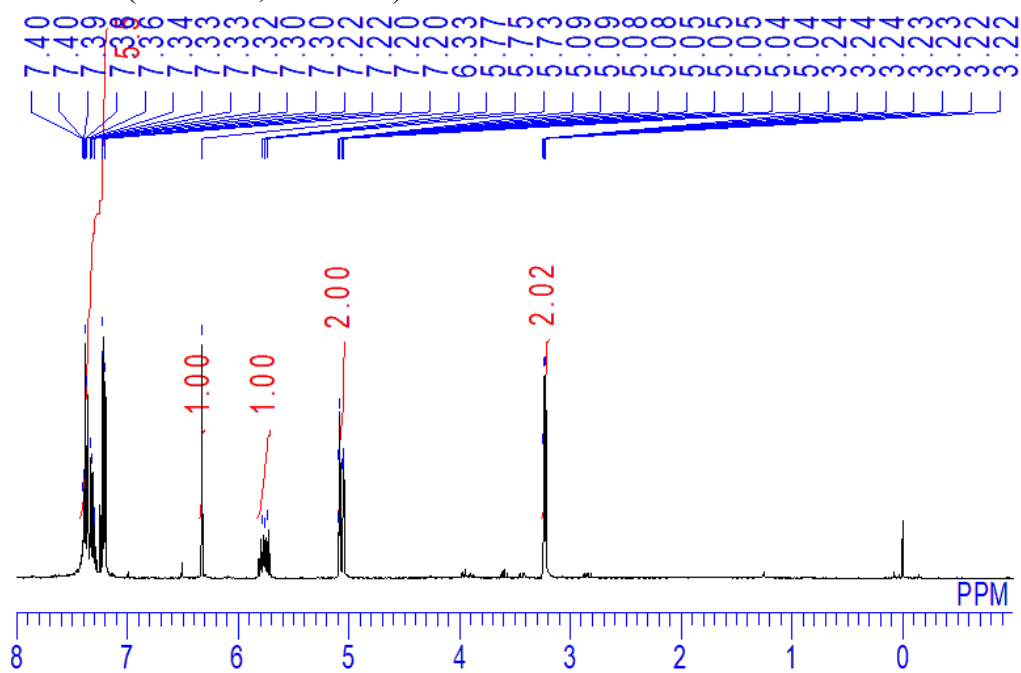
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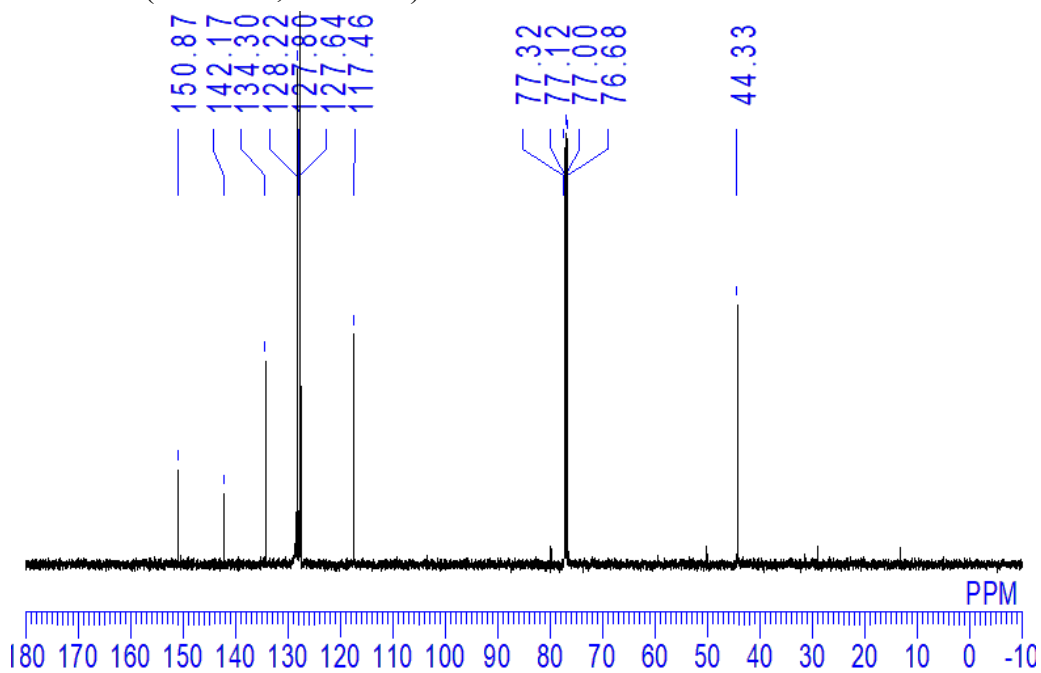
(Z)-(1-iodopenta-1,4-dien-2-yl)benzene (**4hb**)



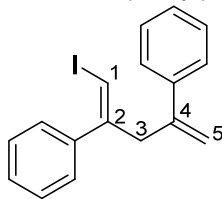
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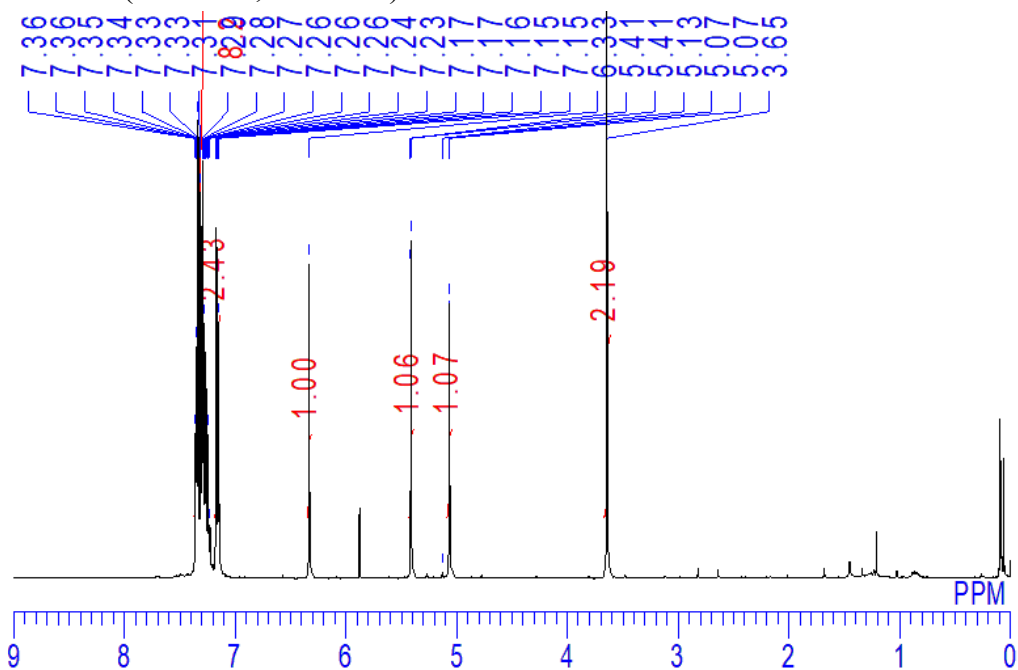
^{13}C NMR (100 MHz, in CDCl_3)



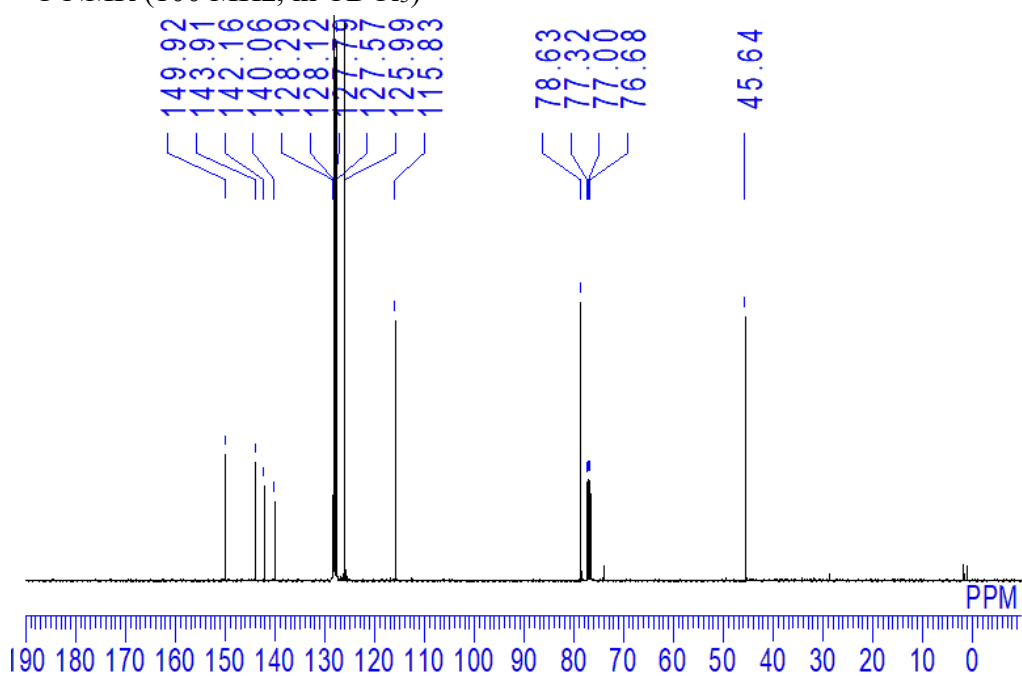
(Z)-1-iodo-2,4-diphenylpenta-1,4-diene (**4hc**)



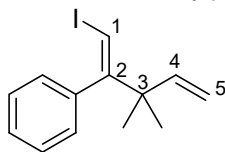
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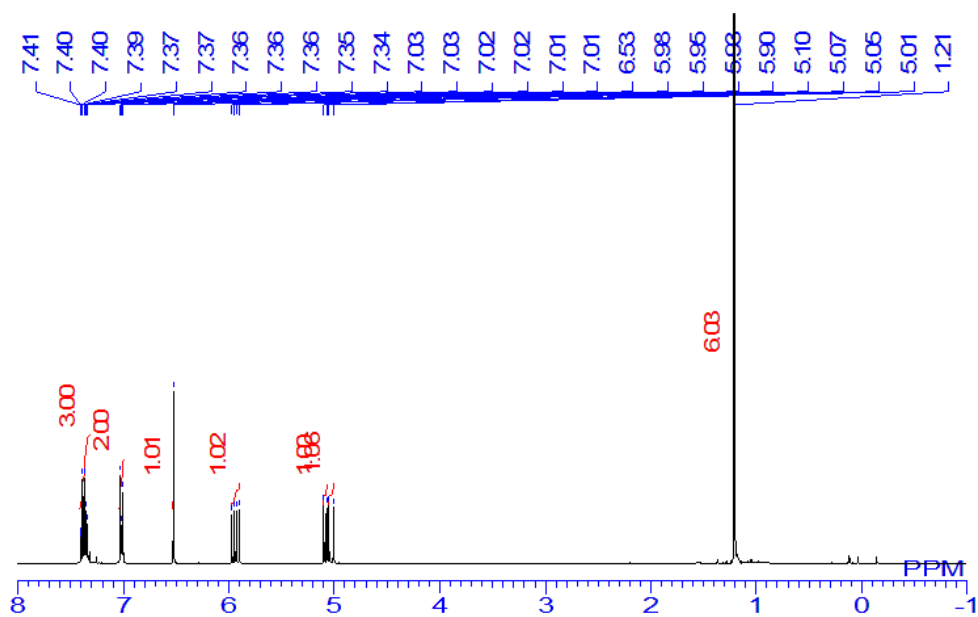
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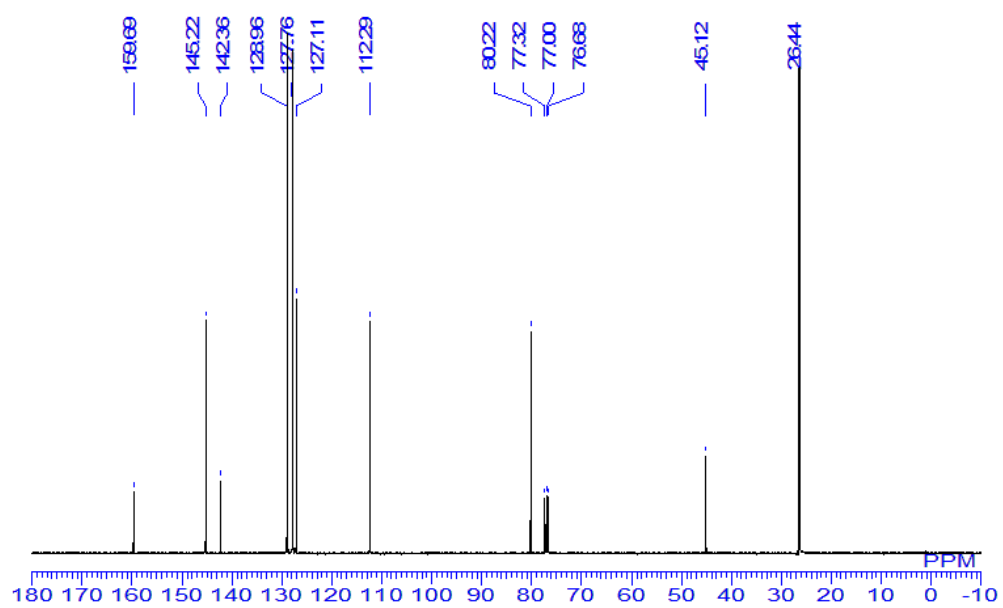
(Z)-(1-iodo-3,3-dimethylpenta-1,4-dien-2-yl)benzene (**4hd**)



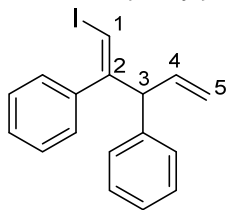
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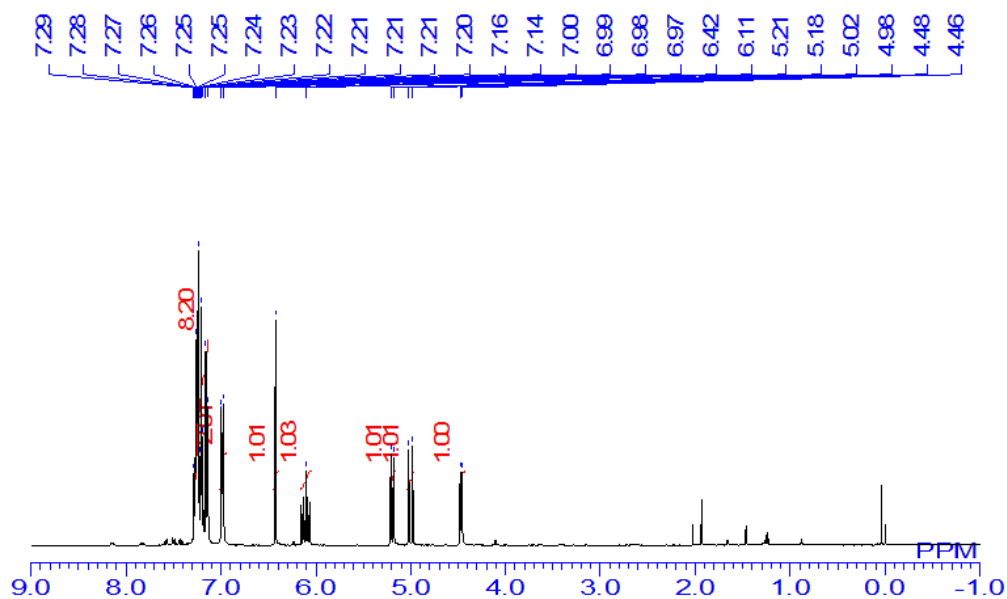
^{13}C NMR (100 MHz, CDCl_3)



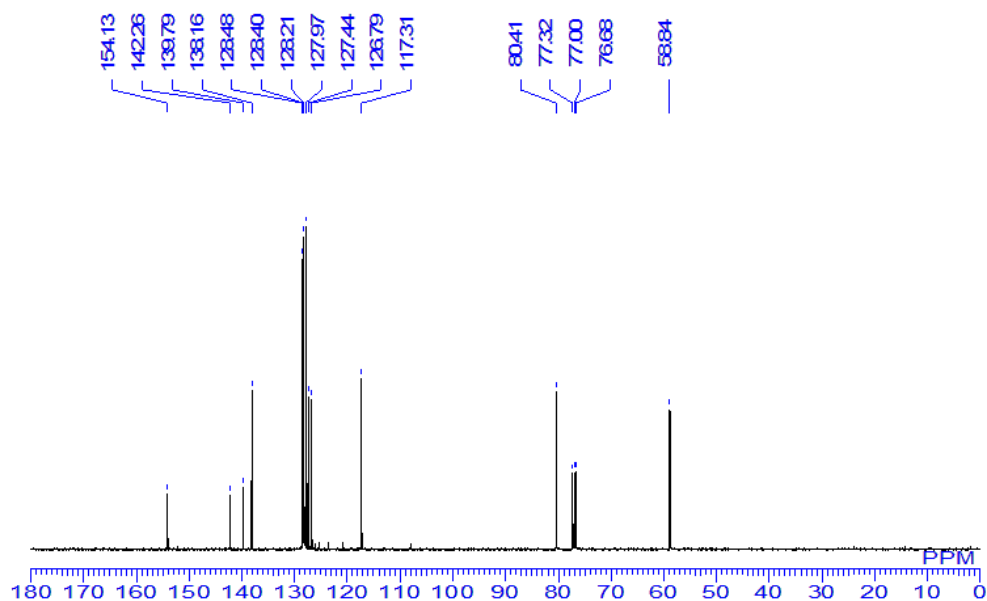
(Z)-1-iodo-2,3-diphenylpenta-1,4-diene (**4he**)



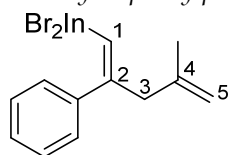
^1H NMR (400 MHz, in CDCl_3)



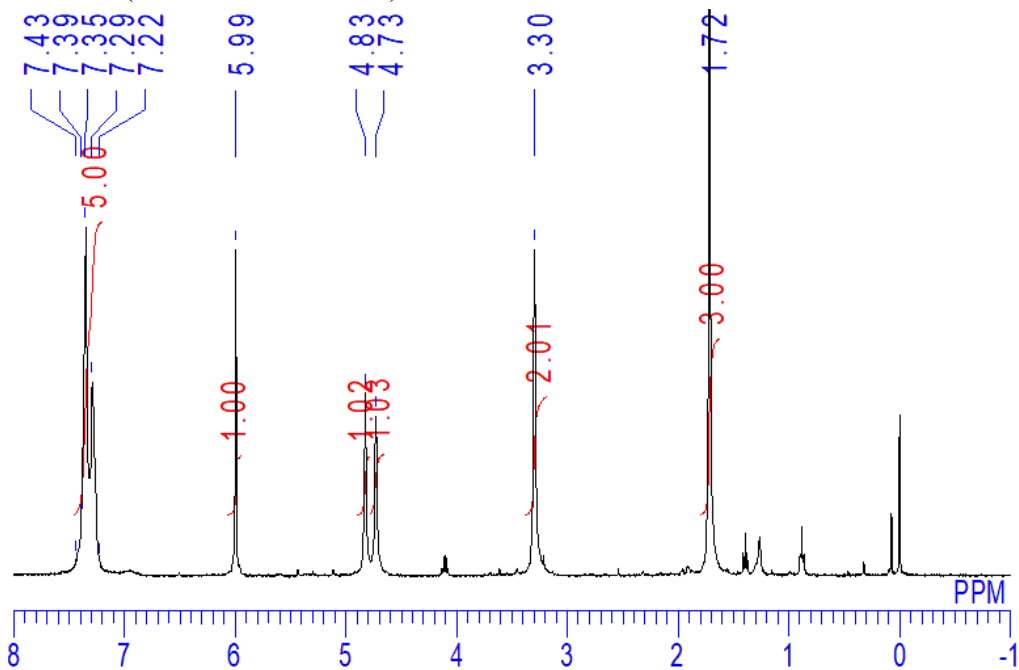
^{13}C NMR (100 MHz, in CDCl_3)



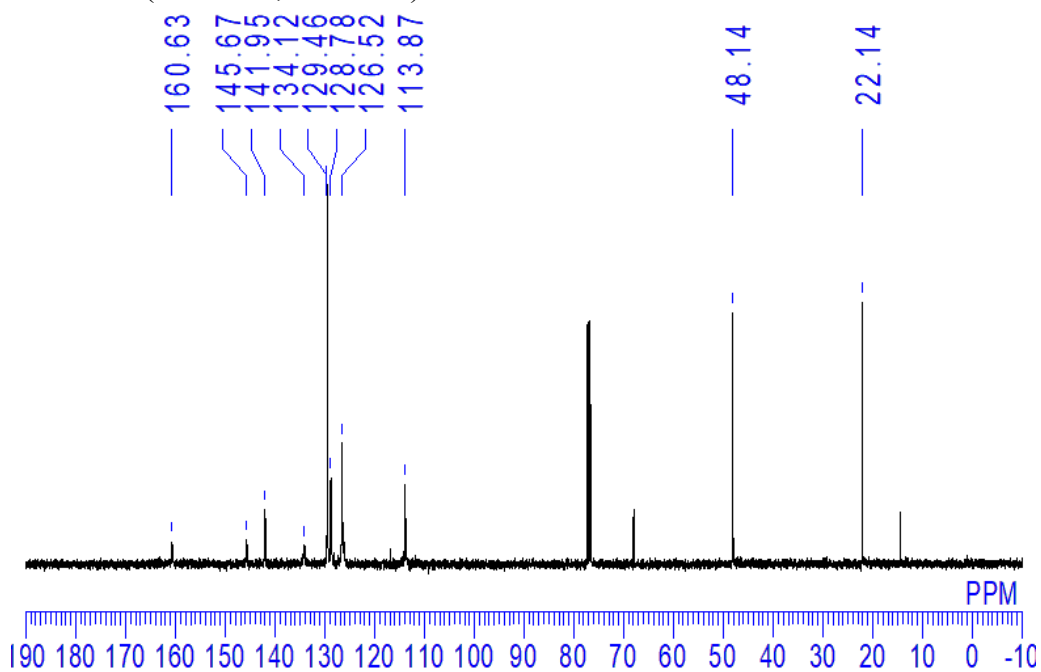
(Z)-(4-methyl-2-phenylpenta-1,4-dien-1-yl)indium(III) bromide (**3ha**)



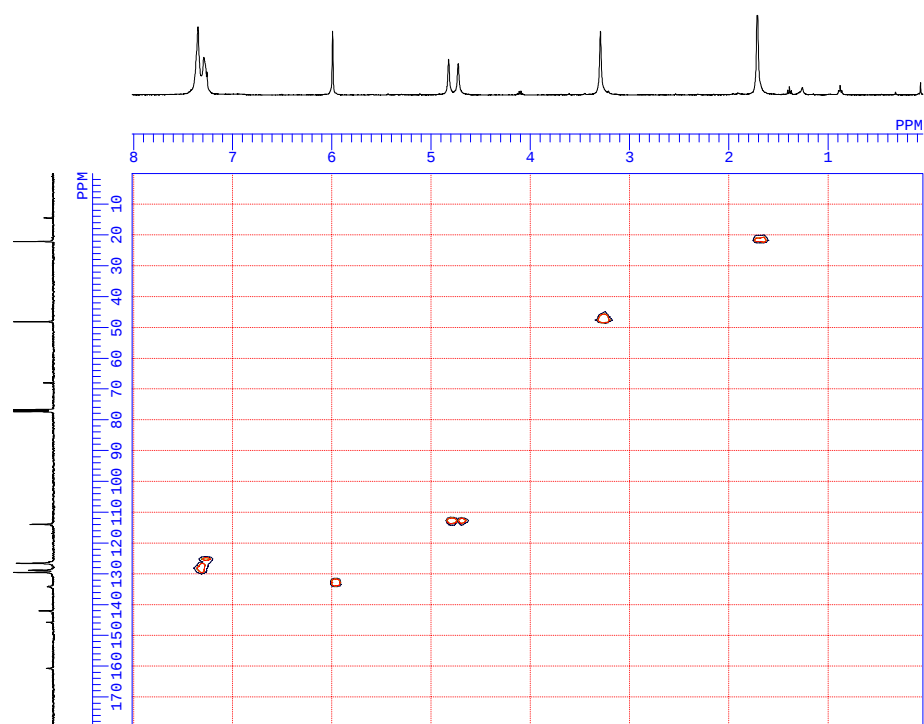
^1H NMR (400 MHz, in CDCl_3)



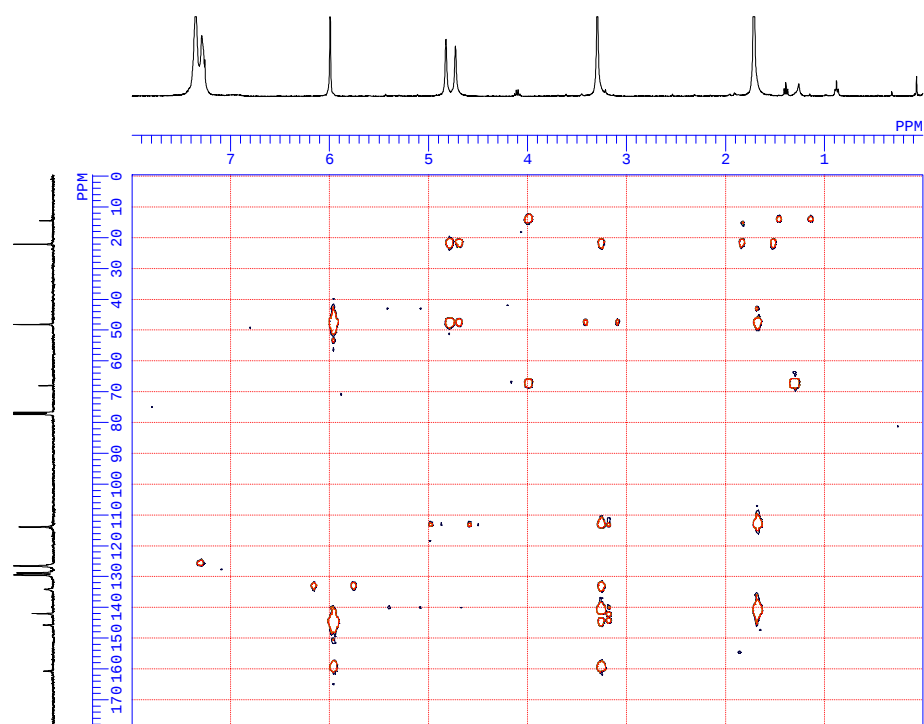
^{13}C NMR (100 MHz, in CDCl_3)



HMQC



HMBC



The chemical structure shows 2,2-diphenyl-3-methylbut-3-ene. The atoms are numbered as follows: 1 is the carbon of the top phenyl ring attached to the double bond; 2 is the carbon of the bottom phenyl ring attached to the double bond; 3 is the methylene carbon between the double bond and the methyl group; 4 is the methyl carbon; and 5 is one of the equivalent protons on the methyl group.

13C NMR spectrum of 1,2-dichloroethane. The spectrum shows peaks at 142.94, 141.02, 140.34, 137.29, 129.01, 128.56, 128.27, 128.07, 127.80, 126.85, 126.25, 113.00, 77.32, 77.00, 76.68, 49.07, and 22.13 ppm. The x-axis is labeled PPM and ranges from 200 to 0.

