Distinctive transformation based diversity oriented synthesis of small ring carbocyles and heterocycles from biocatalytically derived enantiopure α-substituted-β-hydroxyesters

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Supporting Information

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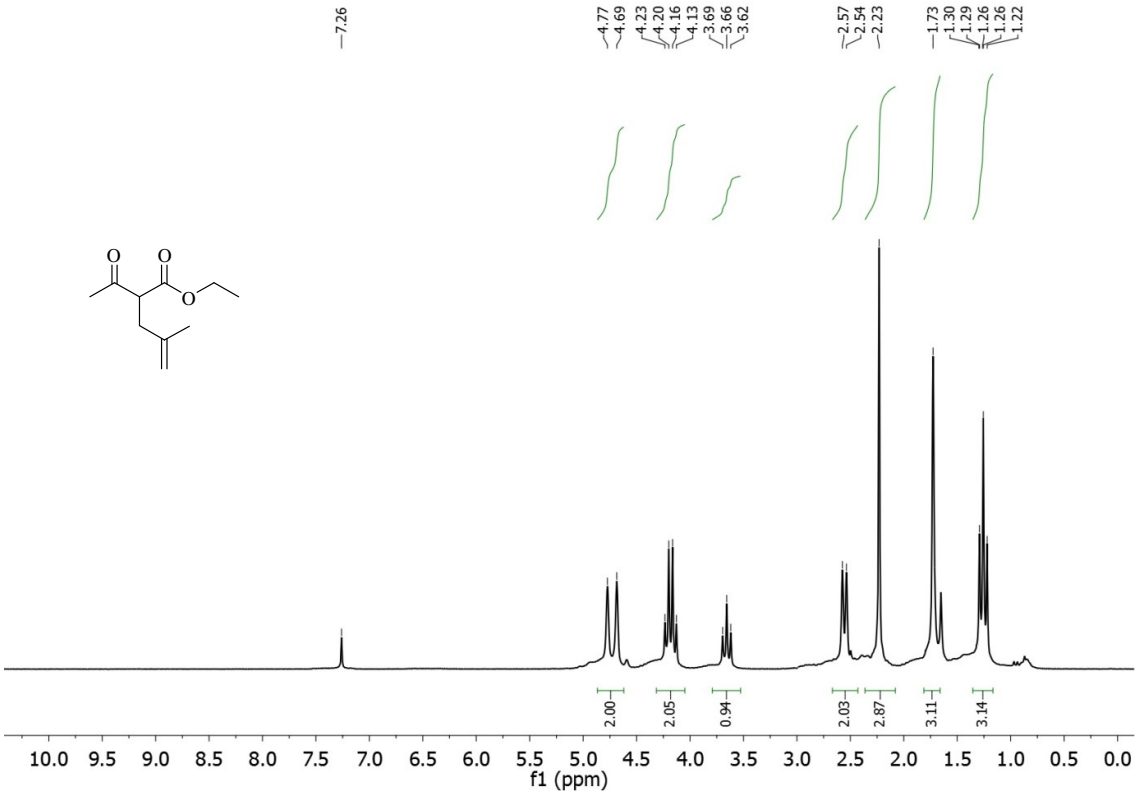
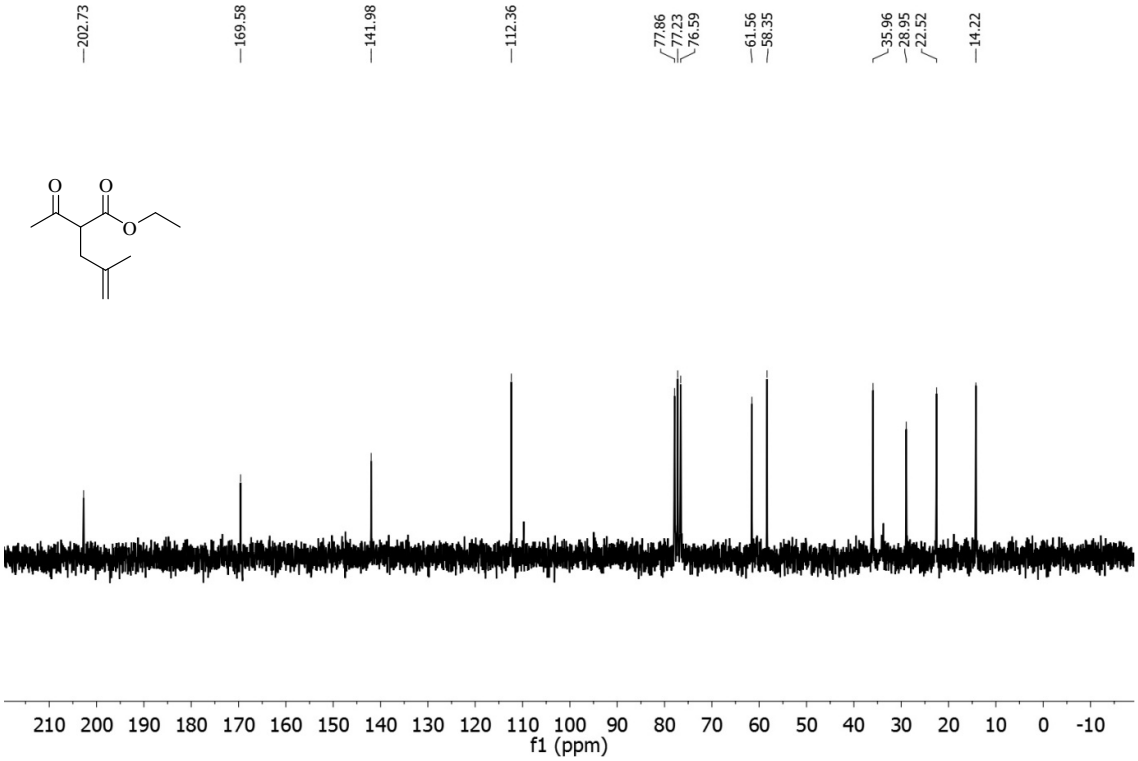
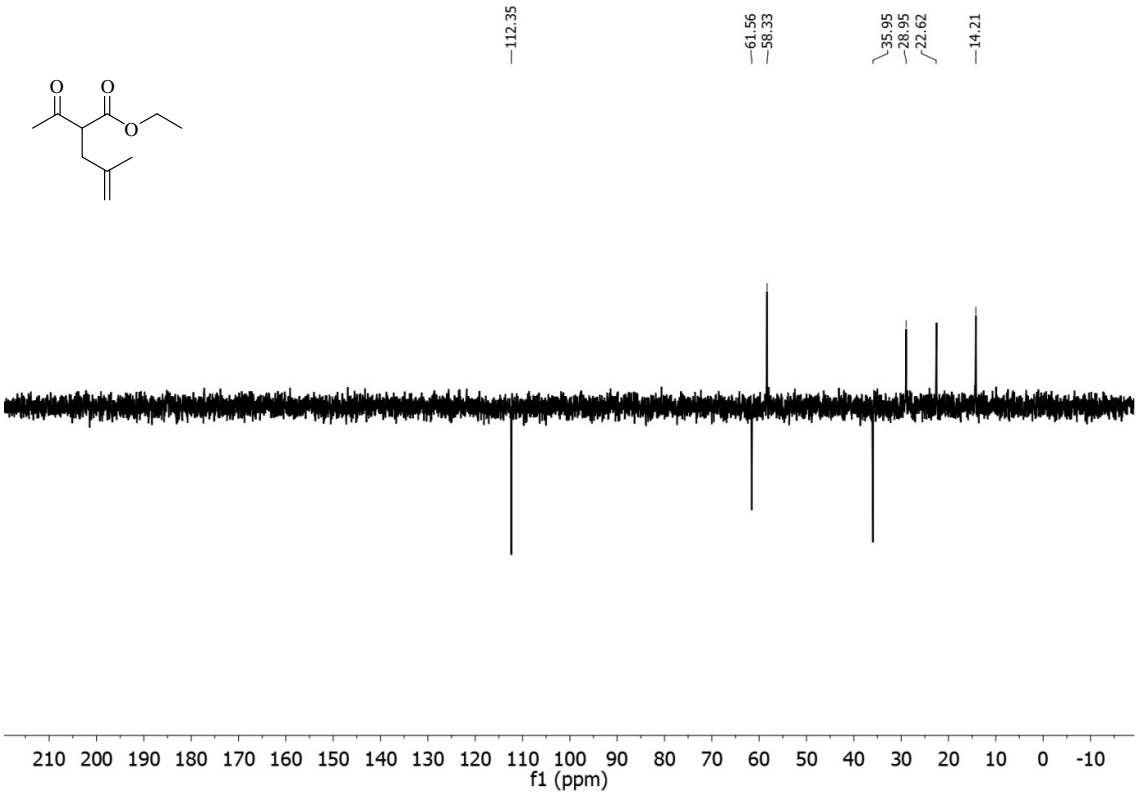
^{1}H - NMR of compound 2 (200 MHz, $CDCl_3$)



^{13}C NMR of compound 2 (50 MHz, $CDCl_3$)



DEPT-135 NMR of compound 2 (50 MHz, $CDCl_3$)



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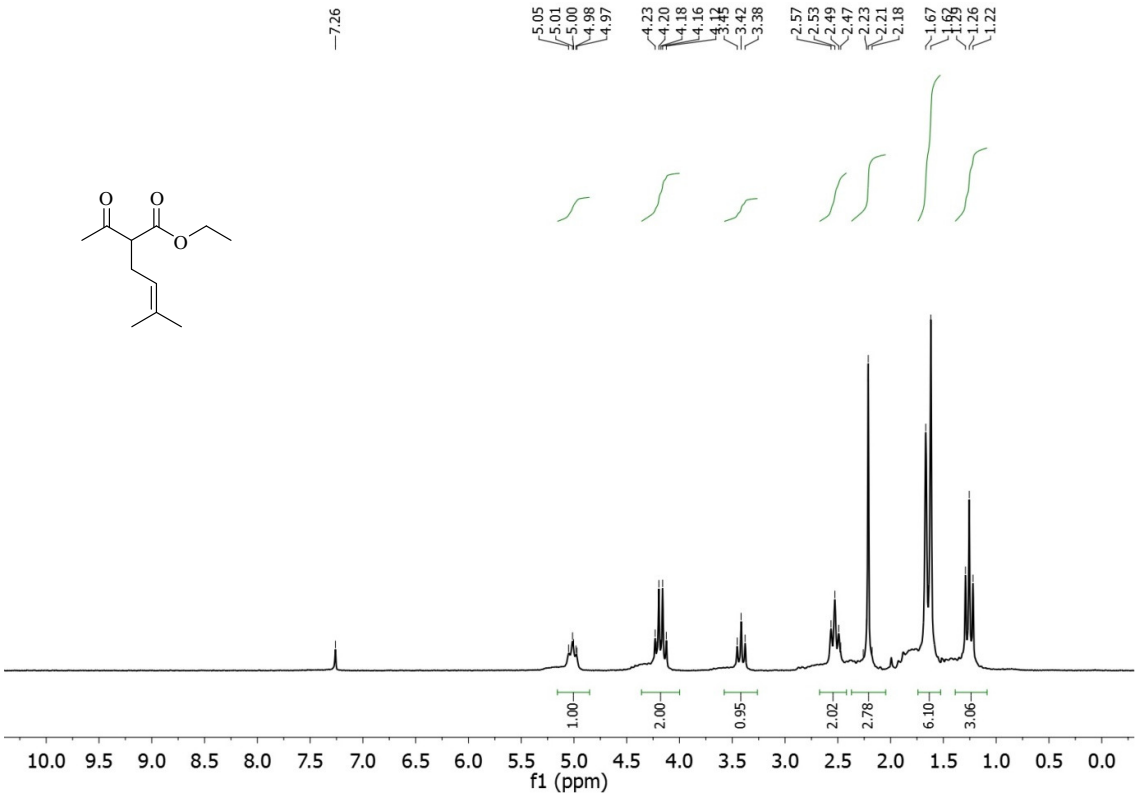

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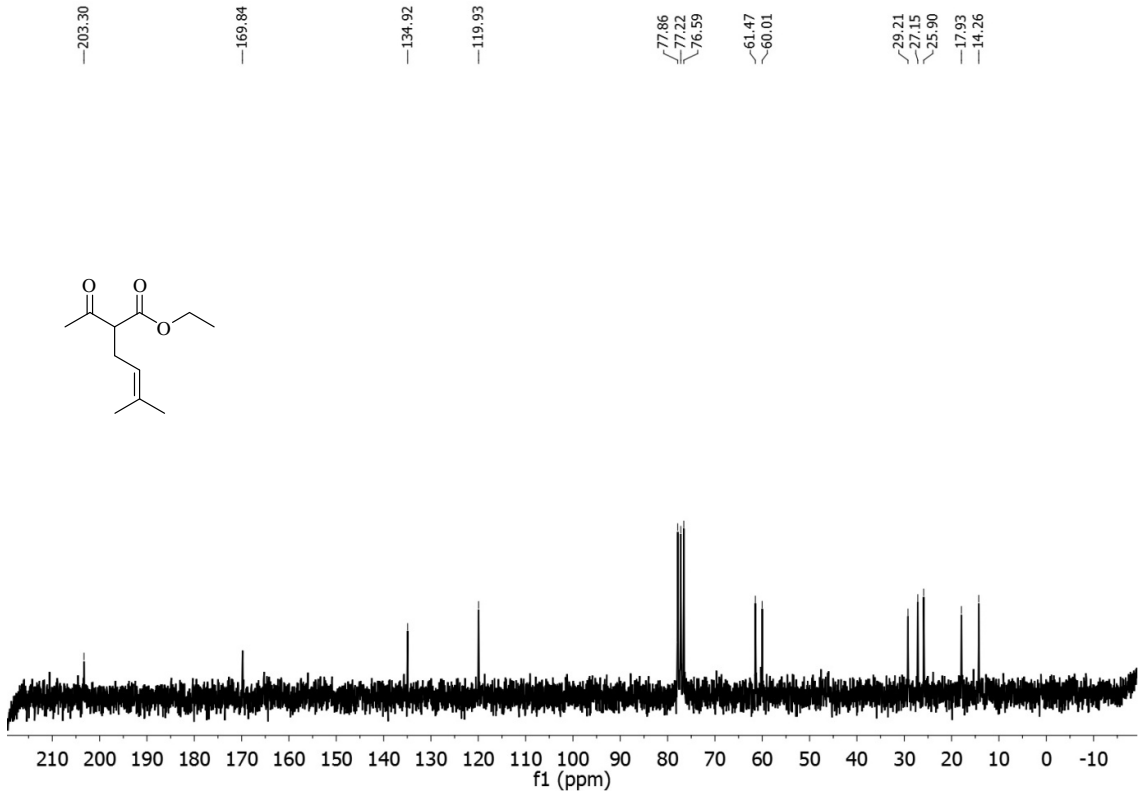

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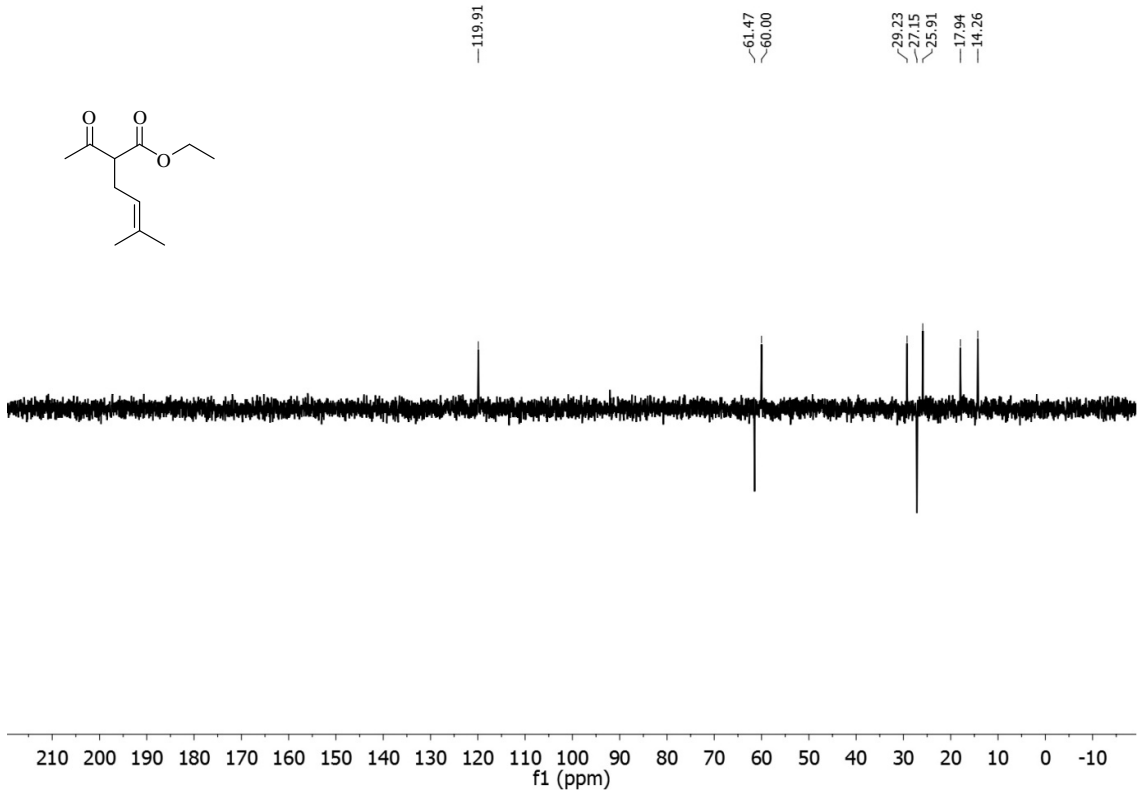

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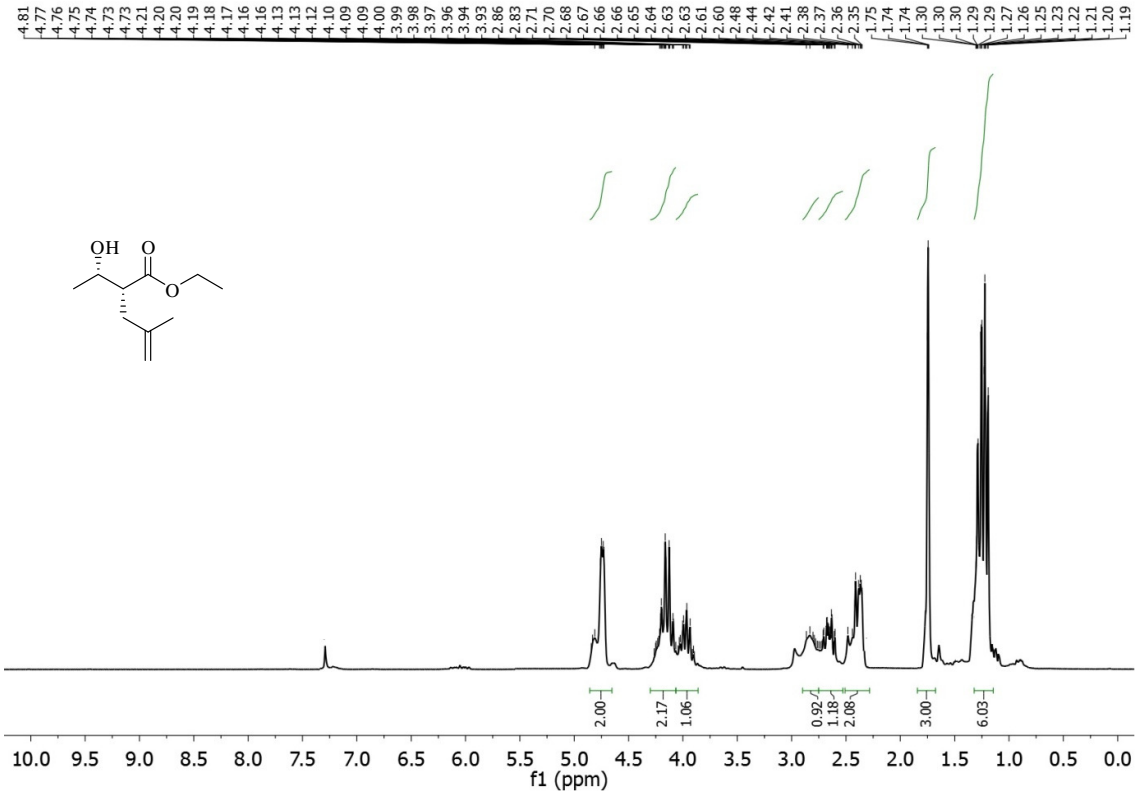

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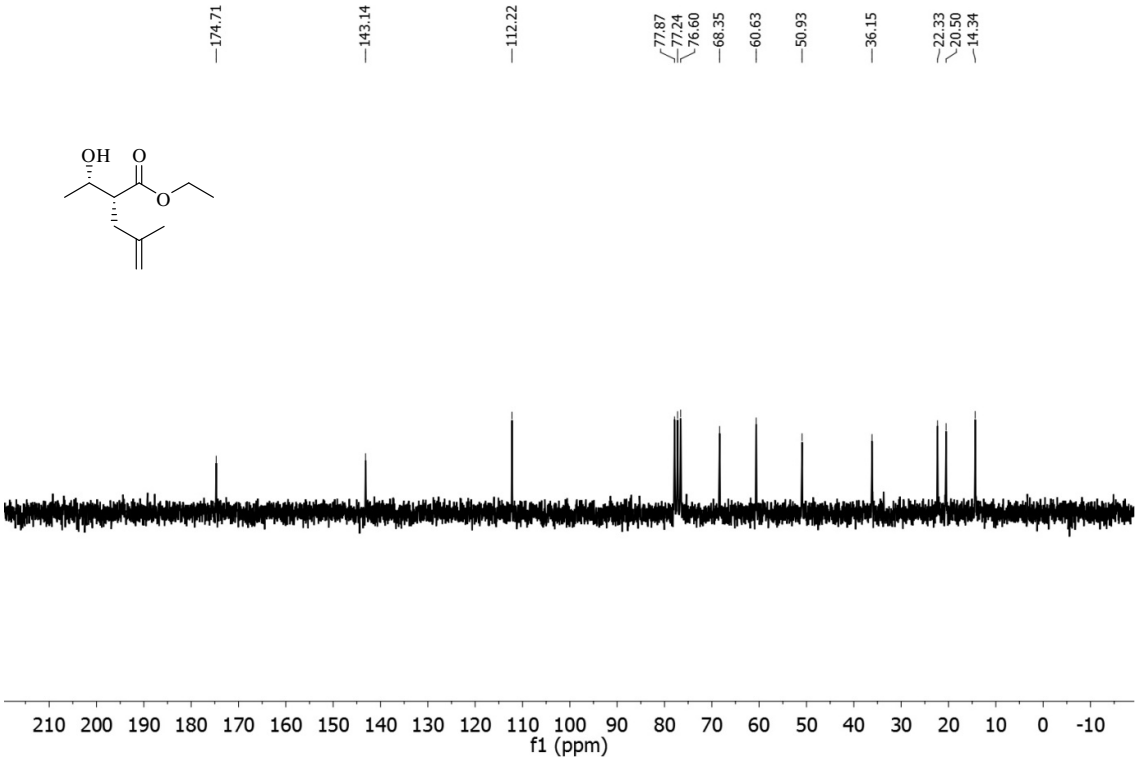

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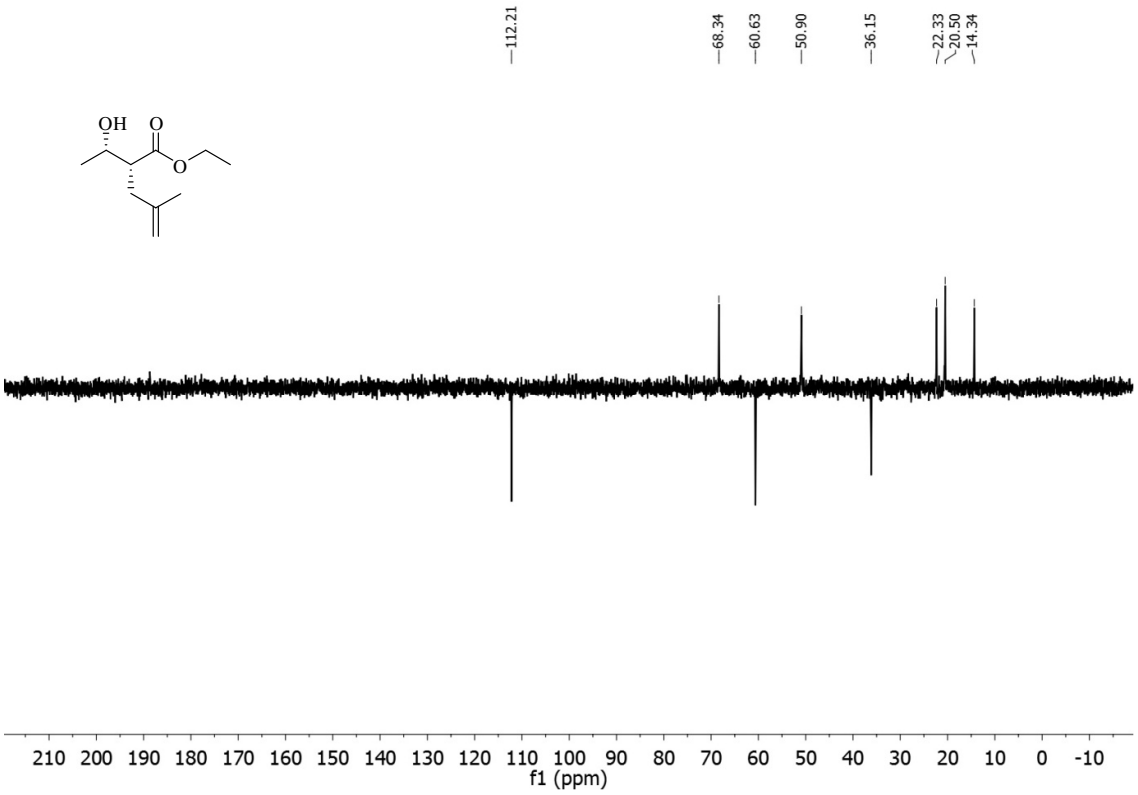

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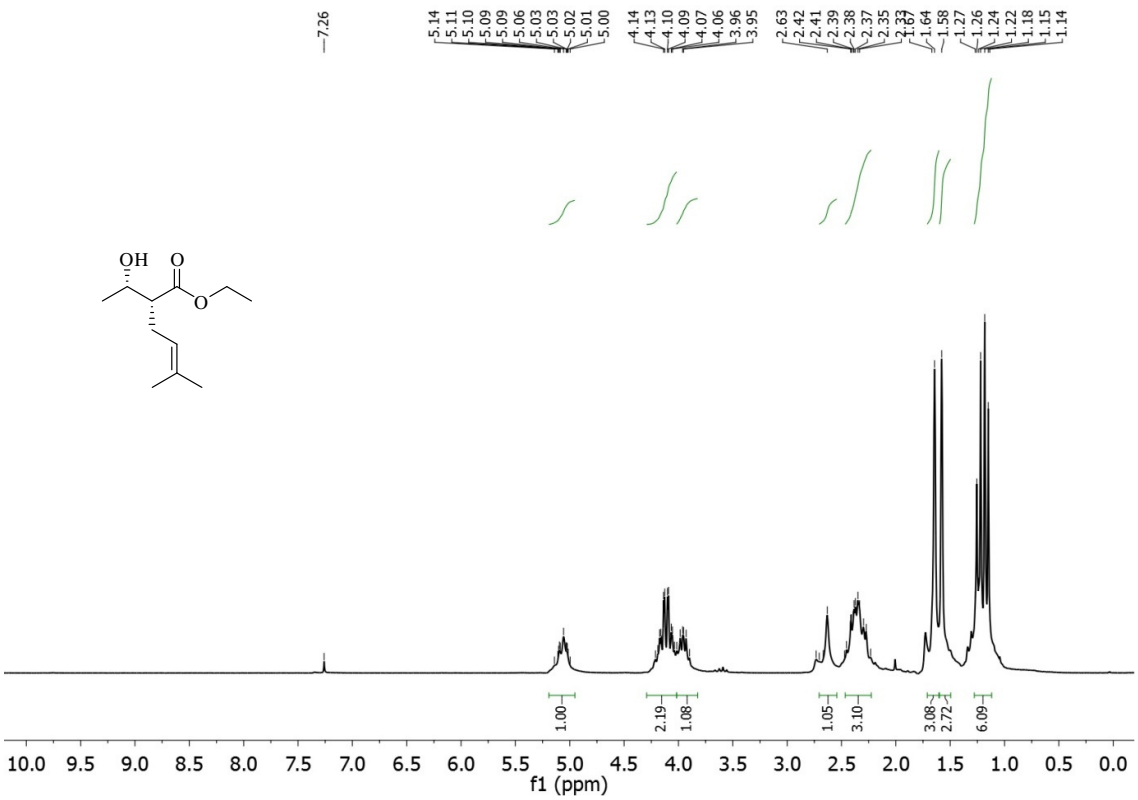

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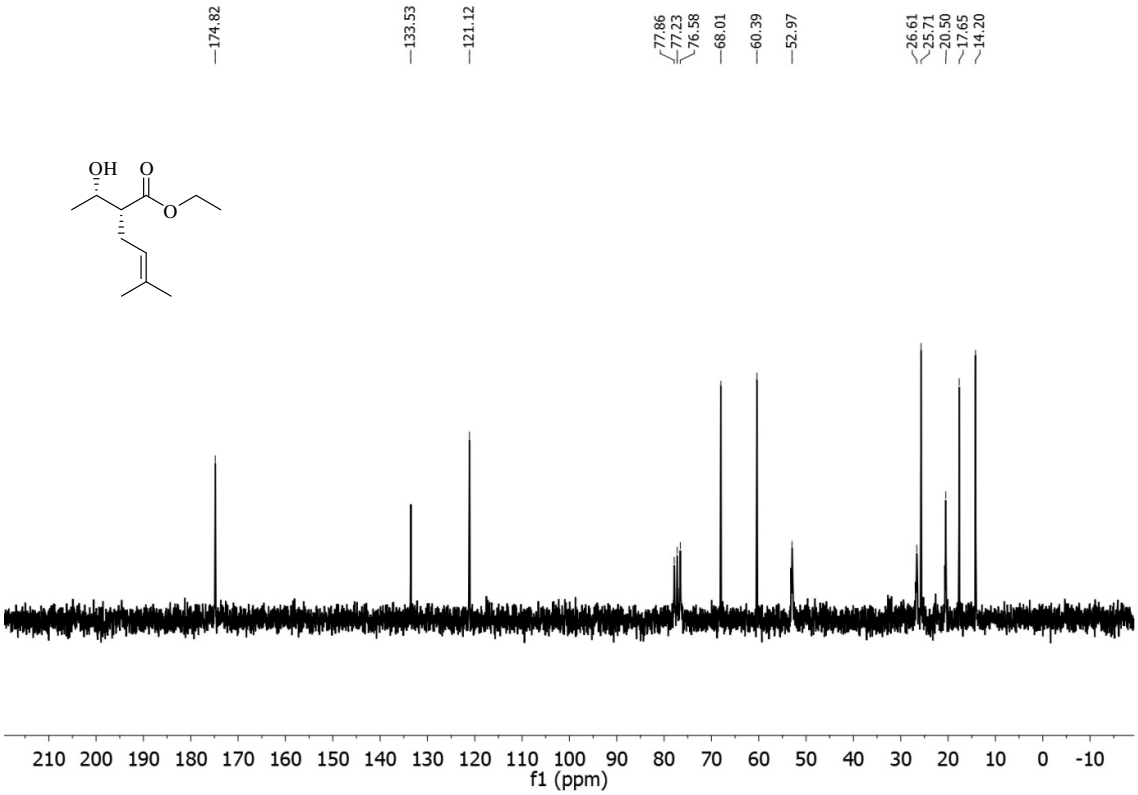

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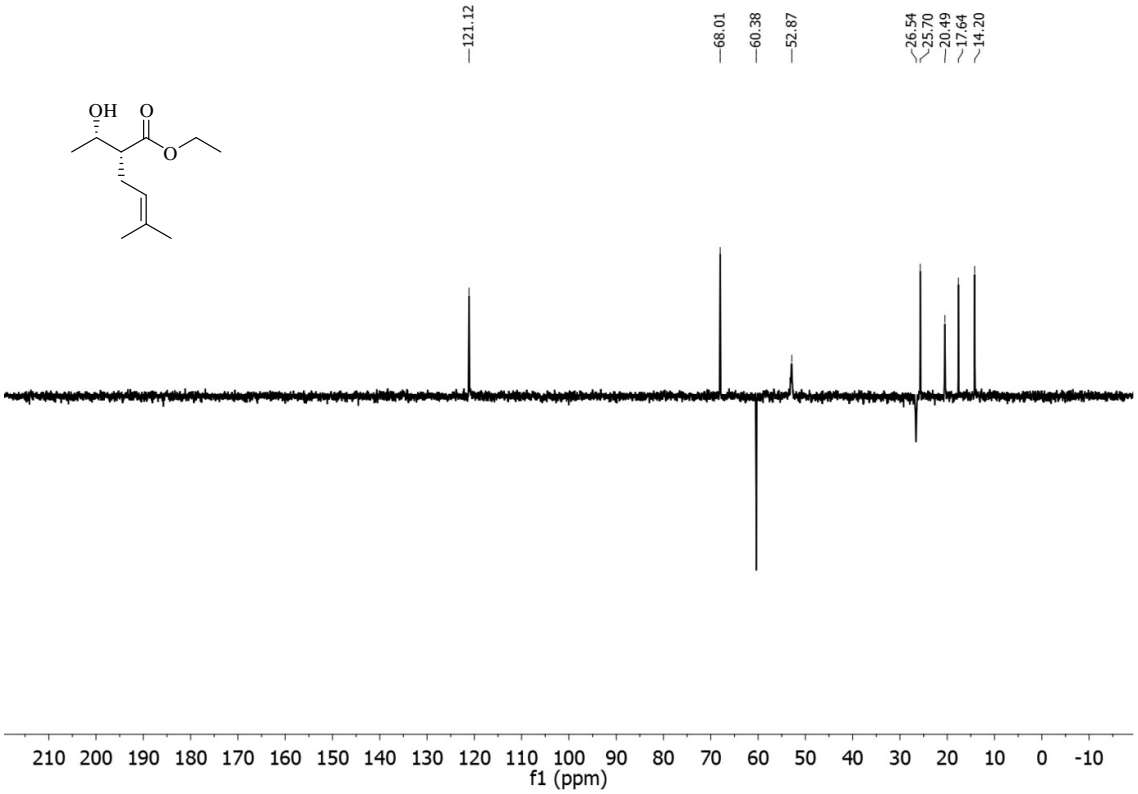

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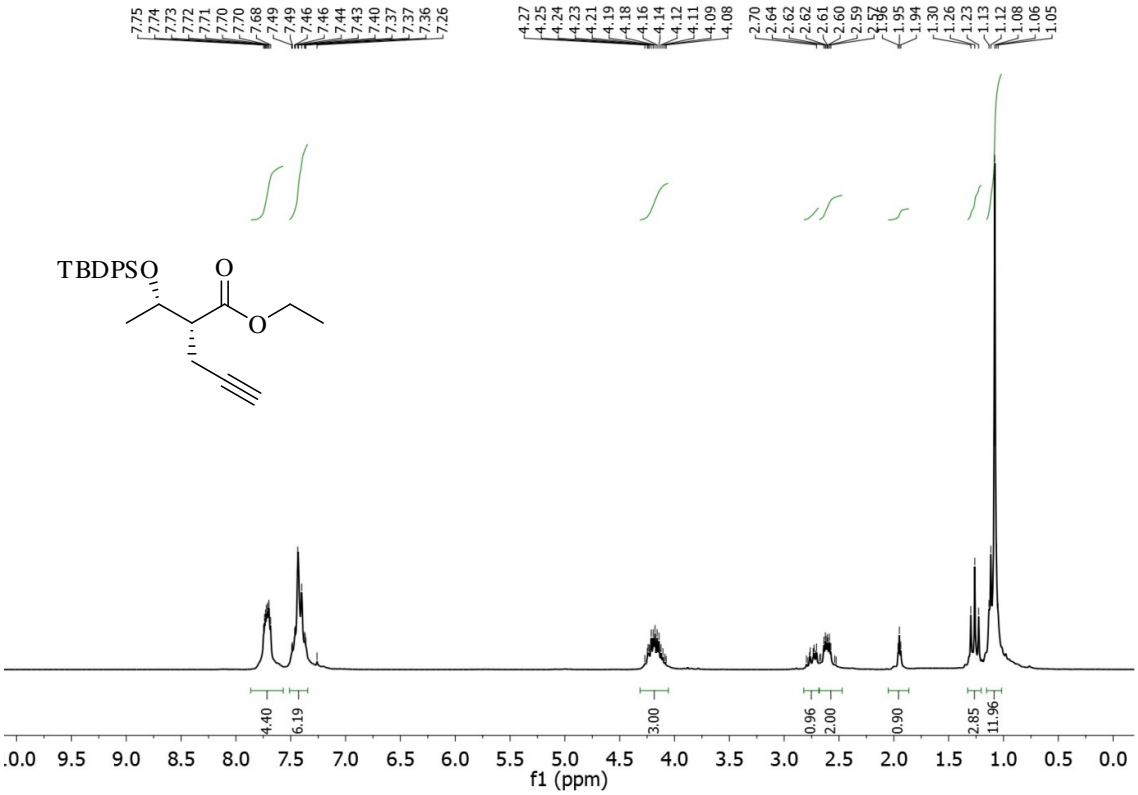

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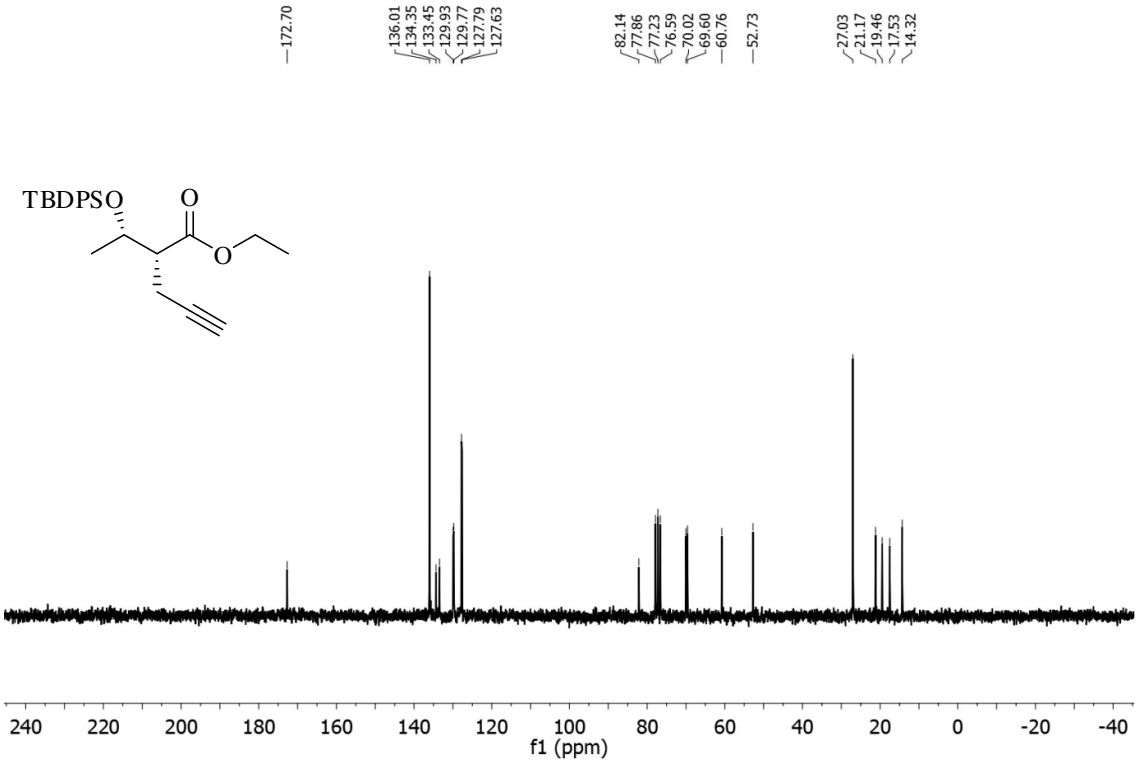

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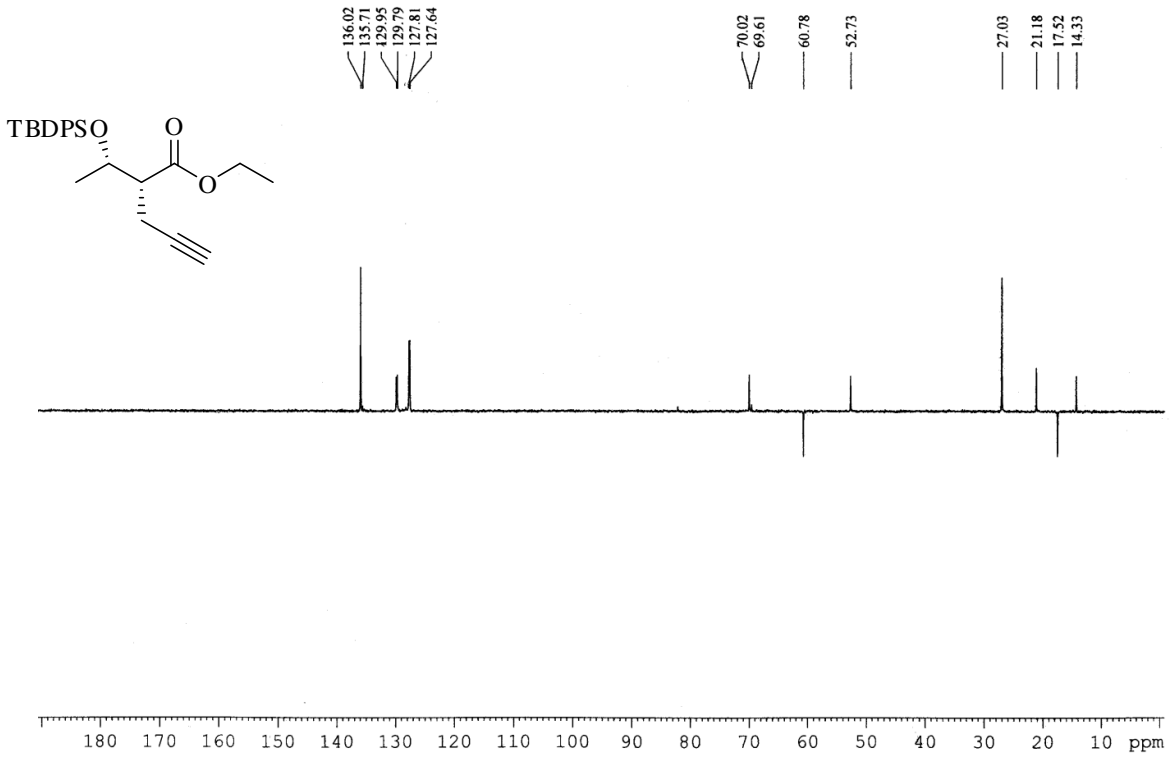

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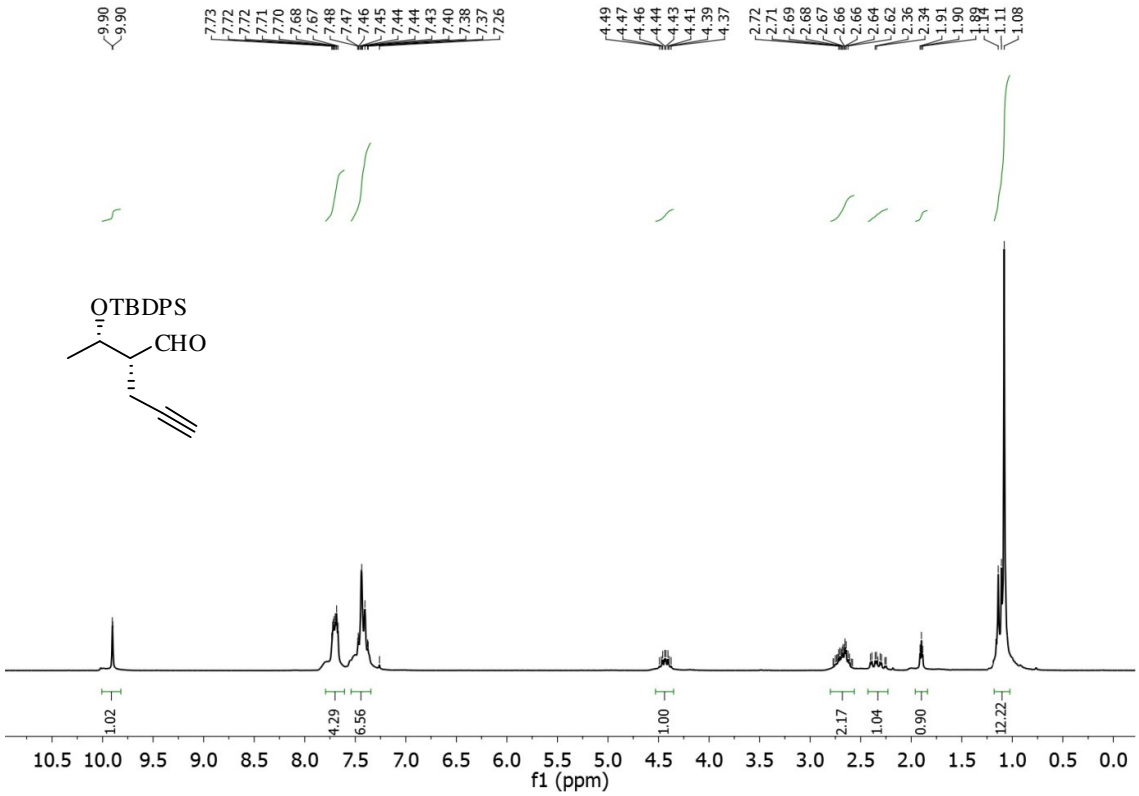

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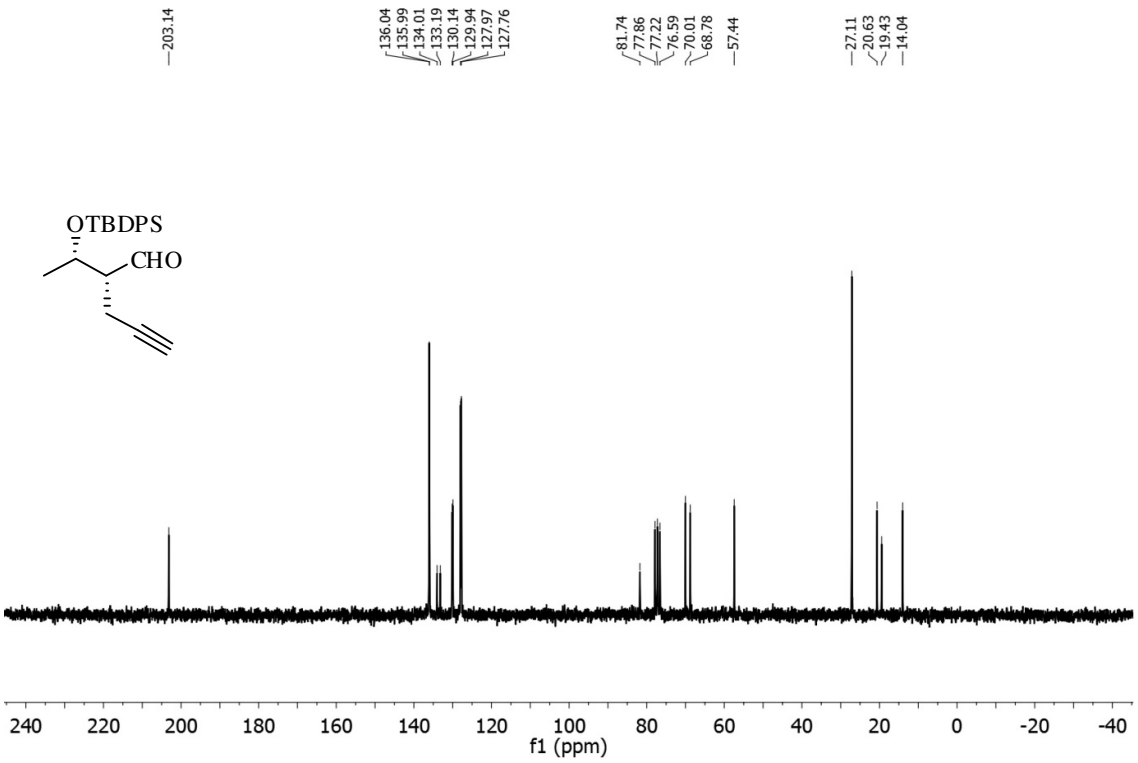

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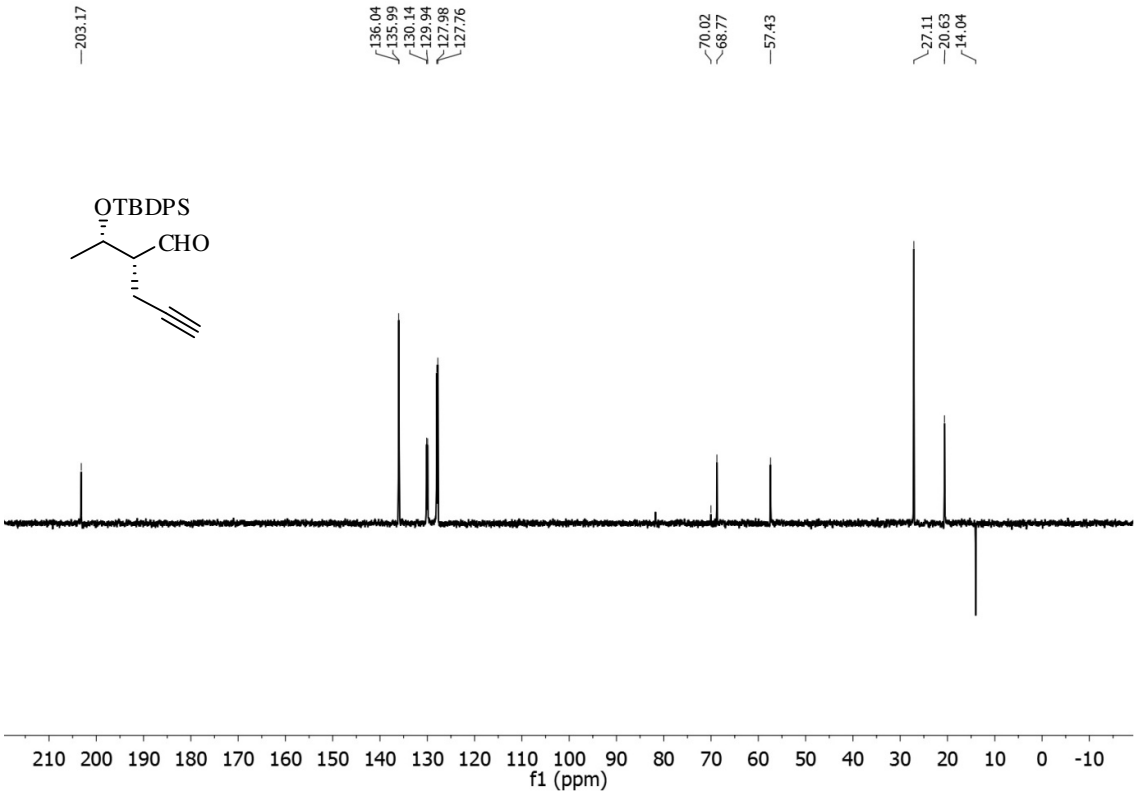

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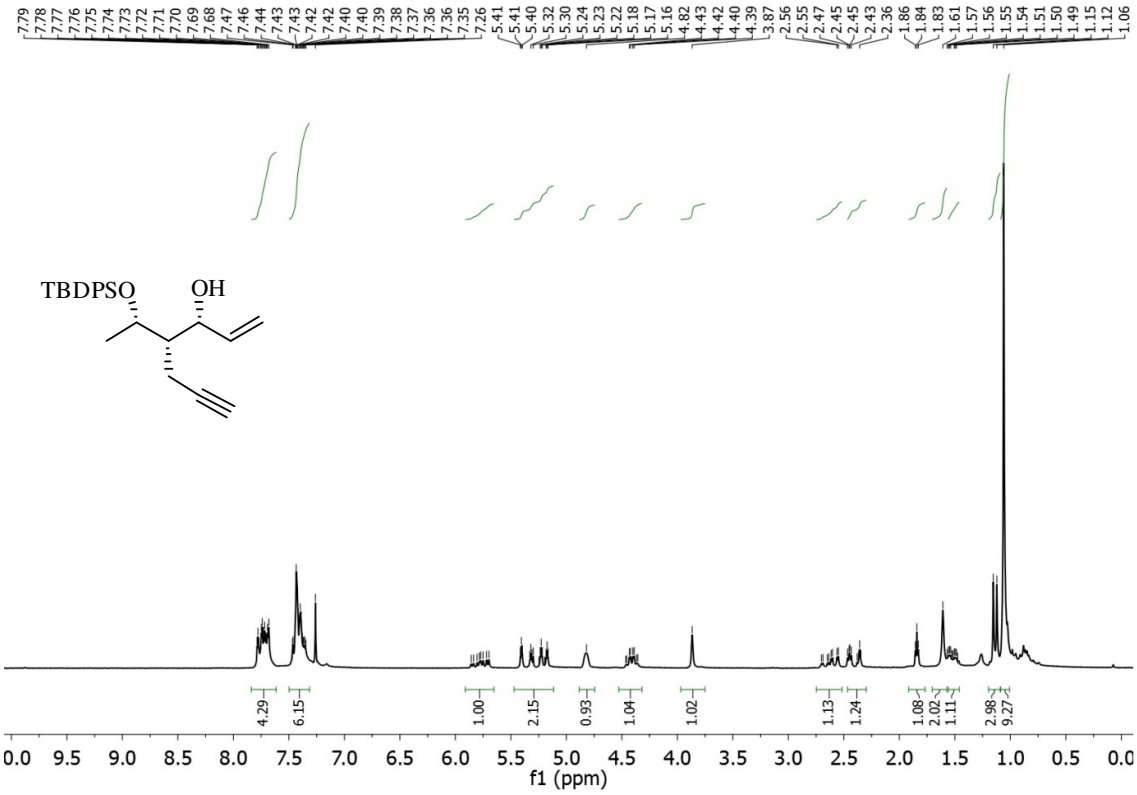

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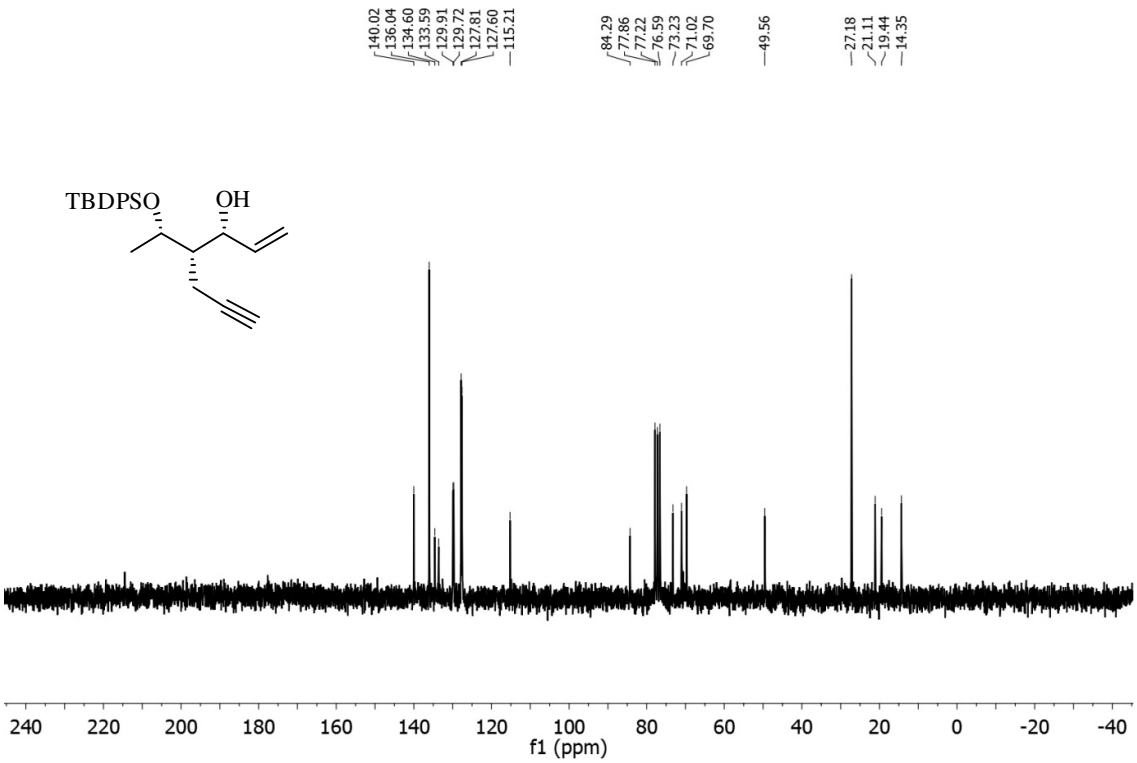

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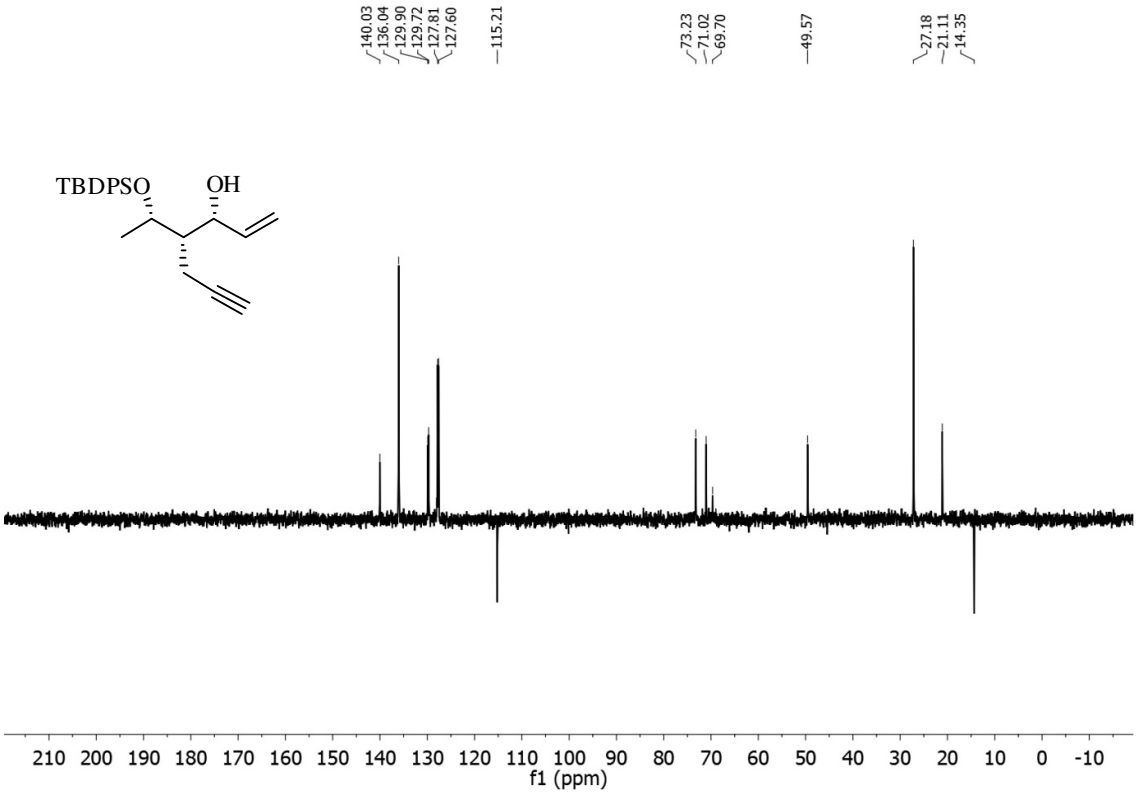

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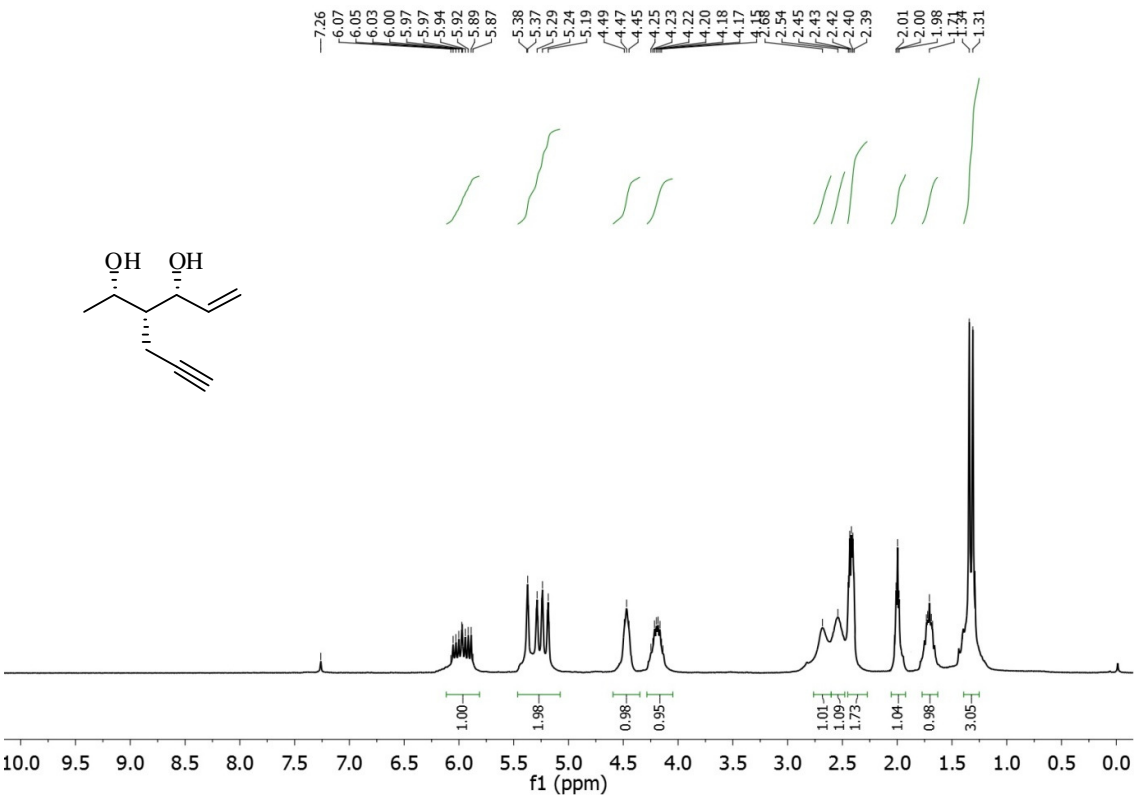

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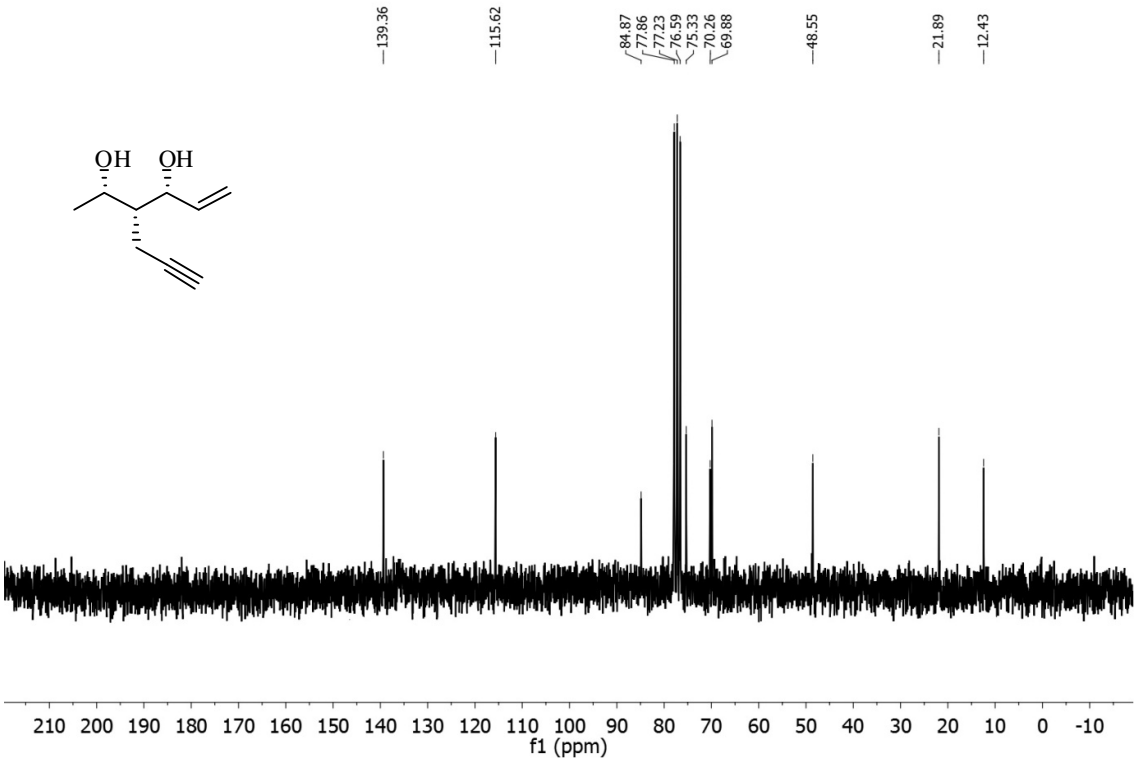

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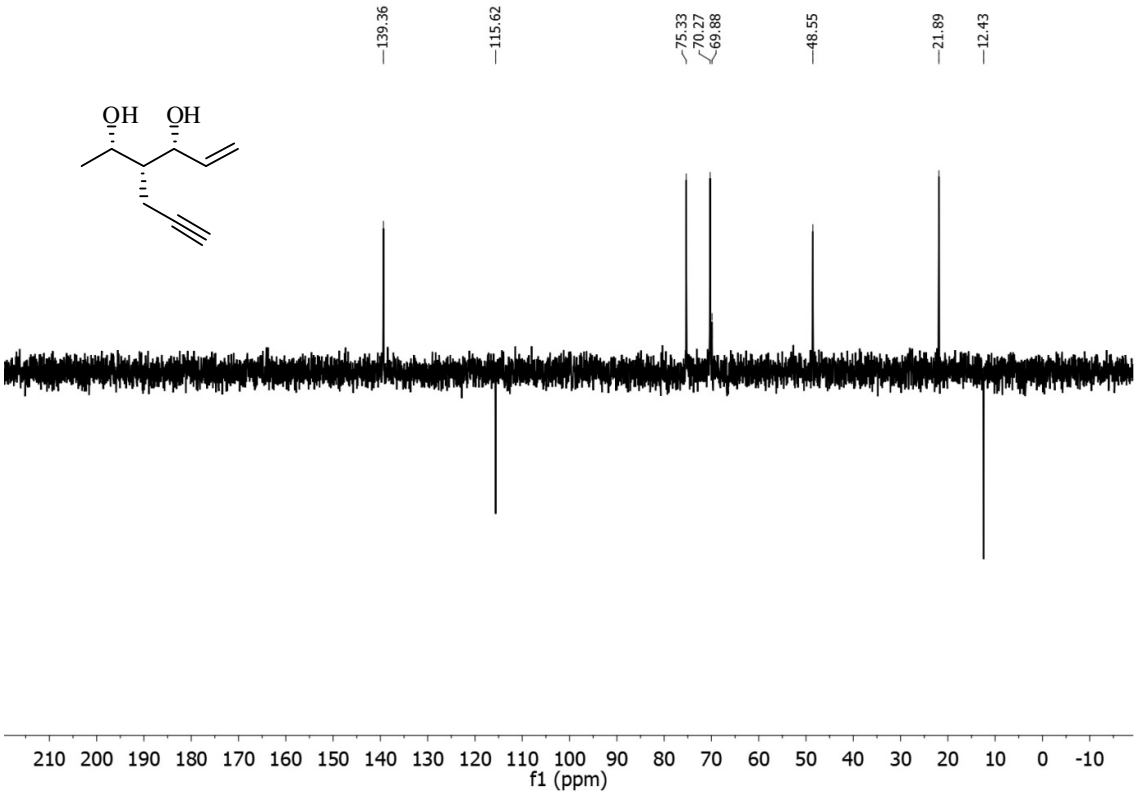
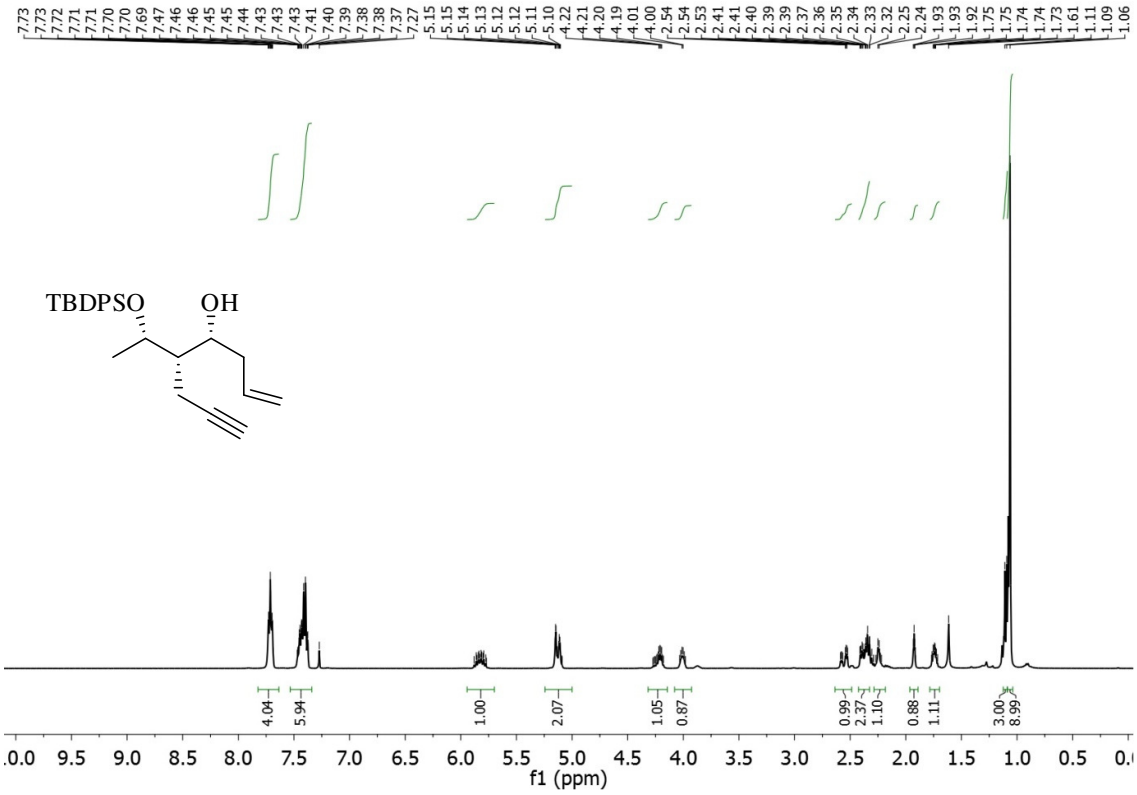


^{1}H - NMR of compound 13a (400 MHz, $CDCl_3$)



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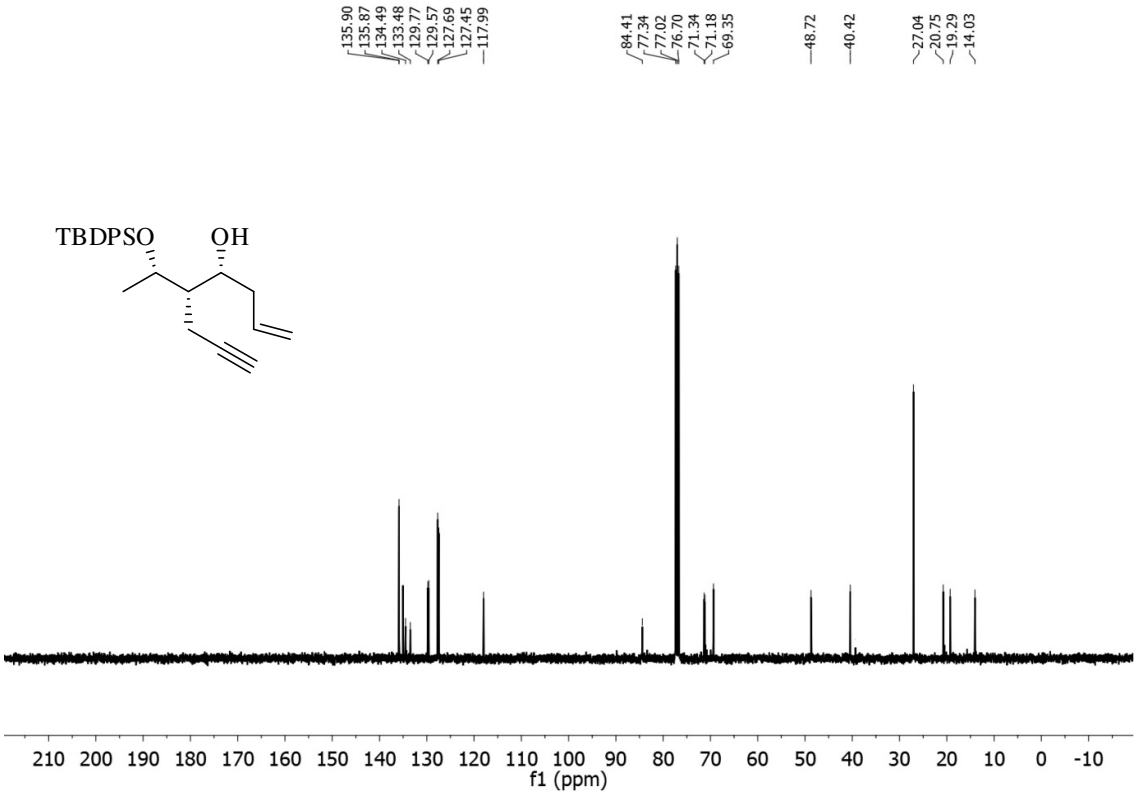

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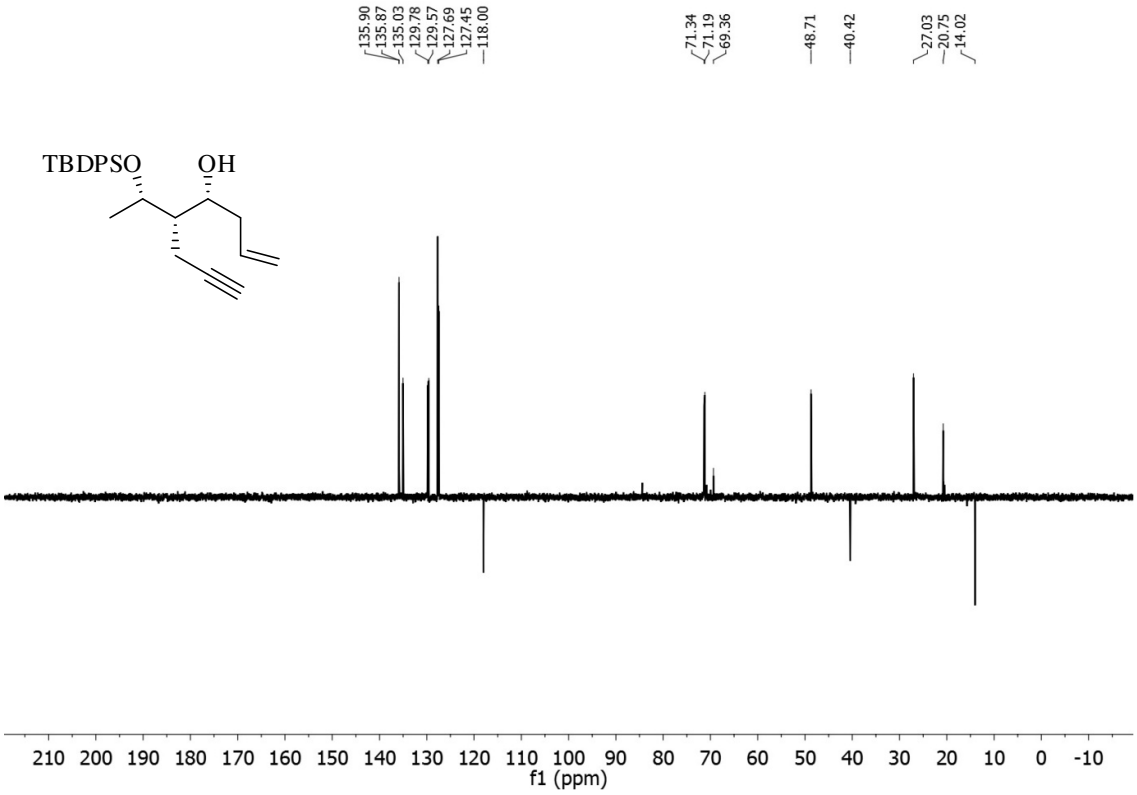

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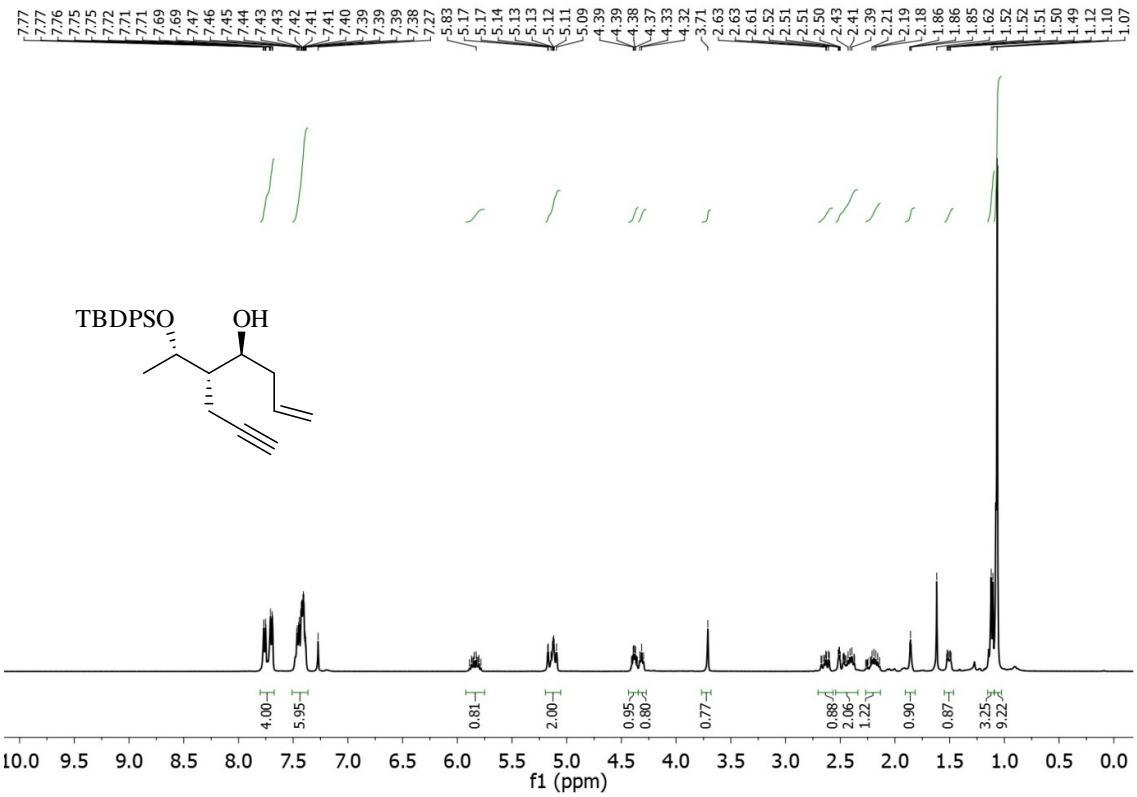

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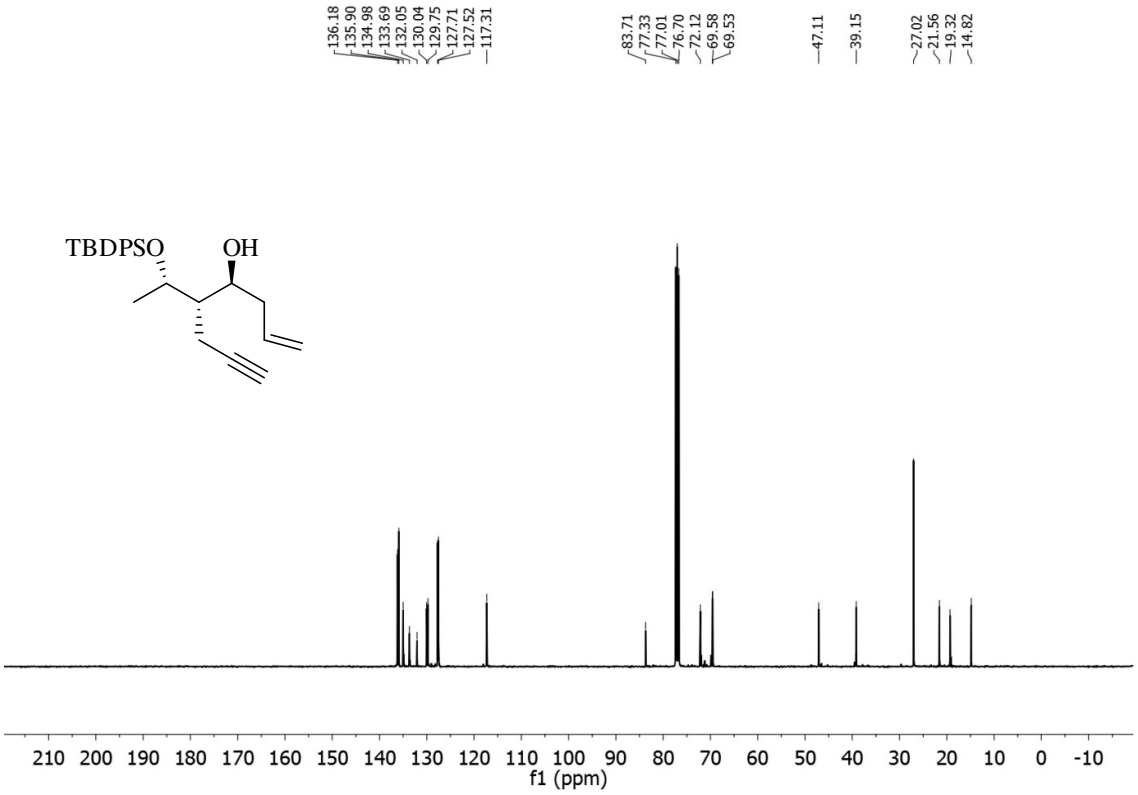

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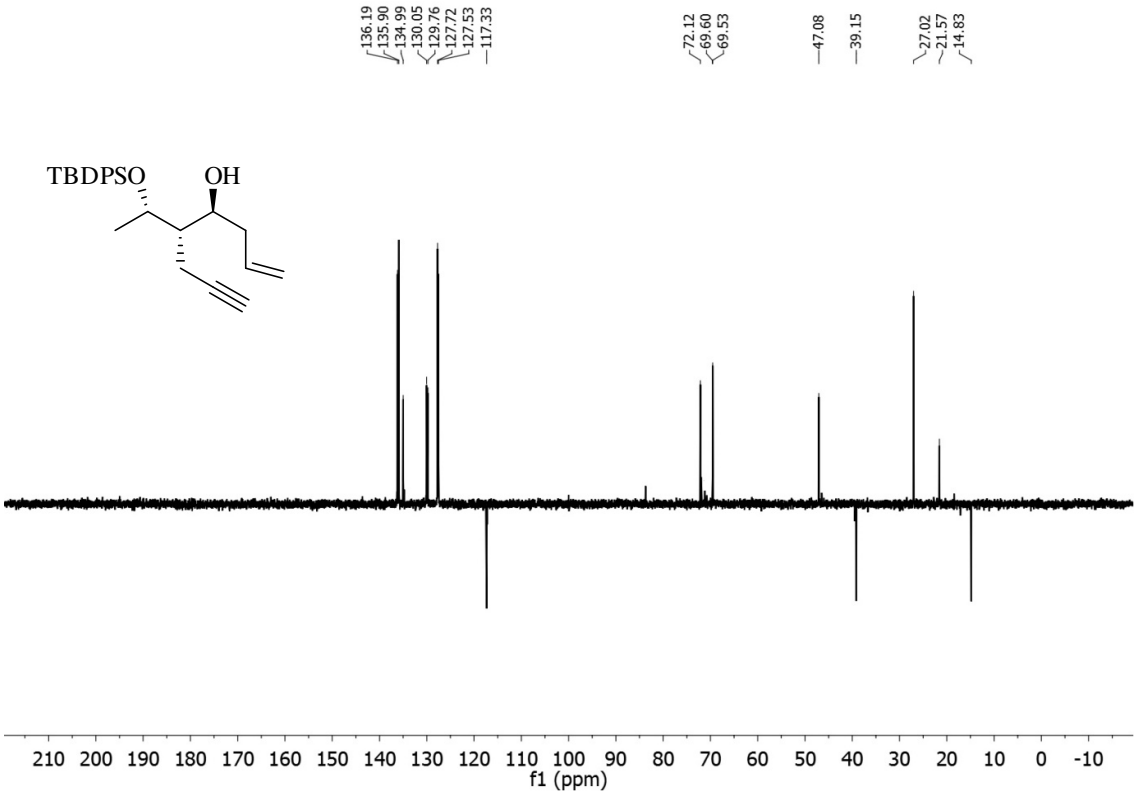

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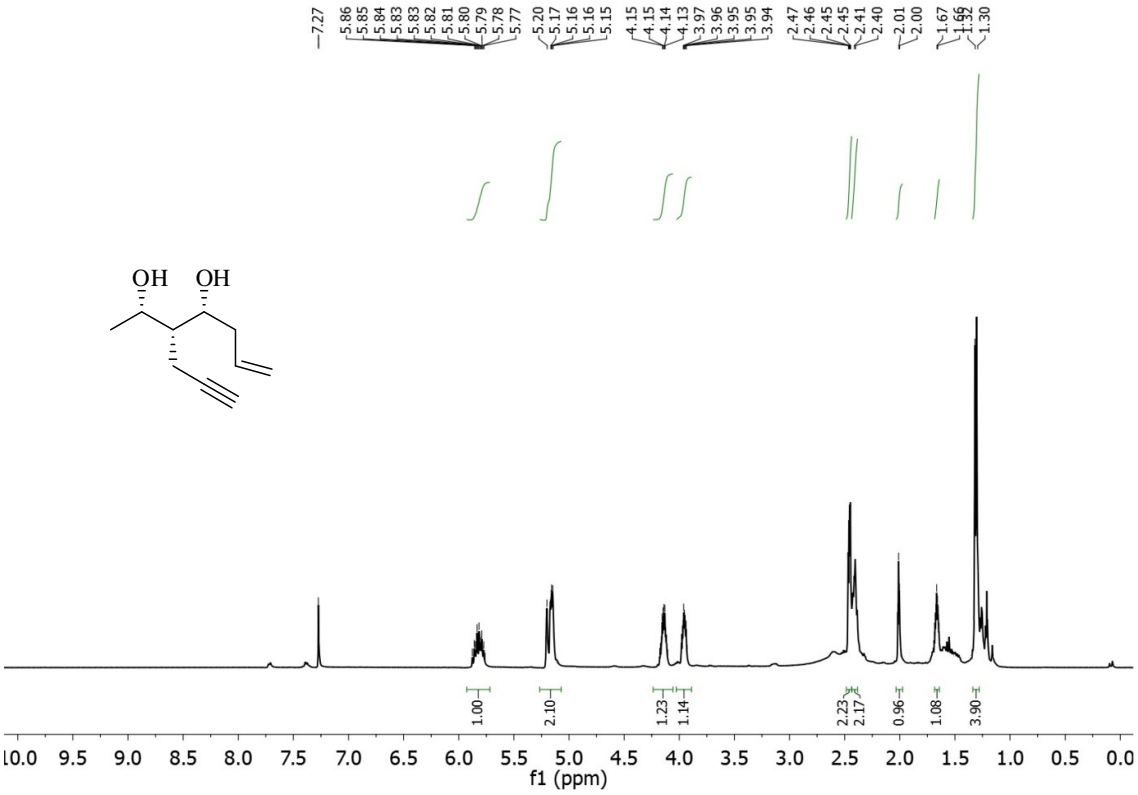

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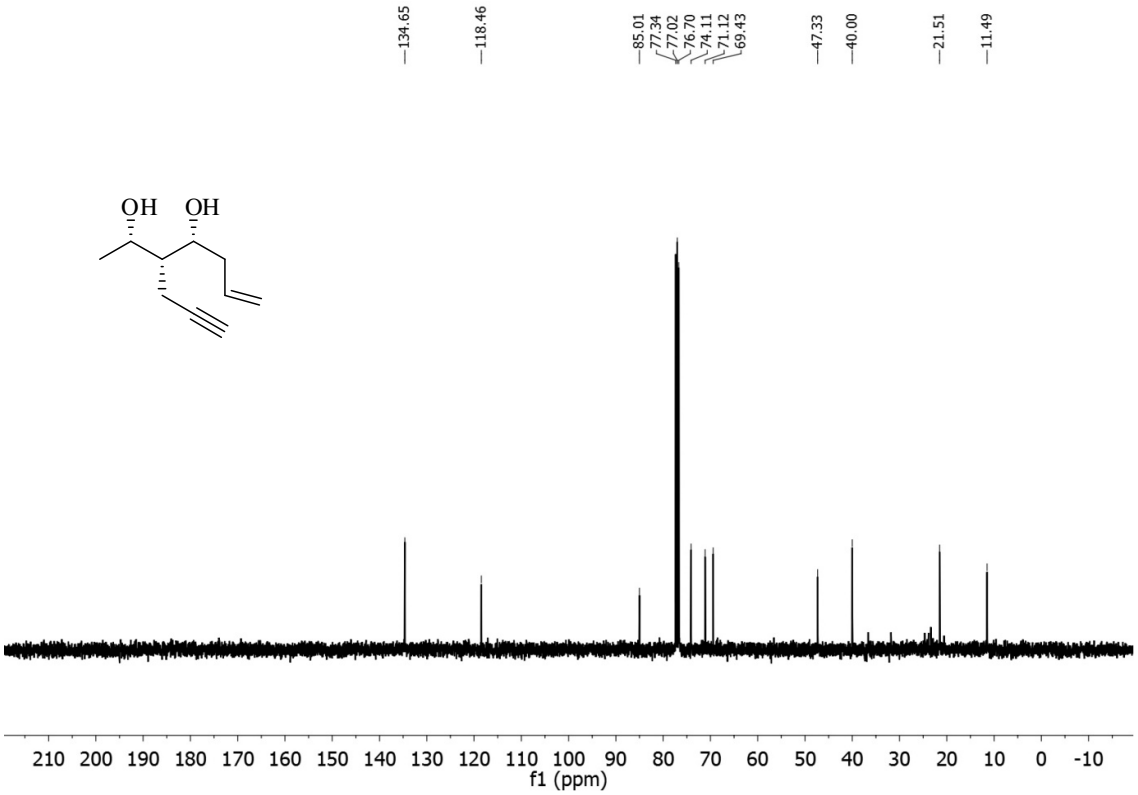

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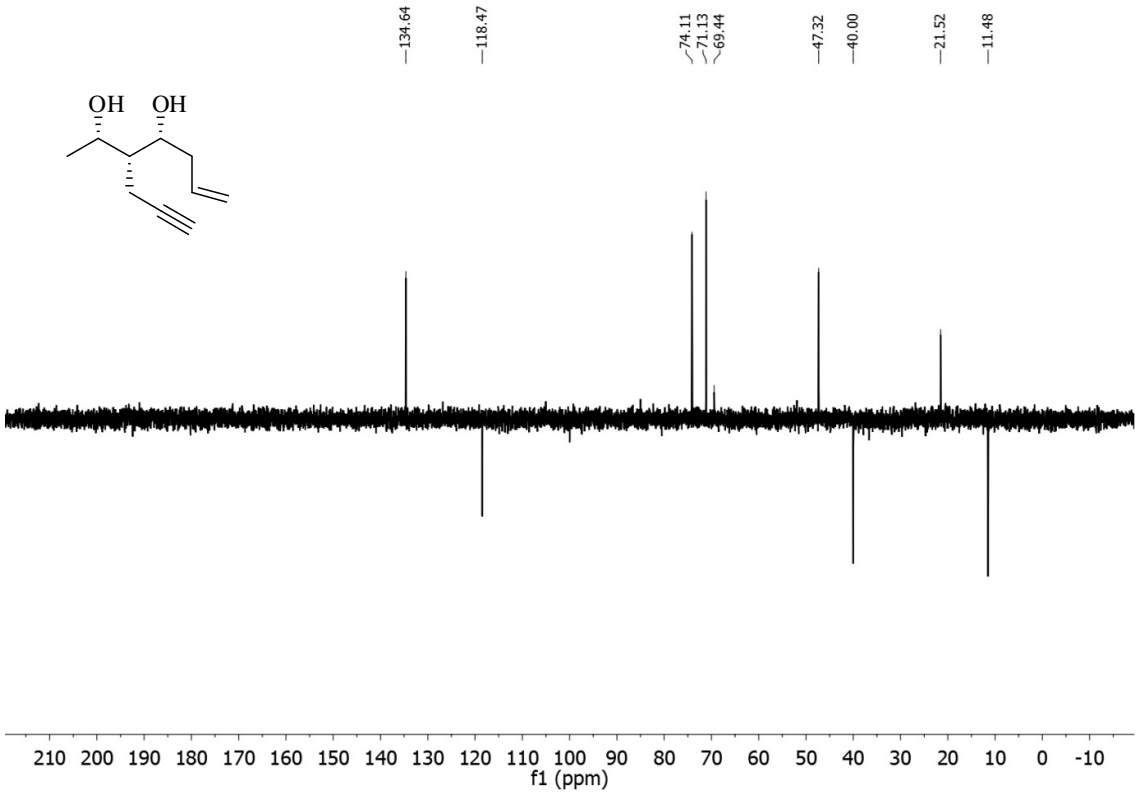

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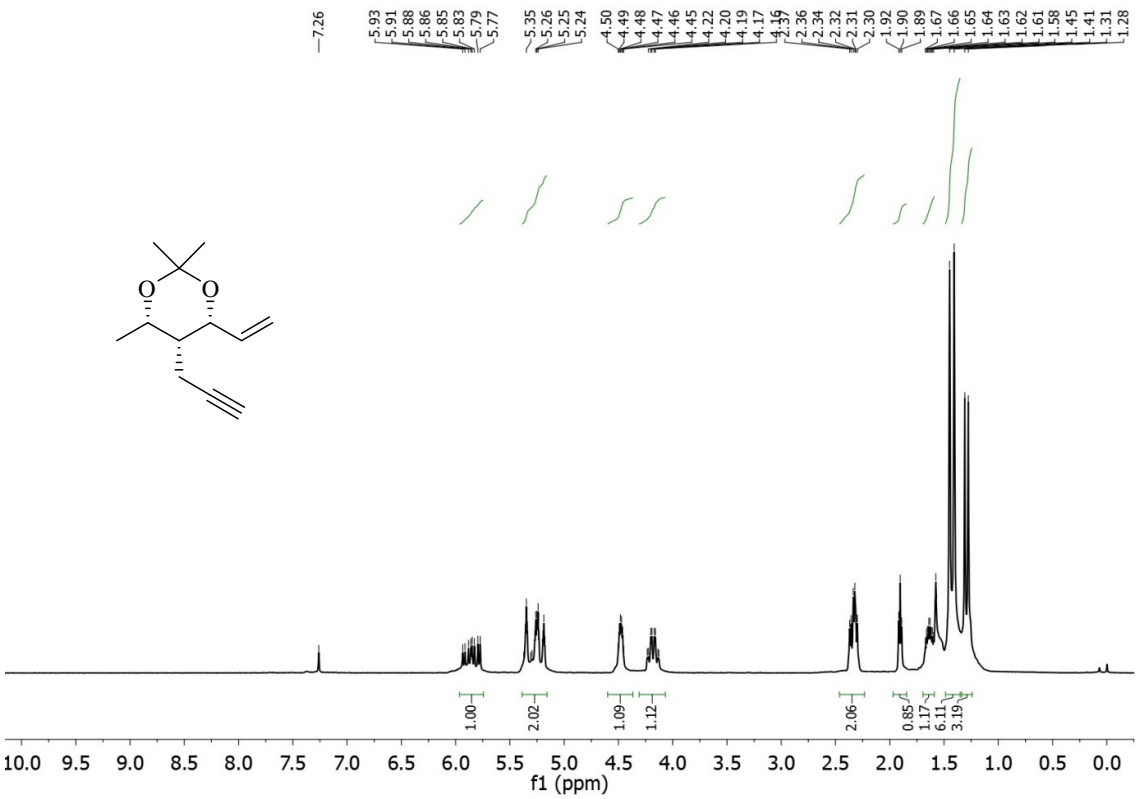

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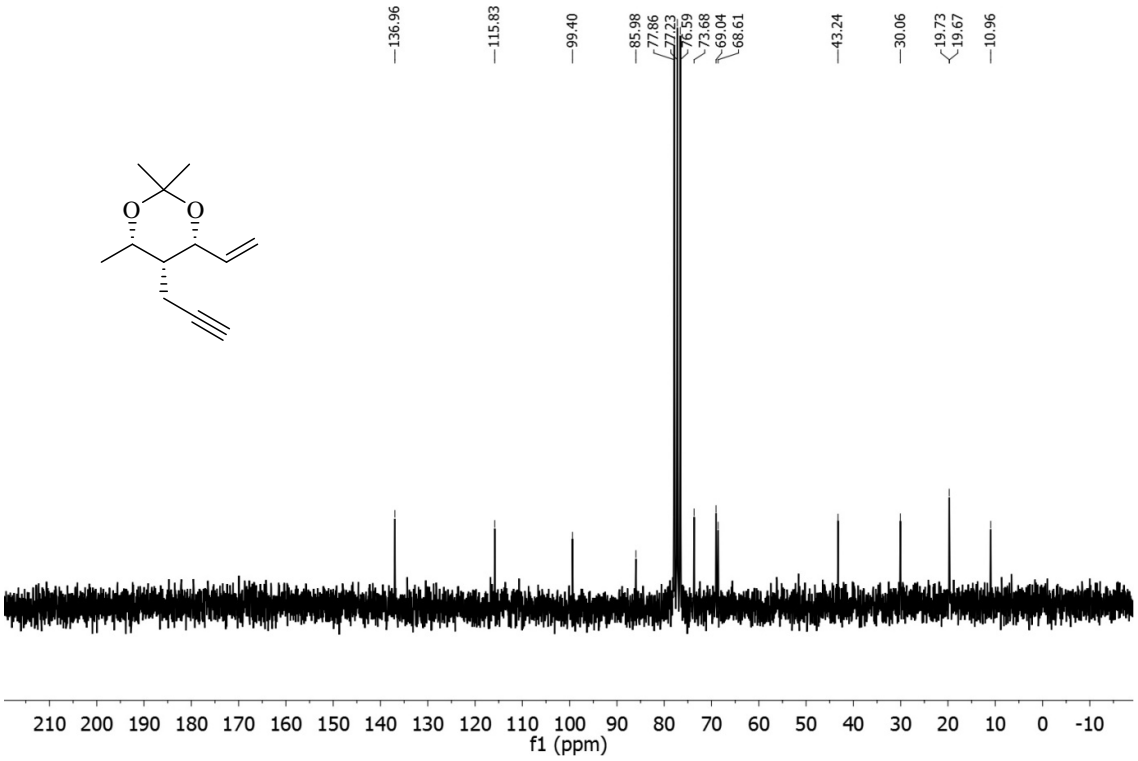
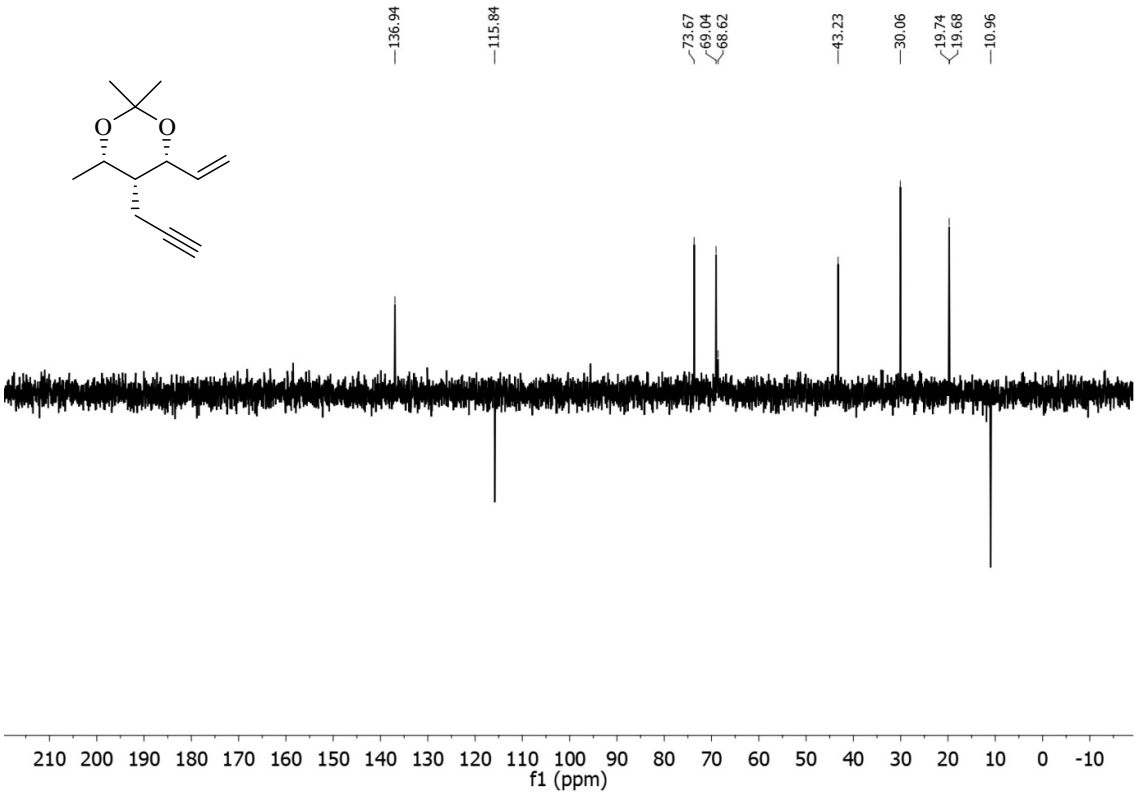


DEPT-135 NMR of compound 15 (50 MHz, $CDCl_3$)



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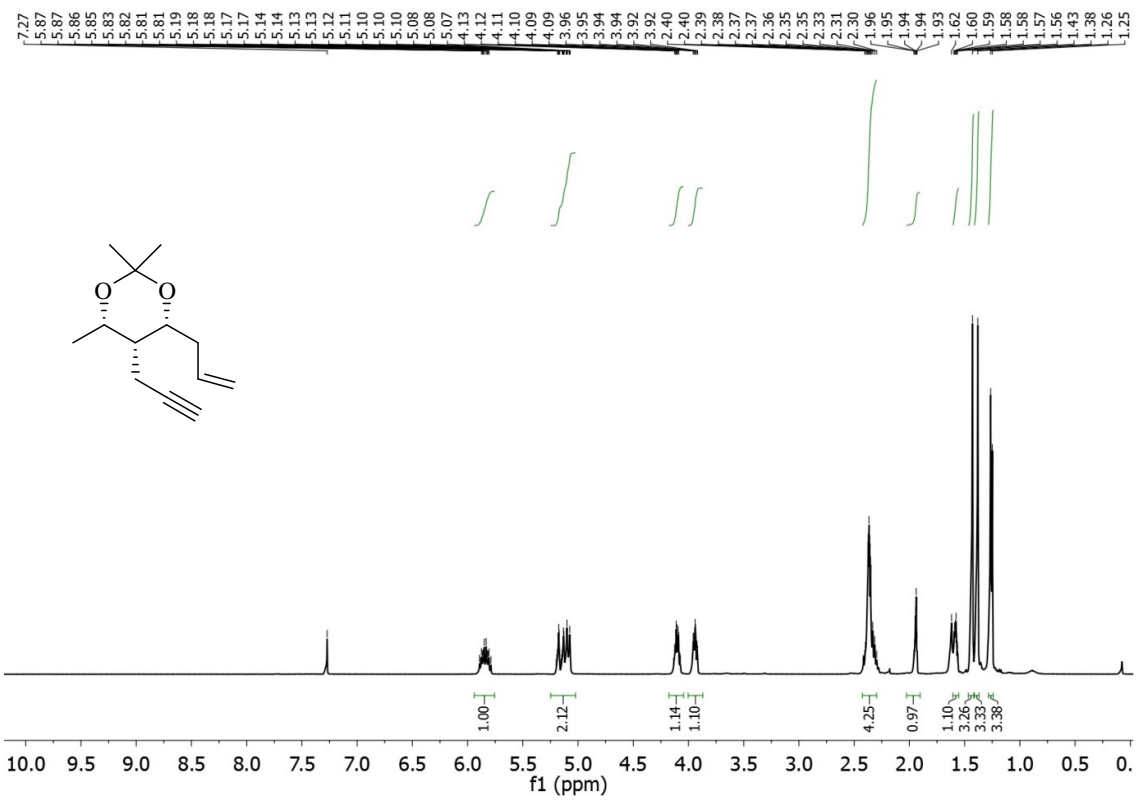

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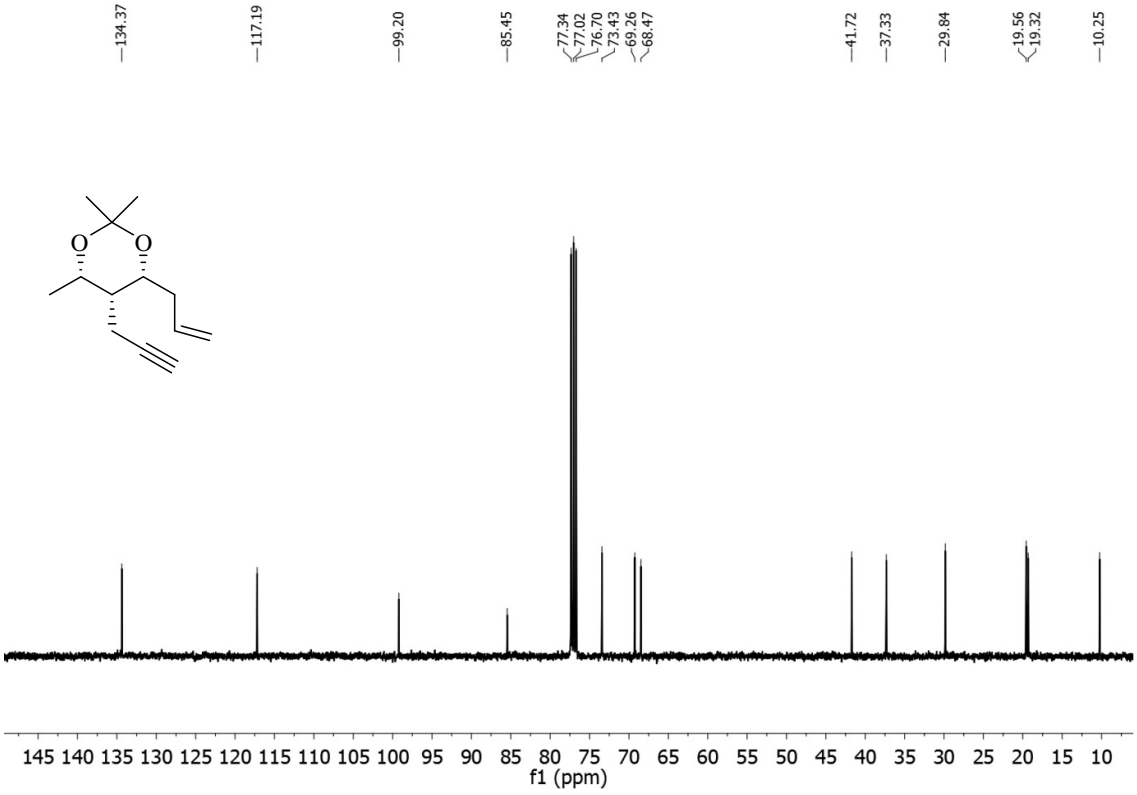

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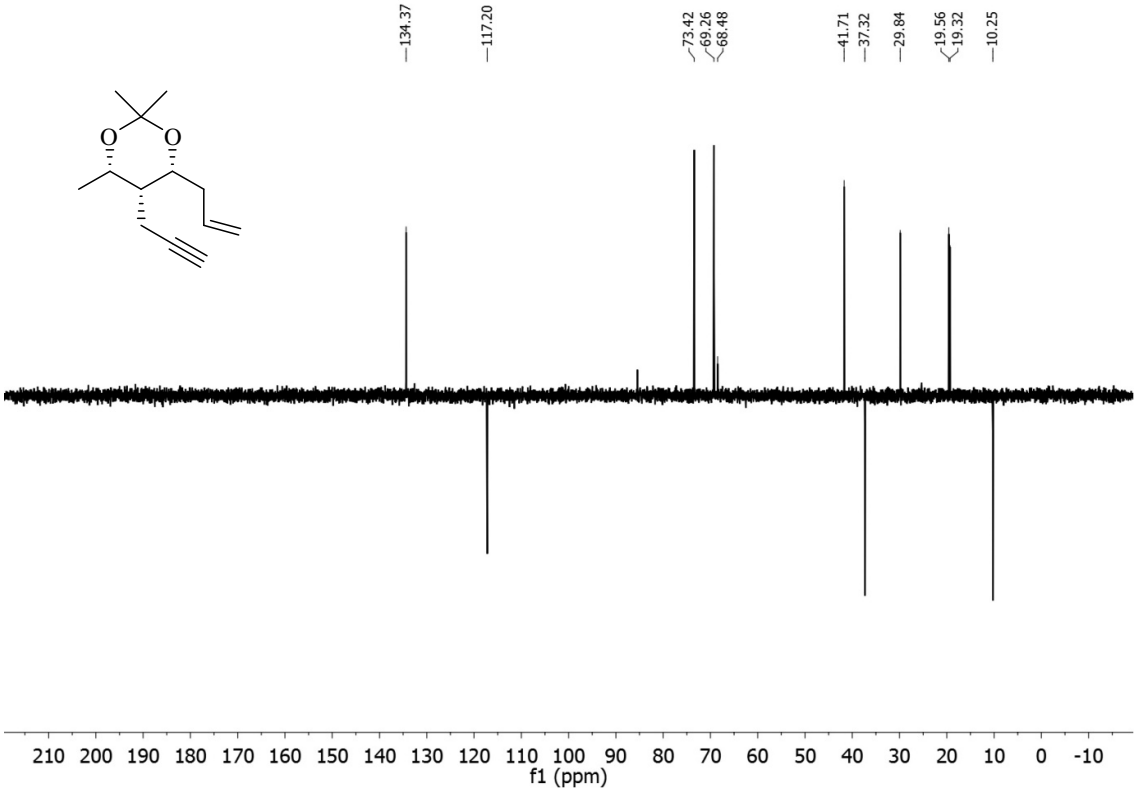

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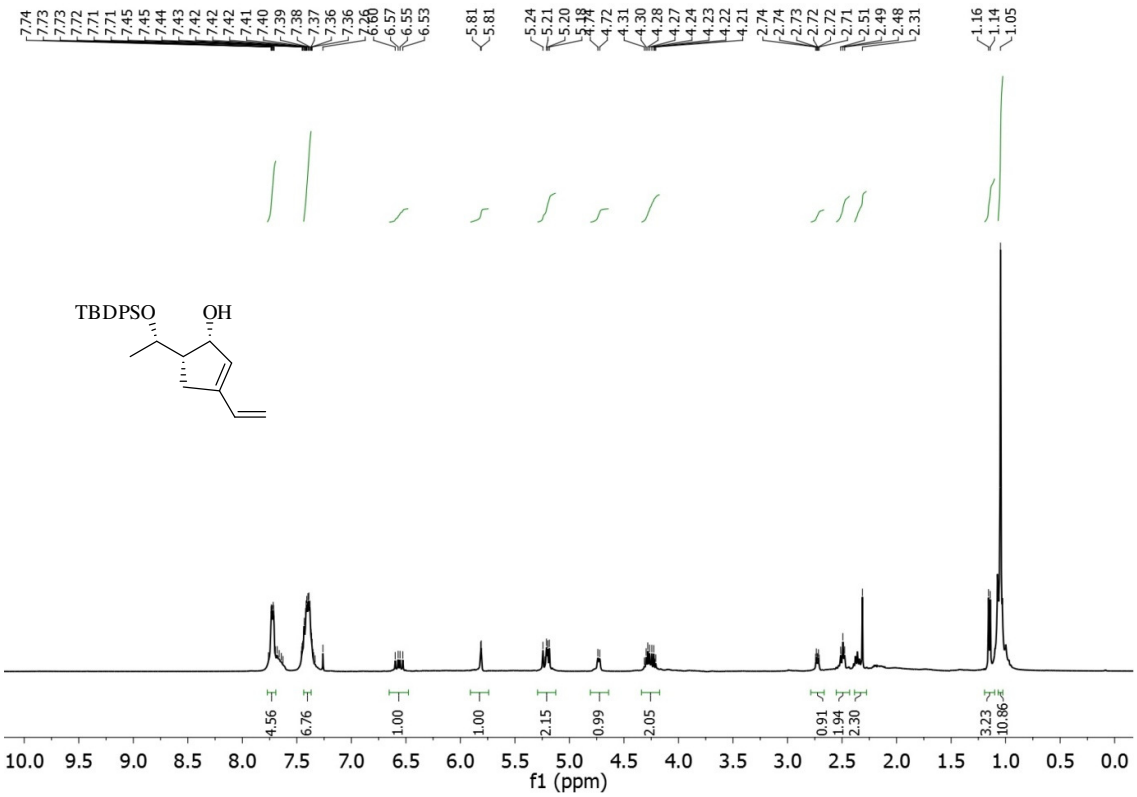

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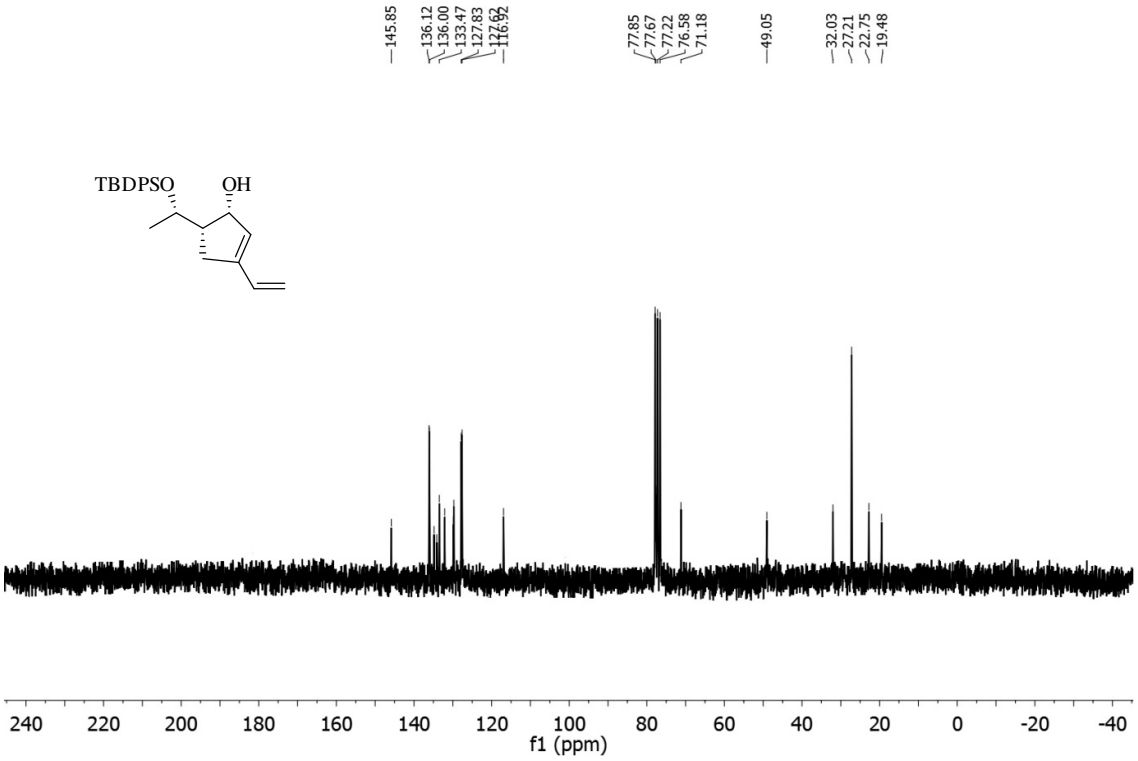

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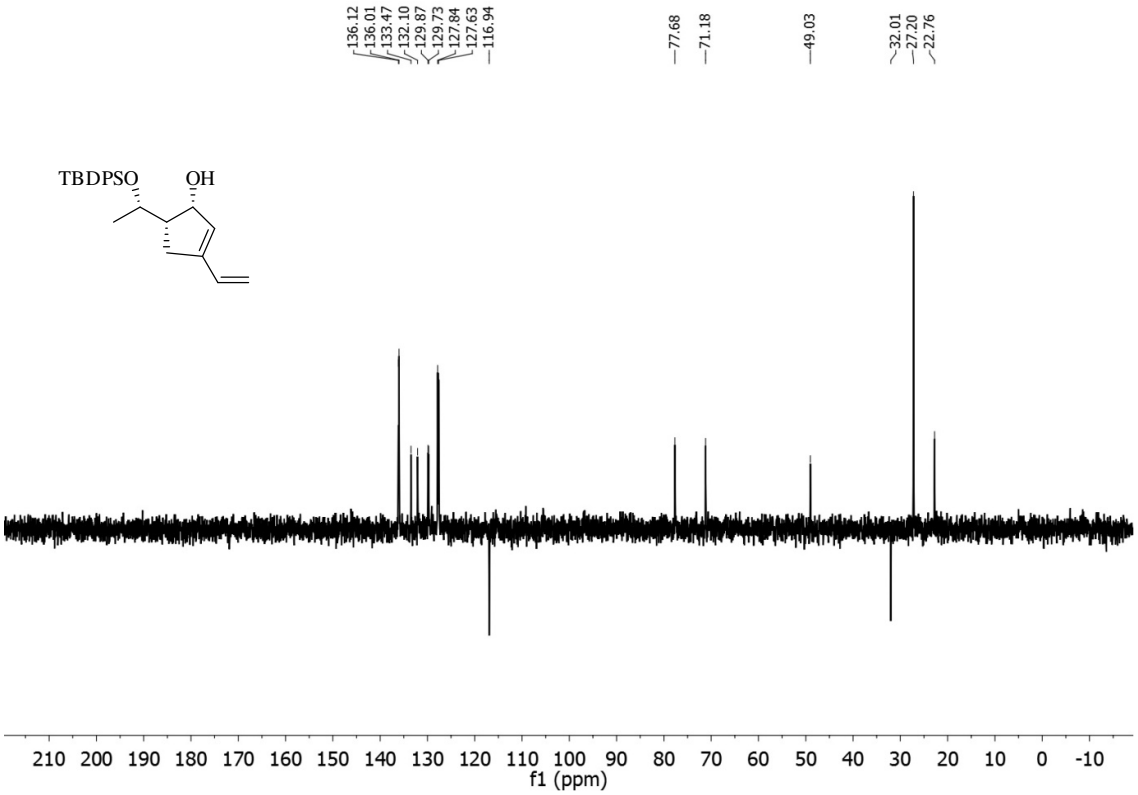

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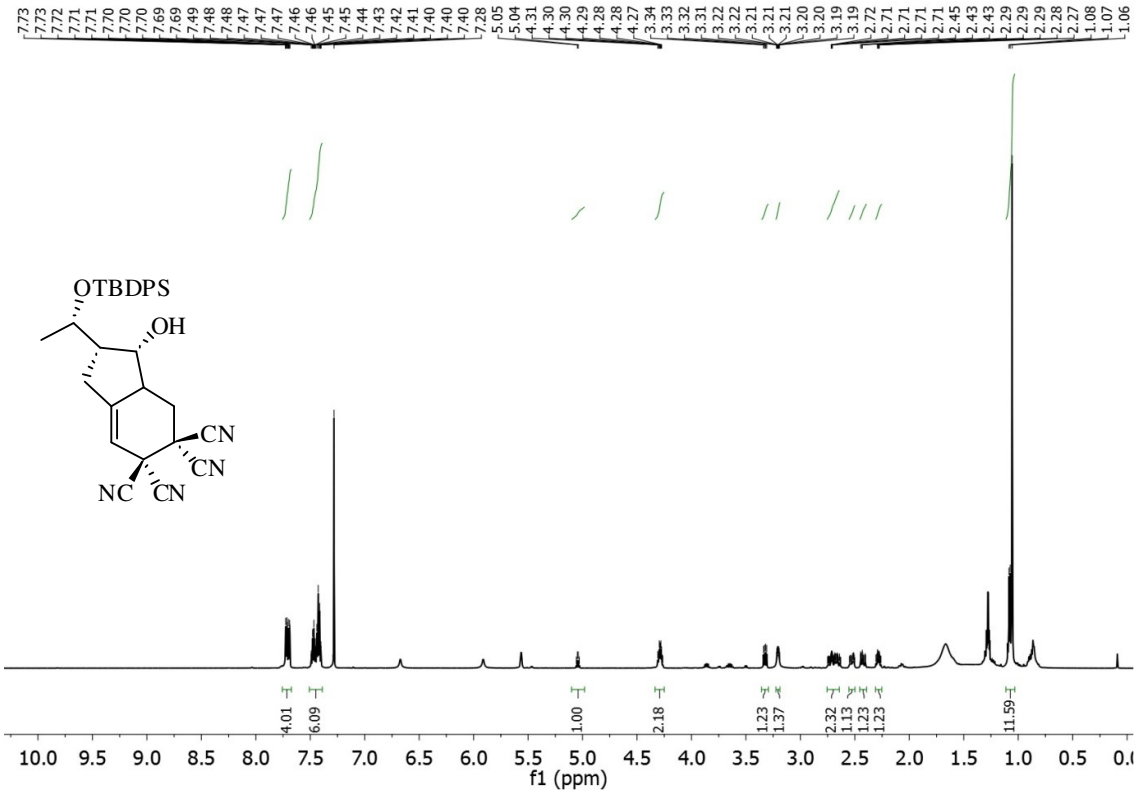

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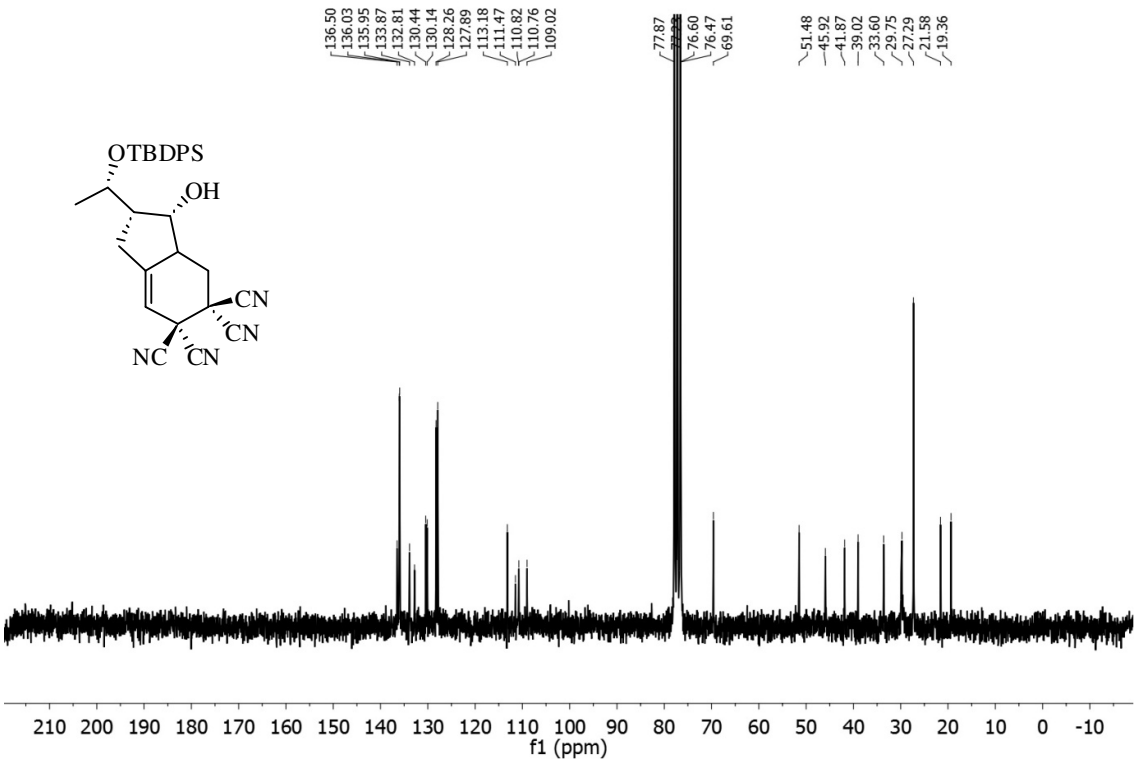

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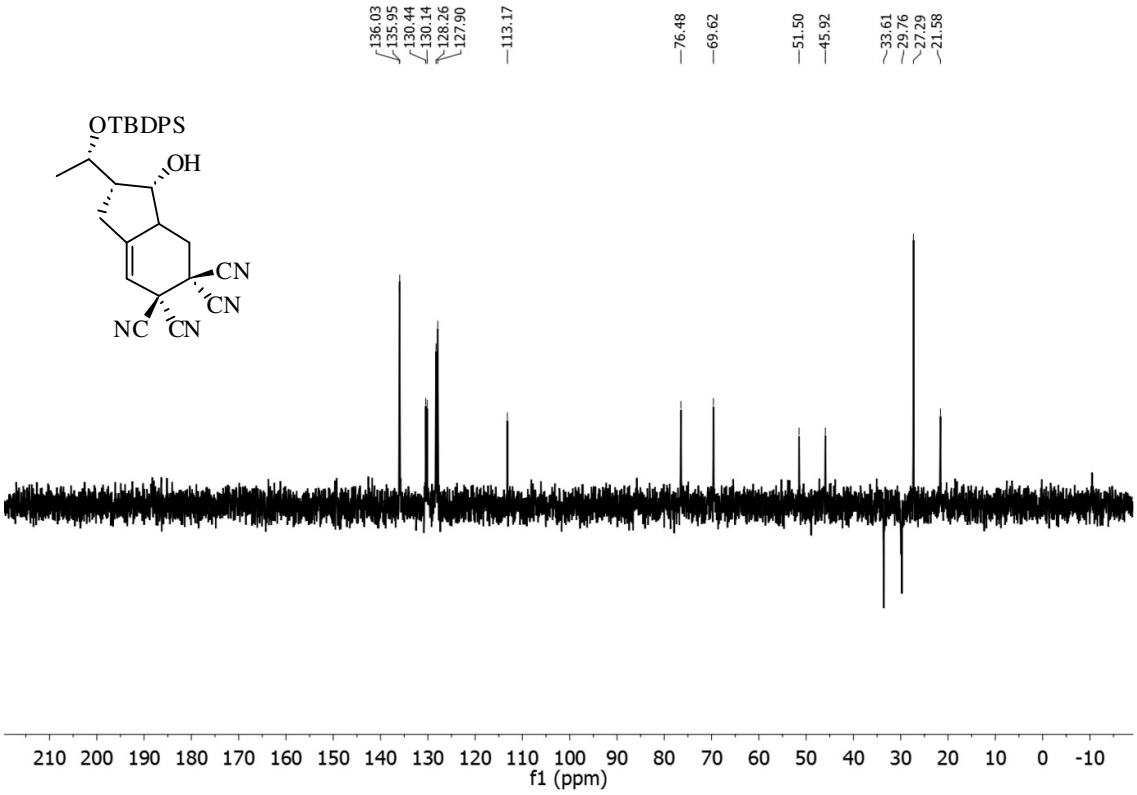

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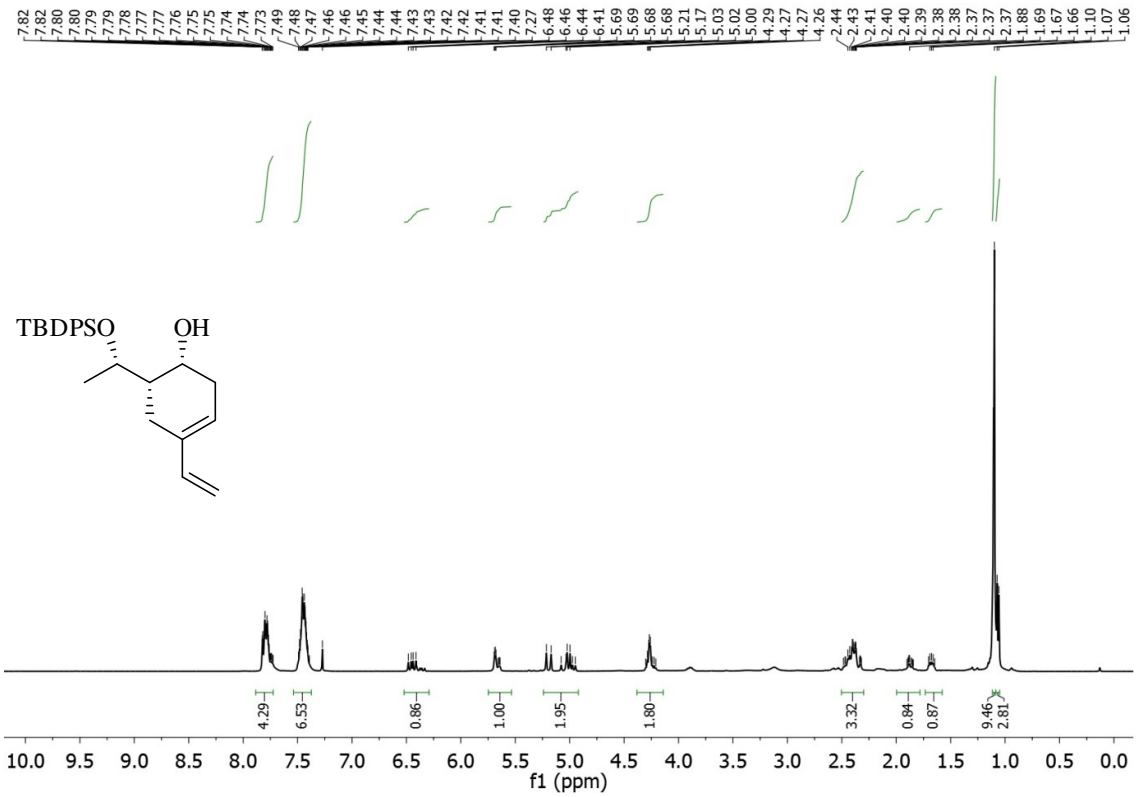

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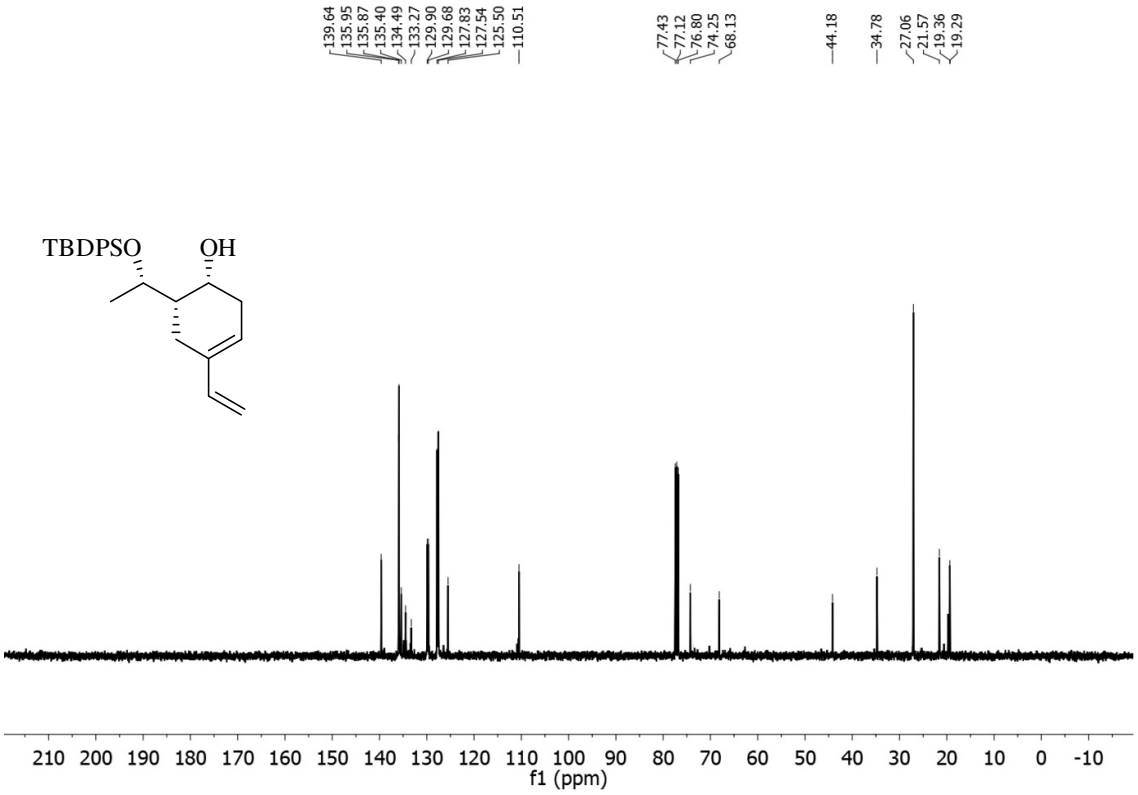

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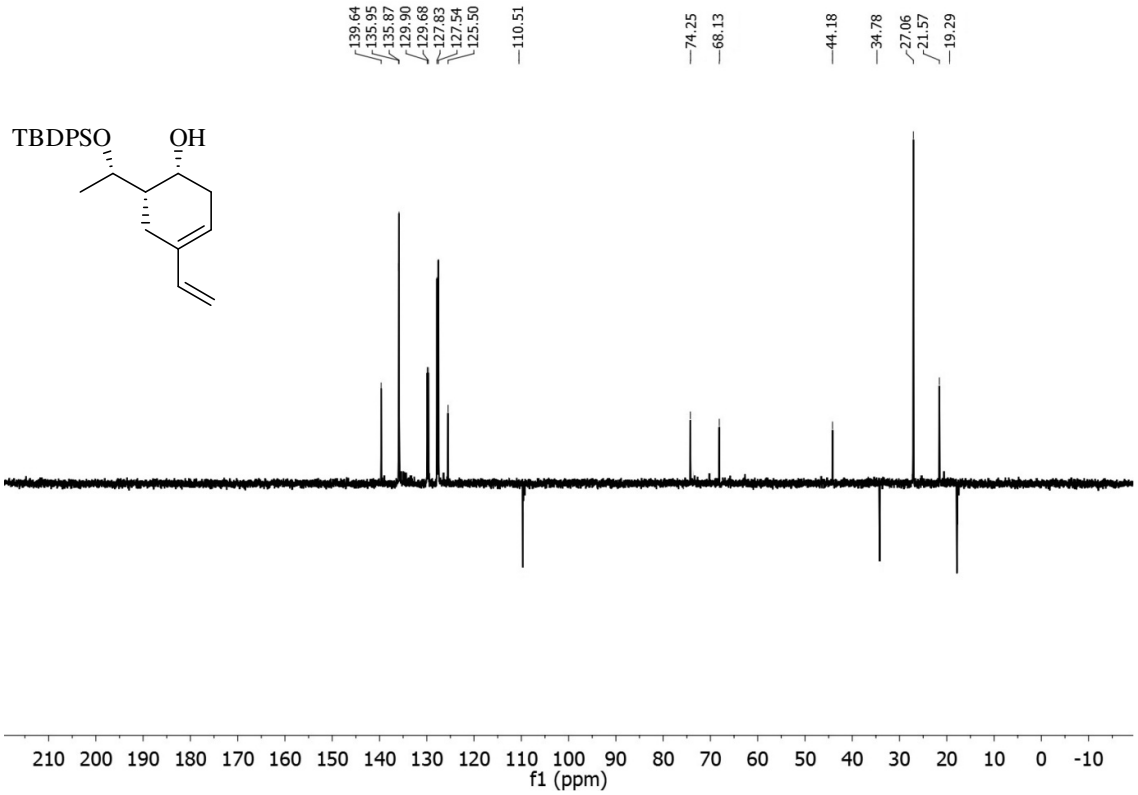

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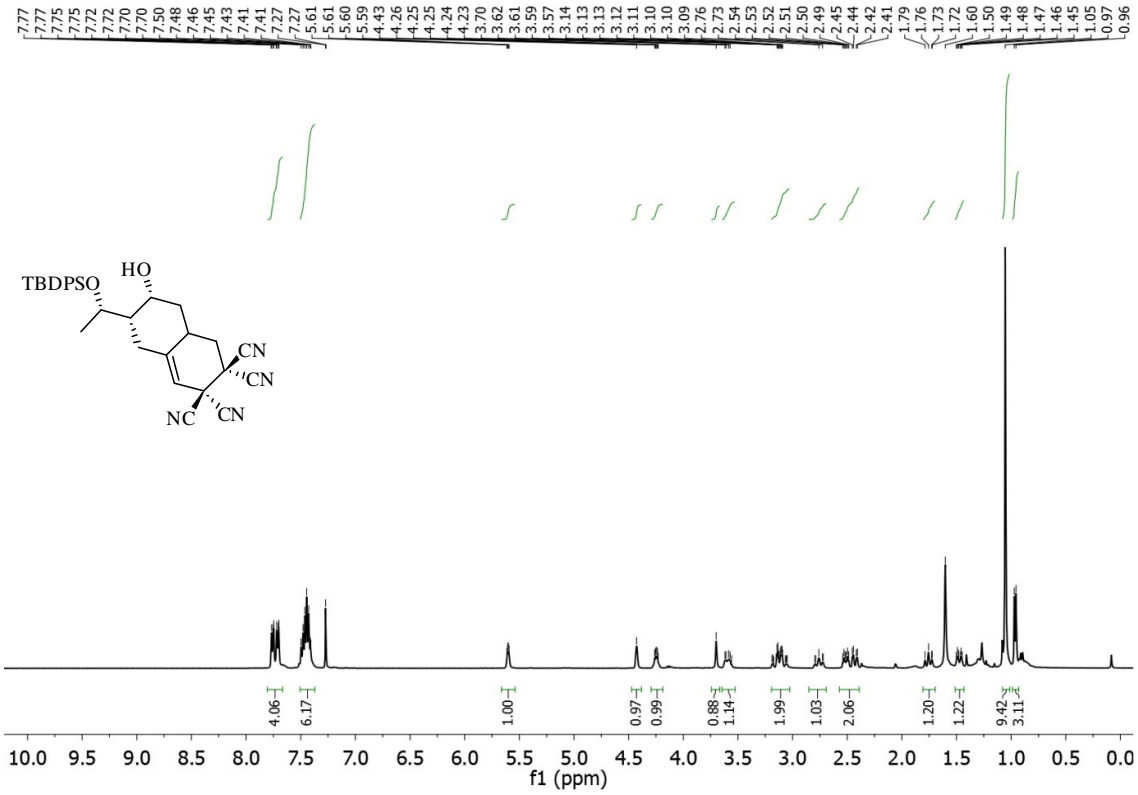

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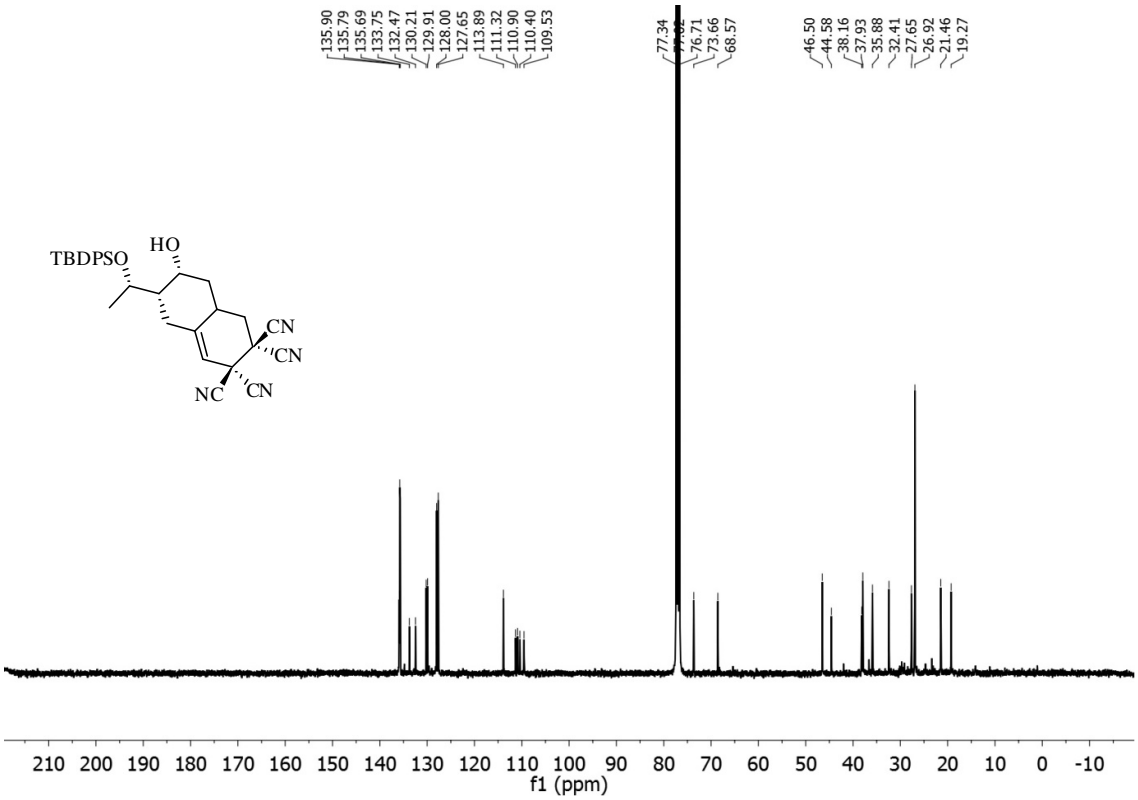

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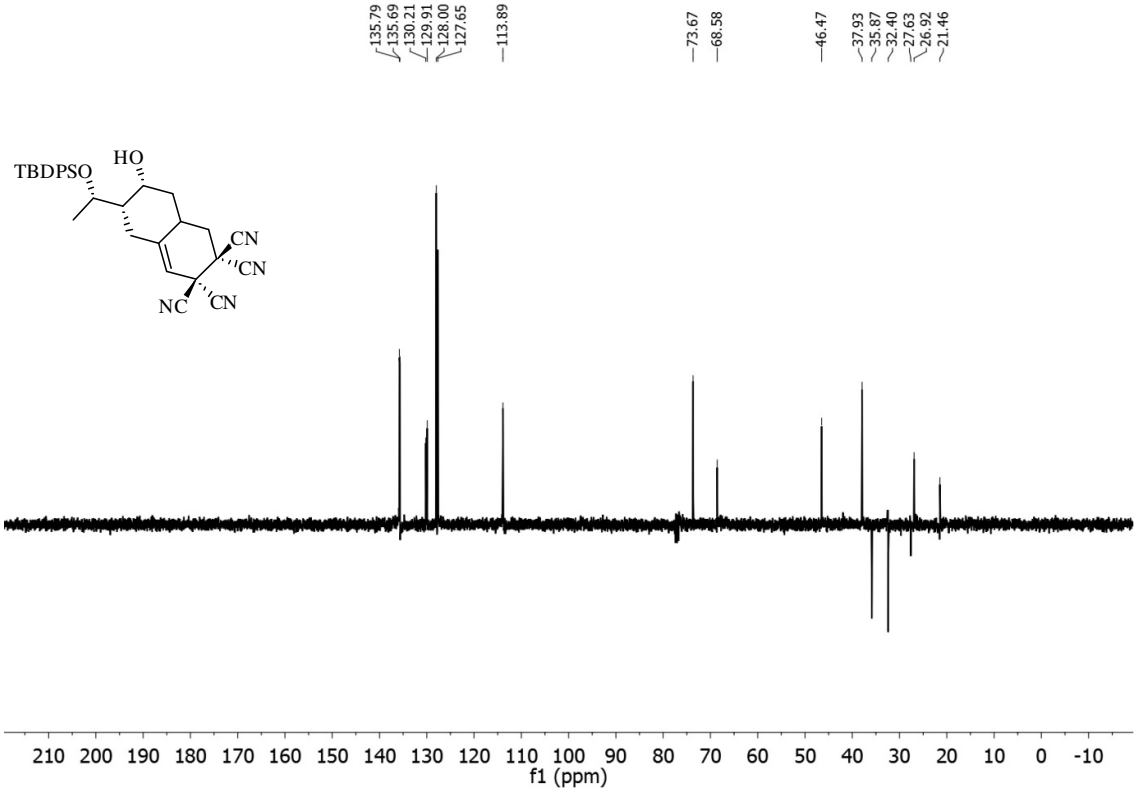

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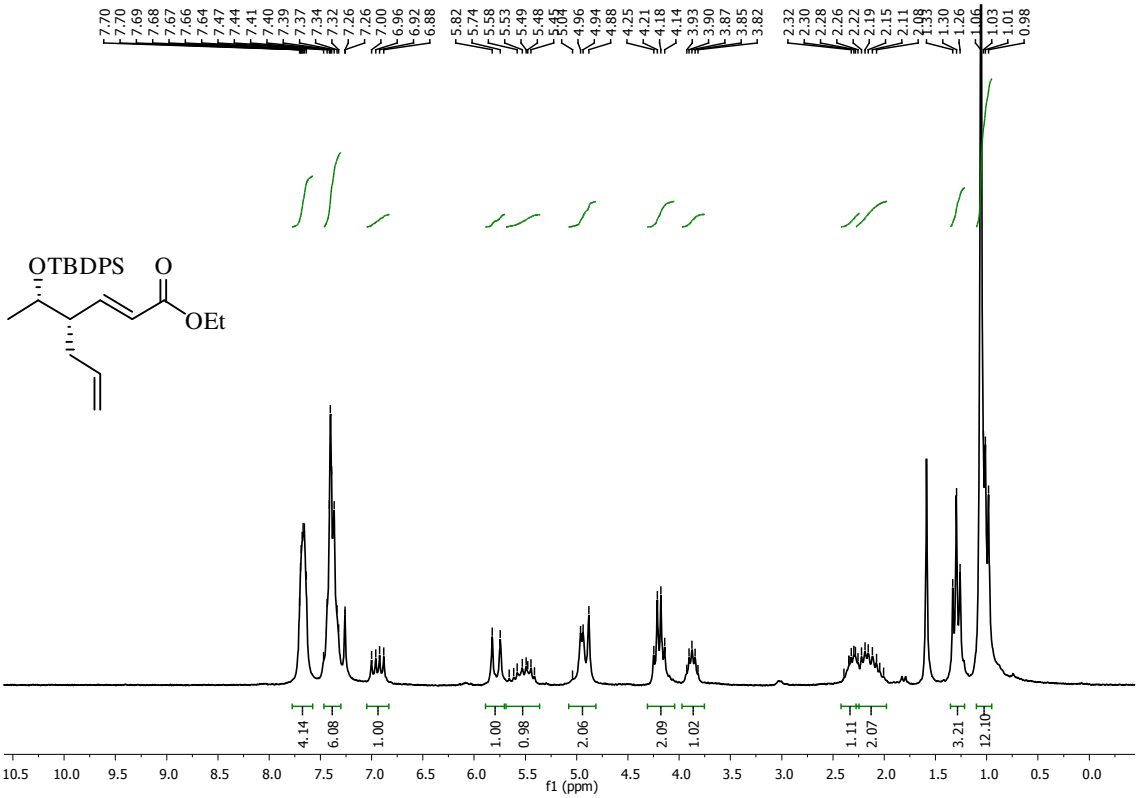
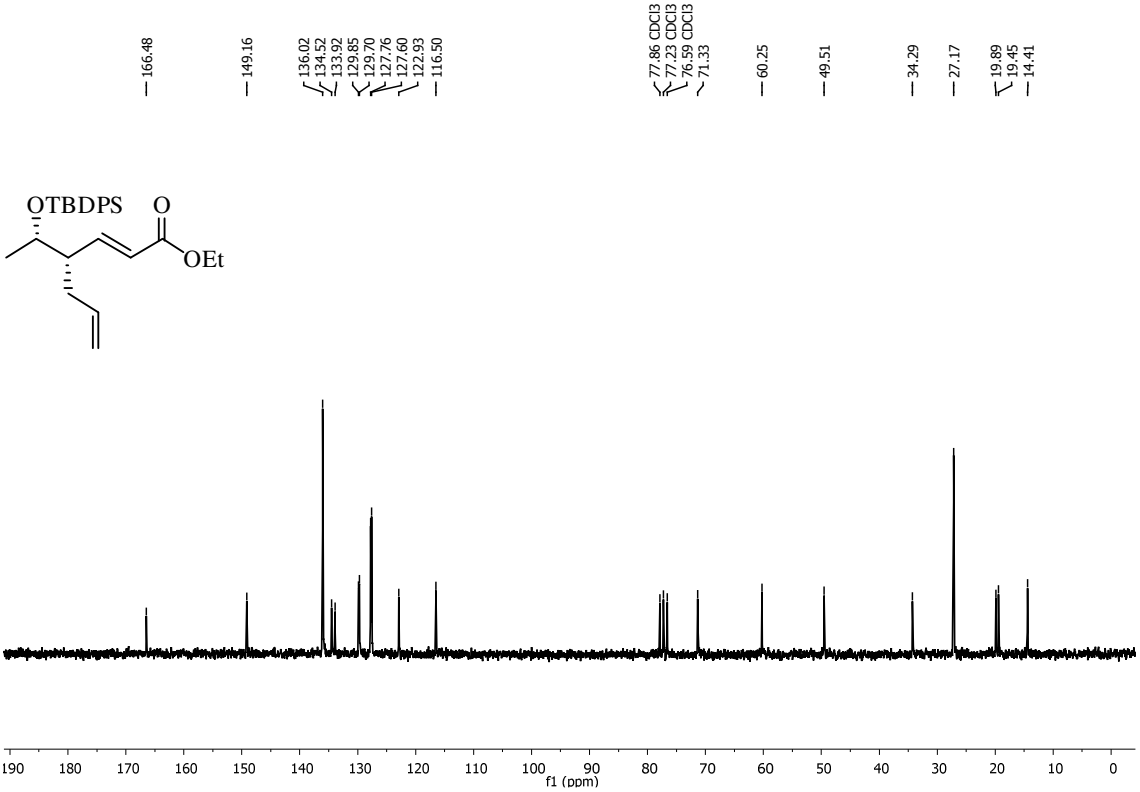
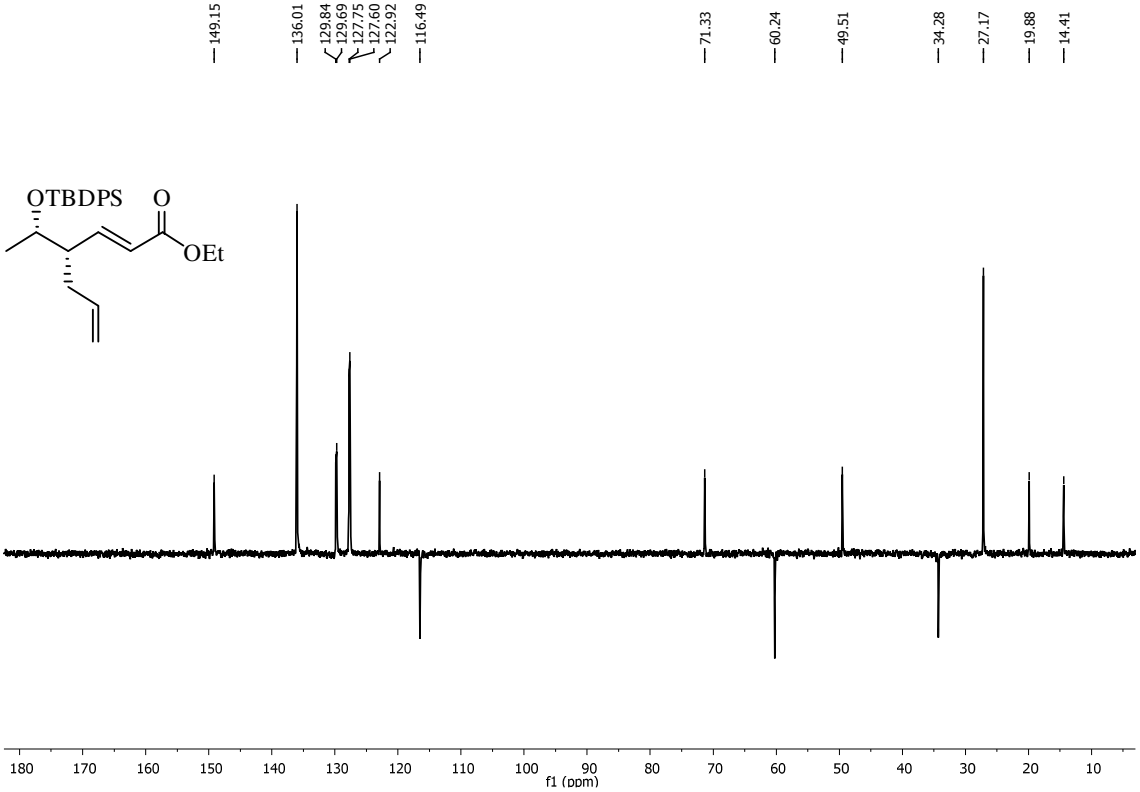


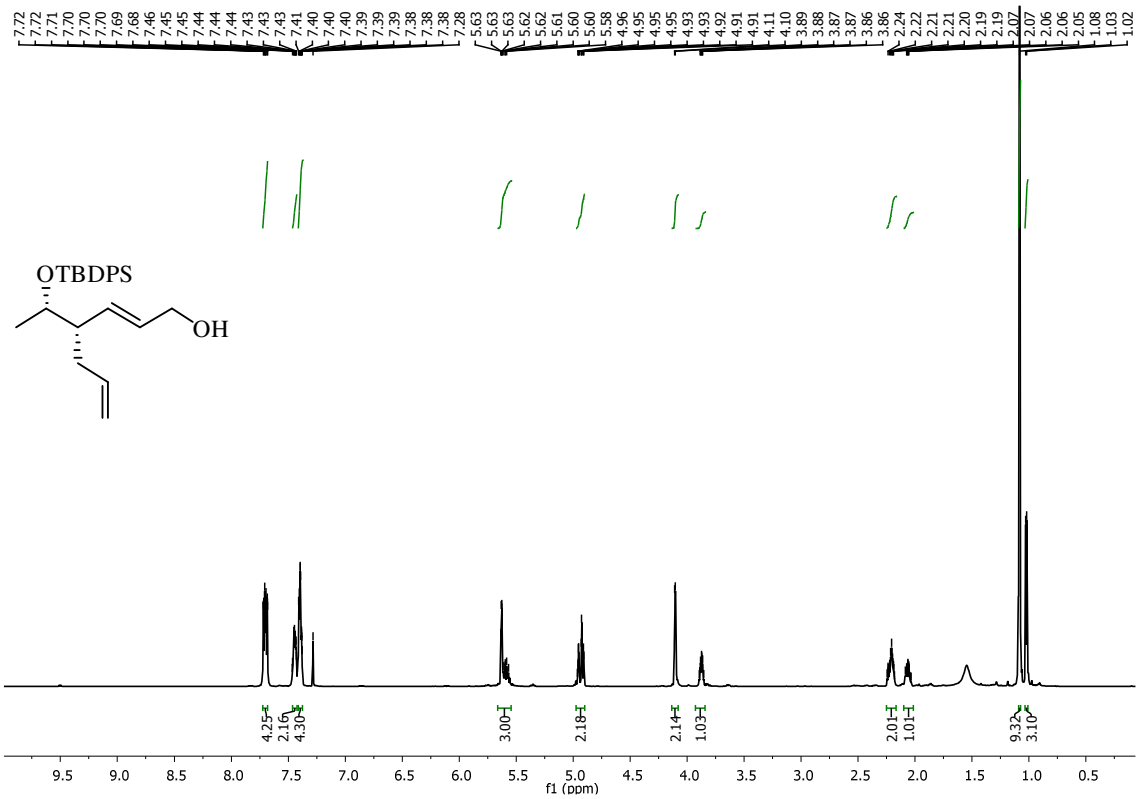
^{13}C NMR of compound 22 (50 MHz, $CDCl_3$)



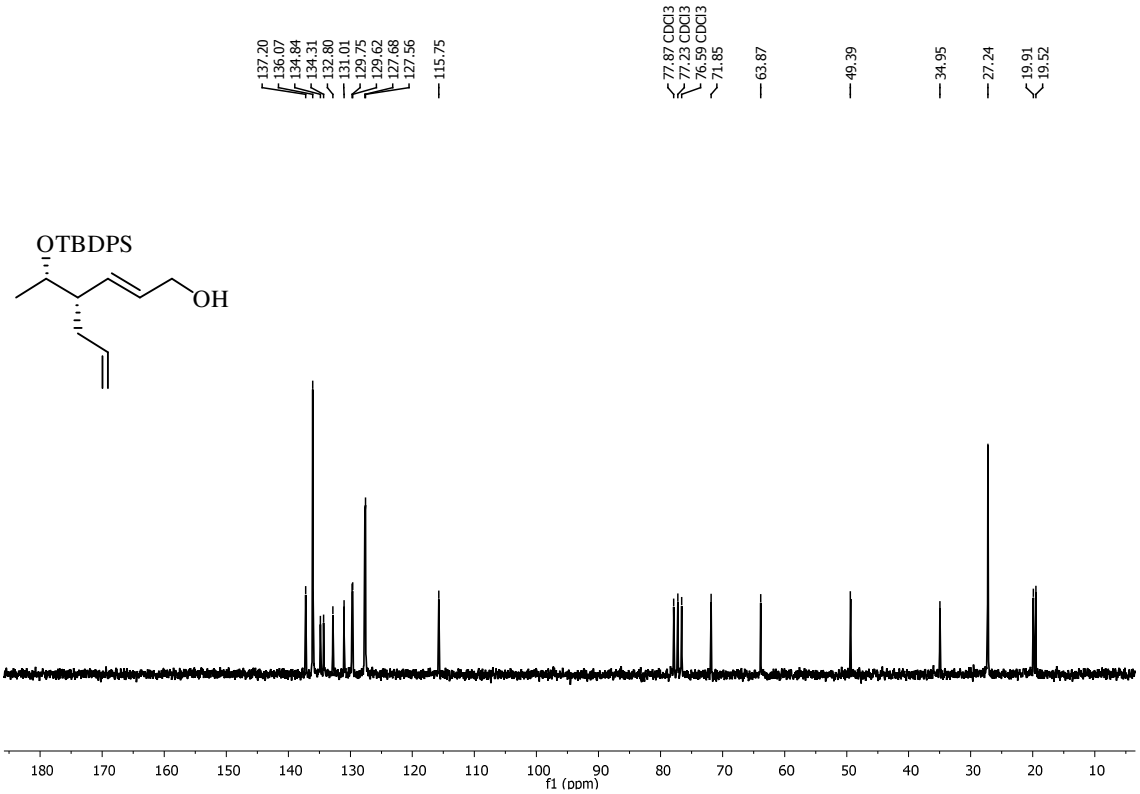
DEPT-135 NMR of compound 22 (50 MHz, $CDCl_3$)



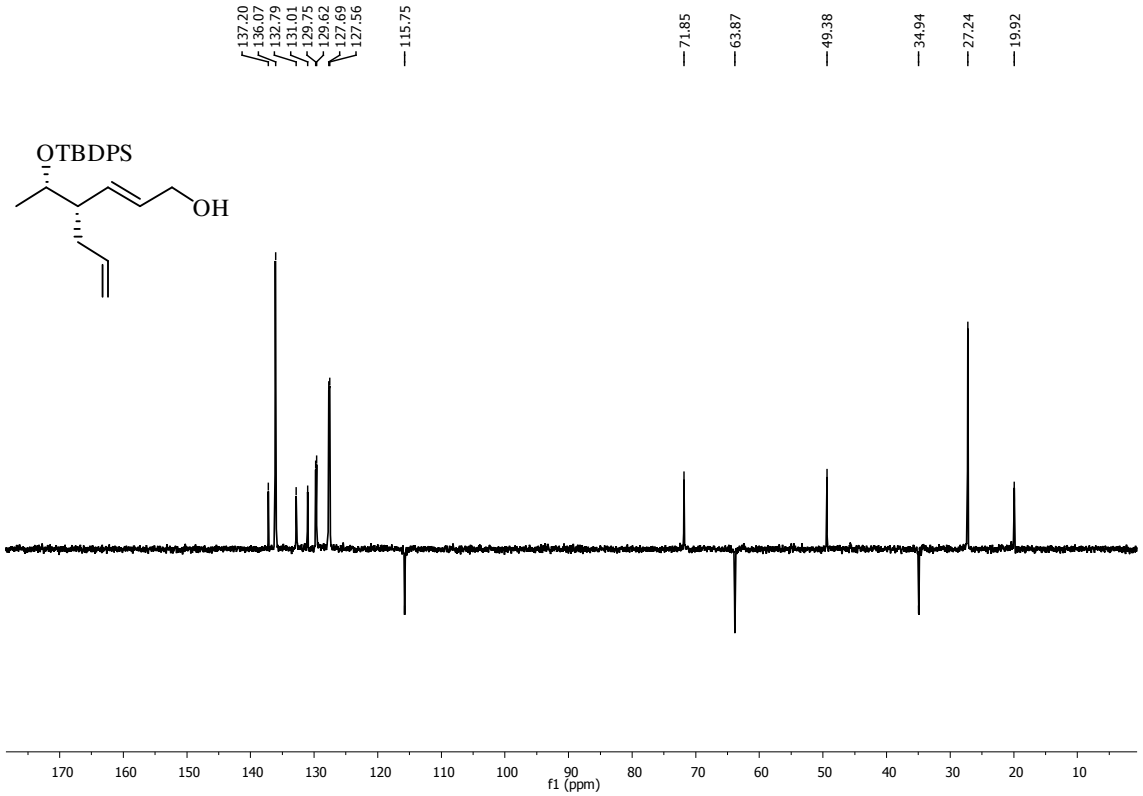
^{1}H - NMR of compound 23 (600 MHz, $CDCl_3$)



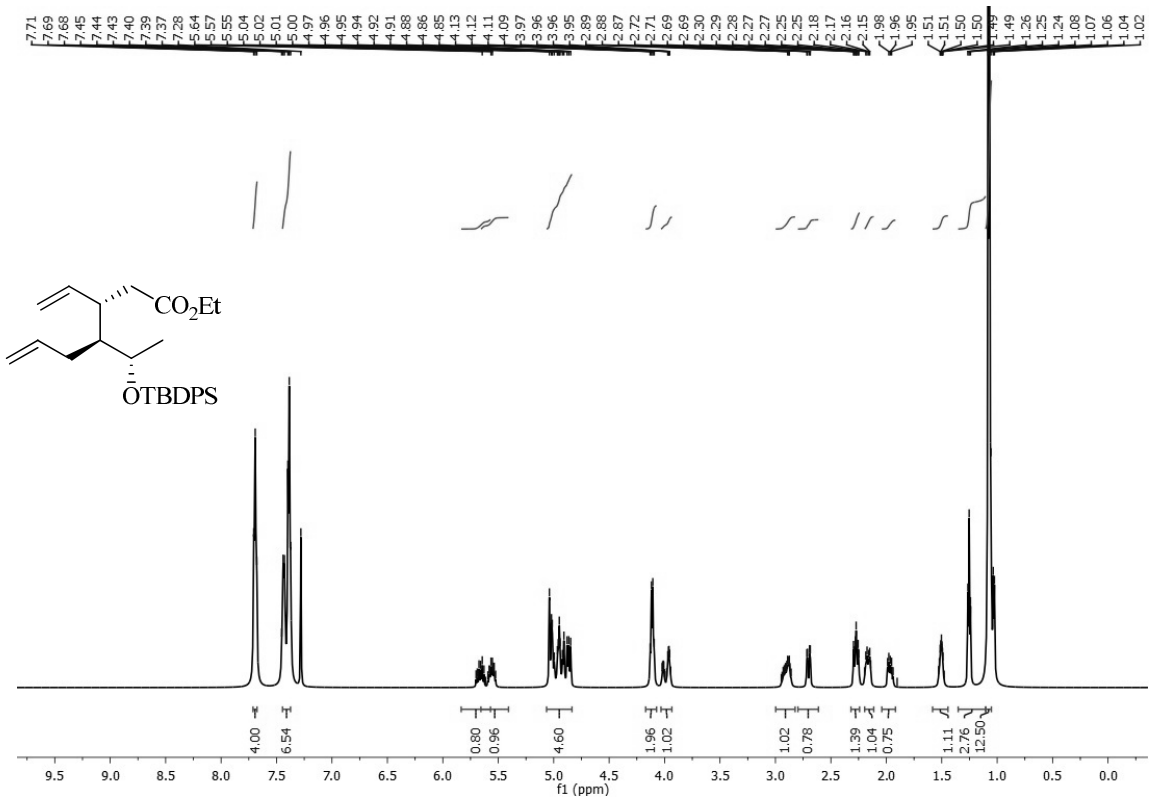
^{13}C NMR of compound 23 (50 MHz, $CDCl_3$)



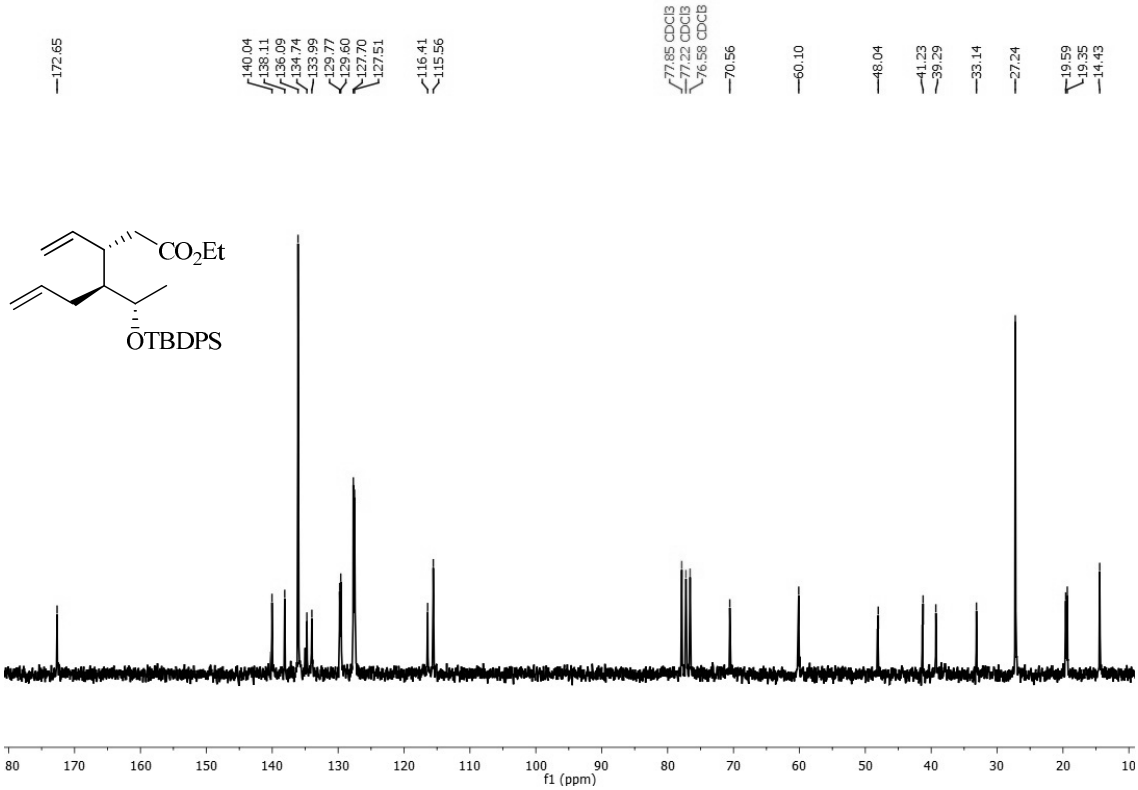
DEPT-135 NMR of compound 23 (50 MHz, $CDCl_3$)



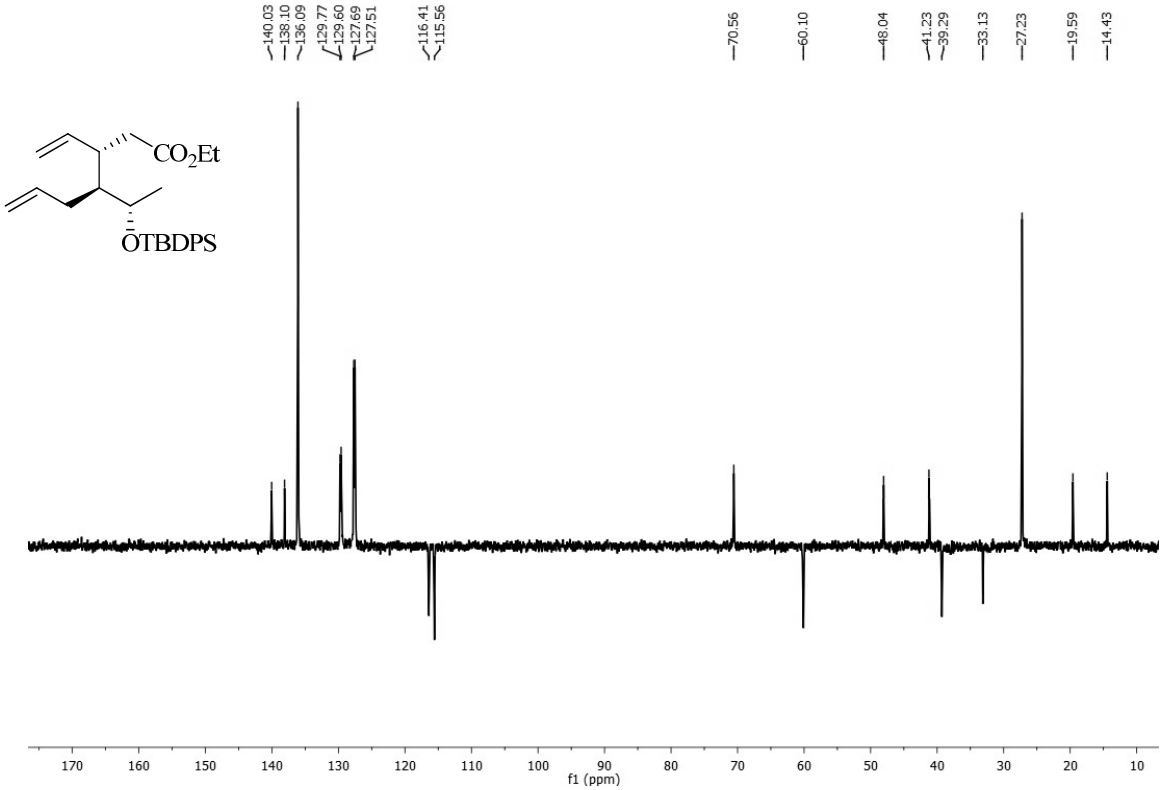
^{1}H - NMR of compound 24 (600 MHz, $CDCl_3$)



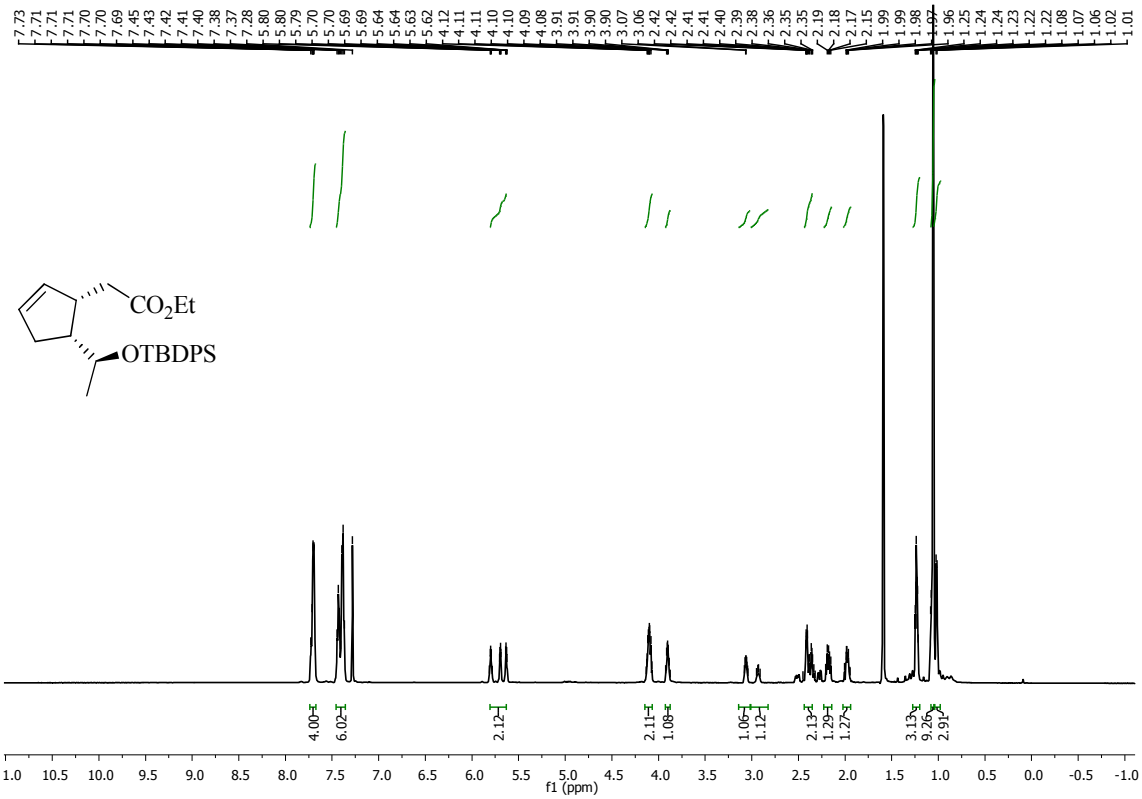
^{13}C NMR of compound 24 (50 MHz, $CDCl_3$)



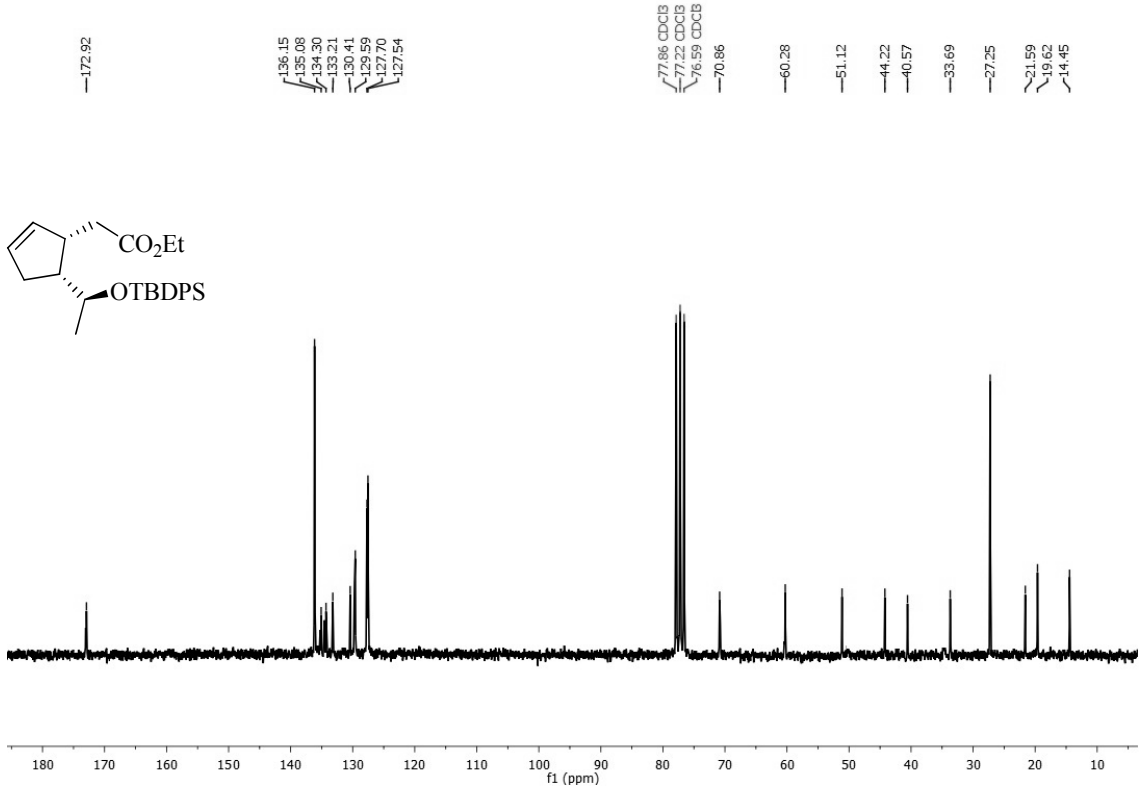
DEPT-135 NMR of compound 24 (50 MHz, $CDCl_3$)



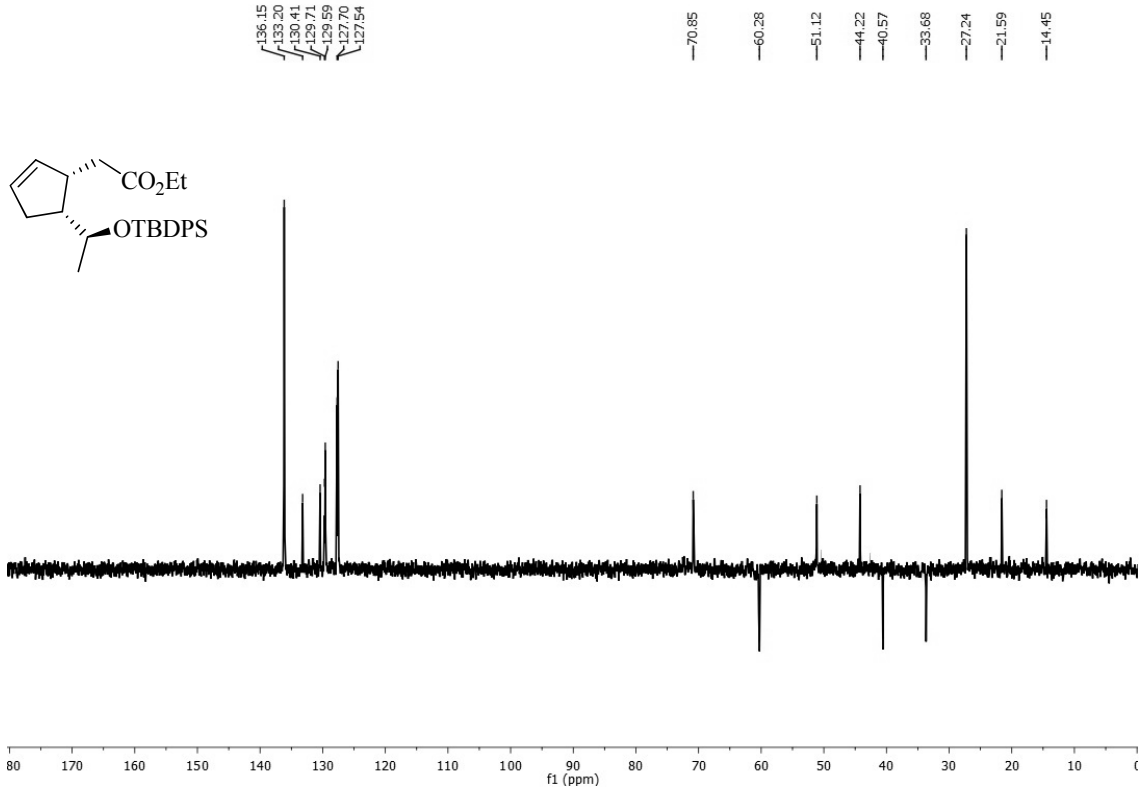
^{1}H - NMR of compound 25 (600 MHz, $CDCl_3$)



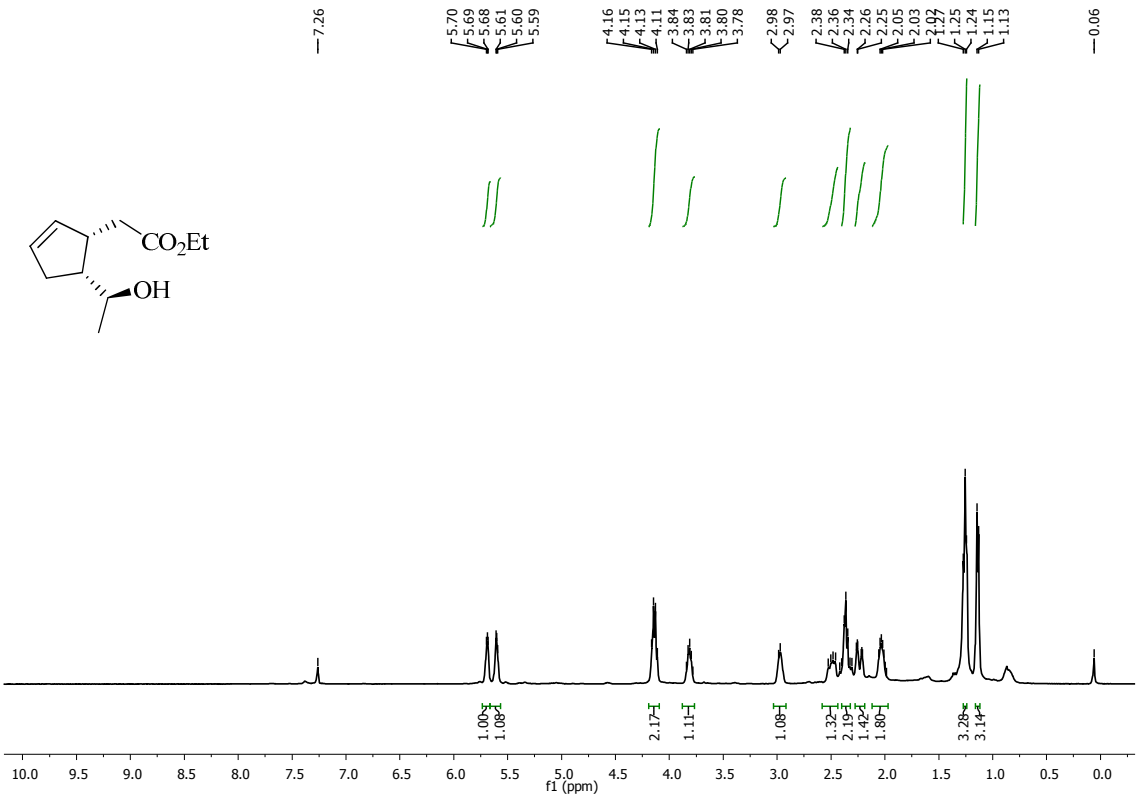
^{13}C NMR of compound 25 (50 MHz, $CDCl_3$)



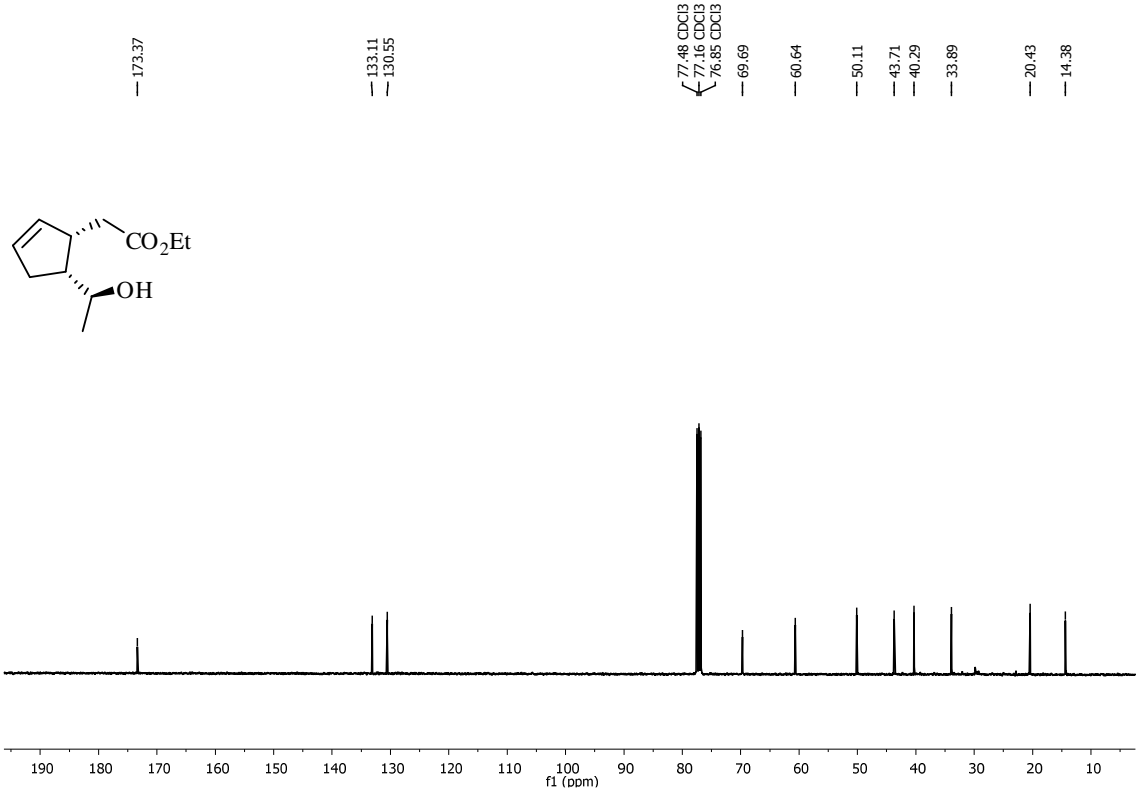
DEPT-135 NMR of compound 25 (50 MHz, $CDCl_3$)



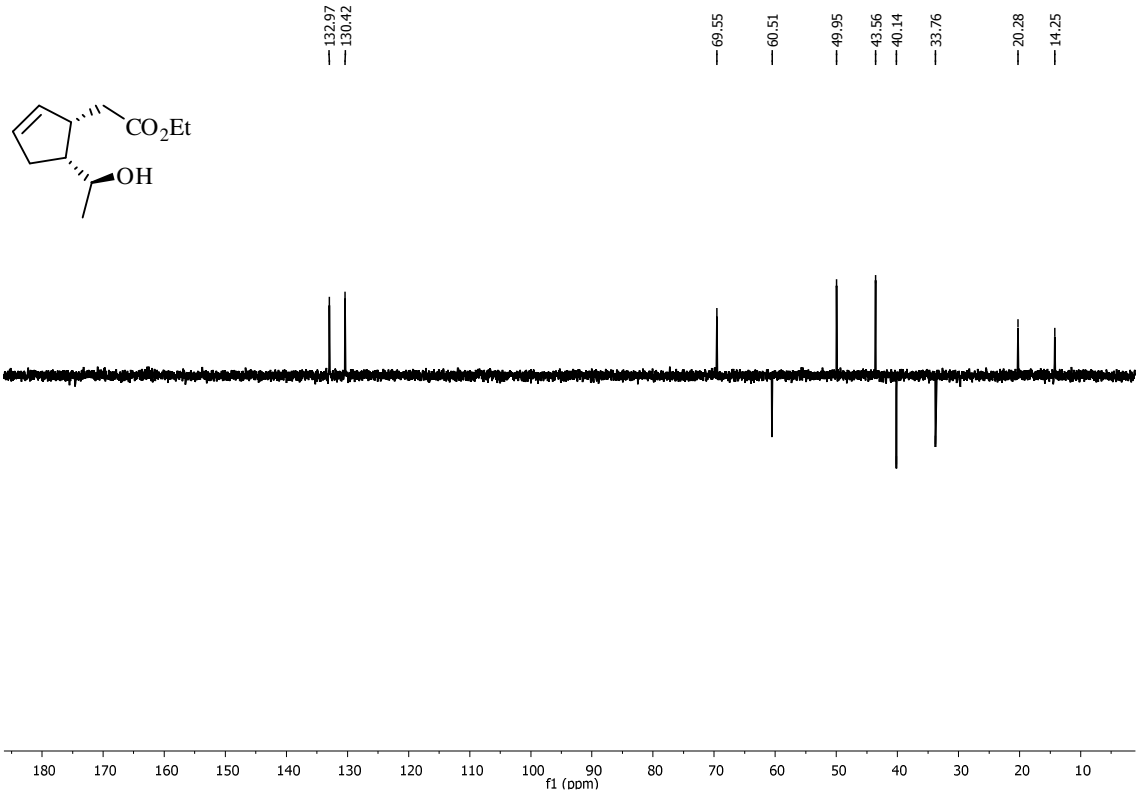
^{1}H - NMR of compound 26 (400 MHz, $CDCl_3$)



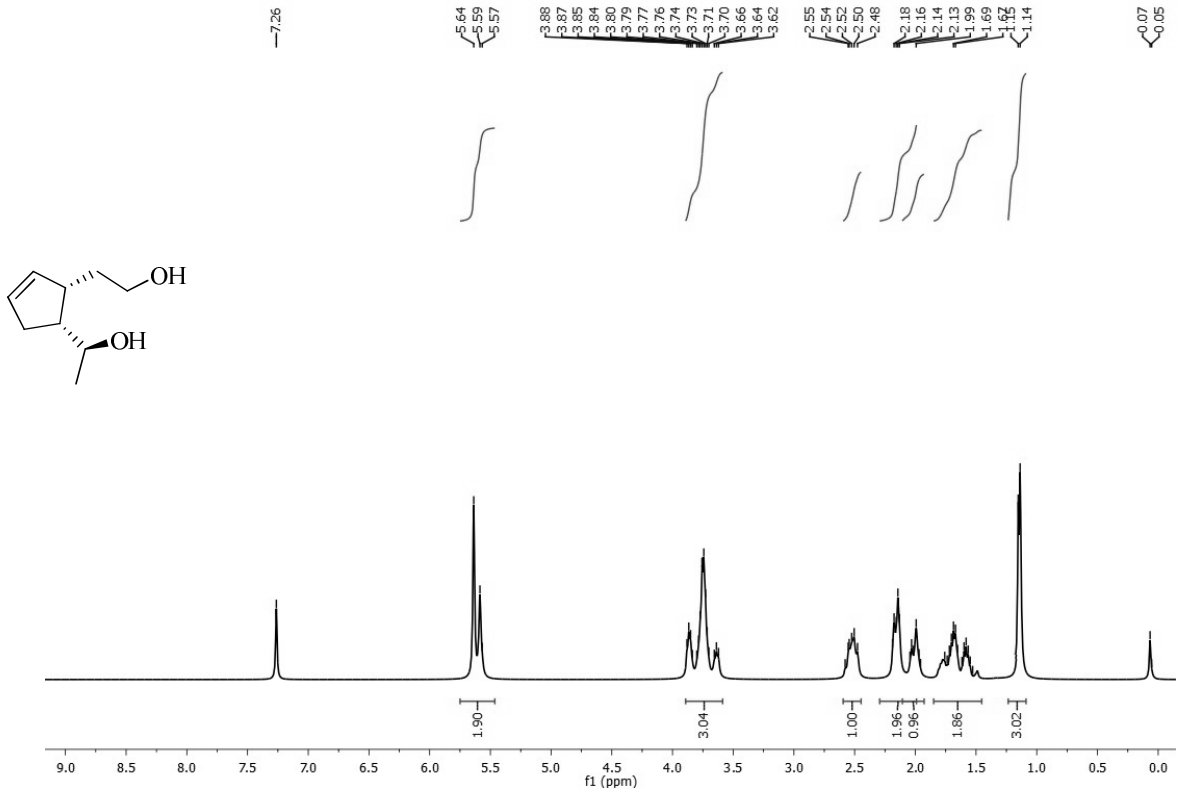
^{13}C NMR of compound 26 (100 MHz, $CDCl_3$)



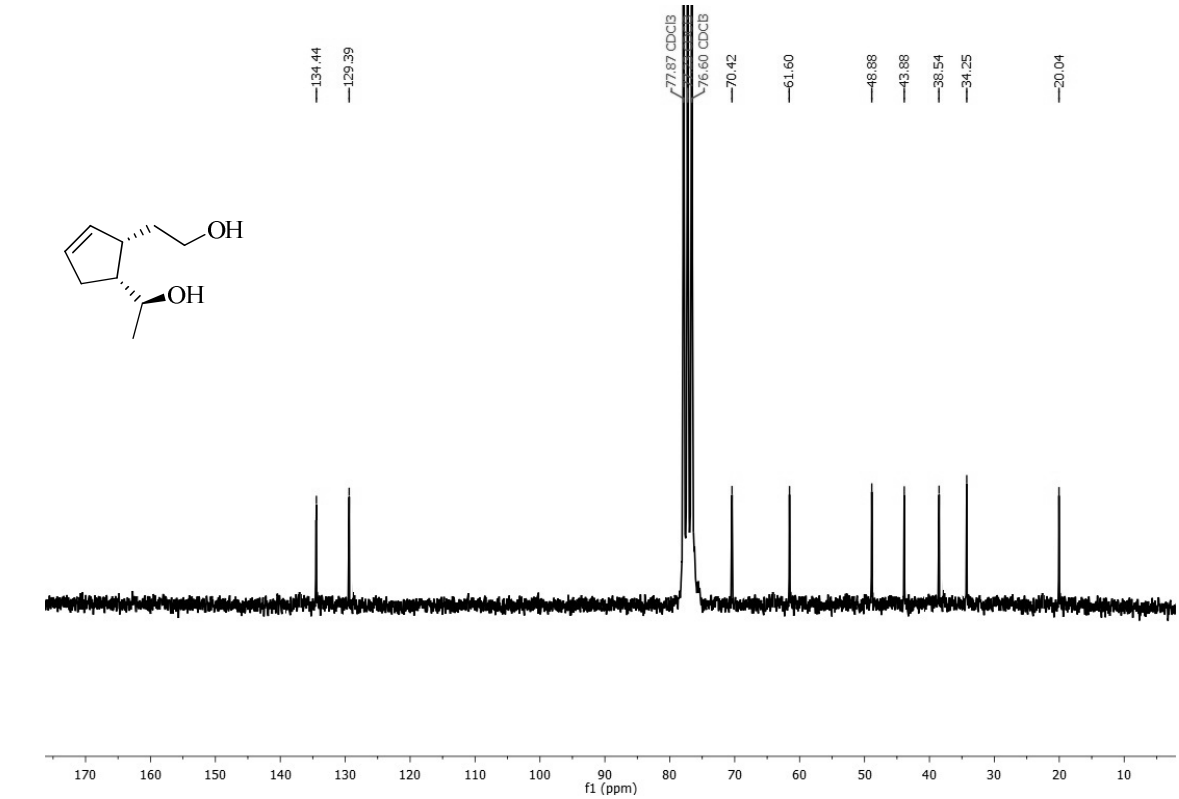
DEPT-135 NMR of compound 26 (100 MHz, $CDCl_3$)



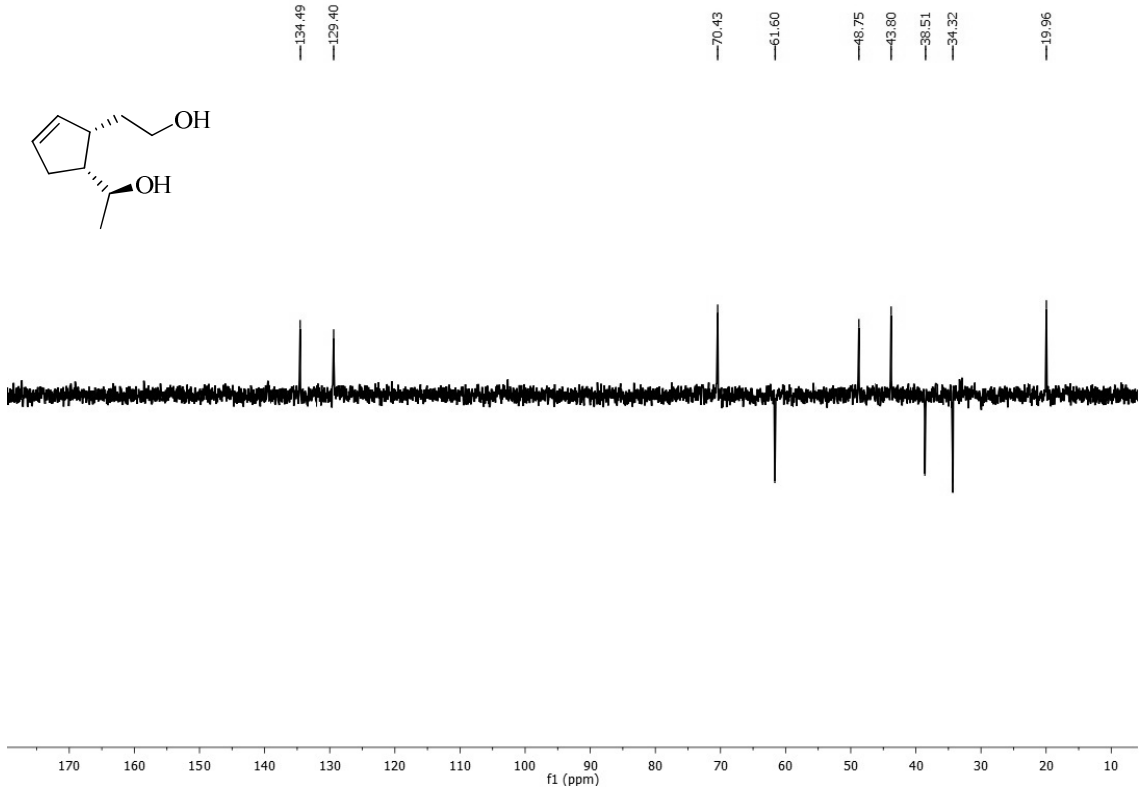
^{1}H - NMR of compound 27 (400 MHz, $CDCl_3$)



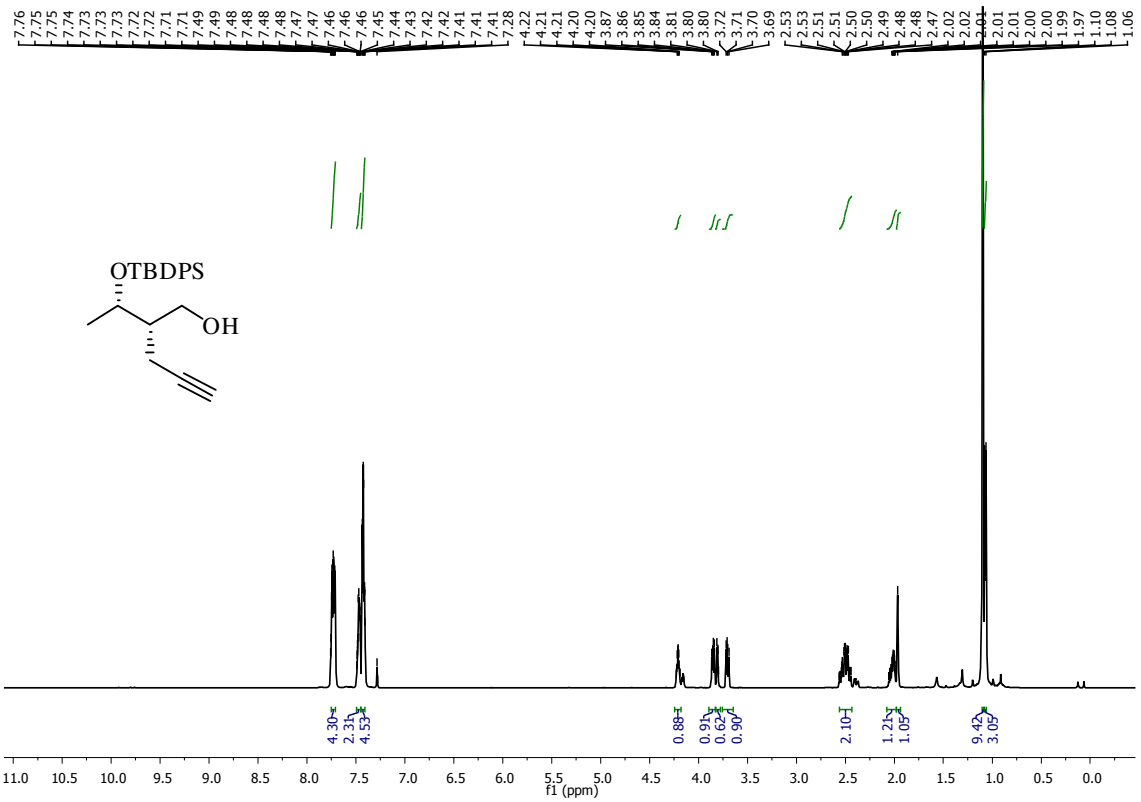
^{13}C NMR of compound 27 (50 MHz, $CDCl_3$)



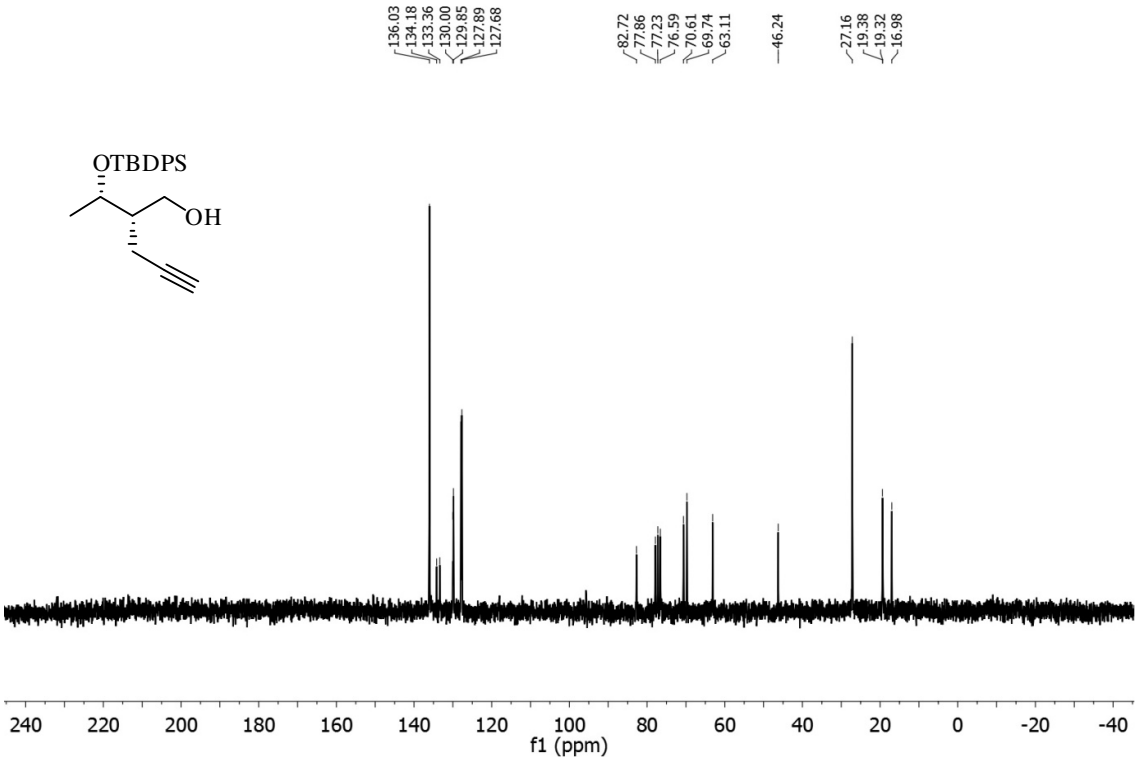
DEPT-135 NMR of compound 27 (50 MHz, $CDCl_3$)



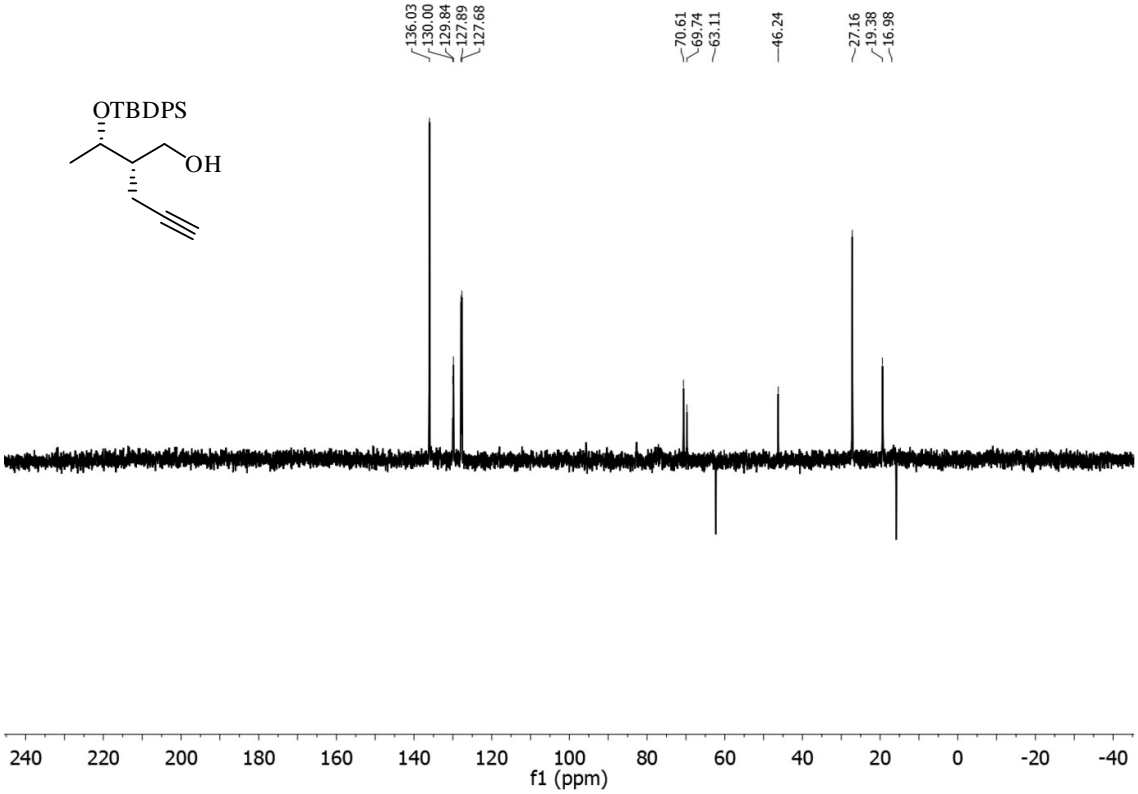
^{1}H - NMR of compound 28 (600 MHz, $CDCl_3$)



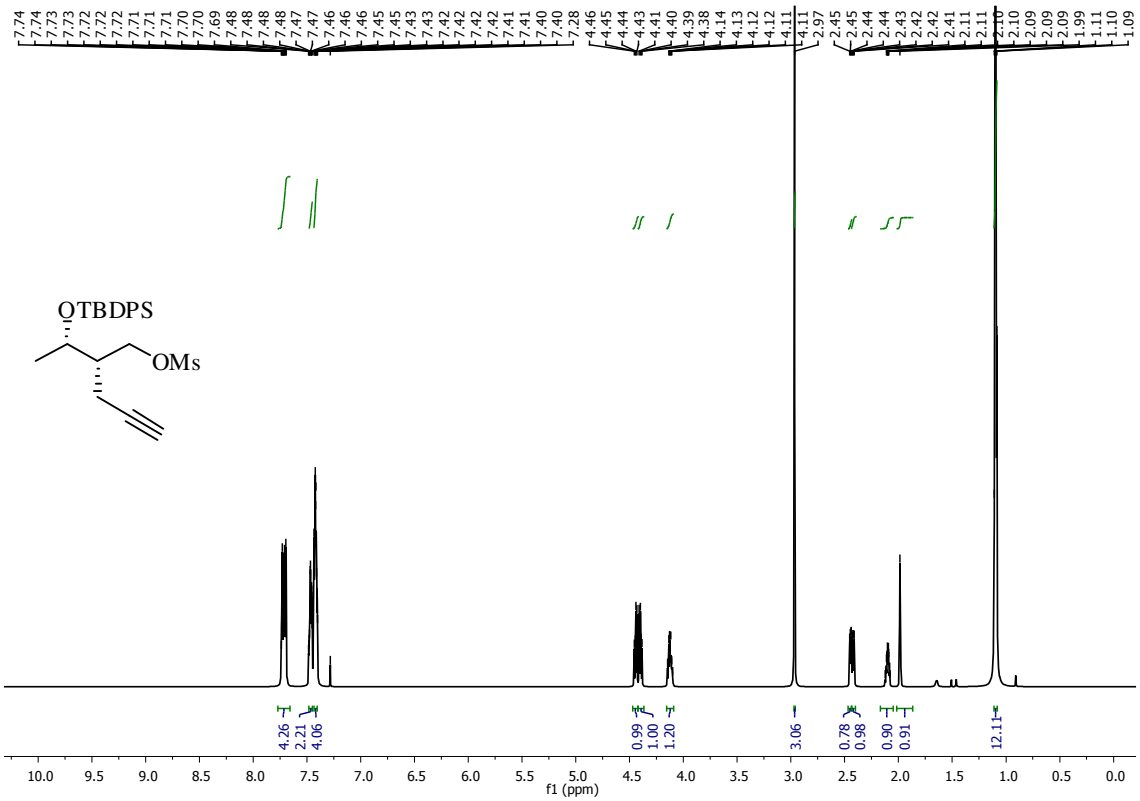
^{13}C NMR of compound 28 (50 MHz, $CDCl_3$)



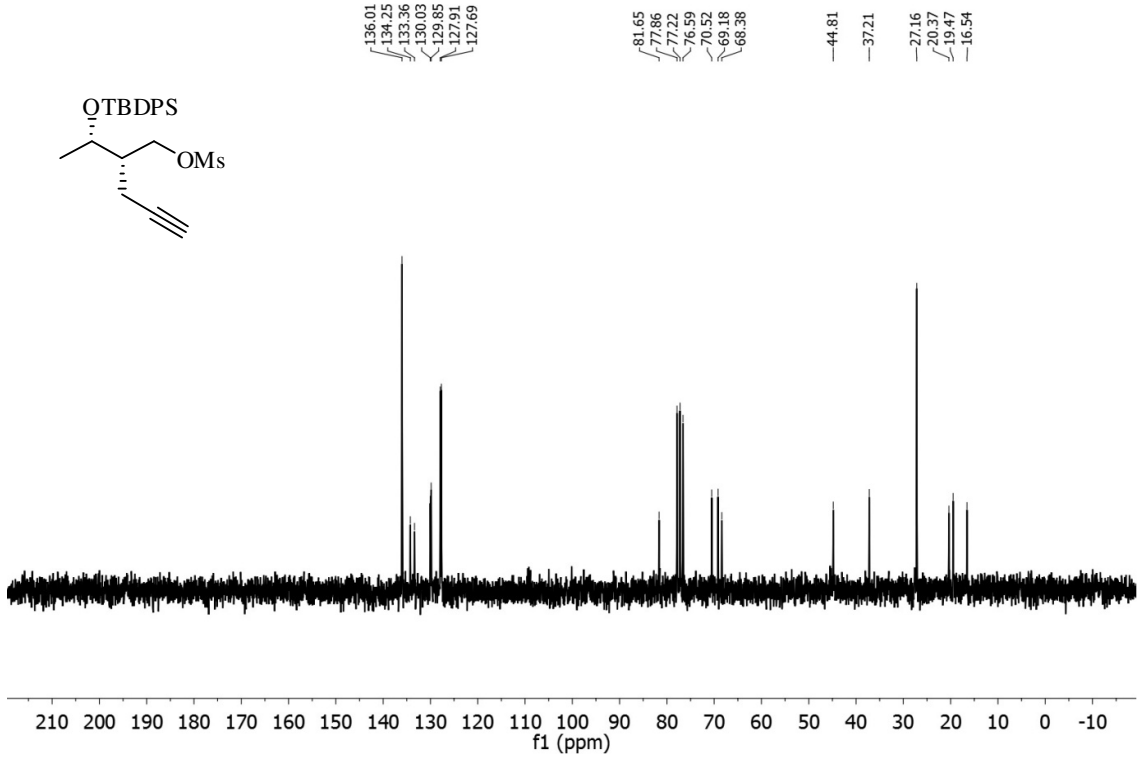
DEPT-135 NMR of compound 28 (50 MHz, $CDCl_3$)



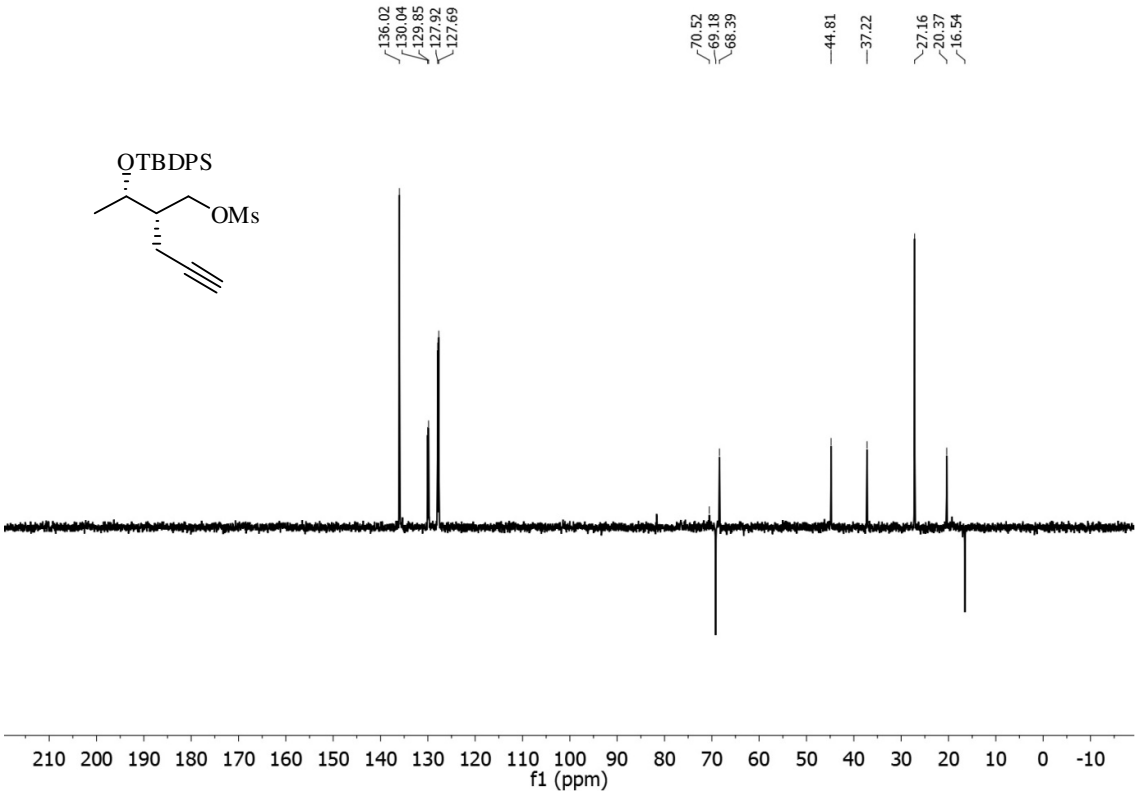
^{1}H - NMR of compound 29 (600 MHz, $CDCl_3$)



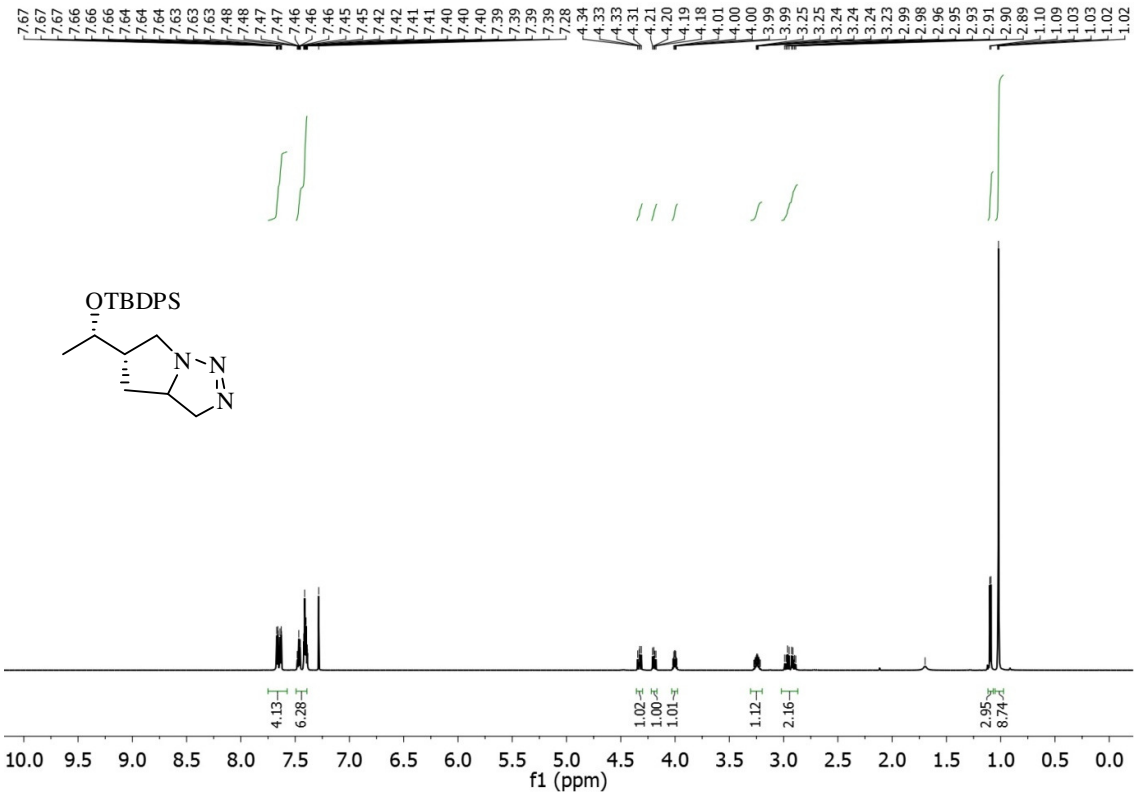
^{13}C NMR of compound 29 (50 MHz, $CDCl_3$)



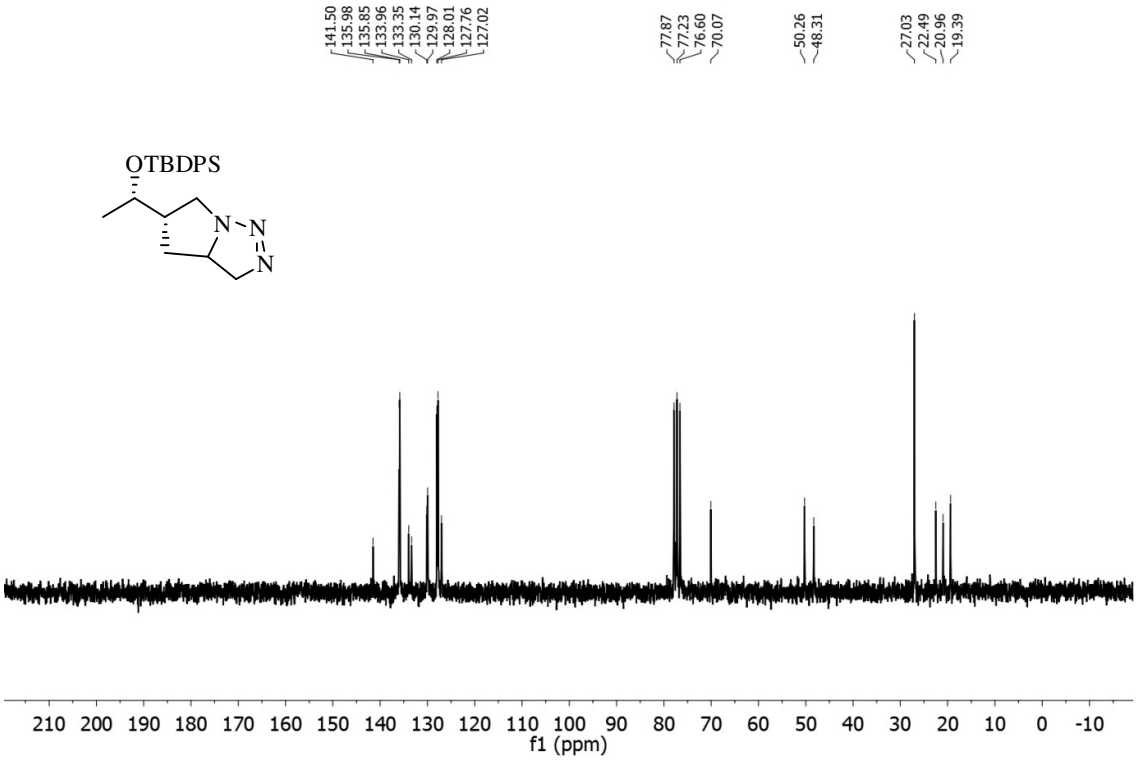
DEPT-135 NMR of compound 29 (50 MHz, $CDCl_3$)



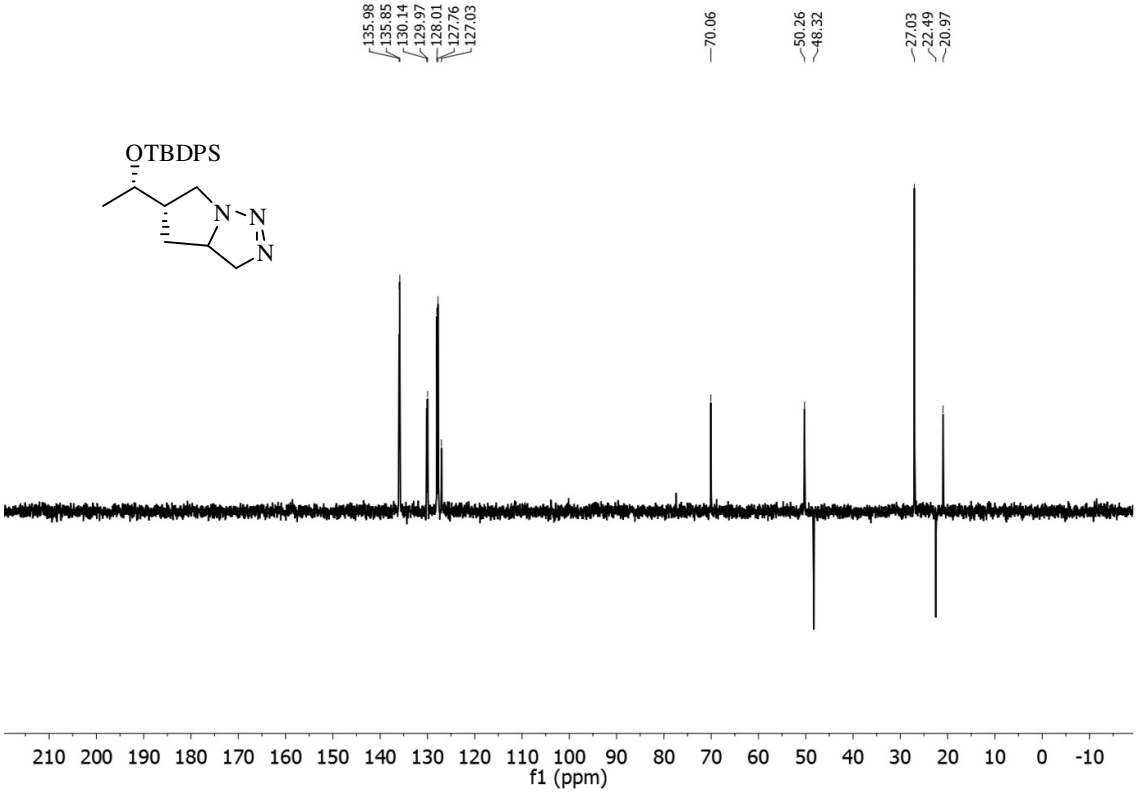
^{1}H - NMR of compound 30 (600 MHz, $CDCl_3$)



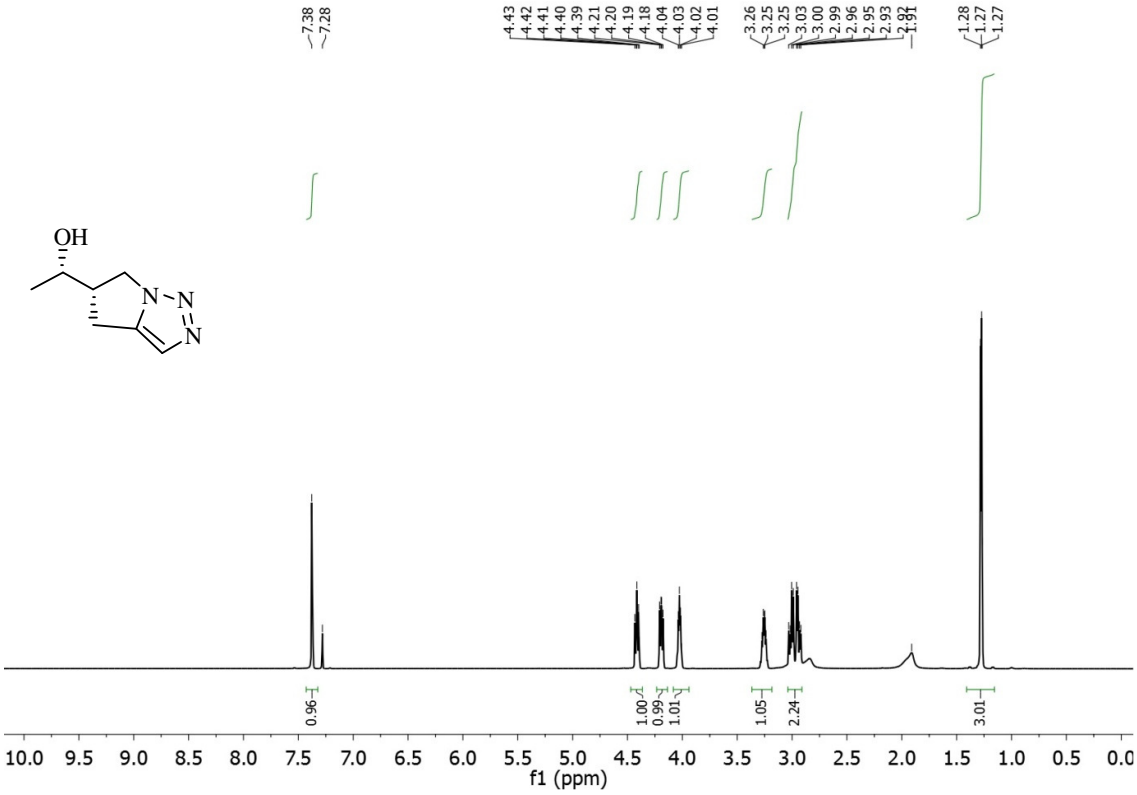
^{13}C NMR of compound 30 (50 MHz, $CDCl_3$)



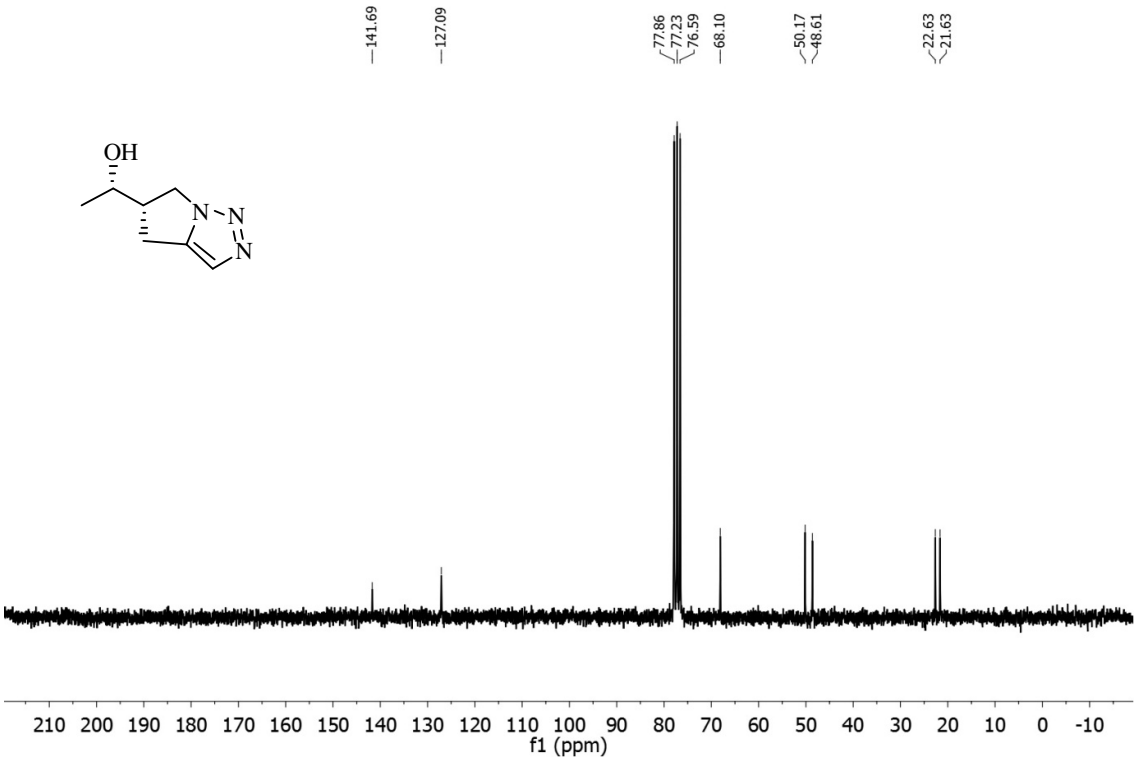
DEPT-135 NMR of compound 30 (50 MHz, $CDCl_3$)



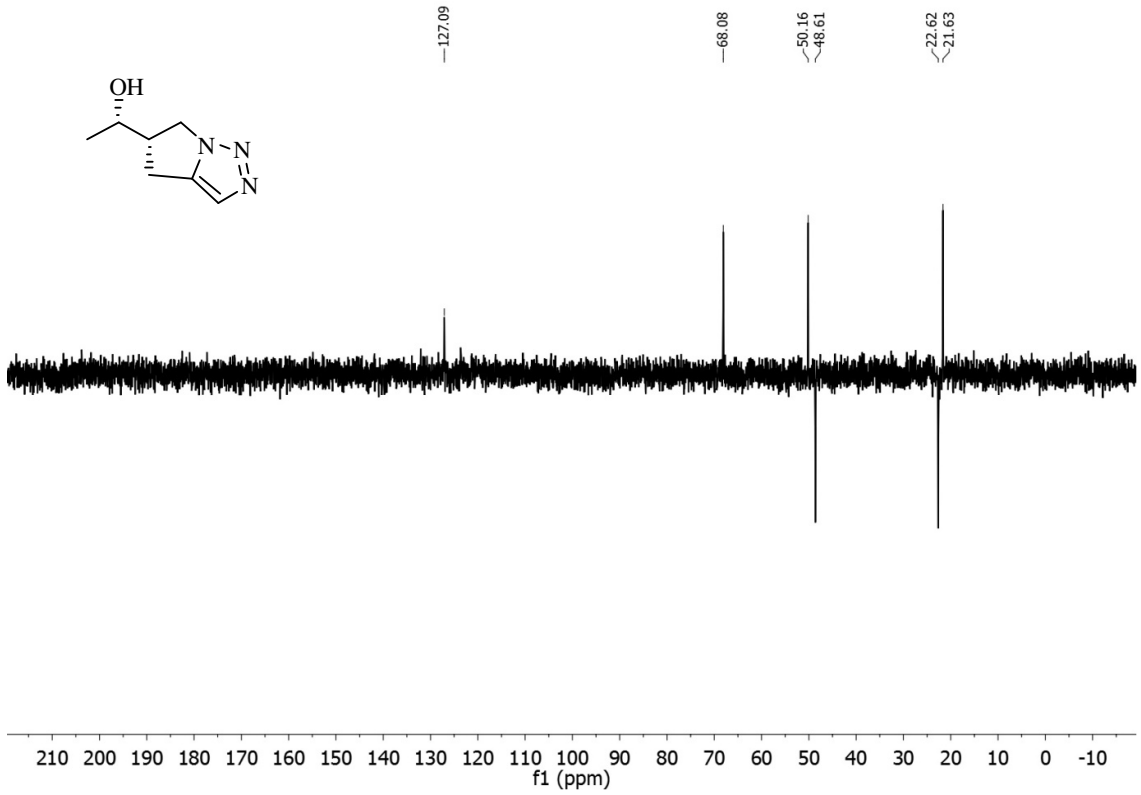
^{1}H - NMR of compound 31 (600 MHz, $CDCl_3$)



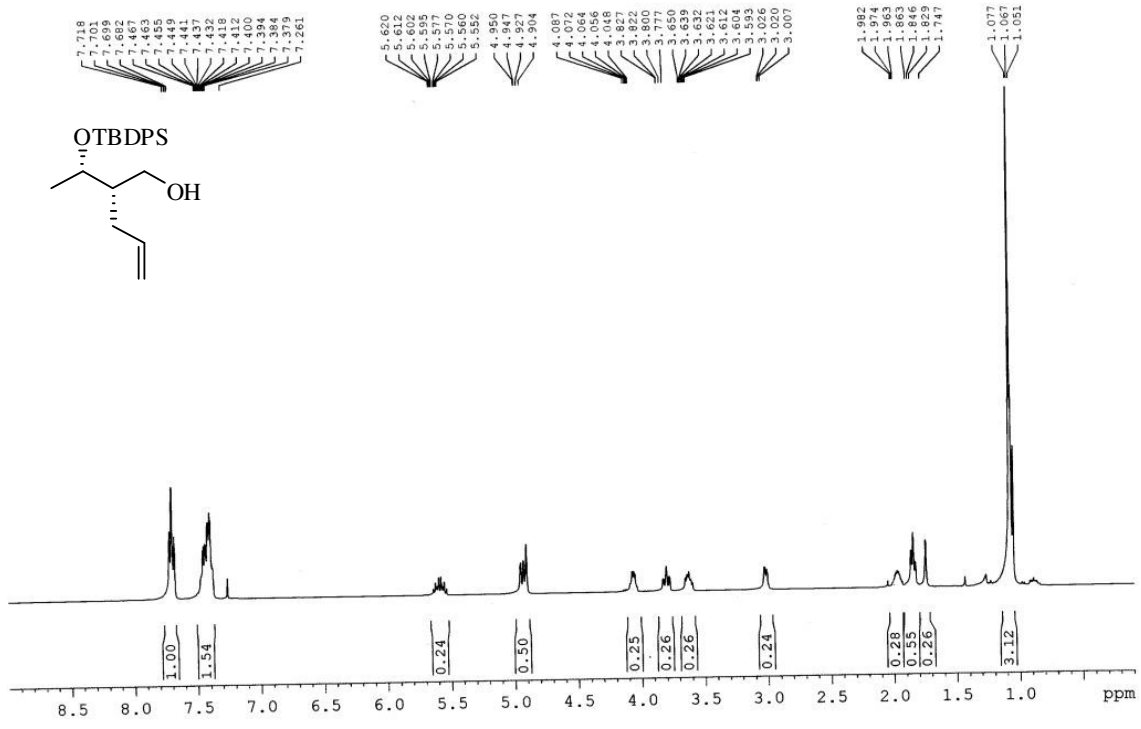
^{13}C NMR of compound 31 (50 MHz, $CDCl_3$)



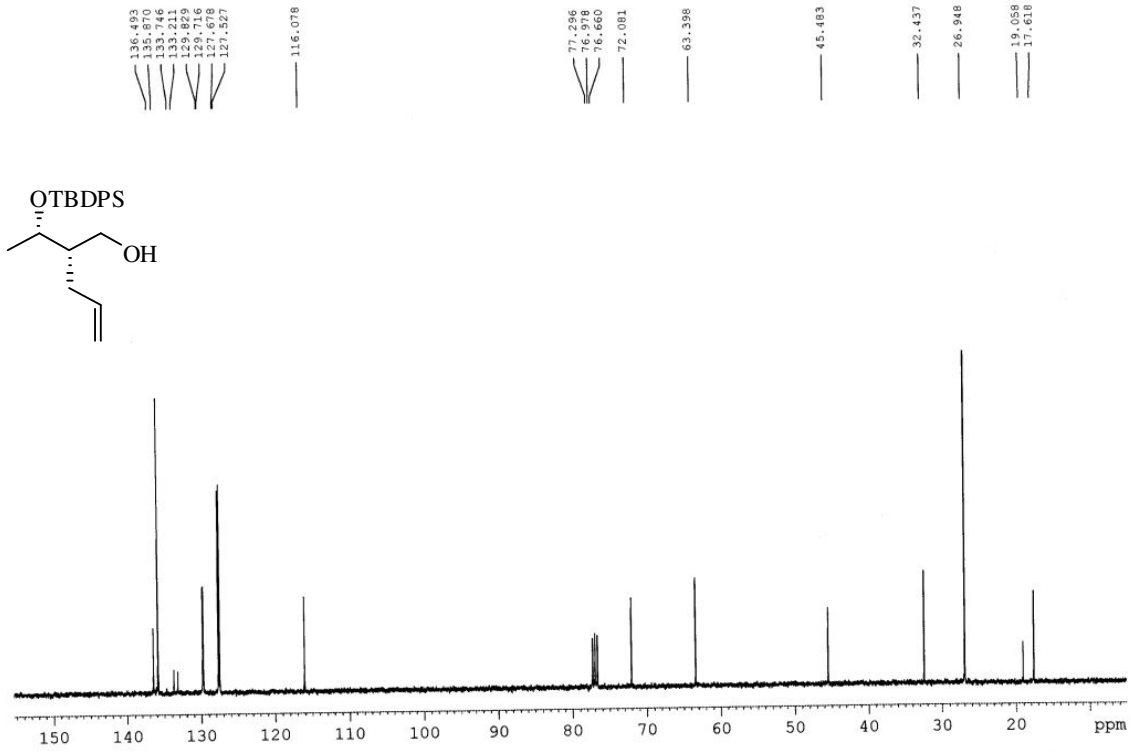
DEPT-135 NMR of compound 31 (50 MHz, $CDCl_3$)



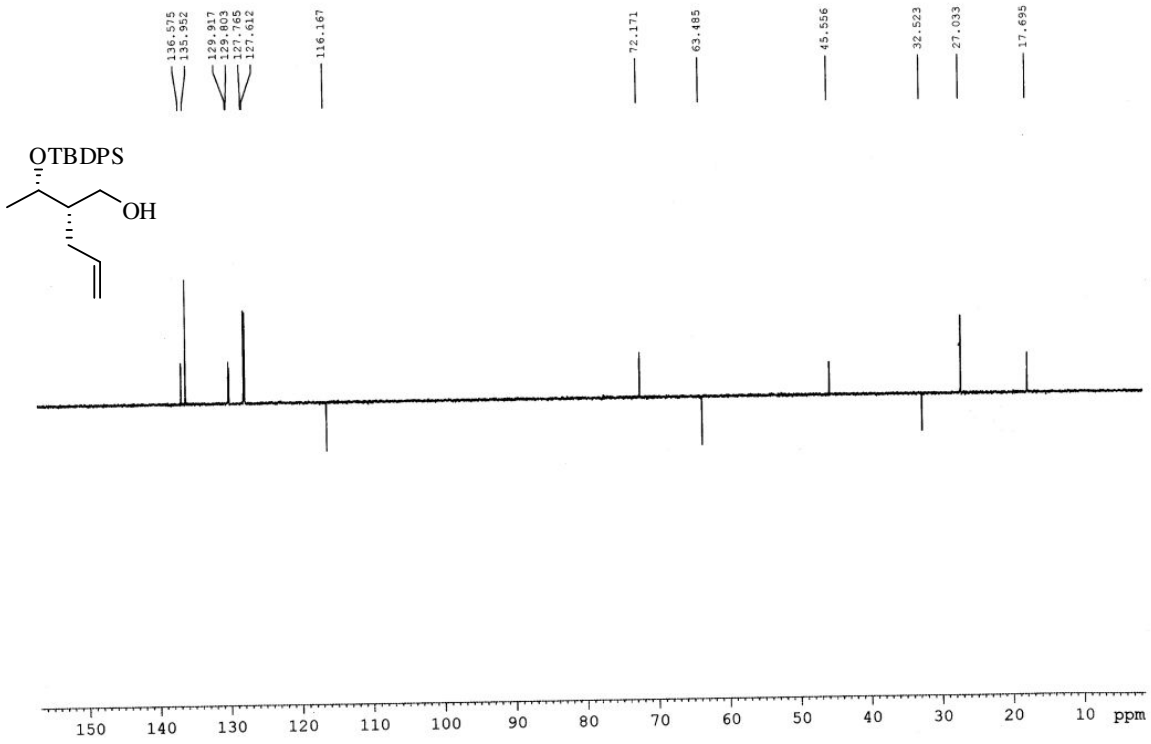
^{1}H - NMR of compound 33 (400 MHz, $CDCl_3$)



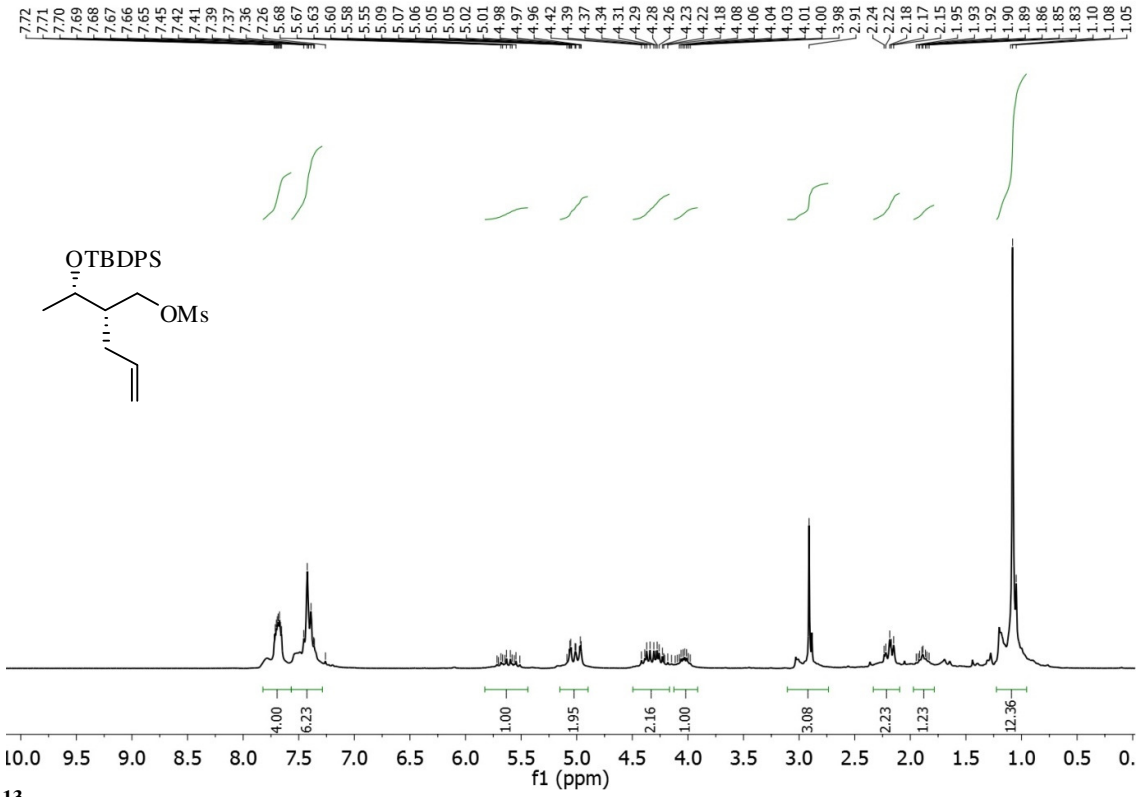
^{13}C NMR of compound 33 (50 MHz, $CDCl_3$)



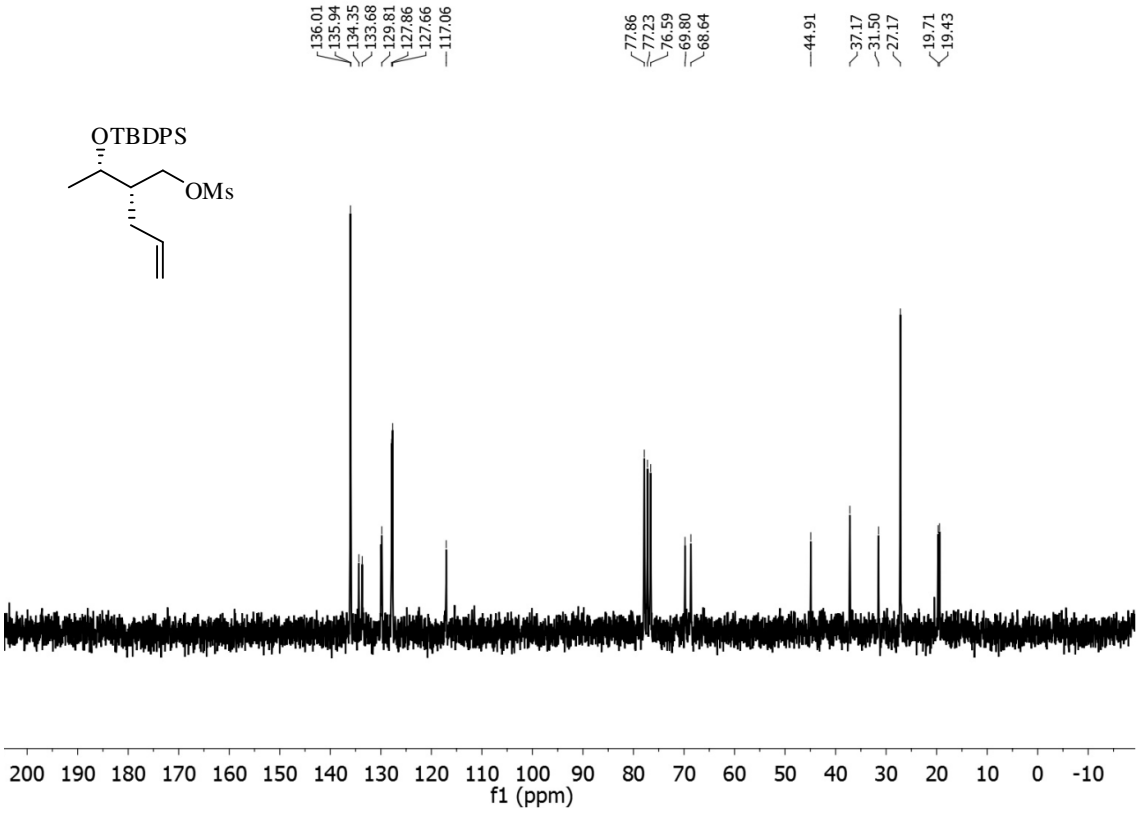
DEPT-135 NMR of compound 33 (50 MHz, $CDCl_3$)



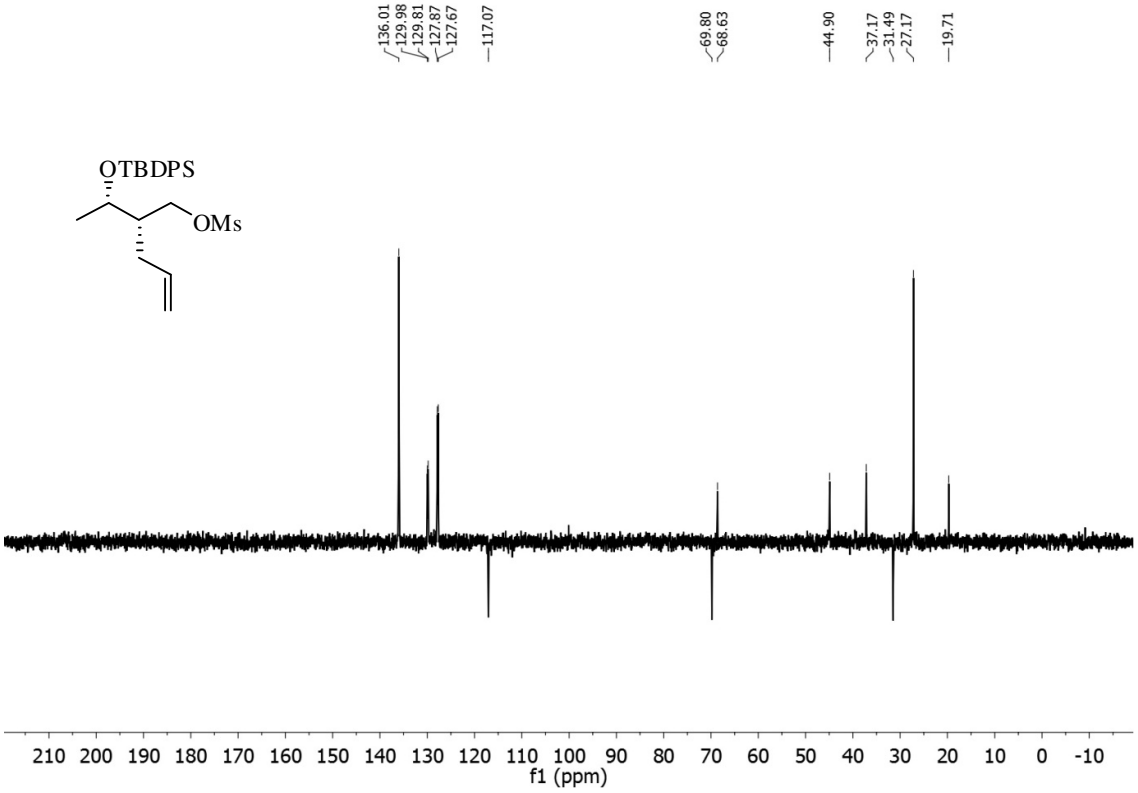
^{1}H - NMR of compound 34 (200 MHz, $CDCl_3$)



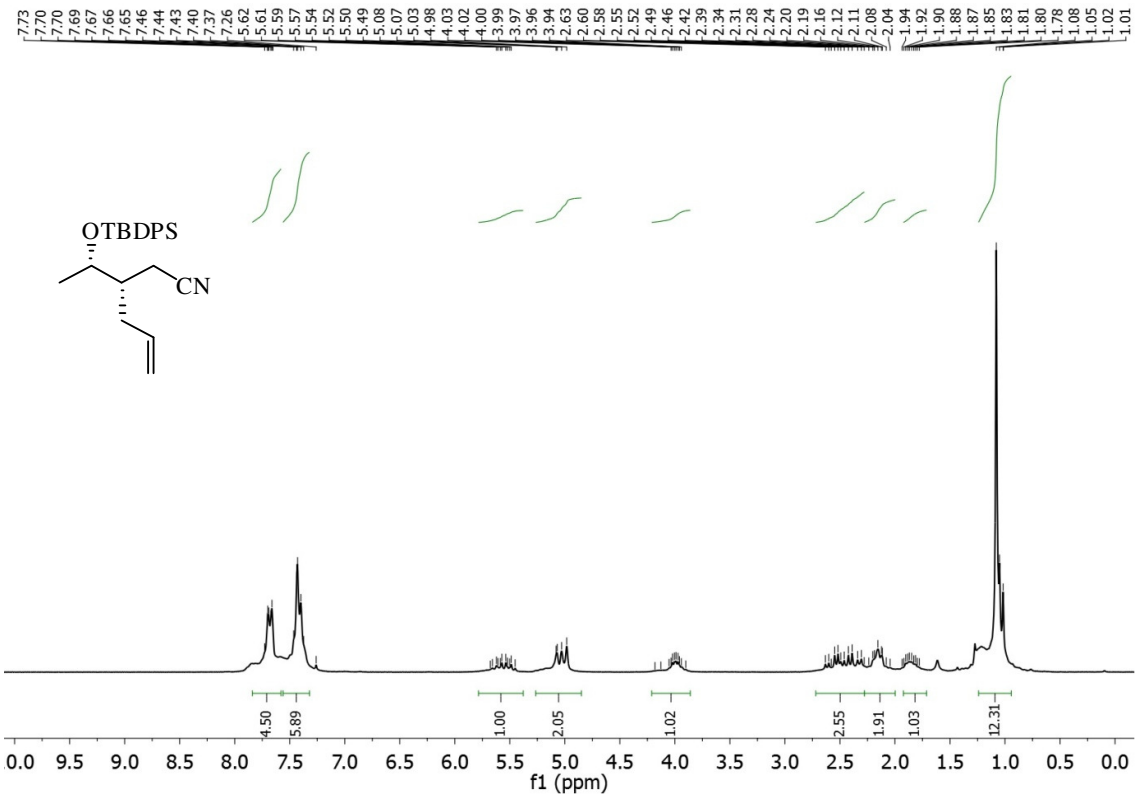
^{13}C NMR of compound 34 (50 MHz, $CDCl_3$)



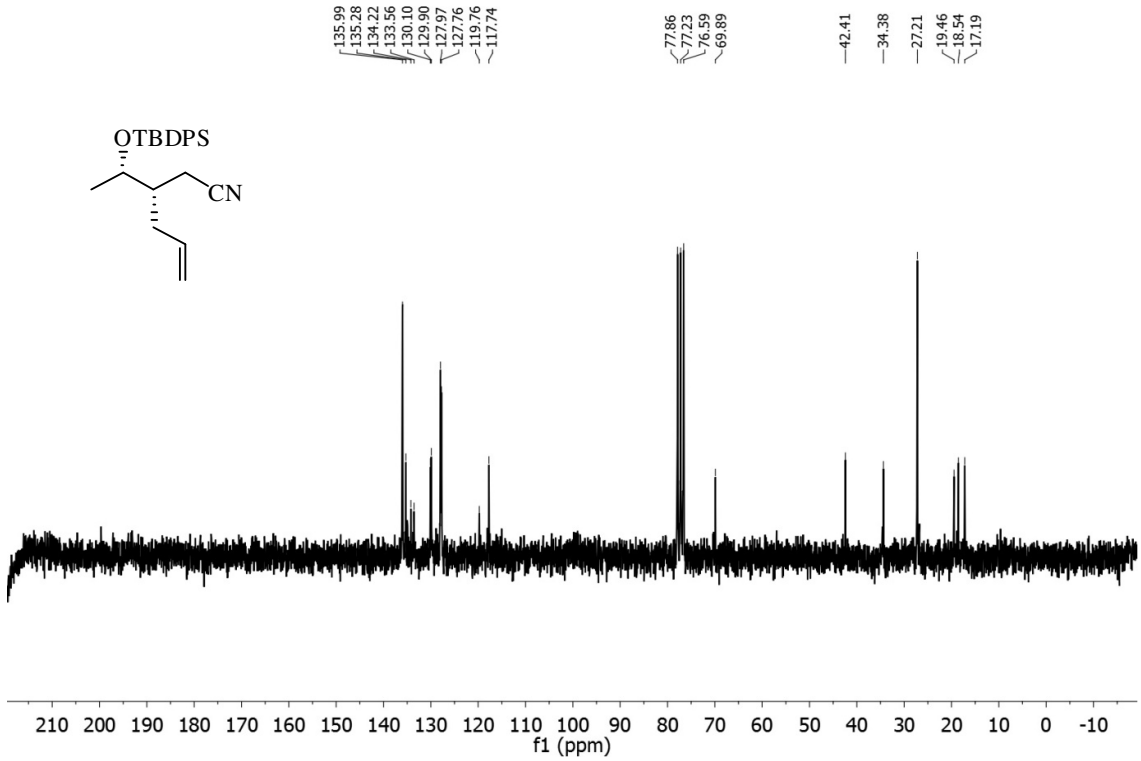
DEPT-135 NMR of compound 34 (50 MHz, $CDCl_3$)



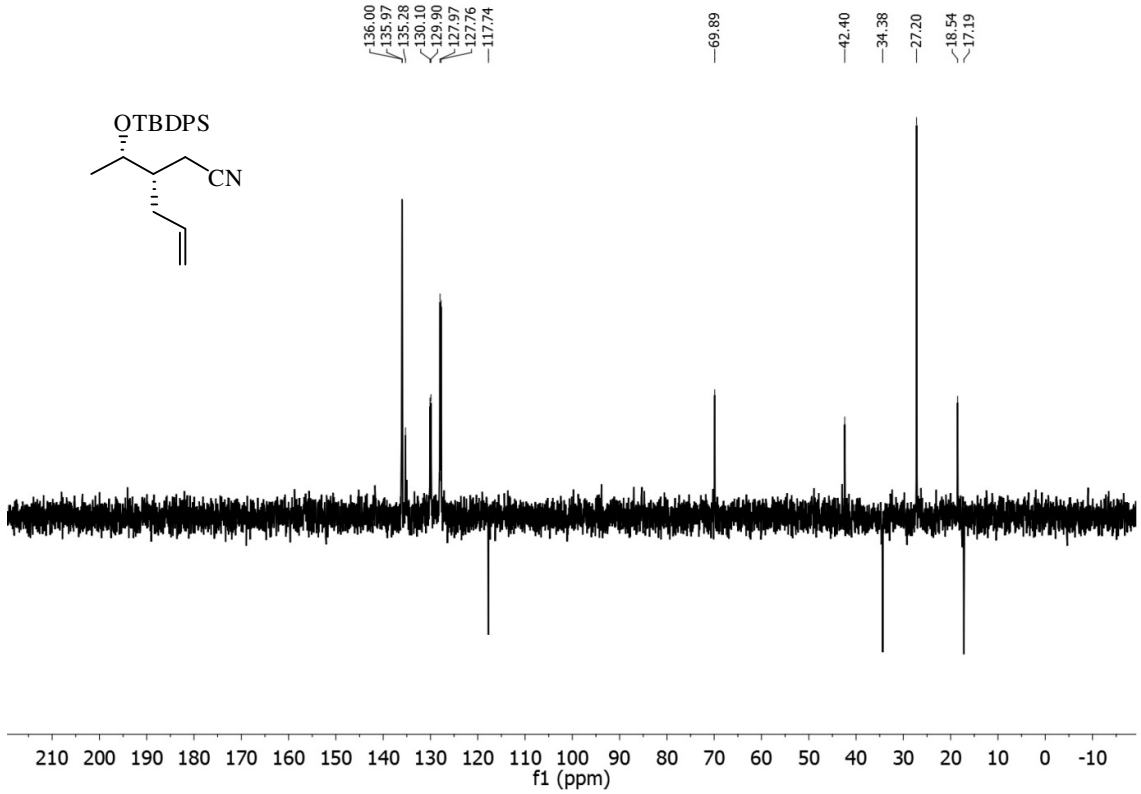
^{1}H - NMR of compound 35 (200 MHz, $CDCl_3$)



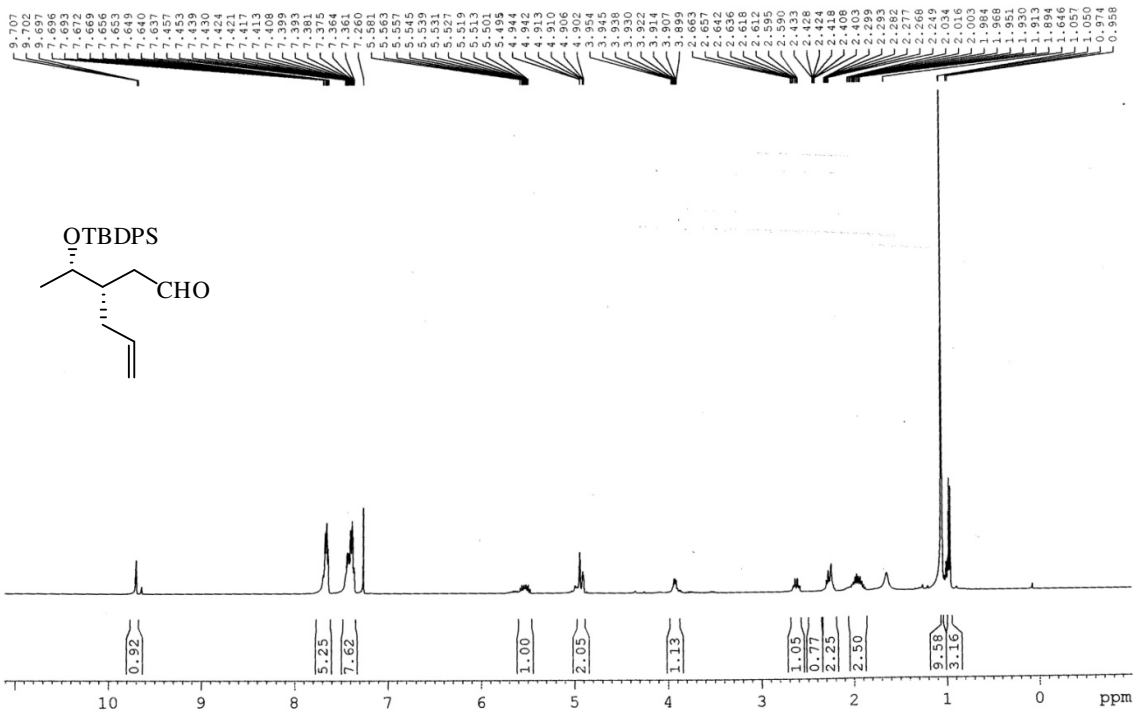
^{13}C NMR of compound 35 (50 MHz, $CDCl_3$)



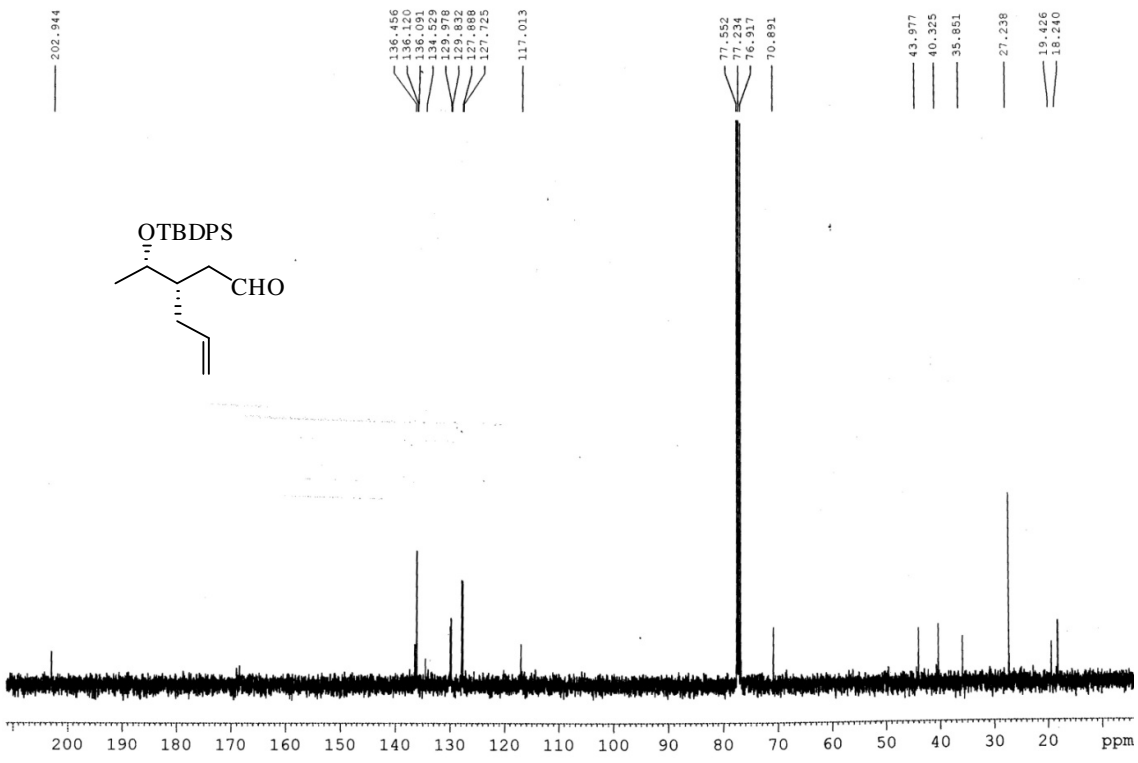
DEPT-135 NMR of compound 35 (50 MHz, $CDCl_3$)



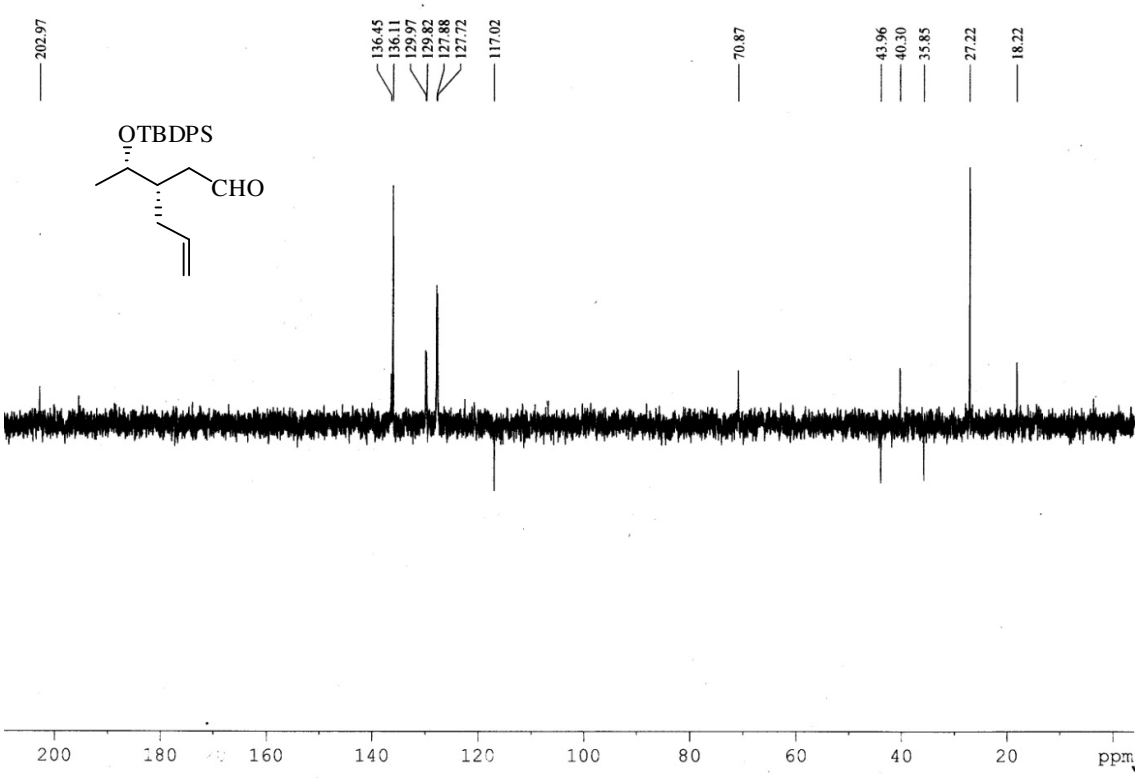
^{1}H - NMR of compound 36 (400 MHz, $CDCl_3$)



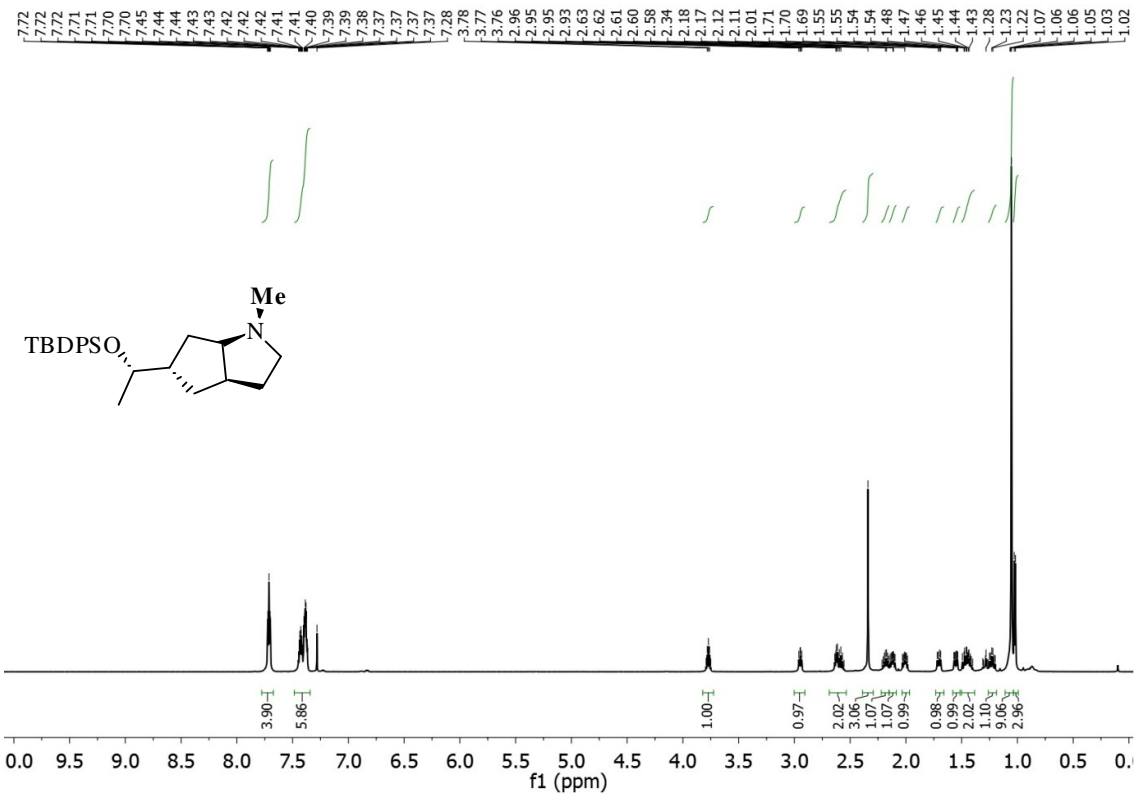
^{13}C NMR of compound 36 (100 MHz, $CDCl_3$)



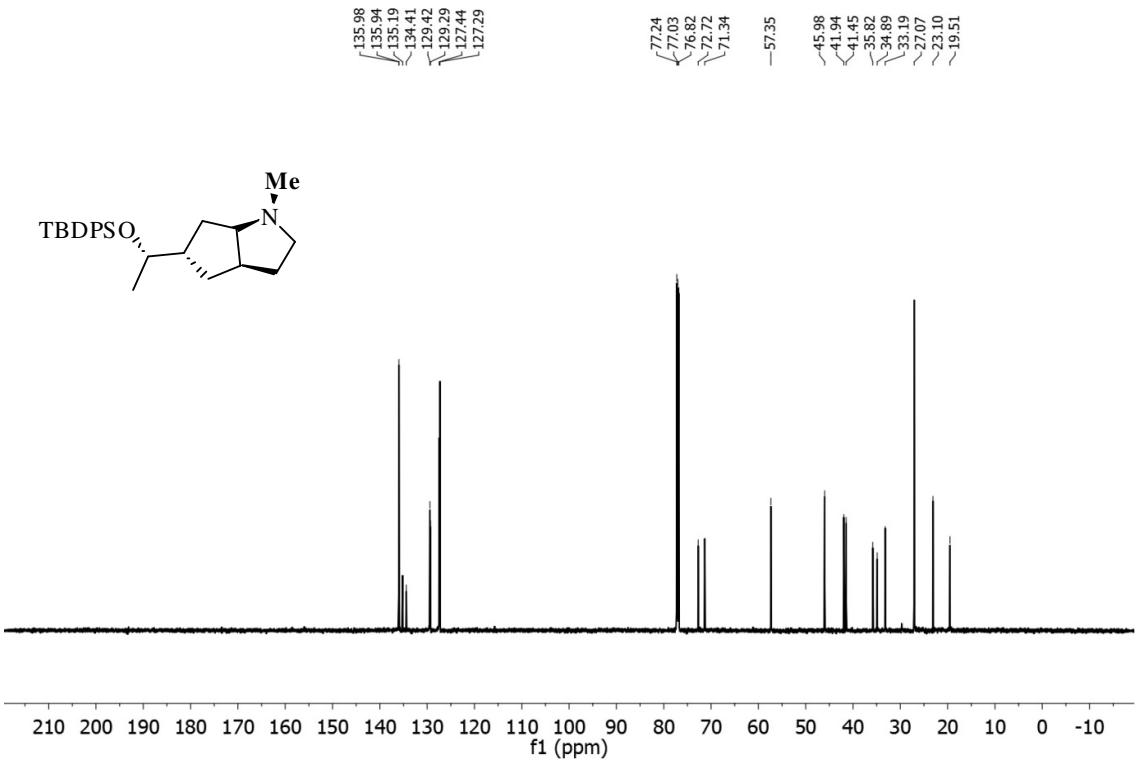
DEPT-135 NMR of compound 36 (50 MHz, $CDCl_3$)



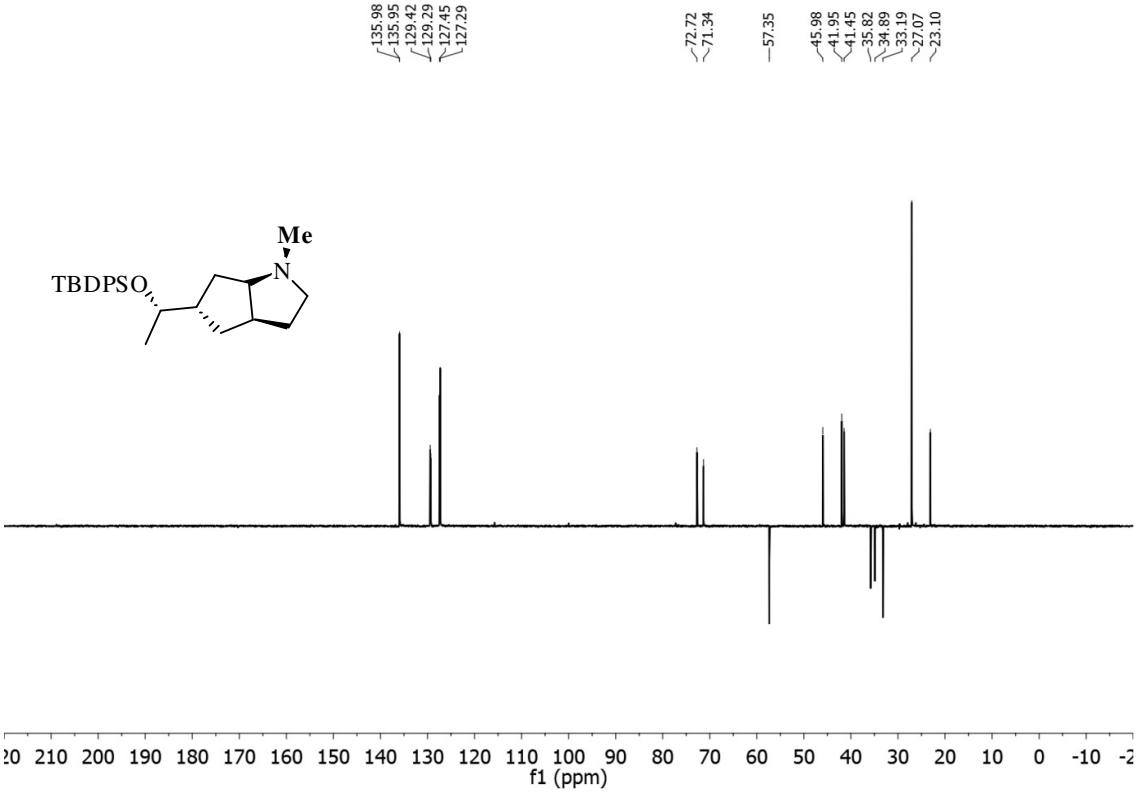
^{1}H - NMR of compound 37 (600 MHz, $CDCl_3$)



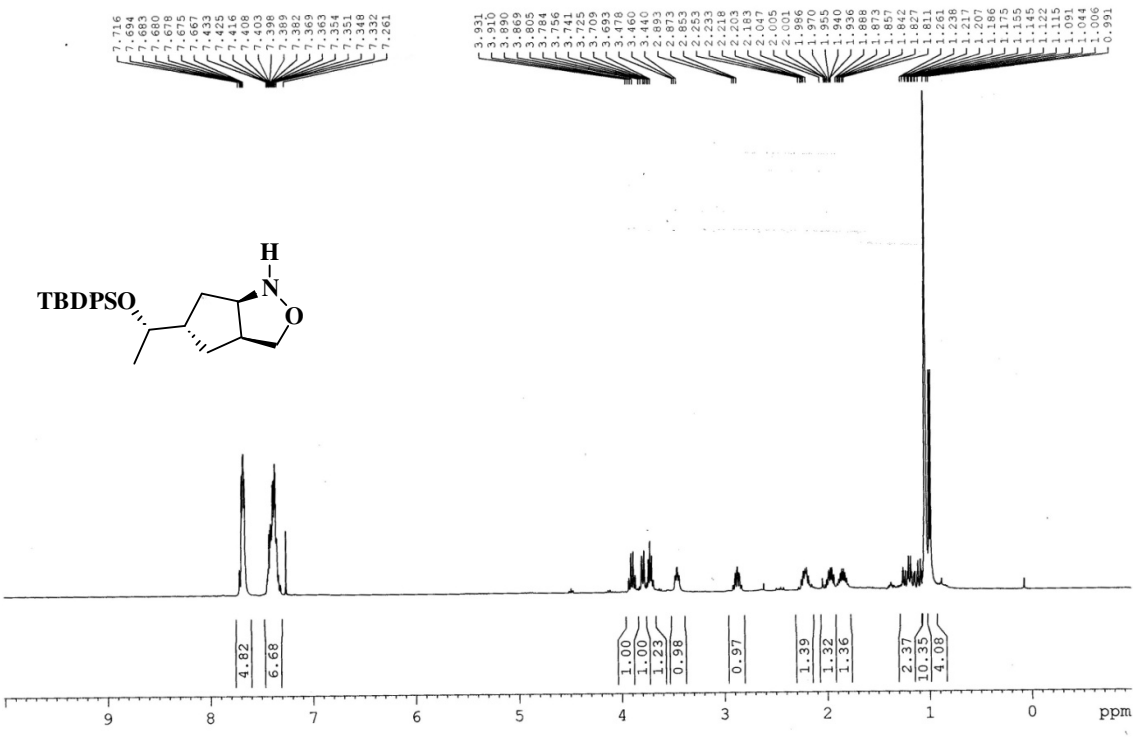
^{13}C NMR of compound 37 (150 MHz, $CDCl_3$)



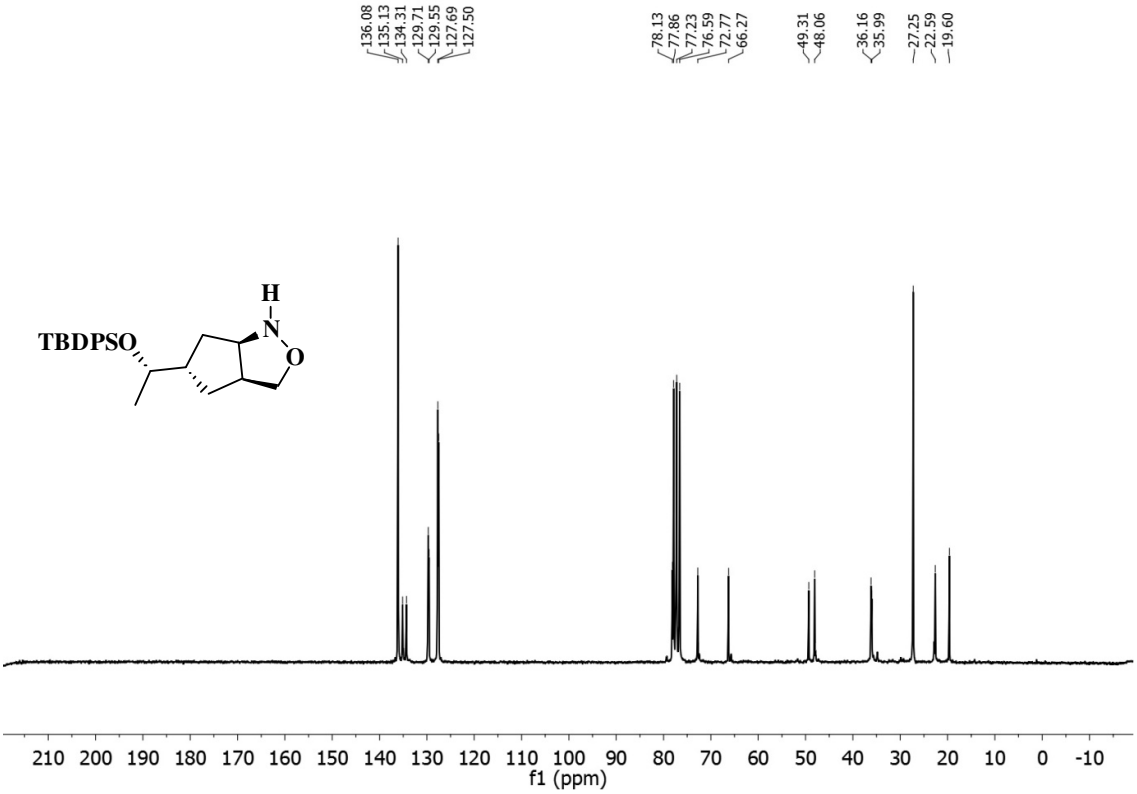
DEPT-135 NMR of compound 37 (150 MHz, $CDCl_3$)



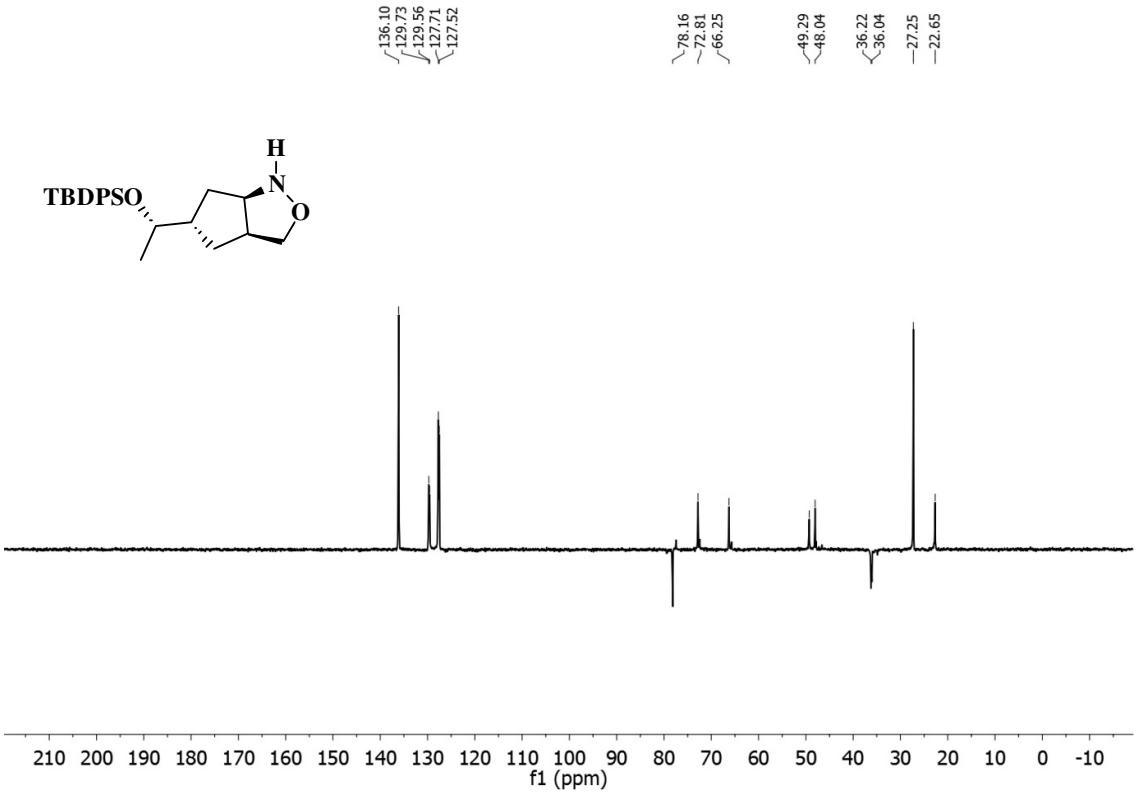
^{1}H - NMR of compound 38 (400 MHz, $CDCl_3$)



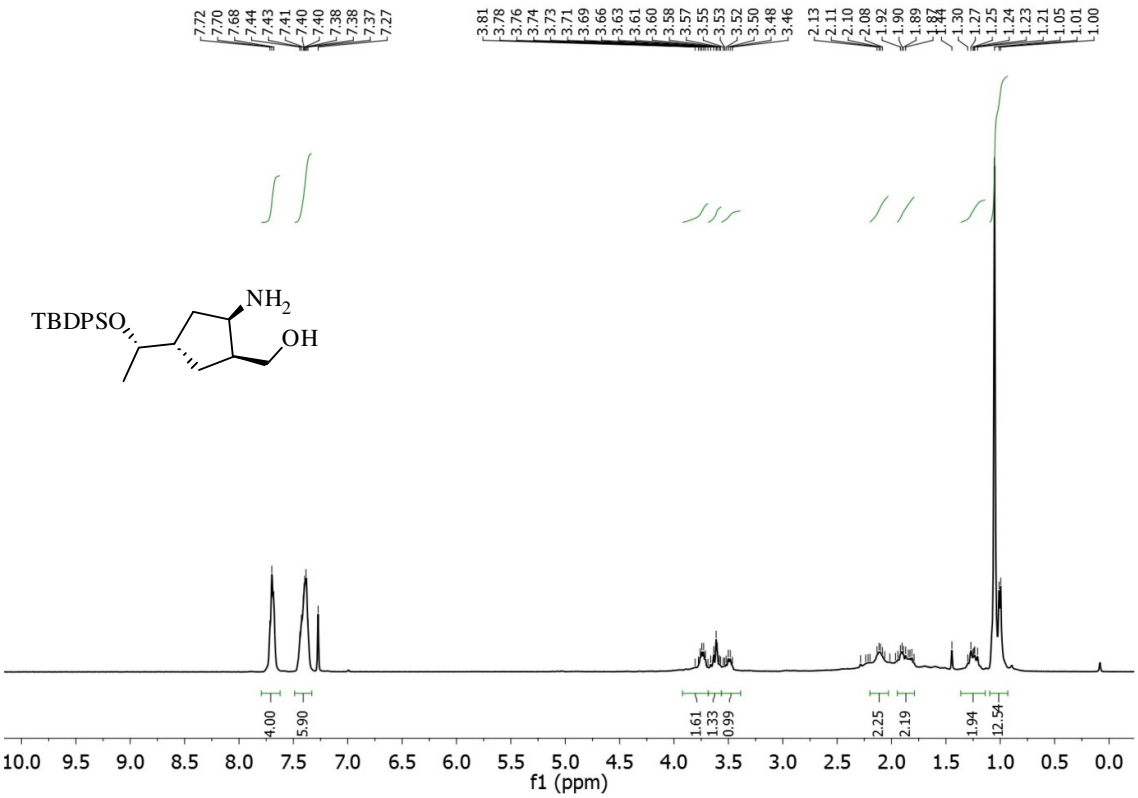
^{13}C NMR of compound 38 (50 MHz, $CDCl_3$)



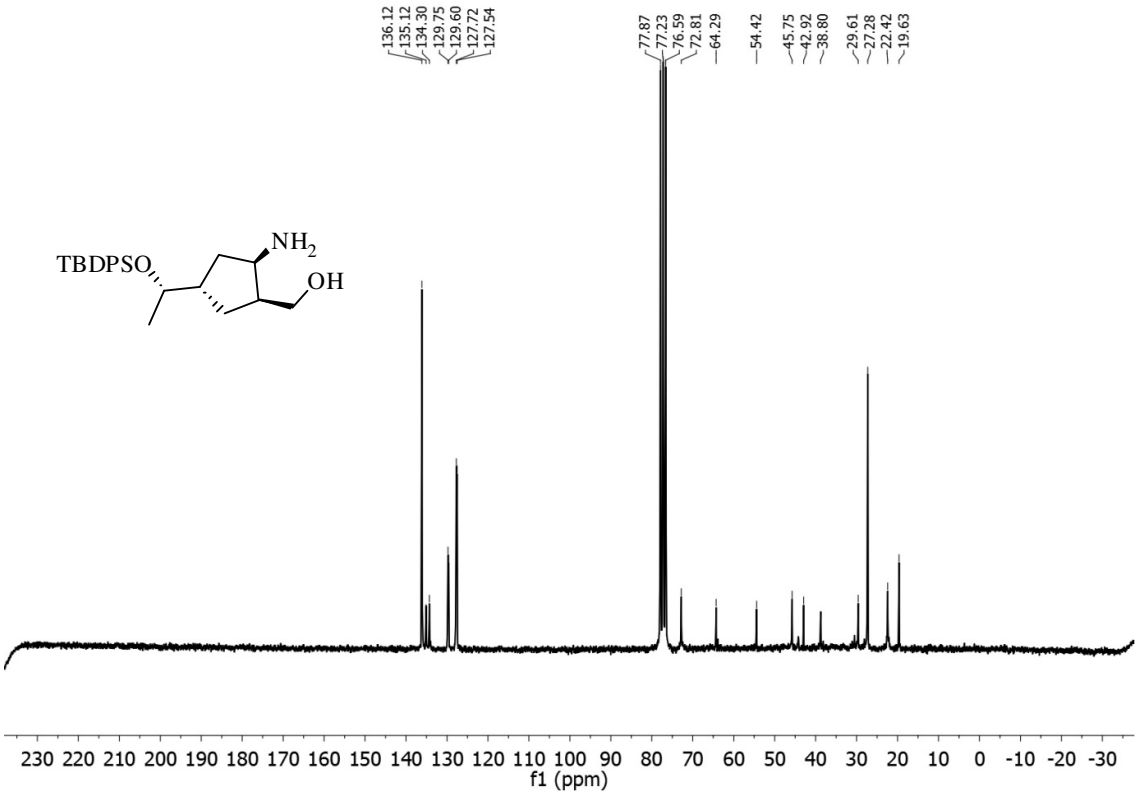
DEPT-135 NMR of compound 38 (50 MHz, $CDCl_3$)



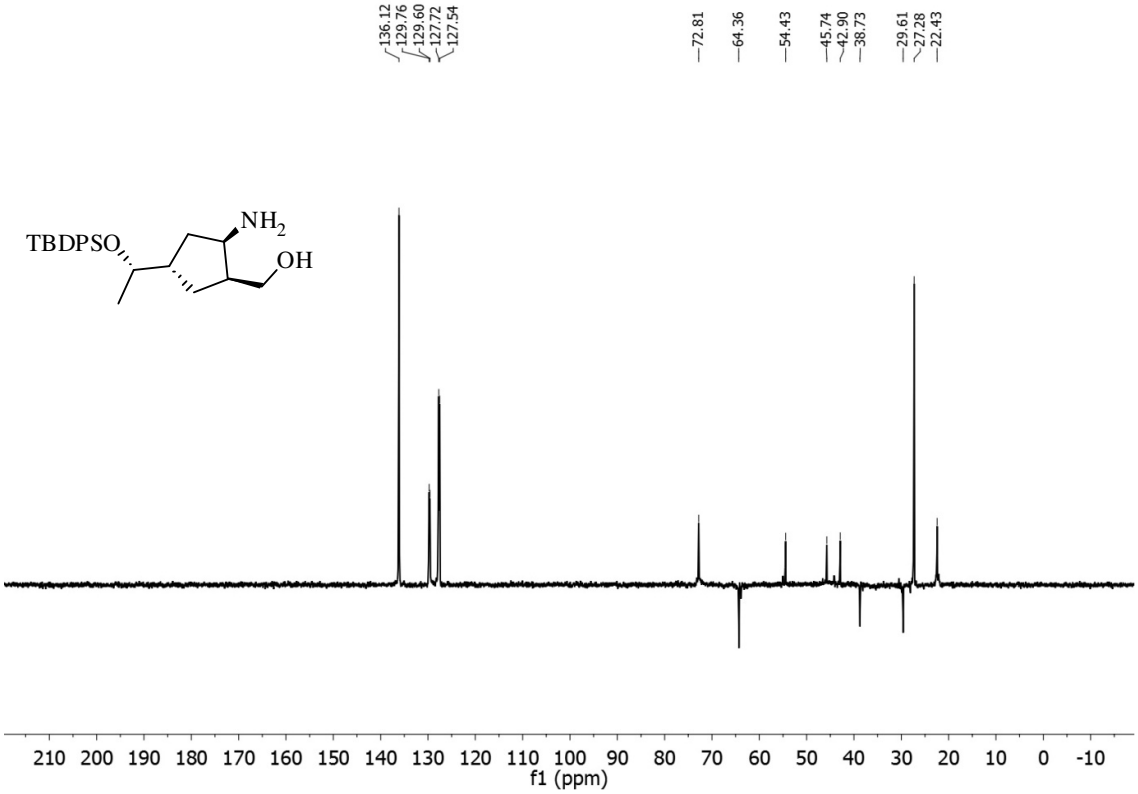
^{1}H - NMR of compound 39 (400 MHz, $CDCl_3$)



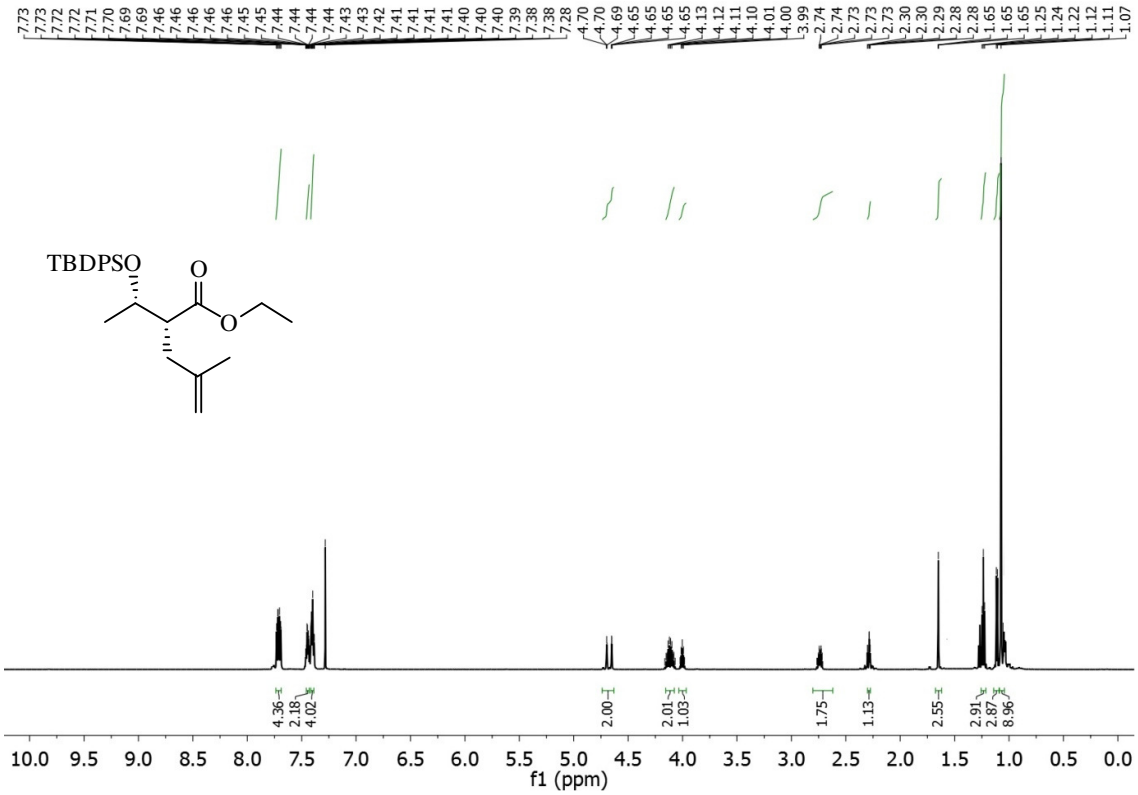
^{13}C NMR of compound 39 (100 MHz, $CDCl_3$)



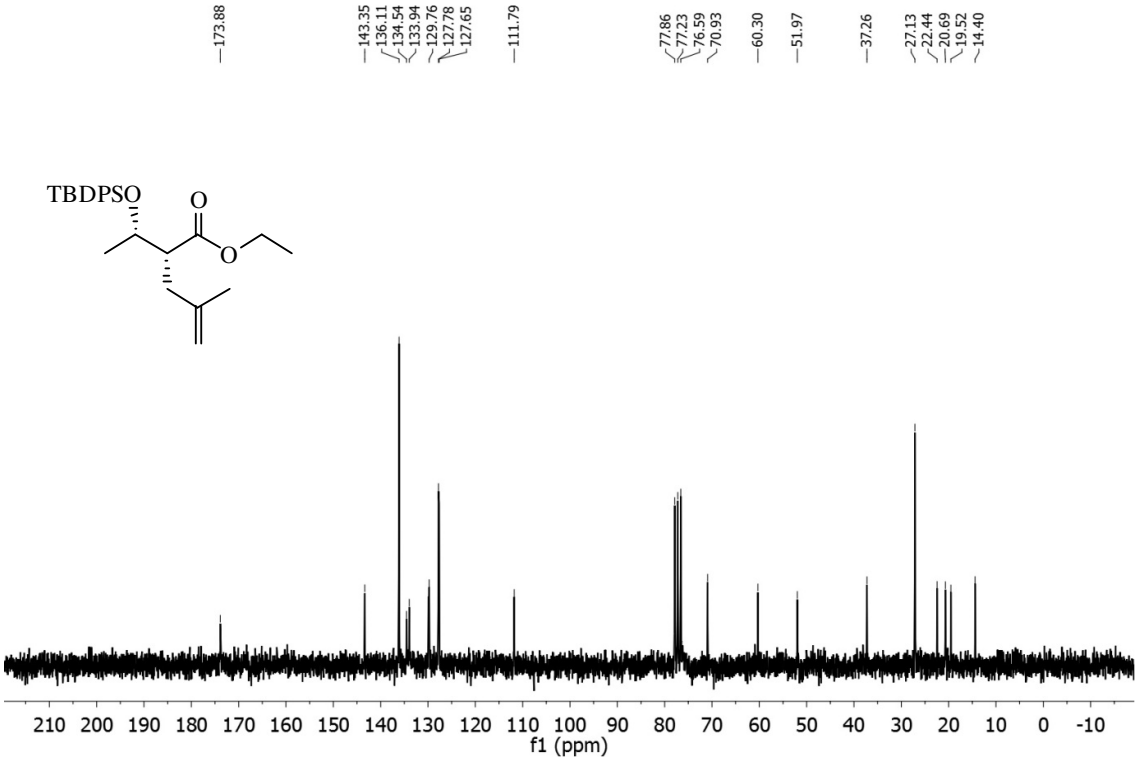
DEPT-135 NMR of compound 39 (100 MHz, $CDCl_3$)



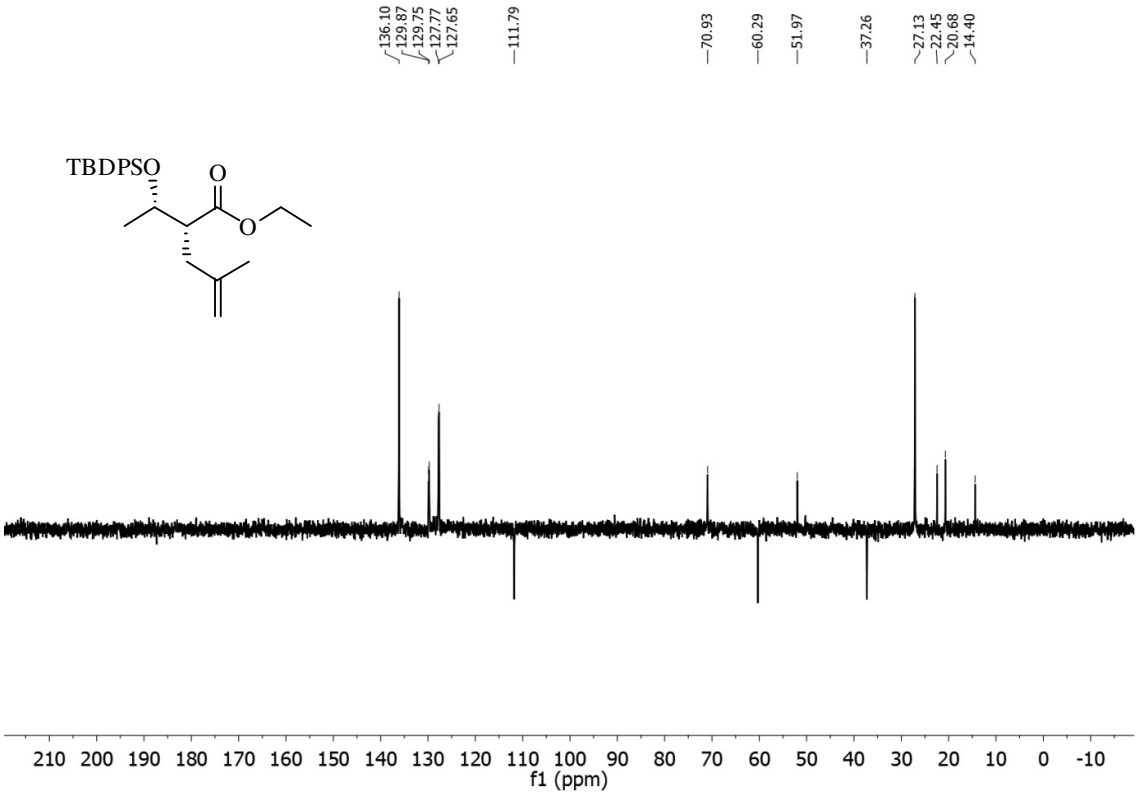
^{1}H - NMR of compound 40 (600 MHz, $CDCl_3$)



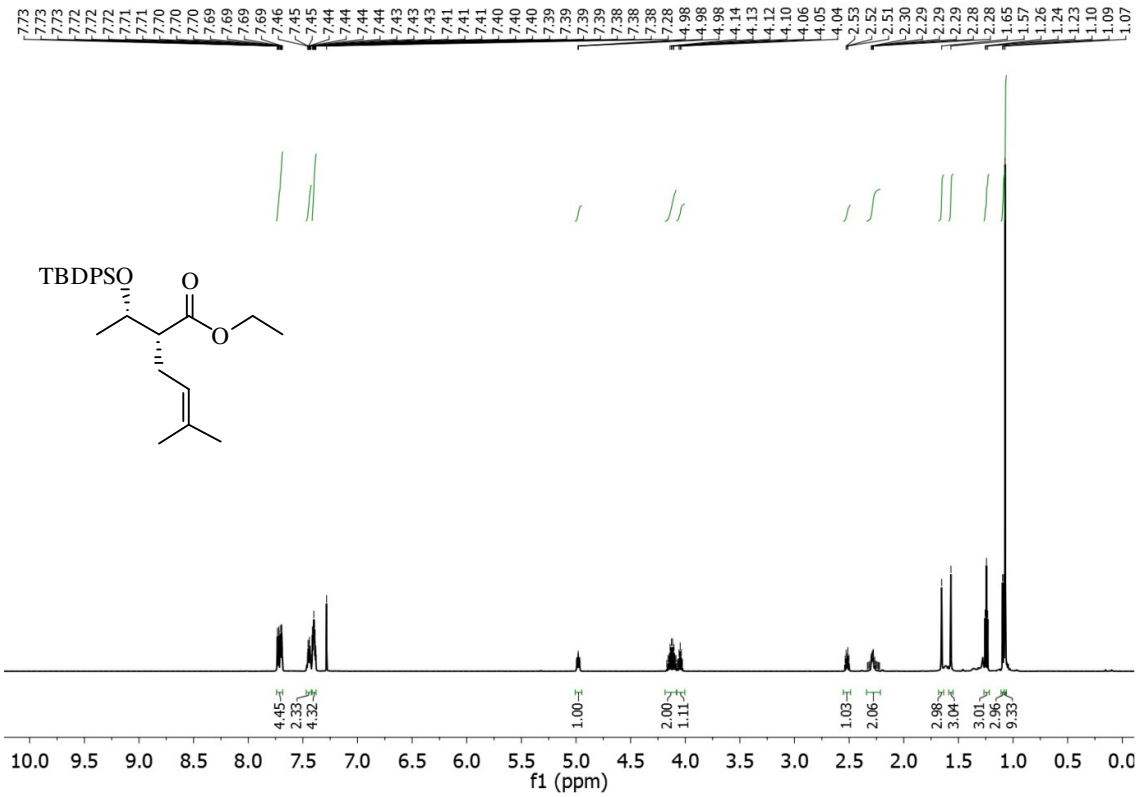
^{13}C NMR of compound 40 (50 MHz, $CDCl_3$)



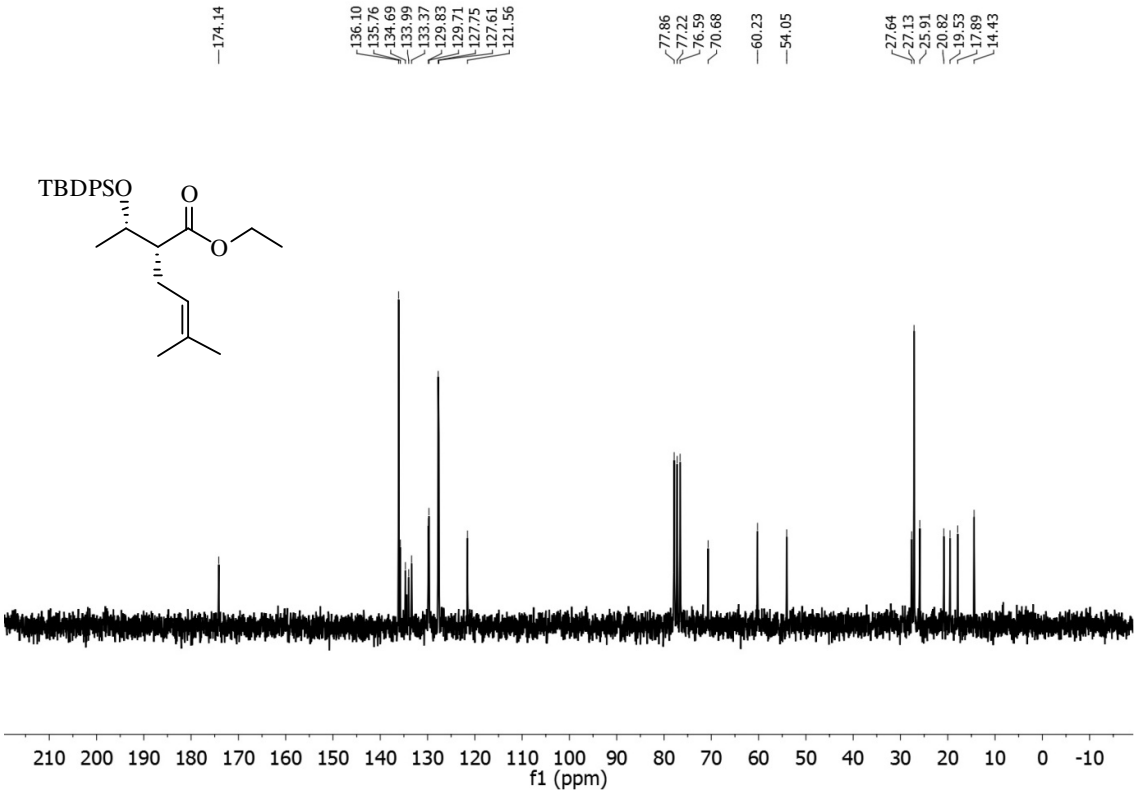
DEPT-135 NMR of compound 40 (50 MHz, $CDCl_3$)



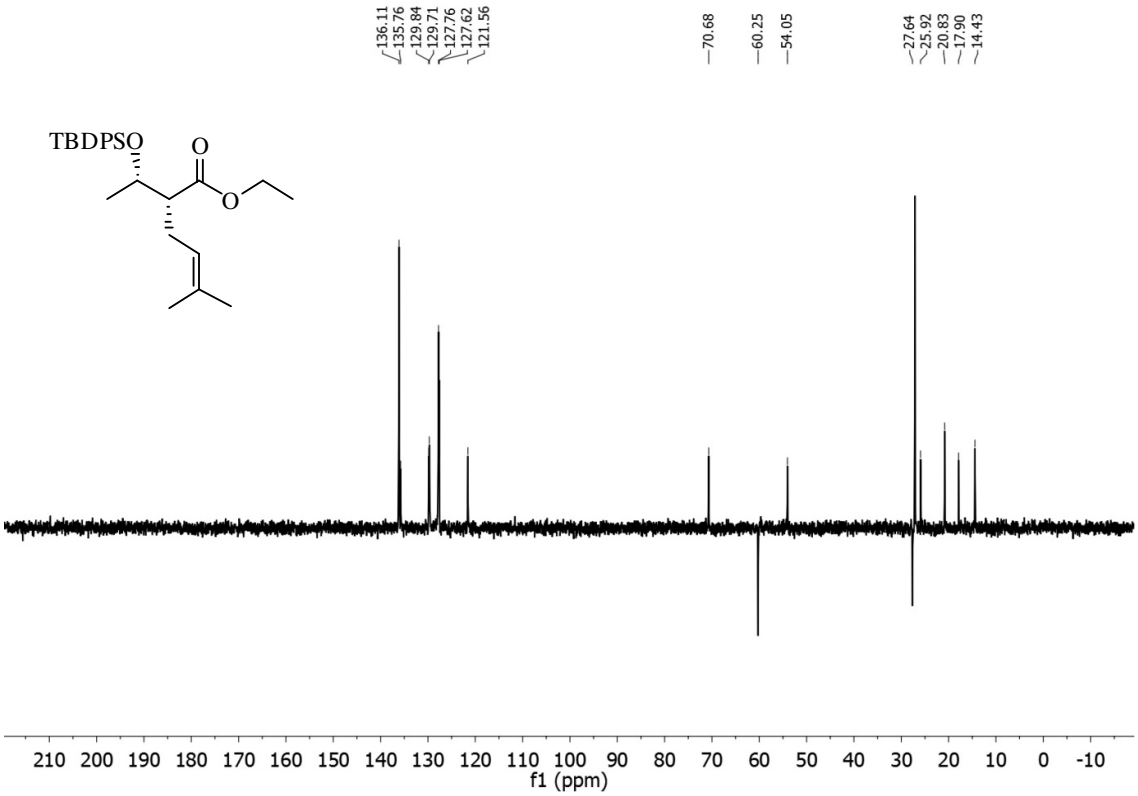
^{1}H - NMR of compound 41 (400 MHz, $CDCl_3$)



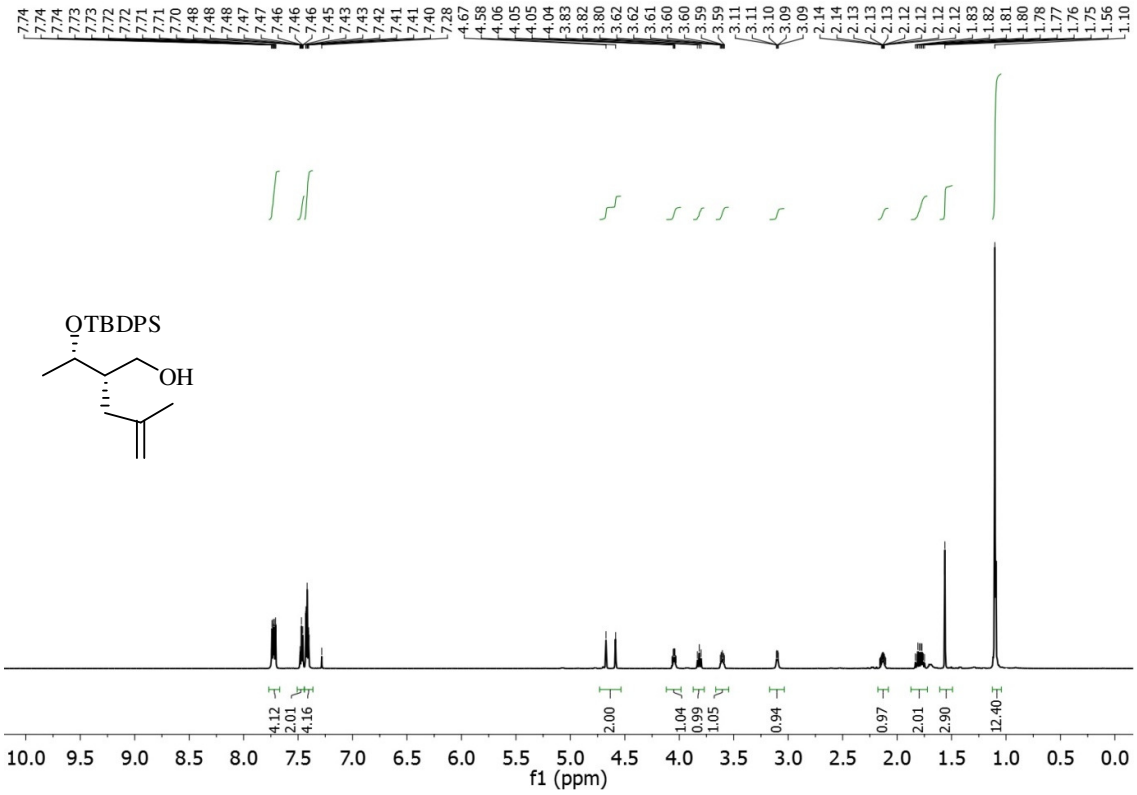
^{13}C NMR of compound 41 (50 MHz, $CDCl_3$)



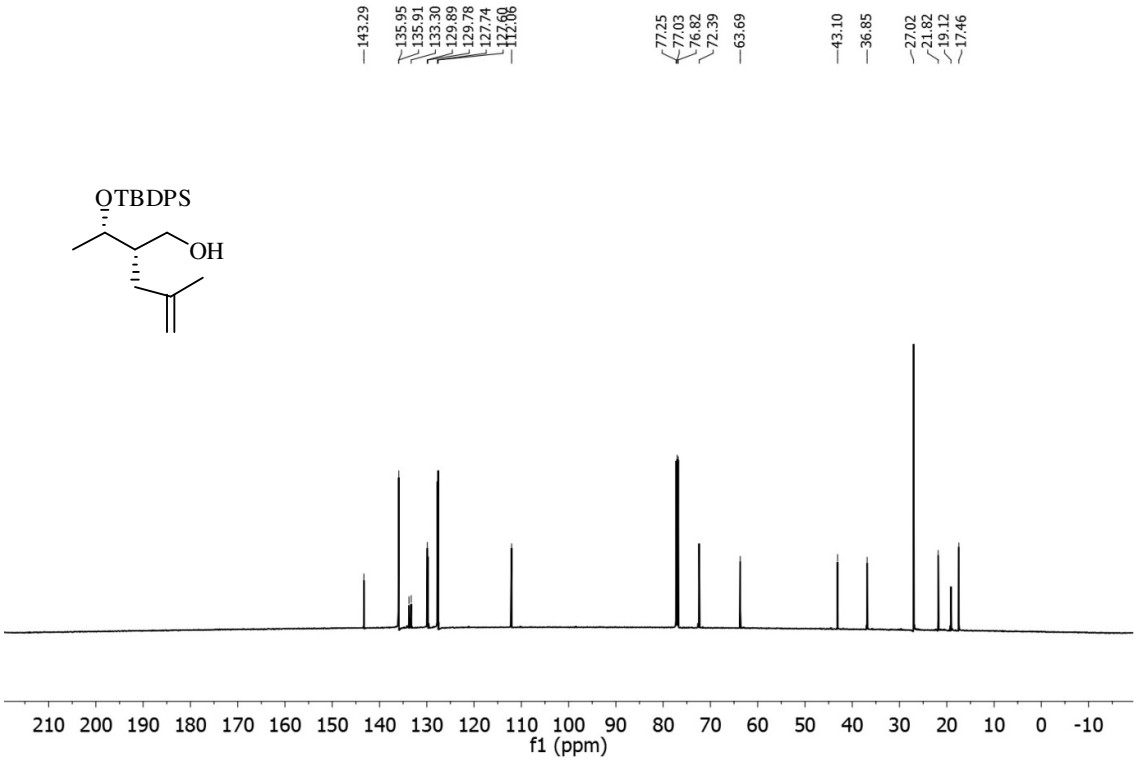
DEPT-135 NMR of compound 41 (50 MHz, $CDCl_3$)



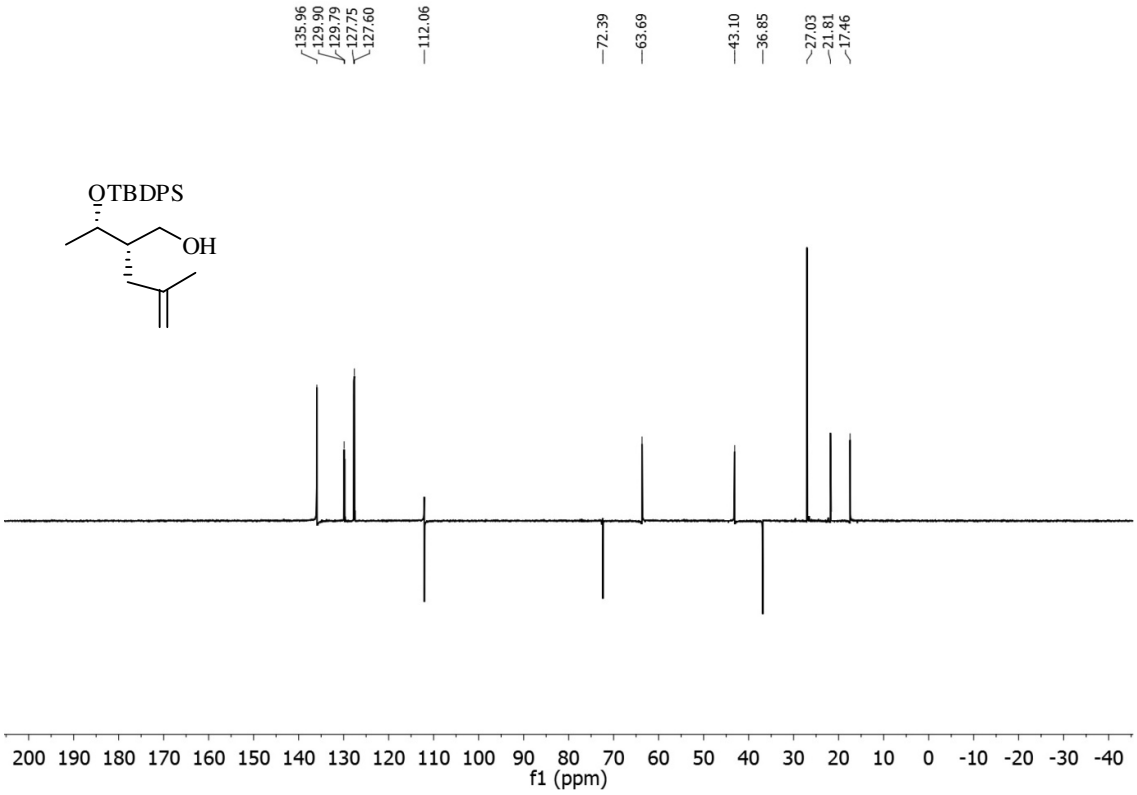
^{1}H - NMR of compound 42 (600 MHz, $CDCl_3$)



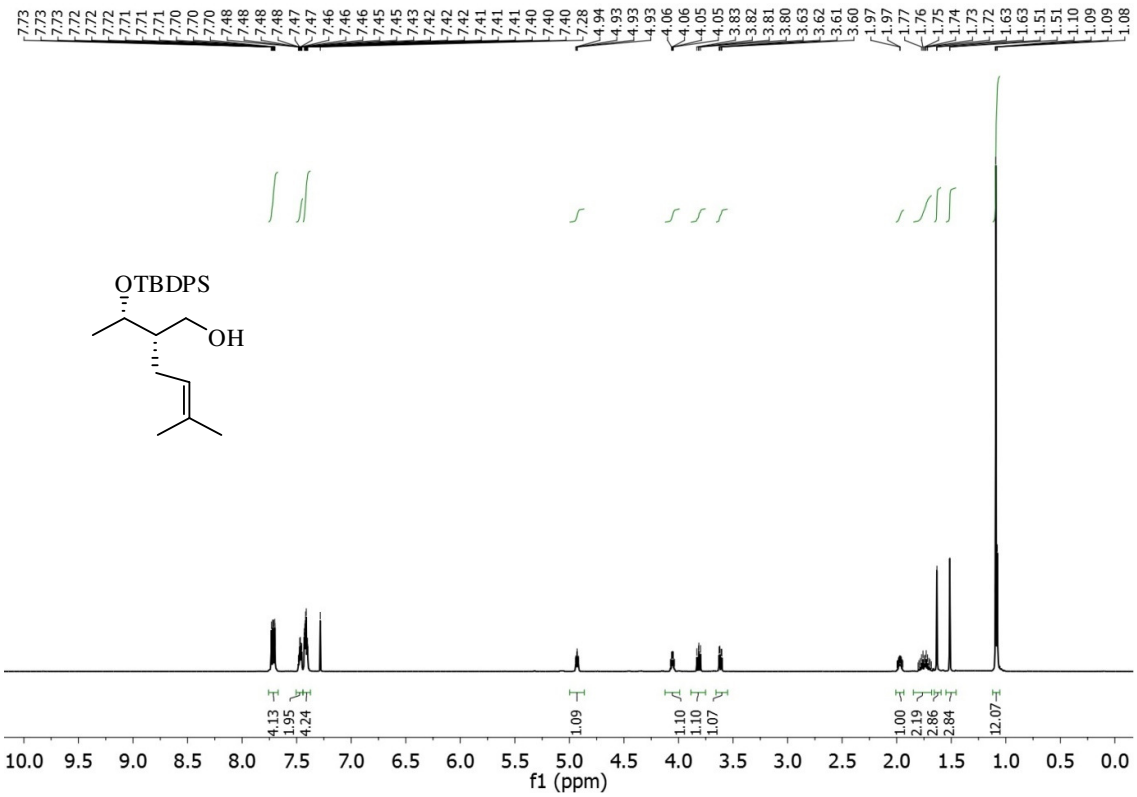
^{13}C NMR of compound 42 (150 MHz, $CDCl_3$)



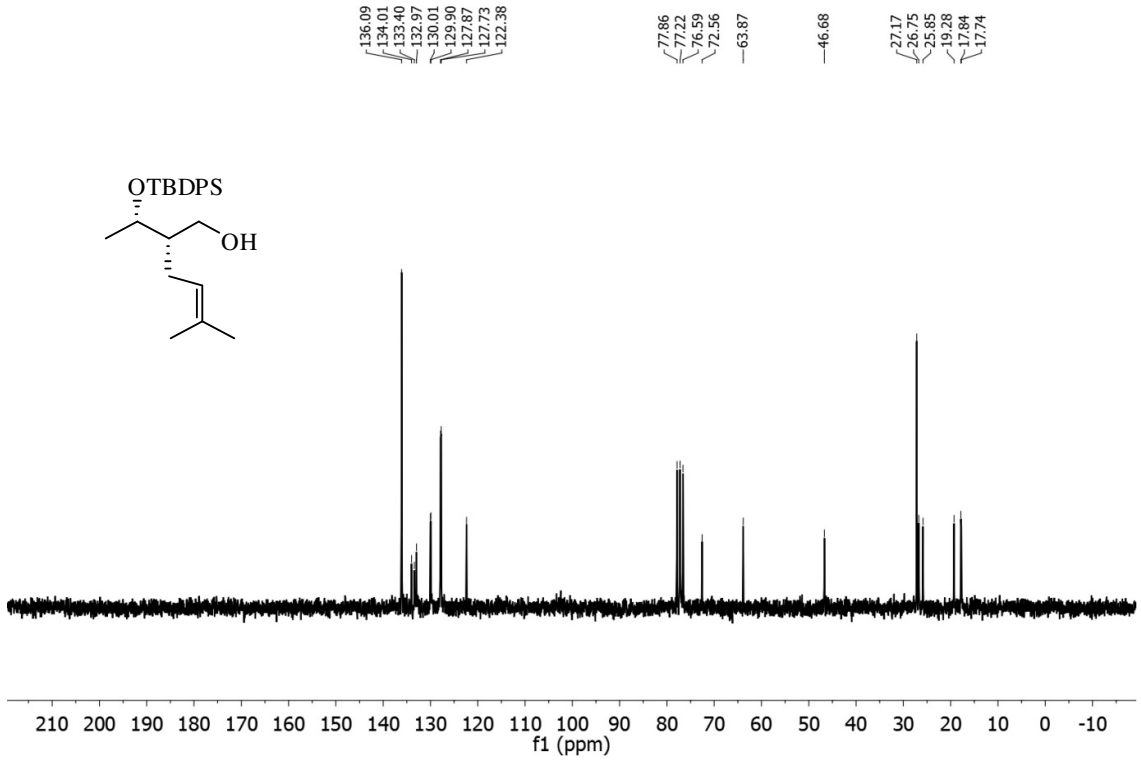
DEPT-135 NMR of compound 42 (150 MHz, $CDCl_3$)



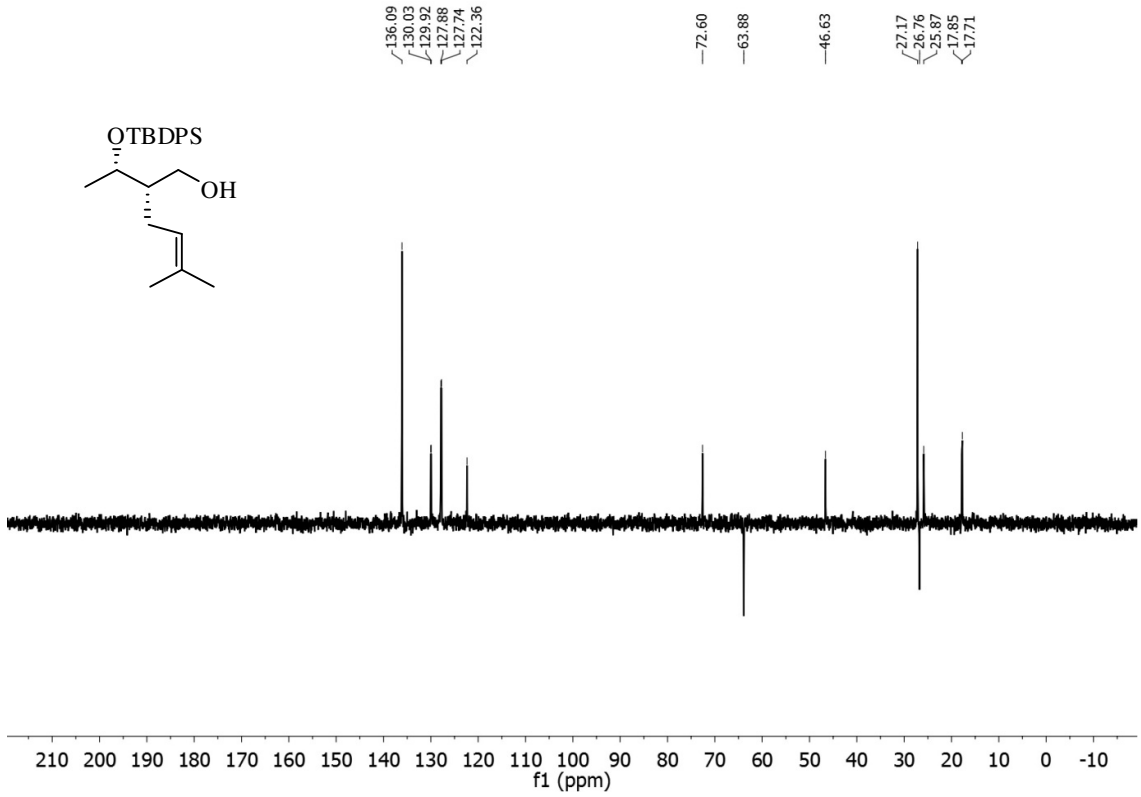
^{1}H - NMR of compound 43 (600 MHz, $CDCl_3$)



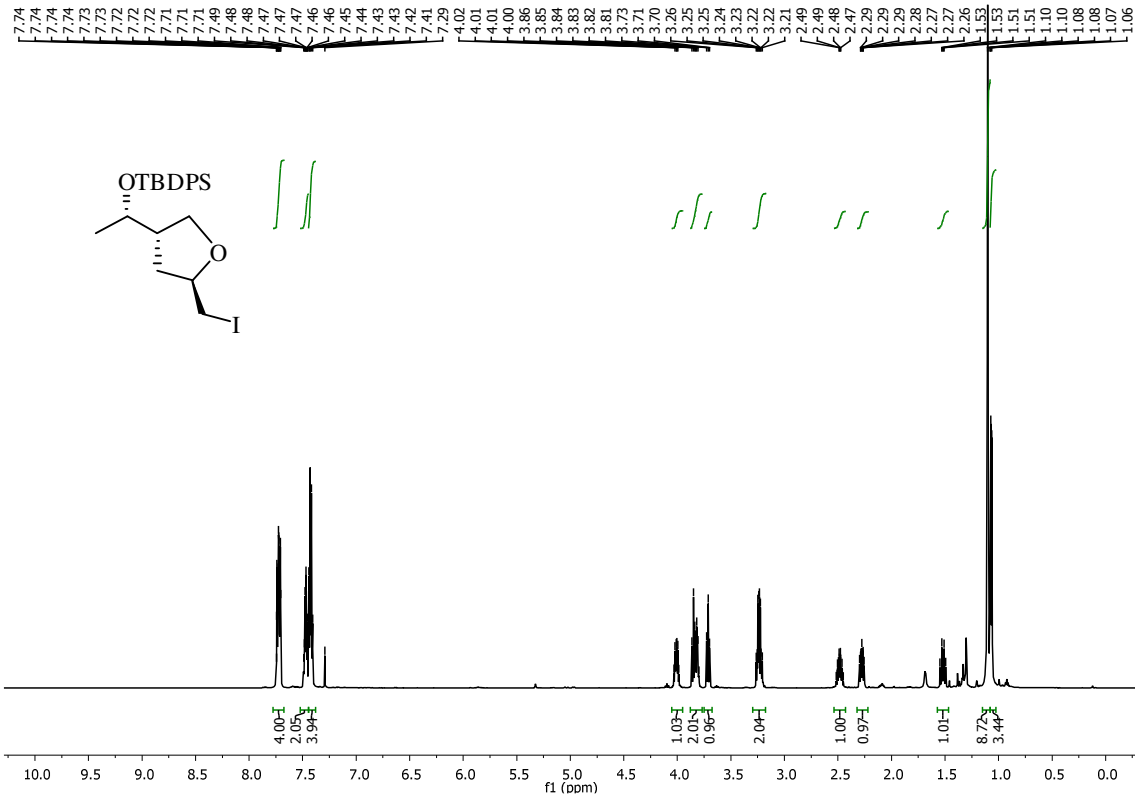
^{13}C NMR of compound 43 (50 MHz, $CDCl_3$)



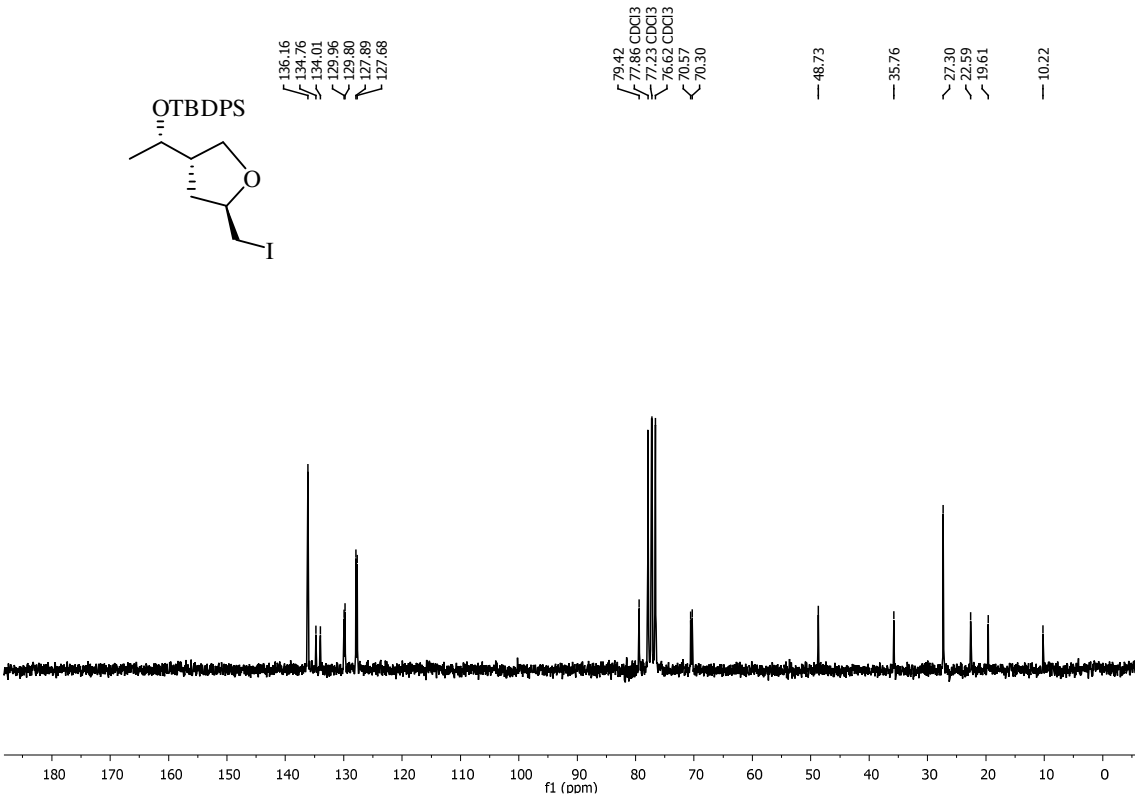
DEPT-135 NMR of compound 43 (50 MHz, $CDCl_3$)



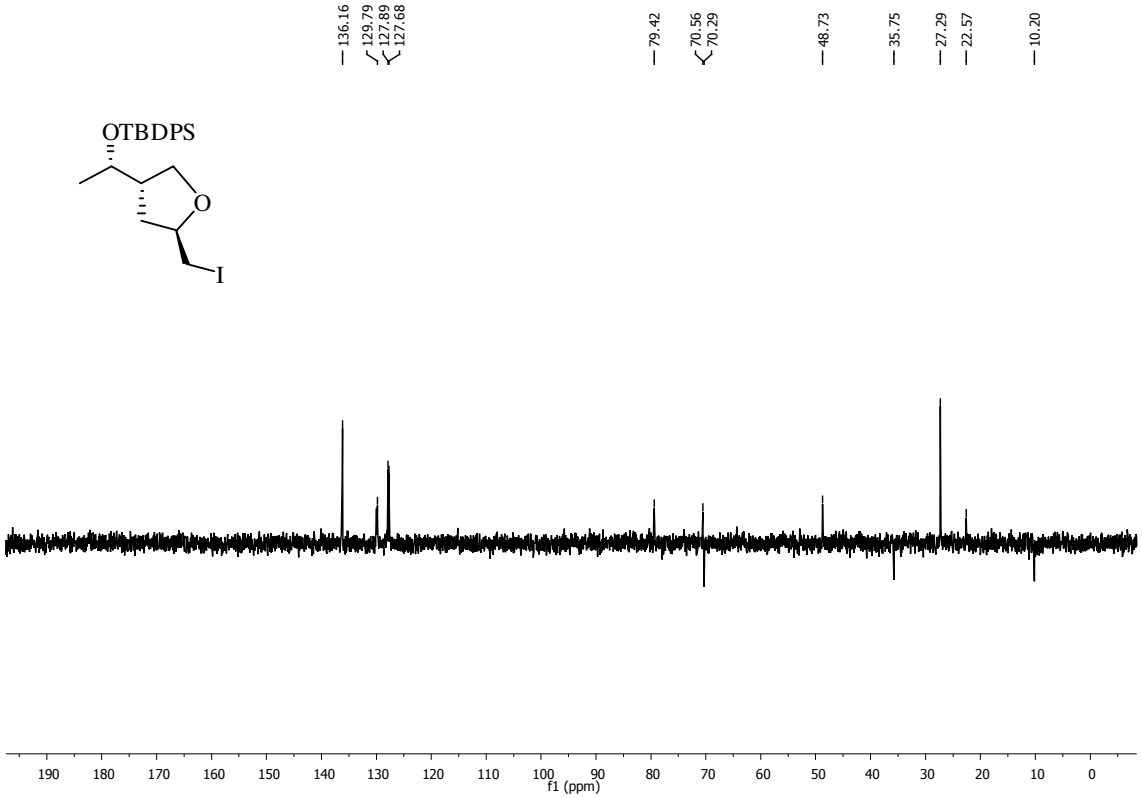
^{1}H - NMR of compound 44 (600 MHz, $CDCl_3$)



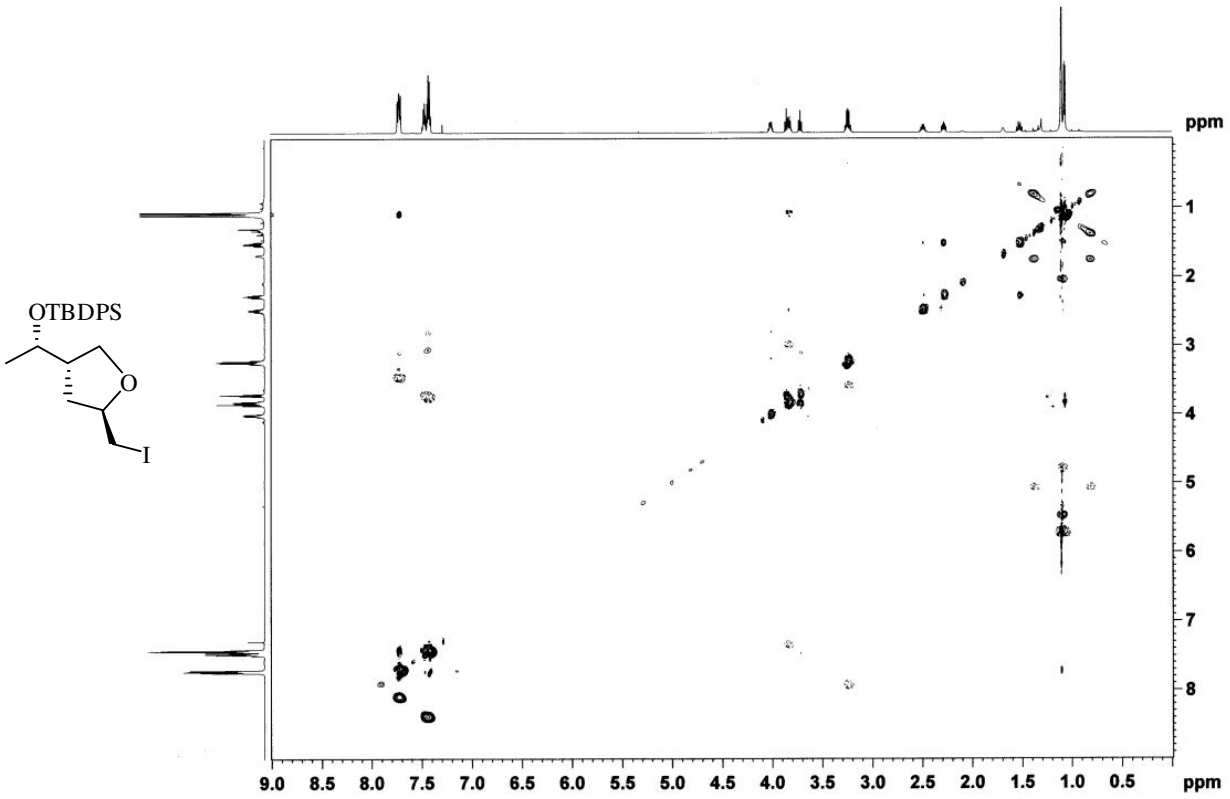
^{13}C NMR of compound 44 (50 MHz, $CDCl_3$)



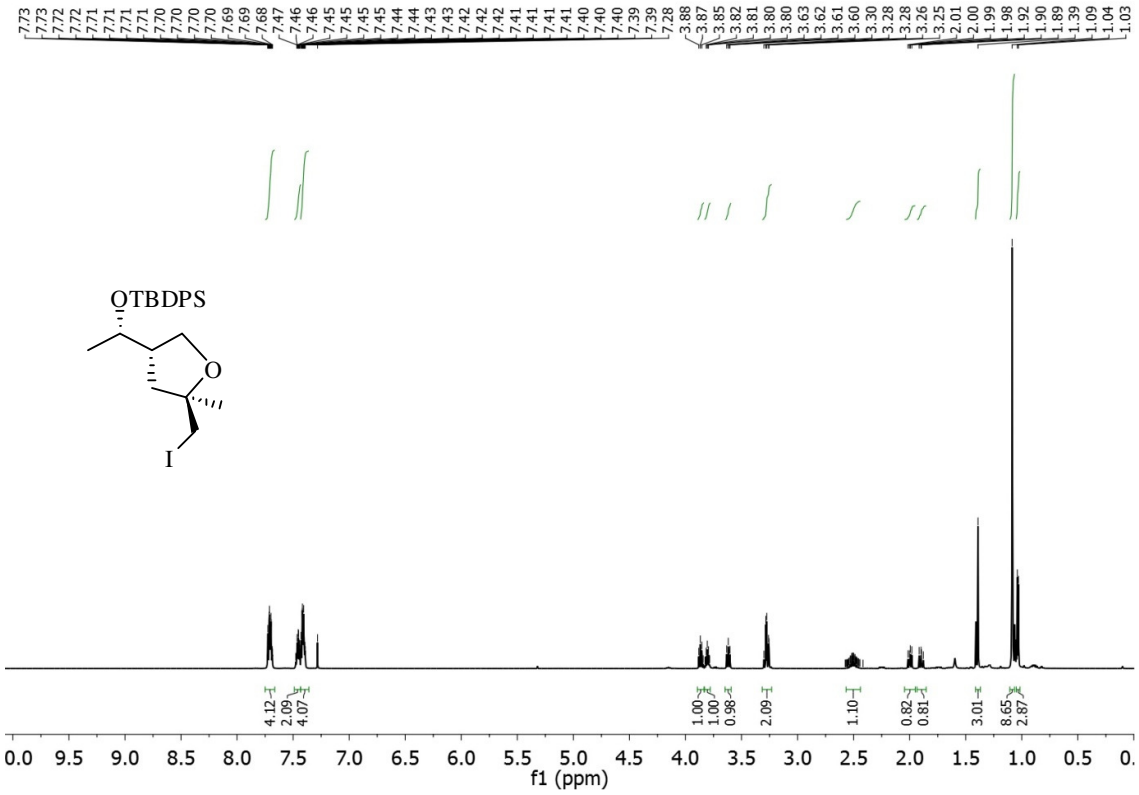
DEPT-135 NMR of compound 44 (50 MHz, $CDCl_3$)



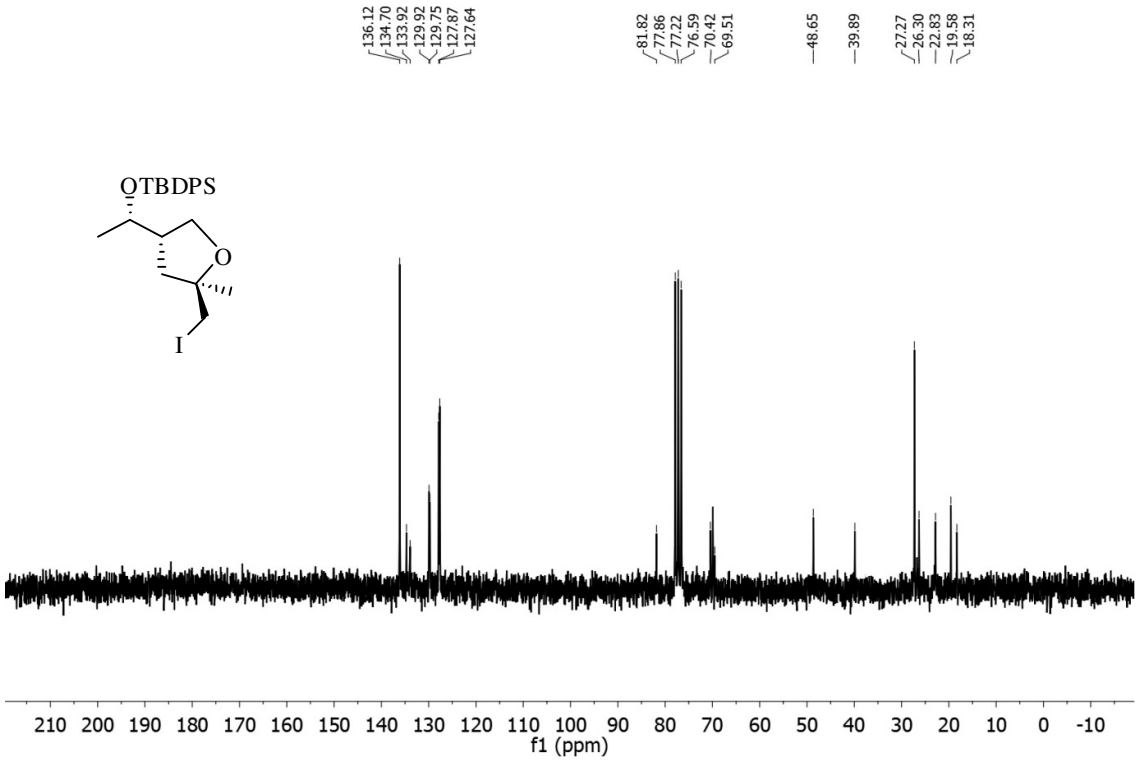
NOESY Spectrum of compound 44 (400 MHz, $CDCl_3$)



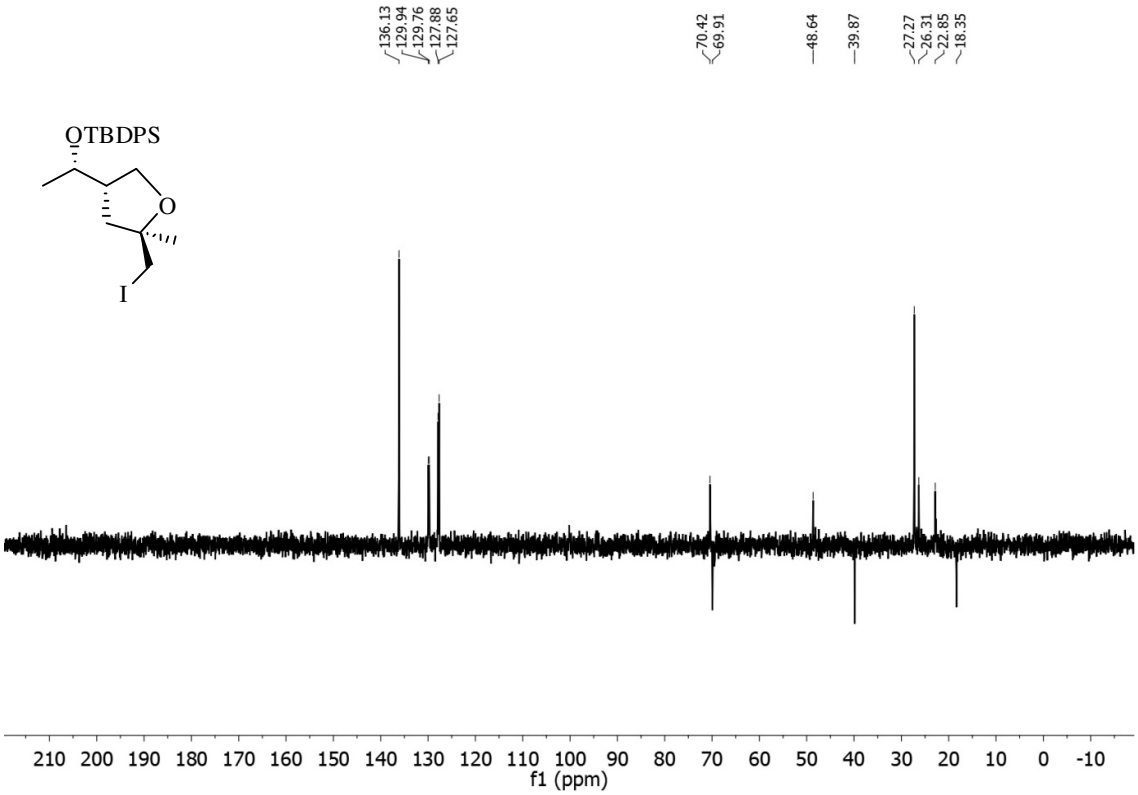
^{1}H - NMR of compound 45 (600 MHz, $CDCl_3$)



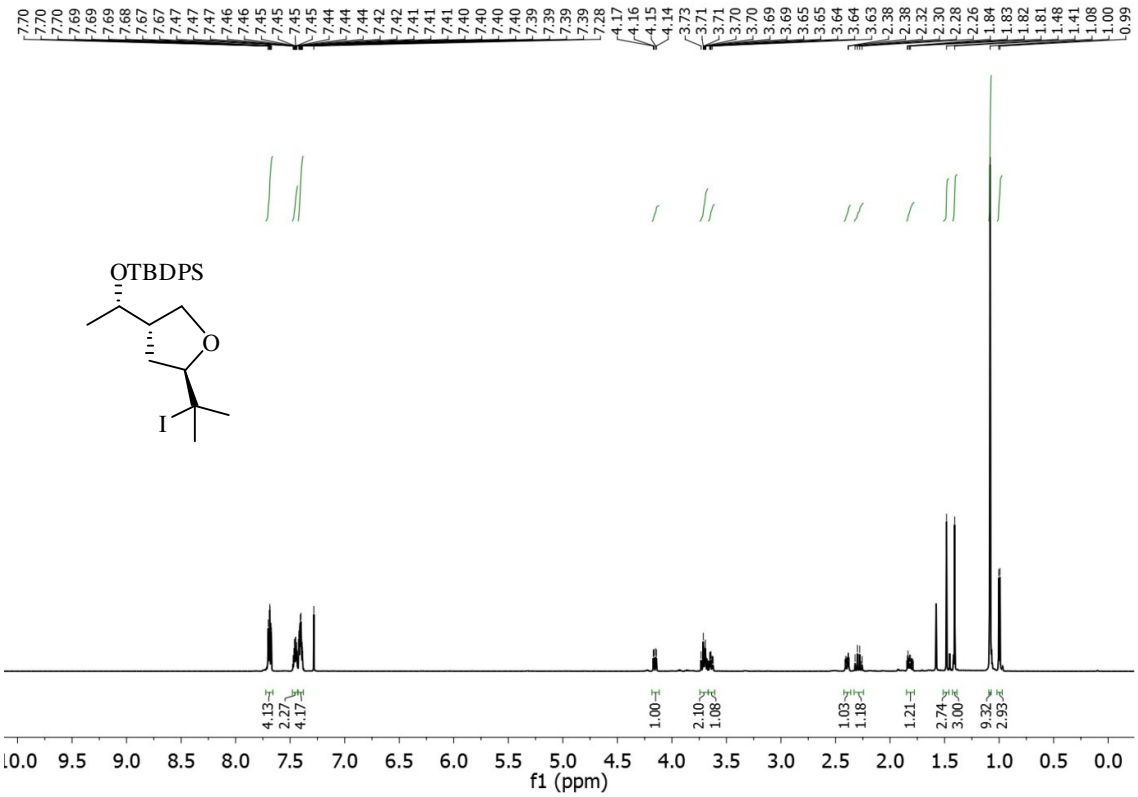
^{13}C NMR of compound 45 (50 MHz, $CDCl_3$)



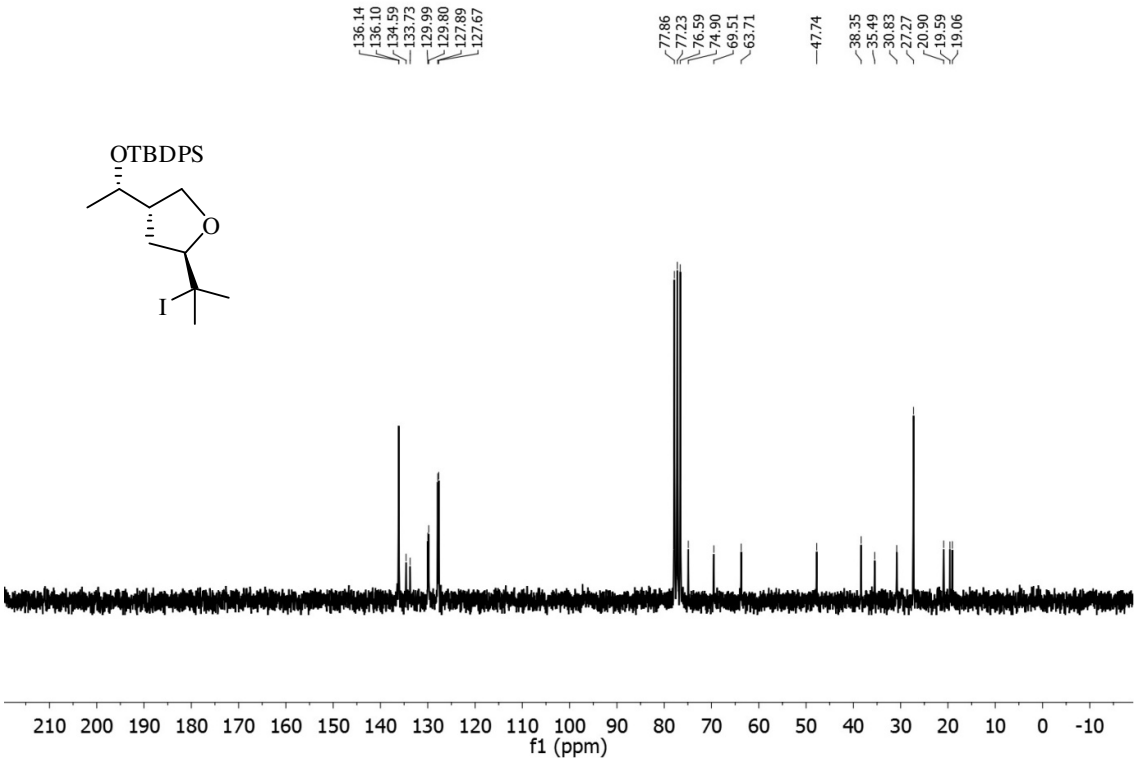
DEPT-135 NMR of compound 45 (50 MHz, $CDCl_3$)



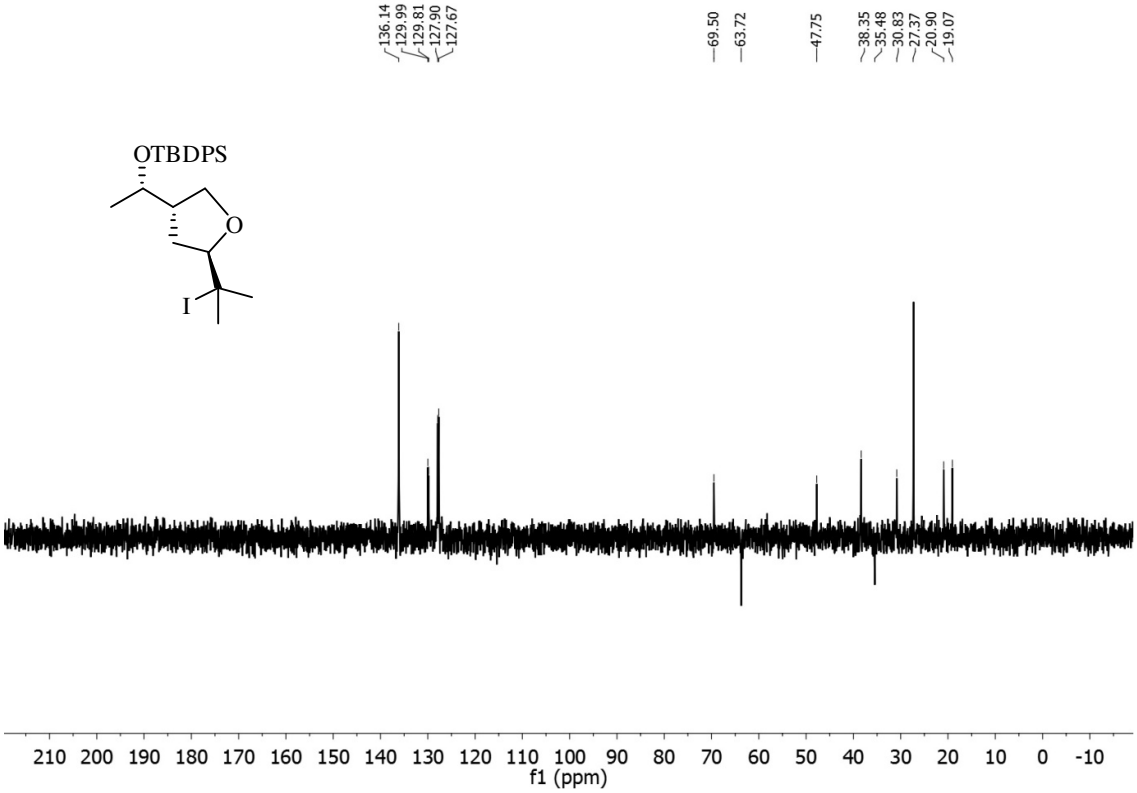
^{1}H - NMR of compound 46 (400 MHz, $CDCl_3$)



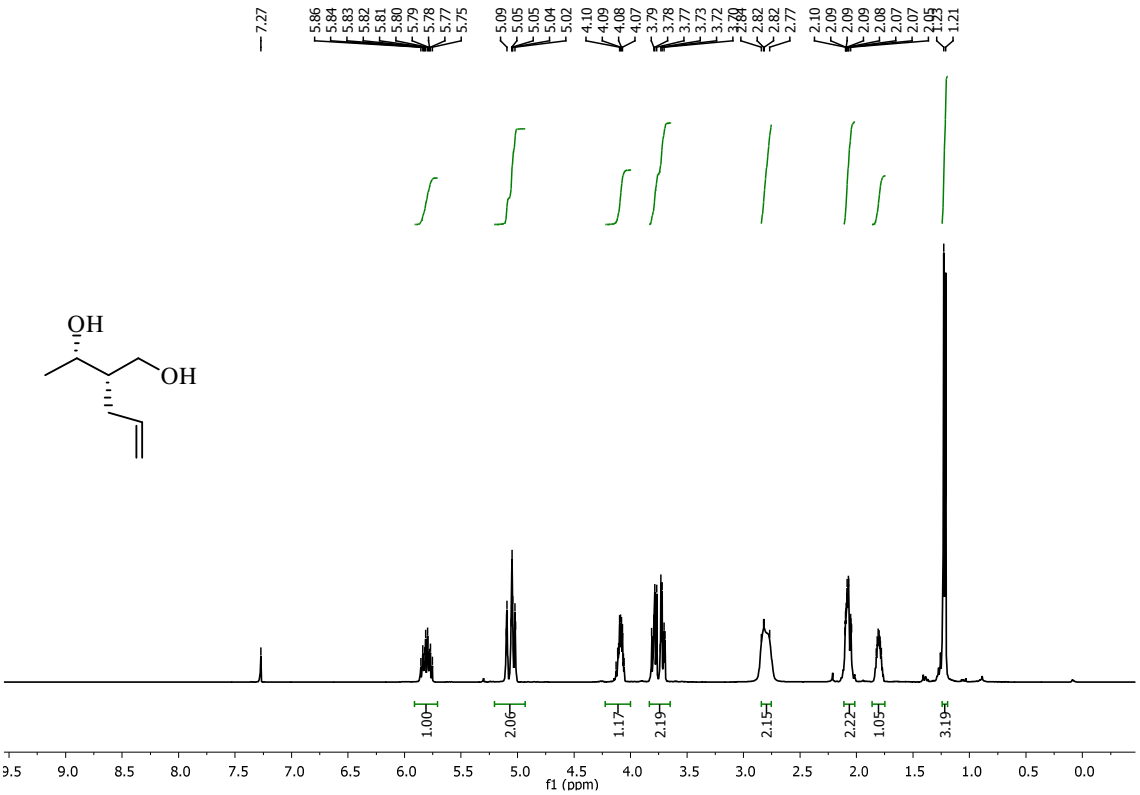
^{13}C NMR of compound 46 (50 MHz, $CDCl_3$)



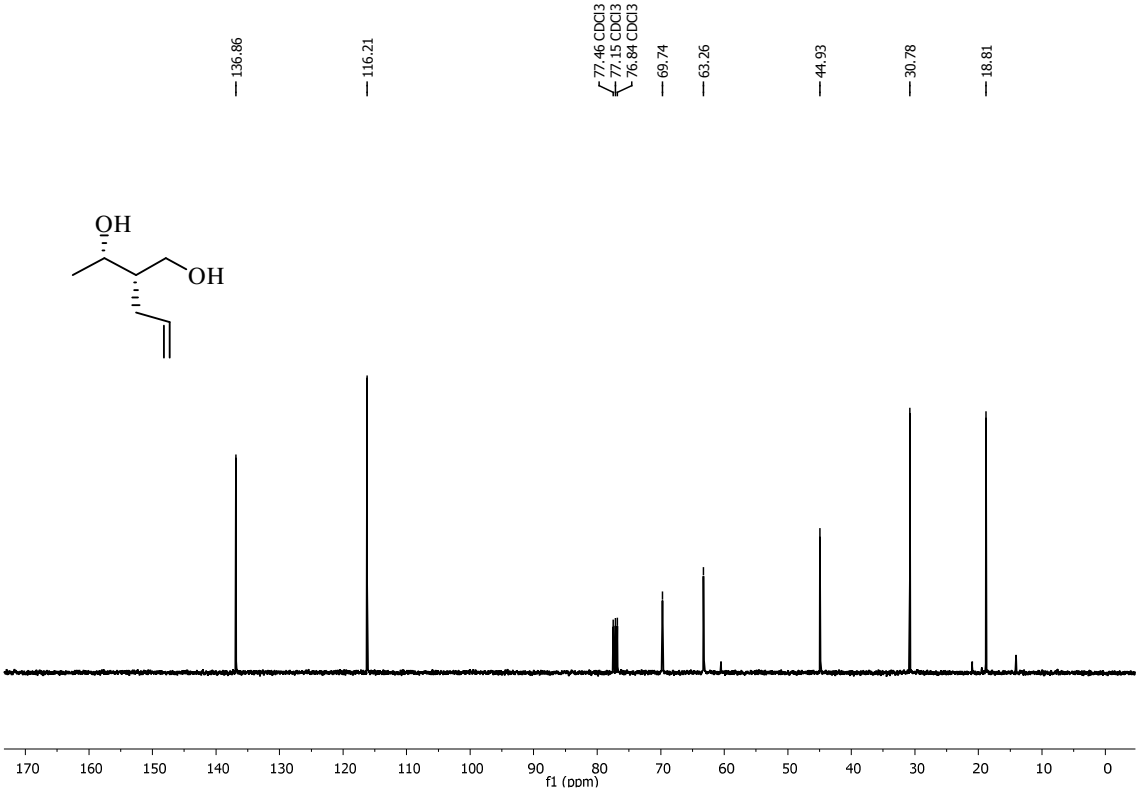
DEPT-135 NMR of compound 46 (50 MHz, $CDCl_3$)



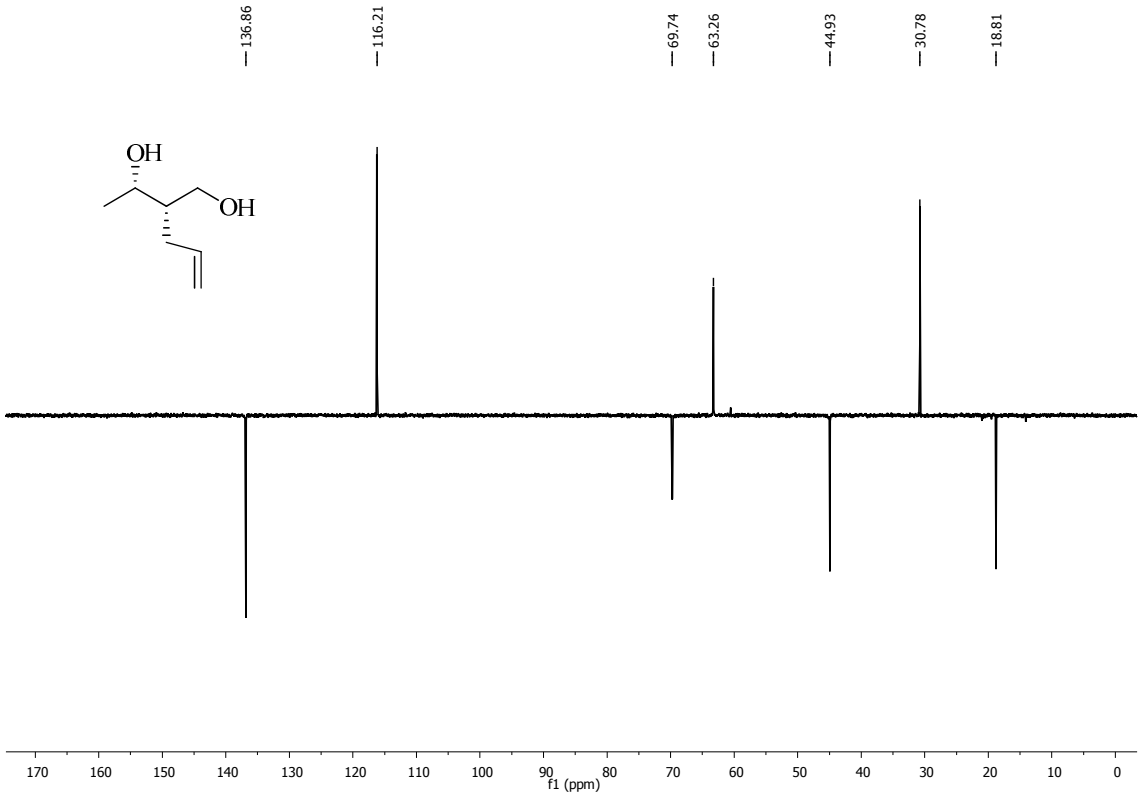
^{1}H - NMR of compound 47 (400 MHz, $CDCl_3$)



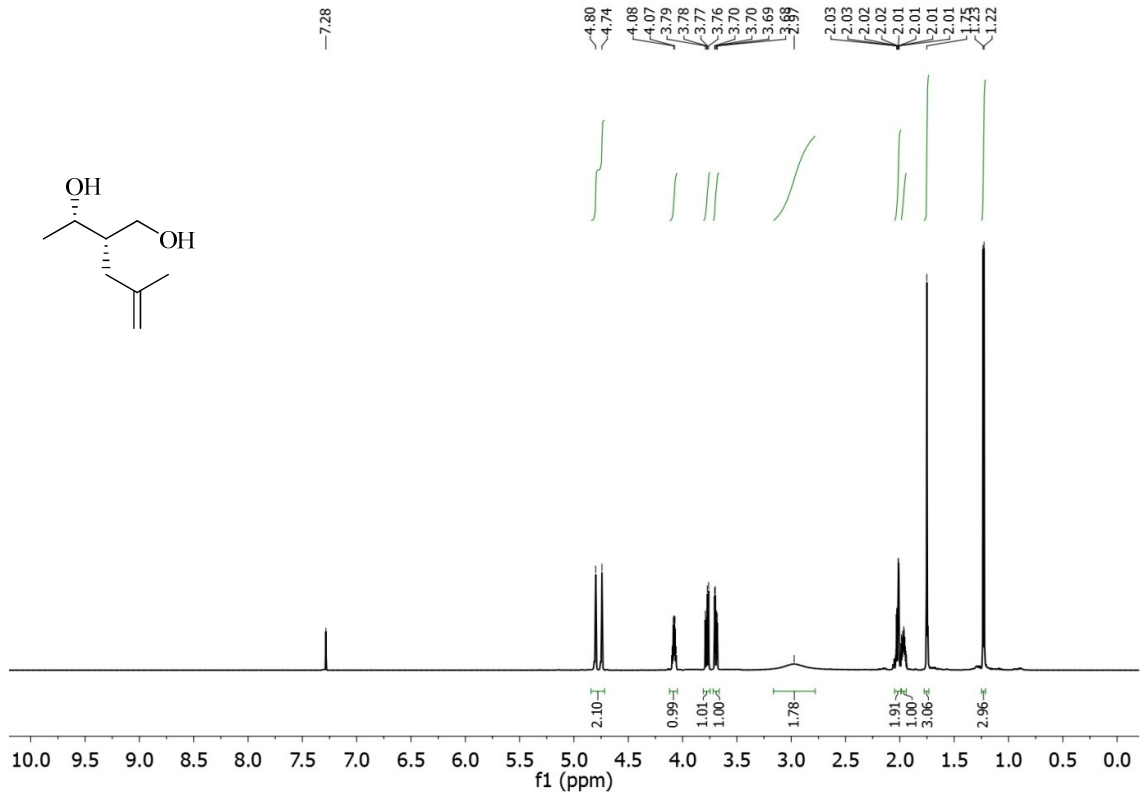
^{13}C NMR of compound 47 (100 MHz, $CDCl_3$)



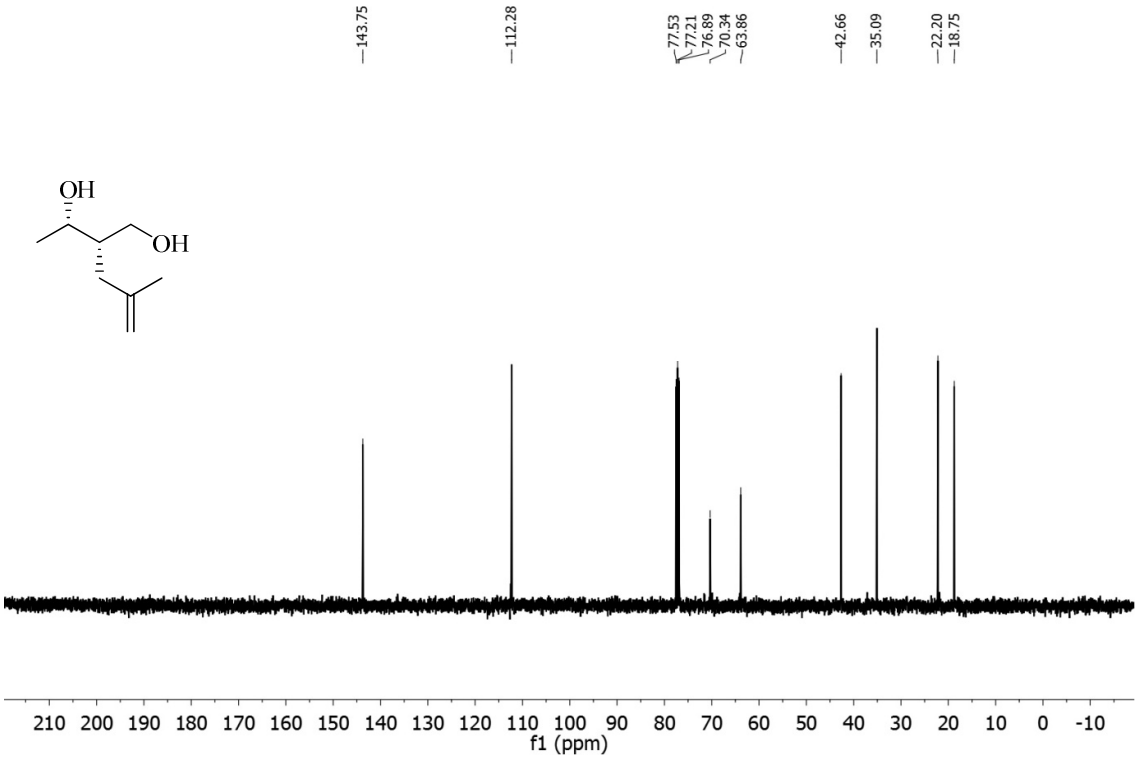
DEPT-135 NMR of compound 47 (100 MHz, $CDCl_3$)



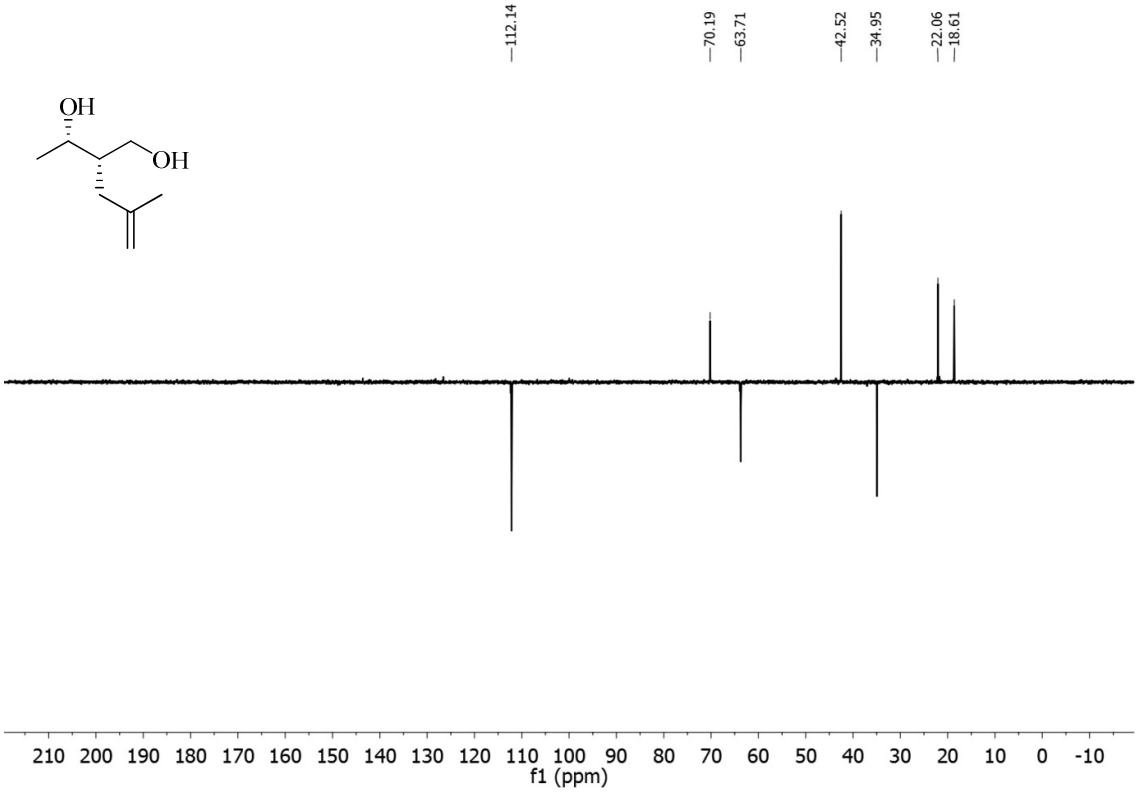
^{1}H - NMR of compound 48 (600 MHz, $CDCl_3$)



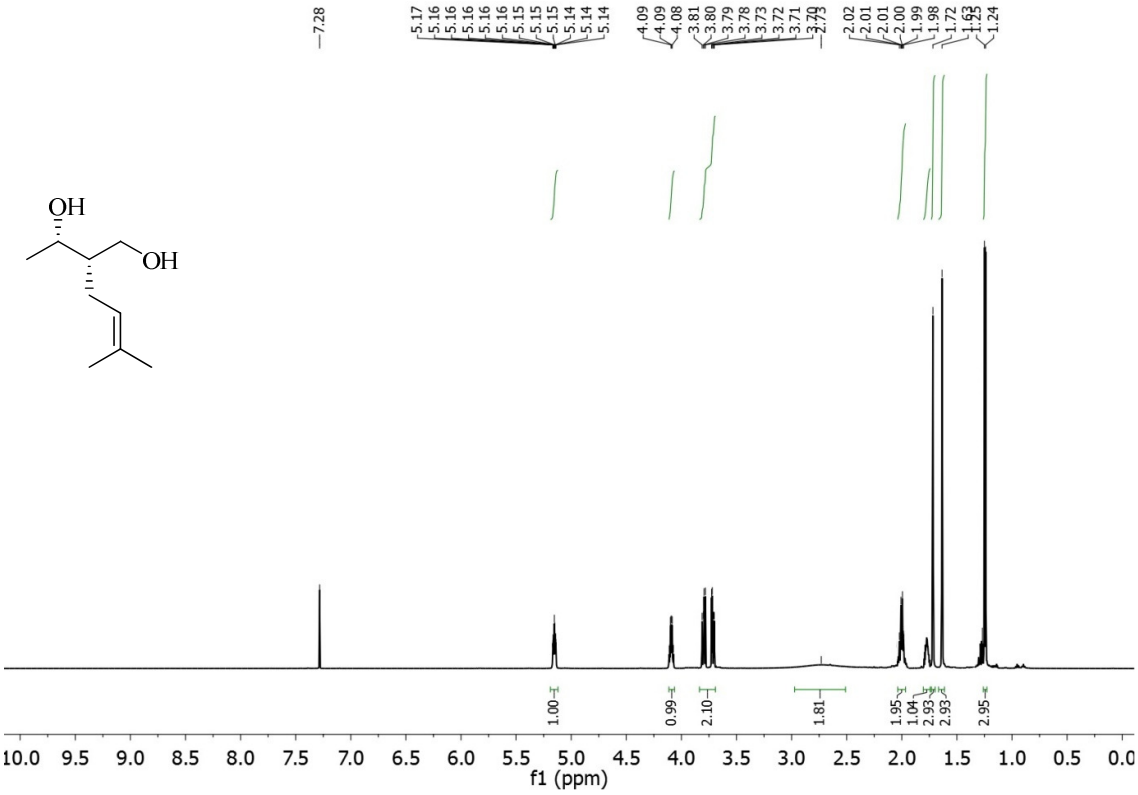
^{13}C NMR of compound 48 (100 MHz, $CDCl_3$)



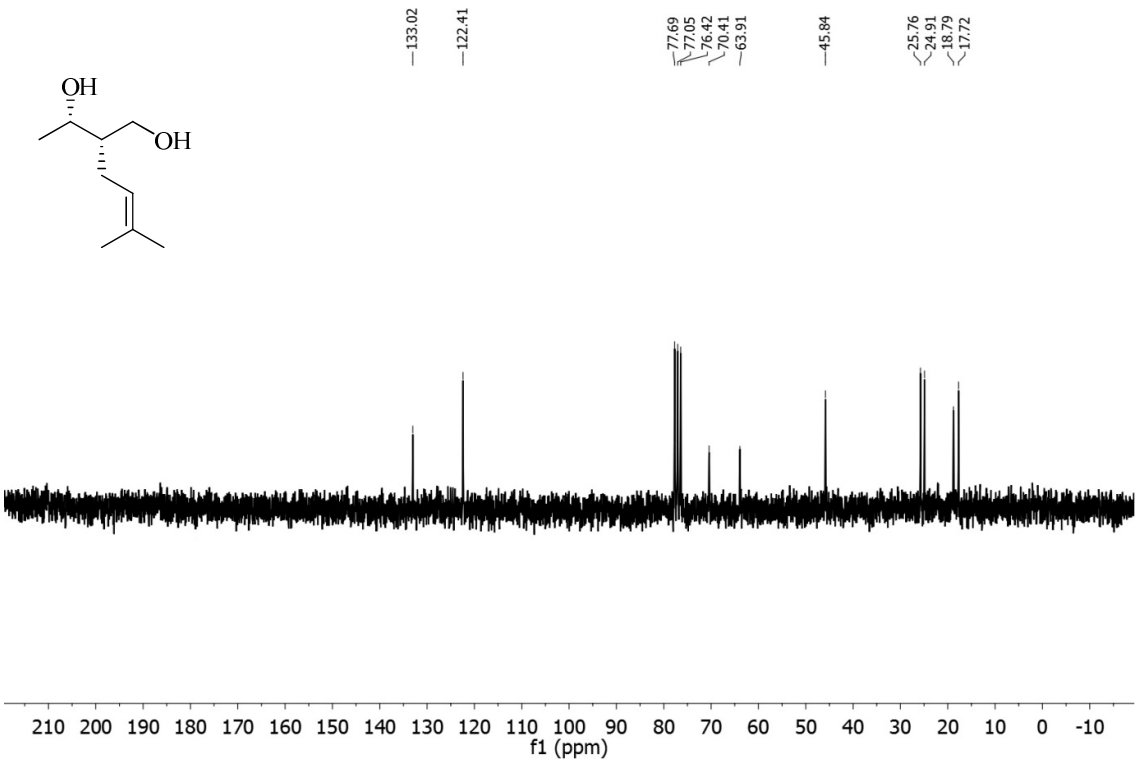
DEPT-135 NMR of compound 48 (100 MHz, $CDCl_3$)



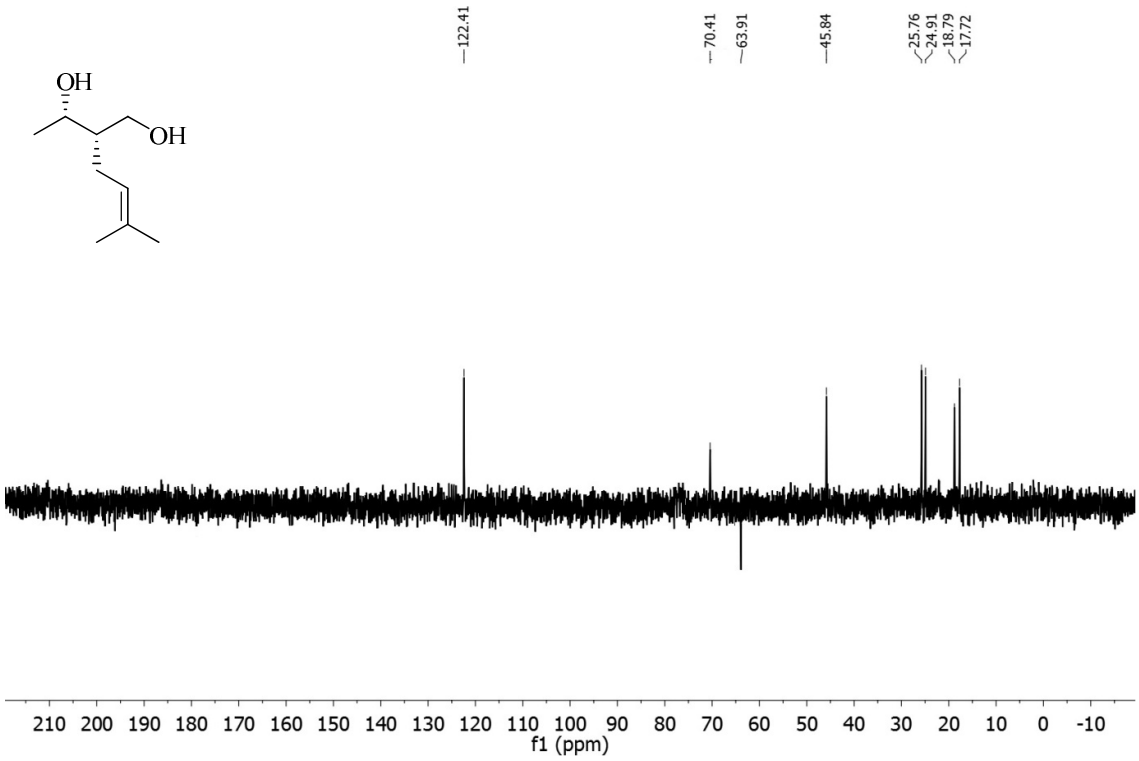
^{1}H - NMR of compound 49 (600 MHz, $CDCl_3$)



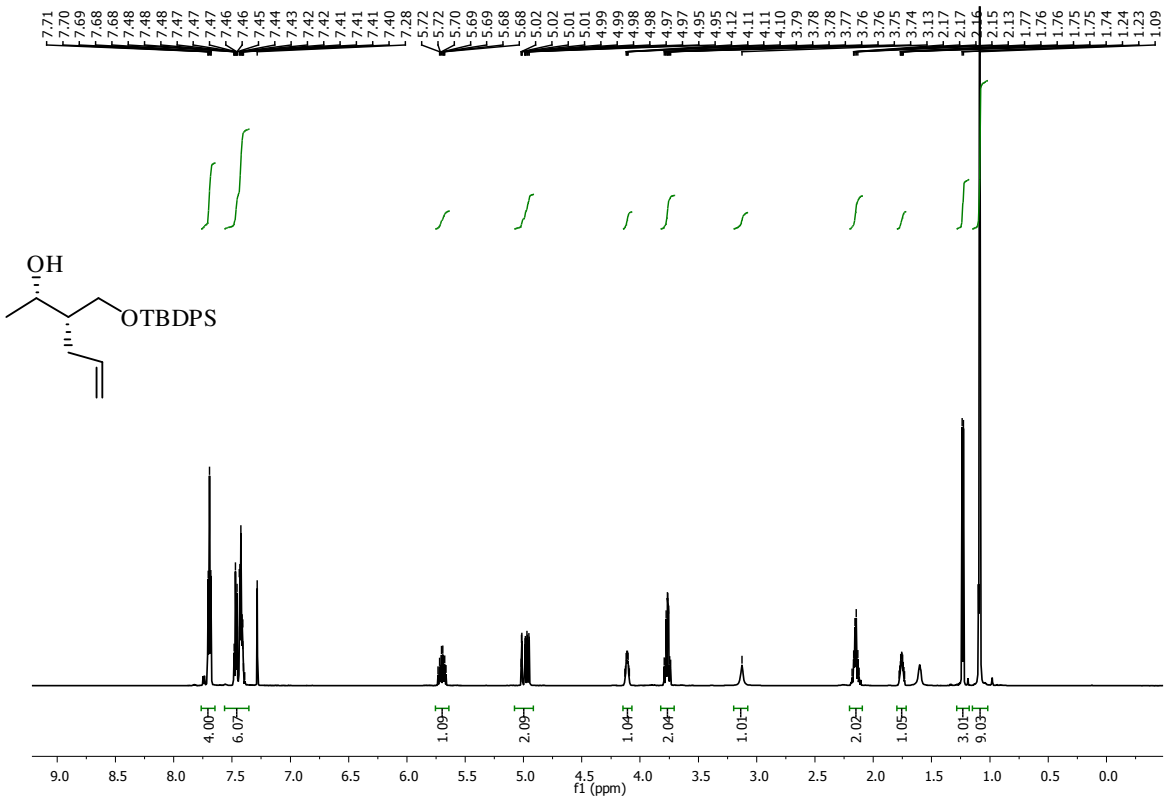
^{13}C NMR of compound 49 (50 MHz, $CDCl_3$)



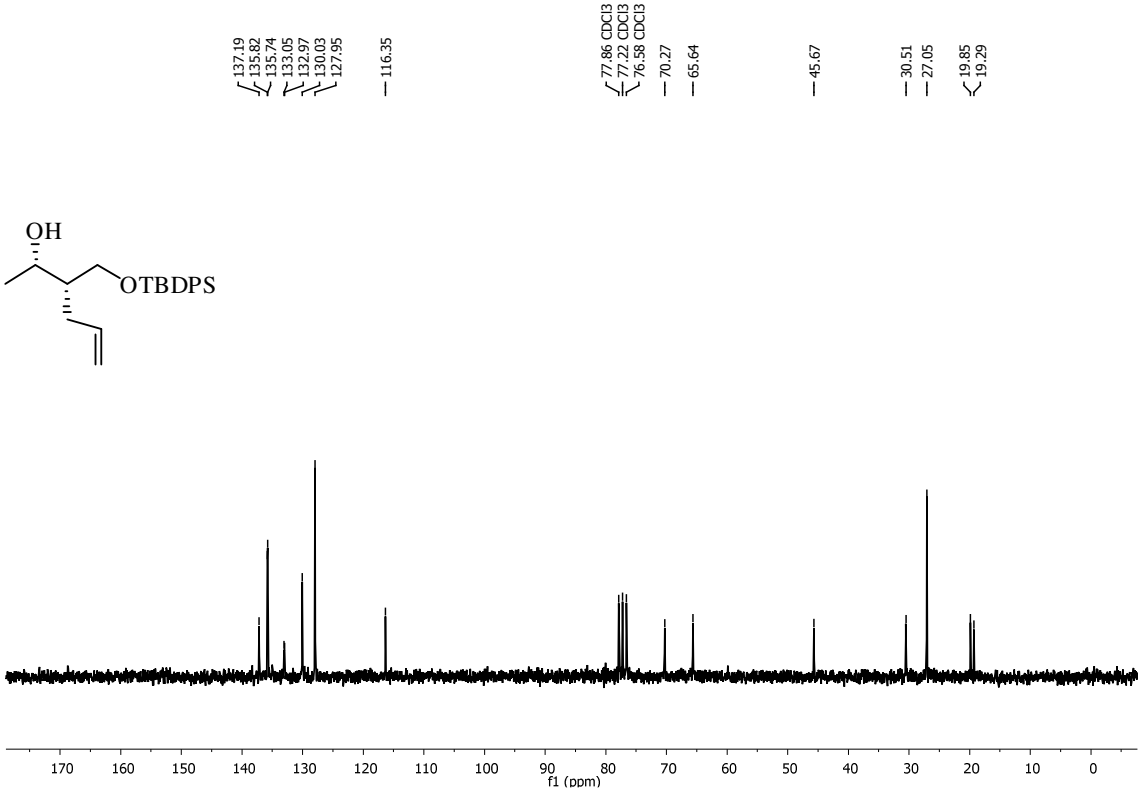
DEPT-135 NMR of compound 49 (50 MHz, $CDCl_3$)



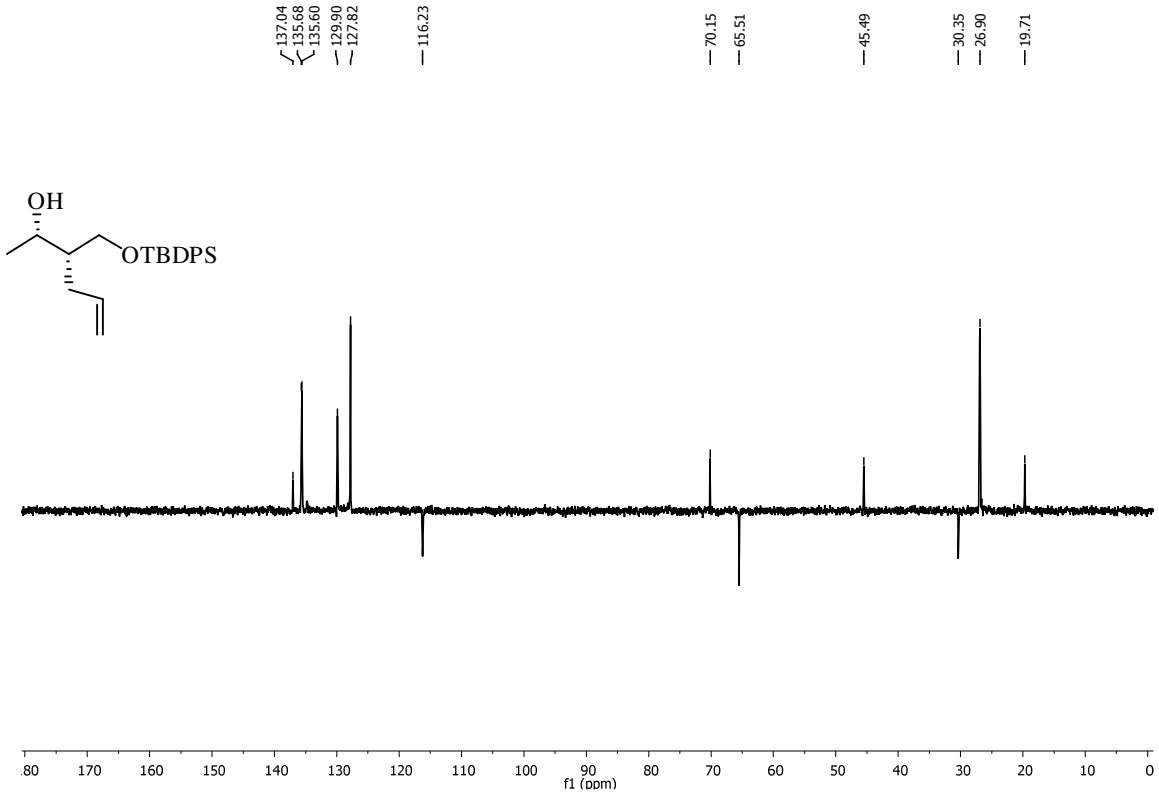
^{1}H - NMR of compound 50 (600 MHz, $CDCl_3$)



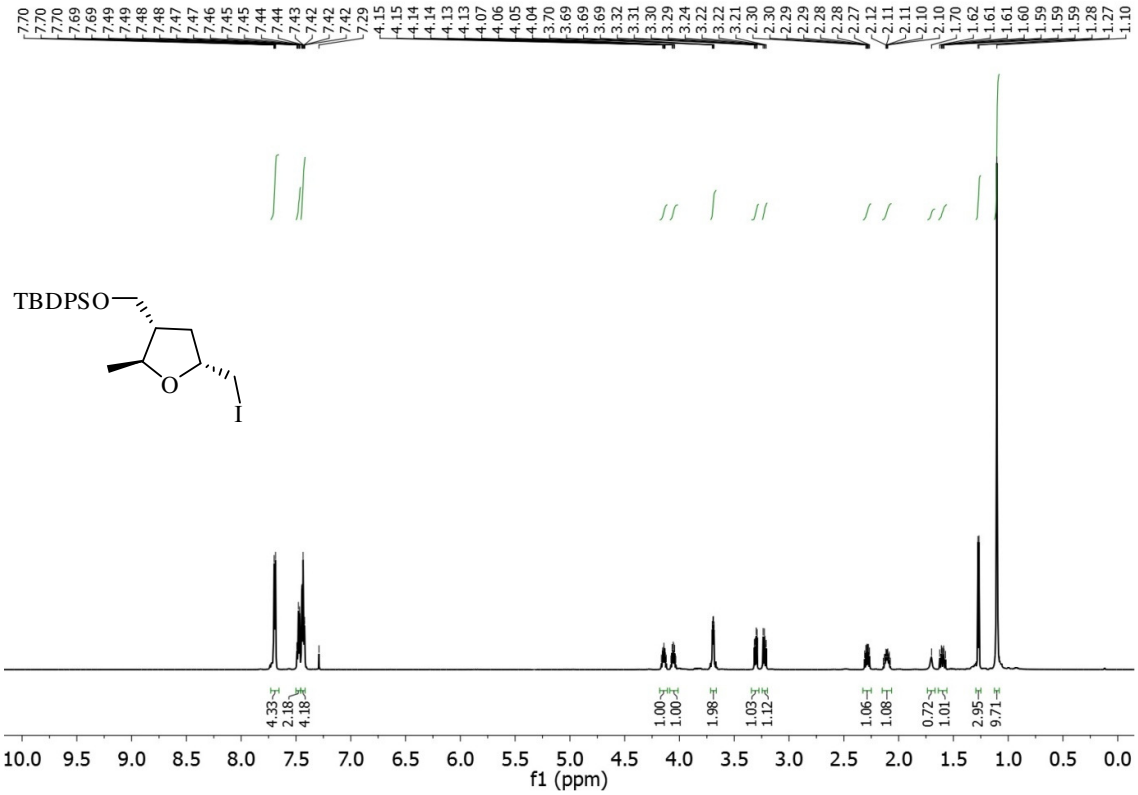
^{13}C NMR of compound 50 (50 MHz, $CDCl_3$)



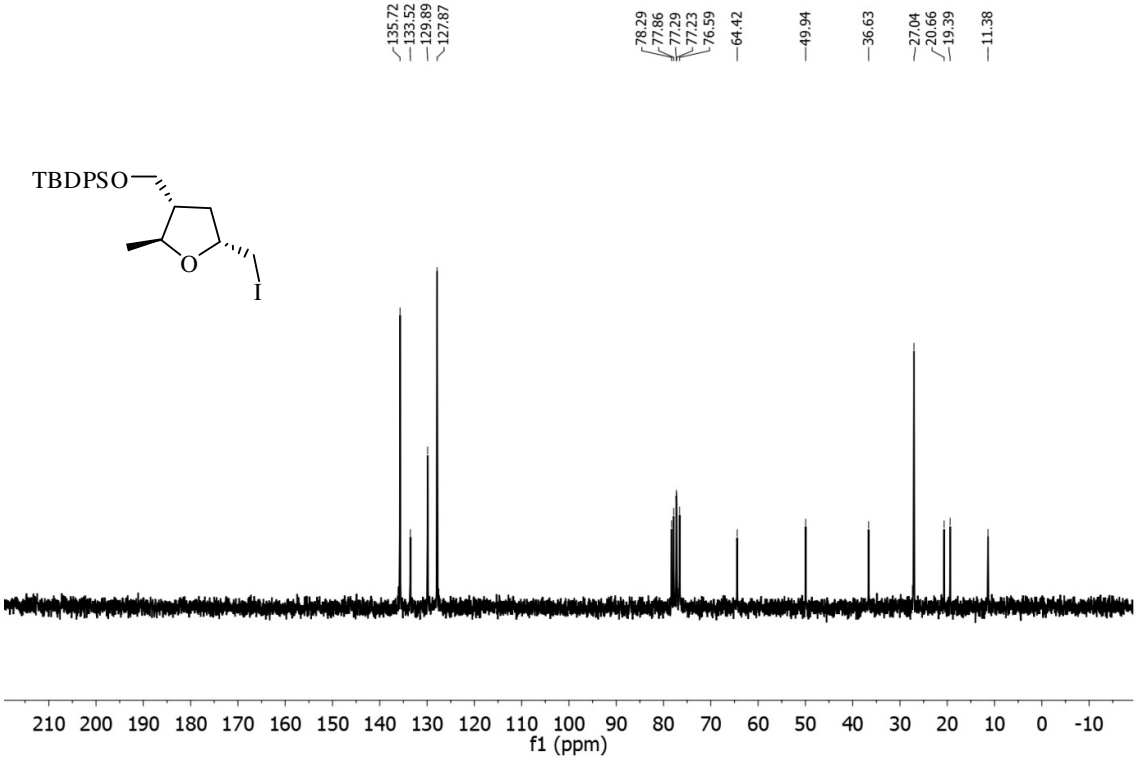
DEPT-135 NMR of compound 50 (50 MHz, $CDCl_3$)



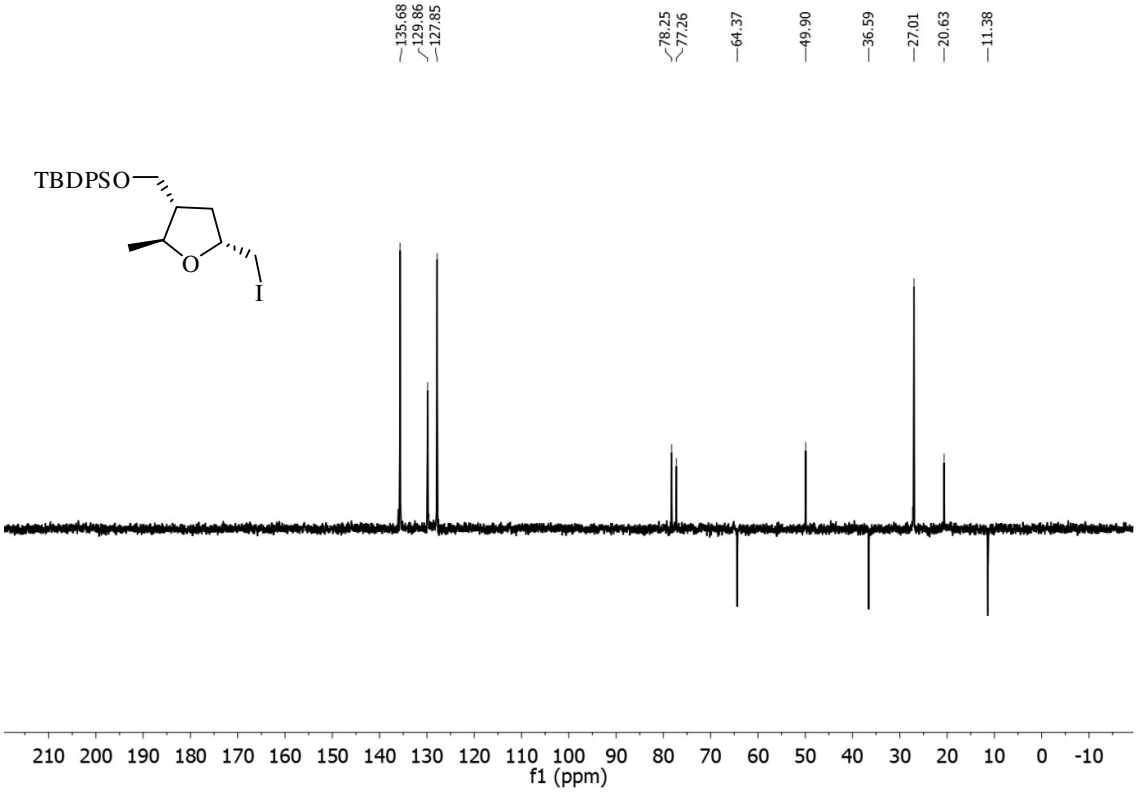
^{1}H - NMR of compound 53 (400 MHz, $CDCl_3$)



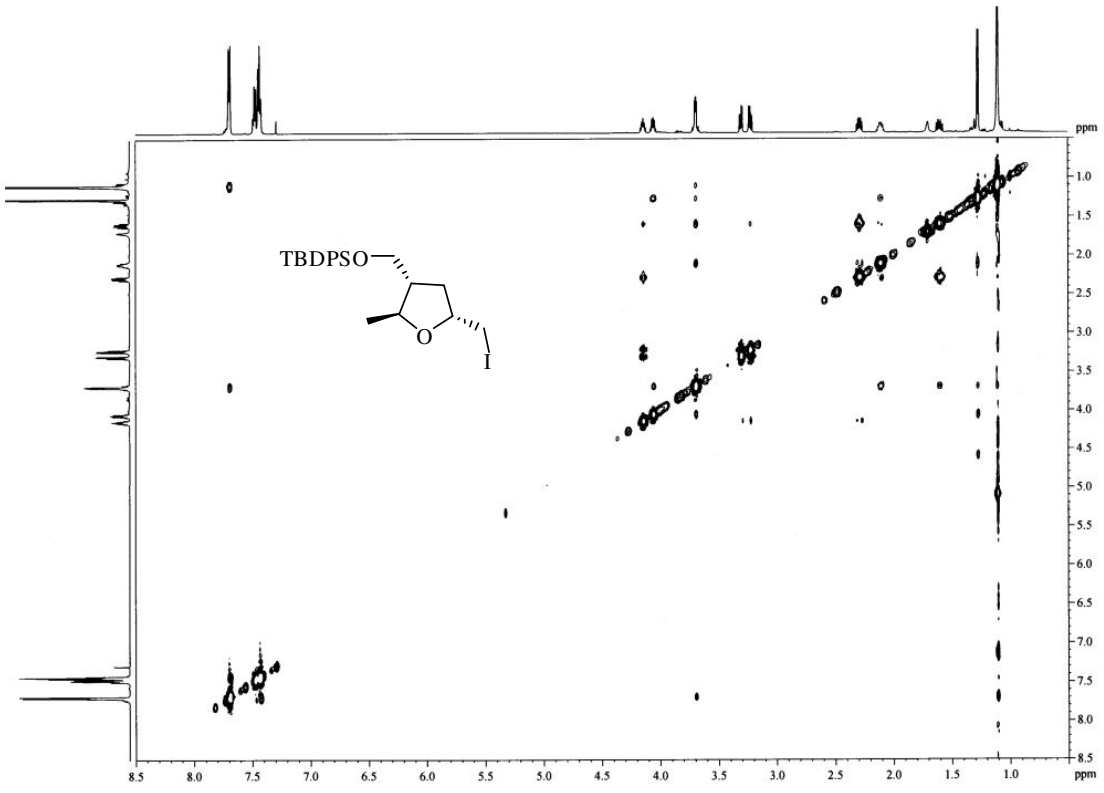
^{13}C NMR of compound 53 (50 MHz, $CDCl_3$)



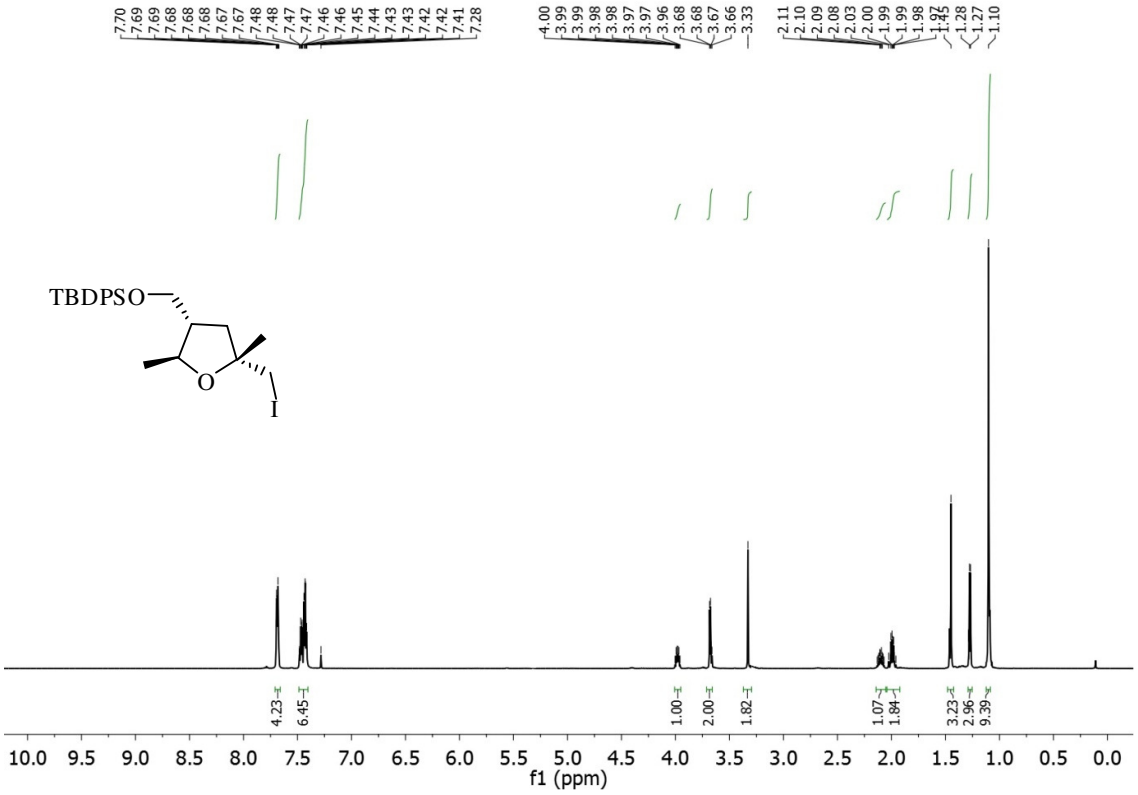
DEPT-135 NMR of compound 53 (50 MHz, $CDCl_3$)



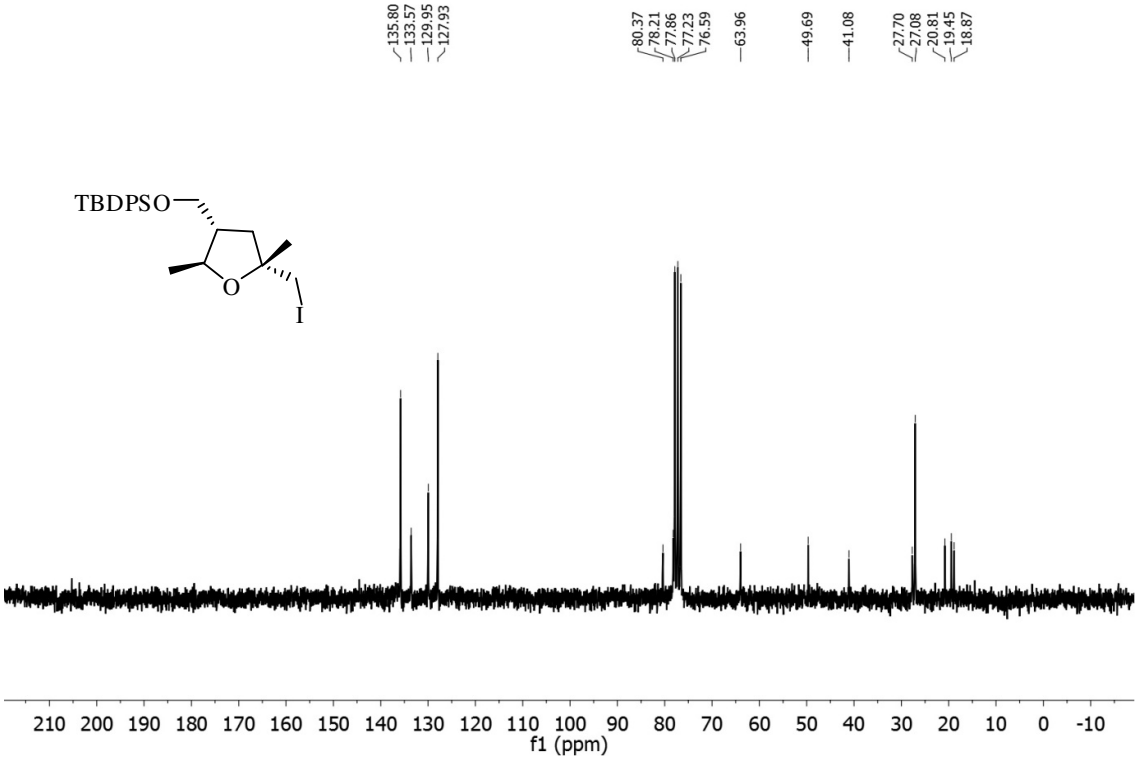
NOESY Spectrum of compound 53 (400 MHz, $CDCl_3$)



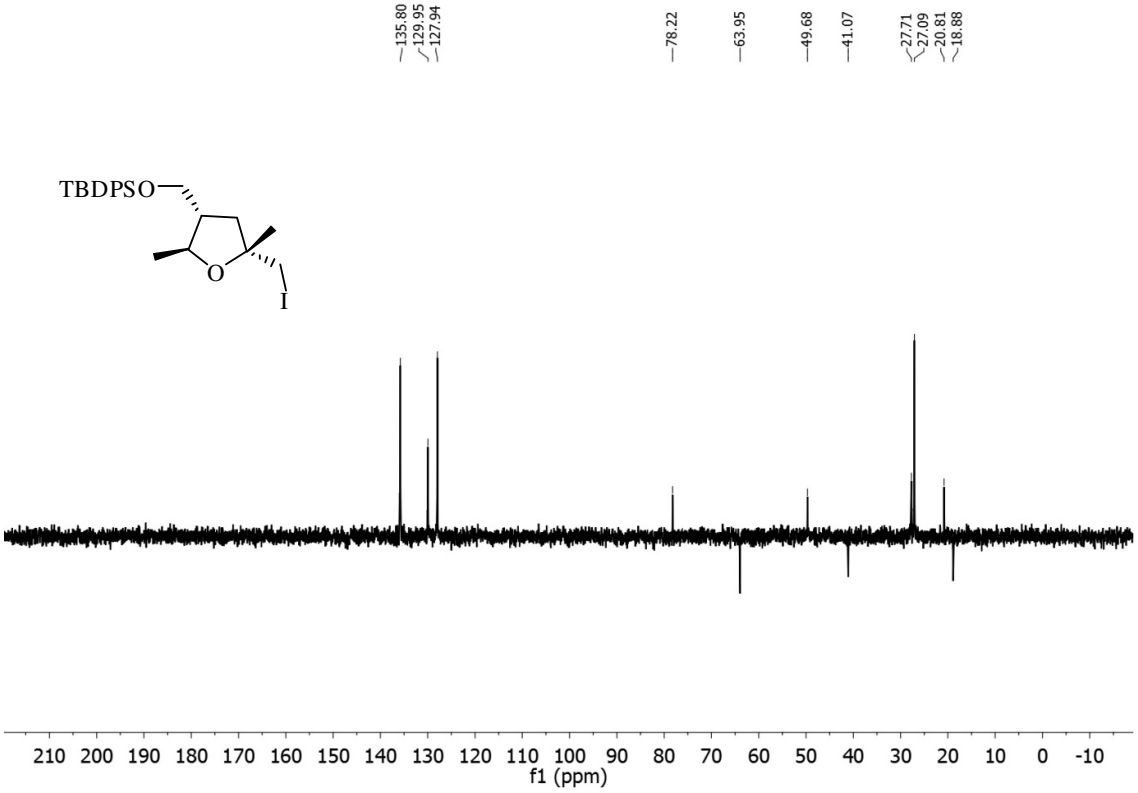
^{1}H - NMR of compound 54 (400 MHz, $CDCl_3$)



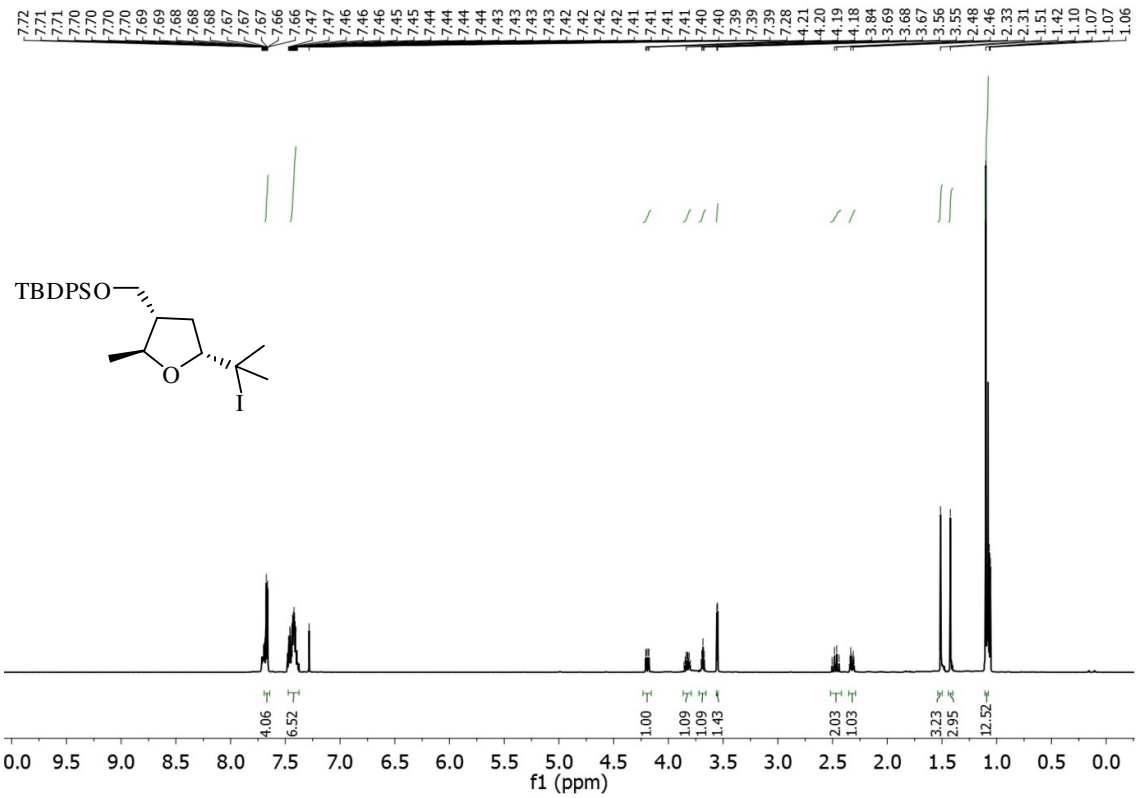
^{13}C NMR of compound 54 (50 MHz, $CDCl_3$)



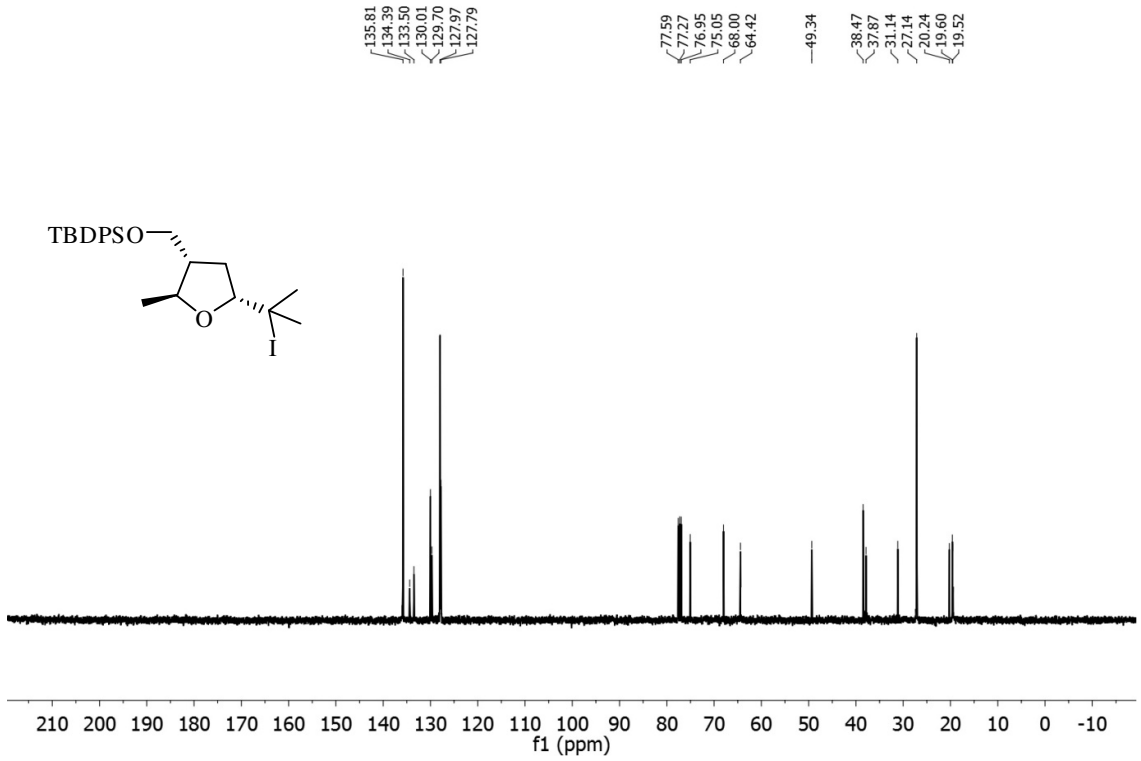
DEPT-135 NMR of compound 54 (50 MHz, $CDCl_3$)



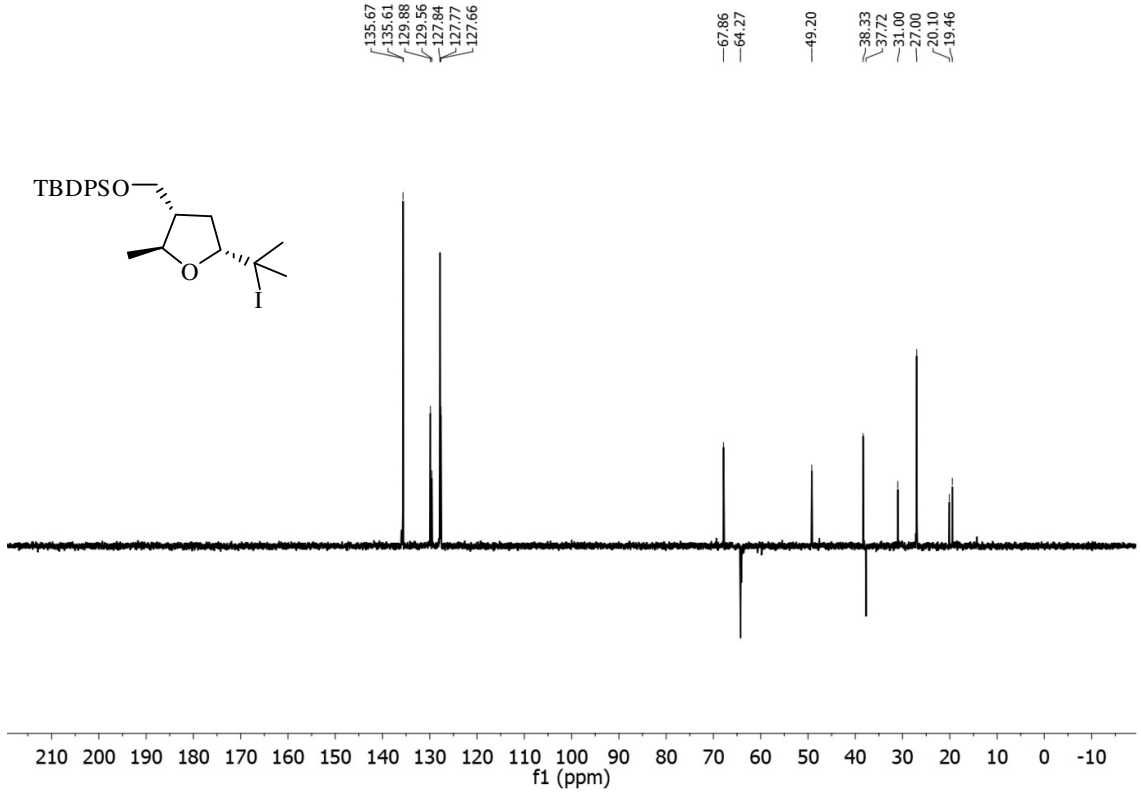
^{1}H - NMR of compound 55 (600 MHz, $CDCl_3$)



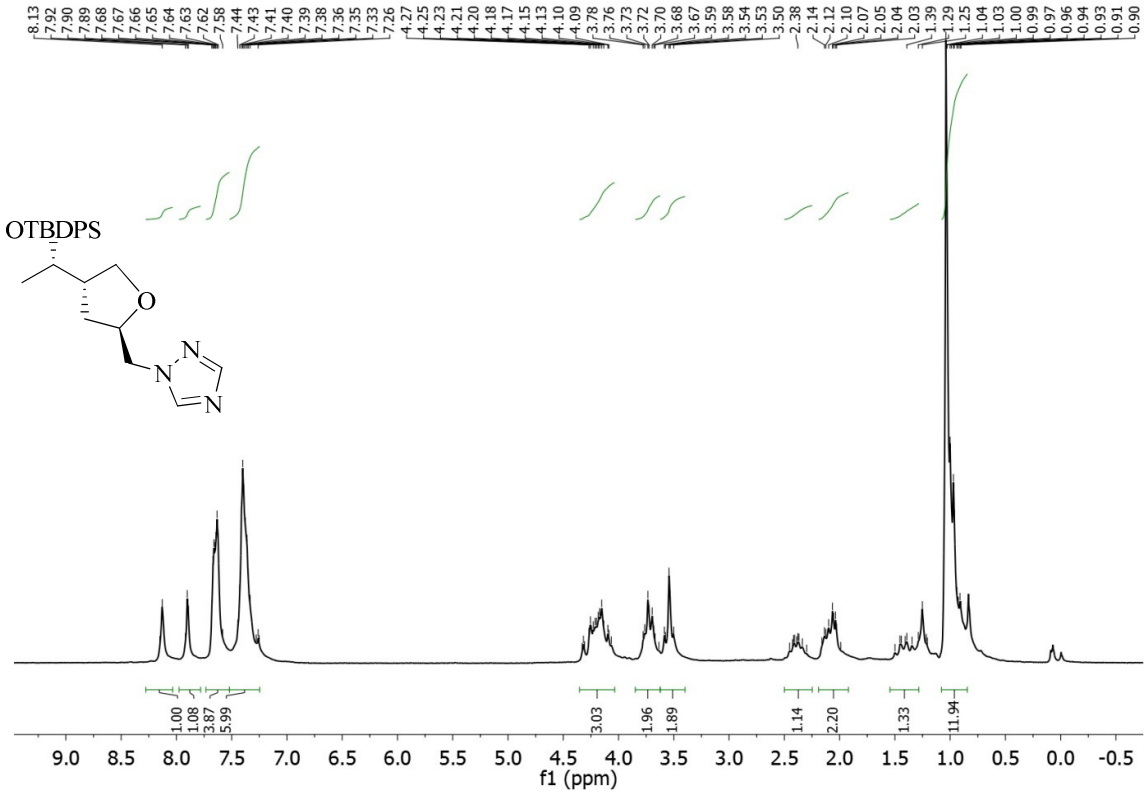
^{13}C NMR of compound 55 (100 MHz, $CDCl_3$)



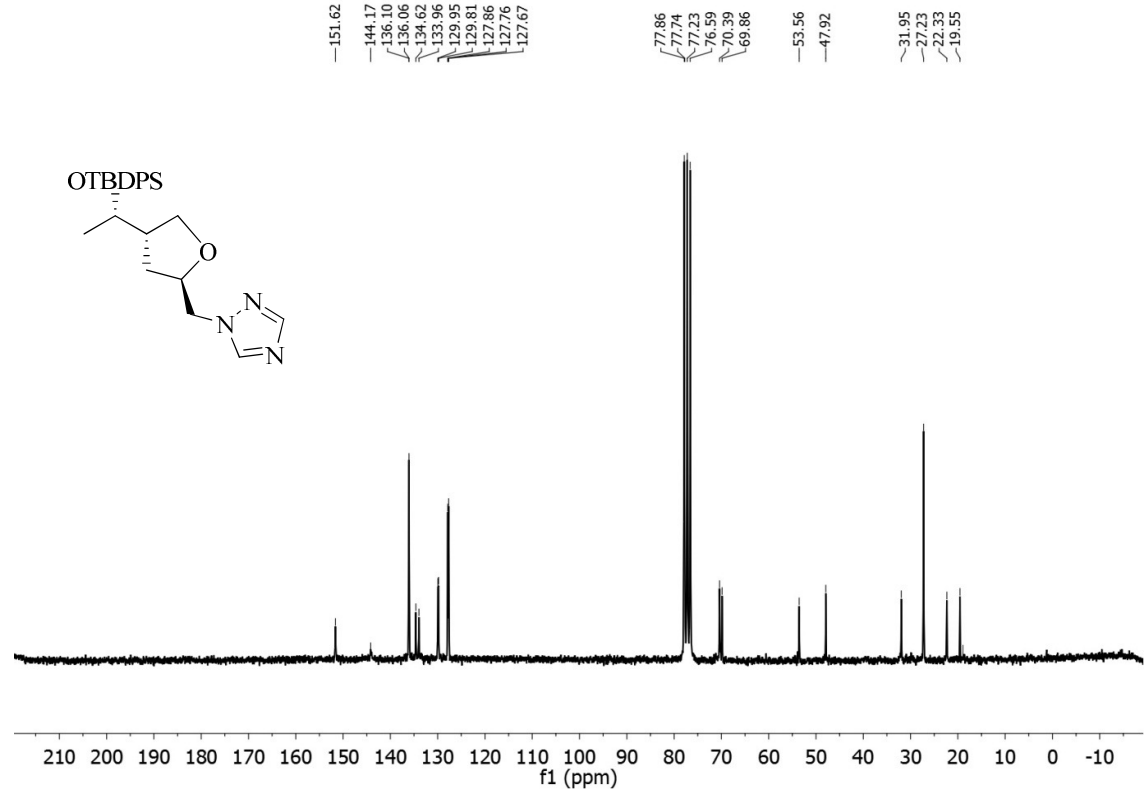
DEPT-135 NMR of compound 55 (100 MHz, $CDCl_3$)



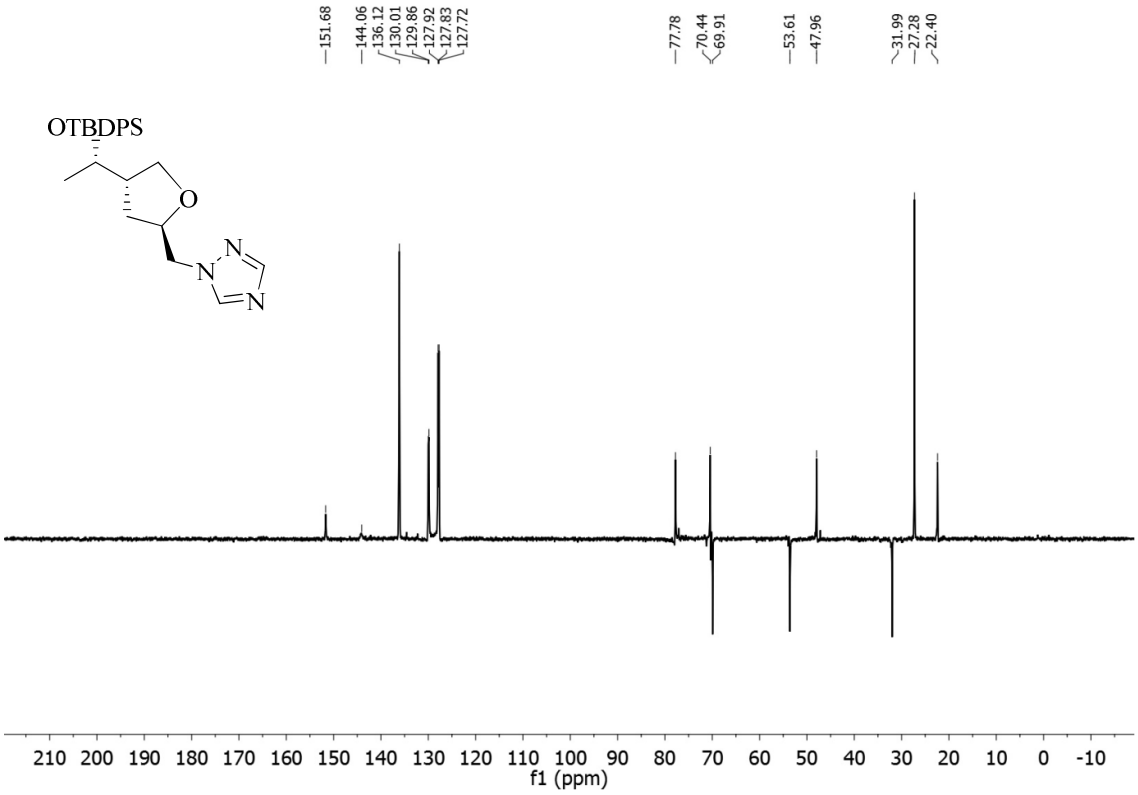
^{1}H - NMR of compound 56 (200 MHz, $CDCl_3$)



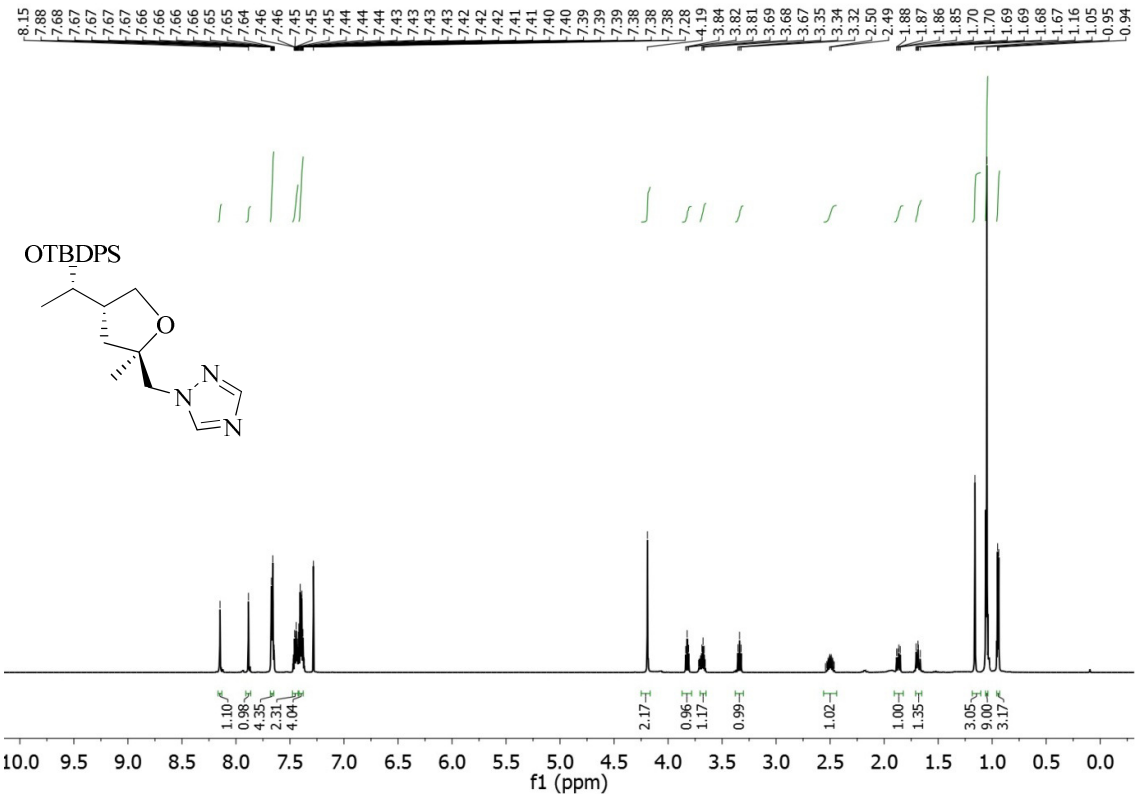
^{13}C NMR of compound 56 (50 MHz, $CDCl_3$)



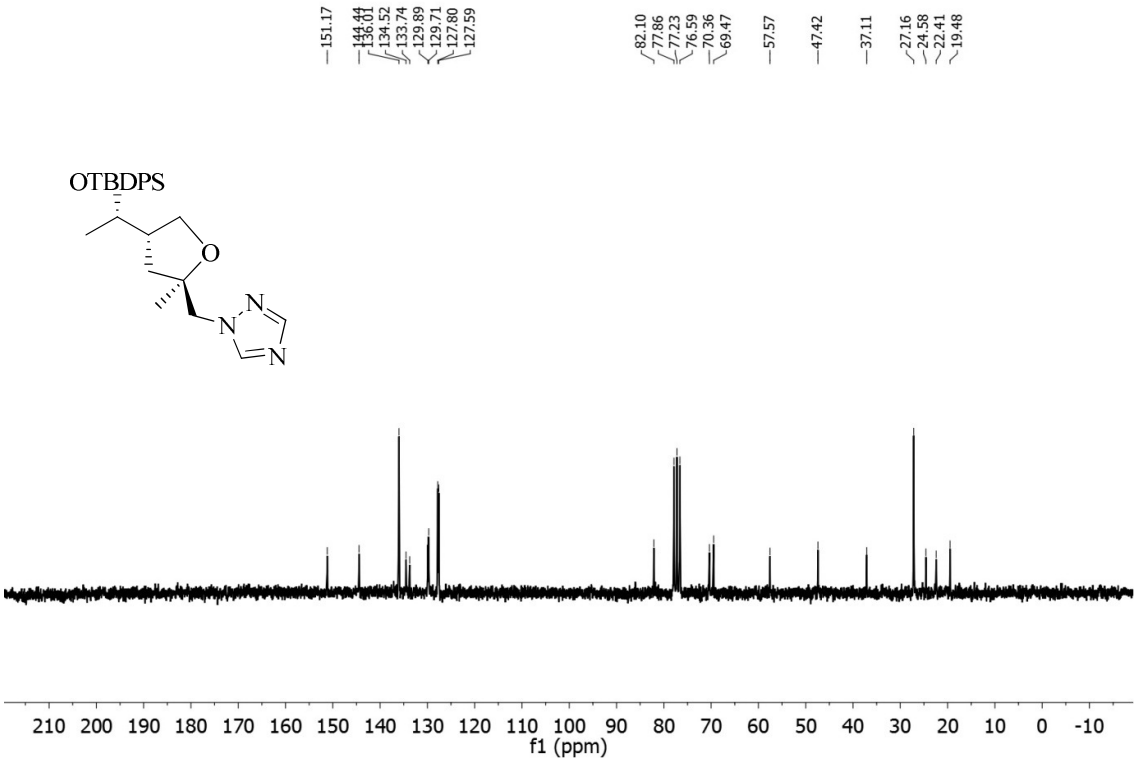
DEPT-135 NMR of compound 56 (50 MHz, $CDCl_3$)



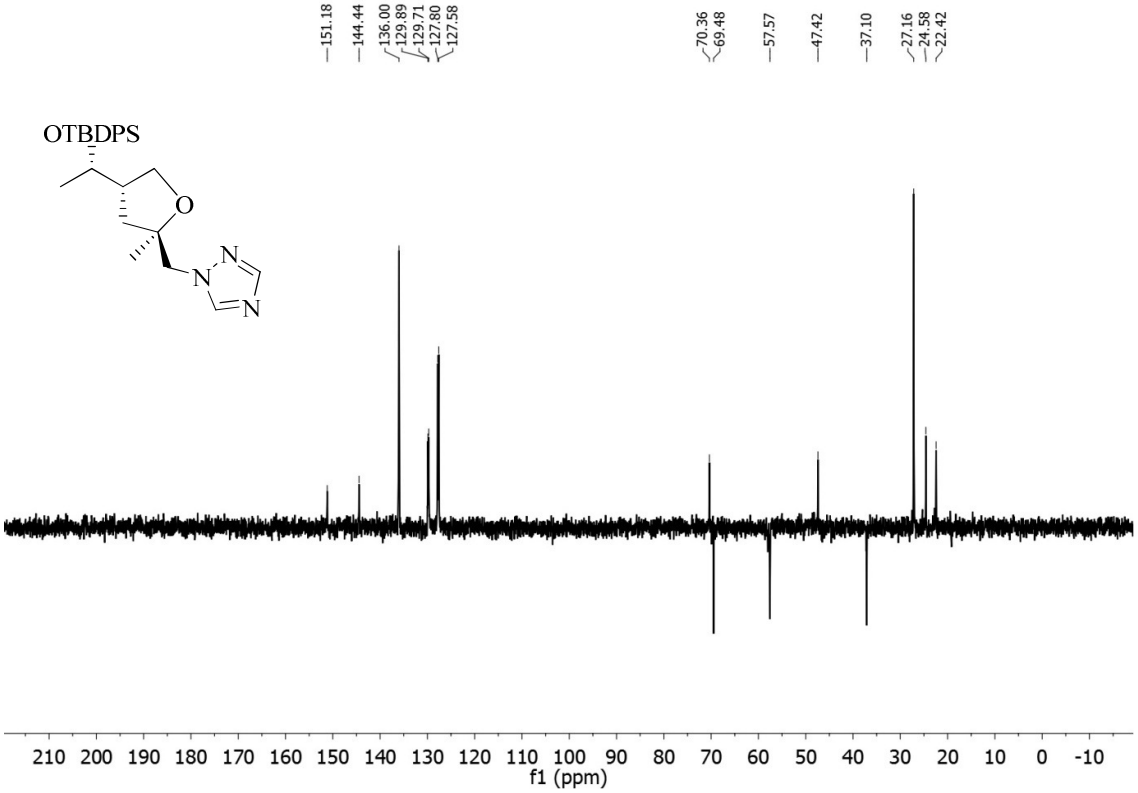
^{1}H - NMR of compound 57 (600 MHz, $CDCl_3$)



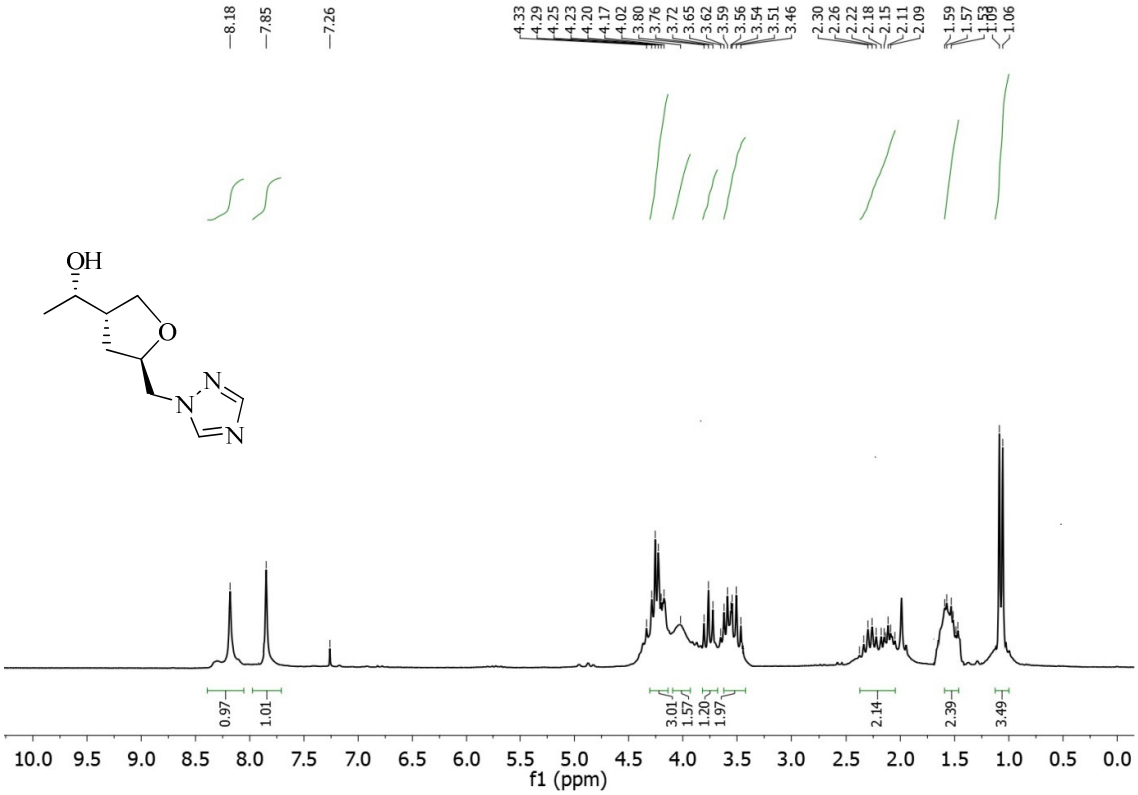
^{13}C NMR of compound 57 (50 MHz, $CDCl_3$)



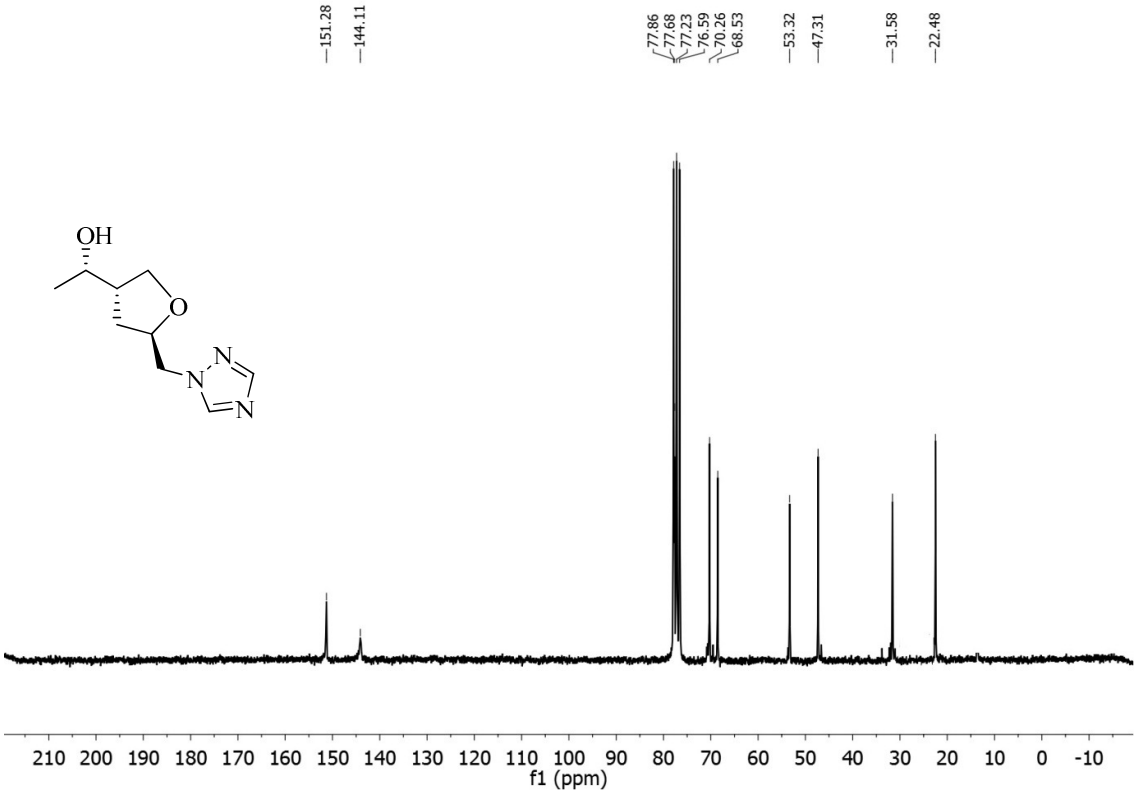
DEPT-135 NMR of compound 57 (50 MHz, $CDCl_3$)



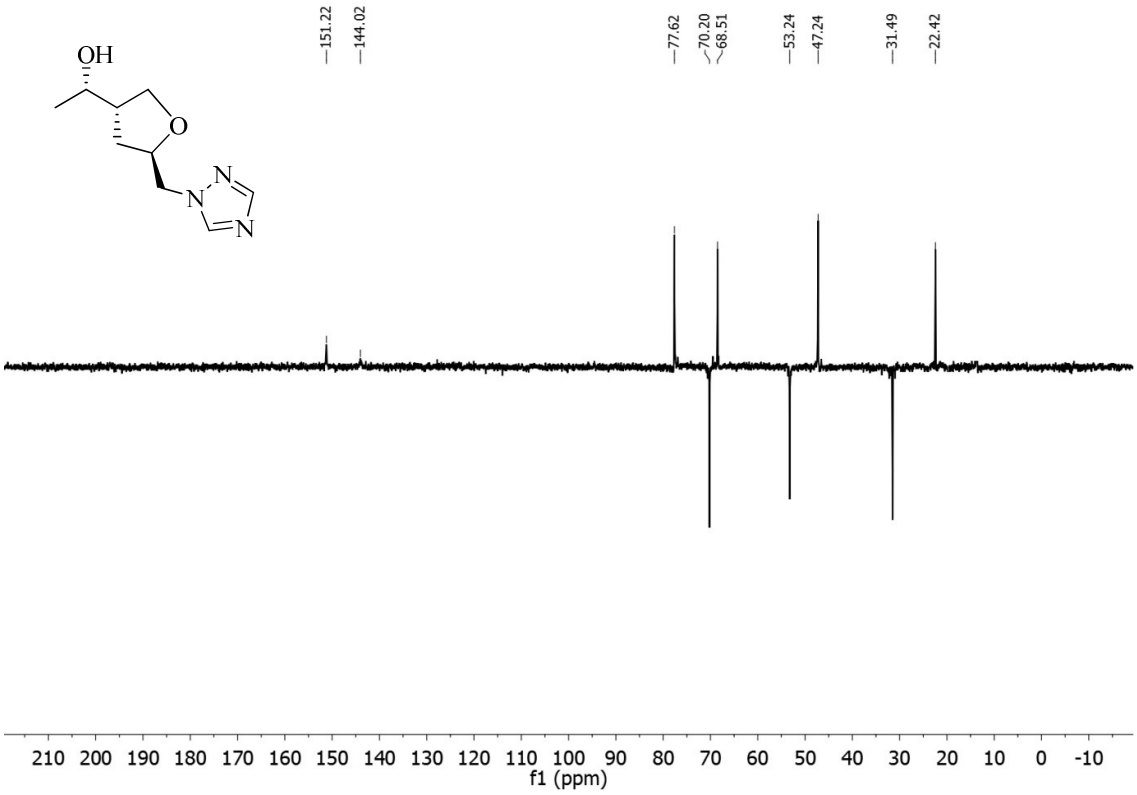
^{1}H - NMR of compound 58 (200 MHz, $CDCl_3$)



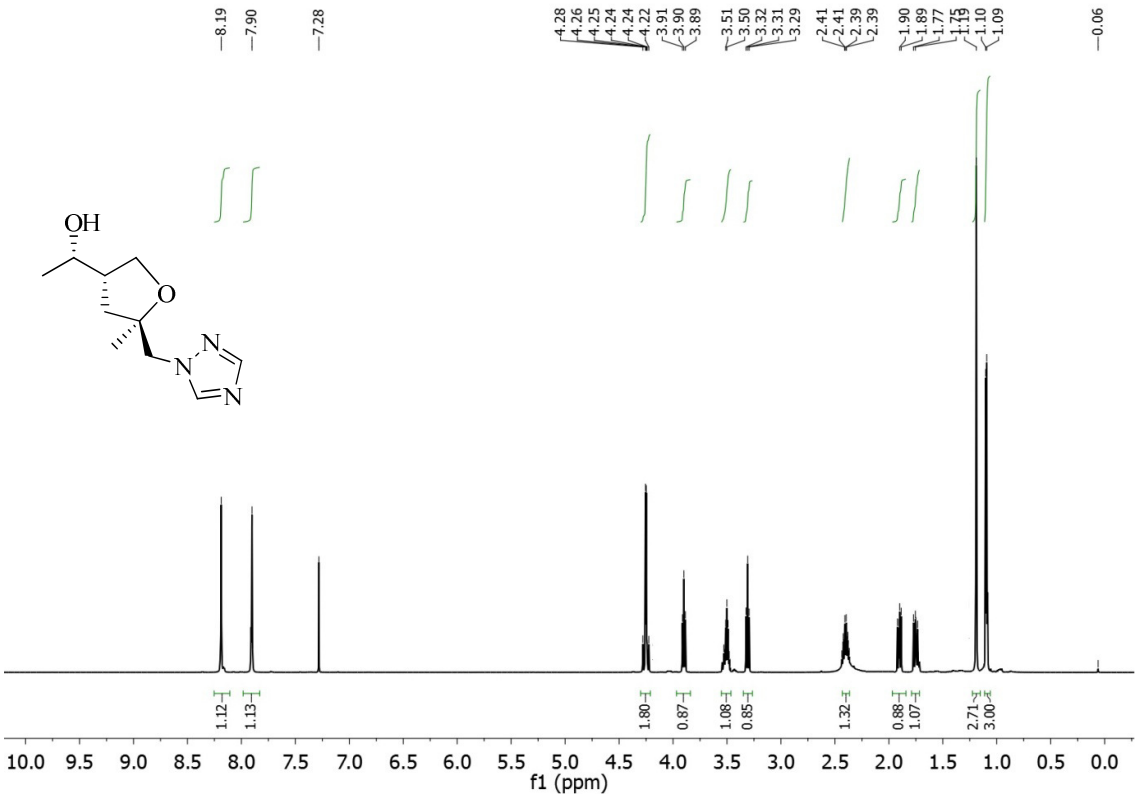
^{13}C NMR of compound 58 (50 MHz, $CDCl_3$)



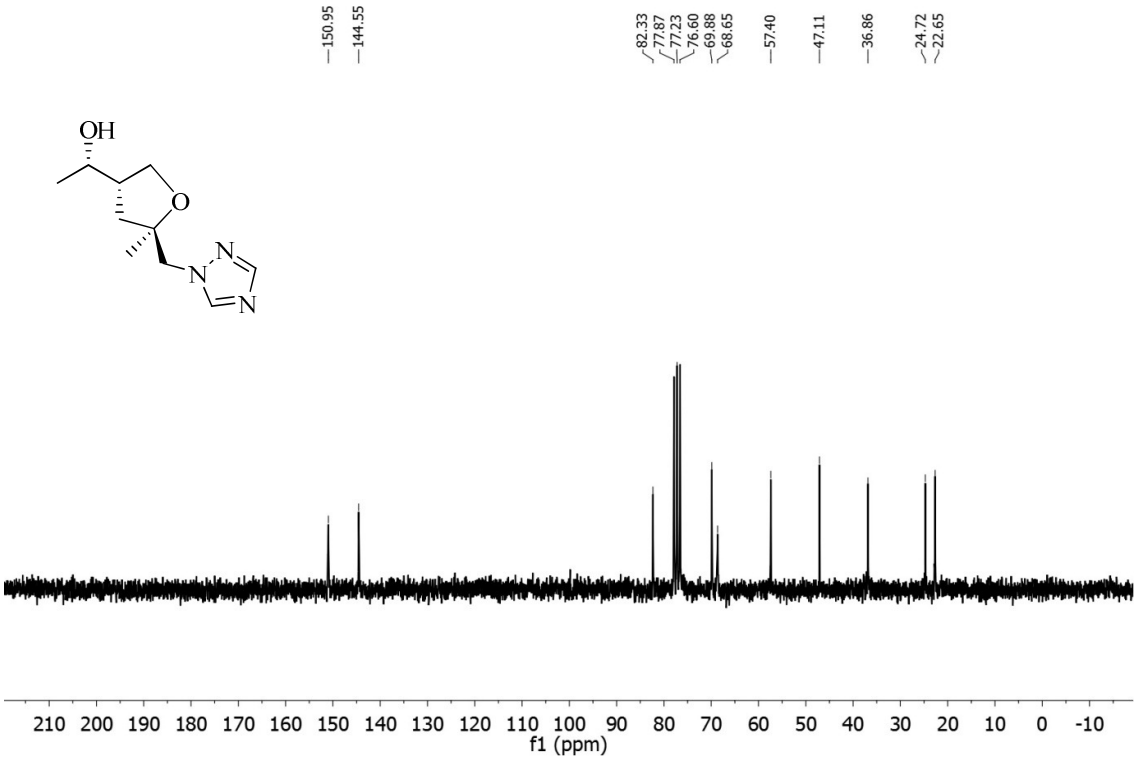
DEPT-135 NMR of compound 58 (50 MHz, $CDCl_3$)



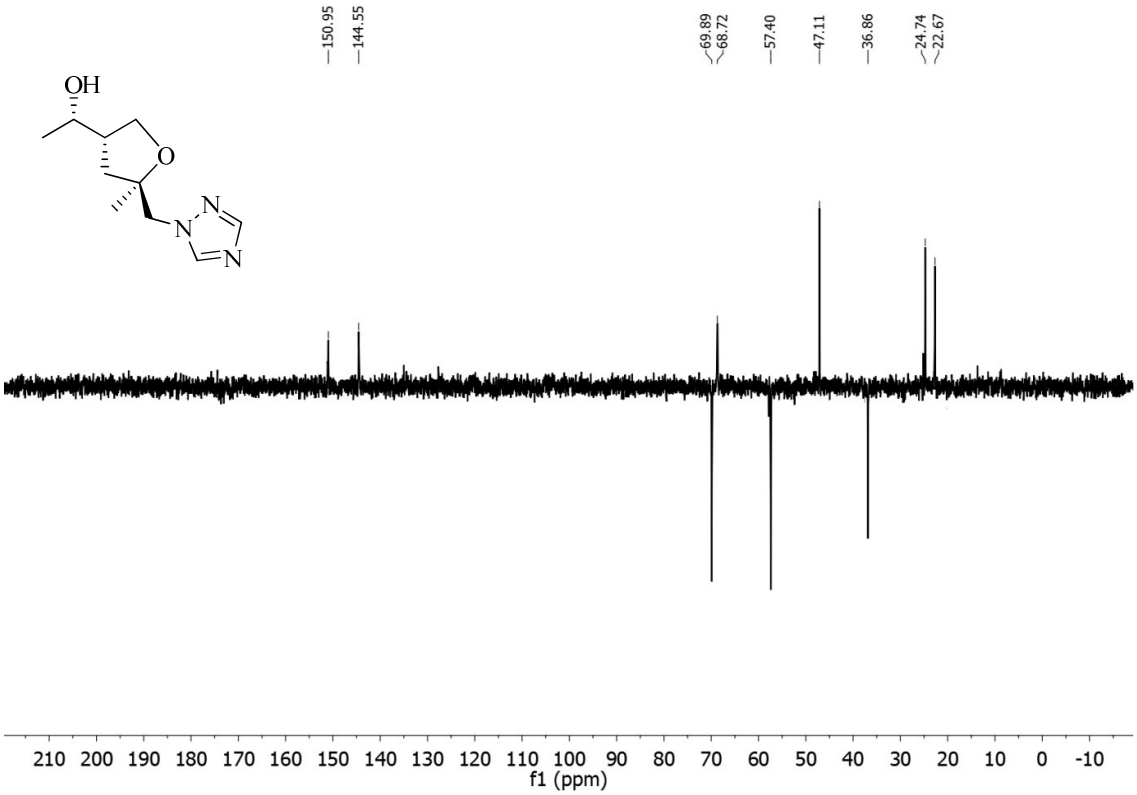
^{1}H - NMR of compound 59 (600 MHz, $CDCl_3$)



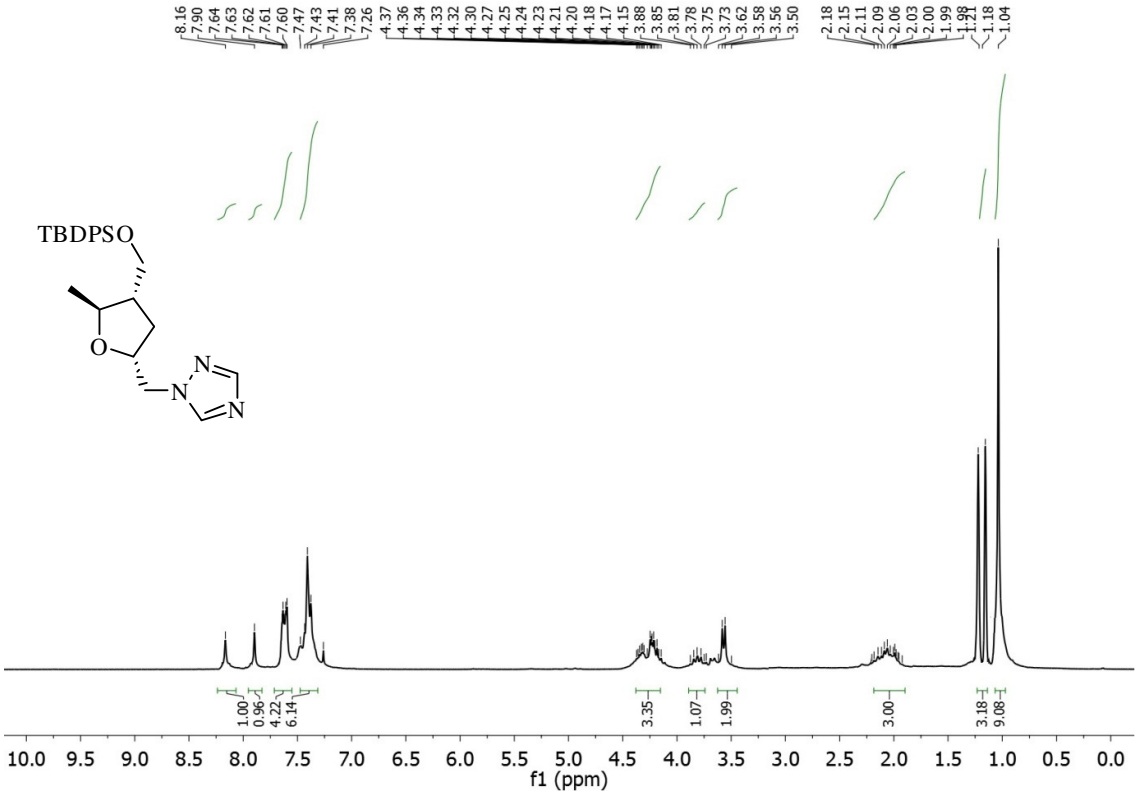
^{13}C NMR of compound 59 (50 MHz, $CDCl_3$)



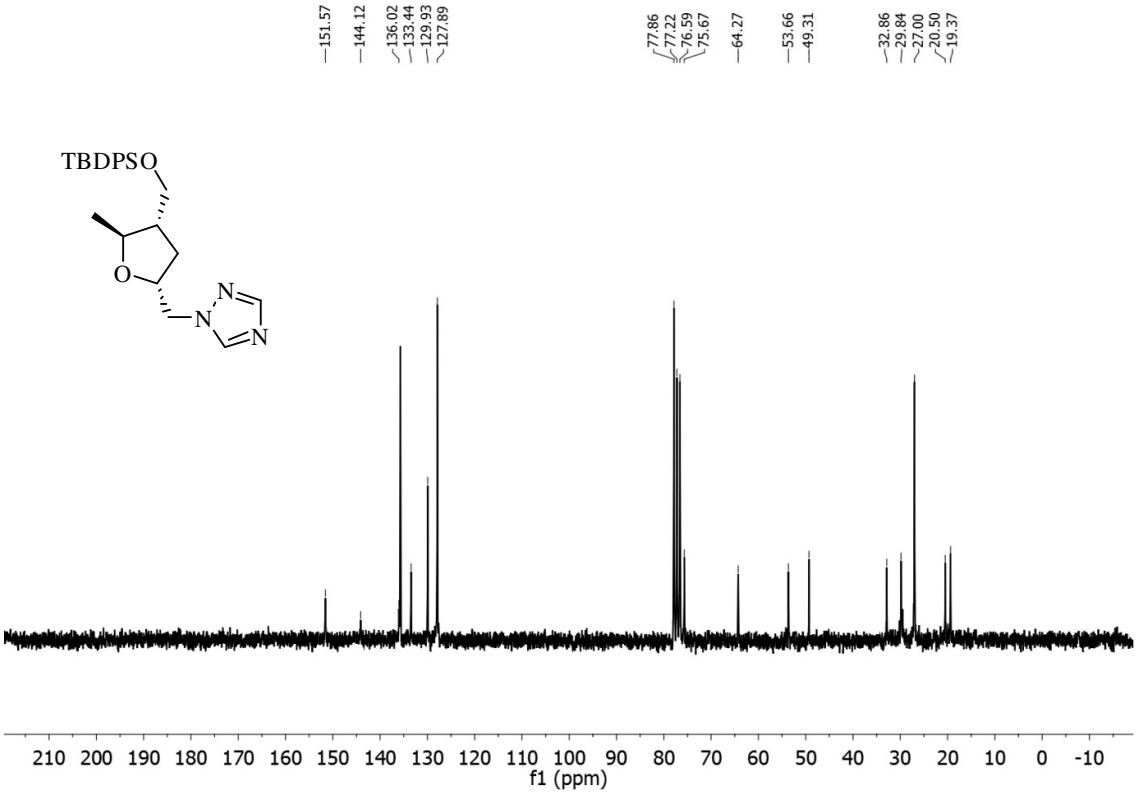
DEPT-135 NMR of compound 59 (50 MHz, $CDCl_3$)



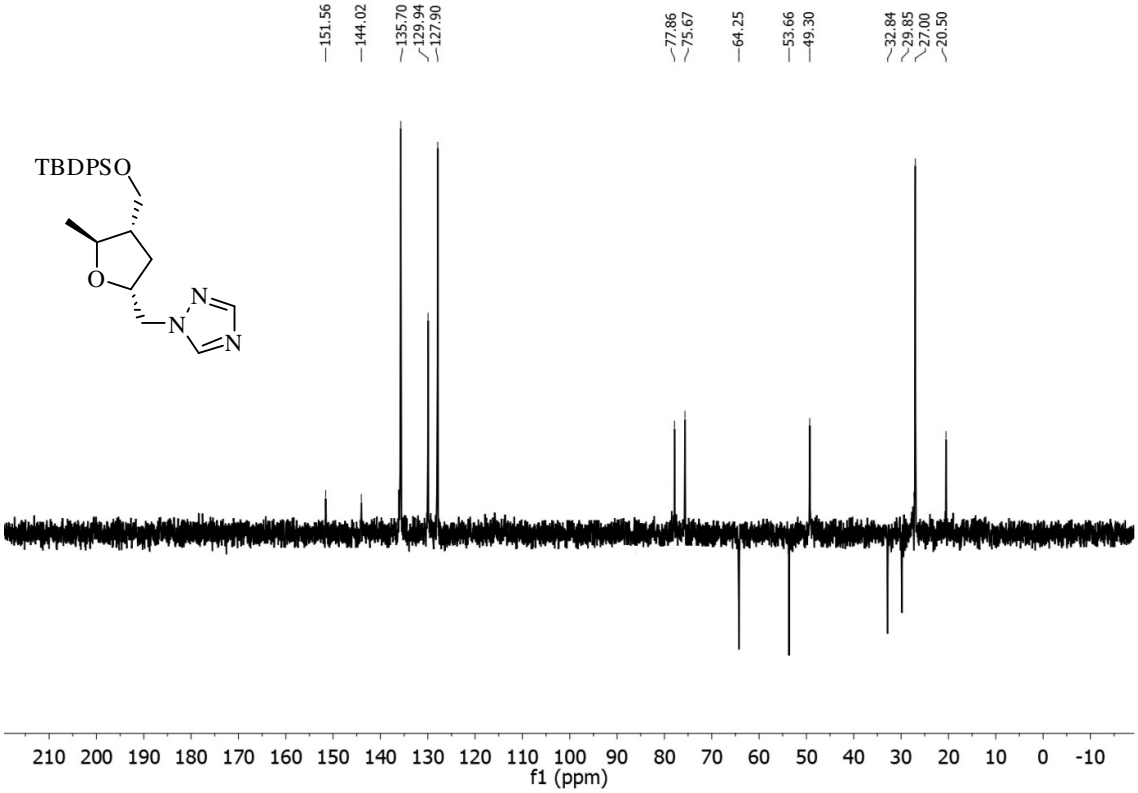
^{1}H - NMR of compound 60 (200 MHz, $CDCl_3$)



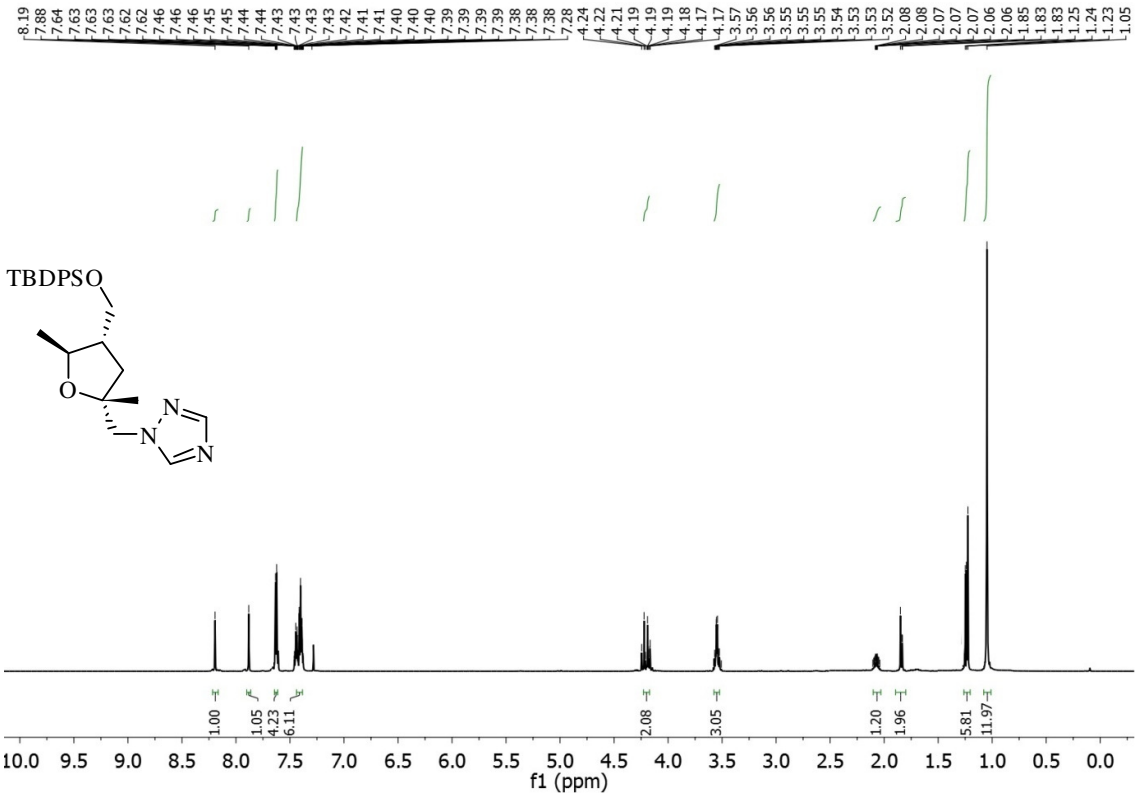
^{13}C NMR of compound 60 (50 MHz, $CDCl_3$)



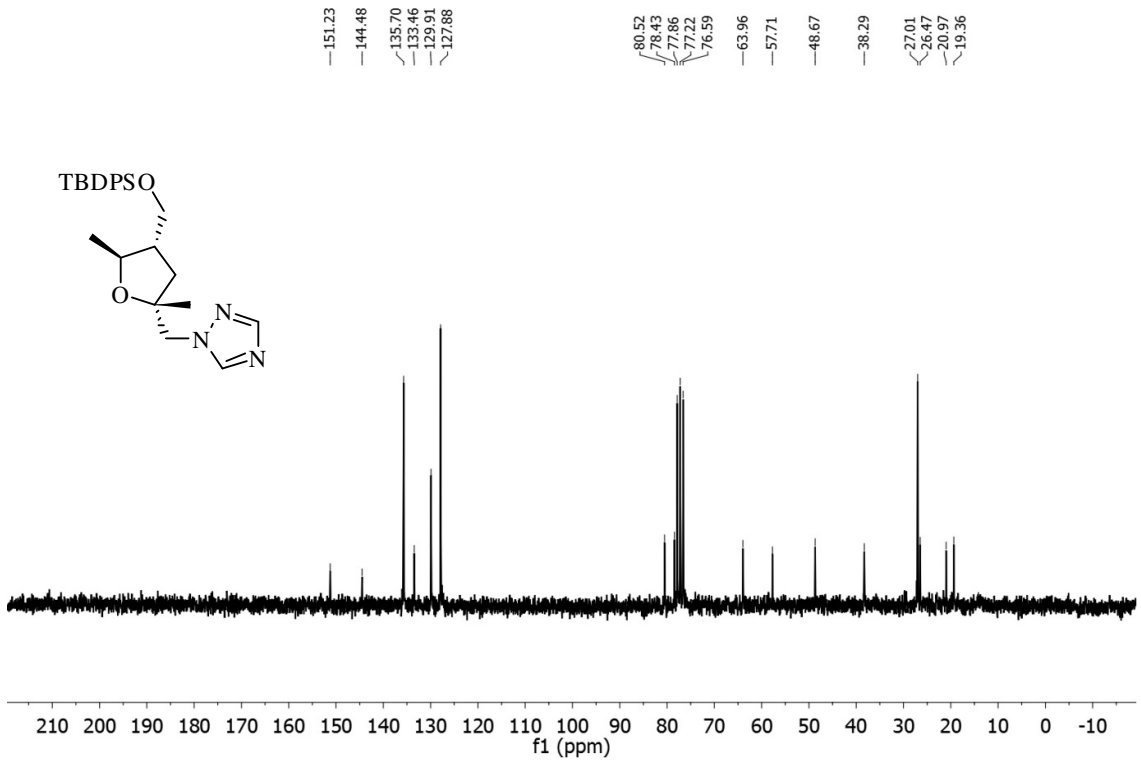
DEPT-135 NMR of compound 60 (50 MHz, $CDCl_3$)



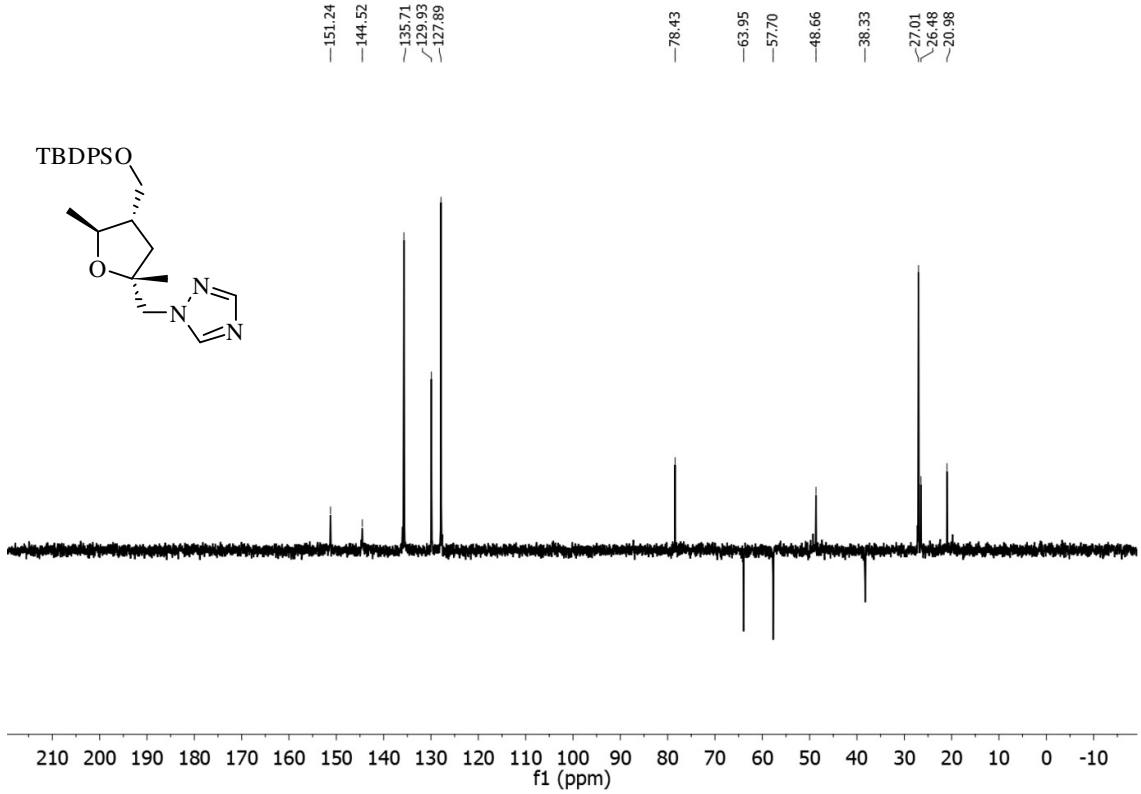
^{1}H - NMR of compound 61 (400 MHz, $CDCl_3$)



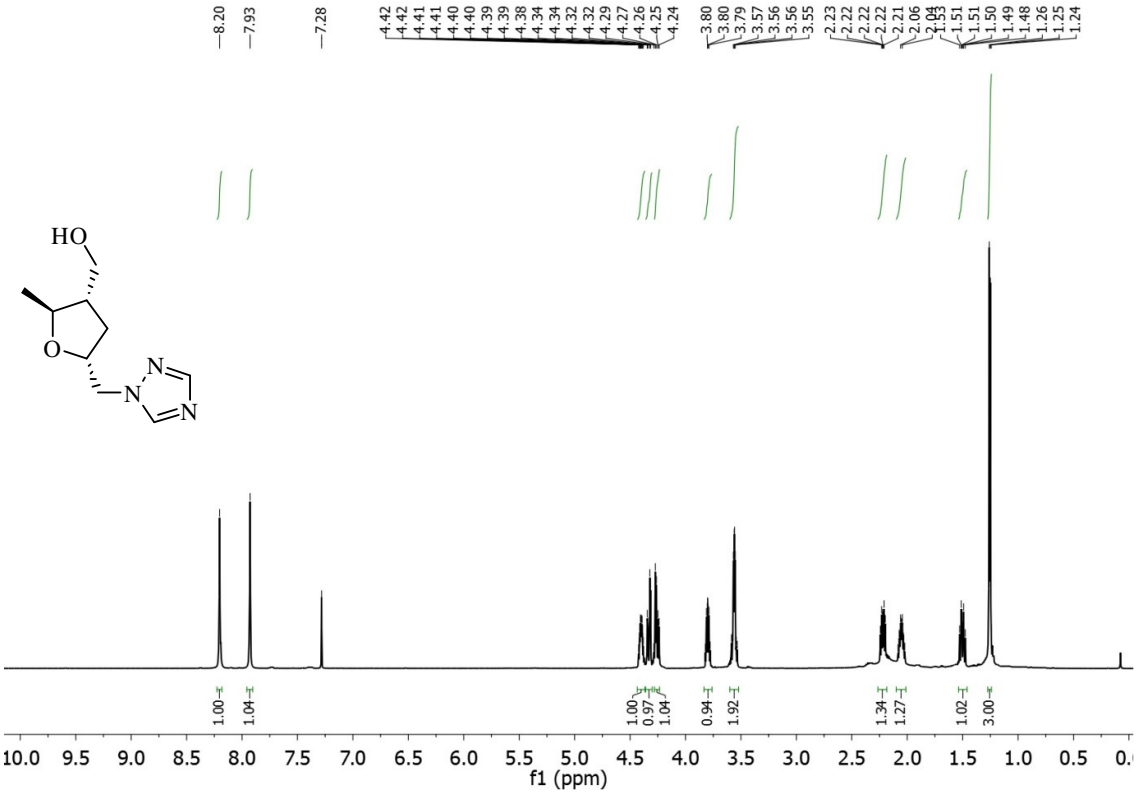
^{13}C NMR of compound 61 (50 MHz, $CDCl_3$)



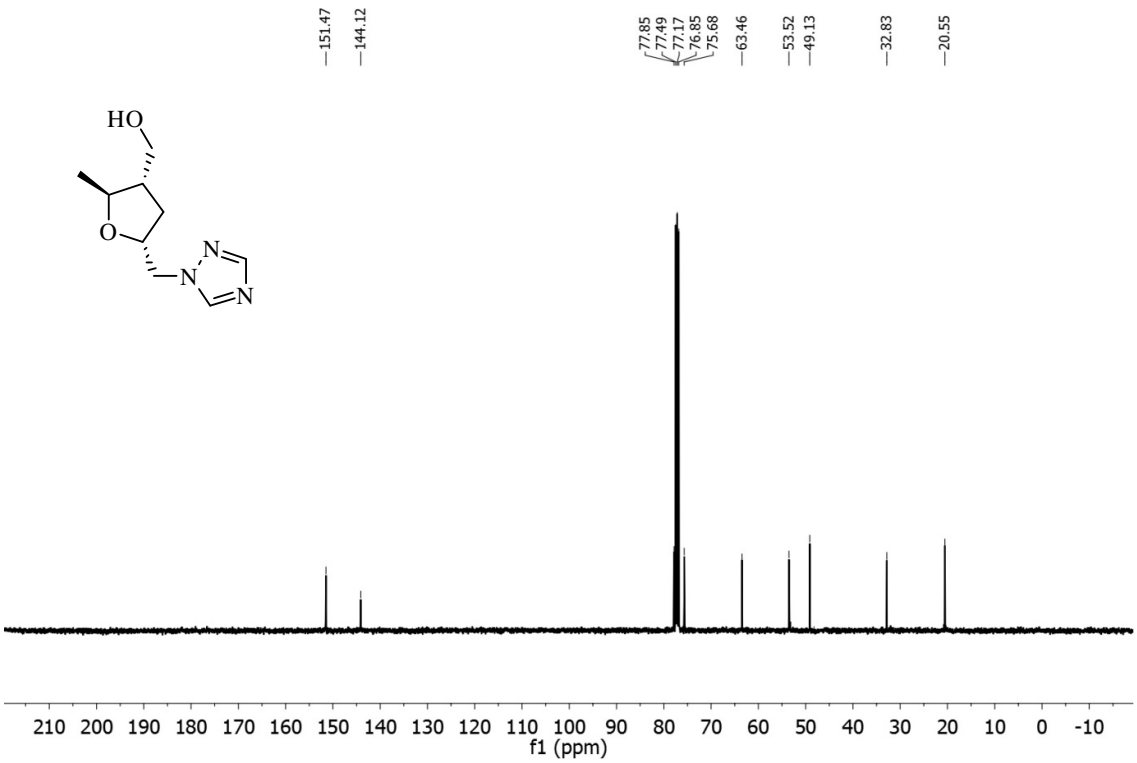
DEPT-135 NMR of compound 61 (50 MHz, $CDCl_3$)



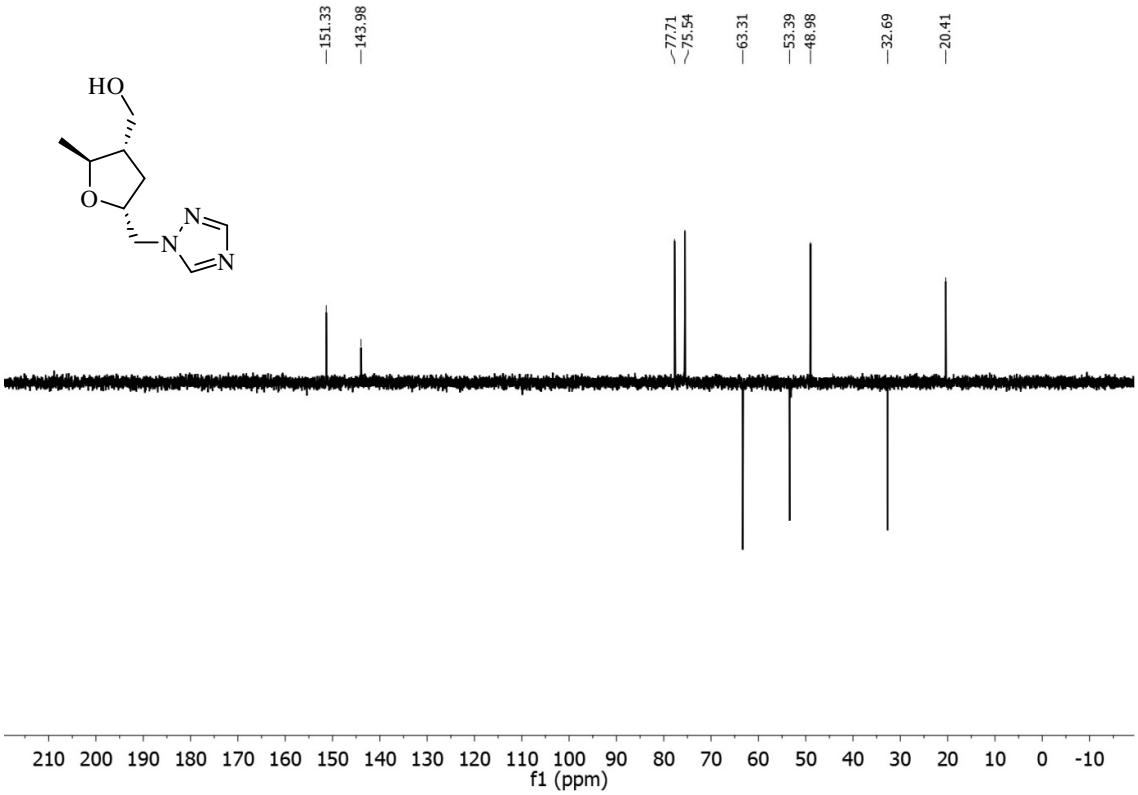
^{1}H - NMR of compound 62 (400 MHz, $CDCl_3$)



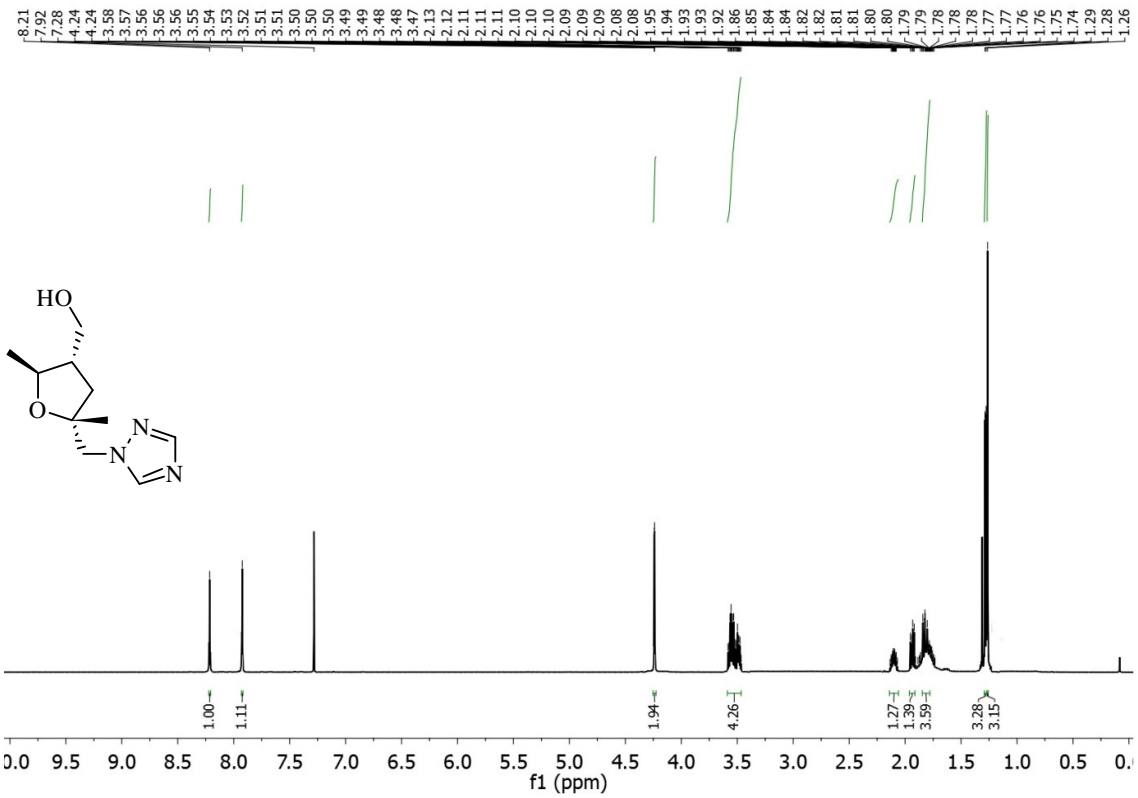
^{13}C NMR of compound 62 (100 MHz, $CDCl_3$)



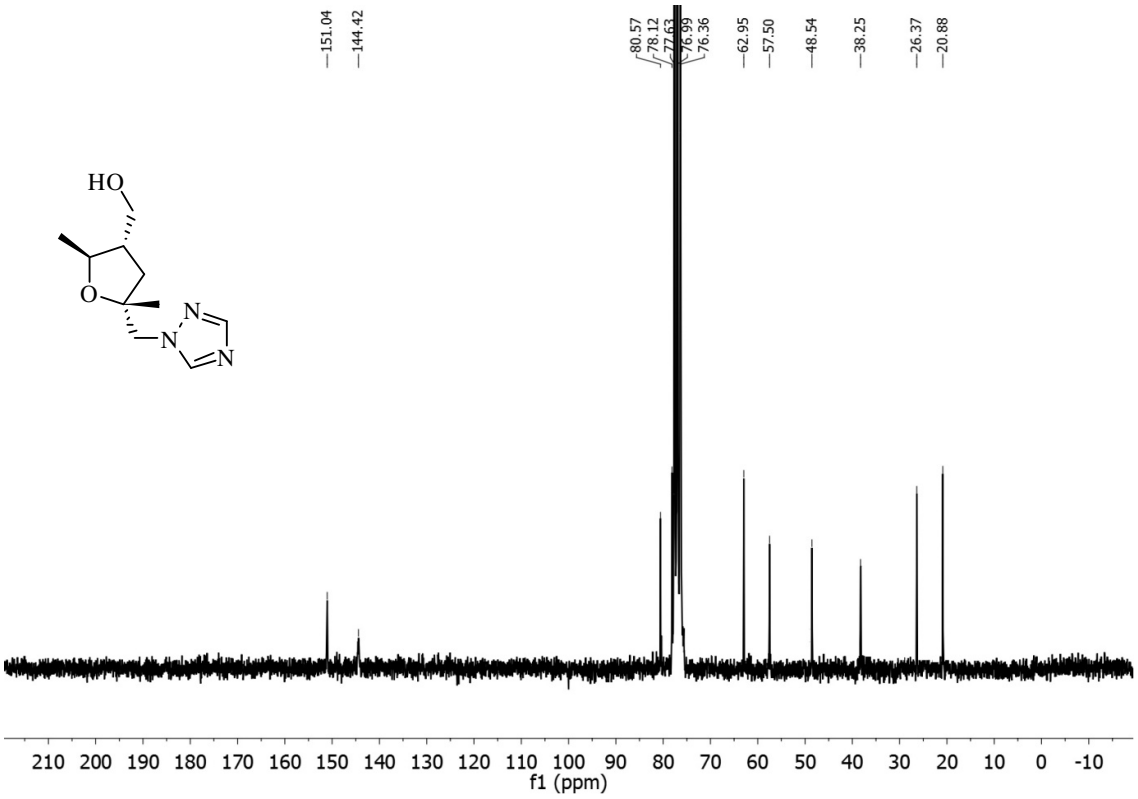
DEPT-135 NMR of compound 62 (100 MHz, $CDCl_3$)



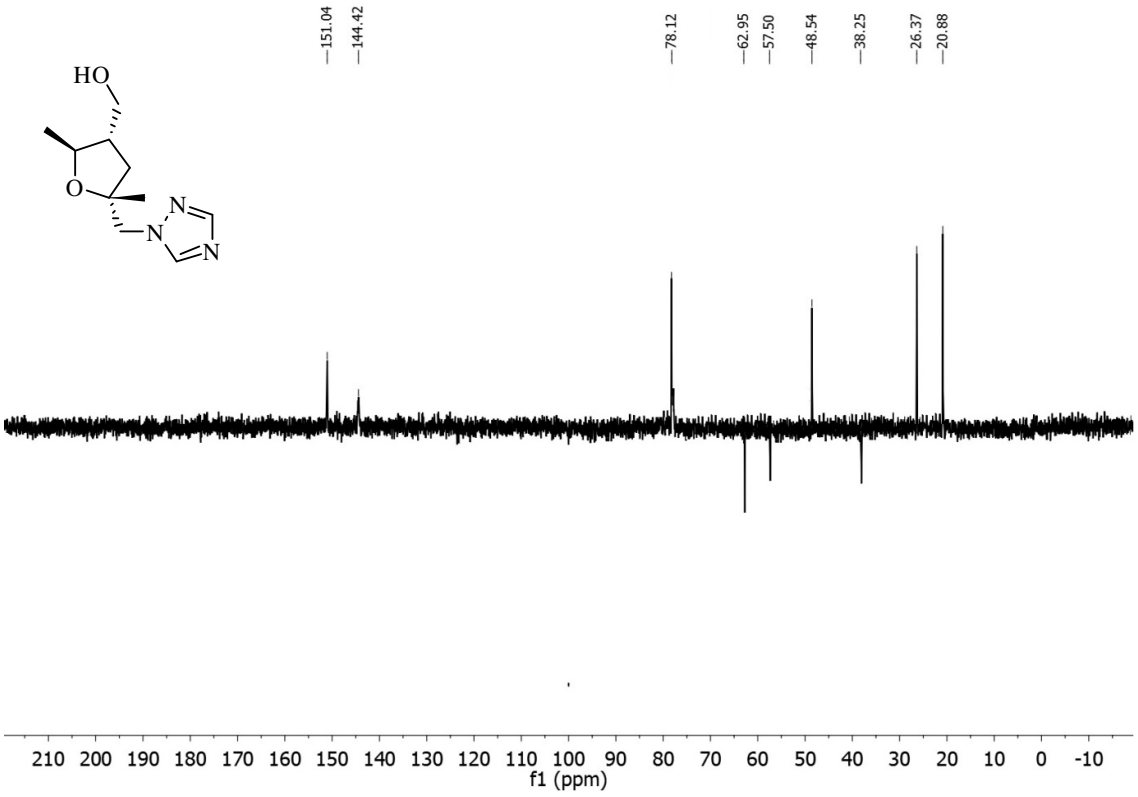
^{1}H - NMR of compound 63 (400 MHz, $CDCl_3$)



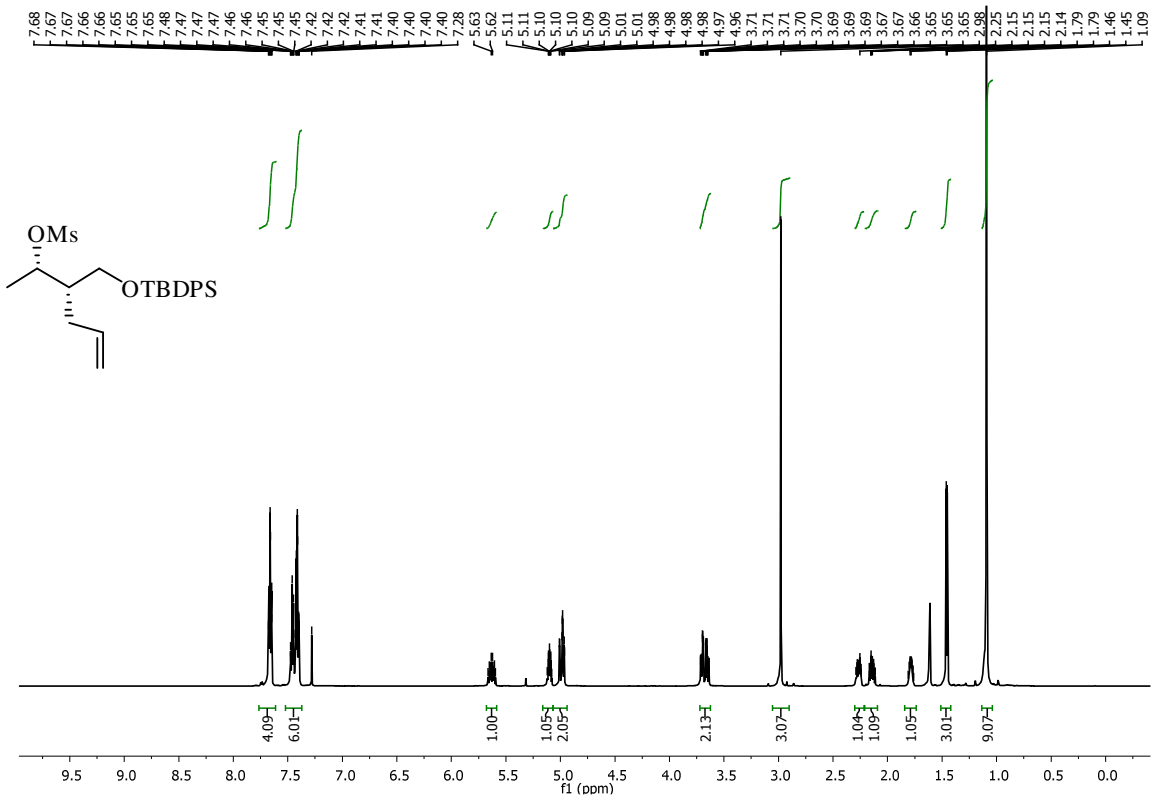
^{13}C NMR of compound 63 (50 MHz, $CDCl_3$)



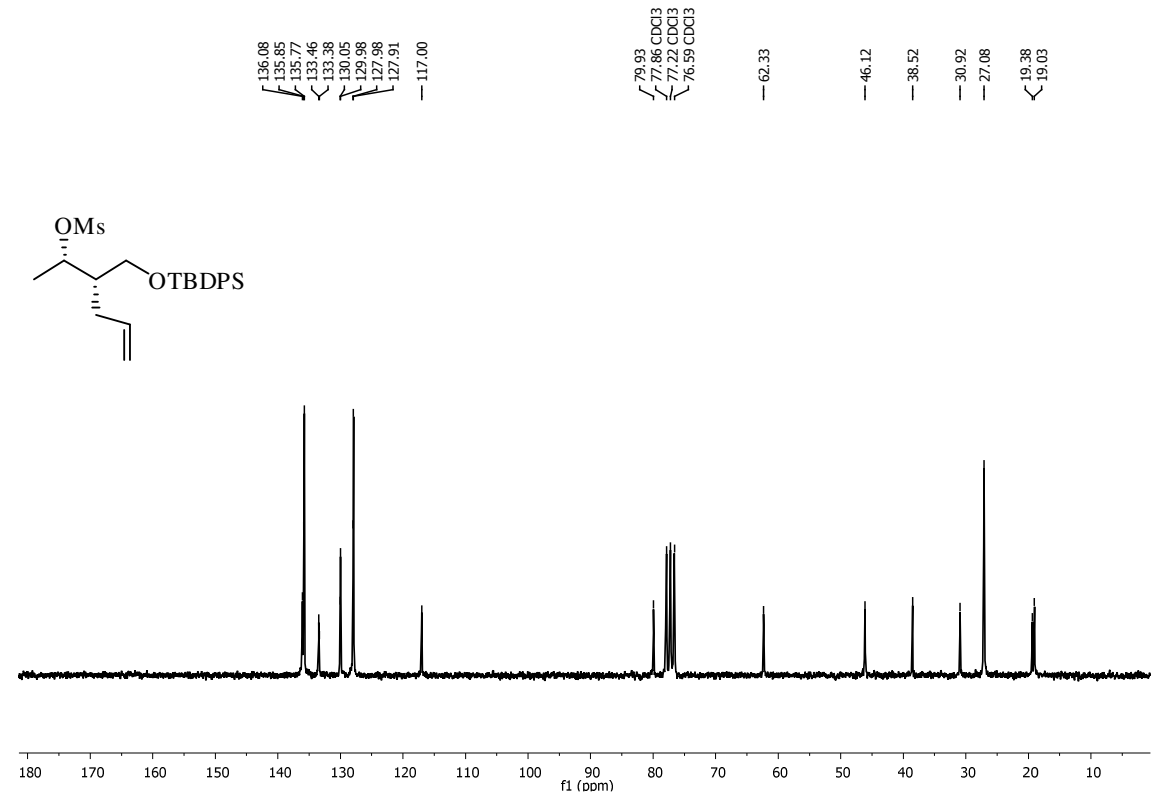
DEPT-135 NMR of compound 63 (50 MHz, $CDCl_3$)



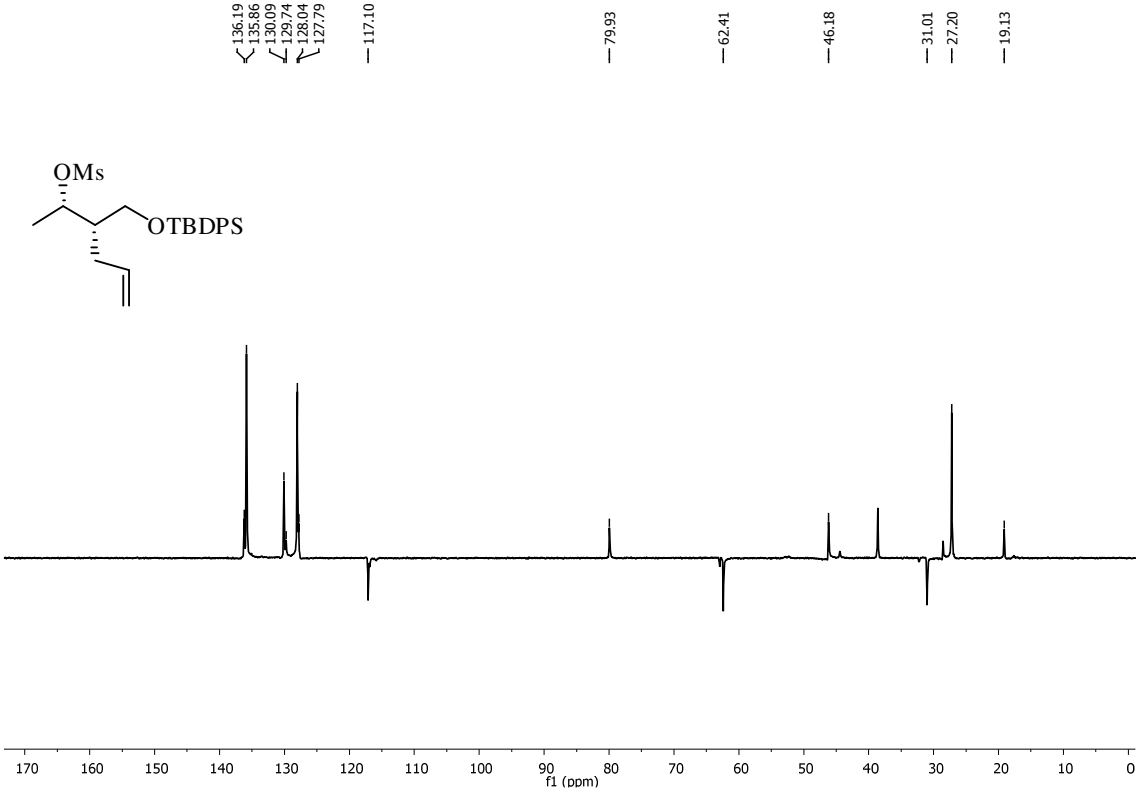
^{1}H - NMR of compound 64 (600 MHz, $CDCl_3$)



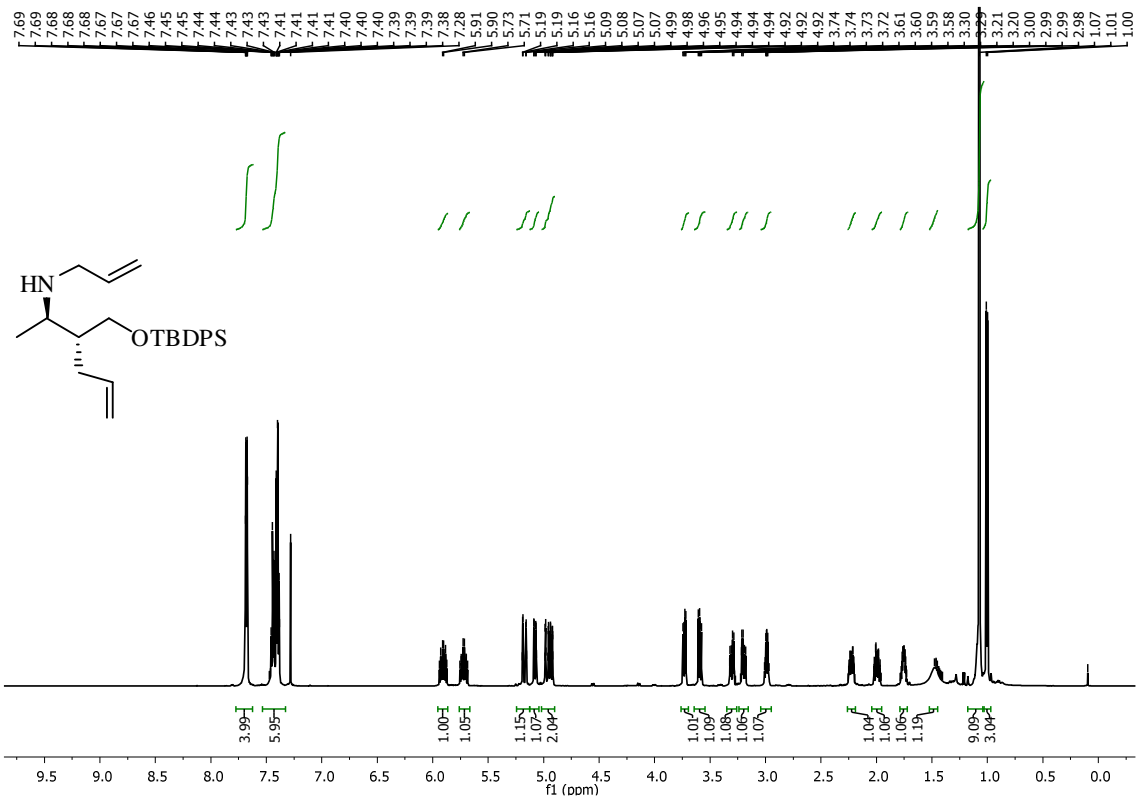
^{13}C NMR of compound 64 (50 MHz, $CDCl_3$)



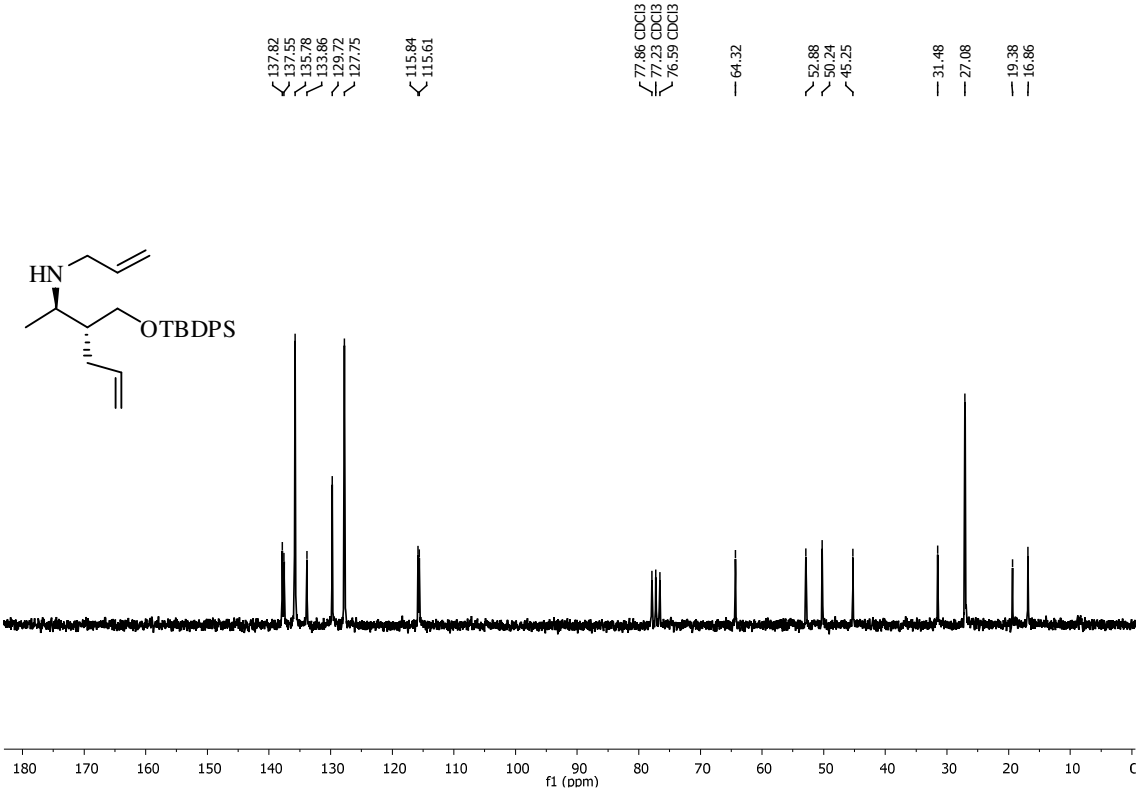
DEPT-135 NMR of compound 64 (50 MHz, $CDCl_3$)



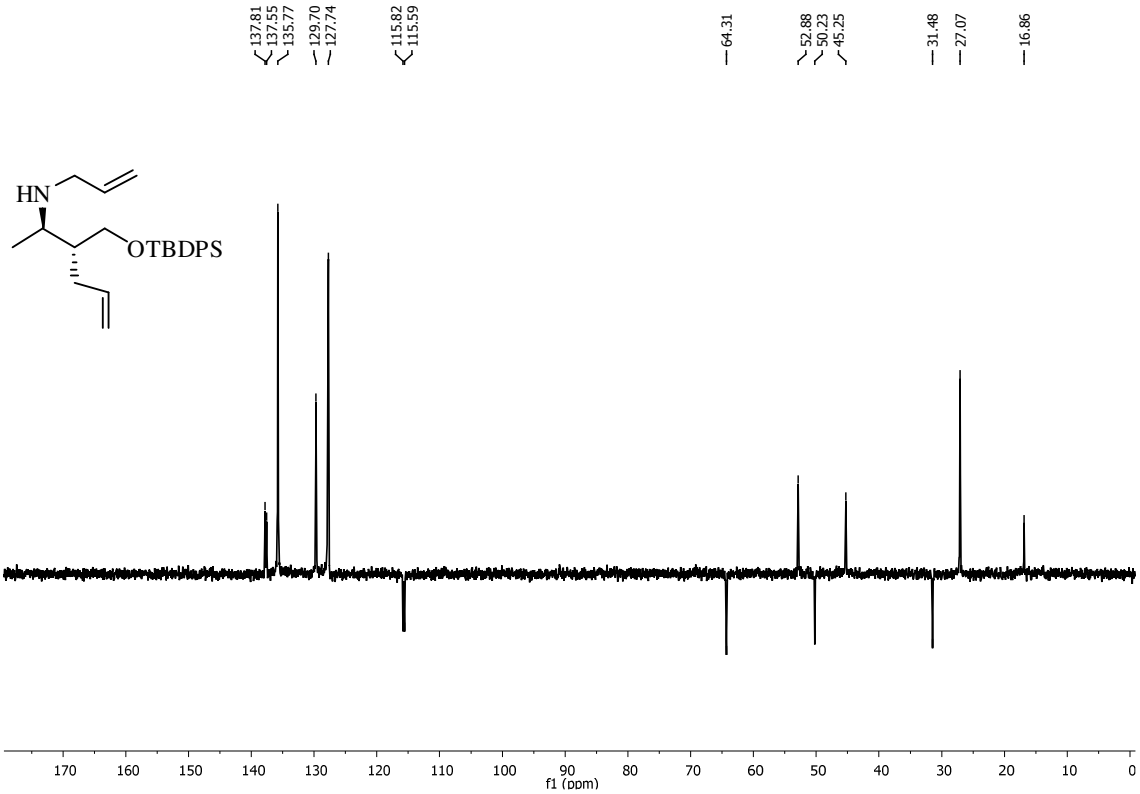
^{1}H - NMR of compound 65 (600 MHz, $CDCl_3$)



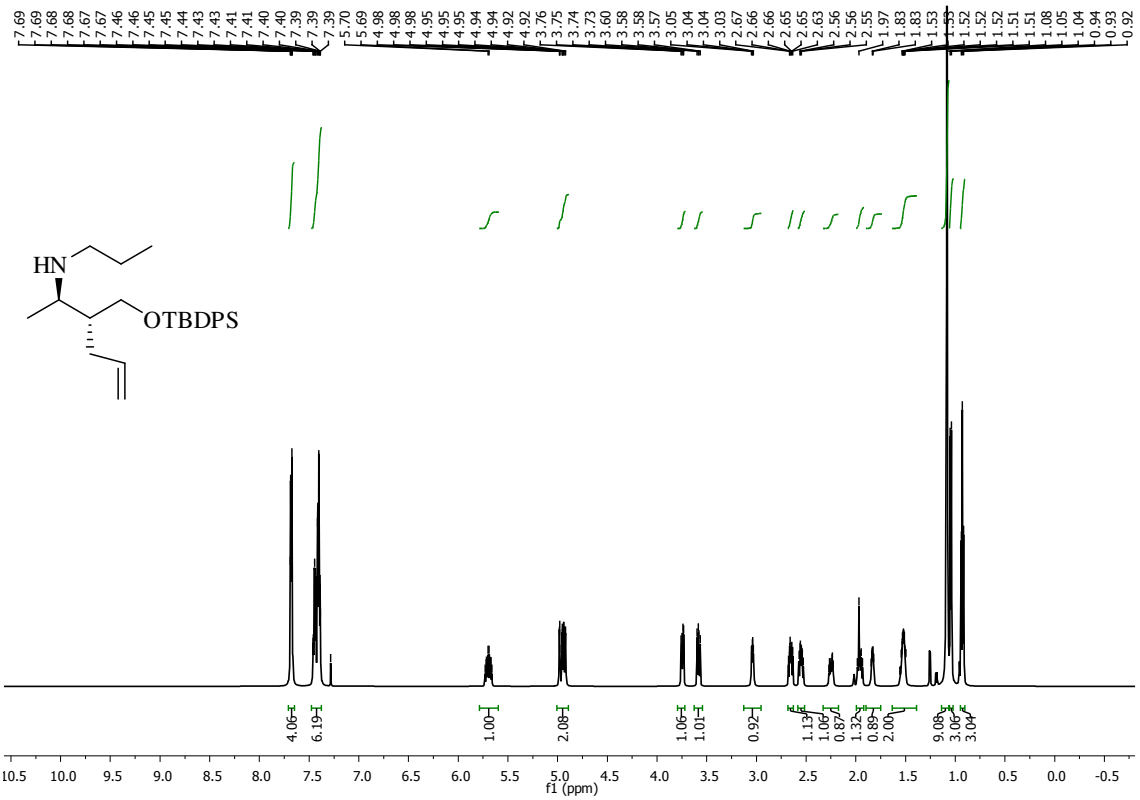
^{13}C NMR of compound 65 (50 MHz, $CDCl_3$)



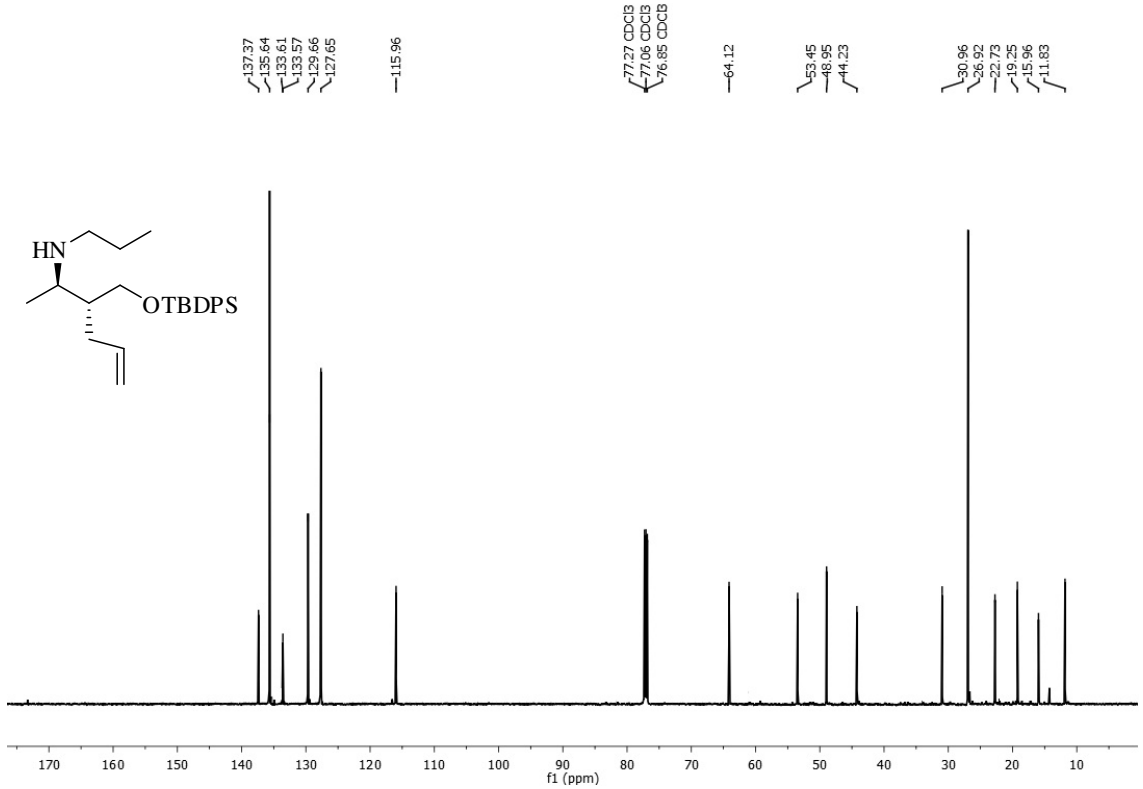
DEPT-135 NMR of compound 65 (50 MHz, $CDCl_3$)



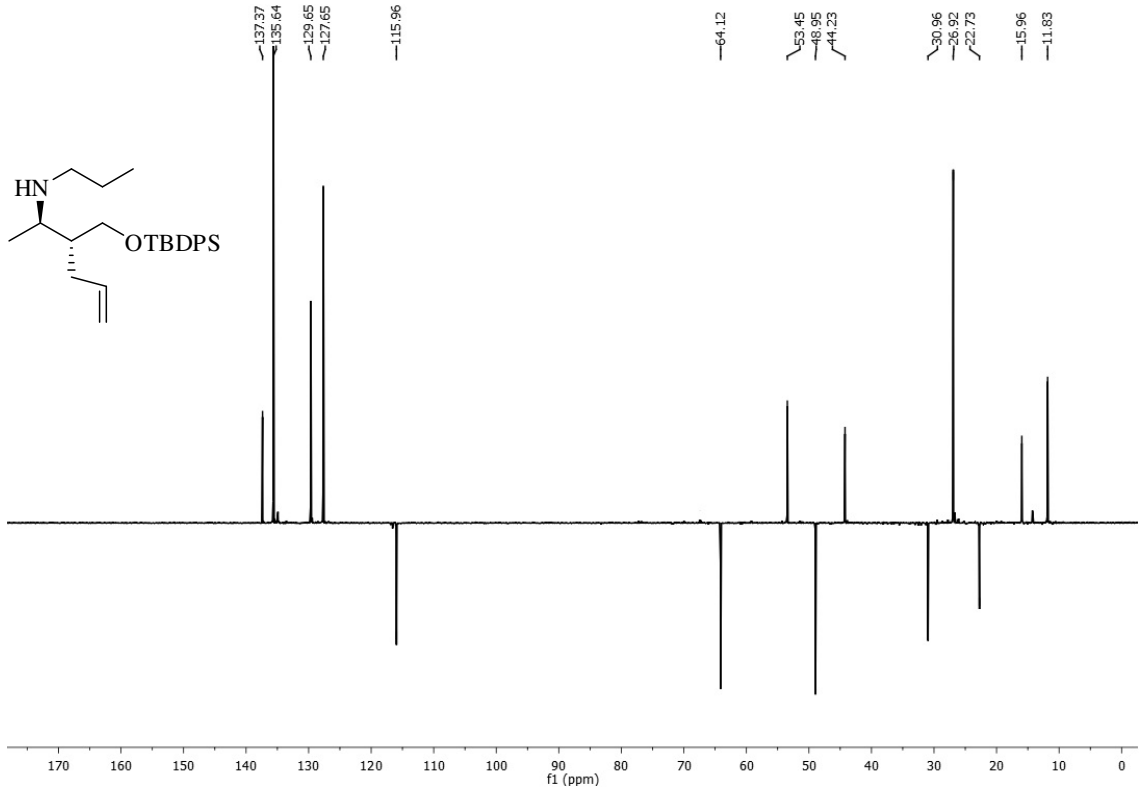
^{1}H - NMR of compound 66 (600 MHz, $CDCl_3$)



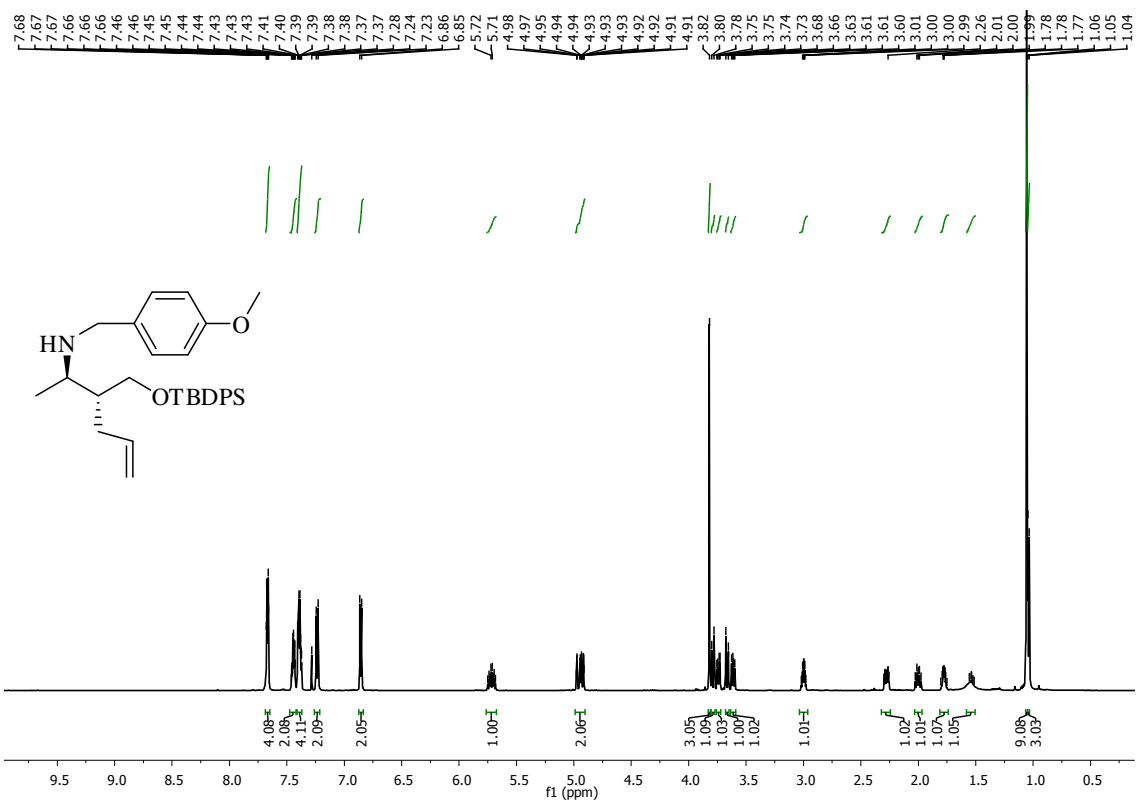
^{13}C NMR of compound 66 (150 MHz, $CDCl_3$)



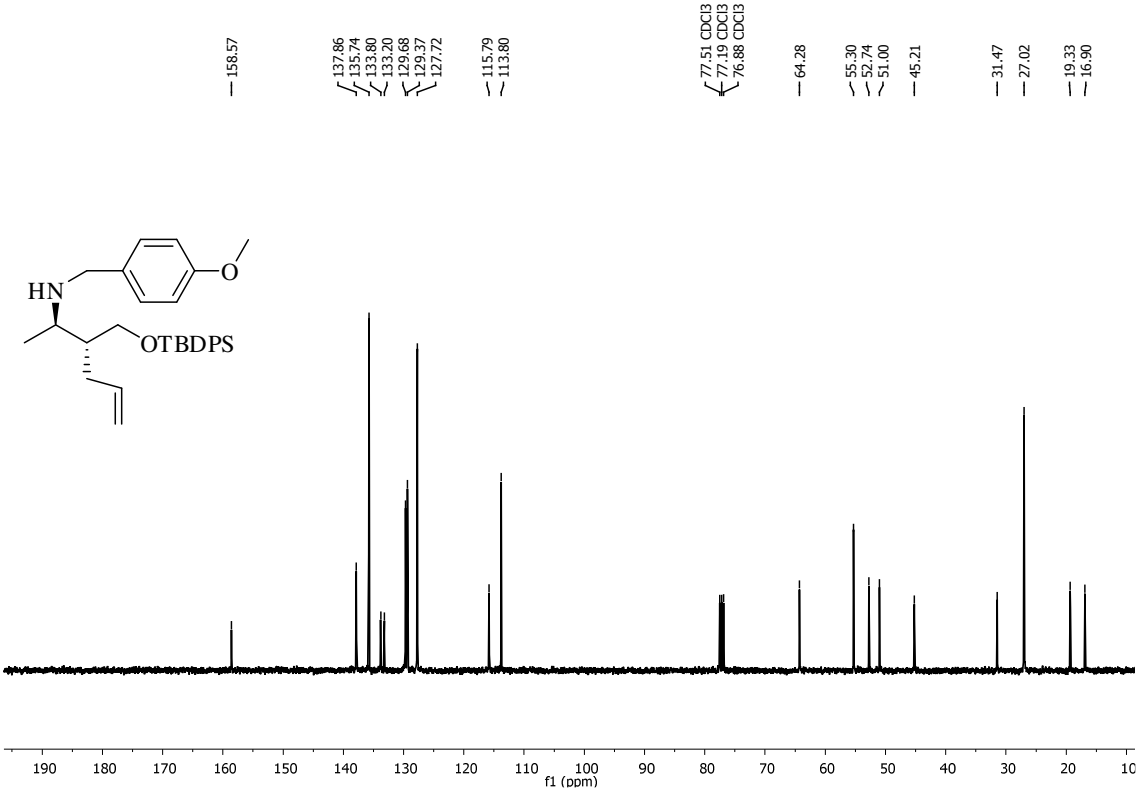
DEPT-135 NMR of compound 66 (150 MHz, $CDCl_3$)



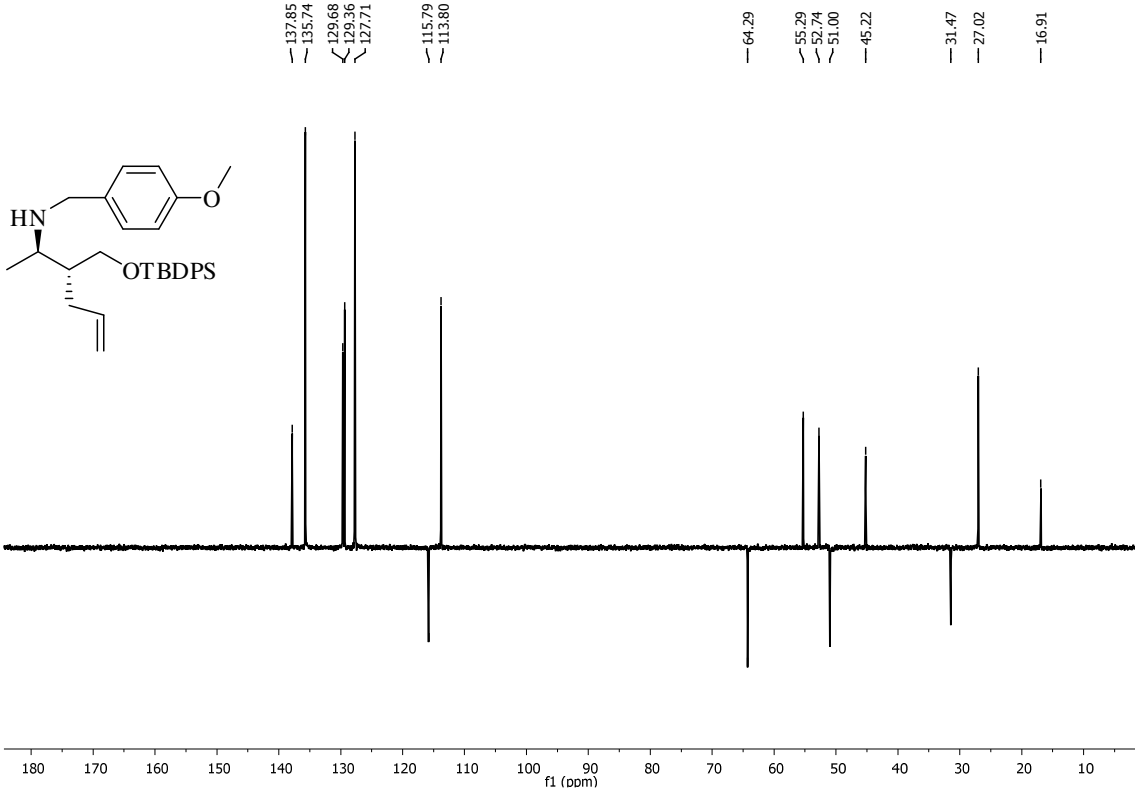
^{1}H - NMR of compound 67 (600 MHz, $CDCl_3$)



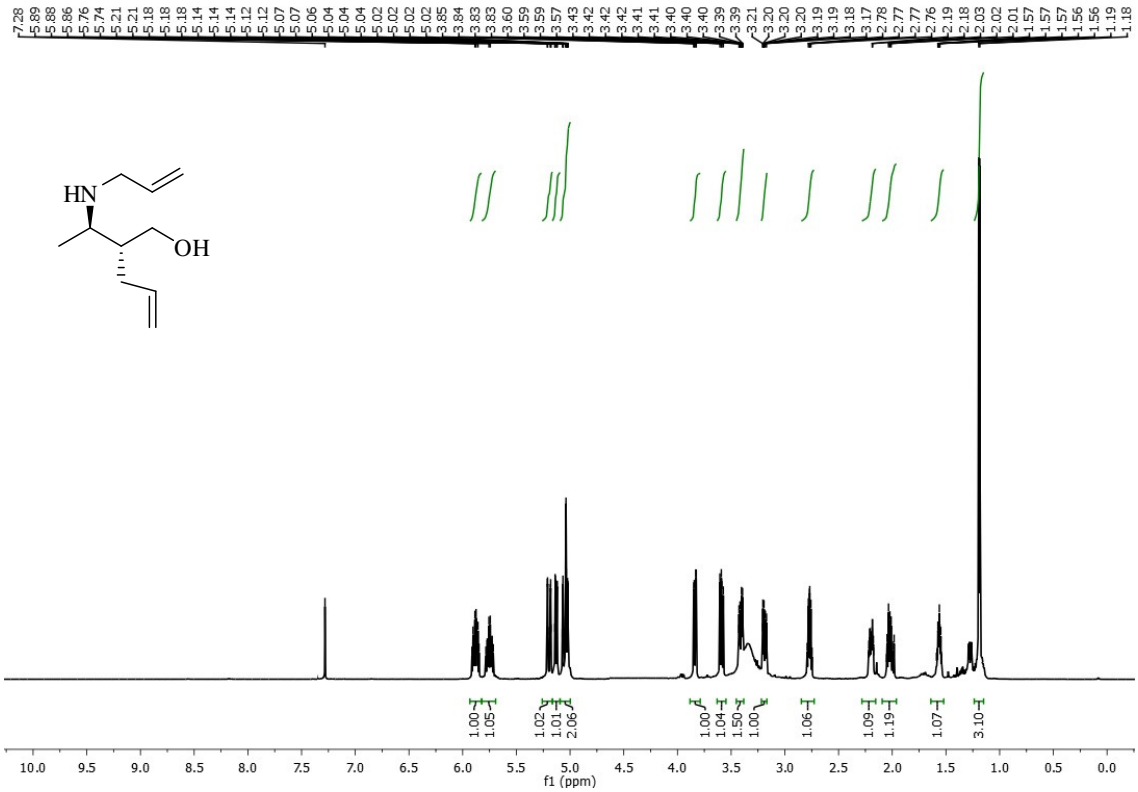
^{13}C NMR of compound 67 (100 MHz, $CDCl_3$)



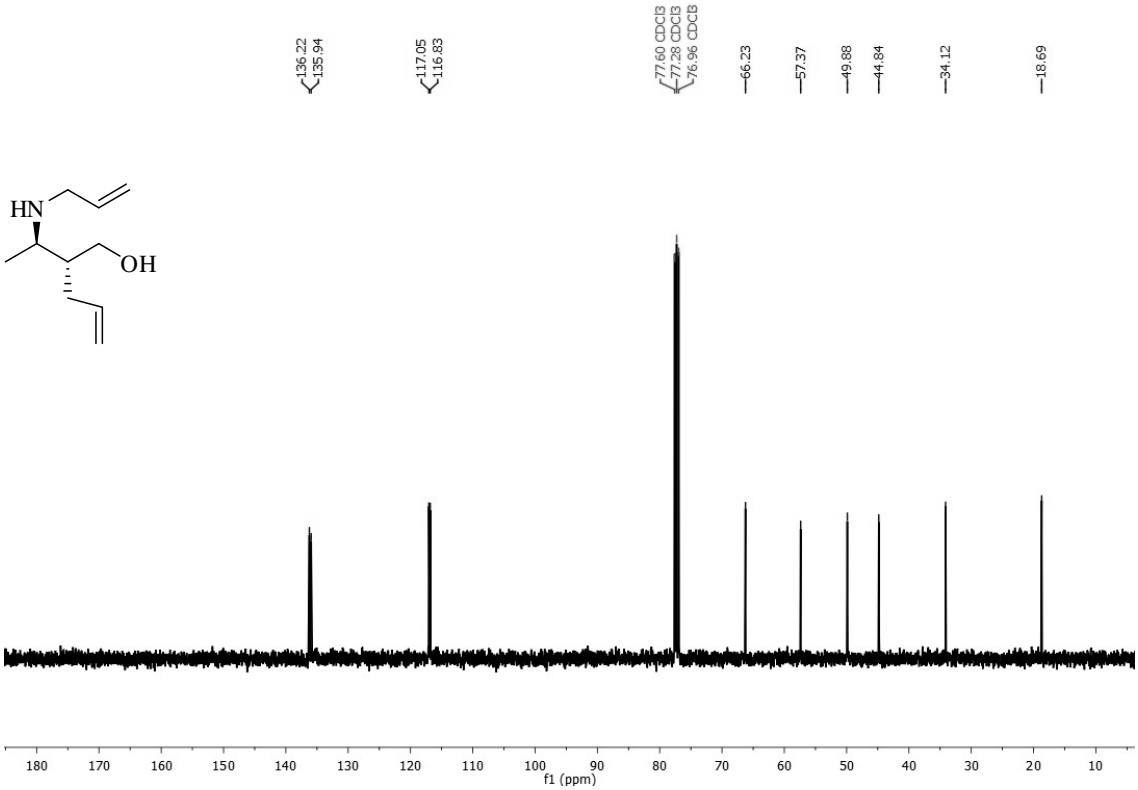
DEPT-135 NMR of compound 67 (100 MHz, $CDCl_3$)



^{1}H - NMR of compound 68 (600 MHz, $CDCl_3$)



^{13}C NMR of compound 68 (100 MHz, $CDCl_3$)



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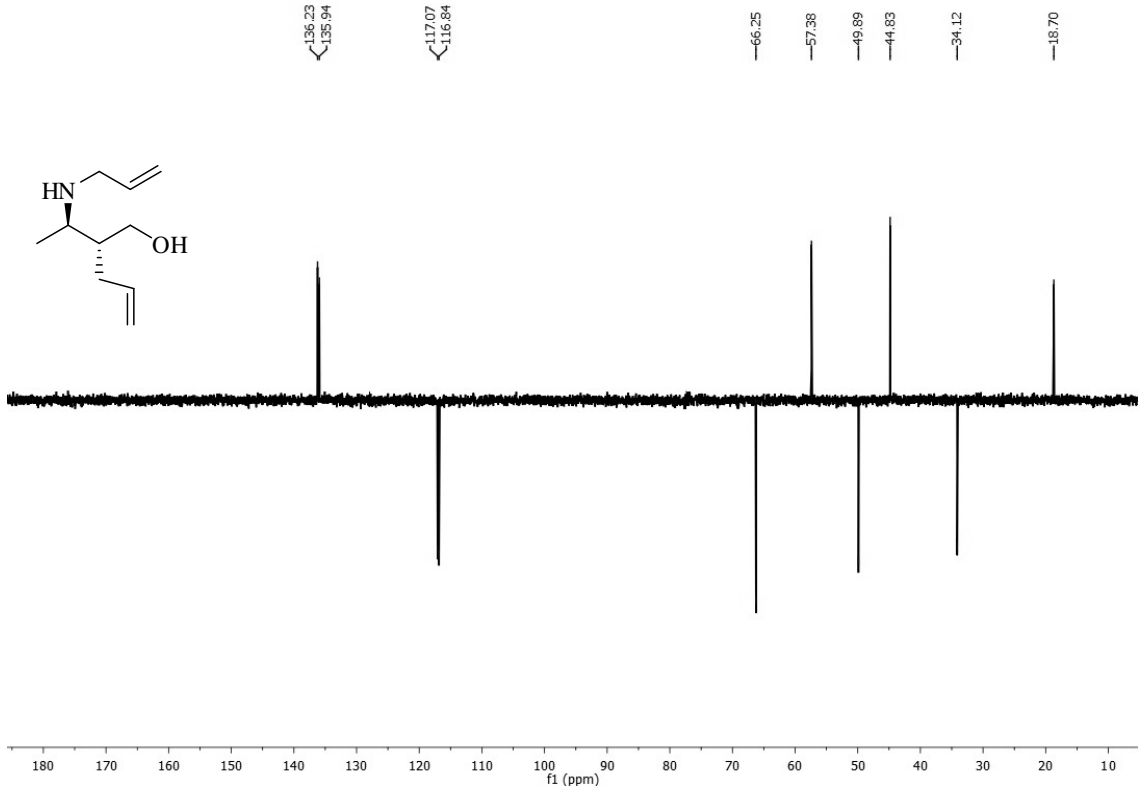

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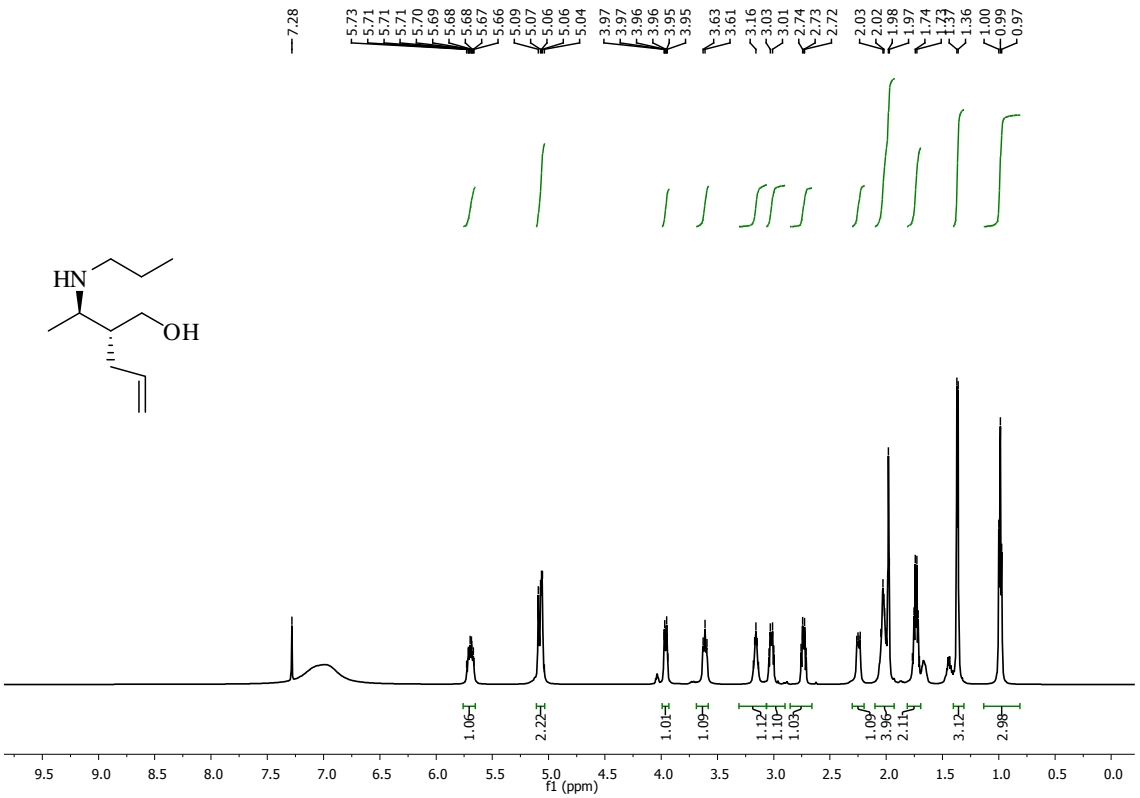
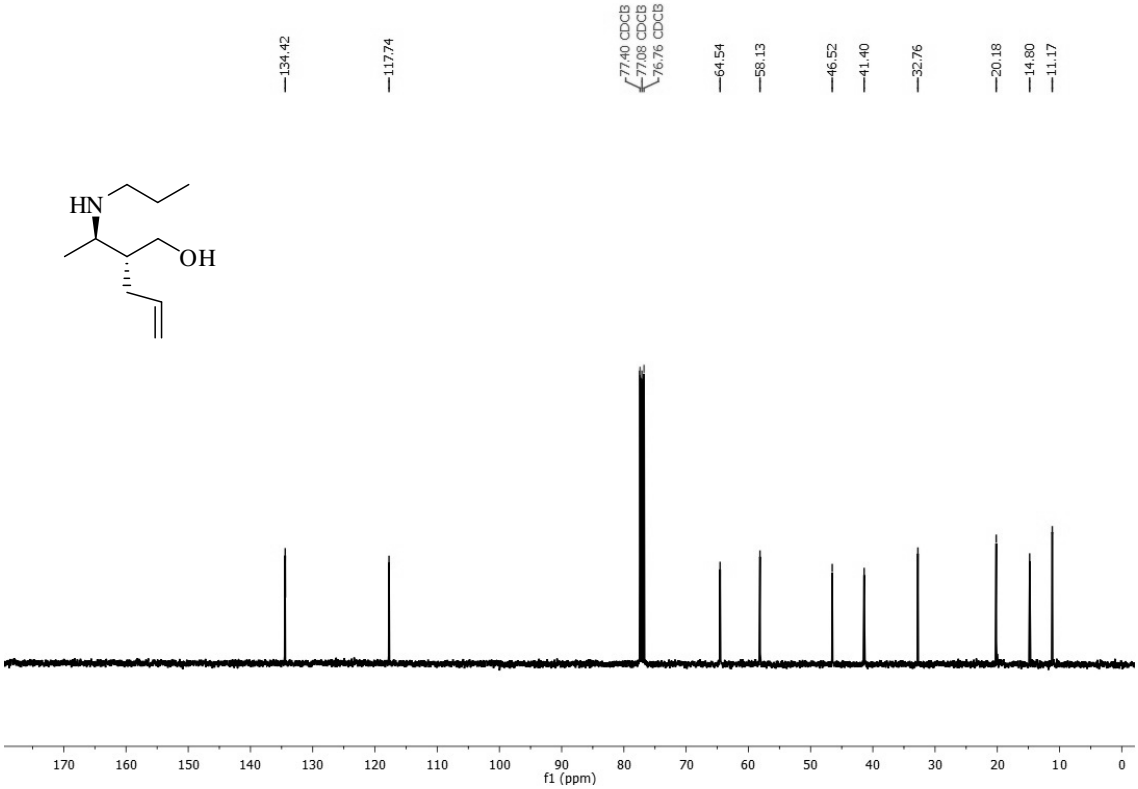
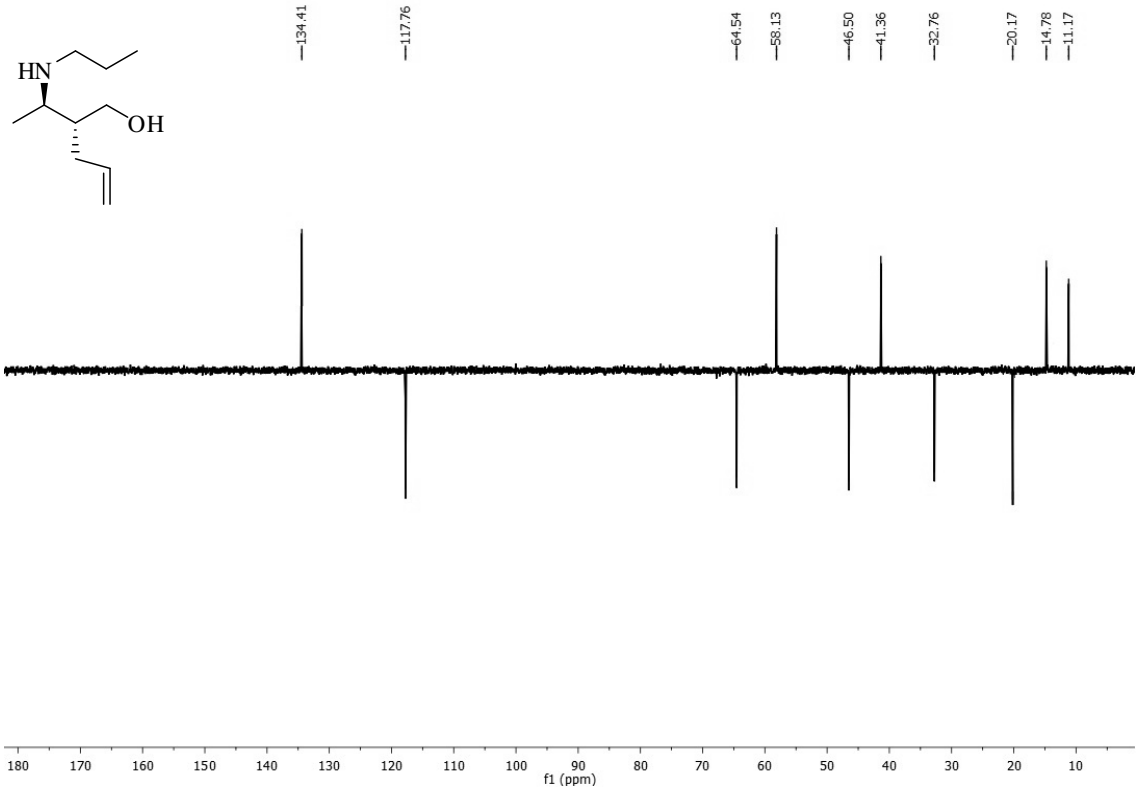


^{13}C NMR of compound 69 (100 MHz, $CDCl_3$)



DEPT-135 NMR of compound 69 (100 MHz, $CDCl_3$)



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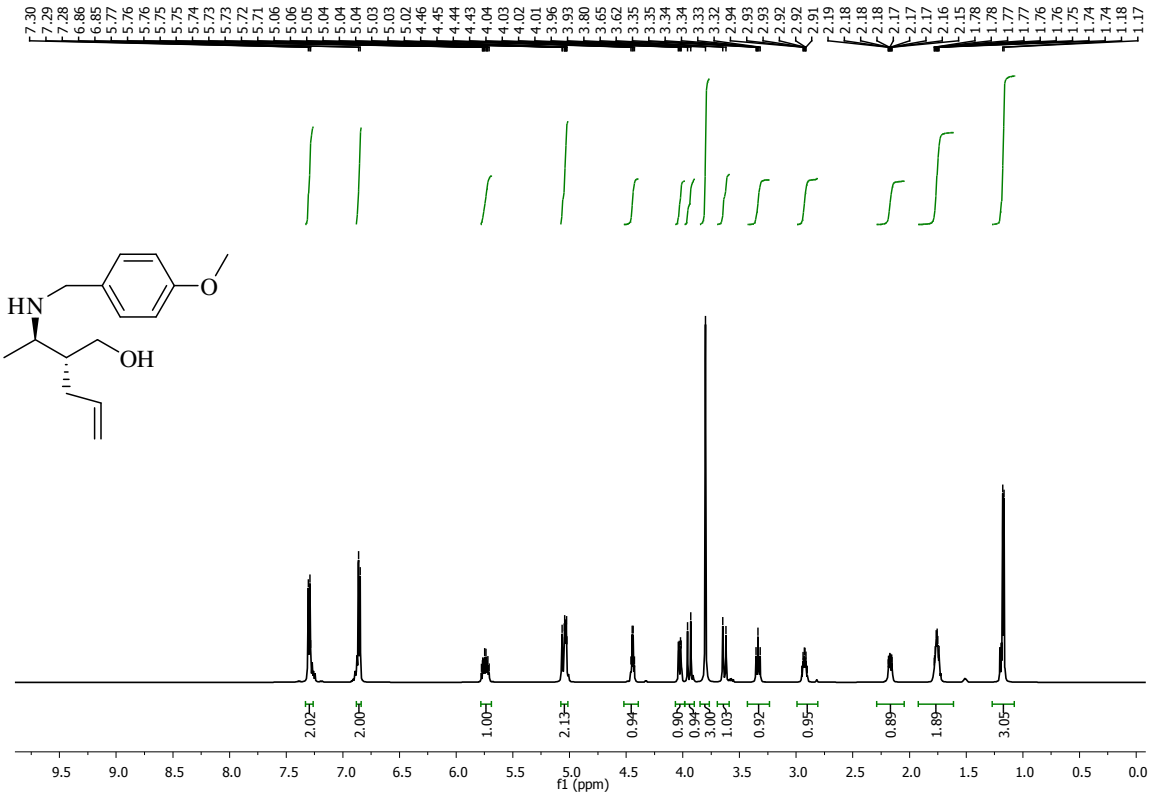

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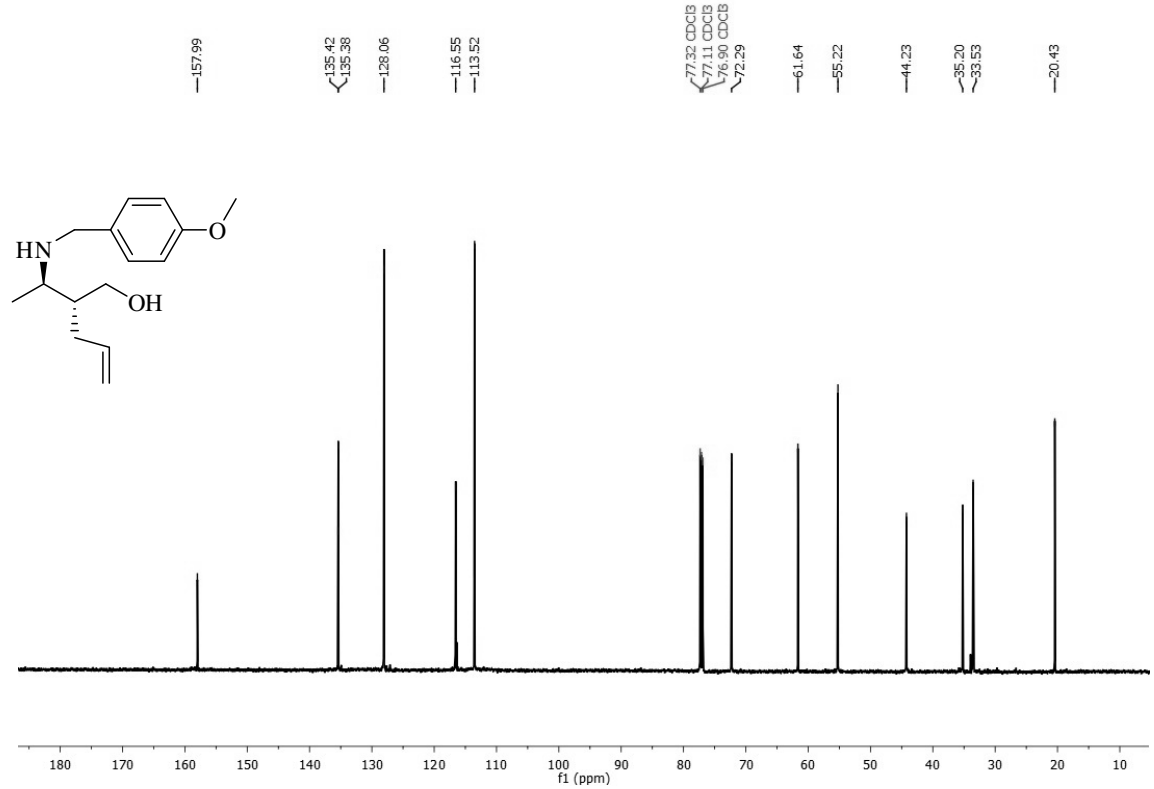
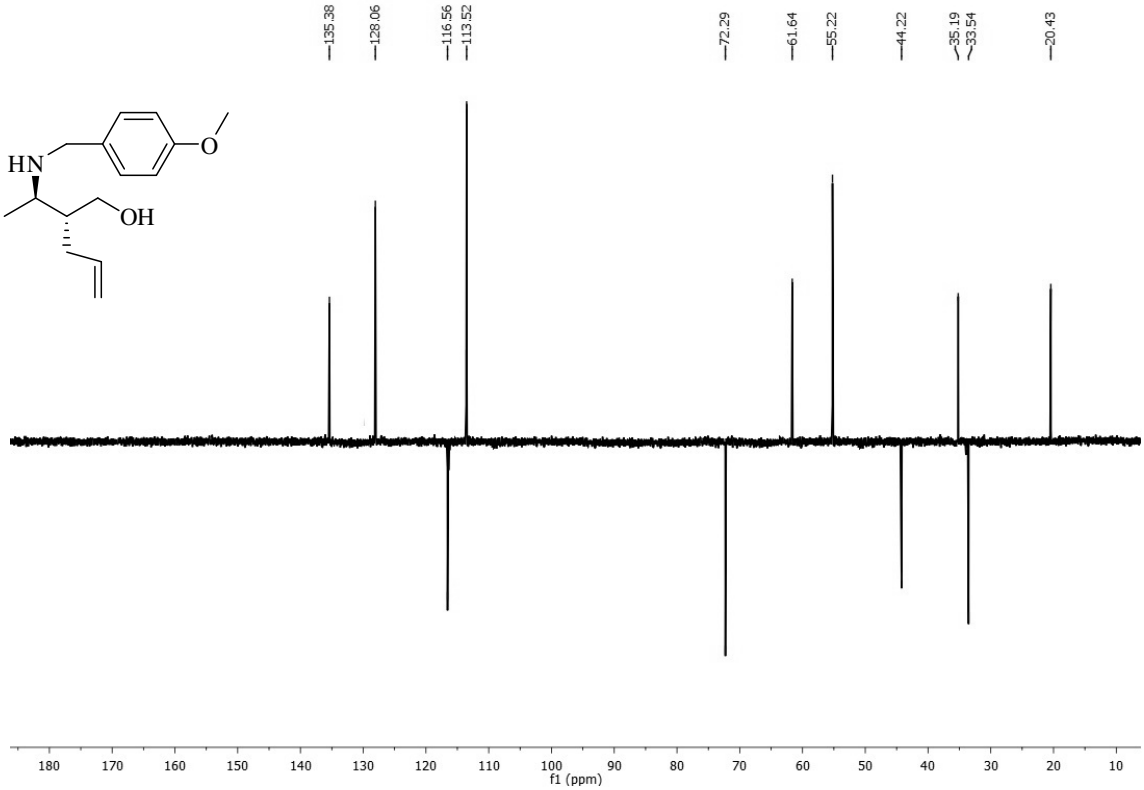
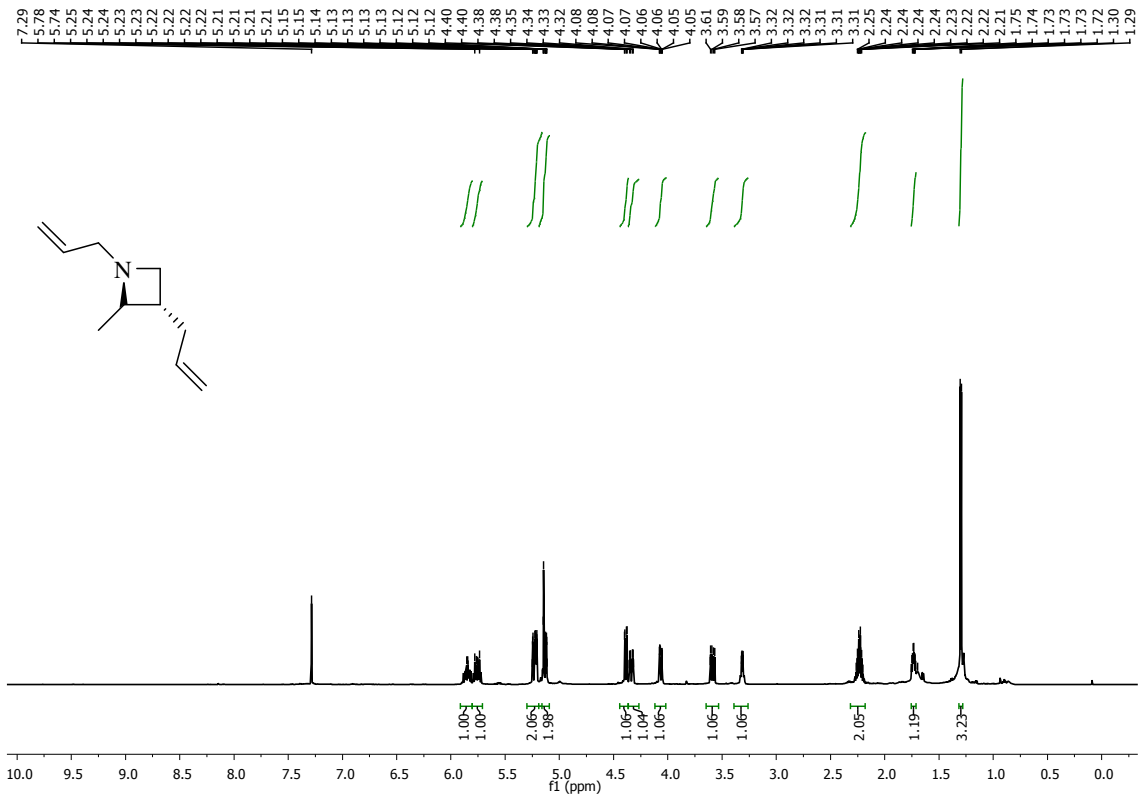


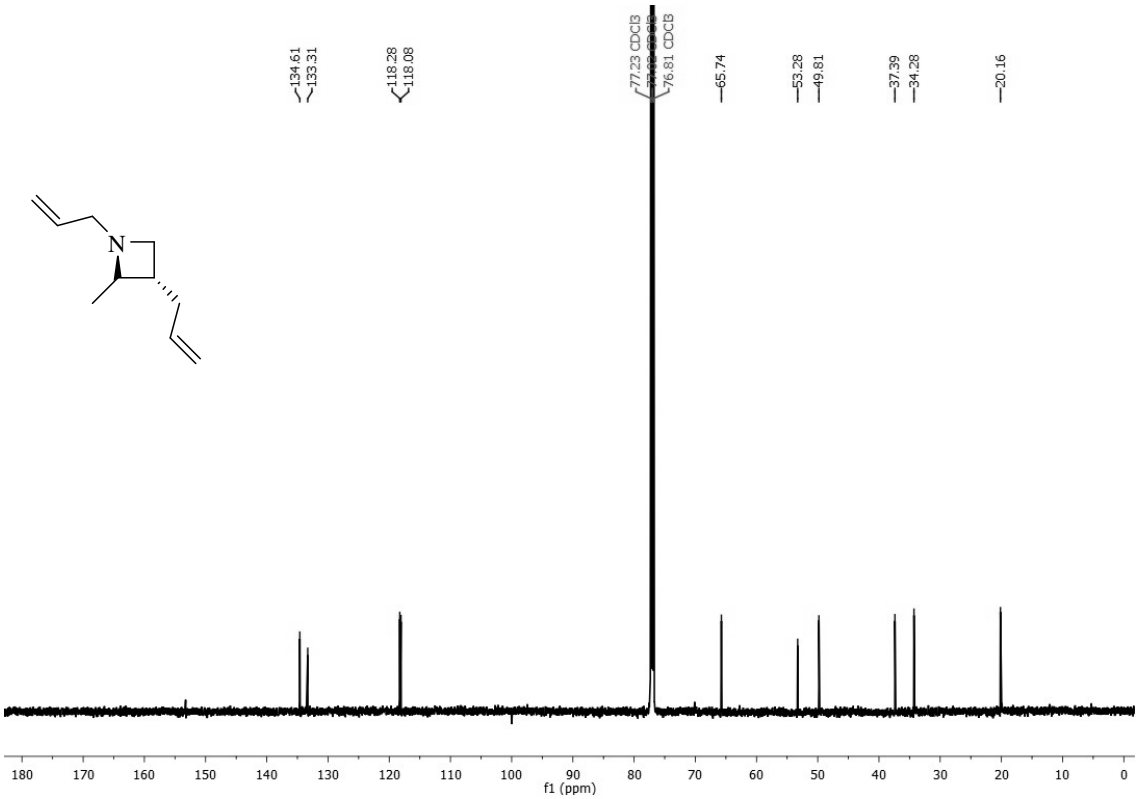
DEPT-135 NMR of compound 70 (150 MHz, $CDCl_3$)



^{1}H - NMR of compound 71 (600 MHz, $CDCl_3$)



^{13}C NMR of compound 71 (150 MHz, $CDCl_3$)



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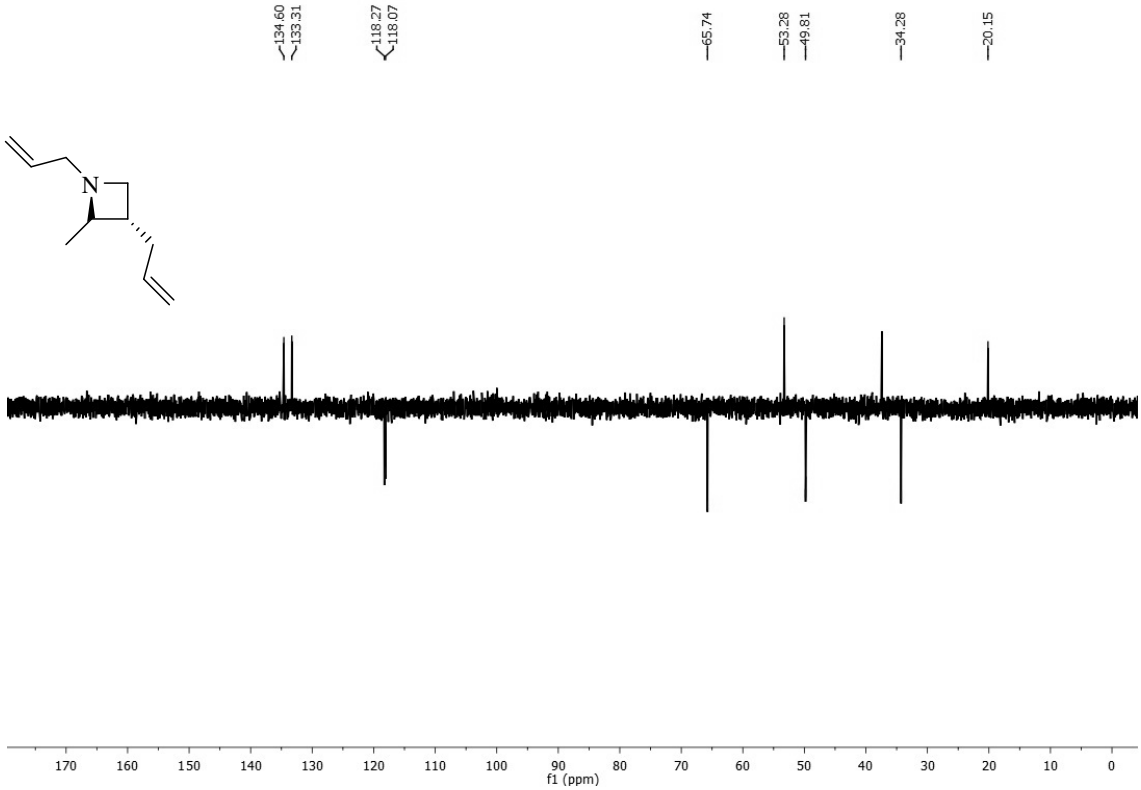
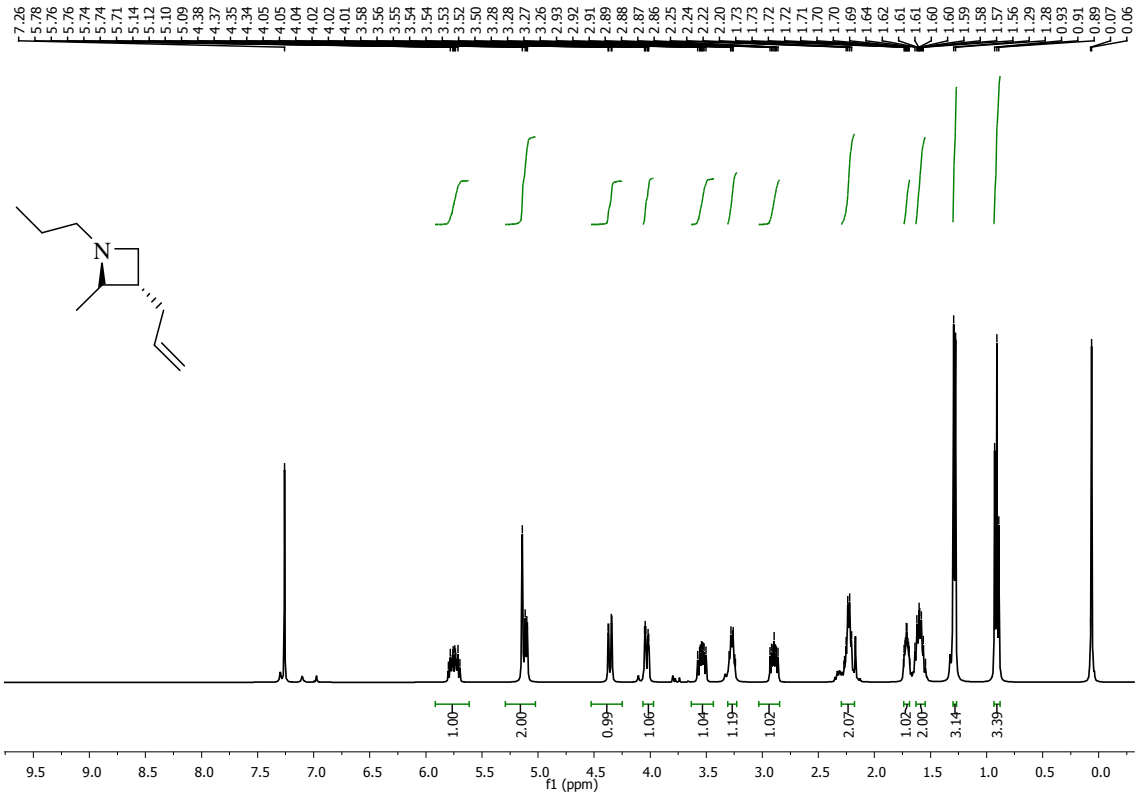
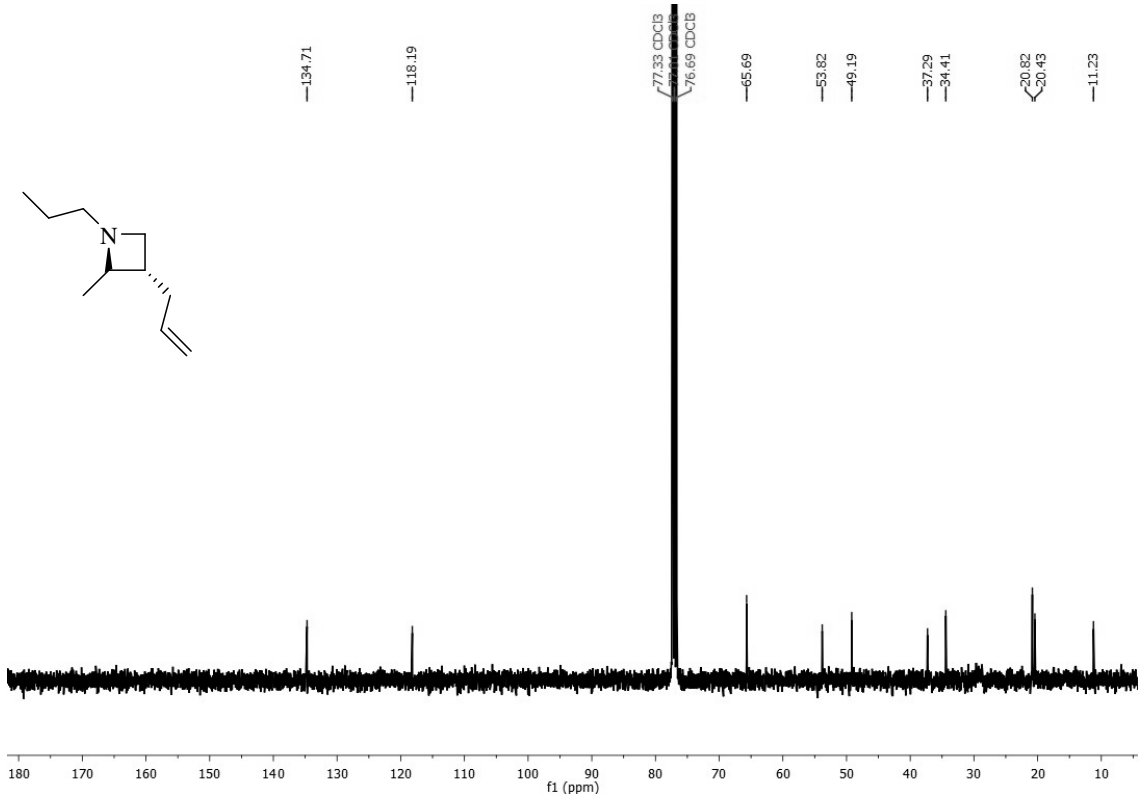


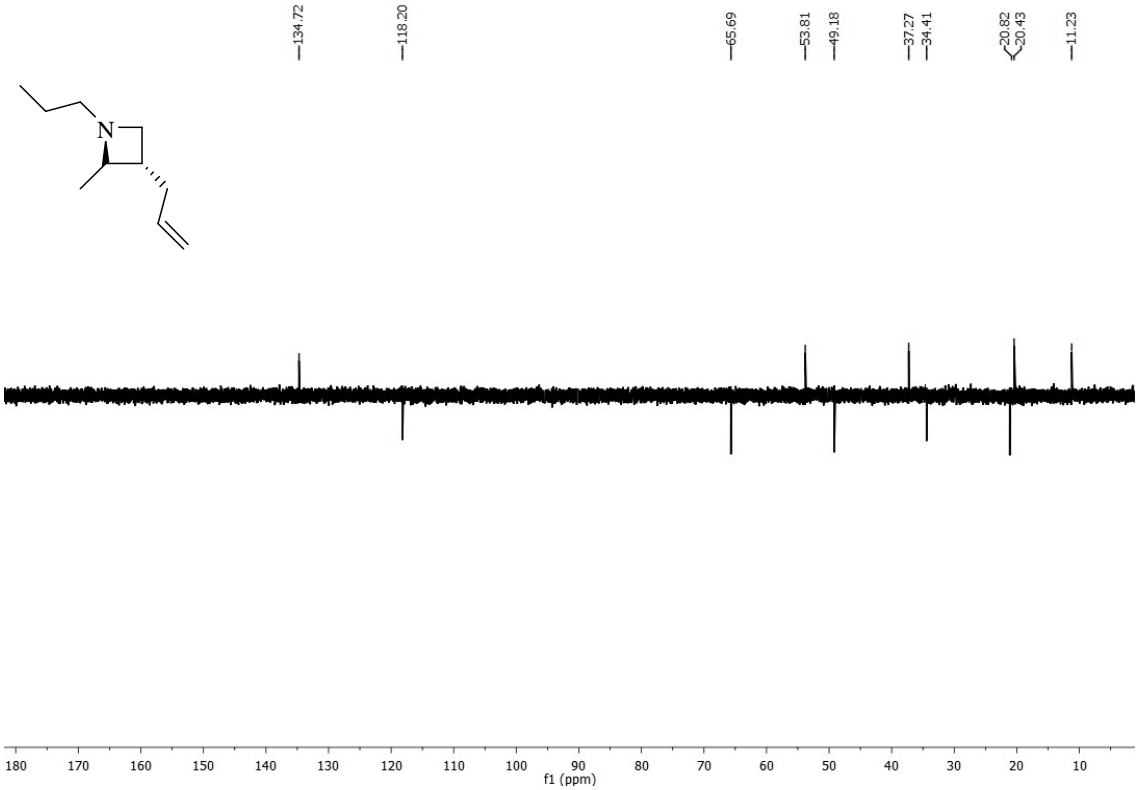
^{1}H - NMR of compound 72 (400 MHz, $CDCl_3$)



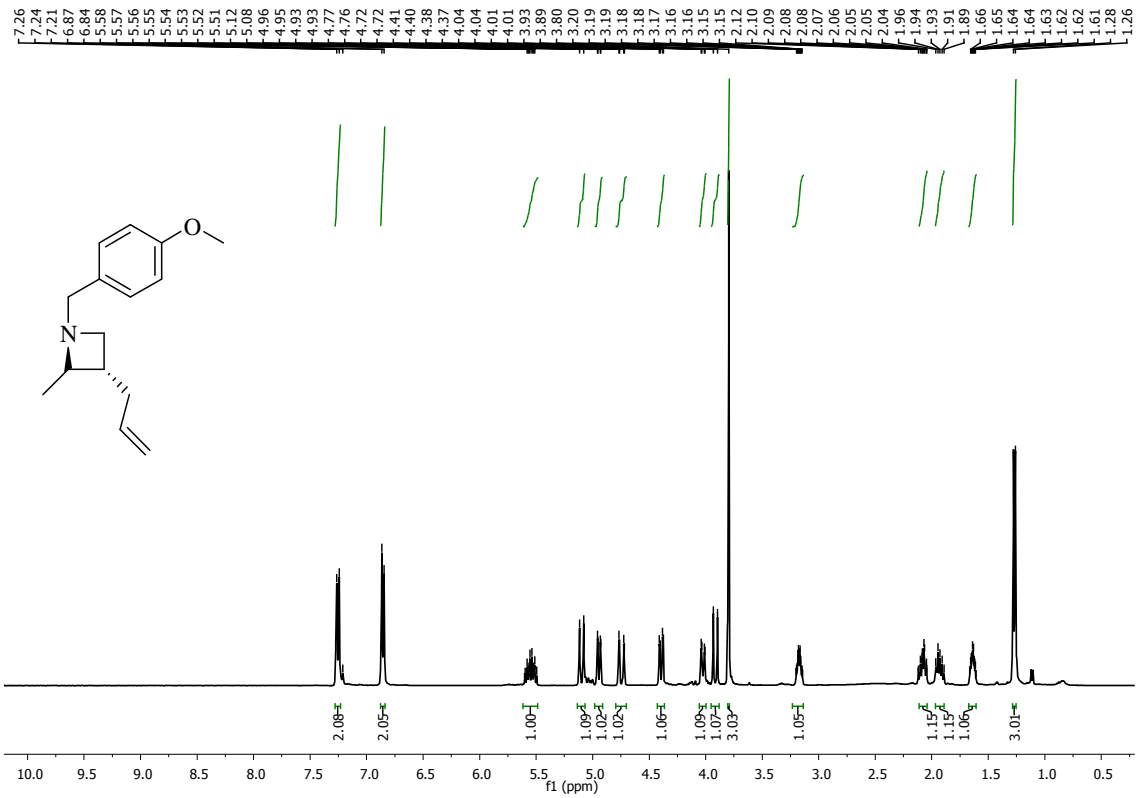
^{13}C NMR of compound 72 (100 MHz, $CDCl_3$)



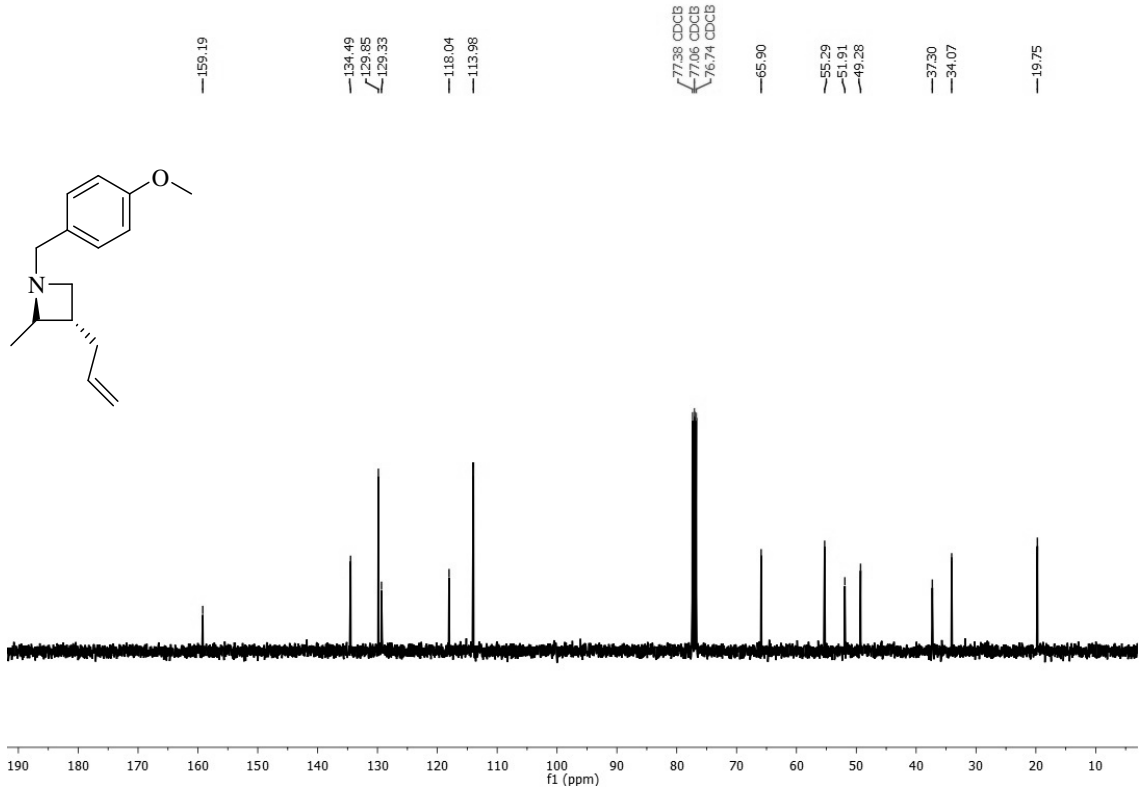
DEPT-135 NMR of compound 72 (125 MHz, $CDCl_3$)



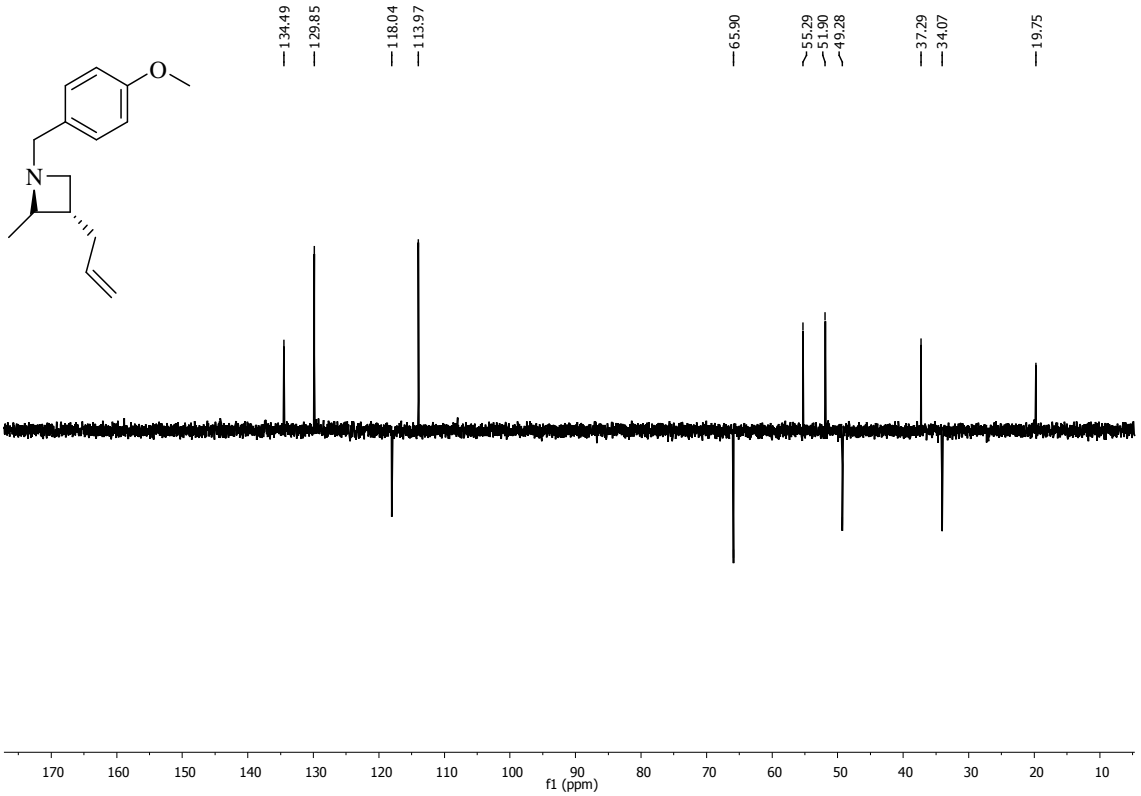
^{1}H - NMR of compound 73 (400 MHz, $CDCl_3$)



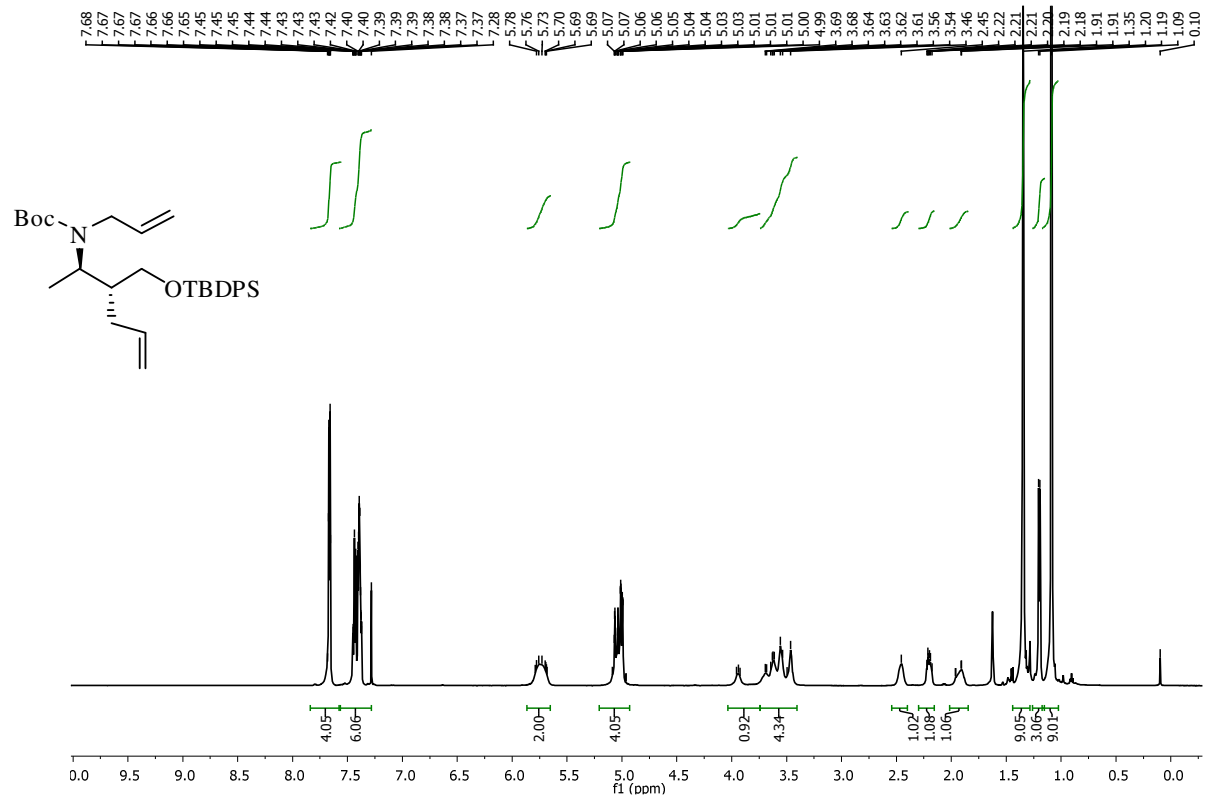
^{13}C NMR of compound 73 (100 MHz, $CDCl_3$)



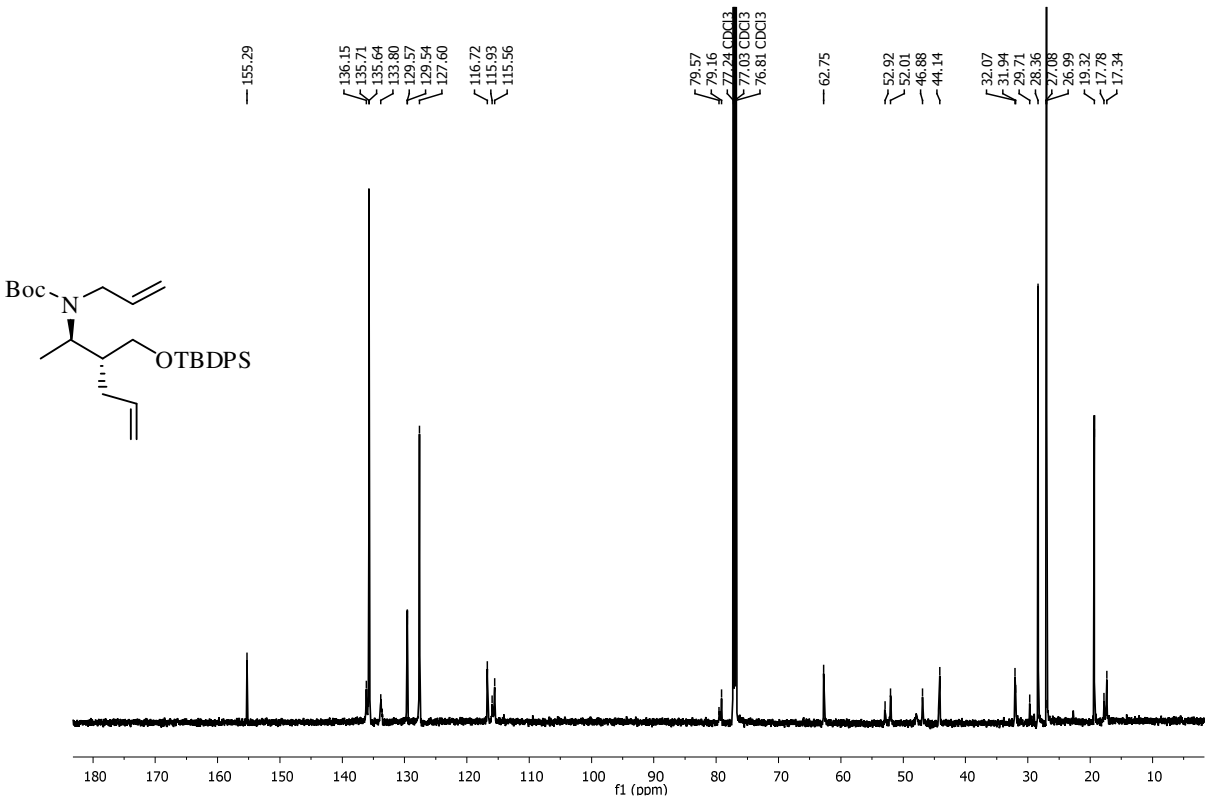
DEPT-135 NMR of compound 73 (100 MHz, $CDCl_3$)



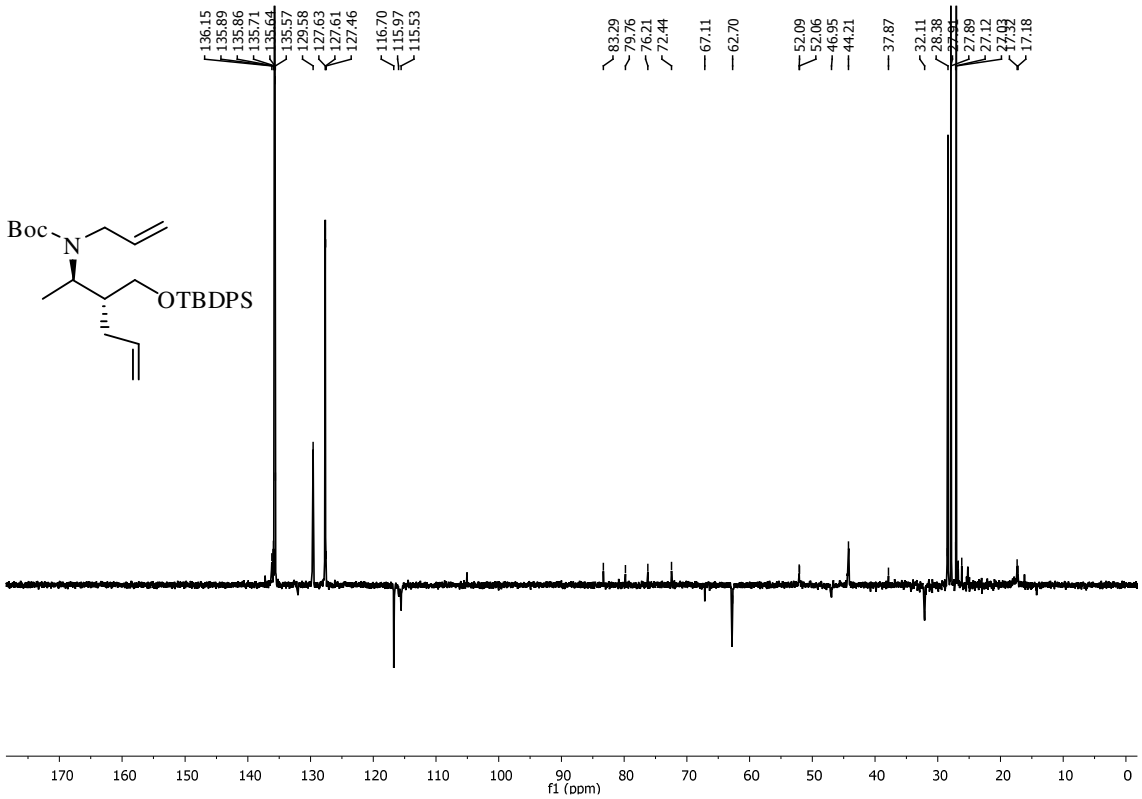
^{1}H - NMR of compound 74 (600 MHz, $CDCl_3$)



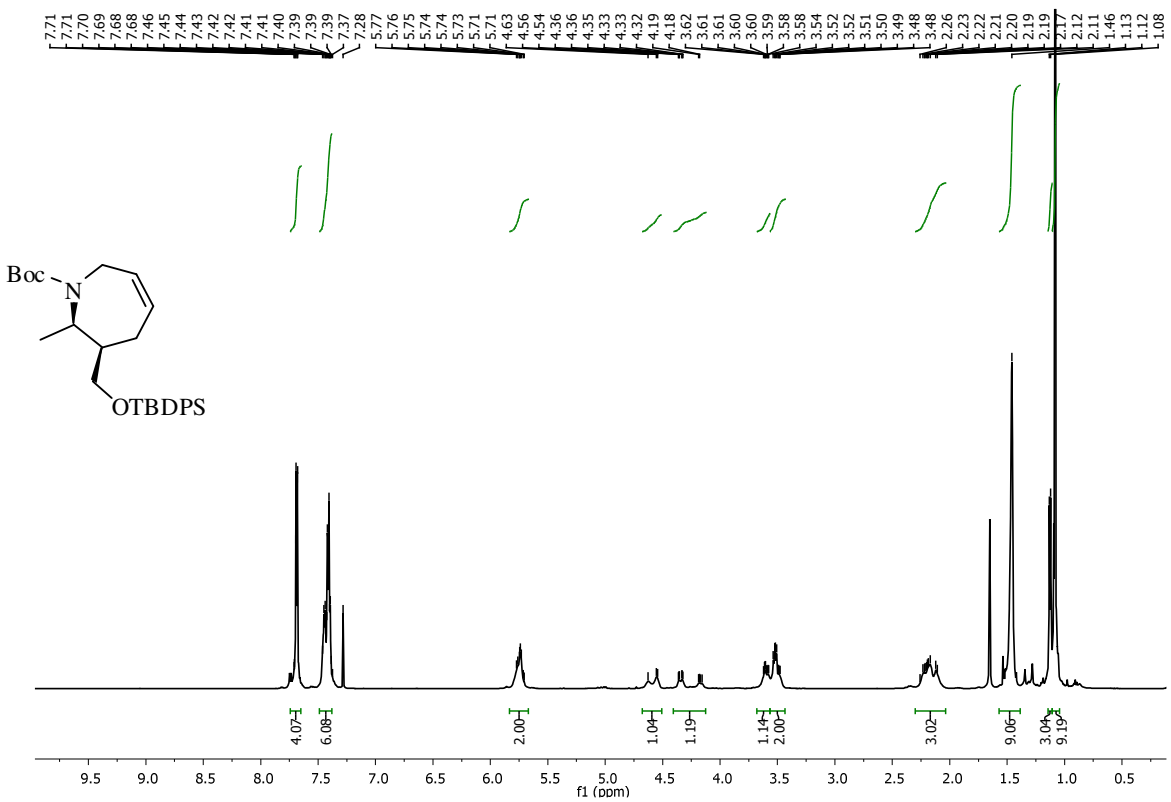
^{13}C NMR of compound 74 (150 MHz, $CDCl_3$)



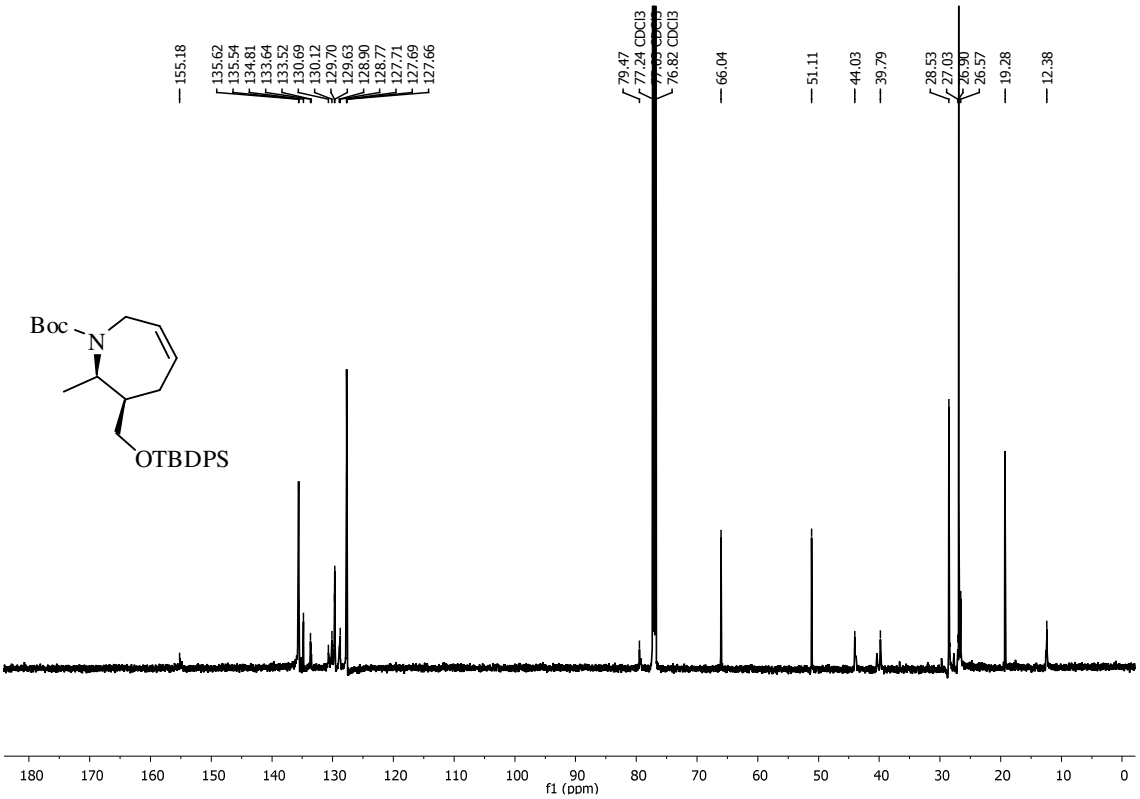
DEPT-135 NMR of compound 74 (150 MHz, $CDCl_3$)



^{1}H - NMR of compound 75 (600 MHz, $CDCl_3$)



^{13}C NMR of compound 75 (150 MHz, $CDCl_3$)



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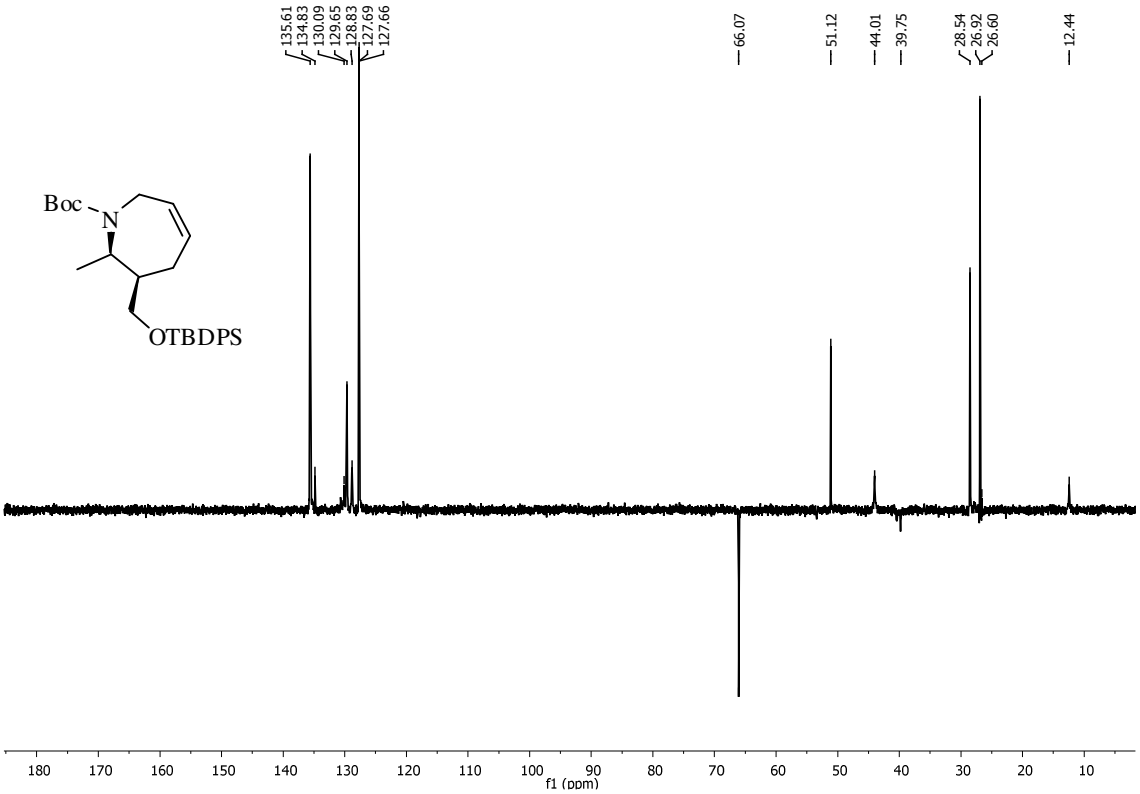
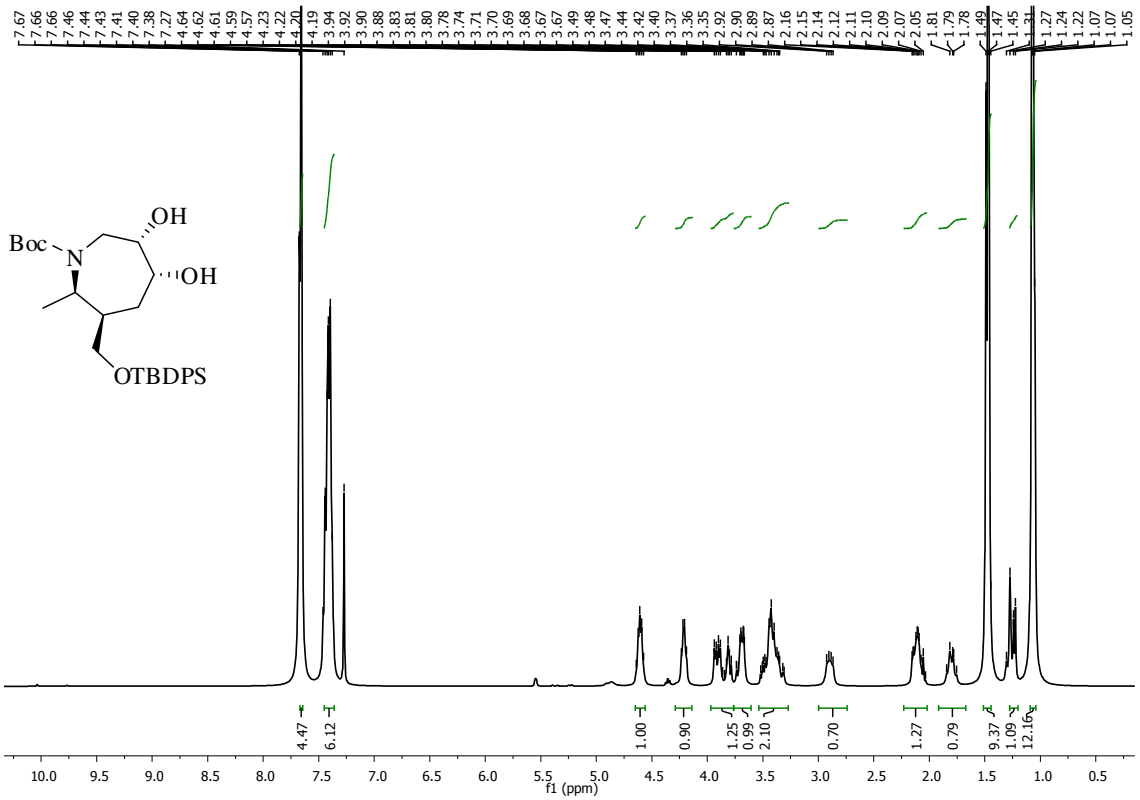
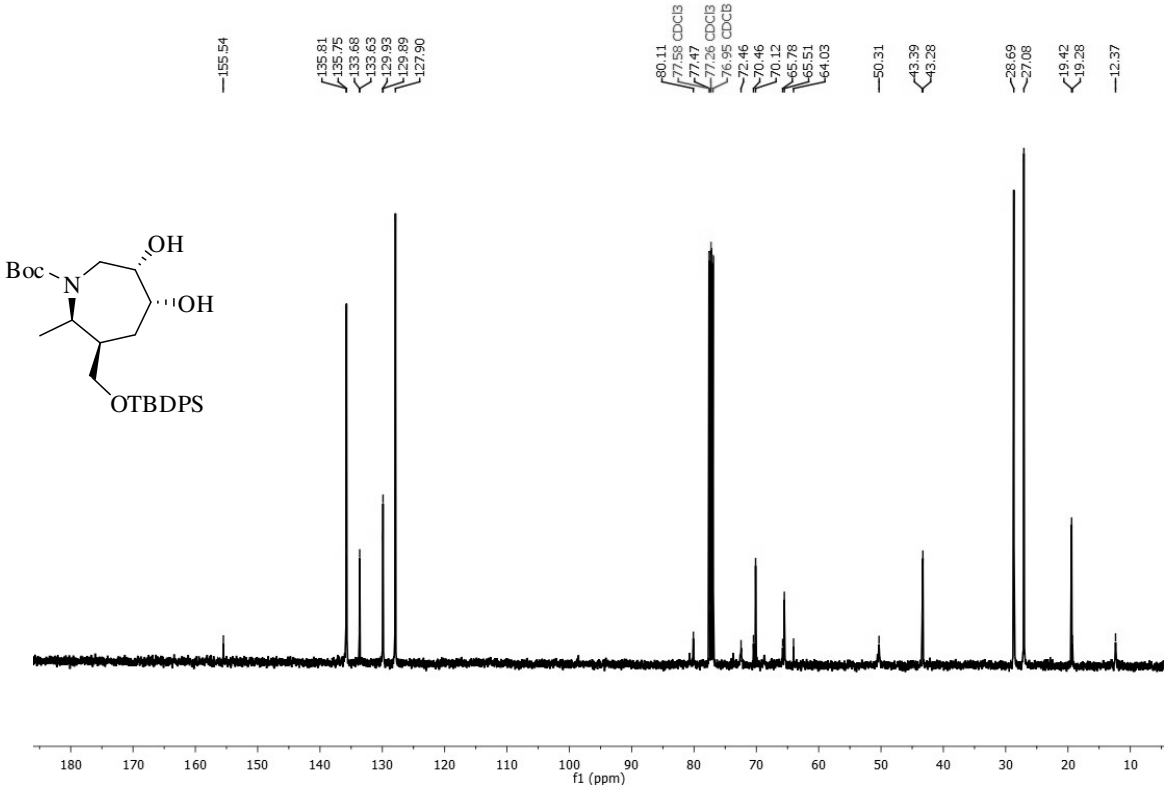


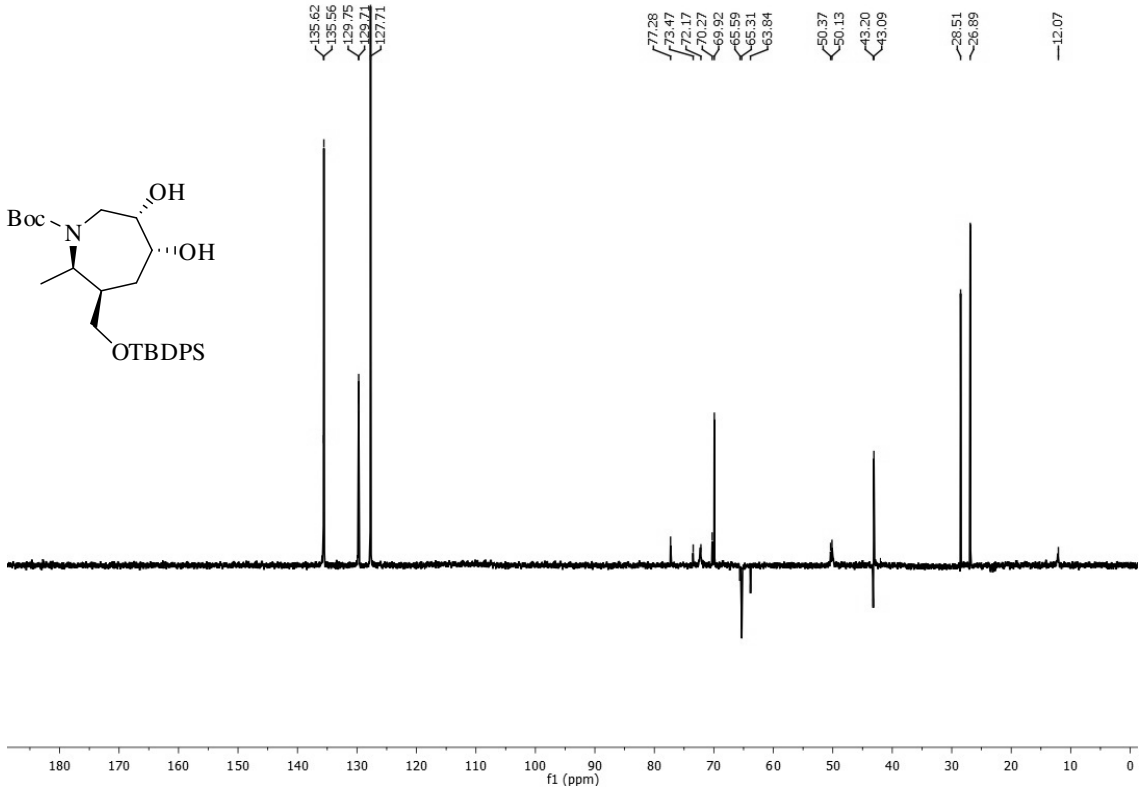
^{1}H - NMR of compound 76 (400 MHz, $CDCl_3$)



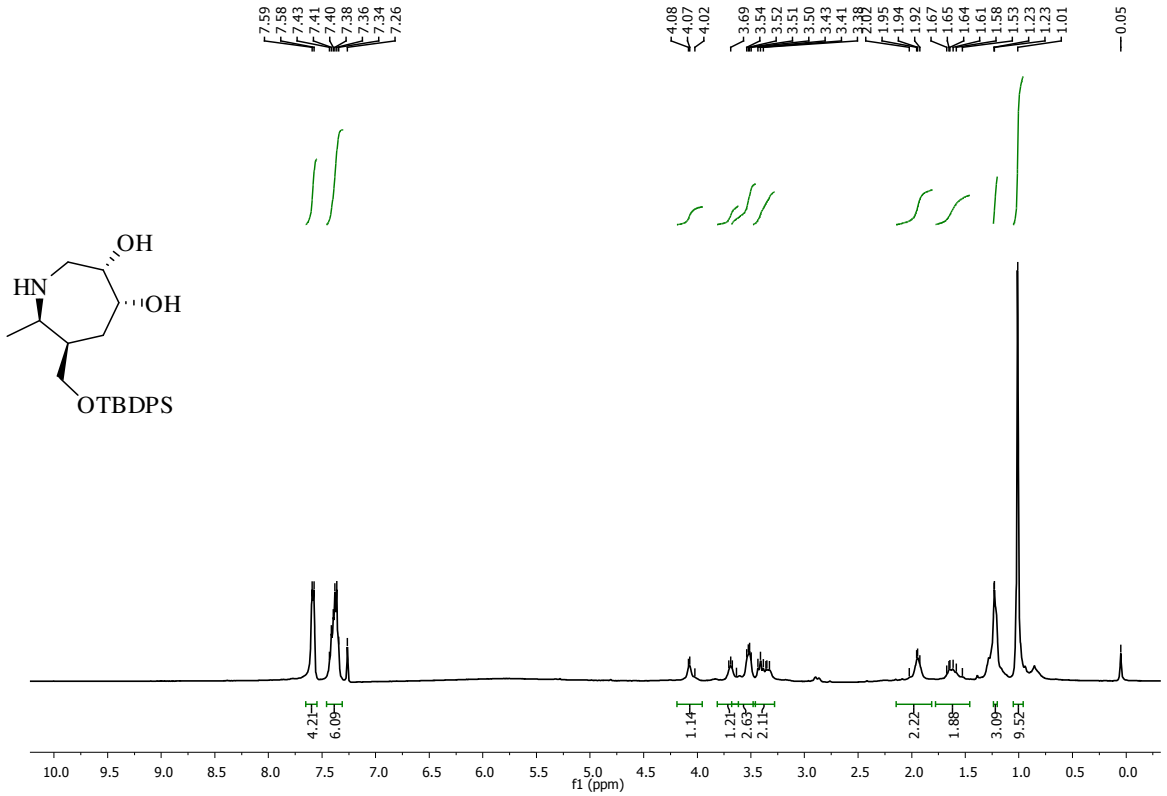
^{13}C NMR of compound 76 (100 MHz, $CDCl_3$)



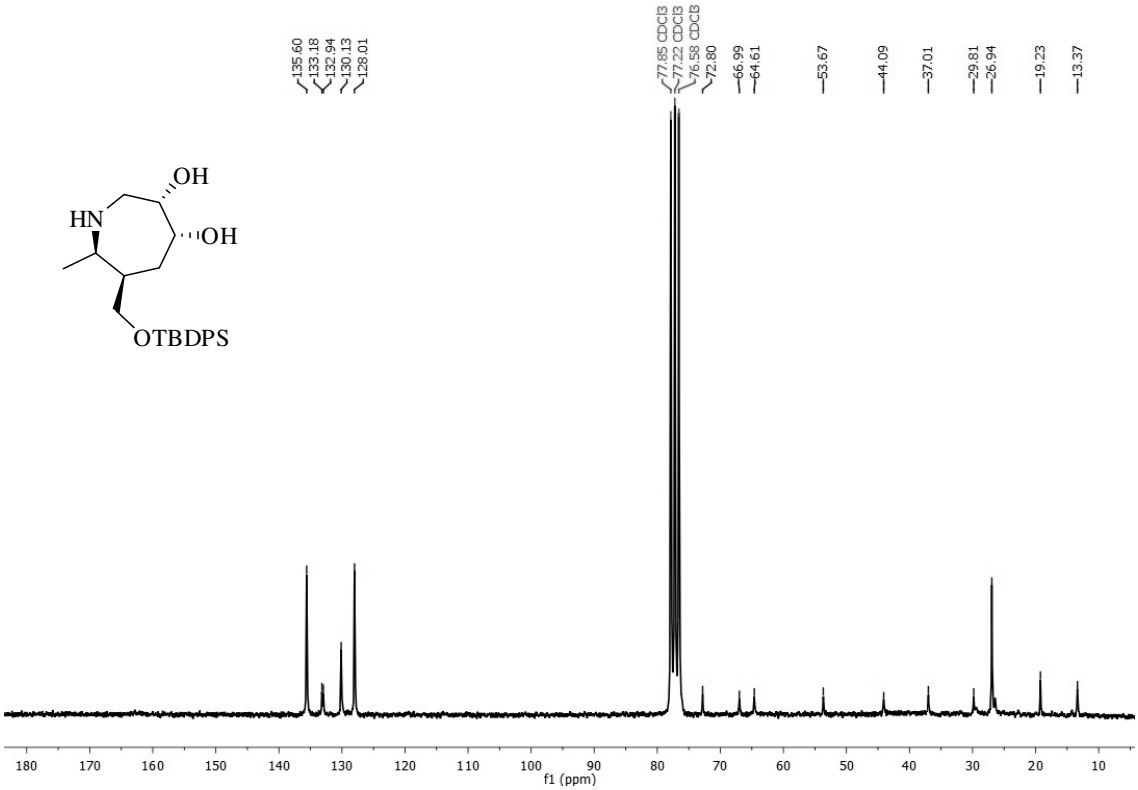
DEPT-135 NMR of compound 76 (100 MHz, $CDCl_3$)



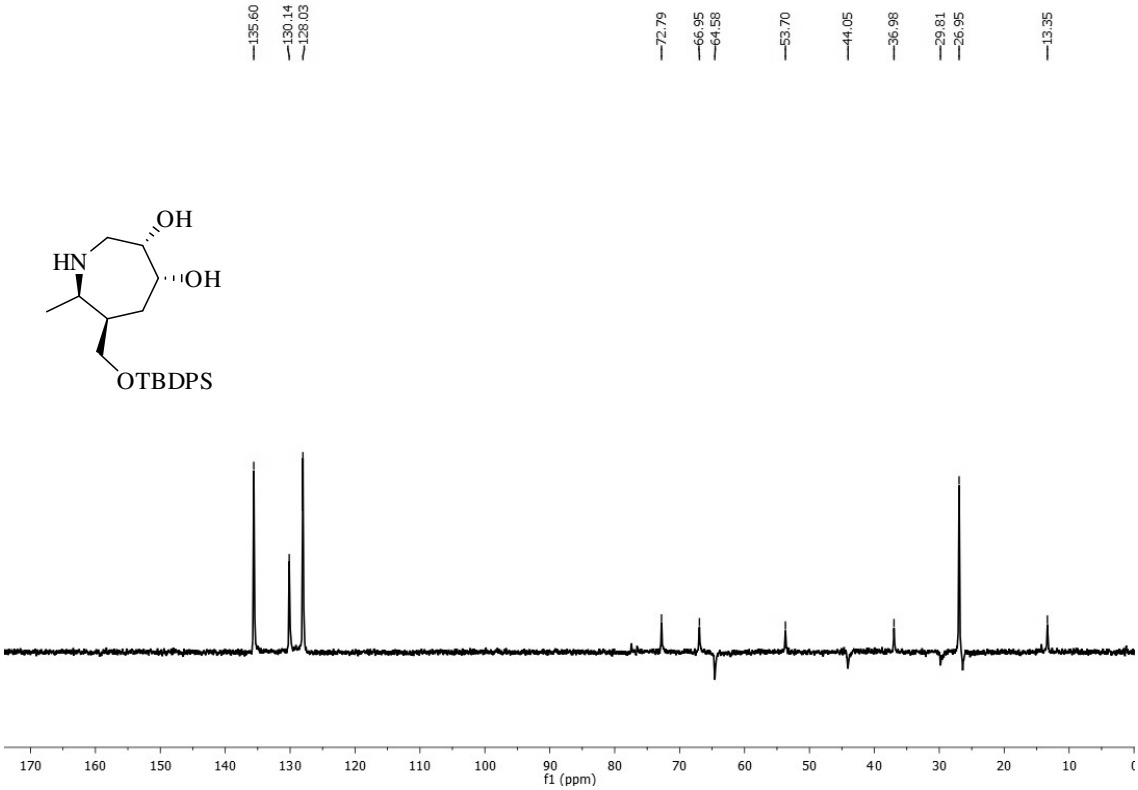
^{1}H - NMR of compound 77 (400 MHz, $CDCl_3$)



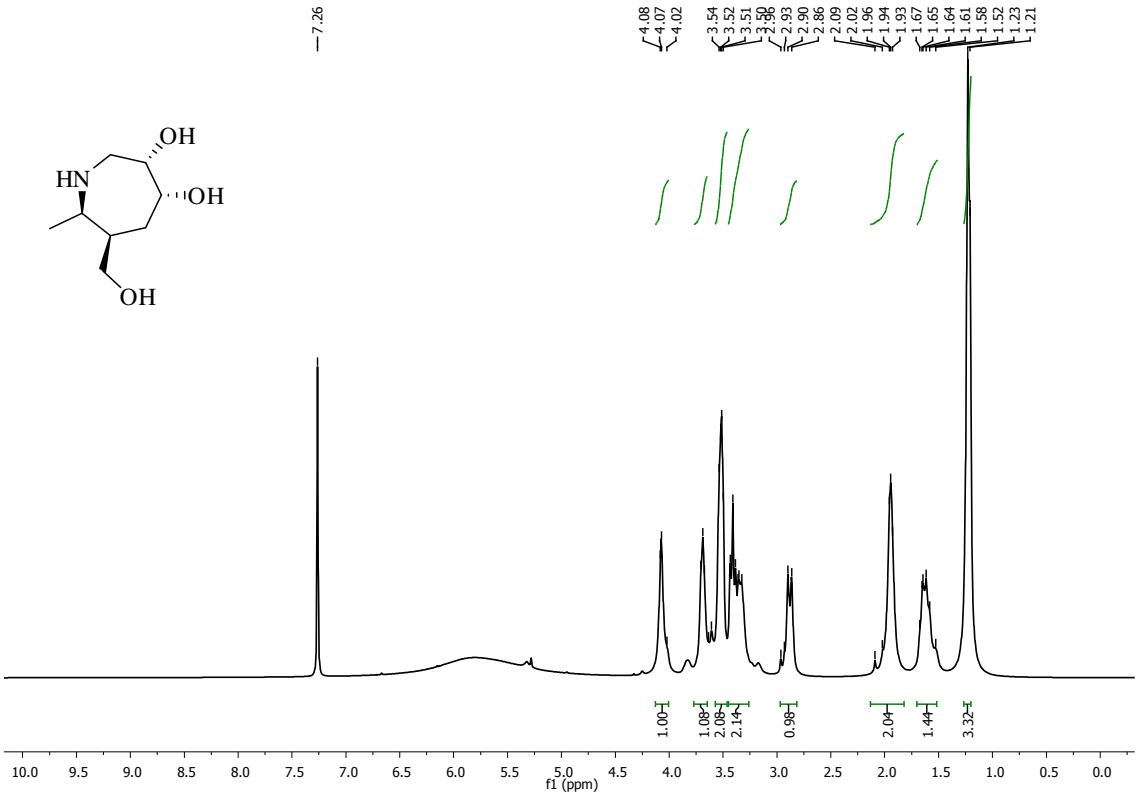
^{13}C NMR of compound 77 (50 MHz, $CDCl_3$)



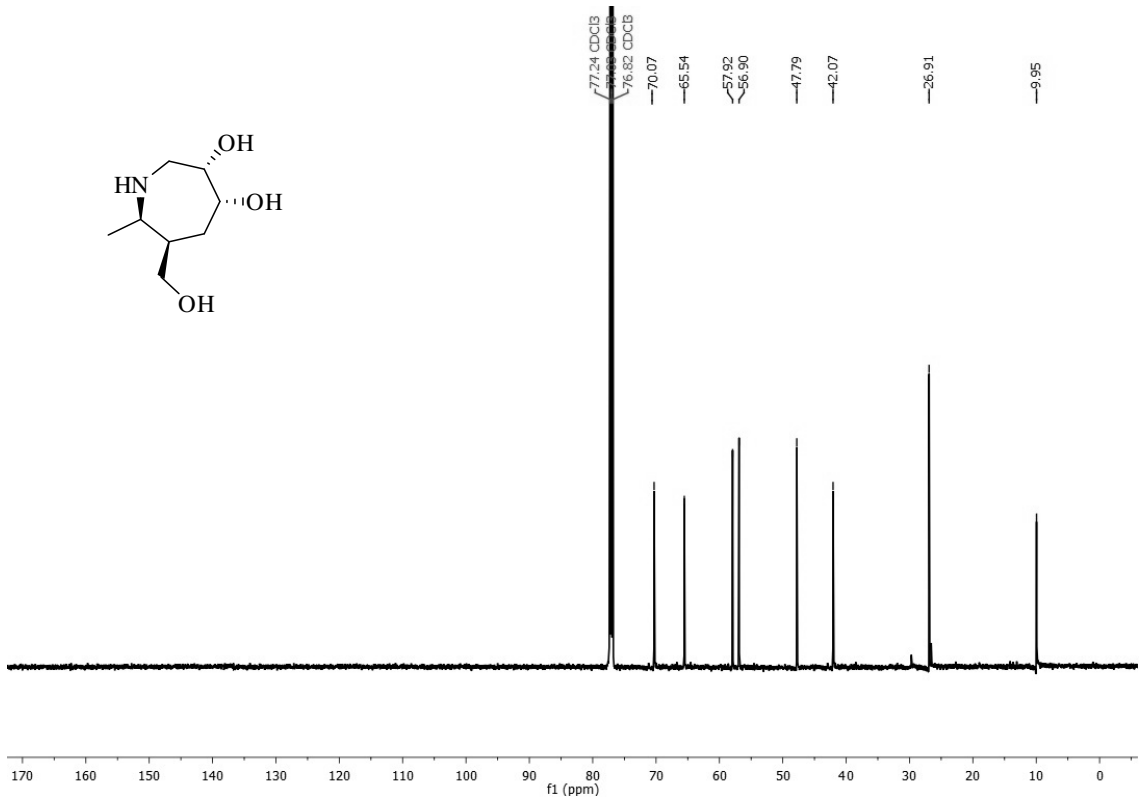
DEPT-135 NMR of compound 77 (50 MHz, $CDCl_3$)



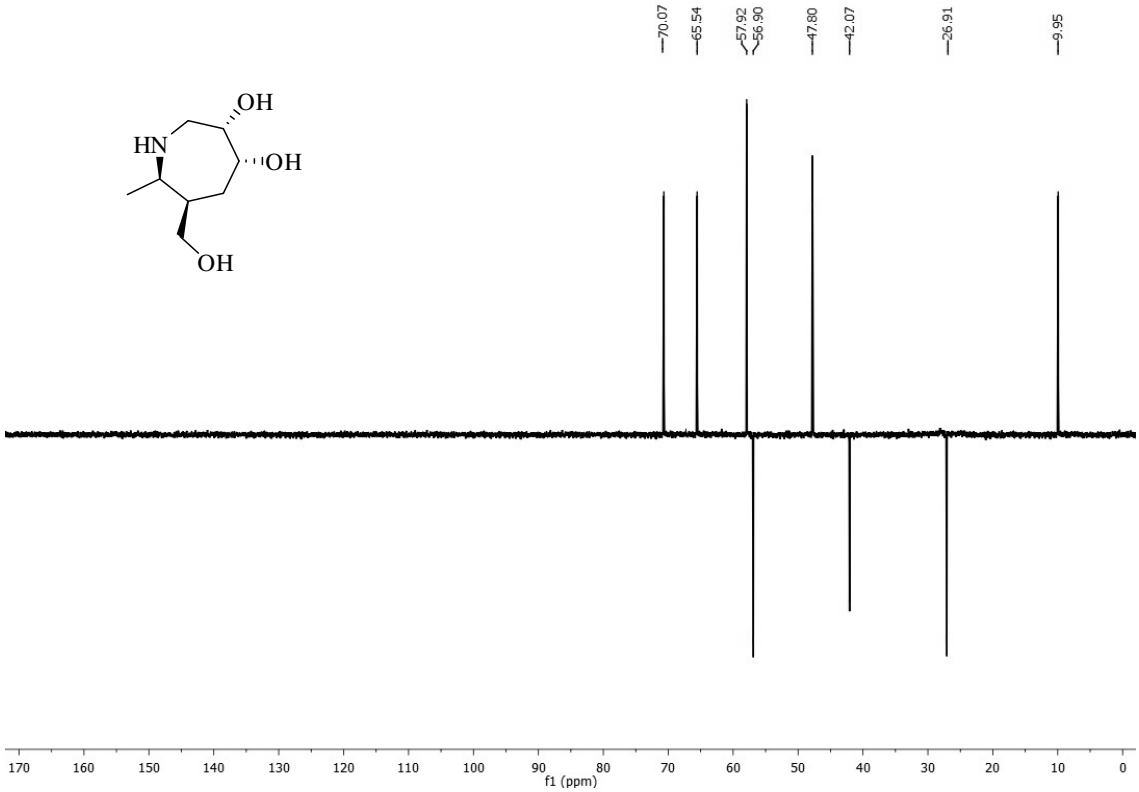
^{1}H - NMR of compound 78 (400 MHz, $CDCl_3$)



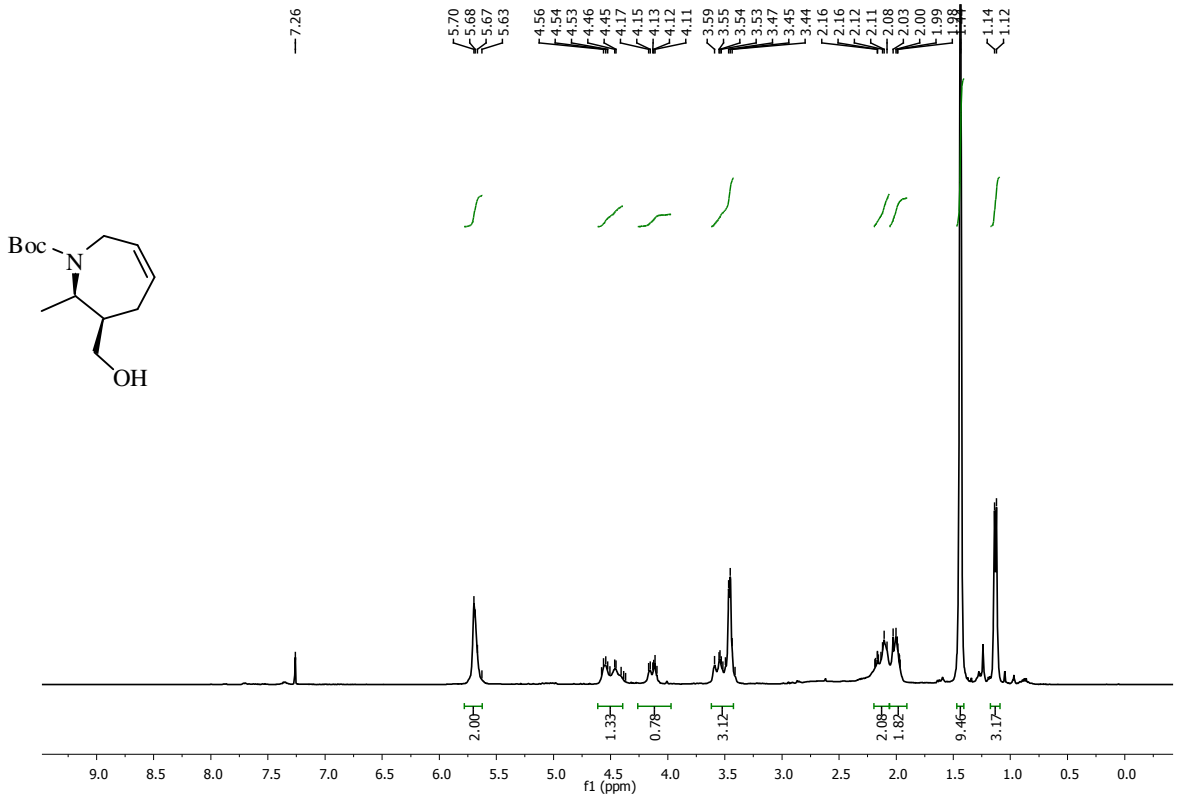
^{13}C NMR of compound 78 (150 MHz, $CDCl_3$)



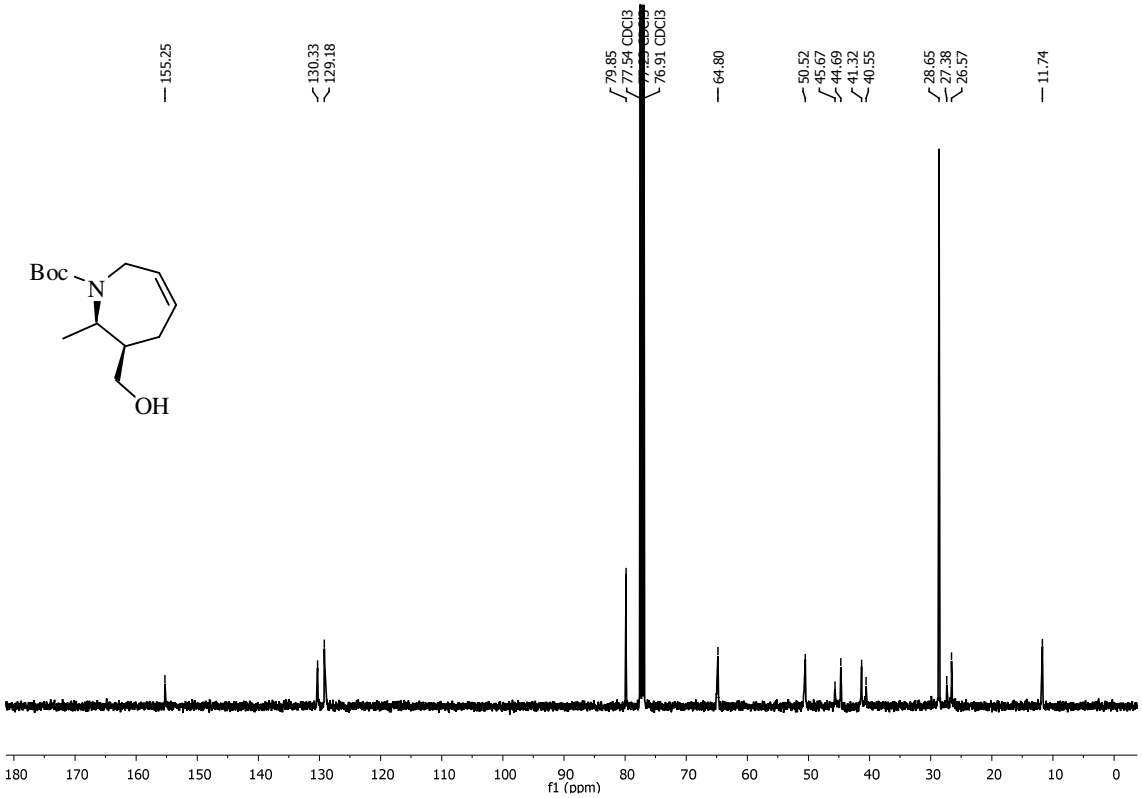
DEPT-135 NMR of compound 78 (150 MHz, $CDCl_3$)



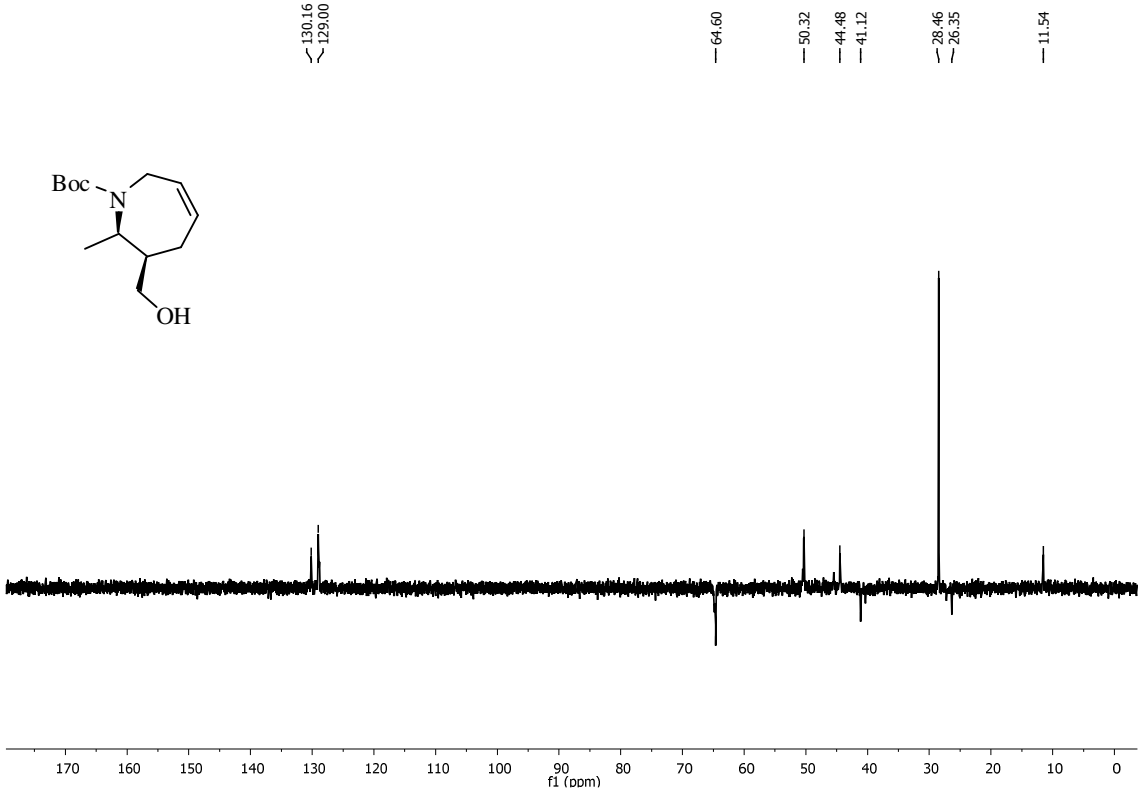
^{1}H - NMR of compound 79 (400 MHz, $CDCl_3$)



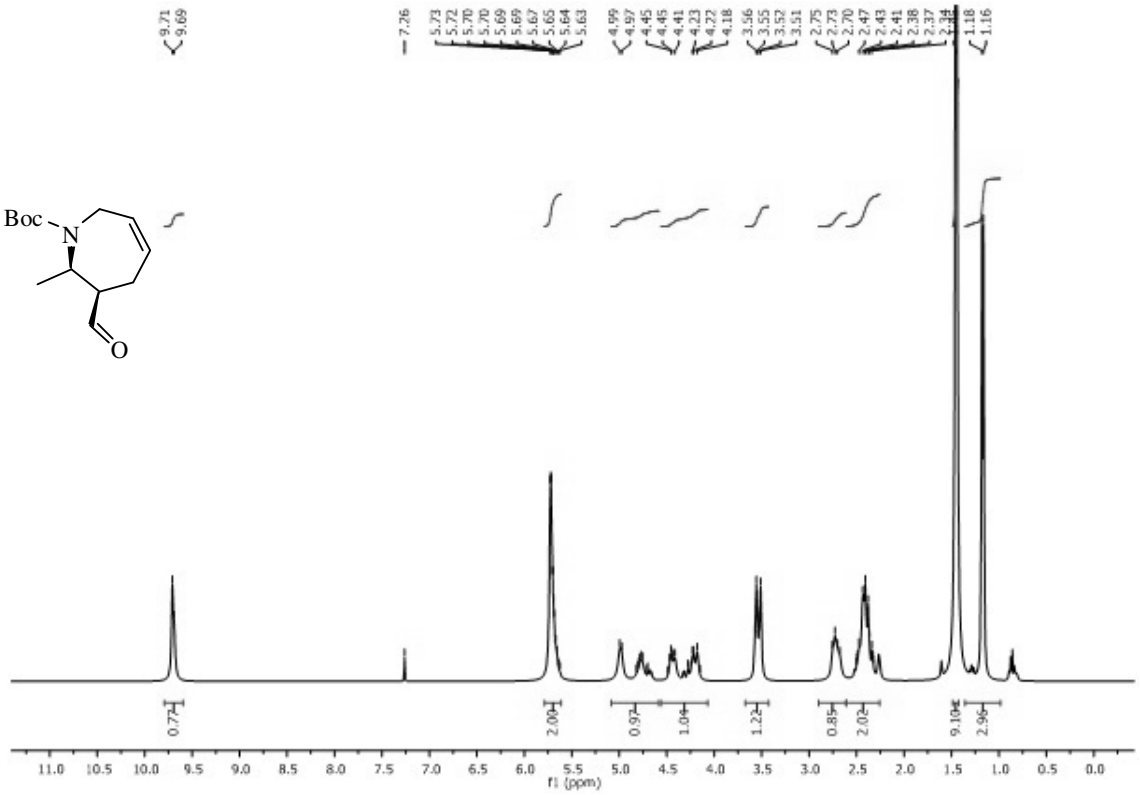
^{13}C NMR of compound 79 (100 MHz, $CDCl_3$)



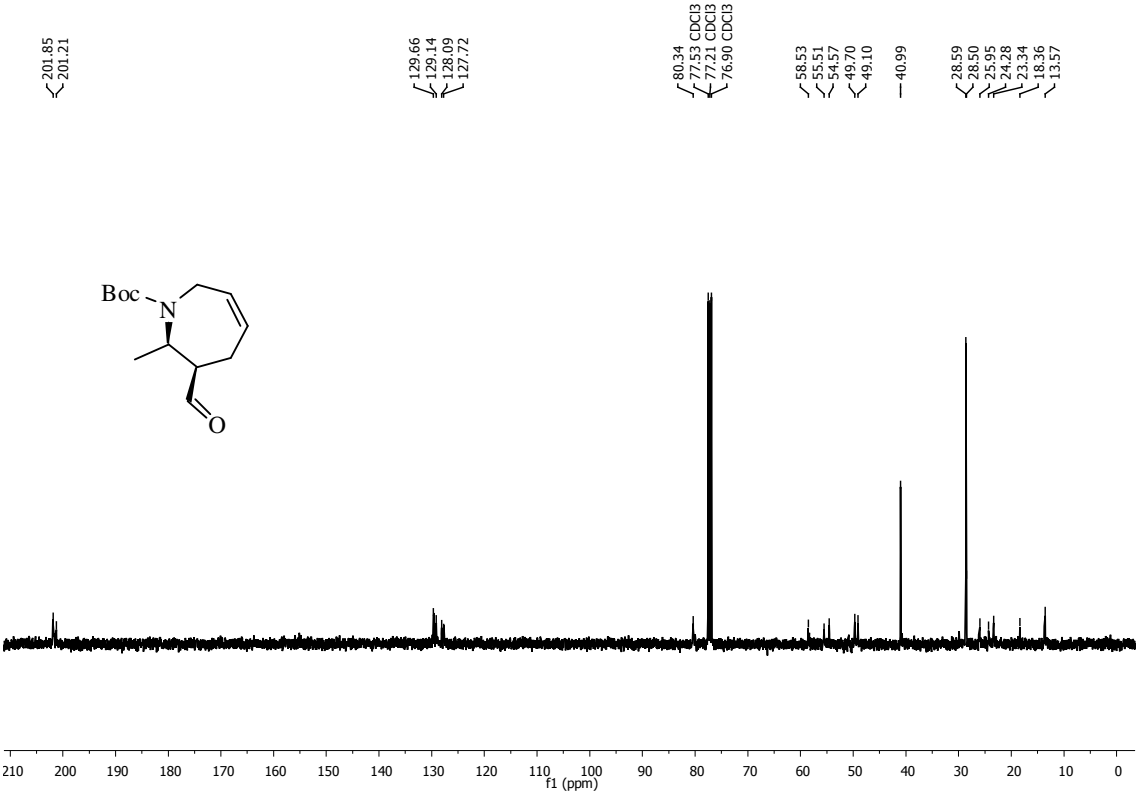
DEPT-135 NMR of compound 79 (100 MHz, $CDCl_3$)



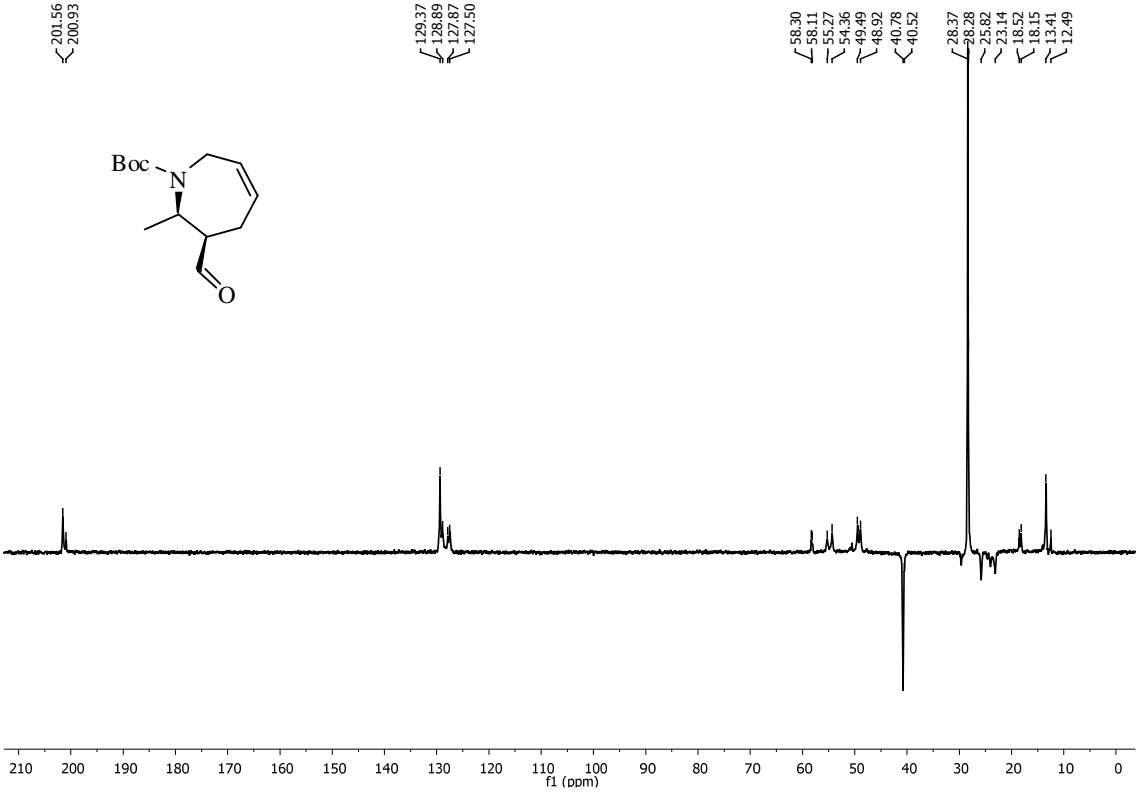
^{1}H - NMR of compound 80 (400 MHz, $CDCl_3$)



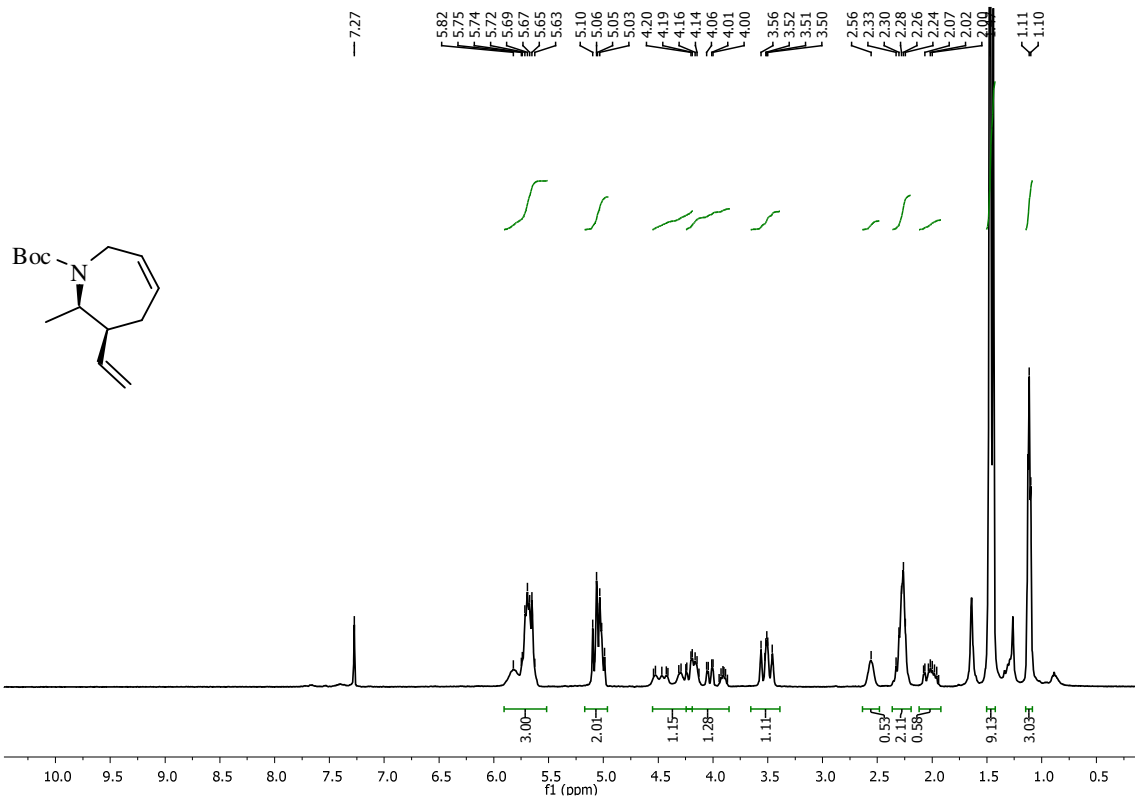
^{13}C NMR of compound 80 (100 MHz, $CDCl_3$)



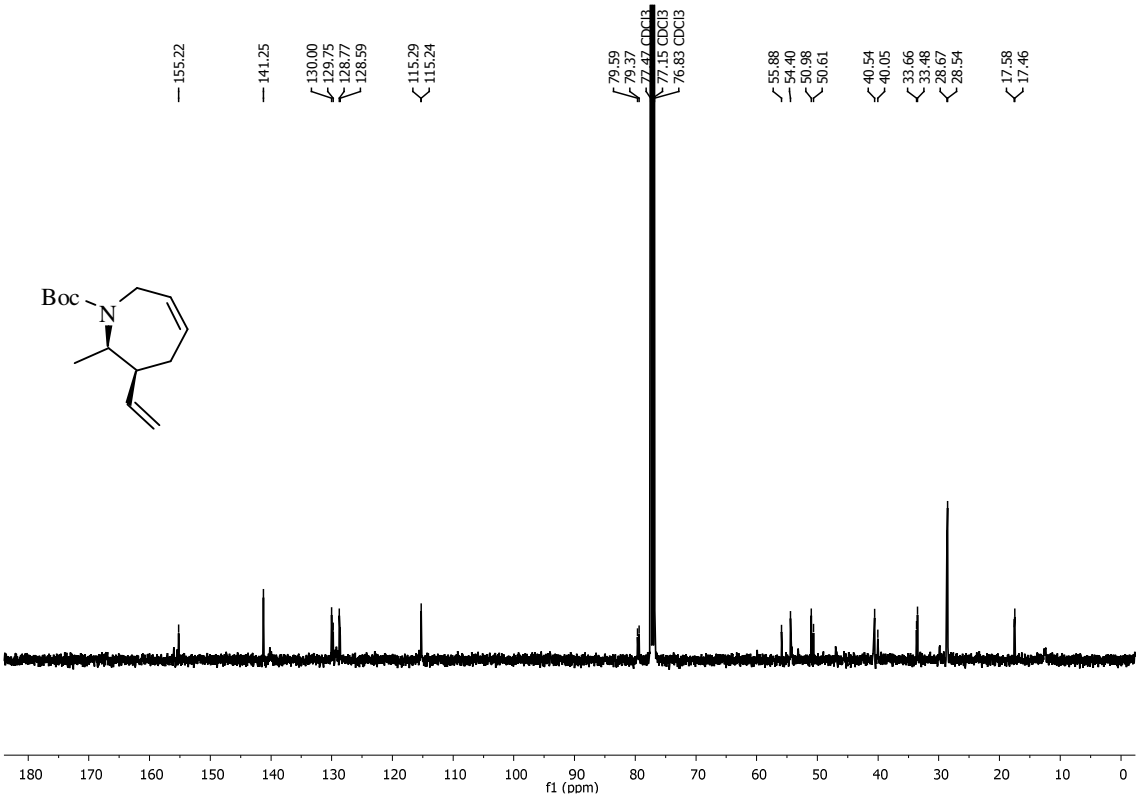
DEPT-135 NMR of compound 80 (50 MHz, $CDCl_3$)



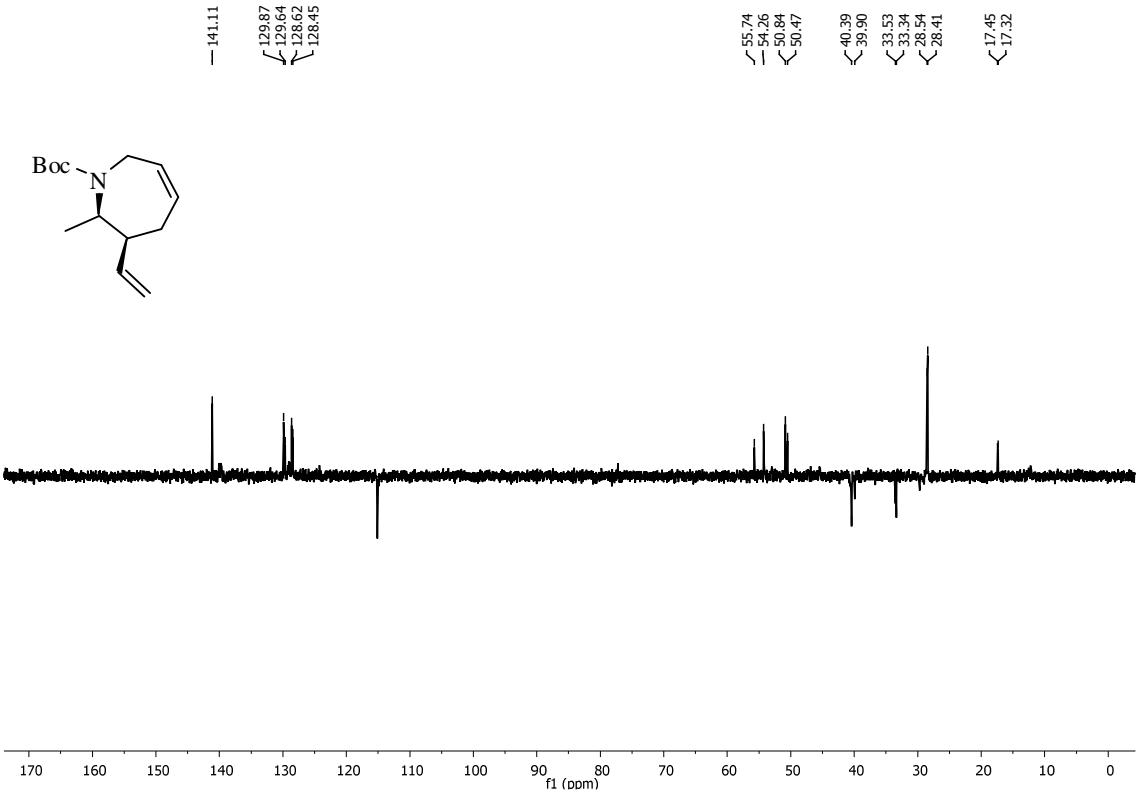
^{1}H - NMR of compound 81 (400 MHz, $CDCl_3$)



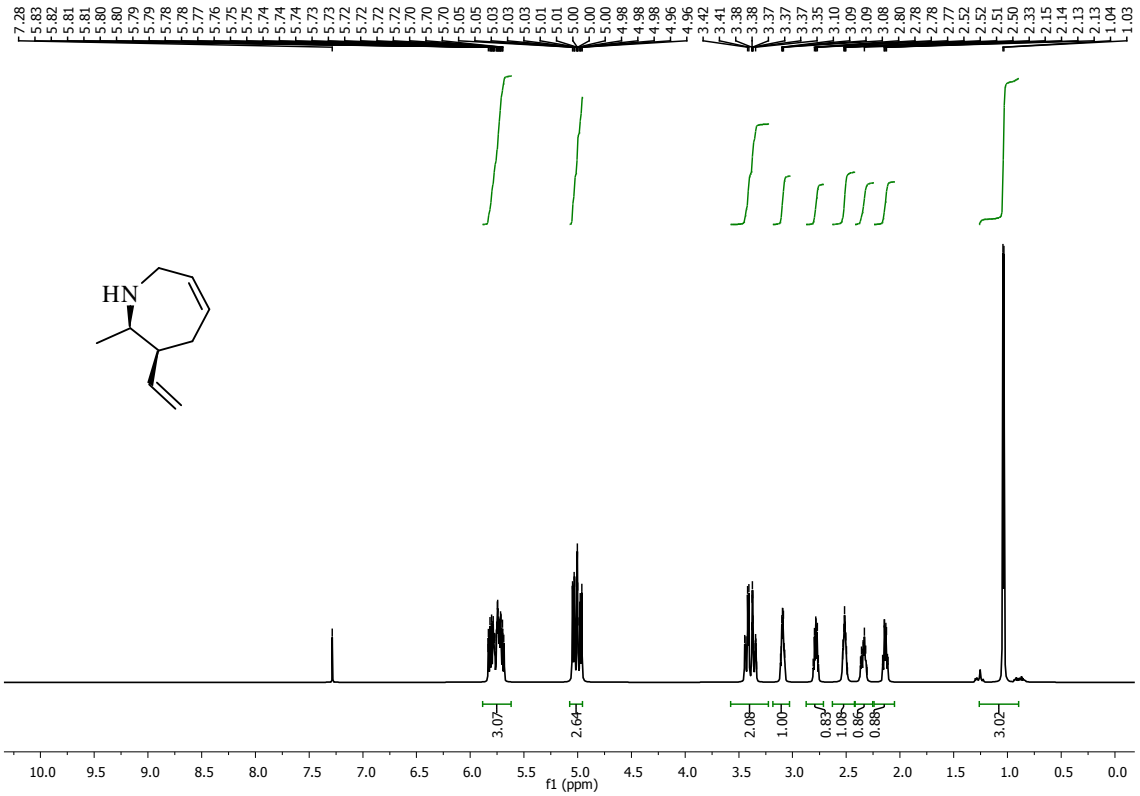
^{13}C NMR of compound 81 (100 MHz, $CDCl_3$)



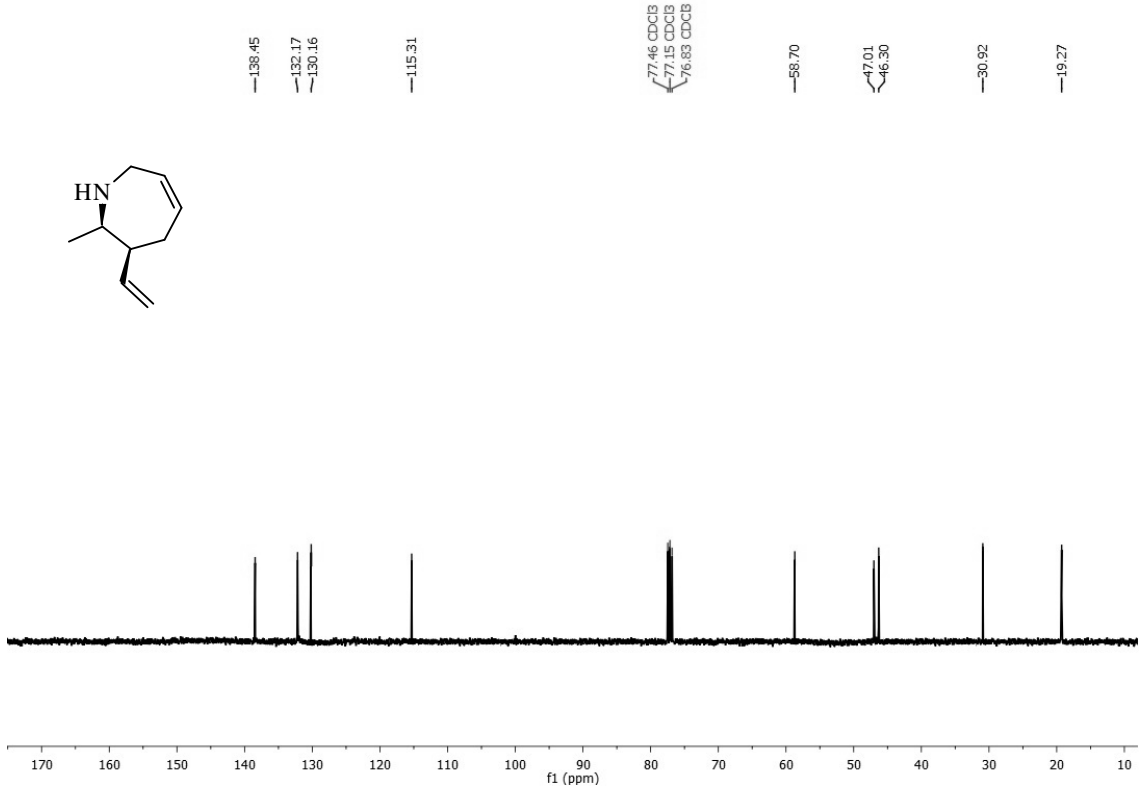
DEPT-135 NMR of compound 81 (100 MHz, $CDCl_3$)



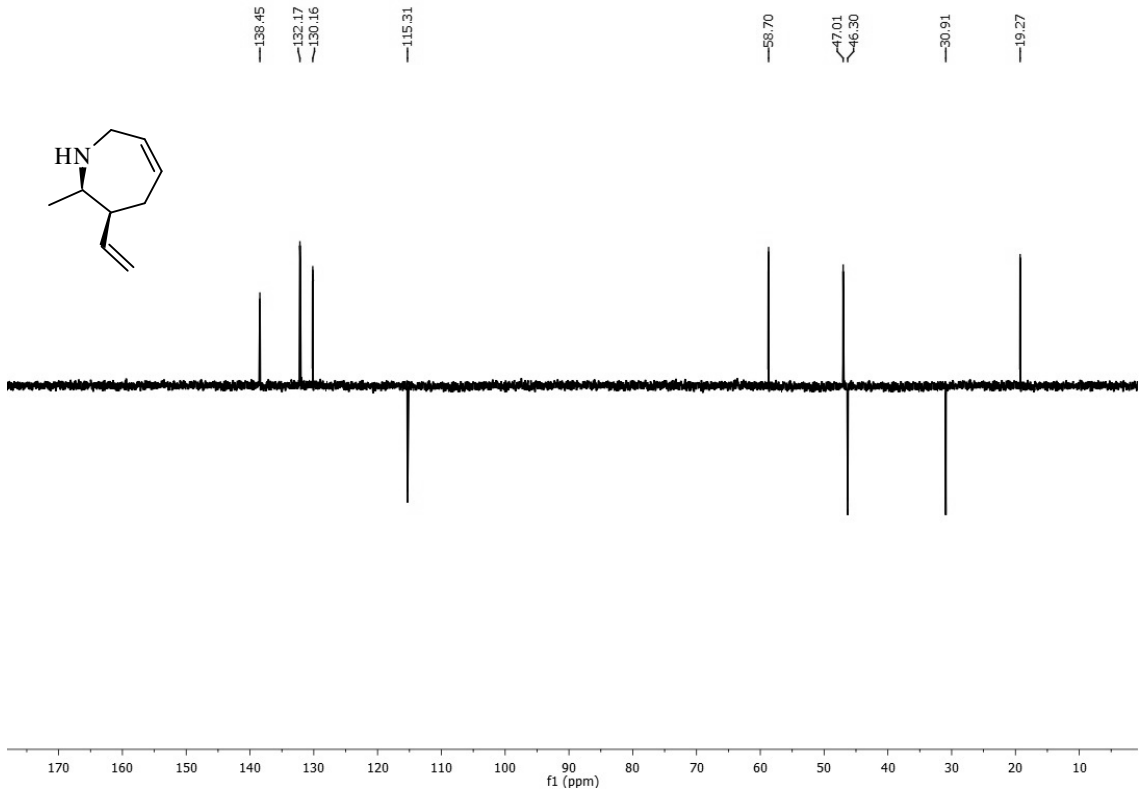
^{1}H - NMR of compound 82 (600 MHz, $CDCl_3$)



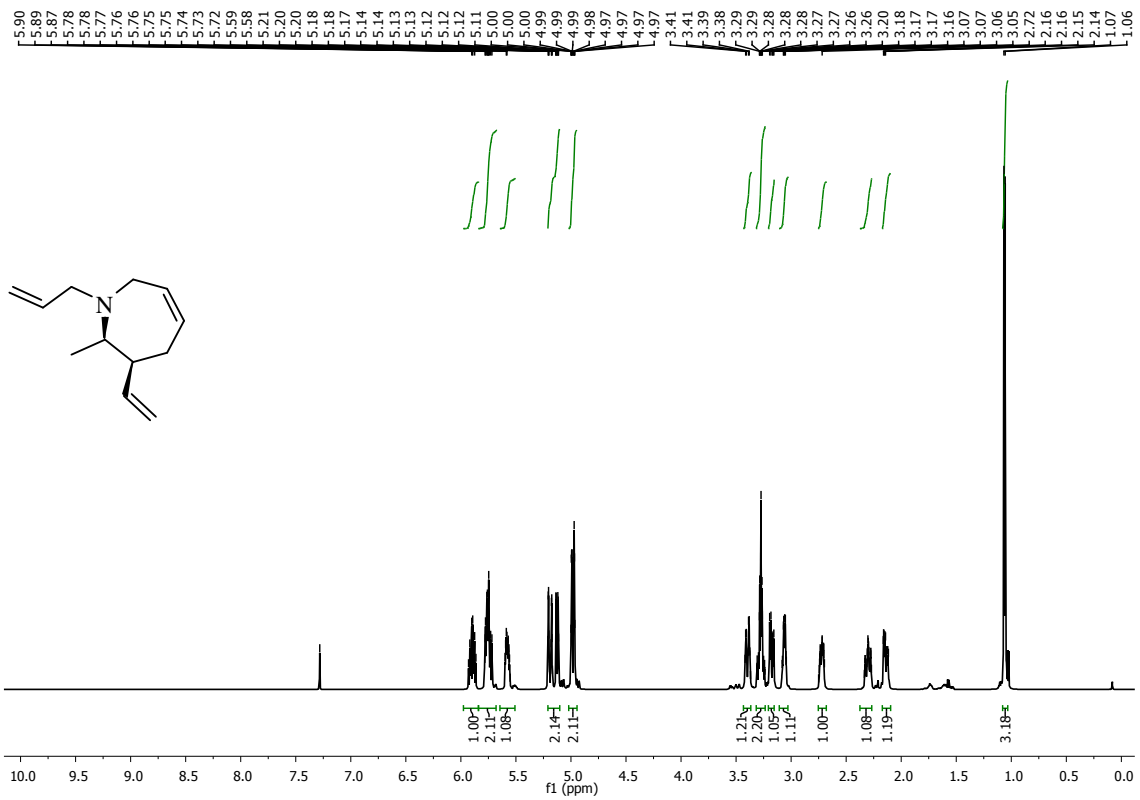
^{13}C NMR of compound 82 (100 MHz, $CDCl_3$)



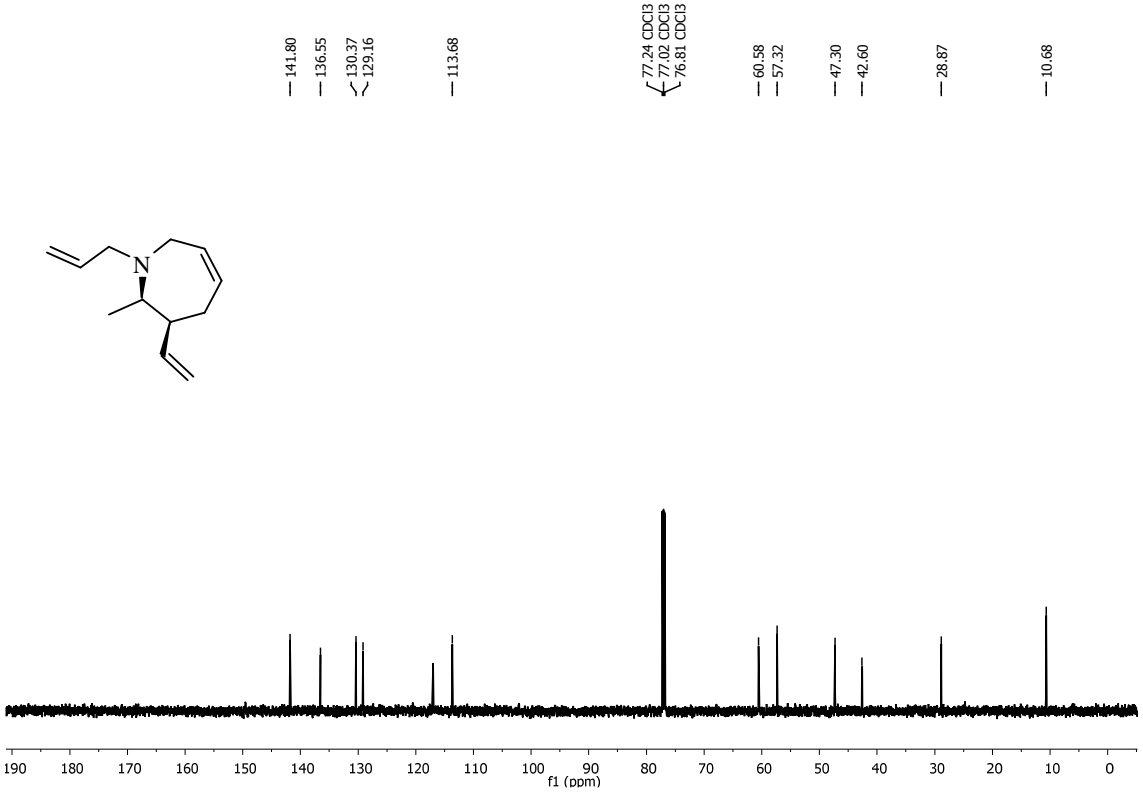
DEPT-135 NMR of compound 82 (100 MHz, $CDCl_3$)



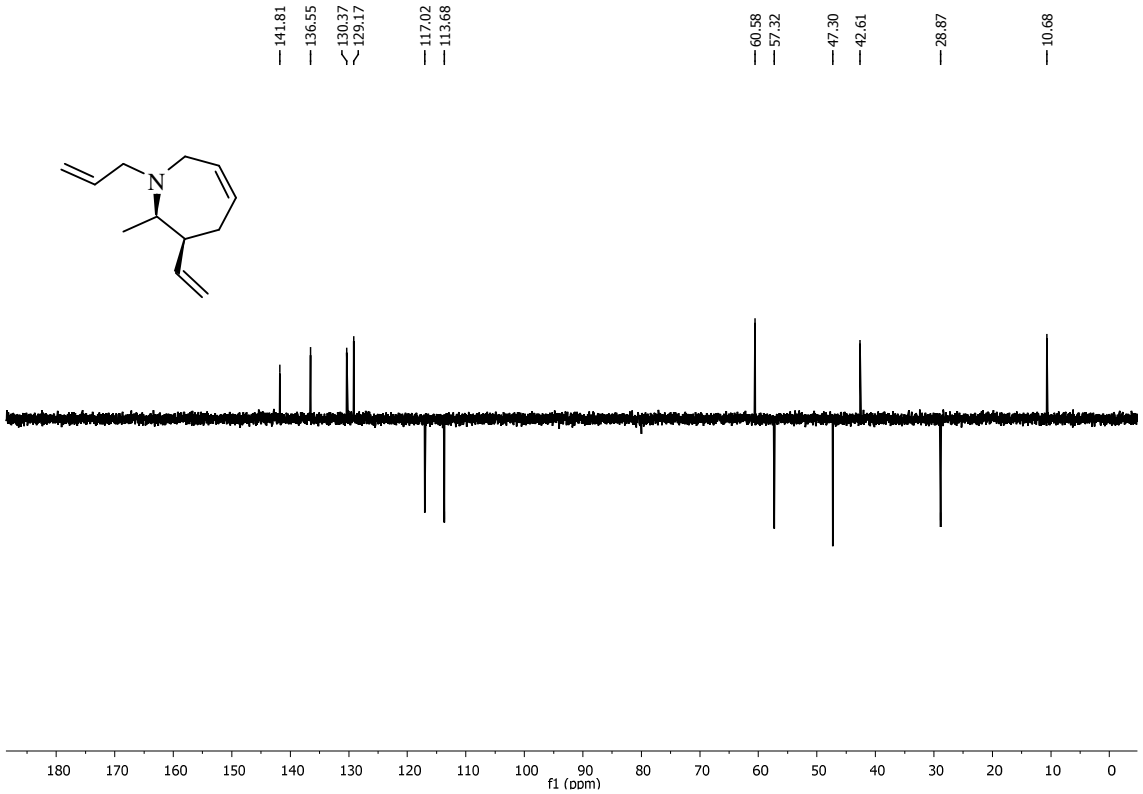
^{1}H - NMR of compound 83 (400 MHz, $CDCl_3$)



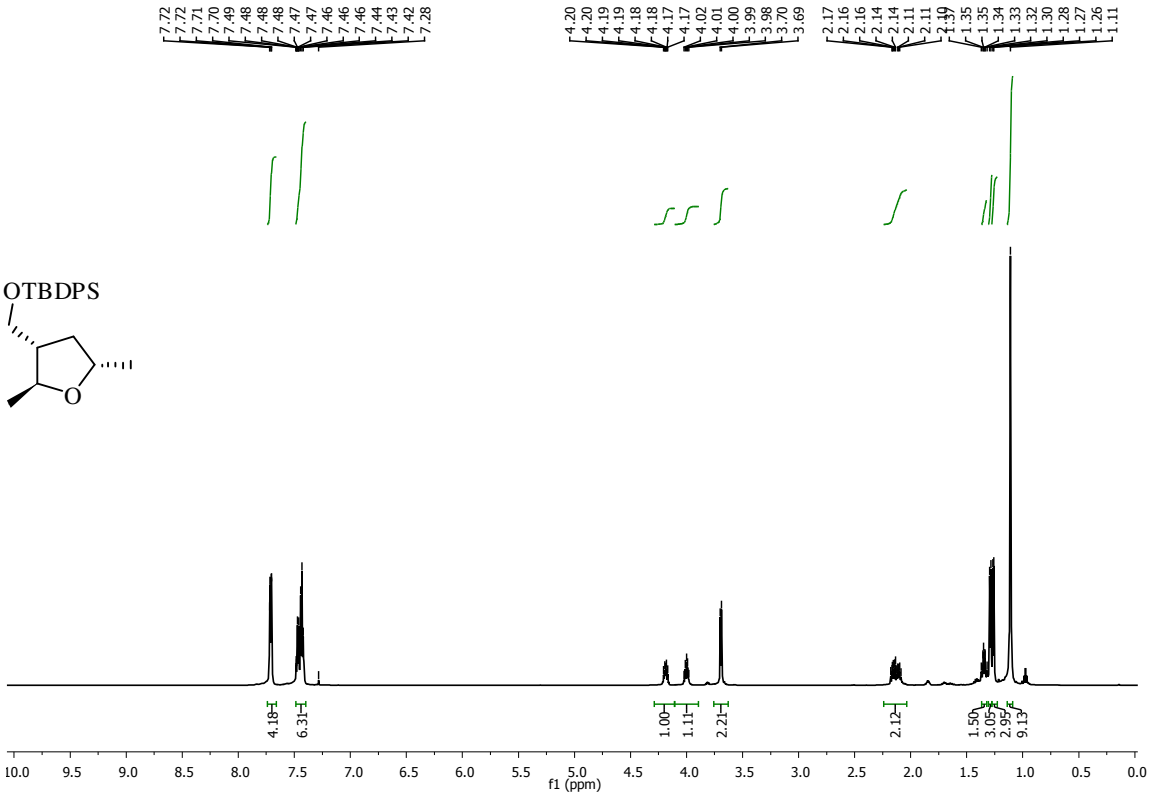
^{13}C NMR of compound 83 (150 MHz, $CDCl_3$)



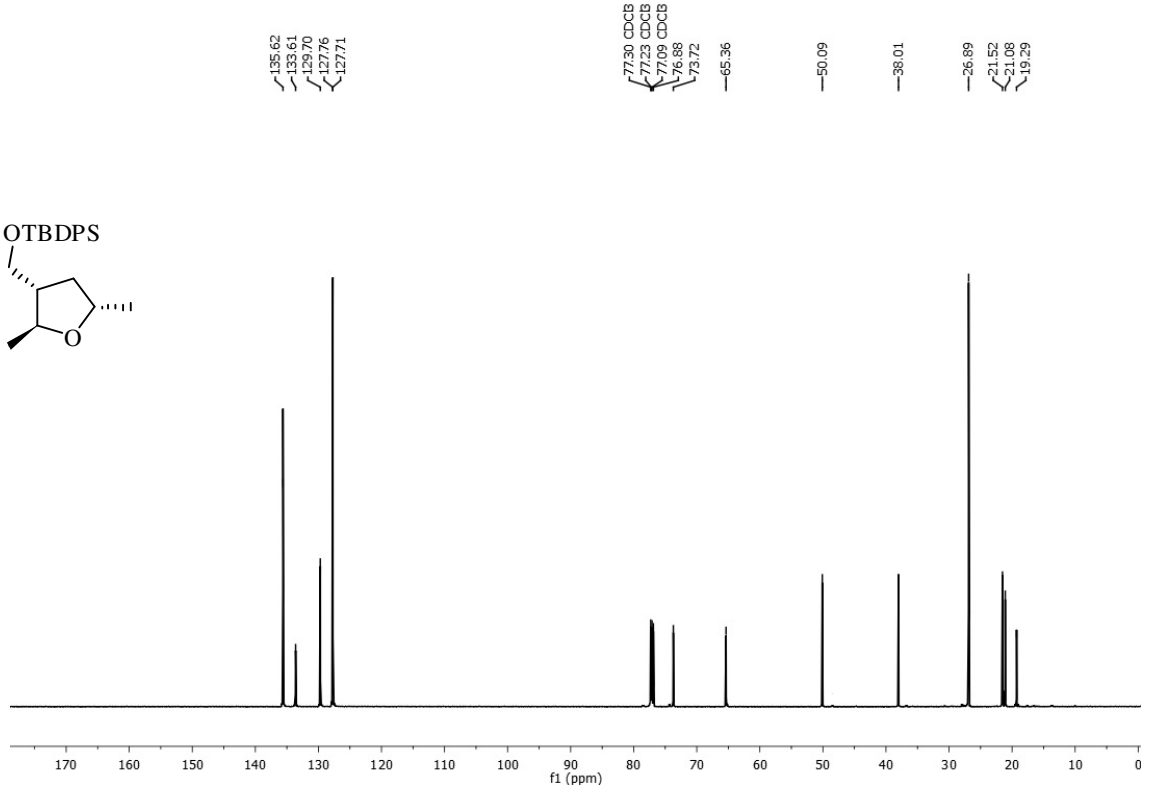
DEPT-135 NMR of compound 83 (150 MHz, $CDCl_3$)



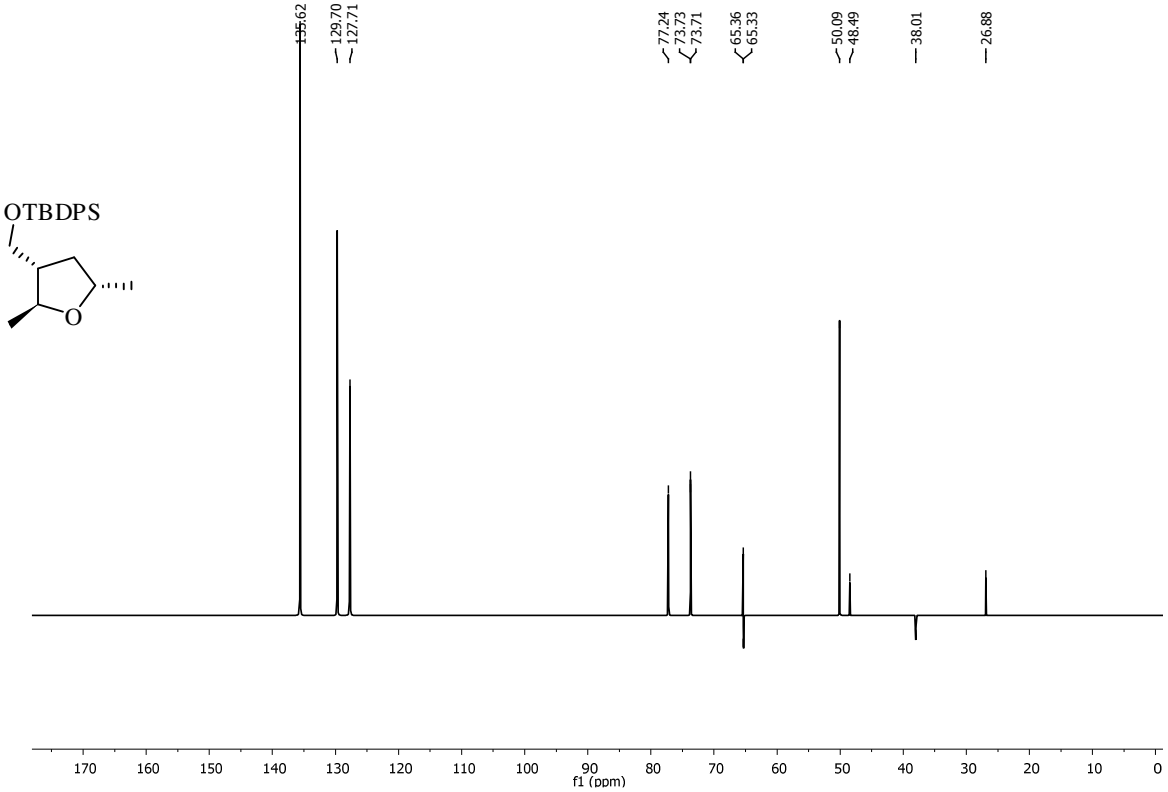
^{1}H - NMR of compound 84 (600 MHz, $CDCl_3$)



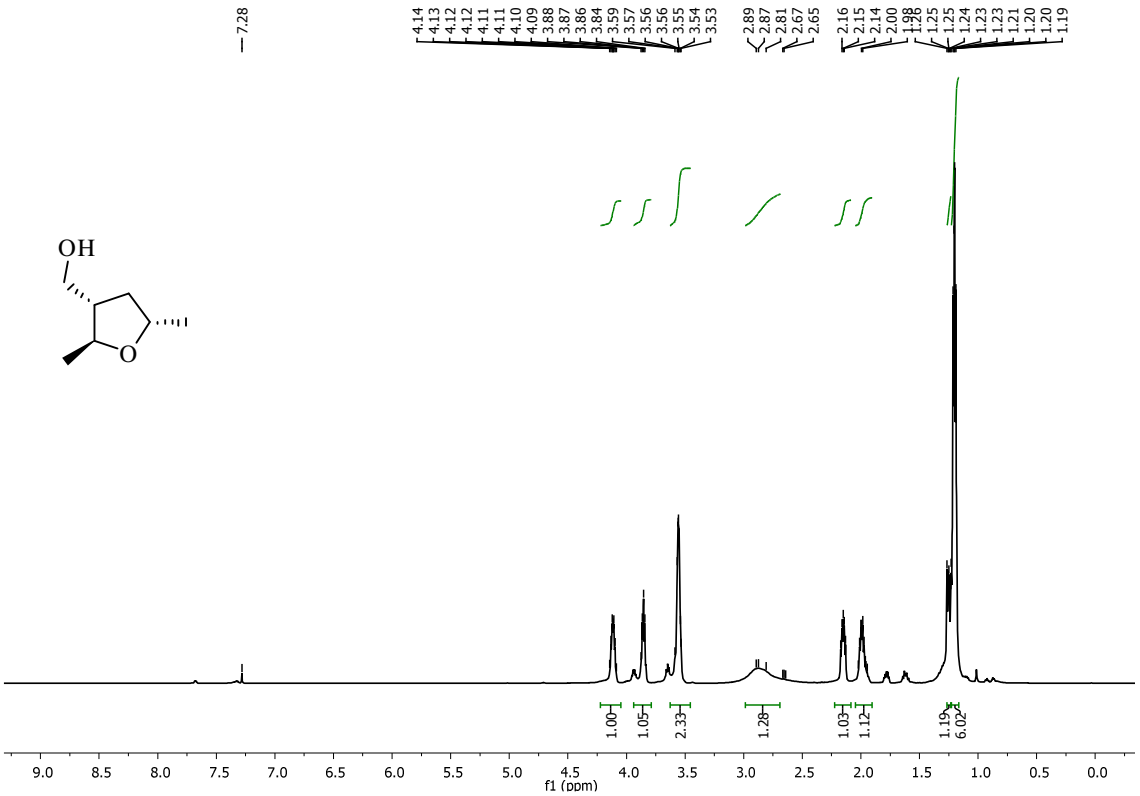
^{13}C NMR of compound 84 (150 MHz, $CDCl_3$)



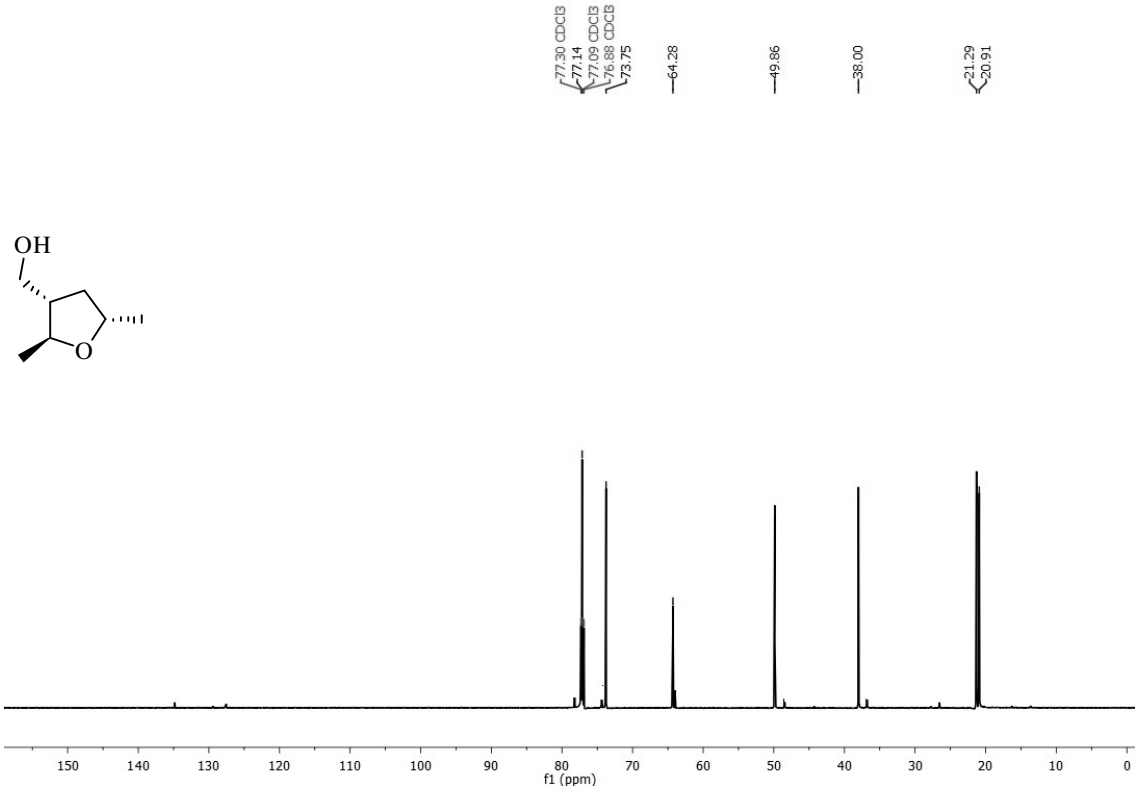
DEPT-135 NMR of compound 84 (150 MHz, $CDCl_3$)



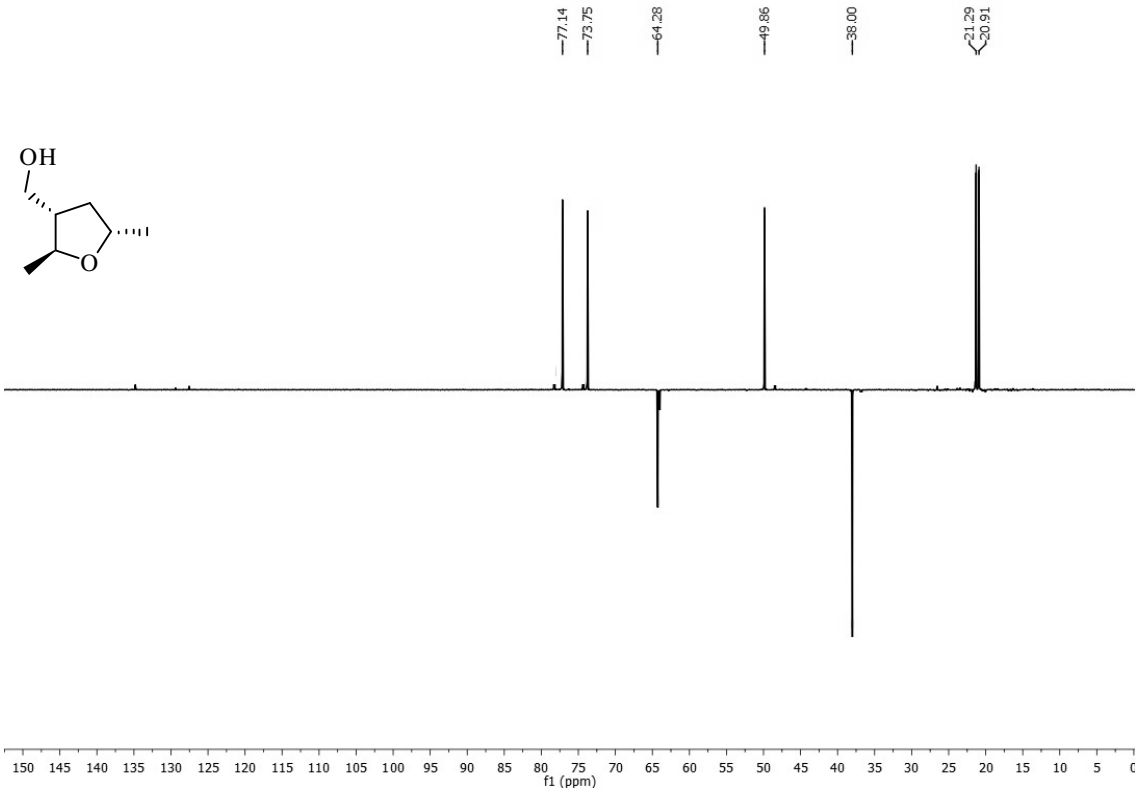
^{1}H - NMR of compound 85 (600 MHz, $CDCl_3$)



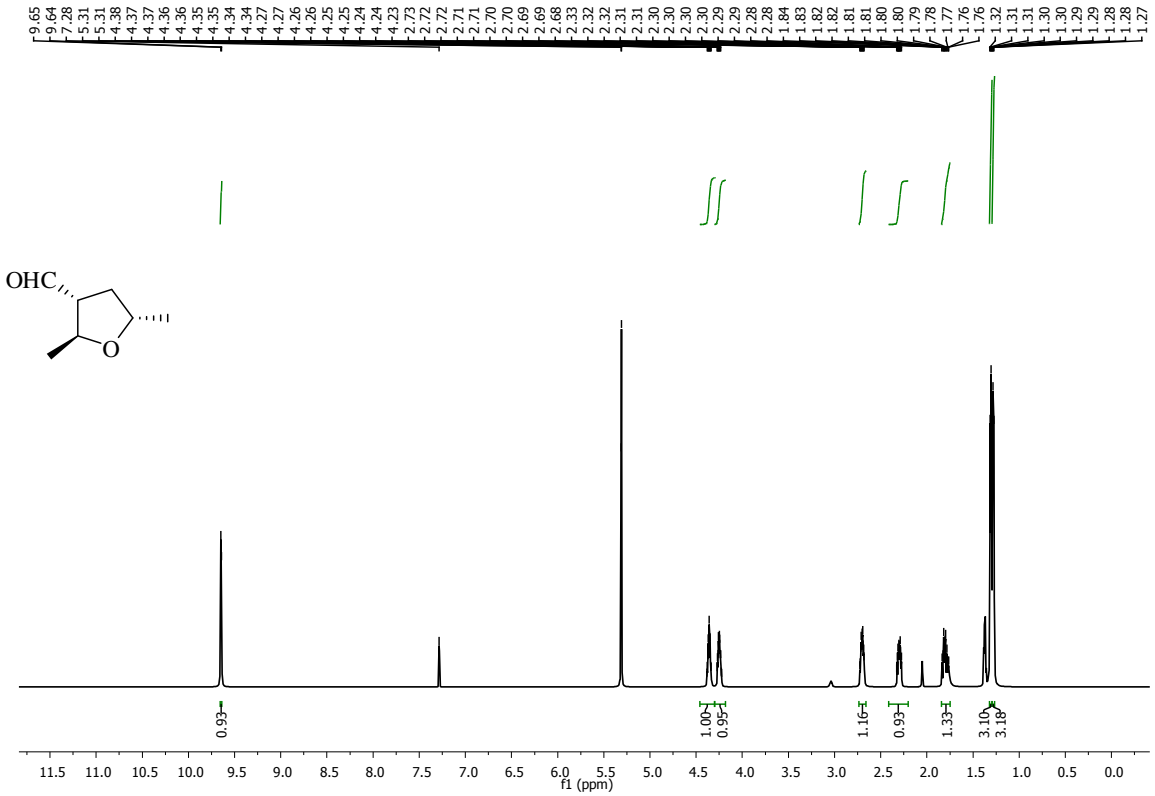
^{13}C NMR of compound 85 (150 MHz, $CDCl_3$)



DEPT-135 NMR of compound 85 (150 MHz, $CDCl_3$)



^{1}H - NMR of compound 86 (600 MHz, $CDCl_3$)



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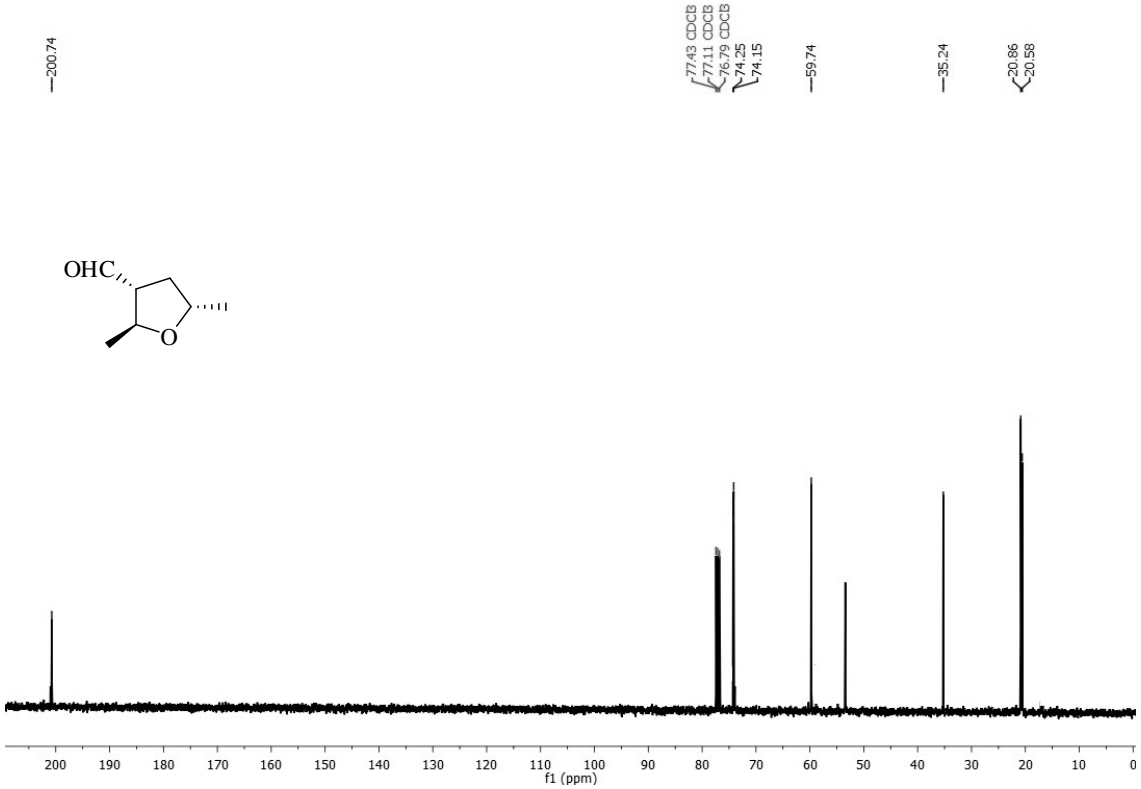
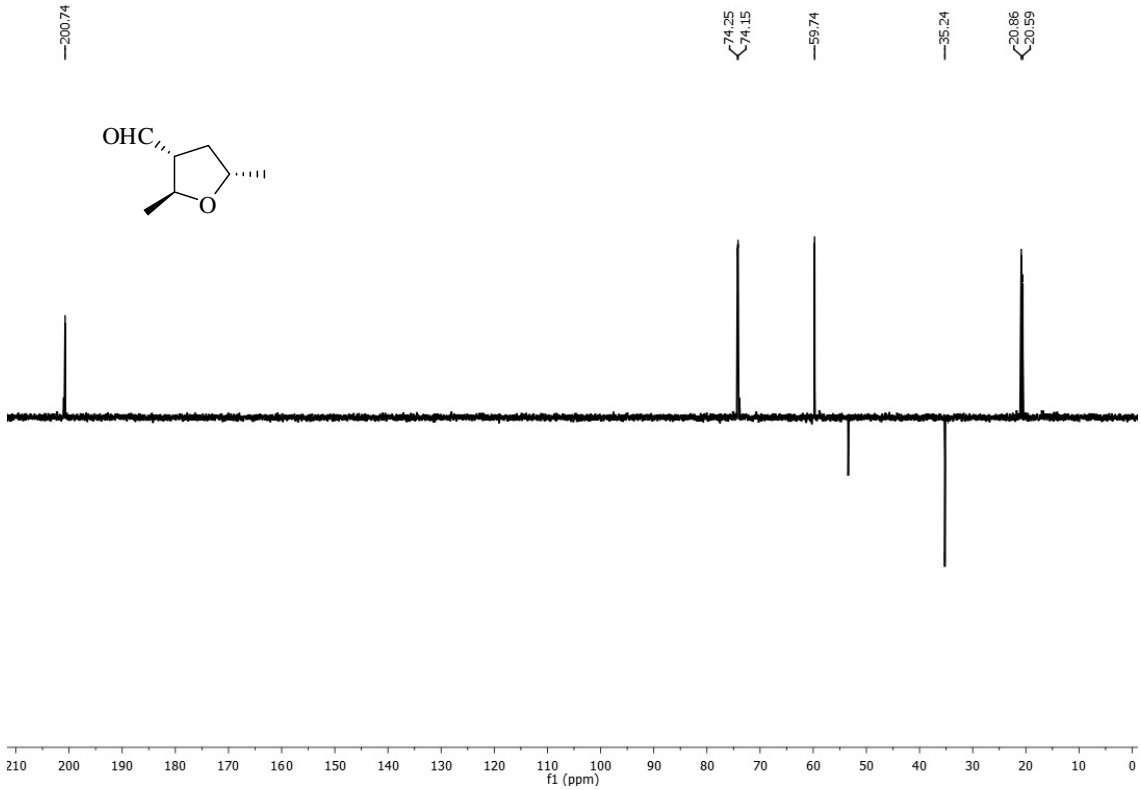
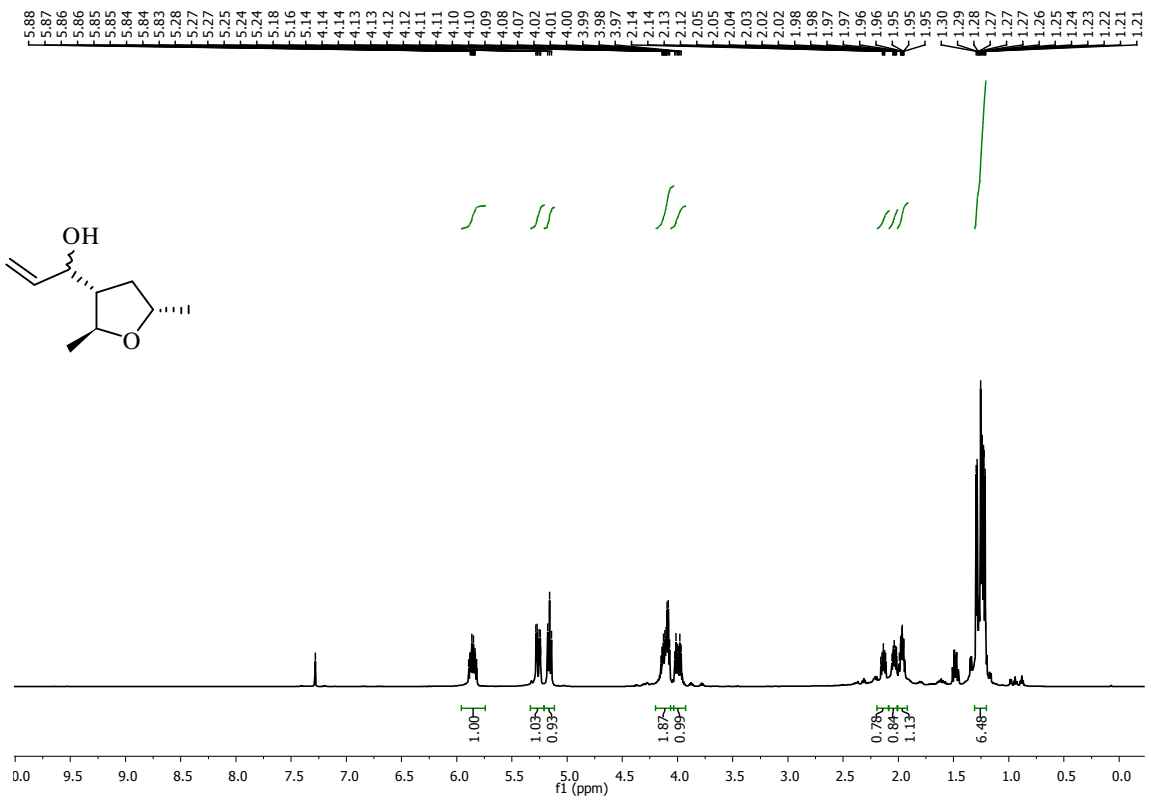


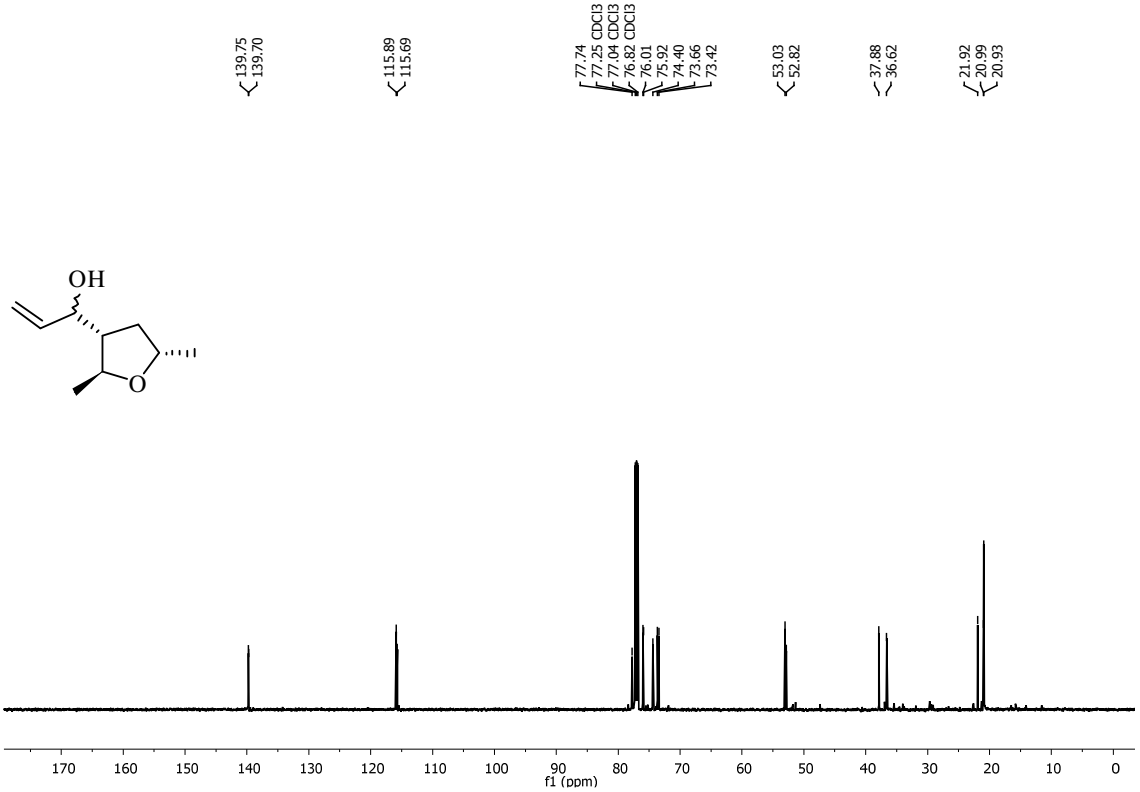
DEPT-135 NMR of compound 86 (100 MHz, $CDCl_3$)



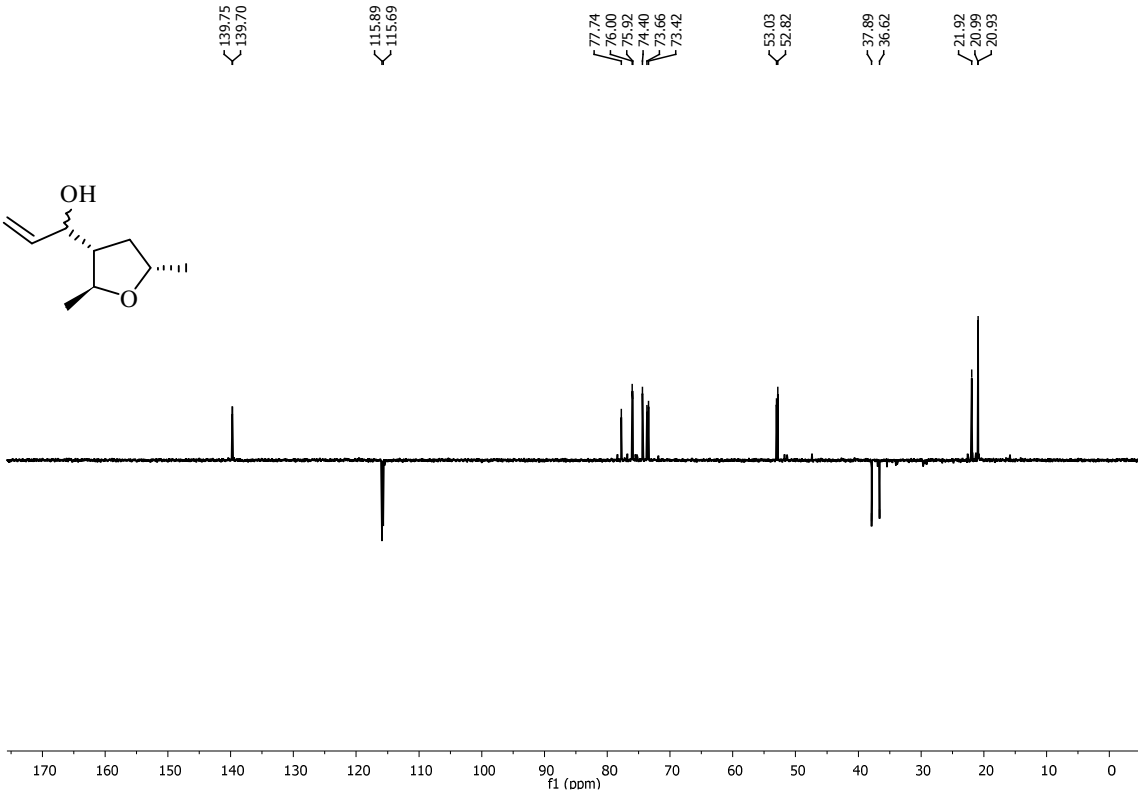
^{1}H - NMR of compound 87 (600 MHz, $CDCl_3$)



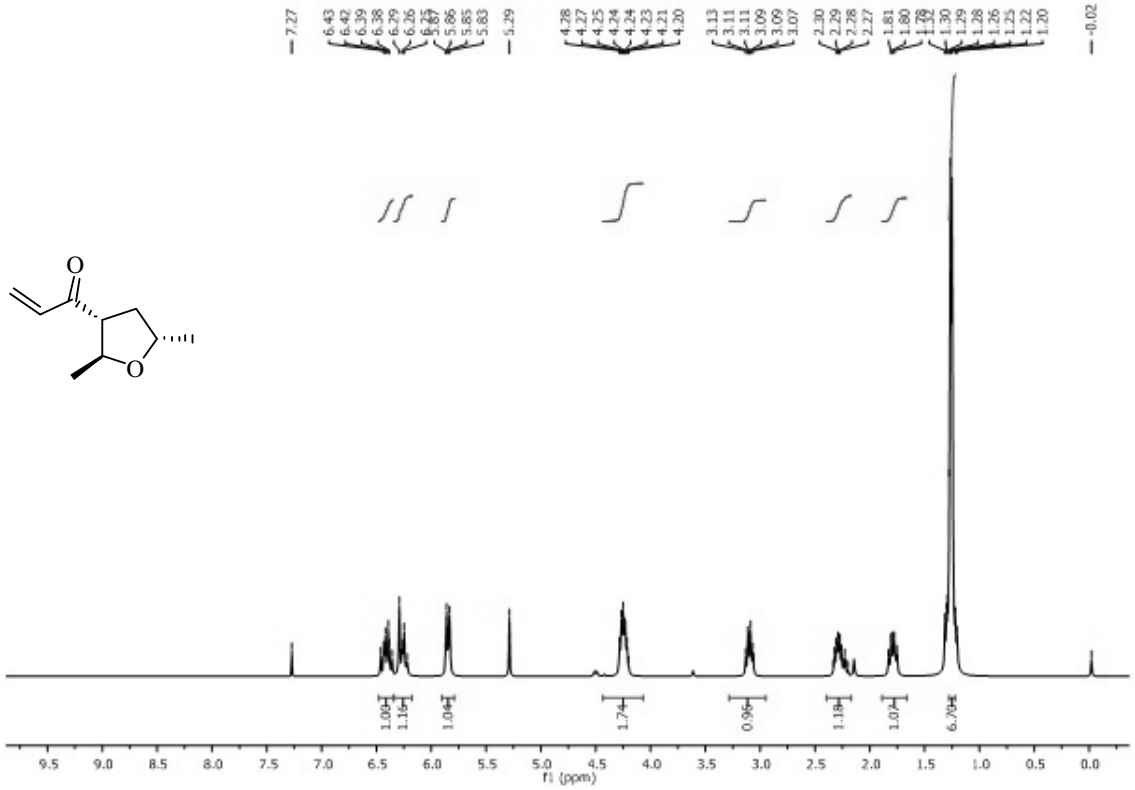
^{13}C NMR of compound 87 (150 MHz, $CDCl_3$)



DEPT-135 NMR of compound 87 (150 MHz, $CDCl_3$)



^{1}H - NMR of compound 88 (400 MHz, $CDCl_3$)



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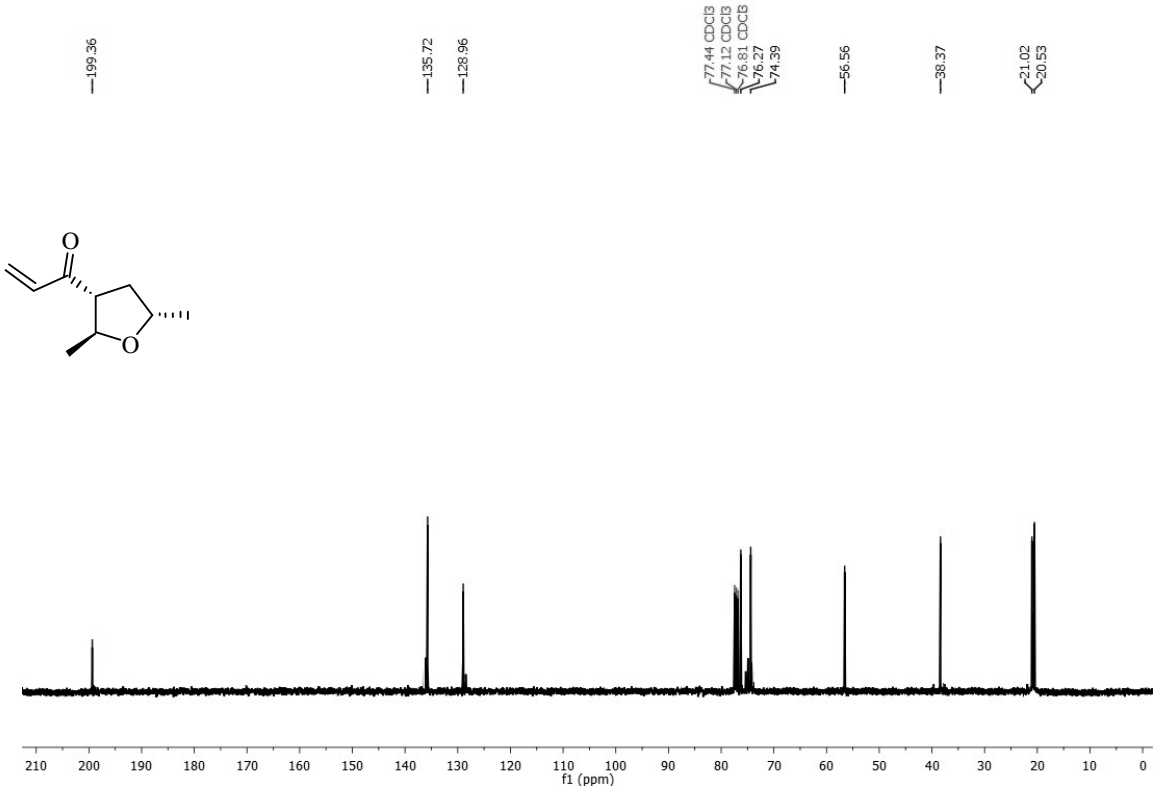
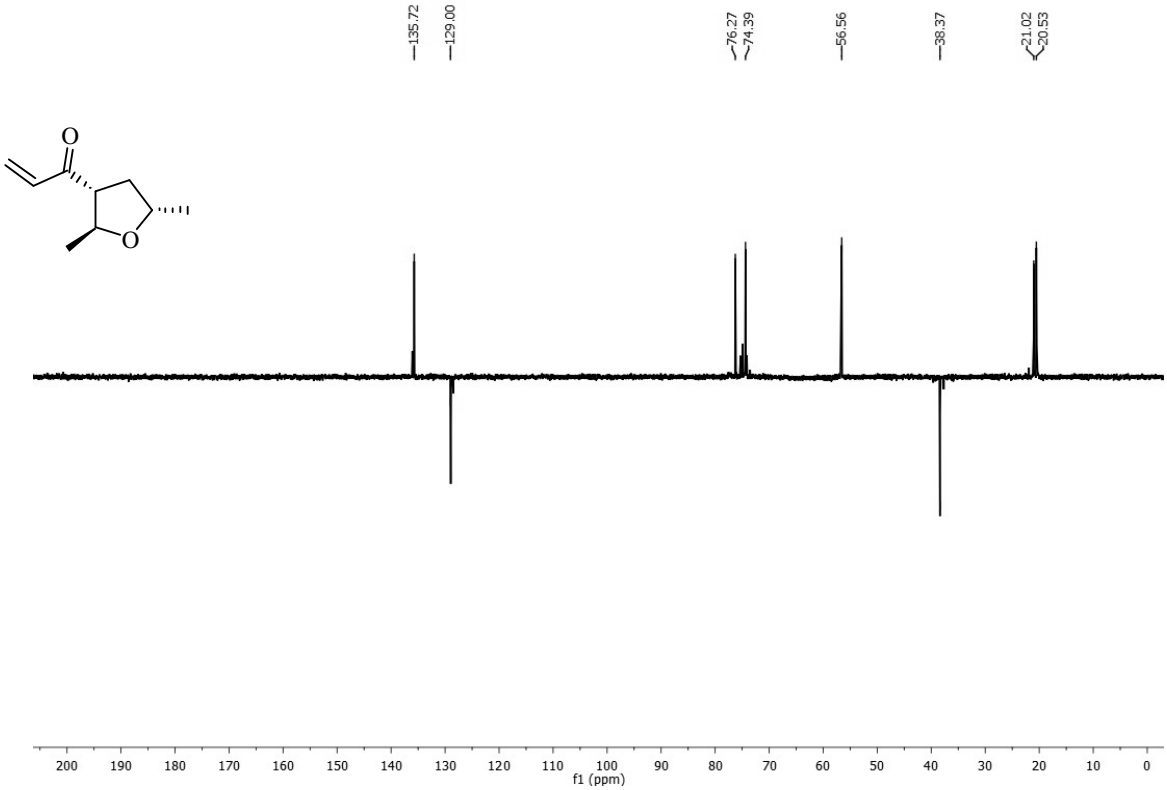
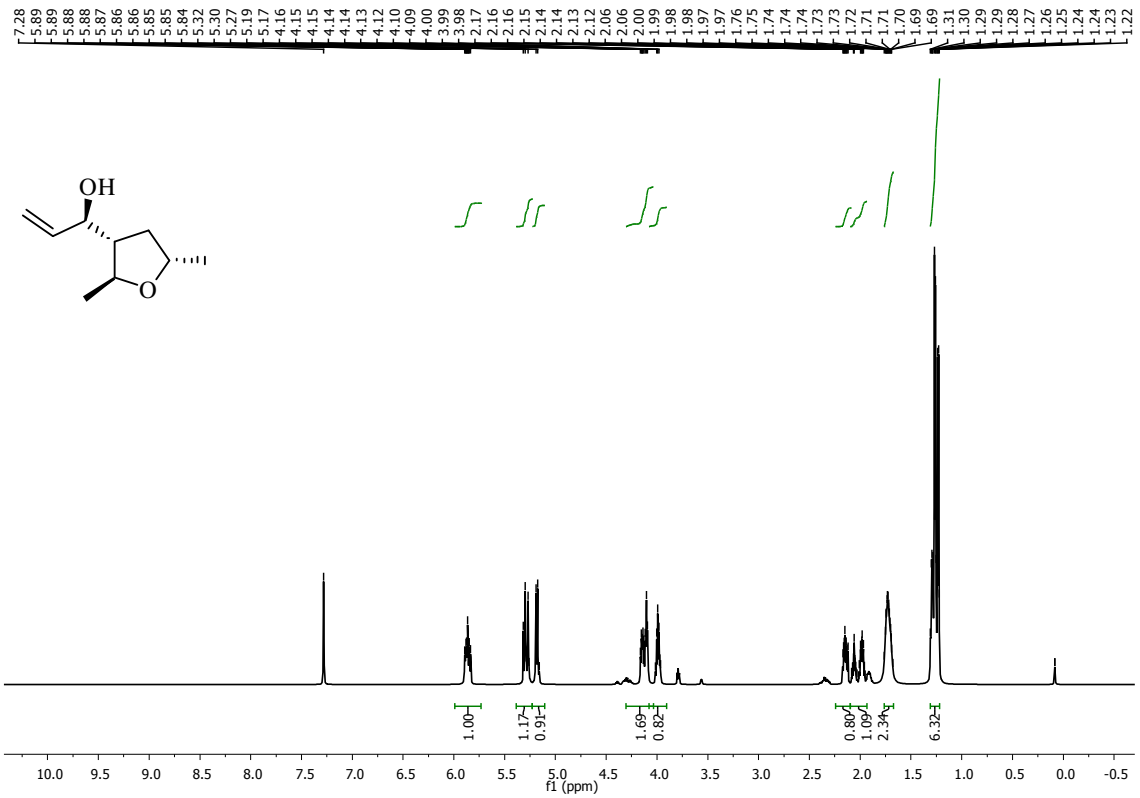


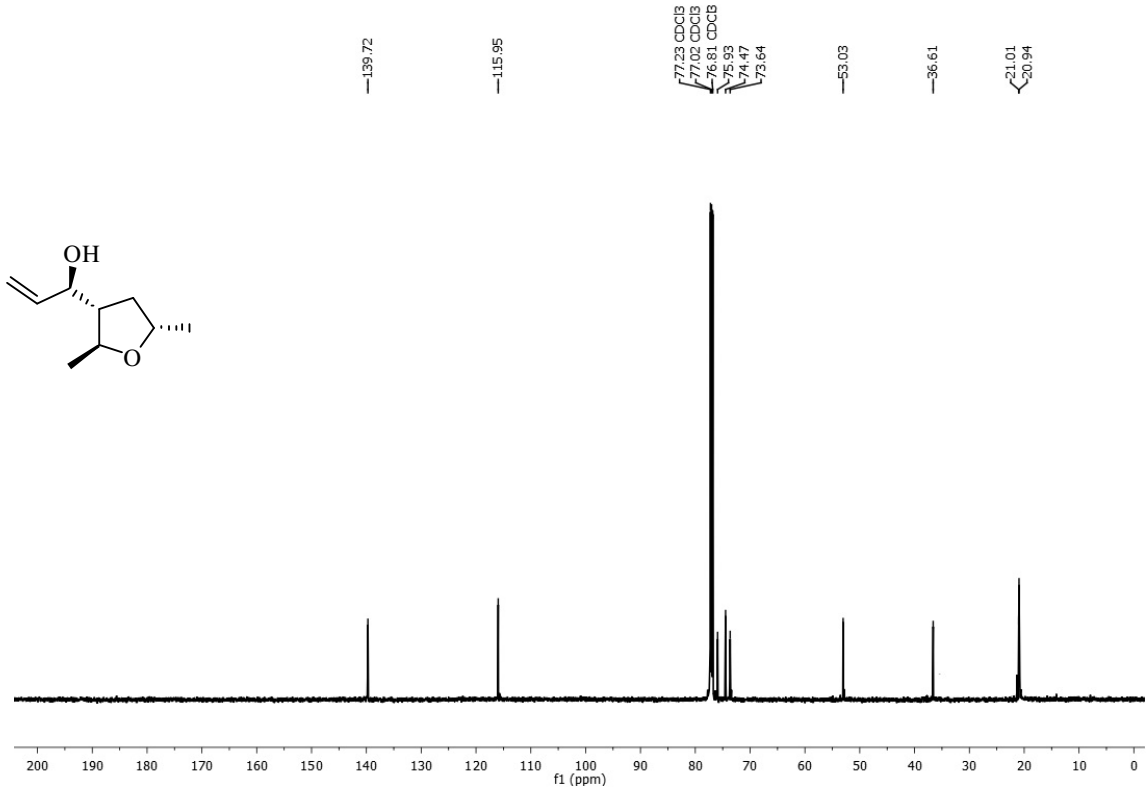
DEPT-135 NMR of compound 88 (100 MHz, $CDCl_3$)



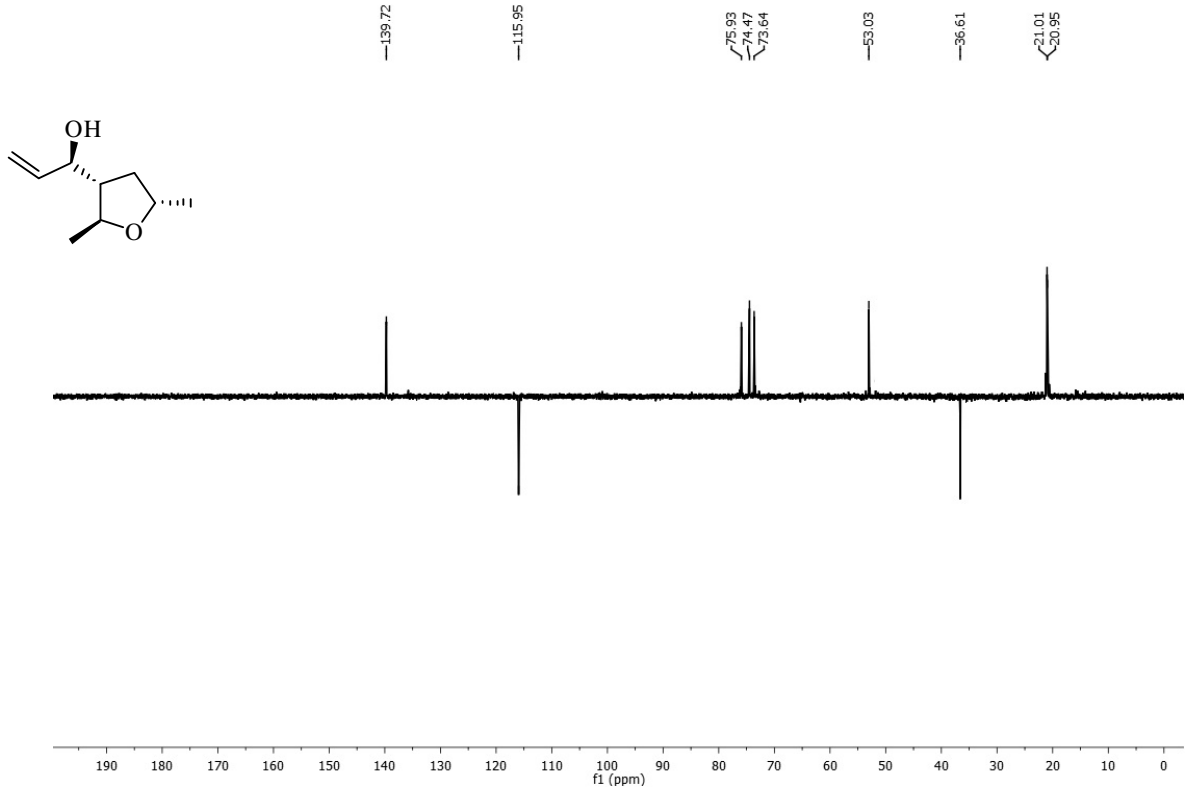
^{1}H - NMR of enantiopure 87 (600 MHz, $CDCl_3$)



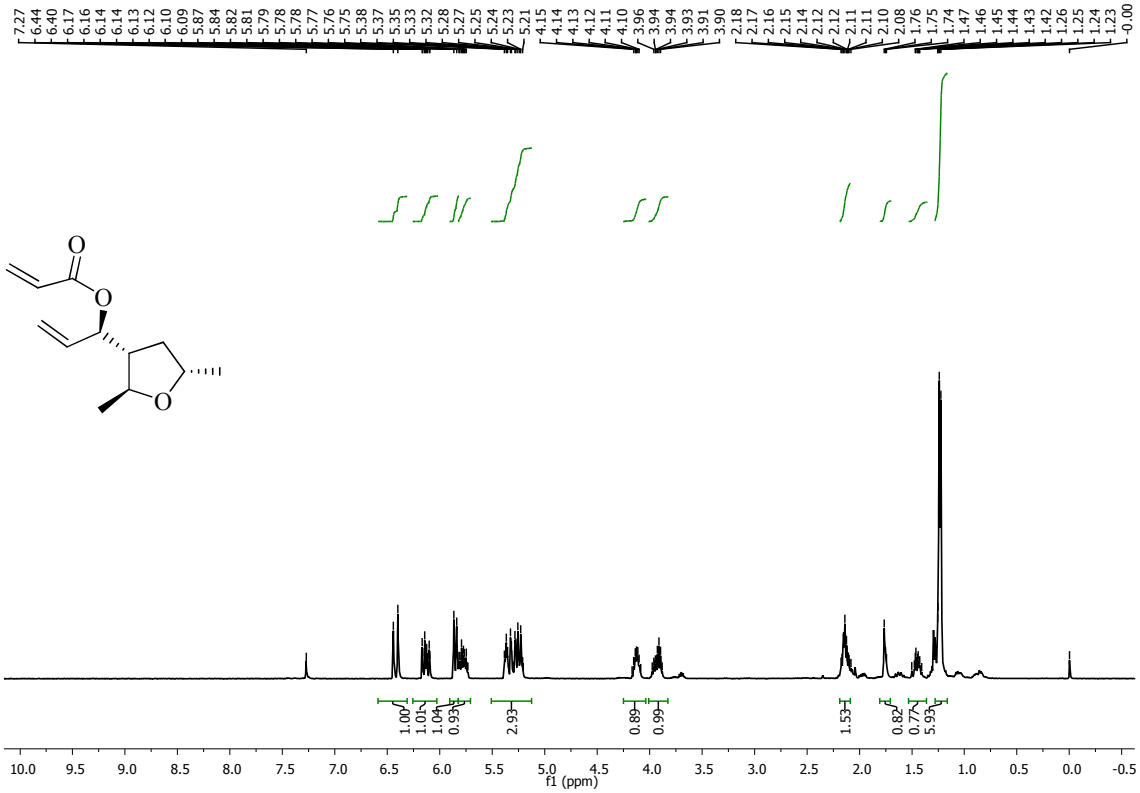
^{13}C NMR of enantiopure 87 (150 MHz, $CDCl_3$)



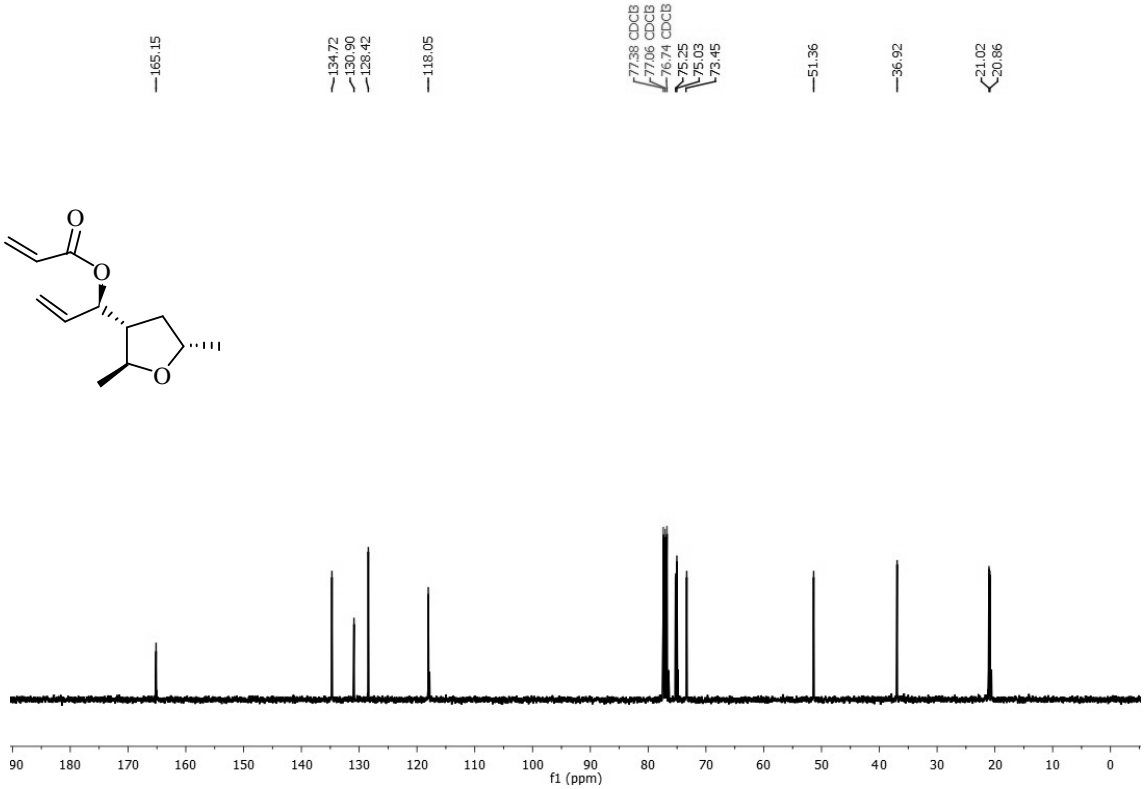
DEPT-135 NMR of enantiopure 87 (150 MHz, $CDCl_3$)



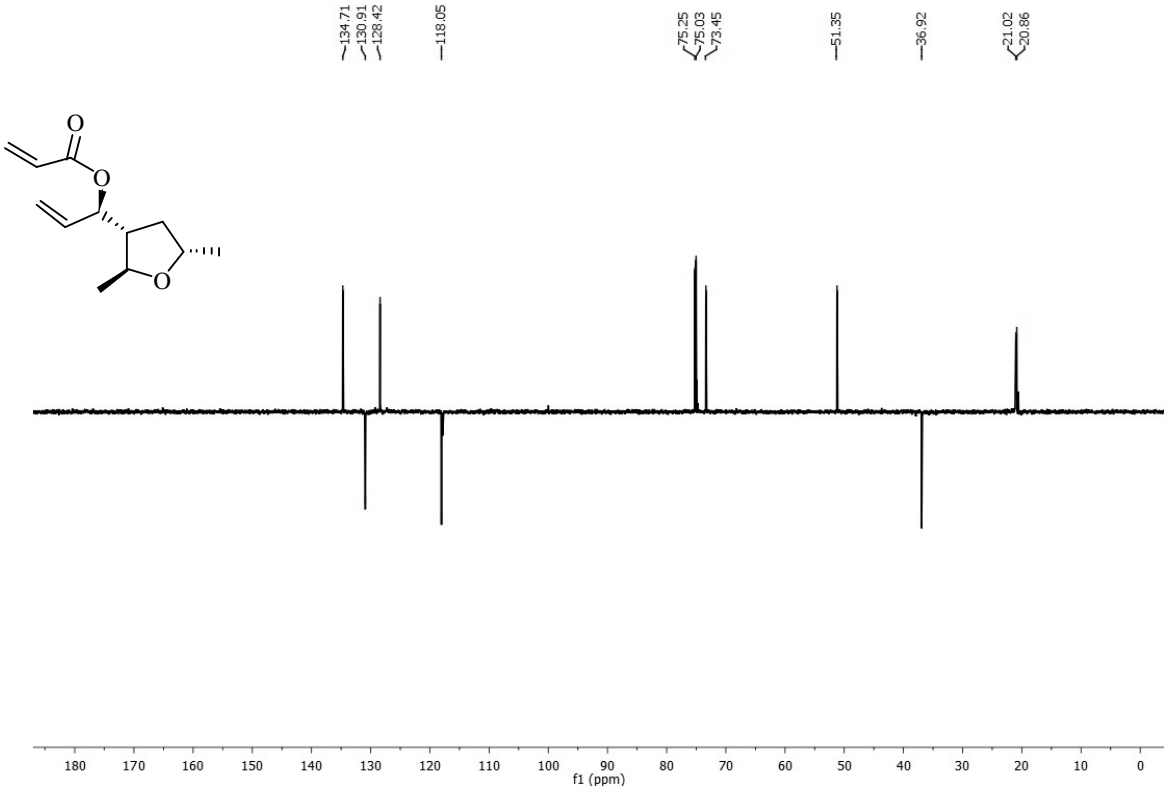
^{1}H - NMR of compound 89 (400 MHz, $CDCl_3$)



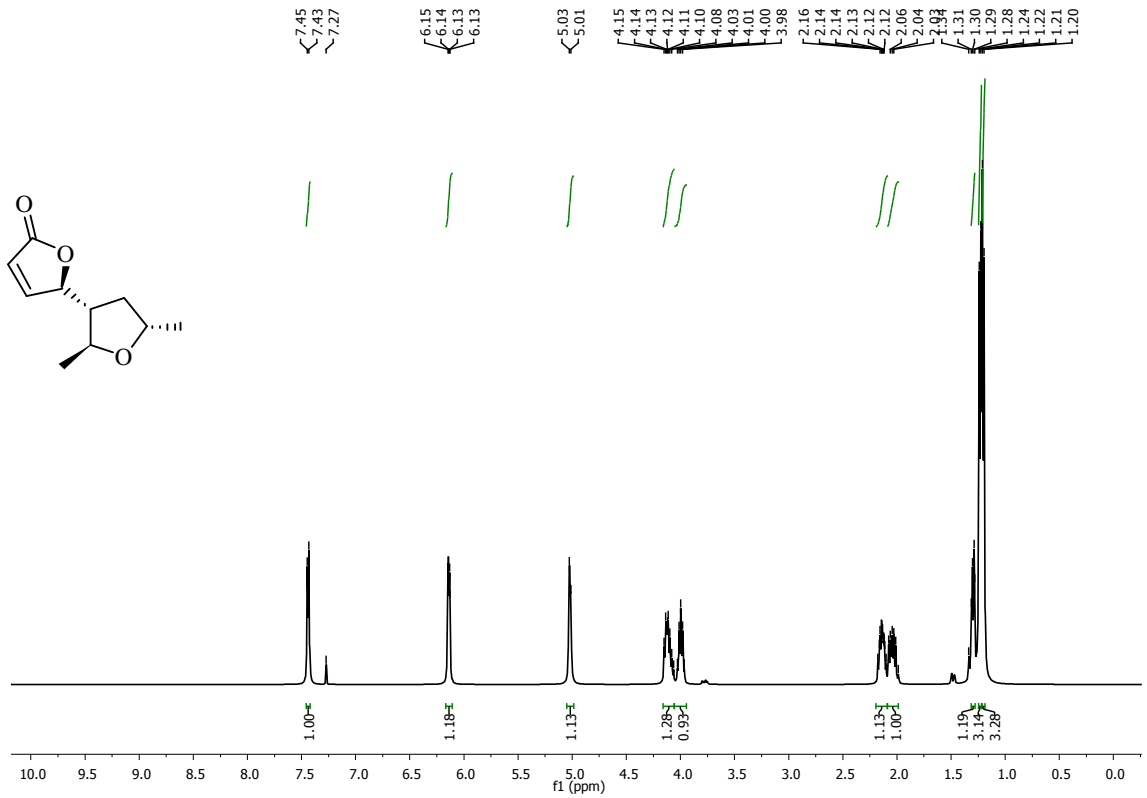
^{13}C NMR of compound 89 (100 MHz, $CDCl_3$)



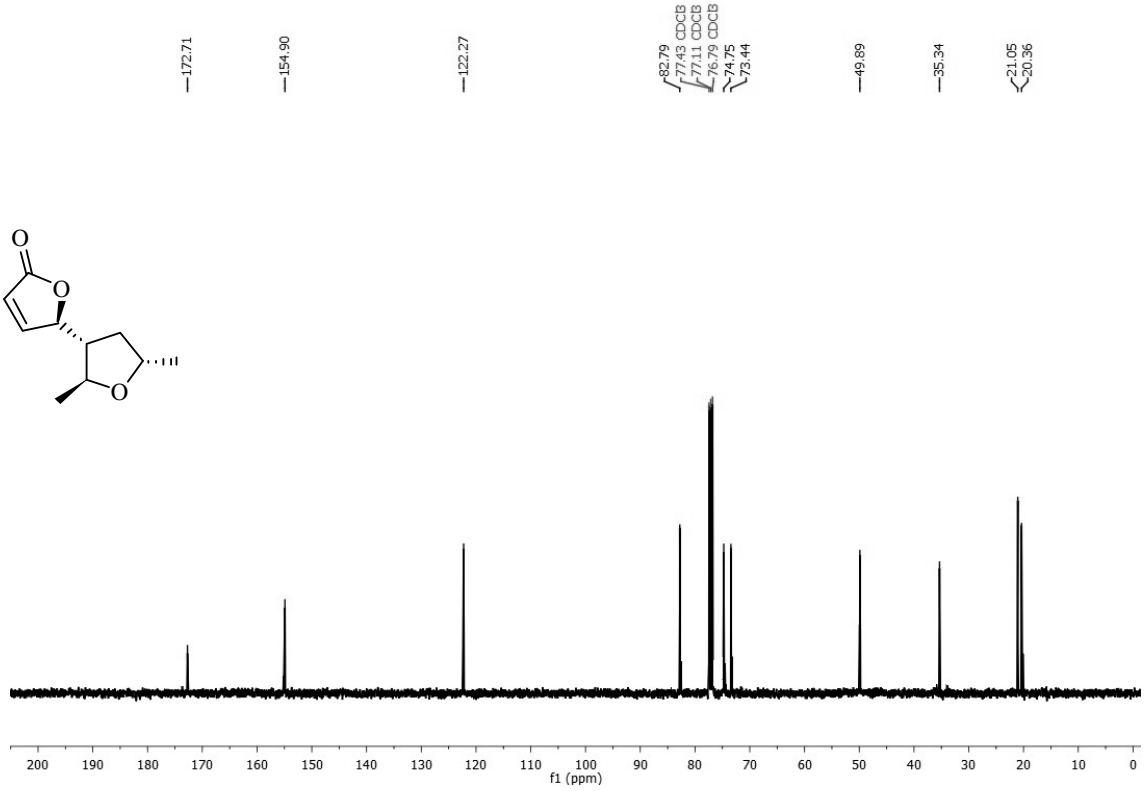
DEPT-135 NMR of compound 89 (100 MHz, $CDCl_3$)



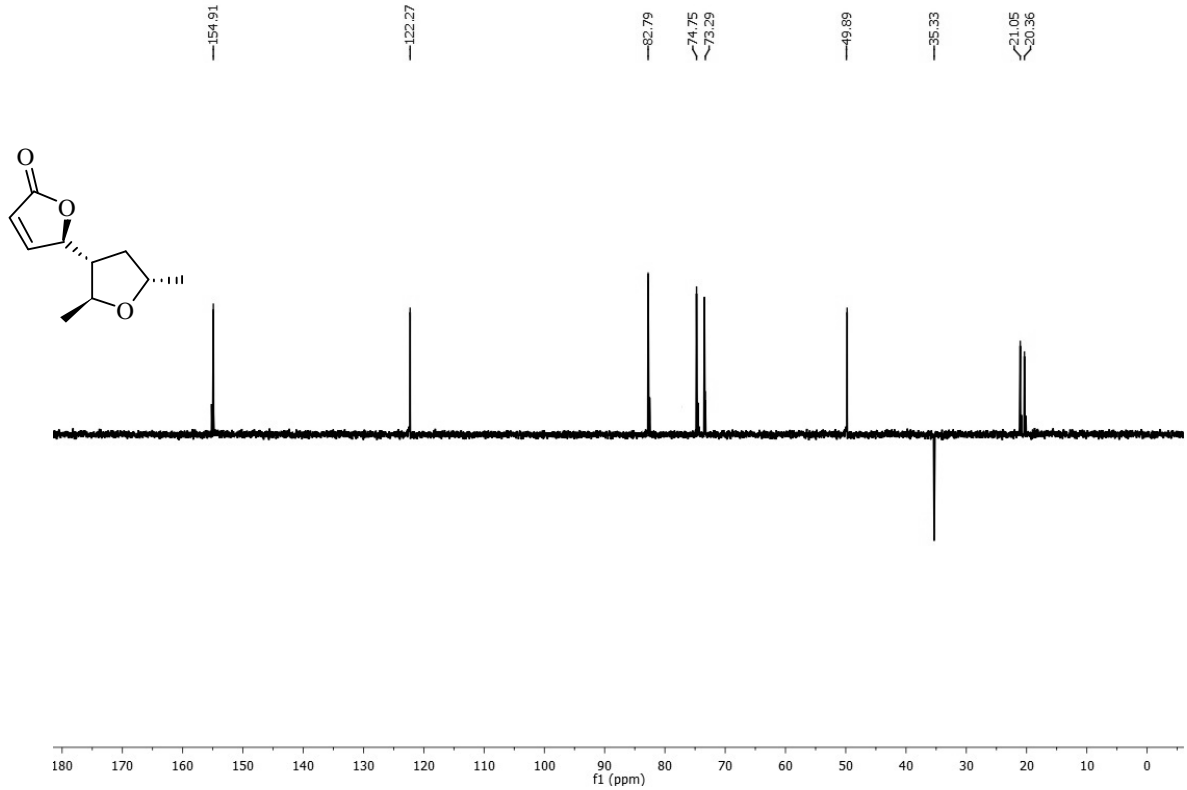
^{1}H - NMR of compound 90 (400 MHz, $CDCl_3$)



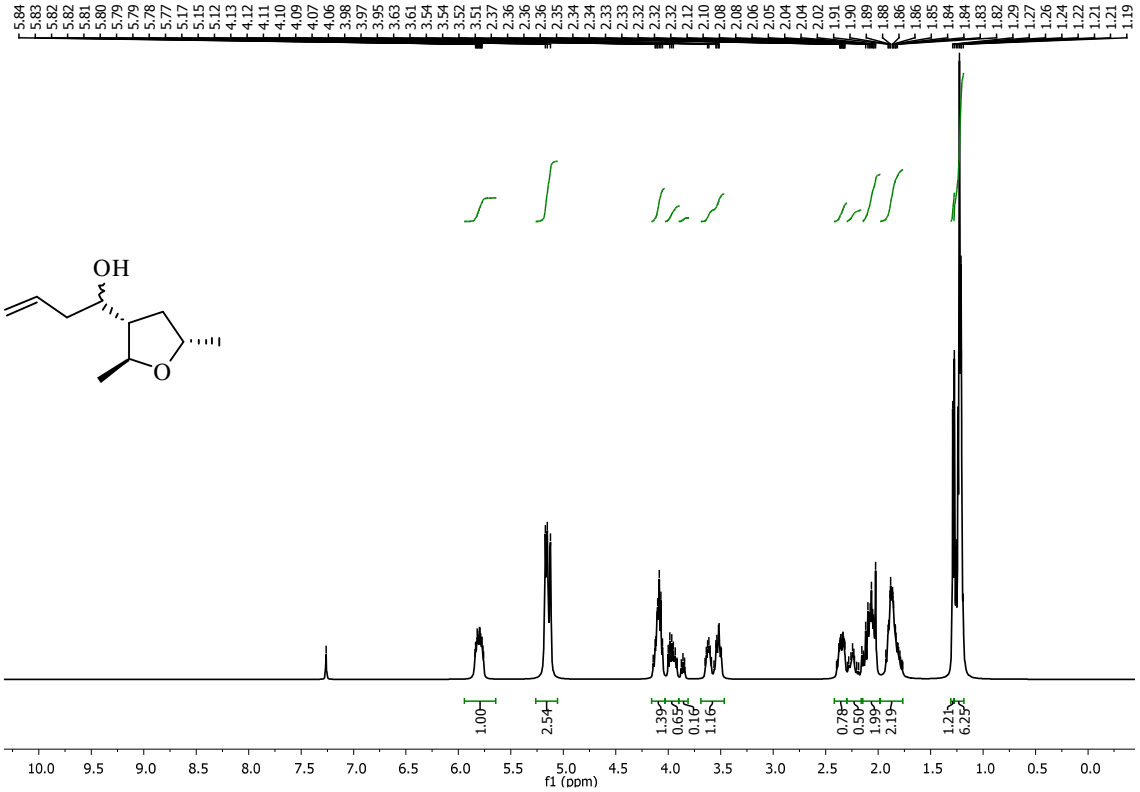
^{13}C NMR of compound 90 (100 MHz, $CDCl_3$)



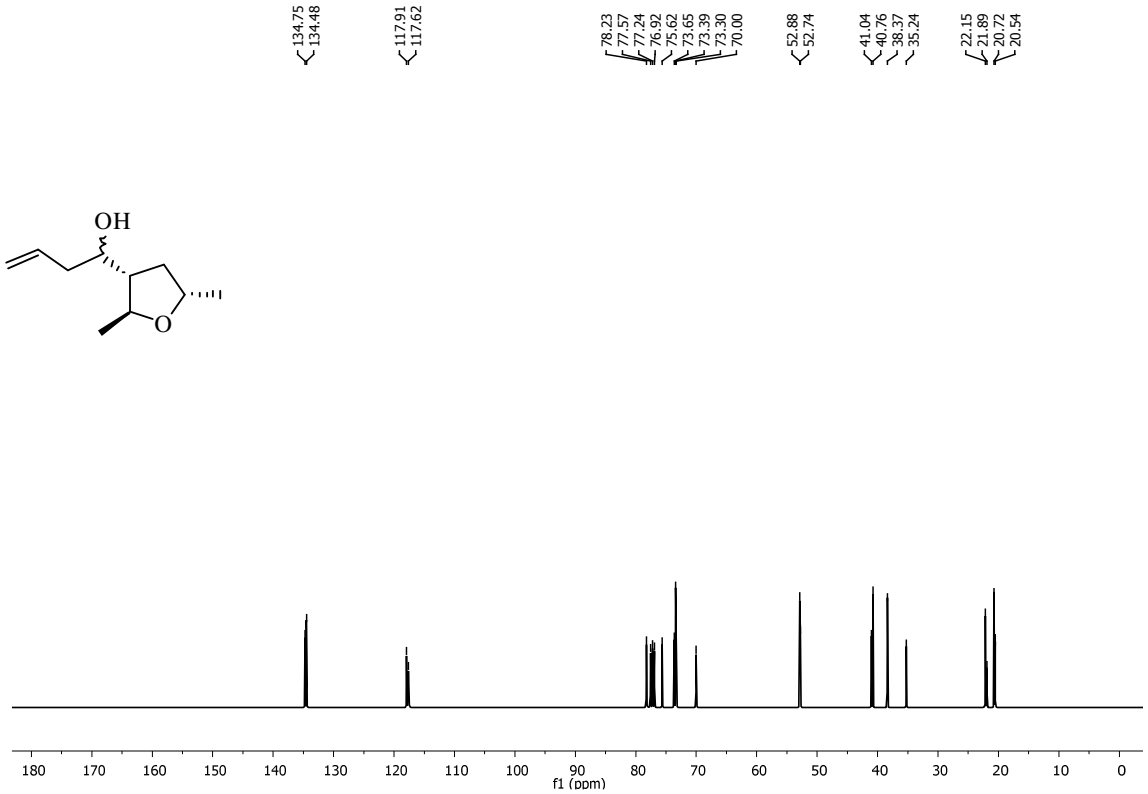
DEPT-135 NMR of compound 90 (100 MHz, $CDCl_3$)



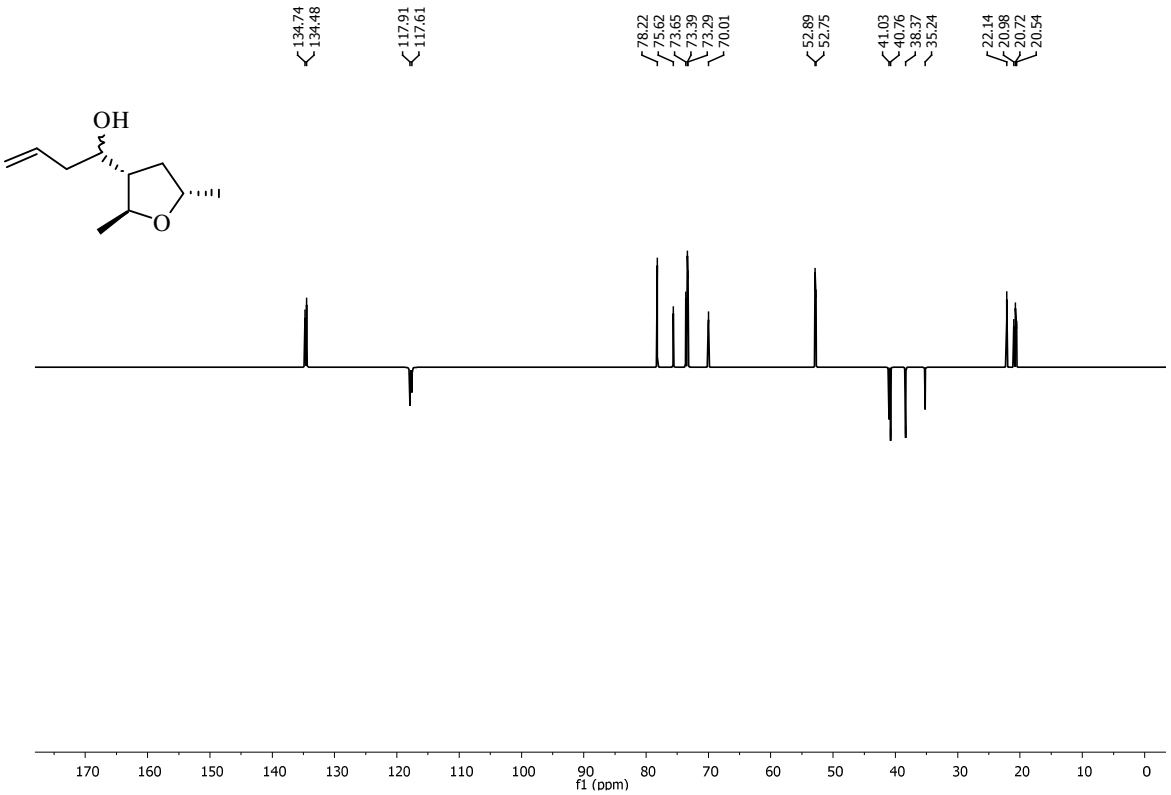
^{1}H - NMR of compound 91 (400 MHz, $CDCl_3$)



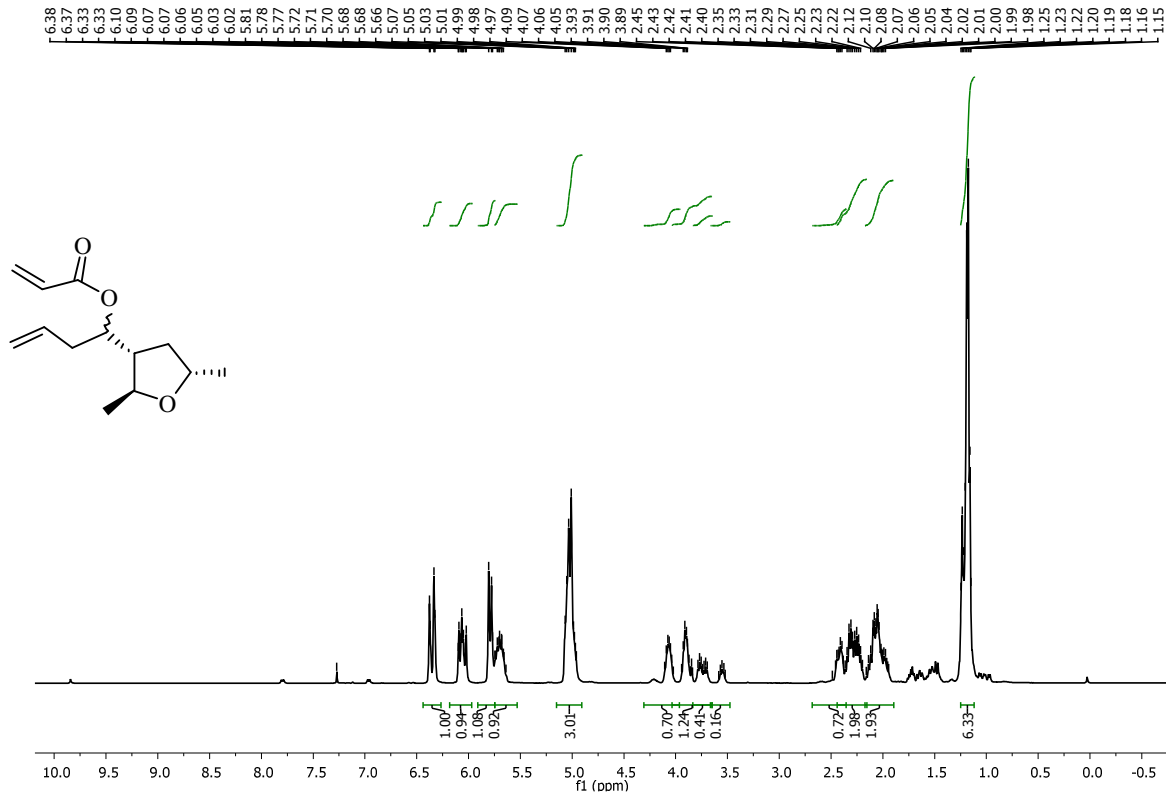
^{13}C NMR of compound 91 (100 MHz, $CDCl_3$)



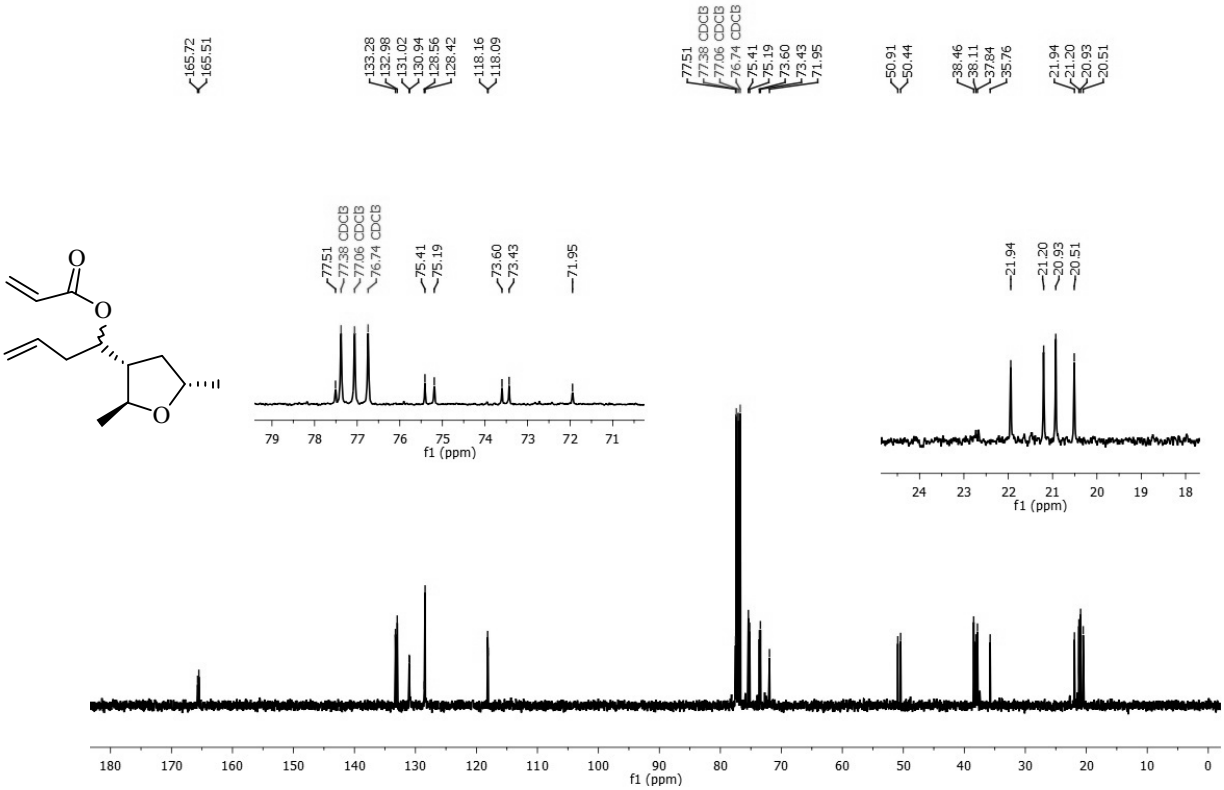
DEPT-135 NMR of compound 91 (100 MHz, $CDCl_3$)



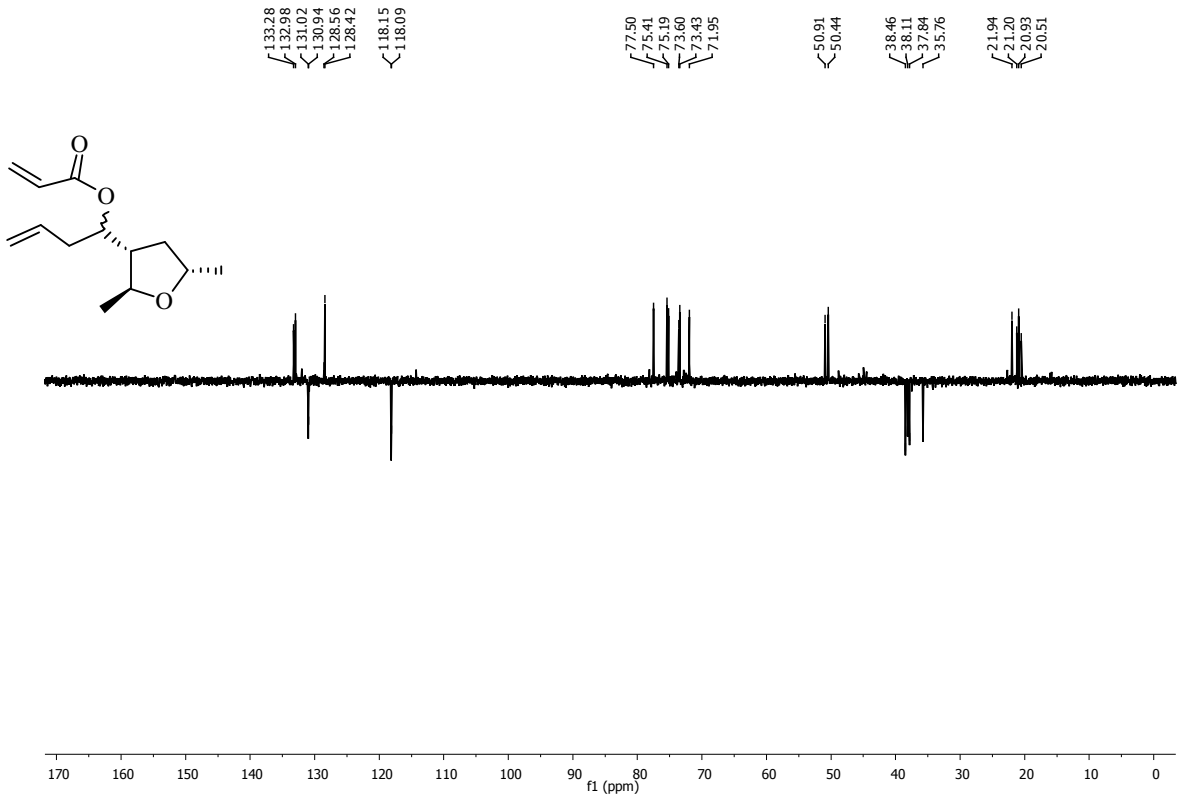
^{1}H - NMR of compound 92 (400 MHz, $CDCl_3$)



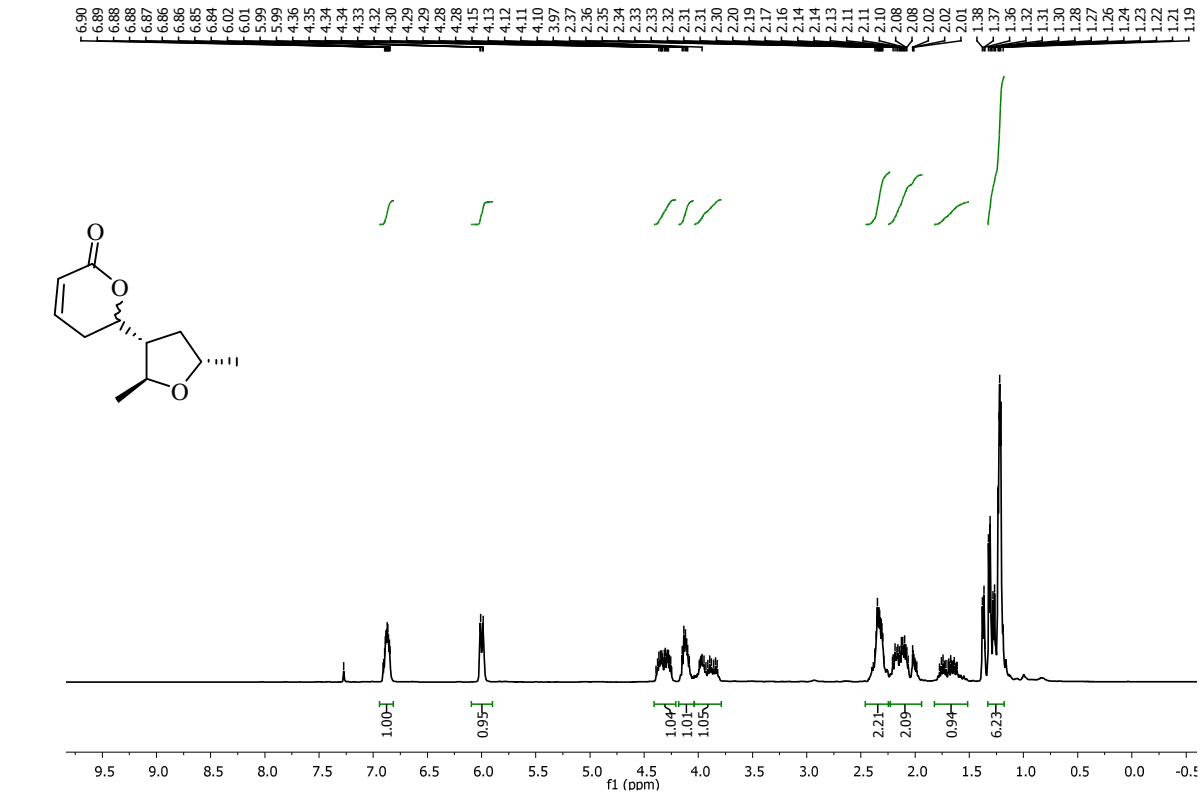
^{13}C NMR of compound 92 (100 MHz, $CDCl_3$)



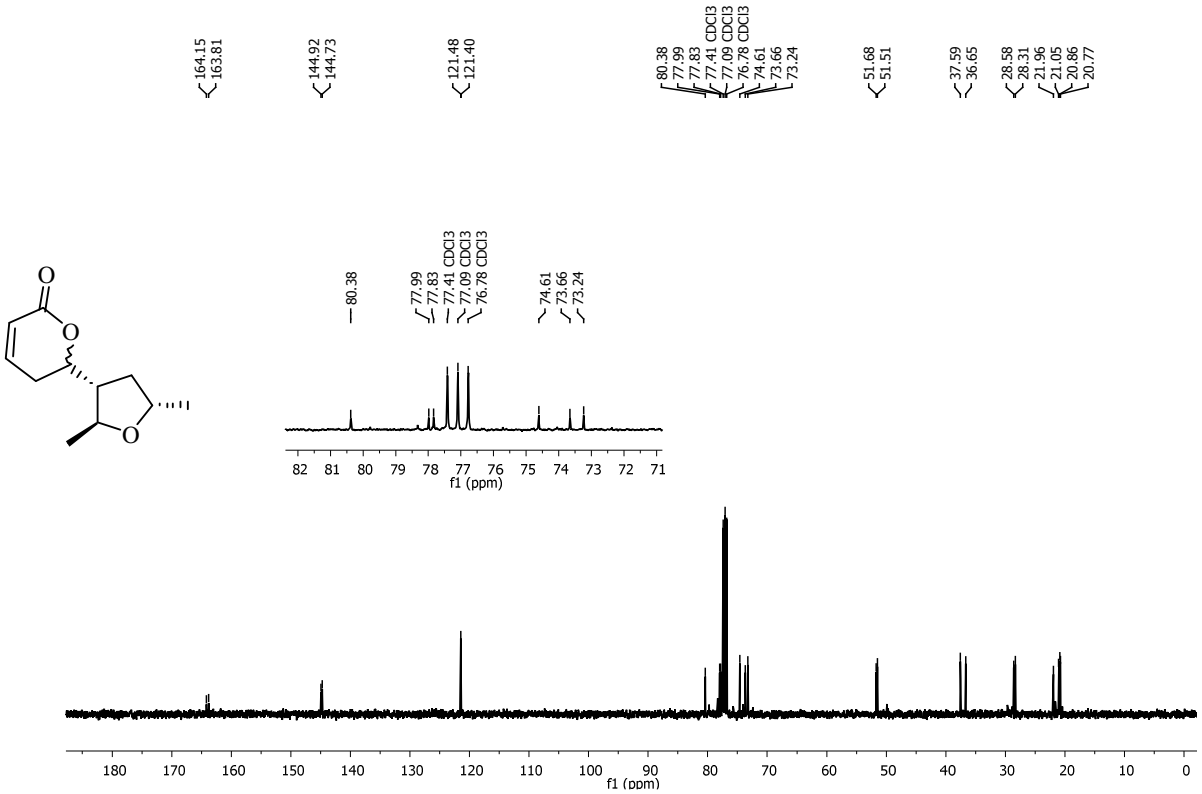
DEPT-135 NMR of compound 92 (100 MHz, $CDCl_3$)



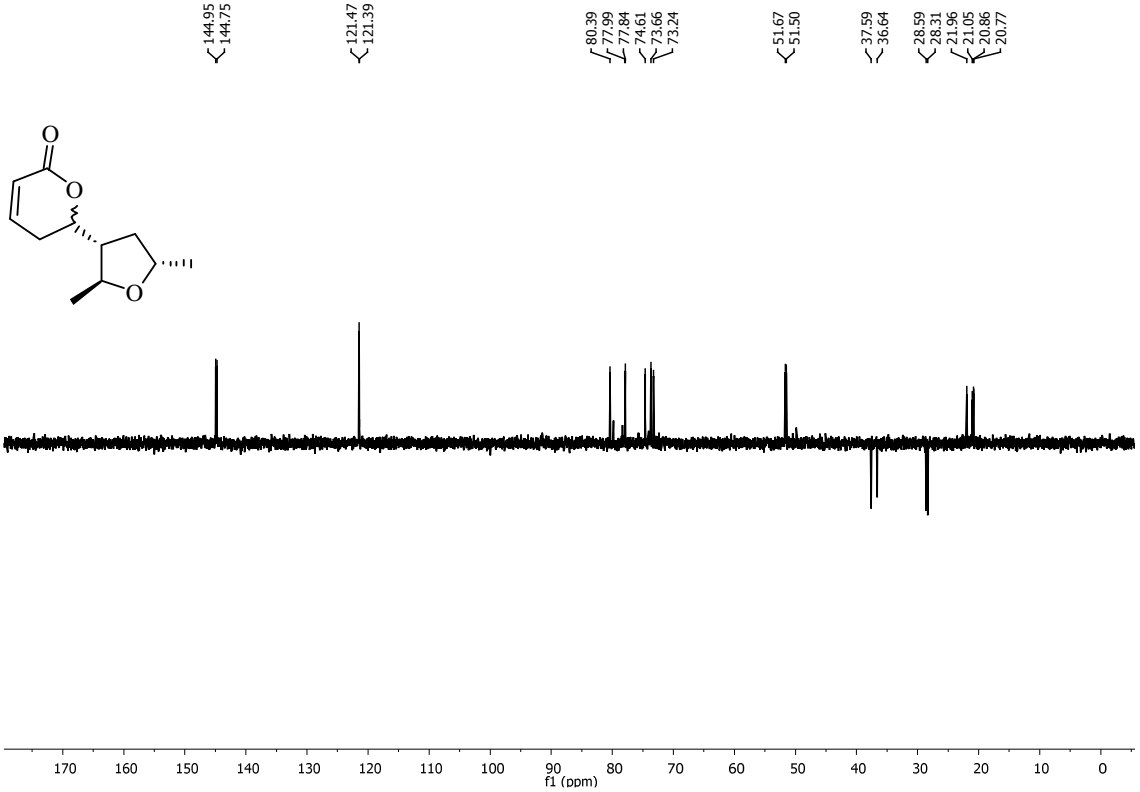
^{1}H - NMR of compound 93 (400 MHz, $CDCl_3$)



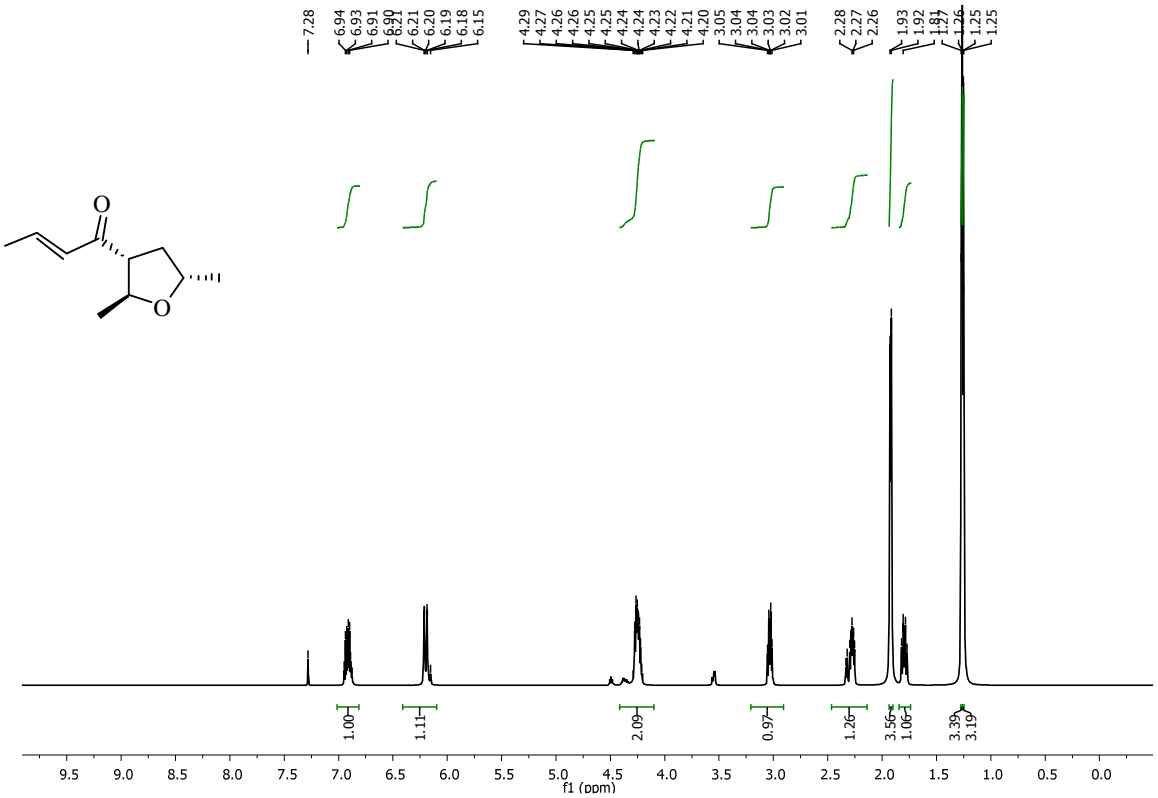
^{13}C NMR of compound 93 (100 MHz, $CDCl_3$)



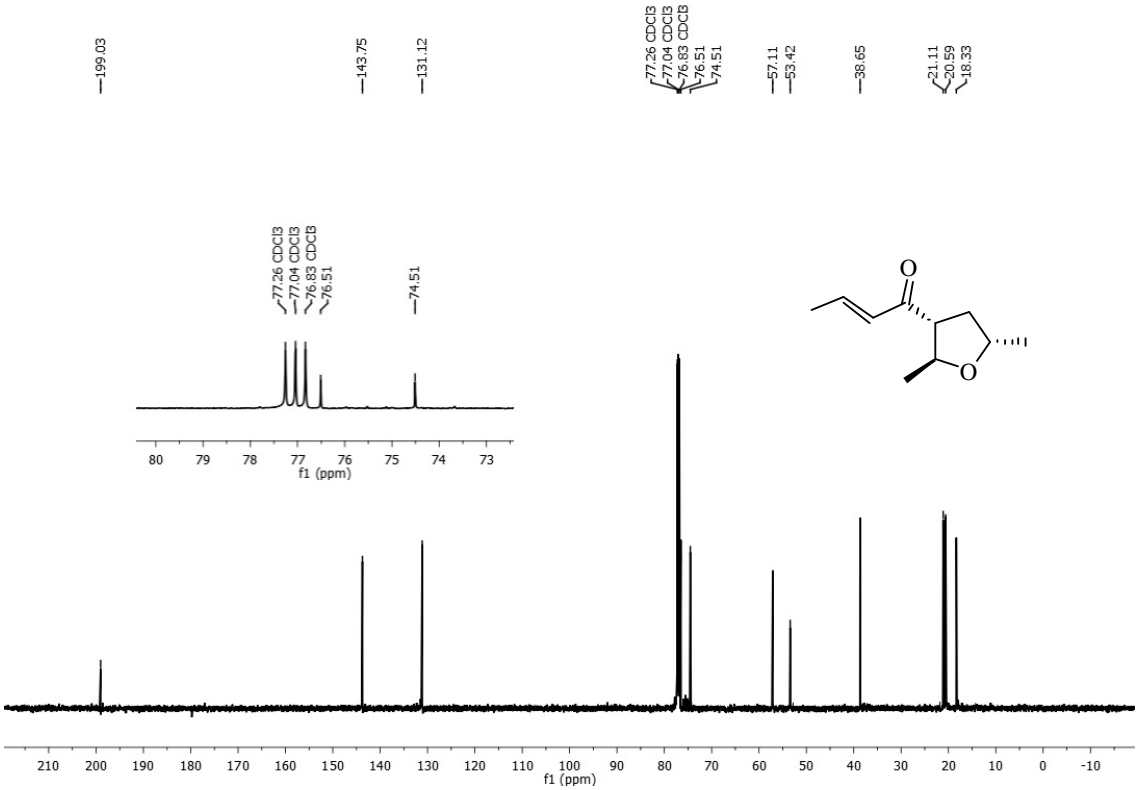
DEPT-135 NMR of compound 93 (100 MHz, $CDCl_3$)



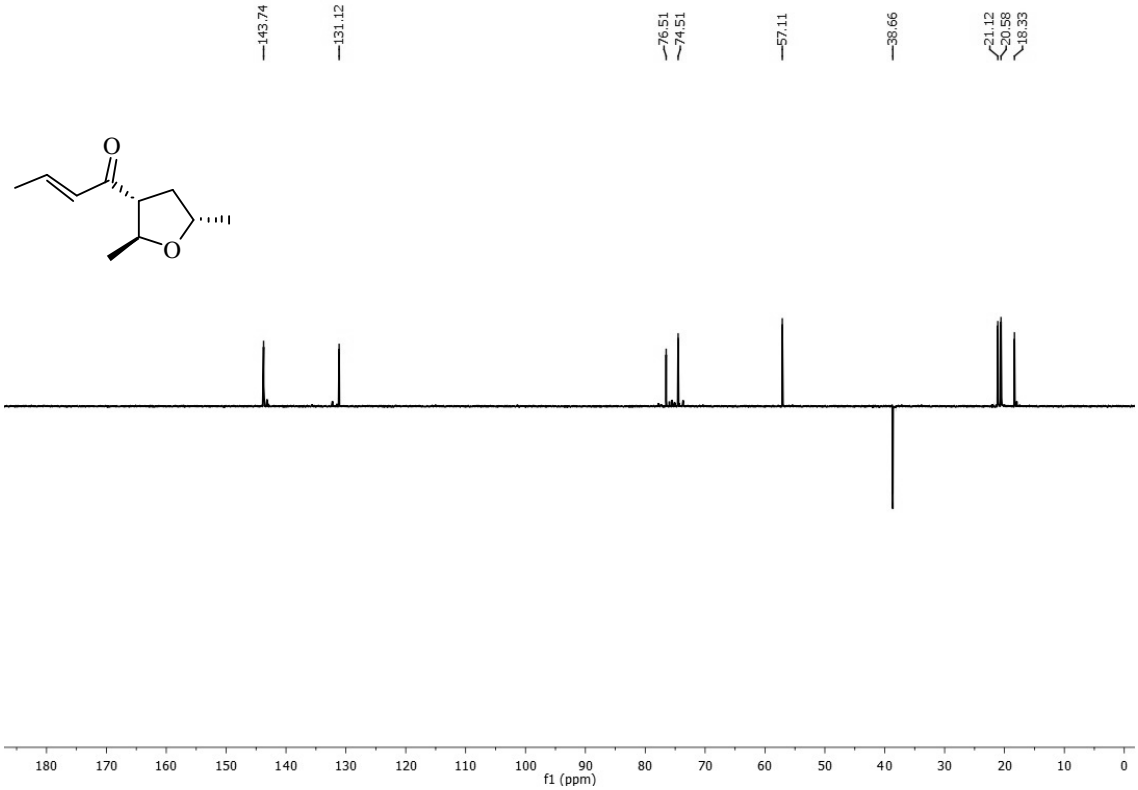
^{1}H - NMR of compound 94 (600 MHz, $CDCl_3$)



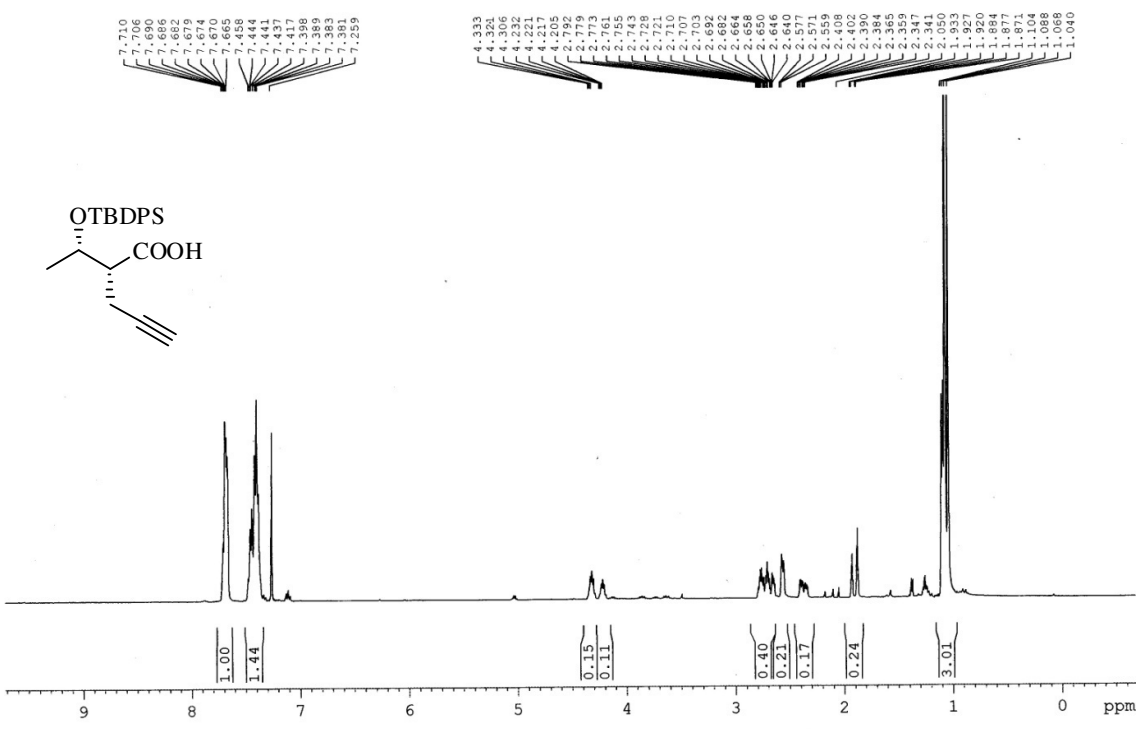
^{13}C NMR of compound 94 (150 MHz, $CDCl_3$)



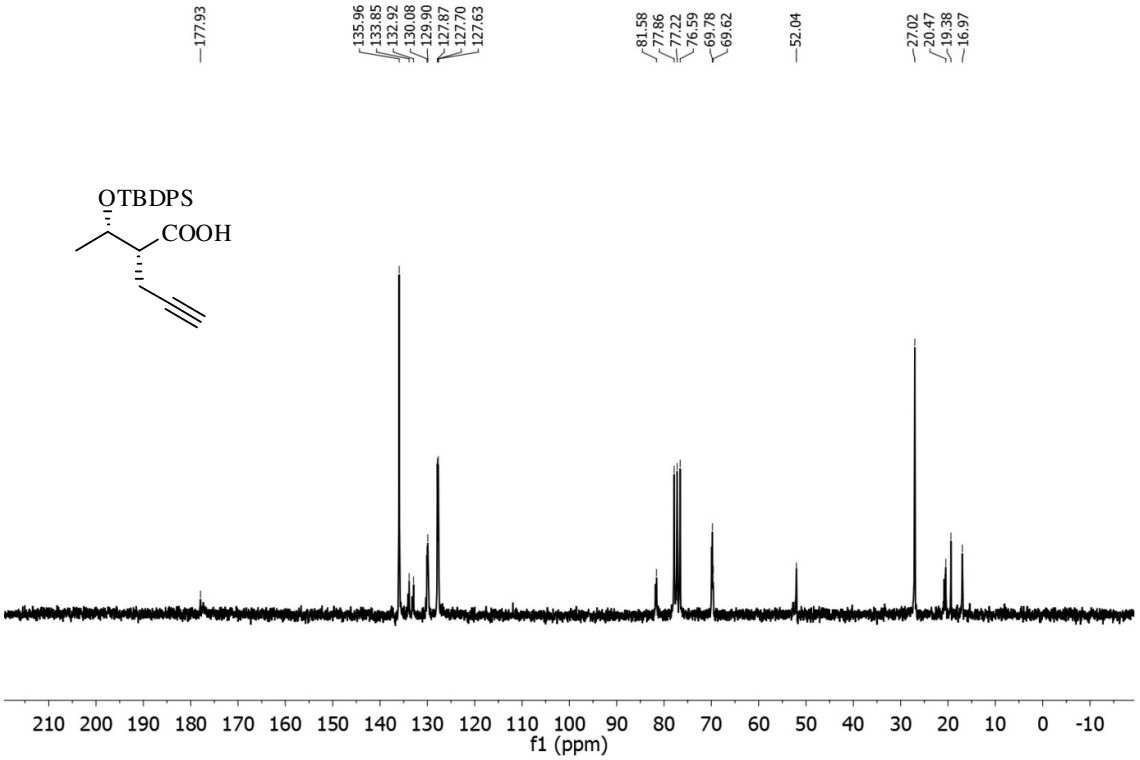
DEPT-135 NMR of compound 94 (150 MHz, $CDCl_3$)



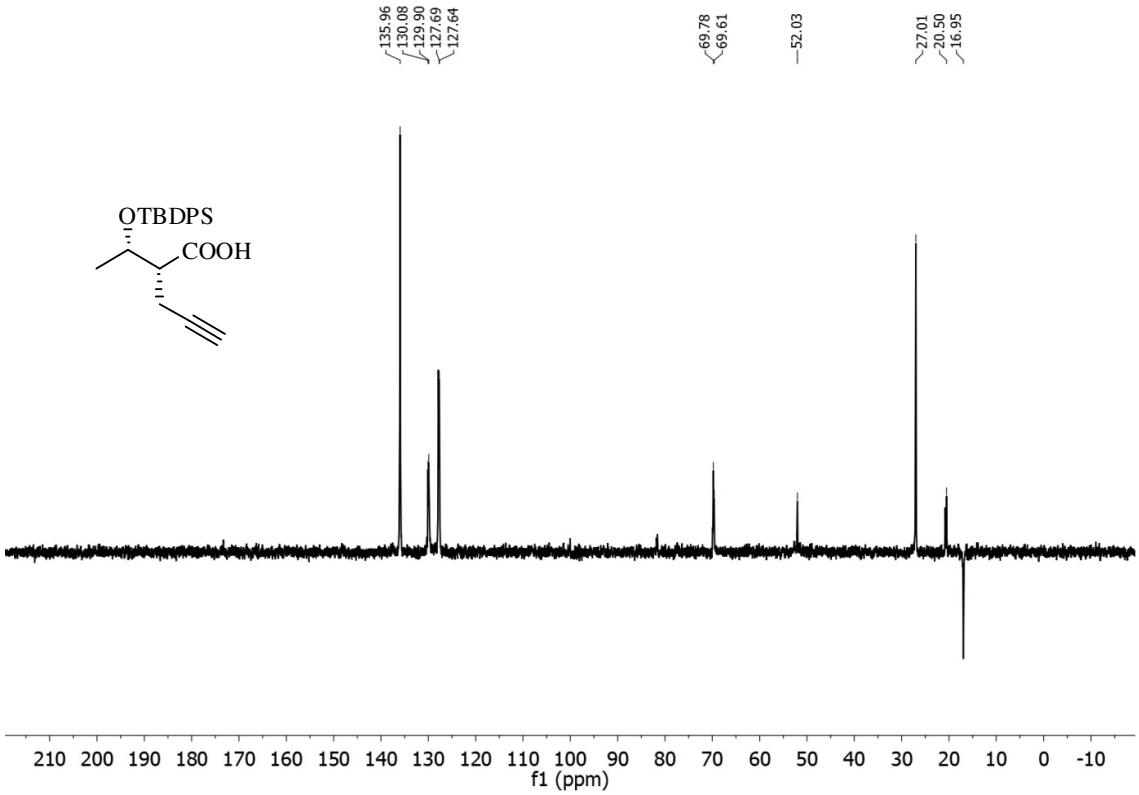
^{1}H - NMR of compound 95 (400 MHz, $CDCl_3$)



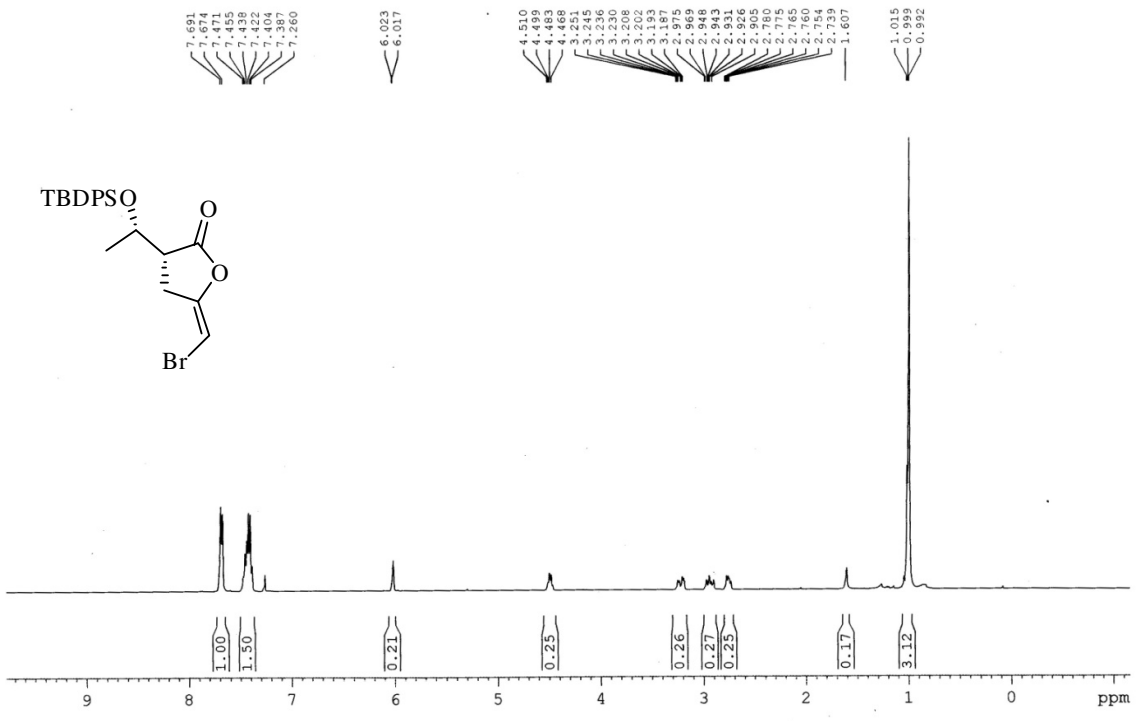
^{13}C NMR of compound 95 (50 MHz, $CDCl_3$)



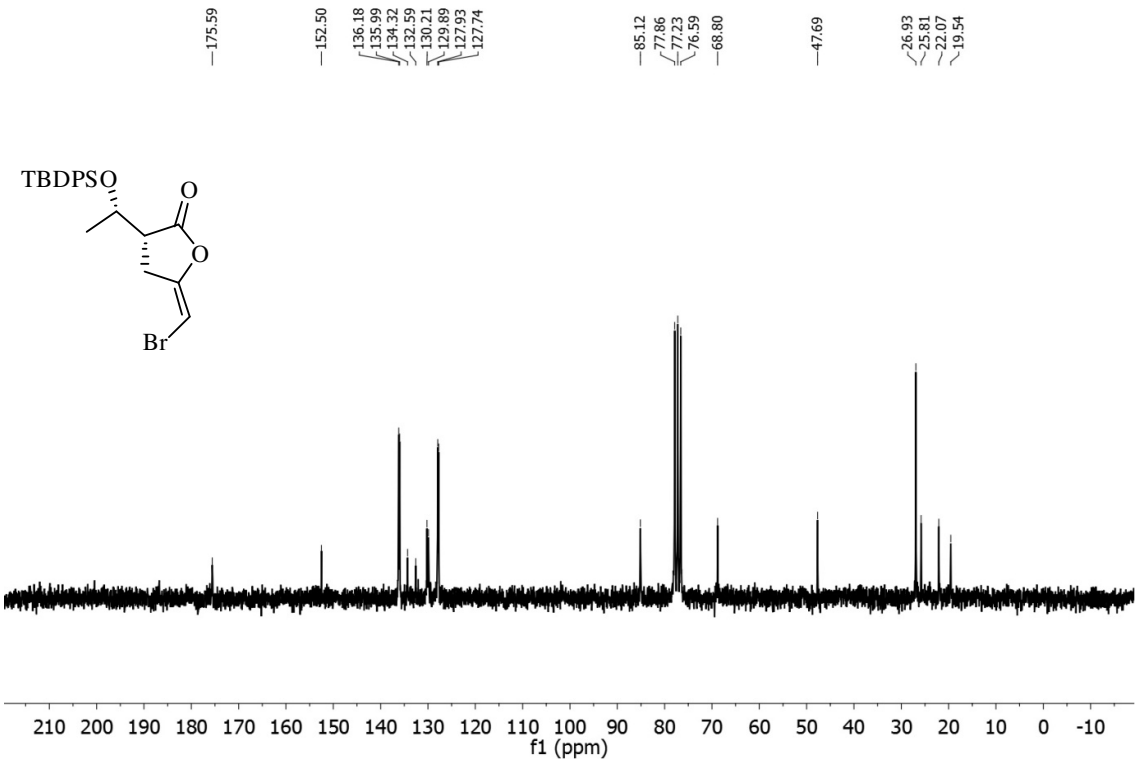
DEPT-135 NMR of compound 95 (50 MHz, $CDCl_3$)



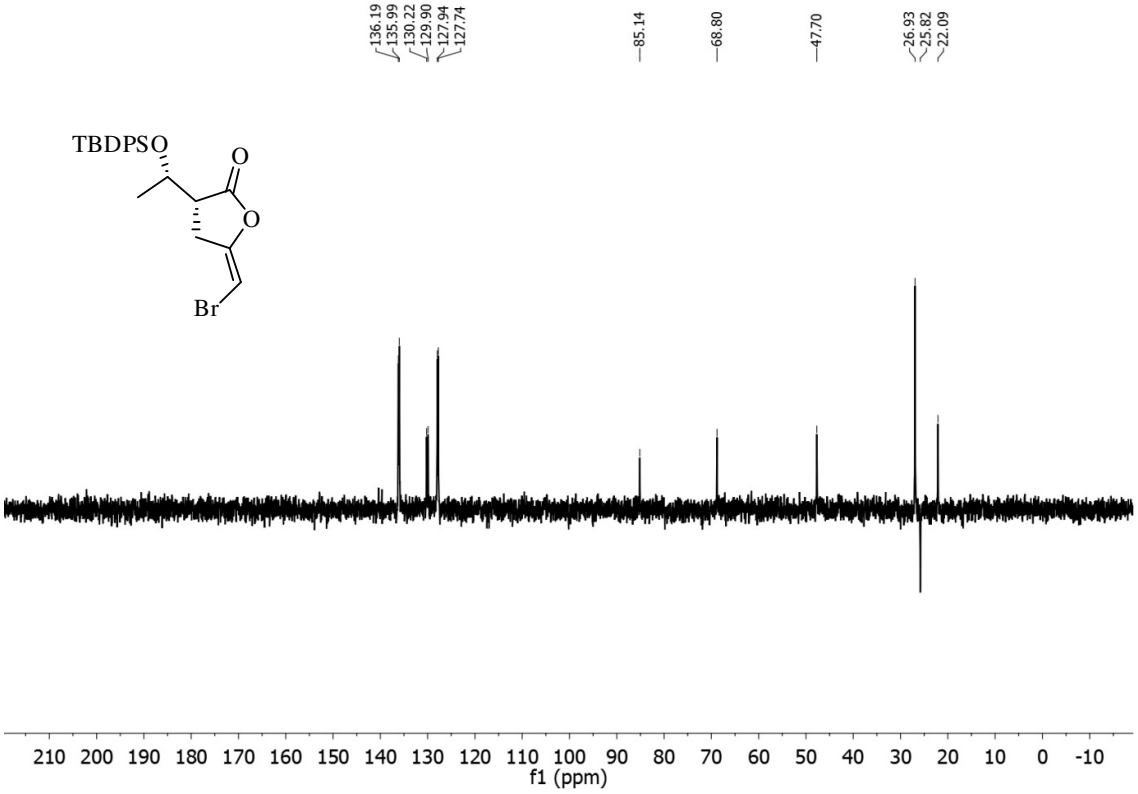
^{1}H - NMR of compound 96 (400 MHz, $CDCl_3$)



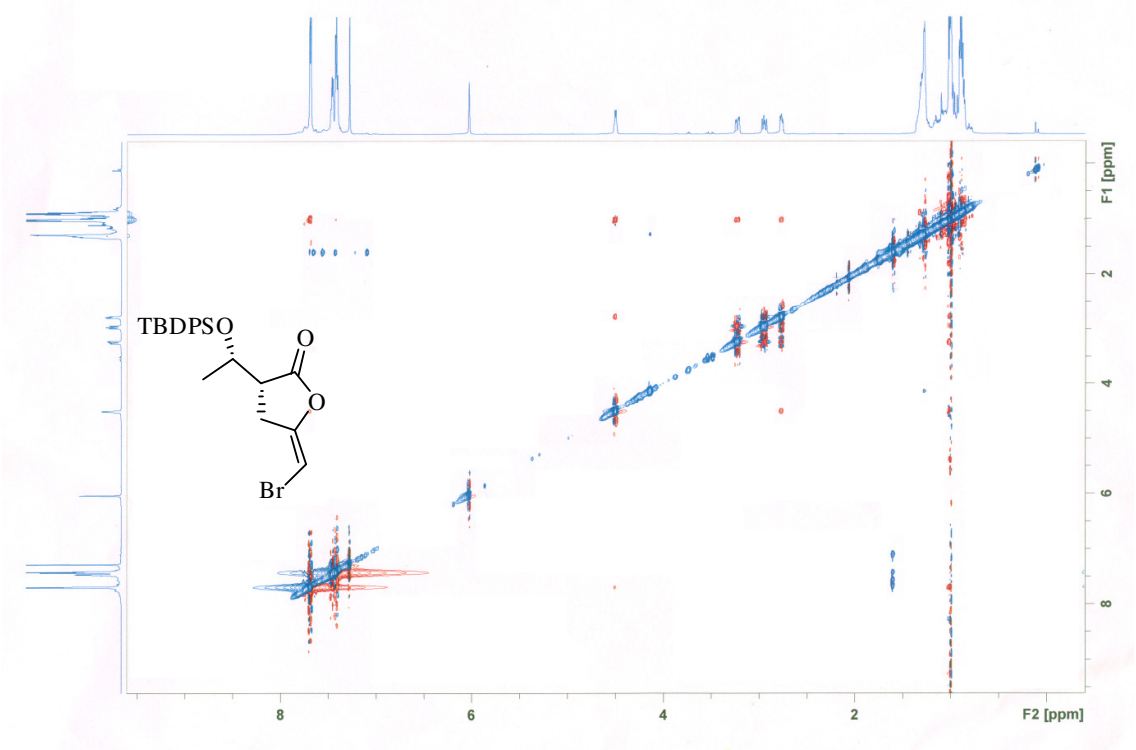
^{13}C NMR of compound 96 (50 MHz, $CDCl_3$)



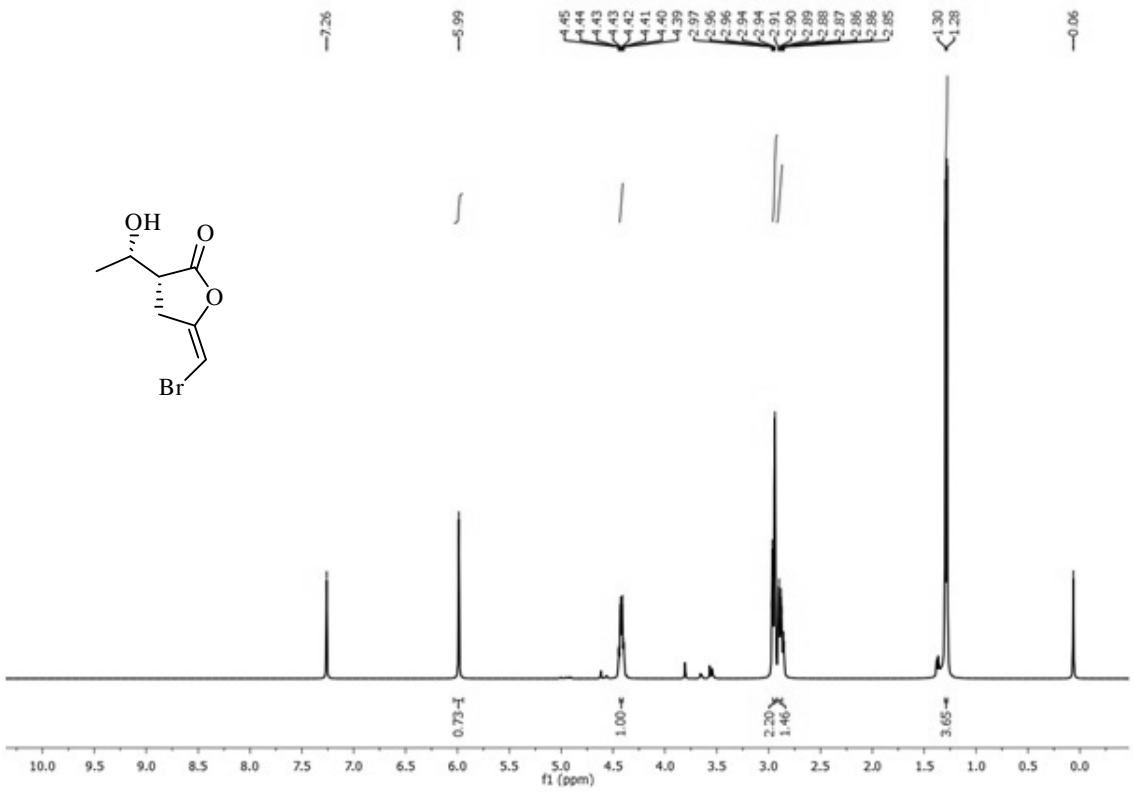
DEPT-135 NMR of compound 96 (50 MHz, $CDCl_3$)



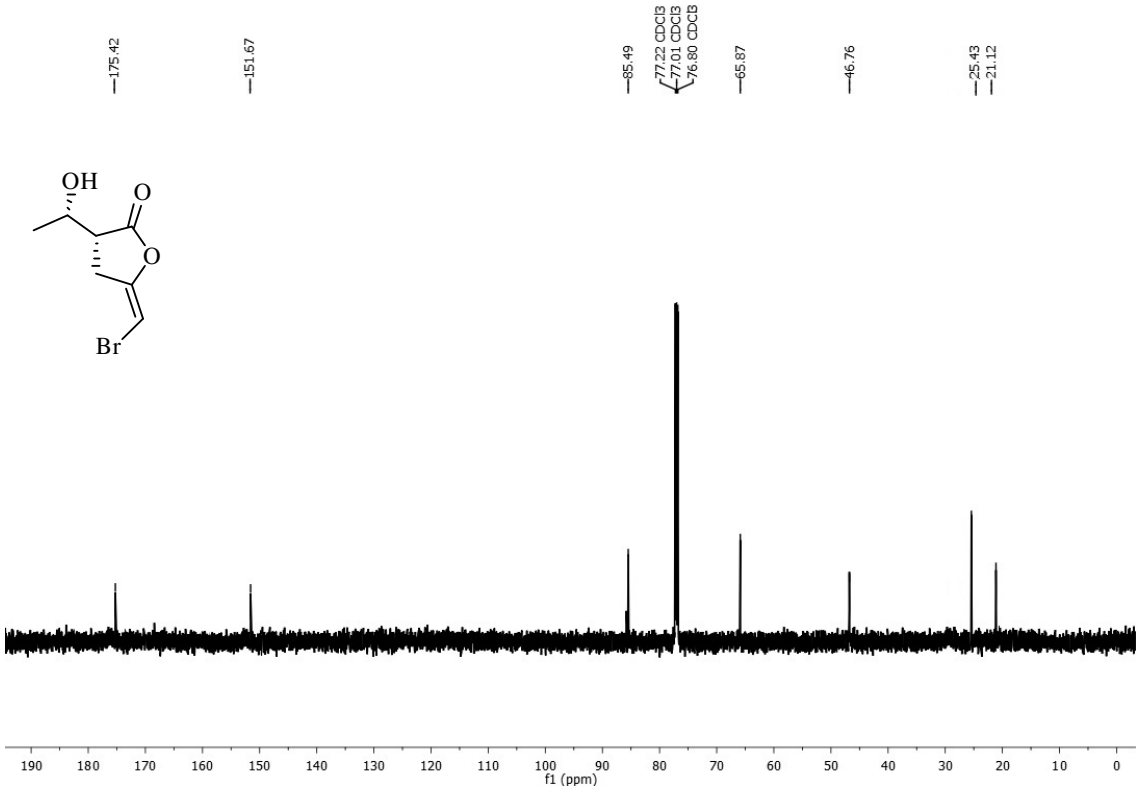
NOESY Spectrum of compound 96 (600 MHz, $CDCl_3$)



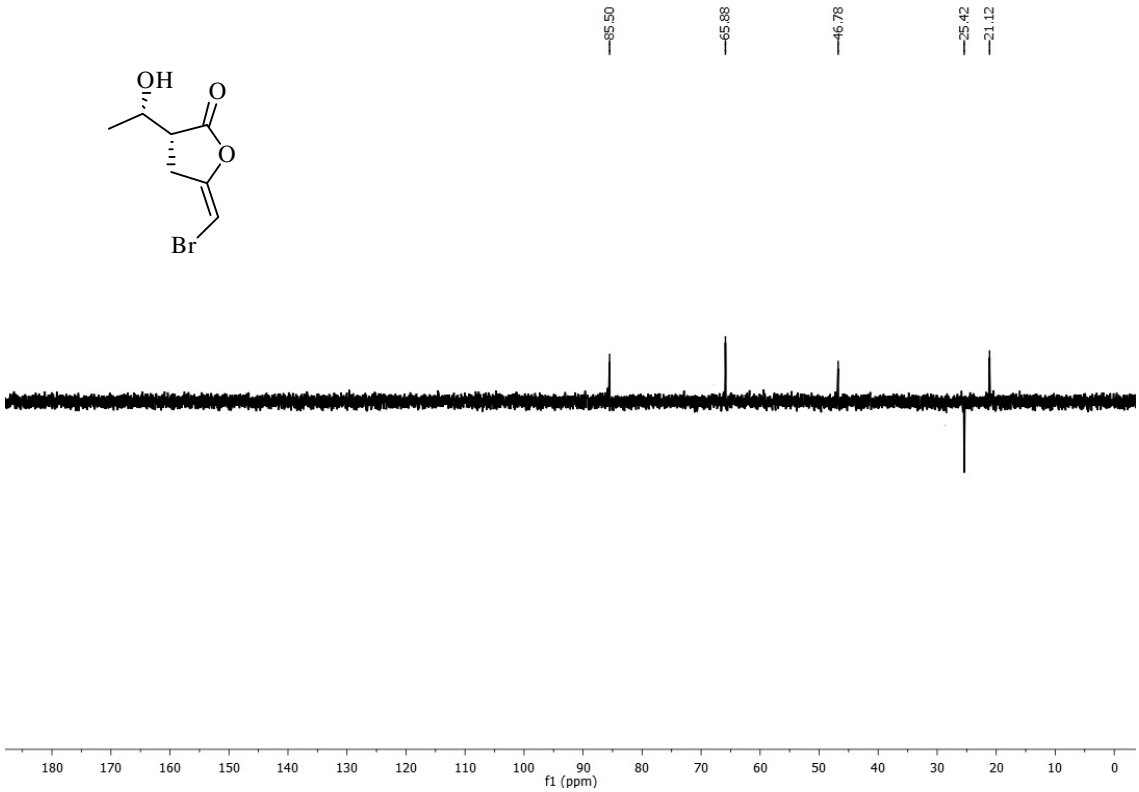
^{1}H - NMR of compound 97 (400 MHz, $CDCl_3$)



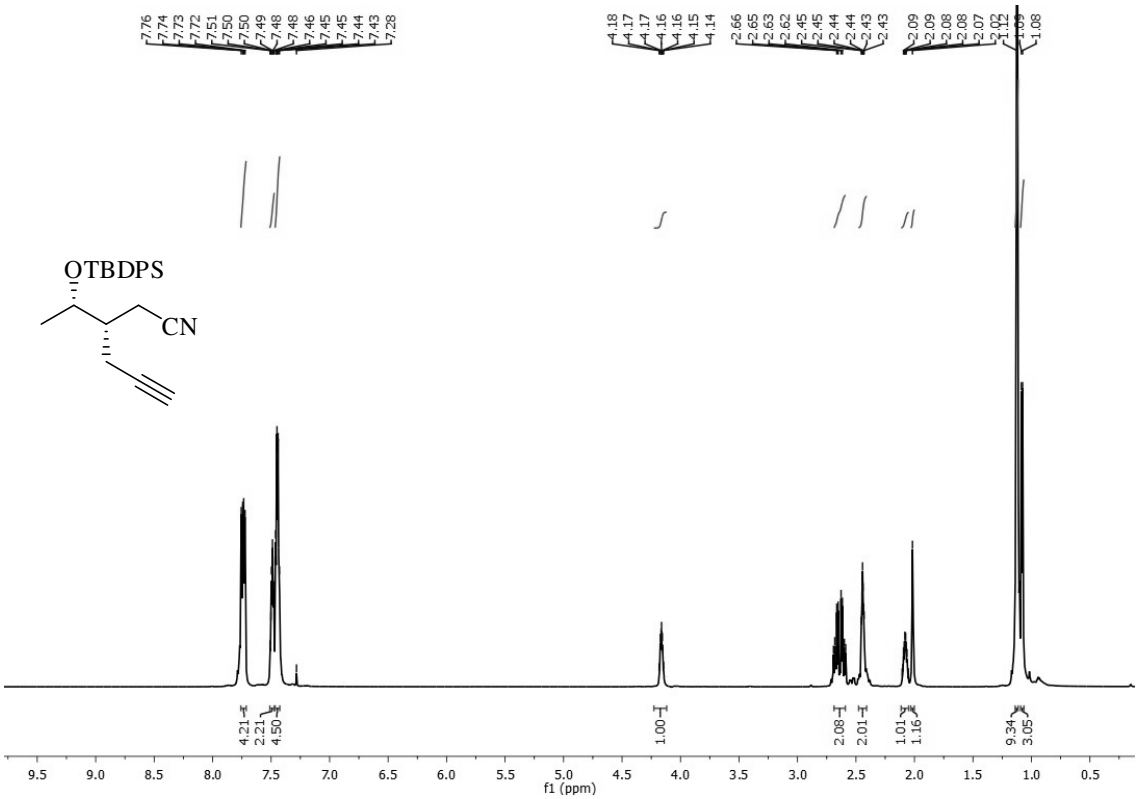
^{13}C NMR of compound 97 (150 MHz, $CDCl_3$)



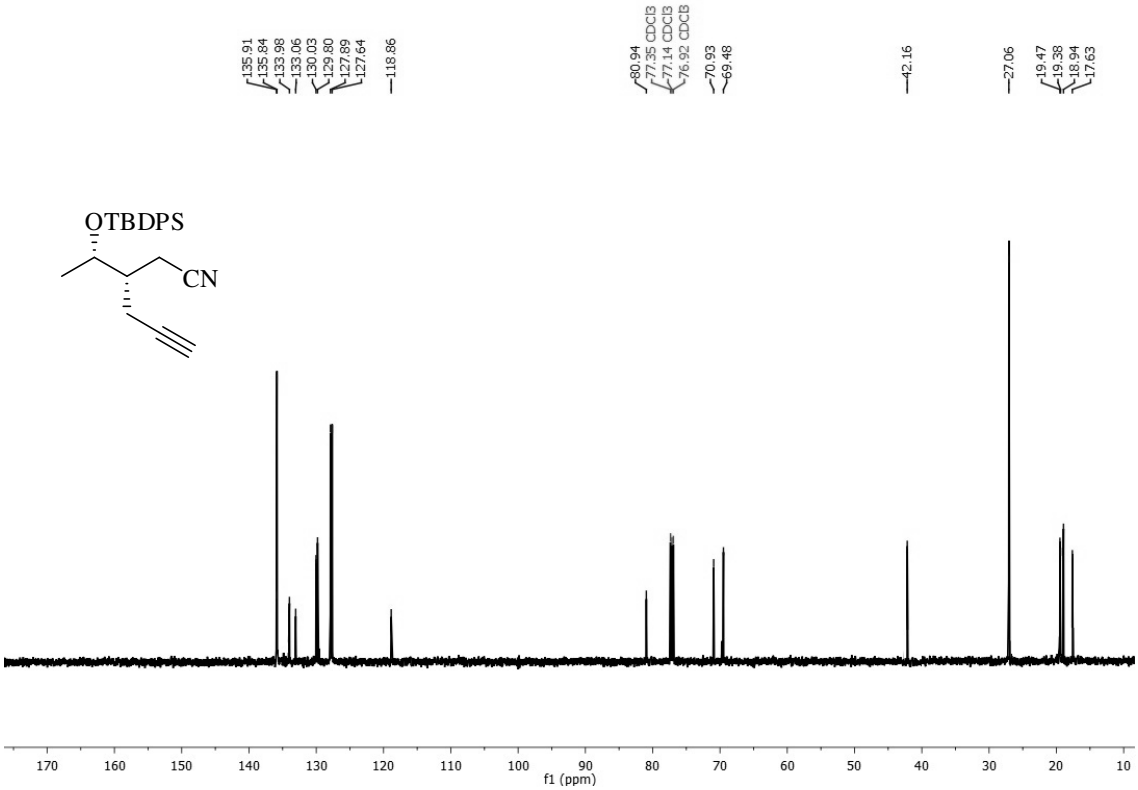
DEPT-135 NMR of compound 97 (150 MHz, $CDCl_3$)



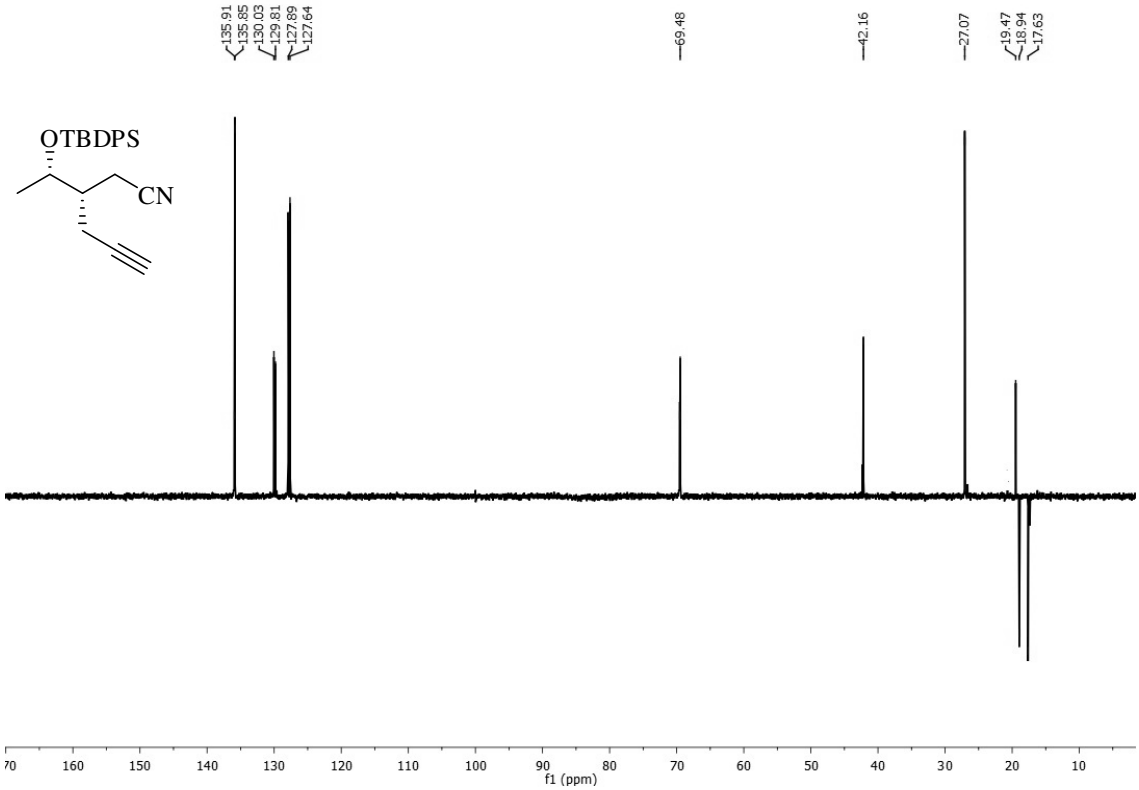
^{1}H - NMR of compound 98 (600 MHz, $CDCl_3$)



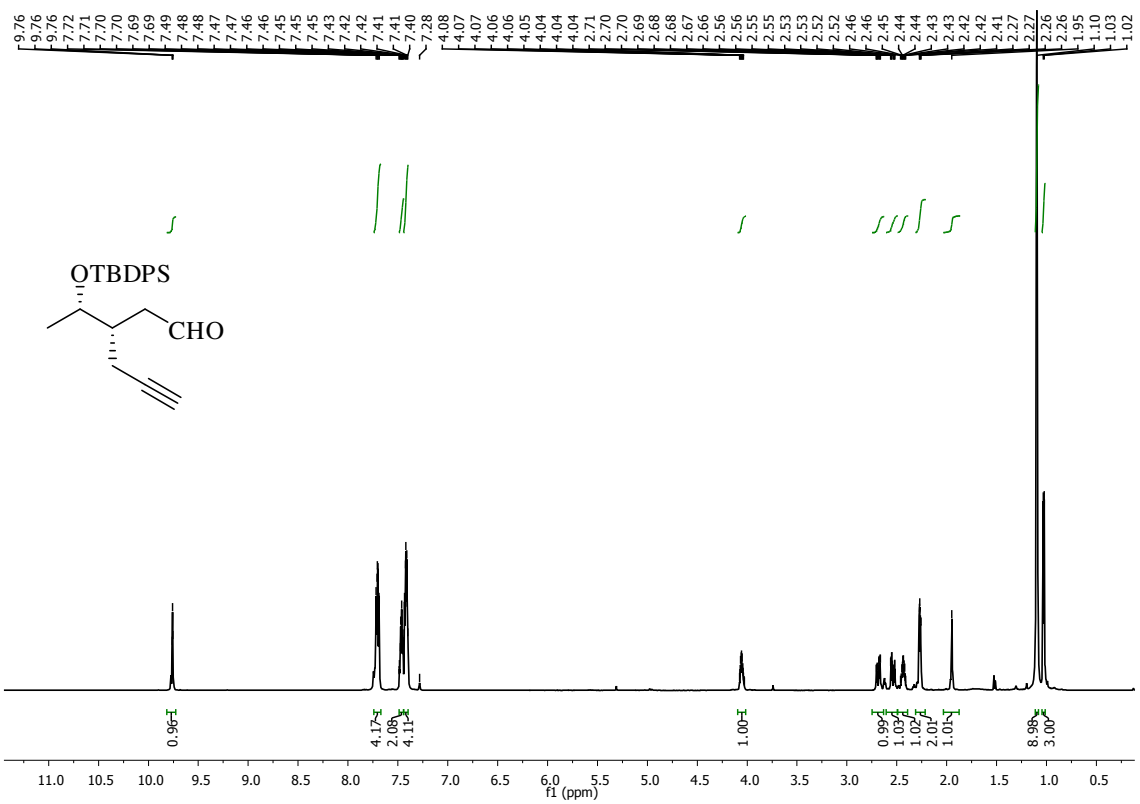
^{13}C NMR of compound 98 (150 MHz, $CDCl_3$)



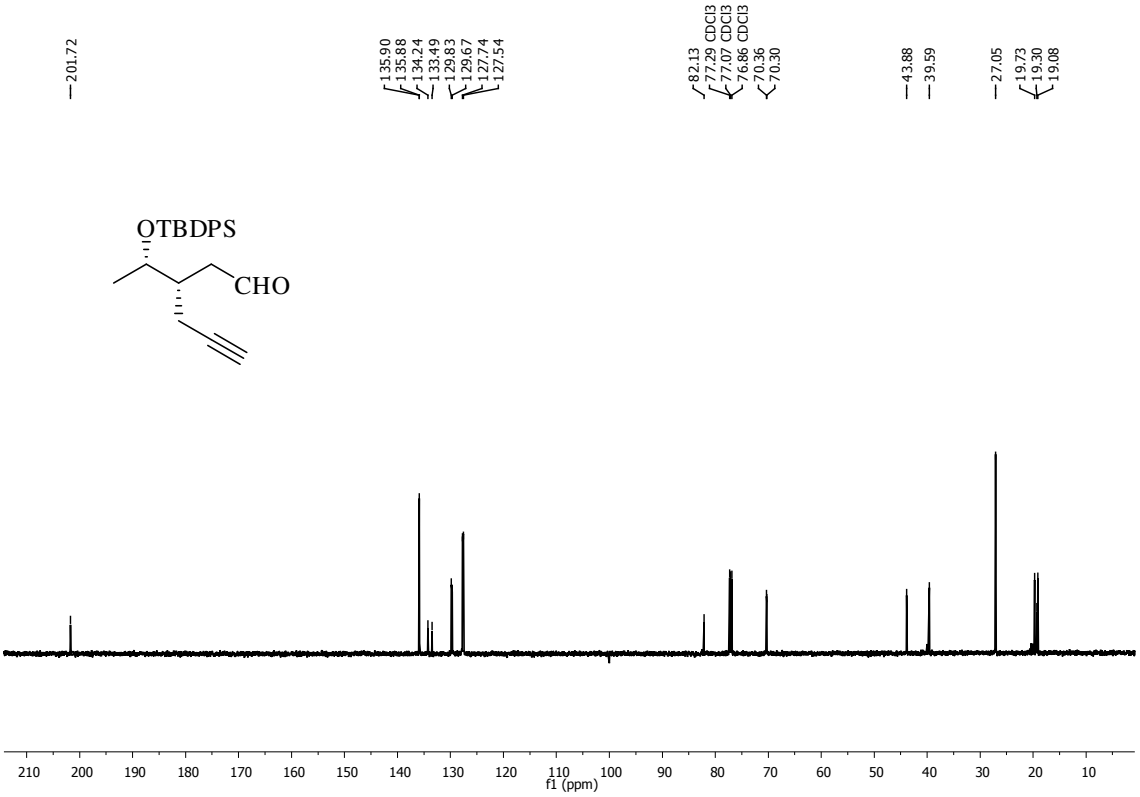
DEPT-135 NMR of compound 98 (150 MHz, $CDCl_3$)



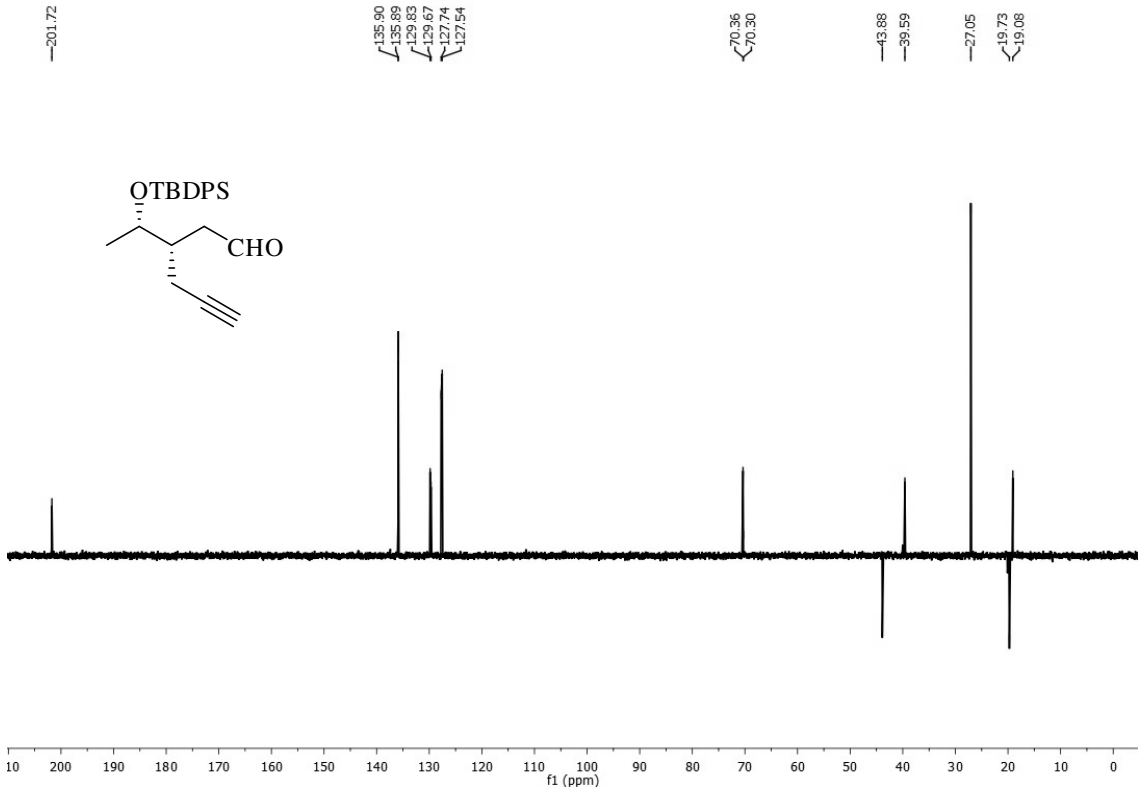
^{1}H - NMR of compound 99 (600 MHz, $CDCl_3$)



^{13}C NMR of compound 99 (150 MHz, $CDCl_3$)



DEPT-135 NMR of compound 99 (150 MHz, $CDCl_3$)



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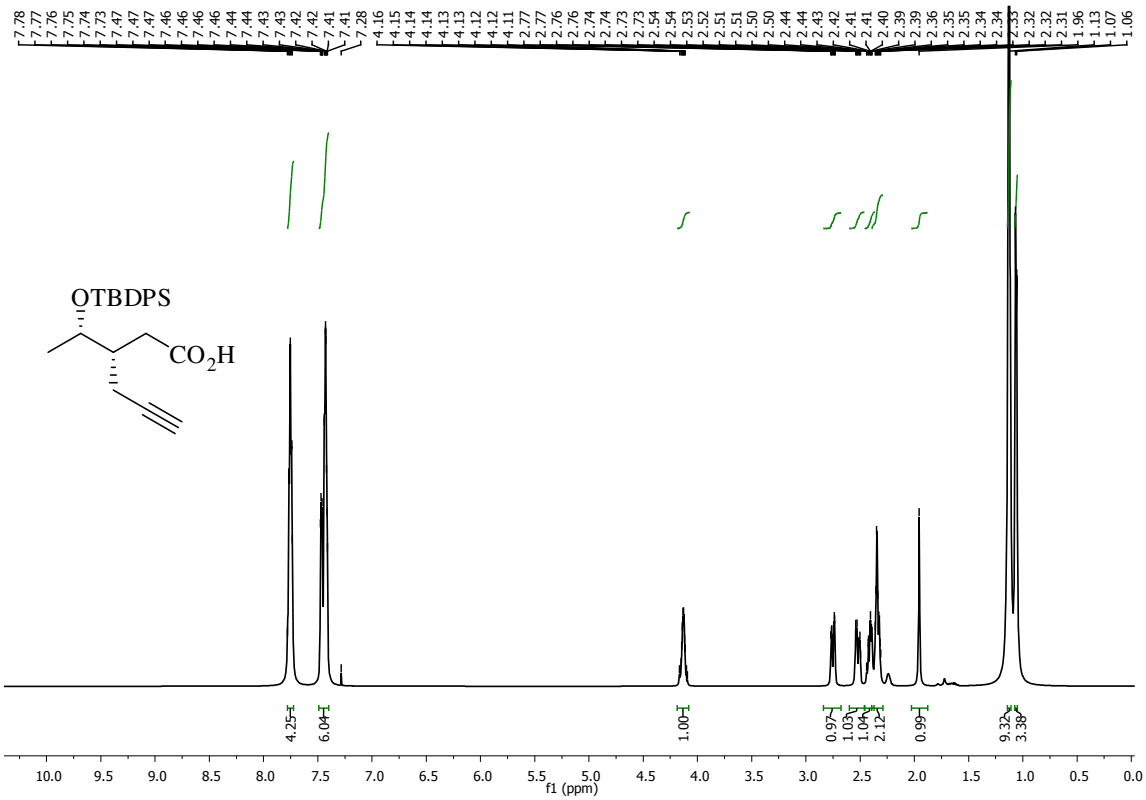
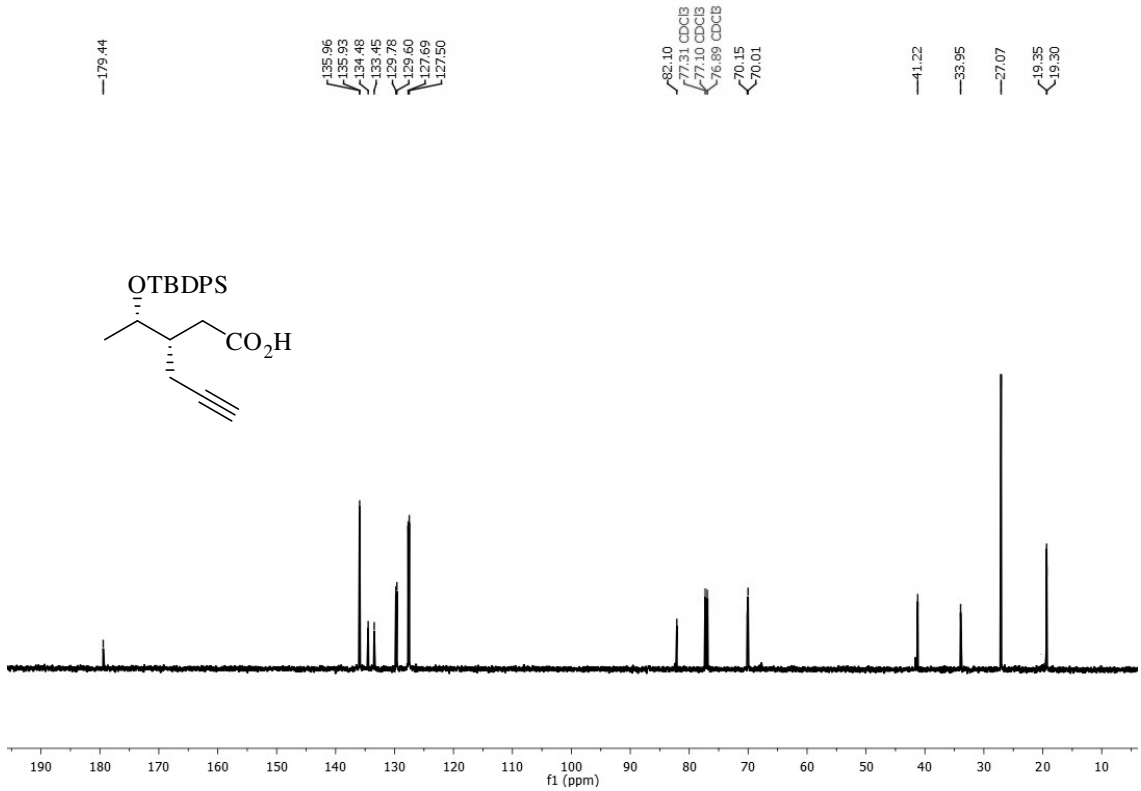
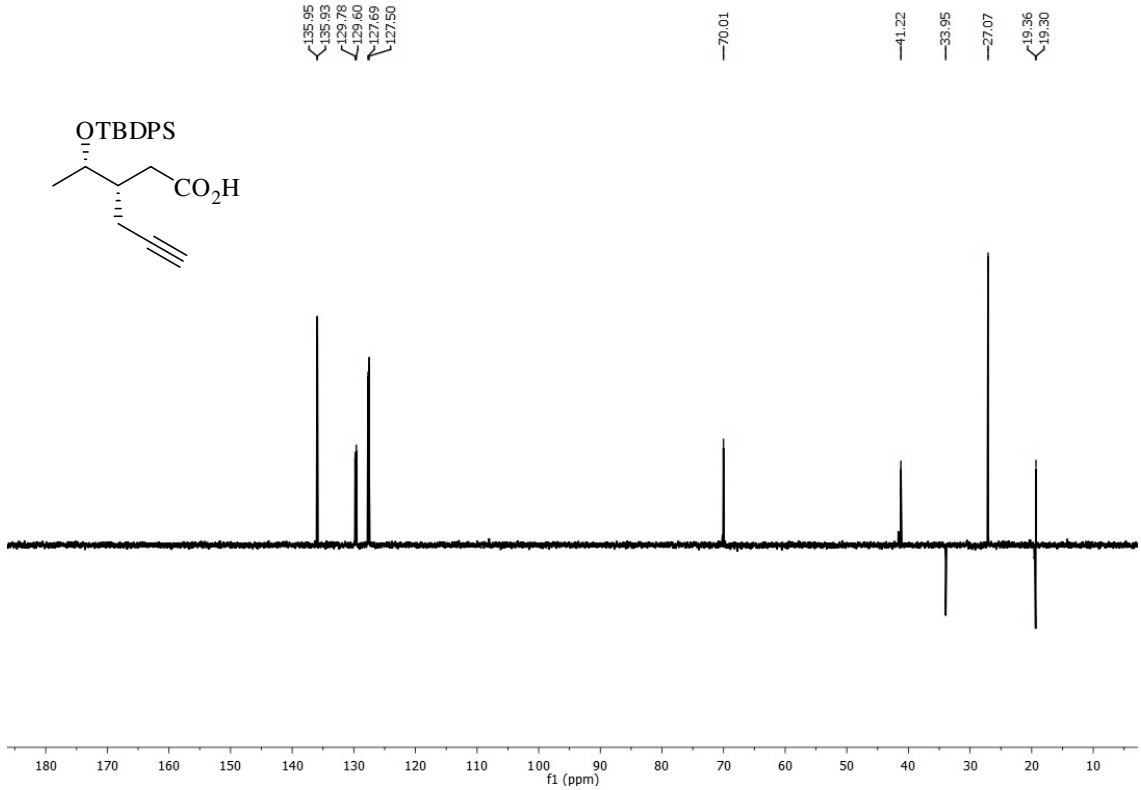


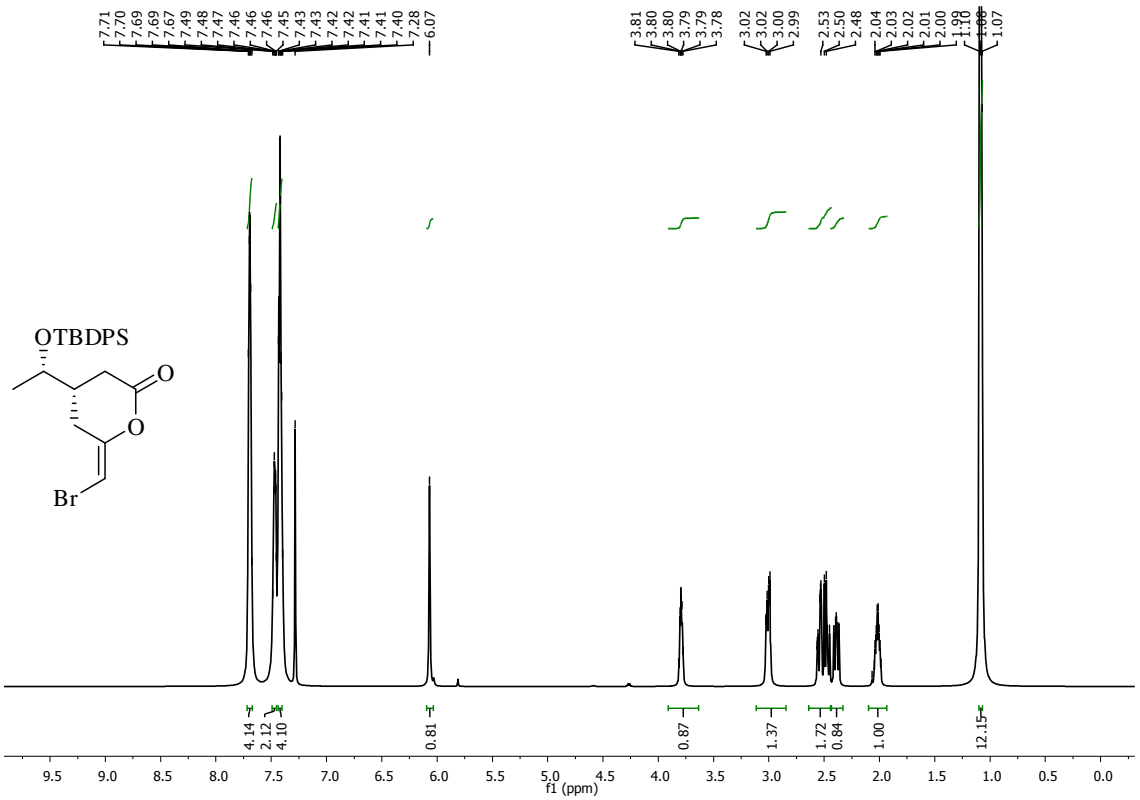
^{13}C NMR of compound 100 (150 MHz, $CDCl_3$)



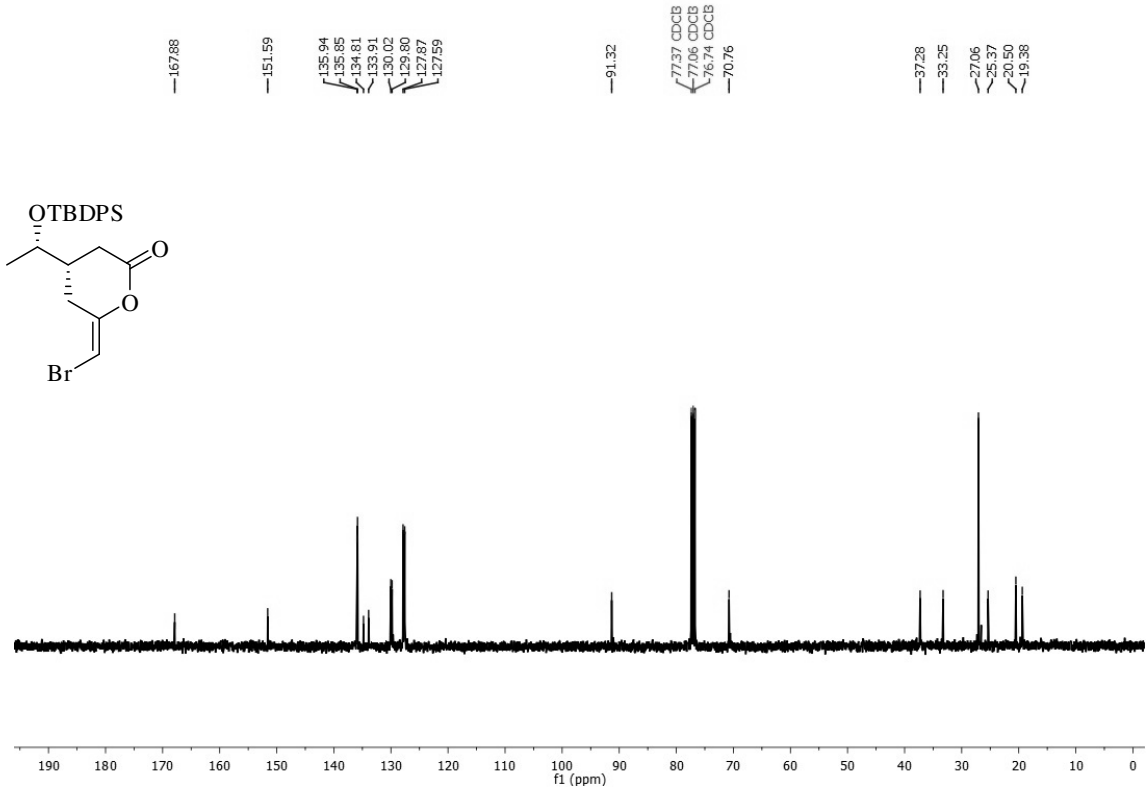
DEPT-135 NMR of compound 100 (150 MHz, $CDCl_3$)



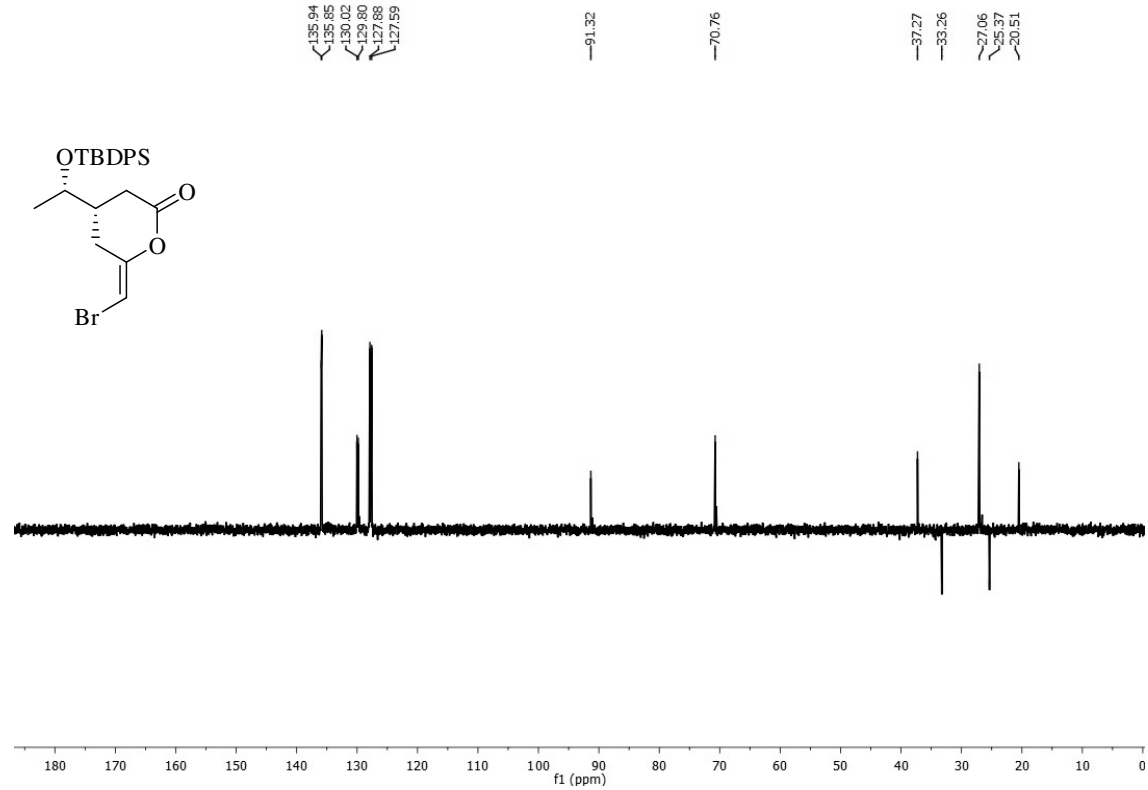
^{1}H - NMR of compound 101 (600 MHz, $CDCl_3$)



^{13}C NMR of compound 101 (100 MHz, $CDCl_3$)



DEPT-135 NMR of compound 101 (100 MHz, $CDCl_3$)



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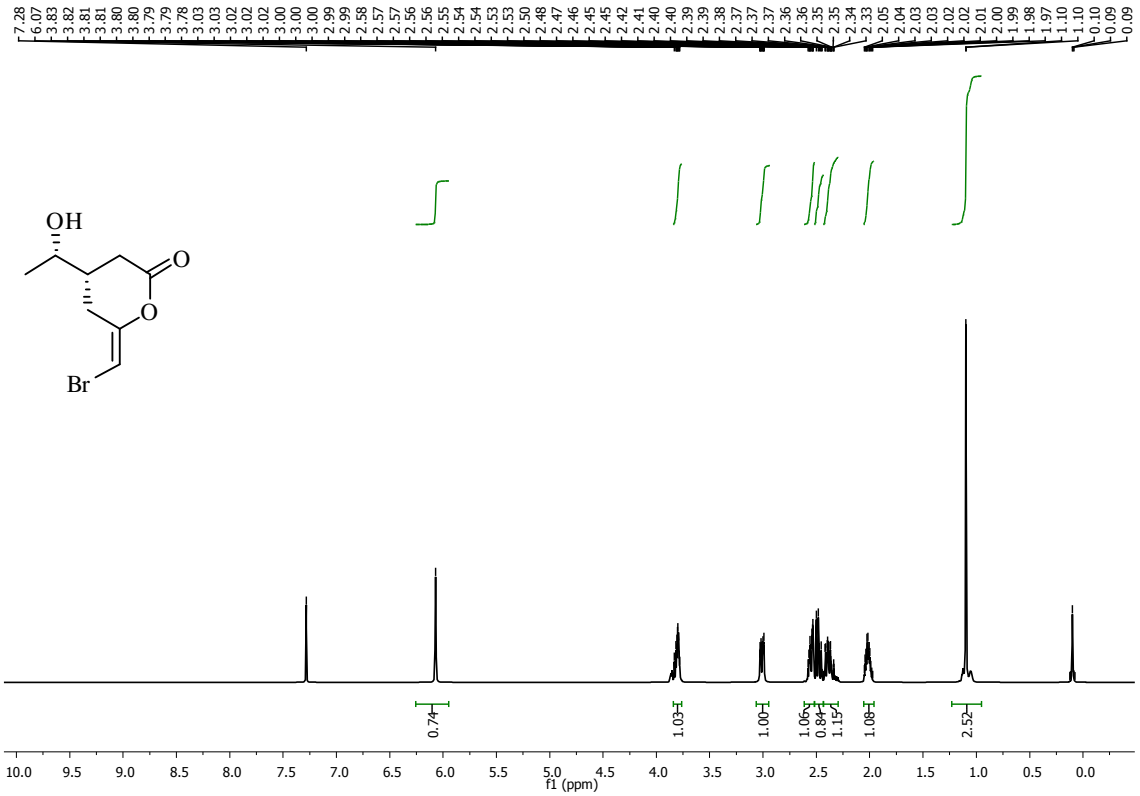

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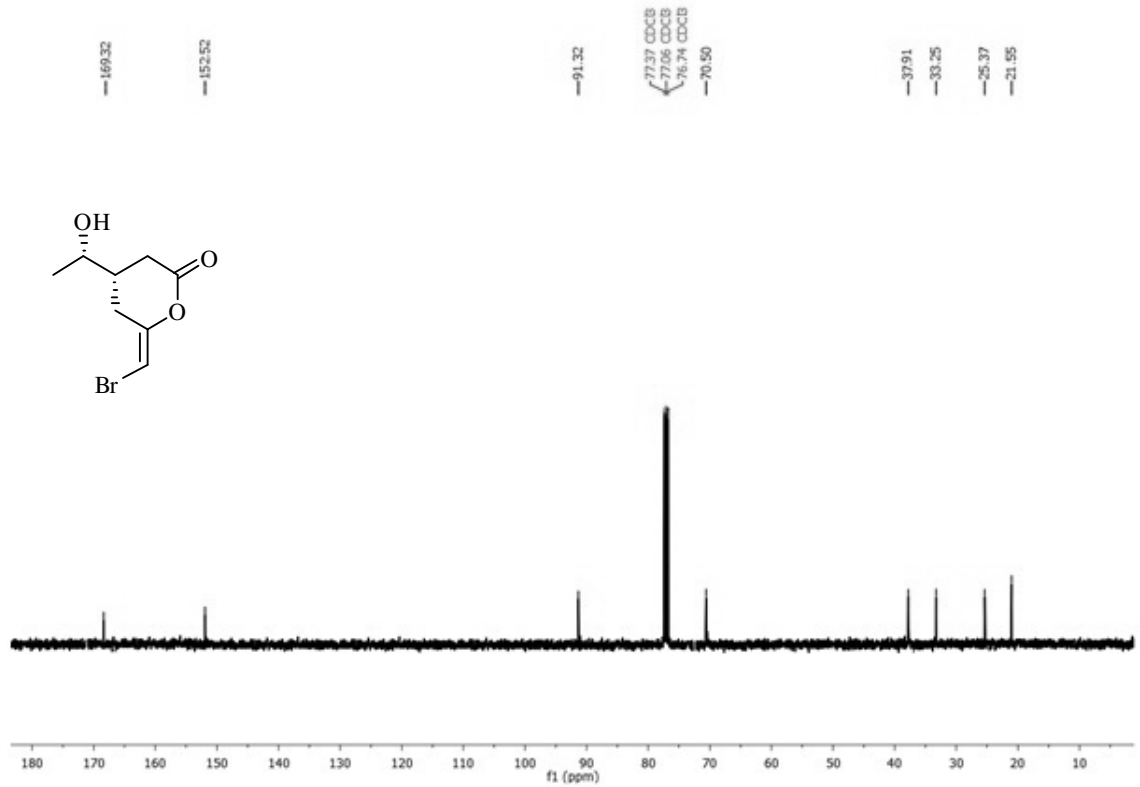

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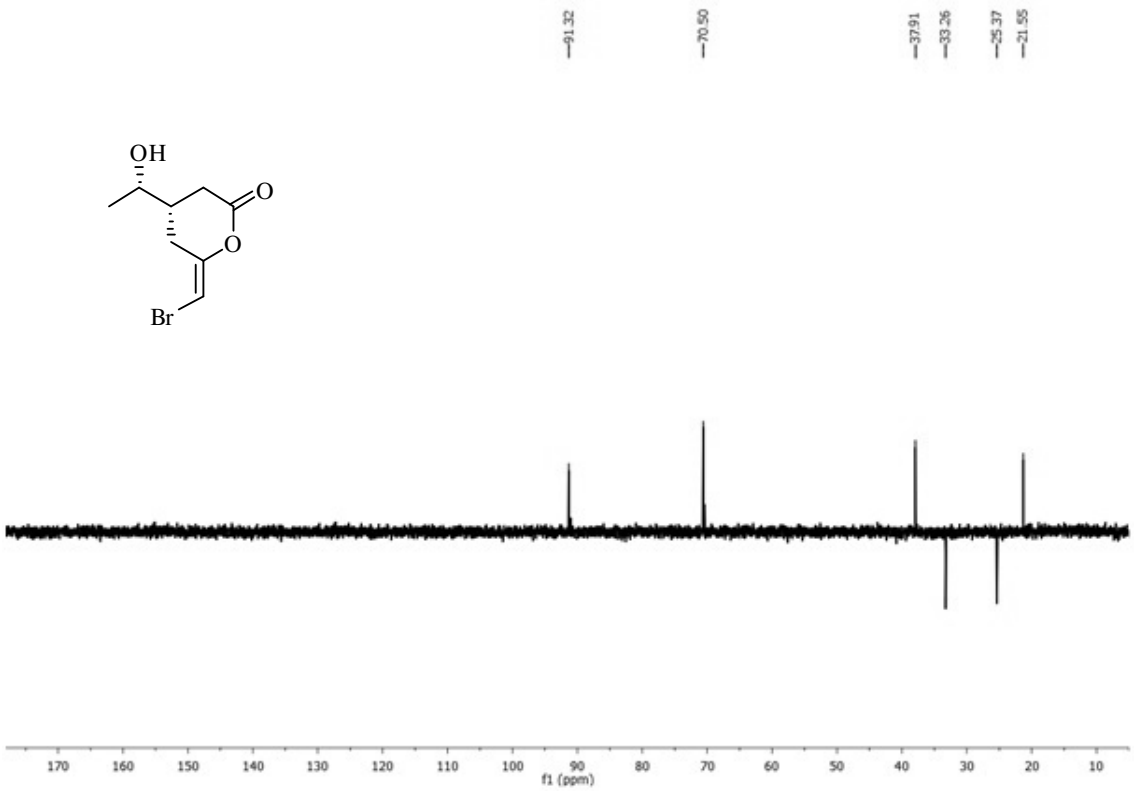

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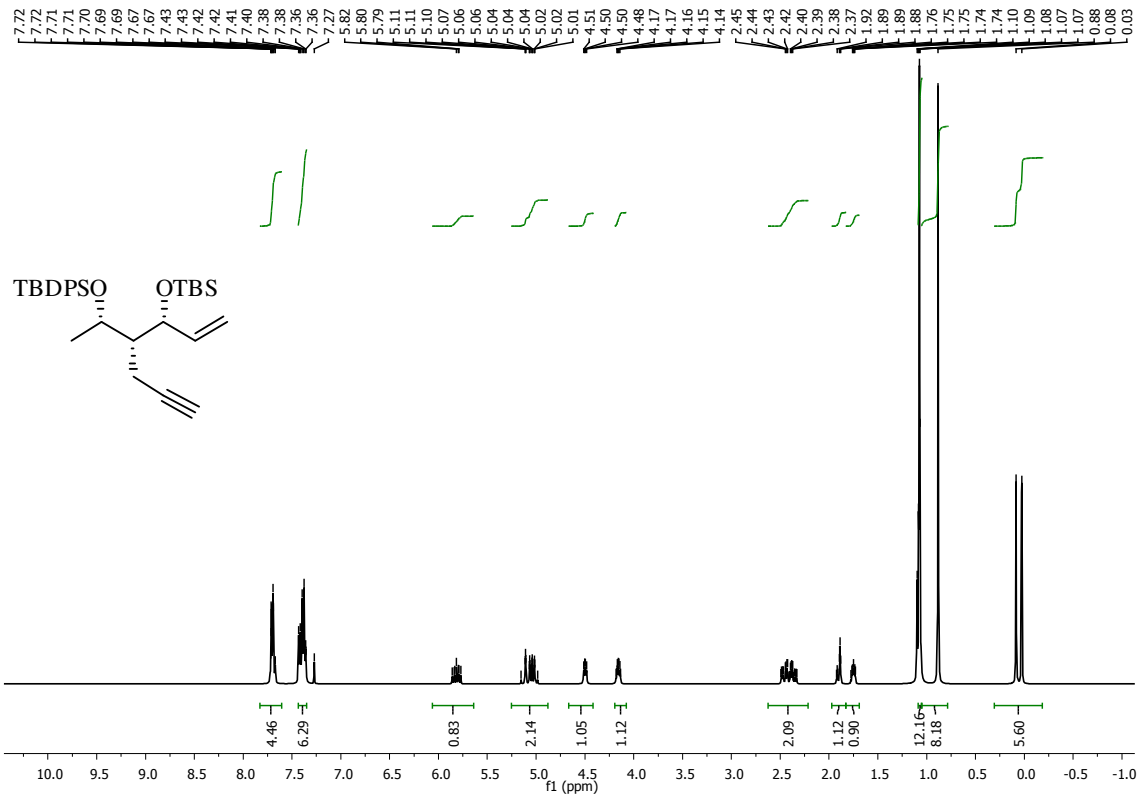
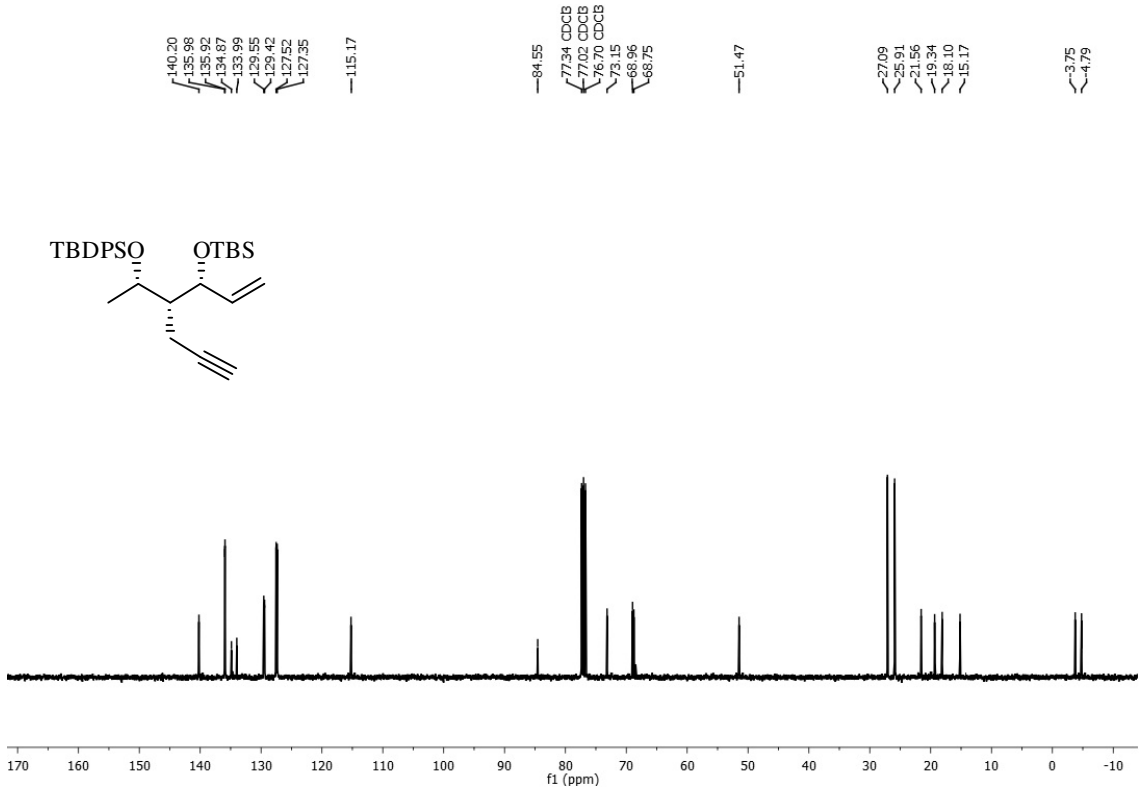
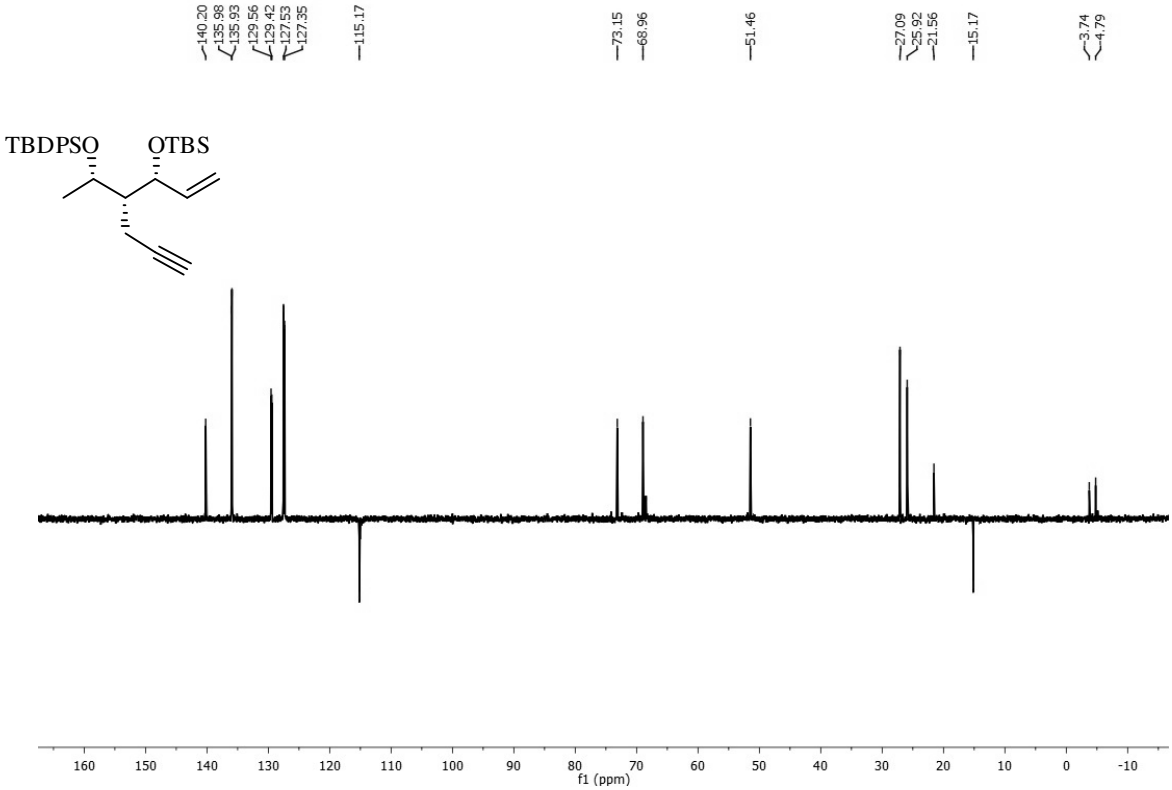


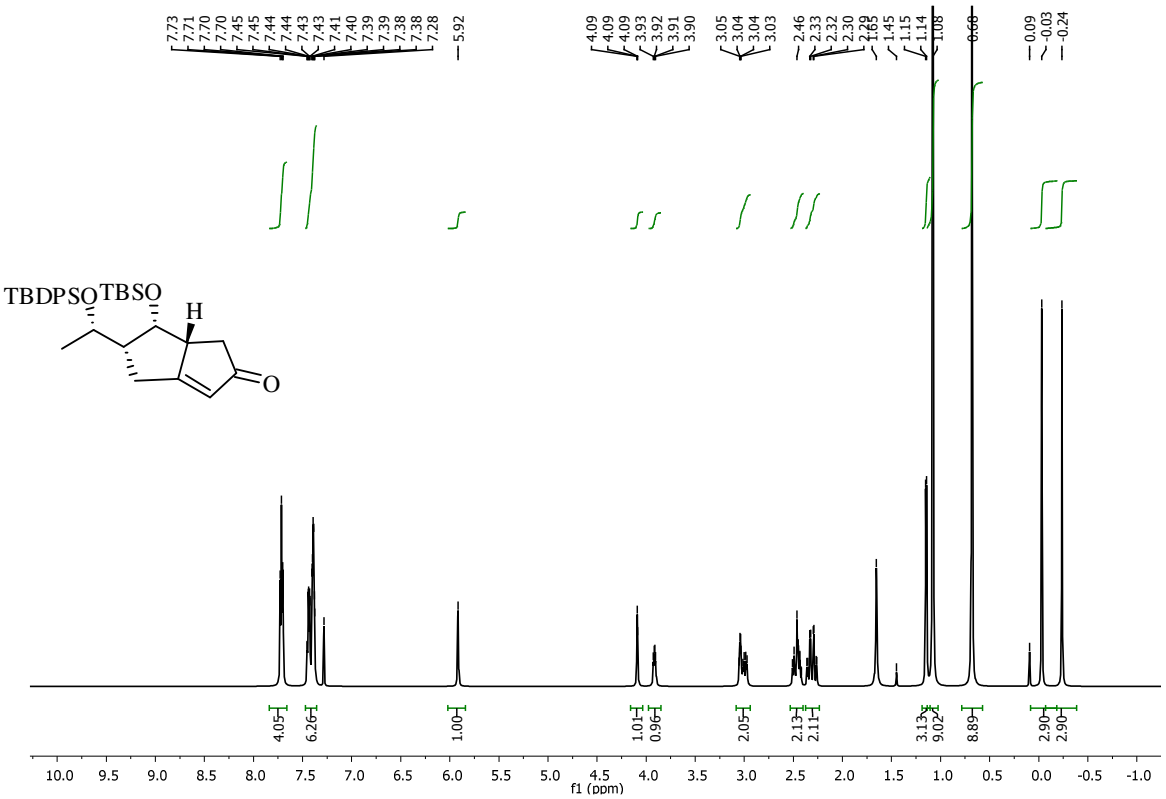
^{13}C NMR of compound 103 (100 MHz, $CDCl_3$)



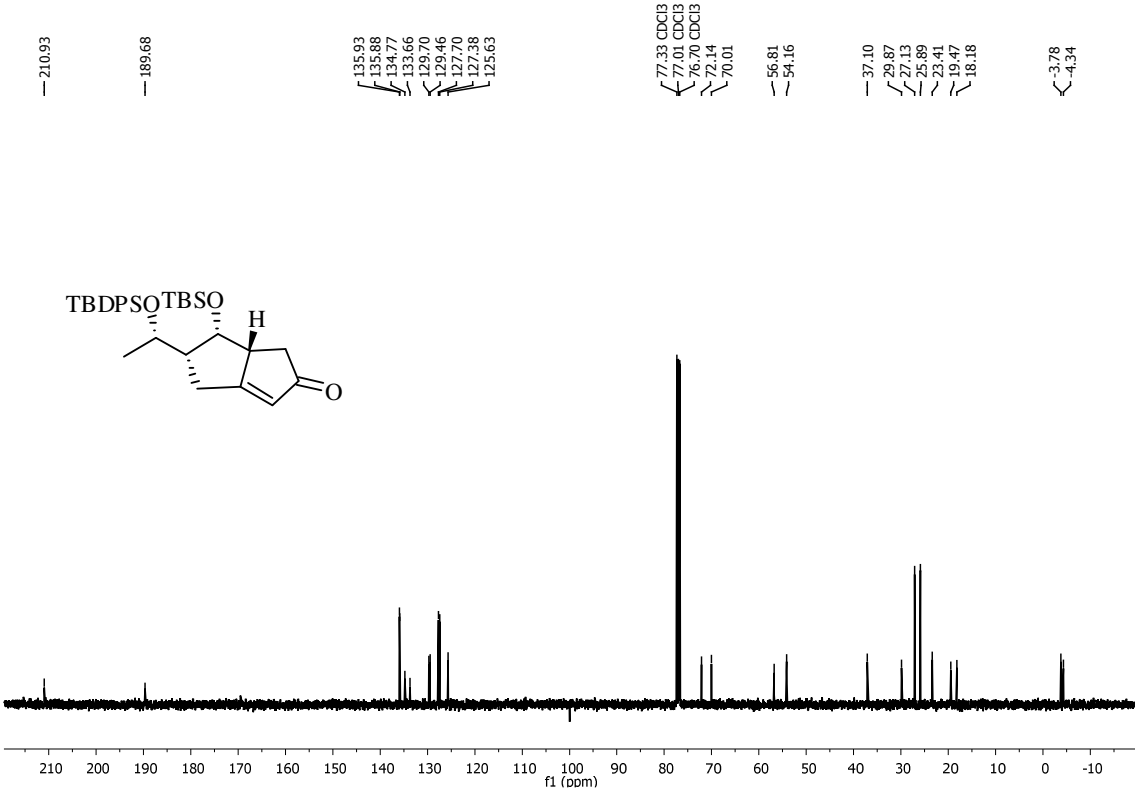
DEPT-135 NMR of compound 103 (100 MHz, $CDCl_3$)



^{1}H - NMR of compound 104a (600 MHz, $CDCl_3$)



^{13}C NMR of compound 104a (100 MHz, $CDCl_3$)



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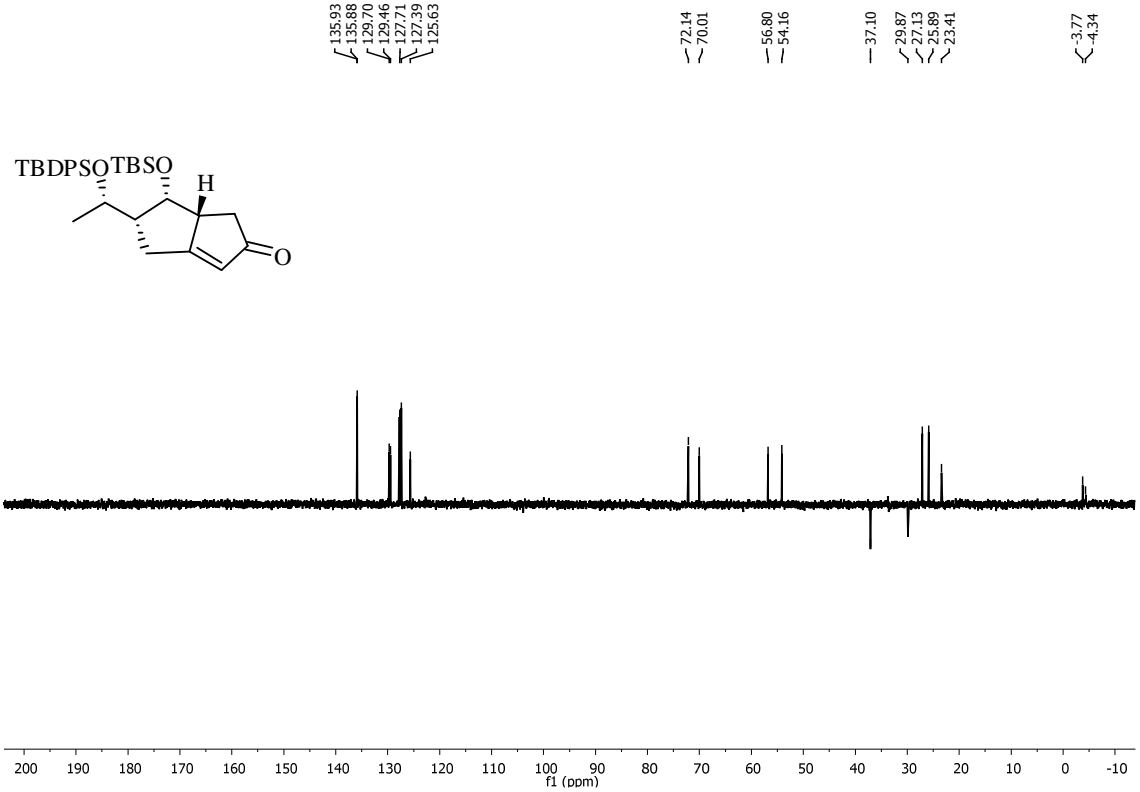
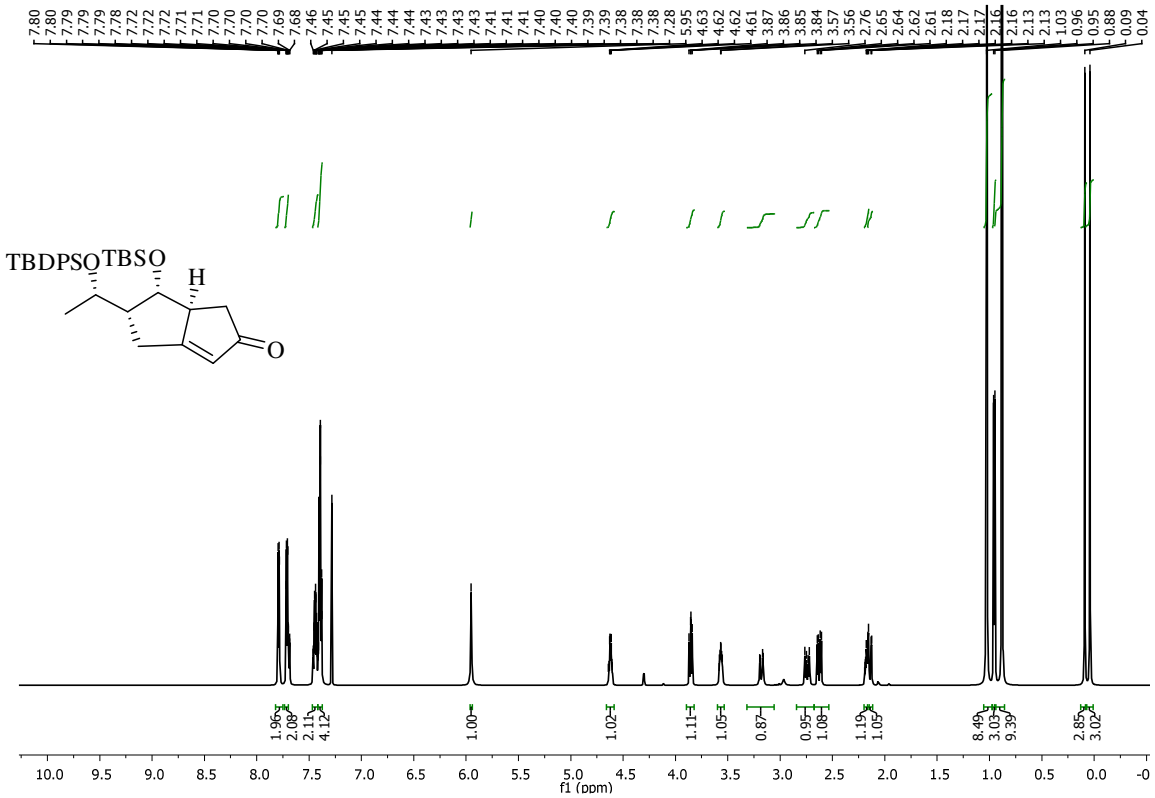
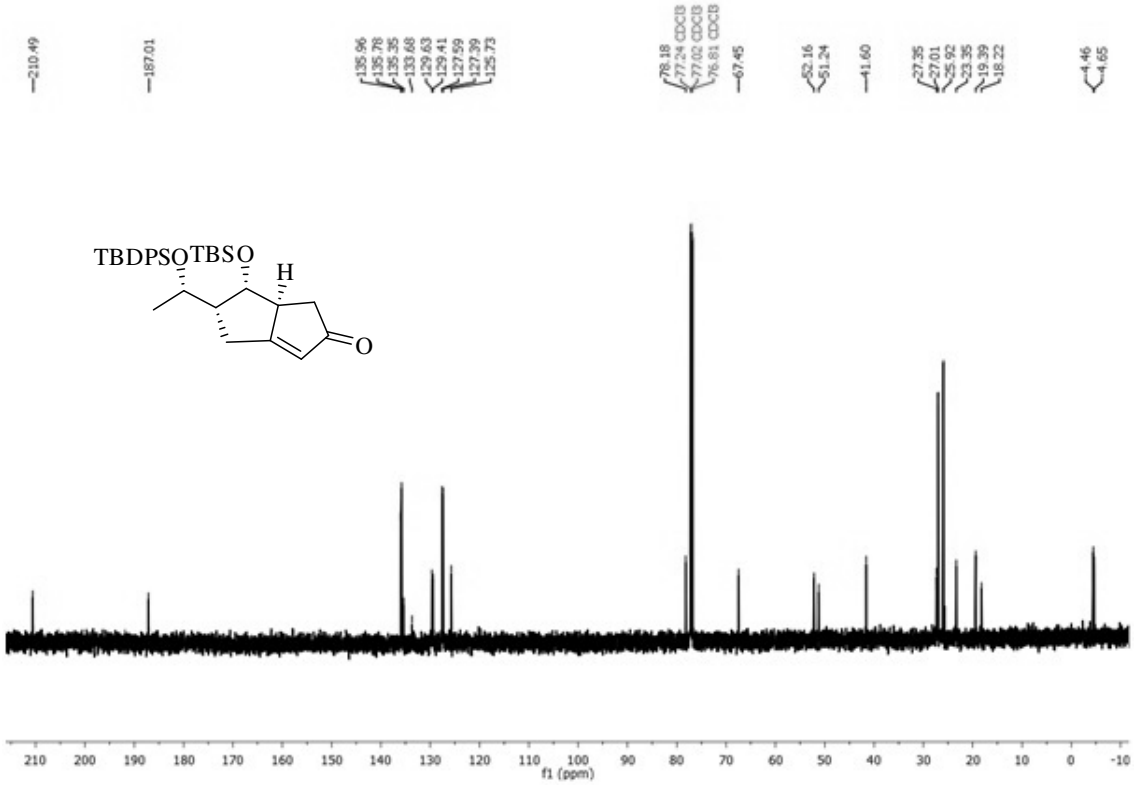


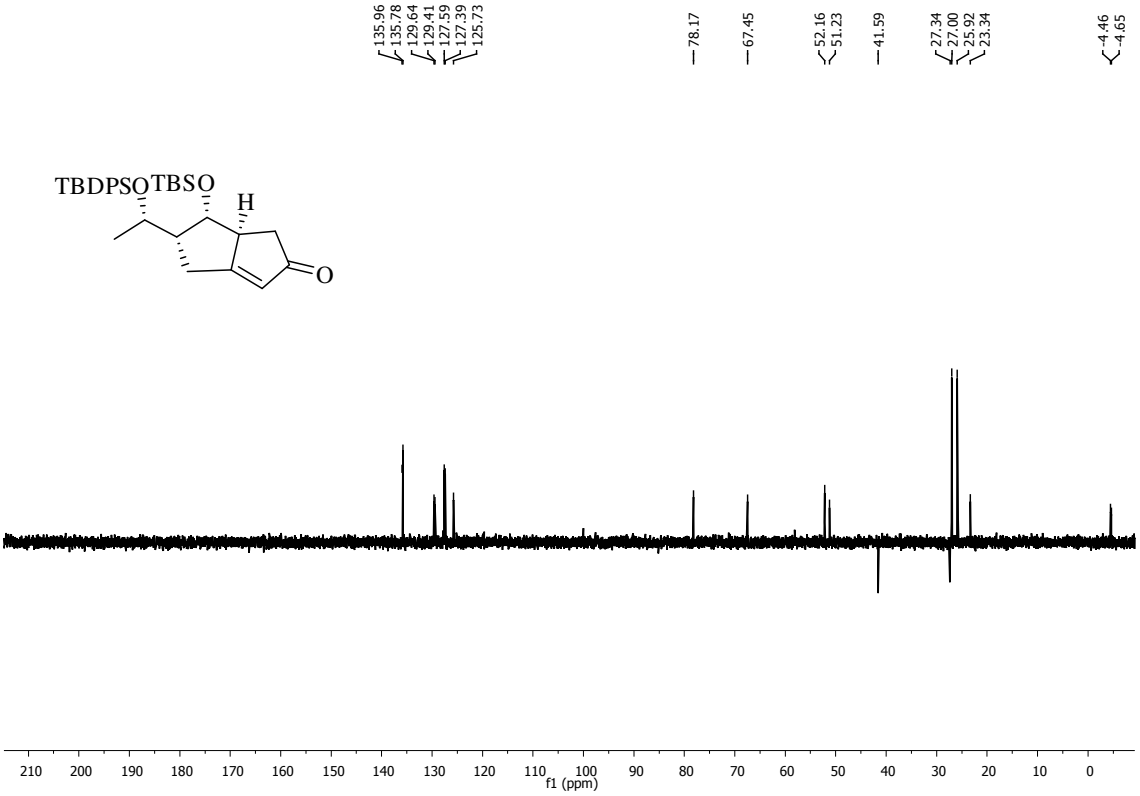
^{1}H - NMR of compound 104b (600 MHz, $CDCl_3$)



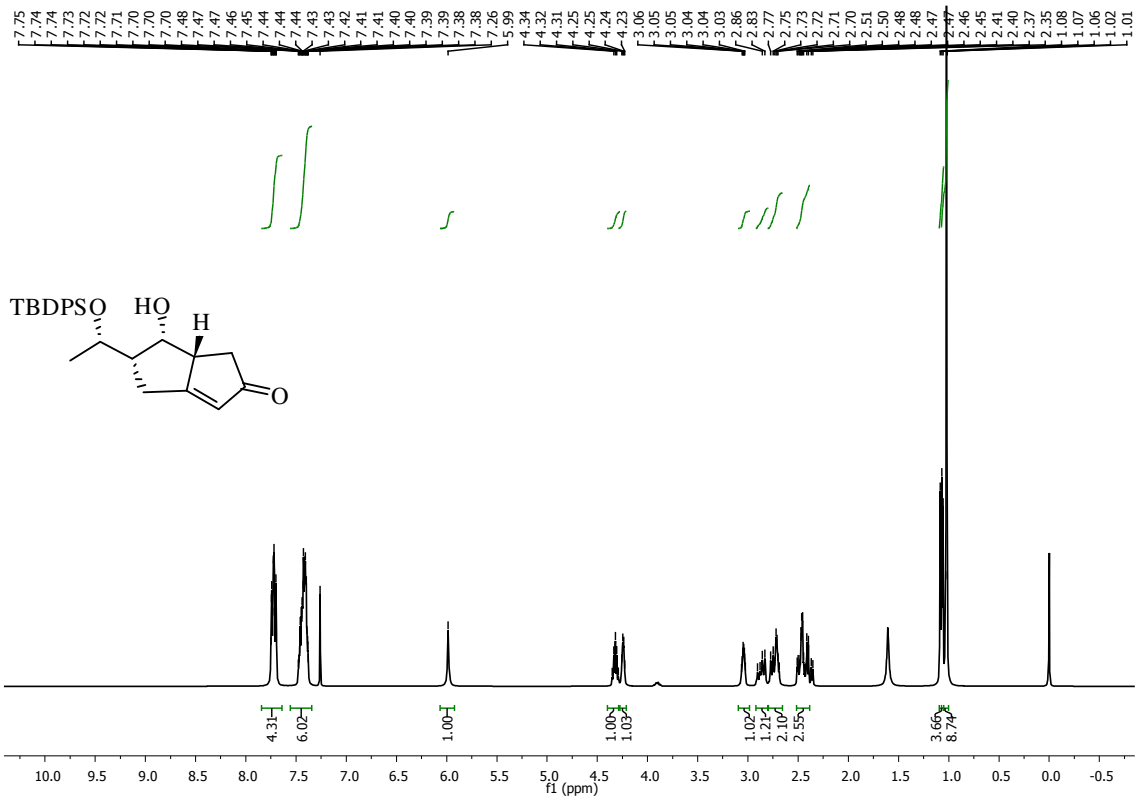
^{13}C NMR of compound 104b (150 MHz, $CDCl_3$)



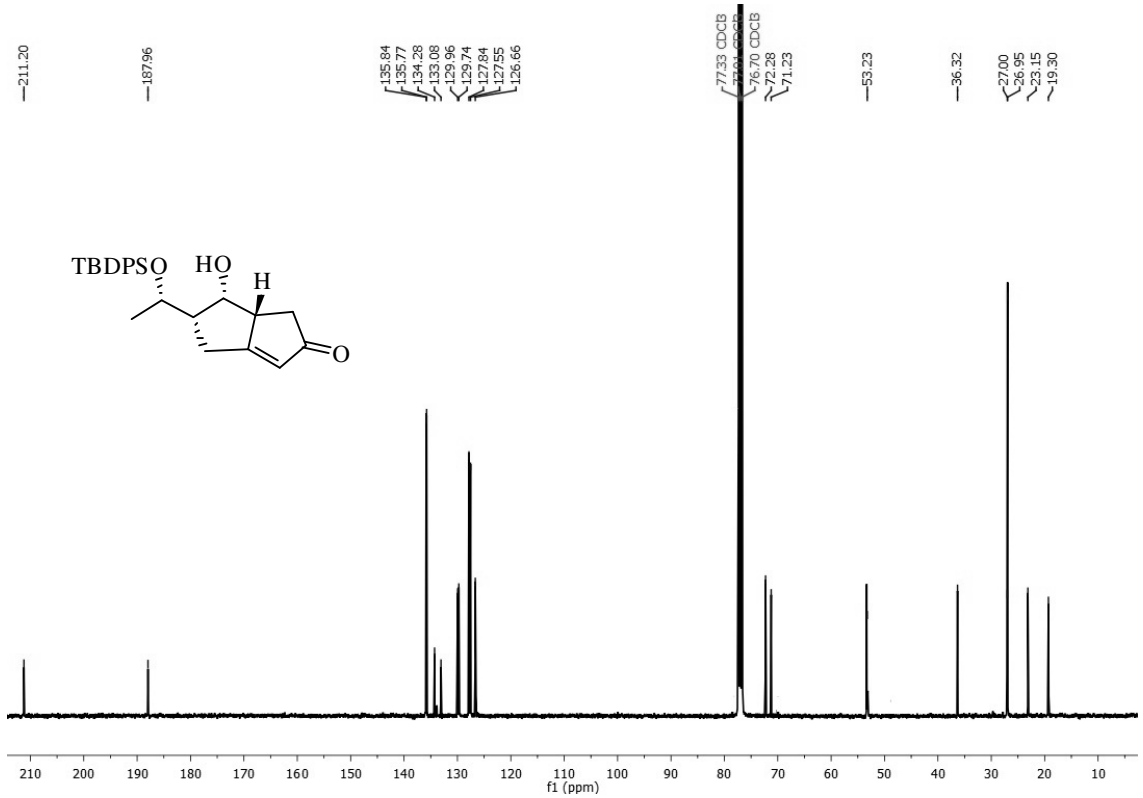
DEPT-135 NMR of compound 104b (150 MHz, $CDCl_3$)



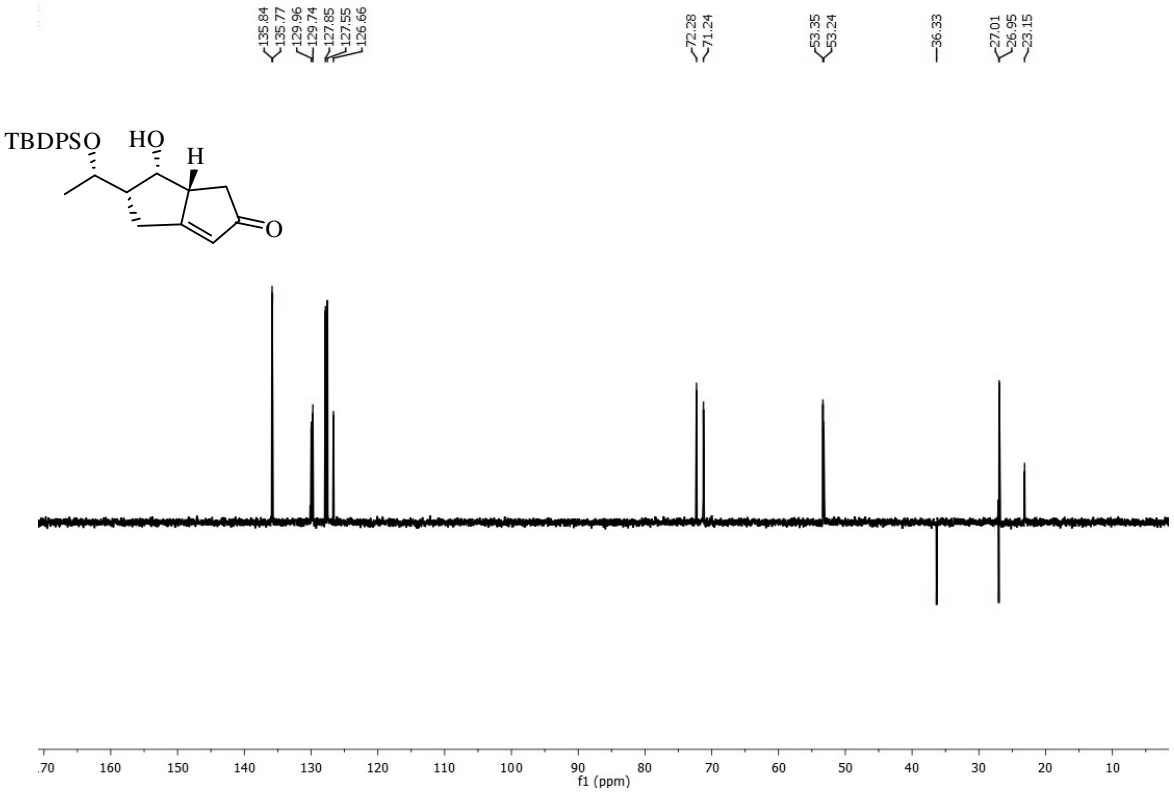
^{1}H - NMR of compound 105 (400 MHz, $CDCl_3$)



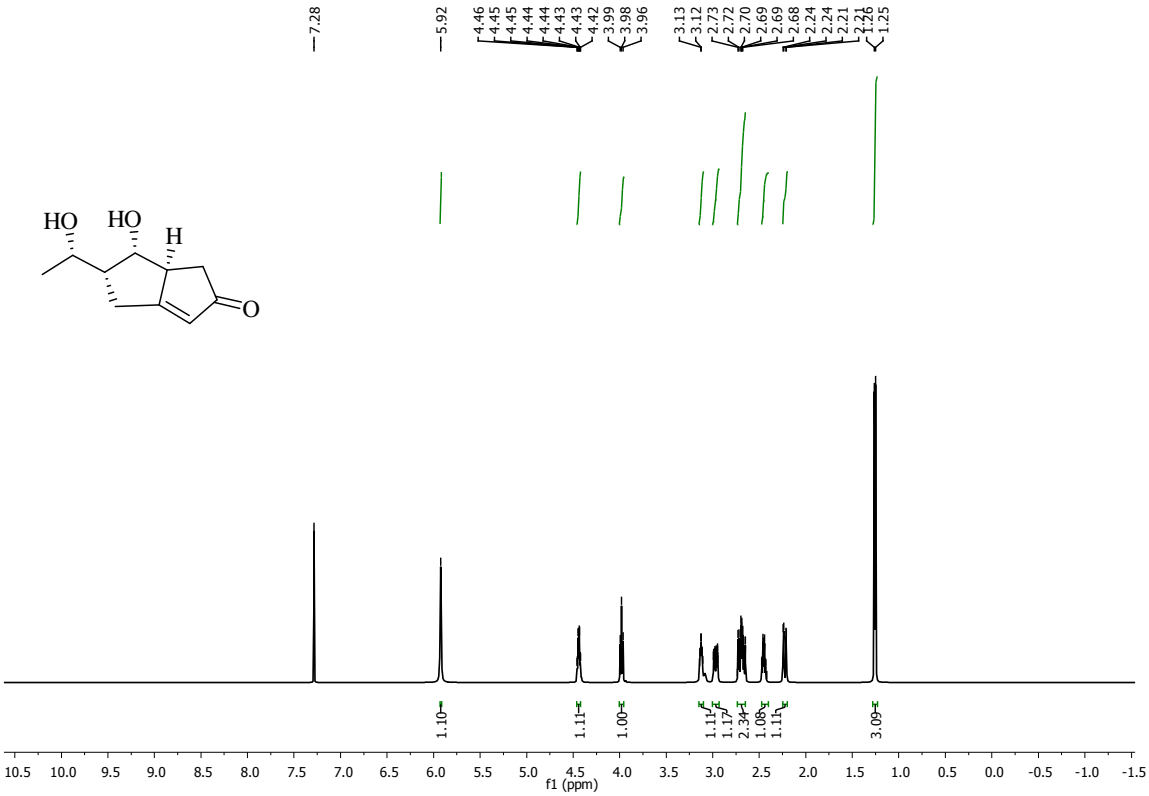
^{13}C NMR of compound 105 (100 MHz, $CDCl_3$)



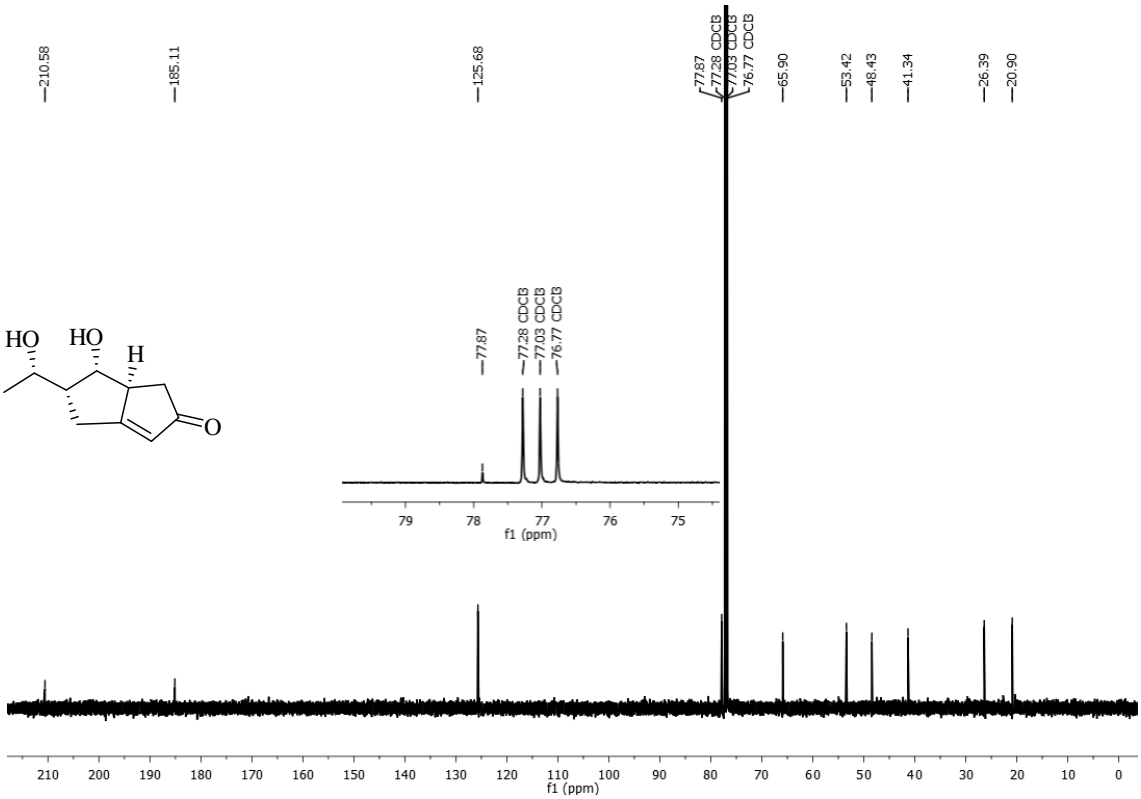
DEPT-135 NMR of compound 105 (100 MHz, $CDCl_3$)



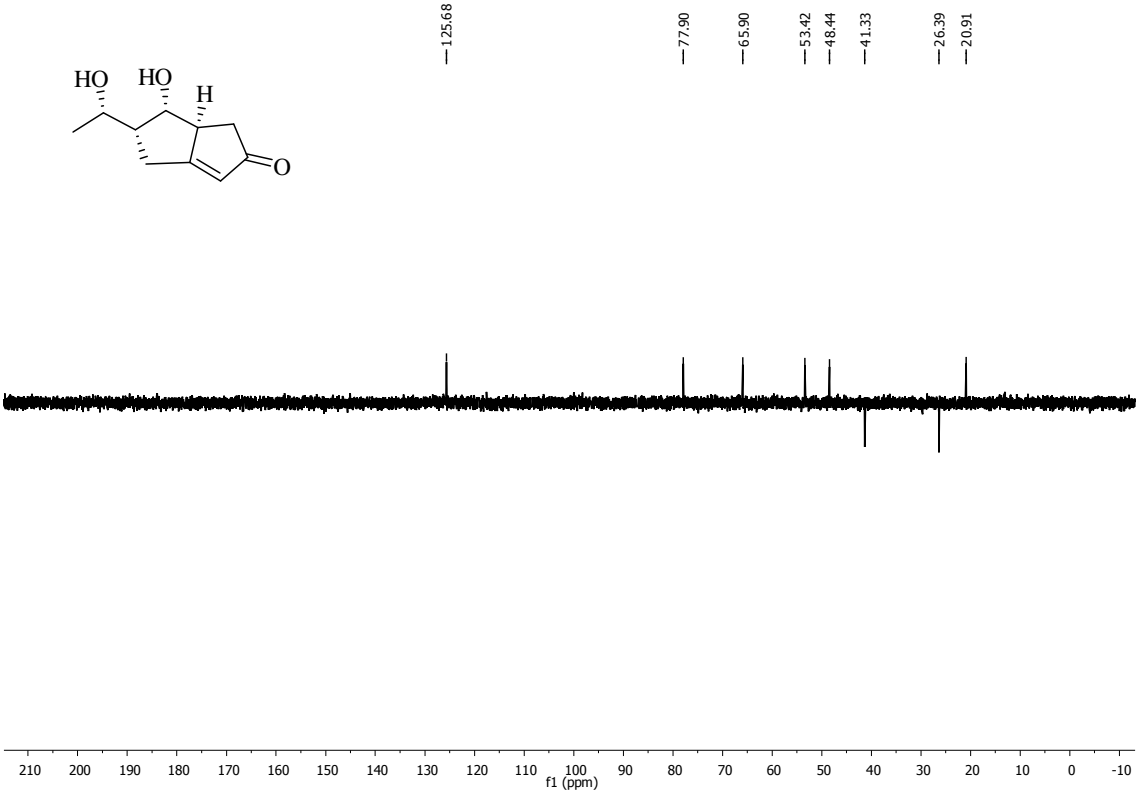
^{1}H - NMR of compound 106 (600 MHz, $CDCl_3$)



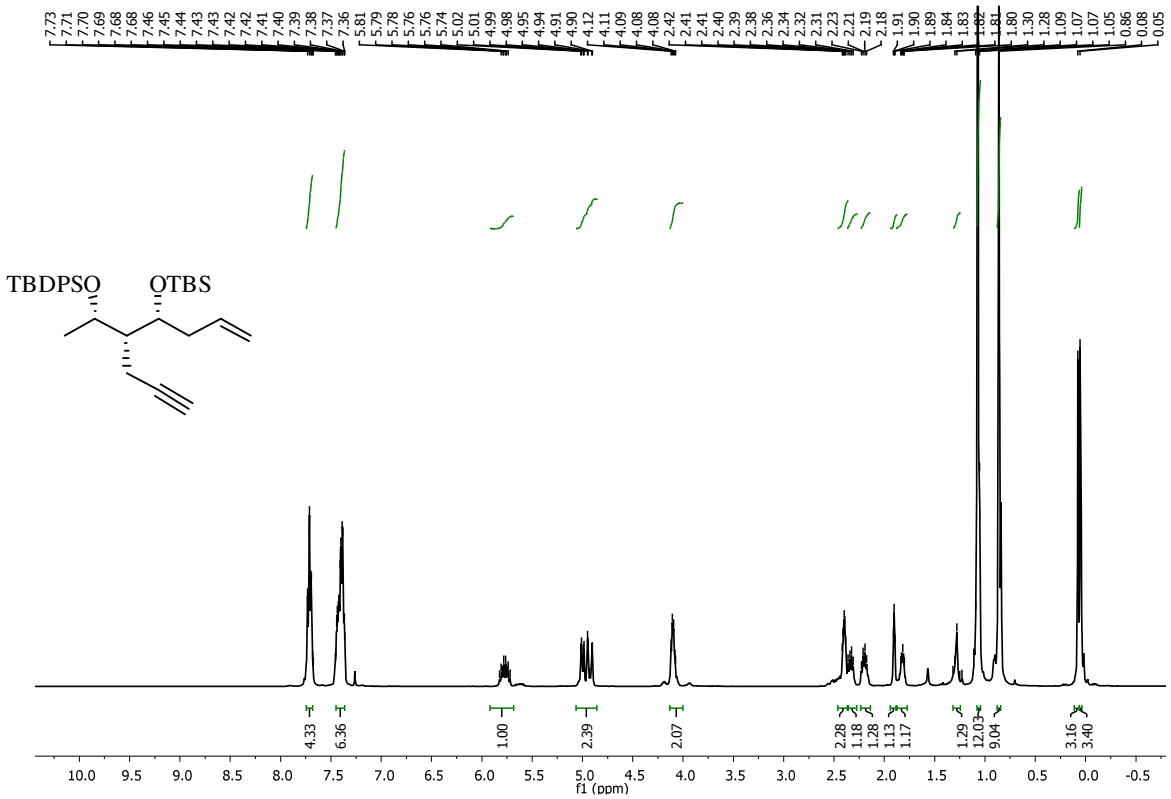
^{13}C NMR of compound 106 (125 MHz, $CDCl_3$)



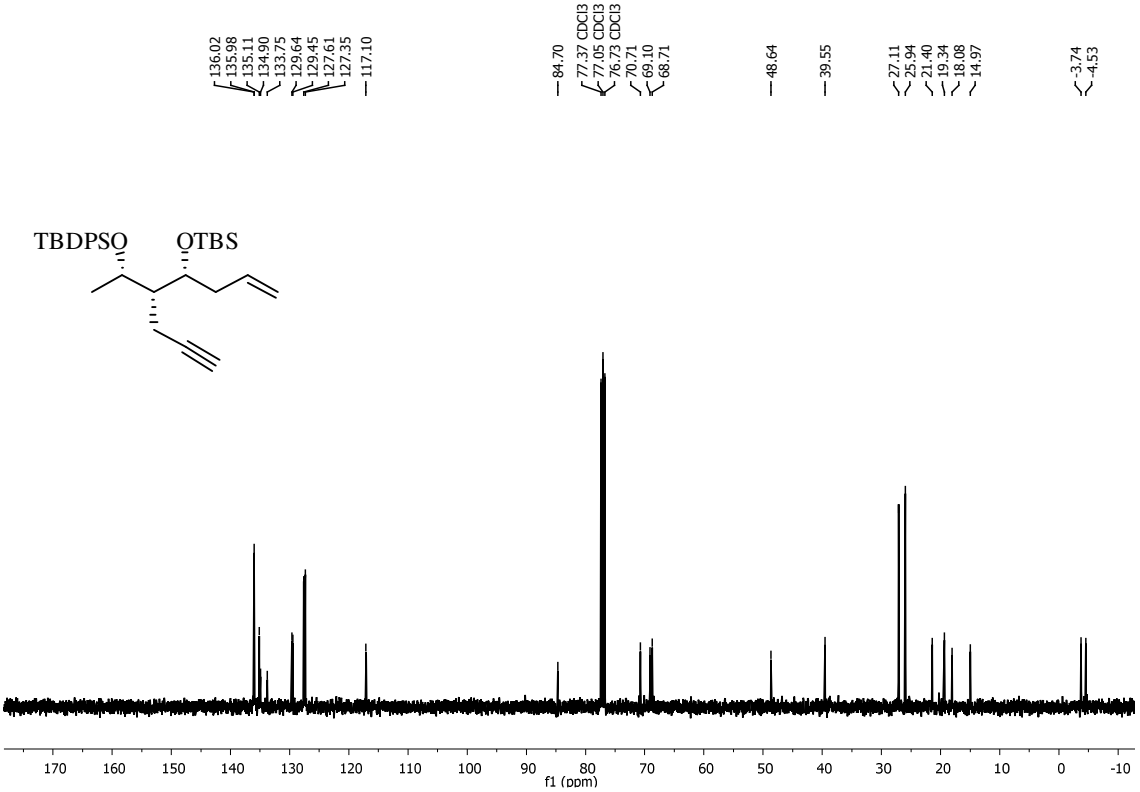
DEPT-135 NMR of compound 106 (150 MHz, $CDCl_3$)



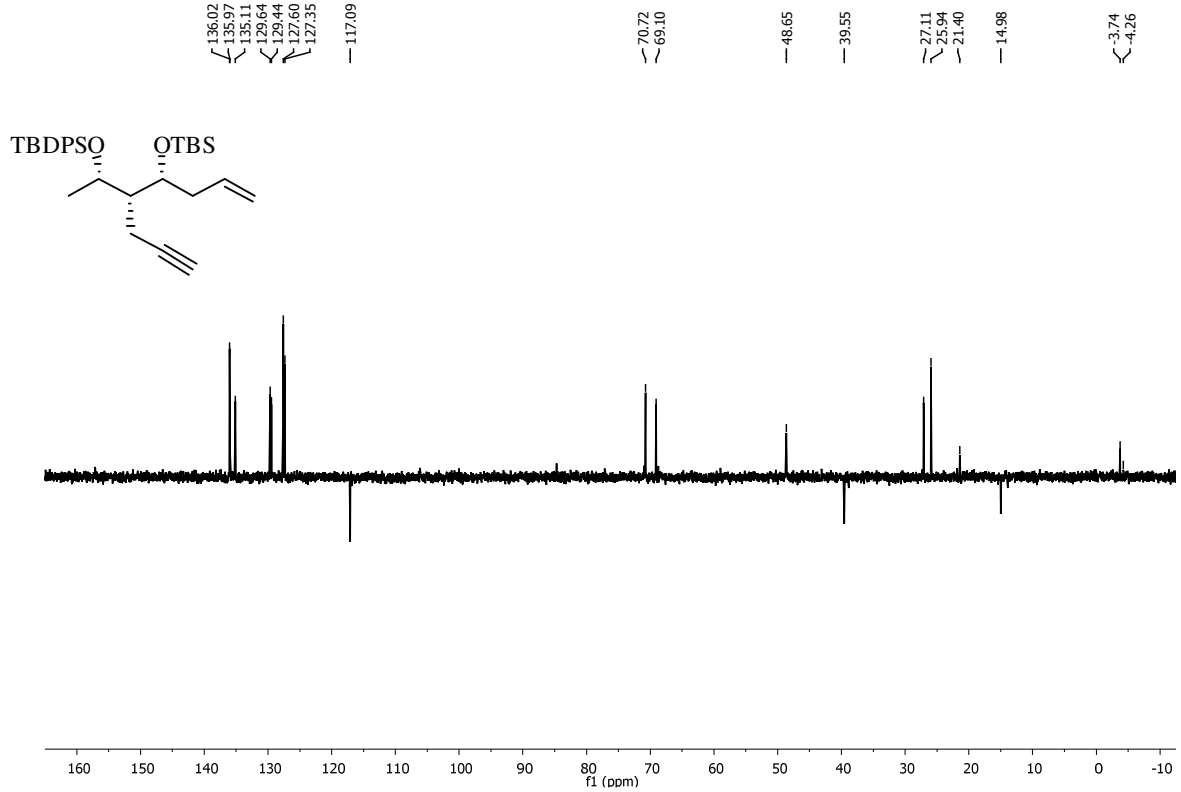
^{1}H - NMR of compound 107 (400 MHz, $CDCl_3$)



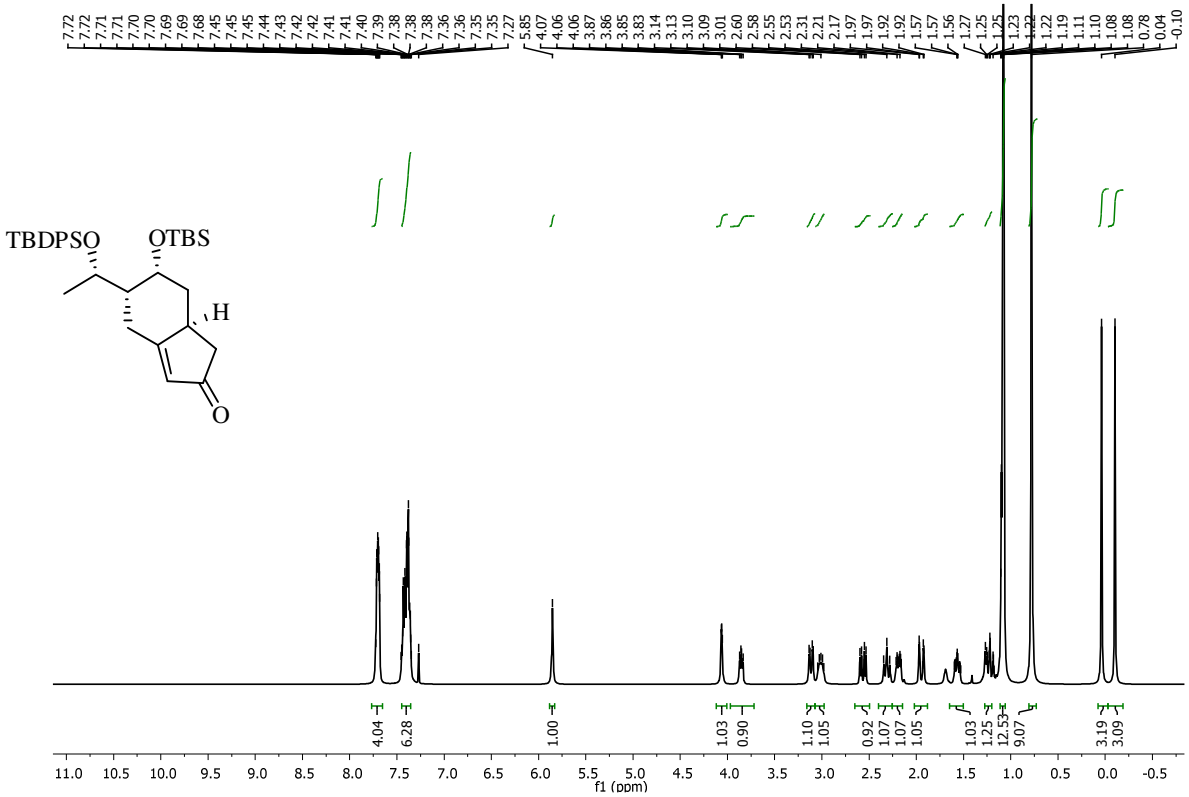
^{13}C NMR of compound 107 (100 MHz, $CDCl_3$)



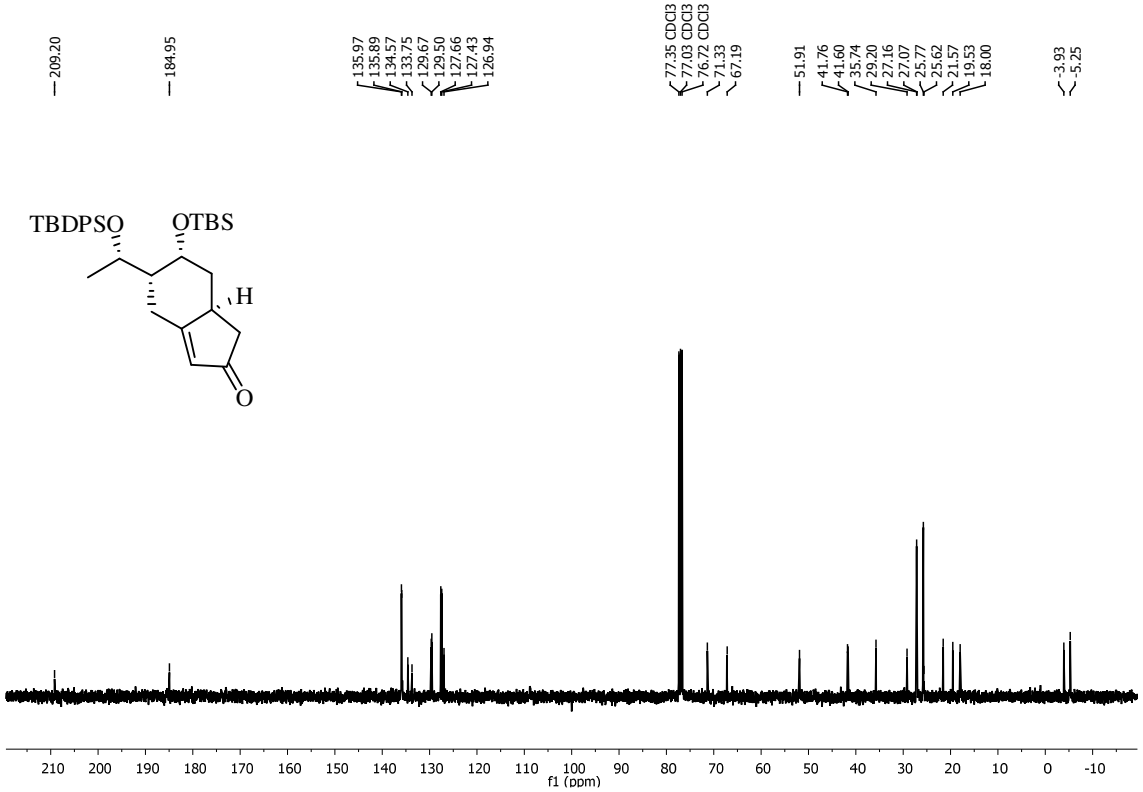
DEPT-135 NMR of compound 107 (100 MHz, $CDCl_3$)



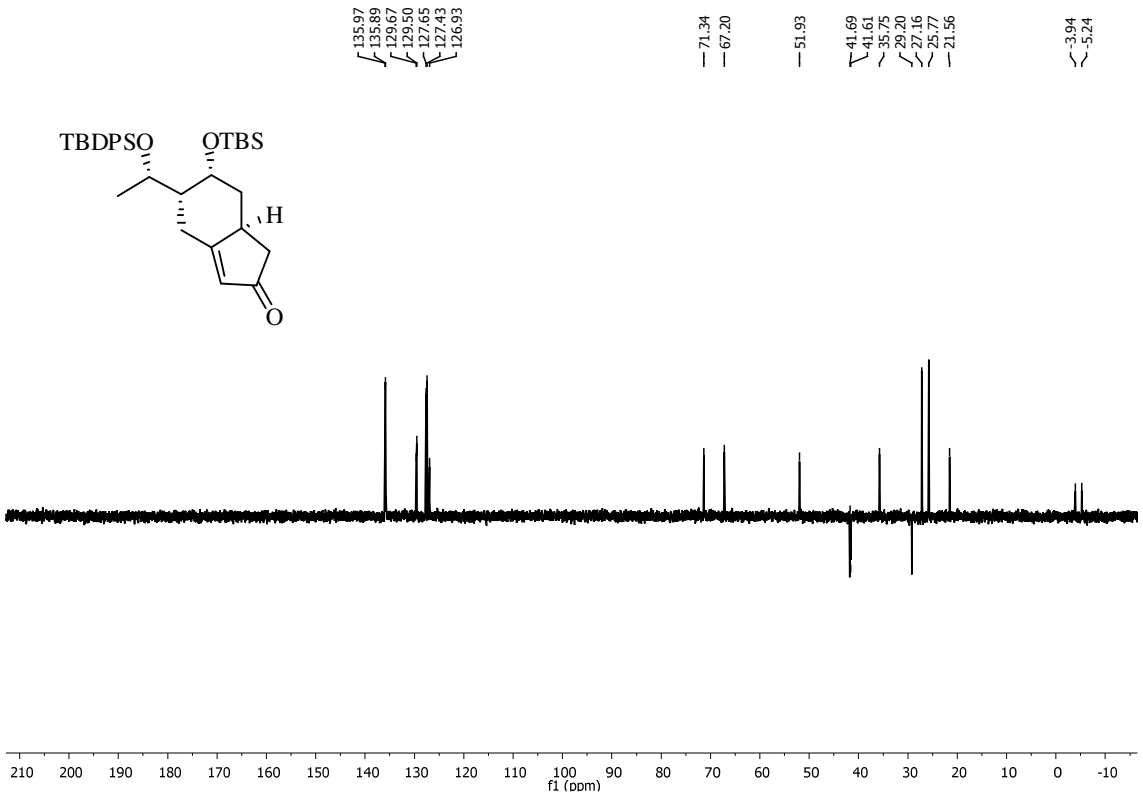
^{1}H - NMR of compound 108 (400 MHz, $CDCl_3$)



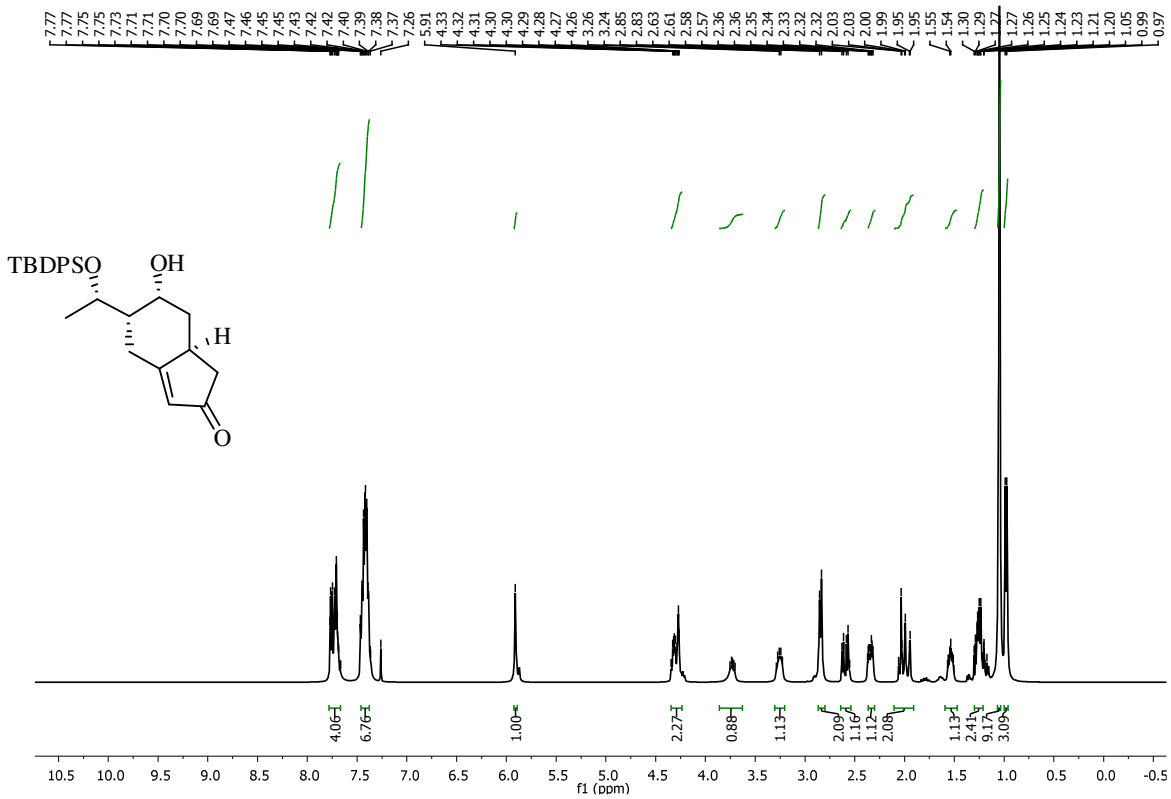
^{13}C NMR of compound 108 (100 MHz, $CDCl_3$)



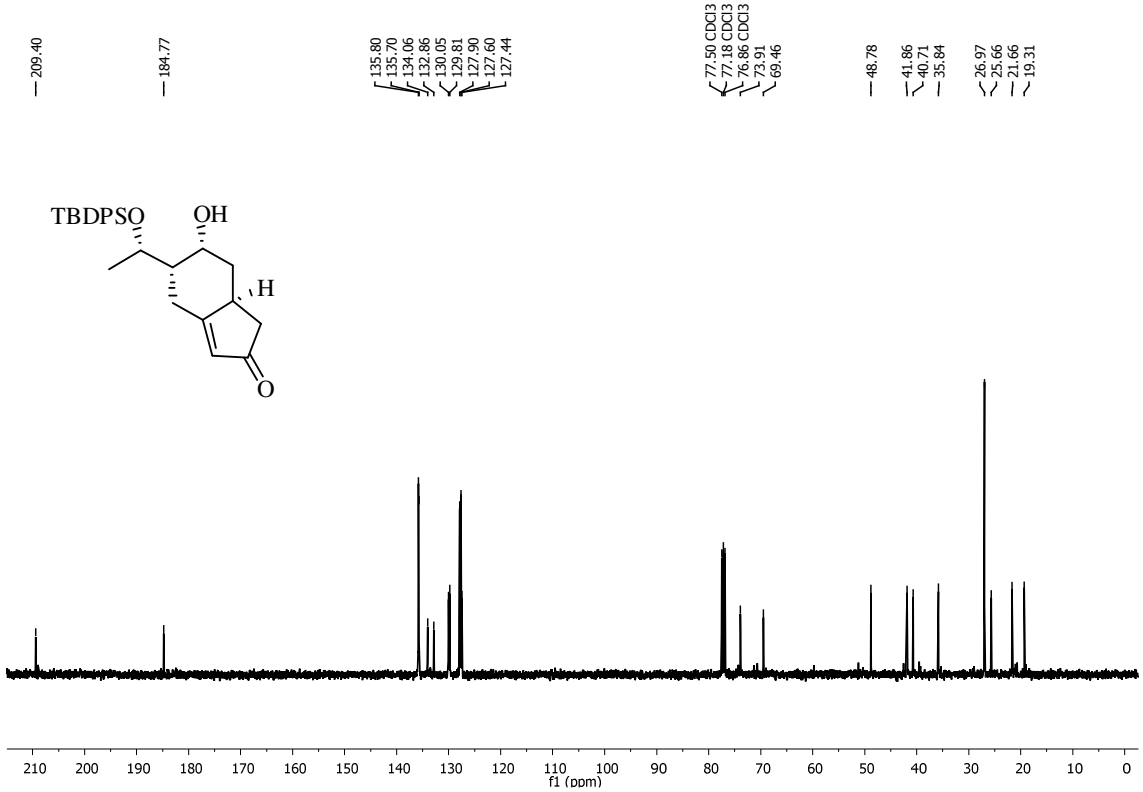
DEPT-135 NMR of compound 108 (150 MHz, $CDCl_3$)



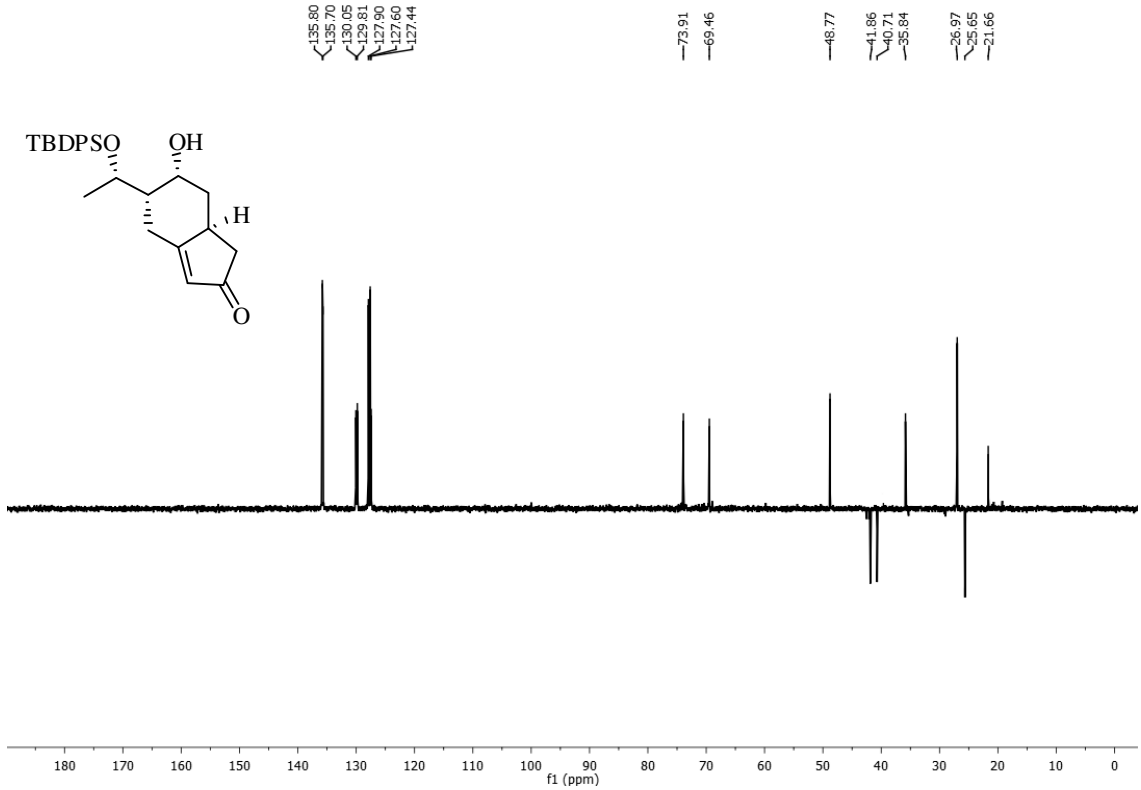
^{1}H - NMR of compound 109 (400 MHz, $CDCl_3$)



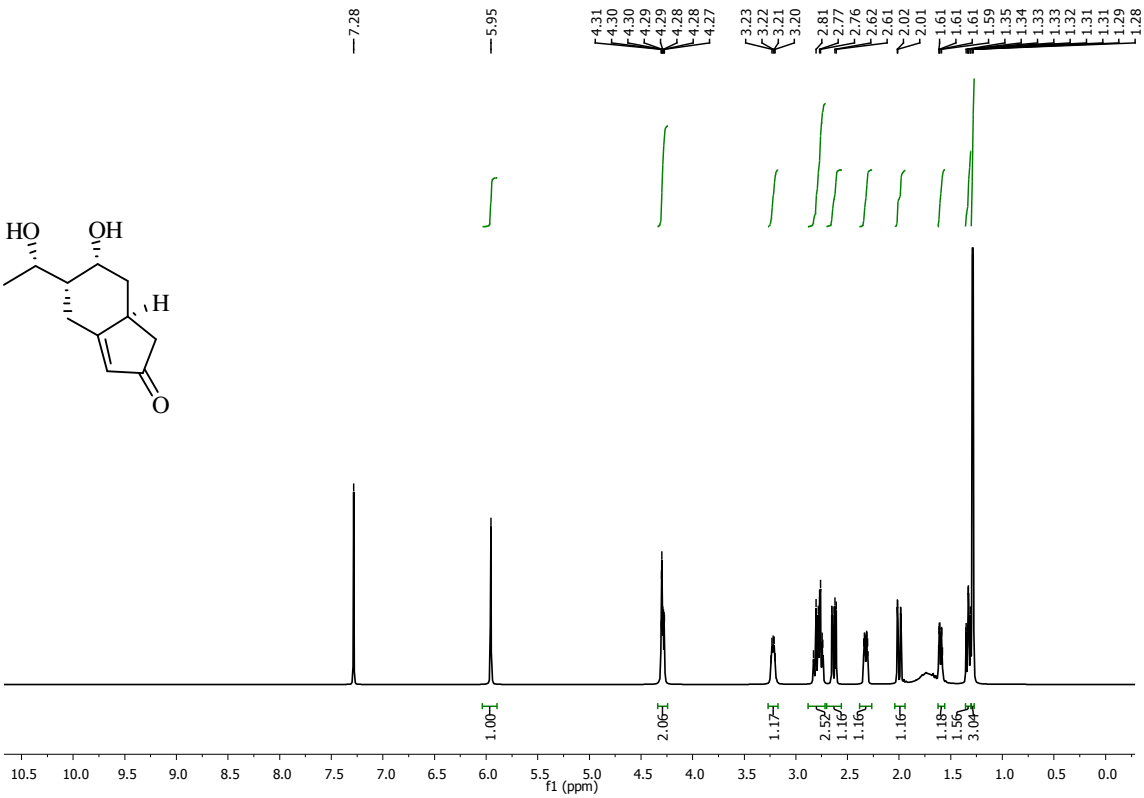
^{13}C NMR of compound 109 (100 MHz, $CDCl_3$)



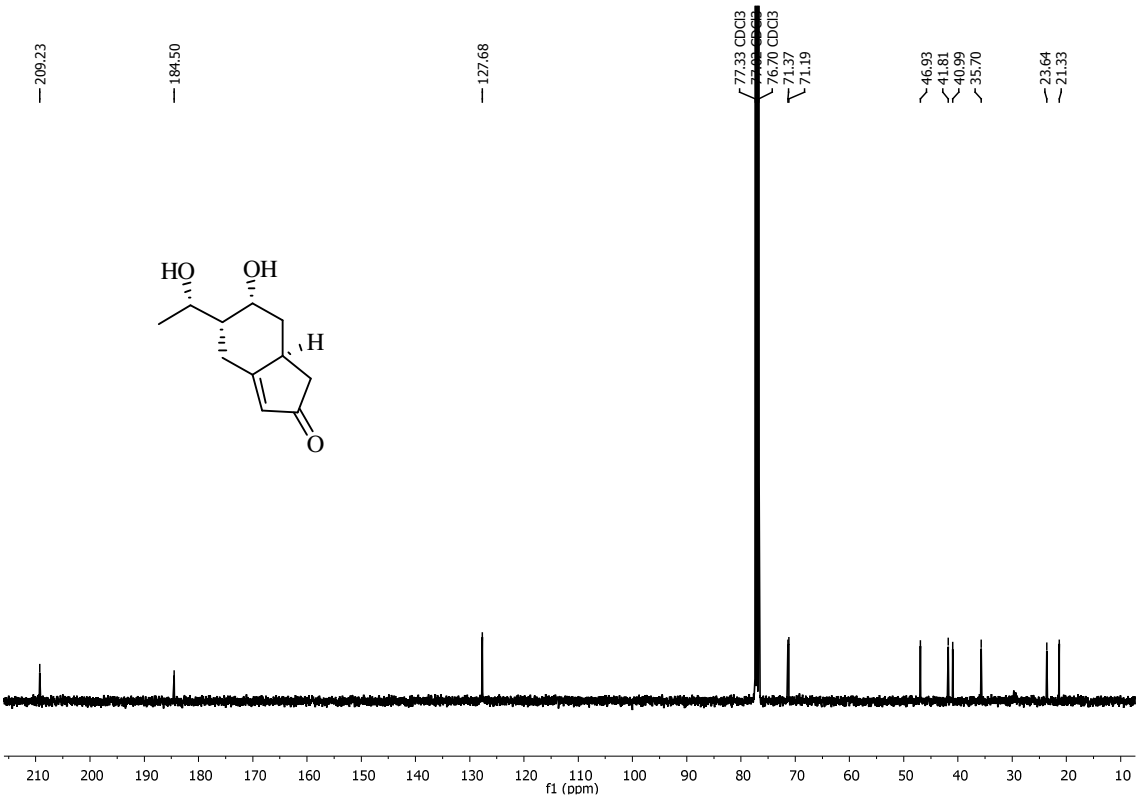
DEPT-135 NMR of compound 109 (100 MHz, $CDCl_3$)



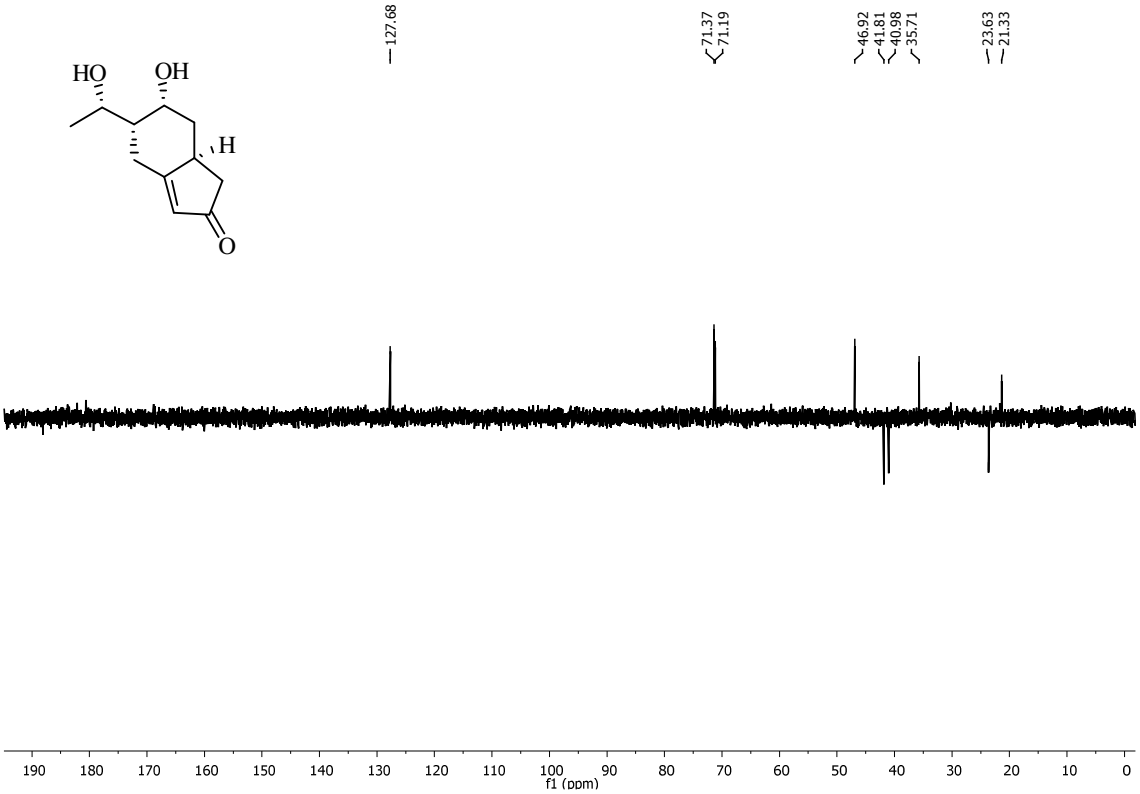
^{1}H - NMR of compound 110 (600 MHz, $CDCl_3$)



^{13}C NMR of compound 110 (100 MHz, $CDCl_3$)

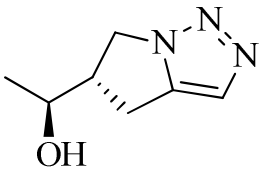


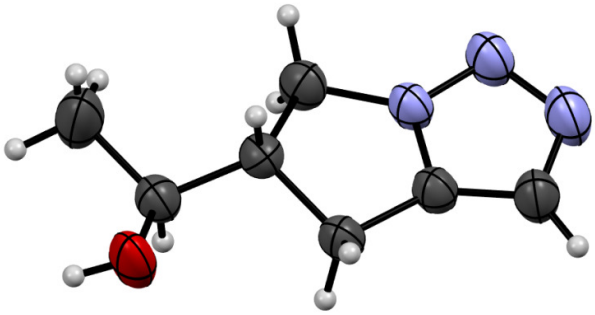
DEPT-135 NMR of compound 110 (100 MHz, $CDCl_3$)



Crystal data and structure refinement for compound 31.

X-ray crystal data of compound **31** (the following crystal has been deposited at the Cambridge Crystallographic Data Centre and has the deposition number CCDC 1402159).



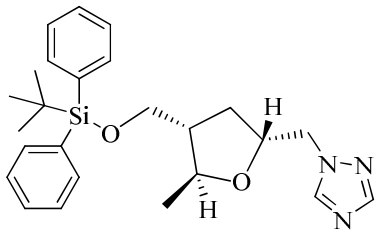


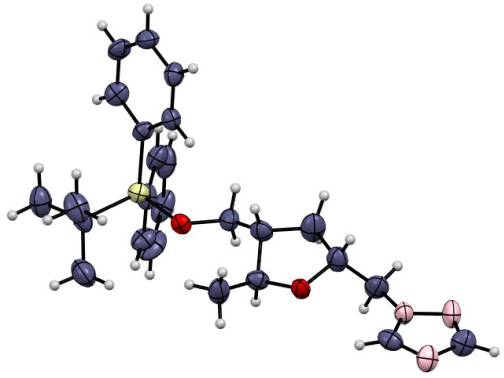
ORTEP presentation (drawn at 50% probability)

Empirical formula	C7 H11 N3 O
Formula weight	153.19
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P21/m
Unit cell dimensions	a = 5.5524(17) Å alpha = 90 °
	b = 7.337(2) Å beta = 91.581(7) °
	c = 9.871(3) Å gamma = 90 °
Volume	402.0(2) $Å^3$
Z, Calculated density	2, 1.266 Mg/m^3
Absorption coefficient	0.089 mm^{-1}
F(000)	164
Crystal size	0.2 x 0.2 x 0.1 mm^3
Theta range for data collection	2.06 to 24.99 °
Limiting indices	-6<=h<=6, -8<=k<=8, -11<=l<=11
Reflections collected / unique	4269 / 1395 [R(int) = 0.0427]
Completeness to theta = 24.99	99.9 %
Absorption correction	none
Max. and min. transmission	0.9880 and 0.9762
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1395 / 1 / 102
Goodness-of-fit on F^2	1.050
Final R indices [I>2sigma(I)]	R1 = 0.0361, wR2 = 0.1209
R indices (all data)	R1 = 0.0480, wR2 = 0.1345
Absolute structure parameter	2(3)
Largest diff. peak and hole	0.155 and -0.192 $e.A^{-3}$

Crystal data and structure refinement for compound 60.

X-ray crystal data of compound **60** (the following crystal has been deposited at the Cambridge Crystallographic Data Centre and has the deposition number CCDC 1407794)



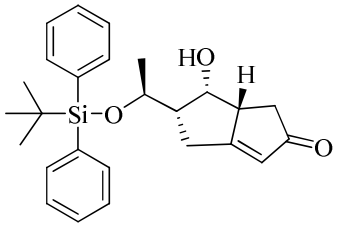


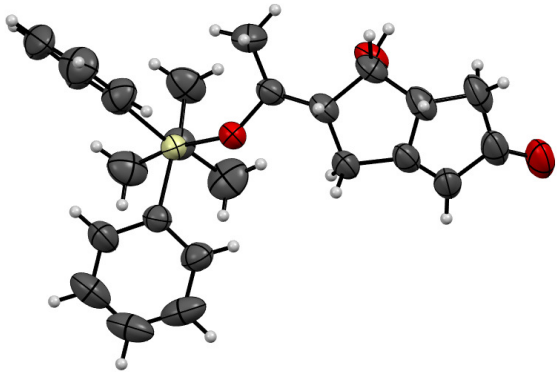
ORTEP presentation (drawn at 50% probability)

Empirical formula	C25 H33 N3 O2 Si
Formula weight	435.63
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 10.558(3) Å alpha = 90 ° b = 39.473(12) Å beta = 90 ° c = 11.458(4) Å gamma = 90 °
Volume	4775(2) Å ^{3}
Z, Calculated density	8, 1.212 Mg/m^3
Absorption coefficient	0.124 mm^{-1}
F(000)	1872
Crystal size	0.14 x 0.11 x 0.09 mm^3
Theta range for data collection	1.03 to 25.00 °
Limiting indices	-12<=h<=12, -44<=k<=46, -13<=l<=13
Reflections collected / unique	56546 / 15822 [R(int) = 0.1453]
Completeness to theta = 25.00	99.5 %
Absorption correction	none
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15822 / 1 / 1118
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.1078, wR2 = 0.2381
R indices (all data)	R1 = 0.1580, wR2 = 0.2781
Absolute structure parameter	0.4(2)
Extinction coefficient	0.078(4)
Largest diff. peak and hole	0.852 and -0.687 e.A^{-3}

Crystal data and structure refinement for compound 105.

X-ray crystal data of compound **105** (the following crystal has been deposited at the Cambridge Crystallographic Data Centre and has the deposition number CCDC 1502161)



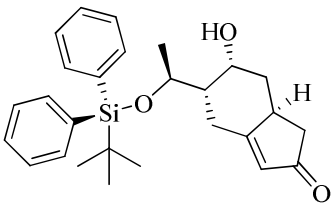


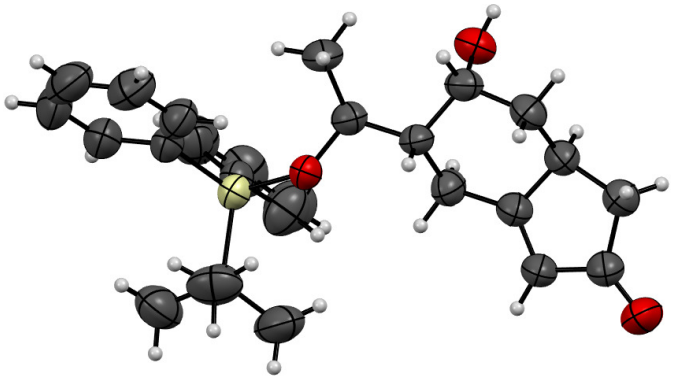
ORTEP presentation (drawn at 50% probability)

Empirical formula	C26 H32 O3 Si
Formula weight	420.61
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P21
Unit cell dimensions	a = 10.523(5) Å alpha = 90.000(5) °
	b = 10.046(5) Å beta = 103.959(5) °
	c = 11.683(5) Å gamma = 90.000(5) °
Volume	1198.6(10) Å ^{3}
Z, Calculated density	2, 1.165 Mg/m^3
Absorption coefficient	0.121 mm^{-1}
F(000)	452
Crystal size	0.20 x 0.20 x 0.10 mm^3
Theta range for data collection	1.80 to 25.00 °
Limiting indices	-12<=h<=12, -11<=k<=11, -11<=l<=13
Reflections collected / unique	13801 / 4156 [R(int) = 0.0253]
Completeness to theta = 25.00	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9880 and 0.9762
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4156 / 1 / 276
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0352, wR2 = 0.0878
R indices (all data)	R1 = 0.0406, wR2 = 0.0917
Absolute structure parameter	0.01(11)
Largest diff. peak and hole	0.151 and -0.143 e.A^{-3}

Crystal data and structure refinement for compound 109.

X-ray crystal data of compound **109** (the following crystal has been deposited at the Cambridge Crystallographic Data Centre and has the deposition number CCDC 1528322)





ORTEP presentation (drawn at 50% probability)

Empirical formula	C27 H34 O3 Si
Formula weight	434.63
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 8.2816(14) Å alpha = 90 °
	b = 11.7445(19) Å beta = 90 °
	c = 25.888(4) Å gamma = 90 °
Volume	2517.9(7) Å ^{3}
Z, Calculated density	4, 1.147 Mg/m^3
Absorption coefficient	0.117 mm^{-1}
F(000)	936
Crystal size	0.20 x 0.20 x 0.10 mm^3
Theta range for data collection	1.57 to 24.99 °
Limiting indices	-9<=h<=9, -13<=k<=13, -30<=l<=30
Reflections collected / unique	29078 / 4417 [R(int) = 0.1226]
Completeness to theta = 24.99	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9884 and 0.9769
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4417 / 0 / 286
Goodness-of-fit on F^2	0.981
Final R indices [I>2sigma(I)]	R1 = 0.0568, wR2 = 0.1161
R indices (all data)	R1 = 0.1160, wR2 = 0.1396
Absolute structure parameter	-0.10(19)
Extinction coefficient	0.0078(12)
Largest diff. peak and hole	0.160 and -0.157 e.A^{-3}