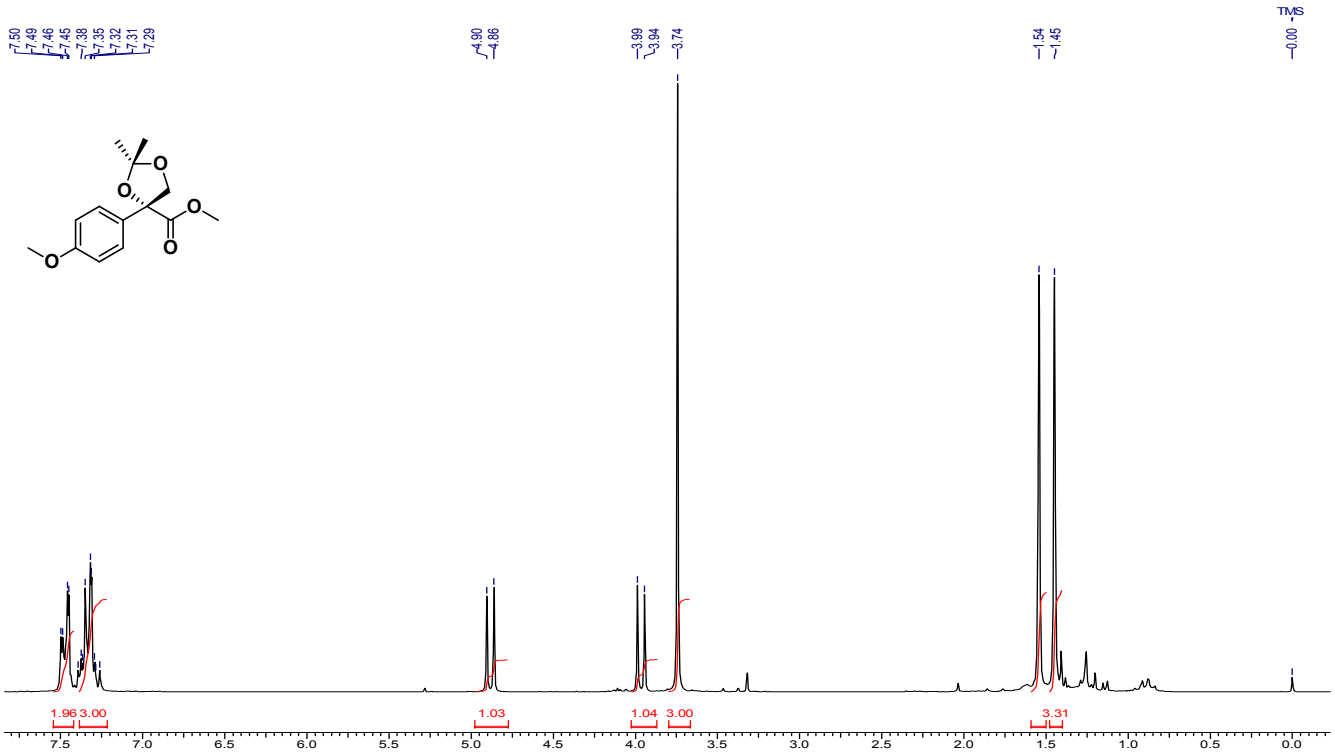
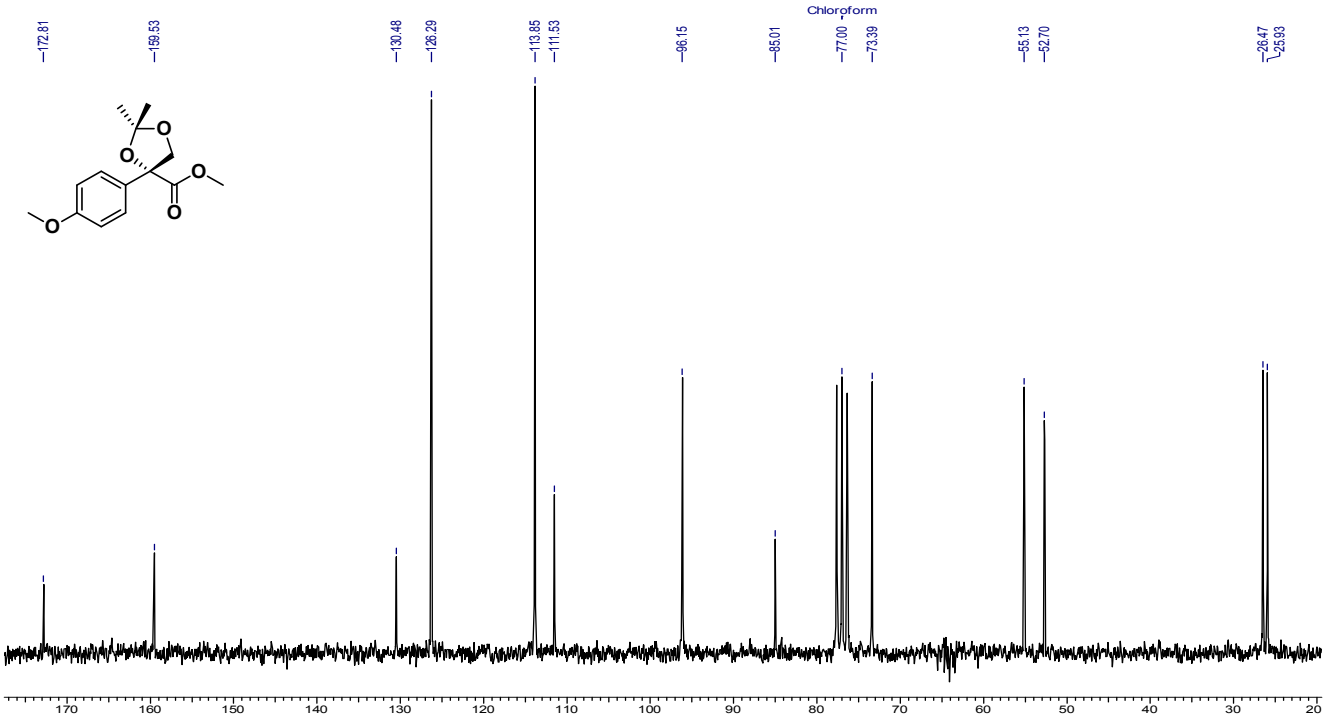
VI. ^{1}H and ^{13}C NMR Spectra

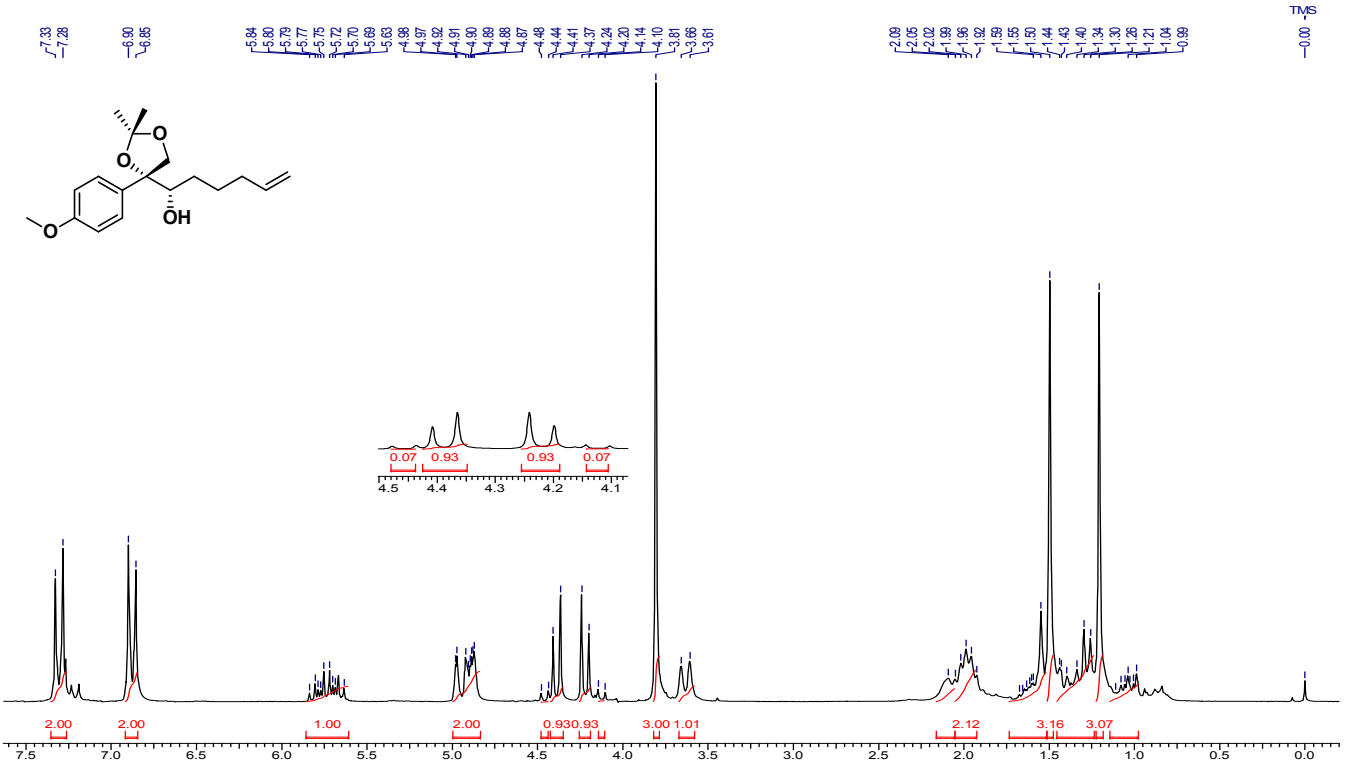
^{1}H NMR of methyl 4-(4-methoxyphenyl)-2,2-dimethyl-1,3-dioxolane-4-carboxylate (3):



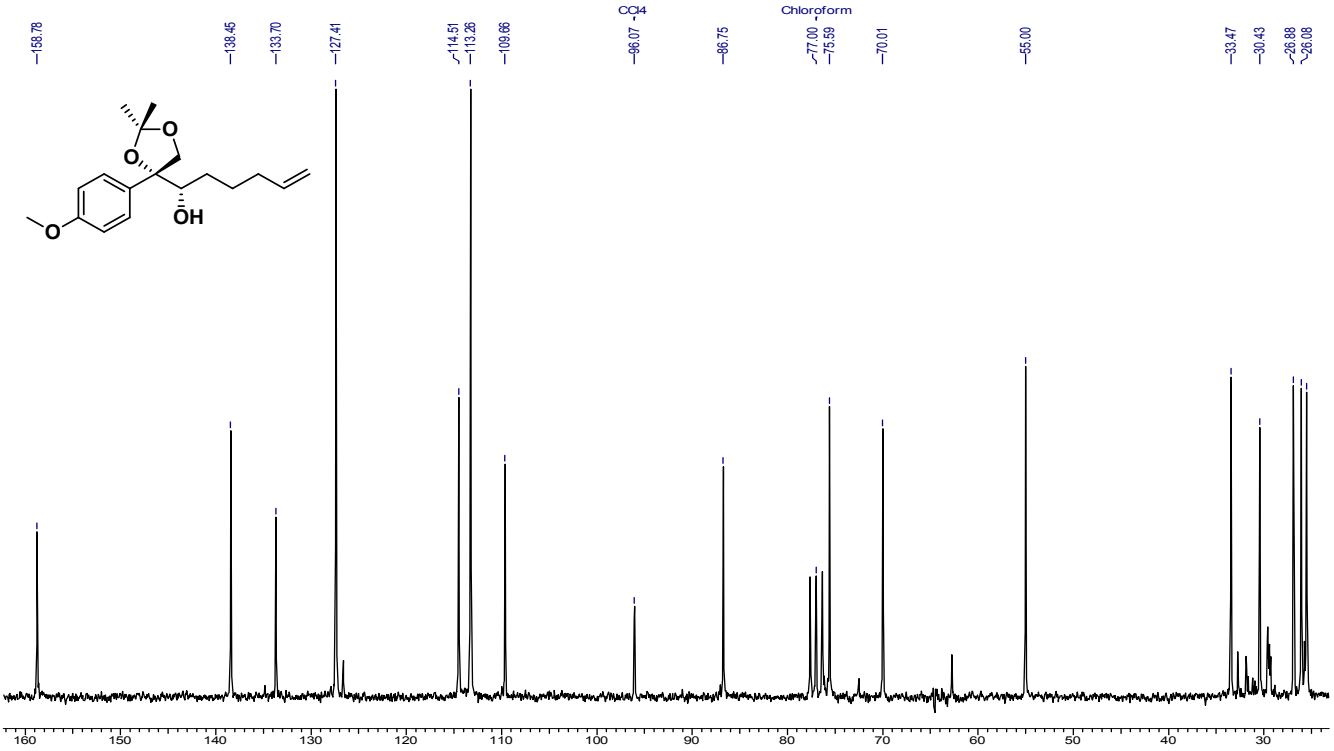
^{13}C NMR of methyl 4-(4-methoxyphenyl)-2,2-dimethyl-1,3-dioxolane-4-carboxylate (3):



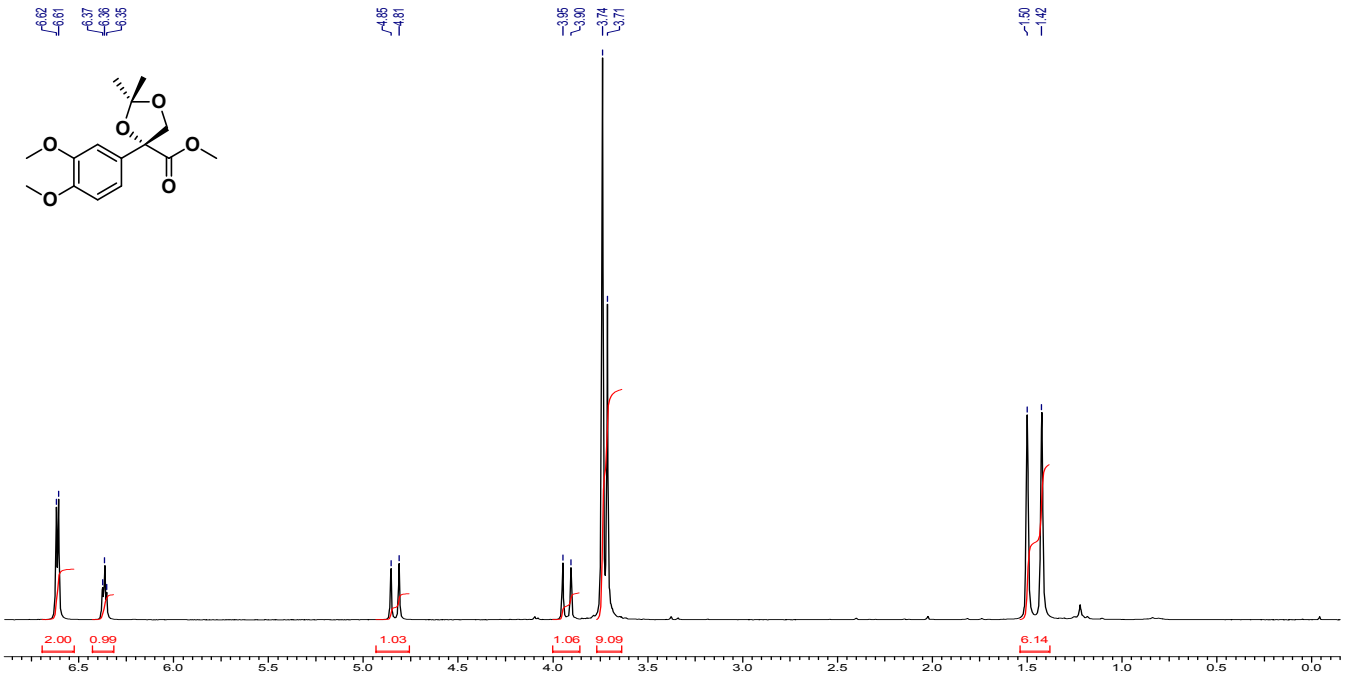
^{1}H NMR of 1-(4-(4-methoxyphenyl)-2,2-dimethyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (3a)



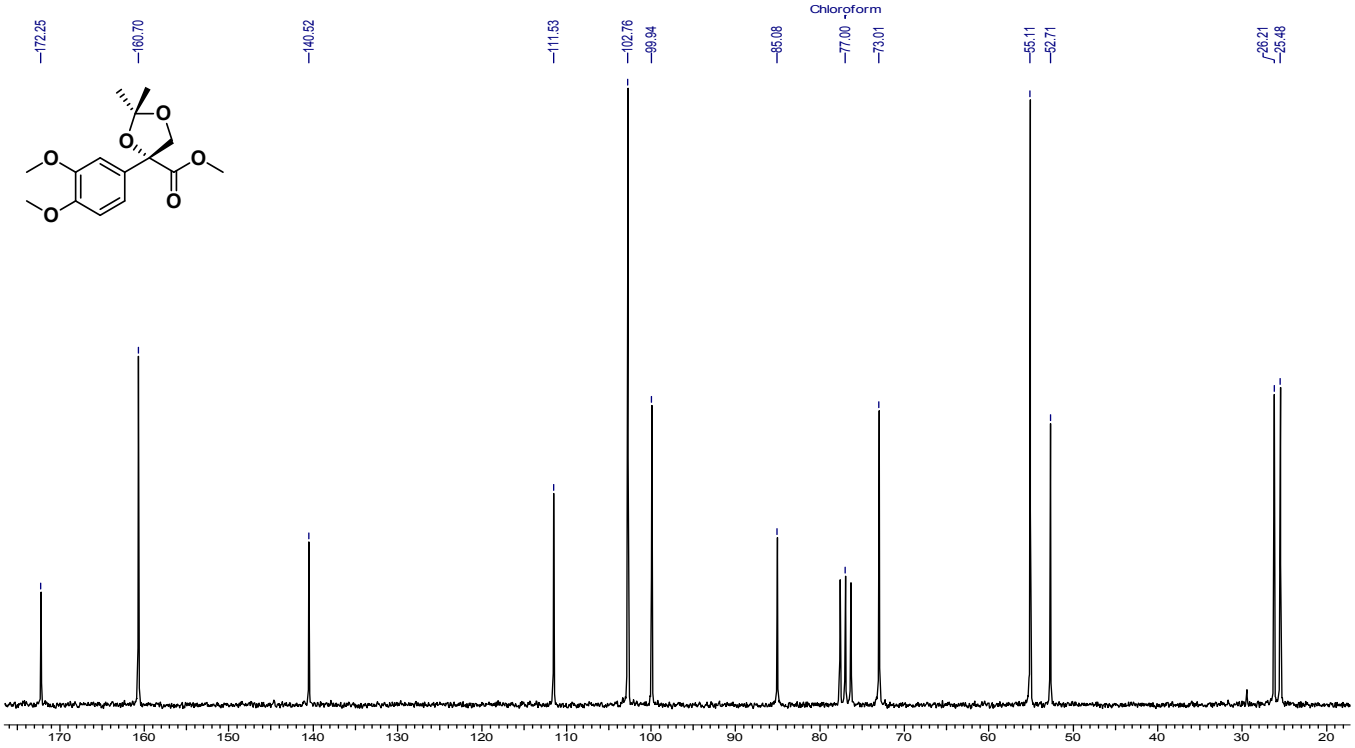
^{13}C NMR of 1-(4-(4-methoxyphenyl)-2,2-dimethyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (3a)



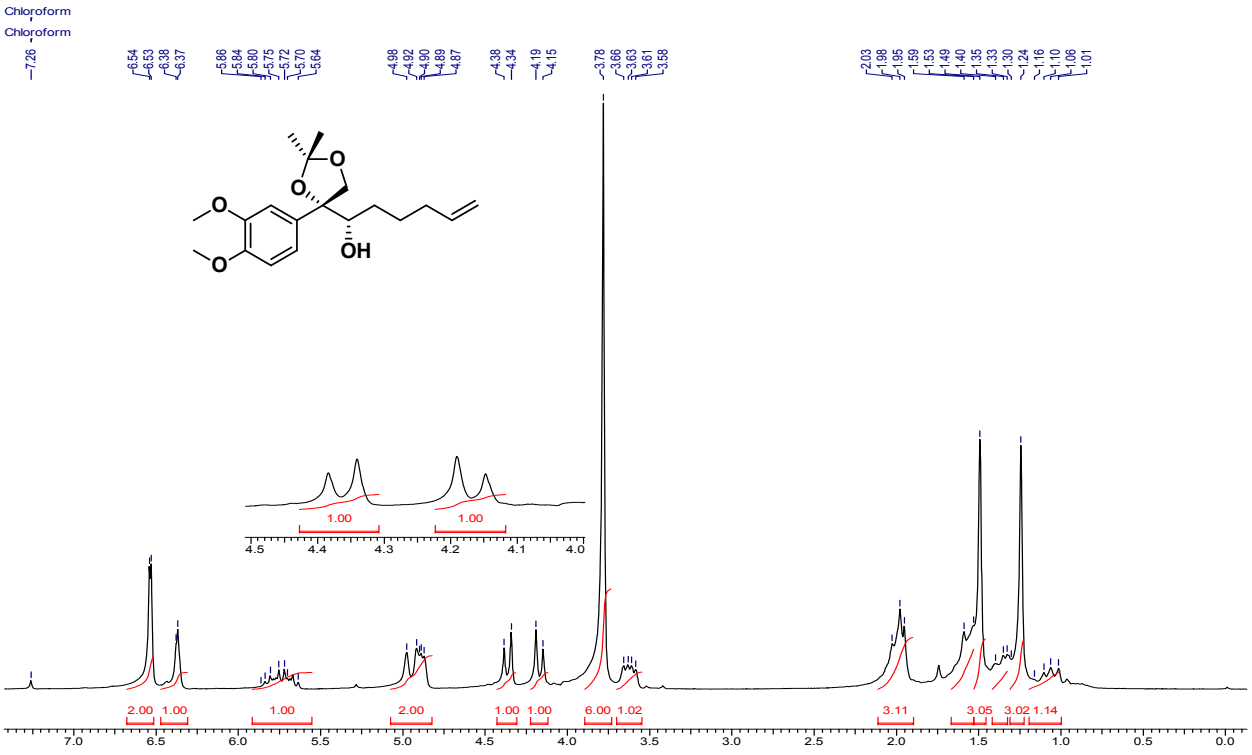
^{1}H NMR of methyl 4-(3,4-dimethoxyphenyl)-2,2-dimethyl-1,3-dioxolane-4-carboxylate (4) :



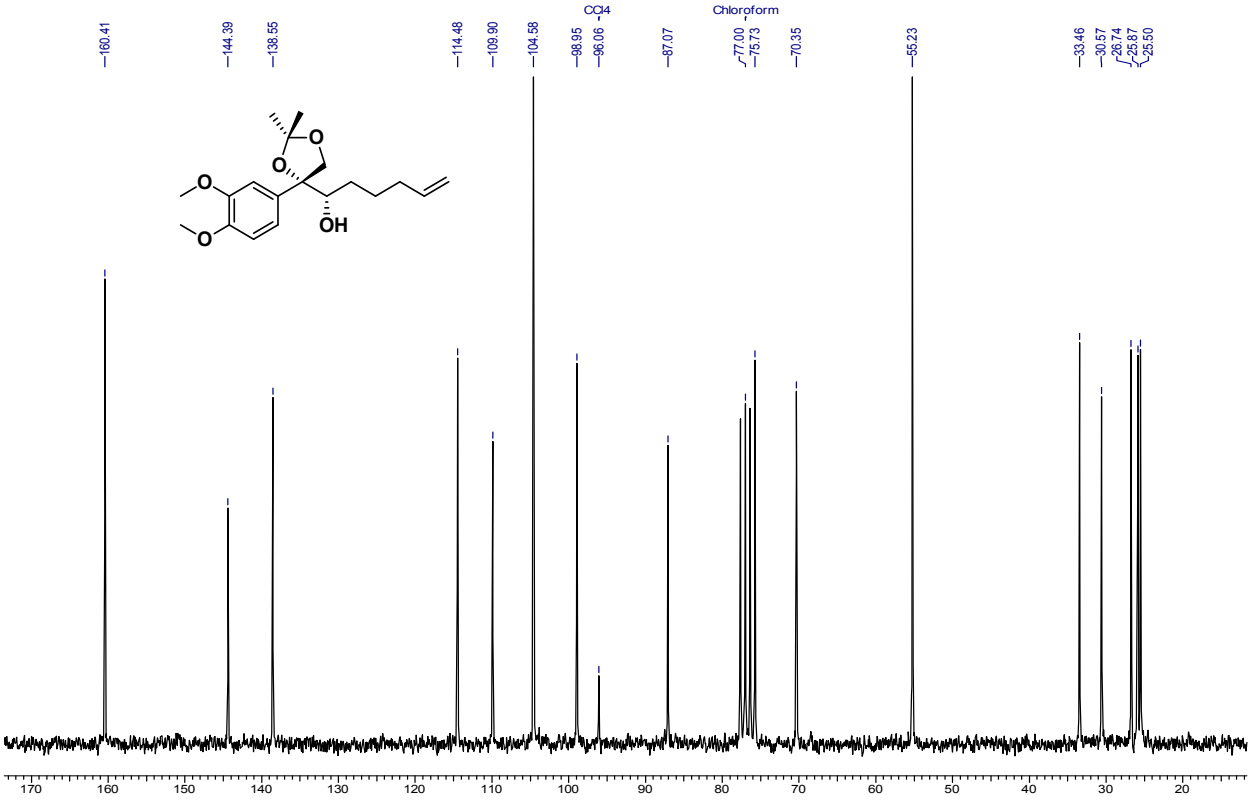
^{13}C NMR of methyl 4-(3,4-dimethoxyphenyl)-2,2-dimethyl-1,3-dioxolane-4-carboxylate (4)



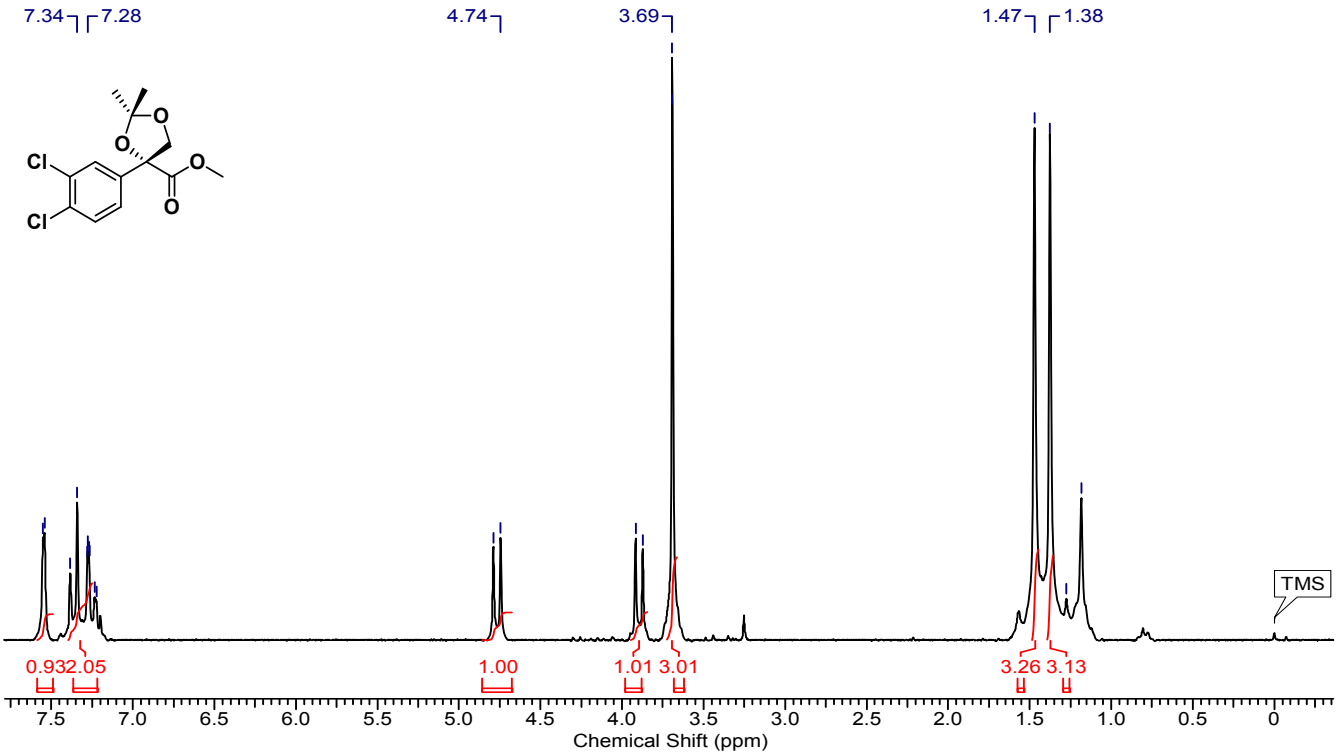
^{1}H NMR of 1-(4-(3,4-dimethoxyphenyl)-2,2-dimethyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (4a):



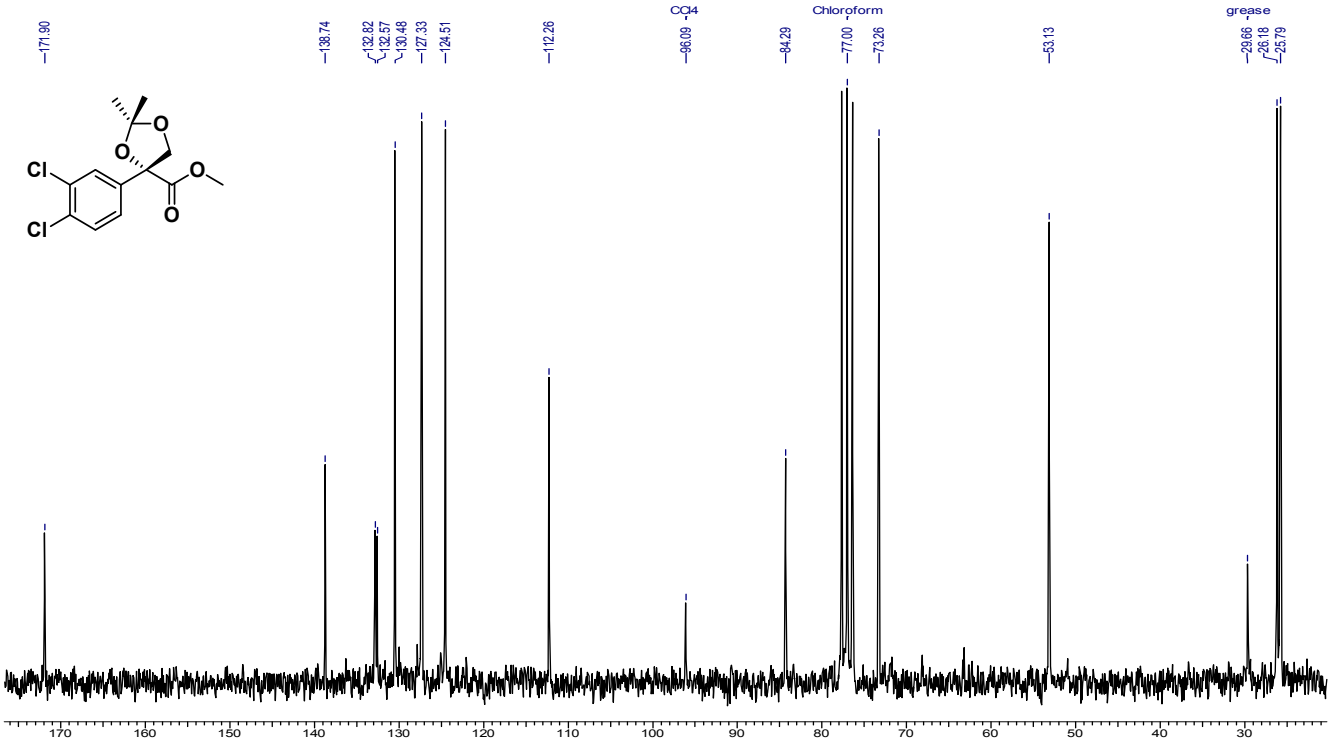
^{13}C NMR of 1-(4-(3,4-dimethoxyphenyl)-2,2-dimethyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (4a):



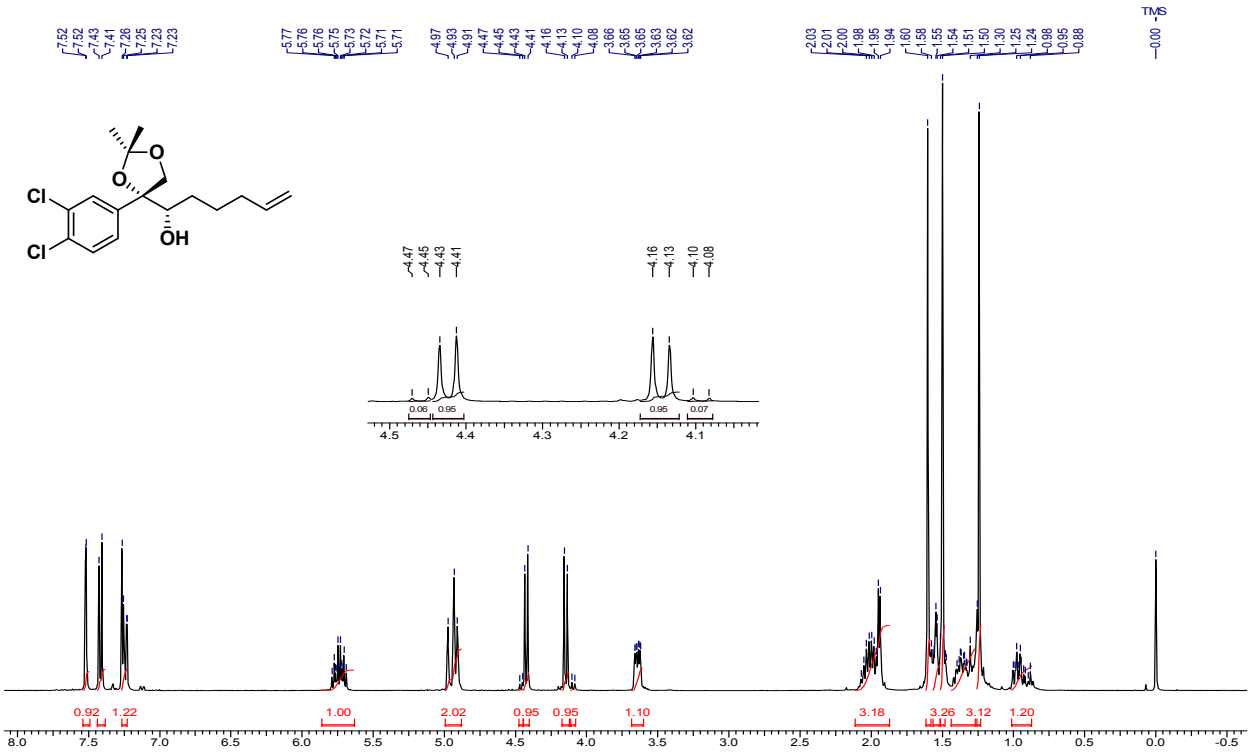
^{1}H NMR of methyl 4-(3,4-dichlorophenyl)-2,2-dimethyl-1,3-dioxolane-4-carboxylate (5)



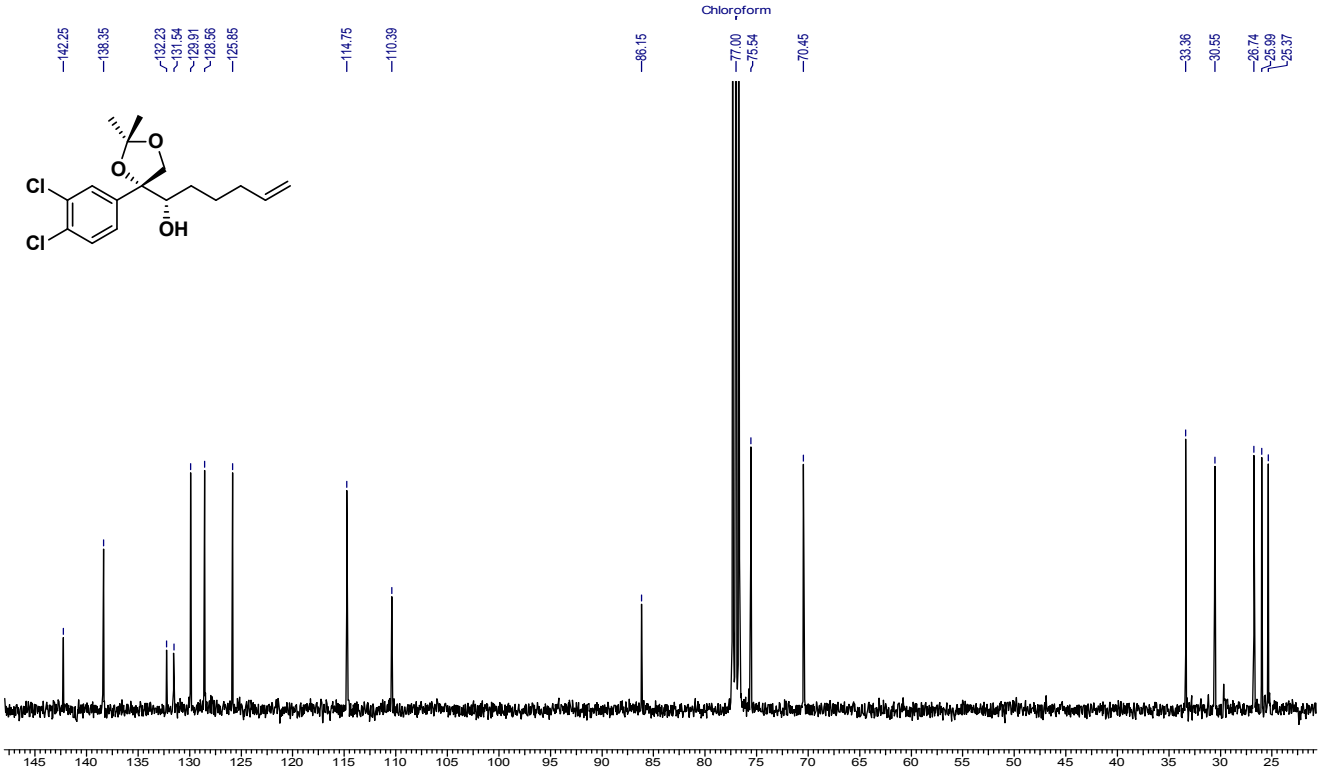
^{13}C NMR of methyl 4-(3,4-dichlorophenyl)-2,2-dimethyl-1,3-dioxolane-4-carboxylate (5)



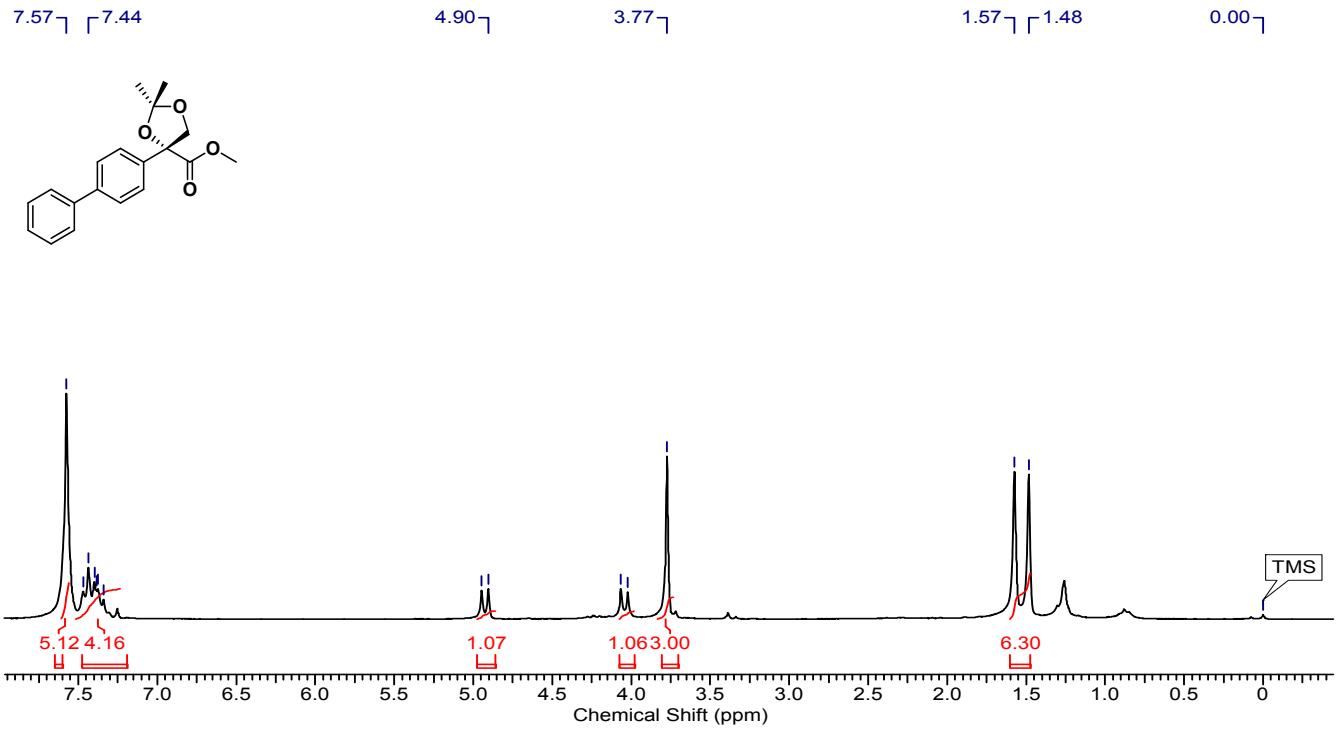
^{1}H NMR of methyl 4-(3,4-dichlorophenyl)-2,2-dimethyl-1,3-dioxolane-4-carboxylate (5a)



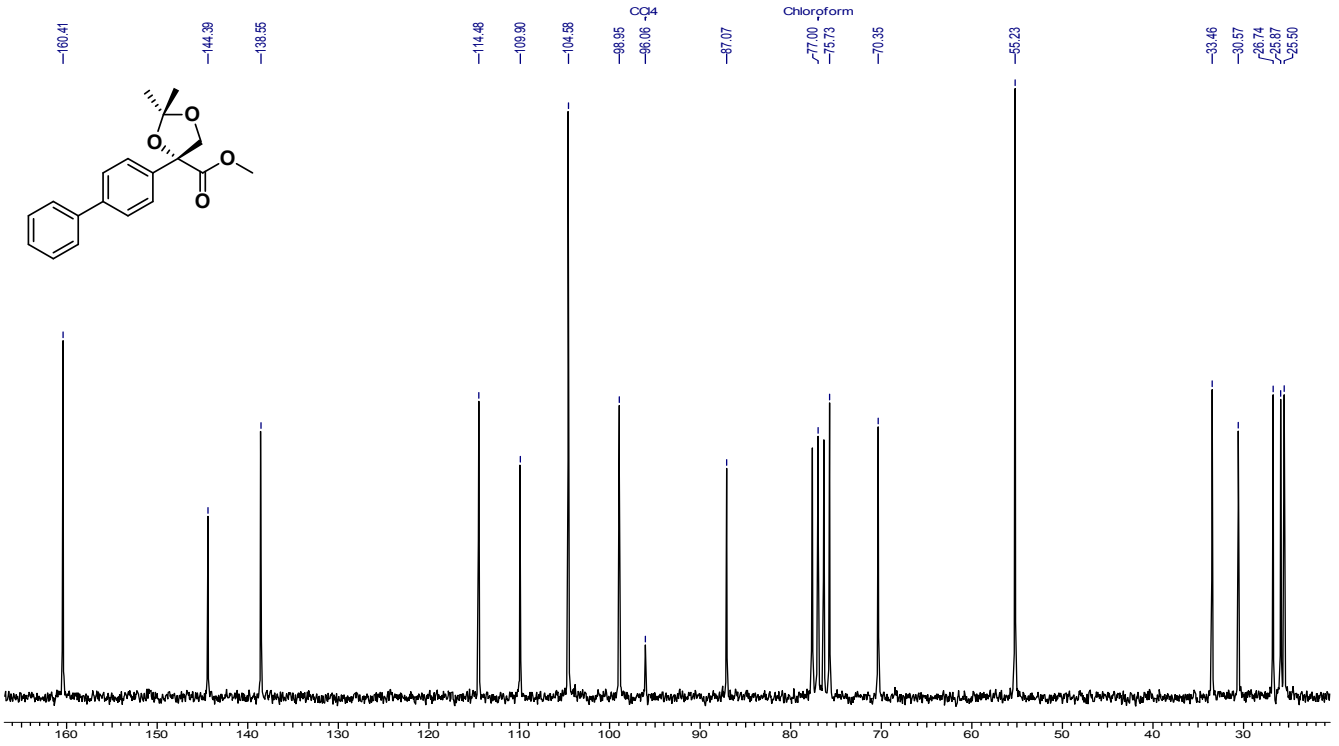
^{13}C NMR of methyl 4-(3,4-dichlorophenyl)-2,2-dimethyl-1,3-dioxolane-4-carboxylate (5a)



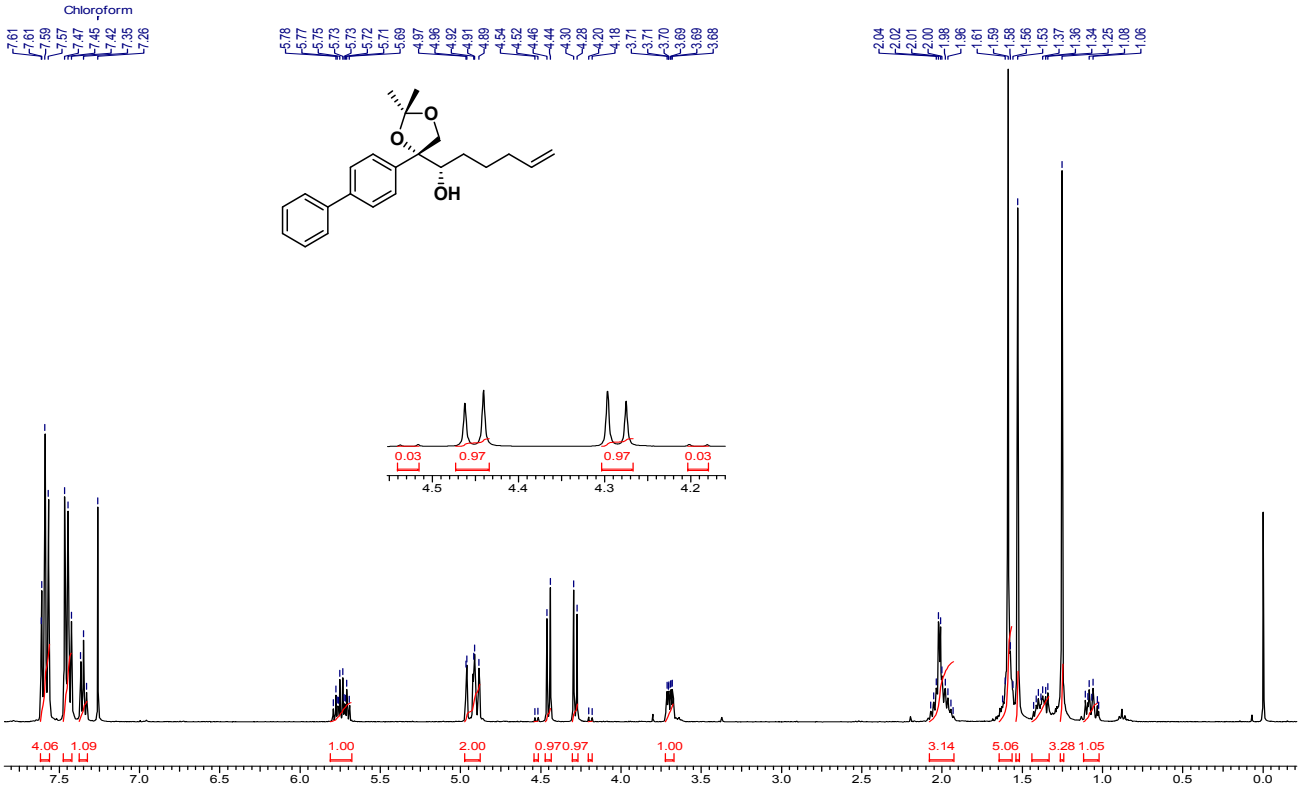
^{1}H NMR of methyl 4-([1,1'-biphenyl]-4-yl)-2,2-dimethyl-1,3-dioxolane-4-carboxylate (6)



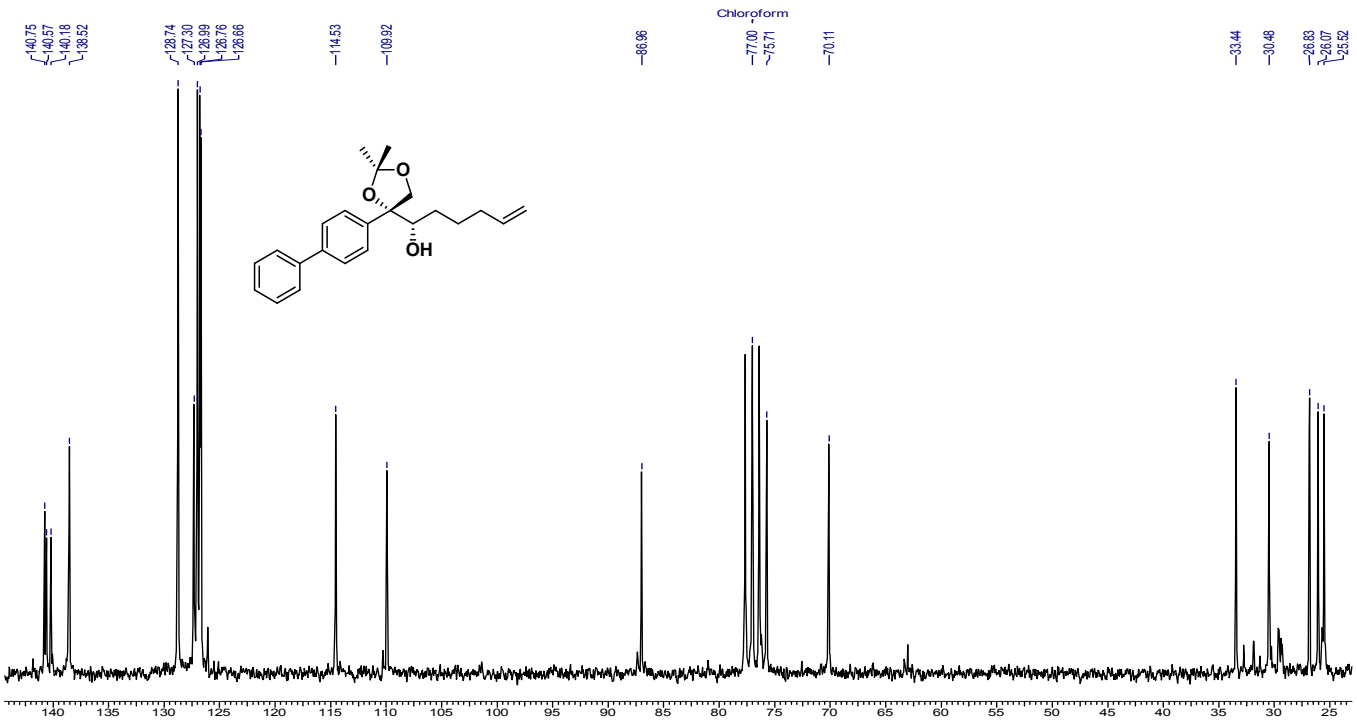
^{13}C NMR of methyl 4-([1,1'-biphenyl]-4-yl)-2,2-dimethyl-1,3-dioxolane-4-carboxylate (6)



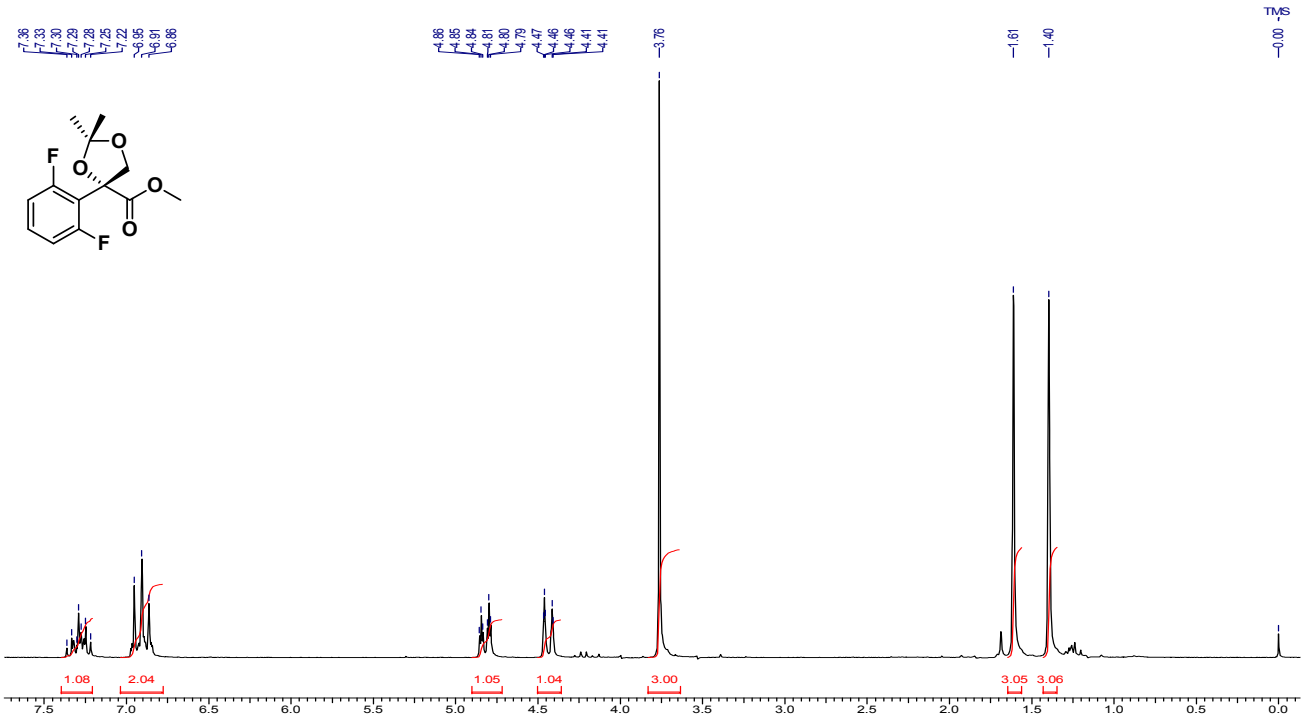
^{1}H NMR of 1-(4-([1,1'-biphenyl]-4-yl)-2,2-dimethyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (6a)



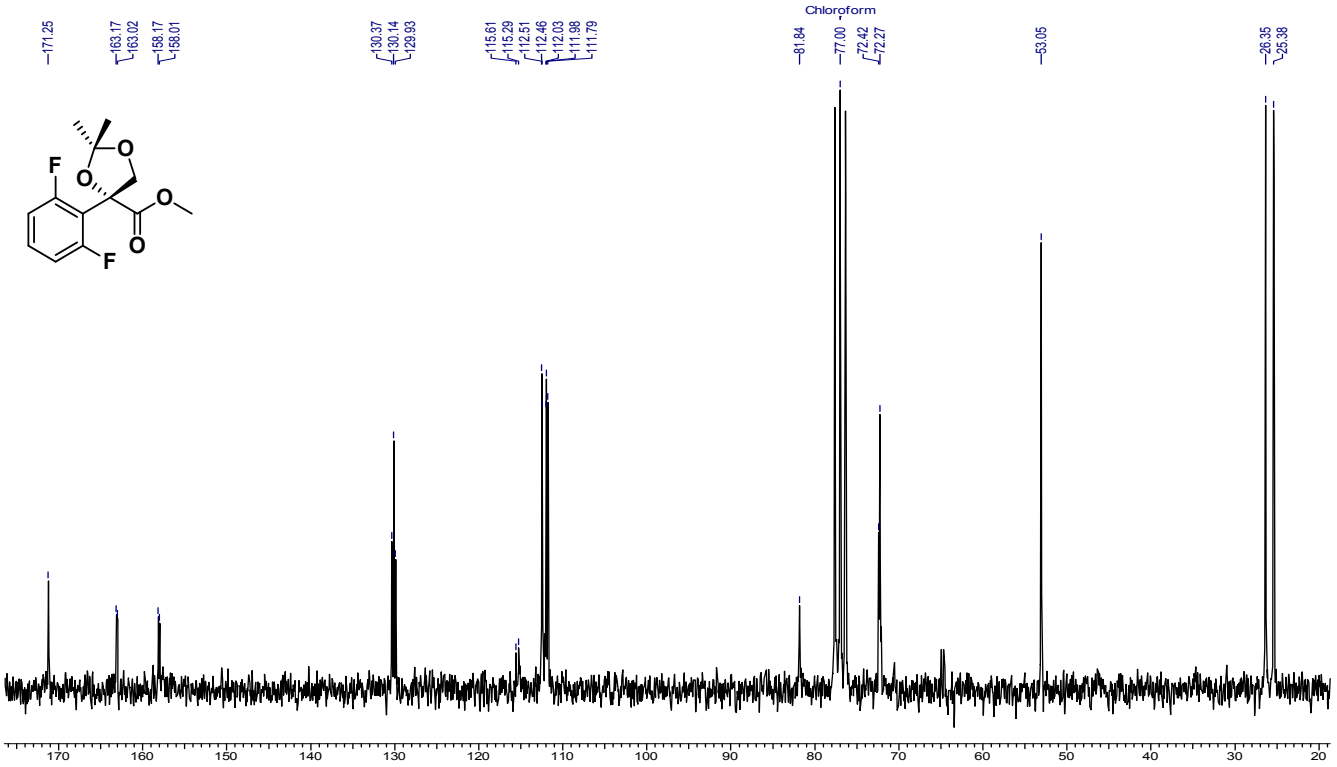
^{13}C NMR of 1-(4-([1,1'-biphenyl]-4-yl)-2,2-dimethyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (6a)



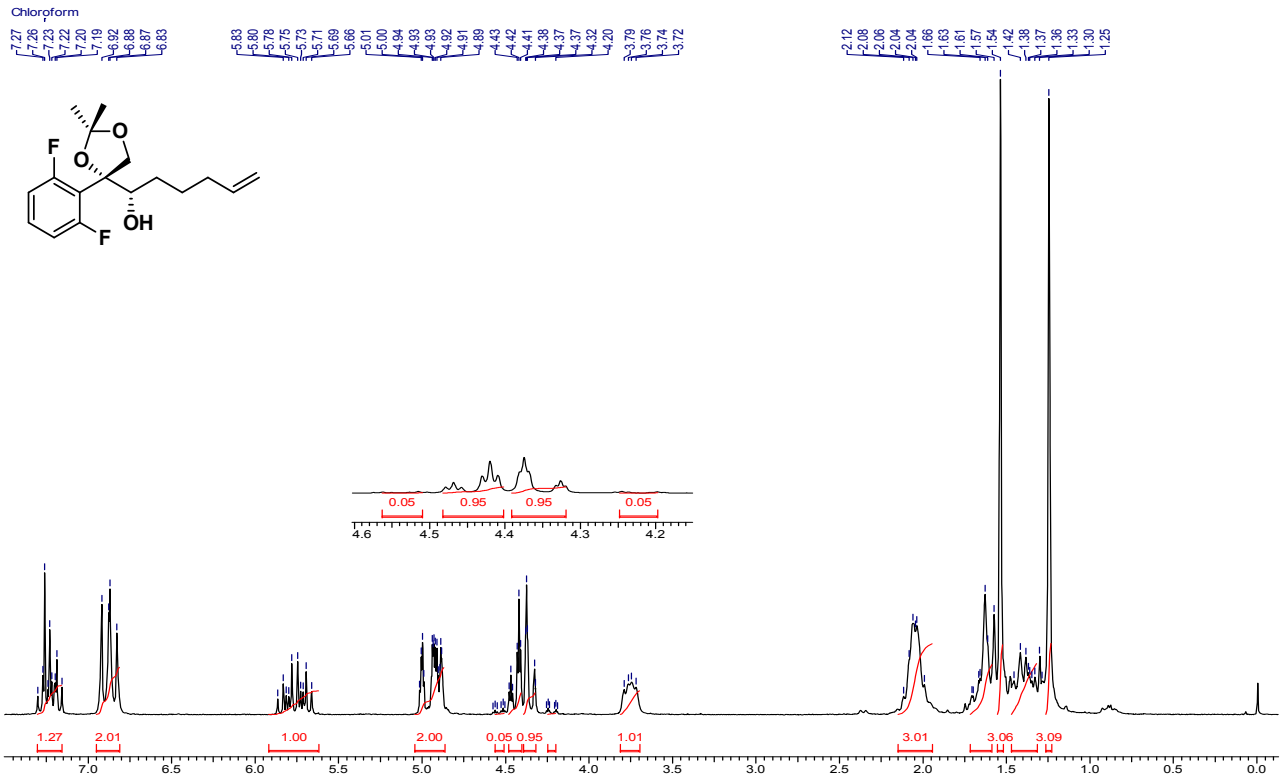
^{1}H NMR of methyl 4-(2,6-difluorophenyl)-2,2-dimethyl-1,3-dioxolane-4-carboxylate (7)



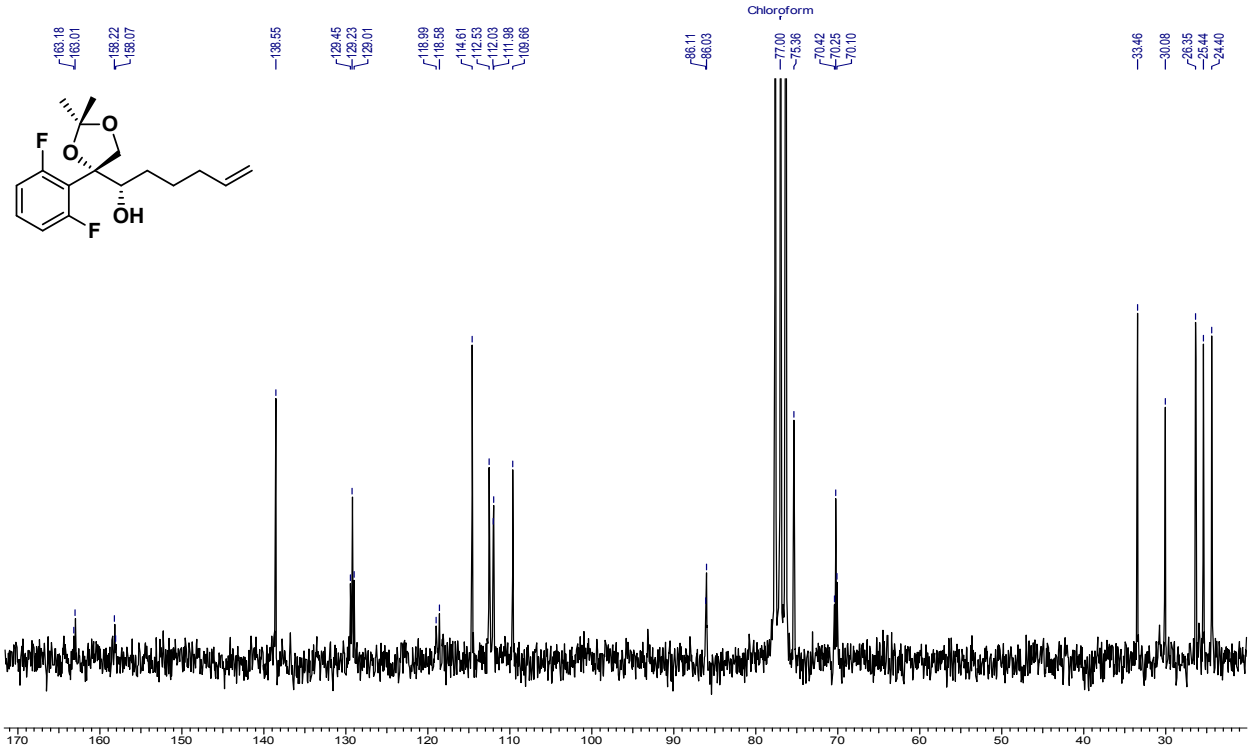
^{13}C NMR of methyl 4-(2,6-difluorophenyl)-2,2-dimethyl-1,3-dioxolane-4-carboxylate (7)



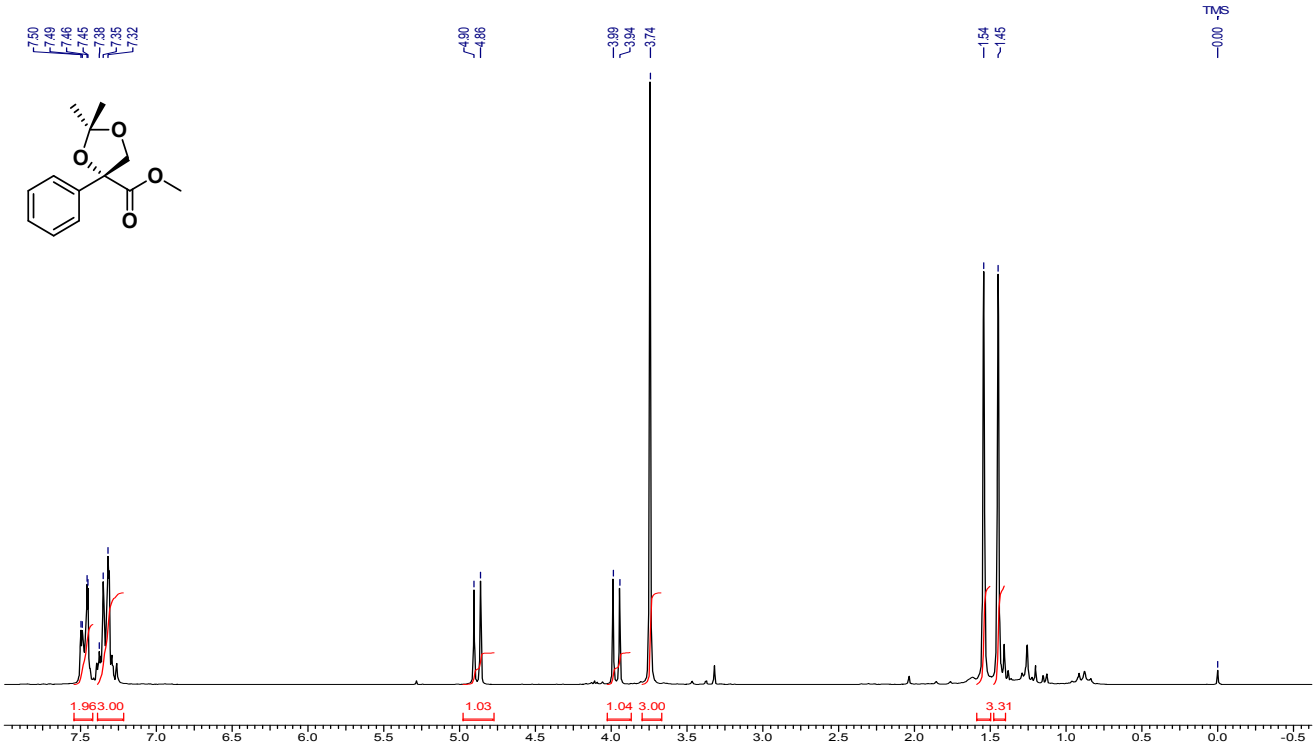
^{1}H NMR of 1-(4-(2,6-difluorophenyl)-2,2-dimethyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (7a)



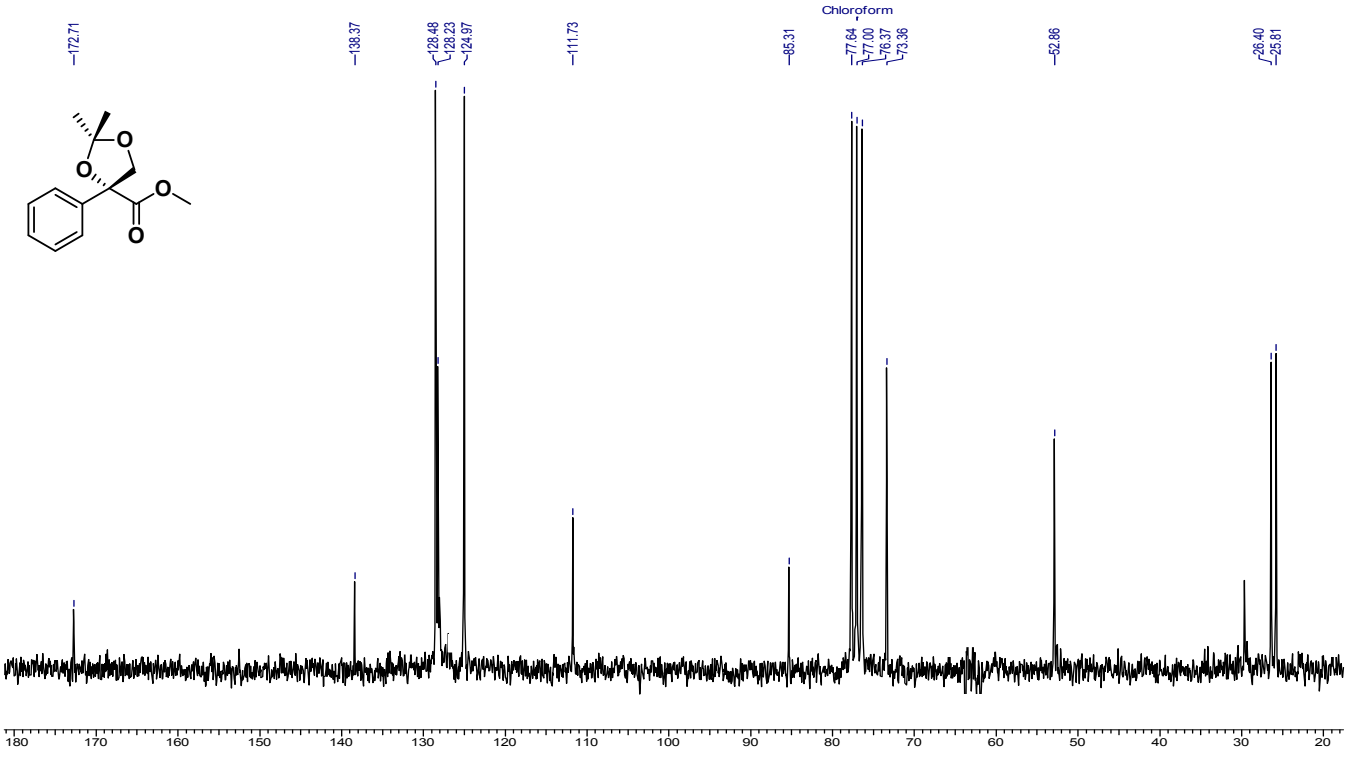
^{13}C NMR of 1-(4-(2,6-difluorophenyl)-2,2-dimethyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (7a)



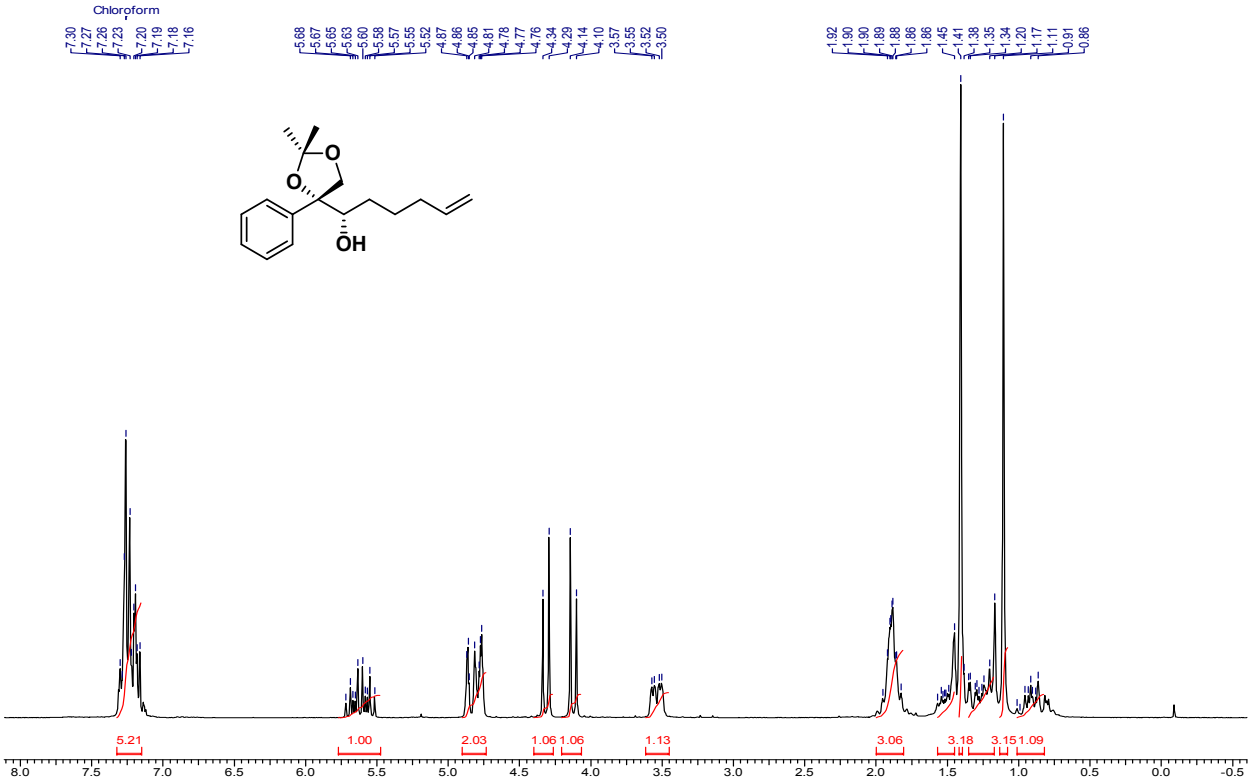
^{1}H NMR of methyl 2,2-dimethyl-4-phenyl-1,3-dioxolane-4-carboxylate (8)



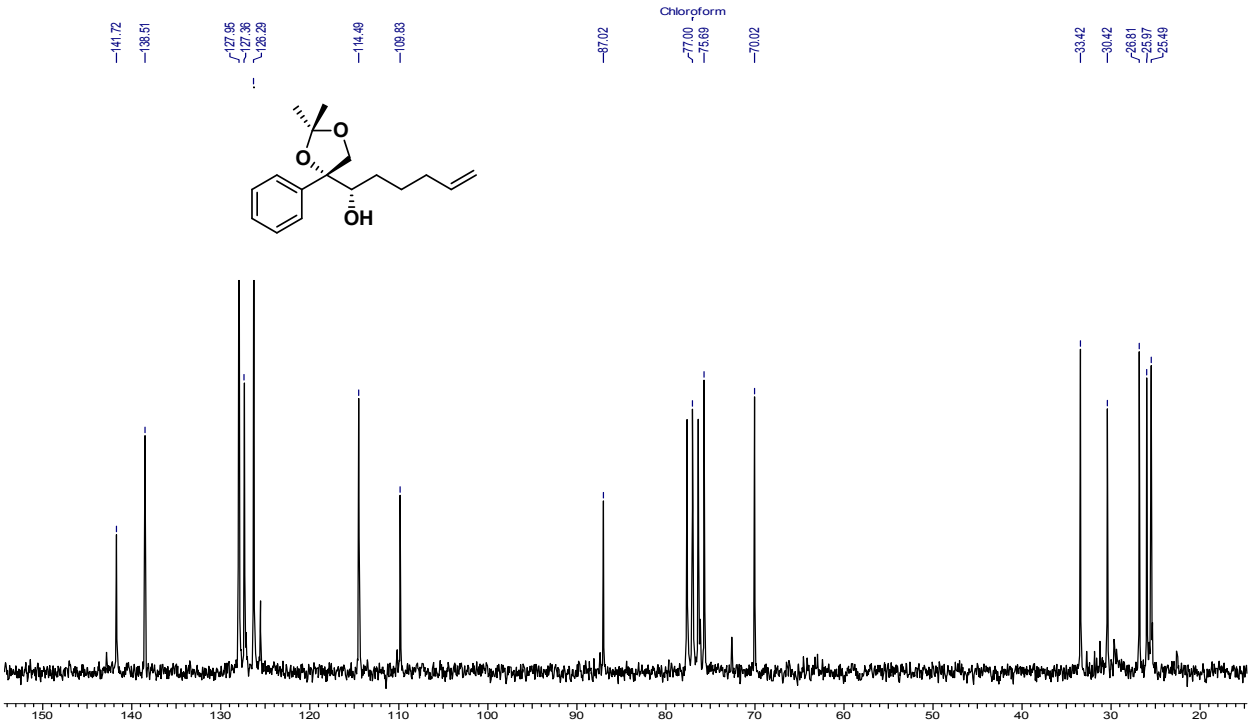
^{13}C NMR of methyl 2,2-dimethyl-4-phenyl-1,3-dioxolane-4-carboxylate (8)



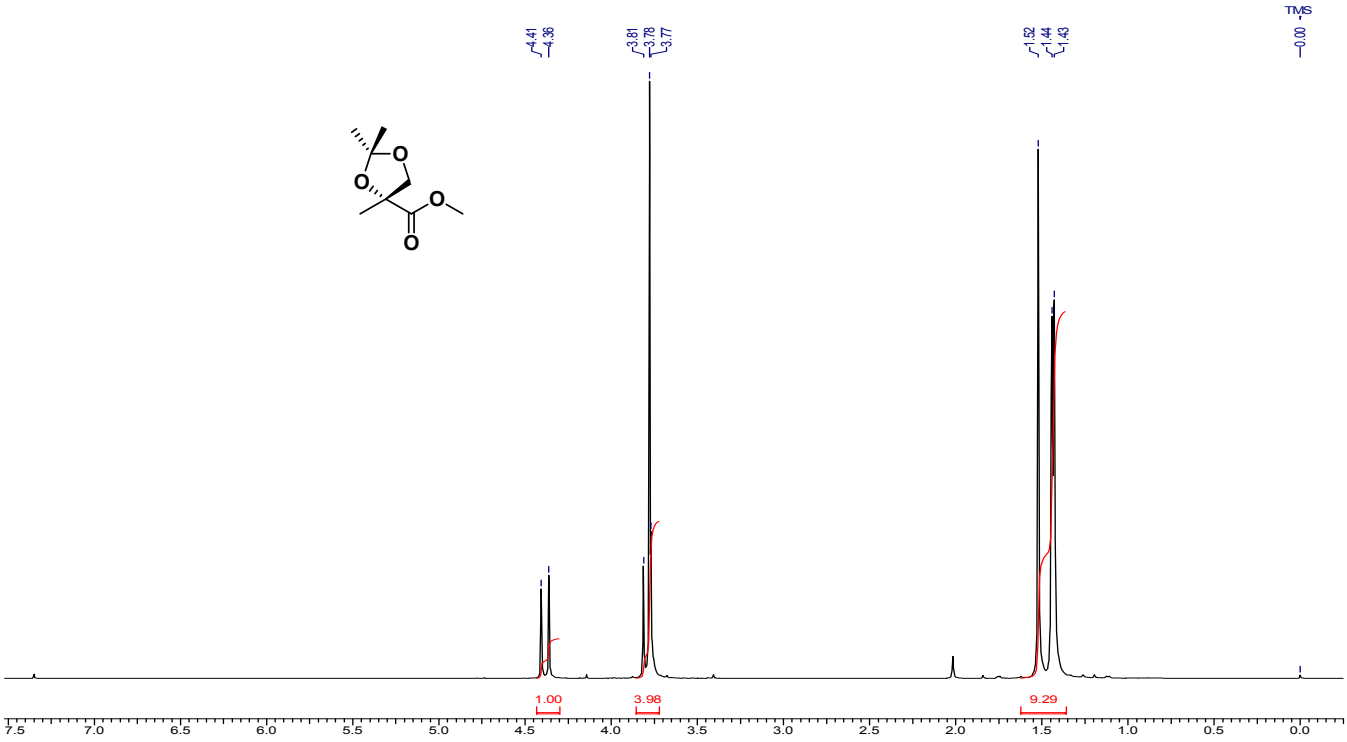
^{1}H NMR of 1-(2,2-dimethyl-4-phenyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (8a)



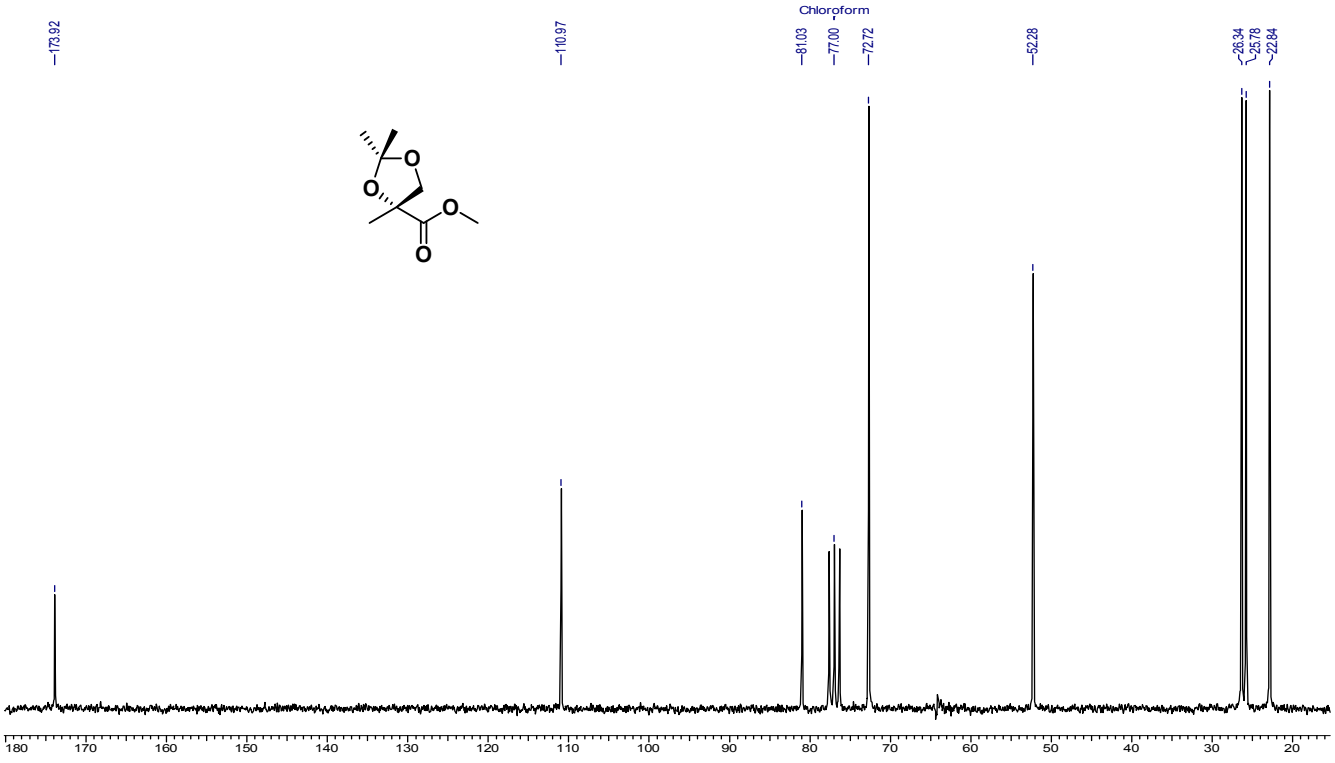
^{13}C NMR of 1-(2,2-dimethyl-4-phenyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (8a)



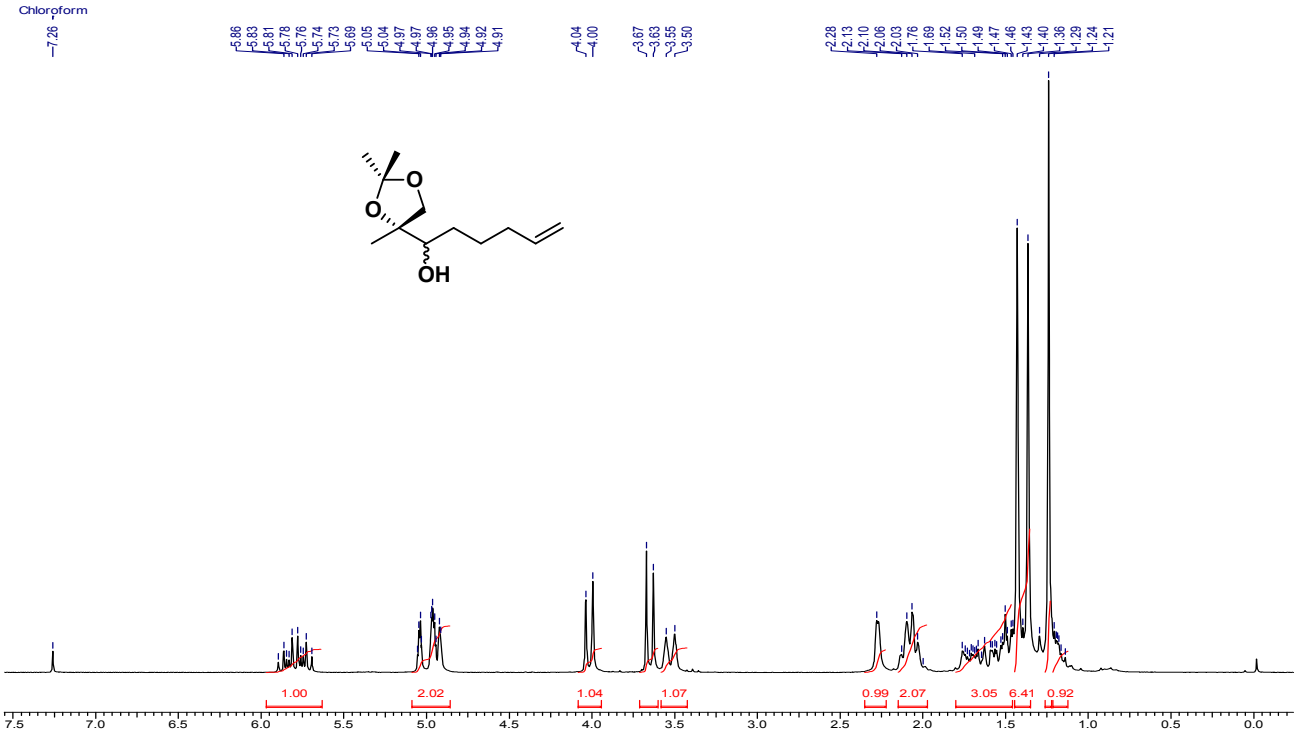
^{1}H NMR of methyl 2,2,4-trimethyl-1,3-dioxolane-4-carboxylate (9)



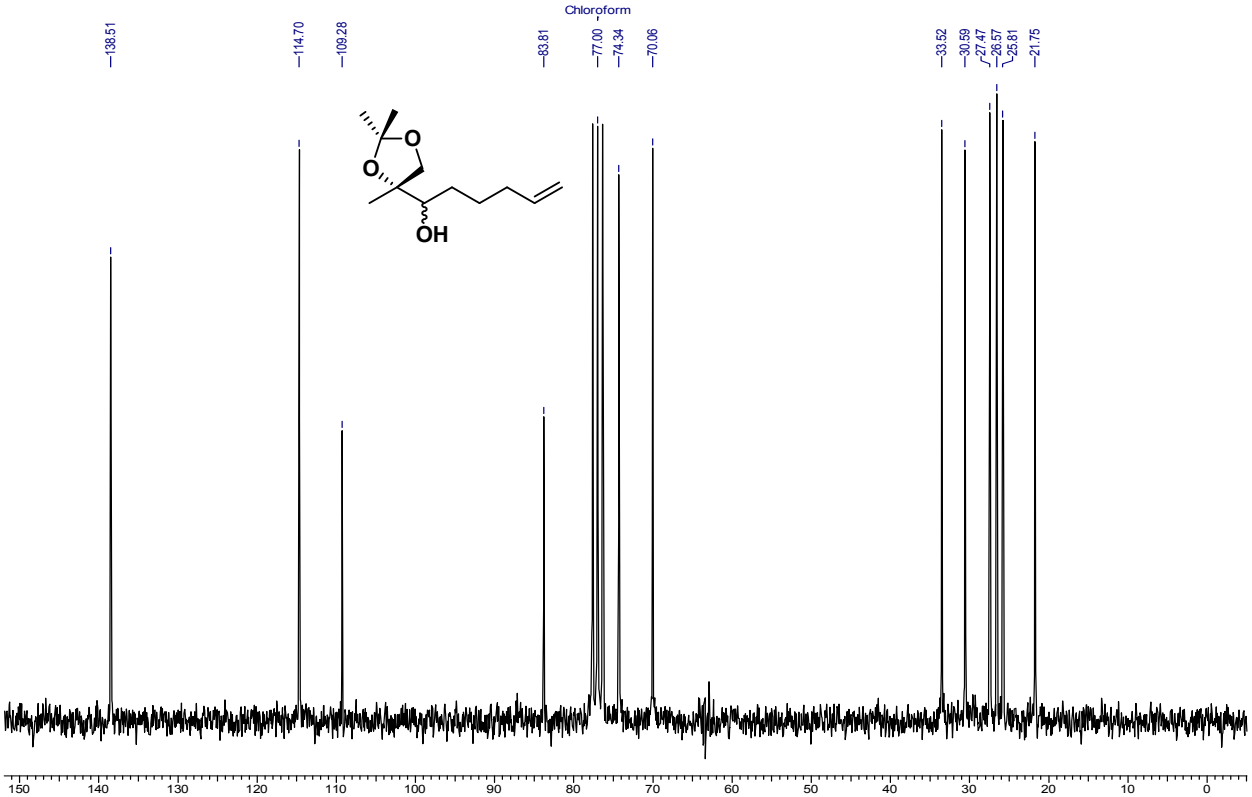
^{13}C NMR of methyl 2,2,4-trimethyl-1,3-dioxolane-4-carboxylate (9)



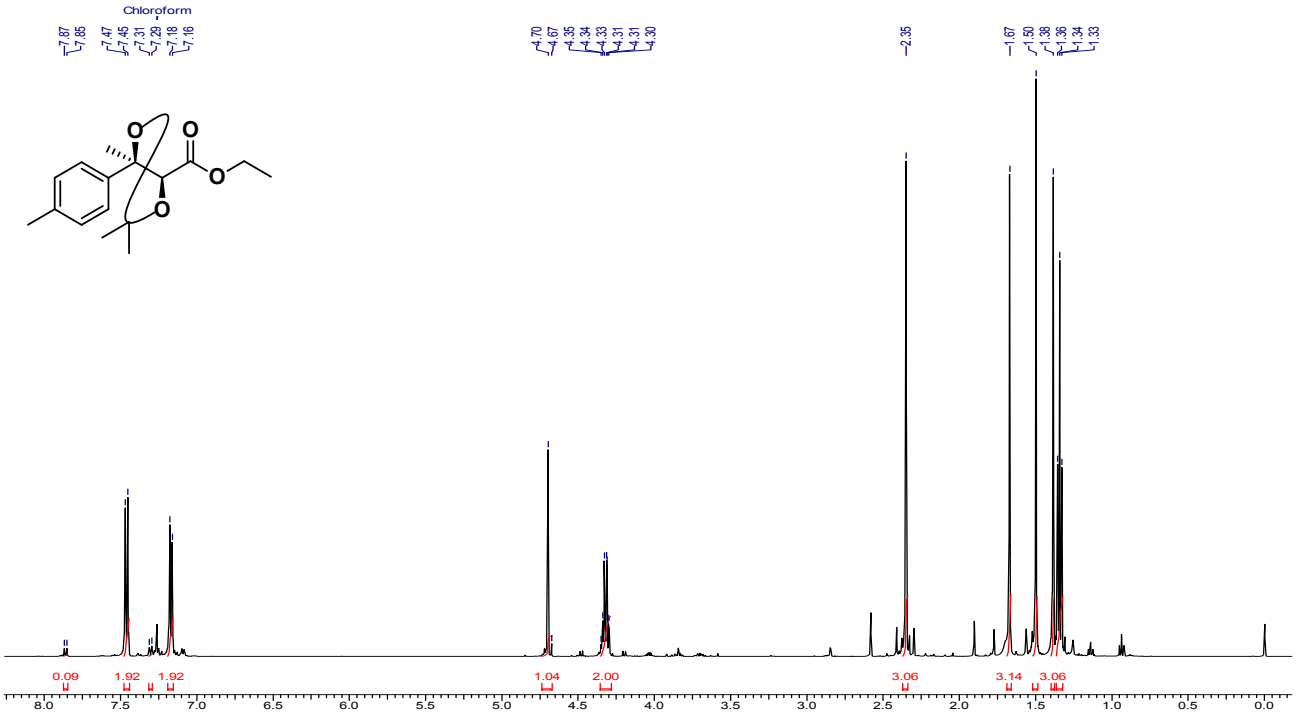
^{1}H NMR of 1-(2,2,4-trimethyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (9a)



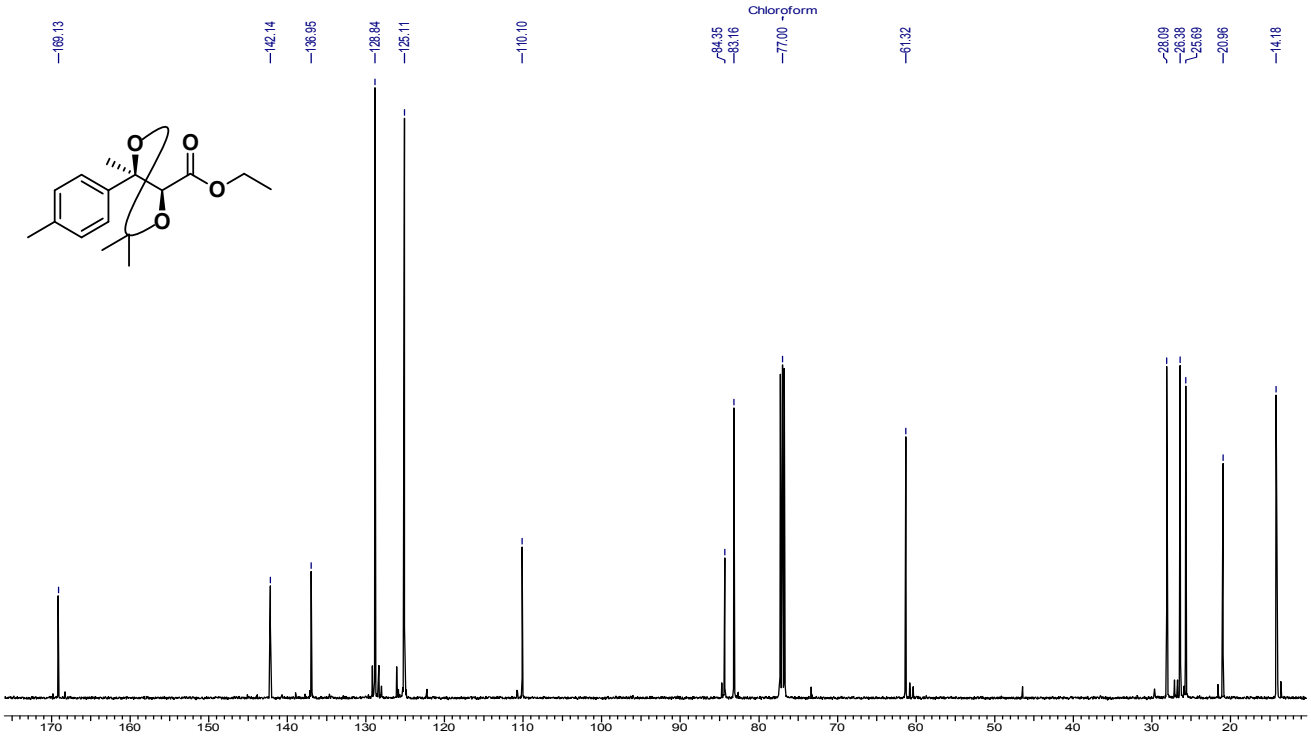
^{13}C NMR of 1-(2,2,4-trimethyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (9a)



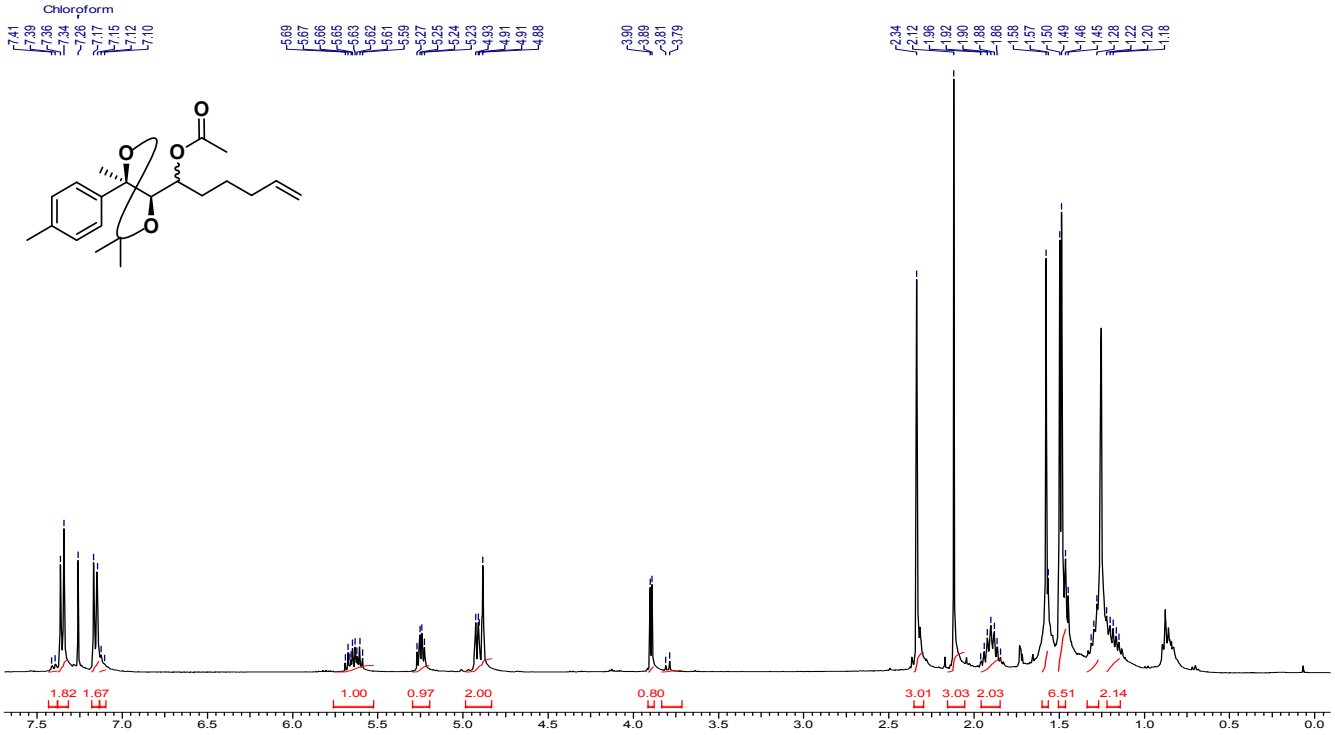
^{1}H NMR of ethyl-2,2,5-trimethyl-5-(*p*-tolyl)-1,3-dioxolane-4-carboxylate (10)



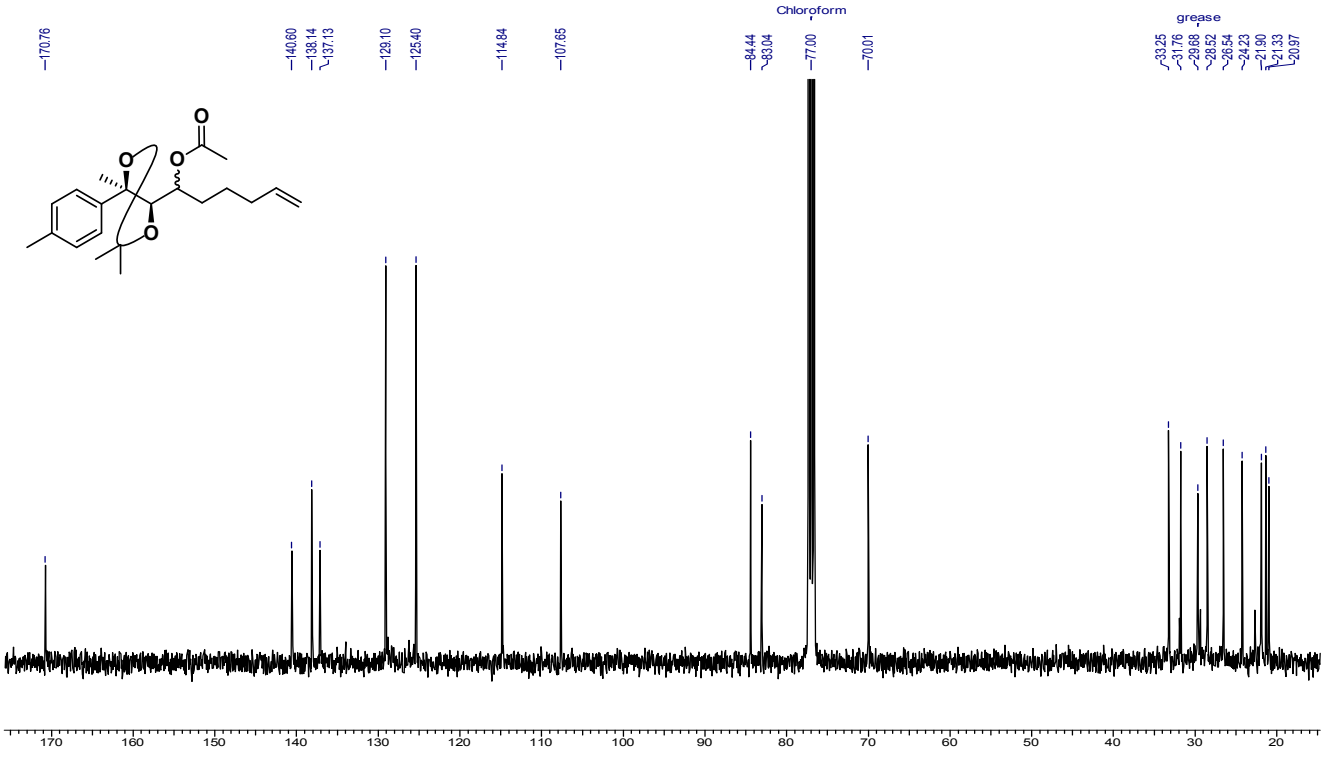
^{13}C NMR of ethyl-2,2,5-trimethyl-5-(*p*-tolyl)-1,3-dioxolane-4-carboxylate (10)



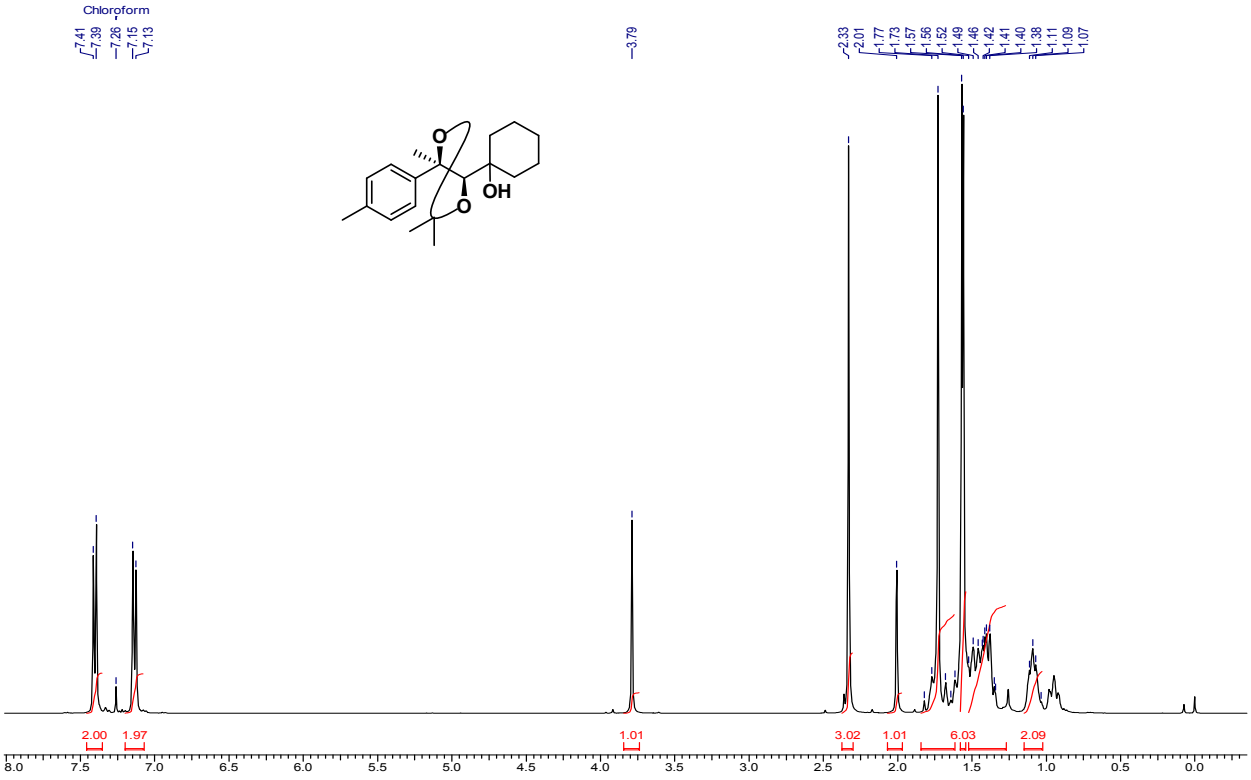
^{1}H NMR of 1-(2,2,5-trimethyl-5-(p-tolyl)-1,3-dioxolan-4-yl)hex-5-en-1-yl acetate (10'a)



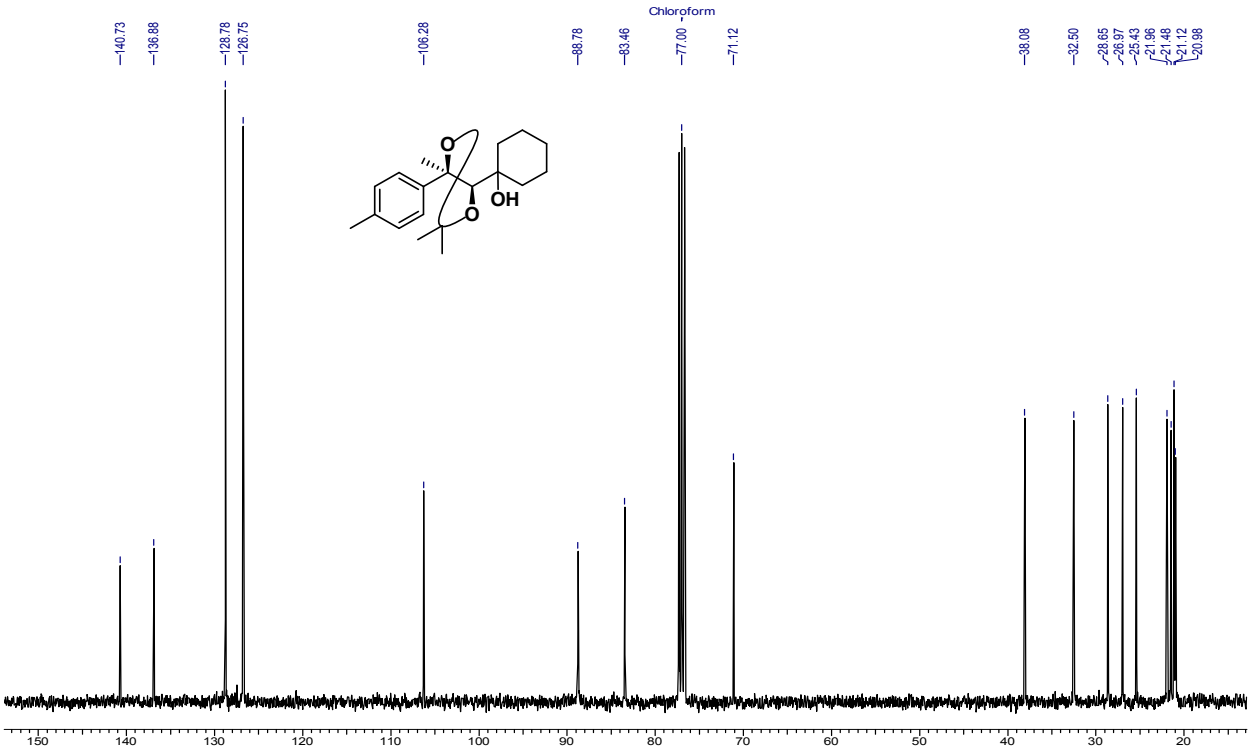
^{13}C NMR of 1-(2,2,5-trimethyl-5-(p-tolyl)-1,3-dioxolan-4-yl)hex-5-en-1-yl acetate (10'a)



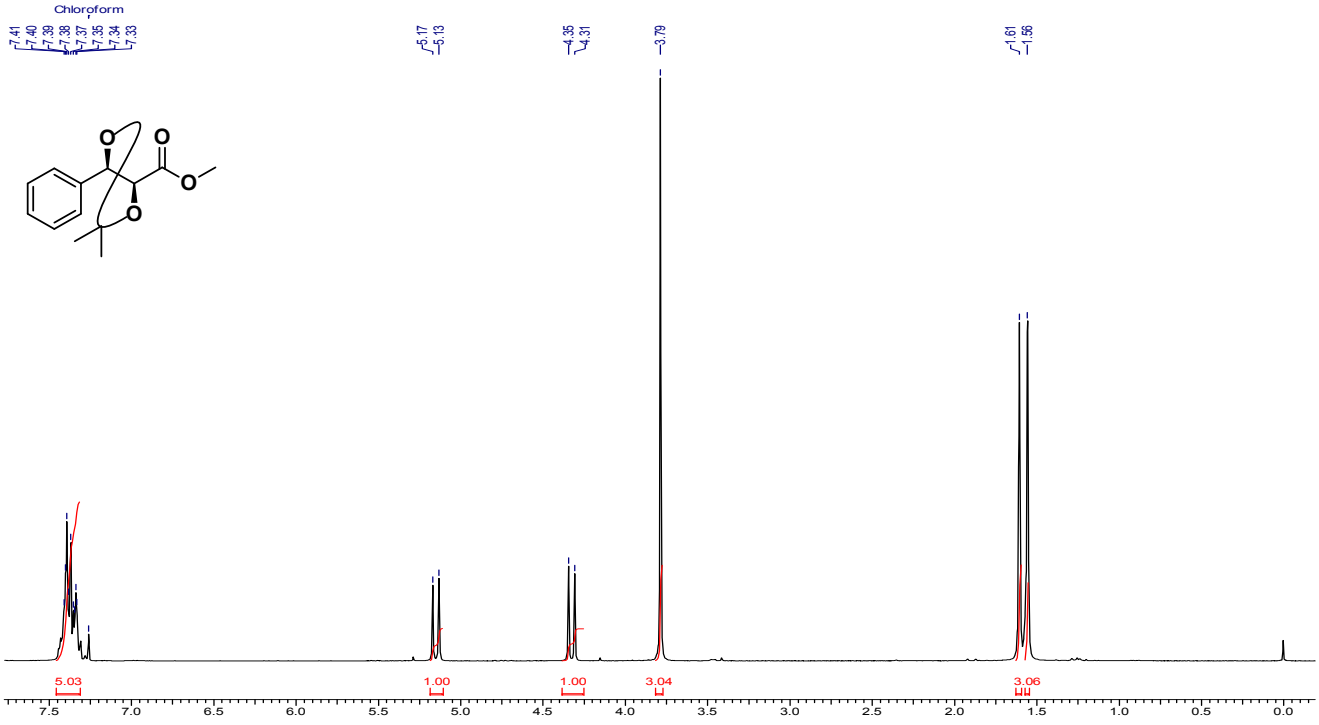
^{1}H NMR of 1-(2,2,5-trimethyl-5-(p-tolyl)-1,3-dioxolan-4-yl)cyclohexanol (10b)



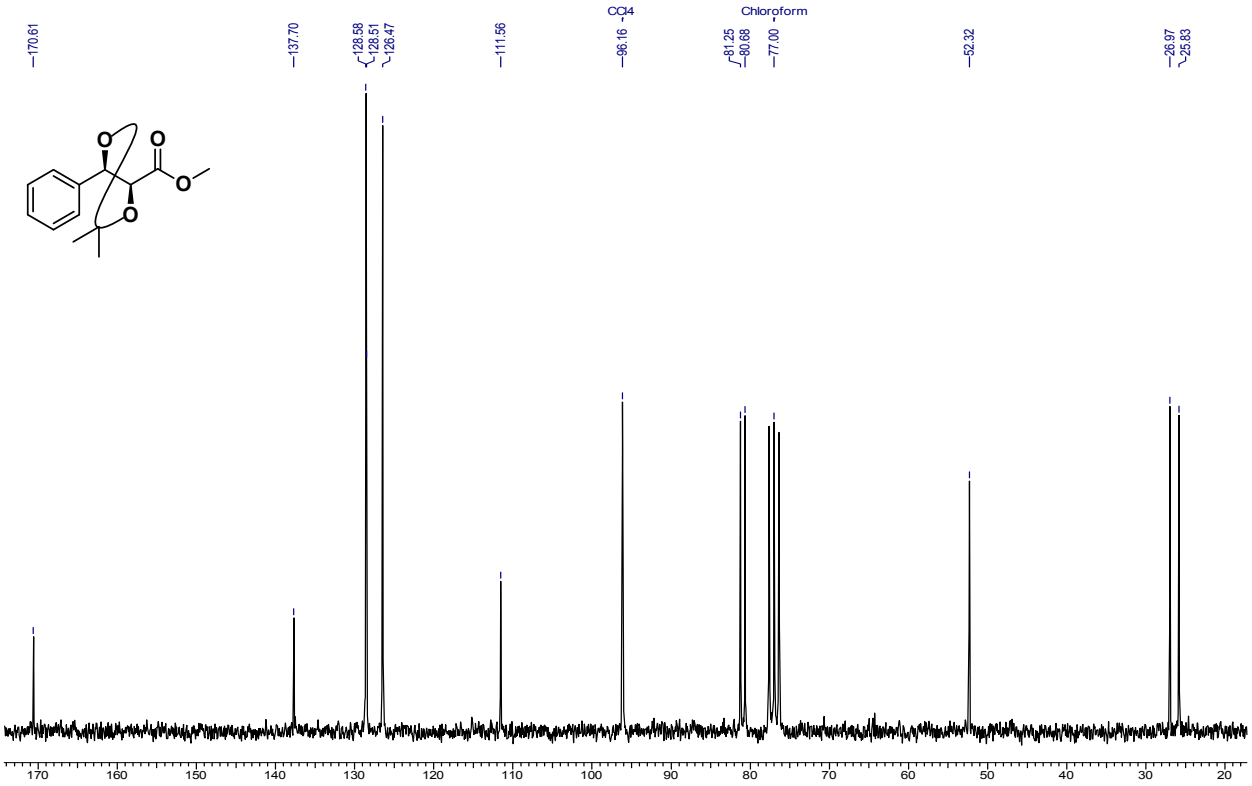
^{13}C NMR of 1-(2,2,5-trimethyl-5-(p-tolyl)-1,3-dioxolan-4-yl)cyclohexanol (10b)



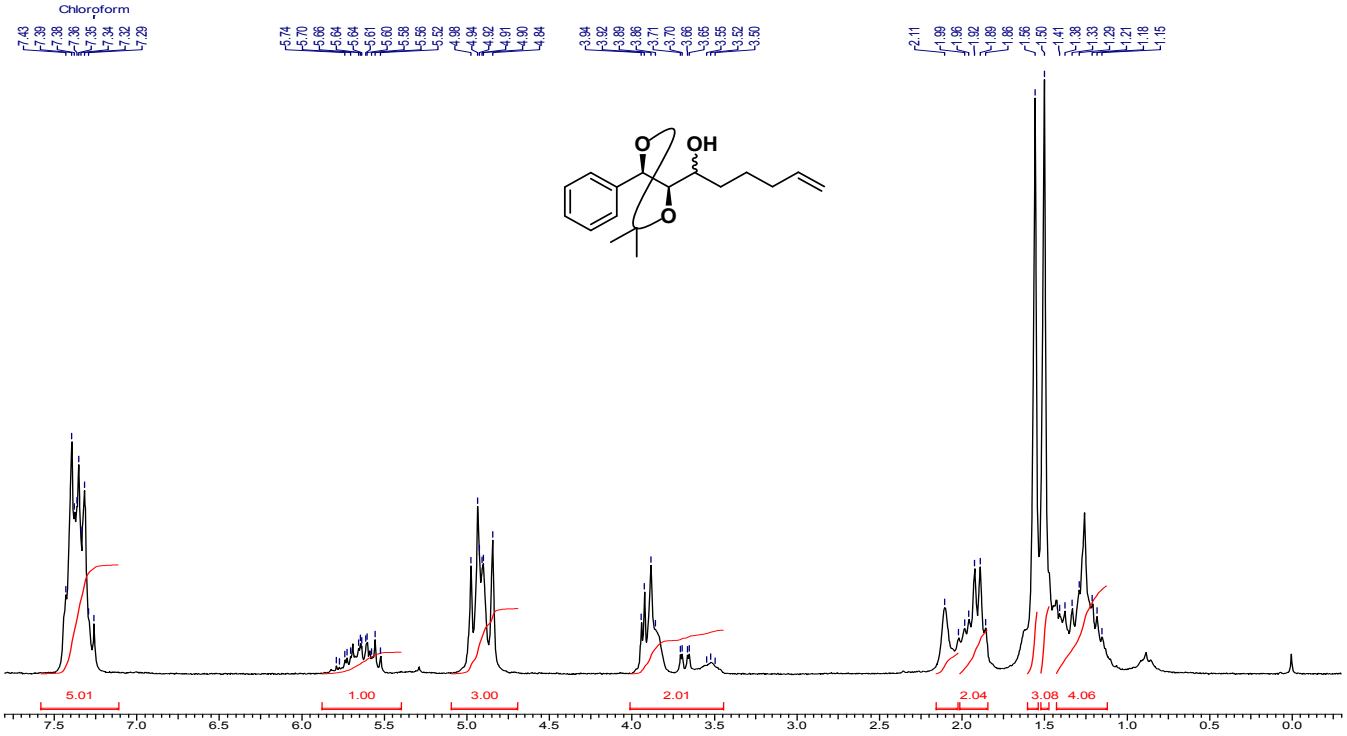
^{1}H NMR of (4*S*, 5*R*)-methyl 2,2-dimethyl-5-phenyl-1,3-dioxolane-4-carboxylate (11)



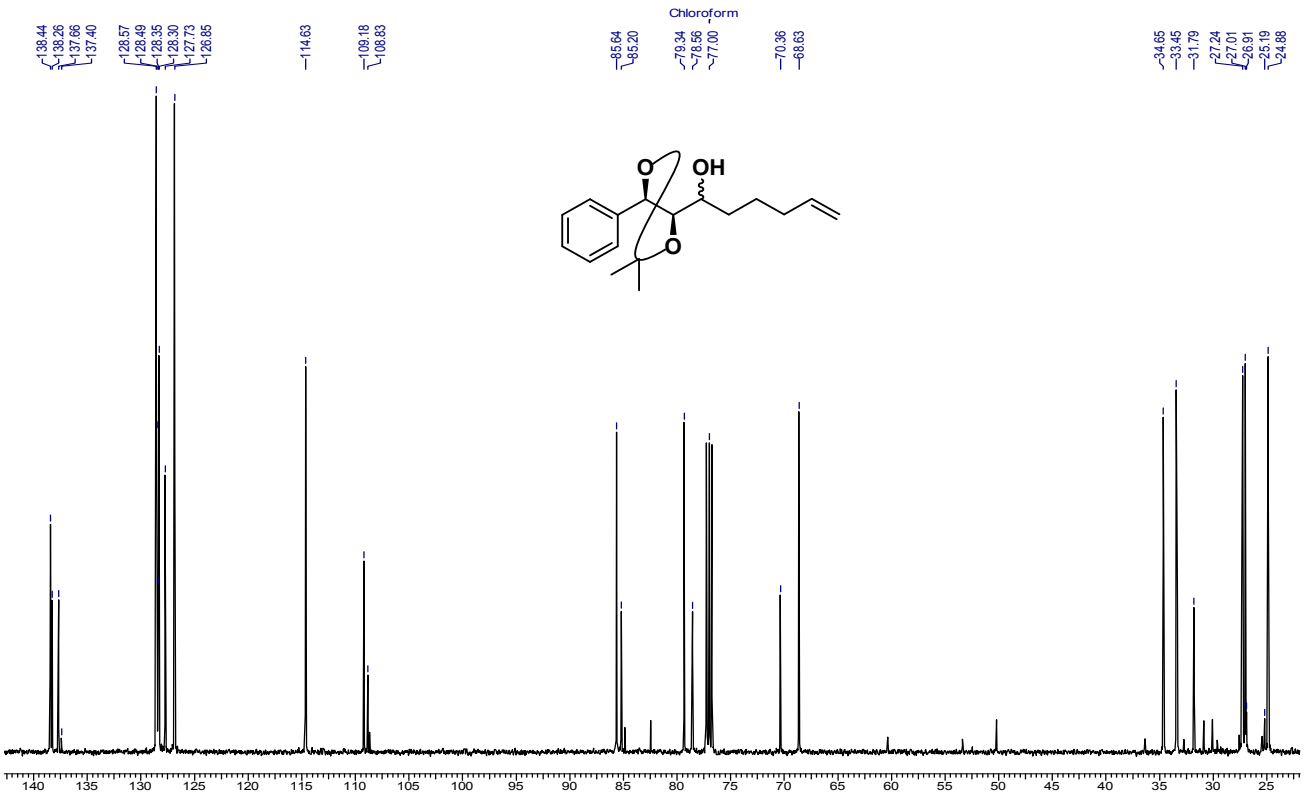
^{13}C NMR of (4*S*,5*R*)-methyl 2,2-dimethyl-5-phenyl-1,3-dioxolane-4-carboxylate (11)



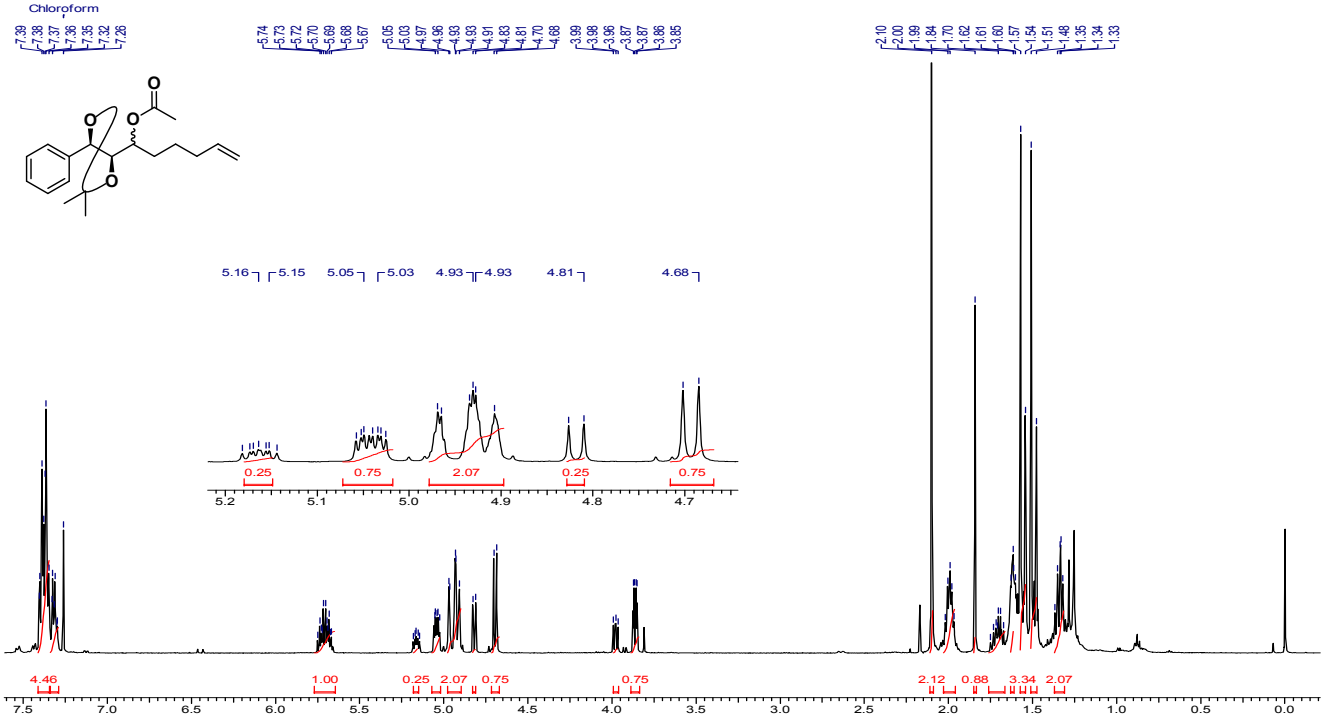
^{1}H NMR of 1-(2,2-dimethyl-5-phenyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (11a)



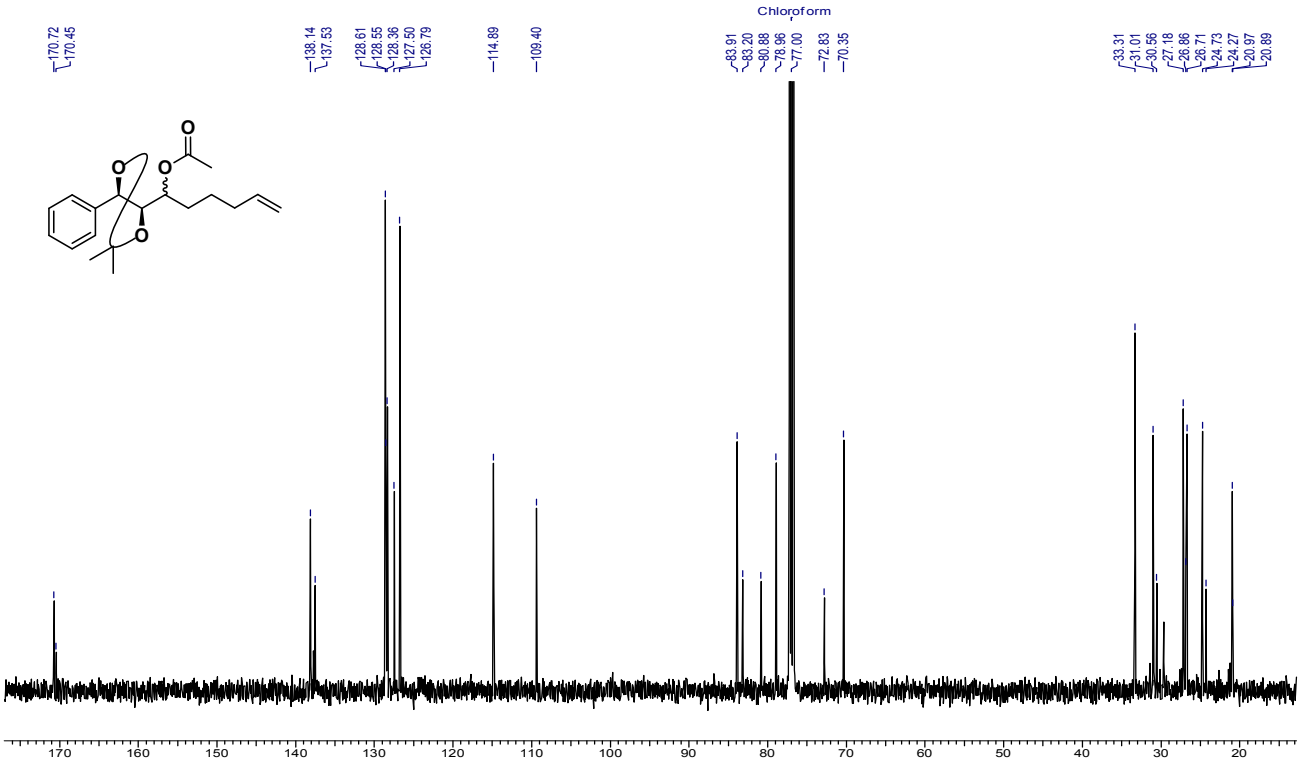
^{13}C NMR of 1-(2,2-dimethyl-5-phenyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (11a)



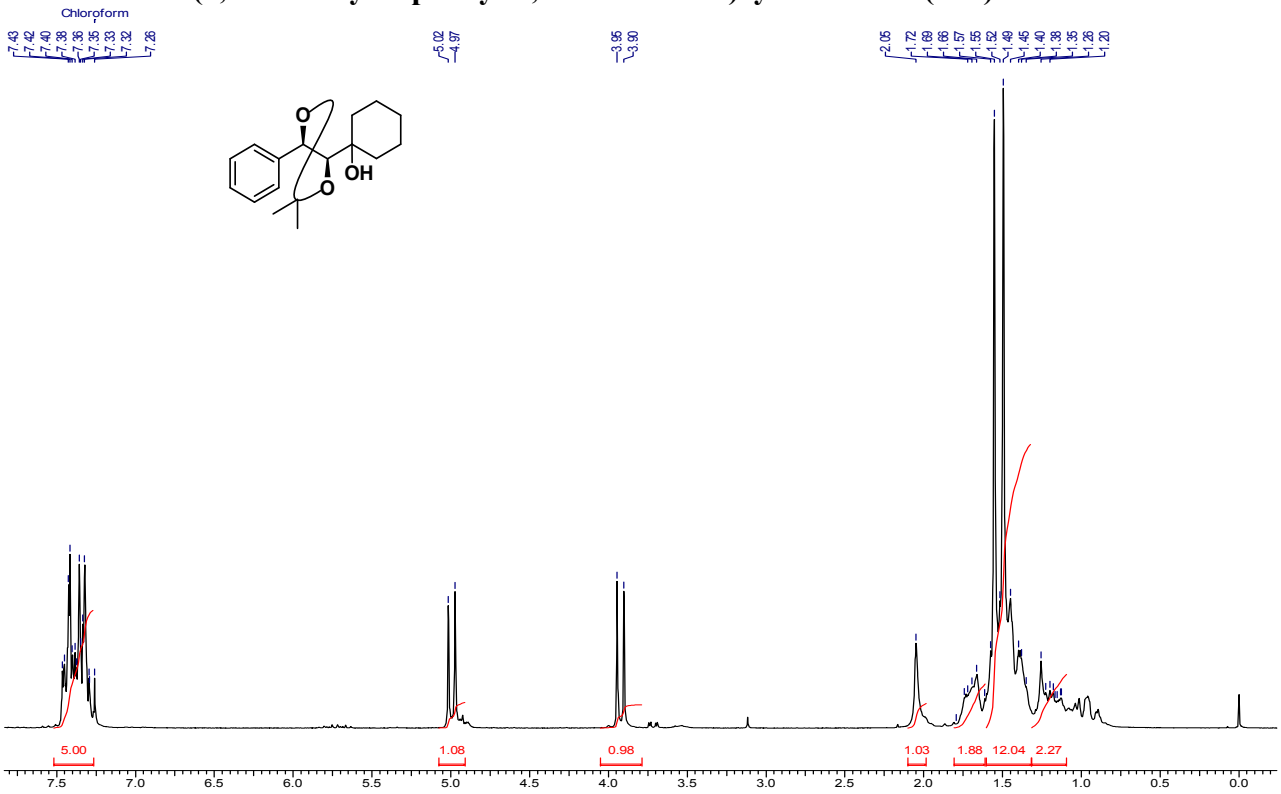
^{1}H NMR of 1-(2,2-dimethyl-5-phenyl-1,3-dioxolan-4-yl)hex-5-en-1-yl acetate (11' a)



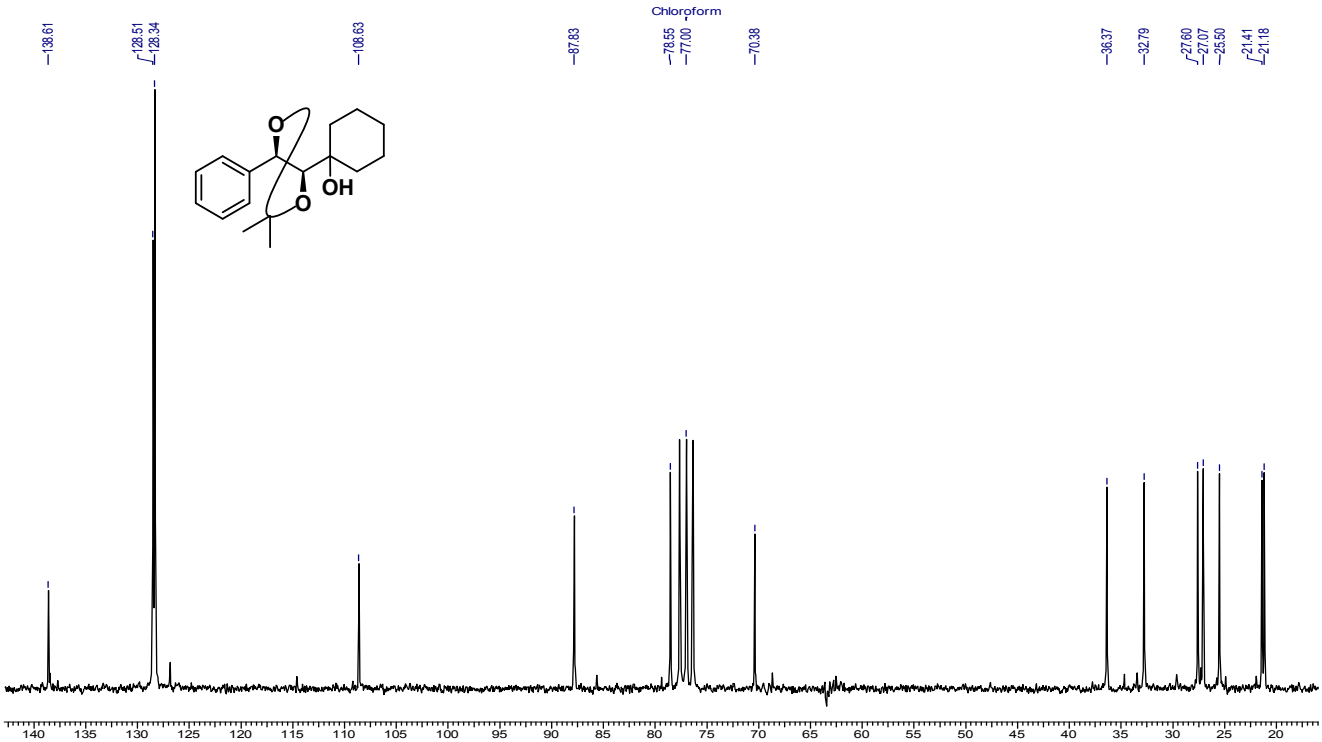
^{13}C NMR of 1-(2,2-dimethyl-5-phenyl-1,3-dioxolan-4-yl)hex-5-en-1-yl acetate (11' a)



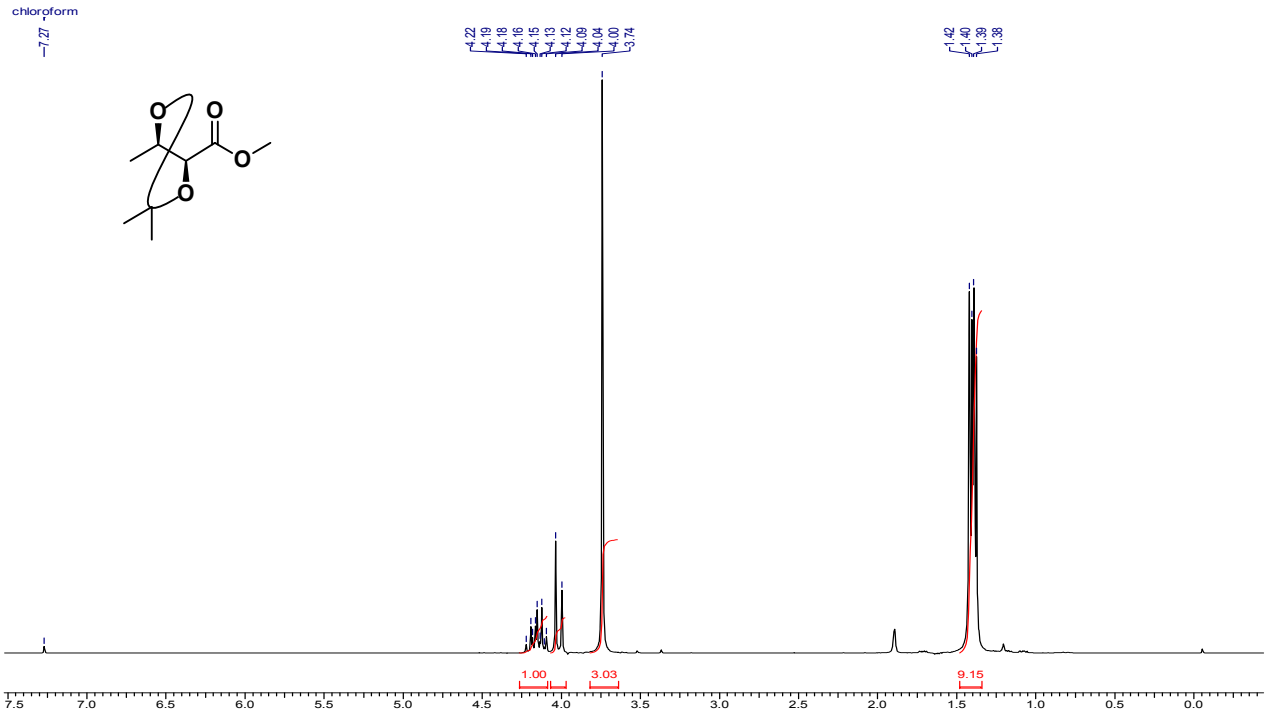
^{1}H NMR of 1-(2,2-dimethyl-5-phenyl-1,3-dioxolan-4-l)cyclohexanol (11b)



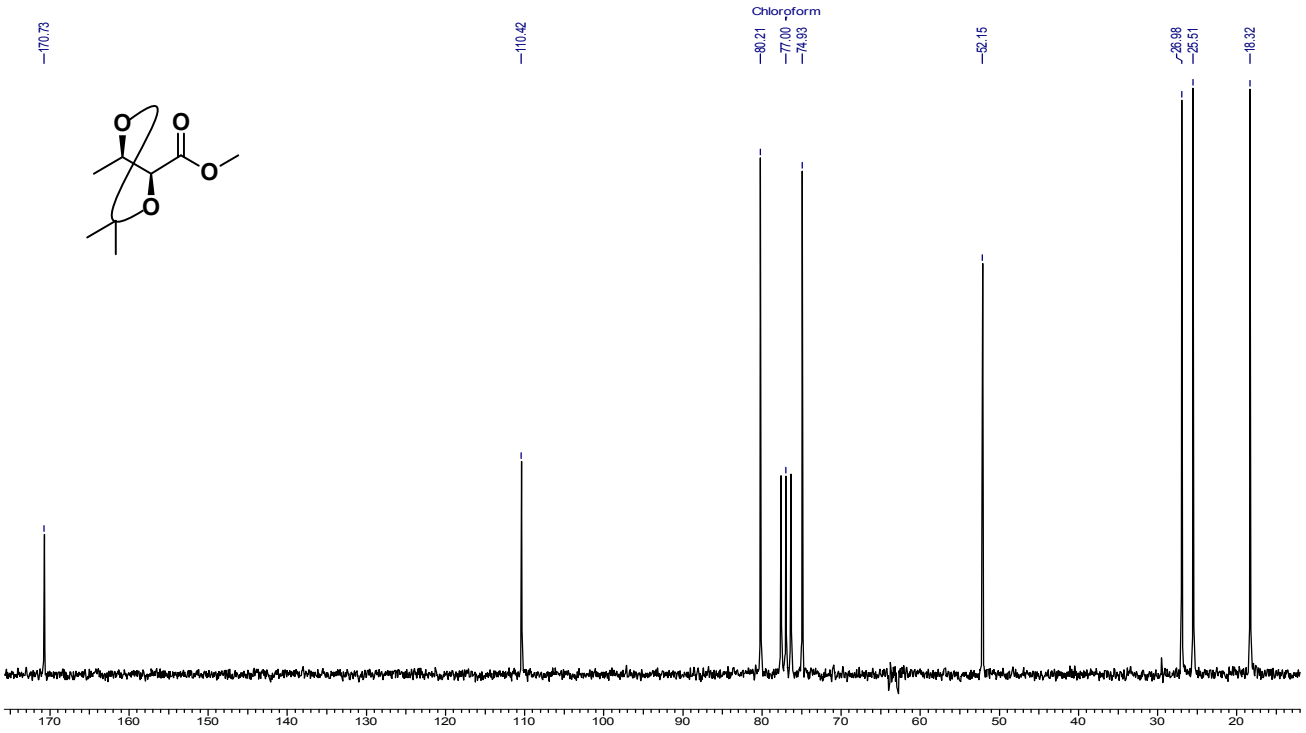
^{13}C NMR of 1-(2,2-dimethyl-5-phenyl-1,3-dioxolan-4-l)cyclohexanol (11b)



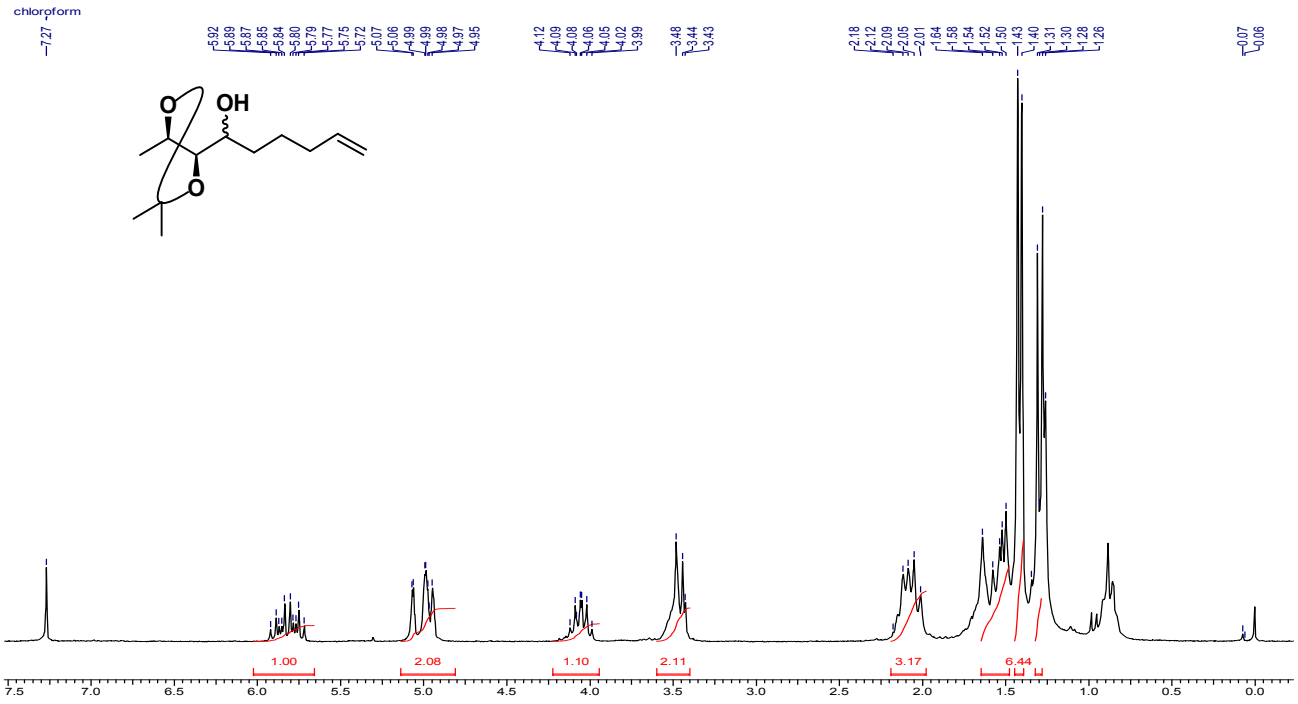
^{1}H NMR of methyl 2,2,5-trimethyl-1,3-dioxolane-4-carboxylate (12)



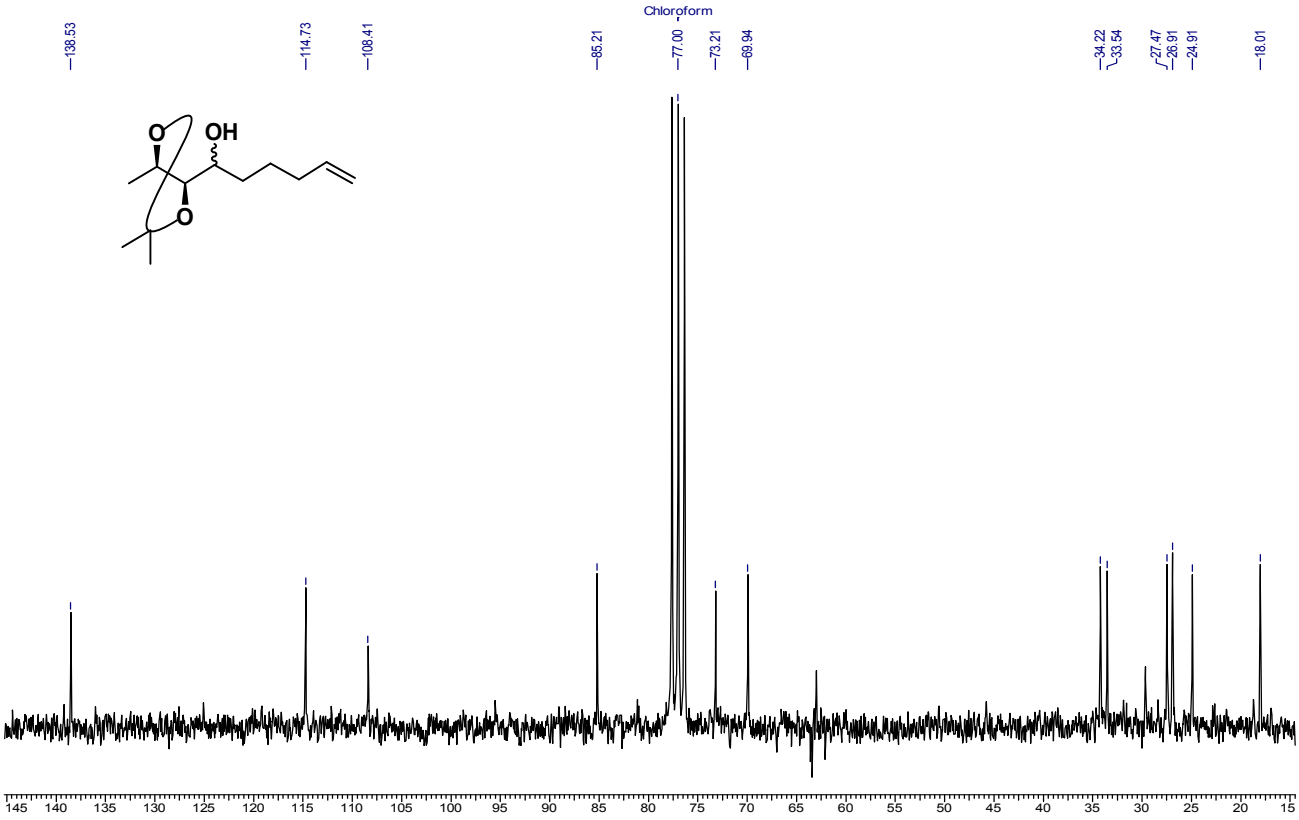
^{13}C NMR of methyl−2,2,5-trimethyl-1,3-dioxolane-4-carboxylate (12)



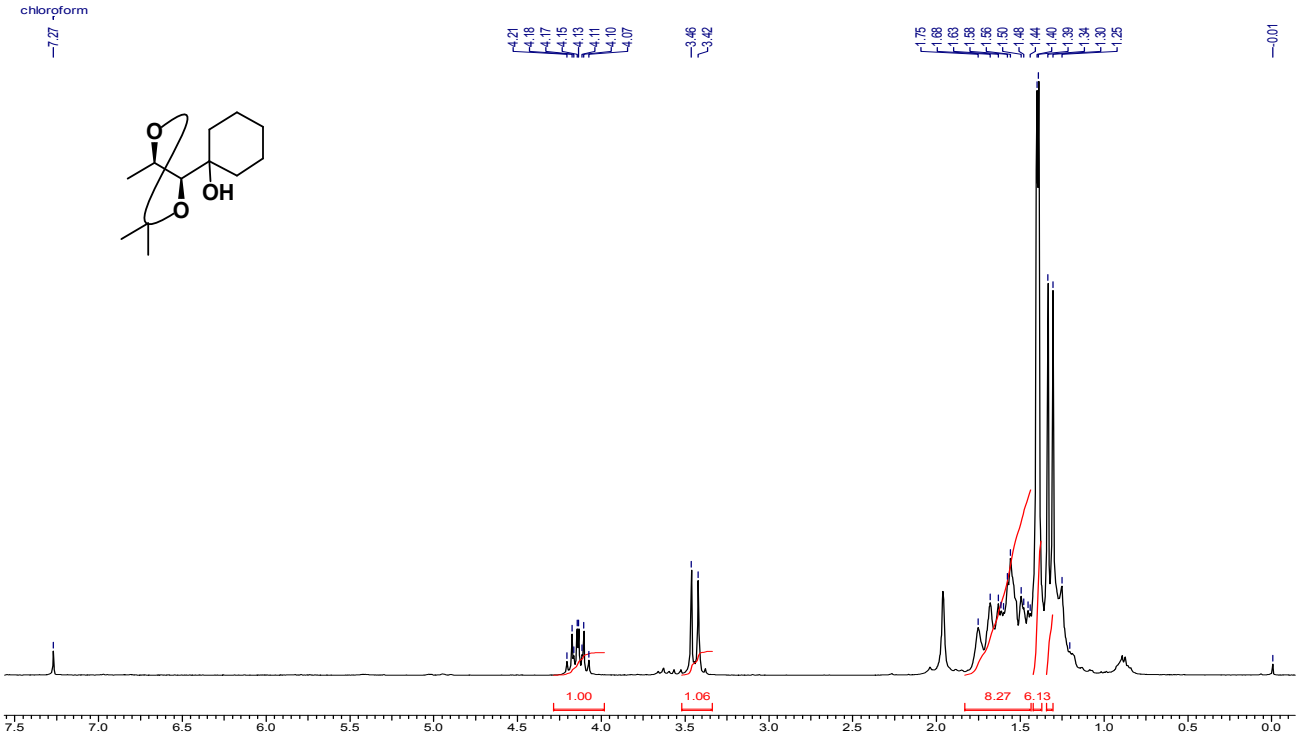
^{1}H NMR of 1-((4*R*,5*R*)-2,2,5-trimethyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (12a)



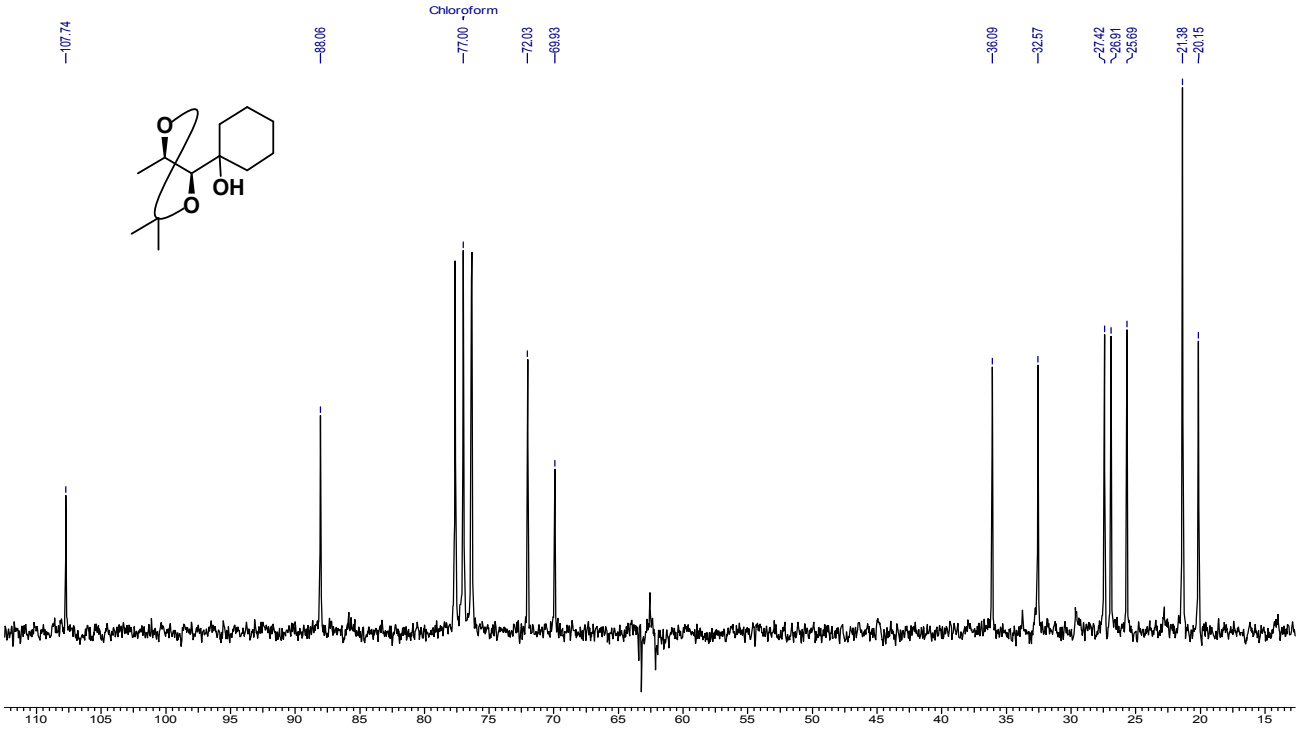
^{13}C NMR of 1-((4*R*,5*R*)-2,2,5-trimethyl-1,3-dioxolan-4-yl)hex-5-en-1-ol (12a)



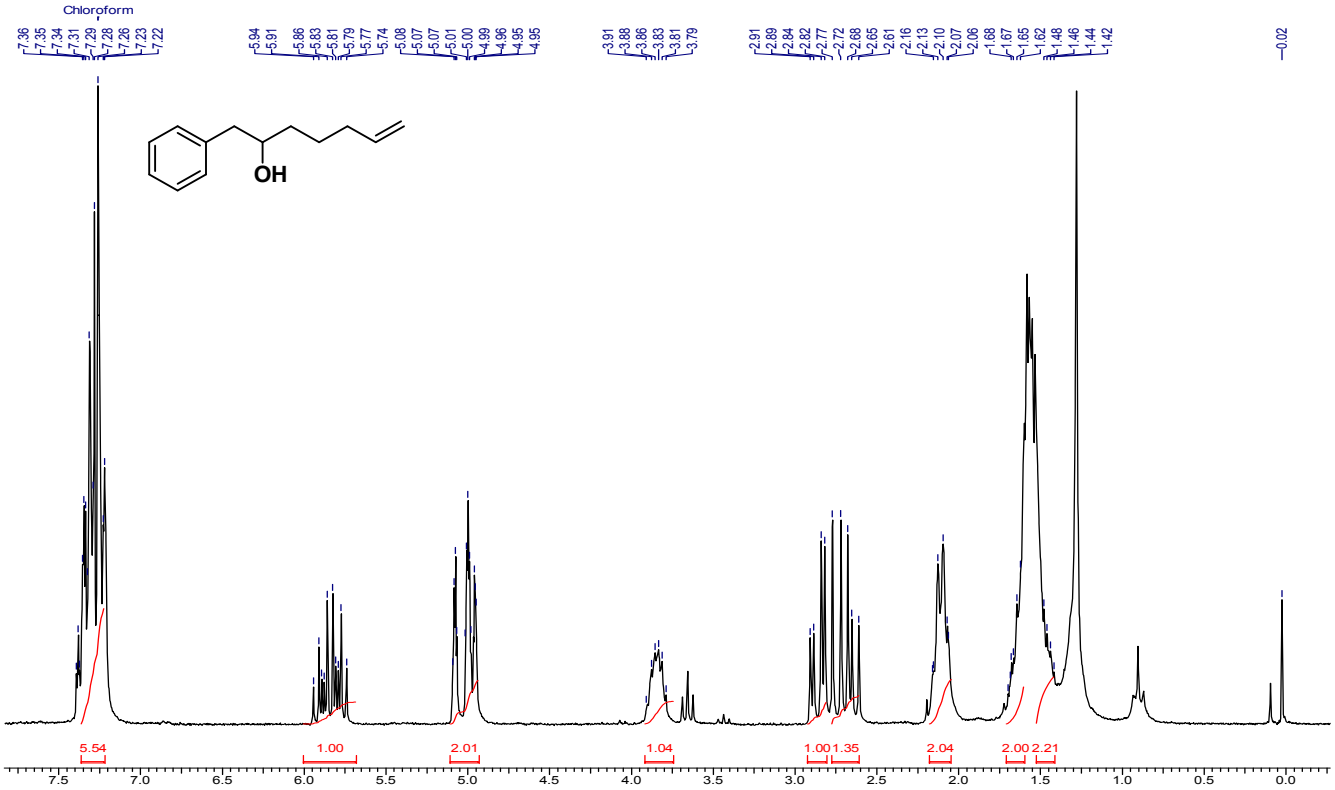
^{1}H NMR of 1-(2,2,5-trimethyl-1,3-dioxolan-4-yl)cyclohexanol (12b)



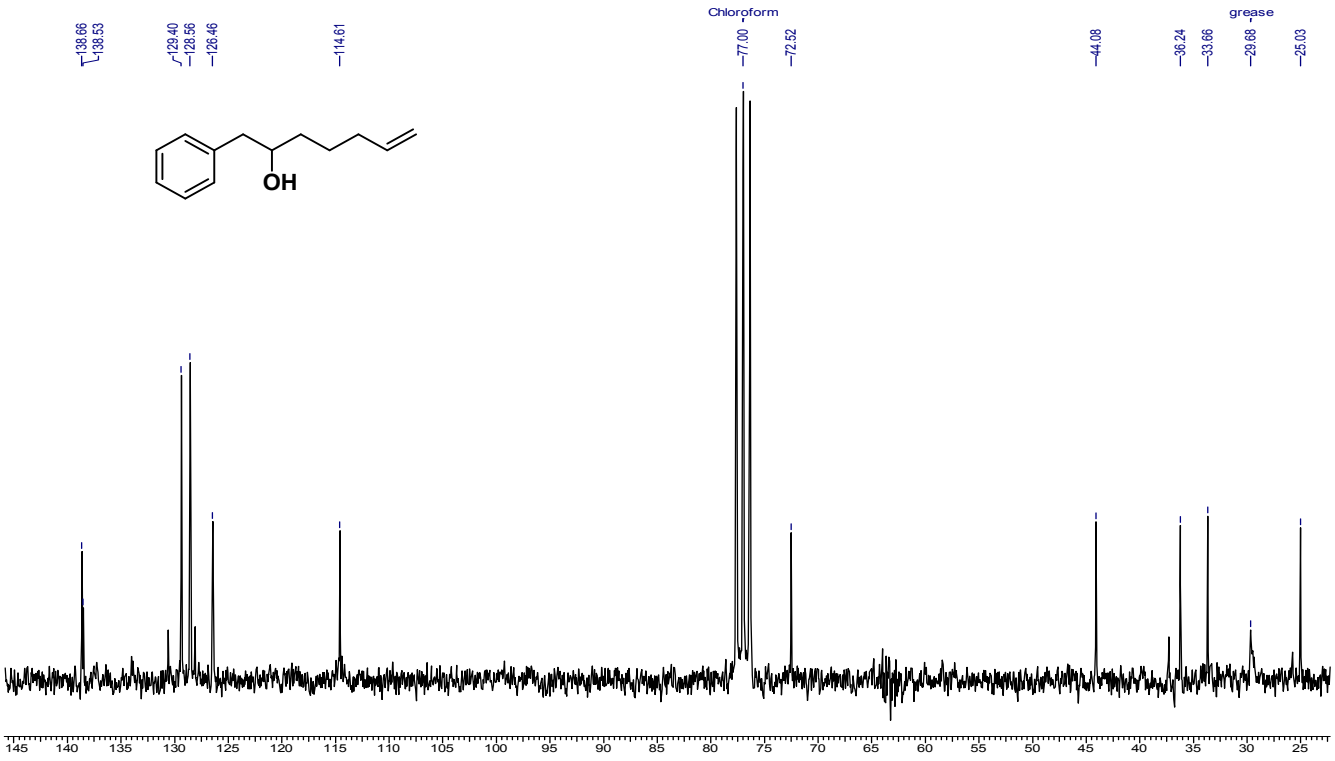
^{13}C NMR of 1-(2,2,5-trimethyl-1,3-dioxolan-4-yl)cyclohexanol (12b)



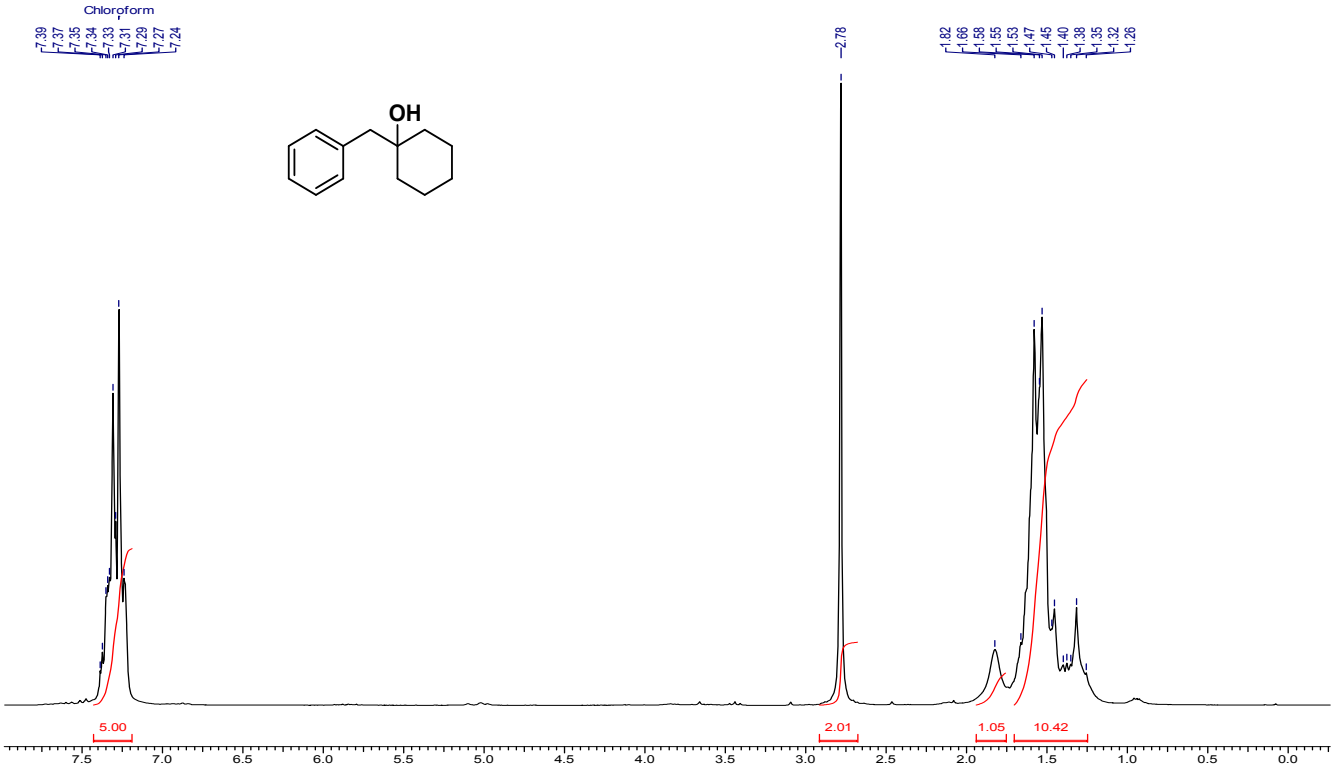
^{1}H NMR of 1-phenylhept-6-en-2-ol (13a)



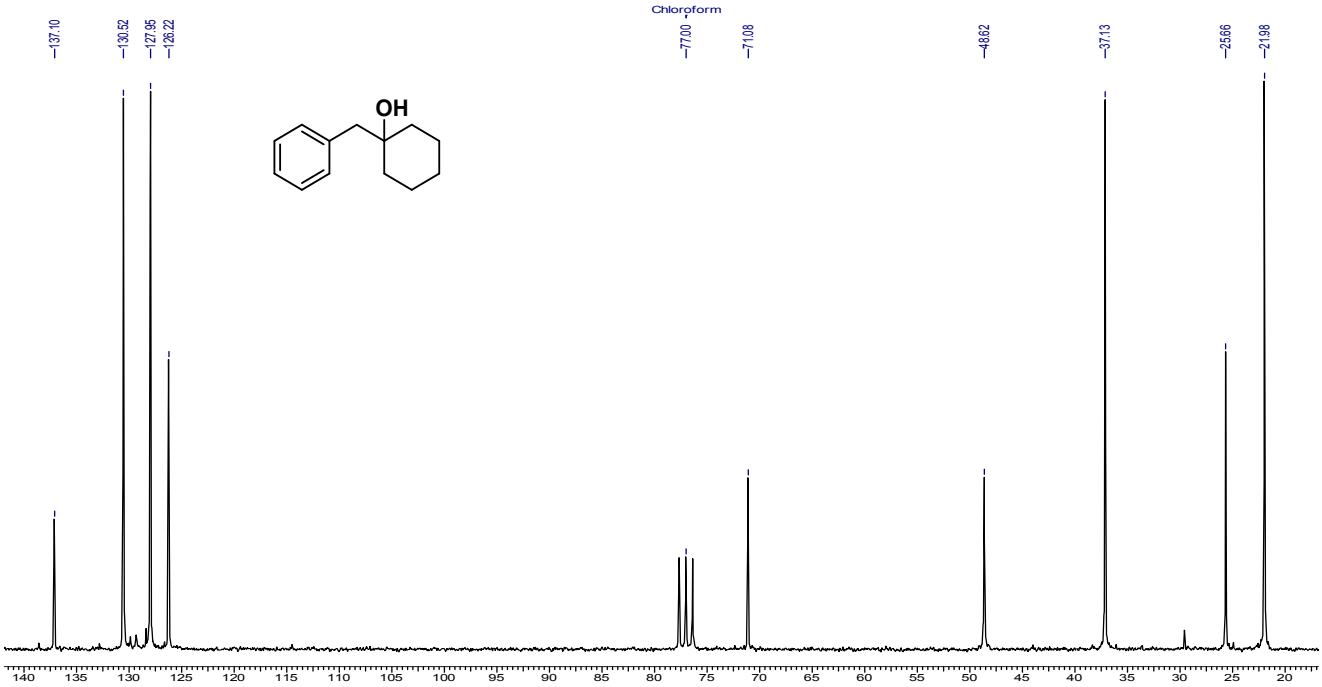
^{13}C NMR of 1-phenylhept-6-en-2-ol (13a)



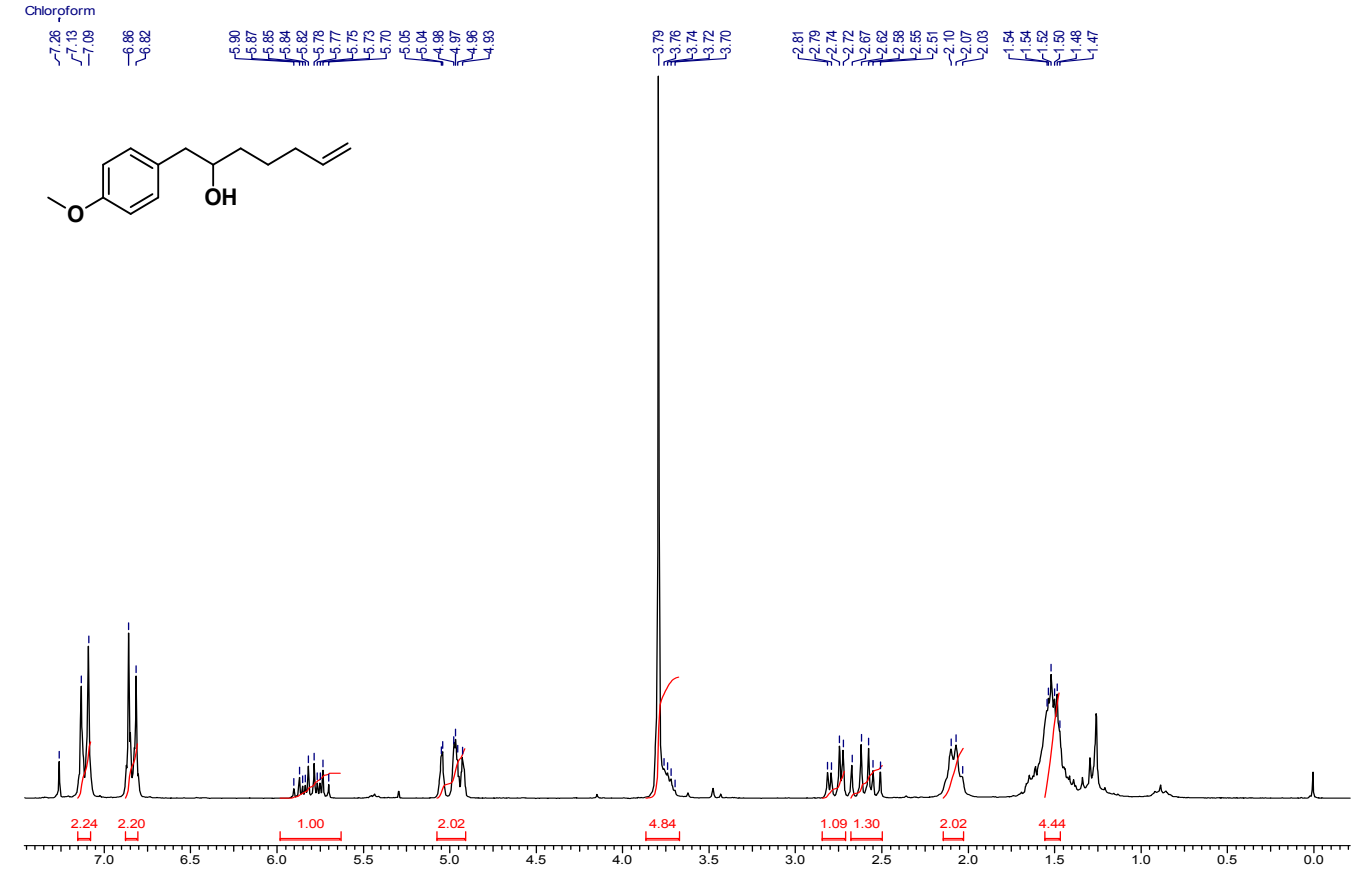
^{1}H NMR of 1-benzylcyclohexanol (13b)



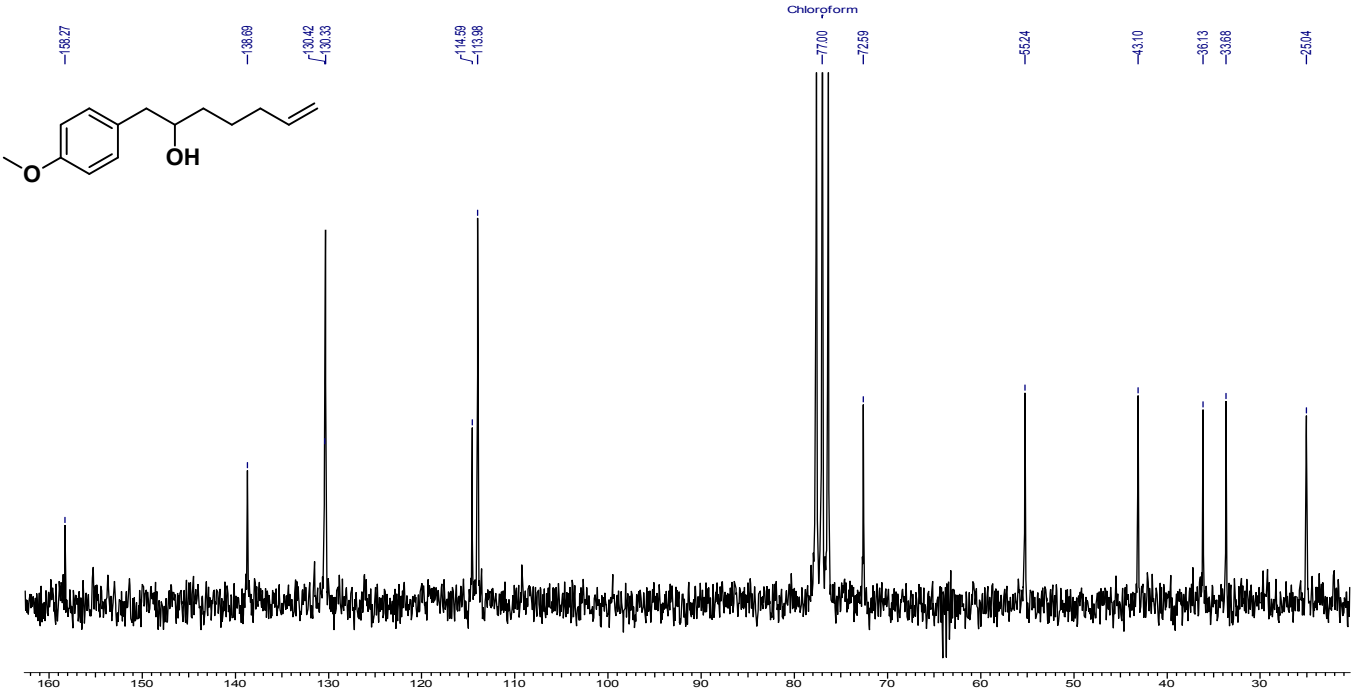
^{13}C NMR of 1-benzylcyclohexanol (13b)



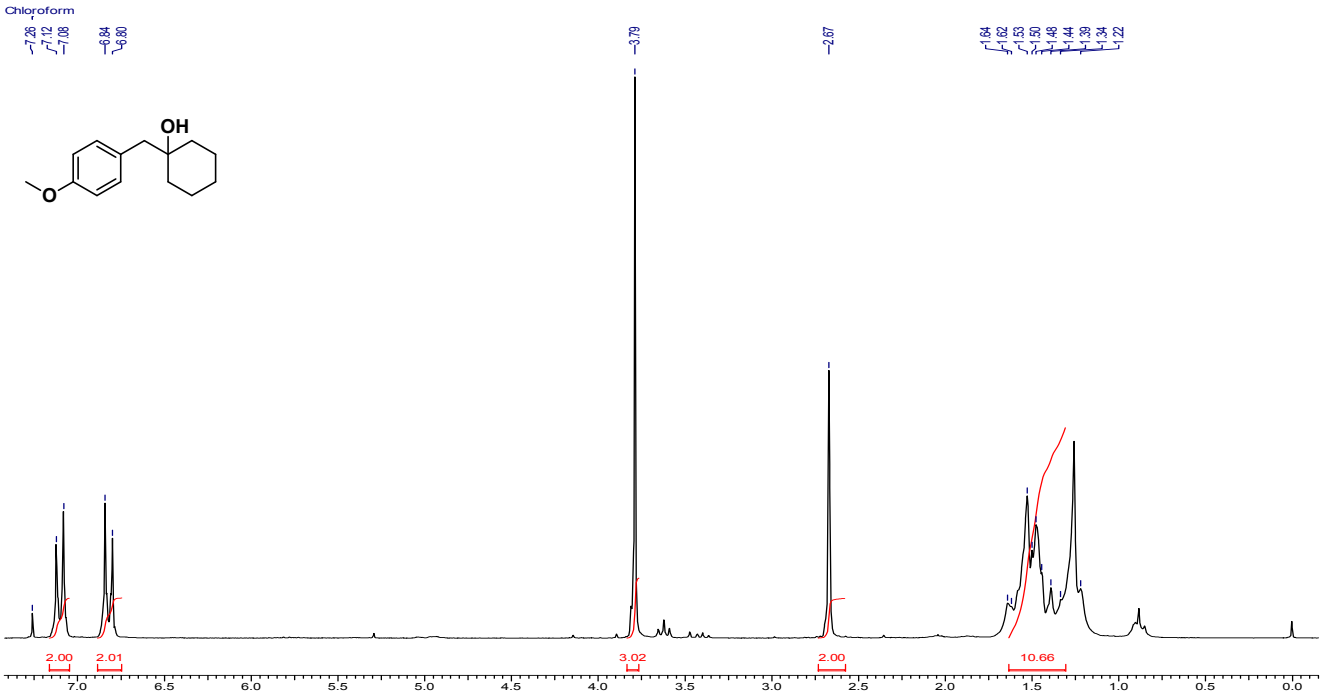
^{1}H NMR of 1-(4-methoxyphenyl)hept-6-en-2-ol (14a)



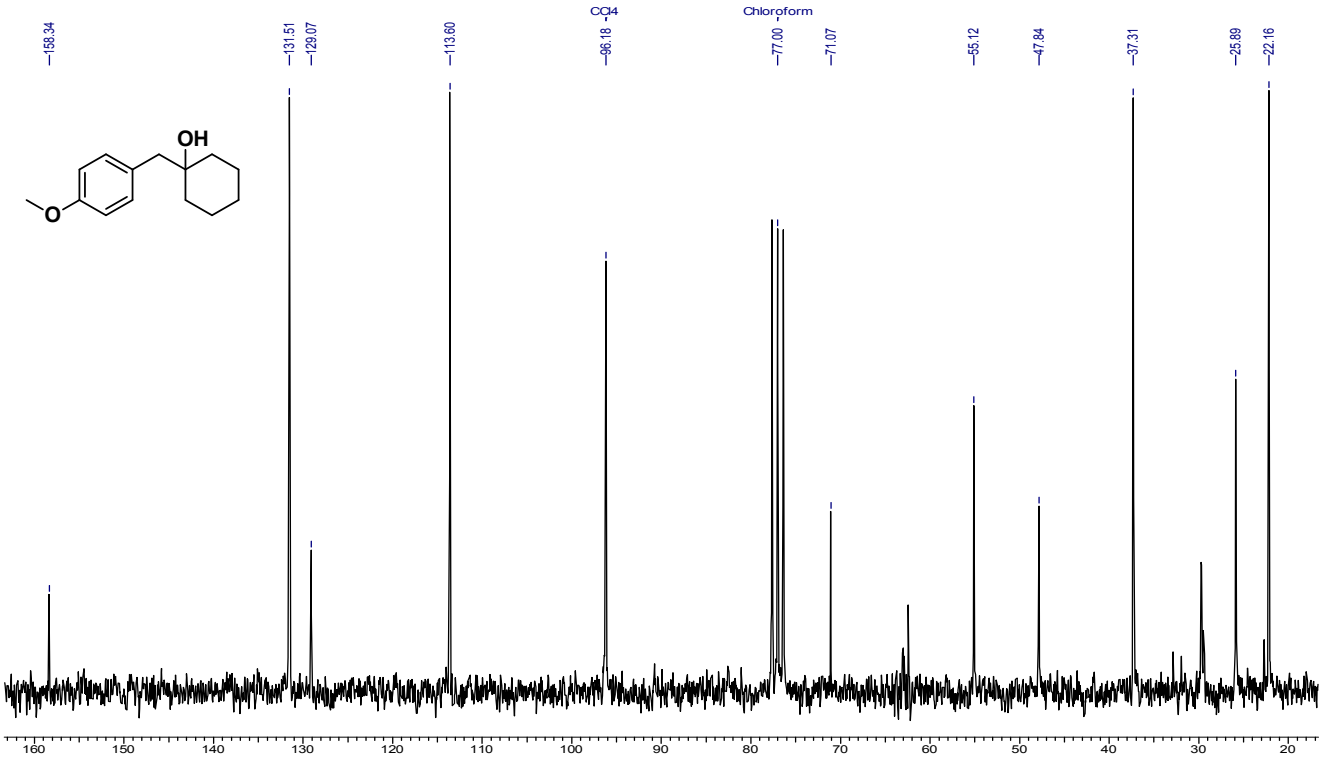
^{13}C NMR of 1-(4-methoxyphenyl)hept-6-en-2-ol (14a)



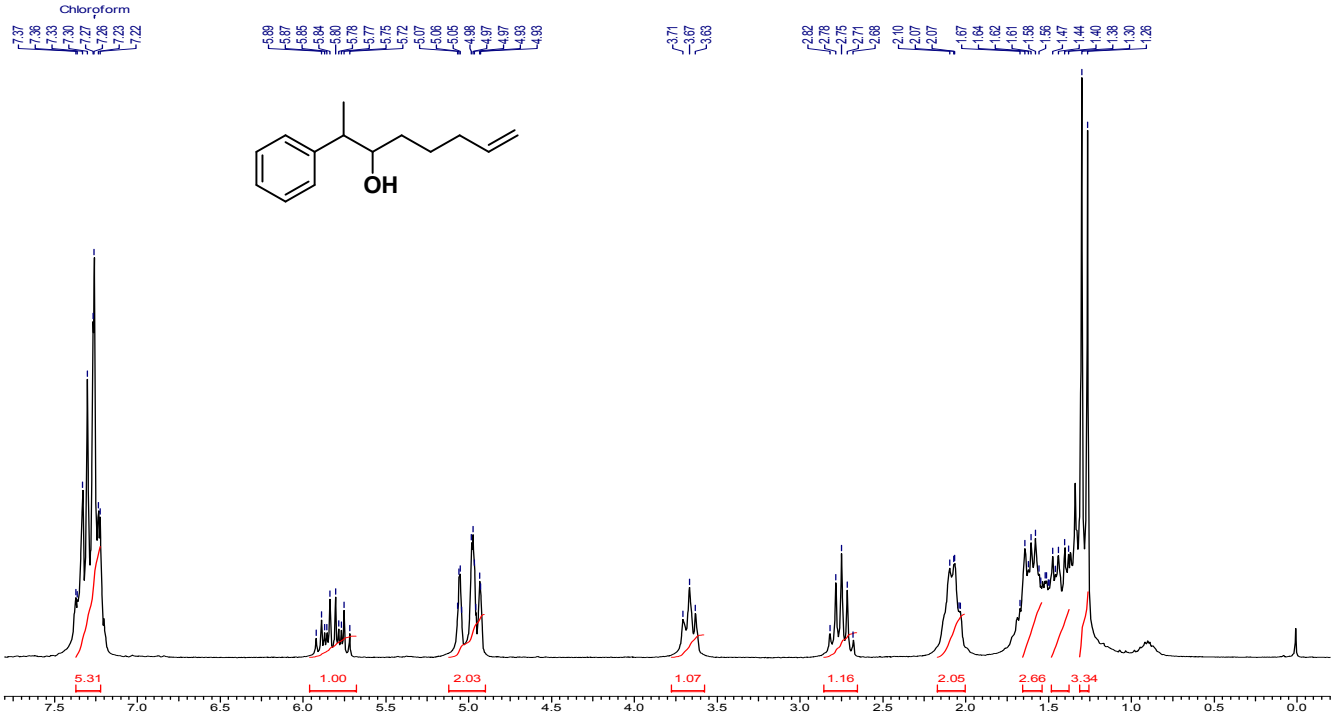
^{1}H NMR of 1-(4-methoxybenzyl)cyclohexanol (14b)



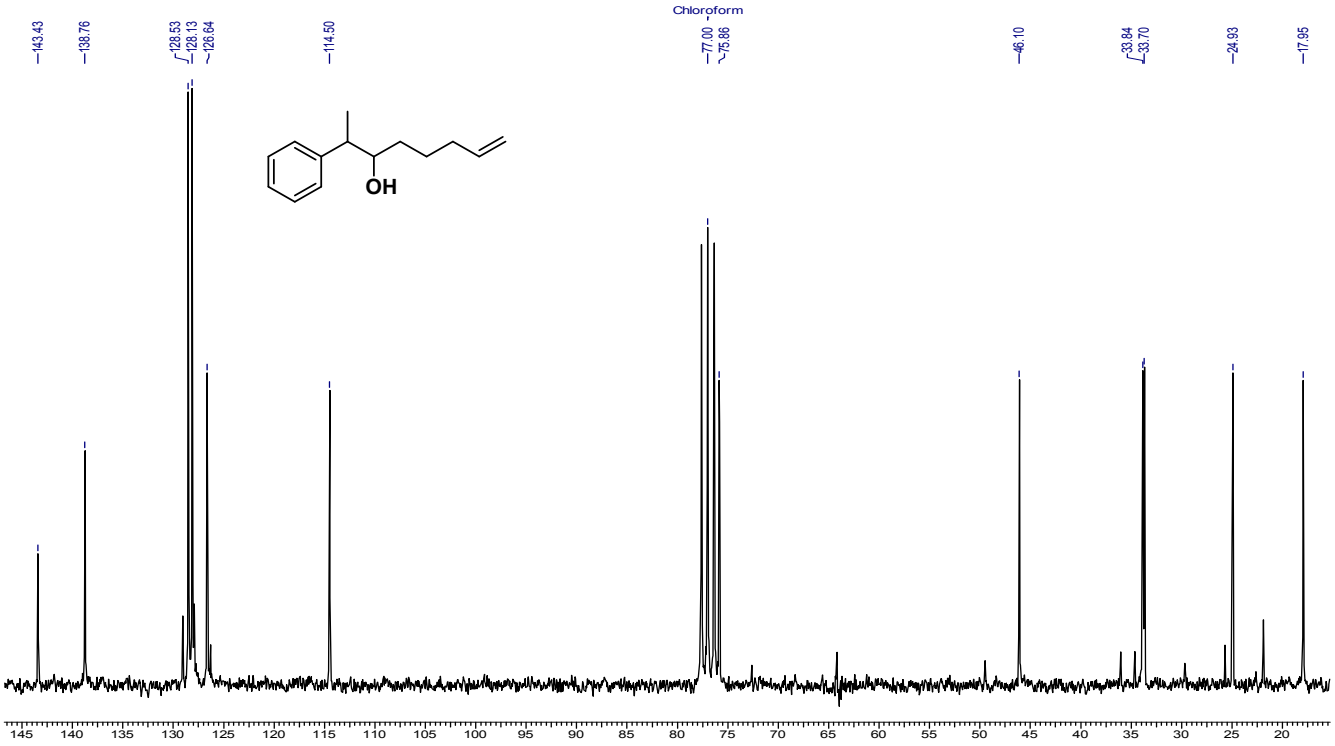
^{13}C NMR of 1-(4-methoxybenzyl)cyclohexanol (14b)



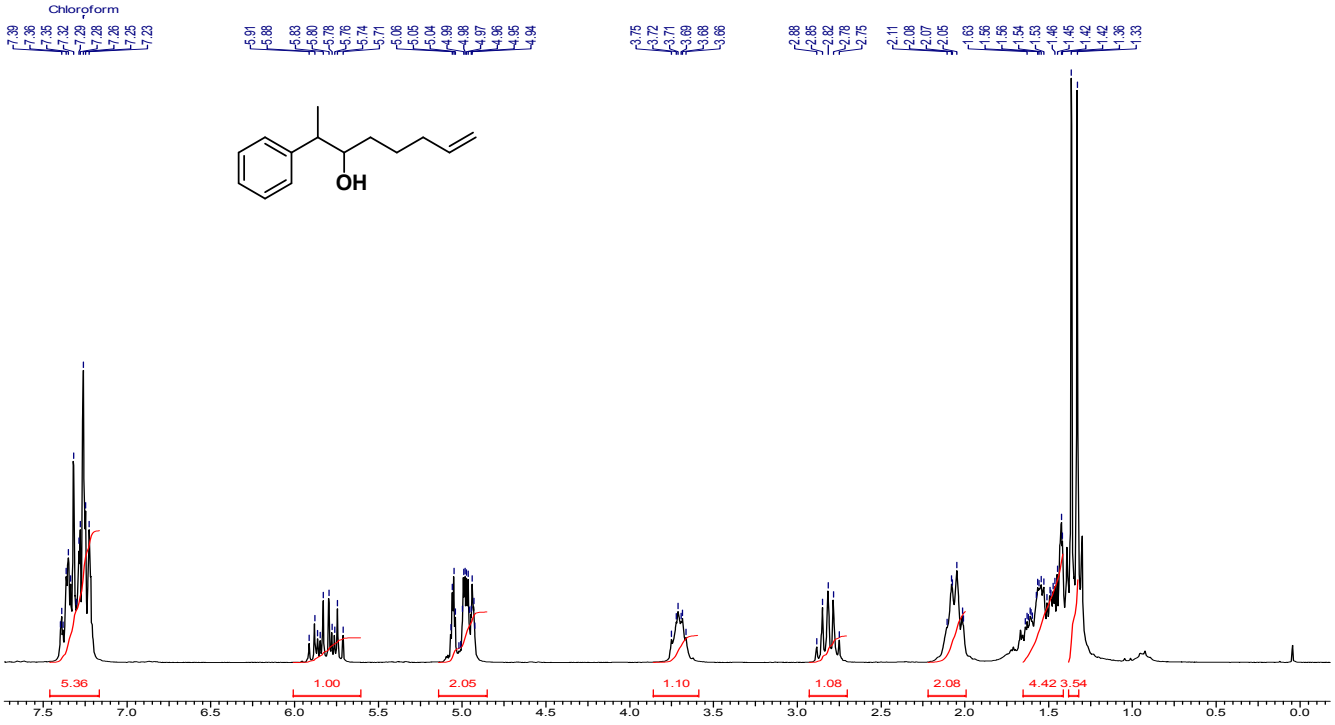
^{1}H NMR of 2-phenyloct-7-en-3-ol (15a) first diastereomer



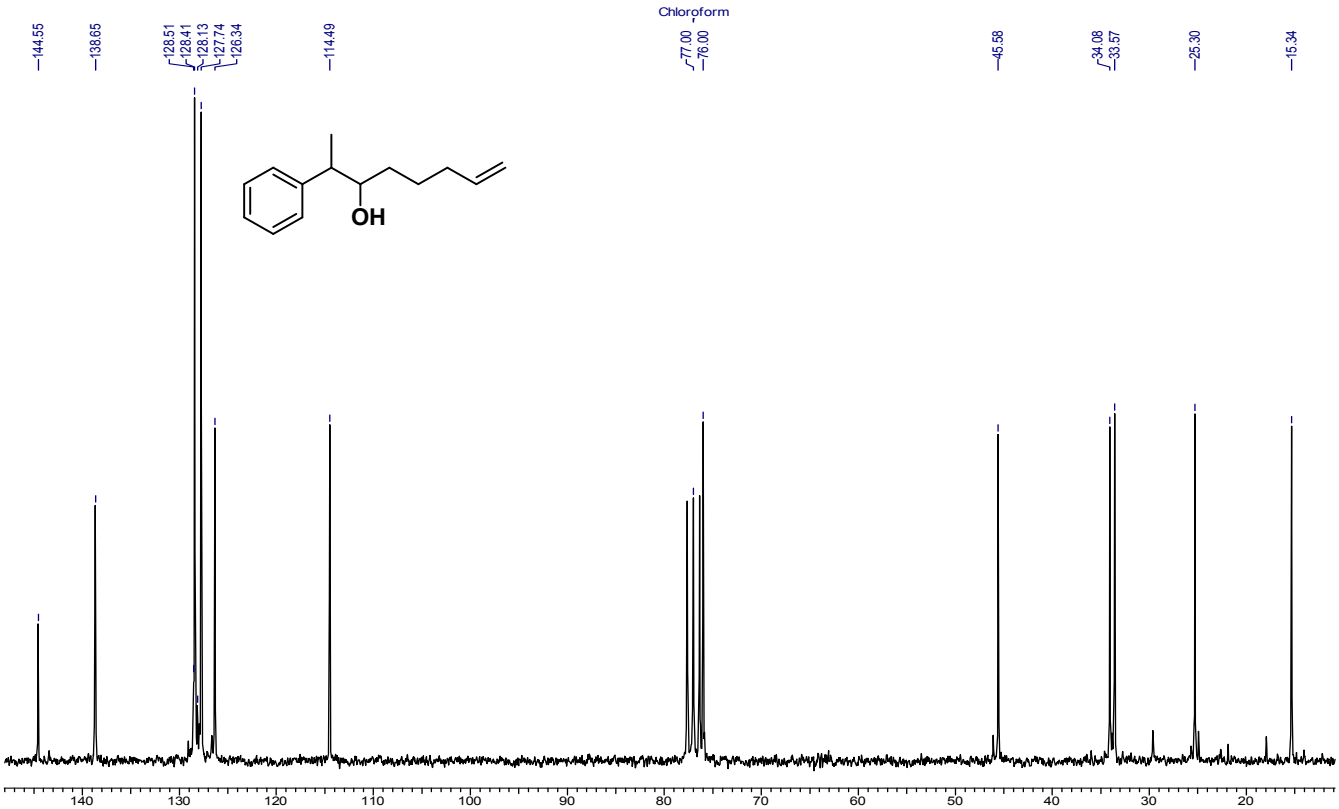
^{13}C NMR of 2-phenyloct-7-en-3-ol (15a) first diastereomer



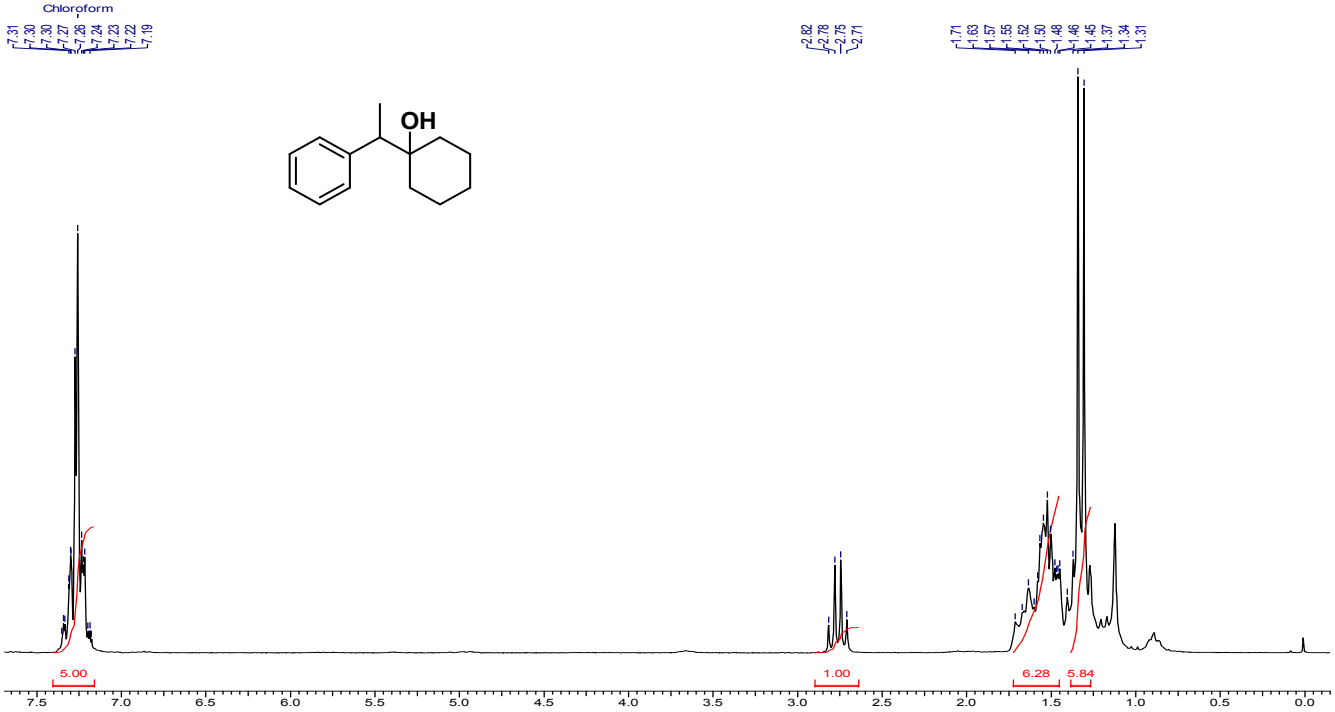
^{1}H NMR of 2-phenyloct-7-en-3-ol (15a) second diastereomer



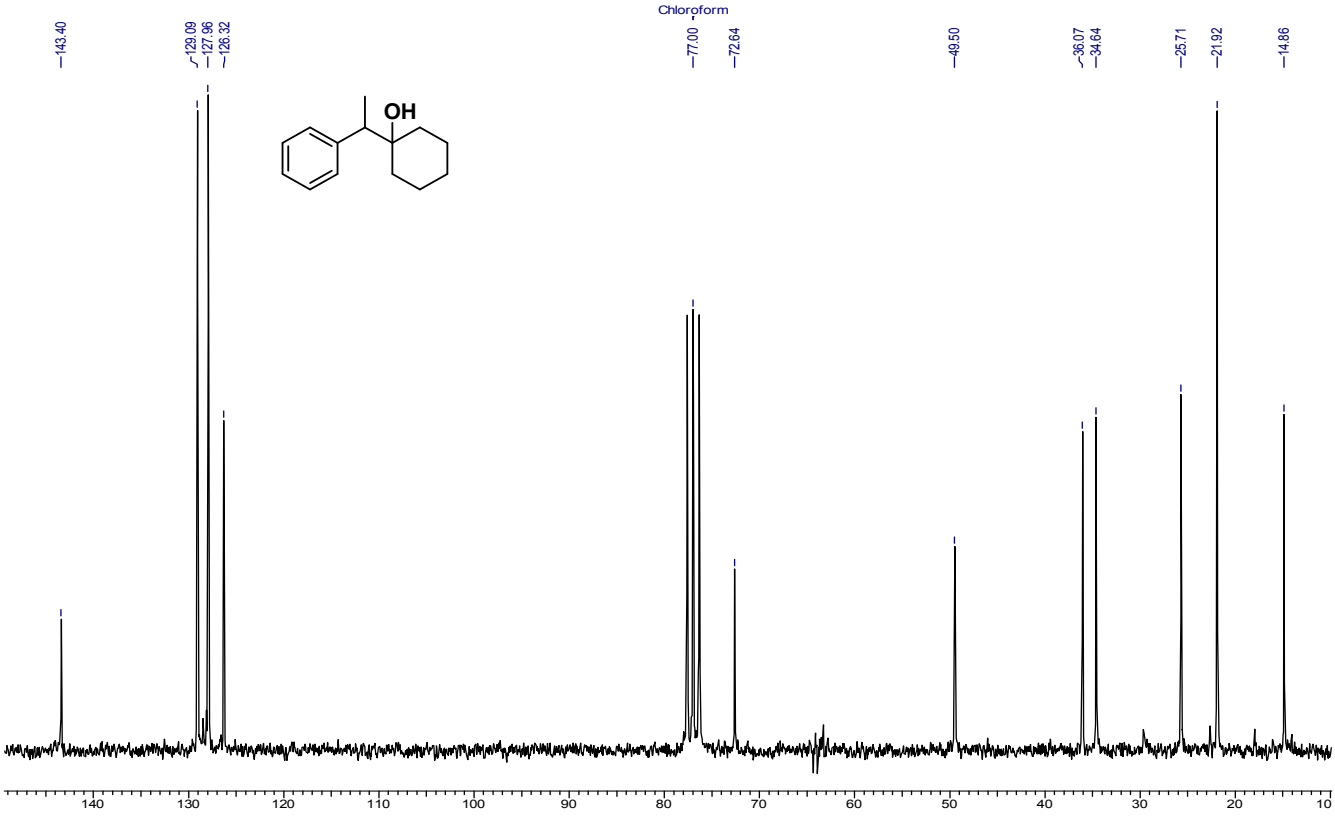
^{13}C NMR of 2-phenyloct-7-en-3-ol (15a) second diastereomer



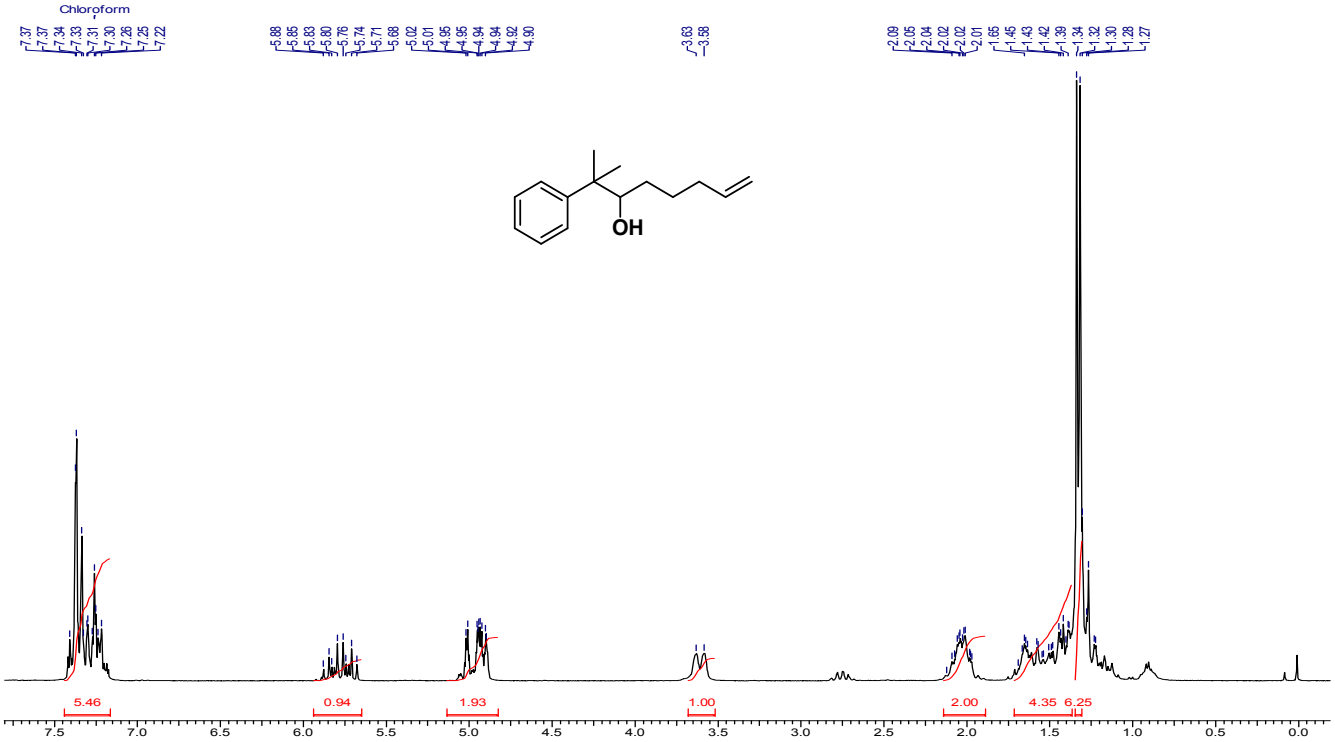
^{1}H NMR of 1-(1-phenylethyl)cyclohexanol (15b)



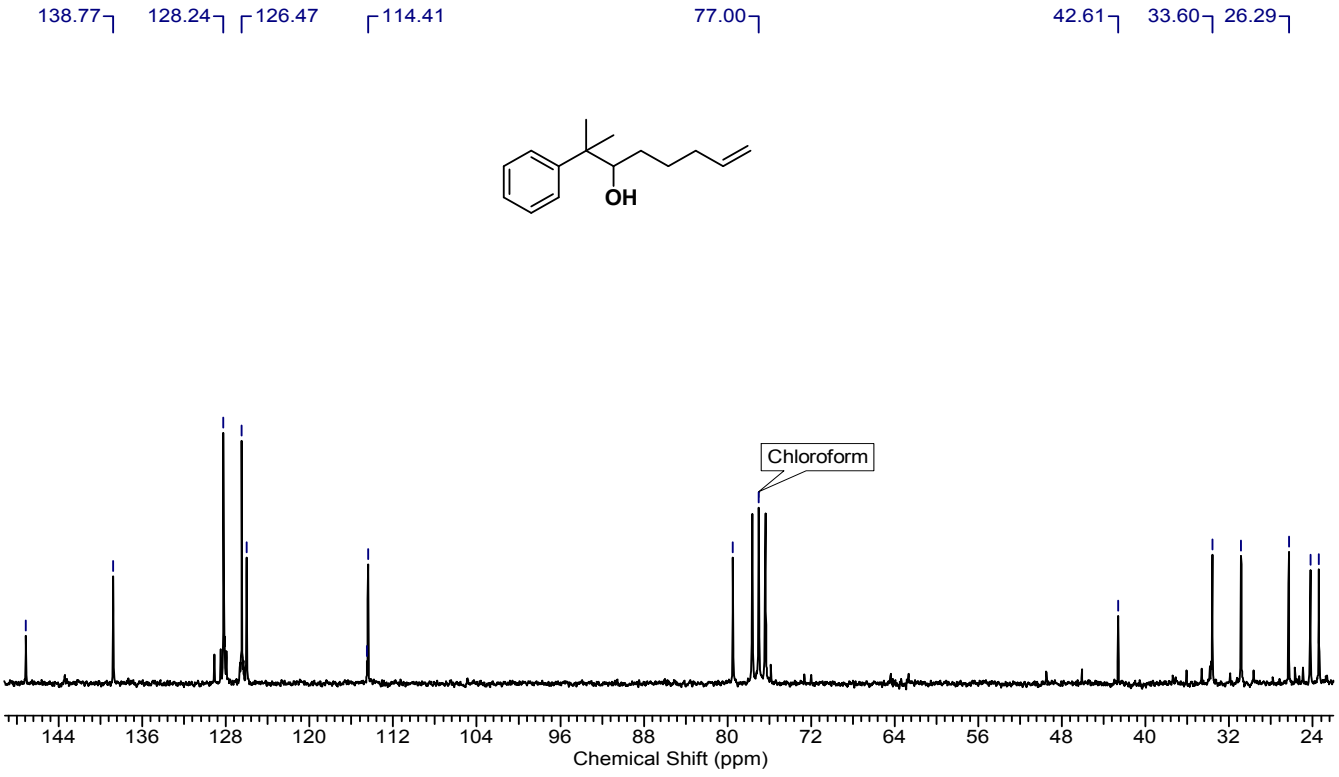
^{13}C NMR of 1-(1-phenylethyl)cyclohexanol (15b)



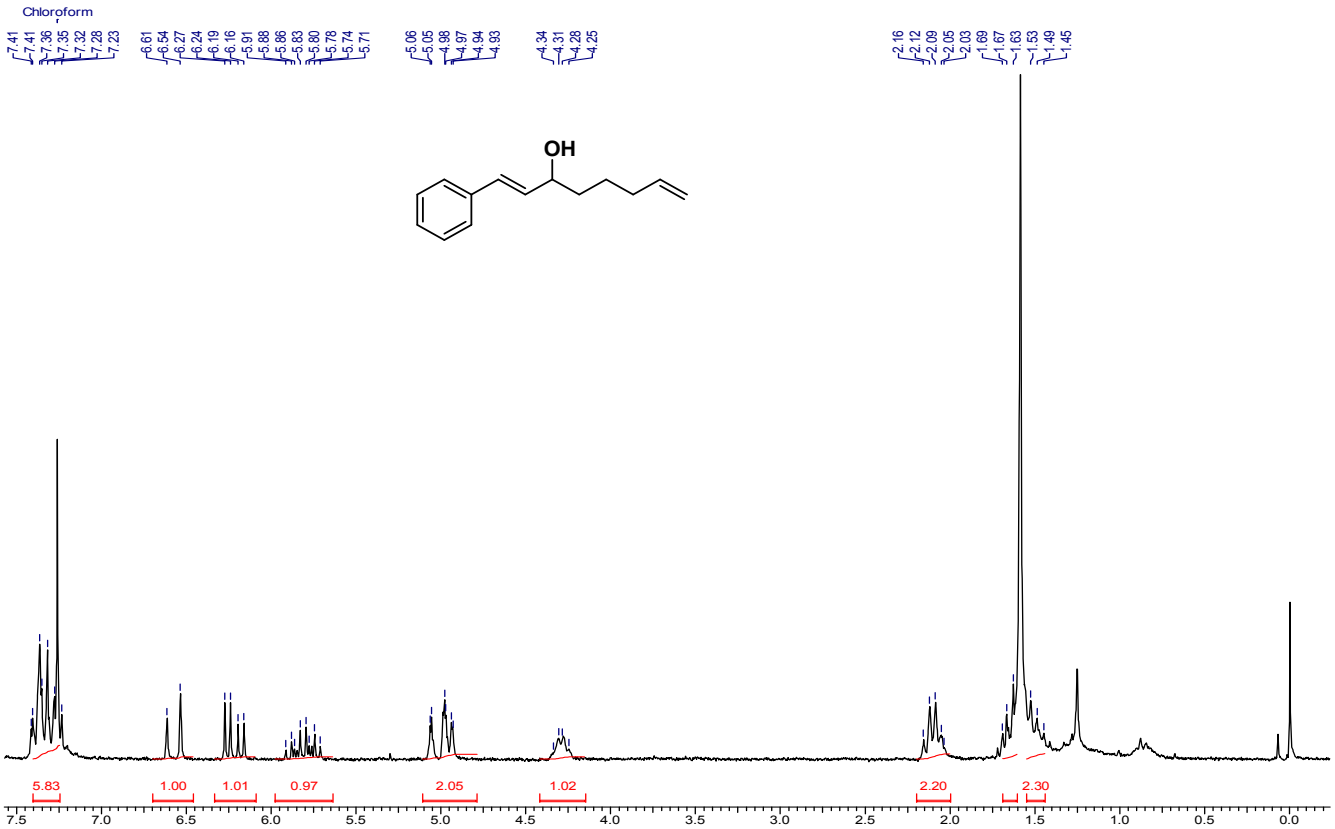
^{1}H NMR of 2-methyl-2-phenyloct-7-en-3-ol (16a)



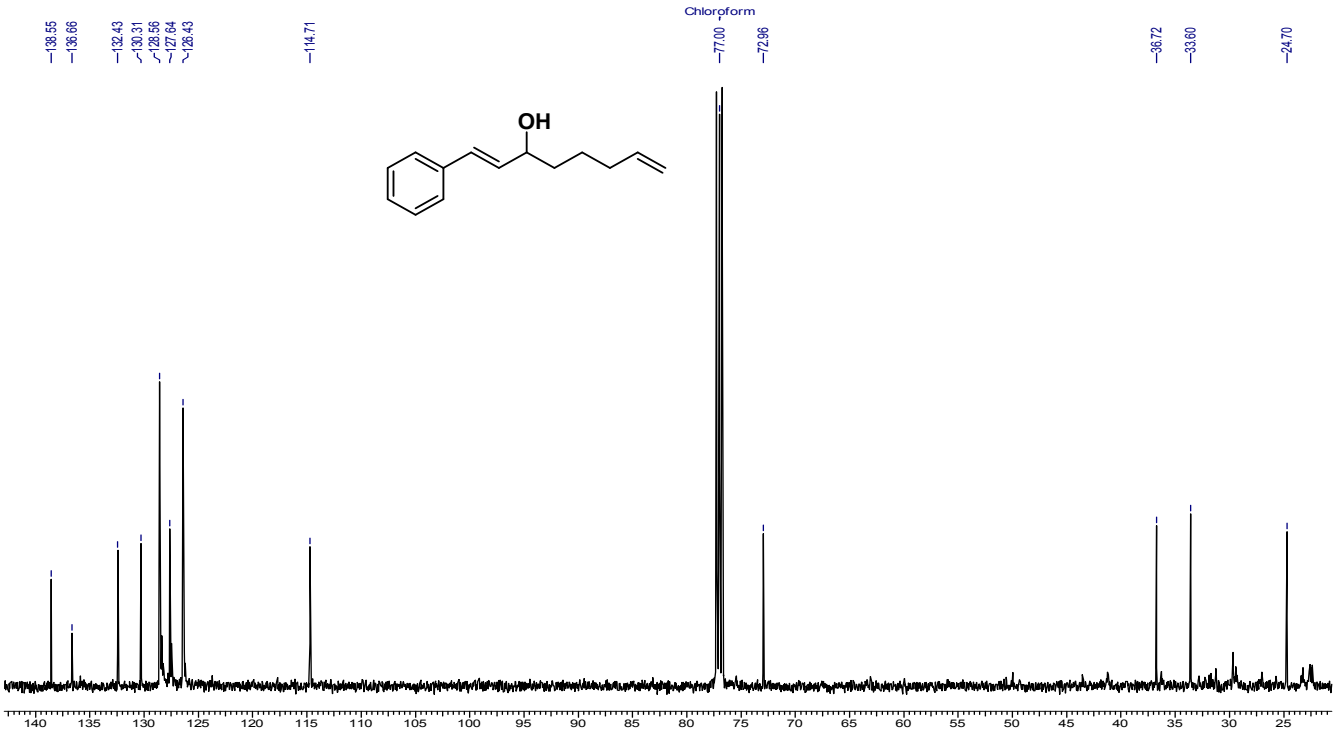
^{13}C NMR of 2-methyl-2-phenyloct-7-en-3-ol (16a)



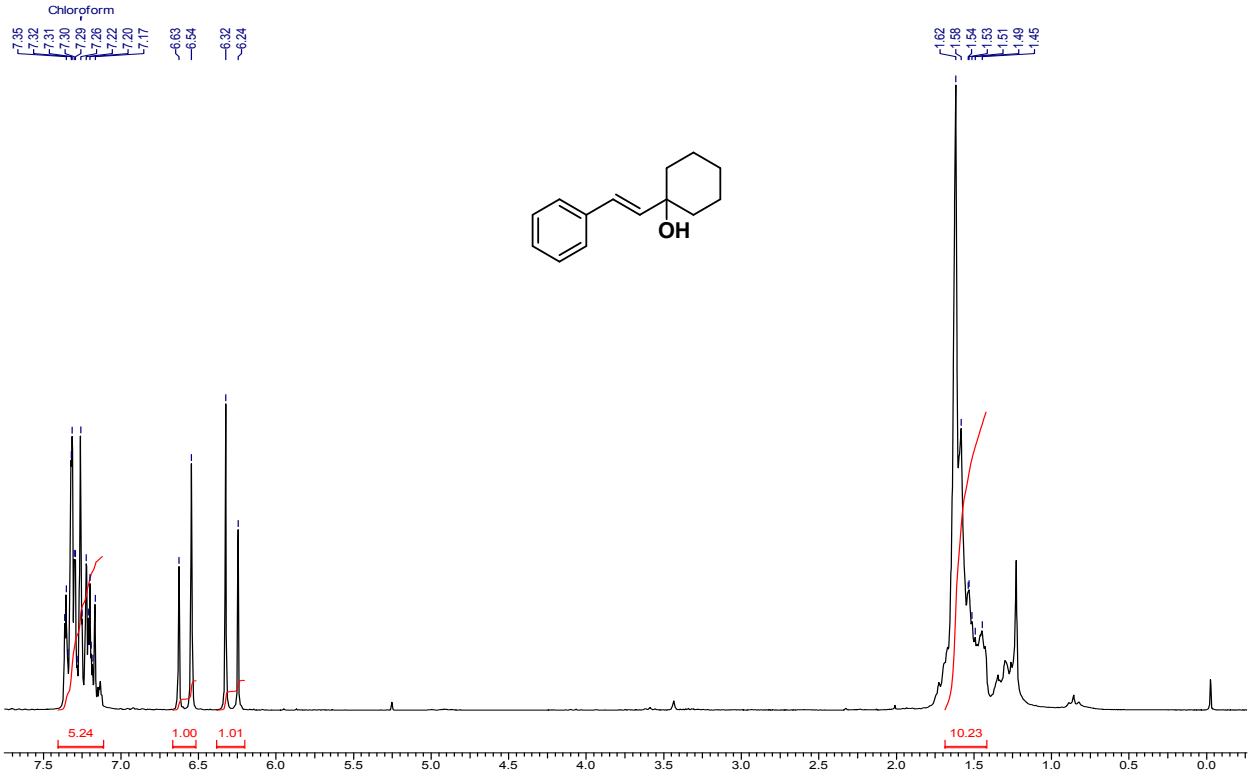
^{1}H NMR of (*E*)-1-phenylocta-1,7-dien-3-ol (17a)



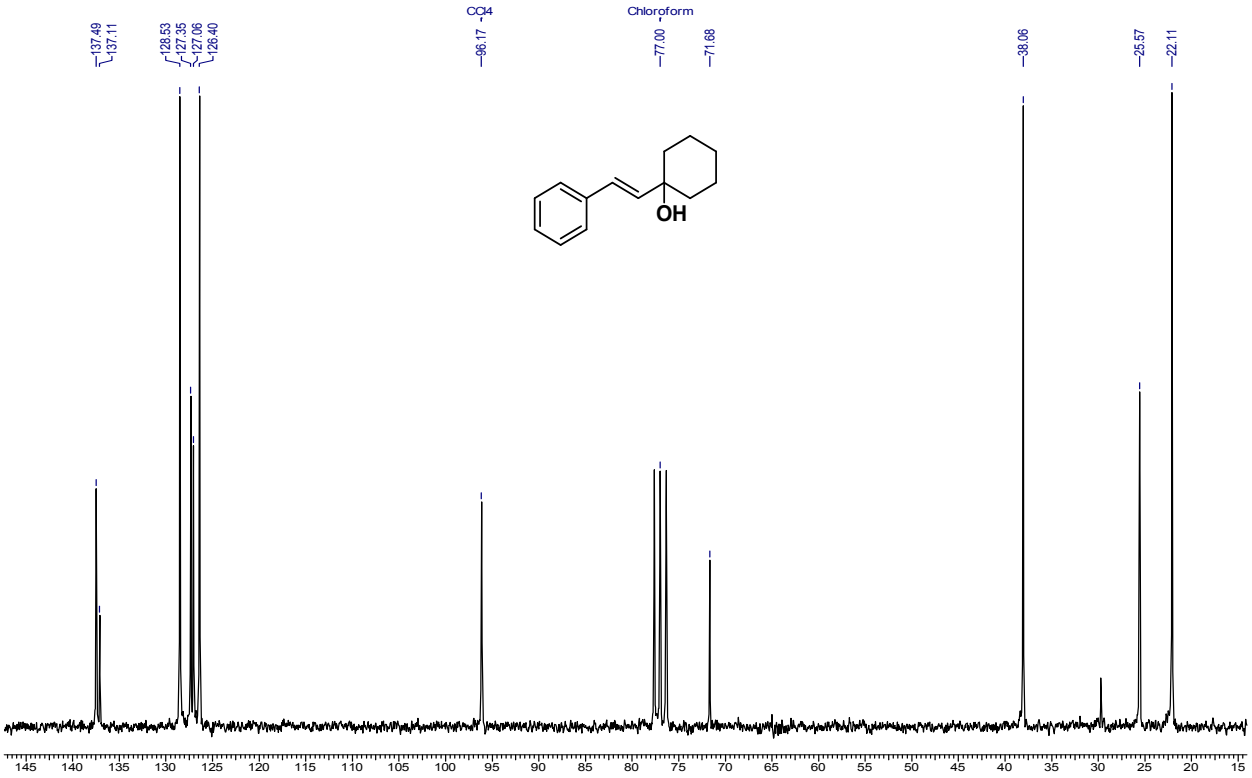
^{13}C NMR of (*E*)-1-phenylocta-1,7-dien-3-ol (17a)



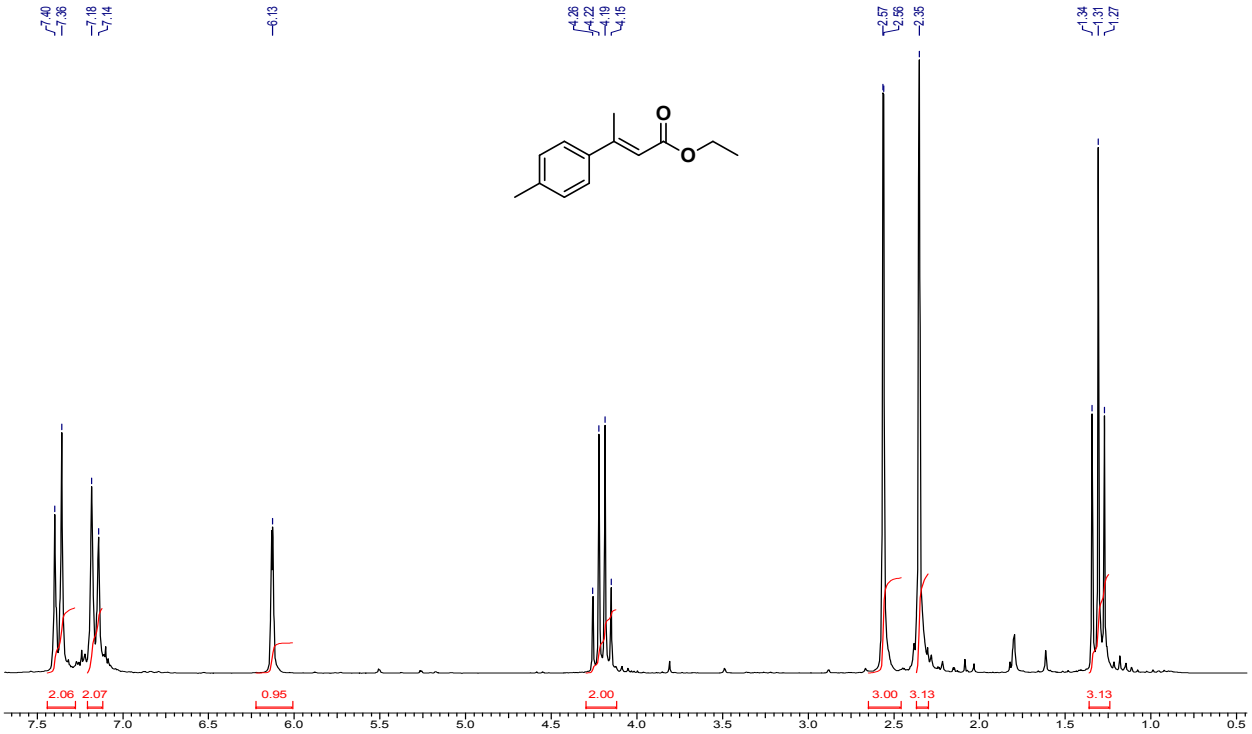
^{1}H NMR of (*E*)-1-styrylcyclohexanol (17b)



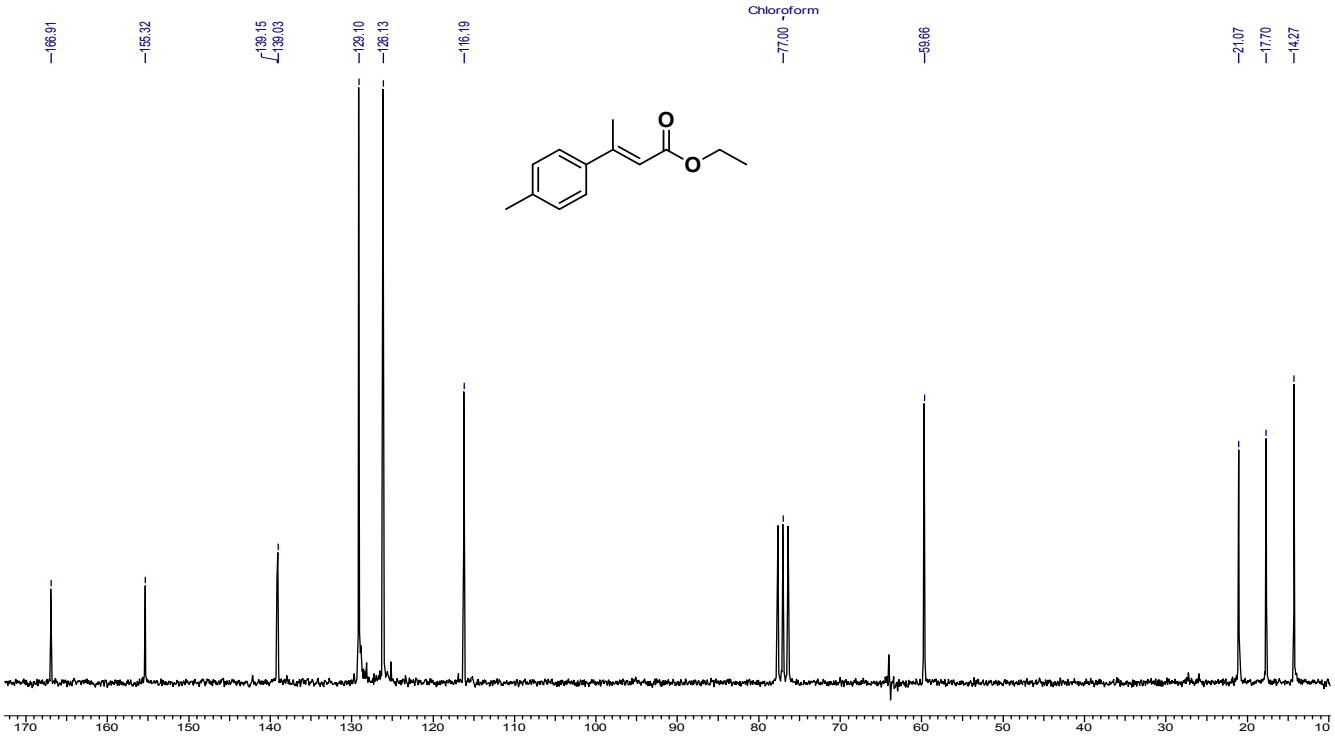
^{13}C NMR of (*E*)-1-styrylcyclohexanol (17b)



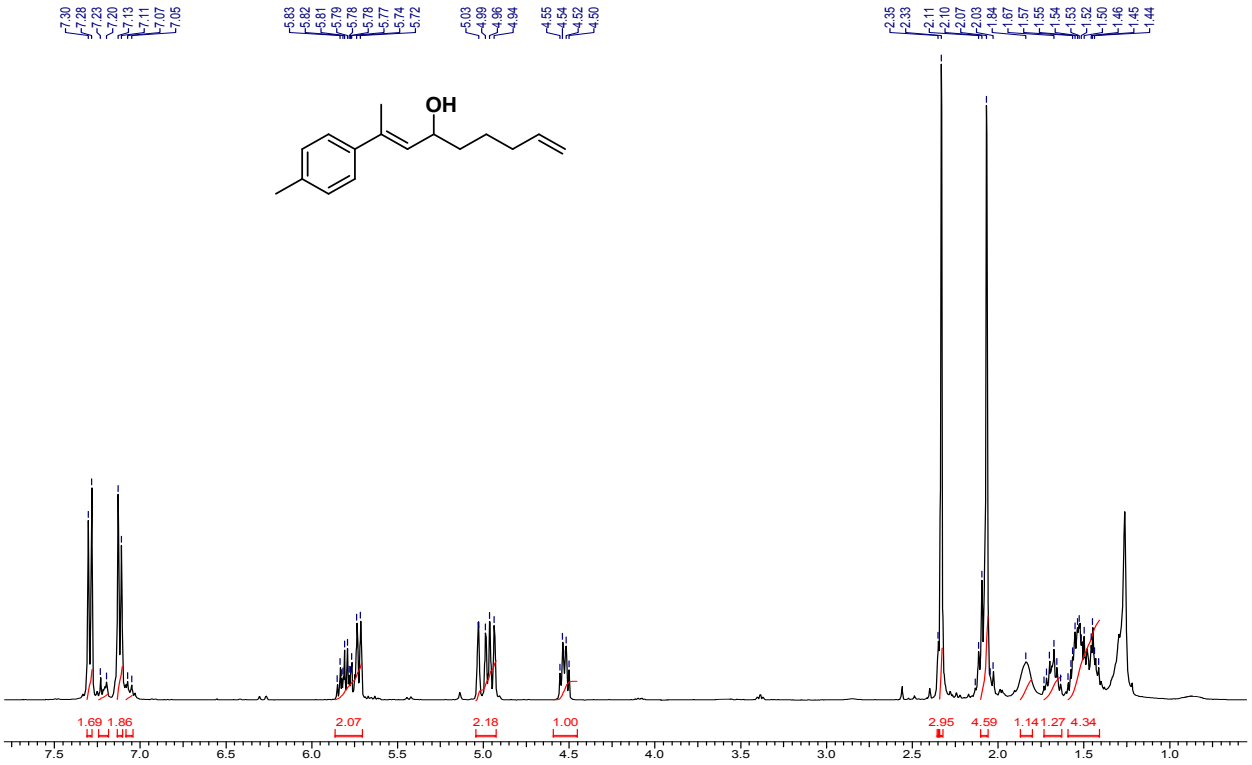
^{1}H NMR of (*E*)-ethyl 3-(*p*-tolyl)but-2-enoate (18)



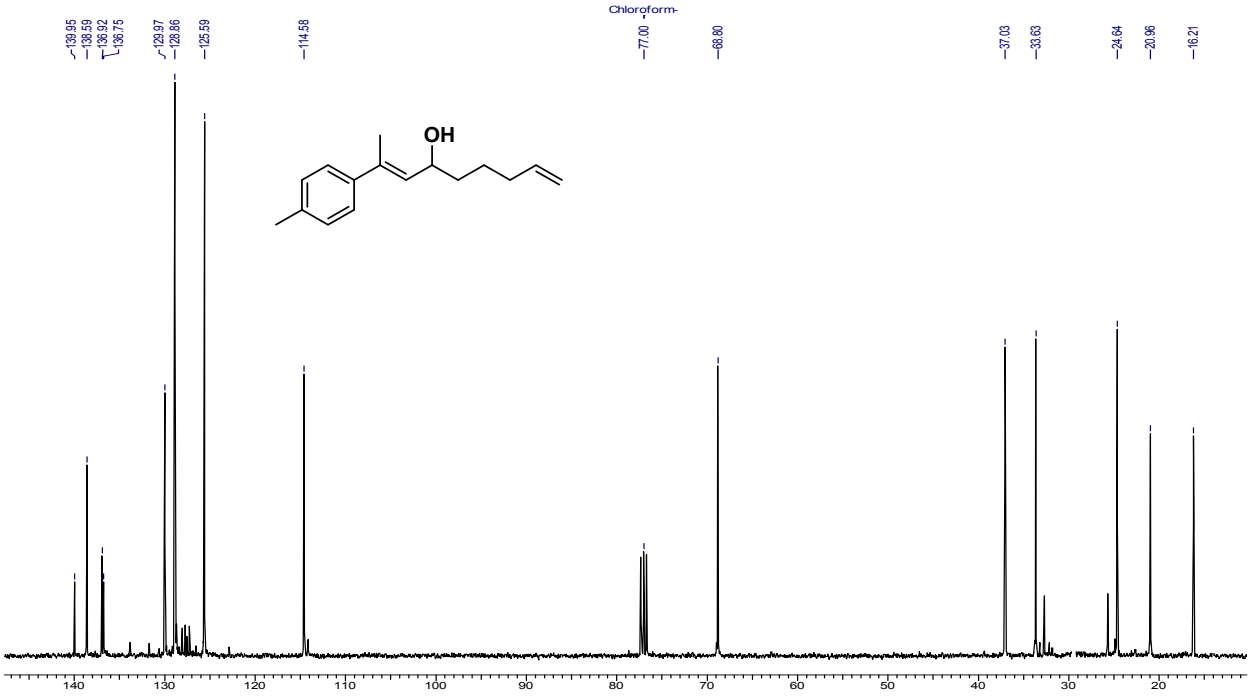
^{13}C NMR of (*E*)-ethyl 3-(*p*-tolyl)but-2-enoate (18)



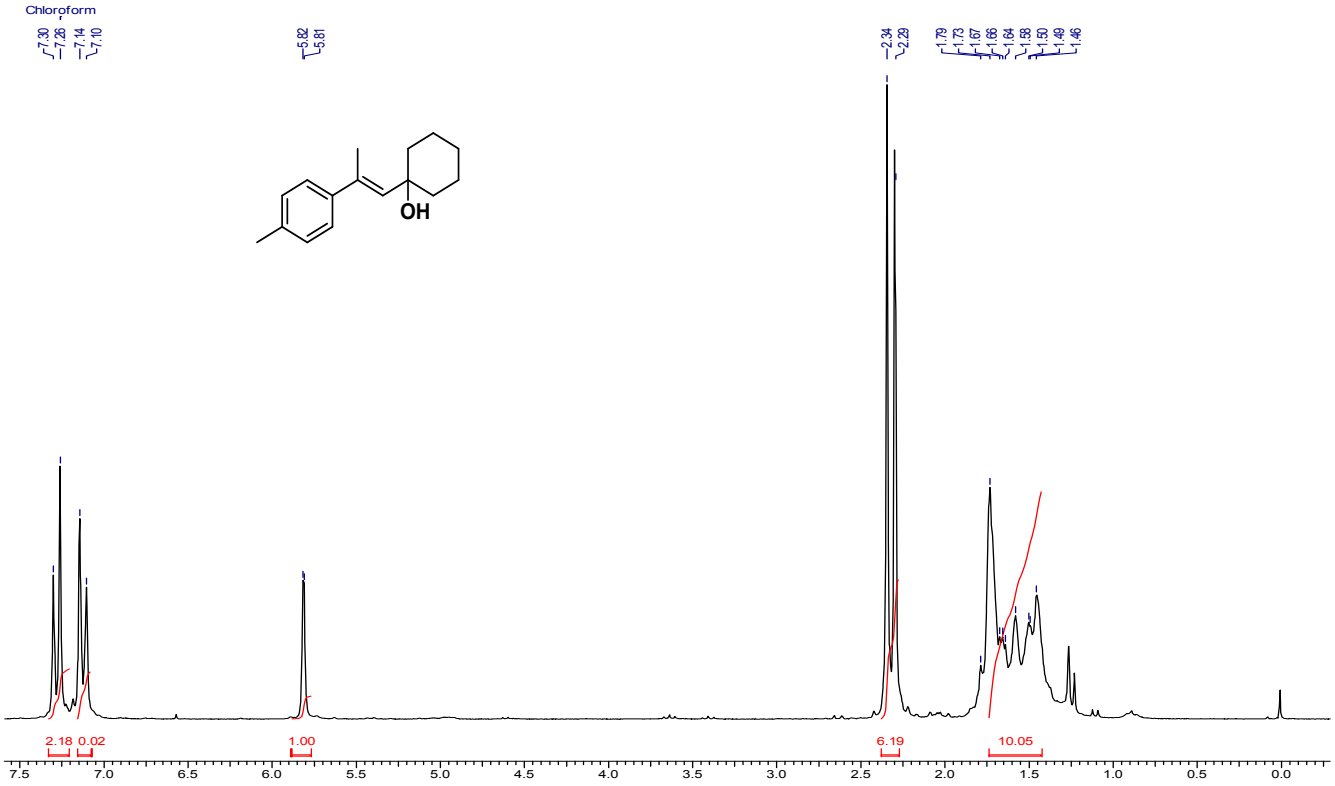
^{1}H NMR of (*E*)-2-(*p*-tolyl)nona-2,8-dien-4-ol (18a)



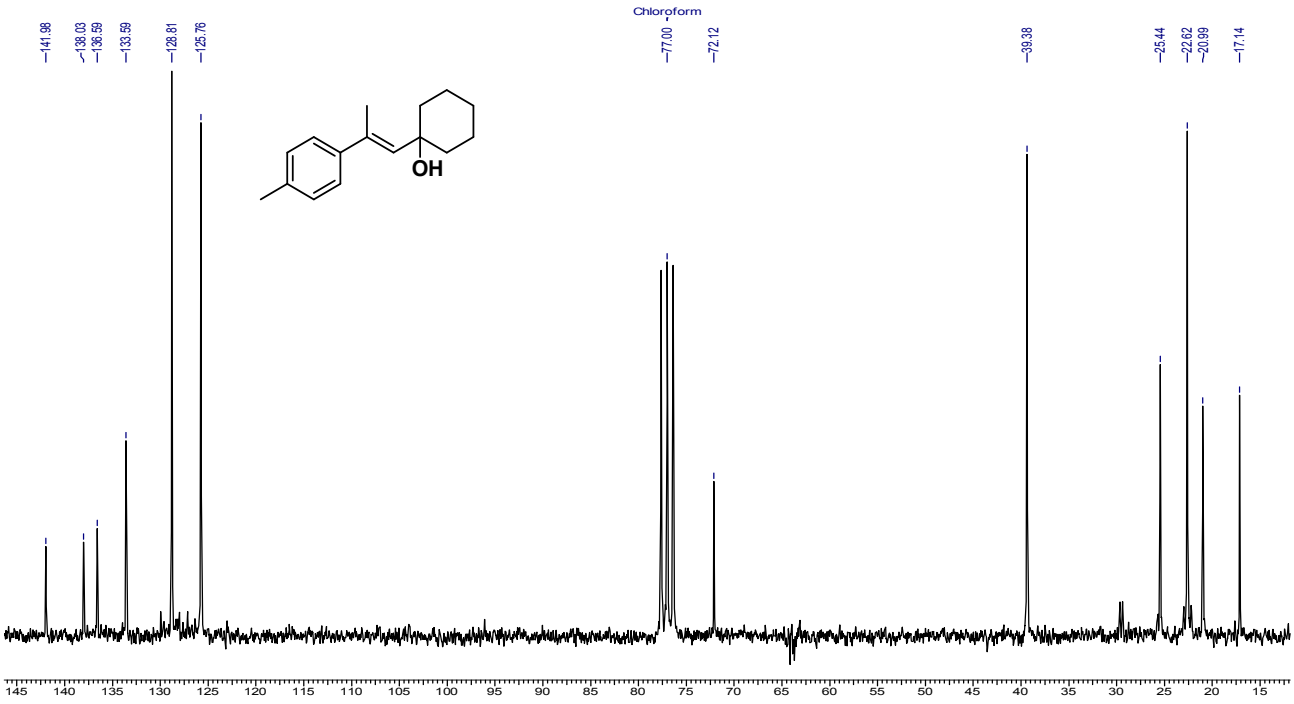
^{13}C NMR of (*E*)-2-(*p*-tolyl)nona-2,8-dien-4-ol (18a)



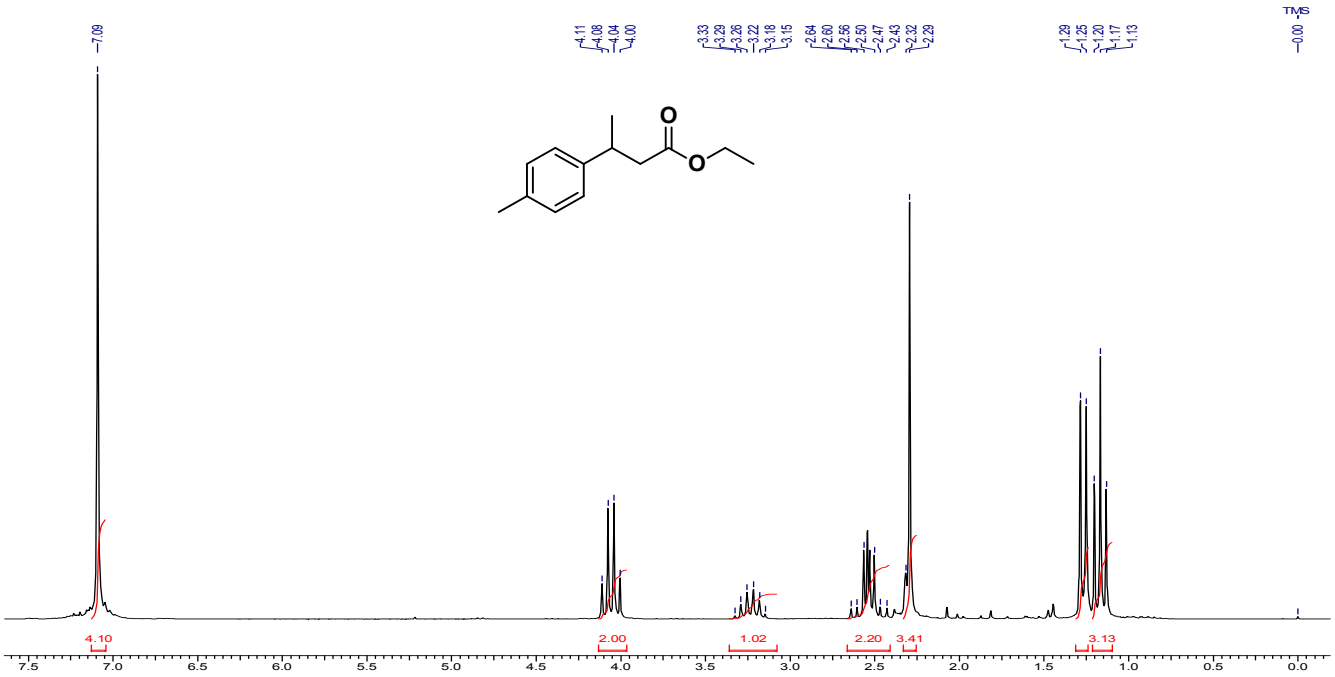
^{1}H NMR of (*E*)-1-(2-(*p*-tolyl)prop-1-en-1-yl)cyclohexanol (18b)



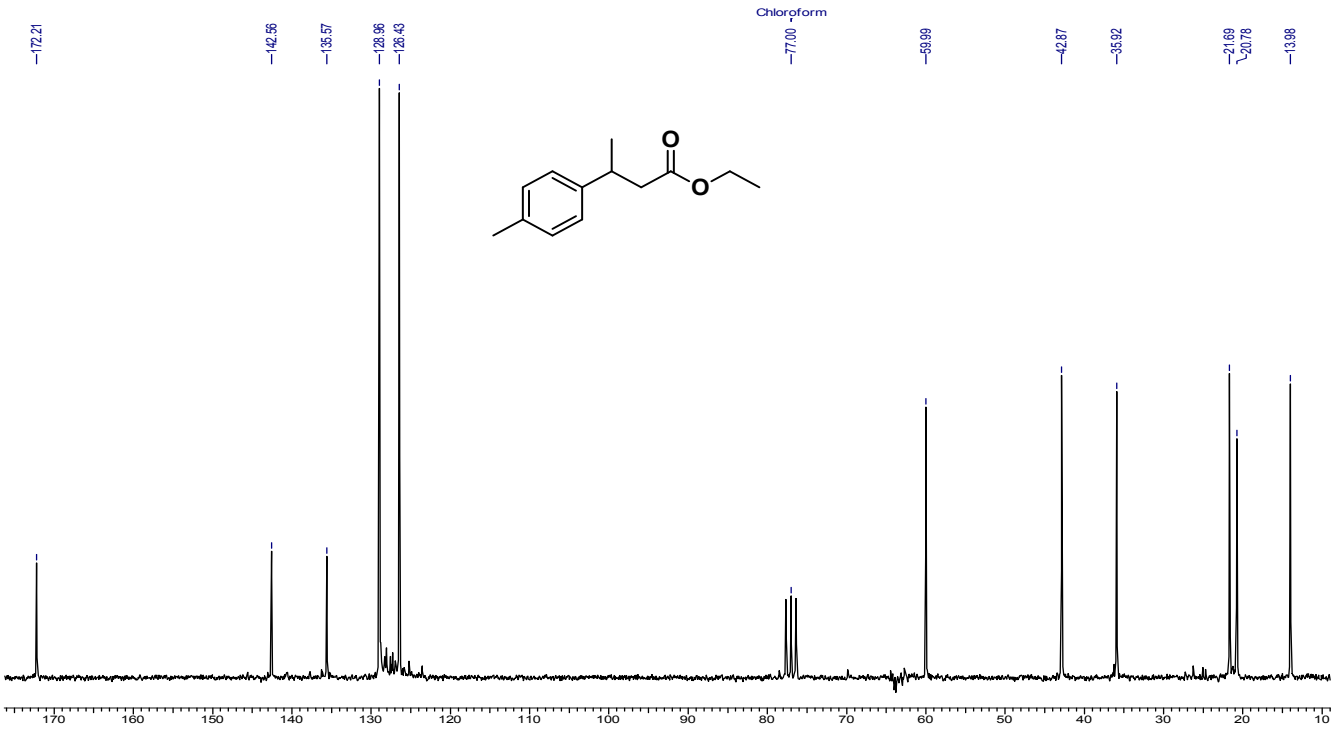
^{13}C NMR of (*E*)-1-(2-(*p*-tolyl)prop-1-en-1-yl)cyclohexanol (18b)



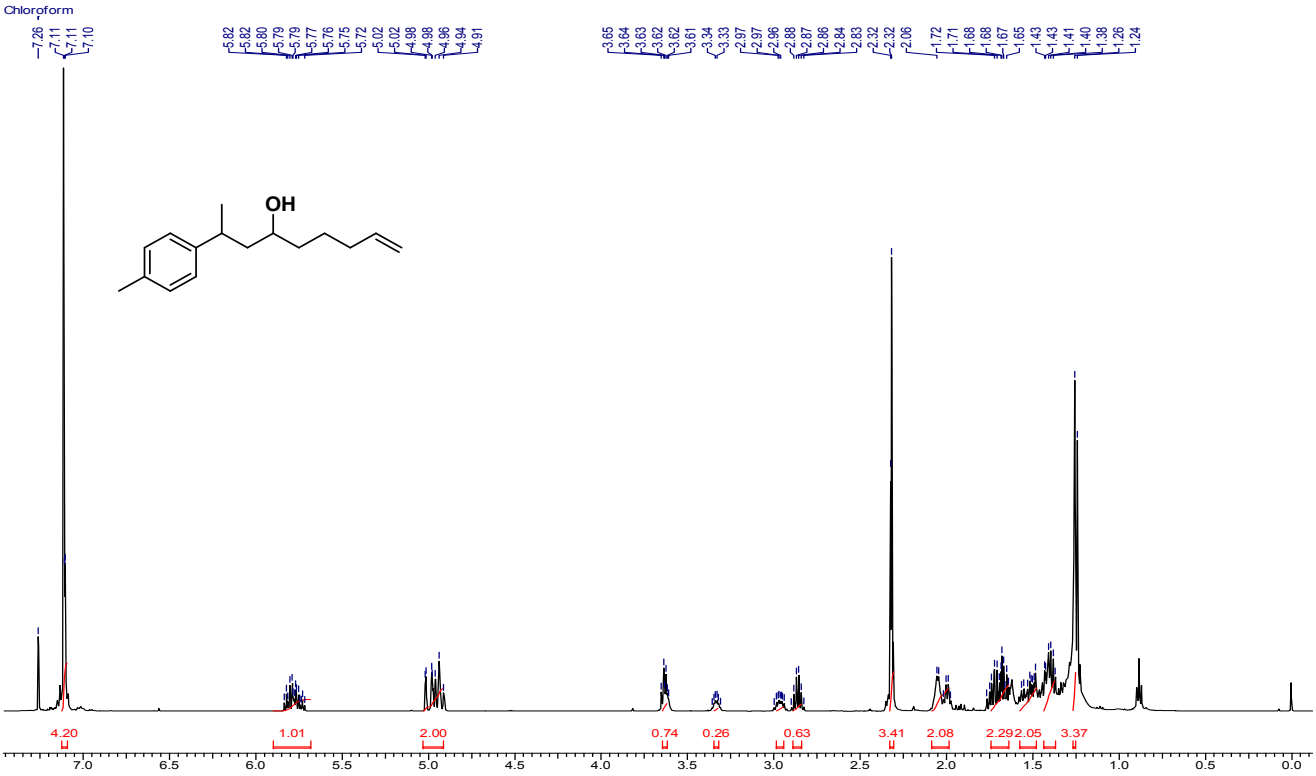
^{1}H NMR of ethyl 3-(*p*-Tolyl)butanoate (19)



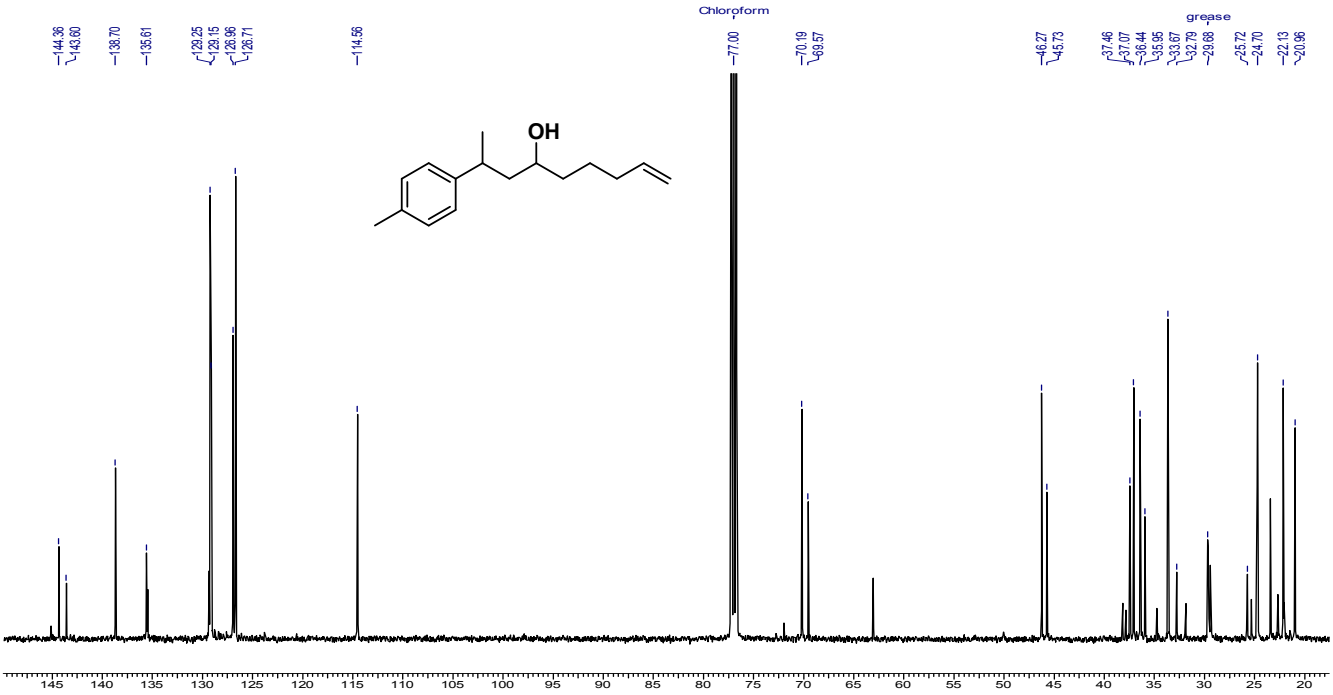
^{13}C NMR of ethyl 3-(*p*-tolyl)butanoate (19)



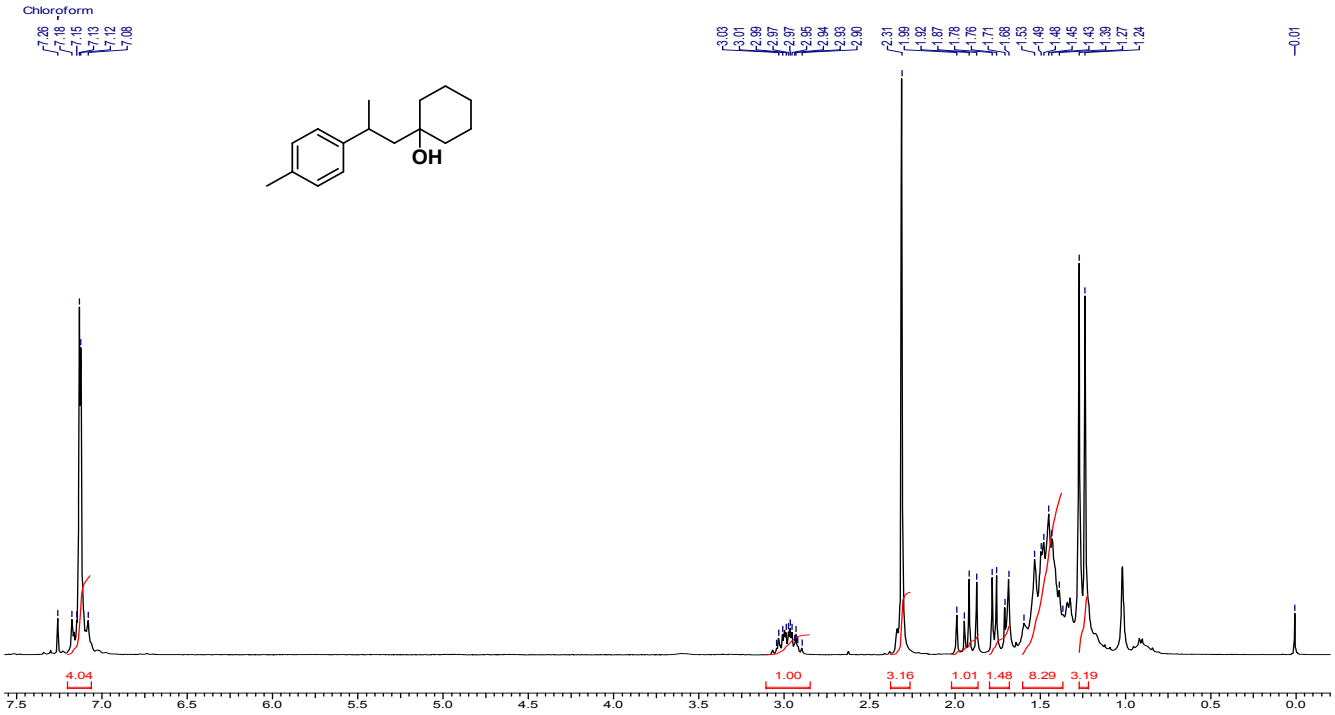
^{1}H NMR of 2-(*p*-tolyl)non-8-en-4-ol (19a)



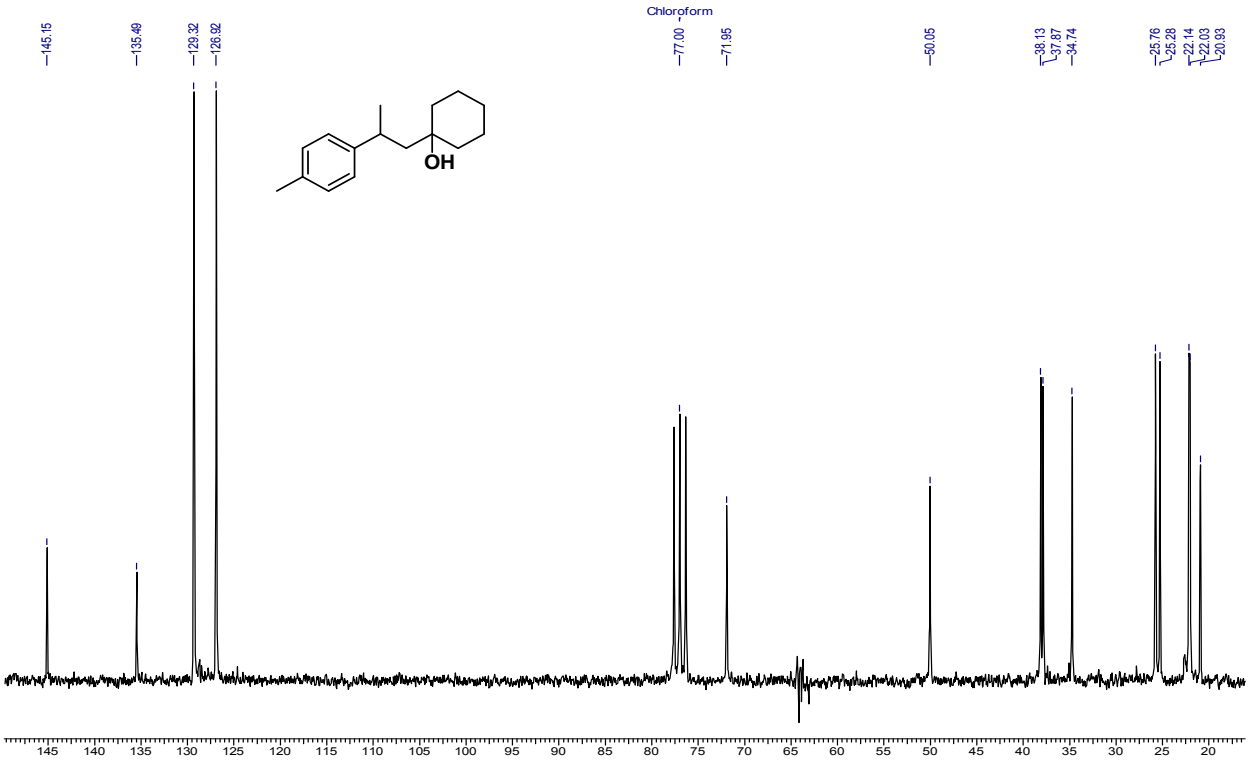
^{13}C NMR of 2-(*p*-tolyl)non-8-en-4-ol (19a)



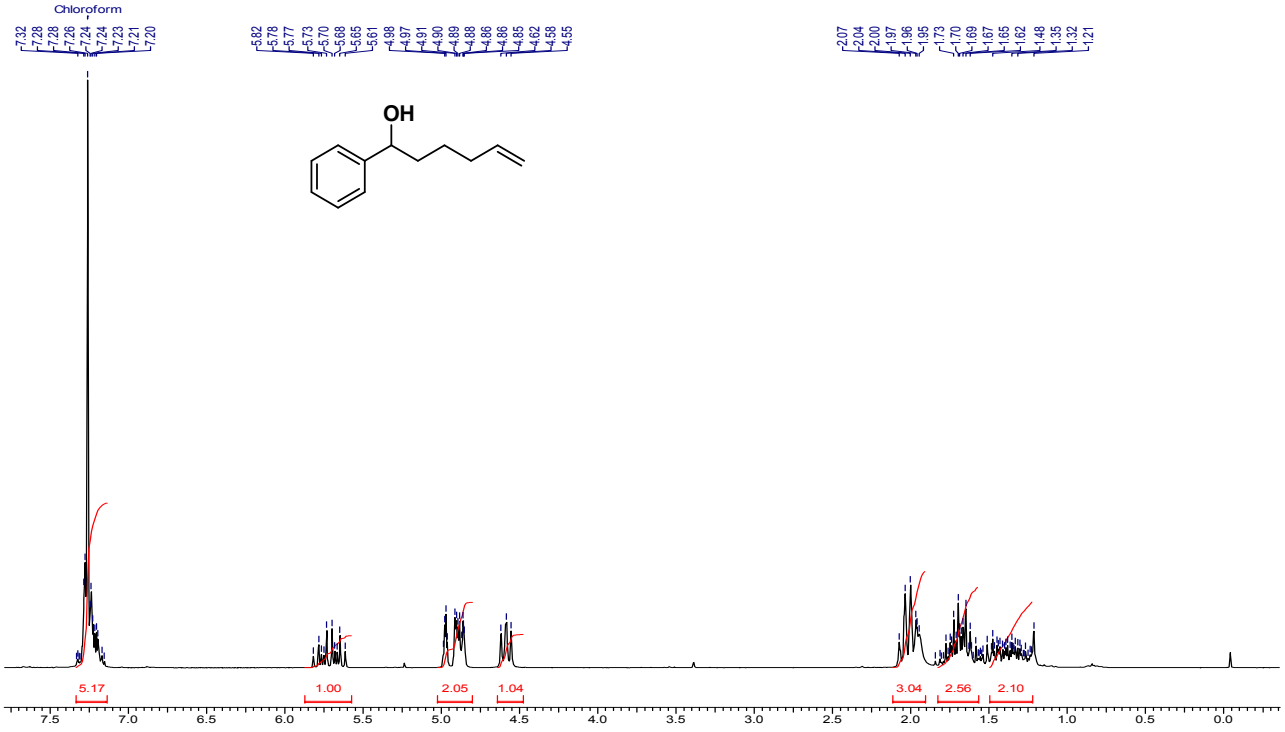
^{1}H NMR of 1-(2-(*p*-tolyl)propyl)cyclohexanol (19b)



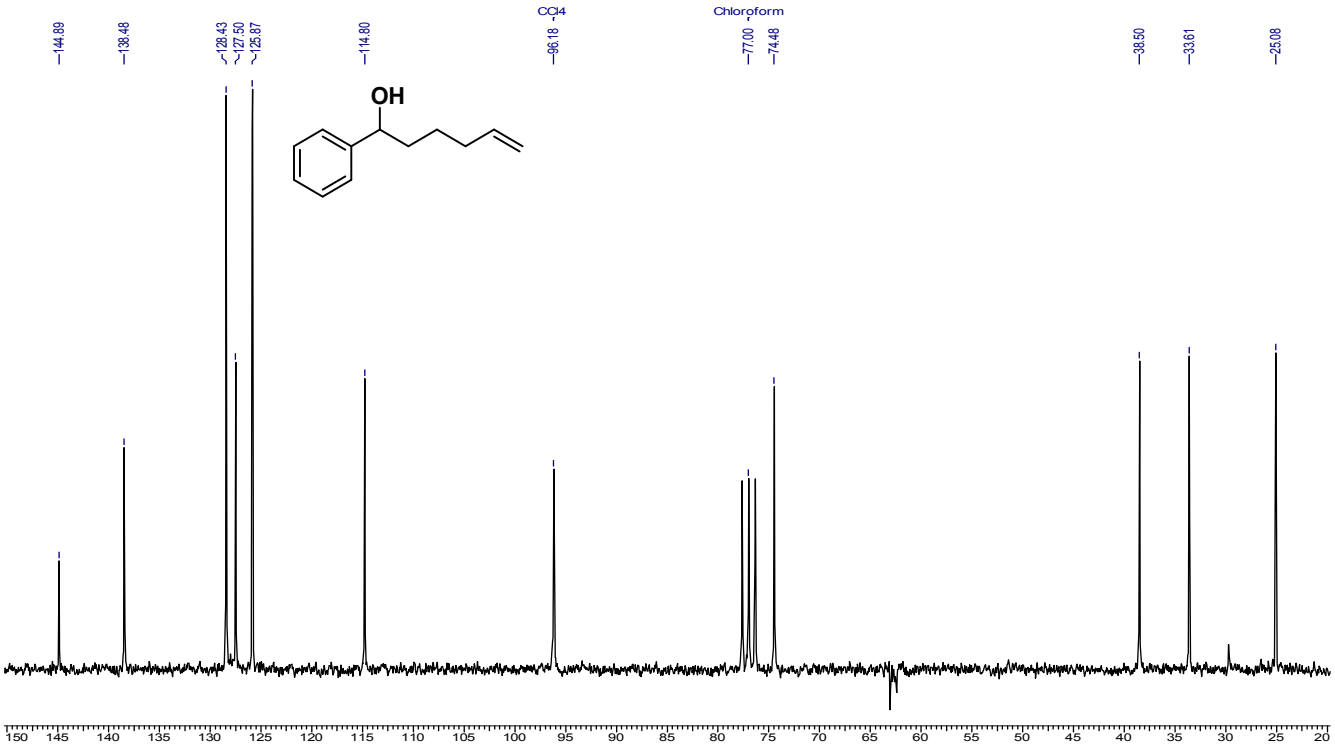
^{13}C NMR of 1-(2-(*p*-tolyl)propyl)cyclohexanol (19b)



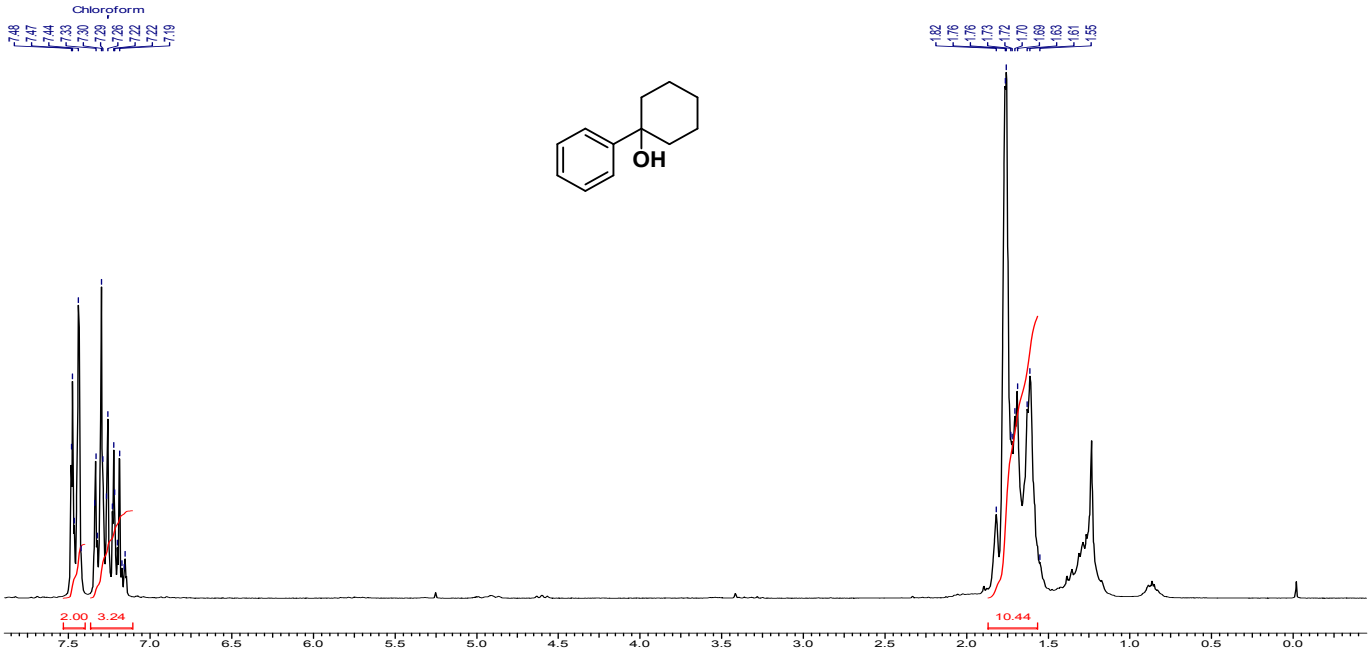
^{1}H NMR of 1-phenylhex-5-en-1-ol (20a)



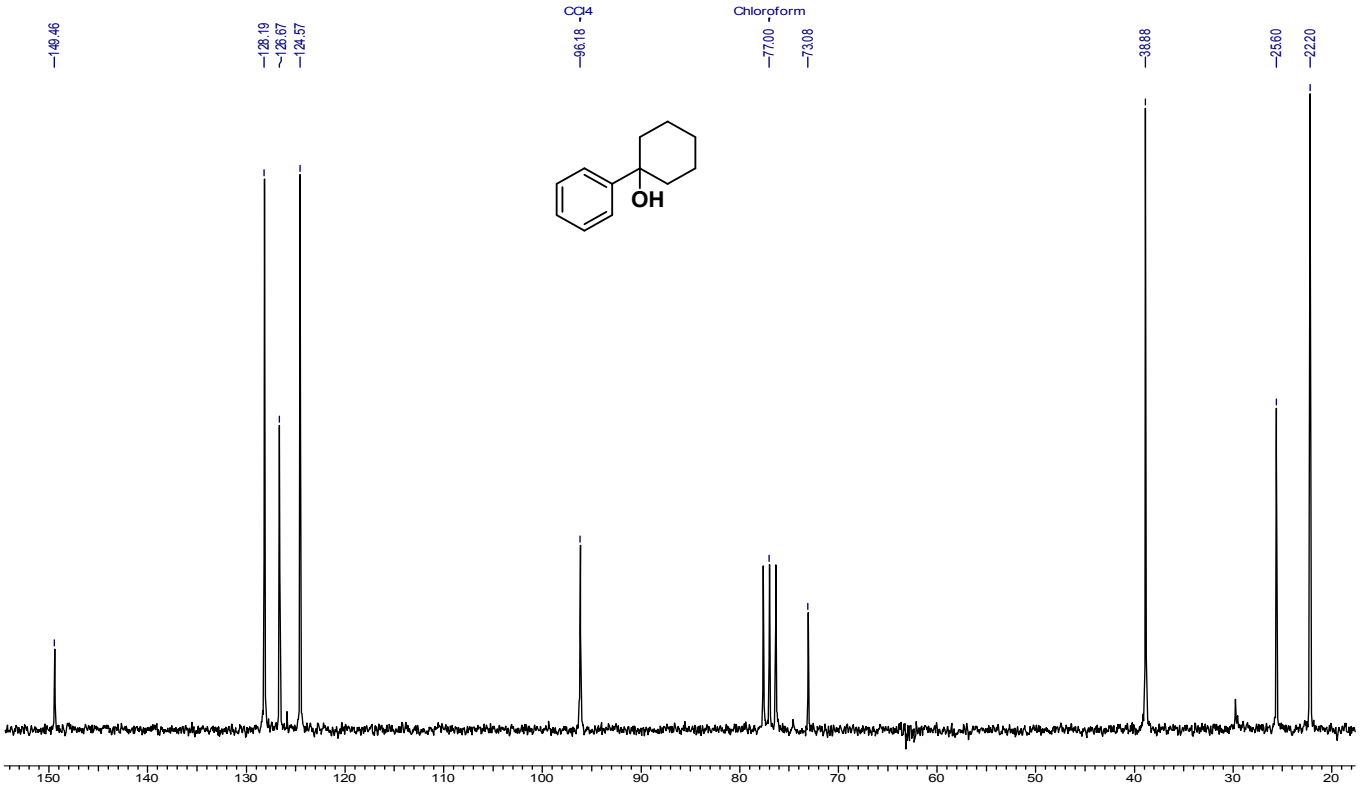
^{13}C NMR of 1-phenylhex-5-en-1-ol (20a)



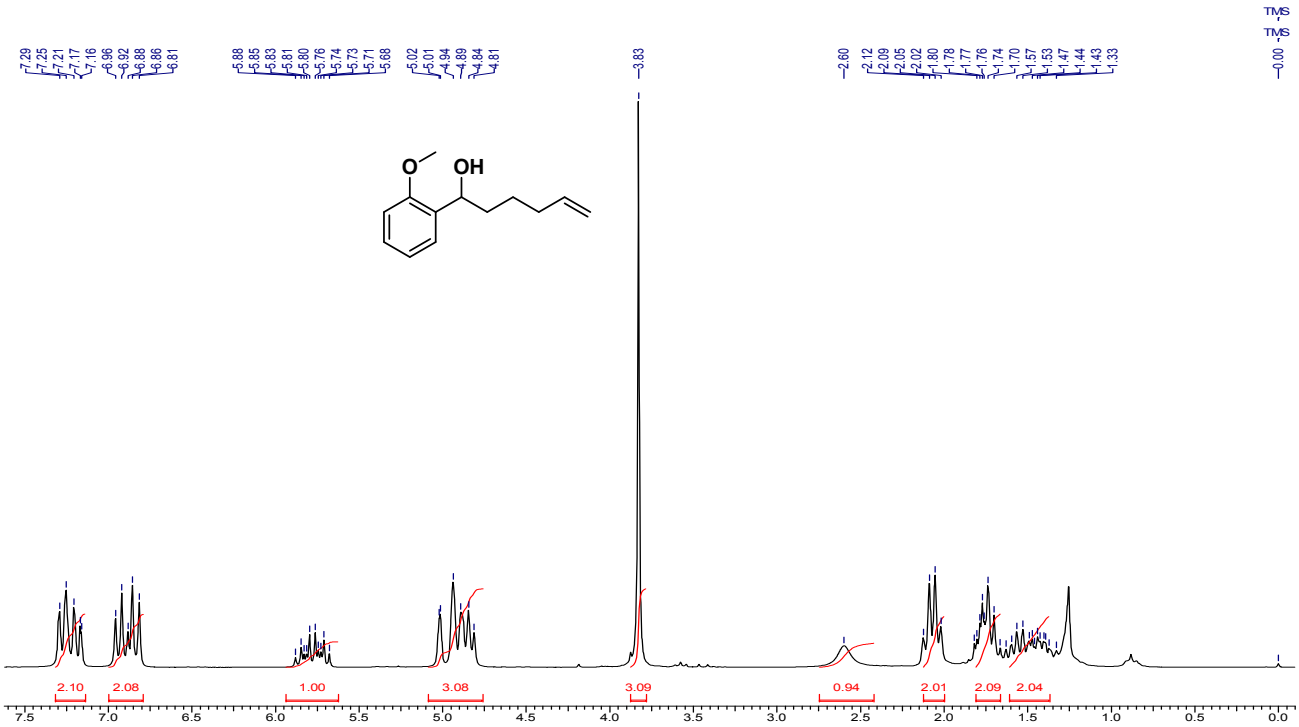
^{1}H NMR of 1-phenylcyclohexanol (20b)



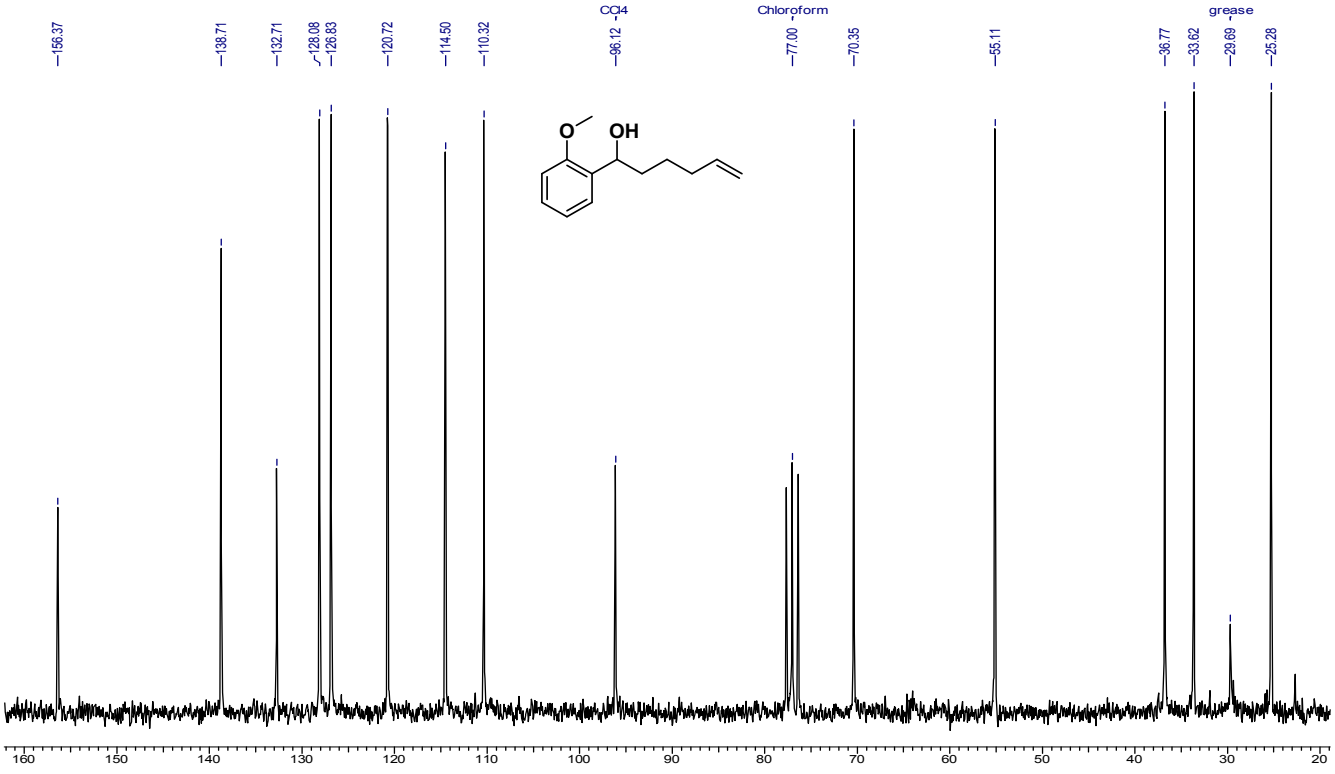
^{13}C NMR of 1-phenylcyclohexanol (20b)



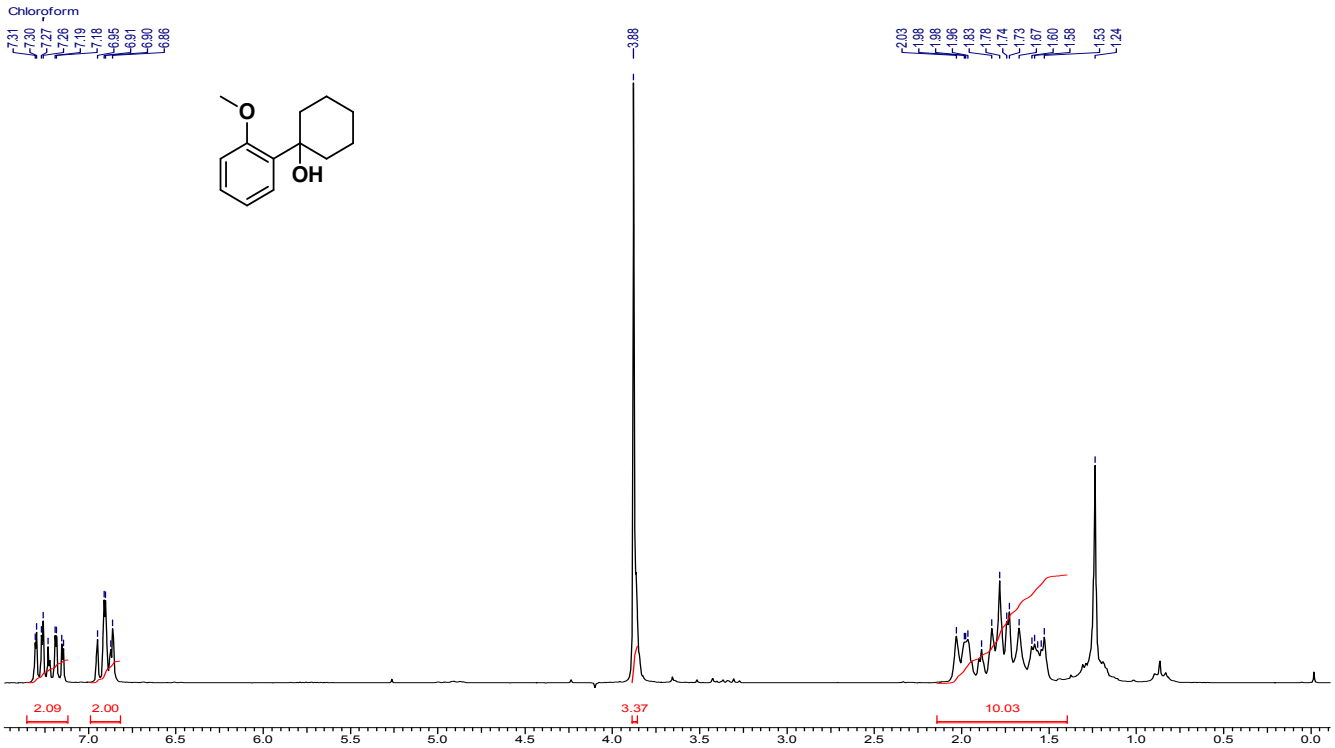
^{1}H NMR of 1-(2-methoxyphenyl)hex-5-en-1-ol (21a)



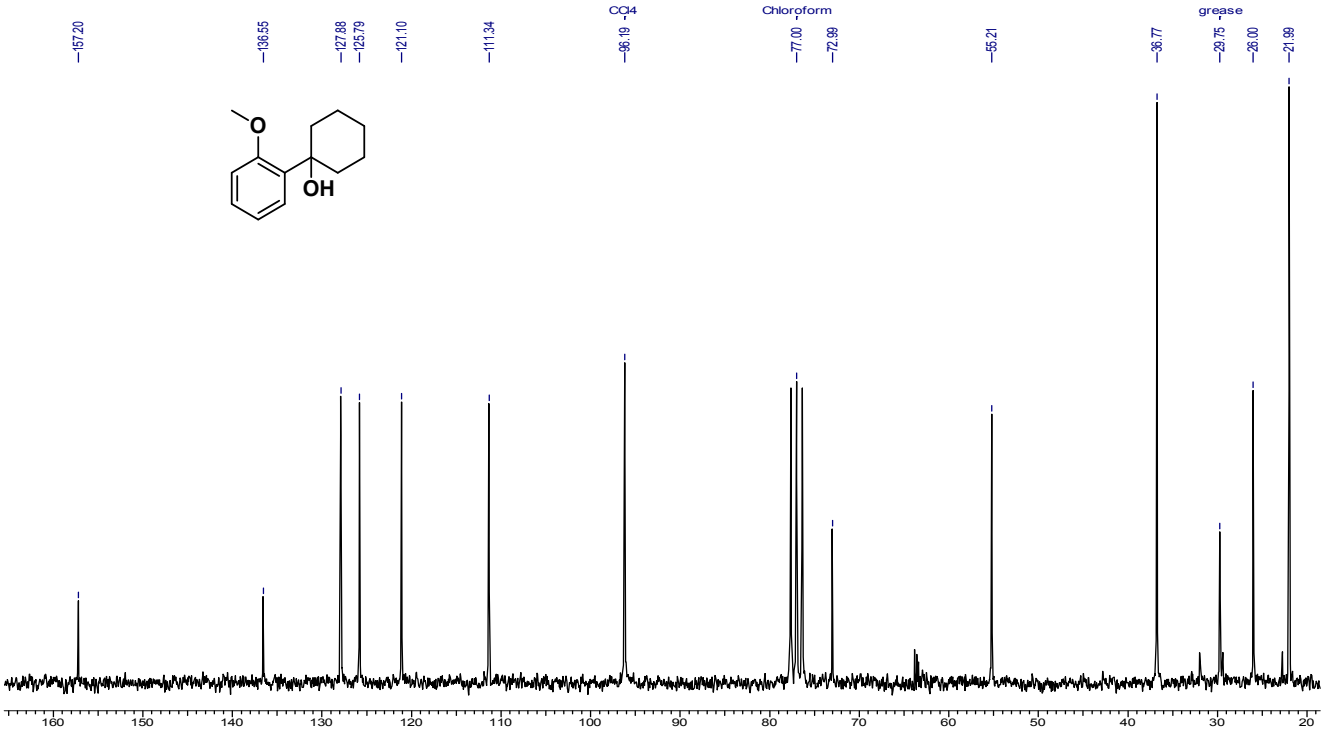
^{13}C NMR of 1-(2-methoxyphenyl)hex-5-en-1-ol (21a)



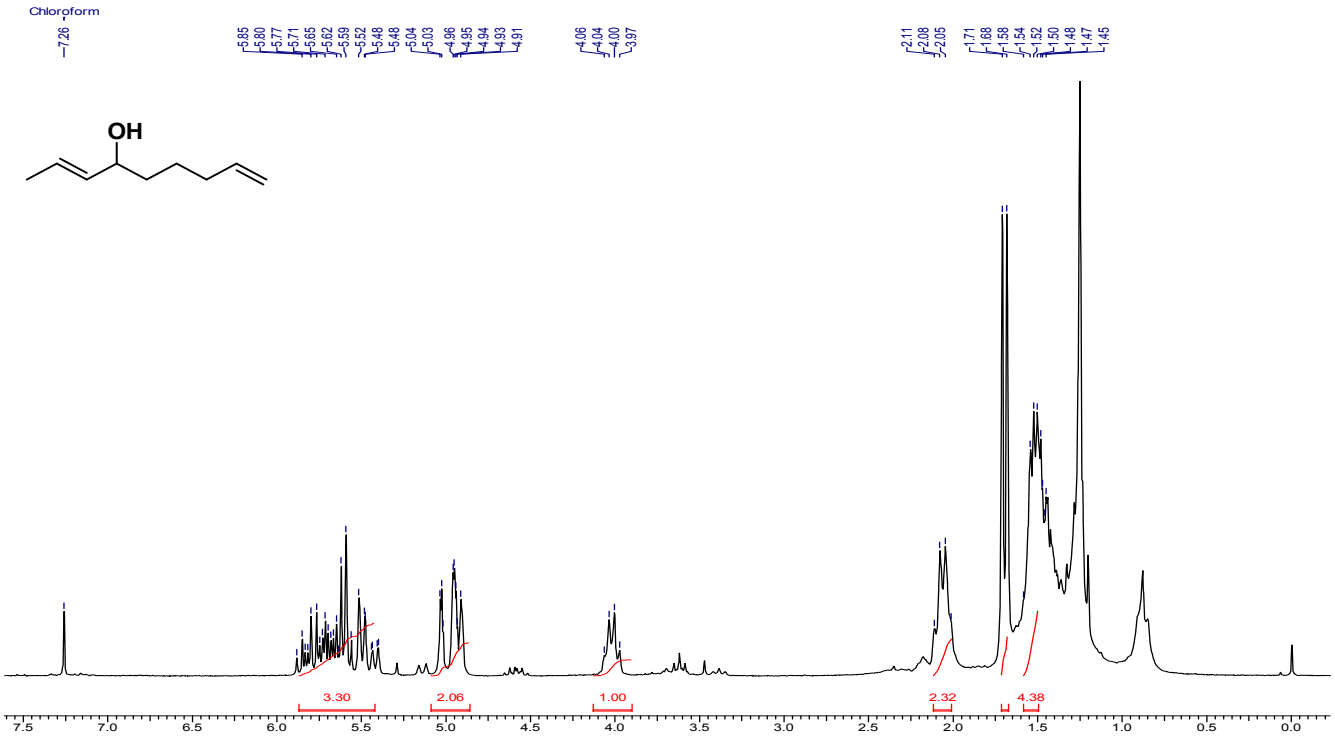
^{1}H NMR of 1-(2-methoxyphenyl)cyclohexanol (21b):



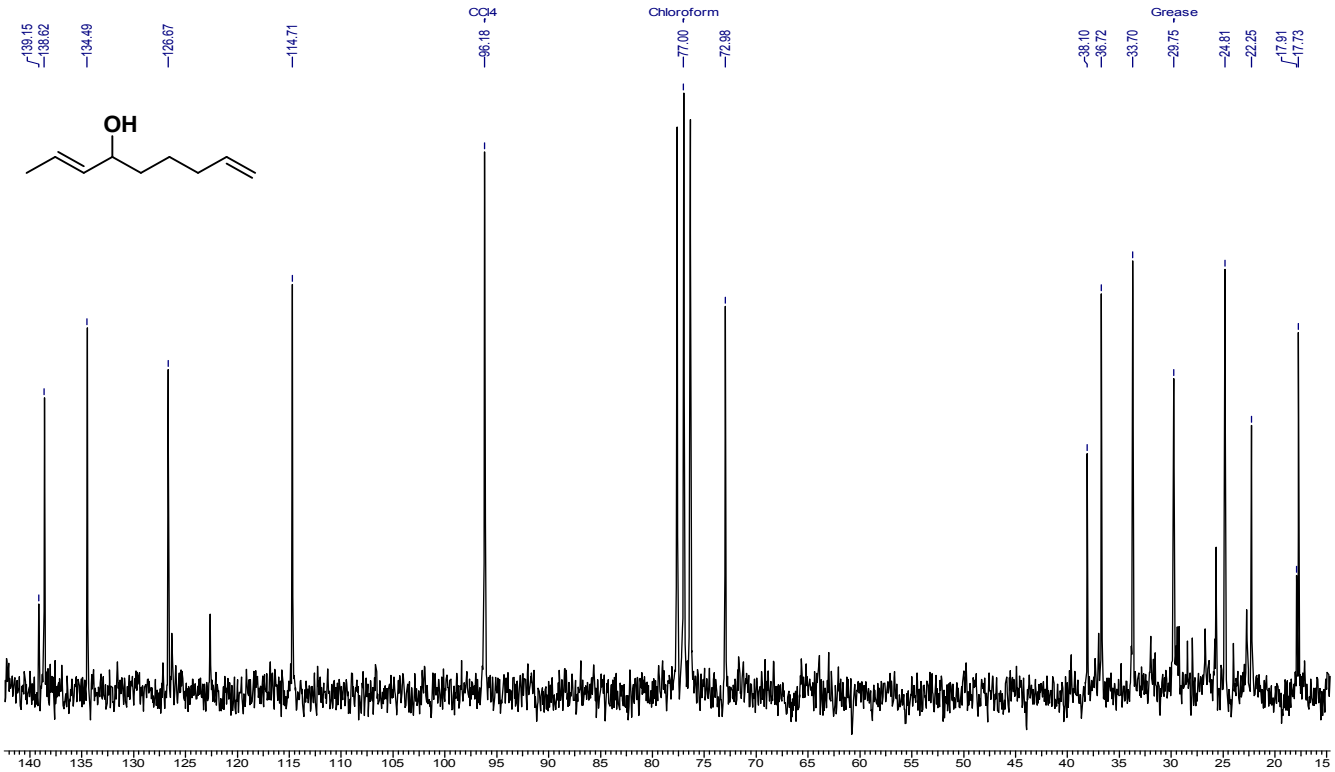
^{13}C NMR of 1-(2-methoxyphenyl)cyclohexanol (21b):



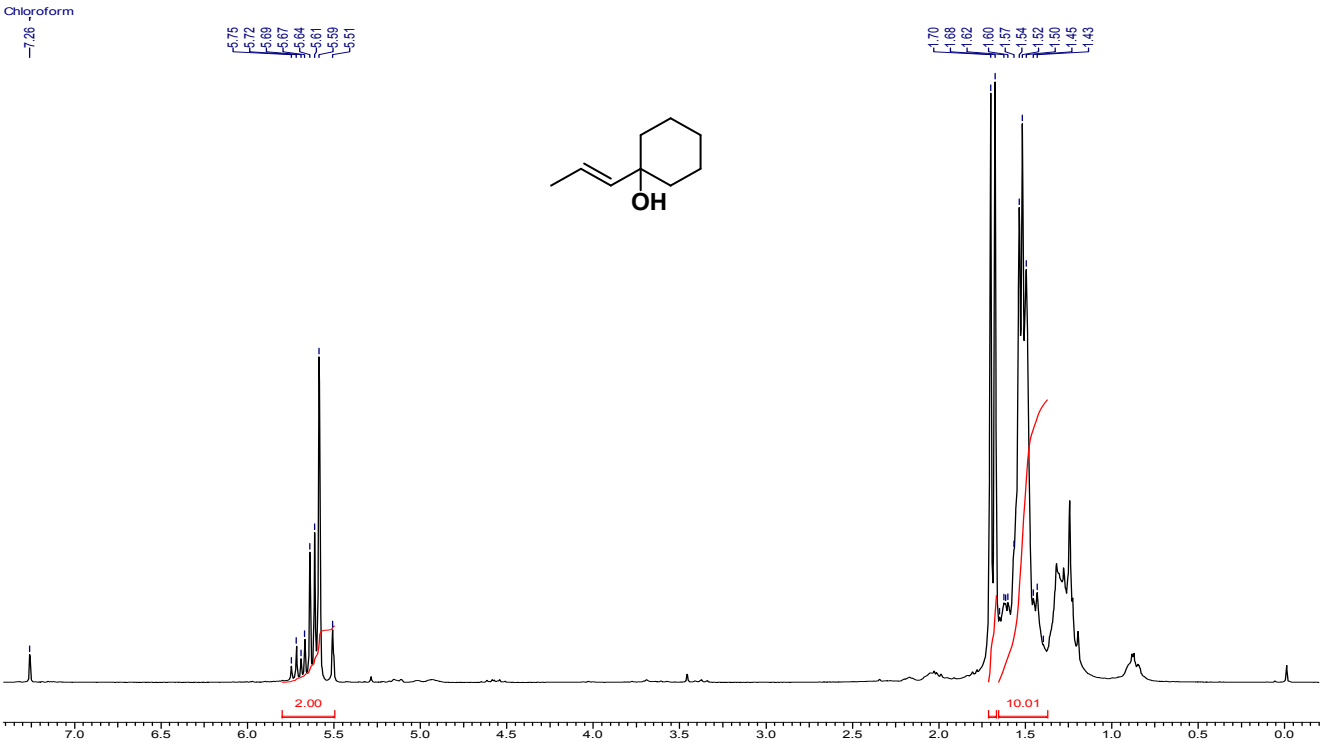
^{1}H NMR of (*E*)-nona-2,8-dien-4-ol (22a)



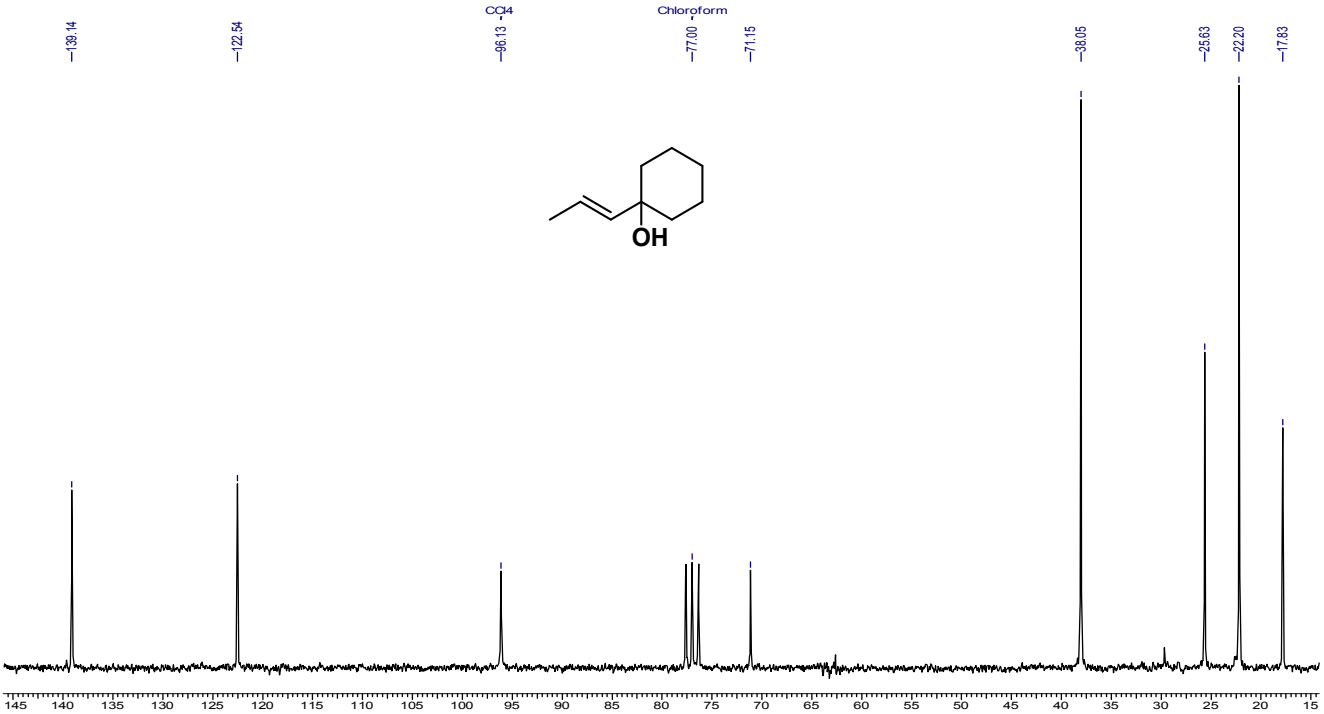
^{13}C NMR of (*E*)-nona-2,8-dien-4-ol (22a)



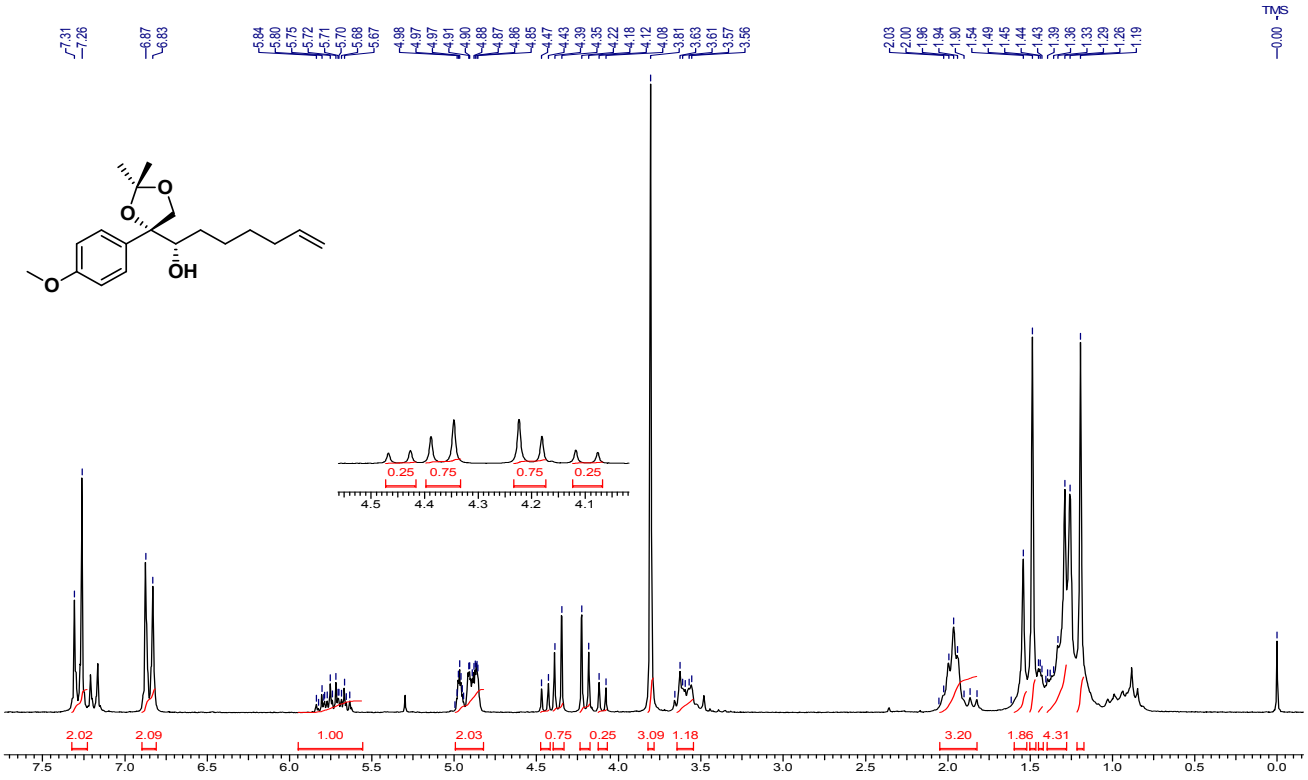
^{1}H NMR of (*E*)-1-(prop-1-en-1-yl)cyclohexanol (22b)



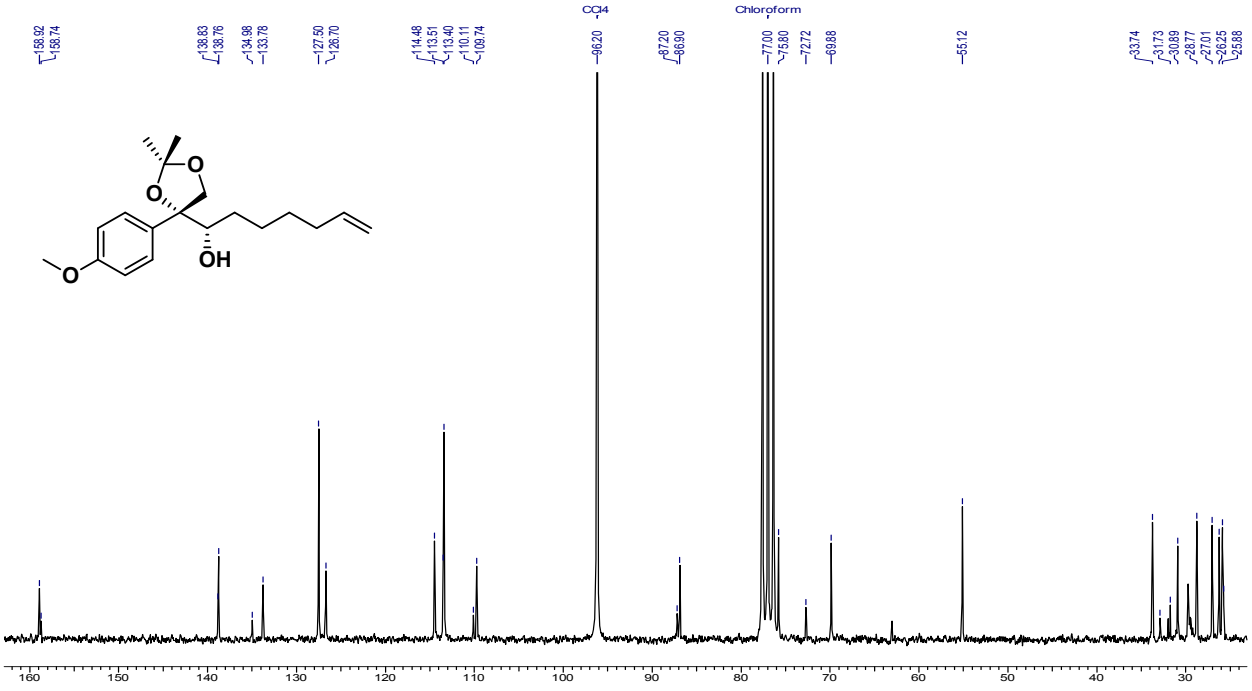
^{13}C NMR of (*E*)-1-(prop-1-en-1-yl)cyclohexanol (22b)



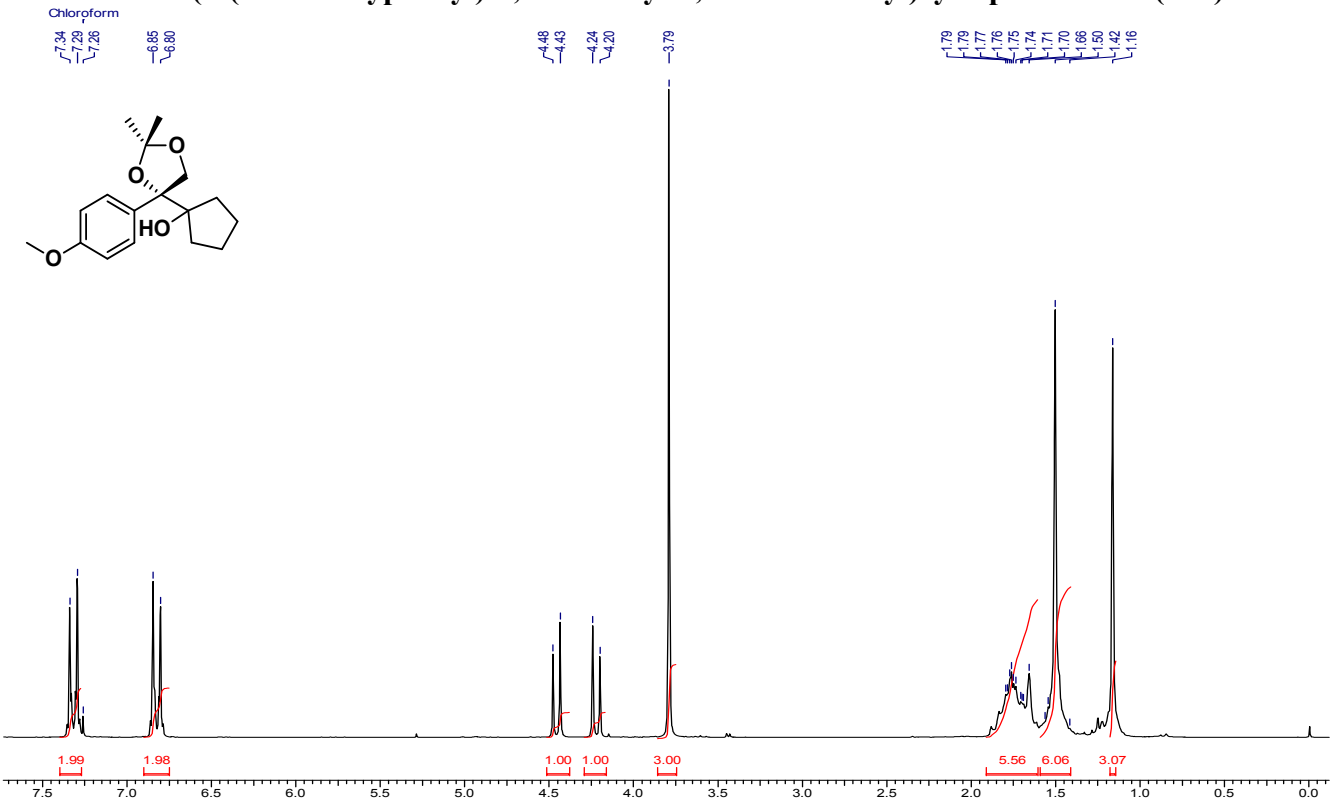
^{1}H NMR of 1-(4-(4-methoxyphenyl)-2,2-dimethyl-1,3-dioxolan-4-yl)hept-6-en-1-ol (23a)



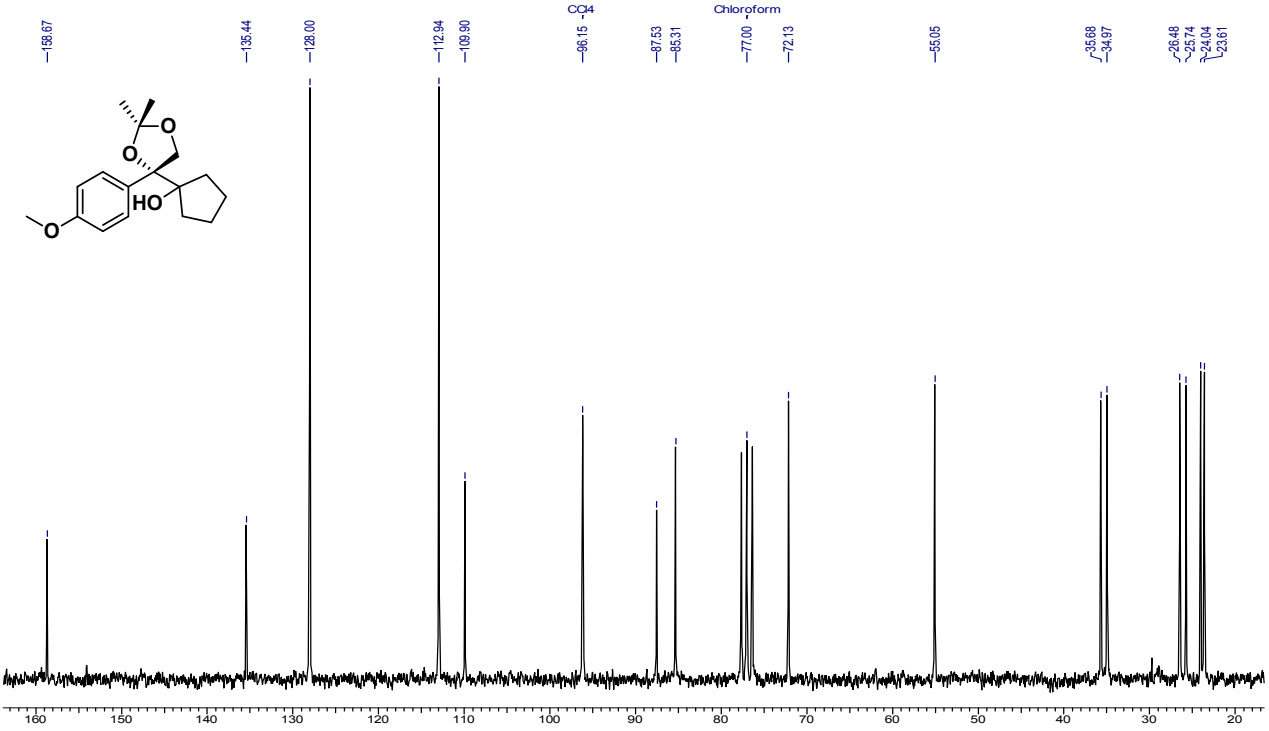
^{13}C NMR of 1-(4-(4-methoxyphenyl)-2,2-dimethyl-1,3-dioxolan-4-yl)hept-6-en-1-ol (23a)



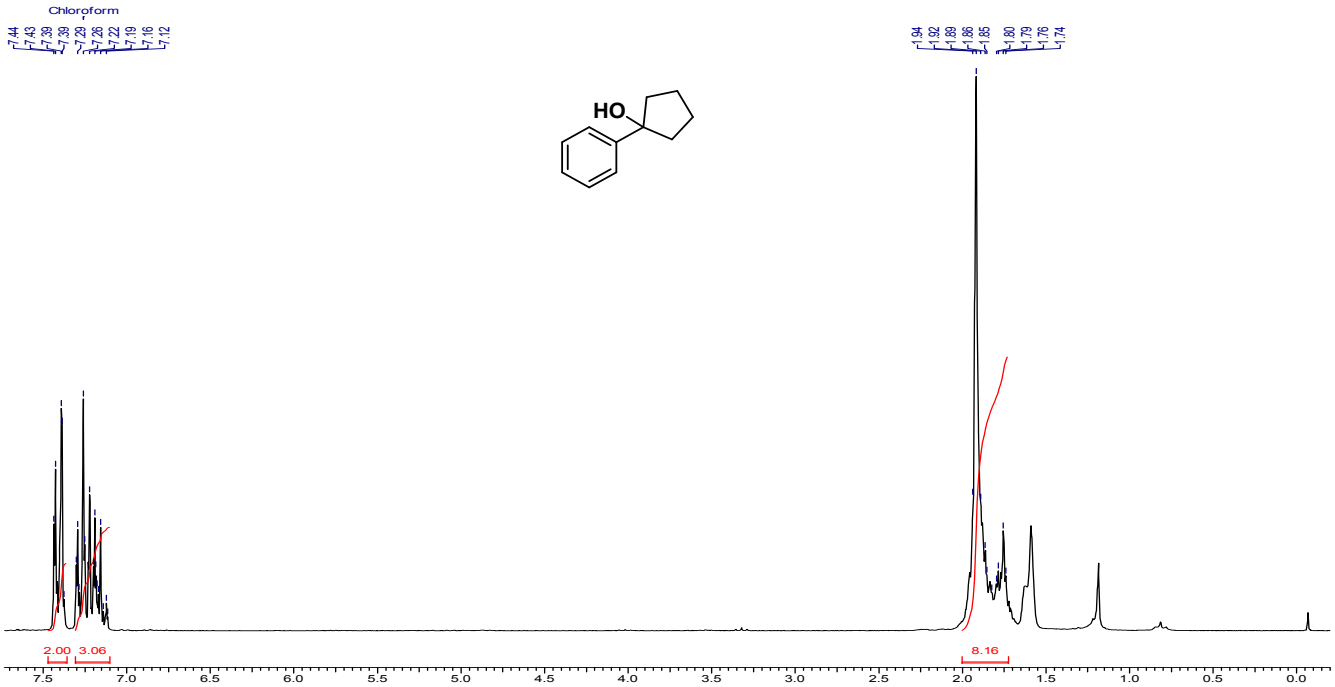
^{1}H NMR of 1-(4-(4-methoxyphenyl)-2,2-dimethyl-1,3-dioxolan-4-yl)cyclopentan-1-ol (24b)



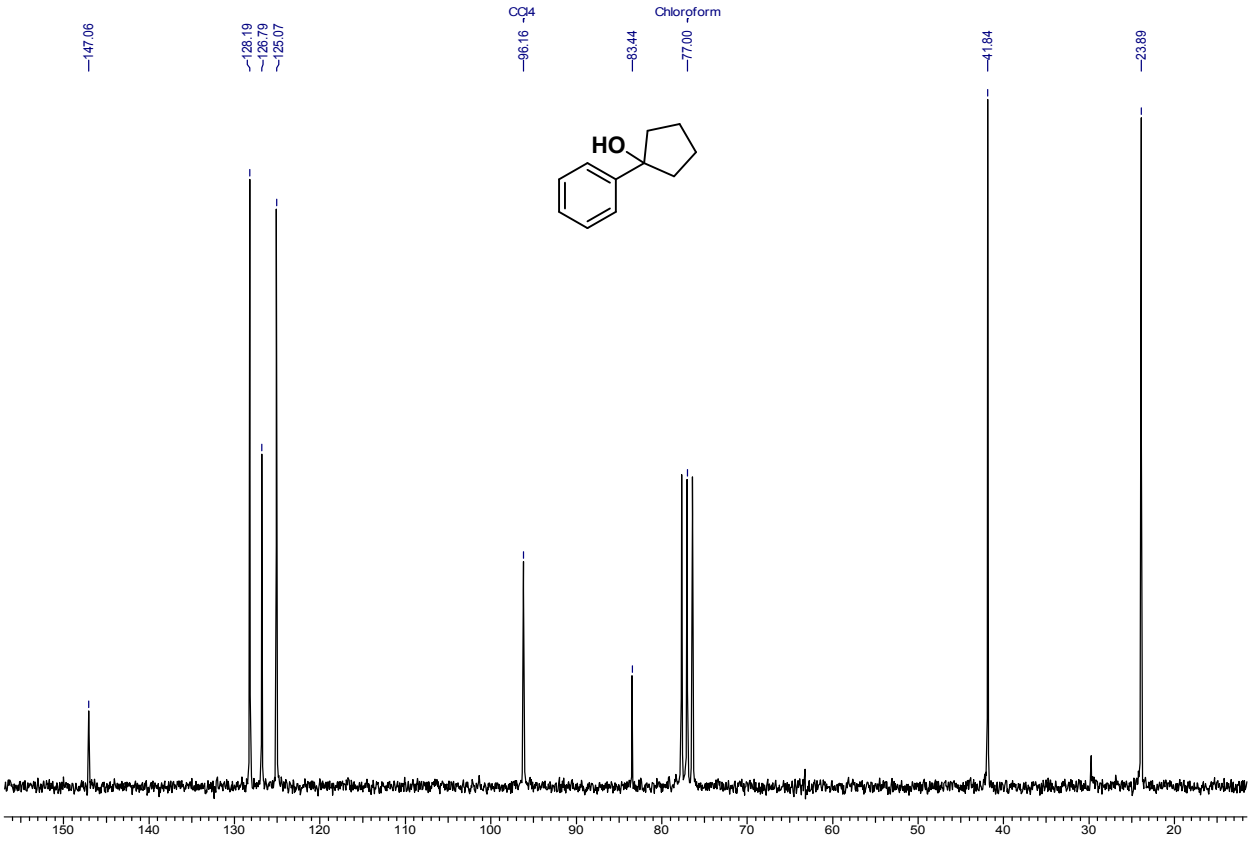
^{13}C NMR of 1-(4-(4-methoxyphenyl)-2,2-dimethyl-1,3-dioxolan-4-yl)cyclopentan-1-ol (24b)



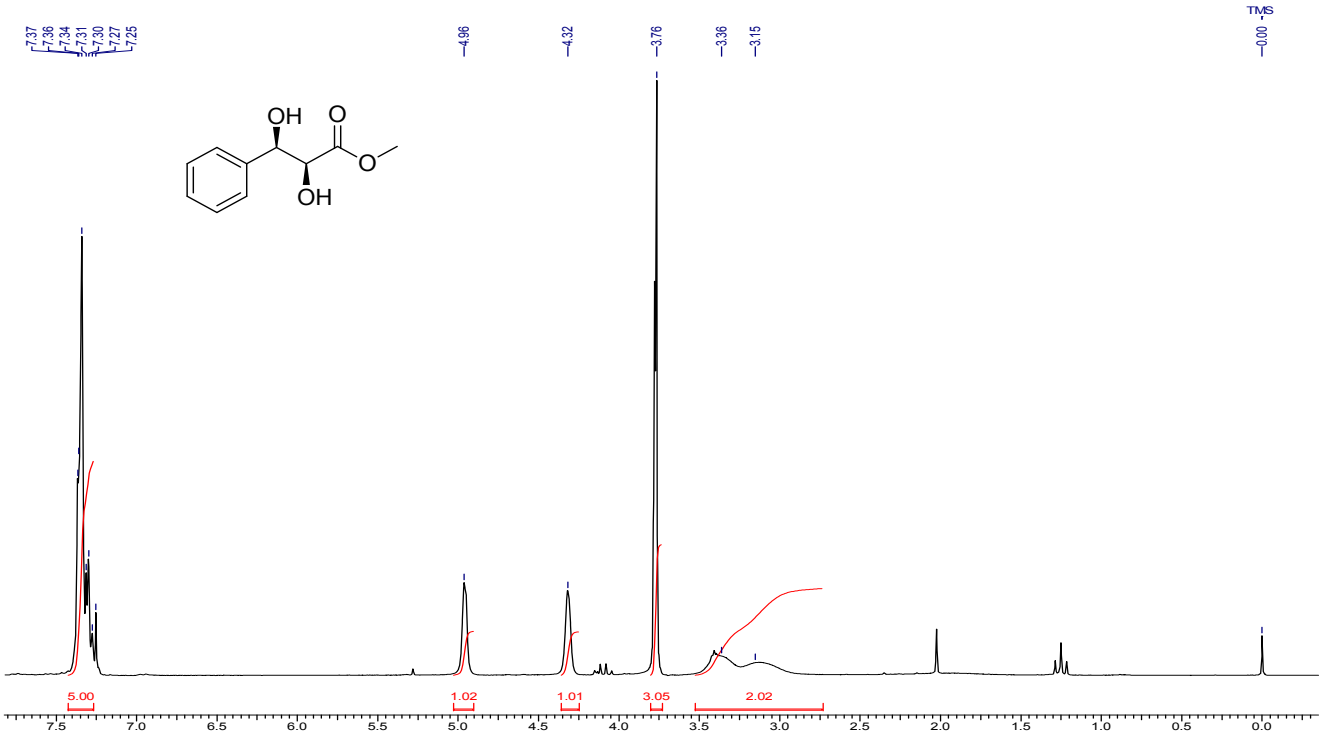
^{1}H NMR of 1-phenylcyclopentanol (25b)



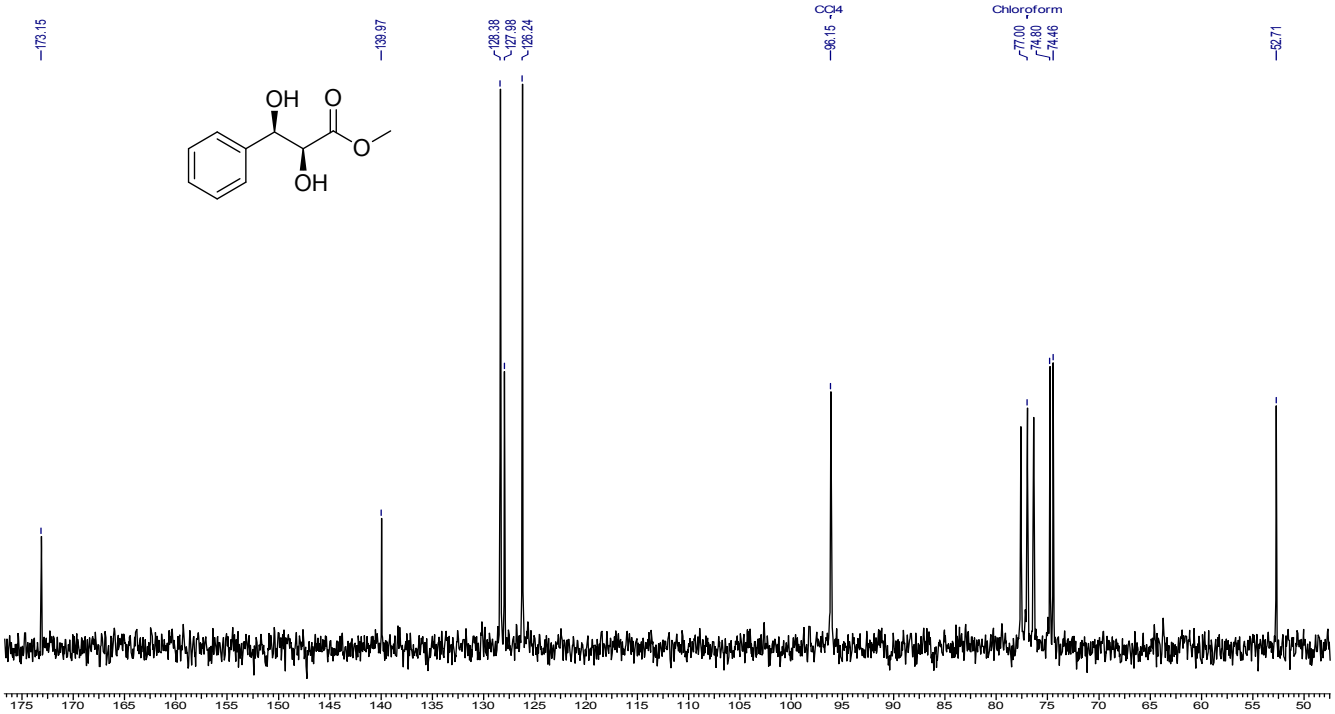
^{13}C NMR of 1-phenylcyclopentanol (25b)



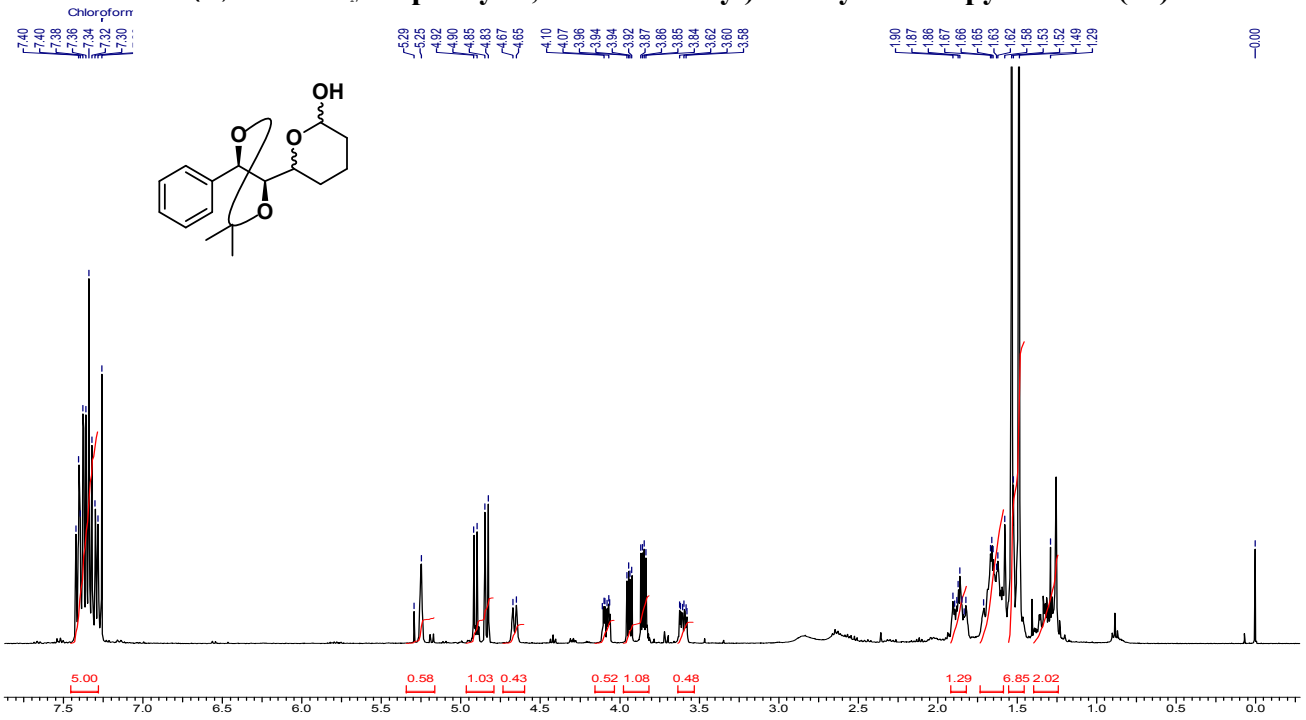
^{1}H NMR of (2*S*,3*R*)-methyl 2,3-dihydroxy-3-phenylpropanoate (37)



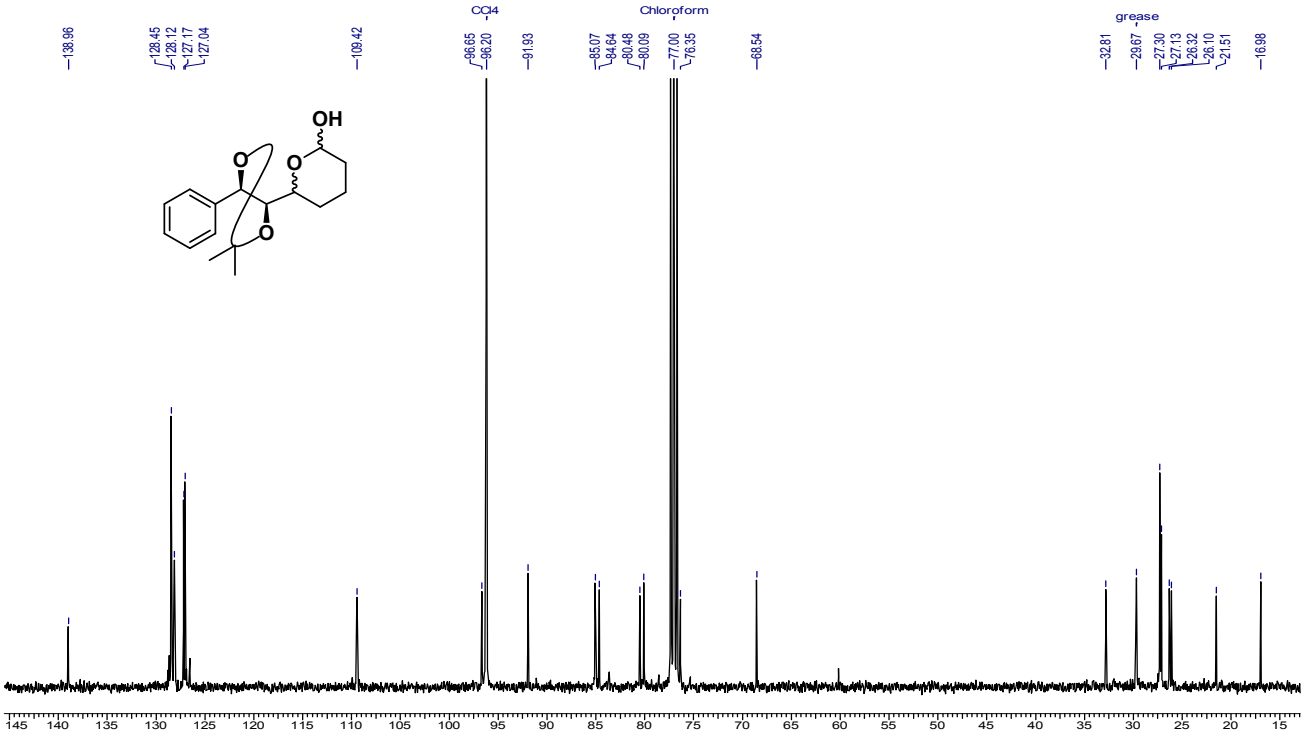
^{13}C NMR of (2*S*,3*R*)-methyl 2,3-dihydroxy-3-phenylpropanoate (37)



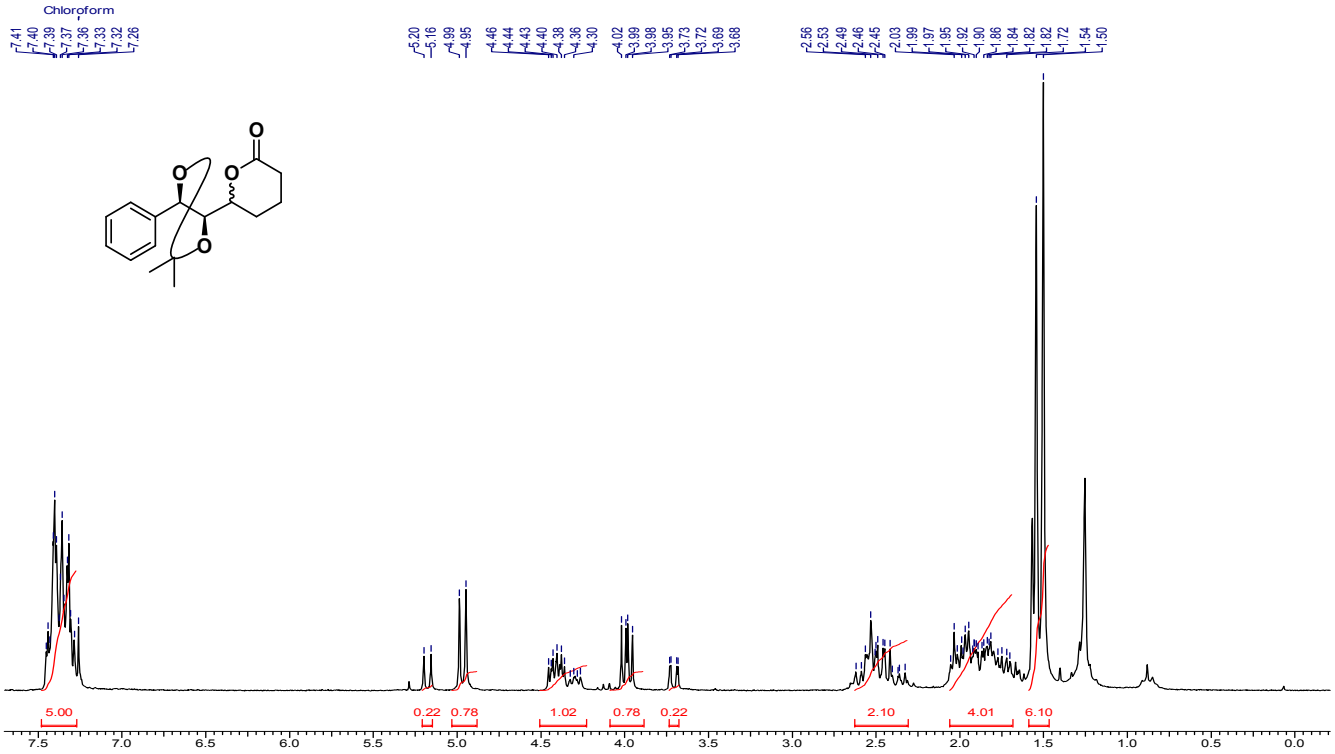
^{1}H NMR of 6-(2,2-dimethyl-5-phenyl-1,3-dioxolan-4-yl)tetrahydro-2H-pyran-2-ol (26)



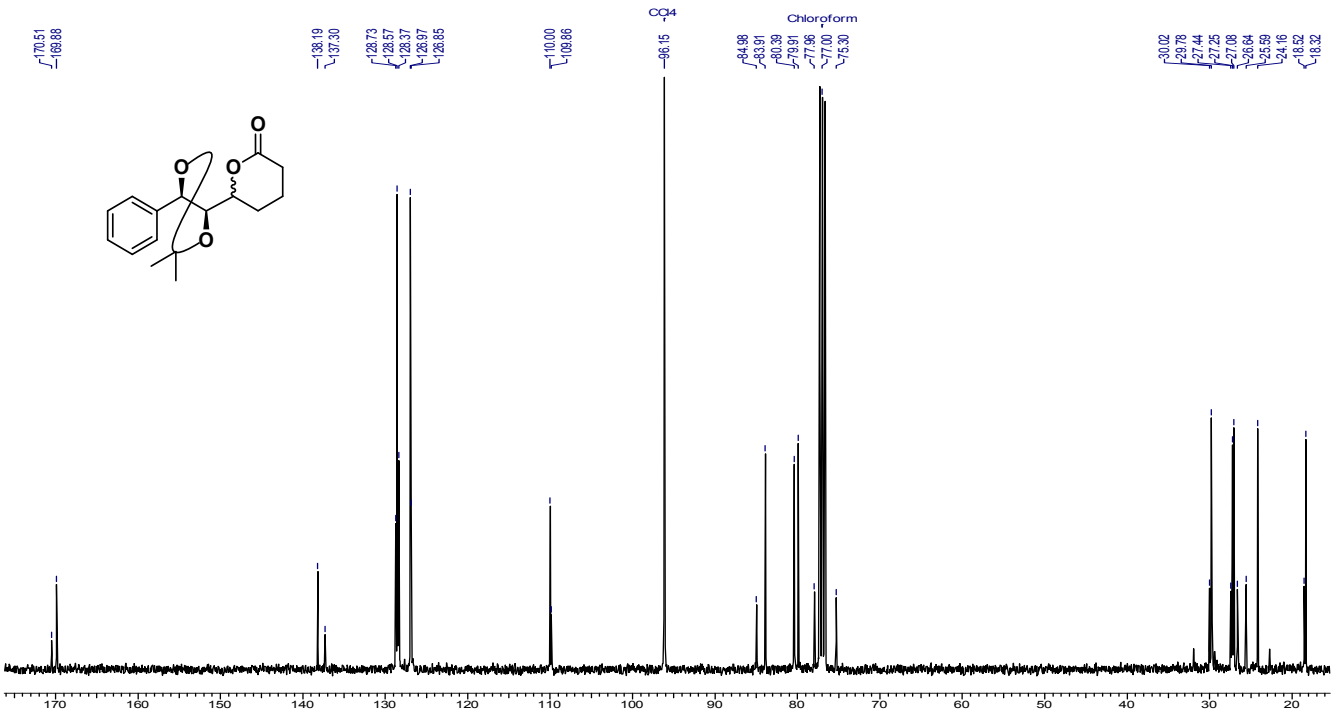
^{13}C NMR of 6-(2,2-dimethyl-5-phenyl-1,3-dioxolan-4-yl)tetrahydro-2H-pyran-2-ol (26)



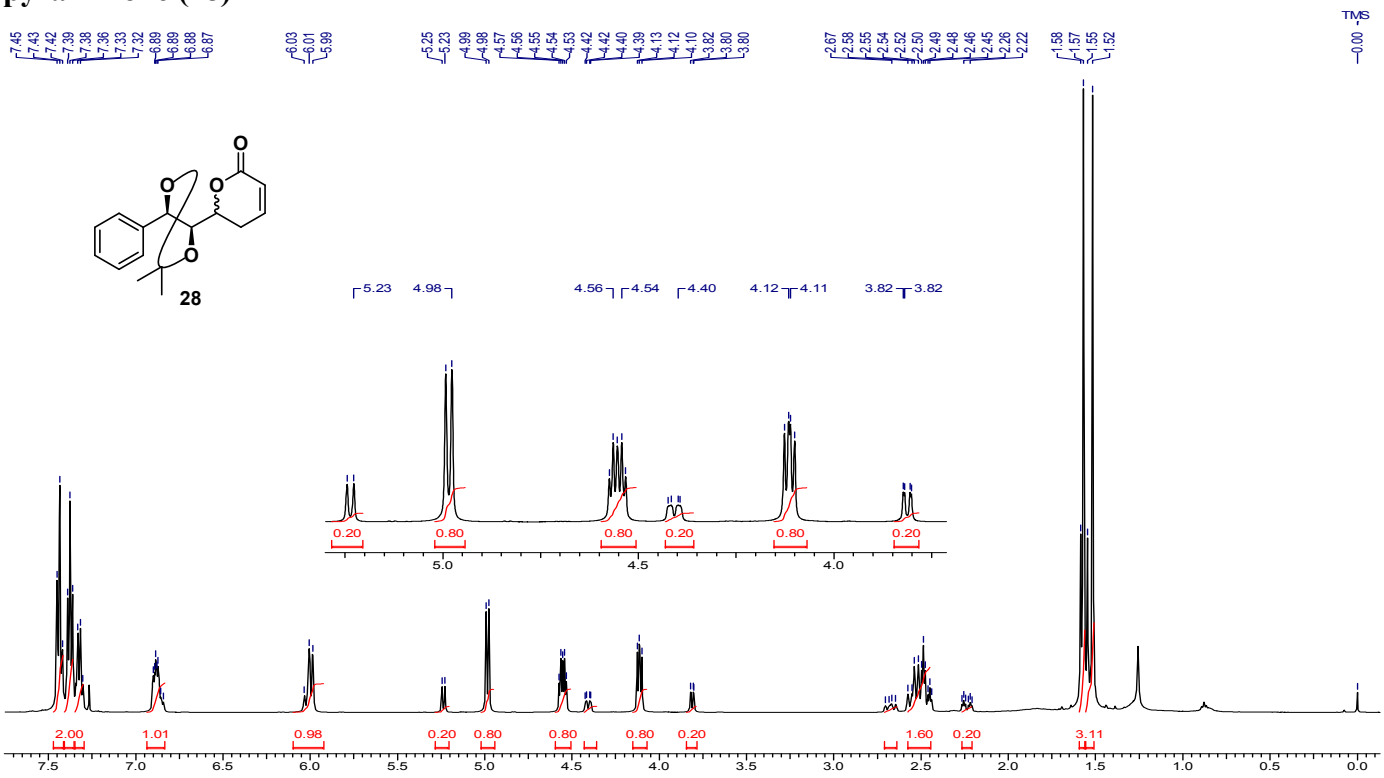
^{1}H NMR of 6-(2,2-dimethyl-5-phenyl-1,3-dioxolan-4-yl)tetrahydro-2H-pyran-2-one (27)



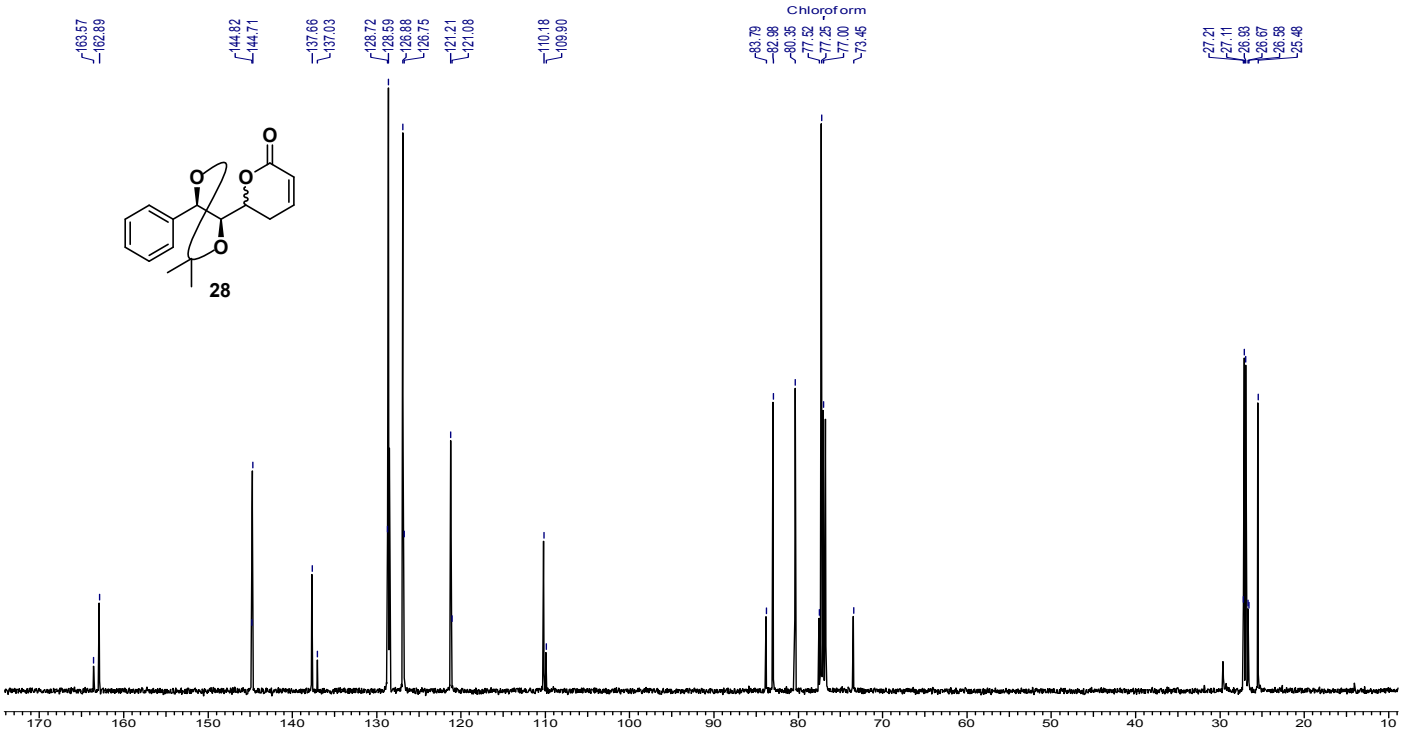
^{13}C NMR of 6-(2,2-dimethyl-5-phenyl-1,3-dioxolan-4-yl)tetrahydro-2H-pyran-2-one (27)



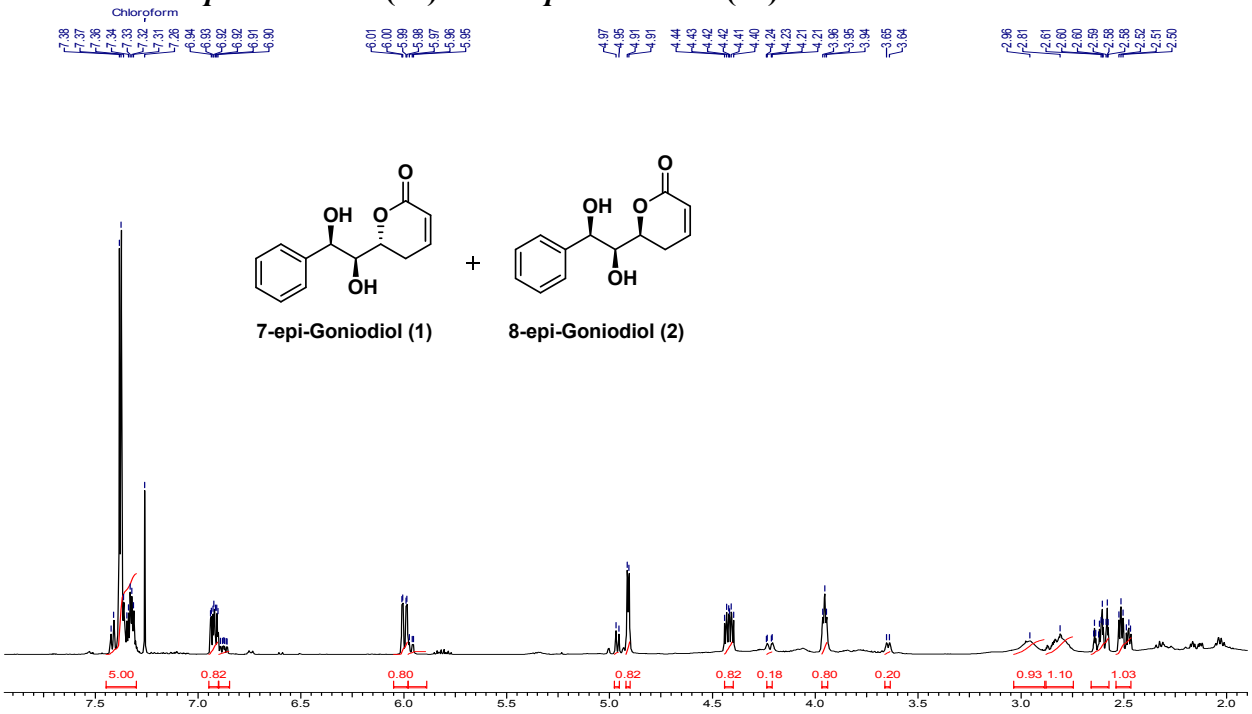
^{1}H NMR of (6*R*)-6-[(4*S*, 5*S*)-2,2-dimethyl-5-phenyl-1,3-dioxolan-4-yl]-5,6-dihydro-2*H*-pyran-2-one (28)



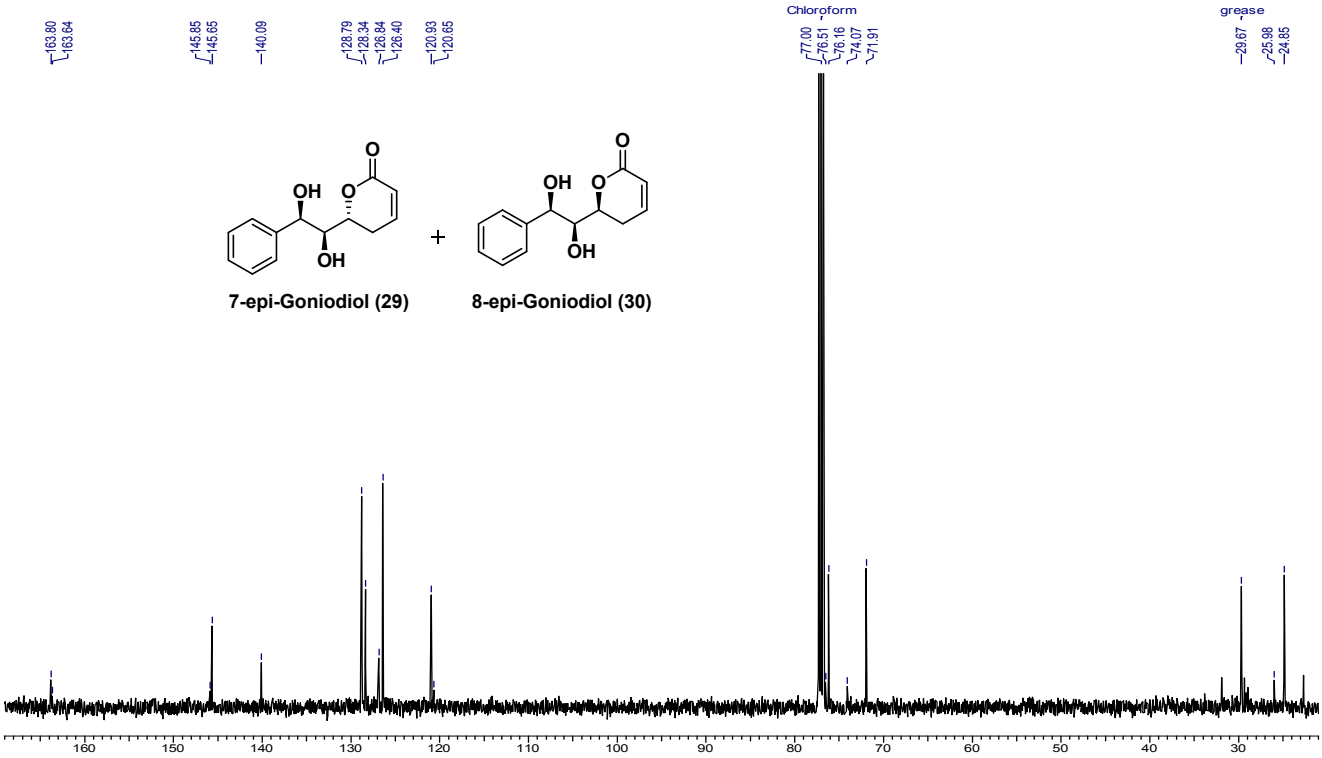
^{13}C NMR of (6*R*)-6-[(4*S*, 5*S*)-2,2-dimethyl-5-phenyl-1,3-dioxolan-4-yl]-5,6-dihydro-2*H*-pyran-2-one (28)



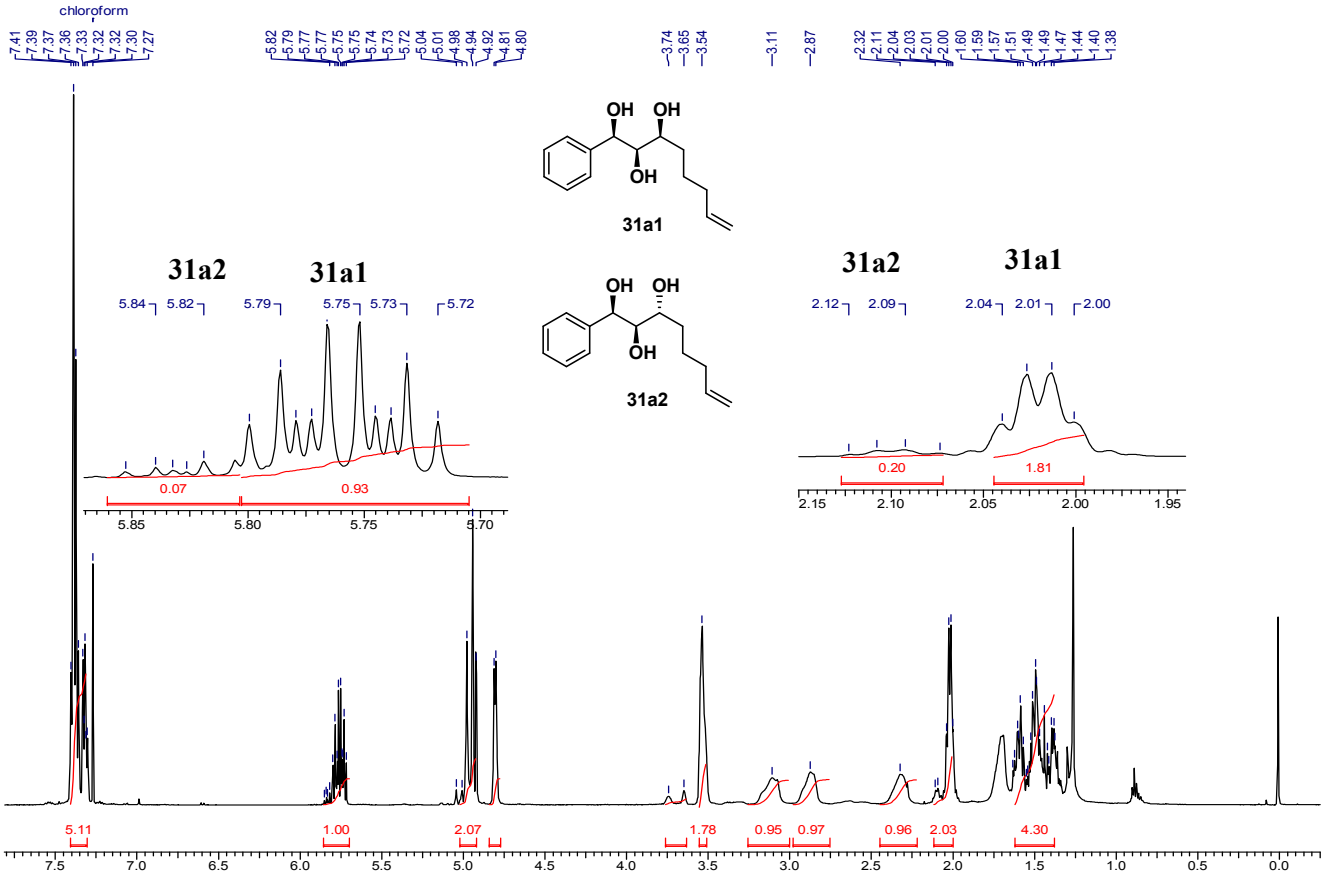
^{1}H NMR of 7-*epi*-Goniodiol (29) and 8-*epi*-Goniodiol (30)



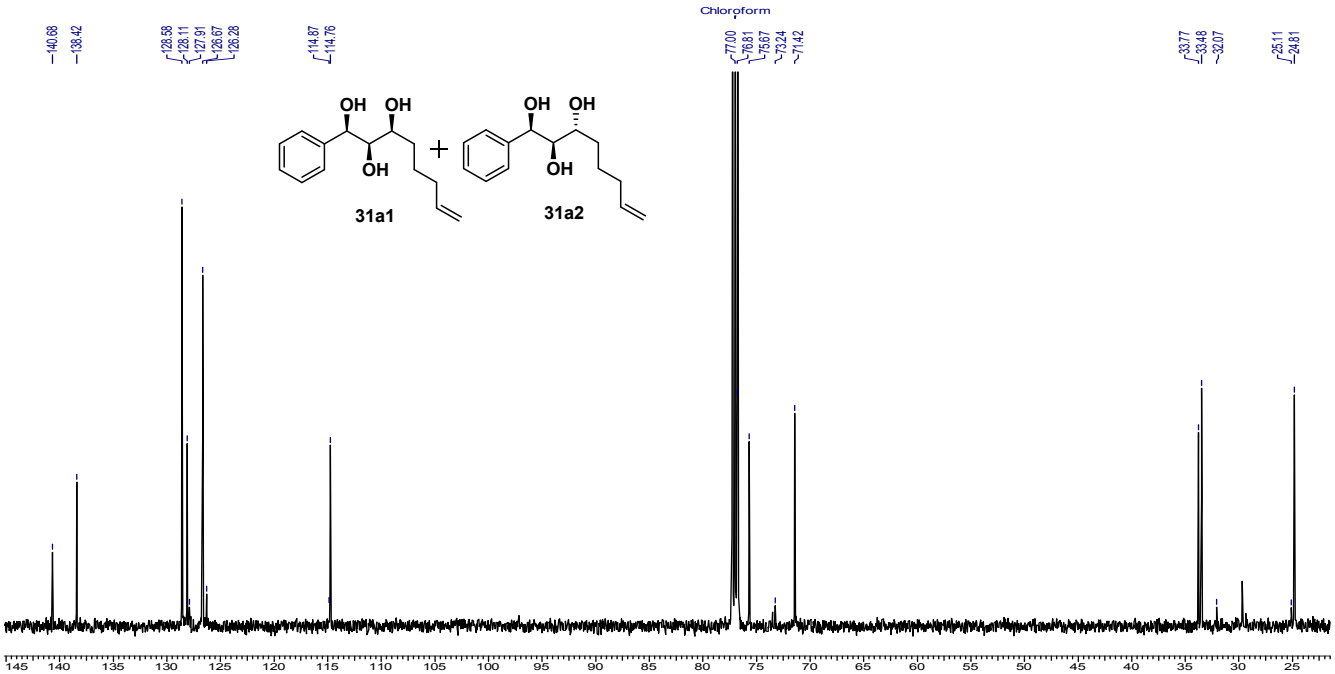
^{13}C NMR of 7-*epi*-Goniodiol (29) and 8-*epi*-Goniodiol (30).



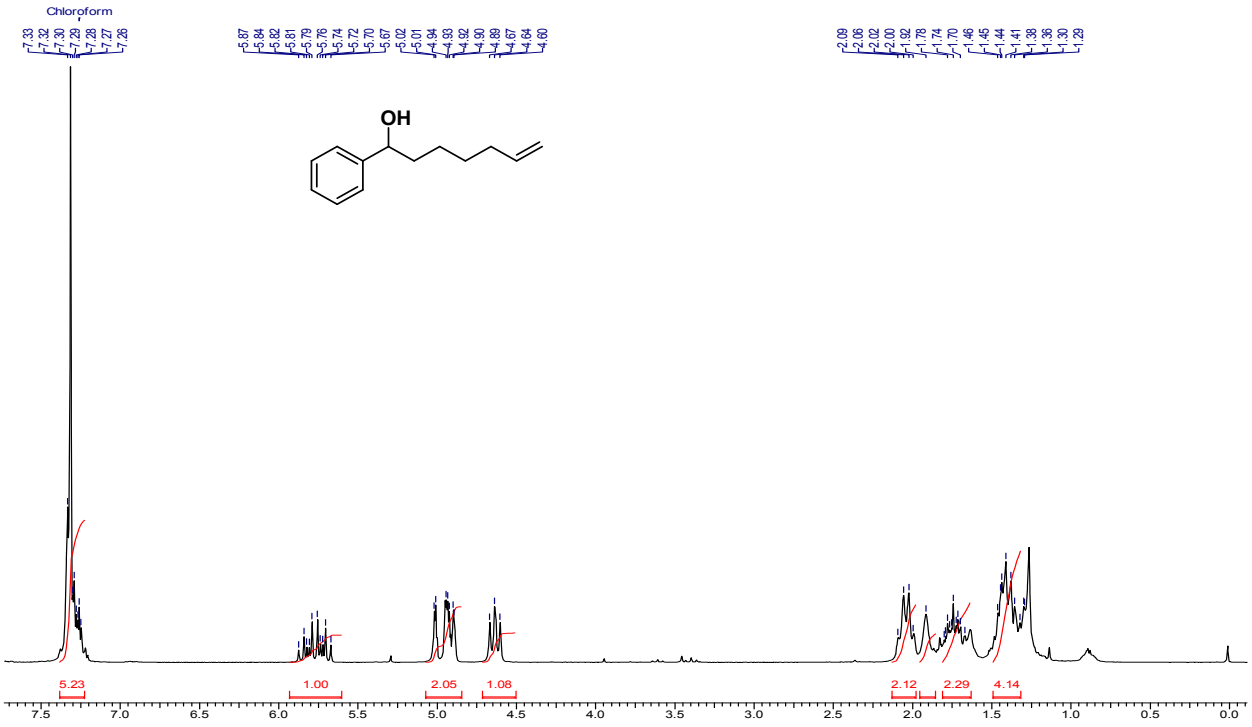
^{1}H NMR of (31a1): (31a2):



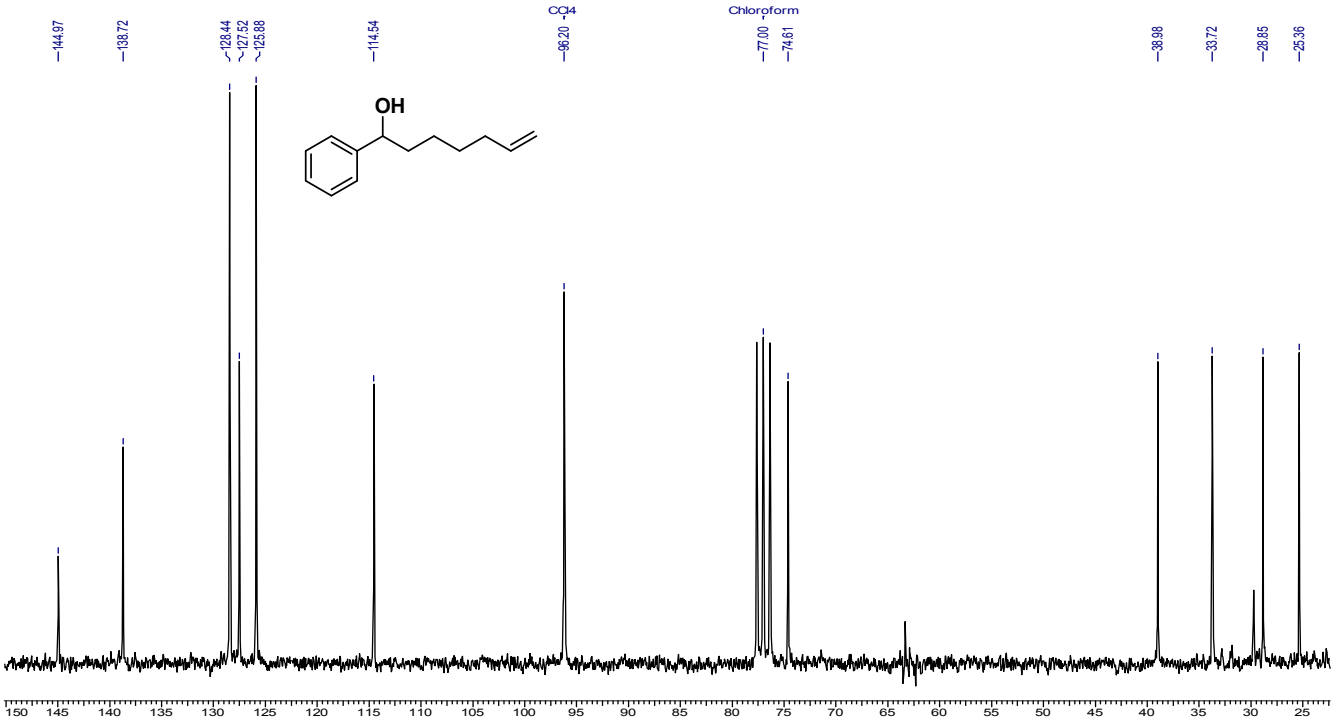
^{13}C NMR of (34a1): (31a2):



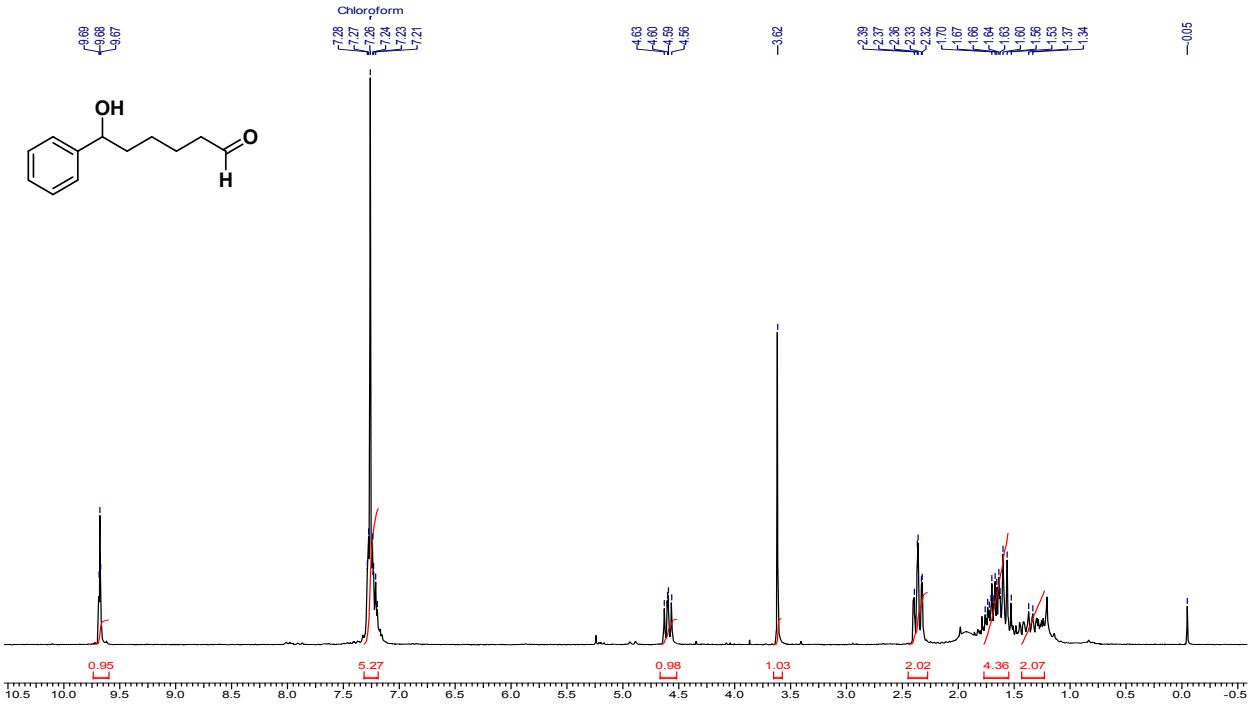
^{1}H NMR of 1−phenylhept−6−en−1−ol (32)



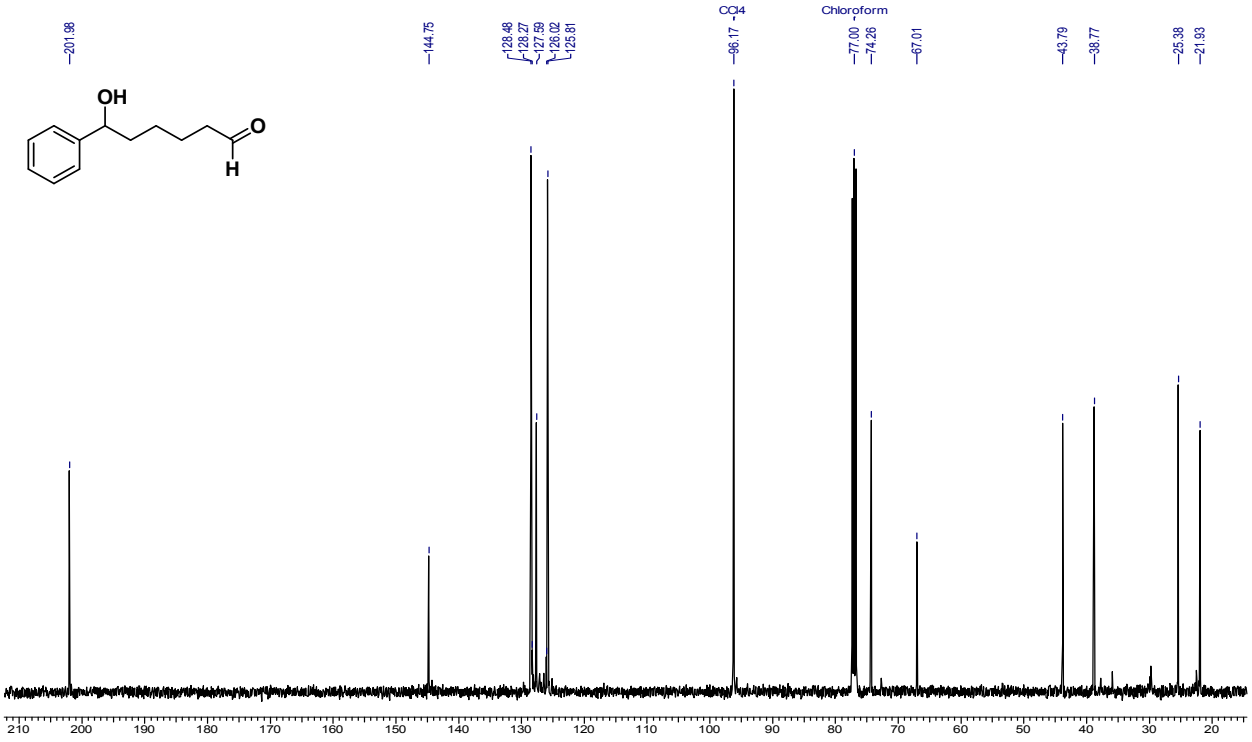
^{13}C NMR of 1−phenylhept−6−en−1−ol (32)



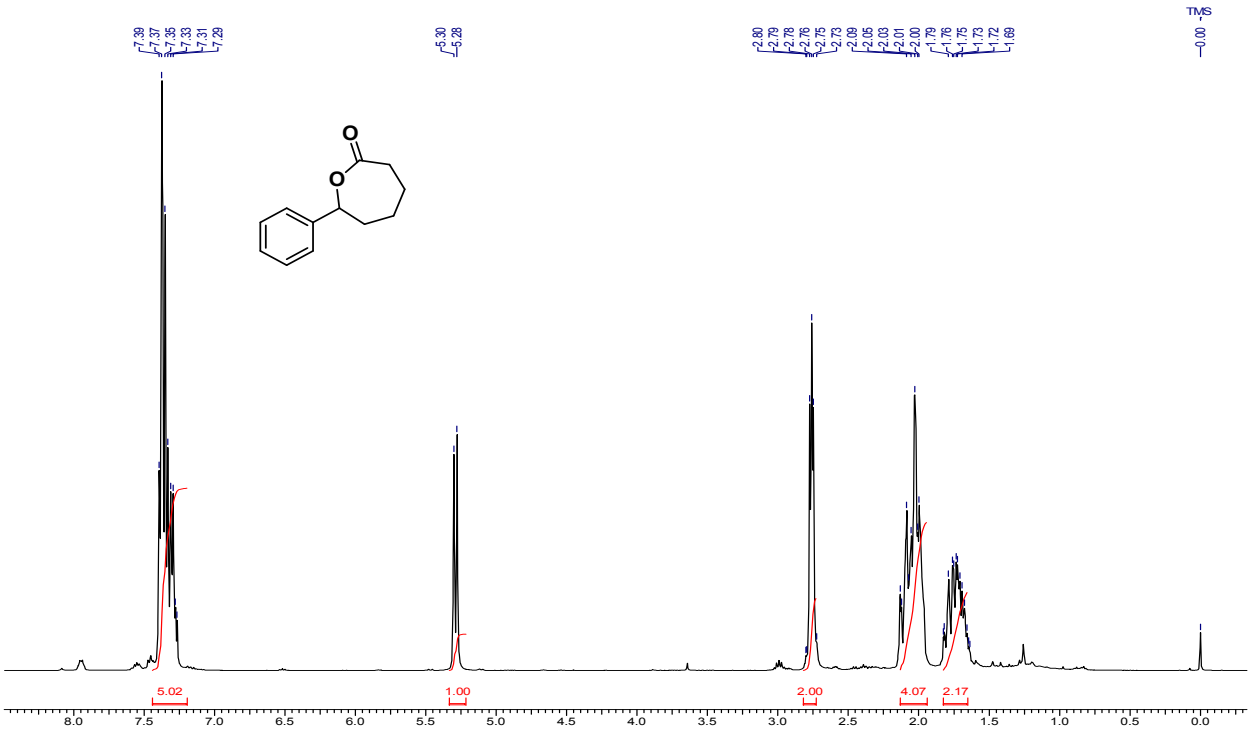
^{1}H NMR of 6−hydroxy−6−phenylhexanal (33):



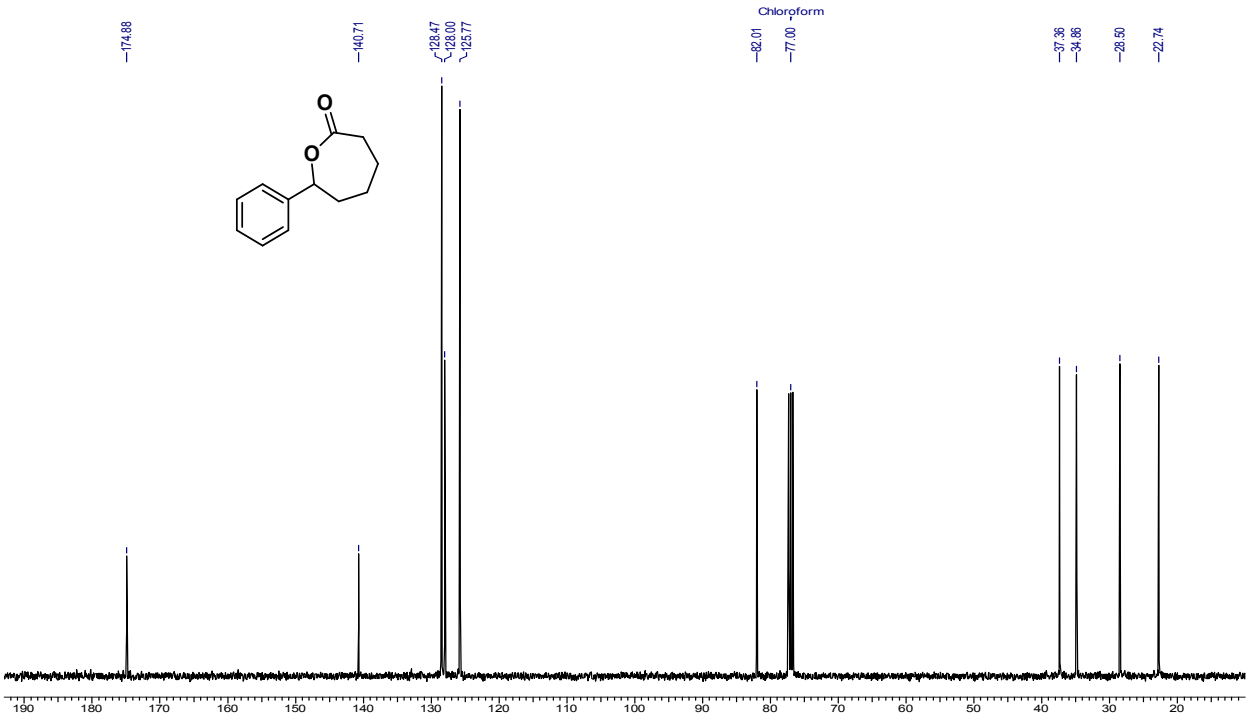
^{13}C NMR of 6−hydroxy−6−phenylhexanal (33):



^{1}H NMR of 7−phenyloxepan−2−one (34):

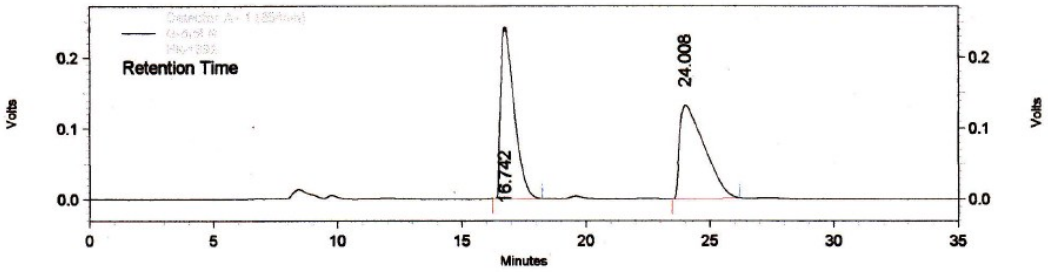


^{13}C NMR of 7−phenyloxepan−2−one (34):



VII. HPLC of racemic 37

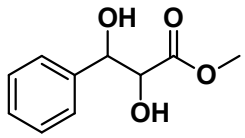
Shimadzu CLASS-VP V6.12 SP5
Method Name: C:\CLASS-VP\Data\Dr. CHAVAN S. P\PAPAL FH10 % IPAPE
Data Name: C:\CLASS-VP\Data\Dr. CHAVAN S. P\Hk-1392
User: System
Acquired: 10/29/12 4:40:31 PM
Printed: 10/29/12 5:57:11 PM
Sample Name G-diol R



Detector A - 1 (254nm)

Retention Time	C Area	Area %
16.742	9082318	50.033
24.008	9070370	49.967
Totals	18152688	100.000

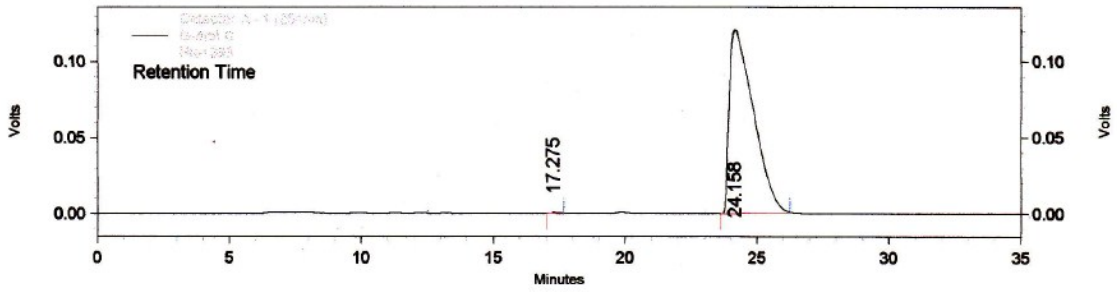
Project Leader : Dr.S.P.Chavan
Column : Chiralcel OJ-H (250x4.6 mm)
Mobile Phase :IPA: Pet ether (30:70)
Wavelength :254nm
Flow Rate :0.5 ml/min(36kgf)
conc. : 1mg/1.0 mL
Inj vol- :20ul



Racemic

HPLC of (-)- 37

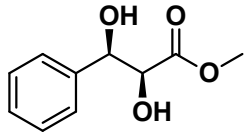
Shimadzu CLASS-VP V6.12 SP5
Method Name: C:\CLASS-VP\Data\Dr. CHAVAN S. P\PAPAL FH10 % IPAPE
Data Name: C:\CLASS-VP\Data\Dr. CHAVAN S. P\Hk-1393
User: System
Acquired: 10/29/12 5:16:17 PM
Printed: 10/29/12 6:22:08 PM
Sample Name G-diol C



Detector A - 1 (254nm)

Retention Time	C Area	Area %
17.275	8428	0.110
24.158	7664366	99.890
Totals	7672794	100.000

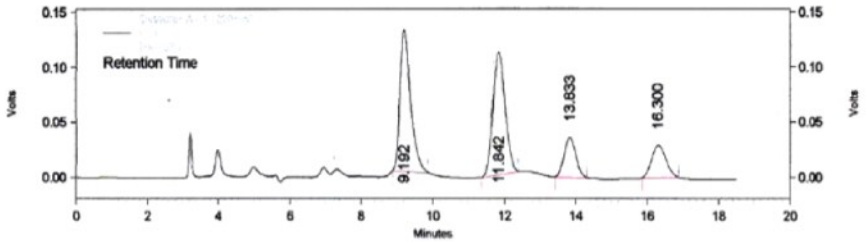
Project Leader : Dr.S.P.Chavan
Column : Chiralcel OJ-H (250x4.6 mm)
Mobile Phase :IPA: Pet ether (30:70)
Wavelength :254nm
Flow Rate :0.5 ml/min(36kgf)
conc. : 1mg/1.0 mL
Inj vol- :20ul



(27) catalyst $(DHQD)_2PHAL$

HPLC of racemic 11

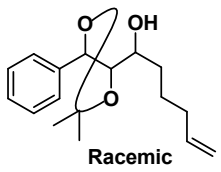
Shimadzu CLASS-VP V6.12 SP5
Method Name: C:\CLASS-VP\Method ch 2.met
Data Name: C:\CLASS-VP\Data\Dr. CHAVAN S. P\Hk-1558
User: System
Acquired: 12/15/15 4:16:30 PM
Printed: 12/15/15 5:28:09 PM
Sample Name G-R



Detector A - 1 (220nm)

Retention Time	C Area	Area %
9.192	1334927	38.785
11.842	1296528	37.669
13.833	406330	11.806
16.300	404068	11.740
Totals	3441853	100.000

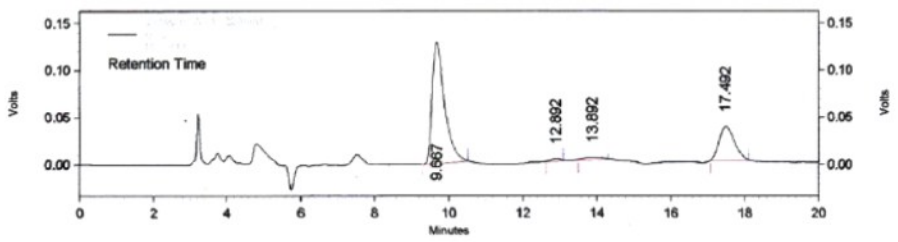
Project Leader :Dr.S. P. Chavan
Column :Chiralpak AD-H (250 X4.6mm)
Mobile Phase :IPA: Pet Ether (01:99)
Flow Rate : 1.0ml/min (515PSI)
Wavelength : 220nm
Con. : 1mg /1.0ml
Inject vol. :5ul



Racemic

HPLC of chiral 11

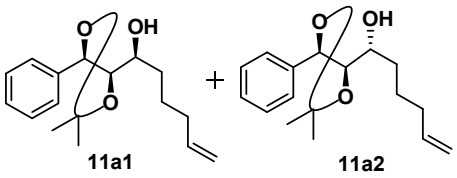
Shimadzu CLASS-VP V6.12 SP5
Method Name: C:\CLASS-VP\Method ch 2.met
Data Name: C:\CLASS-VP\Data\Dr. CHAVAN S. P\Hk-1559
User: System
Acquired: 12/15/15 4:35:35 PM
Printed: 12/15/15 5:24:33 PM
Sample Name G-C



Detector A - 1 (220nm)

Retention Time	C Area	Area %
9.667	1502476	73.385
12.892	14334	0.700
13.892	27732	1.355
17.492	502854	24.561
Totals	2047396	100.000

Project Leader :Dr.S. P. Chavan
Column :Chiralpak AD-H (250 X4.6mm)
Mobile Phase :IPA: Pet Ether (01:99)
Flow Rate : 1.0ml/min (515PSI)
Wavelength : 220nm
Con. : 1mg /1.0ml
Inject vol. :5ul

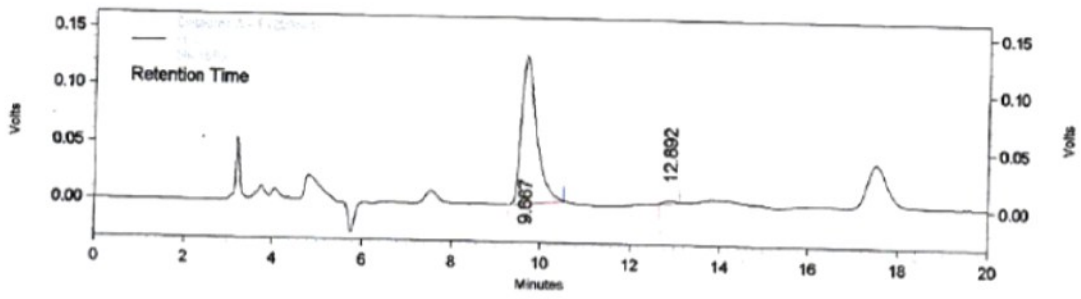


11a1 + **11a2**

dr- 11a1:11a2 (7:3)

HPLC of chiral 11

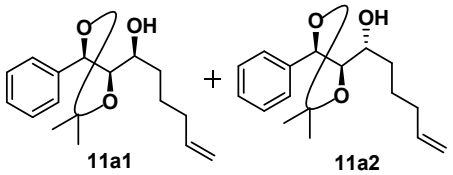
Shimadzu CLASS-VP V6.12 SP5
Method Name: C:\CLASS-VP\Method ch 2.met
Data Name: C:\CLASS-VP\Data\Dr. CHAVAN S. P\Hk-1559
User: System
Acquired: 12/15/15 4:35:35 PM
Printed: 12/15/15 5:25:38 PM
Sample Name G-C



Detector A - 1 (220nm)

Retention Time	C Area	Area %
9.667	1502476	99.055
12.892	14334	0.945
Totals	1516810	100.000

Project Leader :Dr.S. P. Chavan
Column :Chiralpak AD-H (250 X4.6mm)
Mobile Phase :IPA: Pet Ether (01:99)
Flow Rate : 1.0ml/min (515PSI)
Wavelength : 220nm
Con. : 1mg /1.0ml
Inject vol. :5ul



11a1 **11a2**

dr- 11a1:11a2 (7:3)

VIII. Details of DFT calculations

All the calculations in this study have been performed with density functional theory (DFT), with the aid of the Turbomole 6.4 suite of programs, using the PBE functional.[17] The TZVP[18] basis set has been employed. The resolution of identity (RI),[19] along with the multipole accelerated resolution of identity (marij)[20] approximations have been employed for an accurate and efficient treatment of the electronic Coulomb term in the DFT calculations. Solvent correction were incorporated with optimization calculations using the COSMO model,[21] with tetrahydrofuran (ε = 7.58) as the solvent. The values reported are ΔG values, with zero point energy corrections, internal energy and entropic contributions included through frequency calculations on the optimized minima with the temperature taken to be 298.15 K. Harmonic frequency calculations were performed for all stationary points to confirm them as a local minima or transition state structures.

PBE/TZVP optimized geometries for all the reactants, products and transition states

I

C	2.300535	-2.211086	0.423967
C	1.493407	-1.384287	-0.361268
C	0.027894	-1.198902	-0.042400
C	-0.146020	0.060368	0.855235
C	-2.928830	1.710190	-1.812385
Mg	-3.242609	0.244628	-0.282368
O	-1.390737	0.218708	1.333441
C	-1.572346	1.258658	2.370198
H	-0.920589	1.018239	3.216258
C	-1.797906	-2.697774	0.067789
O	-0.527492	-2.311710	0.664686
H	-0.869823	-3.790696	-1.573920
C	-1.617380	-3.941435	-0.785462
H	-1.275828	-4.763823	-0.143686
H	-2.575573	-4.223274	-1.241704
C	-2.839369	-2.854705	1.148659
H	-2.564286	-3.705215	1.785191
H	-2.902839	-1.954314	1.770319
H	-3.821973	-3.058100	0.703503
H	-1.328481	2.242424	1.954986
H	-2.629386	1.185116	2.642455
Br	-5.115245	0.101616	1.326589

H	-1.007868	-0.060122	-1.673574
C	-0.870815	-1.080192	-1.291026
C	2.084645	-0.653613	-1.411957
C	3.454599	-0.747059	-1.657518
Br	4.320049	1.653501	1.427509
C	3.670015	-2.324836	0.177157
H	4.268406	-2.981287	0.807131
C	6.449459	-2.419077	-0.364377
H	6.429881	-2.099053	0.688812
H	6.172709	-3.482425	-0.439590
H	7.453387	-2.271168	-0.775112
O	5.580925	-1.600558	-1.169279
H	1.854073	-2.784103	1.237171
H	3.915059	-0.187956	-2.473286
Mg	2.319579	1.712064	-0.004790
C	1.584394	2.913340	-1.609865
H	2.263514	2.720334	-2.462639
H	1.757681	3.971825	-1.336411
C	0.124874	2.747310	-2.066278
H	-0.084768	3.358475	-2.967691
H	1.478319	-0.030680	-2.075697
C	-0.905004	3.136541	-0.998433
H	-0.774108	2.481691	-0.119271
H	-2.374751	1.305321	-2.680103
C	-2.374378	3.100865	-1.443462
H	-3.961553	1.840098	-2.192353
H	-2.987431	3.534417	-0.633630
H	-2.476947	3.801621	-2.296899
H	-0.658238	4.153802	-0.644579
H	-0.502473	-1.731103	-2.094536
H	-0.056995	1.704862	-2.390327
C	4.259589	-1.580364	-0.858234
O	0.750400	0.859240	1.111716
O	-2.141124	-1.544151	-0.787733

II (TS)

C	-5.429355	-1.008644	0.677974
C	-5.992582	-1.000318	-0.599205
C	-7.457327	-1.288867	-0.822335

C	-8.186249	0.089668	-1.246278
C	-8.606262	-0.171229	-3.550790
Mg	-10.171990	-1.110030	-2.288315
O	-9.529357	0.115680	-0.754809
C	-10.069981	1.431316	-0.431634
H	-9.458547	1.891873	0.351518
C	-9.034067	-2.827403	0.030060
O	-8.088870	-1.778503	0.372760
H	-7.521134	-4.405420	0.028448
C	-8.495489	-4.177709	0.476495
H	-8.368930	-4.157869	1.566688
H	-9.210107	-4.969935	0.217966
C	-10.411300	-2.551827	0.597375
H	-10.375903	-2.663632	1.688453
H	-10.751858	-1.533955	0.379258
H	-11.129714	-3.281885	0.200822
H	-10.089513	2.070694	-1.322885
H	-11.085230	1.238187	-0.070787
Br	-12.530206	-1.203017	-2.794277
H	-7.665671	-2.173582	-2.860715
C	-7.716606	-2.429435	-1.802239
C	-5.180417	-0.638730	-1.693512
C	-3.848171	-0.273358	-1.503645
Br	-4.918733	3.039287	0.475943
C	-4.093032	-0.655176	0.880666
H	-3.694082	-0.655680	1.893864
C	-1.452991	0.322535	1.202152
H	-2.046830	1.047339	1.780192
H	-1.397399	-0.635390	1.742731
H	-0.442223	0.713129	1.045109
O	-2.005952	0.146567	-0.115029
H	-6.046328	-1.283916	1.533044
H	-3.218606	0.005631	-2.350254
Mg	-5.819937	2.100172	-1.644436
C	-5.790091	2.872703	-3.638597
H	-4.788790	2.774676	-4.096966
H	-5.967509	3.963449	-3.558117
C	-6.854045	2.245613	-4.559899
H	-6.826458	2.680654	-5.578687
H	-5.576009	-0.658495	-2.712945

C	-8.301558	2.366571	-4.026222
H	-8.276365	2.626120	-2.956926
H	-7.511618	-0.183692	-3.583204
C	-9.160470	1.101943	-4.219378
H	-8.877554	-1.057132	-4.176724
H	-10.192429	1.317689	-3.884914
H	-9.253686	0.911018	-5.305348
H	-8.811620	3.208470	-4.522036
H	-7.056789	-3.280942	-1.597556
H	-6.610368	1.178291	-4.706984
C	-3.299069	-0.262457	-0.206663
O	-7.561764	1.164072	-1.208523
O	-9.093141	-2.763049	-1.451672

III

C	1.593707	-1.390546	0.114453
C	0.609468	-1.239033	-0.873647
C	-0.821927	-1.000927	-0.453858
C	-0.991013	0.573838	-0.146596
C	-0.898427	1.354198	-1.472879
Mg	-3.149403	-1.054776	1.072071
O	-2.523979	0.634999	0.302512
C	-2.905593	1.859671	0.979269
H	-2.024661	2.284079	1.478694
C	-1.643837	-3.021491	0.418280
O	-1.083771	-1.726248	0.820072
H	-0.222073	-3.577401	-1.158889
C	-0.675048	-3.976924	-0.247813
H	0.130316	-4.217670	0.457379
H	-1.215921	-4.900181	-0.493248
C	-2.302381	-3.658825	1.623449
H	-1.527872	-3.945543	2.344404
H	-3.021480	-3.017581	2.166094
H	-2.853678	-4.552486	1.308160
H	-3.326772	2.569318	0.256689
H	-3.668556	1.614548	1.731548
Br	-5.124384	-1.047898	2.461323
H	-2.638857	-0.869484	-1.762025
C	-1.924214	-1.608106	-1.385440

C	1.015946	-1.218014	-2.219135
C	2.359875	-1.318047	-2.561162
Br	2.514963	0.446447	3.277982
C	2.950691	-1.487390	-0.214202
H	3.678606	-1.600045	0.588707
C	5.667511	-1.562058	-0.996233
H	5.635375	-0.682986	-0.333183
H	5.584603	-2.483023	-0.397957
H	6.610744	-1.568968	-1.552108
O	4.632378	-1.494944	-1.993639
H	1.298839	-1.469517	1.162761
H	2.670984	-1.291813	-3.606526
Mg	1.689401	1.274375	1.046531
C	2.634913	2.696240	-0.235624
H	3.559618	2.300621	-0.694788
H	2.957837	3.549525	0.392932
C	1.670704	3.201209	-1.327023
H	2.092048	4.061158	-1.884294
H	0.282941	-1.108130	-3.021135
C	0.271448	3.607729	-0.792186
H	0.230973	3.435042	0.295833
H	0.049060	1.040025	-1.936391
C	-0.916656	2.894546	-1.461486
H	-1.696806	1.005924	-2.146103
H	-1.857011	3.267602	-1.031788
H	-0.939396	3.195146	-2.523629
H	0.118029	4.691814	-0.922969
H	-1.508837	-2.178205	-2.224140
H	1.550270	2.407994	-2.086117
C	3.342473	-1.433882	-1.561172
O	-0.243516	0.957428	0.852576
O	-2.676158	-2.509919	-0.502539

IV

Br	0.716731	1.741890	2.985334
Mg	0.800860	1.989565	0.510192
C	0.955169	3.405569	-1.127119
C	0.240356	2.824464	-2.345261
H	-0.268495	1.856302	-2.090585

C	0.772876	0.134124	-1.623228
O	1.587571	0.560172	-0.776886
C	1.203663	-0.006384	-3.054219
C	1.055352	2.504953	-3.611042
C	1.959881	1.265476	-3.509548
H	1.888036	-0.870746	-3.108145
H	0.353376	-0.226224	-3.715202
H	2.413924	1.059329	-4.490563
H	0.354835	2.349398	-4.450373
H	1.678673	3.375059	-3.876026
H	2.034075	3.538002	-1.316408
H	0.543201	4.392251	-0.863911
H	-1.845214	3.037801	-0.050687
C	-2.287327	0.928631	0.000462
H	-2.116496	2.366464	1.593861
H	-3.495217	2.631705	0.496046
C	-3.096358	-0.112744	0.763192
H	-2.778933	-0.128476	1.813989
H	-4.162257	0.146697	0.714372
H	-0.208446	-4.950923	-1.847402
C	-0.441011	-2.823809	-1.527838
C	-0.362542	-1.762886	-0.608105
O	-0.860815	0.568107	0.044672
C	0.031038	-2.033830	0.706165
C	0.317723	-3.338414	1.115007
H	0.101424	-1.217639	1.427613
C	0.235214	-4.392014	0.189732
O	0.505856	-5.698760	0.478501
H	0.606377	-3.518014	2.150069
C	0.907562	-6.017545	1.821305
H	1.081449	-7.098745	1.827080
H	0.114604	-5.767361	2.543805
H	1.837533	-5.493685	2.094267
H	-0.619742	3.456020	-2.624212
H	-1.607150	0.122279	-3.007973
C	-1.849120	-0.154218	-1.974133
O	-2.573399	0.935460	-1.397139
H	-2.448378	-1.078056	-1.977703
H	-0.729870	-2.639742	-2.565599
C	-0.595001	-0.332172	-1.068423

C	-0.147712	-4.124910	-1.136944
C	-2.440676	2.331831	0.544985
H	-2.954561	-1.117665	0.344862
H	2.785535	1.444677	-2.804845

V (TS)

Br	-11.193277	1.200920	1.828260
Mg	-9.762422	1.123976	-0.178511
C	-9.775868	2.156332	-2.186299
C	-9.246562	1.188563	-3.118322
H	-8.795111	0.183899	-2.442793
C	-7.885873	-0.281580	-1.520243
O	-7.880584	0.590077	-0.552052
C	-6.698095	-0.256659	-2.459983
C	-7.954722	1.413210	-3.917863
C	-6.657941	1.133461	-3.127488
H	-5.777058	-0.430182	-1.880489
H	-6.772801	-1.047748	-3.222757
H	-5.794659	1.198025	-3.805402
H	-7.972430	0.752658	-4.799504
H	-7.938975	2.450418	-4.287328
H	-9.172965	3.056739	-2.019438
H	-10.848985	2.363057	-2.291451
H	-11.979796	0.050551	-1.990896
C	-11.061137	-1.756328	-1.256644
H	-12.572196	-0.490854	-0.386201
H	-13.078543	-1.349197	-1.866999
C	-11.360337	-3.007130	-0.438797
H	-11.670932	-2.719317	0.574429
H	-12.172845	-3.571943	-0.915253
H	-5.376012	-4.634198	0.082753
C	-6.920177	-3.254852	-0.547850
C	-7.943144	-2.377051	-0.147973
O	-9.947215	-1.027043	-0.639224
C	-8.181986	-2.205694	1.219036
C	-7.439152	-2.903076	2.176551
H	-8.971893	-1.528439	1.547563
C	-6.424652	-3.780709	1.764650
O	-5.637999	-4.511665	2.612728

H	-7.660868	-2.752664	3.232618
C	-5.868774	-4.370425	4.023392
H	-5.143157	-5.032152	4.508392
H	-6.890070	-4.682873	4.294279
H	-5.699248	-3.333318	4.354607
H	-10.014228	0.634538	-3.677080
H	-8.674556	-2.114370	-3.341305
C	-9.182851	-2.390713	-2.408602
O	-10.567370	-2.054960	-2.561737
H	-9.049269	-3.469513	-2.231067
H	-6.697744	-3.398859	-1.608072
C	-8.694675	-1.568933	-1.183705
C	-6.168012	-3.950211	0.392611
C	-12.246809	-0.823426	-1.380750
H	-10.476292	-3.652730	-0.355408
H	-6.516856	1.894164	-2.344785

VI

Br	0.150482	3.083748	2.901954
Mg	0.520008	1.411122	1.184665
C	1.581032	3.750934	-1.917364
C	1.274109	3.537327	-3.203366
H	-0.069415	1.606238	-1.726293
C	0.424132	0.648714	-1.432992
O	1.369054	0.859804	-0.423184
C	1.088884	0.071409	-2.682652
C	1.471416	2.278140	-4.008181
C	2.090874	1.043605	-3.324983
H	1.615026	-0.851841	-2.389111
H	0.329844	-0.208947	-3.433771
H	2.656537	0.483199	-4.085428
H	0.498015	2.000053	-4.456574
H	2.095064	2.558137	-4.877252
H	1.983481	2.959113	-1.278298
H	1.405763	4.726468	-1.457486
H	-2.374616	2.894526	0.480785
C	-2.624827	0.764419	0.288569
H	-2.678695	2.046816	2.026865
H	-4.010404	2.288297	0.866987

C	-3.361508	-0.422542	0.900065
H	-3.098461	-0.518435	1.961891
H	-4.444855	-0.262517	0.815797
H	0.006264	-4.673299	-2.099235
C	-0.376997	-2.611342	-1.569437
C	-0.400792	-1.638171	-0.552461
O	-1.171059	0.510625	0.355308
C	-0.047841	-2.039231	0.738996
C	0.326765	-3.356476	1.027356
H	-0.102871	-1.327271	1.563349
C	0.352105	-4.308533	-0.000985
O	0.696094	-5.623508	0.163014
H	0.584167	-3.623665	2.051732
C	1.054937	-6.057051	1.483968
H	1.289848	-7.122788	1.391110
H	0.218349	-5.925107	2.189050
H	1.940269	-5.516773	1.856129
H	0.847910	4.368429	-3.780492
H	-1.815785	0.307737	-2.764404
C	-2.041031	-0.078899	-1.761552
O	-2.857397	0.900686	-1.106258
H	-2.568096	-1.041963	-1.852748
H	-0.650066	-2.343829	-2.592345
C	-0.768914	-0.209926	-0.882649
C	-0.006708	-3.924899	-1.304896
C	-2.936052	2.082525	0.961107
H	-3.097385	-1.360249	0.394715
H	2.823623	1.354379	-2.563944

VII (TS)

Br	-11.829848	1.974181	1.886558
Mg	-10.521472	1.343445	-0.071040
C	-10.297249	2.562213	-1.872617
C	-8.887699	0.292349	-1.462503
O	-8.705116	0.455425	-0.204631
O	-11.113022	-0.491461	-0.925861
C	-12.349637	-0.724512	-1.699112
C	-13.434287	0.190078	-1.173774
H	-14.364996	0.002151	-1.724257

H	-13.154371	1.242175	-1.318562
H	-13.611436	0.001894	-0.107425
C	-9.423173	-2.571578	-0.120933
H	-13.628424	-2.375211	-2.214308
H	-12.912941	-2.484071	-0.579834
H	-9.952374	-1.977967	0.623854
C	-12.719623	-2.201446	-1.622970
H	-11.915619	-2.840473	-2.009249
C	-8.834572	-3.776489	0.264037
H	-8.915000	-4.098436	1.301509
C	-7.592779	-6.227302	0.935677
H	-7.104519	-5.526340	1.631419
H	-8.632757	-6.401882	1.255247
H	-7.047555	-7.176956	0.930705
O	-7.538068	-5.741839	-0.416647
C	-8.150379	-4.550734	-0.687121
C	-8.070558	-4.101558	-2.016810
C	-8.668506	-2.899632	-2.386104
C	-9.364203	-2.121022	-1.445401
H	-10.612195	-1.742191	-3.683436
C	-10.637648	-0.742454	-3.223304
H	-10.173174	-0.021416	-3.899423
C	-9.983958	-0.775483	-1.813809
H	-8.585742	-2.576957	-3.426374
H	-7.535823	-4.708670	-2.749145
C	-7.714574	0.527538	-2.381760
H	-6.976462	1.063173	-1.766272
H	-7.283473	-0.473823	-2.575984
H	-11.387185	2.762584	-1.766854
H	-9.769832	3.314106	-1.245270
C	-9.925484	2.806959	-3.328236
H	-10.490784	2.120359	-3.982467
H	-10.250330	3.821572	-3.630817
C	-8.427060	2.690560	-3.637160
H	-7.855500	3.261128	-2.882607
H	-8.230187	3.180769	-4.605157
C	-7.876325	1.264863	-3.720396
H	-8.478291	0.679437	-4.432961
H	-6.867313	1.303424	-4.160817
O	-11.985864	-0.311063	-3.009690

VIII

O	-9.149216	-3.180166	-1.140693
C	-8.300197	-2.651997	-2.168274
C	-7.761646	-1.299295	-1.607022
O	-8.226501	-1.317702	-0.230796
C	-8.631906	-2.654014	0.095124
C	-6.244434	-1.200932	-1.644004
C	-5.483159	-1.726759	-2.701811
C	-4.097455	-1.583385	-2.740733
C	-3.432098	-0.899879	-1.711223
C	-4.174645	-0.365201	-0.647404
C	-5.564655	-0.519189	-0.628996
O	-2.066698	-0.811009	-1.831784
C	-1.355060	-0.114298	-0.800064
C	-9.766193	-2.584933	1.101386
C	-7.447312	-3.487820	0.594820
O	-7.959162	1.086654	-1.555850
H	-3.513828	-1.998547	-3.564709
H	-5.970352	-2.255737	-3.523625
H	-6.142926	-0.102671	0.194495
H	-3.685794	0.168949	0.167264
H	-7.475501	-3.349408	-2.386318
H	-8.910528	-2.536856	-3.071774
H	-0.298074	-0.162291	-1.084251
H	-1.492670	-0.598277	0.180961
H	-1.670078	0.940263	-0.736591
H	-10.140519	-3.594254	1.318664
H	-10.584492	-1.975351	0.696061
H	-9.410231	-2.135340	2.037858
H	-7.775121	-4.511998	0.821265
H	-7.033730	-3.035642	1.506600
H	-6.647862	-3.527006	-0.157429
Mg	-8.643585	2.687515	-0.961060
Br	-10.336605	4.395916	-1.270429
C	-8.417467	-0.019135	-2.273514
C	-9.983100	-0.131632	-2.225877
C	-7.964271	0.118528	-3.750999
C	-10.647558	-0.356103	-3.587865

H	-10.366274	0.819536	-1.814312
C	-8.805370	1.177082	-4.471192
H	-8.037561	-0.843161	-4.286769
C	-10.293695	0.762051	-4.583849
H	-10.334808	-1.330822	-3.997652
H	-8.384521	1.387927	-5.466031
H	-10.523525	0.426314	-5.607702
H	-6.903333	0.404691	-3.749260
H	-8.720224	2.118363	-3.901236
H	-10.936385	1.637023	-4.392365
H	-11.740293	-0.421244	-3.464226
H	-10.287329	-0.909086	-1.511143

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