Electronic appendix for:

Novel C-C Bond Formation Strategies for Access to Secondary and Tertiary Amides Enabled by New Synthetic Technologies

Jason D. Williams

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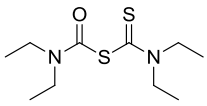
1. NMR spectra of synthesised compounds

1.1. NMR Spectra for compounds synthesised in Chapter 1

1.1.1. Analysis of radical precursors

_N,N_-Diethylcarbamoyl _N,N_-diethyldithiocarbamate



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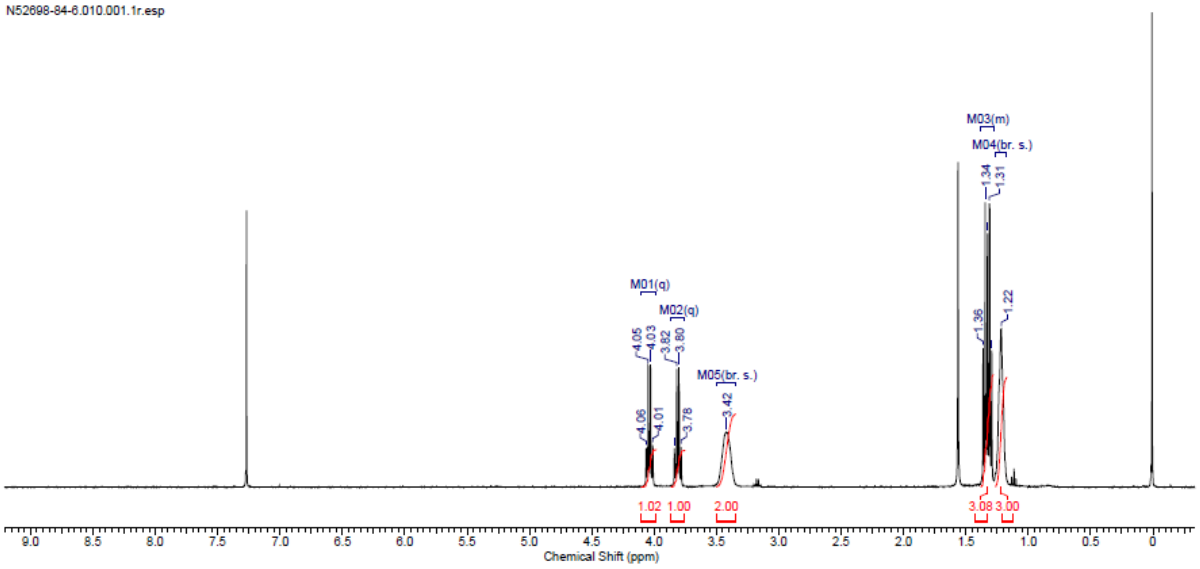
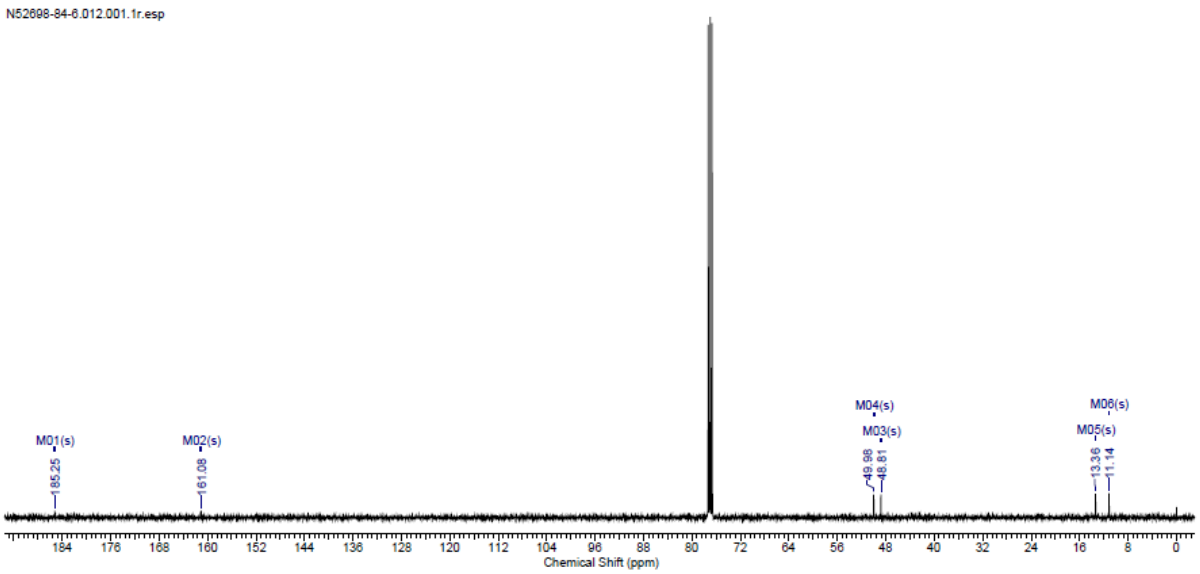
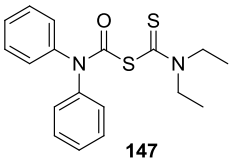




N,N-Diphenylcarbamoyl *N,N*-diethyldithiocarbamate



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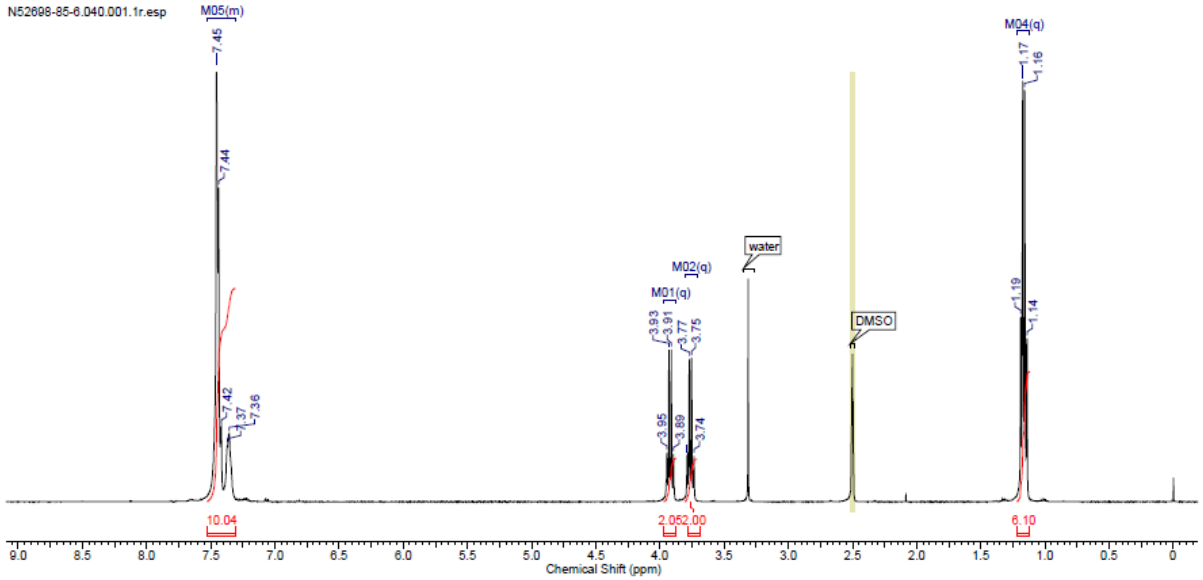
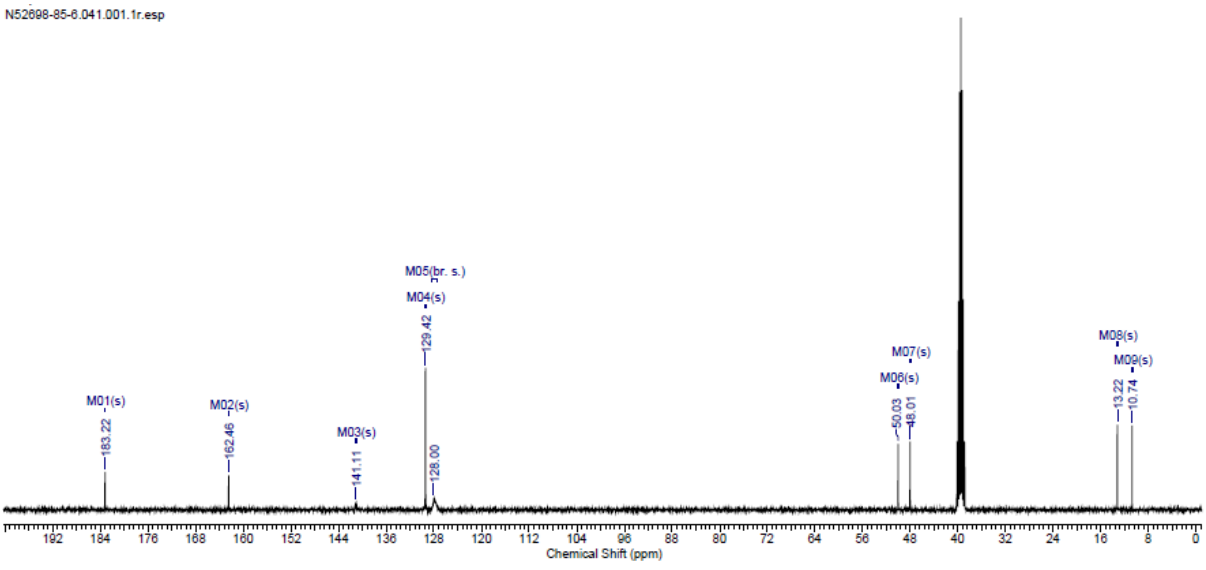
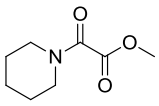




Methyl 2-oxo-2-(piperidin-1-yl)acetate



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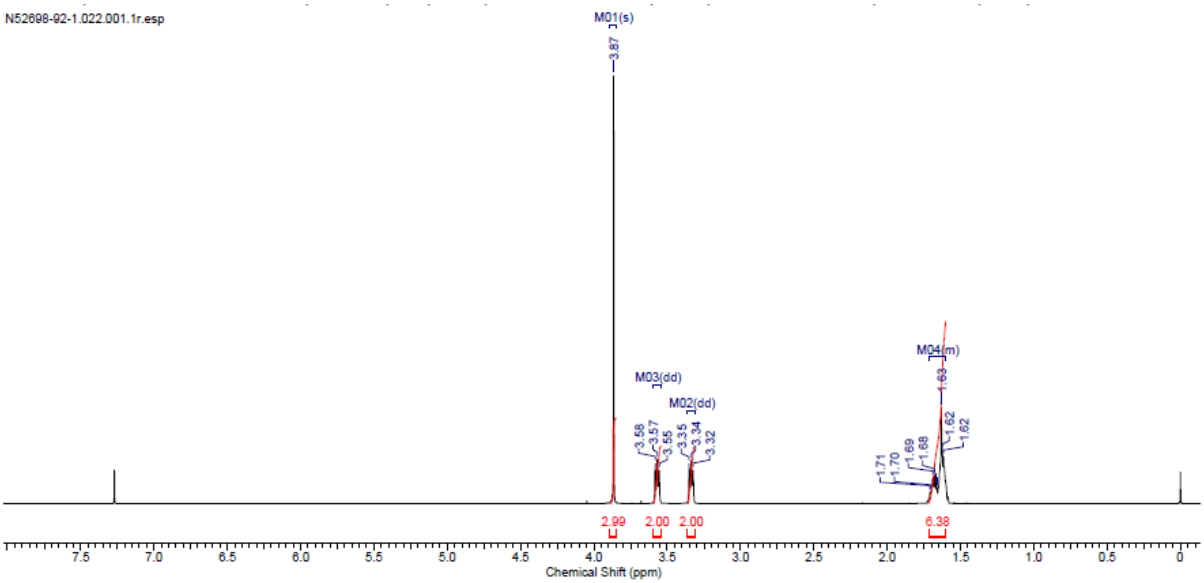

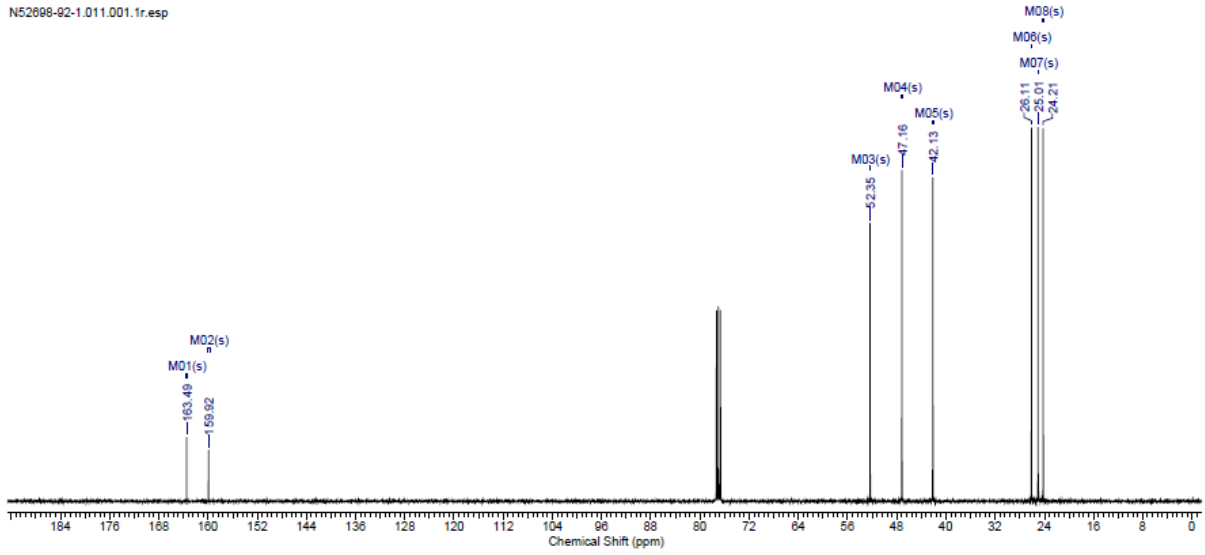

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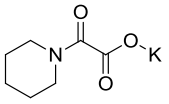

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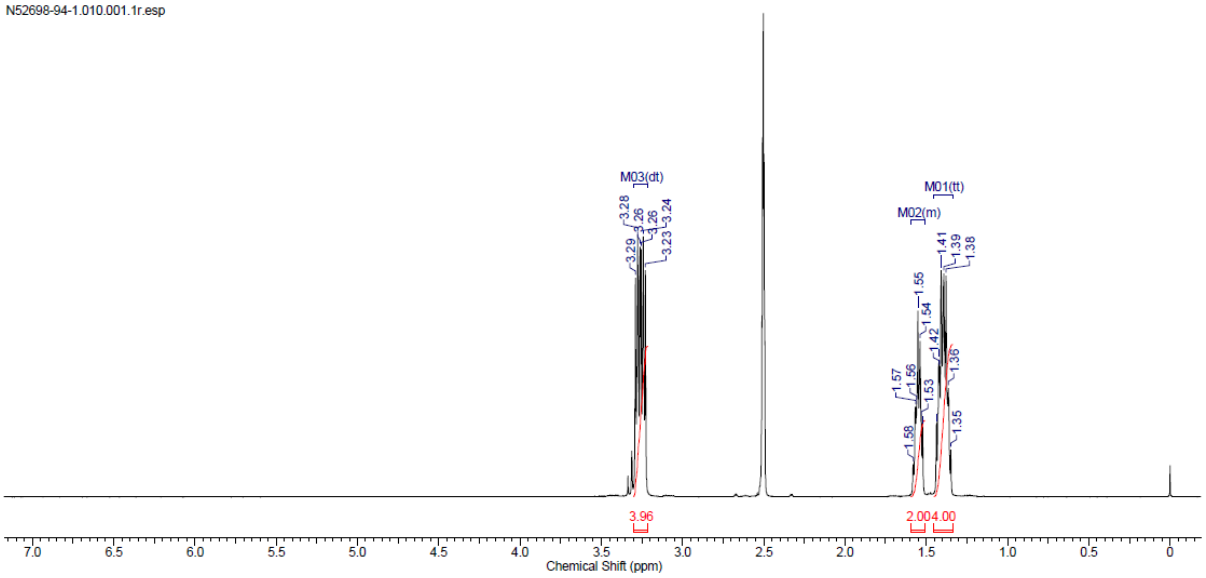
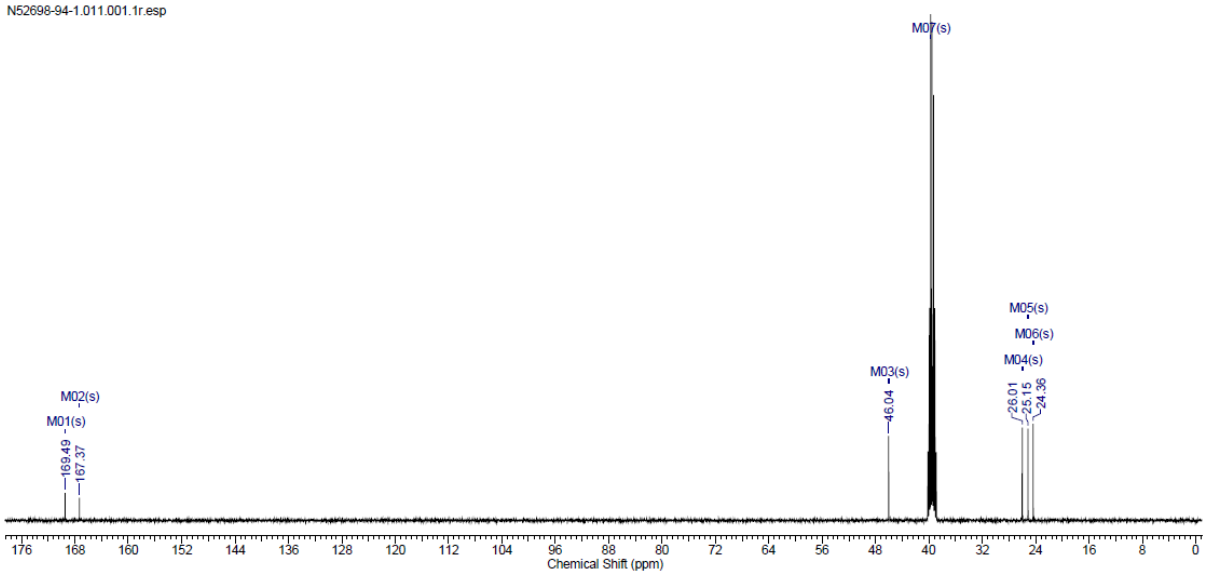
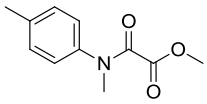




Methyl 2-(methyl(*p*-tolyl)amino)-2-oxoacetate



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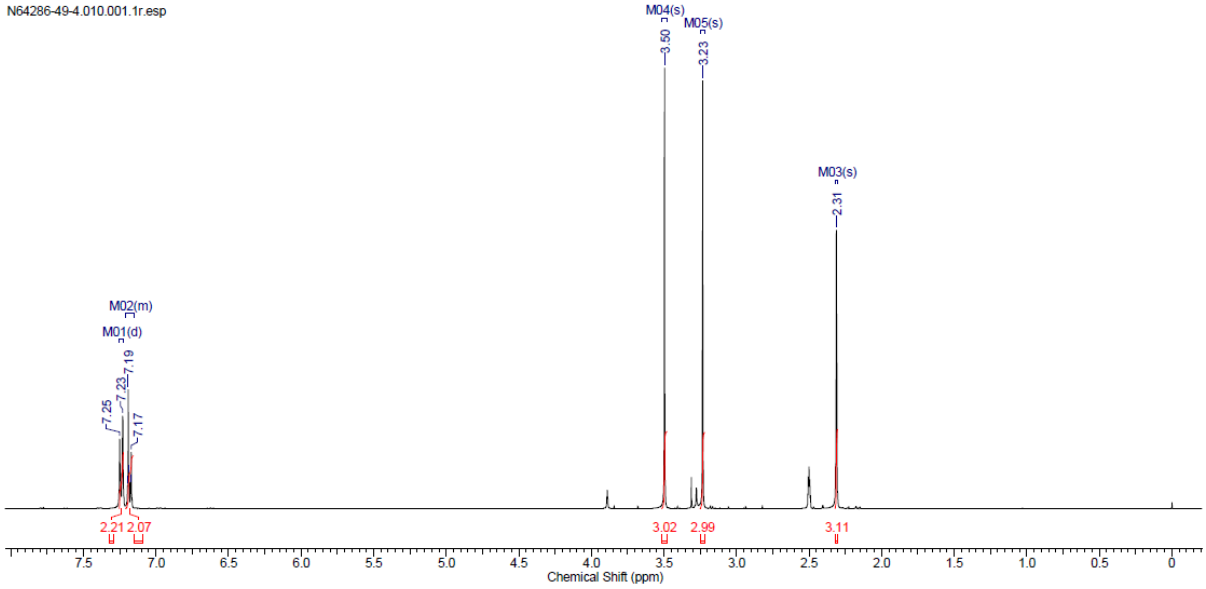
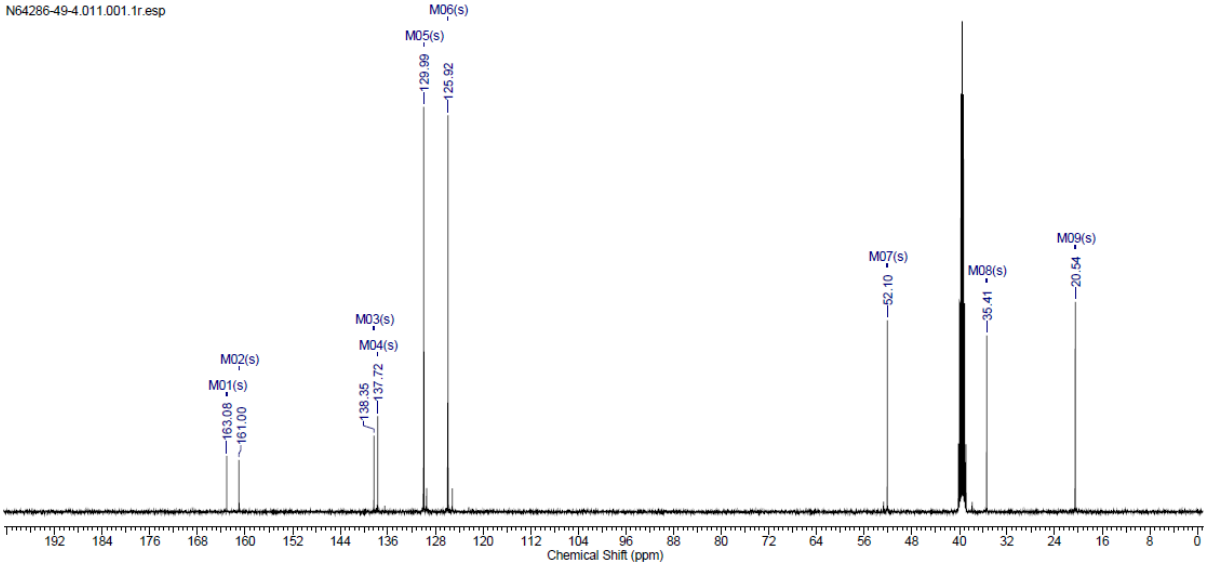
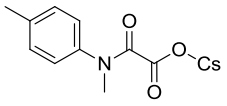




Cesium 2-(methyl(*p*-tolyl)amino)-2-oxoacetate



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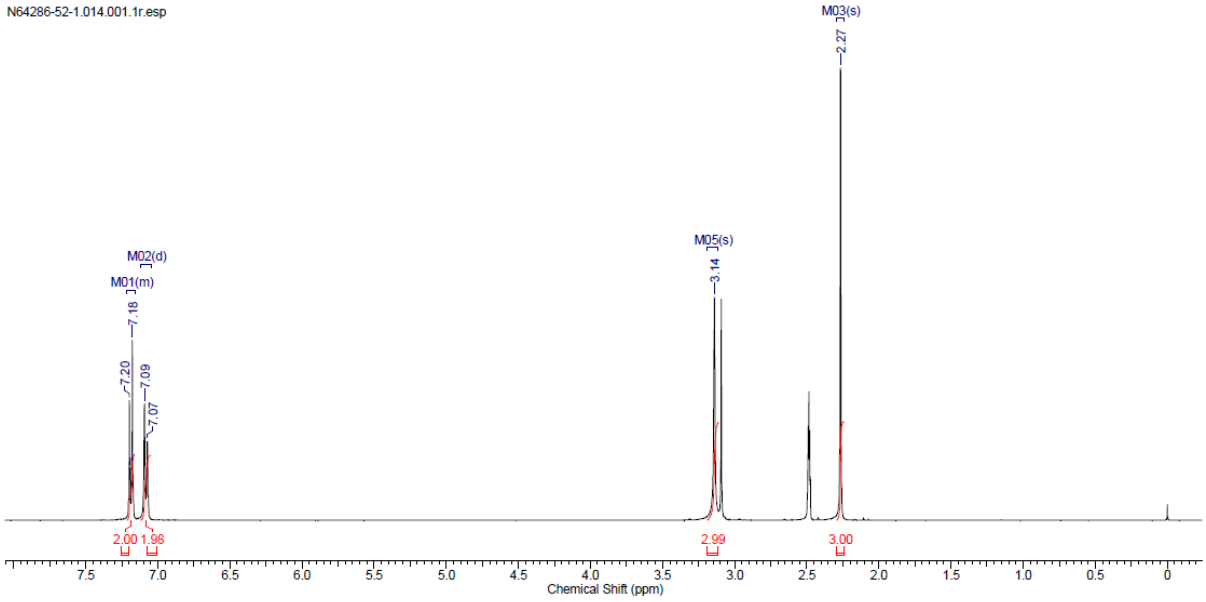
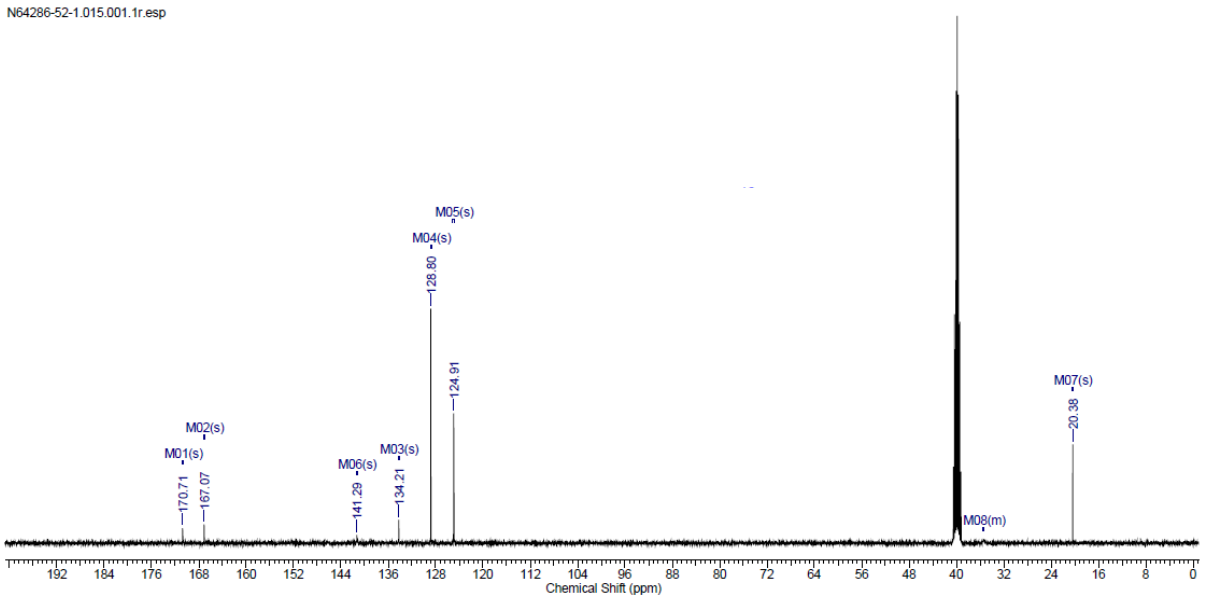
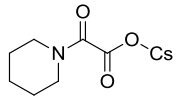




Cesium 2-oxo-2-(piperidin-1-yl)acetate



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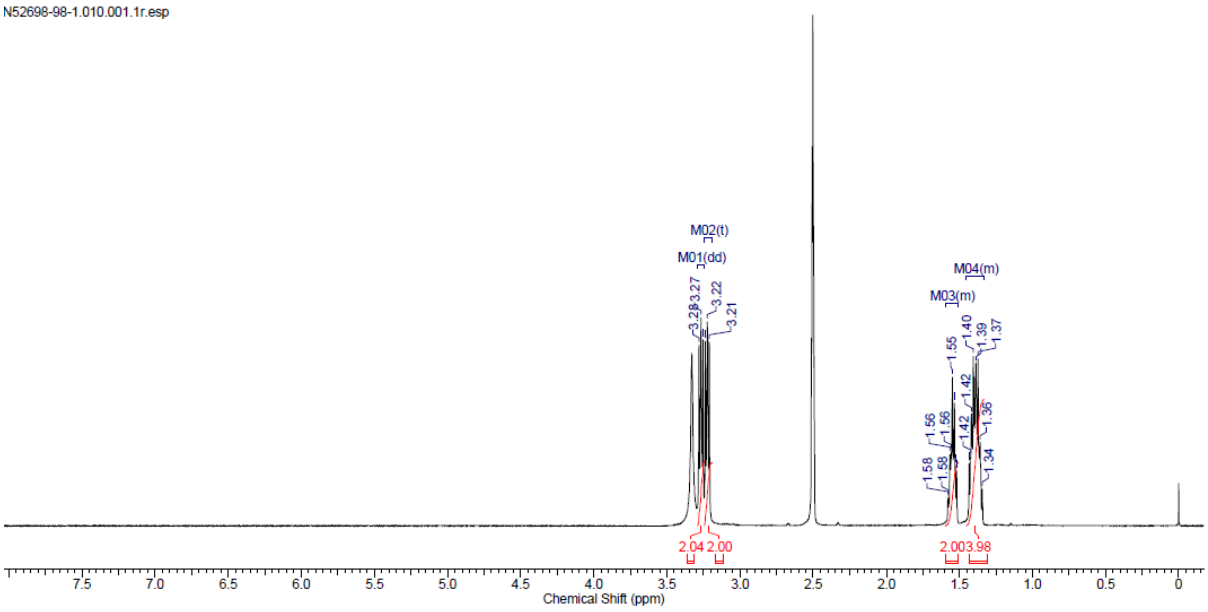
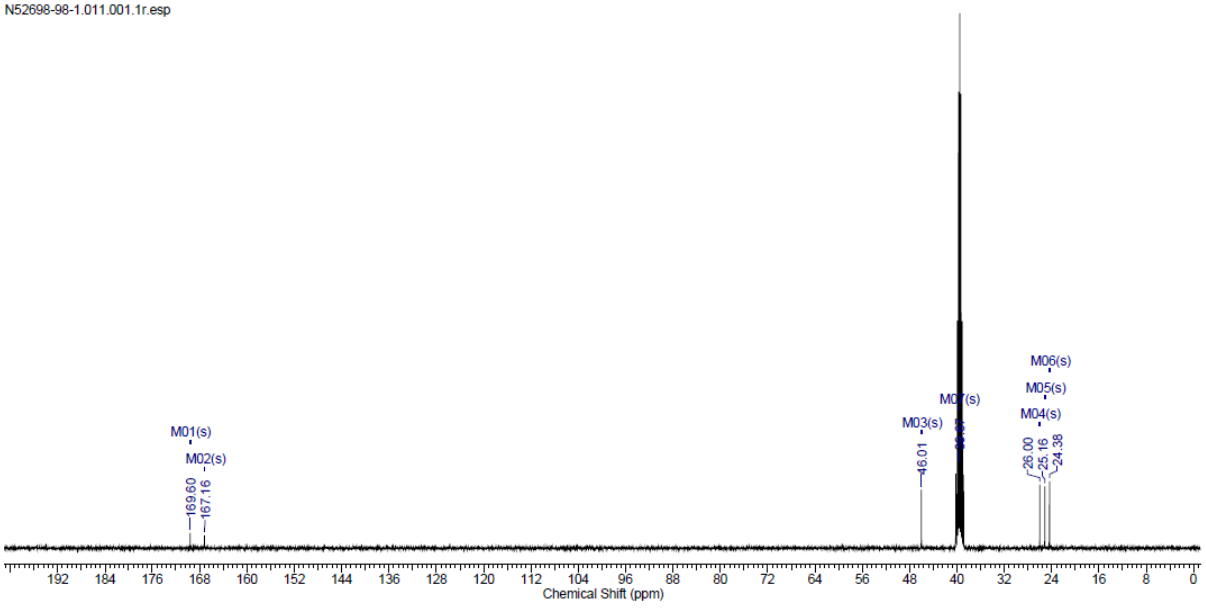
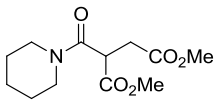




Dimethyl 2-(piperidine-1-carbonyl)succinate



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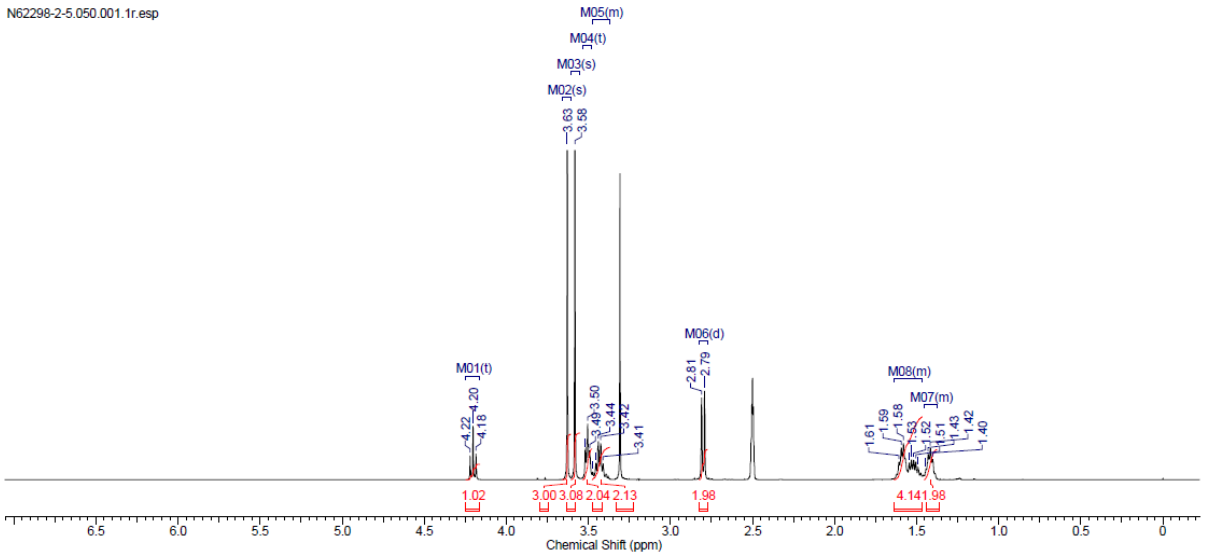
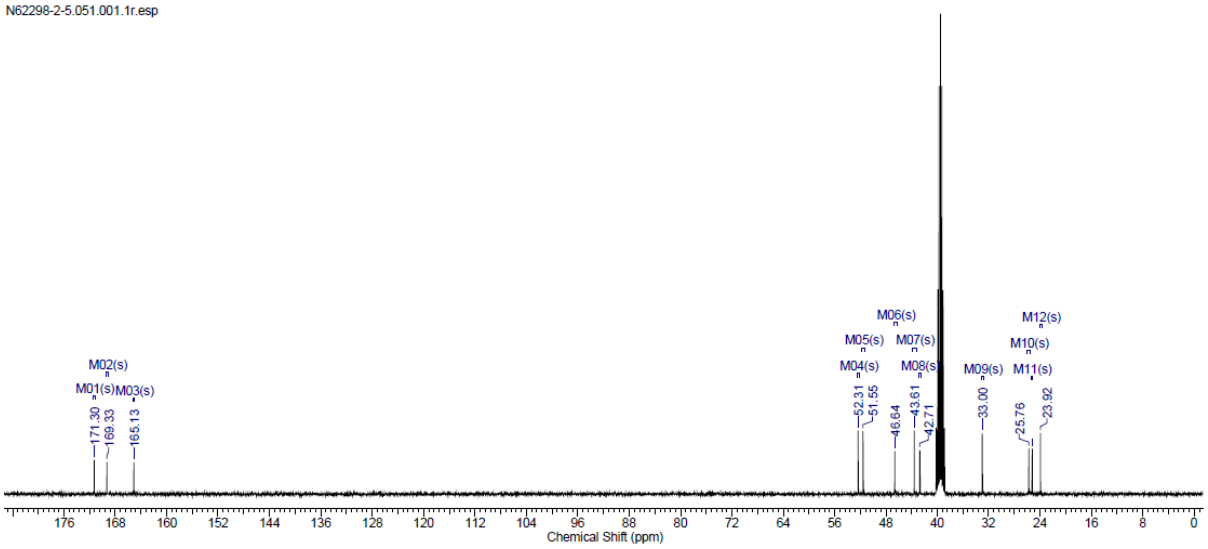
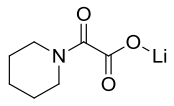




1.1.2. Oxamate salt selection

Lithium 2-oxo-2-(piperidin-1-yl)acetate



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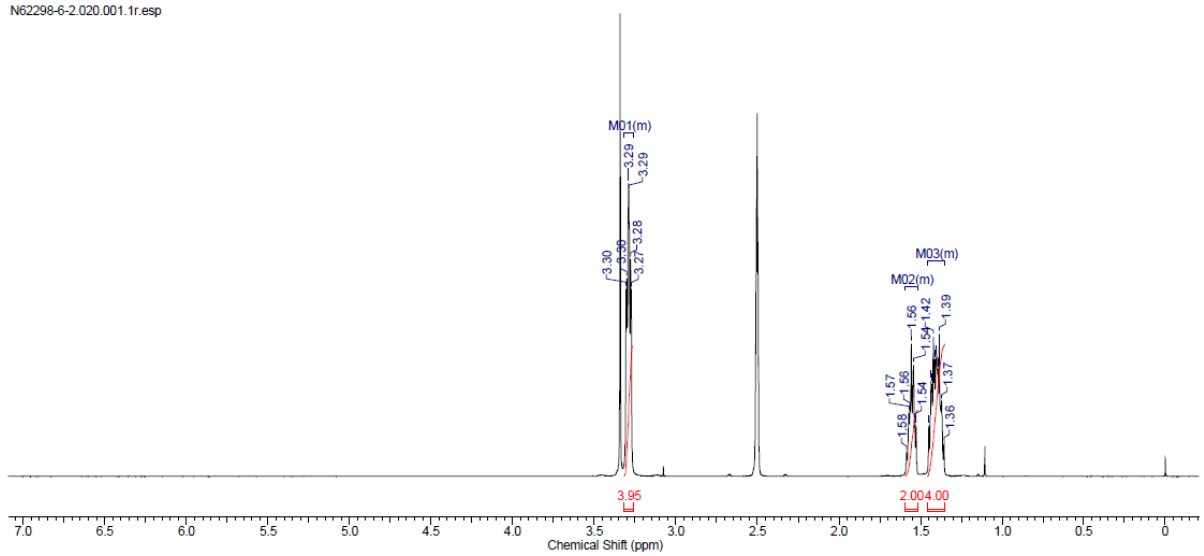
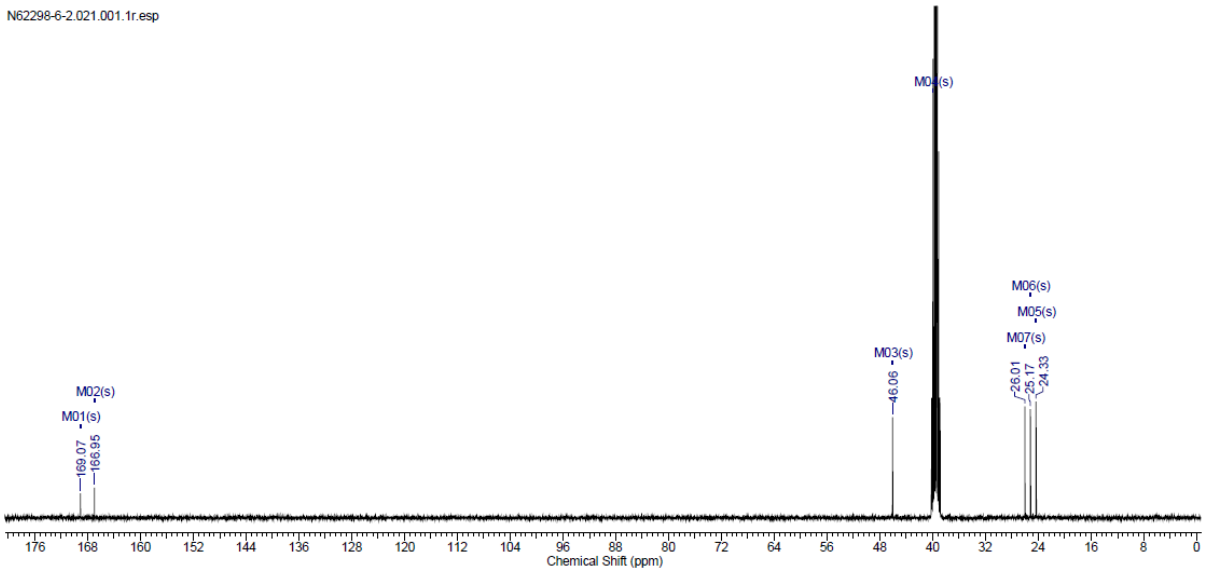
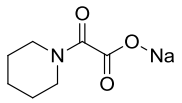




Sodium 2-oxo-2-(piperidin-1-yl)acetate



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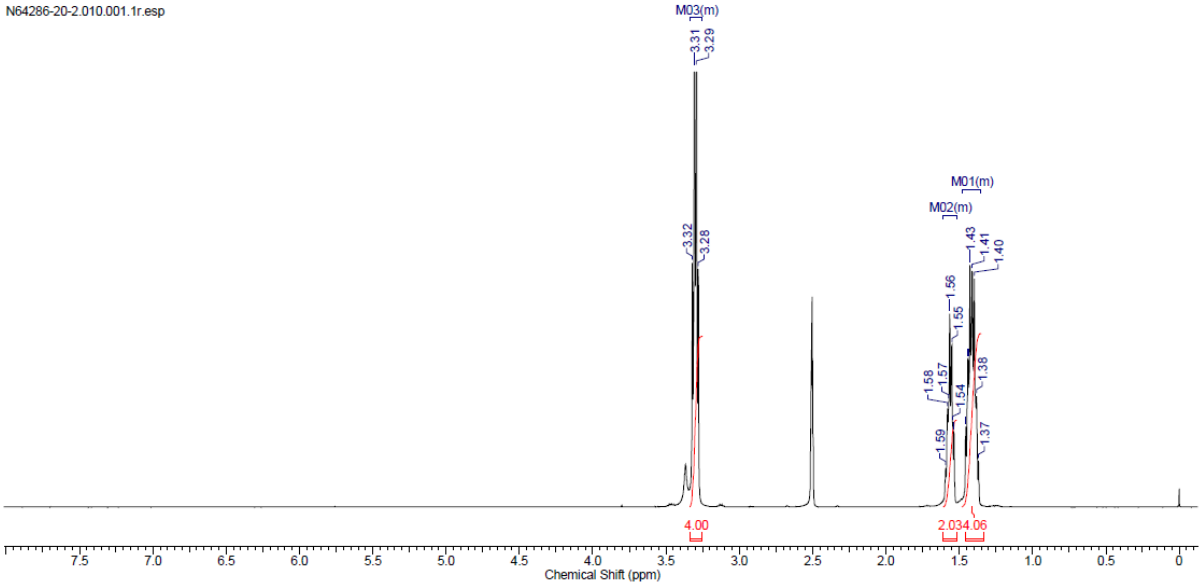
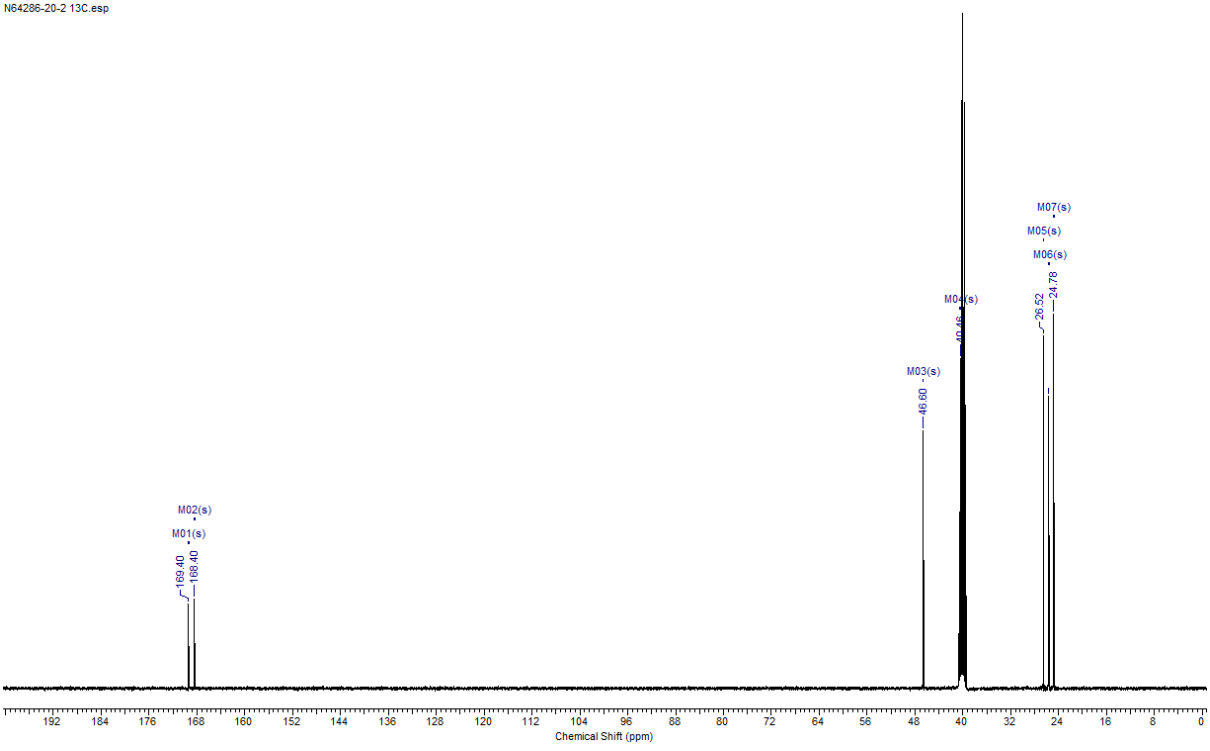
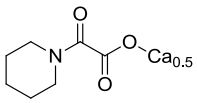




Calcium 2-oxo-2-(piperidin-1-yl)acetate



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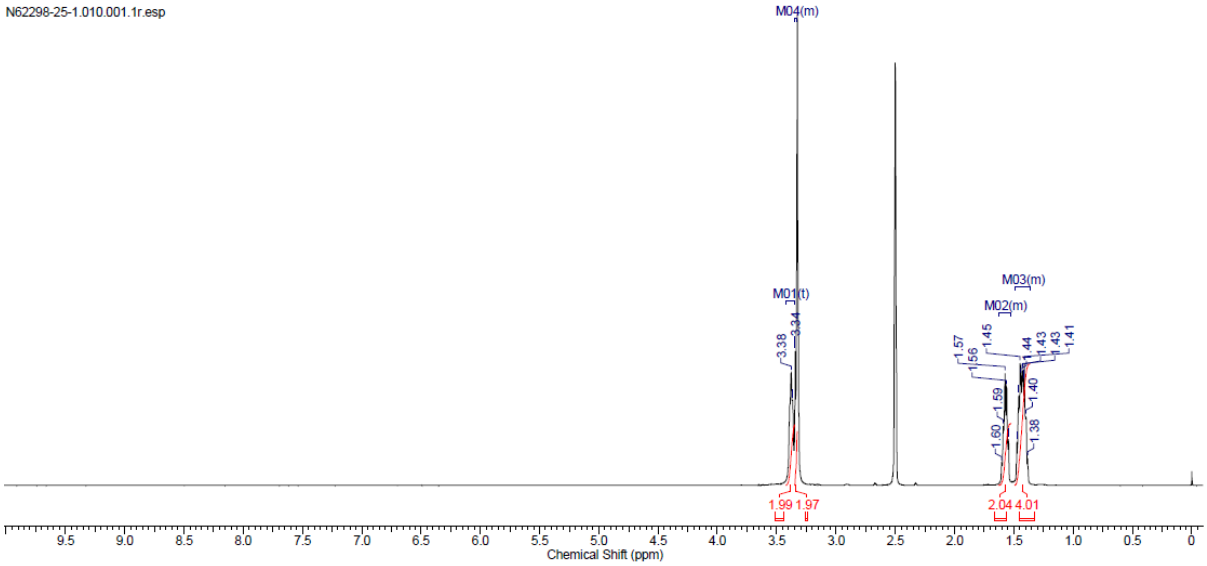
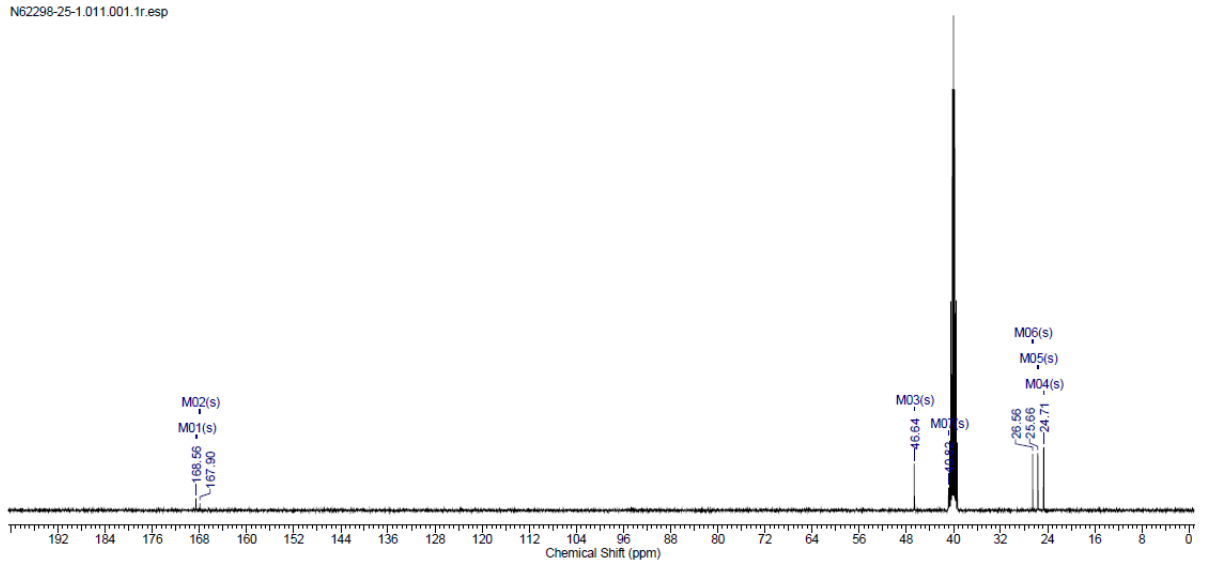
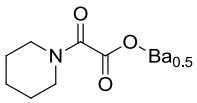




Barium 2-oxo-2-(piperidin-1-yl)acetate



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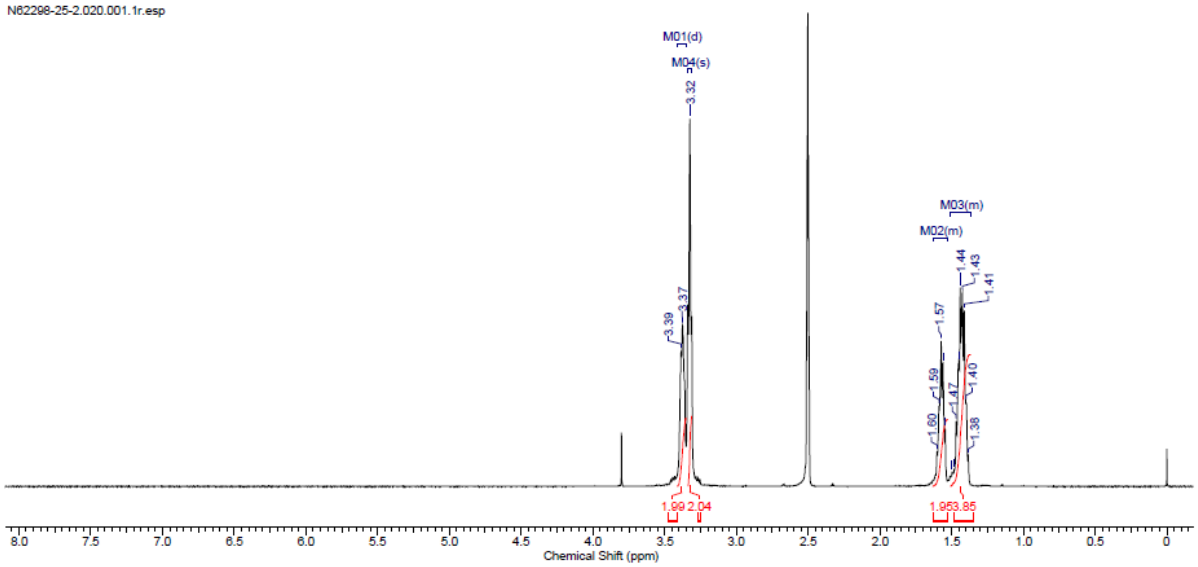
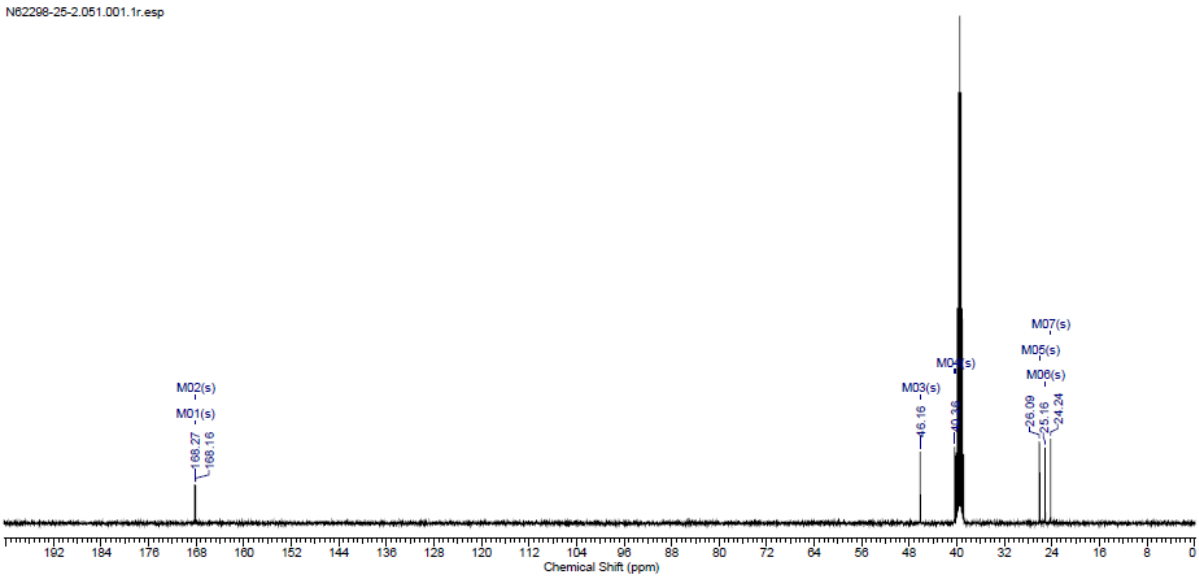
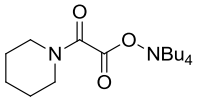




Tetrabutylammonium 2-oxo-2-(piperidin-1-yl)acetate



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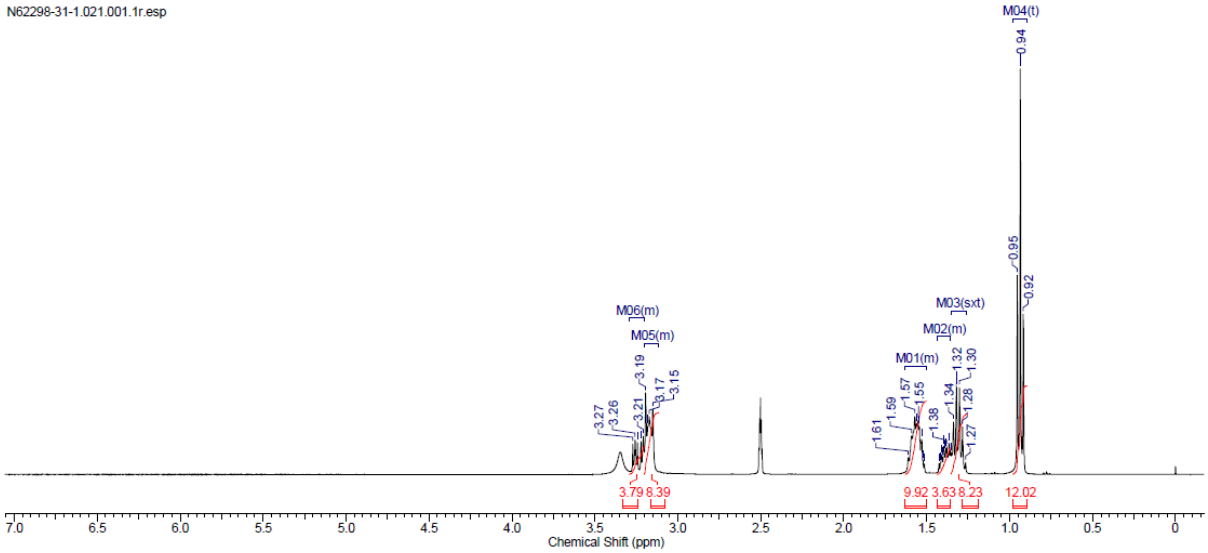
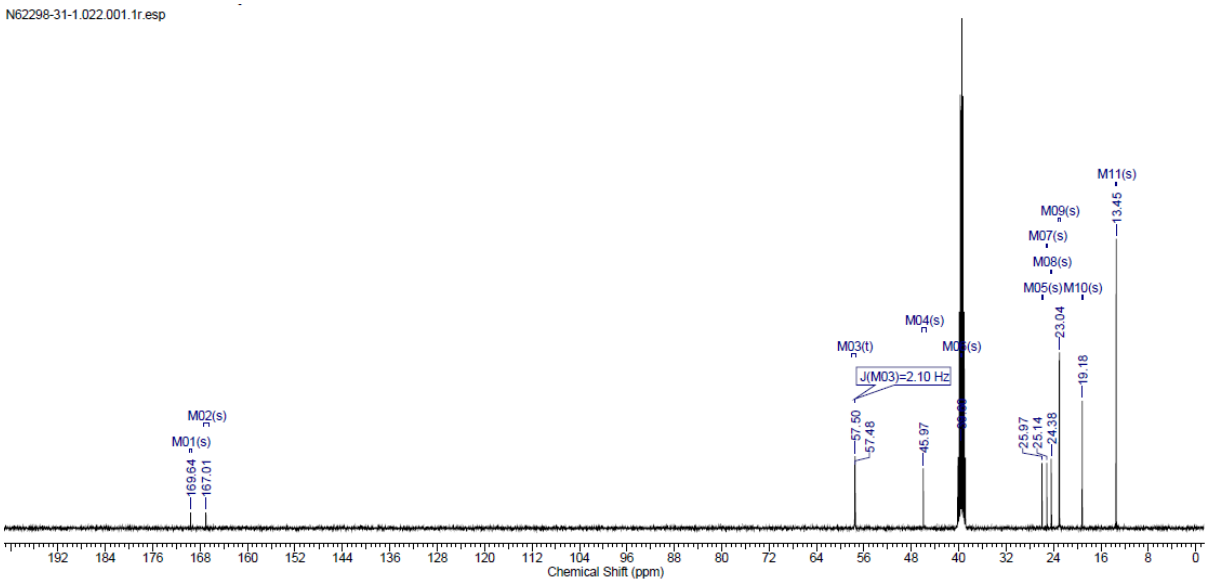
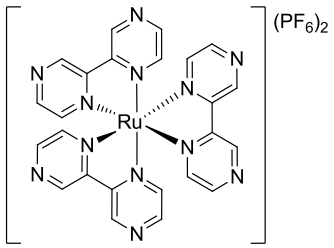




1.1.3. Catalyst selection

Tris(2,2'-bipyrazine)ruthenium(II) hexafluorophosphate



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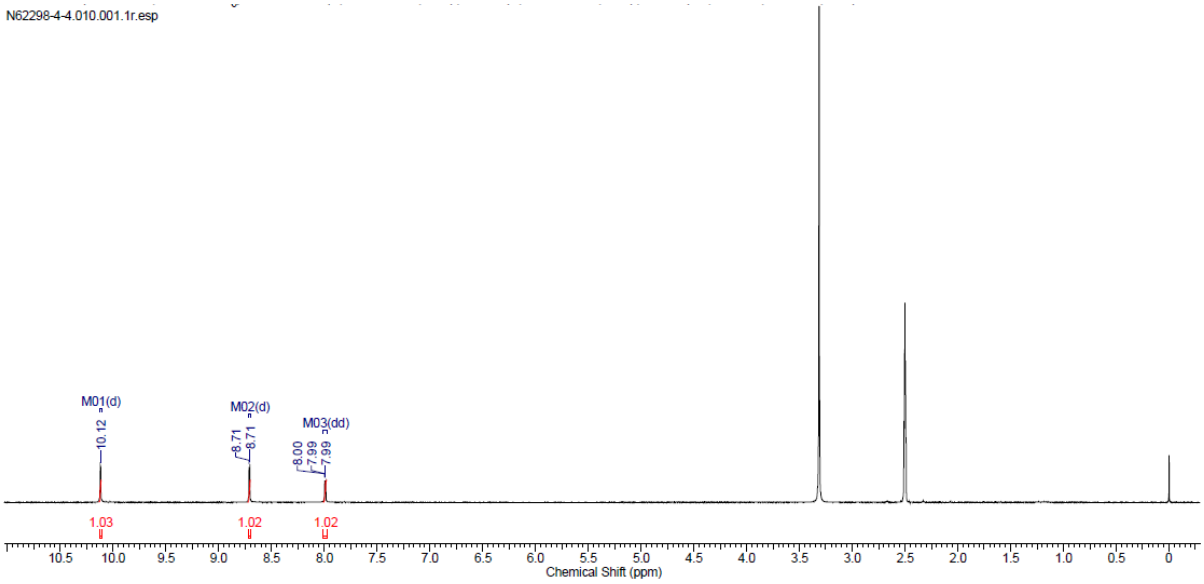

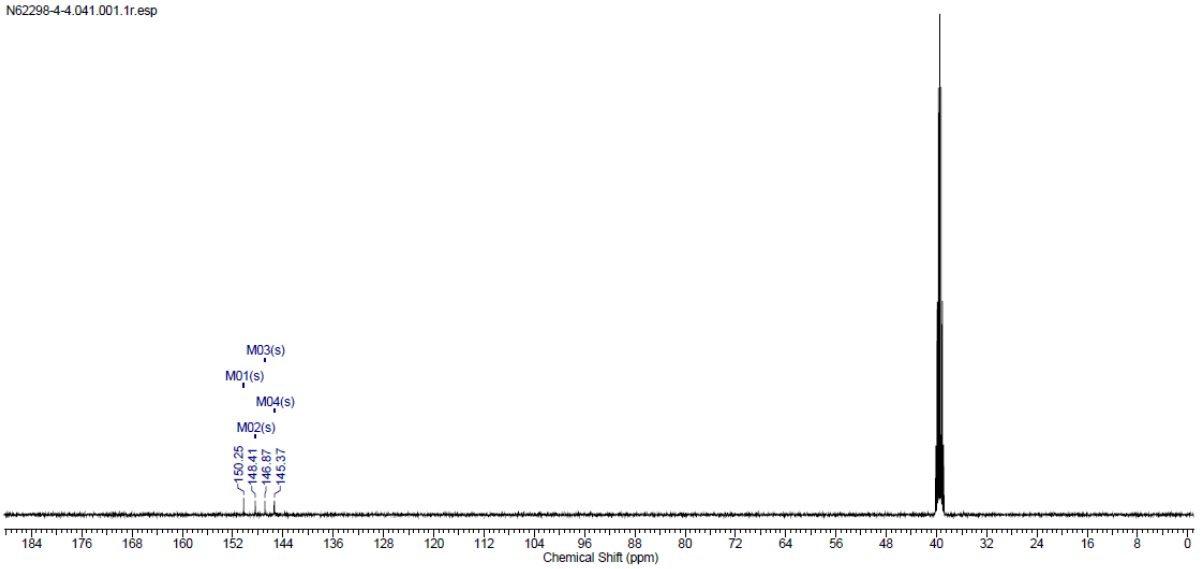

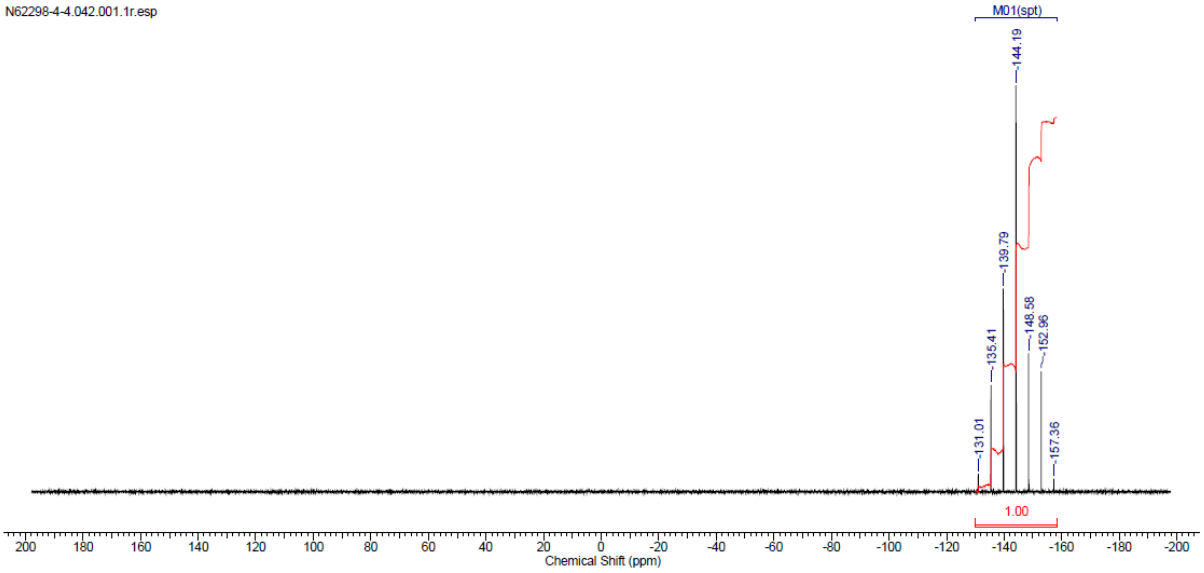
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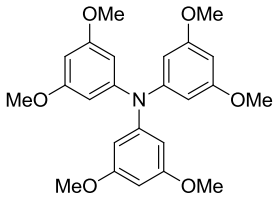
M01(spt)
144.19
139.79
148.58
152.96
135.41
131.01
157.36
1.00
200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200
Chemical Shift (ppm)

Tris(3,5-dimethoxyphenyl)amine[61]



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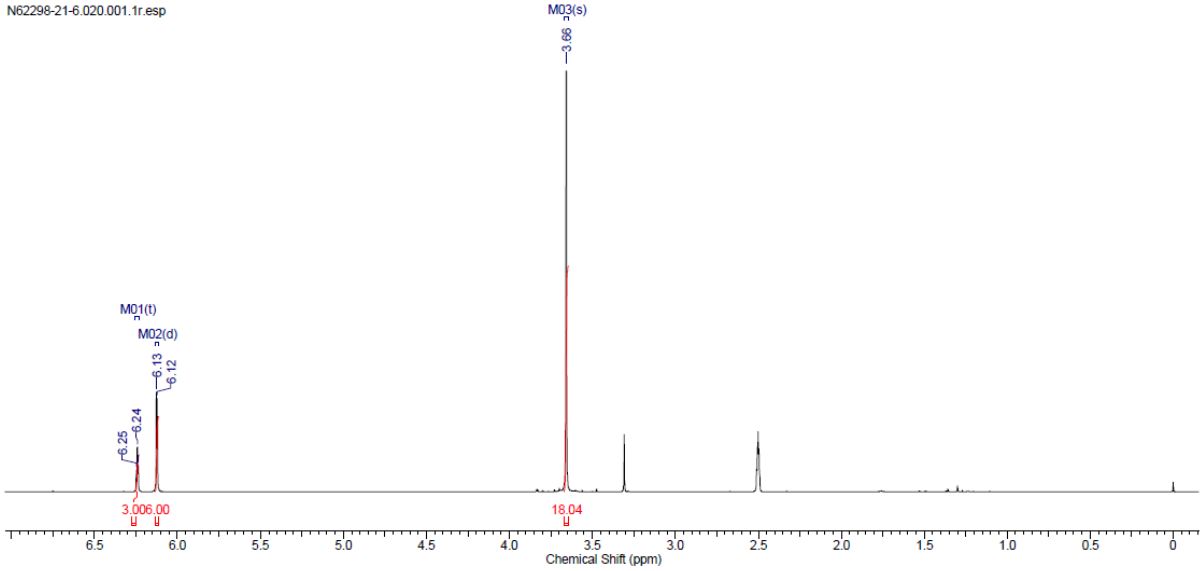
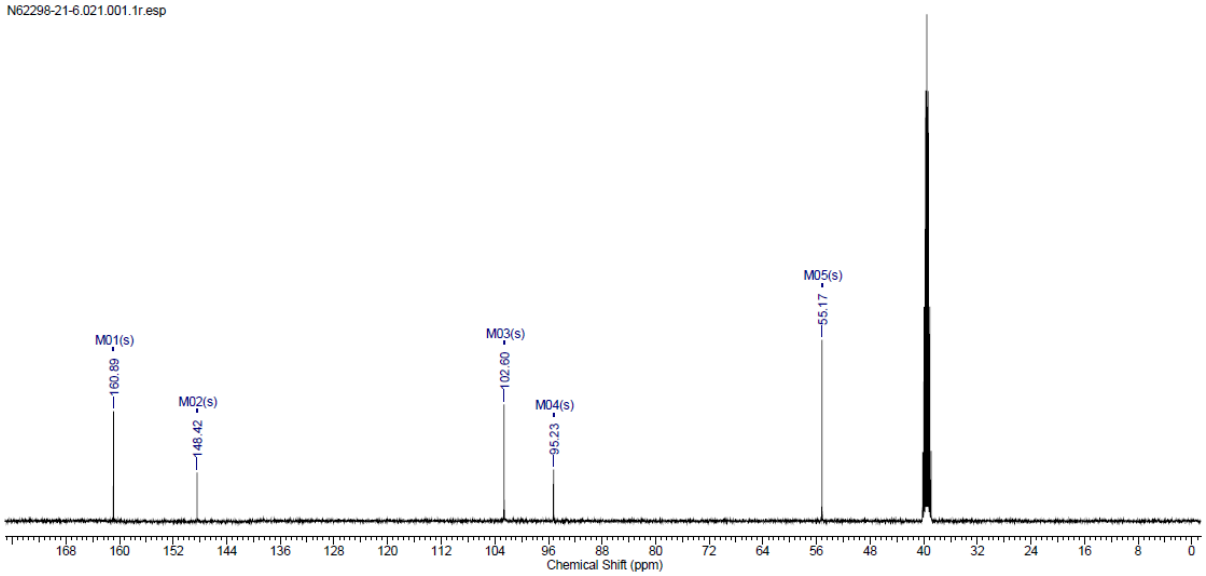
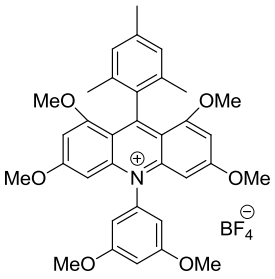




10-(3,5-Dimethoxyphenyl)-9-mesityl-1,3,6,8-tetramethoxyacridin-10-ium tetrafluoroborate



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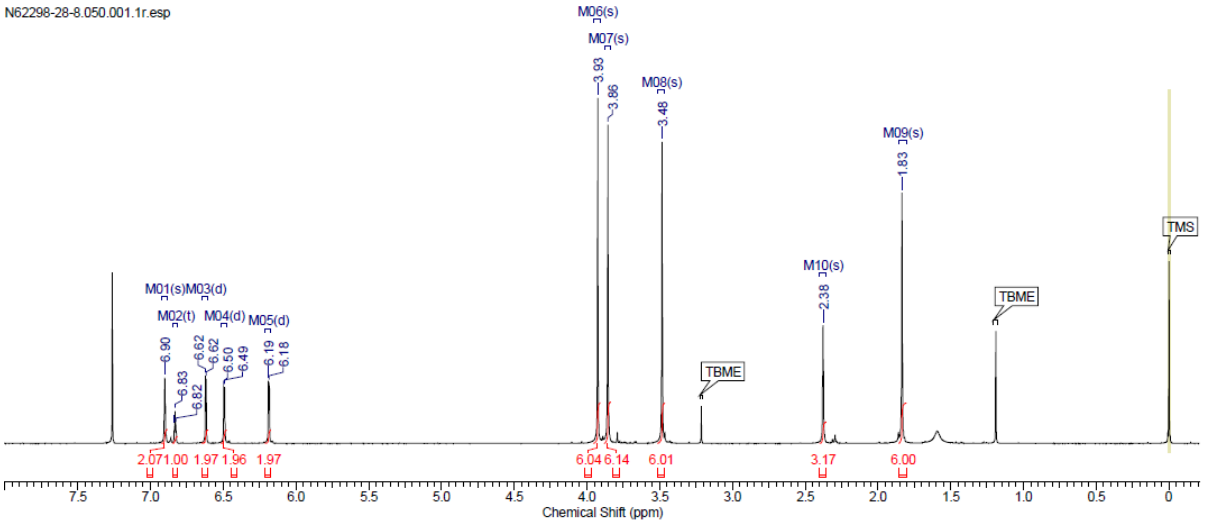
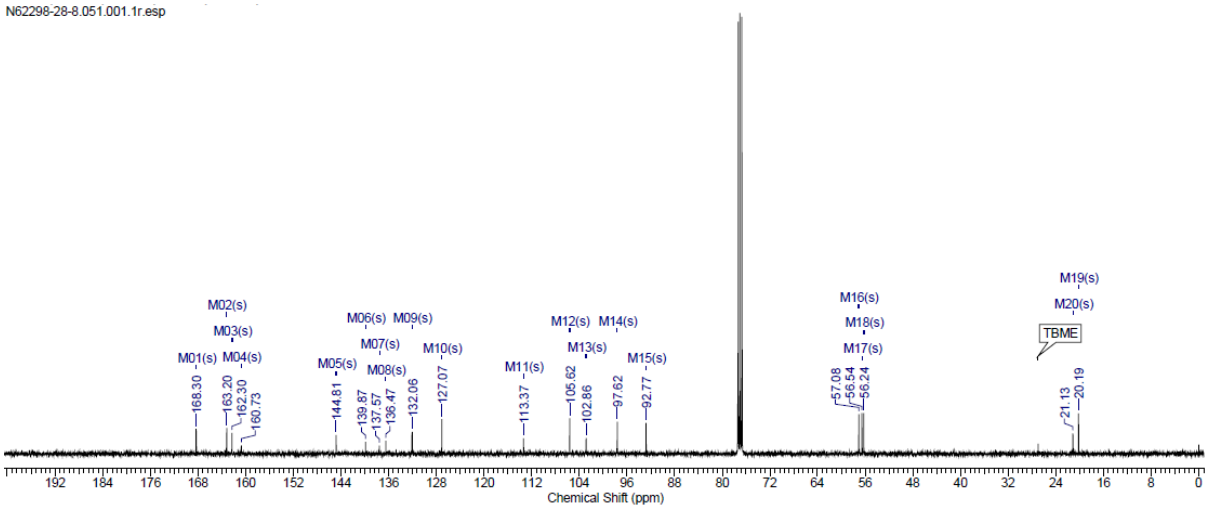
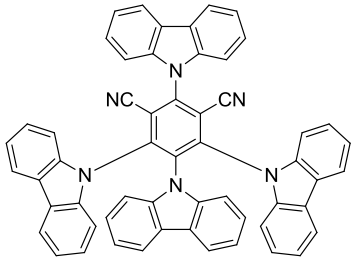




2,4,5,6-tetra(9H-carbazol-9-yl)isophthalonitrile



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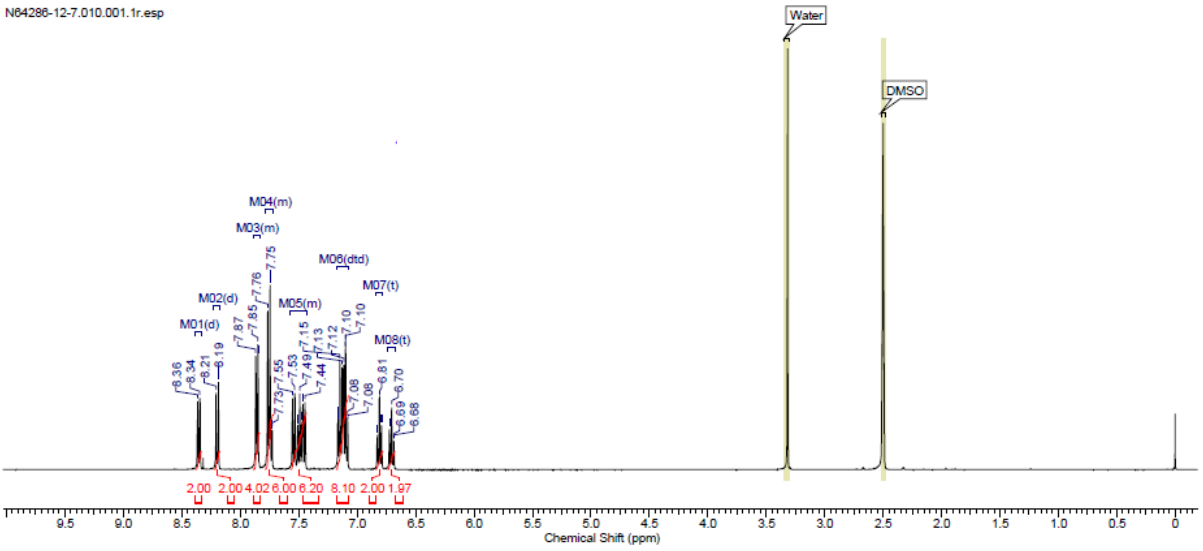
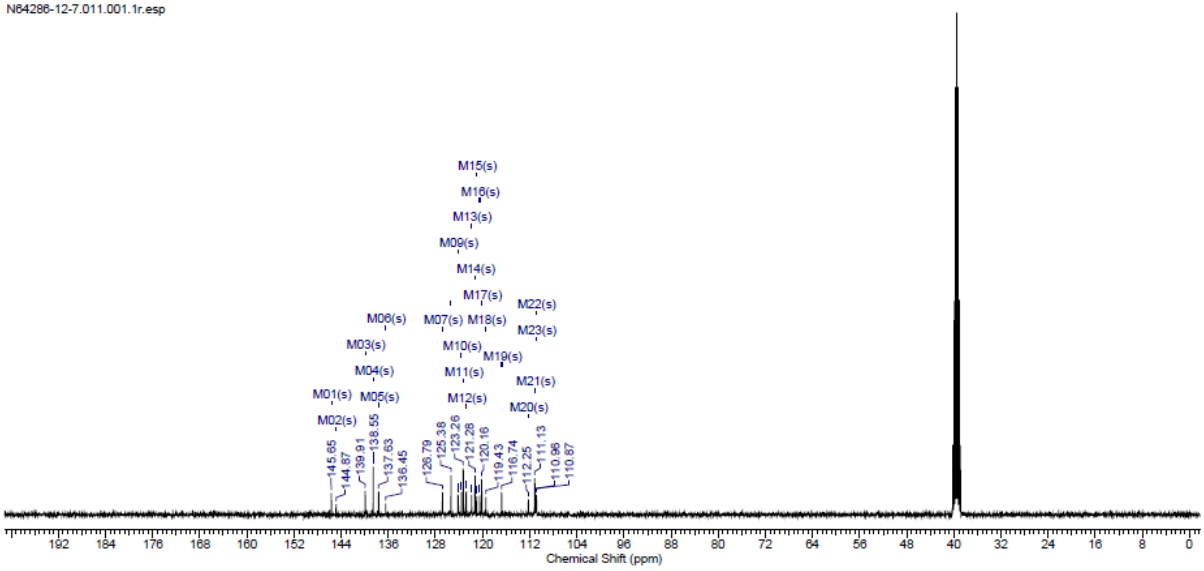
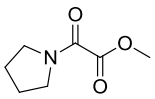




1.1.4. Substrate scope: Starting material synthesis

Methyl 2-oxo-2-(pyrrolidin-1-yl)acetate



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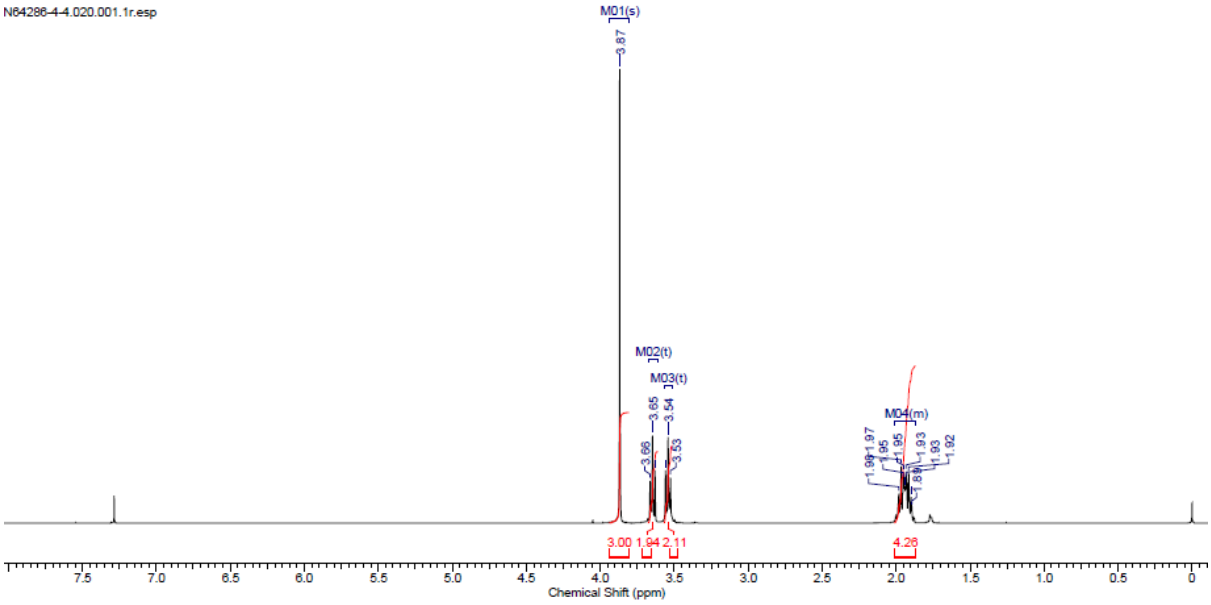
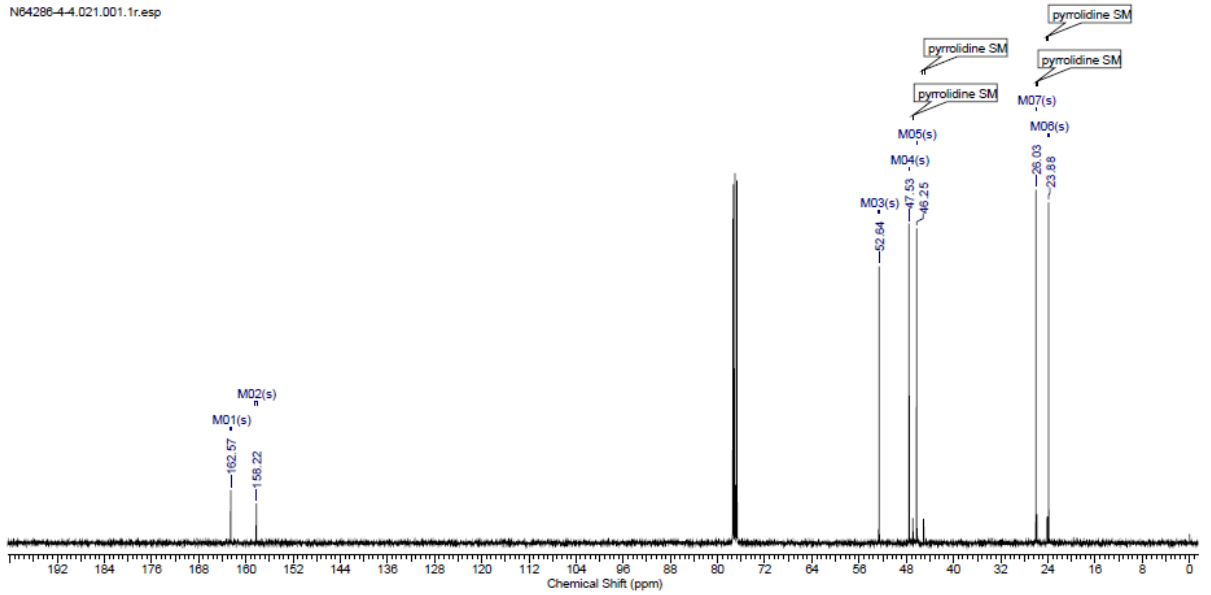
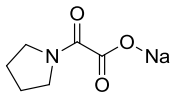




Sodium 2-oxo-2-(pyrrolidin-1-yl)acetate



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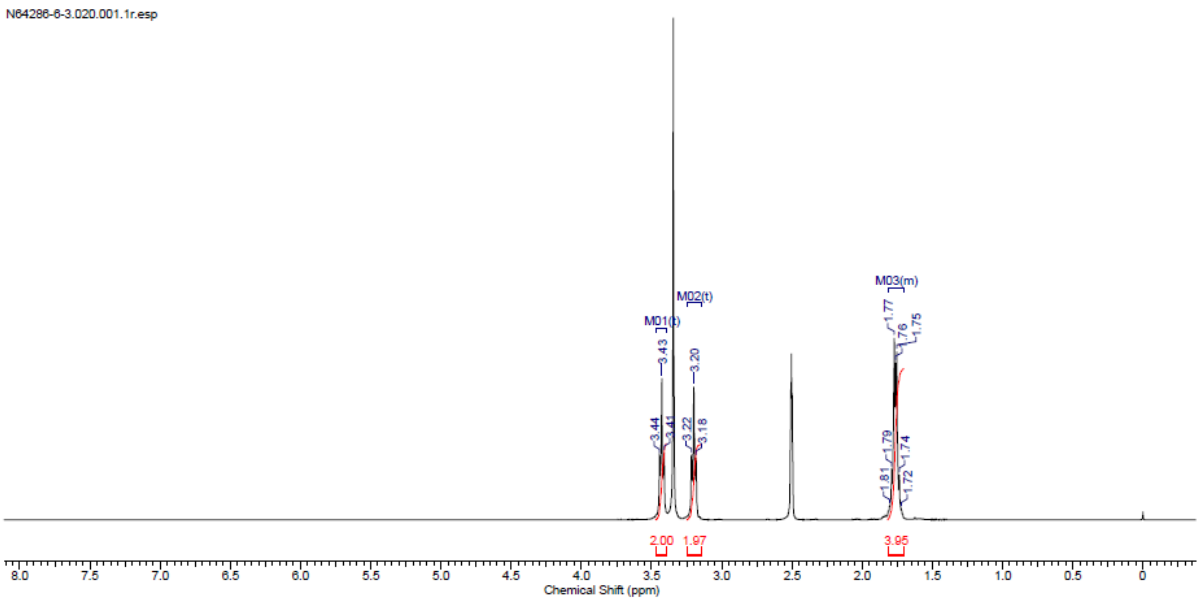
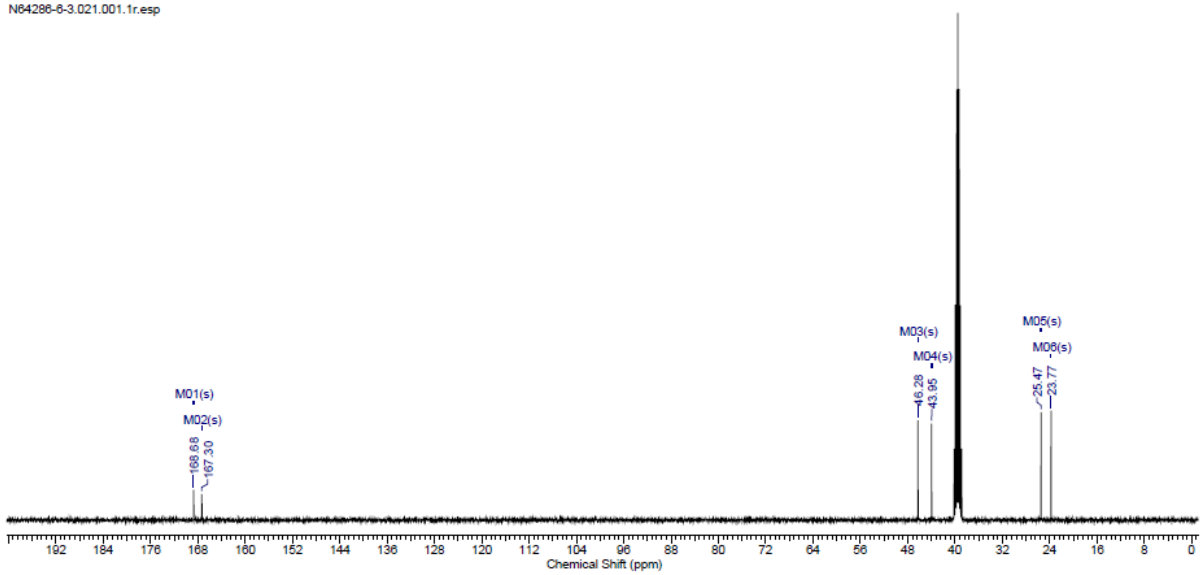
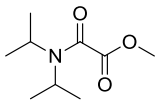




Methyl 2-(diisopropylamino)-2-oxoacetate



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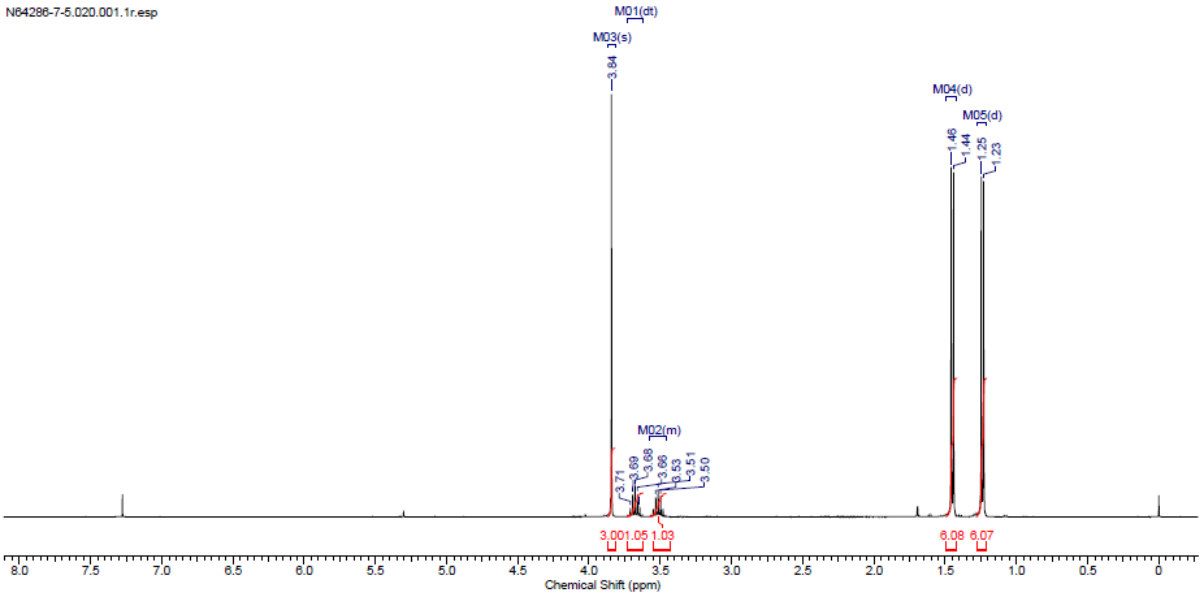
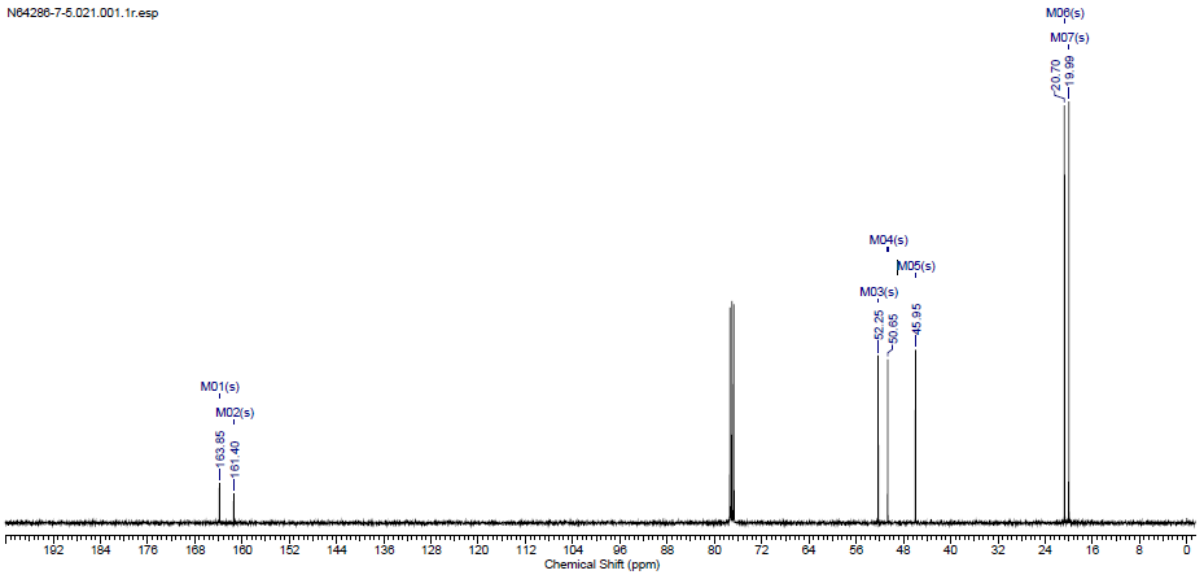
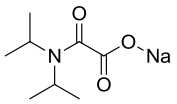




Sodium 2-(diisopropylamino)-2-oxoacetate



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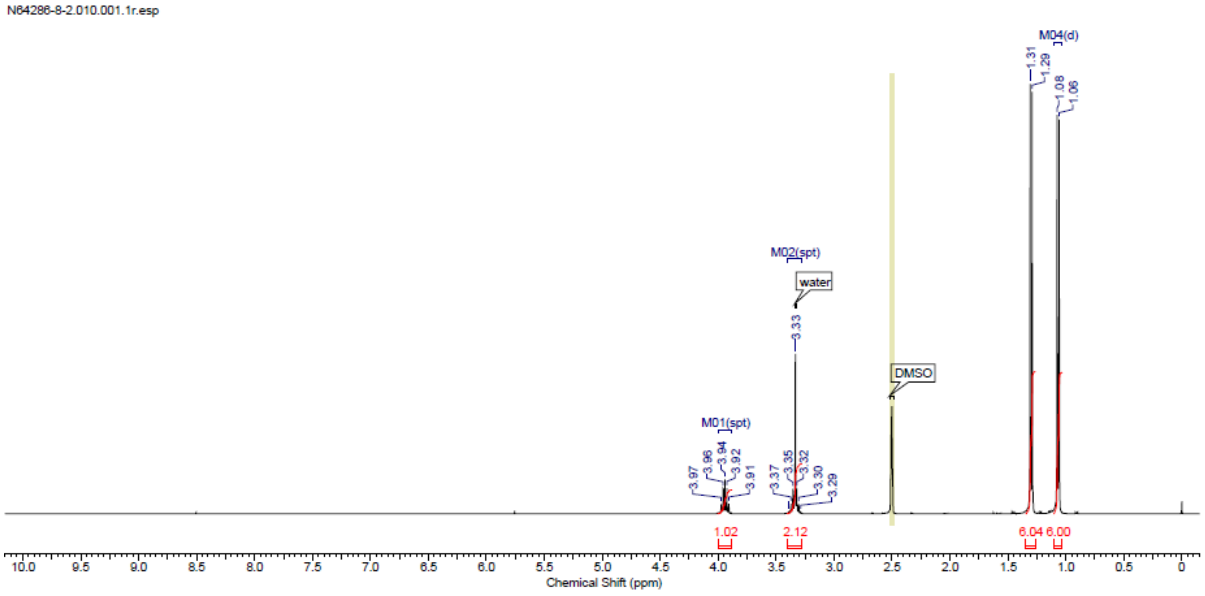
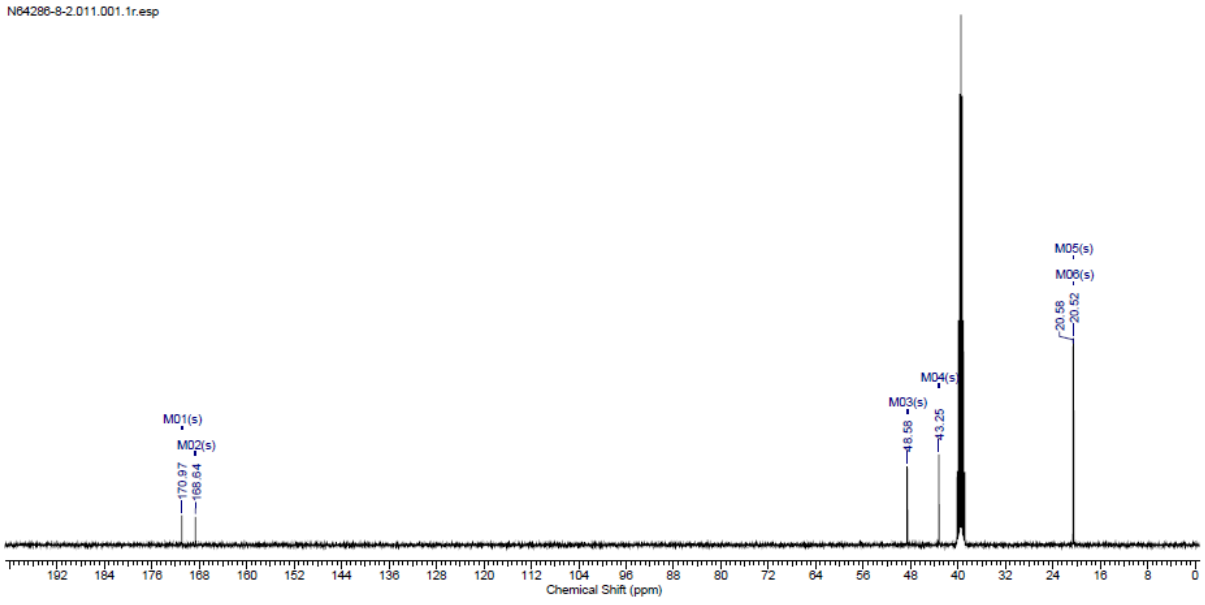
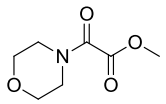




Methyl 2-morpholino-2-oxoacetate



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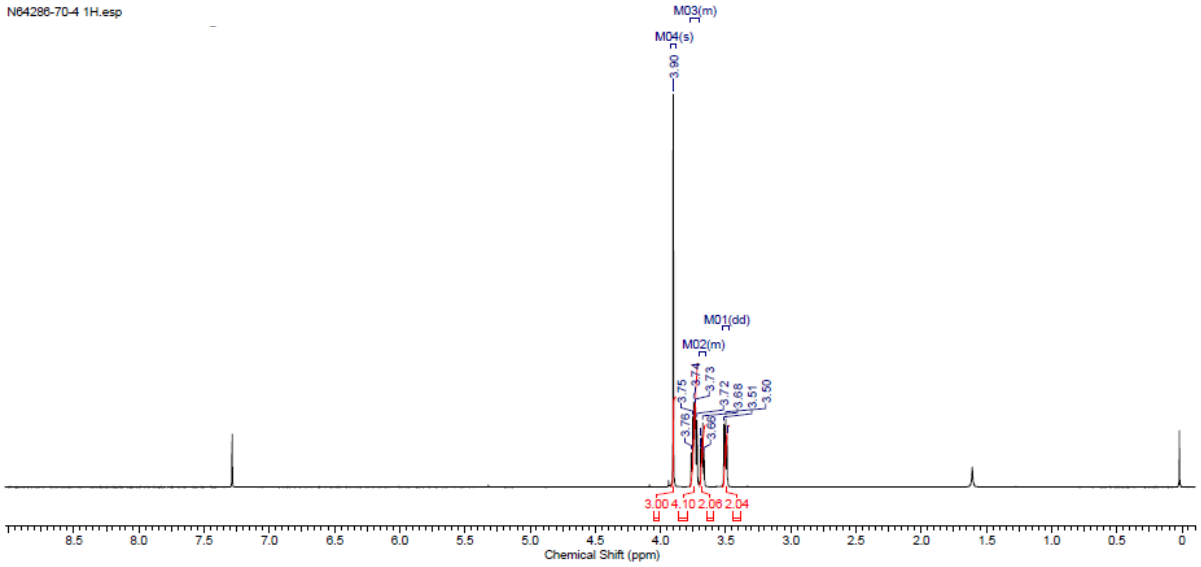
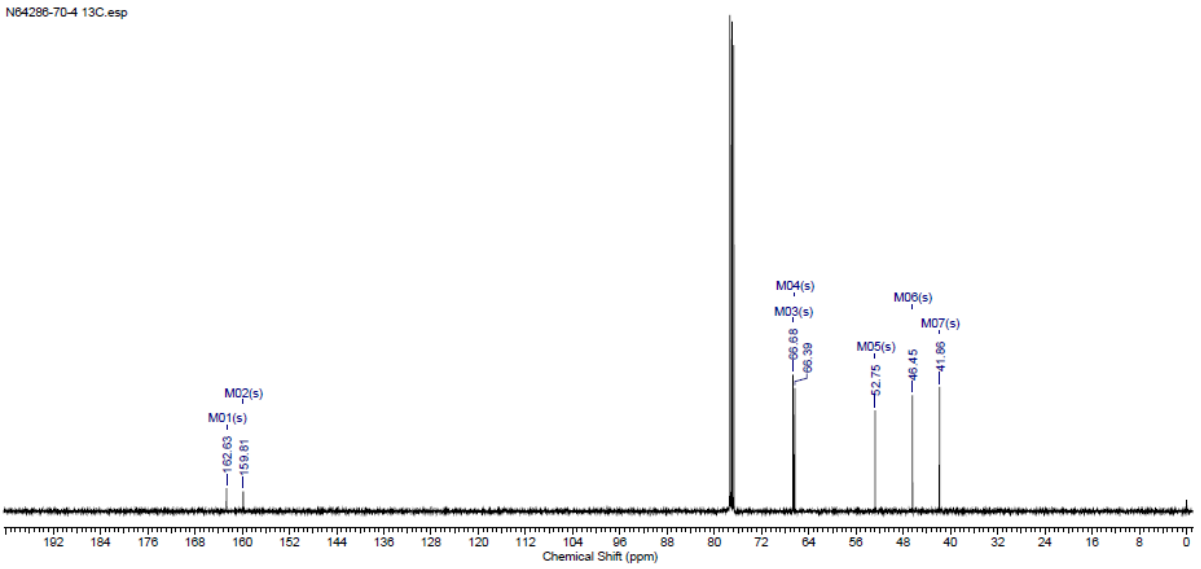
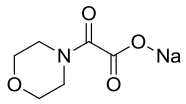




Sodium 2-morpholino-2-oxoacetate



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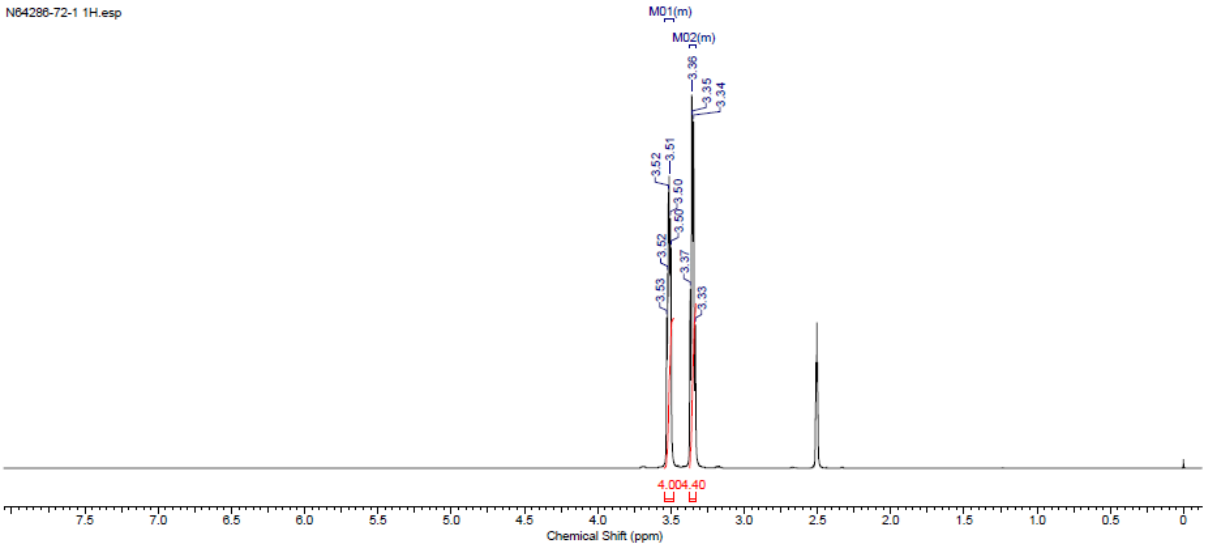
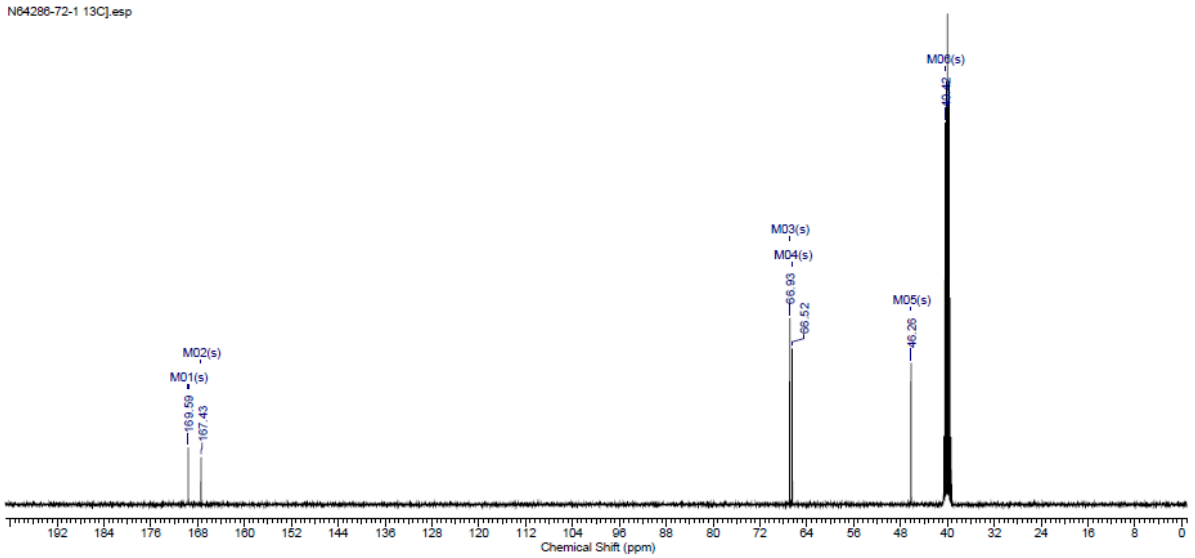
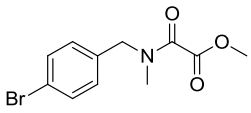




Methyl 2-((4-bromobenzyl)(methyl)amino)-2-oxoacetate



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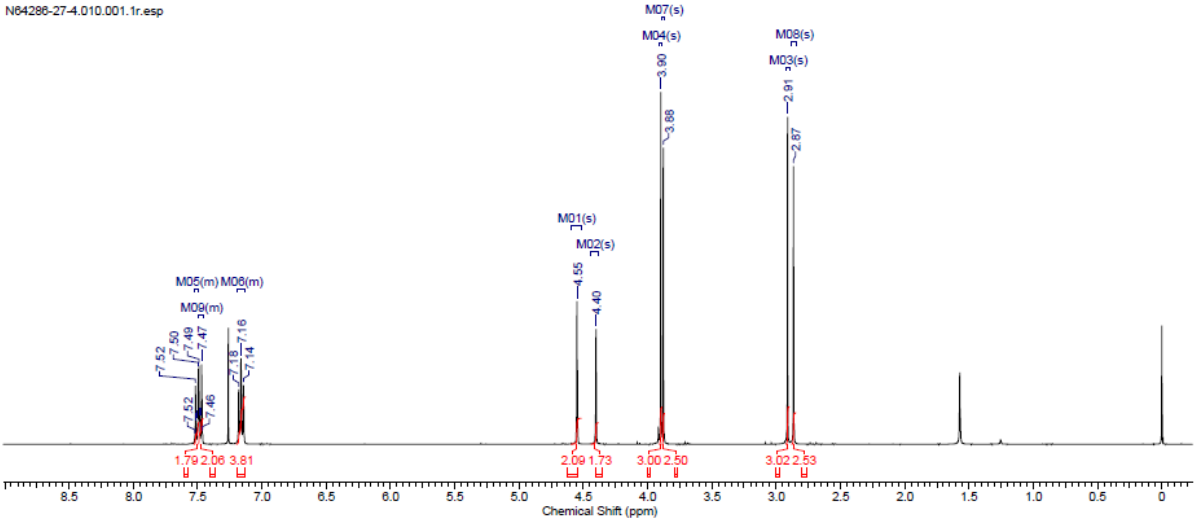

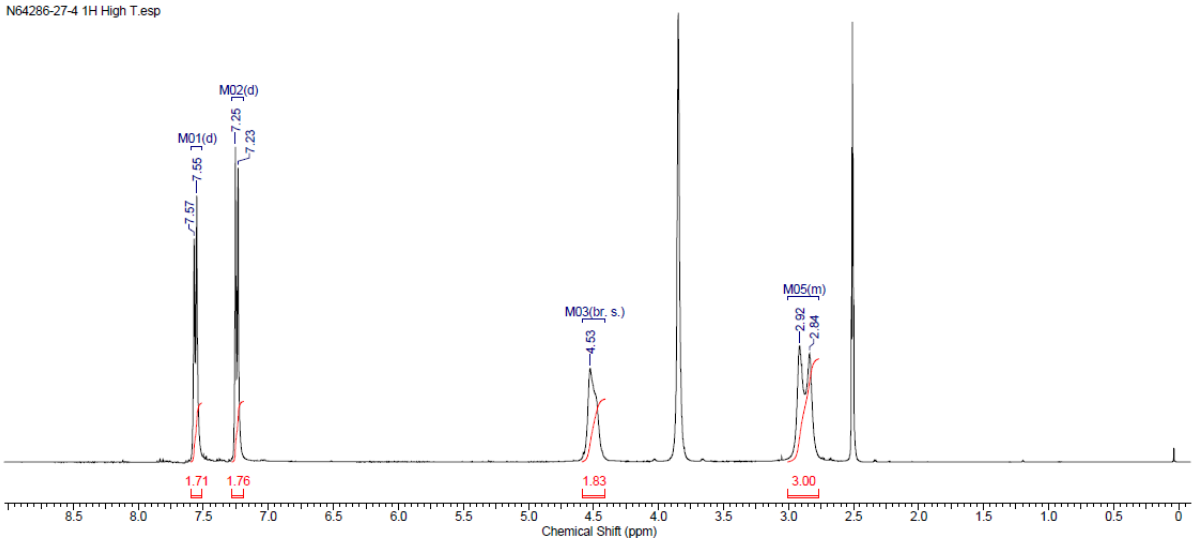

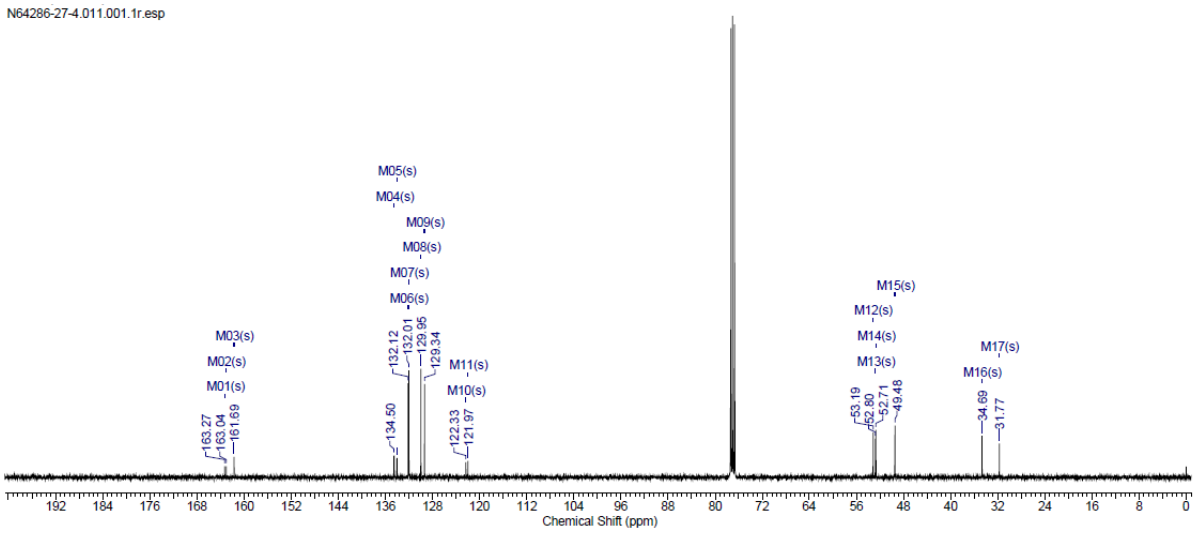
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M15(s)
M12(s)
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M13(s)
M17(s)
M16(s)
M11(s)
M10(s)
132.12
132.01
129.95
129.34
163.27
163.04
161.69
134.50
122.33
121.97
53.19
52.80
52.71
49.48
34.69
31.77
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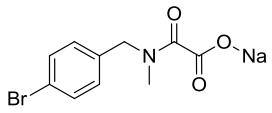
Chemical Shift (ppm)

Sodium 2-((4-bromobenzyl)(methyl)amino)-2-oxoacetate



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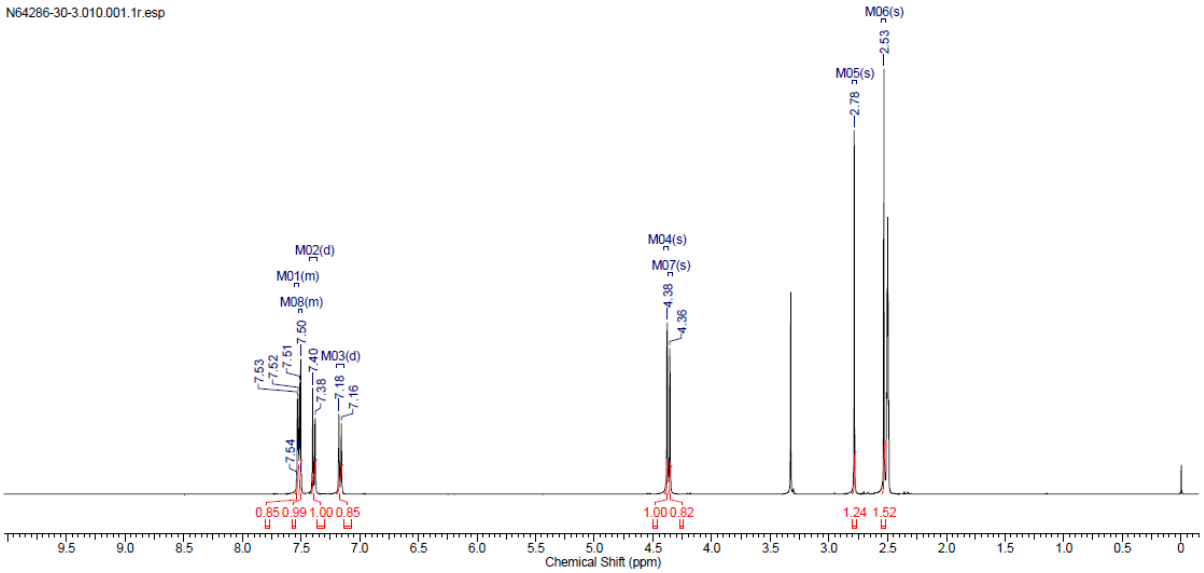
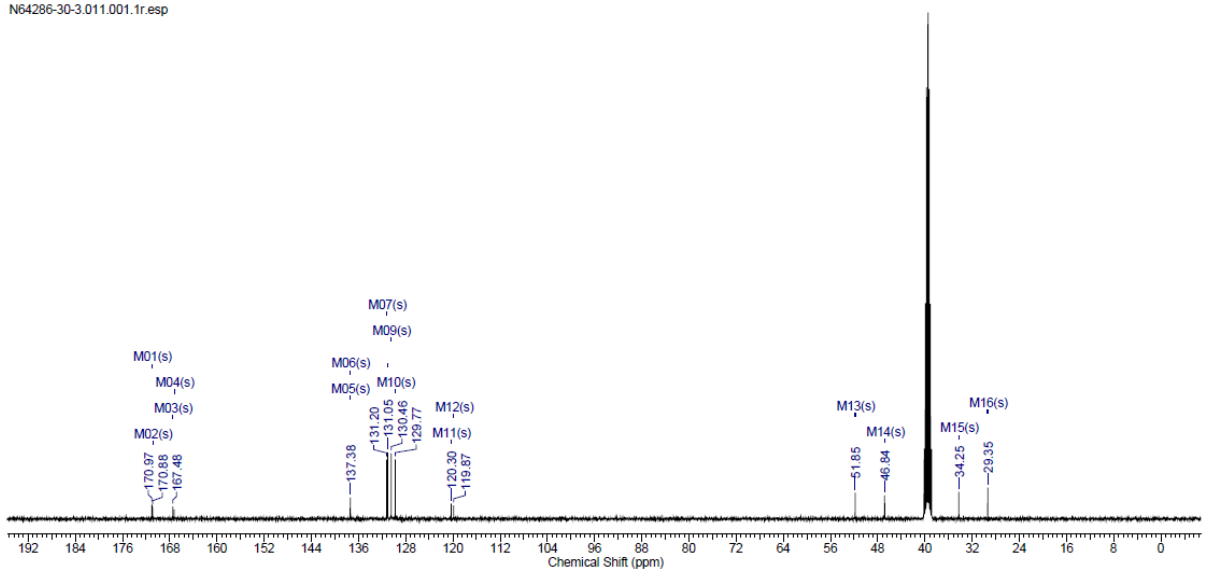
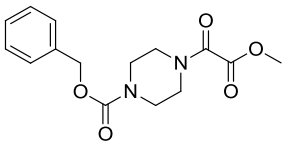




Benzyl 4-(2-methoxy-2-oxoacetyl)piperazine-1-carboxylate



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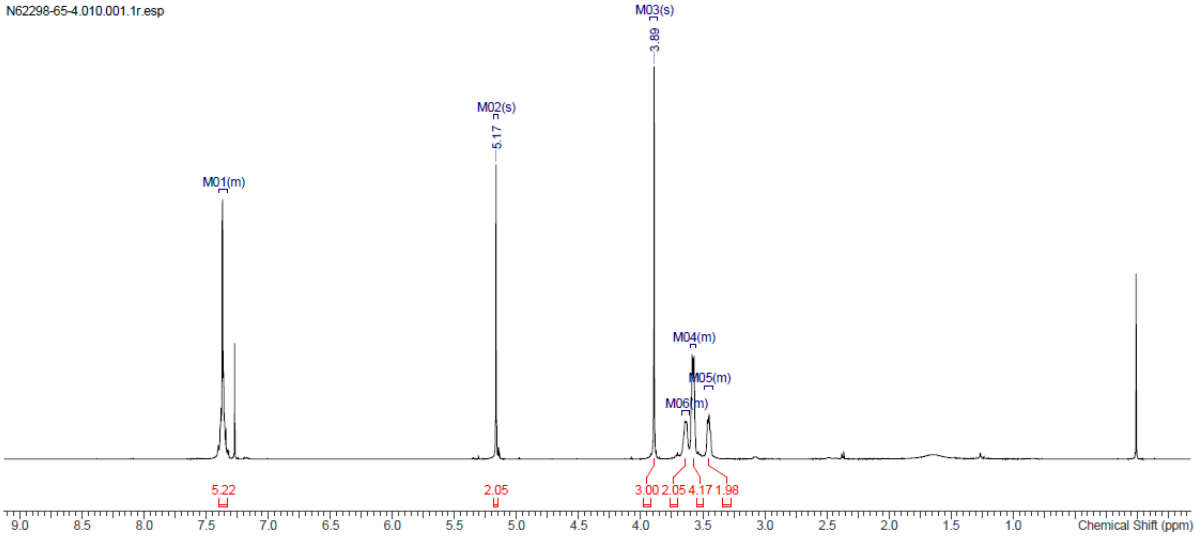
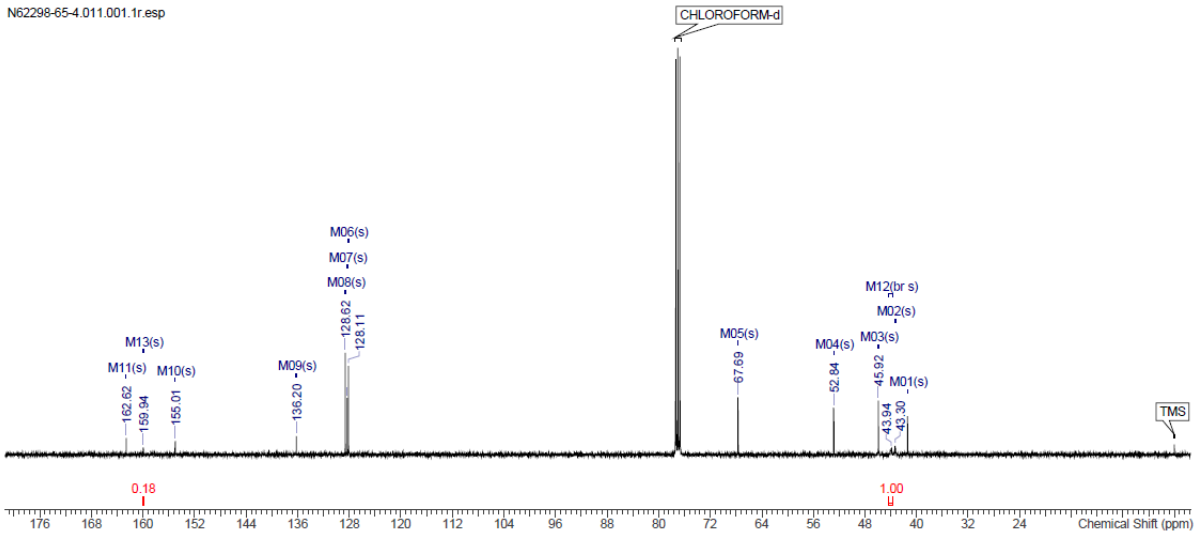
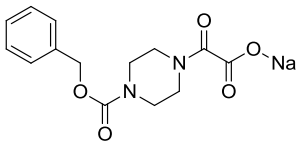




Sodium 2-(4-((benzyloxy)carbonyl)piperazin-1-yl)-2-oxoacetate



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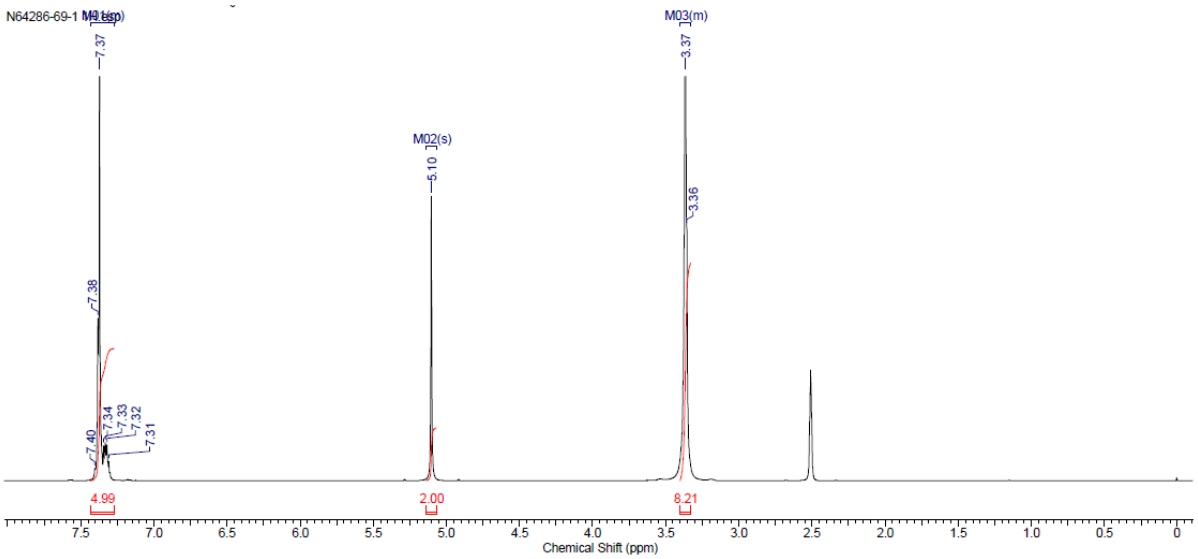
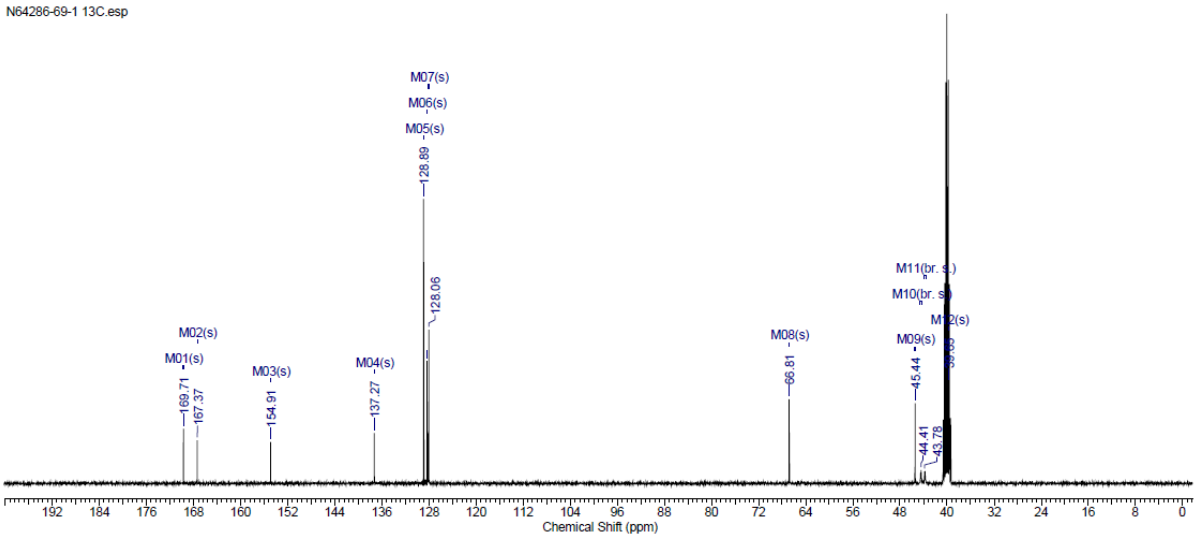
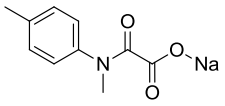




Sodium 2-(methyl(*p*-tolyl)amino)-2-oxoacetate



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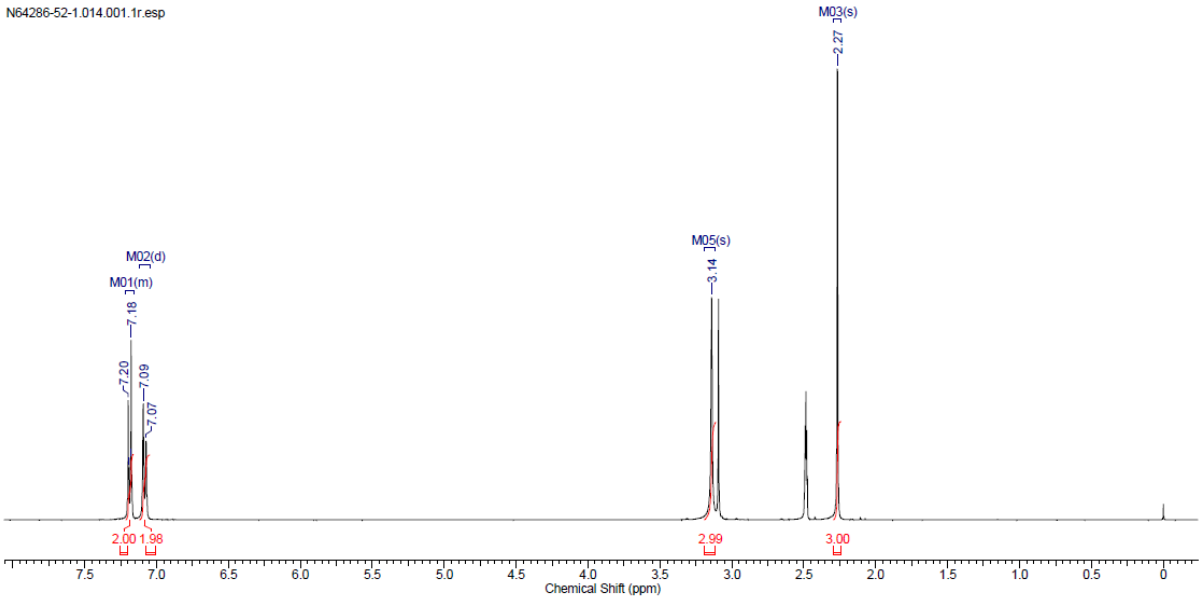
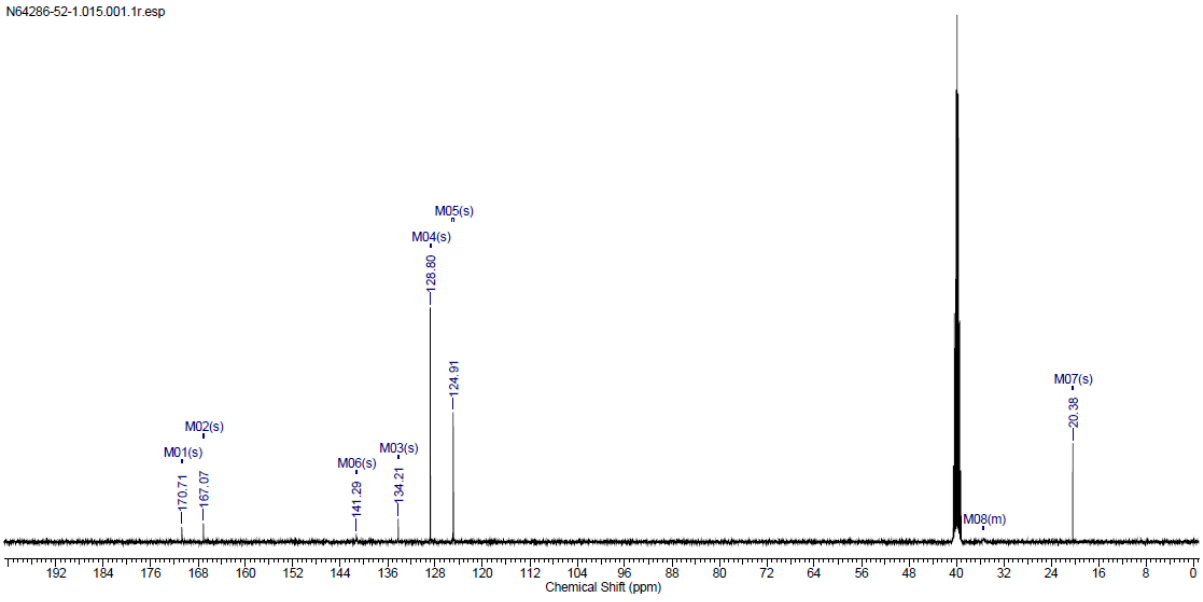
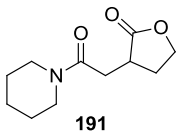




1.1.5. Substrate scope

3-(2-Oxo-2-(piperidin-1-yl)ethyl)dihydrofuran-2(3H)-one



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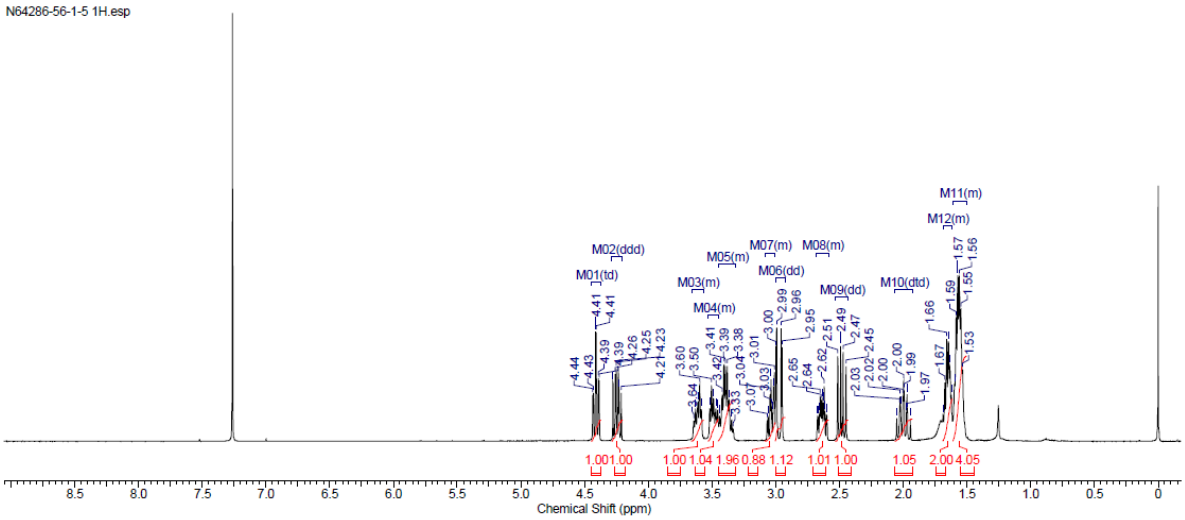
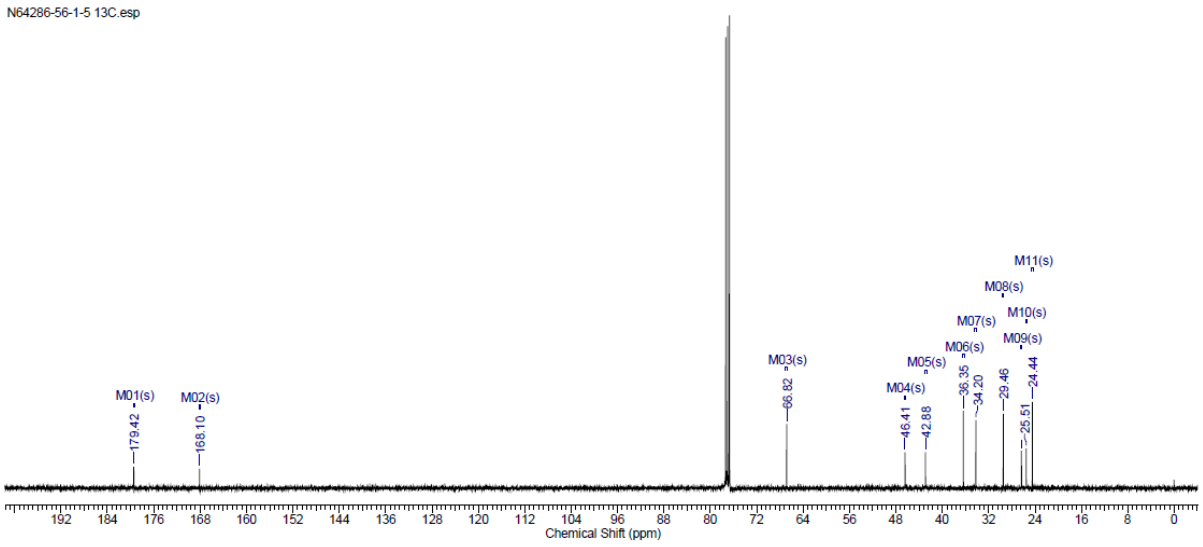
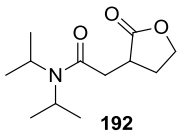




N,N-Diisopropyl-2-(2-oxotetrahydrofuran-3-yl)acetamide



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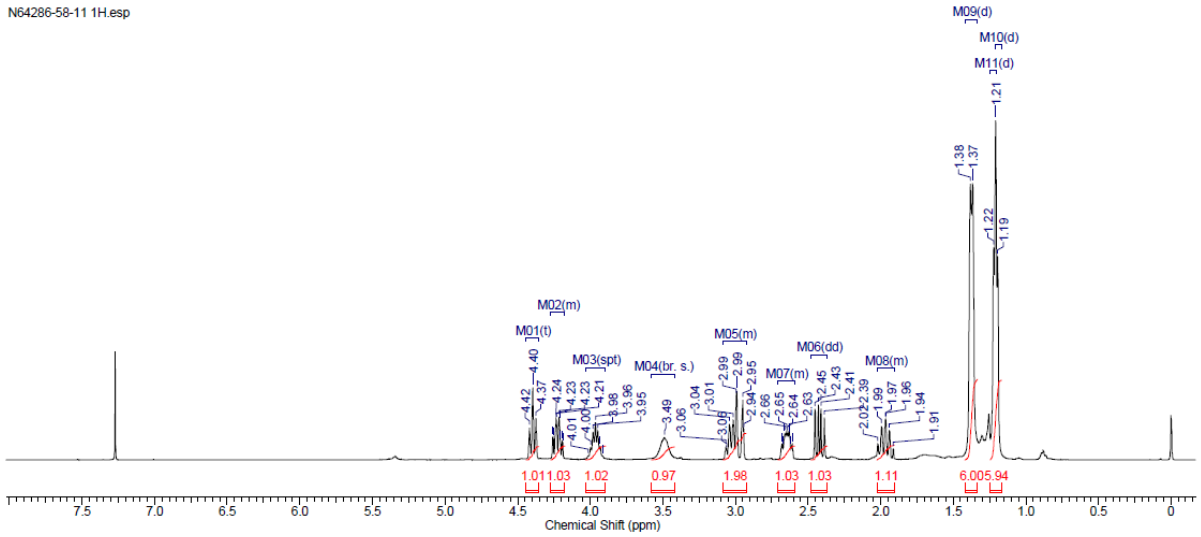
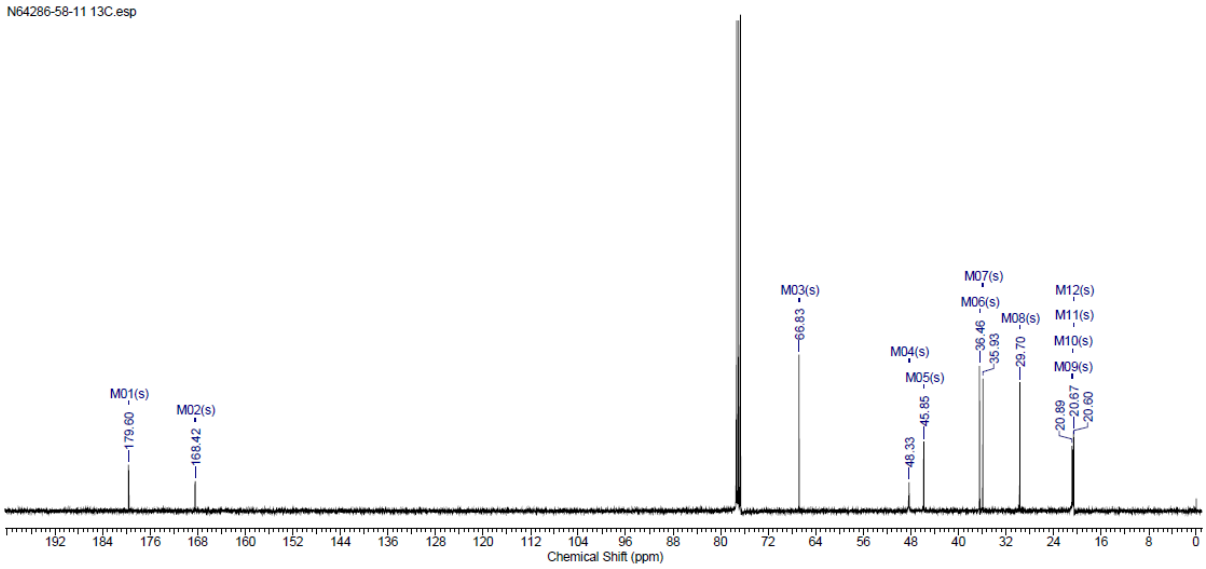
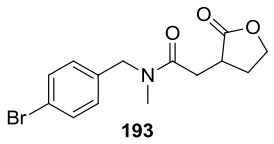




N-(4-Bromobenzyl)-N-methyl-2-(2-oxotetrahydrofuran-3-yl)acetamide



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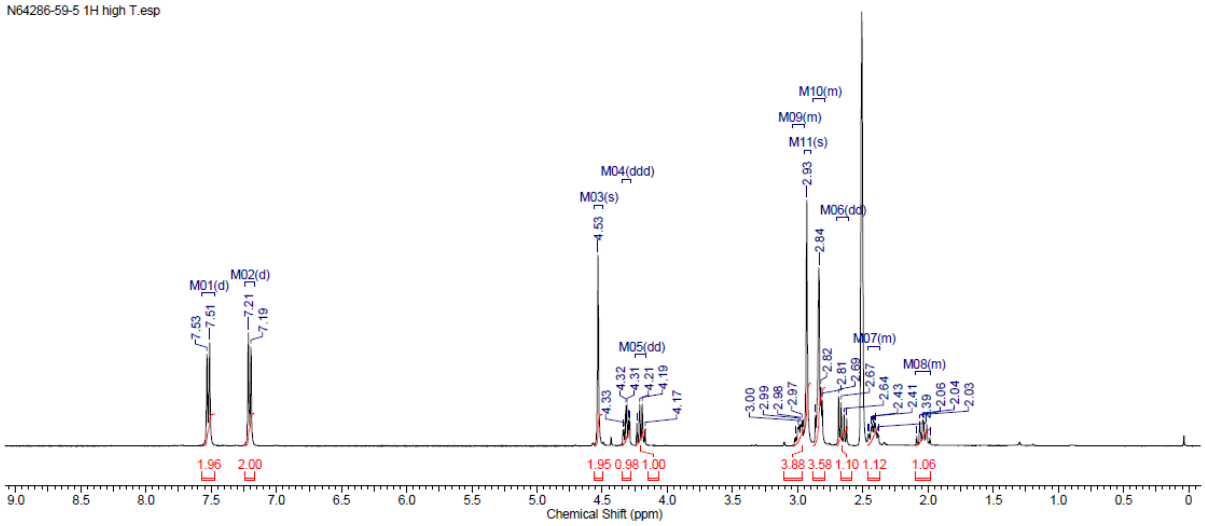
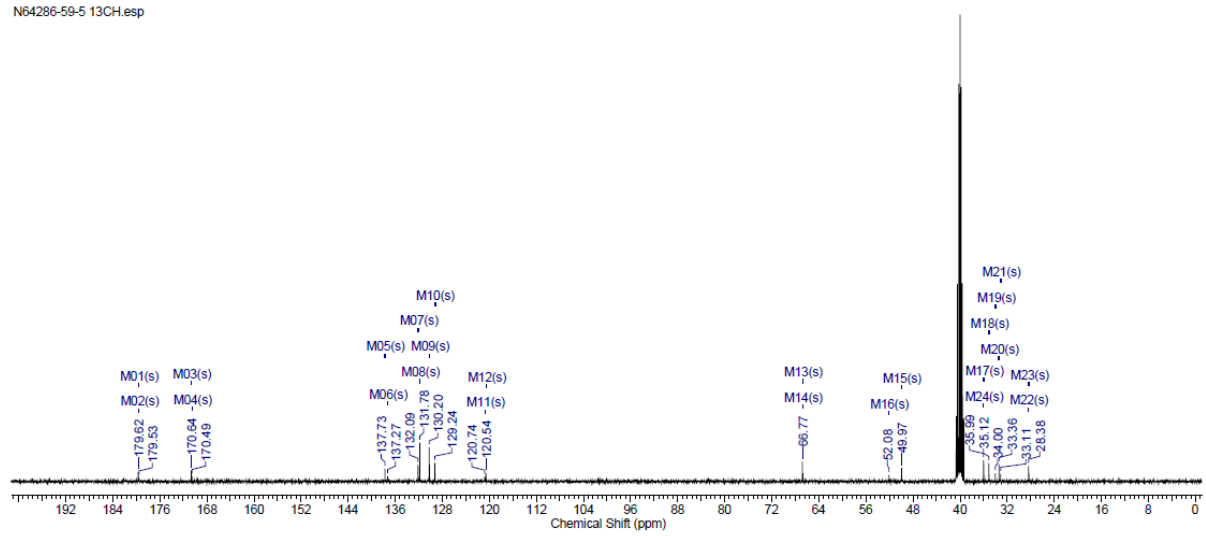
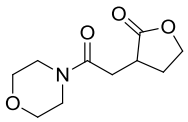




Dimethyl 2-(morpholine-4-carbonyl)succinate



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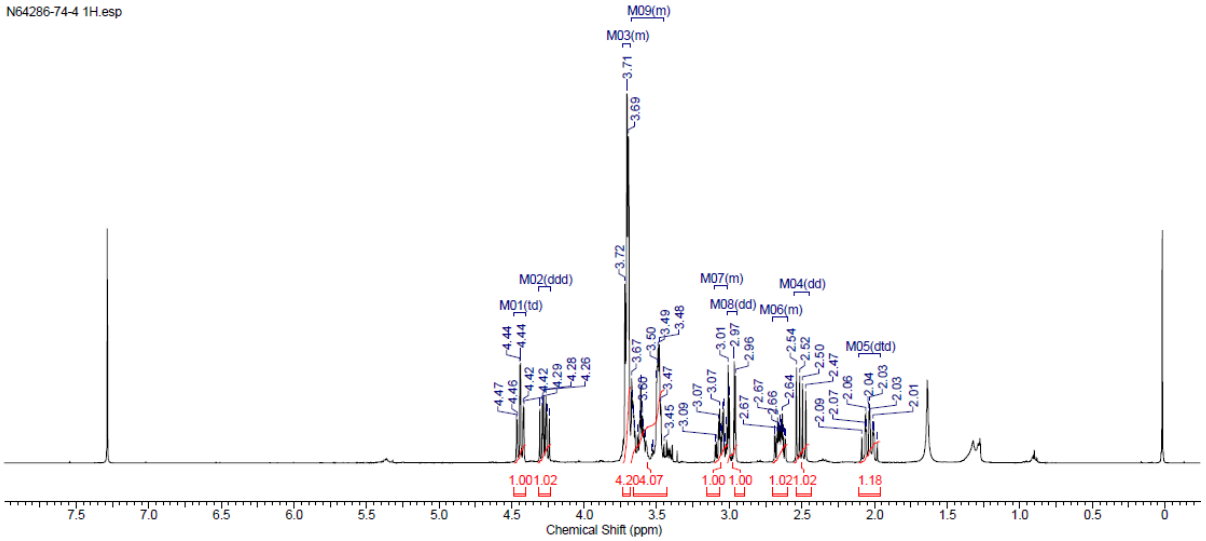
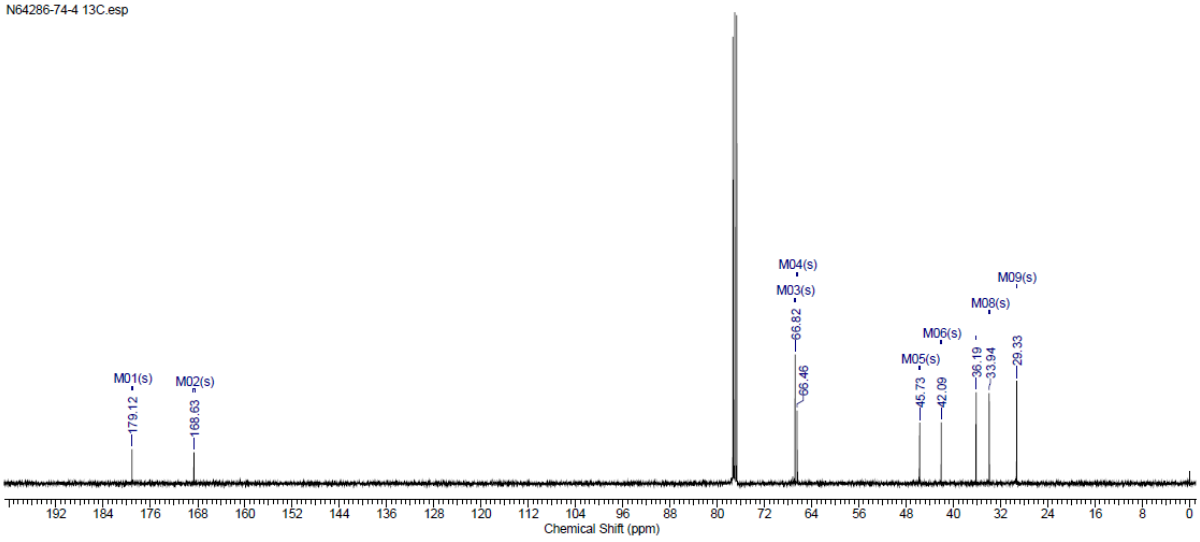
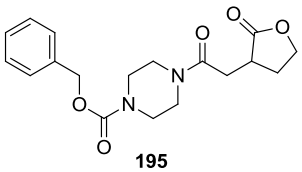




Benzyl4-(2-(2-oxotetrahydrofuran-3-yl)acetyl)piperazine-1-carboxylate



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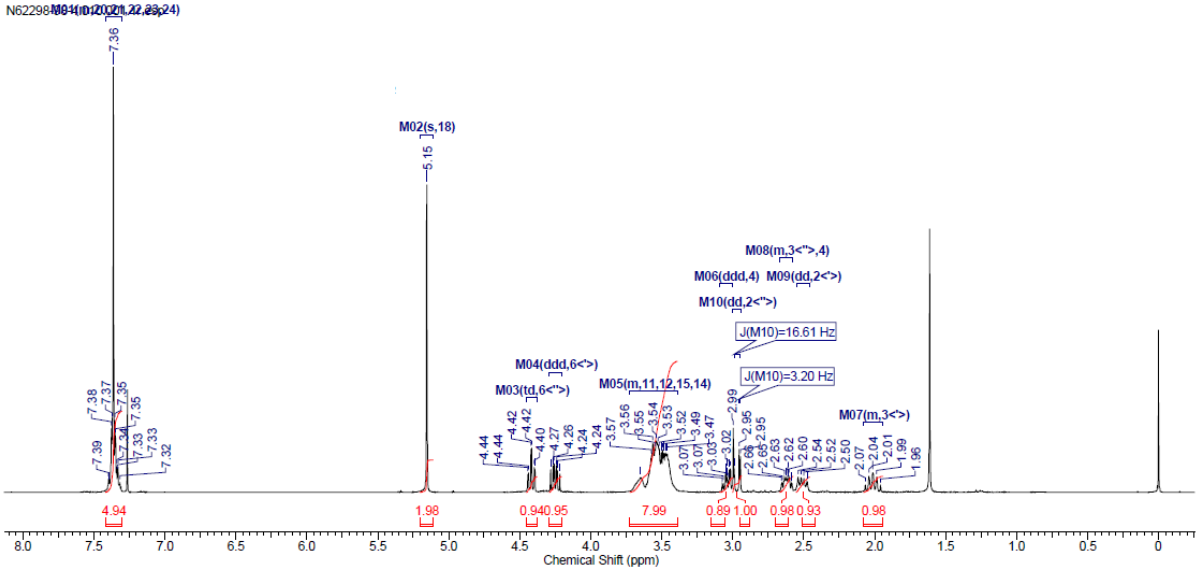
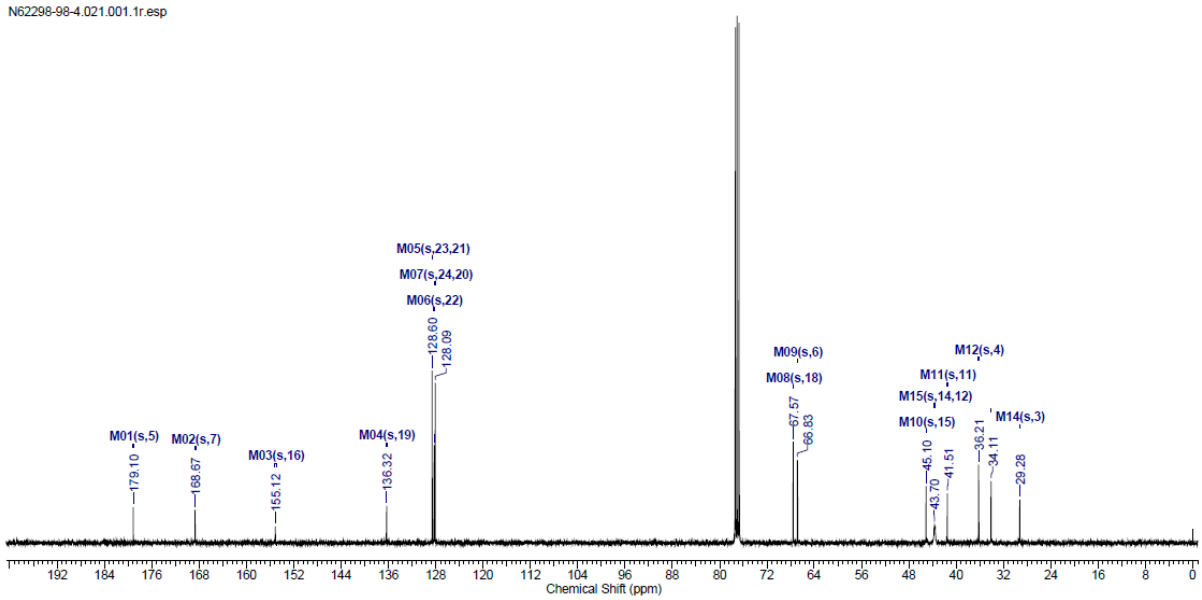
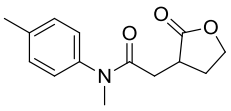




N-Methyl-2-(2-oxotetrahydrofuran-3-yl)-*N*-(*p*-tolyl)acetamide



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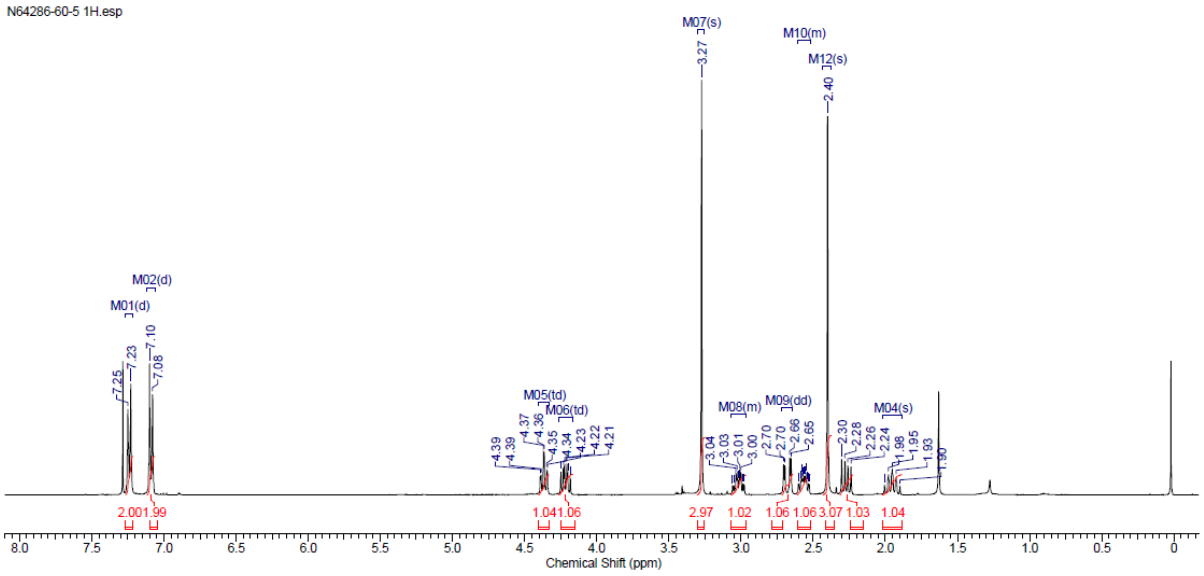
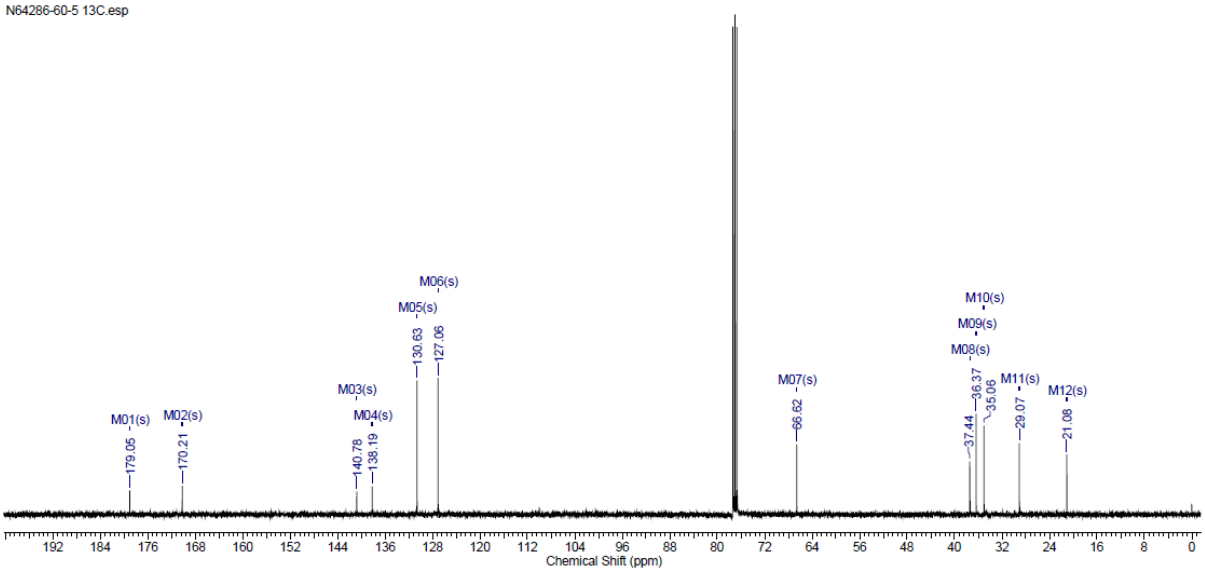
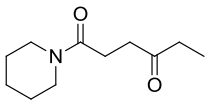




1-(Piperidin-1-yl)hexane-1,4-dione



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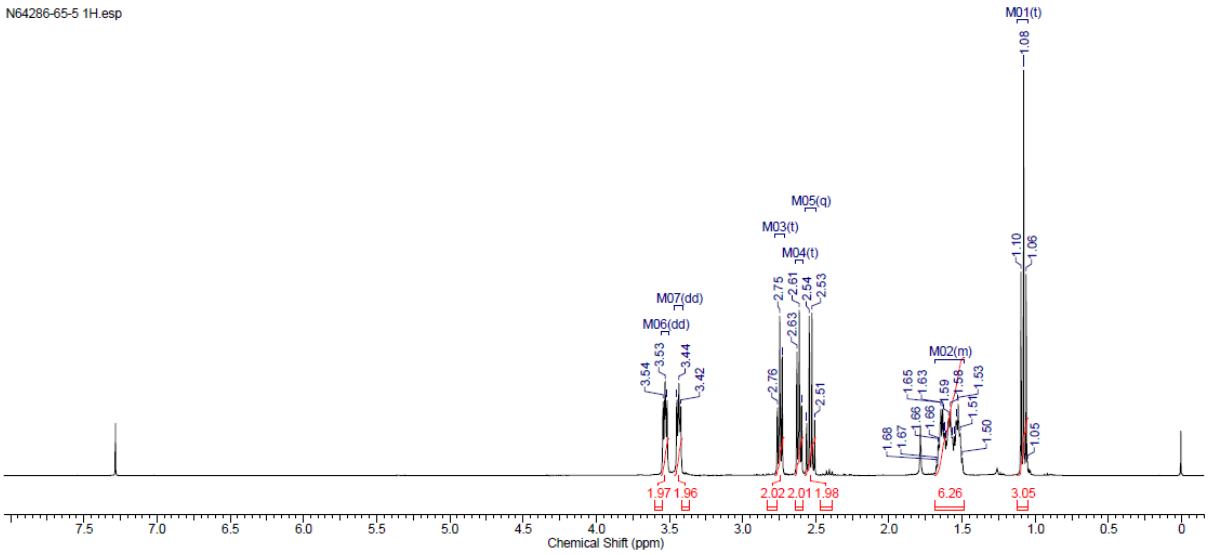
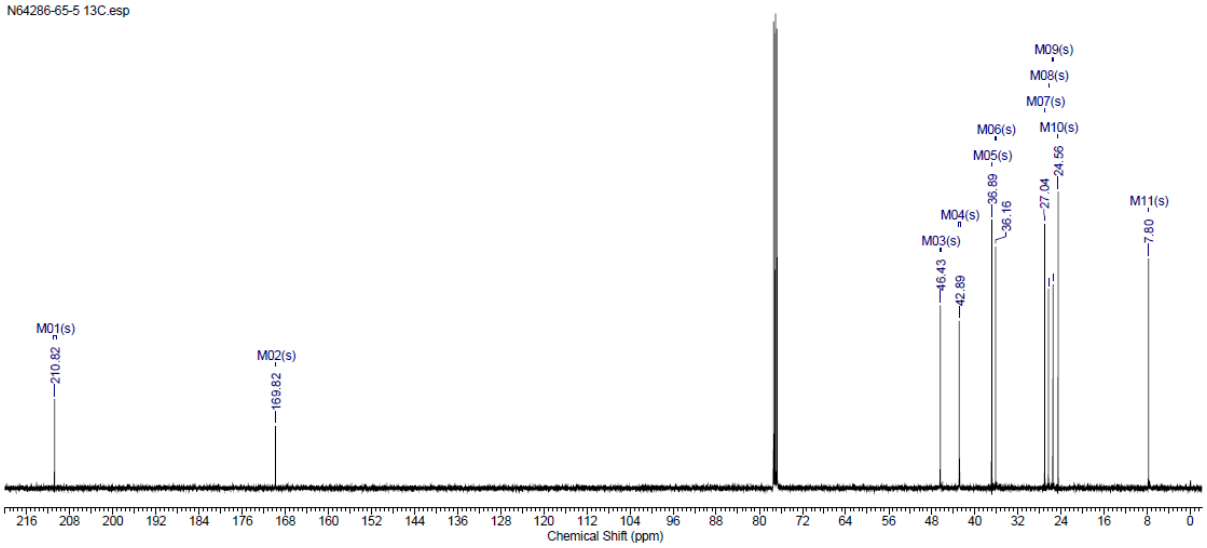
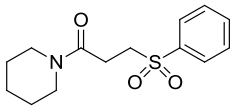




3-(Phenylsulfonyl)-1-(piperidin-1-yl)propan-1-one



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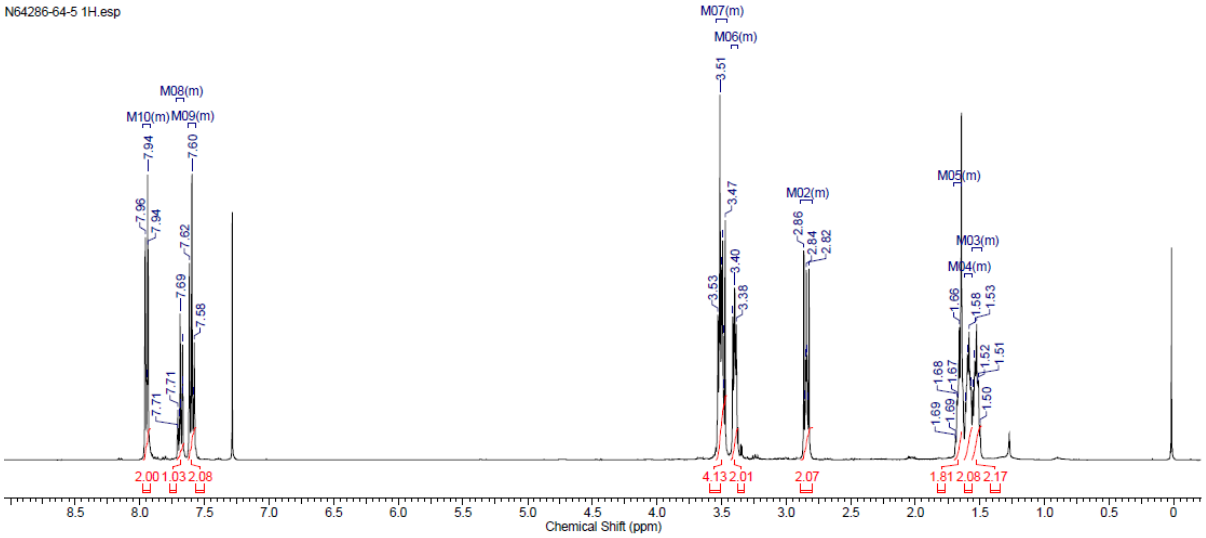
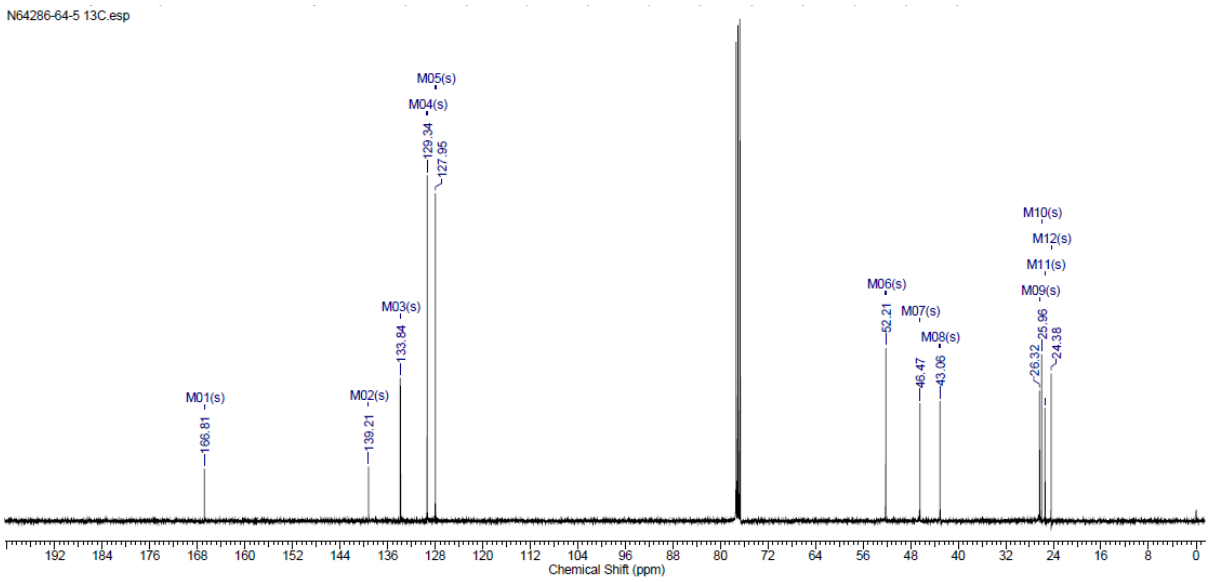
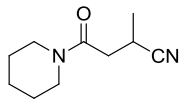




2-Methyl-4-oxo-4-(piperidin-1-yl)butanenitrile



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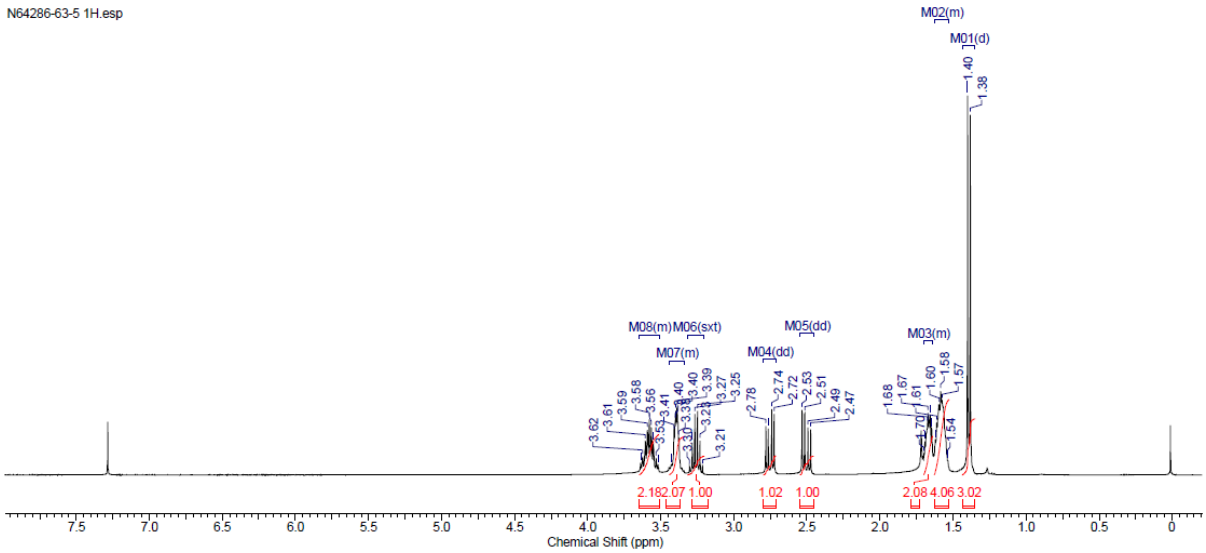
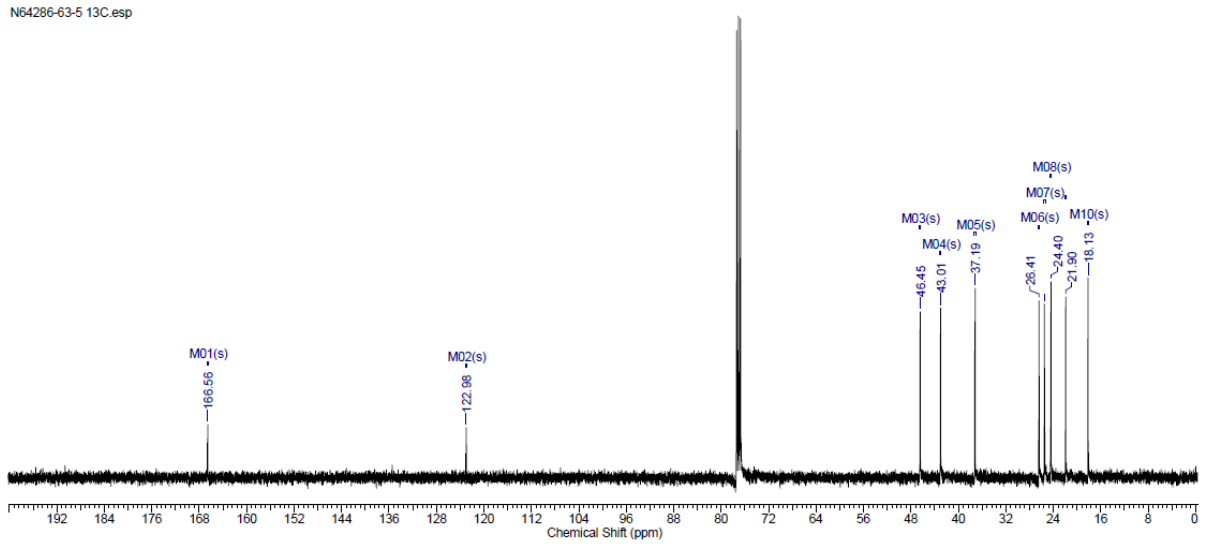
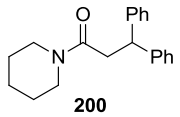




3,3-Diphenyl-1-(piperidin-1-yl)propan-1-one



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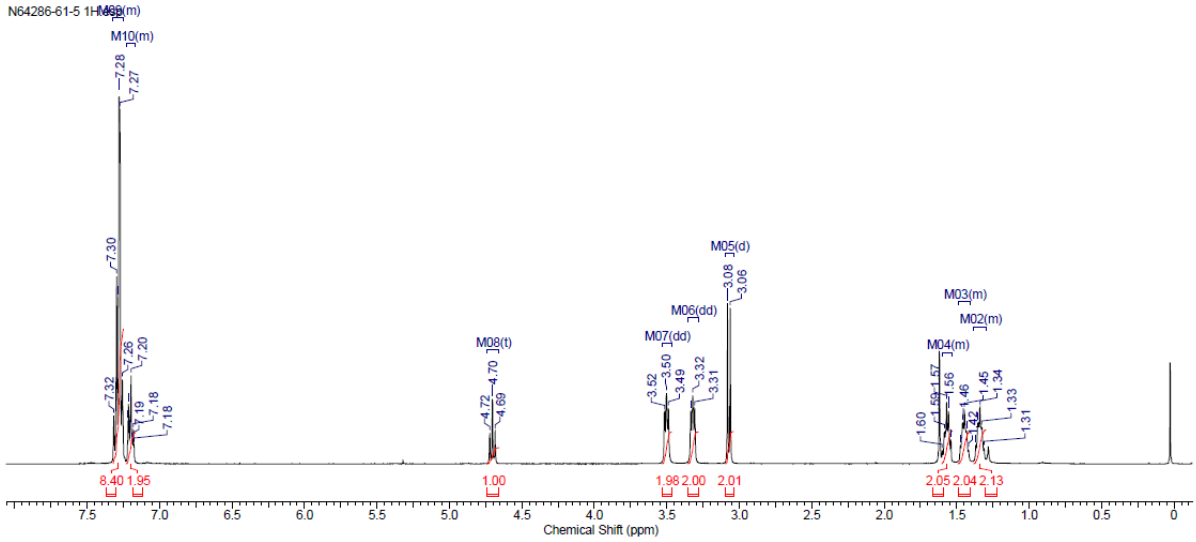
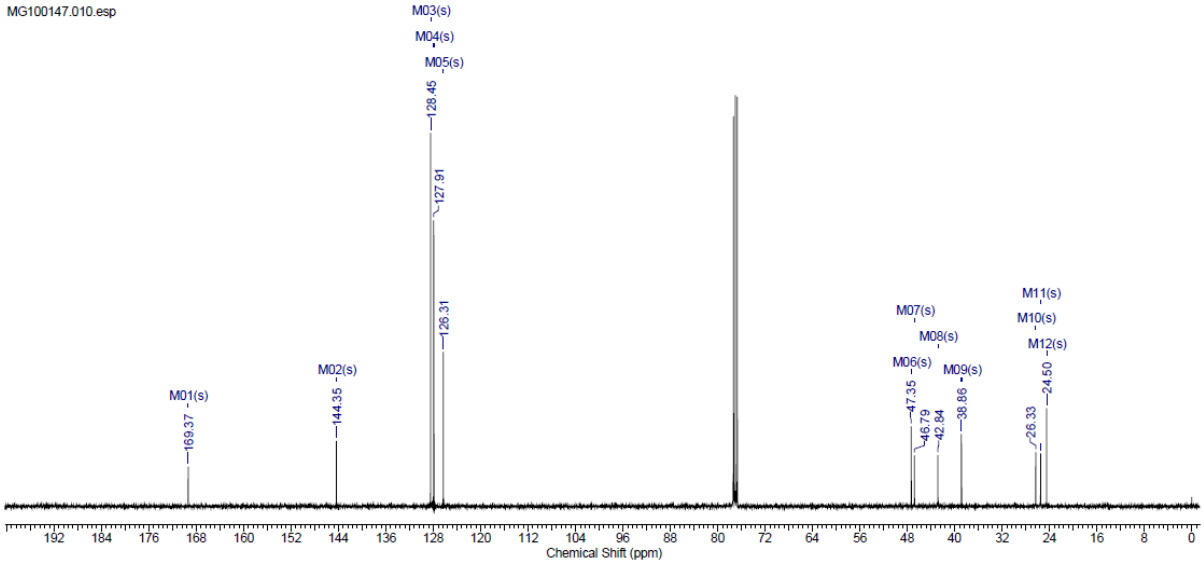
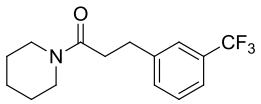




1-(Piperidin-1-yl)-3-(3-(trifluoromethyl)phenyl)propan-1-one



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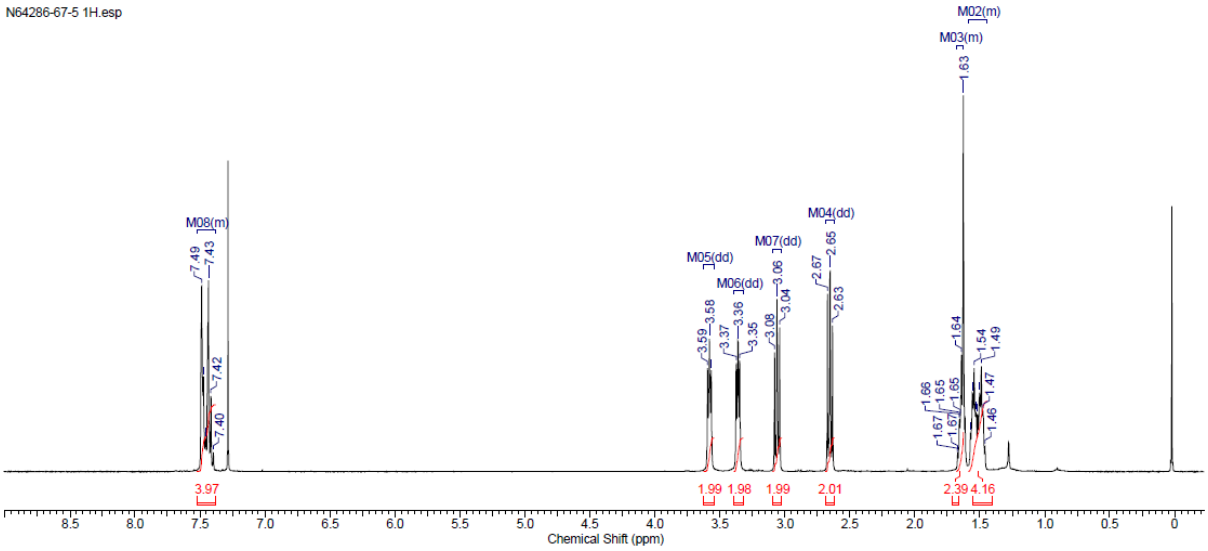

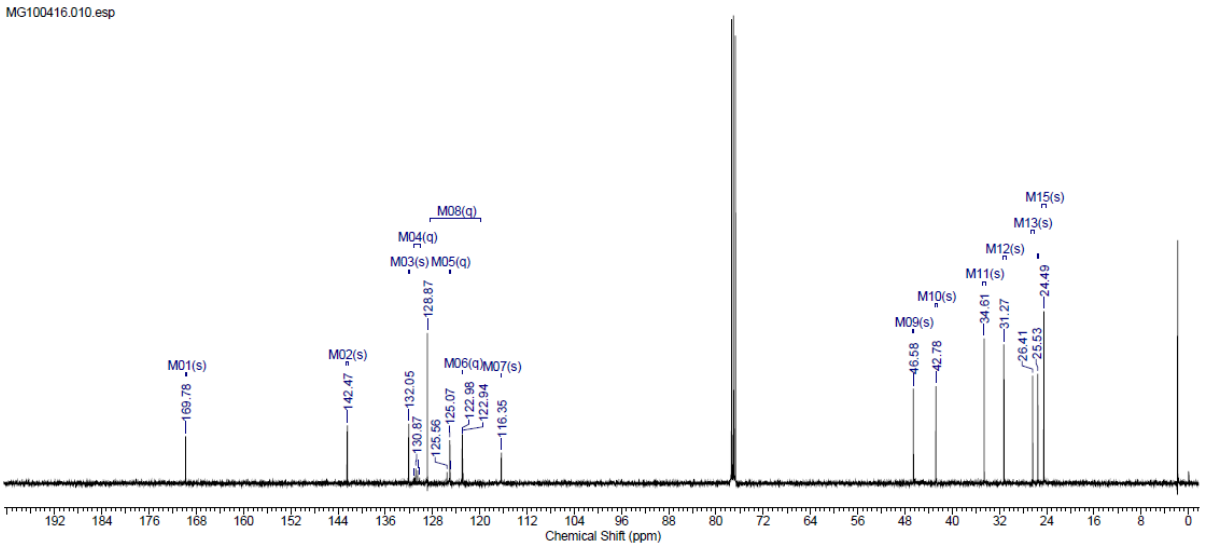

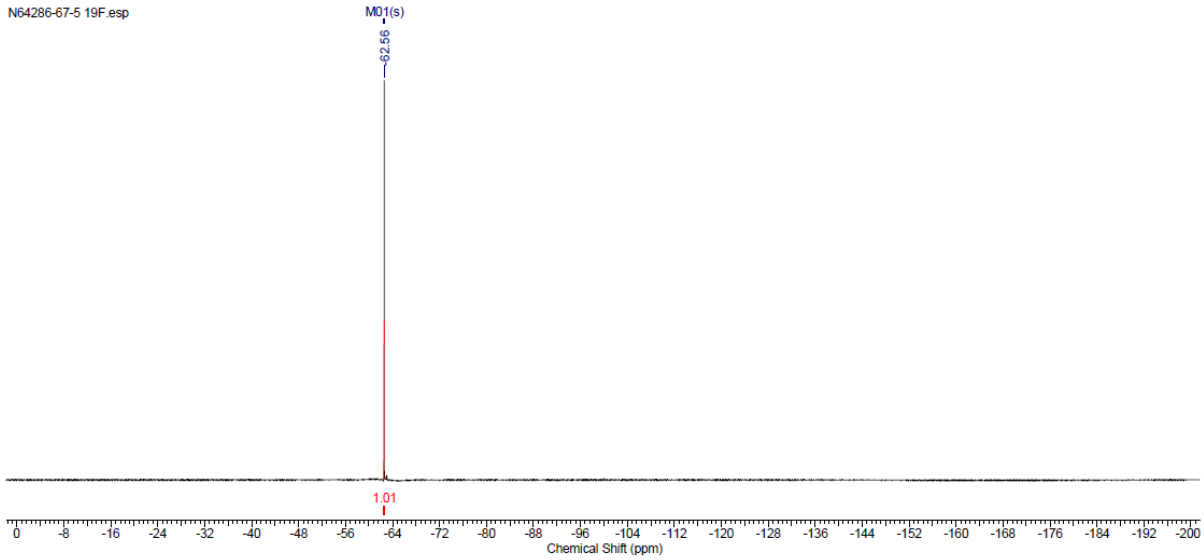
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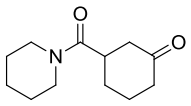
-62.56
1.01
0 -8 -16 -24 -32 -40 -48 -56 -64 -72 -80 -88 -96 -104 -112 -120 -128 -136 -144 -152 -160 -168 -176 -184 -192 -200
Chemical Shift (ppm)

3-(Piperidine-1-carbonyl)cyclohexan-1-one



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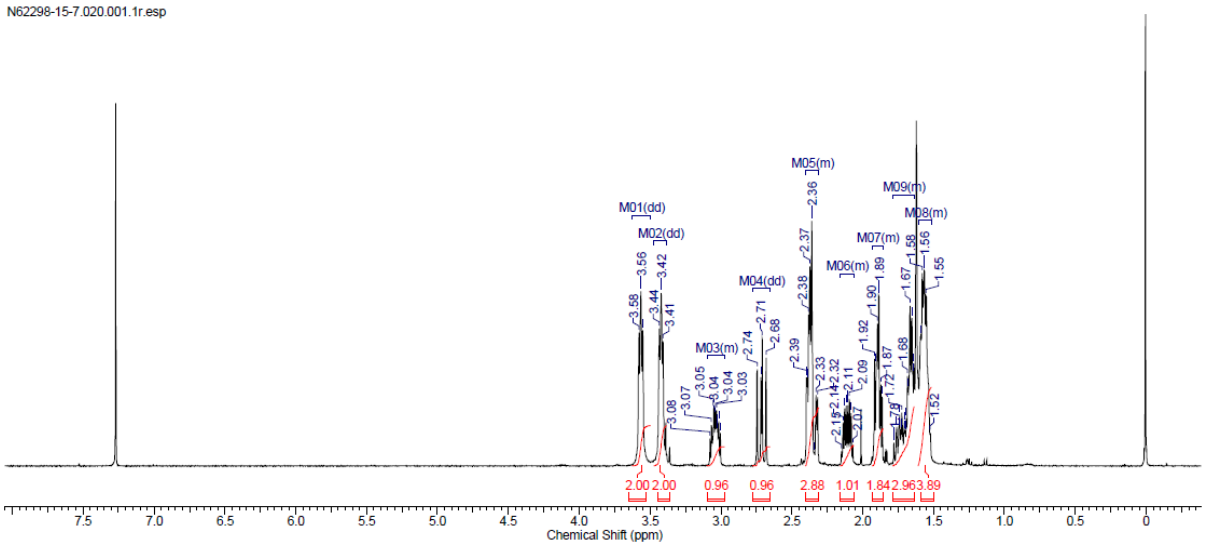
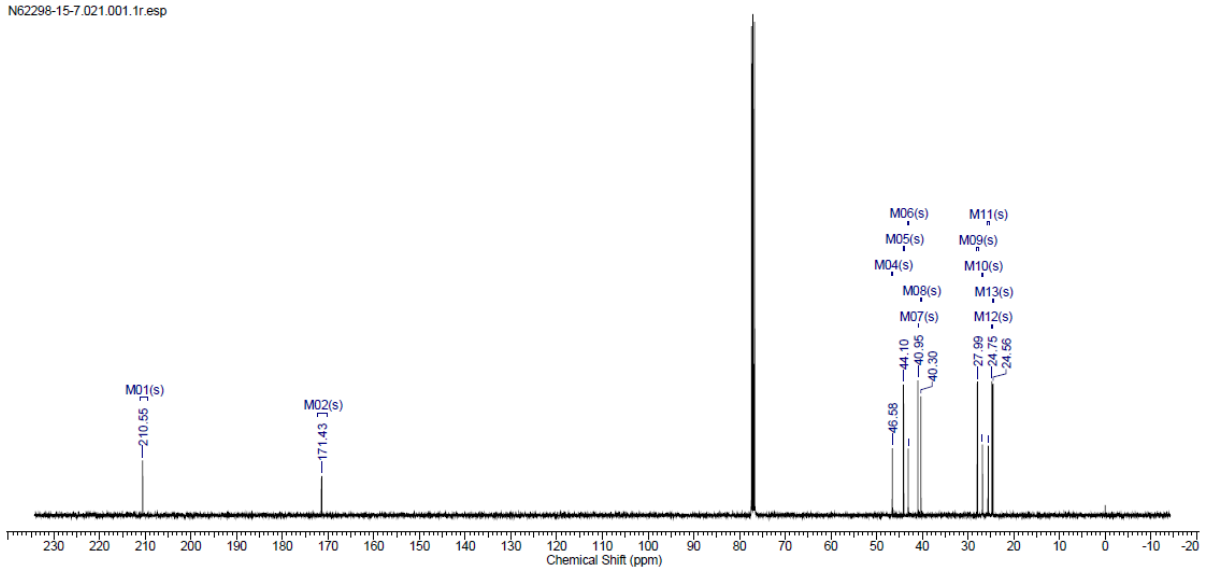
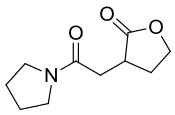




3-(2-Oxo-2-(pyrrolidin-1-yl)ethyl)dihydrofuran-2(3H)-one



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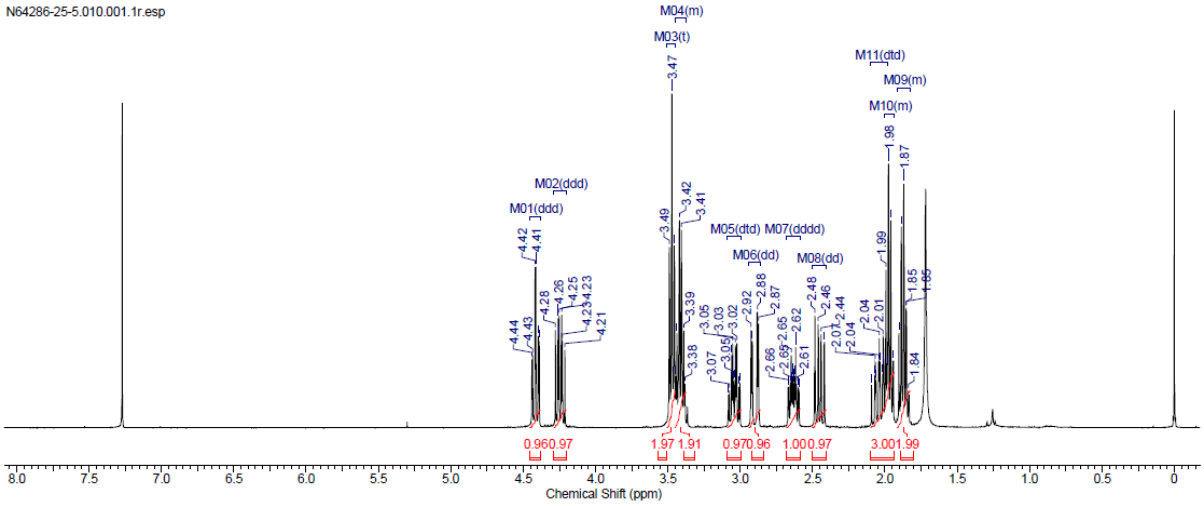
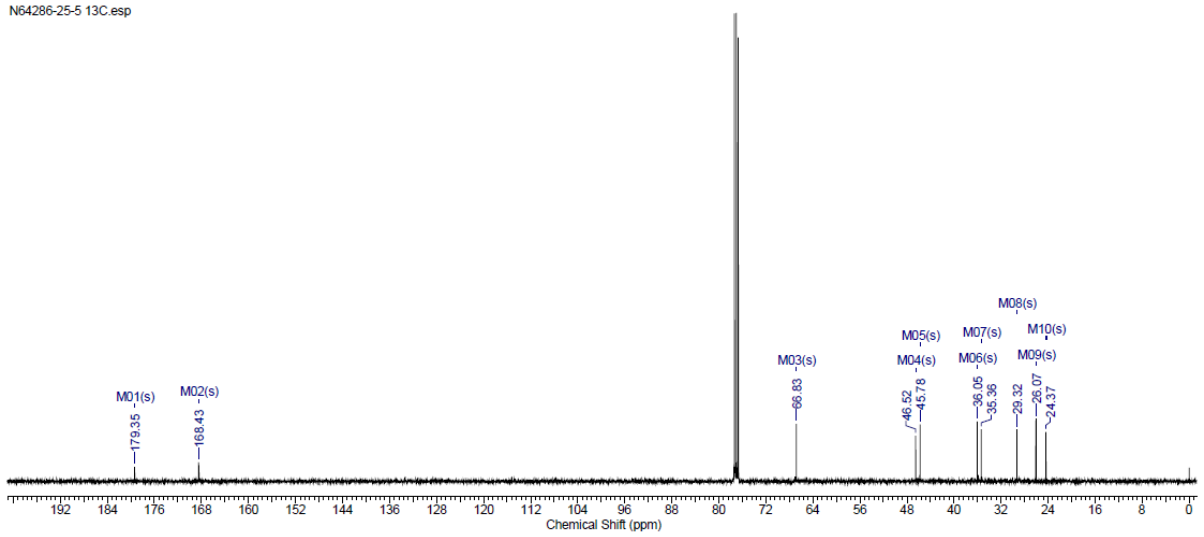
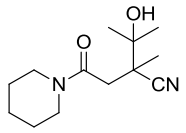




3-Hydroxy-2,3-dimethyl-2-(2-oxo-2-(piperidin-1-yl)ethyl)butanenitrile



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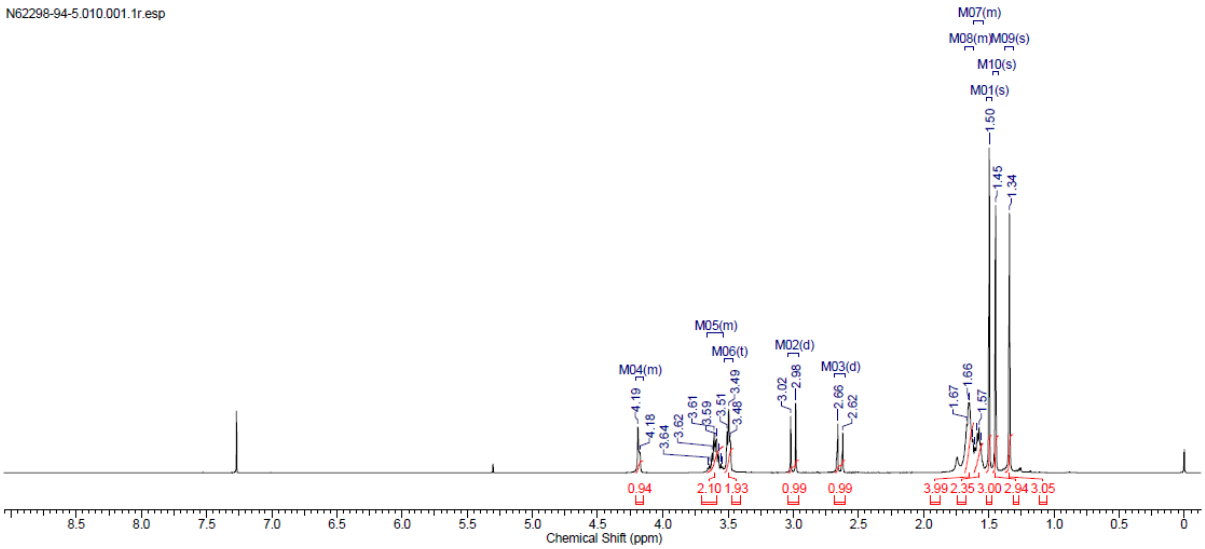

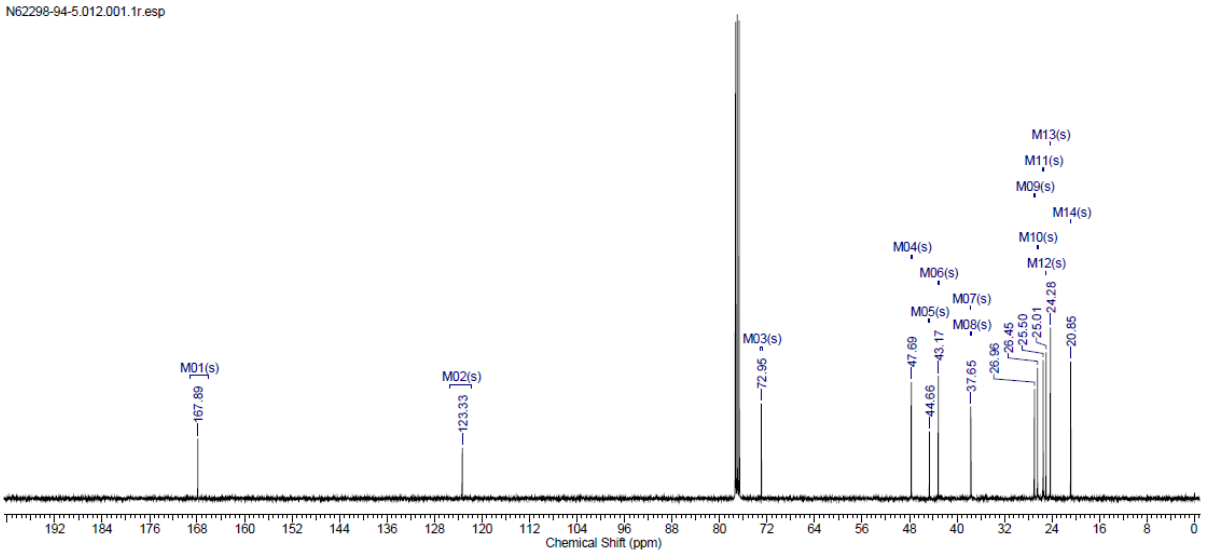

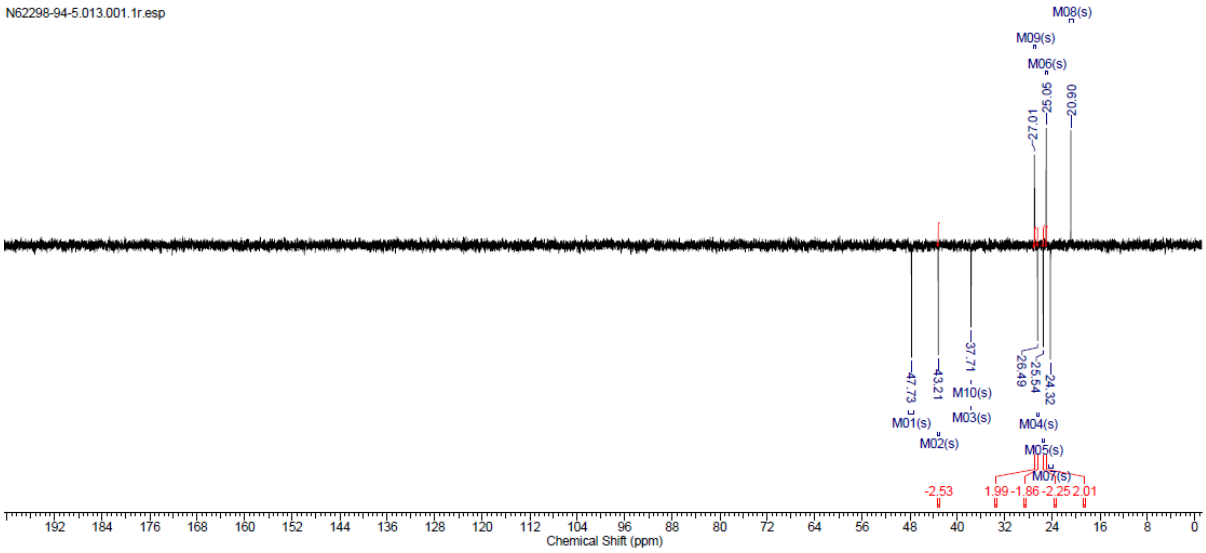
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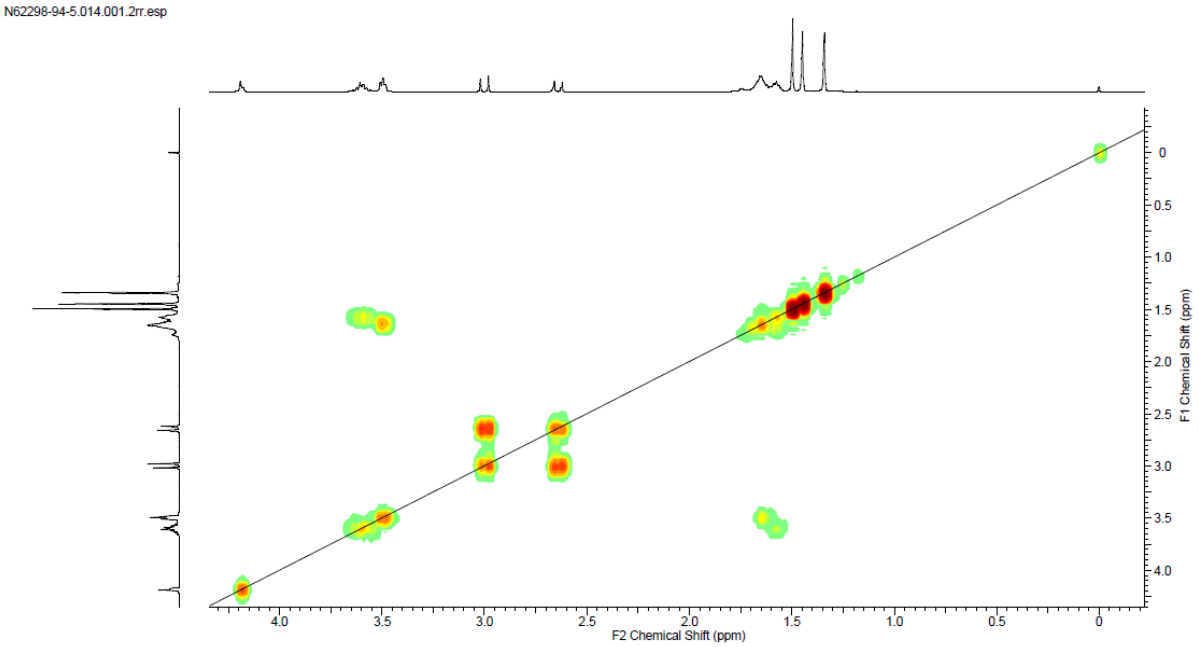
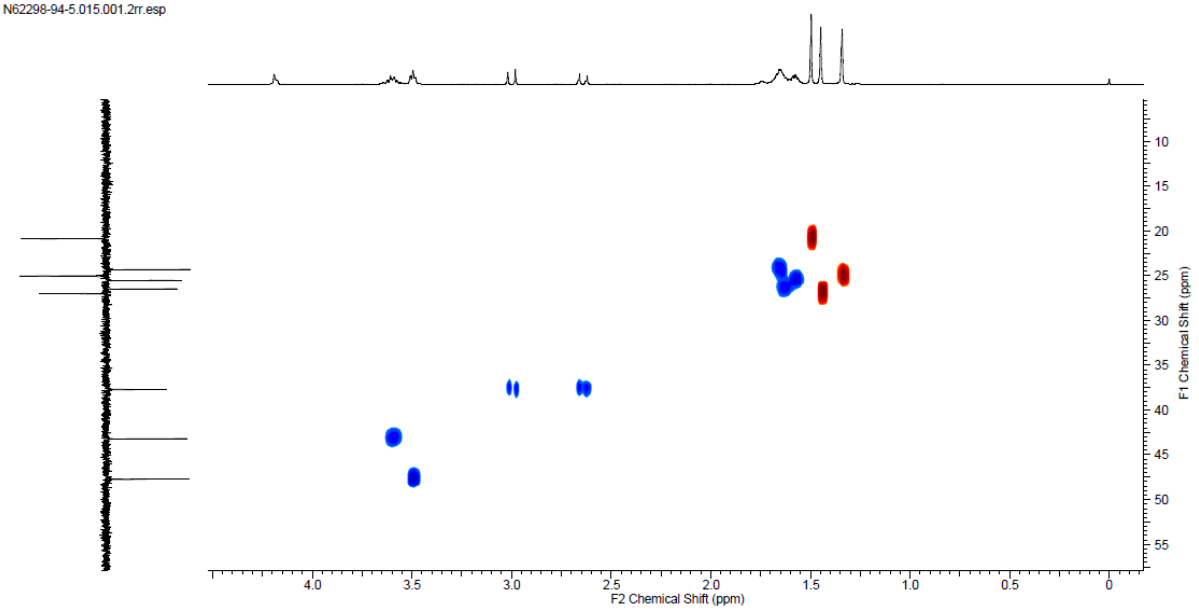
M09(s)
M06(s)
27.01
25.05
20.90
47.73
43.21
37.71
26.49
25.54
24.32
M01(s)
M02(s)
M10(s)
M03(s)
M04(s)
M05(s)
M07(s)
-2.53
1.99
-1.86
-2.25
2.01
Chemical Shift (ppm)


N62298-94-5.014.001.2rr.esp
F1 Chemical Shift (ppm)
F2 Chemical Shift (ppm)

N62298-94-5.015.001.2rr.esp



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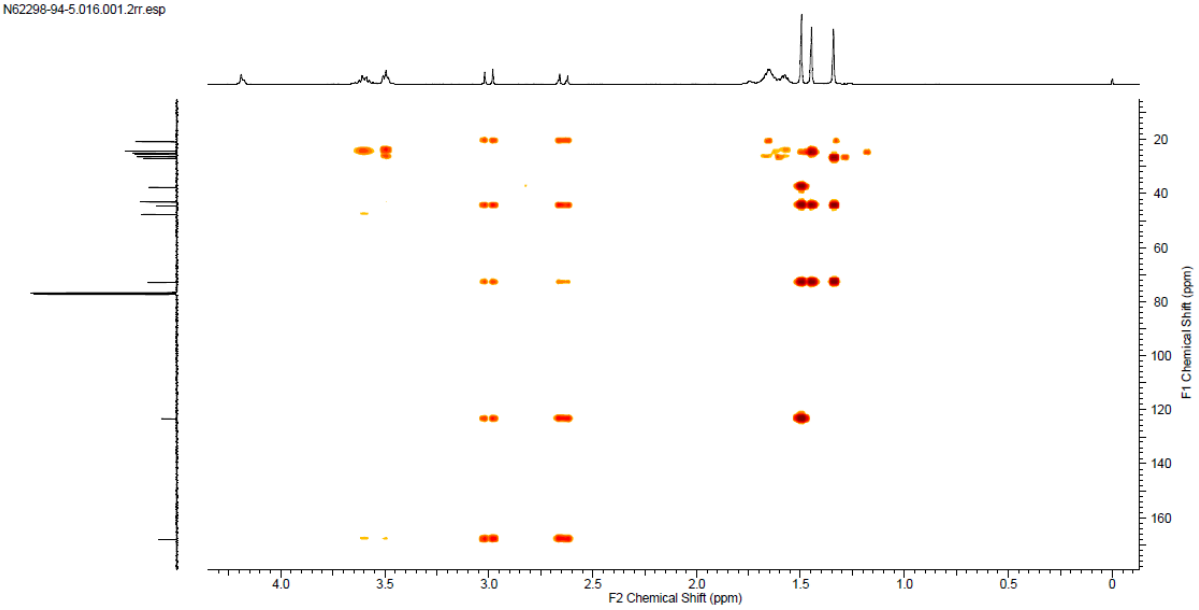
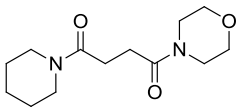


1-Morpholino-4-(piperidin-1-yl)butane-1,4-dione



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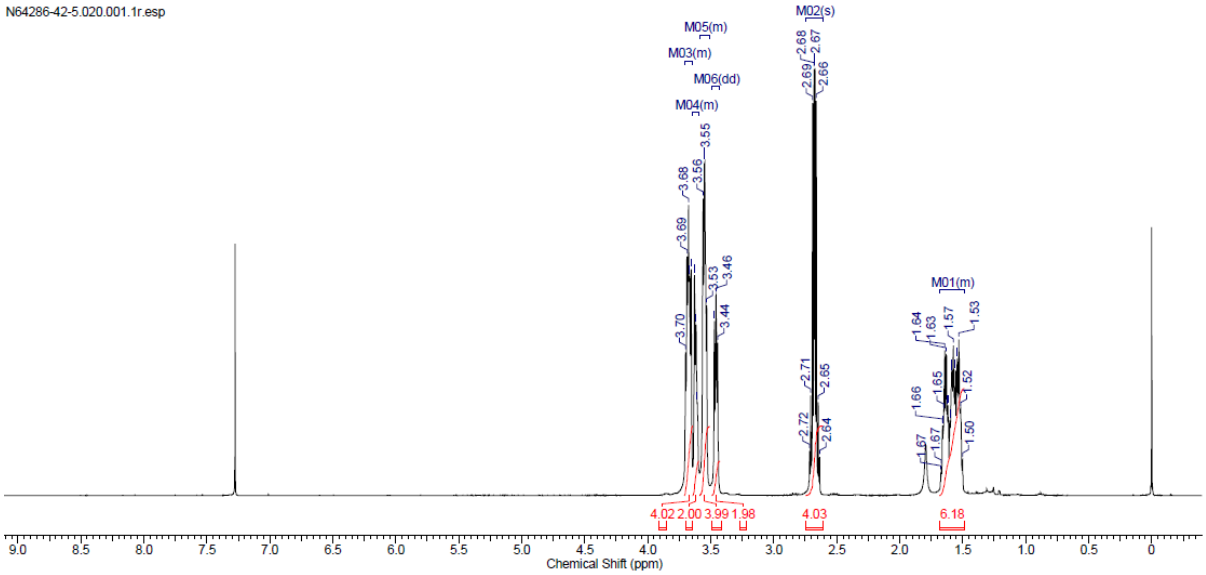
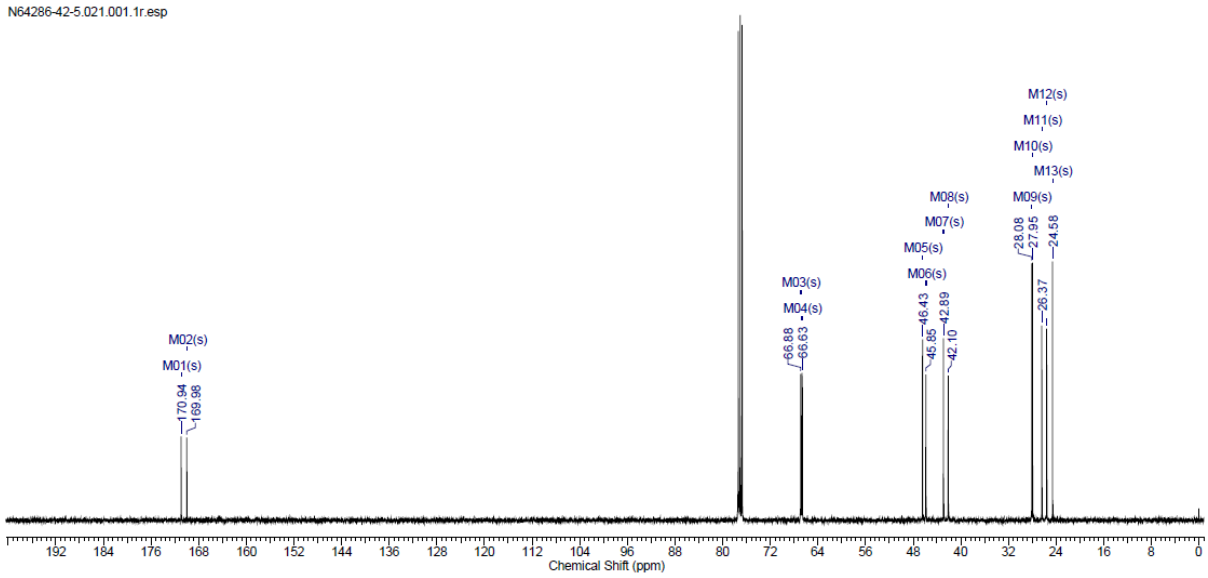
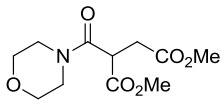




Dimethyl 2-(morpholine-4-carbonyl)succinate



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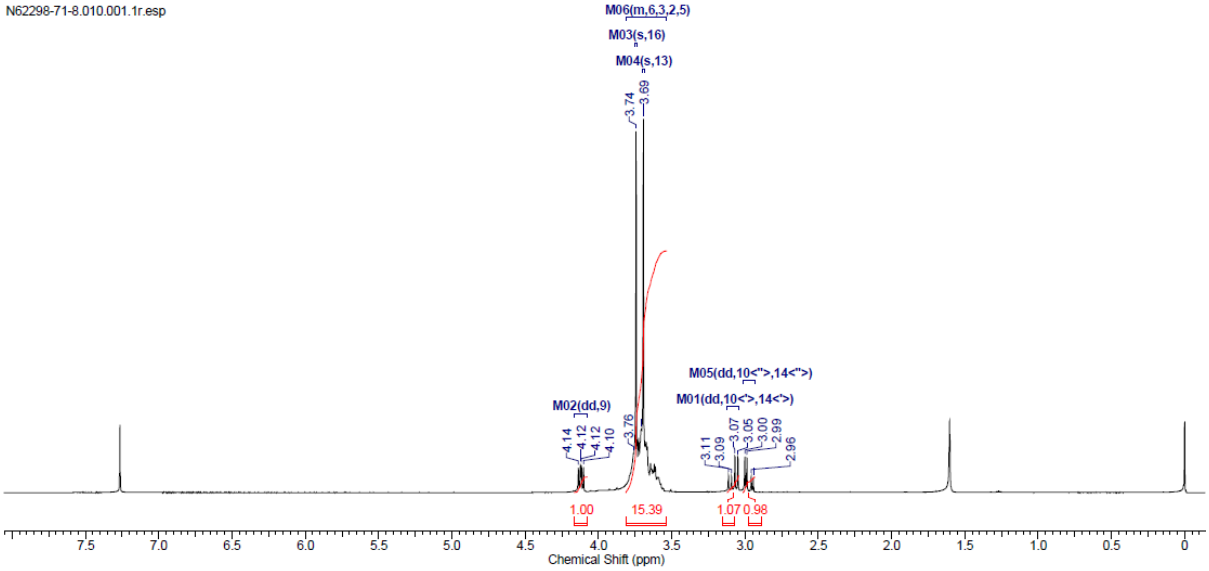
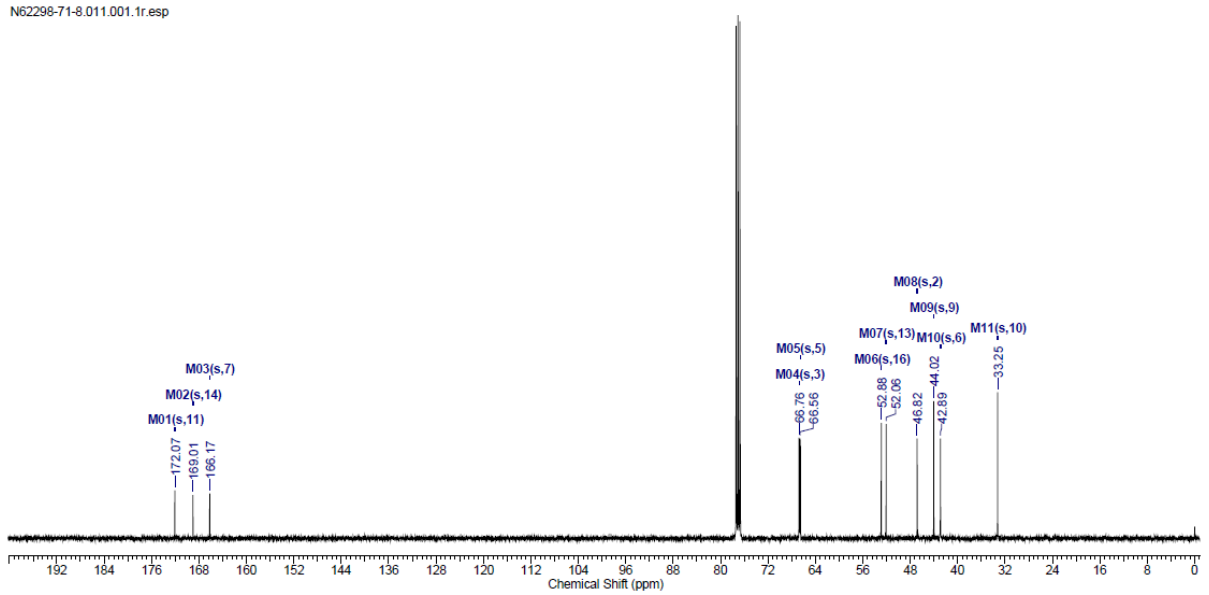
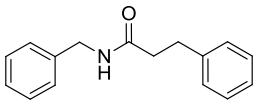




1.2. NMR Spectra for compounds synthesised in Chapter 2

1.2.1. Substrate scope in isocyanate

N-Benzyl-3-phenylpropanamide



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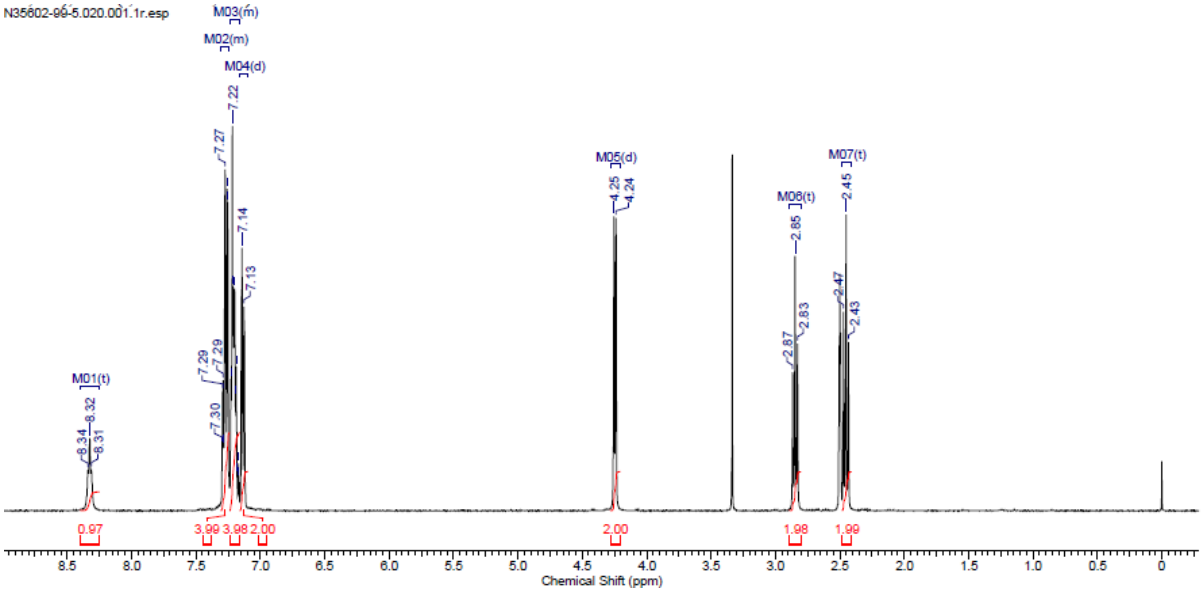
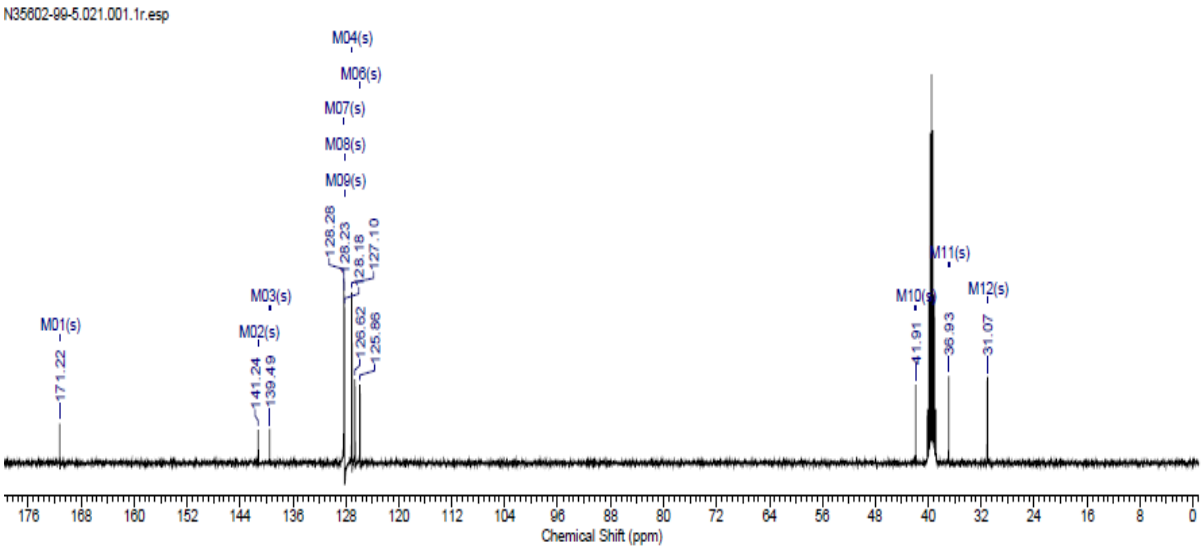
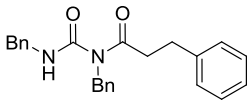




N-Benzyl-*N*-(benzylcarbamoyl)-3-phenylpropanamide



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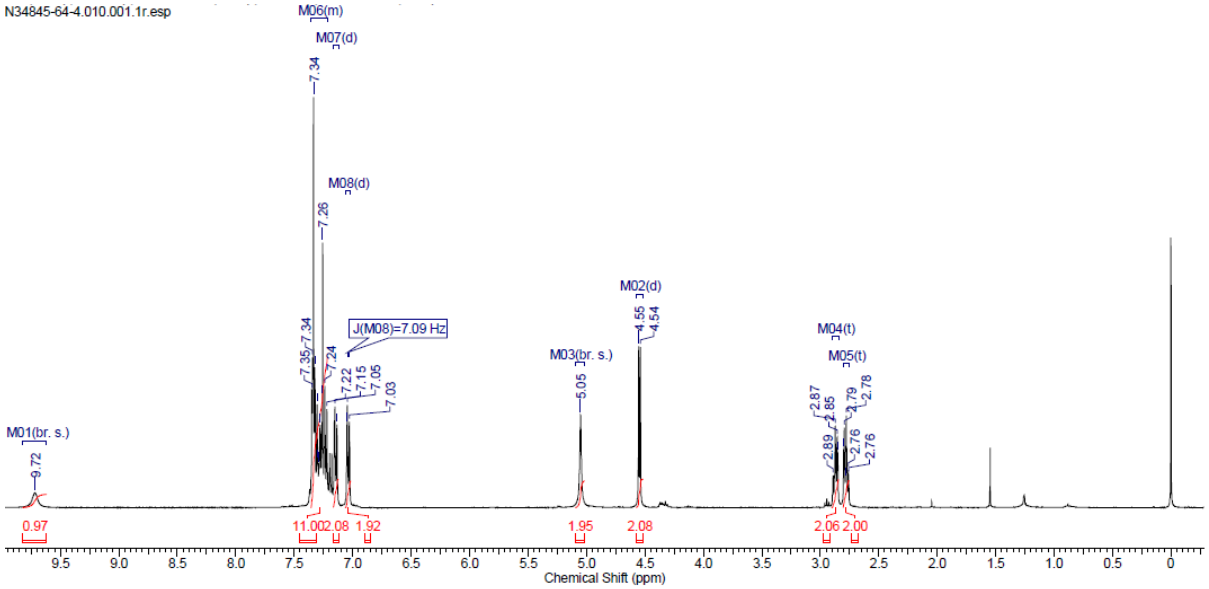
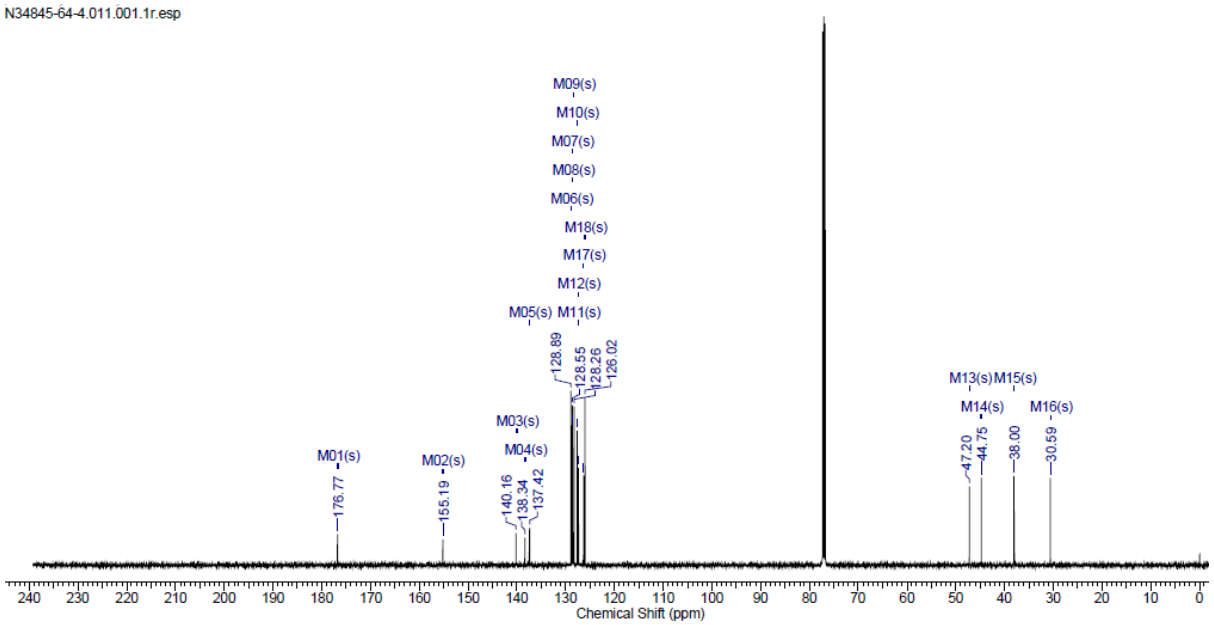
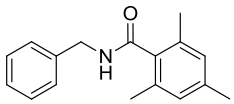




N-Benzyl-2,4,6-trimethylbenzamide



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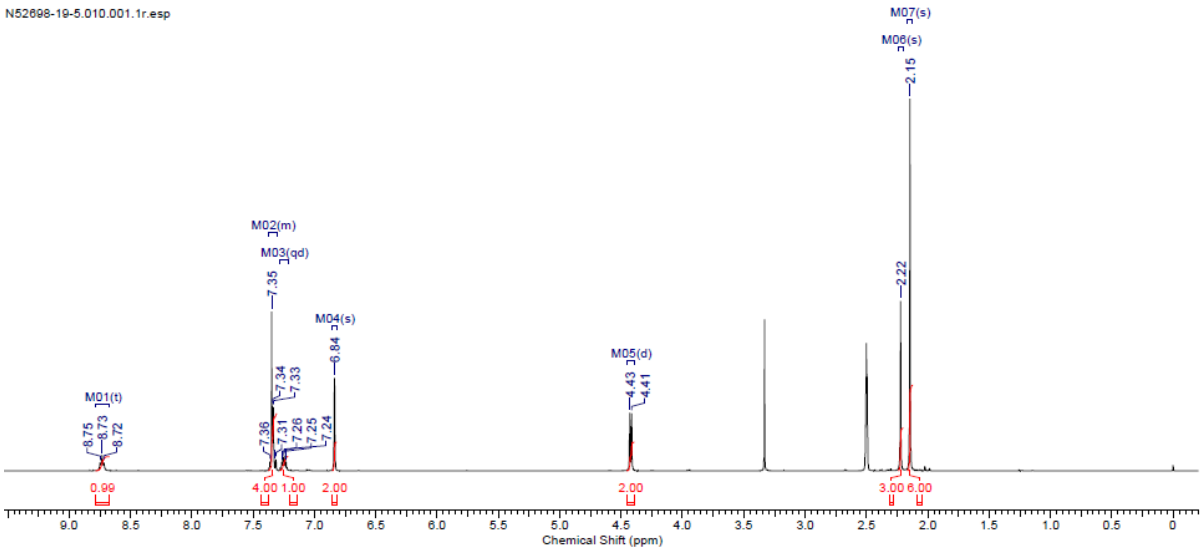
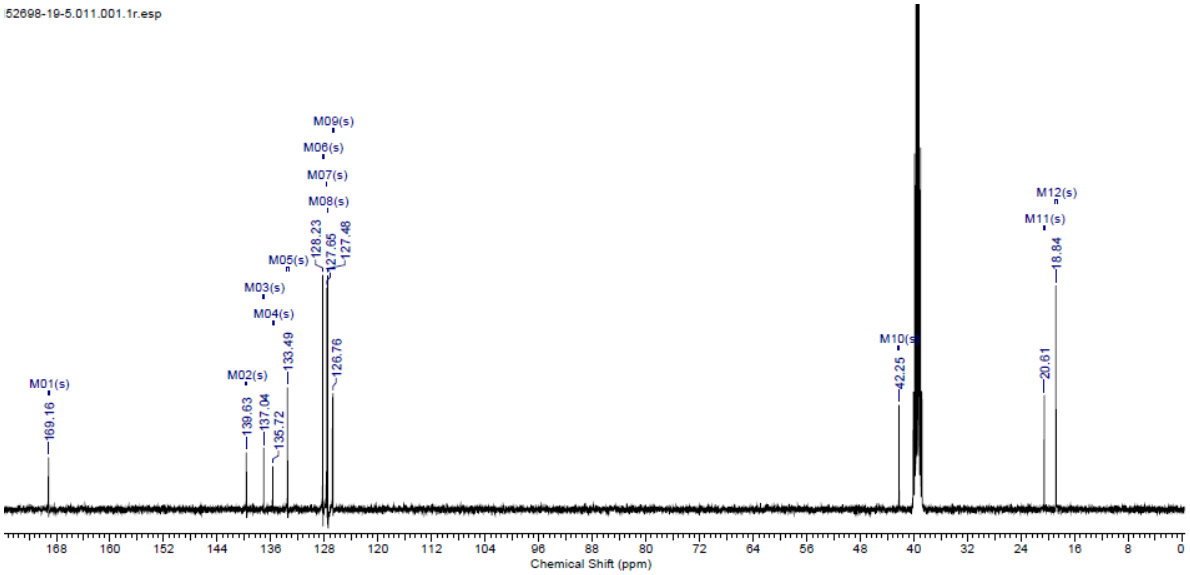
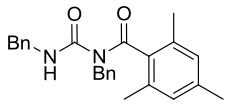




N-Benzyl-*N*-(benzylcarbamoyl)-2,4,6-trimethylbenzamide



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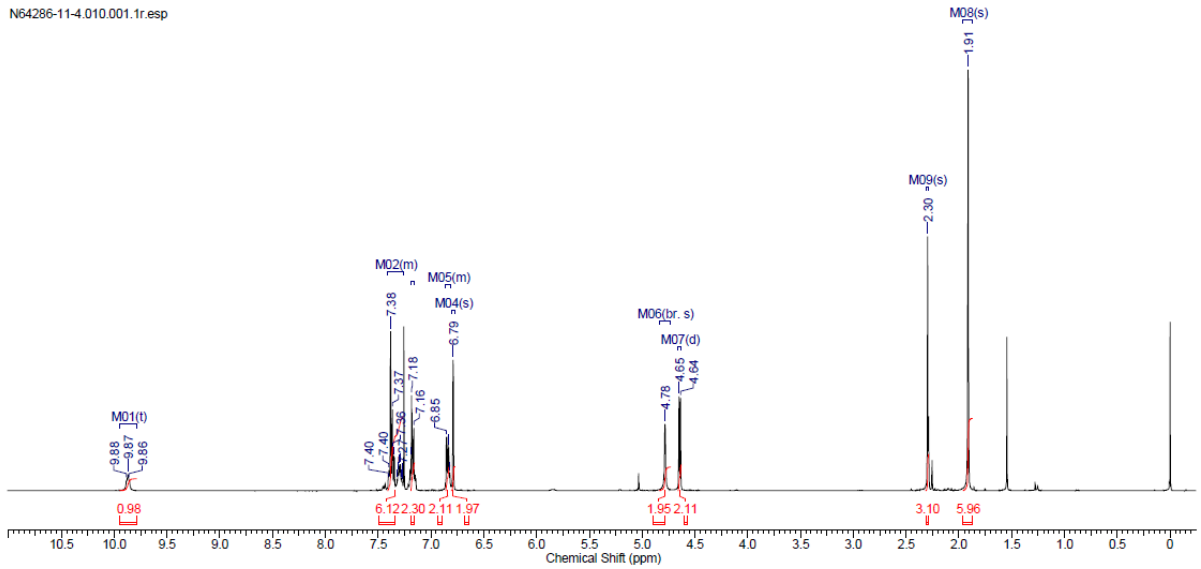
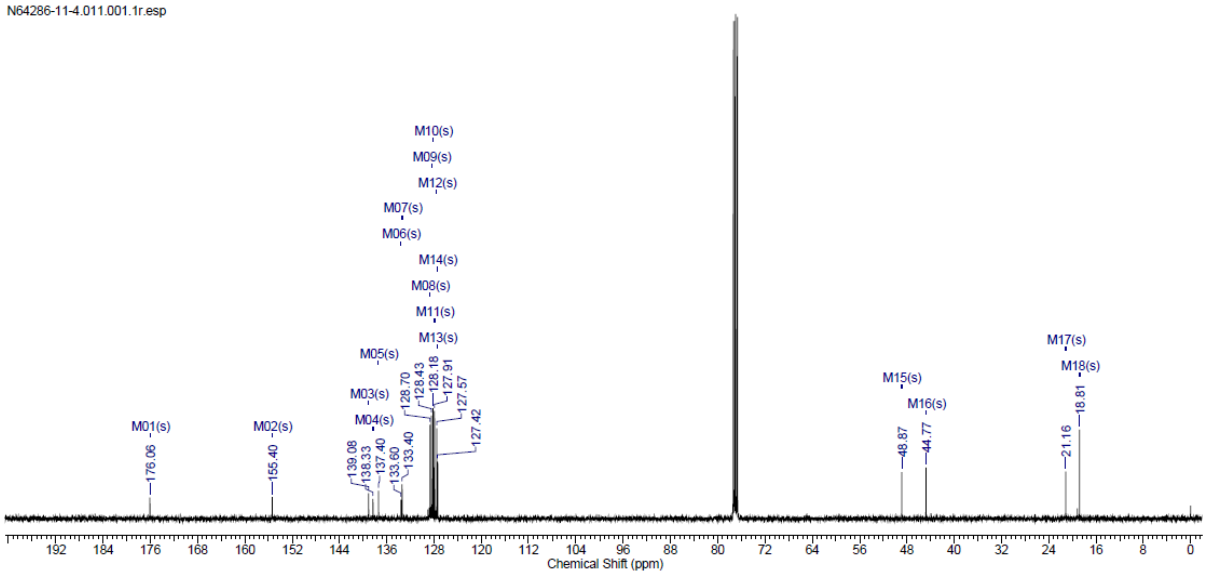
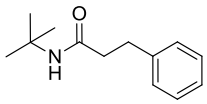




N-(*tert*-Butyl)-3-phenylpropanamide



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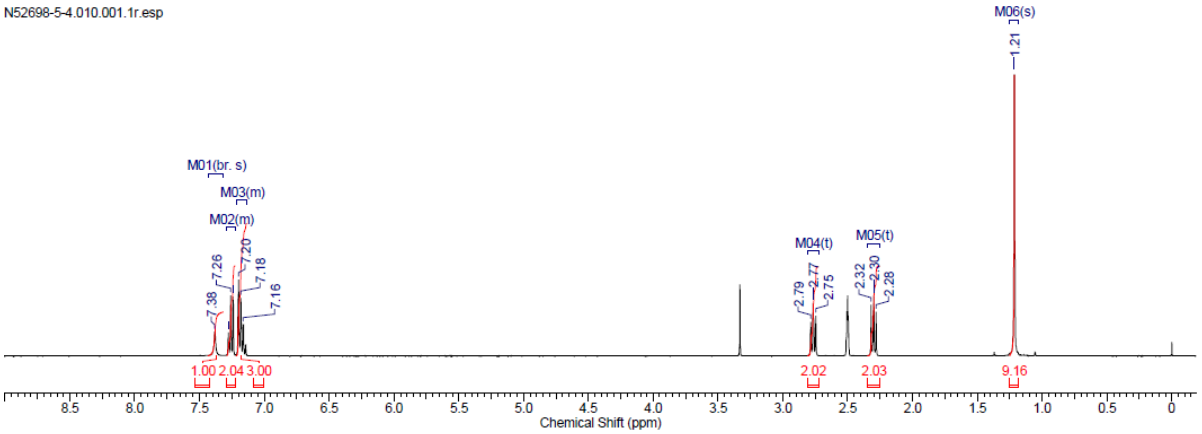
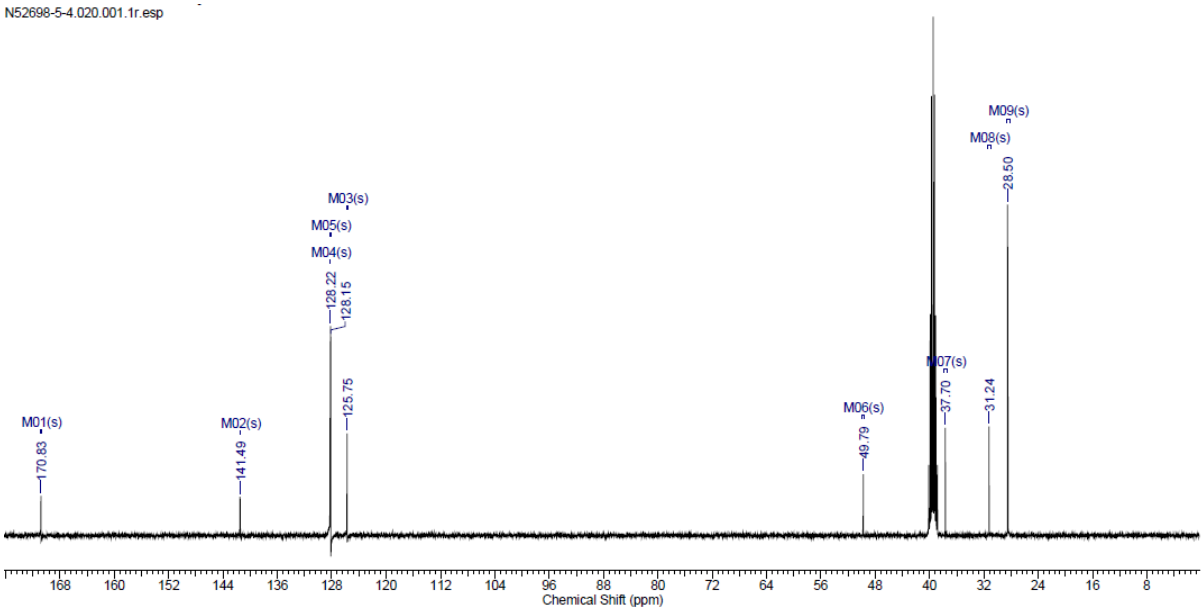
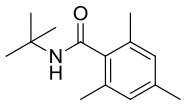




N-(*tert*-Butyl)-2,4,6-trimethylbenzamide



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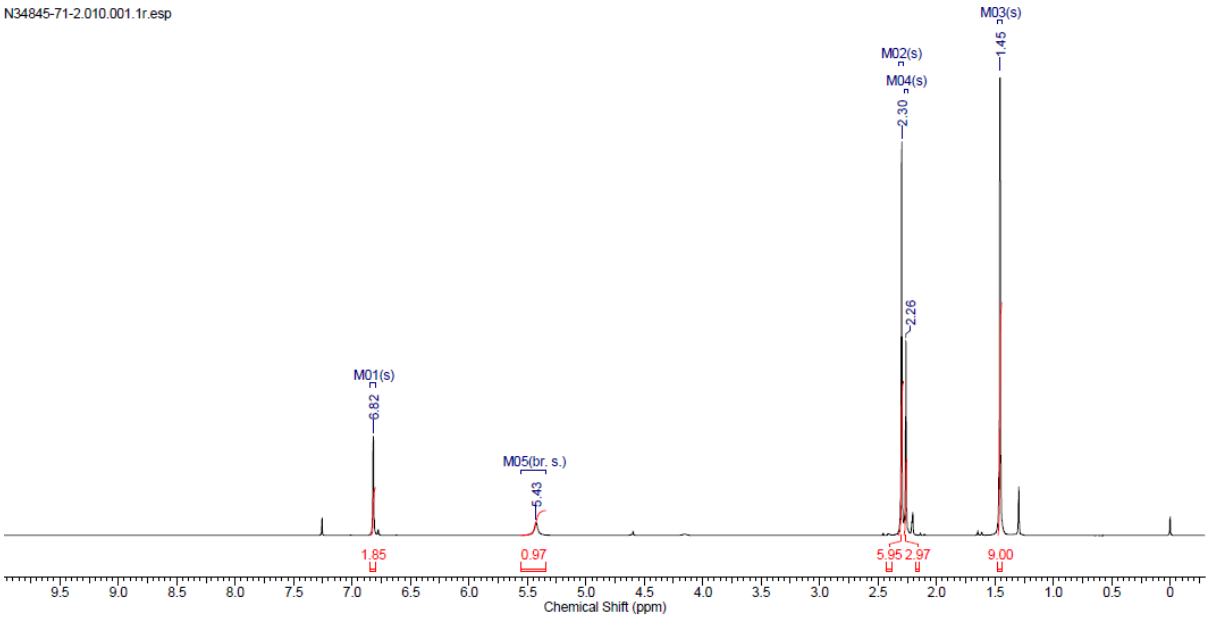
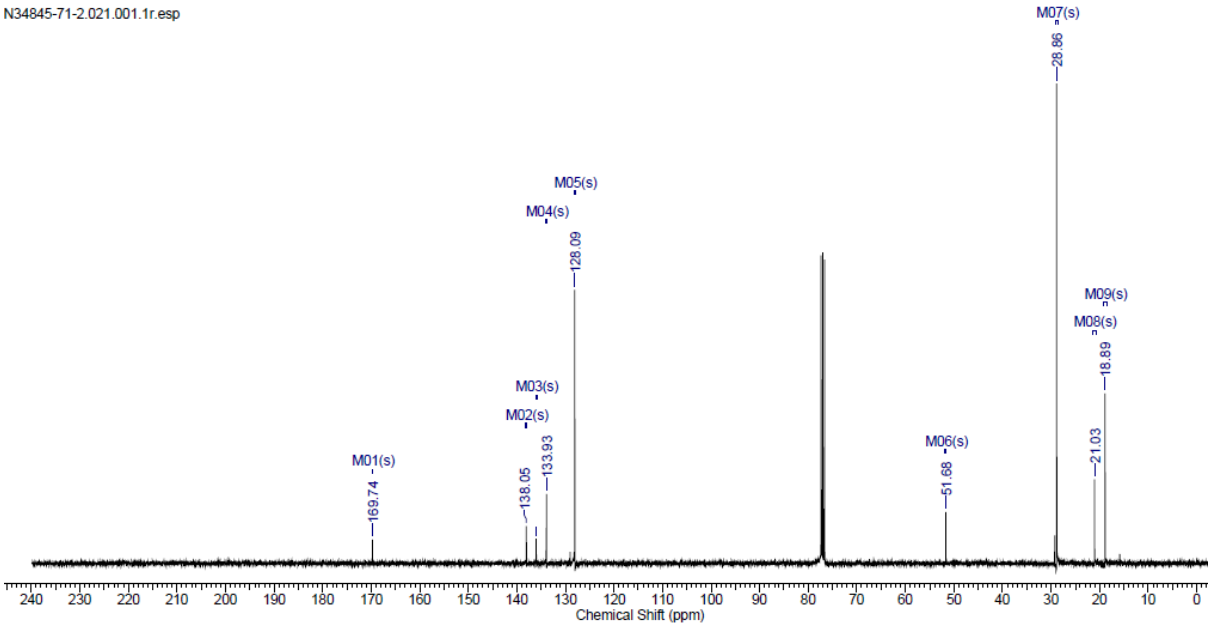
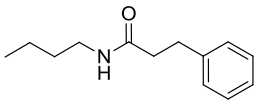




N-Butyl-3-phenylpropanamide



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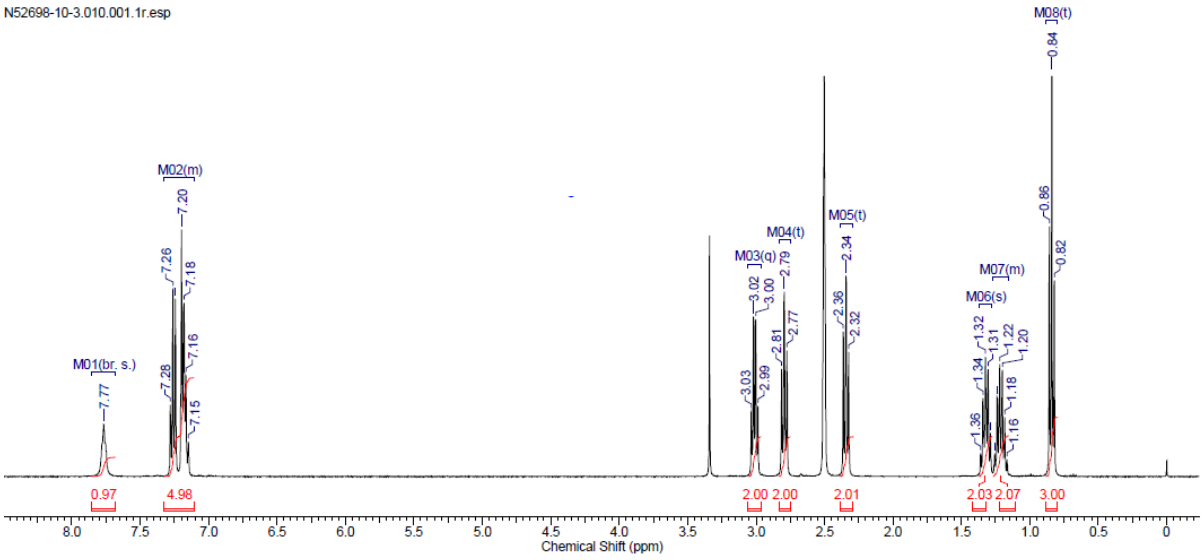
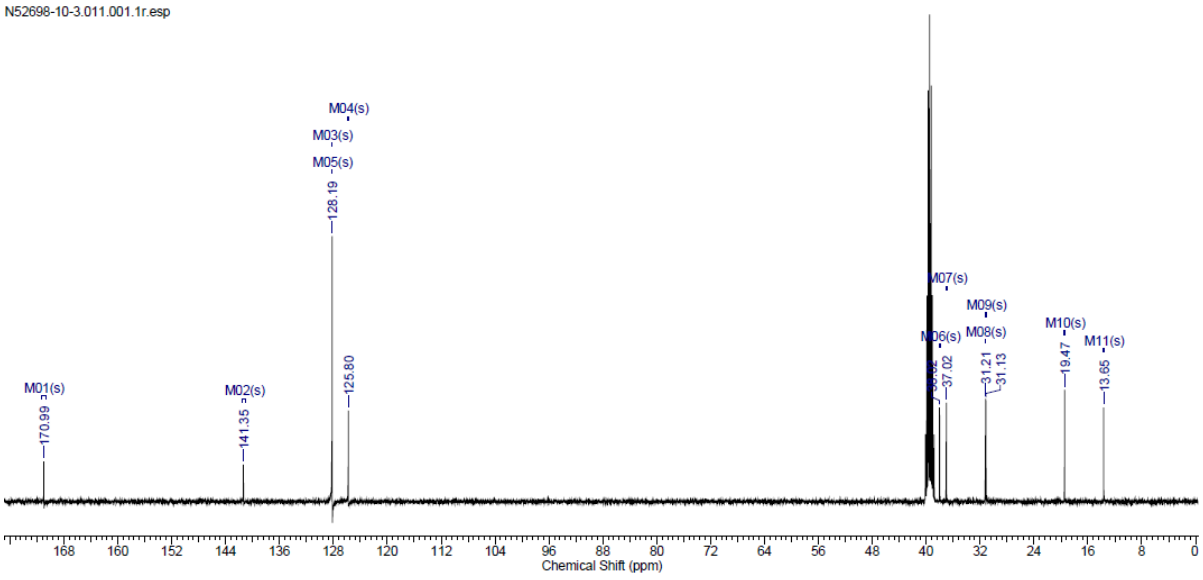
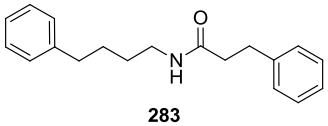




3-Phenyl-*N*-(4-phenylbutyl)propanamide



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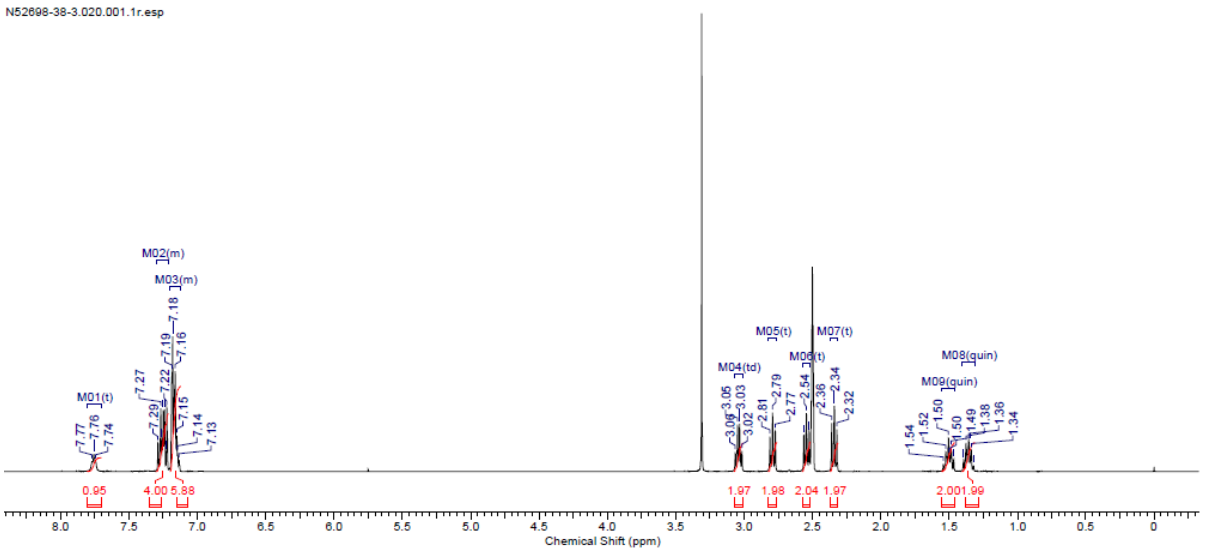
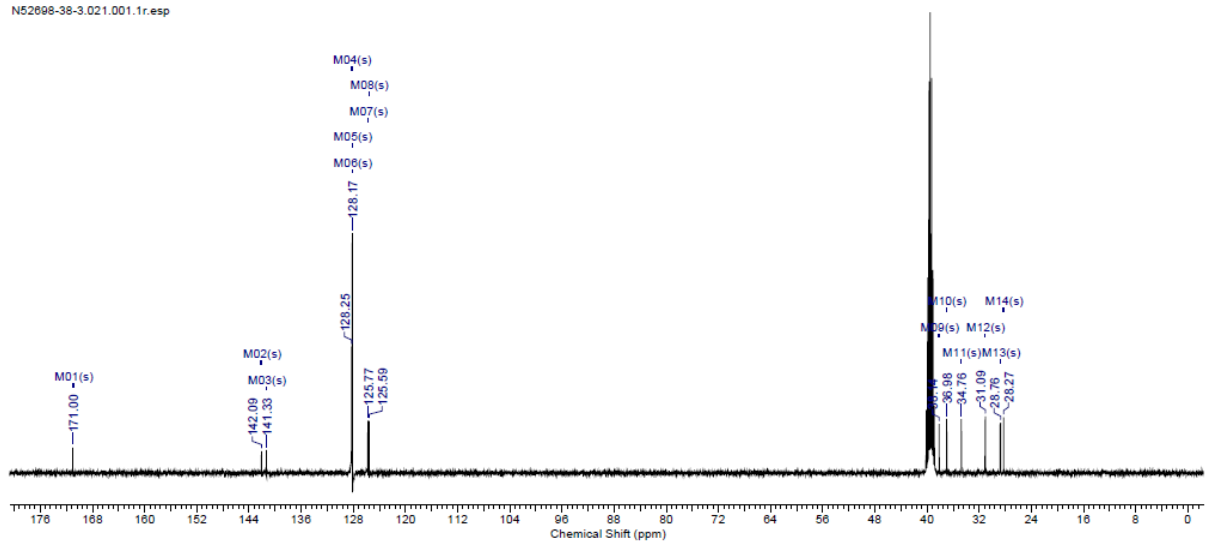
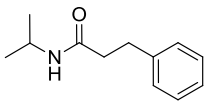




N-Isopropyl-3-phenylpropanamide



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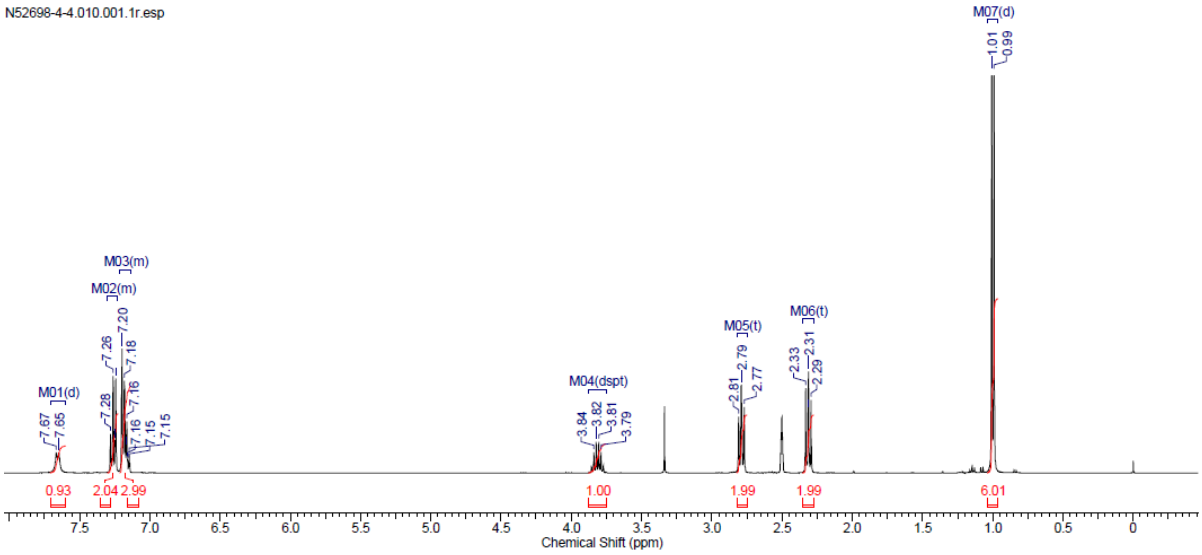
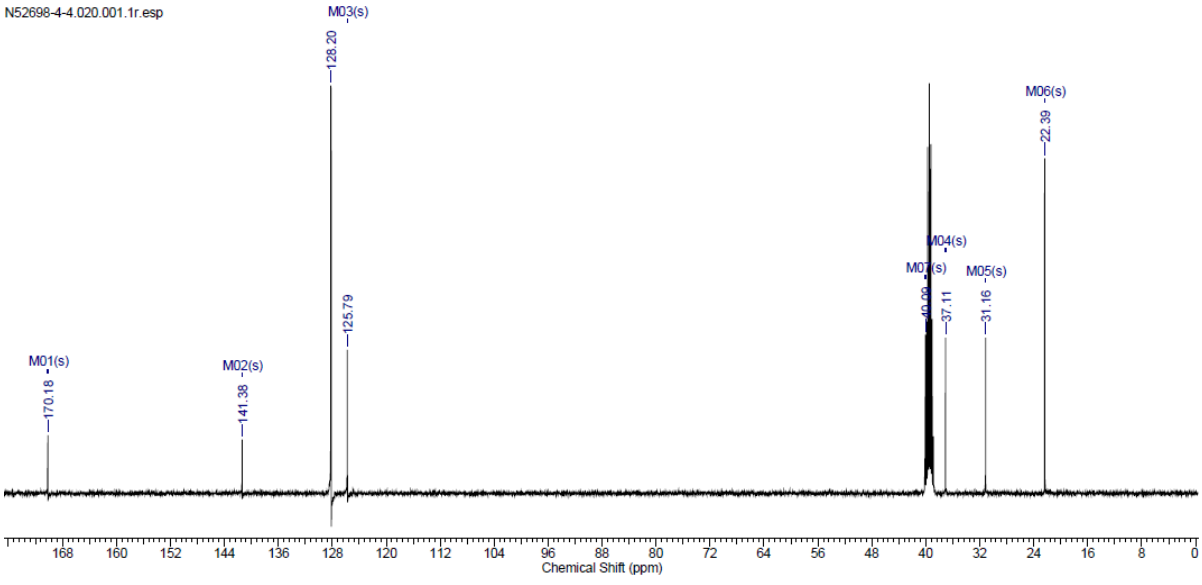
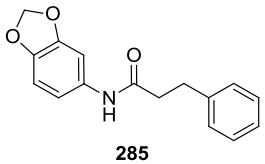




N-(Benzo[*d*][1,3]dioxol-5-yl)-3-phenylpropanamide



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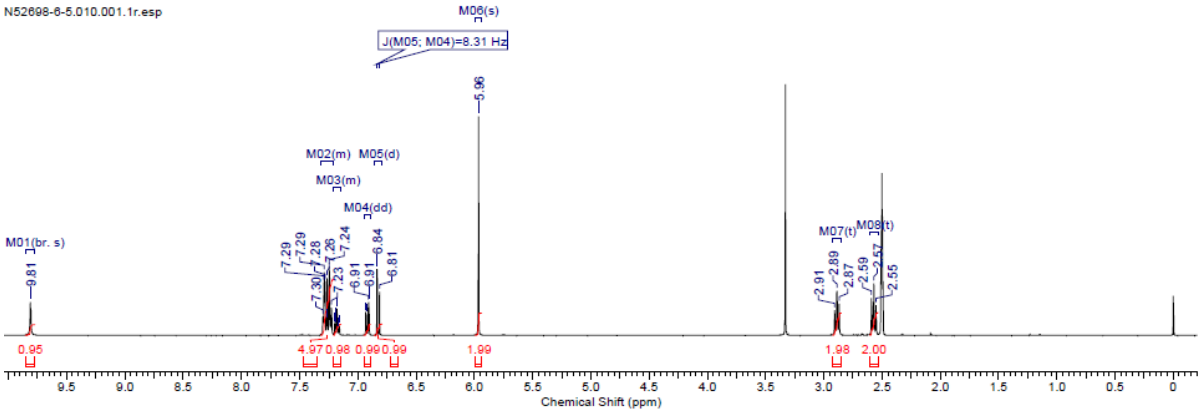
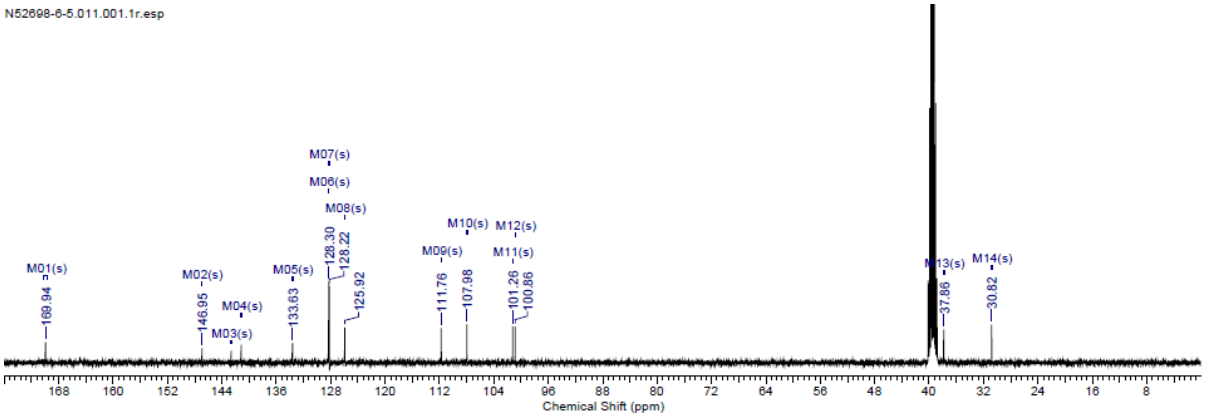
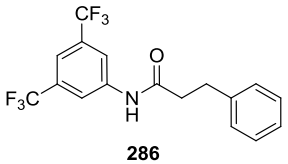




N-(3,5-Bis(trifluoromethyl)phenyl)-3-phenylpropanamide



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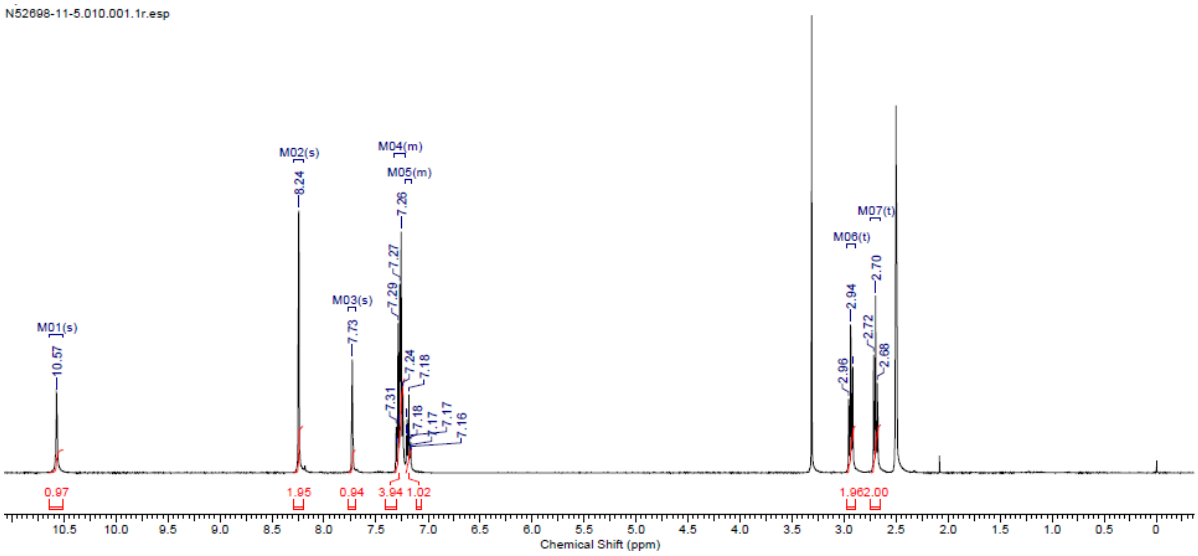

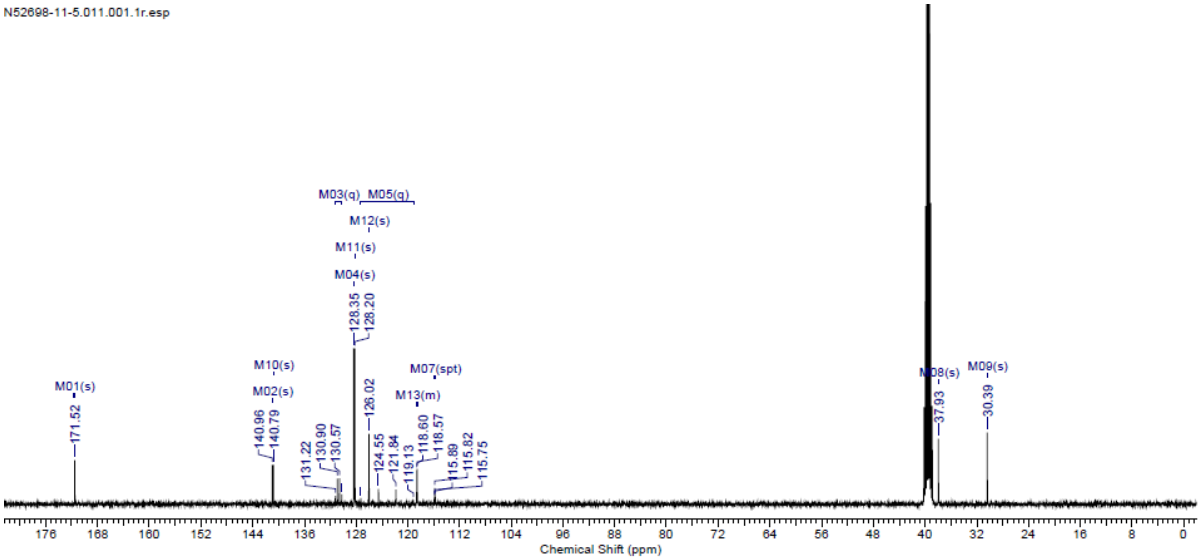

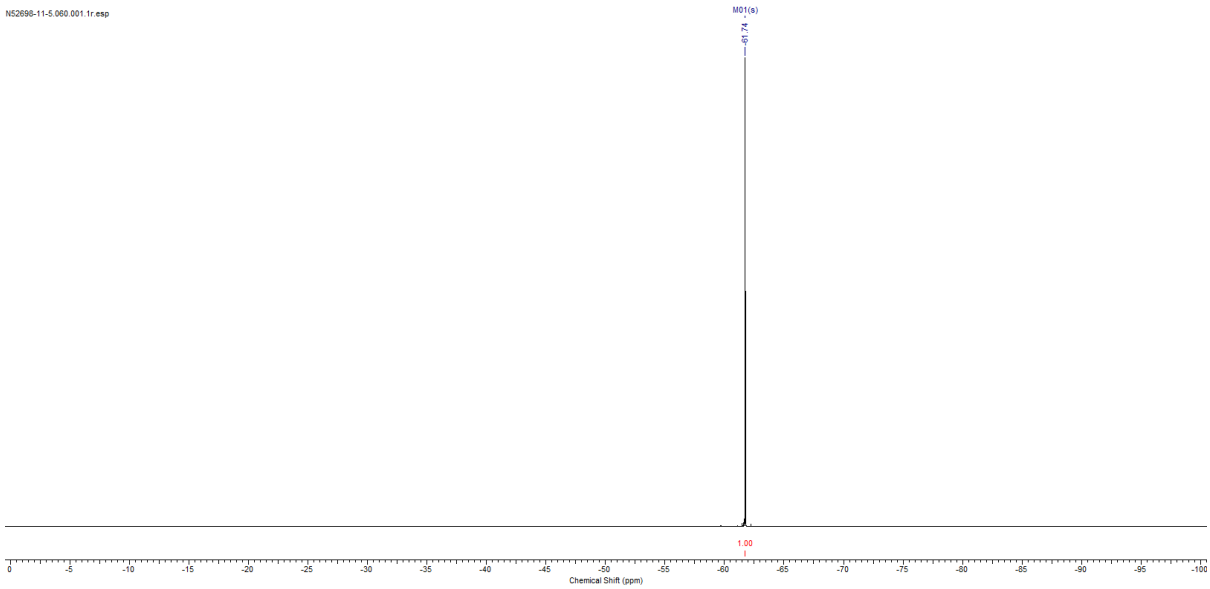
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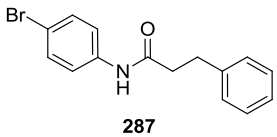
1.00
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
Chemical Shift (ppm)

N-(4-Bromophenyl)-3-phenylpropanamide



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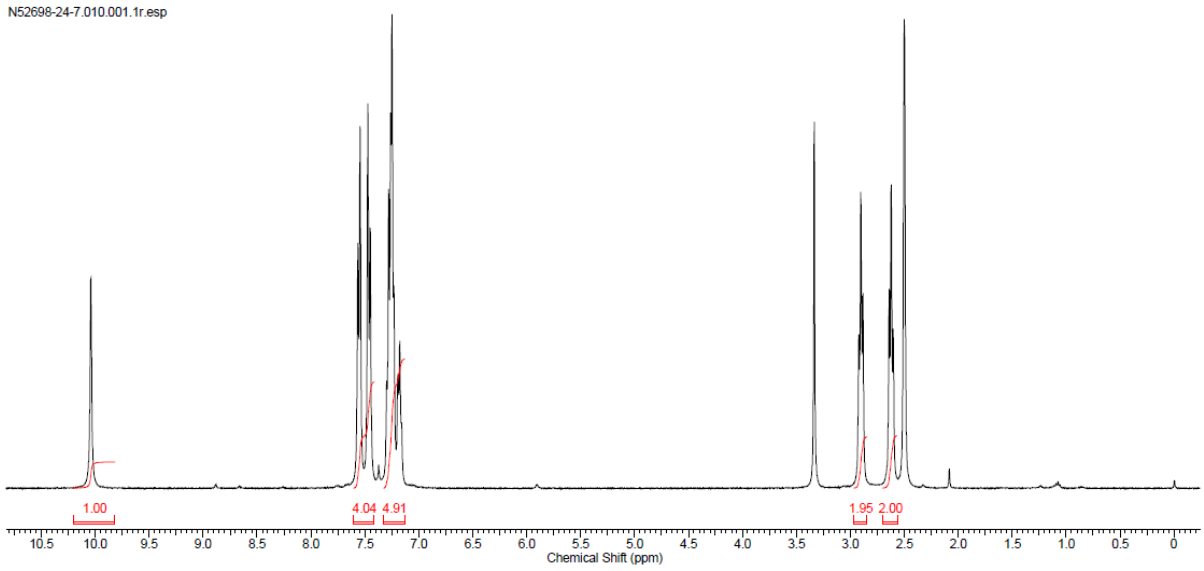
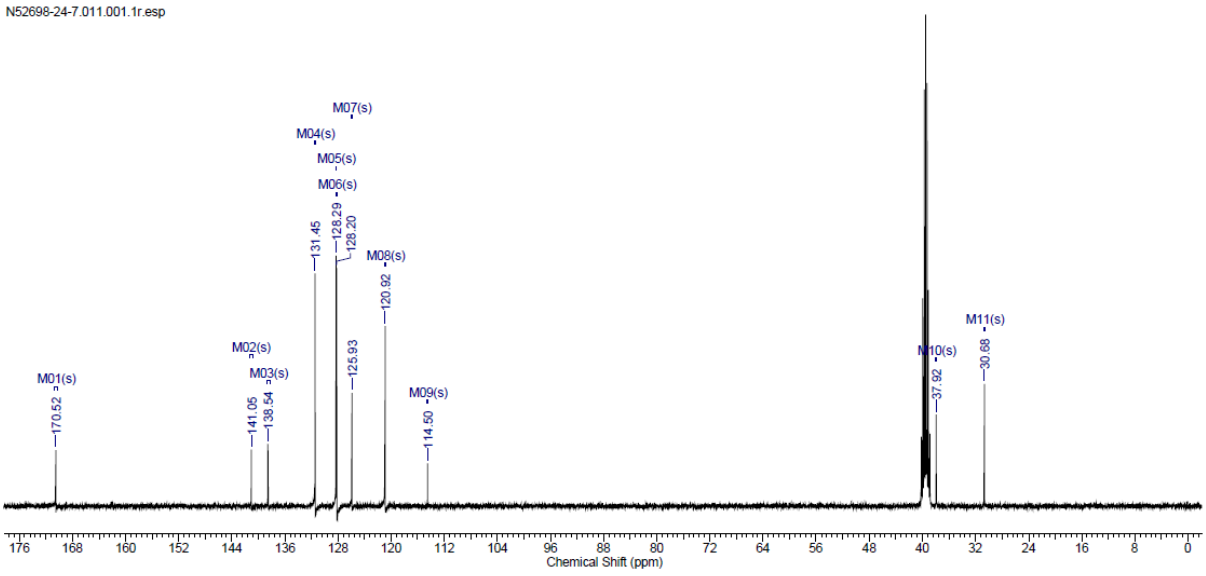
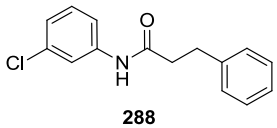




N-(3-chlorophenyl)-3-phenylpropanamide



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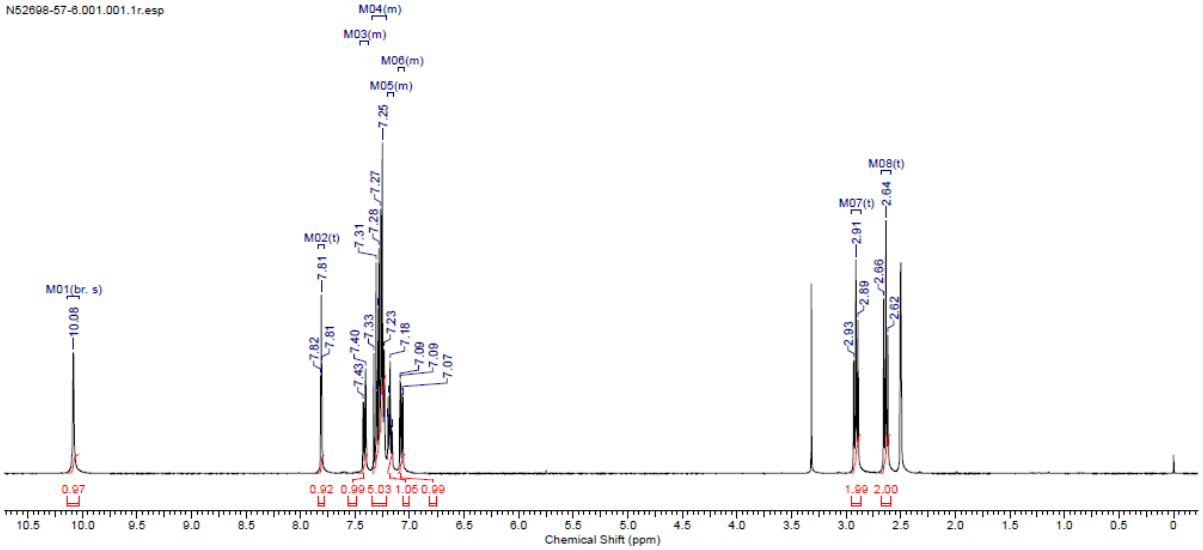
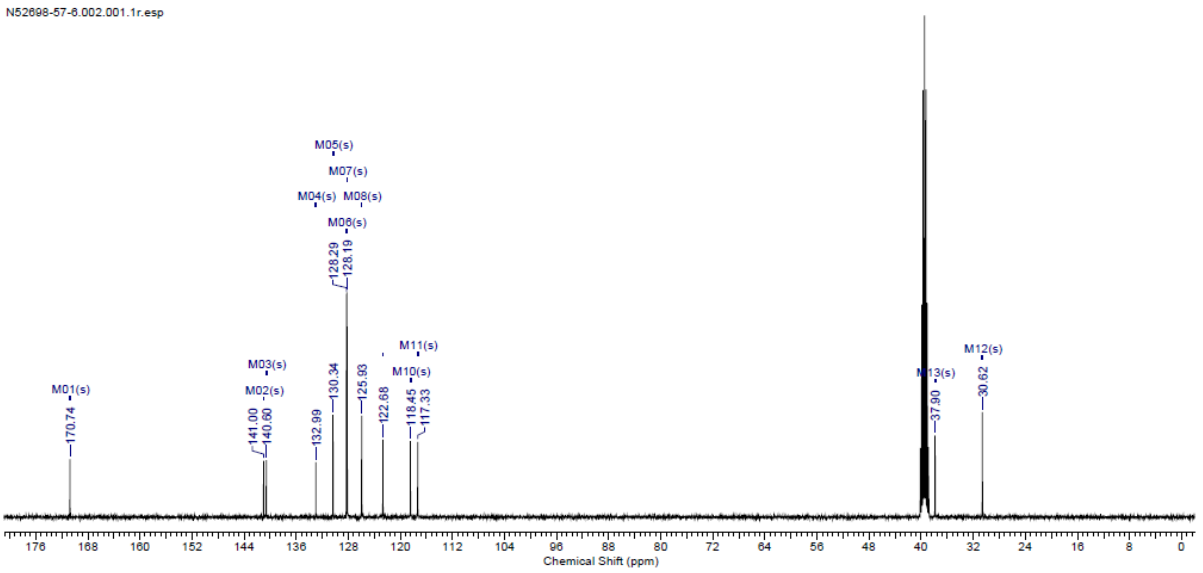
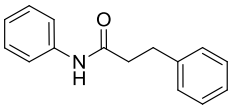




N,3-Diphenylpropanamide



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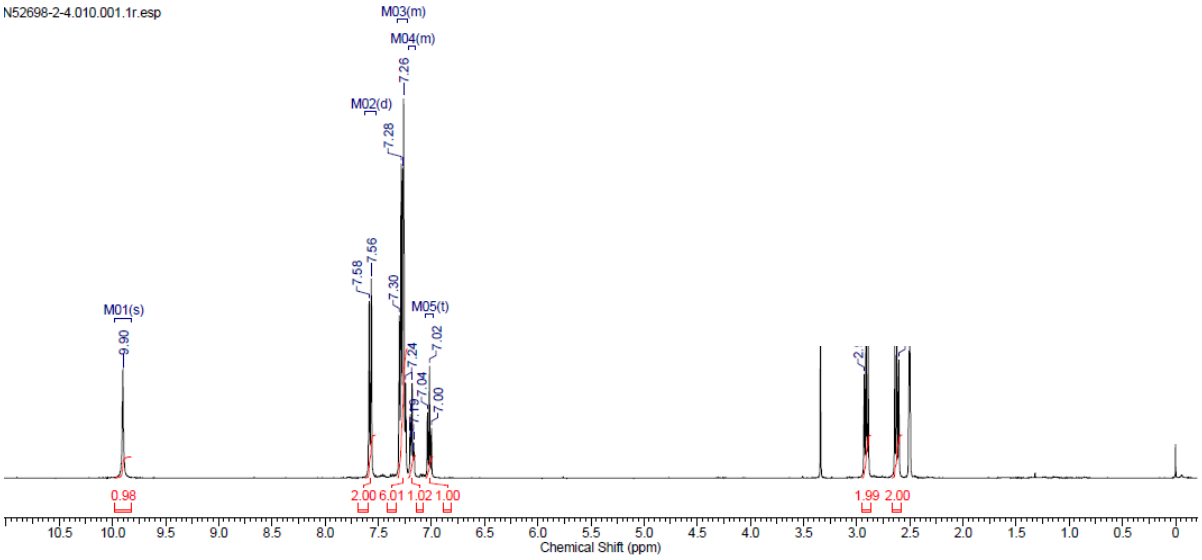
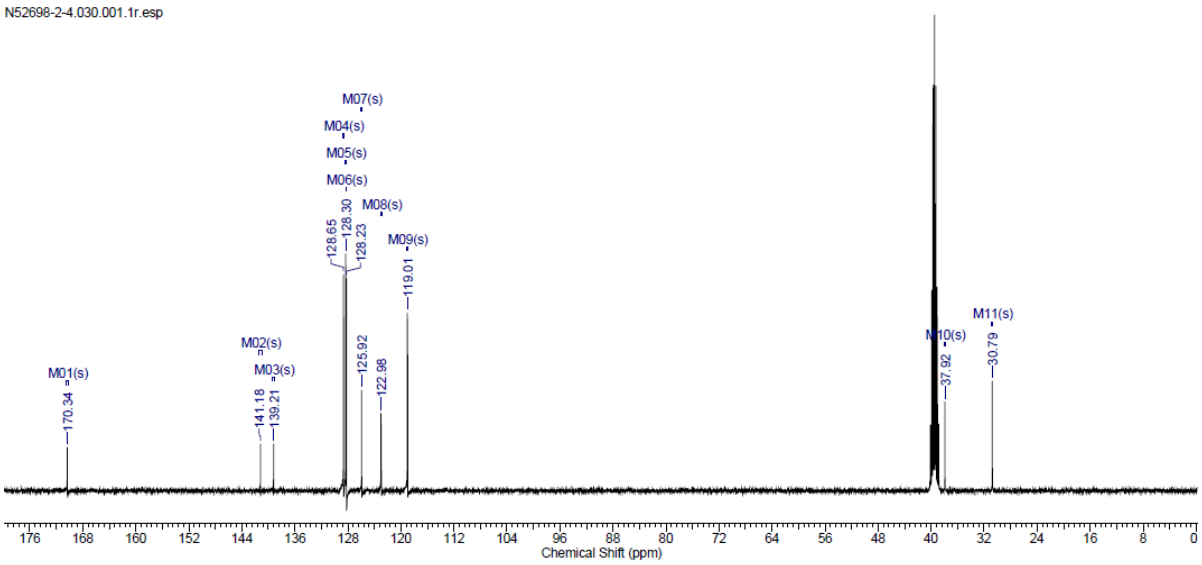
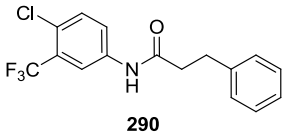




N-(4-Chloro-3-(trifluoromethyl)phenyl)-3-phenylpropanamide



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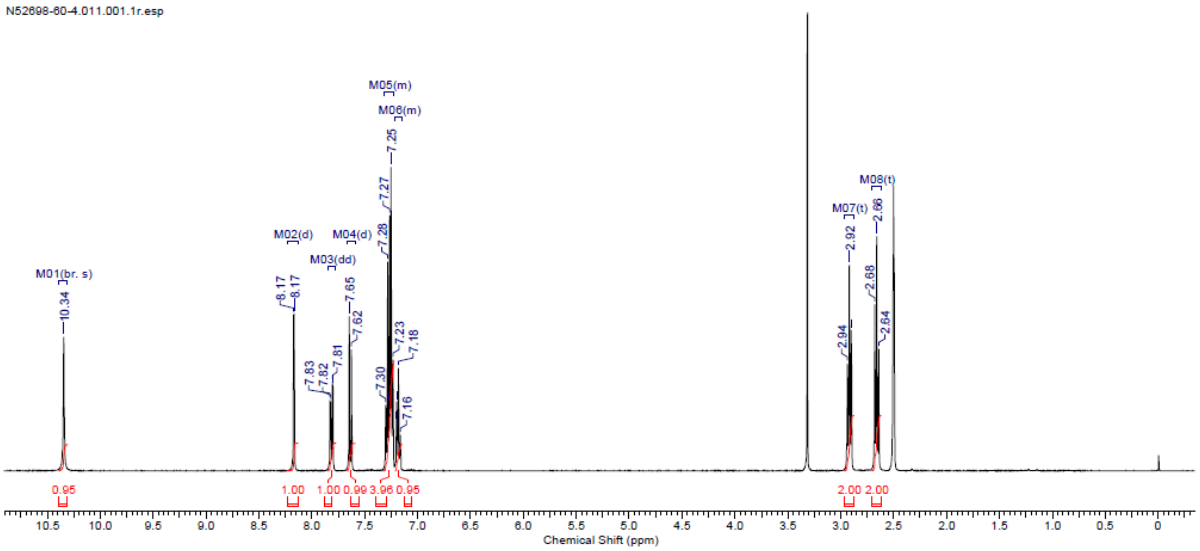

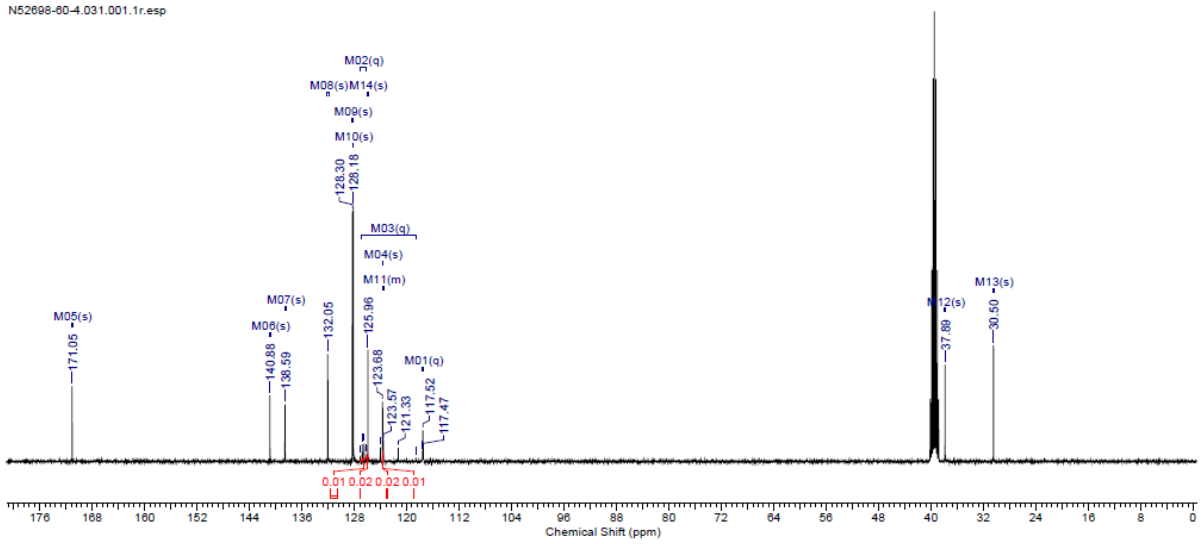

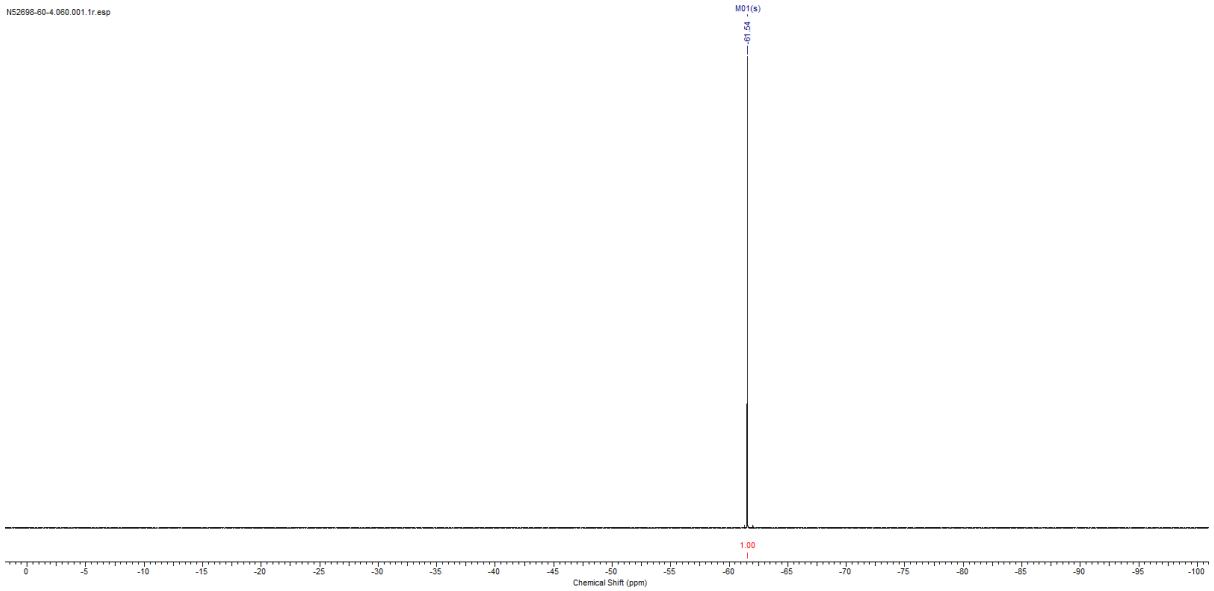
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M01(s)
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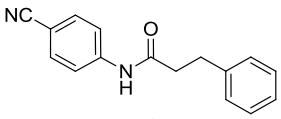
1.00
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
Chemical Shift (ppm)

N-(4-Cyanophenyl)-3-phenylpropanamide



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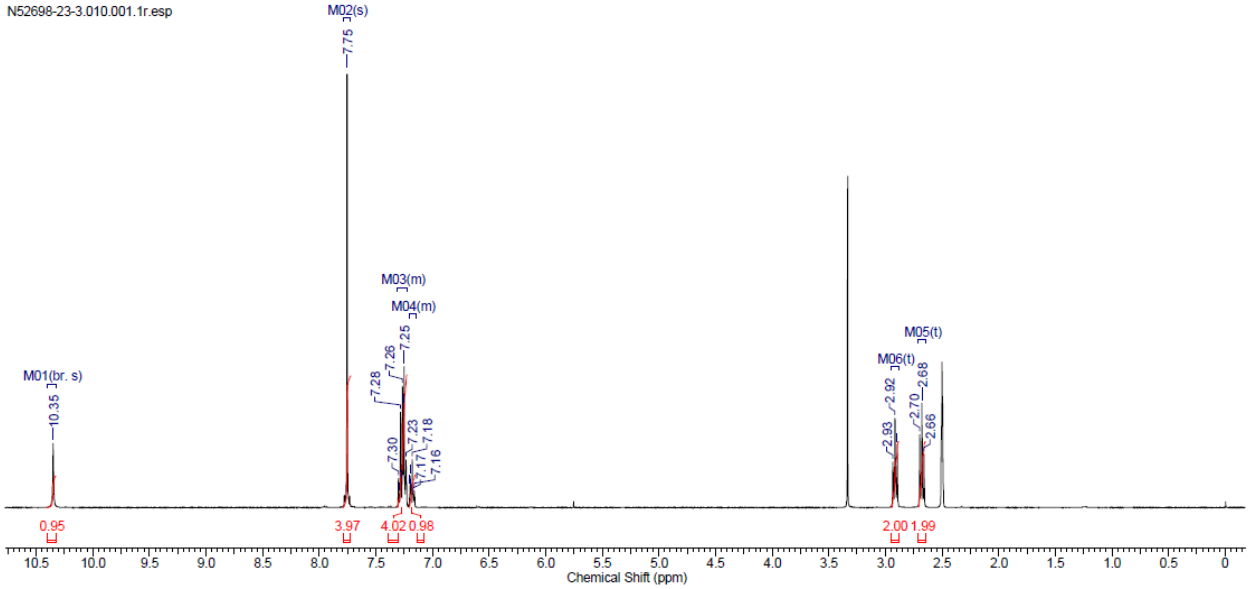
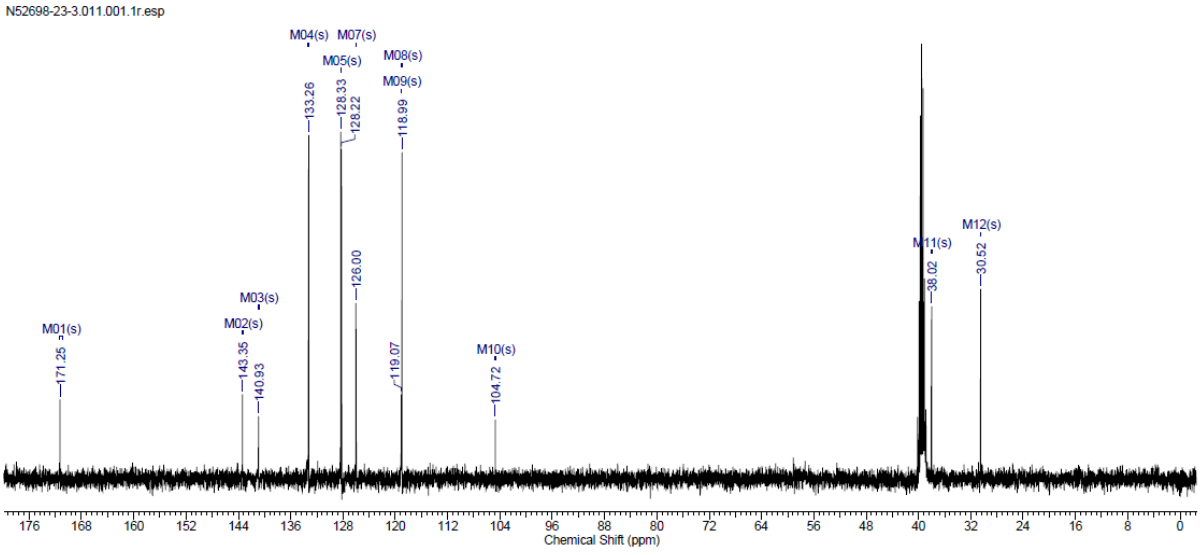
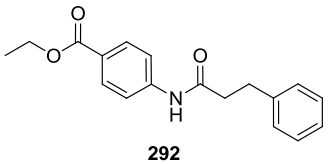




Ethyl 4-(3-phenylpropanamido)benzoate



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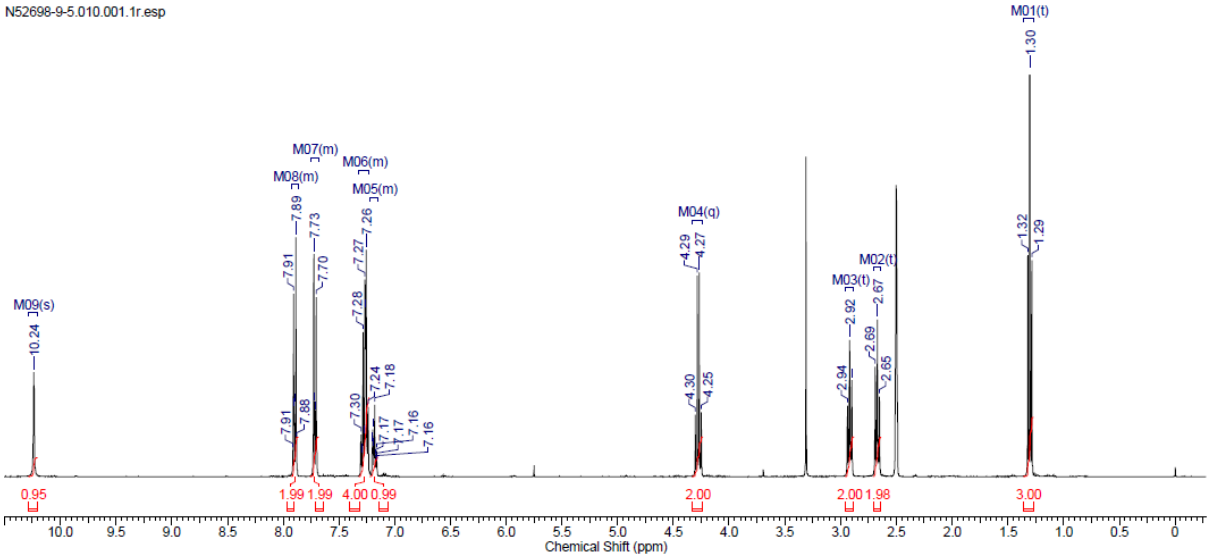
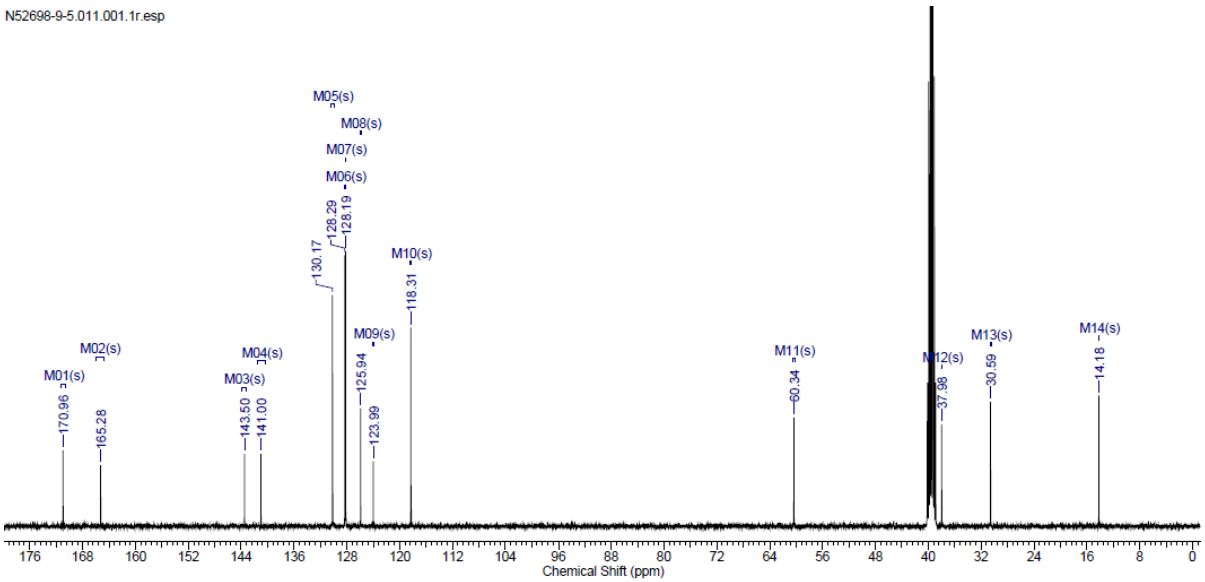
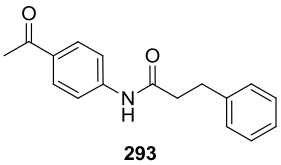




N-(4-Acetylphenyl)-3-phenylpropanamide



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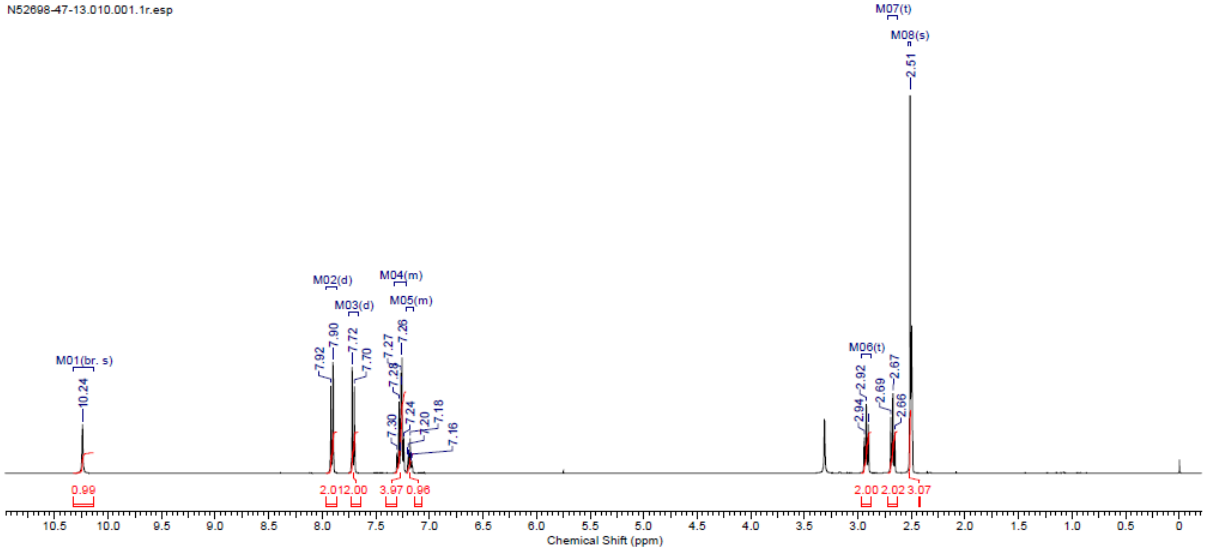
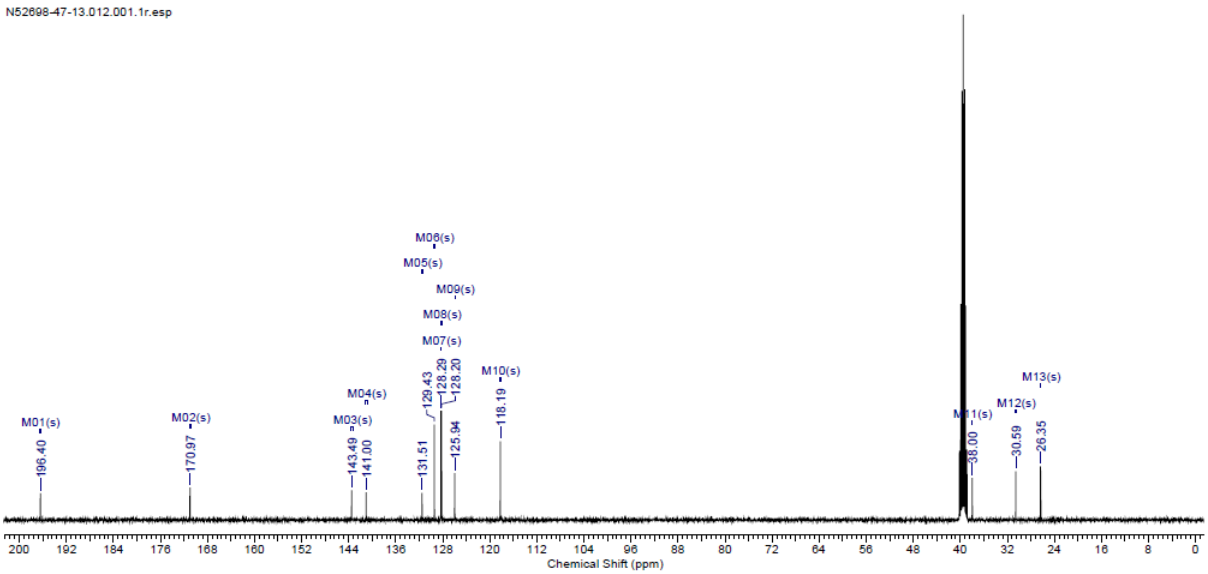
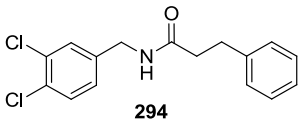




N-(3,4-Dichlorobenzyl)-3-phenylpropanamide



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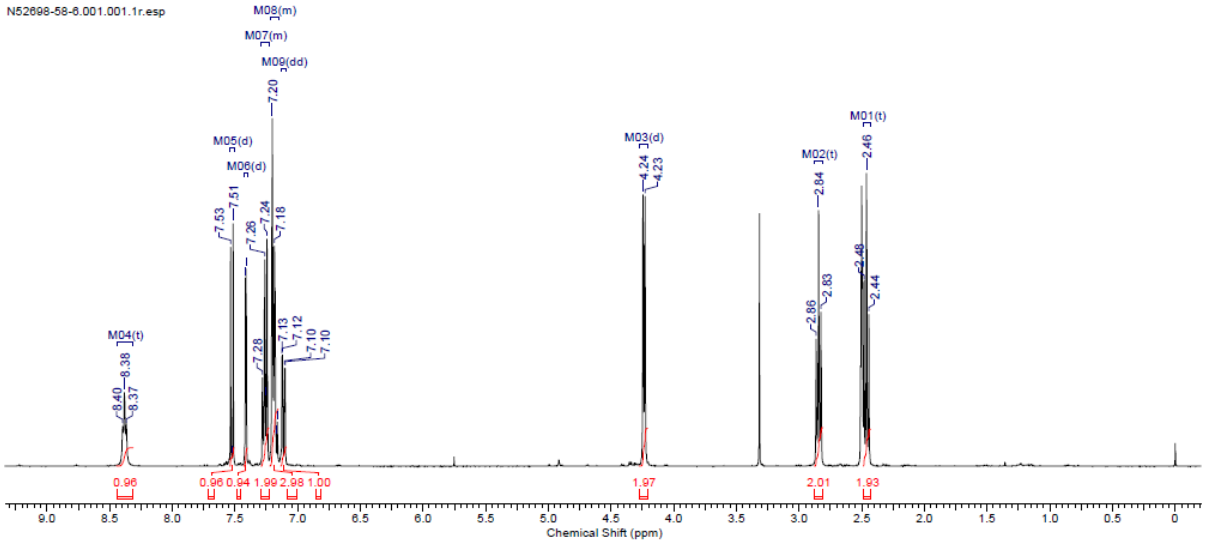
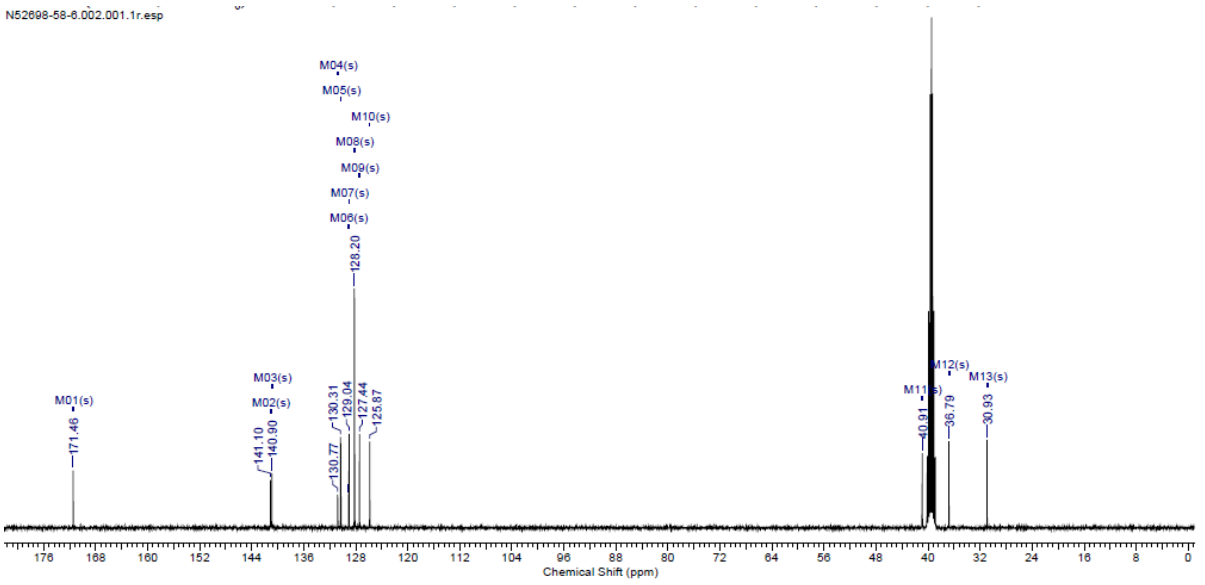
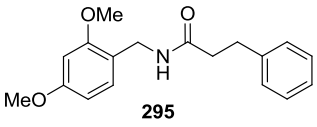




N-(2,4-Dimethoxybenzyl)-3-phenylpropanamide



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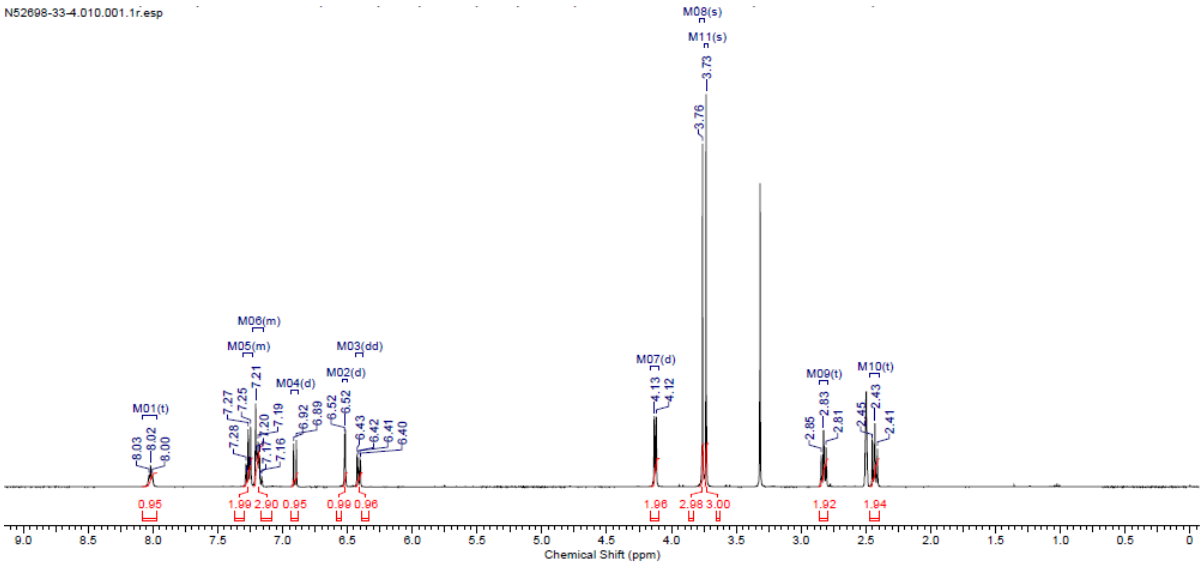
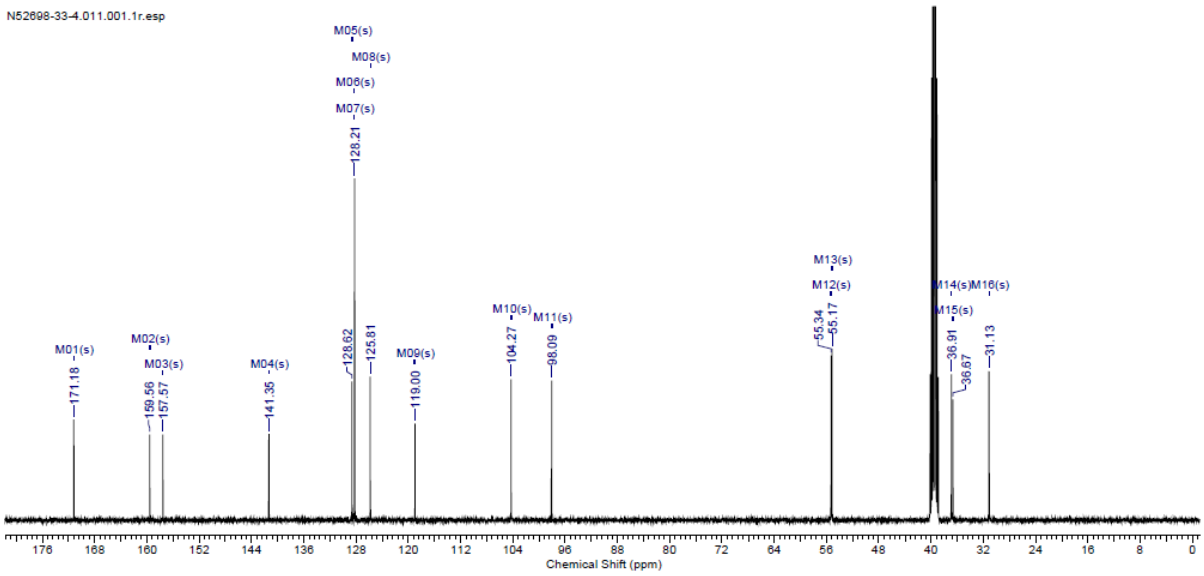
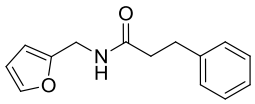




N-(Furan-2-ylmethyl)-3-phenylpropanamide



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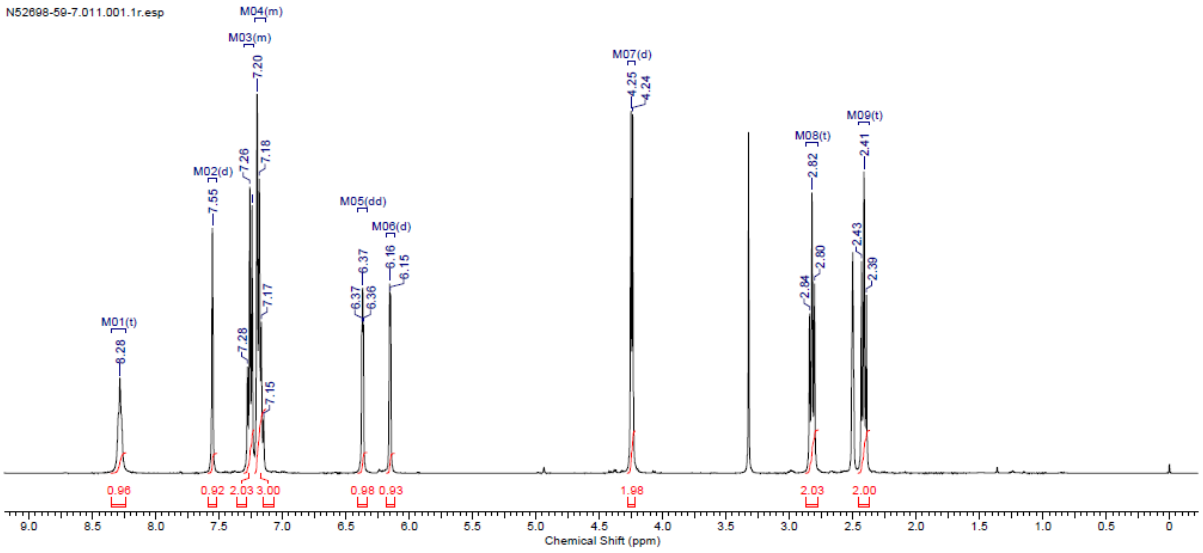
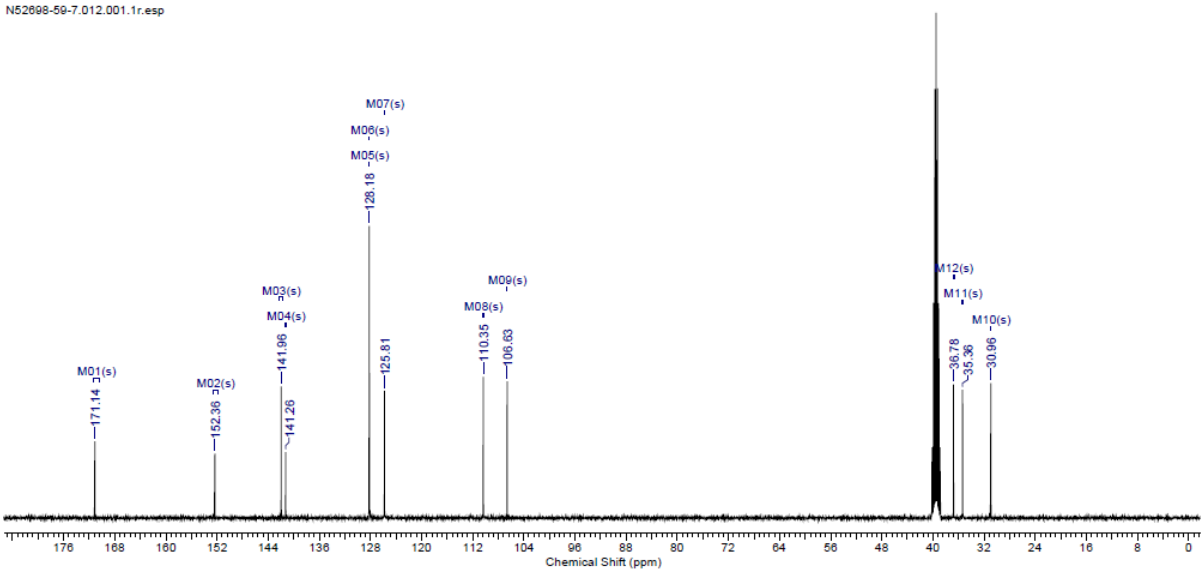
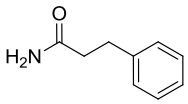




3-Phenylpropanamide



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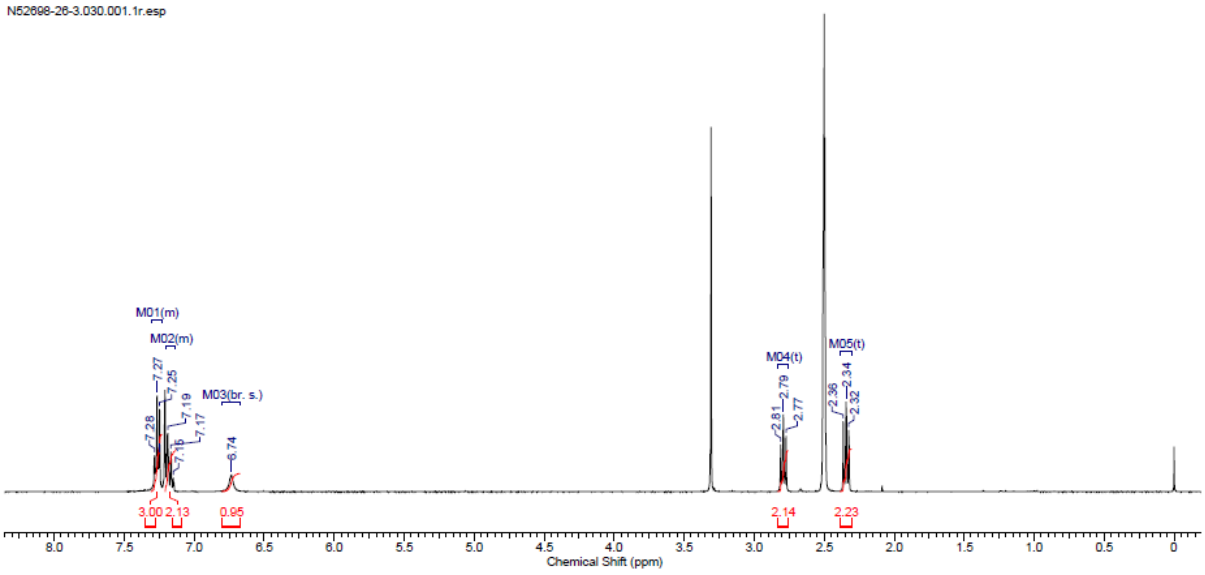
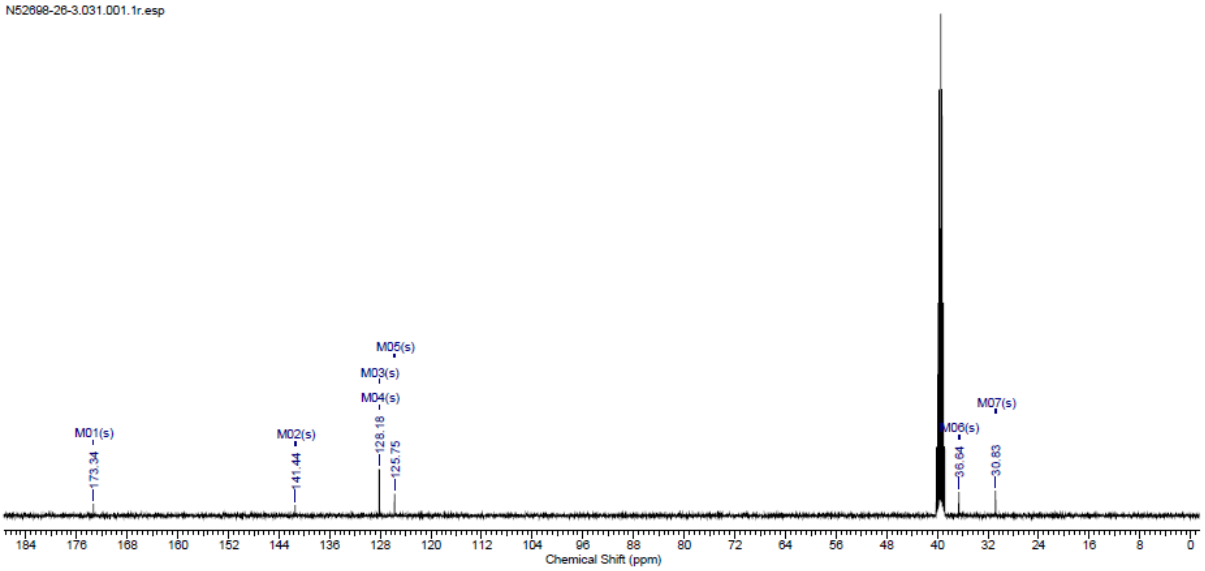
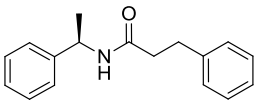




(*R*)-3-Phenyl-*N*-(1-phenylethyl)propanamide



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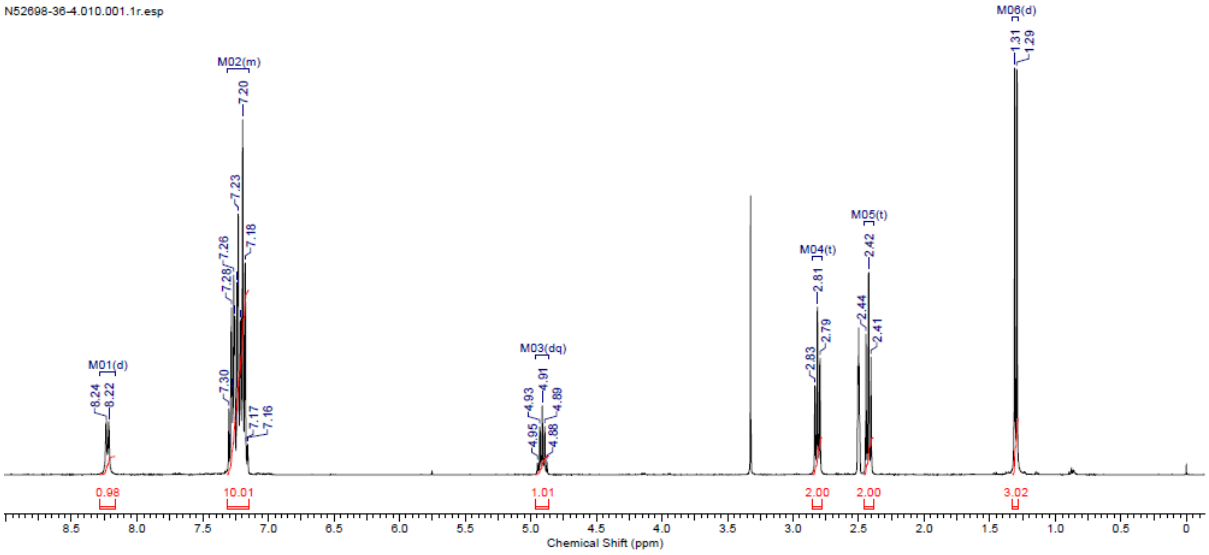
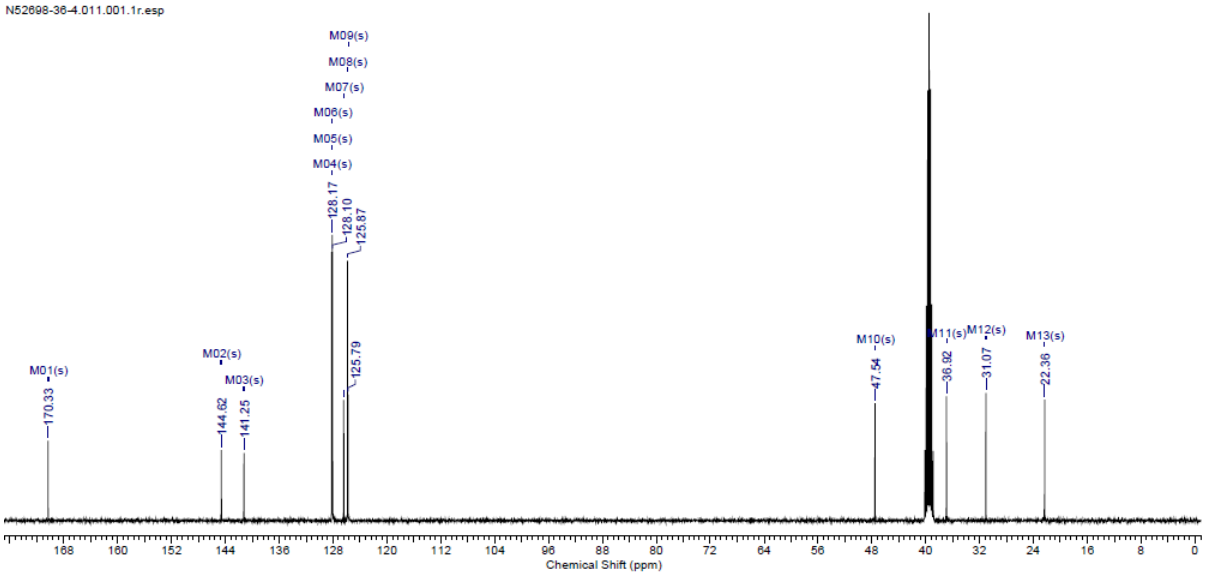
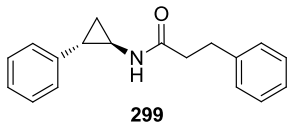




3-Phenyl-*N*-((1*S*,2*R*)-2-phenylcyclopropyl)propanamide



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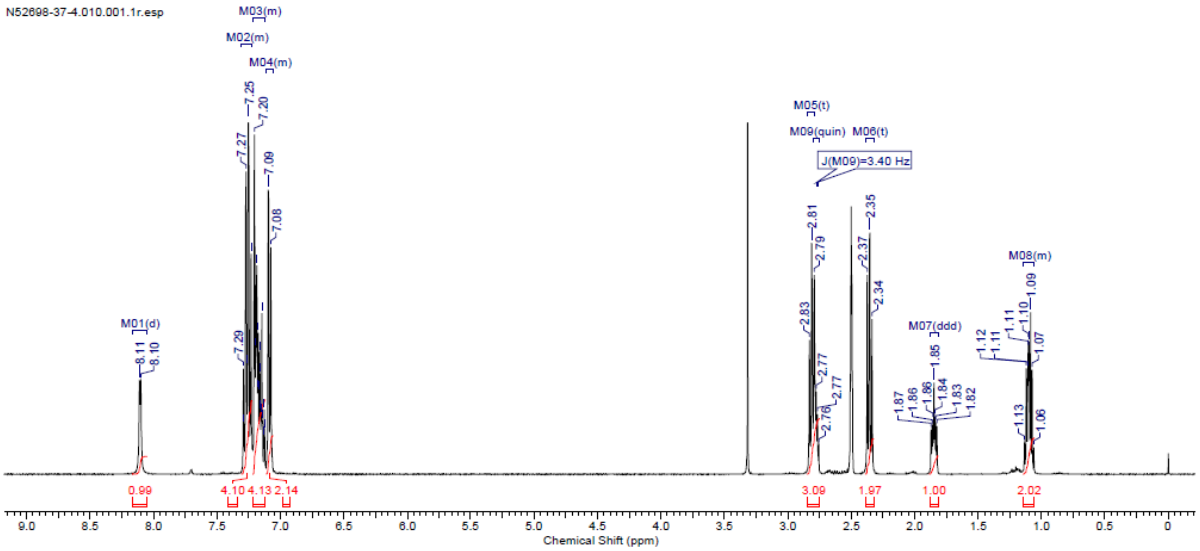
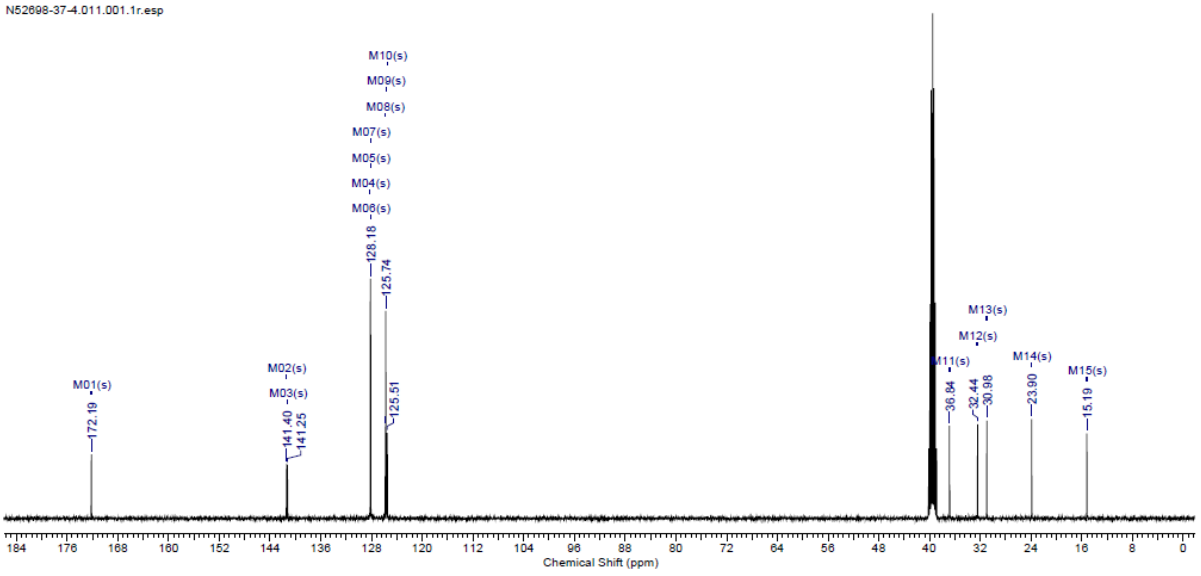
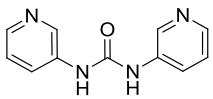




1,3-Di(pyridin-3-yl)urea



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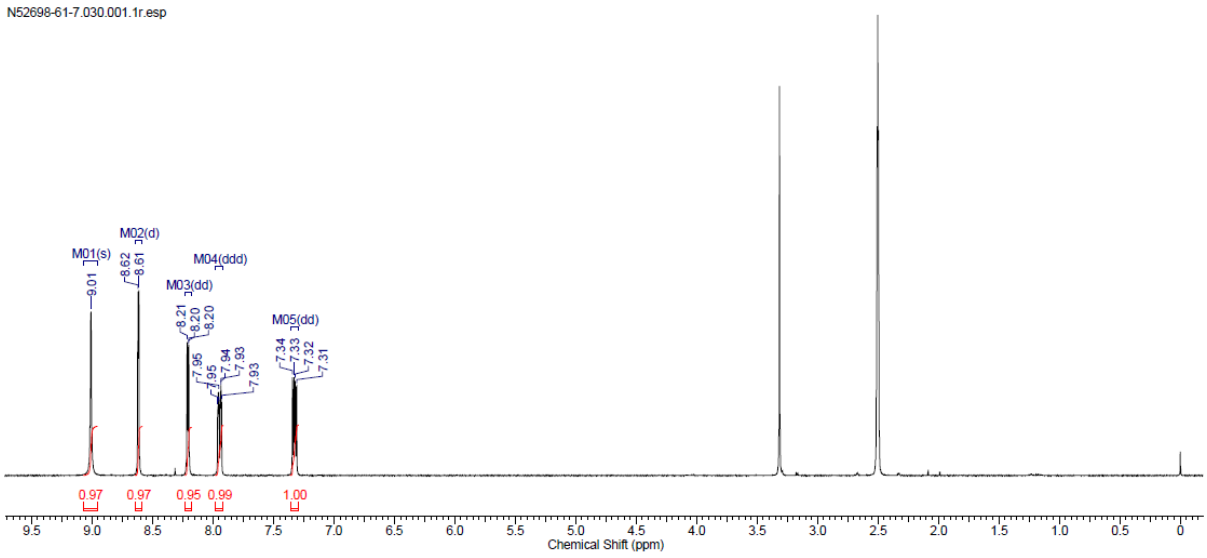
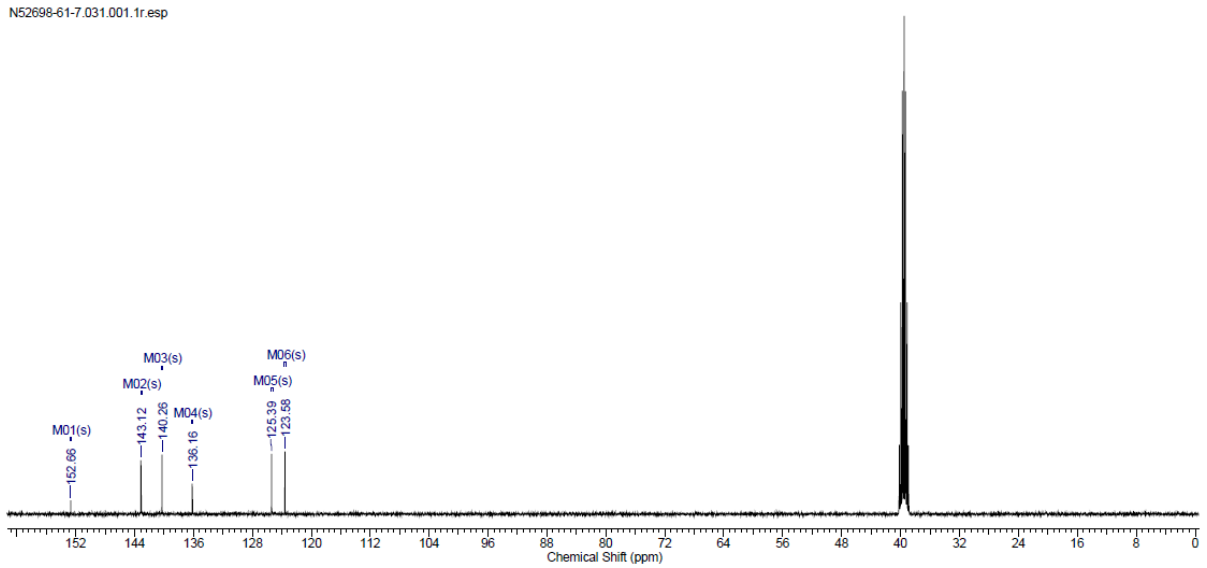
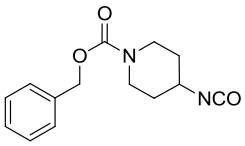




Benzyl 4-isocyanatopiperidine-1-carboxylate



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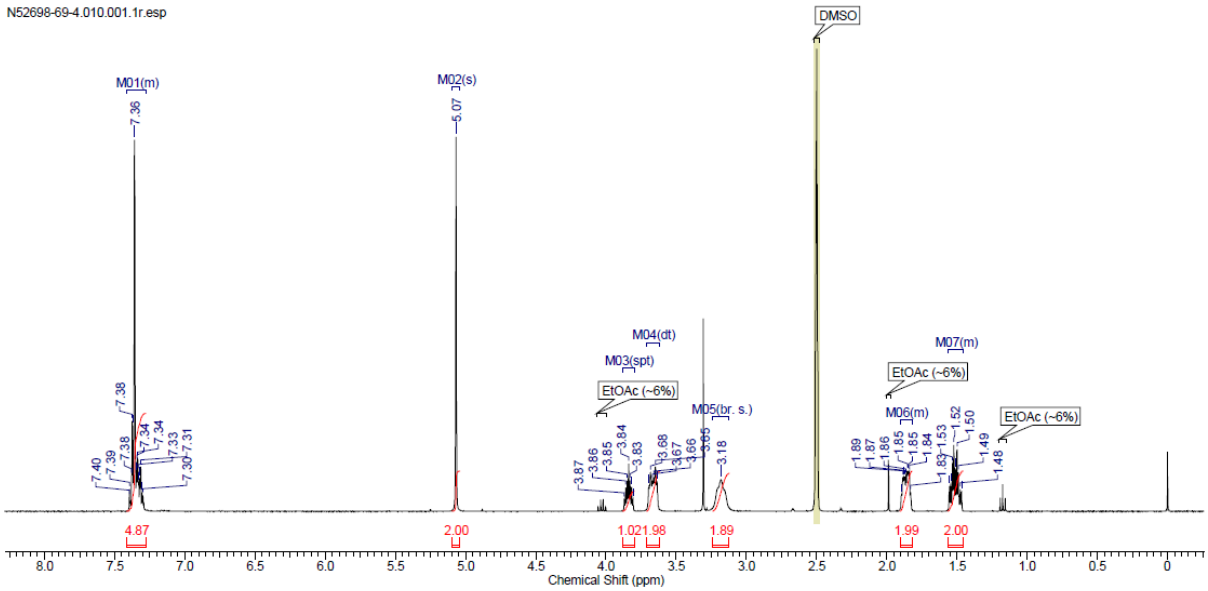
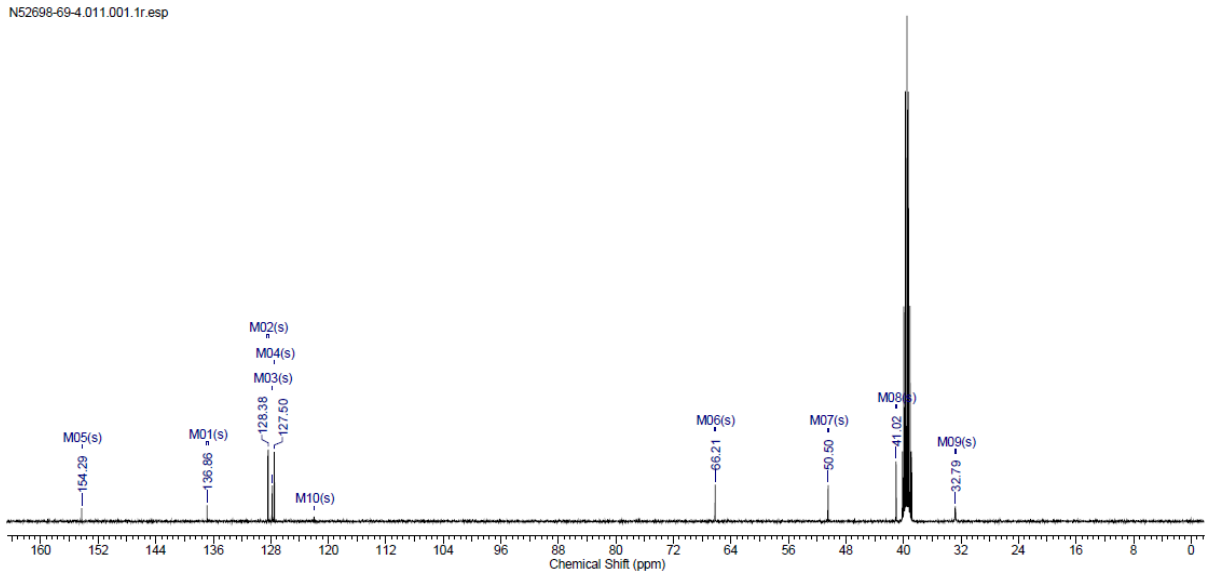
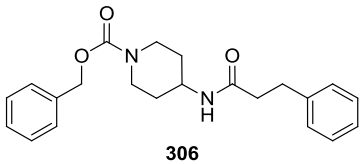




Benzyl 4-(3-phenylpropanamido)piperidine-1-carboxylate



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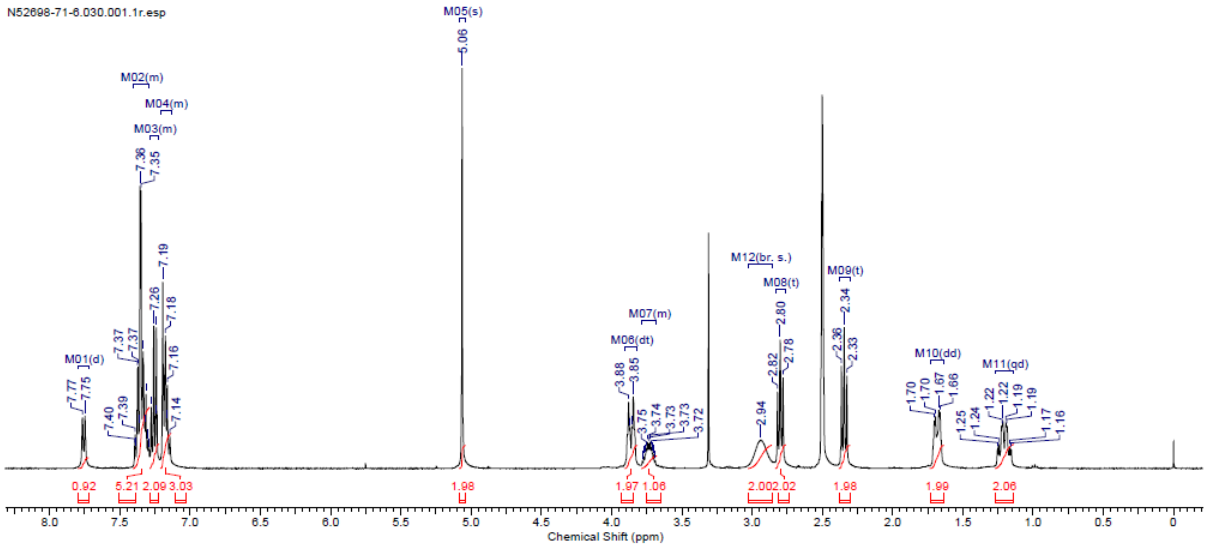
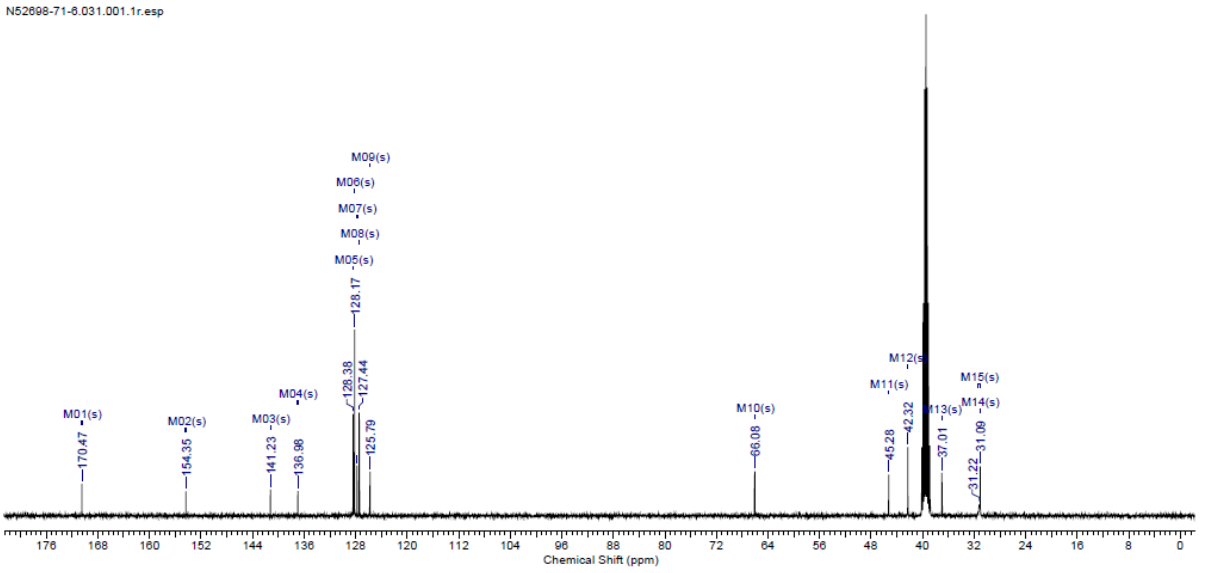
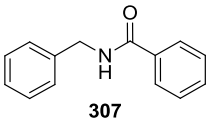




1.2.2. Substrate scope in Grignard reagent

N-Benzylbenzamide



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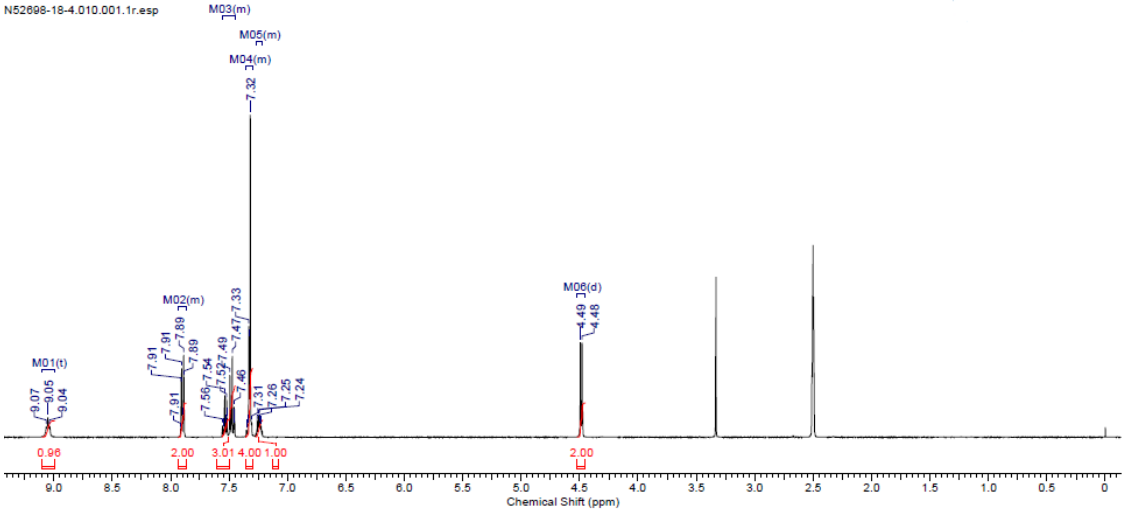
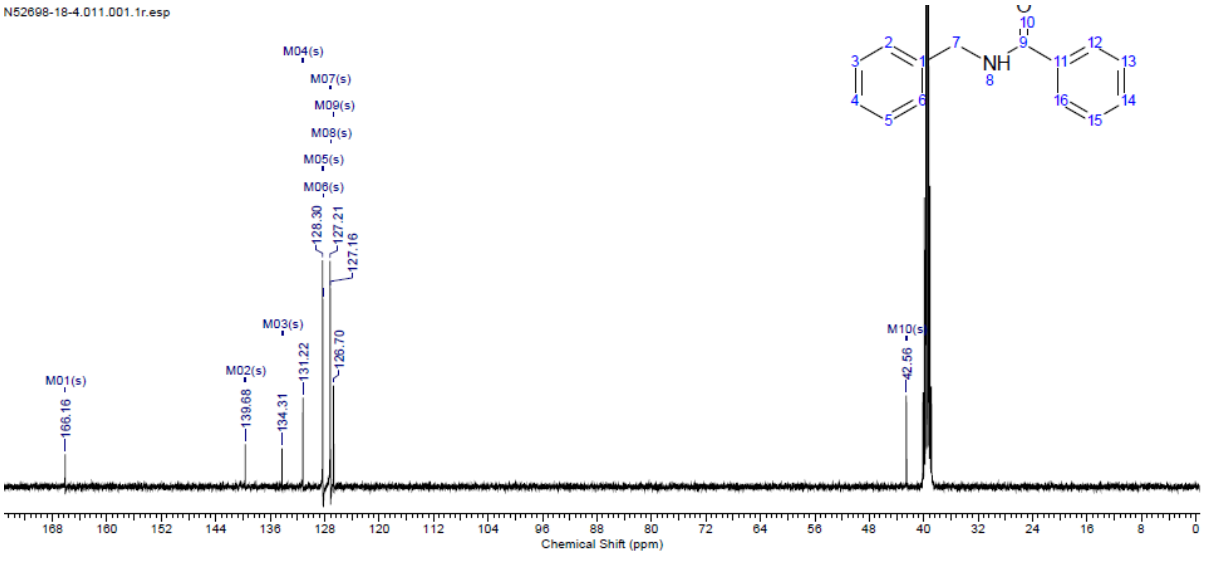
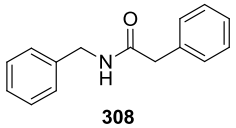




N-Benzyl-2-phenylacetamide



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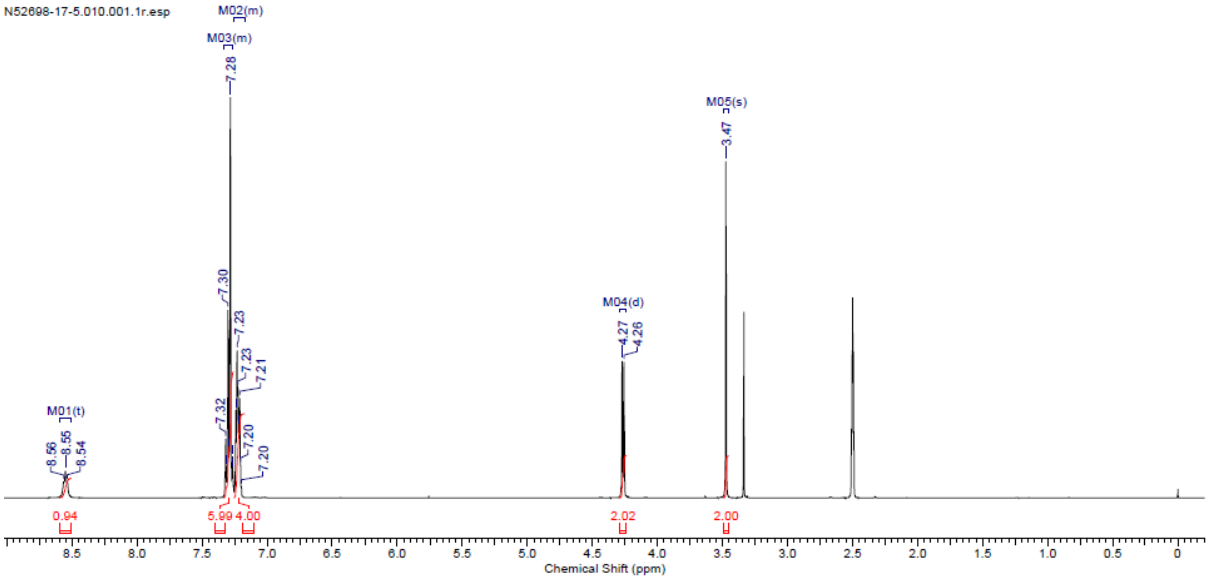
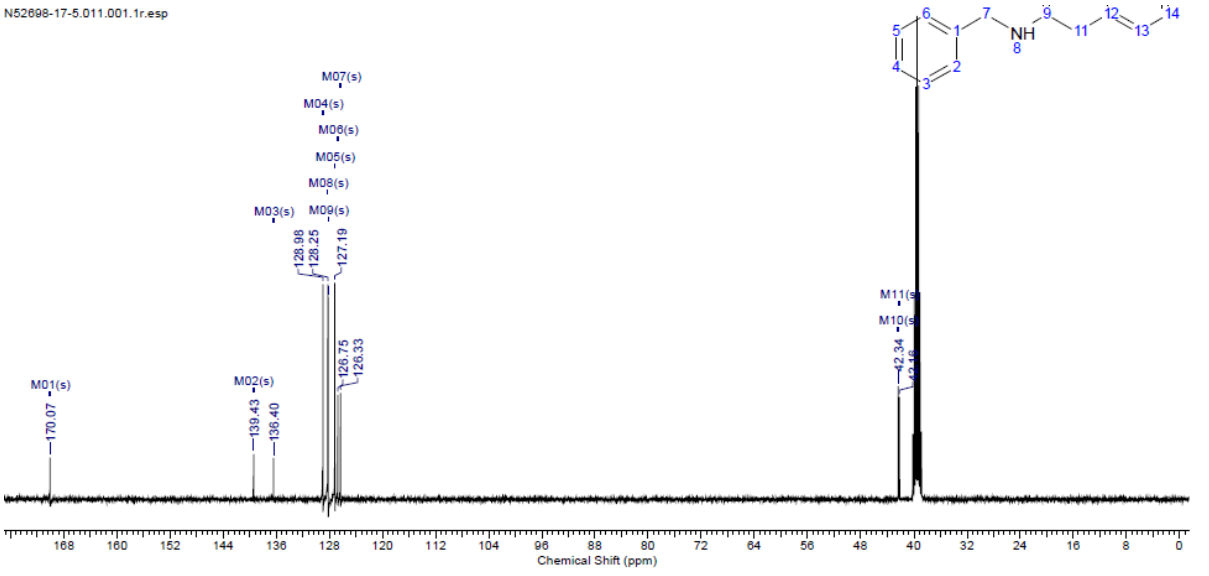
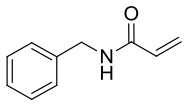




N-Benzylacrylamide



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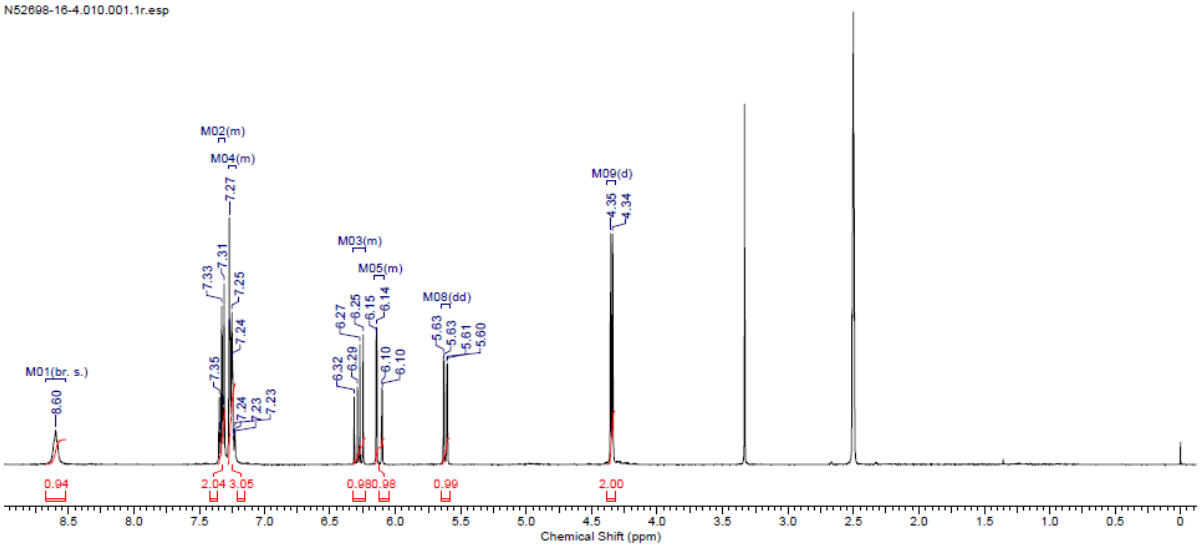
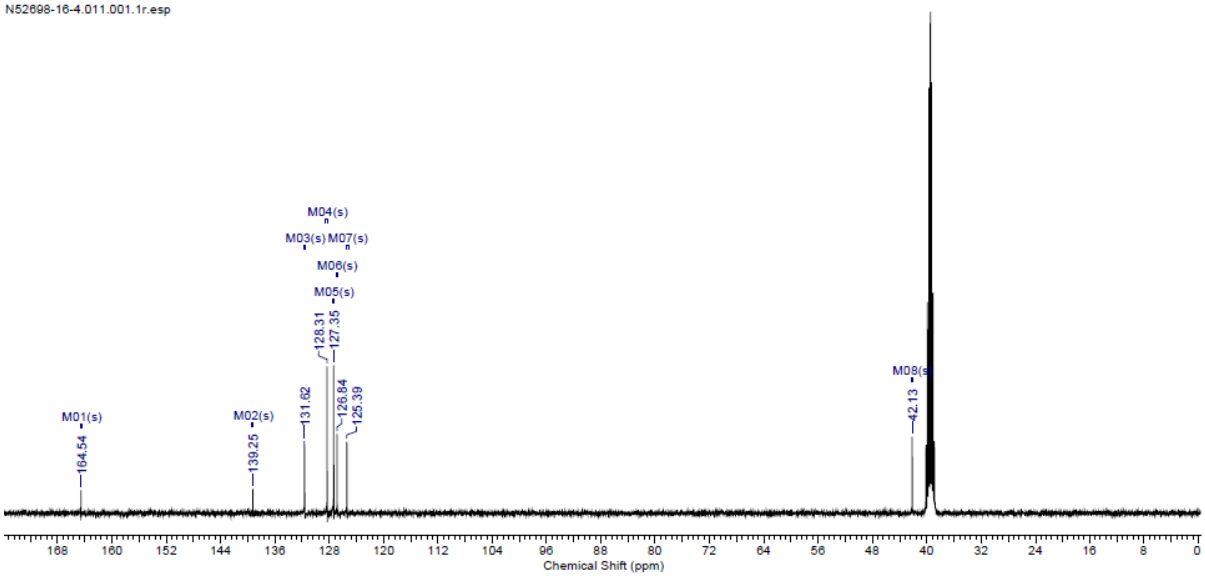
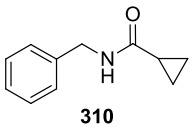




N-Benzylcyclopropanecarboxamide



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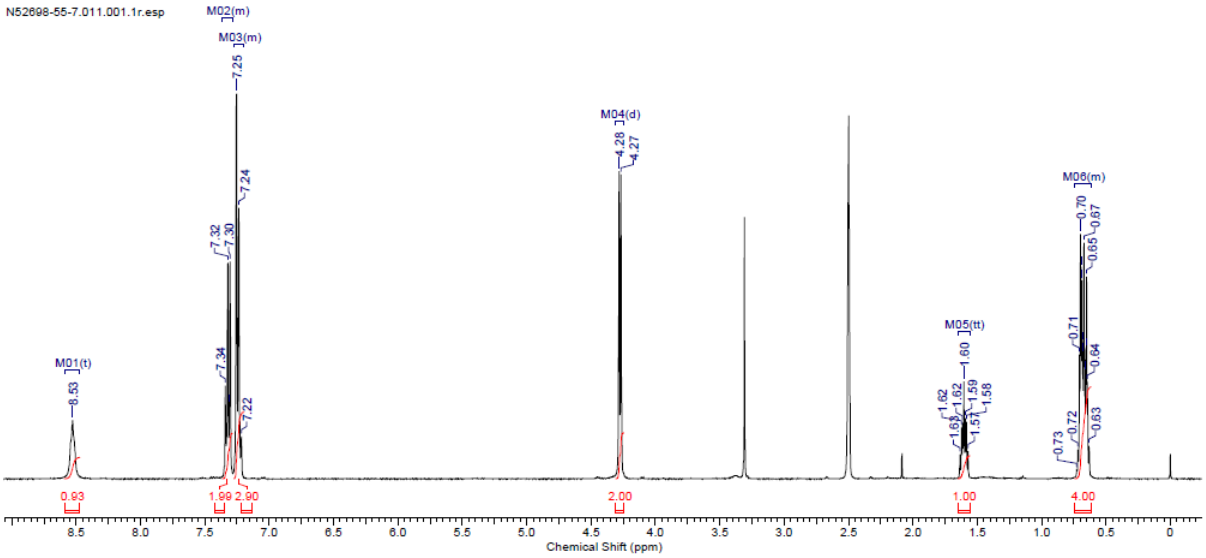
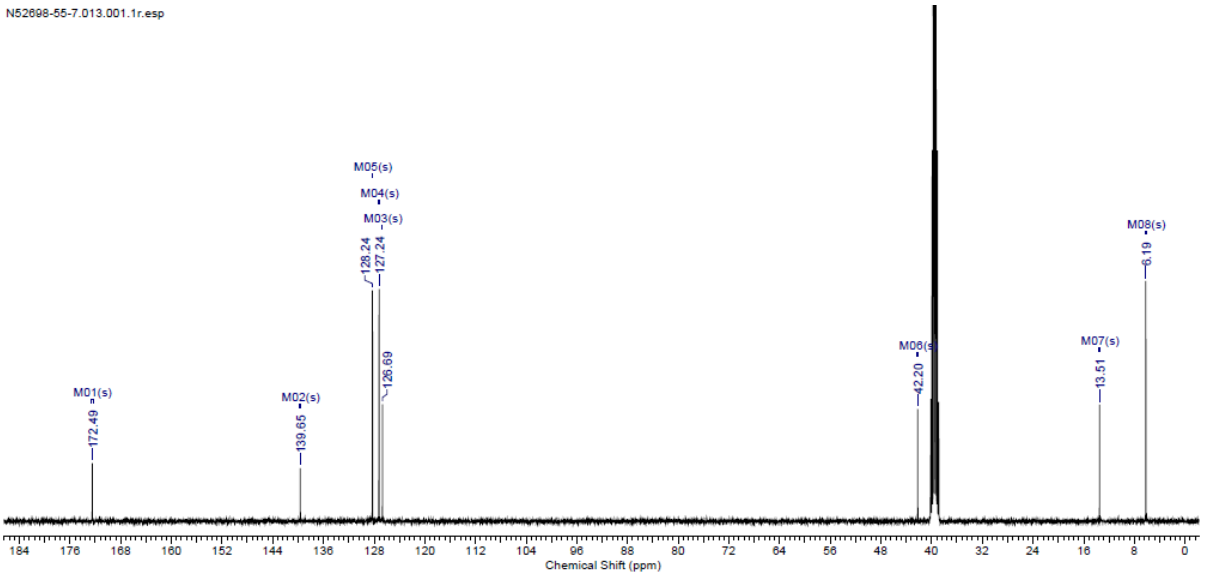
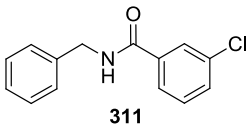




N-Benzyl-3-chlorobenzamide



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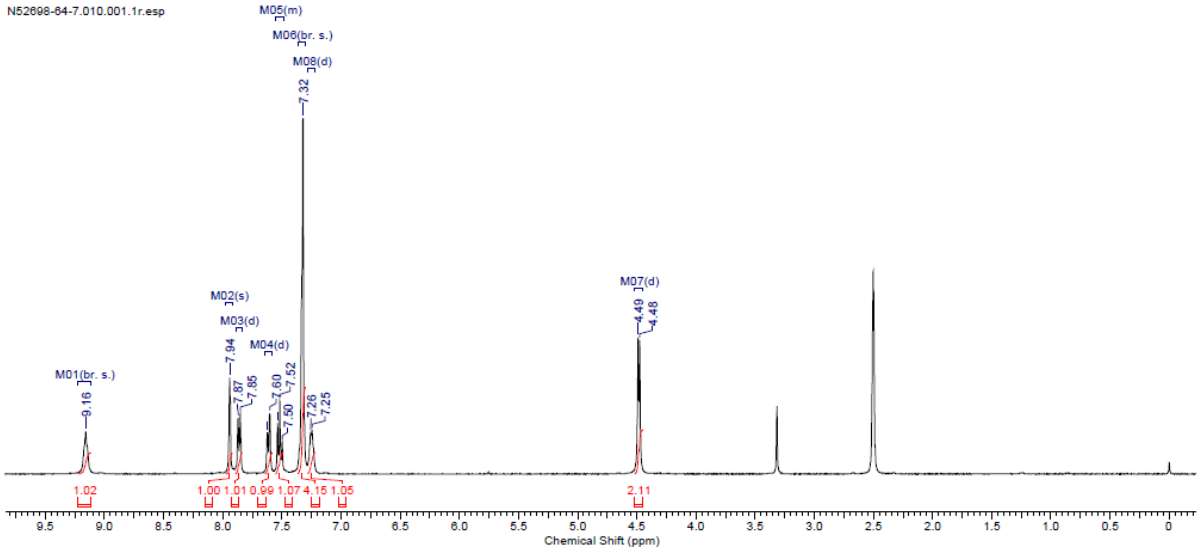
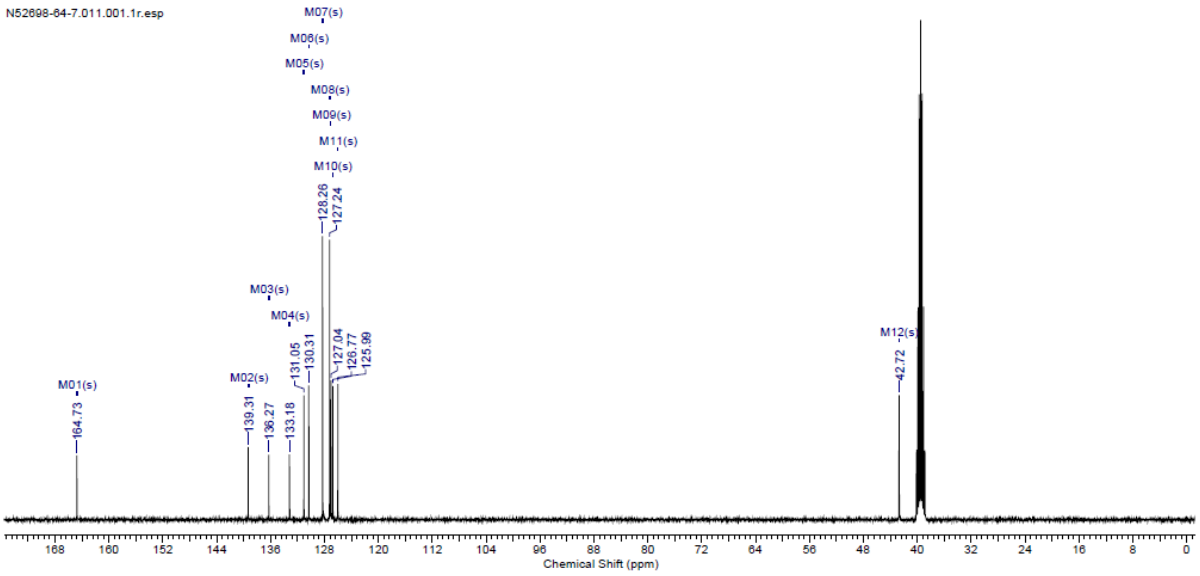
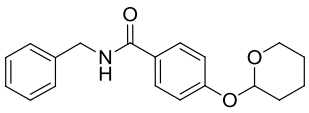




N-Benzyl-4-((tetrahydro-2H-pyran-2-yl)oxy)benzamide



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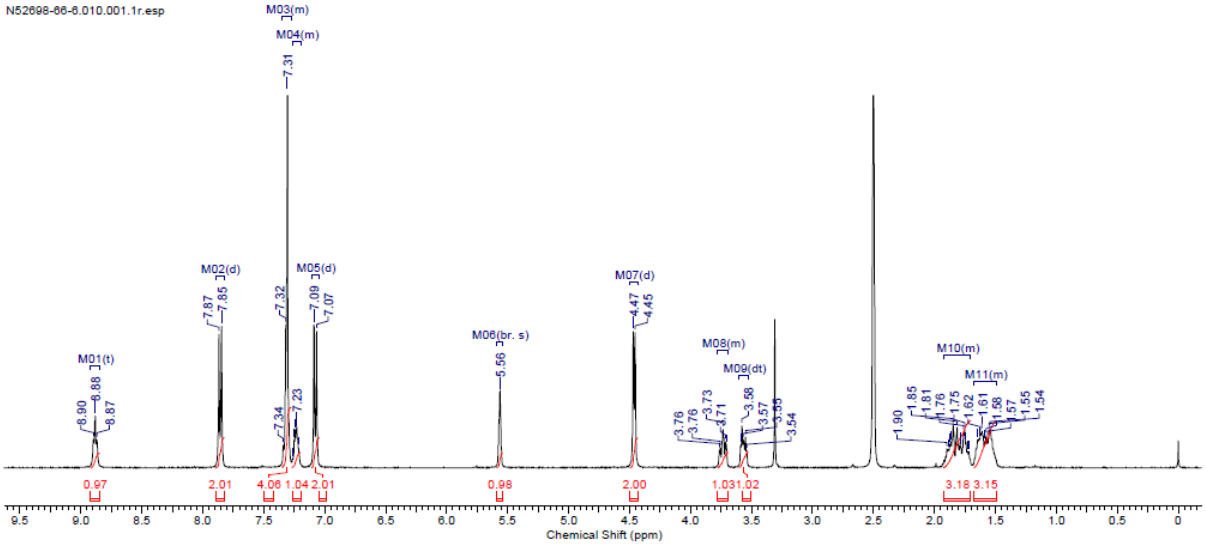
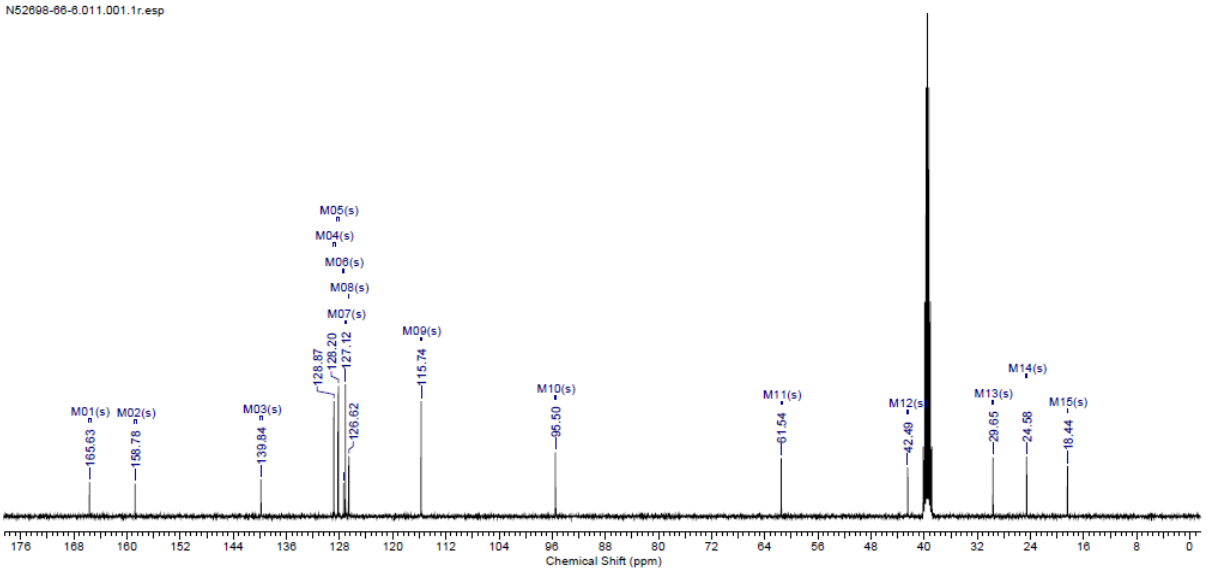
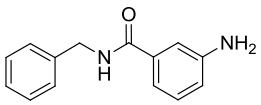




3-Amino-*N*-benzylbenzamide



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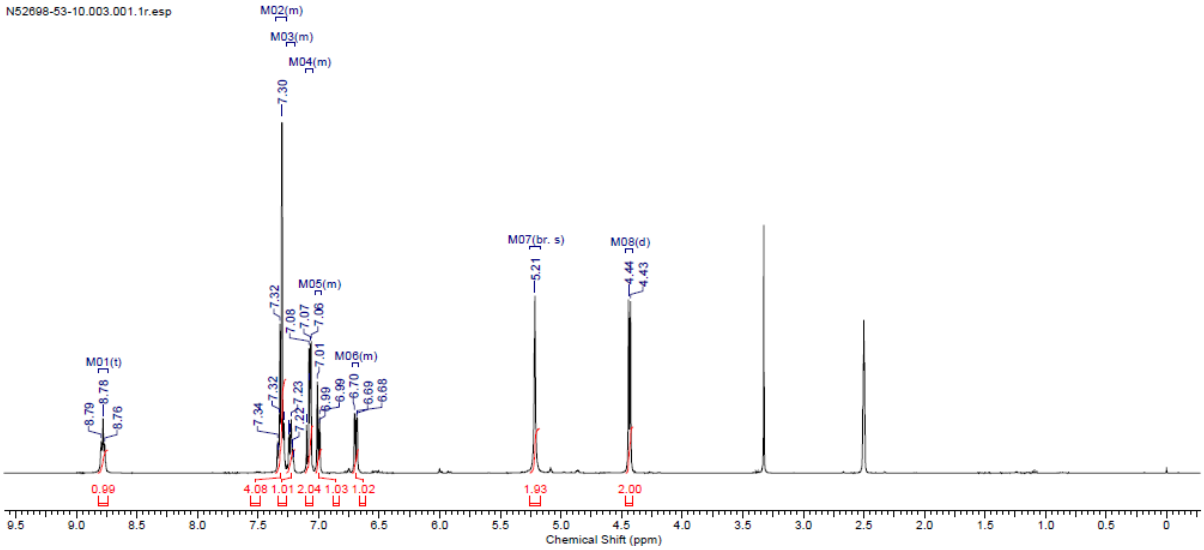
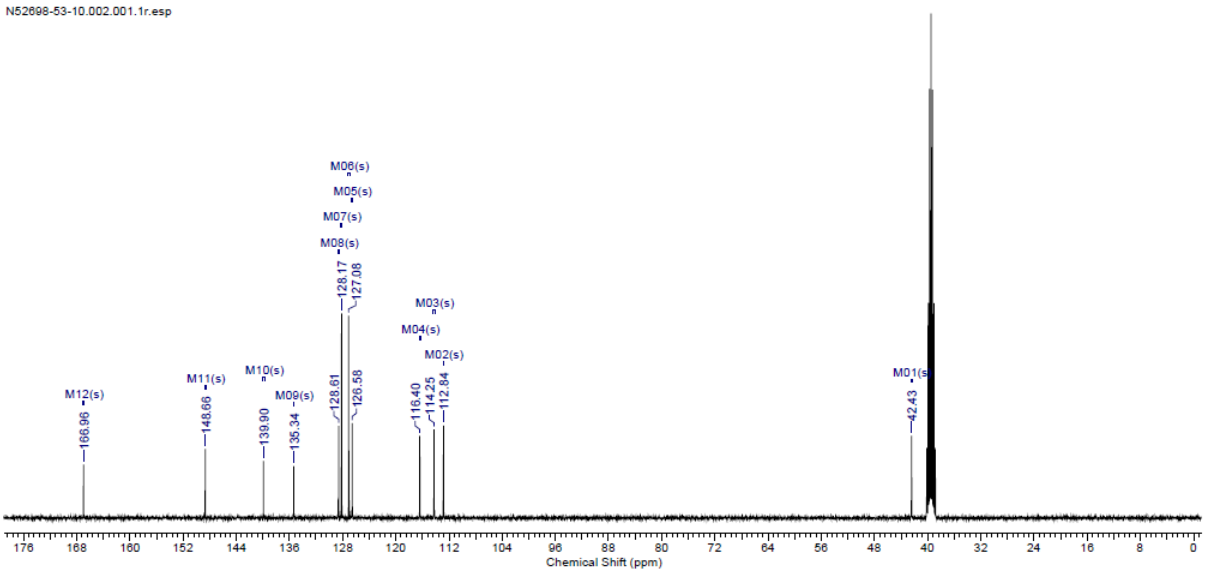
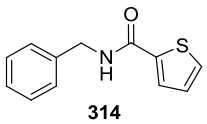




N-Benzylthiophene-2-carboxamide



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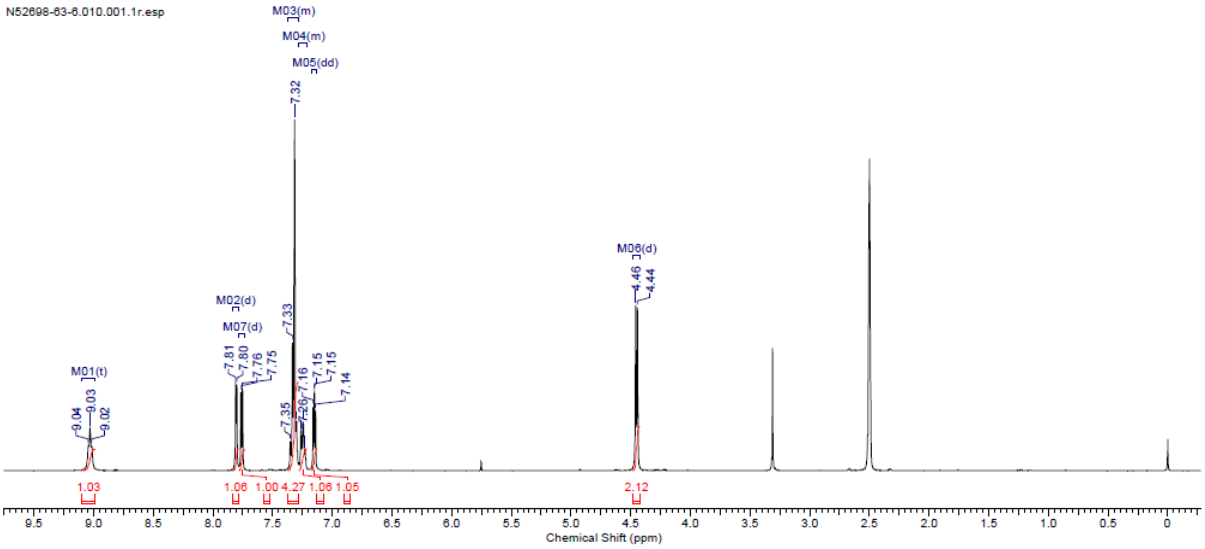
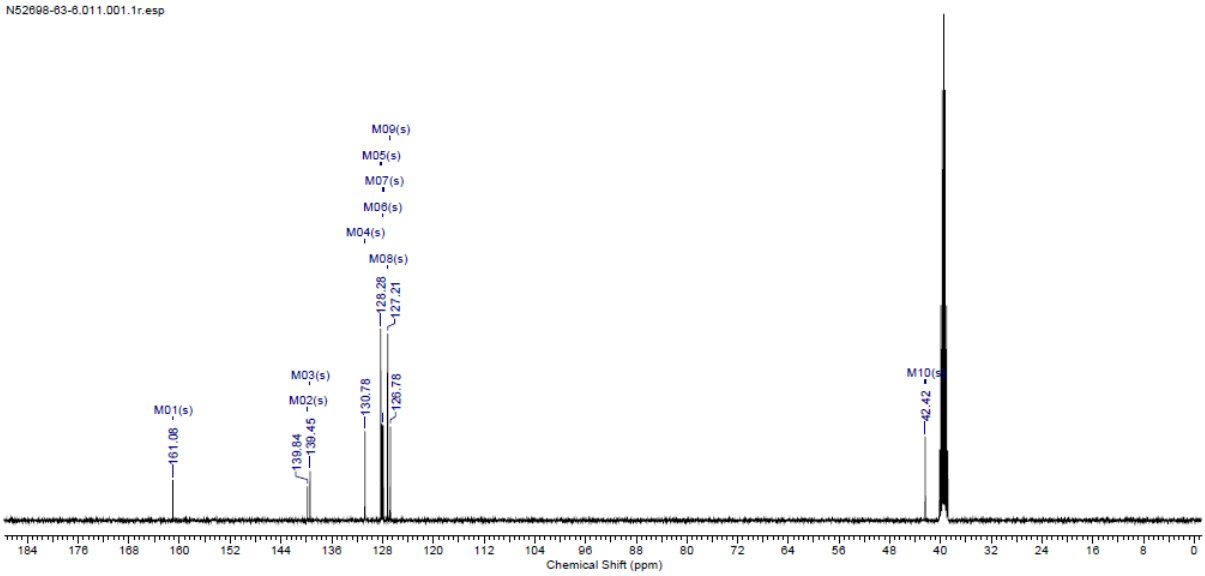
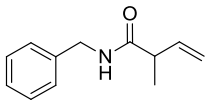




N-Benzyl-2-methylbut-3-enamide



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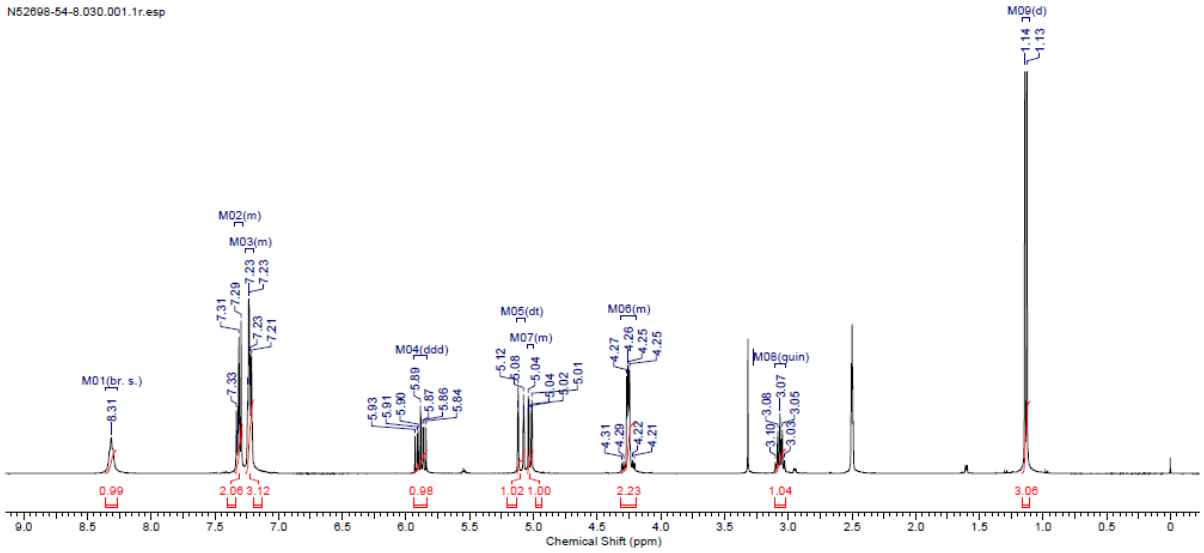
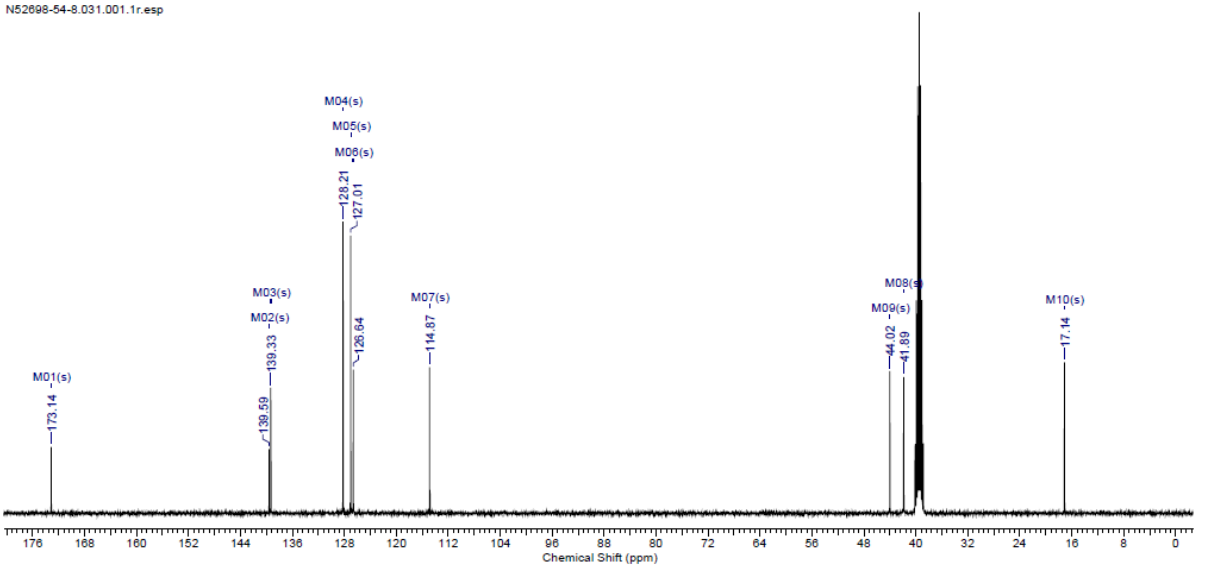
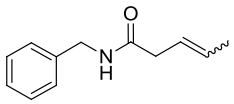




(*E*/*Z*)-*N*-Benzylpent-3-enamide



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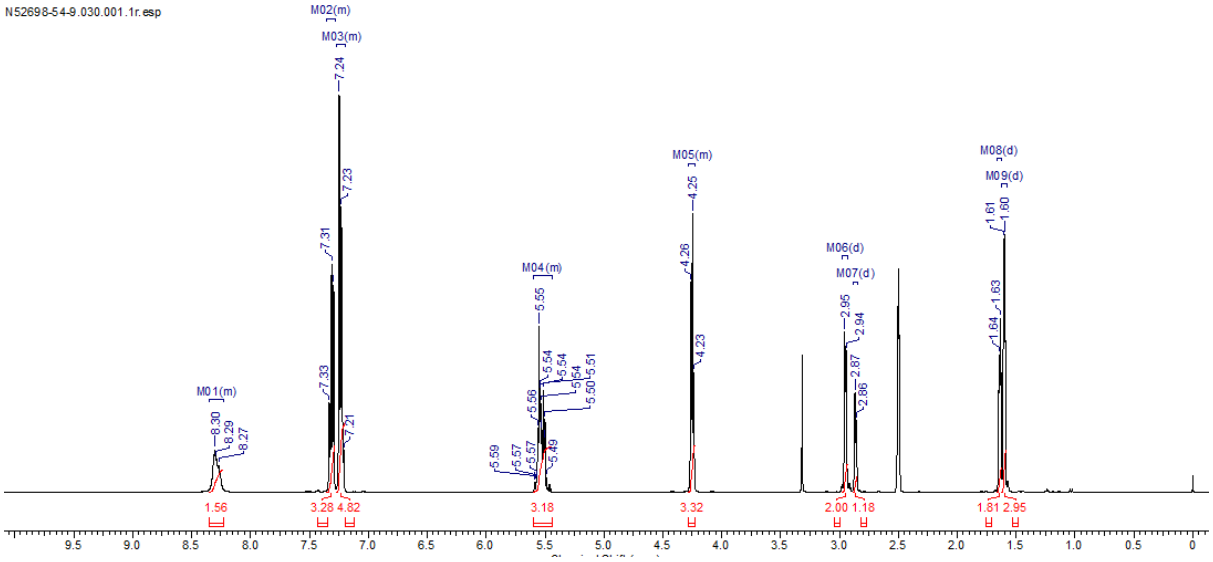
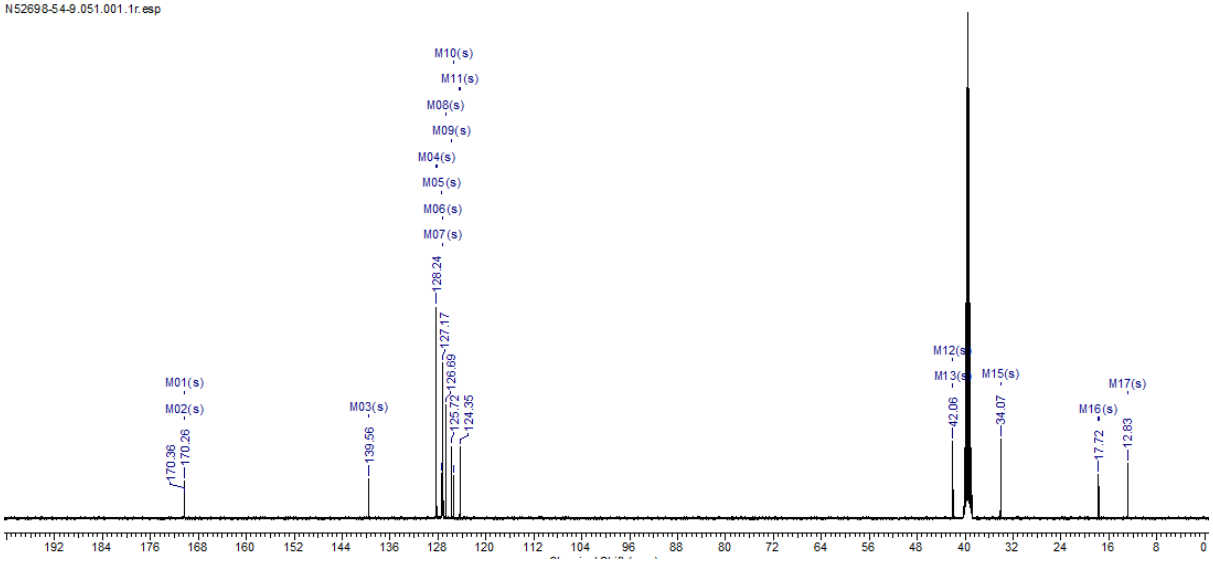
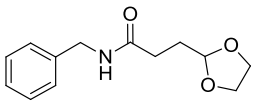




N-Benzyl-3-(1,3-dioxolan-2-yl)propanamide



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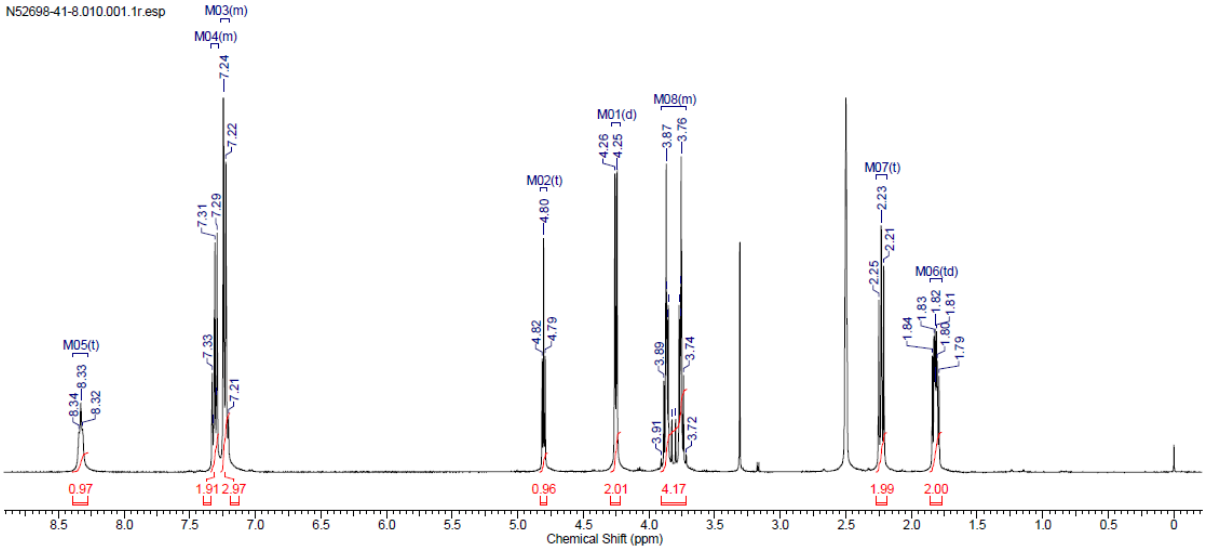
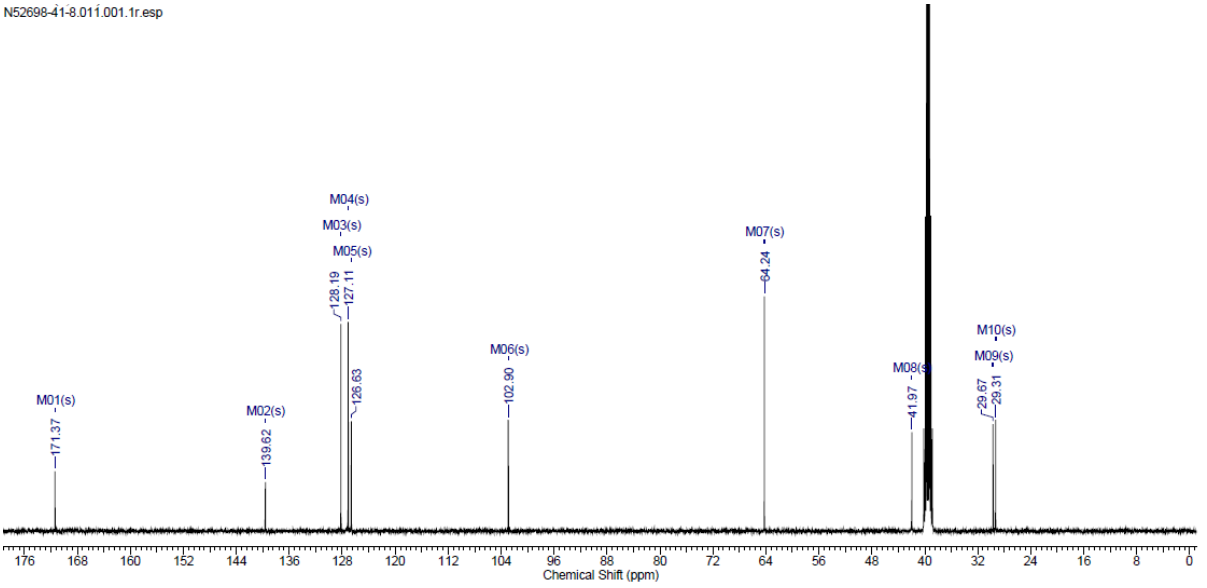
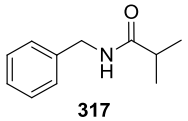




N-Benzylisobutyramide



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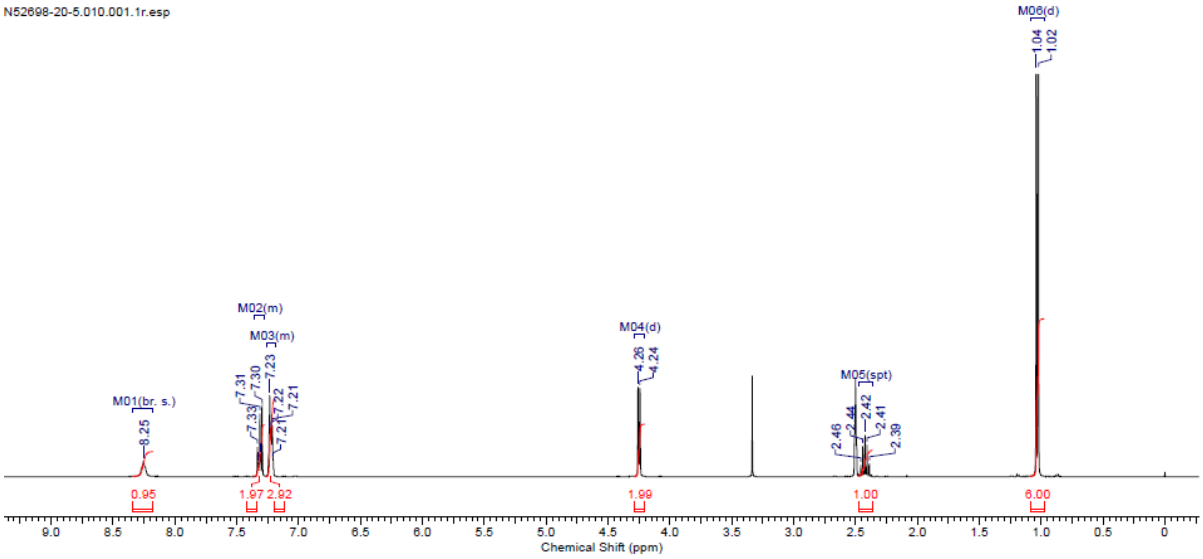
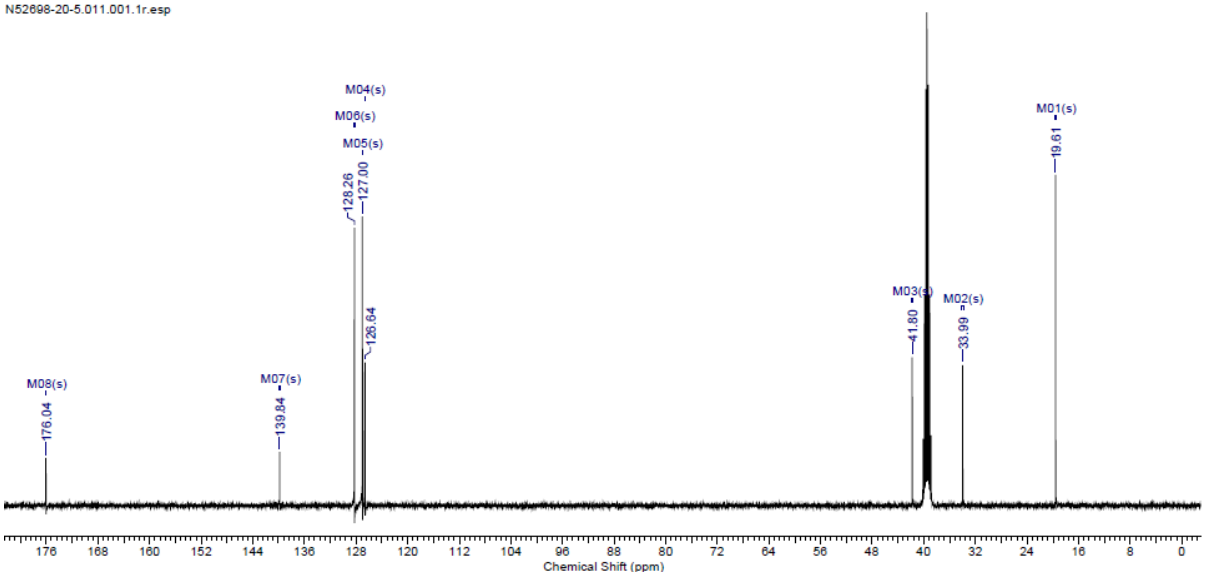
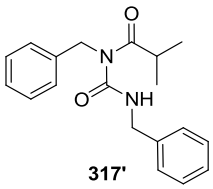




N-Benzylisobutyramide



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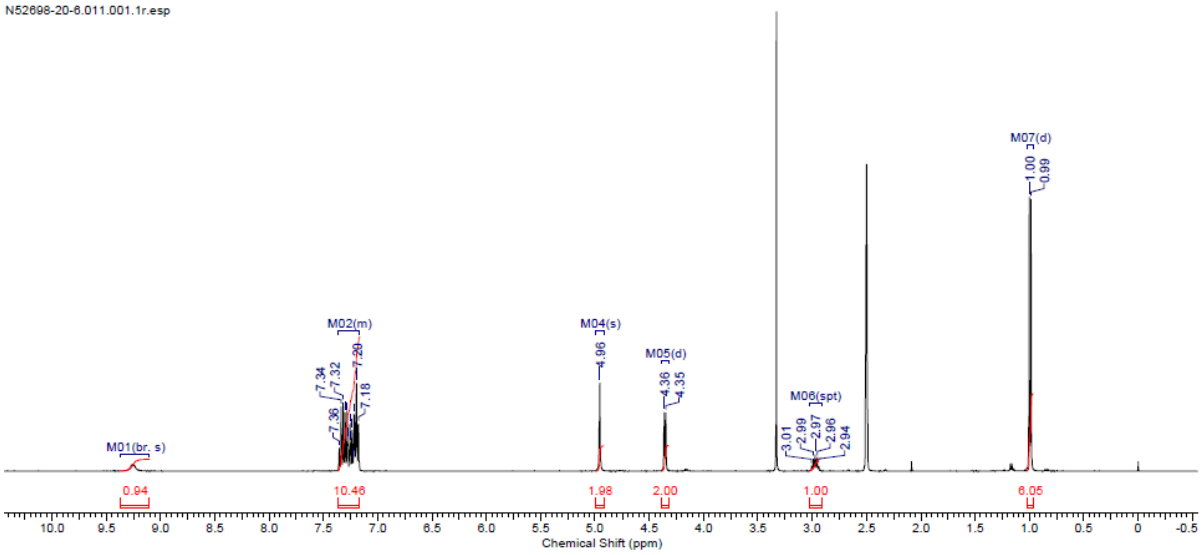
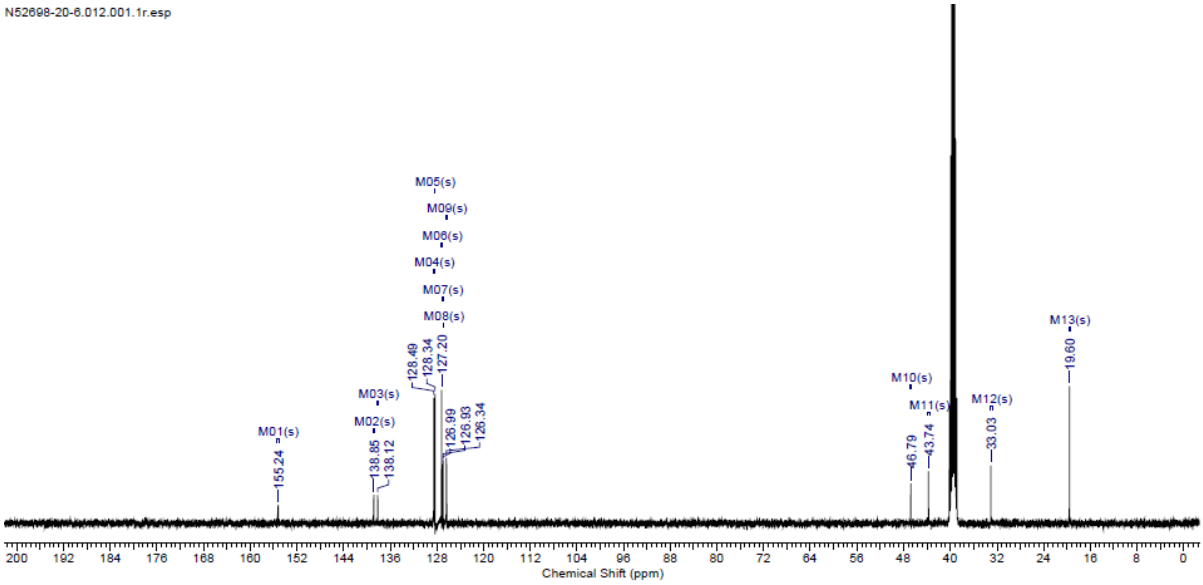
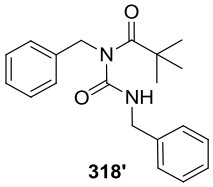
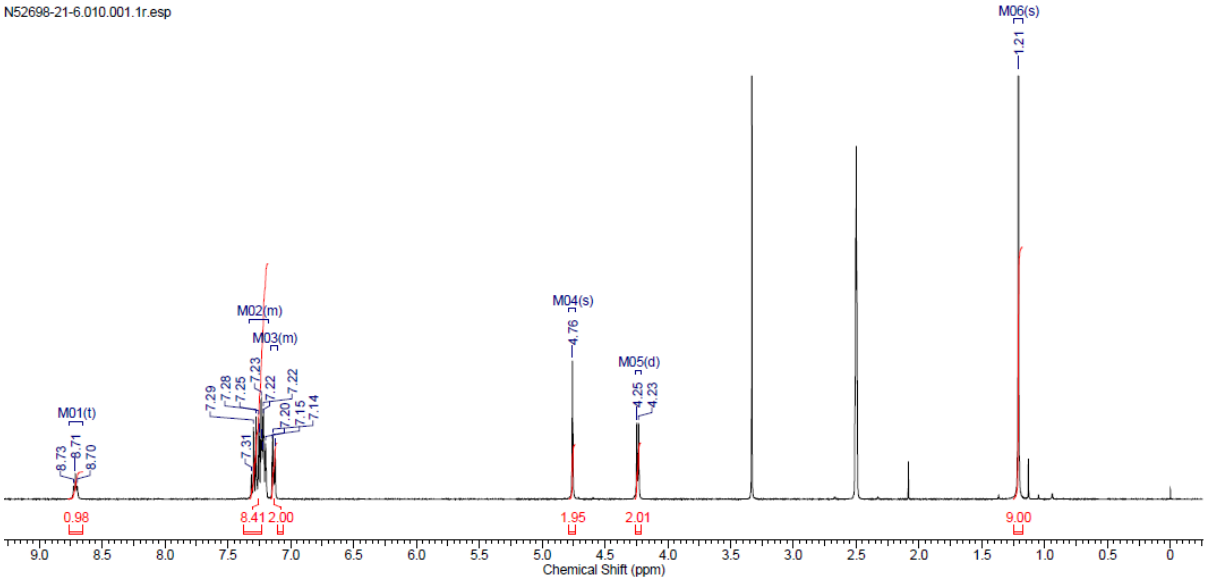


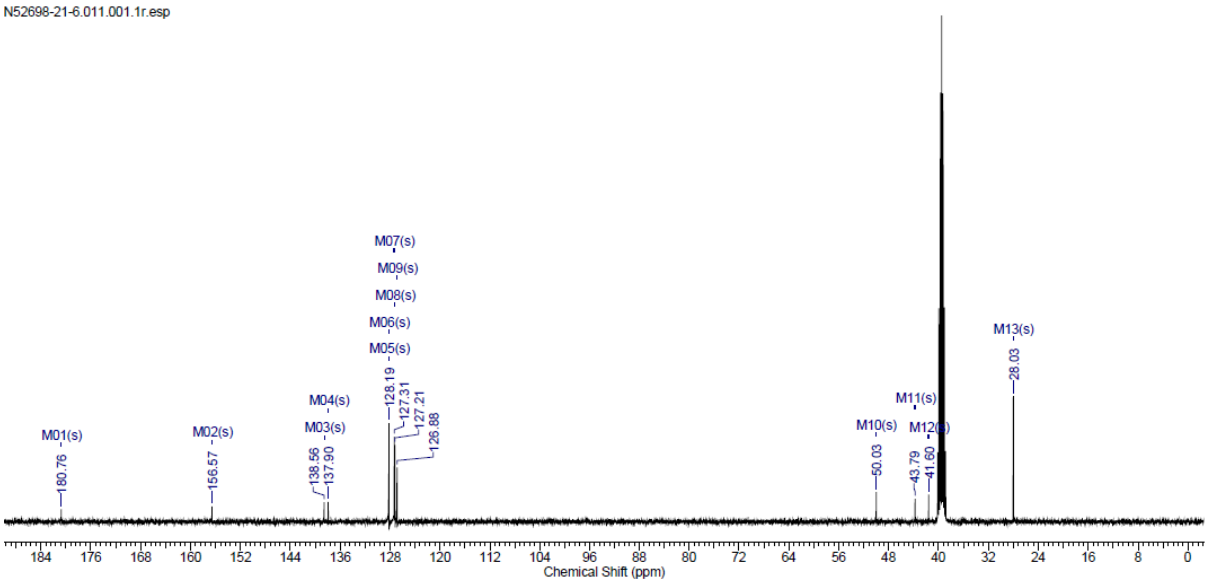


N-Benzyl-*N*-(benzylcarbamoyl)pivalamide

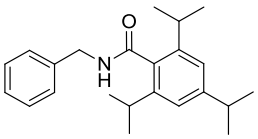


318'





N-Benzyl-2,4,6-triisopropylbenzamide



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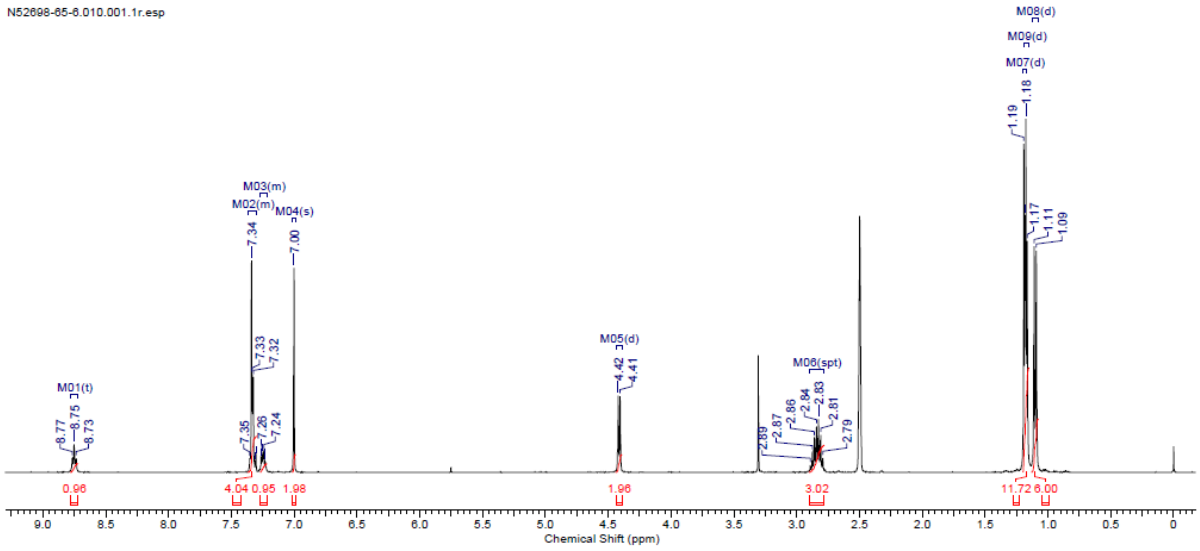
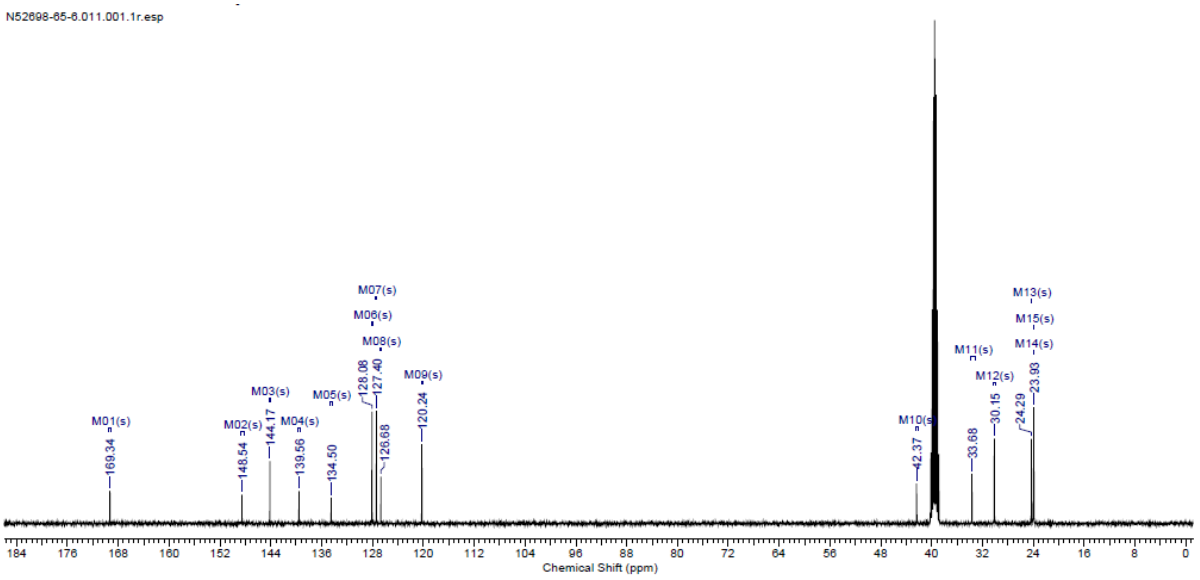
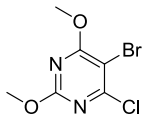




5-Bromo-4-chloro-2,6-dimethoxypyrimidine



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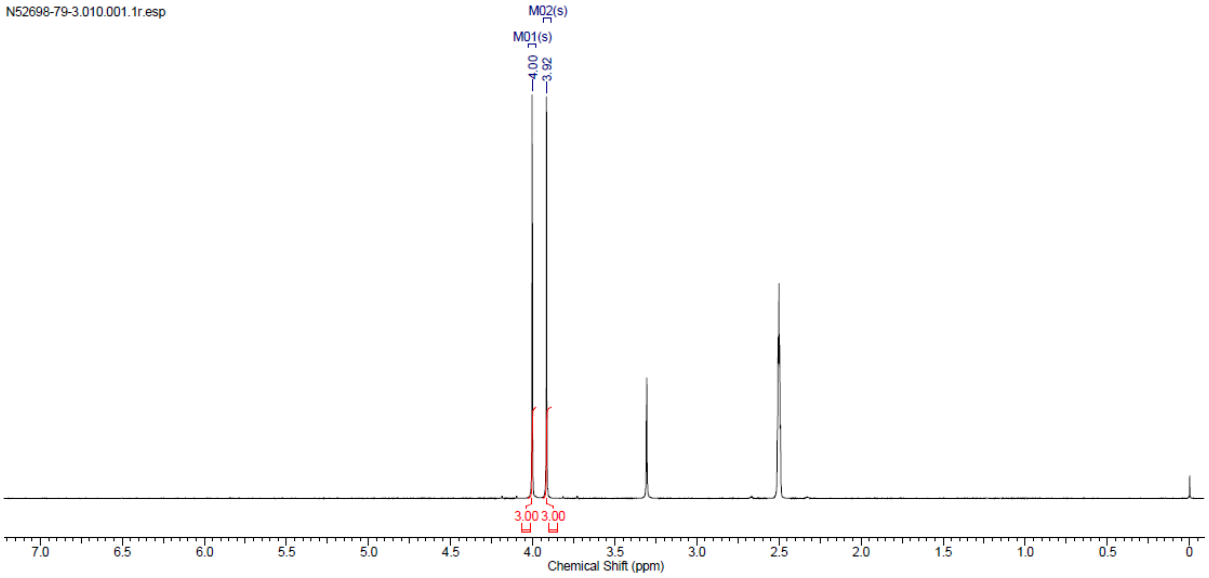
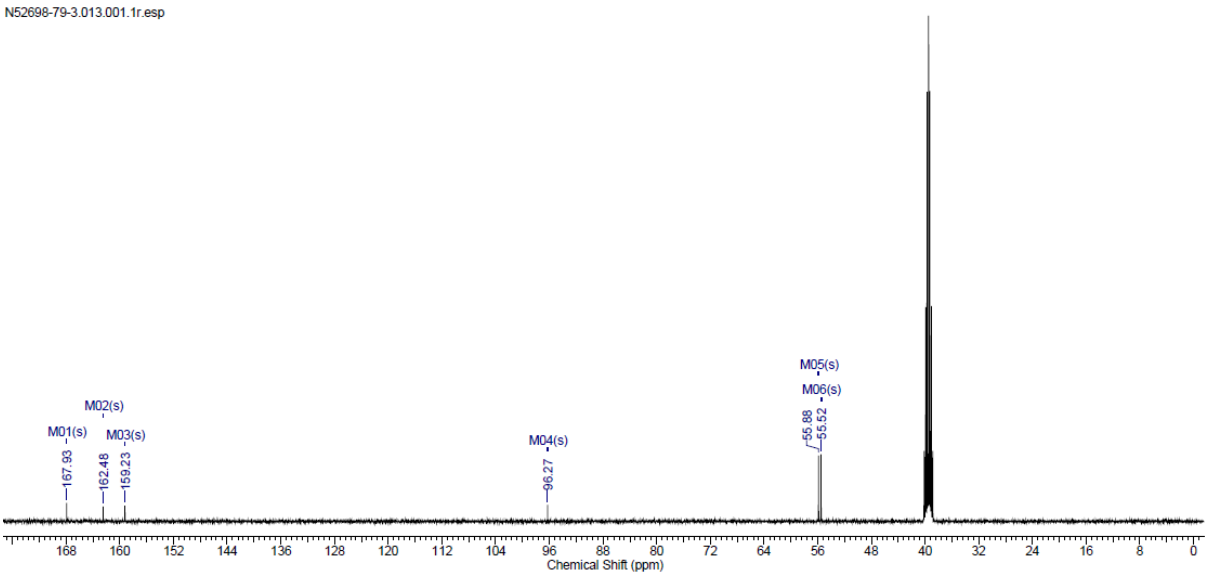
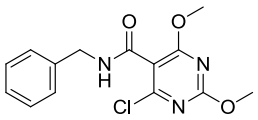




N-Benzyl-4-chloro-2,6-dimethoxypyrimidine-5-carboxamide



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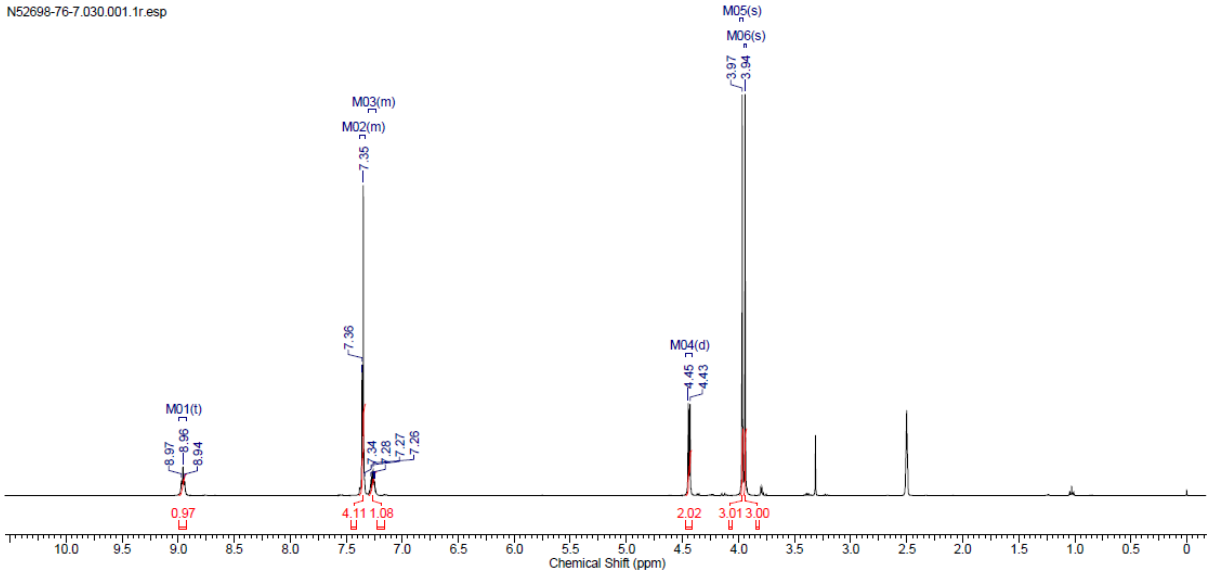
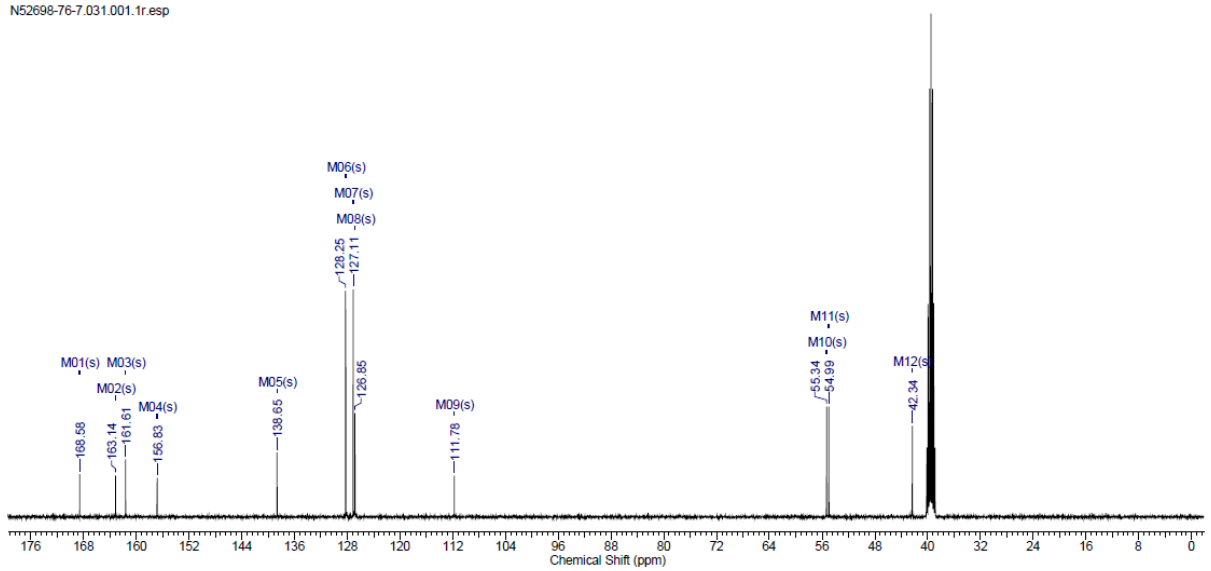
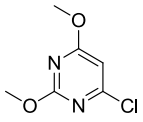




N-Benzyl-4-chloro-2,6-dimethoxypyrimidine-5-carboxamide



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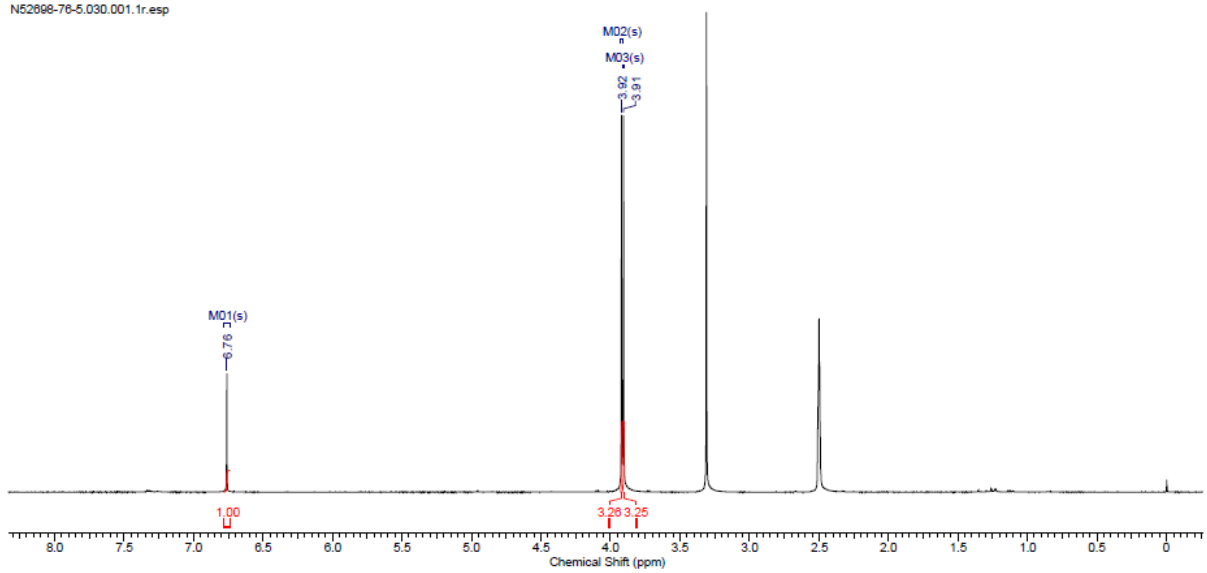
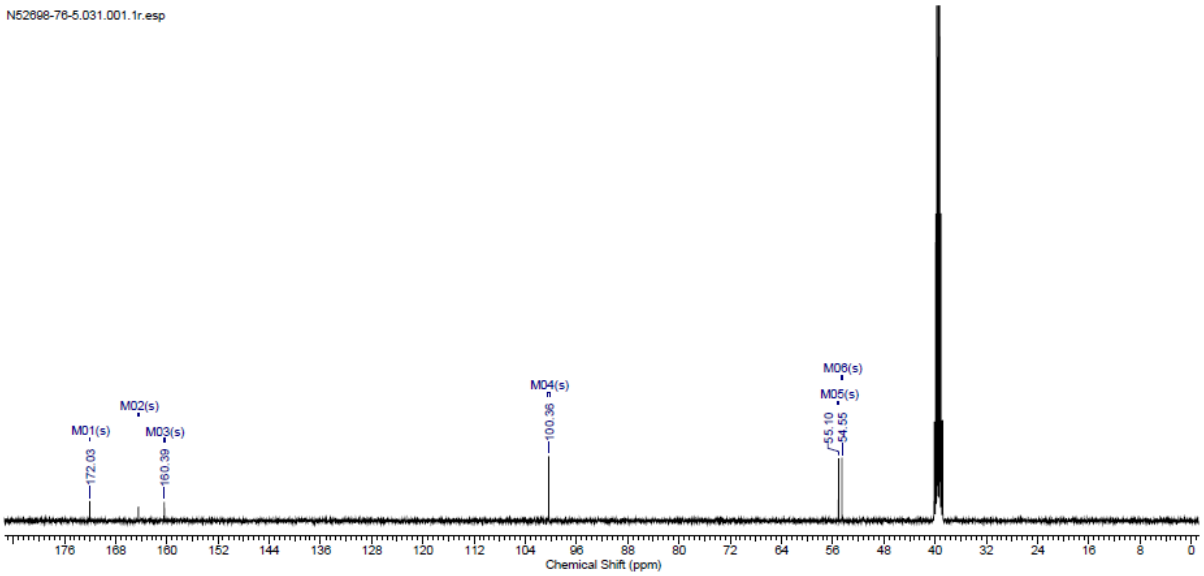
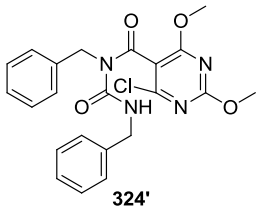




N-Benzyl-4-chloro-2,6-dimethoxypyrimidine-5-carboxamide



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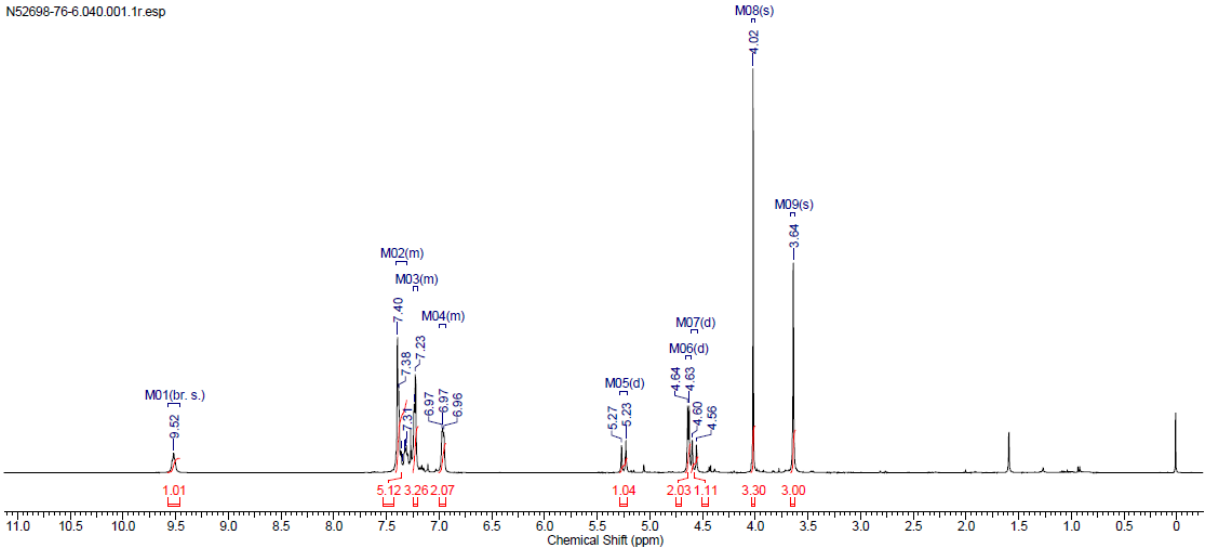
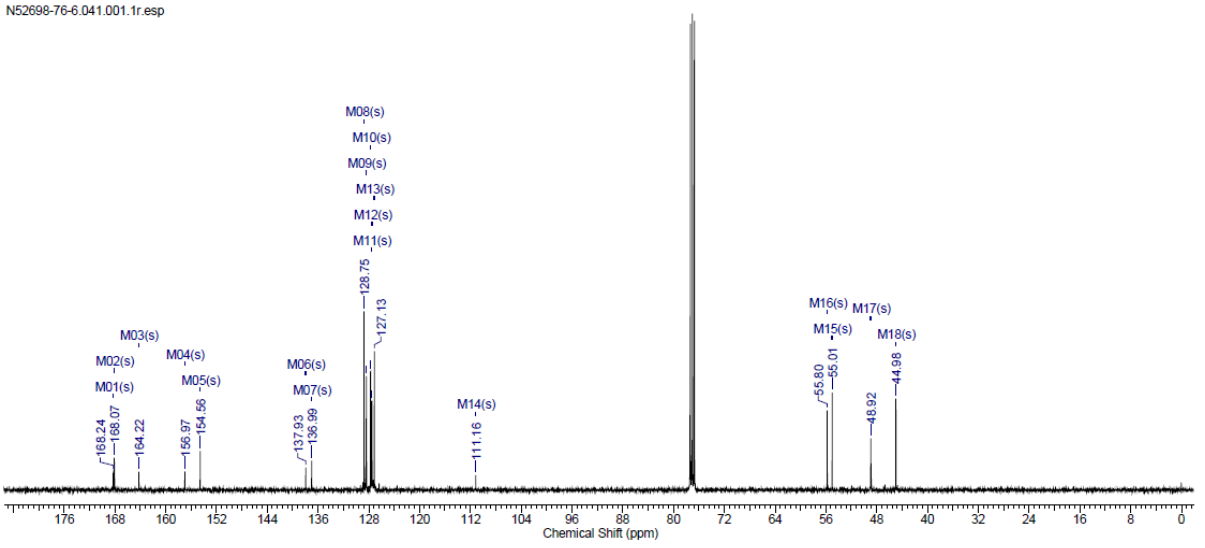
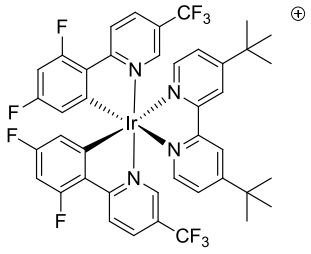




2. Full details of DFT calculations

2.1. Structures



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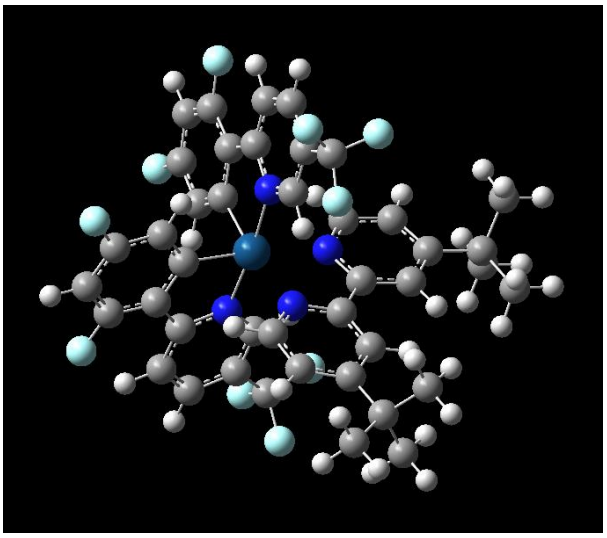
Iridium(III) catalyst

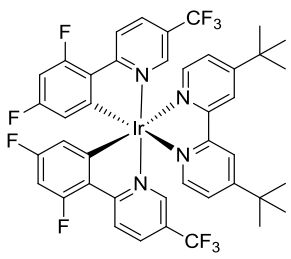


Route	UB3LYP/GEN Pseudo=read FormCheck Opt Freq scrf=(cpcm,solvent=acetone)
Smiles	FC1=C(C2=[N]3C=C(C(F)(F)F)C=C2)C([Ir]435(C6=CC(F)=CC(F)=C6C7=[N]5C=C(C(F)(F)F)C=C7)[N]8=CC=C(C(C)(C)C)C=C8C9=[N]4C=CC(C(C)(C)C)=C9)=CC(F)=C1
Formula	$C_{42}H_{34}F_{10}IrN_4^+$
Charge	1
Multiplicity	1
Dipole (Debye)	10.0250
Gibbs energy (a.u.)	−2942.641912
# Imaginary frequencies	0

Input coordinates:

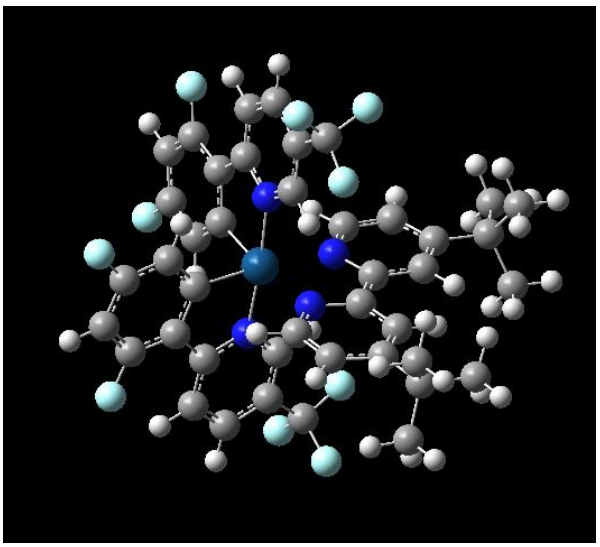
Ir	0.8097410	-0.0856270	0.0034820
C	2.0731130	2.0574420	1.5840340
C	0.5130730	2.9409020	0.0560490
C	2.3557120	3.3605390	2.0358280
C	0.7597900	4.2407510	0.4690080
H	-0.2054980	2.7276160	-0.7234210
C	1.7029000	4.4494420	1.4816950
H	3.0869890	3.5024040	2.8172140
H	1.9164660	5.4538660	1.8328990
C	2.2241580	-0.3789190	1.4165530
C	2.6719390	0.8165580	2.0569210
C	2.7610850	-1.6027750	1.8280170
C	3.6364110	0.7168710	3.0761220
C	3.7135220	-1.6367160	2.8434350
H	2.4671830	-2.5418480	1.3732840
C	4.1707250	-0.4908430	3.4883200
H	4.9137550	-0.5365270	4.2748330
N	1.1422300	1.8803280	0.5912870
F	4.0770390	1.8284580	3.7042930
F	4.2145430	-2.8209930	3.2213780
C	0.0609740	5.3961450	-0.1970230
F	-1.0774480	4.9961300	-0.8073270
F	-0.2586340	6.3497560	0.6976620
F	0.8414120	5.9668860	-1.1354020
C	-0.9190700	-0.3082120	2.6519860
C	-2.1586490	0.1211680	0.7345390
C	-2.0527920	-0.2812790	3.4493000
H	0.0635380	-0.4928080	3.0717460
C	-3.3334060	0.1606570	1.4939890
C	-3.3141140	-0.0416450	2.8786980
H	-1.9407500	-0.4479620	4.5147320
H	-4.2740140	0.3558390	0.9991480
C	-2.1364200	0.3322050	-0.7362930
C	-0.8275450	0.5222880	-2.6457860
C	-3.2878480	0.5285960	-1.4988870
C	-1.9432610	0.7269350	-3.4507400
H	0.1727480	0.5140060	-3.0648000
C	-3.2249700	0.7323210	-2.8867640
H	-4.2539680	0.5200740	-1.0106890
H	-1.7917840	0.8775900	-4.5121590
C	-0.1548610	-2.9705630	-0.0694770
C	1.5714980	-2.4502570	-1.5835470
C	-0.2067000	-4.2897980	-0.4947130
H	-0.8016790	-2.6131830	0.7207320
C	1.5581620	-3.7802360	-2.0426960
C	0.6711120	-4.6986340	-1.5034720
H	2.2492670	-4.0786800	-2.8165070
H	0.6644300	-5.7259130	-1.8523320
C	2.2644580	-0.1110010	-1.3993600
C	2.4377700	-1.3733920	-2.0439620

C	3.0667130	0.9625380	-1.7987210
C	3.4089500	-1.4884470	-3.0551980
C	4.0113460	0.7862920	-2.8065930
H	2.9879780	1.9415060	-1.3401670
C	4.2048750	-0.4300270	-3.4554380
H	4.9460180	-0.5489200	-4.2360410
N	-0.9584210	-0.1151900	1.3207170
N	-0.9075190	0.3285740	-1.3204940
C	-4.5067010	0.9450320	-3.7025730
C	-4.5754900	-0.0073770	3.7506370
C	-5.8491130	0.2610180	2.9271010
H	-5.8147360	1.2321620	2.4193930
H	-6.0274760	-0.5201360	2.1787640
H	-6.7166270	0.2750680	3.5940460
C	-4.4230170	1.1157840	4.8064060
H	-5.3117630	1.1444600	5.4457720
H	-3.5547460	0.9565740	5.4541710
H	-4.3163710	2.0971120	4.3307790
C	-4.7288230	-1.3731010	4.4653000
H	-5.6219100	-1.3590300	5.0991130
H	-4.8391940	-2.1900800	3.7435410
H	-3.8720560	-1.6015250	5.1075930
C	-5.2335220	2.2081810	-3.1781280
H	-6.1541280	2.3687210	-3.7493360
H	-5.5121210	2.1165380	-2.1227080
H	-4.6080180	3.1009790	-3.2874990
C	-4.2106980	1.1354470	-5.2023280
H	-3.7148140	0.2602920	-5.6374090
H	-5.1509160	1.2801240	-5.7433910
H	-3.5878650	2.0174740	-5.3897830
C	-5.4253290	-0.2903870	-3.5336190
H	-6.3430150	-0.1492490	-4.1144320
H	-4.9357380	-1.2026520	-3.8918960
H	-5.7179770	-0.4500470	-2.4901860
N	0.6988980	-2.0744220	-0.5918990
F	4.7689490	1.8293730	-3.1731910
F	3.5941430	-2.6678030	-3.6872410
C	-1.2351890	-5.2202690	0.0911180
F	-0.8355990	-6.5012510	0.0228660
F	-1.4829650	-4.9216950	1.3855150
F	-2.4105740	-5.1238580	-0.5684220



156'

Iridium(II) catalyst

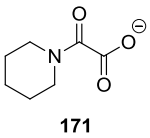


Route	UB3LYP/GEN Pseudo=read FormCheck Opt(MaxCyc=50) Freq scrf=(cpcm,solvent=acetone)
Smiles	FC1=C(C2=[N]3C=C(C(F)(F)F)C=C2)C([Ir]435(C6=CC(F)=CC(F)=C6C7=[N]5C=C(C(F)(F)F)C=C7)[N]8=CC=C(C(C)(C)C)C=C8C9=[N]4C=CC(C(C)(C)C)=C9)=CC(F)=C1
Formula	$C_{42}H_{34}F_{10}IrN_4$
Charge	0
Multiplicity	2
Dipole (Debye)	1.7807
Gibbs energy (a.u.)	−2942.755601
# Imaginary frequencies	0

Input coordinates:

Ir	0.8141500	-0.0403020	-0.0026900
C	1.9397240	2.1702260	1.5881060
C	0.3453410	2.9588310	0.0424510
C	2.1384910	3.4843950	2.0492120
C	0.5127920	4.2697940	0.4654550
H	-0.3450680	2.7069840	-0.7502430
C	1.4271680	4.5352530	1.4917690
H	2.8499490	3.6739950	2.8385210
H	1.5854230	5.5476520	1.8482820
C	2.2372850	-0.2533860	1.4139680
C	2.6135480	0.9635470	2.0610950
C	2.8475440	-1.4486030	1.8204150
C	3.5774070	0.9108800	3.0817250
C	3.7929800	-1.4242100	2.8367010
H	2.6033200	-2.4005820	1.3638120
C	4.1862390	-0.2625920	3.4930770
H	4.9261240	-0.2684880	4.2837370
N	1.0341170	1.9388080	0.5840400
F	3.9586720	2.0497780	3.7239110
F	4.3738250	-2.5934670	3.2174920
C	-0.2826730	5.3838580	-0.1544270
F	-1.0074010	4.9744710	-1.2211140
F	-1.1574550	5.9333480	0.7312340
F	0.5157050	6.3979130	-0.5778140
C	-0.8838940	-0.3605140	2.6418690
C	-2.1445910	0.0118990	0.7244570
C	-2.0188290	-0.4003840	3.4373350
H	0.1033360	-0.4938000	3.0680620
C	-3.3217670	-0.0185660	1.4805610
C	-3.2901140	-0.2286030	2.8639190
H	-1.8940800	-0.5669930	4.5007640
H	-4.2689780	0.1253700	0.9822920
C	-2.1309970	0.2307860	-0.7441910
C	-0.8281640	0.4851580	-2.6520410
C	-3.2902420	0.3803830	-1.5054520
C	-1.9515980	0.6418200	-3.4574590
H	0.1686270	0.5244590	-3.0755330
C	-3.2322360	0.5899980	-2.8927270
H	-4.2527610	0.3303310	-1.0142720
H	-1.8009610	0.8009760	-4.5171870
C	-0.0106260	-2.9631050	-0.0638890
C	1.6773730	-2.3646160	-1.5944020
C	-0.0037180	-4.2810440	-0.4980200
H	-0.6713500	-2.6361260	0.7266850
C	1.7153370	-3.6892660	-2.0664800
C	0.8764730	-4.6488640	-1.5227240
H	2.4014990	-3.9572440	-2.8554330
H	0.9091150	-5.6695000	-1.8890460
C	2.2671220	0.0033430	-1.4047960
C	2.4981050	-1.2476490	-2.0549320

C	3.0264350	1.1152630	-1.7969560
C	3.4721860	-1.3102310	-3.0653670
C	3.9727250	0.9786720	-2.8034780
H	2.8993090	2.0880390	-1.3365260
C	4.2260320	-0.2193570	-3.4633720
H	4.9697710	-0.3012820	-4.2461540
N	-0.9334300	-0.1622350	1.3108520
N	-0.9020510	0.2840040	-1.3266460
C	-4.5219510	0.7467980	-3.7088500
C	-4.5532260	-0.2735700	3.7332900
C	-5.8396230	-0.0754640	2.9088820
H	-5.8614710	0.8994070	2.4100150
H	-5.9665640	-0.8575210	2.1524220
H	-6.7050080	-0.1215310	3.5770820
C	-4.4694820	0.8500340	4.7970520
H	-5.3641330	0.8257210	5.4281580
H	-3.5980430	0.7335590	5.4485230
H	-4.4128080	1.8361620	4.3238820
C	-4.6272340	-1.6507820	4.4396940
H	-5.5233240	-1.6932550	5.0677630
H	-4.6841010	-2.4649960	3.7093420
H	-3.7601520	-1.8291010	5.0827190
C	-5.3151020	1.9653990	-3.1731230
H	-6.2369620	2.0857130	-3.7517840
H	-5.5950650	1.8441500	-2.1223120
H	-4.7312010	2.8872310	-3.2666110
C	-4.2341790	0.9674490	-5.2064240
H	-3.6967570	0.1215500	-5.6480180
H	-5.1817110	1.0729810	-5.7435420
H	-3.6521030	1.8784830	-5.3815000
C	-5.3769890	-0.5362350	-3.5546570
H	-6.3016810	-0.4319840	-4.1320700
H	-4.8394530	-1.4145470	-3.9276530
H	-5.6545020	-0.7231540	-2.5128540
N	0.8007520	-2.0303280	-0.5936890
F	4.6986030	2.0686370	-3.1706620
F	3.7172400	-2.4848540	-3.7099160
C	-0.9309550	-5.2964150	0.1082000
F	-0.2556630	-6.3758560	0.5825070
F	-1.6529270	-4.7951170	1.1365710
F	-1.8190620	-5.7752030	-0.8043090



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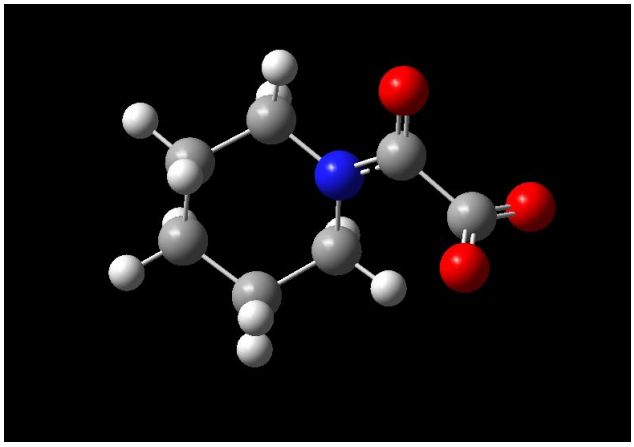
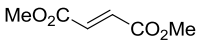


Route	UB3LYP/6-31+G(d,p) FormCheck opt(MaxCyc=1000) freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(C([O-])=O)N1CCCCC1
Formula	$C_7H_{10}NO_3^-$
Charge	−1
Multiplicity	1
Dipole (Debye)	16.5508
Gibbs energy (a.u.)	−553.280058
# Imaginary frequencies	0

Input coordinates:

C	-2.8450240	0.5808480	-0.3369540
C	-1.5928270	1.4980610	-0.4370090
C	-0.5346320	1.1425740	0.6487680
C	-1.3598420	-1.2680910	0.6134860
C	-2.4213700	-0.9063780	-0.4706550
H	0.5309540	1.5877890	0.4406600
H	-1.1460270	1.3749770	-1.4409040
H	-1.8969570	2.5568270	-0.3361170
H	-3.3336670	0.7327810	0.6441680
H	-3.5860510	0.8375080	-1.1181340
H	-0.8574550	-2.2341350	0.3753870
H	-1.8578780	-1.3308890	1.6063860
H	-1.9785260	-1.0646920	-1.4705950
H	-3.3025590	-1.5702340	-0.3833910
H	-0.9499720	1.4227300	1.6424170
N	-0.2258230	-0.3103300	0.6374490
C	1.0281160	-0.7753970	0.0321720
C	2.3159850	0.3860140	-0.1012040
O	3.4301640	-0.1417130	-0.3959520
O	1.1301010	-1.9990950	-0.2308530
O	1.9917930	1.6300400	0.1125980



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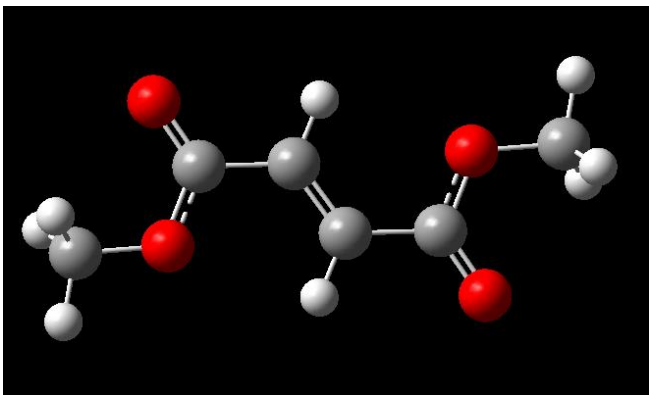
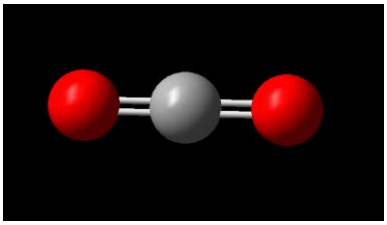


Route	UB3LYP/6-31+G(d,p) FormCheck opt(MaxCyc=1000) freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(OC)/C=C/C(OC)=O
Formula	$C_6H_8O_4$
Charge	0
Multiplicity	1
Dipole (Debye)	0
Gibbs energy (a.u.)	−534.288989
# Imaginary frequencies	0

Input coordinates:

C	-0.3788860	-0.5579410	0.0001630
H	0.0955160	-1.5530000	0.0001390
C	0.3788920	0.5579840	0.0000460
H	-0.0954800	1.5530560	0.0000220
C	1.8975190	0.5782470	0.0000390
C	-1.8975110	-0.5782370	0.0000650
O	2.6327700	1.5886070	0.0000790
O	-2.6327380	-1.5886150	0.0000310
O	2.3920080	-0.7653810	-0.0000030
O	-2.3920290	0.7653800	-0.0000160
C	3.8641200	-0.7375590	-0.0001460
H	4.2625870	-0.2211560	0.8993680
H	4.1894840	-1.7954670	0.0010660
H	4.2624210	-0.2233620	-0.9010060
C	-3.8641430	0.7375280	-0.0001360
H	-4.1895290	1.7954290	-0.0006190
H	-4.2624420	0.2218100	-0.9001220
H	-4.2625870	0.2226280	0.9002550

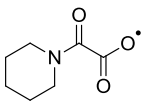
CO_2



Route	UB3LYP/6-31+G(d,p) FormCheck opt(MaxCyc=1000) freq scrf=(cpcm,solvent=acetone)
Smiles	O=C=O
Formula	CO_2
Charge	0
Multiplicity	1
Dipole (Debye)	0
Gibbs energy (a.u.)	−188.602442
# Imaginary frequencies	0

Input coordinates:

C	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.2226540
O	0.0000000	0.0000000	-1.2226540
X	-0.4500375	1.0529453	-0.4811930



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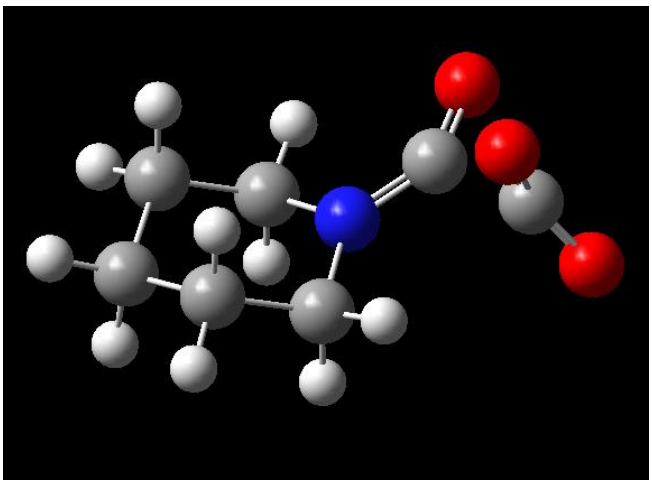
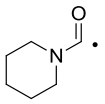


Route	UB3LYP/6-31+G(d,p) FormCheck opt(MaxCyc=1000) freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(C([O])=O)N1CCCCC1
Formula	$C_7H_{10}NO_3$•
Charge	0
Multiplicity	2
Dipole (Debye)	8.6220
Gibbs energy (a.u.)	−553.079468
# Imaginary frequencies	0

Input coordinates:

C	-2.5810860	0.7981740	-0.3336330
C	-1.2641730	1.5867850	-0.1091420
C	-0.4415490	0.9401930	1.0405350
C	-1.4353420	-1.3059070	0.5530080
C	-2.2919530	-0.7037980	-0.5964580
H	0.5269160	1.4525750	1.1924790
H	-0.6465100	1.5784190	-1.0270260
H	-1.4831690	2.6383880	0.1482260
H	-3.2212150	0.8948660	0.5629830
H	-3.1360980	1.2266410	-1.1870380
H	-1.1358450	-2.3495900	0.3356740
H	-1.9904420	-1.2760790	1.5131330
H	-1.7392930	-0.8184550	-1.5468510
H	-3.2364390	-1.2708260	-0.6805400
H	-1.0129880	0.9683620	1.9912040
N	-0.1693550	-0.5064560	0.7407940
C	0.9340280	-0.8787800	-0.0528790
C	2.1578350	0.4238860	-0.1951620
O	1.8822760	1.0854620	-1.2412130
O	1.1339800	-1.9918330	-0.5827840
O	2.9579950	0.3235670	0.7833200



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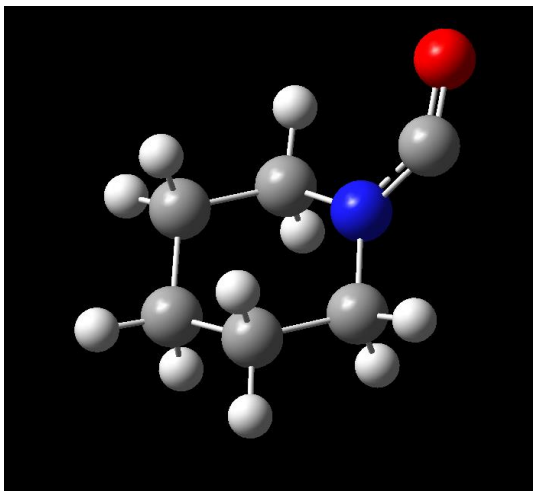
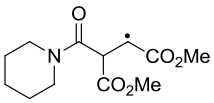


Route	UB3LYP/6-31+G(d,p) FormCheck opt(MaxCyc=1000) freq scrf=(cpcm,solvent=acetone)
Smiles	O=[C]N1CCCCC1
Formula	$C_6H_{10}NO$•
Charge	0
Multiplicity	2
Dipole (Debye)	5.9455
Gibbs energy (a.u.)	−364.508489
# Imaginary frequencies	0

Input coordinates:

C	-2.0804190	-0.3606710	-0.1973140
C	-1.5098450	1.0507540	-0.4932590
C	-0.3508040	1.3820800	0.4913220
C	0.1967760	-1.0632350	0.7096720
C	-0.9556440	-1.4265010	-0.2685990
H	0.1292160	2.3463830	0.2373230
H	-1.1246140	1.0866870	-1.5282610
H	-2.3010900	1.8157000	-0.3964000
H	-2.5295220	-0.3691840	0.8132070
H	-2.8789850	-0.6052590	-0.9203830
H	1.0577330	-1.7502080	0.5950560
H	-0.1673710	-1.1121260	1.7584020
H	-0.5541730	-1.4754780	-1.2968960
H	-1.3529570	-2.4248290	-0.0103250
H	-0.7487080	1.4415020	1.5275200
N	0.7071900	0.3287220	0.4484340
C	1.9020450	0.5730680	-0.2440860
O	2.7884360	-0.2734020	-0.4880870



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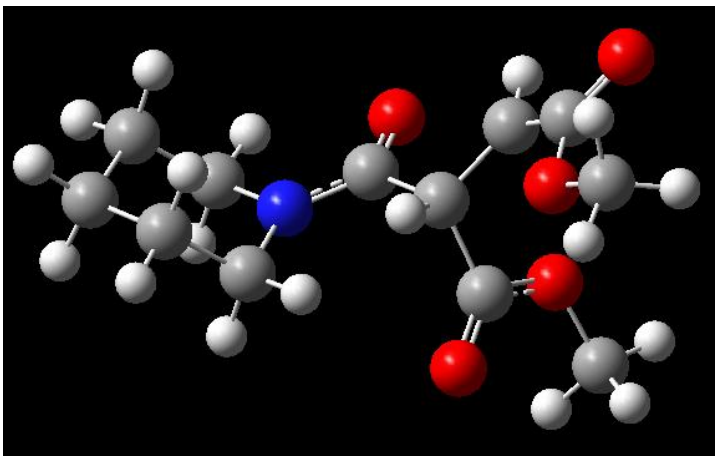
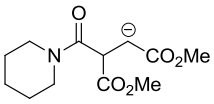


Route	UB3LYP/6-31+G(d,p) FormCheck opt=(Loose, MaxCyc=1000) freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(C(C(OC)=O)[C]C(OC)=O)N1CCCCC1
Formula	$C_{12}H_{18}NO_5$•
Charge	0
Multiplicity	2
Dipole (Debye)	6.2363
Gibbs energy (a.u.)	−898.797993
# Imaginary frequencies	0

Input coordinates:

C	-3.3324860	1.5252950	-0.6729080
C	-2.0294580	1.3168850	-1.4905890
C	-0.8456580	2.0411410	-0.7847040
C	-1.9147060	1.7590120	1.4435180
C	-3.1419740	1.0554280	0.7935370
H	0.1280790	1.9390340	-1.3127000
H	-1.8079990	0.2353810	-1.5619410
H	-2.1497260	1.7114840	-2.5155260
H	-3.5987690	2.5985380	-0.6813570
H	-4.1666760	0.9714470	-1.1401030
H	-1.7075970	1.3429980	2.4485210
H	-2.0841050	2.8522150	1.5190230
H	-2.9672580	-0.0364190	0.8145150
H	-4.0489500	1.2674560	1.3878500
H	-1.0767940	3.1228170	-0.7013110
N	-0.6793440	1.5336890	0.6188390
O	-0.1743750	-0.3379550	1.9683920
C	-0.0275700	0.2795020	0.8973760
C	1.4368260	-1.6136890	-0.0335240
H	2.4545080	-1.8046260	0.3381180
C	2.1249390	0.8372230	-0.4857550
O	3.2156580	0.5074790	0.3614850
C	4.2828560	1.5135400	0.2052570
H	5.0714390	1.2347730	0.9301070
H	4.7008020	1.5058920	-0.8241620
H	3.9116000	2.5367190	0.4263910
O	2.0954180	1.8331130	-1.2396950
C	0.4894980	-2.7465210	-0.1037840
O	0.7085720	-3.9631560	0.1257730
O	-0.8106170	-2.2399470	-0.4935480
C	-1.7648510	-3.3540400	-0.5391090
H	-1.8427510	-3.8706410	0.4419520
H	-2.7441740	-2.9097880	-0.8036270
H	-1.4826880	-4.1106070	-1.3036420
C	0.9770500	-0.2024650	-0.2895400
H	0.3624170	-0.1866380	-1.2118880



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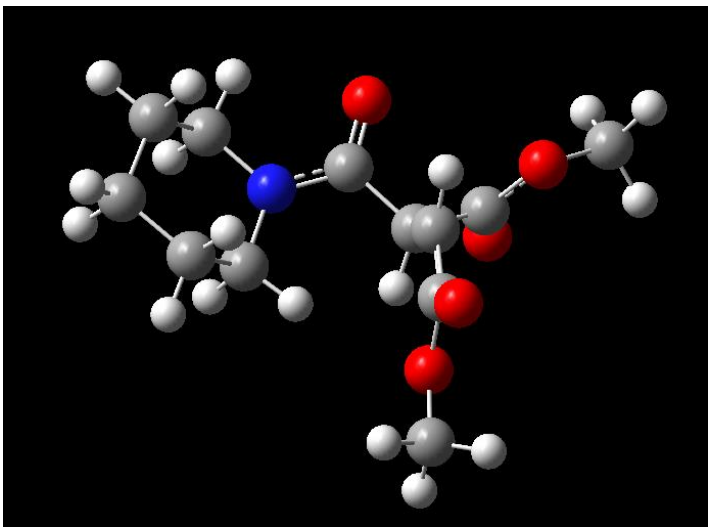
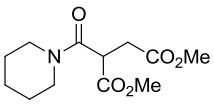


Route	UB3LYP/6-31+G(d,p) FormCheck opt=(Loose, MaxCyc=1000) freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(C(C(OC)=O)[CH-]C(OC)=O)N1CCCCC1
Formula	$C_{12}H_{18}NO_5^-$
Charge	−1
Multiplicity	1
Dipole (Debye)	9.4163
Gibbs energy (a.u.)	−898.943215
# Imaginary frequencies	0

Input coordinates:

C	3.3927880	-0.8209840	-0.0767360
C	2.4191310	-0.2449380	-1.1382830
C	1.3956610	-1.3352760	-1.5683220
C	1.6440760	-2.5752860	0.5453320
C	2.6222600	-1.4909810	1.0917710
H	0.6458460	-0.9157300	-2.2647550
H	1.8554740	0.6657360	-0.7706950
H	2.9984410	0.0582220	-2.0299370
H	4.0533250	-1.5782440	-0.5438110
H	4.0429550	-0.0169500	0.3155890
H	1.0267630	-2.9954420	1.3644940
H	2.2098010	-3.3901000	0.0464360
H	2.0231780	-0.7286500	1.6232820
H	3.3279590	-1.9414080	1.8142820
H	1.9205870	-2.1600320	-2.1004920
N	0.6739850	-1.9731130	-0.4211990
O	-0.9209520	-1.8961730	1.2995750
C	-0.4756380	-1.3408050	0.2702400
C	-0.7145710	1.0868180	0.8312770
H	-1.2715860	0.9296930	1.7570130
C	-2.4856160	0.0696220	-0.6550490
O	-3.2462900	-0.4617110	0.4542090
C	-4.6774590	-0.3448230	0.1550860
H	-5.2137400	-0.7631470	1.0295660
H	-4.9904630	0.7119940	0.0048710
H	-4.9663960	-0.9135750	-0.7566210
O	-3.0407490	0.5296720	-1.6730280
C	0.2537930	2.0968010	0.7939230
O	0.6010230	2.9802660	1.6366380
O	0.9965210	2.1045250	-0.5682240
C	1.9719660	3.1720130	-0.5099230
H	1.8218060	3.6183970	0.5128540
H	3.0094170	2.7857440	-0.6285220
H	1.7916160	3.9313170	-1.3041710
C	-0.9649840	0.0766430	-0.2634700
H	-0.4077420	0.3685060	-1.1694140



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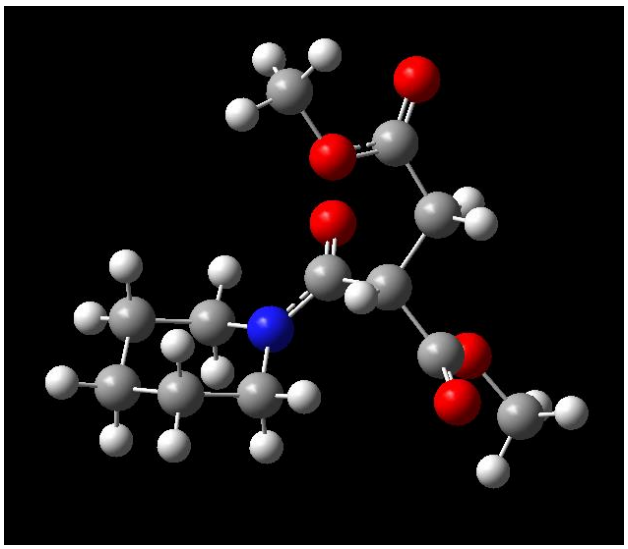

Route	UB3LYP/6-31+G(d,p) FormCheck opt=(Loose, MaxCyc=1000) freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(C(C(OC)=O)CC(OC)=O)N1CCCCC1
Formula	$C_{12}H_{19}NO_5$
Charge	0
Multiplicity	1
Dipole (Debye)	6.5661
Gibbs energy (a.u.)	−899.441512
# Imaginary frequencies	0

Input coordinates:

C	-3.2380390	-1.7084960	0.6323530
C	-1.9464390	-1.4923050	1.4661750
C	-0.7290440	-2.1084310	0.7165070
C	-1.8155920	-1.7403980	-1.4918100
C	-3.0702770	-1.1323260	-0.7984610
H	0.2402690	-1.9820640	1.2473670
H	-1.7774940	-0.4091960	1.6124740
H	-2.0471480	-1.9618100	2.4613320
H	-3.4510110	-2.7917070	0.5672780
H	-4.0985970	-1.2297910	1.1336550
H	-1.6269500	-1.2484630	-2.4658990
H	-1.9414100	-2.8318930	-1.6410570
H	-2.9374190	-0.0359060	-0.7427910
H	-3.9697530	-1.3382120	-1.4061510
H	-0.9006850	-3.1953350	0.5752650
N	-0.5925220	-1.5140130	-0.6542260
O	-0.1601070	0.4460320	-1.8984770
C	0.0114740	-0.2188230	-0.8561310
C	2.1892610	-0.7435750	0.4670800
O	3.2788740	-0.2827050	-0.3215330
C	4.4001190	-1.2348690	-0.2149190
H	5.2101840	-0.8221260	-0.8461830
H	4.7540000	-1.3319290	0.8336270
H	4.1138760	-2.2430720	-0.5832380
O	2.2095800	-1.7932330	1.1442150
C	0.2268400	2.7209160	0.1235780
O	0.2759650	3.9407160	-0.1191330
O	-0.9614510	2.0349480	0.5334140
C	-2.0861290	2.9824210	0.6010440
H	-1.7027030	4.0008920	0.3745920
H	-2.8574570	2.6909420	-0.1413890
H	-2.5255580	2.9457200	1.6189010
C	0.9849250	0.2401100	0.3208640
H	0.4204810	0.1897160	1.2704840
C	1.4148480	1.7057310	0.0590370
H	1.8723260	1.7864200	-0.9446510
H	2.1781280	2.0201070	0.7961770

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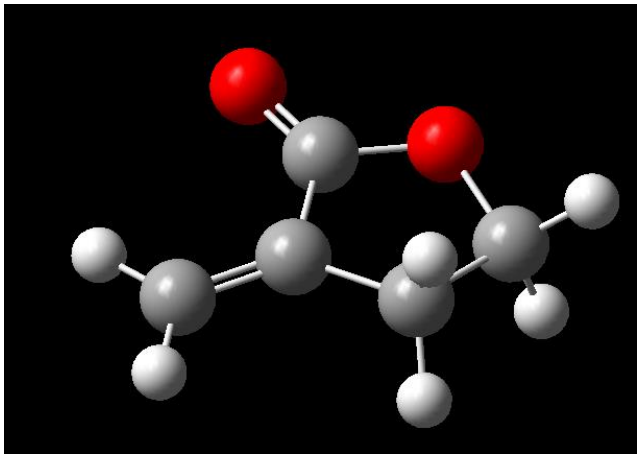
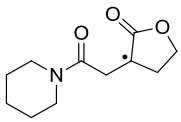


Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(Tight, MaxCyc=100) freq scrf=(cpcm,solvent=acetone)
Smiles	C=C1CCOC1=O
Formula	$C_5H_6O_2$
Charge	1
Multiplicity	1
Dipole (Debye)	6.6588
Gibbs energy (a.u.)	−344.537709
# Imaginary frequencies	0

Input coordinates:

C	-2.0154186	0.0440529	0.0000000
C	-0.4935606	0.0440529	0.0000000
H	-2.4073806	-0.5583921	-0.8575080
H	-2.4055336	-0.4263581	0.9375040
H	-0.1049336	-0.4905451	-0.9032800
H	-0.1001936	-0.4966791	0.8968370
C	-2.4846246	1.4883729	-0.1035900
C	-3.7728720	1.9058432	-0.1555919
H	-3.9985068	2.9493886	-0.2263155
H	-4.5671007	1.1894532	-0.1258242
C	-1.2525276	2.3814859	-0.1331860
O	-1.2457268	3.6346587	-0.2475630
O	-0.0247876	1.4919179	0.0000000



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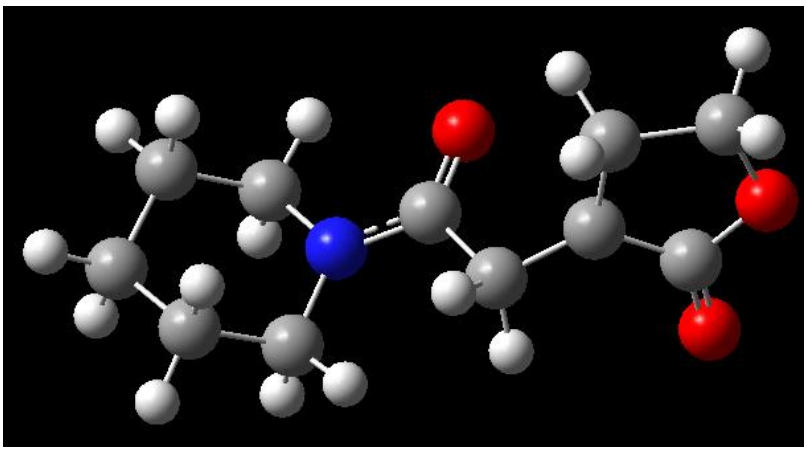
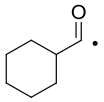


Route	UB3LYP/6-31+G(d,p) FormCheck opt(Tight, MaxCyc=1000) freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(C[C]1CCOC1=O)N2CCCCC2
Formula	$C_{11}H_{16}NO_3$•
Charge	0
Multiplicity	2
Dipole (Debye)	9.3175
Gibbs energy (a.u.)	−709.062690
# Imaginary frequencies	0

Input coordinates:

C	4.3422830	0.5537460	0.2289220
C	3.2834770	1.4032350	-0.4895600
C	2.2667790	0.5190420	-1.2265560
C	2.6536990	-1.3305290	0.3579080
C	3.6778740	-0.4940910	1.1349160
H	1.4909670	1.1287430	-1.6845780
H	2.7488730	2.0274240	0.2383210
H	3.7533820	2.0784280	-1.2139280
H	4.9658050	0.0435900	-0.5190850
H	5.0112200	1.1956220	0.8131690
H	2.1118920	-2.0121270	1.0115790
H	3.1632630	-1.9248000	-0.4140750
H	3.1699820	0.0041910	1.9711080
H	4.4294130	-1.1654530	1.5663770
H	2.7691390	-0.0315780	-2.0346650
N	1.6698090	-0.4641650	-0.3109370
O	-0.0943830	-1.4626340	0.7349400
C	0.3453550	-0.6105270	-0.0536590
C	-0.6284330	0.3386530	-0.7869710
H	-0.3749550	1.3761460	-0.5450760
H	-0.4988880	0.2110350	-1.8696940
C	-2.0459210	0.0885710	-0.4225800
C	-2.6314102	0.0852557	0.9428590
C	-4.1300655	-0.1829805	0.6823826
H	-2.4622162	1.0407984	1.4542019
H	-2.1765653	-0.6934925	1.5717044
H	-4.7638422	0.6646440	0.9505652
H	-4.4995486	-1.0827234	1.1767750
C	-3.0773573	-0.2129152	-1.3929825
O	-2.9853064	-0.3200111	-2.6126761
O	-4.2716654	-0.3906558	-0.7531639



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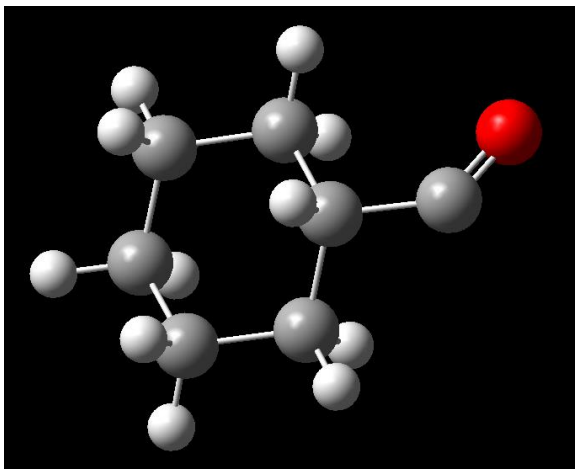
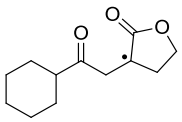


Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(Tight, MaxCyc=1000) Freq scrf=(cpcm,solvent=acetone)
Smiles	O=[C]C1CCCCC1
Formula	$C_7H_{11}O\bullet$
Charge	0
Multiplicity	2
Dipole (Debye)	3.8441
Gibbs energy (a.u.)	−348.445826
# Imaginary frequencies	0

Input coordinates:

C	2.1240950	0.3053170	-0.0740150
C	1.5490280	-1.0824300	-0.4002400
C	0.2795620	-1.3589150	0.4125200
C	-0.2037940	1.0959490	0.5437180
C	1.0619090	1.3998150	-0.2649130
H	-0.2015900	-2.2908840	0.1089450
H	1.3093470	-1.1438570	-1.4697620
H	2.2839990	-1.8664520	-0.1857070
H	2.4765800	0.3175090	0.9670250
H	2.9954110	0.5117650	-0.7052720
H	-1.0090380	1.7974380	0.3202540
H	0.0080940	1.1444170	1.6201540
H	0.7969820	1.4793680	-1.3269720
H	1.4515770	2.3759170	0.0463260
H	0.5247060	-1.4329410	1.4808580
C	-1.6464577	-0.9652055	0.8453399
O	-2.6937281	-0.6163420	1.3608145
C	-0.6946530	-0.2693860	0.2381660
H	-0.9935078	-0.2205531	-0.7880899



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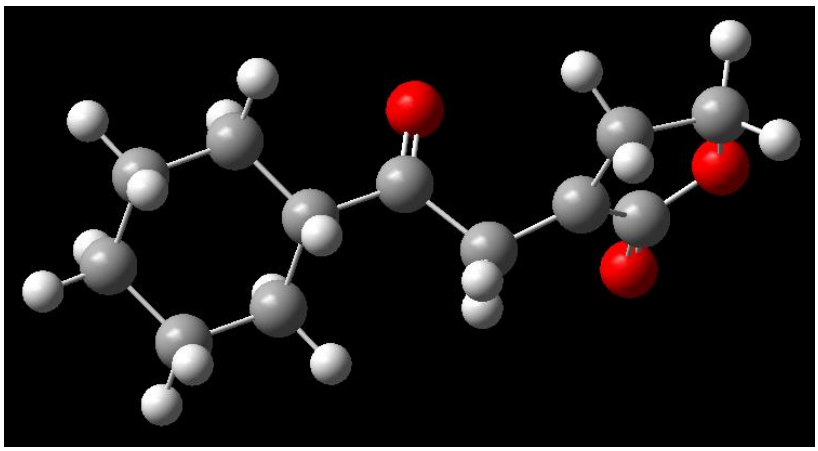
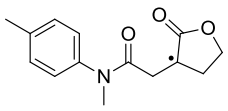


Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(Tight, MaxCyc=1000) freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(C[C]1CCOC1=O)C2CCCCC2
Formula	$C_{12}H_{17}O_3$•
Charge	0
Multiplicity	2
Dipole (Debye)	8.4007
Gibbs energy (a.u.)	−692.998956
# Imaginary frequencies	0

Input coordinates:

C	4.4378220	0.0410840	0.4710810
C	3.3781890	0.8716490	1.2098990
C	2.2413900	1.2886170	0.2660130
C	2.6427240	-0.6799440	-1.1659360
C	3.7883880	-1.1442900	-0.2579610
H	1.4701560	1.8289880	0.8107730
H	2.9561860	0.2876520	2.0381930
H	3.8244540	1.7742680	1.6429750
H	4.9526300	0.6798140	-0.2606240
H	5.2005520	-0.3133400	1.1735490
H	2.1169700	-1.5221660	-1.6127740
H	3.0383170	-0.0519370	-1.9771620
H	3.3947590	-1.8616710	0.4740590
H	4.5279370	-1.6767540	-0.8672200
H	2.6302720	1.9665430	-0.5073740
O	0.1432823	-0.1371720	-2.0887958
C	0.5595997	0.4901904	-1.1016672
C	-0.1829750	1.7569461	-0.6225373
H	-0.4388456	1.6440466	0.4385730
H	0.4885368	2.6182578	-0.7091377
C	-1.4185800	2.0215159	-1.4022616
C	-2.7052322	1.2840415	-1.3119128
C	-3.6047818	2.0179186	-2.3310112
H	-3.1207472	1.3152323	-0.2952813
H	-2.5723153	0.2240925	-1.5641814
H	-4.4709010	2.4959682	-1.8697254
H	-3.9378023	1.3746467	-3.1473501
C	-1.5332707	3.0786745	-2.3848103
O	-0.6914149	3.8972358	-2.7435569
O	-2.7911062	3.0742791	-2.9188030
C	1.6638400	0.1155500	-0.4070940
H	1.2372902	-0.1054032	0.5490100



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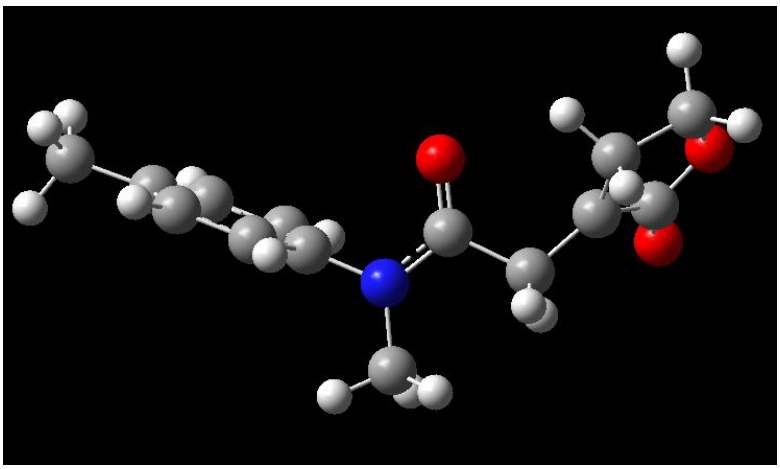
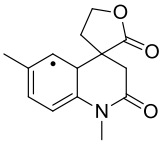


Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(Tight, MaxCyc=1000) freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(C[C]1CCOC1=O)N(C)C2=CC=C(C)C=C2
Formula	$C_{14}H_{16}NO_3$•
Charge	0
Multiplicity	2
Dipole (Debye)	7.9745
Gibbs energy (a.u.)	−823.374738
# Imaginary frequencies	0

Input coordinates:

C	1.8380190	-0.3110180	2.3014210
H	1.0997880	-1.0522260	2.6087420
H	2.7796490	-0.5522970	2.7952340
N	2.0590070	-0.3498010	0.8467230
C	1.0698330	-0.5364200	-0.0719650
O	1.2795550	-0.5045550	-1.2903890
H	1.5133210	0.6823420	2.6321360
C	3.3841990	-0.0142390	0.3834220
C	4.3446380	-1.0175580	0.2289820
C	3.7231690	1.3166440	0.1280340
C	5.6371680	-0.6862470	-0.1829120
H	4.0768960	-2.0515890	0.4253680
C	5.0189970	1.6379030	-0.2844170
H	2.9748080	2.0949300	0.2447750
C	5.9983480	0.6455410	-0.4429290
H	6.3747500	-1.4753230	-0.3049420
H	5.2706420	2.6760710	-0.4850590
C	7.4079020	1.0002150	-0.8564920
H	8.0624760	1.0870680	0.0197250
H	7.8375540	0.2327460	-1.5076770
H	7.4392430	1.9569170	-1.3856200
C	-0.3365390	-0.7967660	0.4824490
H	-0.3389910	-1.7126950	1.0892430
H	-0.6079870	0.0076340	1.1839270
C	-1.3773371	-0.9108795	-0.6468506
C	-2.0129762	-2.2936349	-0.6483199
C	-3.5219964	-2.1159749	-0.5625508
H	-1.6418993	-2.8928614	0.2211456
H	-1.7349913	-2.8533750	-1.5761457
H	-4.0115282	-2.4919054	-1.4961854
H	-3.9402204	-2.7082096	0.2893893
C	-2.4858099	0.1148801	-0.4569809
O	-2.3385366	1.3623604	-0.3816541
O	-3.8088955	-0.6330406	-0.3754413



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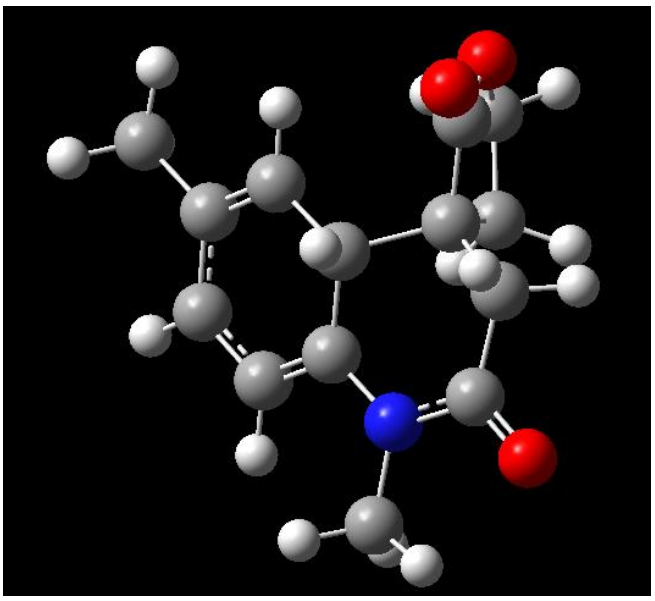

Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(Tight, MaxCyc=1000) Freq scrf=(cpcm,solvent=acetone)
Smiles	CN1C2=CC=C(C)[C]C2C3(C(OCC3)=O)CC1=O
Formula	$C_{14}H_{16}NO_3$•
Charge	0
Multiplicity	2
Dipole (Debye)	7.9256
Gibbs energy (a.u.)	−823.365051
# Imaginary frequencies	0

Input coordinates:

C	2.5272920	-3.1141260	0.5955280
H	2.0674180	-4.0760840	0.3868150
H	3.5577030	-3.1106110	0.2334690
N	1.7558030	-2.0761840	-0.1004560
C	0.5390600	-2.4377690	-0.6399740
O	0.1291850	-3.6036690	-0.6076980
H	2.5213890	-2.9375720	1.6753980
C	2.2489740	-0.7581800	-0.1074370
C	1.5775660	0.2217700	-1.0393390
C	3.3453900	-0.3761460	0.6373100
C	2.1034780	1.6263870	-0.9230740
H	1.7977094	-0.1189759	-2.0749969
C	3.8329100	0.9475650	0.6104250
H	3.8486060	-1.0920700	1.2759250
C	3.1931260	1.9595080	-0.1704360
H	1.5976890	2.3777500	-1.5232940
H	4.6965500	1.2022850	1.2169000
C	3.7263690	3.3730190	-0.1315750
H	4.7703870	3.4083170	-0.4644130
H	3.1422220	4.0382270	-0.7732410
H	3.7011750	3.7743920	0.8884480
C	-0.3124530	-1.3801330	-1.3282430
H	-0.1881223	-1.5282258	-2.4055624
H	-1.3543016	-1.6260212	-1.1107873
C	0.0329150	0.0727110	-1.0098240
C	-0.4873643	0.4669562	0.3652489
C	-1.4482672	1.6337876	0.1870358
H	0.3608328	0.7571827	1.0349679
H	-1.0077564	-0.3971240	0.8495871
H	-1.1155018	2.5127807	0.7939905
H	-2.4707822	1.3542184	0.5457797
C	-0.6329994	0.9740383	-2.0394933
O	-1.4844315	1.9902259	-1.2921731
O	-0.5056795	0.8953787	-3.2889623

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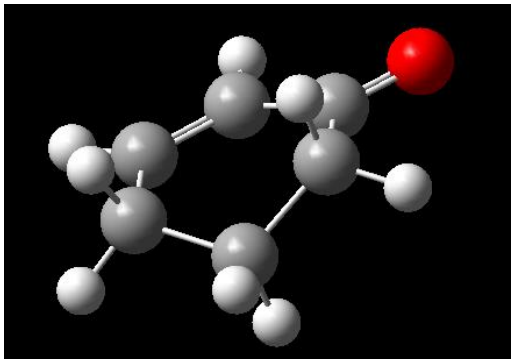
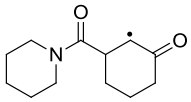


Route	UB3LYP/6-31+G(d,p) FormCheck opt(Tight, MaxCyc=1000) freq scrf=(cpcm,solvent=acetone)
Smiles	O=C1CCCC=C1
Formula	C_6H_8O
Charge	0
Multiplicity	1
Dipole (Debye)	5.7989
Gibbs energy (a.u.)	−308.602408
# Imaginary frequencies	0

Input coordinates:

C	-2.4493960	-1.3201720	1.1092060
C	-3.7441210	-1.3550950	0.2425230
H	-1.6078110	-1.8155410	0.5750670
H	-2.6091740	-1.8663540	2.0557310
C	-3.6179490	-0.3962120	-0.9784270
H	-3.9336500	-2.3846670	-0.1080580
H	-4.6071940	-1.0482930	0.8589550
H	-4.5421930	-0.3998710	-1.5812780
H	-2.7903810	-0.7357870	-1.6292090
C	-3.3064710	1.0766780	-0.5217370
O	-3.7503180	2.0855870	-1.1341140
C	-2.4057360	1.1885370	0.6969560
H	-2.0809930	2.2025510	0.9702600
C	-2.0116410	0.1175760	1.4166210
H	-1.3500750	0.2533760	2.2870320



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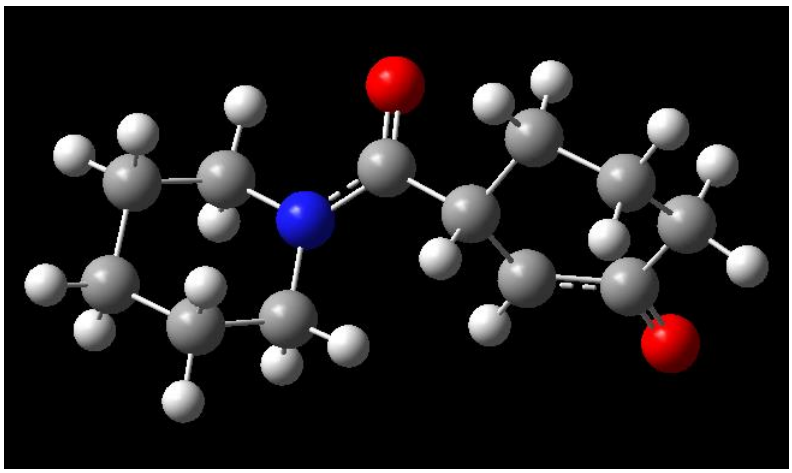
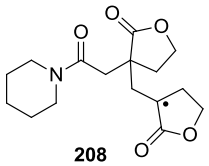


Route	UB3LYP/6-31+G(d,p) FormCheck opt(Tight, MaxCyc=1000) freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(C1CCCC([C]1)=O)N2CCCCC2
Formula	$C_{12}H_{18}NO_2$•
Charge	0
Multiplicity	2
Dipole (Debye)	7.0525
Gibbs energy (a.u.)	−673.112990
# Imaginary frequencies	0

Input coordinates:

C	4.1367070	0.2377100	0.6297890
C	2.9000930	0.6602410	1.4799760
C	1.7986850	1.2914710	0.5633360
C	2.5785100	-0.0652990	-1.3948430
C	3.7107160	-0.7137910	-0.5299530
H	0.9063190	1.5606480	1.1518020
H	2.4825810	-0.2201230	1.9981520
H	3.1957690	1.3990590	2.2446520
H	4.6133260	1.1395960	0.2074010
H	4.8798650	-0.2648440	1.2725150
H	2.1847980	-0.7912580	-2.1304870
H	2.9713670	0.8235530	-1.9266880
H	3.3433440	-1.6670010	-0.1125430
H	4.5758070	-0.9368030	-1.1779730
H	2.1958130	2.2174750	0.1009730
N	1.4051160	0.3660040	-0.5550280
O	0.2554670	-1.5816080	-1.2358060
C	0.3296440	-0.5912650	-0.4671550
C	-1.7497470	-1.5186610	0.7531480
C	-3.2448820	-1.2038480	1.0470080
H	-1.6631190	-2.1012700	-0.1820710
H	-1.3254680	-2.1314310	1.5660430
C	-3.8590640	-0.3553920	-0.1042250
H	-3.8050220	-2.1489790	1.1553000
H	-3.3313310	-0.6527990	1.9997710
H	-4.9079430	-0.0932650	0.1187600
H	-3.8568890	-0.9449200	-1.0398390
C	-3.0454610	0.9667180	-0.3296810
O	-3.6197750	2.0323050	-0.8172710
C	-1.6540590	0.9687760	0.0409830
H	-1.0967060	1.9102790	-0.0871450
C	-0.8798440	-0.2287520	0.5794230
H	-0.4116500	0.0470400	1.5443480



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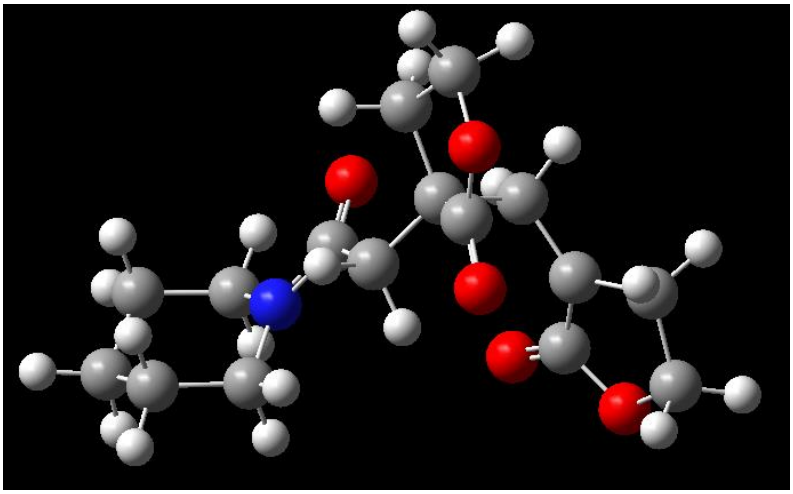
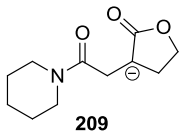


Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(Tight, MaxCyc=1000) Freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(CC1(C[C]2C(OCC2)=O)CCOC1=O)N3CCCCC3
Formula	$C_{16}H_{22}NO_5^{\bullet}$
Charge	0
Multiplicity	2
Dipole (Debye)	4.1672
Gibbs energy (a.u.)	−1053.591813
# Imaginary frequencies	0

Input coordinates:

O	-0.2032110	-1.6729050	0.9554640
C	-0.4630330	-0.5174420	0.5773090
C	0.6707190	0.4576960	0.2453320
H	0.5029530	0.9201550	-0.7332920
H	0.6639420	1.2709750	0.9810180
C	2.0403690	-0.2179340	0.2644850
C	2.4138240	-1.0891250	-0.9451050
C	3.9414070	-0.9896940	-0.9630890
H	1.9939650	-0.6629440	-1.8631740
H	2.0677730	-2.1194160	-0.8526770
H	4.3860180	-1.0138380	-1.9579820
H	4.4209040	-1.7399410	-0.3276410
C	3.1865690	0.7858380	0.3146850
O	3.2293230	1.8536130	0.8947890
O	4.2416420	0.3229120	-0.3920820
C	-2.8674030	-0.9484500	0.8020330
C	-2.1330980	1.3127020	0.1353820
C	-3.9198950	-0.9643950	-0.3134340
H	-3.3174060	-0.5788890	1.7356610
H	-2.4689580	-1.9440300	0.9907210
C	-3.1697070	1.3460260	-0.9960590
H	-2.5618400	1.7630890	1.0430390
H	-1.2569770	1.8989670	-0.1329880
C	-4.3778100	0.4570520	-0.6692360
H	-4.7693380	-1.5761240	0.0119400
H	-3.4920250	-1.4494210	-1.2007190
H	-3.4821950	2.3845870	-1.1547800
H	-2.6948920	1.0031700	-1.9246450
H	-5.0744140	0.4351340	-1.5148920
H	-4.9247370	0.8871520	0.1818360
N	-1.7413270	-0.0691860	0.4511120
C	2.1559654	-1.0576734	1.5502047
H	2.1153707	-2.0721792	1.2125216
C	3.2287892	-1.0611920	2.6550290
C	3.6197431	-2.4875412	3.0150683
C	3.3643924	-2.6832286	4.5027149
H	4.6977154	-2.6689485	2.7757773
H	3.0223665	-3.2202782	2.4165169
H	4.3020390	-3.0014570	5.0235844
H	2.6073942	-3.4913832	4.6646814
C	2.7004309	-0.3877612	3.9133534
O	2.2163372	0.7713626	3.9885591
O	2.8608830	-1.3637246	5.0699915
H	1.2370242	-0.8814050	2.0692197



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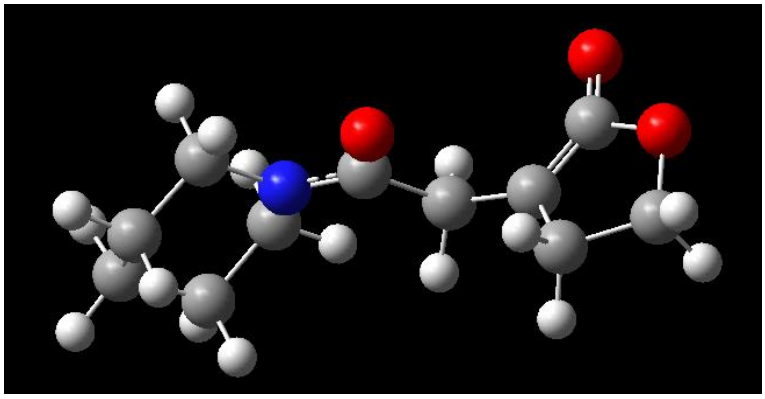
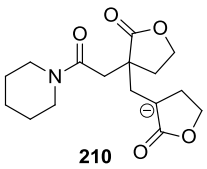


Route	UB3LYP/6-31+G(d,p) FormCheck opt(Tight, MaxCyc=1000) freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(C[C-]1CCOC1=O)N2CCCCC2
Formula	$C_{11}H_{16}NO_3^-$
Charge	−1
Multiplicity	1
Dipole (Debye)	19.3946
Gibbs energy (a.u.)	−709.195396
# Imaginary frequencies	0

Input coordinates:

C	4.4378220	0.0410840	0.4710810
C	3.3781890	0.8716490	1.2098990
C	2.2413900	1.2886170	0.2660130
C	2.6427240	-0.6799440	-1.1659360
C	3.7883880	-1.1442900	-0.2579610
H	1.4701560	1.8289880	0.8107730
H	2.9561860	0.2876520	2.0381930
H	3.8244540	1.7742680	1.6429750
H	4.9526300	0.6798140	-0.2606240
H	5.2005520	-0.3133400	1.1735490
H	2.1169700	-1.5221660	-1.6127740
H	3.0383170	-0.0519370	-1.9771620
H	3.3947590	-1.8616710	0.4740590
H	4.5279370	-1.6767540	-0.8672200
H	2.6302720	1.9665430	-0.5073740
N	1.6638400	0.1155500	-0.4070940
O	-0.0776500	-1.2203040	-1.0290200
C	0.3521060	-0.2329780	-0.4111010
C	-0.6207230	0.6596710	0.3904190
H	-0.2661270	0.7385400	1.4258960
H	-0.6139660	1.6682800	-0.0373050
C	-2.0102320	0.1363120	0.3835650
C	-2.5263940	-1.0334560	1.1403510
C	-4.0213620	-1.0723210	0.7531990
H	-2.3821770	-0.9126640	2.2228370
H	-2.0000880	-1.9532520	0.8543870
H	-4.6871140	-0.9151530	1.6038170
H	-4.3046480	-1.9906920	0.2360390
C	-3.0836290	0.7272240	-0.3876560
O	-3.0548060	1.6997760	-1.1365050
O	-4.2393760	0.0299380	-0.1746800



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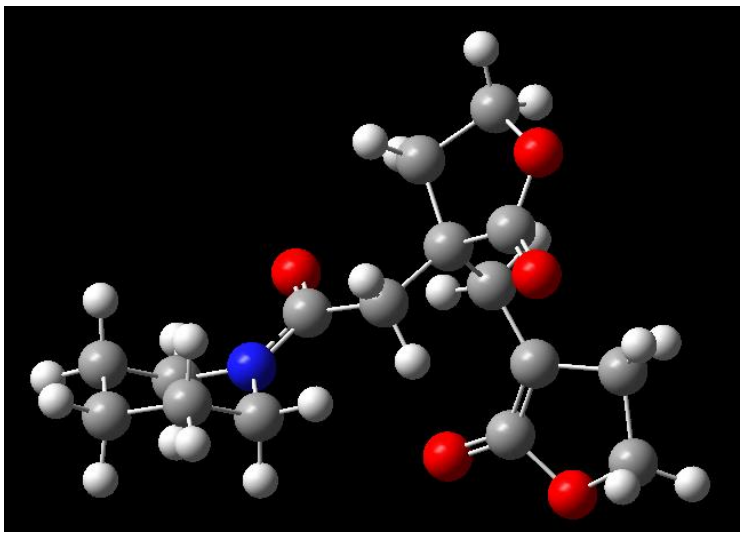
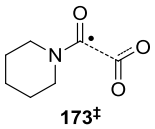


Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(Tight, MaxCyc=1000) Freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(CC1(C[C-]2C(OCC2)=O)CCOC1=O)N3CCCCC3
Formula	$C_{16}H_{22}NO_5^-$
Charge	−1
Multiplicity	1
Dipole (Debye)	15.1696
Gibbs energy (a.u.)	−1053.726981
# Imaginary frequencies	0

Input coordinates:

O	-1.2084500	0.6190550	-1.8246760
C	-1.3567610	0.3122870	-0.6293620
C	-0.2657430	0.6136930	0.4035100
H	-0.6806390	1.2985190	1.1528770
H	-0.0019420	-0.3006850	0.9421540
C	1.0171230	1.2421510	-0.1691510
C	0.8174770	2.6057240	-0.8662550
C	2.0819080	3.3878800	-0.4982830
H	-0.0658800	3.1066230	-0.4582990
H	0.6822280	2.5138200	-1.9439580
H	1.9150580	4.4529270	-0.3369250
H	2.8987500	3.2537800	-1.2126690
C	1.9370860	1.6294600	0.9987290
O	2.1650710	0.9887880	2.0063950
O	2.5195050	2.8250720	0.7766950
C	-3.5777580	-0.6156260	-1.1099840
C	-2.7626360	-0.6805060	1.2149610
C	-4.9005320	0.0199510	-0.6633960
H	-3.6805180	-1.7103050	-1.1381870
H	-3.2829020	-0.2756860	-2.1013390
C	-4.0684660	-0.0498120	1.7209270
H	-2.8432530	-1.7768030	1.2469480
H	-1.9318160	-0.3981400	1.8576270
C	-5.2415460	-0.3678220	0.7828420
H	-5.6956870	-0.2979440	-1.3478480
H	-4.8174360	1.1116350	-0.7472840
H	-4.2683360	-0.4205250	2.7329260
H	-3.9330880	1.0373040	1.7935790
H	-6.1468500	0.1522240	1.1158610
H	-5.4591420	-1.4444960	0.8273490
N	-2.4926400	-0.2831680	-0.1746050
C	1.8048970	0.2585710	-1.1217890
H	2.6211240	0.8206300	-1.5890200
C	2.3707020	-0.9723650	-0.5042430
C	3.7652980	-1.1602780	-0.0136080
C	3.7355790	-2.5786420	0.5885760
H	4.0673140	-0.4049840	0.7199470
H	4.4771550	-1.0885530	-0.8503740
H	3.7251600	-2.5652150	1.6812210
H	4.5449050	-3.2211910	0.2404100
C	1.6735600	-2.2437090	-0.4302660
O	0.5458320	-2.5338980	-0.8169270
O	2.4844090	-3.1805400	0.1488670
H	1.0922140	-0.0143330	-1.9048450

2.2. Transition states



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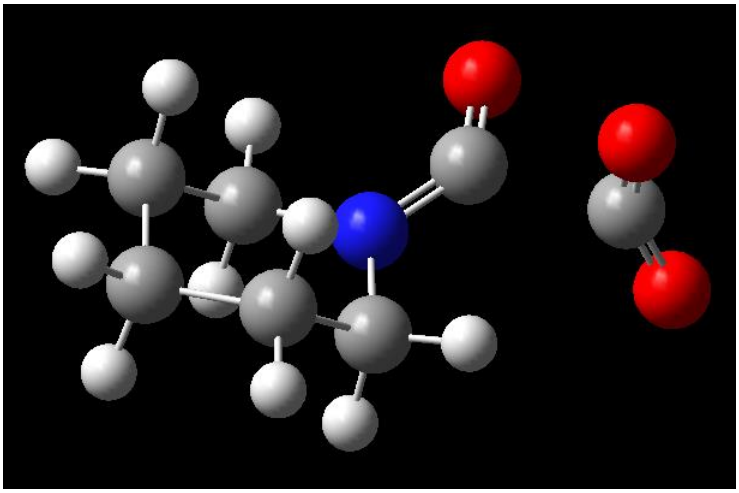
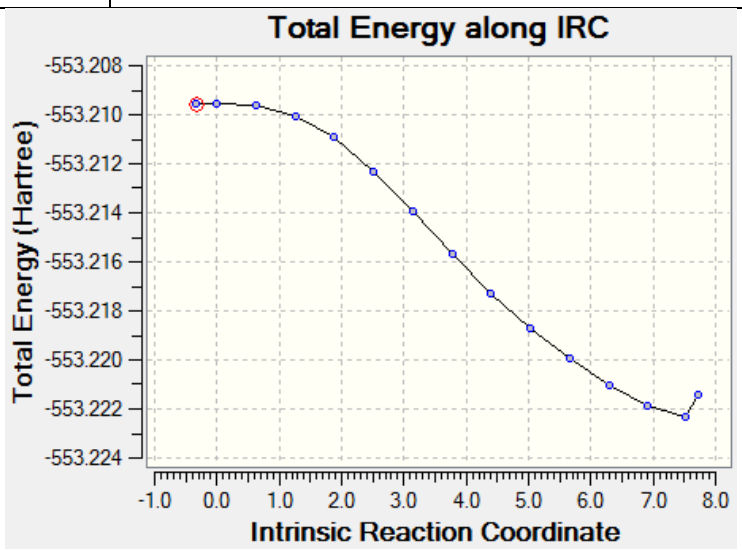


Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(QST3, maxcyc=200, CalcFC, Tight) Freq scrf=(cpcm,solvent=acetone)
Smiles	O=[C](c(o)=O)N1CCCCC1
Formula	$C_7H_{10}NO_3^{\bullet}$
Charge	0
Multiplicity	2
Dipole (Debye)	8.5509
Gibbs energy (a.u.)	−553.078702
# Imaginary frequencies	1



Input coordinates:

SM

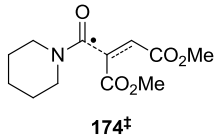
C	-2.9757060	-0.5227670	0.0487520
C	-1.7886570	-1.5072540	0.2800180
C	-0.5409000	-1.1117090	-0.5722500
C	-1.3014470	1.3392960	-0.5088590
C	-2.5396740	0.9420470	0.3556990
H	0.3669130	-1.6807550	-0.2561200
H	-1.5114320	-1.5067910	1.3480140
H	-2.0864390	-2.5344520	0.0078670
H	-3.3174520	-0.5931670	-0.9987730
H	-3.8236000	-0.8012990	0.6976370
H	-0.8956300	2.3235160	-0.2085930
H	-1.5843310	1.3775880	-1.5811660
H	-2.2829670	1.0393300	1.4243690
H	-3.3629810	1.6439190	0.1366610
H	-0.7469770	-1.2631010	-1.6512620
N	-0.1871920	0.3320380	-0.3466030
C	1.0500000	0.7610650	0.1373300
C	2.4395910	-0.4856390	0.0568770
O	1.9836990	-1.6207850	0.4407240
O	1.3498820	1.9238070	0.5023760
O	3.4784190	0.0945670	-0.3528270

Product

C	-2.9347200	-0.8776000	0.3134800
C	-1.5595300	-1.6098900	0.3930520
C	-0.5569610	-1.0257660	-0.6568660
C	-1.7431150	1.2228070	-0.5639670
C	-2.7553500	0.6622810	0.4878720
H	0.4585970	-1.4490030	-0.5215580
H	-1.1345990	-1.4914180	1.4044790
H	-1.6909570	-2.6891430	0.2034640
H	-3.4040210	-1.0830490	-0.6646760
H	-3.6102060	-1.2642910	1.0958430
H	-1.5095020	2.2859860	-0.3685360
H	-2.1705200	1.1311650	-1.5836700
H	-2.3804730	0.8800430	1.5025860
H	-3.7246910	1.1760930	0.3654870
H	-0.9152080	-1.2590450	-1.6806350
N	-0.4384810	0.4641790	-0.5166380
C	0.7435410	1.0348130	-0.0222410
C	3.9036448	-1.1761481	0.1358562
O	3.2021820	-2.1626616	-0.0869215
O	0.9122080	2.2467670	0.2546800
O	4.6028434	-0.1928190	0.3579147

TS Guess

C	-2.9591260	-0.7520270	0.3023270
C	-1.6365380	-1.5750640	0.3869420
C	-0.5892400	-1.0554720	-0.6520760
C	-1.6245540	1.2705210	-0.5515300
C	-2.6795580	0.7714720	0.4886900
H	0.3988620	-1.5391270	-0.5103660
H	-1.2121620	-1.4916030	1.4020700
H	-1.8388430	-2.6418810	0.1896420
H	-3.4337770	-0.9194790	-0.6804690
H	-3.6646450	-1.0974750	1.0773900
H	-1.3202530	2.3138610	-0.3466270
H	-2.0485780	1.2150240	-1.5752800
H	-2.2993260	0.9580130	1.5075760
H	-3.6113660	1.3495190	0.3616060
H	-0.9535100	-1.2572770	-1.6803300
N	-0.3754820	0.4229860	-0.4995330
C	0.8485020	0.9246360	-0.0458050
C	2.9116970	-0.5979320	0.1051150
O	2.3137610	-1.6570320	-0.1071210
O	1.1013570	2.1250900	0.2196830
O	3.7079910	0.3110320	0.3311320



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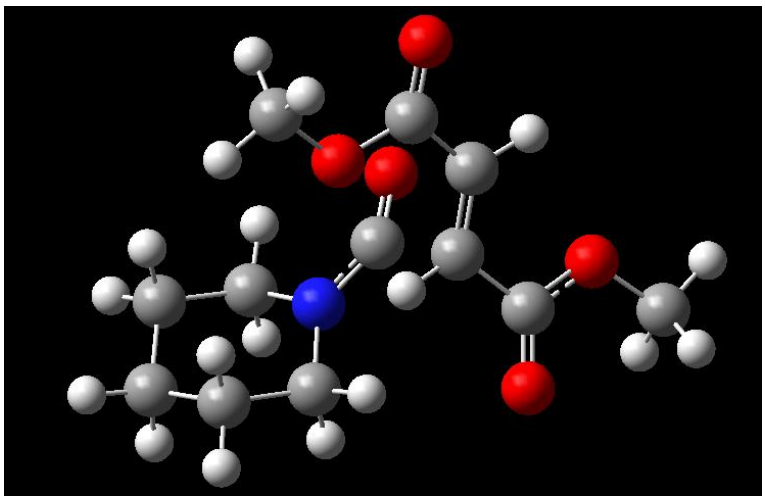
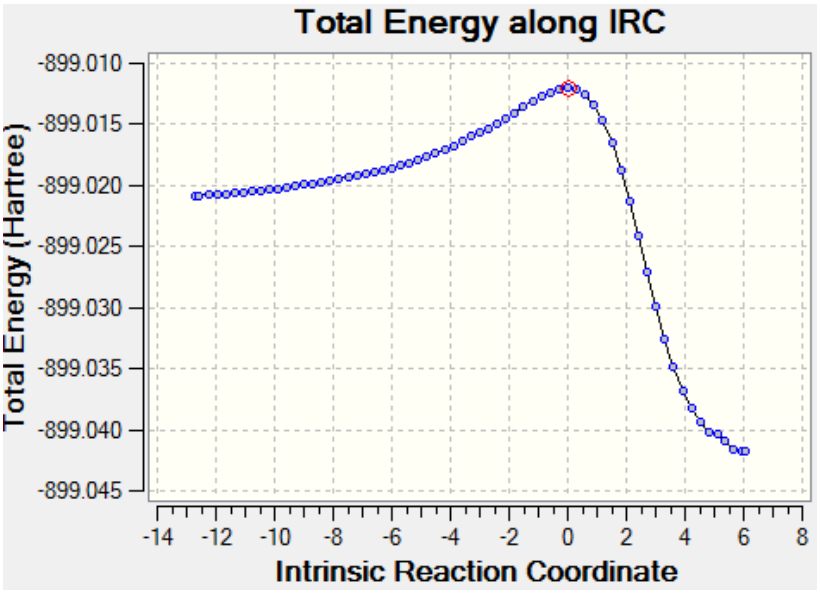


Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(QST3, maxcyc=200, CalcFC, Tight) Freq scrf=(cpcm,solvent=acetone)
Smiles	O=[C](c(C(OC)=O)cC(OC)=O)N1CCCCC1
Formula	$C_{12}H_{17}NO_5^{\bullet}$
Charge	0
Multiplicity	2
Dipole (Debye)	6.4062
Gibbs energy (a.u.)	−898.768608
# Imaginary frequencies	1



Input coordinates:

SM

C	-4.0236650	-0.6956440	-1.1977620
C	-2.7538400	0.1153910	-1.6025930
C	-2.3447050	1.1132600	-0.4693300
C	-3.3817330	-0.4221120	1.2750600
C	-3.8048810	-1.4326770	0.1596210
H	-1.3791390	1.6257260	-0.6984770
H	-1.9180950	-0.5785820	-1.7977990
H	-2.9465260	0.6839350	-2.5287930
H	-4.8828130	-0.0082460	-1.1057680
H	-4.2653860	-1.4309860	-1.9844680
H	-3.1015050	-0.9482550	2.2065410
H	-4.2198060	0.2712990	1.4922800
H	-3.0170680	-2.1969680	0.0452910
H	-4.7326610	-1.9432870	0.4712440
H	-3.1414930	1.8755200	-0.3493110
N	-2.1844920	0.3932030	0.8413000
O	-0.6419560	-0.4872890	2.4083110
C	-0.9122890	0.1971020	1.3914060
C	2.6064920	-0.1613880	0.0355160
H	3.3942180	0.4391260	0.5151580
C	1.2626220	1.9374860	-0.4430250
O	2.3972470	2.6150490	0.0928740
C	2.1519340	4.0766640	0.1210560
H	3.0642060	4.5283010	0.5521120
H	1.9830200	4.4781110	-0.8986260
H	1.2763340	4.3279730	0.7531490
O	0.2255240	2.5350600	-0.8390150
C	2.8626090	-1.6647130	-0.0018750
O	3.8726250	-2.2539140	0.4580960
O	1.7752940	-2.3363620	-0.6472830
C	2.0327590	-3.7945600	-0.6809700
H	2.1282390	-4.2141810	0.3410910
H	1.1598200	-4.2464230	-1.1869070
H	2.9551930	-4.0315630	-1.2491550
C	1.5027480	0.4313740	-0.4696170
H	0.7167210	-0.1653760	-0.9554550

Product

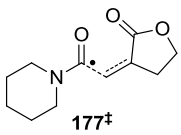
C	-4.2044680	-0.9561730	-1.0792190
C	-2.8205070	-0.6631990	-1.7392110
C	-2.1968610	0.6311860	-1.1204170
C	-3.3953760	0.2581190	1.0487070
C	-4.0826580	-1.0275120	0.4751920
H	-1.2031070	0.8826190	-1.5434490
H	-2.1395020	-1.5166820	-1.5783050
H	-2.9404840	-0.5233740	-2.8274390
H	-4.9122340	-0.1543330	-1.3534060

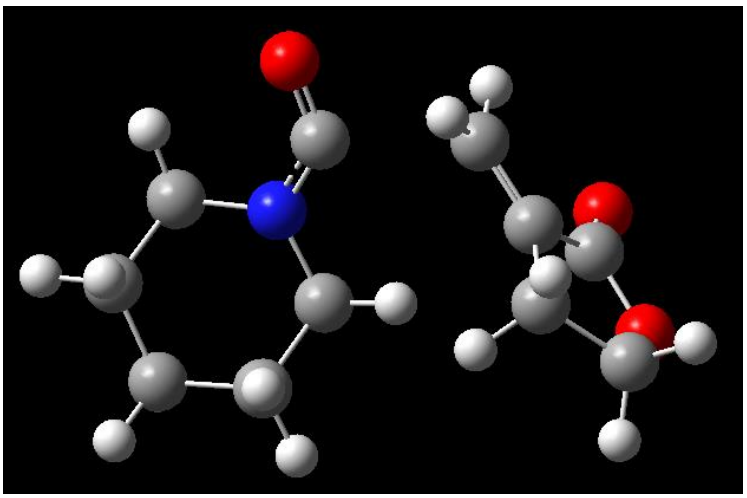
H	-4.6110040	-1.9073480	-1.4642720
H	-3.1801580	0.1373600	2.1269020
H	-4.0489700	1.1396510	0.8991630
H	-3.4827780	-1.9091880	0.7594300
H	-5.0825050	-1.1363600	0.9297990
H	-2.8730780	1.4855340	-1.3223700
N	-2.0753790	0.5224840	0.3764960
O	-0.9754080	-0.3928610	2.2543490
C	-0.9287150	-0.0510920	1.0433610
C	1.4596040	-0.8329500	1.0248350
H	1.2610820	-0.9750130	2.0982400
C	0.8720650	1.2840120	-0.2902080
O	1.7876060	1.8073650	0.6621510
C	2.2596830	3.1503480	0.2395170
H	2.9651920	3.4833630	1.0226130
H	2.7809090	3.1052260	-0.7378540
H	1.4182220	3.8683790	0.1655610
O	0.5180490	1.8682900	-1.3396760
C	2.7290530	-1.3134400	0.4499020
O	3.6607600	-1.9200000	1.0694040
O	2.7989810	-1.0018210	-0.9573600
C	4.0764940	-1.4940660	-1.5157710
H	4.1744550	-2.5942090	-1.4121660
H	4.0646530	-1.2263260	-2.5885370
H	4.9505990	-1.0167470	-1.0270890
C	0.3788660	-0.1457860	0.2017620
H	0.1833670	-0.7244020	-0.7239260

TS guess

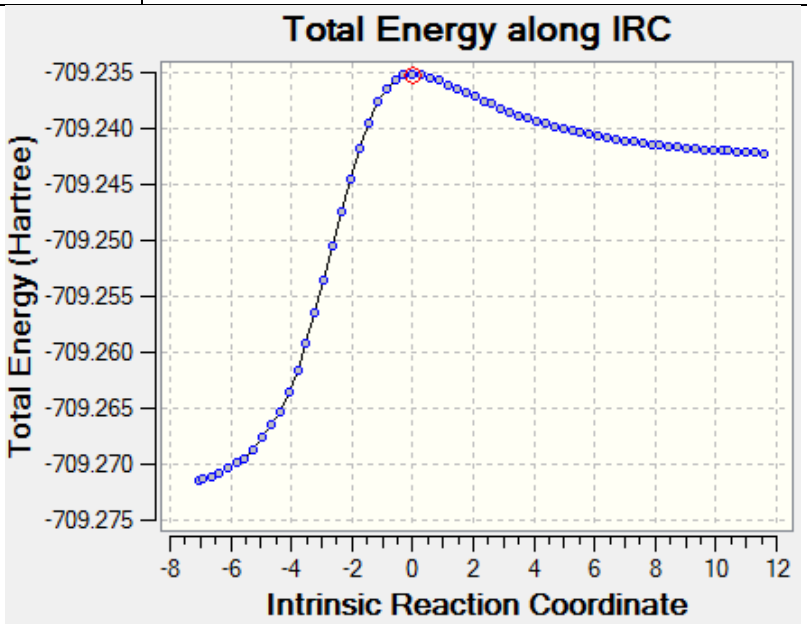
C	-3.8256330	-0.7237260	-0.8575130
C	-2.5556100	-0.1446560	-1.5569840
C	-2.0182610	1.0909380	-0.7647000
C	-2.9644650	0.1902930	1.3921210
C	-3.5471860	-1.0529470	0.6426270
H	-1.0986160	1.5476000	-1.2009270
H	-1.7712850	-0.9191070	-1.6124680
H	-2.8001560	0.1678760	-2.5868170
H	-4.6427270	0.0158960	-0.9215630
H	-4.1580160	-1.6369950	-1.3802150
H	-2.6593590	-0.0689100	2.4227990
H	-3.7142070	1.0049980	1.4279480
H	-2.8261290	-1.8852930	0.7151670
H	-4.4799080	-1.3656330	1.1431290
H	-2.8057310	1.8696110	-0.7329320
N	-1.7405310	0.7241890	0.6733080
O	-0.2244640	-0.1976120	2.2630910
C	-0.4915960	0.2501160	1.1355010
C	2.1663950	-0.3726410	0.2634530
H	2.9116800	0.1612020	0.8685330
C	1.1738190	1.8602790	-0.5182150
O	2.2586210	2.4031750	0.2309840

C	2.3664670	3.8615650	-0.0124100
H	3.2103450	4.2110670	0.6103870
H	2.5763990	4.0803770	-1.0789460
H	1.4394780	4.3925860	0.2843680
O	0.4398280	2.5508060	-1.2747550
C	2.3577200	-1.8344380	0.1004330
O	3.3187930	-2.5261040	0.5560190
O	1.2876800	-2.4116220	-0.6799030
C	1.5165910	-3.8625510	-0.8437150
H	1.5342280	-4.3904640	0.1319050
H	0.6712130	-4.2397590	-1.4485780
H	2.4690250	-4.0734030	-1.3721450
C	1.0195730	0.3497820	-0.2578230
H	0.4969390	-0.1621980	-1.0829380





Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(QST3, maxcyc=200, CalcFC, Tight) Freq scrf=(cpcm,solvent=acetone)
Smiles	O=[C](cc1CCOC1=O)N2CCCCC2
Formula	$C_{11}H_{15}NO_3^{\bullet}$
Charge	0
Multiplicity	2
Dipole (Debye)	8.1756
Gibbs energy (a.u.)	−709.019504
# Imaginary frequencies	1



Input coordinates:

SM

C	-3.9558690	-1.5628220	-0.4802810
C	-2.9289770	-1.7659780	0.6445980
C	-1.6463240	-0.9766260	0.3614490
C	-2.9345630	0.7035720	-0.9767200
C	-4.2331450	-0.0682950	-0.7143920
H	-0.9480210	-1.0024060	1.1977790
H	-3.3526840	-1.4351100	1.6019720
H	-2.6762590	-2.8269600	0.7505560
H	-3.5709250	-2.0089460	-1.4079850
H	-4.8879870	-2.0866820	-0.2406950
H	-3.0985010	1.7815170	-1.0195730
H	-2.4872970	0.3846790	-1.9274180
H	-4.7328230	0.3600430	0.1640710
H	-4.9057970	0.0698500	-1.5688230
H	-1.1378290	-1.3846520	-0.5227740
N	-1.9499880	0.4383110	0.0994010
O	-1.5529590	2.6108970	0.8145930
C	-1.4024970	1.4018840	0.8317550
C	1.8488700	1.0855610	1.2992530
H	1.5612590	2.0288490	0.8454760
H	1.4937000	0.8793260	2.3029780
C	2.5838200	0.2002900	0.6180100
C	3.0800630	-1.1660920	1.0154690
C	4.2124700	-1.4102880	0.0030160
H	2.2851410	-1.9111820	0.8899590
H	3.4296440	-1.2163020	2.0485820
H	4.2517100	-2.4255880	-0.3902320
H	5.1929720	-1.1293320	0.3975070
C	3.0611310	0.4521870	-0.7722260
O	2.7609850	1.3513030	-1.5378710
O	3.9324430	-0.5254050	-1.1263190

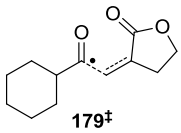
Product

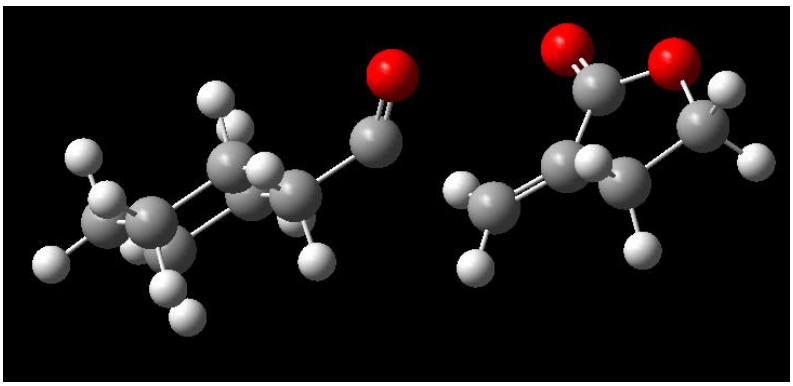
C	4.4378220	0.0410840	0.4710810
C	3.3781890	0.8716490	1.2098990
C	2.2413900	1.2886170	0.2660130
C	2.6427240	-0.6799440	-1.1659360
C	3.7883880	-1.1442900	-0.2579610
H	1.4701560	1.8289880	0.8107730
H	2.9561860	0.2876520	2.0381930
H	3.8244540	1.7742680	1.6429750
H	4.9526300	0.6798140	-0.2606240
H	5.2005520	-0.3133400	1.1735490
H	2.1169700	-1.5221660	-1.6127740
H	3.0383170	-0.0519370	-1.9771620
H	3.3947590	-1.8616710	0.4740590
H	4.5279370	-1.6767540	-0.8672200

H	2.6302720	1.9665430	-0.5073740
N	1.6638400	0.1155500	-0.4070940
O	-0.0776500	-1.2203040	-1.0290200
C	0.3521060	-0.2329780	-0.4111010
C	-0.6207230	0.6596710	0.3904190
H	-0.2661270	0.7385400	1.4258960
H	-0.6139660	1.6682800	-0.0373050
C	-2.0102320	0.1363120	0.3835650
C	-2.5263940	-1.0334560	1.1403510
C	-4.0213620	-1.0723210	0.7531990
H	-2.3821770	-0.9126640	2.2228370
H	-2.0000880	-1.9532520	0.8543870
H	-4.6871140	-0.9151530	1.6038170
H	-4.3046480	-1.9906920	0.2360390
C	-3.0836290	0.7272240	-0.3876560
O	-3.0548060	1.6997760	-1.1365050
O	-4.2393760	0.0299380	-0.1746800

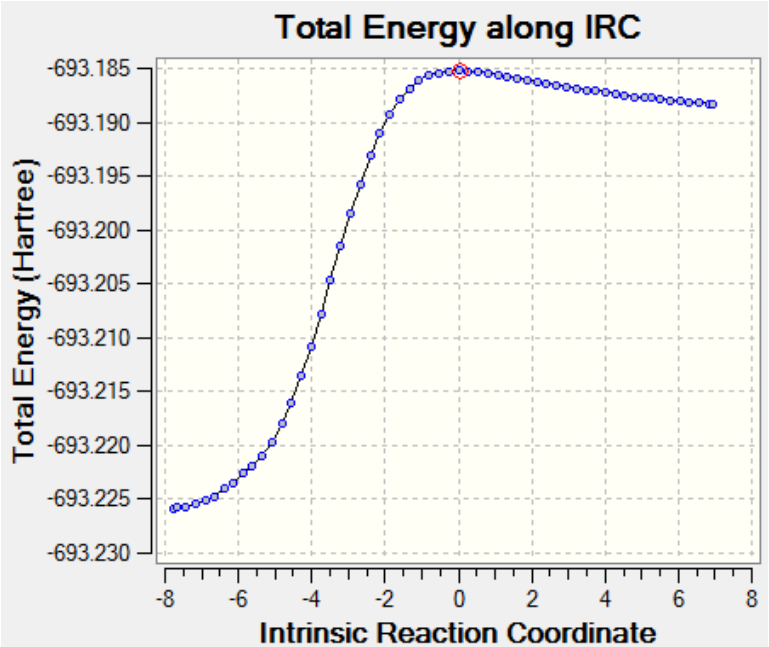
TS guess

C	-3.0064110	-1.9657650	0.1449410
C	-1.4735760	-1.8708260	0.1276160
C	-1.0007010	-0.6896280	-0.7281730
C	-3.1253600	0.5312640	-0.2664870
C	-3.6274870	-0.6345540	0.5913530
H	0.0777380	-0.5613550	-0.6694150
H	-1.0955090	-1.7455770	1.1503440
H	-1.0303780	-2.7901500	-0.2715200
H	-3.3659870	-2.2140860	-0.8636930
H	-3.3301170	-2.7768350	0.8062840
H	-3.4734040	1.4925580	0.1118450
H	-3.4701480	0.4217380	-1.3034600
H	-3.3762600	-0.4377830	1.6412150
H	-4.7209110	-0.6732140	0.5221240
H	-1.2671510	-0.8536750	-1.7809010
N	-1.6392840	0.5597240	-0.2897150
O	-1.4377840	2.7623850	0.3422770
C	-0.9960700	1.6779480	0.0217440
C	1.1959560	1.8245470	-0.0945850
H	1.1811820	2.1704440	-1.1255250
H	1.1121070	2.5945090	0.6654220
C	1.9456640	0.6890840	0.1925630
C	2.3246810	0.1481910	1.5405440
C	3.4110000	-0.8870040	1.1922590
H	1.4600880	-0.3282850	2.0236240
H	2.6947860	0.9191360	2.2241020
H	3.2967410	-1.8410890	1.7073480
H	4.4196480	-0.5003850	1.3604200
C	2.4984510	-0.1982740	-0.8311130
O	2.3467090	-0.1791170	-2.0458300
O	3.2767850	-1.1512570	-0.2357200





Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(QST3, maxcyc=200, CalcFC, Tight) Freq scrf=(cpcm,solvent=acetone)
Smiles	O=[C](cc1CCOC1=O)C2CCCCC2
Formula	$C_{12}H_{16}O_3^{\bullet}$
Charge	0
Multiplicity	2
Dipole (Debye)	9.4237
Gibbs energy (a.u.)	−692.961605
# Imaginary frequencies	1



Input coordinates:

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C	5.1485590	0.1302000	0.3740400
C	4.1761680	1.2154270	0.8622050
C	2.9132270	1.2844710	-0.0104880
C	3.2013080	-1.1930940	-0.5921010
C	4.4618560	-1.2417580	0.2867470
H	2.2063540	2.0210240	0.3860880
H	3.8838660	1.0034040	1.9004760
H	4.6690560	2.1947550	0.8671190
H	5.5302670	0.4073290	-0.6191110
H	6.0171560	0.0754110	1.0410930
H	2.6978280	-2.1659420	-0.5978740
H	3.4817680	-0.9709190	-1.6299930
H	4.1866210	-1.5763640	1.2970620
H	5.1566230	-1.9907820	-0.1121910
H	3.1837750	1.6107120	-1.0237380
O	0.6299000	-0.6277370	-1.8831980
C	0.9632380	-0.0033250	-0.9222260
C	-1.7092140	0.7713510	1.0317140
H	-0.9793460	0.3087940	1.6875490
H	-1.5353160	1.7967580	0.7210690
C	-2.8050650	0.1223880	0.6249210
C	-3.2687270	-1.2838240	0.9068050
C	-4.7523450	-1.2355590	0.5003950
H	-3.1370440	-1.5818050	1.9493990
H	-2.7217440	-1.9977860	0.2802540
H	-5.4151610	-1.0778050	1.3550840
H	-5.0872600	-2.1028140	-0.0679480
C	-3.8262620	0.7575950	-0.2554680
O	-3.7906090	1.8347720	-0.8229270
O	-4.8918460	-0.0723770	-0.3730060
C	2.2314030	-0.1027340	-0.0930250
H	1.8781110	-0.3580580	0.9176020

Product

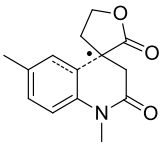
C	4.6266530	0.2970420	-0.1365170
C	3.7314430	1.2589360	0.6580720
C	2.2670310	1.1997460	0.1934150
C	2.6222850	-1.2044760	-0.5657430
C	4.0811080	-1.1378000	-0.0876020
H	1.6563940	1.8610900	0.8170450
H	3.7784200	1.0014160	1.7258630
H	4.0994110	2.2879280	0.5663220
H	4.6759460	0.6298890	-1.1834010
H	5.6515860	0.3282110	0.2525300
H	2.2415920	-2.2291960	-0.4901890
H	2.5707020	-0.9299590	-1.6271550
H	4.1445650	-1.5154410	0.9432370

H	4.7005780	-1.8018520	-0.7024010
H	2.1937340	1.5710140	-0.8381980
O	-0.0943460	-0.9130560	-1.2047840
C	0.2670890	-0.3129950	-0.2036510
C	-0.7535090	0.4461890	0.6710070
H	-0.4785060	0.3028660	1.7241370
H	-0.6325170	1.5147670	0.4530440
C	-2.1629010	0.0514830	0.4364860
C	-2.8057770	-1.2282580	0.8352850
C	-4.2646110	-1.0519750	0.3591090
H	-2.7397170	-1.4032490	1.9171830
H	-2.3170310	-2.0853600	0.3514150
H	-4.9755150	-0.9967170	1.1860090
H	-4.5842120	-1.8233370	-0.3430710
C	-3.1175030	0.8680020	-0.2846350
O	-2.9602640	1.9736550	-0.7939220
O	-4.3201610	0.2226460	-0.3445490
C	1.7224680	-0.2544830	0.2408430
H	1.7300740	-0.5664980	1.2972540

TS guess

C	4.7604060	0.3508400	-0.0517020
C	3.7804060	1.3053190	0.6469670
C	2.3517360	1.1685260	0.0955990
C	2.8546590	-1.2613900	-0.5361020
C	4.2759130	-1.1048370	0.0273360
H	1.6672740	1.8178280	0.6506890
H	3.7703750	1.0946510	1.7255530
H	4.1106100	2.3442990	0.5315440
H	4.8604800	0.6426860	-1.1069220
H	5.7569340	0.4422310	0.3964620
H	2.5104380	-2.2958760	-0.4286280
H	2.8524030	-1.0312160	-1.6090100
H	4.2899870	-1.4381310	1.0747010
H	4.9583570	-1.7653530	-0.5207670
H	2.3277630	1.4903900	-0.9536390
O	0.0594450	-0.8811940	-1.4052210
C	0.4701620	-0.4099090	-0.3697750
C	-1.1798740	0.4884020	1.1236840
H	-0.6887140	-0.0376090	1.9355710
H	-0.8310880	1.4914580	0.8996660
C	-2.3940930	0.0796390	0.6576330
C	-3.1211270	-1.2137380	0.9164960
C	-4.5103280	-0.9441210	0.3072140
H	-3.1841500	-1.4714290	1.9778760
H	-2.6243340	-2.0477790	0.4026500
H	-5.2496610	-0.6683380	1.0643260
H	-4.8975700	-1.7651460	-0.2967480
C	-3.1680950	0.8475390	-0.3258290
O	-2.8886360	1.8990080	-0.8944860
O	-4.3478110	0.2038230	-0.5783720

C	1.8768490	-0.3065530	0.1813120
H	1.8072300	-0.5740670	1.2443060



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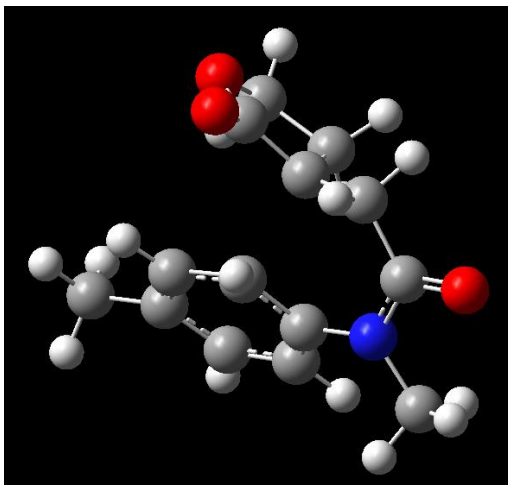
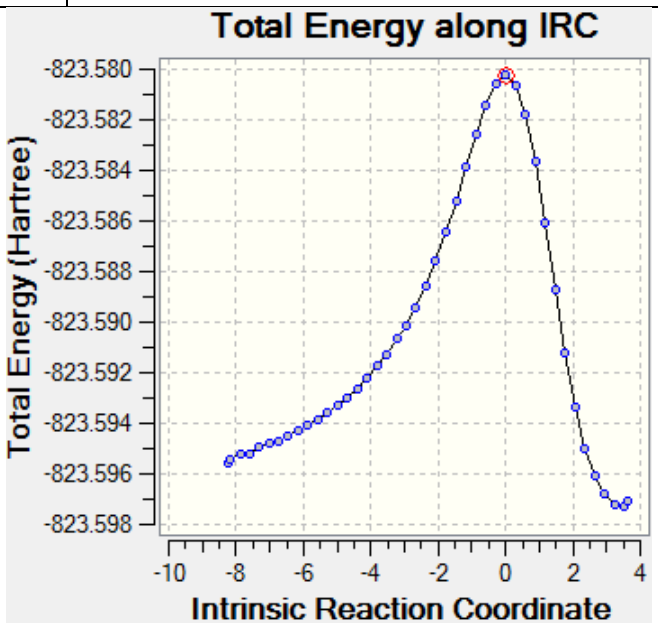


Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(QST3, maxcyc=200, CalcFC, Tight) Freq scrf=(cpcm,solvent=acetone)
Smiles	CN1C2=CC=C(C)cc2[C@]3(C(OCC3)=O)CC1=O
Formula	$C_{14}H_{15}NO_3^{\bullet}$
Charge	0
Multiplicity	2
Dipole (Debye)	9.2978
Gibbs energy (a.u.)	−823.348429
# Imaginary frequencies	1



Input coordinates:

SM

C	2.3447100	2.6220710	0.4406230
H	2.8153970	3.0797310	-0.4354500
H	1.5869320	3.2976830	0.8331620
N	1.6994300	1.3491390	0.0710590
C	2.5277570	0.3337860	-0.3141430
O	3.7530360	0.5022600	-0.3696530
H	3.1122380	2.4499770	1.1975470
C	0.2687340	1.3150780	-0.0185350
C	-0.3718520	1.0152700	-1.2240290
C	-0.5064580	1.6383310	1.1060570
C	-1.7681830	1.0211480	-1.2980880
H	0.2128120	0.7973870	-2.1113880
C	-1.8966010	1.6519270	1.0175820
H	-0.0199170	1.8718500	2.0483340
C	-2.5559330	1.3409340	-0.1851460
H	-2.2462830	0.7808930	-2.2437350
H	-2.4803890	1.9017600	1.8998290
C	-4.0635770	1.3751170	-0.2700000
H	-4.4374430	2.4036740	-0.2005470
H	-4.4187950	0.9531720	-1.2138370
H	-4.5200240	0.8103650	0.5500150
C	1.9508360	-1.0412230	-0.6870700
H	1.7433150	-1.0548820	-1.7626060
H	2.7931100	-1.7289540	-0.5294020
C	0.7650670	-1.5436180	0.0523820
C	0.6504440	-1.7220190	1.5279460
C	-0.7615300	-2.3186600	1.6897070
H	0.7755330	-0.7920670	2.0927320
H	1.4268190	-2.4150350	1.8874730
H	-1.4857360	-1.5790380	2.0392860
H	-0.7955520	-3.1969270	2.3349010
C	-0.3231450	-2.2564820	-0.5911570
O	-1.1777240	-2.7415900	0.3591950
O	-0.5152660	-2.4623610	-1.7846030

Product

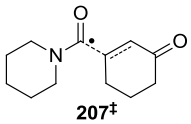
C	3.0190560	2.0393240	0.2052450
H	4.0211270	1.6406520	0.0722290
H	2.8462950	2.8513140	-0.5043870
N	2.0595360	0.9547150	-0.0429160
C	2.5519550	-0.3326560	-0.1289030
O	3.7636190	-0.5714160	-0.0681850
H	2.9157020	2.4207670	1.2255300
C	0.6890830	1.2636720	-0.1257230
C	-0.2232620	0.1960780	-0.6759100
C	0.1963920	2.4973190	0.2506070
C	-1.6761750	0.5880130	-0.6447130

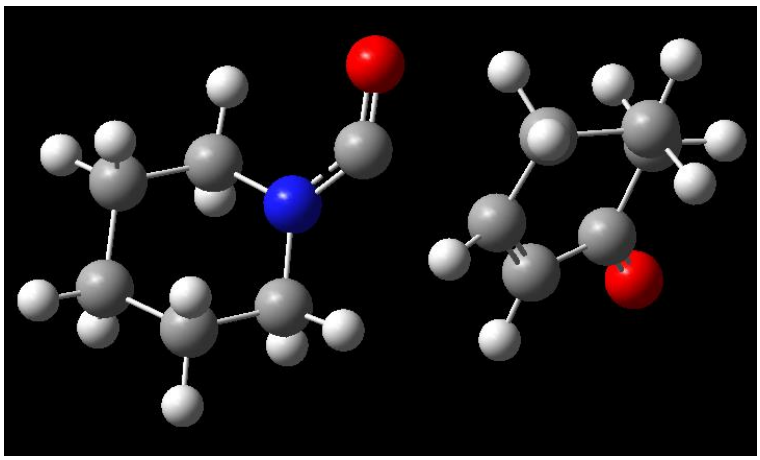
H	0.0552820	0.0192810	-1.7322330
C	-1.1797440	2.7947440	0.1854550
H	0.8675230	3.2630920	0.6205910
C	-2.1256120	1.8196730	-0.2586620
H	-2.3847090	-0.1489610	-1.0158250
H	-1.5233770	3.7763820	0.4963120
C	-3.5936510	2.1759910	-0.2953120
H	-3.7722140	3.0316080	-0.9570290
H	-4.2001210	1.3385950	-0.6505380
H	-3.9533620	2.4603060	0.7004970
C	1.5735920	-1.4792280	-0.3119350
H	1.6353320	-1.7861990	-1.3632150
H	1.9576020	-2.3135950	0.2814070
C	0.1129630	-1.1707850	0.0357660
C	-0.2154780	-1.1833330	1.5441170
C	-1.5838160	-1.8734490	1.6266660
H	-0.2458130	-0.1818090	1.9797500
H	0.5345730	-1.7652350	2.0871040
H	-2.4173830	-1.1685670	1.6513560
H	-1.6735780	-2.5769770	2.4545280
C	-0.7945790	-2.2728340	-0.5168760
O	-1.7101530	-2.6492440	0.3956700
O	-0.7514620	-2.7691930	-1.6255590

TS guess

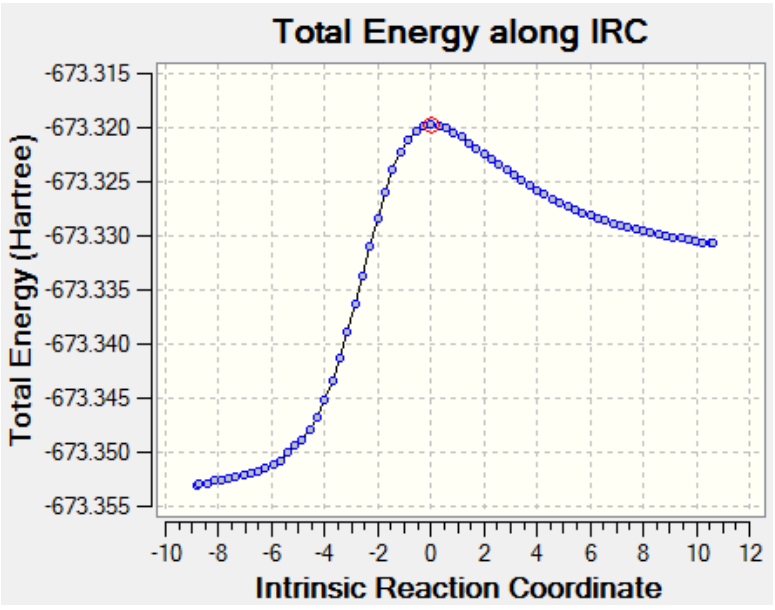
C	3.0259430	2.0633850	0.0702130
H	3.9802220	1.7745260	-0.3661550
H	2.6418330	2.9489110	-0.4362820
N	2.0730740	0.9573930	-0.1145730
C	2.5754930	-0.3240200	-0.0974720
O	3.7932980	-0.5286180	-0.0326080
H	3.1776840	2.2856610	1.1316130
C	0.6919420	1.2502360	-0.1871080
C	-0.1643620	0.3704630	-0.9276760
C	0.1443100	2.3303140	0.5040170
C	-1.5561530	0.7104720	-1.0158940
H	0.2616760	-0.1472540	-1.7831660
C	-1.2290770	2.5920480	0.4404060
H	0.7791350	2.9757050	1.1009300
C	-2.1014000	1.7794200	-0.3228380
H	-2.1901980	0.0994520	-1.6526070
H	-1.6288890	3.4409570	0.9878200
C	-3.5747700	2.1034590	-0.3958910
H	-3.7375500	3.1364520	-0.7226940
H	-4.0942980	1.4394030	-1.0916920
H	-4.0482270	1.9986860	0.5875590
C	1.6368480	-1.5302130	-0.1547810
H	1.7184140	-1.9450470	-1.1666360
H	2.0957700	-2.2688420	0.5143050
C	0.1823920	-1.3622130	0.1896950
C	-0.2841290	-1.1683400	1.6126770

C	-1.7503630	-1.6315570	1.5613370
H	-0.1920460	-0.1398230	1.9735880
H	0.3067070	-1.8034880	2.2868290
H	-2.4494380	-0.7979860	1.4684300
H	-2.0424270	-2.2625770	2.4014860
C	-0.7684370	-2.2986240	-0.4321000
O	-1.8720080	-2.4375930	0.3526620
O	-0.6787050	-2.8769740	-1.5074080





Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(QST3, maxcyc=200, CalcFC, Tight) Freq scrf=(cpcm,solvent=acetone)
Smiles	O=[C](c(CCC1)cC1=O)N2CCCCC2
Formula	$C_{12}H_{17}NO_2^{\bullet}$
Charge	0
Multiplicity	2
Dipole (Debye)	8.0039
Gibbs energy (a.u.)	−673.078693
# Imaginary frequencies	1



Input coordinates:

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C	-4.8826270	-0.5569570	0.1144980
C	-3.8463490	-0.9264430	1.1882440
C	-2.4550290	-1.1129950	0.5724730
C	-3.0310020	0.4636760	-1.2818110
C	-4.4296930	0.6708090	-0.6917170
H	-1.6926890	-1.2727580	1.3377850
H	-3.7971920	-0.1353550	1.9479810
H	-4.1333840	-1.8514940	1.7008320
H	-5.0183410	-1.4092650	-0.5666660
H	-5.8564320	-0.3654330	0.5782060
H	-2.6481060	1.3705060	-1.7524370
H	-3.0471830	-0.3361280	-2.0340750
H	-4.4168790	1.5574620	-0.0450950
H	-5.1294780	0.8761500	-1.5100350
H	-2.4545340	-1.9862220	-0.0945960
N	-2.0763010	0.0679860	-0.2176460
O	-0.4994590	1.7418890	-0.4925250
C	-0.9656070	0.7476310	0.0346400
C	2.5817090	1.2715700	1.0064840
C	4.0681760	1.2452170	0.6202990
H	2.0108010	1.9050110	0.3109400
H	2.4440640	1.7209480	1.9969630
C	4.3016430	0.3812330	-0.6283530
H	4.4348880	2.2619380	0.4471480
H	4.6488690	0.8330490	1.4555030
H	5.3632060	0.2924860	-0.8768590
H	3.8050490	0.8417410	-1.4960770
C	3.7191670	-1.0144690	-0.4828900
O	4.2157130	-1.9851620	-1.0649210
C	2.5058480	-1.1493200	0.3367900
H	2.0438540	-2.1327920	0.3653800
C	1.9686100	-0.0977940	0.9915230
H	1.0384810	-0.2325150	1.5371230

Product

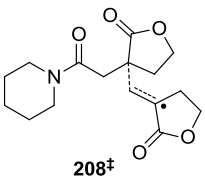
C	-4.1603940	-0.6522140	0.5038770
C	-2.9111510	-1.1028190	1.2737550
C	-1.6903070	-1.1969240	0.3481830
C	-2.6393490	0.5095470	-1.1549500
C	-3.8814320	0.6464400	-0.2663770
H	-0.8047000	-1.4709230	0.9160500
H	-2.6916980	-0.3914290	2.0805050
H	-3.0730800	-2.0820380	1.7387410
H	-4.4517660	-1.4394610	-0.2057410
H	-5.0030820	-0.5171010	1.1910710
H	-2.3841620	1.4520450	-1.6360790
H	-2.8185140	-0.2394210	-1.9396680

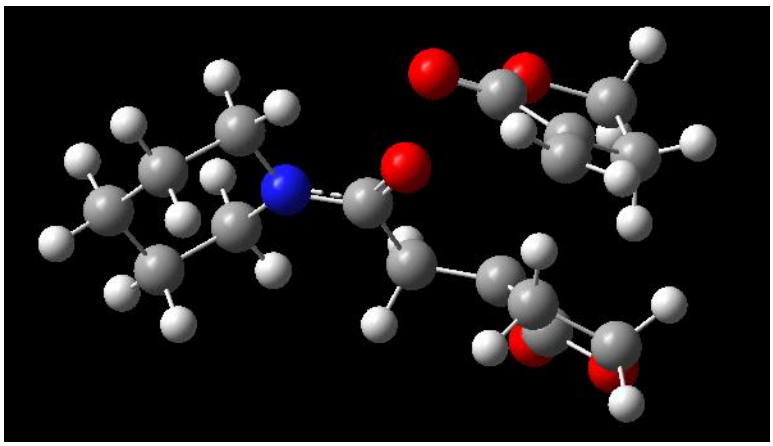
H	-3.7254760	1.4725880	0.4396700
H	-4.7372090	0.9159500	-0.8960880
H	-1.8532910	-1.9838080	-0.4020610
N	-1.4730250	0.0714510	-0.3661430
O	-0.2208850	1.8496640	-1.0469230
C	-0.3294630	0.8010600	-0.3983880
C	1.8877160	1.4273330	0.7814750
C	3.2343200	0.8919040	1.2816420
H	2.0415060	2.0525810	-0.1037130
H	1.4142770	2.0584400	1.5404410
C	3.9416530	0.0884390	0.1804640
H	3.8733530	1.7225330	1.5992190
H	3.0817740	0.2570720	2.1647020
H	4.8338600	-0.4248460	0.5538110
H	4.2821280	0.7660420	-0.6157680
C	3.0427210	-0.9473620	-0.4733170
O	3.5280200	-1.8979260	-1.1270040
C	1.6165820	-0.8209670	-0.3379200
H	1.0225780	-1.6028460	-0.8054550
C	0.9372420	0.2718990	0.4234660
H	0.5587660	-0.1574570	1.3633350

TS guess

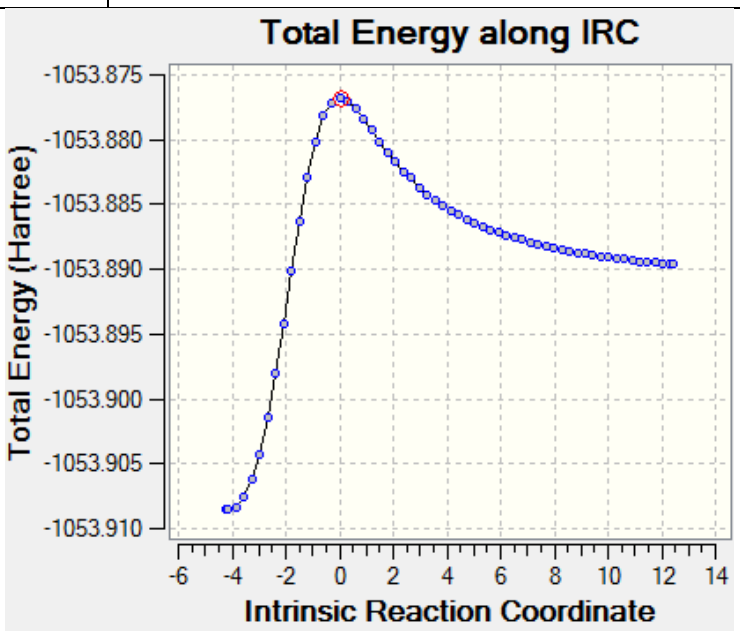
C	-4.2459620	-0.5337720	0.2805850
C	-3.1081210	-0.8950480	1.2464910
C	-1.7780610	-1.0762080	0.5040830
C	-2.5346940	0.4822050	-1.2828360
C	-3.8723490	0.6909590	-0.5672030
H	-0.9652210	-1.2490690	1.2048050
H	-2.9905180	-0.1042400	1.9987140
H	-3.3349900	-1.8227680	1.7838080
H	-4.4460820	-1.3876710	-0.3819140
H	-5.1693580	-0.3422870	0.8380240
H	-2.2084990	1.3811990	-1.8054510
H	-2.6141490	-0.3338840	-2.0132360
H	-3.8013600	1.5806690	0.0714370
H	-4.6433330	0.8924130	-1.3197920
H	-1.8352400	-1.9431840	-0.1673630
N	-1.4729640	0.1093370	-0.3122320
O	-0.0606360	1.8525510	-0.8235500
C	-0.3658530	0.8415440	-0.2236520
C	2.1696580	1.3121830	1.1258720
C	3.6183280	0.9815170	0.7312100
H	1.7831210	2.0880090	0.4537640
H	2.1329810	1.7287370	2.1383040
C	3.6620810	0.1893850	-0.5837520
H	4.1968340	1.9065320	0.6341310
H	4.0941400	0.3891500	1.5232980
H	4.6834910	-0.0873100	-0.8628450
H	3.2602740	0.8034090	-1.4035670
C	2.8279500	-1.0791210	-0.5010630

O	3.1337330	-2.0966880	-1.1558580
C	1.6799210	-1.0591200	0.3772620
H	1.1163510	-1.9845980	0.4591160
C	1.2617110	0.0974960	1.0559670
H	0.5798760	-0.0394820	1.8918700





Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(QST3, maxcyc=200, CalcFC, Tight) Freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(C[C@]1(c[c]2C(OCC2)=O)CCOC1=O)N3CCCCC3
Formula	$C_{16}H_{21}NO_5^{\bullet}$
Charge	0
Multiplicity	2
Dipole (Debye)	4.1827
Gibbs energy (a.u.)	−1053.563162
# Imaginary frequencies	1



Input coordinates:

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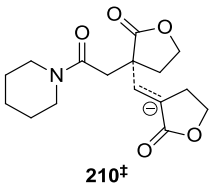
O	-1.1424590	0.4615300	-1.6313680
C	-1.4893410	0.3592850	-0.4436080
C	-0.6472070	0.9927540	0.6759900
H	-1.3026540	1.6443460	1.2765950
H	-0.2872470	0.2164580	1.3599750
C	0.5112270	1.8053980	0.2216390
C	0.5174340	2.8840060	-0.8028620
C	1.9329370	3.4849820	-0.6742690
H	-0.2643810	3.6280830	-0.5881170
H	0.3072550	2.4979050	-1.8052550
H	1.9329980	4.5603700	-0.4904880
H	2.5637800	3.2688960	-1.5395800
C	1.7398930	1.8708400	0.9907370
O	2.0784490	1.2120670	1.9689700
O	2.5489400	2.8486590	0.4823140
C	-3.4535670	-0.9602210	-1.0859920
C	-3.0734040	-0.5236960	1.3106340
C	-4.9116970	-0.5003550	-0.9697120
H	-3.3892340	-2.0472390	-0.9333610
H	-3.0372850	-0.7294690	-2.0650890
C	-4.5236380	-0.0512970	1.4857370
H	-3.0040310	-1.6000980	1.5245590
H	-2.4194310	-0.0125230	2.0135040
C	-5.4512760	-0.7079120	0.4532570
H	-5.5154340	-1.0543300	-1.6978970
H	-4.9728280	0.5621340	-1.2397070
H	-4.8487800	-0.2863420	2.5057560
H	-4.5567430	1.0406680	1.3768050
H	-6.4656630	-0.3027190	0.5409510
H	-5.5204130	-1.7849140	0.6621390
N	-2.6149880	-0.3041870	-0.0698310
C	2.1264140	-0.2410500	-1.5470390
H	2.6631700	0.6182940	-1.9375970
C	2.7535000	-1.1607130	-0.8074170
C	4.1869910	-1.2206180	-0.3447680
C	4.1170260	-2.2161970	0.8251850
H	4.5838950	-0.2498580	-0.0406720
H	4.8272320	-1.6144090	-1.1431290
H	4.0224070	-1.7165600	1.7926130
H	4.9416570	-2.9276840	0.8580550
C	2.0618590	-2.3576520	-0.2496290
O	0.9446880	-2.7822540	-0.4830250
O	2.8940900	-2.9888750	0.6164650
H	1.0740790	-0.3360390	-1.7953850

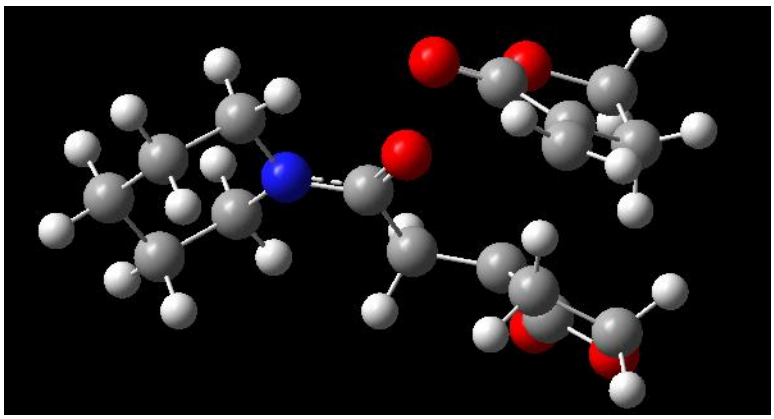
Product

O	-1.2084500	0.6190550	-1.8246760
C	-1.3567610	0.3122870	-0.6293620
C	-0.2657430	0.6136930	0.4035100
H	-0.6806390	1.2985190	1.1528770
H	-0.0019420	-0.3006850	0.9421540
C	1.0171230	1.2421510	-0.1691510
C	0.8174770	2.6057240	-0.8662550
C	2.0819080	3.3878800	-0.4982830
H	-0.0658800	3.1066230	-0.4582990
H	0.6822280	2.5138200	-1.9439580
H	1.9150580	4.4529270	-0.3369250
H	2.8987500	3.2537800	-1.2126690
C	1.9370860	1.6294600	0.9987290
O	2.1650710	0.9887880	2.0063950
O	2.5195050	2.8250720	0.7766950
C	-3.5777580	-0.6156260	-1.1099840
C	-2.7626360	-0.6805060	1.2149610
C	-4.9005320	0.0199510	-0.6633960
H	-3.6805180	-1.7103050	-1.1381870
H	-3.2829020	-0.2756860	-2.1013390
C	-4.0684660	-0.0498120	1.7209270
H	-2.8432530	-1.7768030	1.2469480
H	-1.9318160	-0.3981400	1.8576270
C	-5.2415460	-0.3678220	0.7828420
H	-5.6956870	-0.2979440	-1.3478480
H	-4.8174360	1.1116350	-0.7472840
H	-4.2683360	-0.4205250	2.7329260
H	-3.9330880	1.0373040	1.7935790
H	-6.1468500	0.1522240	1.1158610
H	-5.4591420	-1.4444960	0.8273490
N	-2.4926400	-0.2831680	-0.1746050
C	1.8048970	0.2585710	-1.1217890
H	2.6211240	0.8206300	-1.5890200
C	2.3707020	-0.9723650	-0.5042430
C	3.7652980	-1.1602780	-0.0136080
C	3.7355790	-2.5786420	0.5885760
H	4.0673140	-0.4049840	0.7199470
H	4.4771550	-1.0885530	-0.8503740
H	3.7251600	-2.5652150	1.6812210
H	4.5449050	-3.2211910	0.2404100
C	1.6735600	-2.2437090	-0.4302660
O	0.5458320	-2.5338980	-0.8169270
O	2.4844090	-3.1805400	0.1488670
H	1.0922140	-0.0143330	-1.9048450

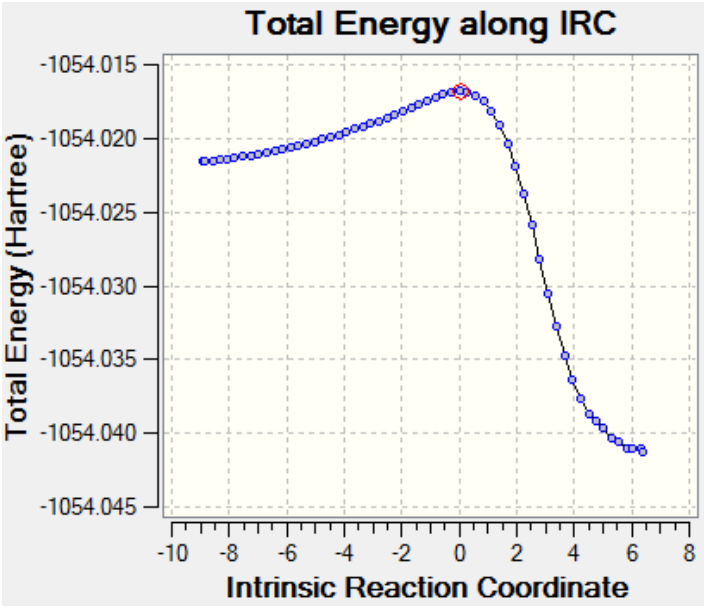
TS guess

O	-1.2057970	0.7787870	-1.7282370
C	-1.4069640	0.4465310	-0.5471970
C	-0.3709530	0.7539590	0.5408460
H	-0.8560320	1.3644810	1.3195360
H	-0.0623690	-0.1693230	1.0410680
C	0.8515360	1.4939530	0.0923150
C	0.8427550	2.7554070	-0.7187290
C	2.2405750	3.3454600	-0.4607230
H	0.0535530	3.4253670	-0.3469400
H	0.6374180	2.5906520	-1.7788120
H	2.2311080	4.4119430	-0.2332600
H	2.9372930	3.1606550	-1.2824220
C	1.9699920	1.5953010	1.0366500
O	2.2293130	0.8902200	1.9805000
O	2.7580870	2.6554410	0.7138630
C	-3.5635780	-0.5513930	-1.1532060
C	-2.8490190	-0.6547410	1.2051070
C	-4.9371780	-0.0046770	-0.7452170
H	-3.6031510	-1.6481180	-1.2239160
H	-3.2455030	-0.1602880	-2.1180510
C	-4.2080010	-0.1125170	1.6704460
H	-2.8713330	-1.7540390	1.1957060
H	-2.0636500	-0.3530800	1.8945410
C	-5.3188390	-0.4618910	0.6700440
H	-5.6824340	-0.3408340	-1.4754430
H	-4.9117130	1.0921160	-0.7886570
H	-4.4304380	-0.5287560	2.6596940
H	-4.1366070	0.9770520	1.7842380
H	-6.2656860	-0.0041660	0.9778760
H	-5.4770670	-1.5496730	0.6693510
N	-2.5399720	-0.1947540	-0.1578160
C	1.9278980	0.0115670	-1.3802140
H	2.5876160	0.8073130	-1.7090650
C	2.4507680	-1.0667200	-0.7294240
C	3.8374450	-1.2595030	-0.1818000
C	3.7173230	-2.5678780	0.6247870
H	4.1576000	-0.4254380	0.4489540
H	4.5676680	-1.3591400	-0.9935810
H	3.7102360	-2.3966270	1.7035110
H	4.4791460	-3.3076600	0.3780240
C	1.6682320	-2.2832660	-0.4367050
O	0.5372420	-2.5548330	-0.7529720
O	2.4264340	-3.1519080	0.2750850
H	0.9499890	-0.0483690	-1.8454120





Route	UB3LYP/6-31+G(d,p) FormCheck Opt=(QST3, maxcyc=200, CalcFC, Tight) Freq scrf=(cpcm,solvent=acetone)
Smiles	O=C(C[C@]1(c[c-]2C(OCC2)=O)CCOC1=O) N3CCCCC3
Formula	$C_{16}H_{21}NO_5^-$
Charge	−1
Multiplicity	1
Dipole (Debye)	10.0524
Gibbs energy (a.u.)	−1053.705008
# Imaginary frequencies	1



Input coordinates:

SM

O	-1.1424590	0.4615300	-1.6313680
C	-1.4893410	0.3592850	-0.4436080
C	-0.6472070	0.9927540	0.6759900
H	-1.3026540	1.6443460	1.2765950
H	-0.2872470	0.2164580	1.3599750
C	0.5112270	1.8053980	0.2216390
C	0.5174340	2.8840060	-0.8028620
C	1.9329370	3.4849820	-0.6742690
H	-0.2643810	3.6280830	-0.5881170
H	0.3072550	2.4979050	-1.8052550
H	1.9329980	4.5603700	-0.4904880
H	2.5637800	3.2688960	-1.5395800
C	1.7398930	1.8708400	0.9907370
O	2.0784490	1.2120670	1.9689700
O	2.5489400	2.8486590	0.4823140
C	-3.4535670	-0.9602210	-1.0859920
C	-3.0734040	-0.5236960	1.3106340
C	-4.9116970	-0.5003550	-0.9697120
H	-3.3892340	-2.0472390	-0.9333610
H	-3.0372850	-0.7294690	-2.0650890
C	-4.5236380	-0.0512970	1.4857370
H	-3.0040310	-1.6000980	1.5245590
H	-2.4194310	-0.0125230	2.0135040
C	-5.4512760	-0.7079120	0.4532570
H	-5.5154340	-1.0543300	-1.6978970
H	-4.9728280	0.5621340	-1.2397070
H	-4.8487800	-0.2863420	2.5057560
H	-4.5567430	1.0406680	1.3768050
H	-6.4656630	-0.3027190	0.5409510
H	-5.5204130	-1.7849140	0.6621390
N	-2.6149880	-0.3041870	-0.0698310
C	2.1264140	-0.2410500	-1.5470390
H	2.6631700	0.6182940	-1.9375970
C	2.7535000	-1.1607130	-0.8074170
C	4.1869910	-1.2206180	-0.3447680
C	4.1170260	-2.2161970	0.8251850
H	4.5838950	-0.2498580	-0.0406720
H	4.8272320	-1.6144090	-1.1431290
H	4.0224070	-1.7165600	1.7926130
H	4.9416570	-2.9276840	0.8580550
C	2.0618590	-2.3576520	-0.2496290
O	0.9446880	-2.7822540	-0.4830250
O	2.8940900	-2.9888750	0.6164650
H	1.0740790	-0.3360390	-1.7953850

Product

O	-1.2084500	0.6190550	-1.8246760
C	-1.3567610	0.3122870	-0.6293620
C	-0.2657430	0.6136930	0.4035100
H	-0.6806390	1.2985190	1.1528770
H	-0.0019420	-0.3006850	0.9421540
C	1.0171230	1.2421510	-0.1691510
C	0.8174770	2.6057240	-0.8662550
C	2.0819080	3.3878800	-0.4982830
H	-0.0658800	3.1066230	-0.4582990
H	0.6822280	2.5138200	-1.9439580
H	1.9150580	4.4529270	-0.3369250
H	2.8987500	3.2537800	-1.2126690
C	1.9370860	1.6294600	0.9987290
O	2.1650710	0.9887880	2.0063950
O	2.5195050	2.8250720	0.7766950
C	-3.5777580	-0.6156260	-1.1099840
C	-2.7626360	-0.6805060	1.2149610
C	-4.9005320	0.0199510	-0.6633960
H	-3.6805180	-1.7103050	-1.1381870
H	-3.2829020	-0.2756860	-2.1013390
C	-4.0684660	-0.0498120	1.7209270
H	-2.8432530	-1.7768030	1.2469480
H	-1.9318160	-0.3981400	1.8576270
C	-5.2415460	-0.3678220	0.7828420
H	-5.6956870	-0.2979440	-1.3478480
H	-4.8174360	1.1116350	-0.7472840
H	-4.2683360	-0.4205250	2.7329260
H	-3.9330880	1.0373040	1.7935790
H	-6.1468500	0.1522240	1.1158610
H	-5.4591420	-1.4444960	0.8273490
N	-2.4926400	-0.2831680	-0.1746050
C	1.8048970	0.2585710	-1.1217890
H	2.6211240	0.8206300	-1.5890200
C	2.3707020	-0.9723650	-0.5042430
C	3.7652980	-1.1602780	-0.0136080
C	3.7355790	-2.5786420	0.5885760
H	4.0673140	-0.4049840	0.7199470
H	4.4771550	-1.0885530	-0.8503740
H	3.7251600	-2.5652150	1.6812210
H	4.5449050	-3.2211910	0.2404100
C	1.6735600	-2.2437090	-0.4302660
O	0.5458320	-2.5338980	-0.8169270
O	2.4844090	-3.1805400	0.1488670
H	1.0922140	-0.0143330	-1.9048450

TS guess

O	-1.2057970	0.7787870	-1.7282370
C	-1.4069640	0.4465310	-0.5471970
C	-0.3709530	0.7539590	0.5408460
H	-0.8560320	1.3644810	1.3195360
H	-0.0623690	-0.1693230	1.0410680
C	0.8515360	1.4939530	0.0923150
C	0.8427550	2.7554070	-0.7187290
C	2.2405750	3.3454600	-0.4607230
H	0.0535530	3.4253670	-0.3469400
H	0.6374180	2.5906520	-1.7788120
H	2.2311080	4.4119430	-0.2332600
H	2.9372930	3.1606550	-1.2824220
C	1.9699920	1.5953010	1.0366500
O	2.2293130	0.8902200	1.9805000
O	2.7580870	2.6554410	0.7138630
C	-3.5635780	-0.5513930	-1.1532060
C	-2.8490190	-0.6547410	1.2051070
C	-4.9371780	-0.0046770	-0.7452170
H	-3.6031510	-1.6481180	-1.2239160
H	-3.2455030	-0.1602880	-2.1180510
C	-4.2080010	-0.1125170	1.6704460
H	-2.8713330	-1.7540390	1.1957060
H	-2.0636500	-0.3530800	1.8945410
C	-5.3188390	-0.4618910	0.6700440
H	-5.6824340	-0.3408340	-1.4754430
H	-4.9117130	1.0921160	-0.7886570
H	-4.4304380	-0.5287560	2.6596940
H	-4.1366070	0.9770520	1.7842380
H	-6.2656860	-0.0041660	0.9778760
H	-5.4770670	-1.5496730	0.6693510
N	-2.5399720	-0.1947540	-0.1578160
C	1.9278980	0.0115670	-1.3802140
H	2.5876160	0.8073130	-1.7090650
C	2.4507680	-1.0667200	-0.7294240
C	3.8374450	-1.2595030	-0.1818000
C	3.7173230	-2.5678780	0.6247870
H	4.1576000	-0.4254380	0.4489540
H	4.5676680	-1.3591400	-0.9935810
H	3.7102360	-2.3966270	1.7035110
H	4.4791460	-3.3076600	0.3780240
C	1.6682320	-2.2832660	-0.4367050
O	0.5372420	-2.5548330	-0.7529720
O	2.4264340	-3.1519080	0.2750850
H	0.9499890	-0.0483690	-1.8454120