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Supporting Information For

Ligand free Cu(II) catalyzed aerobic etherification of aryl halides with silanes: An experimental and theoretical approach

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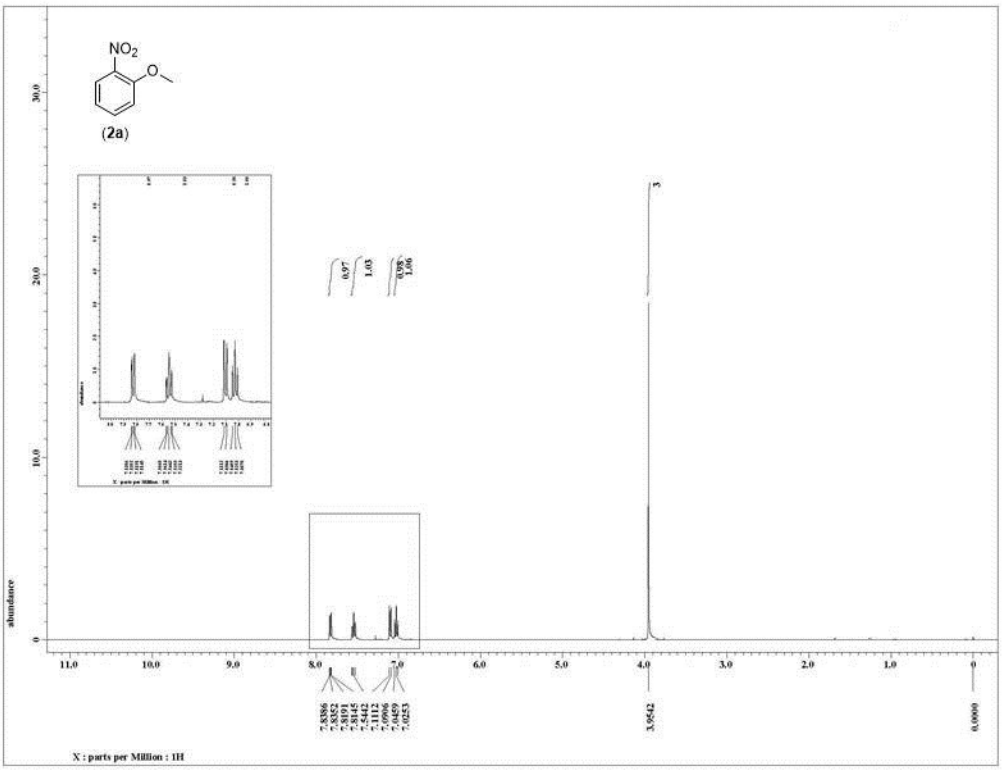
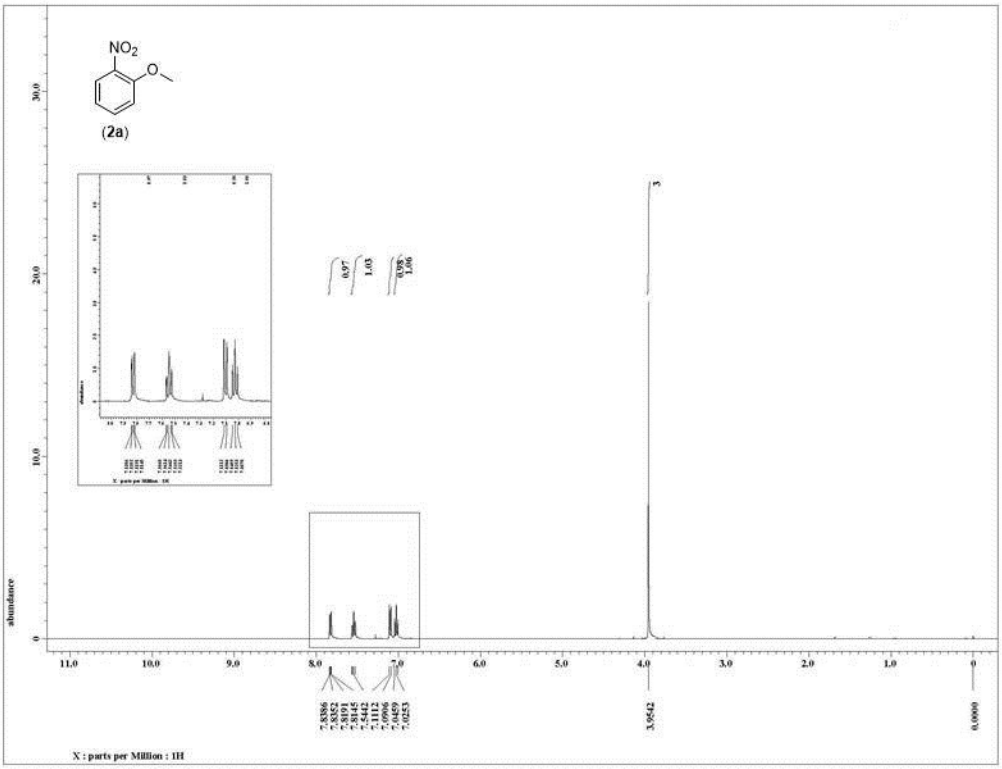
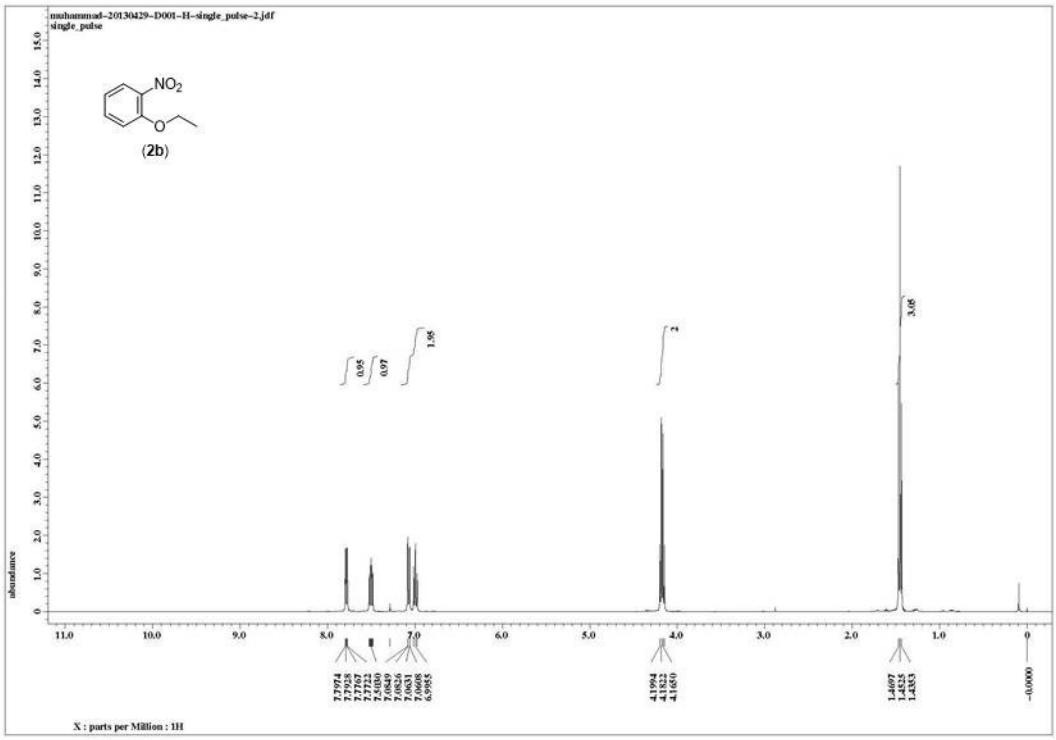

NO2
O
(2a)
0.97
1.03
0.98
1.06
3
abundance
30.0
20.0
10.0
0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.8386
7.8372
7.8191
7.8145
7.5442
7.5112
7.0996
7.0459
7.0253
3.9542
0.0000
X : parts per Million : 1H


NO2
O
(2a)
0.97
1.03
0.98
1.06
3
abundance
30.0
20.0
10.0
0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.8386
7.8372
7.8191
7.8145
7.5442
7.5112
7.0996
7.0459
7.0253
3.9542
0.0000
X : parts per Million : 1H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single_pulse
(2b)
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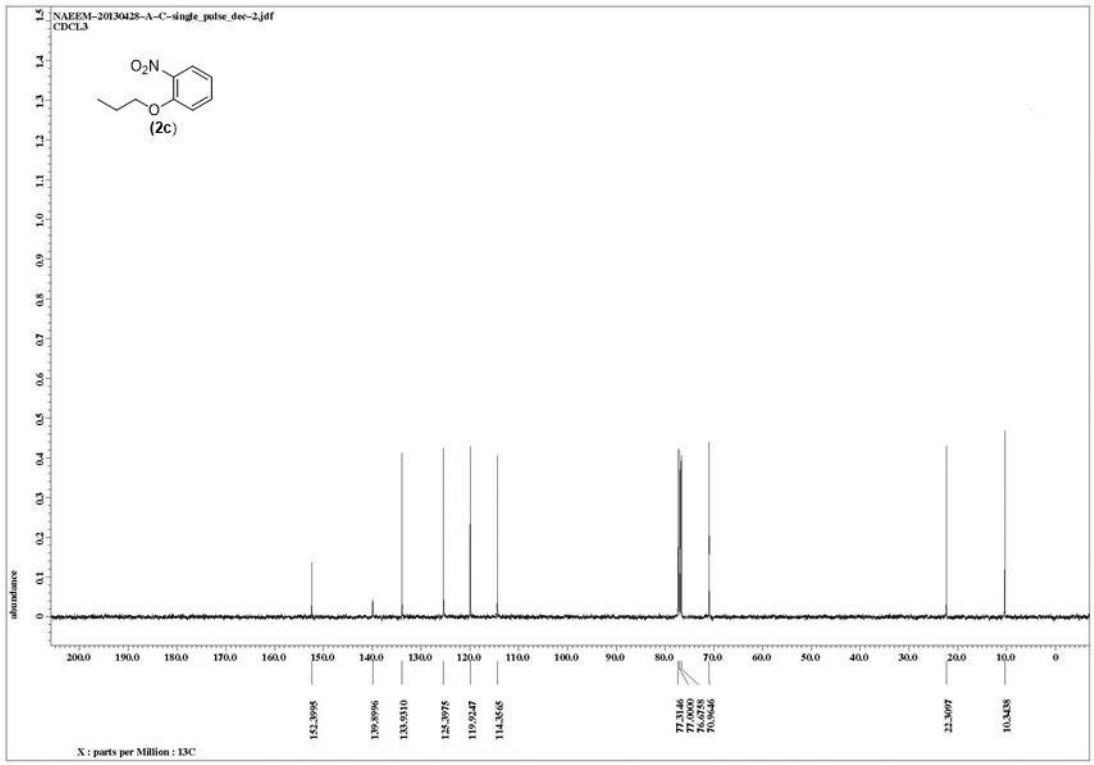
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CDCL3
(2c)
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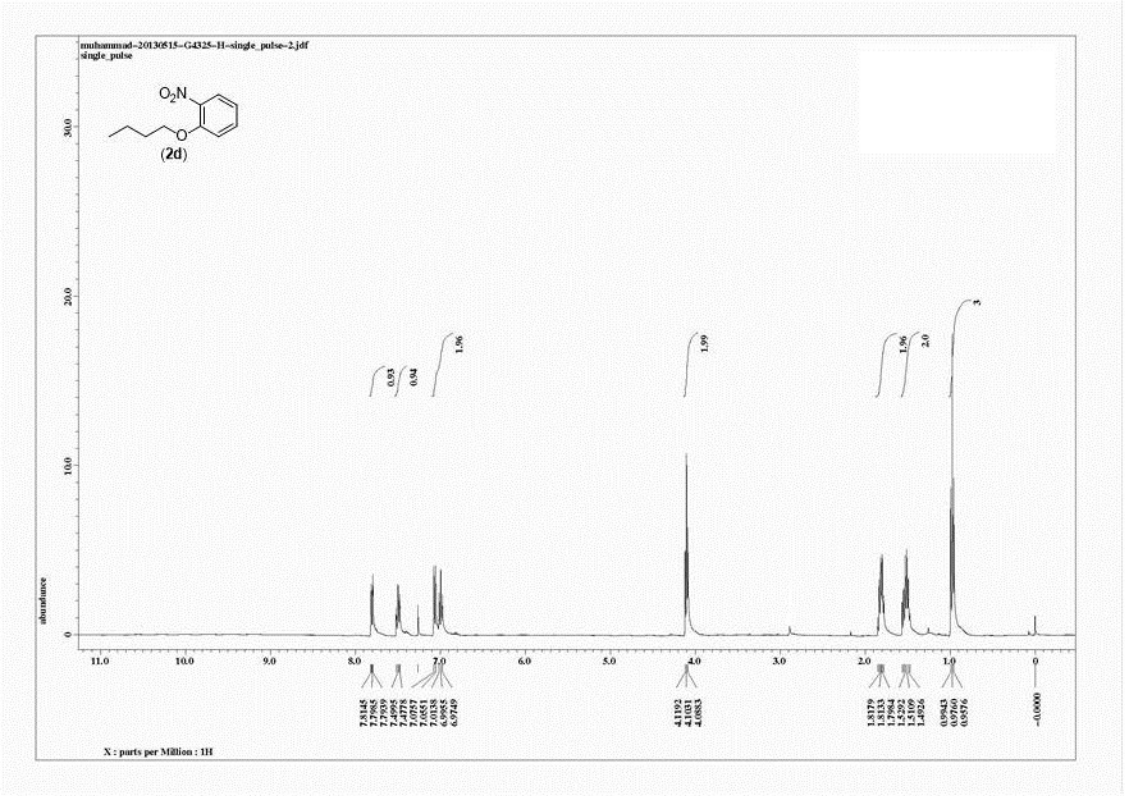
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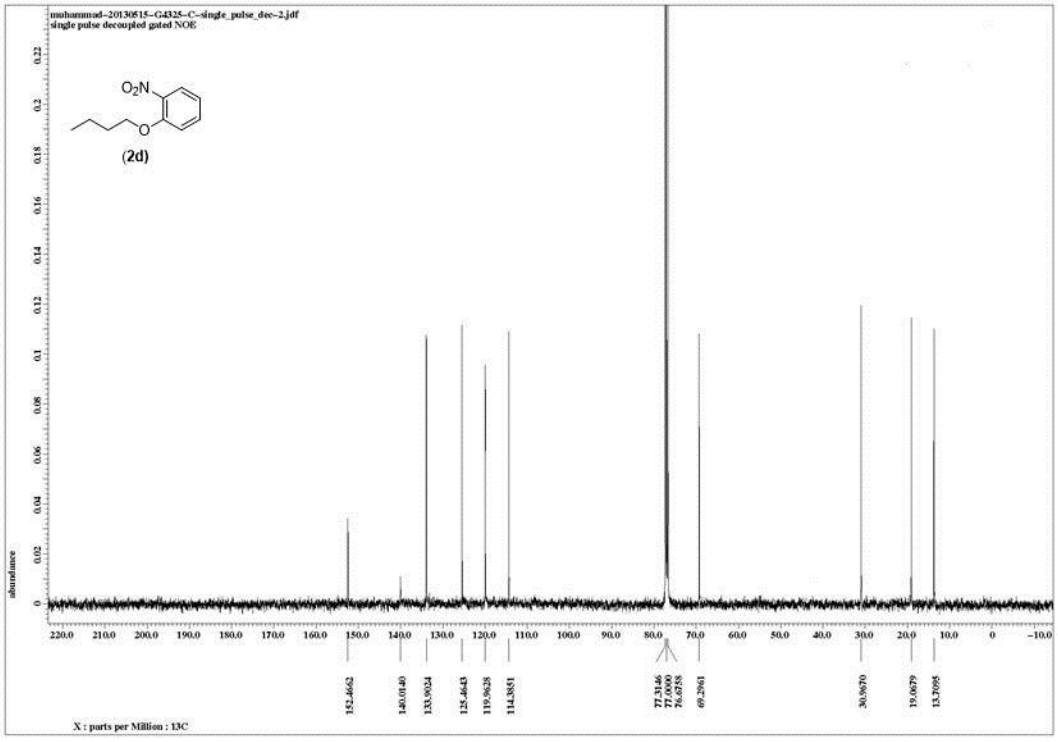
single_pulse
(2d)
abundance
X : parts per Million : 1H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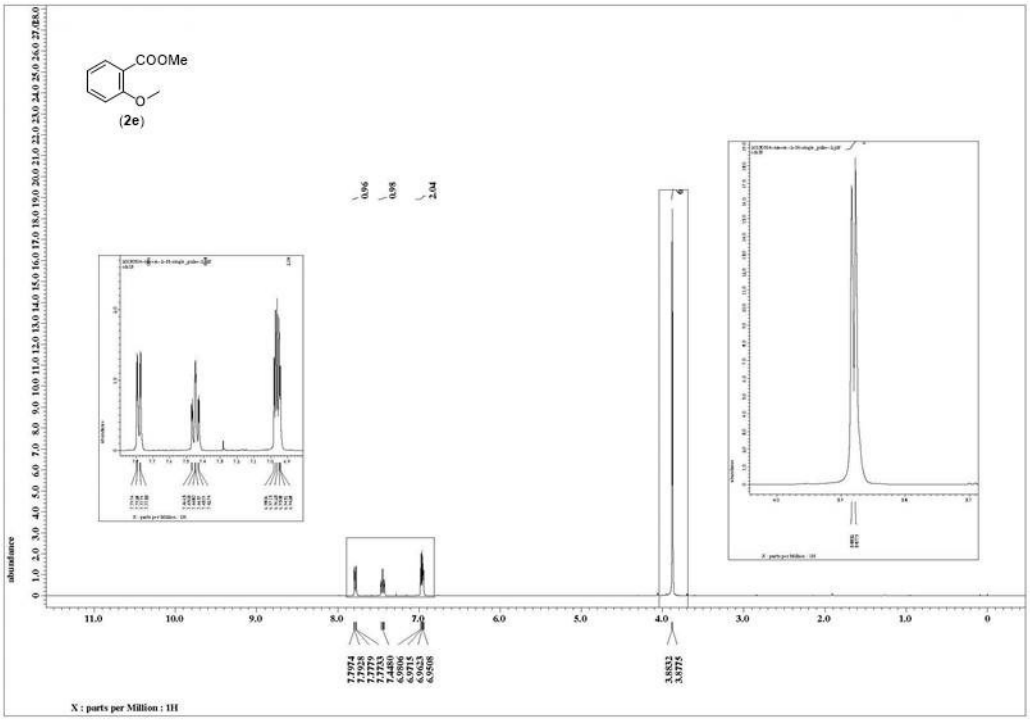
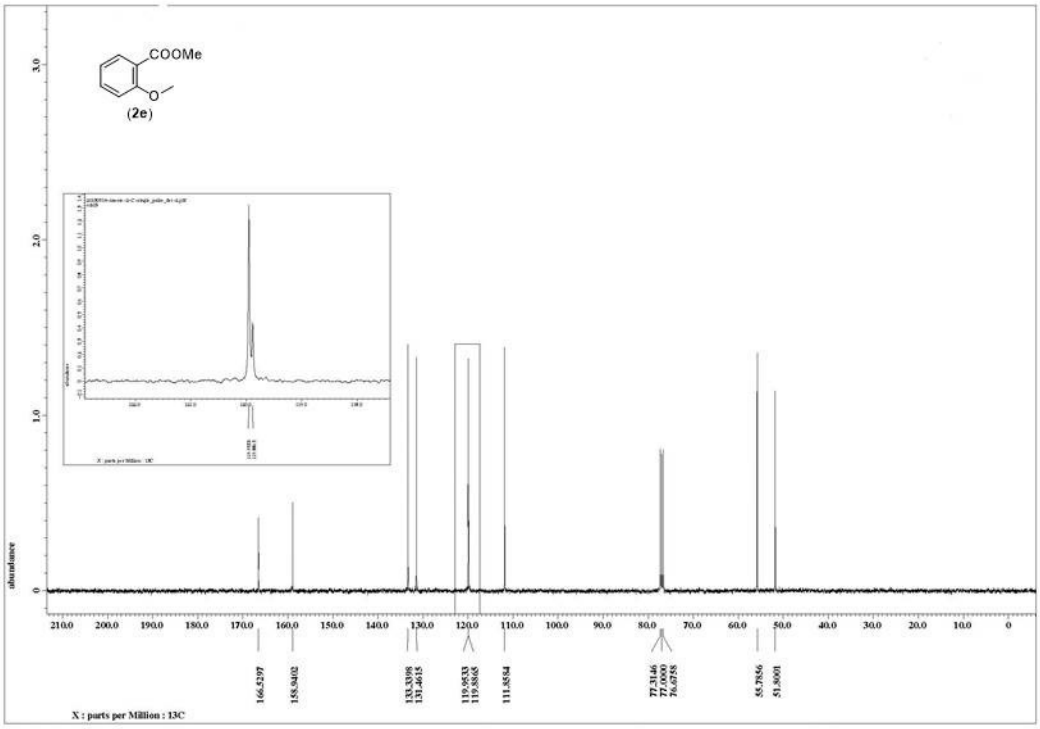
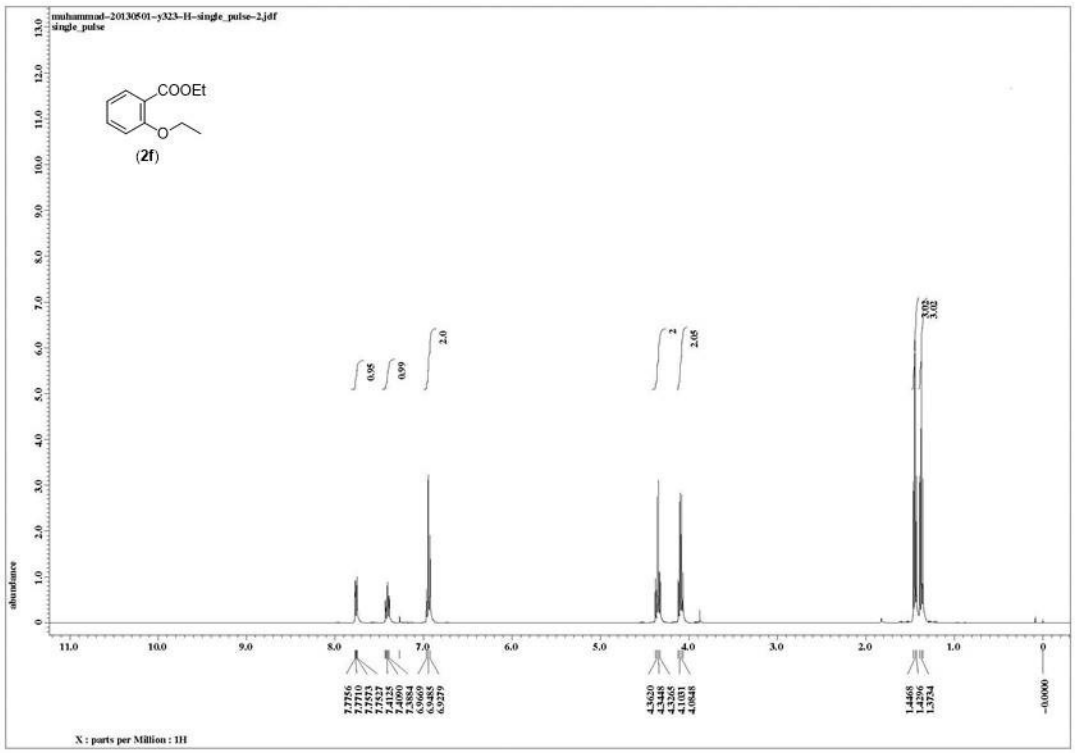
single pulse decoupled gated NOE
(2d)
abundance
X : parts per Million : 13C



1) Cartesian coordinates of relevant stationary points

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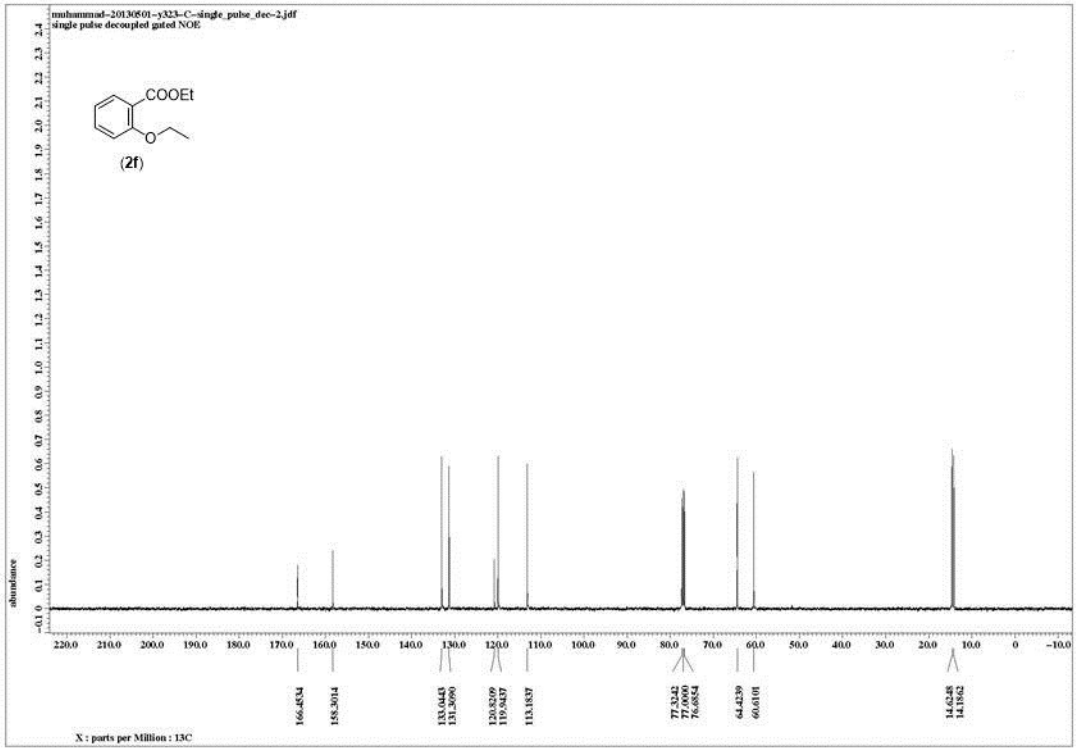
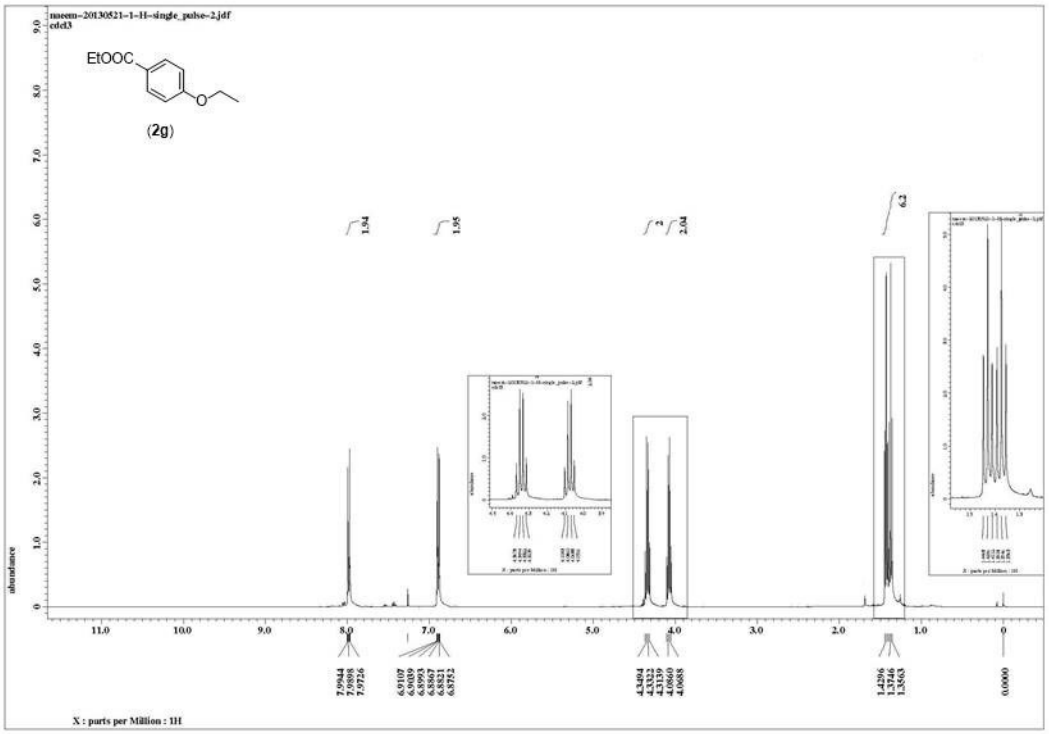
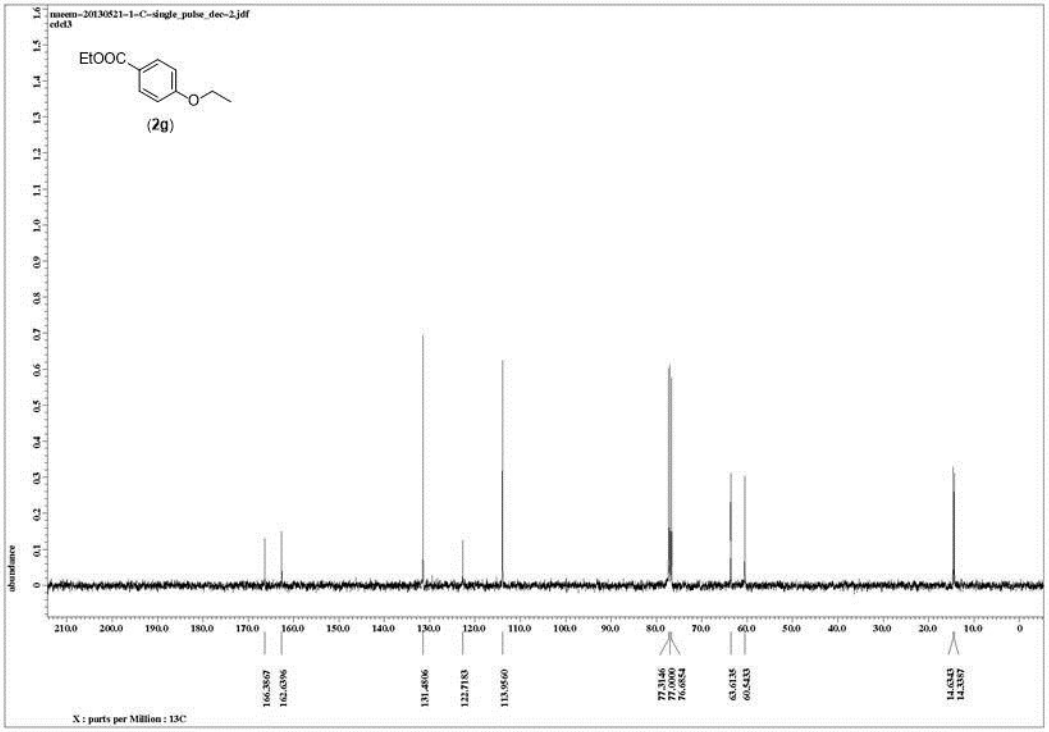
single_pulse
COOEt
O
(2f)
abundance
0.95
0.99
2.0
2
2.05
3.02
3.02
7.7756
7.7710
7.7573
7.7537
7.4125
7.4090
7.3894
6.9660
6.9485
6.9279
4.3620
4.3418
4.3265
4.1031
4.0848
1.4468
1.4296
1.3734
-0.0000
X : parts per Million : 1H


muhammad-20130501-y323-C-single_pulse_dec-2.jdf
single pulse decoupled gated NOE
COOEt
O
(2f)
abundance
166.4534
158.3014
133.0443
131.3990
120.8309
119.9437
113.1837
77.3342
77.0000
76.6854
64.4239
60.6101
14.6248
14.1862
X : parts per Million : 13C


naeem~20130521~1~H~single_pulse~2.jdf
cdcl3
EtOOC
(2g)
1.94
1.95
2.04
6.2
abundance
X : parts per Million : 1H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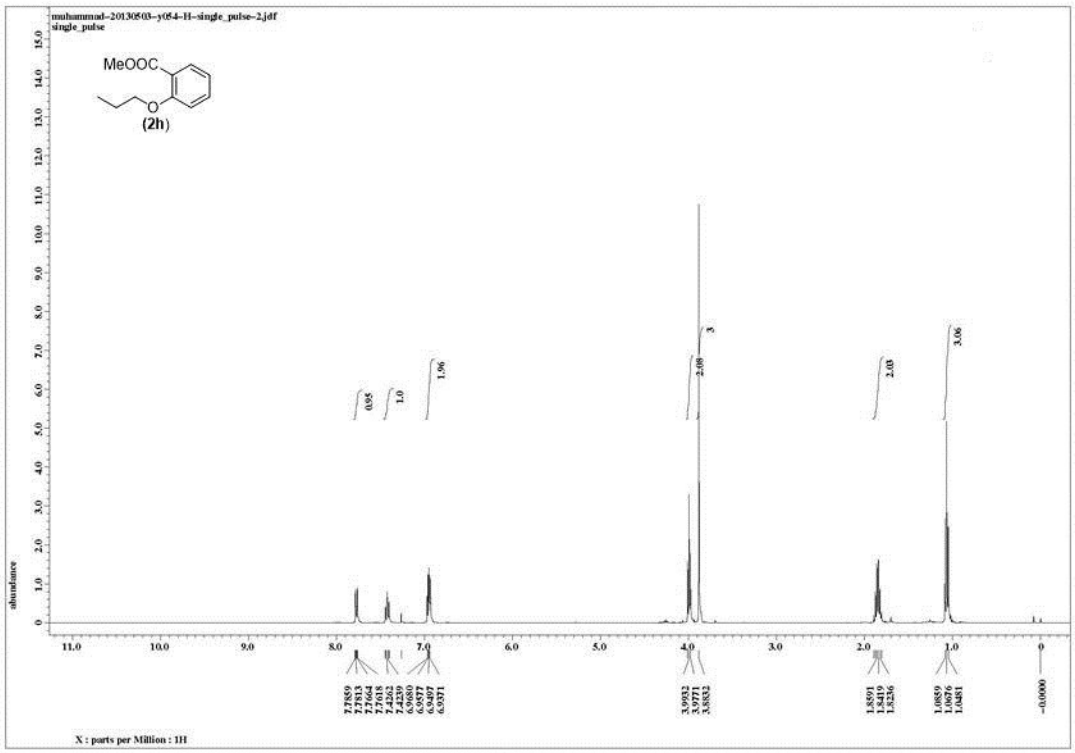
cdcl3
EtOOC
(2g)
abundance
X : parts per Million : 13C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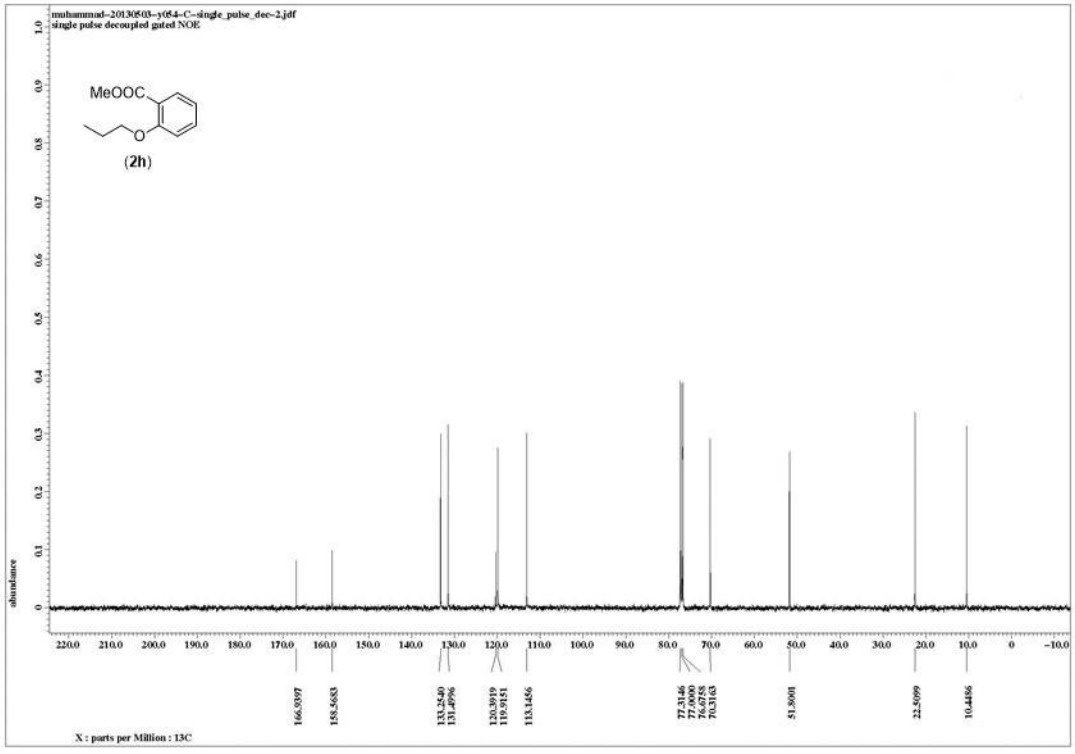
single_pulse
MeOOC
(2h)
abundance
0.95
1.0
1.96
2.98
3
2.03
3.06
7.7859
7.7813
7.7664
7.7618
7.4262
7.4239
6.9569
6.9497
6.9371
3.9932
3.9771
3.8832
1.8591
1.8419
1.8236
1.0859
1.0676
1.0481
-0.0000
X : parts per Million : 1H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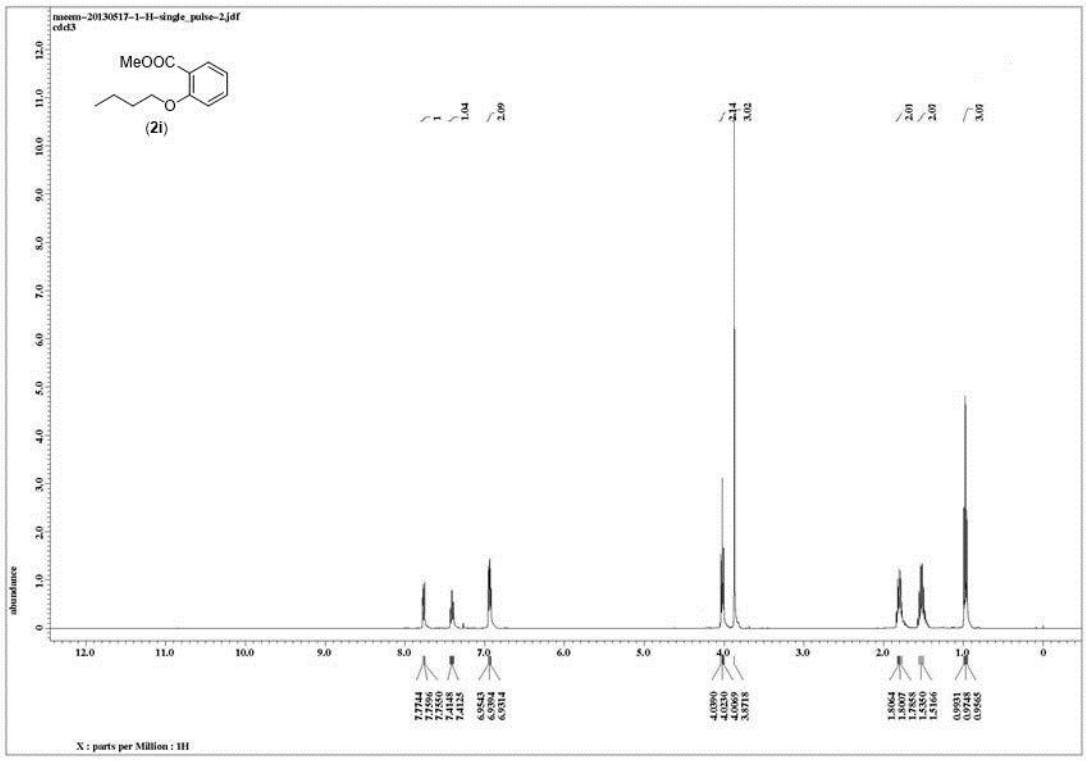
single pulse decoupled gated NOE
MeOOC
(2h)
abundance
166.5397
158.5683
133.2540
131.4996
120.3919
119.9151
113.1456
77.3146
77.0000
76.6858
70.3163
51.8001
22.5099
10.4486
X : parts per Million : 13C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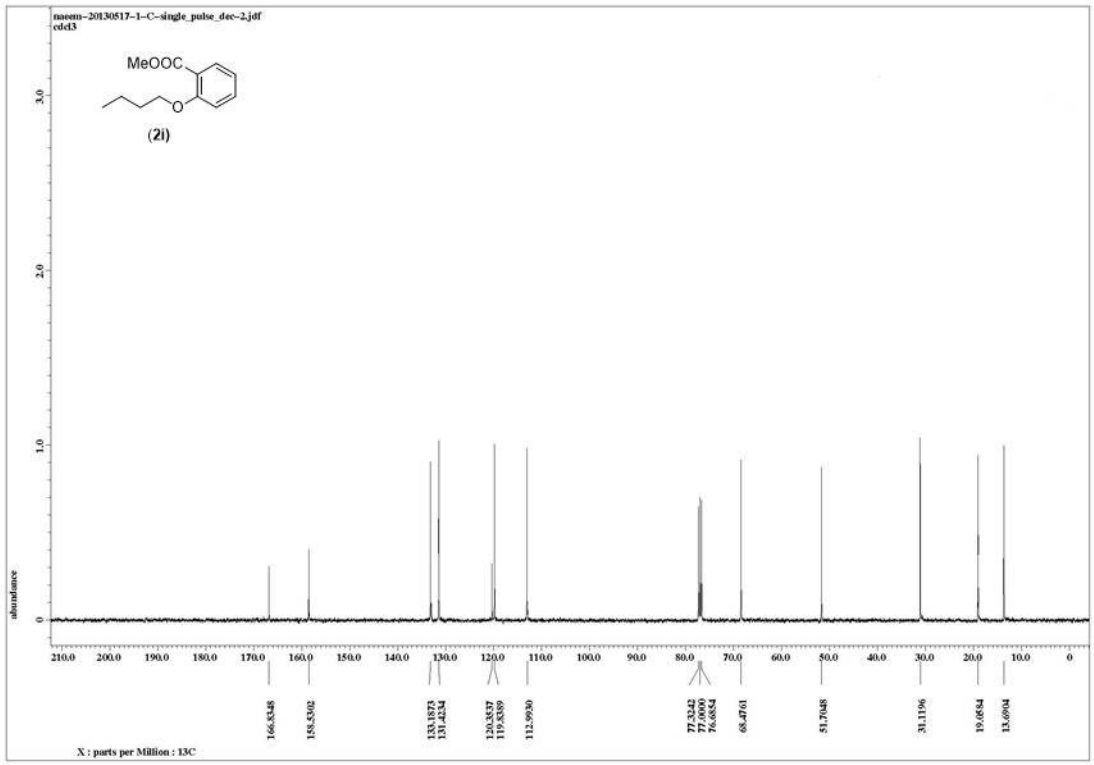
cdcl3
MeOOC
(2i)
1.04
2.09
2.14
3.02
2.01
2.09
3.05
abundance
X : parts per Million : 1H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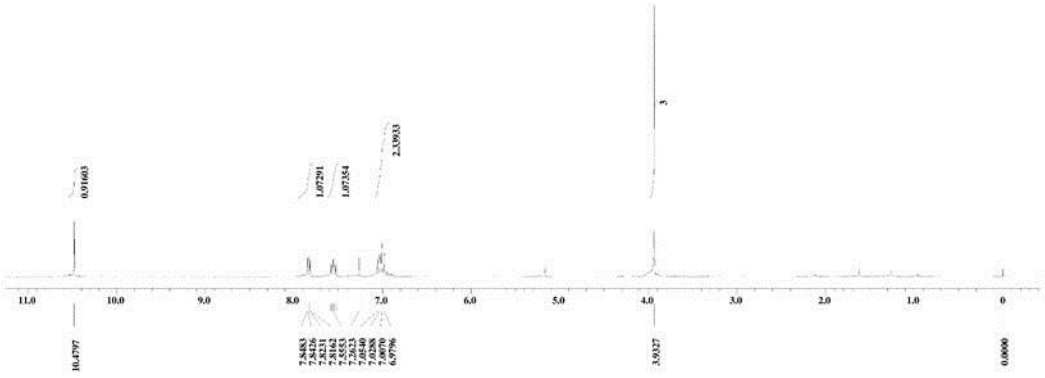
cdcl3
MeOOC
(2i)
166.8348
158.5302
133.1873
131.4234
120.3537
119.5389
112.9930
77.3242
77.0000
76.6854
68.4761
51.7048
31.1196
19.0854
13.6904
abundance
X : parts per Million : 13C

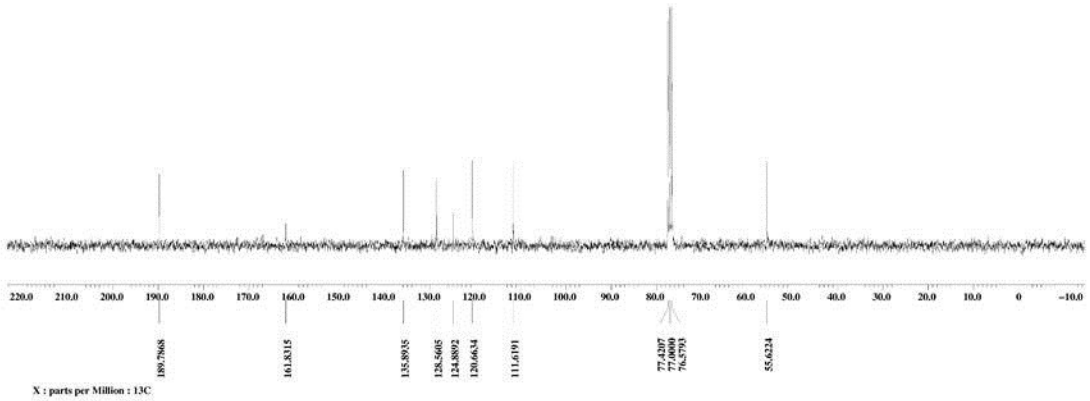
muhammad-20130524-Y777-H-single_pulse-2.jdf
single_pulse

(**2j**)

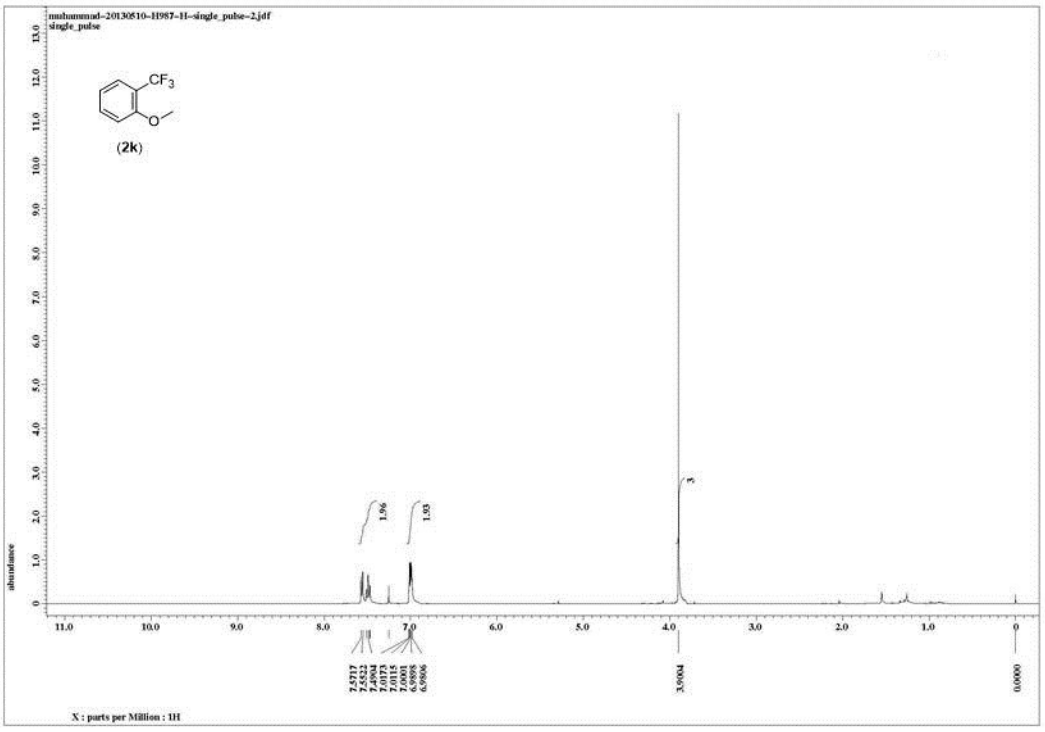


X : parts per Million : 1H

(**2j**)



X : parts per Million : 13C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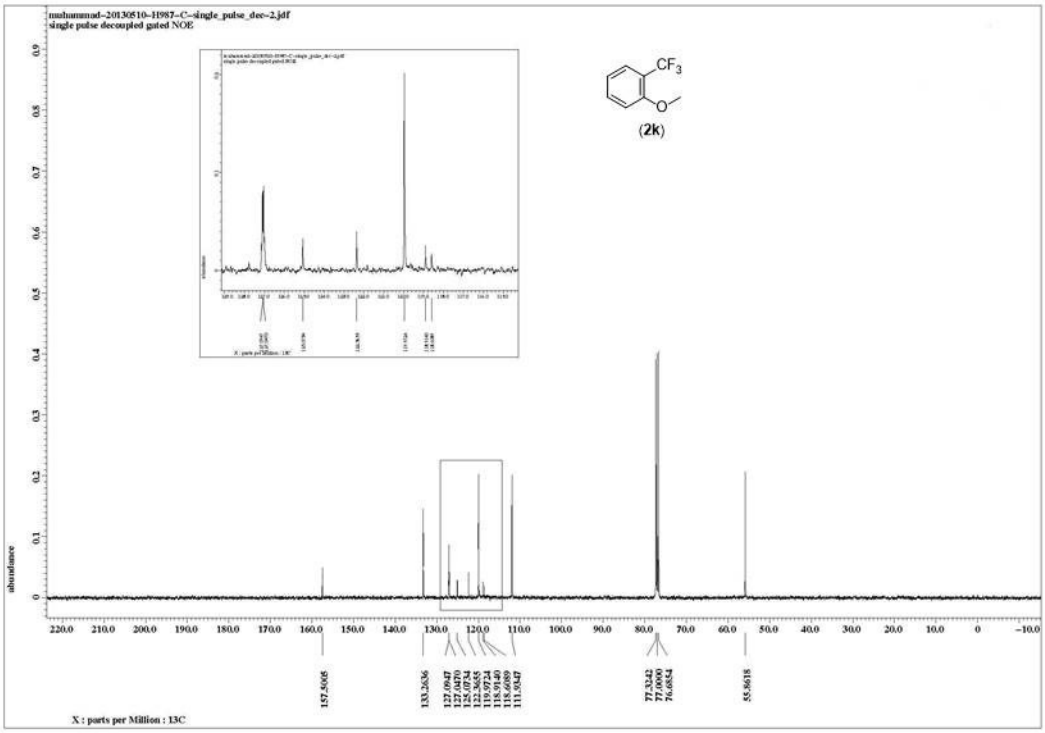
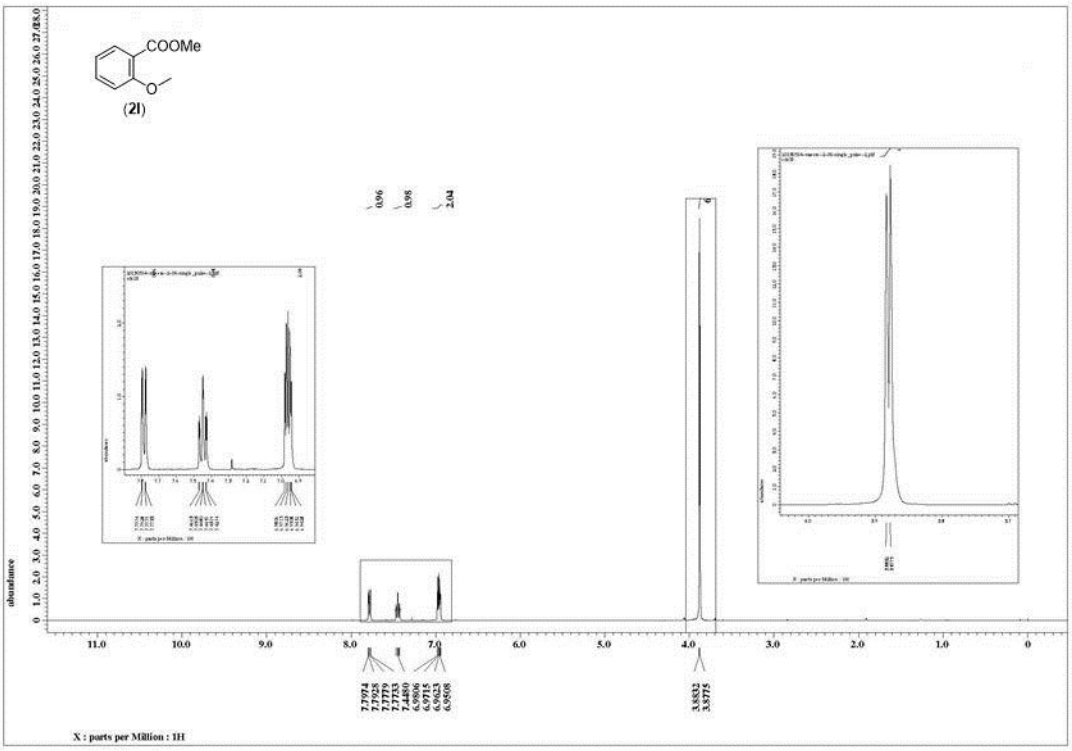
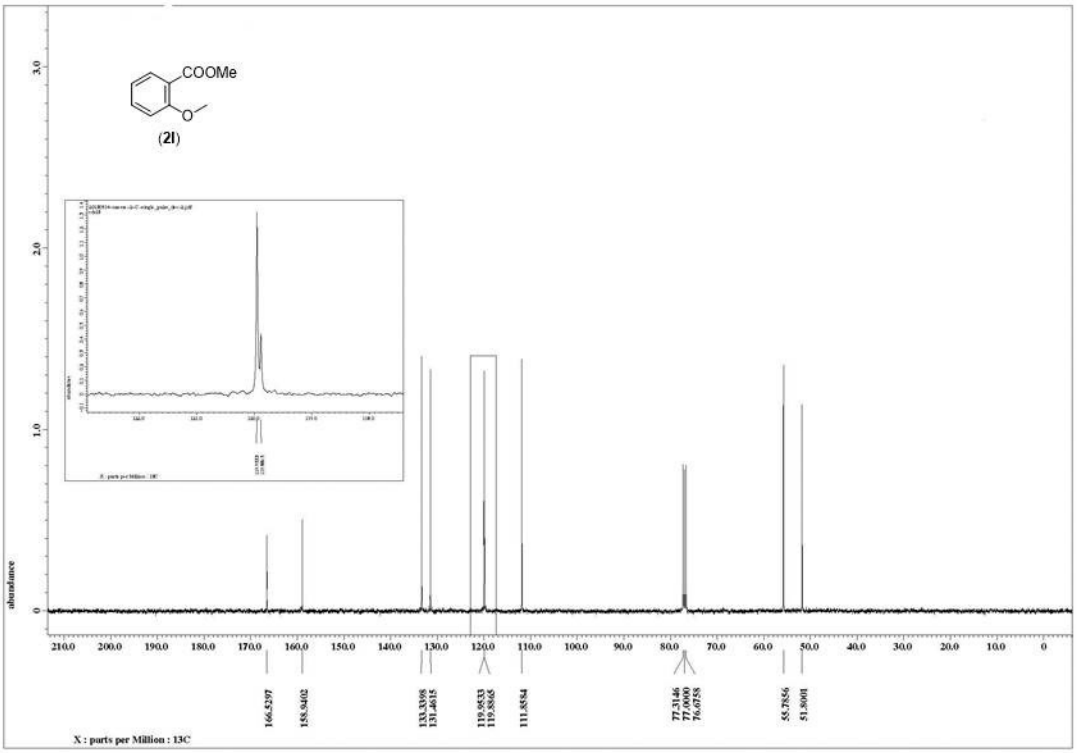
single_pulse
CF3
O
(2k)
abundance
1.96
1.93
3
7.5717
7.5453
7.4904
7.0173
7.0115
7.0055
6.9895
6.9806
3.9004
0.0000
X : parts per Million : 1H


muhummad-20130510-H987-C-single_pulse_dec-2.jdf
single pulse decoupled gated NOE
CF3
O
(2k)
abundance
157.5605
133.2636
127.0947
127.0470
125.0734
122.3653
119.9574
118.9140
118.6089
111.5547
77.3242
77.0000
76.6654
55.5618
X : parts per Million : 13C


COOMe
(2l)
0.96
0.98
2.04
7.7924
7.7935
7.7779
7.7733
7.4810
6.9806
6.9715
6.9623
6.9508
3.8832
3.8775
X : parts per Million : 1H


COOMe
(2l)
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158.8402
133.3398
131.4615
119.9833
119.8868
111.8584
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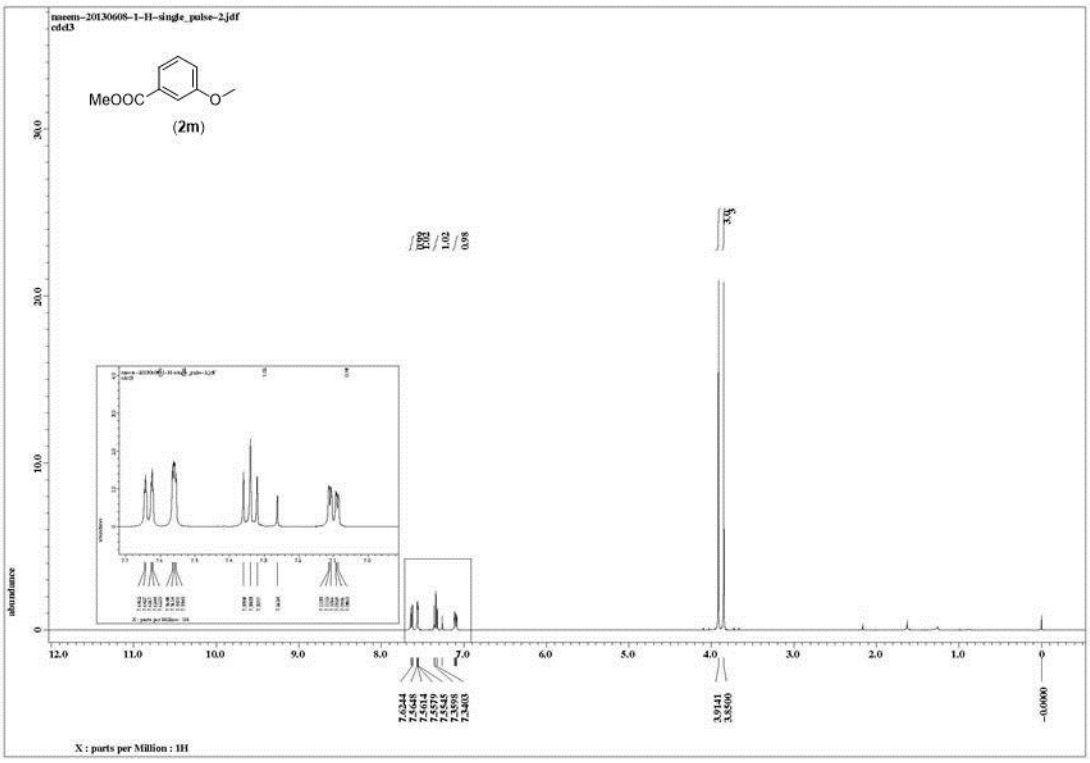
77.0980
76.6758
55.7856
51.8001
X : parts per Million : 13C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MeOOC
O
(2m)
abundance
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.6244
7.5648
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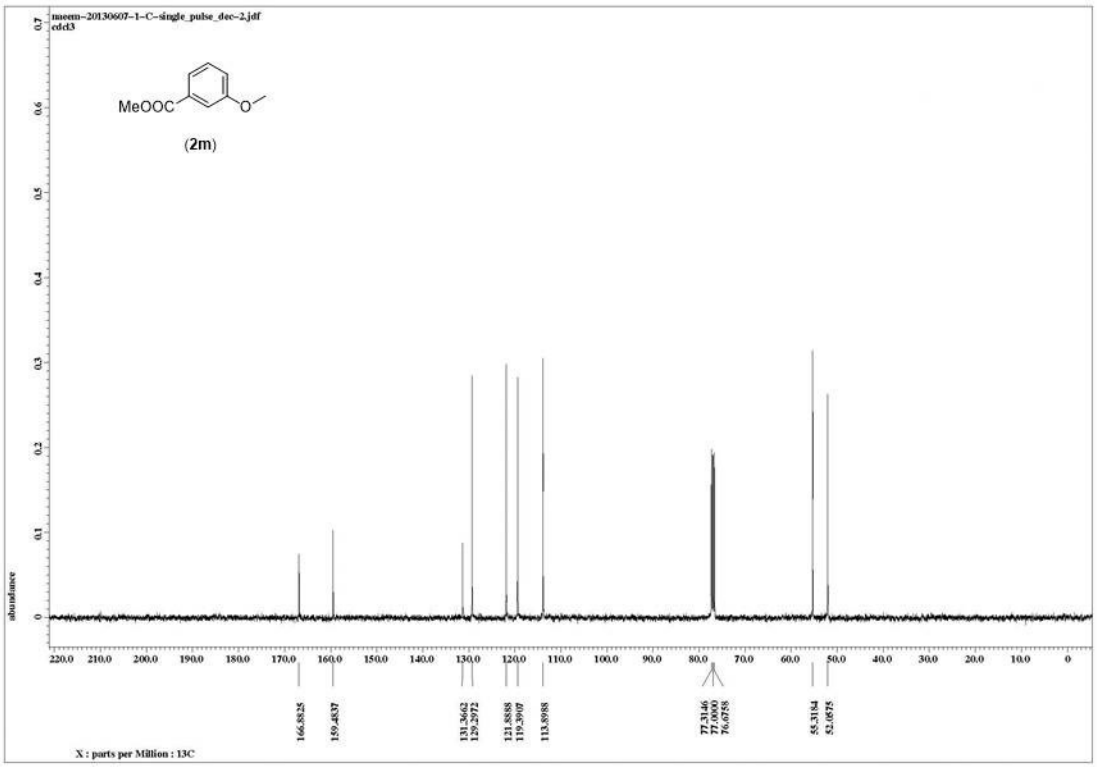
7.5545
7.3598
7.3403
3.9141
3.8500
-0.0000
X : parts per Million : 1H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MeOOC
O
(2m)
abundance
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180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
166.8825
159.4837
131.3662
129.3972
121.8888
119.3907
113.8988
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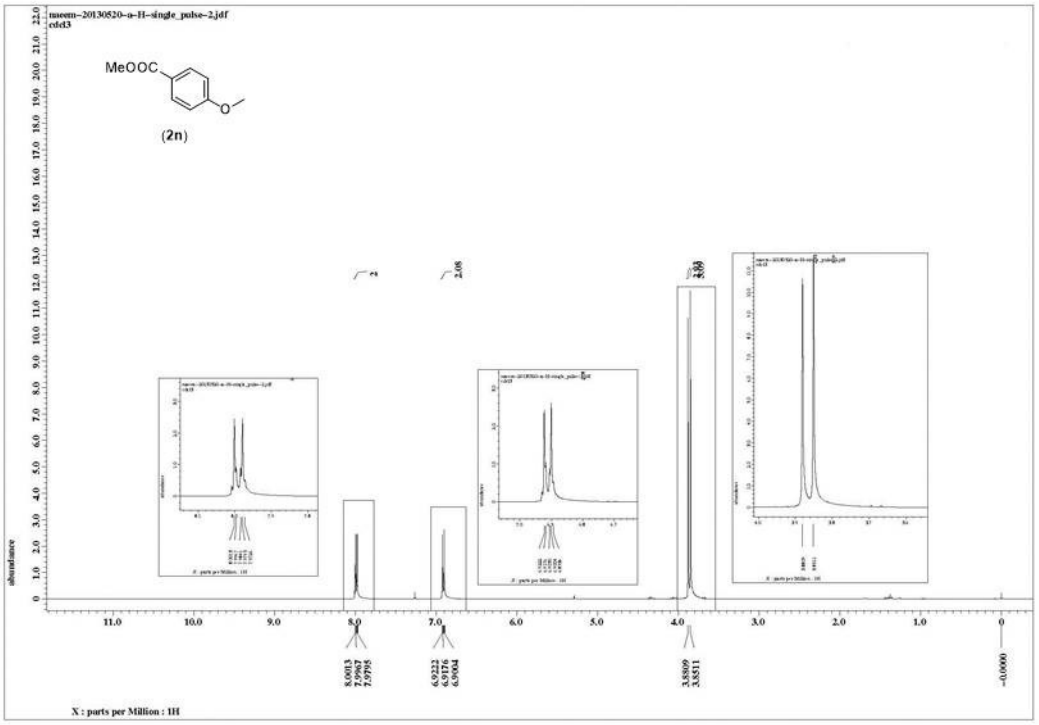
77.0000
76.6858
55.3184
52.0575
X : parts per Million : 13C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MeOOC
O
(2n)
abundance
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10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
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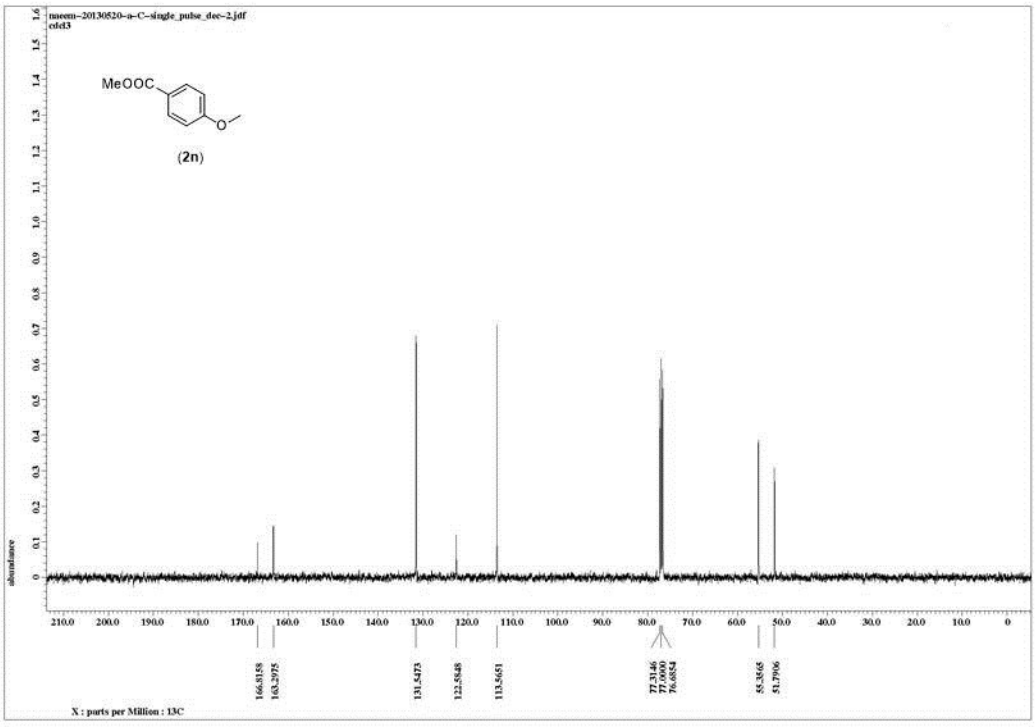
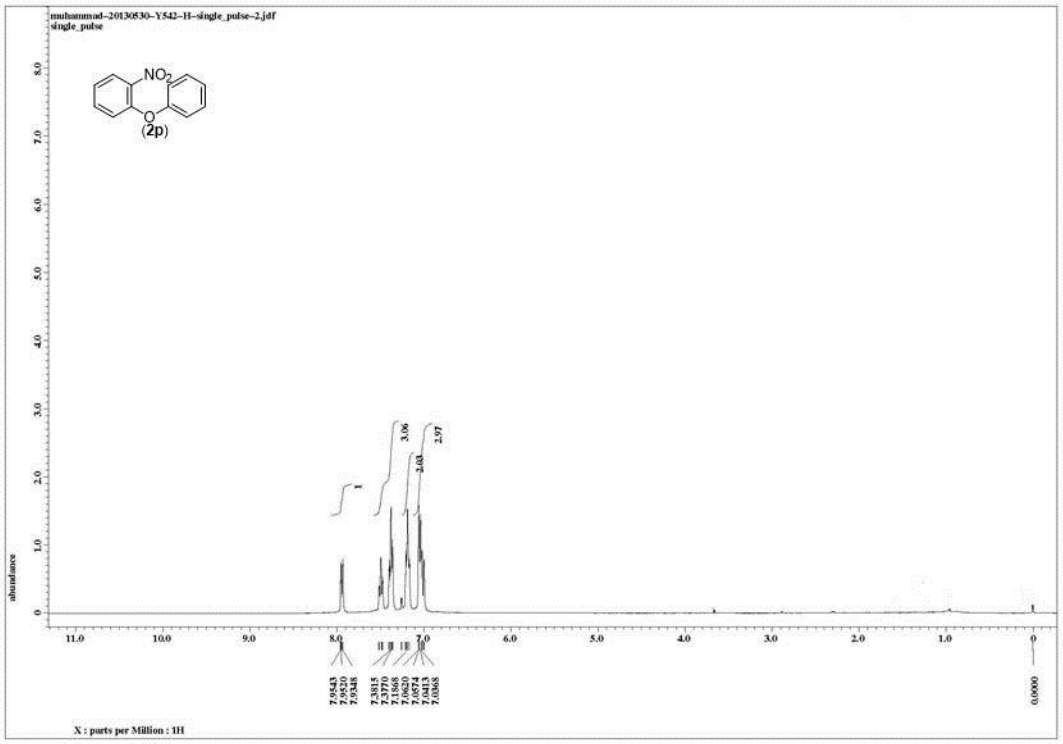
3.8511
0.0000
X : parts per Million : 1H


MeOOC
O
(2n)
abundance
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
166.8158
163.2975
131.5473
122.5848
113.5651
77.3146
77.0000
76.6854
55.3565
51.7906
X : parts per Million : 13C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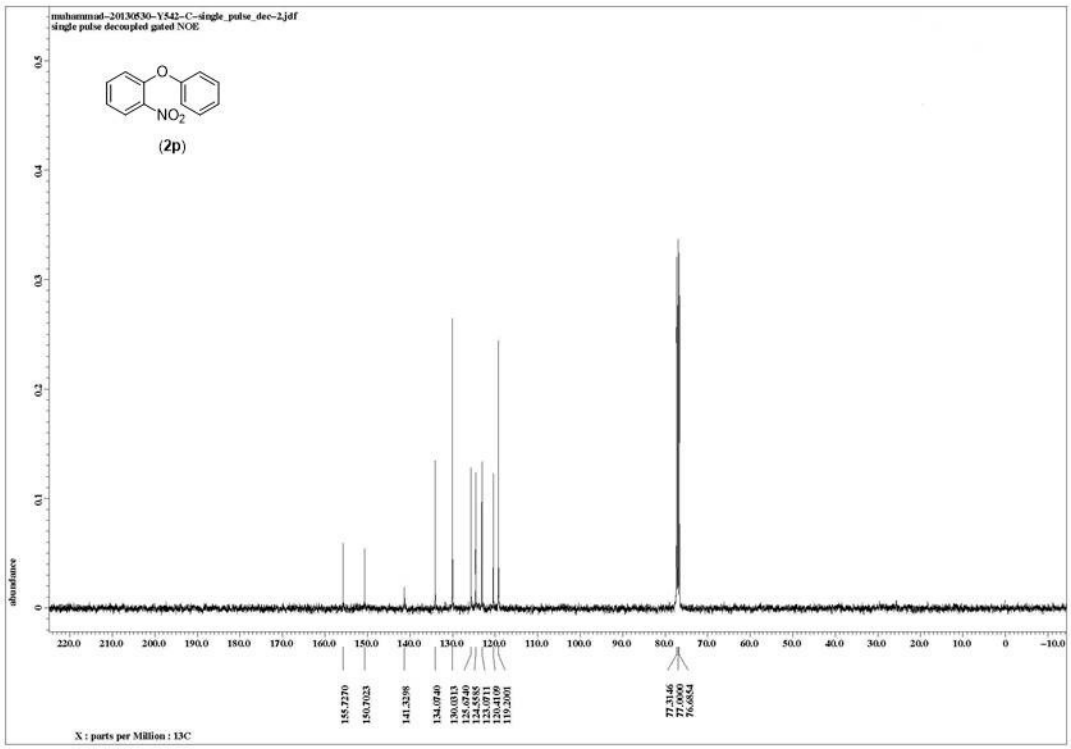
single_pulse
(2p)
abundance
3.06
2.97
2.03
1
7.9543
7.9520
7.9348
7.3815
7.3770
7.1868
7.1650
7.0574
7.0413
7.0368
0.0000
X : parts per Million : 1H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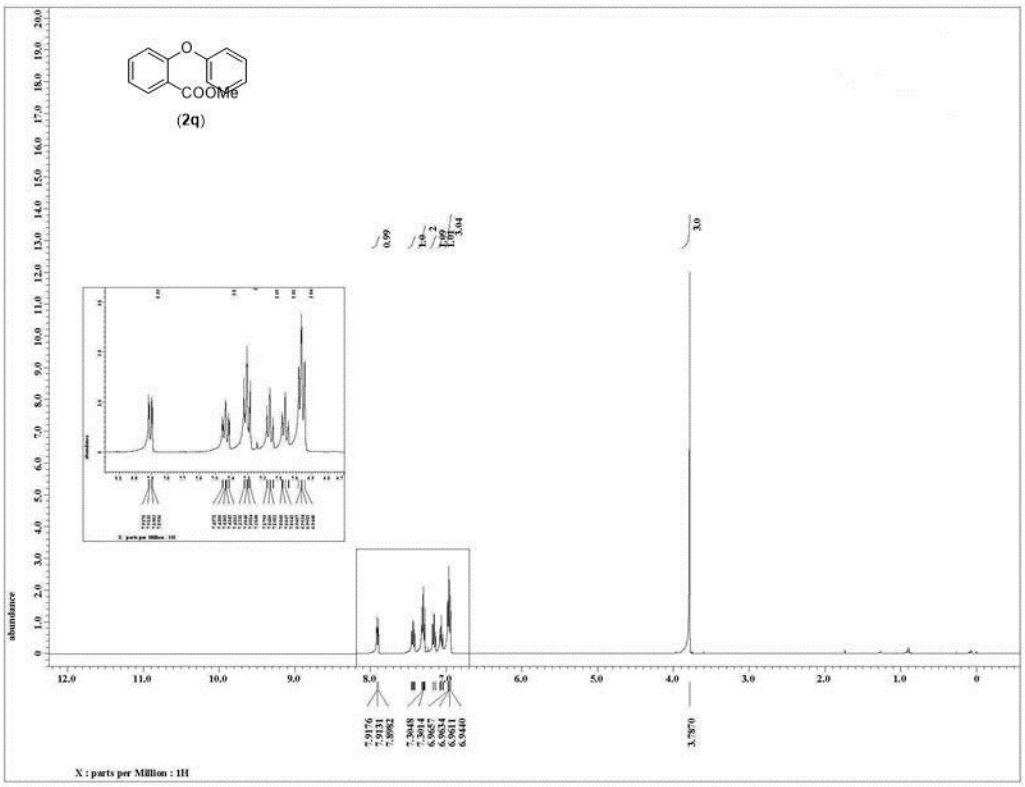
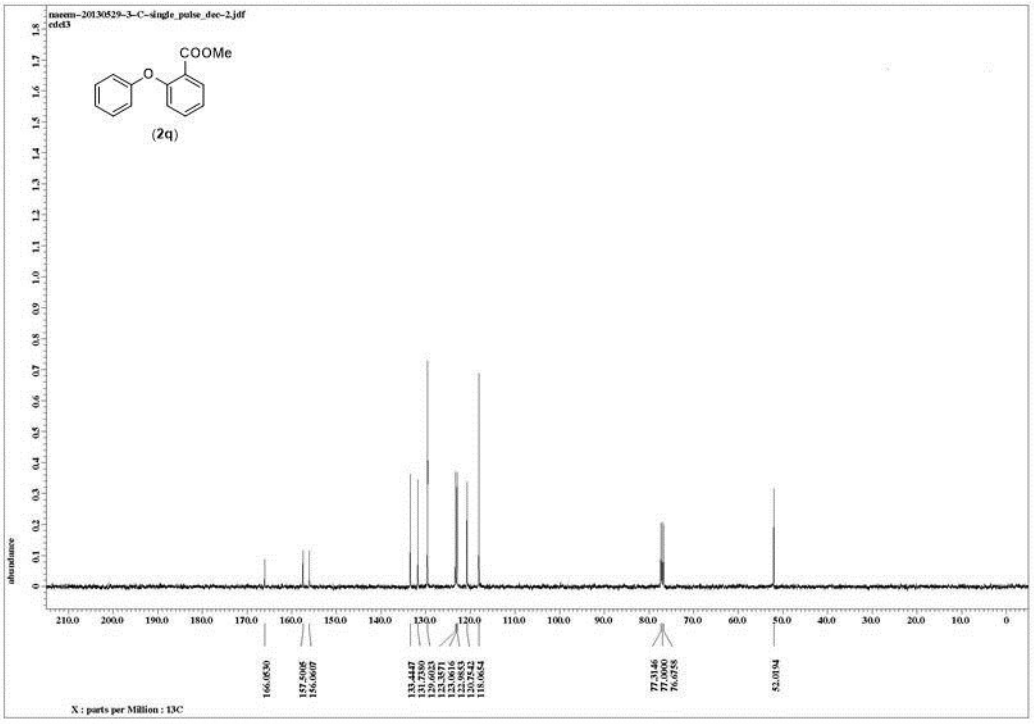
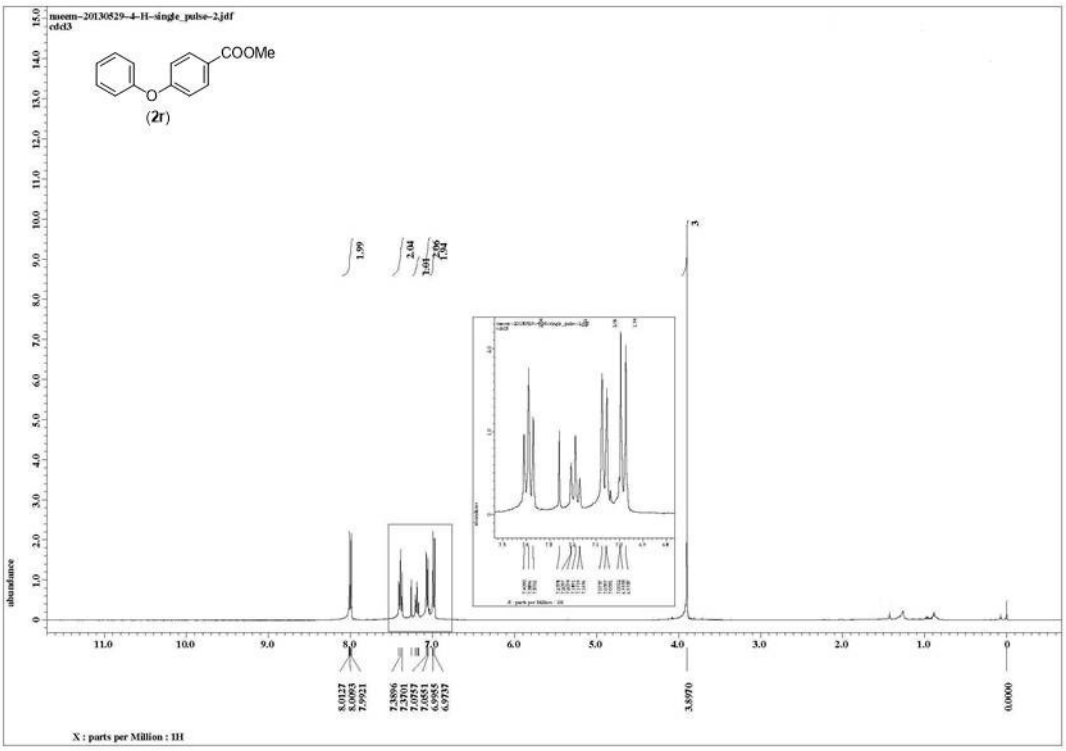
single pulse decoupled gated NOE
(2p)
abundance
155.7270
150.7023
141.3298
134.0740
130.0313
125.6340
124.5456
123.0911
120.4109
119.2001
77.3146
77.0000
76.6854
X : parts per Million : 13C


COOMe
(2q)
abundance
X : parts per Million : 1H


COOMe
(2q)
abundance
X : parts per Million : 13C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cdcl3
COOMe
O
(2r)
1.99
2.04
3.01
2.00
1.04
3.
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.0127
8.0093
7.9921
7.3896
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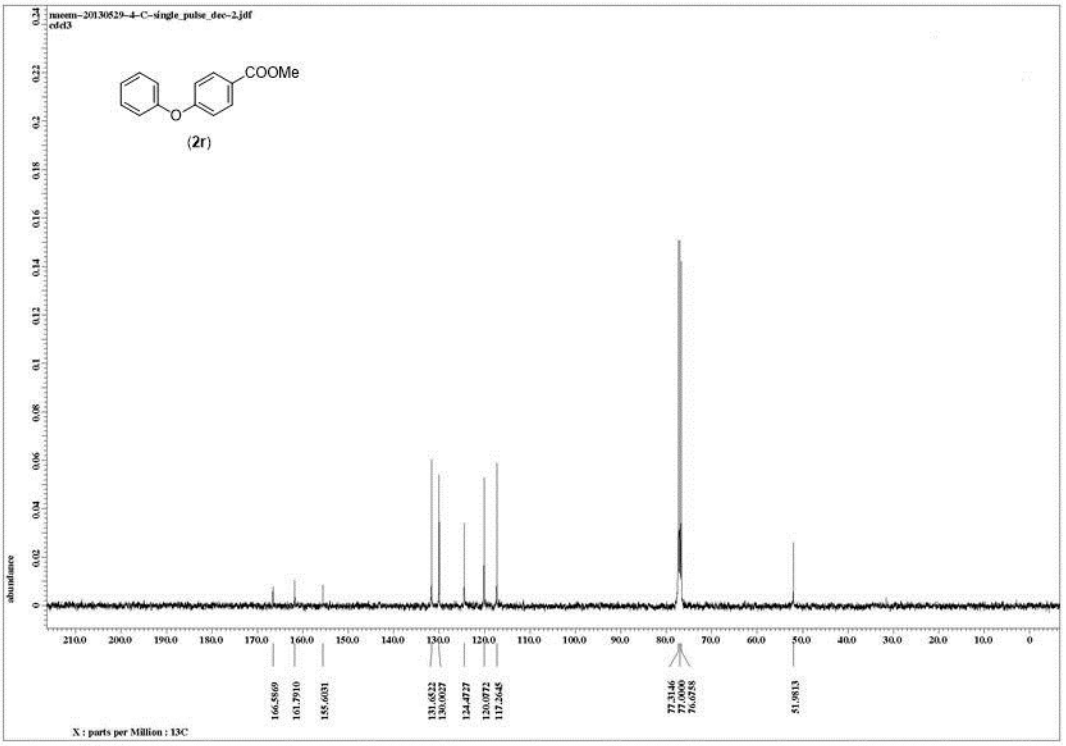
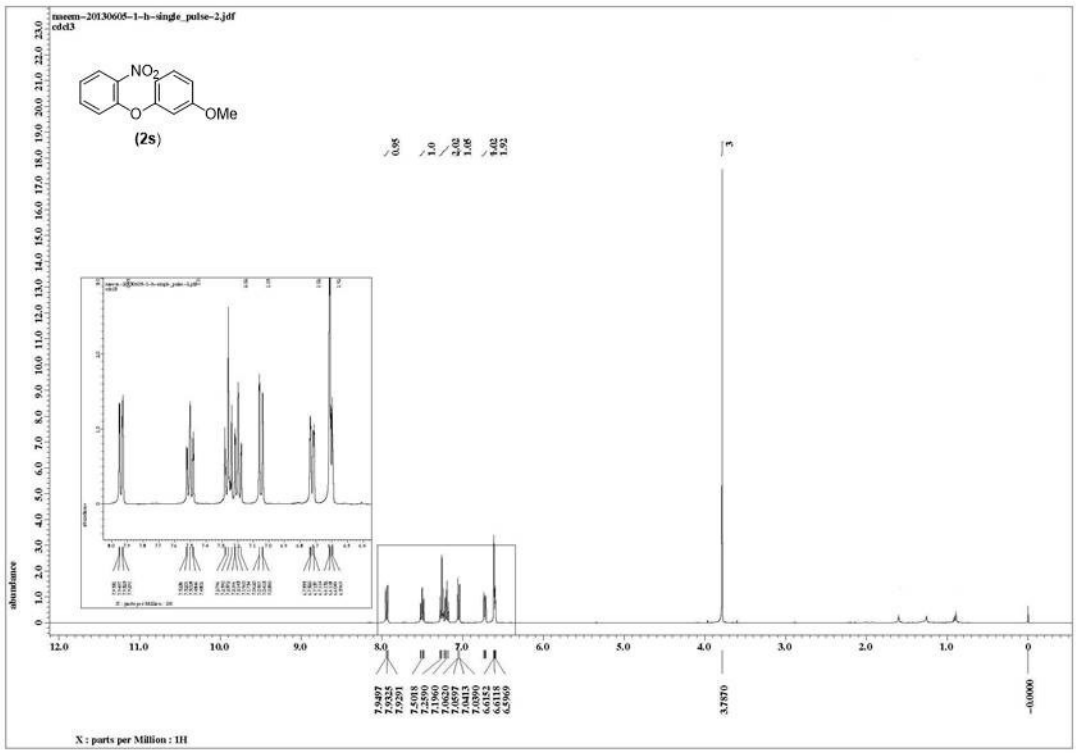
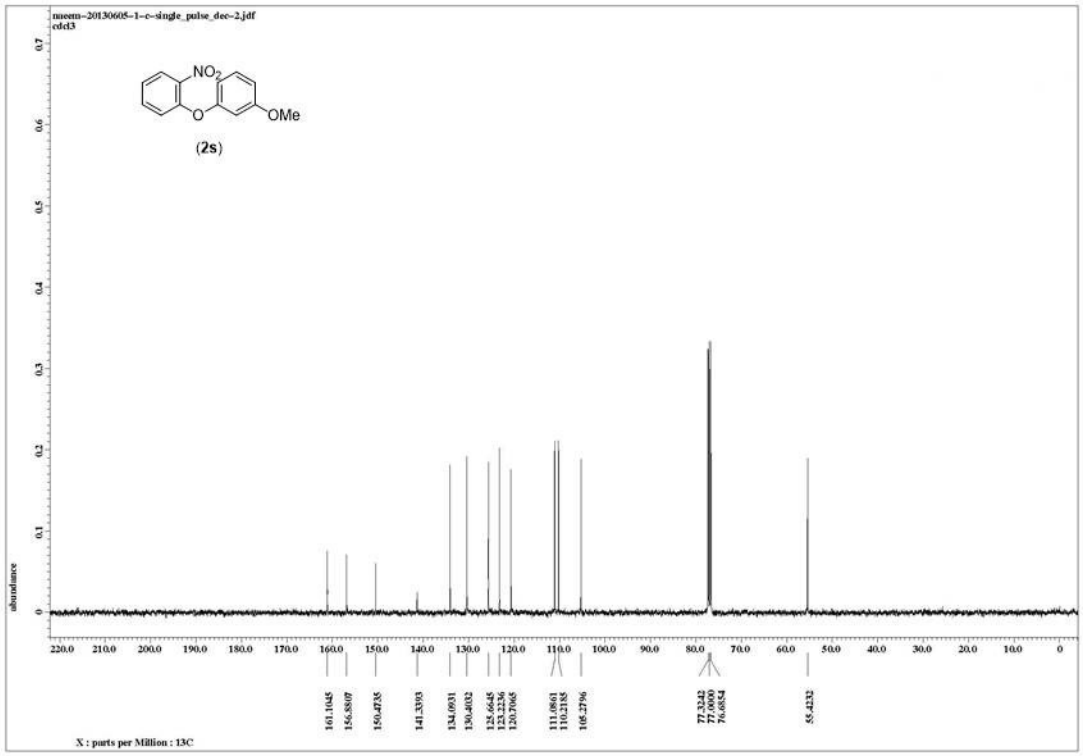
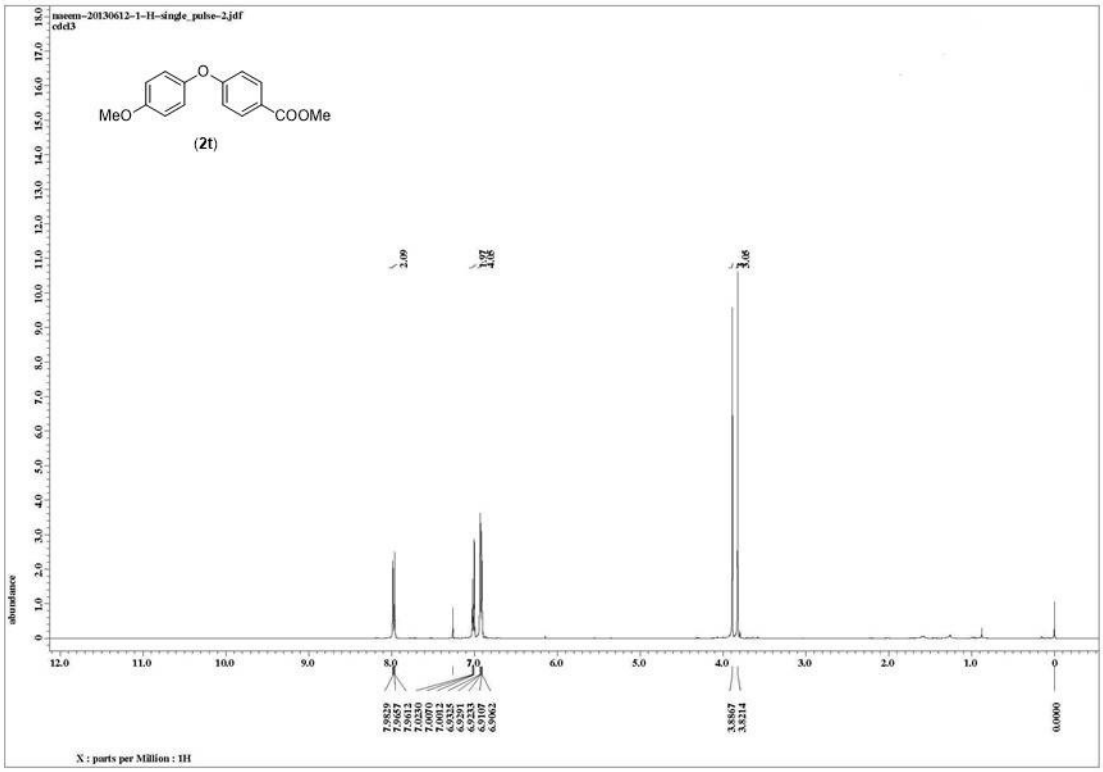
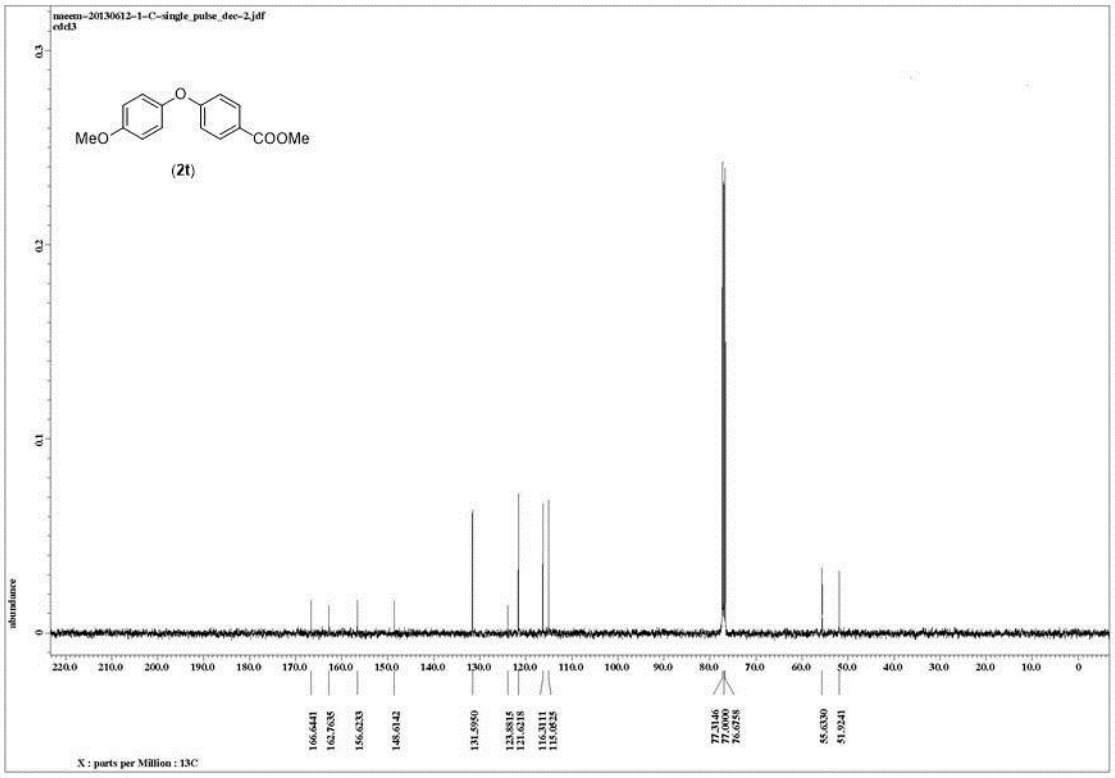
7.0957
7.0851
6.9955
6.9737
3.8970
0.0000
X : parts per Million : 1H

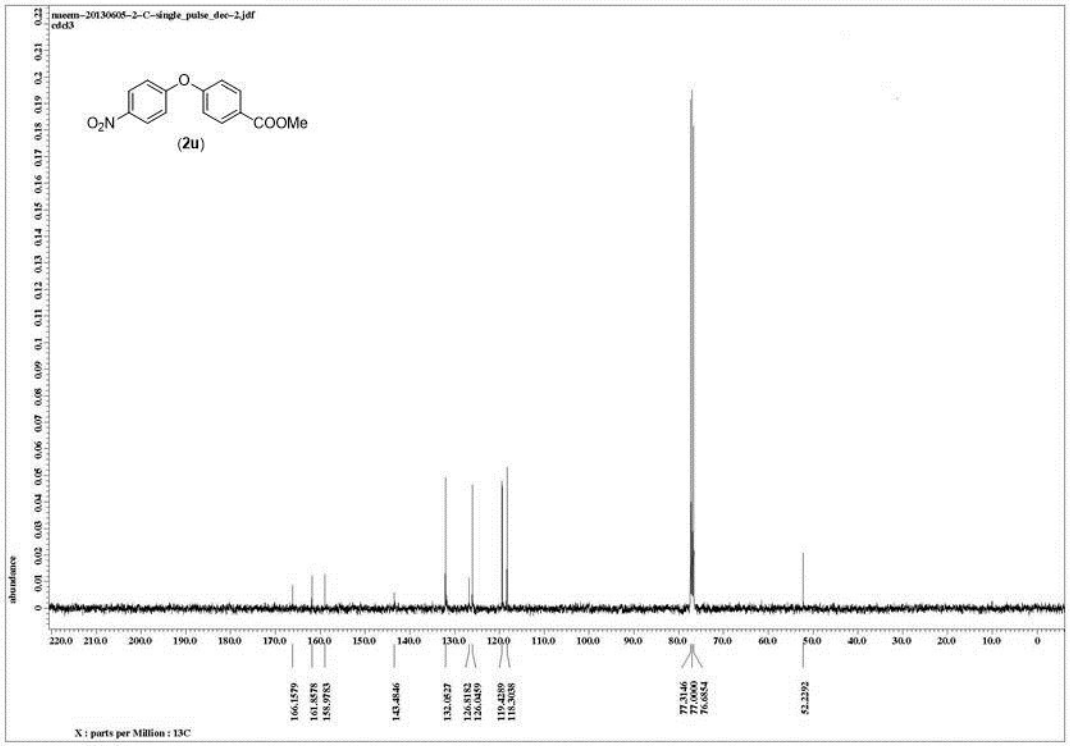

meem-20130529-4-C-single_pulse_dec-2.jdf
cdcl3
COOMe
O
(2r)
abundance
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
166.5869
161.7910
155.6031
131.6522
130.0027
124.4727
120.0772
117.2645
77.3146
77.0990
76.6758
51.9813
X : parts per Million : 13C

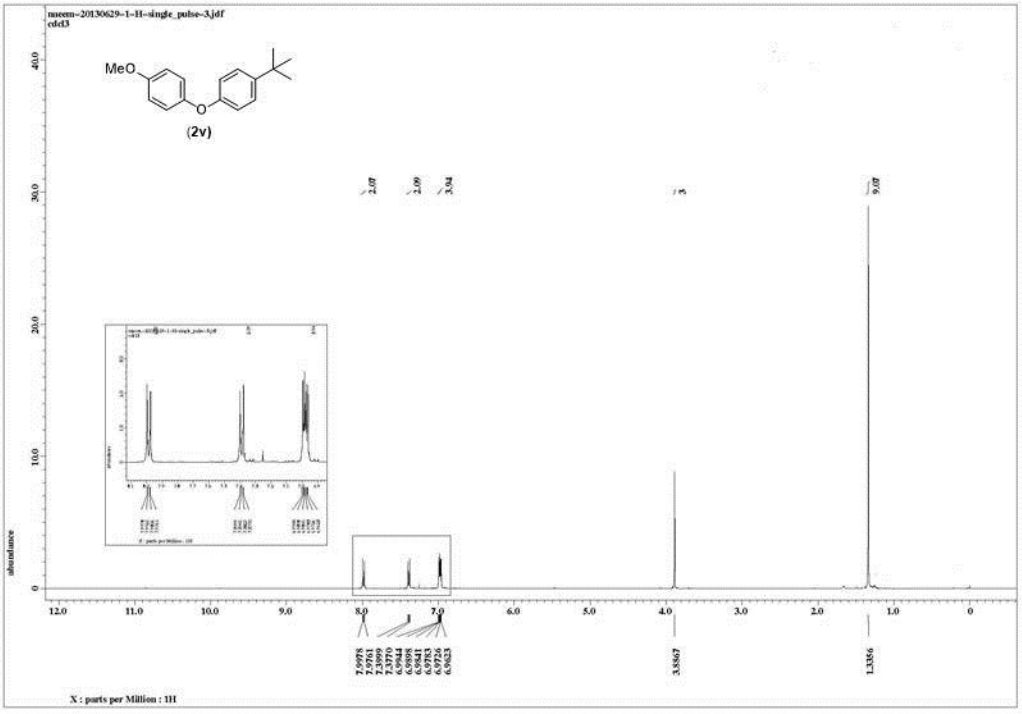

meem-20130605-1-h-single_pulse-2.jdf
cdcl3
NO2
OMe
(2s)
0.95
1.0
2.02
1.08
9.02
1.92
3
abundance
7.9407
7.9325
7.9291
7.5018
7.2590
7.1960
7.0620
7.0497
7.0413
7.0380
6.6152
6.6118
6.5969
3.7870
0.0000
X : parts per Million : 1H

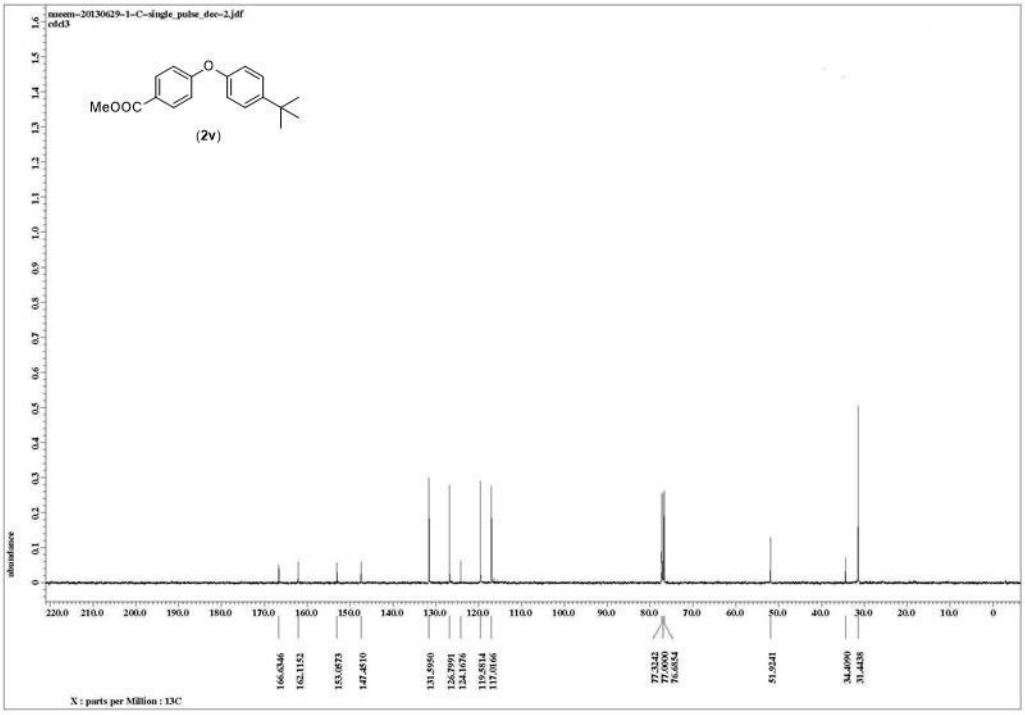

meem-20130605-1-c-single_pulse_dec-2.jdf
cdcl3
NO2
OMe
(2s)
abundance
161.1045
156.8807
150.4735
141.3393
134.0931
130.4032
125.6645
123.2236
120.7065
111.0861
110.2185
105.2796
77.3242
77.0000
76.6854
55.4232
X : parts per Million : 13C


neem-20130612-1-H-single_pulse-2.jdf
cdcl3
MeO
COOMe
(2t)
abundance
X : parts per Million : 1H

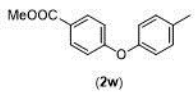

neem-20130612-1-C-single_pulse_dec-2.jdf
cdcl3
MeO
COOMe
(2t)
abundance
X : parts per Million : 13C

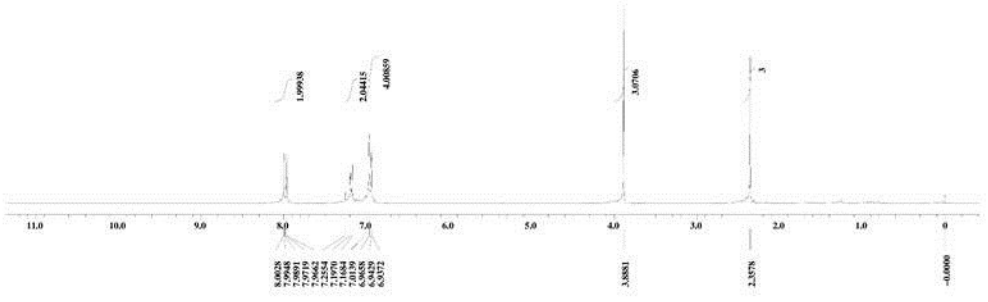

meem-20130605-2-C-single_pulse_dec-2.jdf
cdcl3
O2N
COOMe
(2u)
abundance
X : parts per Million : 13C
166.1579
161.8578
158.9783
143.4846
132.0527
126.8182
126.3459
119.4289
118.3038
77.3146
77.0000
76.6854
52.2292


meem-20130629-1-H-single_pulse-3.jdf
cdcl3
MeO
(2v)
abundance
X : parts per Million : 1H
2.07
2.09
3.04
3
9.07
7.9978
7.9761
7.3990
7.3770
6.9944
6.9838
6.9641
6.9783
6.9726
6.9583
3.8567
1.3356

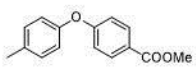


muhammade-20130621-G56-H-single_pulse-2.jdf
single_pulse

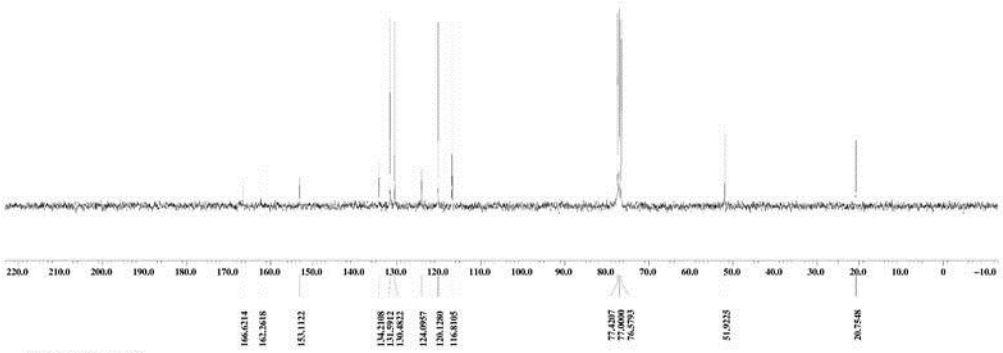




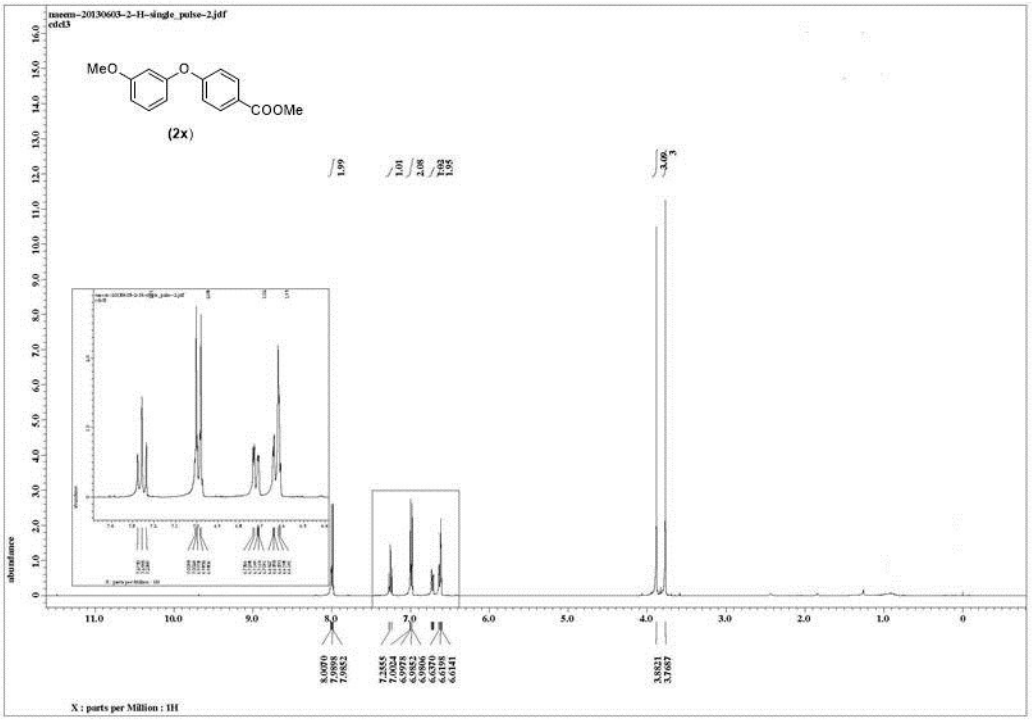
muhammade-20130621-G56-C-single_pulse_dec-2.jdf
single pulse decoupled gated NOE



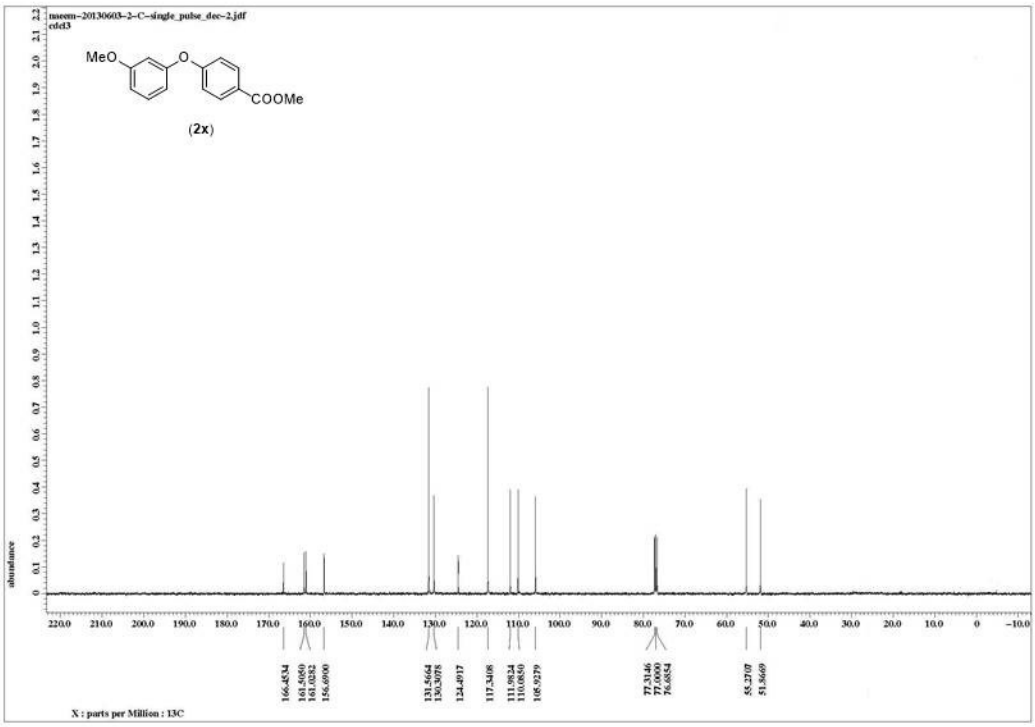
(**2w**)

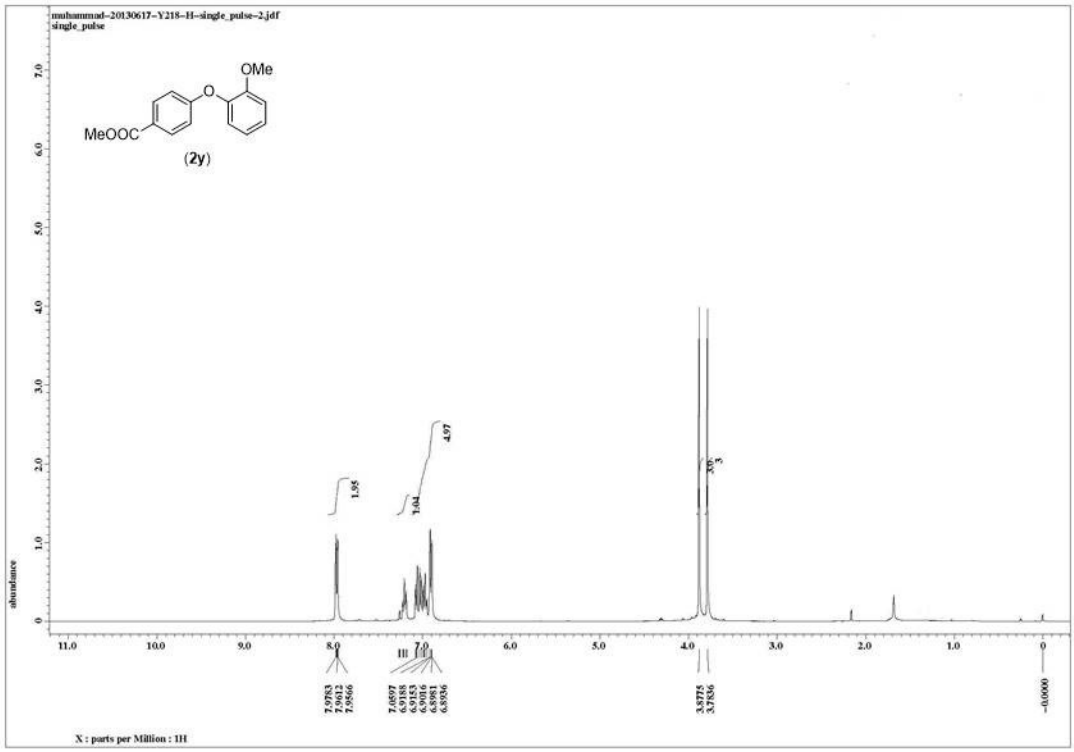


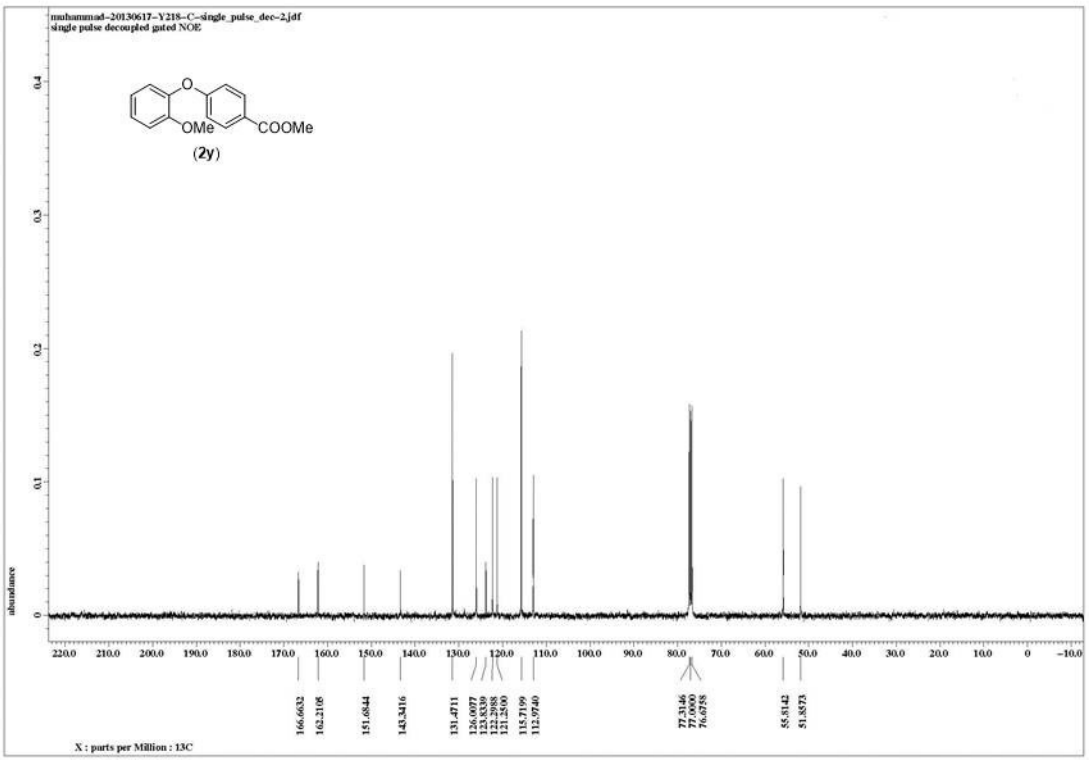
X : parts per Million : 13C

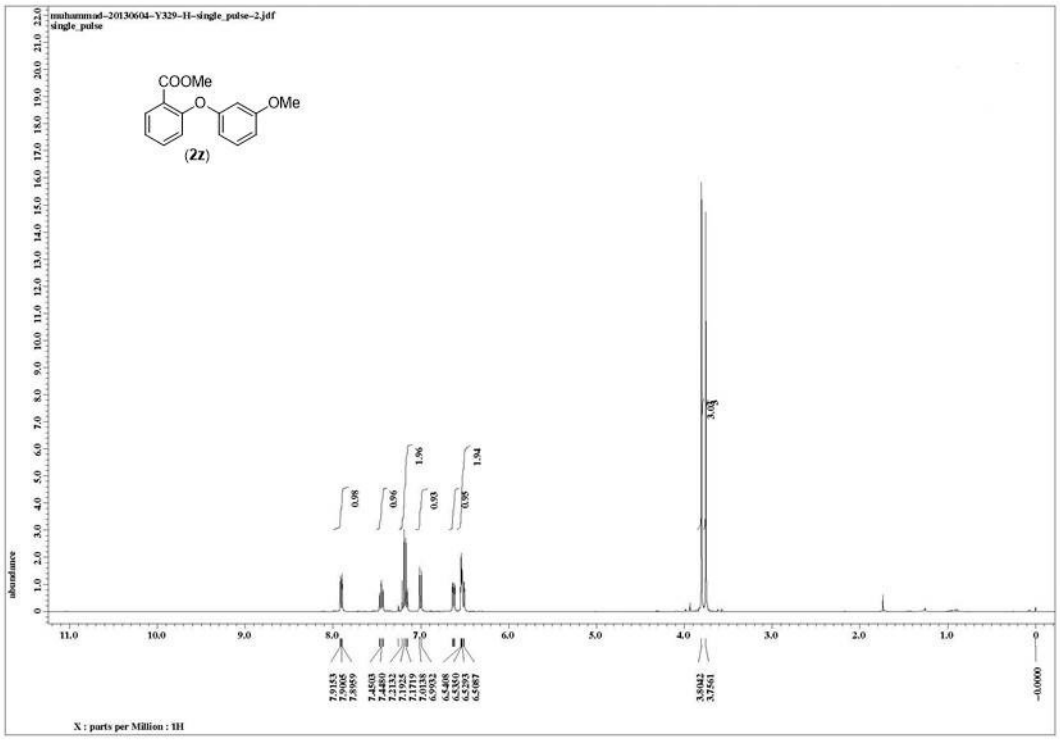


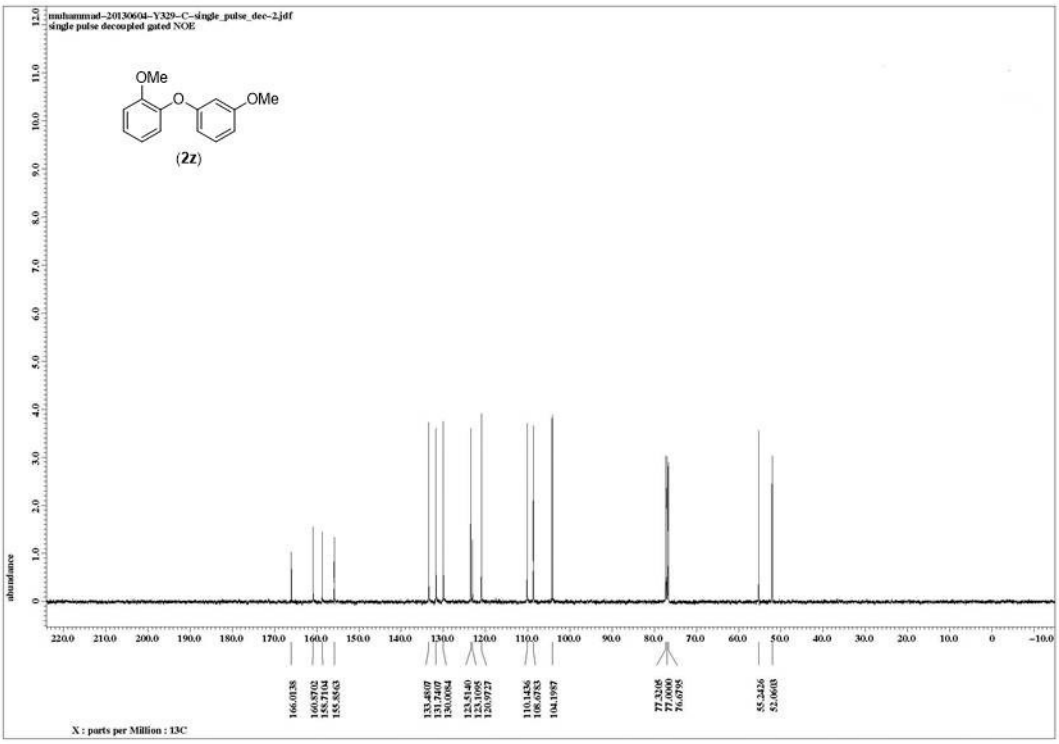
X : parts per Million : 1H


naeem-20130603-2-C-single_pulse_dec-2.jdf
cdcl3
MeO
O
COOMe
(2x)
abundance
166.4534
161.5050
161.0282
156.6900
131.5664
130.3078
124.4917
117.3408
111.9824
110.0850
105.9279
77.3146
77.1600
76.6854
55.2707
51.5669
X : parts per Million : 13C


muhammad-20130617-Y218-H-single_pulse-2.jdf
single_pulse
OMe
O
MeOOC
(2y)
abundance
1.95
1.04
4.97
3.03
3
7.9783
7.9612
7.5946
7.0697
6.9188
6.9153
6.9016
6.8951
6.8936
3.8775
3.7836
-0.0000
X : parts per Million : 1H


muhammad-20130617-Y218-C-single_pulse_dec-2.jdf
single pulse decoupled gated NOE
OMe
COOMe
(2y)
abundance
X : parts per Million : 13C
166.6632
162.2108
151.6844
143.3416
131.4711
126.0077
123.8339
122.2988
121.2600
115.7199
112.9740
77.3146
77.0000
76.6758
55.8142
51.8573


muhammad-20130604-Y329-H-single_pulse-2.jdf
single_pulse
COOMe
OMe
(2z)
abundance
X : parts per Million : 1H
0.98
0.96
1.96
0.93
0.98
1.94
3.03
7.9153
7.9005
7.8959
7.4503
7.4480
7.2133
7.1925
7.1719
7.0138
6.9932
6.5408
6.5380
6.5293
6.5087
3.8042
3.7561
-0.0000



Cartesian coordinates

$Si(OMe)_4$

Charge 0

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
O	-1.38557300	0.00000000	0.88343600
C	-1.87881600	1.12877200	1.59649300
H	-1.97914300	1.99972500	0.93912000
H	-1.21654200	1.38923400	2.43200300
H	-2.86255700	0.86820600	1.99824800
Si	0.00000000	0.00000000	0.00000000
O	0.00000000	1.38557300	-0.88343600

O	1.38557300	0.00000000	0.88343600
O	0.00000000	-1.38557300	-0.88343600
C	1.12877200	1.87881600	-1.59649300
H	1.38923400	1.21654200	-2.43200300
H	0.86820600	2.86255700	-1.99824800
H	1.99972500	1.97914300	-0.93912000
C	-1.12877200	-1.87881600	-1.59649300
H	-0.86820600	-2.86255700	-1.99824800
H	-1.99972500	-1.97914300	-0.93912000
H	-1.38923400	-1.21654200	-2.43200300
C	1.87881600	-1.12877200	1.59649300
H	2.86255700	-0.86820600	1.99824800
H	1.21654200	-1.38923400	2.43200300
H	1.97914300	-1.99972500	0.93912000

Sum of electronic and zero-point Energies= -750.008391

Sum of electronic and thermal Energies= -749.994373

Sum of electronic and thermal Enthalpies= -749.993429

Sum of electronic and thermal Free Energies= -750.050540

1

Charge -2

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
O	-1.70133100	0.87978600	-0.82064900
C	-2.10760100	2.14626100	-0.42609800
H	-3.21669200	2.19476700	-0.37775300
H	-1.79724800	2.92702500	-1.15219100
H	-1.70779900	2.43406500	0.55466100
Si	-0.42777500	-0.09246800	-0.11559600
O	-0.84105500	-0.85957800	1.36826300

O	-1.13634000	-1.46766000	-1.00518200
O	0.19584600	1.31228500	0.84020000
C	-0.11049800	-0.70669300	2.55437200
H	-0.31397700	0.25447200	3.05828400
H	-0.40756800	-1.51831400	3.24976200
H	0.96723500	-0.77933900	2.36689400
C	1.05194200	2.27854900	0.32925200
H	0.51715200	3.08608500	-0.22457400
H	1.58337200	2.78797800	1.16112900
H	1.81218700	1.87255200	-0.35115300
C	-2.41670100	-1.91234400	-0.75606300
H	-3.18860700	-1.12394100	-0.87869800
H	-2.68270300	-2.72635800	-1.46711700
H	-2.54643300	-2.32725900	0.26423500
C	2.29662900	-0.53565400	-0.55579200
O	0.98103200	-0.24572700	-1.03121800
O	2.37811900	-1.17688000	0.52042200
O	3.20964300	-0.11821300	-1.30422900

Sum of electronic and zero-point Energies= -1013.735129

Sum of electronic and thermal Energies= -1013.718315

Sum of electronic and thermal Enthalpies= -1013.717371

Sum of electronic and thermal Free Energies= -1013.779963

2

Charge 0

Spin multiplicity 2

Atom	Coordinates		
Type	X	Y	Z
C	2.33398000	0.00001300	-0.00787300
O	1.66922100	-1.09078000	-0.01000100
O	1.66921400	1.09080000	-0.00999700

Cu	0.00000000	-0.00000800	-0.00902900
C	-2.33397900	-0.00002500	-0.00783400
O	-1.66922300	-1.09081500	-0.00996100
O	-1.66921100	1.09076500	-0.00996900
C	-3.83457100	0.00002300	0.02812500
H	-4.22567000	-0.89976100	-0.45157200
H	-4.16231500	0.00162100	1.07453100
H	-4.22559500	0.89848000	-0.45413700
C	3.83457000	0.00001200	0.02815500
H	4.16223900	-0.00018800	1.07459000
H	4.22566300	-0.89903600	-0.45293800
H	4.22566600	0.89922400	-0.45262100

Sum of electronic and zero-point Energies= -654.272395

Sum of electronic and thermal Energies= -654.261269

Sum of electronic and thermal Enthalpies= -654.260325

Sum of electronic and thermal Free Energies= -654.312745

3

Charge -1

Spin multiplicity 2

Atom	Coordinates		
Type	X	Y	Z
O	2.34672100	0.05896400	-0.32988800
C	2.79923300	0.30531000	-1.62710300
H	2.45433200	-0.46104900	-2.34074700
H	3.90221100	0.29691900	-1.63357700
H	2.46982900	1.28791700	-2.00361300
Si	0.66811400	-0.00852300	0.05402100
O	0.40047200	-1.29094400	-0.99818600
O	0.89958300	-0.32491900	1.68930300
O	0.41438600	1.57507300	-0.44649000

C	-0.64986200	-2.22026200	-1.08510000
H	-0.30085300	-3.06394600	-1.69916000
H	-0.94156000	-2.61277200	-0.10180400
H	-1.53868200	-1.79054300	-1.56147300
C	-0.64680800	2.46739600	-0.21815000
H	-0.30228100	3.47478600	-0.49570200
H	-1.52617700	2.22290800	-0.82496000
H	-0.95182000	2.49039400	0.83668600
C	2.16495500	-0.43980300	2.29412500
H	2.75973700	0.47846600	2.19929100
H	2.00478700	-0.64370700	3.36342900
H	2.76021000	-1.25840800	1.86800400
C	-2.44092200	-0.03705700	0.20314900
O	-1.25960500	-0.11903000	0.66649200
O	-3.46793300	-0.18702300	0.95481400
O	-2.77148700	0.19348700	-1.00656900

Sum of electronic and zero-point Energies= -1013.792368

Sum of electronic and thermal Energies= -1013.774835

Sum of electronic and thermal Enthalpies= -1013.773891

Sum of electronic and thermal Free Energies= -1013.839648

4

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
C	2.76070200	-0.16017200	-0.00023700
O	2.73851500	-1.39279300	-0.00102900
O	1.74406500	0.64852300	0.00050800
Cu	-0.00019400	-0.00042100	0.00041300
C	-2.76042600	0.16040000	-0.00023000

O	-1.74452800	-0.64922300	0.00054400
O	-2.73699400	1.39299900	-0.00102200
C	-4.10578300	-0.58427100	-0.00008800
H	-4.17509100	-1.23385000	-0.88077700
H	-4.17542400	-1.23295300	0.88123500
H	-4.93819200	0.12448100	-0.00061200
C	4.10534800	0.58581000	-0.00007000
H	4.17438500	1.23448400	0.88130600
H	4.93844100	-0.12214000	-0.00067300
H	4.17400700	1.23553200	-0.88070400

Sum of electronic and zero-point Energies= -654.357108

Sum of electronic and thermal Energies= -654.345325

Sum of electronic and thermal Enthalpies= -654.344381

Sum of electronic and thermal Free Energies= -654.398942

5

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
O	1.57525000	0.51265700	-0.84176900
C	1.58095800	0.42695300	-2.23871900
H	2.53327400	0.83052500	-2.61962400
H	0.76282100	1.00652100	-2.69413500
H	1.49302500	-0.61428400	-2.58988800
Si	0.21787500	0.00328800	0.07621800
O	0.88178000	0.39024100	1.57427700
O	0.33546900	-1.61436000	-0.40252400
C	-0.50773500	-2.65013900	0.04314800
H	-1.53352200	-2.54498000	-0.33464700
H	-0.09789400	-3.60284900	-0.32503600

H	-0.56728000	-2.70089000	1.13886400
C	2.23157100	0.73265800	1.77721100
H	2.51211500	1.64975300	1.24320900
H	2.38046300	0.89422700	2.85543300
H	2.92001600	-0.05969200	1.44949600
C	-1.96705700	0.68310600	0.03190400
O	-0.91575300	1.05588500	-0.76520600
O	-1.45358100	-0.19160700	0.88717100
O	-3.10812600	1.08970500	-0.06094800

Sum of electronic and zero-point Energies= -898.771087

Sum of electronic and thermal Energies= -898.757648

Sum of electronic and thermal Enthalpies= -898.756704

Sum of electronic and thermal Free Energies= -898.811624

6

Charge 0

Spin multiplicity 2

Atom	Coordinates		
Type	X	Y	Z
Cu	-0.46738300	0.00073500	0.15822000
C	1.85464100	-0.00068300	-0.08425800
O	1.19515700	1.09054900	-0.01870500
O	1.19440200	-1.09123300	-0.01718800
C	3.35177400	-0.00075800	-0.20294100
H	3.78542600	0.01974400	0.80399500
H	3.69364000	-0.90834800	-0.70486400
H	3.69013400	0.88940700	-0.73770400
O	-2.21206900	0.00060100	0.42313500
C	-3.26103800	-0.00122700	-0.51190500
H	-2.92419700	0.00103500	-1.55815200
H	-3.89405200	0.88307300	-0.34632600

H	-3.88901500	-0.88955400	-0.34862500

Sum of electronic and zero-point Energies= -540.892254

Sum of electronic and thermal Energies= -540.883354

Sum of electronic and thermal Enthalpies= -540.882410

Sum of electronic and thermal Free Energies= -540.929621

7

Charge -2

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
O	1.90494400	0.13781900	-0.12461100
C	2.70599800	-0.78232600	0.28486600
Si	-0.08694400	0.30234500	-0.16109600
O	0.11974400	0.29950800	1.52351200
O	0.18801500	1.84105600	-0.86485400
O	0.08914200	-1.00096900	-1.23406800
C	-0.94569200	0.43151000	2.43653400
H	-0.52252500	0.36290700	3.45524200
H	-1.45202700	1.40735000	2.35058900
H	-1.69562100	-0.35354600	2.29548500
C	-0.98150400	-1.60405900	-1.92213700
H	-0.56040000	-2.40451000	-2.55755800
H	-1.71384800	-2.03256400	-1.23034600
H	-1.50943700	-0.89591100	-2.58092200
C	1.31285500	2.64344700	-0.71404900
H	2.16012200	2.32391600	-1.34370000
H	1.04660500	3.67820400	-1.00625800
H	1.68612100	2.67577500	0.32210100
C	-2.92537600	-0.21812600	0.06793900
O	-1.78291800	0.54735900	-0.27475200

O	-4.01265200	0.32165100	-0.22436200
O	-2.72243200	-1.33620400	0.62304100
C	4.18399800	-0.41988200	-0.03292500
H	4.42330800	0.58299600	0.34319200
H	4.86690000	-1.15330600	0.41043600
H	4.33562200	-0.39837700	-1.12041900
O	2.47249700	-1.85136300	0.85060900

Sum of electronic and zero-point Energies= -1127.109758

Sum of electronic and thermal Energies= -1127.090647

Sum of electronic and thermal Enthalpies= -1127.089703

Sum of electronic and thermal Free Energies= -1127.159148

8

Charge -2

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
O	-1.91965100	0.21703200	0.00018300
C	-2.67960500	-0.86071000	0.00030700
Si	-0.12356200	0.31883900	-0.00001300
O	-0.09492300	-0.43187100	-1.49291200
O	-0.12334000	1.99990200	-0.00032700
O	-0.09459700	-0.43136000	1.49313300
C	0.94603500	-0.55590600	-2.43033000
H	0.49906400	-0.87133100	-3.38343400
H	1.47557300	0.39196100	-2.59785100
H	1.67755000	-1.31338700	-2.12623400
C	0.94653900	-0.55501700	2.43040800
H	0.49972900	-0.86996500	3.38374400
H	1.67794100	-1.31269500	2.12652800
H	1.47617200	0.39289100	2.59738300

C	-1.26025900	2.82531100	-0.00032600
H	-1.89205700	2.67034500	0.88503300
H	-0.91468800	3.86933300	-0.00026200
H	-1.89196500	2.67043800	-0.88577600
C	2.83534400	-0.18531200	-0.00011100
O	1.79644600	0.55807900	-0.00027400
O	4.01177300	0.31362000	-0.00004500
O	2.85935200	-1.45694700	-0.00001800
C	-4.16377900	-0.48559100	-0.00013400
H	-4.39799500	0.12107500	-0.88266600
H	-4.77954100	-1.38807400	0.00074000
H	-4.39814000	0.12298800	0.88103200
O	-2.31598600	-2.02395100	0.00064200

Sum of electronic and zero-point Energies= -1127.152703

Sum of electronic and thermal Energies= -1127.133306

Sum of electronic and thermal Enthalpies= -1127.132361

Sum of electronic and thermal Free Energies= -1127.203341

9

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	-0.66519800	-0.41420000	-0.00000200
C	2.02979700	0.30228800	0.00000400
O	1.78444600	1.51107200	-0.00005600
O	1.18379700	-0.68085400	0.00008600
C	3.49187200	-0.18071800	-0.00000100
H	3.68145700	-0.80550900	0.88126700
H	3.68143100	-0.80563500	-0.88118700
H	4.17876600	0.67011700	-0.00007600

O	-2.48572900	-0.37377400	-0.00013700
C	-3.17155000	0.83038400	0.00007800
H	-2.97141900	1.46962000	0.88705400
H	-4.26919000	0.64985300	-0.00014400
H	-2.97112900	1.47008900	-0.88649100

Sum of electronic and zero-point Energies= -540.977690

Sum of electronic and thermal Energies= -540.967728

Sum of electronic and thermal Enthalpies= -540.966784

Sum of electronic and thermal Free Energies= -541.016457

10

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
O	1.41183900	0.15985400	-0.28256500
C	2.18979800	-0.84964400	0.07380100
Si	-0.34043700	0.31887300	0.00792800
O	-0.13088100	0.35332400	1.67016000
O	-0.45403700	1.82947700	-0.71368800
C	-1.18265500	0.44249300	2.60522700
H	-0.73427500	0.55737100	3.60200600
H	-1.83932800	1.30332000	2.41859700
H	-1.80913300	-0.45797500	2.60555400
C	0.62772600	2.67294100	-1.02392500
H	1.27154000	2.25126500	-1.80737000
H	0.21895200	3.62726500	-1.38543700
H	1.26254300	2.88086500	-0.15036900
C	-2.04934200	-0.94631000	-0.77449500
O	-2.16634100	0.10880400	0.03283600
O	-2.91531300	-1.65492500	-1.23831400

O	-0.69931800	-1.07277900	-0.98179900
C	3.61705500	-0.65080500	-0.43423500
H	4.01718300	0.30409400	-0.07475200
H	4.25362800	-1.47137900	-0.09584300
H	3.61900300	-0.61068000	-1.52965100
O	1.86536500	-1.83130800	0.71687300

Sum of electronic and zero-point Energies= -1012.130267

Sum of electronic and thermal Energies= -1012.114781

Sum of electronic and thermal Enthalpies= -1012.113836

Sum of electronic and thermal Free Energies= -1012.174800

11

Charge 0

Spin multiplicity 2

Atom	Coordinates		
Type	X	Y	Z
Cu	-0.00000400	0.00002200	0.00005100
O	-1.66042500	-0.54964800	-0.00000500
O	1.66044400	0.54963700	-0.00000200
C	2.82930600	-0.23275500	-0.00007500
H	2.64015000	-1.31490400	0.00002900
H	3.43140100	0.01766100	0.88603100
H	3.43123000	0.01754600	-0.88632800
C	-2.82931000	0.23269700	-0.00007500
H	-3.43133600	-0.01777900	-0.88620100
H	-3.43128600	-0.01756000	0.88615000
H	-2.64016300	1.31484500	-0.00020400

Sum of electronic and zero-point Energies= -427.517844

Sum of electronic and thermal Energies= -427.509708

Sum of electronic and thermal Enthalpies= -427.508764

Sum of electronic and thermal Free Energies= -427.553182

$TS_{(b)}$

Charge -1

Spin multiplicity 2

Atom	Coordinates		
Type	X	Y	Z
O	-2.47318200	-0.47730900	0.26344300
C	-2.66765300	-1.12096500	1.45743600
H	-2.05173600	-2.03964300	1.48398800
H	-3.72546200	-1.39636300	1.62960900
H	-2.30531400	-0.50326600	2.29946800
Si	-0.27941800	0.10227300	-0.24569700
O	-0.28559400	-1.56588000	-0.15597400
O	-0.97148400	0.74494700	-1.61642000
O	-0.60855100	0.97438700	1.13845100
C	0.73370300	-2.38929400	-0.70061400
H	0.31486700	-3.39709600	-0.82491900
H	1.07618000	-2.03340900	-1.68030500
H	1.59339300	-2.43010000	-0.02528900
C	0.34148500	1.82508400	1.76225700
H	-0.13961600	2.26075100	2.64846200
H	1.22999000	1.26161900	2.06350700
H	0.65117600	2.64477000	1.09952000
C	-2.23416600	1.34823600	-1.74741100
H	-2.53209400	1.89042900	-0.84068400
H	-2.18438600	2.06301400	-2.58172500
H	-3.01440800	0.60725900	-1.96208600
C	2.48450500	0.12180100	-0.01864100
O	1.31324400	0.49811700	-0.67183200
O	3.54472500	0.38218400	-0.61178600
O	2.36234400	-0.44006700	1.10562400

Sum of electronic and zero-point Energies= -1013.564610

Sum of electronic and thermal Energies= -1013.547222

Sum of electronic and thermal Enthalpies= -1013.546277

Sum of electronic and thermal Free Energies= -1013.611529

$TS_{(f)}$

Charge -1

Spin multiplicity 2

Atom	Coordinates		
Type	X	Y	Z
O	1.80610600	1.50083300	0.27146500
C	1.58750100	2.69912600	0.90362500
Si	-0.04492300	0.17043200	-0.14919600
O	-0.37792200	1.56245200	-0.98240100
O	1.16281600	-0.71329700	-0.94677700
O	0.06685100	0.23249200	1.51110000
C	-1.49389800	1.71673100	-1.84994700
H	-1.45344400	2.73676100	-2.25238300
H	-1.45154500	1.01071900	-2.68928900
H	-2.42965700	1.56999600	-1.30243800
C	-0.71796300	-0.55233900	2.40205600
H	-0.25377900	-0.48259100	3.39390700
H	-1.74351400	-0.17733500	2.44188700
H	-0.74783200	-1.60743500	2.10288200
C	2.34998600	-1.25711900	-0.64958900
C	-2.62338900	-0.81543000	-0.07141000
O	-1.28307700	-0.92084500	-0.48285000
O	-3.32374300	-1.81733000	-0.27547800
O	-2.96627700	0.27452300	0.46077400
O	3.12199000	-1.58760100	-1.52595700
C	2.64141400	-1.48516100	0.82306400

H	2.60857300	-0.53369900	1.35853700
H	1.87821200	-2.13682900	1.26319200
H	3.62409600	-1.95051700	0.92334700
H	1.07470800	2.52024700	1.86722800
H	2.51912300	3.26363800	1.08397200
H	0.88811400	3.31632400	0.31210700

Sum of electronic and zero-point Energies= -1127.113687

Sum of electronic and thermal Energies= -1127.094583

Sum of electronic and thermal Enthalpies= -1127.093639

Sum of electronic and thermal Free Energies= -1127.163196

2-iodonitrobenzene

Charge 0

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
C	2.01939600	-2.31599100	0.05321500
C	0.67696600	-1.93820000	0.04489600
C	0.31014100	-0.58682700	0.04424000
C	1.33112200	0.37458600	0.03096700
C	2.67704600	-0.00243600	0.01192400
C	3.02463000	-1.34792300	0.03557400
H	2.27383400	-3.37184000	0.06573200
H	-0.09677700	-2.69735300	0.03665600
H	3.42810100	0.77786200	-0.01670300
H	4.07105300	-1.63623500	0.03612400
I	-1.76006000	-0.17255900	-0.05266000
N	1.07527600	1.82755000	0.04881400
O	0.08378100	2.22955600	0.64886300
O	1.89674800	2.54308200	-0.52354100

Sum of electronic and zero-point Energies= -447.419645

Sum of electronic and thermal Energies= -447.411221

Sum of electronic and thermal Enthalpies= -447.410277

Sum of electronic and thermal Free Energies= -447.455488

Int1

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	-0.66519800	-0.41420000	-0.00000200
C	2.02979700	0.30228800	0.00000400
O	1.78444600	1.51107200	-0.00005600
O	1.18379700	-0.68085400	0.00008600
C	3.49187200	-0.18071800	-0.00000100
H	3.68145700	-0.80550900	0.88126700
H	3.68143100	-0.80563500	-0.88118700
H	4.17876600	0.67011700	-0.00007600
O	-2.48572900	-0.37377400	-0.00013700
C	-3.17155000	0.83038400	0.00007800
H	-2.97141900	1.46962000	0.88705400
H	-4.26919000	0.64985300	-0.00014400
H	-2.97112900	1.47008900	-0.88649100

Sum of electronic and zero-point Energies= -540.977690

Sum of electronic and thermal Energies= -540.967728

Sum of electronic and thermal Enthalpies= -540.966784

Sum of electronic and thermal Free Energies= -541.016456

Int2

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z

Cu	-0.66519800	-0.41420000	-0.00000200
C	2.02979700	0.30228800	0.00000400
O	1.78444600	1.51107200	-0.00005600
O	1.18379700	-0.68085400	0.00008600
C	3.49187200	-0.18071800	-0.00000100
H	3.68145700	-0.80550900	0.88126700
H	3.68143100	-0.80563500	-0.88118700
H	4.17876600	0.67011700	-0.00007600
O	-2.48572900	-0.37377400	-0.00013700
C	-3.17155000	0.83038400	0.00007800
H	-2.97141900	1.46962000	0.88705400
H	-4.26919000	0.64985300	-0.00014400
H	-2.97112900	1.47008900	-0.88649100

Sum of electronic and zero-point Energies= -540.977690

Sum of electronic and thermal Energies= -540.967728

Sum of electronic and thermal Enthalpies= -540.966784

Sum of electronic and thermal Free Energies= -541.016456

Int3

Charge 0

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	-1.29739500	-0.02721300	-0.10379400
O	-3.00874400	-0.51488700	-0.20773300
C	-4.04287600	0.25497900	0.33954300
H	-3.98012700	0.36249600	1.43867900
H	-5.00864400	-0.23496100	0.12493400
H	-4.10582200	1.27580200	-0.08096700
O	0.56076500	0.38053800	-0.05486600
C	1.51279700	-0.42188200	0.01706000

H	1.35019800	-1.50501100	0.06397100
N	2.79792200	-0.04683900	0.04370200
C	3.87038300	-1.02889500	0.13303100
H	4.53125600	-0.95131400	-0.73799500
H	4.46386500	-0.86316700	1.03952100
H	3.44993300	-2.03668400	0.16698300
C	3.17685900	1.36227500	-0.01181600
H	3.81230500	1.54278900	-0.88609400
H	2.27440400	1.96780600	-0.08345400
H	3.73248300	1.63522100	0.89243000

Sum of electronic and zero-point Energies= -560.872269

Sum of electronic and thermal Energies= -560.860443

Sum of electronic and thermal Enthalpies= -560.859499

Sum of electronic and thermal Free Energies= -560.912900

Int1-TS_{OA}

Charge -1

Spin multiplicity 1

Atom Type	Coordinates X	Y	Z
Cu	0.22054000	1.69127100	0.15910100
C	1.02979700	-1.02105400	2.83851500
C	0.14697100	-0.30572000	2.04699900
C	0.30533400	-0.25862600	0.63759200
C	1.37411700	-0.99946100	0.08292800
C	2.25020600	-1.74314200	0.88898400
C	2.08803900	-1.75280000	2.26364200
H	0.89422400	-1.02040300	3.91821800
H	-0.67902100	0.24484800	2.48301400
H	3.04439800	-2.29376800	0.39887400

H	2.77033600	-2.32082400	2.88995800
I	-1.90835700	-1.12047500	-0.40899400
O	-1.34243700	2.21768200	0.95539000
N	1.58107000	-1.03659700	-1.35068300
O	0.88012200	-0.30945900	-2.06145200
O	2.44178400	-1.81214200	-1.80262300
O	1.86708100	2.30706300	-0.29385300
C	2.86275300	1.88719000	-1.15710900
H	2.53981600	1.82393800	-2.21041800
H	3.71787500	2.58782800	-1.10718800
H	3.26685700	0.89441600	-0.87998500
C	-2.44294400	2.58791500	0.18462600
H	-2.84191000	1.74354400	-0.40289800
H	-3.26055800	2.92547400	0.84827500
H	-2.23031100	3.41845600	-0.51709400

Sum of electronic and zero-point Energies= -875.009418

Sum of electronic and thermal Energies= -874.992104

Sum of electronic and thermal Enthalpies= -874.991160

Sum of electronic and thermal Free Energies= -875.057678

Int2-TS_{OA}

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	-1.03502600	-0.65314500	0.46017300
C	1.20121800	1.80464500	2.60947200
C	0.99851100	0.59585000	1.96377300
C	0.54288300	0.55744500	0.62489900
C	0.31672500	1.79471300	-0.02053200
C	0.54721200	3.01631200	0.62886100

C	0.98968400	3.02723500	1.94092800
H	1.53499000	1.80463200	3.64531900
H	1.16413100	-0.35239300	2.46319800
H	0.35732400	3.92899300	0.07644200
H	1.16389500	3.97125300	2.45000700
I	2.21901300	-0.84645700	-0.73890500
C	-3.33826000	-0.24526000	-0.20742200
O	-2.97651300	-1.45236800	-0.15160000
O	-2.52516900	0.69132100	0.09620500
C	-4.73610400	0.12809500	-0.66142800
H	-5.15338200	0.89730400	-0.00383500
H	-4.68043400	0.55251800	-1.67071600
H	-5.38663700	-0.74947500	-0.67764400
O	-0.26975100	-2.00190100	1.47338400
C	-0.30231200	-3.27437200	0.90116400
H	-1.31180600	-3.57881200	0.57262100
H	0.03381100	-4.00960500	1.65623200
H	0.38603000	-3.36511600	0.04186100
N	-0.16659300	1.83182500	-1.38520700
O	-0.48595600	0.76503400	-1.92126600
O	-0.22399300	2.92958800	-1.96151800

Sum of electronic and zero-point Energies= -988.387656

Sum of electronic and thermal Energies= -988.368432

Sum of electronic and thermal Enthalpies= -988.367488

Sum of electronic and thermal Free Energies= -988.439015

Int1-M1

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z

Cu	0.62541600	0.69223100	-0.20695400
C	-2.86717600	-0.93005400	-1.95492200
C	-1.55041700	-0.52230000	-1.74471900
C	-1.12177900	-0.05821100	-0.49208300
C	-2.07919000	-0.03591600	0.52520900
C	-3.40460600	-0.45019300	0.34371200
C	-3.80068100	-0.89842100	-0.90925100
H	-3.16921400	-1.28478900	-2.93868200
H	-0.83868900	-0.57834200	-2.56404500
H	-4.08983400	-0.40948100	1.18209900
H	-4.82439500	-1.22499900	-1.07257800
I	1.52826300	-1.73793200	0.05709600
C	2.49061500	2.58653800	0.61356200
O	2.32655400	1.42984000	-0.14315800
O	-0.22751700	2.32909500	-0.56632200
C	-0.01663400	2.76043200	-1.87646300
H	1.05313800	2.85398600	-2.13029000
H	-0.47787600	3.75844400	-1.98468600
H	-0.49474200	2.10815000	-2.63391600
N	-1.69976200	0.44395300	1.85686500
O	-0.52875500	0.78687100	2.04890700
O	-2.56668100	0.48073700	2.73685800
H	3.43644300	3.07916900	0.31686500
H	1.67837100	3.31823800	0.46150100
H	2.56050200	2.38407600	1.70069400

Sum of electronic and zero-point Energies= -875.047613

Sum of electronic and thermal Energies= -875.030053

Sum of electronic and thermal Enthalpies= -875.029108

Sum of electronic and thermal Free Energies= -875.096111

Int2-M1

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	-0.48459100	-0.47656400	0.21441200
C	2.81965600	-0.46100400	-2.35906600
C	1.51626600	-0.44989800	-1.86117000
C	1.27777100	-0.33975300	-0.48595400
C	2.38701800	-0.24501300	0.35612700
C	3.70089300	-0.24930500	-0.12563600
C	3.91685900	-0.35800900	-1.49365200
H	2.98138900	-0.54270400	-3.43195600
H	0.67522100	-0.51179900	-2.54558800
H	4.51806100	-0.17007600	0.58132400
H	4.93050200	-0.36067500	-1.88535600
I	-0.73048700	2.07132200	-0.22898700
C	-3.10140700	-1.02351300	-0.06063500
O	-2.80484700	-1.21732700	-1.24724200
O	-2.27887600	-0.66820800	0.87410700
C	-4.54312400	-1.19125900	0.42474200
H	-4.58126100	-1.91913600	1.24309700
H	-4.91159600	-0.23806600	0.82058600
H	-5.18510000	-1.52146900	-0.39578600
O	-0.00485900	-2.27195200	0.46690000
C	-0.21144800	-3.14245300	-0.60817500
H	-1.23264300	-3.09517000	-1.01071000
H	-0.03106600	-4.16589900	-0.23342000
H	0.49720400	-2.97931600	-1.44278000
N	2.19301200	-0.13808000	1.80404700

O	1.04060800	-0.07930500	2.23932400
O	3.19575400	-0.10415900	2.52580200

Sum of electronic and zero-point Energies= -988.420224

Sum of electronic and thermal Energies= -988.400676

Sum of electronic and thermal Enthalpies= -988.399731

Sum of electronic and thermal Free Energies= -988.472381

Int1-TS_{RE}

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	0.57149000	0.77621500	-0.02842600
C	-2.72962100	-0.95647900	-2.01666800
C	-1.54296700	-0.27786900	-1.79504900
C	-1.21870000	0.21054700	-0.50336700
C	-2.12862100	-0.09224400	0.53956600
C	-3.33720900	-0.76173200	0.30511700
C	-3.65121500	-1.18769200	-0.97469700
H	-2.94321700	-1.33247800	-3.01576400
H	-0.83605900	-0.14773700	-2.60811000
H	-3.99016500	-0.94619900	1.15061000
H	-4.58067200	-1.71597900	-1.16630600
I	1.66473700	-1.53393600	-0.04713600
C	3.29510100	1.78147000	0.32097700
O	1.96297100	2.01928600	0.02093800
O	-0.87549400	2.02230000	-0.47146700
C	-0.63412600	2.67060700	-1.70487100
H	0.43862400	2.82222500	-1.87611100
H	-1.12641200	3.65162500	-1.64597000

H	-1.07679300	2.12003200	-2.55092000
N	-1.79125700	0.26641700	1.88906000
O	-0.65675500	0.73319300	2.10656000
O	-2.62780700	0.09571700	2.78749800
H	3.86296000	2.73324800	0.27747000
H	3.45176900	1.37204300	1.33835900
H	3.79532600	1.08305900	-0.37837600

Sum of electronic and zero-point Energies= -875.034411

Sum of electronic and thermal Energies= -875.017383

Sum of electronic and thermal Enthalpies= -875.016438

Sum of electronic and thermal Free Energies= -875.082106

Int2-TS_{RE}

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	-0.53125400	-0.39770700	0.24309600
C	2.79078700	-0.49967800	-2.29868400
C	1.50234600	-0.67333900	-1.81111400
C	1.25171400	-0.60829000	-0.42513900
C	2.34468300	-0.34876600	0.42668900
C	3.64451400	-0.19036200	-0.06746000
C	3.87499500	-0.26937700	-1.43272400
H	2.95630400	-0.53131600	-3.37370600
H	0.67416500	-0.82384000	-2.49596500
H	4.44031300	0.00694100	0.64142300
H	4.87849600	-0.13921100	-1.82716200
I	-0.68764300	2.11972400	-0.28172200
C	-3.13045800	-1.10780100	0.00863800
O	-2.80783500	-1.37003200	-1.16239000

O	-2.33105300	-0.69131200	0.93253300
C	-4.58778700	-1.24743500	0.45569200
H	-5.17835600	-1.76036500	-0.30795700
H	-4.64591700	-1.79083600	1.40504300
H	-5.00836600	-0.24922300	0.62672000
O	0.30081000	-2.14587400	0.24266400
C	-0.07593800	-3.05205400	-0.77810600
H	-1.07184300	-2.83690000	-1.17846600
H	-0.07638300	-4.04804000	-0.31118000
H	0.65908900	-3.06348300	-1.59994200
N	2.12150700	-0.21120500	1.84599200
O	0.95031400	-0.22887700	2.25702300
O	3.09829400	-0.07822600	2.59441800

Sum of electronic and zero-point Energies= -988.412544

Sum of electronic and thermal Energies= -988.393728

Sum of electronic and thermal Enthalpies= -988.392784

Sum of electronic and thermal Free Energies= -988.463194

Int1-M2

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	0.00000000	0.93522800	0.00000000
I	0.26095900	-1.52567600	0.00000000
C	-1.31981700	3.43478100	0.00000000
O	-0.10518700	2.76810600	0.00000000
H	-1.15818700	4.53485200	0.00000000
H	-1.95611800	3.22542800	-0.88748700
H	-1.95611800	3.22542800	0.88748700

Sum of electronic and zero-point Energies= -323.980649

Sum of electronic and thermal Energies= -323.974221

Sum of electronic and thermal Enthalpies= -323.973277

Sum of electronic and thermal Free Energies= -324.013604

Int2-M2

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	-0.35147200	-0.24480500	0.00004600
I	2.08842000	0.06363100	0.00003200
C	-3.07371400	0.22199800	-0.00007700
O	-2.87365100	1.43832600	-0.00019000
O	-2.17773600	-0.71942100	-0.00072300
C	-4.51058500	-0.32356900	0.00049600
H	-4.67209200	-0.95560900	-0.88076900
H	-4.67139400	-0.95595000	0.88163300
H	-5.23319300	0.49664600	0.00088200

Sum of electronic and zero-point Energies= -437.359643

Sum of electronic and thermal Energies= -437.351371

Sum of electronic and thermal Enthalpies= -437.350426

Sum of electronic and thermal Free Energies= -437.396555

Int1-TSSig

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	2.23286900	0.50050200	-0.65203300
C	-3.02042500	1.53851400	0.49025200
C	-2.20303800	0.53082000	-0.06696500

C	-0.87830800	0.30106100	0.40825700
C	-0.47464400	1.10099500	1.52741700
C	-1.27831800	2.09233100	2.04136200
C	-2.57558300	2.32690200	1.52818600
H	-4.00808800	1.65963100	0.06212100
H	0.50732700	0.91717800	1.94949000
H	-0.90756500	2.68755400	2.87384100
H	-3.20968500	3.10261400	1.94713900
I	-0.10755100	-1.78188700	0.56426500
C	4.73681000	0.74063600	0.58847100
O	4.02076600	0.24664000	-0.49378900
O	0.39087500	0.76906100	-0.96521200
C	0.03005500	2.01314800	-1.52270000
H	-1.01573900	1.99082800	-1.86214200
H	0.66187000	2.21438800	-2.39779000
H	0.14417000	2.84604800	-0.80957200
N	-2.76726200	-0.22755200	-1.15806300
O	-2.03187700	-0.98210500	-1.80271700
O	-3.97990300	-0.08629200	-1.40889600
H	4.41111300	0.33438200	1.56912200
H	5.80938100	0.47371900	0.48988200
H	4.70682200	1.84708800	0.68650400

Sum of electronic and zero-point Energies= -875.015259

Sum of electronic and thermal Energies= -874.997707

Sum of electronic and thermal Enthalpies= -874.996763

Sum of electronic and thermal Free Energies= -875.065690

Int2-TSSig

Charge -1

Spin multiplicity 1

Atom Coordinates

Type	X	Y	Z
Cu	-1.85125800	0.25040000	0.34115000
C	3.47805700	1.57802600	-0.30577100
C	2.59649600	0.60705700	0.21600100
C	1.37893200	0.28024900	-0.44758600
C	1.15134600	0.94295700	-1.69561000
C	2.01438100	1.90119400	-2.17738600
C	3.20218000	2.23270900	-1.48649400
H	4.37627300	1.78143700	0.26445800
H	0.25517000	0.68382500	-2.24870300
H	1.77822900	2.39247700	-3.11939200
H	3.88541400	2.98015800	-1.87846900
I	0.66213300	-1.82760500	-0.49331000
C	-4.53951900	0.52368900	0.10485800
O	-4.41079500	1.73582600	0.29457700
O	-3.58888100	-0.36405400	0.07269400
C	-5.92986300	-0.08305600	-0.12202700
H	-5.95714500	-0.60986700	-1.08292100
H	-6.14431700	-0.82486100	0.65627500
H	-6.69629200	0.69578300	-0.10677000
O	-0.10063100	0.85223600	0.66181800
C	0.05132500	2.21833000	0.98332800
H	1.06083500	2.40189700	1.38046100
H	-0.67314400	2.49160200	1.76123800
H	-0.10636800	2.87769700	0.11532400
N	2.98045400	-0.01190800	1.46455600
O	2.17403000	-0.74989700	2.03820500
O	4.11772900	0.22685600	1.91305600

Sum of electronic and zero-point Energies= -988.393968

Sum of electronic and thermal Energies= -988.374576

Sum of electronic and thermal Enthalpies= -988.373632

Sum of electronic and thermal Free Energies= -988.447787

P (2-nitroanisole)

Charge 0

Spin multiplicity 1

Atom Type	Coordinates X	Y	Z
C	1.61404500	1.99582300	-0.05944000
C	1.80518700	0.61596000	-0.01912200
C	0.71040300	-0.26359500	0.00104400
C	-0.58533900	0.30596000	-0.01488500
C	-0.76617700	1.68845800	-0.03238700
C	0.33043200	2.54252100	-0.06429300
H	2.48378800	2.64671300	-0.08167400
H	2.81322900	0.22026000	-0.00139300
H	-1.78108100	2.06719900	-0.02338000
H	0.18404500	3.61726400	-0.09229200
O	0.82851600	-1.60469000	0.07352200
C	2.12843300	-2.17832500	0.15080800
H	1.96480600	-3.25456200	0.21516500
H	2.66691600	-1.83487400	1.04286300
H	2.71941900	-1.95256000	-0.74531000
N	-1.79907300	-0.52049300	-0.02190400
O	-1.74178700	-1.64388900	-0.51446200
O	-2.82166900	-0.01477100	0.44956500

Sum of electronic and zero-point Energies= -551.127132

Sum of electronic and thermal Energies= -551.117754

Sum of electronic and thermal Enthalpies= -551.116810

Sum of electronic and thermal Free Energies= -551.162481

Int1-DMF

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	1.94897000	0.19772200	-0.16036100
O	3.54148500	-0.42524600	-0.78925100
O	0.28795600	0.81389600	0.35702900
C	0.19039400	1.89376200	1.22987000
H	0.65923700	1.71490300	2.21951200
H	-0.87612200	2.13119000	1.43160300
H	0.64249200	2.82670100	0.83821100
C	4.37631400	-1.20946600	-0.01169400
H	5.29013800	-1.48676400	-0.58160500
H	4.74055800	-0.71221100	0.91441300
H	3.92583800	-2.17163300	0.31839700
O	-3.71418100	1.02959500	-1.36076900
C	-2.86528200	0.48147100	-0.66088300
H	-1.81462300	0.81455500	-0.58991000
N	-3.10541100	-0.61697500	0.12176400
C	-2.05416600	-1.21926500	0.92545100
H	-2.35157500	-1.24554800	1.98506100
H	-1.86456700	-2.25459100	0.60403600
H	-1.13128300	-0.62992200	0.82041900
C	-4.42022800	-1.21846100	0.14191100
H	-4.84093700	-1.21449500	1.15870500
H	-5.06412900	-0.63871400	-0.52219000
H	-4.38155300	-2.26278400	-0.20252500

Sum of electronic and zero-point Energies= -809.276002

Sum of electronic and thermal Energies= -809.256695

Sum of electronic and thermal Enthalpies= -809.255750

Sum of electronic and thermal Free Energies= -809.326616

Int1-TS_{OA}-DMF

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	-0.44358700	-0.13419600	-0.45513000
C	1.13827800	1.23693500	2.89371400
C	0.81703700	0.24655800	1.97840300
C	1.15241400	0.38712200	0.60868200
C	1.84421600	1.55714400	0.22960500
C	2.19681800	2.54173500	1.16435100
C	1.84036200	2.39024700	2.49405900
H	0.85339500	1.10889500	3.93587900
H	0.30477600	-0.65573500	2.29317400
H	2.74192200	3.40811100	0.80883800
H	2.10391900	3.15431500	3.21988100
I	2.69641000	-1.66078900	-0.00179100
O	-1.04850100	-1.77335000	0.10590900
N	2.24509400	1.75856100	-1.15093200
O	1.84557700	0.95338900	-1.99749700
O	2.97774400	2.72509300	-1.41557900
O	-1.24091800	1.39087600	-1.07625200
C	-0.78671500	2.55959200	-1.66301500
H	-0.36994800	2.40946900	-2.67295800
H	-1.61860900	3.28417100	-1.74342300
H	-0.00646900	3.05698400	-1.05639800
C	-0.84819800	-2.95692000	-0.60424800
H	0.22262400	-3.20340300	-0.69139300
H	-1.32973300	-3.79711600	-0.07227000

H	-1.27018000	-2.92718900	-1.62689200
O	-7.00306000	-0.83506300	-0.22056800
C	-6.25925800	0.13764200	-0.16137500
H	-6.56800200	1.13546500	-0.53679500
N	-4.99786200	0.16189700	0.33800100
C	-4.22933500	1.39548600	0.41867300
H	-4.03371500	1.65734700	1.46920200
H	-3.26772800	1.31078600	-0.10314800
H	-4.80671400	2.20845400	-0.03435300
C	-4.40072200	-1.04647800	0.89255800
H	-4.30399000	-0.95847000	1.98472700
H	-5.06120200	-1.88312700	0.66040200
H	-3.40284100	-1.22062500	0.47320600

Sum of electronic and zero-point Energies= -1123.426117

Sum of electronic and thermal Energies= -1123.400568

Sum of electronic and thermal Enthalpies= -1123.399624

Sum of electronic and thermal Free Energies= -1123.489578

Int1-TSSig-DMF

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	-0.63998500	1.45398600	0.45179000
C	4.65239800	0.30450400	-0.52235100
C	3.48547600	-0.19906900	0.09241400
C	2.19235800	0.04812200	-0.45436700
C	2.16917900	0.77597400	-1.68858200
C	3.31697400	1.27591700	-2.26009600
C	4.58688400	1.04340100	-1.68308700
H	5.59531400	0.08231800	-0.03765900

H	1.20616000	0.93986300	-2.15986500
H	3.23649700	1.84162900	-3.18643800
H	5.48971700	1.42918600	-2.14687000
I	0.65342300	-1.57132500	-0.42773100
C	-2.97226800	2.97710400	0.03216100
O	-2.43440400	1.70560700	0.23486100
O	1.19283700	1.14286900	0.75659800
C	1.97452400	2.25097400	1.14691900
H	2.96013000	1.91431900	1.49918200
H	1.47930200	2.76730600	1.97965400
H	2.12813400	2.97134200	0.32721000
N	3.66948300	-0.95107800	1.31186200
O	2.67545900	-1.26241400	1.97551200
O	4.83038600	-1.25271100	1.64767400
H	-2.58319100	3.48723700	-0.87092900
H	-4.06970400	2.90496200	-0.09976600
H	-2.80520400	3.67189800	0.87923000
O	-7.30089000	-0.94161000	-0.82370200
C	-6.57874400	-0.80864100	0.15967900
H	-6.98848900	-0.80749000	1.19185800
N	-5.23621000	-0.63433200	0.15722000
C	-4.46192900	-0.53998800	1.38834100
H	-3.87558000	-1.45611600	1.55395300
H	-3.76874400	0.30705500	1.31639000
H	-5.14135500	-0.40560200	2.23685800
C	-4.49139100	-0.59496800	-1.09599400
H	-5.19888000	-0.42678000	-1.90959300
H	-3.74630700	0.20575700	-1.03815900
H	-3.97044600	-1.54827000	-1.26854500

Sum of electronic and zero-point Energies= -1123.434045

Sum of electronic and thermal Energies= -1123.408554

Sum of electronic and thermal Enthalpies= -1123.407610

Sum of electronic and thermal Free Energies= -1123.498315

Int1-TS_{OA}-PhI

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	-0.50594300	1.40821000	-0.01680000
C	2.97890100	0.14593200	1.42369400
C	1.59261100	0.00748000	1.34612000
C	0.98244600	-0.08051700	0.08304100
C	1.76753200	-0.10865400	-1.08154800
C	3.15105500	0.03913300	-0.98003000
C	3.76825900	0.16084100	0.26898500
H	3.44292100	0.24454700	2.40366000
H	0.96958400	0.04061700	2.23080000
H	3.74875600	0.04663200	-1.88981900
H	4.84896700	0.25979400	0.34128400
I	-0.80725800	-1.78987000	-0.03603200
O	-0.80652000	1.53754600	1.82246400
O	-0.60141900	2.00381300	-1.75911700
C	-1.13298600	1.25848500	-2.79617600
H	-2.18269500	0.94045400	-2.63383000
H	-1.11893700	1.84056400	-3.74007700
H	-0.56221300	0.32686800	-3.00449600
C	-2.13044200	1.52051200	2.24522300
H	-2.63749000	0.55084100	2.06323700
H	-2.18533400	1.69751000	3.33908000
H	-2.76485400	2.30384800	1.77689800

H	1.29757100	-0.21681000	-2.05245800

Sum of electronic and zero-point Energies= -670.514578

Sum of electronic and thermal Energies= -670.499267

Sum of electronic and thermal Enthalpies= -670.498323

Sum of electronic and thermal Free Energies= -670.560705

Int1-M1-PhI

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	0.32211700	-0.43278900	-0.46691800
C	-3.24944600	-0.73828700	1.61410500
C	-1.89553600	-0.69416200	1.25406400
C	-1.54388600	-0.35018400	-0.05099200
C	-2.52471700	-0.06039800	-0.99823200
C	-3.87244700	-0.10330800	-0.63011200
C	-4.23948600	-0.44207400	0.67629700
H	-3.52279000	-1.00170000	2.63449900
H	-1.12583100	-0.91800600	1.98828600
H	-4.63778300	0.12606200	-1.36975100
H	-5.28980100	-0.47405300	0.95873500
I	0.50697900	2.10348800	0.00853200
C	2.64154500	-1.16677800	0.47476500
O	1.87502500	-1.42901600	1.42042500
O	2.26703900	-0.66845600	-0.65296800
C	4.14545900	-1.41090500	0.60254000
H	4.51298300	-1.97900100	-0.25909400
H	4.66943000	-0.44772300	0.60520800
H	4.37054600	-1.94737300	1.52795300
O	-0.12582700	-2.02877200	-1.31908600

C	-0.19484100	-3.18286400	-0.53620100
H	0.71565000	-3.36195100	0.05627400
H	-0.33272100	-4.03994800	-1.21981600
H	-1.05538000	-3.18141300	0.15799100
H	-2.24535000	0.19482500	-2.01622700

Sum of electronic and zero-point Energies= -783.916509

Sum of electronic and thermal Energies= -783.899221

Sum of electronic and thermal Enthalpies= -783.898277

Sum of electronic and thermal Free Energies= -783.966011

Int1-TS_{RE}-PhI

Charge -2

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	0.35919900	0.79826100	0.20978600
C	-3.22400800	-0.47523700	-1.42995200
C	-2.09070300	0.29543100	-1.14081200
C	-1.52036900	0.22843200	0.13752200
C	-2.11496600	-0.56069600	1.13531100
C	-3.24185900	-1.31582400	0.83086300
C	-3.80821500	-1.28021600	-0.45312800
H	-3.64416500	-0.44157400	-2.43399600
H	-1.63747100	0.90502000	-1.91789100
H	-3.68449400	-1.94357000	1.60252800
H	-4.69045500	-1.87334300	-0.68164100
I	1.51760100	-1.49153800	-0.00786600
C	2.92306400	1.97060800	-0.61384100
O	1.65212700	2.14917900	-0.09498700
O	-1.05557900	1.90949400	0.92293900
C	-1.28319900	3.05133000	0.12215100

H	-0.37153700	3.37362100	-0.39544600
H	-1.61236500	3.85253700	0.80055600
H	-2.09094300	2.87310500	-0.60887100
H	3.43021400	2.95015300	-0.74907400
H	3.58452600	1.36782500	0.03953500
H	2.93889700	1.47239600	-1.60564500
H	-1.68269100	-0.58657200	2.13077800

Sum of electronic and zero-point Energies= -670.527020

Sum of electronic and thermal Energies= -670.512366

Sum of electronic and thermal Enthalpies= -670.511422

Sum of electronic and thermal Free Energies= -670.571677

Int1-TSSig-PhI

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	-1.77876800	-1.05482200	-0.08038600
C	3.73251800	-0.51958500	-0.65613500
C	2.45558800	-0.06021600	-0.98306800
C	1.43108500	-0.09982600	-0.01881500
C	1.71548700	-0.58561900	1.27197800
C	2.99718000	-1.04354000	1.57081300
C	4.02298300	-1.01622400	0.61799300
H	4.51295800	-0.47485600	-1.41501000
H	0.93237700	-0.60291500	2.02297500
H	3.19468600	-1.42197100	2.57298300
H	5.02194700	-1.36626000	0.86530000
I	0.01565100	1.79971700	-0.06026400
O	-3.47906600	-1.14789500	0.55098600
O	-0.01224100	-1.14737700	-0.74844700

C	0.48216700	-2.44907500	-0.98139200
H	1.47122800	-2.39307000	-1.46099700
H	-0.19725000	-2.98325900	-1.66014700
H	0.58419200	-3.03872900	-0.05616200
H	2.24713900	0.33433200	-1.97205400
C	-4.36068700	-0.08794000	0.37882600
H	-3.99757800	0.87353800	0.79664300
H	-4.62079900	0.11520800	-0.68210900
H	-5.32159900	-0.30285300	0.89222800

Sum of electronic and zero-point Energies= -670.512127

Sum of electronic and thermal Energies= -670.497092

Sum of electronic and thermal Enthalpies= -670.496148

Sum of electronic and thermal Free Energies= -670.558838

9-O_2-singlet

Charge -1

Spin multiplicity 1

Atom	Coordinates		
Type	X	Y	Z
Cu	0.55645200	-0.24623700	-0.18502900
C	2.31139600	1.85416600	0.25203700
O	1.07258700	1.51694400	-0.28851100
H	2.50074900	2.92955500	0.06716600
H	2.37217300	1.70834000	1.34830200
H	3.15993600	1.30054100	-0.19408300
O	0.89369600	-2.06627900	0.00798300
O	2.00219700	-1.26487600	0.22981600
C	-2.08738900	0.11258900	0.19276600
O	-1.83672000	0.04491300	1.39770700
O	-1.23768400	-0.02388500	-0.78068400
C	-3.51475500	0.39171500	-0.29566500

H	-3.54493300	1.36133900	-0.80660300
H	-3.82396400	-0.36763600	-1.02266900
H	-4.20917700	0.40336500	0.54840900

Sum of electronic and zero-point Energies= -691.286979

Sum of electronic and thermal Energies= -691.274827

Sum of electronic and thermal Enthalpies= -691.273883

Sum of electronic and thermal Free Energies= -691.327434

9-O_2-triplet

Charge -1

Spin multiplicity 3

Atom	Coordinates		
Type	X	Y	Z
Cu	0.50039200	0.12724600	-0.21368600
C	2.60773800	-1.64663400	0.37531000
O	1.38428300	-1.52333100	-0.26592700
H	3.07051400	-2.62425900	0.12650900
H	3.35244700	-0.87409600	0.08897100
H	2.53902500	-1.61580600	1.48433300
O	0.75414300	2.22716700	-0.13801500
O	1.81358500	1.53742500	0.24560700
C	-2.11351700	-0.16593700	0.17894600
O	-1.32166700	-0.23351200	-0.84008000
O	-1.77872300	0.12618400	1.33608500
C	-3.57625700	-0.50015100	-0.13960100
H	-3.65252100	-1.54736600	-0.45602200
H	-4.20889800	-0.33911500	0.73732400
H	-3.93268900	0.11536000	-0.97350600

Sum of electronic and zero-point Energies= -691.296913

Sum of electronic and thermal Energies= -691.283684

Sum of electronic and thermal Enthalpies= -691.282740

Sum of electronic and thermal Free Energies= -691.340823