Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Highly Atom-Economic, Catalyst-free, and Solvent-free Phosphorylation of Chalcogenides

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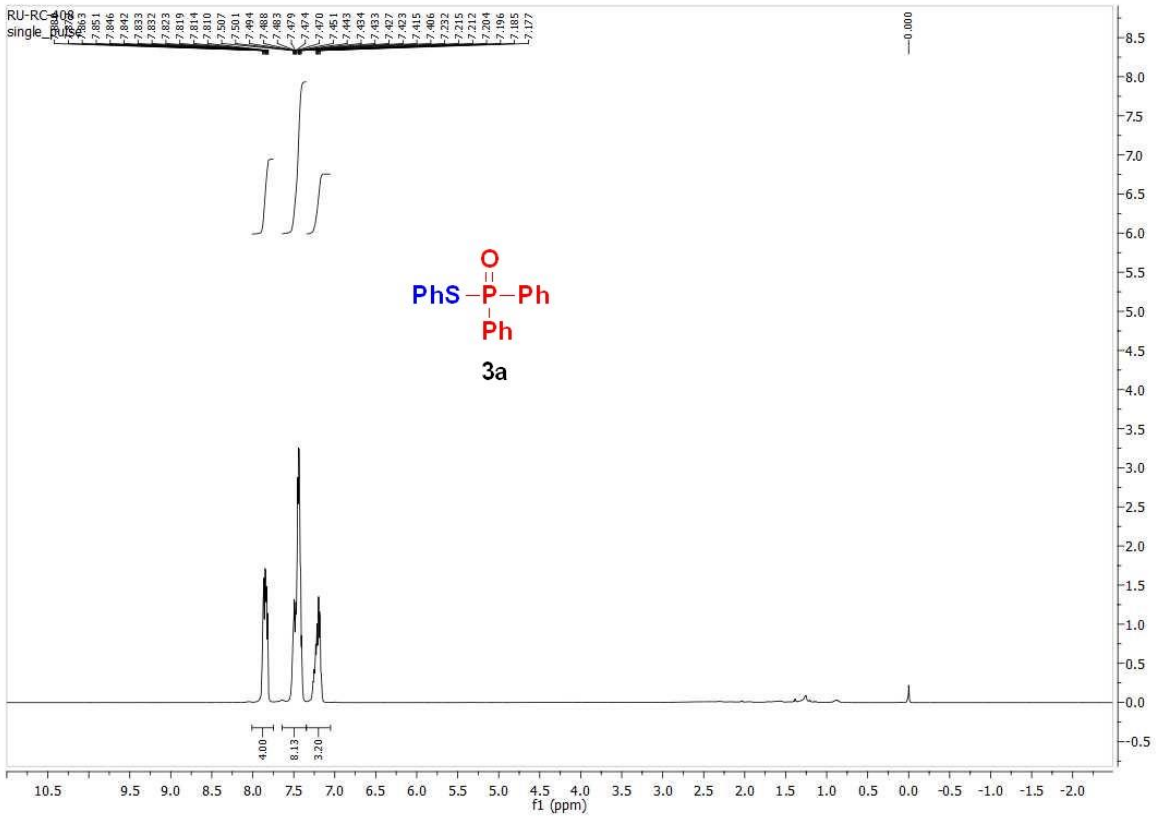
^{1}H, ^{13}C, ^{31}P NMR spectra and mass spectra of products 3, 5, 7 & 8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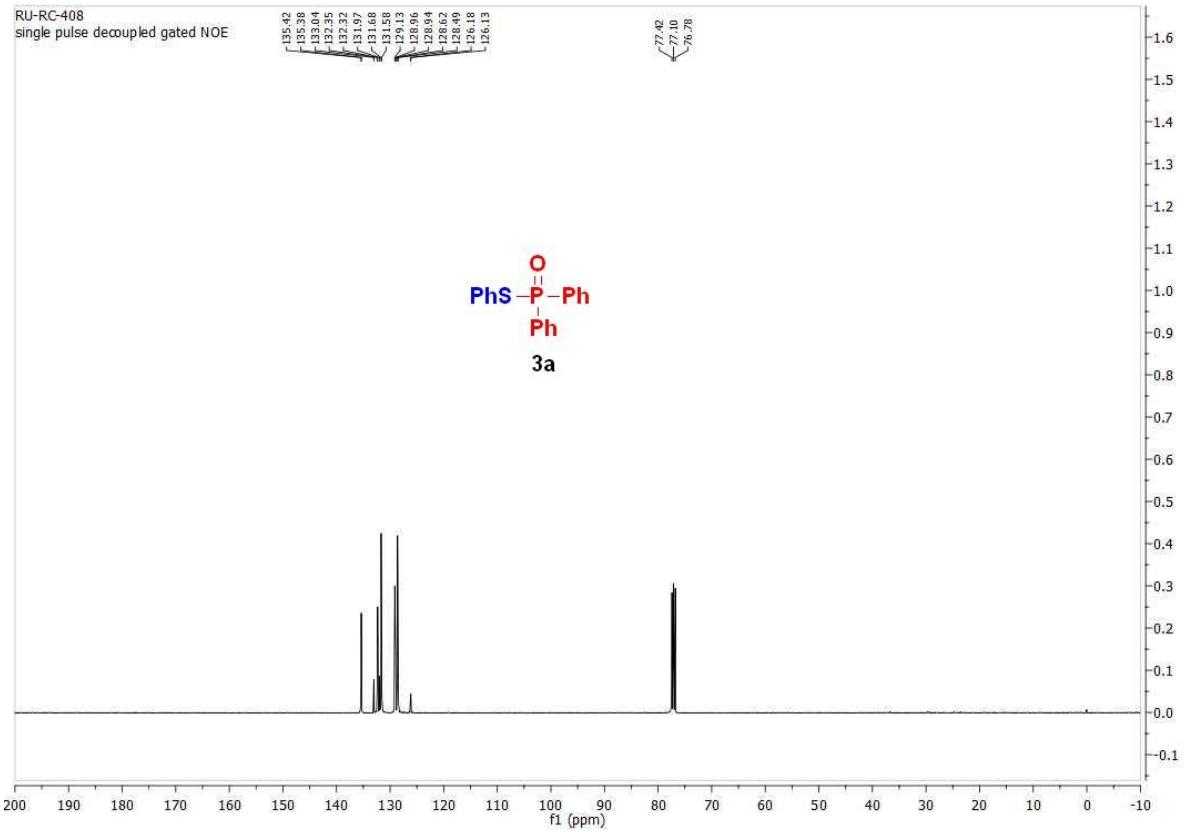
PhS–P(=O)–Ph
Ph
3a
f1 (ppm)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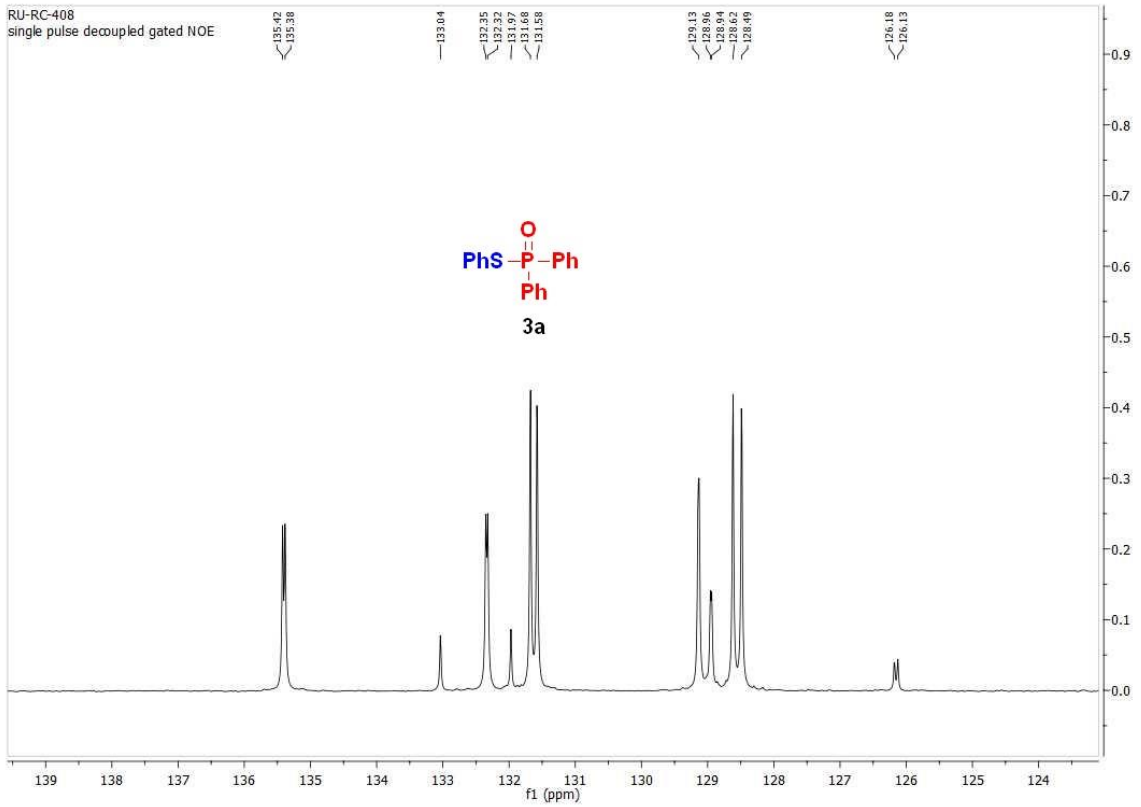
PhS–P(=O)–Ph
Ph
3a
f1 (ppm)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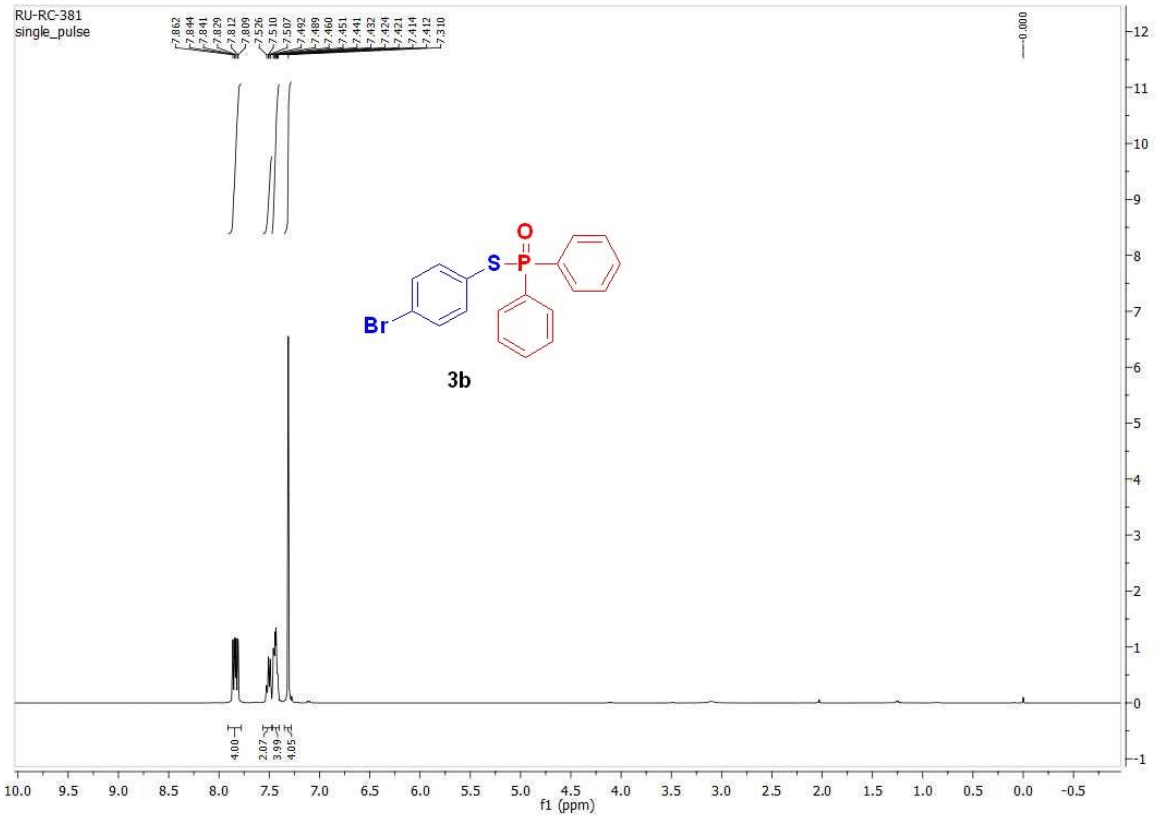
126.13
PhS
P
Ph
Ph
O
3a
f1 (ppm)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7.489
7.460
7.451
7.441
7.432
7.424
7.421
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4.00
2.07
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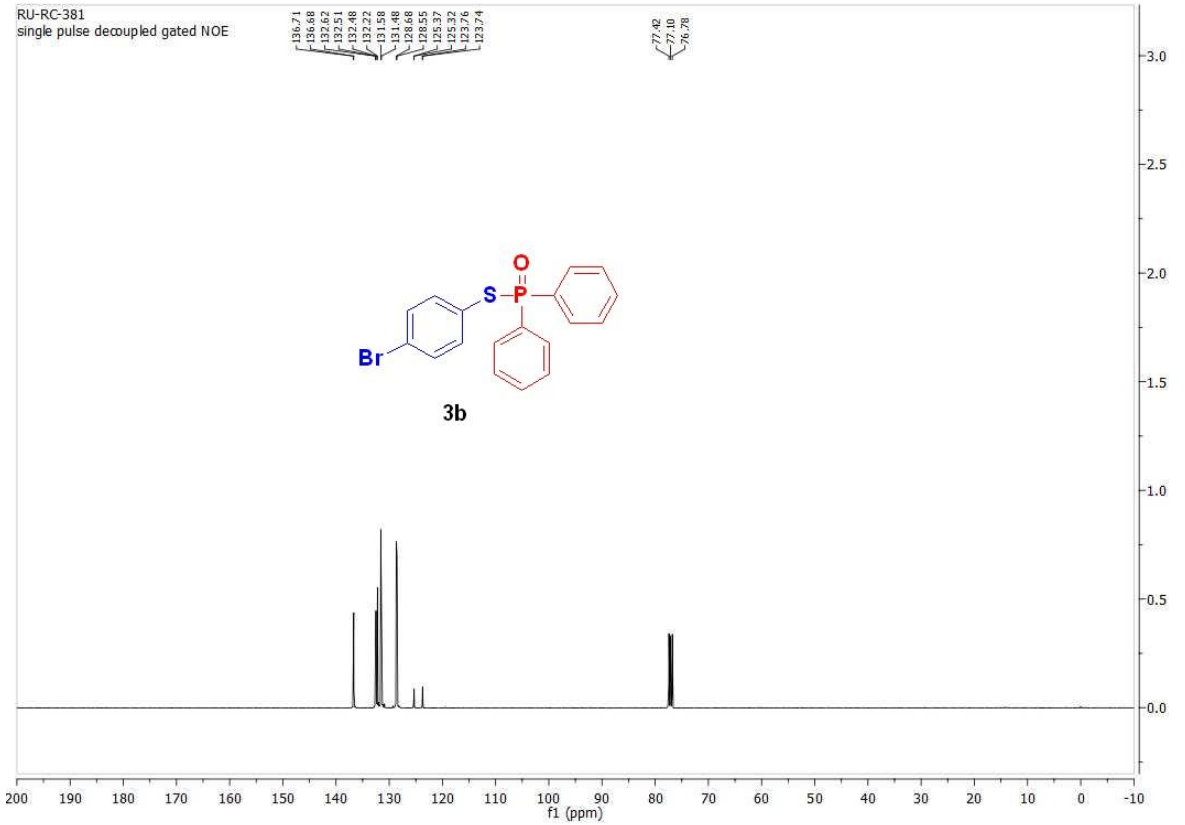
Br
S
P
O
3b
f1 (ppm)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131.48
128.68
128.55
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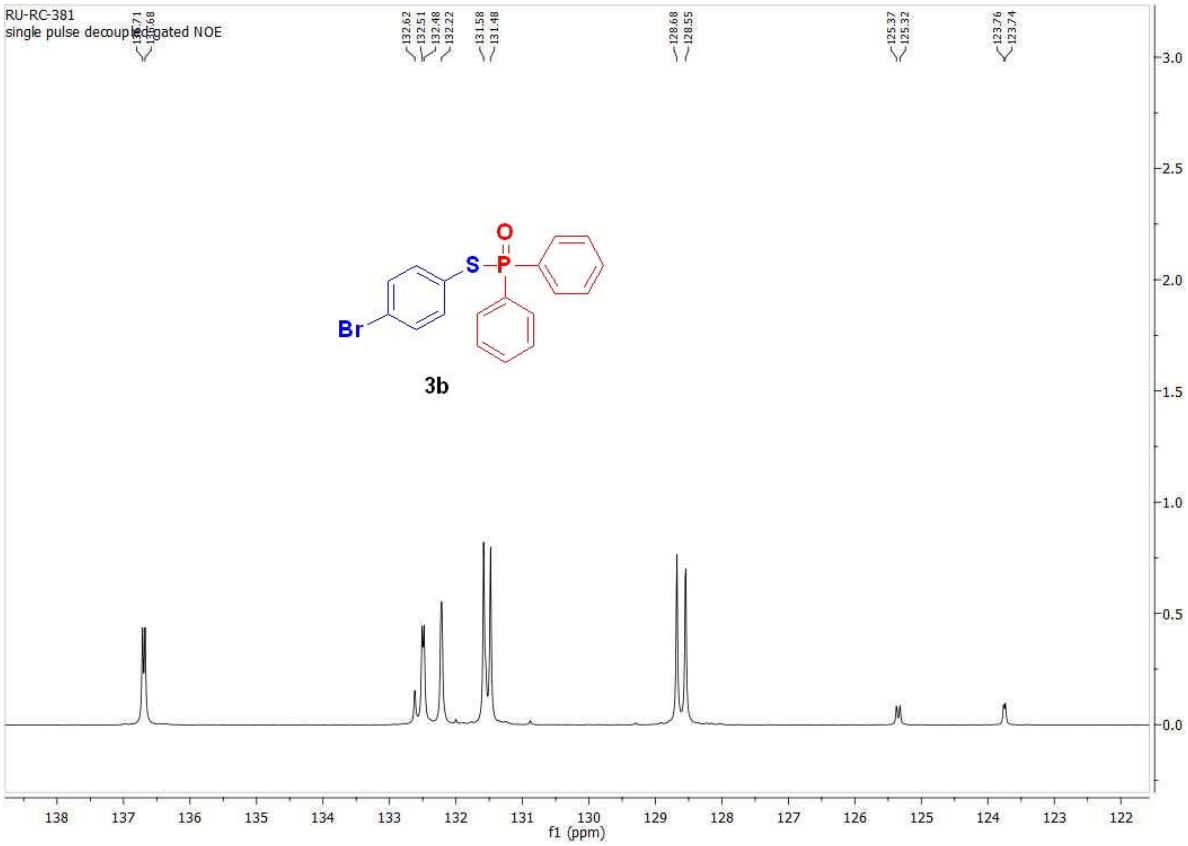
125.32
123.76
123.74
77.42
77.10
76.78
Br
S
P
O
3b
f1 (ppm)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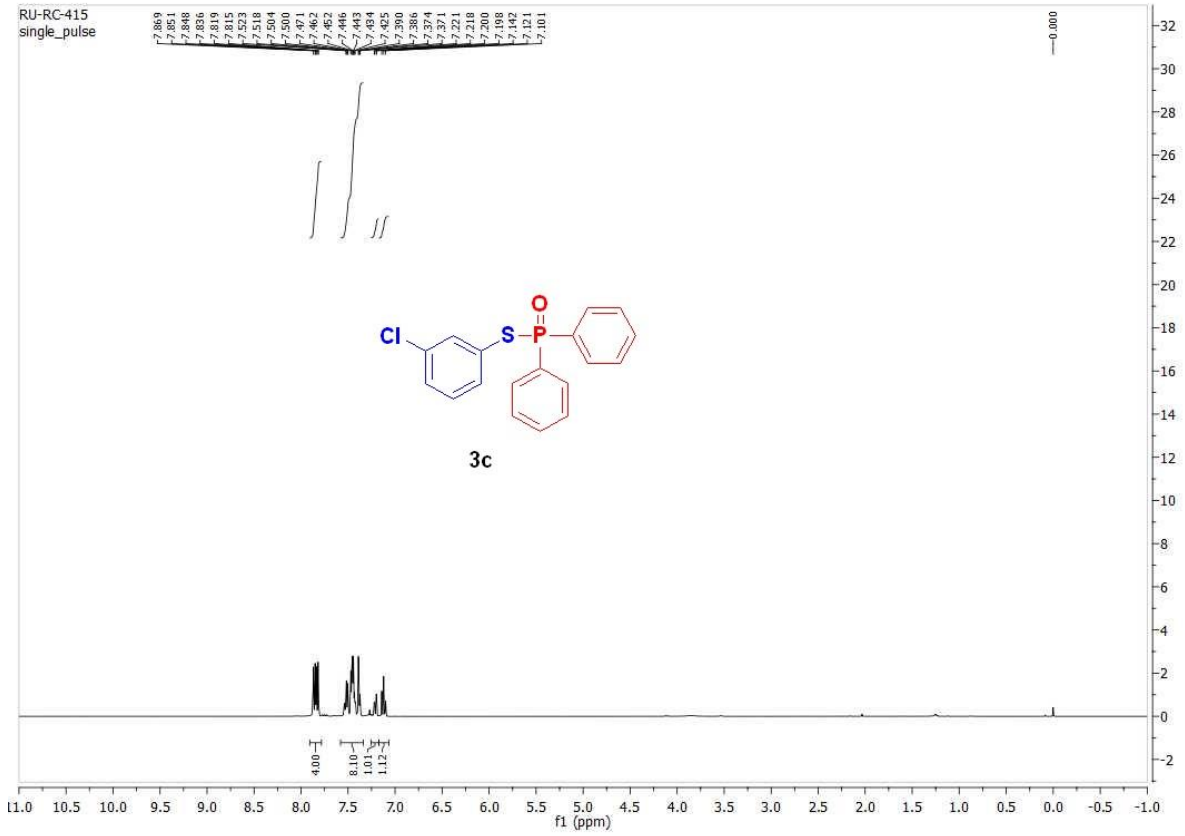
125.32
123.76
123.74
Br
S
P
O
3b
f1 (ppm)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7.836
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7.504
7.500
7.471
7.462
7.452
7.446
7.443
7.434
7.425
7.390
7.386
7.374
7.371
7.221
7.218
7.200
7.198
7.192
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Cl
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P
O
3c
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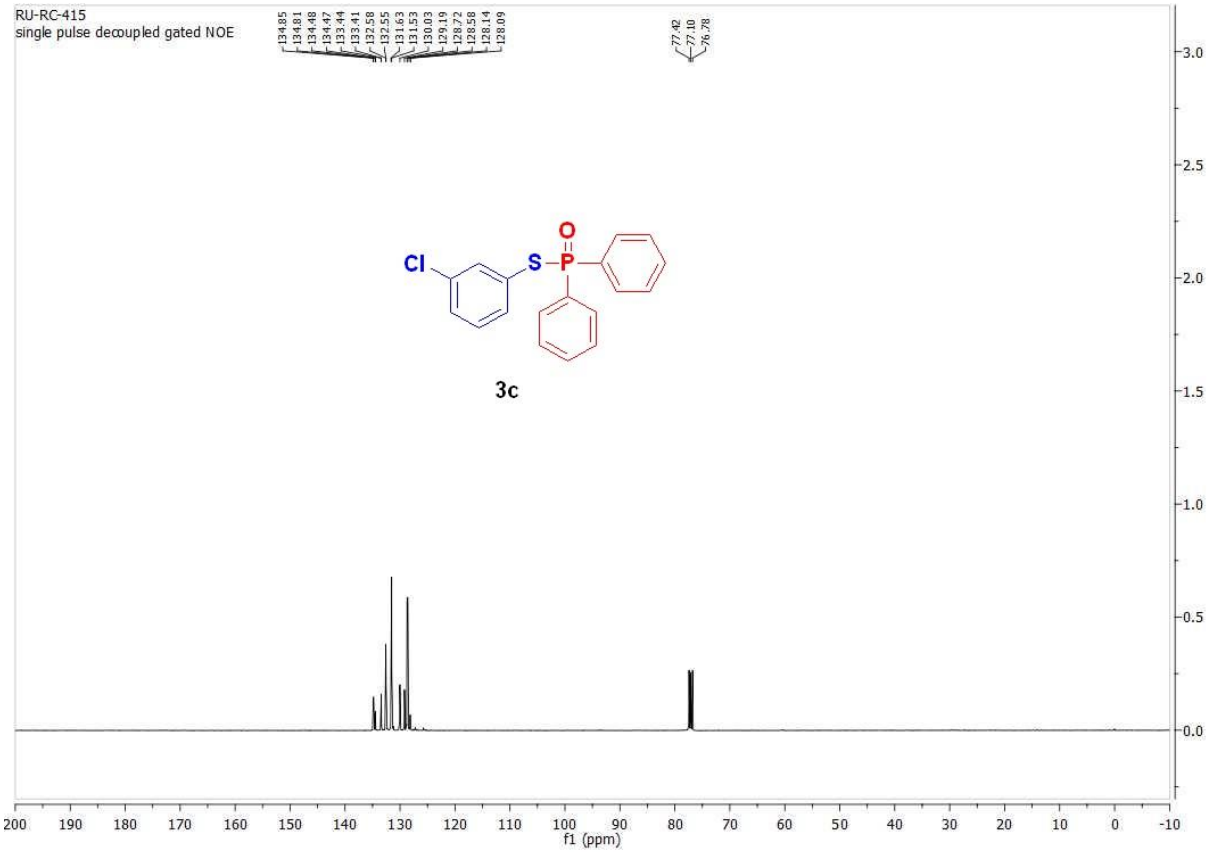
1.12
f1 (ppm)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131.63
131.53
130.03
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128.14
128.09
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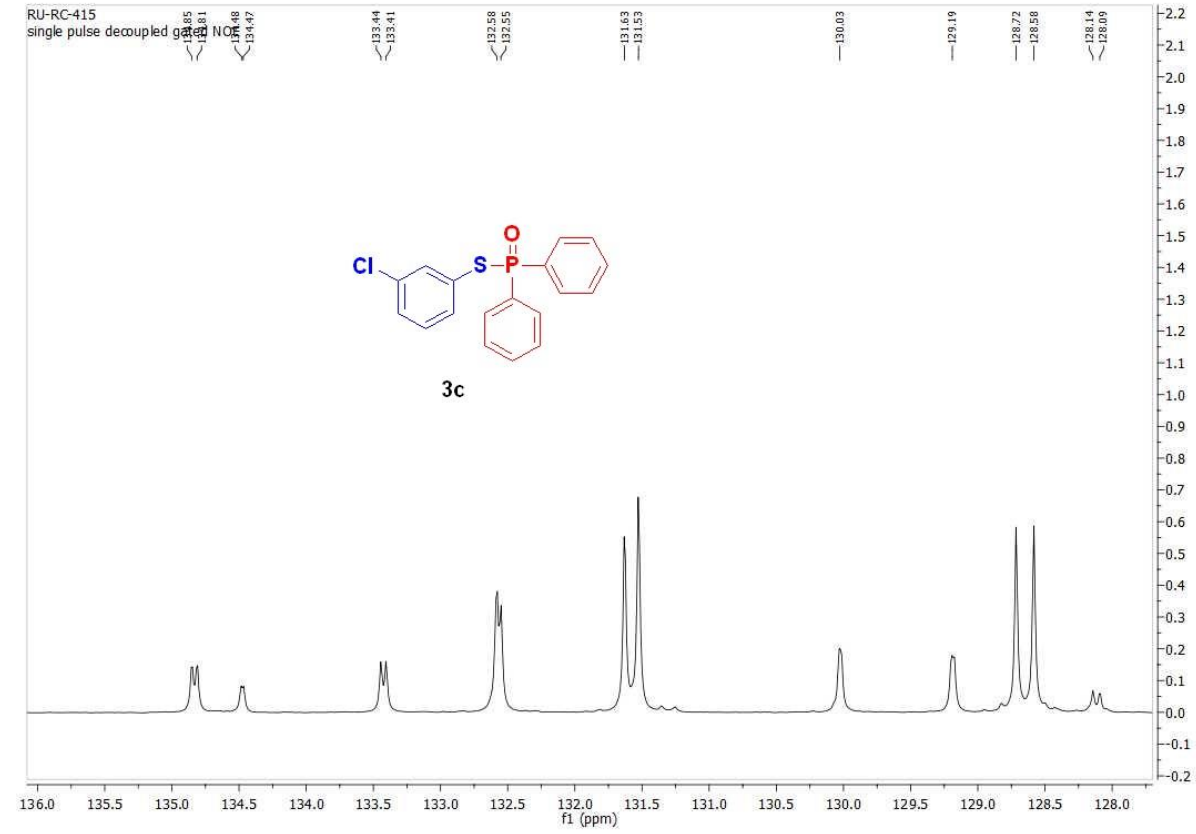
77.10
76.78
Cl
S
P
O
3c
f1 (ppm)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single pulse decoupled gated NOE
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134.81
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134.47
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132.55
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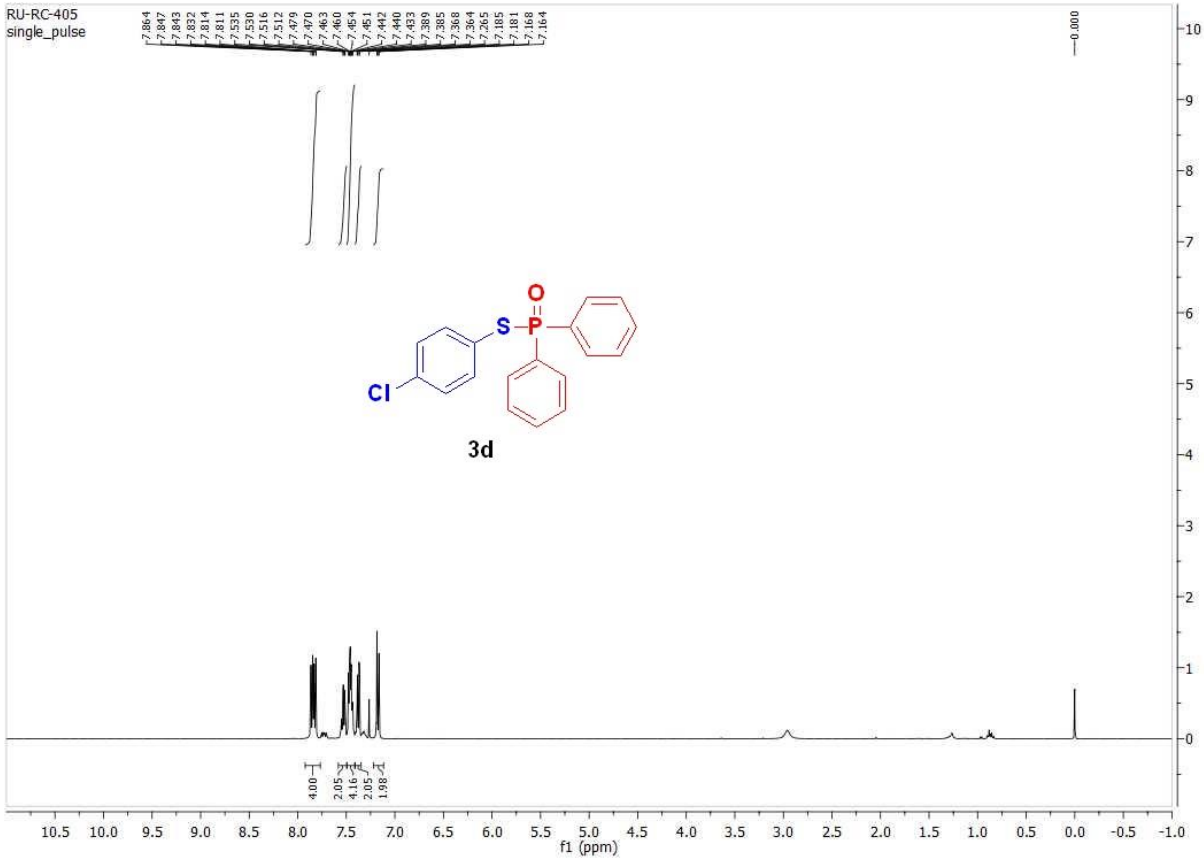
131.53
130.03
129.19
128.72
128.58
128.14
128.09
Cl
S
P
O
3c
f1 (ppm)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7.814
7.811
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7.512
7.479
7.470
7.463
7.460
7.454
7.451
7.442
7.440
7.433
7.389
7.385
7.368
7.364
7.265
7.185
7.181
7.168
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4.00
2.05
4.16
2.05
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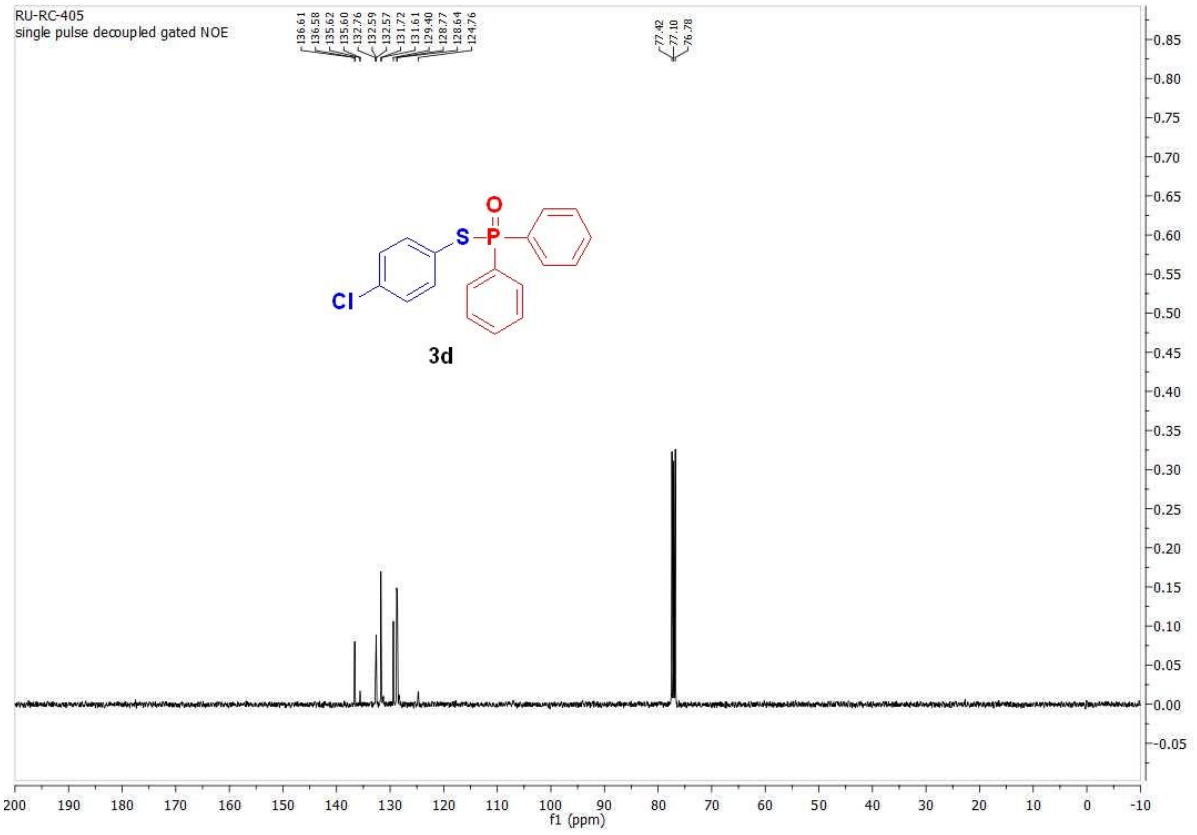
Cl
S
P
O
3d
f1 (ppm)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136.61
136.58
135.62
135.60
132.76
132.59
132.57
131.72
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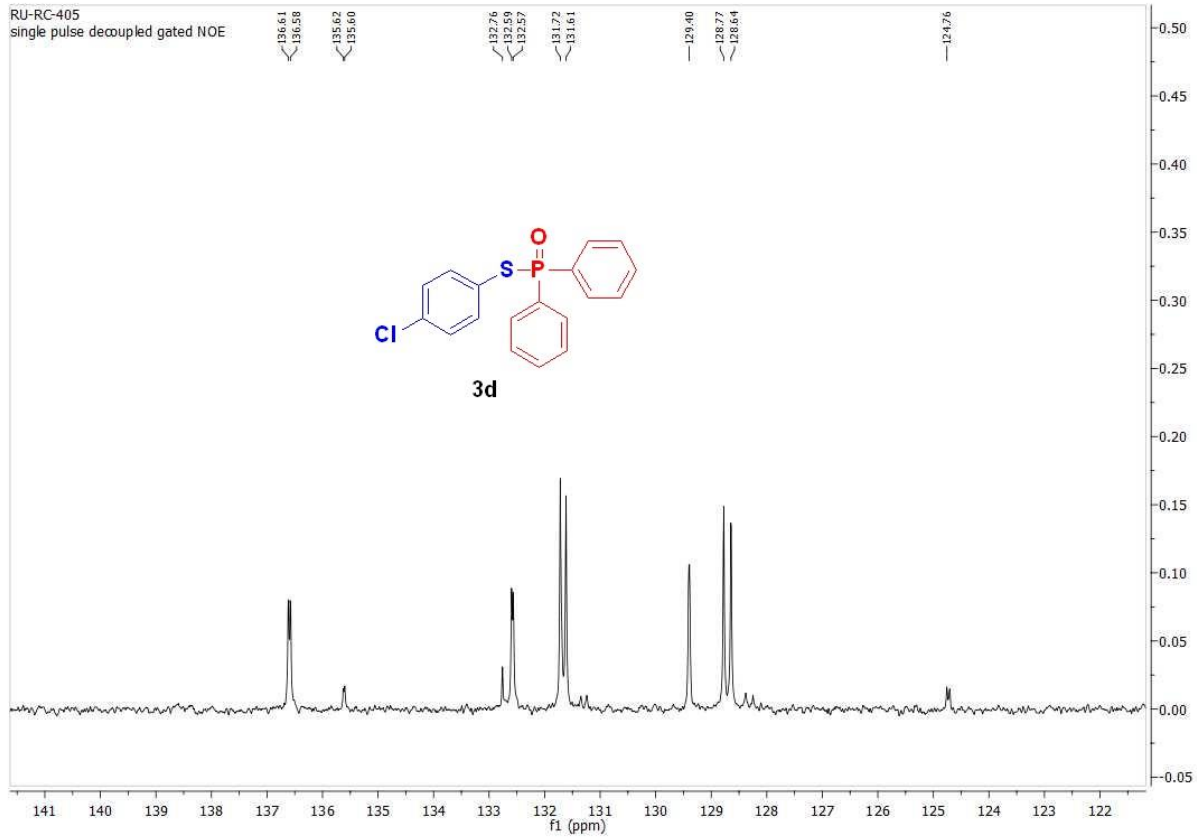
128.64
124.76
77.42
77.10
76.78
O
S
P
Cl
3d
f1 (ppm)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single pulse decoupled gated NOE
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136.58
135.62
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132.76
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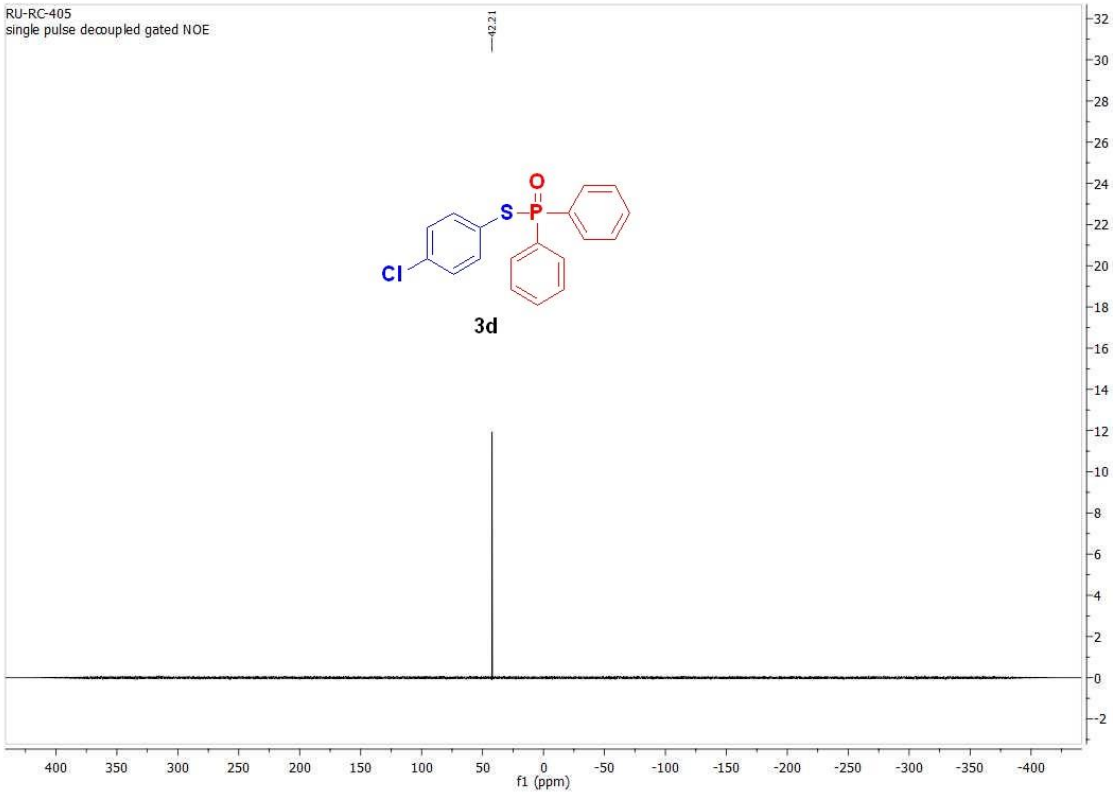
131.61
129.40
128.77
128.64
124.76
O
S
P
Cl
3d
f1 (ppm)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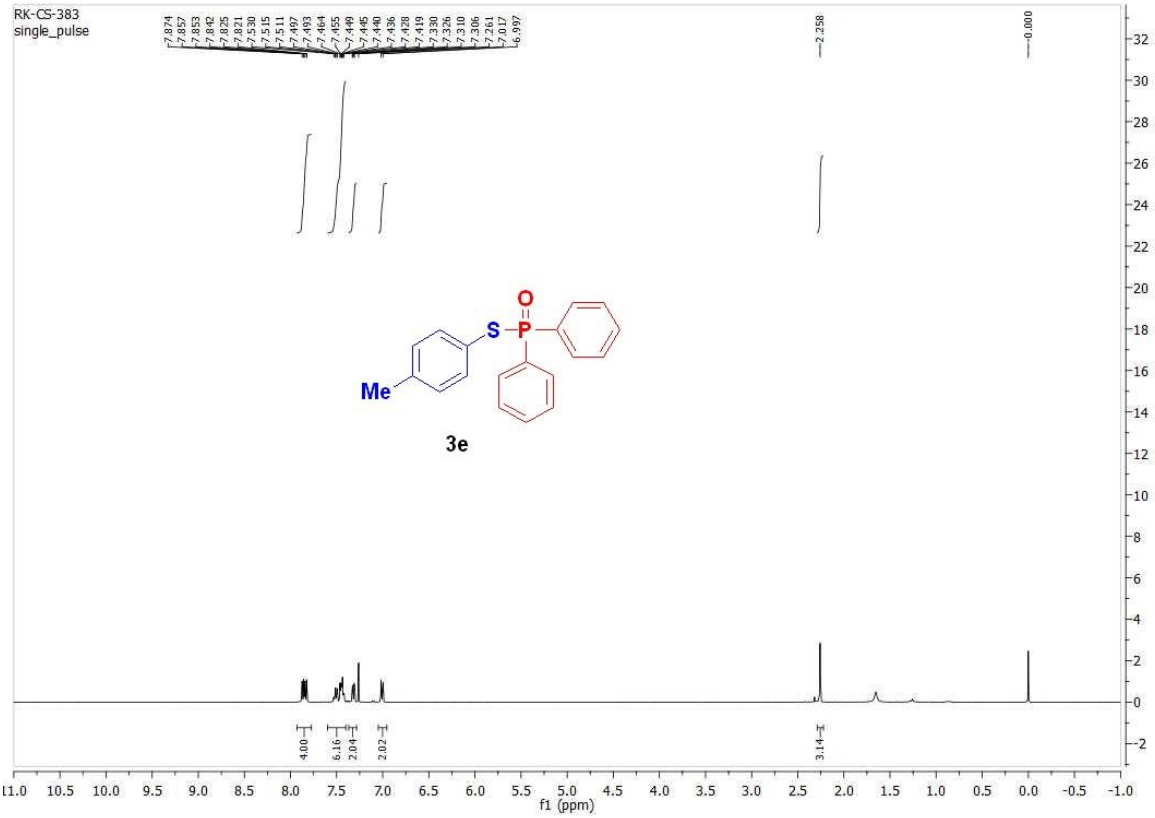
P
Cl
3d
f1 (ppm)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7.853
7.842
7.825
7.821
7.530
7.515
7.511
7.497
7.493
7.464
7.455
7.449
7.445
7.440
7.436
7.428
7.419
7.330
7.326
7.310
7.306
7.261
7.017
6.997
2.258
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O
S
P
Me
3e
4.00
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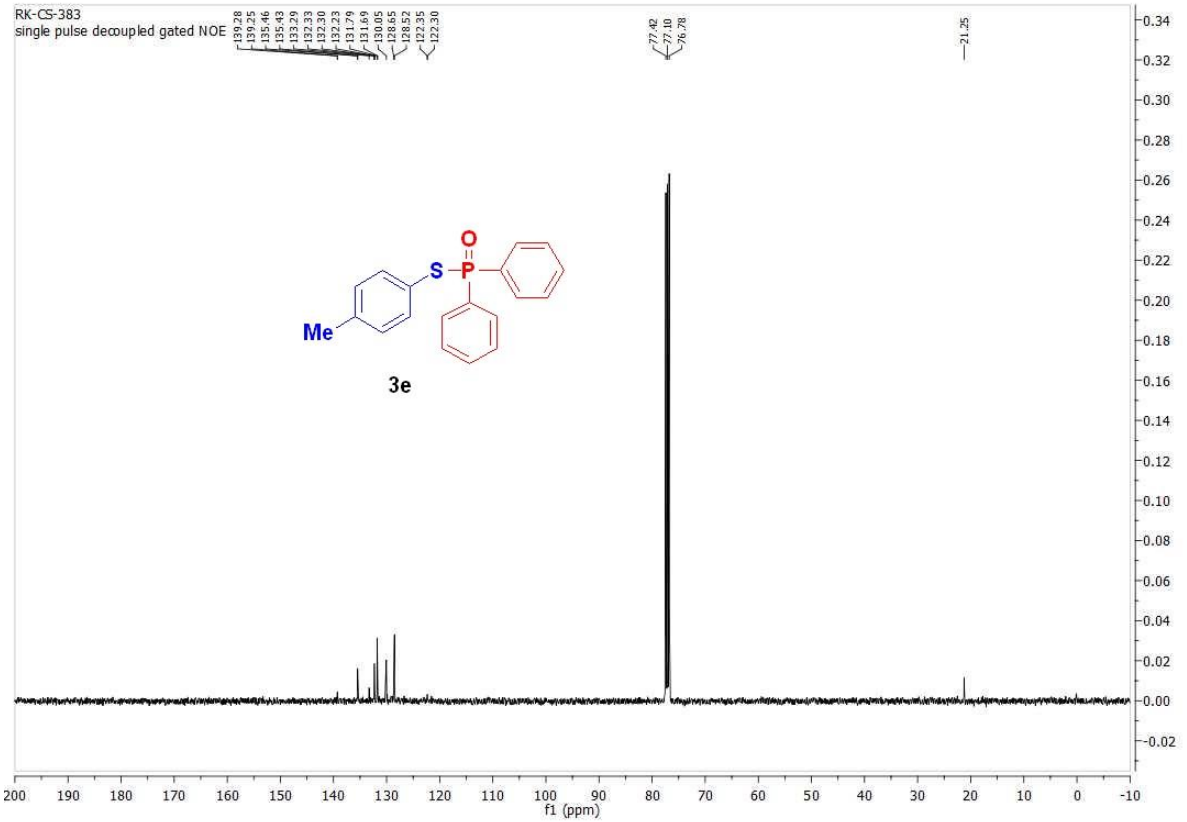
2.04
2.02
3.14
f1 (ppm)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135.46
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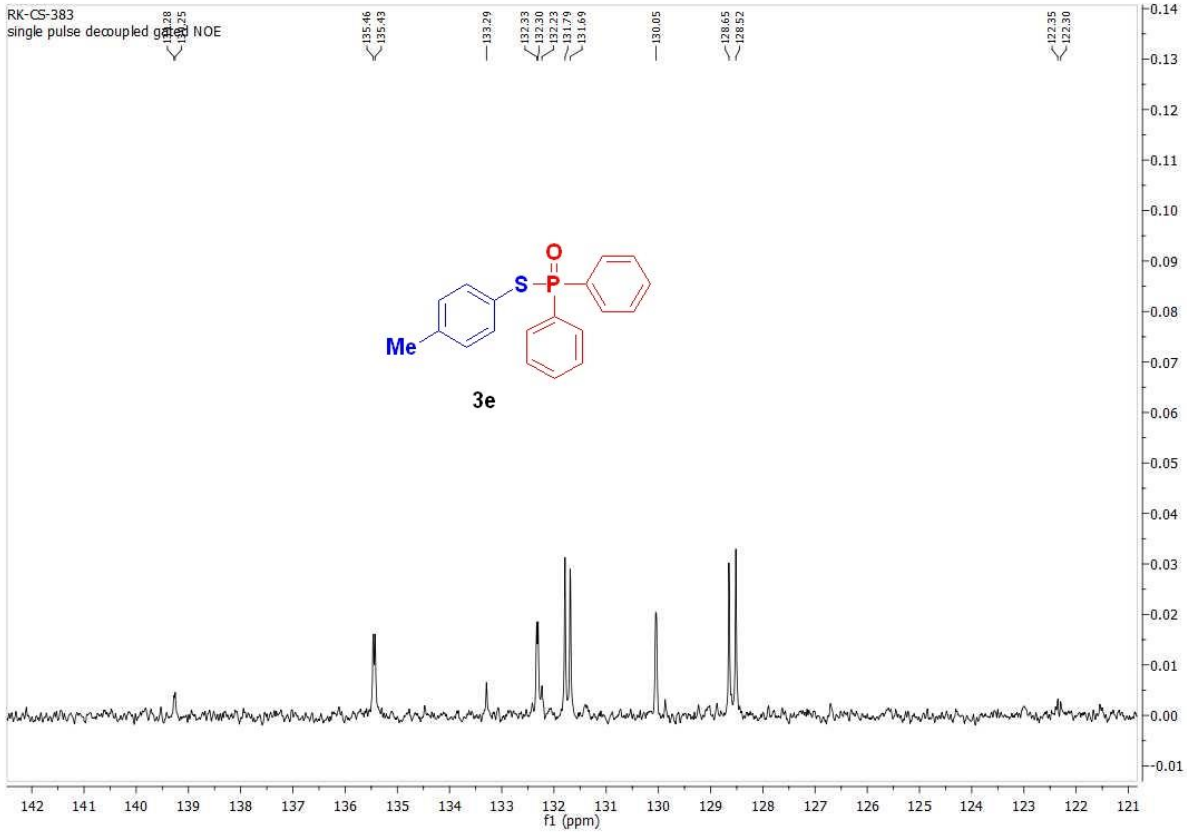
133.29
132.33
132.30
132.23
131.79
131.69
130.05
128.65
128.52
122.35
122.30
77.42
77.10
76.78
21.25
O
S
P
Me
3e
f1 (ppm)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single pulse decoupled gated NOE
135.46
135.43
133.29
132.33
132.30
132.23
131.79
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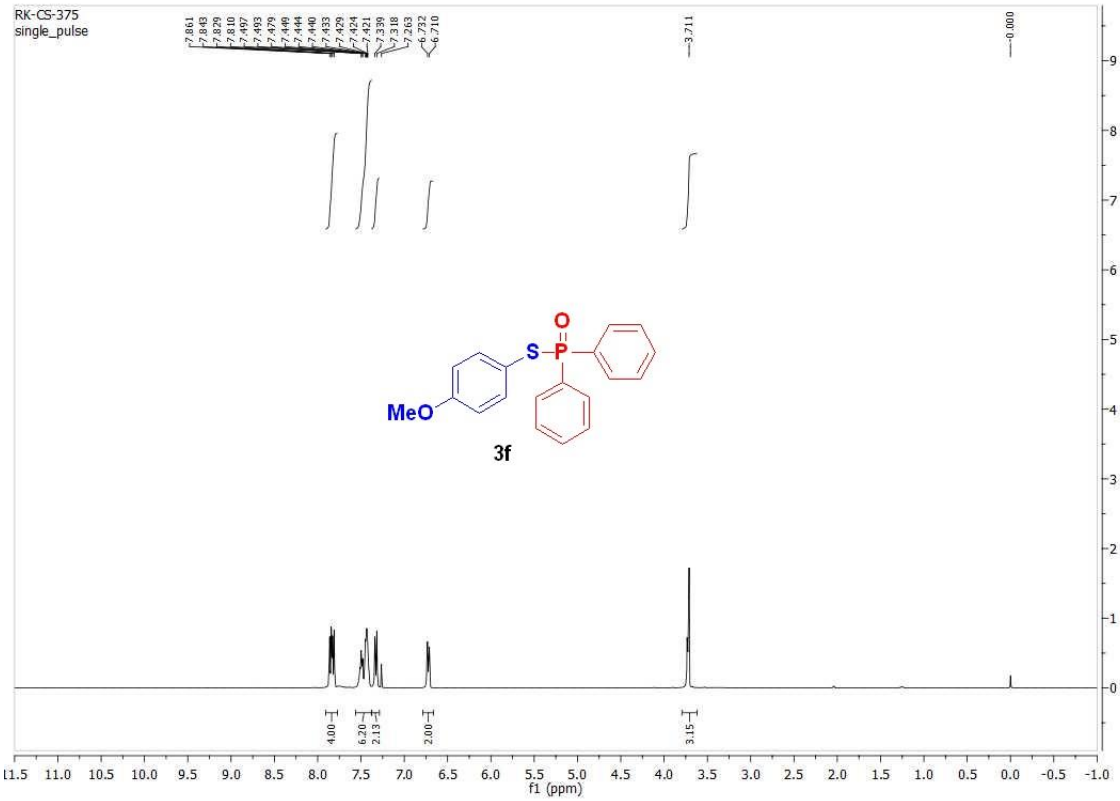
130.05
128.65
128.52
122.35
122.30
O
S
P
Me
3e
f1 (ppm)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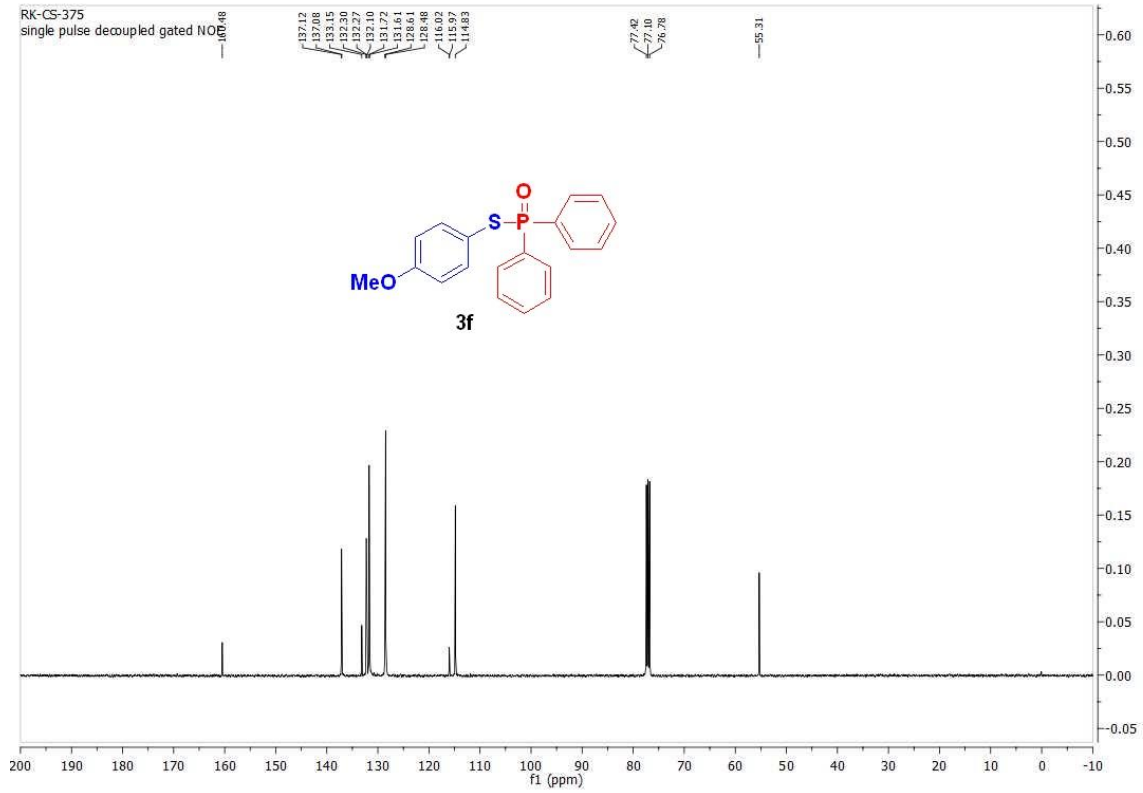
7.444
7.440
7.433
7.429
7.424
7.421
7.339
7.318
7.263
6.732
6.710
3.711
0.000
MeO
S
P
O
3f
4.00
6.20
2.13
2.00
3.15
f1 (ppm)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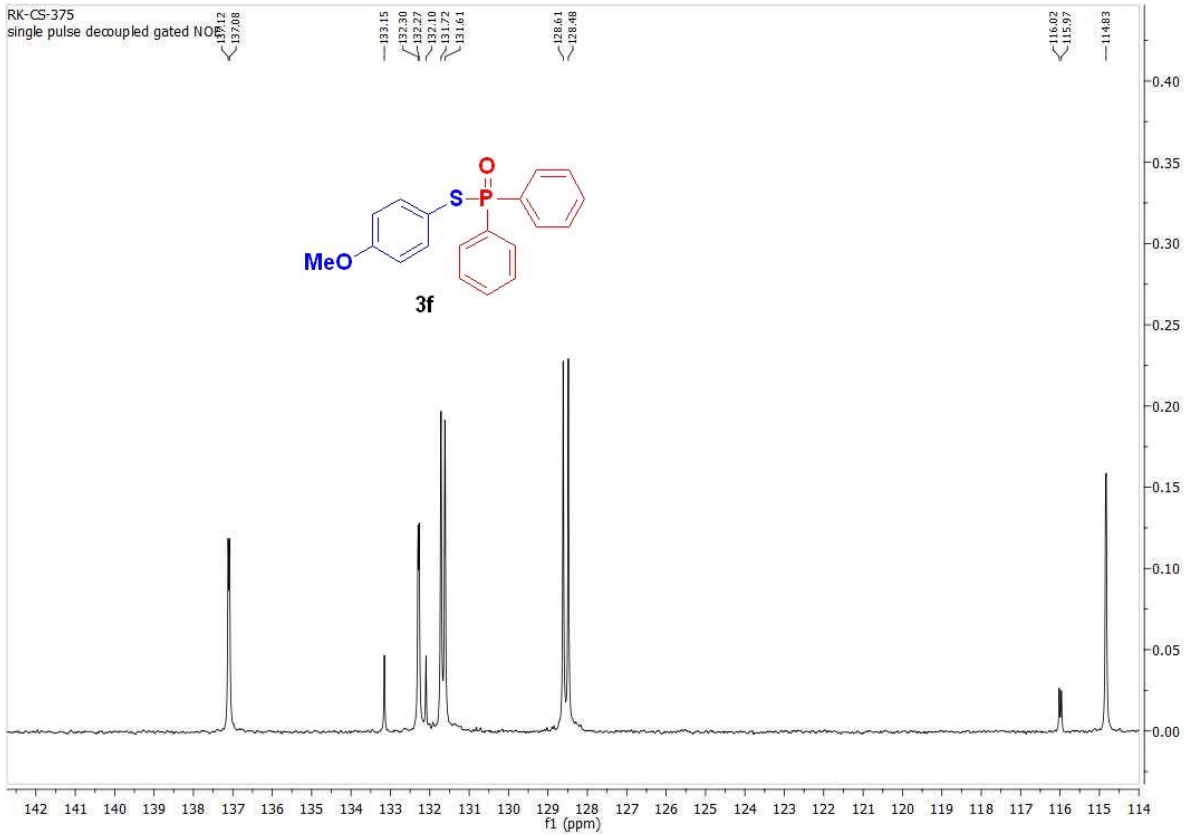
137.12
137.08
133.15
132.30
132.27
132.10
131.72
131.61
128.61
128.48
116.02
115.97
114.83
77.42
77.10
76.78
55.31
MeO
S
P
O
3f
f1 (ppm)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133.15
132.30
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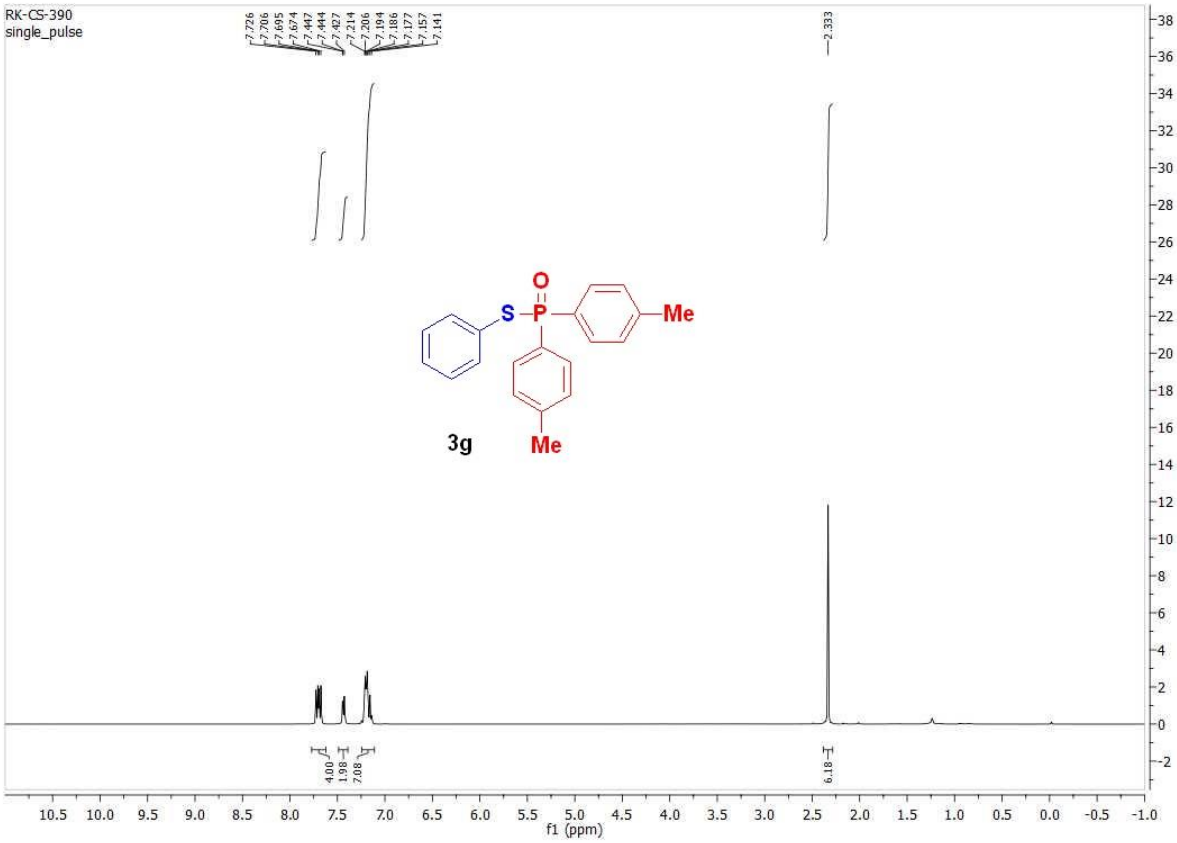
131.61
128.61
128.48
116.02
115.97
114.83
MeO
3f
f1 (ppm)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7.194
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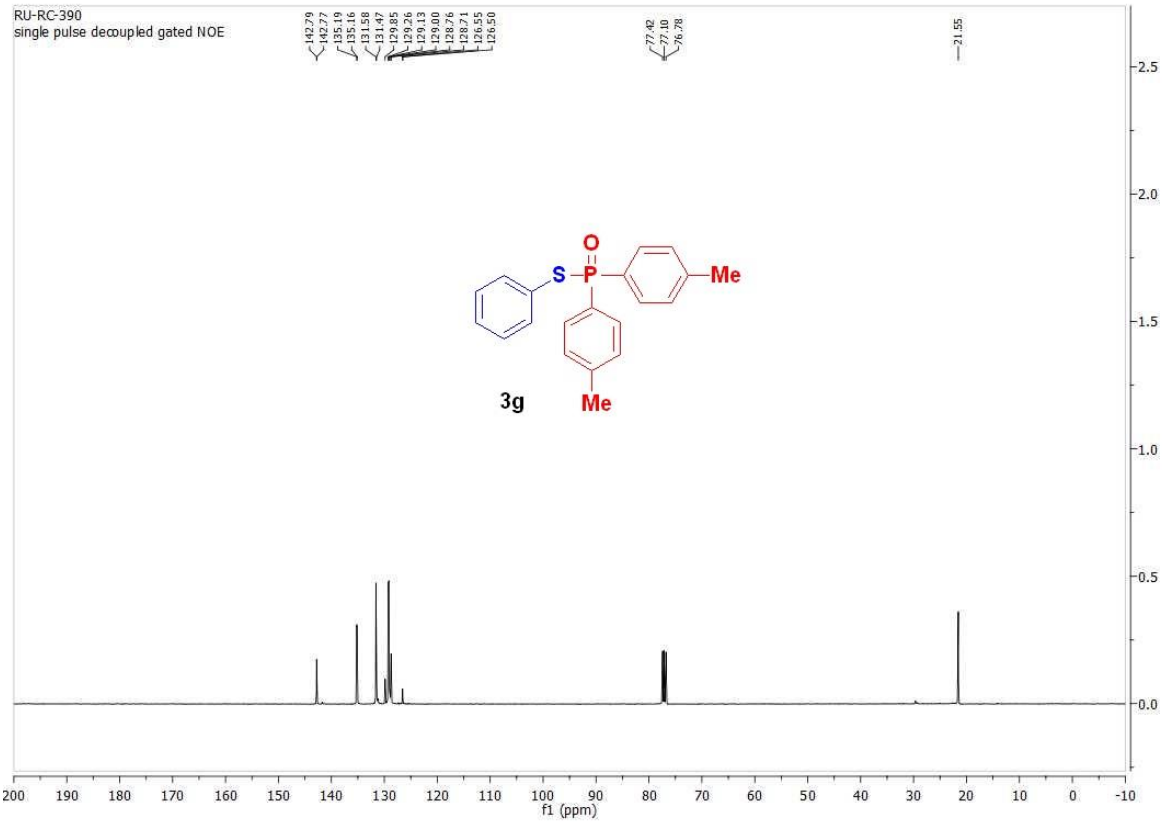
7.157
7.141
2.333
4.00
1.98
7.08
6.18
3g
Me
Me
f1 (ppm)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129.13
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128.76
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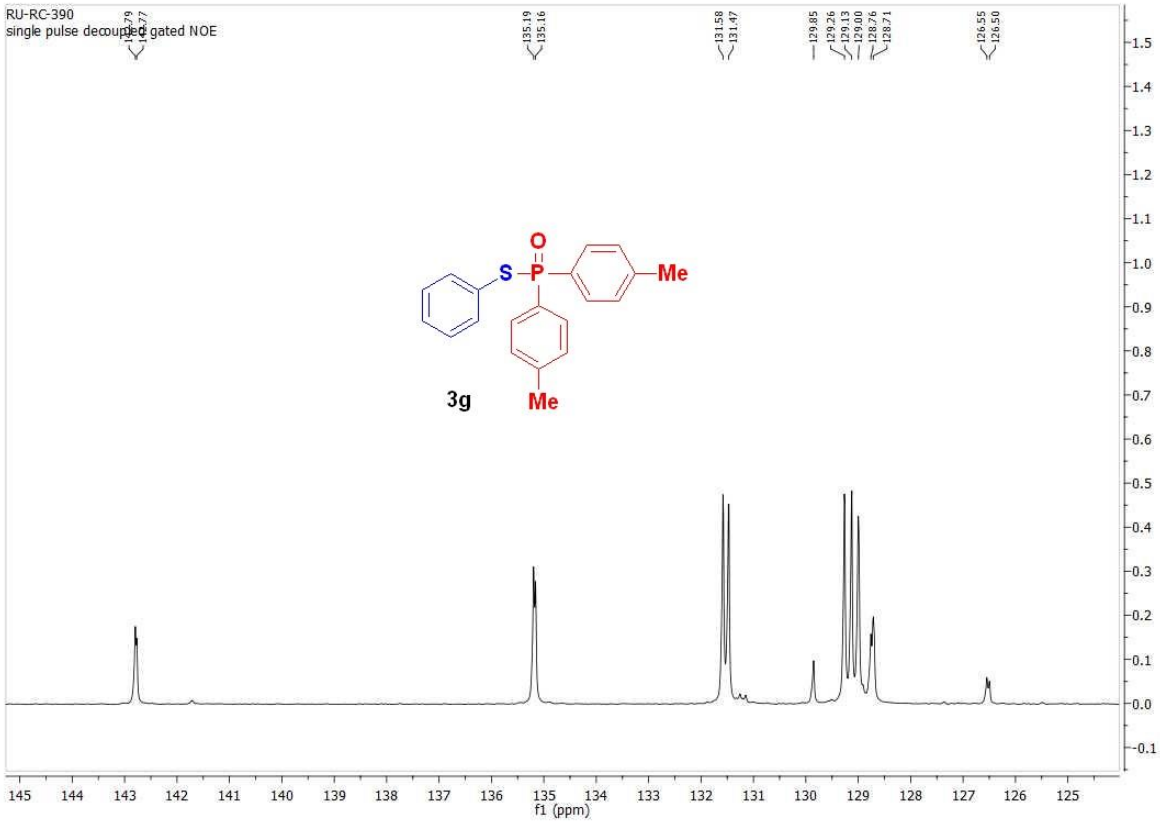
77.42
77.10
76.78
21.55
O
S
P
Me
3g
Me
f1 (ppm)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135.16
131.58
131.47
129.85
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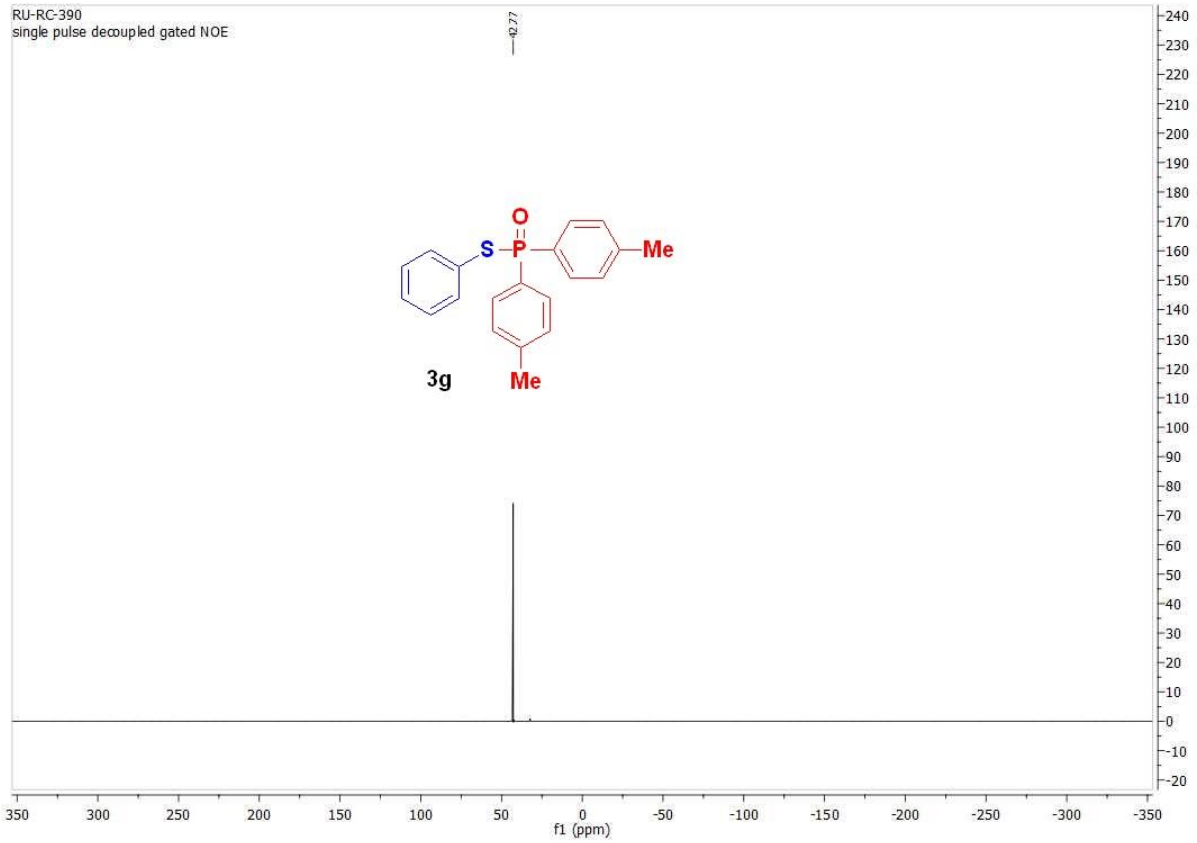
128.76
128.71
126.55
126.50
O
S
P
Me
3g
Me
f1 (ppm)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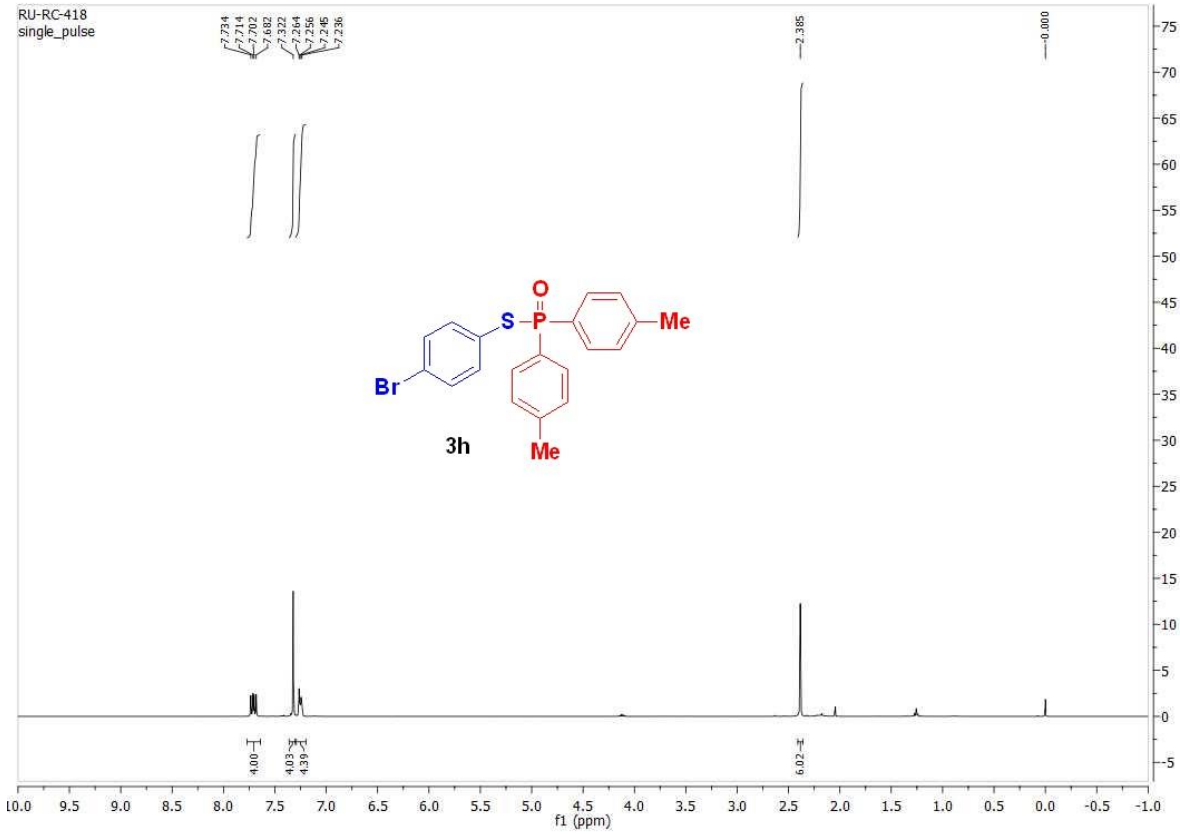
Me
3g
Me
f1 (ppm)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S
P
Me
Br
3h
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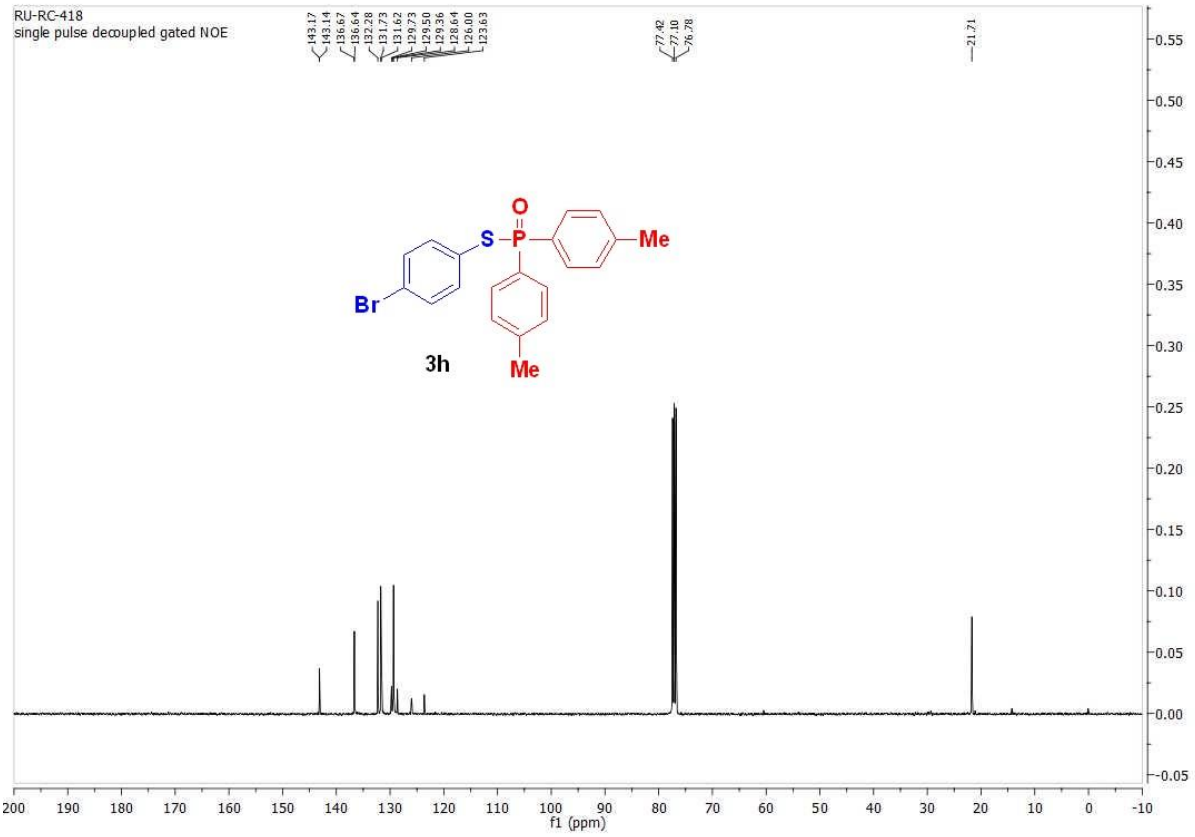
4.03
4.39
6.02
f1 (ppm)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single pulse decoupled gated NOE
143.17
143.14
136.67
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129.50
129.36
128.64
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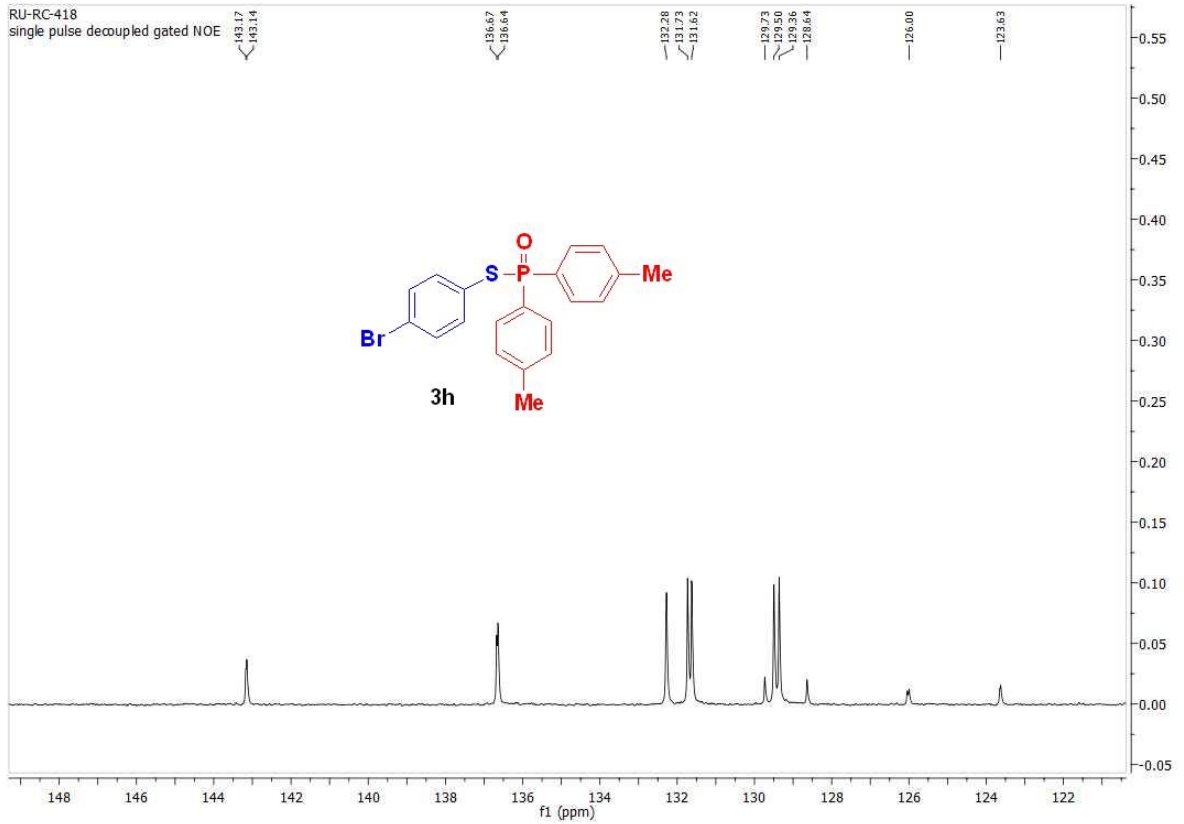
123.63
77.42
77.10
76.78
21.71
O
S
P
Me
Br
Me
3h
f1 (ppm)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single pulse decoupled gated NOE
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143.14
136.67
136.64
132.28
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131.62
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128.64
126.00
123.63
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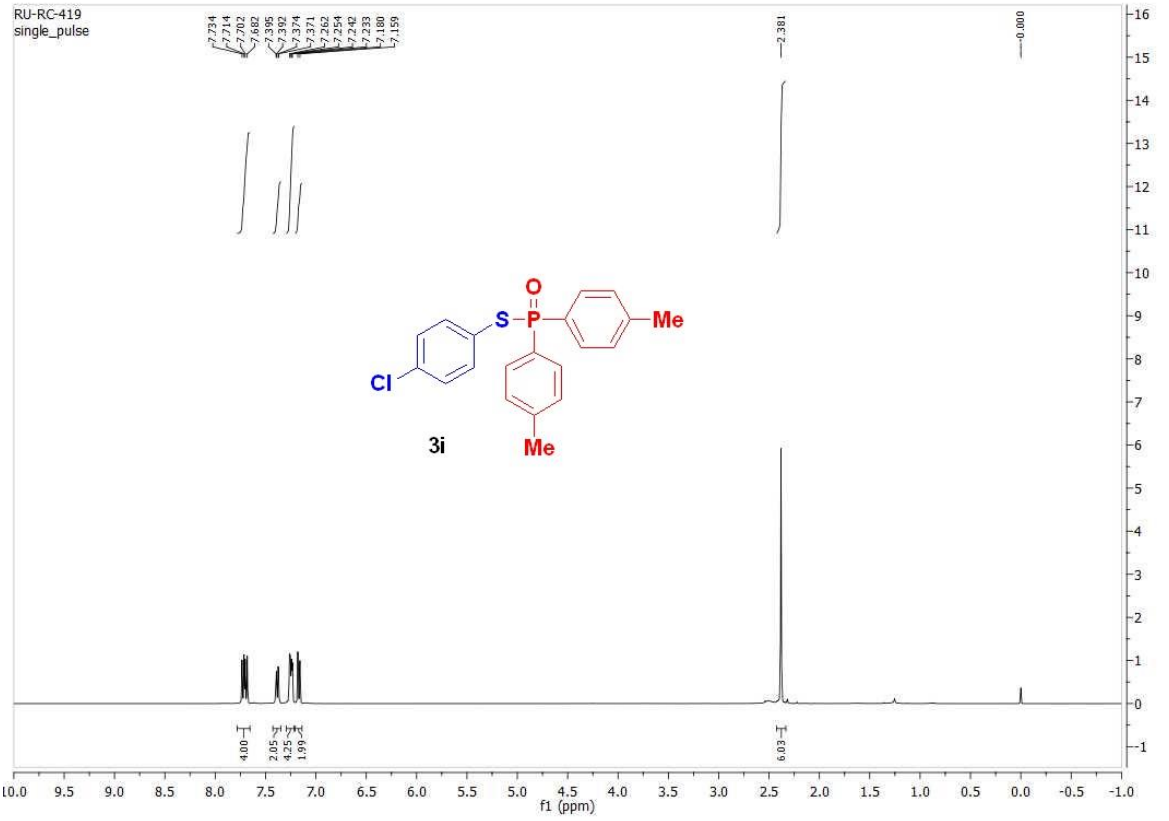
S
P
Me
Br
Me
3h
f1 (ppm)


RU-RC-419
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7.734
7.714
7.702
7.682
7.395
7.392
7.374
7.371
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7.254
7.242
7.233
7.180
7.159
2.381
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P
Me
Cl
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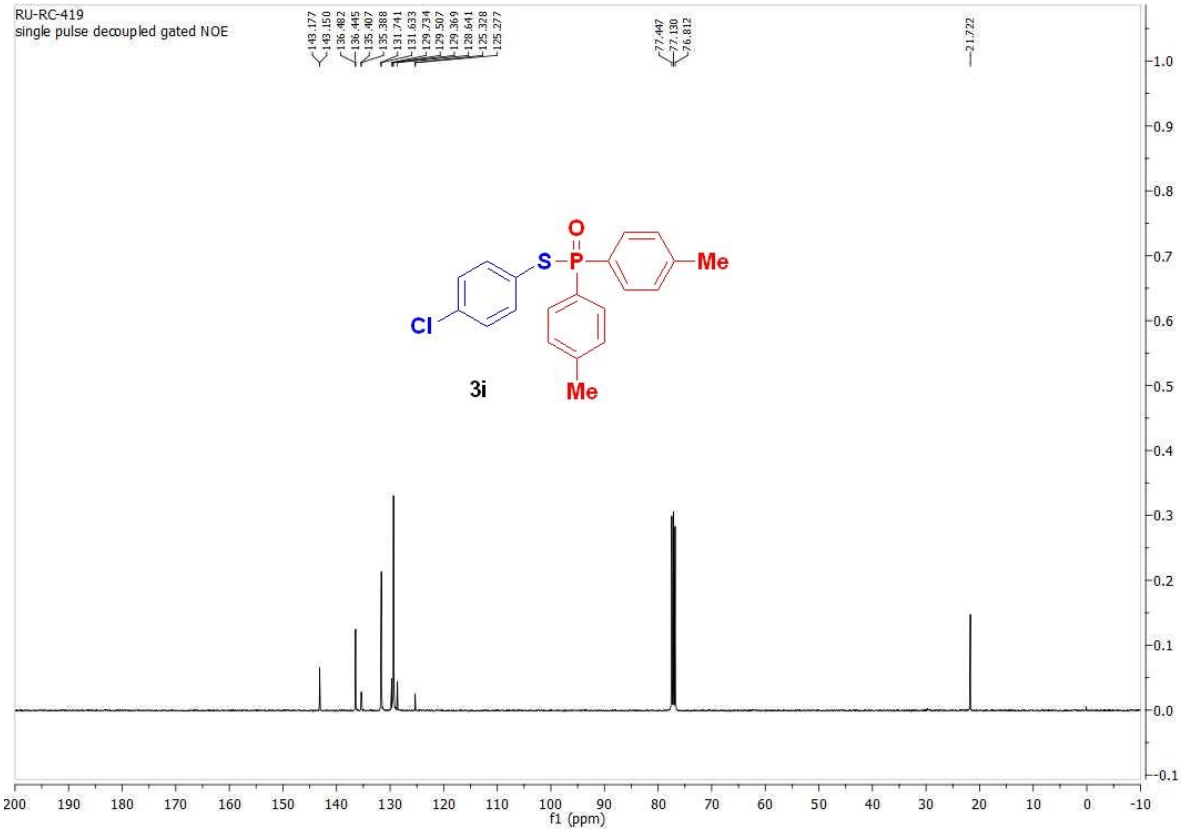
1.99
6.03
f1 (ppm)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single pulse decoupled gated NOE
148.177
146.150
136.482
136.445
135.467
135.388
131.741
131.633
129.734
129.507
129.369
128.641
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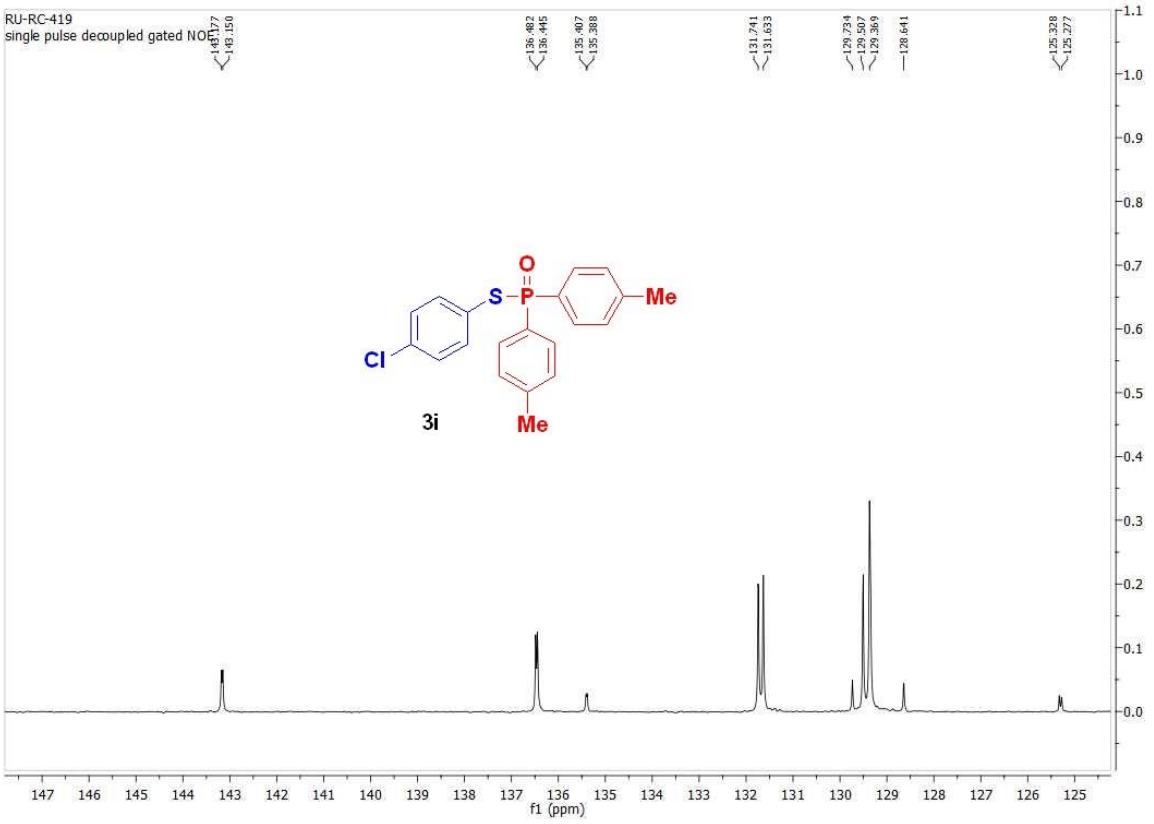
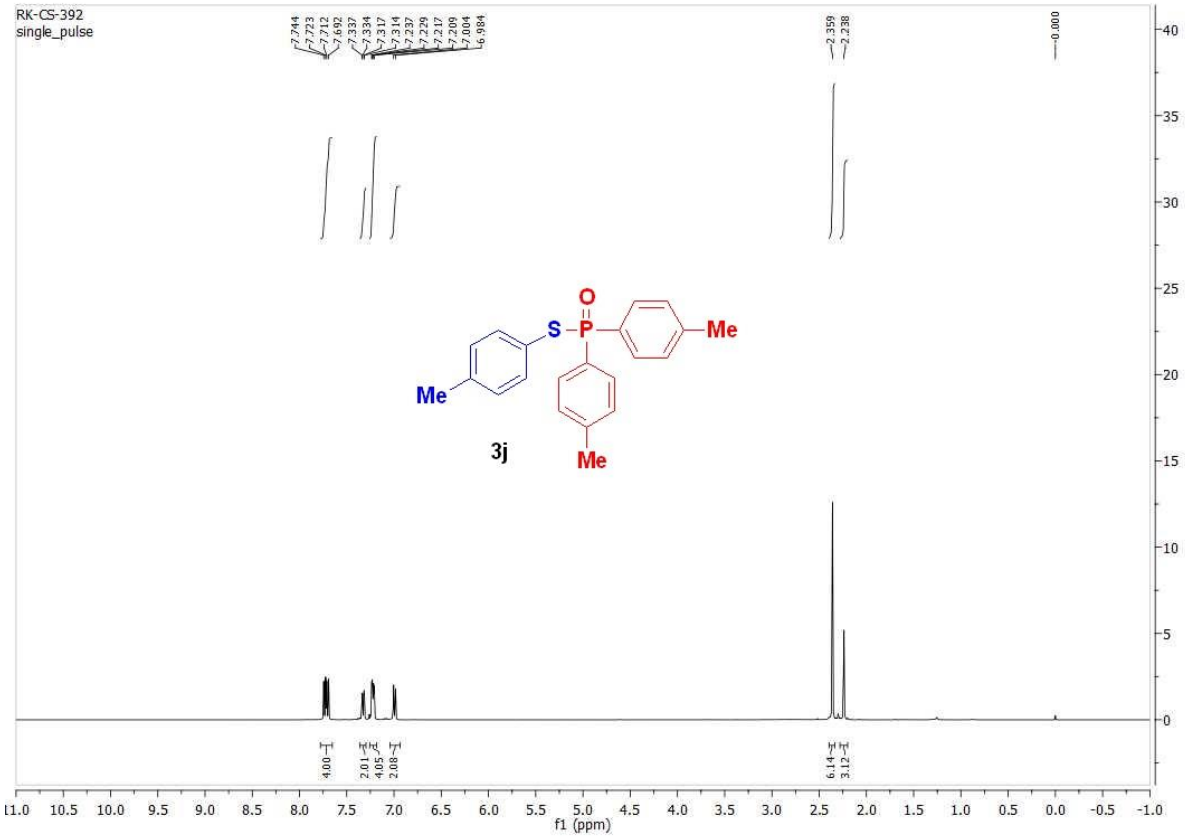
125.277
77.447
77.130
76.812
21.722
O
S
P
Me
Cl
Me
3i
f1 (ppm)


RU-RC-419
single pulse decoupled gated NOE
143.177
143.150
136.482
136.445
135.407
135.388
131.741
131.633
129.734
129.507
129.369
128.641
125.328
125.277
O
S
P
Me
Cl
Me
3i
f1 (ppm)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7.723
7.712
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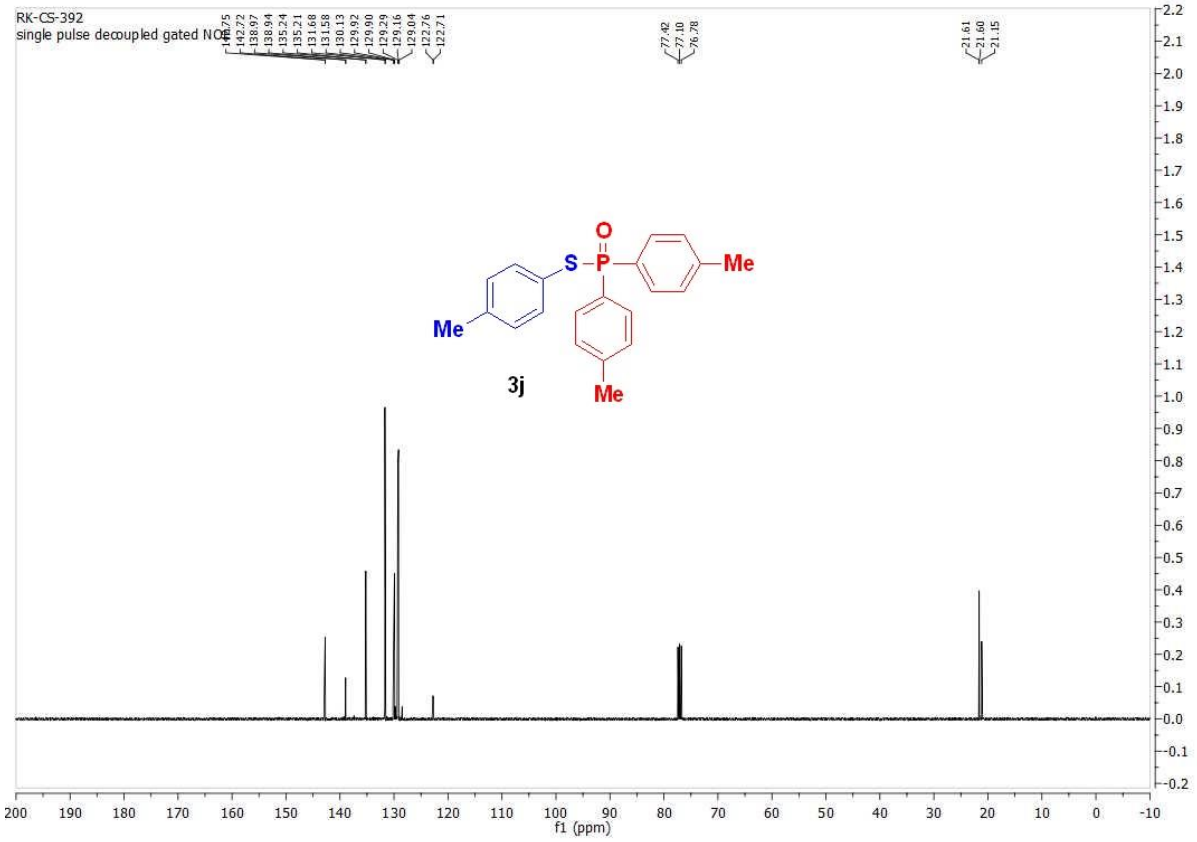
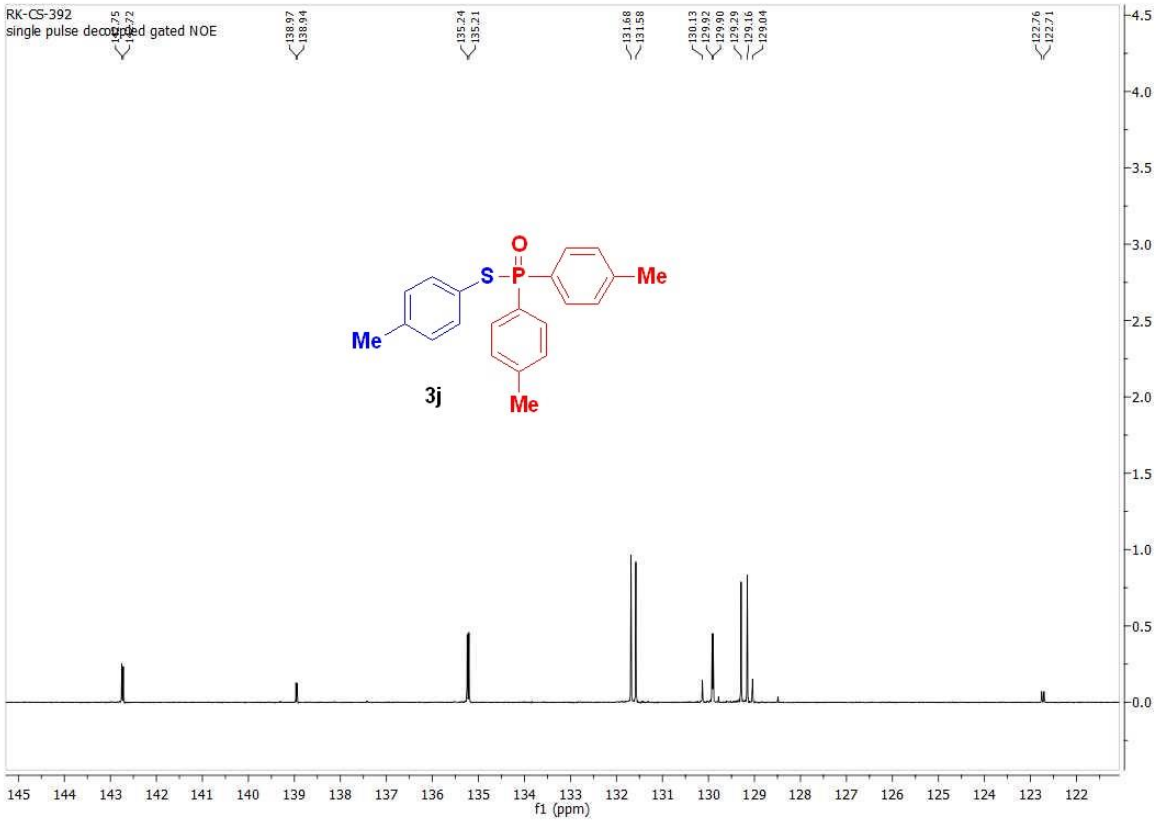
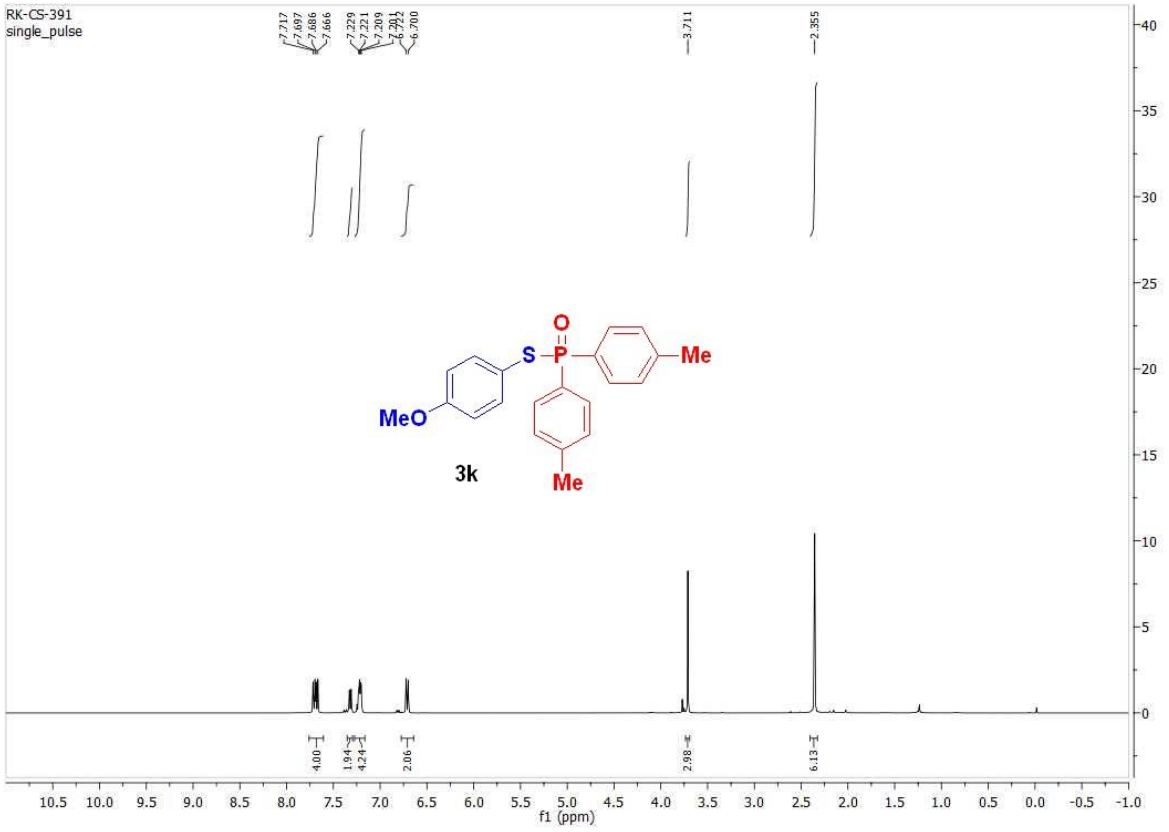
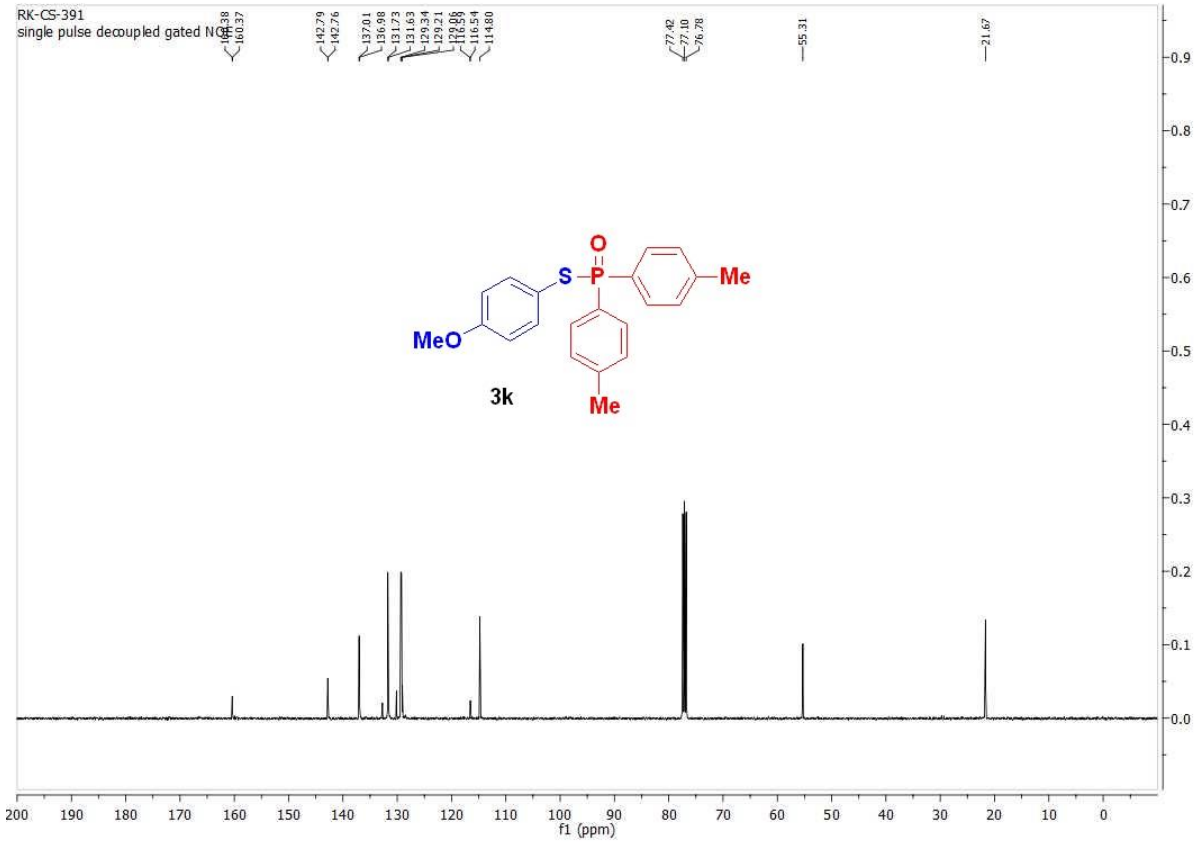
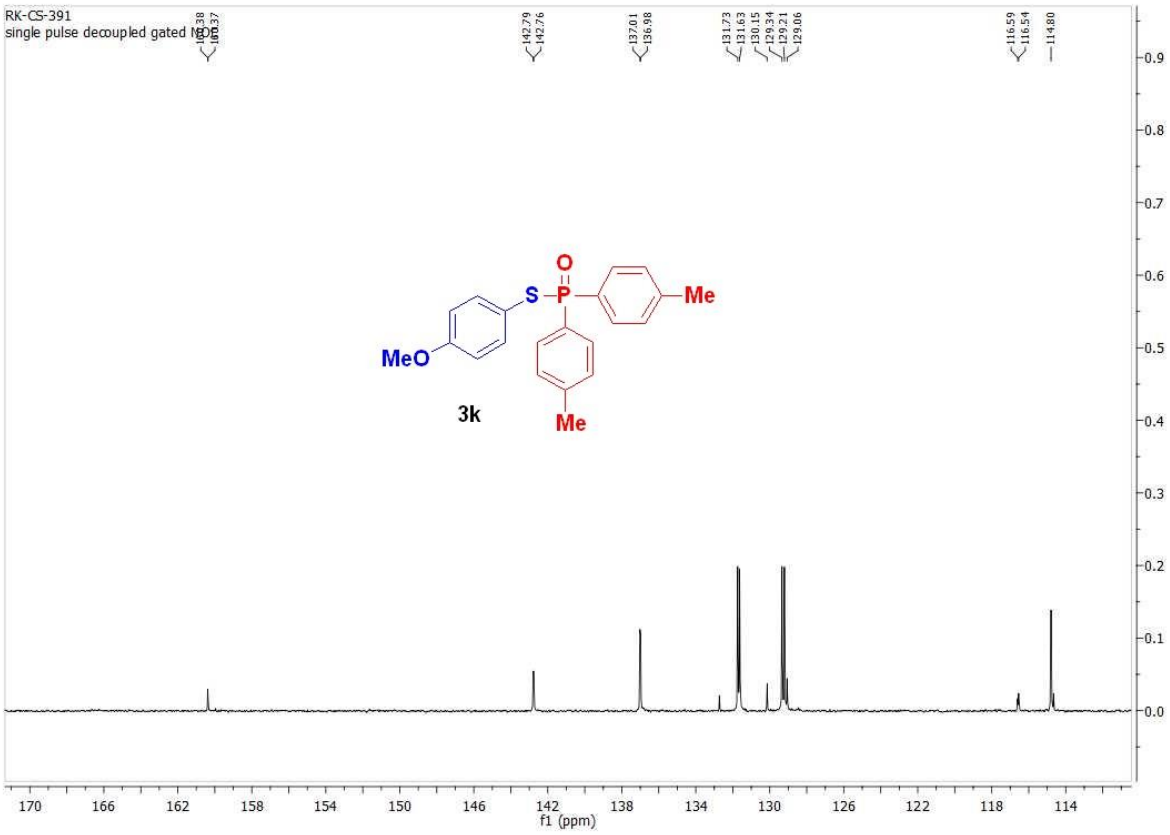
7.229
7.217
7.209
7.004
6.984
2.359
2.238
0.000
O
S
P
Me
Me
Me
3j
4.00
2.01
4.05
2.08
6.14
3.12
f1 (ppm)

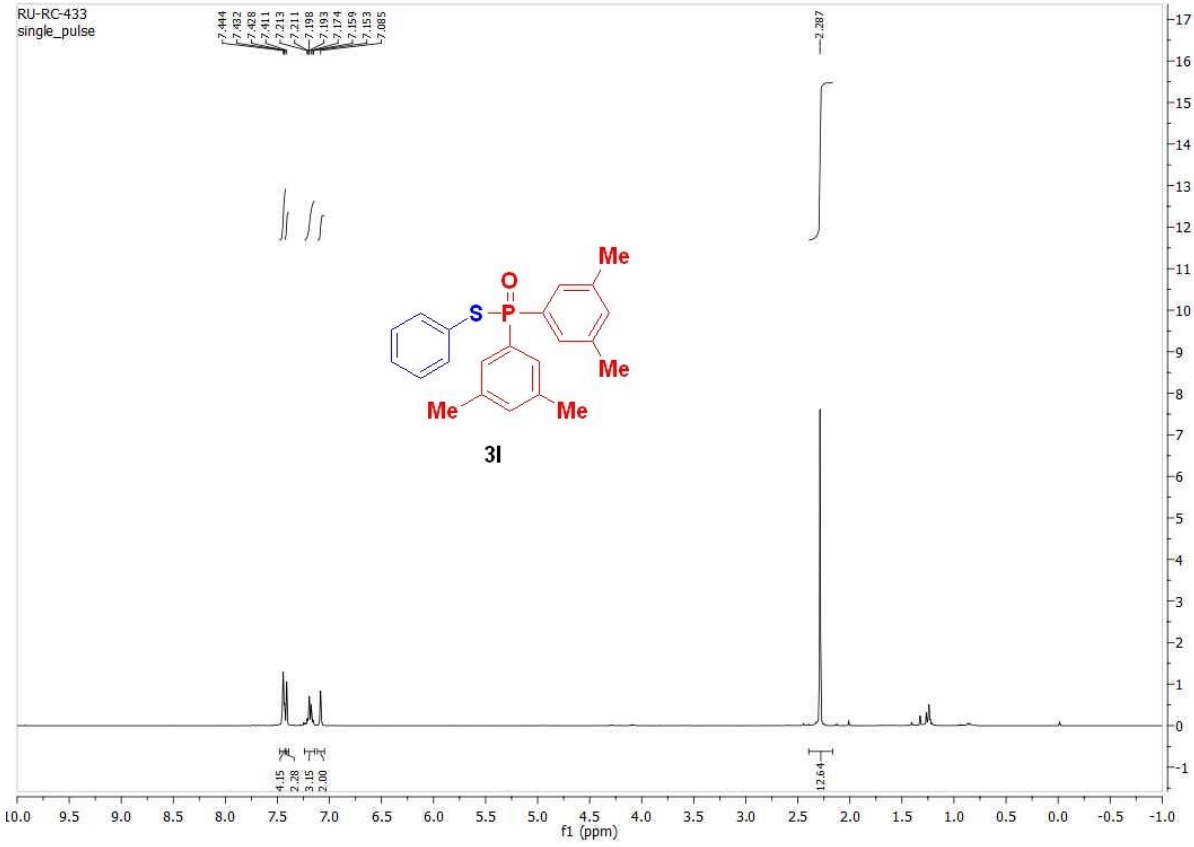

RK-CS-392
single pulse decoupled gated NOE
142.75
142.72
138.97
138.94
135.24
135.21
131.68
131.58
130.13
129.92
129.90
129.29
129.16
129.04
122.76
122.71
77.42
77.10
76.78
21.61
21.60
21.15
O
S
P
Me
Me
Me
3j
f1 (ppm)

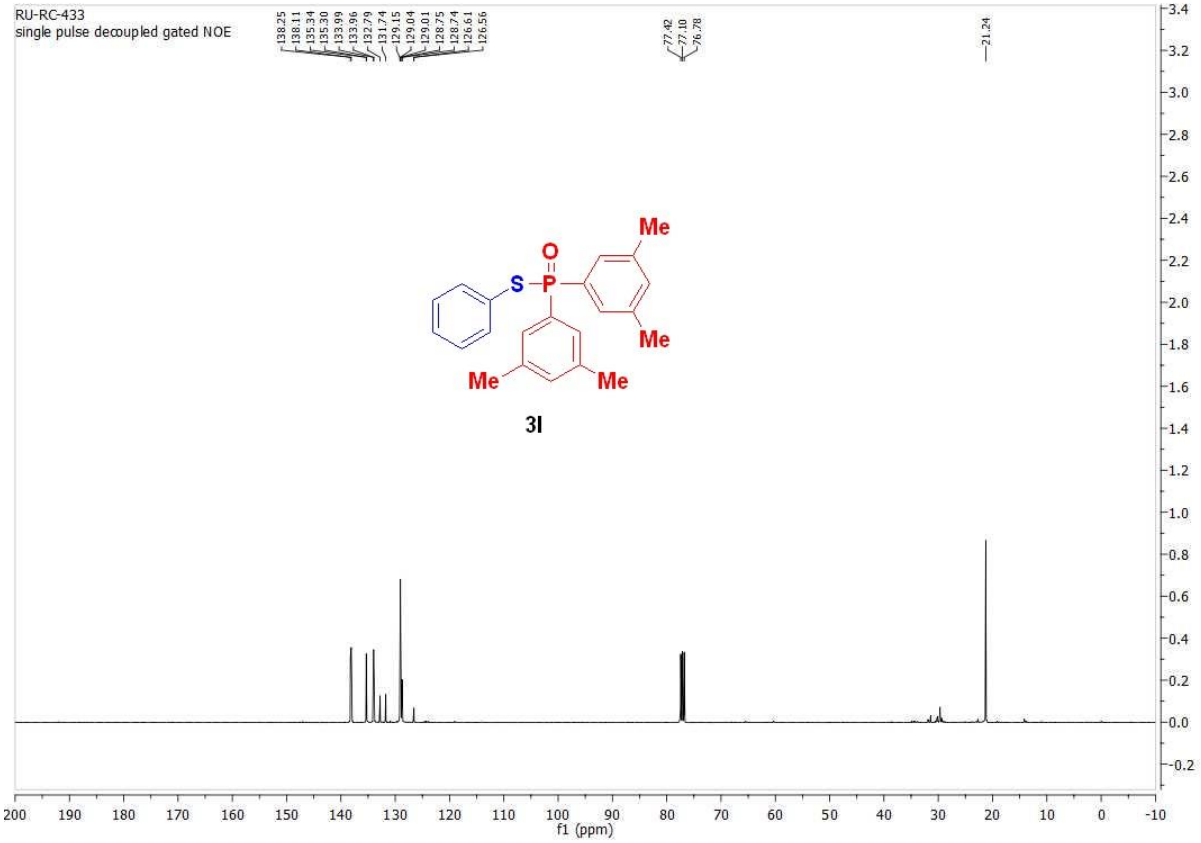

RK-CS-392
single pulse decoupled gated NOE
142.75
142.72
138.97
138.94
135.24
135.21
131.68
131.58
130.13
129.92
129.90
129.29
129.16
129.04
122.76
122.71
O
S
P
Me
Me
Me
3j
f1 (ppm)


RK-CS-391
single_pulse
7.717
7.697
7.686
7.666
7.229
7.221
7.209
7.201
6.722
6.700
3.711
2.355
O
S
P
Me
MeO
Me
3k
4.00
1.94
4.24
2.06
2.98
6.13
f1 (ppm)

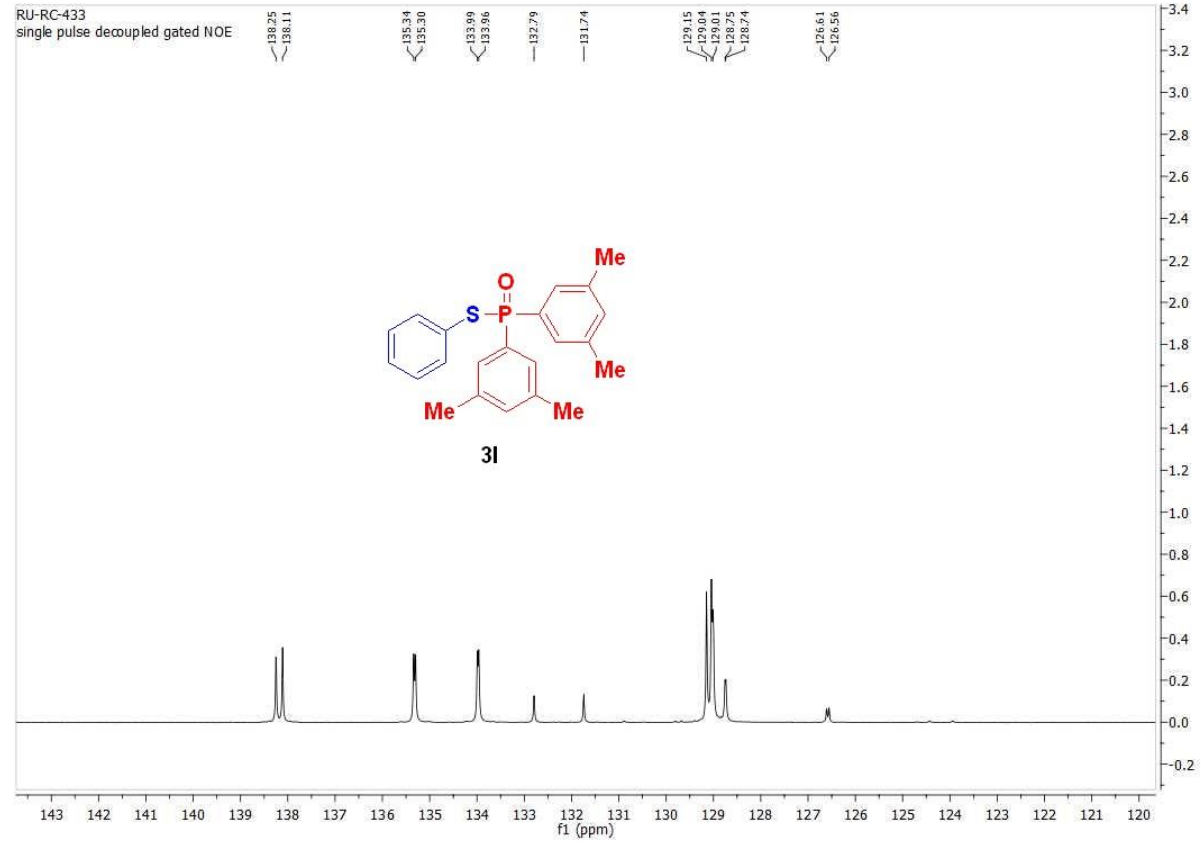

RK-CS-391
single pulse decoupled gated NOE
160.38
160.37
142.79
142.76
137.01
136.98
131.73
131.63
129.34
129.21
116.54
114.80
77.42
77.10
76.78
55.31
21.67
O
S
P
Me
MeO
Me
3k
f1 (ppm)


RK-CS-391
single pulse decoupled gated NO
142.79
142.76
137.01
136.98
131.73
131.63
130.15
129.34
129.21
129.06
116.59
116.54
114.80
O
S
P
Me
MeO
Me
3k
f1 (ppm)

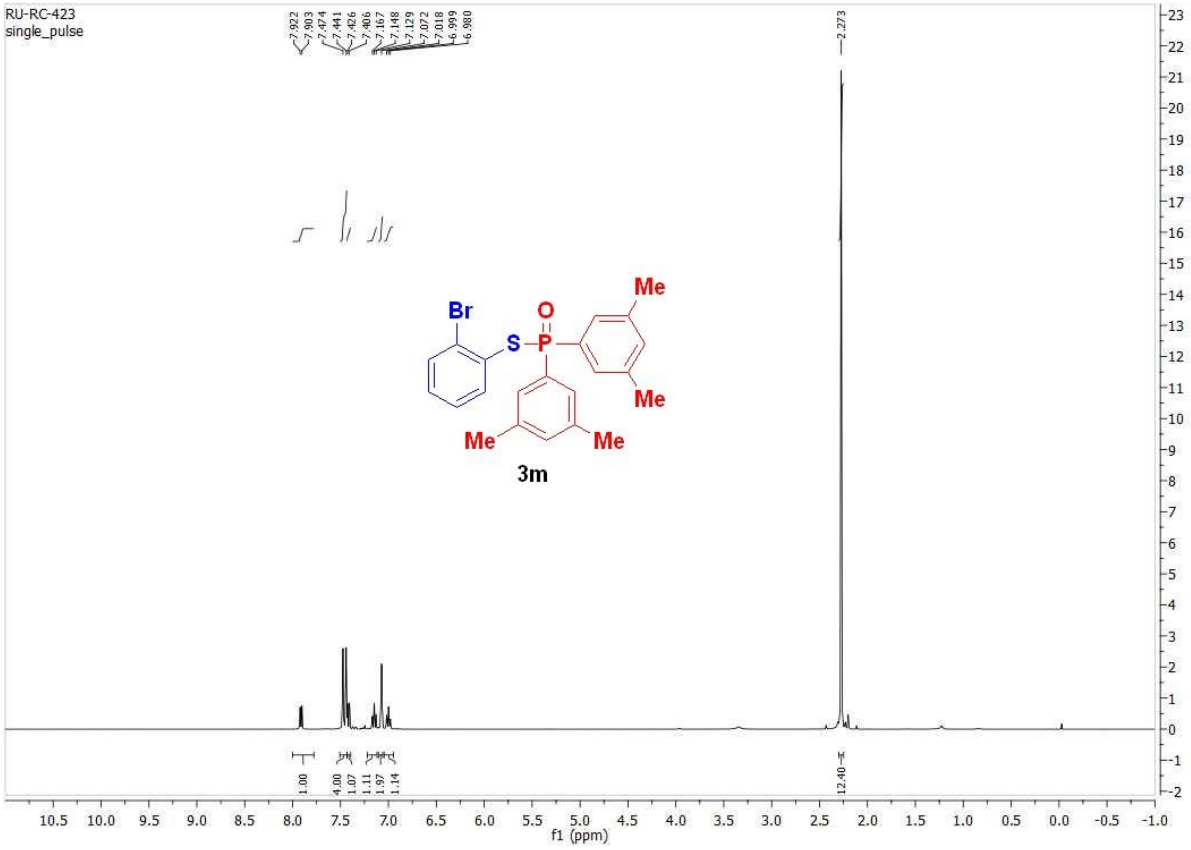

RU-RC-433
single_pulse
7.444
7.432
7.428
7.411
7.213
7.211
7.198
7.193
7.174
7.159
7.153
7.085
2.287
O
S
P
Me
Me
Me
Me
3l
4.15
2.38
3.15
2.00
12.64
f1 (ppm)

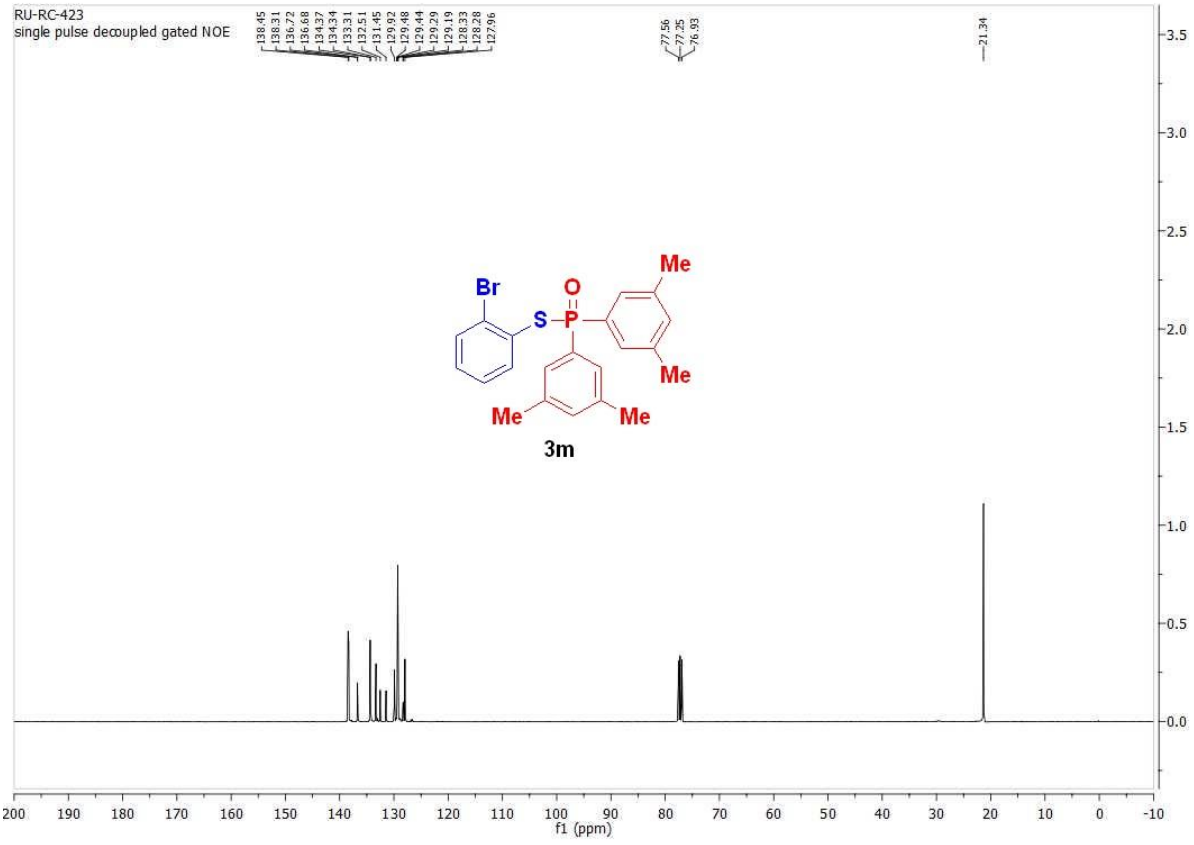

RU-RC-433
single pulse decoupled gated NOE
138.25
138.11
135.34
135.30
133.99
133.96
132.79
131.74
129.15
129.04
129.01
128.75
128.74
126.61
126.56
77.42
77.10
76.78
21.24
Me
O
S
P
Me
Me
Me
f1 (ppm)

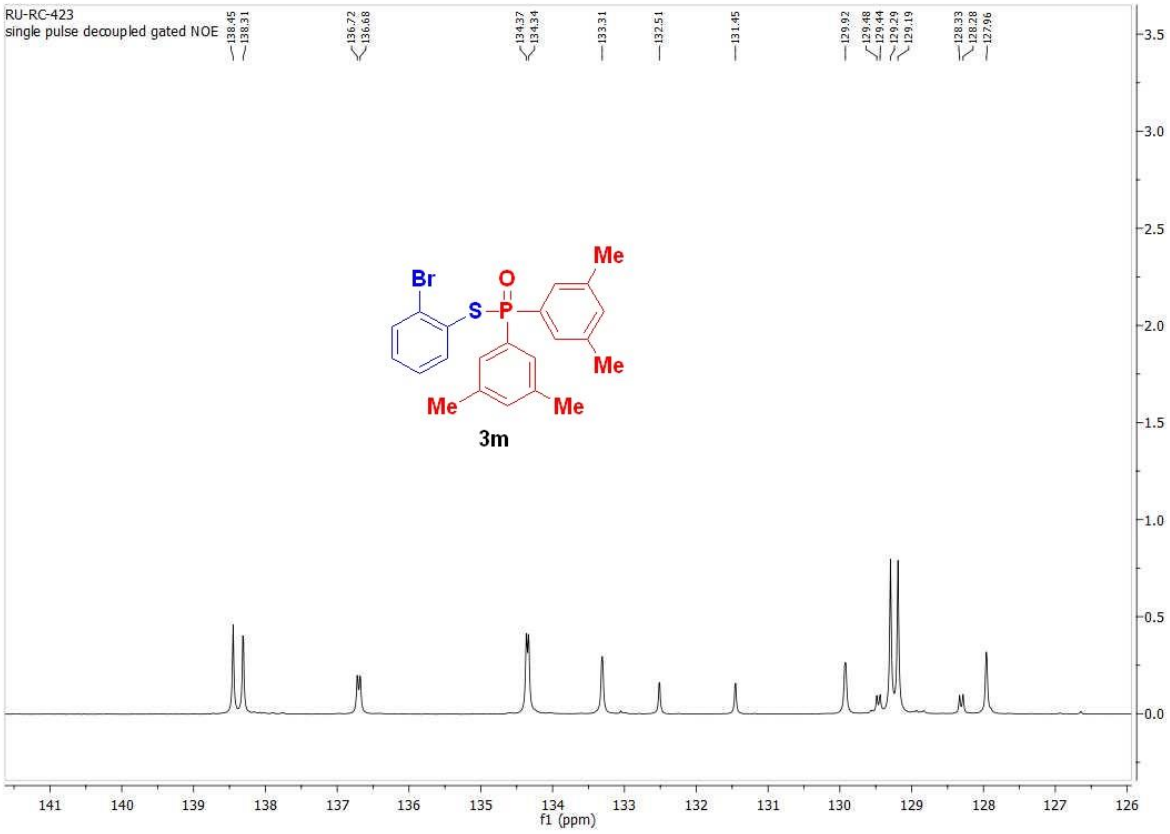
3l

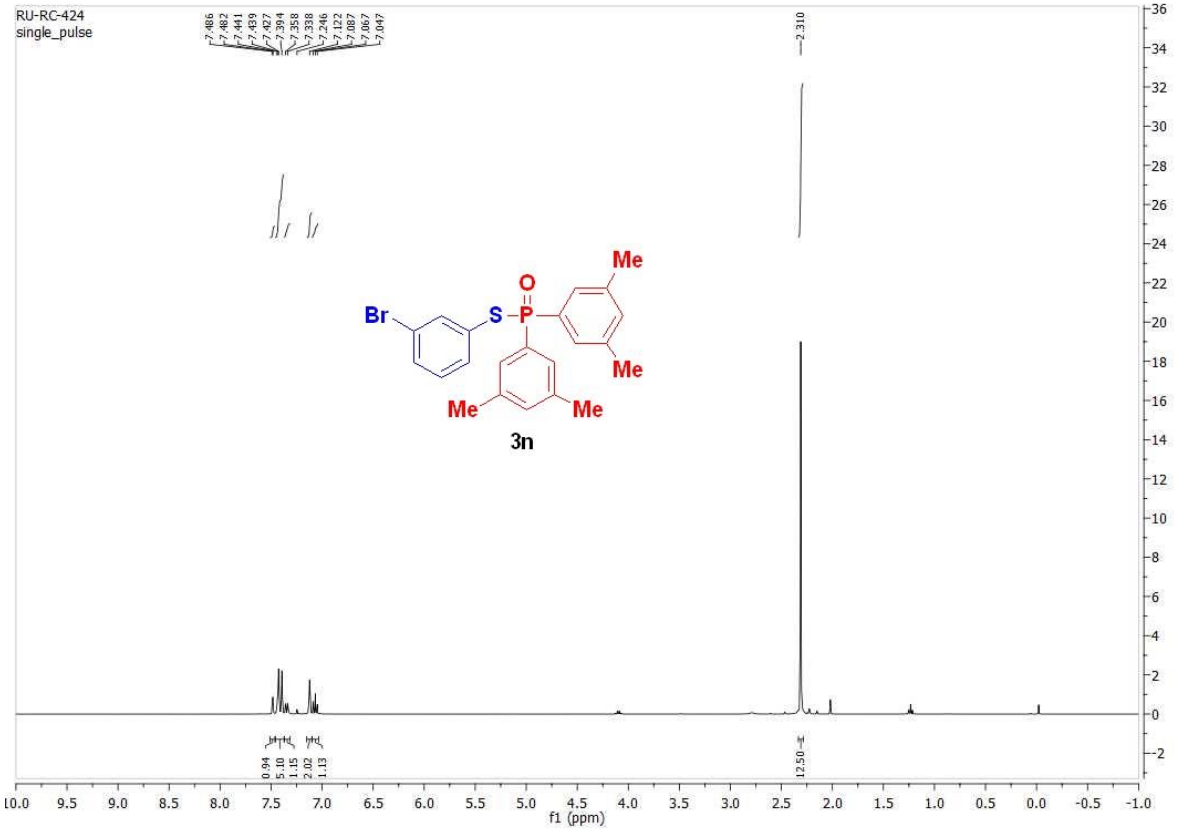

RU-RC-433
single pulse decoupled gated NOE
138.25
138.11
135.34
135.30
133.99
133.96
132.79
131.74
129.15
129.04
129.01
128.75
128.74
126.61
126.56
Me
O
S
P
Me
Me
Me
f1 (ppm)

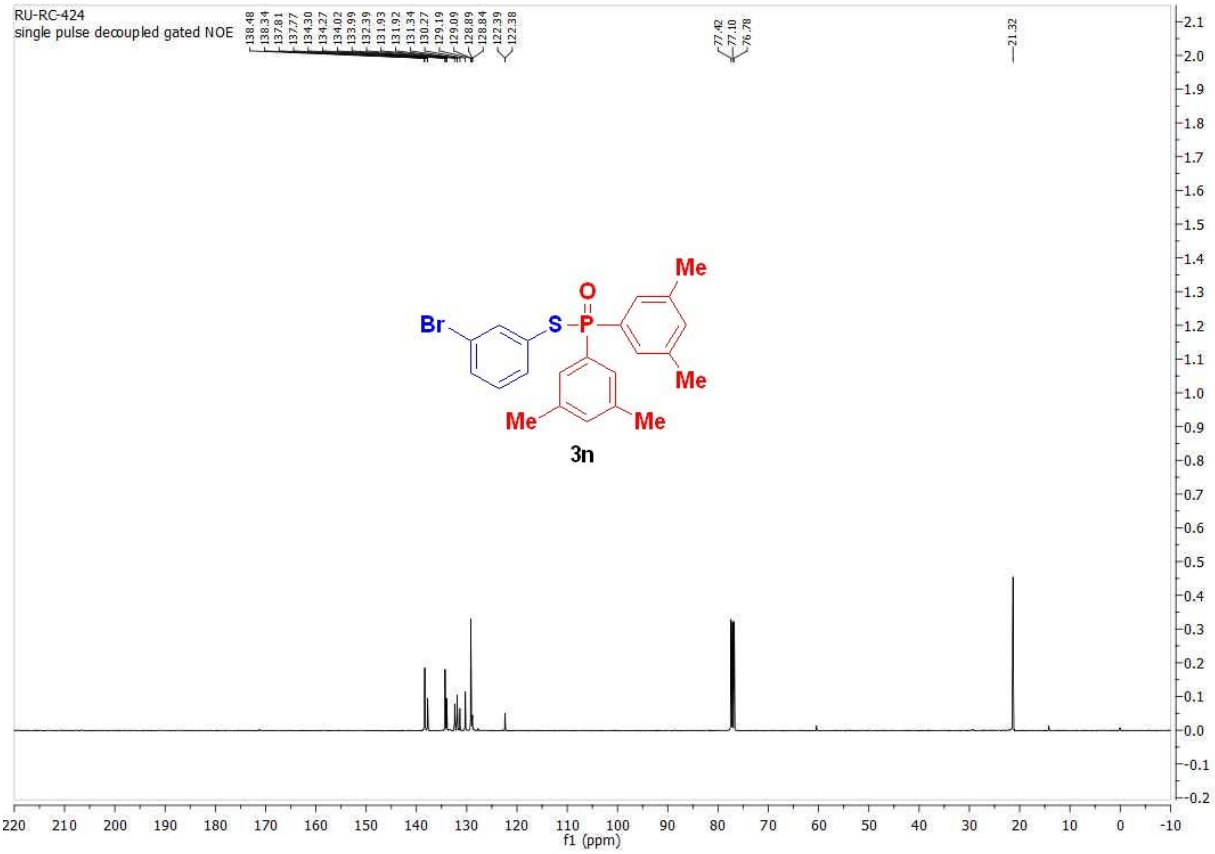
3l

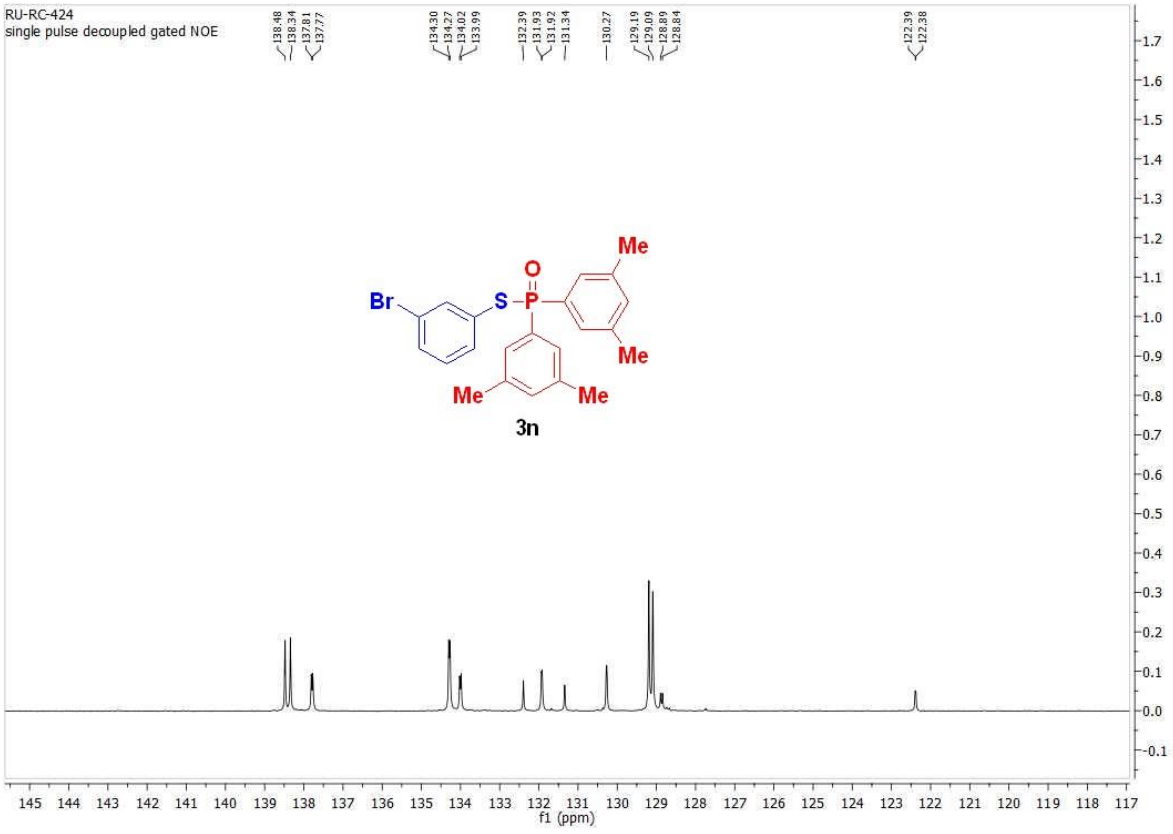

RU-RC-423
single_pulse
7.922
7.903
7.474
7.441
7.426
7.406
7.167
7.148
7.129
7.072
7.018
6.999
6.980
2.273
Br
O
S
P
Me
Me
Me
Me
3m
1.00
4.00
1.07
1.11
1.97
1.14
12.40
f1 (ppm)

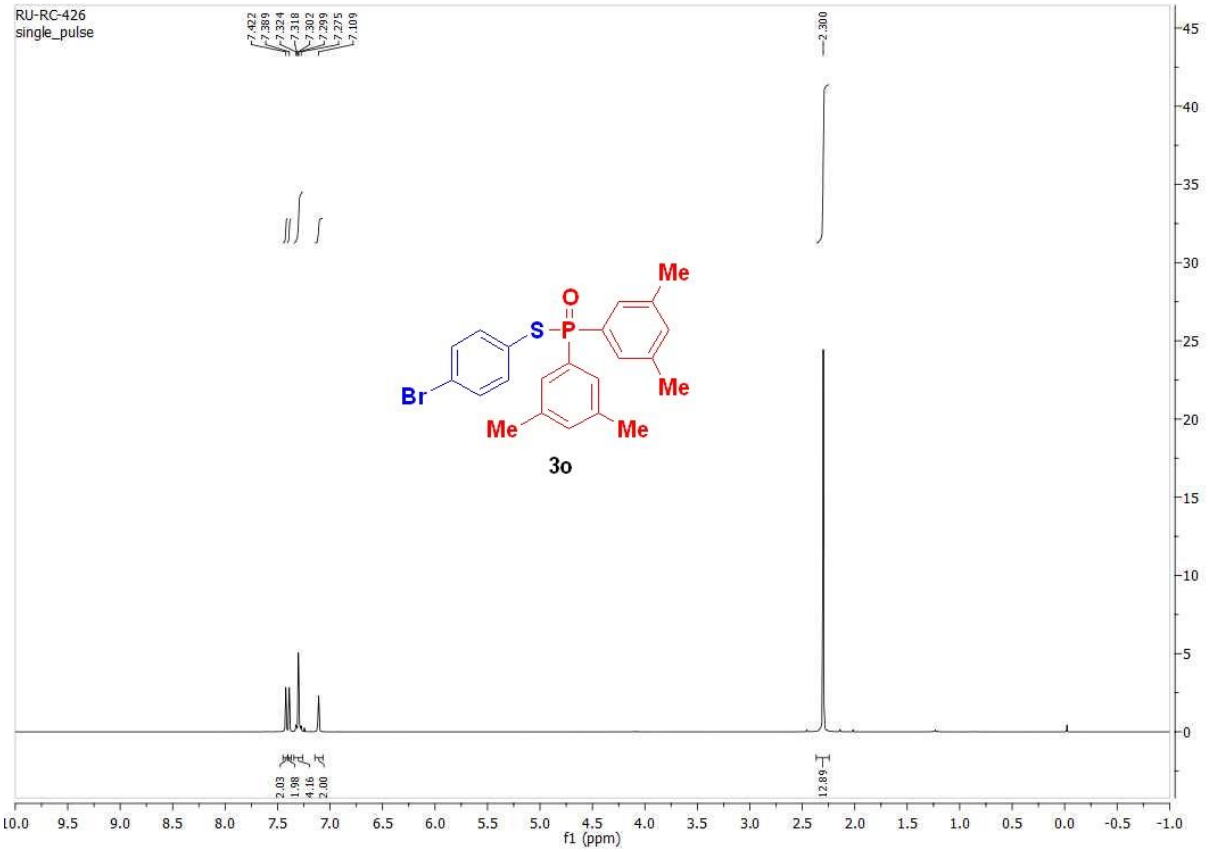

RU-RC-423
single pulse decoupled gated NOE
138.45
138.31
136.72
136.68
134.37
134.34
133.31
132.51
131.45
129.92
129.48
129.44
129.29
129.19
128.33
128.28
127.96
77.56
77.25
76.93
21.34
Br
O
S
P
Me
Me
Me
Me
3m
f1 (ppm)

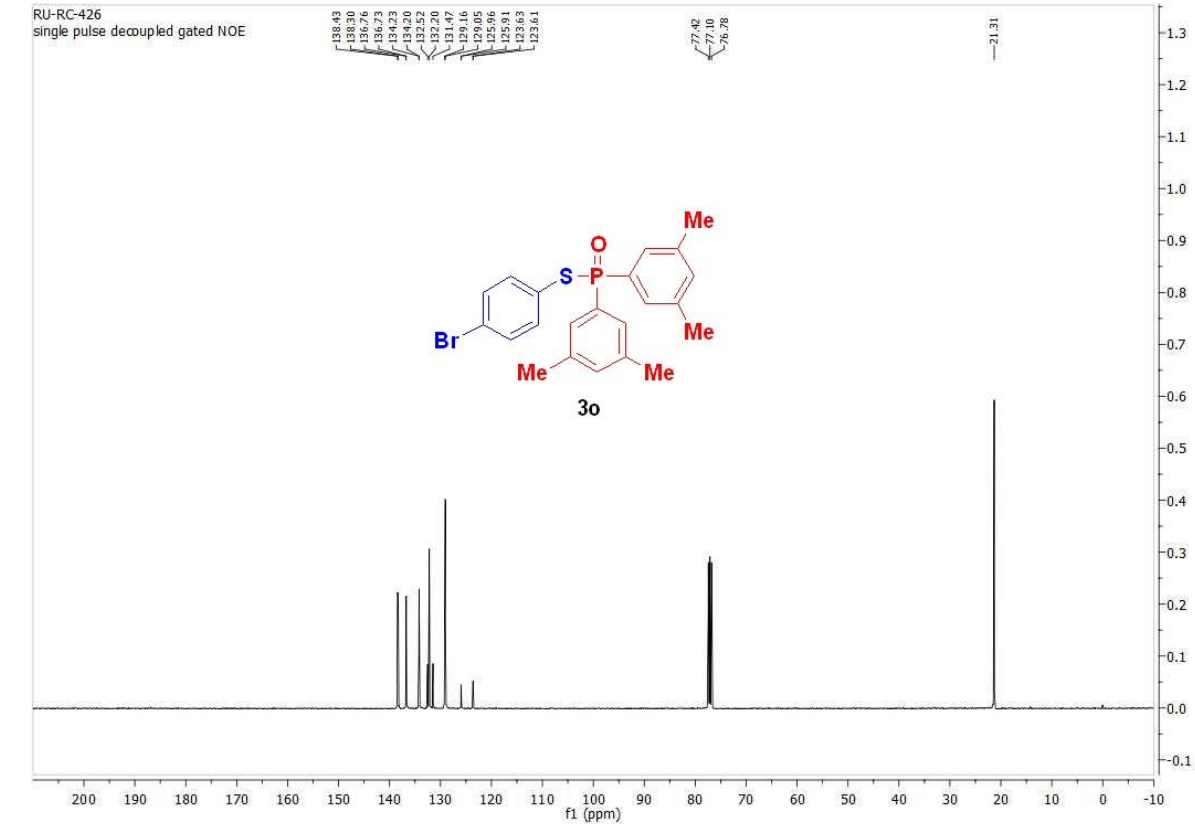

RU-RC-423
single pulse decoupled gated NOE
138.45
138.31
136.72
136.68
134.37
134.34
133.31
132.51
131.45
129.92
129.48
129.44
129.29
129.19
128.33
128.28
127.96
Br
S
O
P
Me
Me
Me
Me
3m
f1 (ppm)

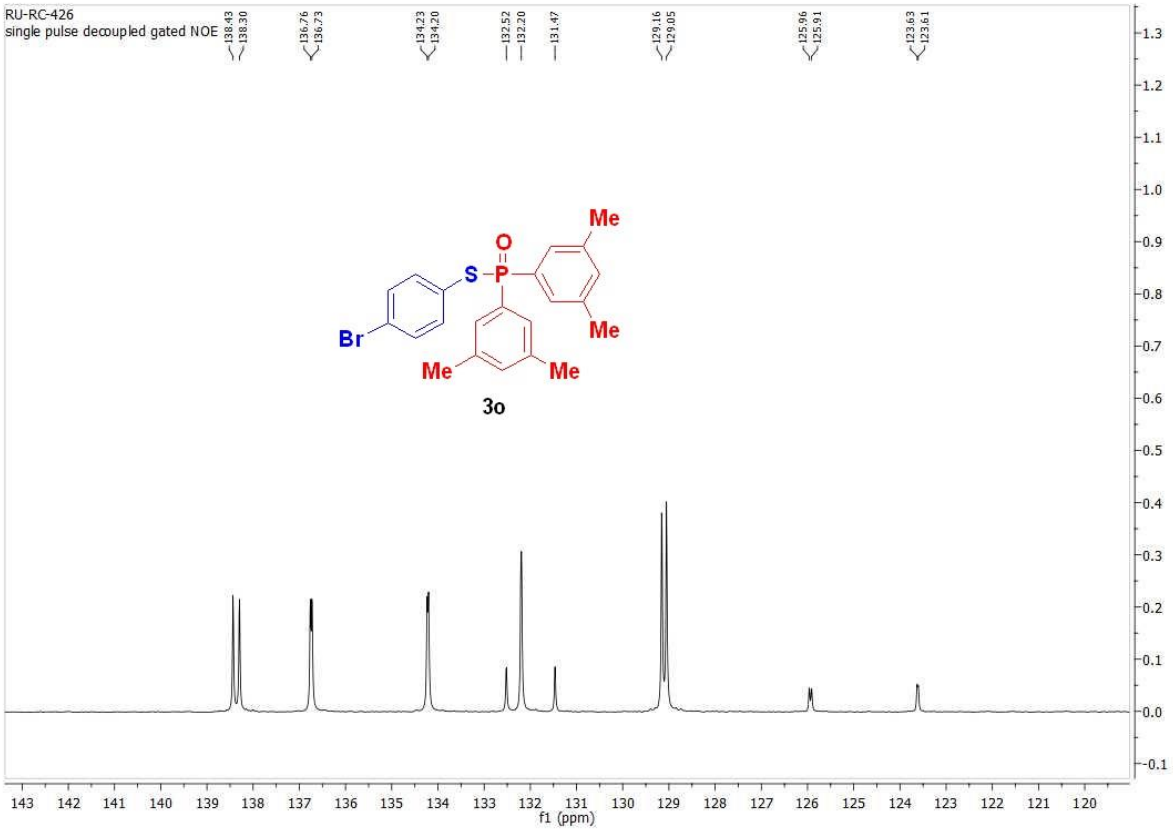

RU-RC-424
single_pulse
7.486
7.482
7.441
7.439
7.427
7.394
7.358
7.338
7.246
7.122
7.087
7.067
7.047
2.310
0.94
5.10
1.15
2.02
1.13
12.50
Br
S
O
P
Me
Me
Me
Me
3n
f1 (ppm)


RU-RC-424
single pulse decoupled gated NOE
138.48
138.34
137.81
137.77
134.30
134.27
134.02
133.99
132.39
131.93
131.92
131.34
130.27
129.19
129.09
128.89
128.84
122.39
122.38
77.42
77.10
76.78
21.32
Br
S
O
P
Me
Me
Me
Me
3n
f1 (ppm)

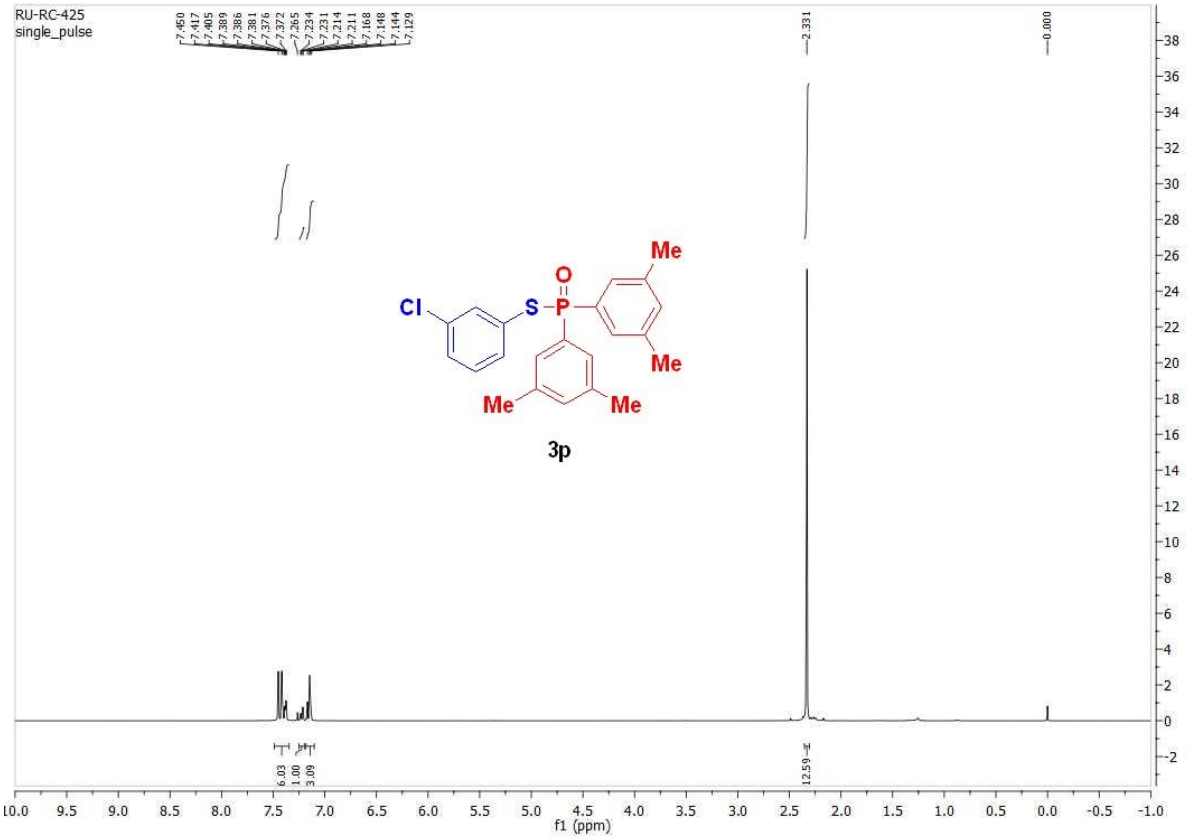

RU-RC-424
single pulse decoupled gated NOE
138.48
138.34
137.81
137.77
134.30
134.27
134.02
133.99
132.39
131.93
131.92
131.34
130.27
129.19
129.09
128.89
128.84
122.39
122.38
Br
S
O
P
Me
Me
Me
Me
3n
f1 (ppm)


RU-RC-426
single_pulse
7.422
7.389
7.324
7.318
7.302
7.299
7.275
7.109
2.300
Me
O
S
P
Me
Br
Me
Me
3o
2.03
1.98
4.16
2.00
12.89
f1 (ppm)

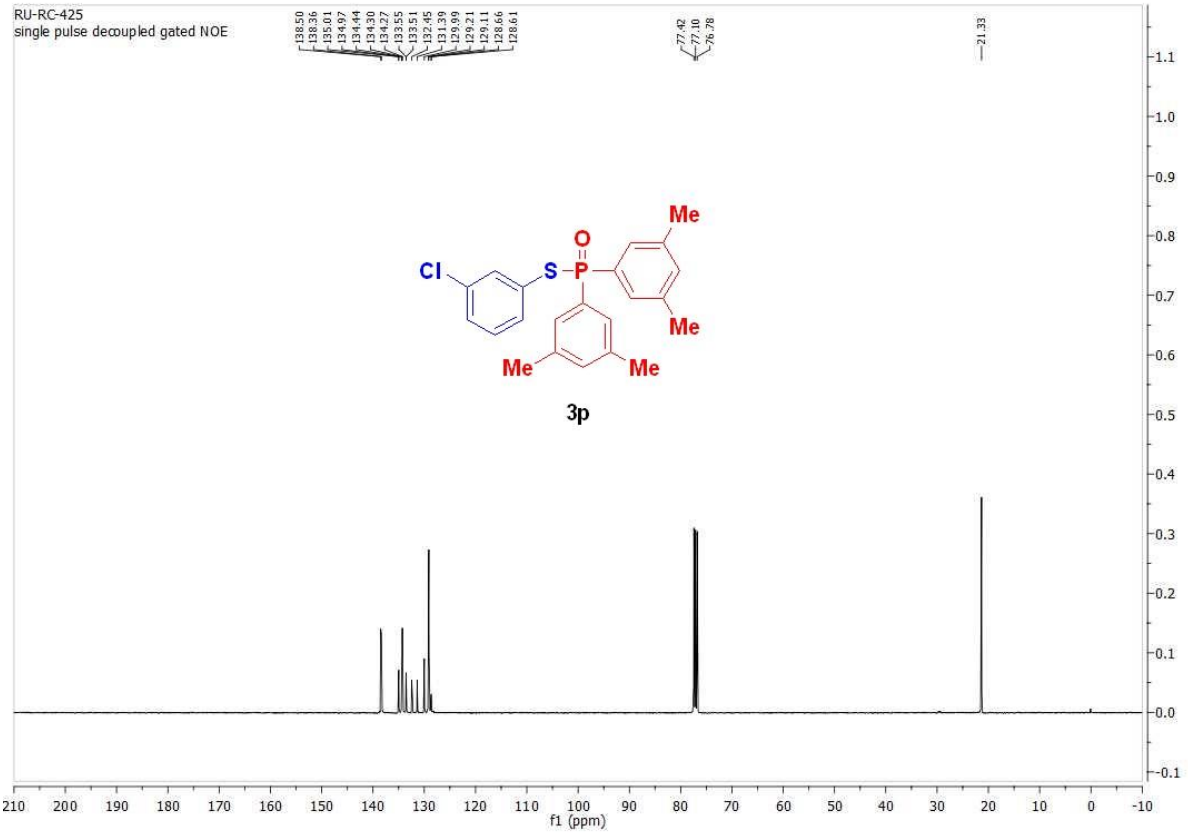

RU-RC-426
single pulse decoupled gated NOE
138.43
138.30
136.76
136.73
134.23
134.20
132.52
132.20
131.47
129.16
129.05
125.96
125.91
123.63
123.61
77.42
77.10
76.78
21.31
Me
O
S
P
Me
Br
Me
Me
3o
f1 (ppm)

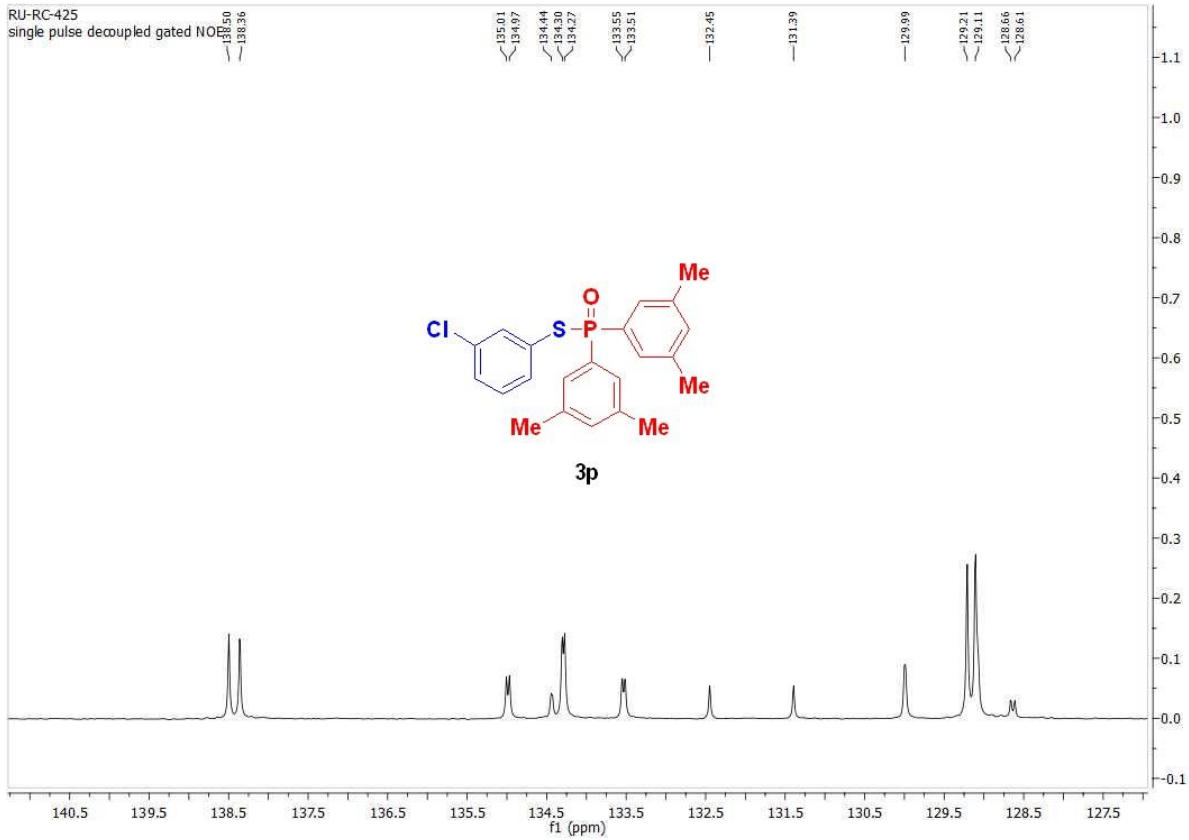

RU-RC-426
single pulse decoupled gated NOE
138.43
138.30
136.76
136.73
134.23
134.20
132.52
132.20
131.47
129.16
129.05
125.96
125.91
123.63
123.61
Me
O
S
P
Me
Br
Me
Me
f1 (ppm)

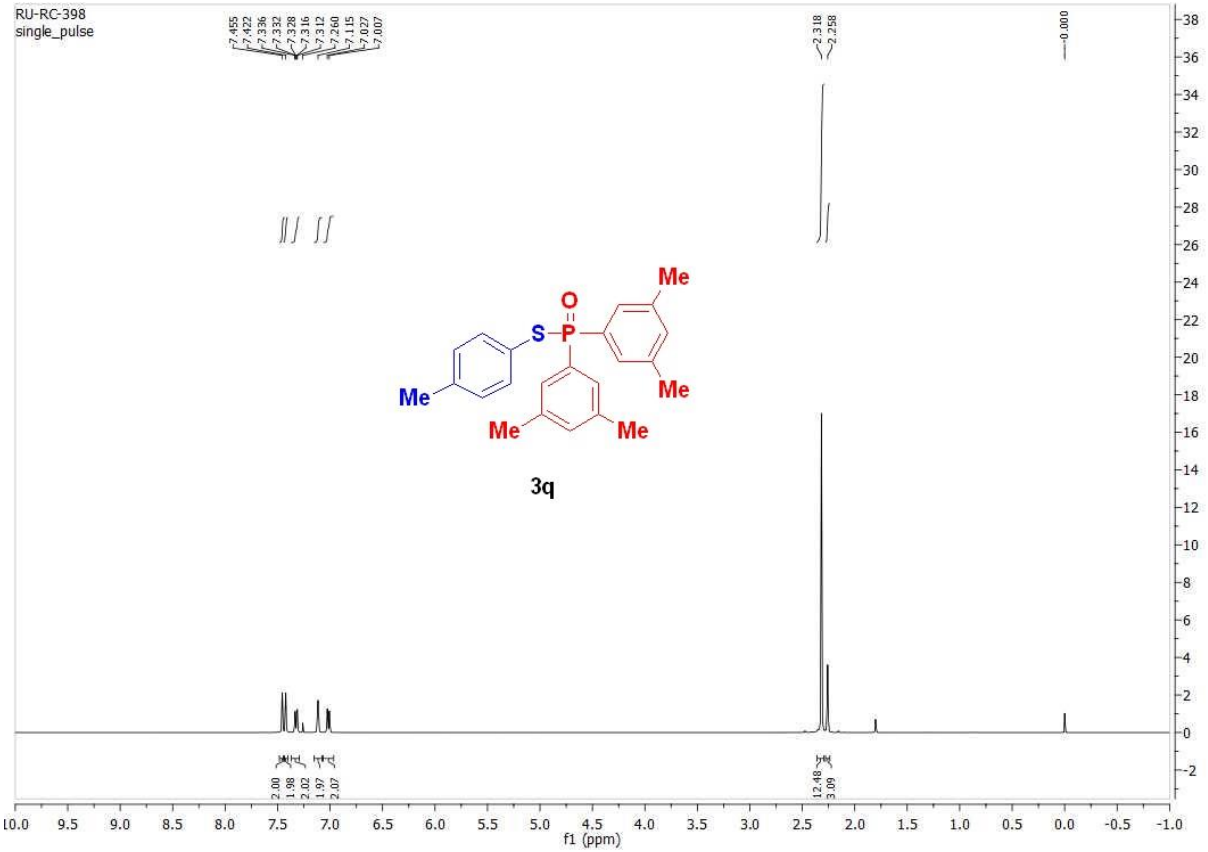
3o

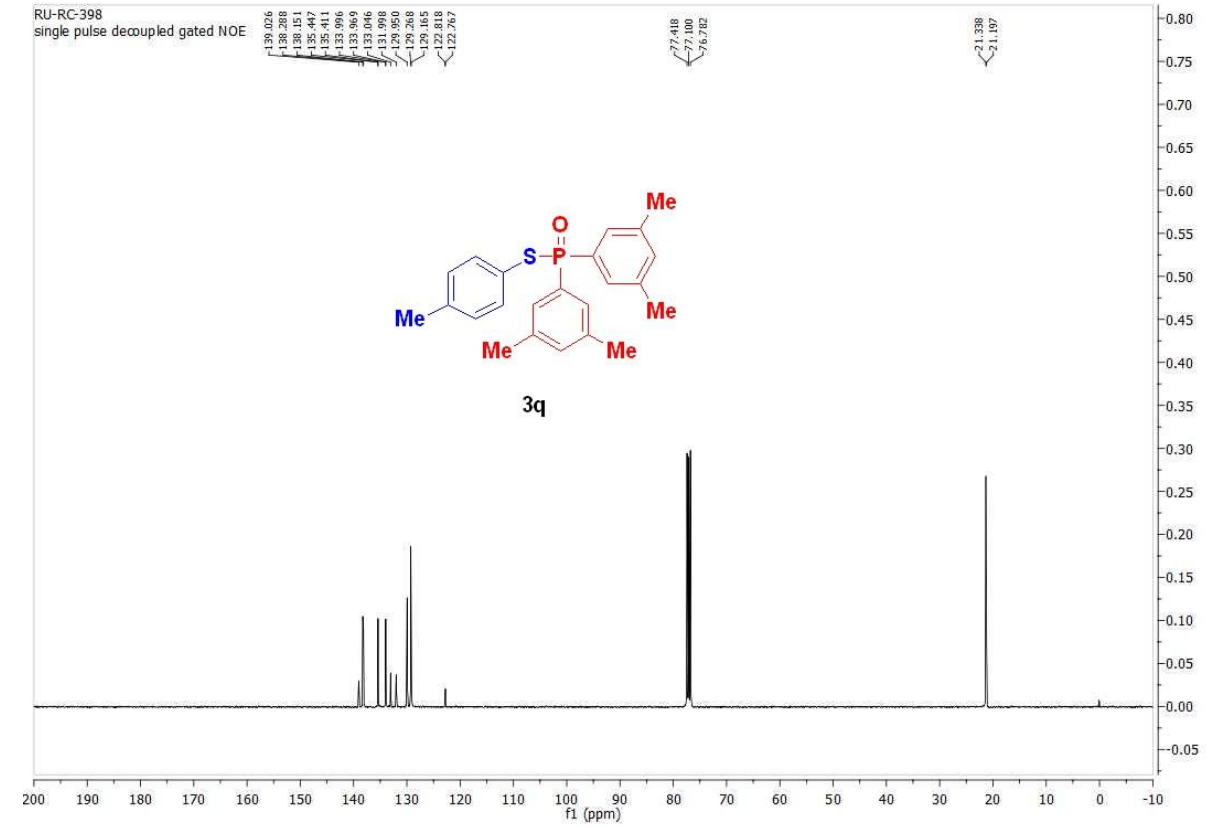

RU-RC-425
single_pulse
7.460
7.417
7.405
7.389
7.386
7.381
7.376
7.372
7.265
7.234
7.231
7.214
7.211
7.168
7.148
7.144
7.129
2.331
0.000
6.03
1.00
3.09
12.59
Me
O
Cl
S
P
Me
Me
Me
f1 (ppm)

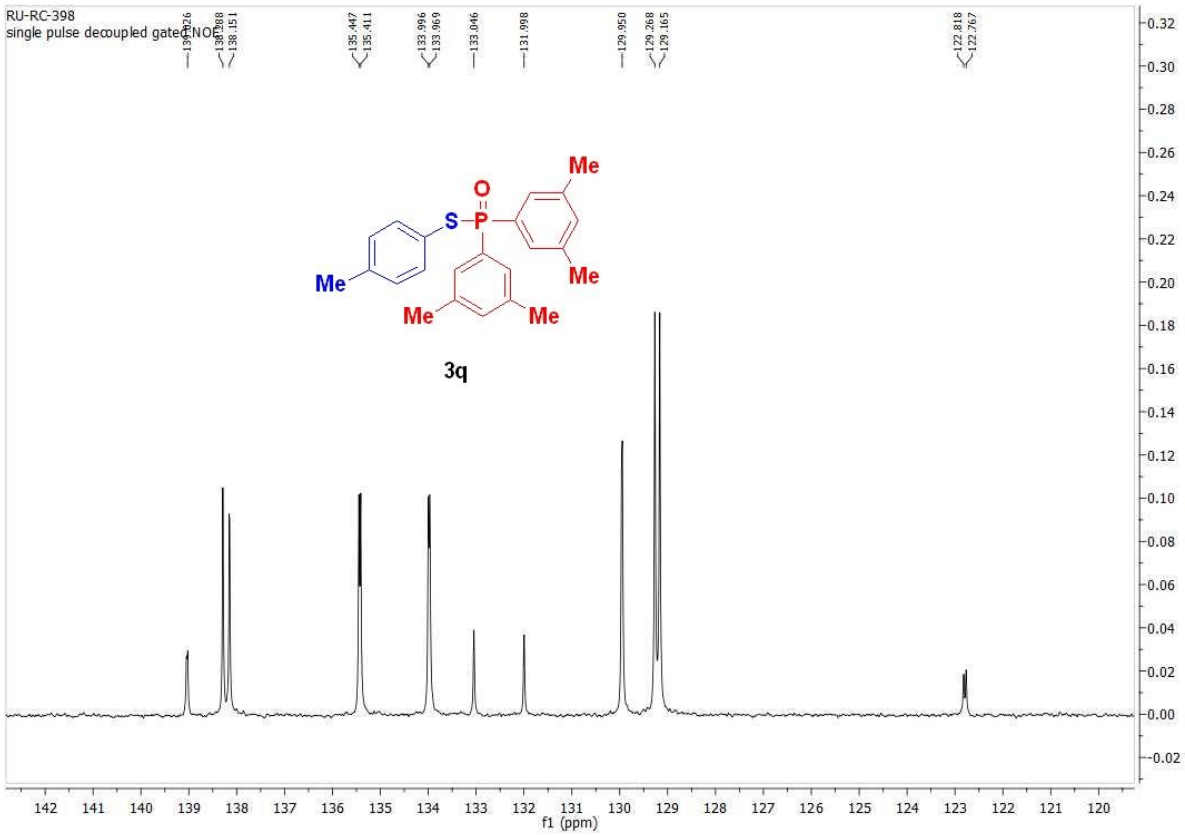
3p

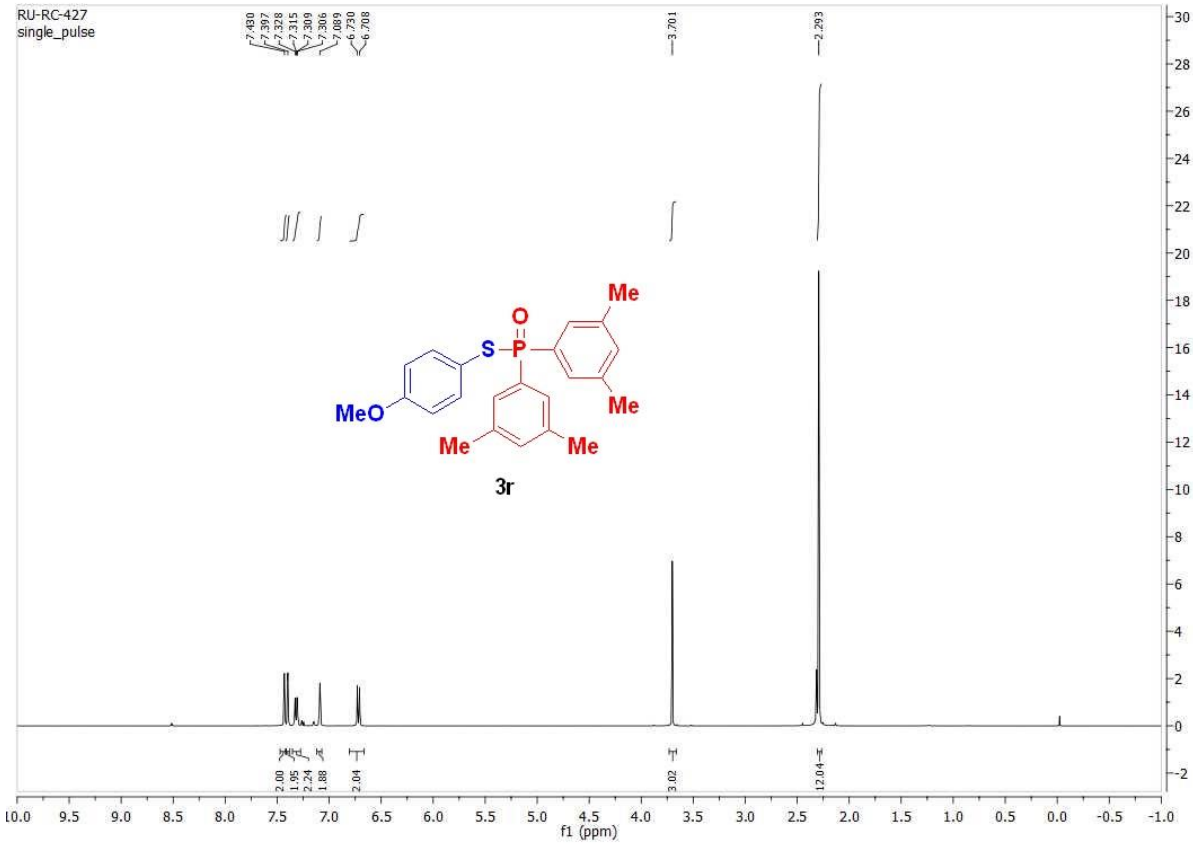

RU-RC-425
single pulse decoupled gated NOE
138.50
138.36
135.01
134.97
134.44
134.30
134.27
133.55
133.51
132.45
131.39
129.99
129.21
129.11
128.66
128.61
77.42
77.10
76.78
21.33
Cl
S
O
P
Me
Me
Me
Me
3p
f1 (ppm)

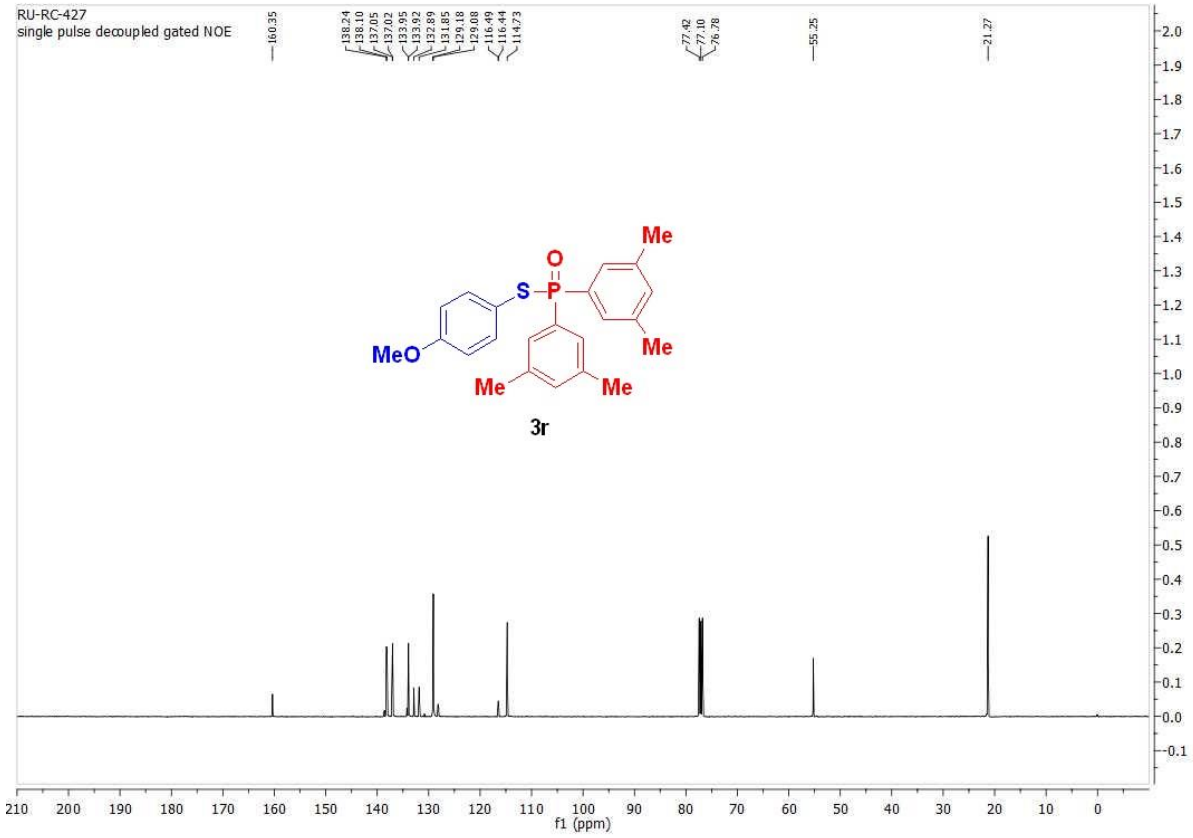

RU-RC-425
single pulse decoupled gated NOE
138.50
138.36
135.01
134.97
134.44
134.30
134.27
133.55
133.51
132.45
131.39
129.99
129.21
129.11
128.66
128.61
Cl
S
O
P
Me
Me
Me
Me
3p
f1 (ppm)

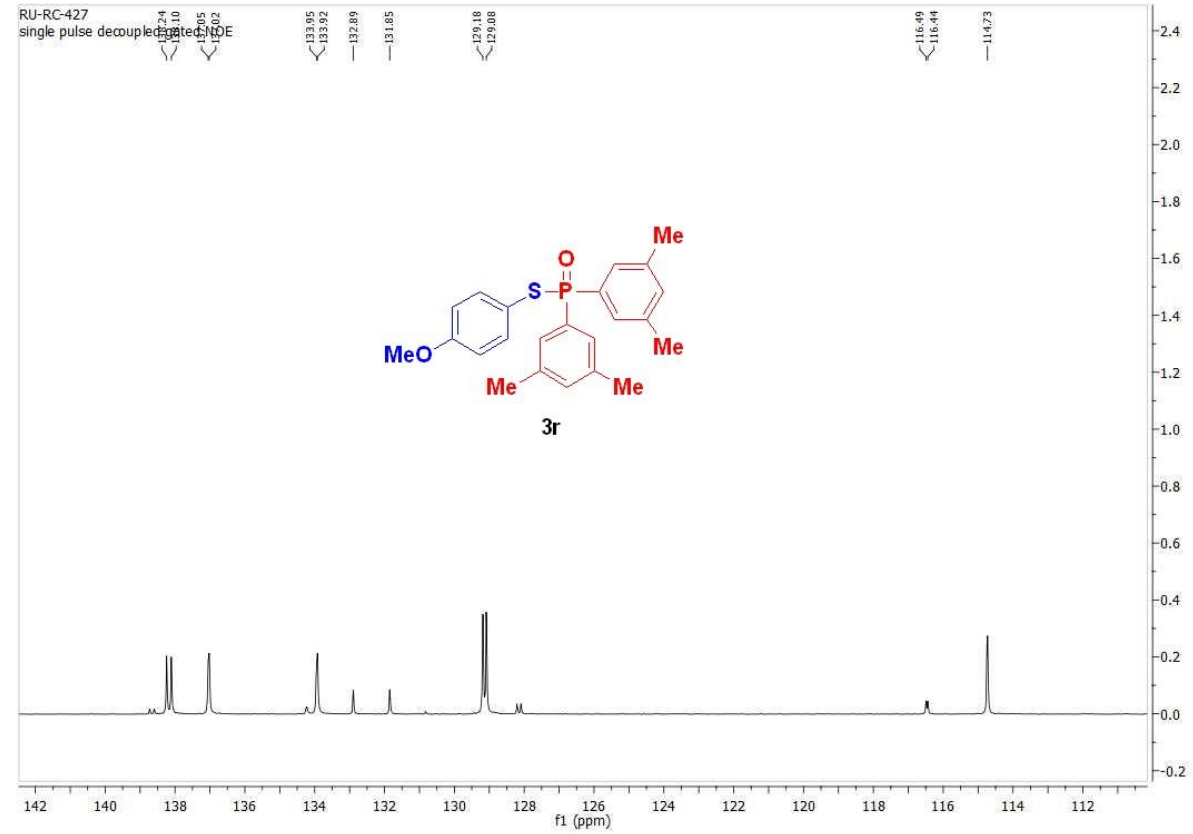

RU-RC-398
single_pulse
7.455
7.422
7.336
7.332
7.328
7.316
7.312
7.260
7.115
7.027
7.007
2.318
2.258
0.000
Me
O
S
P
Me
Me
Me
Me
3q
2.00
1.98
2.02
1.97
2.07
12.48
3.09
f1 (ppm)

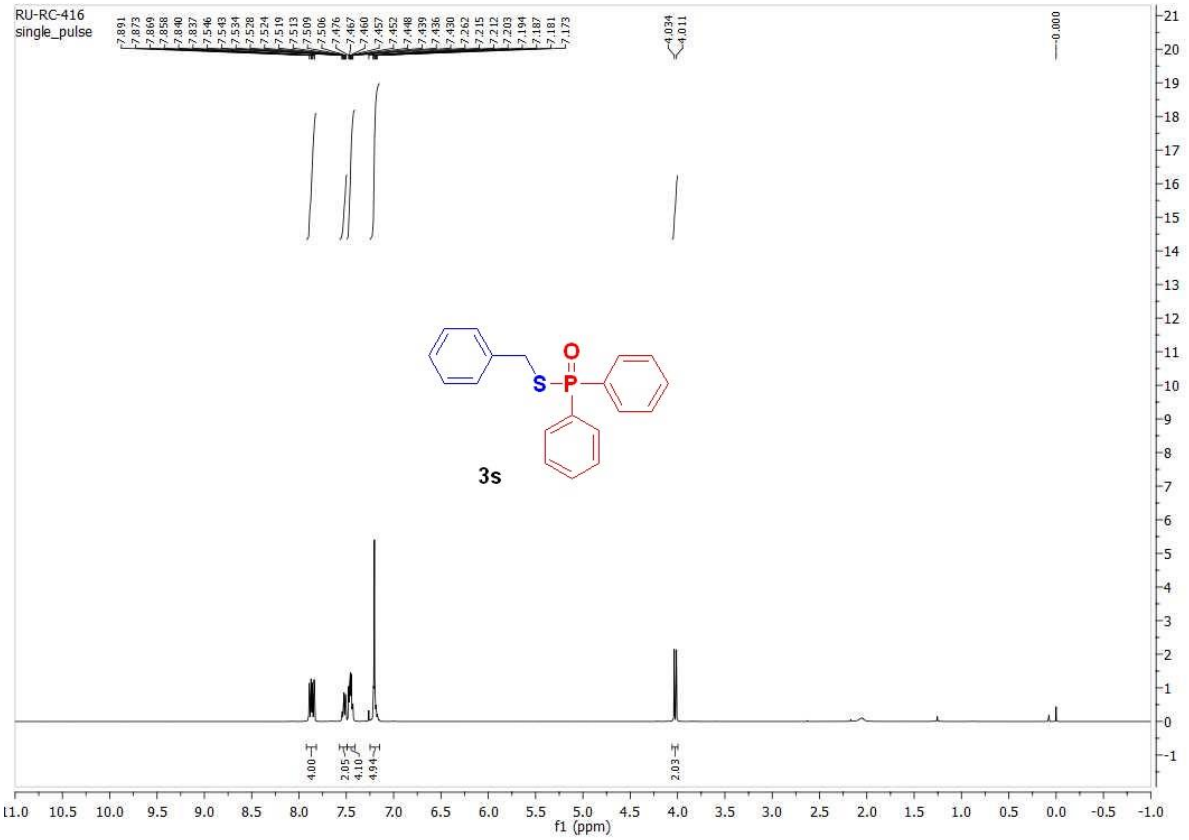

RU-RC-398
single pulse decoupled gated NOE
139.026
138.288
138.151
135.447
135.411
133.996
133.969
133.046
131.998
129.950
129.268
129.165
122.818
122.767
77.418
77.100
76.782
21.338
21.197
Me
O
S
P
Me
Me
Me
Me
3q
f1 (ppm)

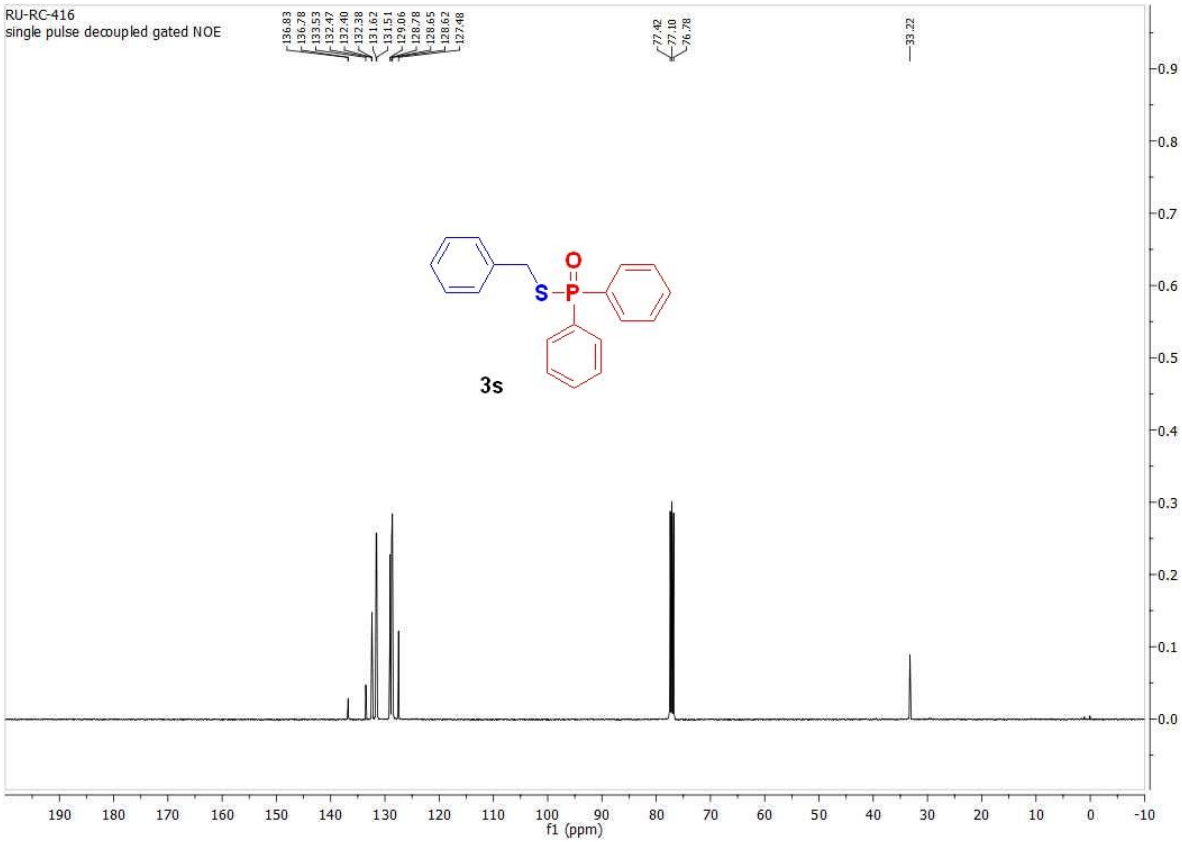

RU-RC-398
single pulse decoupled gated NOE
Me
O
S
P
Me
Me
Me
Me
3q
f1 (ppm)

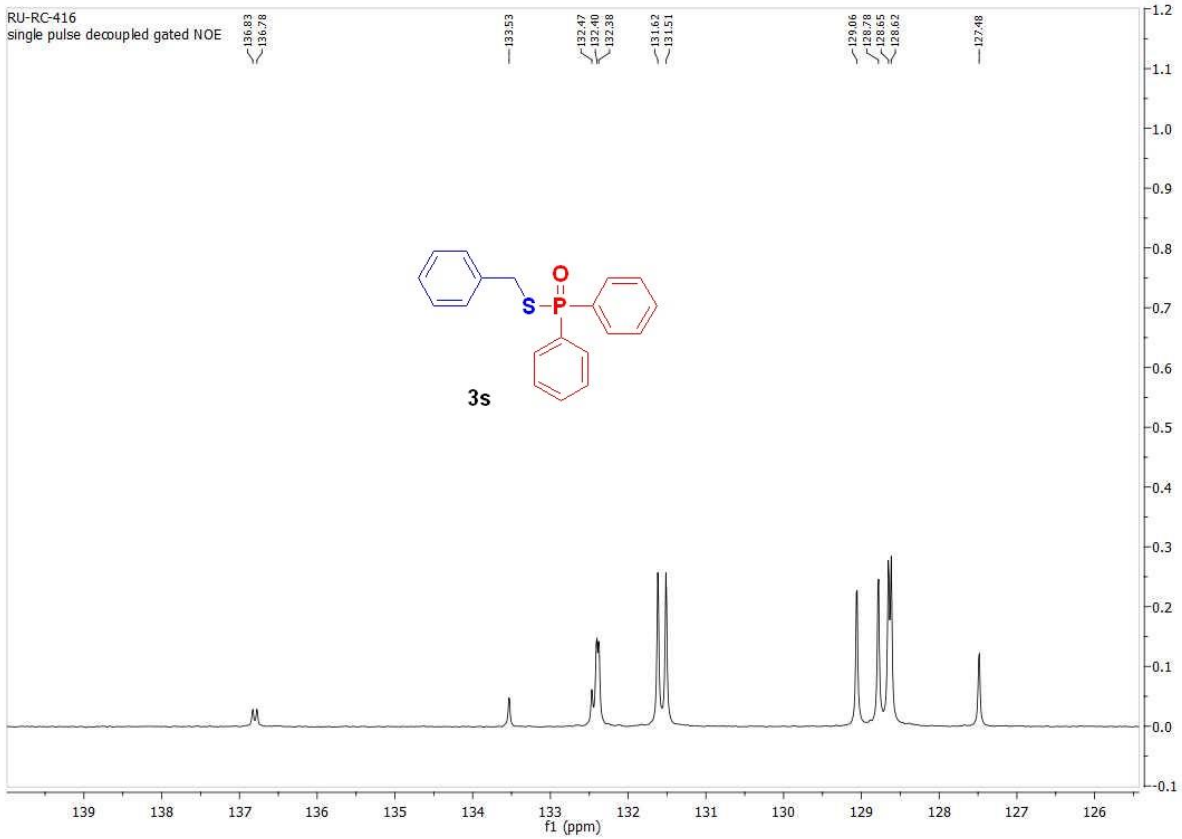

RU-RC-427
single_pulse
Me
O
S
P
Me
MeO
Me
Me
3r
f1 (ppm)

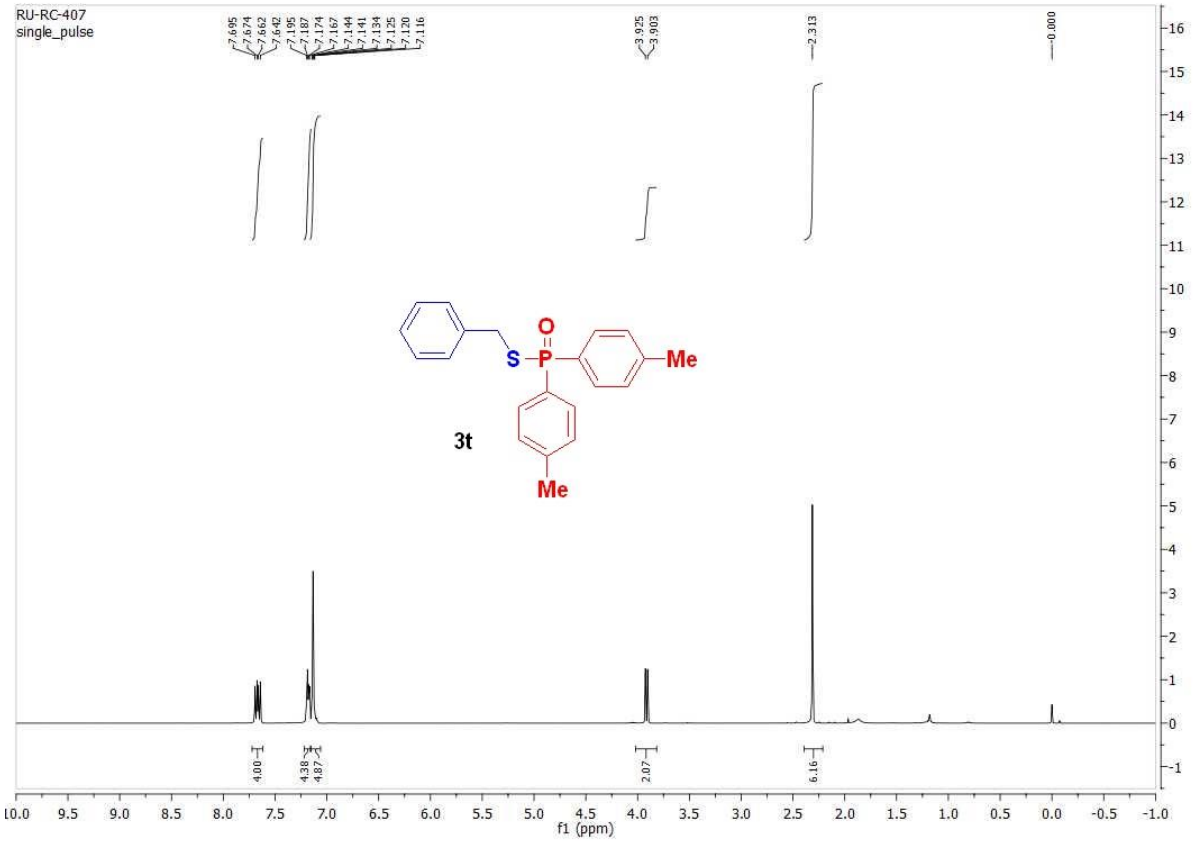

RU-RC-427
single pulse decoupled gated NOE
160.35
138.24
138.10
137.05
137.02
133.95
133.92
132.89
131.85
129.18
129.08
116.49
116.44
114.73
77.42
77.10
76.78
55.25
21.27
Me
O
S
P
Me
MeO
Me
Me
3r
f1 (ppm)

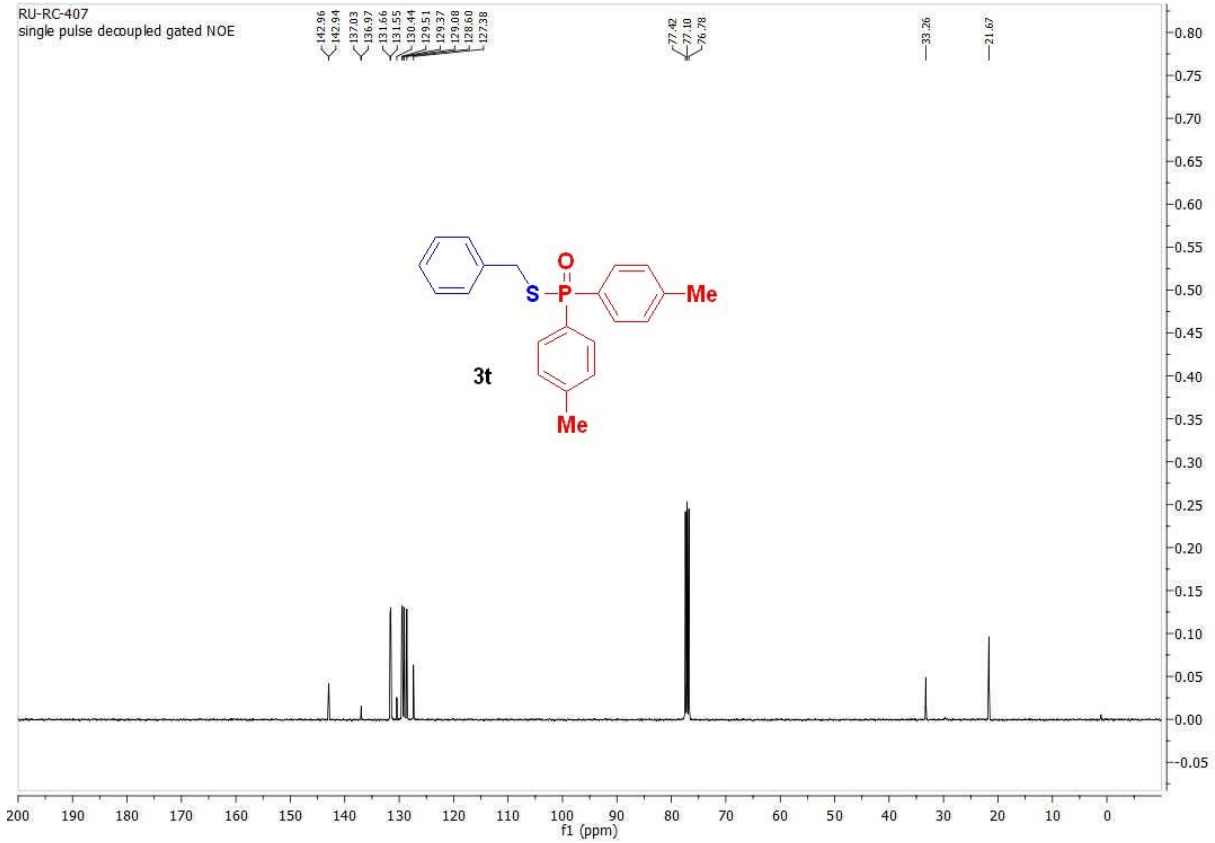

RU-RC-427
single pulse decoupled gated NOE
133.95
133.92
132.89
131.85
129.18
129.08
116.49
116.44
114.73
Me
O
S
P
Me
MeO
Me
Me
3r
f1 (ppm)

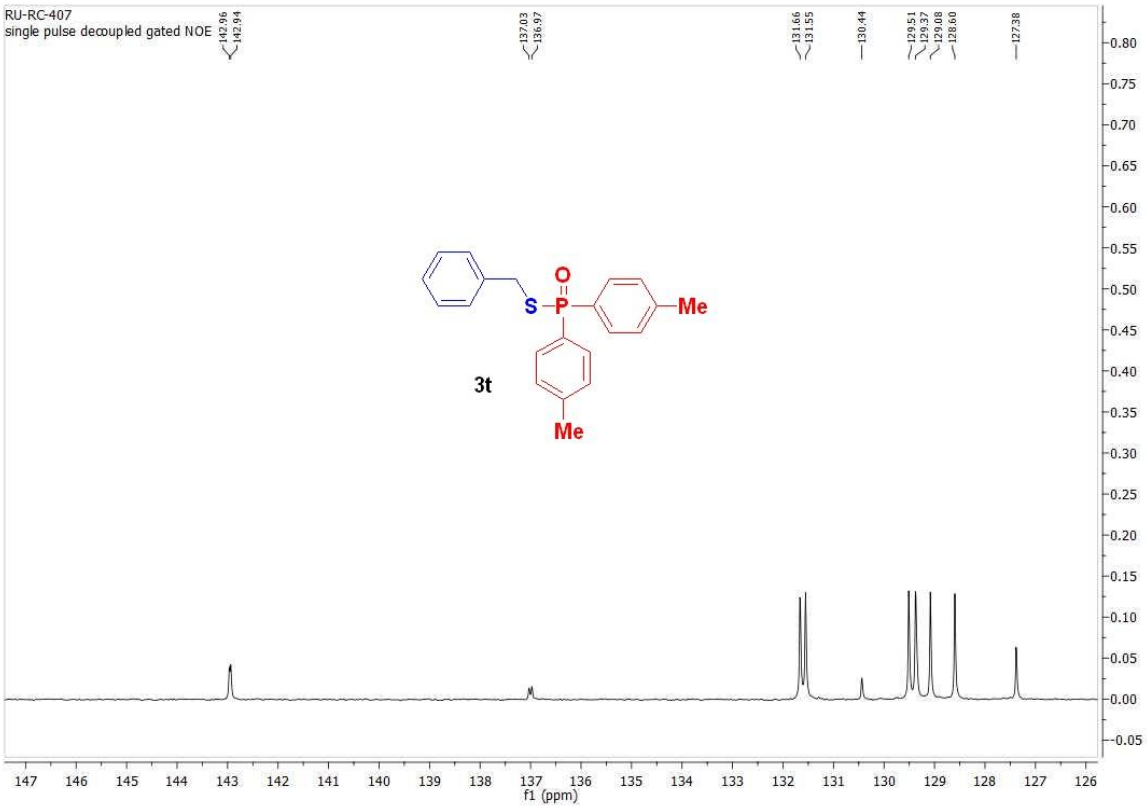

RU-RC-416
single_pulse
3s
f1 (ppm)

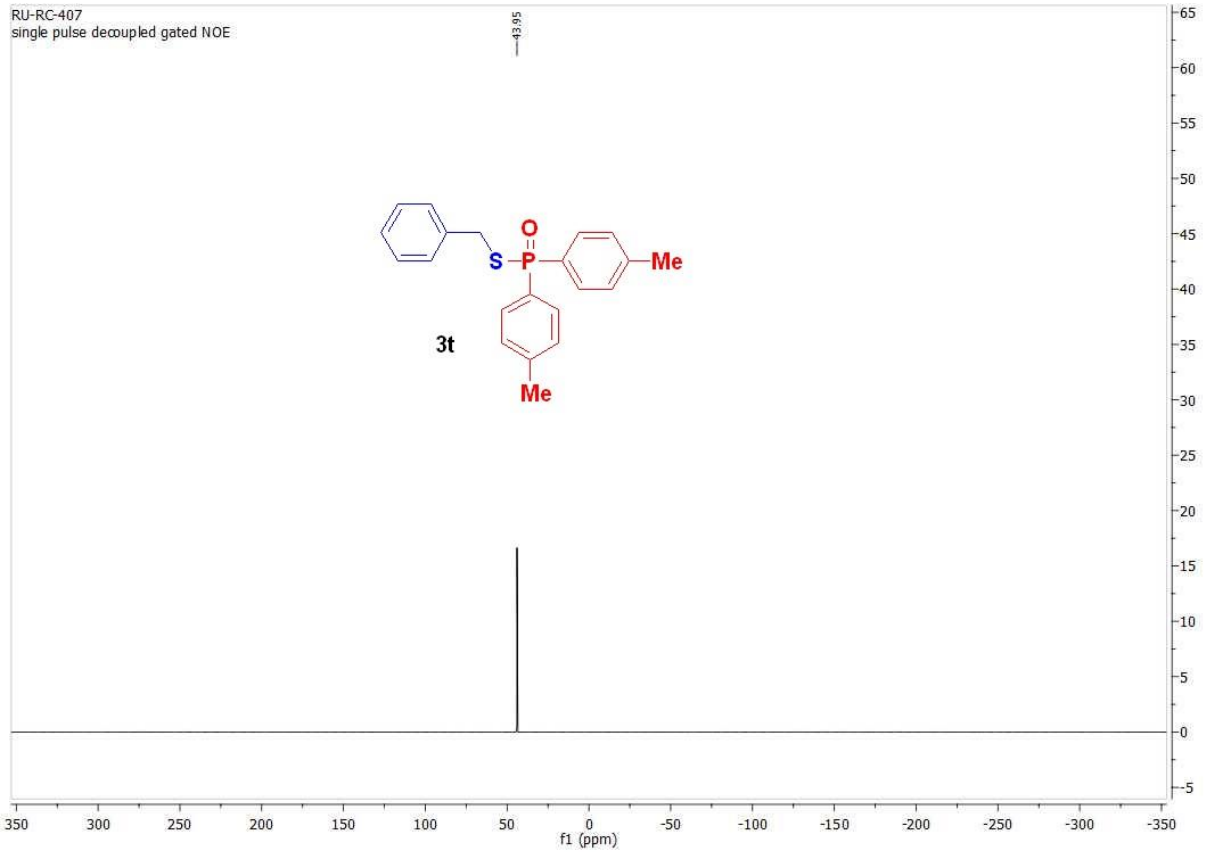

RU-RC-416
single pulse decoupled gated NOE
3s
f1 (ppm)

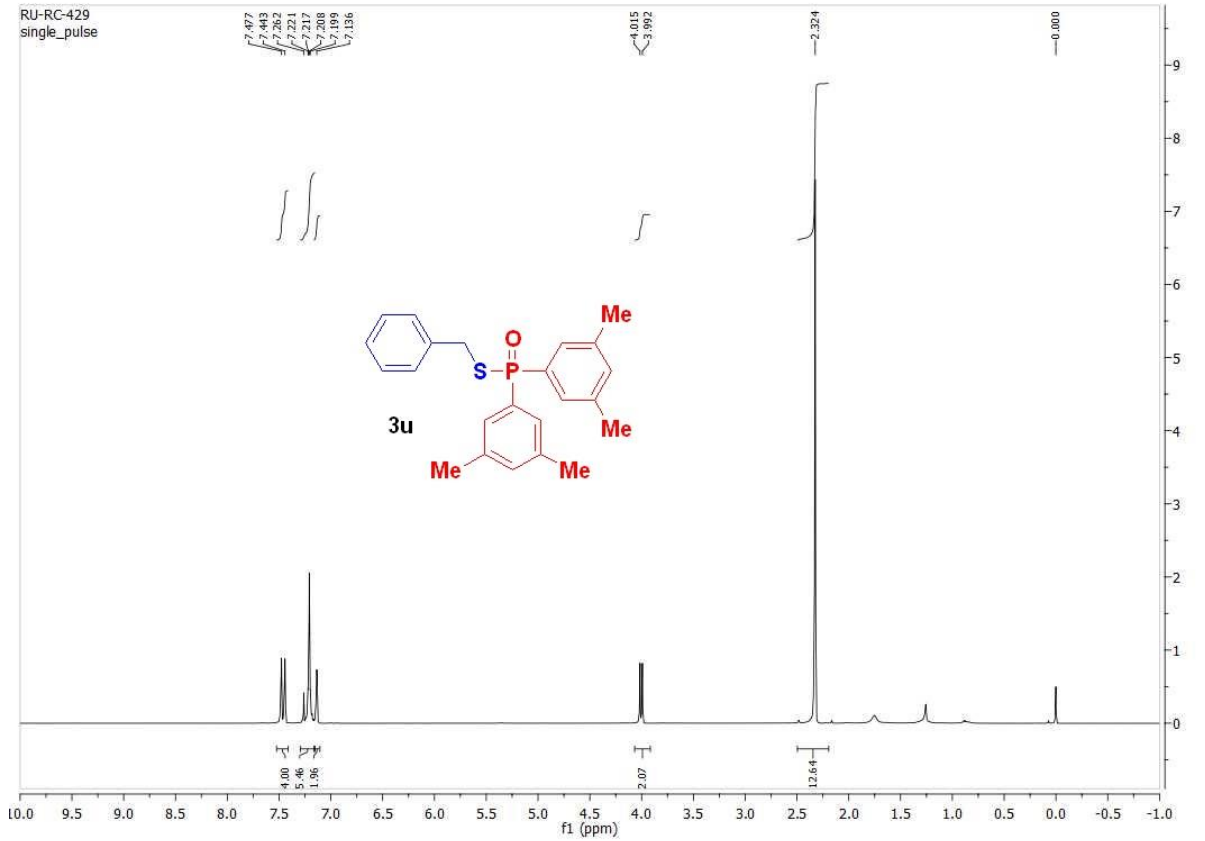

RU-RC-416
single pulse decoupled gated NOE
136.83
136.78
133.53
132.47
132.40
132.38
131.62
131.51
129.06
128.78
128.65
128.62
127.48
O
S
P
3s
f1 (ppm)

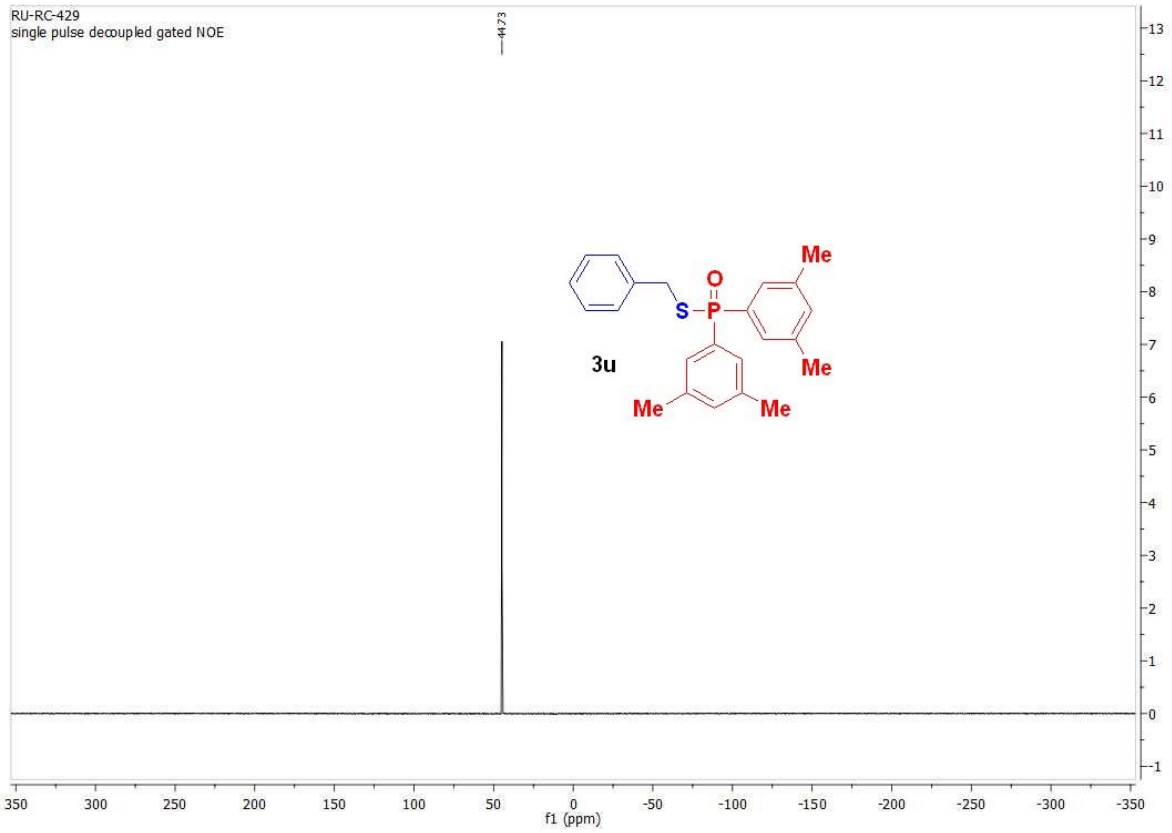

RU-RC-407
single_pulse
7.695
7.674
7.662
7.642
7.196
7.187
7.174
7.167
7.144
7.141
7.134
7.125
7.120
7.116
3.925
3.903
2.313
0.000
O
S
P
Me
Me
3t
4.00
4.38
4.87
2.07
6.16
f1 (ppm)

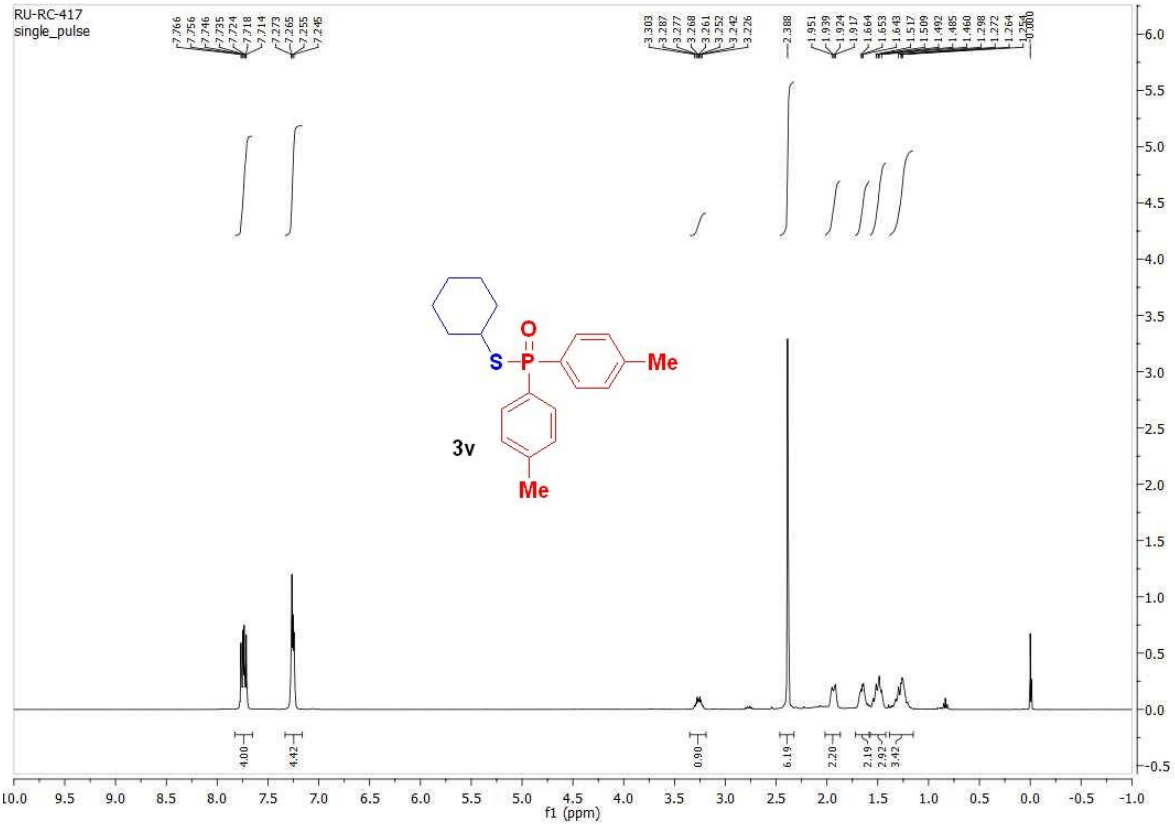

RU-RC-407
single pulse decoupled gated NOE
142.96
142.94
137.03
136.97
131.66
131.55
130.44
129.51
129.37
129.08
128.60
127.38
77.42
77.10
76.78
33.26
21.67
O
S
P
Me
3t
Me
f1 (ppm)

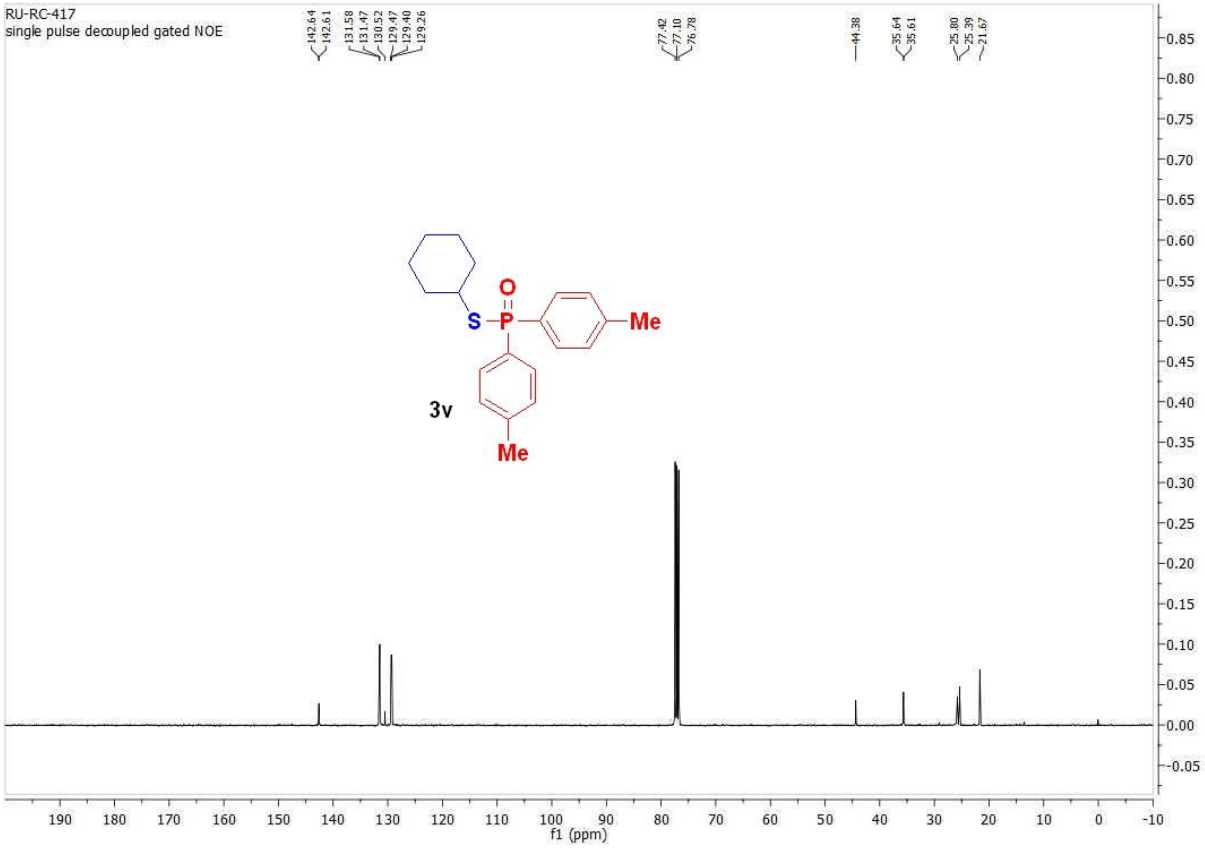

RU-RC-407
single pulse decoupled gated NOE
142.96
142.94
137.03
136.97
131.66
131.55
130.44
129.51
129.37
129.08
128.60
127.38
O
S
P
Me
3t
Me
f1 (ppm)

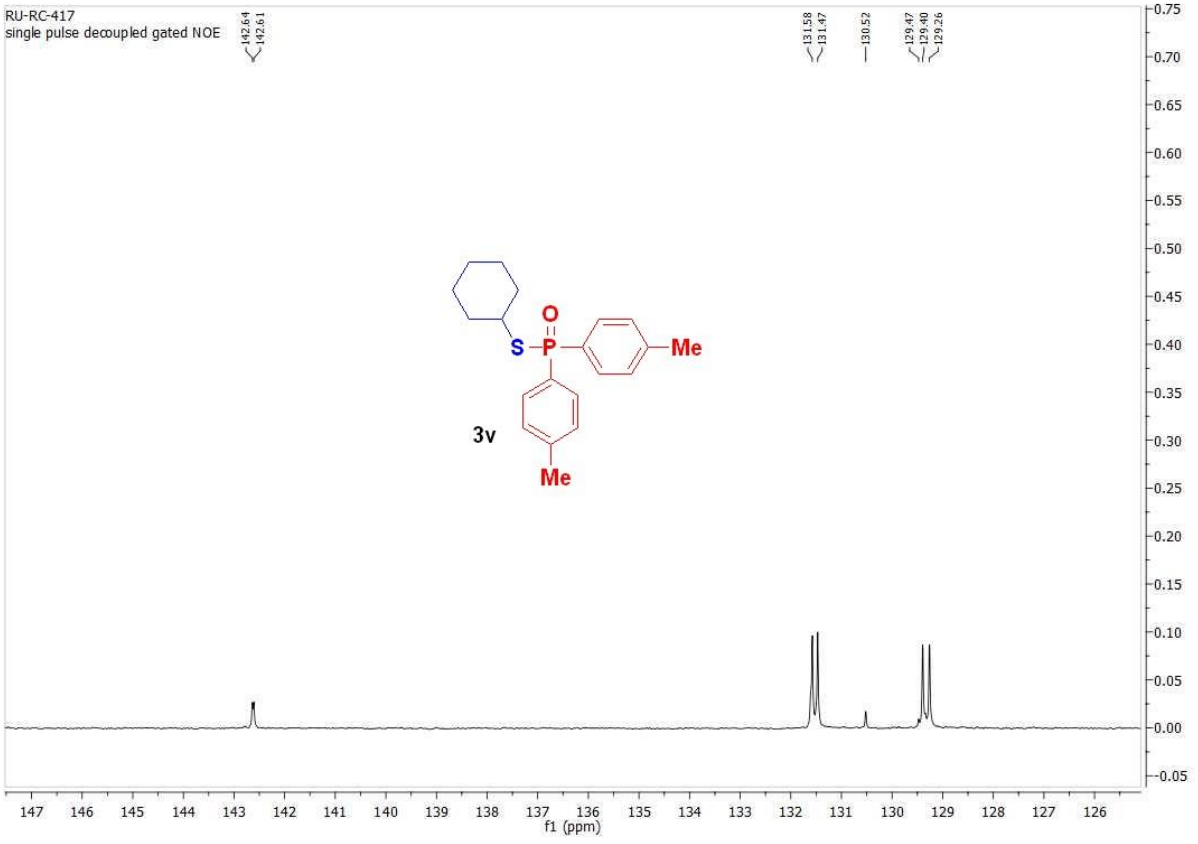

RU-RC-407
single pulse decoupled gated NOE
43.95
O
S
P
Me
Me
3t
f1 (ppm)

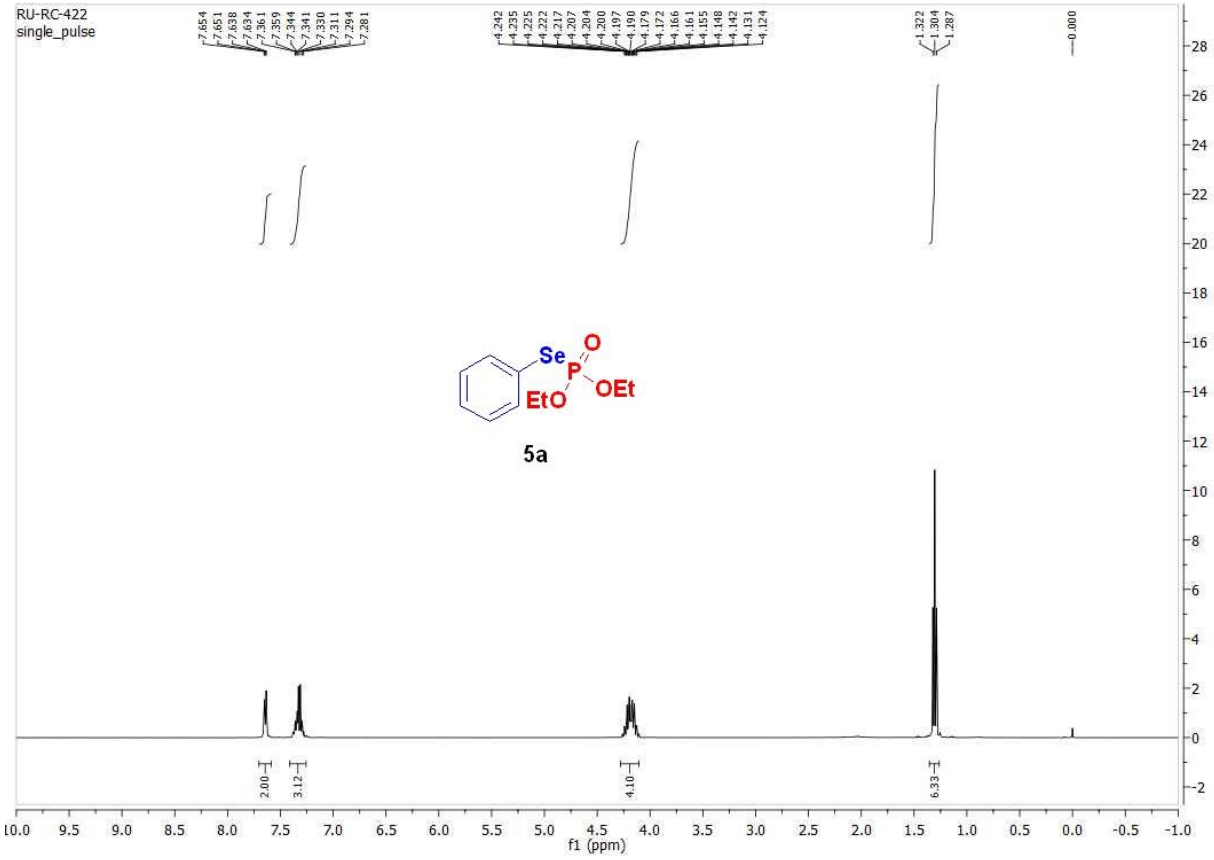

RU-RC-429
single_pulse
7.497
7.443
7.262
7.221
7.217
7.208
7.199
7.136
4.015
3.992
2.324
0.000
Me
O
S
P
Me
3u
Me
Me
4.00
5.46
1.96
2.07
12.64
f1 (ppm)

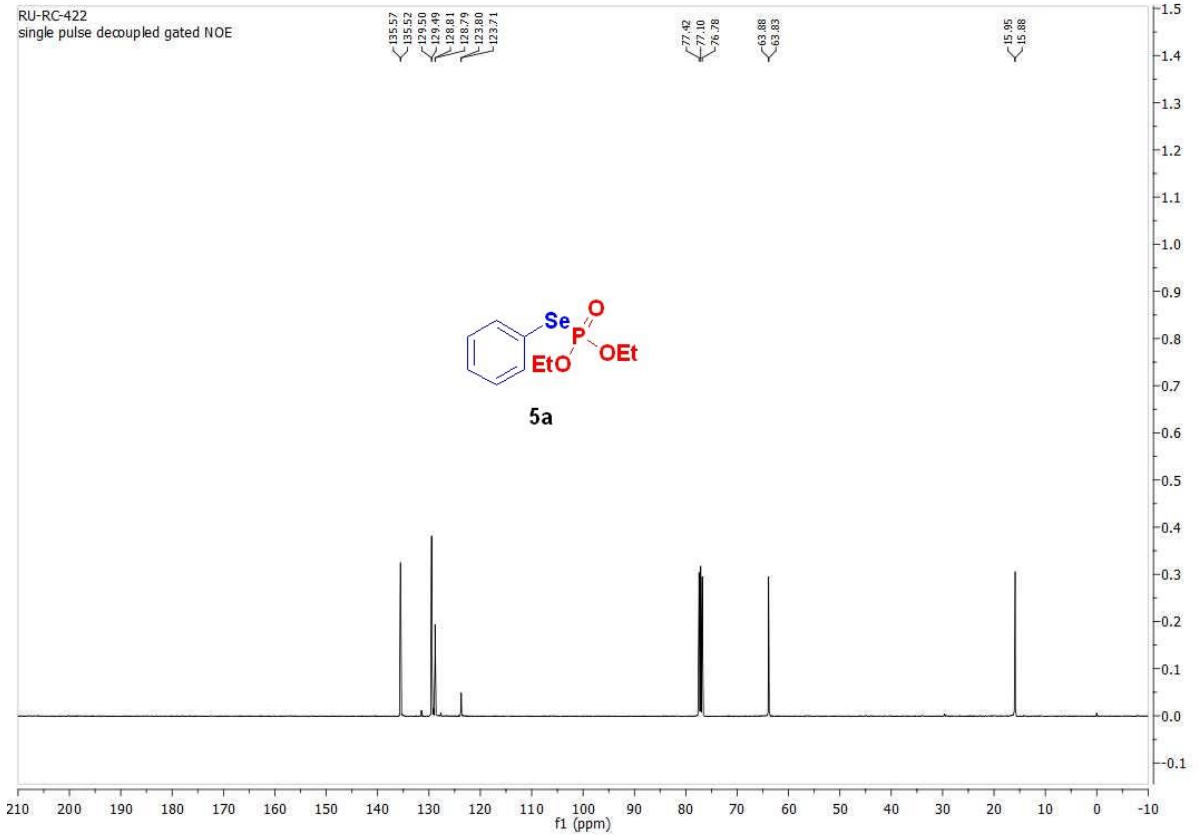

RU-RC-429
single pulse decoupled gated NOE
44.73
3u
Me
Me
Me
Me
O
S
P
f1 (ppm)

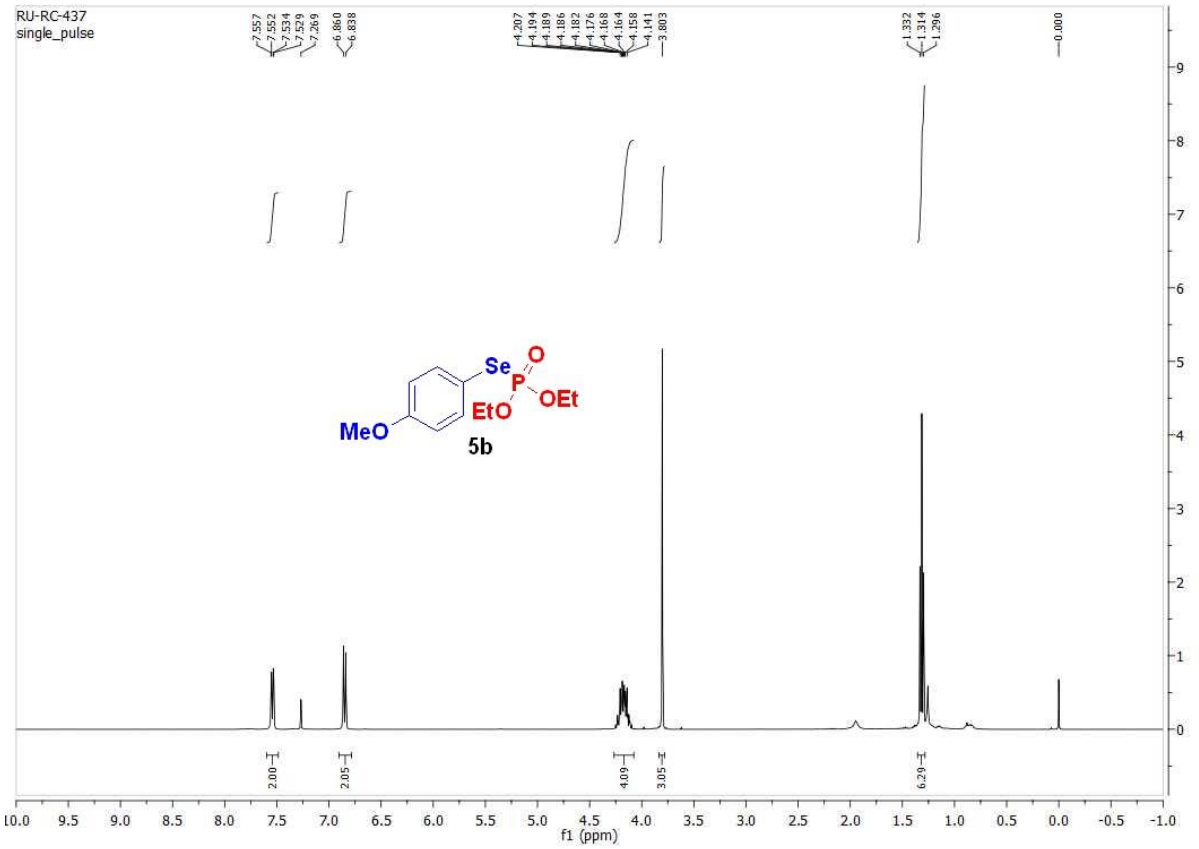

RU-RC-417
single_pulse
3v
Me
Me
O
S
P
4.00
4.42
0.90
6.19
2.20
2.19
2.92
3.42
f1 (ppm)

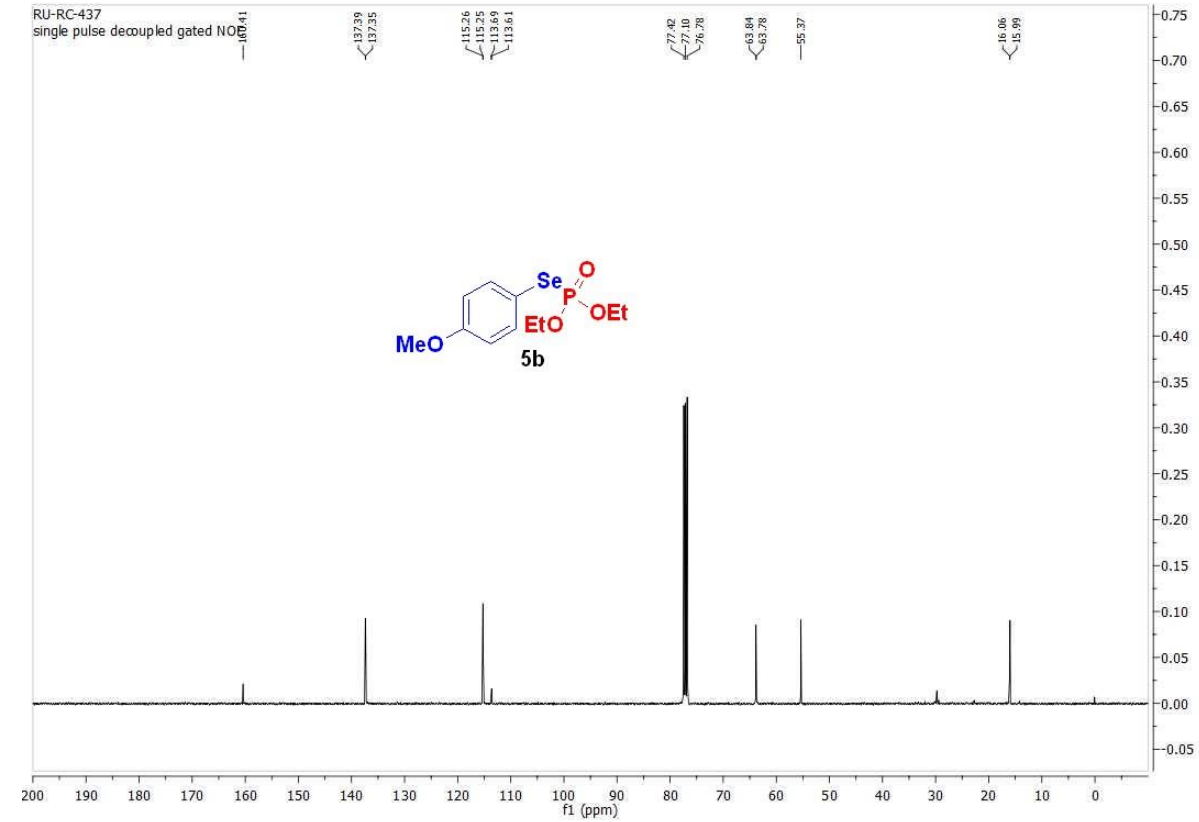

RU-RC-417
single pulse decoupled gated NOE
142.64
142.61
131.58
131.47
130.52
129.47
129.40
129.26
77.42
77.10
76.78
44.38
35.64
35.61
25.80
25.39
21.67
O
S
P
Me
3v
Me
f1 (ppm)

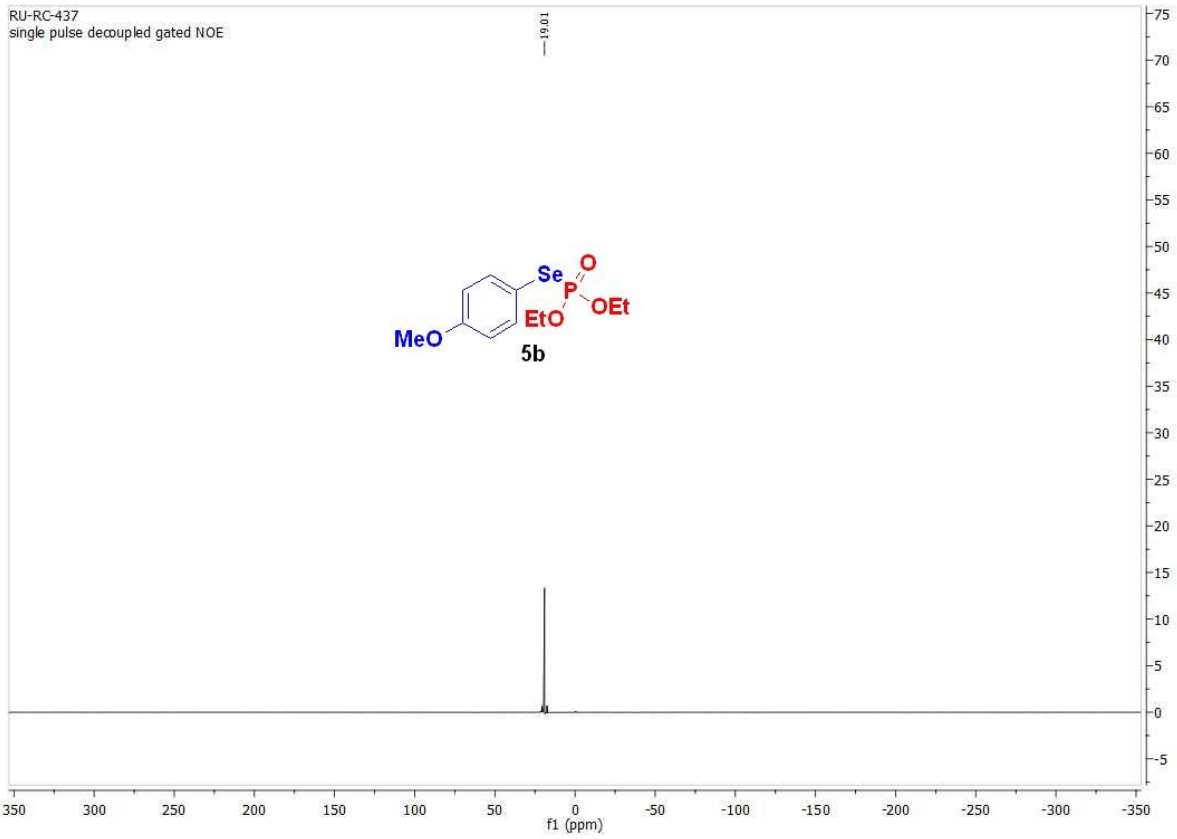

RU-RC-417
single pulse decoupled gated NOE
142.64
142.61
131.58
131.47
130.52
129.47
129.40
129.26
O
S
P
Me
3v
Me
f1 (ppm)


RU-RC-422
single_pulse
7.654
7.651
7.638
7.634
7.361
7.359
7.344
7.341
7.330
7.311
7.294
7.281
4.242
4.235
4.225
4.222
4.217
4.207
4.204
4.200
4.197
4.190
4.179
4.172
4.166
4.161
4.155
4.148
4.142
4.131
4.124
1.322
1.304
1.287
0.000
Se
O
P
OEt
EtO
5a
2.00
3.12
4.10
6.33
f1 (ppm)

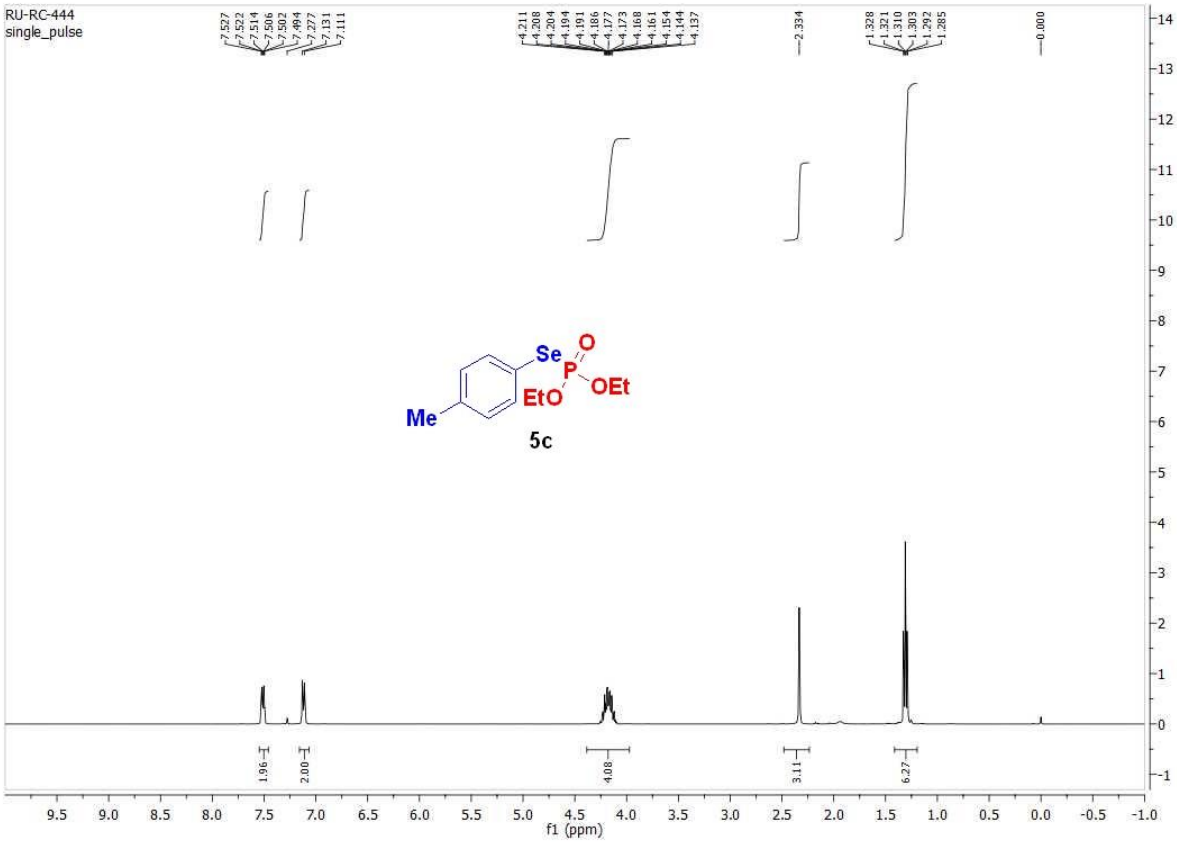

RU-RC-422
single pulse decoupled gated NOE
135.57
135.52
129.50
129.49
128.81
128.79
123.80
123.71
77.42
77.10
76.78
63.88
63.83
15.95
15.88
Se
O
P
OEt
EtO
5a
f1 (ppm)


RU-RC-437
single_pulse
7.557
7.552
7.534
7.529
7.269
6.860
6.838
4.207
4.194
4.189
4.186
4.182
4.176
4.168
4.164
4.158
4.141
3.803
1.332
1.314
1.296
0.000
Se
O
P
OEt
EtO
MeO
5b
2.00
2.05
4.09
3.05
6.29
f1 (ppm)

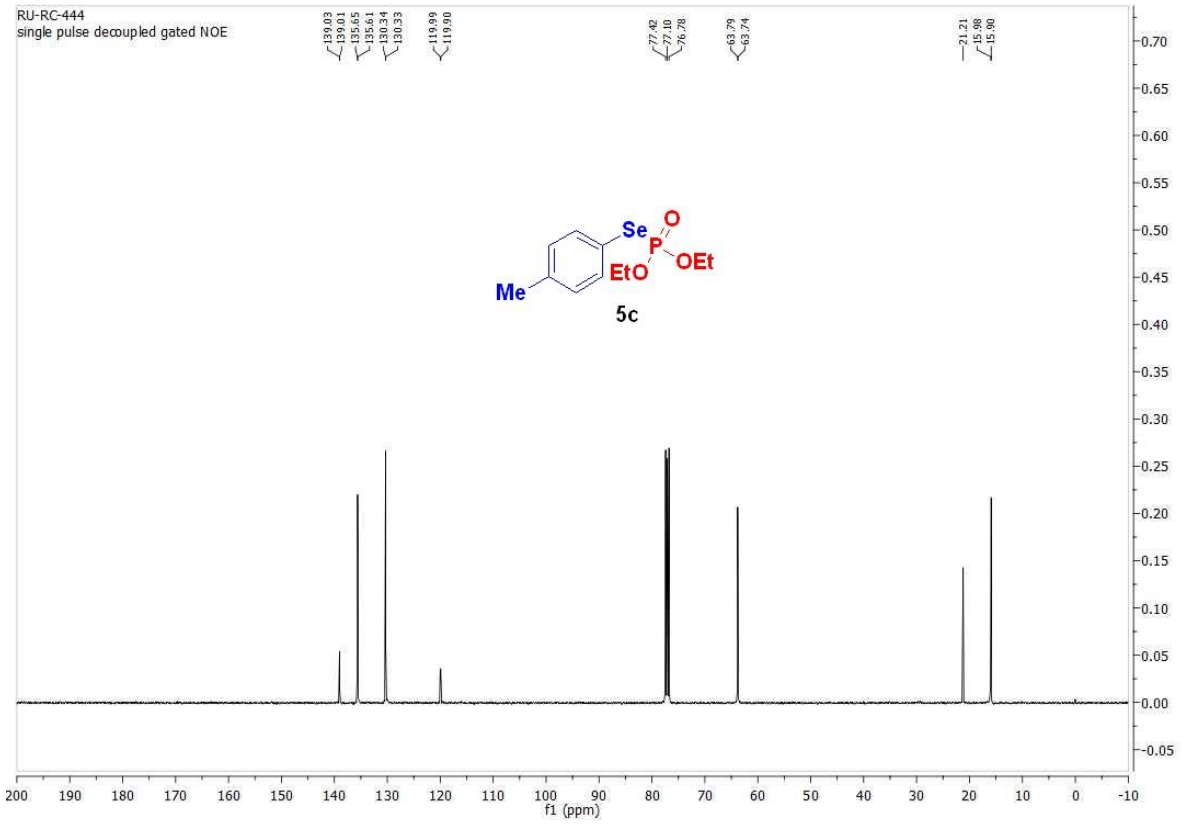

RU-RC-437
single pulse decoupled gated NOE
160.41
137.39
137.35
115.26
115.25
113.69
113.61
77.42
77.10
76.78
63.84
63.78
55.37
16.06
15.99
Se
O
P
OEt
EtO
MeO
5b
f1 (ppm)

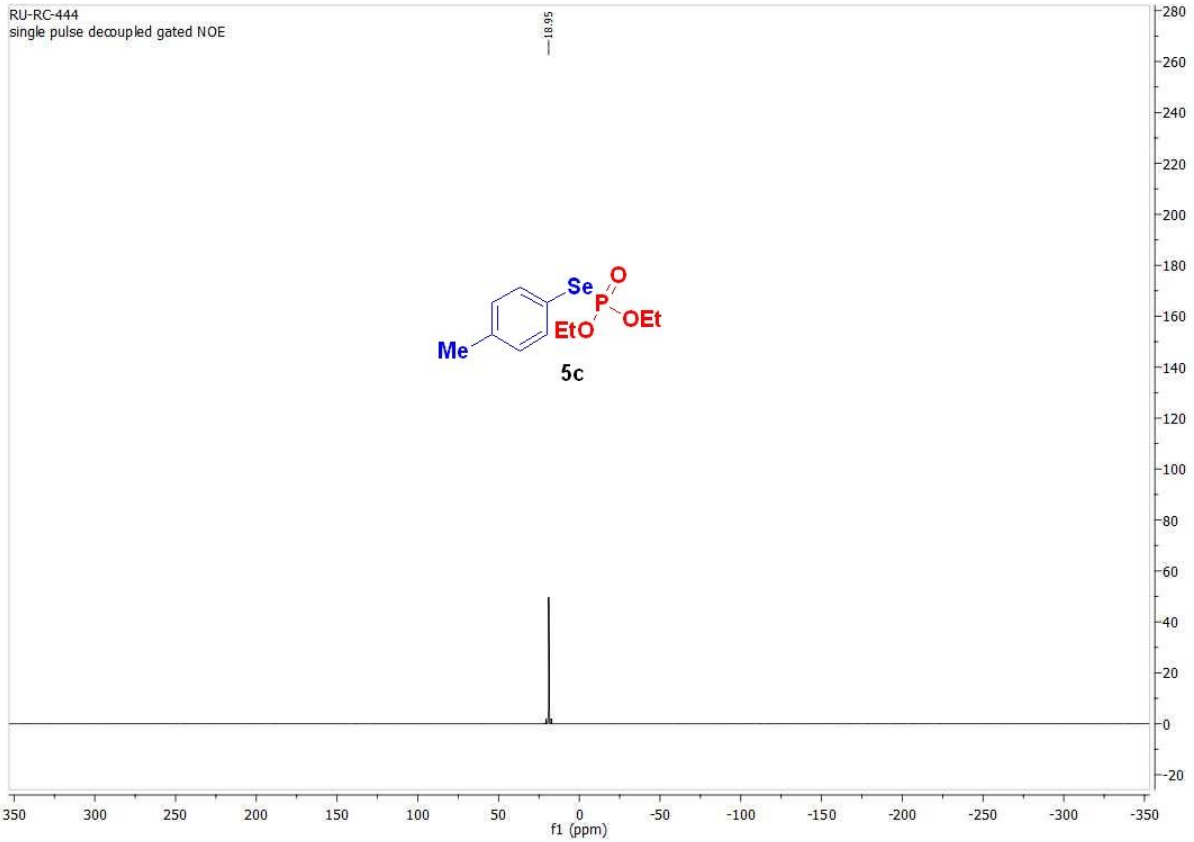

RU-RC-437
single pulse decoupled gated NOE
19.01
Se
O
P
OEt
EtO
MeO
f1 (ppm)

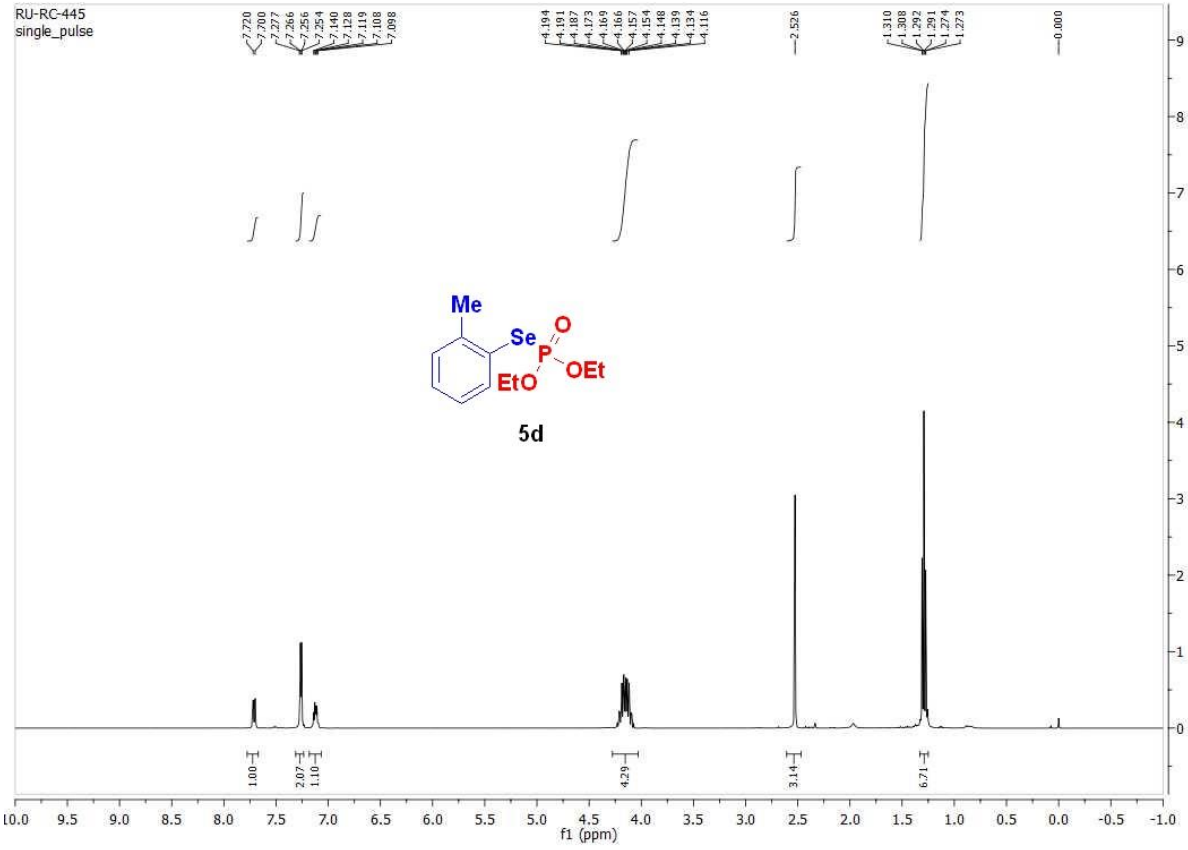
5b

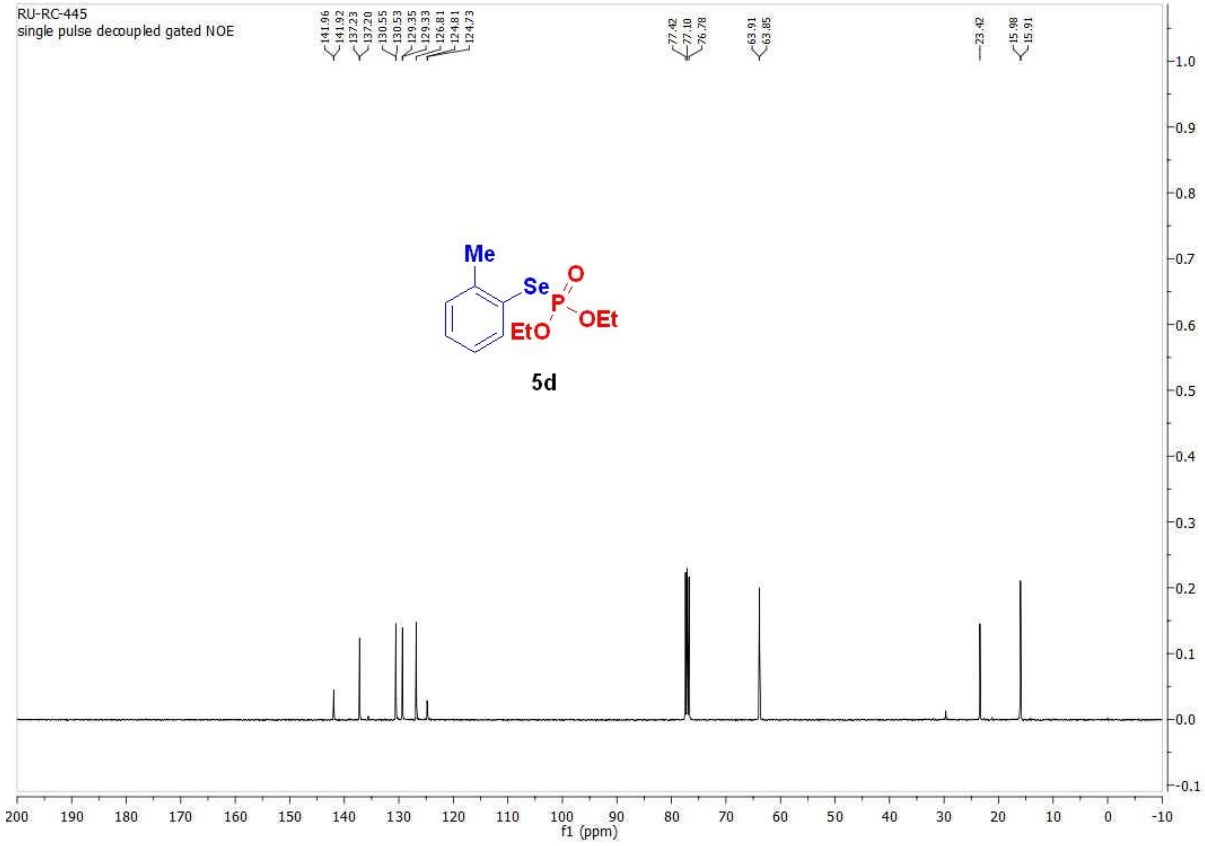

RU-RC-444
single_pulse
7.527
7.522
7.514
7.506
7.502
7.494
7.277
7.131
7.111
4.211
4.208
4.204
4.194
4.191
4.186
4.177
4.173
4.168
4.161
4.154
4.144
4.137
2.334
1.328
1.321
1.310
1.303
1.292
1.285
0.000
Se
O
P
OEt
EtO
Me
1.96
2.00
4.08
3.11
6.27
f1 (ppm)

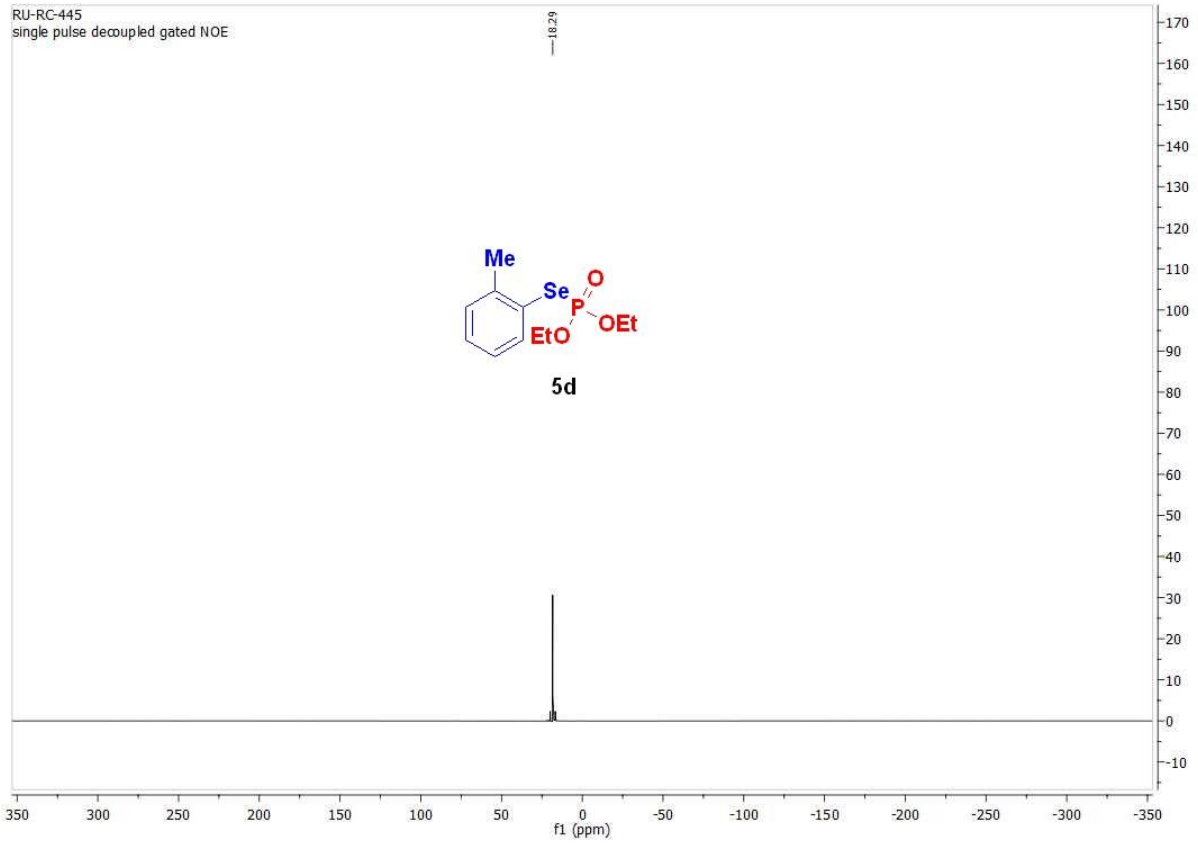
5c


RU-RC-444
single pulse decoupled gated NOE
139.03
139.01
135.65
135.61
130.34
130.33
119.99
119.90
77.42
77.10
76.78
63.79
63.74
21.21
15.98
15.90
Se
O
P
EtO
OEt
Me
5c
f1 (ppm)

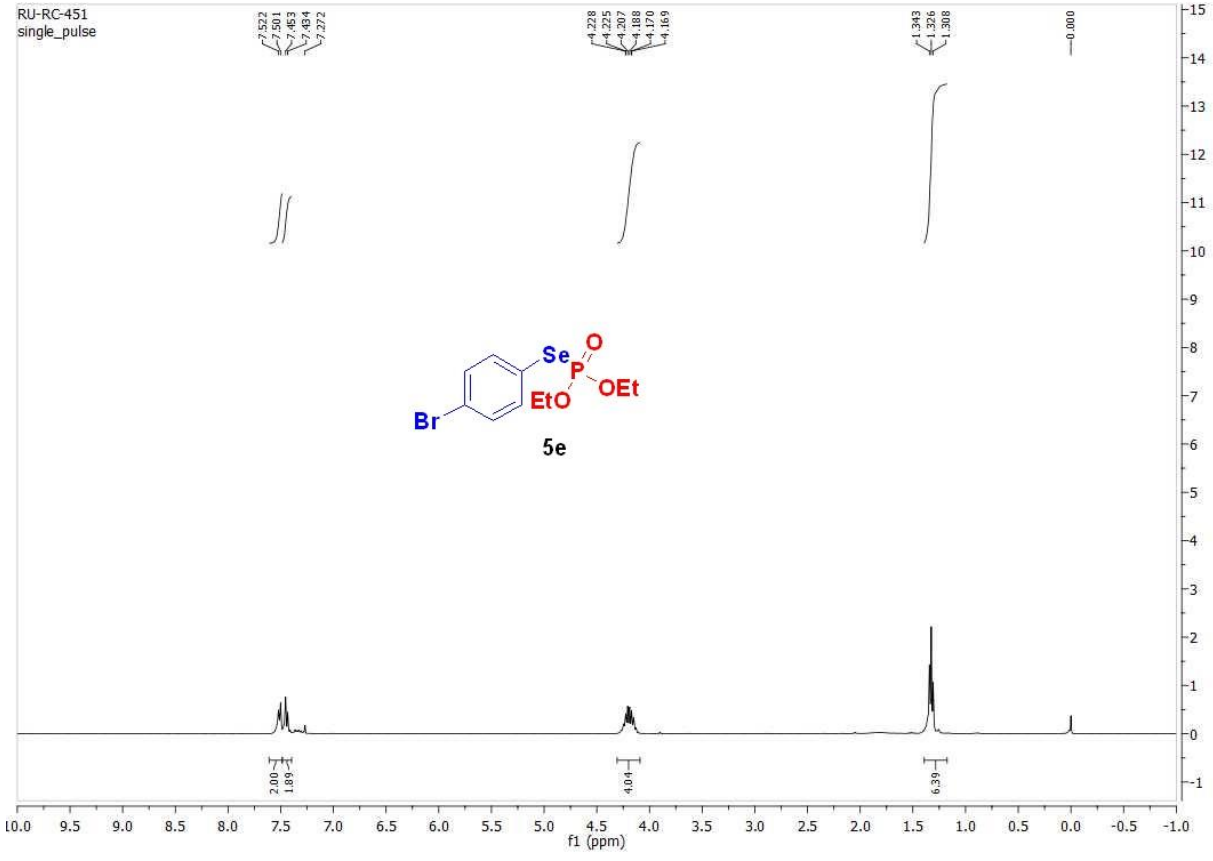

RU-RC-444
single pulse decoupled gated NOE
18.95
Se
O
P
EtO
OEt
Me
5c
f1 (ppm)


RU-RC-445
single_pulse
7.720
7.700
7.277
7.266
7.256
7.254
7.140
7.128
7.119
7.108
7.098
4.194
4.191
4.187
4.173
4.169
4.166
4.157
4.154
4.148
4.139
4.134
4.116
2.526
1.310
1.308
1.292
1.291
1.274
1.273
0.000
Me
Se
O
P
OEt
EtO
5d
1.00
2.07
1.10
4.29
3.14
6.71
f1 (ppm)

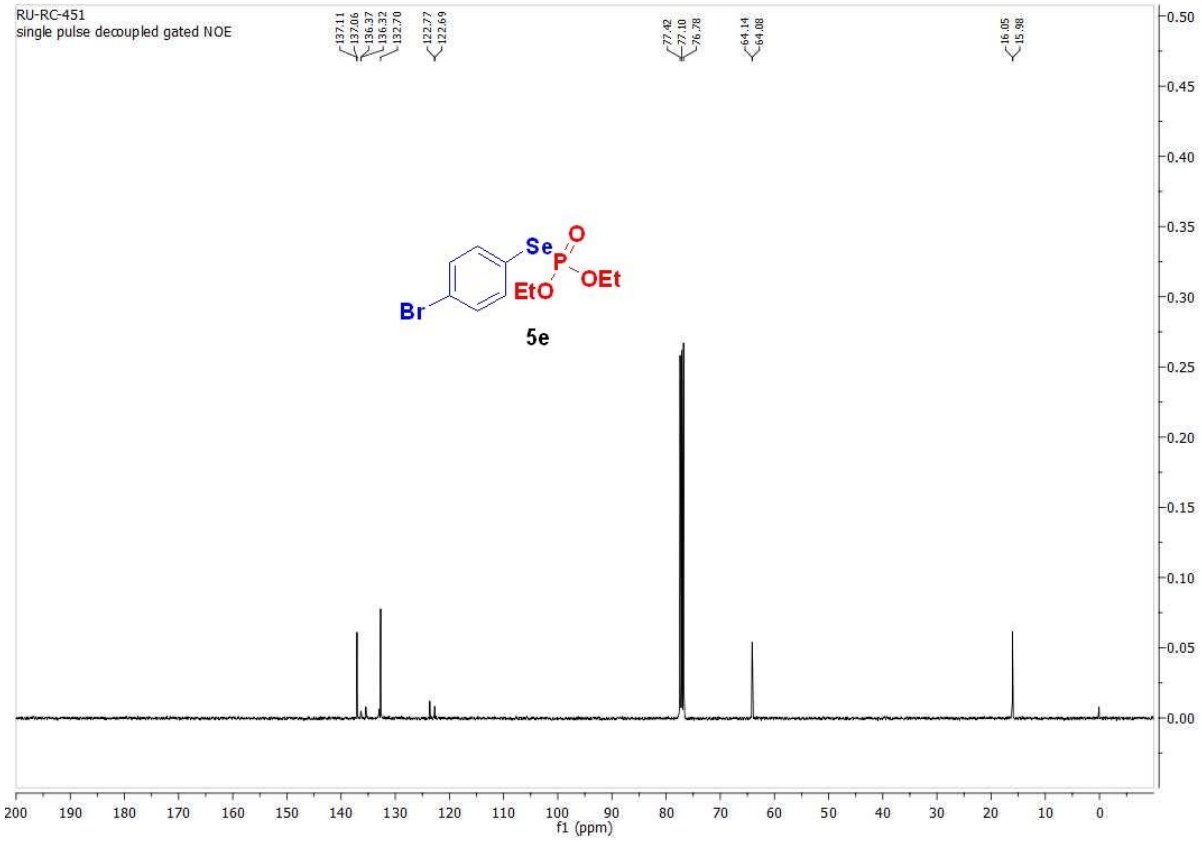

RU-RC-445
single pulse decoupled gated NOE
141.96
141.92
137.23
137.20
130.55
130.53
129.35
129.33
126.81
124.81
124.73
77.42
77.10
76.78
63.91
63.85
23.42
15.98
15.91
Me
Se
O
P
OEt
EtO
5d
f1 (ppm)

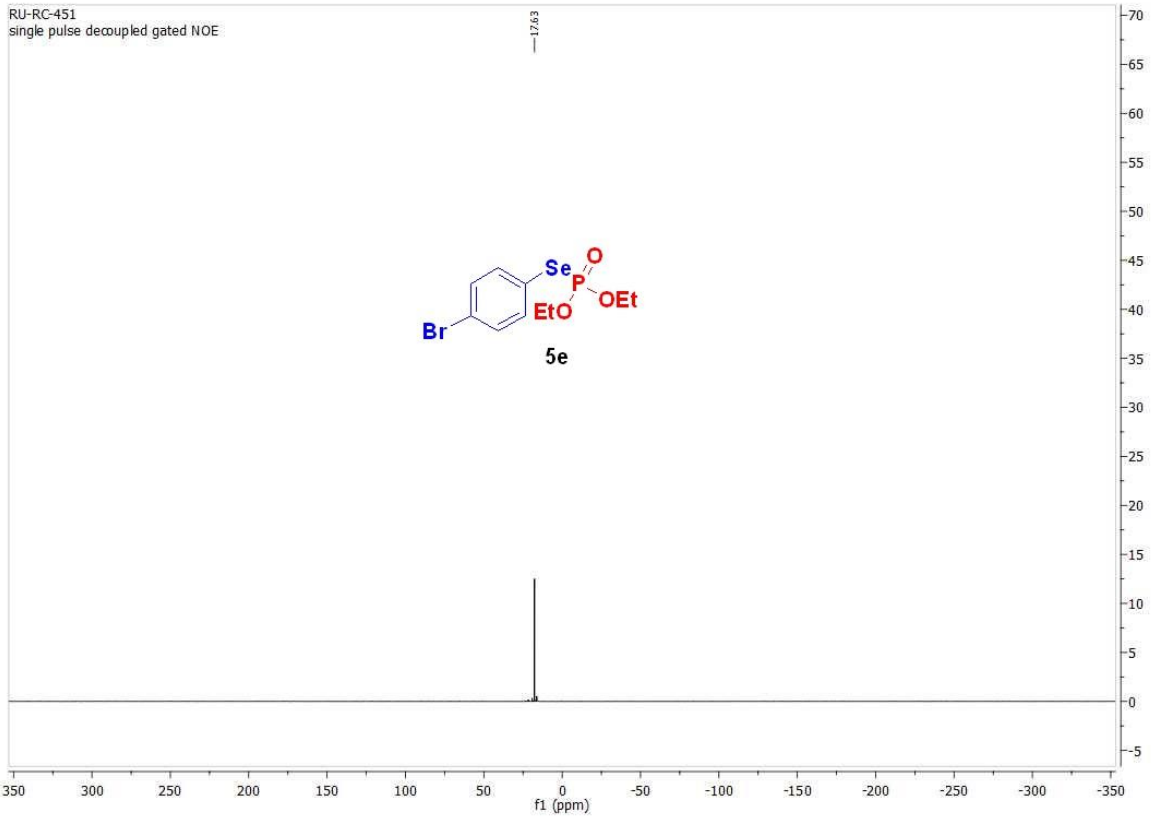

RU-RC-445
single pulse decoupled gated NOE
18.29
Me
Se
O
P
OEt
EtO
f1 (ppm)

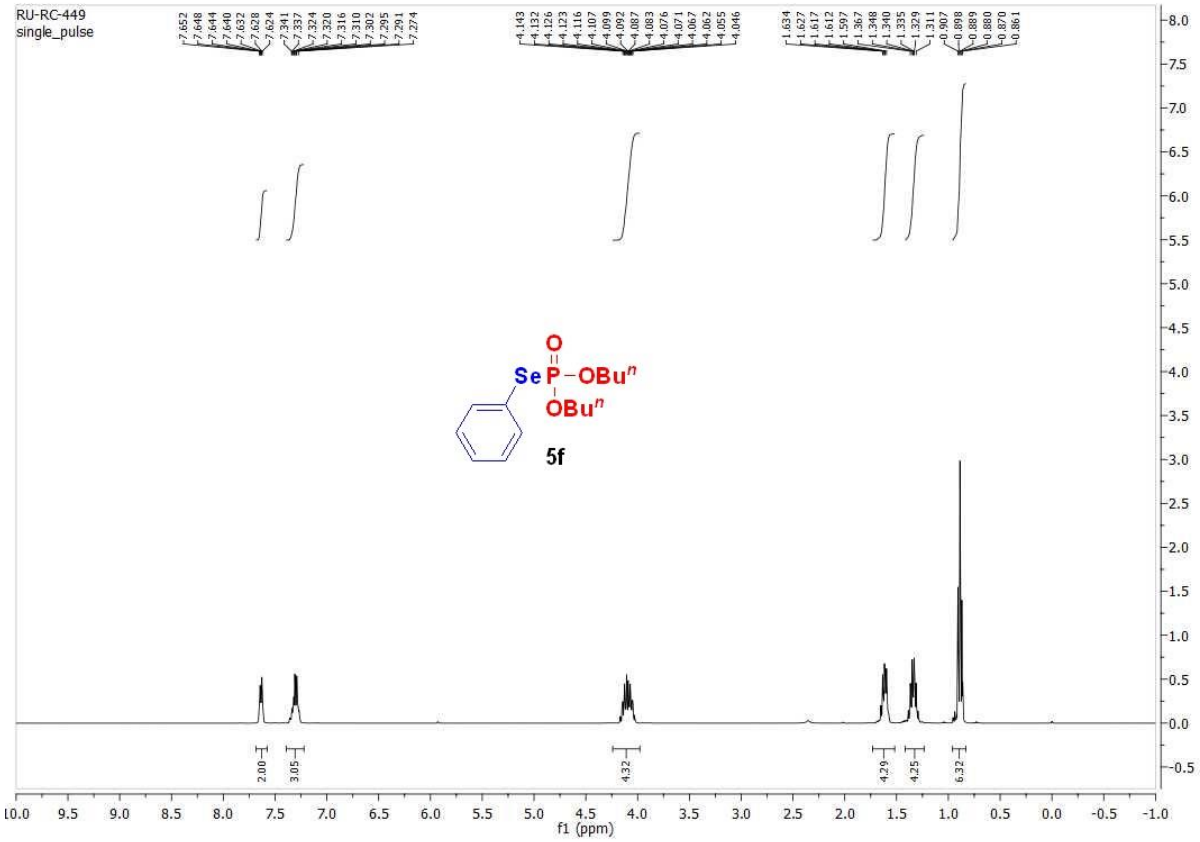
5d

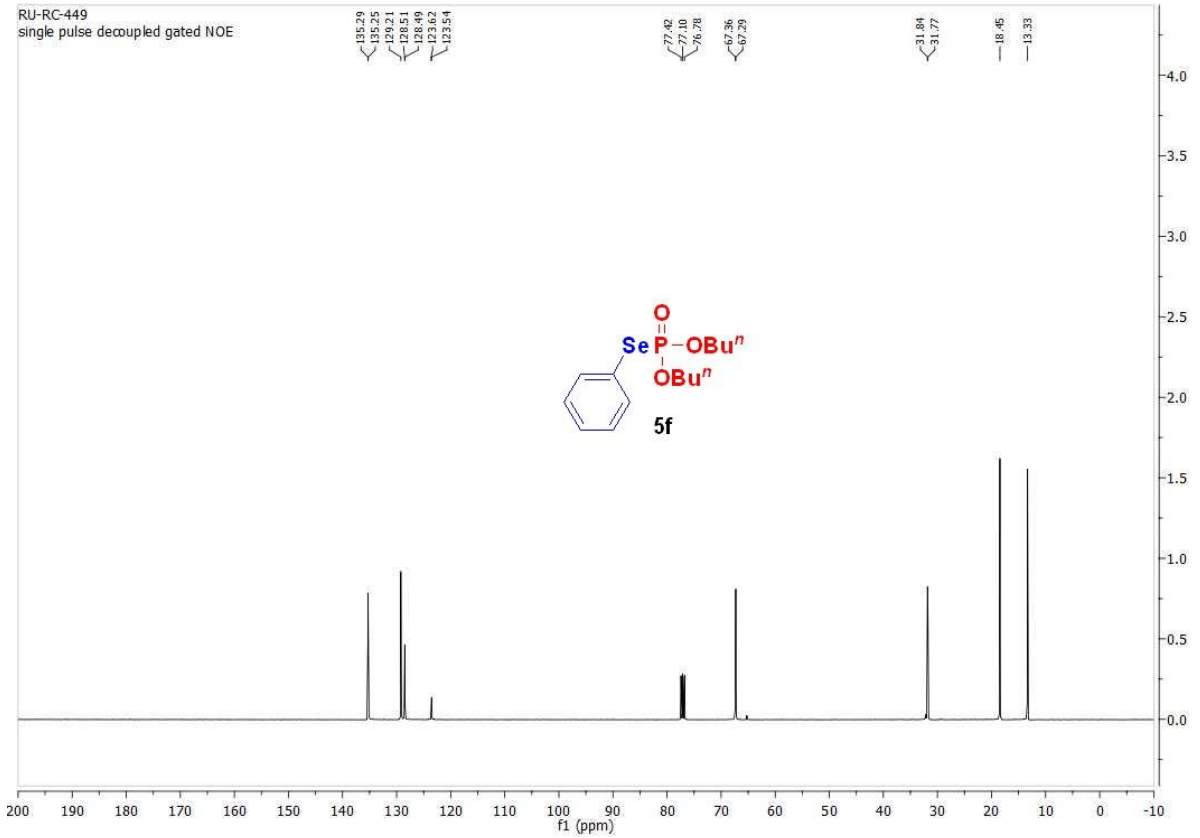

RU-RC-451
single_pulse
7.522
7.501
7.483
7.484
7.272
4.228
4.225
4.207
4.188
4.170
4.169
1.343
1.326
1.308
0.000
Se
O
P
OEt
EtO
Br
2.00
1.89
4.04
6.39
f1 (ppm)

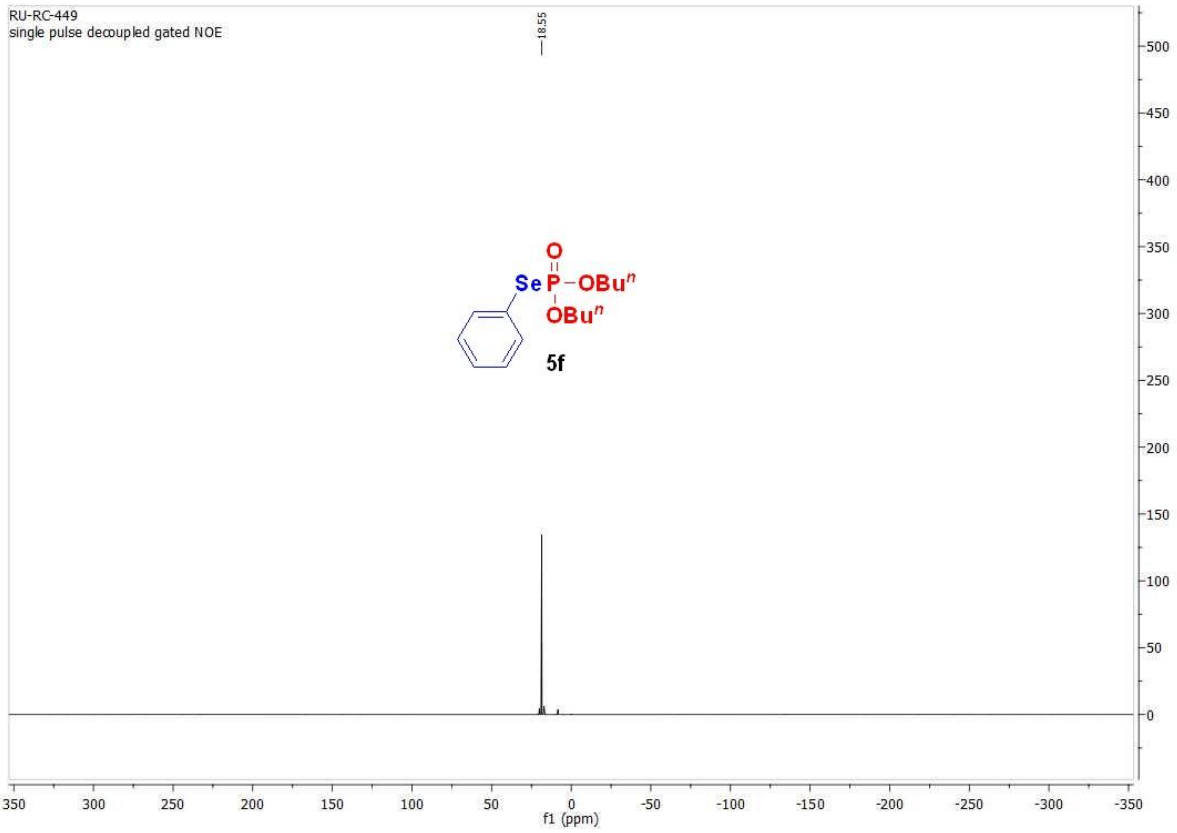
5e

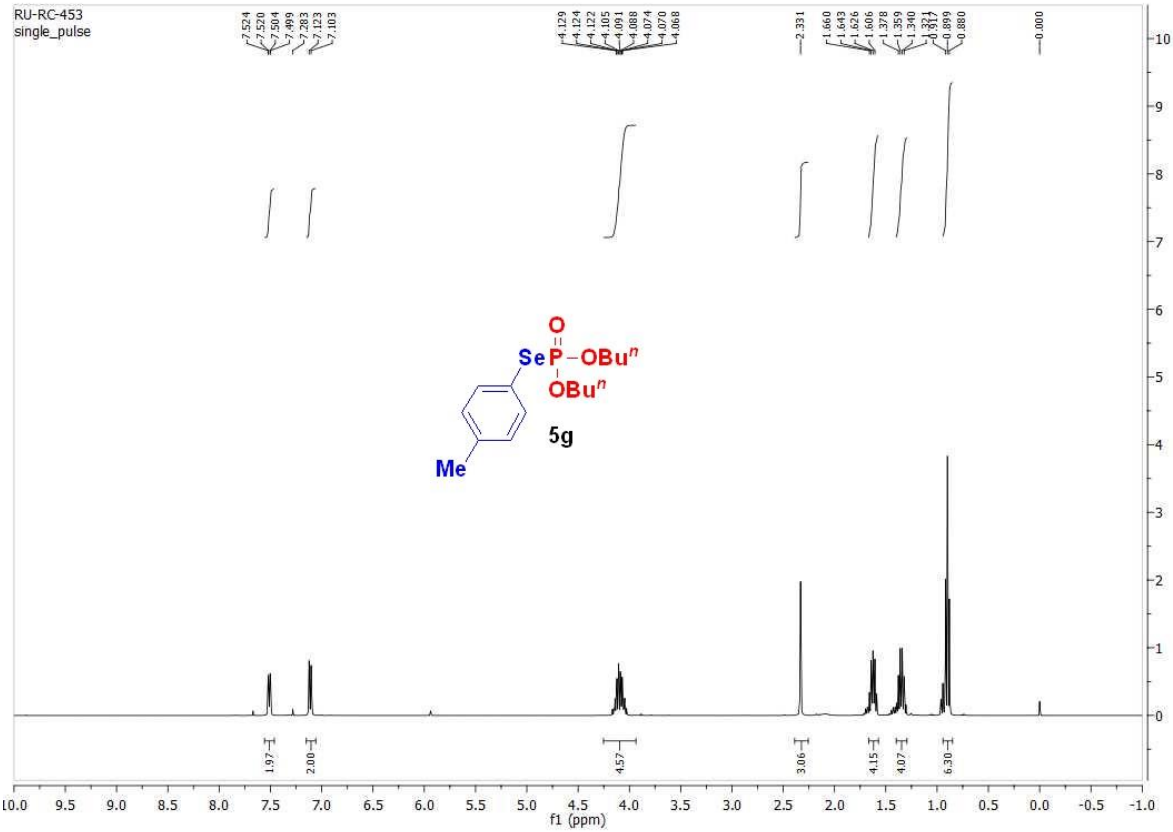

RU-RC-451
single pulse decoupled gated NOE
137.11
137.06
136.37
136.32
132.70
122.77
122.69
77.42
77.10
76.78
64.14
64.08
16.05
15.98
Se
O
P
OEt
EtO
Br
5e
f1 (ppm)

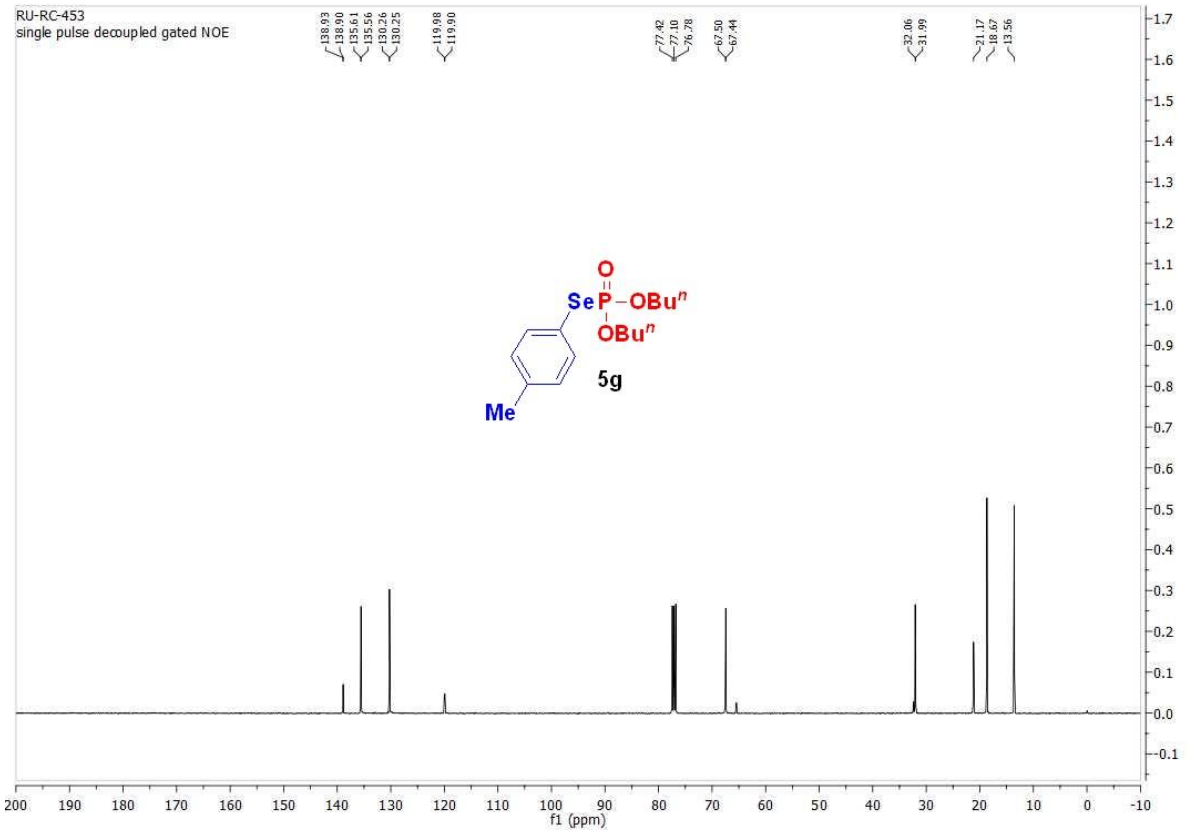

RU-RC-451
single pulse decoupled gated NOE
17.63
Se
O
P
OEt
EtO
Br
5e
f1 (ppm)

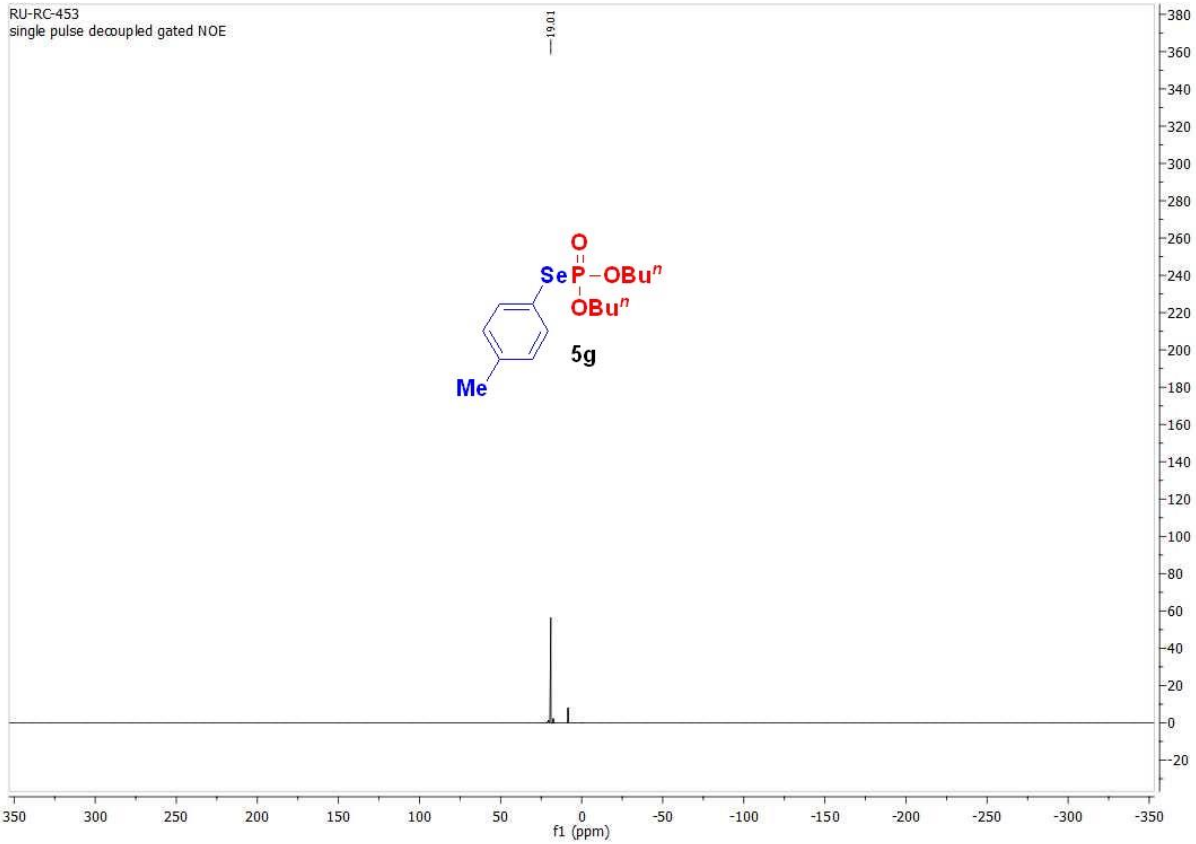

RU-RC-449
single_pulse
7.652 7.648 7.644 7.640 7.632 7.628 7.624 7.341 7.337 7.324 7.320 7.316 7.310 7.302 7.295 7.291 7.274
4.143 4.132 4.126 4.123 4.116 4.107 4.099 4.092 4.087 4.083 4.076 4.071 4.067 4.062 4.055 4.046
1.634 1.627 1.617 1.612 1.597 1.367 1.348 1.340 1.335 1.329 1.311 0.907 0.898 0.889 0.880 0.870 0.861
O
Se P –OBu^n
OBu^n
5f
2.00 3.05 4.32 4.29 4.25 6.32
f1 (ppm)

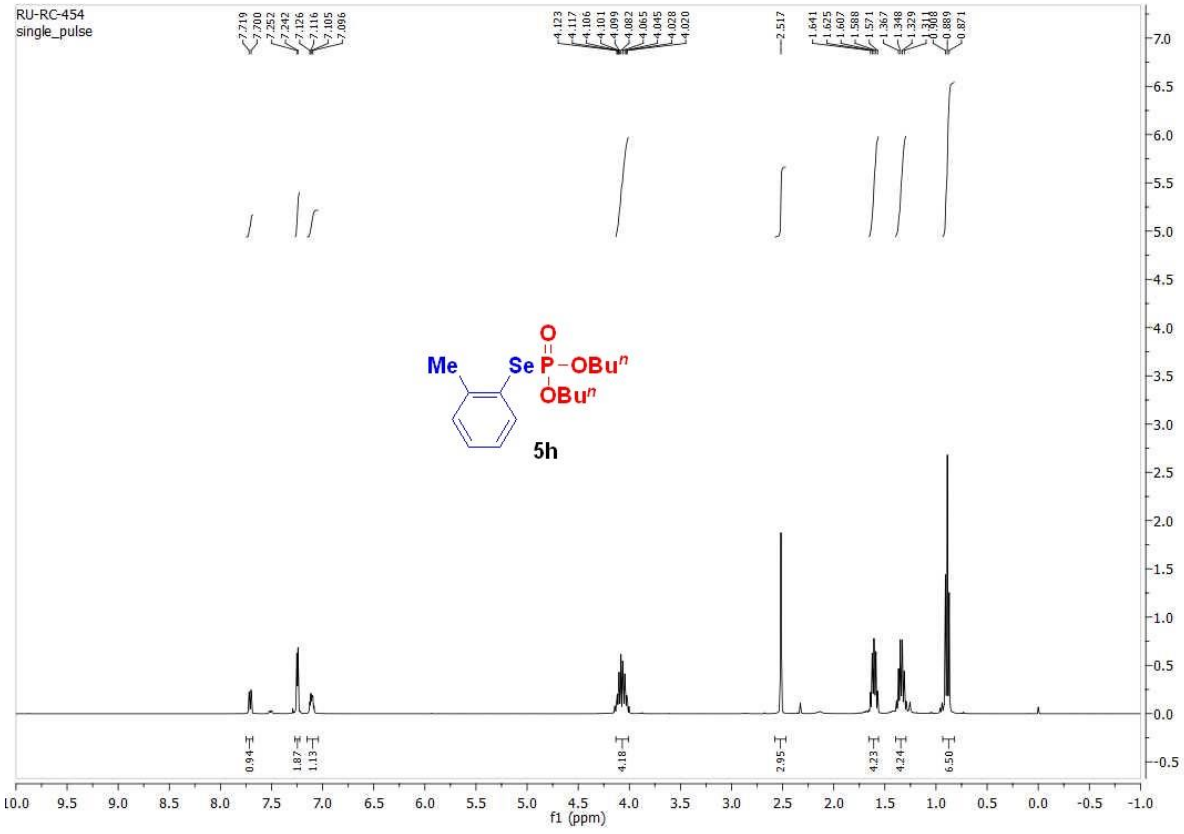

RU-RC-449
single pulse decoupled gated NOE
135.29 135.25 129.21 128.51 128.49 123.62 123.54
77.42 77.10 76.78 67.36 67.29
31.84 31.77 18.45 13.33
O
Se P –OBu^n
OBu^n
5f
f1 (ppm)

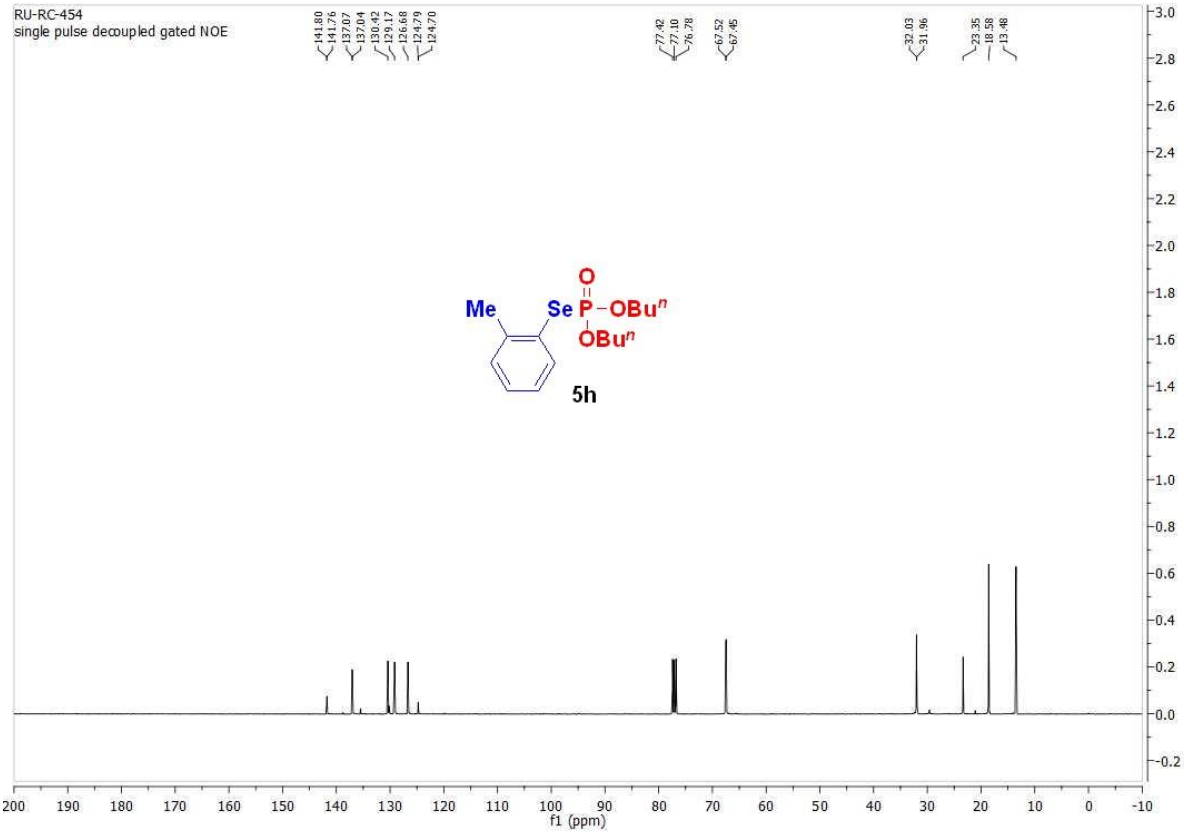

RU-RC-449
single pulse decoupled gated NOE
18.55
O
Se P –OBu^n
OBu^n
5f
f1 (ppm)

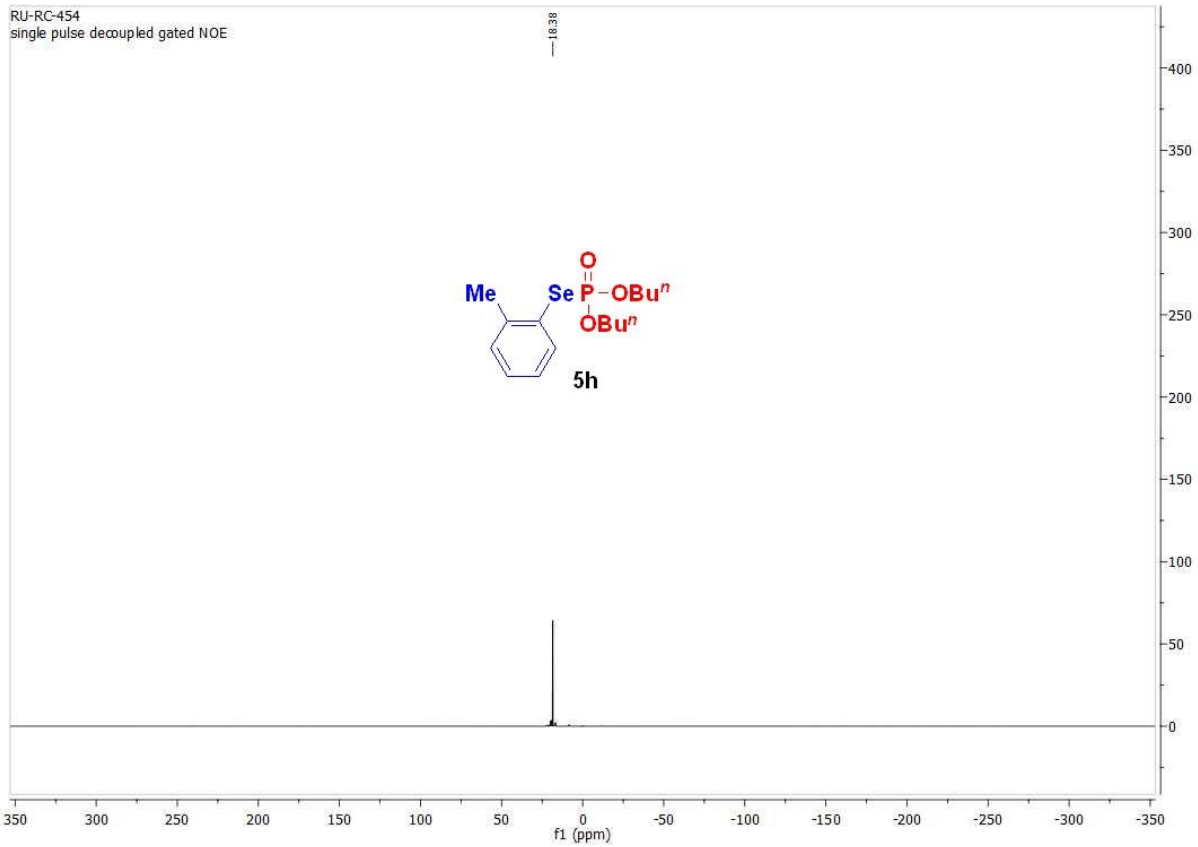

RU-RC-453
single_pulse
7.524
7.520
7.504
7.499
7.283
7.123
7.103
4.129
4.124
4.122
4.105
4.091
4.088
4.074
4.070
4.068
2.331
1.660
1.643
1.626
1.606
1.378
1.359
1.340
0.899
0.880
0.000
O
Se P –OBu^n
OBu^n
5g
Me
1.97
2.00
4.57
3.06
4.15
4.07
6.30
f1 (ppm)

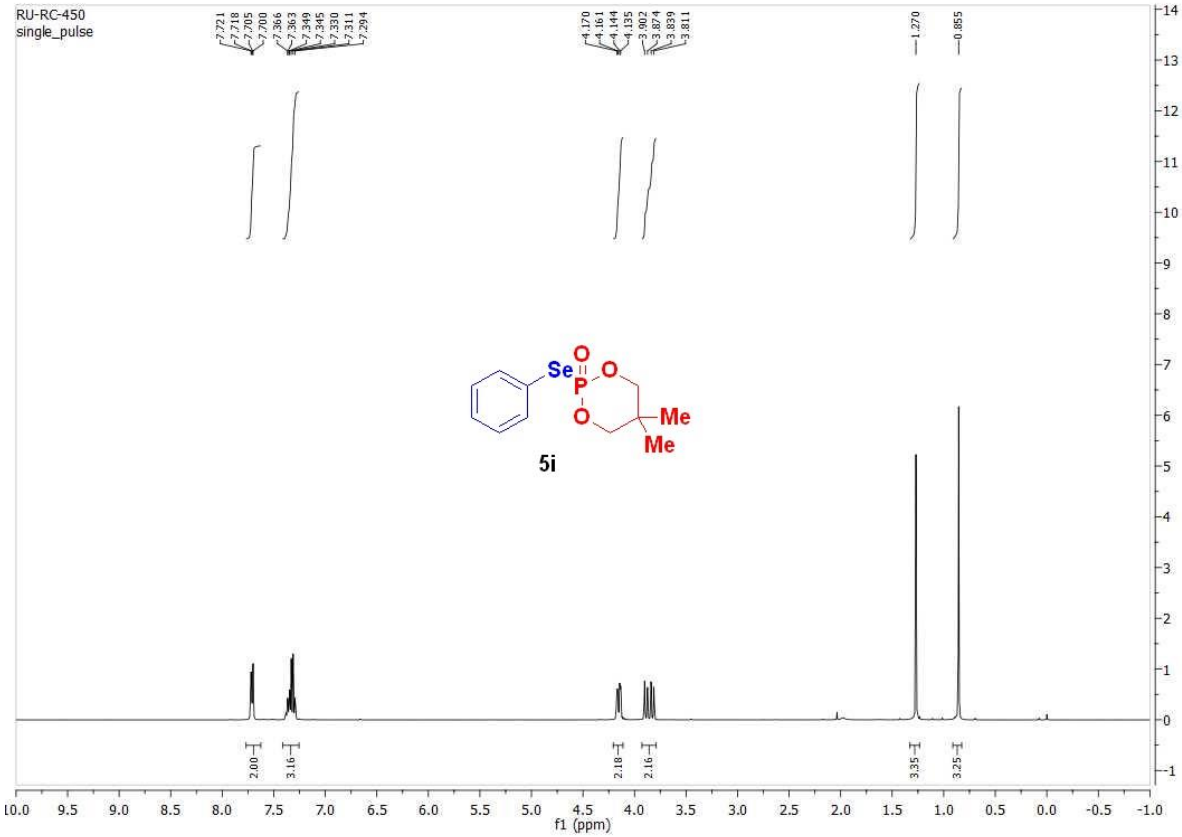

RU-RC-453
single pulse decoupled gated NOE
138.93
138.90
135.61
135.56
130.26
130.25
119.98
119.90
77.42
77.10
76.78
67.50
67.44
32.06
31.99
21.17
18.67
13.56
O
Se P –OBu^n
OBu^n
5g
Me
f1 (ppm)

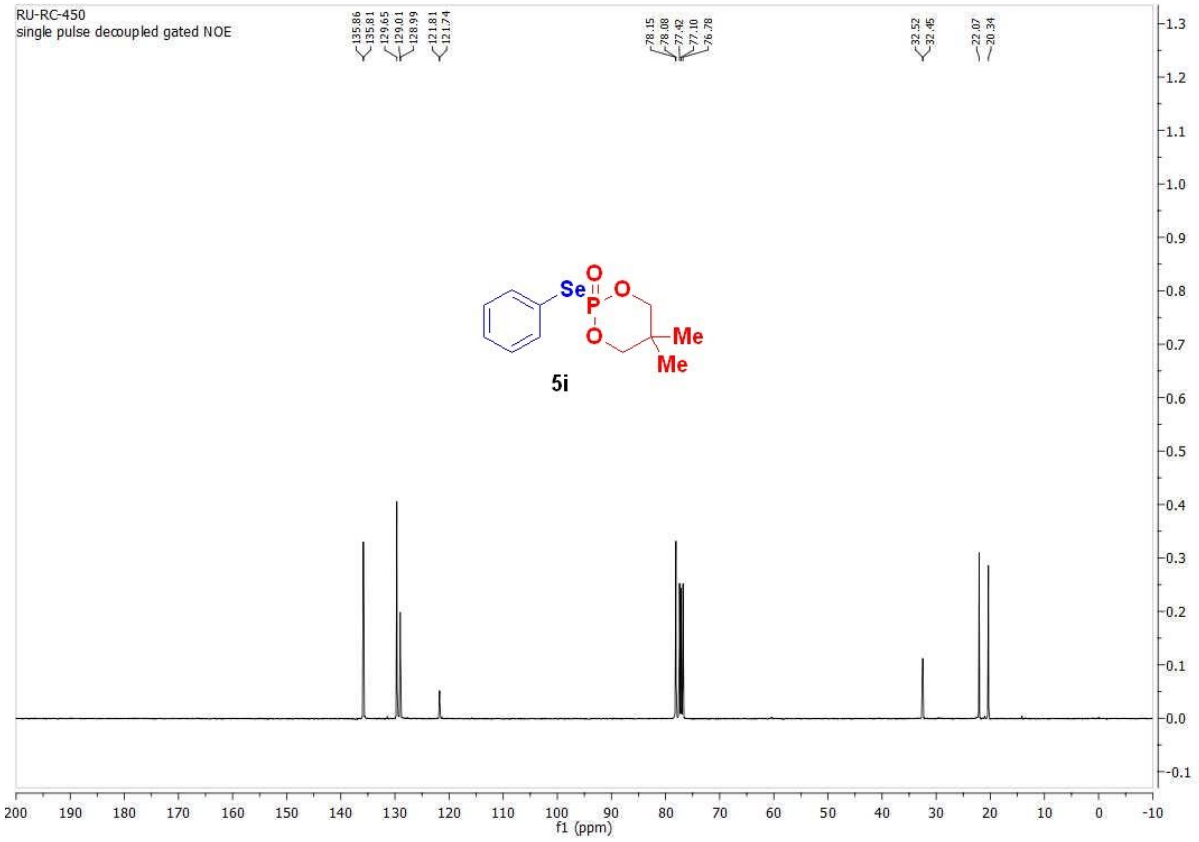

RU-RC-453
single pulse decoupled gated NOE
19.01
O
Se P –OBu^n
OBu^n
5g
Me
f1 (ppm)

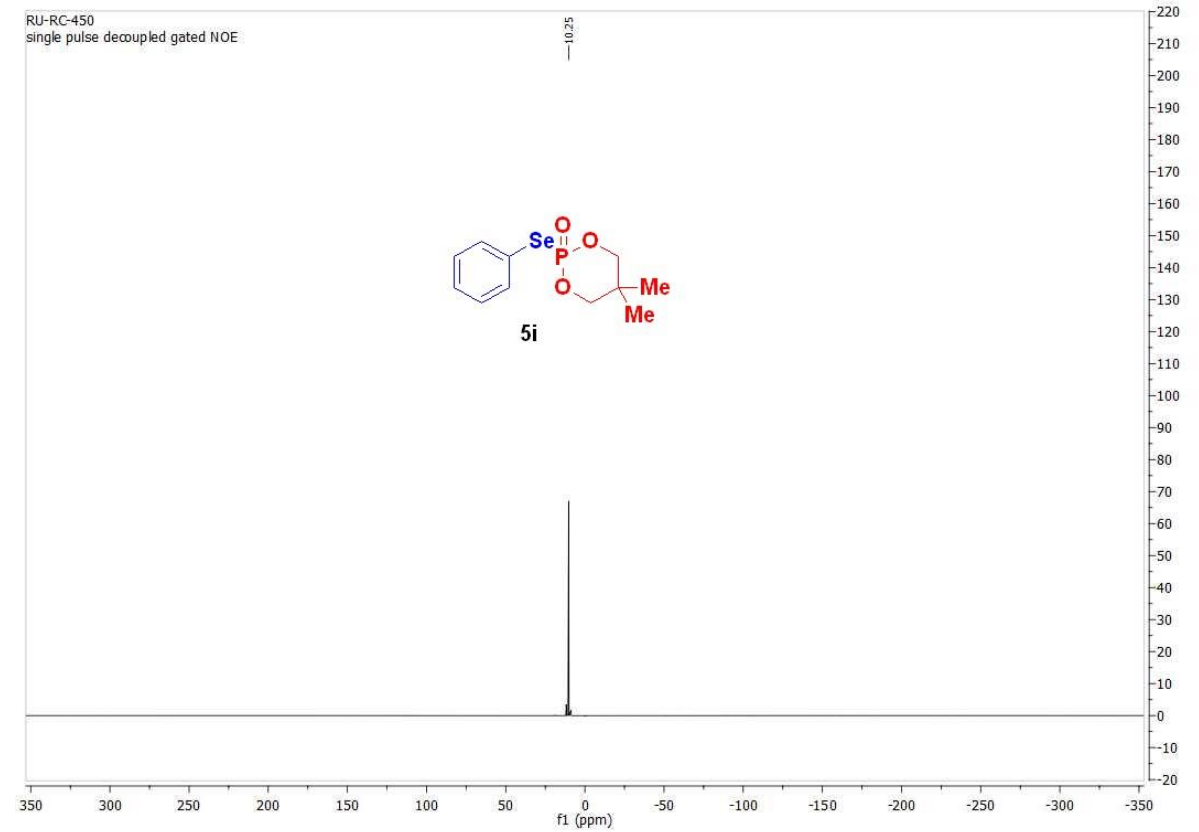

RU-RC-454
single_pulse
7.719
7.700
7.252
7.242
7.126
7.116
7.105
7.096
4.123
4.117
4.106
4.101
4.099
4.082
4.065
4.045
4.028
4.020
2.517
1.641
1.625
1.607
1.588
1.571
1.367
1.348
1.329
0.911
0.908
0.889
0.871
Me
Se
P
O
OBu^n
OBu^n
5h
0.94
1.87
1.13
4.18
2.95
4.23
4.24
6.50
f1 (ppm)

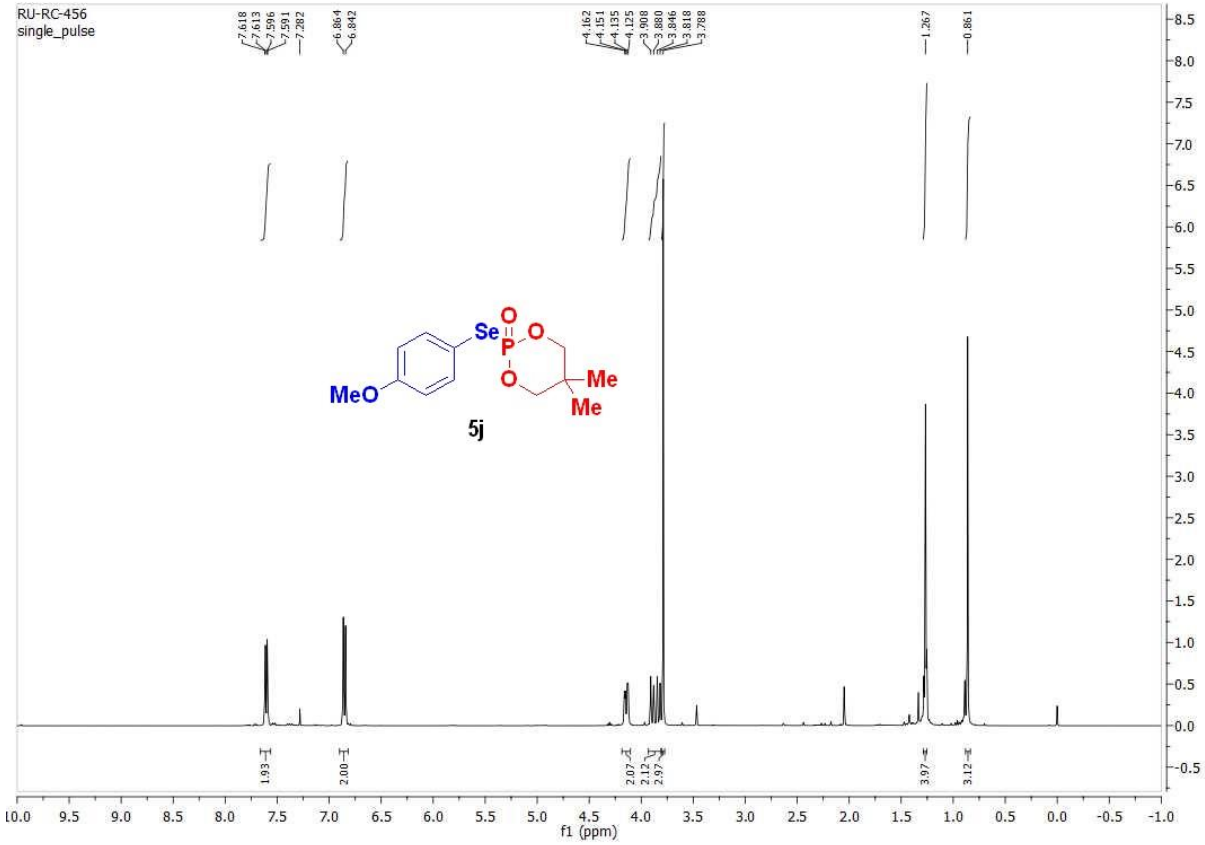

RU-RC-454
single pulse decoupled gated NOE
141.80
141.76
137.07
137.04
130.42
129.17
126.68
124.79
124.70
77.42
77.10
76.78
67.52
67.45
32.03
31.96
23.35
18.58
13.48
Me
Se
P
O
OBu^n
OBu^n
5h
f1 (ppm)

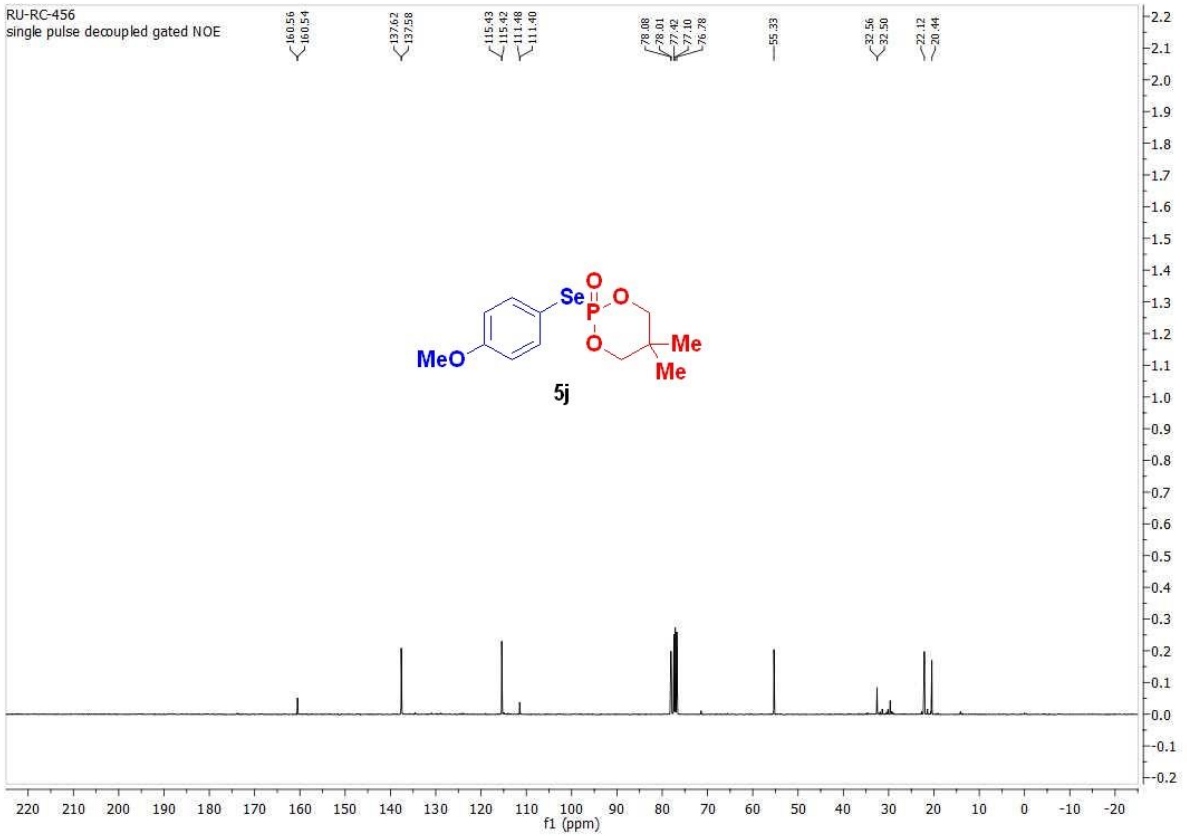

RU-RC-454
single pulse decoupled gated NOE
18.38
Me
Se
O
P
OBu^n
OBu^n
5h
f1 (ppm)


RU-RC-450
single_pulse
7.721
7.718
7.705
7.700
7.366
7.363
7.349
7.345
7.330
7.311
7.294
4.170
4.161
4.144
4.135
3.902
3.874
3.839
3.811
1.270
0.855
Se
O
P
O
O
Me
Me
5i
2.00
3.16
2.18
2.16
3.35
3.25
f1 (ppm)


RU-RC-450
single pulse decoupled gated NOE
135.86
135.81
129.65
129.01
128.99
121.81
121.74
78.15
78.08
77.42
77.10
76.78
32.52
32.45
22.07
20.34
Se
O
P
O
O
Me
Me
5i
f1 (ppm)


RU-RC-450
single pulse decoupled gated NOE
10.25
Se
O
P
O
O
Me
Me
5i
f1 (ppm)


RU-RC-456
single_pulse
7.618
7.613
7.596
7.591
7.282
6.864
6.842
4.162
4.151
4.135
4.125
3.908
3.880
3.846
3.818
3.788
1.267
0.861
1.93
2.00
2.07
2.12
2.97
3.97
3.12
Se
O
P
O
O
Me
Me
MeO
5j
f1 (ppm)


RU-RC-456
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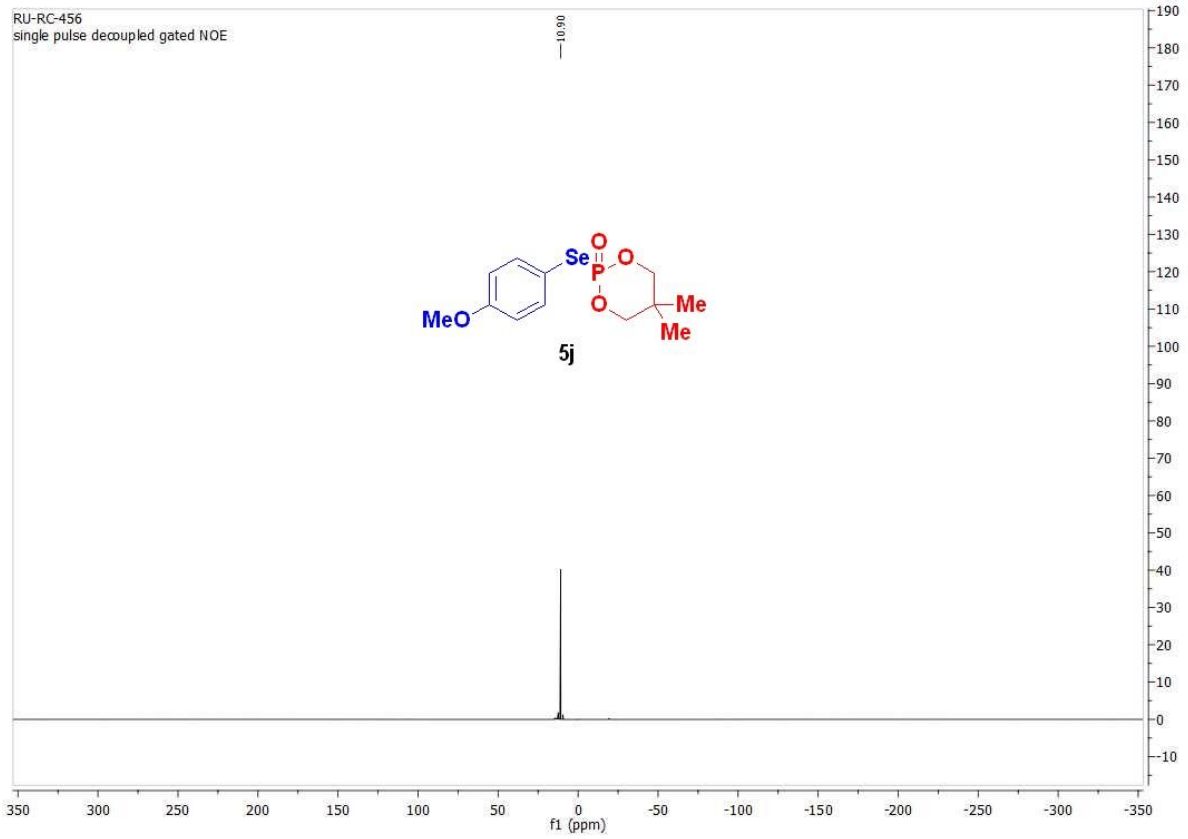
160.56
160.54
137.62
137.58
115.43
115.42
111.48
111.40
78.08
78.01
77.42
77.10
76.78
55.33
32.56
32.50
22.12
20.44
Se
O
P
O
O
Me
Me
MeO
5j
f1 (ppm)


RU-RC-456
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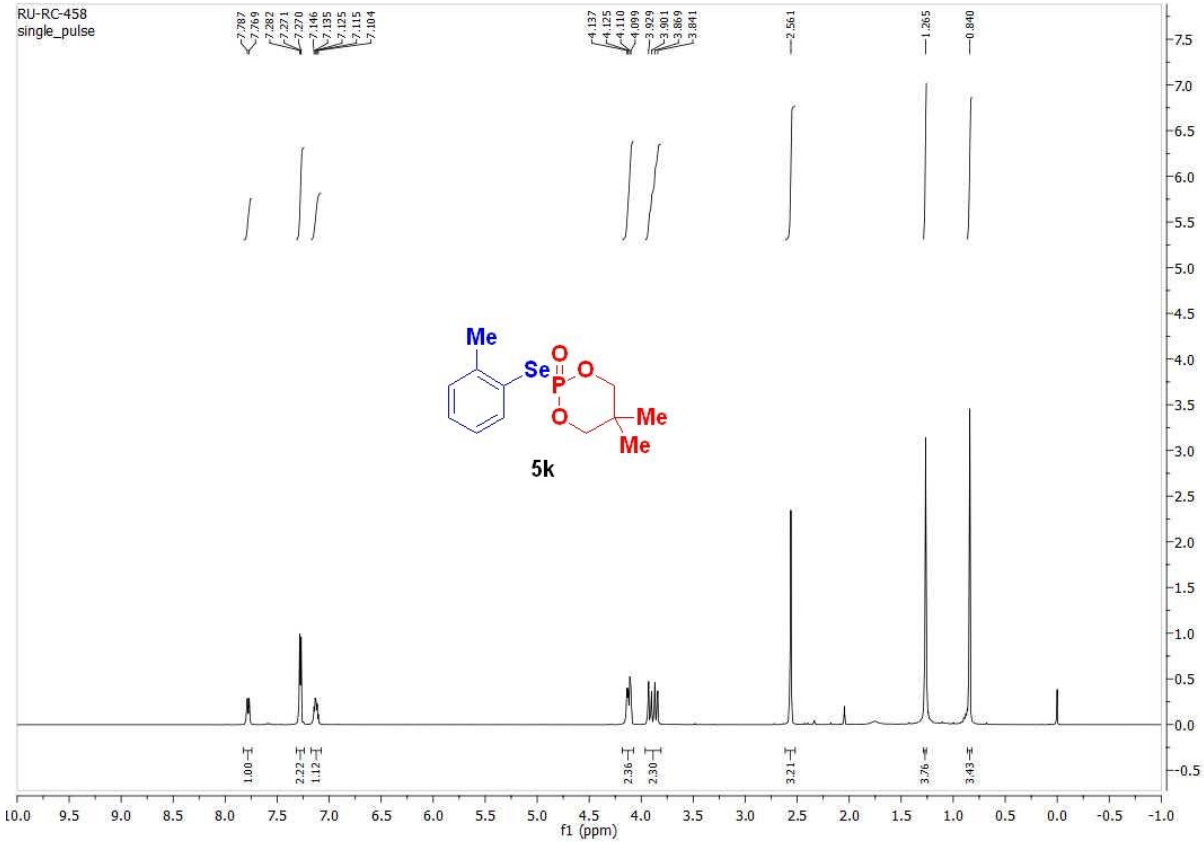
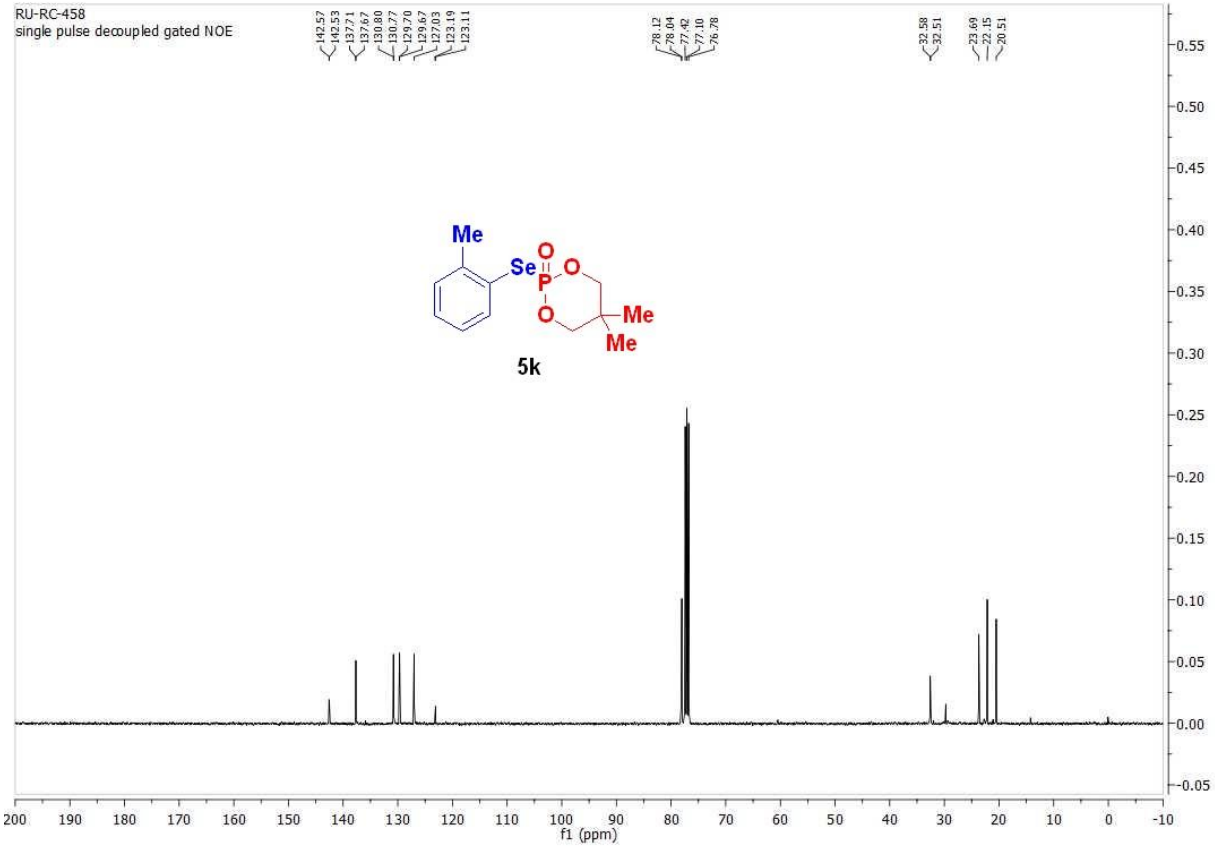
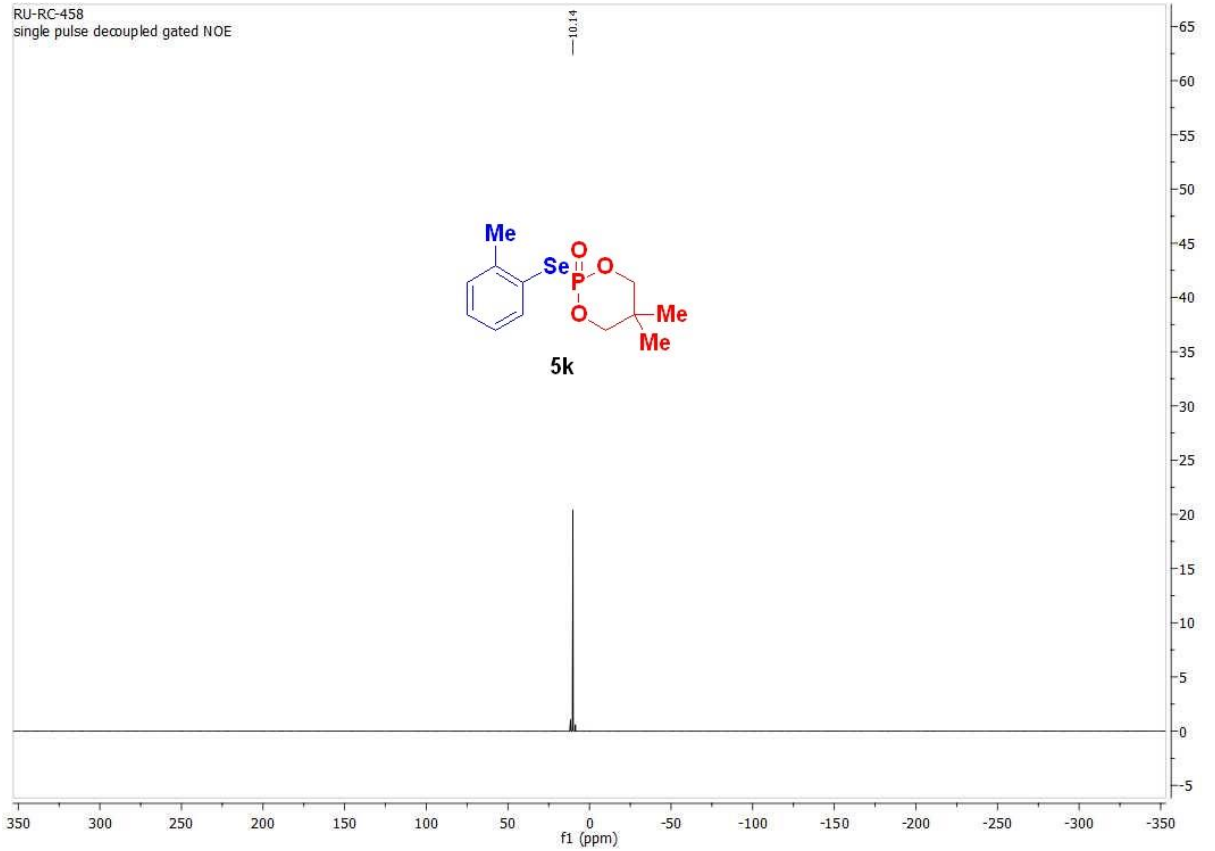
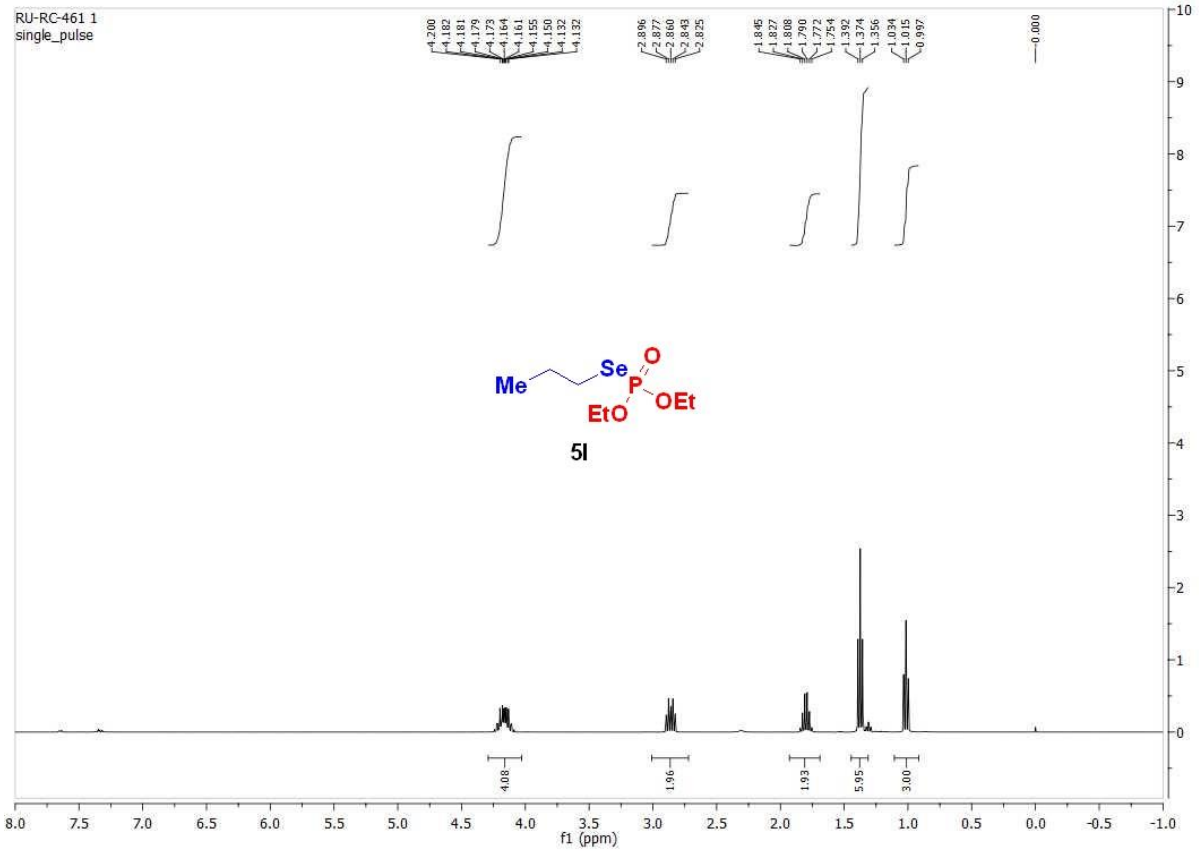
10.90
Se
O
P
O
O
Me
Me
MeO
5j
f1 (ppm)


RU-RC-458
single_pulse
7.787
7.769
7.282
7.271
7.270
7.146
7.135
7.125
7.115
7.104
4.137
4.125
4.110
4.099
3.929
3.901
3.869
3.841
2.561
1.265
0.840
Me
Se
O
P
O
O
Me
Me
5k
1.00
2.22
1.12
2.36
2.30
3.21
3.76
3.43
f1 (ppm)


RU-RC-458
single pulse decoupled gated NOE
142.57
142.53
137.71
137.67
130.80
130.77
129.70
129.67
127.03
123.19
123.11
78.12
78.04
77.42
77.10
76.78
32.58
32.51
23.69
22.15
20.51
Me
Se
O
P
O
O
Me
Me
5k
f1 (ppm)


RU-RC-458
single pulse decoupled gated NOE
10.14
Me
Se
O
P
O
O
Me
Me
5k
f1 (ppm)


RU-RC-461 1
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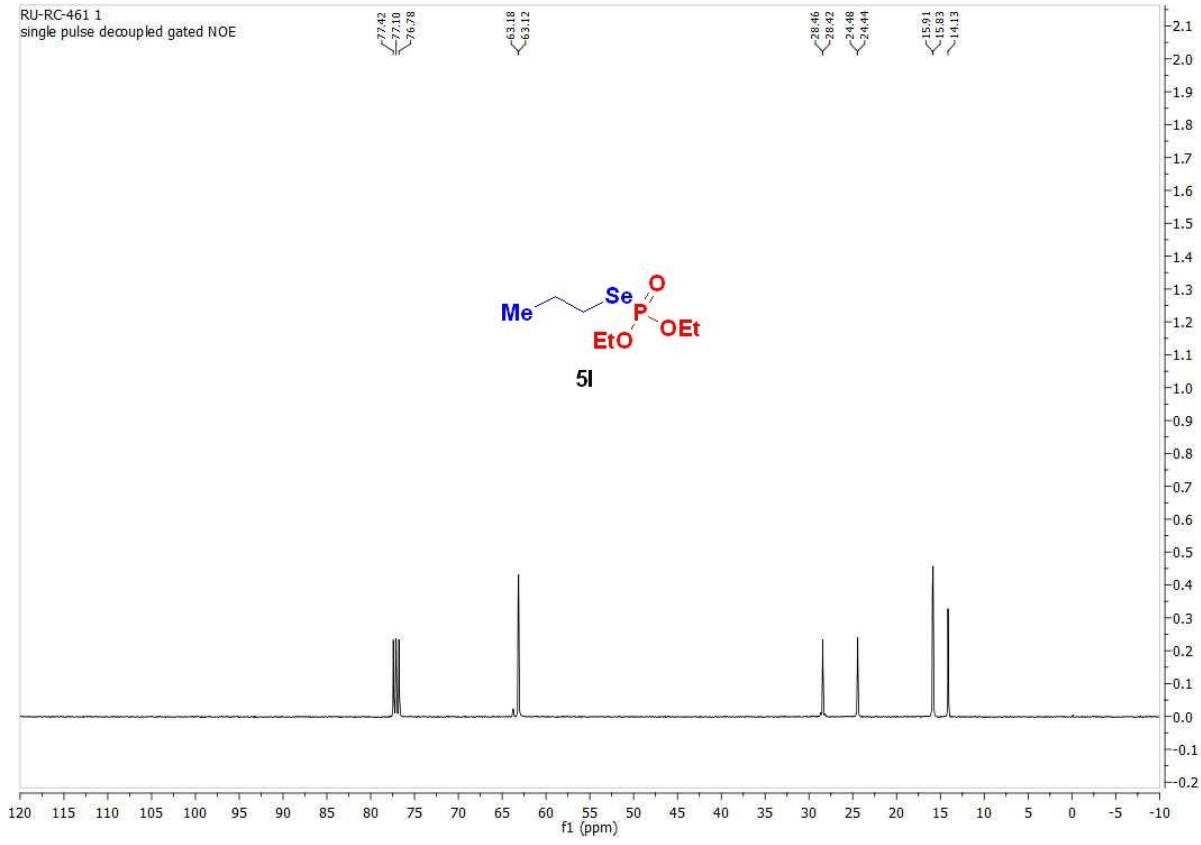
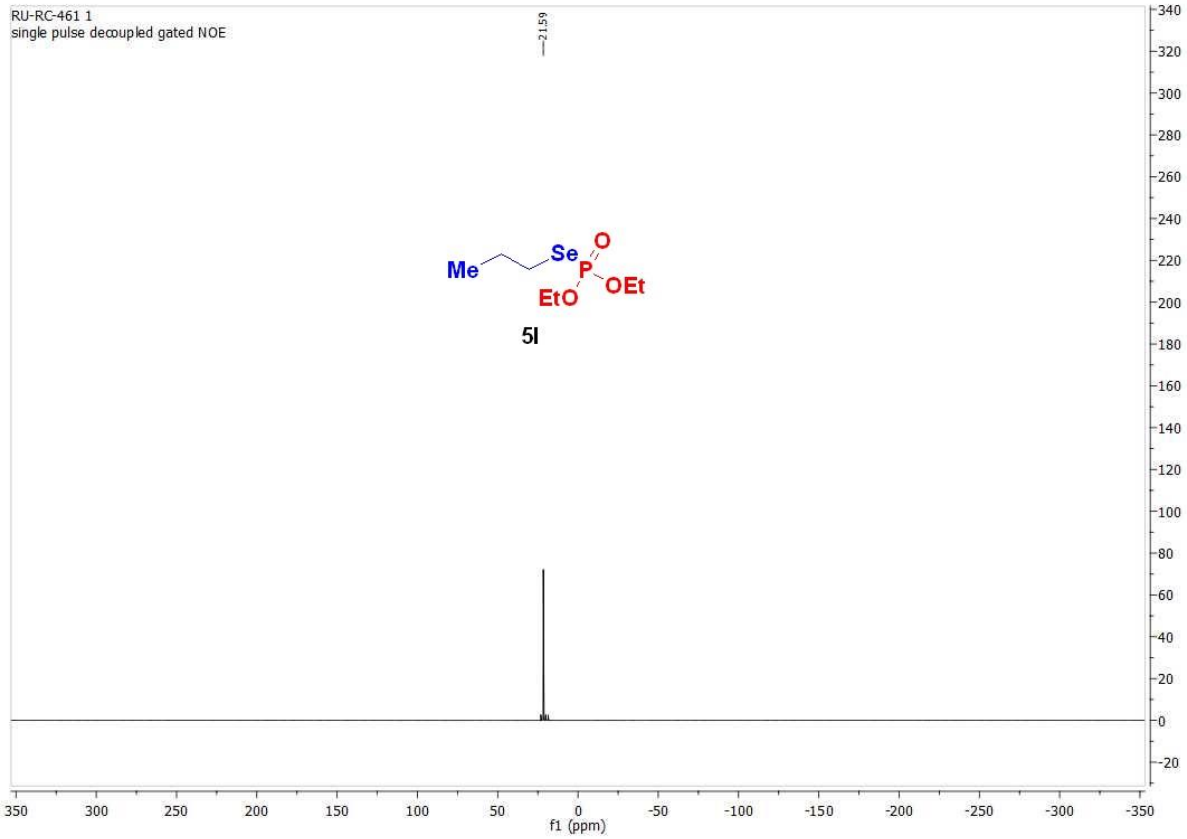
4.200
4.182
4.181
4.179
4.173
4.164
4.161
4.155
4.150
4.132
4.132
2.896
2.877
2.860
2.843
2.825
1.845
1.827
1.808
1.790
1.772
1.754
1.392
1.374
1.356
1.034
1.015
0.997
0.000
Me
Se
O
P
OEt
EtO
5l
4.08
1.96
1.93
5.95
3.00
f1 (ppm)


RU-RC-461 1
single pulse decoupled gated NOE
77.42
77.10
76.78
63.18
63.12
28.46
28.42
24.48
24.44
15.91
15.93
14.13
Me
Se
O
P
OEt
EtO
5l
f1 (ppm)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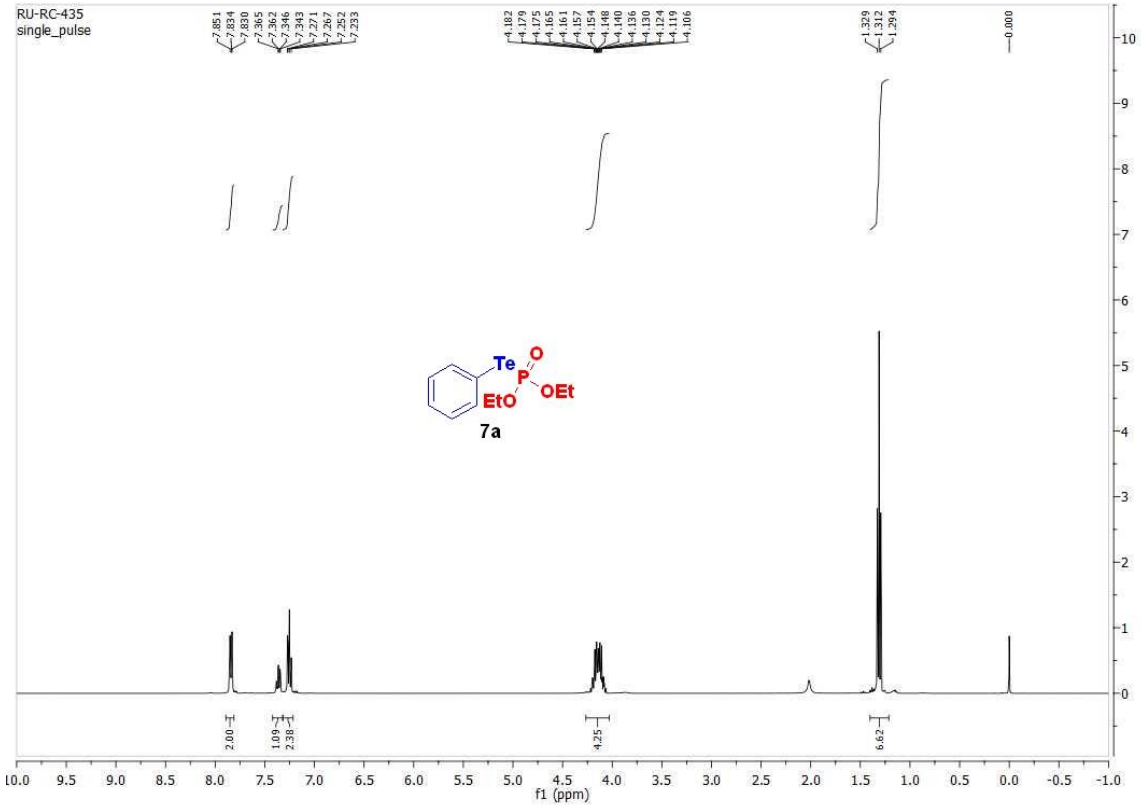
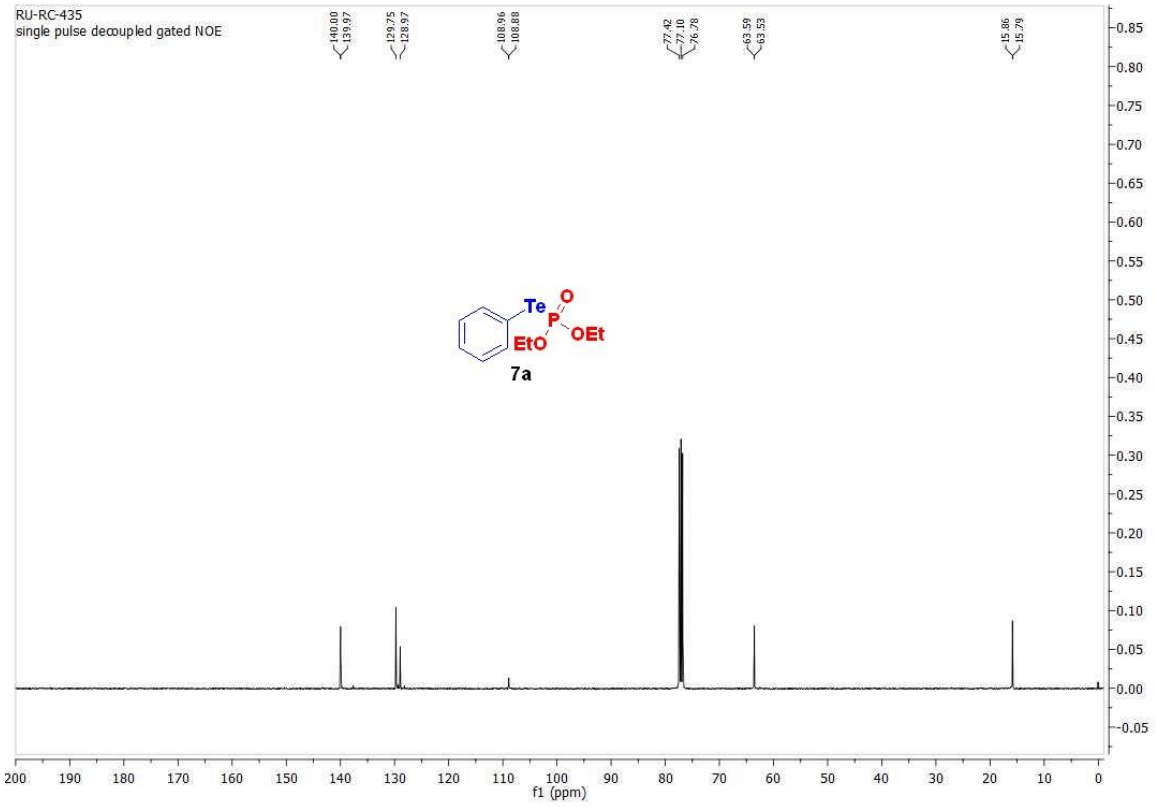
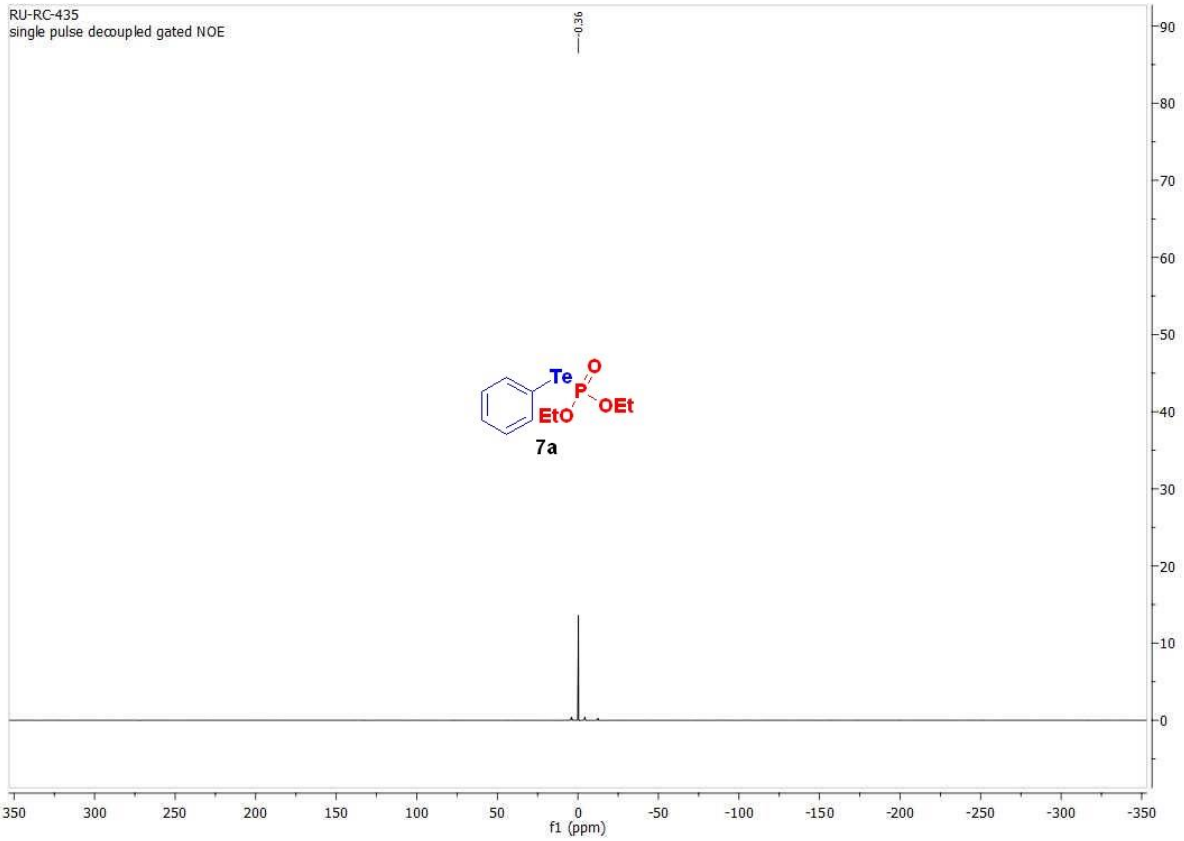
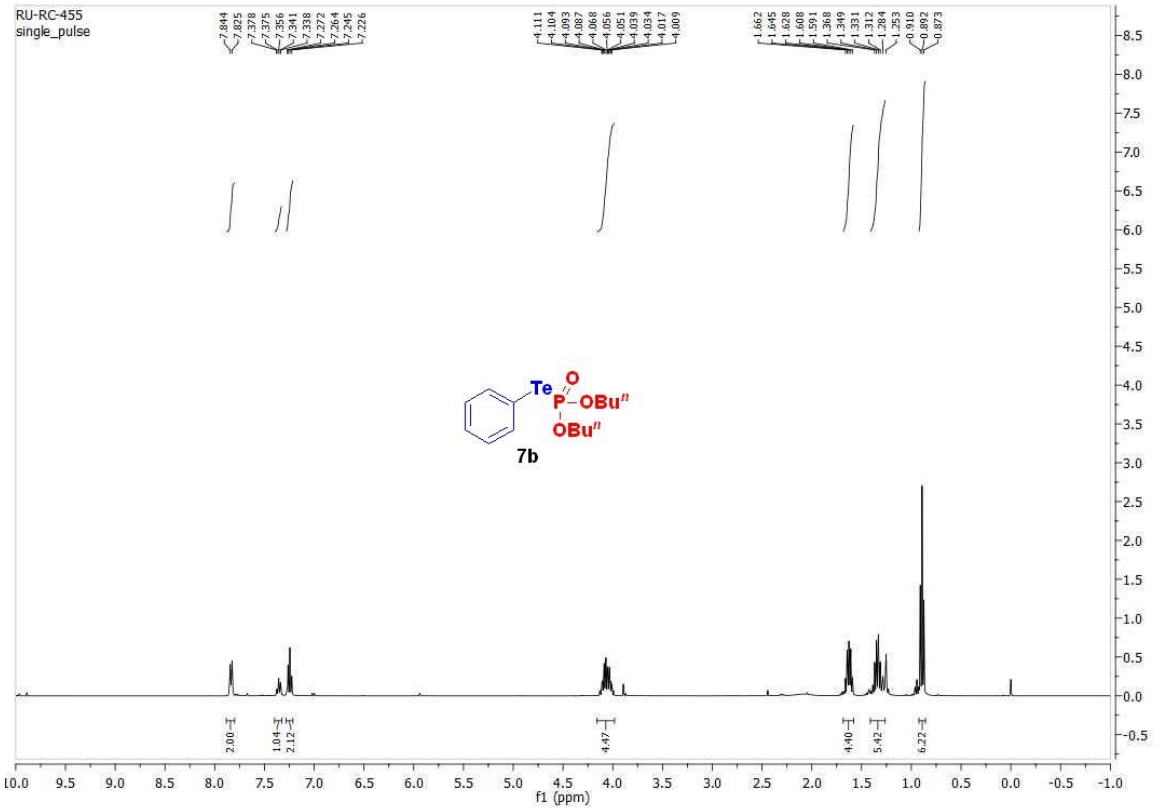
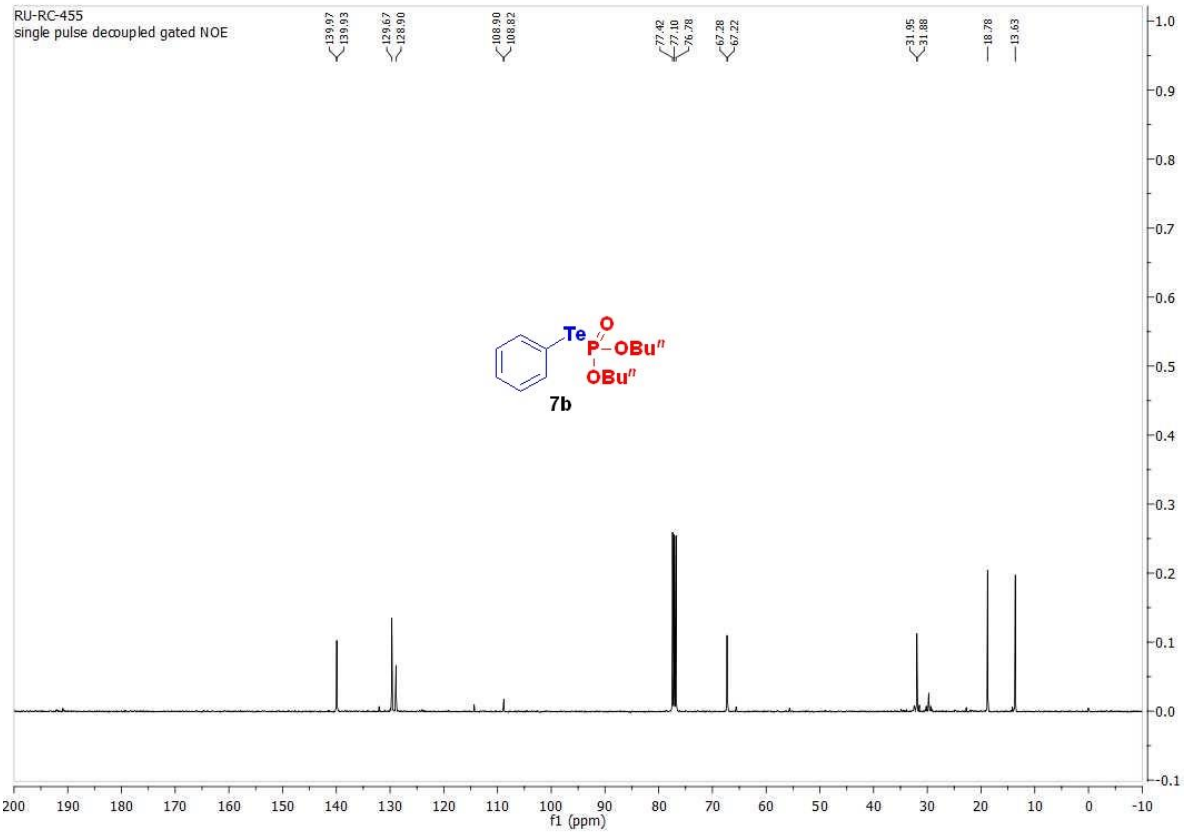
single pulse decoupled gated NOE
21.59
Me
Se
O
P
EtO
OEt
5l
f1 (ppm)

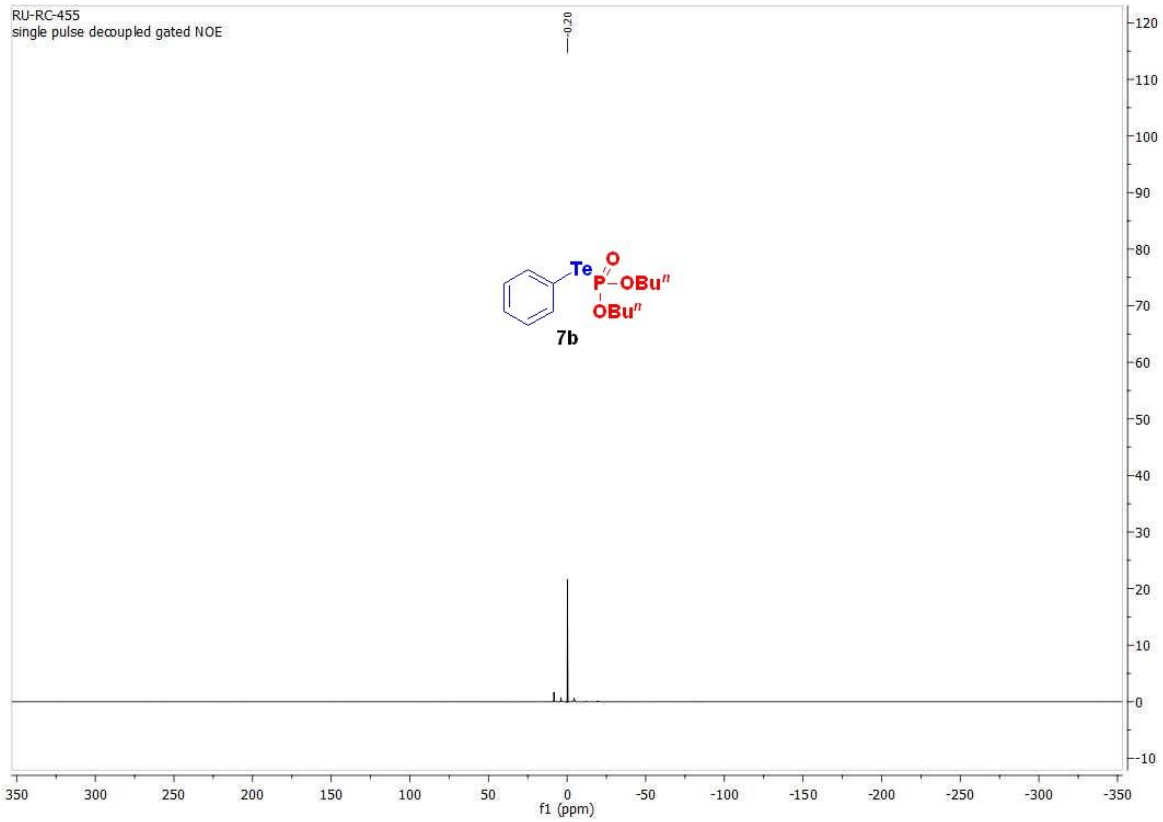

RU-RC-435
single_pulse
7.851
7.834
7.830
7.365
7.362
7.346
7.343
7.271
7.267
7.252
7.233
4.182
4.179
4.175
4.165
4.161
4.157
4.154
4.148
4.140
4.136
4.130
4.124
4.119
4.106
1.329
1.312
1.294
0.000
Te
O
P
EtO
OEt
7a
2.00
1.09
2.38
4.25
6.62
f1 (ppm)

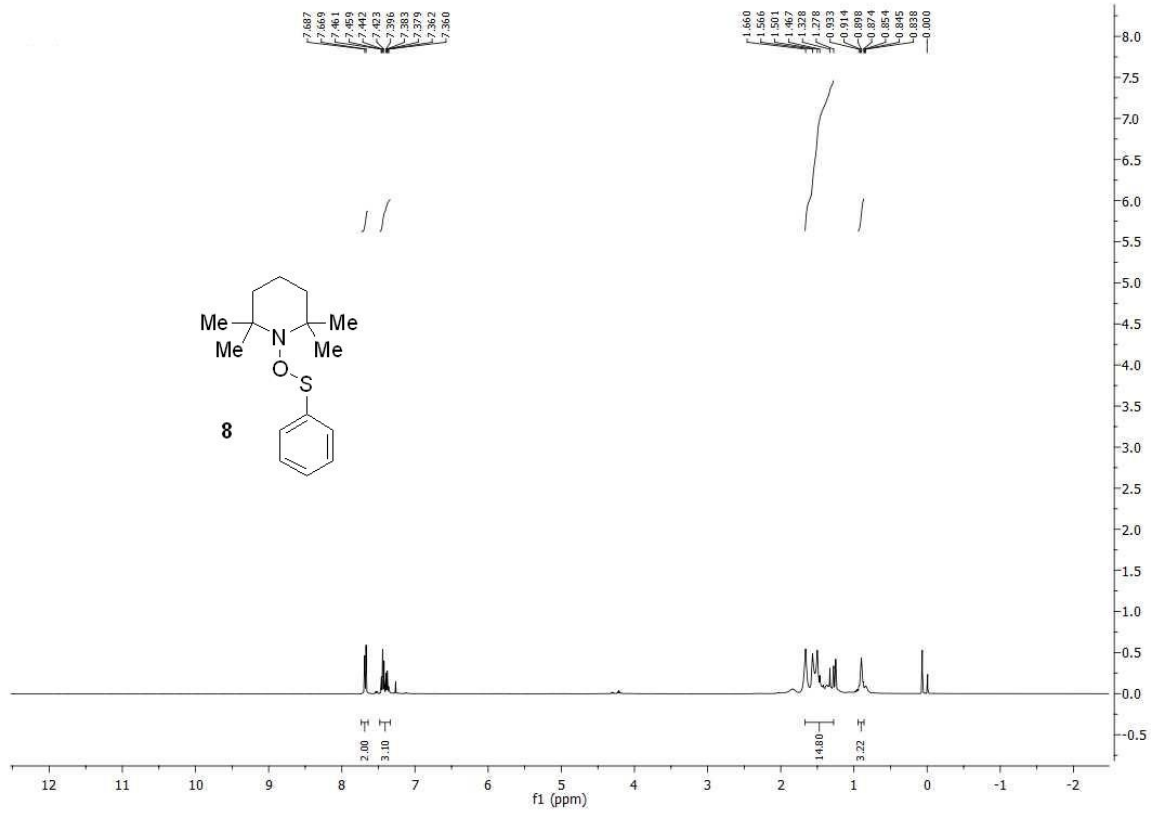

RU-RC-435
single pulse decoupled gated NOE
140.00
139.97
129.75
128.97
108.96
108.88
77.42
77.10
76.78
63.59
63.53
15.86
15.79
Te
O
P
OEt
EtO
7a
f1 (ppm)


RU-RC-435
single pulse decoupled gated NOE
0.36
Te
O
P
OEt
EtO
7a
f1 (ppm)


RU-RC-455
single_pulse
7b
f1 (ppm)


RU-RC-455
single pulse decoupled gated NOE
7b
f1 (ppm)


RU-RC-455
single pulse decoupled gated NOE
0.20
Te
O
P
OBu^n
OBu^n
7b
f1 (ppm)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7.459
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7.423
7.386
7.383
7.379
7.362
7.360
1.660
1.566
1.501
1.467
1.328
1.278
0.933
0.914
0.898
0.874
0.854
0.845
0.838
0.000
Me
Me
N
Me
Me
O
S
8
2.00
3.10
14.80
3.22
f1 (ppm)

HRMS Spectrum of compound 3g

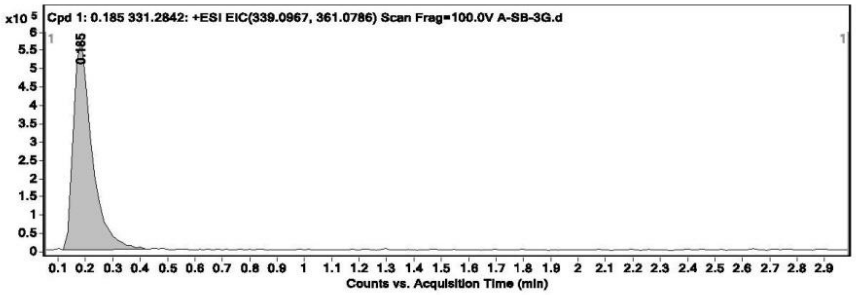
Data File	A-SB-3G.d	**Sample Name**	AK-SB-3G
Sample Type	Sample	**Position**	P2-E1
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACN_H20_40_60_esi_positive_bintu3min.m	**Acquired Time**	10/1/2019 11:51:01 AM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

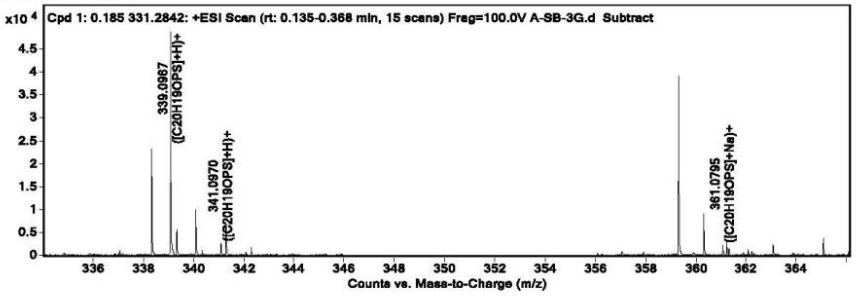
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.185 331.2842	0.185	338.0894	49401	C20 H19 O P S	338.0894	0.07

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.185 331.2842	339.0967	0.185	Find By Formula	338.0894



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
339.0967	339.0967	0.03	1	49400.85	C20H19OPS	(M+H)+
340.0998	340.0999	0.46	1	10096.57	C20H19OPS	(M+H)+
341.097	341.0964	-1.82	1	2575.77	C20H19OPS	(M+H)+
361.0795	361.0786	-2.3	1	2283.12	C20H19OPS	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 3h

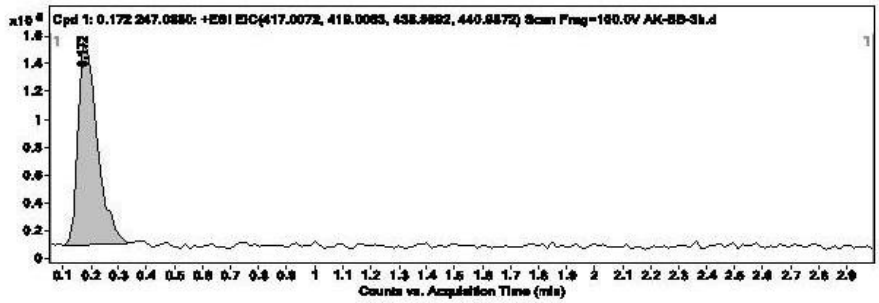
Data File	AK-SB-3h.d	**Sample Name**	AK-SB-3h
Sample Type	Sample	**Position**	P2-E2
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACN_H20_40_60_esi_positive_bintu3min.m	**Acquired Time**	10/1/2019 11:59:21 AM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

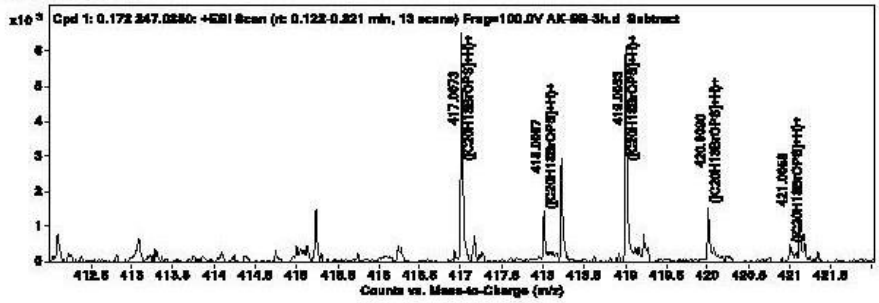
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.172 247.0880	0.172	416.0001	6528	C20 H18 Br O P S	415.9999	0.48

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.172 247.0880	417.0073	0.172	Find By Formula	416.0001



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
417.0073	417.0072	-0.29	1	6527.71	C20H18BrOPS	(M+H)+
418.0097	418.0105	1.7	1	1440.15	C20H18BrOPS	(M+H)+
419.0053	419.0053	-0.14	1	6302.2	C20H18BrOPS	(M+H)+
420.009	420.0084	-1.38	1	1599.37	C20H18BrOPS	(M+H)+
421.0058	421.005	-1.87	1	482.77	C20H18BrOPS	(M+H)+
422.0216	422.0062	-36.49	1	119.72	C20H18BrOPS	(M+H)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 3i

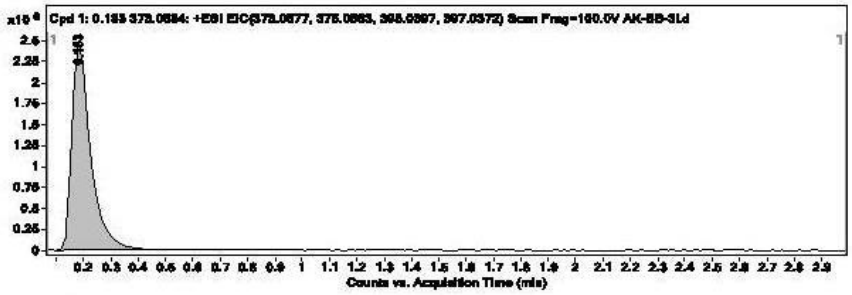
Data File	AK-SB-3i.d	**Sample Name**	AK-SB-3i
Sample Type	Sample	**Position**	P2-E3
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACN_H20_40_60_esi_positive_bintu3min.m	**Acquired Time**	10/1/2019 12:07:40 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

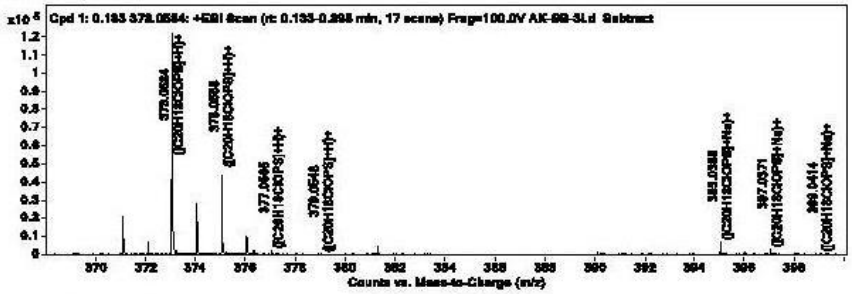
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.183 373.0584	0.183	372.0511	6557	C20 H18 Cl O P S	372.0505	1.68

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.183 373.0584	395.0398	0.183	Find By Formula	372.0511



MS Zoomed Spectrum

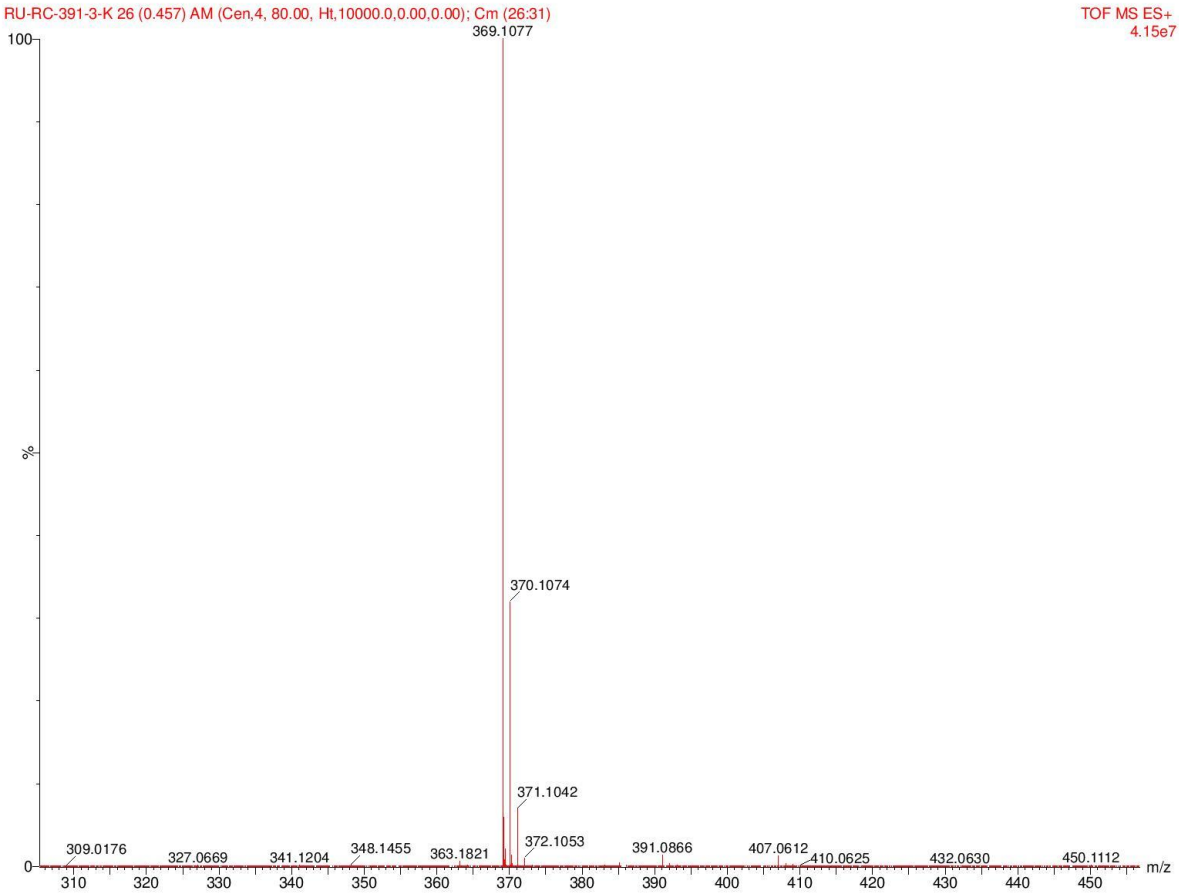


MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
373.0584	373.0577	-1.76	1	124382.36	C20H18ClOPS	(M+H)+
374.0616	374.061	-1.79	1	28376.43	C20H18ClOPS	(M+H)+
375.0558	375.0553	-1.5	1	47022.79	C20H18ClOPS	(M+H)+
376.0588	376.0581	-1.88	1	10409.05	C20H18ClOPS	(M+H)+
377.0565	377.0548	-4.32	1	2150.7	C20H18ClOPS	(M+H)+
378.0594	378.056	-9.07	1	465.74	C20H18ClOPS	(M+H)+
379.0548	379.0576	7.49	1	131.61	C20H18ClOPS	(M+H)+
395.0398	395.0397	-0.28	1	6556.57	C20H18ClOPS	(M+Na)+
396.0432	396.0429	-0.63	1	1380.1	C20H18ClOPS	(M+Na)+
397.0371	397.0372	0.23	1	2724.51	C20H18ClOPS	(M+Na)+
398.0386	398.0401	3.56	1	589.86	C20H18ClOPS	(M+Na)+
399.0414	399.0368	-11.64	1	209.21	C20H18ClOPS	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 3k



HRMS Spectrum of compound 3l

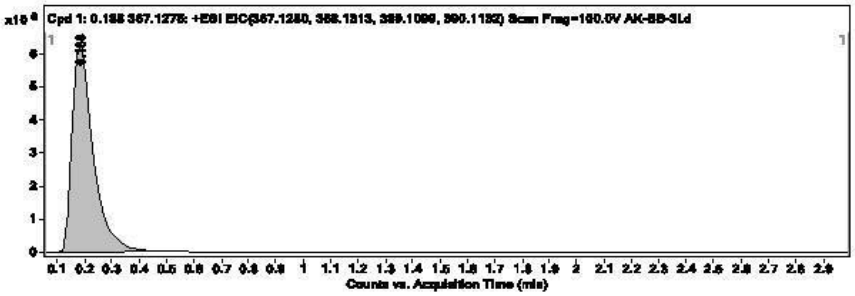
Data File	AK-SB-3l.d	**Sample Name**	AK-SB-3l
Sample Type	Sample	**Position**	P2-E5
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACN_H20_40_60_esi_positive_bintu3min.m	**Acquired Time**	10/1/2019 12:24:20 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

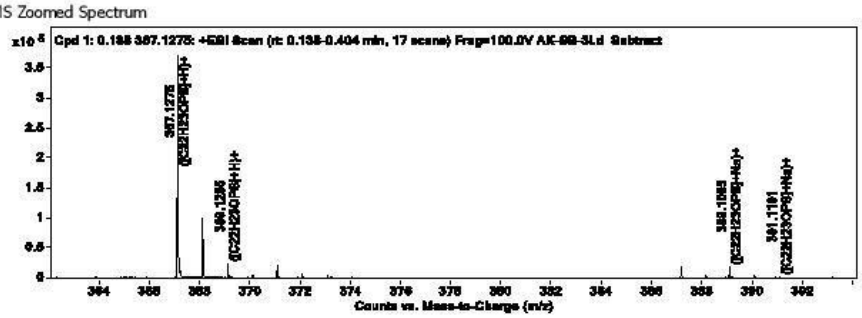
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.188 367.1275	0.188	366.1203	18023	C22 H23 O P S	366.1207	-1.21

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.188 367.1275	389.1095	0.188	Find By Formula	366.1203



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
367.1275	367.128	1.29	1	389170.92	C22H23OPS	(M+H)+
368.1308	368.1313	1.32	1	100243.58	C22H23OPS	(M+H)+
369.1285	369.1282	-0.9	1	23661.2	C22H23OPS	(M+H)+
389.1095	389.1099	1.18	1	18022.98	C22H23OPS	(M+Na)+
390.1123	390.1132	2.22	1	4689.46	C22H23OPS	(M+Na)+
391.1101	391.1101	0.16	1	1473.28	C22H23OPS	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 3m

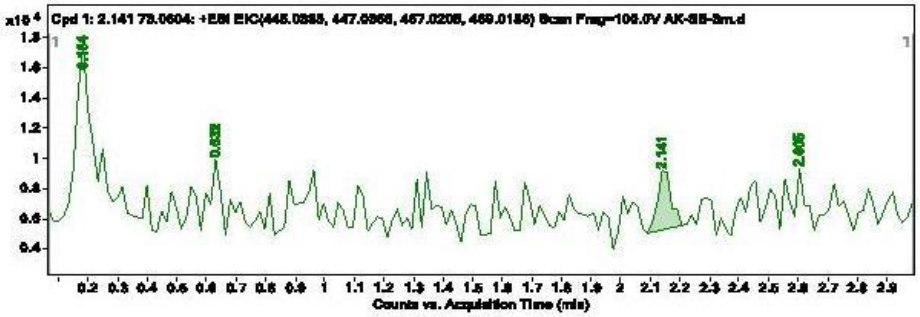
Data File	AK-SB-3m.d	**Sample Name**	AK-SB-3m
Sample Type	Sample	**Position**	P2-E6
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACN_H20_40_60_esi_positive_bintu3min.m	**Acquired Time**	10/1/2019 12:32:36 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

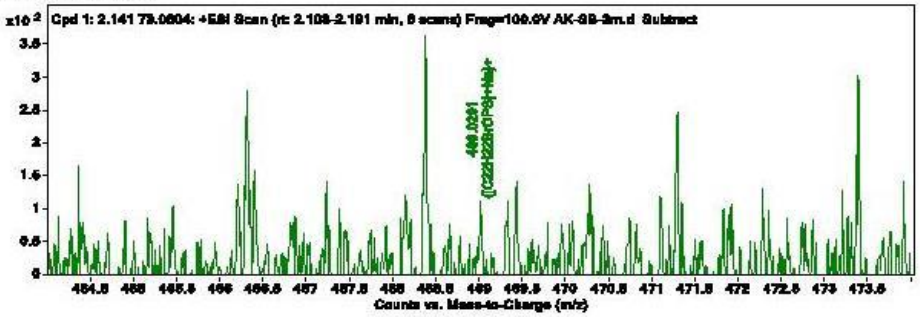
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 2.141 73.0604	2.141	444.0328	113	C22 H22 Br O P S	444.0312	3.43

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 2.141 73.0604	469.0201	2.141	Find By Formula	444.0328



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
469.0201	469.0186	-3.24	1	112.52	C22H22BrOPS	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 3n

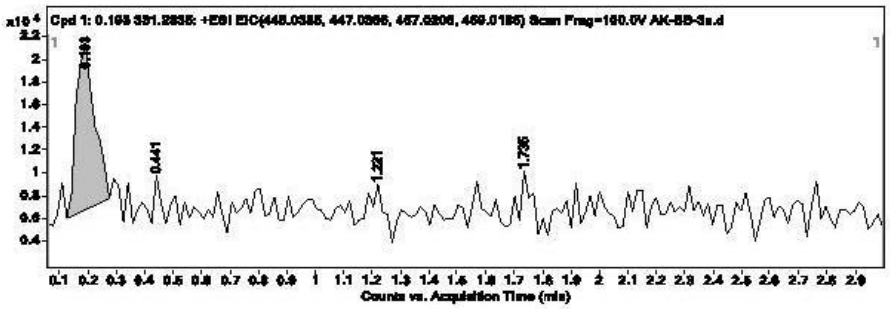
Data File	AK-SB-3n.d	**Sample Name**	AK-SB-3n
Sample Type	Sample	**Position**	P2-E7
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACN_H20_40_60_esi_positive_bintu3min.m	**Acquired Time**	10/1/2019 12:40:52 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

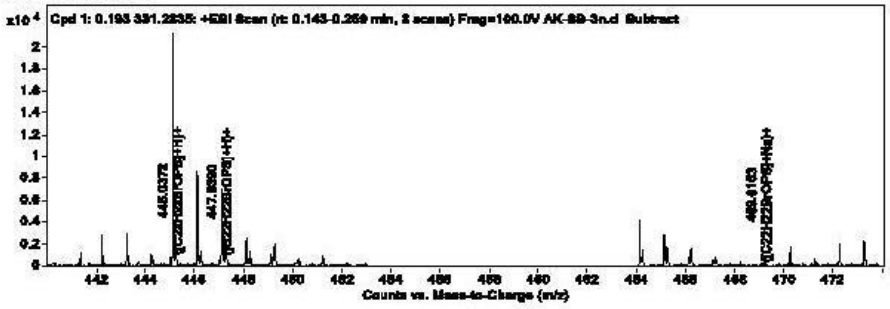
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.193 331.2835	0.193	444.0306	819	C22 H22 Br O P S	444.0312	-1.34

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.193 331.2835	445.0372	0.193	Find By Formula	444.0306



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
445.0372	445.0385	2.85	1	819.46	C22H22BrOPS	(M+H)+
446.0377	446.0418	9.13	1	271.35	C22H22BrOPS	(M+H)+
447.039	447.0366	-5.24	1	724.77	C22H22BrOPS	(M+H)+
448.0376	448.0397	4.65	1	214.35	C22H22BrOPS	(M+H)+
469.0163	469.0186	4.93	1	116.83	C22H22BrOPS	(M+Na)+
470.0181	470.0217	7.62	1	36.91	C22H22BrOPS	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 3o

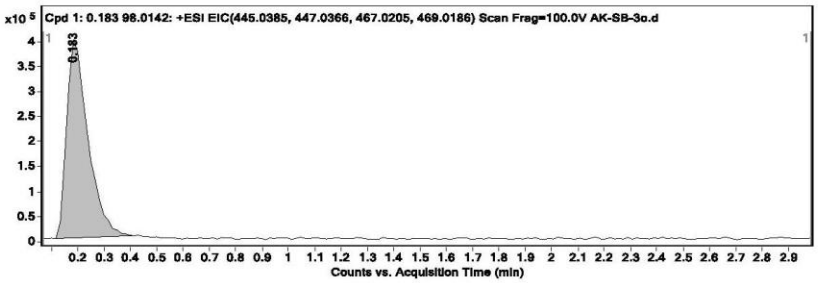
Data File	AK-SB-3o.d	**Sample Name**	AK-SB-3o
Sample Type	Sample	**Position**	P2-E8
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACN_H20_40_60_esi_positive_bintu3min.m	**Acquired Time**	10/1/2019 12:49:08 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

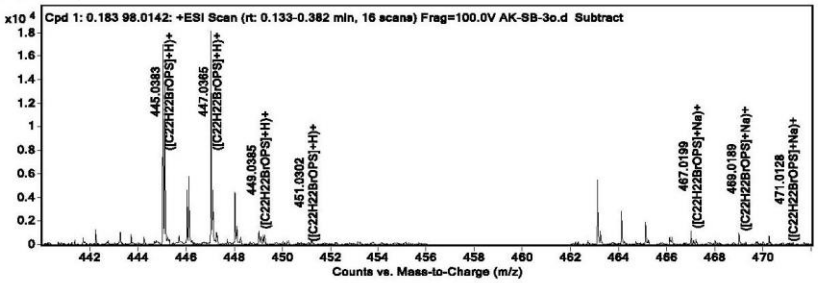
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.183 98.0142	0.183	444.0311	18368	C22 H22 Br O P S	444.0312	-0.21

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.183 98.0142	447.0365	0.183	Find By Formula	444.0311



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
445.0383	445.0385	0.46	1	17810.47	C22H22BrOPS	(M+H)+
446.0419	446.0418	-0.22	1	4653.61	C22H22BrOPS	(M+H)+
447.0365	447.0366	0.31	1	18368.06	C22H22BrOPS	(M+H)+
448.0398	448.0397	-0.16	1	4707.37	C22H22BrOPS	(M+H)+
449.0385	449.0368	-3.9	1	1171.43	C22H22BrOPS	(M+H)+
450.0398	450.0378	-4.55	1	283.28	C22H22BrOPS	(M+H)+
451.0302	451.0395	20.79	1	95.73	C22H22BrOPS	(M+H)+
467.0199	467.0205	1.15	1	1213.25	C22H22BrOPS	(M+Na)+
468.0239	468.0237	-0.47	1	355.45	C22H22BrOPS	(M+Na)+
469.0189	469.0186	-0.7	1	996.16	C22H22BrOPS	(M+Na)+
470.0215	470.0217	0.27	1	263.53	C22H22BrOPS	(M+Na)+
471.0128	471.0187	12.55	1	99.4	C22H22BrOPS	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 3p

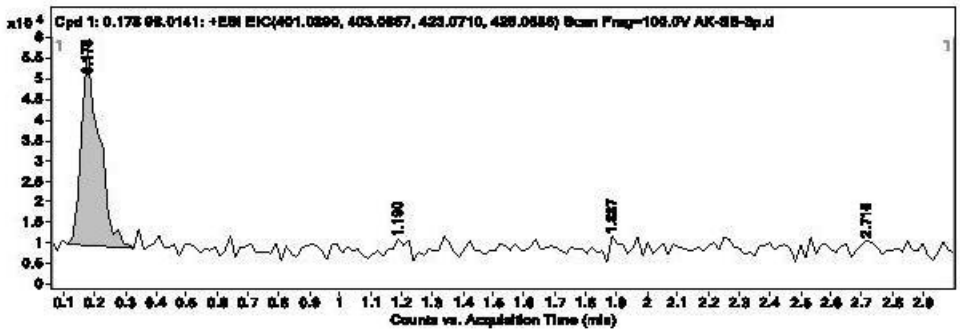
Data File	AK-SB-3p.d	**Sample Name**	AK-SB-3p
Sample Type	Sample	**Position**	P2-E9
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACN_H20_40_60_esi_positive_bintu3min.m	**Acquired Time**	10/1/2019 12:57:30 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

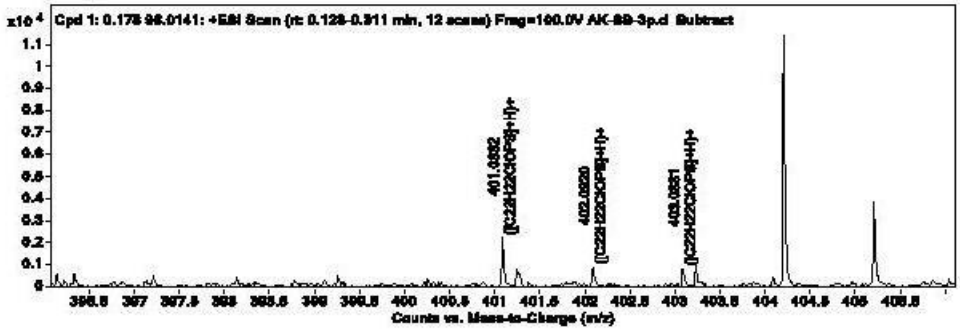
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.178 98.0141	0.178	400.0815	2217	C22 H22 Cl O P S	400.0818	-0.51

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.178 98.0141	401.0882	0.178	Find By Formula	400.0815



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
401.0882	401.089	1.97	1	2217.09	C22H22ClOPS	(M+H)+
402.092	402.0923	0.65	1	892.14	C22H22ClOPS	(M+H)+
403.0881	403.0867	-3.56	1	823.48	C22H22ClOPS	(M+H)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 3r

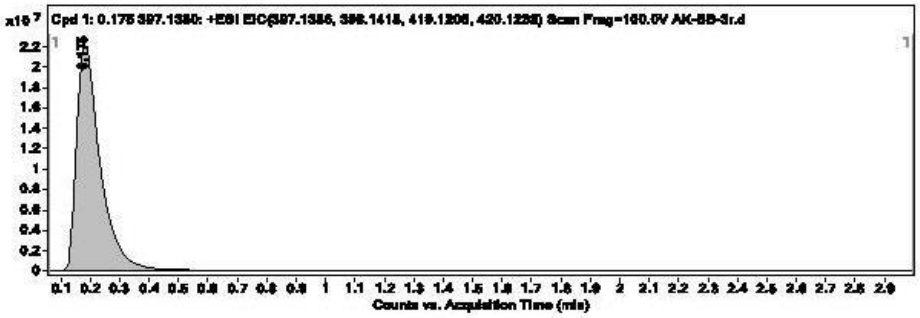
Data File	AK-SB-3r.d	**Sample Name**	AK-SB-3r
Sample Type	Sample	**Position**	P2-E10
Instrument Name	Instrument 1	**User Name**	
Acq Method	ACN_H20_40_60_esi_positive_bintu3min.m	**Acquired Time**	10/1/2019 1:05:51 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

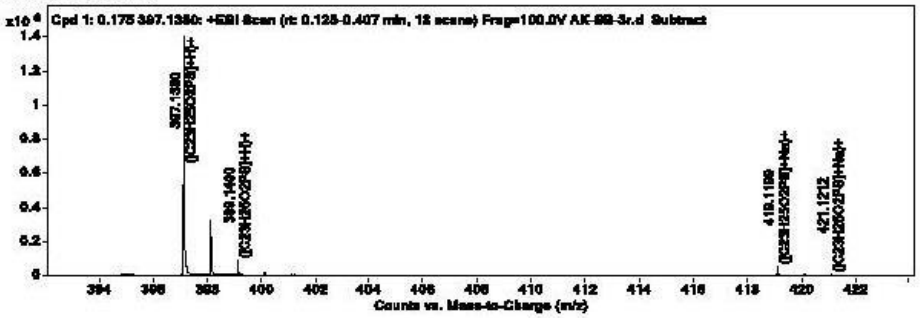
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.175 397.1380	0.175	396.1309	50166	C23 H25 O2 P S	396.1313	-1.07

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.175 397.1380	419.1199	0.175	Find By Formula	396.1309



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
397.138	397.1386	1.35	1	1409909.75	C23H25O2PS	(M+H)+
398.1416	398.1418	0.61	1	340891.69	C23H25O2PS	(M+H)+
399.14	399.1391	-2.24	1	85673.02	C23H25O2PS	(M+H)+
419.1199	419.1205	1.39	1	50165.6	C23H25O2PS	(M+Na)+
420.123	420.1238	1.97	1	12085.31	C23H25O2PS	(M+Na)+
421.1212	421.121	-0.38	1	3416.94	C23H25O2PS	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 3t

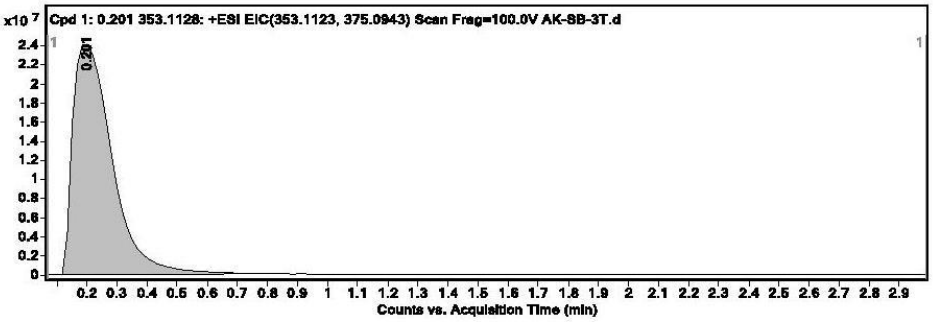
Data File	AK-SB-3T.d	**Sample Name**	AK-SB-3T
Sample Type	Sample	**Position**	P2-D1
Instrument Name	Instrument 1	**User Name**	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	**Acquired Time**	10/3/2019 12:15:22 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

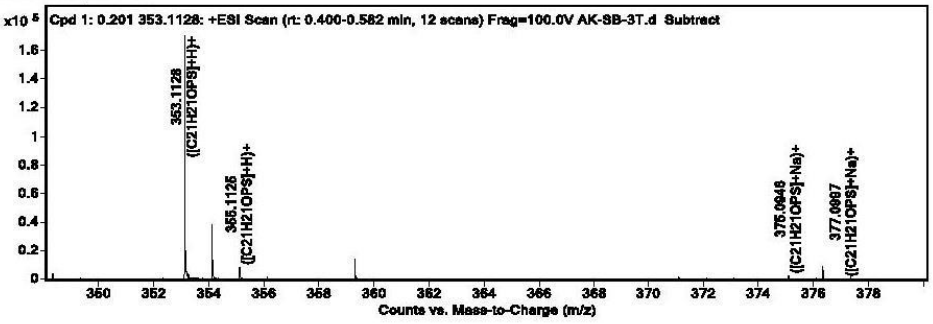
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.201 353.1128	0.201	352.1055	174621	C21 H21 O P S	352.1051	1.32

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.201 353.1128	353.1128	0.201	Find By Formula	352.1055



MS Zoomed Spectrum

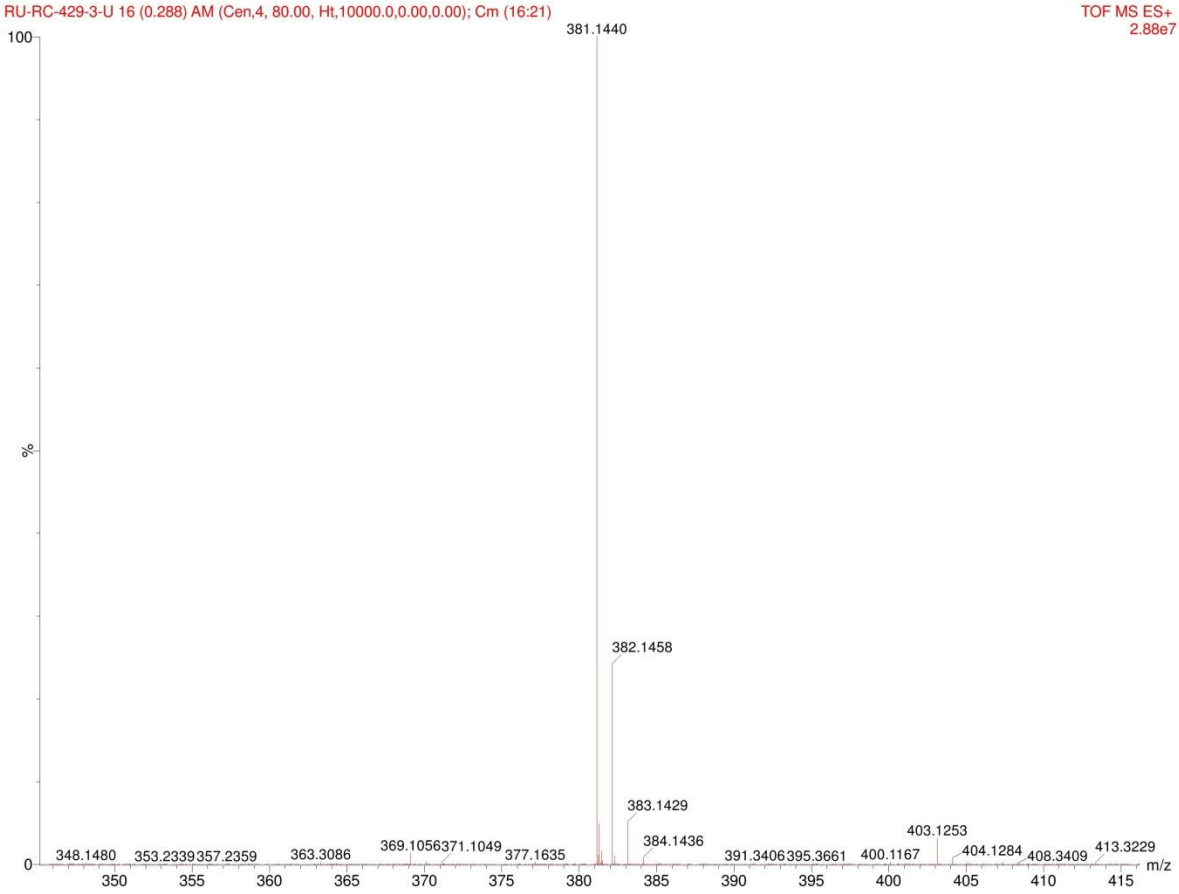


MS Spectrum Peak List

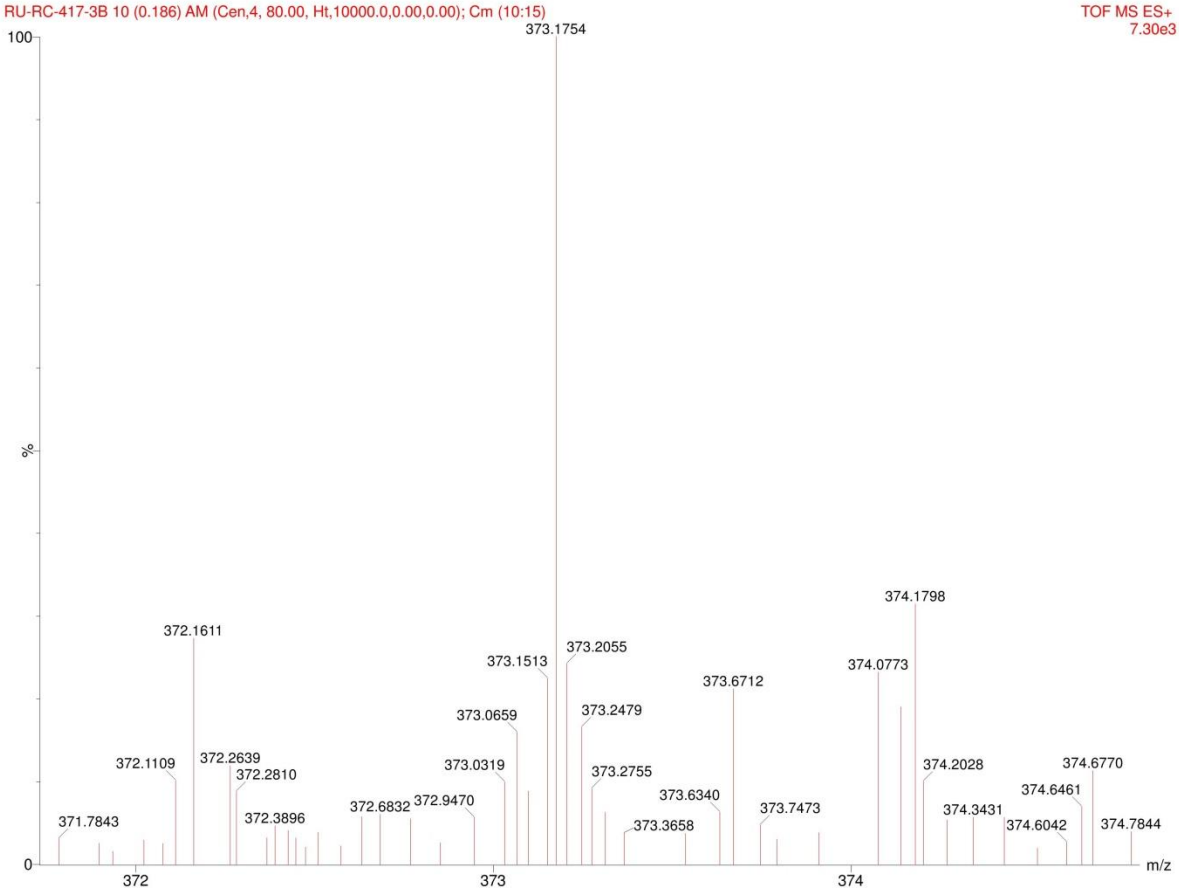
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
353.1128	353.1123	-1.35	1	174620.74	C21H21OPS	(M+H)+
354.116	354.1156	-1.25	1	39249.14	C21H21OPS	(M+H)+
355.1125	355.1123	-0.41	1	8483.23	C21H21OPS	(M+H)+
375.0946	375.0943	-0.86	1	2487.16	C21H21OPS	(M+Na)+
376.0983	376.0975	-2.12	1	424.69	C21H21OPS	(M+Na)+
377.0997	377.0942	-14.36	1	309.7	C21H21OPS	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 3u



HRMS Spectrum of compound 3v



HRMS Spectrum of compound 5b

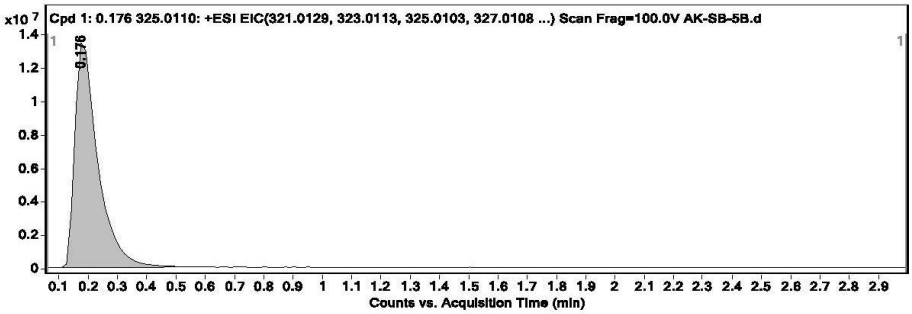
Data File	AK-SB-5B.d	**Sample Name**	AK-SB-5B
Sample Type	Sample	**Position**	P2-D4
Instrument Name	Instrument 1	**User Name**	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	**Acquired Time**	10/3/2019 12:40:09 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

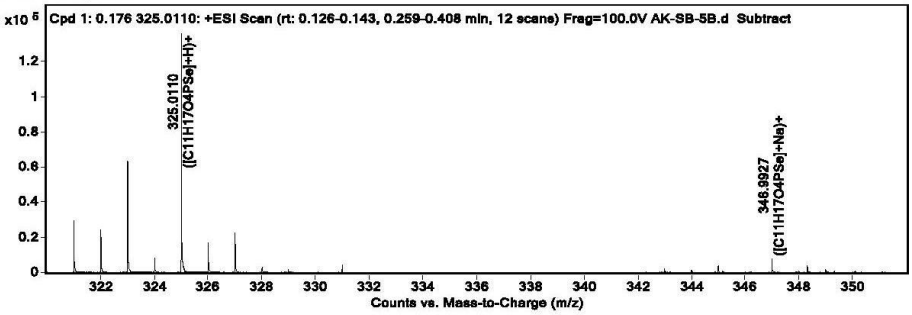
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.176 325.0110	0.176	318.0096	8135	C11 H17 O4 P Se	318.0089	2.09

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.176 325.0110	346.9927	0.176	Find By Formula	318.0096



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
325.011	325.0103	-2.12	1	136999.18	C11H17O4PSe	(M+H)+
326.0143	326.0137	-1.85	1	16884.26	C11H17O4PSe	(M+H)+
346.9927	346.9922	-1.29	1	8135.31	C11H17O4PSe	(M+Na)+
347.996	347.9956	-1.12	1	910.83	C11H17O4PSe	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 5d

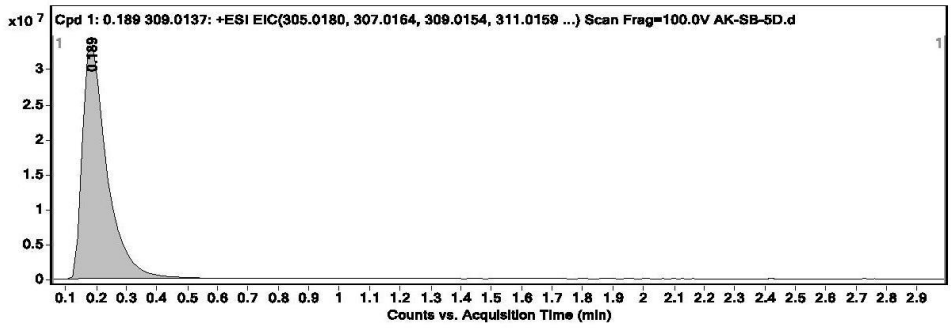
Data File	AK-SB-5D.d	**Sample Name**	AK-SB-5D
Sample Type	Sample	**Position**	P2-D5
Instrument Name	Instrument 1	**User Name**	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	**Acquired Time**	10/3/2019 12:48:26 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

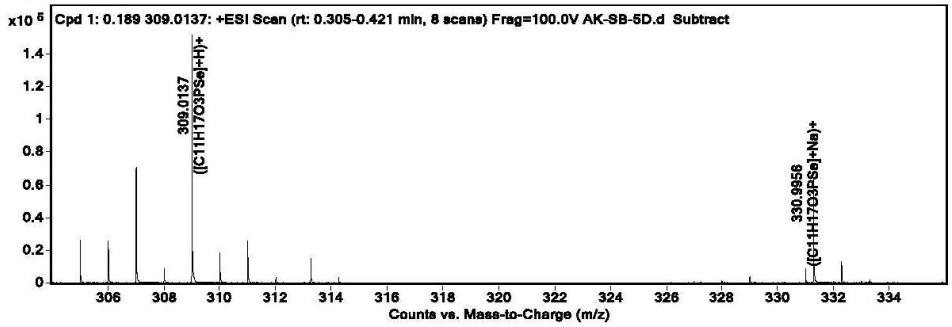
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.189 309.0137	0.189	302.0123	8666	C11 H17 O3 P Se	302.014	-5.54

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.189 309.0137	330.9956	0.189	Find By Formula	302.0123



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
309.0137	309.0154	5.42	1	152145.06	C11H17O3PSe	(M+H)+
310.0171	310.0188	5.23	1	18248.33	C11H17O3PSe	(M+H)+
330.9956	330.9973	5.13	1	8666.43	C11H17O3PSe	(M+Na)+
331.9988	332.0007	5.66	1	1157	C11H17O3PSe	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 5e

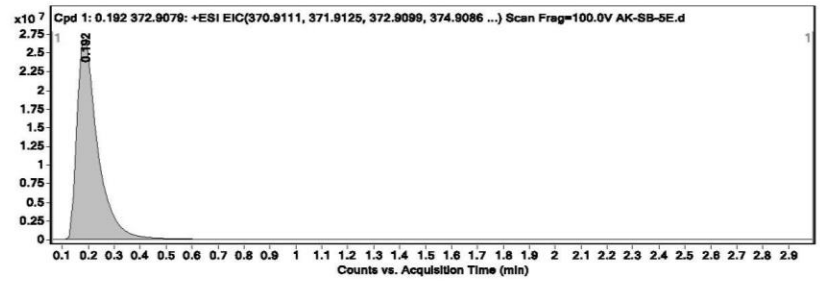
Data File	AK-SB-5E.d	**Sample Name**	AK-SB-5E
Sample Type	Sample	**Position**	P2-D6
Instrument Name	Instrument 1	**User Name**	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	**Acquired Time**	10/3/2019 12:56:42 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

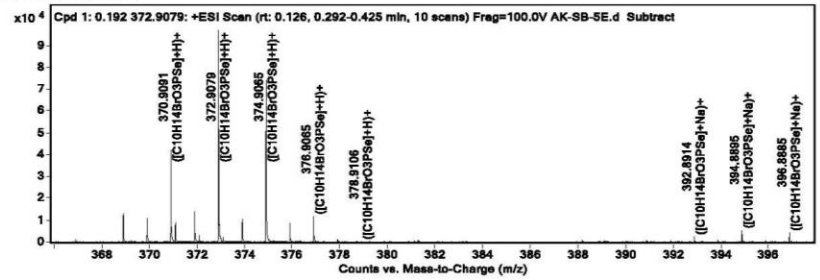
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.192 372.9079	0.192	365.9068	5379	C10 H14 Br O3 P Se	365.9089	-5.59

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.192 372.9079	394.8895	0.192	Find By Formula	365.9068



MS Zoomed Spectrum

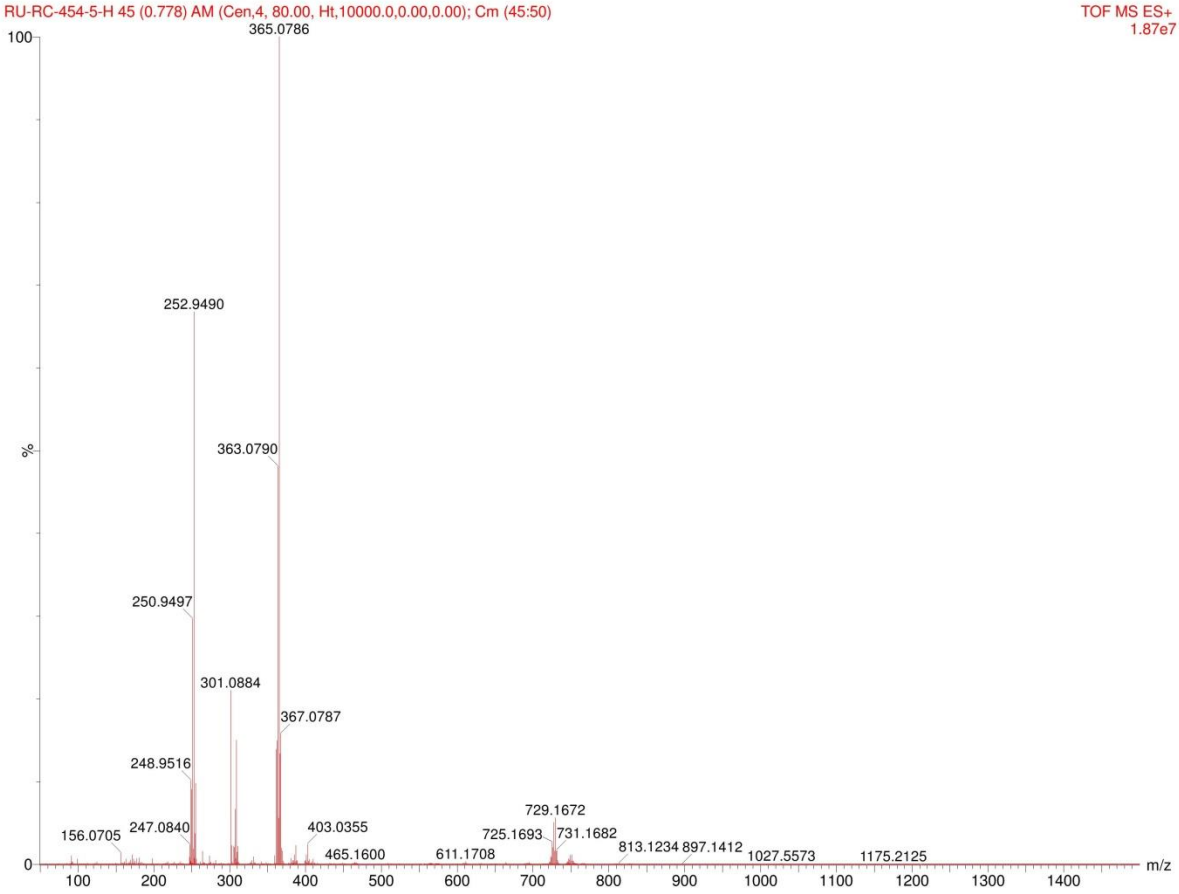


MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
370.9091	370.9111	5.35	1	42435.1	C10H14BrO3PSe	(M+H)+
371.9105	371.9125	5.57	1	13903.93	C10H14BrO3PSe	(M+H)+
372.9079	372.9099	5.33	1	97119.04	C10H14BrO3PSe	(M+H)+
373.9111	373.9133	5.92	1	10842.53	C10H14BrO3PSe	(M+H)+
374.9065	374.9086	5.55	1	75129.39	C10H14BrO3PSe	(M+H)+
375.9098	375.912	5.61	1	8617.62	C10H14BrO3PSe	(M+H)+
376.9065	376.9087	5.81	1	11772.72	C10H14BrO3PSe	(M+H)+
377.9092	377.912	7.23	1	1241.46	C10H14BrO3PSe	(M+H)+
378.9106	378.9139	8.79	1	247.23	C10H14BrO3PSe	(M+H)+
392.8914	392.8931	4.14	1	2389.1	C10H14BrO3PSe	(M+Na)+
393.8929	393.8945	3.86	1	772.18	C10H14BrO3PSe	(M+Na)+
394.8895	394.8918	5.98	1	5378.82	C10H14BrO3PSe	(M+Na)+
395.8932	395.8952	4.97	1	515.42	C10H14BrO3PSe	(M+Na)+
396.8885	396.8905	5.07	1	4225.32	C10H14BrO3PSe	(M+Na)+
397.8927	397.8939	2.99	1	363.53	C10H14BrO3PSe	(M+Na)+
398.8892	398.8907	3.71	1	682.65	C10H14BrO3PSe	(M+Na)+
399.8823	399.8939	29.09	1	54.13	C10H14BrO3PSe	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 5h



HRMS Spectrum of compound 5j

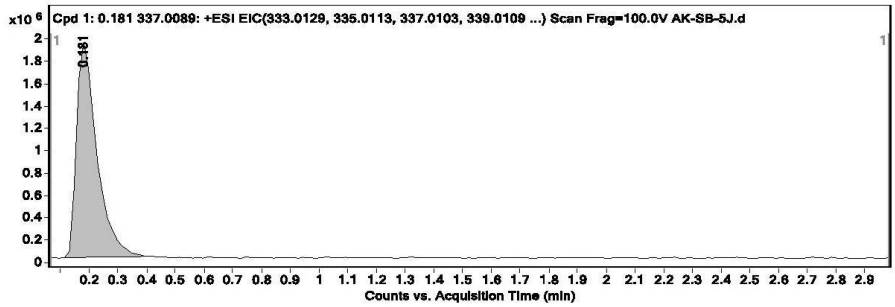
Data File	AK-SB-5J.d	**Sample Name**	AK-SB-5J
Sample Type	Sample	**Position**	P2-D7
Instrument Name	Instrument 1	**User Name**	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	**Acquired Time**	10/3/2019 1:04:55 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

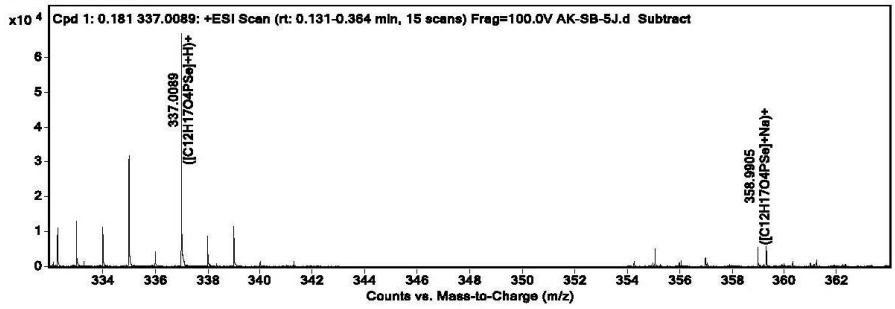
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.181 337.0089	0.181	330.0075	66802	C12 H17 O4 P Se	330.0089	-4.32

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.181 337.0089	337.0089	0.181	Find By Formula	330.0075



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
337.0089	337.0103	4.2	1	66801.91	C12H17O4PSe	(M+H)+
338.0124	338.0137	3.79	1	8742.53	C12H17O4PSe	(M+H)+
358.9905	358.9922	4.71	1	5565.78	C12H17O4PSe	(M+Na)+
359.9936	359.9956	5.58	1	799.78	C12H17O4PSe	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 5k

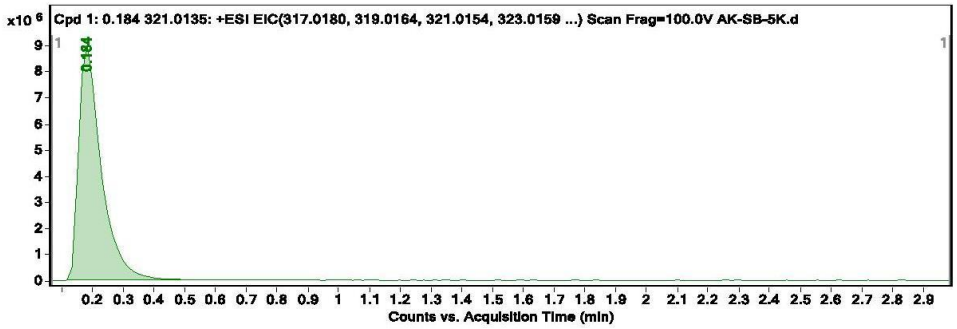
Data File	AK-SB-5K.d	**Sample Name**	AK-SB-5K
Sample Type	Sample	**Position**	P2-D9
Instrument Name	Instrument 1	**User Name**	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	**Acquired Time**	10/3/2019 1:21:18 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

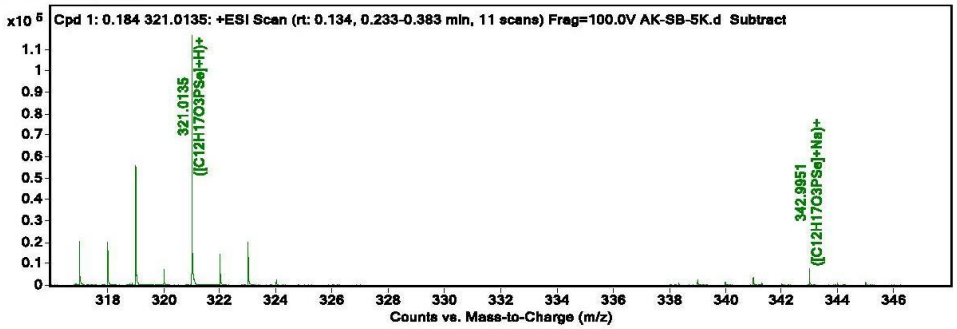
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.184 321.0135	0.184	314.0121	116716	C12 H17 O3 P Se	314.014	-6.14

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.184 321.0135	321.0135	0.184	Find By Formula	314.0121



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
321.0135	321.0154	5.88	1	116716.3	C12H17O3PSe	(M+H)+
322.0168	322.0188	6.23	1	14837.48	C12H17O3PSe	(M+H)+
342.9951	342.9973	6.58	1	7932.92	C12H17O3PSe	(M+Na)+
343.9976	344.0007	8.89	1	963.54	C12H17O3PSe	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

HRMS Spectrum of compound 8

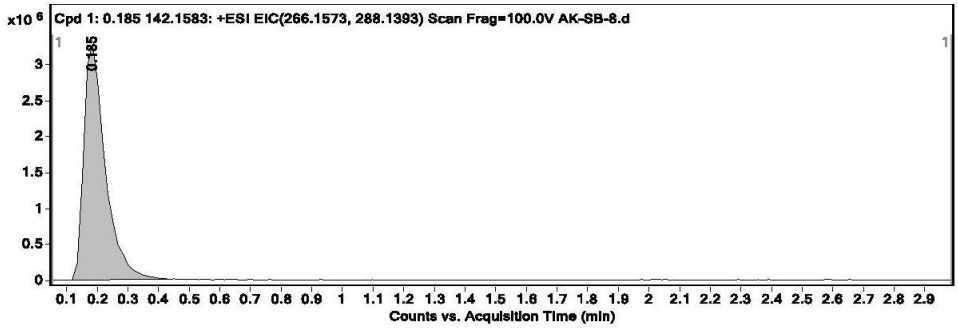
Data File	AK-SB-8.d	**Sample Name**	AK-SB-8
Sample Type	Sample	**Position**	P2-D8
Instrument Name	Instrument 1	**User Name**	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	**Acquired Time**	10/3/2019 1:13:06 PM
IRM Calibration Status	Success	**DA Method**	PROCESSNEW.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

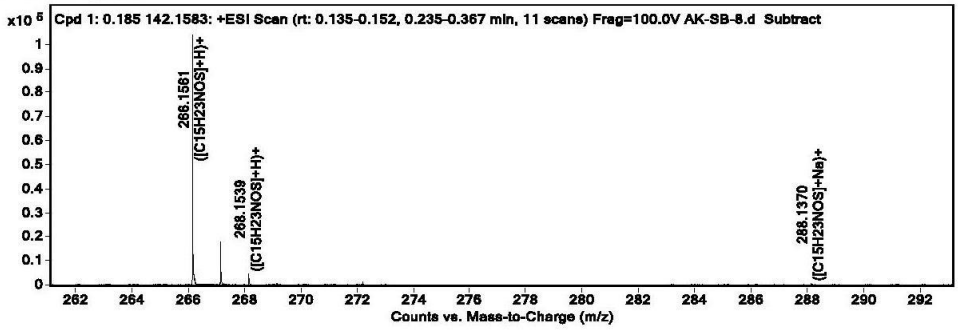
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.185 142.1583	0.185	265.1488	106439	C15 H23 N O S	265.15	-4.81

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.185 142.1583	266.1561	0.185	Find By Formula	265.1488



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
266.1561	266.1573	4.67	1	106438.68	C15H23NOS	(M+H)+
267.1593	267.1604	4.25	1	17821.39	C15H23NOS	(M+H)+
268.1539	268.1559	7.29	1	4639.62	C15H23NOS	(M+H)+
288.137	288.1393	7.67	1	713.26	C15H23NOS	(M+Na)+
289.1316	289.1423	37.01	1	220.37	C15H23NOS	(M+Na)+

Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS