Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Experimental and computational studies on the formation and biological properties of the simplest polyfluoroalkyl phosphonates

Piotr M. Zagórski[1], Paulina Tokarz[2], Bartłomiej Gostyński[3], Paweł Tokarz[4]*

[1]University of Lodz, Faculty of Chemistry, Department of Organic Chemistry, Tamka 12, 91-403 Lodz

[2]University of Lodz, Faculty of Biology and Environmental Protection, Department of Molecular Genetics, Pomorska 141/143, 90-236 Lodz, Poland

[3]Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Sienkiewicza 112, Lodz 90-363, Poland

[4]University of Lodz, Faculty of Chemistry, Molecular Spectroscopy Laboratory, Tamka 12, 91-403 Lodz

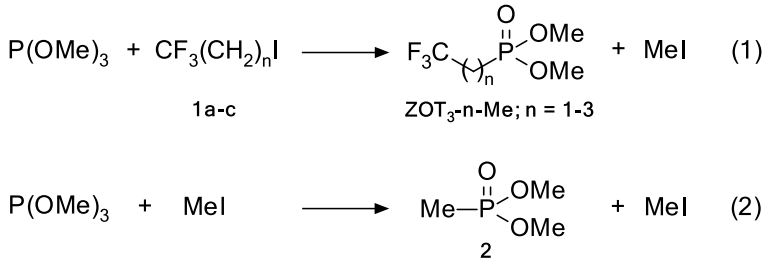
**pawel.tokarz@chemia.uni.lodz.pl*

Supplementary Material

Contents

Derivation of the mathematical model for the kinetic experiments

A mixture of trimethyl phosphite and polyfluorinated alkyl iodide is expected to undergo the following chemical processes:



The kinetics of the competitive processes can be expressed by the following system of differential equations:

$$\frac{\partial x_{MeI}}{\partial t} = k_1 x_{CF_3(CH_2)_nI} x_{P(OMe)_3} = k_1 x_{CF_3(CH_2)_nI}\left(x_{0,P(OMe)_3} - x_{MeP(O)(OMe)_2}\right), \quad (1)$$

$$\frac{\partial x_{MeP(O)(OMe)_2}}{\partial t} = k_2 x_{MeI}\, x_{P(OMe)_3} = k_2 x_{MeI}\left(x_{0,P(OMe)_3} - x_{MeP(O)(OMe)_2}\right), \quad (2)$$

where k_n is the rate constant of a reaction *n*, x_S is a time-dependent molar fraction of any substance S and $x_{0,P(OMe)_3}$ is the initial molar fraction of trimethyl phosphite. The use of molar fractions instead of molar concentrations is justified by solvent-free conditions of the process. The reaction rate constants are of dimension of s^{-1}.

Reaction 1 is considered to be significantly slower than 2, from which the constancy of $x_{CF_3(CH_2)_nI}$ follows naturally. Moreover, the reasonable boundary conditions are:

$$x_{MeP(O)(OMe)_2} = 0 \quad \text{and} \quad x_{MeI} = 0 \quad \text{for} \quad t = 0.$$

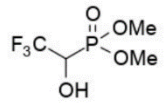
Under these assumptions the equation system becomes analytically solvable. With aid of the computer algebra system built into the Wolfram Development Platform at Wolfram Cloud[28] the following solution has been found:

$$x_{MeP(O)(OMe)_2} = x_{0,P(OMe)_3} \tanh^2\left(t\sqrt{\frac{1}{2}k_1 k_2 x_{CF_3(CH_2)_nI}\, x_{0,P(OMe)_3}}\right).$$

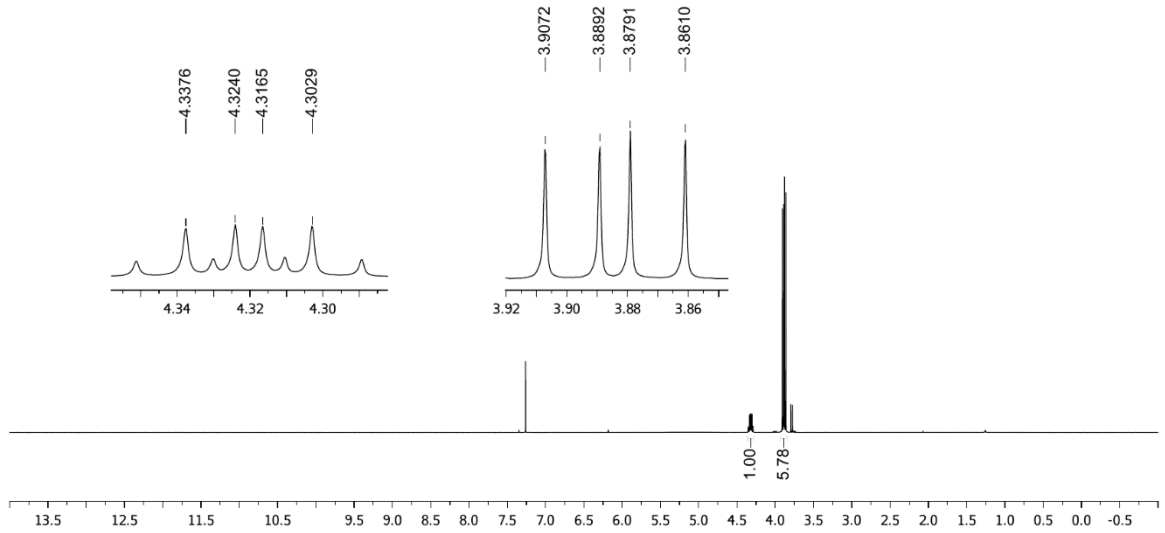
Moreover, from the **Equation 2,** it is visible that in a reaction system containing only methyl iodide and trimethyl phosphite the initial reaction rate v_0 is linearly proportional to the reaction rate constant k_2 and the methyl iodide concentration:

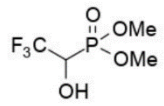
$$\frac{v_0}{x_{0,P(OMe)_3}} = k_2 x_{MeI}$$

NMR spectra

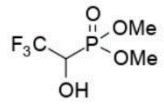


1H NMR

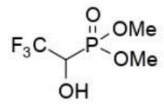




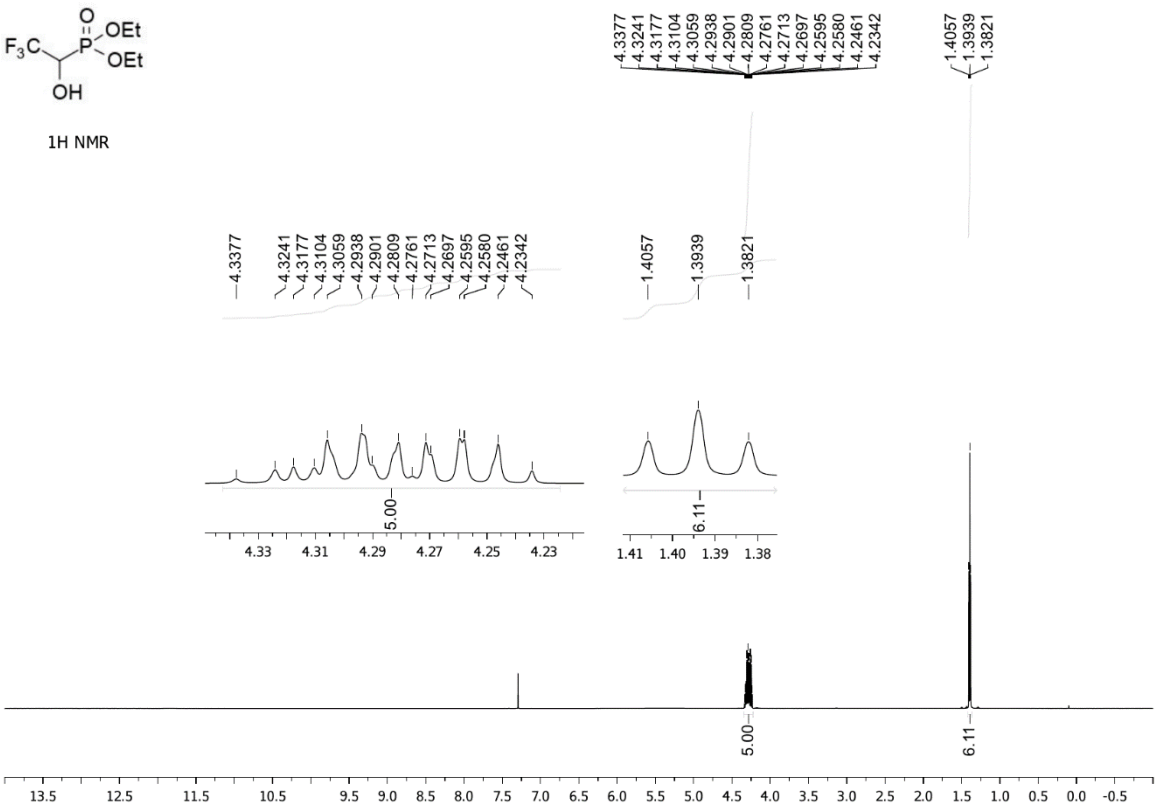
13C NMR



31P NMR



19F NMR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4.2938
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4.2713
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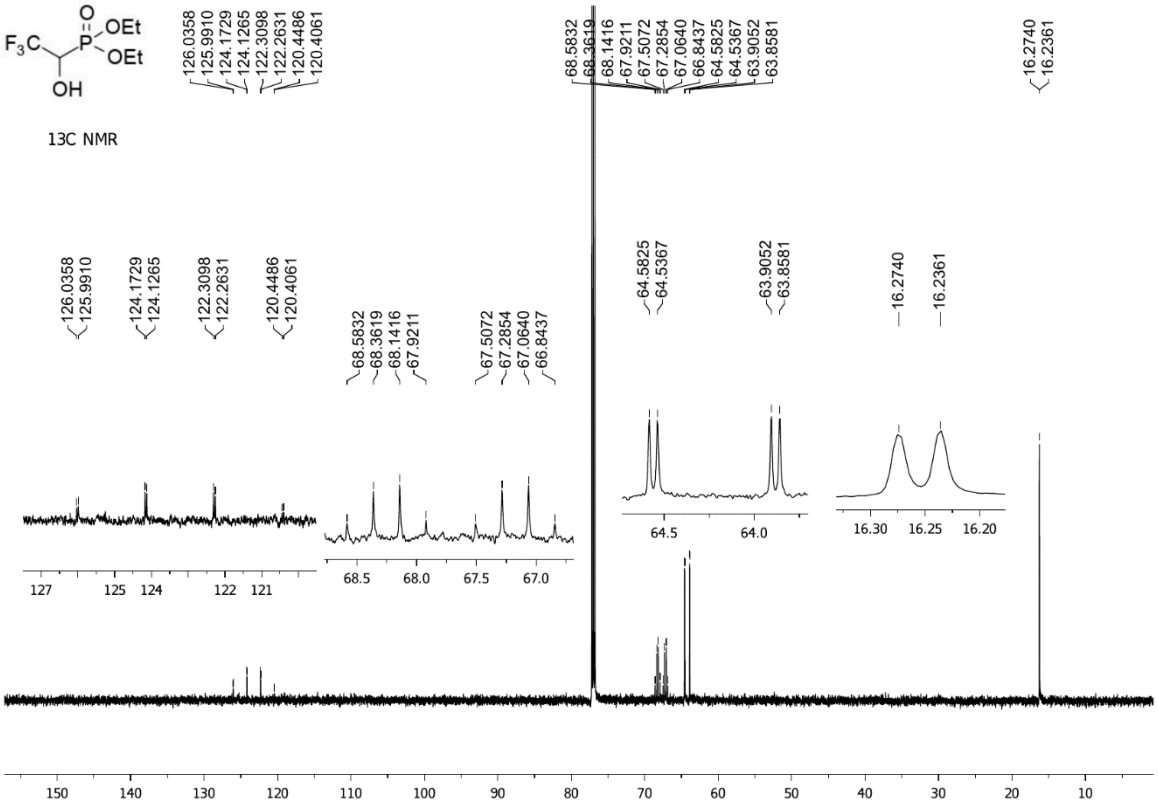
5.00
6.11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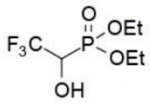
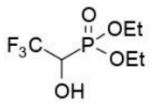
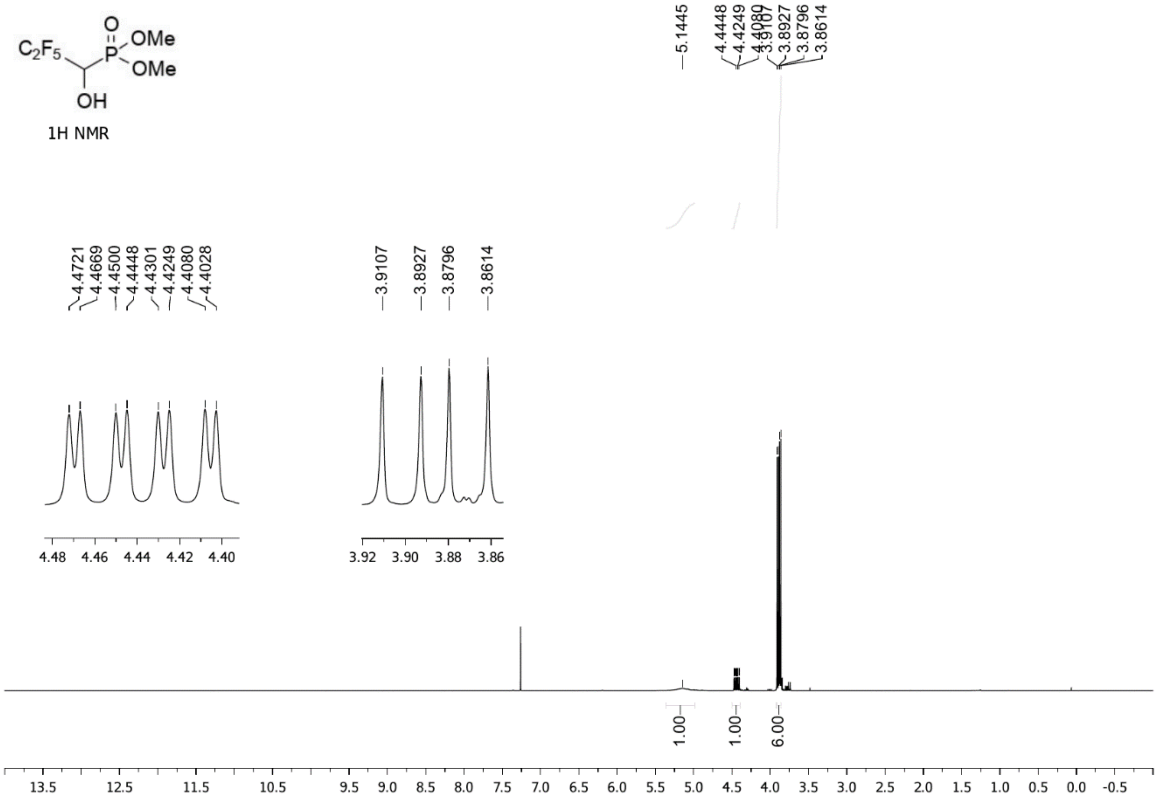


31P NMR



19F NMR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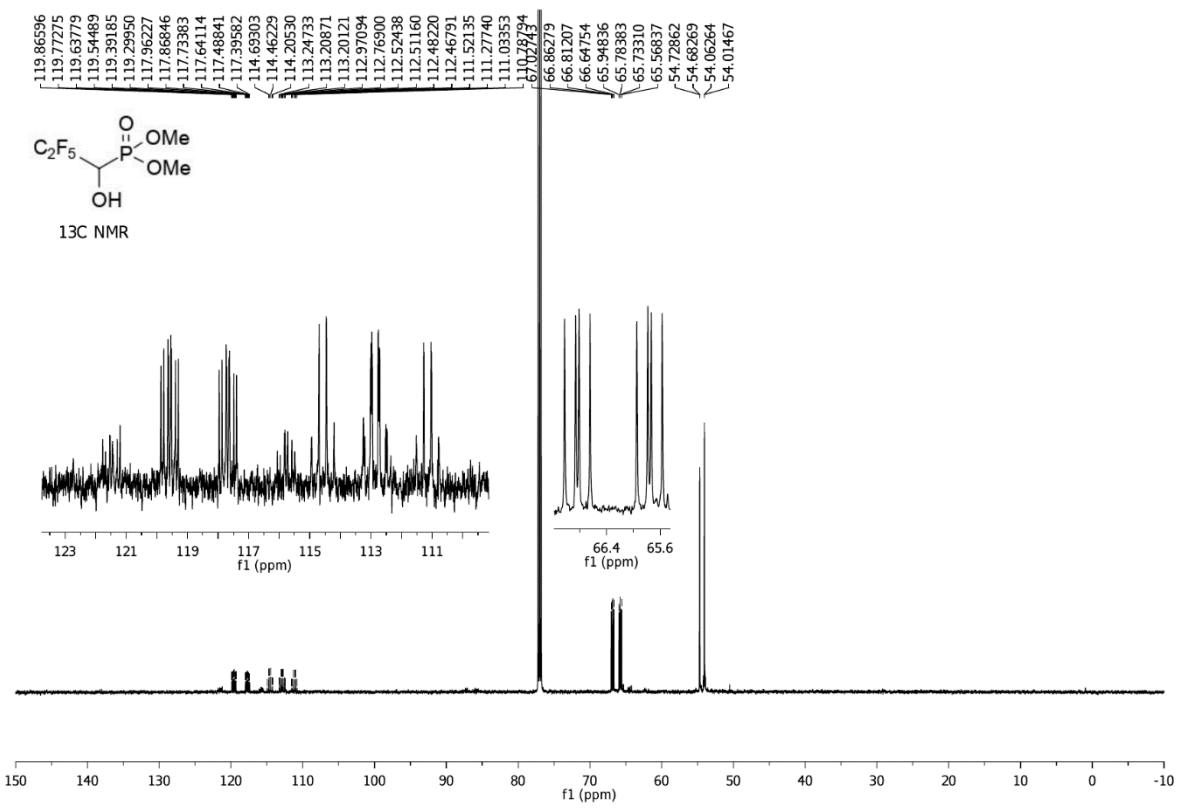
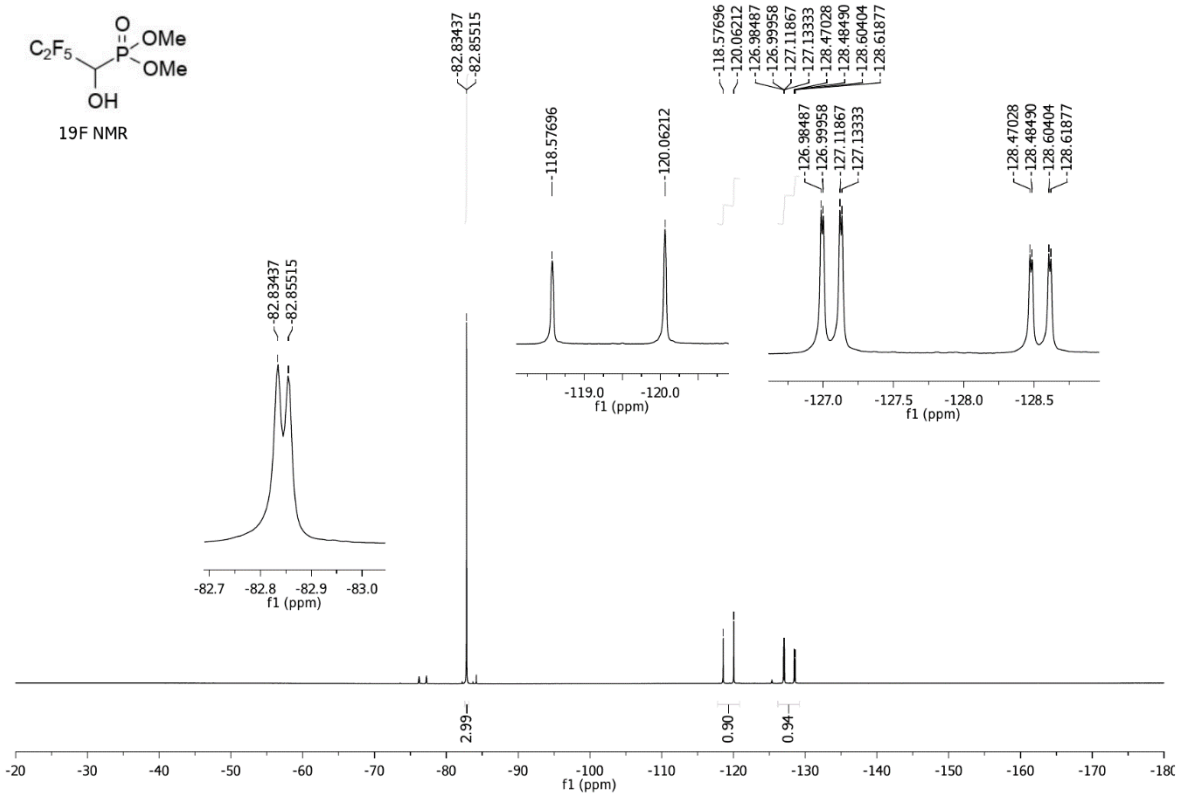
1.00
6.00


13C NMR
f1 (ppm)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O
OMe
P
OMe
OH
19F NMR
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-126.99958
-127.11867
-127.13333
-128.47028
-128.48490
-128.60404
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-82.7
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-83.0
f1 (ppm)
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-120.0
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-128.5
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0.94
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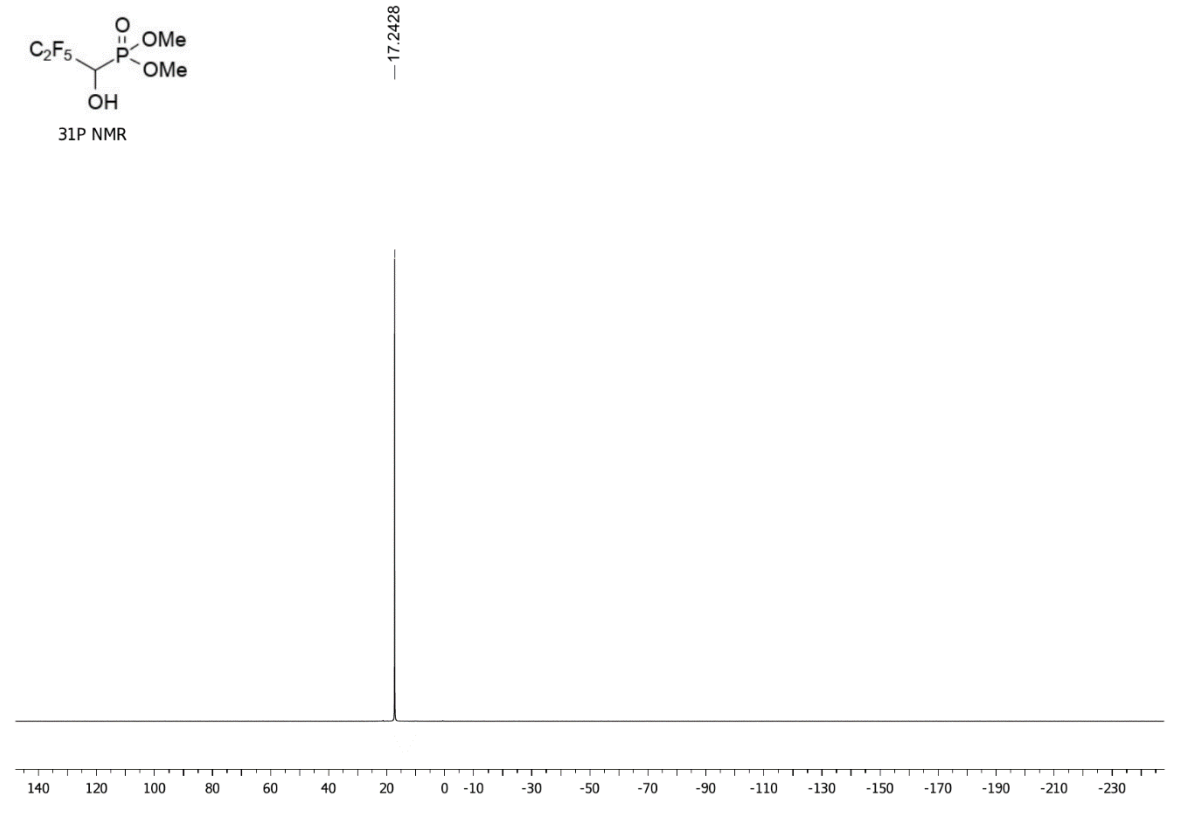
C2F5
O
OMe
P
OMe
OH
31P NMR
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140
120
100
80
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0
-10
-30
-50
-70
-90
-110
-130
-150
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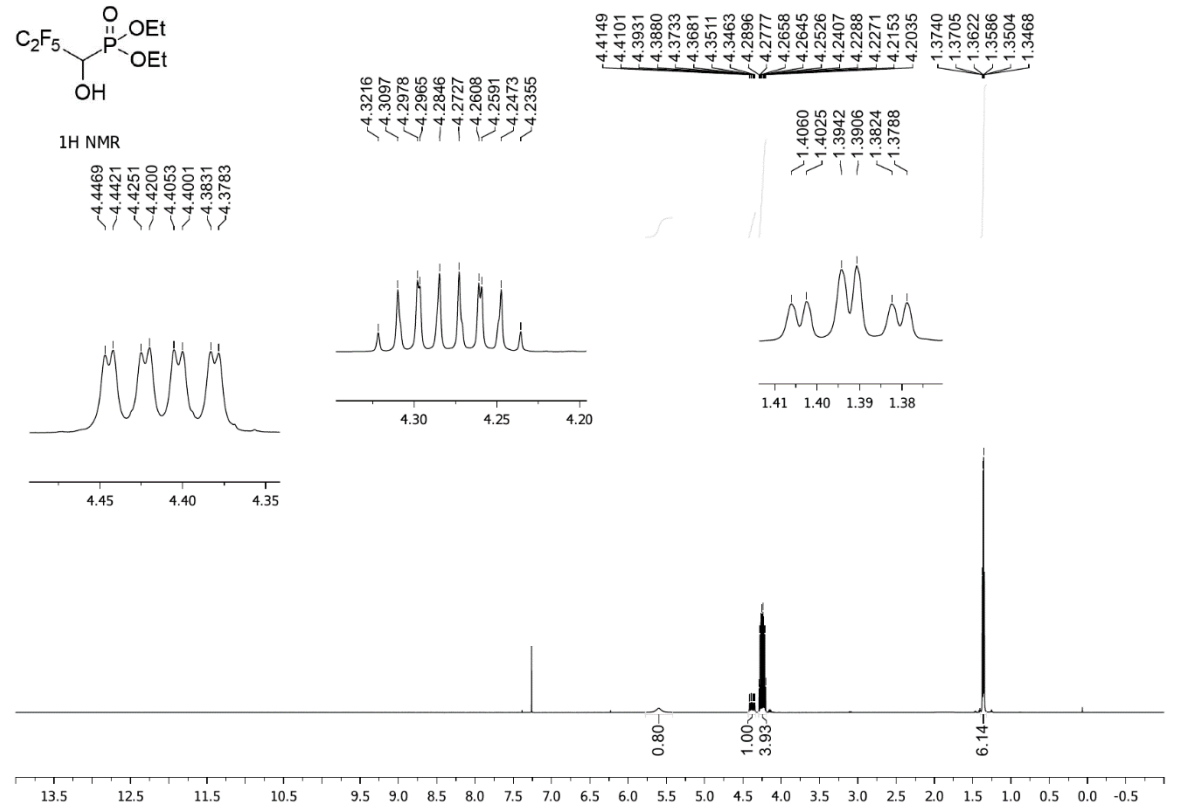
-190
-210
-230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4.4200
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4.4001
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4.2978
4.2965
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4.2727
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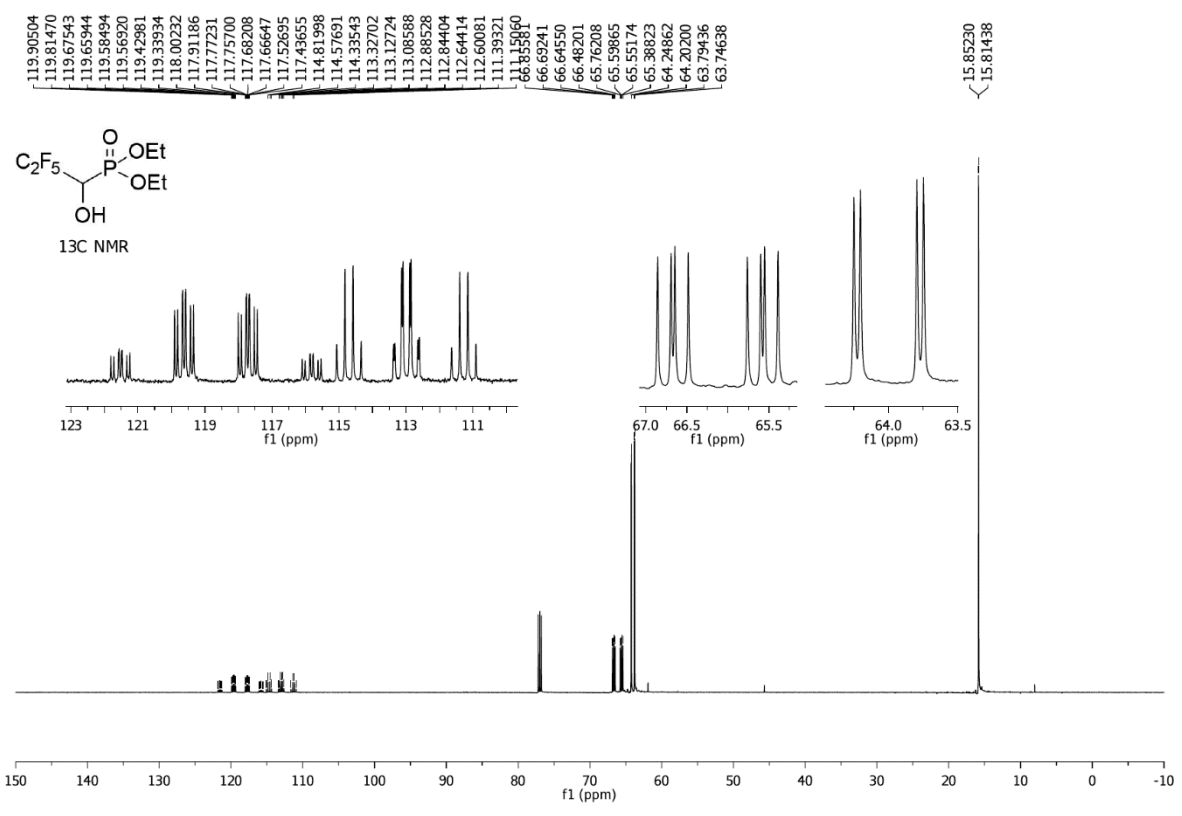
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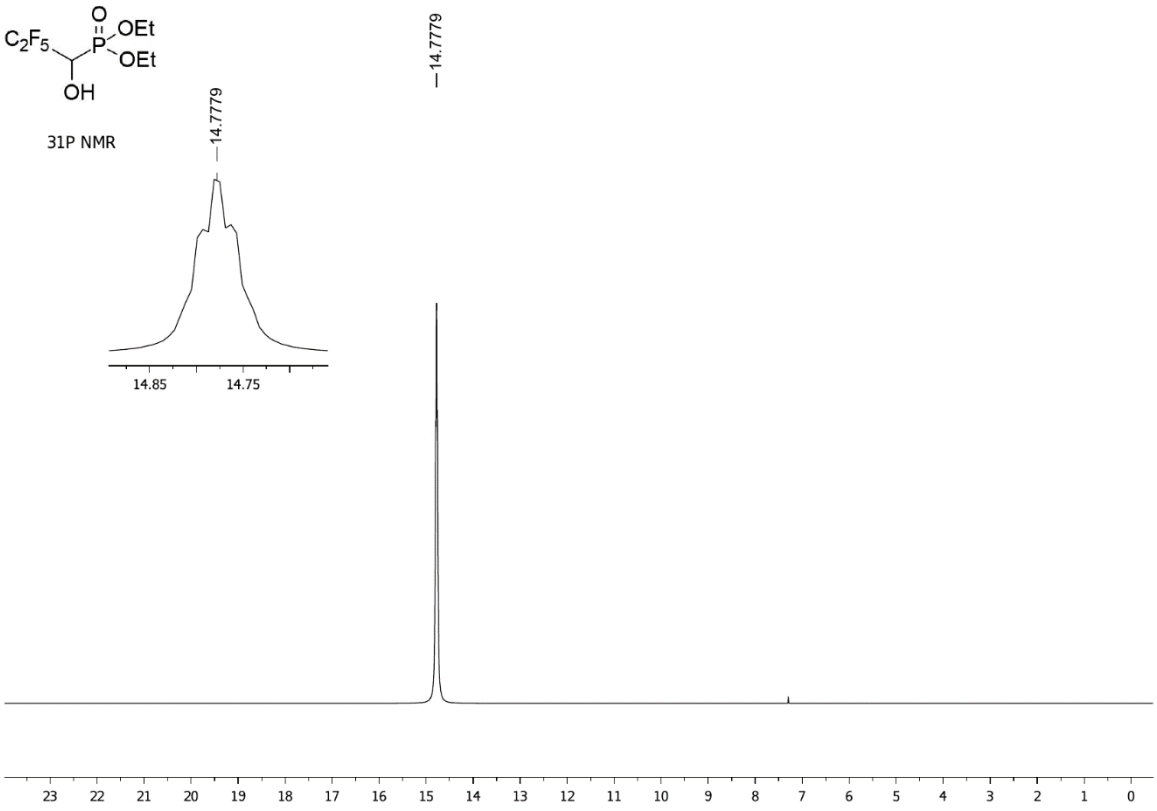
C2F5
O
OEt
P
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OH
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14.75
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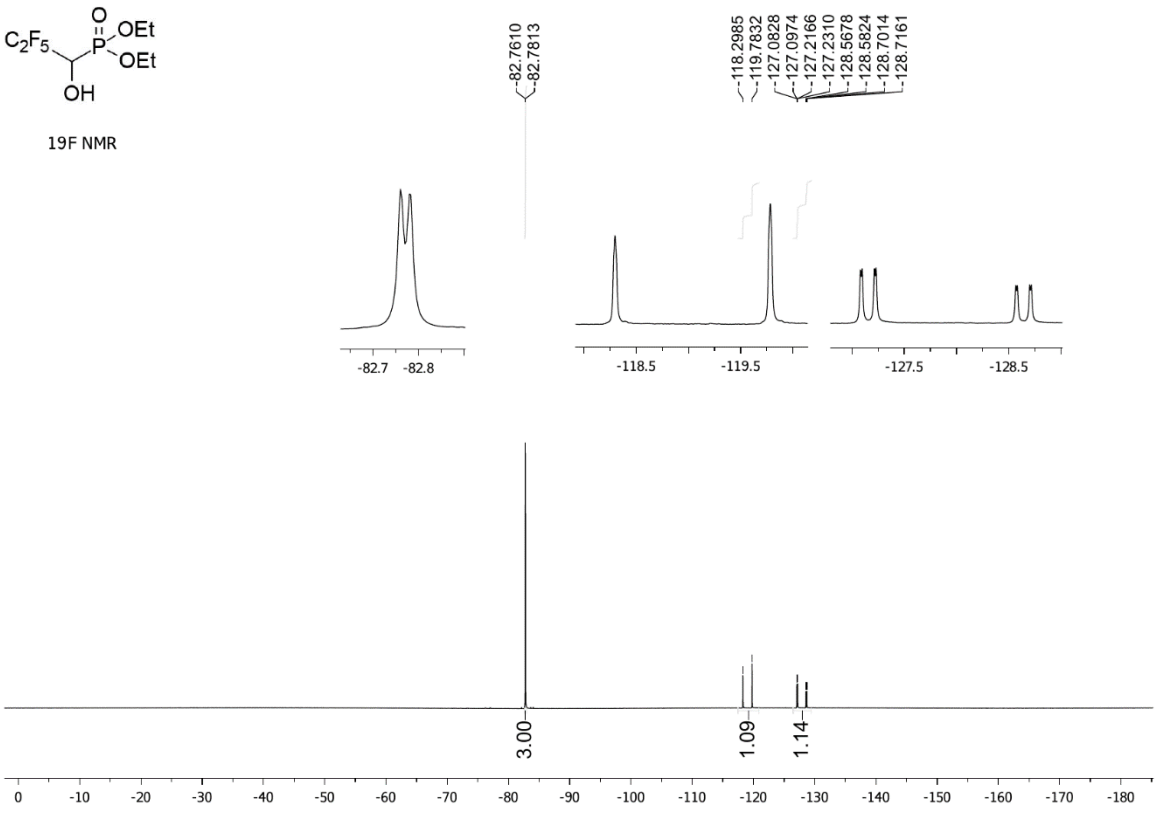
C2F5
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OEt
P
OEt
OH
19F NMR
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-127.2310
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-82.7 -82.8
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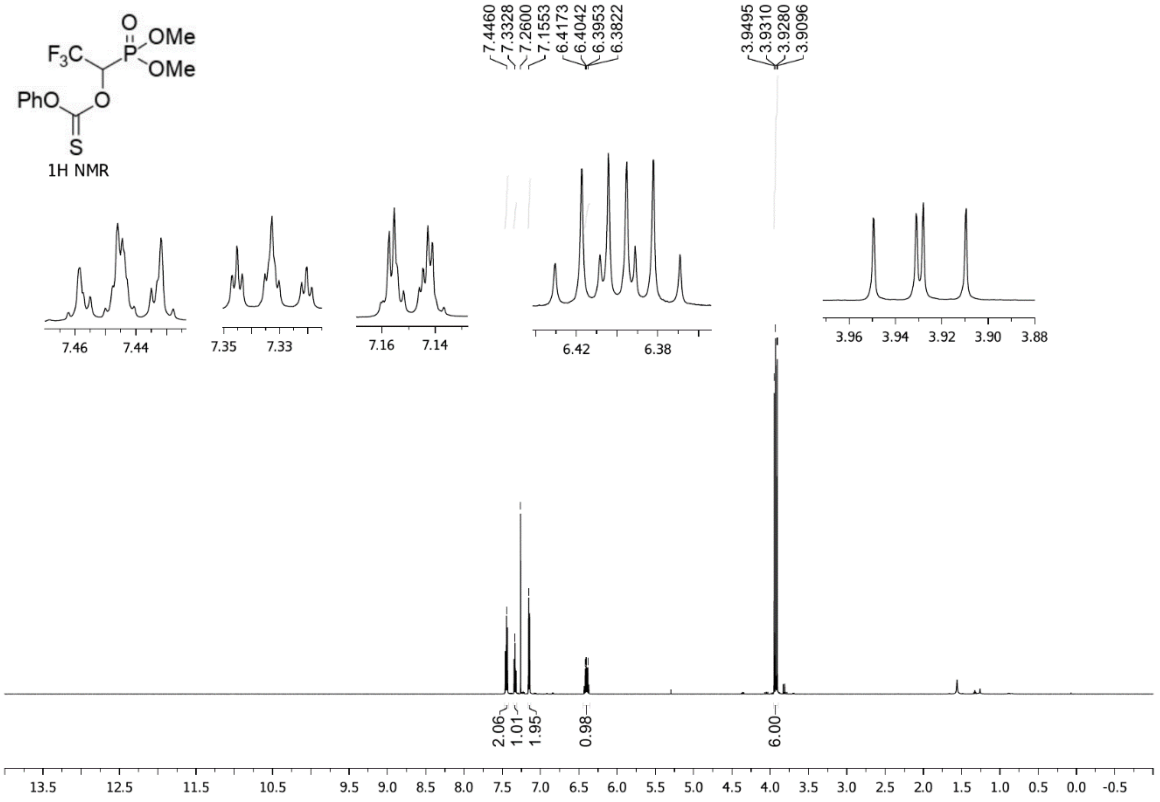
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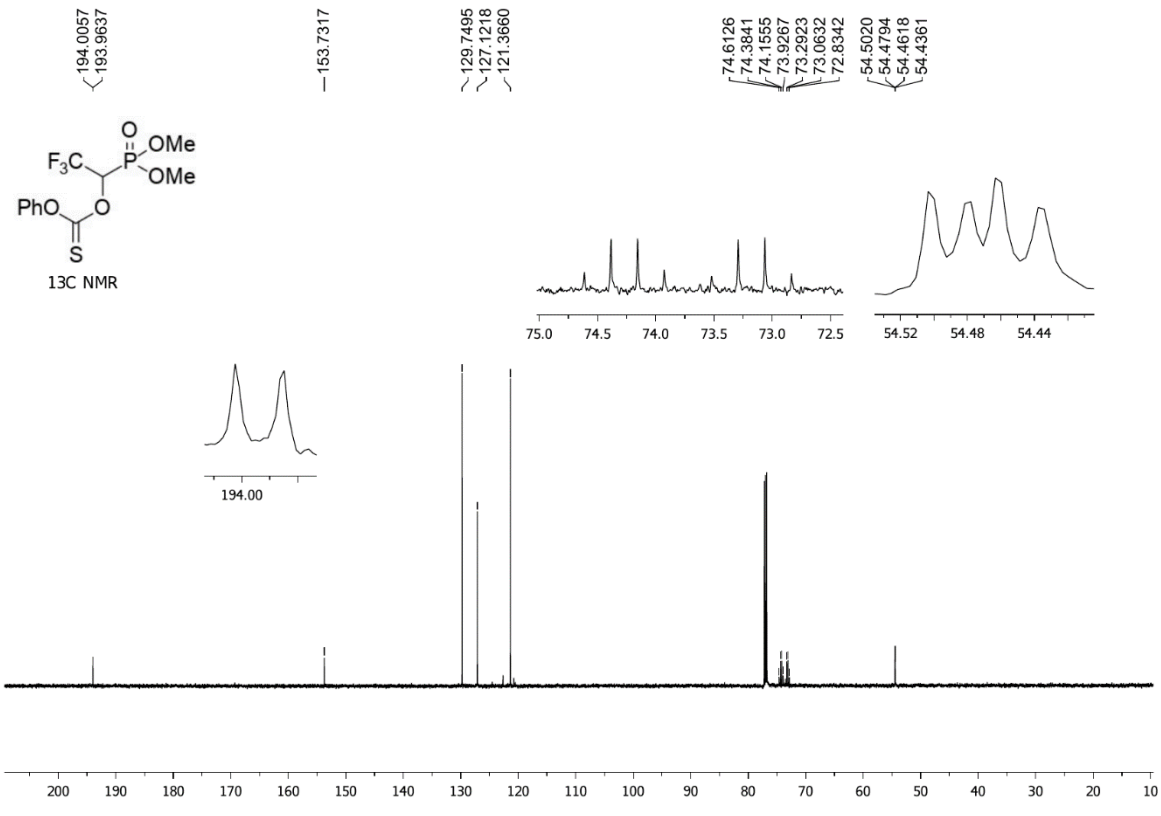
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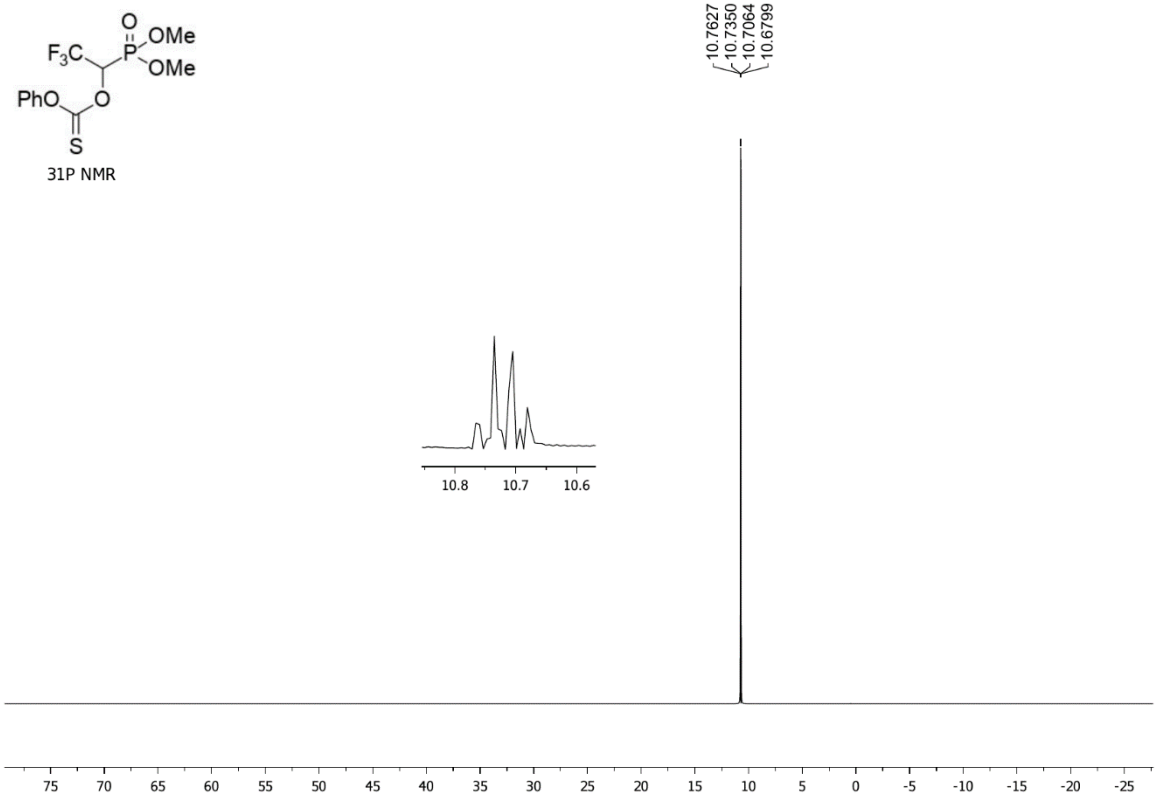
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P
OMe
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O
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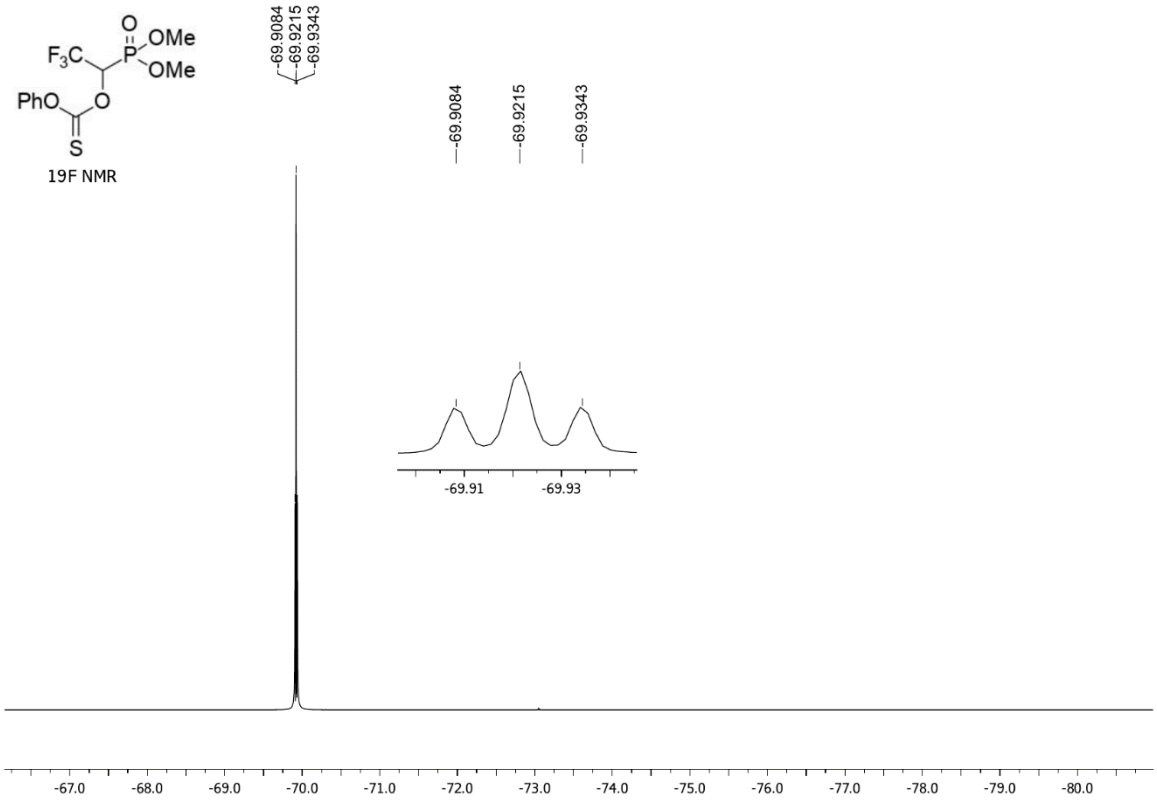
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OMe
PhO
O
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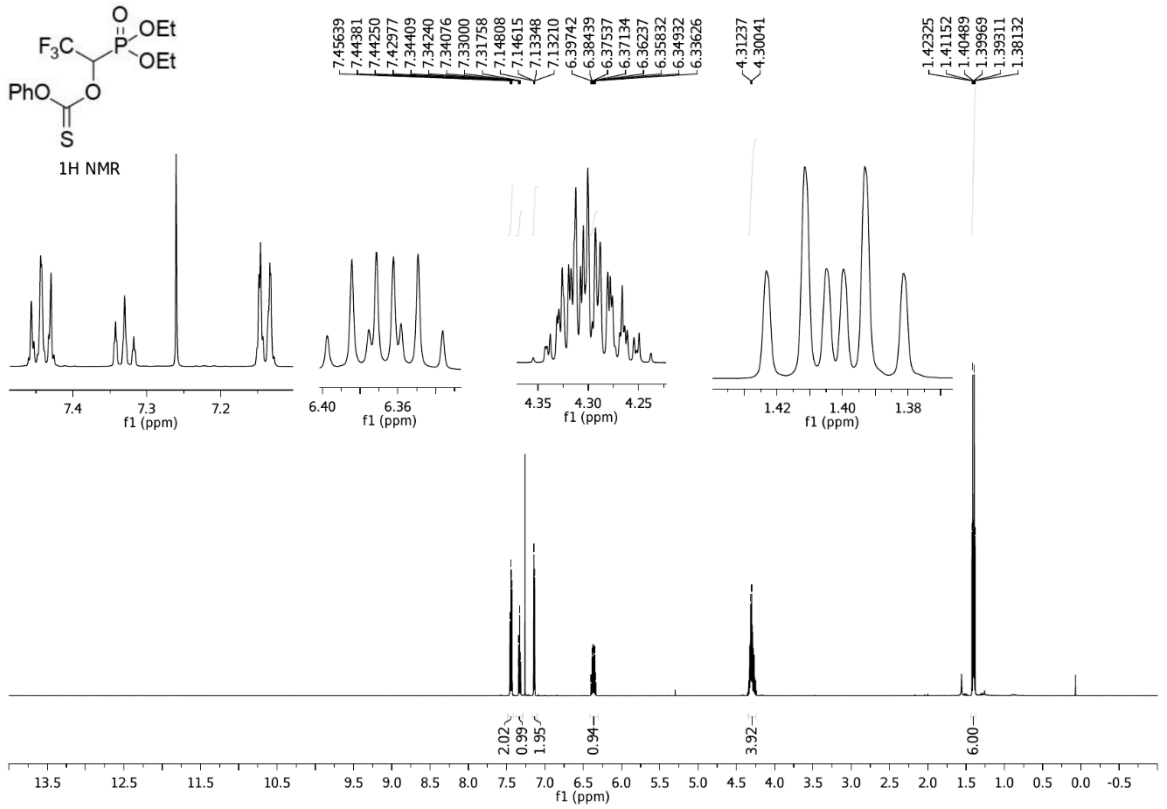
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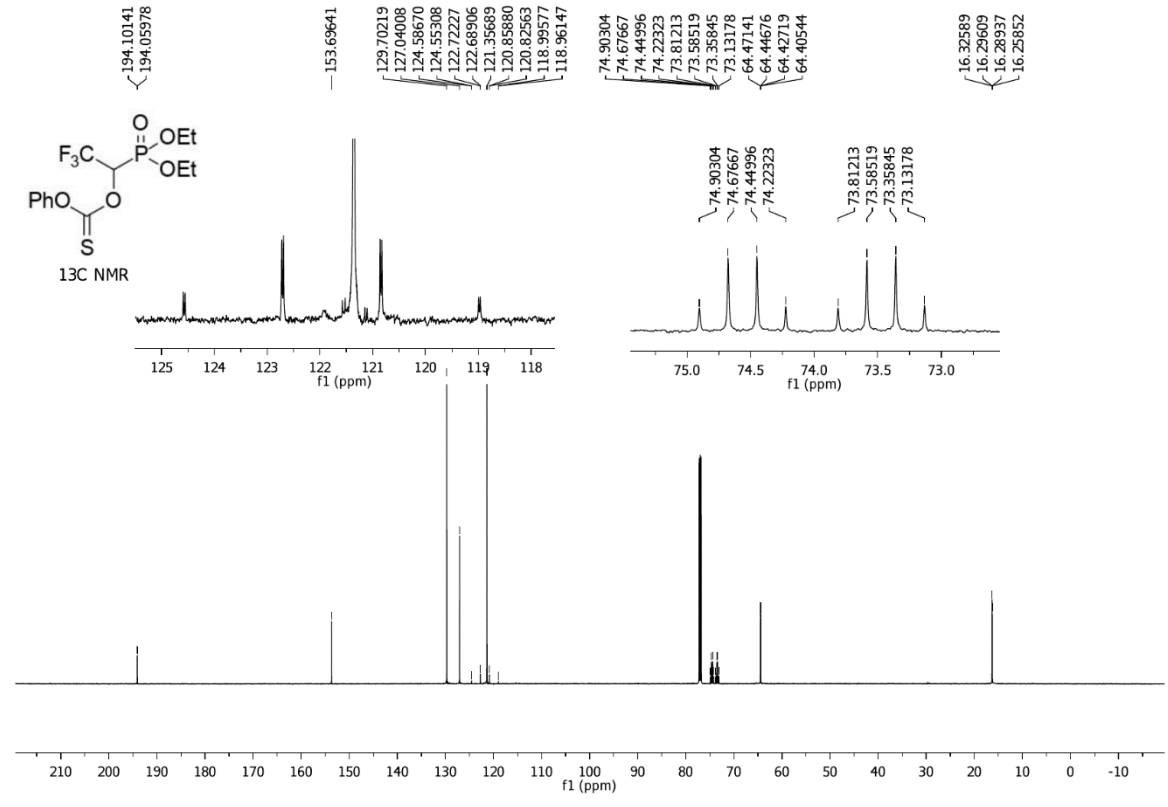
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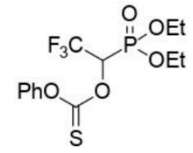

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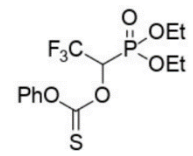
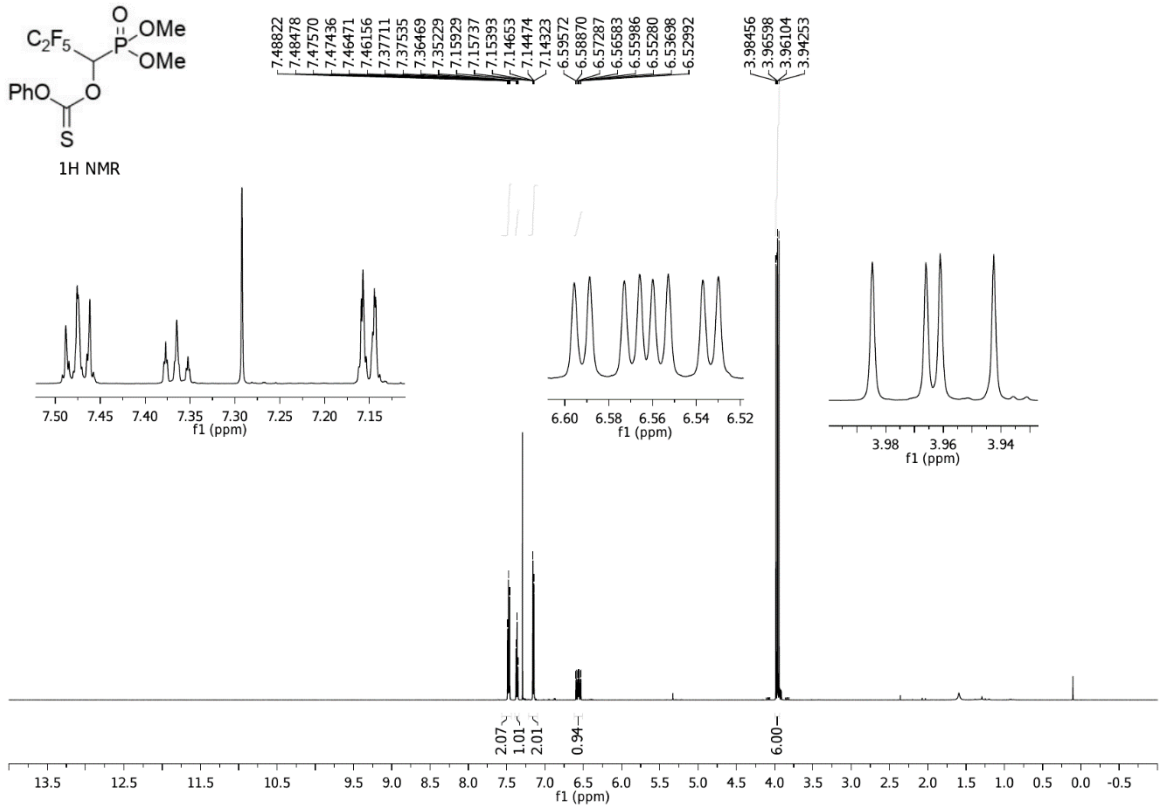


19F NMR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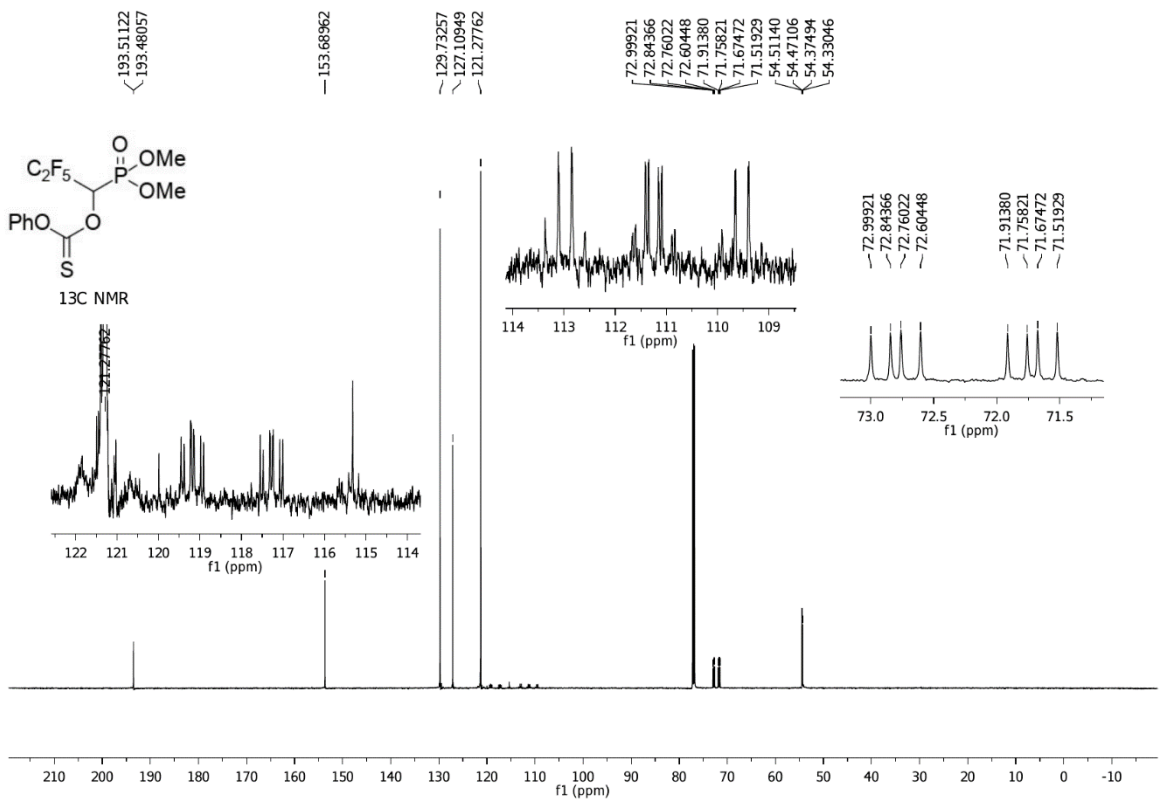
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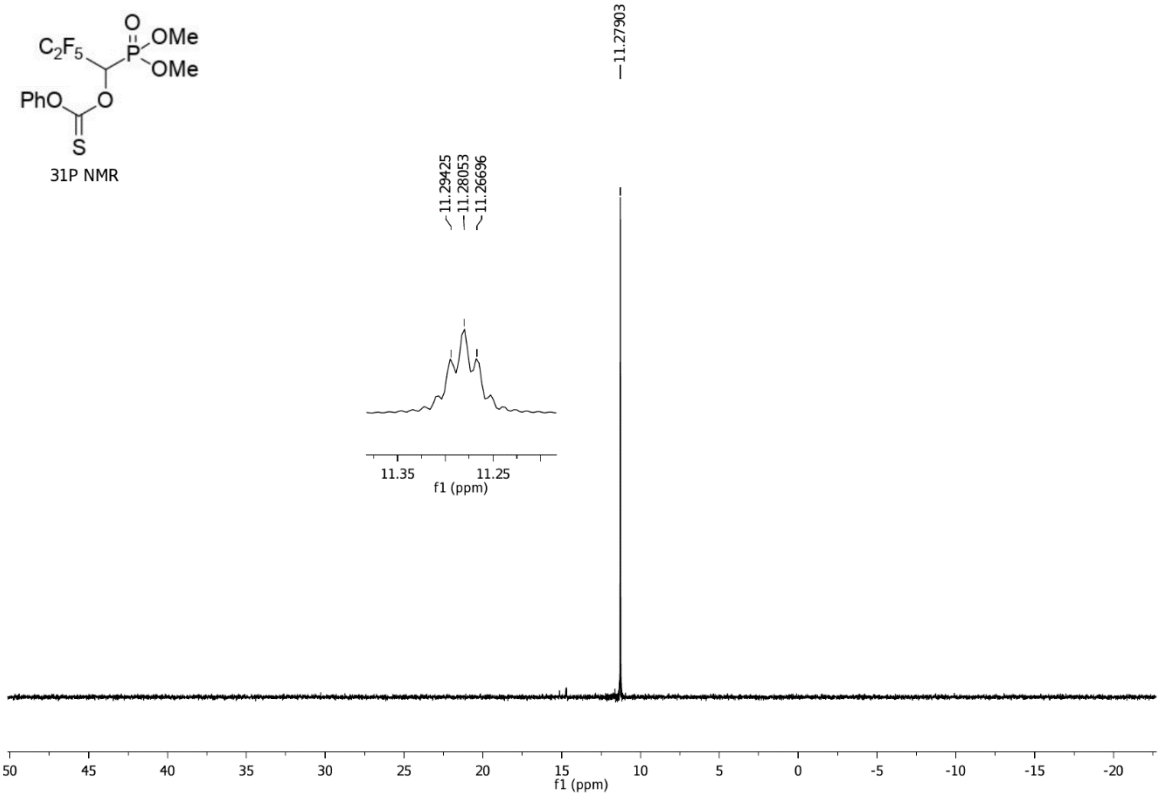
f1 (ppm)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11.35
11.25
f1 (ppm)
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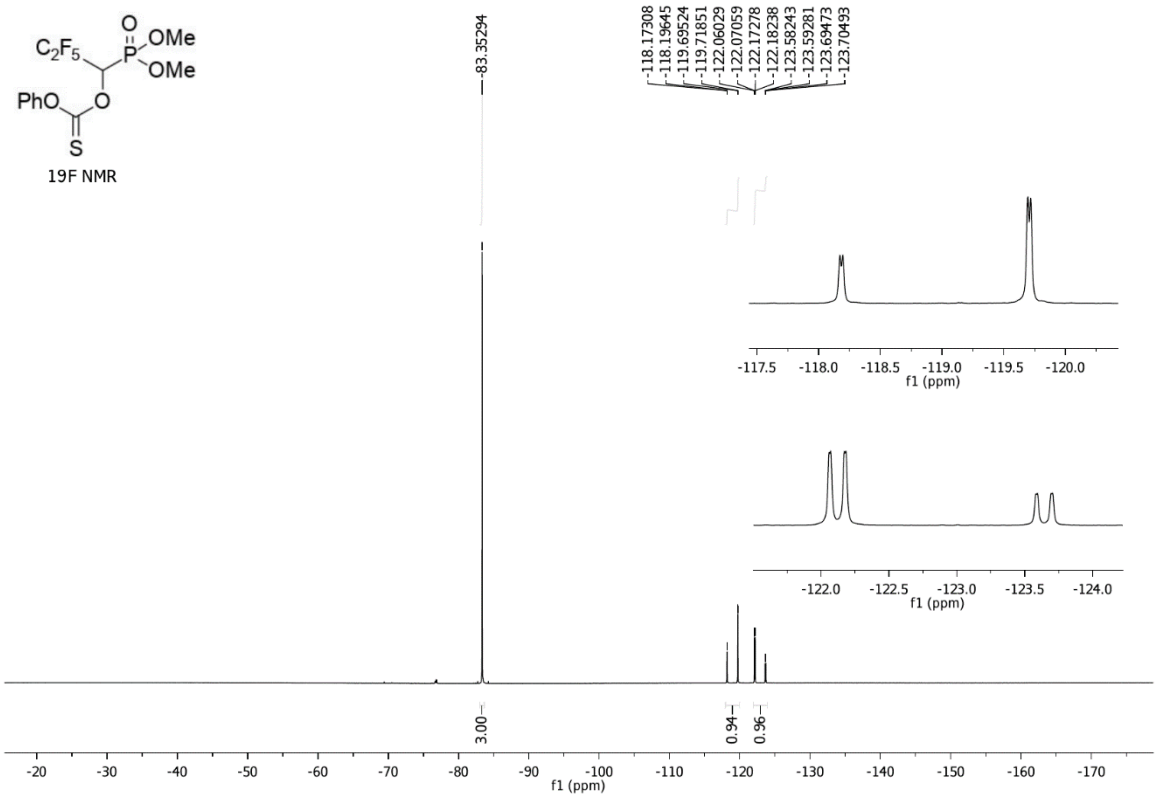
f1 (ppm)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f1 (ppm)
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0.96
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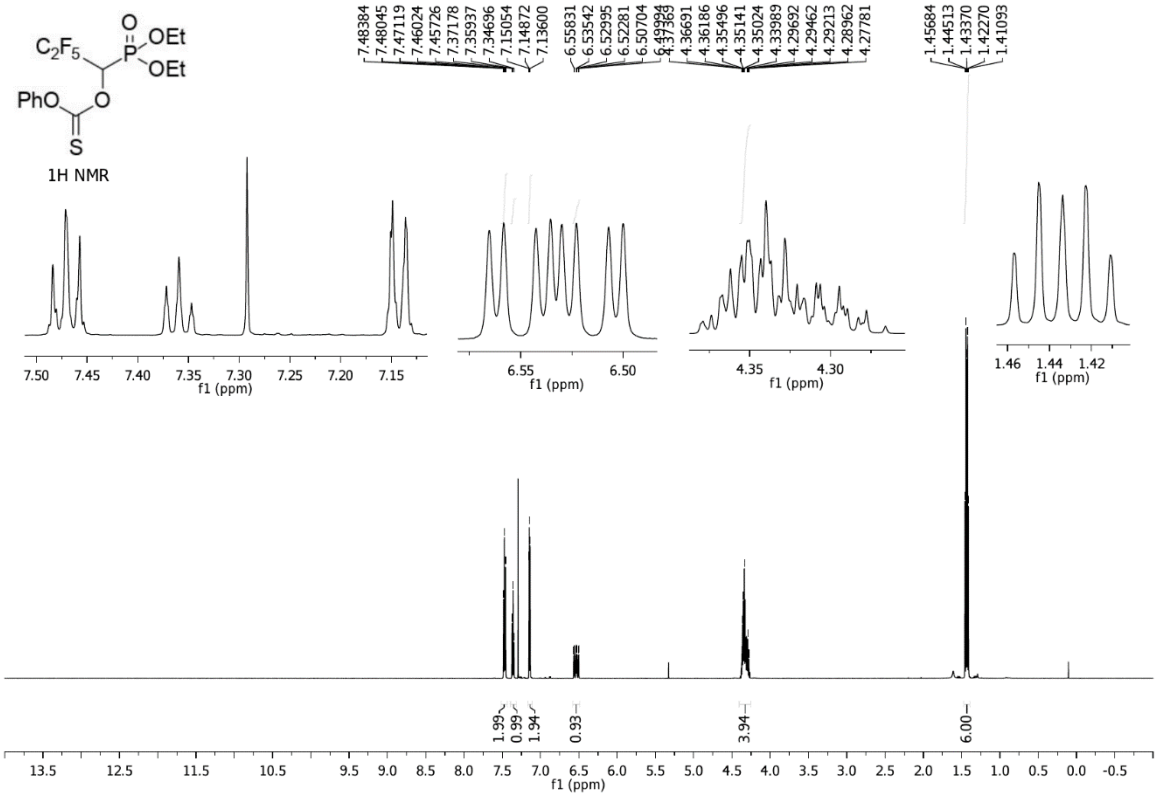
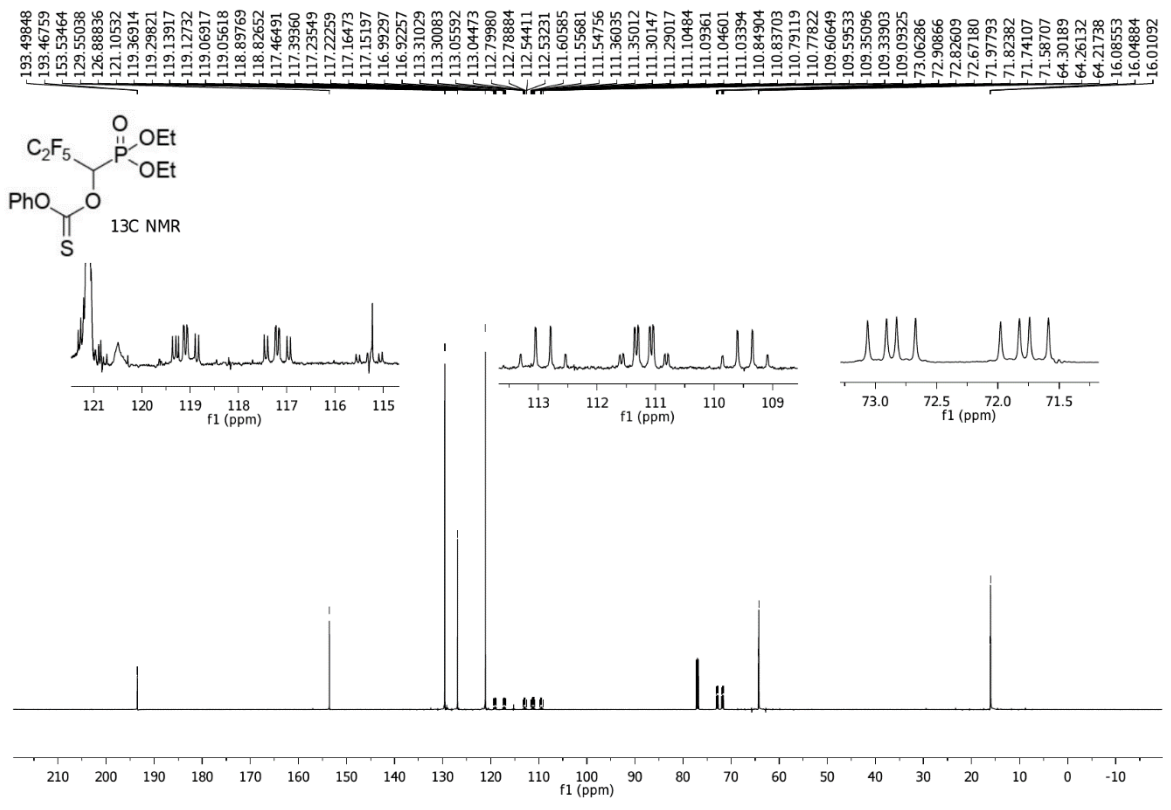
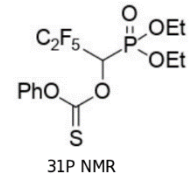
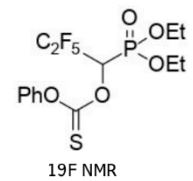
f1 (ppm)


1H NMR
f1 (ppm)

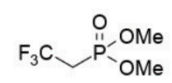

13C NMR
f1 (ppm)



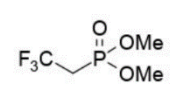
31P NMR



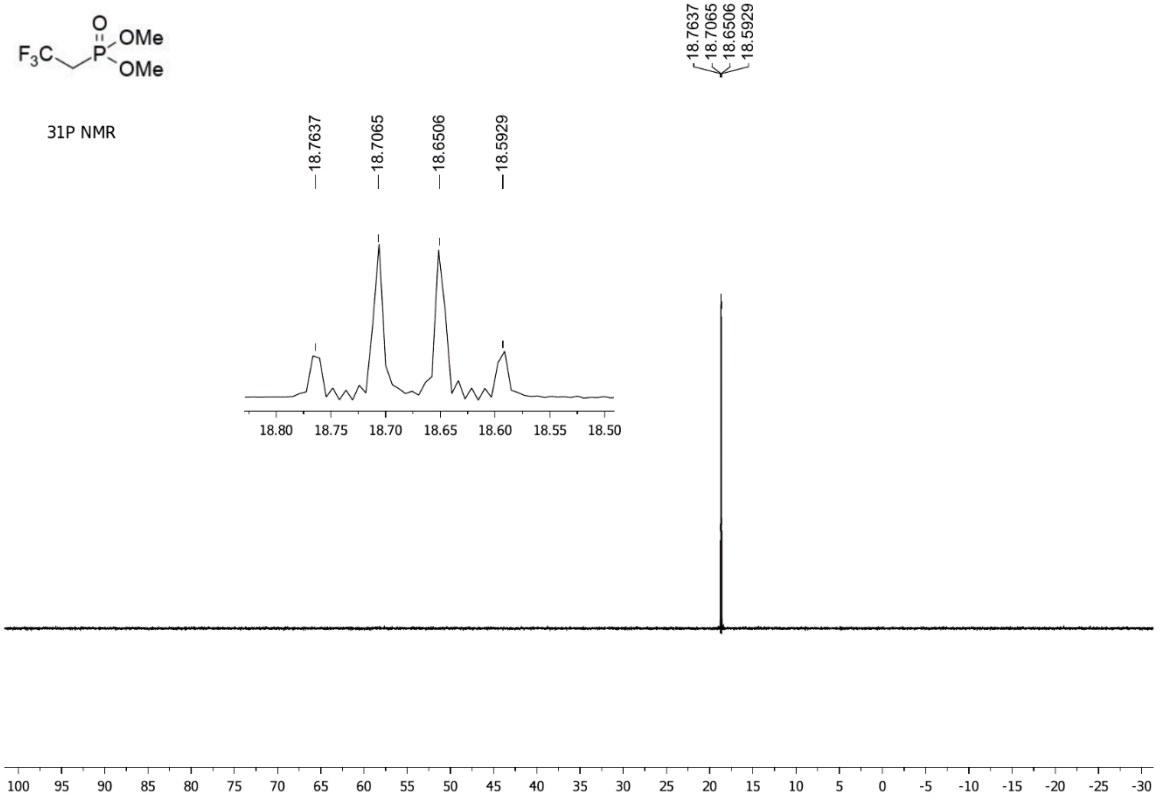
19F NMR

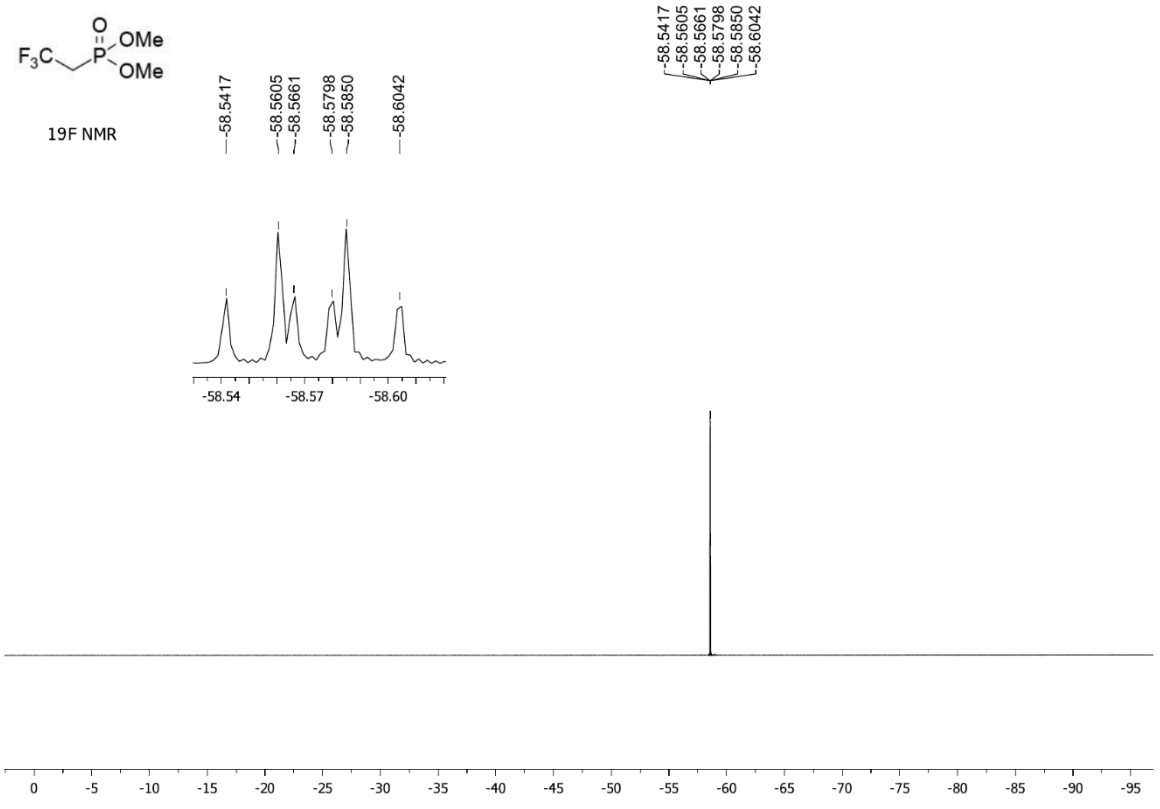


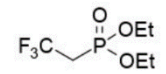
1H NMR



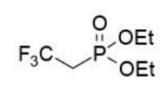
13C NMR


F3C
O
P
OMe
OMe
31P NMR
18.7637
18.7065
18.6506
18.5929
18.80 18.75 18.70 18.65 18.60 18.55 18.50
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30

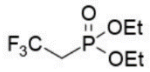

F3C
O
P
OMe
OMe
19F NMR
-58.5417
-58.5605
-58.5661
-58.5798
-58.5850
-58.6042
-58.54 -58.57 -58.60
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95



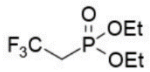
1H NMR



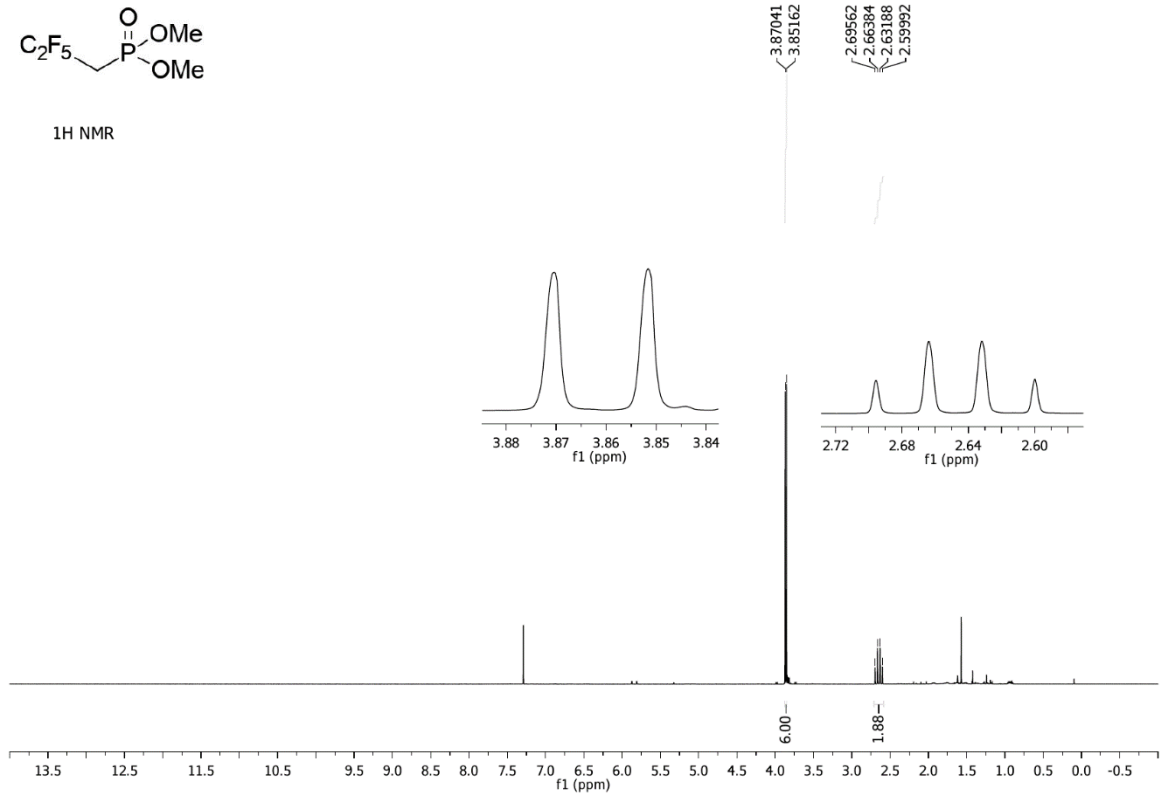
13C NMR

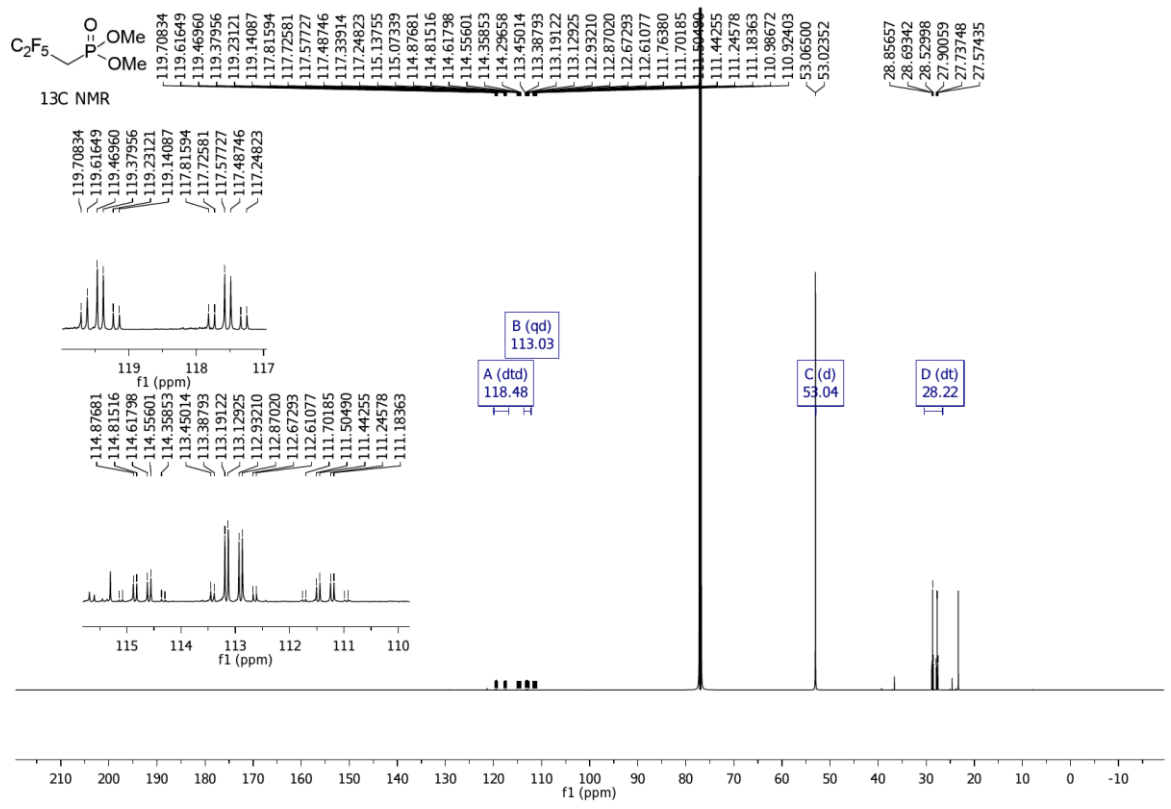


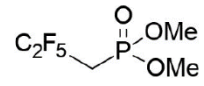
31P NMR



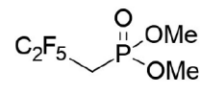
19F NMR


1H NMR
3.87041
3.85162
2.69562
2.66384
2.63188
2.59992
6.00
1.88
f1 (ppm)

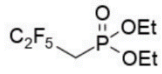

13C NMR
B (qd)
113.03
A (dtd)
118.48
C (d)
53.04
D (dt)
28.22
f1 (ppm)



31P NMR

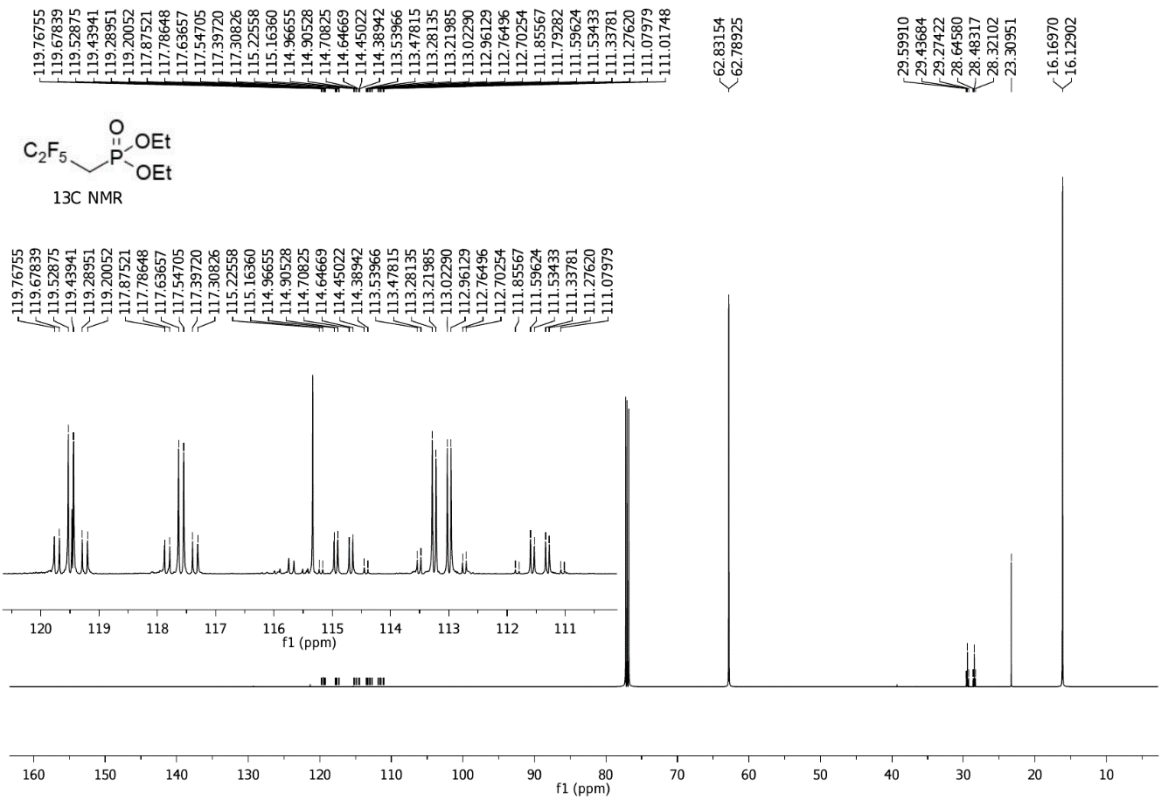


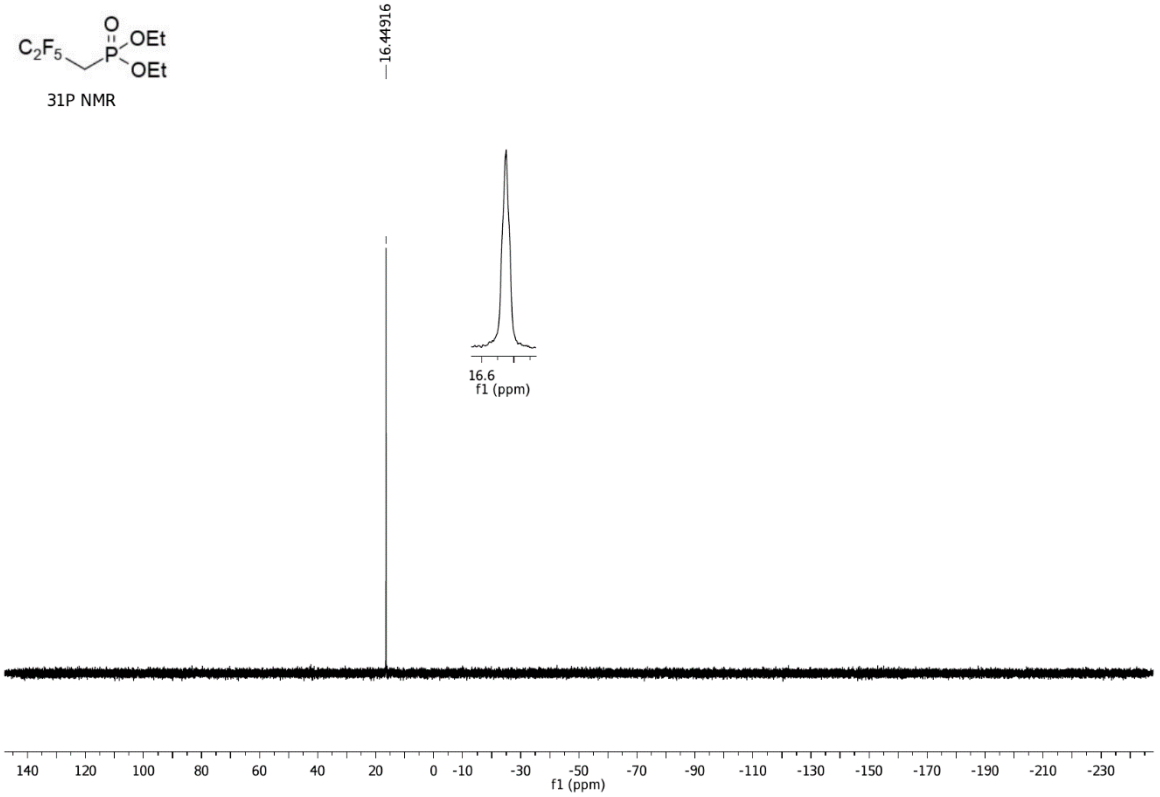
19F NMR

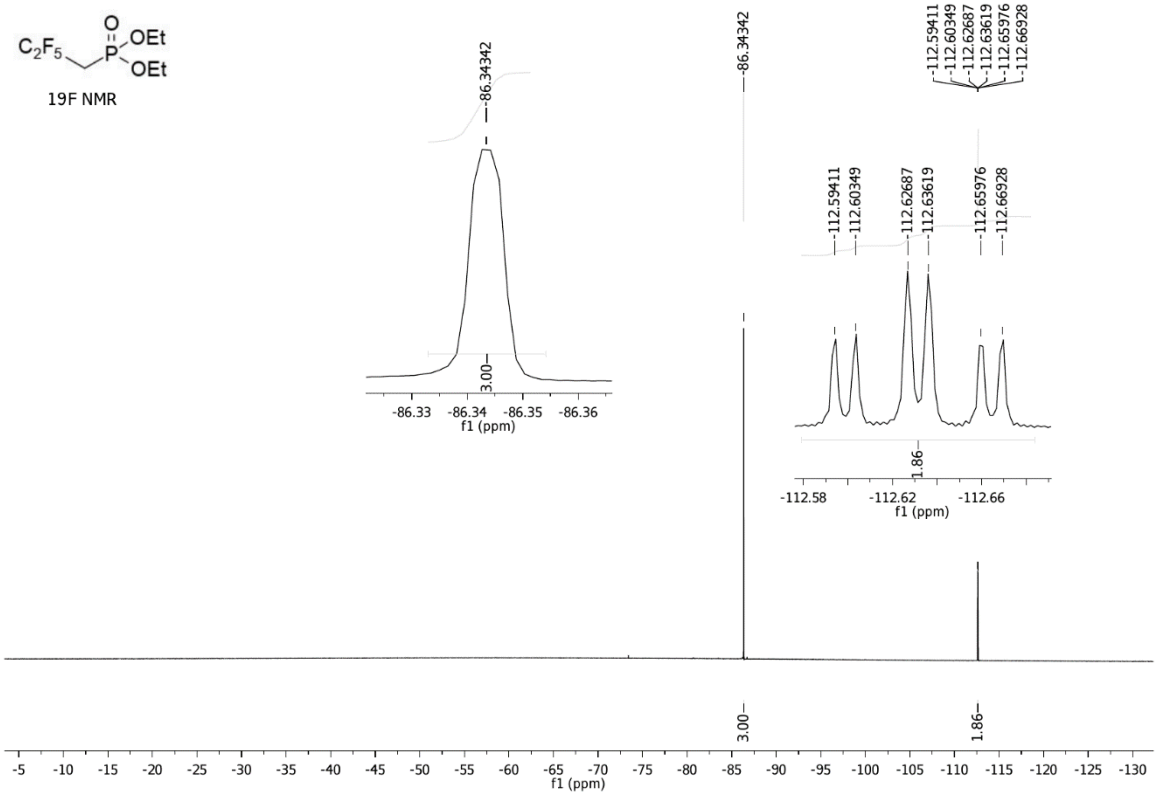

O
C2F5
P
OEt
OEt

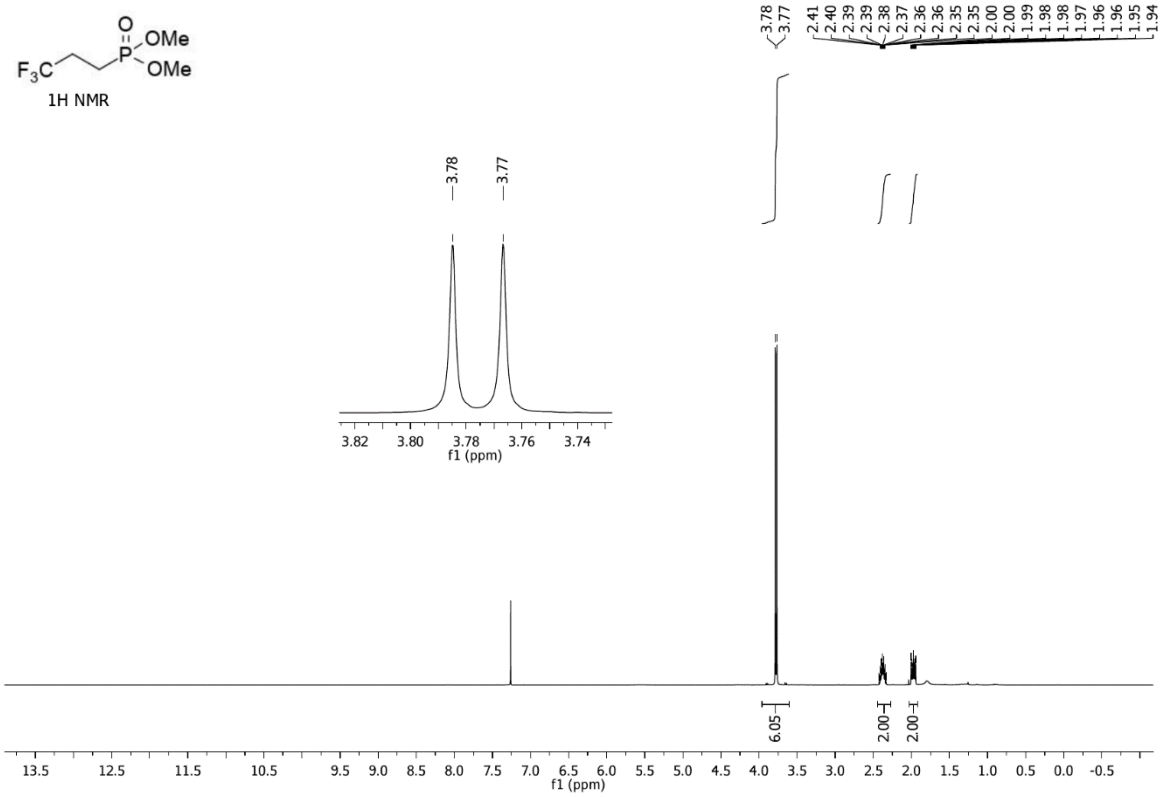
1H NMR

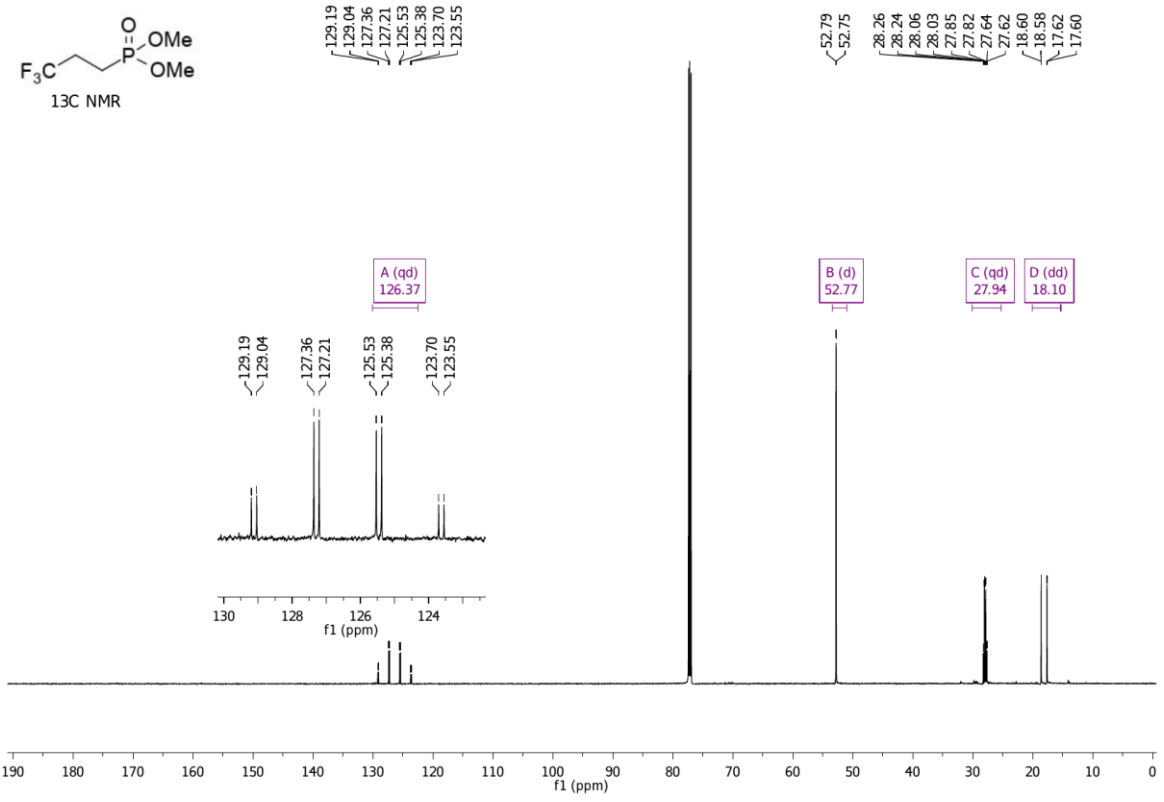
4.22136
4.20950
4.19754
4.19621
4.18395
4.17210
2.64925
2.61752
2.58566
2.55380
1.37388
1.36212
1.35033
4.22 4.20 4.18
f1 (ppm)
2.65 2.60 2.55
f1 (ppm)
1.37 1.35
f1 (ppm)
4.00
2.04
6.08
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

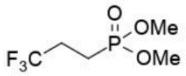

119.76755
119.67839
119.52875
119.43941
119.28951
119.20052
117.87521
117.78648
117.63657
117.54705
117.39720
117.30826
115.22558
115.16360
114.96655
114.90528
114.70825
114.64669
114.45022
114.38942
113.53966
113.47815
113.28135
113.21985
113.02290
112.96129
112.76496
112.70254
111.85567
111.79282
111.59624
111.53433
111.33781
111.27620
111.07979
111.01748
62.83154
62.78925
29.59910
29.43684
29.27422
28.64580
28.48317
28.32102
23.30951
16.16970
16.12902
O
C2F5
P
OEt
OEt
13C NMR
120 119 118 117 116 115 114 113 112 111
f1 (ppm)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


31P NMR
16.44916
16.6
f1 (ppm)
140 120 100 80 60 40 20 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230
f1 (ppm)

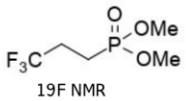

19F NMR
-86.34342
3.00
-86.33 -86.34 -86.35 -86.36
f1 (ppm)
-112.59411
-112.60349
-112.62687
-112.63619
-112.65976
-112.66928
1.86
-112.58 -112.62 -112.66
f1 (ppm)
3.00
1.86
-5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130
f1 (ppm)


1H NMR
3.78
3.77
2.41
2.40
2.39
2.39
2.38
2.37
2.36
2.36
2.35
2.35
2.00
2.00
1.99
1.98
1.98
1.97
1.96
1.96
1.95
1.94
3.82 3.80 3.78 3.76 3.74
f1 (ppm)
6.05
2.00
2.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


13C NMR
129.19
129.04
127.36
127.21
125.53
125.38
123.70
123.55
52.79
52.75
28.26
28.24
28.06
28.03
27.85
27.82
27.64
27.62
18.60
18.58
17.62
17.60
A (qd)
126.37
B (d)
52.77
C (qd)
27.94
D (dd)
18.10
130 128 126 124
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

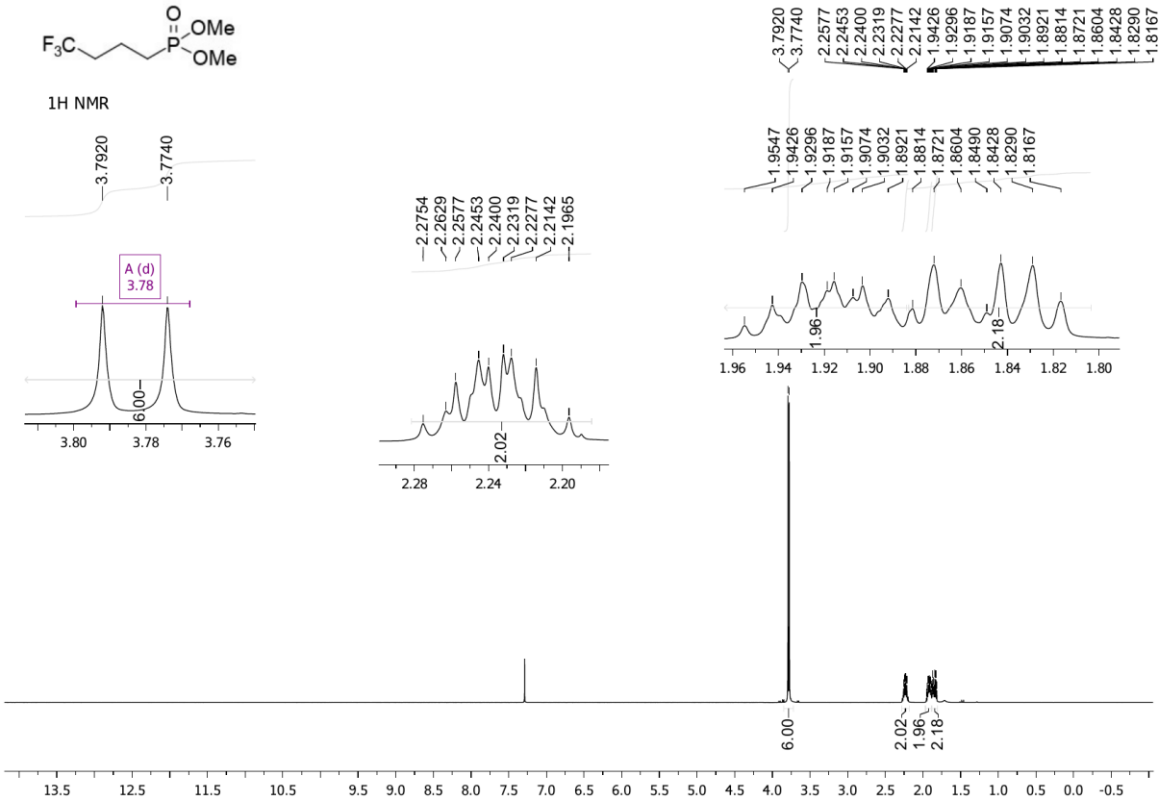


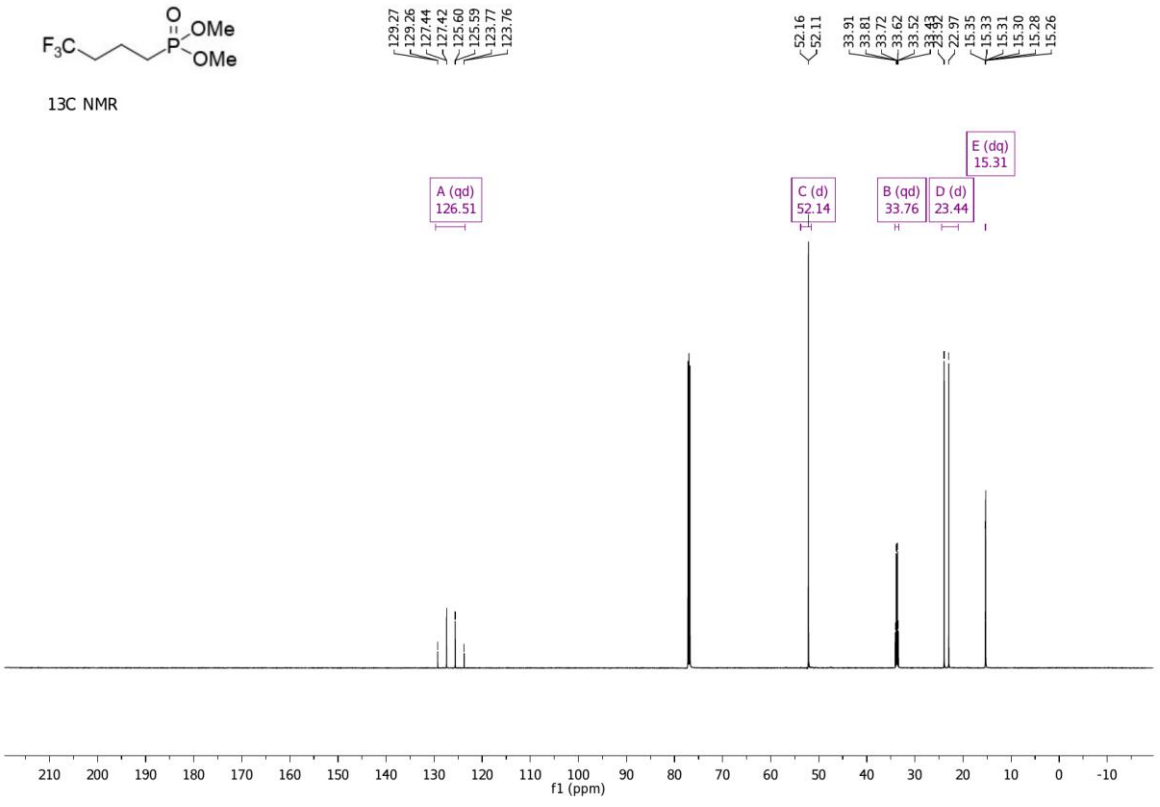
31P NMR

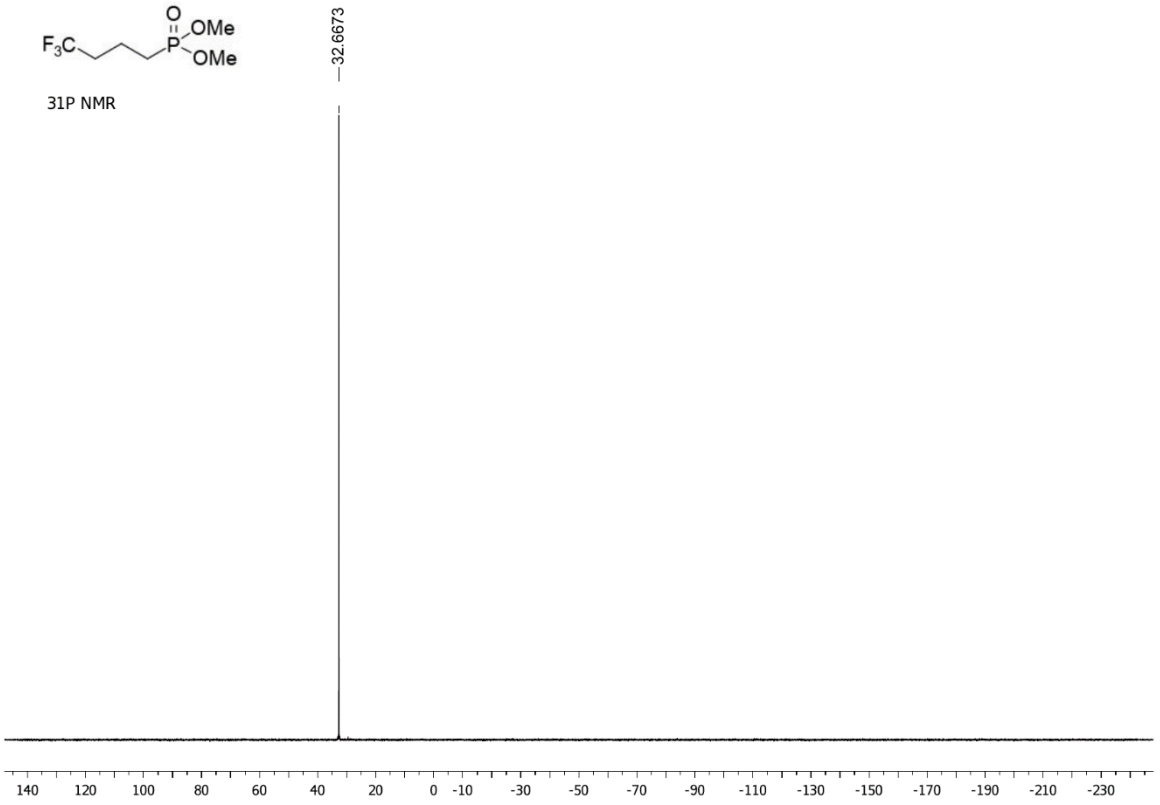


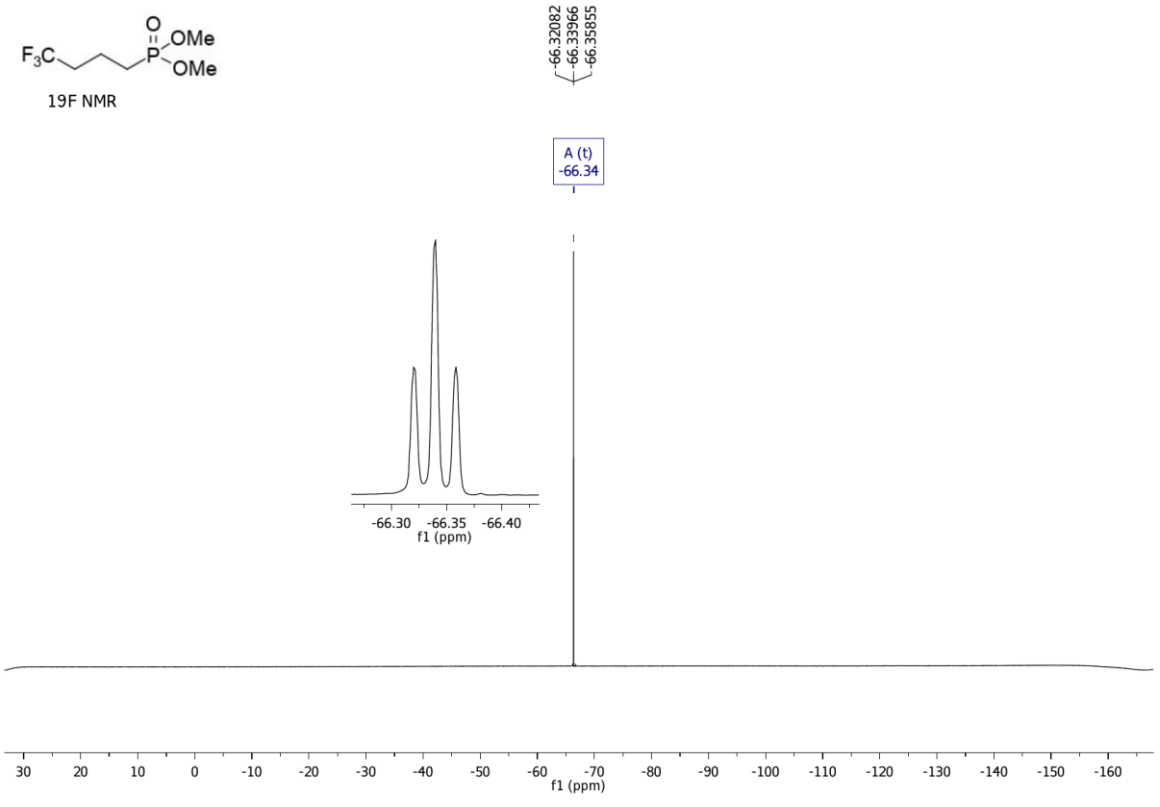
19F NMR

-67.95 (t, J = 10.2 Hz)


1H NMR
3.7920
3.7740
A (d)
3.78
6.00
2.2754
2.2629
2.2577
2.2453
2.2400
2.2319
2.2277
2.2142
2.1965
2.02
1.9547
1.9426
1.9296
1.9187
1.9157
1.9074
1.9032
1.8921
1.8814
1.8721
1.8604
1.8490
1.8428
1.8290
1.8167
1.96
2.18
6.00
2.02
1.96
2.18


13C NMR
129.27
129.26
127.44
127.42
125.60
125.59
123.77
123.76
52.16
52.11
33.91
33.81
33.72
33.62
33.52
22.97
15.35
15.33
15.31
15.30
15.28
15.26
A (qd)
126.51
C (d)
52.14
B (qd)
33.76
D (d)
23.44
E (dq)
15.31
f1 (ppm)


F3C
O
OMe
P
OMe
31P NMR
32.6673
140 120 100 80 60 40 20 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230


F3C
O
OMe
P
OMe
19F NMR
-66.32082
-66.33966
-66.35855
A (t)
-66.34
-66.30 -66.35 -66.40
f1 (ppm)
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160
f1 (ppm)

ADME data

Molecule	ZOT_3-1-Me	ZOT_3-1-Et	ZOT_5-1-Me	ZOT_5-1-Et	ZOT_3-2-Me	ZOT_3-3-Me
MW	192,07	220,13	242,08	270,13	206,1	220,13
#Heavy atoms	11	13	14	16	12	13
#Aromatic heavy atoms	0	0	0	0	0	0
Fraction Csp3	1	1	1	1	1	1
#Rotatable bonds	4	6	5	7	5	6
#H-bond acceptors	6	6	8	8	6	6
#H-bond donors	0	0	0	0	0	0
MR	32,37	41,98	37,31	46,93	37,17	41,98
TPSA	45,34	45,34	45,34	45,34	45,34	45,34
iLOGP	1,65	1,93	1,95	2,07	1,88	2,14
XLOGP3	0,59	1,32	1,26	1,99	0,94	1,3
WLOGP	3,3	4,08	4,77	5,55	3,69	4,08
MLOGP	0,61	1,32	1,32	1,96	0,98	1,32
Silicos-IT Log P	0,77	1,34	1,53	2,14	1,02	1,34
Consensus Log P	1,38	2	2,17	2,74	1,7	2,04
ESOL Log S	-1,14	-1,64	-1,8	-2,31	-1,38	-1,63
ESOL Solubility (mg/ml)	14	5,04	3,8	1,33	8,59	5,19
ESOL Solubility (mol/l)	0,0727	0,0229	0,0157	0,00494	0,0417	0,0236
ESOL Class	Very soluble	Very soluble	Very soluble	Soluble	Very soluble	Very soluble
Ali Log S	-1,12	-1,87	-1,81	-2,57	-1,48	-1,85
Ali Solubility (mg/ml)	14,7	2,95	3,74	0,73	6,84	3,09
Ali Solubility (mol/l)	0,0766	0,0134	0,0155	0,0027	0,0332	0,014
Ali Class	Very soluble	Very soluble	Very soluble	Soluble	Very soluble	Very soluble
Silicos-IT LogSw	-1,45	-2,26	-2,06	-2,86	-1,85	-2,26
Silicos-IT Solubility (mg/ml)	6,85	1,2	2,12	0,371	2,88	1,2
Silicos-IT Solubility (mol/l)	0,0356	0,00547	0,00875	0,00137	0,014	0,00547
Silicos-IT class	Soluble	Soluble	Soluble	Soluble	Soluble	Soluble
GI absorption	High	High	High	High	High	High
BBB permeant	Yes	Yes	Yes	Yes	Yes	Yes
P-gp substrate	No	No	No	No	No	No
CYP1A2 inhibitor	No	No	No	No	No	No
CYP2C19 inhibitor	No	No	No	No	No	No
CYP2C9 inhibitor	No	No	No	No	No	No
CYP2D6 inhibitor	No	No	No	No	No	No
CYP3A4 inhibitor	No	No	No	No	No	No
log Kp (cm/s)	-7,05	-6,71	-6,88	-6,53	-6,89	-6,72
Lipinski #violations	0	0	0	0	0	0
Ghose #violations	2	0	1	0	1	0
Veber #violations	0	0	0	0	0	0
Egan #violations	0	0	0	0	0	0
Muegge #violations	2	0	0	0	0	0
Bioavailability Score	0,55	0,55	0,55	0,55	0,55	0,55
PAINS #alerts	0	0	0	0	0	0
Brenk #alerts	1	1	2	2	1	1
Leadlikeness #violations	1	1	1	0	1	1
Synthetic Accessibility	3,52	3,68	3,8	3,95	3,75	3,75

Geometries of DFT-optimized structures

The following supplementary info comprises Cartesian coordinates of PES stationary points corresponding to structures necessary for calculating total free energy changes (ΔG) for reactions 3a and 3b as well as total G=G(ξ) dependence for both reactions in solution; ξ – reaction coordinate.

DMF SOLUTION

SUBSTRATES + PRODUCTS

$P(OMe)_3$

E_{el} = -686.990790 Hartree

P	0.00183300	-0.00569300	0.41305200
O	-0.51957300	1.32117300	-0.38635800
O	1.40379800	-0.22300300	-0.39748000
O	-0.89476700	-1.11450600	-0.38559800
C	-0.09944800	2.61323700	0.07852300
H	0.88485400	2.86049600	-0.32367600
H	-0.82880900	3.33785100	-0.27838000
H	-0.06108600	2.65129000	1.17070400
C	-2.22680600	-1.38340600	0.07866000
H	-2.92525200	-0.64671700	-0.32285100
H	-2.49987000	-2.37417500	-0.27936400
H	-2.27923700	-1.36960200	1.17083500
C	2.33131600	-1.20909300	0.08176500
H	2.06539500	-2.19784700	-0.29700300
H	3.31654000	-0.93272900	-0.28887800
H	2.35394400	-1.23690700	1.17462800

CH_3I

E_{el} = -337.737630 Hartree

C	1.83673000	-0.00000100	-0.00001800
H	2.15649900	-0.03784300	1.03512200
H	2.15659700	0.91545300	-0.48468700
H	2.15677300	-0.87754300	-0.55026400
I	-0.33000500	-0.00000100	-0.00000100

CF_3CH_2I

E_{el} = -674.933283 Hartree

C	-1.72028100	0.00414900	0.00004200
C	-0.55646800	0.96451200	-0.00007600

H	-0.60536500	1.58026500	0.89187800
H	-0.60541100	1.58009600	-0.89214400
I	1.36154500	-0.01984900	-0.00003200
F	-1.74399500	-0.79313200	-1.08490500
F	-2.87769800	0.70603500	0.00001400
F	-1.74393300	-0.79294300	1.08513000

$CF_3(CH_2)_2I$

E_{el} = -714.271178 Hartree

C	-0.11125900	-2.49419700	0.00000000
I	-0.01561100	1.97197500	0.00000000
F	-1.17171600	-3.32950600	0.00000000
F	0.63425400	-2.80305100	1.08518000
F	0.63425400	-2.80305100	-1.08518000
C	0.63425400	-0.10205000	0.00000000
H	1.24667600	-0.20851300	-0.88940200
H	1.24667600	-0.20851300	0.88940200
C	-0.55381400	-1.04814100	0.00000000
H	-1.17610600	-0.90543600	0.88279900
H	-1.17610600	-0.90543600	-0.88279900

$CF_3(CH_2)_3I$

E_{el} = -753.605421 Hartree

C	3.14338500	-0.05304600	0.00003600
F	4.28276000	0.67607200	0.00007200
F	3.19772400	-0.86007100	-1.08512800
F	3.19770500	-0.86014800	1.08514300
C	0.61732100	0.02328700	0.00000600
H	0.58426300	-0.62062300	0.87961600
H	0.58428300	-0.62054400	-0.87966300
C	1.92216600	0.82814500	0.00005600
H	1.99162200	1.46609900	-0.88205600
H	1.99159900	1.46602500	0.88222400
C	-0.57125000	0.96609400	0.00003500
H	-0.60938900	1.58992500	-0.88855500
H	-0.60940900	1.58984700	0.88867900
I	-2.46615800	-0.11434500	-0.00003400

$P(O)(OMe)_2CH_2CF_3$

E_{el} = -1024.246782 Hartree

P	0.93420400	0.02193200	0.49261200
C	-0.78881900	-0.14515200	1.05139100
H	-0.99946300	0.70086100	1.70535400
H	-0.85258600	-1.05423800	1.64914600

O	1.82588300	0.42772800	1.59382400
O	0.95251900	0.98765800	-0.76782100
O	1.19395600	-1.39038200	-0.16584500
C	2.46457900	-1.70341200	-0.78546500
H	2.40683000	-2.74621200	-1.08335400
H	2.61769800	-1.07281400	-1.66061900
H	3.27730500	-1.56406900	-0.07322100
C	1.05153000	2.42337800	-0.62976900
H	1.76210600	2.68113700	0.15387500
H	1.39831200	2.80095600	-1.58781400
H	0.07024800	2.83947800	-0.40184200
C	-1.87089500	-0.18959400	-0.00025100
F	-3.07633700	-0.42017100	0.56875500
F	-1.68076500	-1.15935300	-0.91666600
F	-1.97742600	0.97669700	-0.67291100

$P(O)(OMe)_2(CH_2)_2CF_3$

E_{el} = -1063.585035 Hartree

P	1.46267500	-0.01381600	0.42402500
C	-0.30344600	0.06568100	0.77515600
H	-0.48434800	1.05460400	1.20116700
H	-0.50355600	-0.66592500	1.55965900
O	2.32367400	0.26252200	1.59112500
O	1.73439800	0.94188900	-0.82572400
O	1.59331300	-1.45007400	-0.23701300
C	2.86520500	-1.93038000	-0.72743700
H	2.69372800	-2.94326400	-1.08070100
H	3.21100300	-1.30349600	-1.54922500
H	3.60282300	-1.93664100	0.07481200
C	2.10819600	2.32590100	-0.65596700
H	2.85167800	2.42523800	0.13347300
H	2.52650100	2.65100800	-1.60505700
H	1.22912500	2.92614300	-0.41805200
C	-2.65905100	-0.06433800	-0.10529900
F	-2.98757200	1.16055000	0.36671400
F	-3.03942500	-0.95732400	0.83744100
F	-3.43358900	-0.28645800	-1.19029400
C	-1.19471700	-0.17494900	-0.44340100
H	-0.99389900	0.55272200	-1.22949300
H	-1.03609900	-1.17023700	-0.85711100

$P(O)(OMe)_2(CH_2)_3CF_3$

E_{el} = -1102.917653 Hartree

P	2.03322500	0.00143300	0.42740300
C	0.39002600	0.19002000	1.13816900
H	0.35626200	1.20503500	1.54380000
H	0.33545400	-0.49128300	1.99071700

O	3.14255600	0.28368400	1.36238800
O	2.07490300	0.88594100	-0.90431300
O	1.97167400	-1.46749300	-0.17307300
C	3.10299800	-2.02886500	-0.87383300
H	2.84172600	-3.05828300	-1.10315000
H	3.28414700	-1.47779000	-1.79674000
H	3.99173800	-2.00379000	-0.24330100
C	2.46458100	2.27397500	-0.87054700
H	3.35568300	2.40575500	-0.25808900
H	2.67379300	2.56204600	-1.89767000
H	1.65020300	2.88559500	-0.47901500
C	-0.76695400	-0.04746000	0.16368300
H	-0.66971500	0.62146900	-0.69251000
H	-0.72184100	-1.06821900	-0.21754900
C	-2.11463700	0.18771000	0.84582100
H	-2.24654500	-0.48235000	1.69674900
H	-2.19536400	1.21221500	1.21252800
C	-3.28295900	-0.04033000	-0.07530200
F	-3.32815400	-1.30789900	-0.54946900
F	-4.46290200	0.18243700	0.54888000
F	-3.25620100	0.77443600	-1.15660800

TRANSITION STATES + INTERMEDIATES

Reaction $P(OMe)_3 + CF_3CH_2I$

SUBSTRATE COMPLEX

E_{el} = -1361.930336 Hartree

P	2.35641500	-0.23318800	-0.04630700
O	3.42649500	-1.44865600	-0.25126300
O	3.39914800	1.01697700	-0.16328400
O	2.24882700	-0.28903400	1.58028000
C	3.72580700	-1.88252900	-1.58777300
H	4.49726200	-1.24864800	-2.02886100
H	4.09133400	-2.90530500	-1.52101600
H	2.83539900	-1.85987300	-2.22190300
C	1.31012300	-1.19540300	2.18192800
H	1.75494600	-2.18693400	2.28404300
H	1.06844600	-0.80209700	3.16739200
H	0.39341400	-1.27061200	1.59224900
C	2.87478800	2.35433300	-0.21444500
H	2.59948500	2.69611300	0.78515300
H	3.66367200	2.99098200	-0.60963100
H	2.00150900	2.41529700	-0.86803500
C	-1.31489200	1.78413600	-0.09074200
C	-1.34697600	0.58058100	-0.99869100
H	-1.86336500	0.83882500	-1.91722000

H	-0.32572300	0.26632000	-1.19483000
I	-2.36551900	-1.11008800	-0.13283500
F	-0.66016000	1.55154100	1.06373200
F	-2.53986300	2.24355800	0.22829500
F	-0.66430300	2.79572700	-0.71425400

TS1

E_{el} = -1361.892502 Hartree

P	2.22461500	0.43744100	-0.02620600
O	2.44941400	1.94486200	-0.51977400
O	3.02809200	0.43993400	1.35917100
O	3.22990000	-0.36401400	-0.97994900
C	1.71533300	3.04359700	0.06967300
H	2.01797900	3.18417900	1.10691500
H	1.96901700	3.92473600	-0.51271100
H	0.63990900	2.86938700	0.01407500
C	2.83766300	-0.77555600	-2.30980600
H	2.74677500	0.09265300	-2.96198900
H	3.62819900	-1.42764500	-2.67021800
H	1.89666400	-1.32520900	-2.28232200
C	3.06602800	-0.72986900	2.21011800
H	3.63903200	-1.52318100	1.73091700
H	3.55744000	-0.41998200	3.12795000
H	2.05871000	-1.08096300	2.43336500
C	-0.36066500	-1.52857600	0.04629900
C	-0.32471100	-0.01109500	0.01965000
H	-0.28445800	0.52014300	0.94898400
H	-0.29576300	0.49203500	-0.92456900
I	-2.95045500	0.51144400	-0.00342000
F	-0.91861600	-2.02533200	-1.07169500
F	-1.04212100	-1.99512200	1.10641300
F	0.86854500	-2.10527700	0.12892200

SALT

E_{el} = -1361.975963 Hartree

P	1.46758200	-0.71144700	-0.00311600
O	0.58249300	-1.92999700	-0.36025100
O	2.92562200	-0.83193900	-0.50245000
O	1.49666000	-0.63393200	1.53832100
C	0.07042500	-2.28288600	-1.68557200
H	0.87973300	-2.26939300	-2.41211000
H	-0.32689200	-3.28613200	-1.57903600
H	-0.72294400	-1.58664900	-1.94757400
C	0.35661800	-0.88429700	2.42984100
H	0.39056000	-1.92984100	2.72210400
H	0.50888100	-0.23362900	3.28415500

H	-0.57884600	-0.65157800	1.92371100
C	3.85980000	-1.87692400	-0.07661200
H	3.44993700	-2.85325100	-0.32445000
H	4.76999300	-1.69041300	-0.63530200
H	4.03571100	-1.78479500	0.99209000
C	1.33689000	2.08589600	-0.23273500
C	0.82513900	0.77027700	-0.78433900
H	1.05987600	0.72306500	-1.84816500
H	-0.26525400	0.74636800	-0.66533000
I	-2.91059000	-0.04276000	-0.02191100
F	0.97930900	2.26342900	1.05354200
F	0.82208100	3.10842600	-0.93820400
F	2.67809400	2.18911700	-0.29428700

TS2

E_{el} = -1361.951521 Hartree

P	-1.47577000	0.10843600	-0.14574400
O	-1.52142000	1.62823000	0.21018300
O	-1.57241400	-0.60745900	1.24865700
O	-0.31370300	-0.35726700	-0.97938800
C	-0.63572300	2.27318700	1.16758100
H	0.36307500	2.35813200	0.74399000
H	-1.05449300	3.25955200	1.33811200
H	-0.61414100	1.70516600	2.09517800
C	1.53756900	-0.21631600	-0.56365800
H	1.45918500	-0.32531100	0.50283700
H	1.77170900	-1.07782500	-1.15897200
H	1.64399100	0.76344400	-0.98986300
C	-1.34489700	-2.03049900	1.44122700
H	-1.08777900	-2.15376400	2.48848600
H	-2.26030500	-2.57124800	1.20951900
H	-0.52793300	-2.37272500	0.80891100
C	-2.97788000	-0.15442100	-1.11697800
H	-2.90297300	-1.13956500	-1.57713700
H	-2.98707200	0.59013500	-1.91286200
I	4.33305100	-0.05423400	-0.09138400
C	-4.29313900	-0.08336400	-0.37138700
F	-4.40486300	-1.06234700	0.55047600
F	-4.46894300	1.08816800	0.26761500
F	-5.32327200	-0.22889300	-1.22865000

PRODUCT COMPLEX

E_{el} = -1361.990944 Hartree

P	1.24894600	0.55207500	0.55842900
O	1.22089800	1.62312200	-0.60169700
O	0.74045200	-0.75812300	-0.17642500

O	0.52053500	0.88522900	1.79725000
C	-0.03717600	2.09954700	-1.13957200
H	-0.60342100	2.61485600	-0.36452300
H	0.21760600	2.79125200	-1.93705700
H	-0.61812000	1.26702800	-1.53432300
C	-2.88843300	0.85356400	1.43879500
H	-1.81750900	0.83003400	1.61205500
H	-3.44314500	0.39981000	2.25242500
H	-3.24252700	1.85615200	1.22602300
C	0.28687000	-1.92240100	0.55064700
H	-0.40276000	-2.44541400	-0.10528000
H	1.14064600	-2.55779700	0.78495200
H	-0.22705200	-1.62491600	1.46301600
C	3.03400100	0.37763900	0.85908200
H	3.15026900	-0.17249600	1.79273500
H	3.44193900	1.37743300	1.00642800
I	-3.27779100	-0.33958700	-0.32932600
C	3.85986400	-0.32383800	-0.19176700
F	3.52244700	-1.62478400	-0.32255300
F	3.75126700	0.23840800	-1.41201400
F	5.17150700	-0.29449600	0.13737600

Reaction $P(OMe)_3 + CF_3(CH_2)_2I$

SUBSTRATE COMPLEX

E_{el} = -1401.268444 Hartree

P	-2.23440500	0.29051800	-0.01490900
O	-3.59311000	-0.26302200	-0.73277000
O	-2.54633000	-0.23793600	1.49948800
O	-2.69390400	1.84370600	0.18763100
C	-3.59563200	-1.60957400	-1.23438400
H	-3.82094500	-2.31377600	-0.43133200
H	-4.36991000	-1.66846900	-1.99670800
H	-2.63139100	-1.86915800	-1.67970500
C	-2.42798500	2.77955500	-0.87032400
H	-3.22274900	2.74283000	-1.61758100
H	-2.39600800	3.77103300	-0.42290700
H	-1.46865200	2.57344100	-1.35097700
C	-1.50045800	-0.17709200	2.48254200
H	-1.28117000	0.85724300	2.75578100
H	-1.86043500	-0.71052400	3.35978900
H	-0.59102200	-0.66165800	2.11902100
C	2.03573200	0.76472300	0.40847800
C	1.52556400	-0.09171000	-0.73689100
H	0.52484300	0.19262100	-1.04653700
H	2.20483700	-0.09925300	-1.58300700

I	1.32869200	-2.16836800	-0.13344600
H	3.02695900	0.45038900	0.73366700
H	1.36693400	0.72147500	1.26720500
C	2.13932300	2.21921500	0.00900100
F	2.97653200	2.40730500	-1.03606700
F	2.60321900	2.97480100	1.02690000
F	0.94325100	2.73866200	-0.35271800

TS1

E_{el} = -1401.236848 Hartree

P	2.22173200	-0.62091000	-0.01019700
O	2.30073100	-1.98381700	0.84071700
O	3.05031000	-1.02899000	-1.32544400
O	3.31496300	0.25847500	0.77103600
C	1.43760800	-3.10322000	0.54588200
H	1.54902000	-3.41218900	-0.49384100
H	1.75278600	-3.91124700	1.20045600
H	0.39592600	-2.85616900	0.75430400
C	3.09768200	0.68547700	2.13508200
H	3.21765500	-0.16127600	2.80999100
H	3.85391200	1.43754000	2.34353100
H	2.10718900	1.12317100	2.25740400
C	2.97585600	-0.25026900	-2.54089400
H	3.26488300	0.78501900	-2.35885000
H	3.67776800	-0.70500900	-3.23454500
H	1.97195500	-0.29343100	-2.96385100
C	-0.37740400	1.17368100	-0.96273800
C	-0.34369100	-0.15349000	-0.25252100
H	-0.28993000	-1.04888900	-0.84075500
H	-0.31340900	-0.22671700	0.81695600
I	-2.96779500	-0.77748100	0.01894100
H	-1.32102100	1.28784500	-1.49316300
H	0.40862700	1.24306100	-1.71281900
C	-0.23478000	2.37094300	-0.05318000
F	-1.10997600	2.35331200	0.97241700
F	-0.44199100	3.51433100	-0.73802000
F	0.99998200	2.46062000	0.49271600

SALT

E_{el} = -1401.316149 Hartree

P	-0.74565300	0.66973000	-0.16002100
O	-0.58437300	1.12999500	1.30701200
O	-0.00309800	-0.69043500	-0.26387900
O	-0.22235200	1.68182600	-1.21343400
C	0.61734900	1.03036700	2.14104500
H	1.37742000	0.42598800	1.64981900

H	0.97586100	2.04224100	2.30660700
H	0.30229000	0.57310800	3.07362300
C	1.13777500	2.22855900	-1.25265800
H	1.86226800	1.48005700	-0.93203200
H	1.31026500	2.50643300	-2.28696300
H	1.16955000	3.10360200	-0.60853700
C	0.39225900	-1.36231700	-1.50124200
H	-0.26036900	-2.22138400	-1.62806500
H	0.30416200	-0.68439000	-2.34769600
H	1.42684500	-1.65912400	-1.35888400
C	-2.49600800	0.55287900	-0.47000100
H	-2.61324000	0.29422300	-1.52418200
H	-2.90693500	1.55393700	-0.32775900
I	3.94413200	-0.49360500	0.13316800
C	-3.18419400	-0.47103400	0.43780000
H	-2.78320800	-1.47274600	0.28681000
H	-3.06823700	-0.21101400	1.48931400
C	-4.66649000	-0.53920700	0.15813600
F	-4.92830200	-0.89593700	-1.11839900
F	-5.26880500	-1.44291800	0.95601200
F	-5.27805000	0.64748200	0.36619600

TS2

E_{el} = -1401.291676 Hartree

P	1.03285800	-0.23911300	0.01926200
O	1.13880900	-1.79650800	0.16601900
O	0.86642300	0.25132000	1.51042200
O	-0.05616900	0.27531100	-0.88558800
C	0.12073700	-2.62236800	0.79057400
H	-0.76657000	-2.65538000	0.16059300
H	0.55287400	-3.61436000	0.87534200
H	-0.12263300	-2.23256800	1.77731300
C	-1.94207700	0.20994100	-0.54554400
H	-1.89121400	0.10797200	0.52292400
H	-2.08562000	1.18400500	-0.97189200
H	-2.08719400	-0.66124200	-1.15506600
C	0.50601100	1.61188100	1.86557000
H	0.00173700	1.55328200	2.82547400
H	1.41075600	2.21118300	1.95178800
H	-0.16004900	2.04011400	1.11850900
C	2.63927400	0.23705800	-0.61844000
H	2.62267800	1.32456500	-0.71246000
H	2.71351900	-0.17602000	-1.62544000
I	-4.73521600	0.16356500	-0.17637400
C	3.80223900	-0.22587400	0.26225200
H	3.71831400	0.16997000	1.27408400
H	3.84006100	-1.31253100	0.32603700

C	5.13128600	0.23508300	-0.28262300
F	5.21334600	1.58242800	-0.36096900
F	6.14979200	-0.17740400	0.50075900
F	5.36904000	-0.24241600	-1.52488900

PRODUCT COMPLEX

E_{el} = -1401.329215 Hartree

P	0.79014000	0.50323300	0.52976400
O	0.73466100	1.57362600	-0.63832700
O	0.25506600	-0.80997400	-0.19979900
O	0.05950600	0.83951600	1.76957000
C	-0.53110600	2.07949000	-1.12143300
H	-1.05514500	2.60318400	-0.32236800
H	-0.29673800	2.77005300	-1.92654300
H	-1.14764900	1.26299600	-1.49613500
C	-3.34912600	0.84524700	1.38821900
H	-2.27643900	0.80489900	1.54698900
H	-3.90015700	0.41301100	2.21596000
H	-3.68836700	1.85094800	1.16611900
C	-0.24040900	-1.94463200	0.54307400
H	-0.93616300	-2.46379700	-0.10998300
H	0.58892700	-2.60211200	0.80561100
H	-0.75804100	-1.61547000	1.44257900
C	2.56560800	0.29491200	0.75572600
H	2.68447600	-0.47891400	1.51704500
H	2.94400600	1.22692300	1.17834900
I	-3.78460600	-0.36531800	-0.35710300
C	3.31956700	-0.07800100	-0.52114900
H	2.93229200	-1.00040600	-0.95369000
H	3.23655000	0.70722100	-1.27182000
C	4.78912300	-0.29362800	-0.26563400
F	5.01676200	-1.29403500	0.61682300
F	5.44595000	-0.61642000	-1.40145800
F	5.39158300	0.80925000	0.23613500

<u>Reaction $P(OMe)_3 + CF_3(CH_2)_3I$</u>

SUBSTRATE COMPLEX

E_{el} = -1440.602912 Hartree

P	-3.18966100	0.14978100	0.24347600
O	-2.49647900	-0.92039300	-0.78433800
O	-4.74196500	-0.29388500	-0.00203900
O	-3.15648000	1.45412300	-0.73688800
C	-2.35814600	-2.28466700	-0.35572300
H	-3.28667200	-2.83063100	-0.52877800

H	-1.55742900	-2.72914300	-0.94357000
H	-2.09847700	-2.34751900	0.70484000
C	-2.05046100	2.36598500	-0.66442200
H	-1.26040300	2.05386200	-1.34949600
H	-2.41661400	3.34742300	-0.95954600
H	-1.64572800	2.42499800	0.34917200
C	-5.76288000	0.26949400	0.83674100
H	-6.07377500	1.24353400	0.45432300
H	-6.60941100	-0.41405200	0.81770600
H	-5.41545300	0.38182800	1.86733800
C	1.30707000	0.62046000	0.91085200
C	0.66182200	-0.71097000	0.58998600
H	0.18059400	-1.14486900	1.46019900
H	-0.04849400	-0.64307000	-0.22777000
I	2.08086800	-2.25318800	-0.05115500
H	2.04722100	0.50627300	1.70353600
H	0.50870300	1.25446500	1.31037300
C	1.93434000	1.30531700	-0.30140000
H	2.81609400	0.76512400	-0.64678600
H	1.22923800	1.35477300	-1.13242500
C	2.36472800	2.71732700	-0.00974400
F	3.26095300	2.78682600	1.00227300
F	2.94521600	3.29500100	-1.08570300
F	1.32384000	3.51070800	0.34213600

TS1

E_{el} = -1440.574658 Hartree

P	-2.51752900	-0.42860600	-0.01472200
O	-3.21915200	-1.06014500	-1.31426300
O	-3.27358900	-1.23002900	1.15595900
O	-3.26890700	0.99164000	0.07012200
C	-2.81256400	-2.35057800	-1.82176100
H	-3.16426400	-3.14118900	-1.15913100
H	-3.27508200	-2.45498500	-2.79939400
H	-1.72809200	-2.40962600	-1.92590500
C	-2.96072000	2.06548400	-0.84583400
H	-3.17551300	1.76488800	-1.87104200
H	-3.60079100	2.89718000	-0.56452100
H	-1.91759500	2.36824600	-0.75547400
C	-2.88890000	-1.06423300	2.53809600
H	-3.18666400	-0.07912000	2.89725500
H	-3.41331300	-1.83456200	3.09681800
H	-1.81320000	-1.19473600	2.66511200
C	0.46528100	0.72842700	0.61700300
C	0.08969200	-0.64769600	0.13912300
H	-0.13840100	-1.42665300	0.84290200
H	0.01413400	-0.87814200	-0.90669000

I	2.56250900	-1.80941300	-0.03433500
H	1.18820100	0.63245400	1.42655800
H	-0.40523300	1.21502700	1.06026900
C	1.03384800	1.59996100	-0.50074600
H	1.97941500	1.19205300	-0.85789500
H	0.35224200	1.65348000	-1.35087700
C	1.28857300	3.01419200	-0.05496700
F	2.14125600	3.08097600	0.99249100
F	1.82376000	3.75977600	-1.04571800
F	0.15010100	3.64131200	0.33351000

SALT

E_{el} = -1440.649087 Hartree

P	2.20135400	-0.88103000	0.16243200
O	3.23579500	0.05036300	-0.52652300
O	2.07278400	-0.65416000	1.69258900
O	2.80705700	-2.30907000	0.11672000
C	3.10109400	1.45942300	-0.88860500
H	3.53832500	2.05334800	-0.09056400
H	3.65950700	1.58380000	-1.81054200
H	2.05712300	1.73038700	-1.03537000
C	3.31991900	-2.93920100	-1.09556800
H	4.06662200	-2.29586800	-1.55493900
H	3.76825400	-3.87055200	-0.76712400
H	2.49951500	-3.13665900	-1.78259900
C	1.52054200	0.53400100	2.34135500
H	1.13691100	0.19251500	3.29703500
H	2.32484000	1.25098600	2.48609800
H	0.72063000	0.97289800	1.74589700
C	-0.48082000	-1.59948400	0.02752800
C	0.61855400	-0.76788400	-0.64672700
H	0.33340400	0.29030400	-0.66228400
H	0.77423200	-1.06725200	-1.68676900
I	-0.90886000	2.82843700	-0.15787100
H	-0.57257700	-1.31310400	1.07581700
H	-0.22587200	-2.65945300	0.00144100
C	-1.81595200	-1.36296200	-0.67820100
H	-2.08087800	-0.30437500	-0.64907200
H	-1.76972500	-1.67250300	-1.72305500
C	-2.94579900	-2.12564800	-0.04015000
F	-3.13060500	-1.78245500	1.25633200
F	-4.11804600	-1.90131000	-0.67444200
F	-2.74150000	-3.46431600	-0.05893100

TS2

E_{el} = -1440.625467 Hartree

P	-0.57765900	0.12518400	-0.17435400
O	-0.72604700	1.63576200	0.22878400
O	-0.47670000	-0.60348500	1.22543100
O	0.58441300	-0.20457500	-1.07690200
C	0.26665100	2.35336900	1.00641600
H	1.17089400	2.49241200	0.41596800
H	-0.17510400	3.31709500	1.23955200
H	0.48771400	1.81071300	1.92402700
C	2.45266500	-0.13846100	-0.61019700
H	2.33058100	-0.14460700	0.45720600
H	2.64227000	-1.06207800	-1.12195000
H	2.60476600	0.79287800	-1.12104400
C	-0.10223100	-1.99723100	1.36451800
H	0.31962300	-2.10232500	2.35972700
H	-0.98905200	-2.62122400	1.26556800
H	0.63759500	-2.27274100	0.61476300
C	-2.12814000	-0.26648500	-0.97950100
H	-2.07218500	-1.32531900	-1.24449500
H	-2.13905900	0.29463500	-1.91694100
I	5.20670900	-0.07835100	-0.07145500
C	-3.37141000	0.03096600	-0.13457500
H	-3.32280200	-0.52017300	0.80555300
H	-3.40230400	1.09234900	0.11254100
C	-4.64129900	-0.35896000	-0.89100500
H	-4.64219500	-1.42203900	-1.13643600
H	-4.73029400	0.20029700	-1.82332700
C	-5.89219600	-0.09156100	-0.09649100
F	-7.00332200	-0.43860100	-0.78462200
F	-5.92134000	-0.78415500	1.06635600
F	-6.02741700	1.21537300	0.22918000

PRODUCT COMPLEX

E_{el} = -1440.661911 Hartree

P	-0.29816000	-0.84463300	0.54257900
O	-0.35636200	-1.42908700	-0.93193100
O	0.06541100	0.68628600	0.26701100
O	0.63122300	-1.51611700	1.47739100
C	0.84804000	-1.59590400	-1.71241000
H	1.49935600	-2.33434500	-1.24548300
H	0.53264500	-1.94767100	-2.69078500
H	1.37352700	-0.64599300	-1.80970400
C	3.90693900	-1.33152500	0.59683100
H	2.87465700	-1.43999400	0.91383000
H	4.59645200	-1.36276300	1.43308200
H	4.17779400	-2.05023300	-0.16864100
C	0.55270700	1.54216600	1.32045600
H	0.97638200	2.41757600	0.83578600

H	-0.26978600	1.84299500	1.97142400
H	1.32288000	1.03409000	1.89839500
C	-2.02550000	-0.90039200	1.04504500
H	-2.05801600	-0.45830400	2.04471000
H	-2.28546800	-1.95558100	1.15859600
I	4.08768200	0.63623000	-0.29516200
C	-2.99739200	-0.18756500	0.10105100
H	-2.69739100	0.85464600	-0.01732000
H	-2.95552100	-0.64947200	-0.88590300
C	-4.42748500	-0.24941600	0.63745800
H	-4.49999400	0.22507600	1.61741400
H	-4.76455000	-1.28198100	0.74099500
C	-5.41606400	0.44651600	-0.25919200
F	-6.67300700	0.38541600	0.23849000
F	-5.12742900	1.75923400	-0.42513100
F	-5.46260600	-0.09694700	-1.49854600

Reaction $P(OMe)_3 + CH_3I$

SUBSTRATE COMPLEX

E_{el} = -1024.736927 Hartree

P	-1.81132600	0.01576900	0.52081600
O	-1.56186500	-0.66548600	-0.95513600
O	-3.30882400	-0.46115400	0.91020600
O	-2.16557100	1.51699300	-0.02070800
C	-1.05592600	-2.00646600	-1.01413800
H	-1.87492200	-2.72507300	-0.94046400
H	-0.55607000	-2.12410700	-1.97375900
H	-0.33577300	-2.19855700	-0.21455200
C	-1.09999200	2.35652900	-0.48859900
H	-0.77422000	2.04350900	-1.48206400
H	-1.49047900	3.37120600	-0.53533900
H	-0.24439200	2.32890700	0.19111300
C	-4.43236600	-0.35301000	0.01064600
H	-4.17394000	-0.73957400	-0.97550000
H	-5.23539500	-0.94851900	0.43939600
H	-4.74783100	0.68653800	-0.07518400
C	1.94220300	-0.53695500	1.85089200
H	0.87532900	-0.40648000	1.99651300
H	2.23985600	-1.57397800	1.95838000
H	2.52320000	0.11536800	2.49303300
I	2.36096400	0.03869500	-0.19474600

TS1

E_{el} = -1024.713058 Hartree

P	1.97355000	0.07236700	-0.08122300
O	2.78203700	-0.43042600	1.22876100
O	2.40043800	-0.89520500	-1.27658300
O	2.83404500	1.38859500	-0.42532200
C	2.26829000	-1.52102200	2.02231200
H	2.44018300	-2.47103100	1.51536000
H	2.81267300	-1.50358700	2.96286900
H	1.20204900	-1.39570500	2.21821000
C	2.81170000	2.52785700	0.46060800
H	3.34157600	2.29610600	1.38426800
H	3.31609800	3.33509000	-0.06380400
H	1.78582500	2.82525200	0.68633400
C	3.78284000	-1.17662100	-1.61726900
H	4.33649400	-1.48208700	-0.73010400
H	3.75931000	-1.98847800	-2.33892900
H	4.24182000	-0.29361600	-2.05864400
C	-0.57358600	0.06669200	-0.04277900
H	-0.50572100	-1.00425700	-0.09404200
H	-0.53078800	0.64782400	-0.94562200
H	-0.54867700	0.56122200	0.91012500
I	-3.19097600	-0.00938500	-0.06376900

SALT

E_{el} = -1024.786924 Hartree

P	-2.31393700	-0.01336700	-0.09696000
O	-2.12869400	0.22985700	1.42951400
O	-2.15069000	-1.49337300	-0.52272400
O	-1.24063300	0.77216200	-0.90484700
C	-0.90593400	-0.07315700	2.17516700
H	-0.02333500	0.11574400	1.56388700
H	-0.91800200	0.58356700	3.03870700
H	-0.94281200	-1.11430200	2.48660600
C	-0.82671600	2.14878000	-0.64925000
H	0.25496200	2.15671200	-0.74305300
H	-1.29725100	2.78162000	-1.39688300
H	-1.11883800	2.45805300	0.35261800
C	-0.88232300	-2.21529000	-0.65441100
H	-0.04275300	-1.52190800	-0.66855600
H	-0.80702300	-2.89742100	0.18796500
H	-0.94225600	-2.76359400	-1.58928000
C	-3.97716200	0.45836500	-0.46051400
H	-4.66331500	-0.18318200	0.09027400
H	-4.14293500	0.35228700	-1.53153700
H	-4.12535500	1.49579600	-0.16254100
I	2.58850800	0.01426000	-0.05010000

TS2

E_{el} = -1024.760547 Hartree

P	2.42240500	-0.03428200	0.29599500
O	2.64281000	1.50402800	0.53913000
O	3.83093600	-0.54954400	-0.19651100
O	1.36385100	-0.36558600	-0.72723000
C	2.91371000	2.41303000	-0.55950500
H	2.13442200	2.32916400	-1.31562200
H	2.91319700	3.41020700	-0.13041500
H	3.88796000	2.18965100	-0.99178600
C	-0.54185000	-0.20247200	-0.40654600
H	-0.74532600	-0.42628400	-1.43618200
H	-0.57112500	-0.99104800	0.32116300
H	-0.50565600	0.82230300	-0.08759400
C	4.01381200	-1.78478300	-0.93290100
H	5.02496400	-1.75092100	-1.32761600
H	3.90462000	-2.63727200	-0.26330600
H	3.29316100	-1.84712600	-1.74566300
C	2.08463700	-0.66364200	1.92729700
H	2.90877900	-0.41753500	2.59474200
H	1.96614900	-1.74553600	1.87308900
H	1.16428500	-0.21980600	2.30546500
I	-3.30630400	-0.02802900	-0.02508300

PRODUCT COMPLEX

E_{el} = -1024.796545 Hartree

P	-2.38561100	-0.01695500	0.15825200
O	-2.33283700	-1.35973700	-0.68875400
O	-1.52181100	0.97547100	-0.74989000
O	-1.89411100	-0.11188300	1.55115000
C	-1.12814800	-2.15689000	-0.72316300
H	-0.83843500	-2.44682400	0.28660100
H	-1.36256000	-3.04120600	-1.30930700
H	-0.31789600	-1.60115400	-1.19526600
C	1.49557600	-0.60600100	1.66534800
H	0.44063900	-0.35098600	1.65172500
H	2.02773500	-0.09906600	2.46247500
H	1.65081000	-1.67851500	1.70272200
C	-1.00664500	2.21081200	-0.21390700
H	-0.50443100	2.03443600	0.73607900
H	-0.29334600	2.58980900	-0.94058200
H	-1.81485500	2.93196100	-0.08045100
C	-4.09812300	0.47369600	-0.01460400
H	-4.38449300	0.48480100	-1.06511600
H	-4.21983000	1.47236800	0.40512400
H	-4.73274600	-0.22145900	0.53370900
I	2.34995600	0.08716300	-0.20270900