

Deoxyfluorinating reagents as tools for γ -amino- α -hydroxyphosphonates modification

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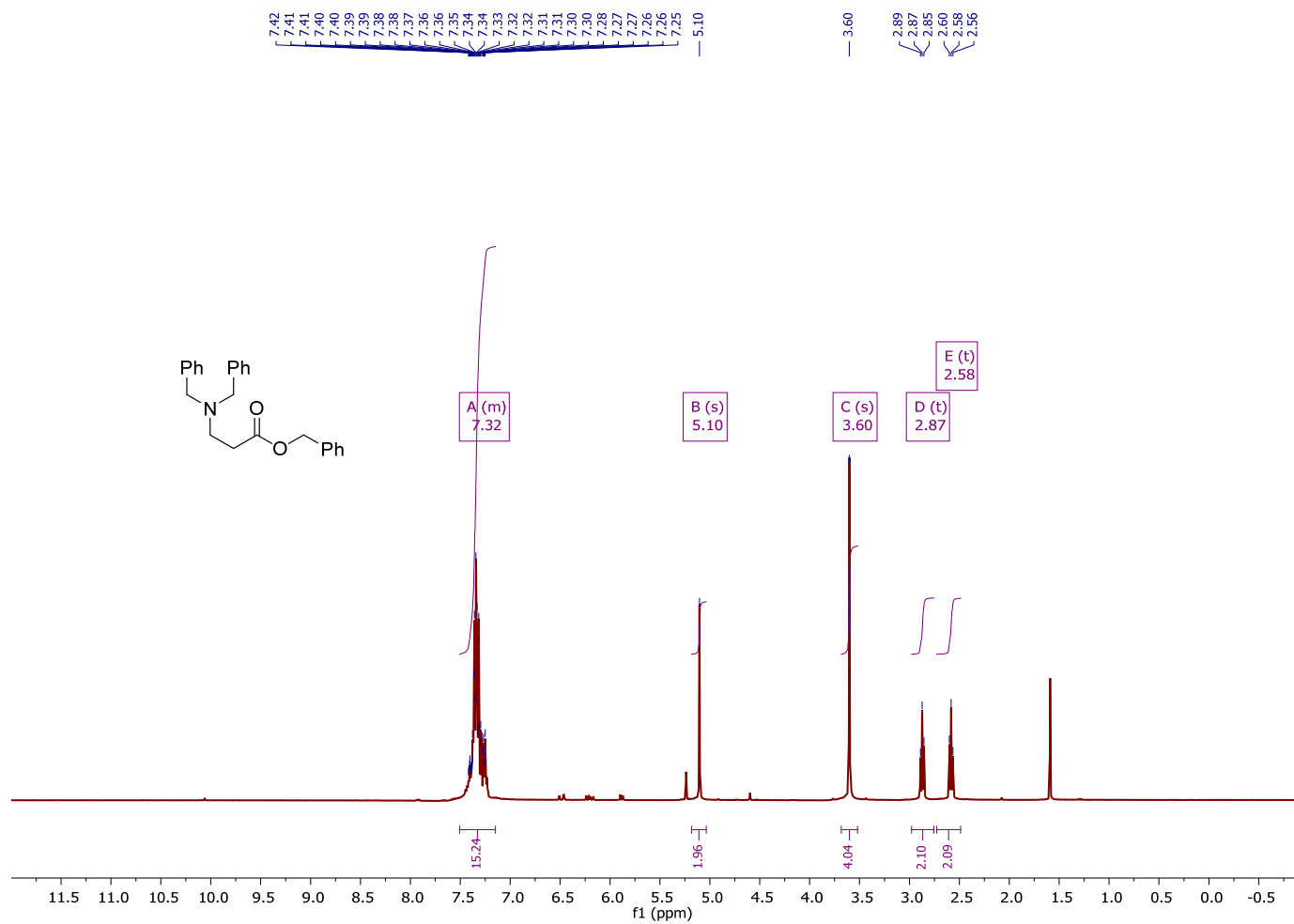
^b*Centre for Advanced Technologies, Adam Mickiewicz University in Poznań, Uniwersytetu
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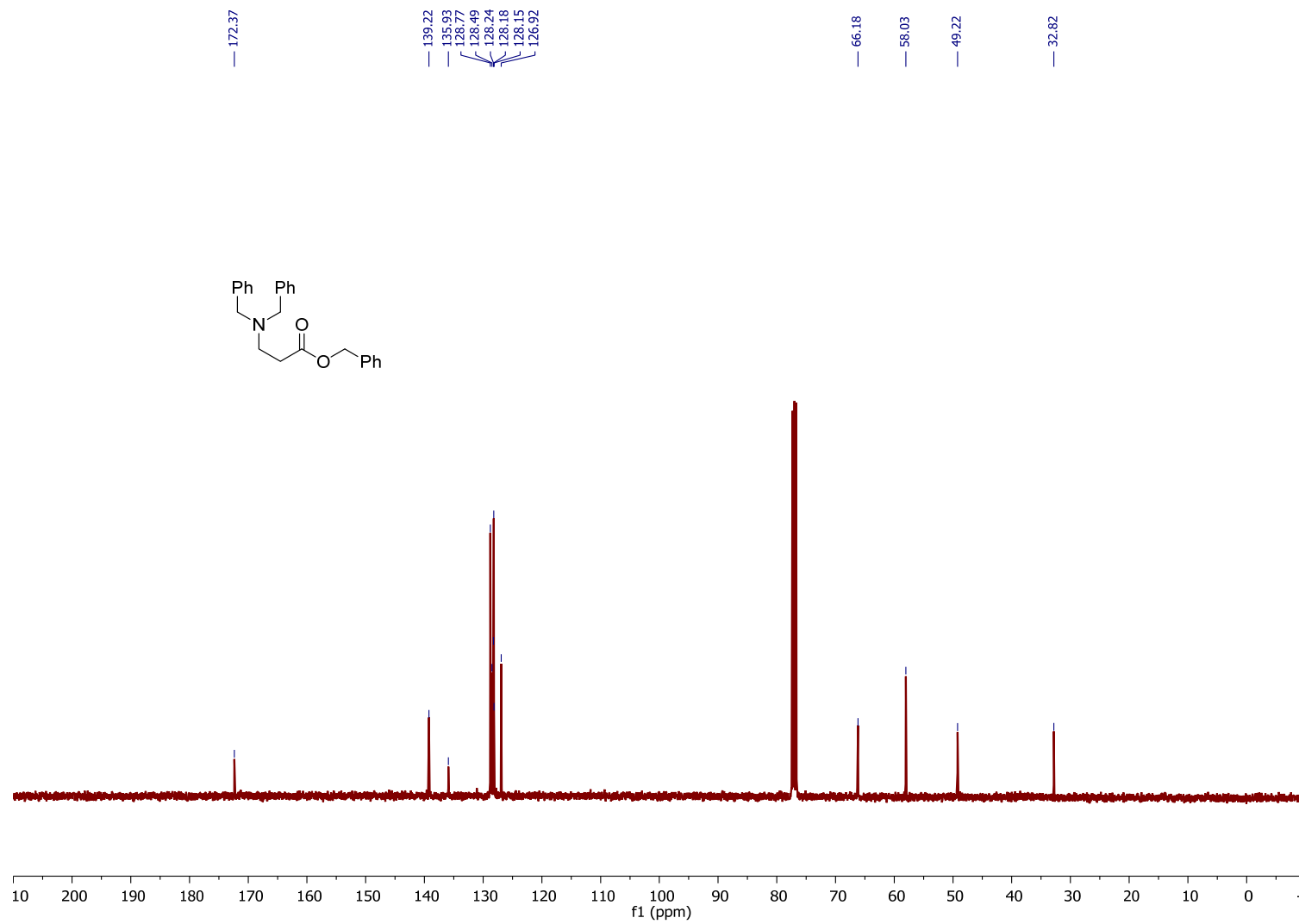
* Corresponding author

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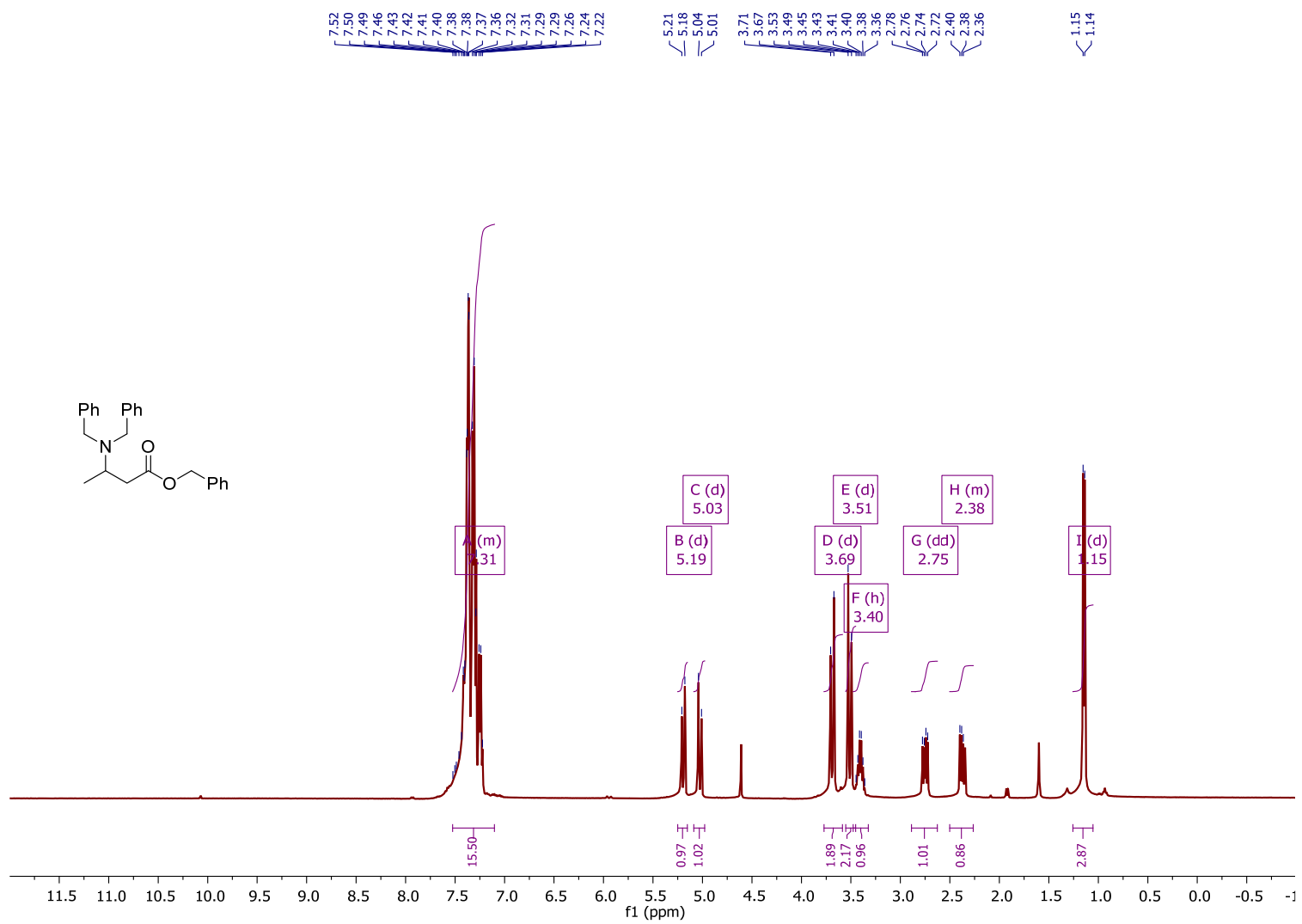
NMR Data:



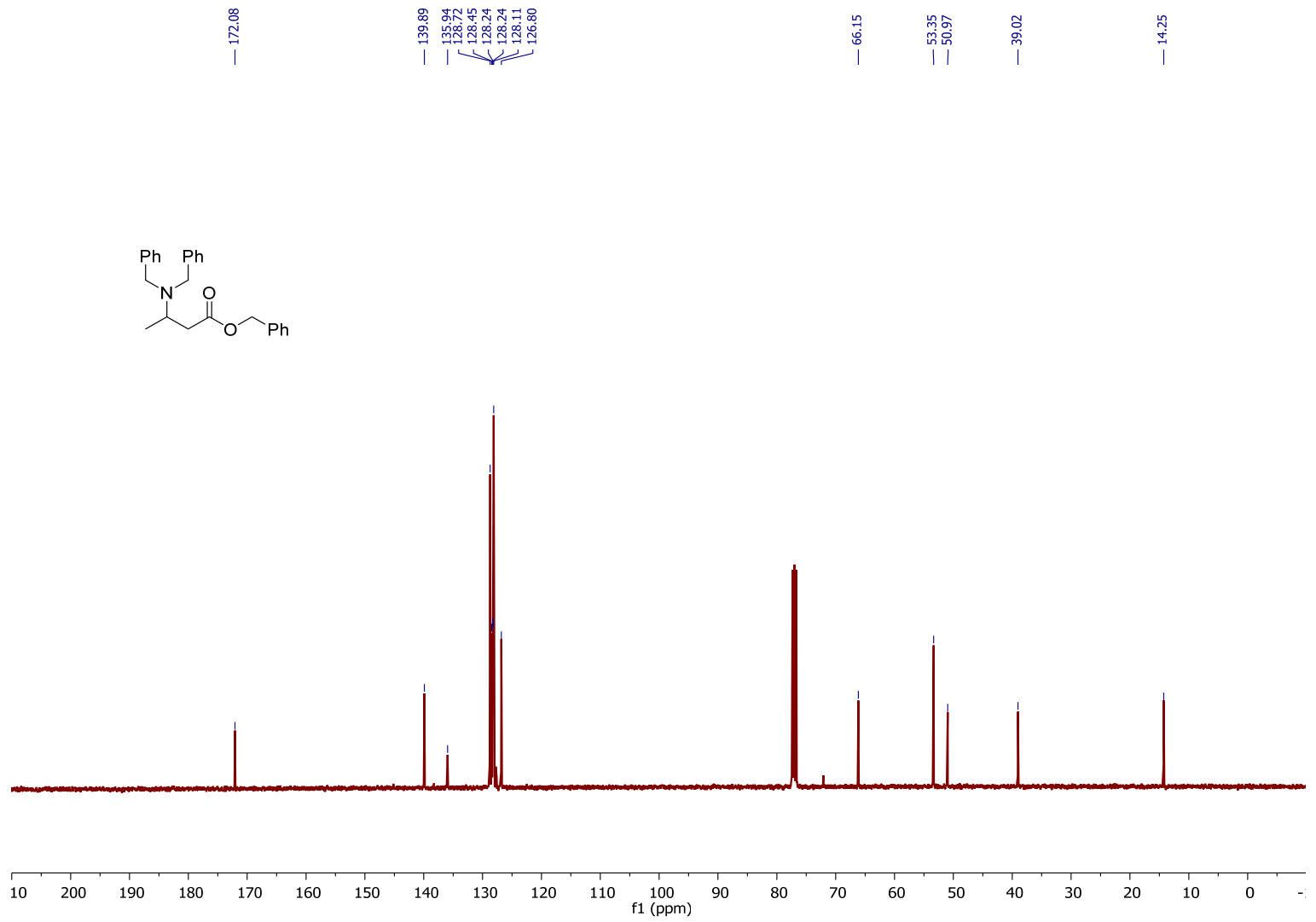
¹H NMR of rac-4a.



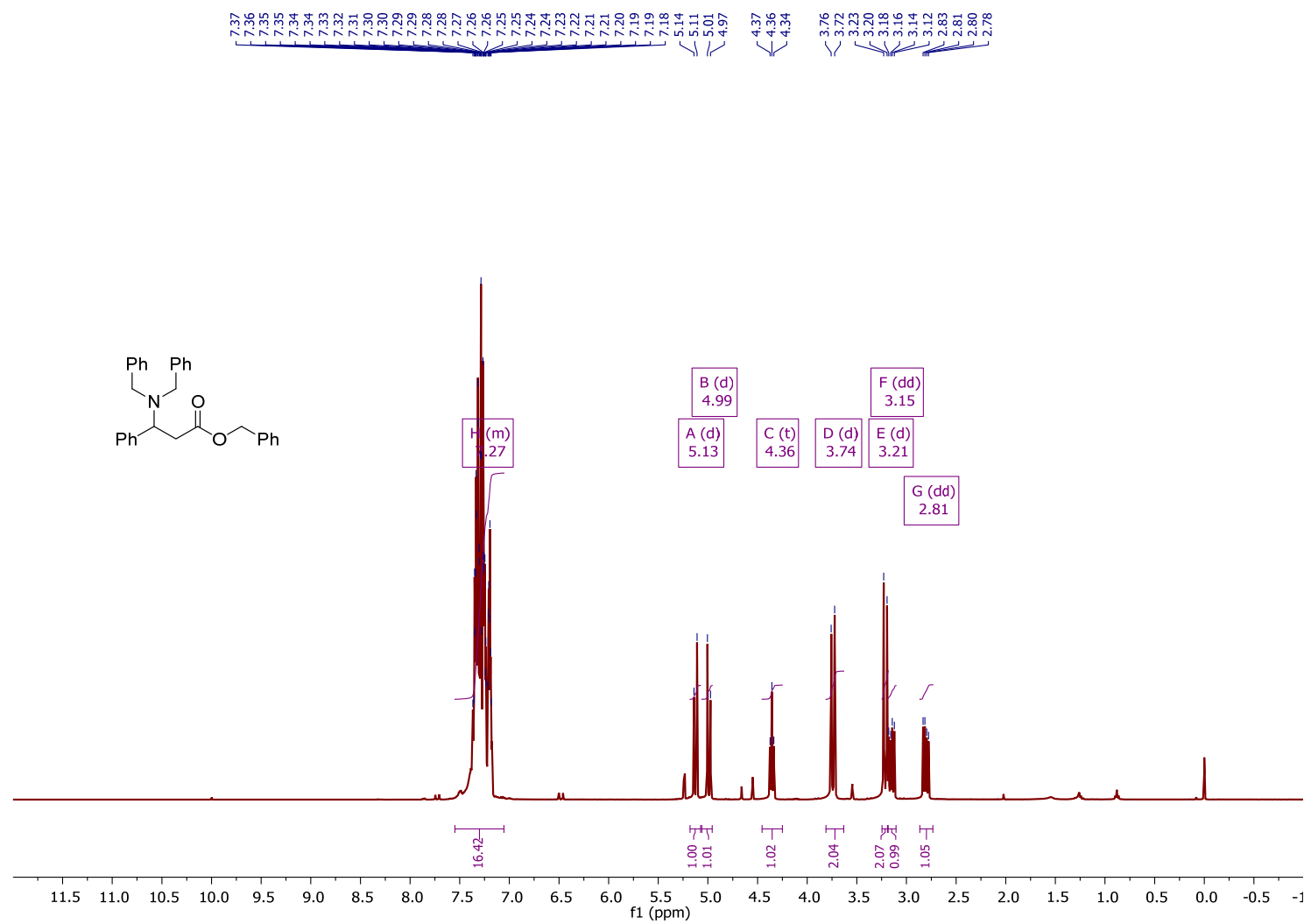
¹³C NMR of rac-4a.



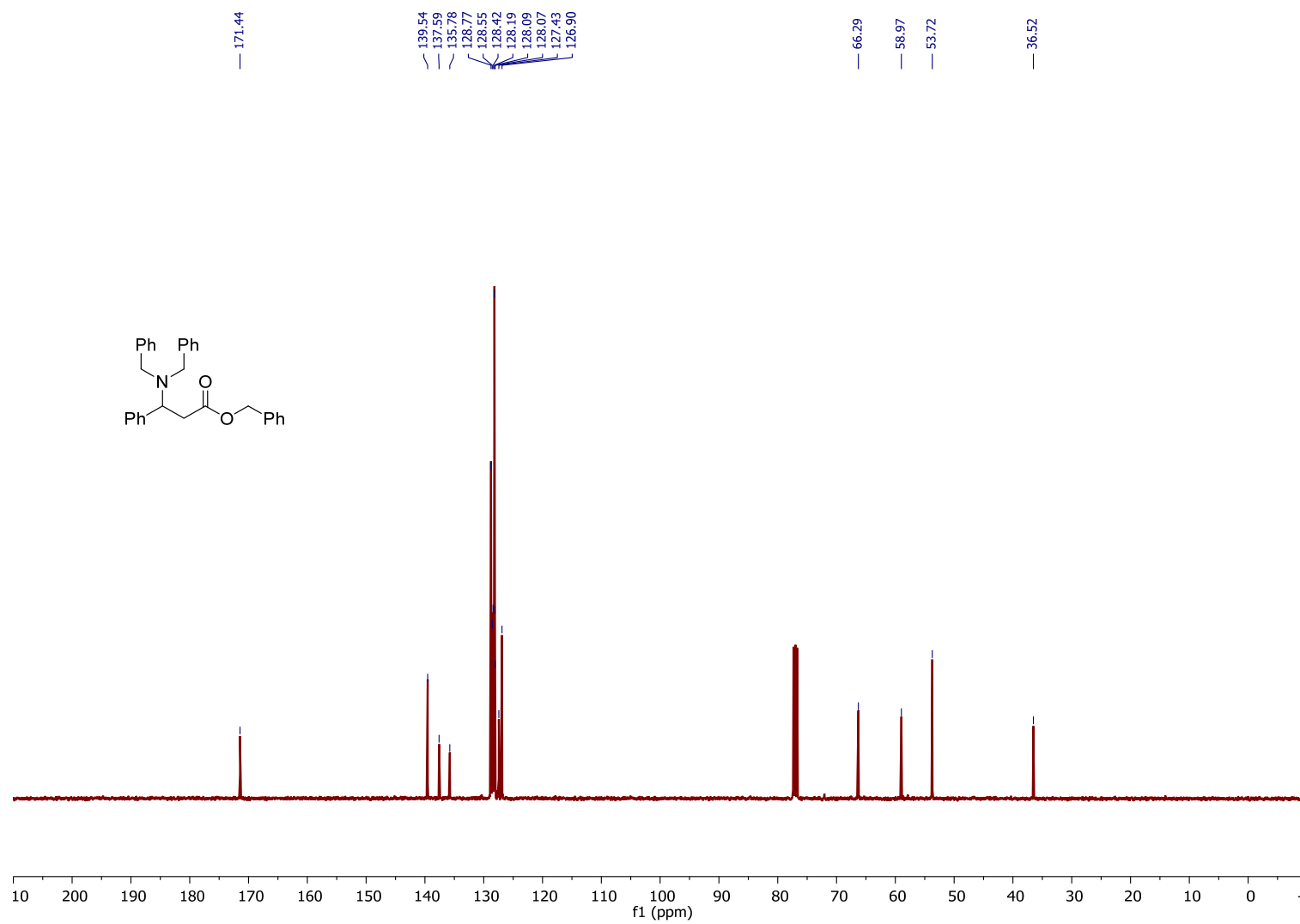
¹H NMR of **rac-4b**.



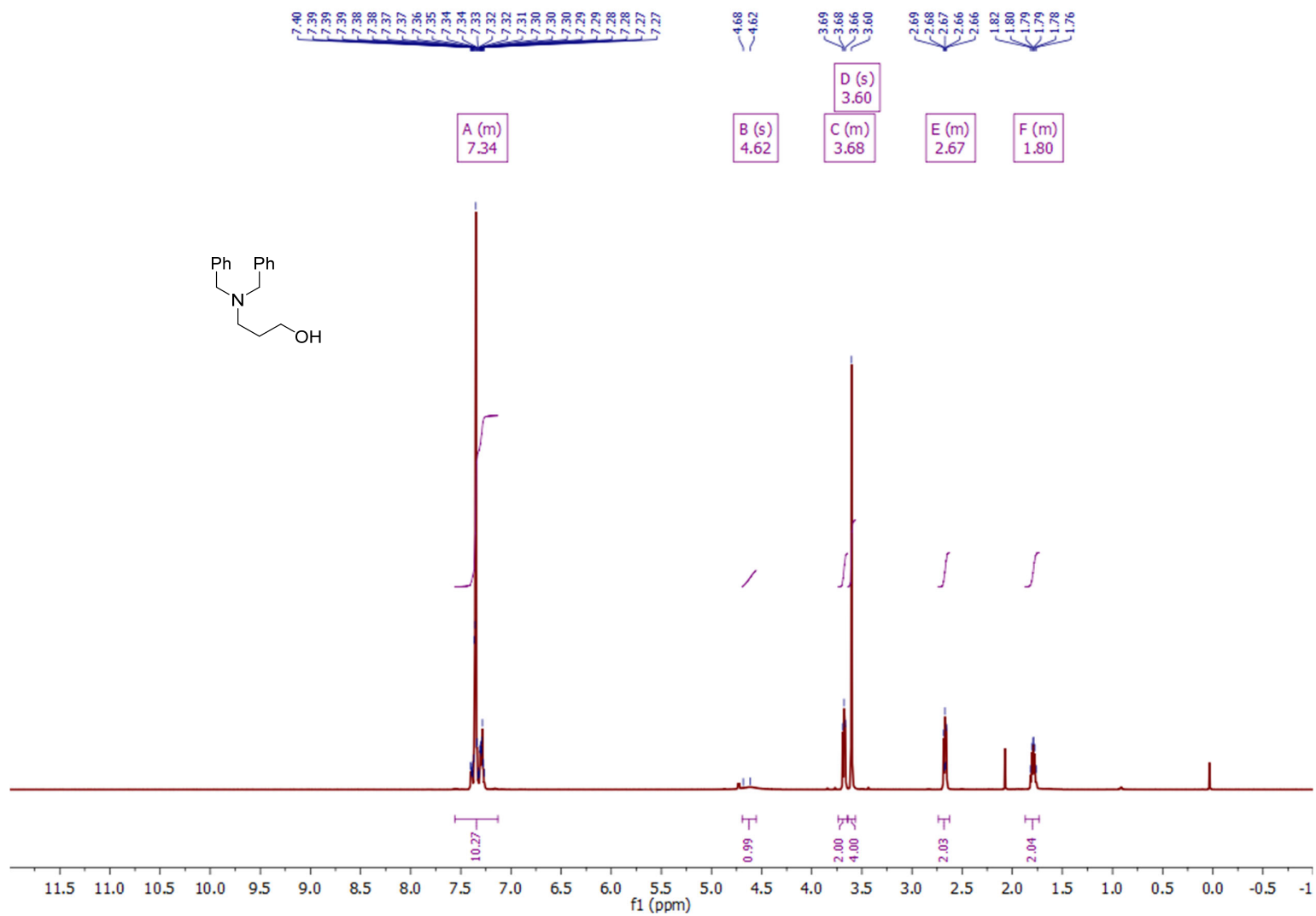
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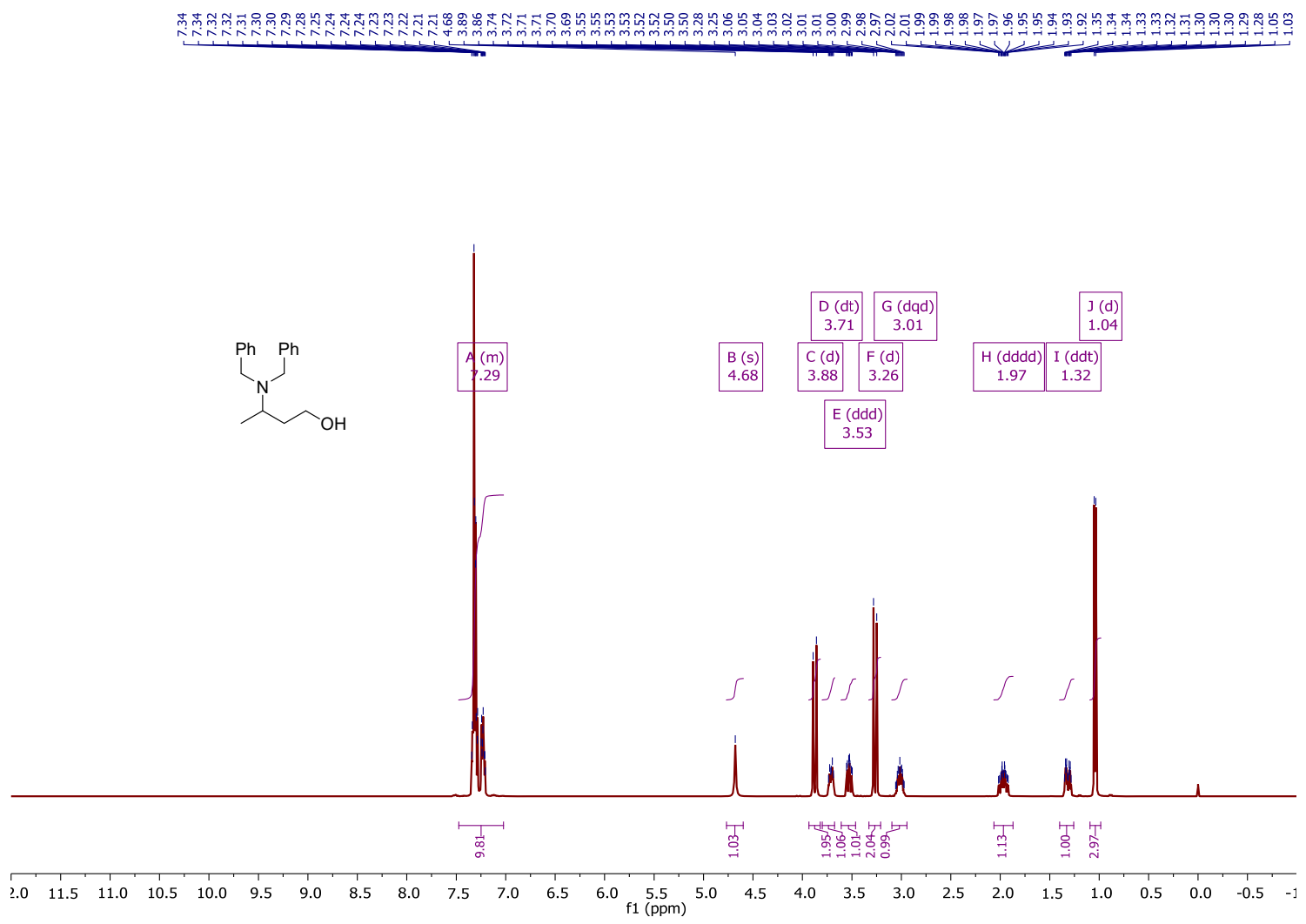
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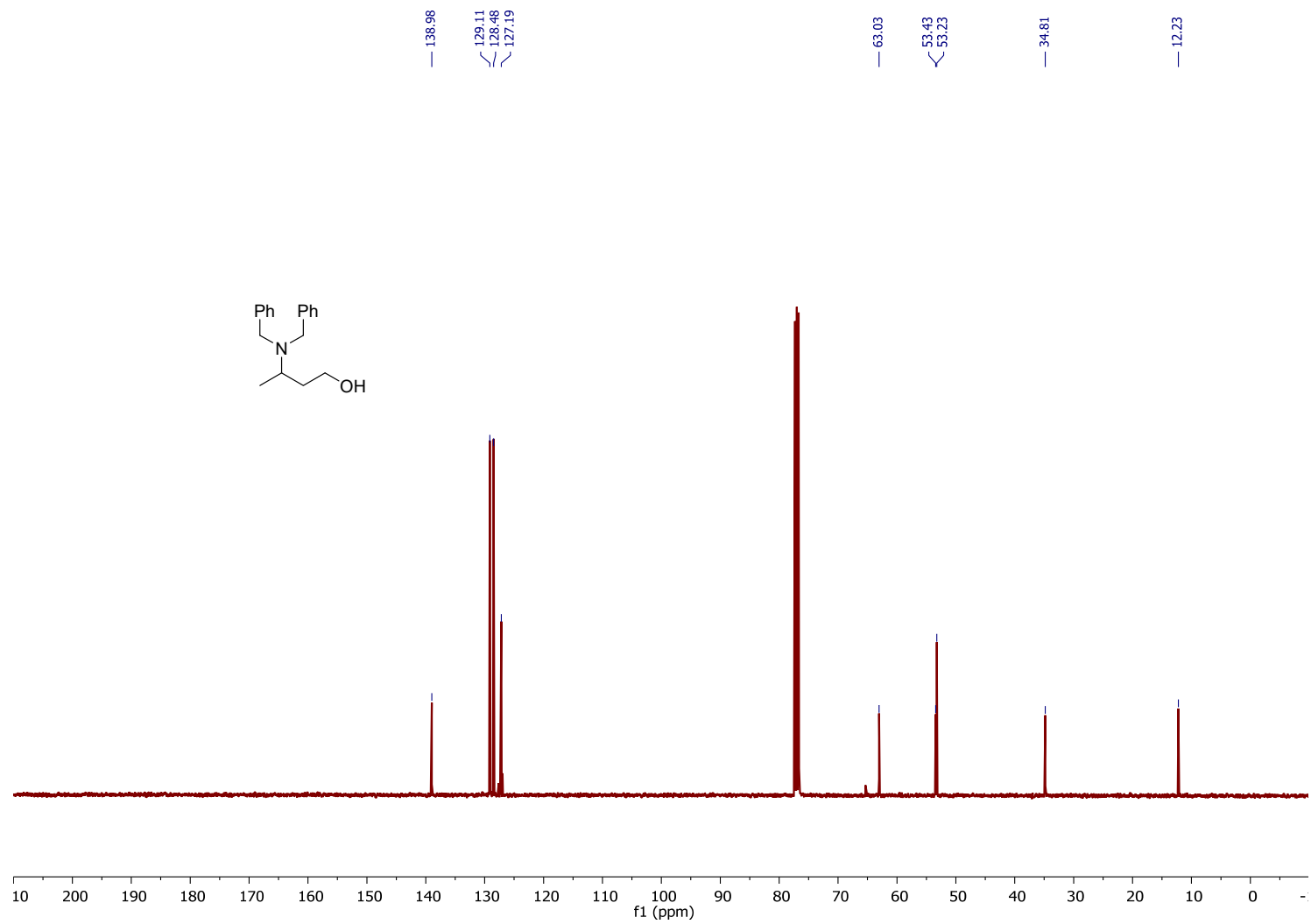
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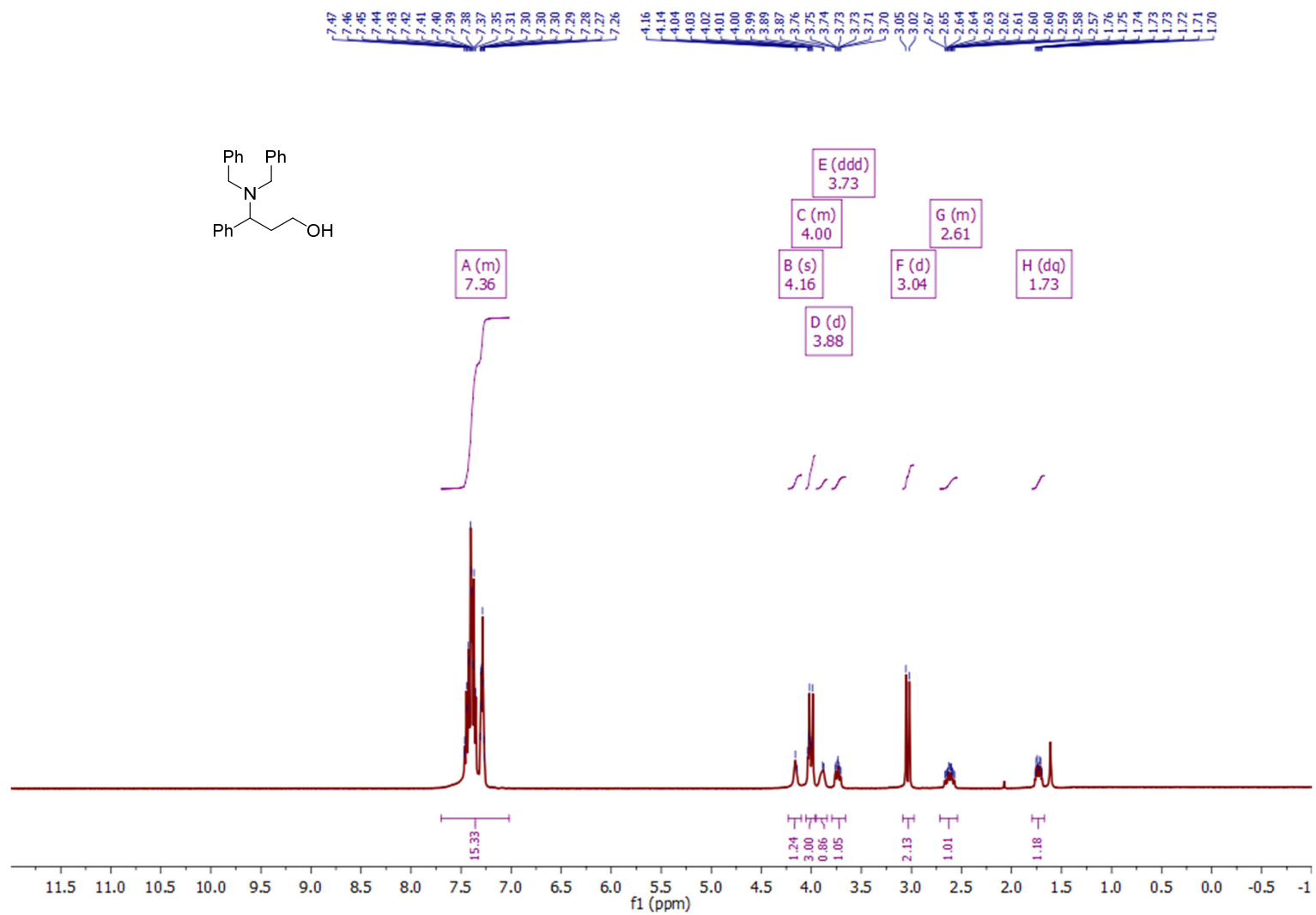
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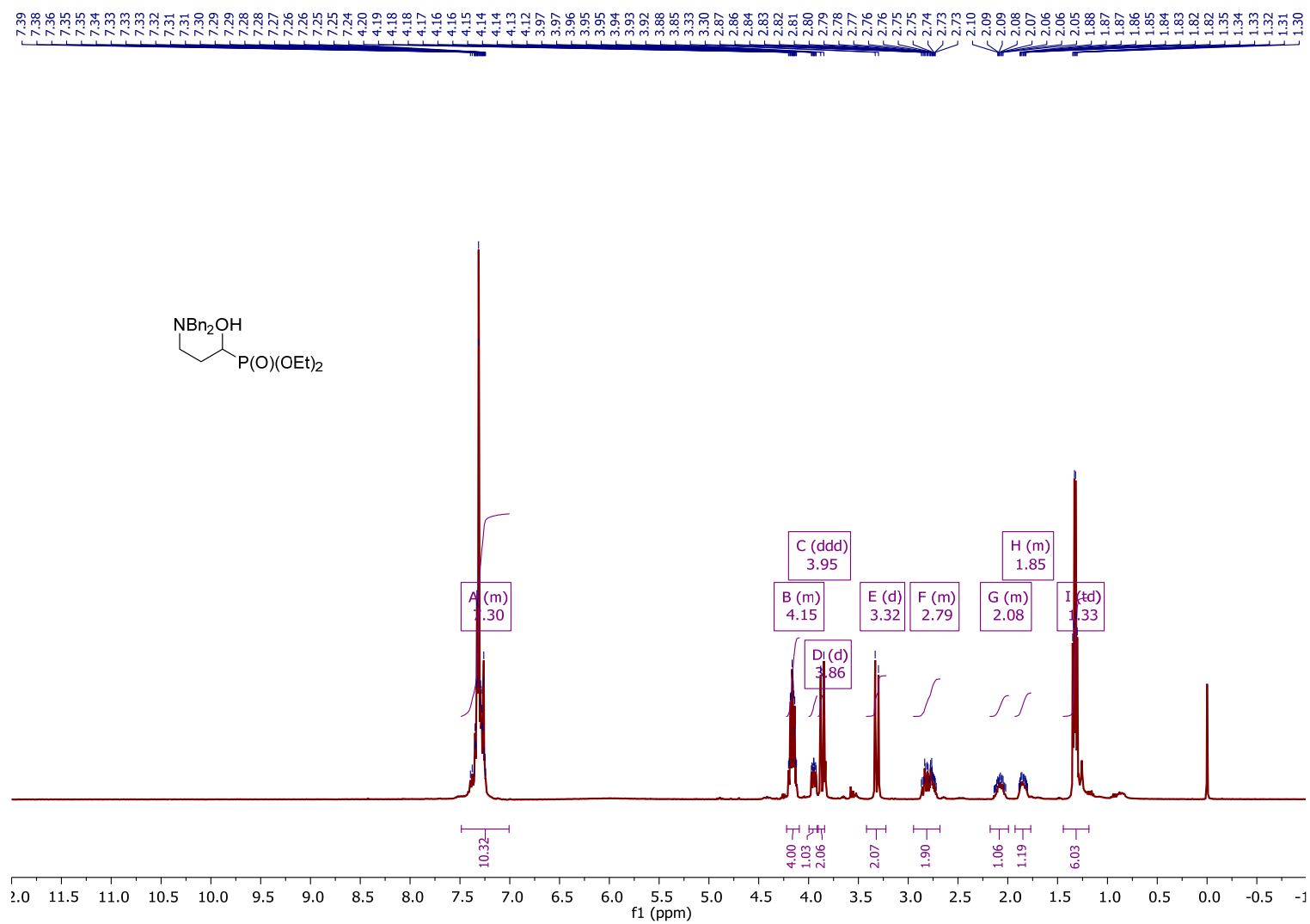
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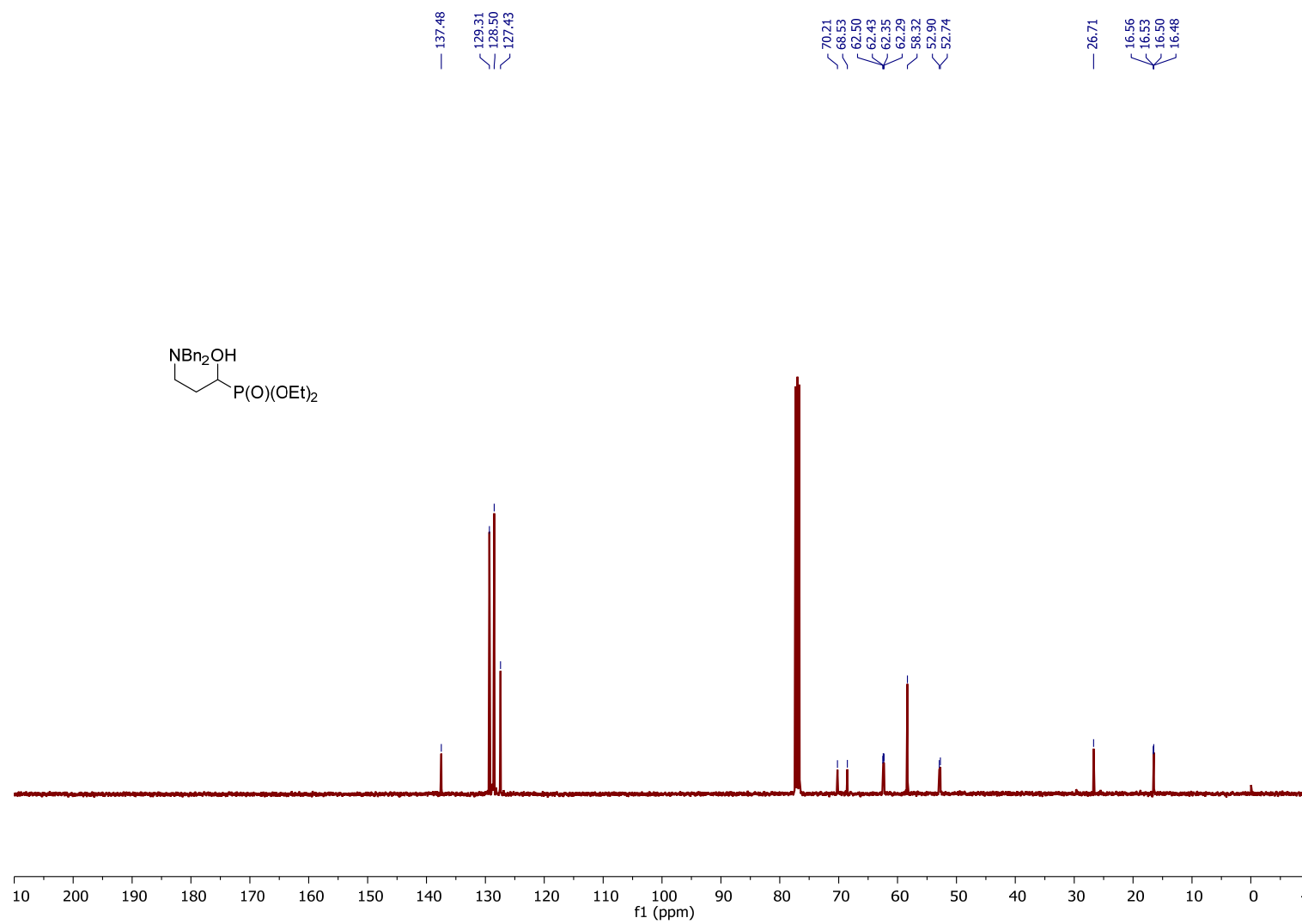
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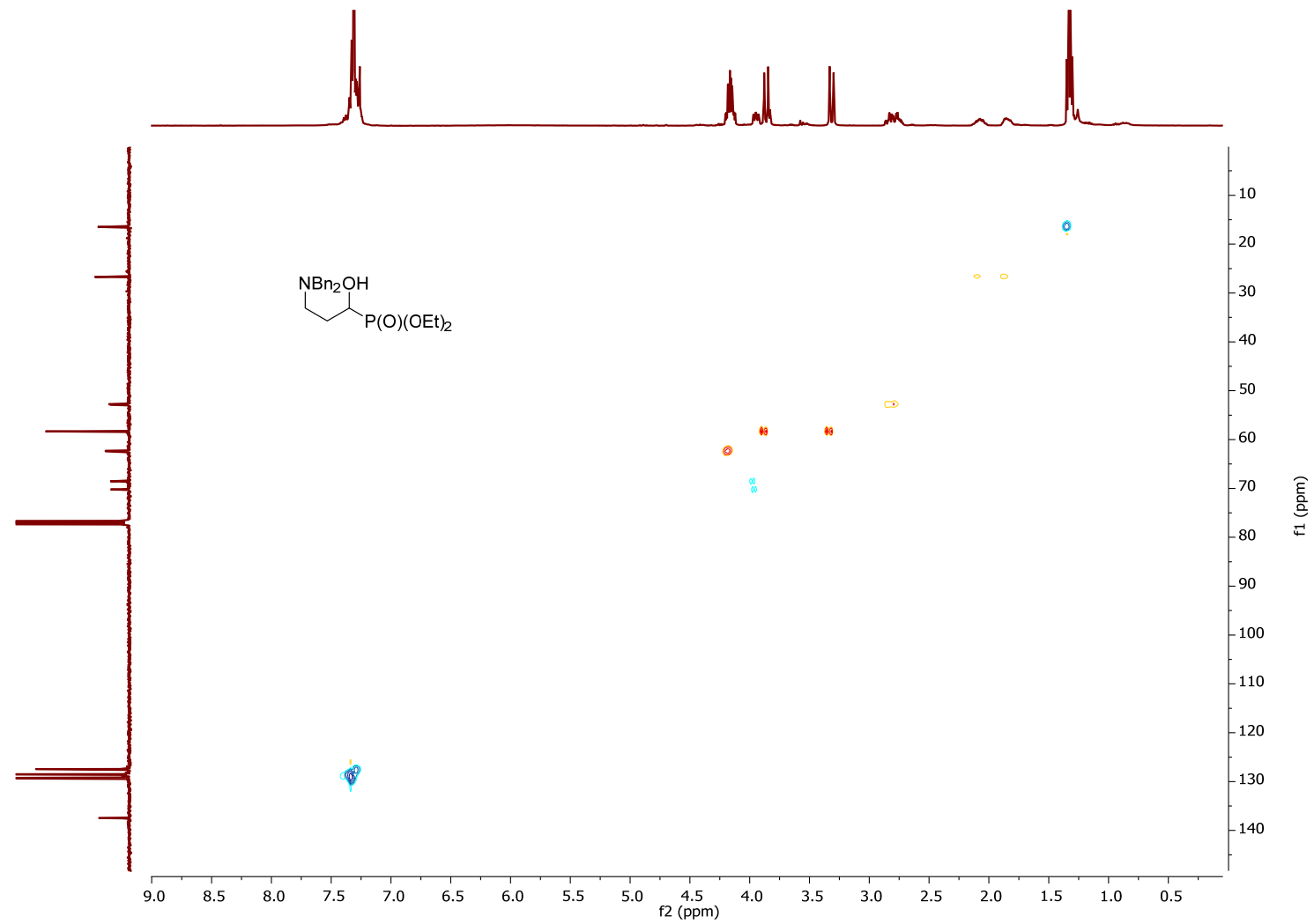
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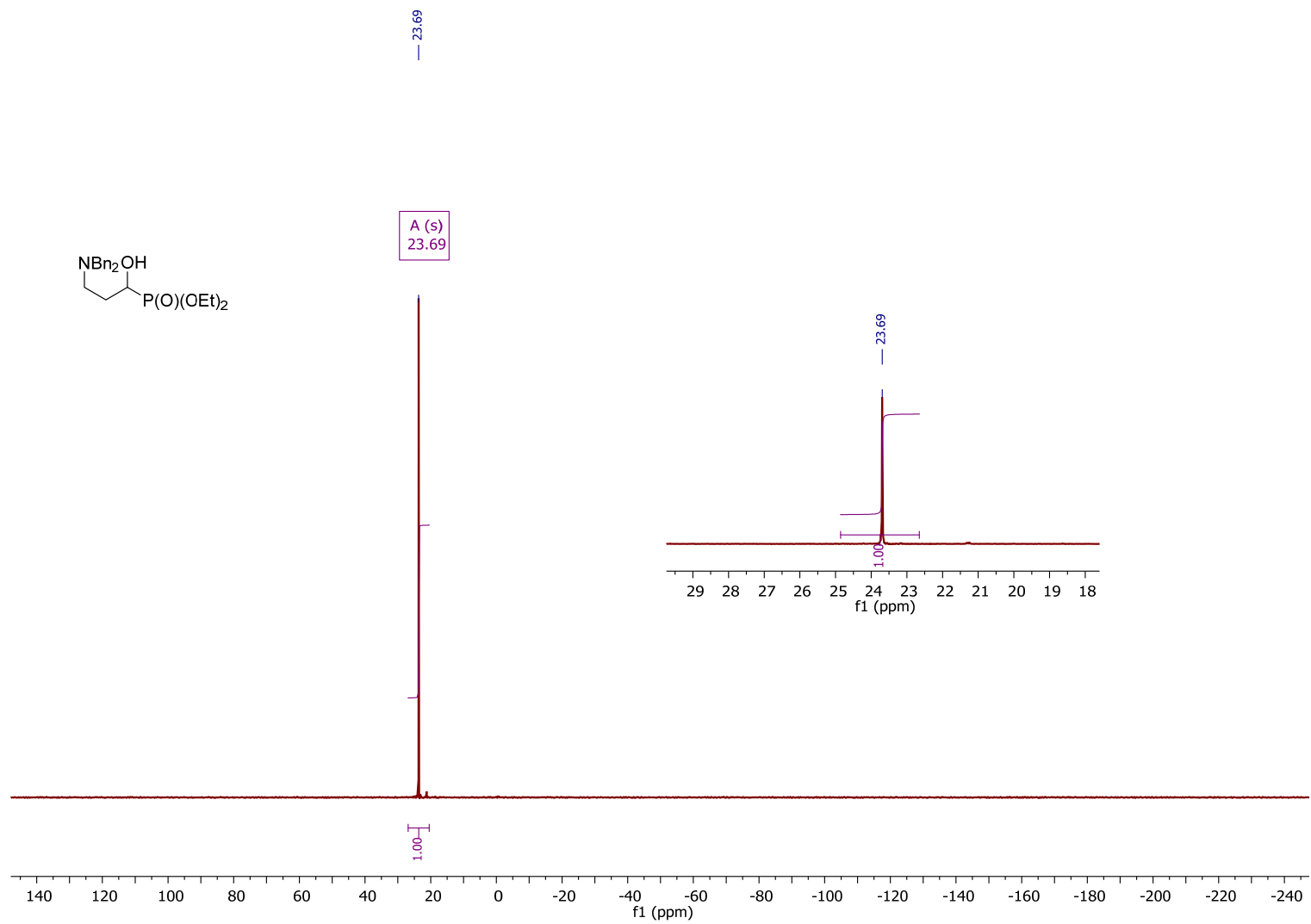
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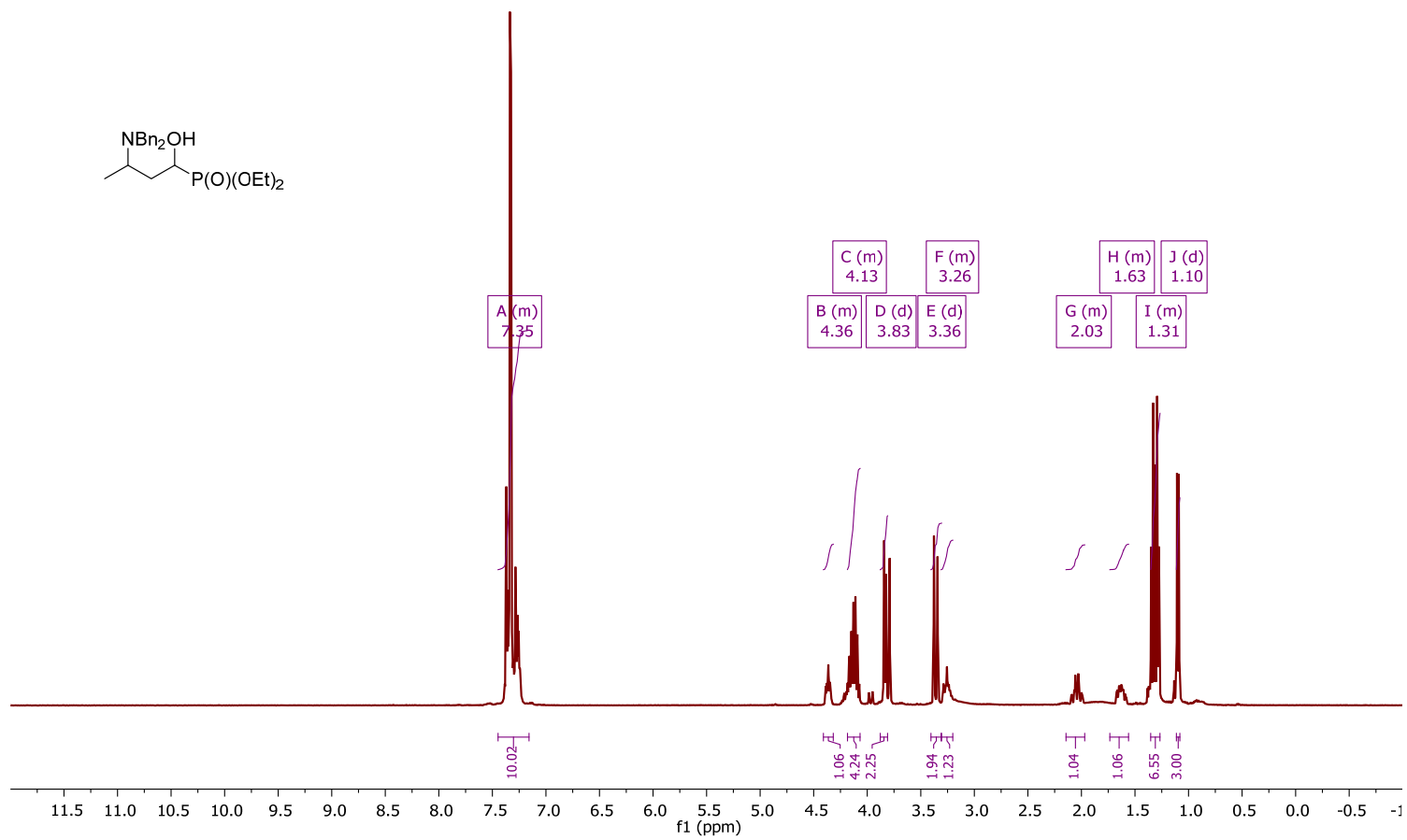
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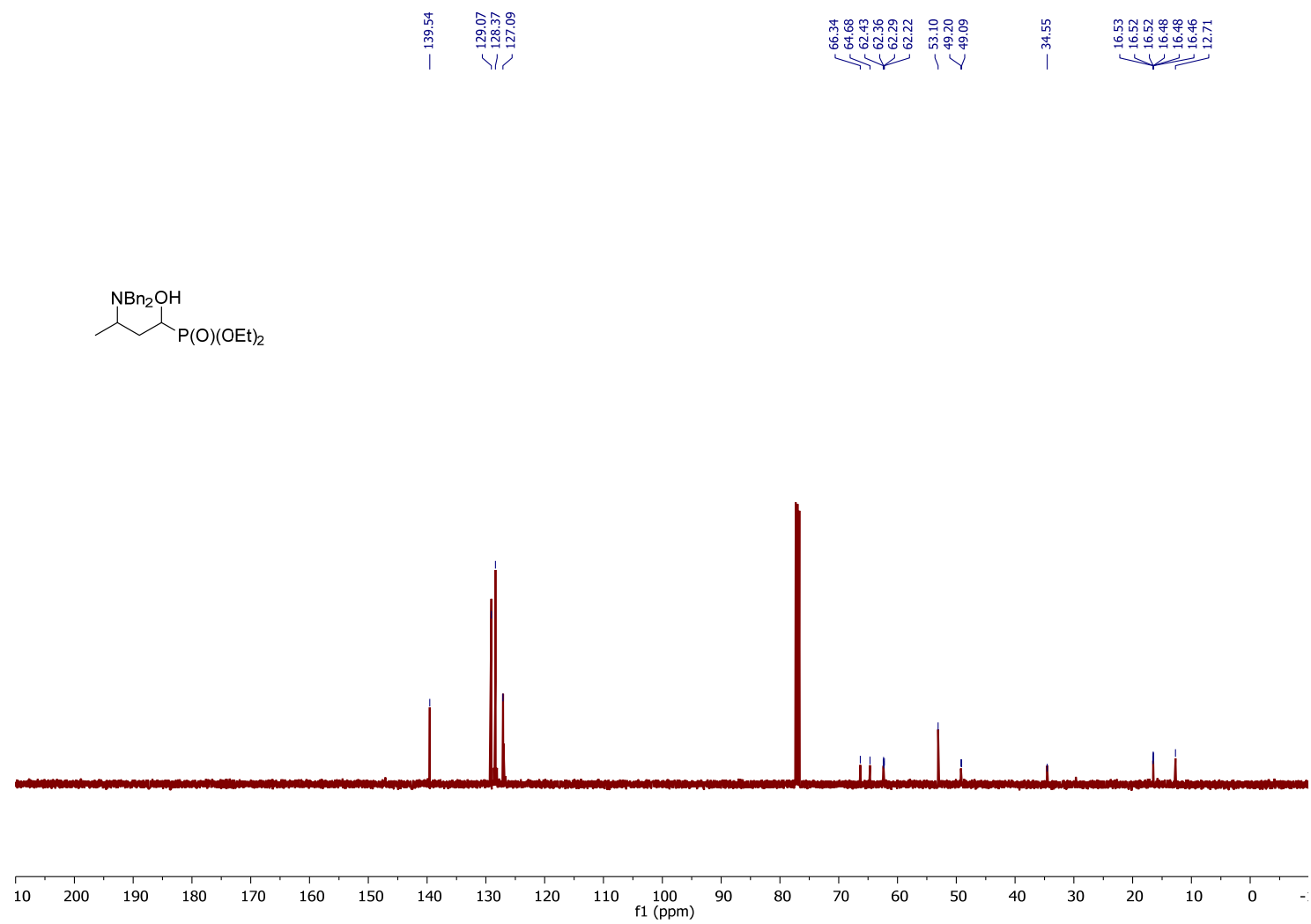
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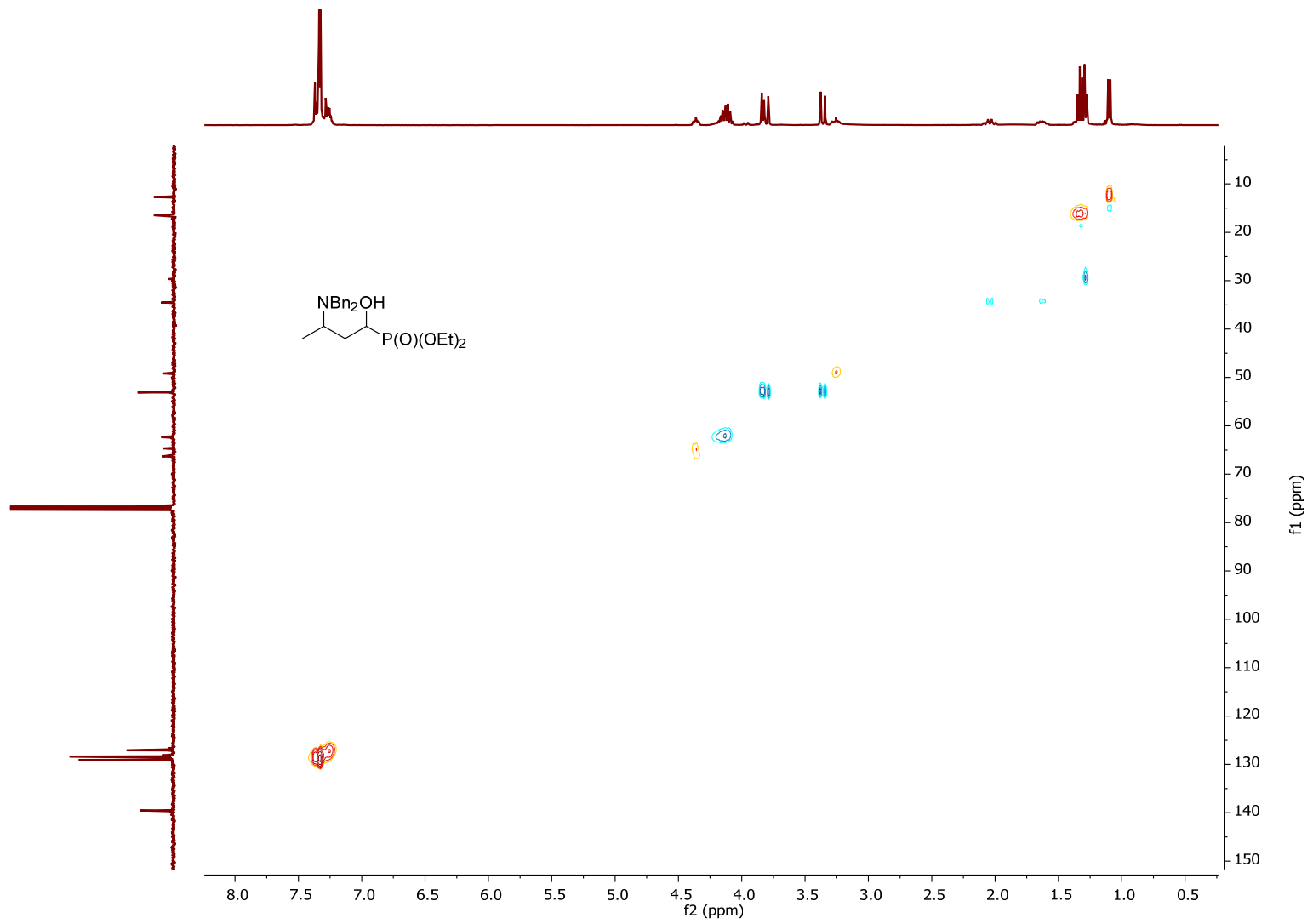
$^{31}\text{P}\{^1\text{H}\}$ NMR of **rac-6a**.



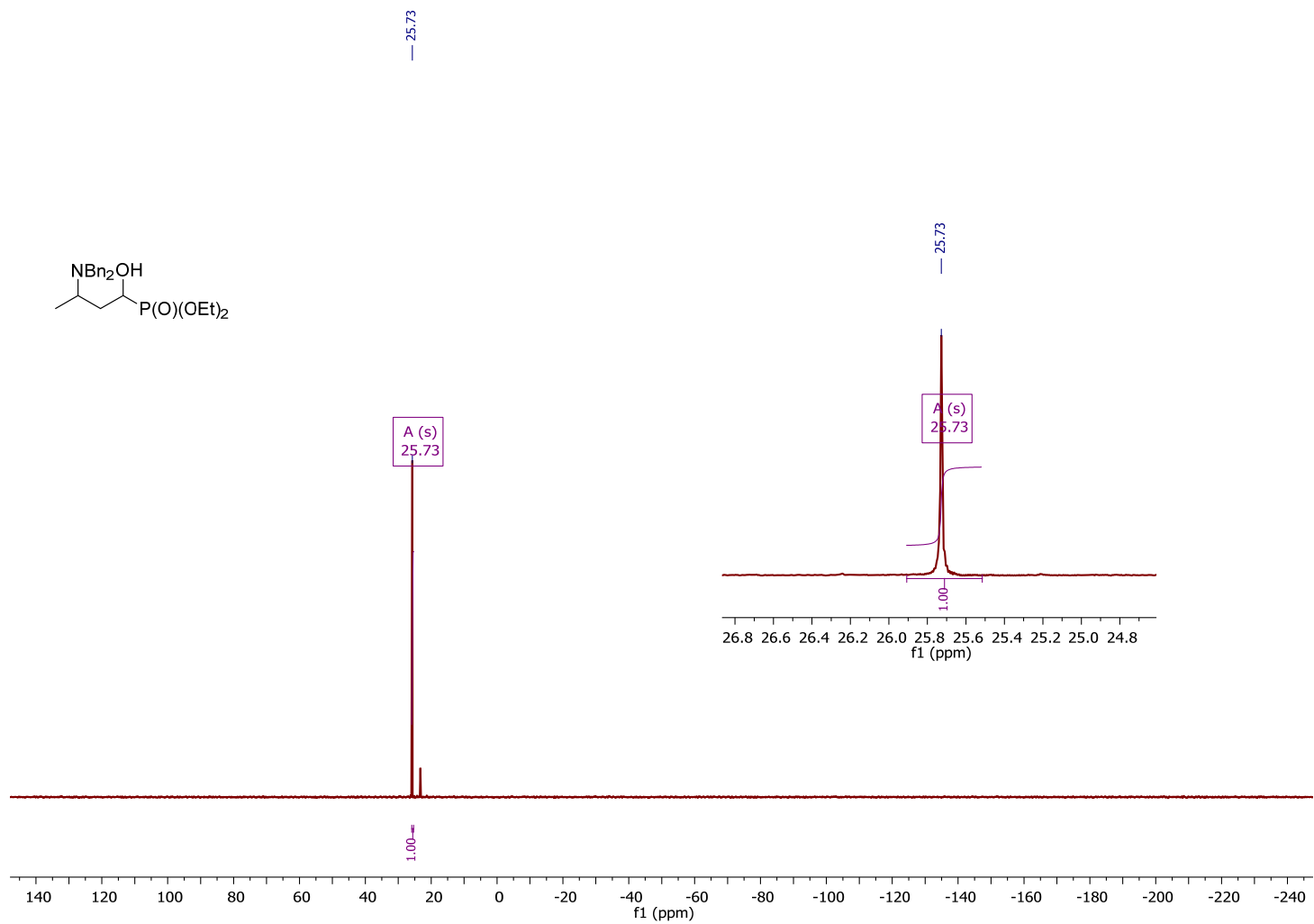
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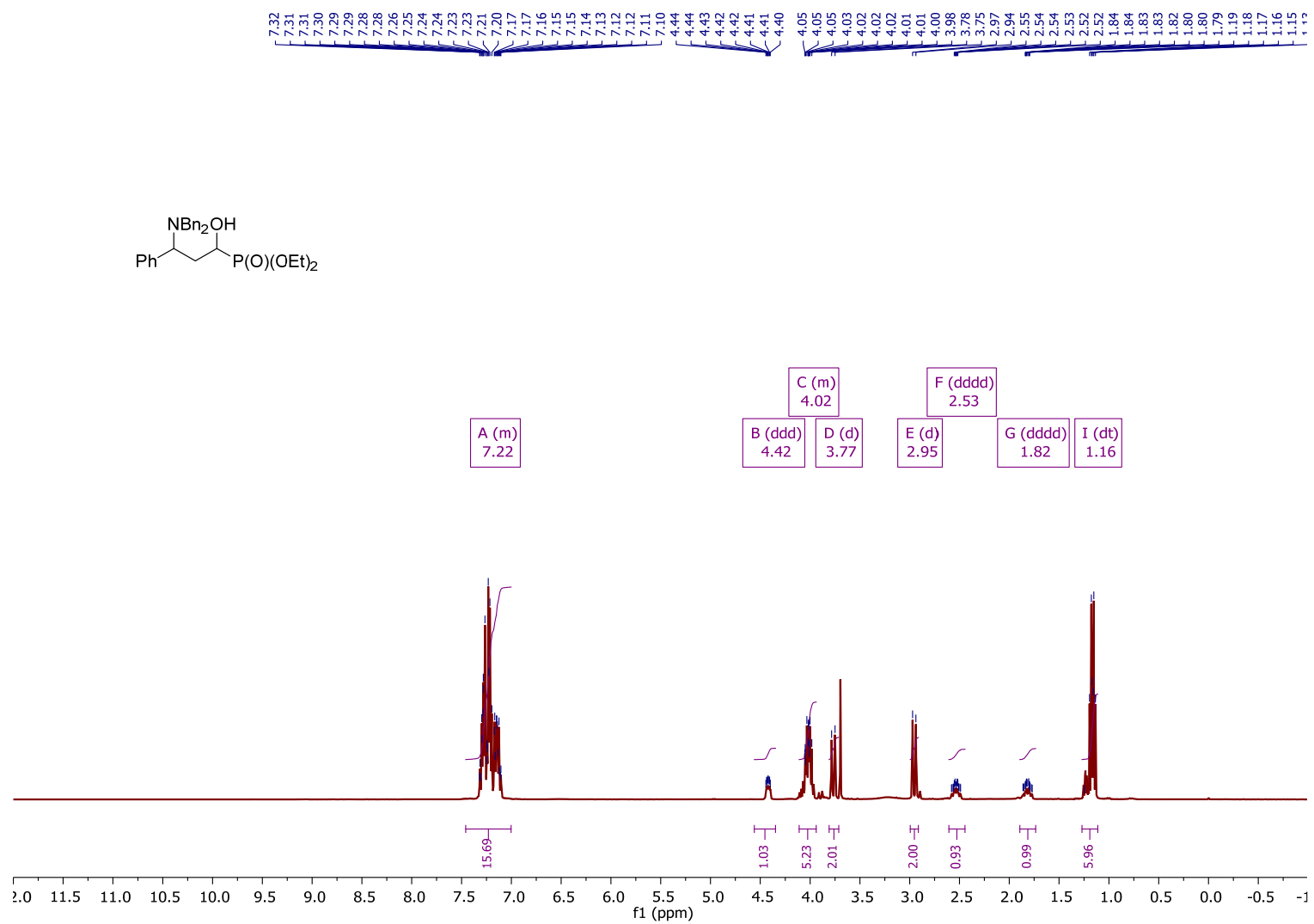
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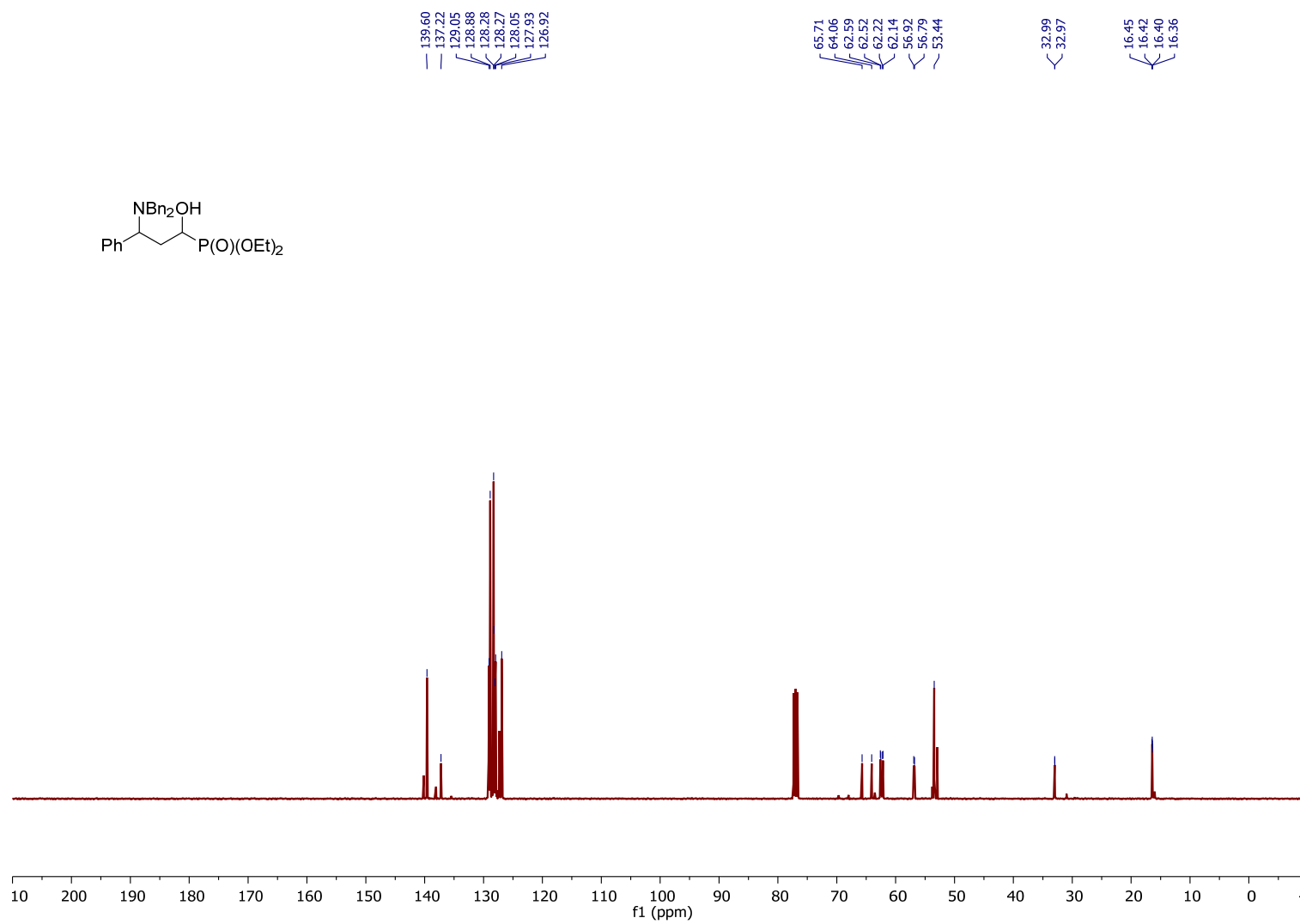
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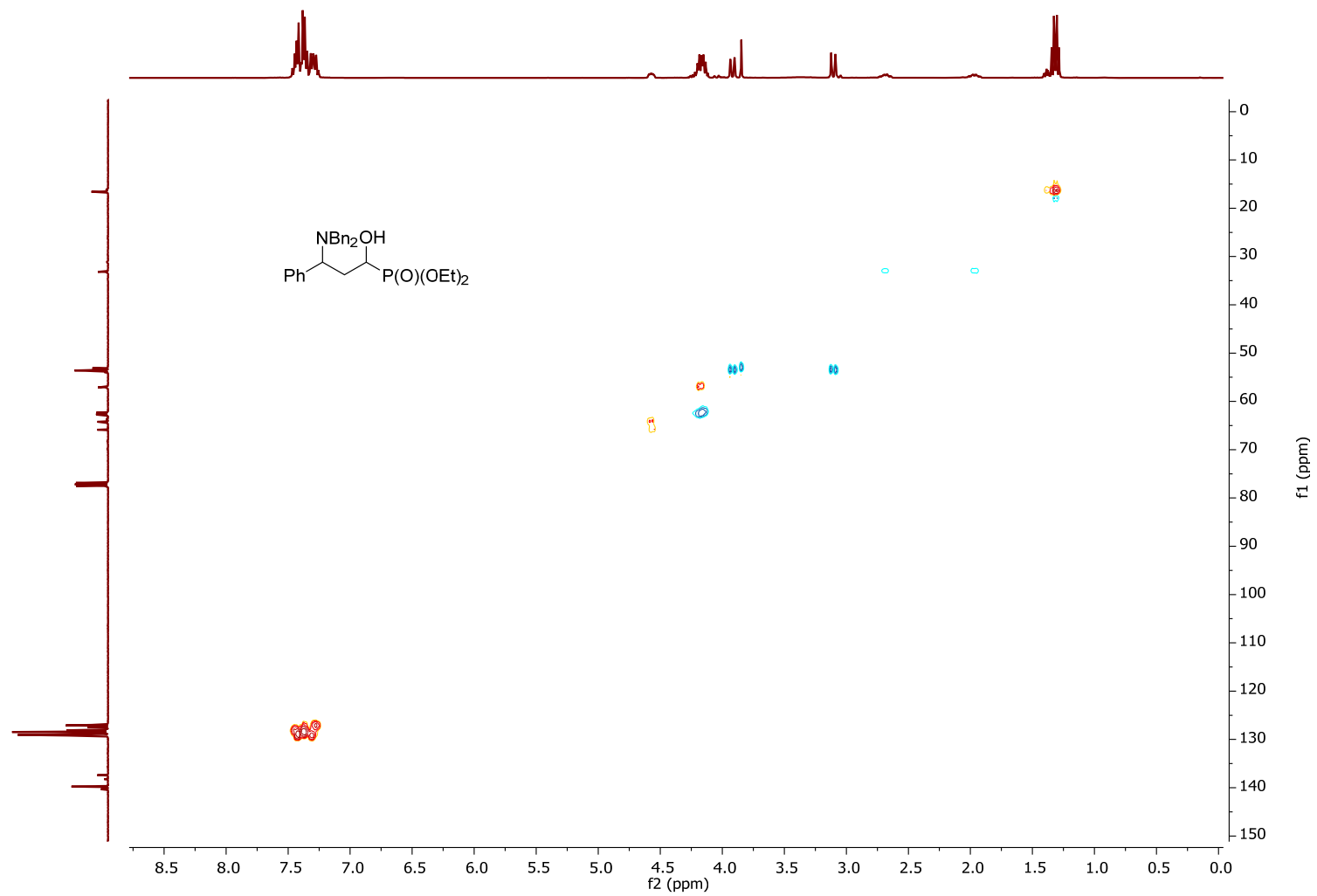
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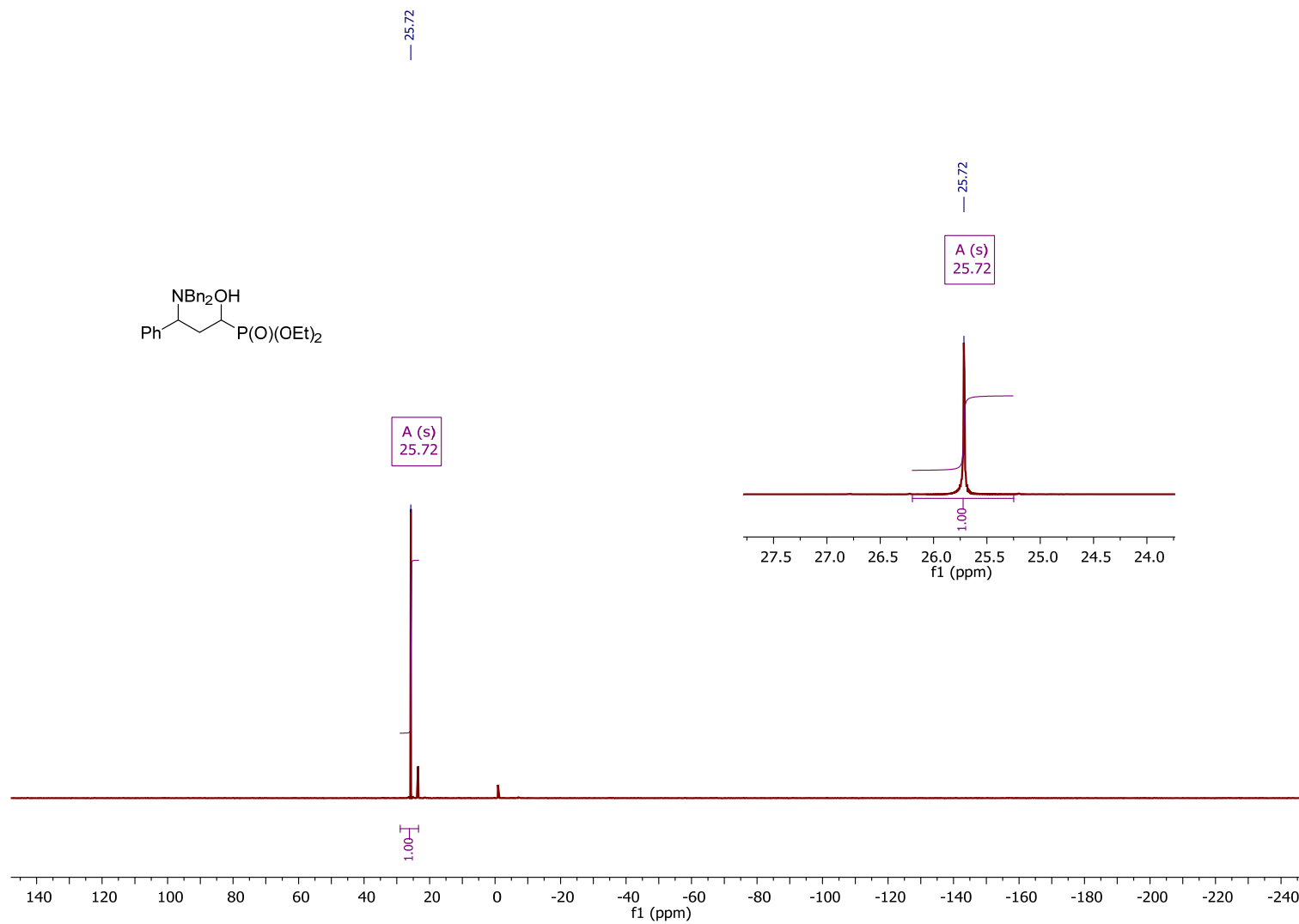
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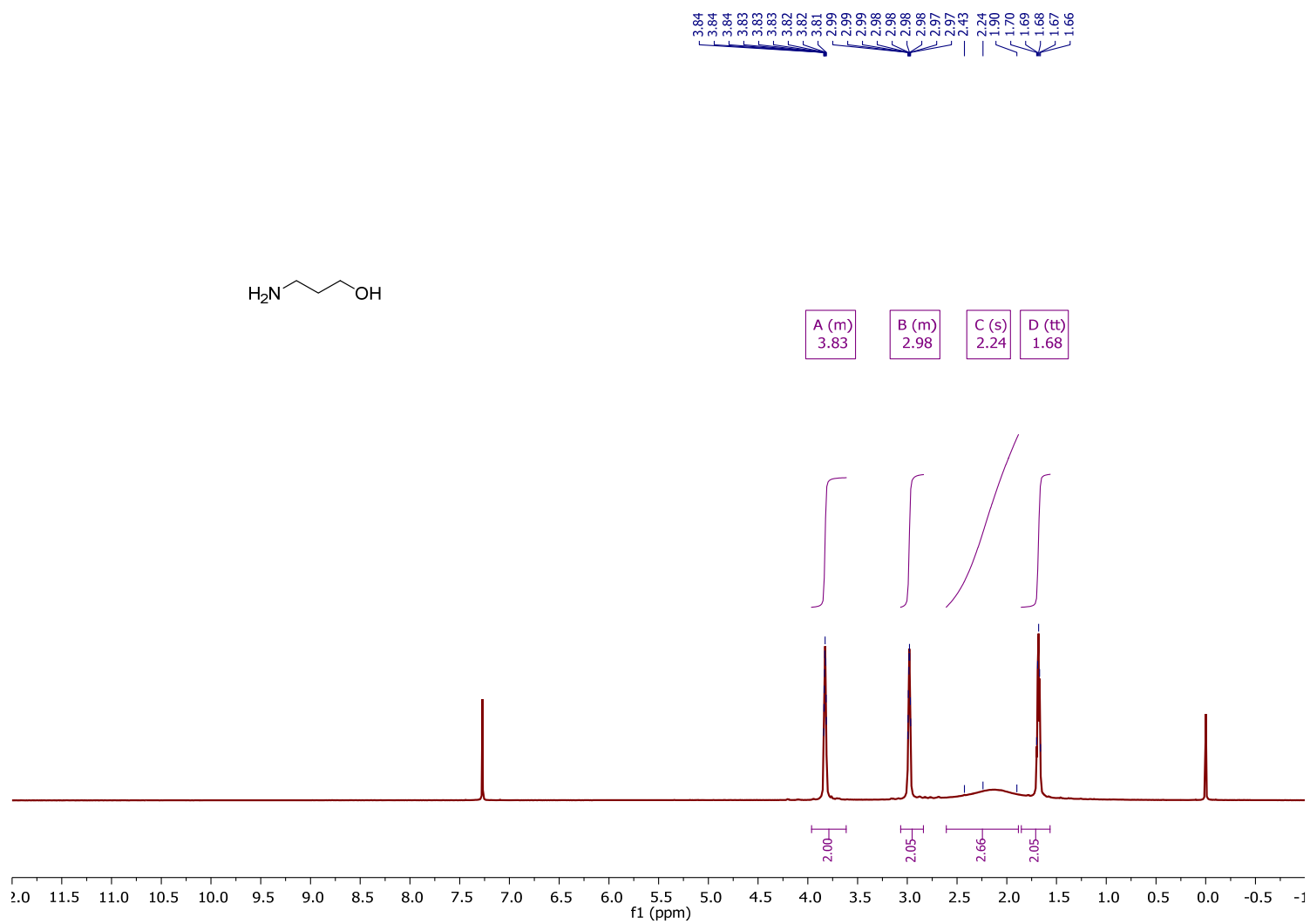
¹³C NMR of **rac-6c**.



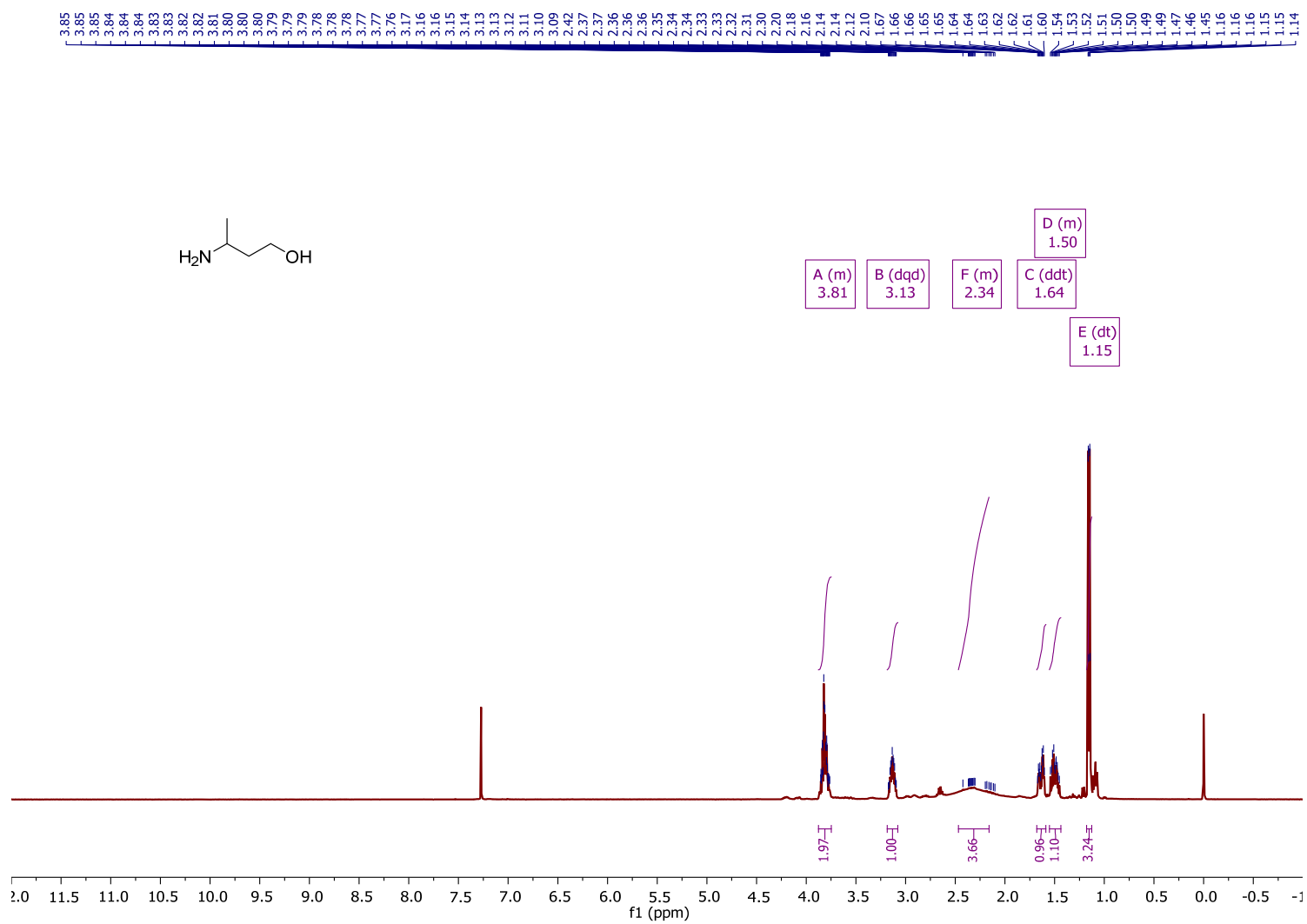
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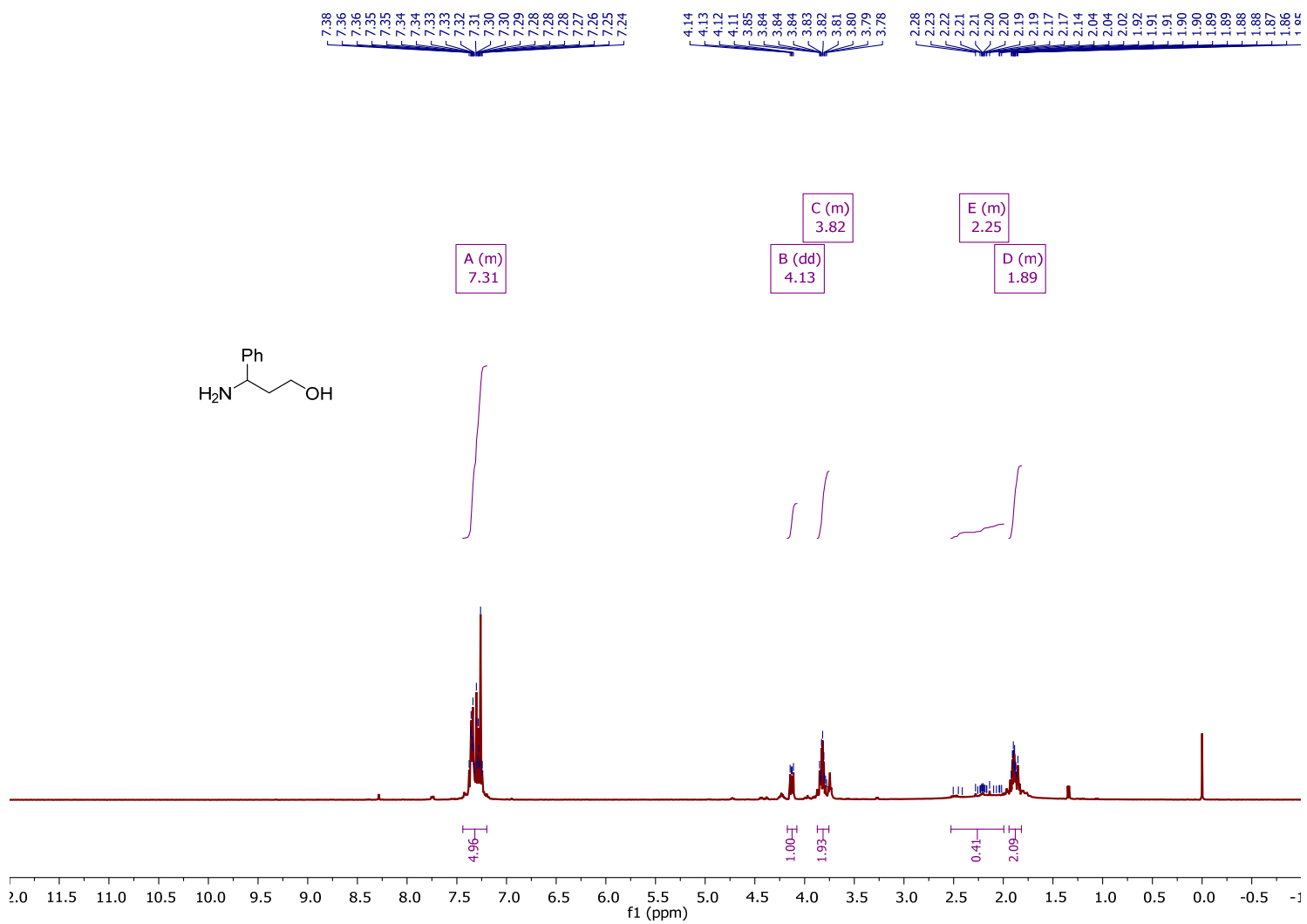
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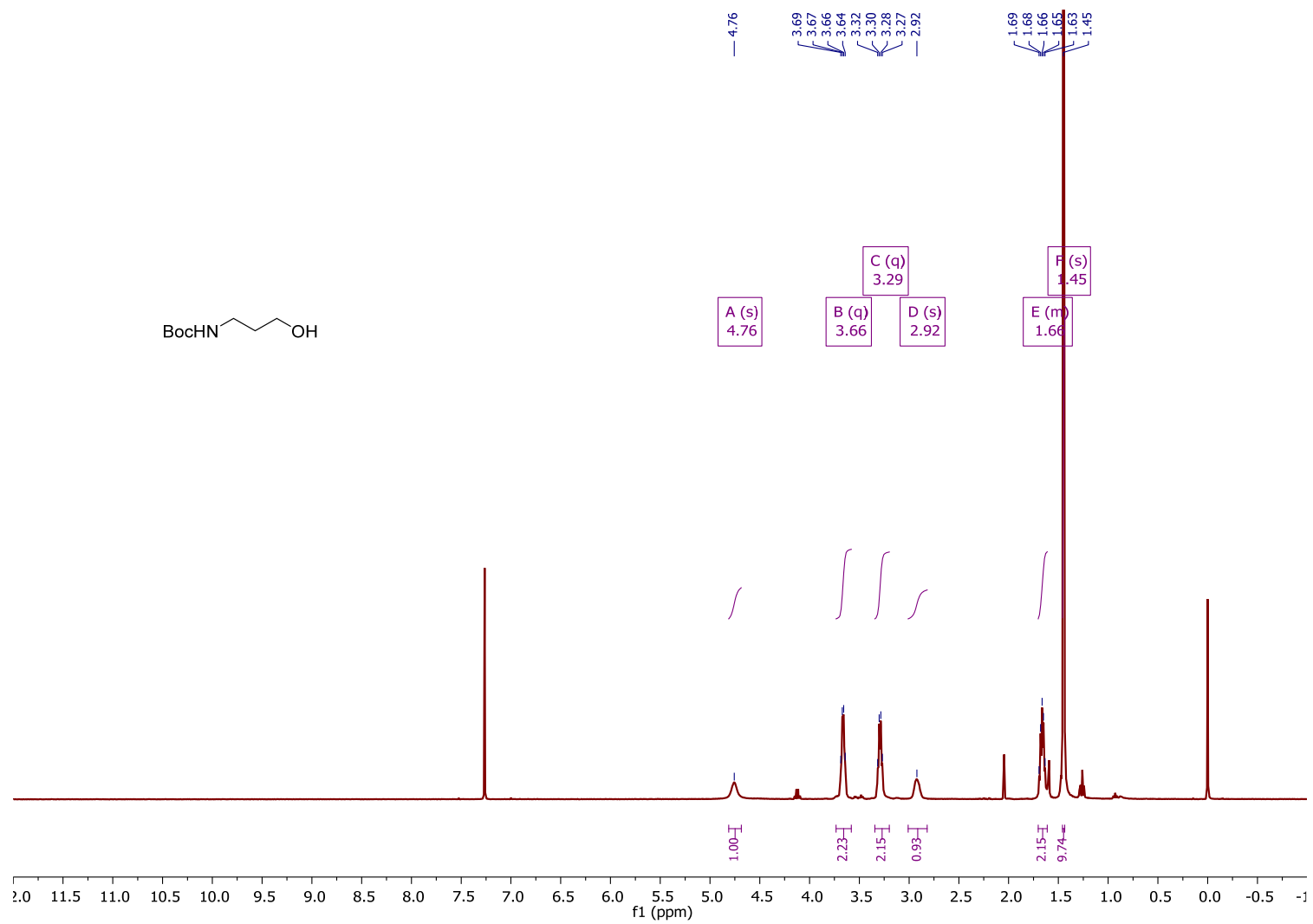
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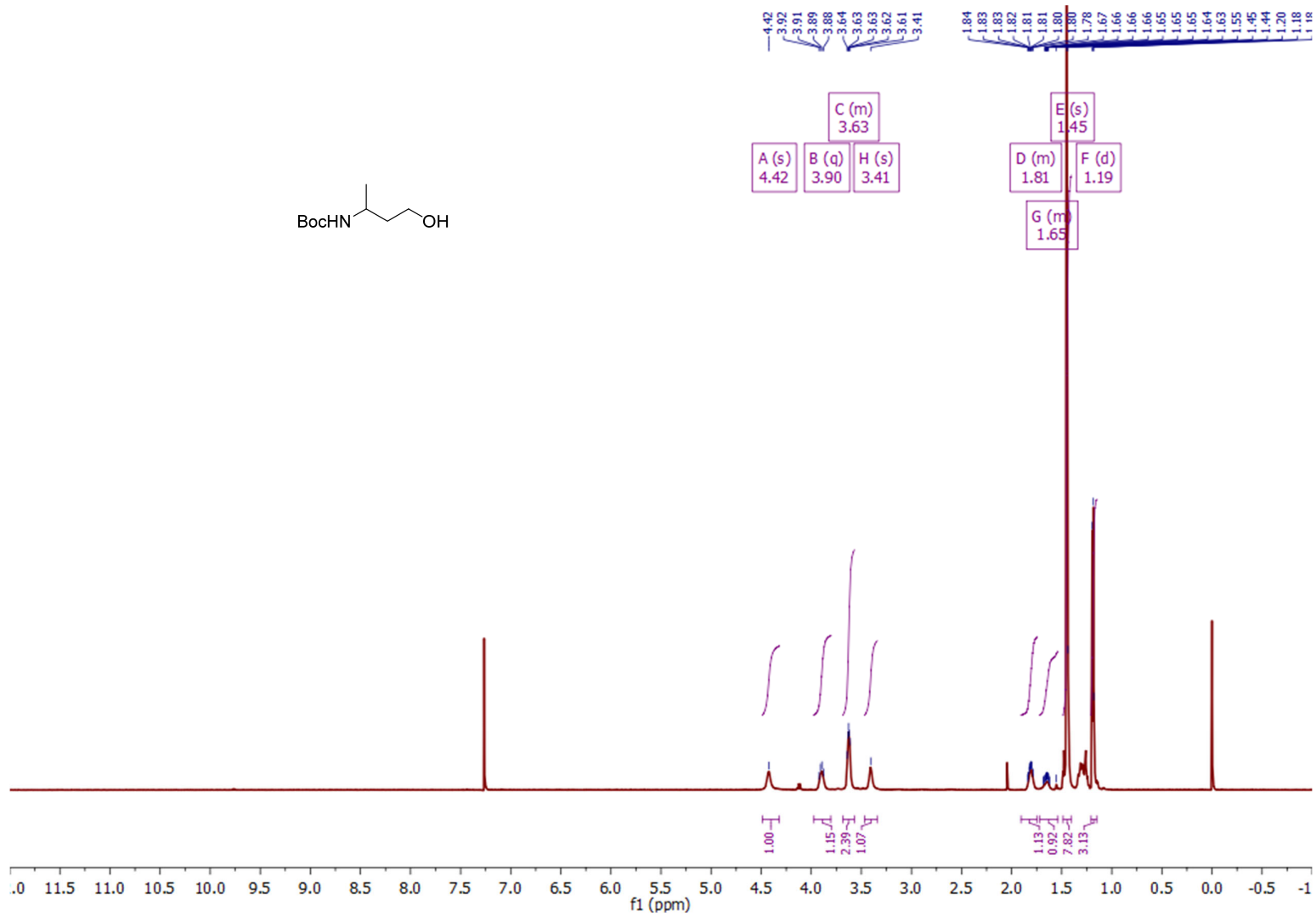
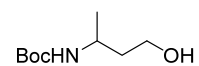
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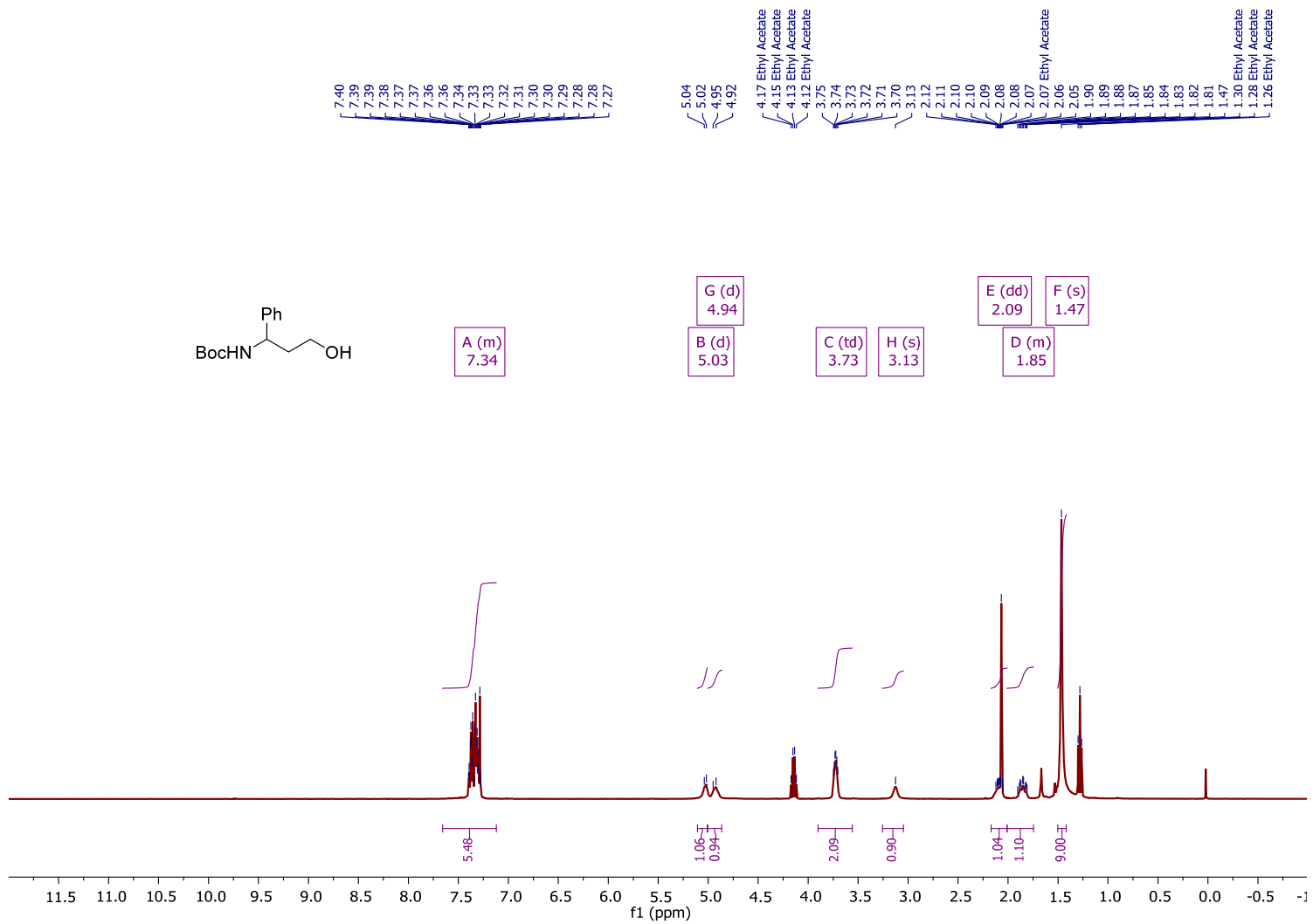
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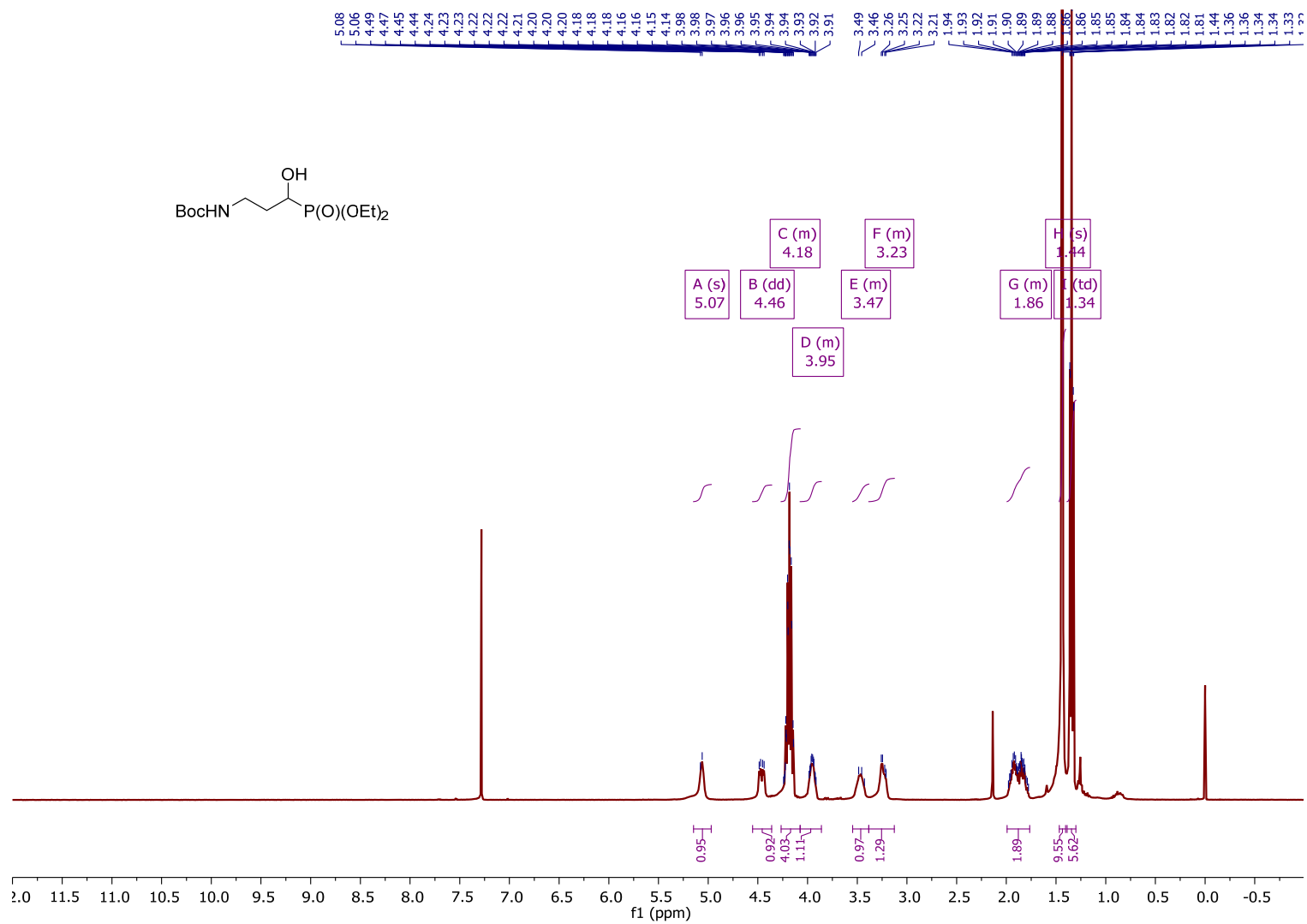
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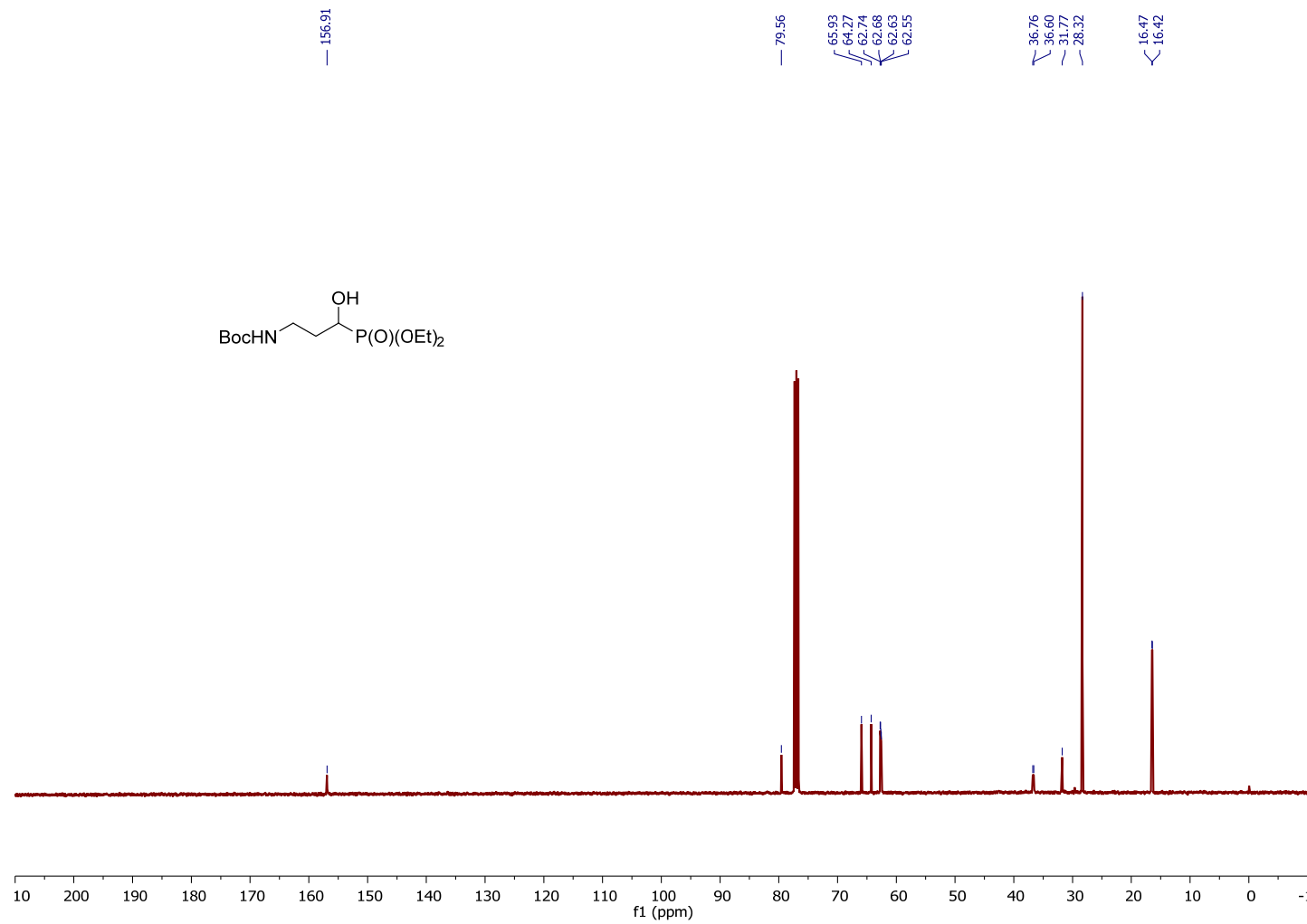
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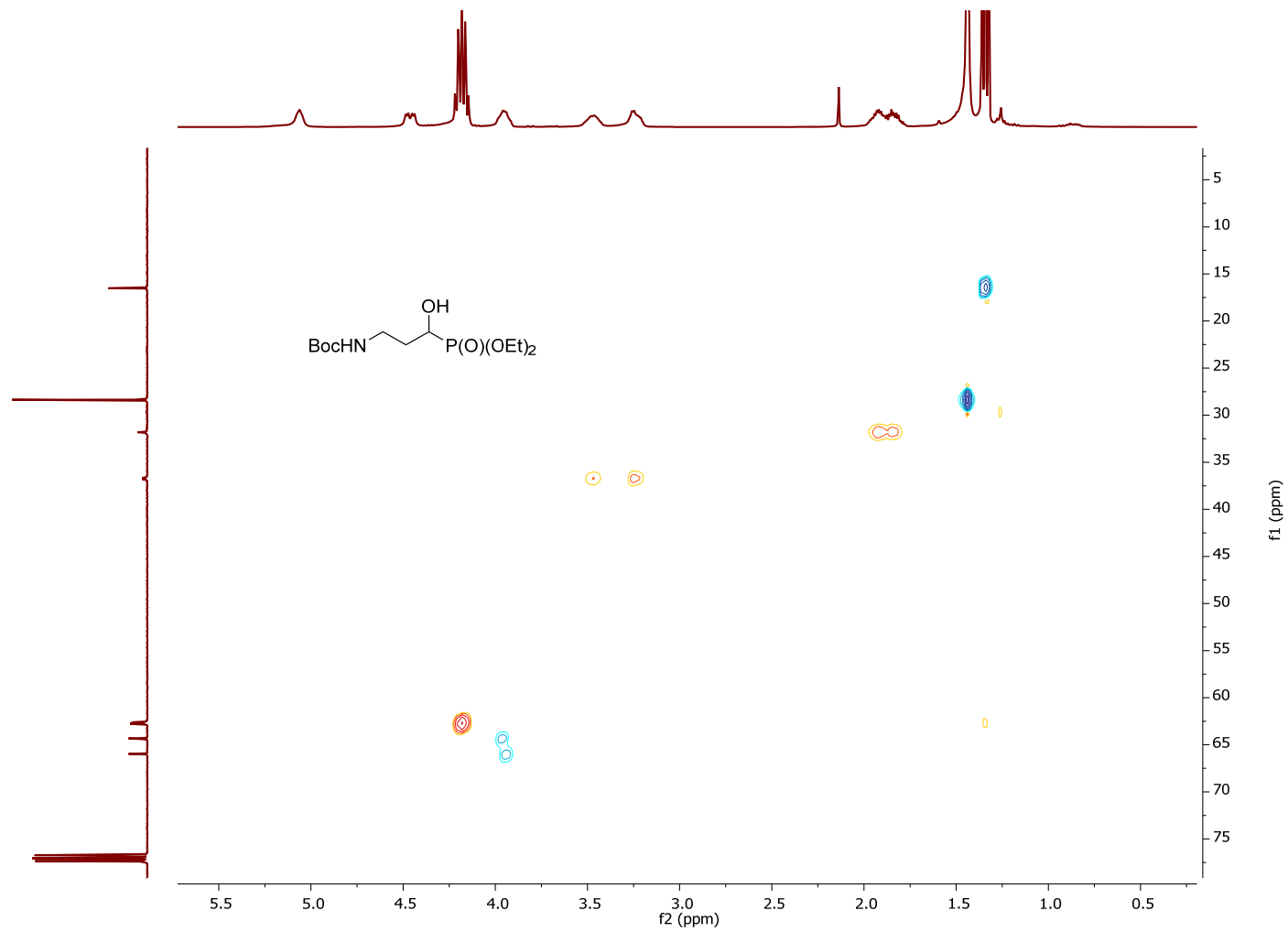
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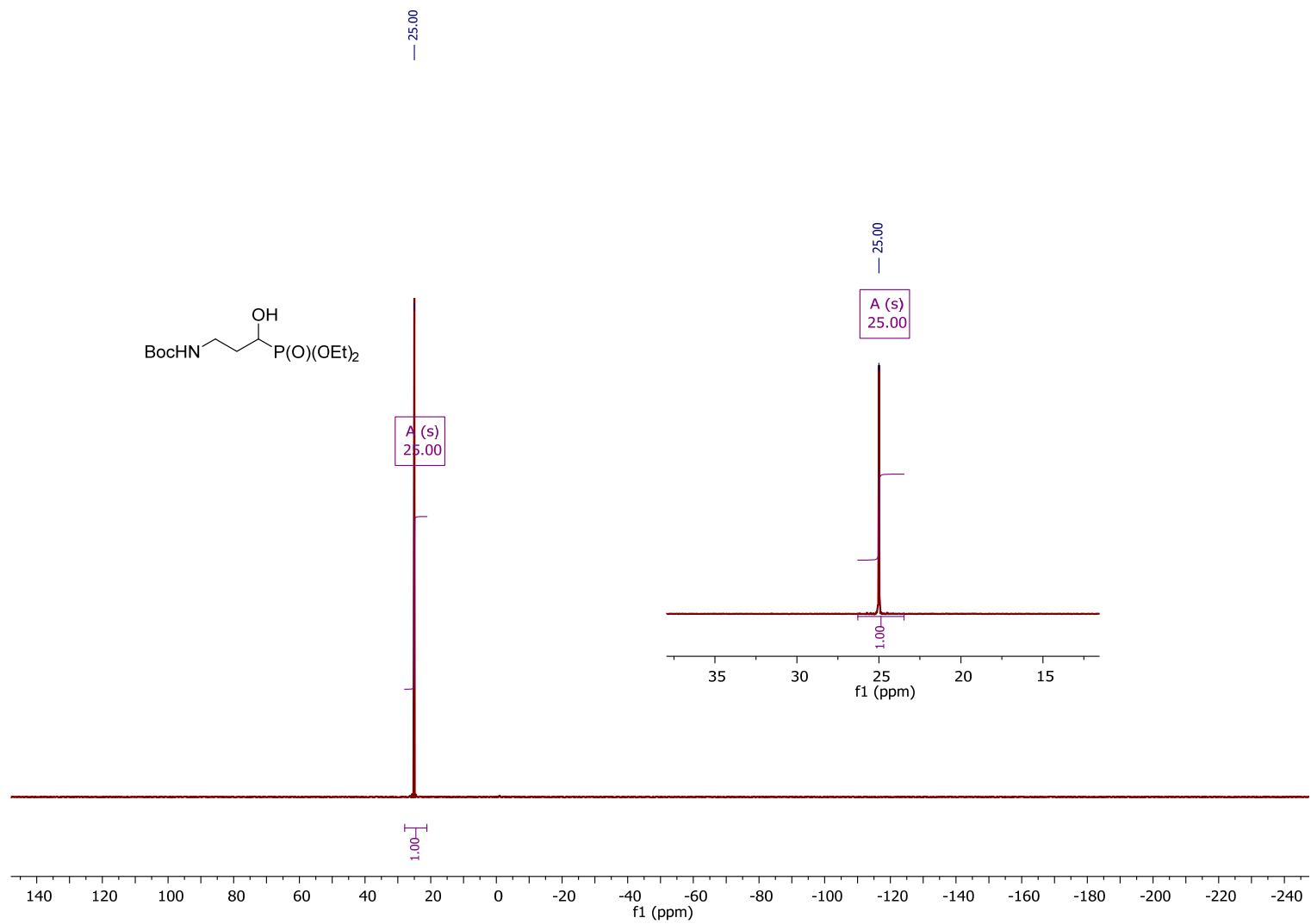
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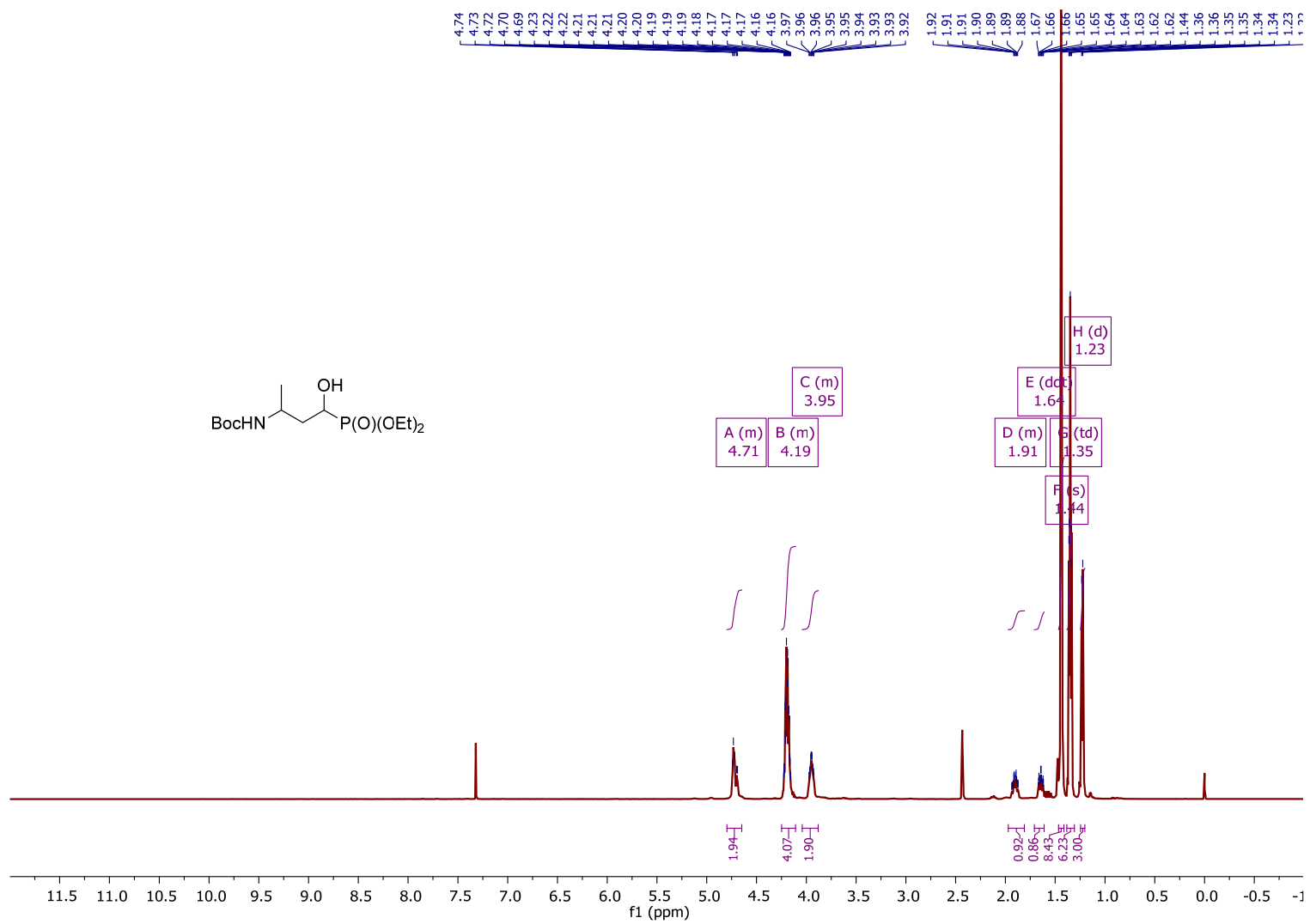
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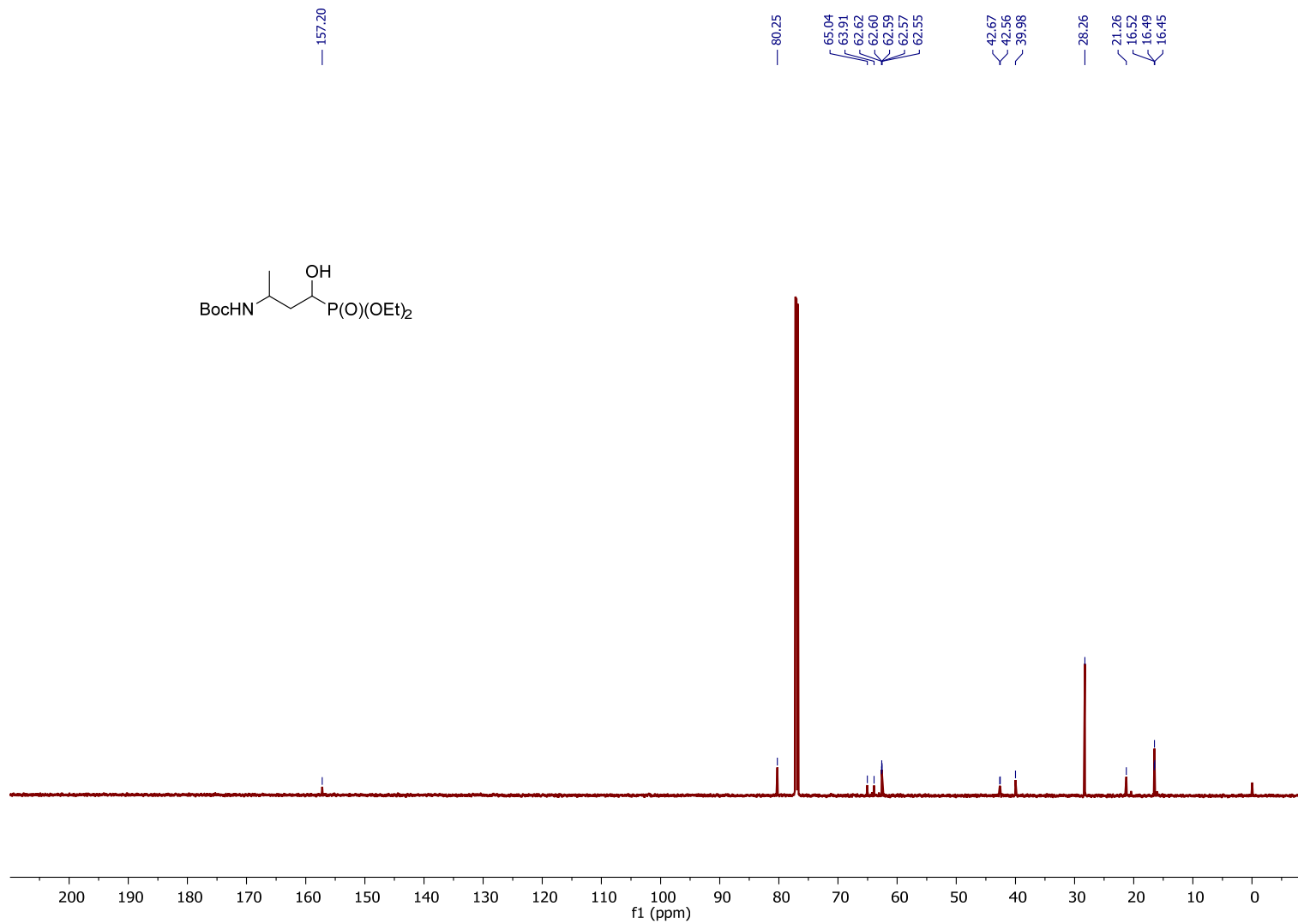
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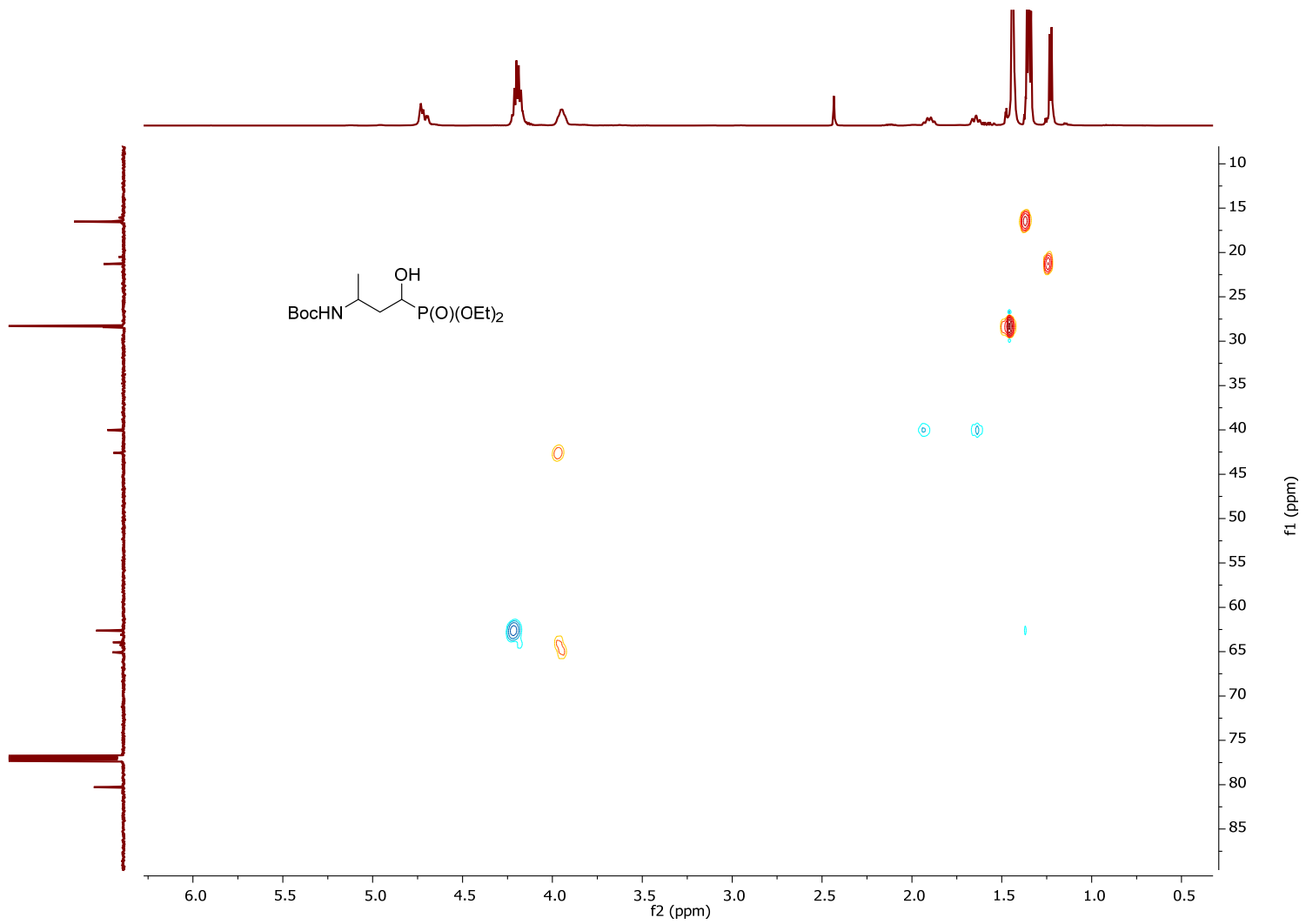
$^{31}\text{P}\{^1\text{H}\}$ NMR of **rac-9a**.



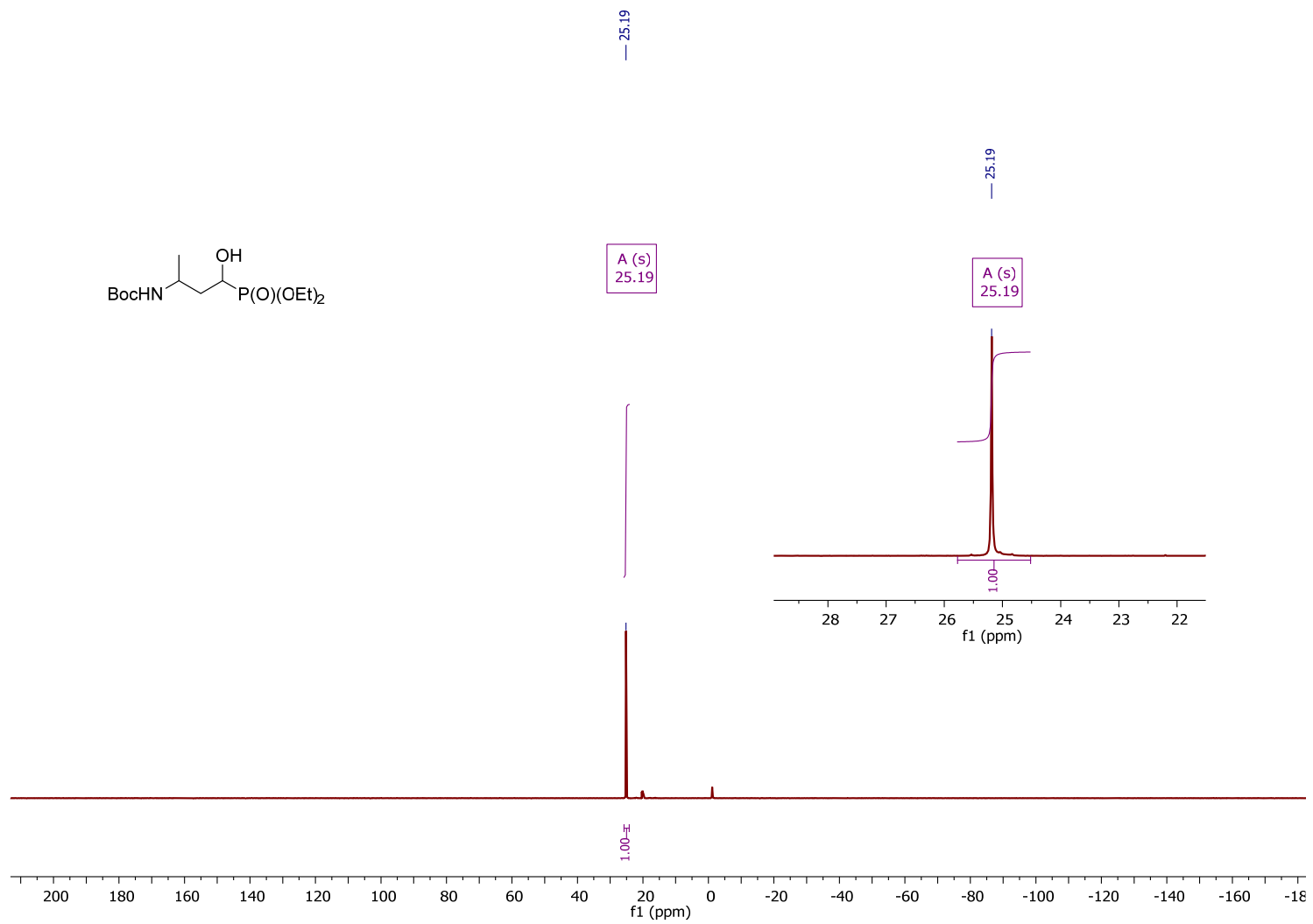
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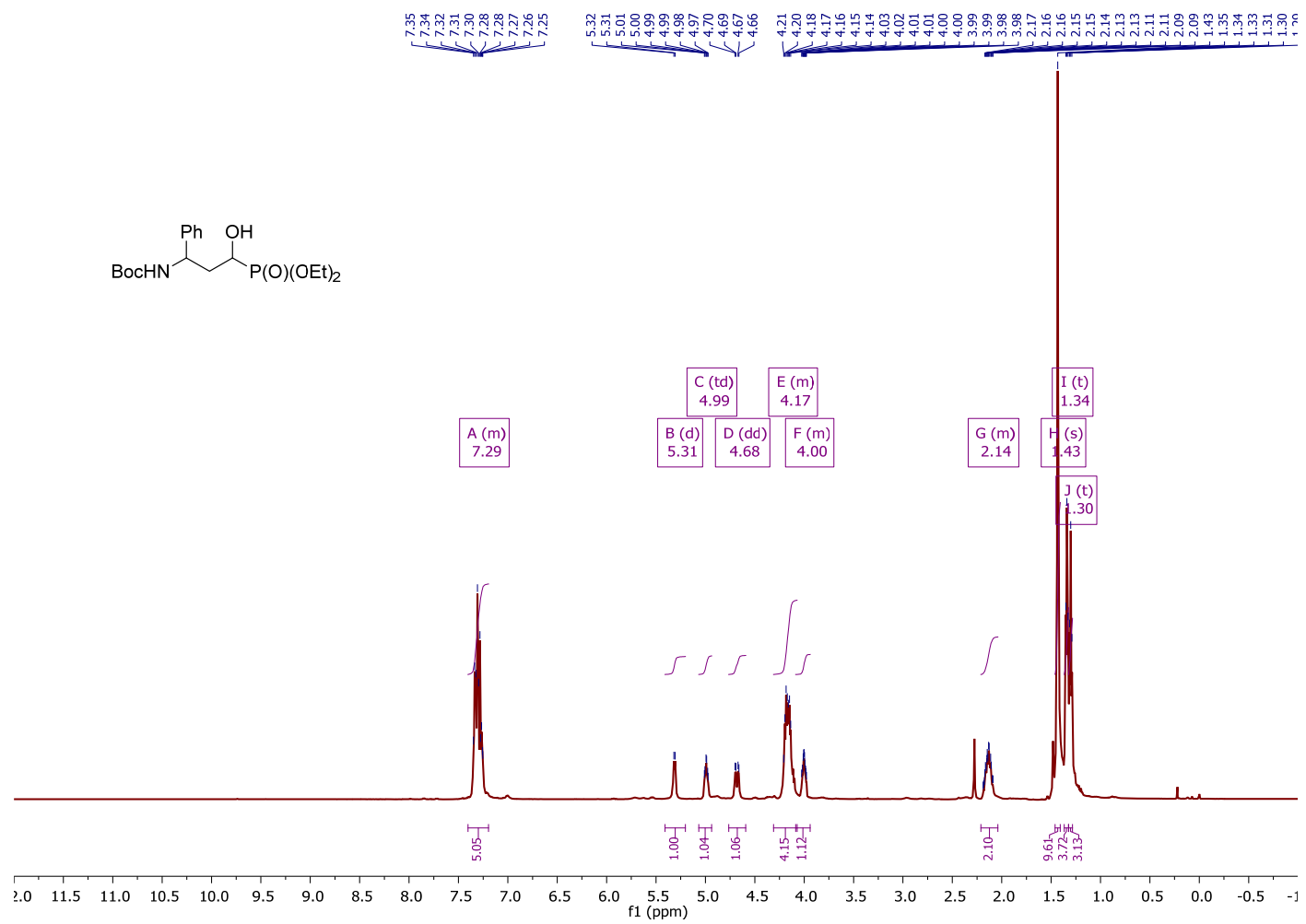
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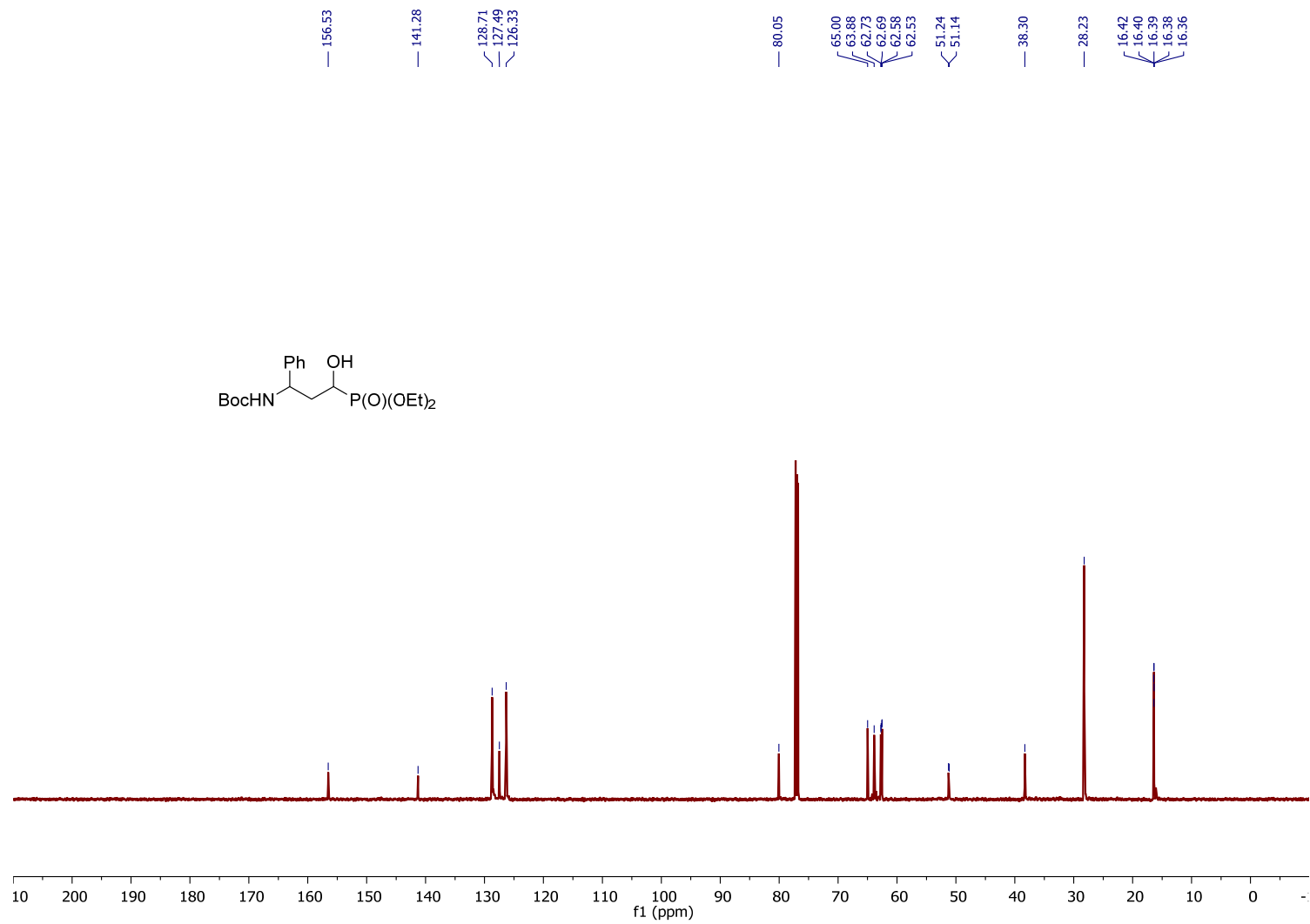
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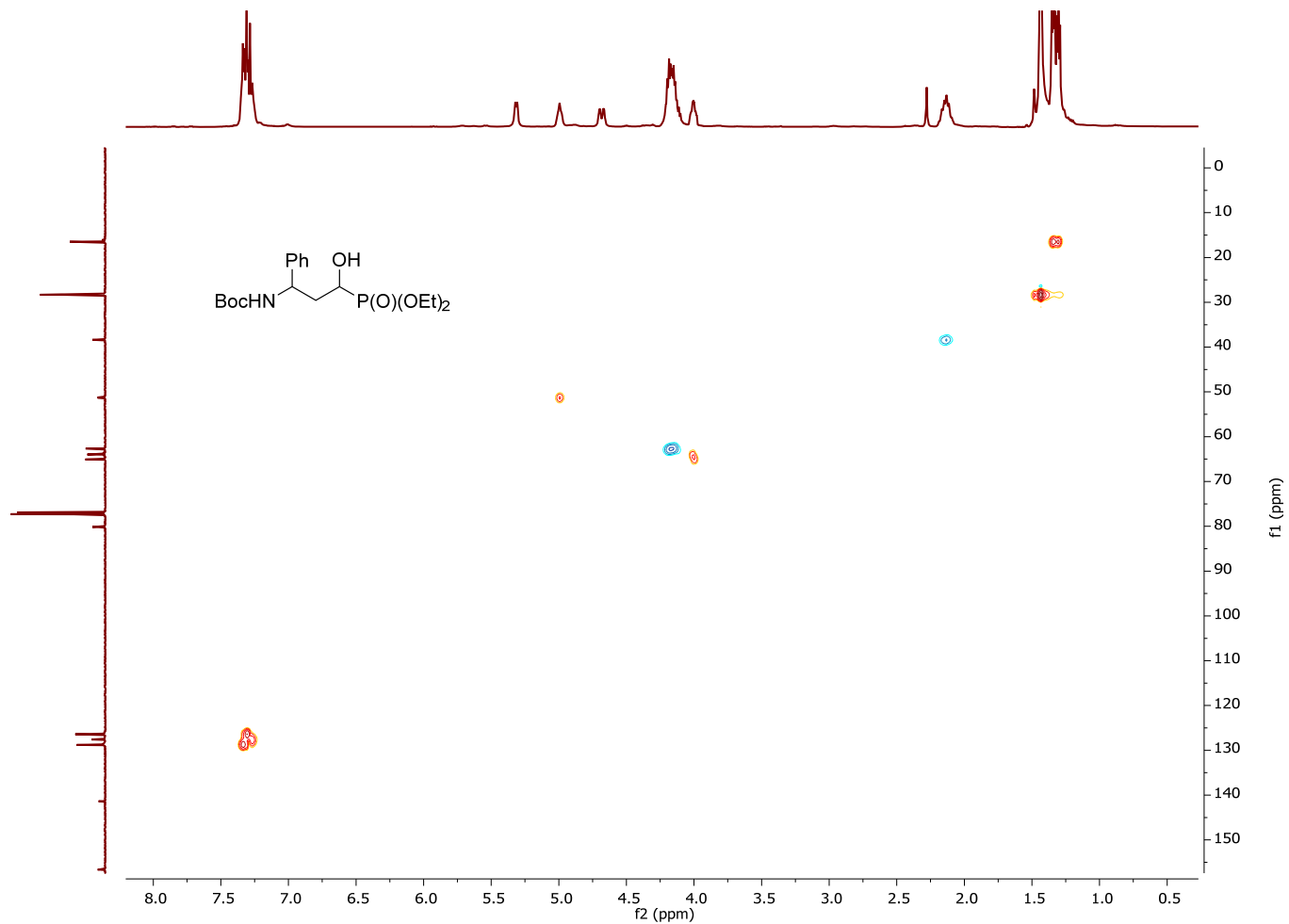
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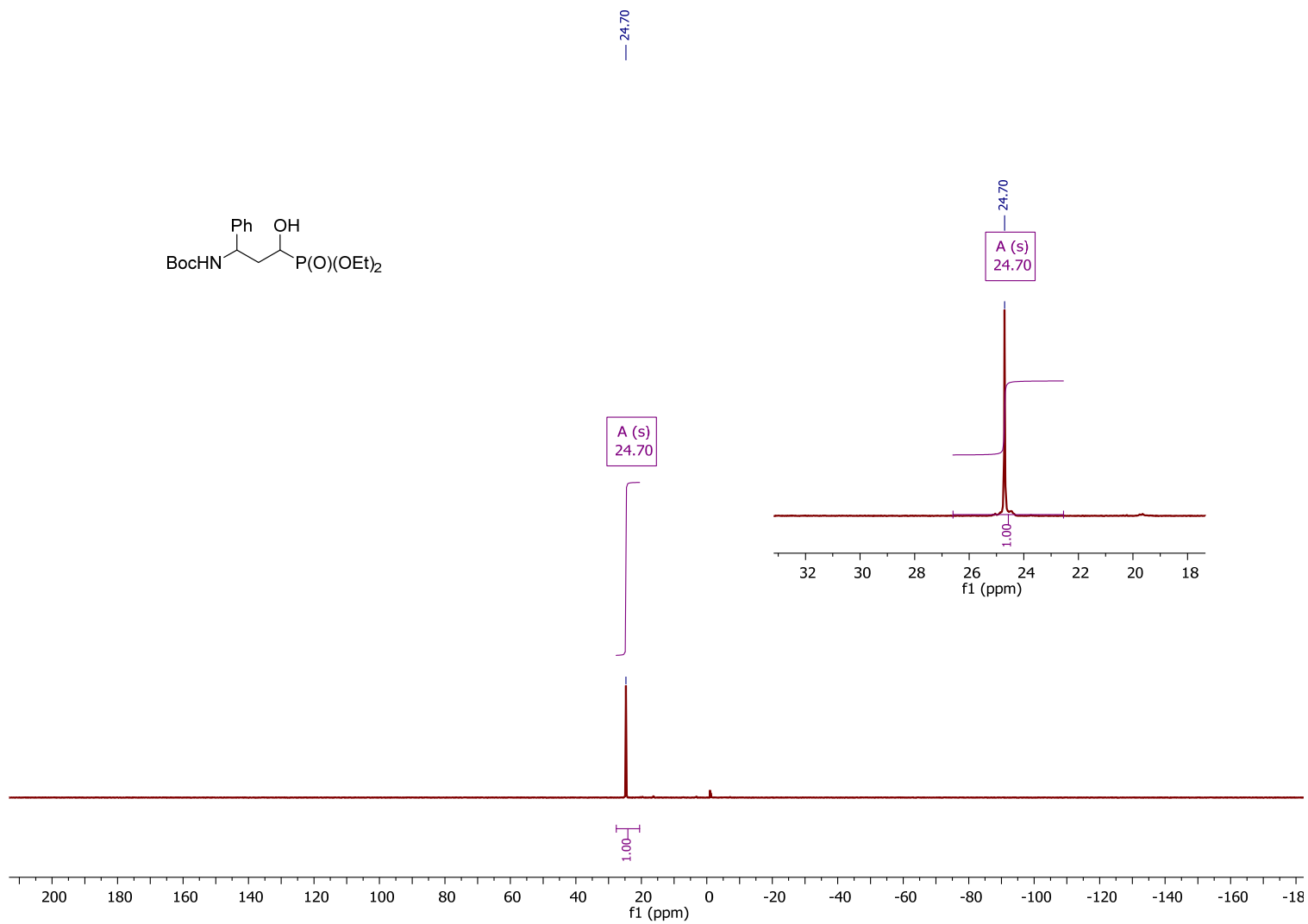
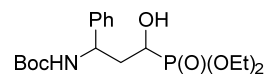
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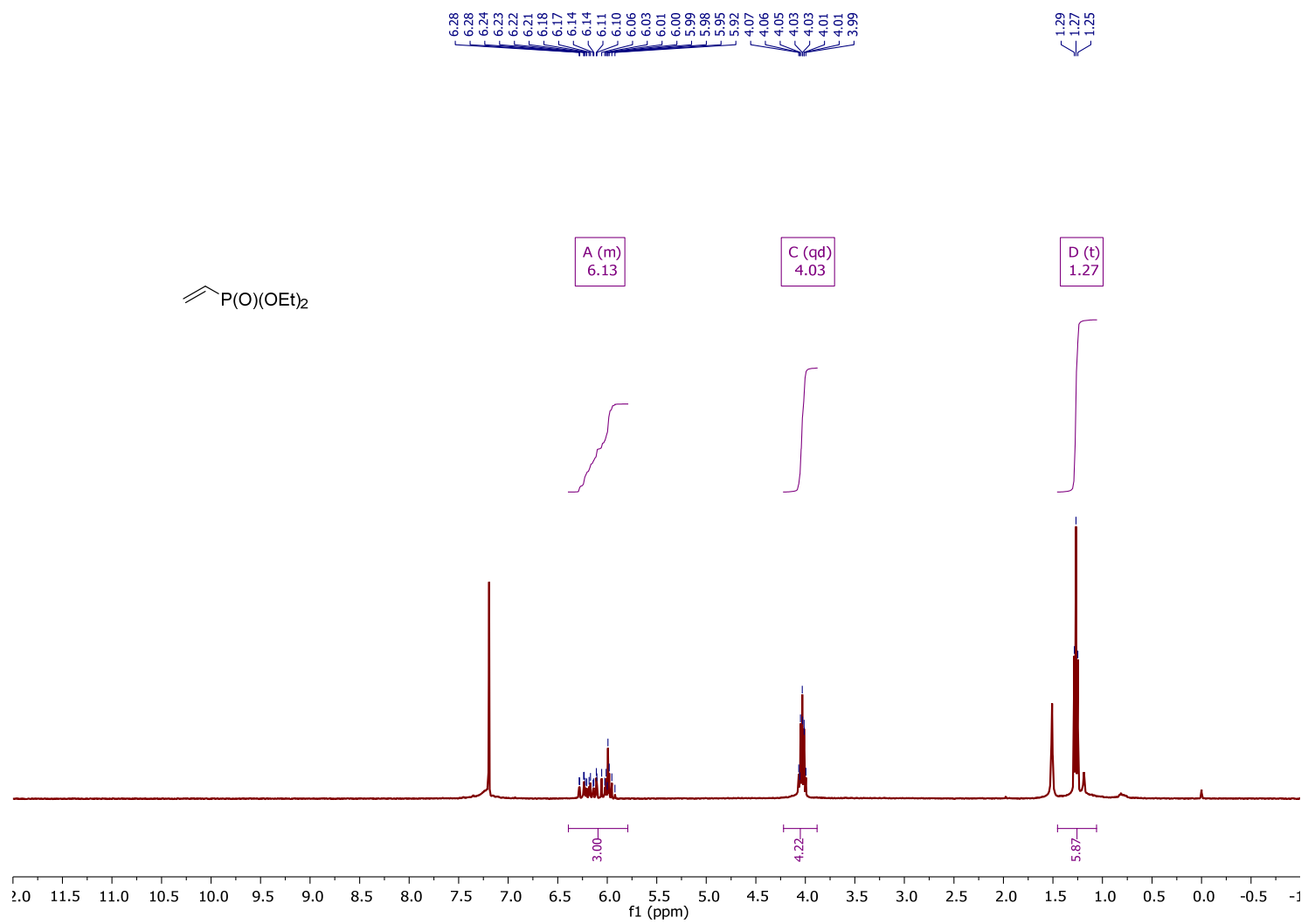
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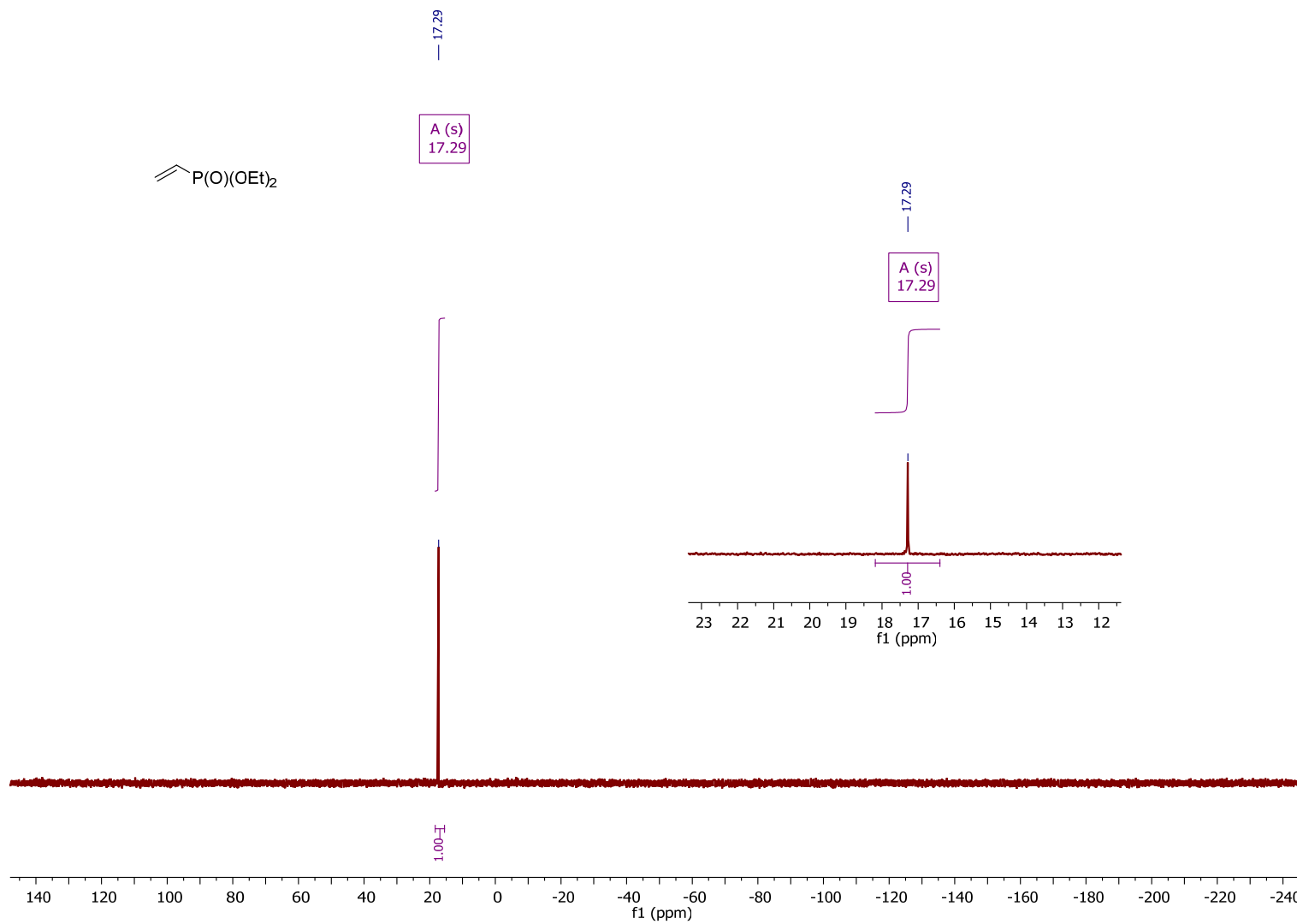
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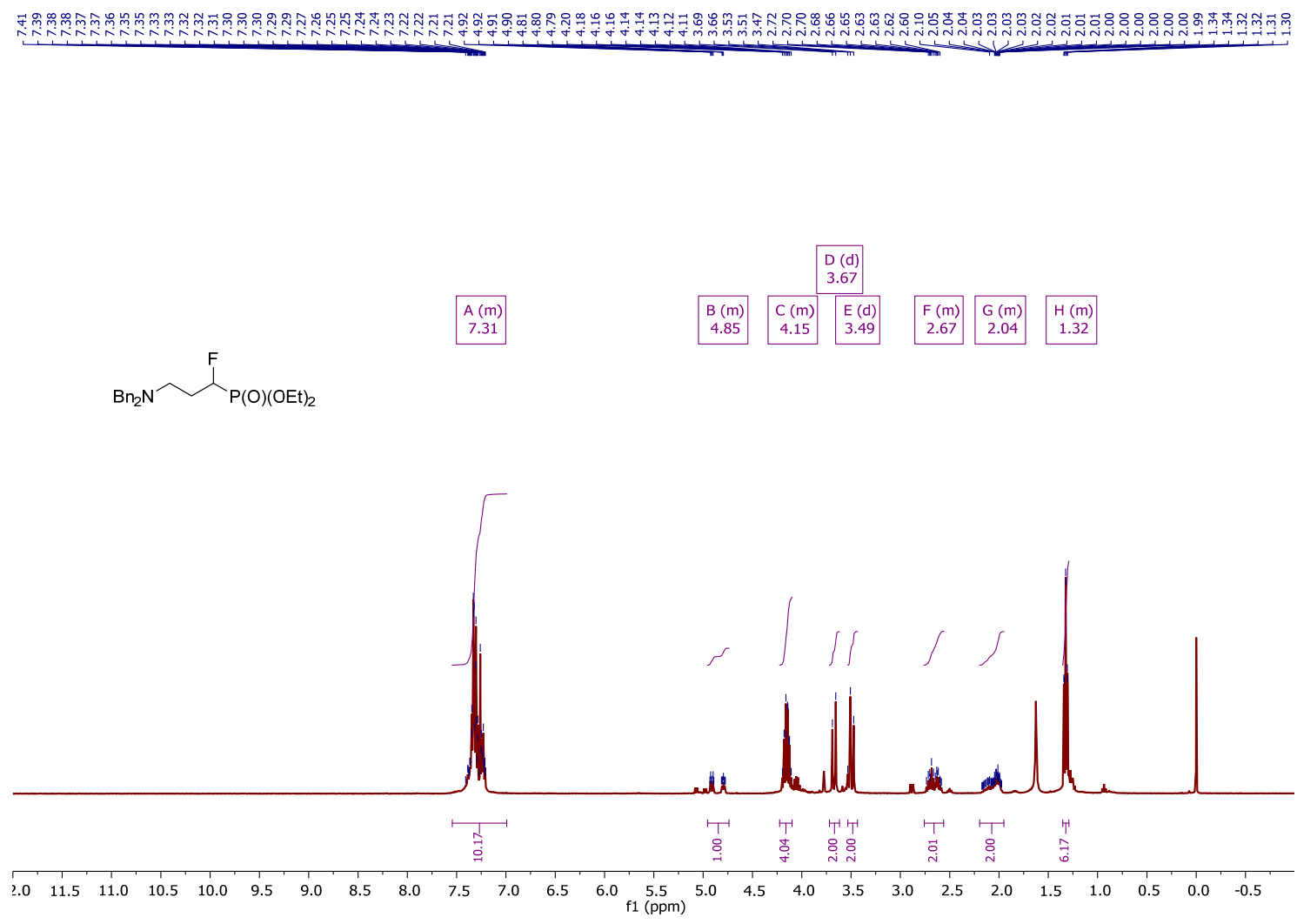
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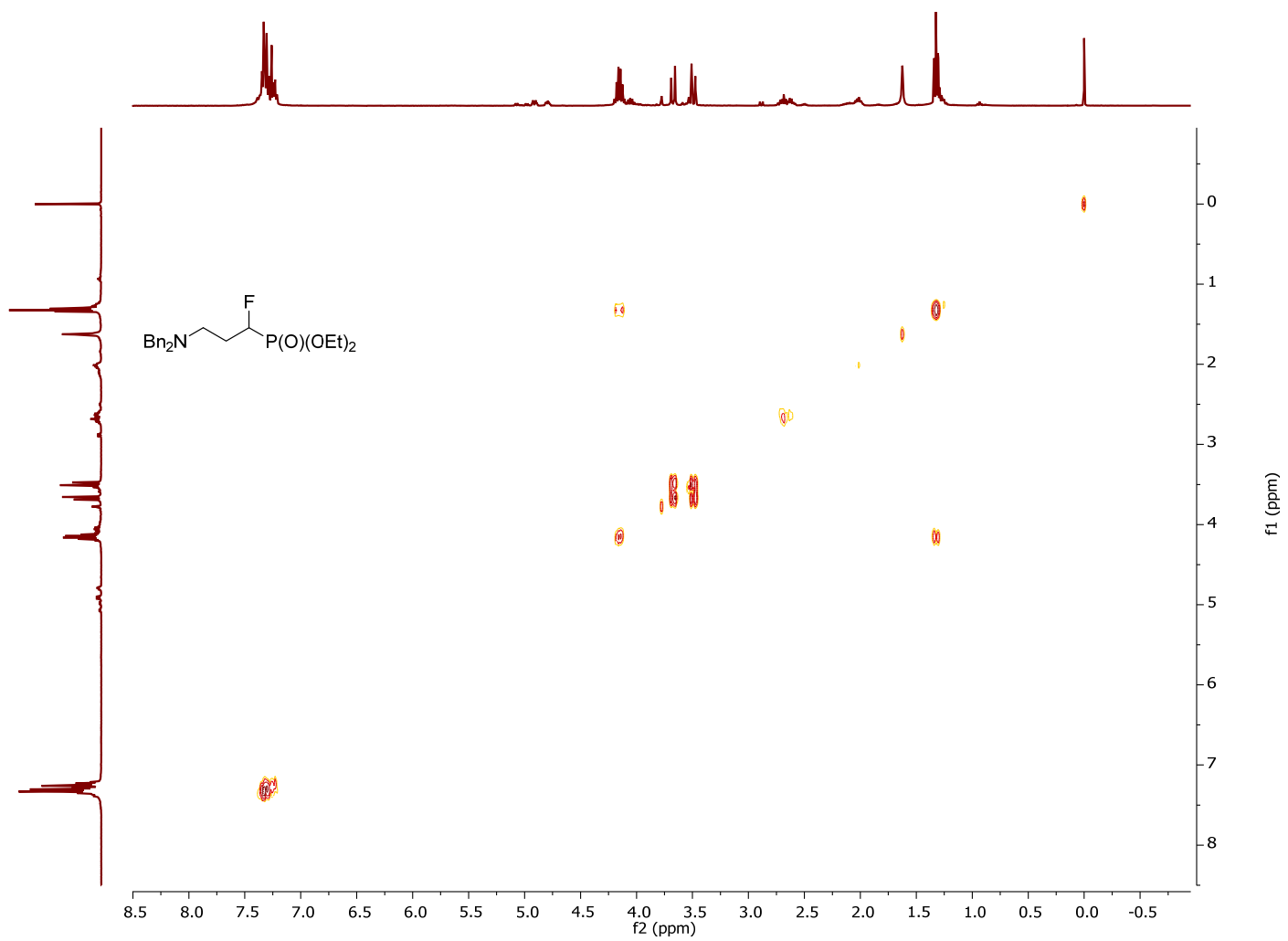
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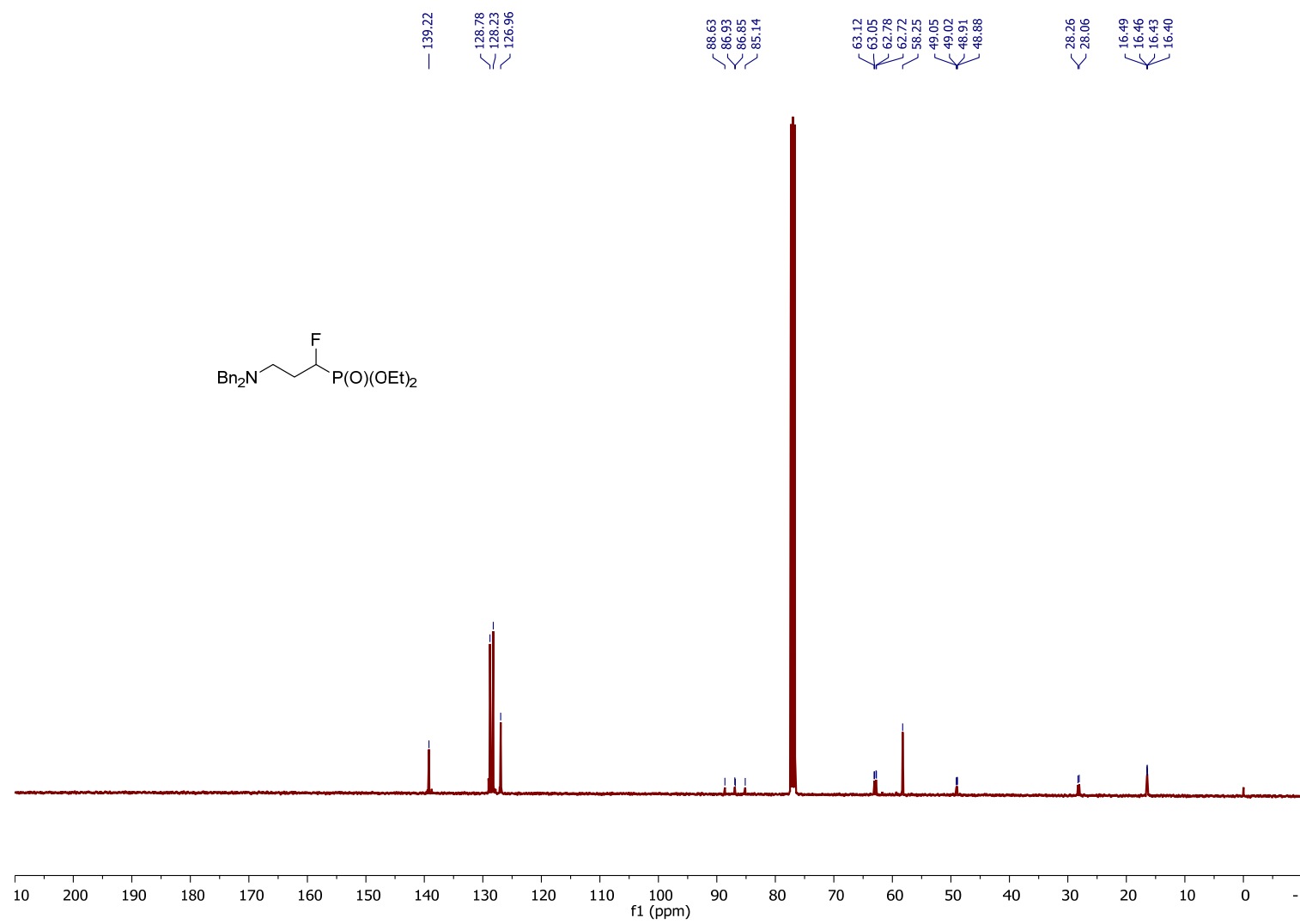
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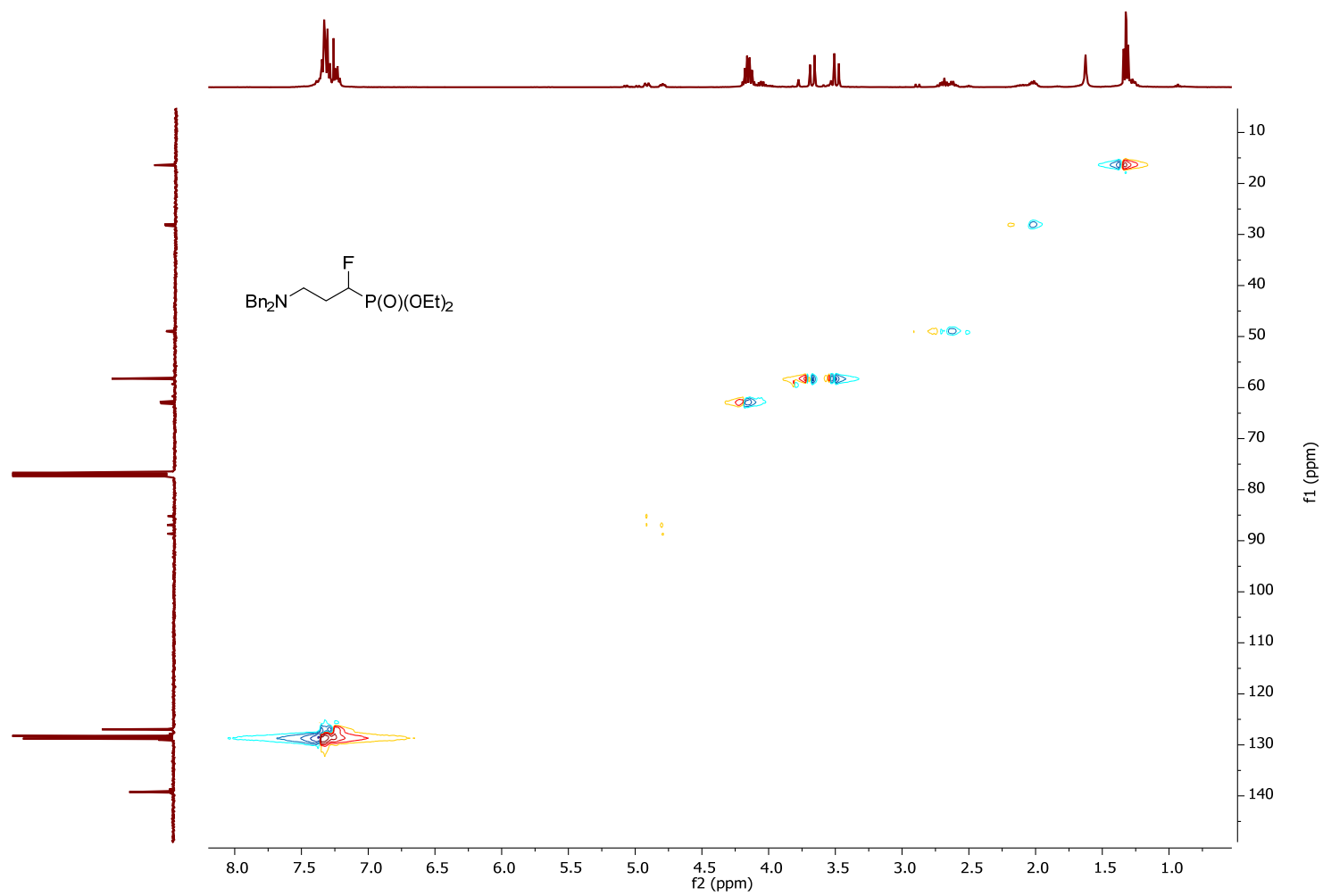
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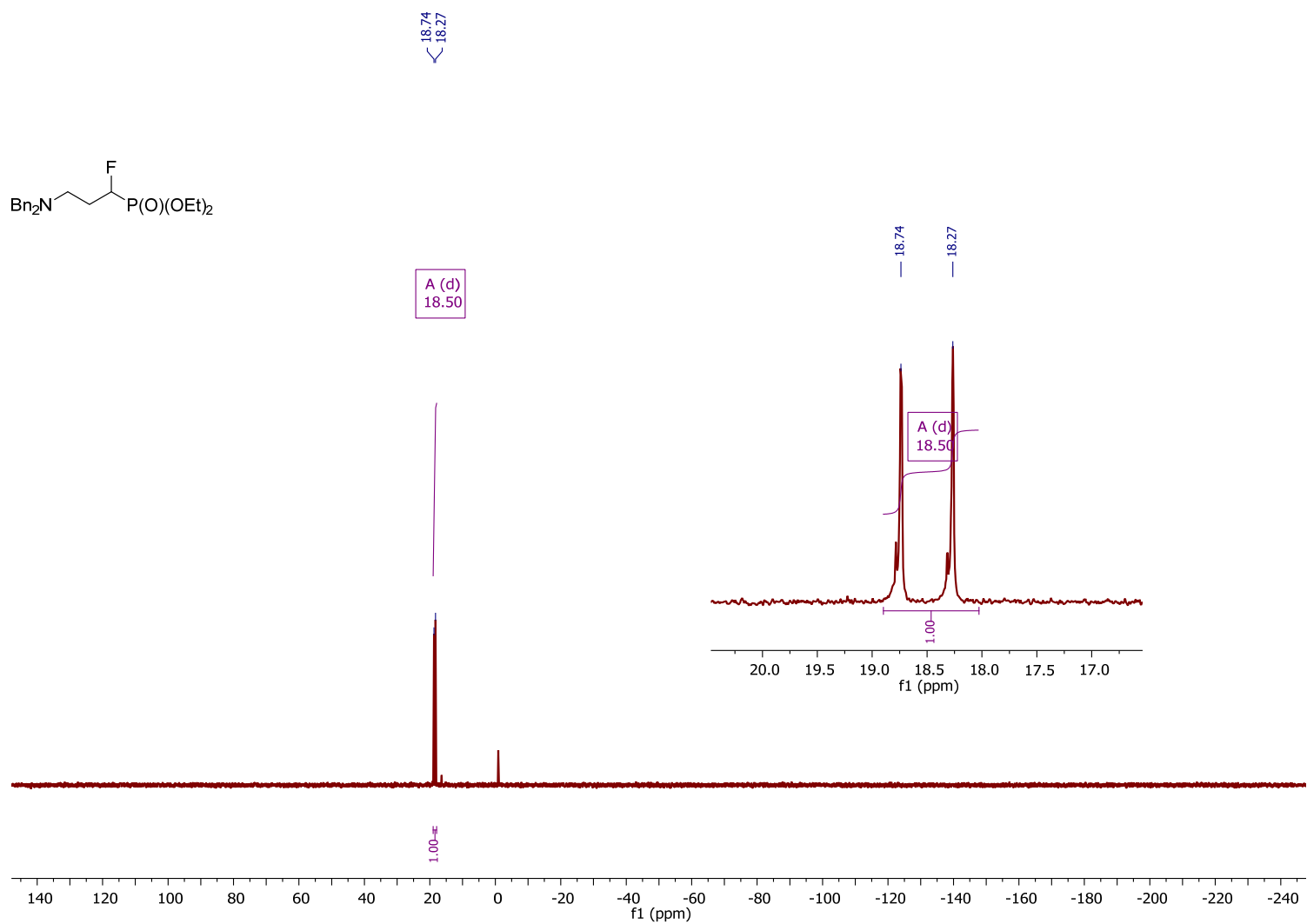
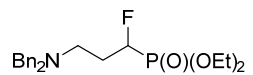
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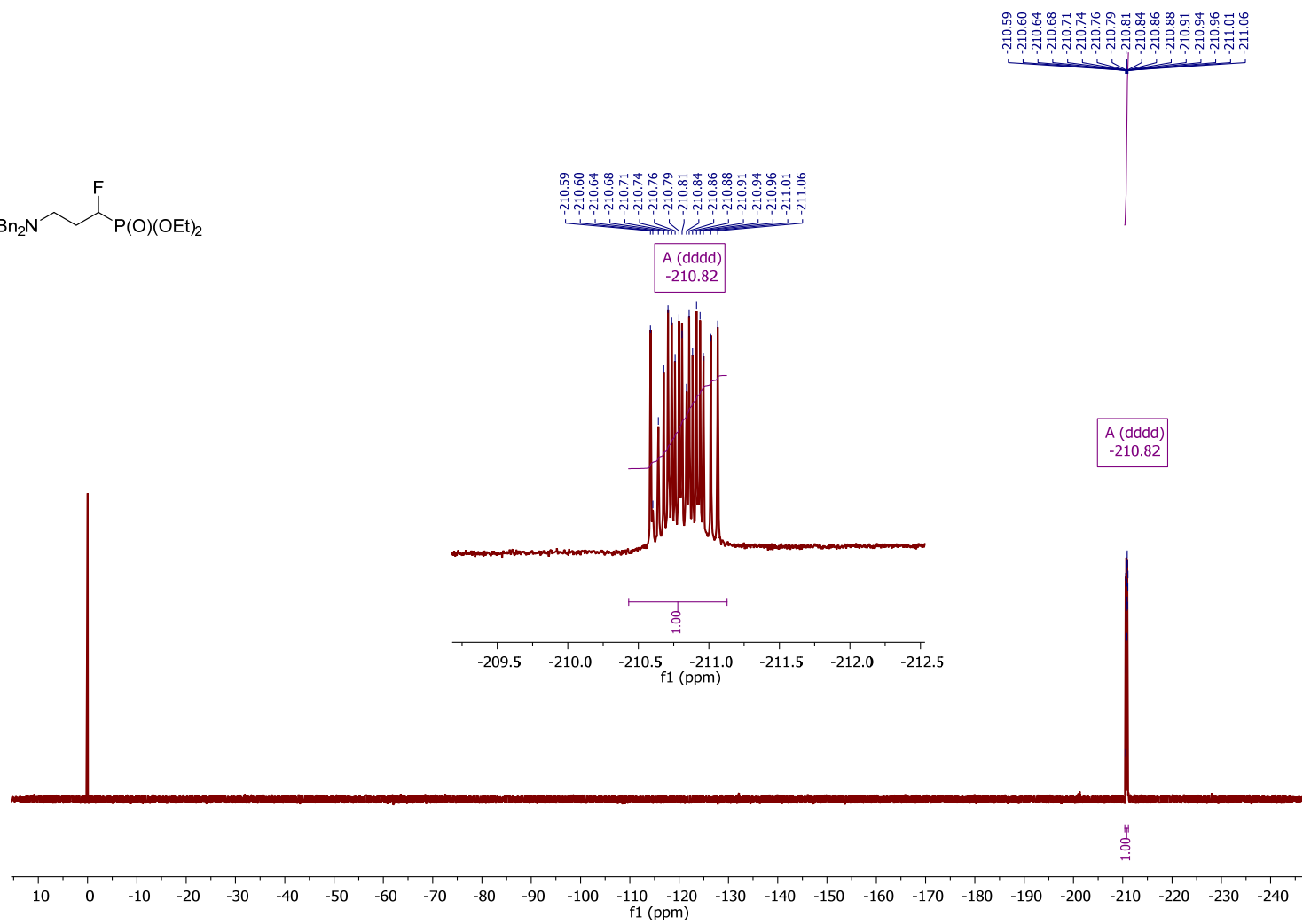
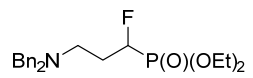
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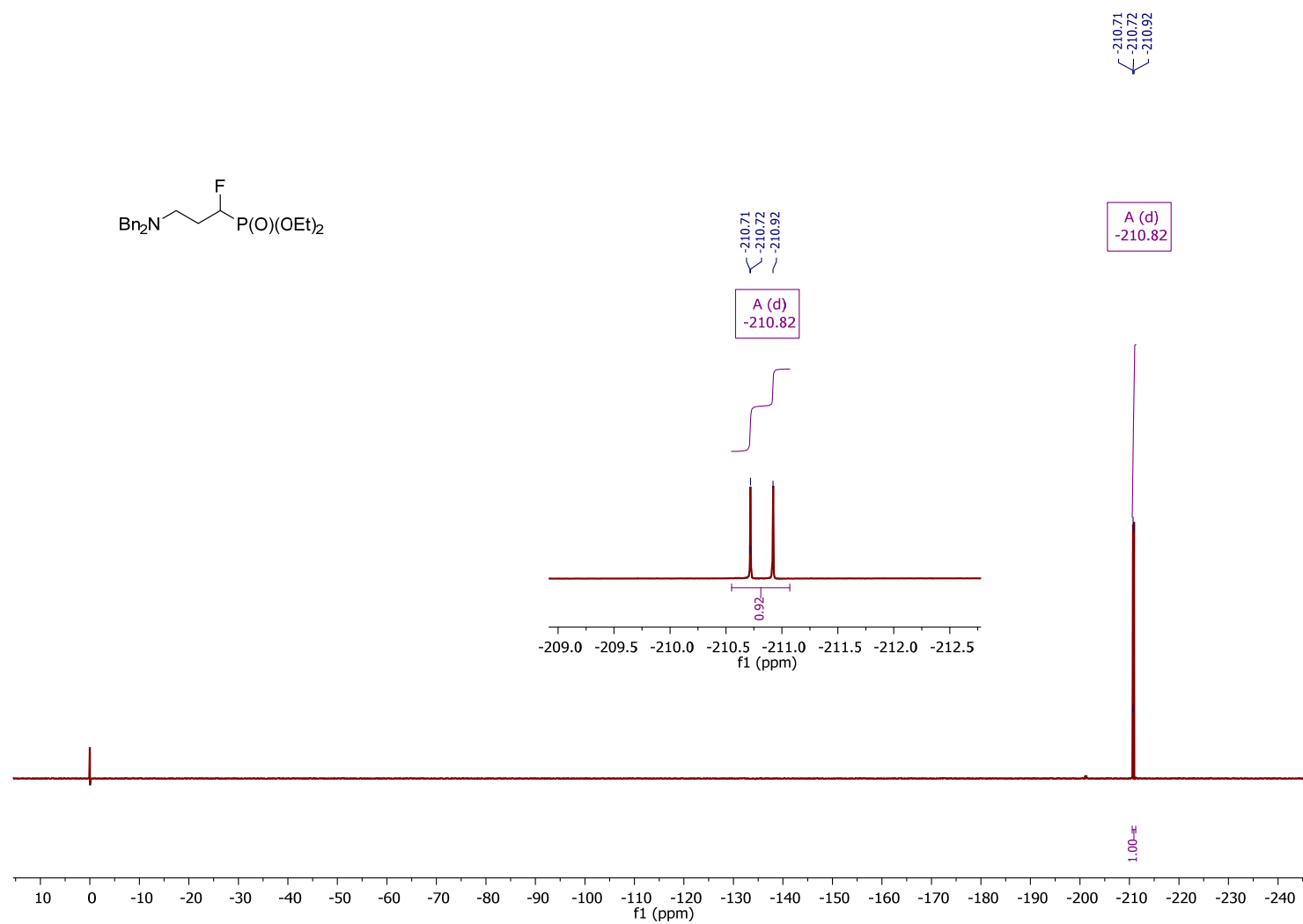
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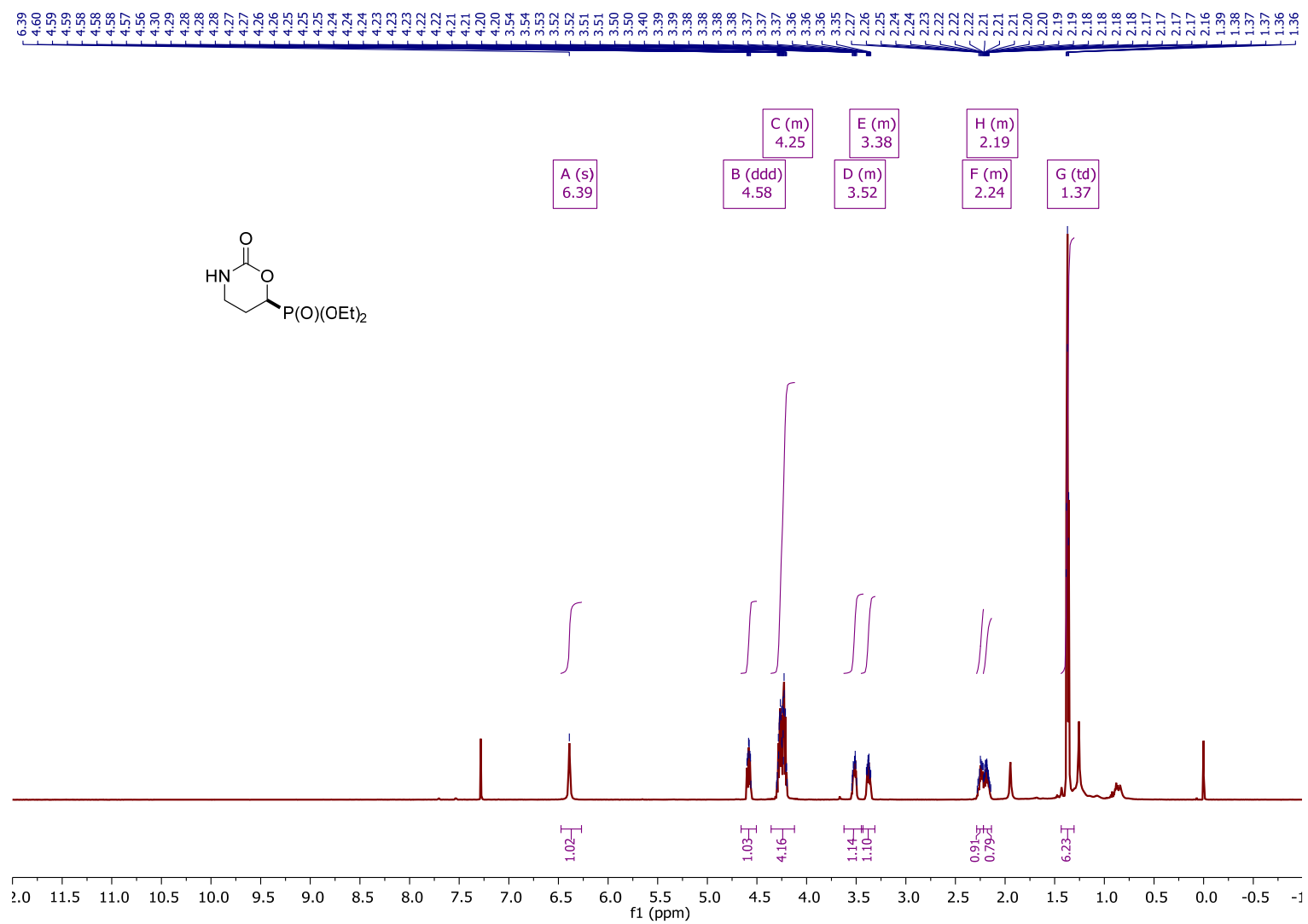
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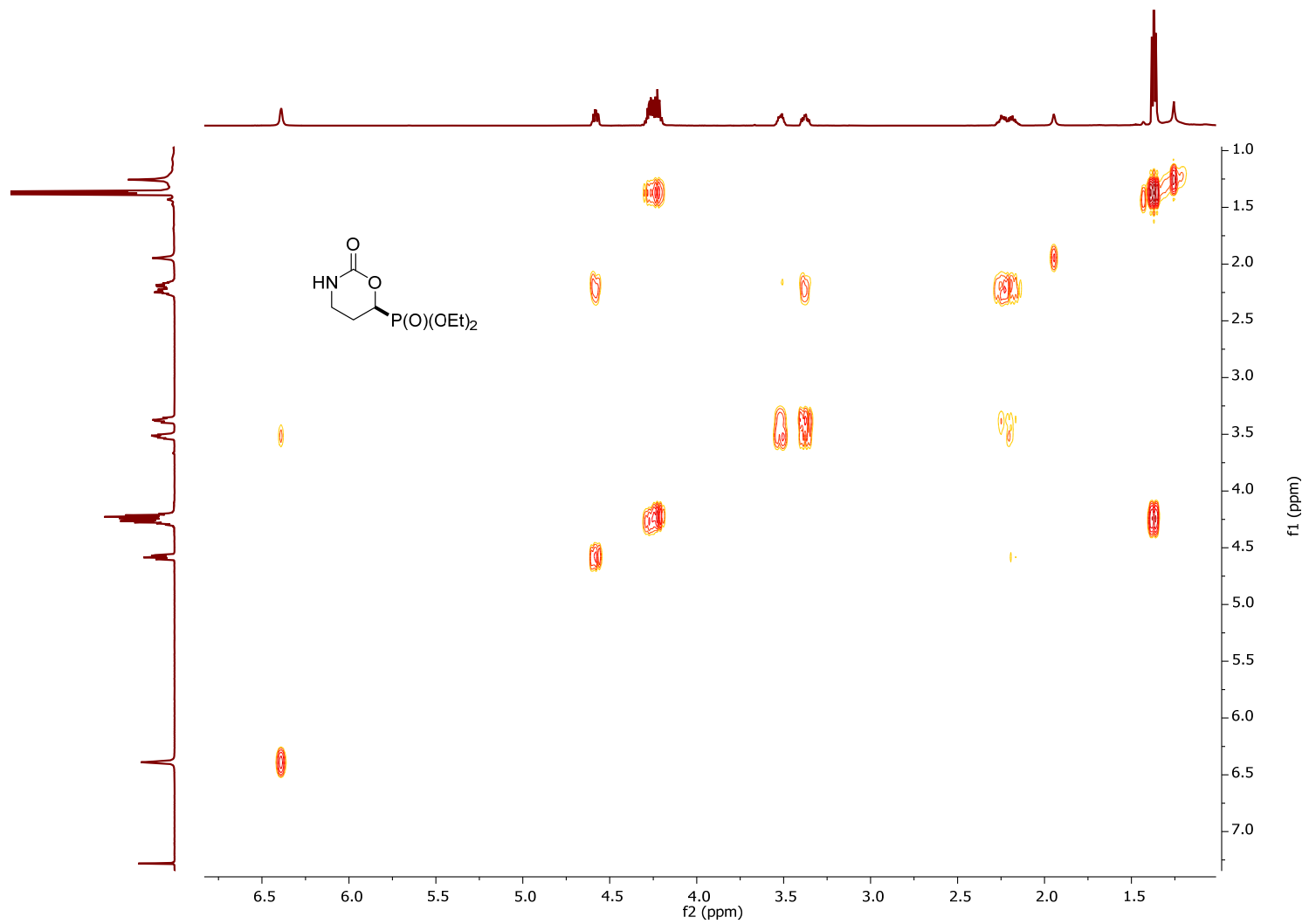
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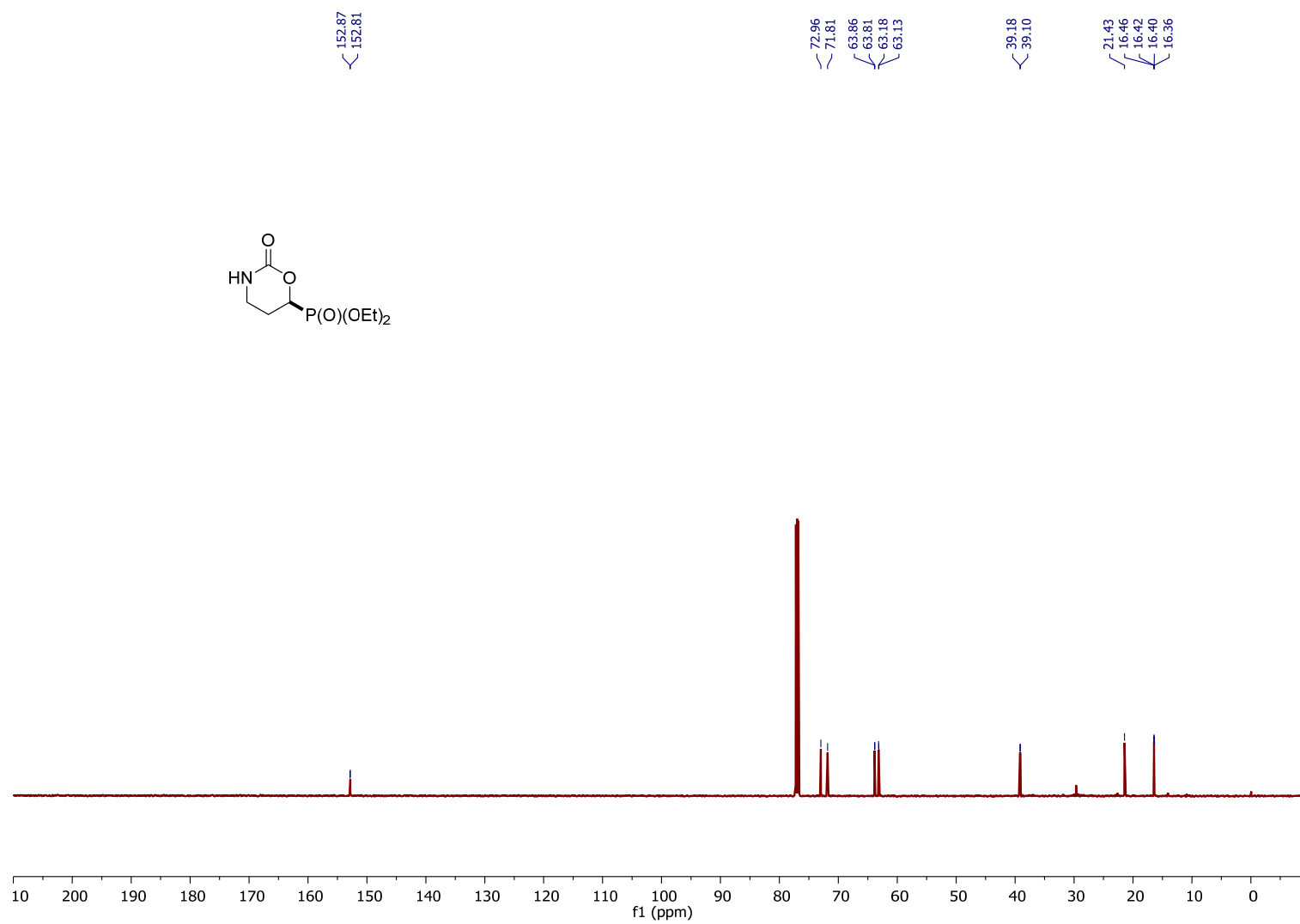
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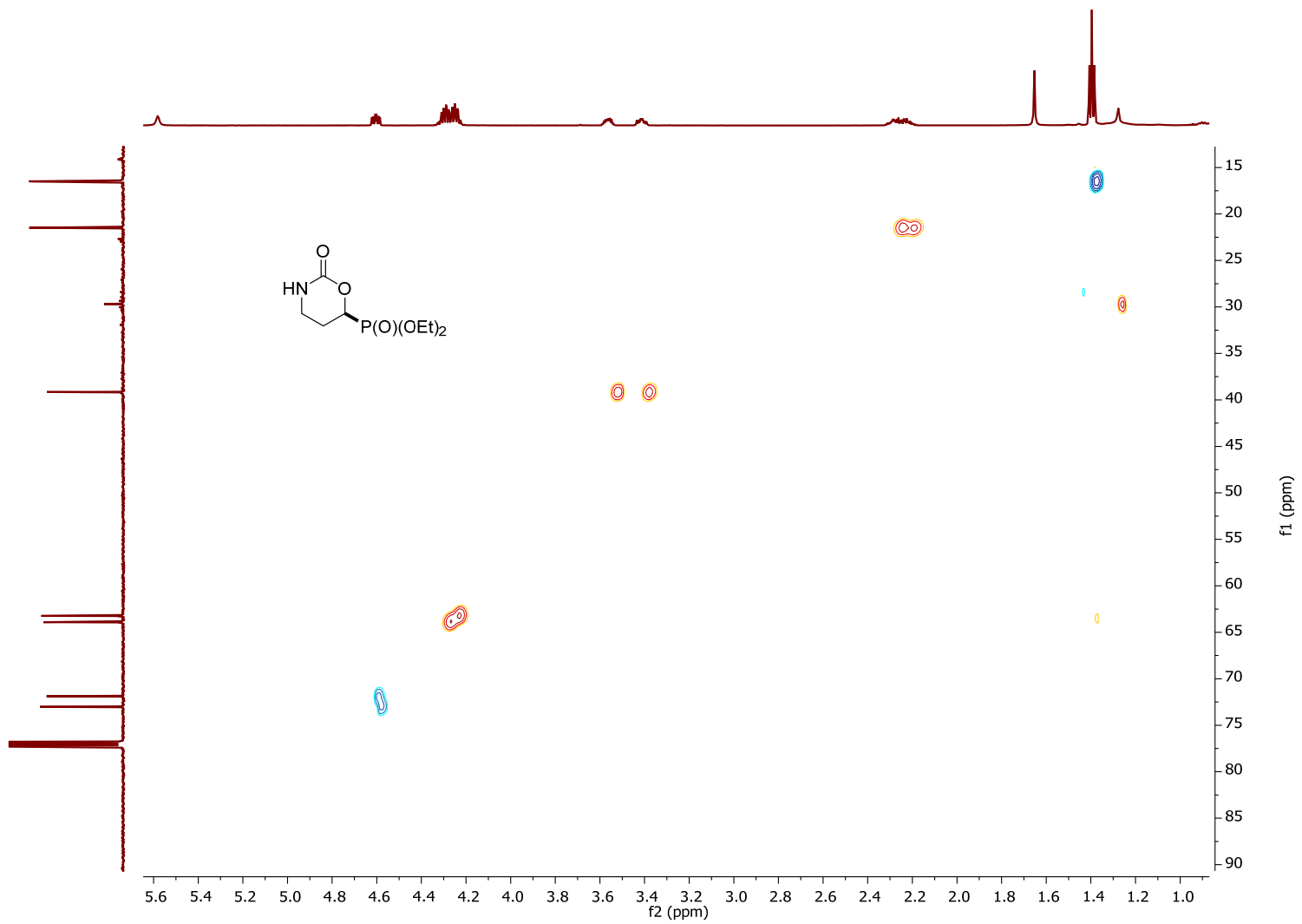
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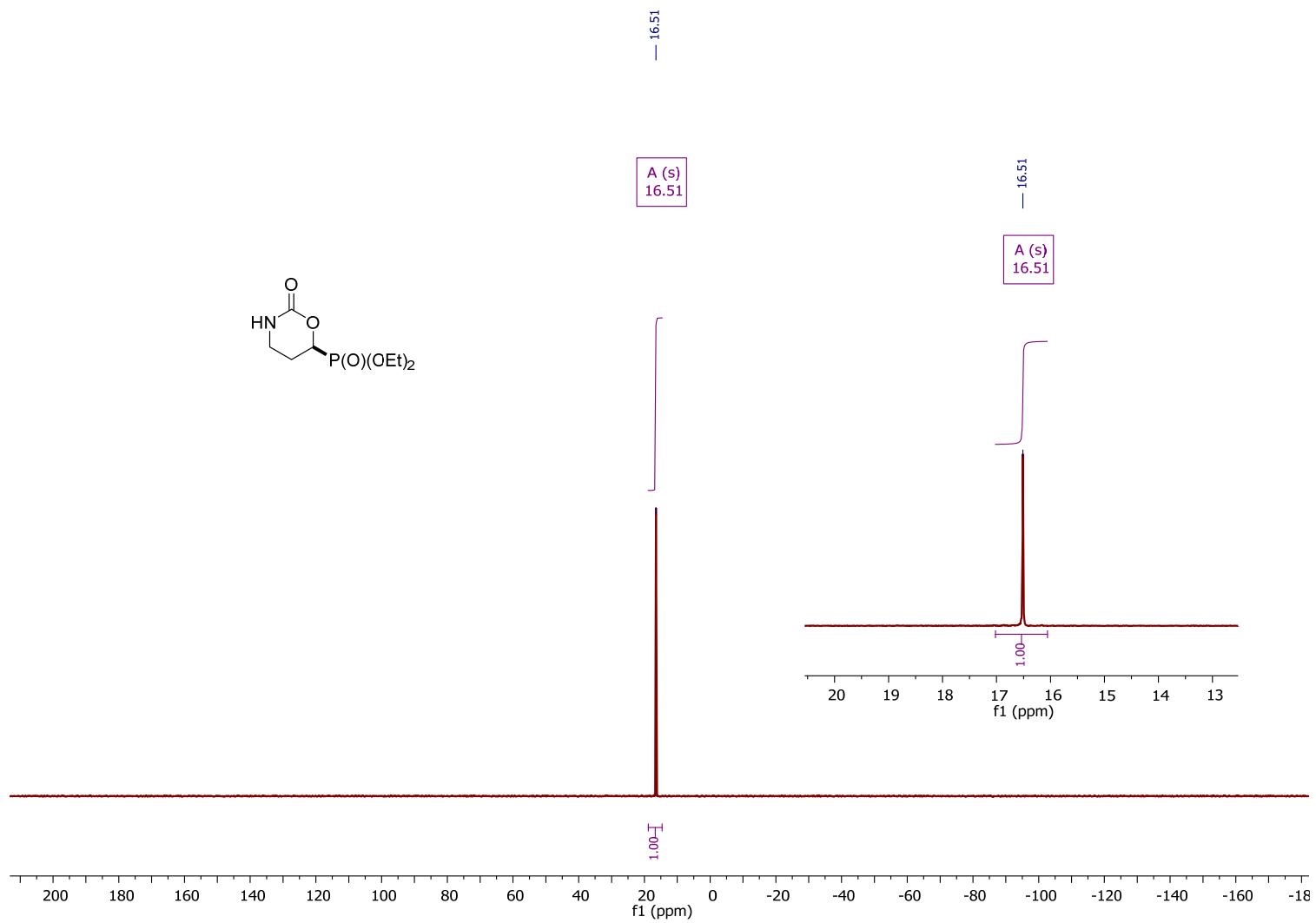
¹H-¹H COSY of rac-16a.



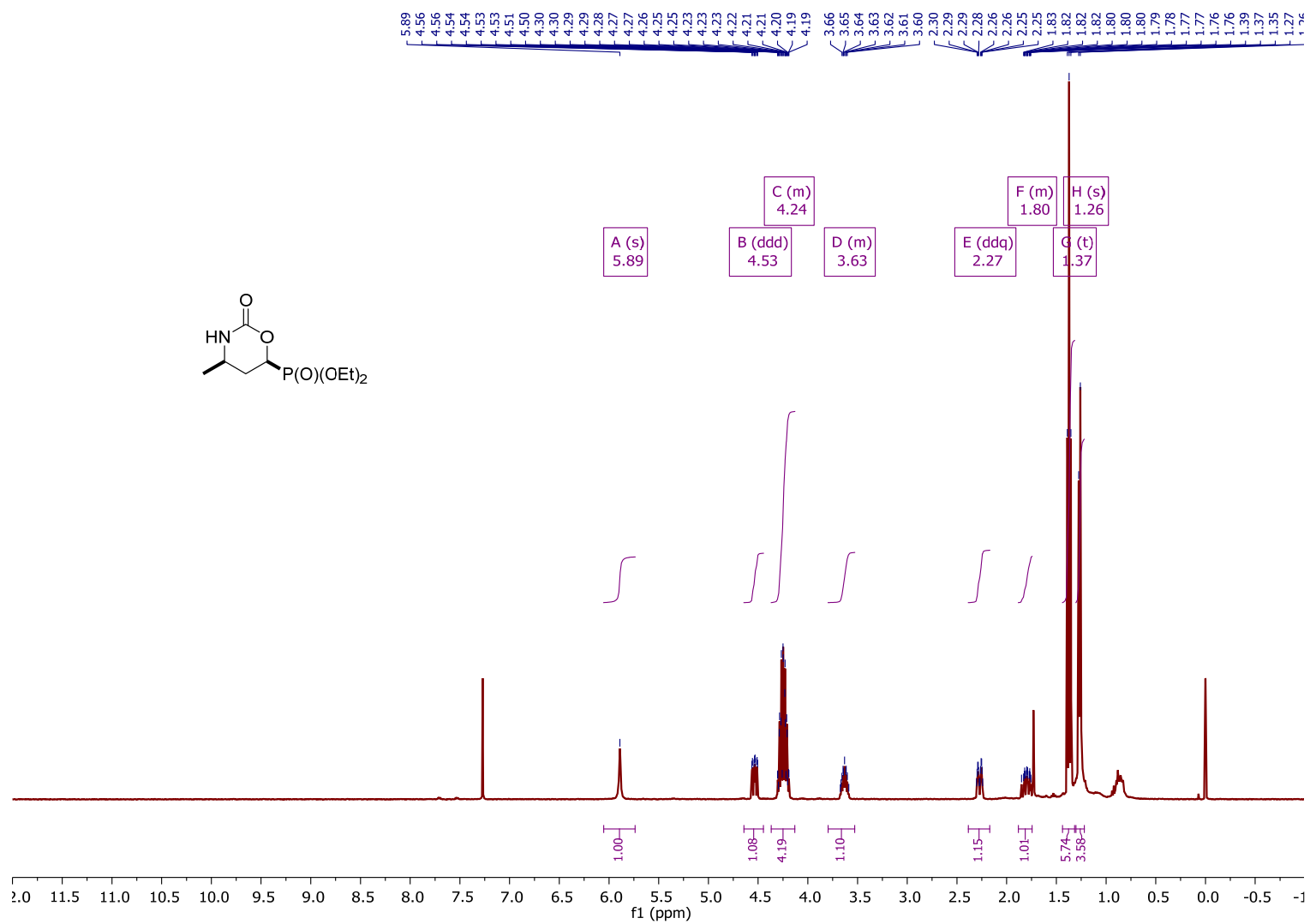
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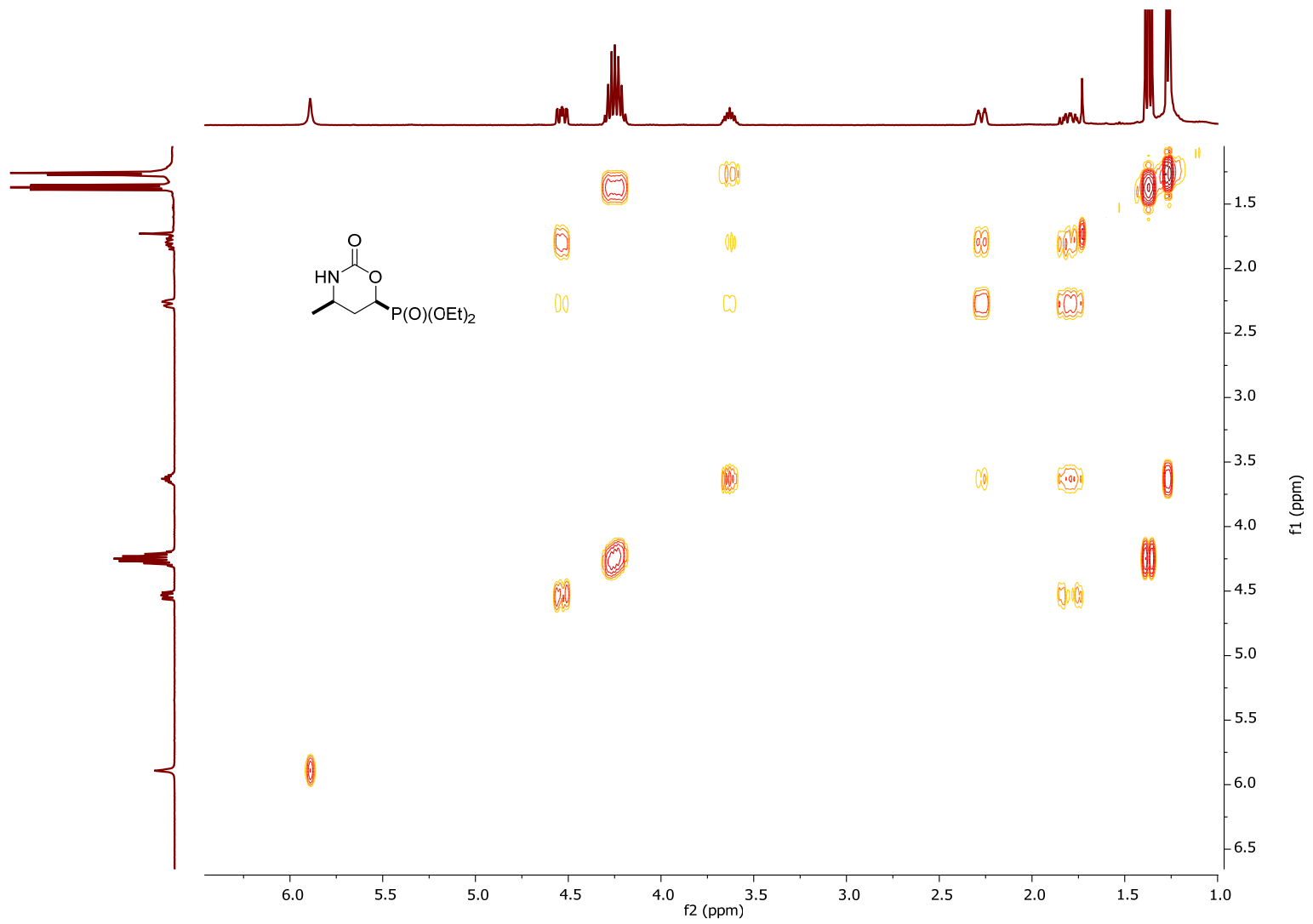
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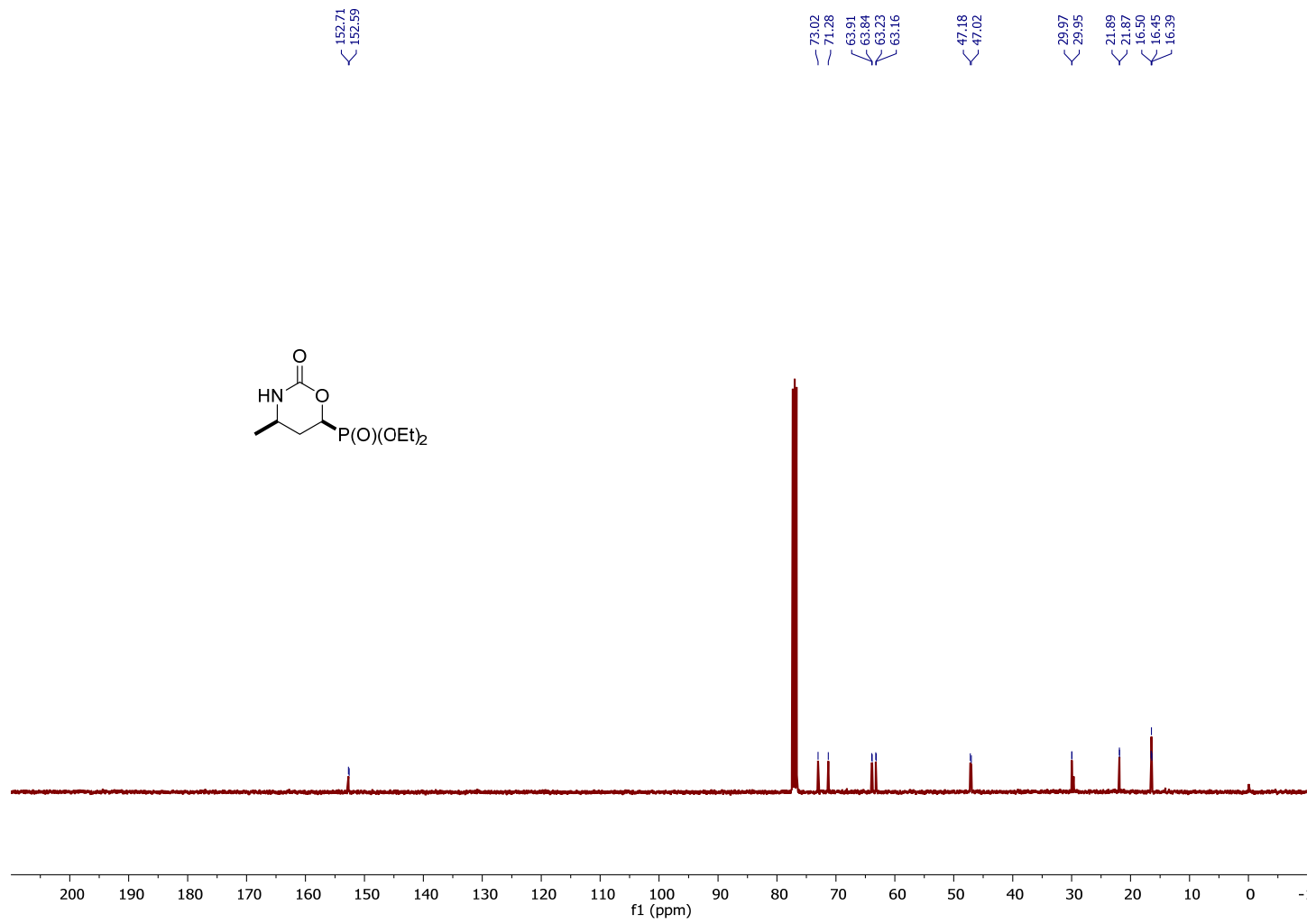
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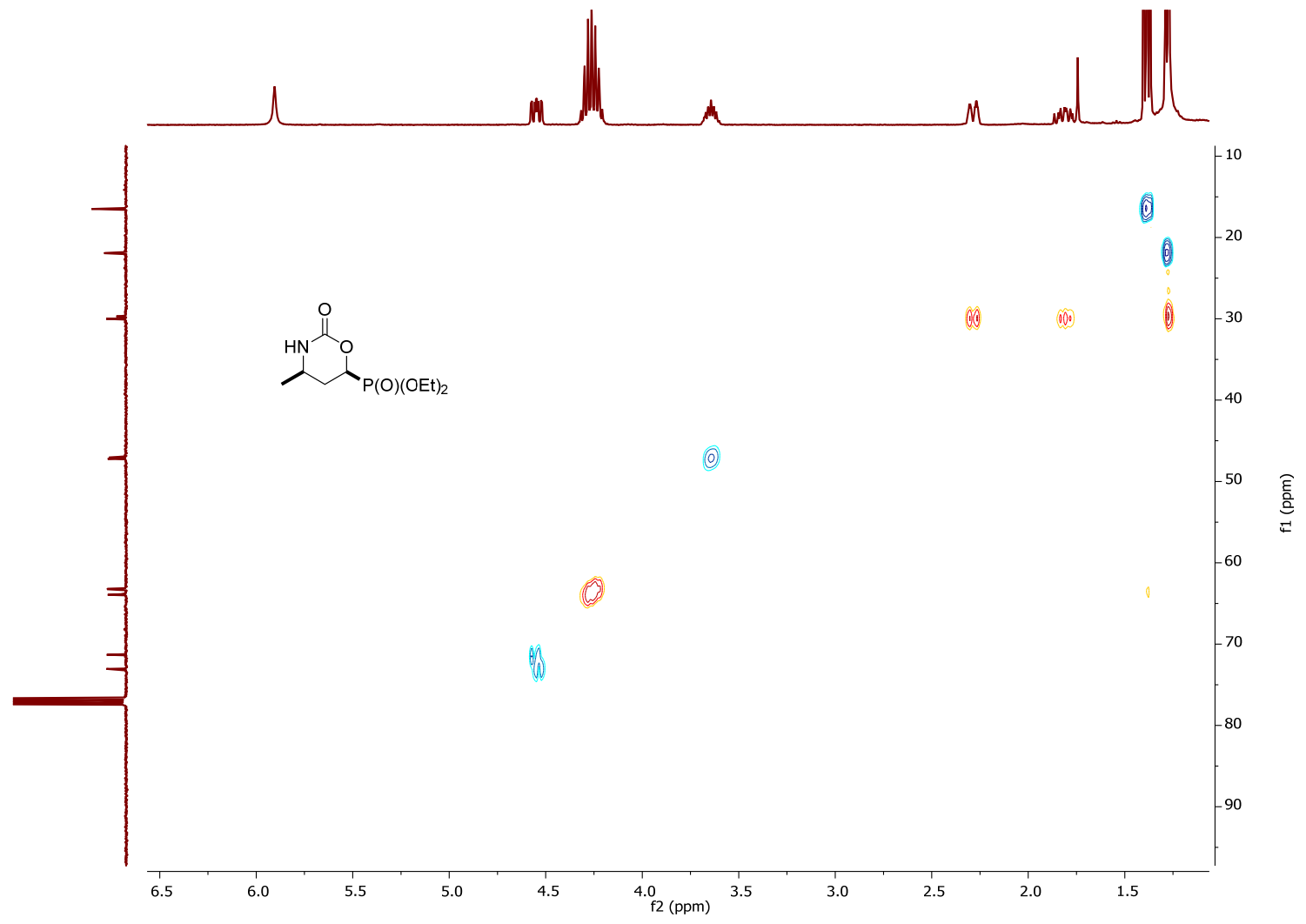
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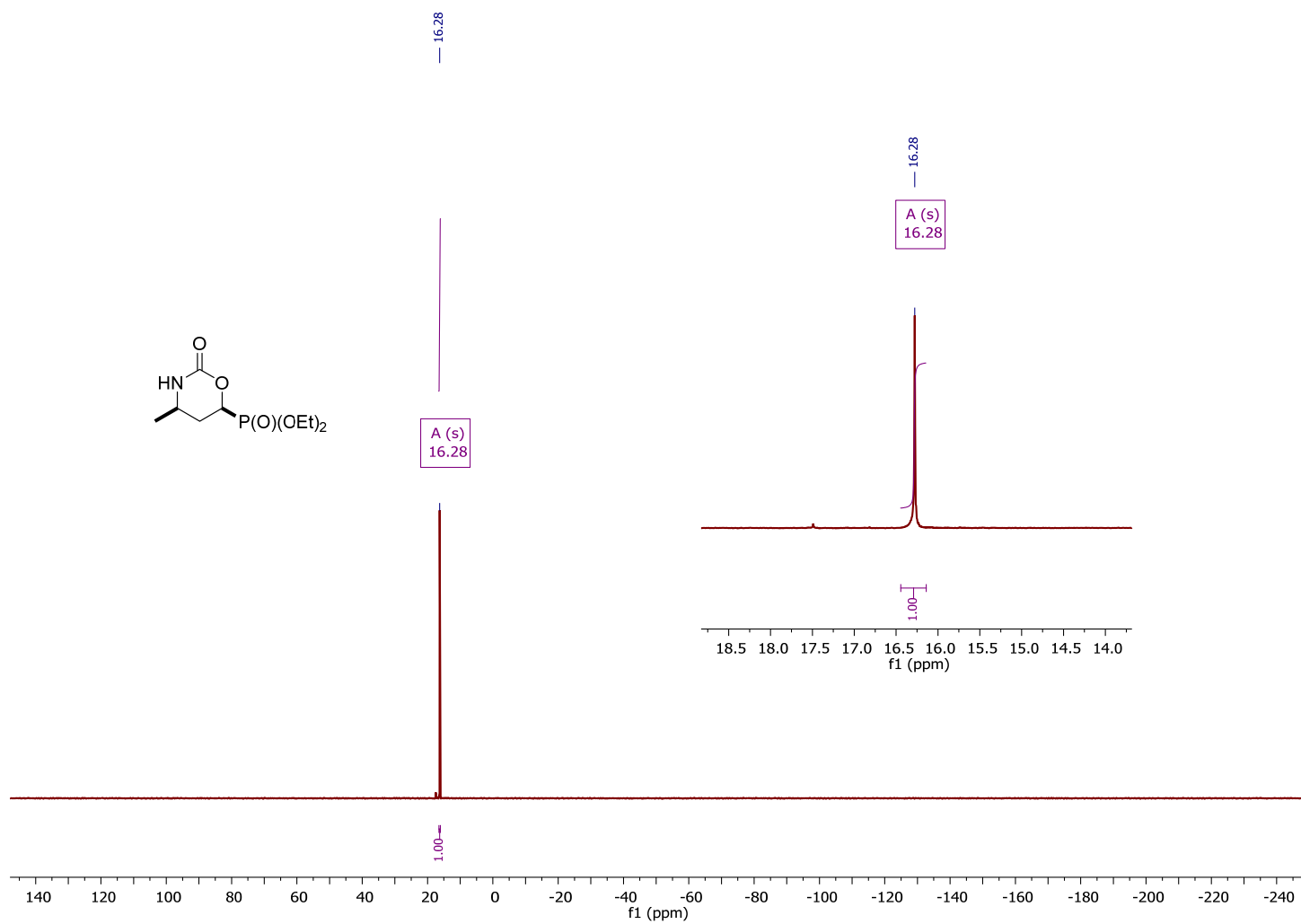
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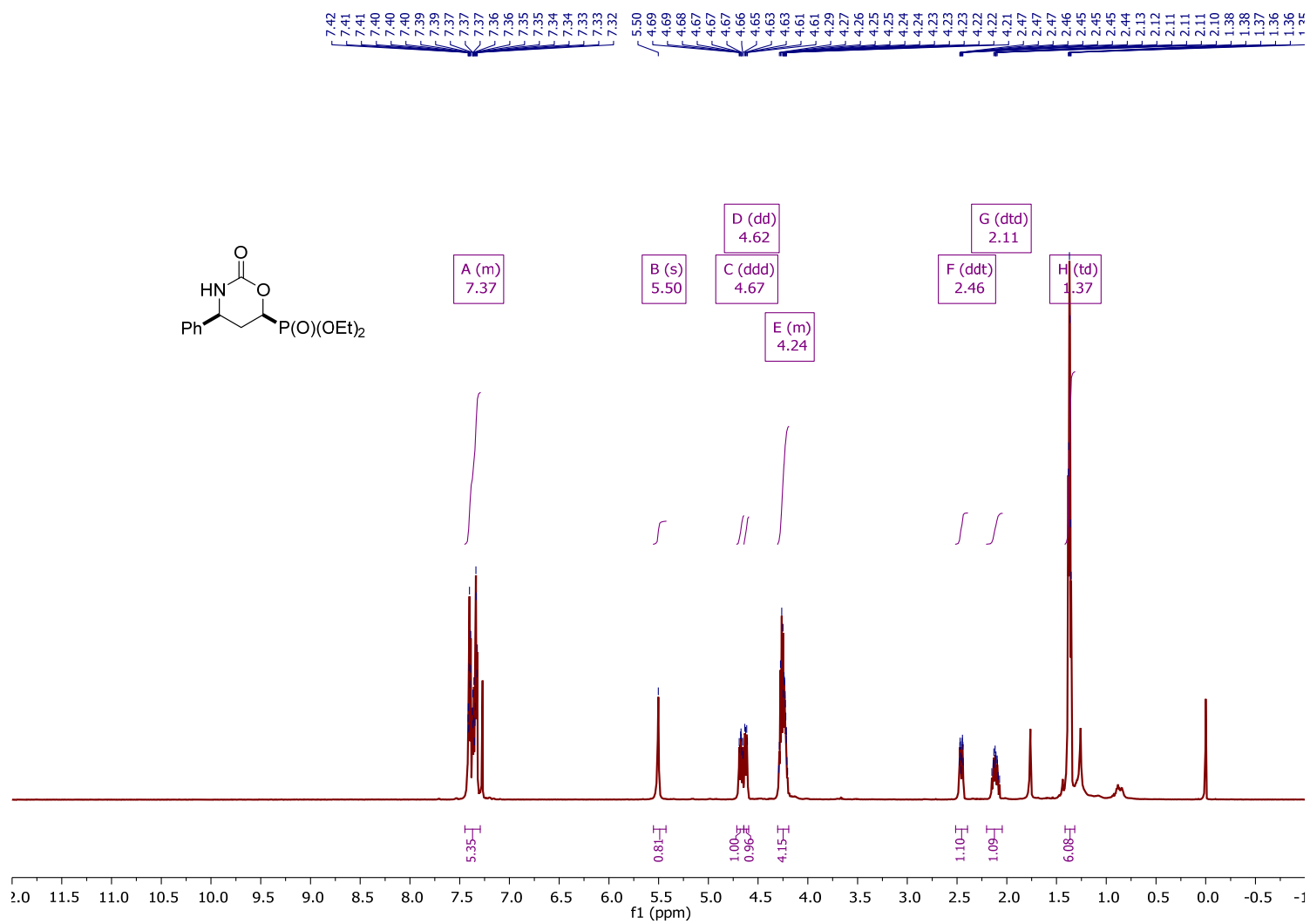
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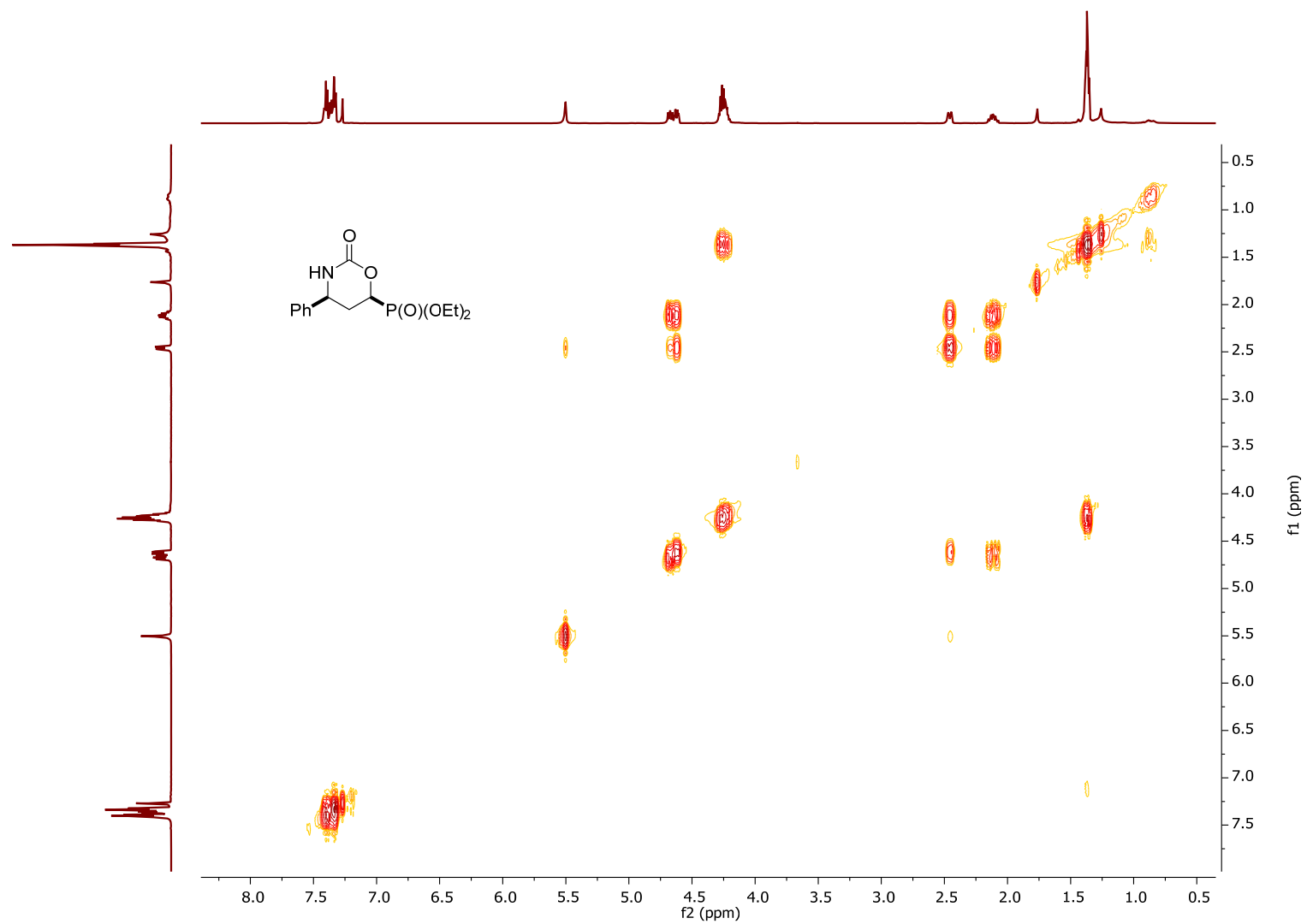
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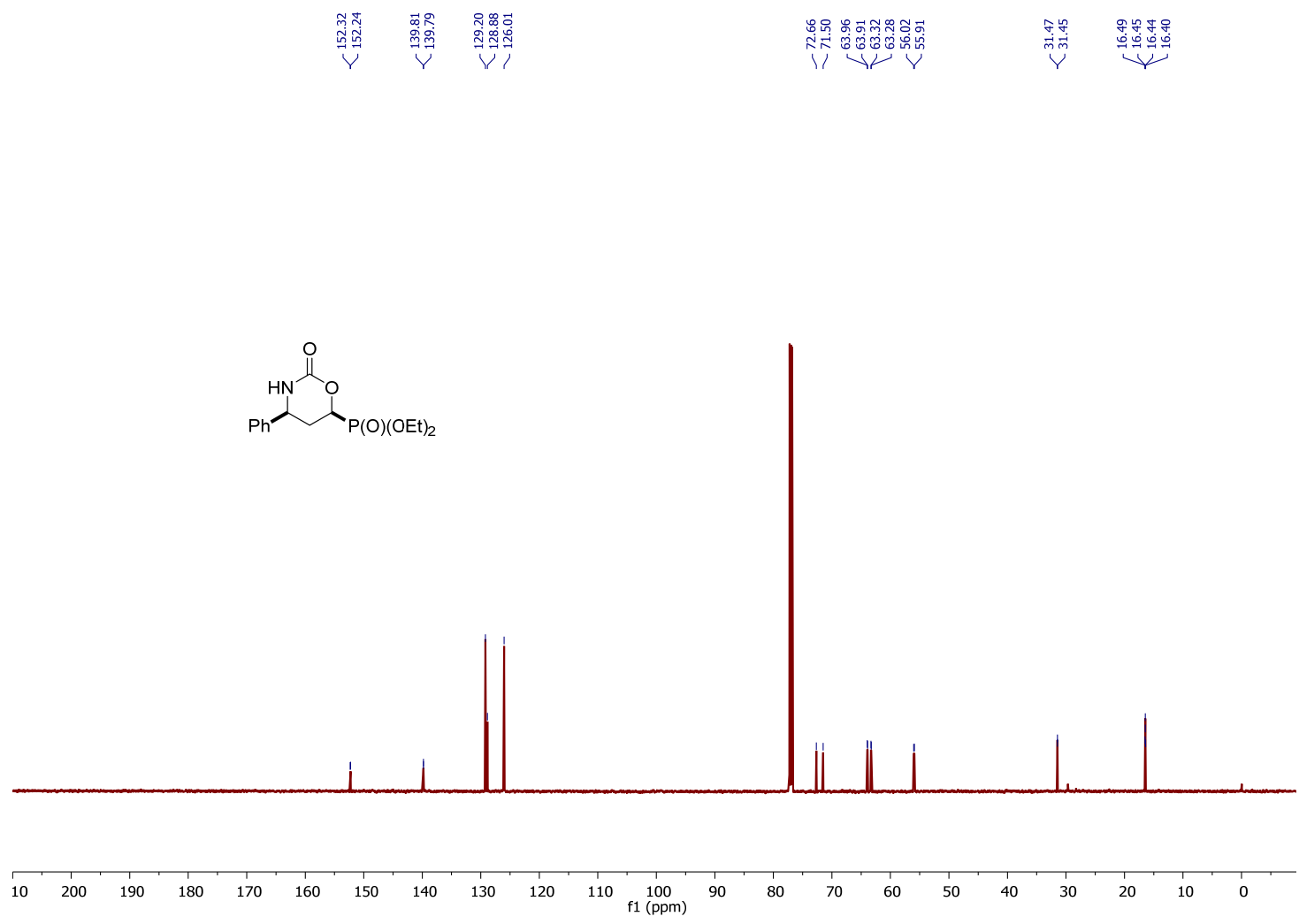
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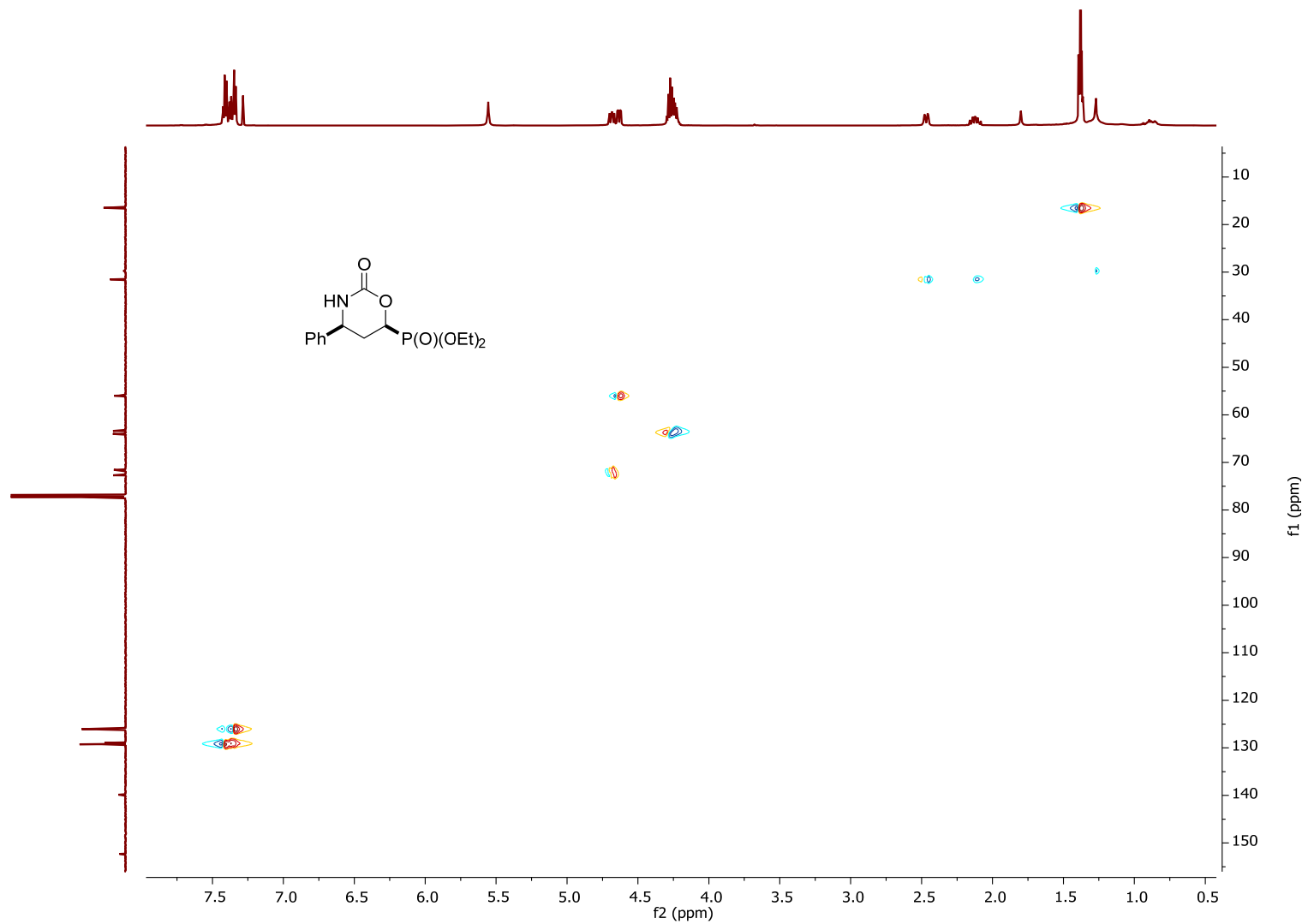
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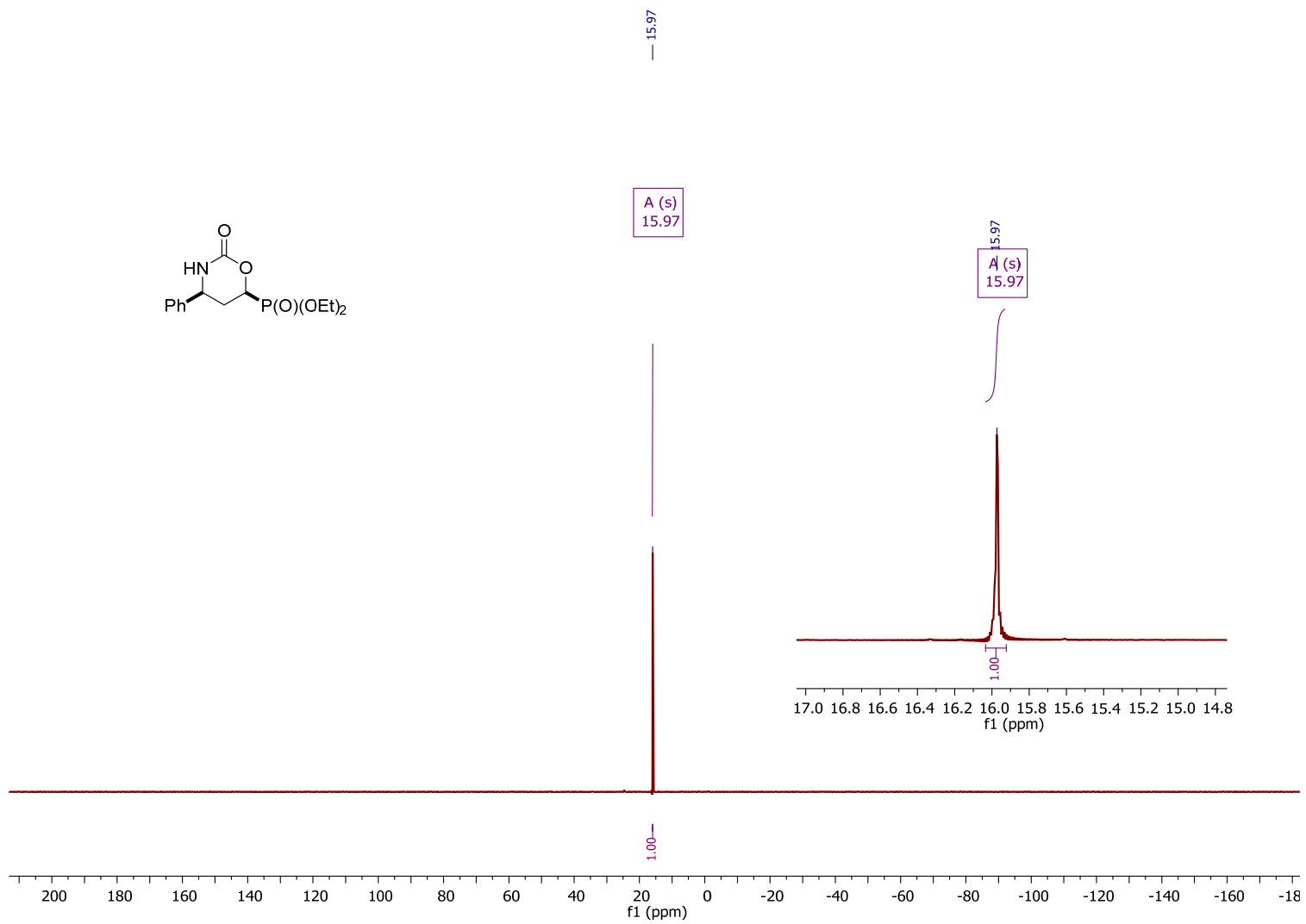
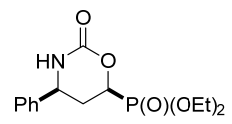


^1H - ^1H COSY of **rac-16c**.

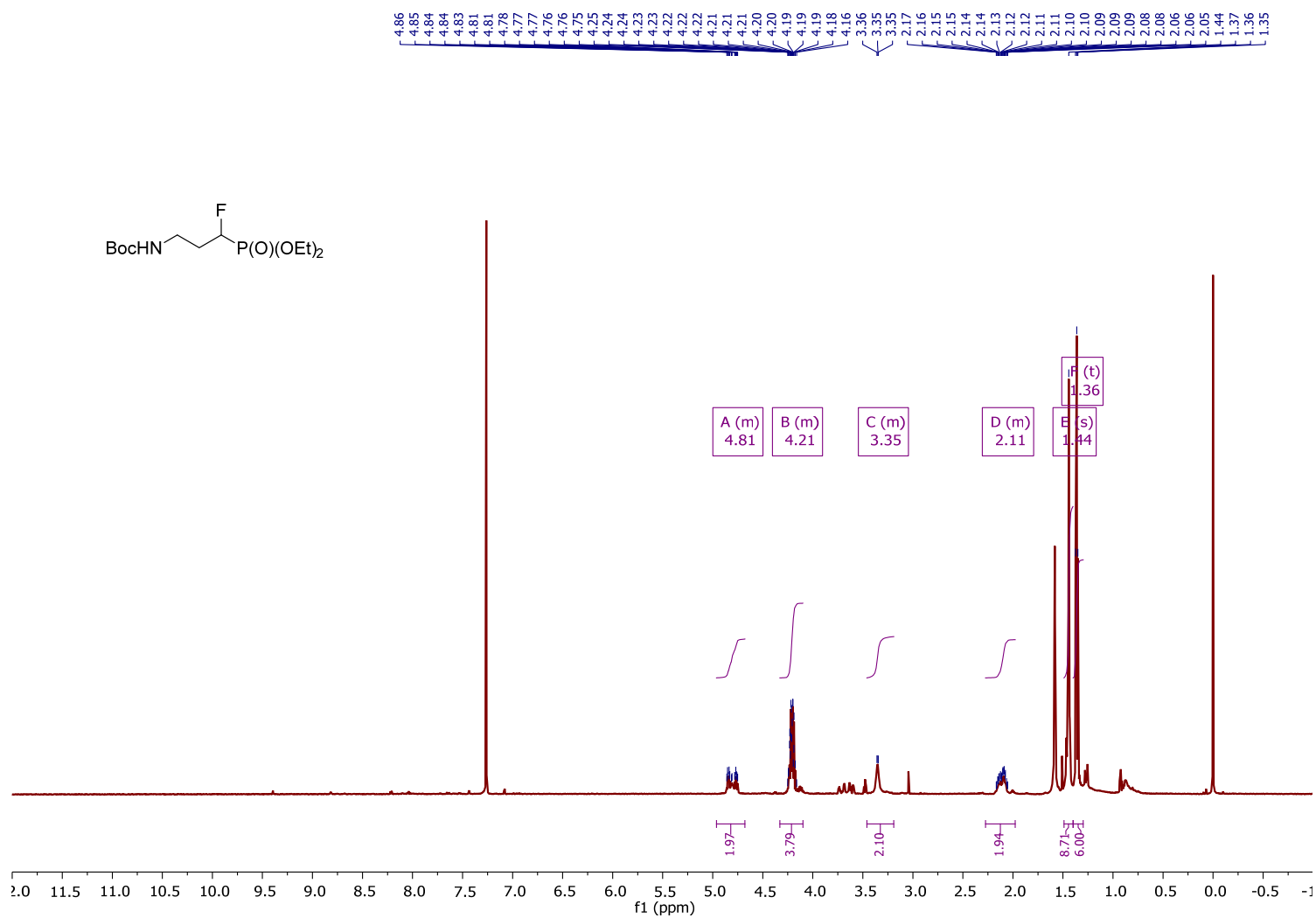


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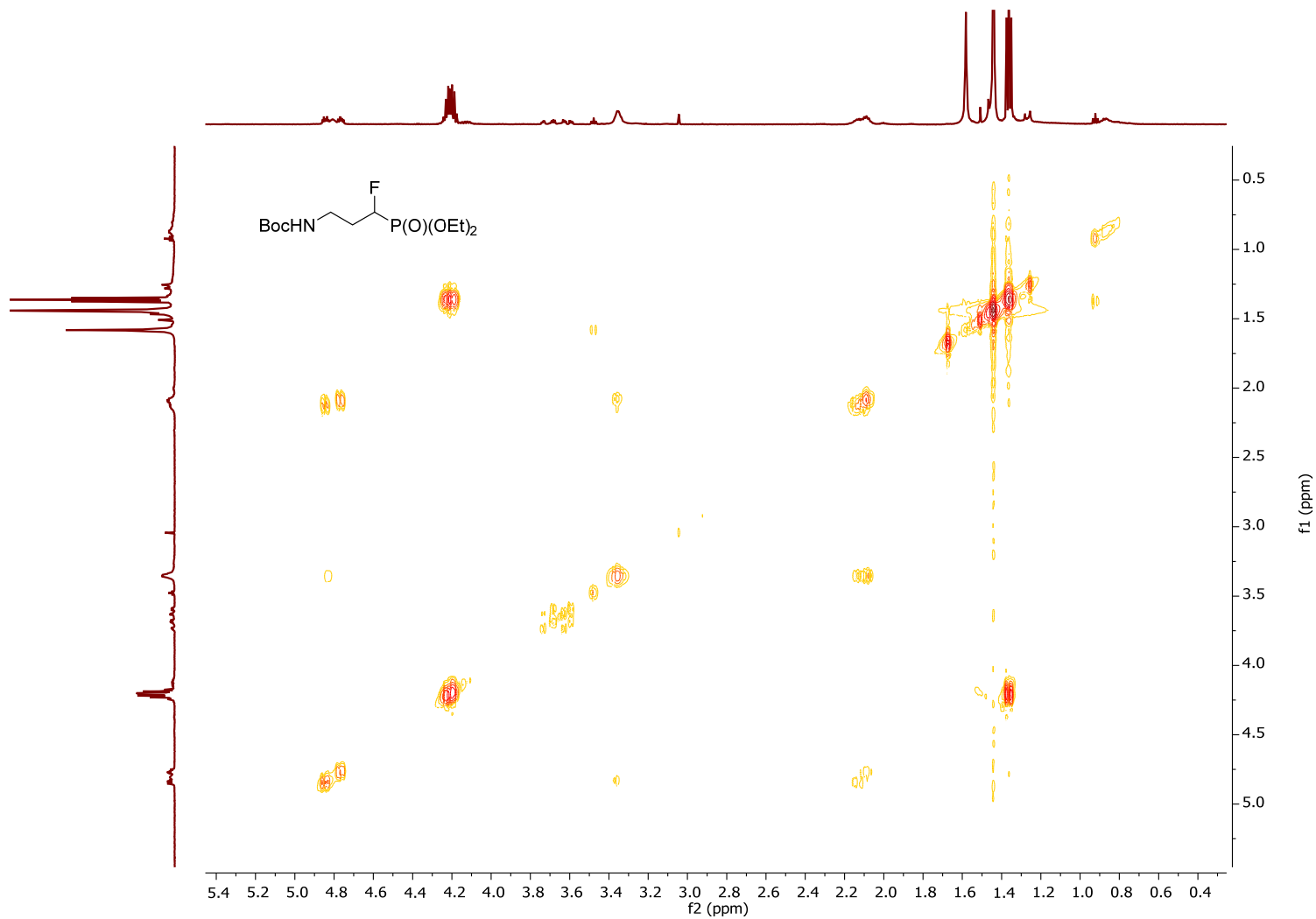




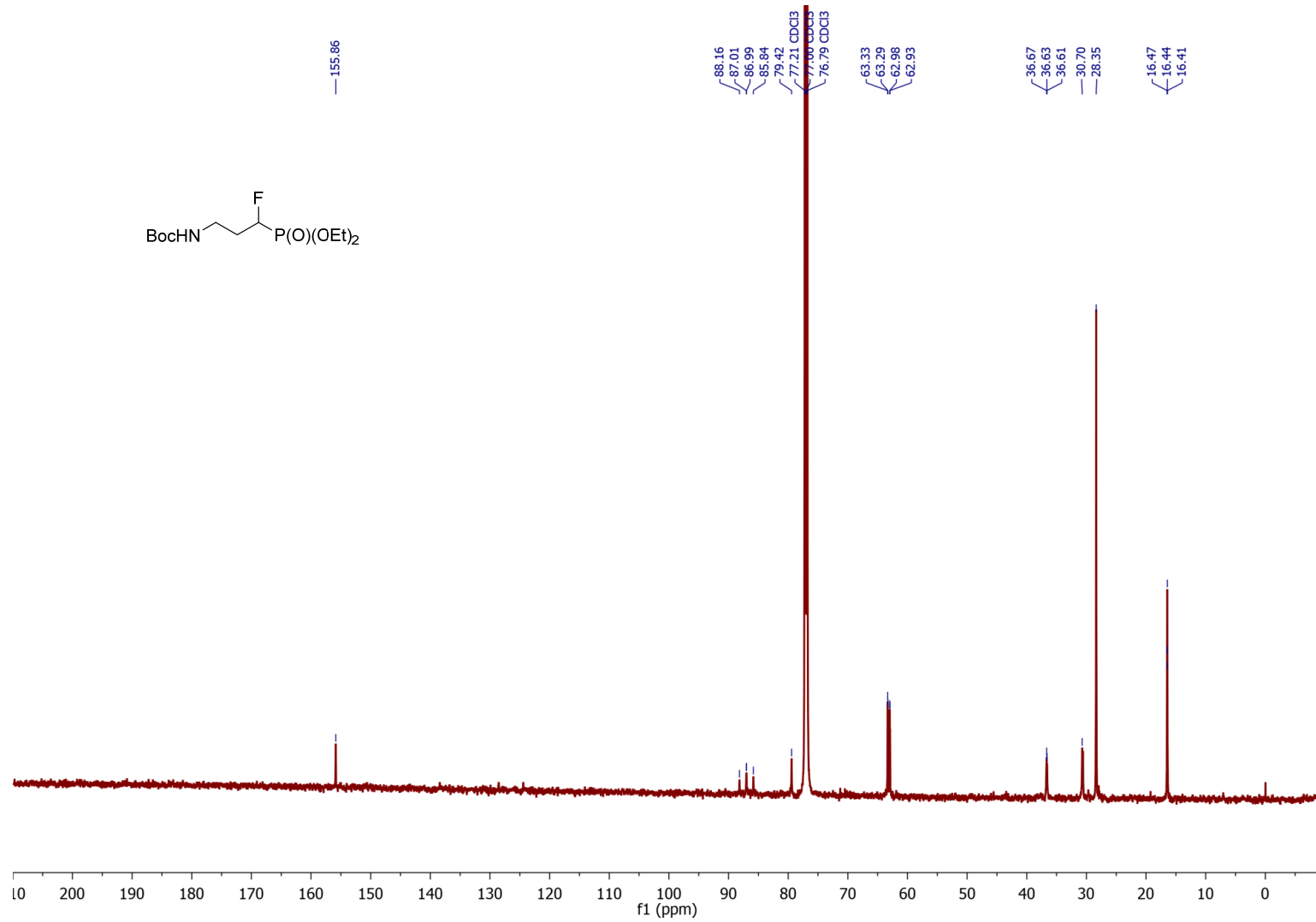
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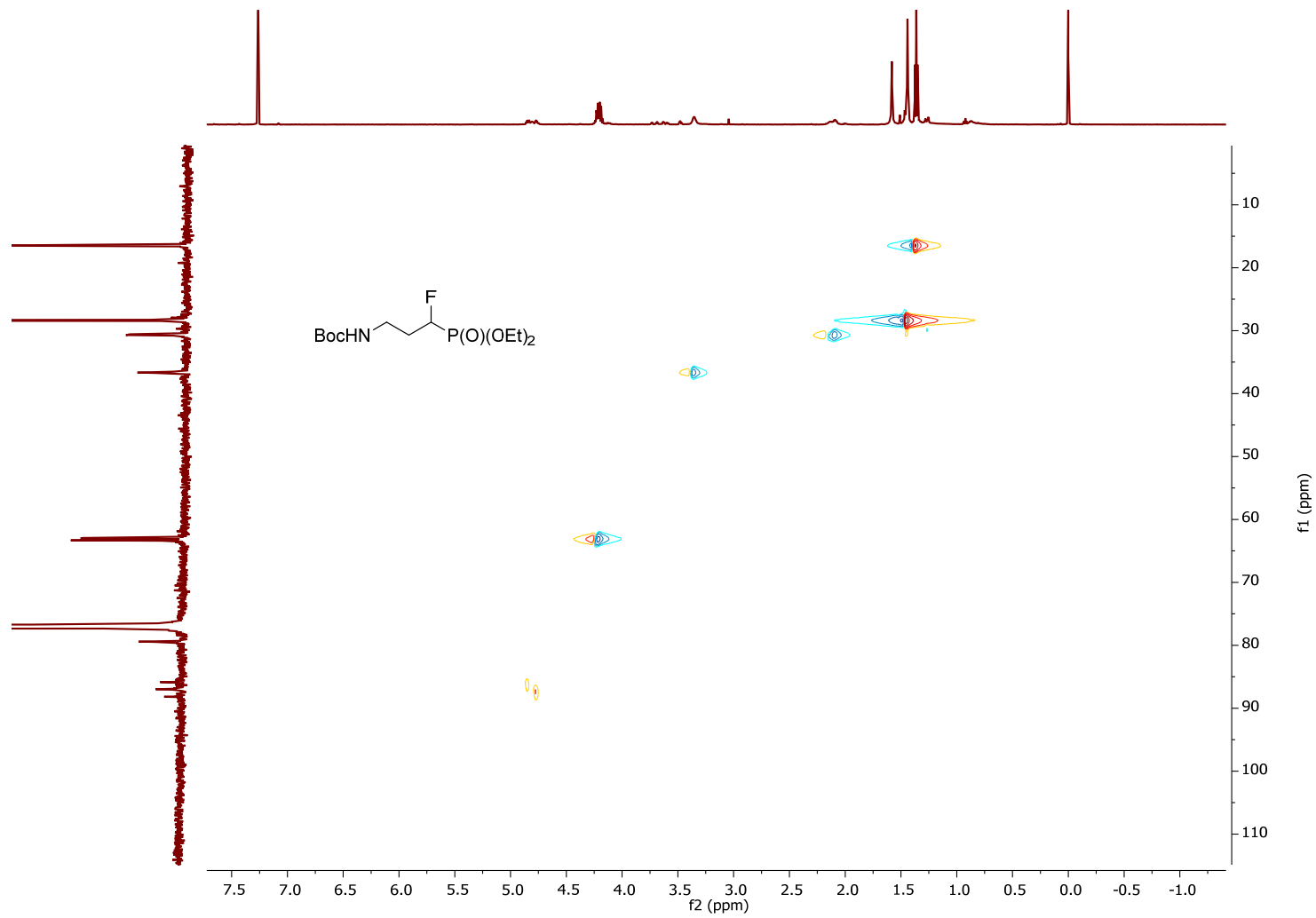
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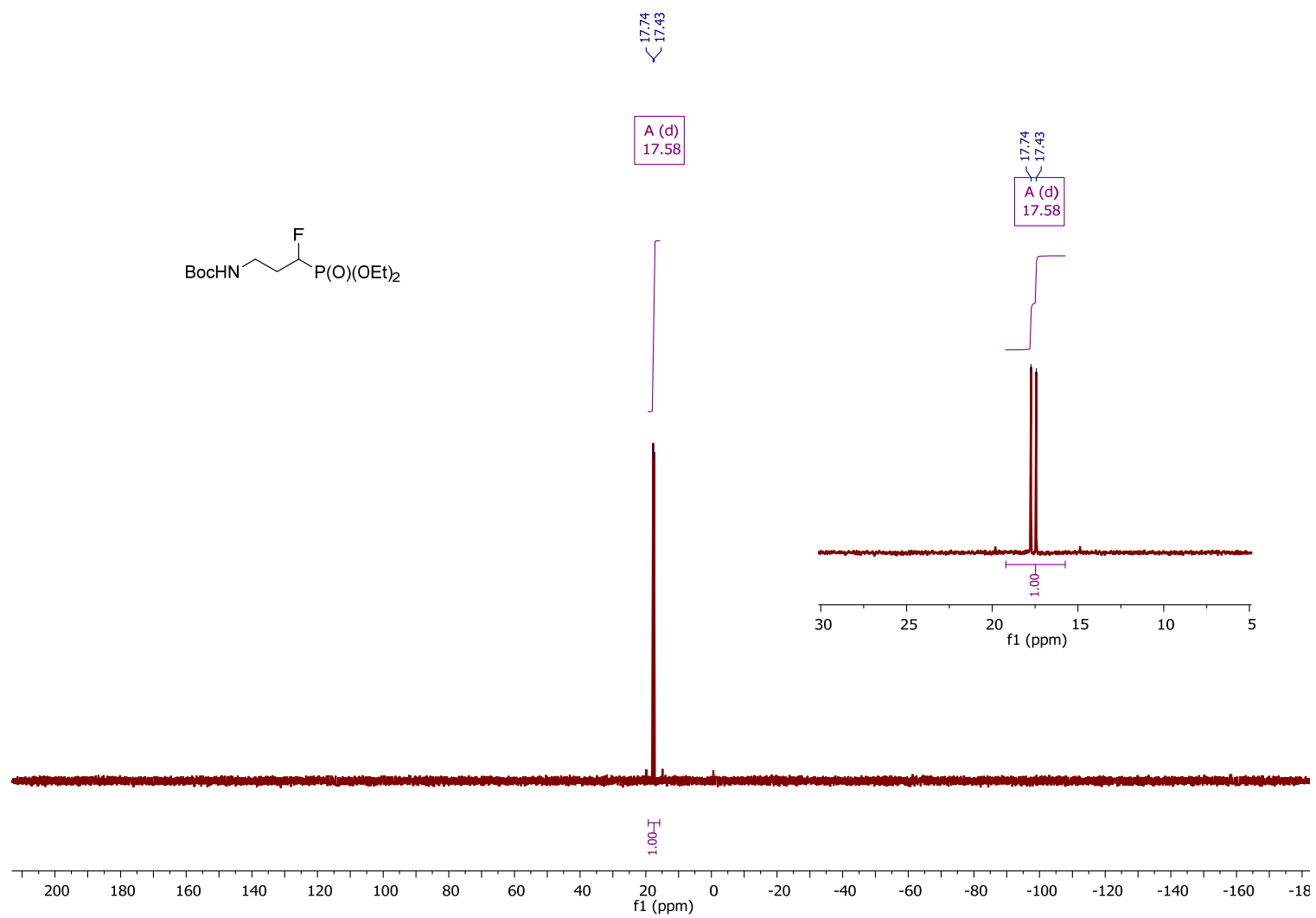
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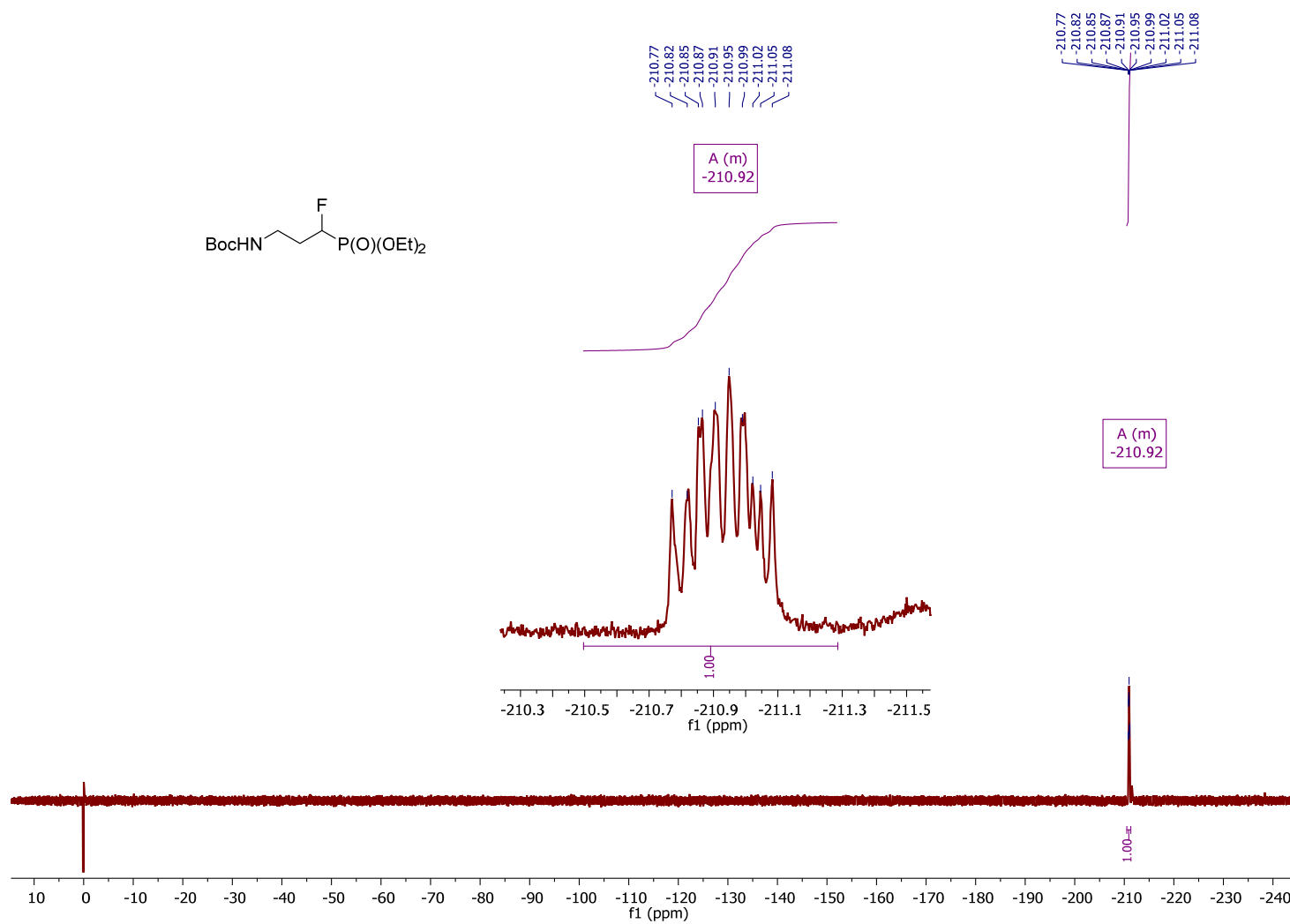
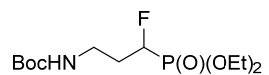
^{13}C NMR of **rac-17a**.



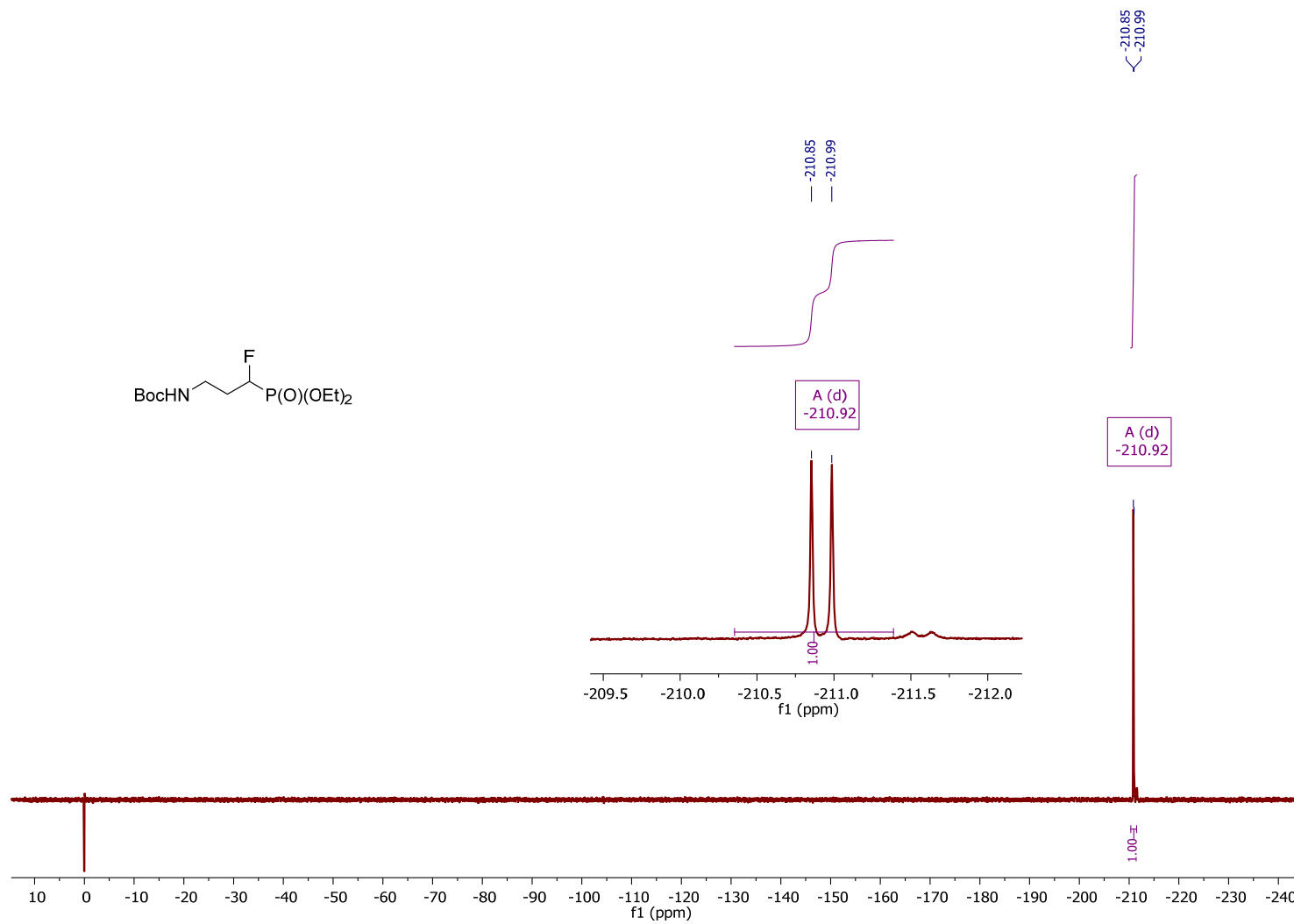
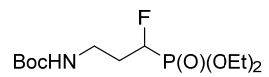
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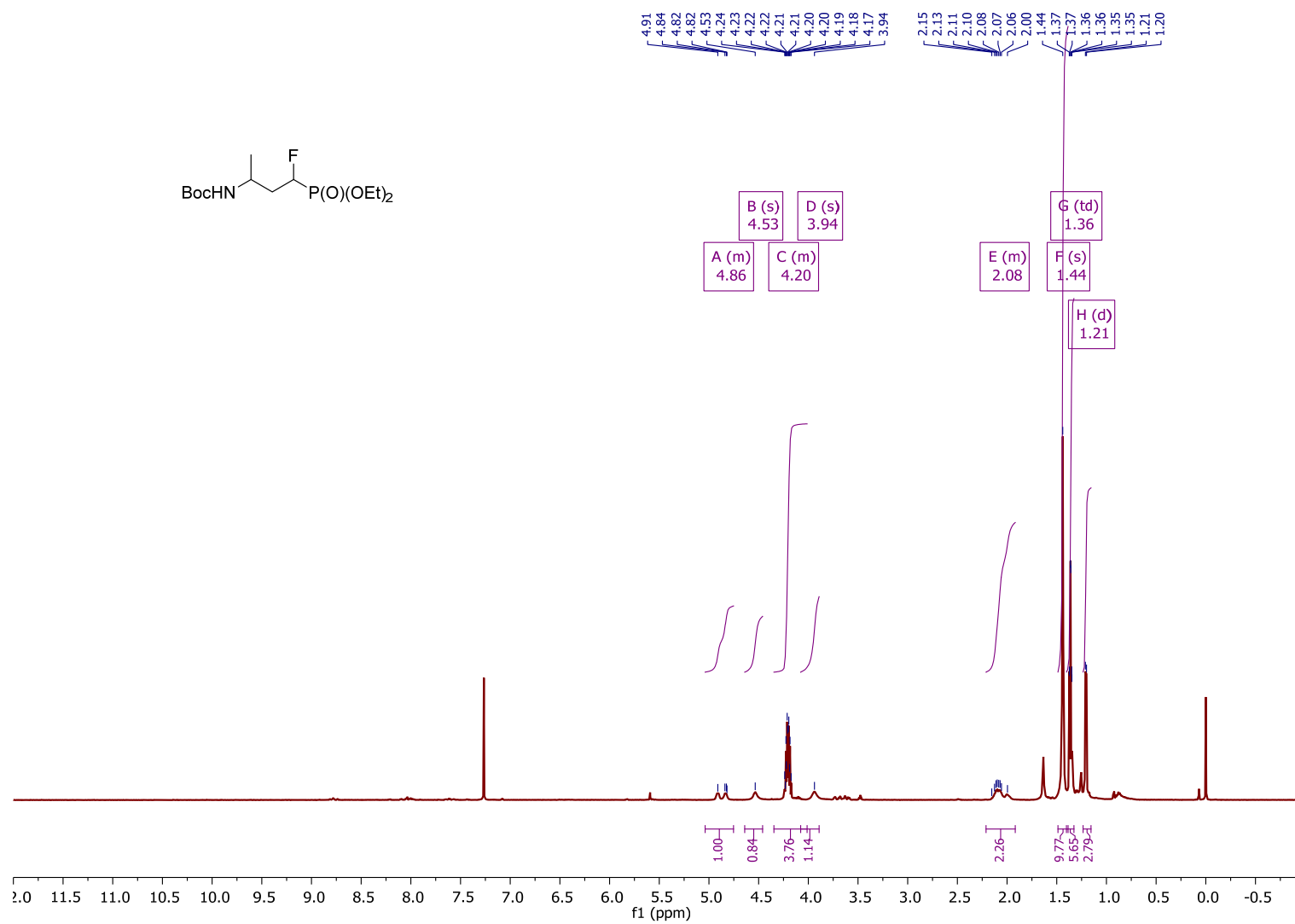
$^{31}\text{P}\{^1\text{H}\}$ NMR of rac-17a.



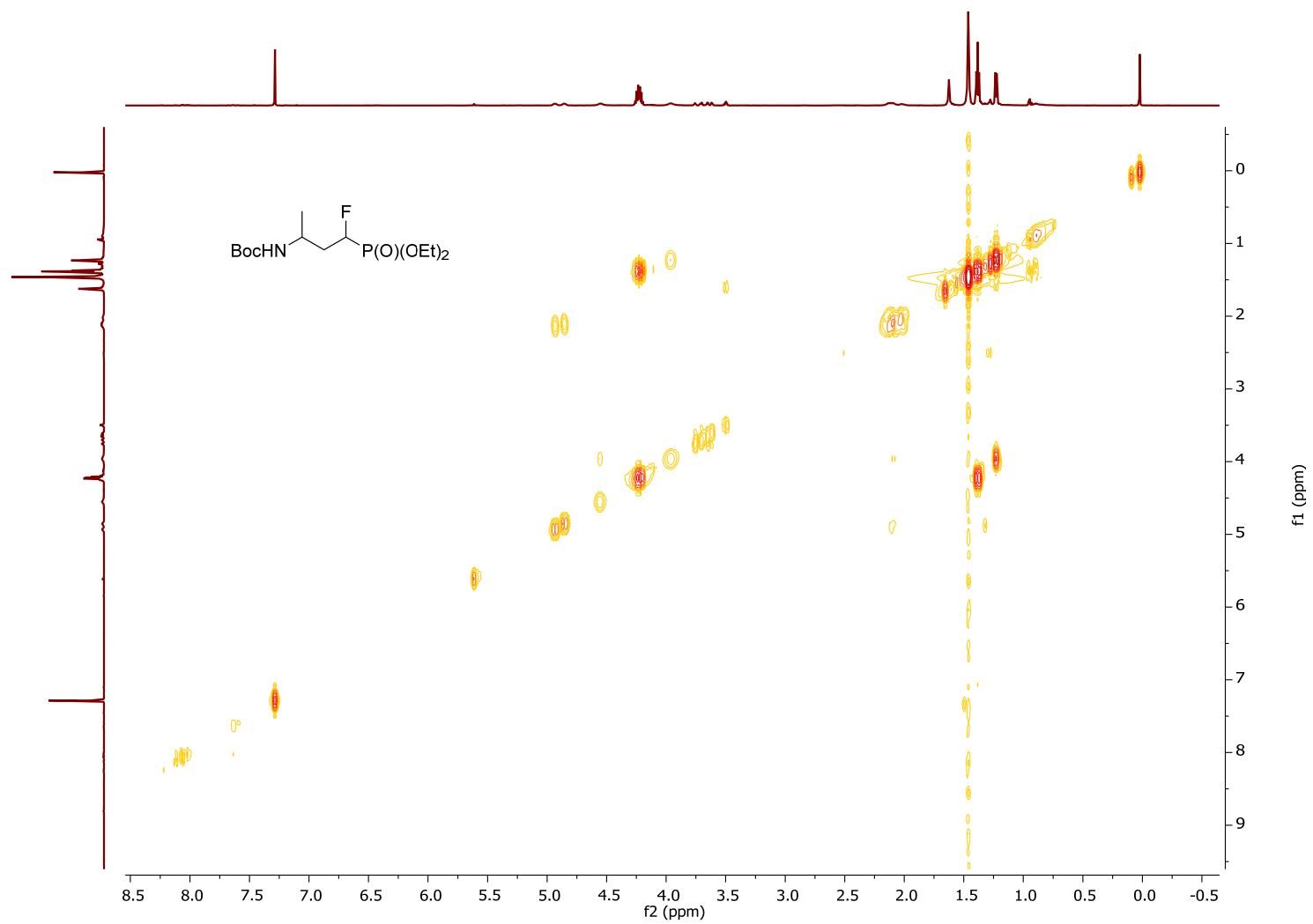
^{19}F NMR of rac-17a.



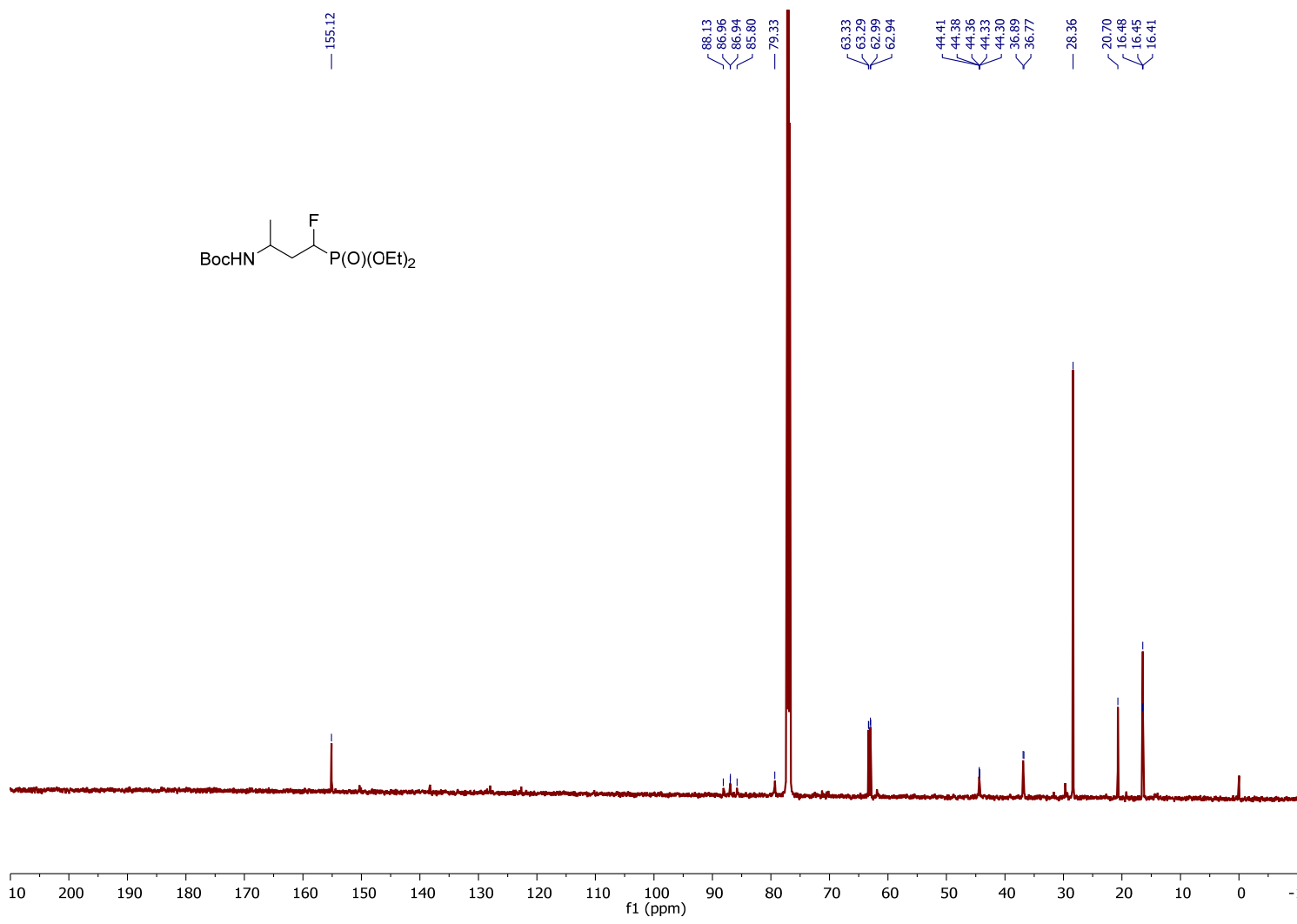
¹⁹F{¹H} NMR of rac-17a.



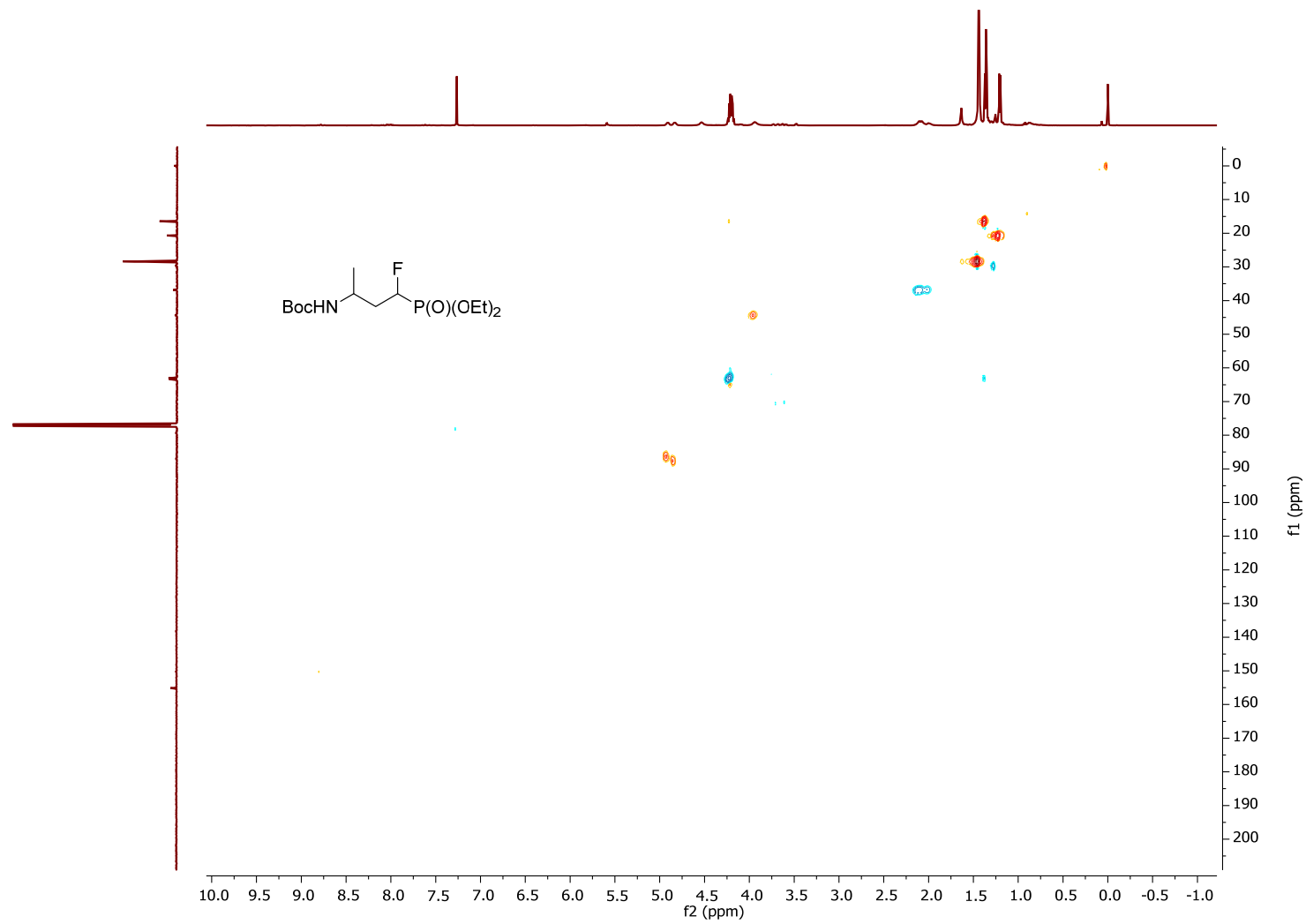
^1H NMR of rac-17b.



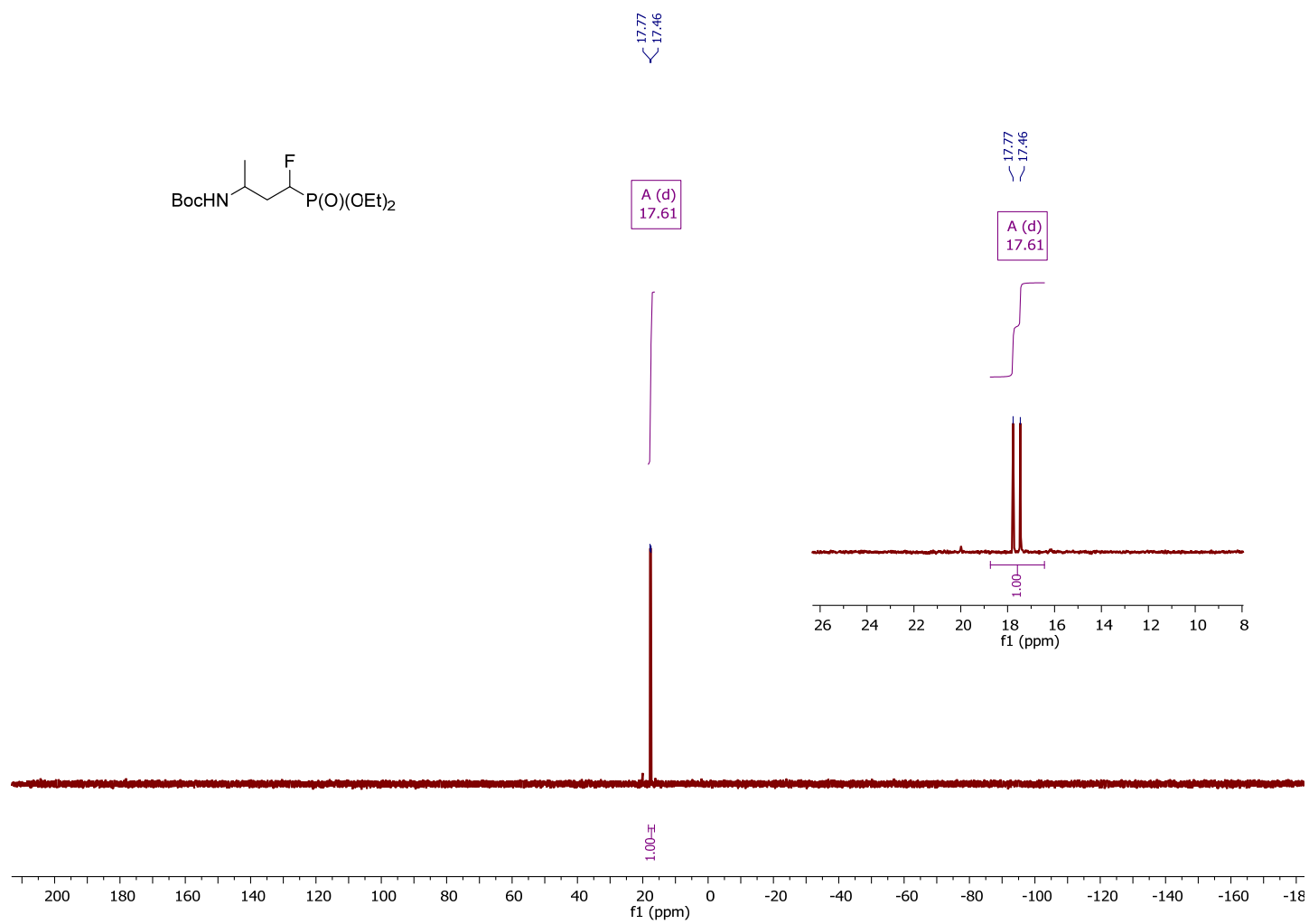
¹H-¹H COSY of rac-**17b**.



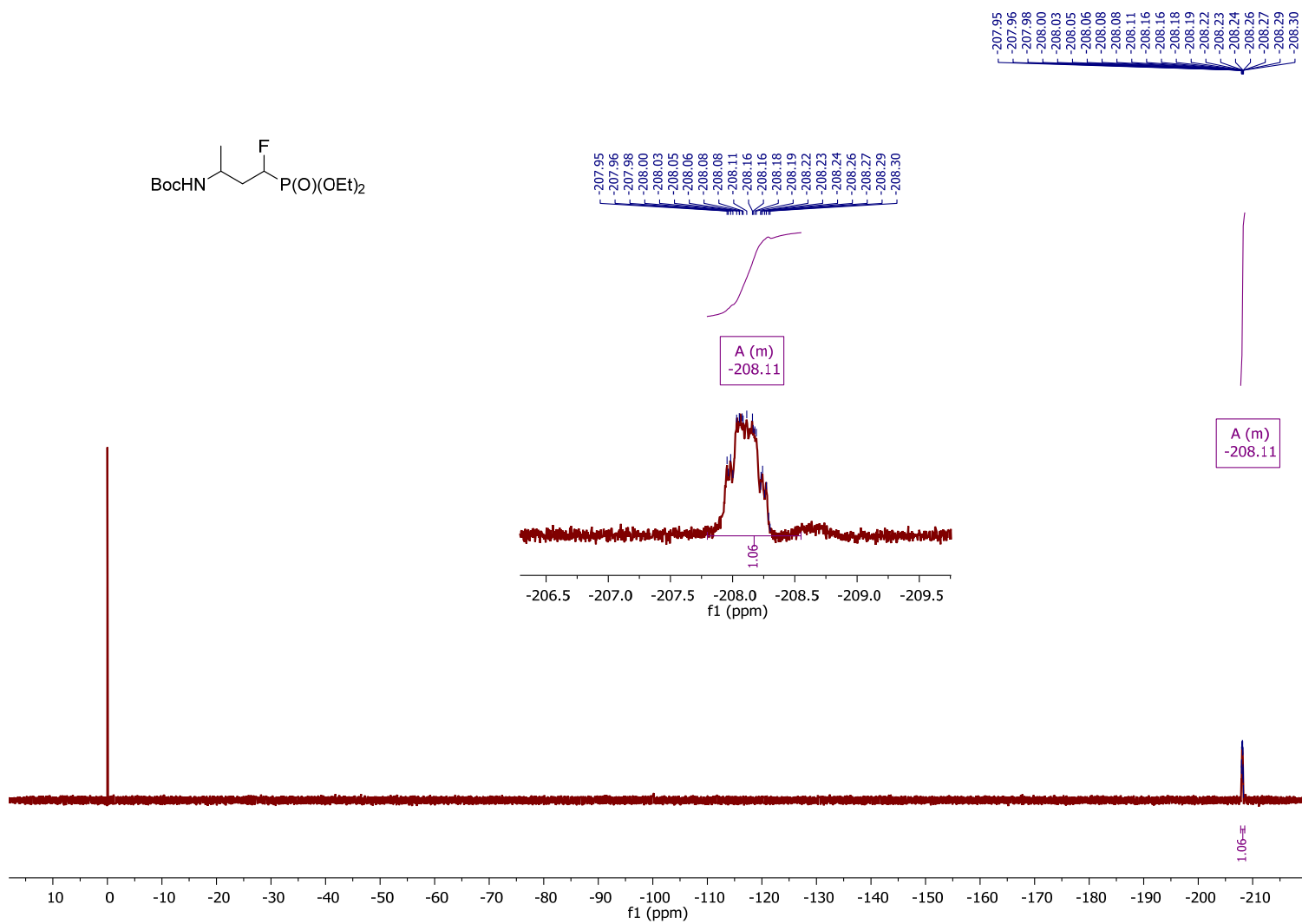
¹³C NMR of rac-17b.



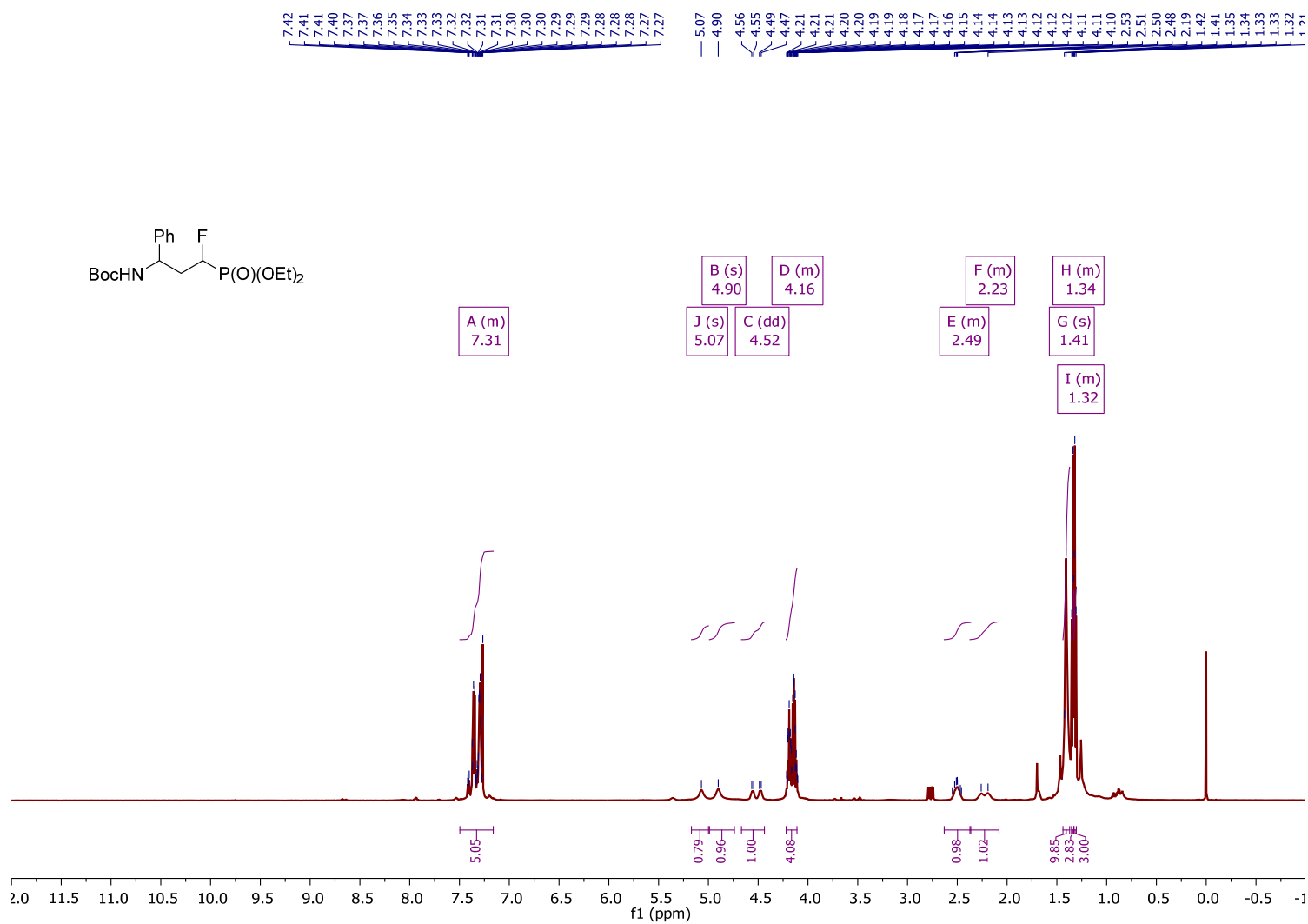
^1H - ^{13}C HSQC of rac-17b.



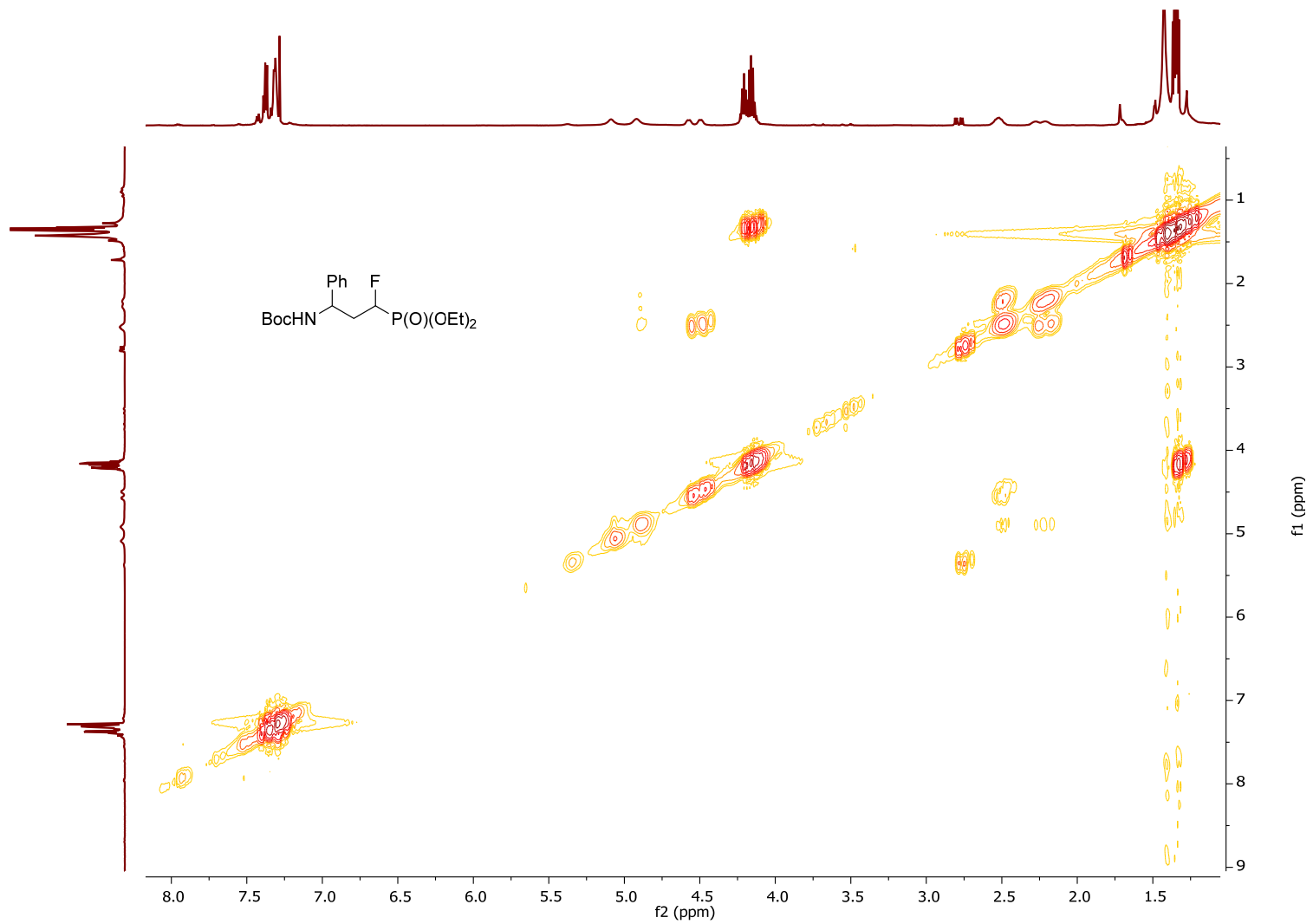
$^{31}\text{P}\{^1\text{H}\}$ NMR of rac-**17b**.

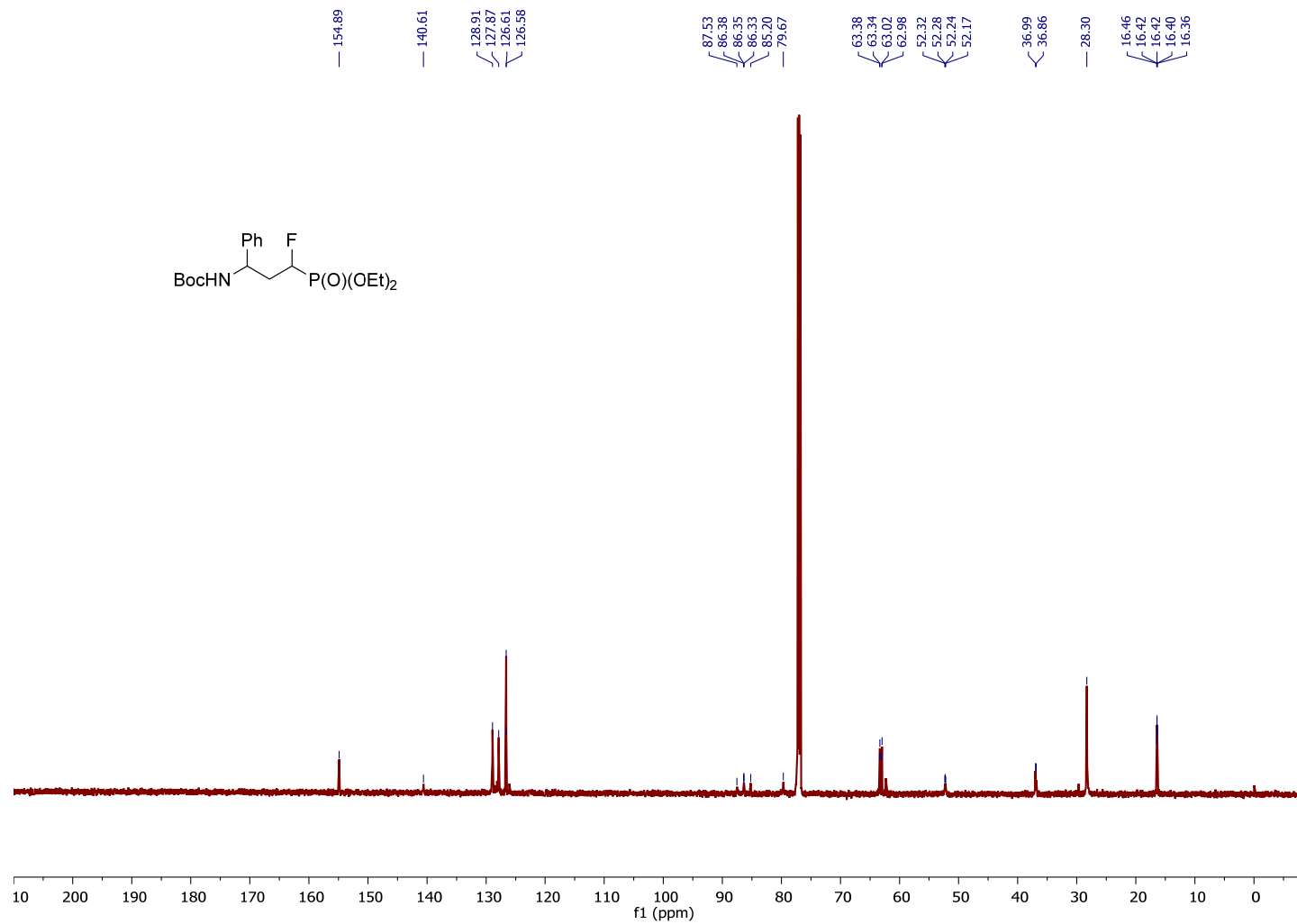


^{19}F NMR of rac-17b.

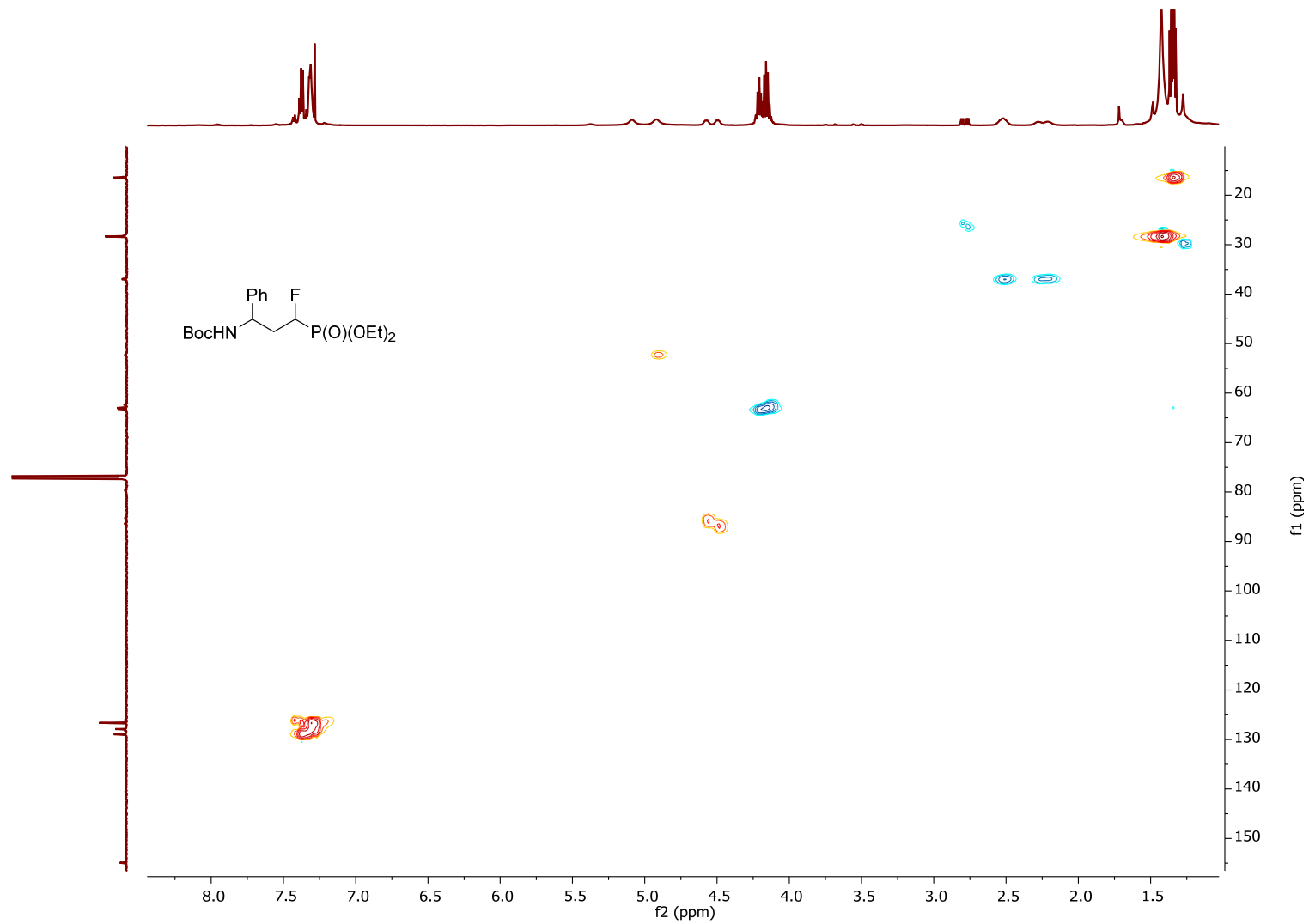


¹H NMR of rac-17c.

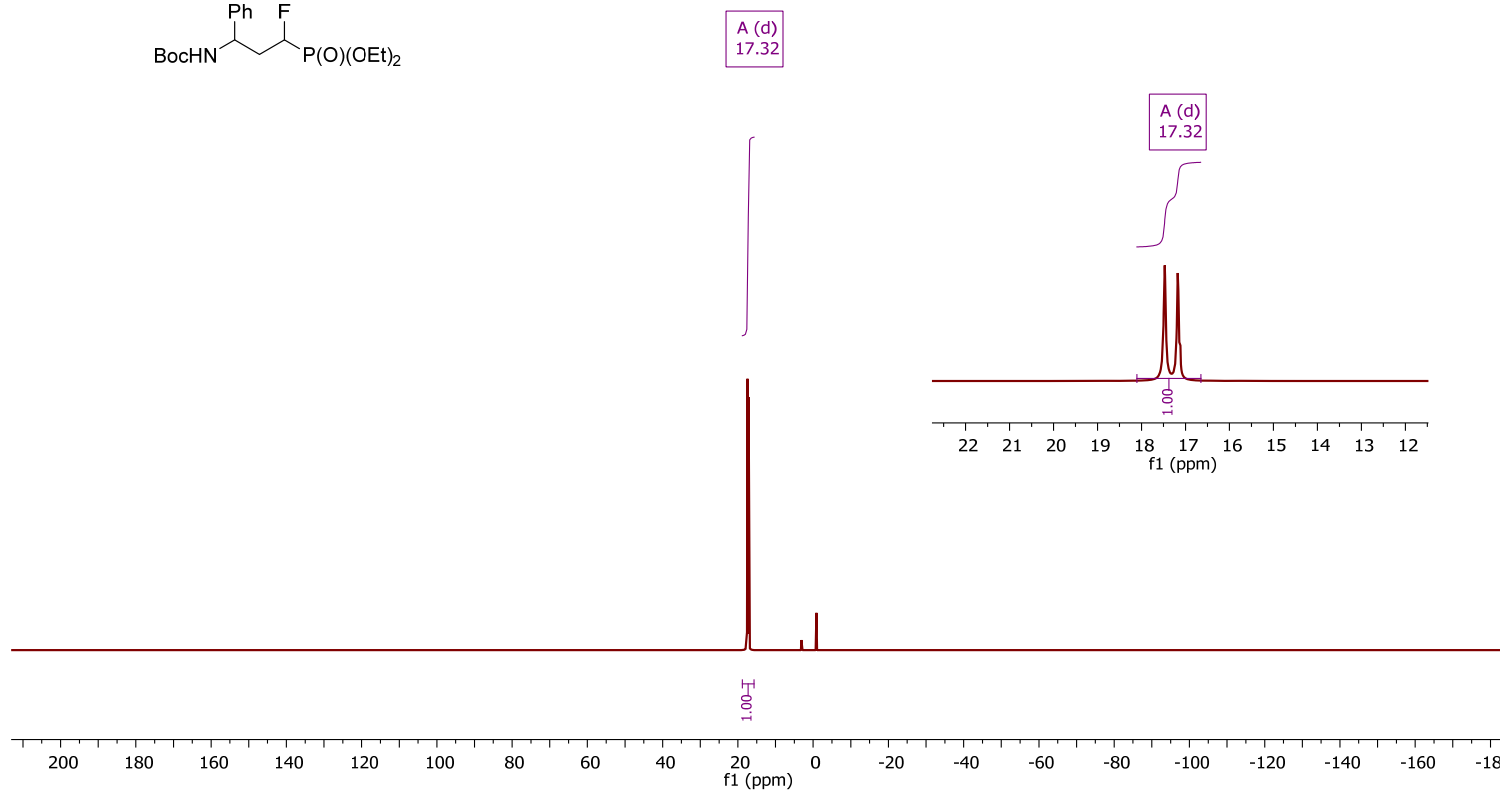
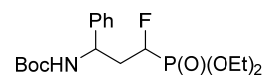




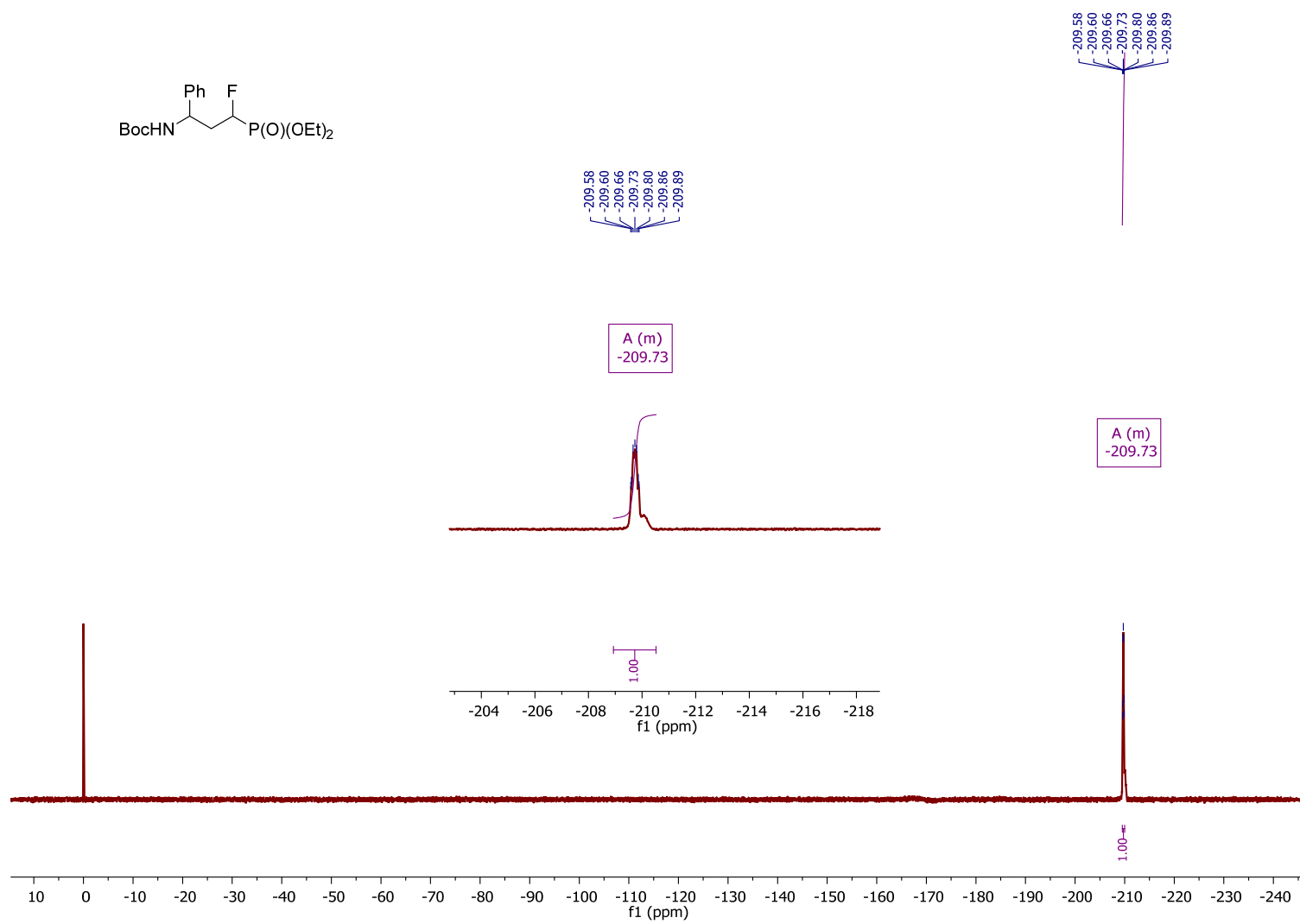
¹³C NMR of rac-17c.



¹H-¹³C HSQC of rac-17c.



$^{31}\text{P}\{^1\text{H}\}$ NMR of rac-17c.



^{19}F NMR of rac-17c.

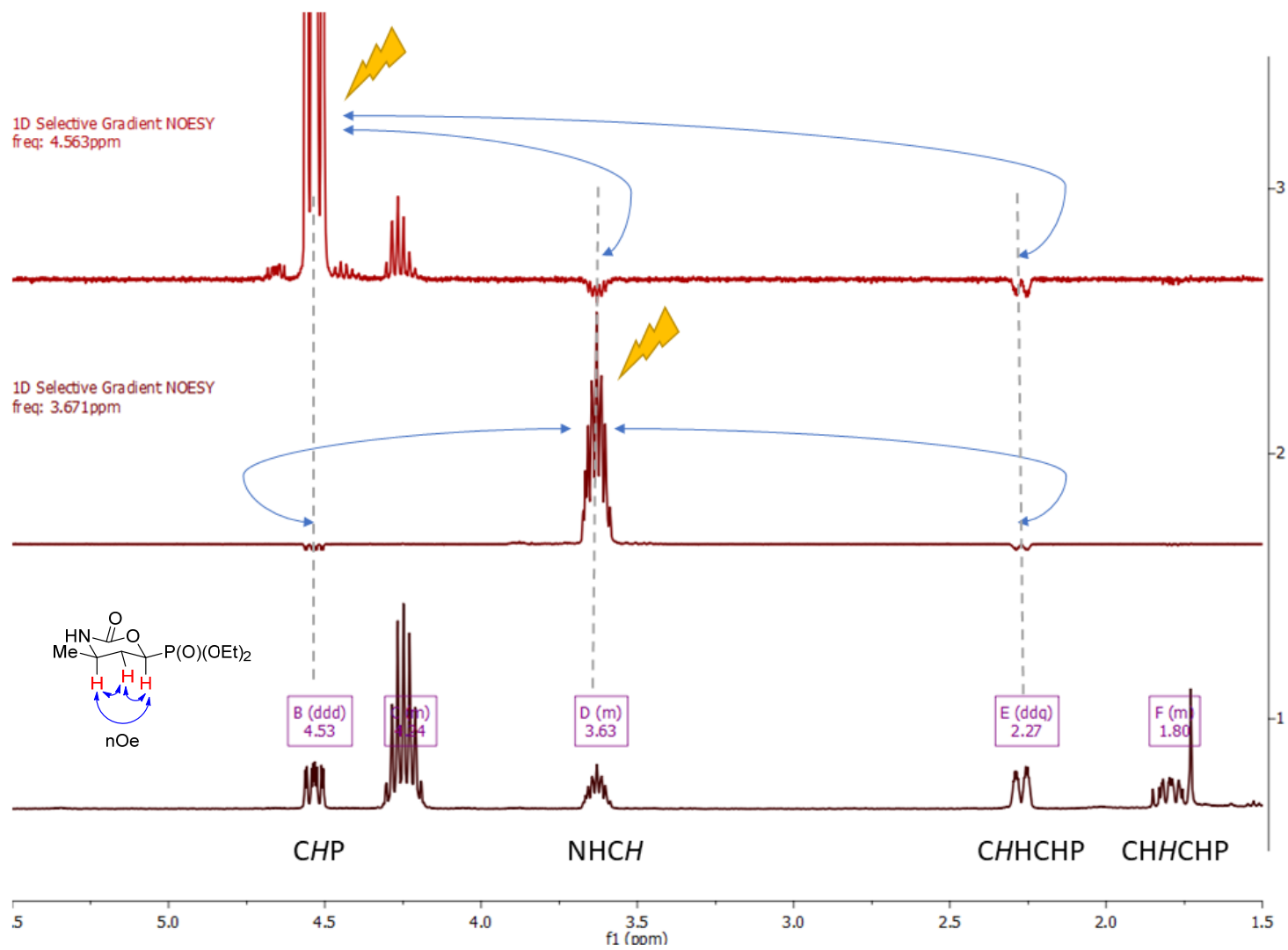


Figure S4. ^1H - ^1H NOEs of rac-16b.

X-Ray Data:

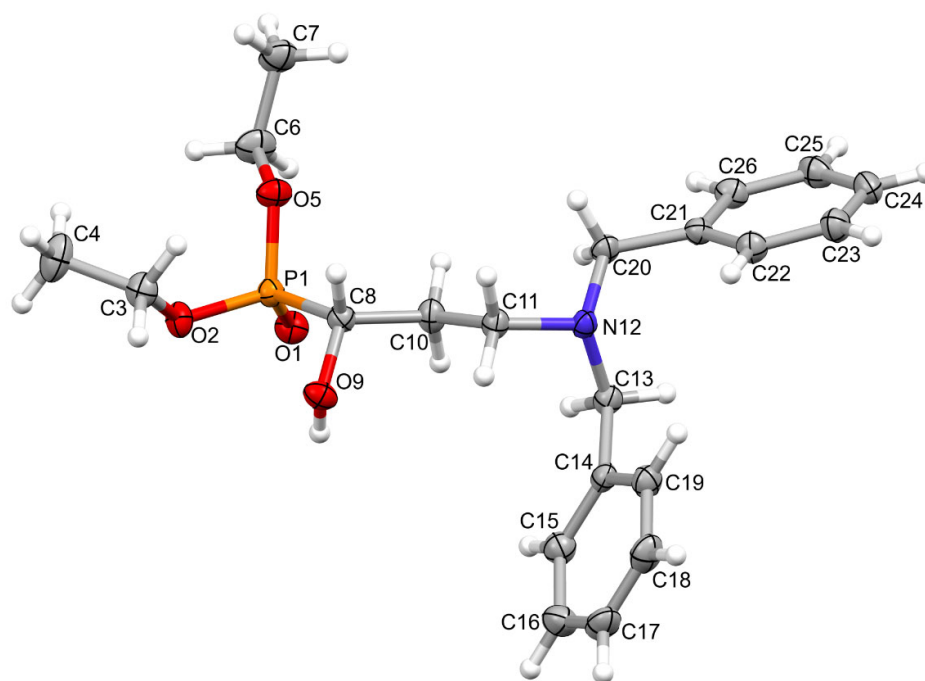


Figure S1. Perspective view of the molecule **rac-6a**; ellipsoids are drawn at the 50% probability level; hydrogen atoms are shown as spheres of arbitrary radii.

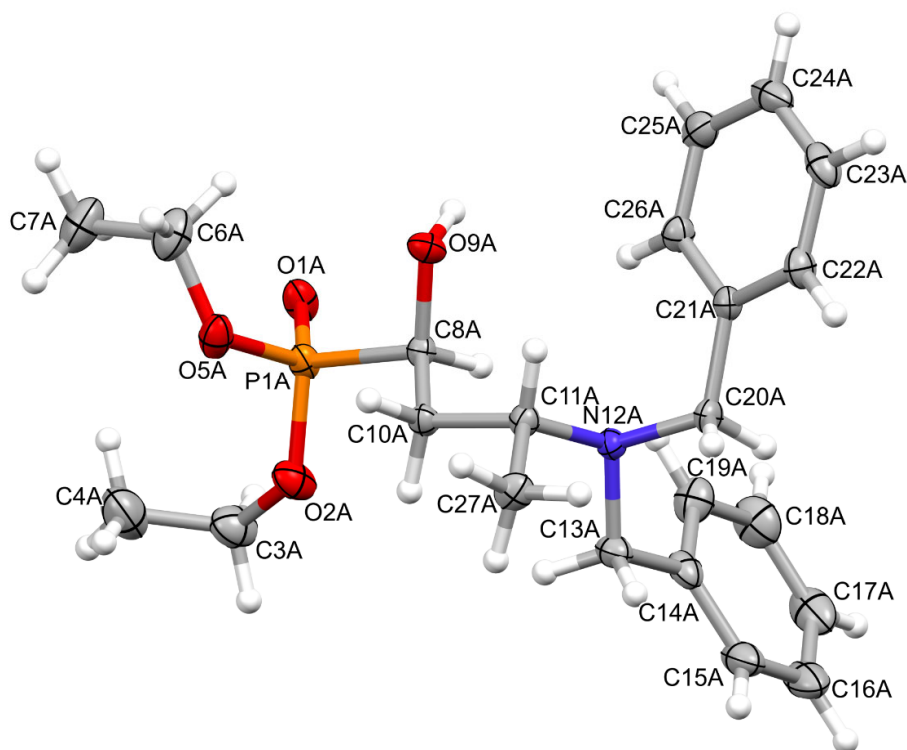


Figure S2. Perspective view of the molecule **rac-6b**; ellipsoids are drawn at the 50% probability level; hydrogen atoms are shown as spheres of arbitrary radii.

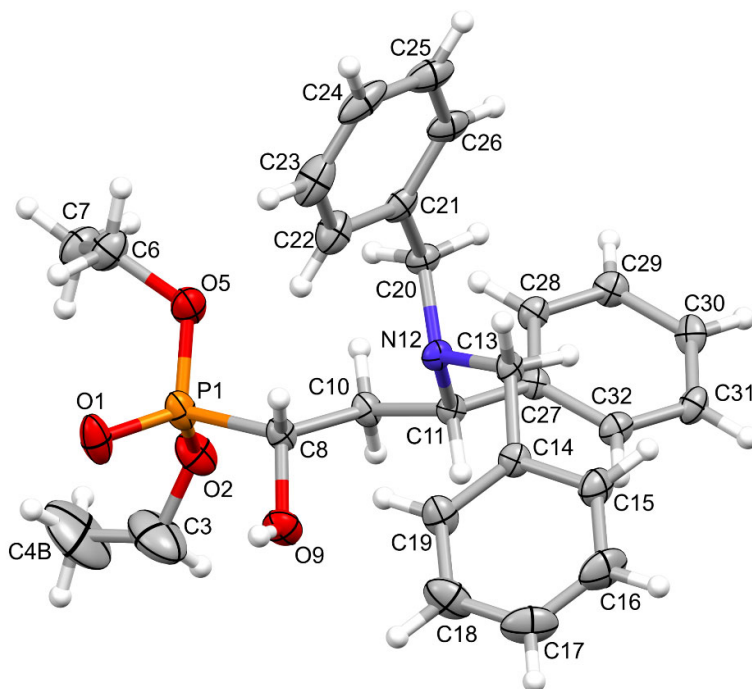


Figure S3. Perspective view of the molecule **rac-6c**; ellipsoids are drawn at the 50% probability level; hydrogen atoms are shown as spheres of arbitrary radii.

Table S1. Crystal data, data collection and structure refinement

Compound	rac-6a	rac-6b	rac-6c
Formula	C ₂₁ H ₃₀ NO ₄ P	C ₂₂ H ₃₂ NO ₄ P	C ₂₇ H ₃₄ NO ₄ P
Formula weight	391.43	405.45	467.52
Crystal system	triclinic	triclinic	triclinic
Space group	P-1	P-1	P-1
a (Å)	8.5489(2)	10.7214(4)	10.0312(6)
b (Å)	9.9570(2)	11.9743(6)	10.9576(9)
c (Å)	12.8587(3)	18.1464(8)	13.1760(13)
α (°)	71.144(2)	88.453(4)	72.616(8)
β (°)	81.512(2)	77.487(4)	81.716(7)
γ (°)	81.501(2)	74.219(4)	67.437(7)
V(Å ³)	1018.59(4)	2187.33(18)	1275.6(2)
Z	2	4	2
D _x (g cm ⁻³)	1.276	1.231	1.217
F(000)	420	872	500
μ(mm ⁻¹)	1.409	0.152	0.140
Reflections:			

collected	19681	15919	14455
unique (R_{int})	4211 (0.0189)	8706 (0.0160)	4957 (0.0344)
with $I > 2\sigma(I)$	4170	7298	4117
R(F) [$I > 2\sigma(I)$]	0.0327	0.0626	0.0531
wR(F^2) [$I > 2\sigma(I)$]	0.0844	0.1714	0.1295
R(F) [all data]	0.0329	0.0735	0.0654
wR(F^2) [all data]	0.0845	0.1818	0.1387
Goodness of fit	1.061	1.056	1.034
max/min $\Delta\rho$ ($e \cdot \text{\AA}^{-3}$)	0.28/-0.38	1.14/-0.55	0.92/-0.44
CCDC number	2172329	2172330	2172331

Table S2. Hydrogen bond data; symmetry codes: ⁱ: 1-x,1-y,-z; ⁱⁱ: 1-x,1-y,1-z; ⁱⁱⁱ-x,1-y,-z

D	H	A	D-H	H...A	D...A	D-H...A
rac-6a						
O9	H9	O1 ⁱ	0.844(19)	1.82(2)	2.6583(12)	1701.1(18)
rac-6b						
O9A	H9A	O1A ⁱⁱ	0.84	1.86	2.700(2)	175
O9B	H9B	O1 ⁱⁱⁱ	0.84	1.87	2.698(2)	170
rac-6c						
O9	H9	O1 ⁱ	0.84	1.89	2.704(2)	162