Supplemental Material

Clarifying the use of benzylidene protecting group for D-(+)-ribono-1,4-lactone, an essential building block in the synthesis of C-nucleosides.

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[2] *Dipartimento di Scienze Biomediche, Chirurgiche e Odontoiatriche, Università degli Studi di Milano, Via Saldini 50, 20122 Milano, Italy; pietro.allevi@unimi.it, paola.rota@unimi.it.*

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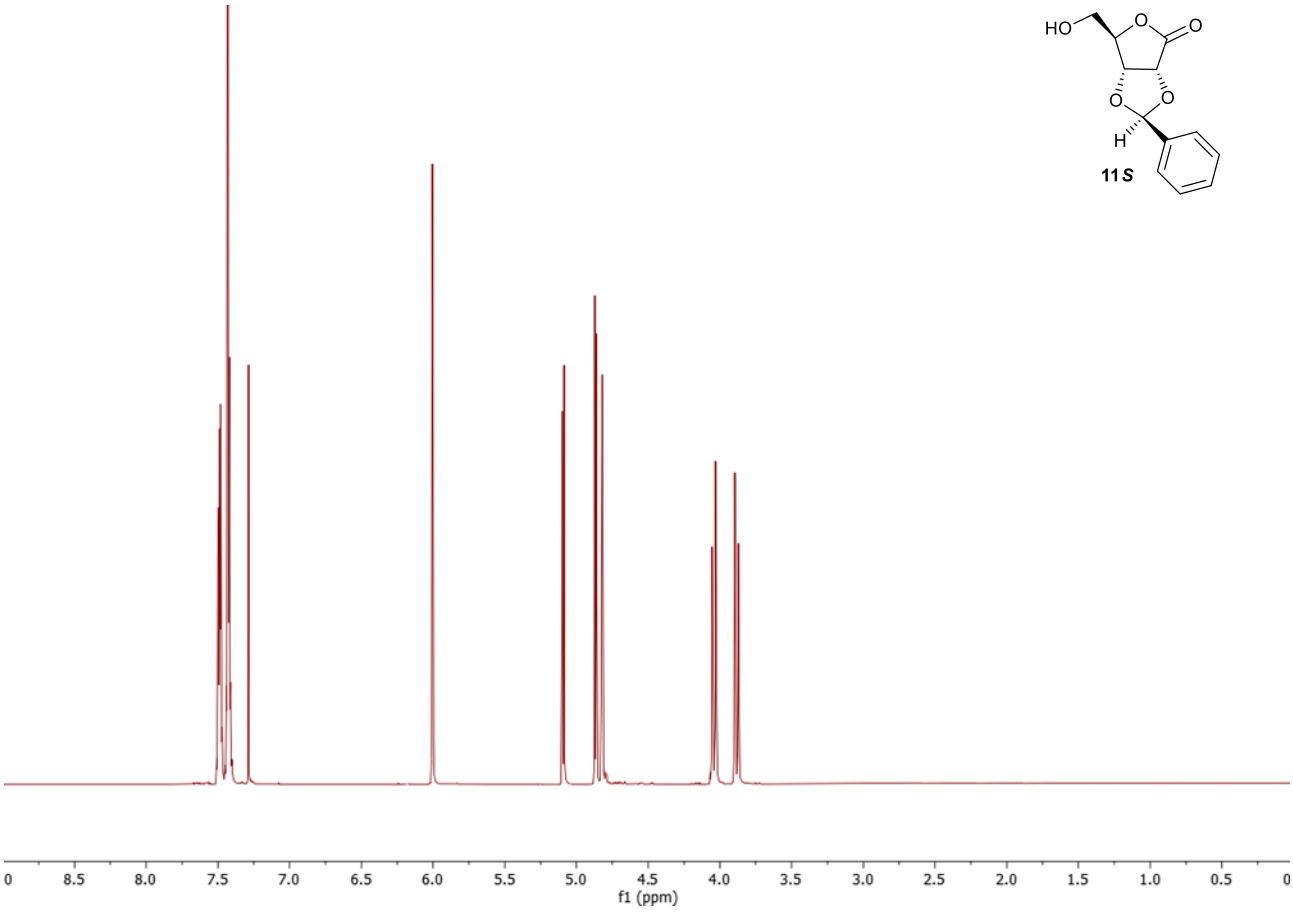
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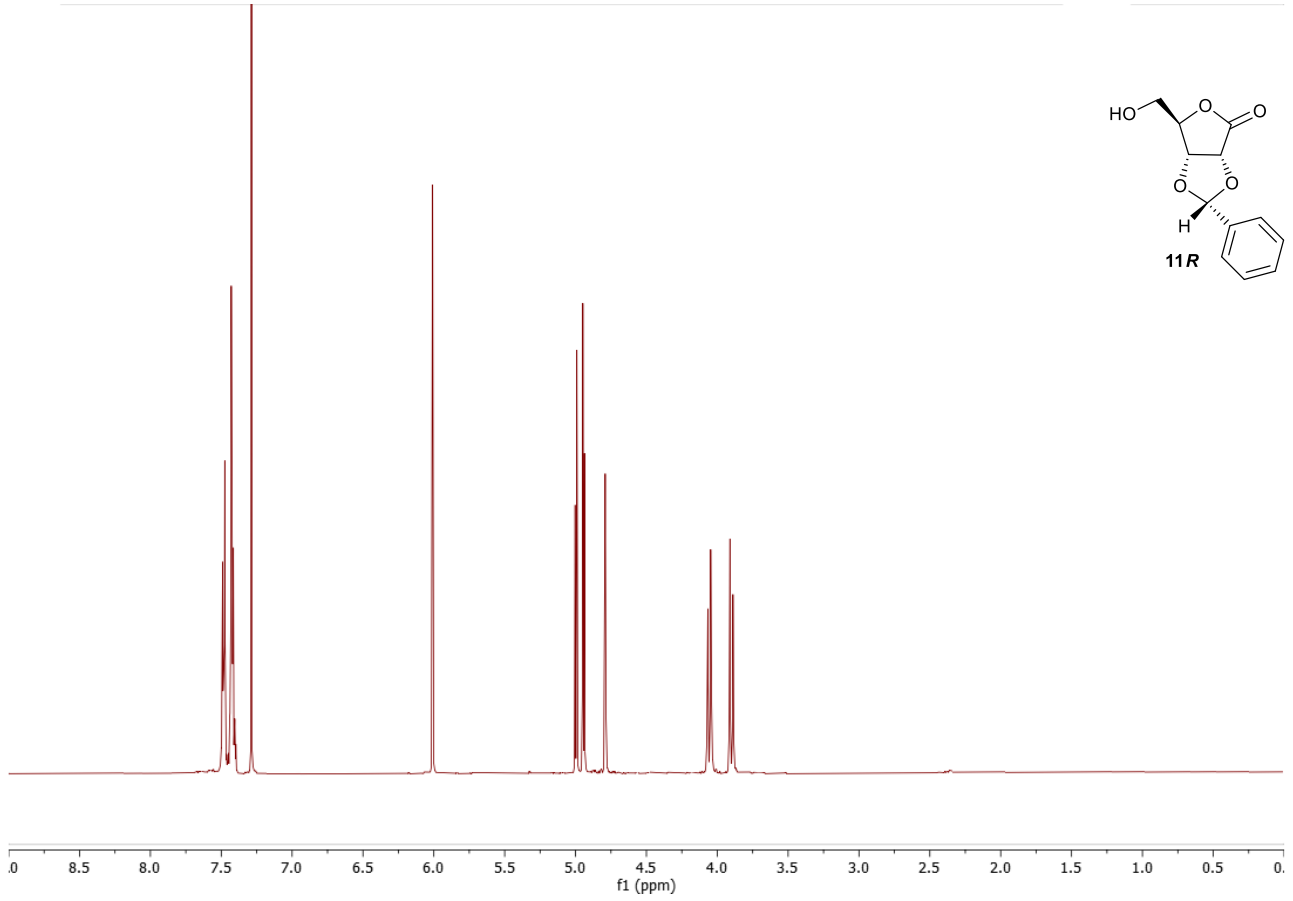
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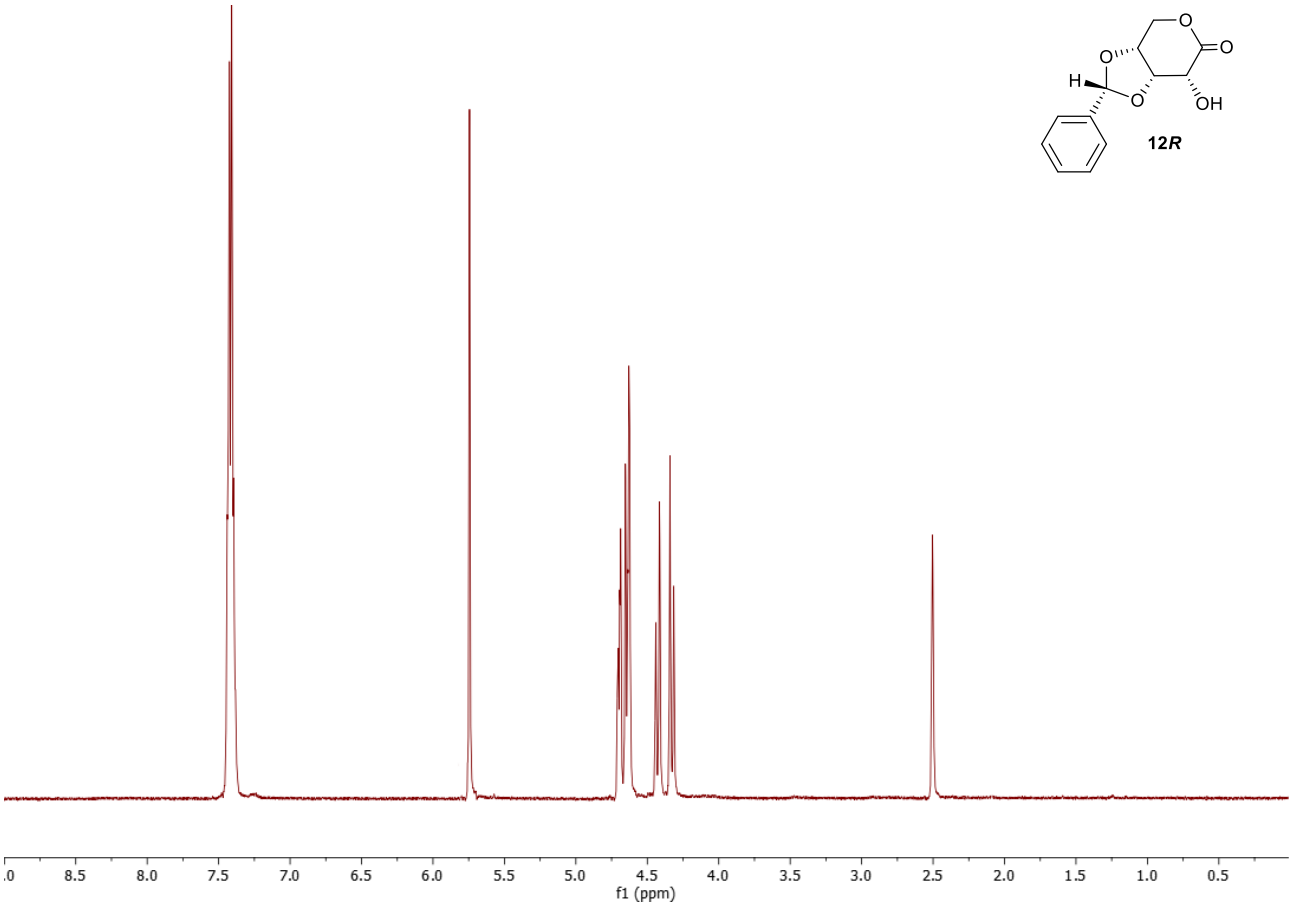
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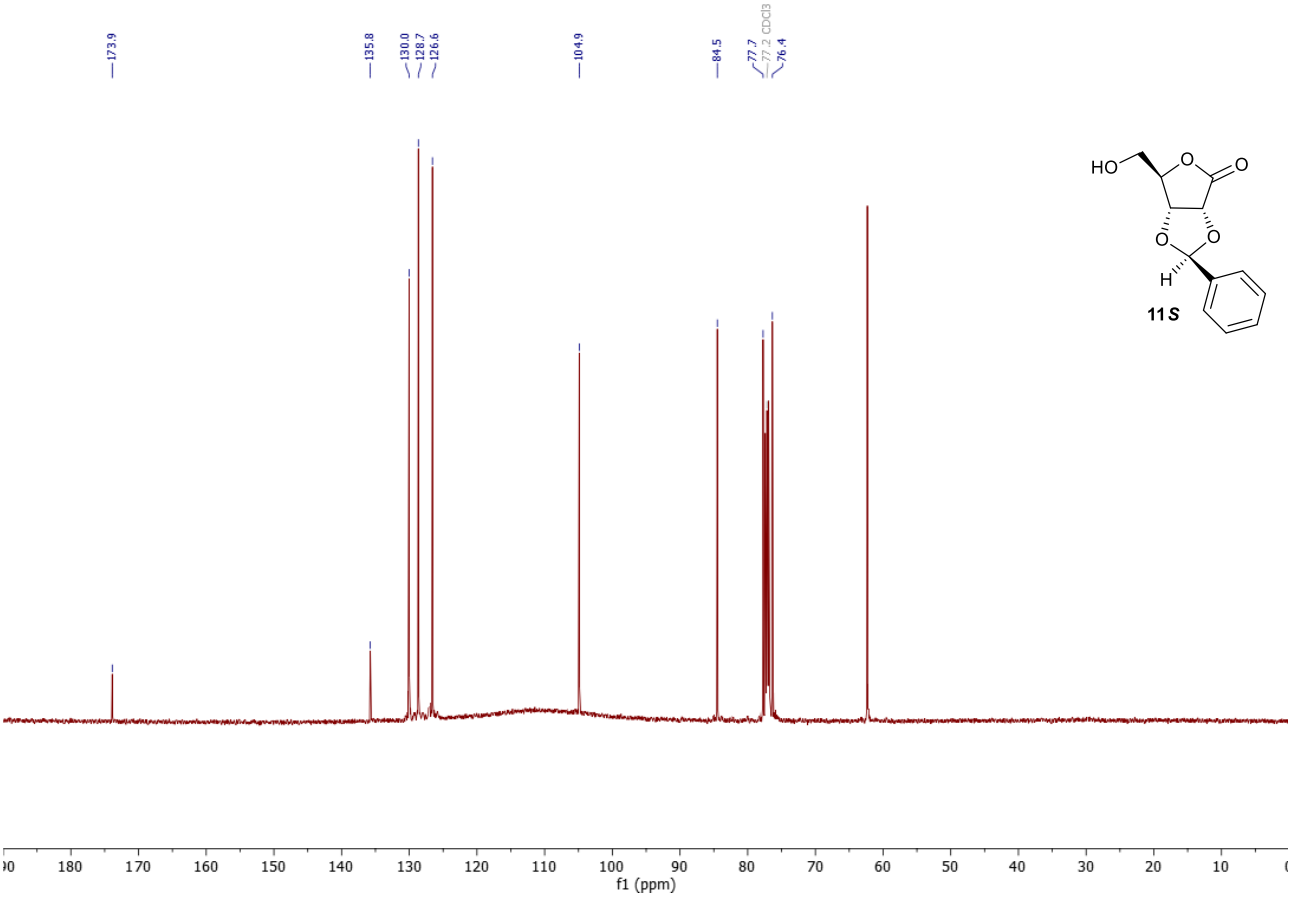
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O
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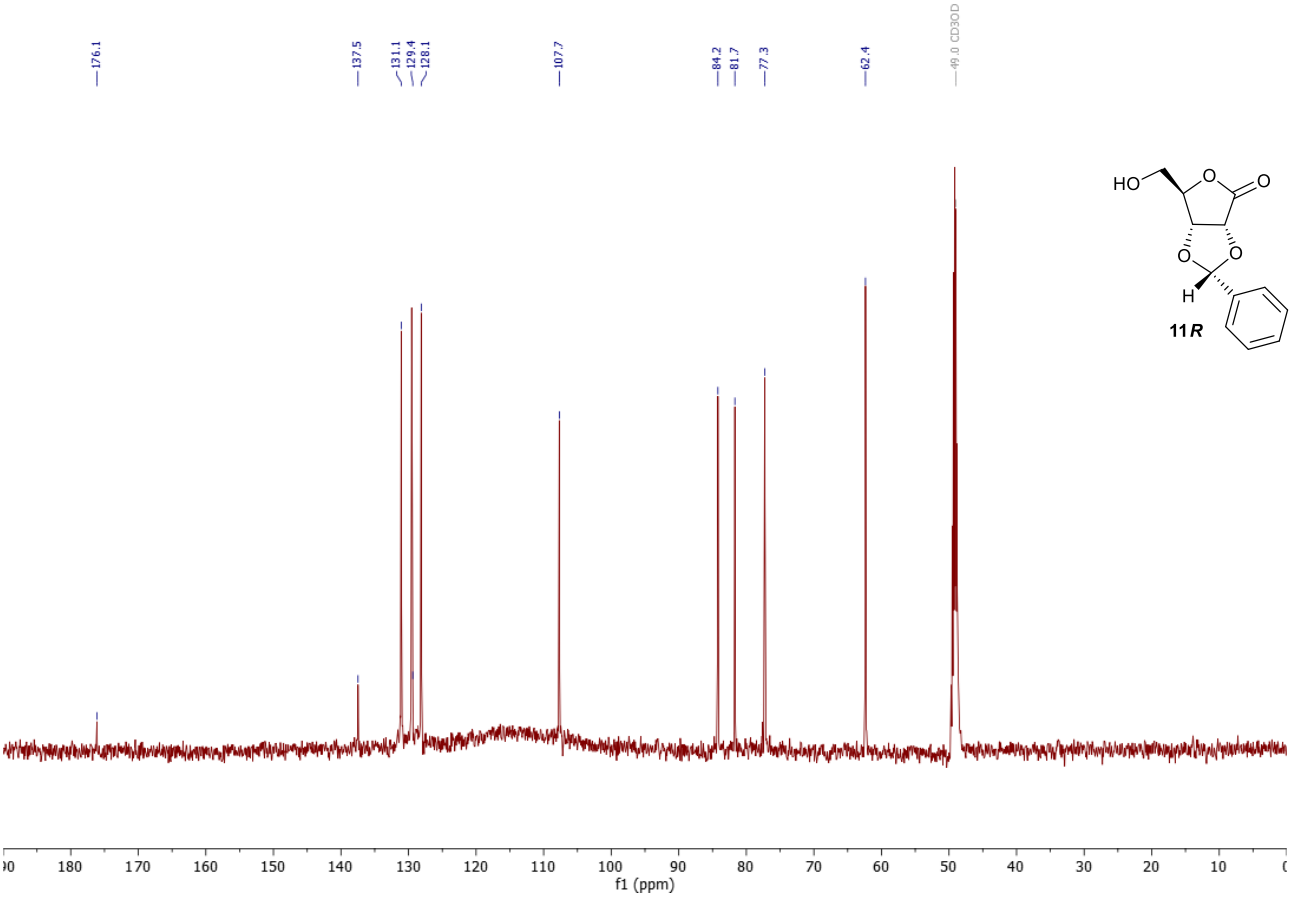
O
H
11S
f1 (ppm)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11R
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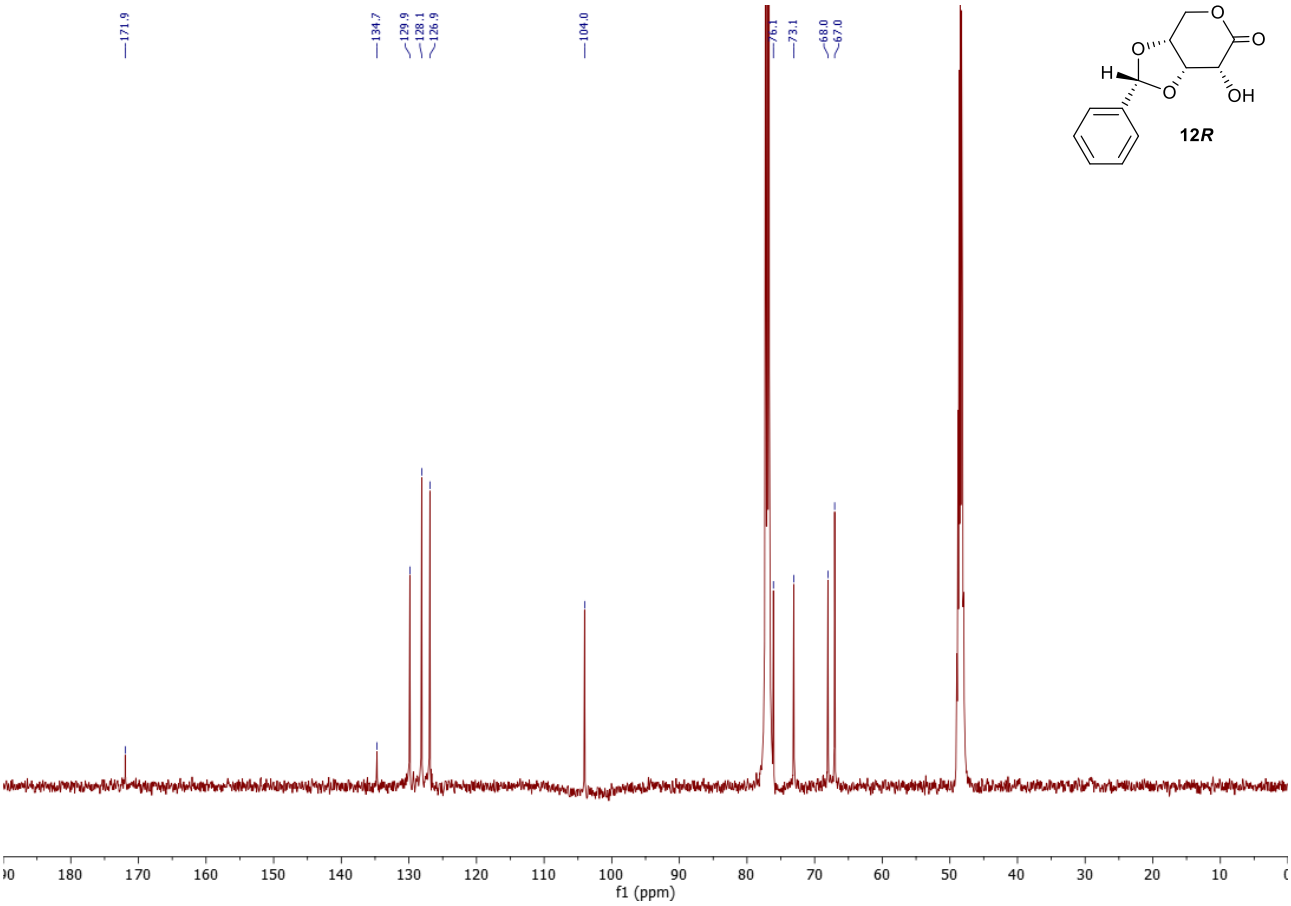
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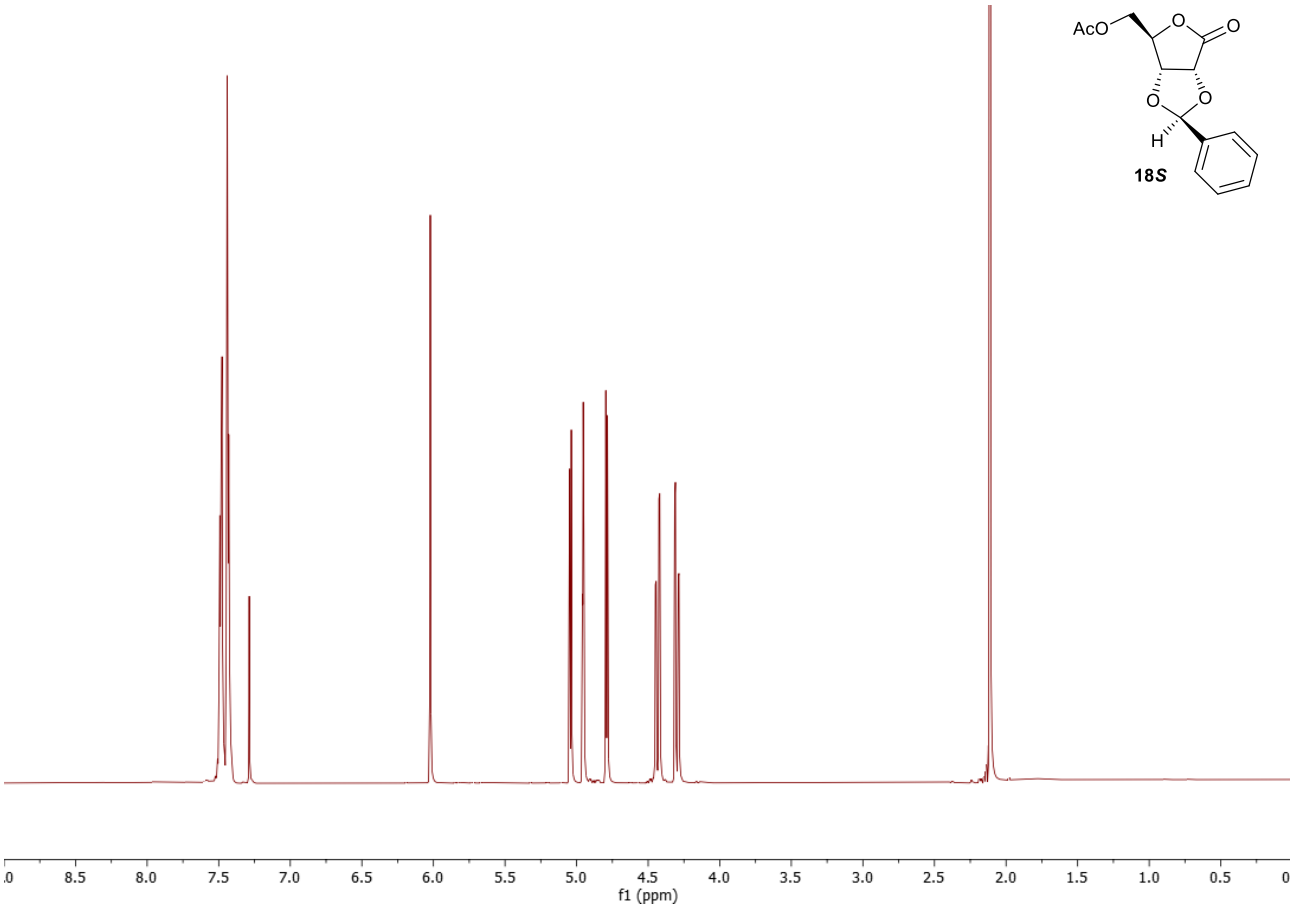
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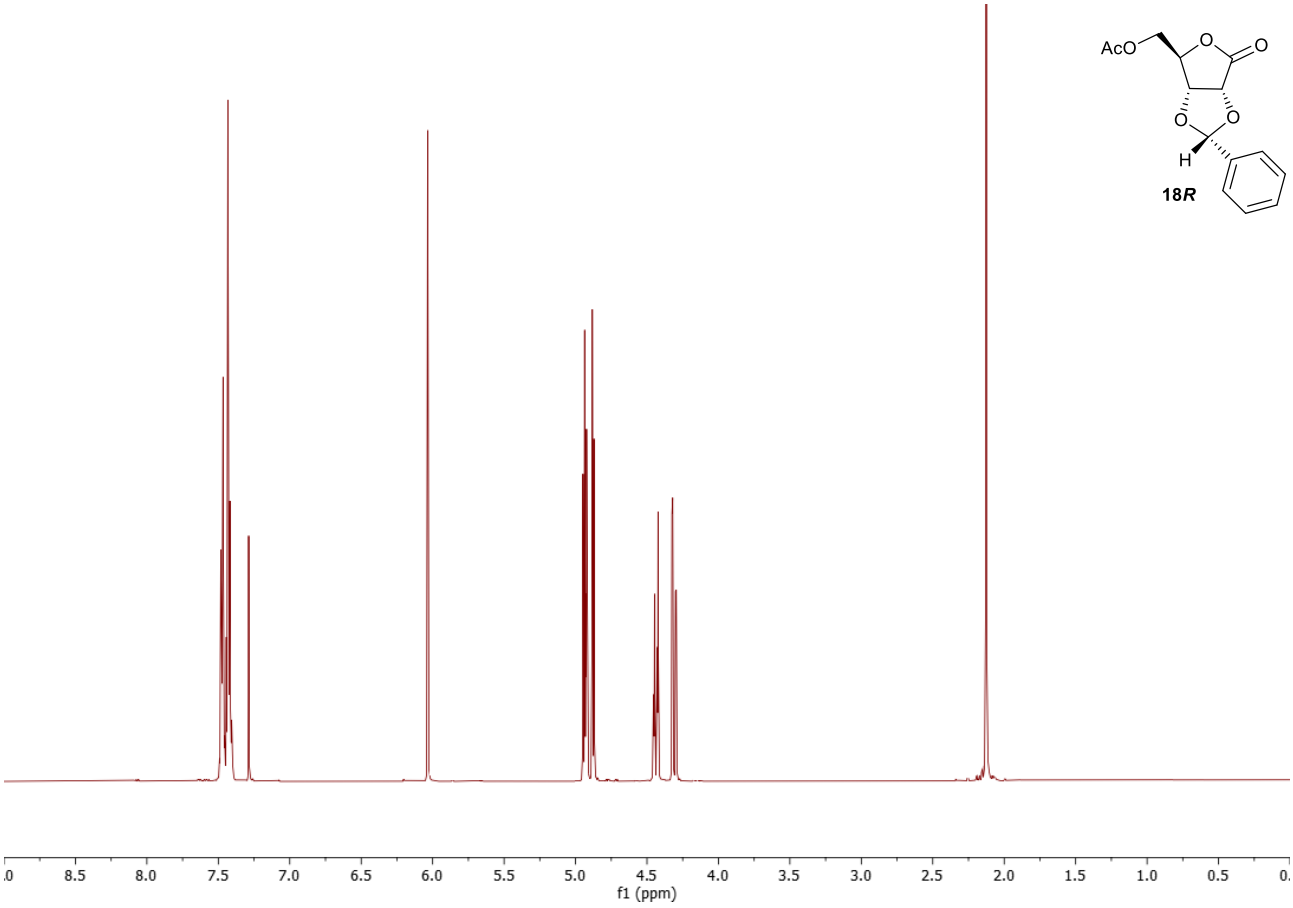
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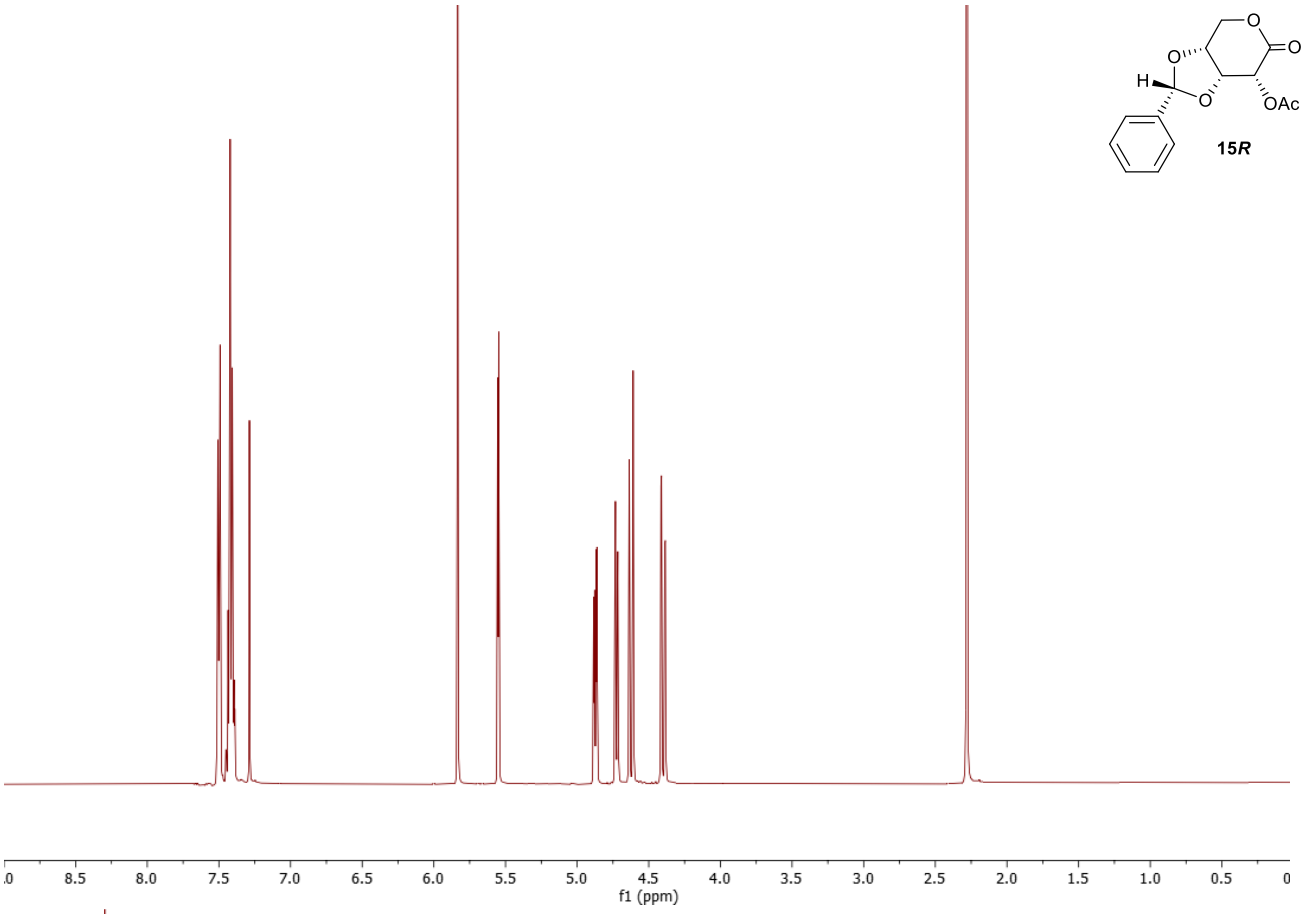
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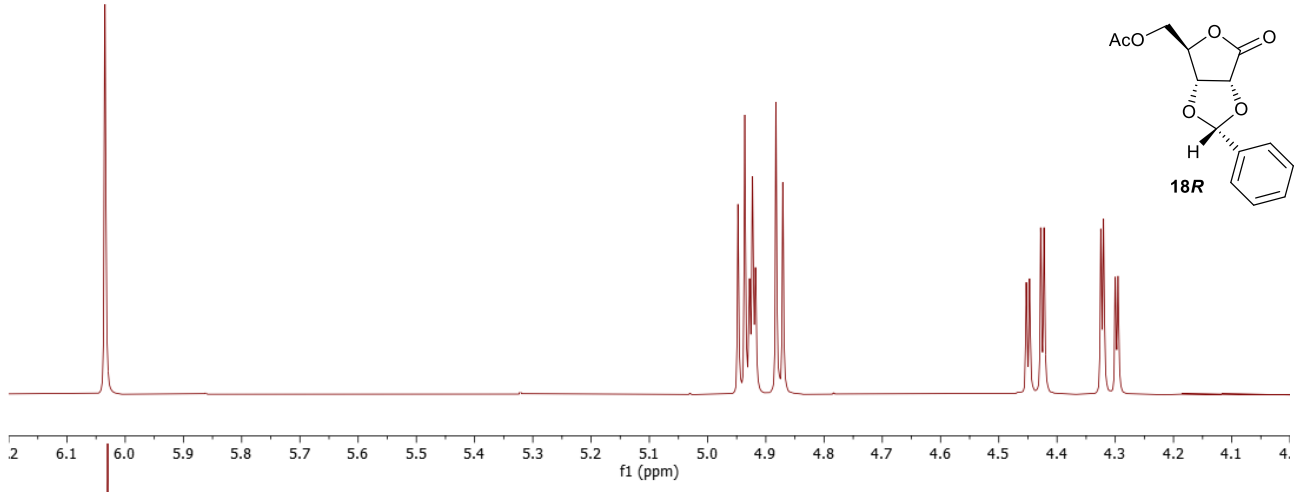
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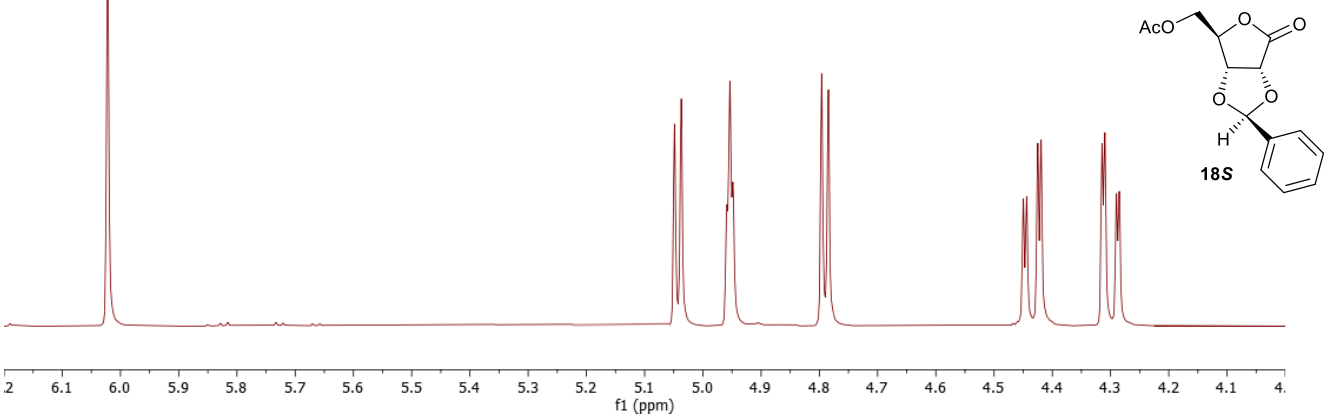
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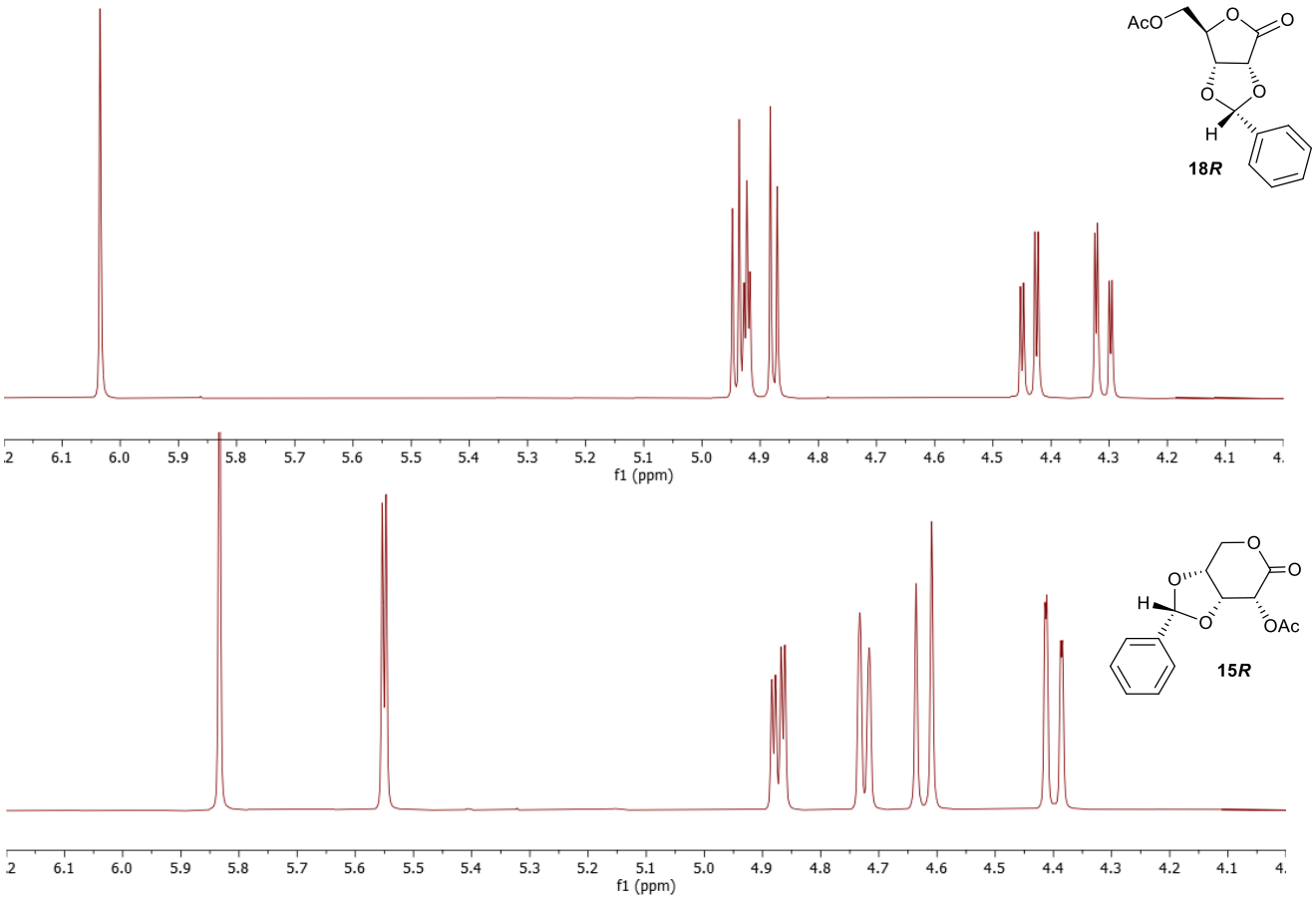
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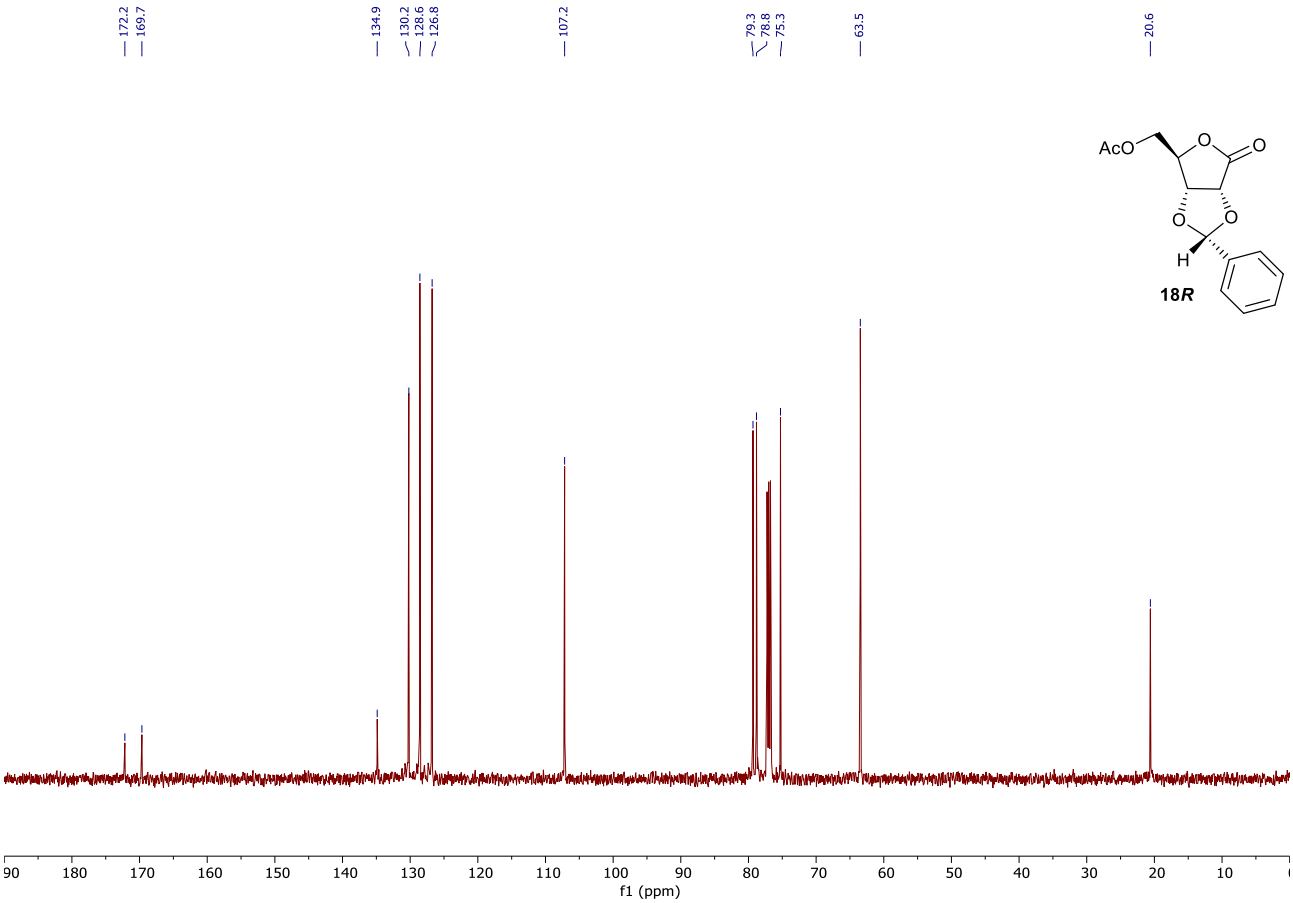
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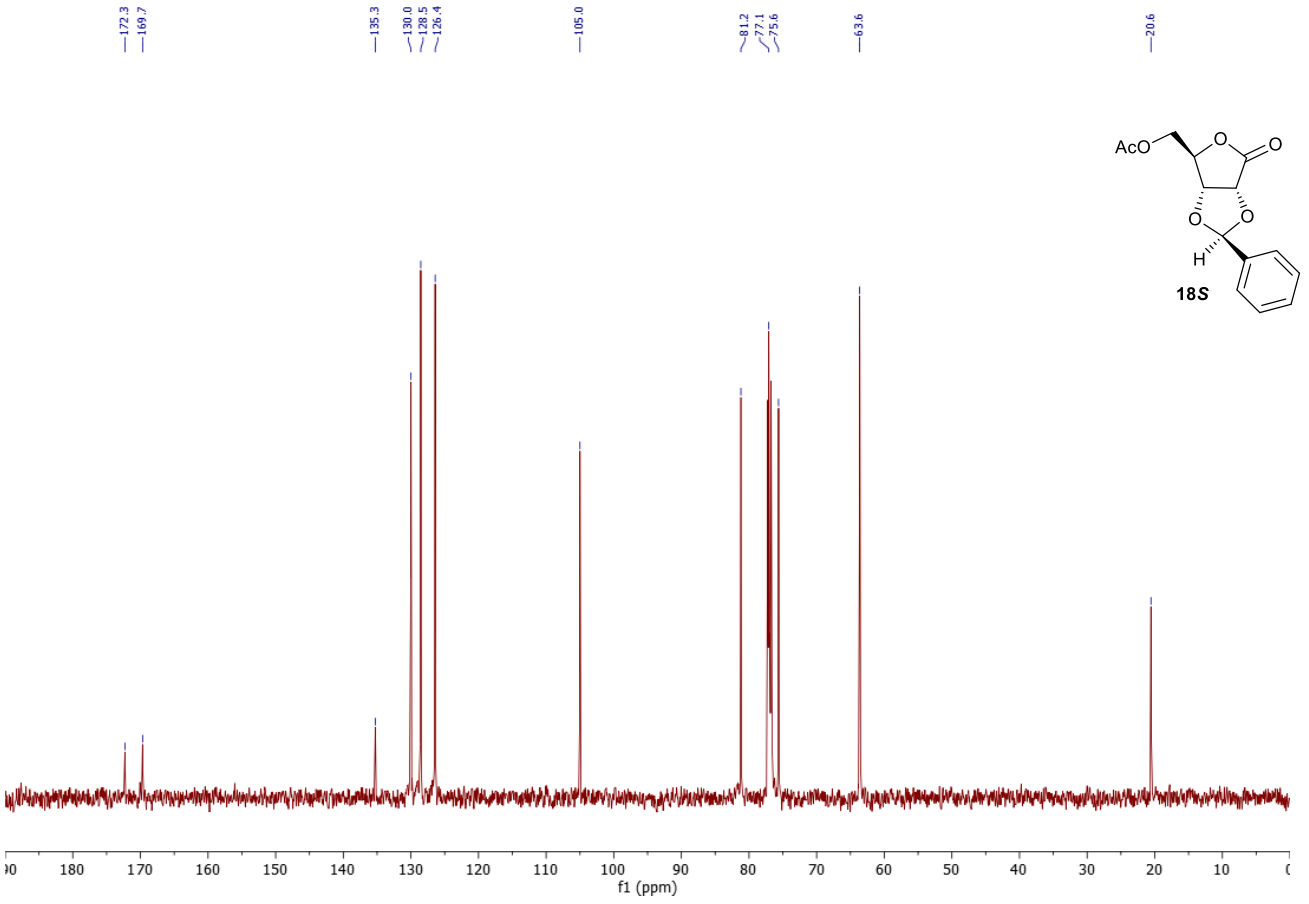
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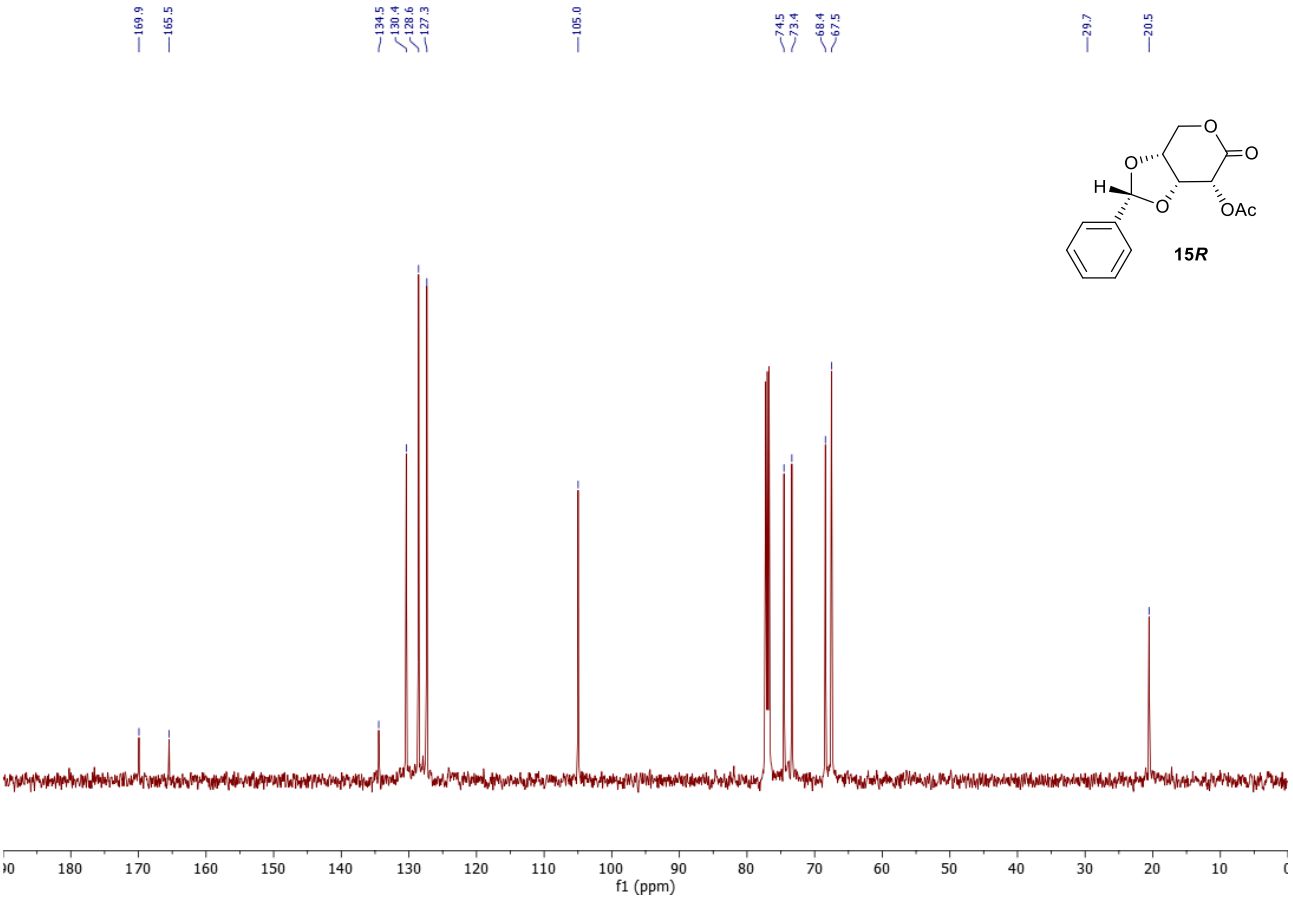
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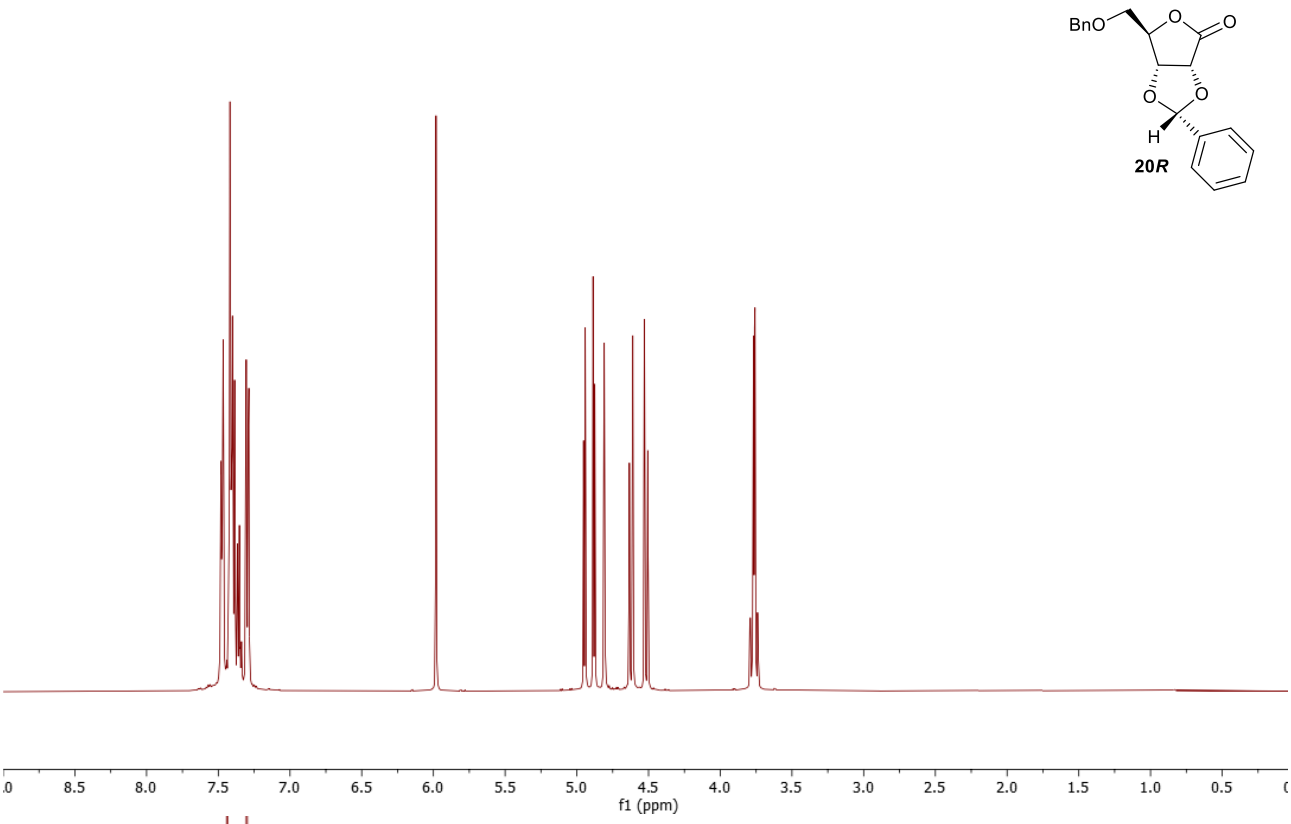
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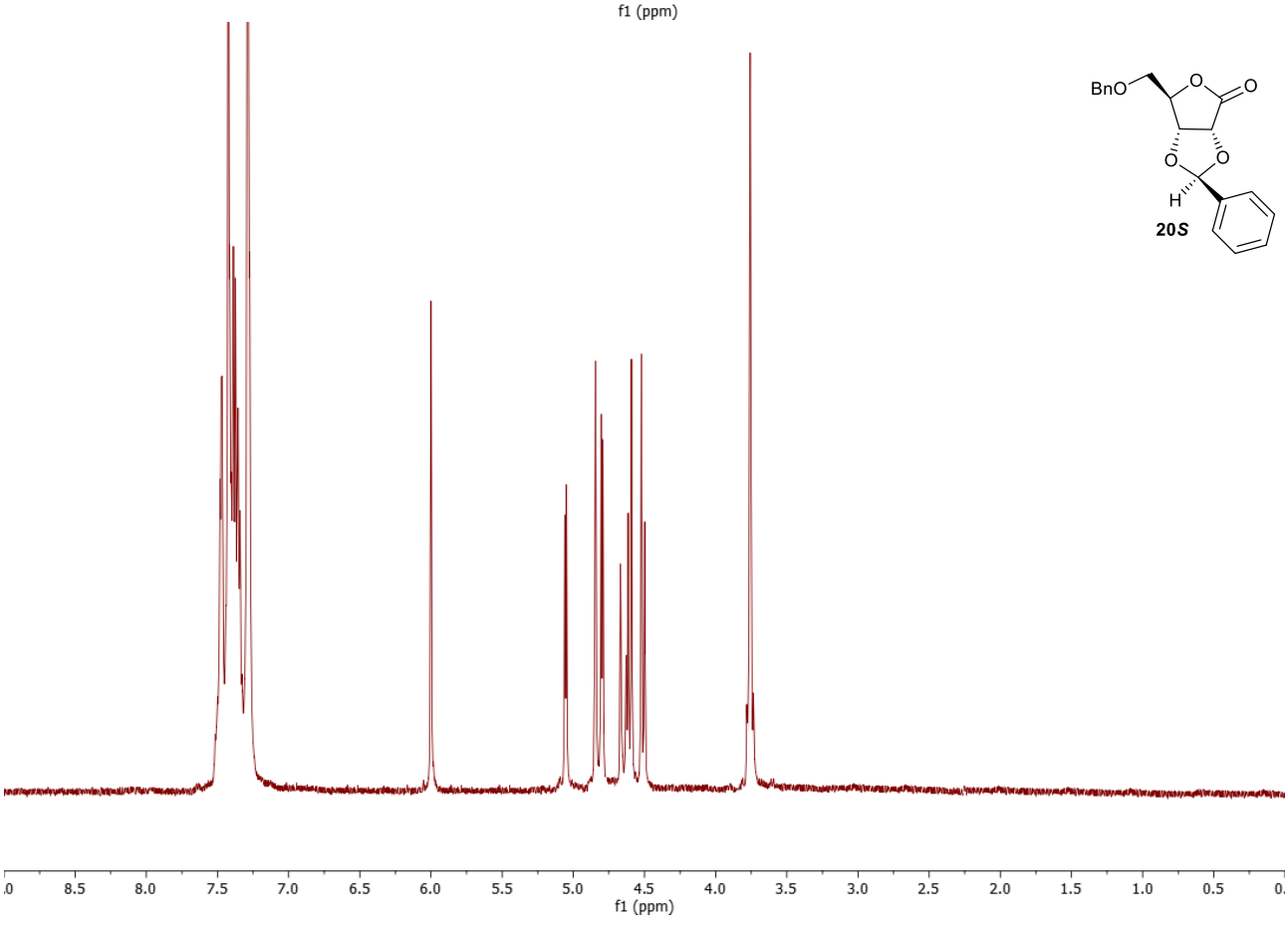
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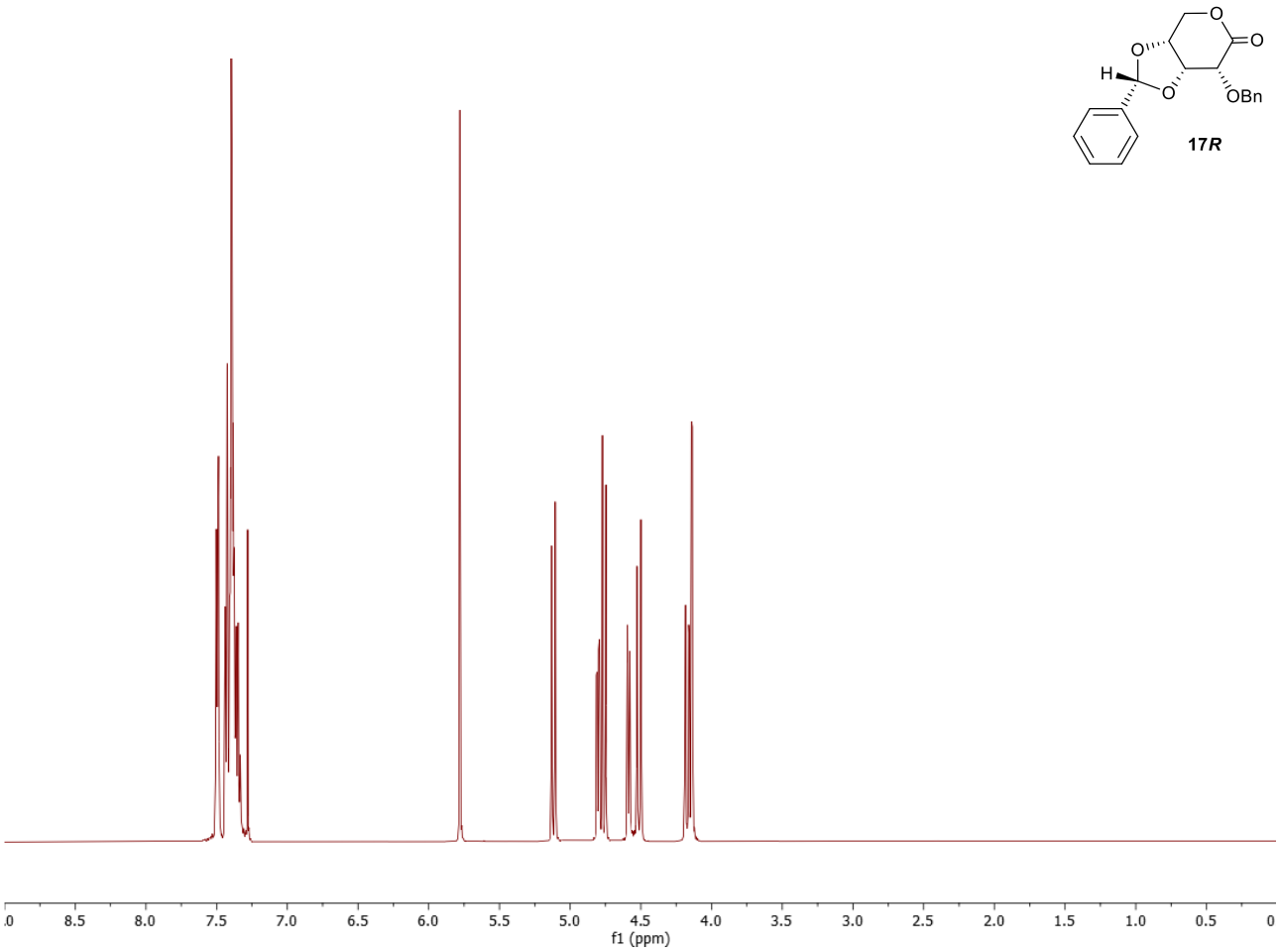
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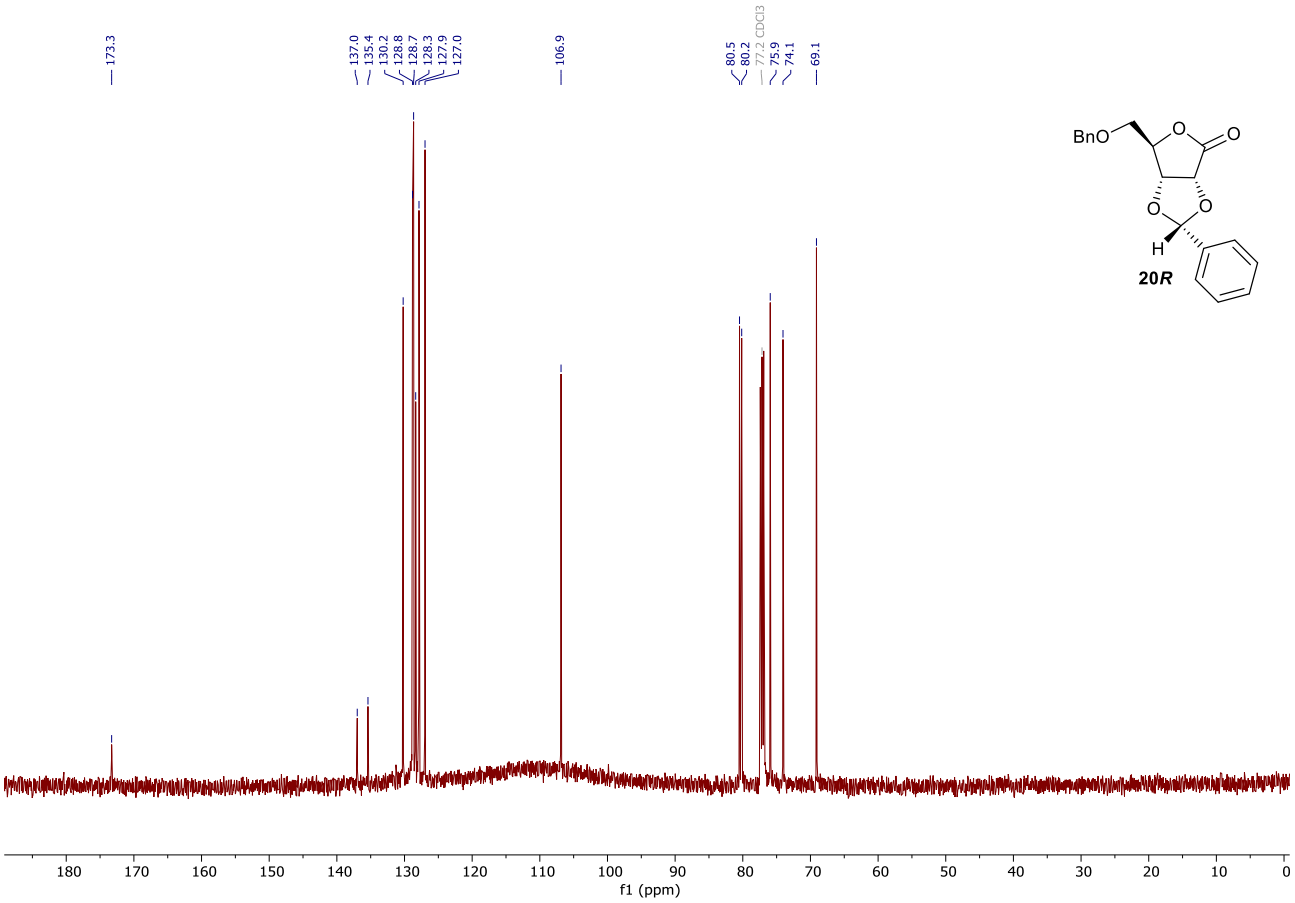
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77.2 CDCl3
75.9
74.1
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O
O
H
20R
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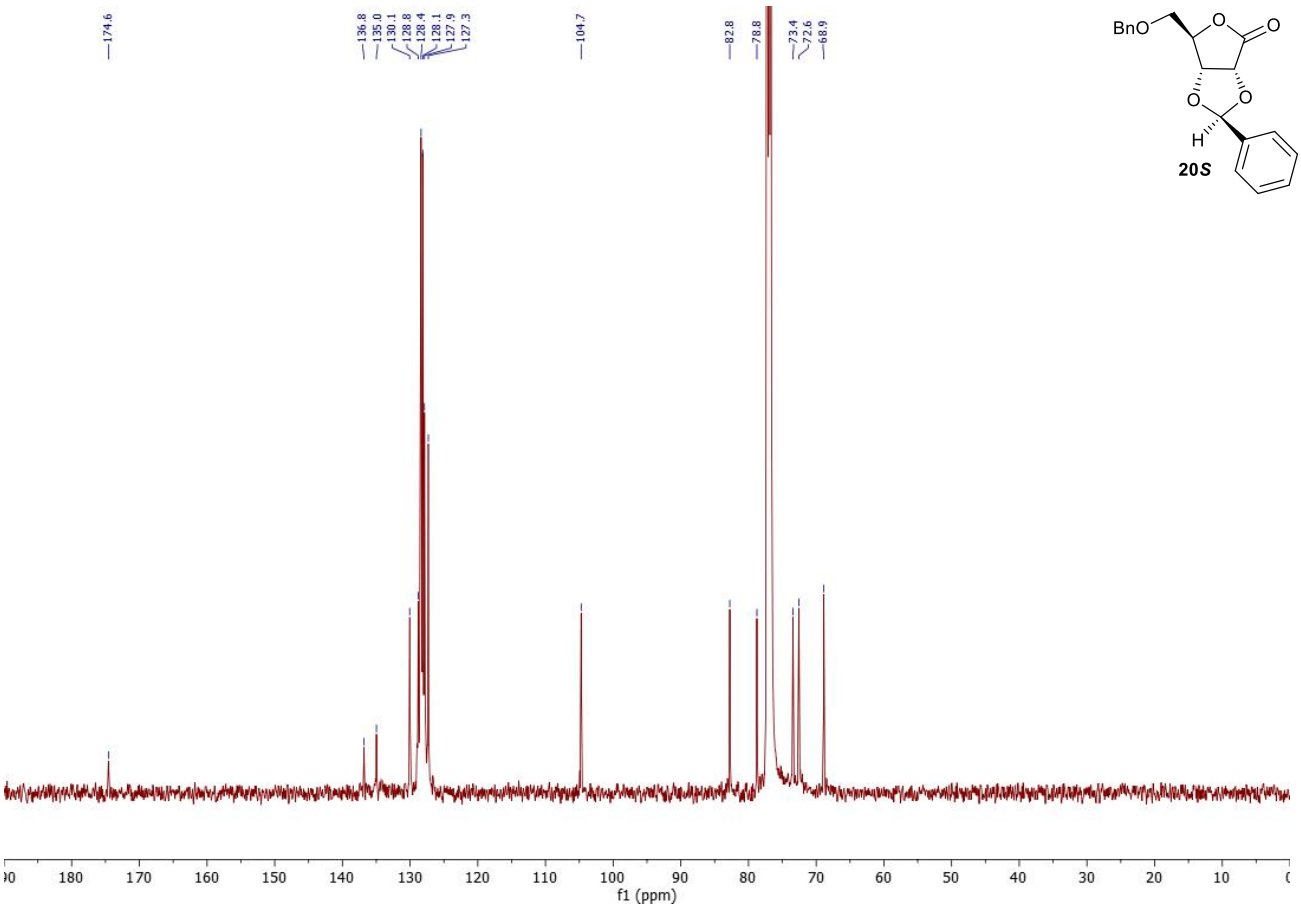
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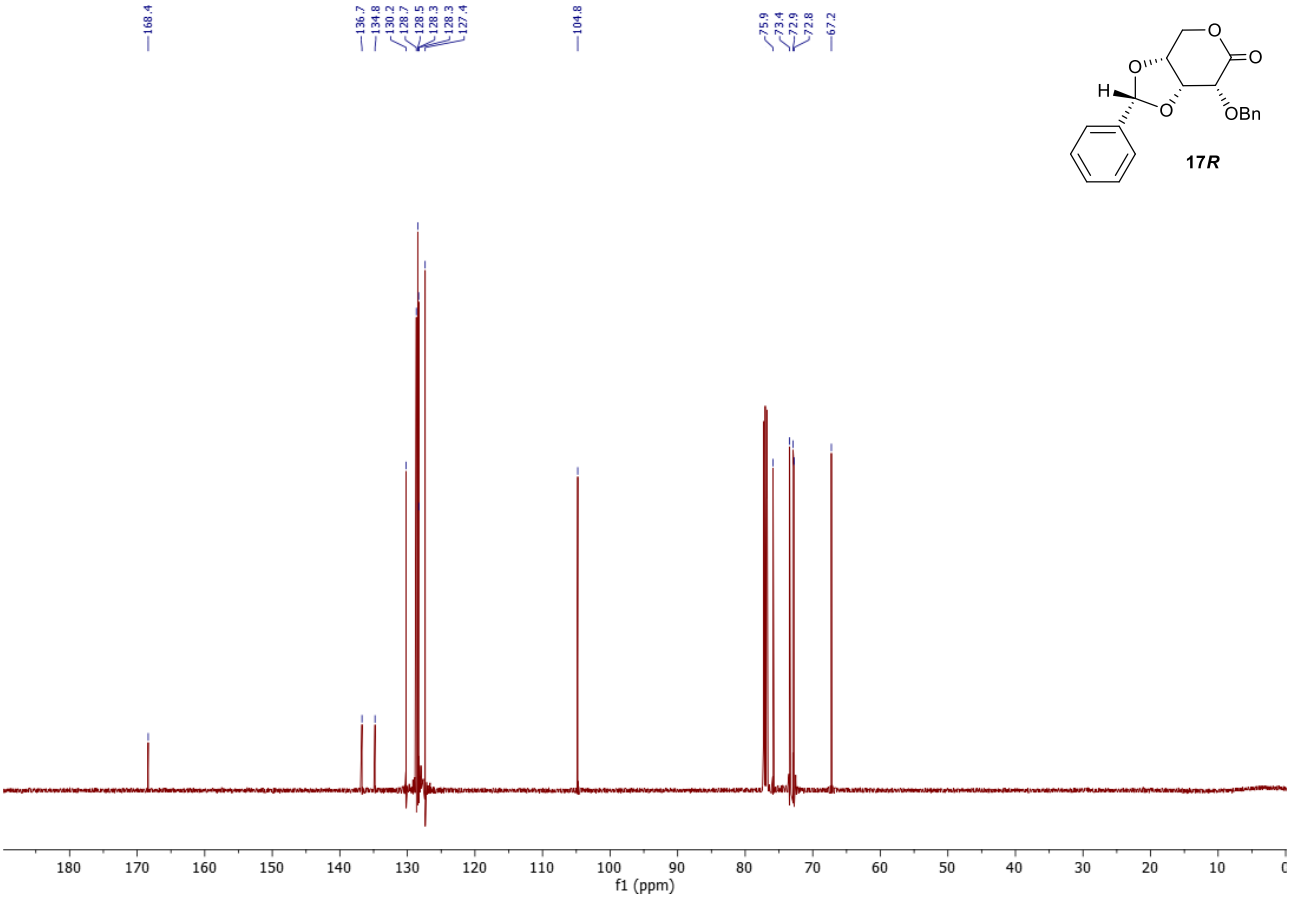
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OBn
17R
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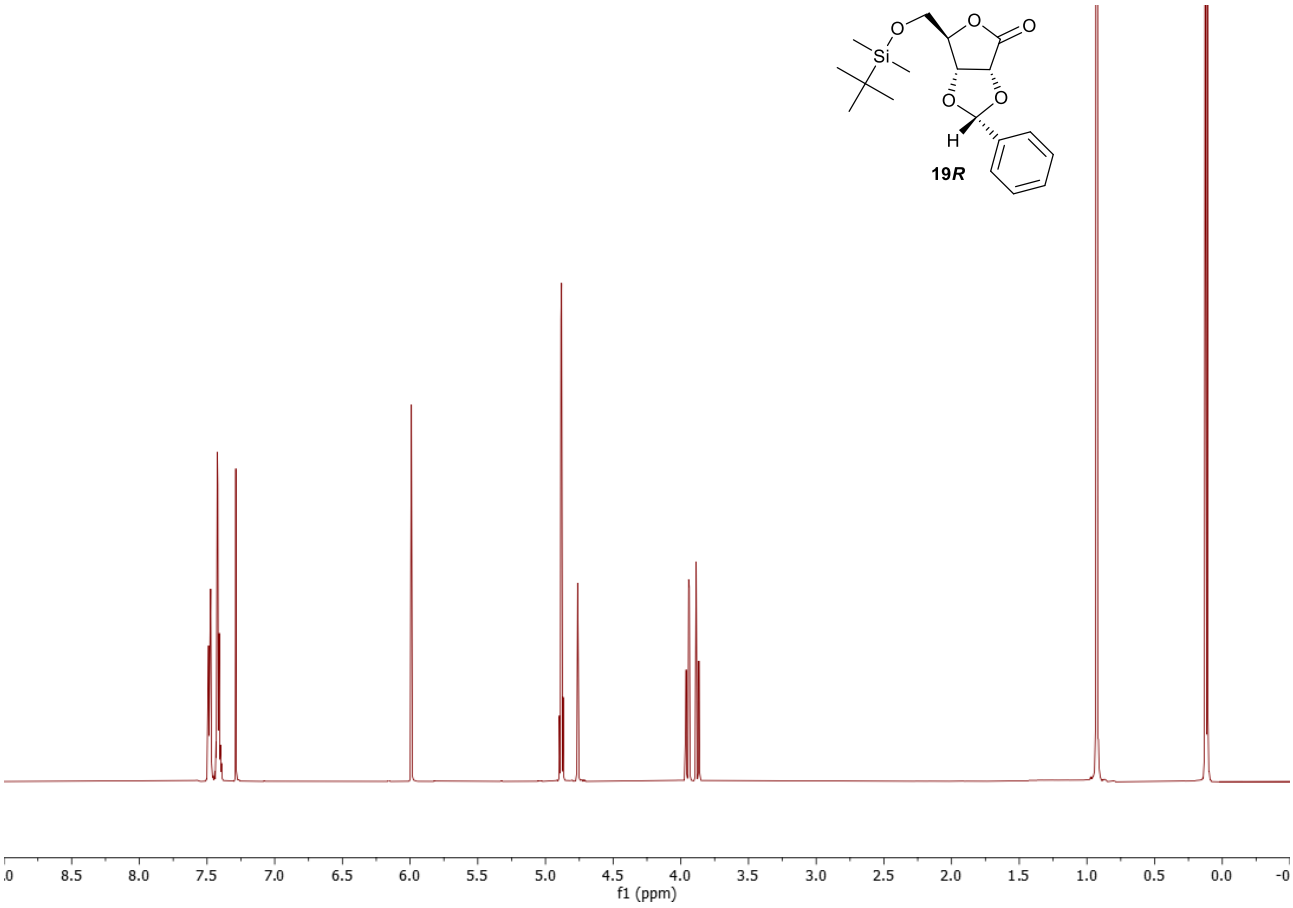
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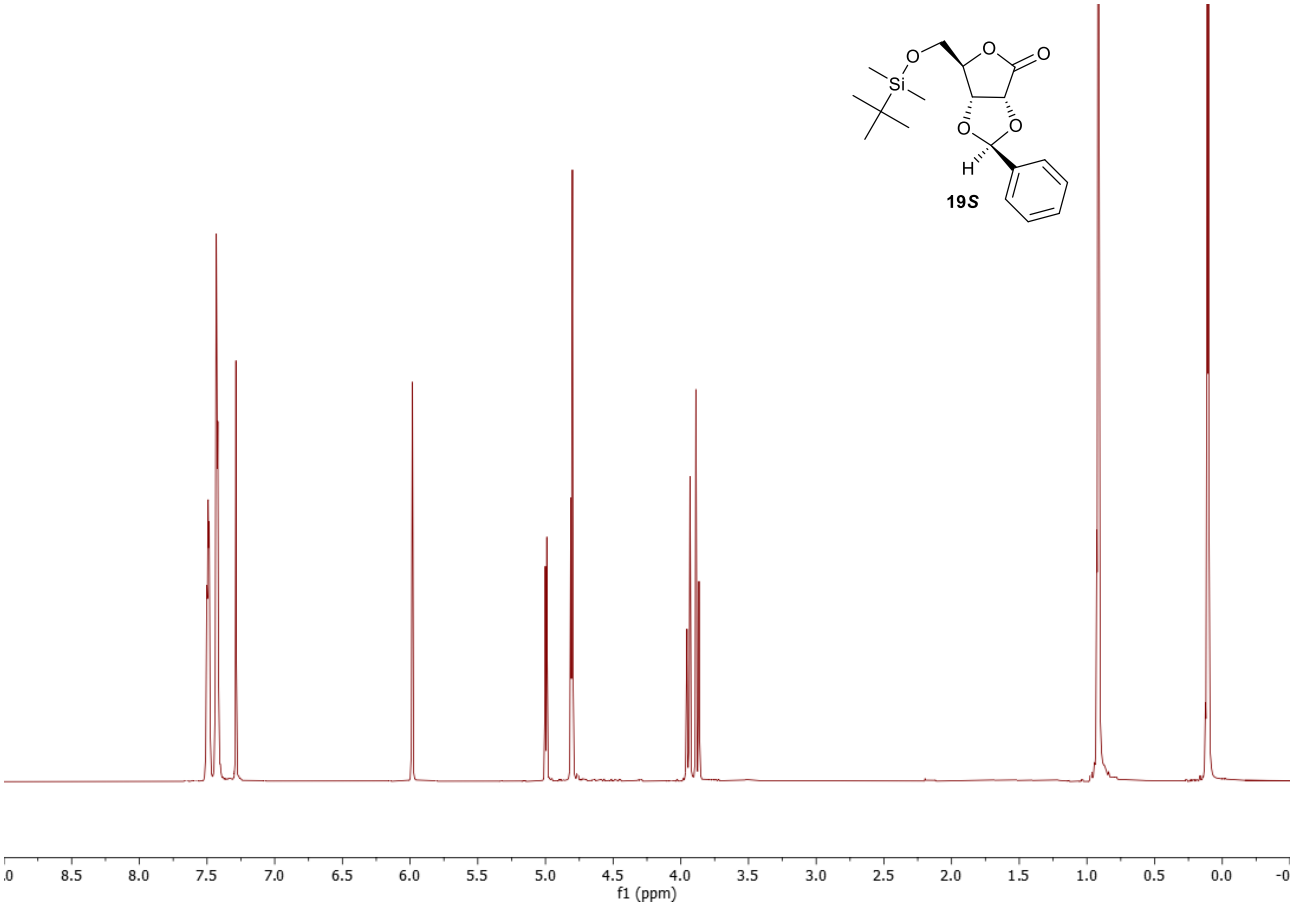
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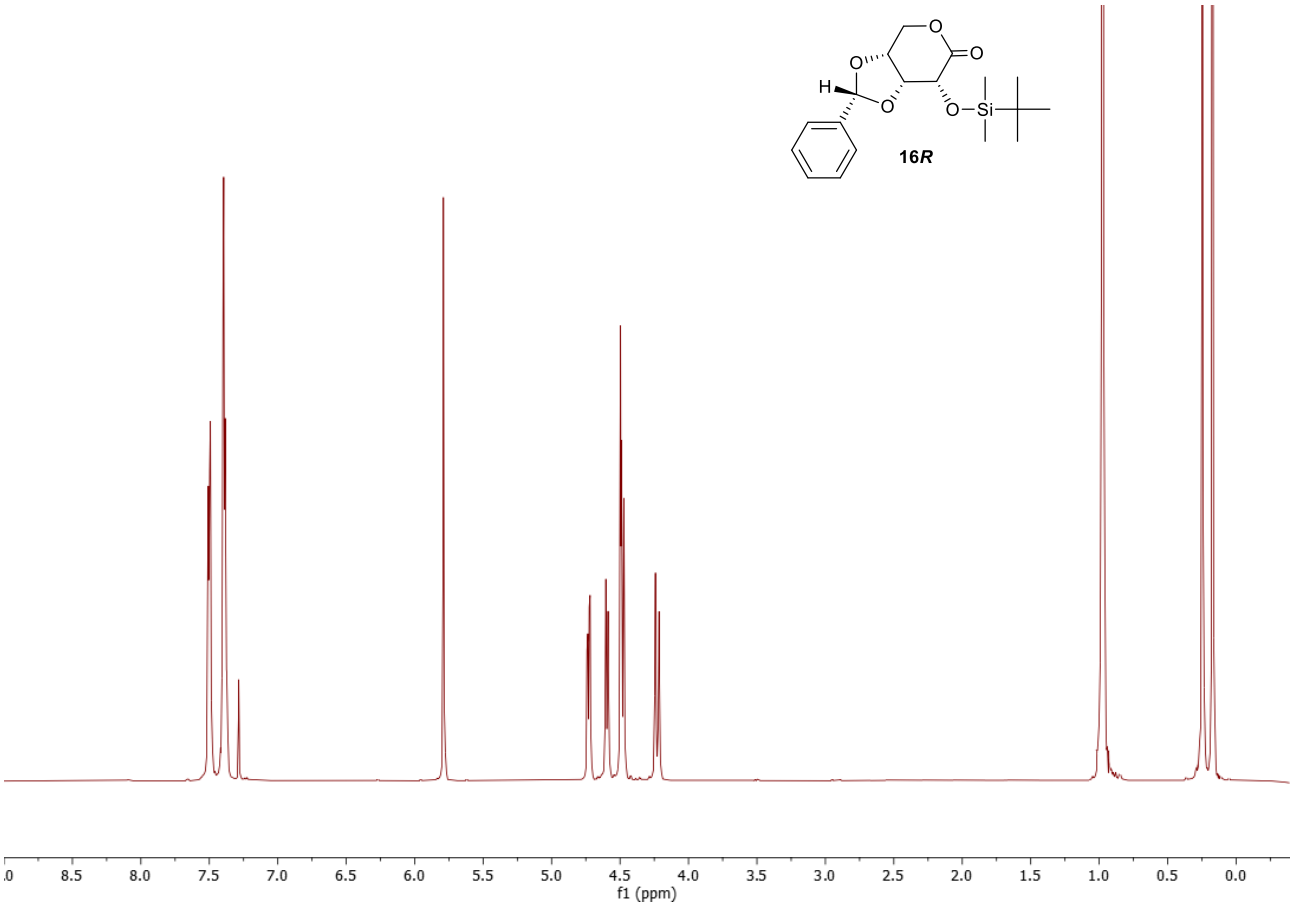
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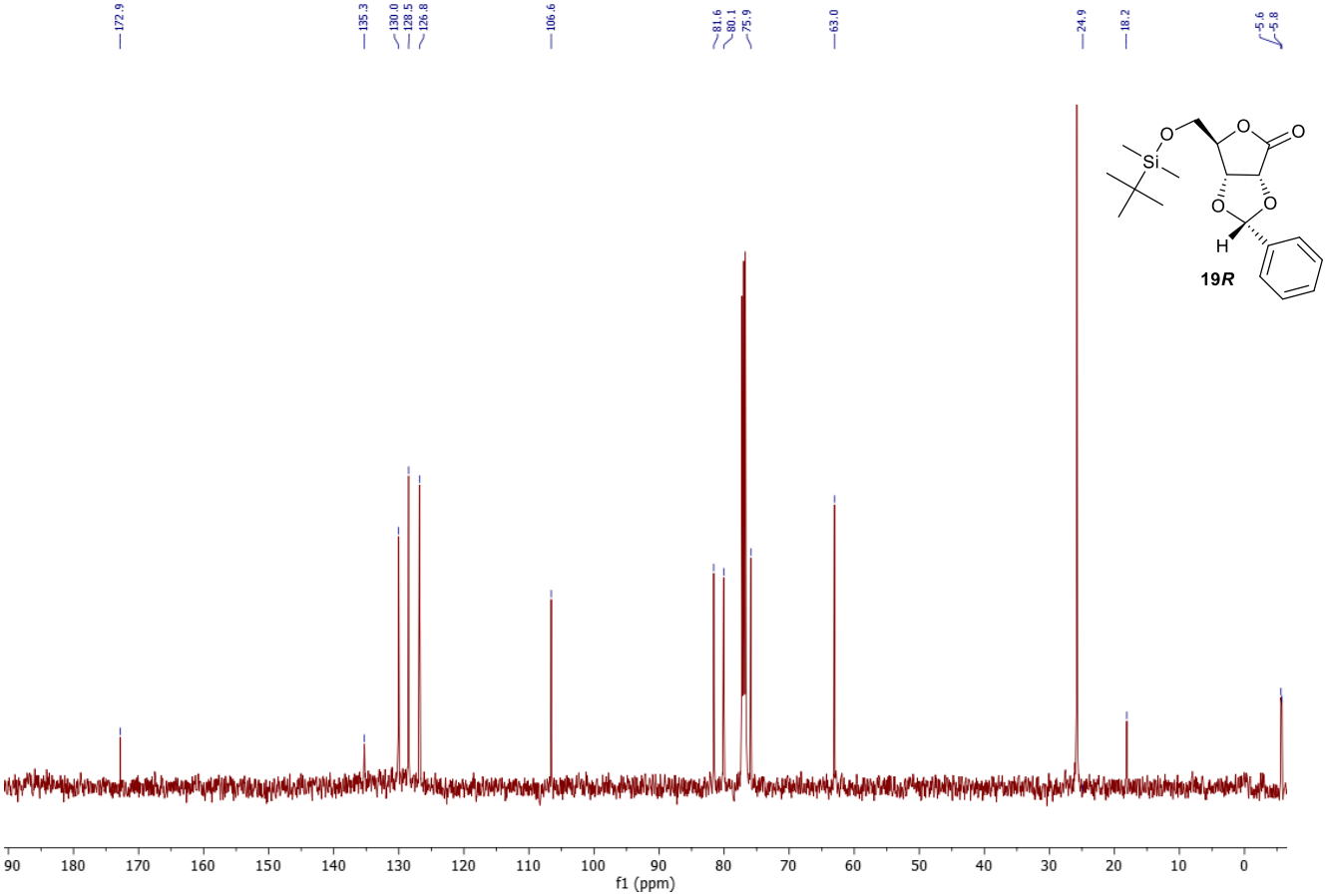
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-5.8
19R
90
180
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120
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100
90
80
70
60
50
40
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10
0
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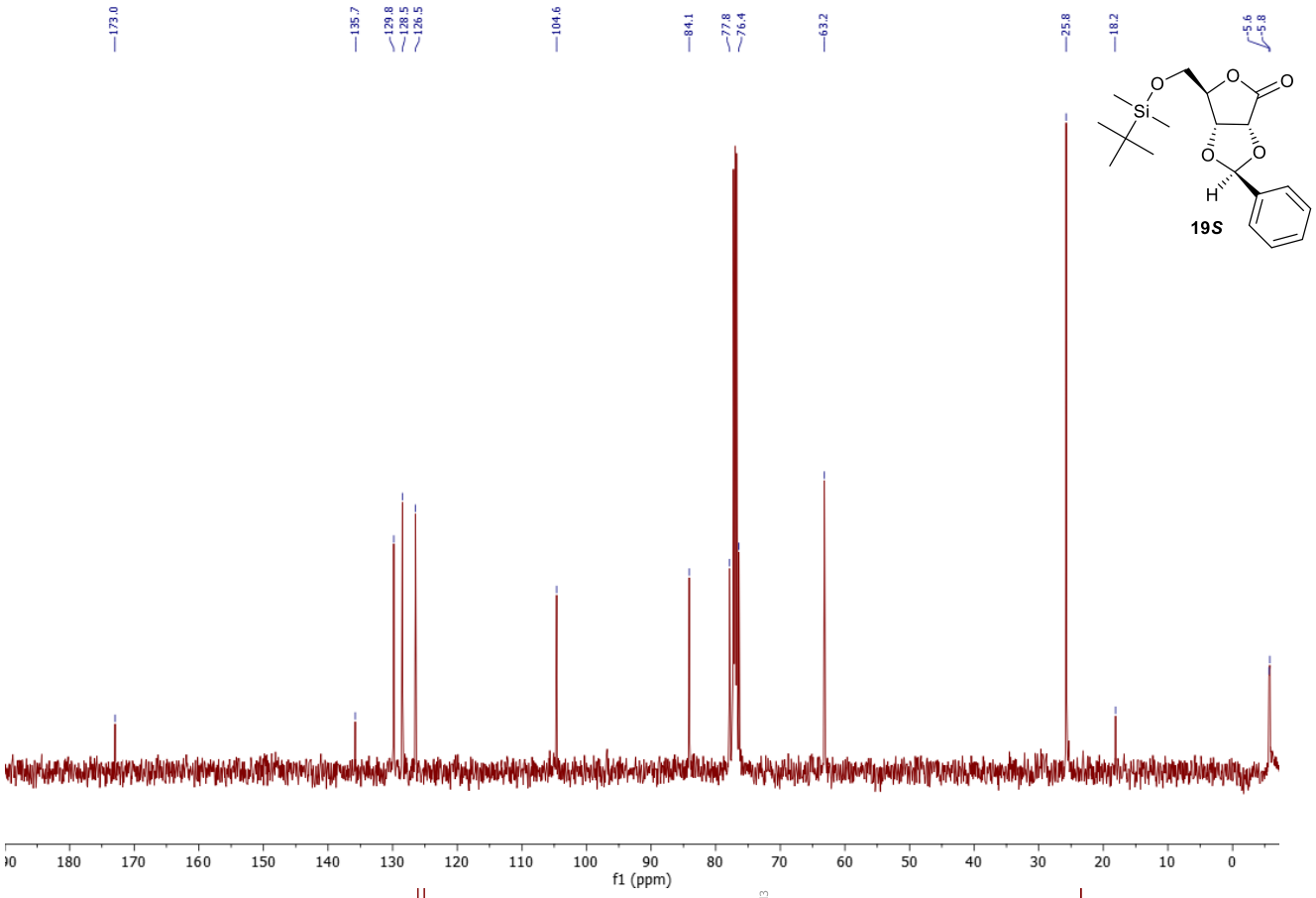
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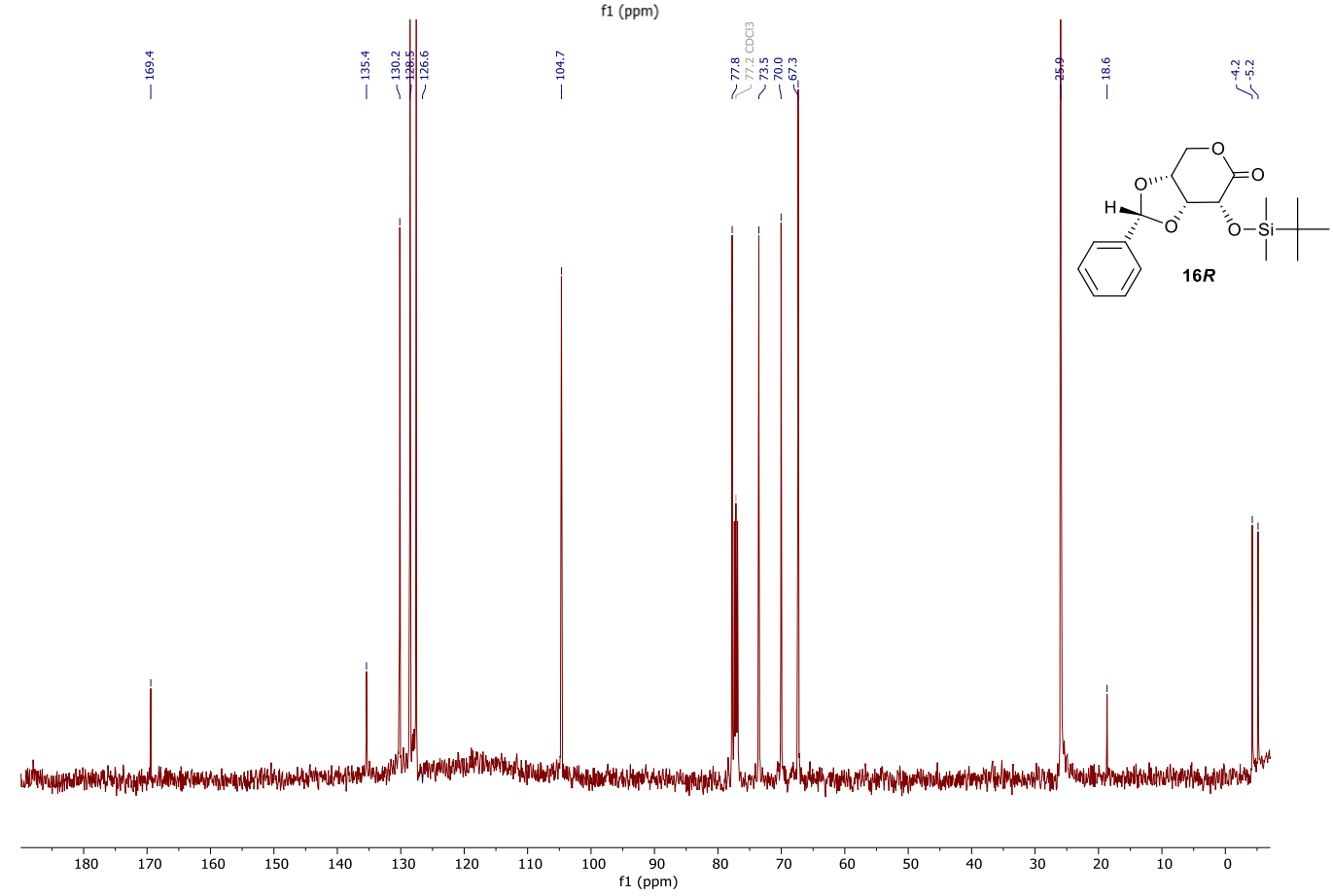
O
O
O
O
H
19S
f1 (ppm)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18.6
-4.2
-5.2
O
O
O
H
O
O
Si
16R
f1 (ppm)

Table S1. Energies (E), relative energies (ΔE) in kJ/mol and Boltzmann population distribution at 298 K of conformers of the compound **12*R***, in a range of 50 kJ/mol (12 kcal/mol), calculated with a hybrid DFT (B3LYP) approach with 6-31G* basis set using SM8 (DMSO) solvation model.

E (kJ/mol)	ΔE (kJ/mol)	% in the population
-2207062.42	0.00	99.99
-2207039.64	22.78	1.00×10^{-4}
-2207031.86	30.56	4.30×10^{-6}
-2207026.05	36.37	4.11×10^{-7}
-2207025.94	36.48	3.93×10^{-7}
-2207019.50	42.92	2.90×10^{-8}

Table S2. Energies (E), relative energies (ΔE) in kJ/mol and Boltzmann population distribution at 298 K of conformers of the compound **12*S***, in a range of 50 kJ/mol (12 kcal/mol), calculated with a hybrid DFT (B3LYP) approach with 6-31G* basis set using SM8 (DMSO) solvation model.

E (kJ/mol)	ΔE (kJ/mol)	% in the population
-2207059.06	0.00	99.94
-2207038.82	20.24	0.028
-2207038.68	20.39	0.027
-2207027.14	31.92	2.56×10^{-4}
-2207027.08	31.98	2.50×10^{-4}
-2207022.11	36.95	3.36×10^{-5}
-2207021.70	37.36	2.84×10^{-5}

Table S3. Energies (E), relative energies (ΔE) in kJ/mol and Boltzmann population distribution at 298 K of conformers of the compound **11*R***, in a range of 50 kJ/mol (12 kcal/mol), calculated with a hybrid DFT (B3LYP) approach with 6-31G* basis set using SM8 ($CHCl_3$) solvation model.

E (kJ/mol)	ΔE (kJ/mol)	% in the population
-2207031.58	0.00	84.42
-2207026.44	5.14	10.63
-2207022.56	9.02	2.22
-2207022.02	9.56	1.78
-2207020.38	11.21	0.92
-2207011.68	19.90	0.03

Table S4. Energies (E), relative energies (ΔE) in kJ/mol and Boltzmann population distribution at 298 K of conformers of the compound **11*S***, in a range of 50 kJ/mol (12 kcal/mol), calculated with a hybrid DFT (B3LYP) approach with 6-31G* basis set using SM8 ($CHCl_3$) solvation model.

E (kJ/mol)	ΔE (kJ/mol)	% in the population
-2207029.90	0.00	62.68
-2207027.67	2.23	25.45
-2207025.27	4.63	9.68
-2207020.40	9.50	1.36
-2207018.62	11.28	0.66
-2207015.21	14.69	0.17