

ELECTRONIC SUPPLEMENTARY INFORMATION

for

Orthogonal synthesis of a heterodimeric ligand for the development of the Gd^{III}/Ga^{III} ditopic complex as potential pH-sensitive MRI/PET probe

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HPLC methods

Method 1:

Solvent A: H₂O TFA 0.1%; Solvent B: MeOH TFA 0.1%

HPLC gradient conditions, at flow: 1 ml/min

Time (min)	Solvent A (%)	Solvent B (%)
0	25	75
15	0	100
17	0	100

Method 2:

Solvent A: H₂O TFA 0.1%; Solvent B: MeOH TFA 0.1%

HPLC gradient conditions, at flow: 1 ml/min

Time (min)	Solvent A (%)	Solvent B (%)
0	30	70
10	20	80
15	0	100

Method 3:

Solvent A: H₂O TFA 0.1%; Solvent B: MeOH TFA 0.1%

HPLC gradient conditions, at flow: 1 ml/min

Time (min)	Solvent A (%)	Solvent B (%)
0	20	80
15	0	100
17	0	100

Method 4:

Solvent A: H₂O TFA 0.1%; Solvent B: MeOH TFA 0.1%

HPLC gradient conditions, at flow: 1 ml/min

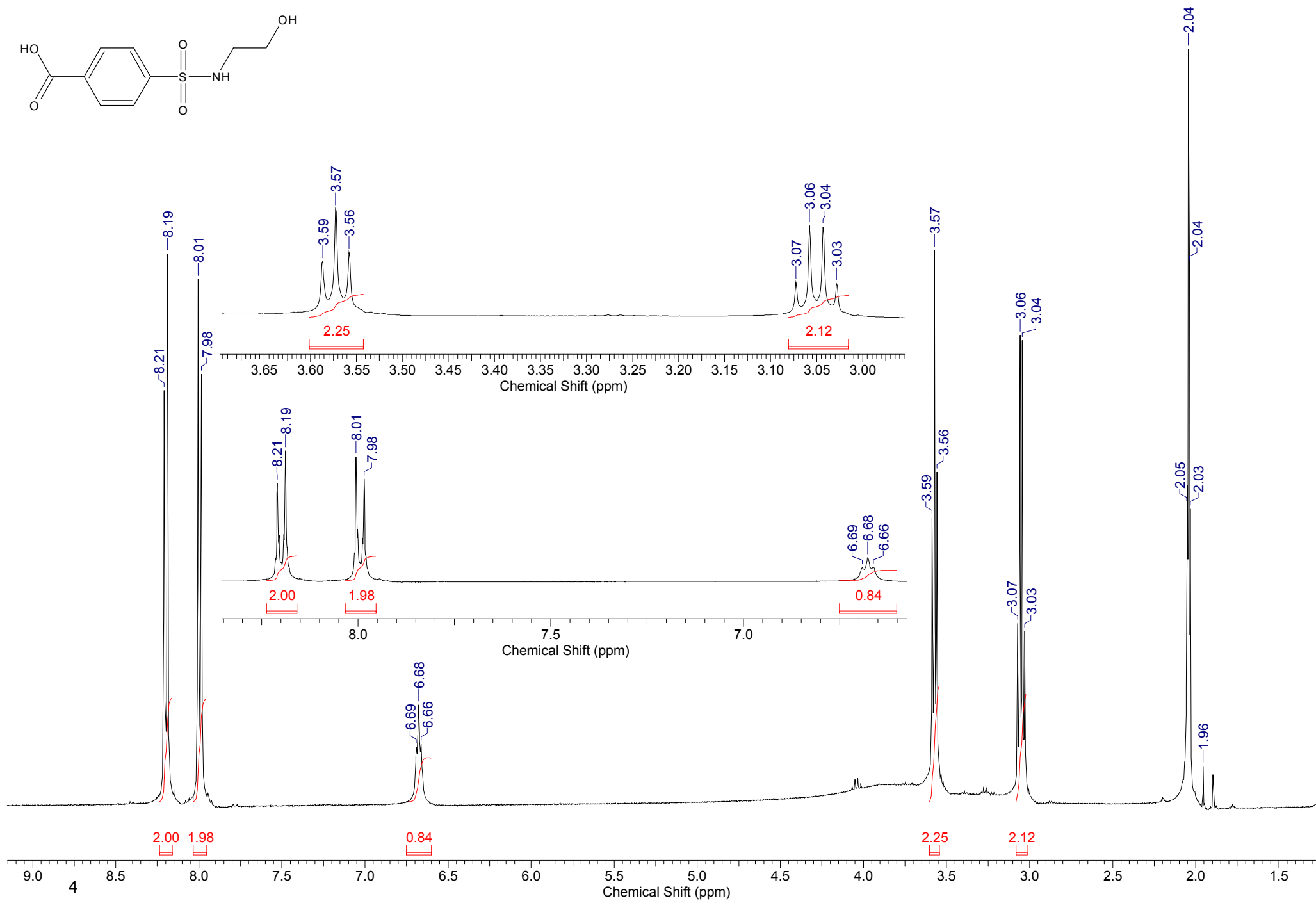
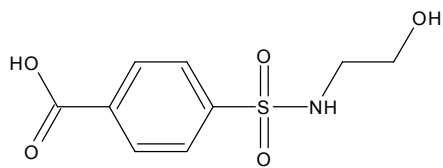
Time (min)	Solvent A (%)	Solvent B (%)
0	100	0
5	100	0
8	90	10
12	90	10
14	0	100

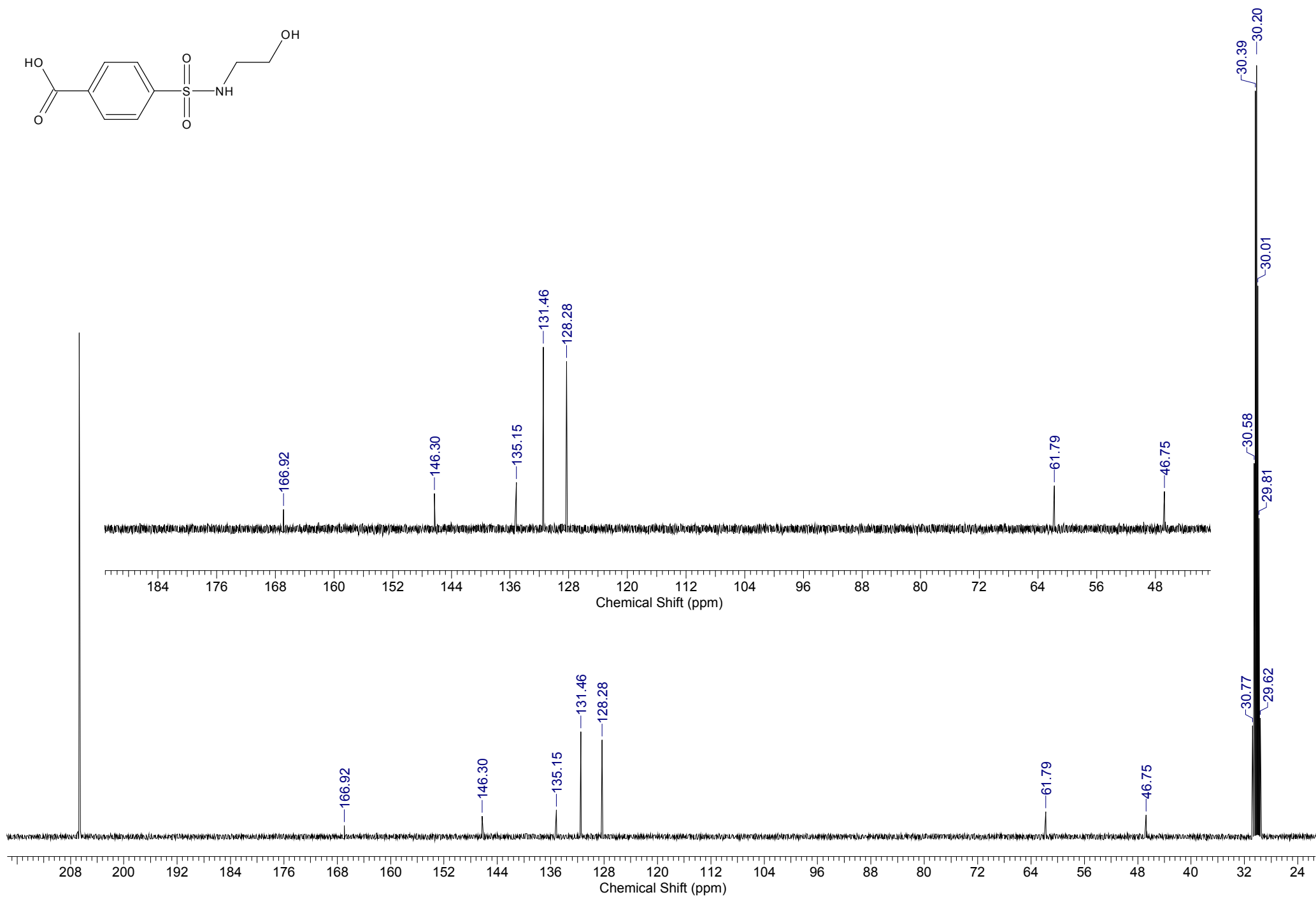
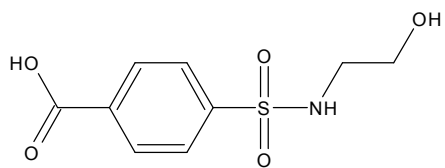
Method 5:

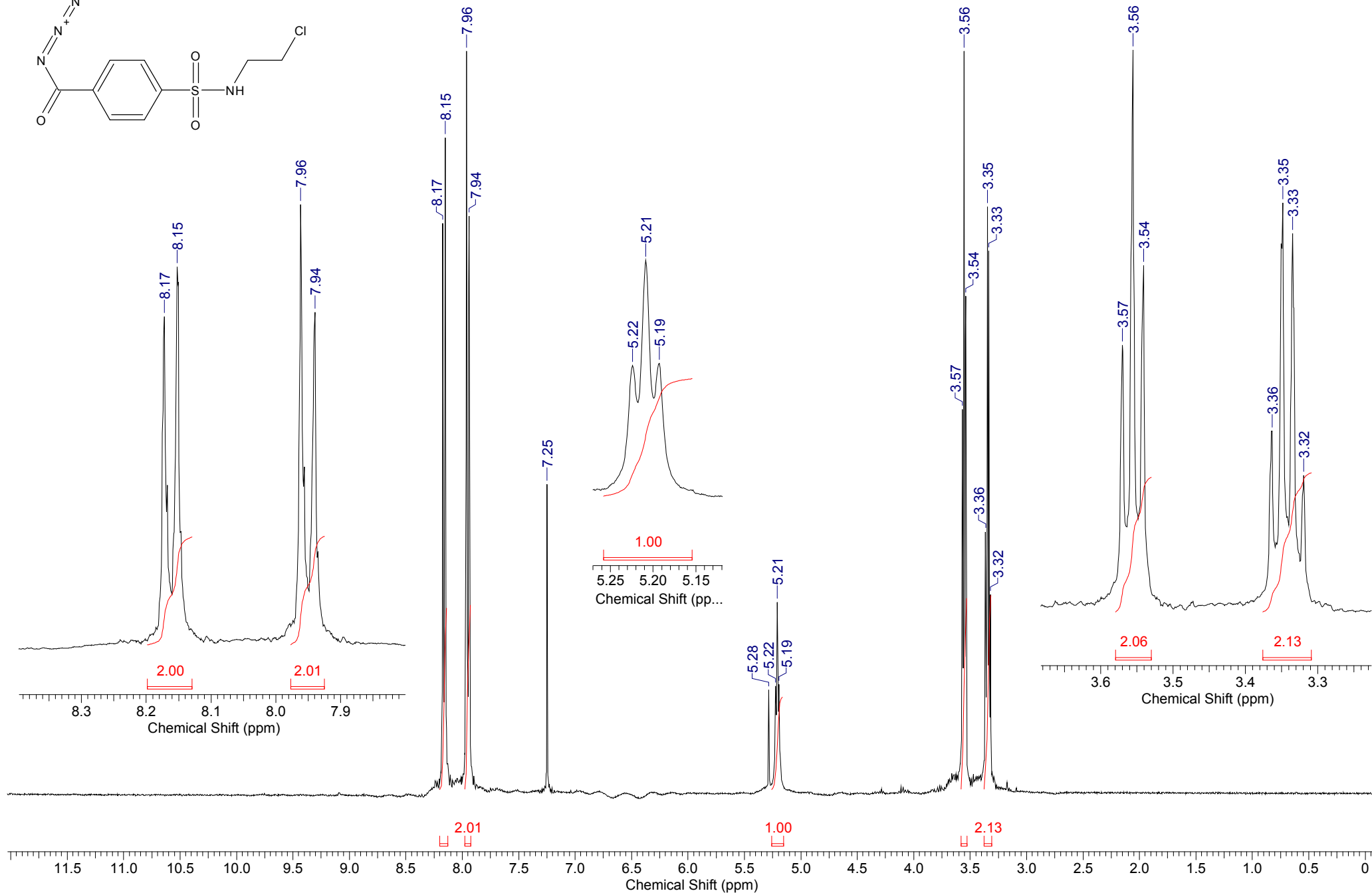
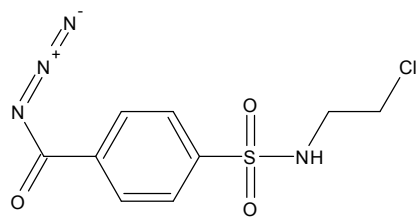
Solvent A: H₂O TFA 0.1%; Solvent B: MeOH TFA 0.1%

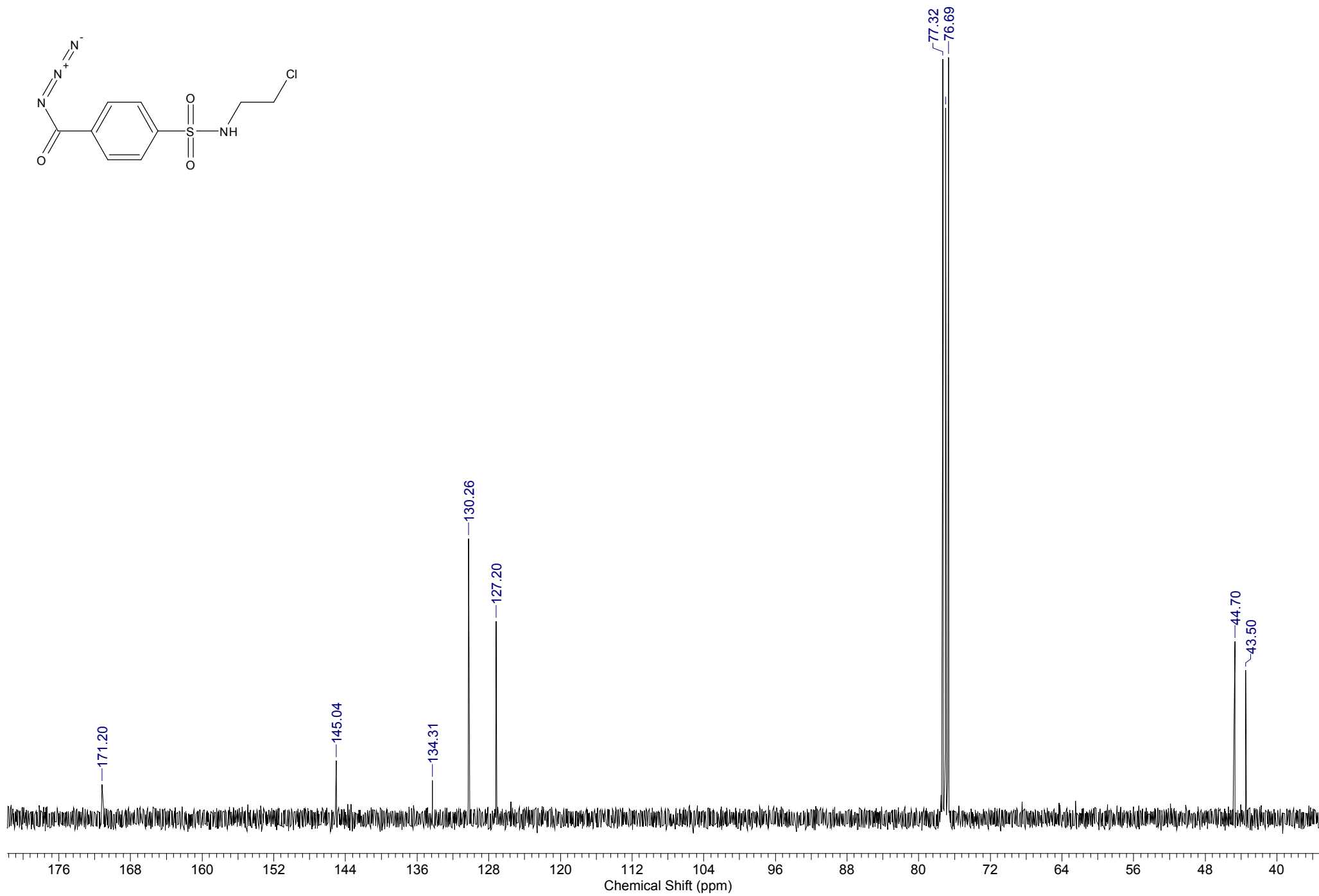
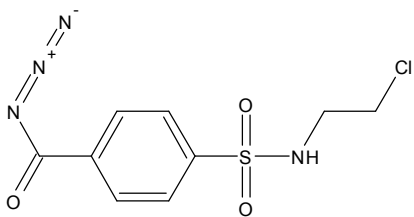
HPLC gradient conditions, at flow: 20 ml/min

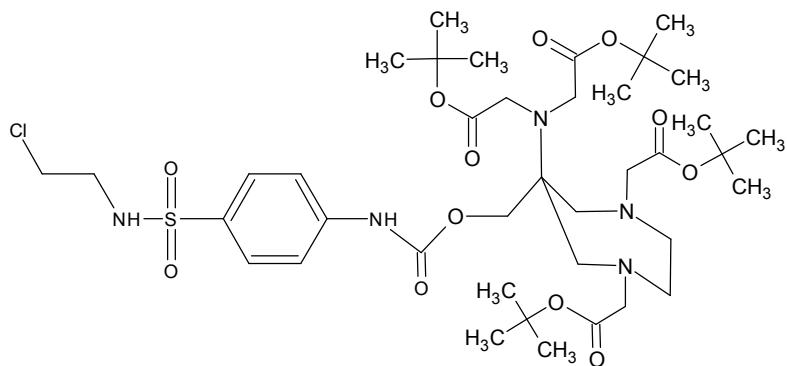
Time (min)	Solvent A (%)	Solvent B (%)
0	30	70
6.67	20	80
10	0	100



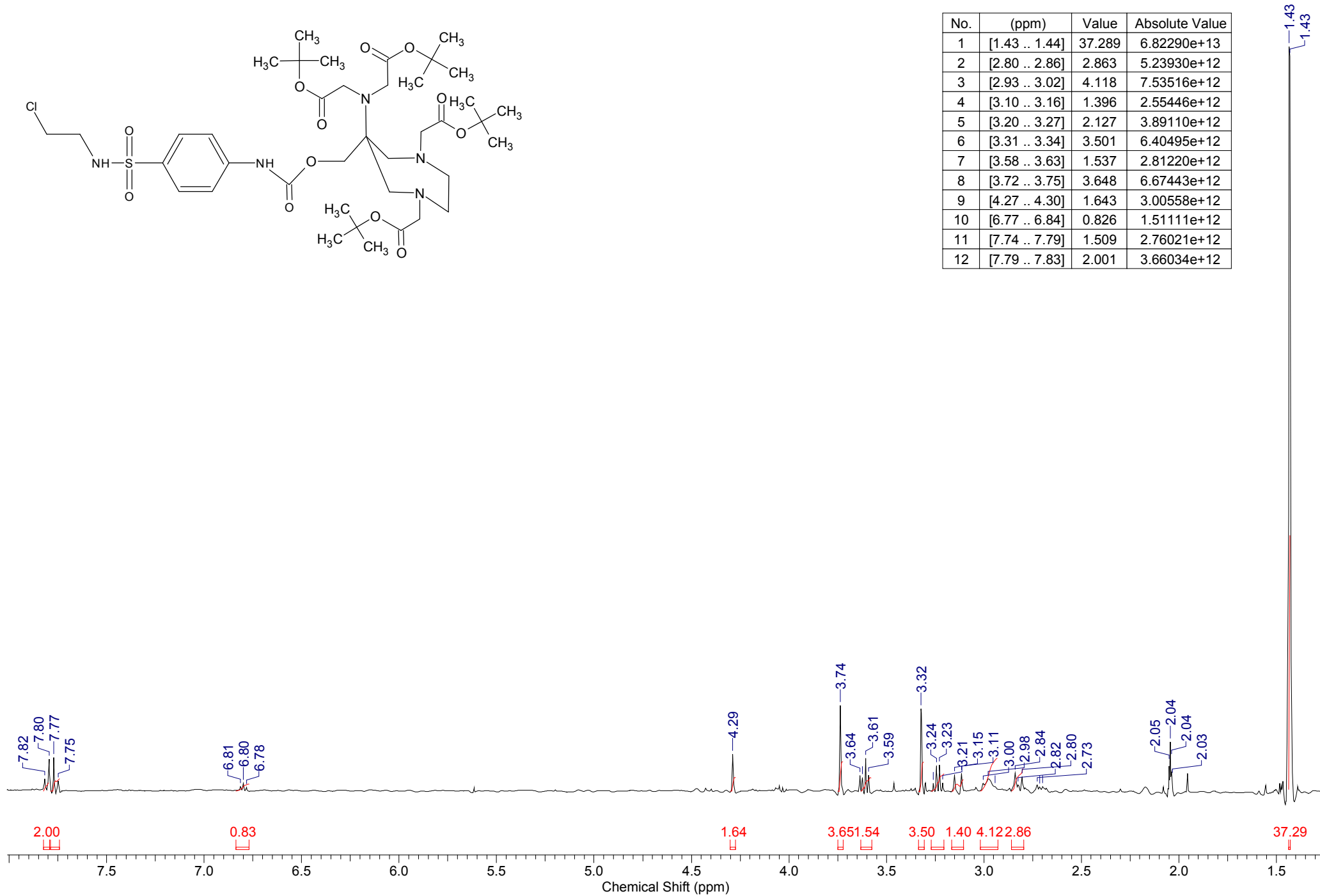


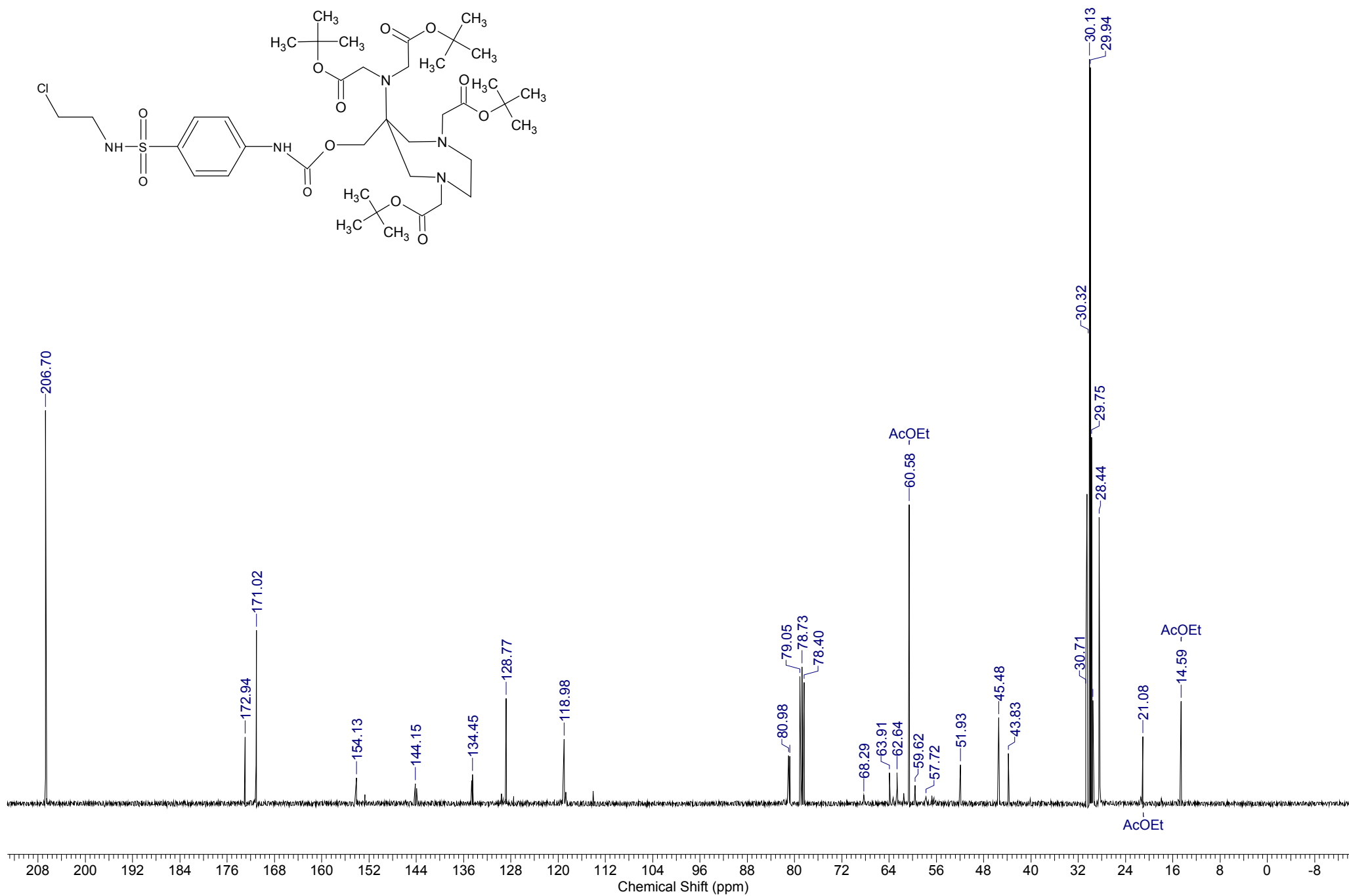
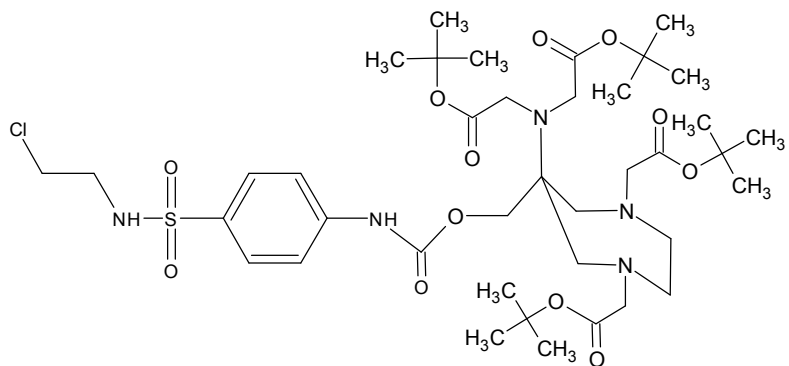


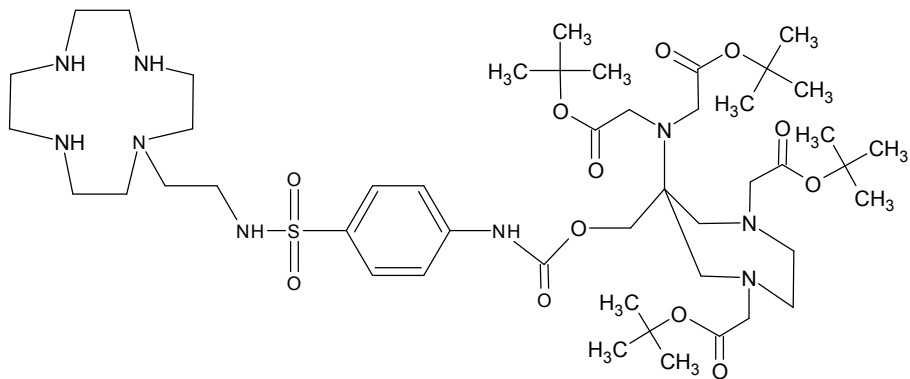




No.	(ppm)	Value	Absolute Value
1	[1.43 .. 1.44]	37.289	6.82290e+13
2	[2.80 .. 2.86]	2.863	5.23930e+12
3	[2.93 .. 3.02]	4.118	7.53516e+12
4	[3.10 .. 3.16]	1.396	2.55446e+12
5	[3.20 .. 3.27]	2.127	3.89110e+12
6	[3.31 .. 3.34]	3.501	6.40495e+12
7	[3.58 .. 3.63]	1.537	2.81220e+12
8	[3.72 .. 3.75]	3.648	6.67443e+12
9	[4.27 .. 4.30]	1.643	3.00558e+12
10	[6.77 .. 6.84]	0.826	1.51111e+12
11	[7.74 .. 7.79]	1.509	2.76021e+12
12	[7.79 .. 7.83]	2.001	3.66034e+12







No.	(ppm)	Value	Absolute Value
1	[1.37 .. 1.39]	36.357	1.73412e+12
2	[2.51 .. 2.55]	4.301	2.05126e+11
3	[2.57 .. 2.63]	8.022	3.82640e+11
4	[2.69 .. 2.72]	2.158	1.02953e+11
5	[2.72 .. 2.79]	8.005	3.81810e+11
6	[2.83 .. 2.96]	4.220	2.01264e+11
7	[2.98 .. 3.09]	2.445	1.16617e+11
8	[3.18 .. 3.23]	4.066	1.93948e+11
9	[3.63 .. 3.67]	3.960	1.88887e+11
10	[4.14 .. 4.21]	2.140	1.02064e+11
11	[7.48 .. 7.54]	2.045	9.75365e+10
12	[7.69 .. 7.75]	2.000	9.53957e+10

