

SUPPORTING INFORMATION

Synthesis of Glutathione-Sulfur Mustard Bioadducts for the Verification of Potential Biomarkers

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Christian G. Bochet^[b], Christophe Curty*^[a]

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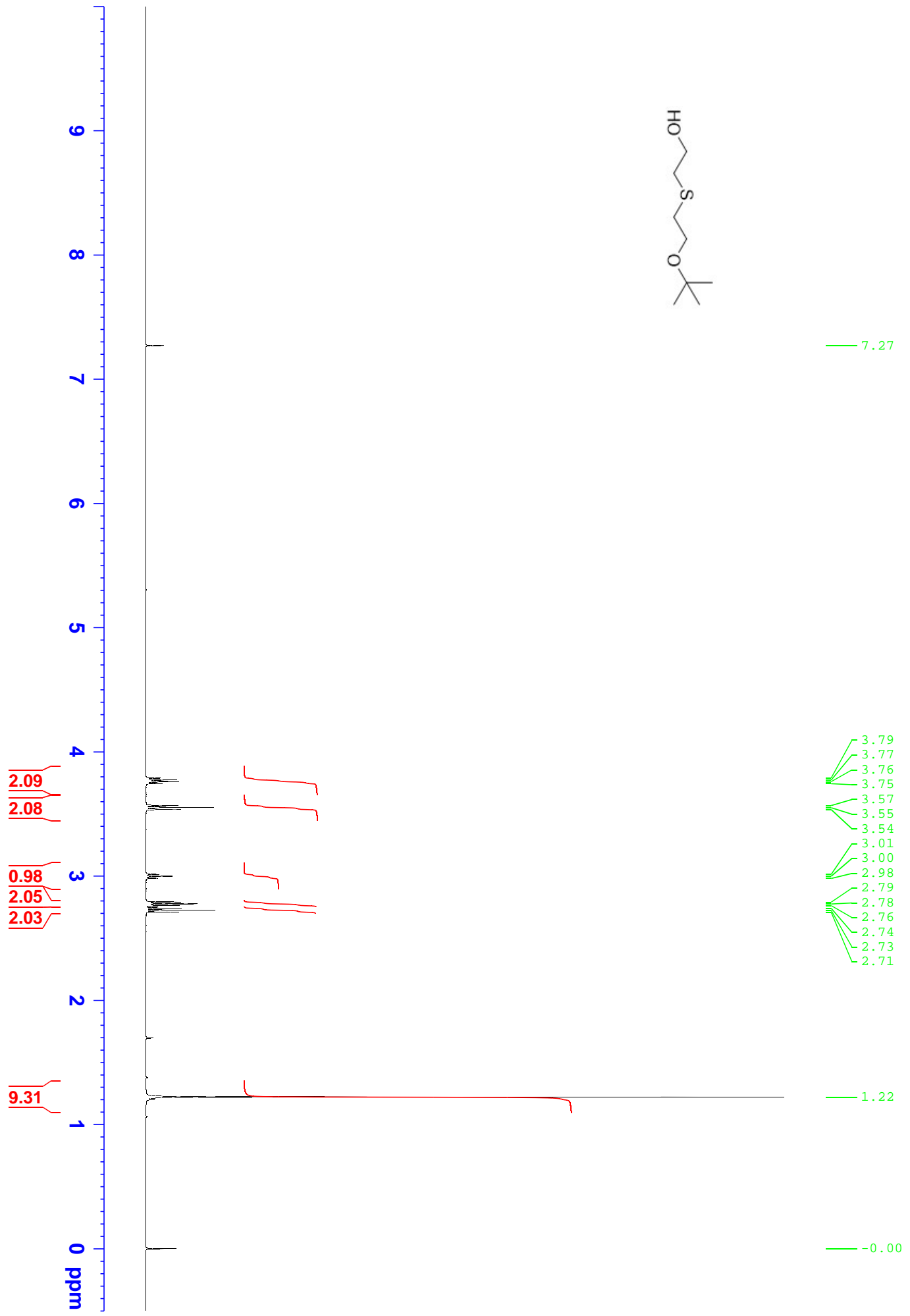
^[b]University of Fribourg, Departement of Chemistry, Chemin du Musée 9, 1700 Fribourg,
Switzerland

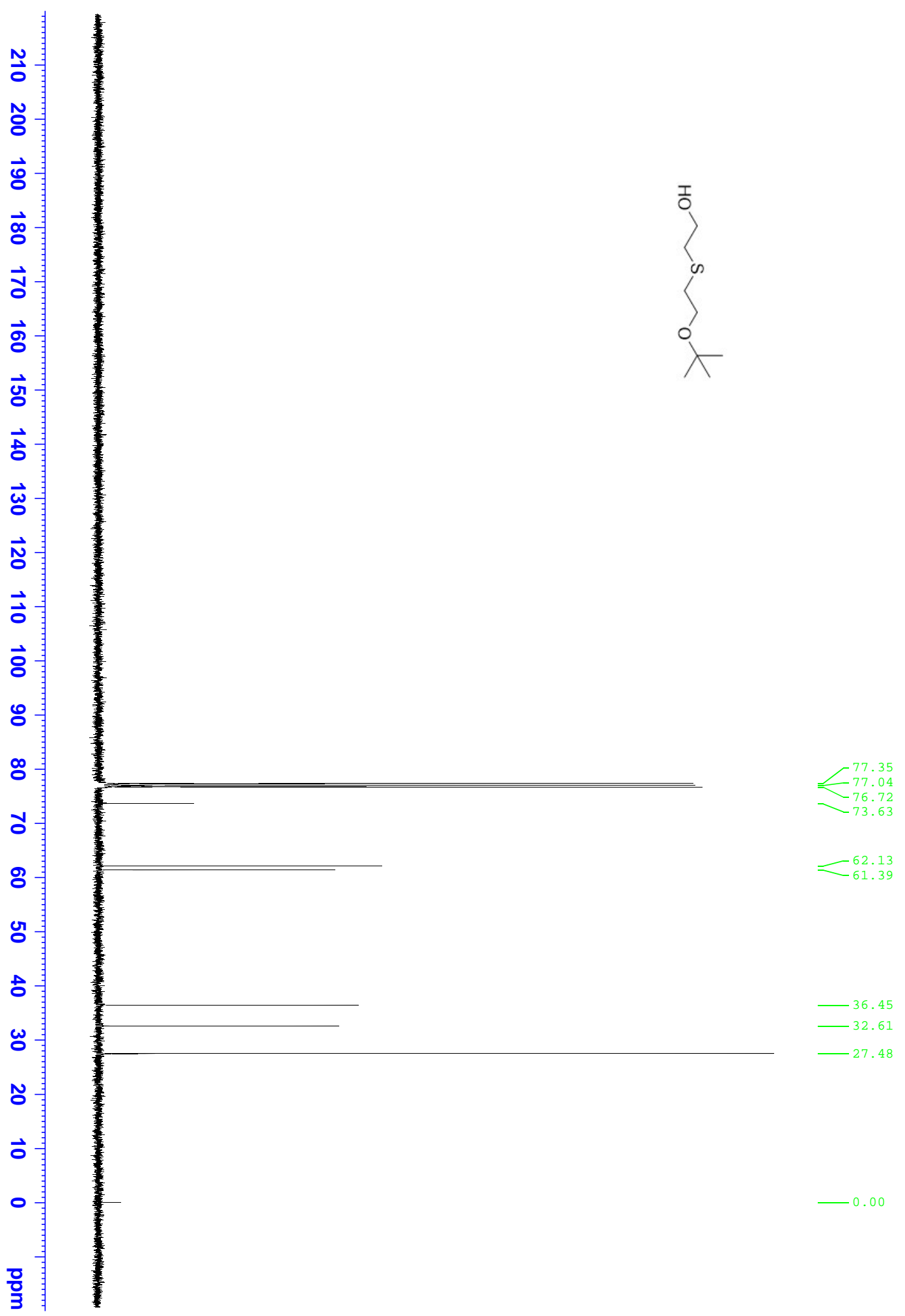
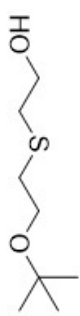
^[c]Ecole Polytechnique Fédéral de Lausanne, Institute of Chemical Sciences and Engineering,
Station 6, 1015 Lausanne, Switzerland

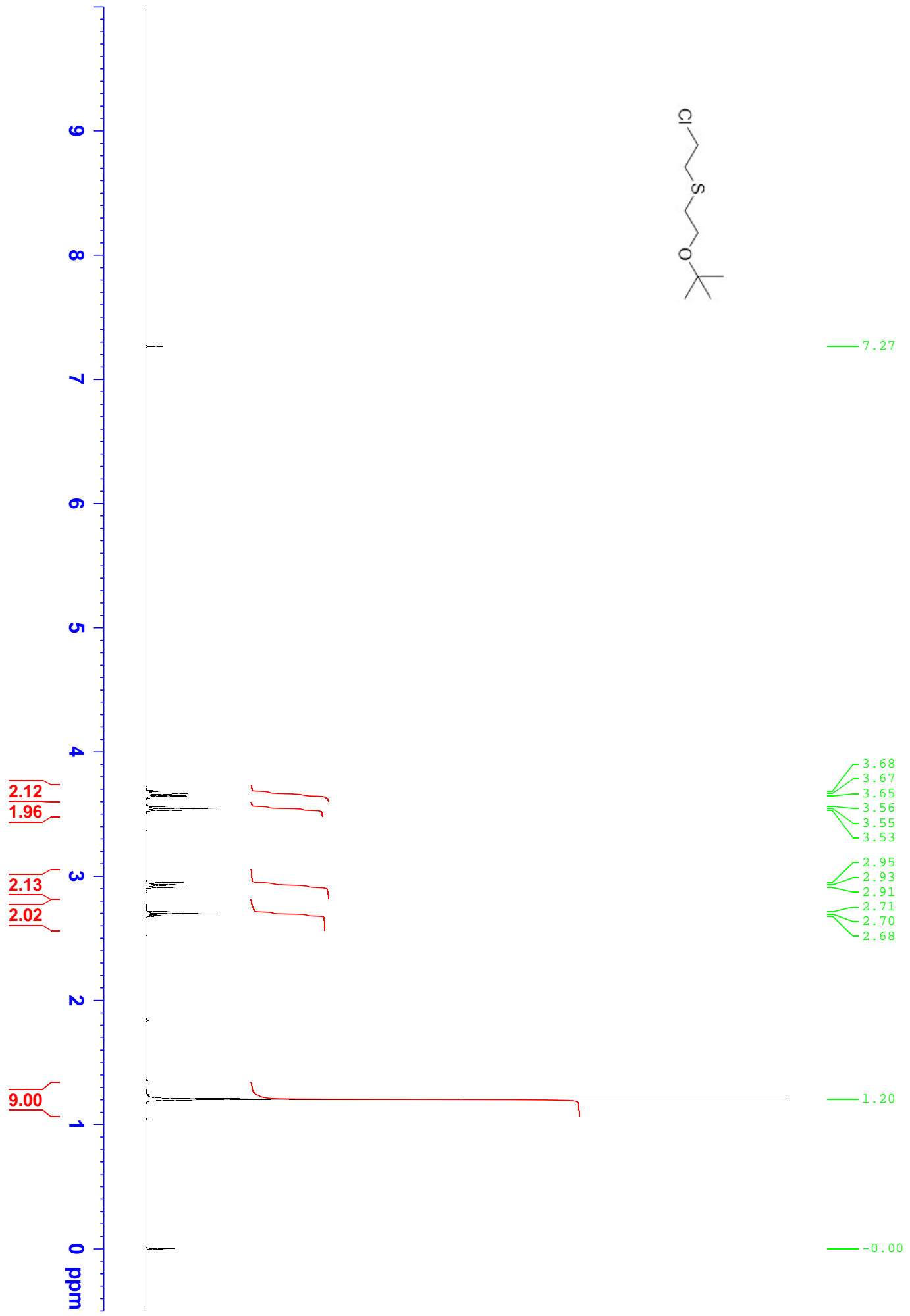
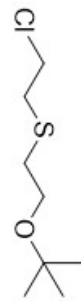
christophe.curty@babs.admin.ch

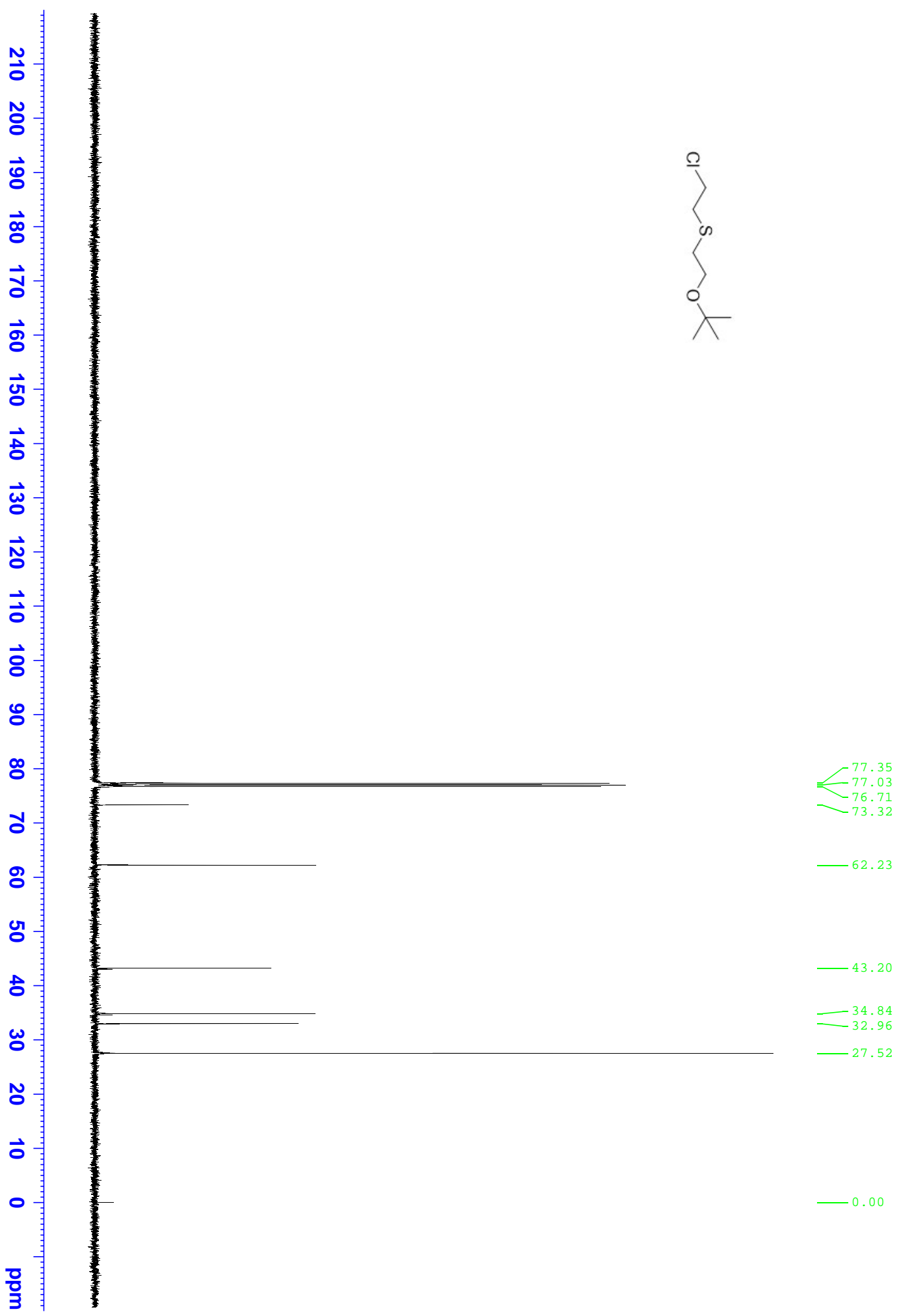
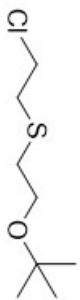
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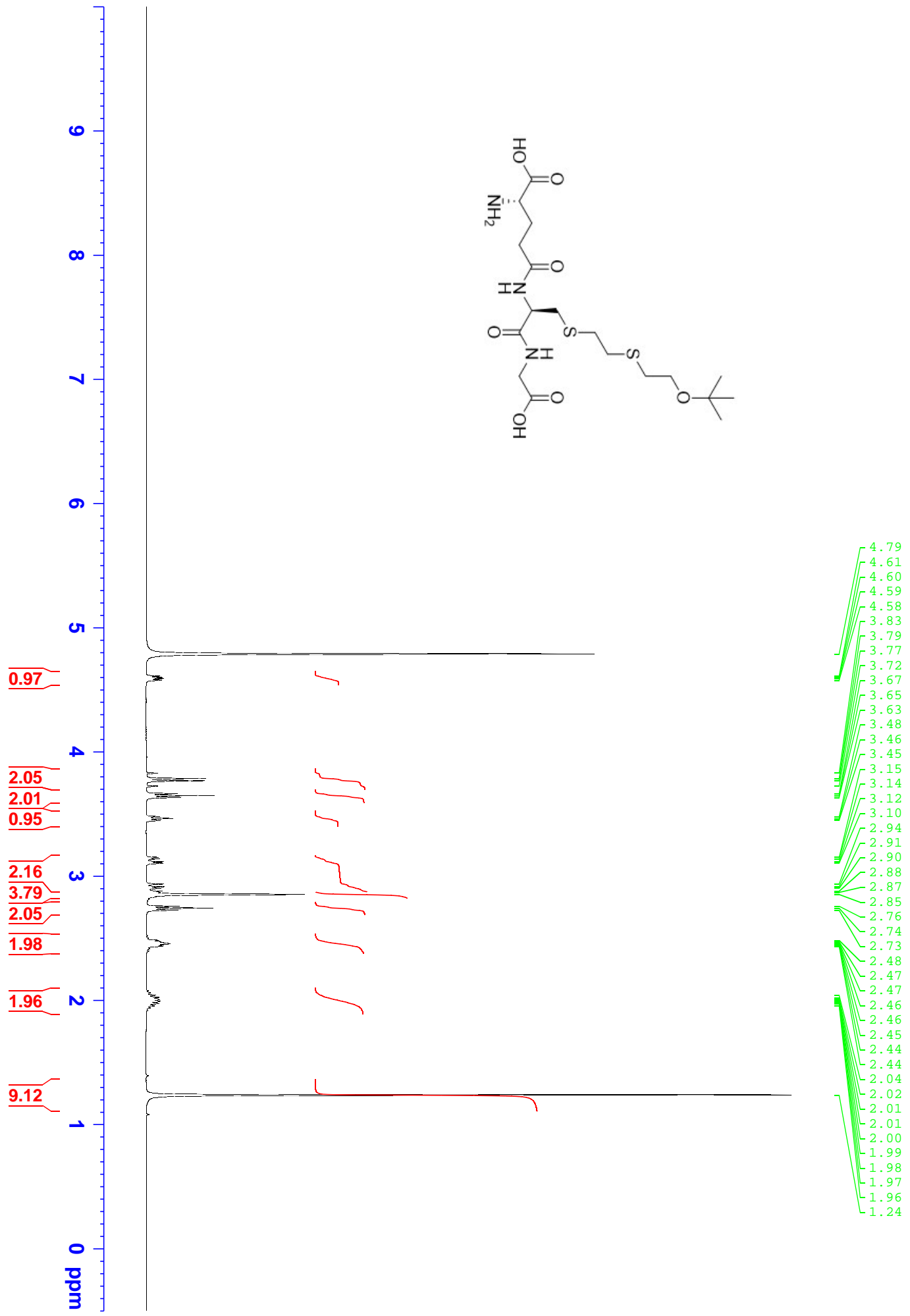
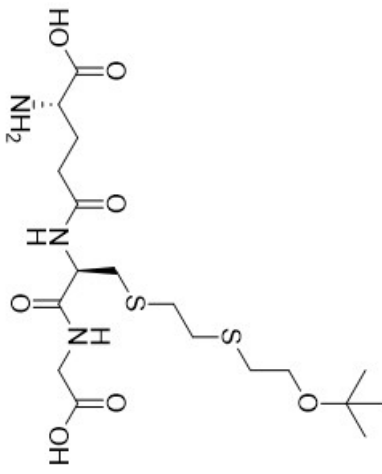
¹ H NMR and ¹³ C NMR of 1	S2
¹ H NMR and ¹³ C NMR of 2	S4
¹ H NMR and ¹³ C NMR of 3	S6
¹ H NMR and ¹³ C NMR of 4 by alkylation of GSH	S7
¹ H NMR and ¹³ C NMR of 5	S10
¹ H NMR and ¹³ C NMR of 6	S12
¹ H NMR and ¹³ C NMR of 4 by SPPS	S14
¹ H NMR and ¹³ C NMR of 7	S16
¹ H NMR and ¹³ C NMR of 11	S18
¹ H NMR and ¹³ C NMR of 12	S20
¹ H NMR and ¹³ C NMR of 8	S22
¹ H NMR and ¹³ C NMR of 14	S24
¹ H NMR and ¹³ C NMR of 15	S26
¹ H NMR and ¹³ C NMR of 9	S28

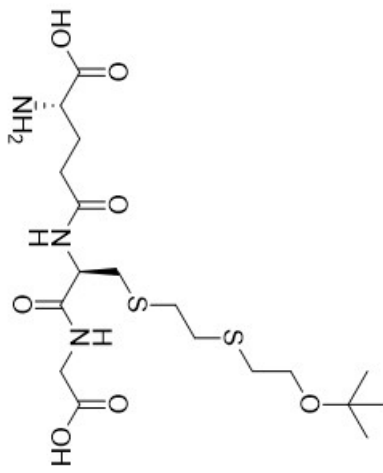






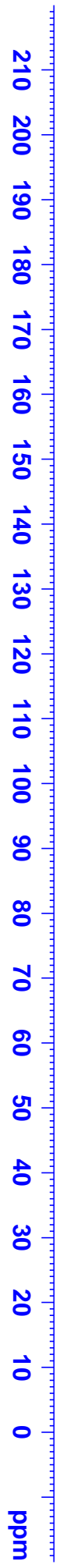


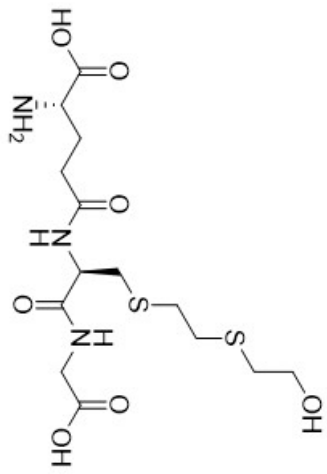




179.24
176.20
175.82
171.92

75.16
60.98
55.01
53.11
43.39
32.92
31.97
31.57
31.52
31.29
29.08
26.59



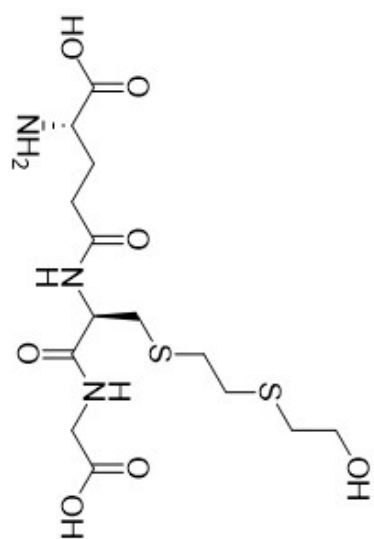


Integration values (from left to right):

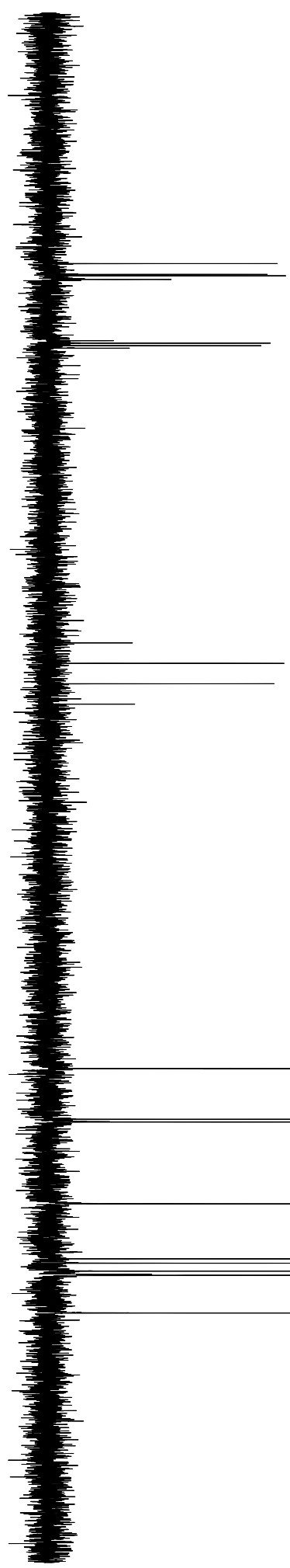
- 0.90
- 1.06
- 1.91
- 2.32
- 2.36
- 4.44
- 2.18
- 2.04
- 2.02

Peak chemical shifts (from top to bottom):

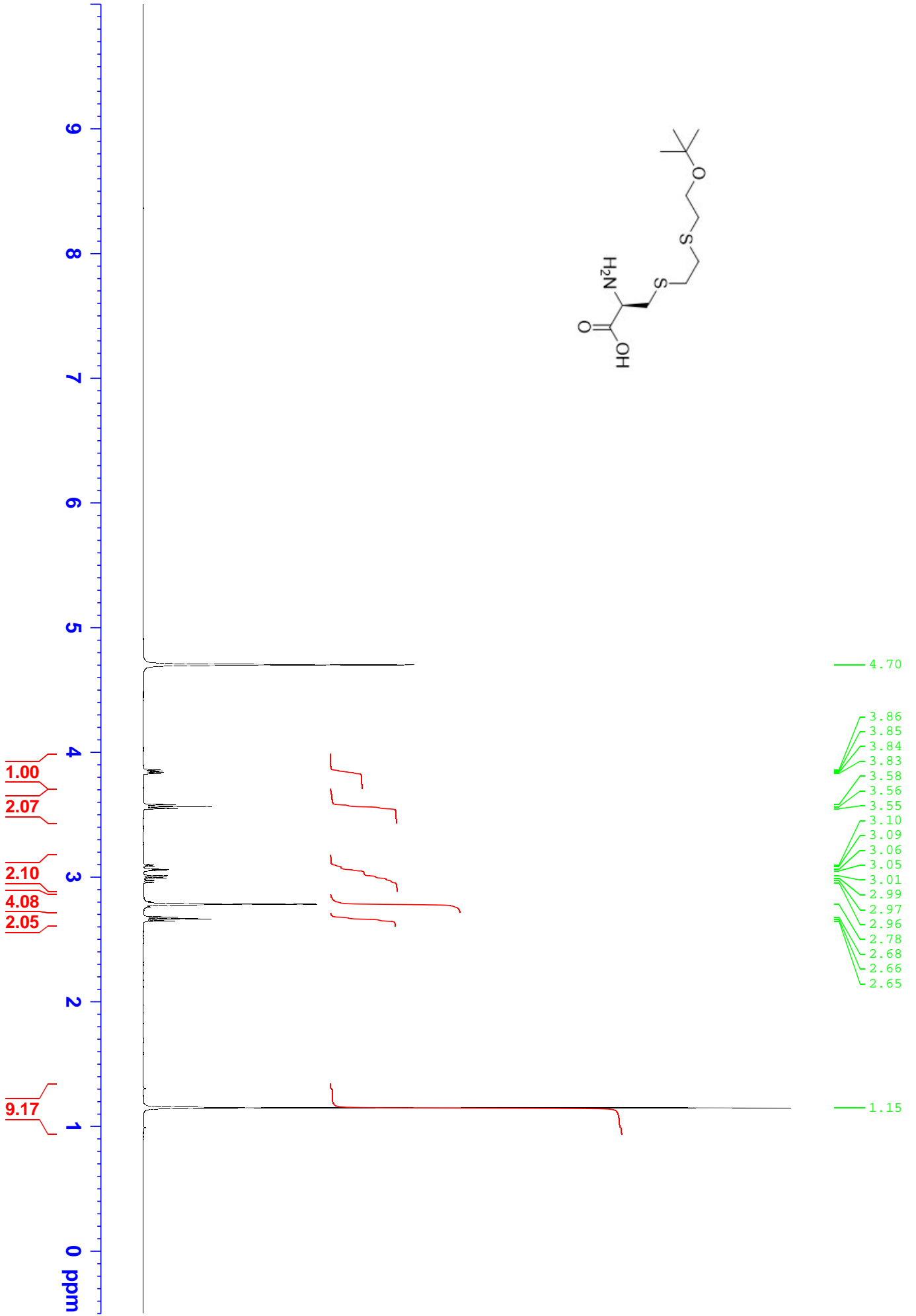
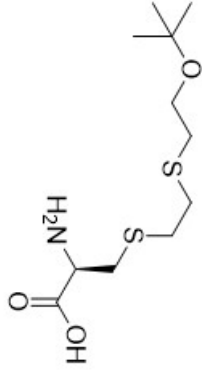
- 4.79
- 4.61
- 4.59
- 4.58
- 4.57
- 4.10
- 4.08
- 4.07
- 4.02
- 3.76
- 3.74
- 3.73
- 3.11
- 3.10
- 3.08
- 3.06
- 2.94
- 2.92
- 2.90
- 2.88
- 2.83
- 2.76
- 2.75
- 2.73
- 2.66
- 2.64
- 2.62
- 2.61
- 2.59
- 2.57
- 2.55
- 2.53
- 2.31
- 2.30
- 2.28
- 2.26
- 2.24
- 2.22
- 2.20
- 2.18
- 2.17



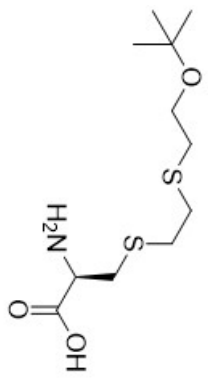
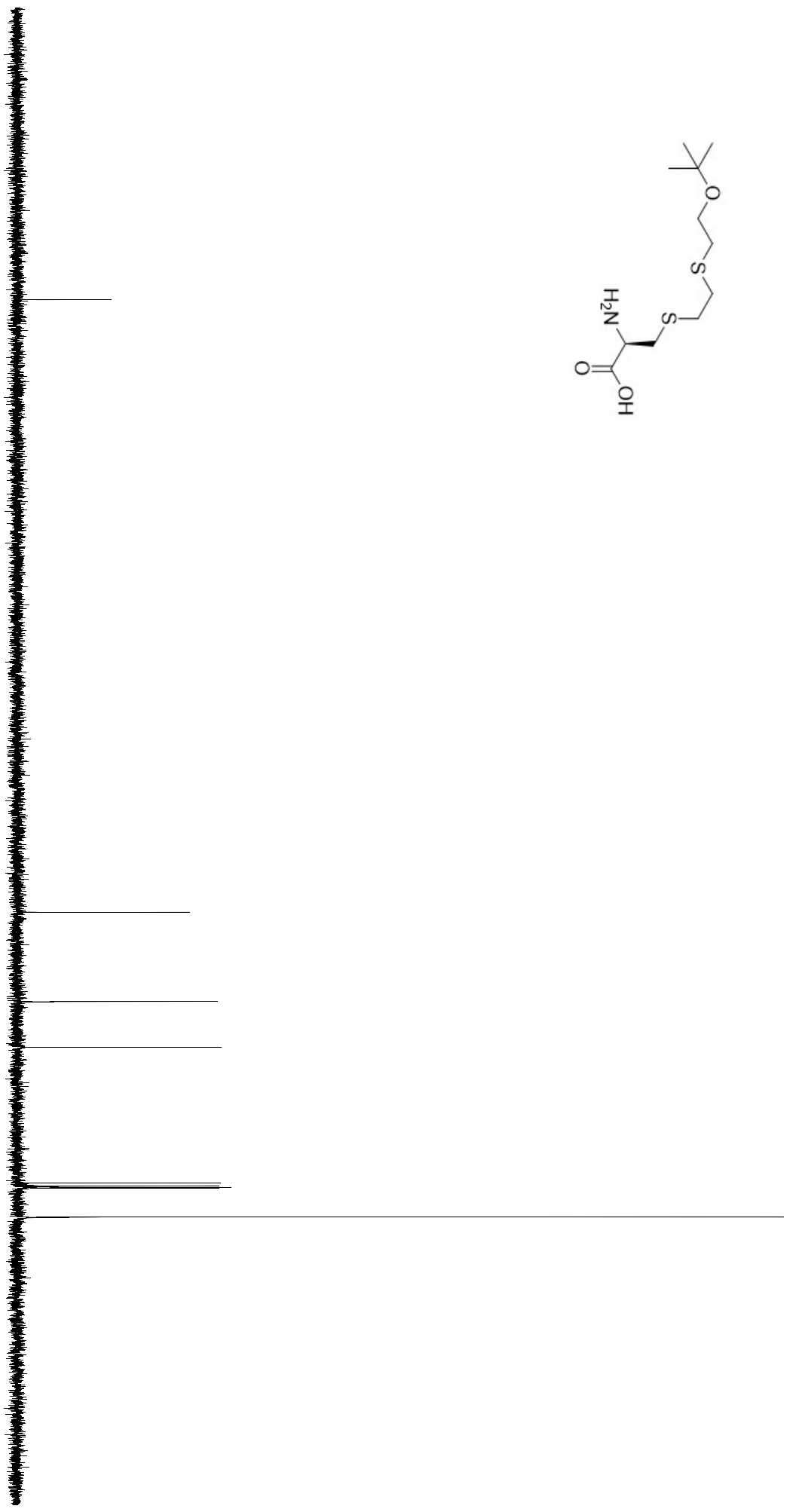
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



- 174.46
- 172.93
- 172.74
- 172.21
- 163.52
- 163.17
- 162.82
- 162.47
- 120.66
- 117.77
- 114.87
- 111.98
- 60.28
- 53.10
- 52.71
- 41.11
- 33.31
- 32.69
- 31.56
- 31.11
- 30.98
- 25.62



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



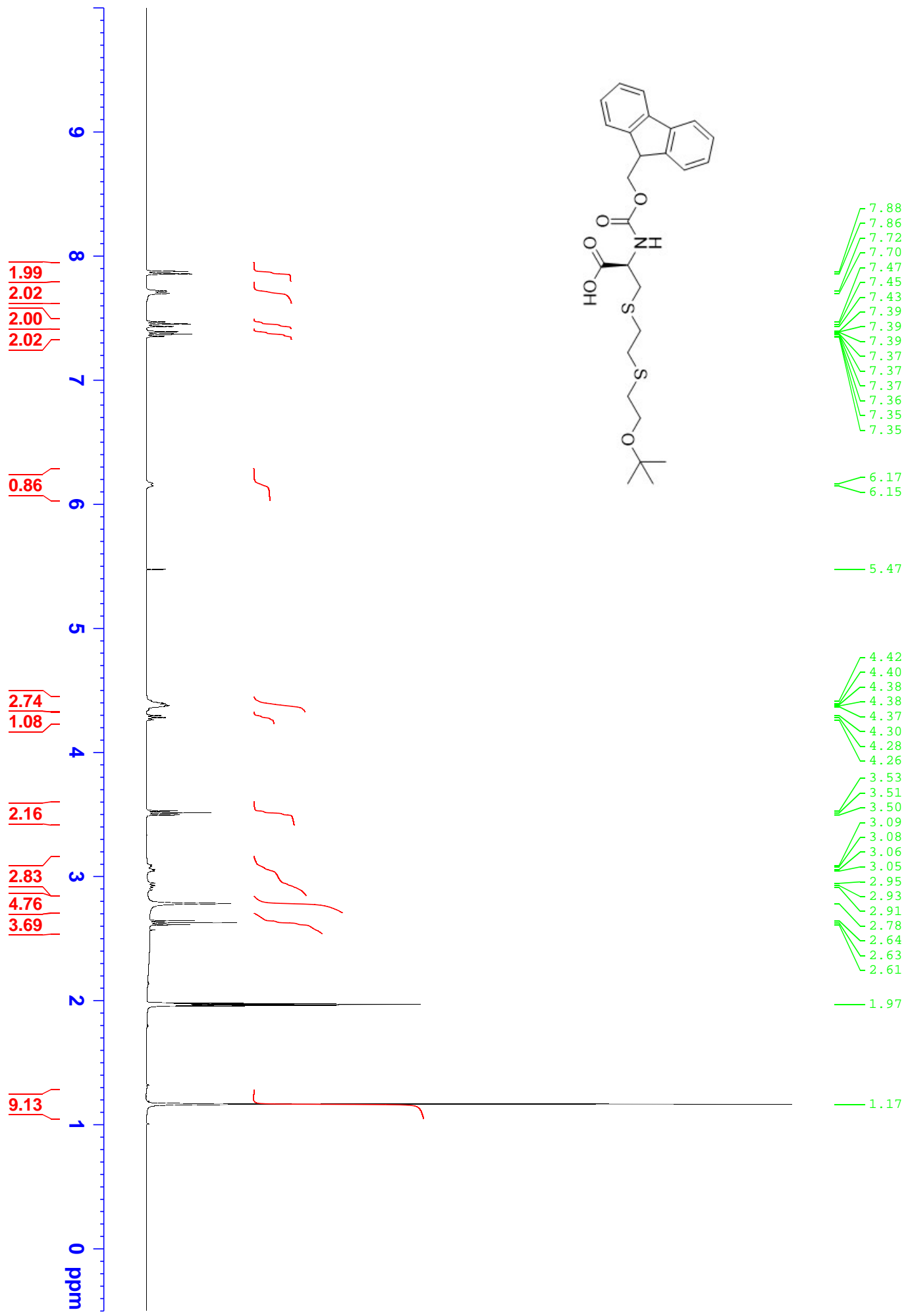
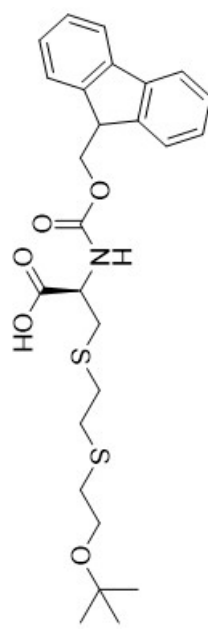
172.78

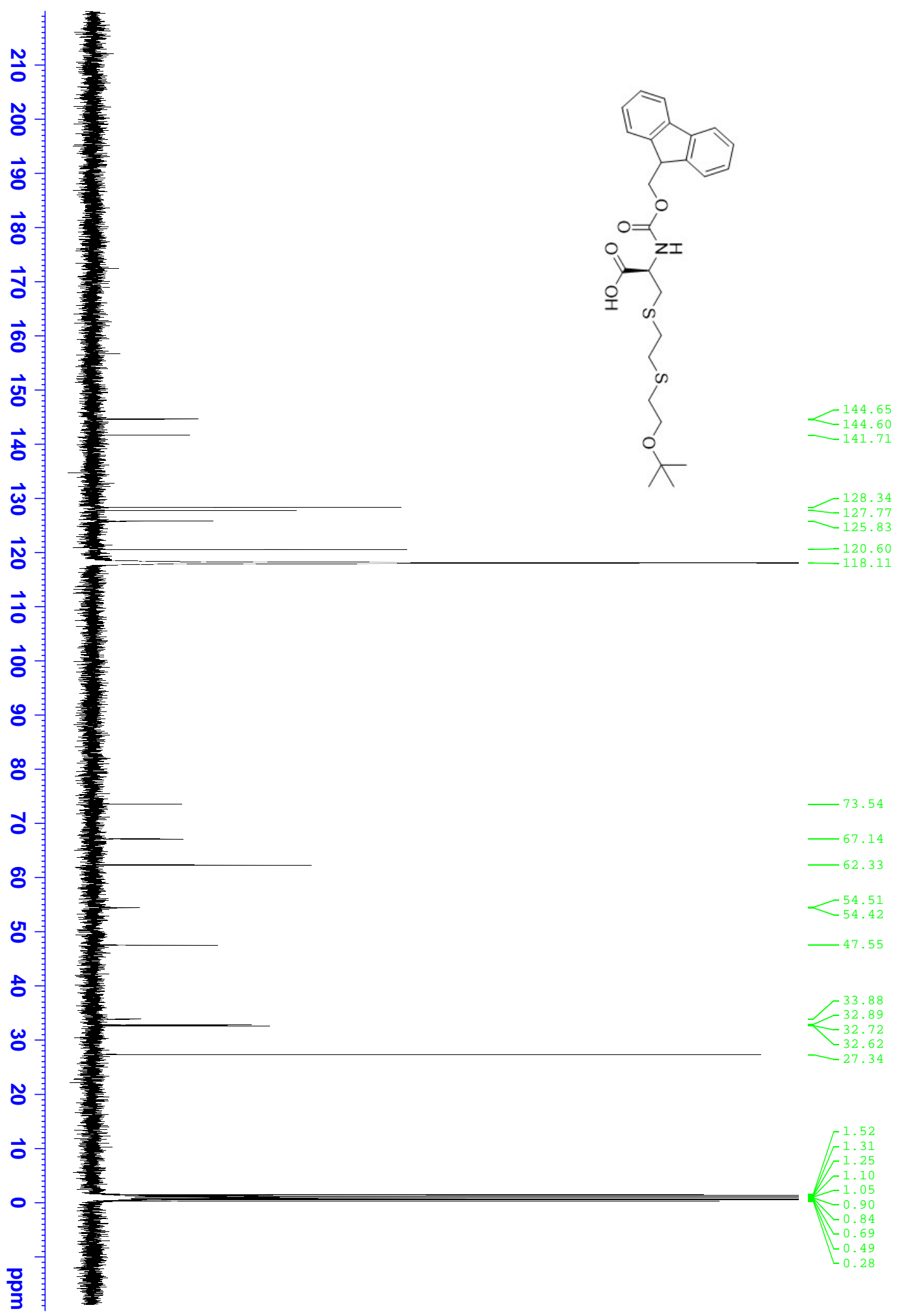
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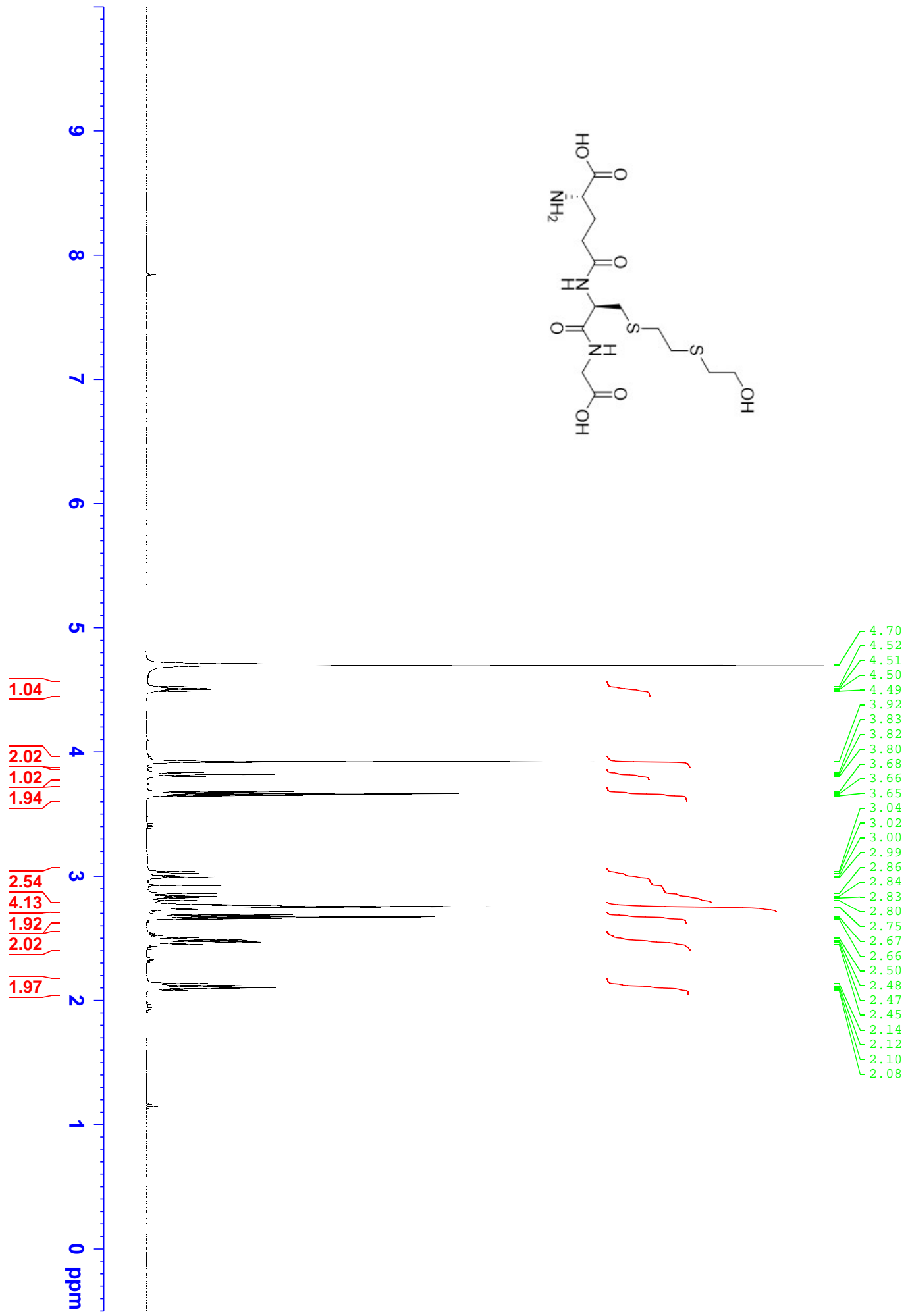
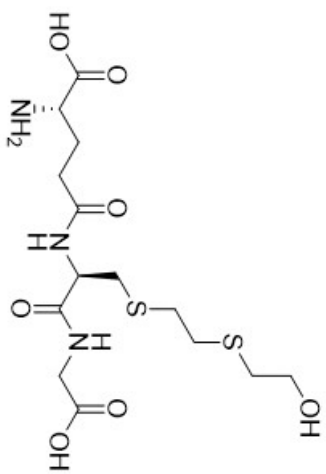
60.89

53.61

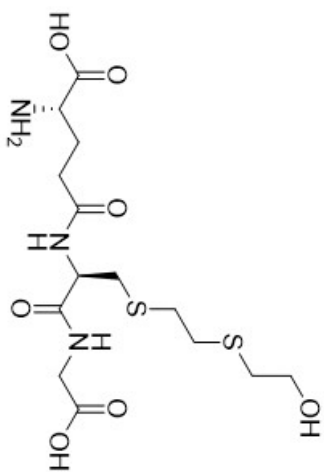
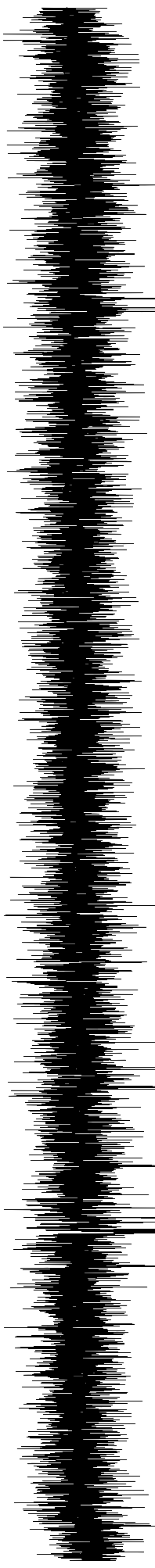
32.00
31.54
31.29
31.14
26.52







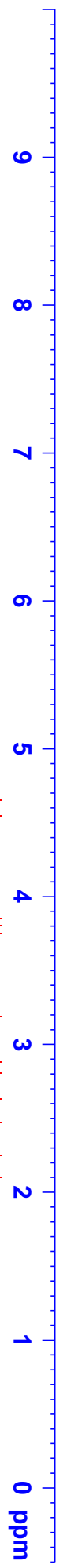
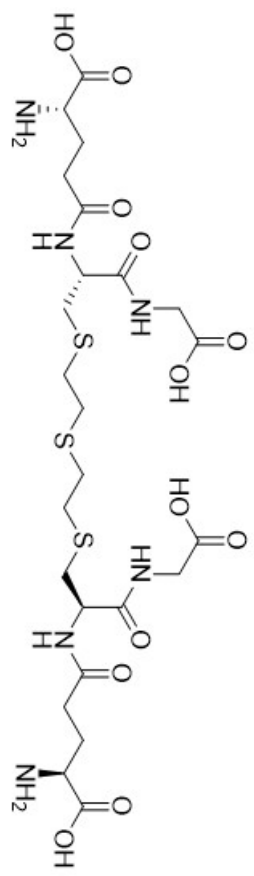
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174.66
173.14
173.09
172.71

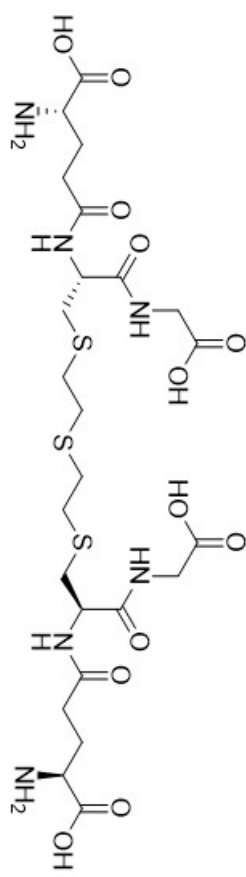
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53.39
53.14

41.26
33.32
32.69
31.57
31.10
31.00
25.88



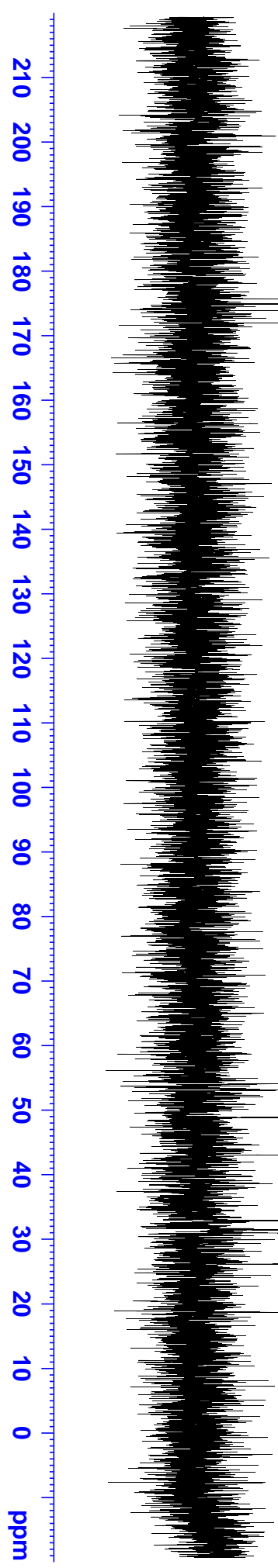
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3.67
2.35
4.80
7.65
4.16
4.04

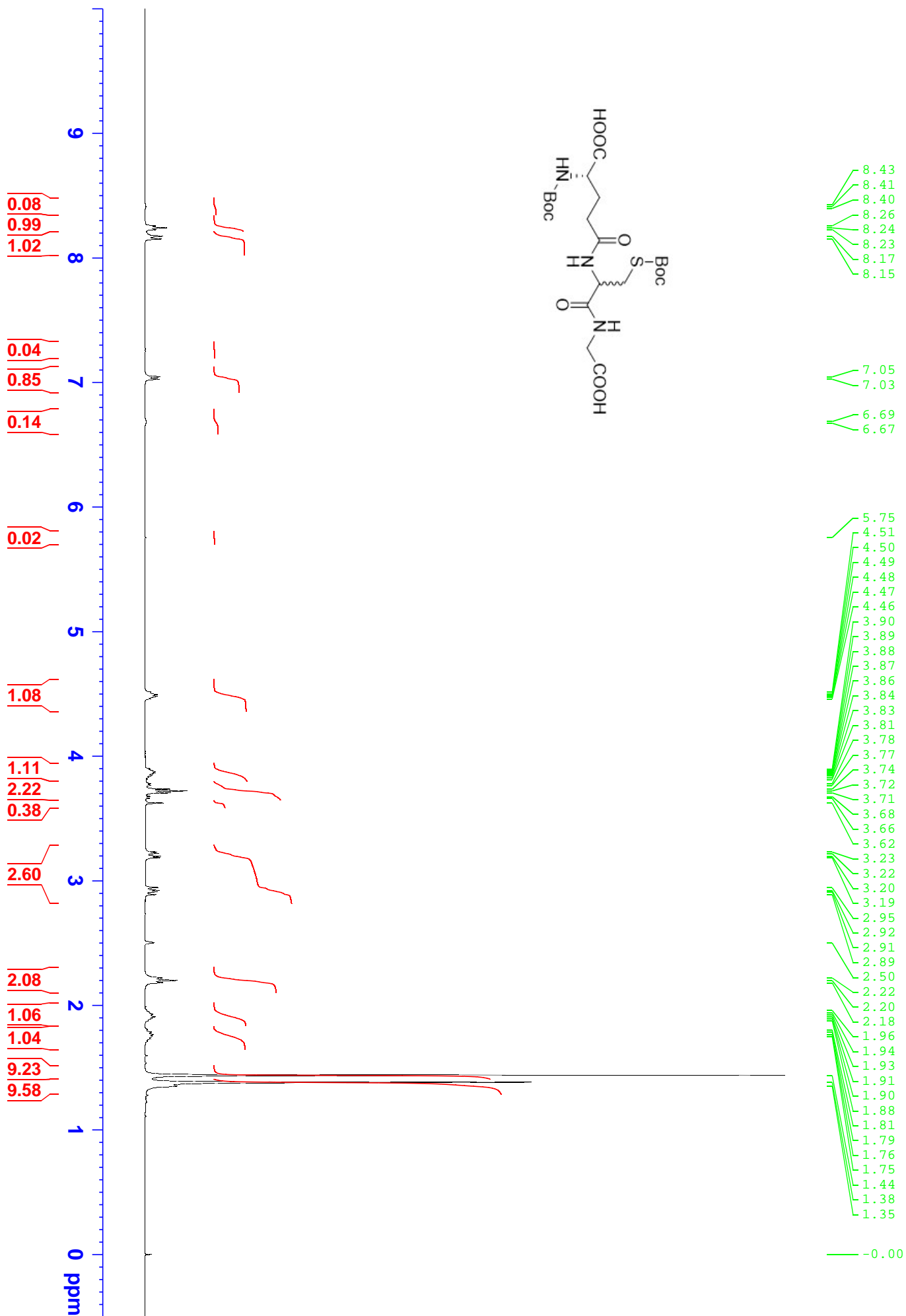
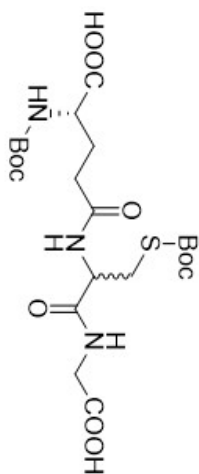
4.79
4.62
4.61
4.60
4.59
3.82
3.81
3.80
3.79
3.77
3.35
3.15
3.13
3.11
3.10
2.94
2.92
2.91
2.89
2.85
2.57
2.56
2.55
2.54
2.54
2.53
2.21
2.20
2.18
2.16
2.14

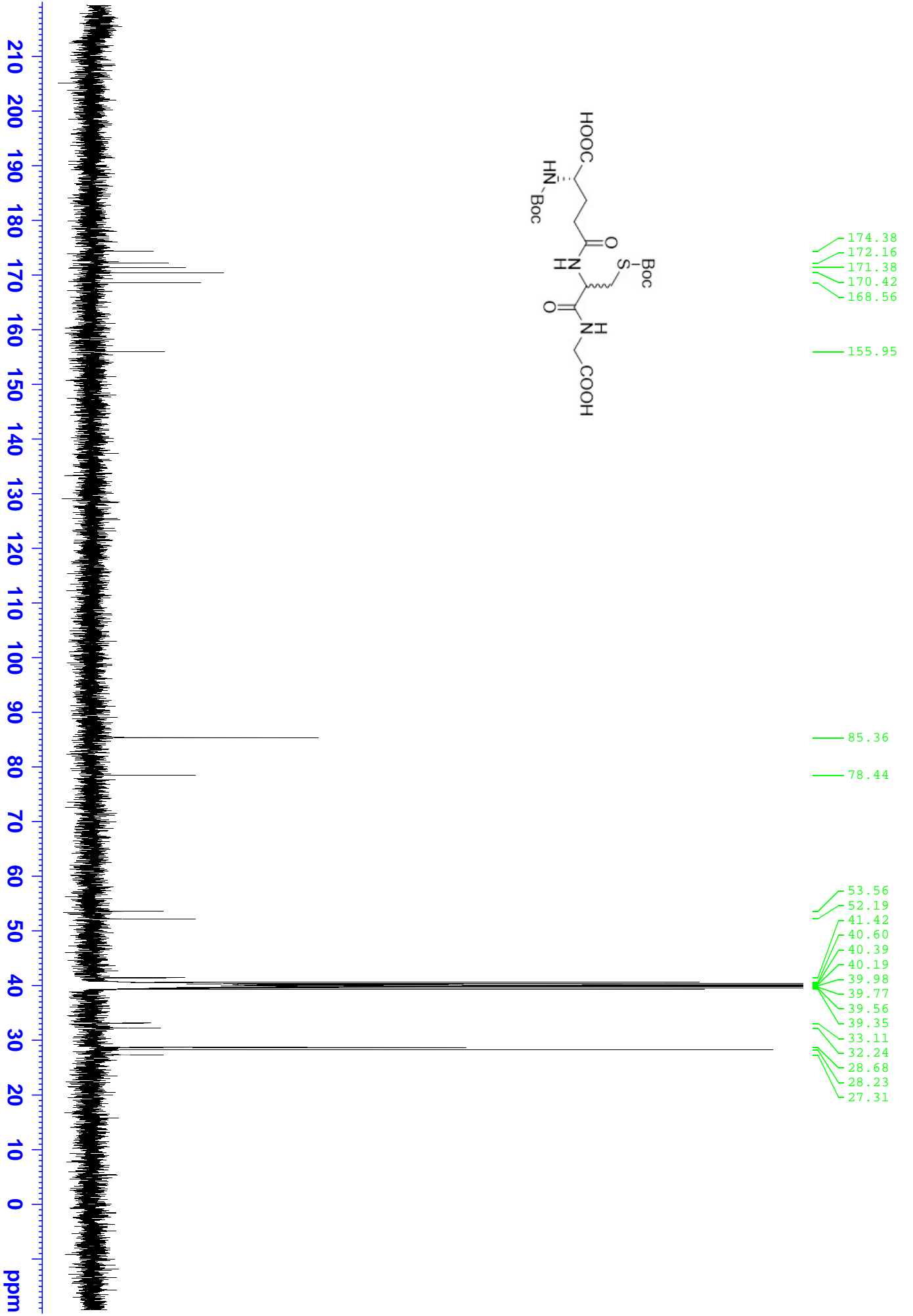
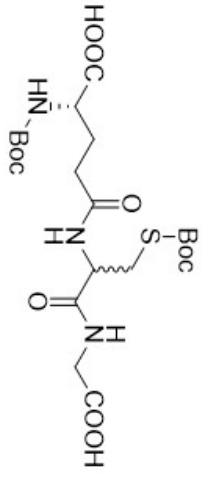


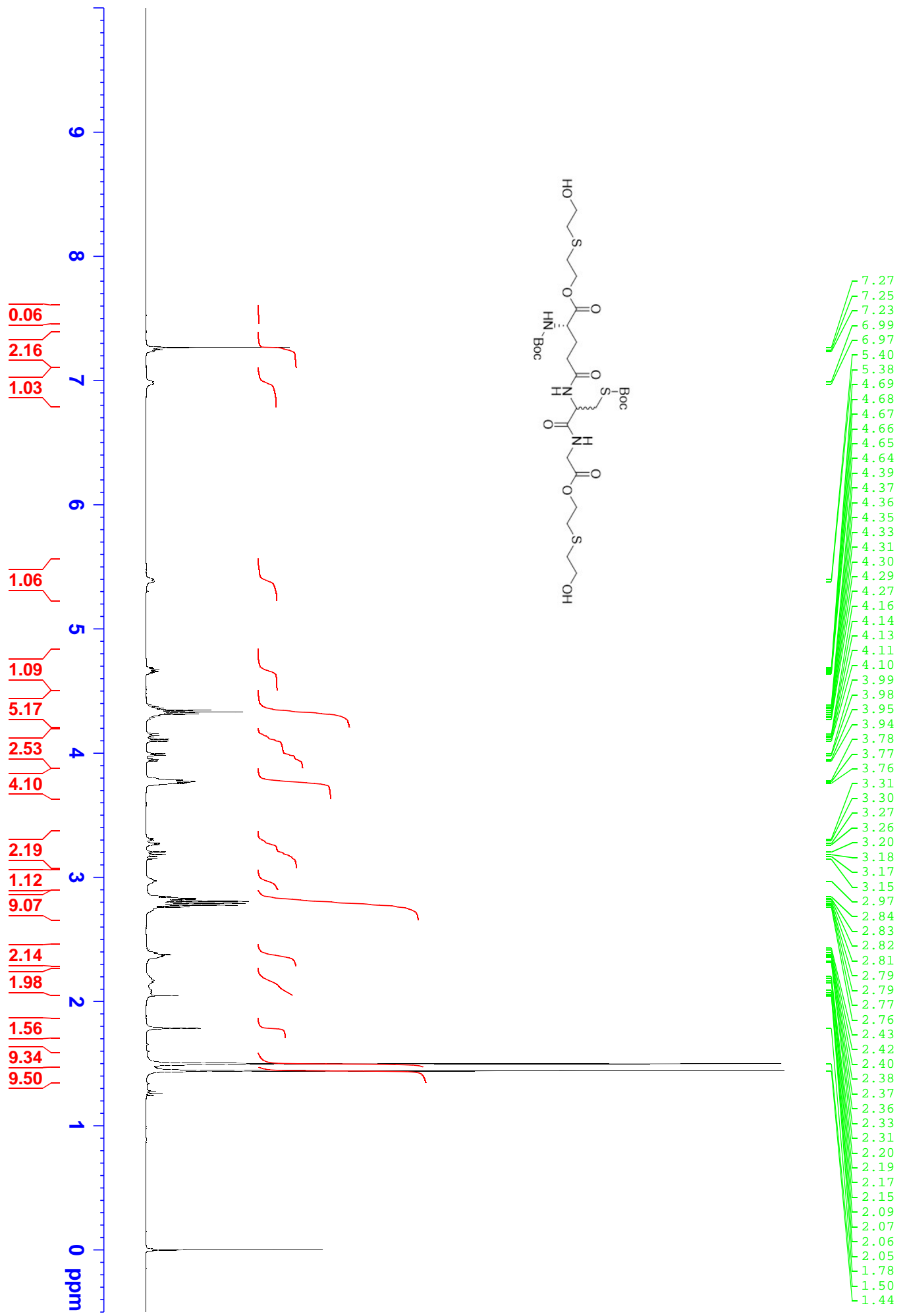
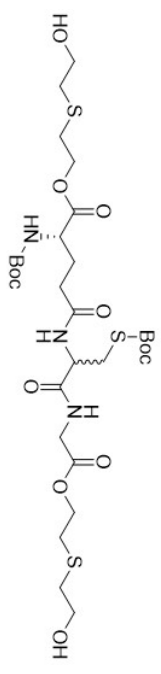
175.71
174.87
173.90
172.01

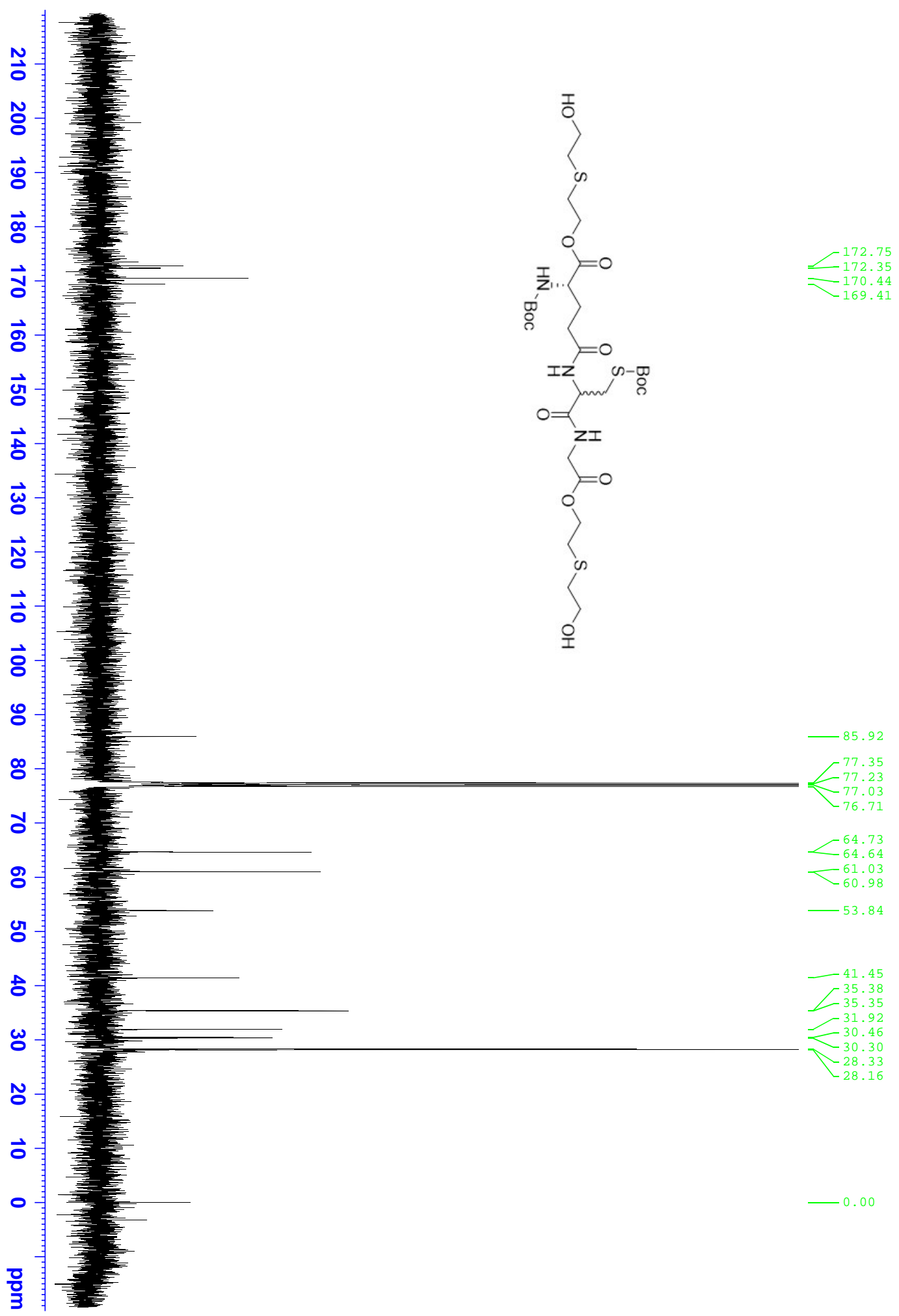
54.07
53.14
48.85
43.03
32.84
31.52
31.37
30.95
26.17

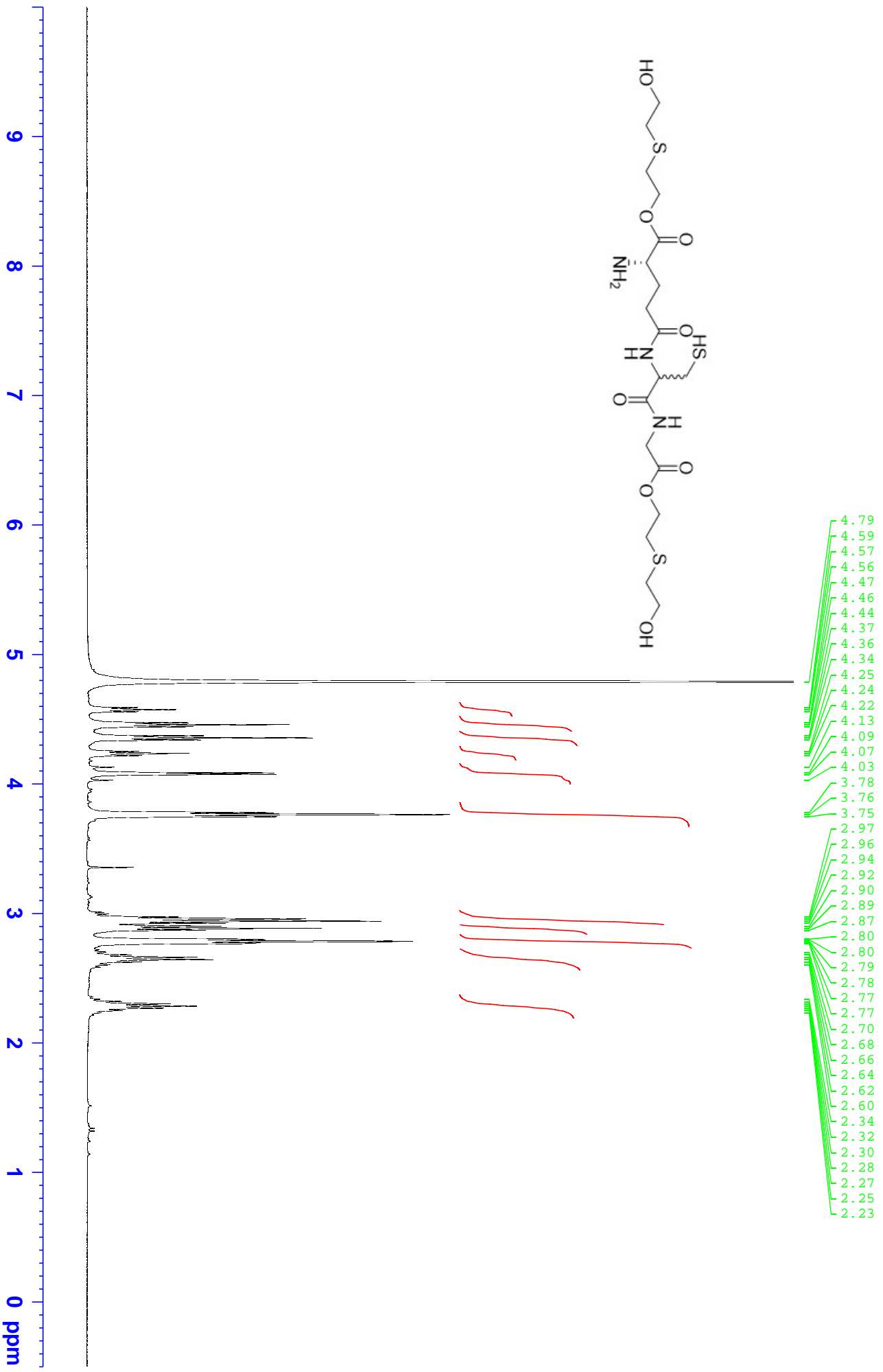
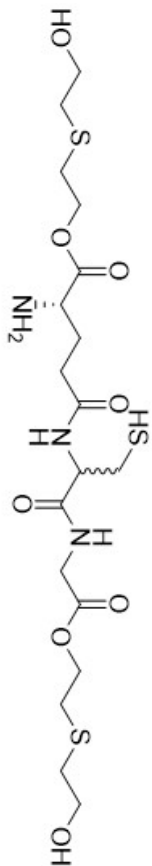


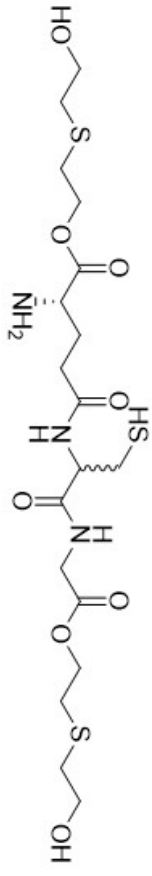








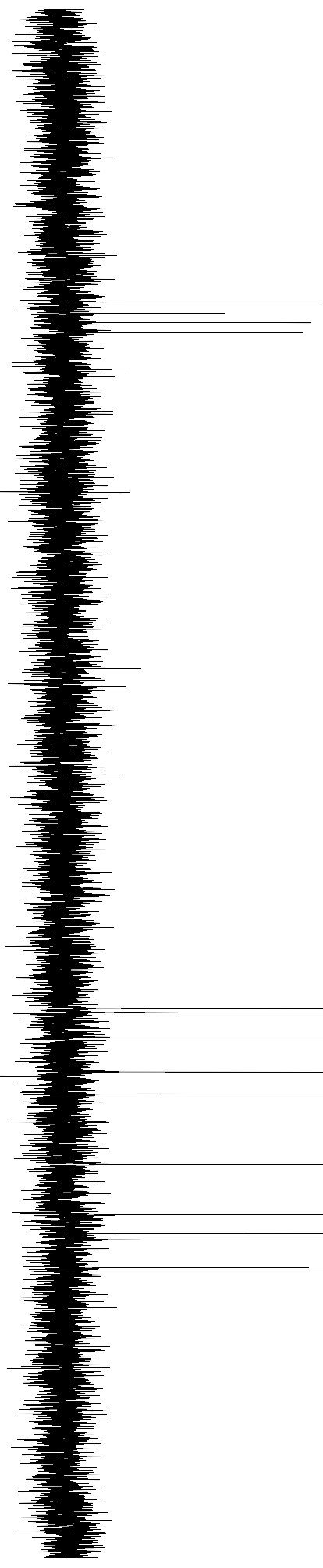
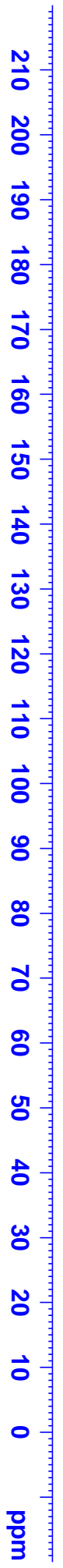


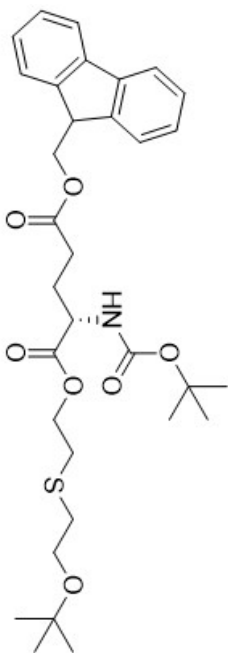
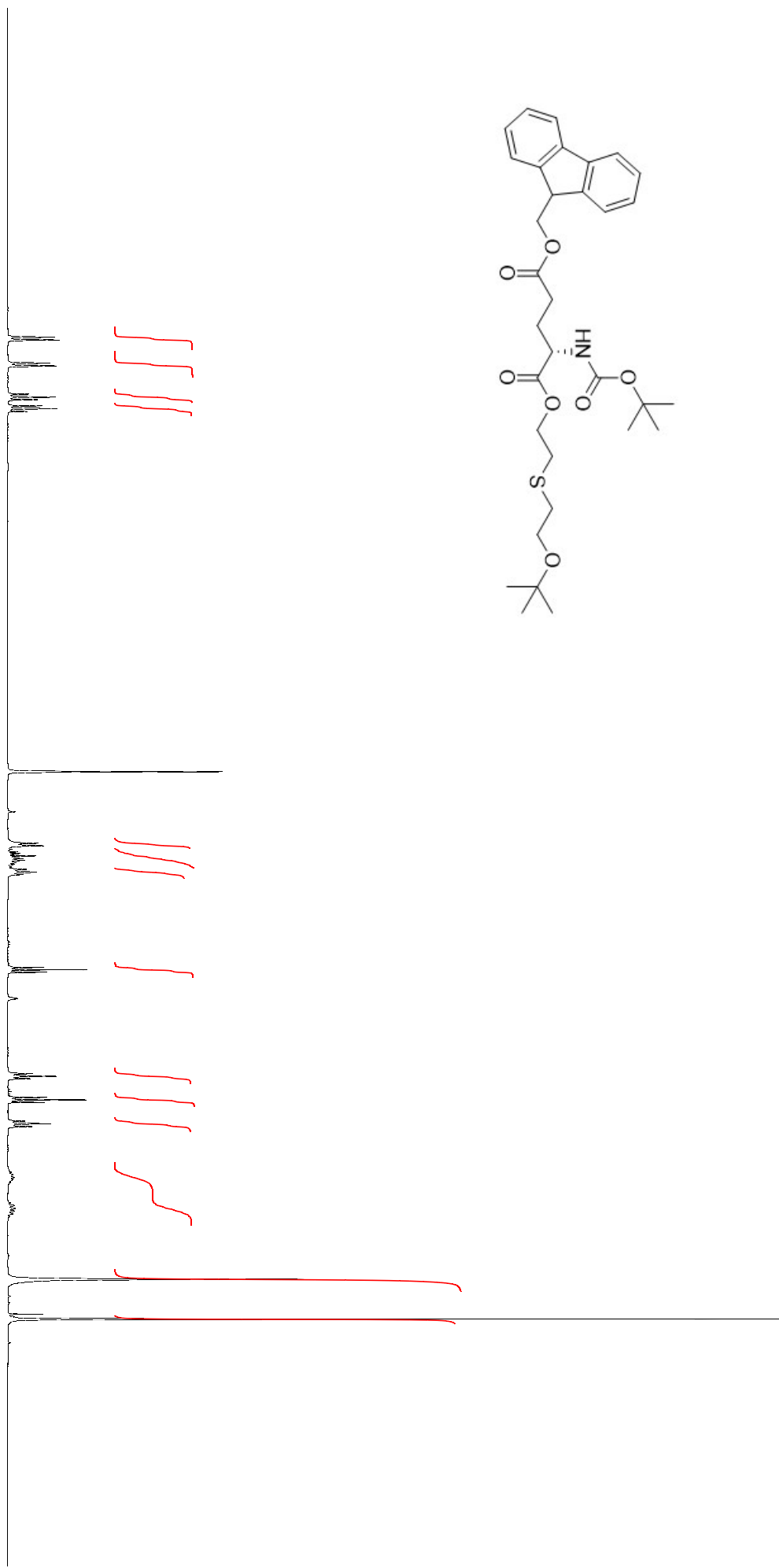
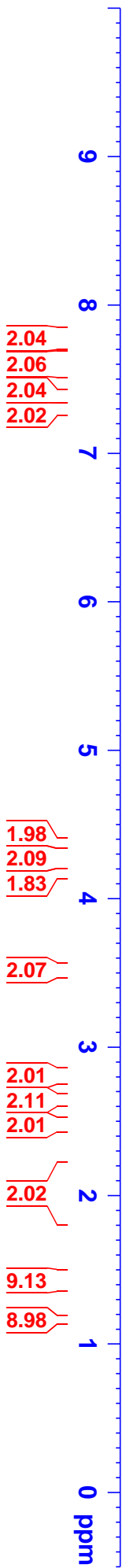


174.09
172.49
171.03
169.49

65.30
64.70
60.29
55.53
52.15

41.31
33.62
33.54
30.64
29.69
29.66
25.41
25.31

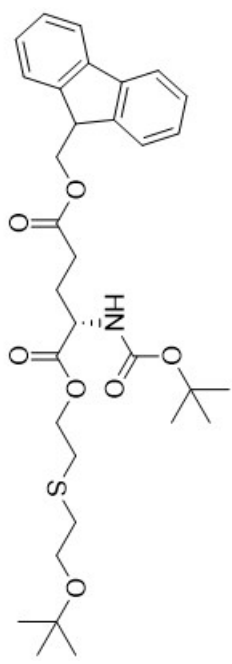




- 7.78
- 7.76
- 7.61
- 7.59
- 7.40
- 7.38
- 7.36
- 7.32
- 7.30
- 7.28

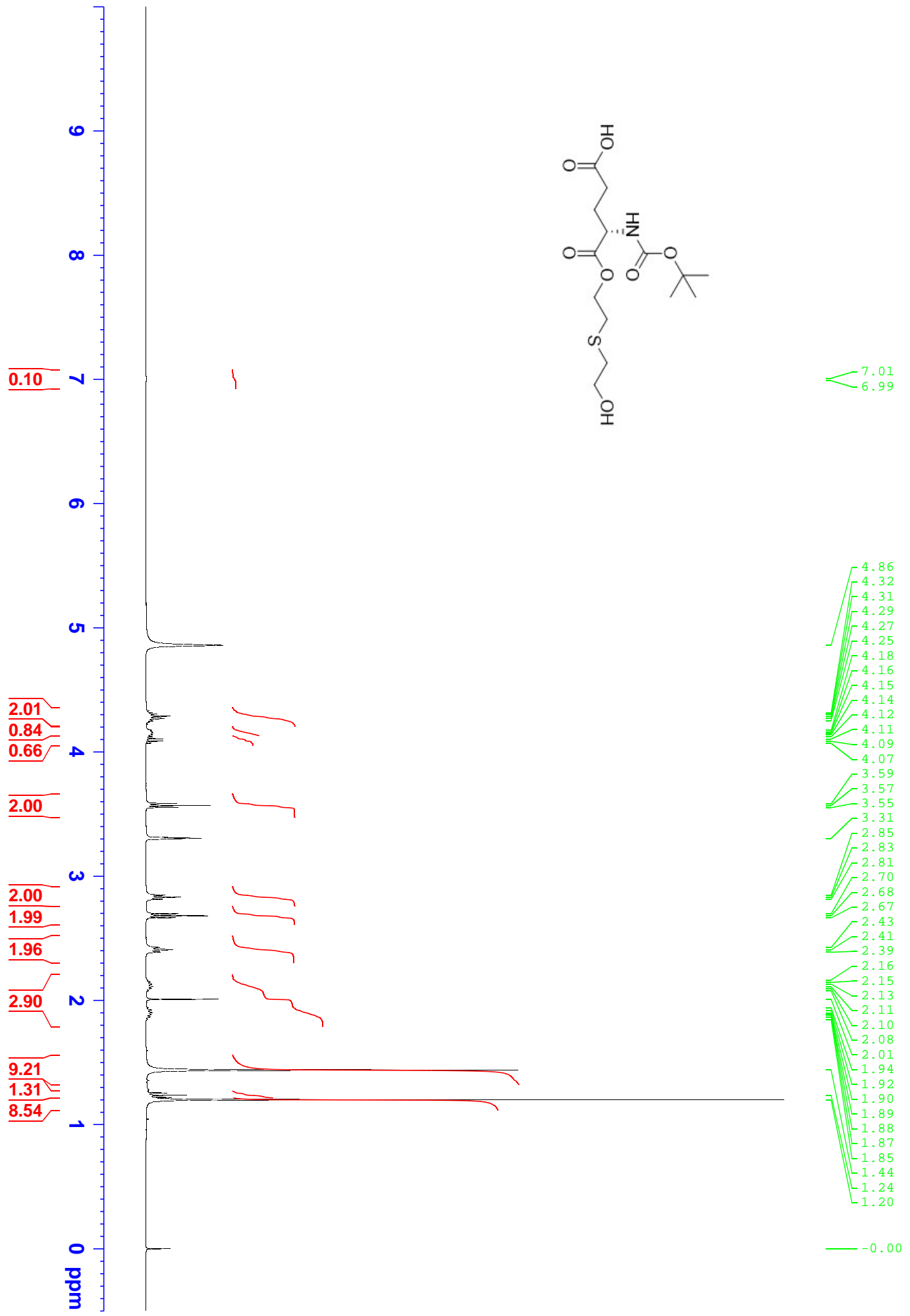
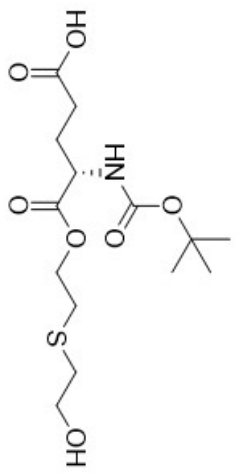
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- 4.37
- 4.36
- 4.31
- 4.30
- 4.29
- 4.27
- 4.27
- 4.26
- 4.24
- 4.20
- 4.18
- 4.16
- 3.54
- 3.52
- 3.50
- 2.82
- 2.80
- 2.79
- 2.66
- 2.64
- 2.63
- 2.50
- 2.48
- 2.46
- 2.16
- 2.14
- 2.12
- 2.11
- 2.09
- 1.95
- 1.93
- 1.91
- 1.90
- 1.89
- 1.87
- 1.86
- 1.44
- 1.17

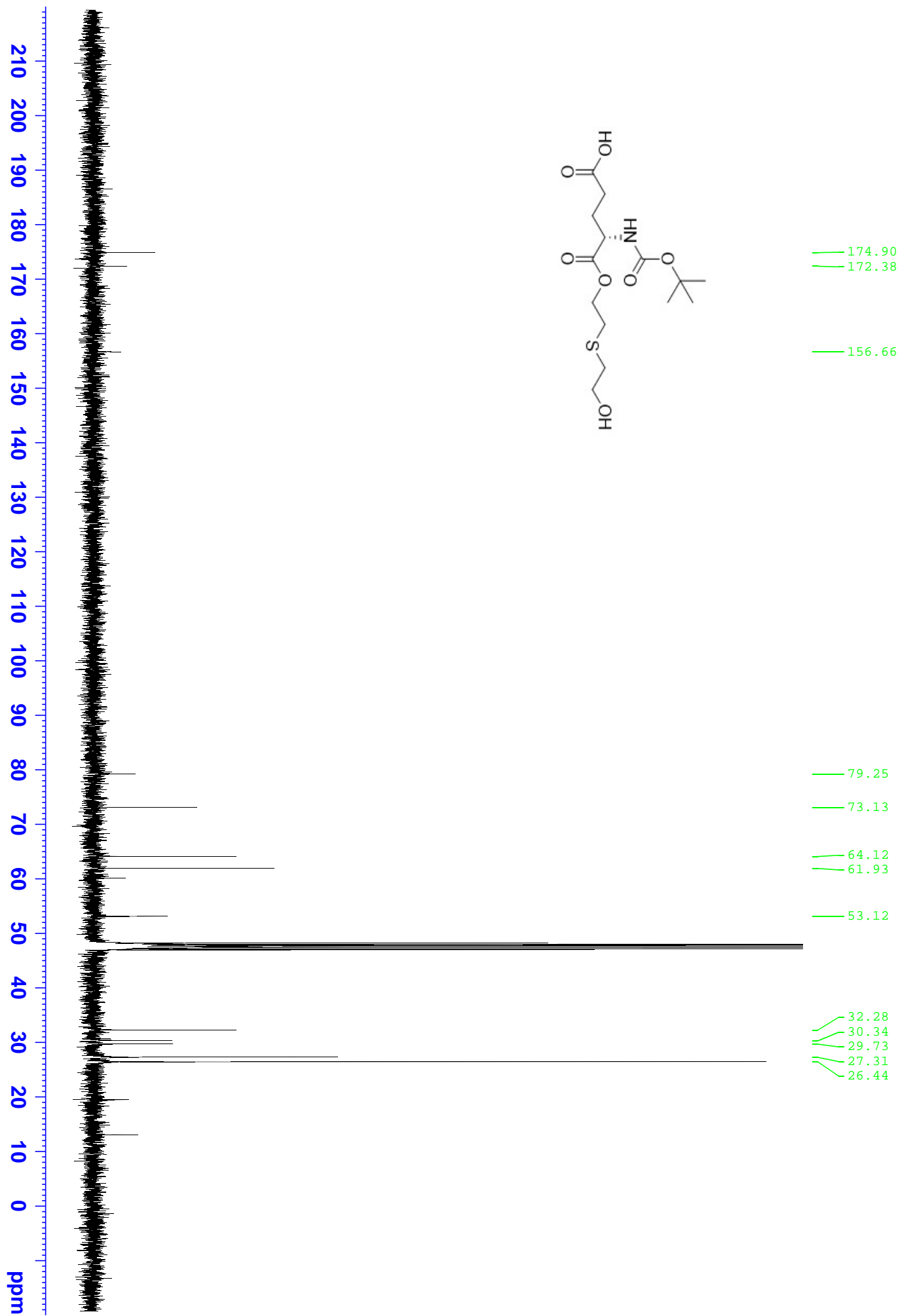
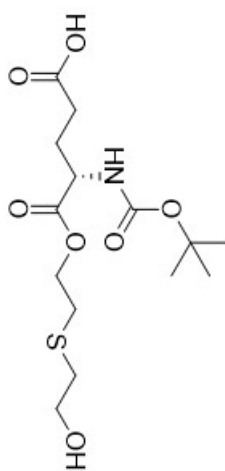
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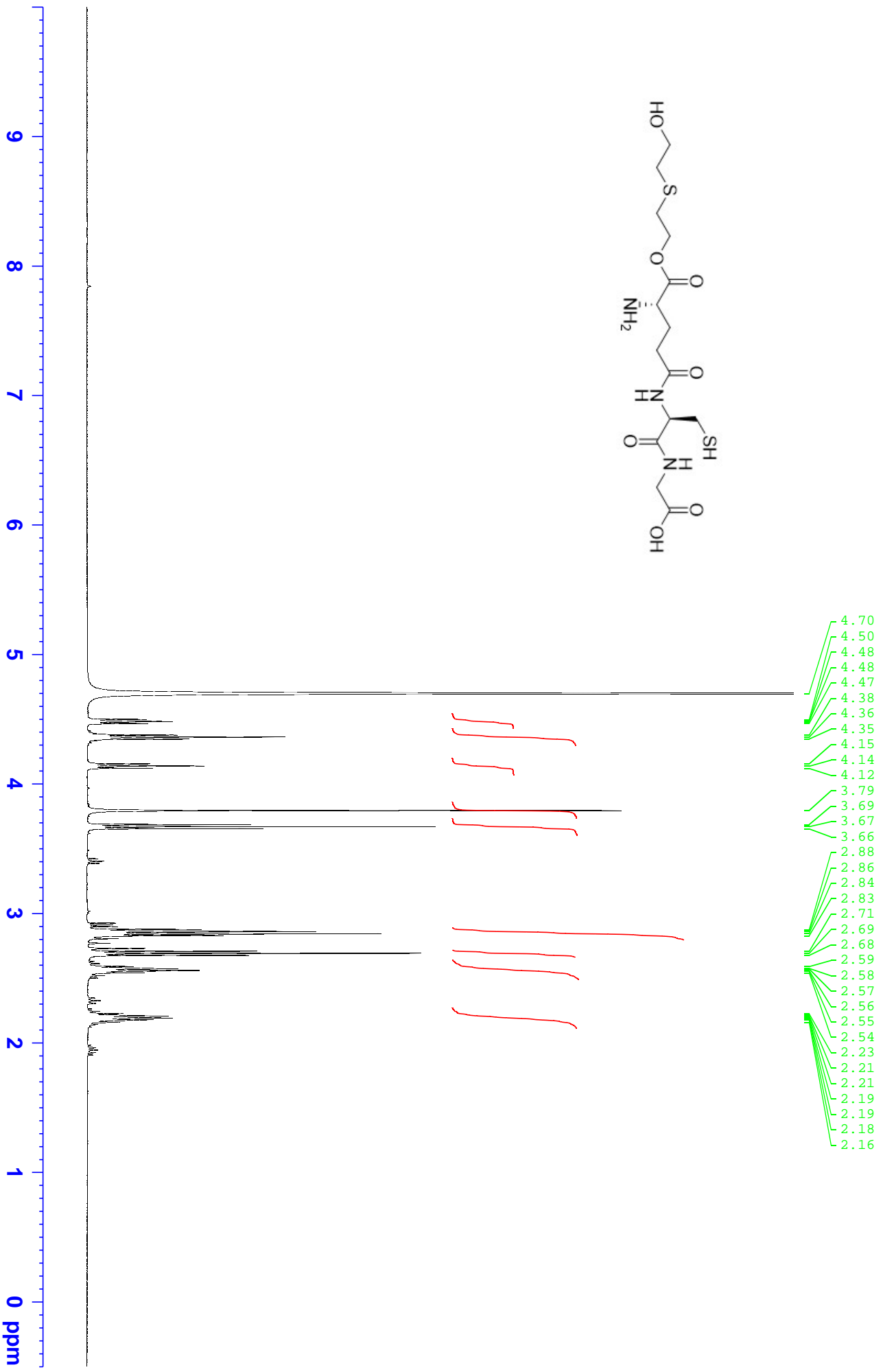
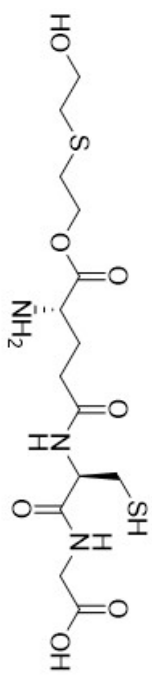


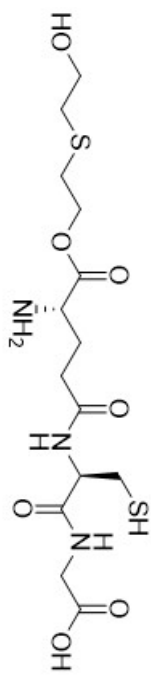
- 172.76
- 172.21
- 156.55
- 143.78
- 141.18
- 127.52
- 126.87
- 124.76
- 119.68

- 79.32
- 73.12
- 66.18
- 64.15
- 61.91
- 61.31
- 52.98
- 48.32
- 48.23
- 48.10
- 48.02
- 47.89
- 47.81
- 47.68
- 47.60
- 47.47
- 47.25
- 47.04
- 46.63
- 34.50
- 32.32
- 30.44
- 29.91
- 27.41
- 26.53
- 26.49
- 26.42









174.84
174.15
171.82
169.47

65.26
60.25
55.54
52.11
42.40
33.50
30.72
29.61
25.44
25.30

