Supporting Information

Synthesis and Anticancer Activity Comparison of Phenylalkyl Isoselenocyanates with Corresponding Naturally Occurring and Synthetic Isothiocyanates

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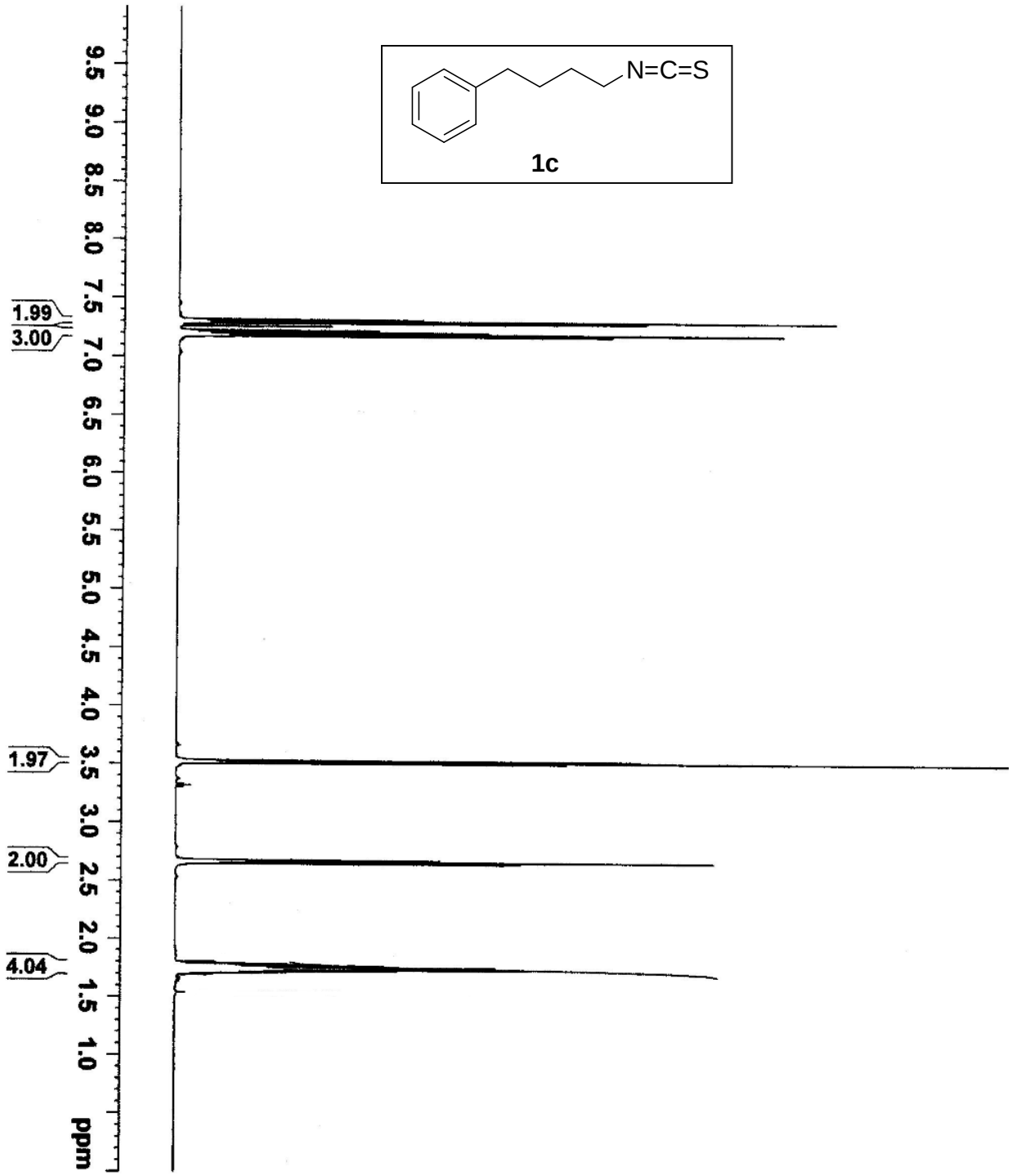
Phenylbutyl isothiocyanate (1c) and Phenylhexyl isothiocyanate (1d) were synthesized according to a literature method and their purity was confirmed by 500 MHz ^{1}H NMR spectra.

Phenylbutyl isothiocyanate (1c). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 1.72-1.80 (m, 4H), 2.66 (t, 2H, *J* = 7.0 Hz), 3.52 (t, 2H, *J* = 6.5 Hz), 7.17-7.22 (m, 3H), 7.28-7.31 (m, 2H).

Phenylhexyl isothiocyanate (1d). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 1.34-1.40 (m, 2H), 1.42-1.48 (m, 2H), 1.62-1.72 (m, 4H), 2.63 (t, 2H, *J* = 7.5 Hz), 3.50 (t, 2H, *J* = 6.5 Hz), 7.18-7.21 (m, 3H), 7.28-7.31 (m, 2H).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3.00
1.97
2.00
4.04
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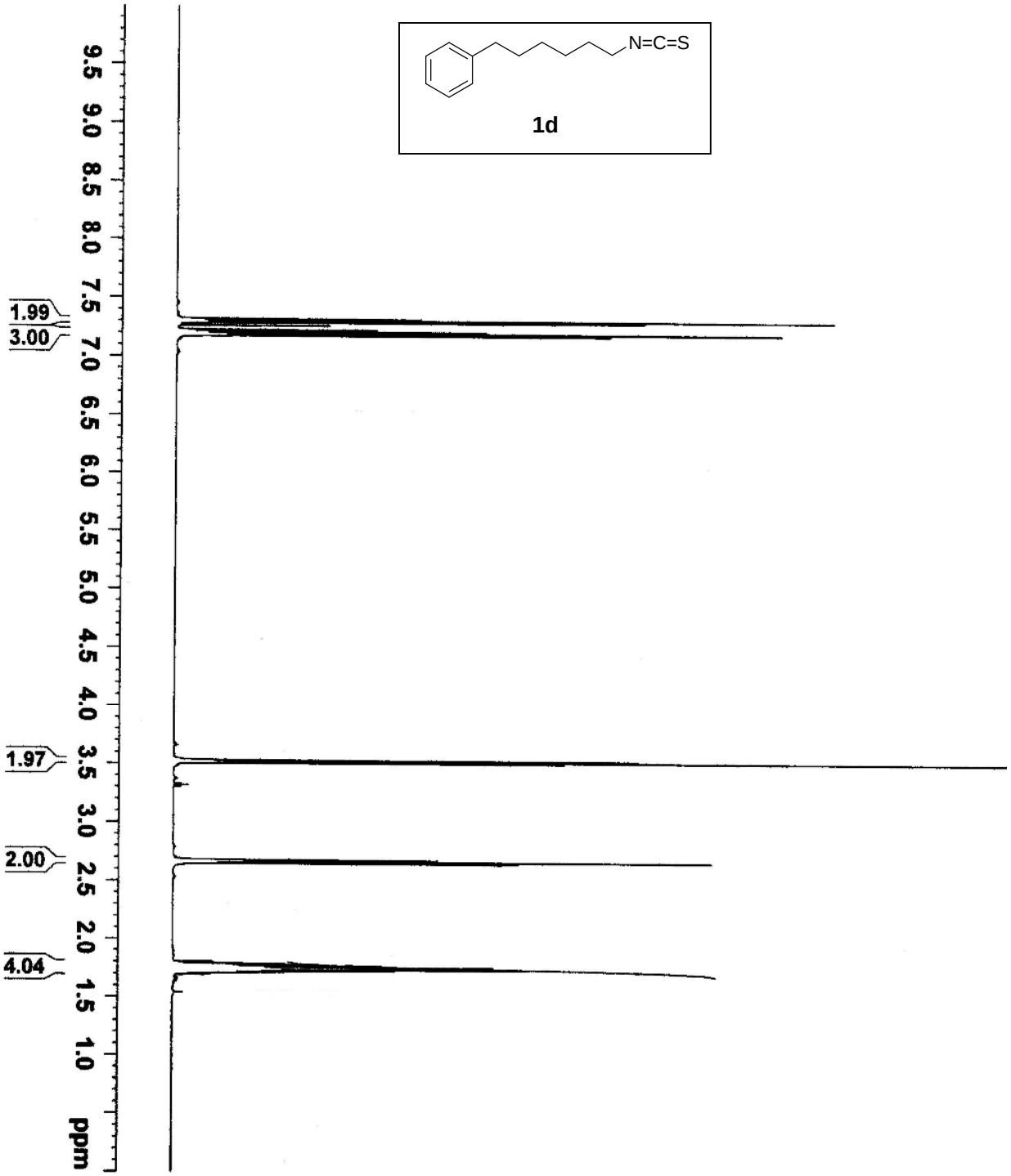
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3.00
1.97
2.00
4.04
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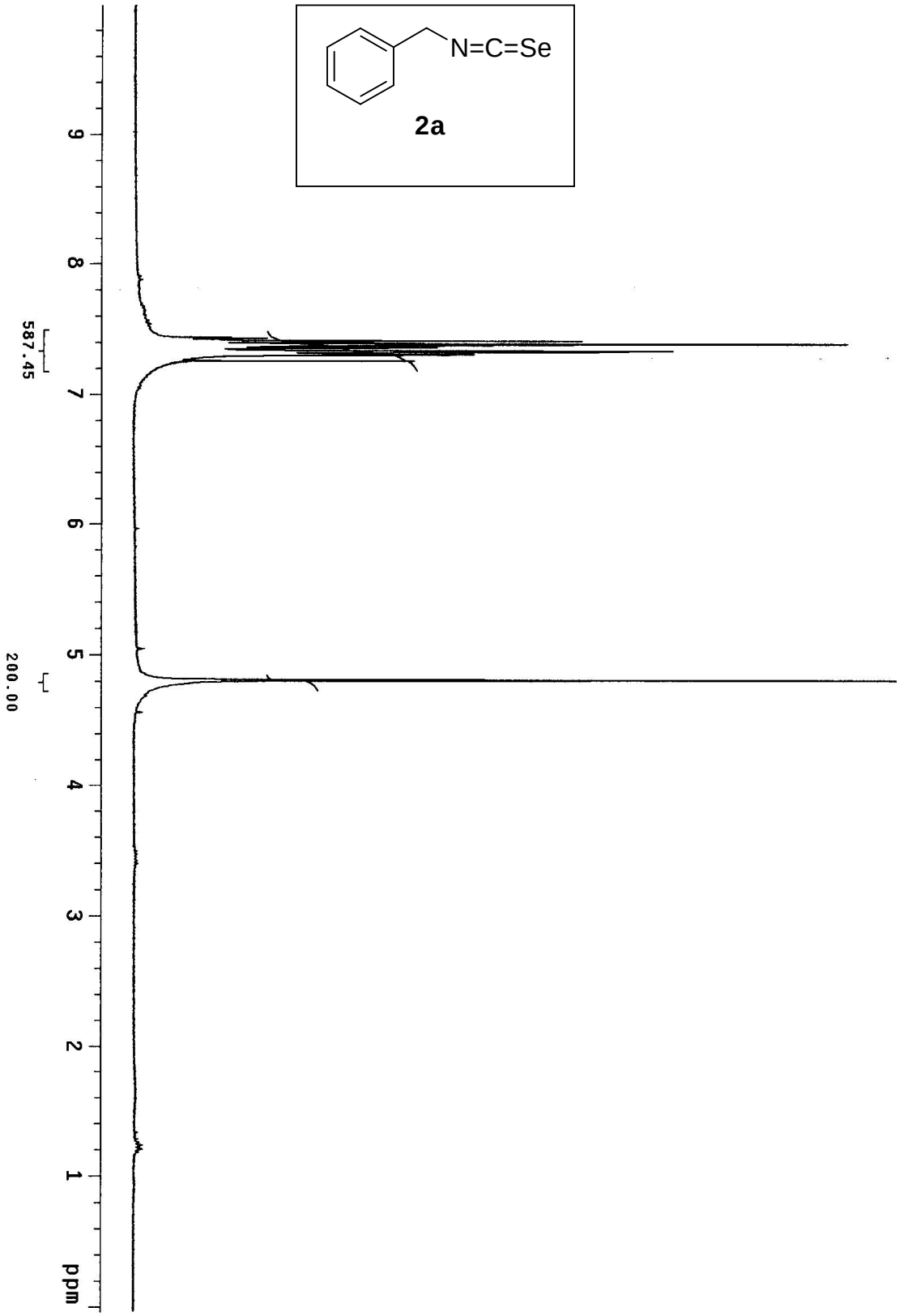
ppm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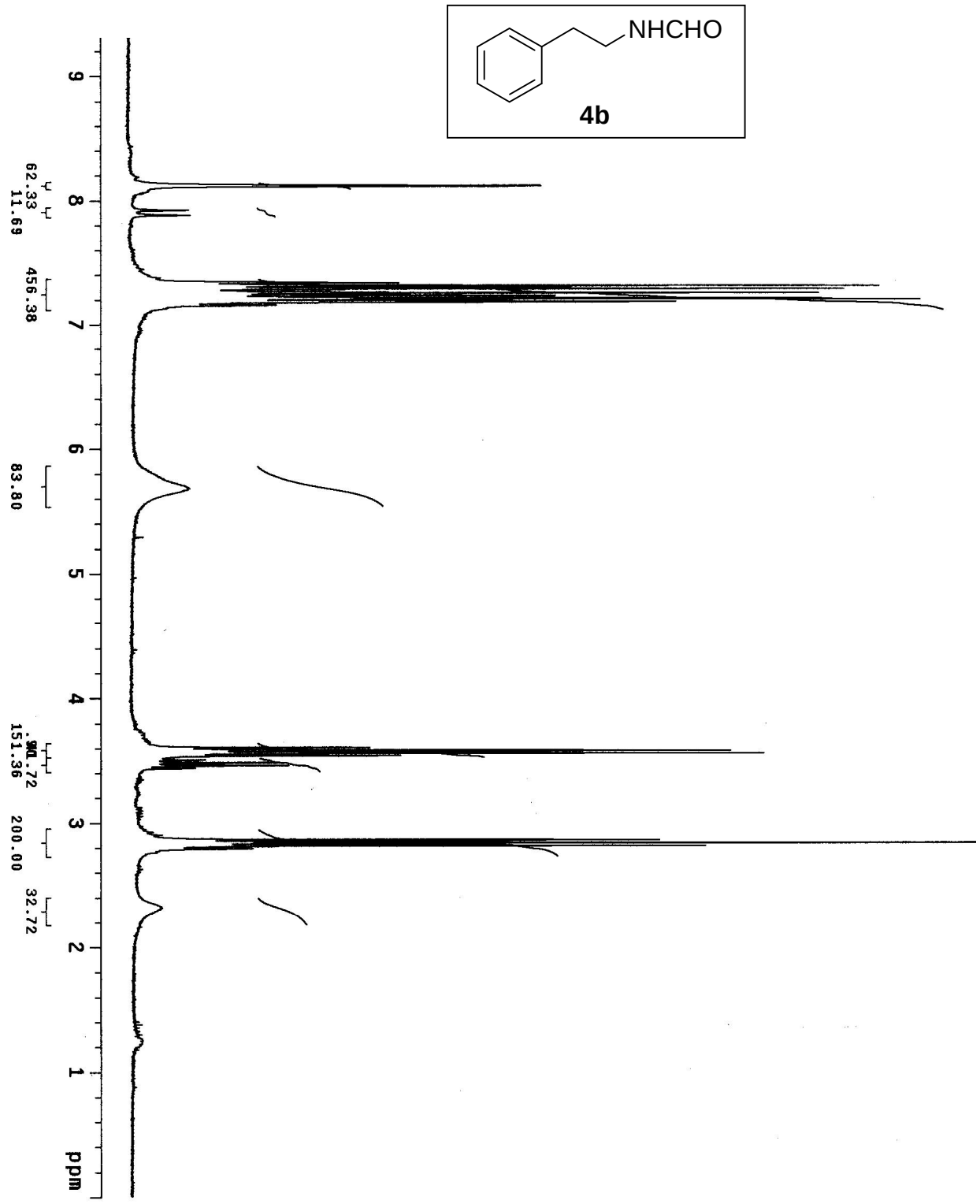
200.00
9
8
7
6
5
4
3
2
1
ppm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456.38
83.80
151.36
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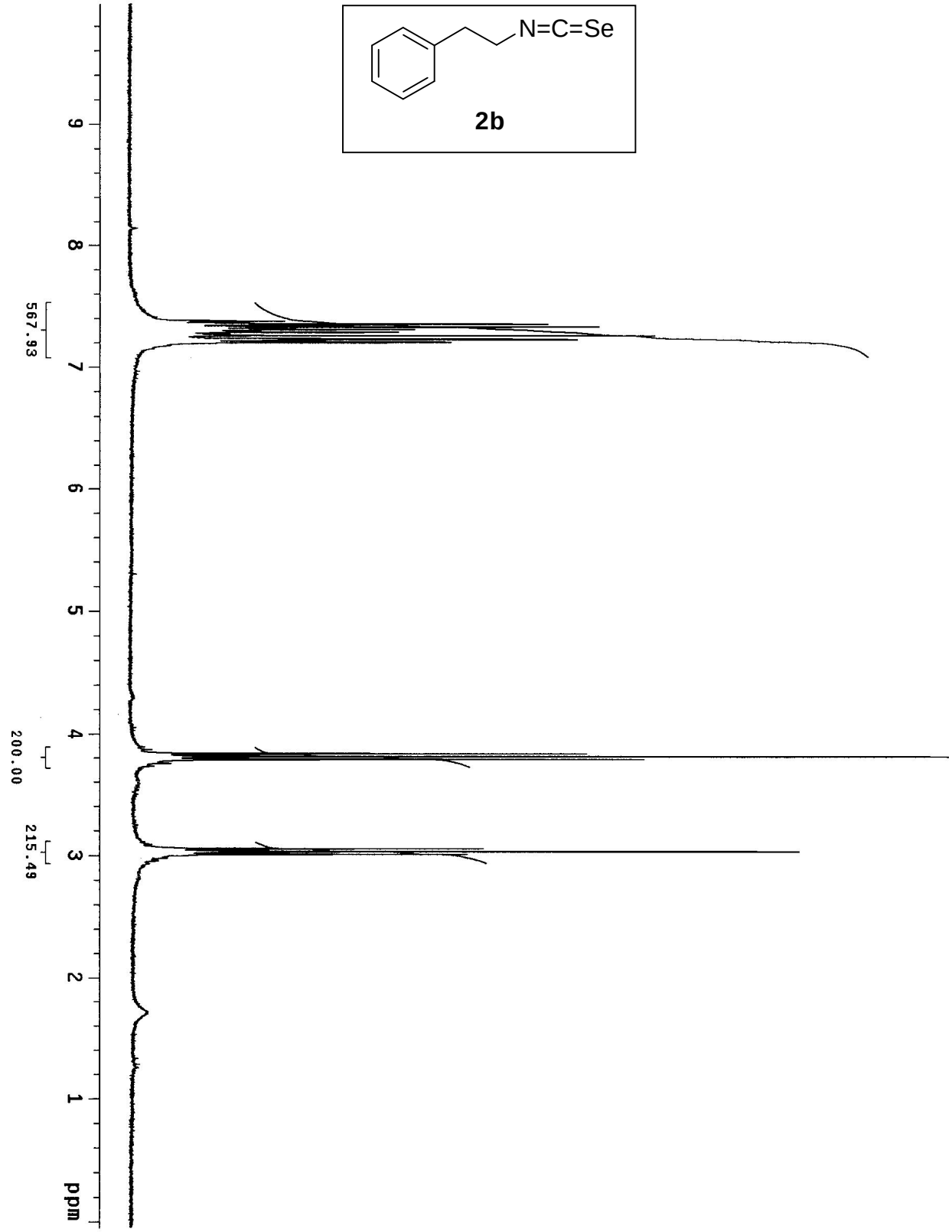
32.72
ppm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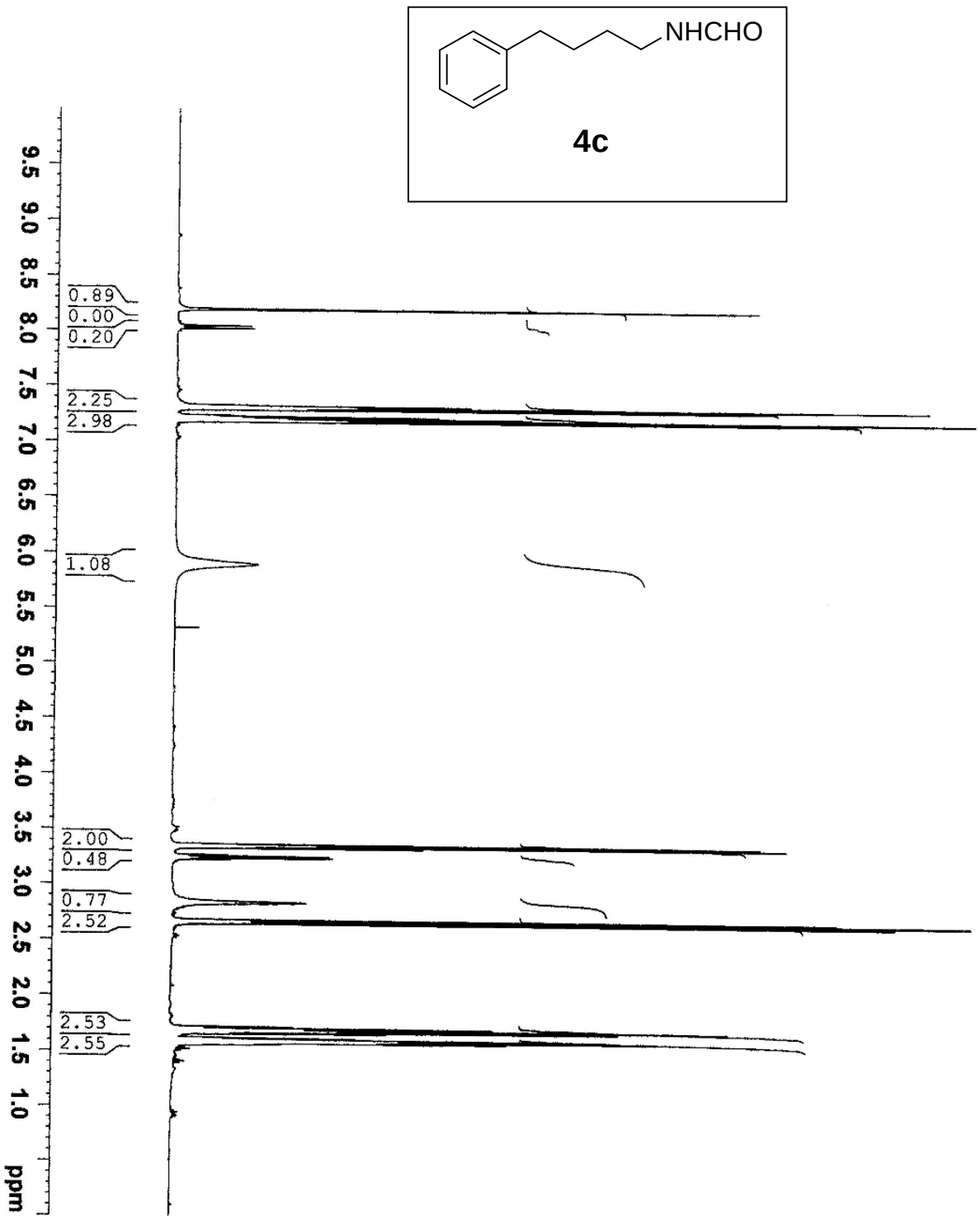
2b
567.93
200.00
215.49
ppm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4c
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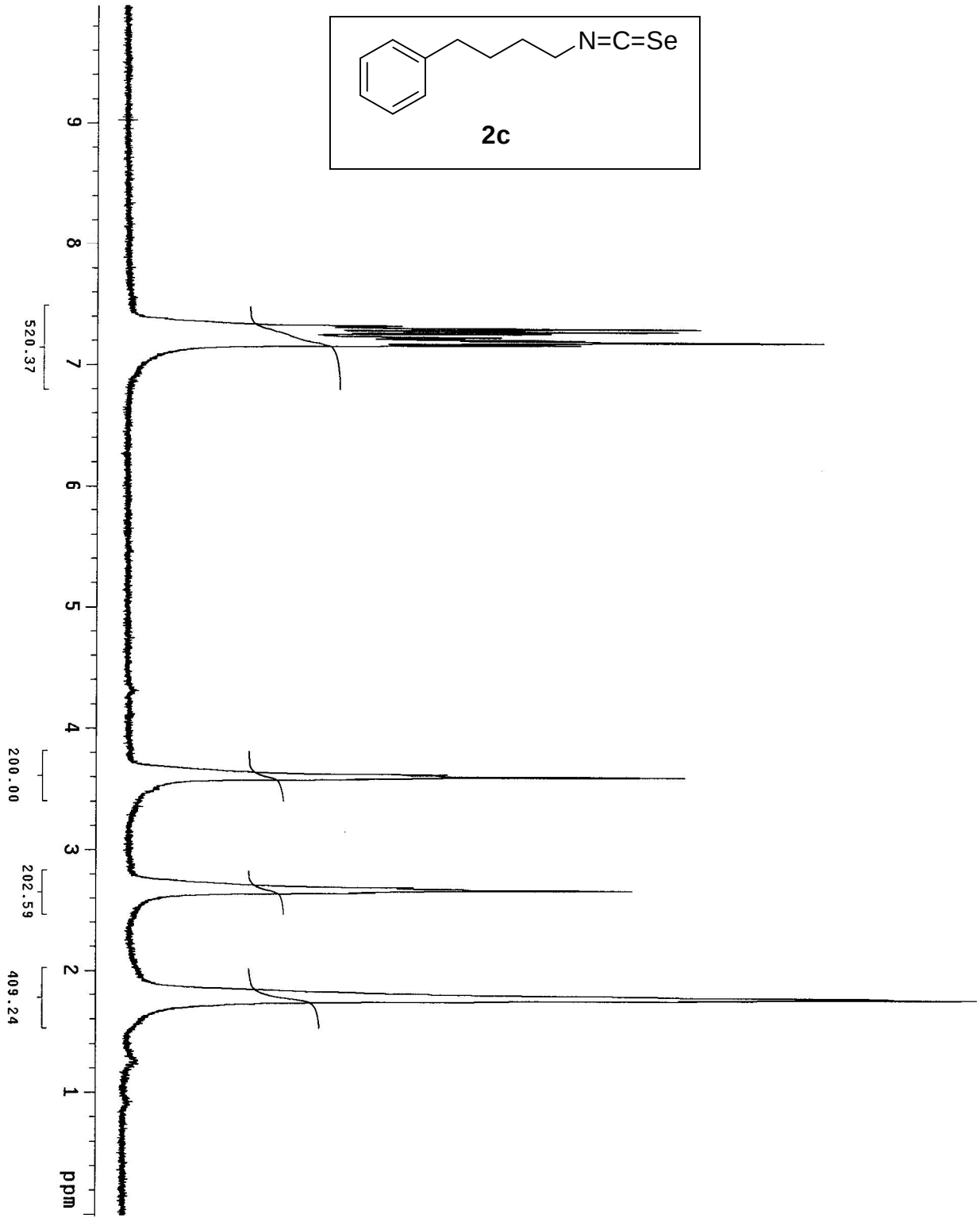
0.89
0.00
0.20
2.25
2.98
1.08
2.00
0.48
0.77
2.52
2.53
2.55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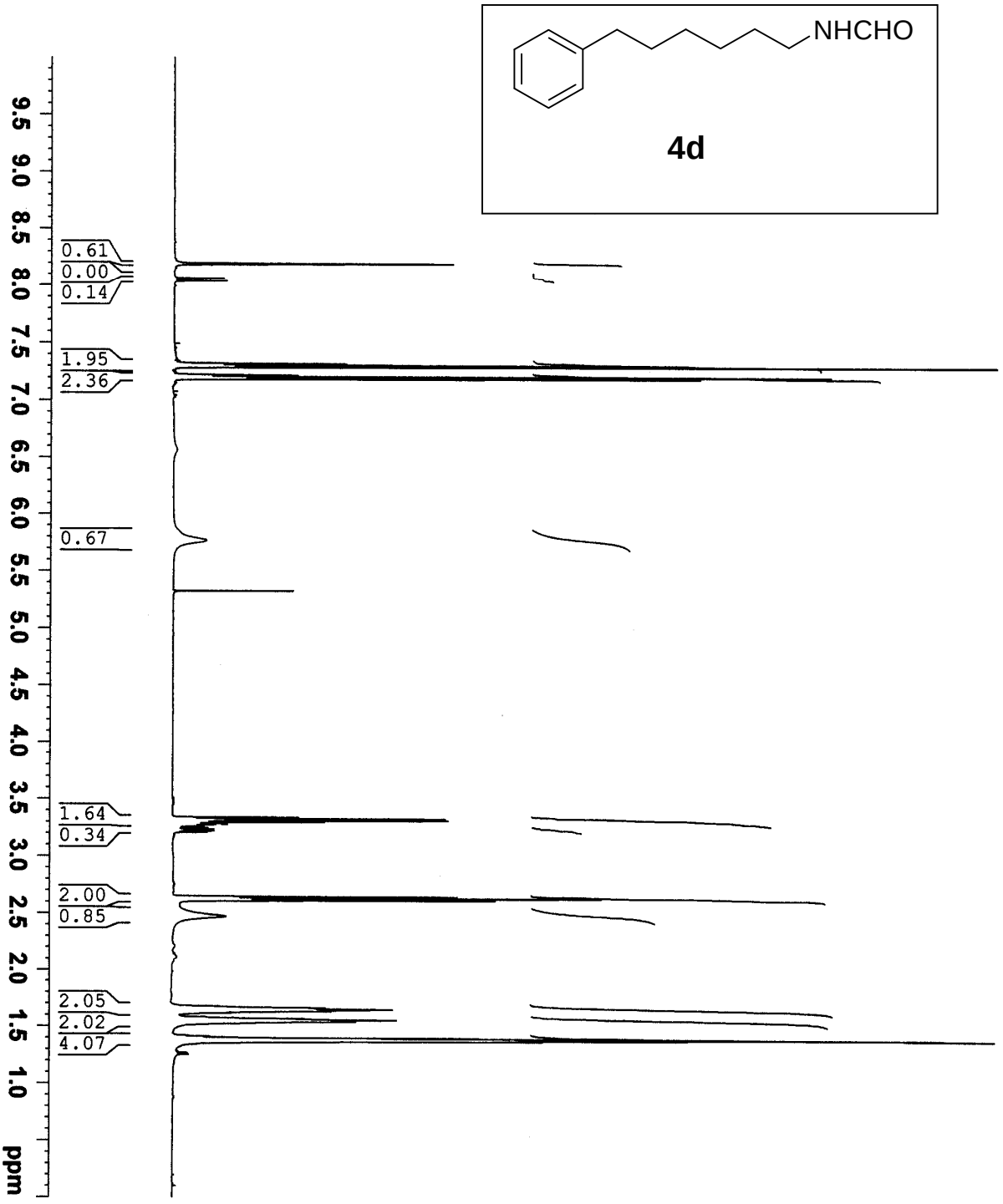
202.59
409.24
9
8
7
6
5
4
3
2
1
ppm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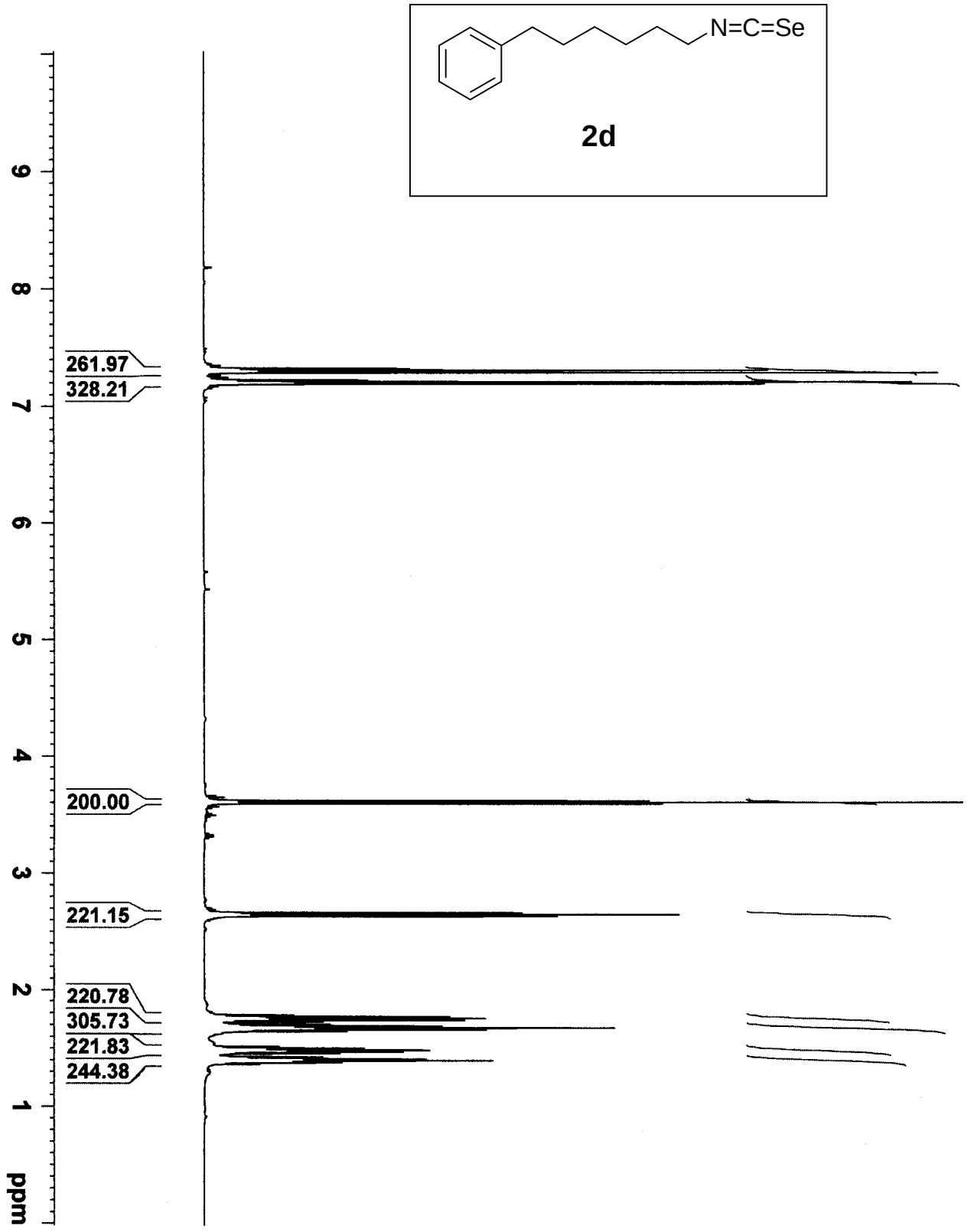
4d
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.61
0.00
0.14
1.95
2.36
0.67
1.64
0.34
2.00
0.85
2.05
2.02
4.07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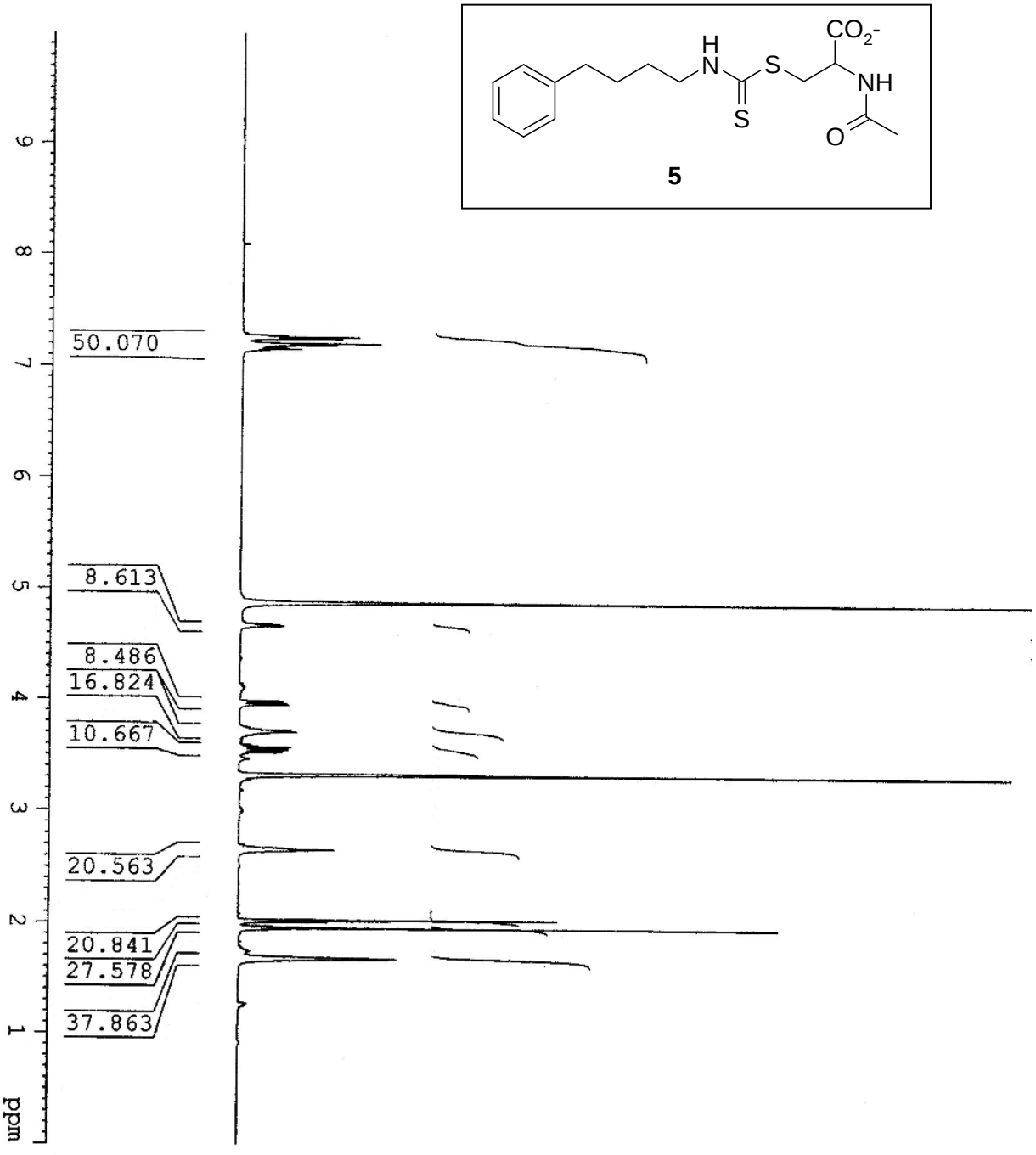
221.83
244.38
ppm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H
N
S
NH
S
O
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16.824
10.667
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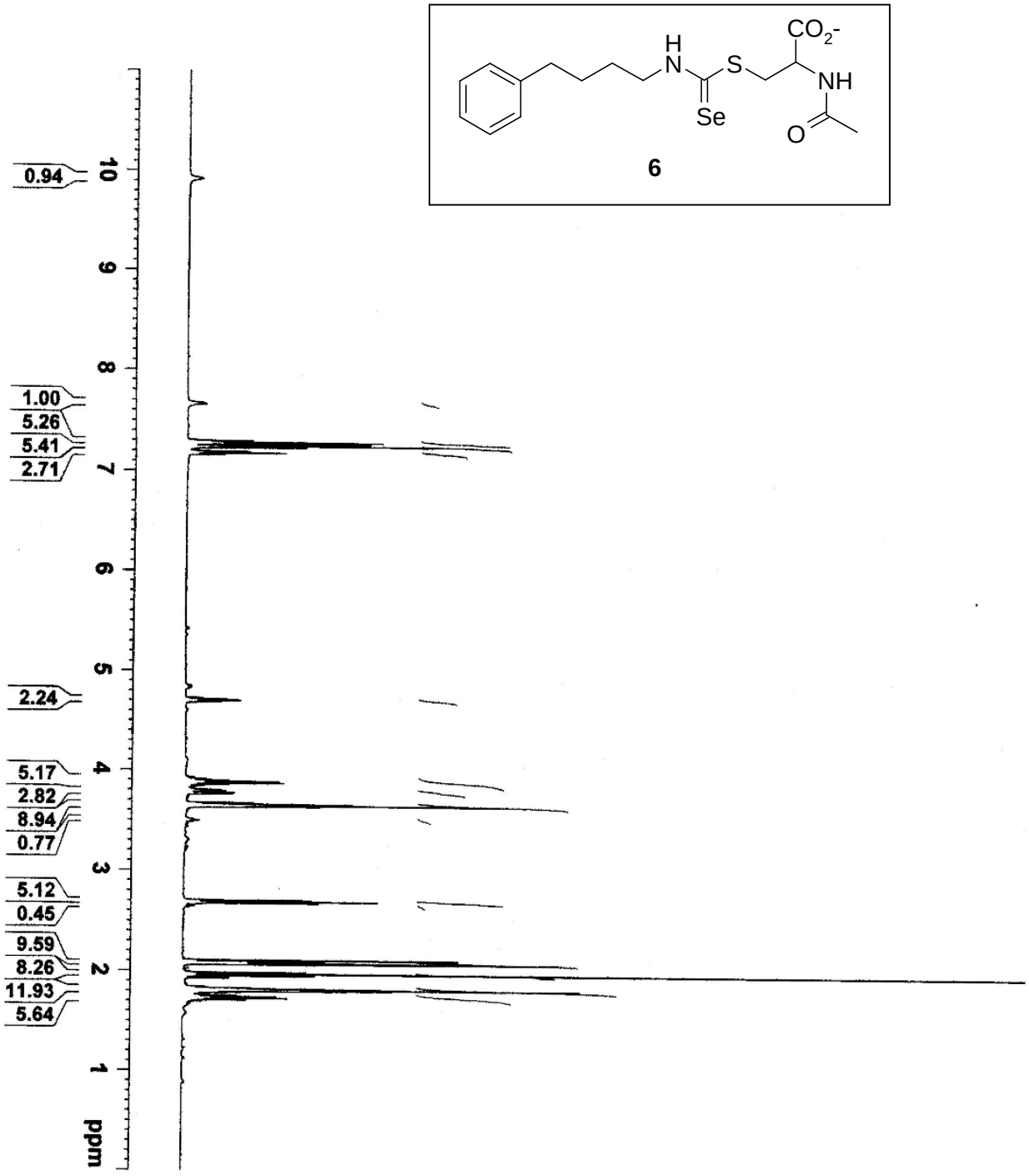
27.578
37.863
ppm


CO2-
H
N
S
NH
Se
O
6
0.94
1.00
5.26
5.41
2.71
2.24
5.17
2.82
8.94
0.77
5.12
0.45
9.59
8.26
11.93
5.64
10
9
8
7
6
5
4
3
2
1
ppm