SUPPORTING INFORMATION

S-Alkylated Homocysteine Derivatives: New Inhibitors of Human Betaine-Homocysteine *S*-Methyltransferase

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1. HPLC purity data for target compounds. HPLC analyses for target compounds were measured using two different HPLC systems.

Analytical **RP-HPLC** was performed using a Watrex (Nucleosil 120, 5μm, C18, 25 x 0.46 cm; Prague, Czech Republic) column. For gradient RP-HPLC analysis, a Waters LC 625 System (Milford, MA, USA) was used. Different gradients of acetonitrile (% v/v) in water containing 0.1% (v/v) of TFA at 1 ml/min were used for elution of compounds: a) 0 min - 0 %; 5 min - 0 %; 25 min - 16 %; 35 min - 80 %; 36 min - 0%; b) 0 min - 2 %; 5 min - 2 %; 25 min - 18 %; 35 min - 80 %; 36 min - 2%; c) 0 min - 4 %; 5 min - 4 %; 25 min - 22 %; 35 min - 80 %; 36 min - 4 %; d) 0 min - 4 %; 5 min - 4 %; 25 min - 28 %; 35 min - 80 %; 36 min - 4%. The purity data resulted from integration of peaks at 218 nm and are summarized in Table 1.

Analytical **Ion-exchange chromatography** was performed at 0.25 ml/min using AS11-HC (0.2 x 25 cm, Dionex Corporation, Sunnyvale, CA) column and using BioLC system (GP50 gradient pump, ED50 electrochemical detector) from Dionex Corporation (Sunnyvale, CA). The following gradient of water (A), 0.25 M sodium hydroxide (B), 1 M sodium acetate (C) and 0.1 M acetic acid (D) was used for elution of compounds: 0 min - 76% A, 24% B; 2 min - 76% A, 24% B; 8 min - 64% A, 36% B; 11 min - 64% A, 36% B; 18 min - 40% A, 20% B, 40% C; 21 min - 44% A, 16% B, 40% C; 23 min - 14% A, 16% B, 70% C; 45 min - 4% A, 16% B, 70% C; 45.1 min - 100% D; 47.1% min - 100% D; 47.2 min - 20% A, 80% B; 49.2 min - 20% A, 80% B; 49.3 min - 76% A, 24% B; 74 min - 76% A, 24% B. The purity data resulted from integration of peaks after amperometric detection and are given in Table 1. na means that the data are not available due to the low amperometric signal.

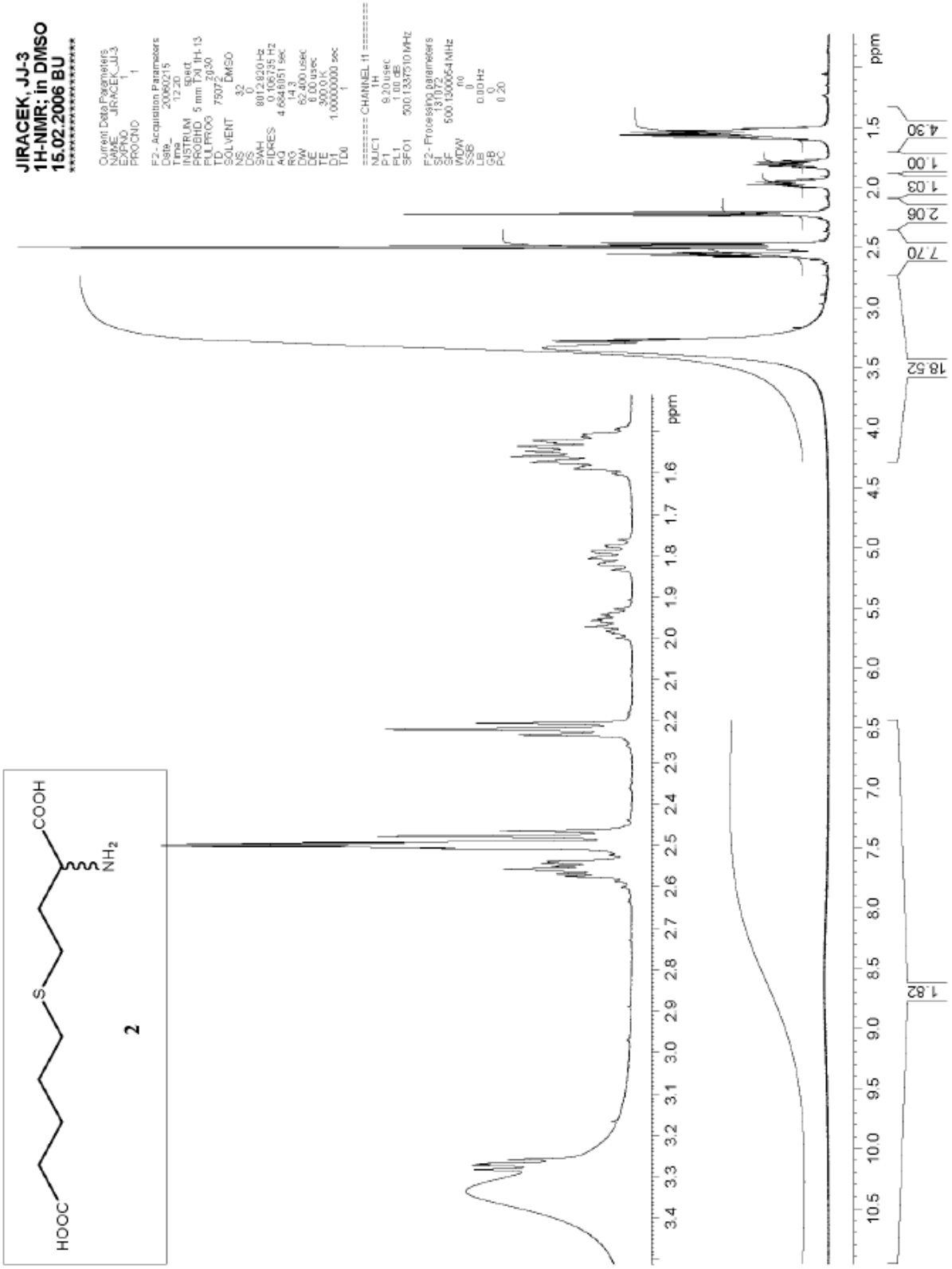
Table 1. HPLC purity data for target compounds. [a-b]Different gradients of acetonitrile in water.

Compound	RP-HPLC		Ion-exchange HPLC	
	E_t (min)	Purity (%)	E_t (min)	Purity (%)
2	23.05[b]	99.0	39.62	98.1
8	15.03[b]	97.4	36.83	95.8
9	26.99[b]	99.1	46.08	99.1
10	11.82[a]	95.8	30.47	95.3
11	9.55[a]	96.9	34.45	98.2
12	21.63[b]	98.7	33.75	98.5

13	29.74[b]	99.3	na	na
14	23.96[d]	97.5	na	na
15	24.13[c]	95.8	na	na
16	31.69[b]	99.6	na	na
17	25.32[d]	99.5	32.01	99.9
18	19.01[b]	95.2	33.59	98.8
19	16.09[b]	97.6	47.29	97.9
20	14.51[b]	97.9	41.23	98.3
21	18.53[b]	97.3	32.90	96.2
22	17.65[a]	99.4	33.91	99.8
23	5.94[a]	99.6	33.04	96.7
24	4.82[a]	96.1	33.54	97.9
25	14.63[a]	95.1	33.74	95.6

3. ^{1}H and ^{13}C NMR spectra records for target compounds 2, 9 and 19.

4.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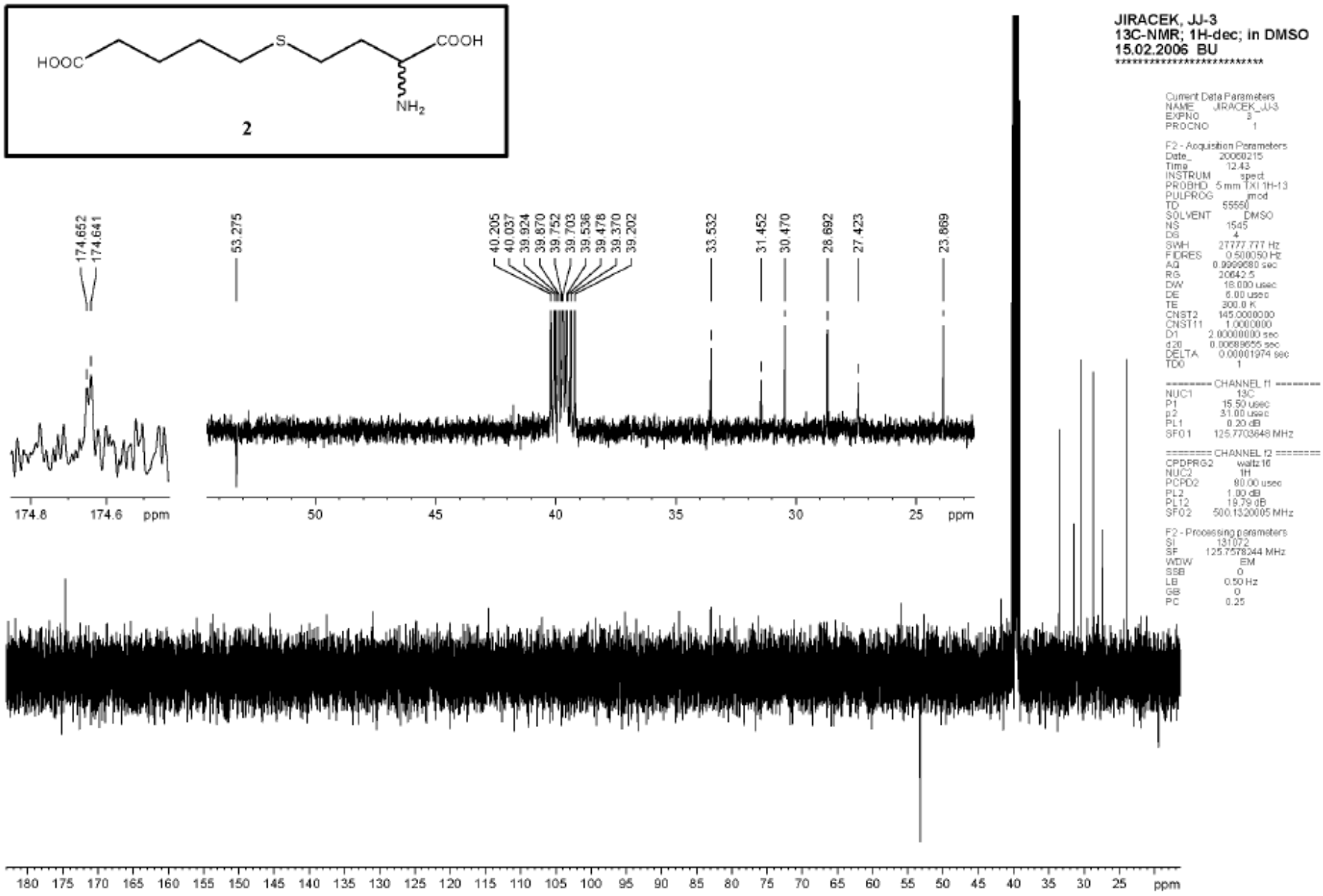
1.03
1.00
4.30
1.82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COOH
NH2
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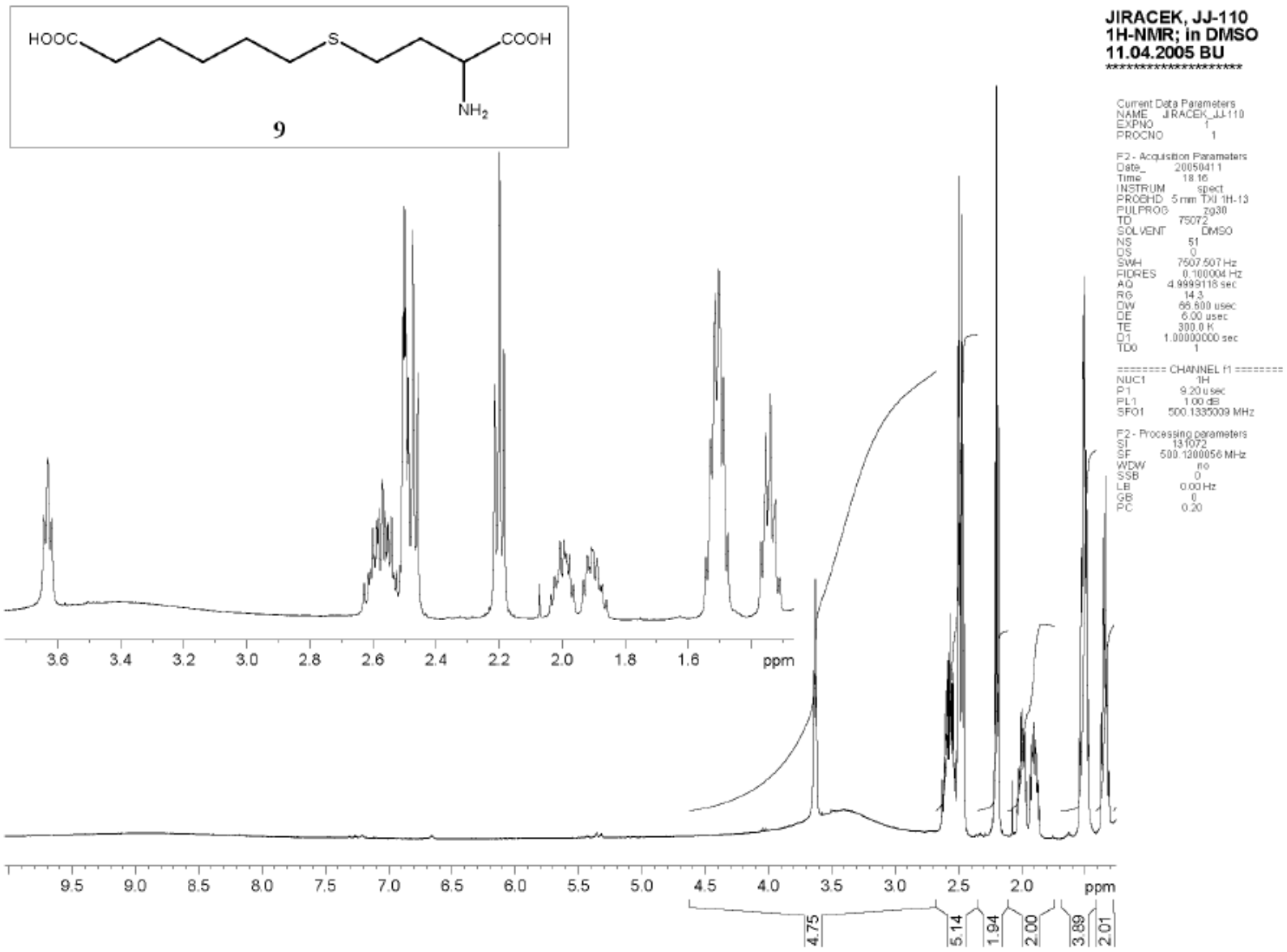
ppm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COOH
NH2
9
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11.04.2005 BU
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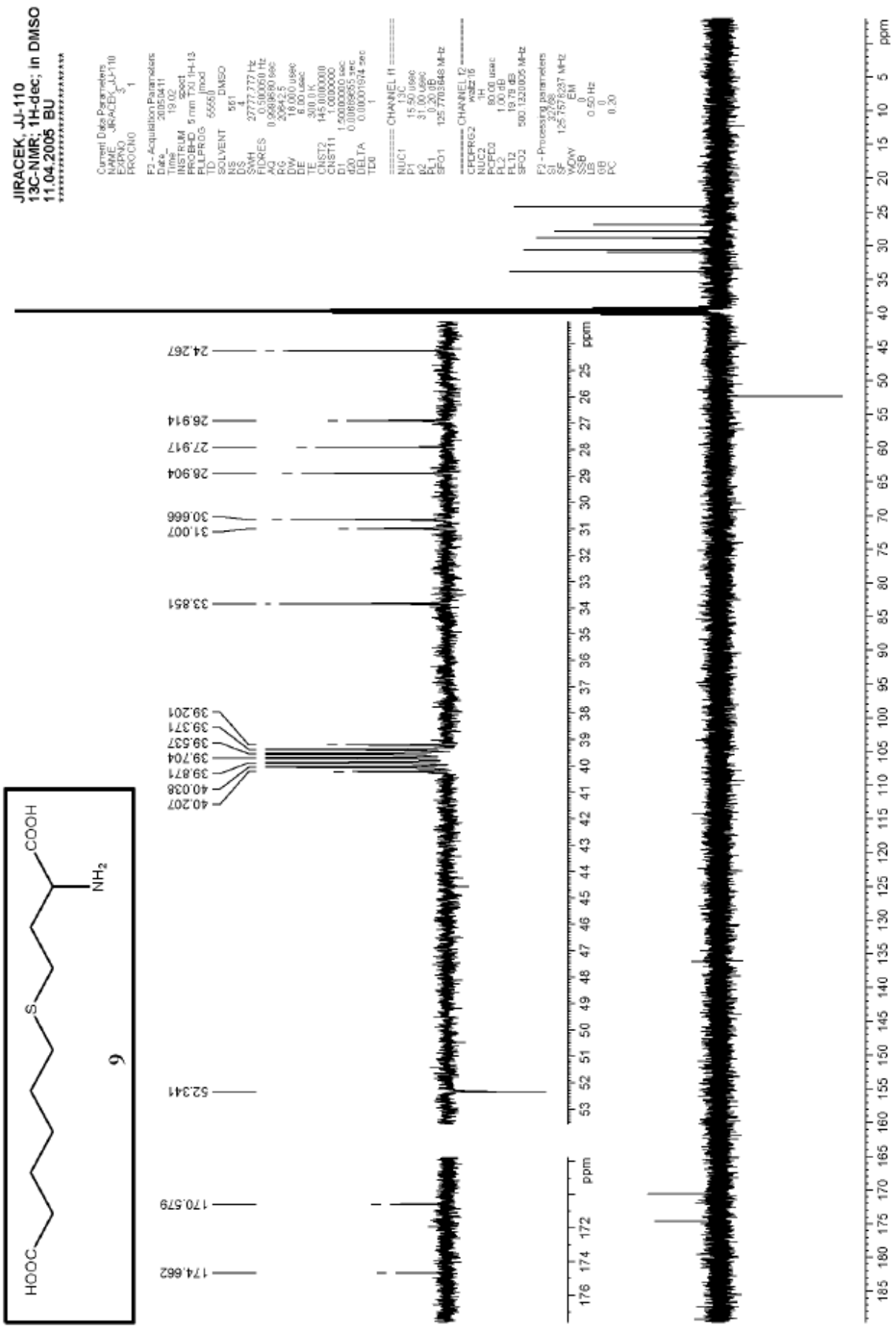
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HOOC
COOH
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40.038
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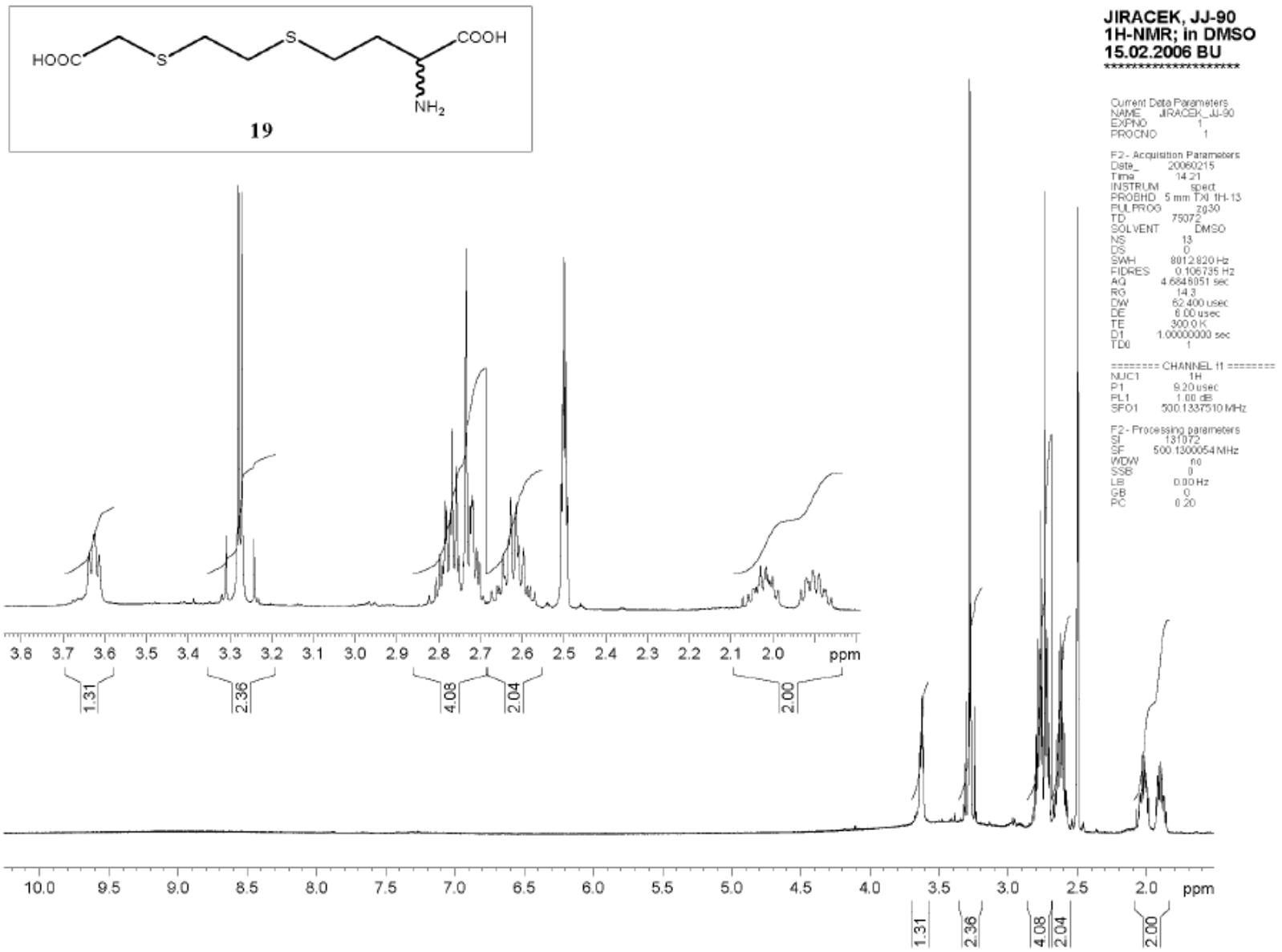
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COOH
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LB 0.00 Hz
GB 0
PC 0.20
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1.31
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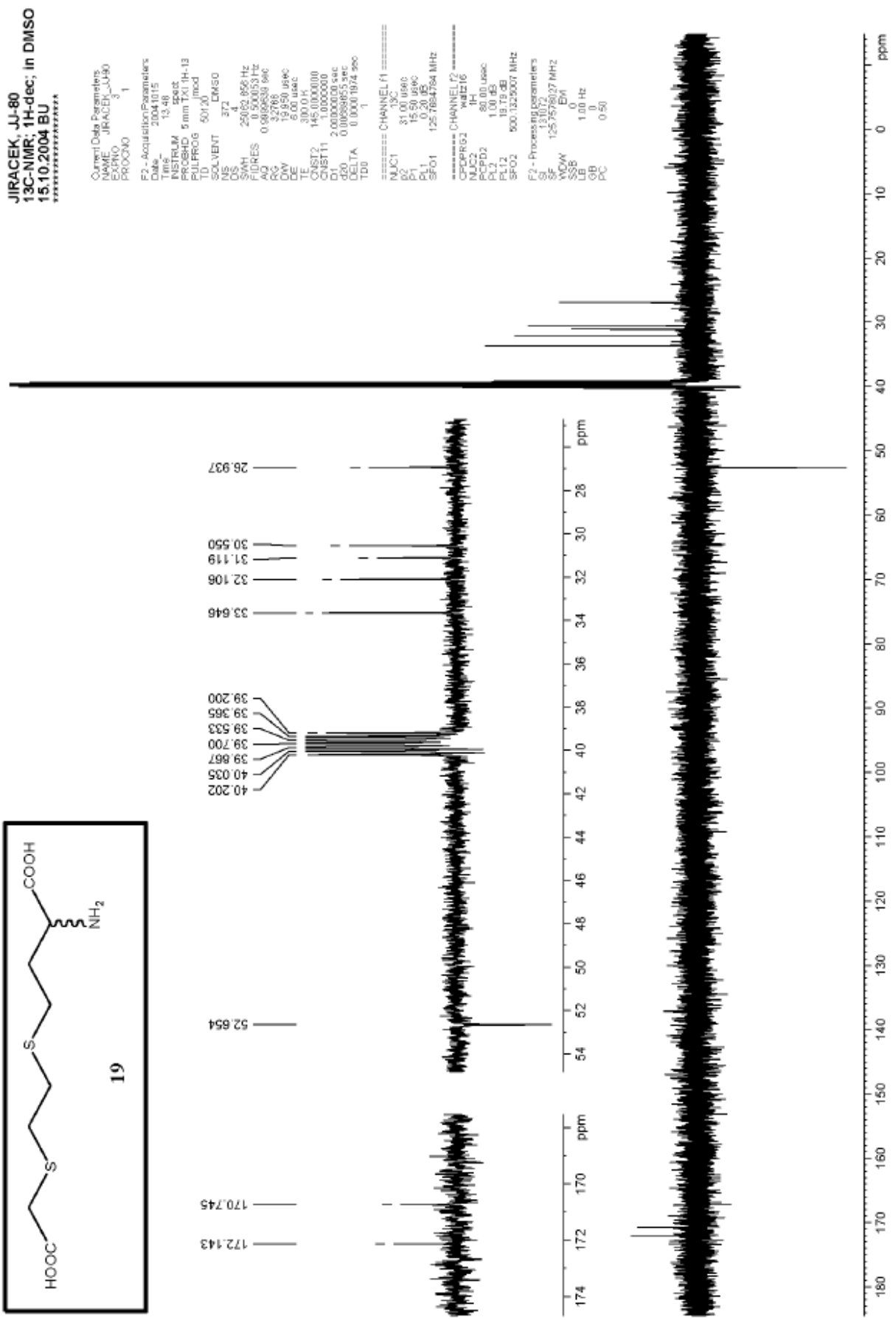
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COOH
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39.200
33.646
32.106
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30.550
26.937
ppm