

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.
2. ¹H and ¹³C NMR spectra records for target compounds **2**, **9** and **19**.

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, 5 μ m, 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.

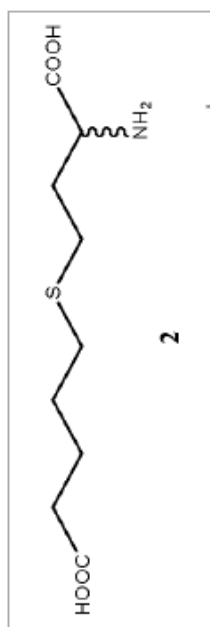
Table 1. HPLC purity data for target compounds. ^{a-b}Different gradients of acetonitrile in water.

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

4.



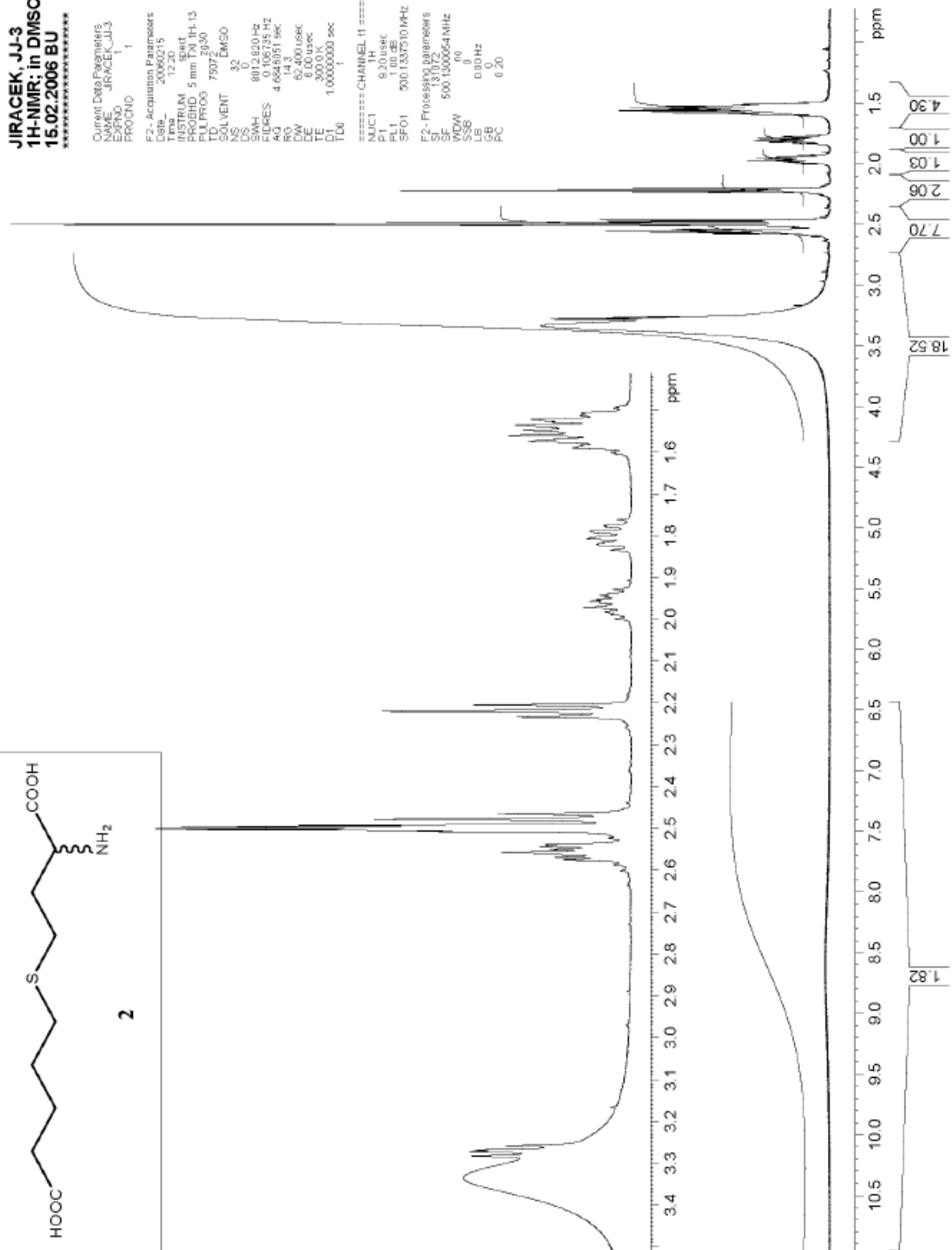
JIRACEK, JJ-3
1H-NMR: in DMSO
15.02.2006 BU

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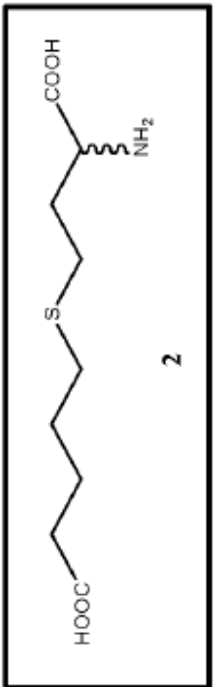
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JIRACEK, JJ-3
 13C-NMR, 1H-dec; in DMSO
 15.02.2006 BU



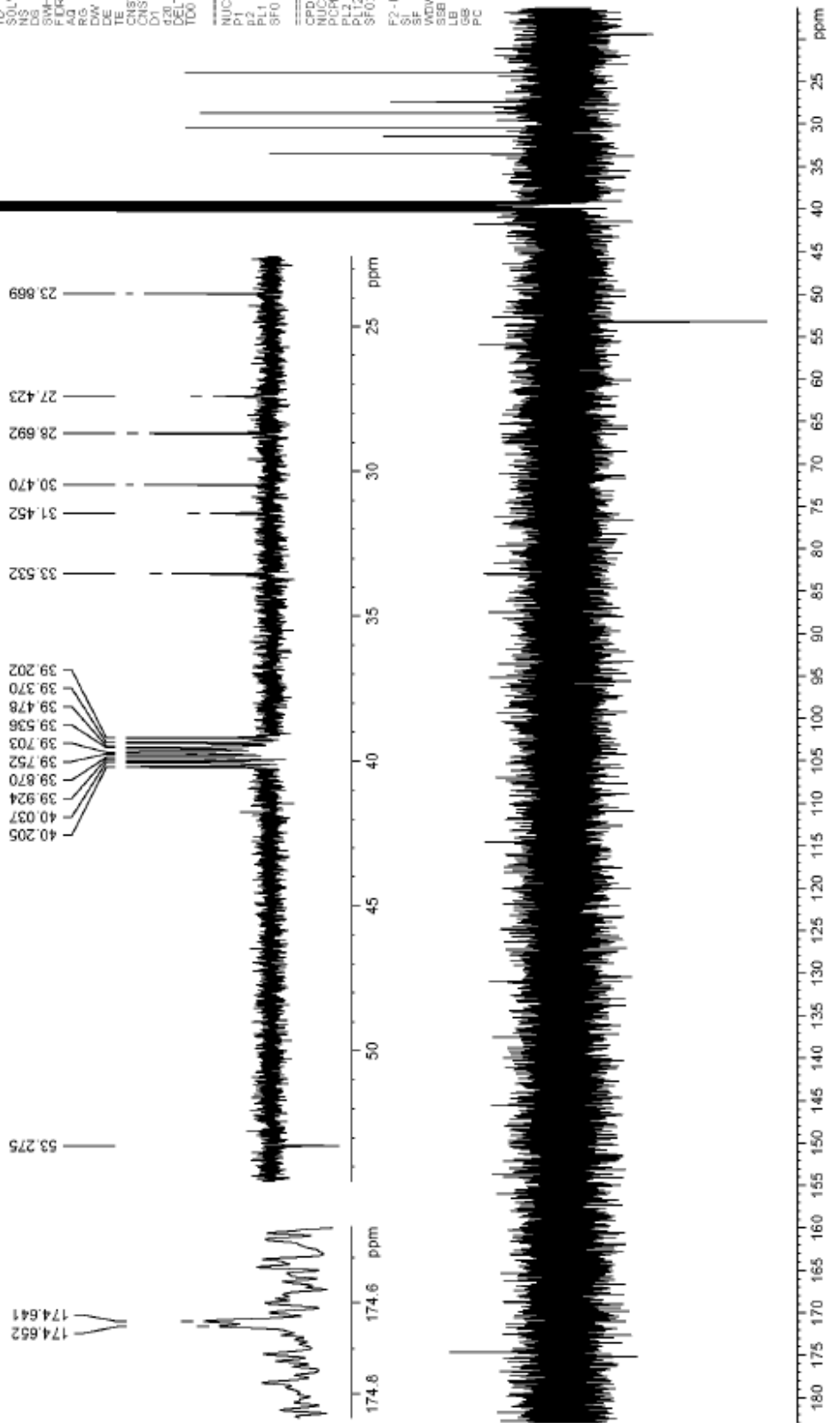
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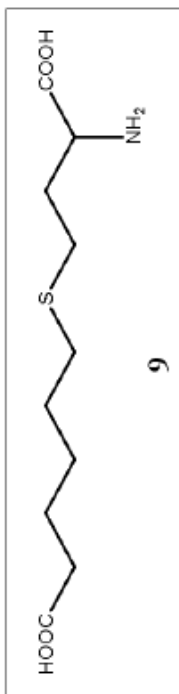
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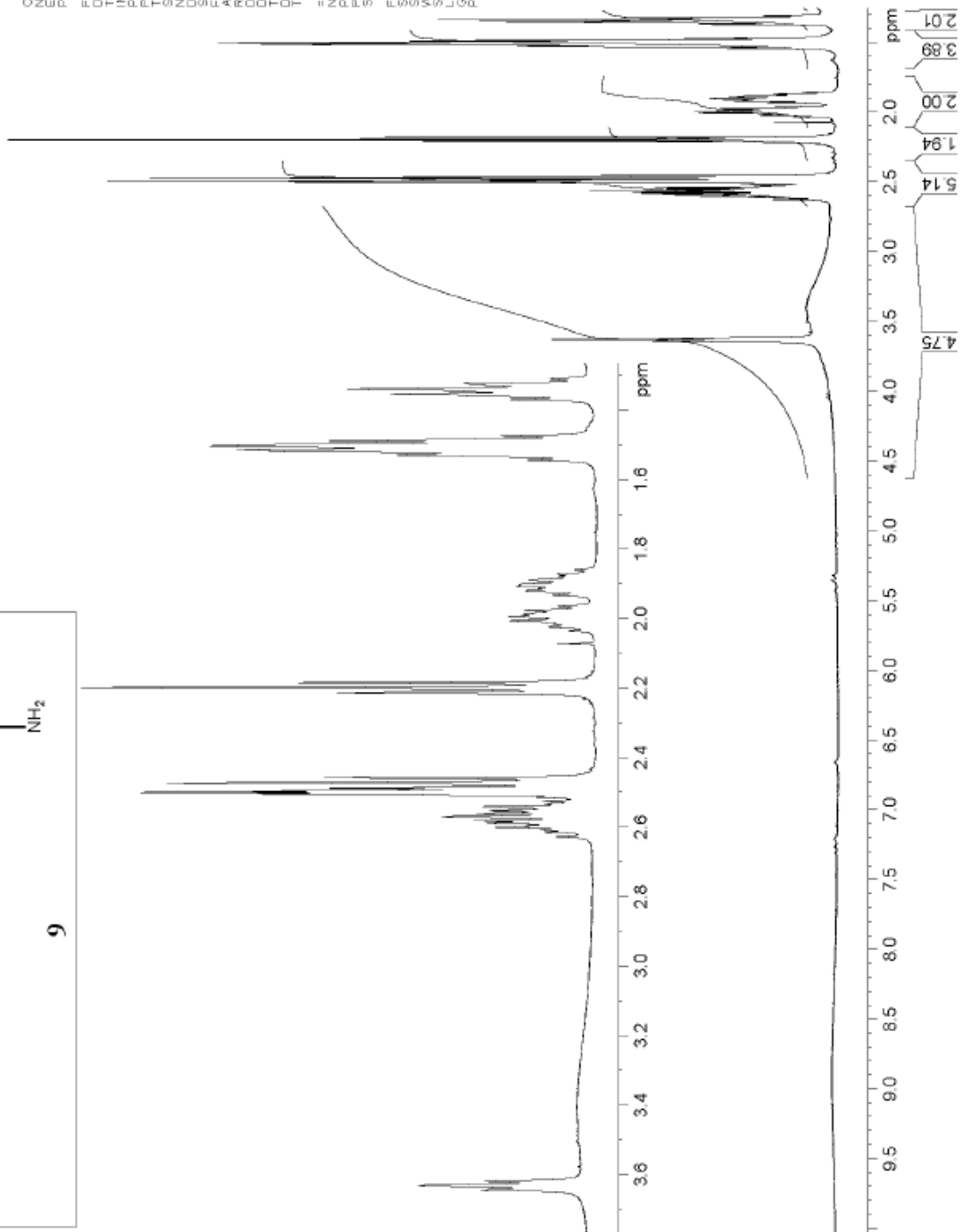


JIRACEK, JJ-110
¹H-NMR: in DMSO
11.04.2005 BU



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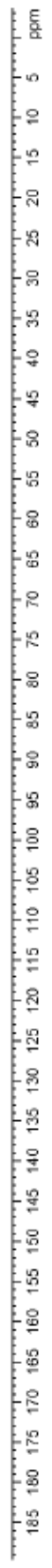
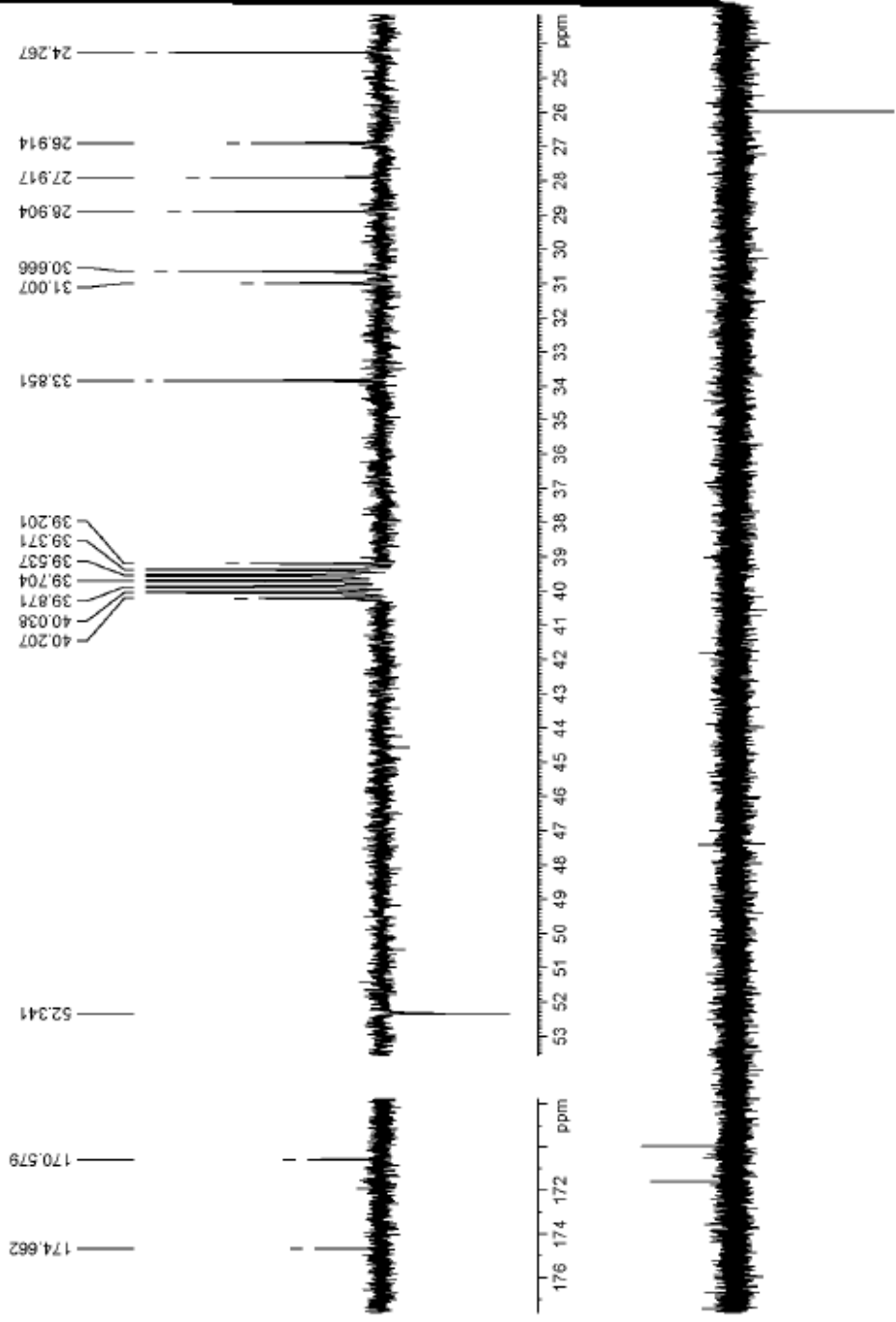
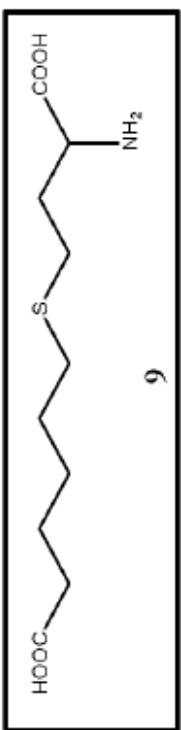
JIRACEK, JJ-110
 13C-NMR, 1H-dec; in DMSO
 11.04.2005 BU

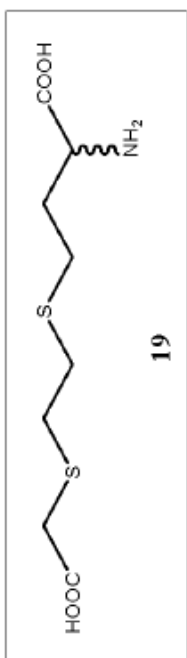
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 FIDRES 0.000001 Hz
 AQ 0.000001 sec
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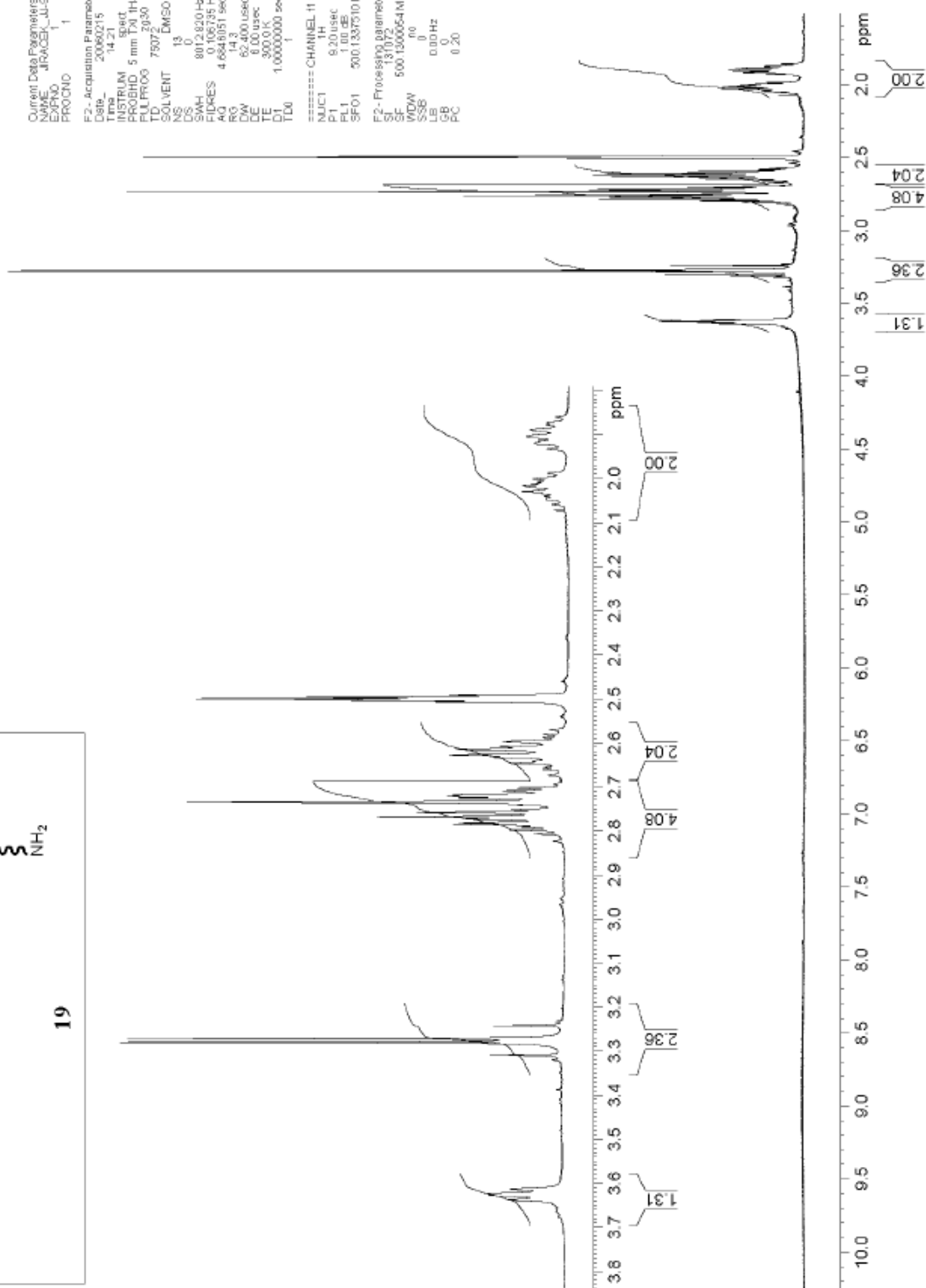




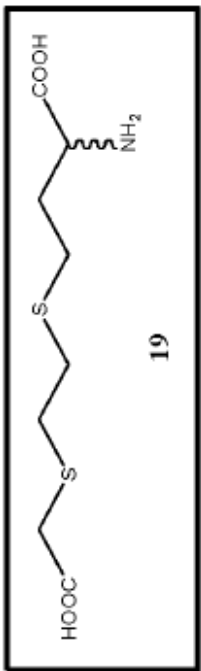
JIRACEK, JJ-90
1H-NMR: in DMSO
15.02.2006 BU

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SOLVENT: DMSO
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CWA: 62.400 usec
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PL1: 1.00 dB
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F2 - Processing parameters
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PC: 0.20
  
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JIRACEK, JI-80
 13C-NMR; 1H-dec; in DMSO
 15.10.2004 BU



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RG      : 32768
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TE      : 300.0 K
CHST2   : 145.0000000
CHST1   : 1.0000000
D1      : 2.0000000 sec
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DELTA   : 0.0000000 sec
TD0     : 1
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NUC1    : 13C
P1      : 31.00 usec
PL1     : 0.00 dB
PL12    : 19.30 dB
SFO1    : 125.7634764 MHz

===== CHANNEL f2 =====
CPDPRG2 : waltz16
NUC2    : 13C
P2      : 80.00 usec
PL2     : 1.00 dB
PL12    : 19.78 dB
SFO2    : 900.1322007 MHz

C2 - Processing parameters
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WDW     : EM
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