Electronic Supplementary Information (ESI)

Preparation of sulfur-MOF composites and their application in Willgerodt-Kindler reaction

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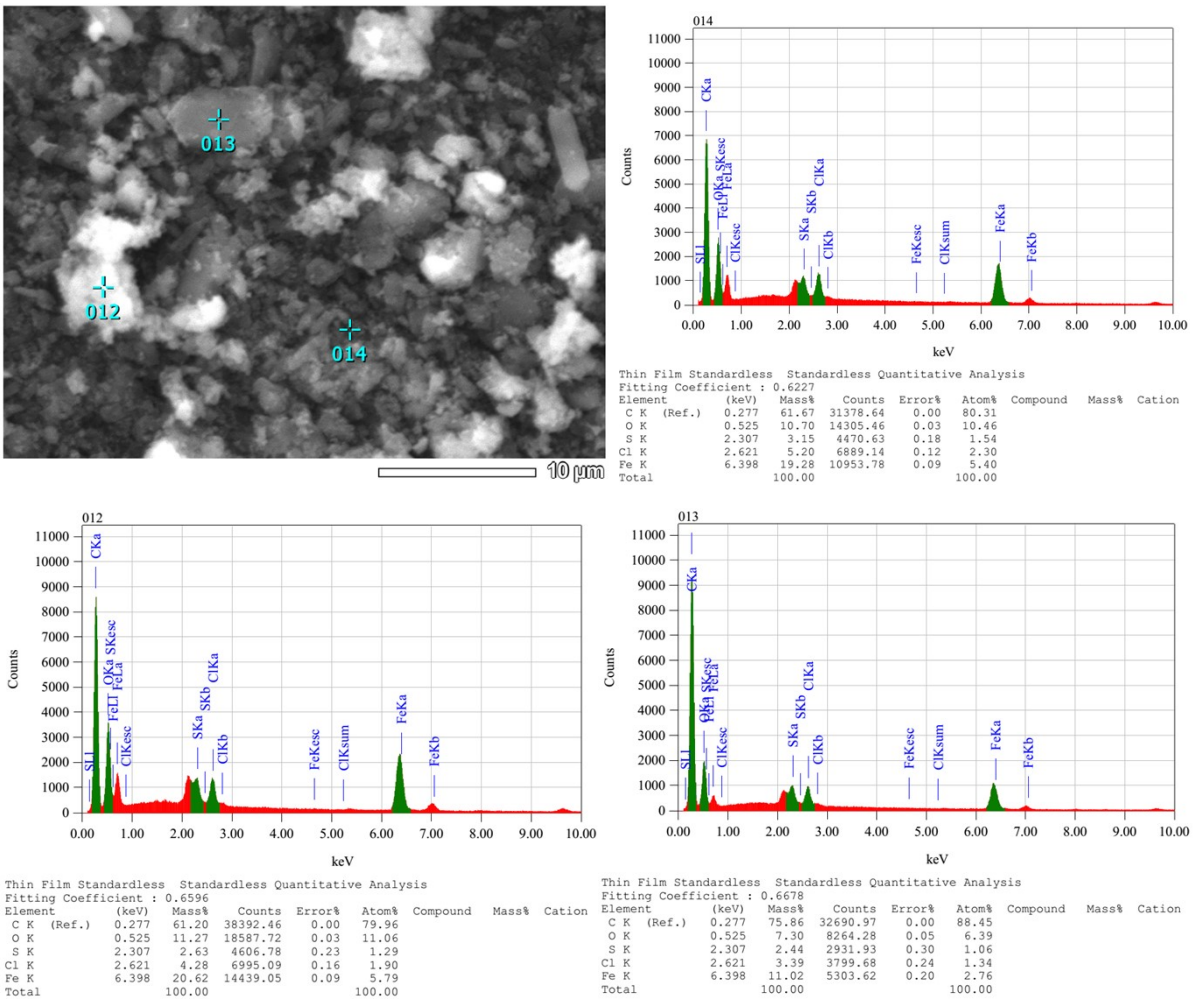
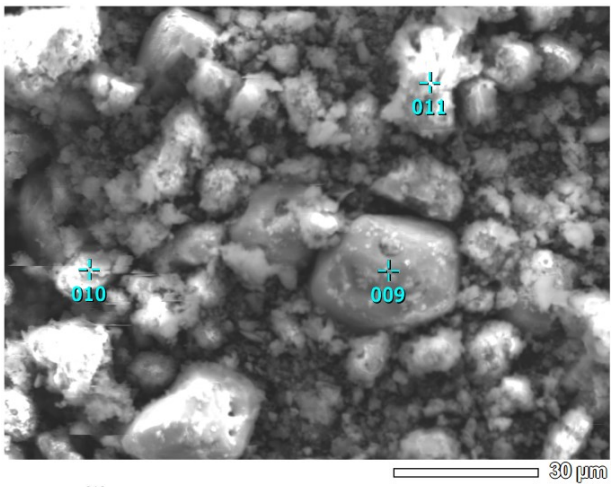
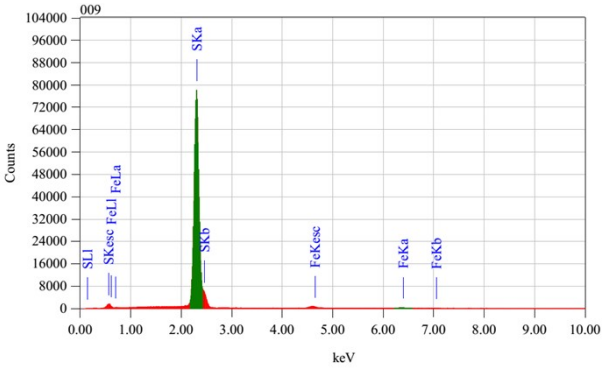


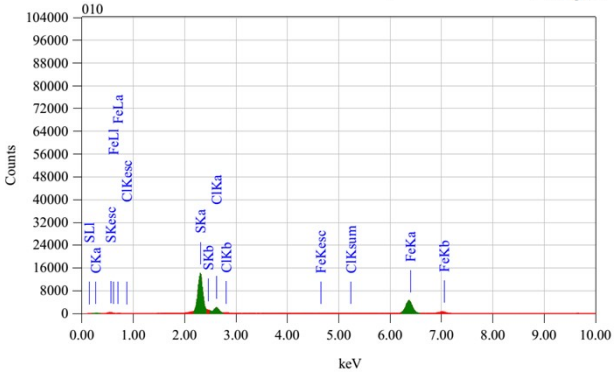
Fig S1. EDX analysis of S@MIL101(Fe) particles





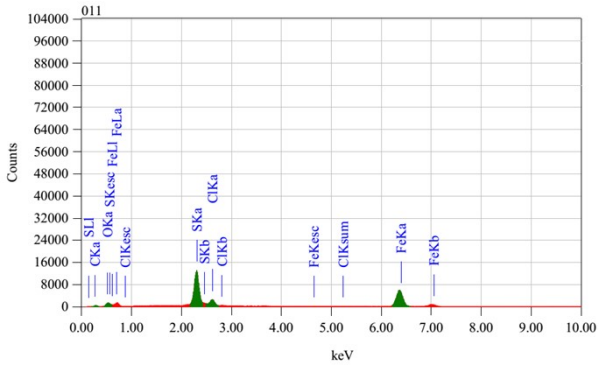
Thin Film Standardless Standardless Quantitative Analysis
Fitting Coefficient : 0.6205

Element		(keV)	Mass%	Counts	Error%	Atom%	Compound	Mass%	Cation
S K	(Ref.)	2.307	99.42	609391.50	0.02	99.67			
Fe K		6.398	0.58	1417.35	7.84	0.33			
Total			100.00			100.00			



Thin Film Standardless Standardless Quantitative Analysis
Fitting Coefficient : 0.6376

Element		(keV)	Mass%	Counts	Error%	Atom%	Compound	Mass%	Cation
C K		0.277	1.01	705.50	0.31	3.19			
S K	(Ref.)	2.307	51.85	101371.03	0.01	61.53			
Cl K		2.621	8.06	14691.05	0.11	8.65			
Fe K		6.398	39.08	30555.65	0.06	26.63			
Total			100.00			100.00			



Thin Film Standardless Standardless Quantitative Analysis
Fitting Coefficient : 0.6677

Element		(keV)	Mass%	Counts	Error%	Atom%	Compound	Mass%	Cation
C K		0.277	2.68	2058.23	0.12	8.27			
O K		0.525	2.79	5628.12	0.14	6.46			
S K	(Ref.)	2.307	39.50	84631.27	0.02	45.64			
Cl K		2.621	8.15	16272.83	0.11	8.51			
Fe K		6.398	46.89	40171.28	0.05	31.11			
Total			100.00			100.00			

Fig S2. EDX analysis of S@MIL88A particles

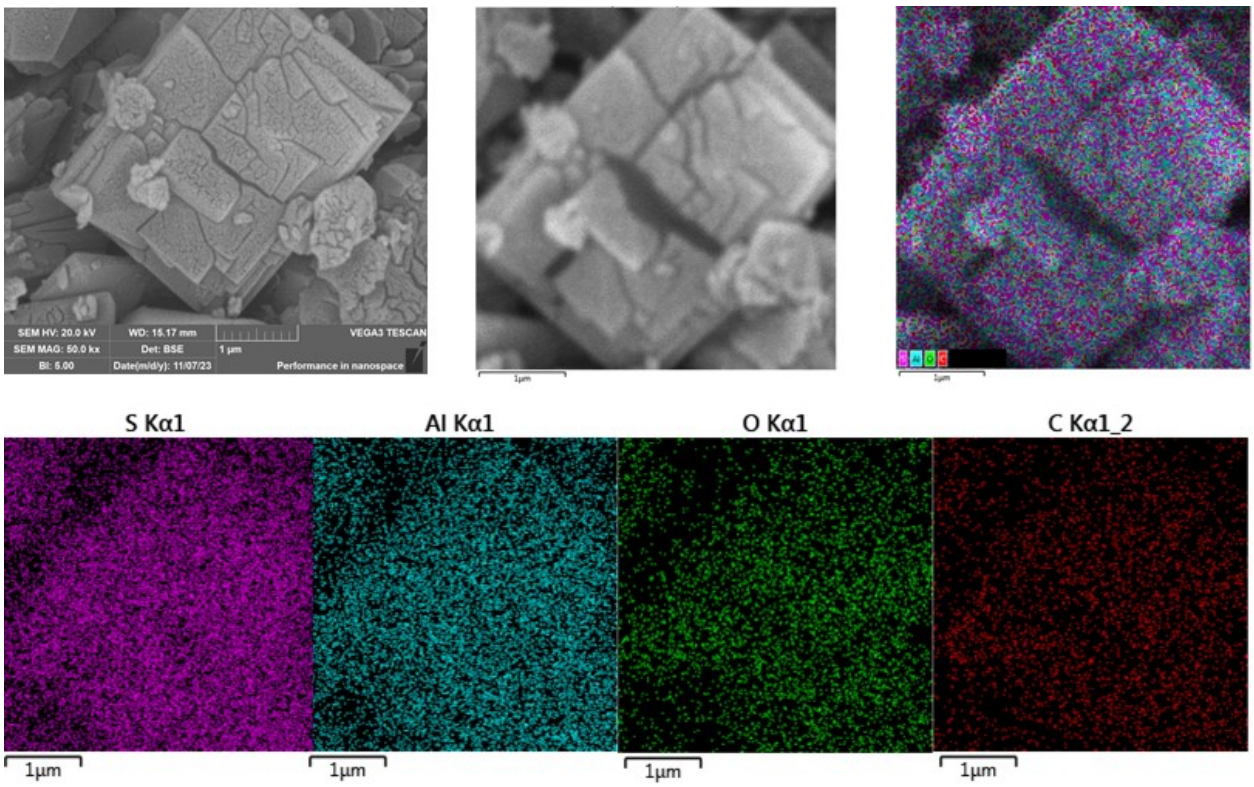


Fig S3. S@CAU-10(H) atom mapping.

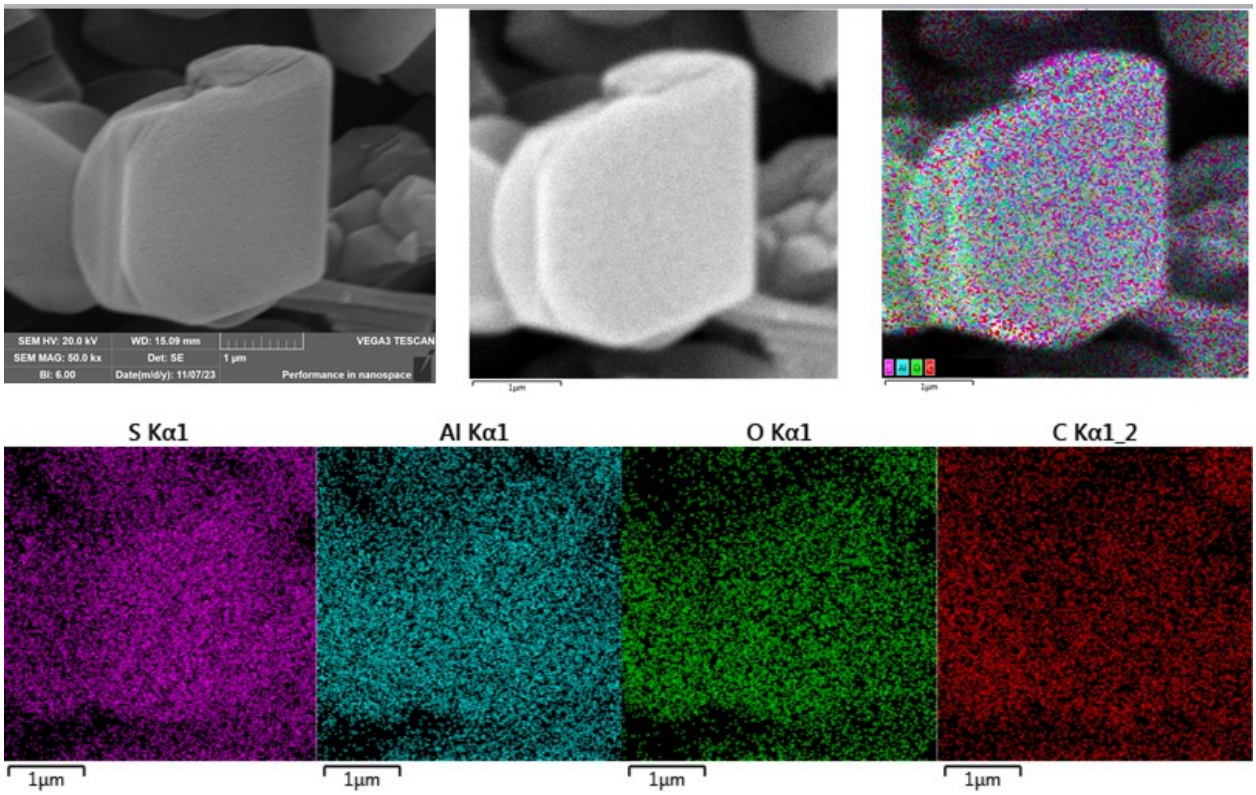


Fig S4. S@MIL-53(Al) atom mapping.

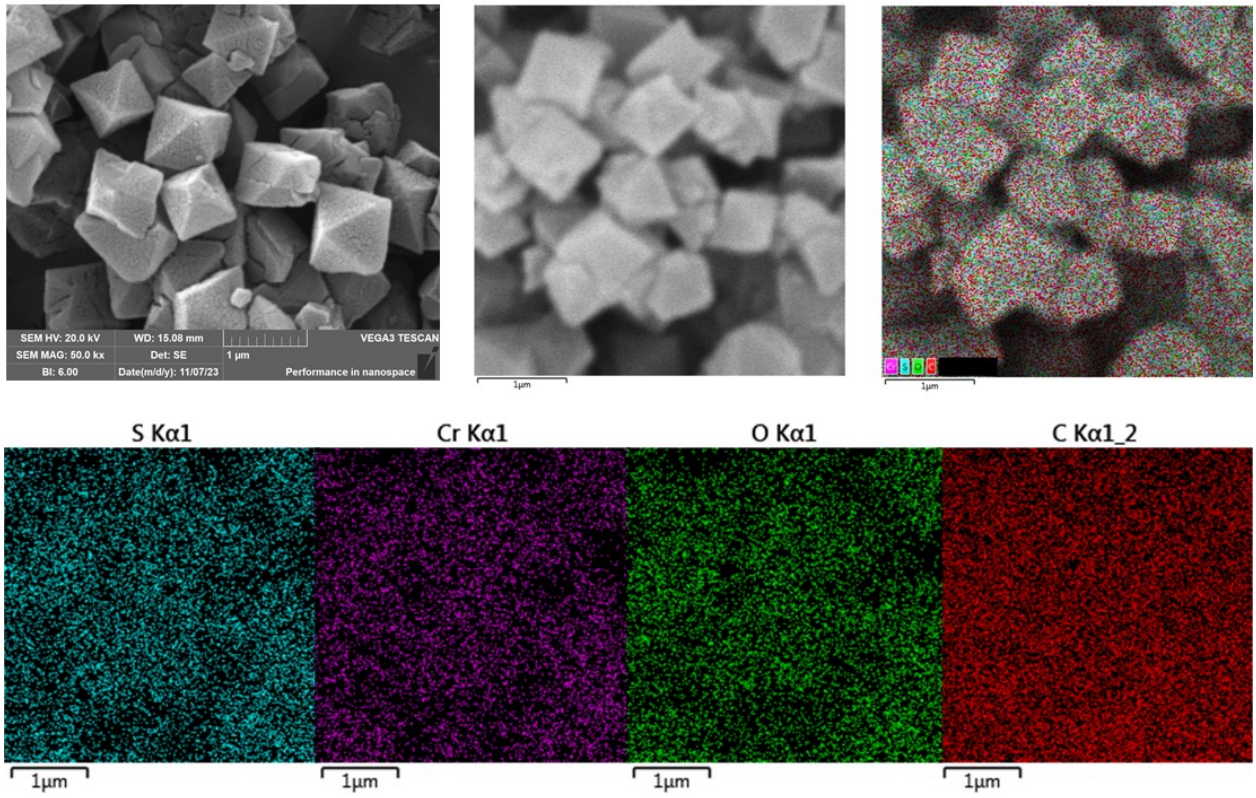


Fig S5. S@MIL-101(Cr) atom mapping.

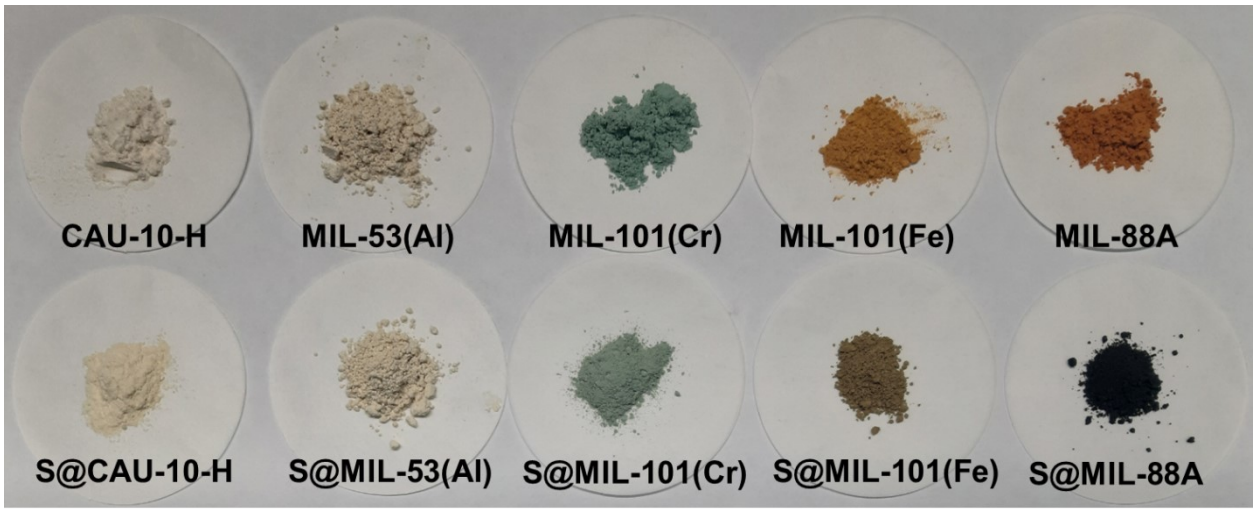
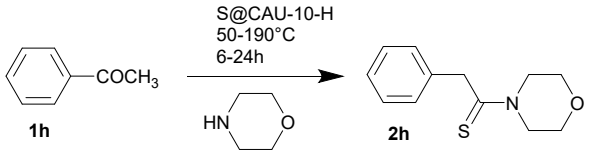


Fig S6. Activated MOF and MOF after sulfur sorption (20% w/w) photo.

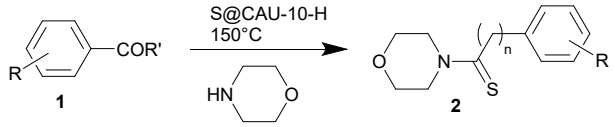


Scheme S1. CAU-10-H-assisted phenylacetic thiomorpholide synthesis.

Entry	S_8 mass fraction in CAU-10-H, %	Sulfur, equiv.	Morpholine, equiv.	Temperature, °C	Reaction time, h	Isolated yield, %
1	20	1	1	160	10	59
2	20	1	1.5	160	10	66
3	20	1	2	160	10	62
4	20	1	3	160	10	61
5	20	1.2	1.2	160	10	83
6	20	1.5	1.5	160	10	79
7	20	1.5	2	160	10	77
8	20	2	1	160	10	75
9	20	2	2	160	10	57
10	20	2	3	160	10	56
11	20[a]	1.2	1.2	160	10	72
12	-[b]	1.2	1.2	160	10	0
13	15	1.2	1.2	160	10	66
14	10	1.2	1.2	160	10	63
15	20	1.2	1.2	50	24	0
16	20	1.2	1.2	100	8	11
17	20	1.2	1.2	100	24	22
18	20	1.2	1.2	120	24	36
19	20	1.2	1.2	150	6	71
20	**20**	**1.2**	**1.2**	**150**	**8**	**83**
21	20	1.2	1.2	150	16	80
22	20	1.2	1.2	150	24	75
23	20	1.2	1.2	170	8	72
24	20	1.2	1.2	190	8	40

[a]Grounded sulfur and CAU-10(H) mixture, [b]without MOF

Table S1. Reaction parameters screening for the synthesis of phenylacetic acid thiomorpholide.



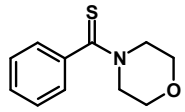
Scheme S2. CAU-10-H-assisted thiomorpholides synthesis.

Entry	Substrate	R	R’	Product	n	Reaction time, h	Isolated yield, %
1	1a	H	H	2a	0	8	86
2	1b	4-Me	H	2b	0	8	91
3	1c	4-Cl	H	2c	0	8	78
4	1d	4-OMe	H	2d	0	8	81
5	1e	4-NMe_2	H	2e	0	8	70
6	1f	4-NO_2	H	2f	0	8	68
7	1g	3- NO_2	H	2g	0	8	56
8	1h	H	Me	2h	1	8	83
9	1i	4-Me	Me	2i	1	8	79
10	1j	4-Ph	Me	2j	1	8	82
11	1k	4-OMe	Me	2k	1	8	83
12	1l	4- NMe_2	Me	2l	1	8	62
13	1m	C_6H_4 (α-naphthyl)	Me	2m	1	16	58
14	1n	H	Et	2n	2	16	79
15	1o	4-Me	Et	2o	2	16	76
16	1p	4-OMe	Et	2p	2	16	63

Table S2. CAU-10-H-assisted WK-reaction products yields.

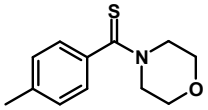
Characterization of compounds **2a-2p, 4a, 4b**

Benzoic acid thiomorpholide (**2a**)



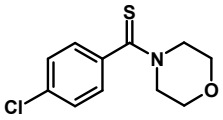
Mp 137 °C (from EtOH) (lit.,[1] 138 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): **δ_H** = 7.24-7.38 (m, 5H, Ar-H), 4.28 (t, J_{H-H} = 4.8 Hz, 2H, CH_2,), 3.74 (t, J_{H-H} = 5.0 Hz, 2H, CH_2), 3.49-3.56 (m, 4H, CH_2) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): **δ_C** = 199.2 (CS), 142.9 (C_{Ar}), 129.8 (CH_{Ar}), 128.8 (CH_{Ar}), 126.4 (CH_{Ar}), 66.5 (OCH_2), 66.2 (OCH_2), 52.8 (NCH_2), 49.7 (NCH_2) ppm; **Elemental analysis**: Found: C, 63.69; H, 6.3. Calc. for $C_{11}H_{13}NOS$: C, 63.72; H, 6.32%; **IR-ATR**: 2981, 2917, 2845, 1573, 1492, 1475, 1108, 1223, 1022 cm^{-1}.

p-Toluic acid thiomorpholide (**2b**)



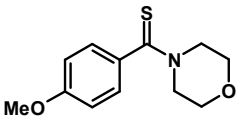
Mp 127 °C (from EtOH) (lit.,[2] 127-129 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): **δ_H** = 7.12-7.20 (m, 4H, Ar-H), 4.27 (t, J_{H-H} = 4.9 Hz, 2H, CH_2), 3.73 (t, J_{H-H} = 5.0 Hz, 2H, CH_2), 3.50-3.56 (m, 4H, CH_2), 2.28 (s, 3H, CH_3) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): **δ_C** = 199.6 (CS), 140.2 (C_{Ar}),138.7 ($\underline{C}_{Ar}CH_3$), 129.2 (CH_{Ar}), 126.6 (CH_{Ar}), 66.6 (OCH_2), 66.2 (OCH_2), 52.8 (NCH_2), 49.9 (NCH_2), 21.3 ($Ar\underline{C}H_3$) ppm. **Elemental analysis**: Found: C, 65.10; H, 6.85. Calc. for $C_{12}H_{15}NOS$: C, 65.12; H, 6.83%; **IR-ATR**: 2974, 2915, 2852, 1605, 1510, 1473, 1429, 1105, 1290, 1255, 1222 cm^{-1}.

4-Chlorobenzoic acid thiomorpholide (**2c**)



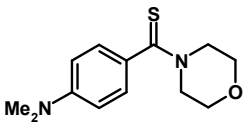
Mp 138-139 °C (from EtOH) (lit.,[3] 136-138 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): **δ_H** = 7.42 (d, J_{H-H} = 8.5 Hz, 2H, Ar-H), 7.28 (d, J_{H-H} = 8.5 Hz, 2H, Ar-H), 4.26 (t, J_{H-H} = 4.9 Hz, 2H, CH_2), 3.74 (t, J_{H-H} = 5.0 Hz, 2H, CH_2), 3.49-3.56 (m, 4H, CH_2) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): **δ_C** = 197.7 (CS), 141.6 (C_{Ar}), 133.7 (CCl_{Ar}), 128.9 (CH_{Ar}), 128.3 (CH_{Ar}), 66.5 (OCH_2), 66.2 (OCH_2), 52.9 (NCH_2), 49.8 (NCH_2) ppm; **Elemental analysis**: Found: C, 54.69; H, 5.05. Calc. for $C_{11}H_{12}ClNOS$: C, 54.64; H, 5.00%; **IR-ATR**: 2983, 2916, 2851, 1590, 1498, 1473, 1110, 1289, 1233, 1030 cm^{-1}.

4-Methoxybenzoic acid thiomorpholide (**2d**)



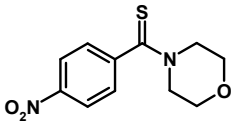
Mp 102-103 °C (from *i*-PrOH) (lit.,[4] 100 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): **δ_H** = 7.25 (d, J_{H-H} = 8.7 Hz, 2H, Ar-H), 6.90 (d, J_{H-H} = 8.8 Hz, 2H, Ar-H), 4.26 (br.s, 2H, CH_2), 3.74 (s, 3H, OMe), 3.23 (br.s, 2H, CH_2), 3.55 (br.s, 4H, CH_2) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): **δ_C** = 199.5 (CS), 160.1 (CO_{Ar}), 135.2 (C_{Ar}), 128.6 (CH_{Ar}), 113.0 (CH_{Ar}), 66.6(OCH_2), 66.3 (OCH_2), 55.8 (OCH_3), 53.0 (NCH_2), 50.2 (NCH_2) ppm; **Elemental analysis**: Found: C, 60.70; H, 6.40. Calc. for $C_{12}H_{15}NO_2S$: C, 60.73; H, 6.37%; **IR-ATR**: 3005, 2953, 2846, 1603, 1508, 1478, 1108, 1224, 1029 cm^{-1}.

4-(Dimethylamino)benzoic acid thiomorpholide (**2e**)



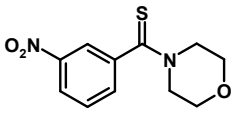
Mp 147-148 °C (from *i*-PrOH) (lit.,[5] 149-150 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): **δ_H** = 7.20 (d, J_{H-H} = 8.8 Hz, 2H, Ar-H), 6.63 (d, J_{H-H} = 8.9 Hz, 2H, Ar-H), 4.20 (br.s, 2H, CH_2), 3.63 (br.s, 6H, CH_2), 2.90 (s, 6H, NMe_2) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): **δ_C** = 200.5 (CS), 151.3 (CN_{Ar}), 129.9 (C_{Ar}), 129.1 (CH_{Ar}), 111.3 (CH_{Ar}), 66.5 (OCH_2), 53.2 (NCH_2), 50.8 (NCH_2), 40.4 (NCH_3) ppm; **Elemental analysis**: Found: C, 62.34; H, 7.29. Calc. for $C_{13}H_{18}N_2OS$: C, 62.37; H, 7.25%; **IR-ATR**: 2960, 2882, 2848, 1598, 1517, 1361, 1113, 1280, 1218 cm^{-1}.

4-Nitrobenzoic acid thiomorpholide (**2f**)



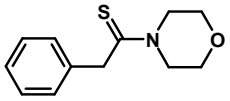
Mp 202 °C (from *i*-PrOH/DMF) (lit.,[6] 202-203 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): δ_H = 8.19 (d, J_{H-H} = 8.7 Hz, 2H, Ar-H), 7.51 (d, J_{H-H} = 8.7 Hz, 2H, Ar-H), 4.27 (t, J_{H-H} = 4.9 Hz, 2H, CH_2), 3.76 (t, J_{H-H} = 5.0 Hz, 2H, CH_2), 3.46-3.57 (m, 4H, CH_2) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): δ_C = 196.0 (CS), 148.3 (CN_{Ar}), 147.4 (CN_{Ar}), 127.5 (CH_{Ar}), 124.3 (CH_{Ar}), 66.4 (OCH_2), 66.1 (OCH_2), 52.8 (NCH_2), 49.4 (NCH_2) ppm; **Elemental analysis**: Found: C, 52.34; H, 4.81. Calc. for $C_{11}H_{12}N_2O_3S$: C, 52.37; H, 4.79%; **IR-ATR**: 3059, 2857, 1591, 1509, 1501, 1476, 1342, 1105, 1232, 1030 cm^{-1}.

3-Nitrobenzoic acid thiomorpholide (**2g**)



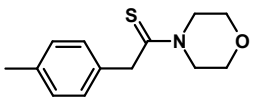
Mp 149-150 °C (from *i*-PrOH/DMF) (lit.,[6] 151 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): δ_H = 8.15-8.18 (m, 1H, Ar-H), 8.09 (t, J_{H-H} = 2.0 Hz, 1H, Ar-H), 7.62-7.71 (m, 2H, Ar-H), 4.28 (t, J_{H-H} = 4.5 Hz, 2H, CH_2), 3.77 (t, J_{H-H} = 4.2 Hz, 2H, CH_2), 3.52-3.57 (m, 4H, CH_2) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): δ_C = 195.7 (CS), 148.1 (CN_{Ar}), 144.0 (C_{Ar}), 132.6 (CH_{Ar}), 130.6 (CH_{Ar}), 123.7 (CH_{Ar}), 121.3 (CH_{Ar}), 66.4 (OCH_2), 66.1 (OCH_2), 52.9 (NCH_2), 49.7 (NCH_2) ppm; **Elemental analysis**: Found: C, 52.38; H, 4.83. Calc. for $C_{11}H_{12}N_2O_3S$: C, 52.37; H, 4.79%; **IR-ATR**: 3072, 2978, 2860, 1523, 1489, 1438, 1348, 1106 cm^{-1}.

Phenylacetic acid thiomorpholide (**2h**)



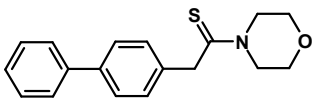
Mp 79 °C (from EtOH) (lit.,[7] 79-80 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): δ_H = 7.18-7.30 (m, 5H, Ar-H), 4.28 (s, 2H, $ArCH_2$), 4.20 (t, J_{H-H} = 4.9 Hz, 2H, CH_2), 3.65 (t, J_{H-H} = 4.8 Hz, 2H, CH_2), 3.60 (t, J_{H-H} = 5.0 Hz, 2H, CH_2), 3.36 (t, J_{H-H} = 5.1 Hz, 2H, CH_2) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): δ_C = 199.3 (CS), 136.9 (C_{Ar}), 129.1 (CH_{Ar}), 128.5 (CH_{Ar}), 127.2 (CH_{Ar}), 66.3 (OCH_2), 66.2 (OCH_2), 51.2 (NCH_2), 50.4 (NCH_2), 49.7 ($Ar\underline{C}H_2$) ppm; **Elemental analysis**: Found: C, 65.11; H, 6.85. Calc. for $C_{12}H_{15}NOS$: C, 65.12; H, 6.83%; **IR-ATR**: 2963, 2907, 2849, 1603, 1493, 1453, 1111, 1433, 1263, 1033 cm^{-1}.

4-Methylphenylacetic acid thiomorpholide (**2i**)



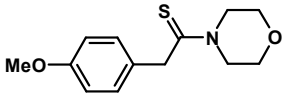
Mp 103-104 °C (from *i*-PrOH) (lit.,[8] 105 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): δ_H = 7.18 (d, J_{H-H} = 8.7 Hz, 2H, Ar-H), 7.09 (d, J_{H-H} = 8.7 Hz, 2H, Ar-H), 4.22 (s, 2H, $ArCH_2$), 4.18 (t, J_{H-H} = 4.9 Hz, 2H, CH_2), 3.64 (t, J_{H-H} = 4.9 Hz, 2H, CH_2), 3.59 (t, J_{H-H} = 4.9 Hz, 2H, CH_2), 3.36 (t, J_{H-H} = 4.9 Hz, 2H, CH_2), 2.23 (s, 3H, CH_3) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): δ_C = 199.6 (CS), 136.3 ($\underline{C}_{Ar}CH_2$), 133.8 ($C_{Ar}CH_3$), 129.7 (CH_{Ar}), 128.3 (CH_{Ar}), 66.3 (OCH_2), 66.2 (OCH_2), 51.1 (NCH_2), 50.4 (NCH_2), 49.3 ($C_{Ar}\underline{C}H_2$), 21.2 (CH_3) ppm; **Elemental analysis**: Found: C, 66.32; H, 7.30. Calc. for $C_{13}H_{17}NOS$: C, 66.35; H, 7.28%; **IR-ATR**: 2845, 1492, 1429, 1284, 1255, 1106, 1096, 1026, 957 cm^{-1}.

4-Biphenylacetic acid thiomorpholide (**2j**)



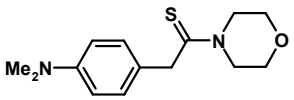
Mp 72-73 °C (from EtOH/DMF) (lit.,[9] 73-74 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): δ_H = 7.59-7.63 (m, 4H, Ar-H), 7.30-7.44 (m, 5H, Ar-H), 4.32 (s, 2H, $ArCH_2$), 4.21 (t, J_{H-H} = 4.4 Hz, 2H, CH_2), 3.71 (t, J_{H-H} = 4.4 Hz, 2H, CH_2), 3.62 (t, J_{H-H} = 5.3 Hz, 2H, CH_2), 3.43 (t, J_{H-H} = 5.1 Hz, 2H, CH_2) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): δ_C = 199.3 (CS), 140.3 (CH_{Ar}), 139.0 (C_{Ar}), 136.1 (C_{Ar}), 129.5 (CH_{Ar}), 129.1 (CH_{Ar}), 127.9 (C_{Ar}),127.4 (CH_{Ar}), 127.1 (CH_{Ar}), 66.4 (OCH_2), 66.2 (OCH_2), 51.2 (NCH_2), 50.4 (NCH_2), 49.2 (CH_2) ppm; **Elemental analysis**: Found: C, 72.66; H, 6.47. Calc. for $C_{18}H_{19}NOS$: C, 72.69; H, 6.44%; **IR-ATR**: 2960, 2914, 2847, 1597, 1496, 1490, 1439, 1102, 1302, 1259cm^{-1}.

4-Methoxyphenylacetic acid thiomorpholide (**2k**)



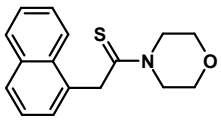
Mp 64 °C (from MeOH) (lit.,[8] 70 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): δ_H = 7.22 (d, $J_{H\text{-}H}$ = 8.7 Hz, 2H, Ar-H), 6.86 (d, $J_{H\text{-}H}$ = 8.7 Hz, 2H, Ar-H), 4.19 (s, 2H, $ArCH_2$), 4.18 (t, $J_{H\text{-}H}$ = 4.7 Hz, 2H, CH_2), 3.66 (t, $J_{H\text{-}H}$ = 4.4 Hz, 2H, CH_2), 3.59 (t, $J_{H\text{-}H}$ = 5.0 Hz, 2H, CH_2), 3.37 (t, $J_{H\text{-}H}$ = 5.0 Hz, 2H, CH_2), 3.69 (s, 3H, CH_3) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): δ_C = 199.8 (CS), 158.5 (CO_{Ar}), 129.5 (CH_{Ar}), 128.6 (C_{Ar}), 114,5 (CH_{Ar}), 66.3 (OCH_2), 66.2 (OCH_2), 55.5 (OCH_3), 51.1 (NCH_2), 50.4 (NCH_2), 48.8 (CH_2) ppm; **Elemental analysis**: Found: C, 62.1; H, 6.84. Calc. for $C_{13}H_{17}NO_2S$: C, 62.12; H, 6.82%; **IR-ATR**: 2994, 2854, 2837, 1610, 1580, 1512, 1495, 1108, 1249, 1029 cm^{-1}.

4-(Dimethylamino)phenylacetic acid thiomorpholide (**2l**)



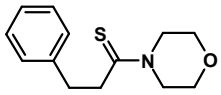
Mp 139-140 °C (from *i*-PrOH) (lit.,[10] 138-140 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): δ_H = 7.11 (d, $J_{H\text{-}H}$ = 8.7 Hz, 2H, Ar-H), 6.64 (d, $J_{H\text{-}H}$ = 8.7 Hz, 2H, Ar-H), 4.13 (s, 2H, $ArCH_2$), 4.16 (t, $J_{H\text{-}H}$ = 4.9 Hz, 2H, CH_2), 3.65 (t, $J_{H\text{-}H}$ = 4.7 Hz, 2H, CH_2), 3.58 (t, $J_{H\text{-}H}$ = 5.0 Hz, 2H, CH_2), 3.35 (t, $J_{H\text{-}H}$ = 4.9 Hz, 2H, CH_2), 2.82 (s, 6H, NMe_2) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): δ_C = 200.3 (CS), 149.8 (CN_{Ar}), 129.0 (CH_{Ar}), 123.9 (C_{Ar}), 113.1 (CH_{Ar}), 66.3 (OCH_2), 66.2 (OCH_2), 51.1 (NCH_2), 50.4 (NCH_2), 48.9 (CH_2), 40.7 (NCH_3) ppm; **Elemental analysis**: Found: C, 63.62; H, 7.65. Calc. for $C_{14}H_{20}N_2OS$: C, 63.60; H, 7.62%; **IR-ATR**: 2963, 2846, 2802, 1621, 1527, 1496, 1113, 1433, 1264, 1101 cm^{-1}.

1-Naphthylacetic acid thiomorpholide (**2m**)



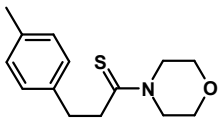
Mp 210-212 °C (from *i*-PrOH) (lit.,[11] 208-210 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): δ_H = 7.79-7.99 (m, 3H, Ar-H), 7.43-7.55 (m, 3H, Ar-H), 7.26 (d, $J_{H\text{-}H}$ = 7.2 Hz, 1H, Ar-H), 4.68 (s, 2H, $ArCH_2$), 4.31 (t, $J_{H\text{-}H}$ = 4.9 Hz, 2H, CH_2), 3.71 (t, $J_{H\text{-}H}$ = 4.9 Hz, 2H, CH_2), 3.57 (t, $J_{H\text{-}H}$ = 5.3 Hz, 2H, CH_2), 3.45 (t, $J_{H\text{-}H}$ = 5.3 Hz, 2H, CH_2) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): δ_C = 199.6 (CS), 133.9 ($\underline{C}_{Ar}CH_2$), 133.1 (CH_{Ar}), 131.7 (CH_{Ar}), 129.1 (CH_{Ar}), 127.7 (C_{Ar}), 126.8 (C_{Ar}), 126.4 (CH_{Ar}), 126.2 (CH_{Ar}), 125.3 (CH_{Ar}), 124.0 (CH_{Ar}), 66.3 (OCH_2), 66.2 (OCH_2), 51.1 (NCH_2), 50.2 (NCH_2), 46.8 (CH_2) ppm; **Elemental analysis**: Found: C, 70.85; H, 6.33. Calc. for $C_{16}H_{17}NOS$: C, 70.81; H, 6.31%; **IR-ATR**: 3052, 2854, 1596, 1491, 1433, 1111, 1100, 963 cm^{-1}.

3-Phenylpropionic acid thiomorpholide (**2n**)



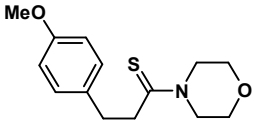
Oil; **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): δ_H = 7.15-7.27 (m, 5H, Ar-H), 4.17 (t, $J_{H\text{-}H}$ = 4.5 Hz, 2H, CH_2), 3.67 (t, $J_{H\text{-}H}$ = 4.4 Hz, 2H, CH_2), 3.58 (t, $J_{H\text{-}H}$ = 5.0 Hz, 2H, CH_2), 3.41 (t, $J_{H\text{-}H}$ = 5.2 Hz, 2H, CH_2), 3.03-3.07 (m, 2H, CH_2CS), 2.92-2.96 (m, 2H, $ArCH_2$) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): δ_C = 201.8 (CS), 141.0 (C_{Ar}), 129.1 (CH_{Ar}), 128.9 (CH_{Ar}), 126.7 (CH_{Ar}), 66.4 (OCH_2), 66.2 (OCH_2), 50.5 (NCH_2), 50.2 (NCH_2), 44.1 ($\underline{C}H_2CS$), 35.4 ($Ph\underline{C}H_2$) ppm; **Elemental analysis**: Found: C, 66.33; H, 7.30. Calc. for $C_{13}H_{17}NOS$: C, 66.35; H, 7.28%; **IR-ATR**: 3023, 2962, 2916, 2853, 1601, 1479, 1452, 1428, 1273, 1237, 1110 cm^{-1}.

3-(4-methylphenyl)propionic acid thiomorpholide (**2o**)



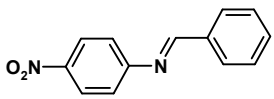
Mp 101-102 °C (from *i*-PrOH) (lit.,[12] 102-104 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): δ_H = 7.04-7.11 (m, 4H, Ar-H), 4.16 (t, $J_{H\text{-}H}$ = 4.8 Hz, 2H, CH_2), 3.67 (t, $J_{H\text{-}H}$ = 4.8 Hz, 2H, CH_2), 3.58 (t, $J_{H\text{-}H}$ = 5.0 Hz, 2H, CH_2), 3.43 (t, $J_{H\text{-}H}$ = 5.2 Hz, 2H, CH_2), 2.99-3.03 (m, 2H, CH_2CS), 2.85-2.88 (m, 2H, $ArCH_2$), 2.23 (s, 3H, CH_3) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): δ_C = 201.2 (CS), 137.8 ($\underline{C}_{Ar}CH_2$), 135.7 ($\underline{C}_{Ar}CH_3$), 129.4 (CH_{Ar}), 128.9 (CH_{Ar}), 66.4 (OCH_2), 66.2 (OCH_2), 50.5 (NCH_2), 50.1 (NCH_2), 44.4 ($\underline{C}H_2CS$), 34.9 ($Ar\underline{C}H_2$), 21.2 ($Ar\underline{C}H_3$) ppm; **Elemental analysis**: Found: C, 67.40; H, 7.71. Calc. for $C_{14}H_{19}NOS$: C, 67.43; H, 7.68%; **IR-ATR**: 2962, 2916, 2847, 1512, 1484, 1462, 1427, 1284, 1236, 1110, 1095 cm^{-1}.

3-(4-methoxylphenyl)propionic acid thiomorpholide (**2p**)



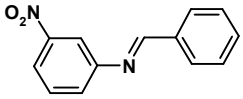
Mp 90-91 °C (from MeOH) (lit.,[12] 89-90 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): **δ_H** = 7.11-7.15 (m, 2H, Ar-H), 6.79-6.83 (m, 2H, Ar-H), 4.16 (t, J_{H-H} = 4.8 Hz, 2H, CH_2), 3.68 (s, 3H, OMe), 3.67 (t, J_{H-H} = 6 Hz, 2H, CH_2), 3.58 (t, J_{H-H} = 5.2 Hz, 2H, CH_2), 3.43 (t, J_{H-H} = 5.2 Hz, 2H, CH_2), 2.98-3.02 (m, 2H, CH_2CS), 2.83-2.87 (m, 2H, $ArCH_2$) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): **δ_C =** 201.8 (CS), 158.3 (CO_{Ar}), 132.8 (C_{Ar}), 129.9 (CH_{Ar}), 114.3 (CH_{Ar}), 66.4 (OCH_2), 66.2 (OCH_2), 55.5 (OCH_3), 50.4 (NCH_2), 50.1 (NCH_2), 44.6 ($\underline{C}H_2CS$), 34.4 ($Ar\underline{C}H_2$) ppm; **Elemental analysis**: Found: C, 63.32; H, 7.25. Calc. for $C_{14}H_{19}NO_2S$: C, 63.36; H, 7.22%; **IR-ATR**: 2969, 2862, 2827, 1608, 1511, 1484, 1431, 1245, 1113, 1093, 983 cm^{-1}.

N-(4-Nitrophenyl)phenylmethanimine (**4a**)



Mp 140-141 °C (from *i*-PrOH) (lit.,[13] 144 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): **δ_H** = 8.62 (s, 1H, CH), 8.22-8.26 (m, 2H, Ar-H), 7.92-7.95 (m, 2H, Ar-H), 7.49-7.58 (m, 3H, Ar-H), 7.38-7.42 (m, 2H, Ar-H) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): **δ_C =** 164.4 (CHN), 158.1 ($C_{Ar}N$), 145.5 ($C_{Ar}NO_2$), 135.9 ($\underline{C}_{Ar}CH$), 132.9 ($C_{Ar}H$), 129.8 ($C_{Ar}H$), 129.5 ($C_{Ar}H$), 125.5 ($C_{Ar}H$), 122.4 ($C_{Ar}H$) ppm; **Elemental analysis**: Found: C, 69.07; H, 4.50. Calc. for $C_{13}H_{10}N_2O_2$: C, 69.02; H, 4.46%; **IR-ATR**: 1623, 1596, 1570, 1506, 1475, 1451, 1317, 1285, 1191, 1162, 1102 cm^{-1}.

N-(4-Nitrophenyl)phenylmethanimine (**4b**)



Mp 65-66 °C (from *i*-PrOH) (lit.,[13] 66 °C); **^{1}H NMR** (DMSO-d_6, 298 K, 400 MHz): **δ_H** = 8.72 (s, 1H, CH), 8.06-8.09 (m, 1H, Ar-H), 8.03-8.04 (m, 1H, Ar-H), 7.94-7.96 (m, 2H, Ar-H), 7.66-7.72 (m, 2H, Ar-H), 7.49-7.56 (m, 3H, Ar-H) ppm; **^{13}C NMR** (DMSO-d_6, 298 K, 100 MHz): **δ_C** = 164.2 (CHN), 153.1 ($C_{Ar}N$), 149.1 ($C_{Ar}NO_2$), 136.1 ($\underline{C}_{Ar}CH$), 132.7 ($C_{Ar}H$), 131.2 ($C_{Ar}H$), 129.6 ($C_{Ar}H$), 129.5 ($C_{Ar}H$), 128.8 ($C_{Ar}H$), 120.9 ($C_{Ar}H$), 115.8 ($C_{Ar}H$) ppm; **Elemental analysis**: Found: C, 69.00; H, 4.39. Calc. for $C_{13}H_{10}N_2O_2$: C, 69.02; H, 4.46%; **IR-ATR**: 1629, 1577, 1508, 1470, 1453, 1349, 1312, 1193, 1172, 1073 cm^{-1}.

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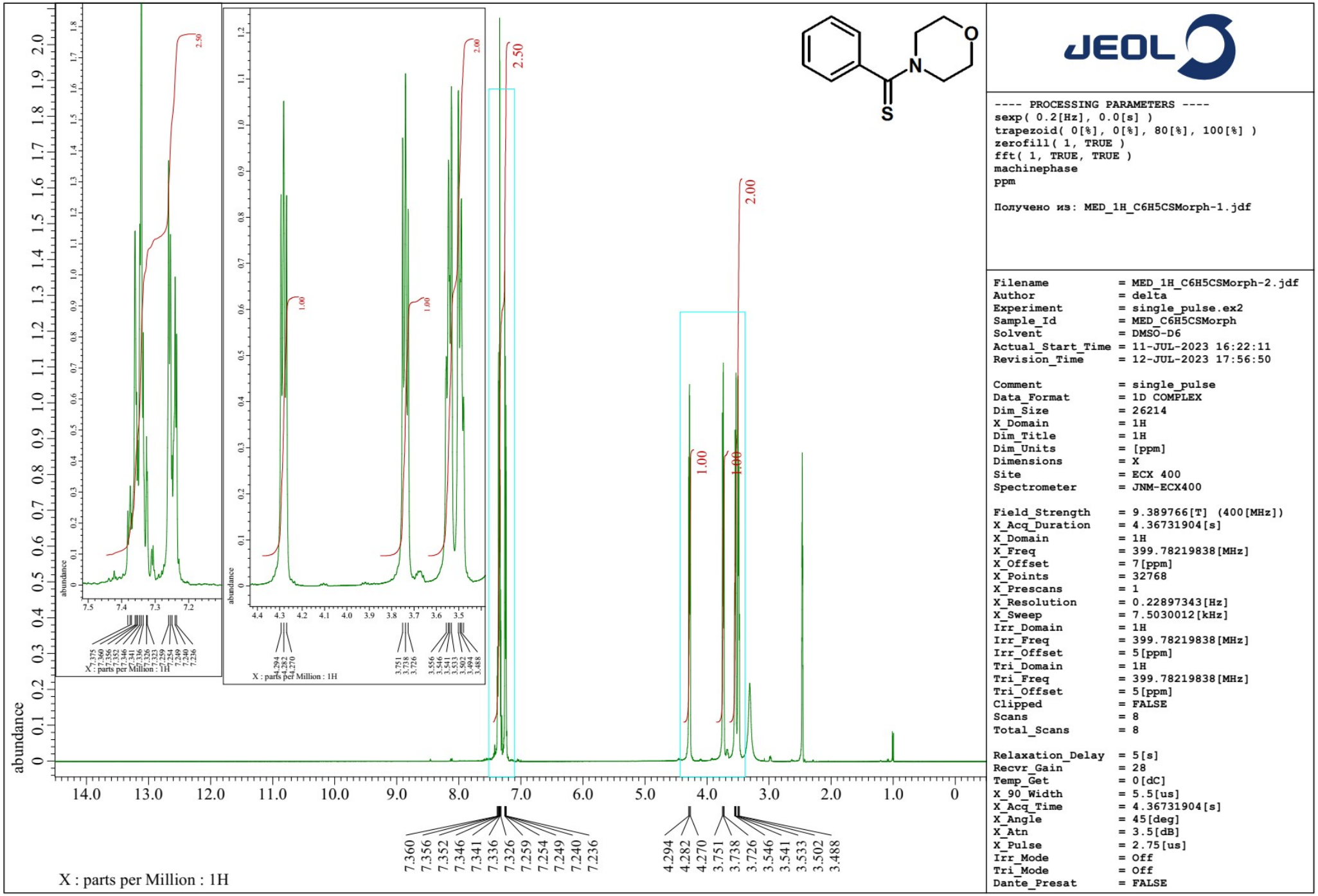


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fft( 1, TRUE, TRUE )
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ppm

Получено из: MED_1H_C6H5CSMorph-1.jdf
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Revision_Time       = 12-JUL-2023 17:56:50

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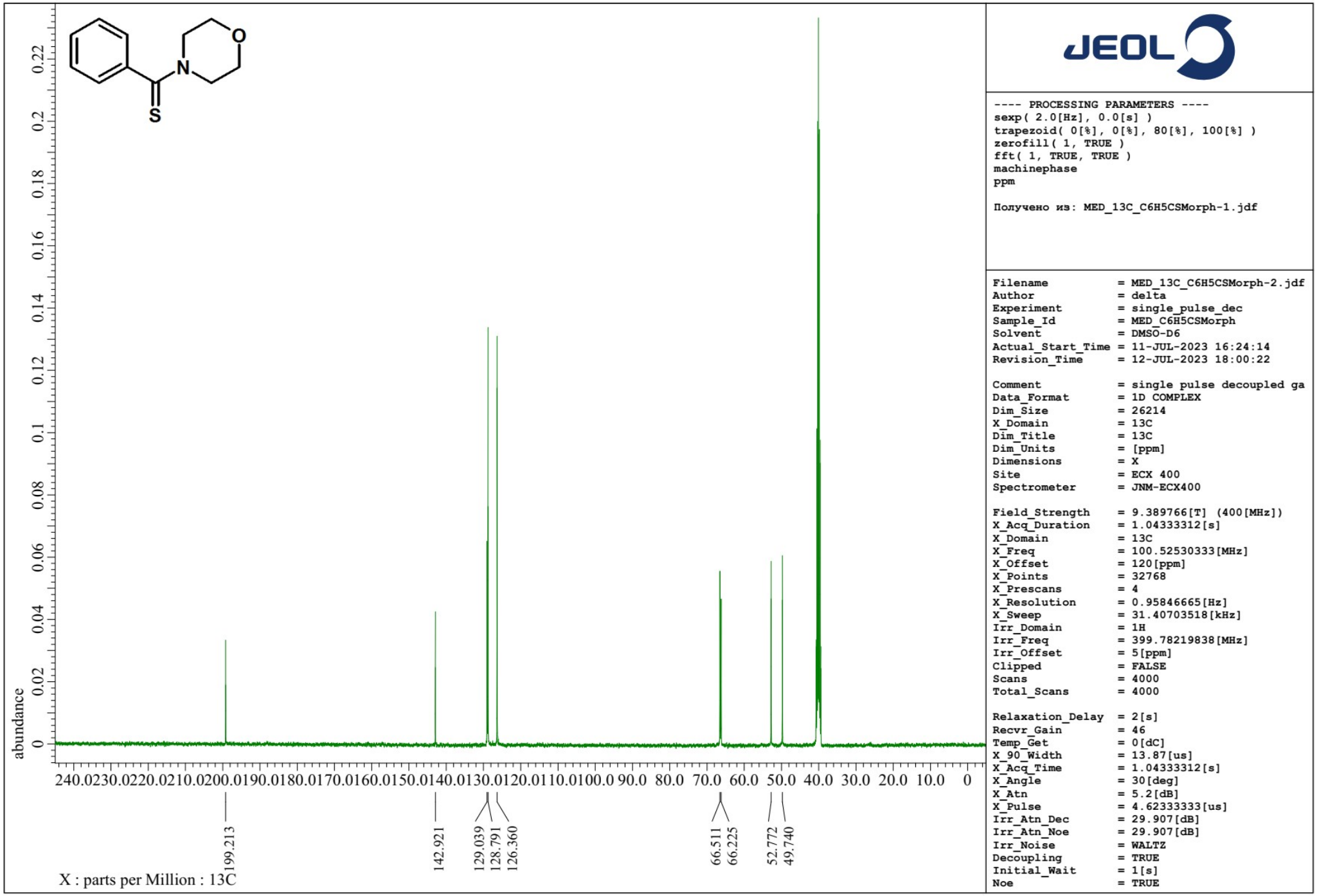


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Получено из: MED_13C_C6H5CSMorph-1.jdf
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Spectrometer      = JNM-ECX400

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Noe               = TRUE
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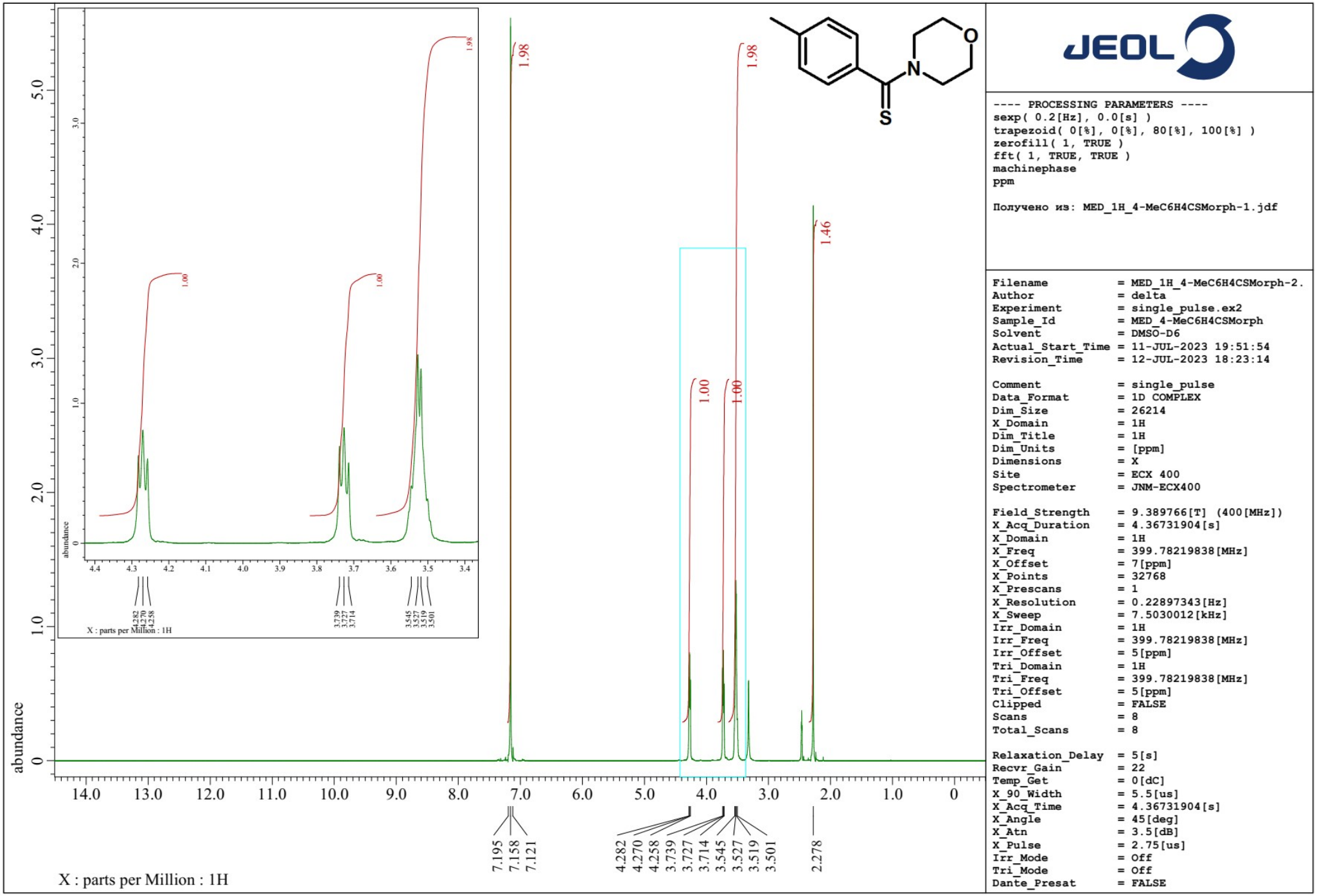
JEOL
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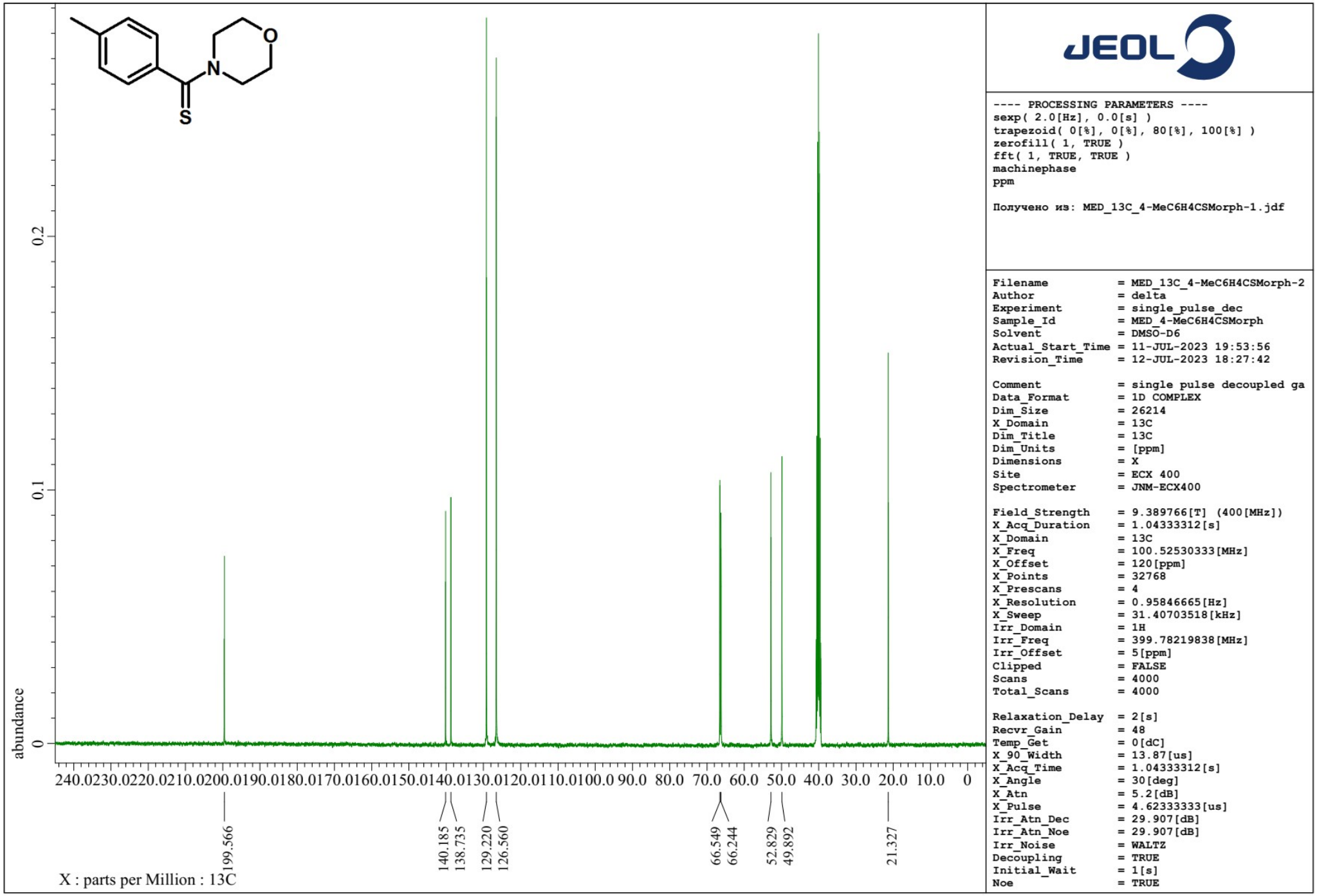
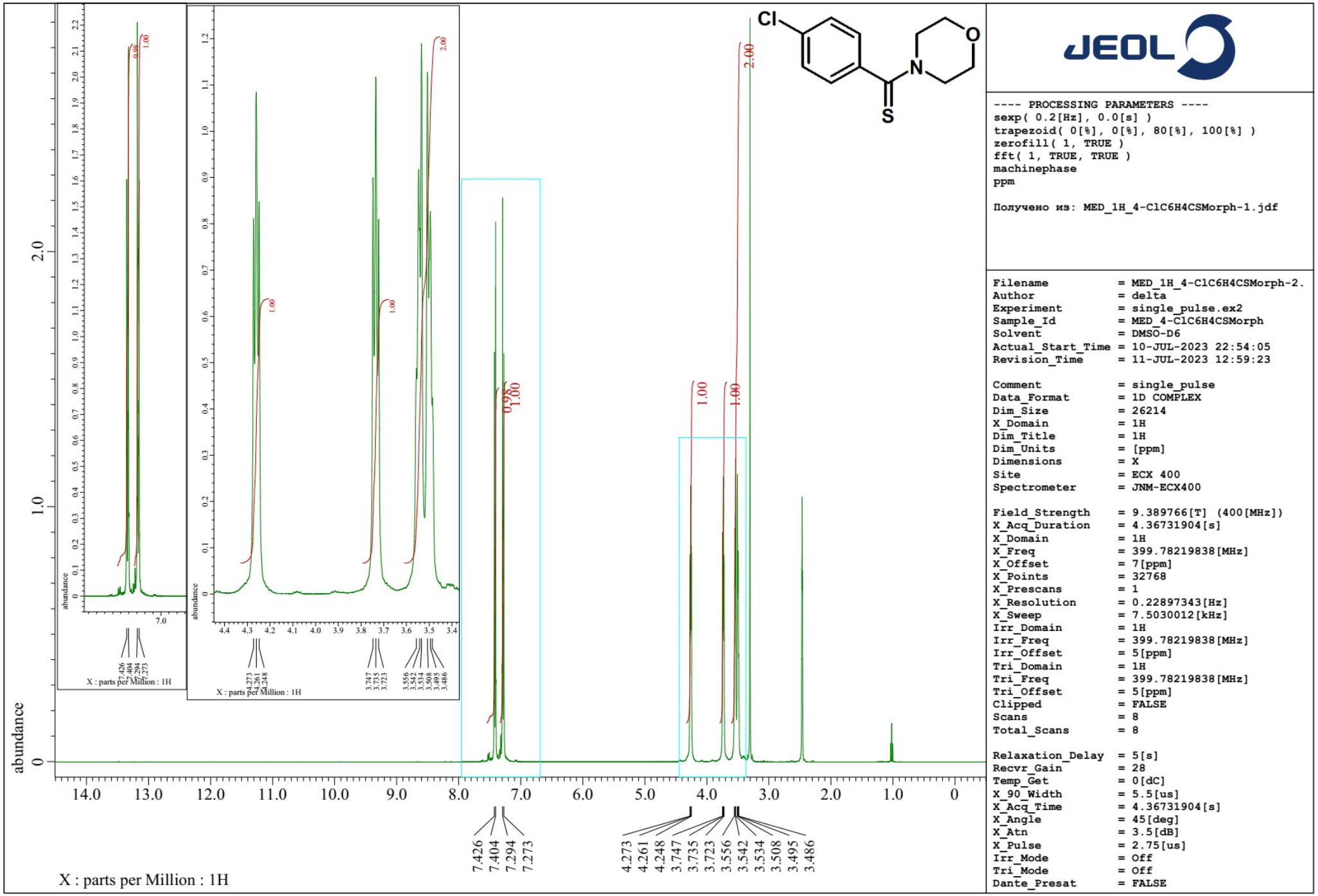
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 7[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 22
Temp_Get = 0[dC]
X_90_Width = 5.5[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 2.75[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
abundance
X : parts per Million : 1H
7.195
7.158
7.121
4.282
4.270
4.258
3.739
3.727
3.714
3.545
3.527
3.519
3.501
2.278
1.98
1.98
1.46
1.00
1.00
1.00

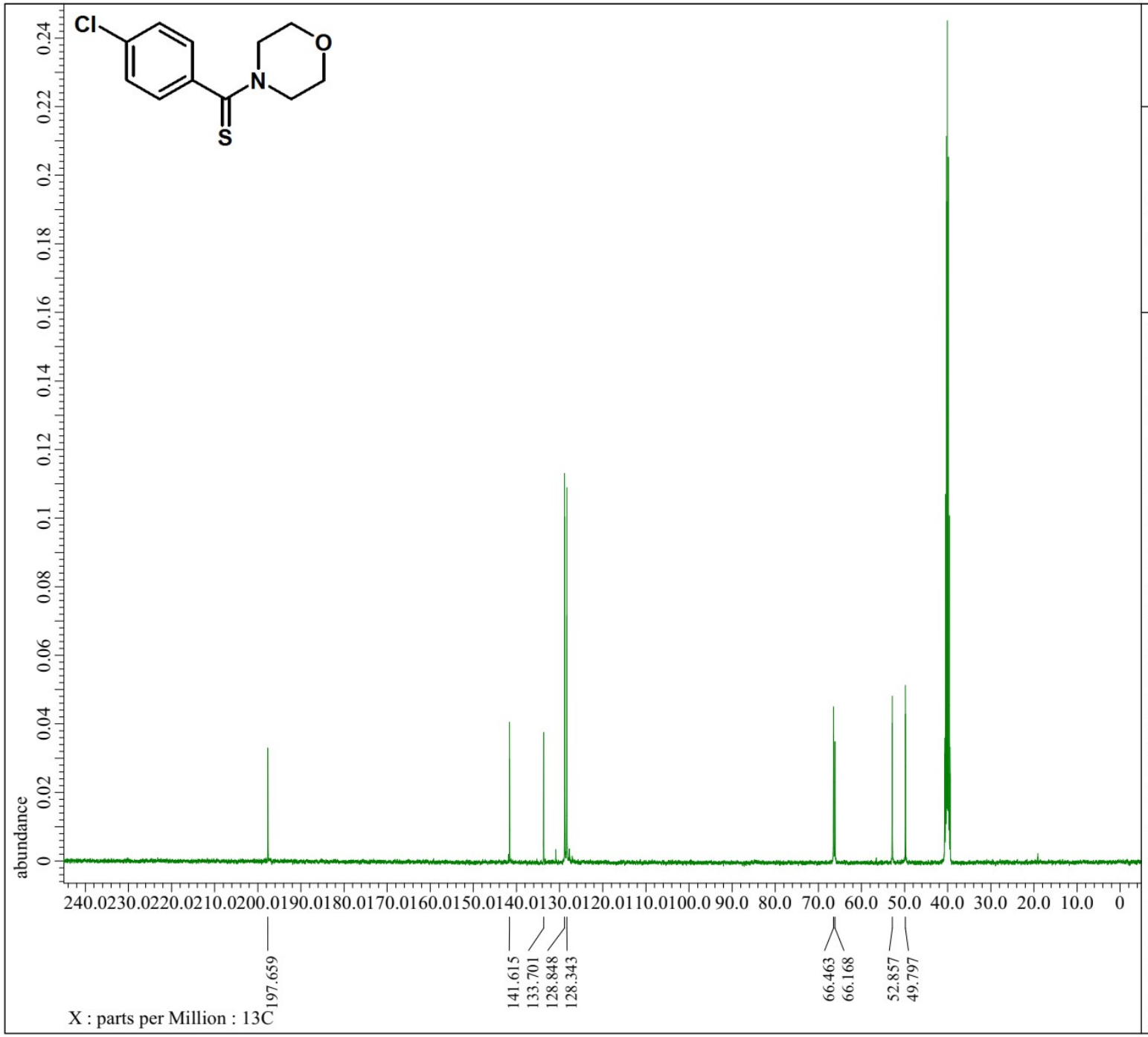

O
N
S
abundance
0
0.1
0.2
240.0 230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
199.566
140.185
138.735
129.220
126.560
66.549
66.244
52.829
49.892
21.327
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Получено из: MED_13C_4-MeC6H4CSMorph-1.jdf
Filename = MED_13C_4-MeC6H4CSMorph-2
Author = delta
Experiment = single_pulse_dec
Sample_Id = MED_4-MeC6H4CSMorph
Solvent = DMSO-D6
Actual_Start_Time = 11-JUL-2023 19:53:56
Revision_Time = 12-JUL-2023 18:27:42
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 120[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 4000
Total_Scans = 4000
Relaxation_Delay = 2[s]
Recvr_Gain = 48
Temp_Get = 0[dC]
X_90_Width = 13.87[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 5.2[dB]
X_Pulse = 4.62333333[us]
Irr_Atn_Dec = 29.907[dB]
Irr_Atn_Noe = 29.907[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE



JEOL

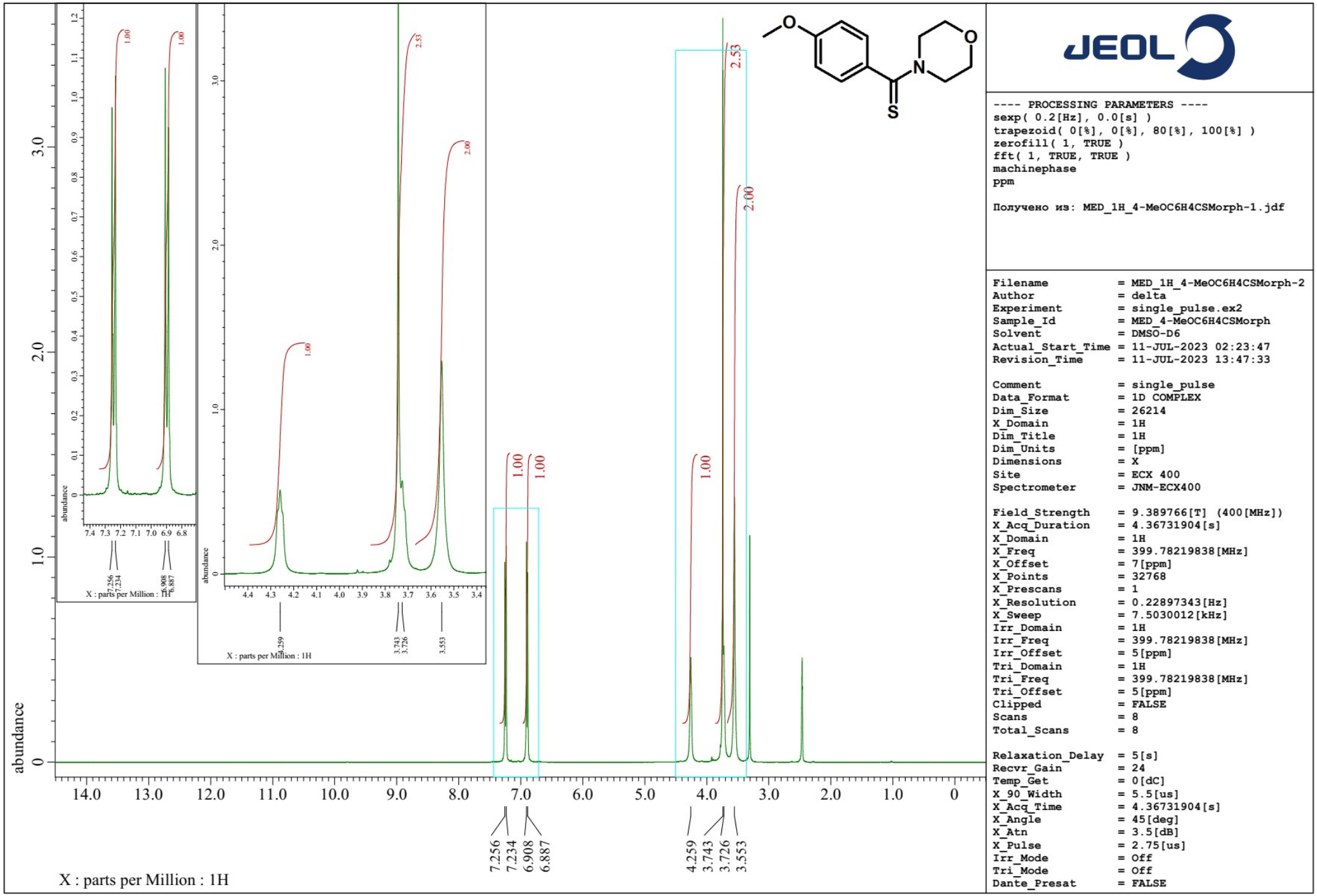
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_1H_4-ClC6H4CSMorph-1.jdf
```

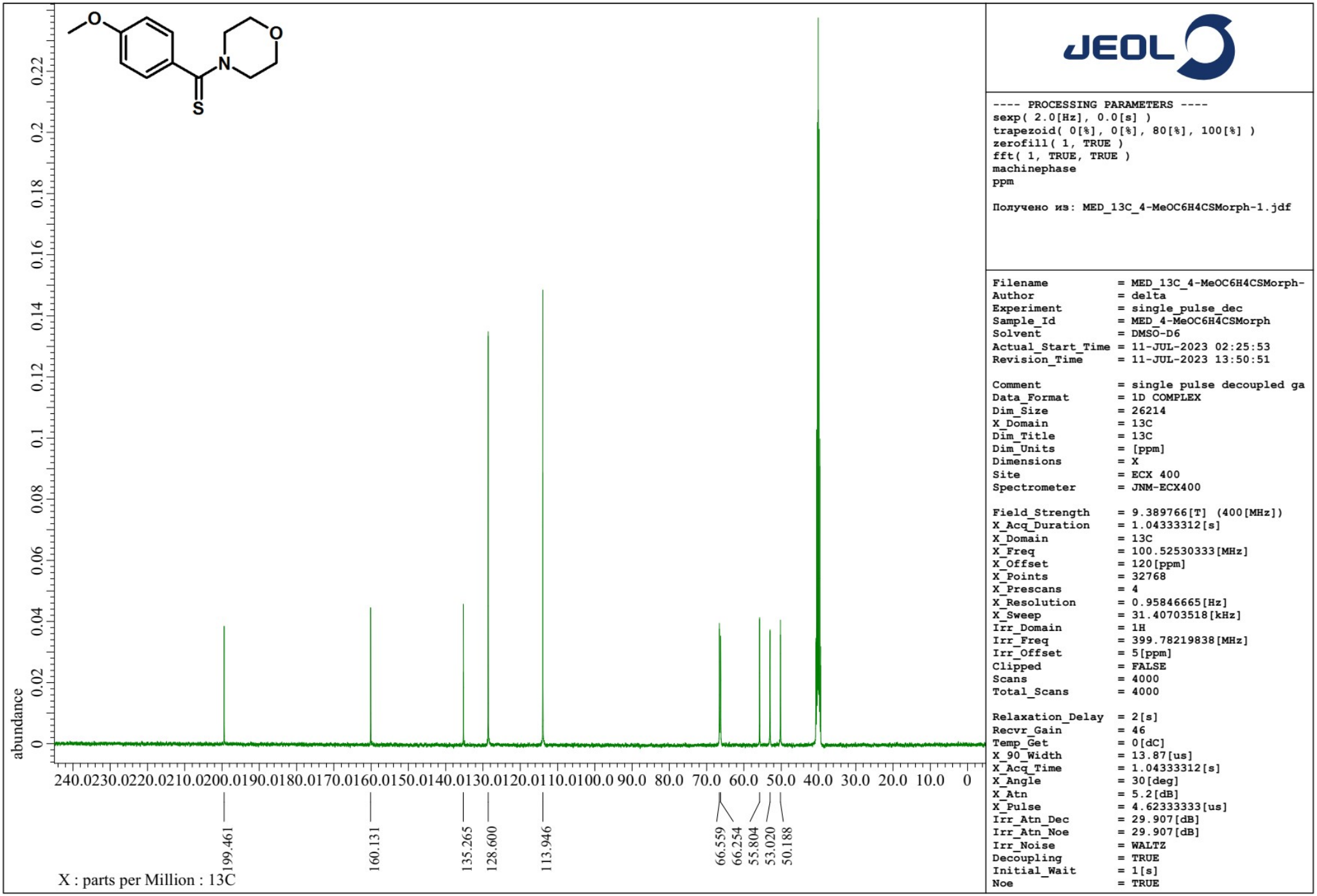
```
Filename            = MED_1H_4-ClC6H4CSMorph-2.
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = MED_4-ClC6H4CSMorph
Solvent             = DMSO-D6
Actual_Start_Time   = 10-JUL-2023 22:54:05
Revision_Time       = 11-JUL-2023 12:59:23

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 1H
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400
Spectrometer        = JNM-ECX400

Field_Strength      = 9.389766[T] (400[MHz])
X_Acq_Duration      = 4.36731904[s]
X_Domain            = 1H
X_Freq              = 399.78219838[MHz]
X_Offset            = 7[ppm]
X_Points            = 32768
X_Prescans          = 1
X_Resolution        = 0.22897343[Hz]
X_Sweep             = 7.5030012[kHz]
Irr_Domain          = 1H
Irr_Freq            = 399.78219838[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = 1H
Tri_Freq            = 399.78219838[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 28
Temp_Get            = 0[dC]
X_90_Width          = 5.5[us]
X_Acq_Time          = 4.36731904[s]
X_Angle             = 45[deg]
X_Atn               = 3.5[dB]
X_Pulse             = 2.75[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_13C_4-ClC6H4CSMorph-1.jdf
```

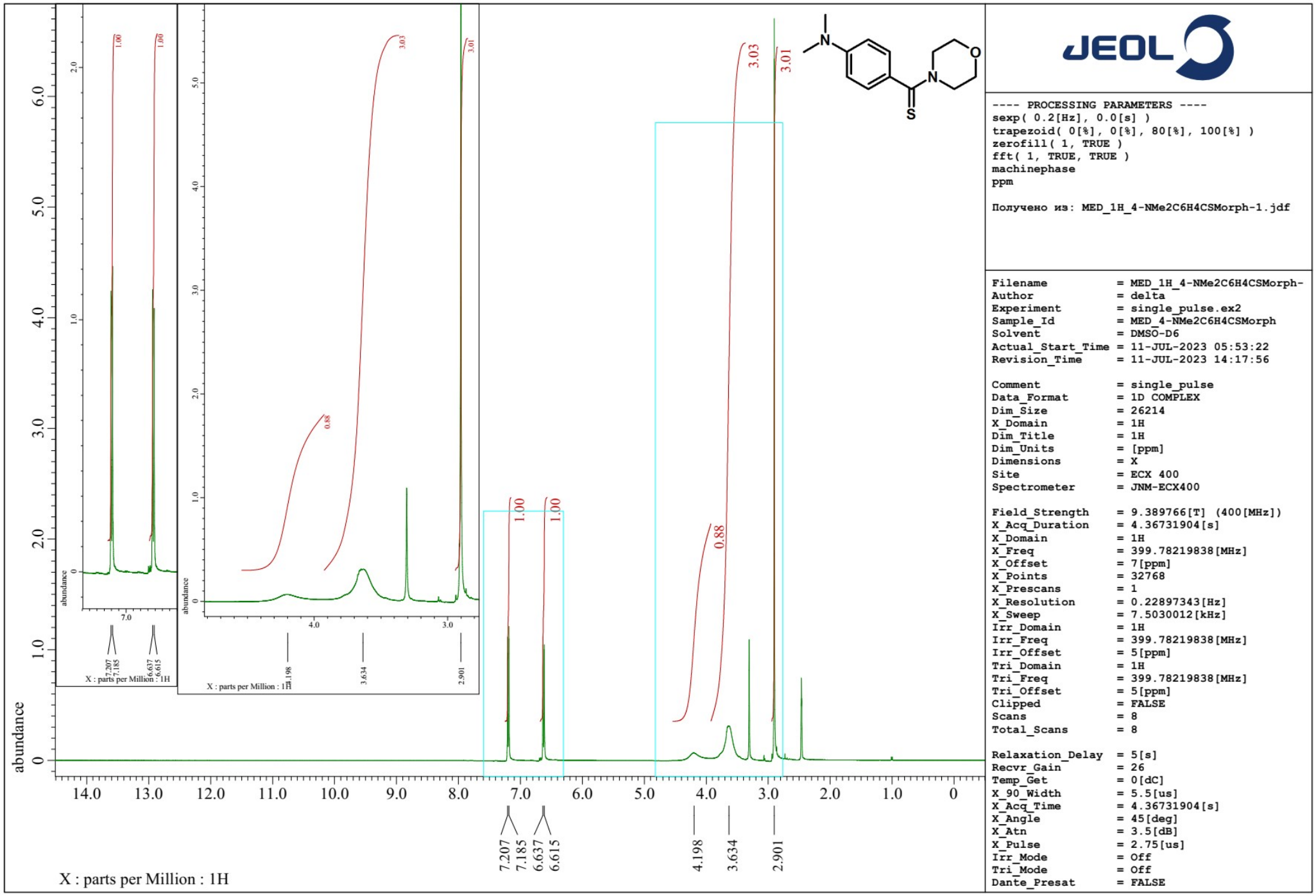
```
Filename          = MED_13C_4-ClC6H4CSMorph-2
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = MED_4-ClC6H4CSMorph
Solvent           = DMSO-D6
Actual_Start_Time = 10-JUL-2023 22:56:07
Revision_Time     = 11-JUL-2023 12:42:40

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = 13C
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 120[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 4000
Total_Scans       = 4000

Relaxation_Delay  = 2[s]
Recvr_Gain        = 46
Temp_Get          = 0[dC]
X_90_Width        = 13.87[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 5.2[dB]
X_Pulse           = 4.62333333[us]
Irr_Atn_Dec       = 29.907[dB]
Irr_Atn_Noe       = 29.907[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
```


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Получено из: MED_1H_4-MeOC6H4CSMorph-1.jdf
Filename = MED_1H_4-MeOC6H4CSMorph-2
Author = delta
Experiment = single_pulse.ex2
Sample_Id = MED_4-MeOC6H4CSMorph
Solvent = DMSO-D6
Actual_Start_Time = 11-JUL-2023 02:23:47
Revision_Time = 11-JUL-2023 13:47:33
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 7[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 24
Temp_Get = 0[dC]
X_90_Width = 5.5[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 2.75[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
abundance
X : parts per Million : 1H
7.256
7.234
6.908
6.887
4.259
3.743
3.726
3.553
1.00
2.53
2.00



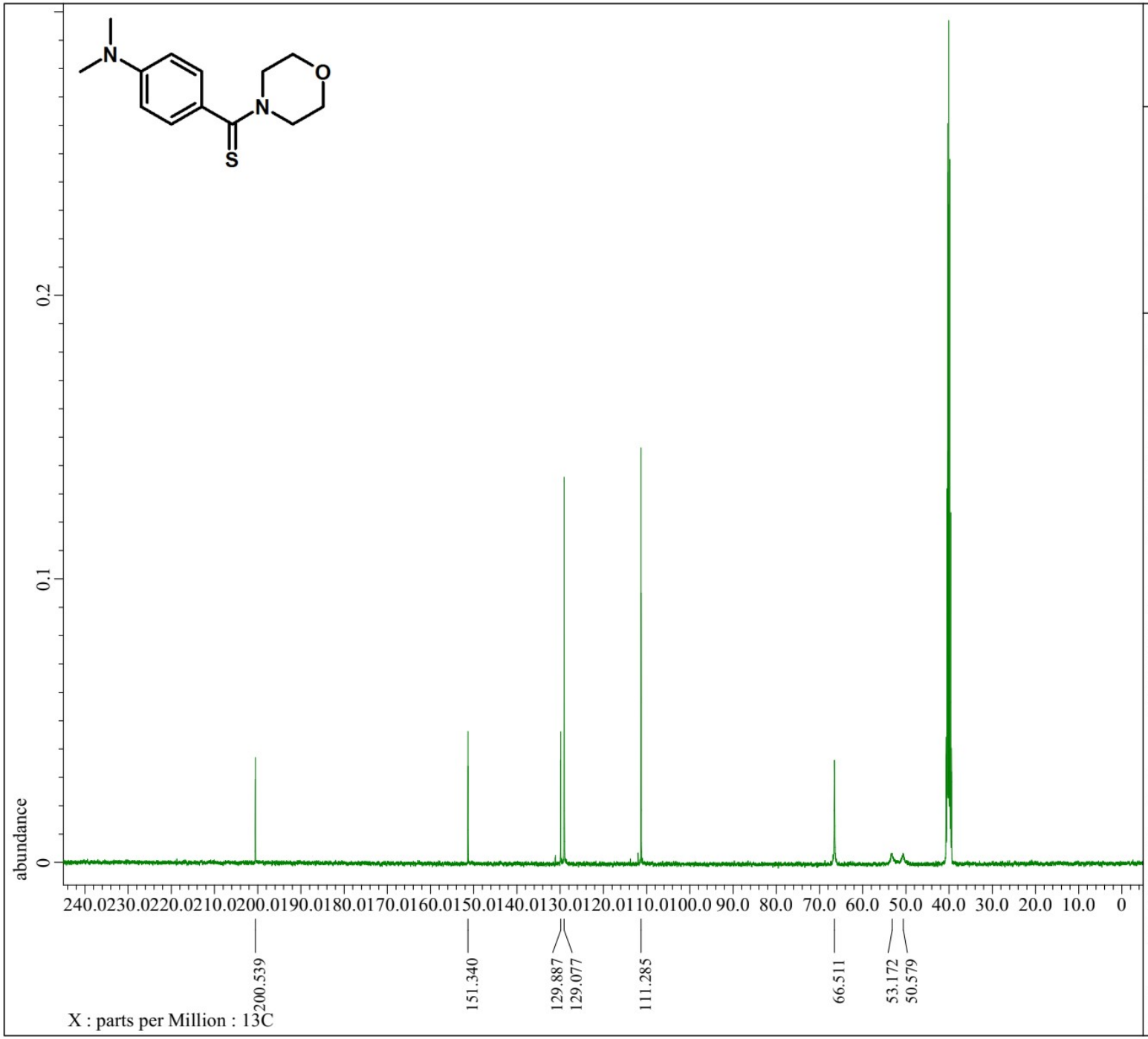

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_13C_4-MeOC6H4CSMorph-1.jdf
```

```
Filename          = MED_13C_4-MeOC6H4CSMorph-
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = MED_4-MeOC6H4CSMorph
Solvent           = DMSO-D6
Actual_Start_Time = 11-JUL-2023 02:25:53
Revision_Time     = 11-JUL-2023 13:50:51

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = 13C
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 120[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 4000
Total_Scans       = 4000

Relaxation_Delay  = 2[s]
Recvr_Gain        = 46
Temp_Get          = 0[dC]
X_90_Width        = 13.87[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 5.2[dB]
X_Pulse           = 4.62333333[us]
Irr_Atn_Dec       = 29.907[dB]
Irr_Atn_Noe       = 29.907[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
```



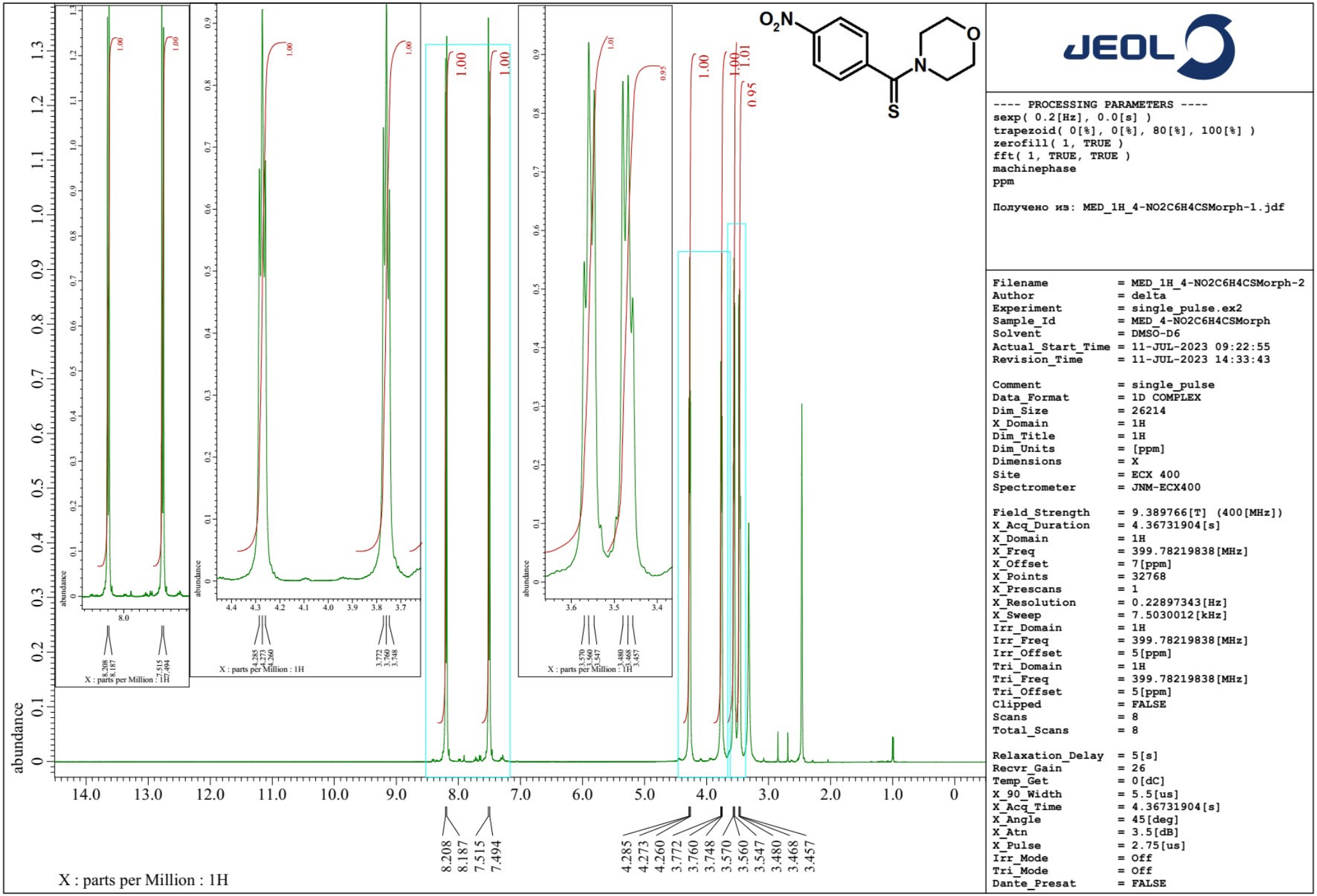

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_1H_4-NMe2C6H4CSMorph-1.jdf
```

```
Filename            = MED_1H_4-NMe2C6H4CSMorph-
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = MED_4-NMe2C6H4CSMorph
Solvent             = DMSO-D6
Actual_Start_Time   = 11-JUL-2023 05:53:22
Revision_Time       = 11-JUL-2023 14:17:56

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 1H
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400
Spectrometer        = JNM-ECX400

Field_Strength      = 9.389766[T] (400[MHz])
X_Acq_Duration      = 4.36731904[s]
X_Domain            = 1H
X_Freq              = 399.78219838[MHz]
X_Offset            = 7[ppm]
X_Points            = 32768
X_Prescans          = 1
X_Resolution        = 0.22897343[Hz]
X_Sweep             = 7.5030012[kHz]
Irr_Domain          = 1H
Irr_Freq            = 399.78219838[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = 1H
Tri_Freq            = 399.78219838[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 26
Temp_Get            = 0[dC]
X_90_Width          = 5.5[us]
X_Acq_Time          = 4.36731904[s]
X_Angle             = 45[deg]
X_Atn               = 3.5[dB]
X_Pulse             = 2.75[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_13C_4-NMe2C6H4CSMorph-1.jdf
```

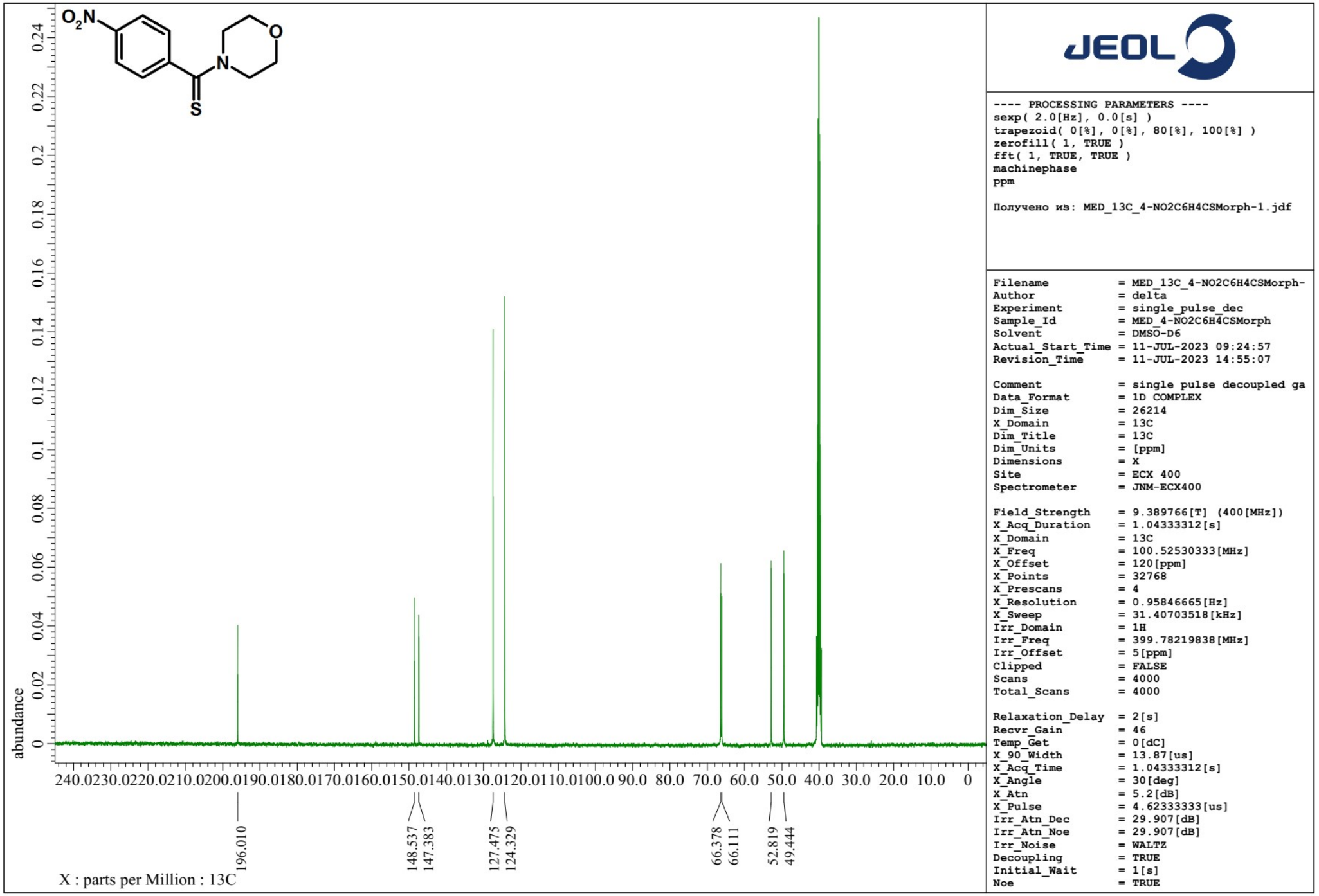
```
Filename           = MED_13C_4-NMe2C6H4CSMorph
Author             = delta
Experiment         = single_pulse_dec
Sample_Id          = MED_4-NMe2C6H4CSMorph
Solvent            = DMSO-D6
Actual_Start_Time  = 11-JUL-2023 05:55:30
Revision_Time      = 11-JUL-2023 14:22:16

Comment            = single pulse decoupled ga
Data_Format        = 1D COMPLEX
Dim_Size           = 26214
X_Domain           = 13C
Dim_Title          = 13C
Dim_Units          = [ppm]
Dimensions         = X
Site               = ECX 400
Spectrometer       = JNM-ECX400

Field_Strength     = 9.389766[T] (400[MHz])
X_Acq_Duration     = 1.04333312[s]
X_Domain           = 13C
X_Freq             = 100.52530333[MHz]
X_Offset           = 120[ppm]
X_Points           = 32768
X_Prescans         = 4
X_Resolution       = 0.95846665[Hz]
X_Sweep            = 31.40703518[kHz]
Irr_Domain         = 1H
Irr_Freq           = 399.78219838[MHz]
Irr_Offset         = 5[ppm]
Clipped            = FALSE
Scans              = 4000
Total_Scans        = 4000

Relaxation_Delay   = 2[s]
Recvr_Gain         = 48
Temp_Get           = 0[dC]
X_90_Width         = 13.87[us]
X_Acq_Time         = 1.04333312[s]
X_Angle            = 30[deg]
X_Atn              = 5.2[dB]
X_Pulse            = 4.62333333[us]
Irr_Atn_Dec        = 29.907[dB]
Irr_Atn_Noe        = 29.907[dB]
Irr_Noise          = WALTZ
Decoupling         = TRUE
Initial_Wait       = 1[s]
Noe                = TRUE
```



JEOL

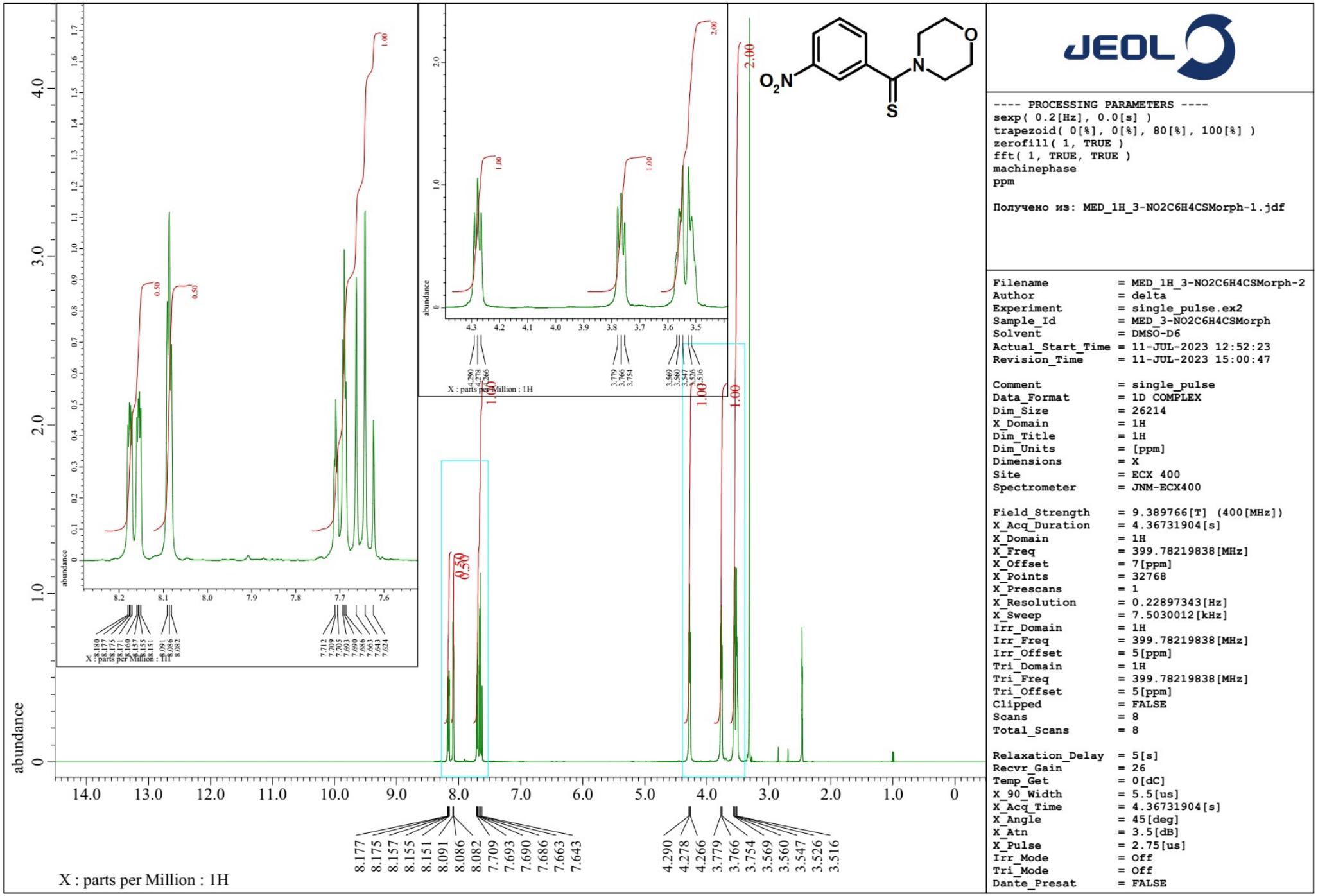
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_1H_4-NO2C6H4CSMorph-1.jdf
```

```
Filename            = MED_1H_4-NO2C6H4CSMorph-2
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = MED_4-NO2C6H4CSMorph
Solvent             = DMSO-D6
Actual_Start_Time   = 11-JUL-2023 09:22:55
Revision_Time       = 11-JUL-2023 14:33:43

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 1H
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400
Spectrometer        = JNM-ECX400

Field_Strength      = 9.389766[T] (400[MHz])
X_Acq_Duration      = 4.36731904[s]
X_Domain            = 1H
X_Freq              = 399.78219838[MHz]
X_Offset            = 7[ppm]
X_Points            = 32768
X_Prescans          = 1
X_Resolution        = 0.22897343[Hz]
X_Sweep             = 7.5030012[kHz]
Irr_Domain          = 1H
Irr_Freq            = 399.78219838[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = 1H
Tri_Freq            = 399.78219838[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 26
Temp_Get            = 0[dC]
X_90_Width          = 5.5[us]
X_Acq_Time          = 4.36731904[s]
X_Angle             = 45[deg]
X_Atn               = 3.5[dB]
X_Pulse             = 2.75[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_13C_4-NO2C6H4CSMorph-1.jdf
```

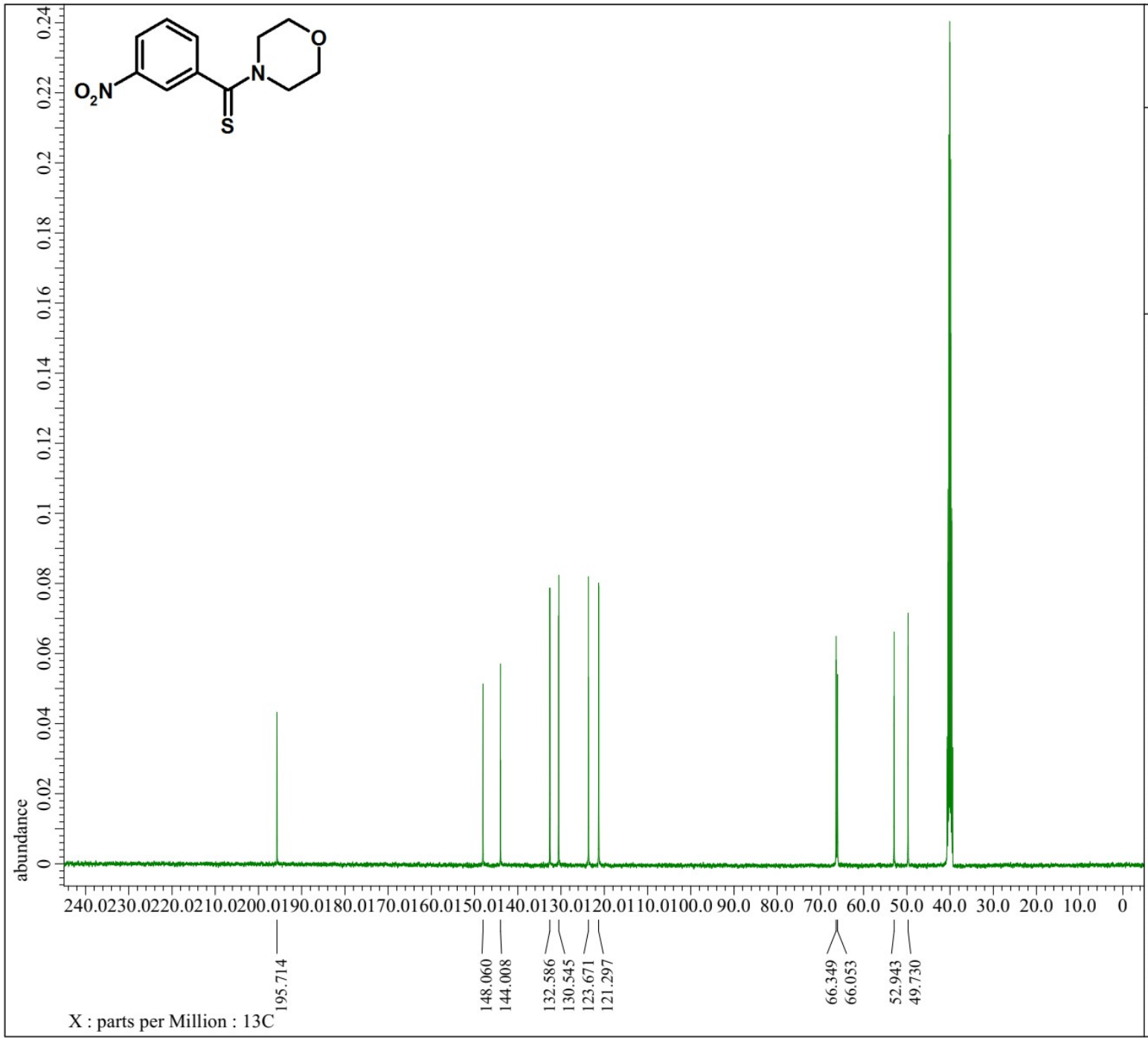
```
Filename          = MED_13C_4-NO2C6H4CSMorph-
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = MED_4-NO2C6H4CSMorph
Solvent           = DMSO-D6
Actual_Start_Time = 11-JUL-2023 09:24:57
Revision_Time     = 11-JUL-2023 14:55:07

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = 13C
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 120[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 4000
Total_Scans       = 4000

Relaxation_Delay  = 2[s]
Recvr_Gain        = 46
Temp_Get          = 0[dC]
X_90_Width        = 13.87[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 5.2[dB]
X_Pulse           = 4.62333333[us]
Irr_Atn_Dec       = 29.907[dB]
Irr_Atn_Noe       = 29.907[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
```



JEOL

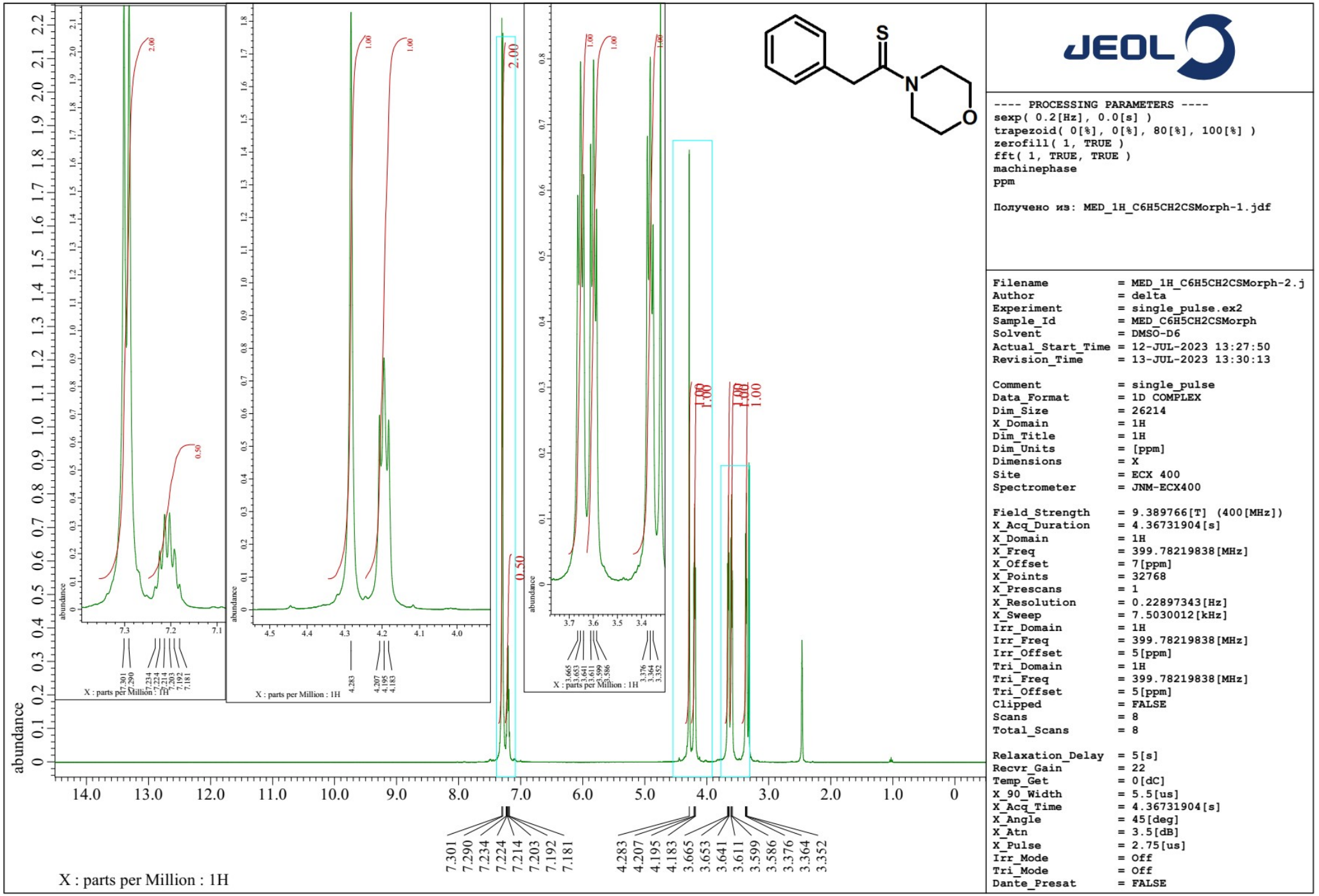
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_1H_3-NO2C6H4CSMorph-1.jdf
```

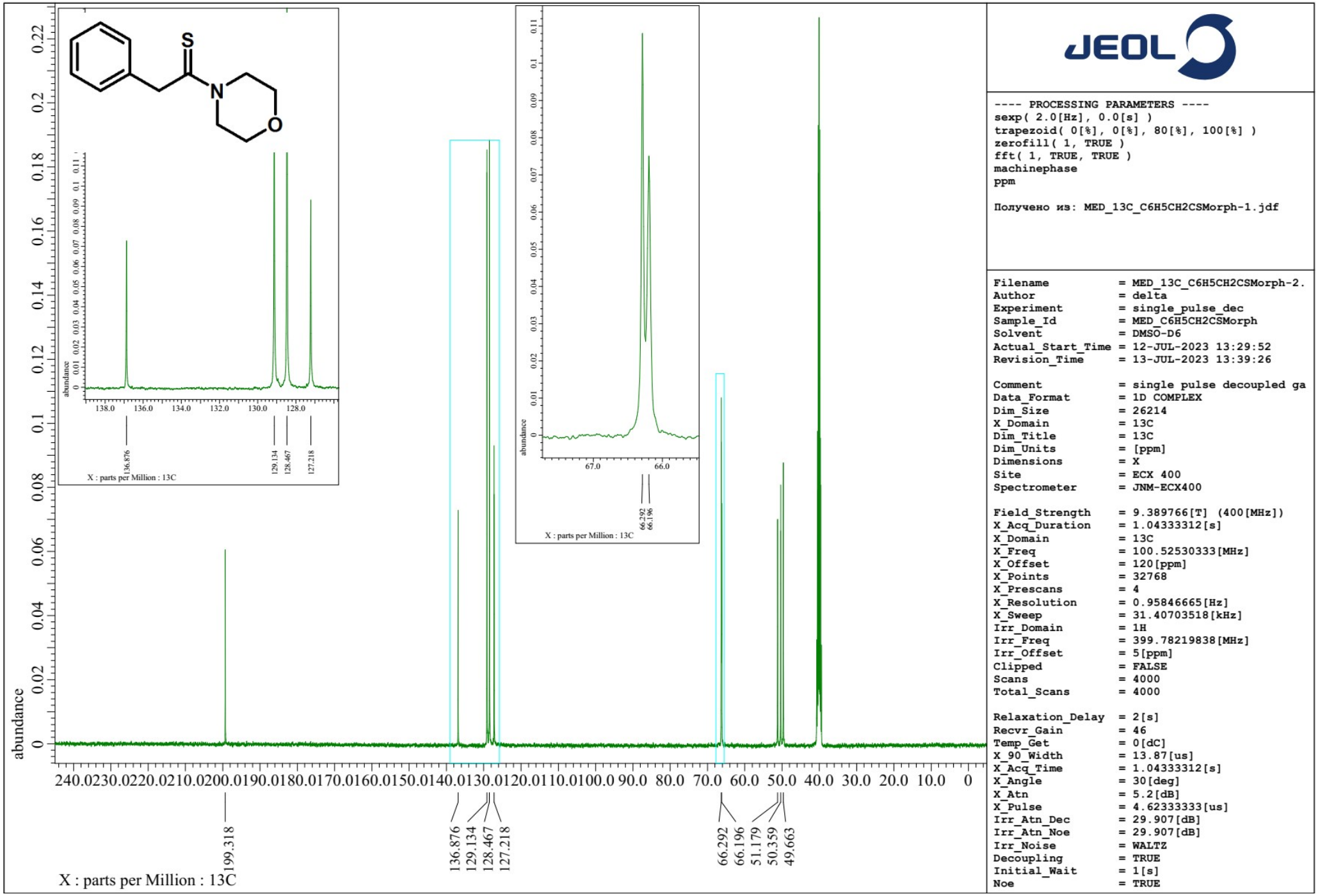
```
Filename            = MED_1H_3-NO2C6H4CSMorph-2
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = MED_3-NO2C6H4CSMorph
Solvent             = DMSO-D6
Actual_Start_Time   = 11-JUL-2023 12:52:23
Revision_Time       = 11-JUL-2023 15:00:47

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 1H
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400
Spectrometer        = JNM-ECX400

Field_Strength      = 9.389766[T] (400[MHz])
X_Acq_Duration      = 4.36731904[s]
X_Domain            = 1H
X_Freq              = 399.78219838[MHz]
X_Offset            = 7[ppm]
X_Points            = 32768
X_Prescans          = 1
X_Resolution        = 0.22897343[Hz]
X_Sweep             = 7.5030012[kHz]
Irr_Domain          = 1H
Irr_Freq            = 399.78219838[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = 1H
Tri_Freq            = 399.78219838[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 26
Temp_Get            = 0[dC]
X_90_Width          = 5.5[us]
X_Acq_Time          = 4.36731904[s]
X_Angle             = 45[deg]
X_Atn               = 3.5[dB]
X_Pulse             = 2.75[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_13C_3-NO2C6H4CSMorph-1.jdf
```

```
Filename          = MED_13C_3-NO2C6H4CSMorph-
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = MED_3-NO2C6H4CSMorph
Solvent           = DMSO-D6
Actual_Start_Time = 11-JUL-2023 12:54:26
Revision_Time     = 11-JUL-2023 15:26:04

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = 13C
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 120[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 4000
Total_Scans       = 4000

Relaxation_Delay  = 2[s]
Recvr_Gain        = 46
Temp_Get          = 0[dC]
X_90_Width        = 13.87[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 5.2[dB]
X_Pulse           = 4.62333333[us]
Irr_Atn_Dec       = 29.907[dB]
Irr_Atn_Noe       = 29.907[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
```

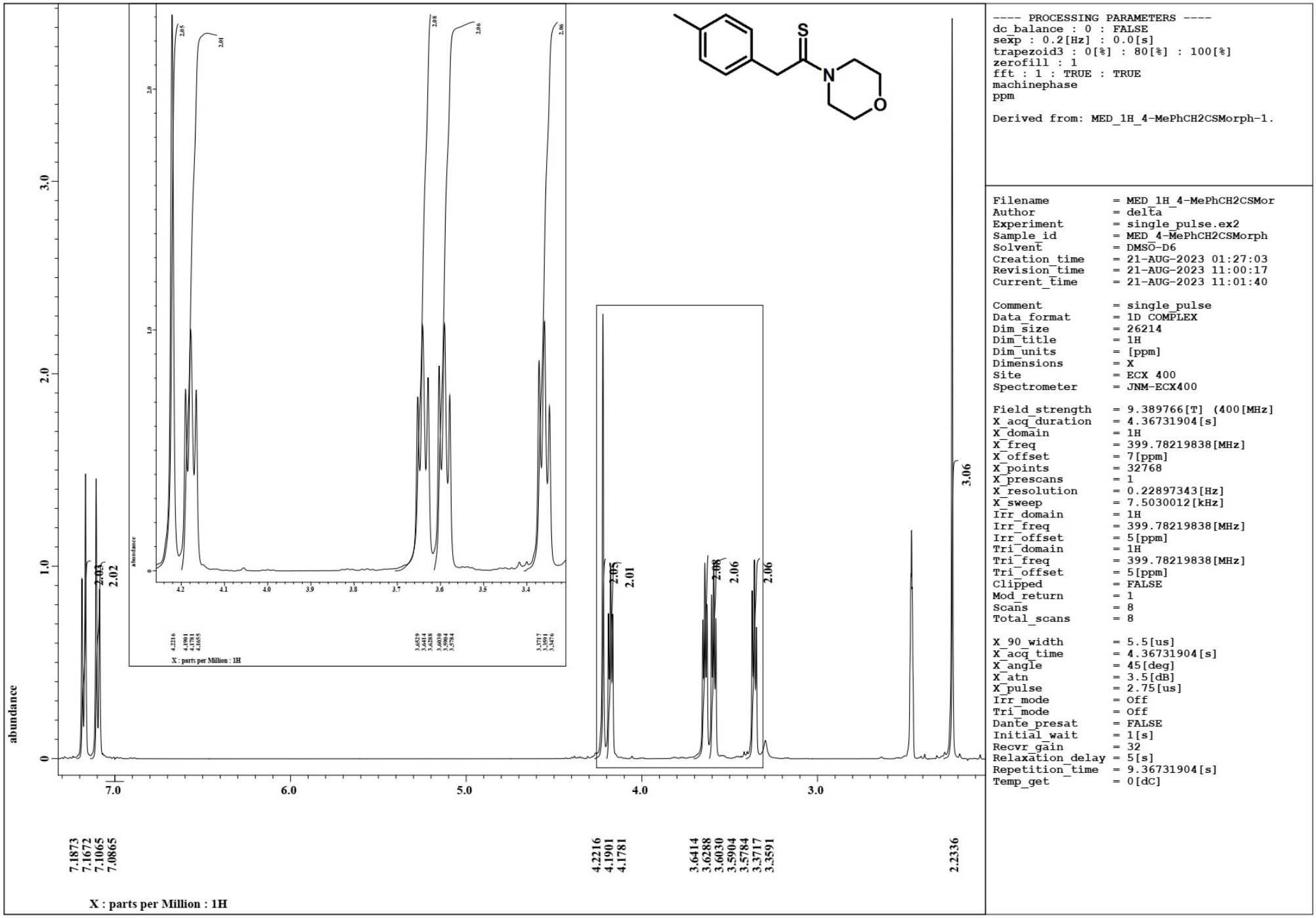

JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Получено из: MED_1H_C6H5CH2CSMorph-1.jdf
Filename = MED_1H_C6H5CH2CSMorph-2.j
Author = delta
Experiment = single_pulse.ex2
Sample_Id = MED_C6H5CH2CSMorph
Solvent = DMSO-D6
Actual_Start_Time = 12-JUL-2023 13:27:50
Revision_Time = 13-JUL-2023 13:30:13
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 7[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 22
Temp_Get = 0[dC]
X_90_Width = 5.5[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 2.75[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
abundance
X : parts per Million : 1H
7.301
7.290
7.234
7.224
7.214
7.203
7.192
7.181
4.283
4.207
4.195
4.183
3.665
3.653
3.641
3.611
3.599
3.586
3.376
3.364
3.352
S
N
O



JEOL

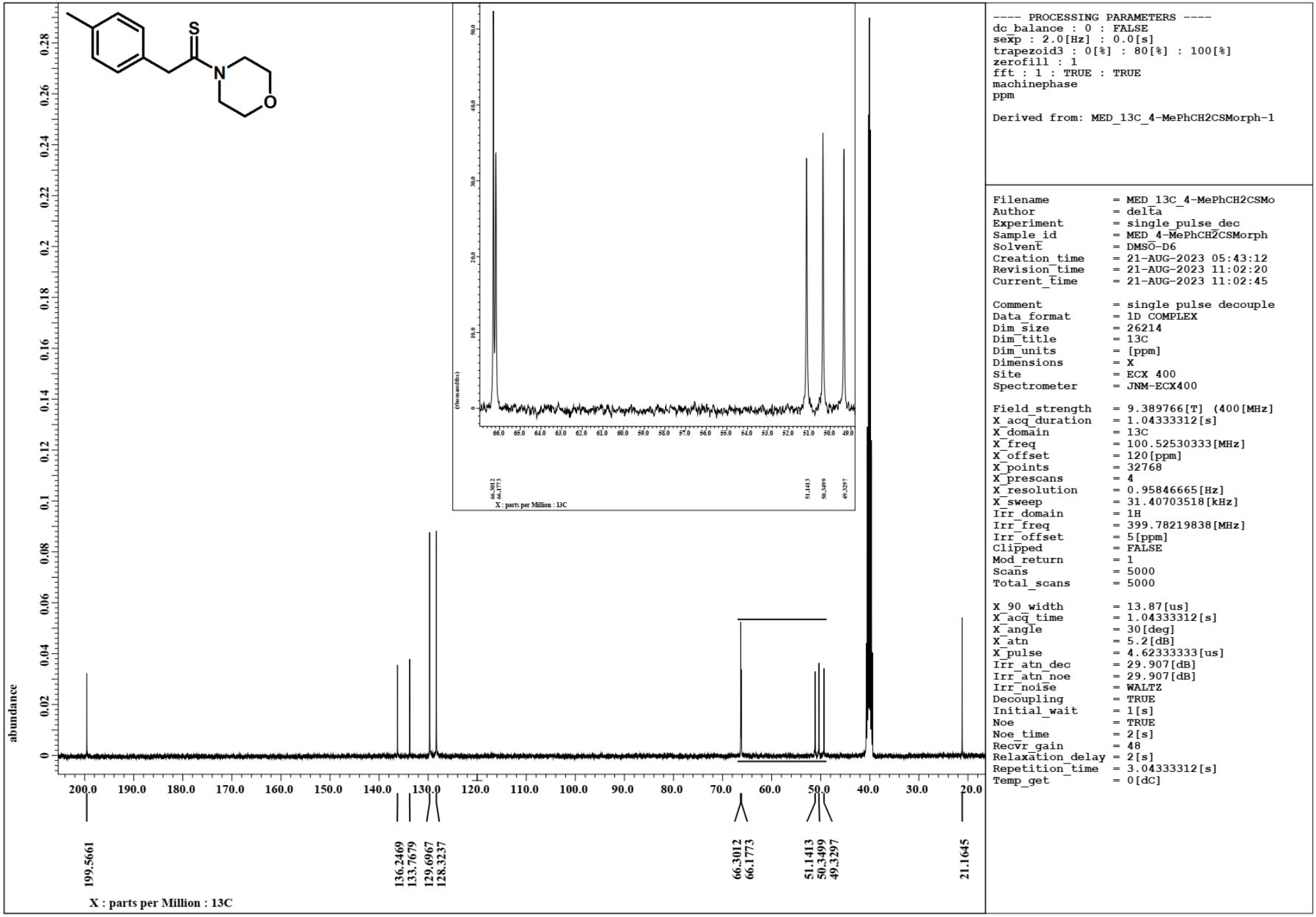
```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_13C_C6H5CH2CSMorph-1.jdf
```

```
Filename          = MED_13C_C6H5CH2CSMorph-2.
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = MED_C6H5CH2CSMorph
Solvent           = DMSO-D6
Actual_Start_Time = 12-JUL-2023 13:29:52
Revision_Time     = 13-JUL-2023 13:39:26

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = 13C
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 120[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 4000
Total_Scans       = 4000

Relaxation_Delay  = 2[s]
Recvr_Gain        = 46
Temp_Get          = 0[dC]
X_90_Width        = 13.87[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 5.2[dB]
X_Pulse           = 4.62333333[us]
Irr_Atn_Dec       = 29.907[dB]
Irr_Atn_Noe       = 29.907[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
```



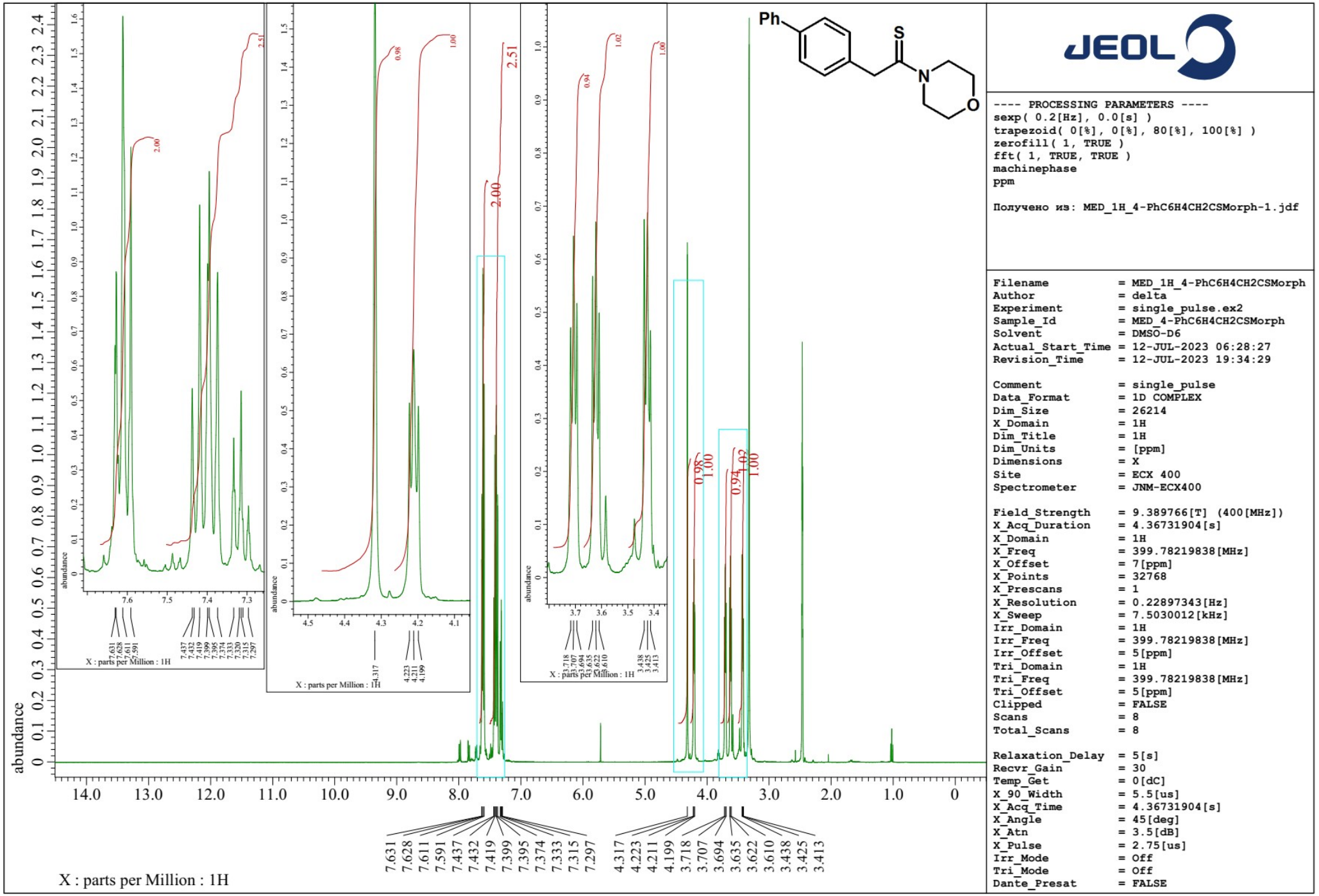

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: MED_1H_4-MePhCH2CSMorph-1.
```

```
Filename          = MED_1H_4-MePhCH2CSMor
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = MED_4-MePhCH2CSMorph
Solvent           = DMSO-D6
Creation_time     = 21-AUG-2023 01:27:03
Revision_time     = 21-AUG-2023 11:00:17
Current_time      = 21-AUG-2023 11:01:40

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 4.36731904[s]
X_domain          = 1H
X_freq            = 399.78219838[MHz]
X_offset          = 7[ppm]
X_points          = 32768
X_prescans        = 1
X_resolution      = 0.22897343[Hz]
X_sweep           = 7.5030012[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 399.78219838[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 5.5[us]
X_acq_time        = 4.36731904[s]
X_angle           = 45[deg]
X_atn             = 3.5[dB]
X_pulse           = 2.75[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 32
Relaxation_delay  = 5[s]
Repetition_time   = 9.36731904[s]
Temp_get          = 0[dC]
```




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: MED_13C_4-MePhCH2CSMorph-1
```

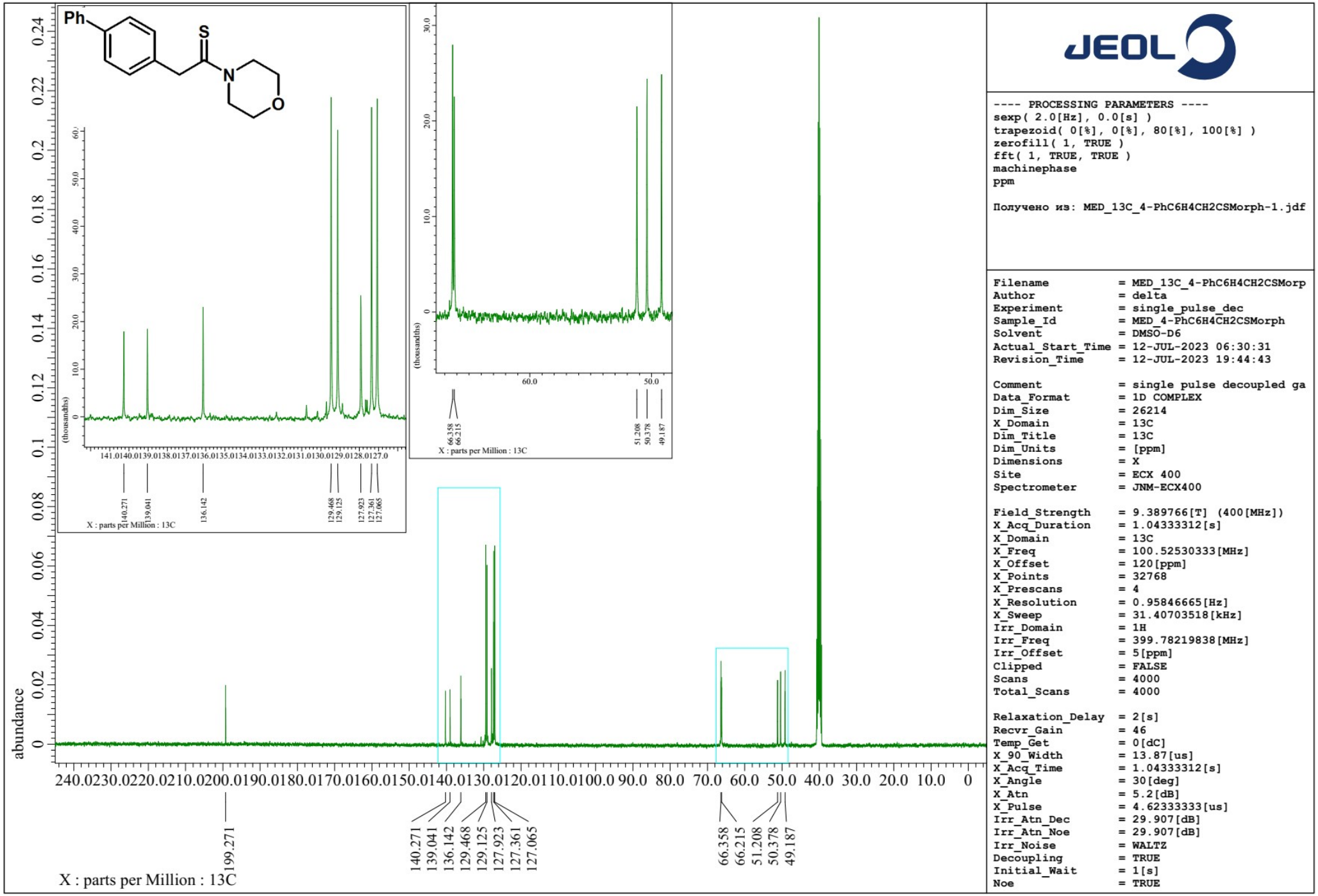
```
Filename          = MED_13C_4-MePhCH2CSMo
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = MED_4-MePhCH2CSMorph
Solvent           = DMSO-D6
Creation_time     = 21-AUG-2023 05:43:12
Revision_time     = 21-AUG-2023 11:02:20
Current_time      = 21-AUG-2023 11:02:45

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 120[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 5000
Total_scans       = 5000

X_90_width        = 13.87[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 5.2[dB]
X_pulse           = 4.62333333[us]
Irr_atn_dec       = 29.907[dB]
Irr_atn_noe       = 29.907[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 48
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 0[dC]
```



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_1H_4-PhC6H4CH2CSMorph-1.jdf
```

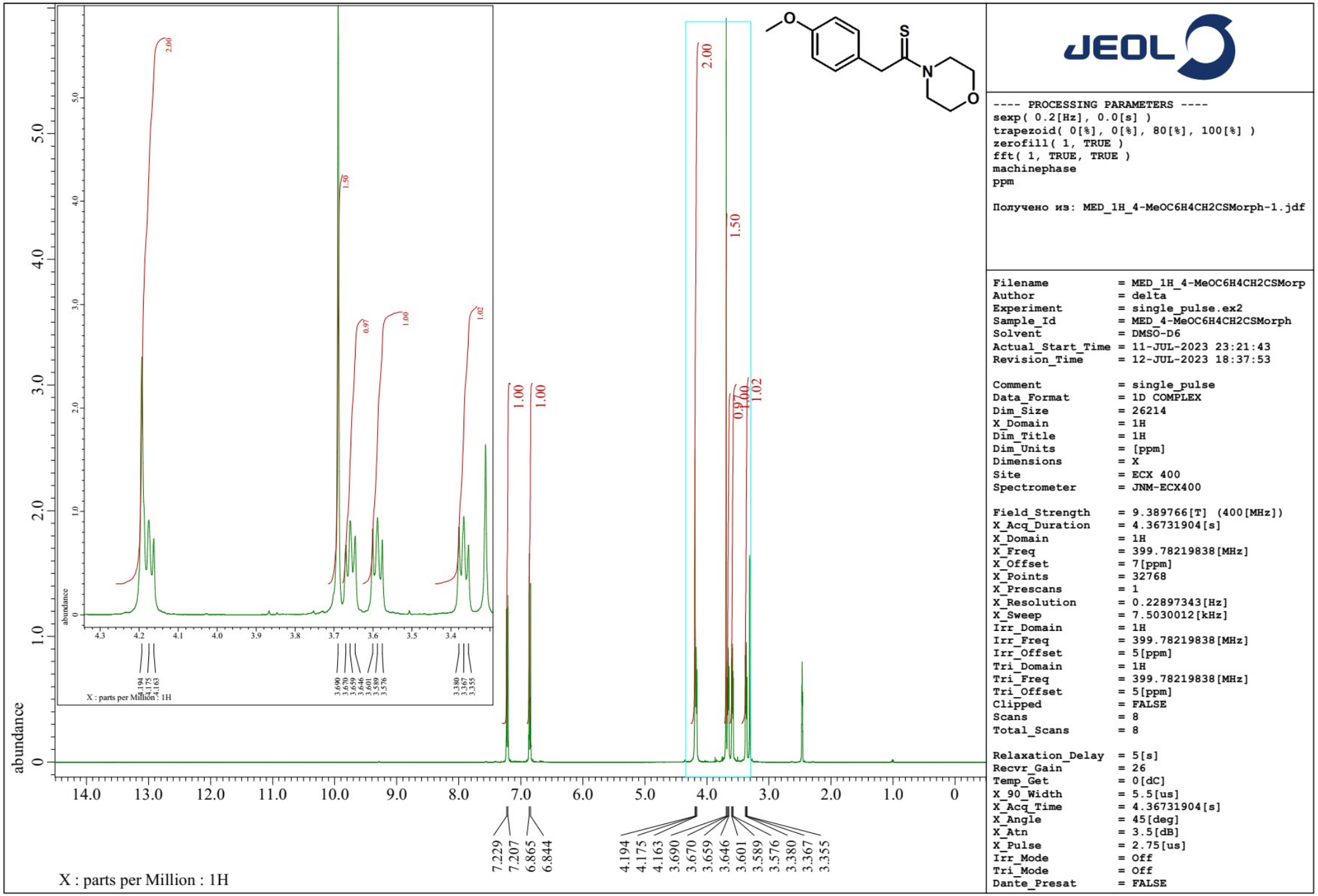
```
Filename            = MED_1H_4-PhC6H4CH2CSMorph
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = MED_4-PhC6H4CH2CSMorph
Solvent             = DMSO-D6
Actual_Start_Time   = 12-JUL-2023 06:28:27
Revision_Time       = 12-JUL-2023 19:34:29

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 1H
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400
Spectrometer        = JNM-ECX400

Field_Strength      = 9.389766[T] (400[MHz])
X_Acq_Duration      = 4.36731904[s]
X_Domain            = 1H
X_Freq              = 399.78219838[MHz]
X_Offset            = 7[ppm]
X_Points            = 32768
X_Prescans          = 1
X_Resolution        = 0.22897343[Hz]
X_Sweep             = 7.5030012[kHz]
Irr_Domain          = 1H
Irr_Freq            = 399.78219838[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = 1H
Tri_Freq            = 399.78219838[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 30
Temp_Get            = 0[dC]
X_90_Width          = 5.5[us]
X_Acq_Time          = 4.36731904[s]
X_Angle             = 45[deg]
X_Atn               = 3.5[dB]
X_Pulse             = 2.75[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
```

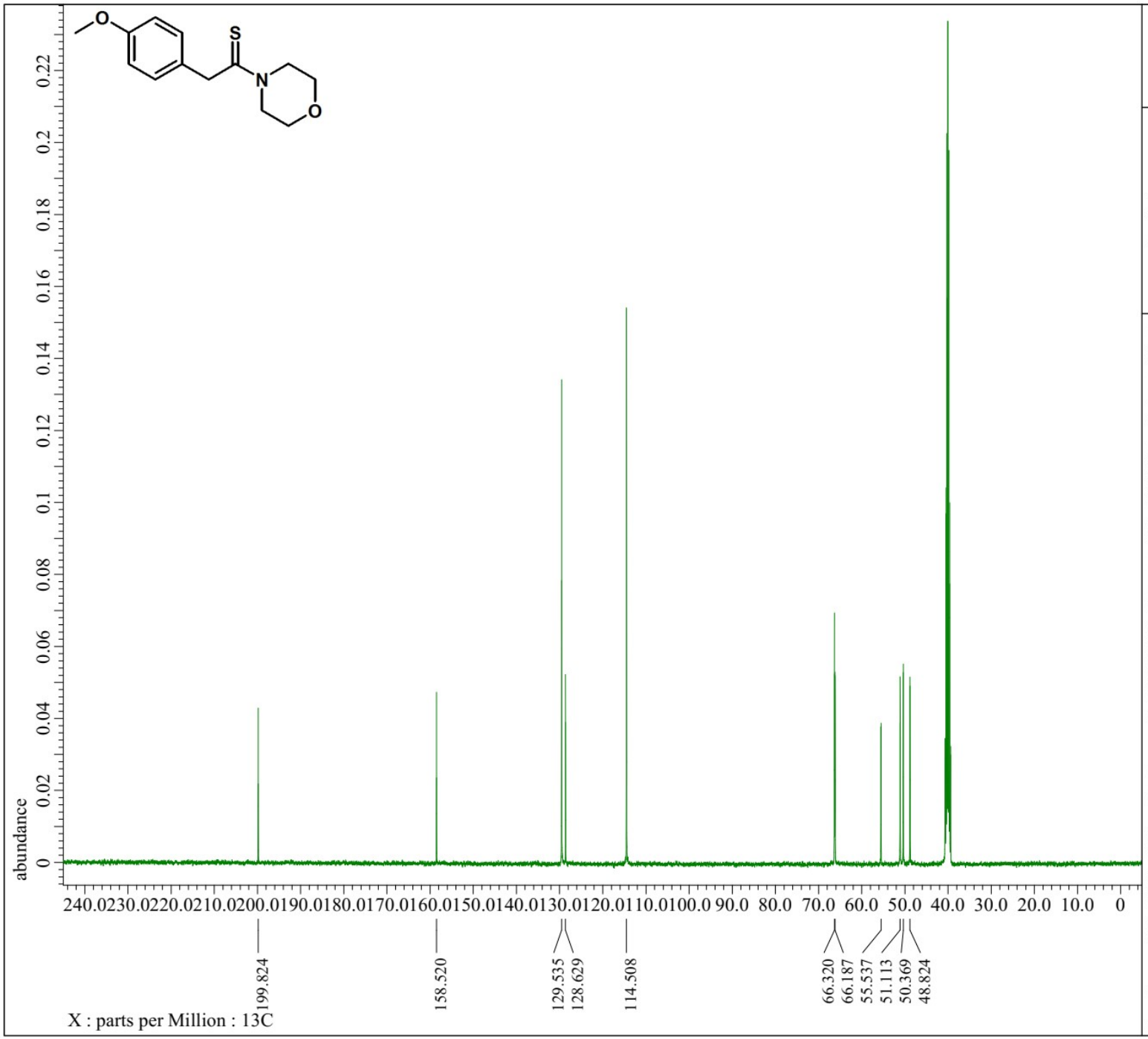


JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_13C_4-PhC6H4CH2CSMorph-1.jdf
```

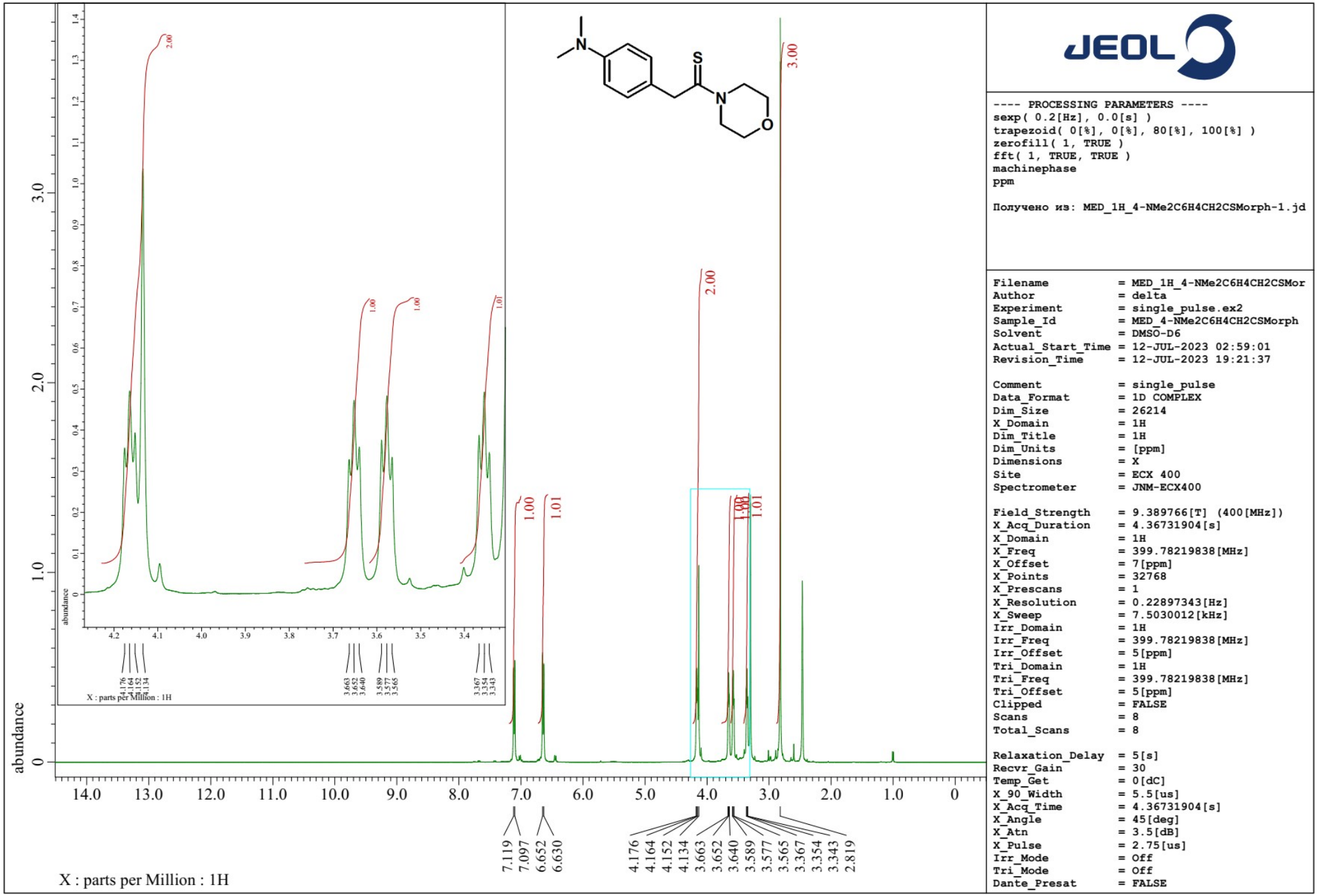
```
Filename            = MED_13C_4-PhC6H4CH2CSMorp
Author              = delta
Experiment          = single_pulse_dec
Sample_Id           = MED_4-PhC6H4CH2CSMorph
Solvent             = DMSO-D6
Actual_Start_Time   = 12-JUL-2023 06:30:31
Revision_Time       = 12-JUL-2023 19:44:43

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 13C
Dim_Title           = 13C
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400
Spectrometer        = JNM-ECX400

Field_Strength      = 9.389766[T] (400[MHz])
X_Acq_Duration      = 1.04333312[s]
X_Domain            = 13C
X_Freq              = 100.52530333[MHz]
X_Offset            = 120[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 0.95846665[Hz]
X_Sweep             = 31.40703518[kHz]
Irr_Domain          = 1H
Irr_Freq            = 399.78219838[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 4000
Total_Scans         = 4000

Relaxation_Delay    = 2[s]
Recvr_Gain          = 46
Temp_Get            = 0[dC]
X_90_Width          = 13.87[us]
X_Acq_Time          = 1.04333312[s]
X_Angle             = 30[deg]
X_Atn               = 5.2[dB]
X_Pulse             = 4.62333333[us]
Irr_Atn_Dec         = 29.907[dB]
Irr_Atn_Noe         = 29.907[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
```

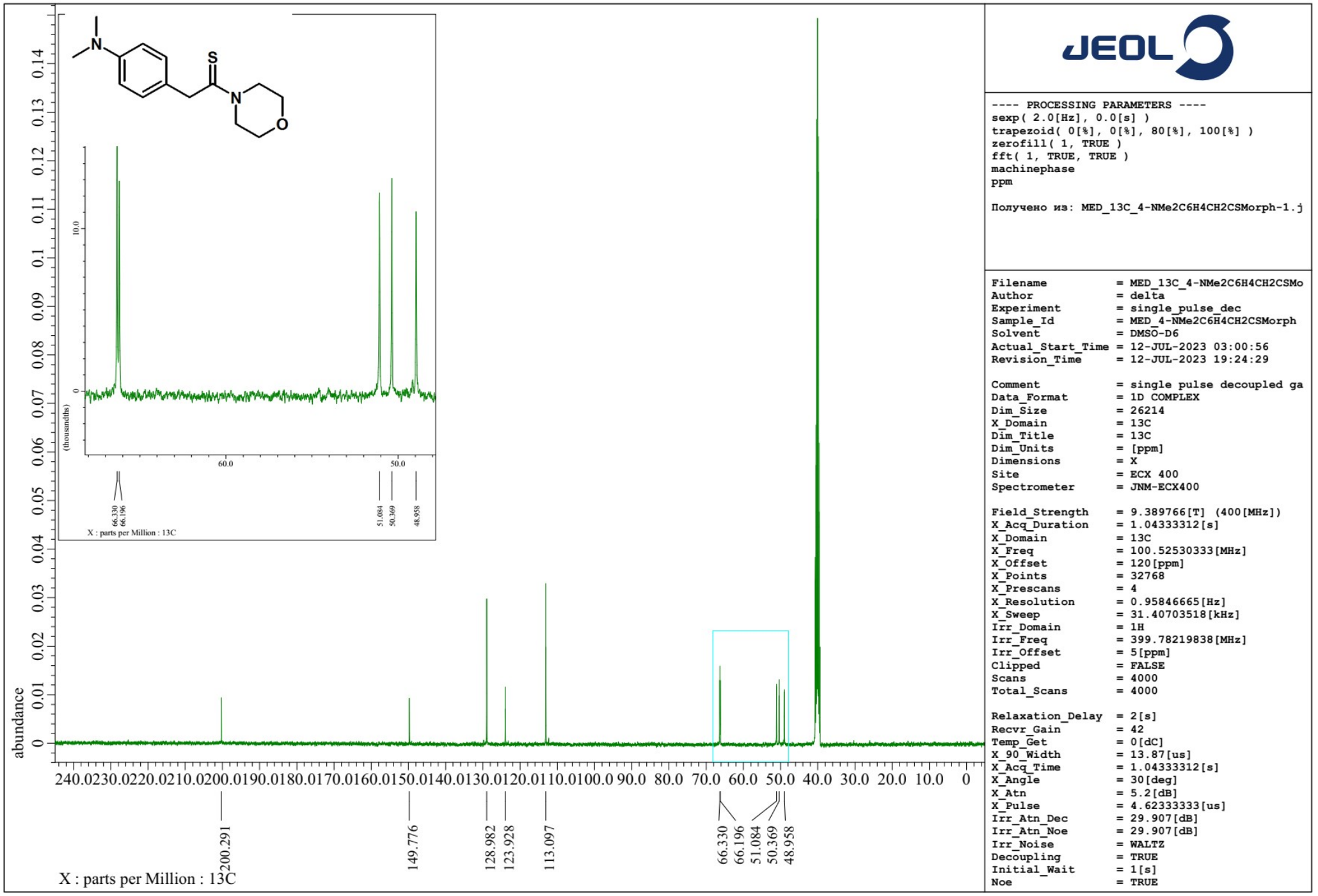

JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Получено из: MED_1H_4-MeOC6H4CH2CSMorph-1.jdf
Filename = MED_1H_4-MeOC6H4CH2CSMorp
Author = delta
Experiment = single_pulse.ex2
Sample_Id = MED_4-MeOC6H4CH2CSMorph
Solvent = DMSO-D6
Actual_Start_Time = 11-JUL-2023 23:21:43
Revision_Time = 12-JUL-2023 18:37:53
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 7[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 26
Temp_Get = 0[dC]
X_90_Width = 5.5[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 2.75[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
abundance
X : parts per Million : 1H
7.229
7.207
6.865
6.844
4.194
4.175
4.163
3.690
3.670
3.659
3.646
3.601
3.589
3.576
3.380
3.367
3.355
2.00
1.50
1.00
1.00
0.97
1.00
1.02

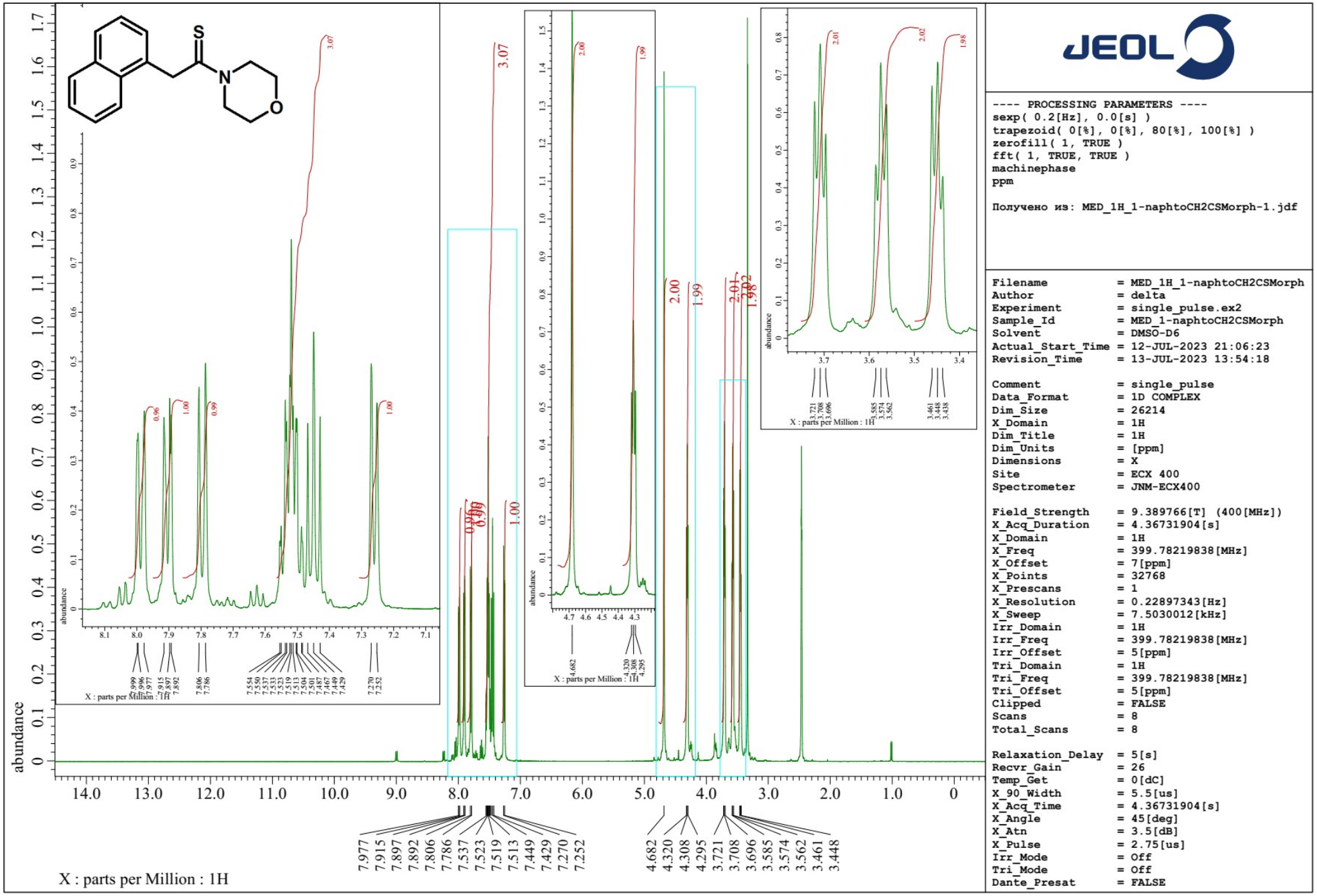



```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_13C_4-MeOC6H4CH2CSMorph-1.jd
```

```
Filename          = MED_13C_4-MeOC6H4CH2CSMor
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = MED_4-MeOC6H4CH2CSMorph
Solvent           = DMSO-D6
Actual_Start_Time = 11-JUL-2023 23:23:44
Revision_Time     = 12-JUL-2023 18:42:28

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = 13C
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 120[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 4000
Total_Scans       = 4000

Relaxation_Delay  = 2[s]
Recvr_Gain        = 46
Temp_Get          = 0[dC]
X_90_Width        = 13.87[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 5.2[dB]
X_Pulse           = 4.62333333[us]
Irr_Atn_Dec       = 29.907[dB]
Irr_Atn_Noe       = 29.907[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
```


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Получено из: MED_1H_4-NMe2C6H4CH2CSMorph-1.jd
Filename = MED_1H_4-NMe2C6H4CH2CSMor
Author = delta
Experiment = single_pulse.ex2
Sample_Id = MED_4-NMe2C6H4CH2CSMorph
Solvent = DMSO-D6
Actual_Start_Time = 12-JUL-2023 02:59:01
Revision_Time = 12-JUL-2023 19:21:37
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 7[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 30
Temp_Get = 0[dC]
X_90_Width = 5.5[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 2.75[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
abundance
X : parts per Million : 1H
7.119
7.097
6.652
6.630
4.176
4.164
4.152
4.134
3.663
3.652
3.640
3.589
3.577
3.565
3.367
3.354
3.343
2.819

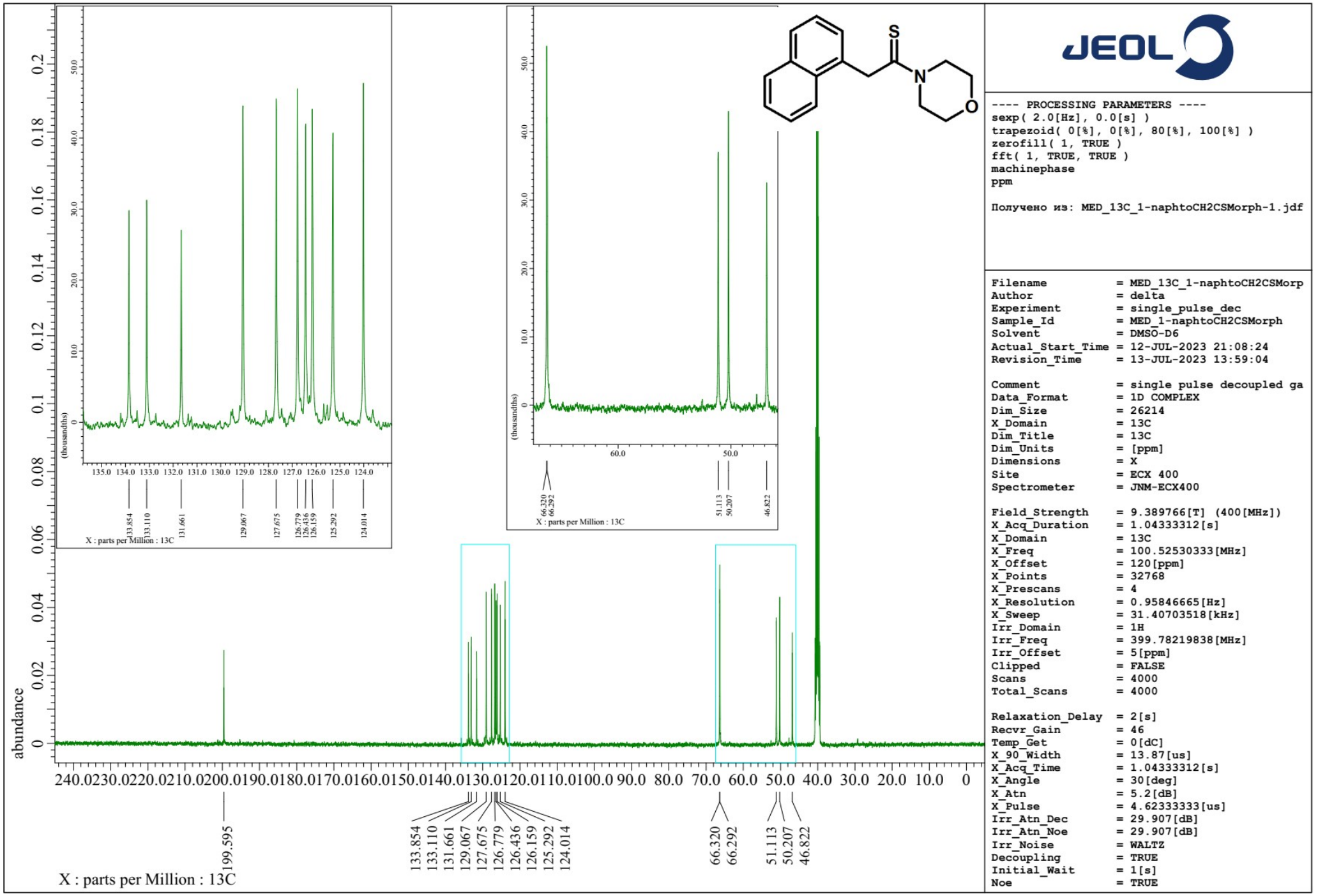

JEOL
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Получено из: MED_13C_4-NMe2C6H4CH2CSMorph-1.j
Filename = MED_13C_4-NMe2C6H4CH2CSMo
Author = delta
Experiment = single_pulse_dec
Sample_Id = MED_4-NMe2C6H4CH2CSMorph
Solvent = DMSO-D6
Actual_Start_Time = 12-JUL-2023 03:00:56
Revision_Time = 12-JUL-2023 19:24:29
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 120[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 4000
Total_Scans = 4000
Relaxation_Delay = 2[s]
Recvr_Gain = 42
Temp_Get = 0[dC]
X_90_Width = 13.87[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 5.2[dB]
X_Pulse = 4.62333333[us]
Irr_Atn_Dec = 29.907[dB]
Irr_Atn_Noe = 29.907[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
abundance
X : parts per Million : 13C
200.291
149.776
128.982
123.928
113.097
66.330
66.196
51.084
50.369
48.958

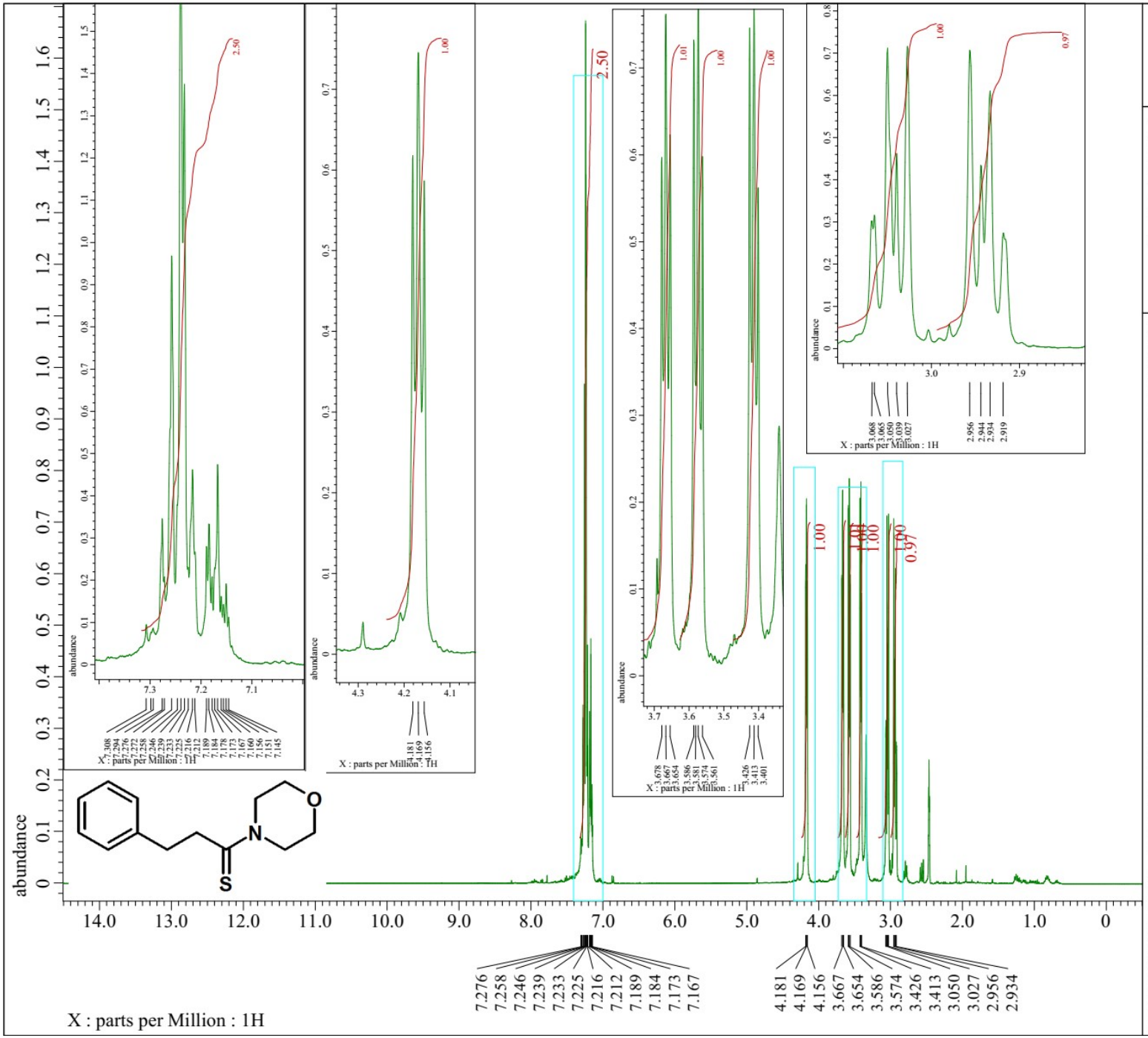


JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_1H_1-naphtoCH2CSMorph-1.jdf
```

Filename	= MED_1H_1-naphtoCH2CSMorph
Author	= delta
Experiment	= single_pulse.ex2
Sample_Id	= MED_1-naphtoCH2CSMorph
Solvent	= DMSO-D6
Actual_Start_Time	= 12-JUL-2023 21:06:23
Revision_Time	= 13-JUL-2023 13:54:18
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400
Spectrometer	= JNM-ECX400
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 4.36731904[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 7[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.22897343[Hz]
X_Sweep	= 7.5030012[kHz]
Irr_Domain	= 1H
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 26
Temp_Get	= 0[dC]
X_90_Width	= 5.5[us]
X_Acq_Time	= 4.36731904[s]
X_Angle	= 45[deg]
X_Atn	= 3.5[dB]
X_Pulse	= 2.75[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE

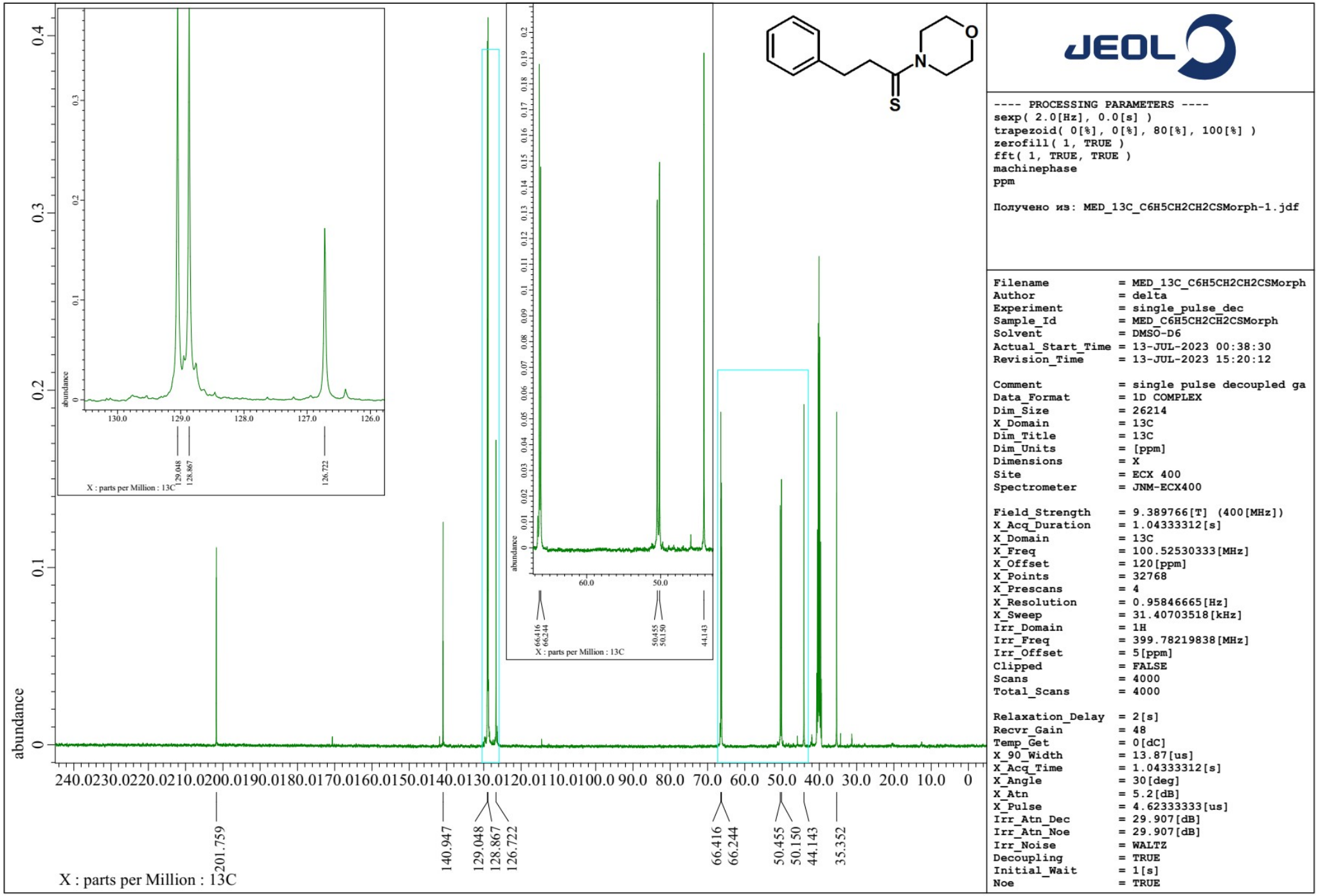

abundance
X : parts per Million : 13C
199.595
133.854
133.110
131.661
129.067
127.675
126.779
126.436
126.159
125.292
124.014
66.320
66.292
51.113
50.207
46.822
S
N
O
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Получено из: MED_13C_1-naphtoCH2CSMorph-1.jdf
Filename = MED_13C_1-naphtoCH2CSMorp
Author = delta
Experiment = single_pulse_dec
Sample_Id = MED_1-naphtoCH2CSMorph
Solvent = DMSO-D6
Actual_Start_Time = 12-JUL-2023 21:08:24
Revision_Time = 13-JUL-2023 13:59:04
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 120[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 4000
Total_Scans = 4000
Relaxation_Delay = 2[s]
Recvr_Gain = 46
Temp_Get = 0[dC]
X_90_Width = 13.87[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 5.2[dB]
X_Pulse = 4.62333333[us]
Irr_Atn_Dec = 29.907[dB]
Irr_Atn_Noe = 29.907[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_1H_C6H5CH2CH2CSMorph-1.jdf
```

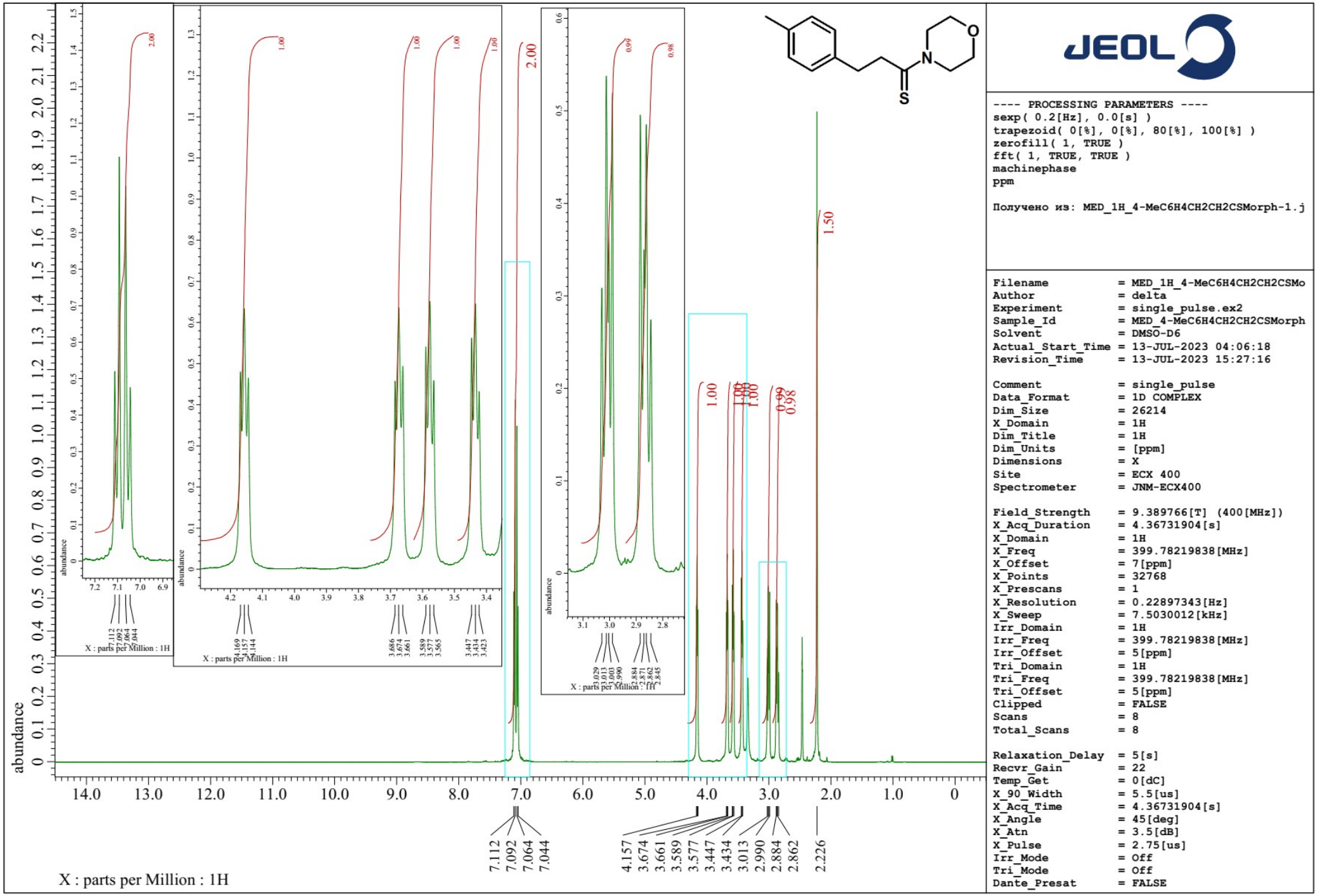
```
Filename            = MED_1H_C6H5CH2CH2CSMorph-
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = MED_C6H5CH2CH2CSMorph
Solvent             = DMSO-D6
Actual_Start_Time   = 13-JUL-2023 00:36:23
Revision_Time       = 13-JUL-2023 15:03:59

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 1H
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400
Spectrometer        = JNM-ECX400

Field_Strength      = 9.389766[T] (400[MHz])
X_Acq_Duration      = 4.36731904[s]
X_Domain            = 1H
X_Freq              = 399.78219838[MHz]
X_Offset            = 7[ppm]
X_Points            = 32768
X_Prescans          = 1
X_Resolution        = 0.22897343[Hz]
X_Sweep             = 7.5030012[kHz]
Irr_Domain          = 1H
Irr_Freq            = 399.78219838[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = 1H
Tri_Freq            = 399.78219838[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 18
Temp_Get            = 0[dC]
X_90_Width          = 5.5[us]
X_Acq_Time          = 4.36731904[s]
X_Angle             = 45[deg]
X_Atn               = 3.5[dB]
X_Pulse             = 2.75[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
```

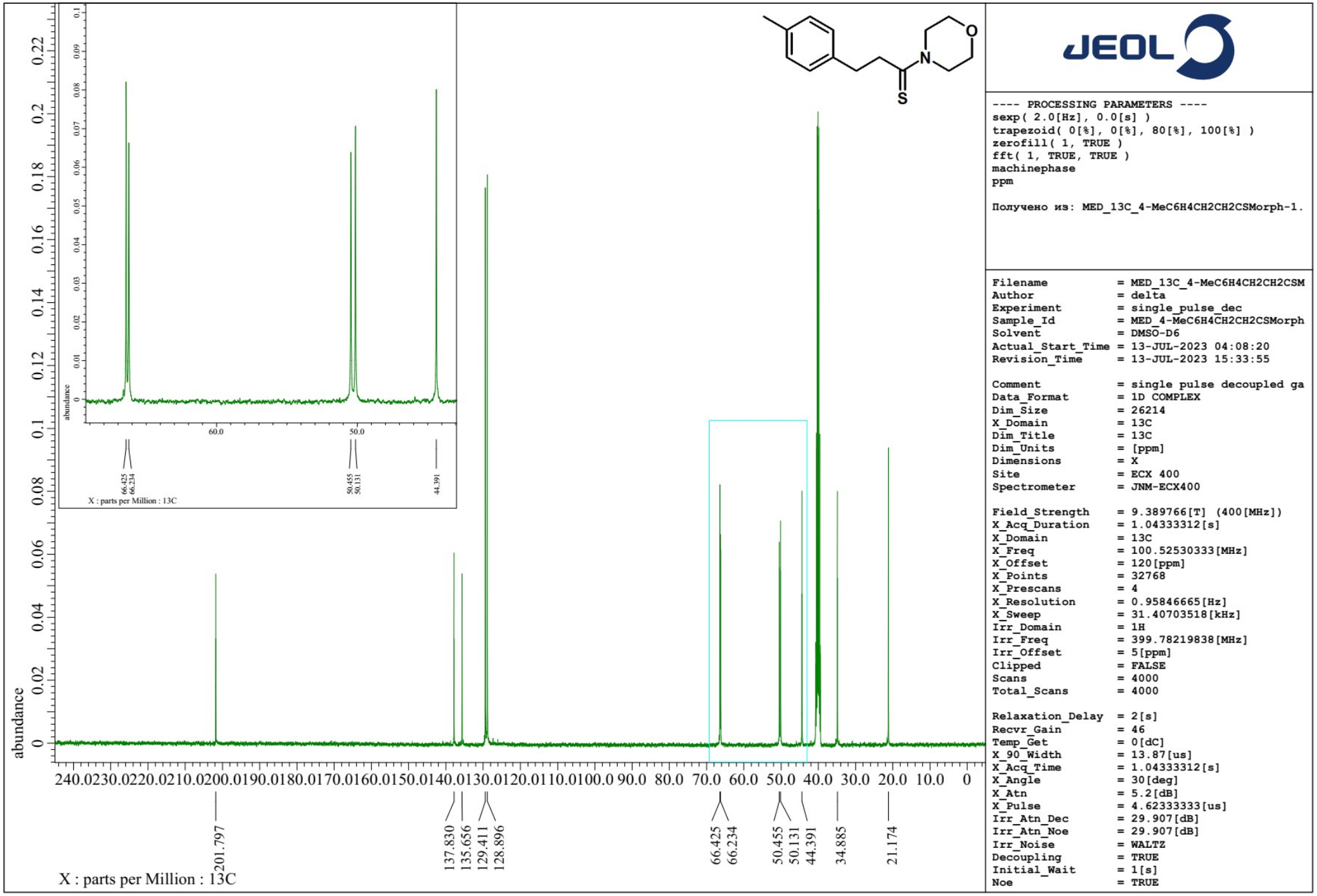


JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Получено из: MED_13C_C6H5CH2CH2CSMorph-1.jdf
```

```
Filename          = MED_13C_C6H5CH2CH2CSMorph
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = MED_C6H5CH2CH2CSMorph
Solvent           = DMSO-D6
Actual_Start_Time = 13-JUL-2023 00:38:30
Revision_Time     = 13-JUL-2023 15:20:12

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = 13C
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 120[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 4000
Total_Scans       = 4000

Relaxation_Delay  = 2[s]
Recvr_Gain        = 48
Temp_Get          = 0[dC]
X_90_Width        = 13.87[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 5.2[dB]
X_Pulse           = 4.62333333[us]
Irr_Atn_Dec       = 29.907[dB]
Irr_Atn_Noe       = 29.907[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
```

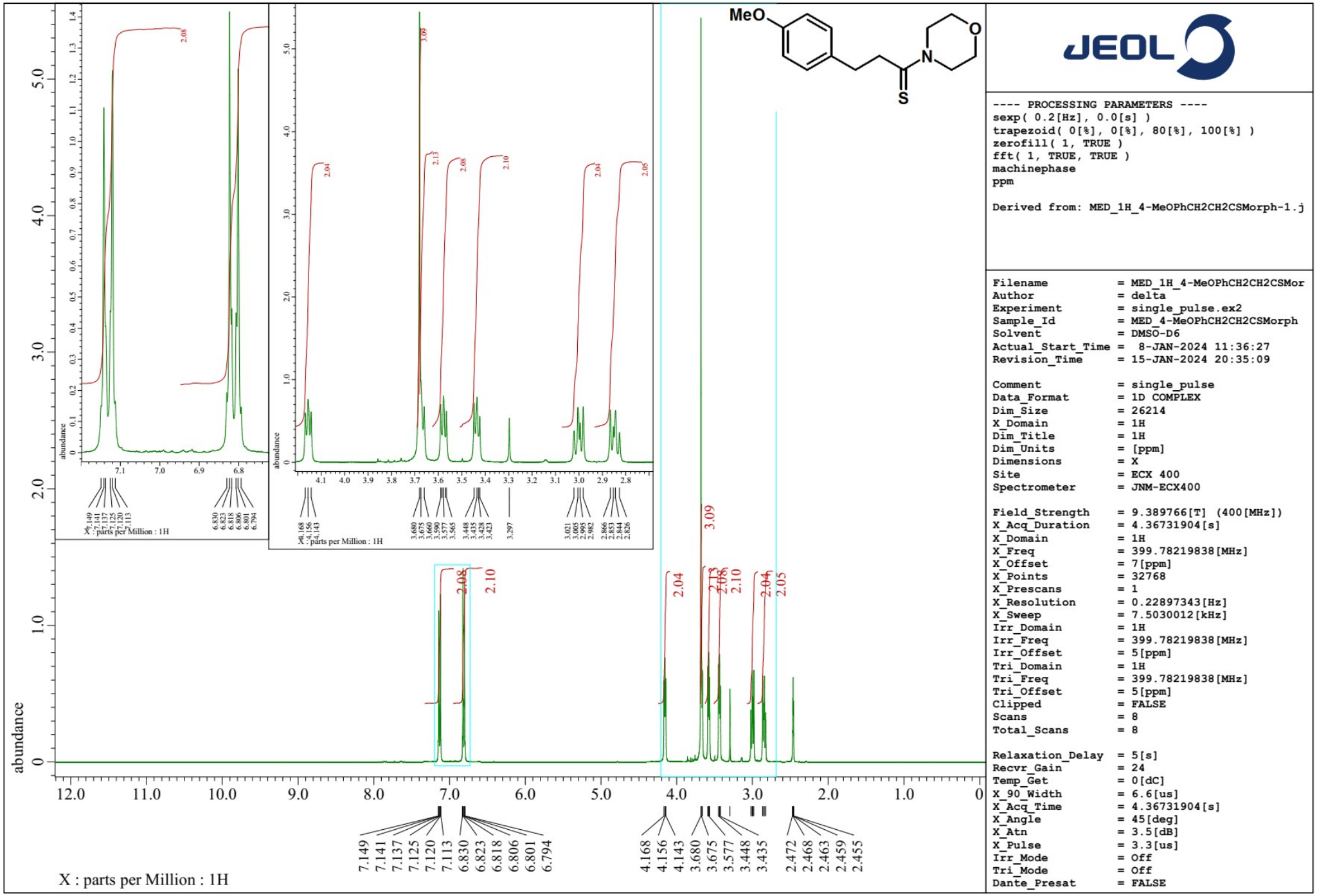

JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Получено из: MED_1H_4-MeC6H4CH2CH2CSMorph-1.j
Filename = MED_1H_4-MeC6H4CH2CH2CSMo
Author = delta
Experiment = single_pulse.ex2
Sample_Id = MED_4-MeC6H4CH2CH2CSMorph
Solvent = DMSO-D6
Actual_Start_Time = 13-JUL-2023 04:06:18
Revision_Time = 13-JUL-2023 15:27:16
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 7[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 22
Temp_Get = 0[dC]
X_90_Width = 5.5[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 2.75[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
abundance
X : parts per Million : 1H
7.112
7.092
7.064
7.044
4.157
3.674
3.661
3.589
3.577
3.447
3.434
3.013
2.990
2.884
2.862
2.226
2.00
1.00
0.99
0.98
1.50



---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm

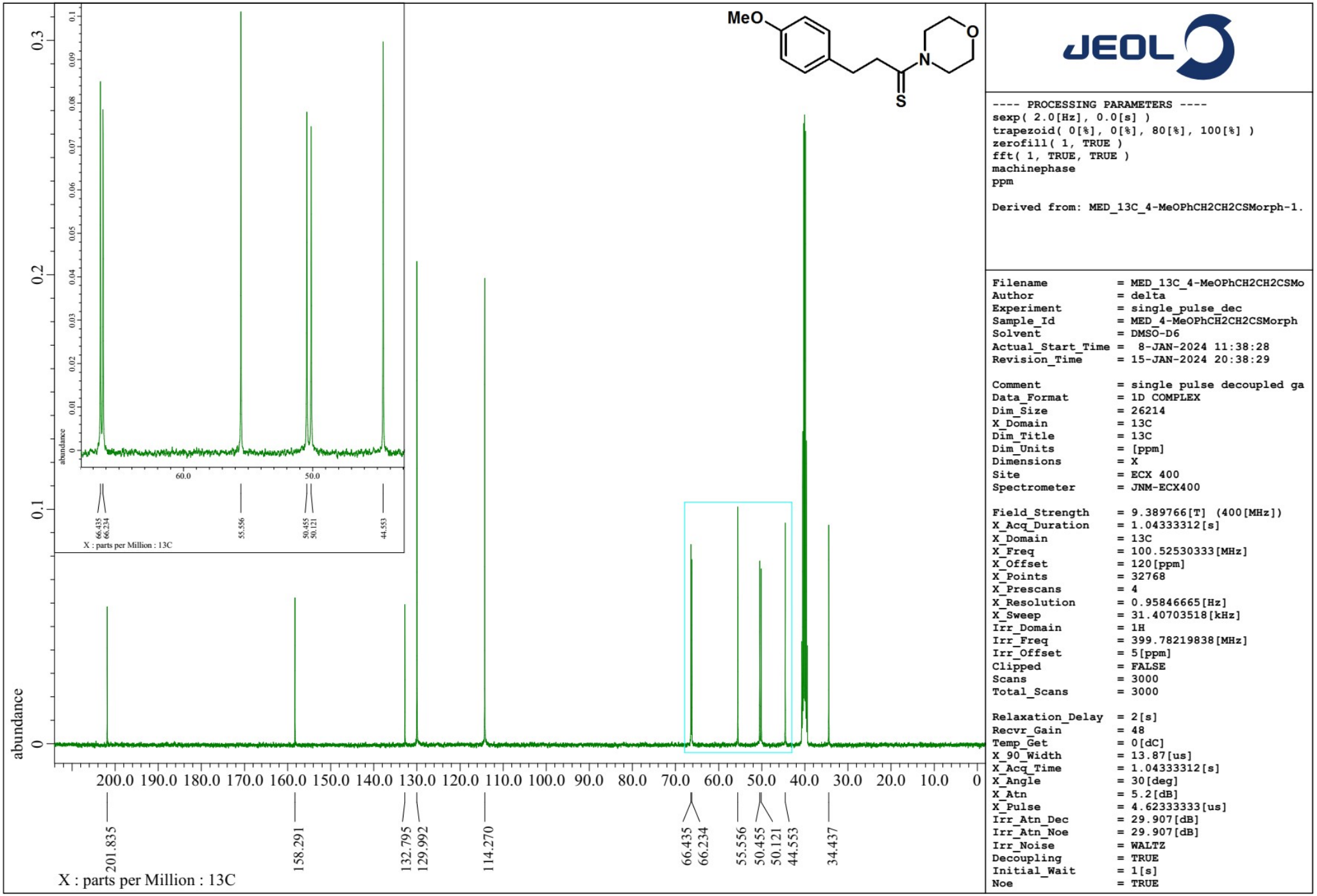
Получено из: MED_13C_4-MeC6H4CH2CH2CSMorph-1.

Filename	= MED_13C_4-MeC6H4CH2CH2CSM
Author	= delta
Experiment	= single_pulse_dec
Sample_Id	= MED_4-MeC6H4CH2CH2CSMorph
Solvent	= DMSO-D6
Actual_Start_Time	= 13-JUL-2023 04:08:20
Revision_Time	= 13-JUL-2023 15:33:55
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400
Spectrometer	= JNM-ECX400
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.52530333[MHz]
X_Offset	= 120[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
Irr_Domain	= 1H
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 4000
Total_Scans	= 4000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 46
Temp_Get	= 0[dC]
X_90_Width	= 13.87[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.2[dB]
X_Pulse	= 4.62333333[us]
Irr_Atn_Dec	= 29.907[dB]
Irr_Atn_Noe	= 29.907[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE



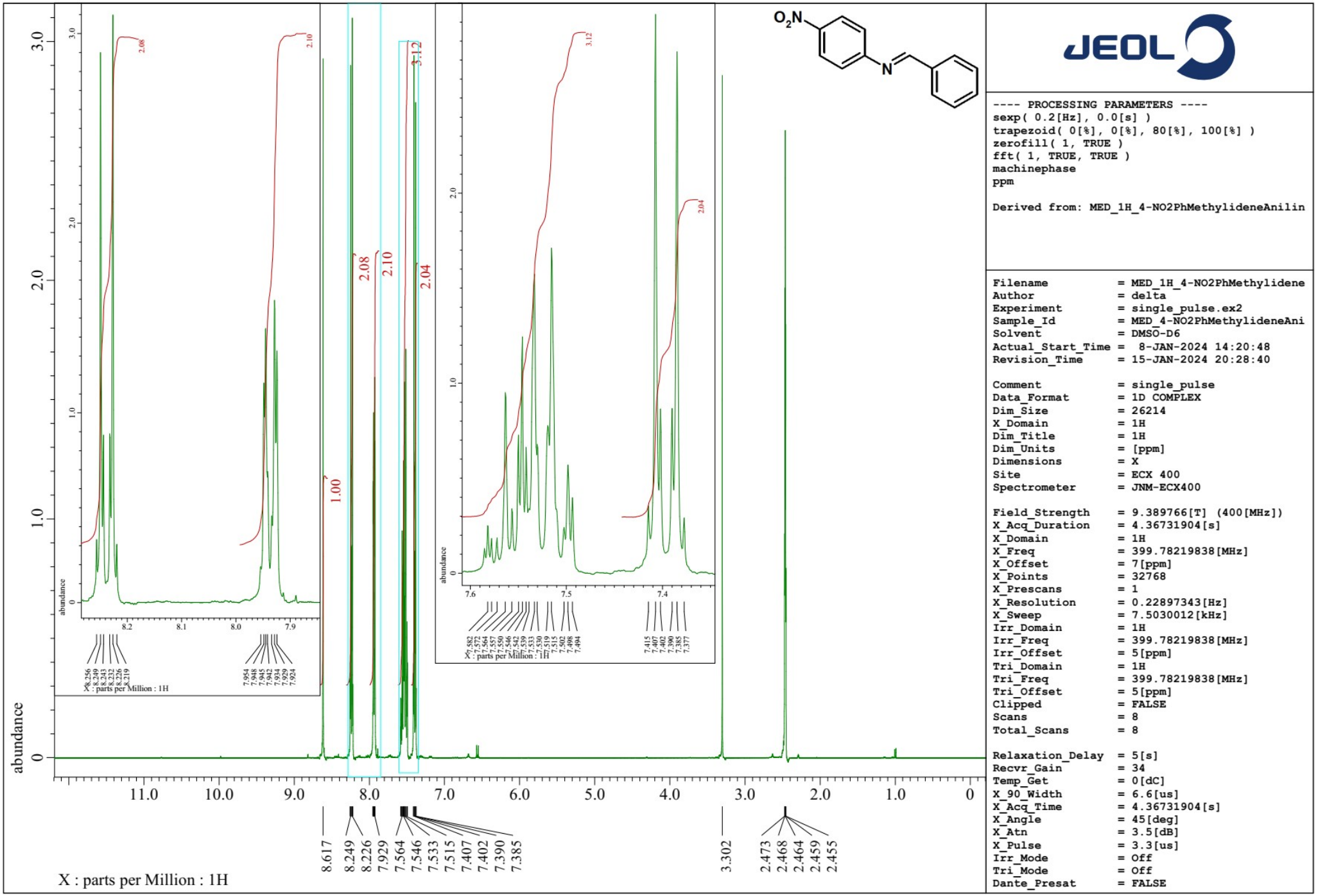

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MED_1H_4-MeOPhCH2CH2CSMorph-1.j
```

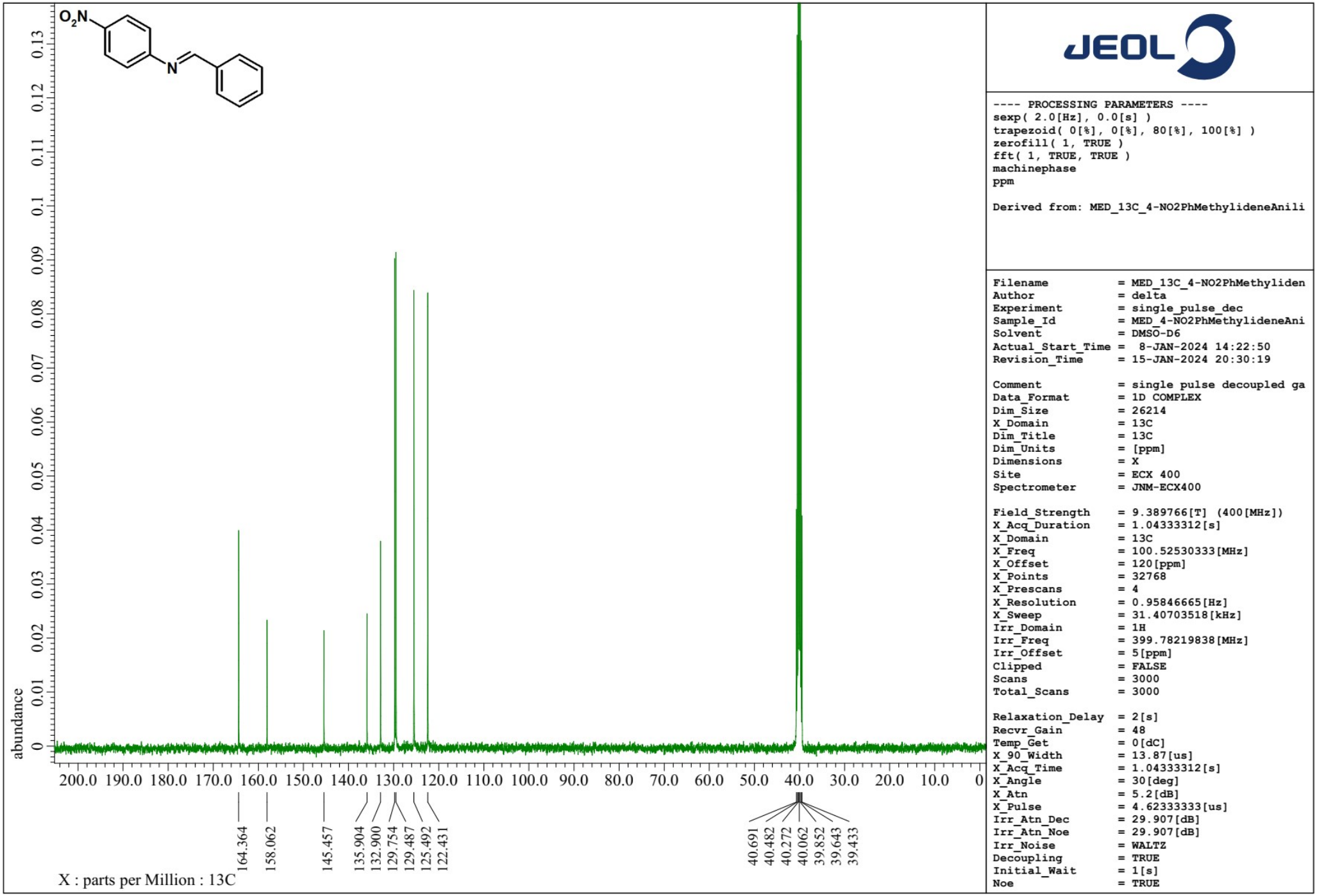
Filename	= MED_1H_4-MeOPhCH2CH2CSMor
Author	= delta
Experiment	= single_pulse.ex2
Sample_Id	= MED_4-MeOPhCH2CH2CSMorph
Solvent	= DMSO-D6
Actual_Start_Time	= 8-JAN-2024 11:36:27
Revision_Time	= 15-JAN-2024 20:35:09
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400
Spectrometer	= JNM-ECX400
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 4.36731904[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 7[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.22897343[Hz]
X_Sweep	= 7.5030012[kHz]
Irr_Domain	= 1H
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 24
Temp_Get	= 0[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 4.36731904[s]
X_Angle	= 45[deg]
X_Atn	= 3.5[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MED_13C_4-MeOPhCH2CH2CSMorph-1.
```

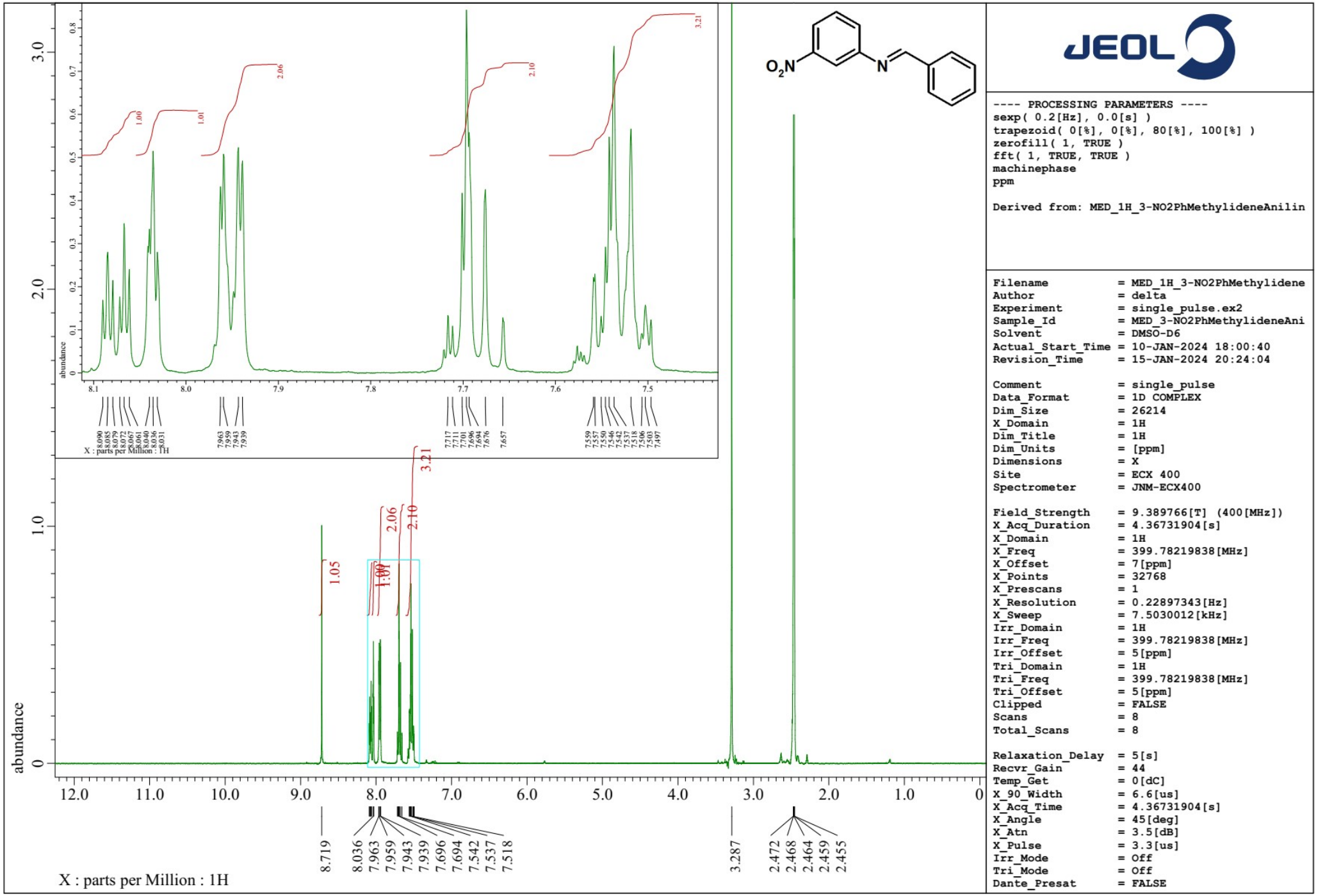
Filename	= MED_13C_4-MeOPhCH2CH2CSMo
Author	= delta
Experiment	= single_pulse_dec
Sample_Id	= MED_4-MeOPhCH2CH2CSMorph
Solvent	= DMSO-D6
Actual_Start_Time	= 8-JAN-2024 11:38:28
Revision_Time	= 15-JAN-2024 20:38:29
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400
Spectrometer	= JNM-ECX400
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.52530333[MHz]
X_Offset	= 120[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
Irr_Domain	= 1H
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 3000
Total_Scans	= 3000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 48
Temp_Get	= 0[dC]
X_90_Width	= 13.87[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.2[dB]
X_Pulse	= 4.62333333[us]
Irr_Atn_Dec	= 29.907[dB]
Irr_Atn_Noe	= 29.907[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE

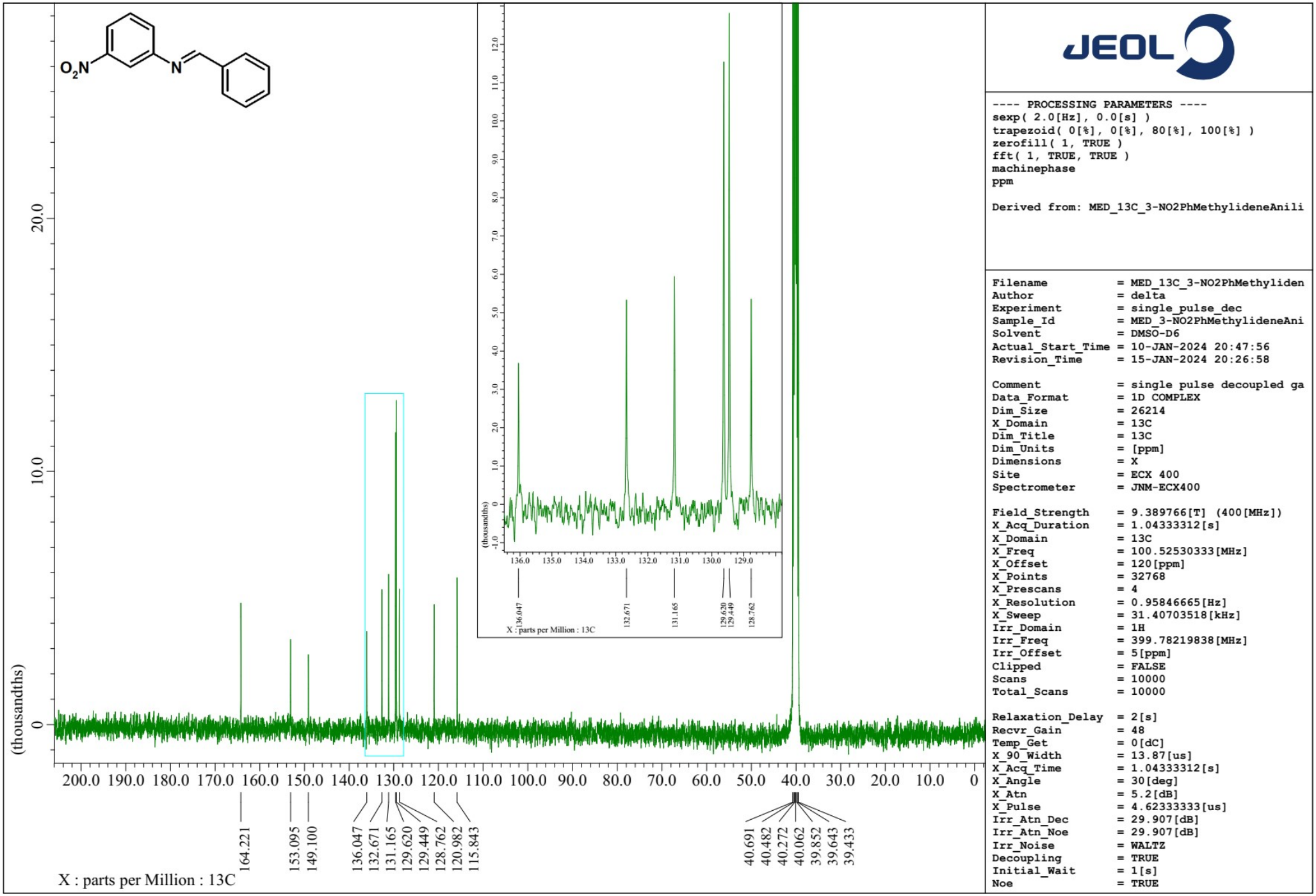

JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MED_1H_4-NO2PhMethylideneAnilin
Filename = MED_1H_4-NO2PhMethylidene
Author = delta
Experiment = single_pulse.ex2
Sample_Id = MED_4-NO2PhMethylideneAni
Solvent = DMSO-D6
Actual_Start_Time = 8-JAN-2024 14:20:48
Revision_Time = 15-JAN-2024 20:28:40
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 7[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 34
Temp_Get = 0[dC]
X_90_Width = 6.6[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 3.3[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
abundance
X : parts per Million : 1H
1.00
2.08
2.10
2.04
3.12
8.617
8.249
8.226
7.929
7.564
7.546
7.533
7.515
7.407
7.402
7.390
7.385
3.302
2.473
2.468
2.464
2.459
2.455




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MED_13C_4-NO2PhMethylideneAnili
```

Filename	= MED_13C_4-NO2PhMethyliden
Author	= delta
Experiment	= single_pulse_dec
Sample_Id	= MED_4-NO2PhMethylideneAni
Solvent	= DMSO-D6
Actual_Start_Time	= 8-JAN-2024 14:22:50
Revision_Time	= 15-JAN-2024 20:30:19
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400
Spectrometer	= JNM-ECX400
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.52530333[MHz]
X_Offset	= 120[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
Irr_Domain	= 1H
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 3000
Total_Scans	= 3000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 48
Temp_Get	= 0[dC]
X_90_Width	= 13.87[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.2[dB]
X_Pulse	= 4.62333333[us]
Irr_Atn_Dec	= 29.907[dB]
Irr_Atn_Noe	= 29.907[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MED_1H_3-NO2PhMethylideneAnilin
Filename = MED_1H_3-NO2PhMethylidene
Author = delta
Experiment = single_pulse.ex2
Sample_Id = MED_3-NO2PhMethylideneAni
Solvent = DMSO-D6
Actual_Start_Time = 10-JAN-2024 18:00:40
Revision_Time = 15-JAN-2024 20:24:04
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 7[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 44
Temp_Get = 0[dC]
X_90_Width = 6.6[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 3.3[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
abundance
X : parts per Million : 1H


O2N
N
(thousandths)
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
164.221
153.095
149.100
136.047
132.671
131.165
129.620
129.449
128.762
120.982
115.843
40.691
40.482
40.272
40.062
39.852
39.643
39.433
X : parts per Million : 13C
136.0 135.0 134.0 133.0 132.0 131.0 130.0 129.0
136.047
132.671
131.165
129.620
129.449
128.762
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MED_13C_3-NO2PhMethylideneAnili
Filename = MED_13C_3-NO2PhMethyliden
Author = delta
Experiment = single_pulse_dec
Sample_Id = MED_3-NO2PhMethylideneAni
Solvent = DMSO-D6
Actual_Start_Time = 10-JAN-2024 20:47:56
Revision_Time = 15-JAN-2024 20:26:58
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 120[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 10000
Total_Scans = 10000
Relaxation_Delay = 2[s]
Recvr_Gain = 48
Temp_Get = 0[dC]
X_90_Width = 13.87[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 5.2[dB]
X_Pulse = 4.62333333[us]
Irr_Atn_Dec = 29.907[dB]
Irr_Atn_Noe = 29.907[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE