

Supporting Information

Domino reactions of 1-(2-alkoxyaryl)-3-alkylprop-2-yn-1-ones with sodium sulfide leading to thiochromen-4-one derivatives

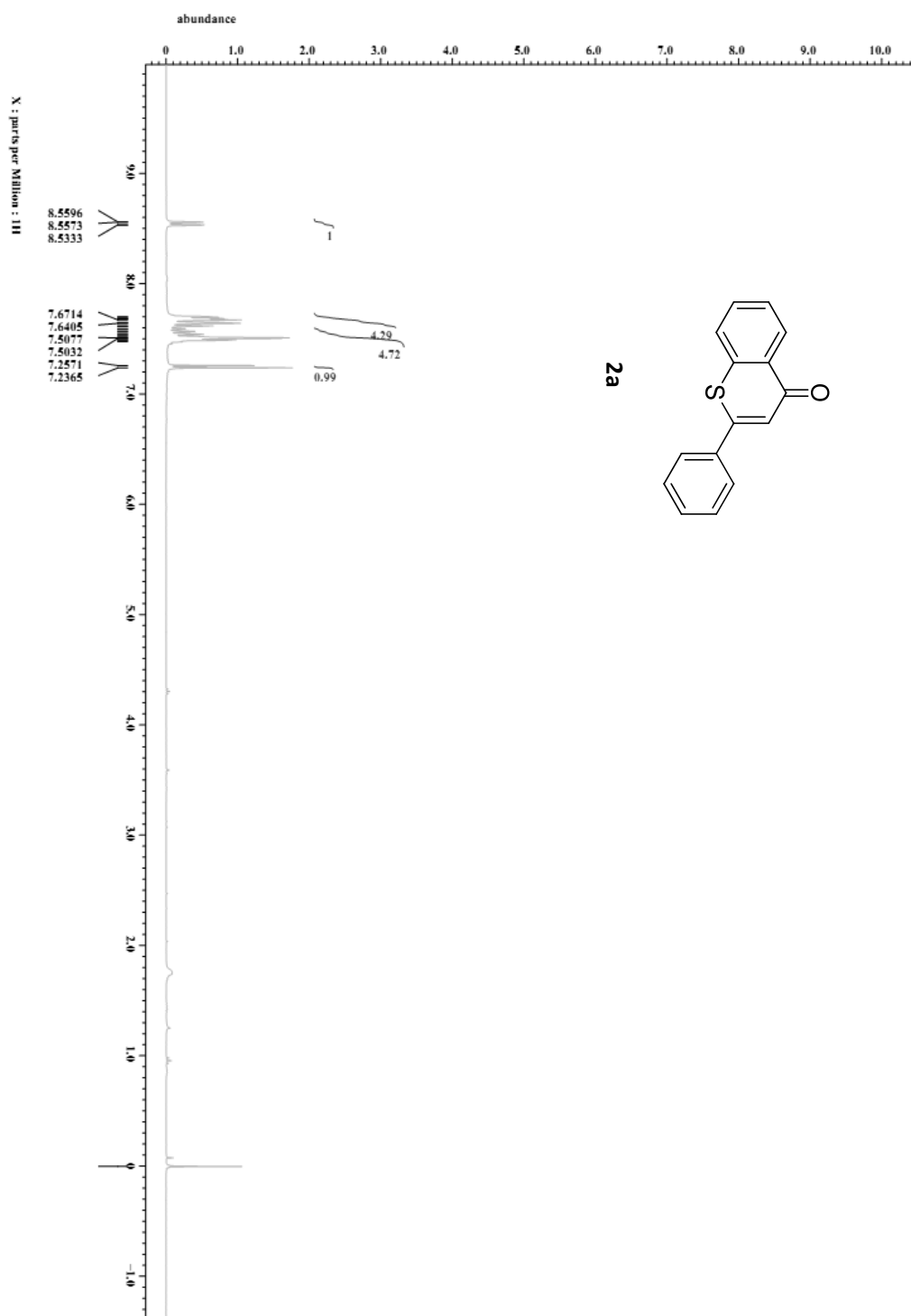
Xiaobo Yang,^a Shangfu Li,^b Hongxia Liu,^b Yuyang Jiang,^b and Hua Fu^{*a,b}

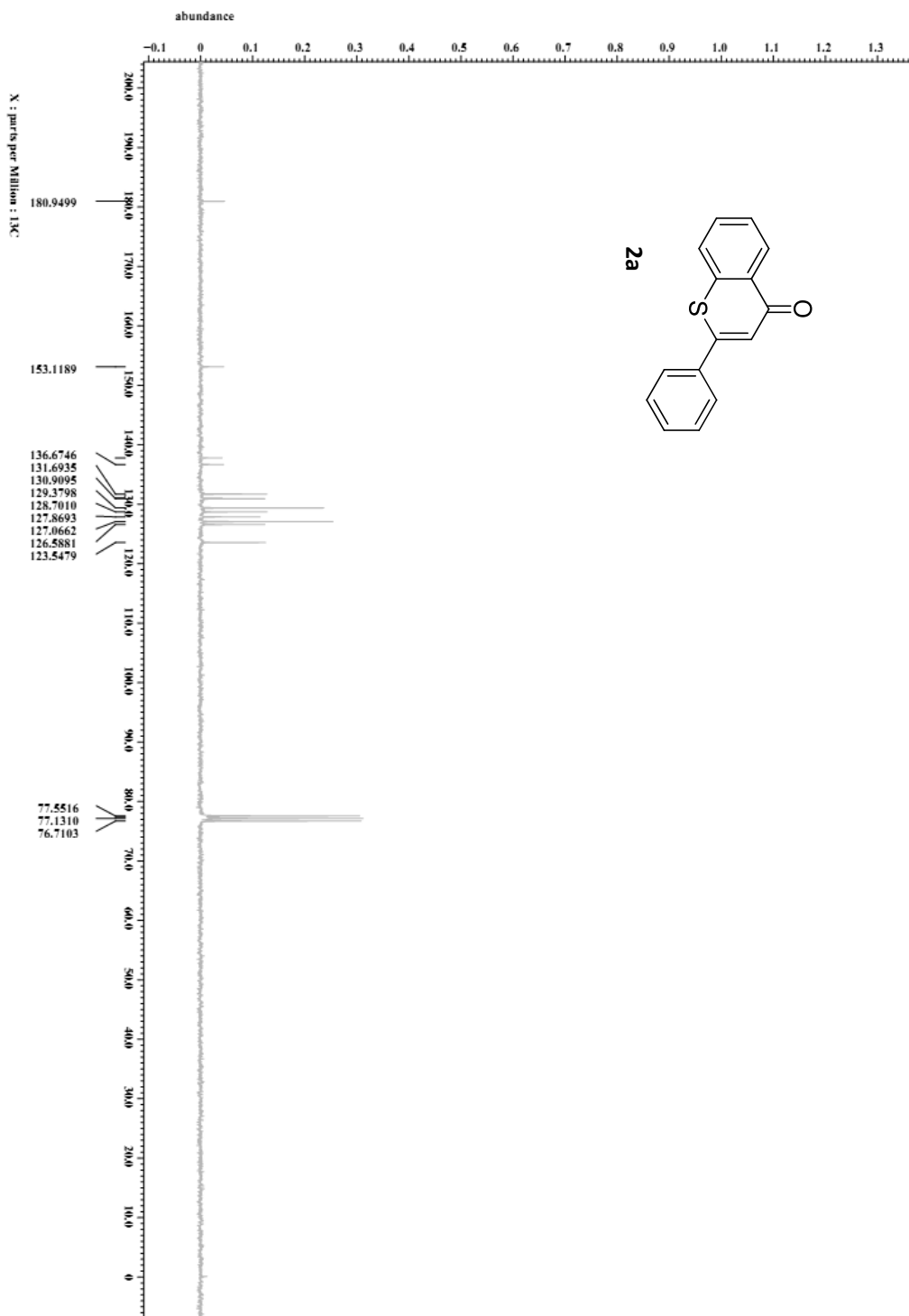
^a Key Laboratory of Bioorganic Phosphorus Chemistry and Chemical Biology (Ministry of Education), Department of Chemistry, Tsinghua University, Beijing 100084, P. R. China

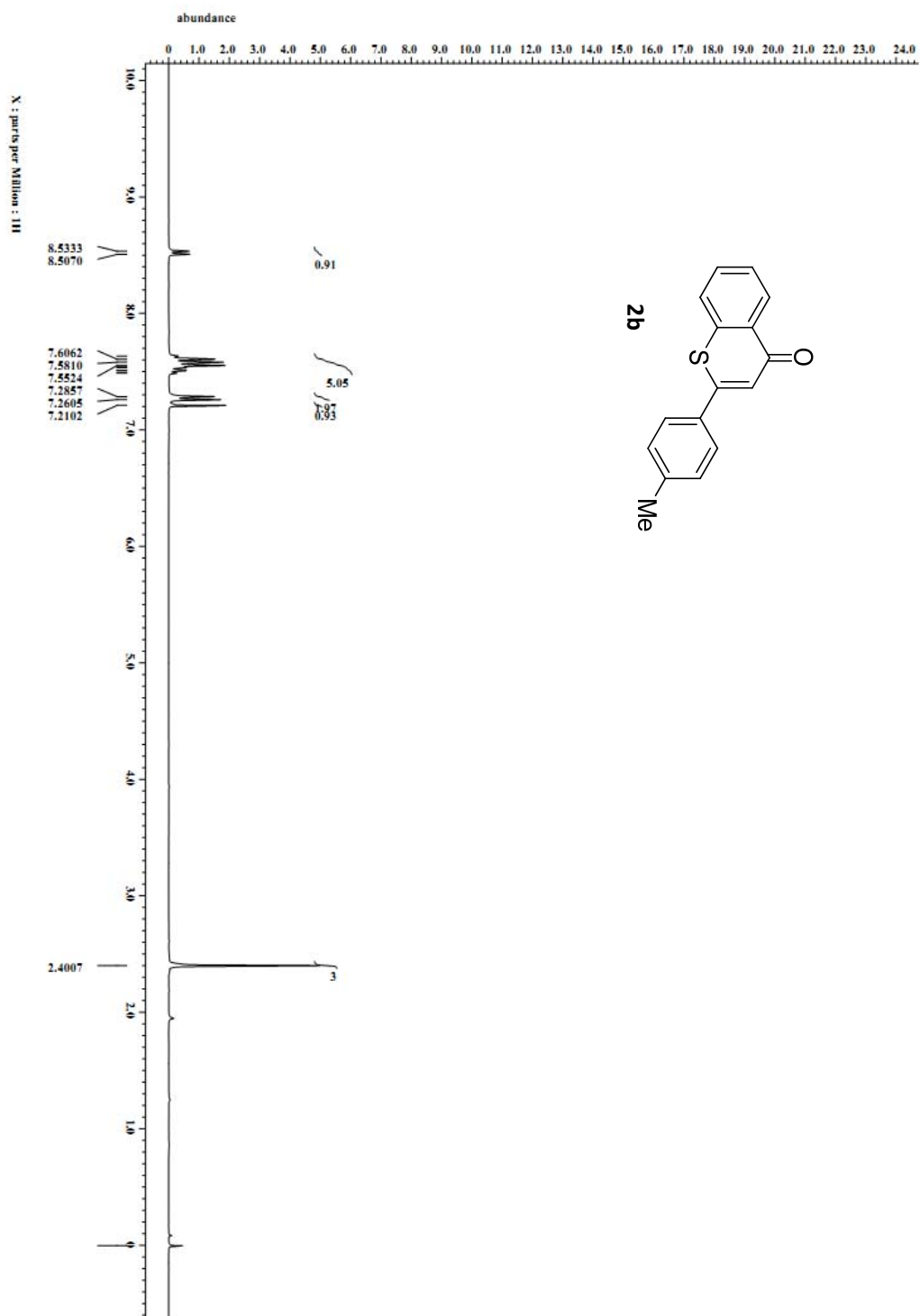
^b Key Laboratory of Chemical Biology (Guangdong Province), Graduate School of Shenzhen, Tsinghua University, Shenzhen 518057, P. R. China

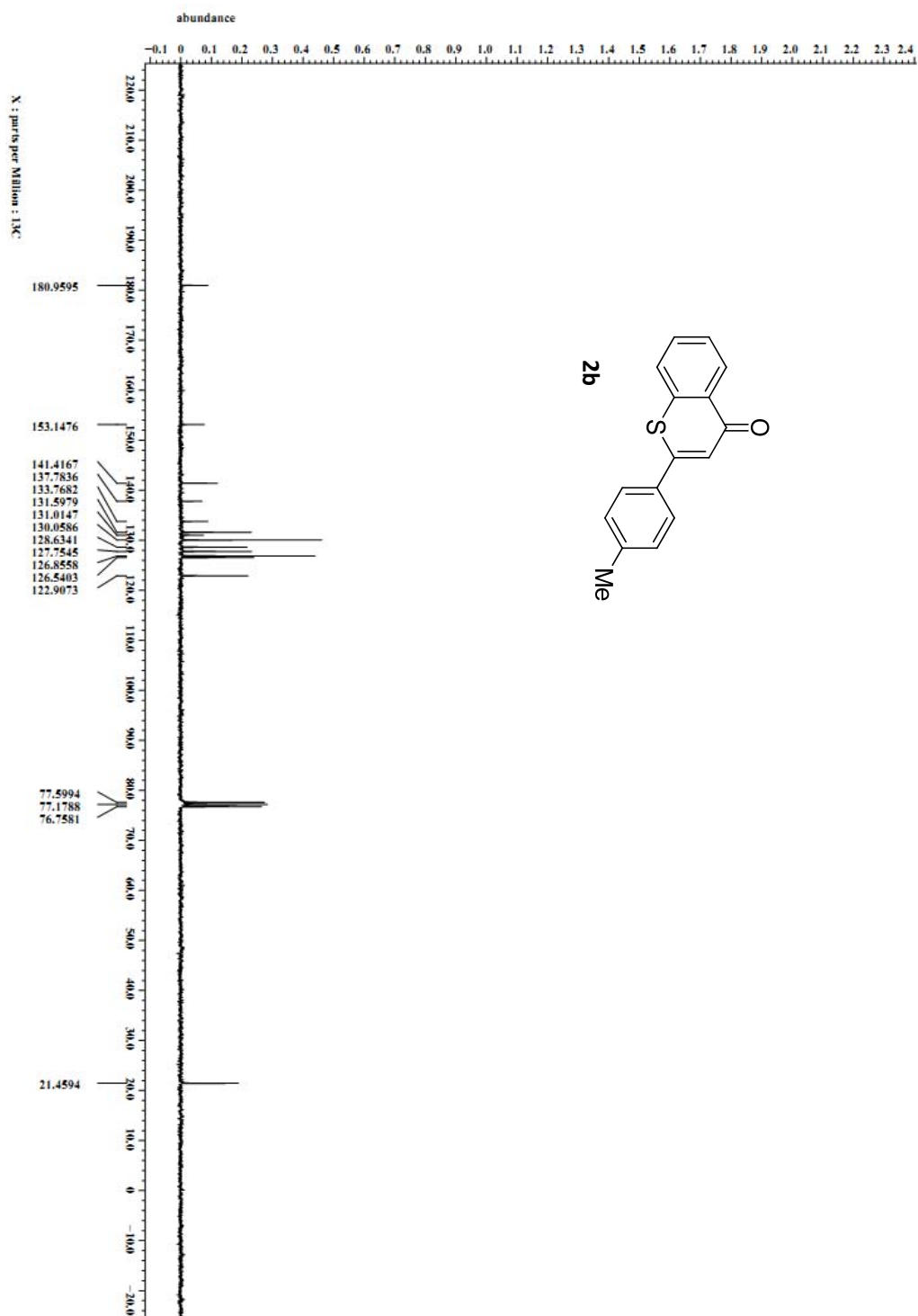
*To whom correspondence should be addressed. E-mail: fuhua@mail.tsinghua.edu.cn

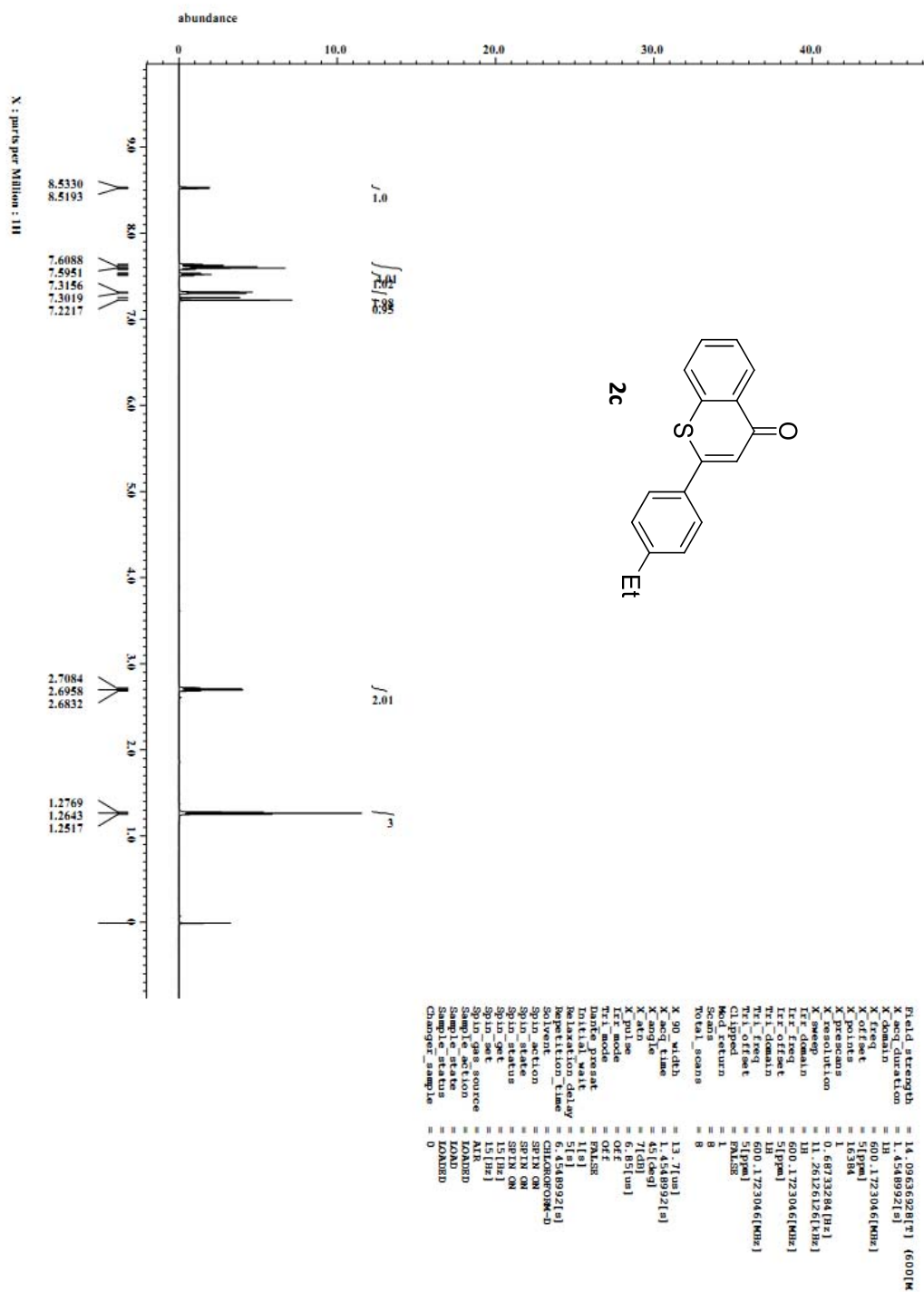
The ¹H and ¹³C NMR spectra of compounds **2a-v** and **Ia**

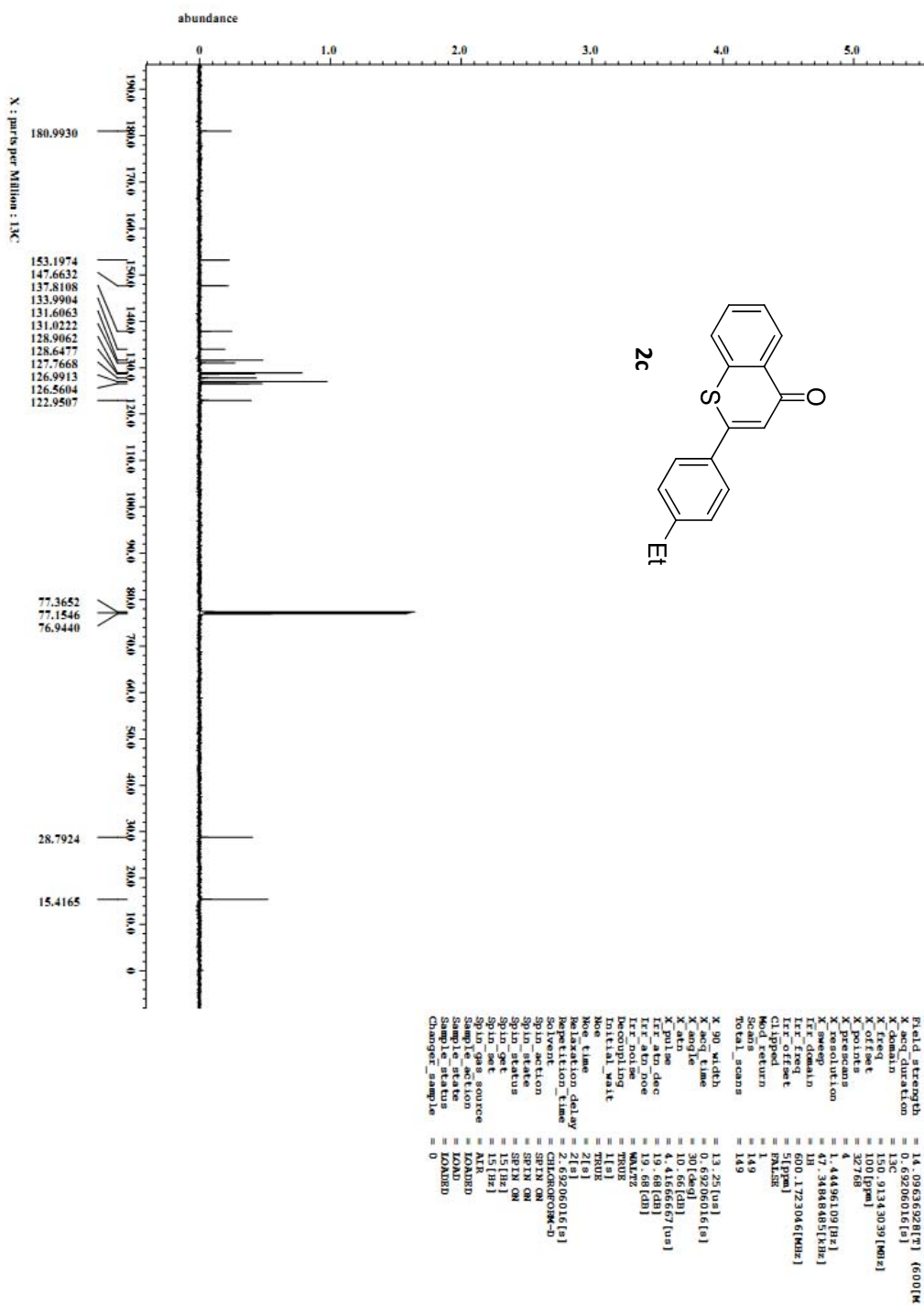


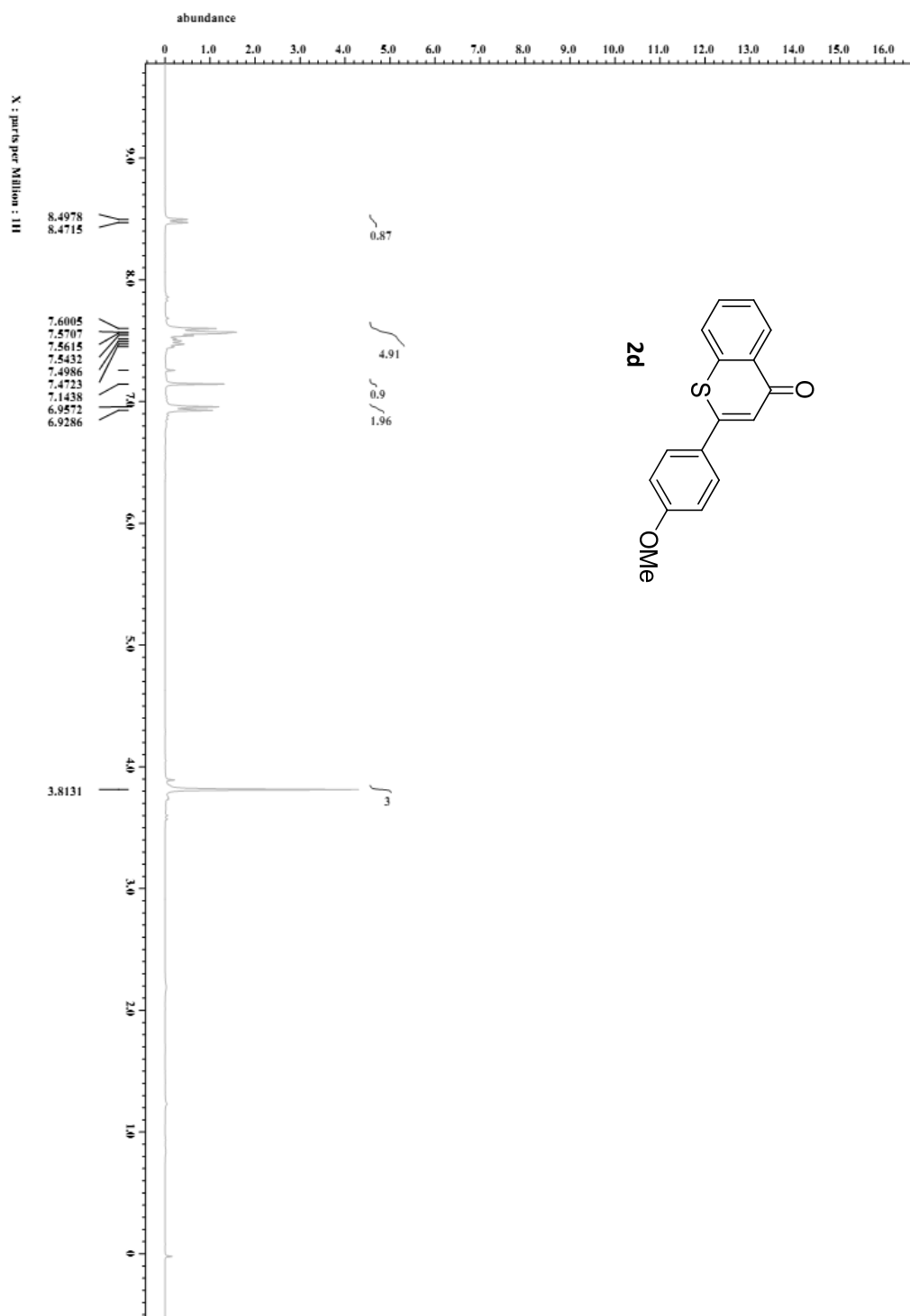


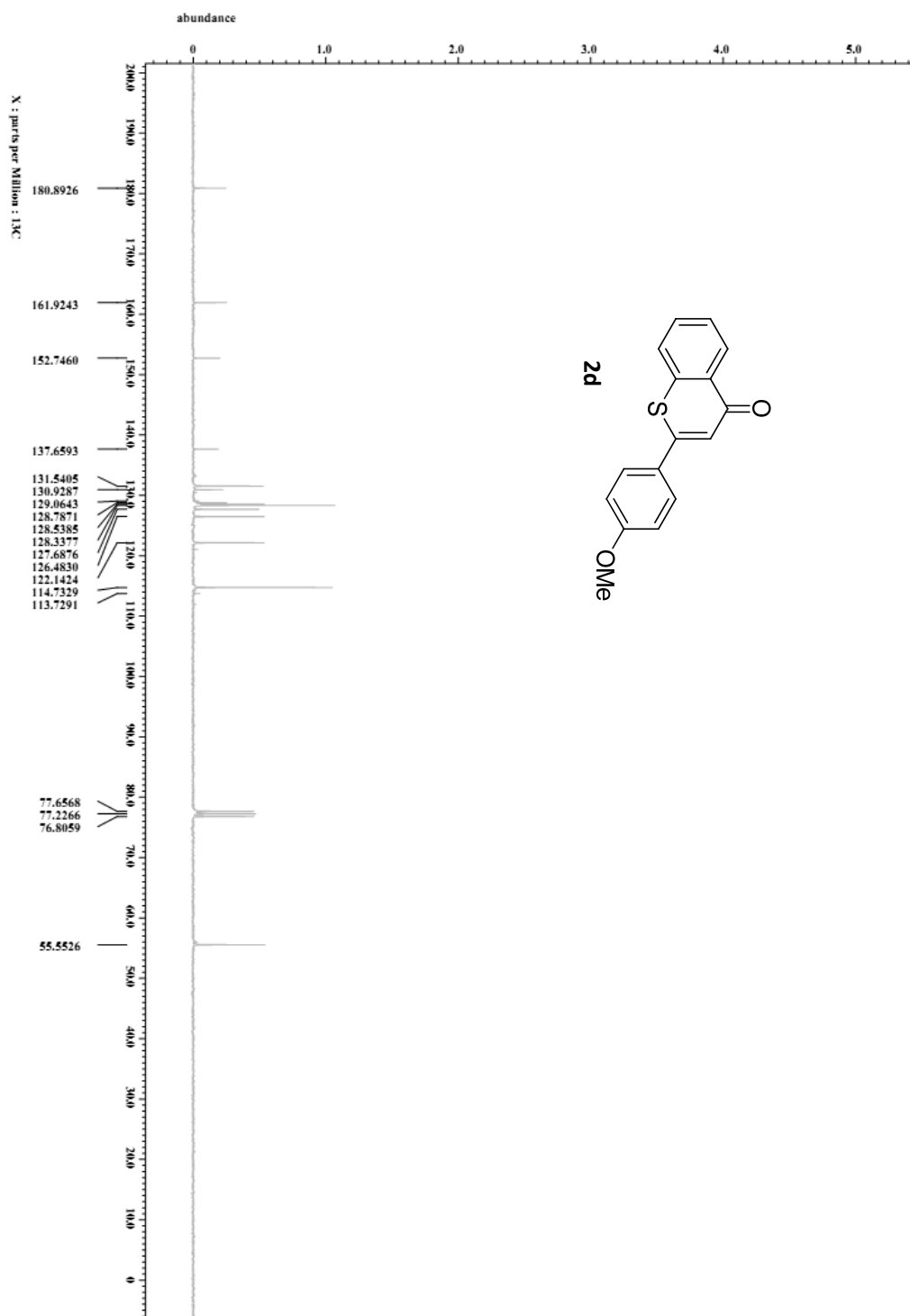


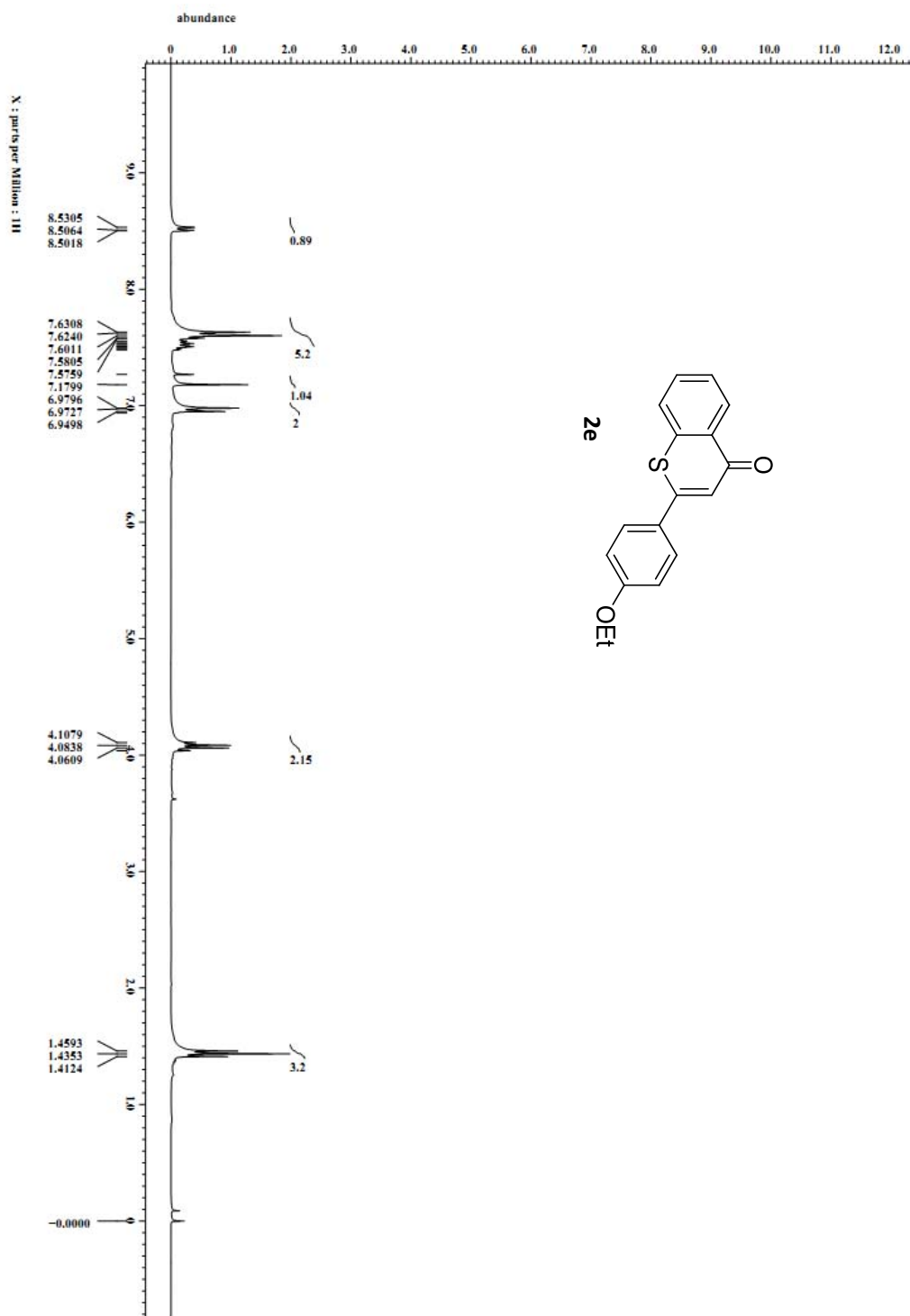


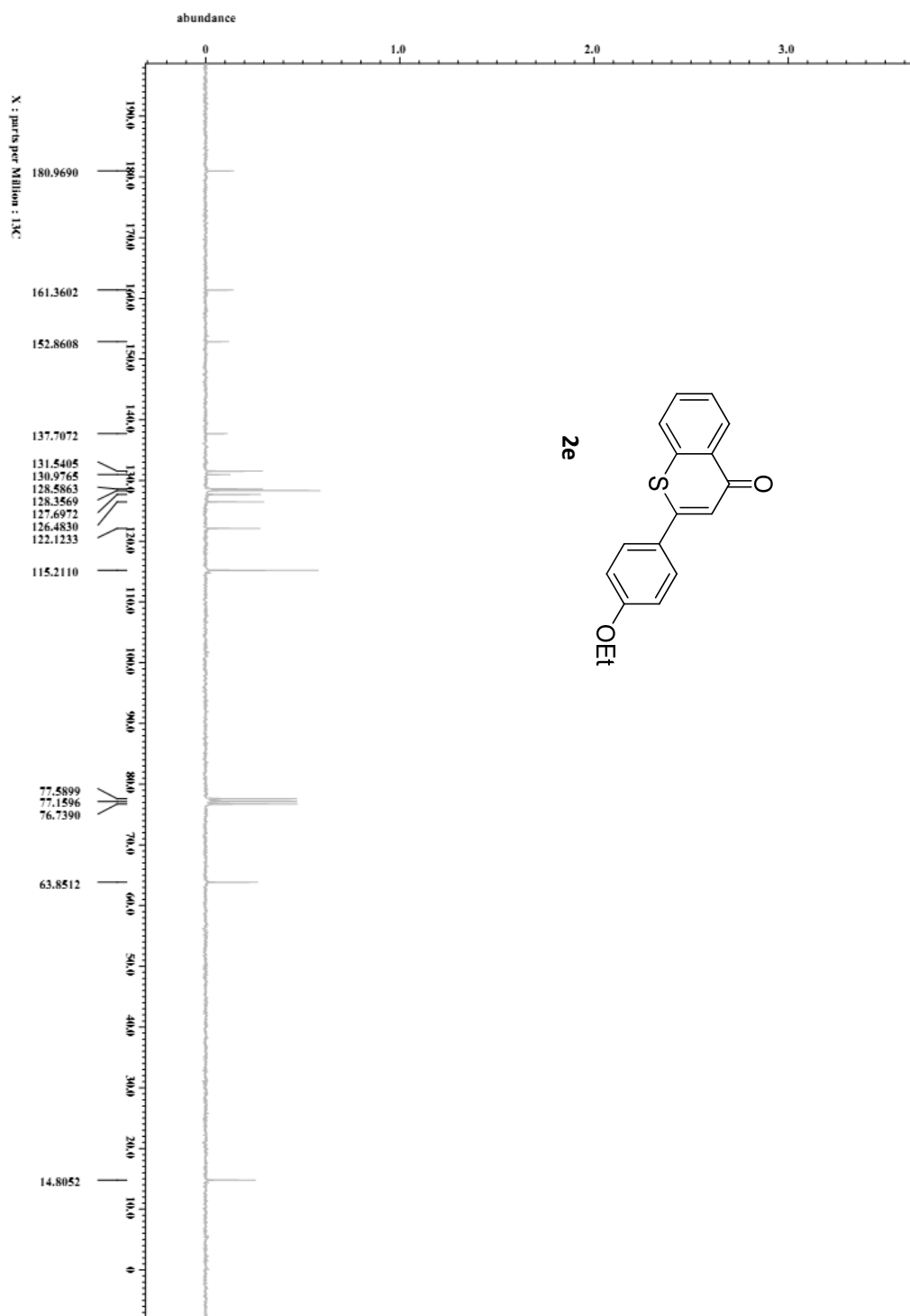


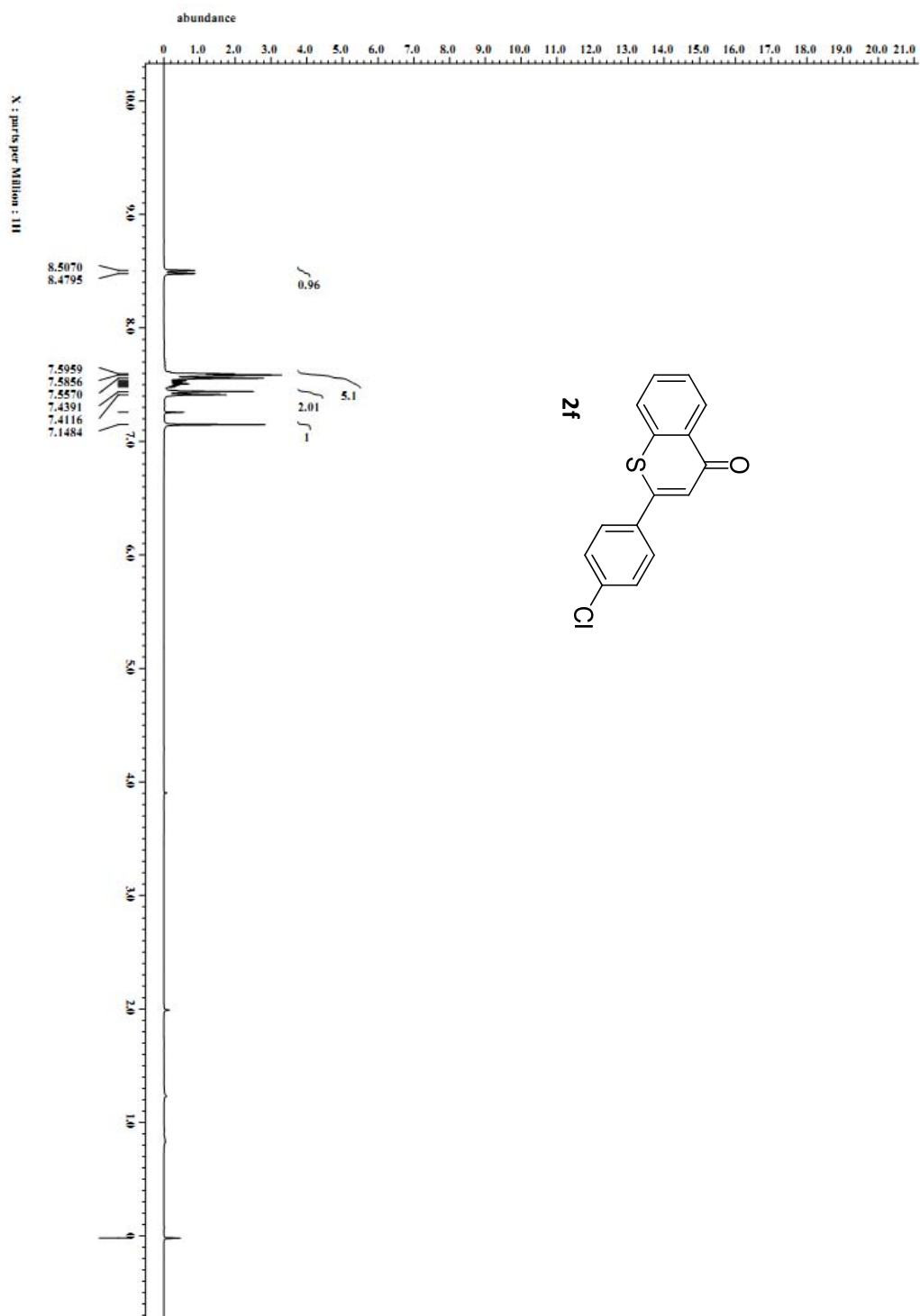


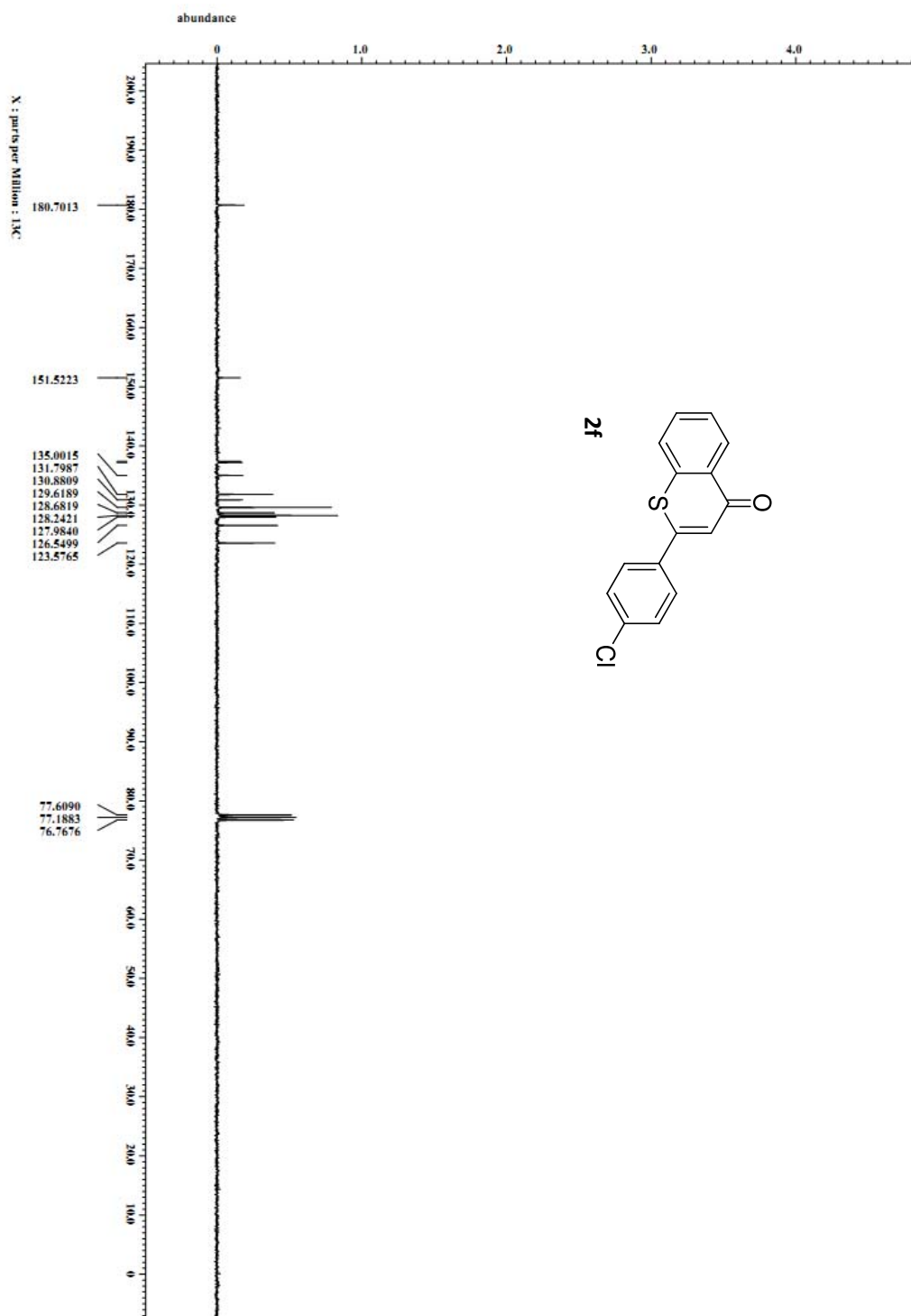


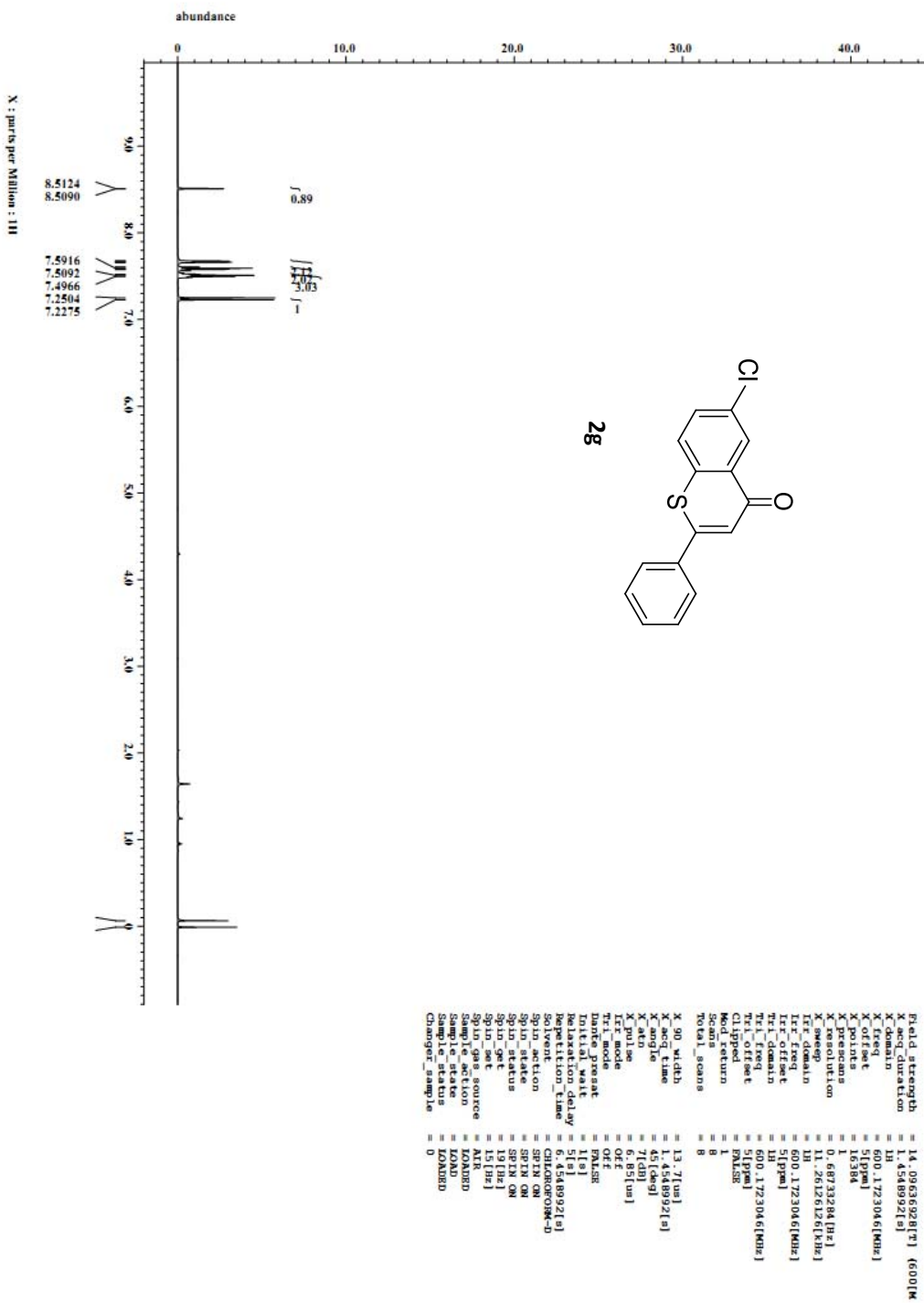


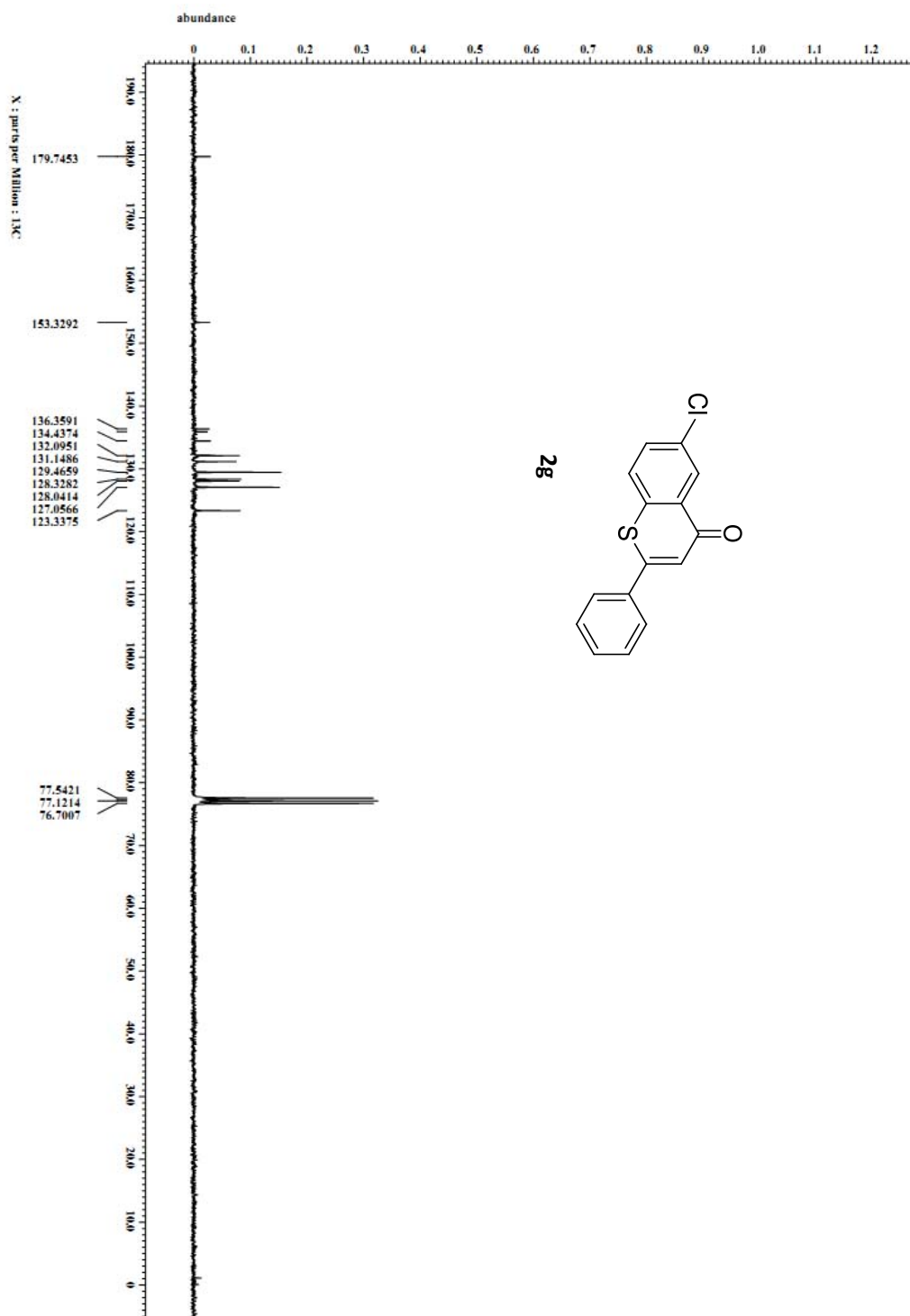


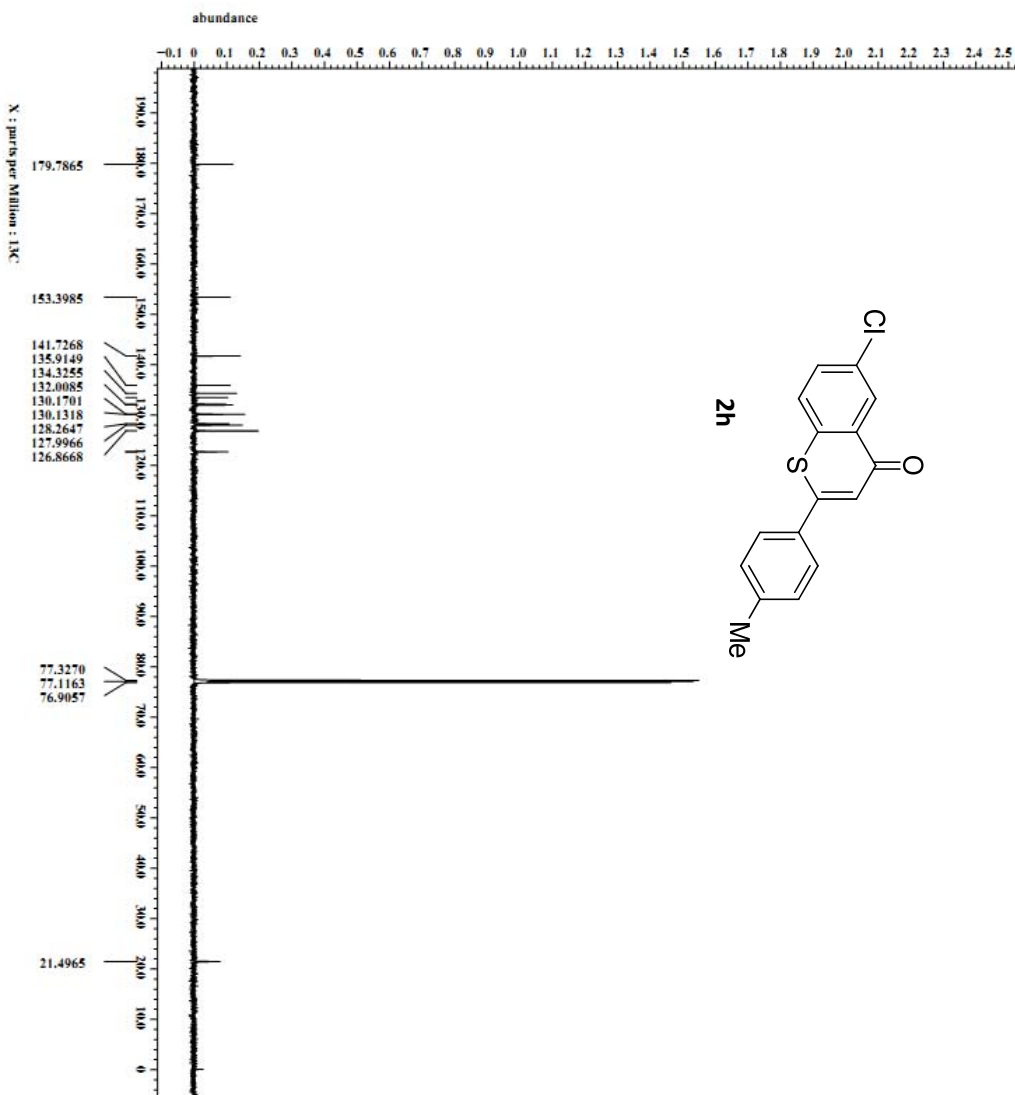






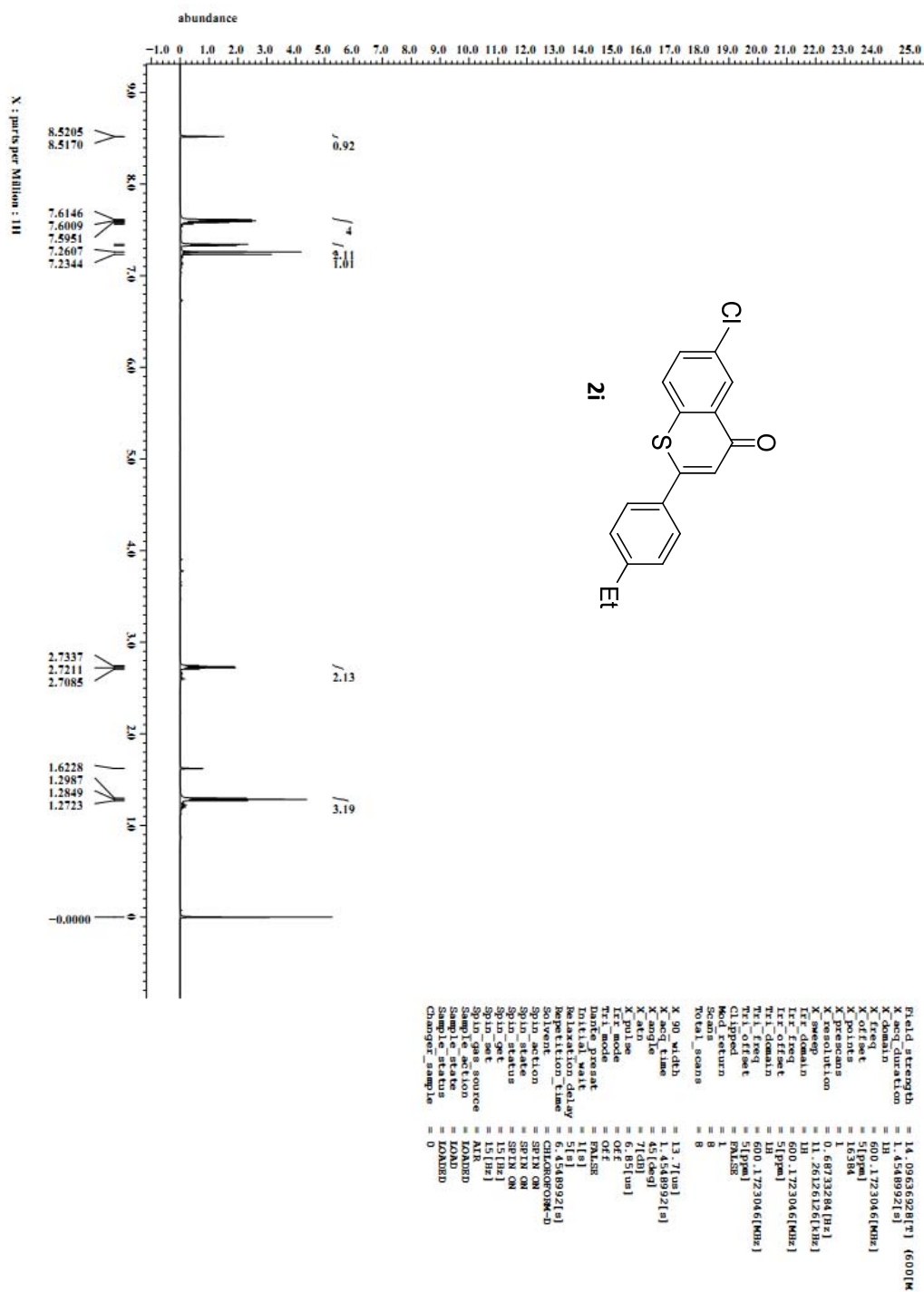


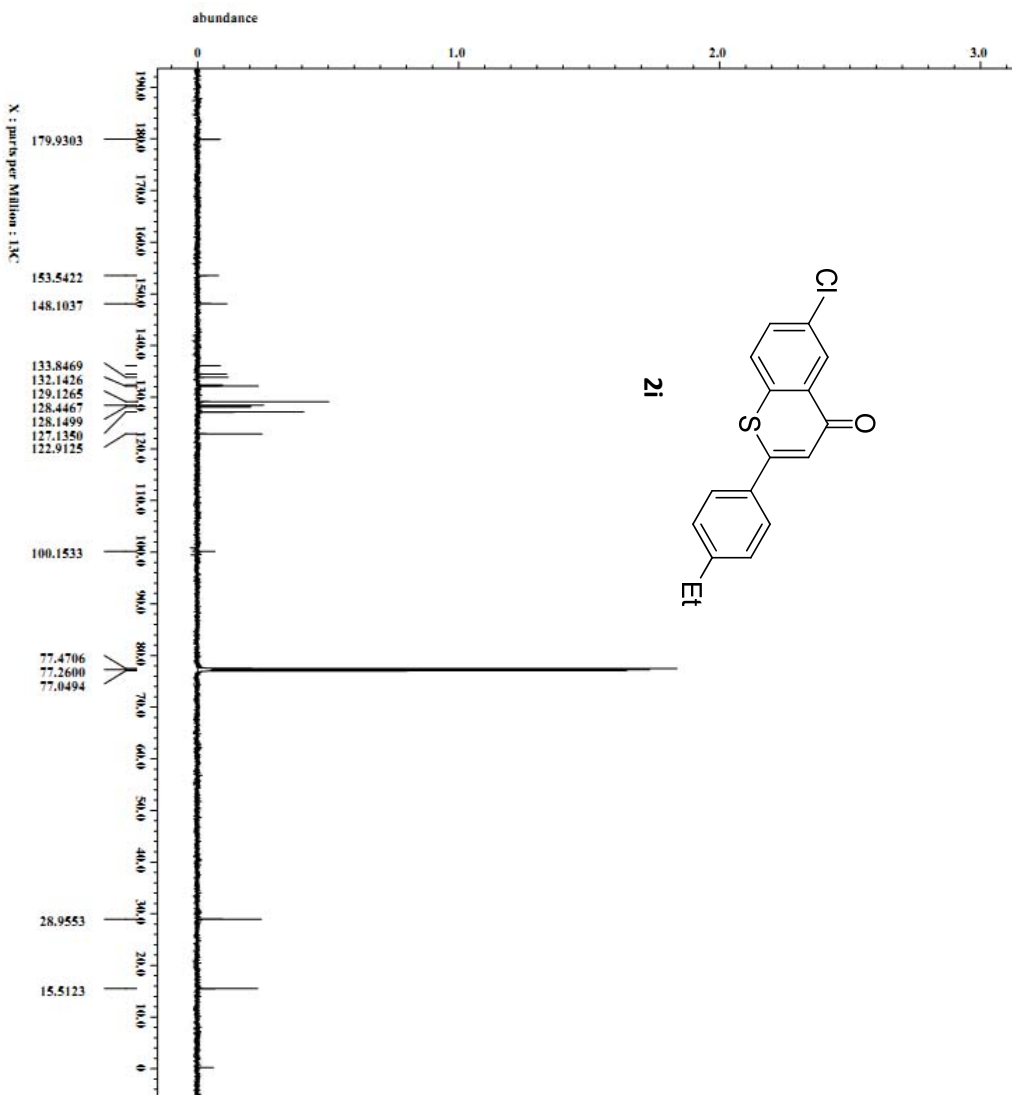




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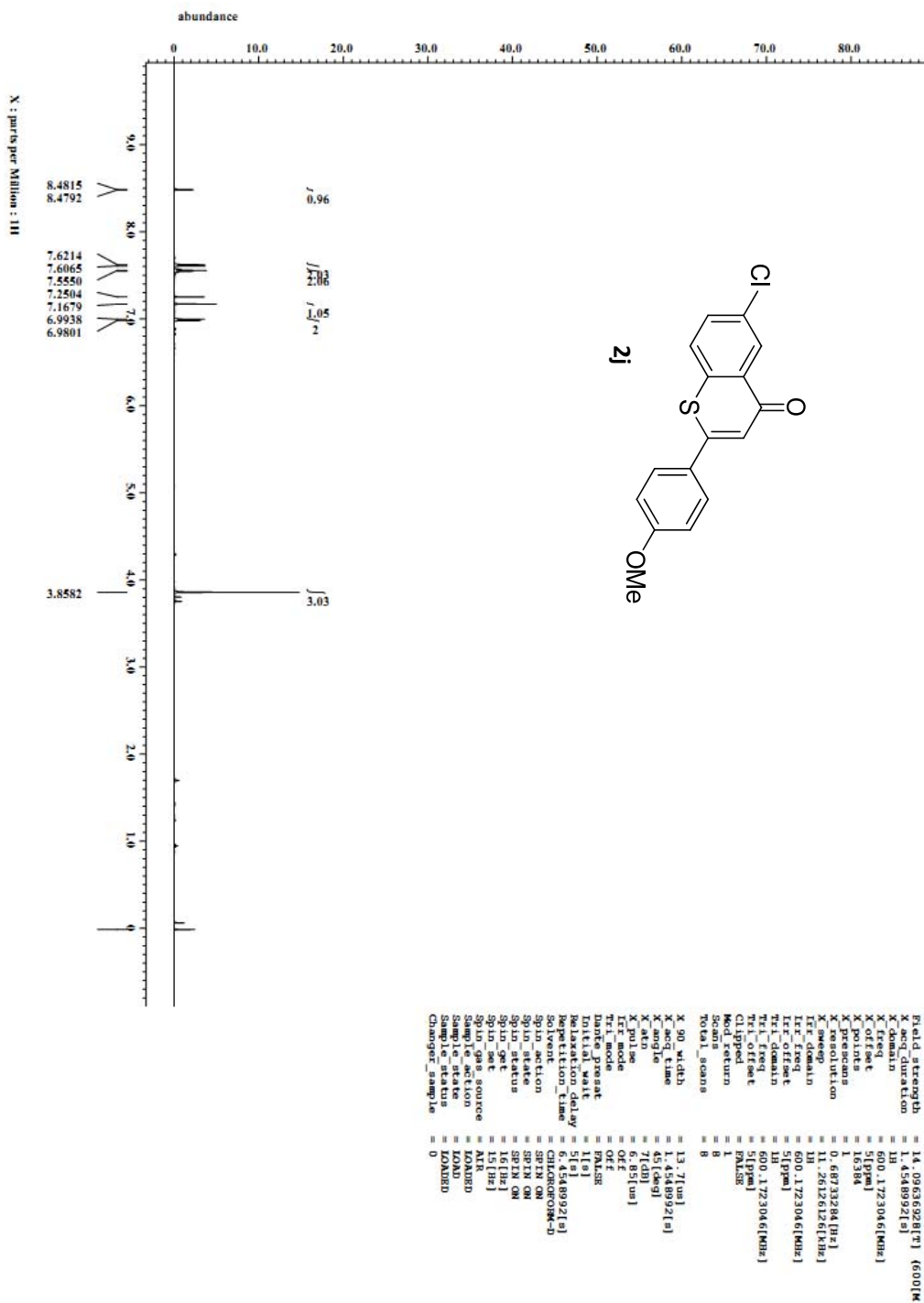
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X_freq = 150.91343030 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 4.44496100 [Hz]
X_resolution = 47.34848485 [kHz]
X_domain = 600.17230461 [MHz]
X_offset = 51 [ppm]
Clipped_spectrum_copy = 1
Mod_return = 1
Seams = 487
Total_scans = 487
X_90_width = 13.25 [us]
X_acq_time = 0.69206016 [s]
X_angle = 30 [deg]
X_atn = 10.66 [dB]
X_pulse = 4.4166667 [us]
X_pulse_dac = 10.66 [dB]
X_pulse_noise = 19.68 [dB]
X_noise = WALTZ
Decoupling = TRUE
Inletial_wait = 1[s]
Noe_time = 2[s]
Relaxation_delay = 2[s]
Repetition_time = 2.69206016 [s]
Solvent = CDCl3
Spin_action = SPIN ON
Spin_delay = 18 [Hz]
Spin_get = 15 [Hz]
Spin_set = 15 [Hz]
Spin_gate_source = AIRBURST
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Sample_status = LOAHD
Charger_sample = 0
    
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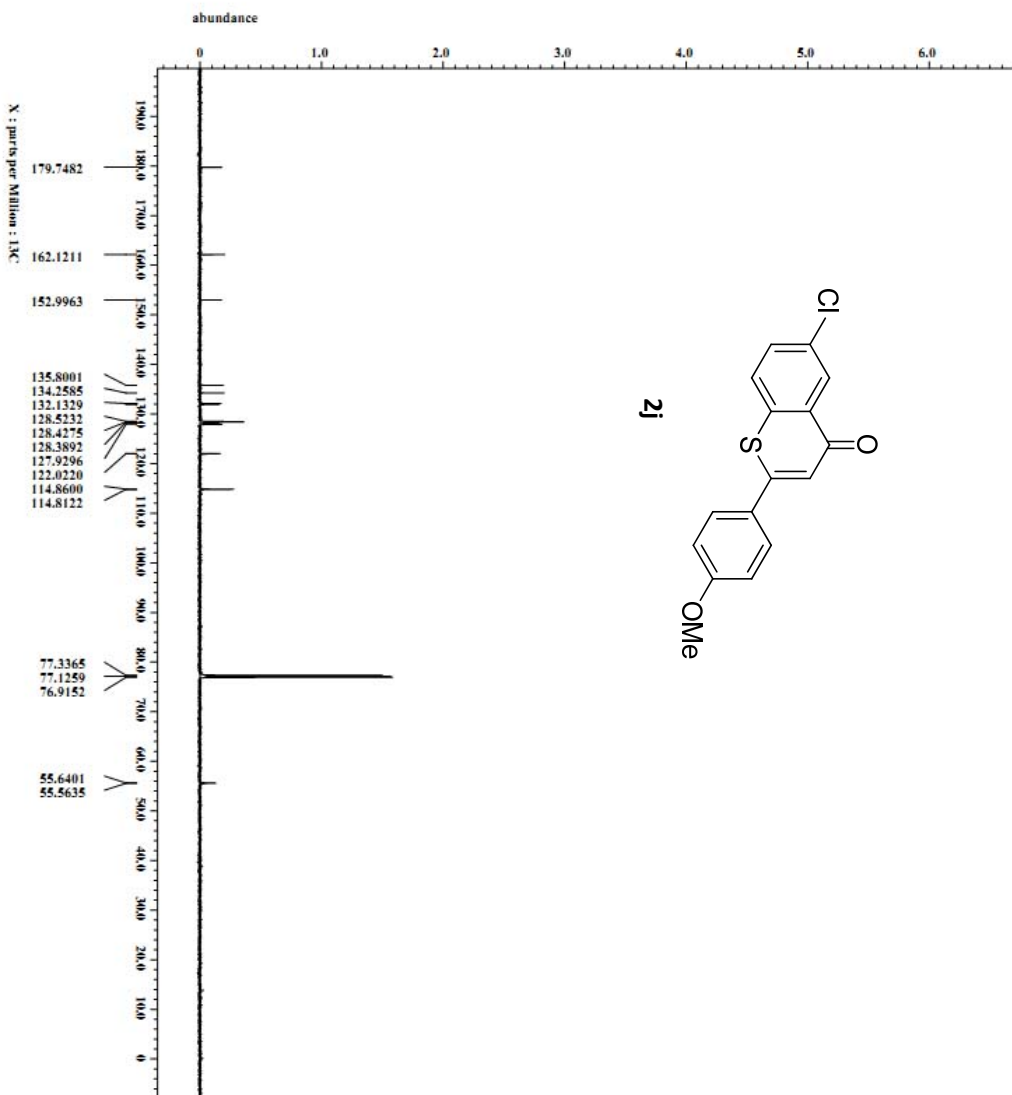




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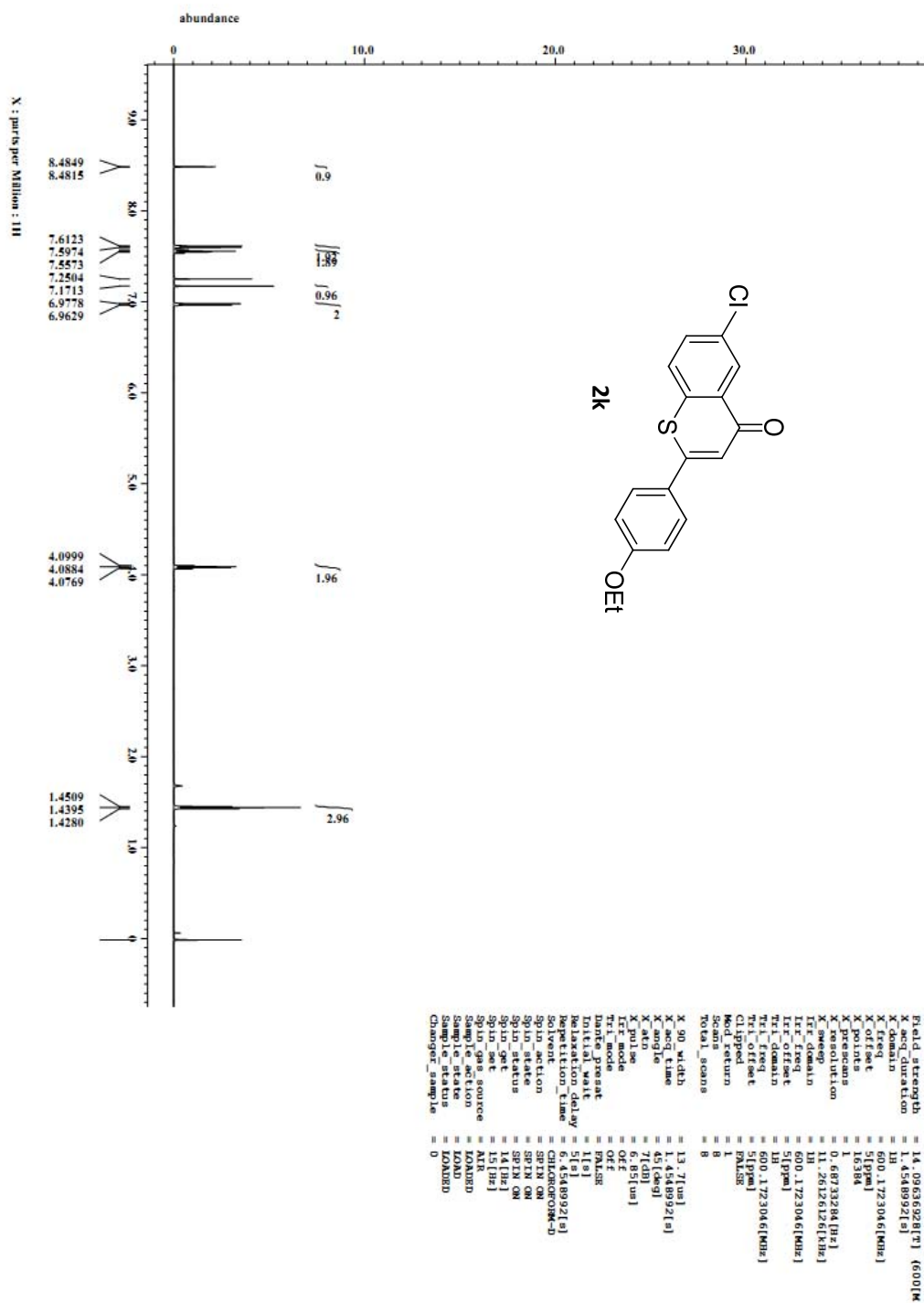
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X_freq = 150.91343030 [MHz]
X_ofset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 4.44196100 [Hz]
X_sweep = 47.34848485 [kHz]
Ir_domain = 600.1723046 [kHz]
Ir_freq = 51 [ppm]
Ir_ofset = TRUE
Clipped = TRUE
No_return = 441
Total_scans = 441
X_90_width = 13.25 [us]
X_delay = 0.69206016 [s]
X_angle = 30 [deg]
X_atn = 10.66 [dB]
X_pulse = 4.4166667 [us]
Ir_atn_dec = 19.68 [dB]
Ir_on_time = 19.68 [us]
Ir_noise = MAVE
Decoupling = TRUE
Initial_wait = 1[s]
Noe_time = TRUE
Noe_delay = 2[s]
Repetition_delay = 2[s]
Repetition_time = 2.69206016 [s]
Solvent = CHLOROFORM-D
Spin_action = SPTX ON
Spin_delay = 30 [us]
Spin_echo = 14 [Hz]
Spin_get = 14 [Hz]
Spin_set = 15 [Hz]
Spin_gas_source = AIR
Sample_action = LOCKED
Sample_status = LOCKED
Changer_sample = 0
    
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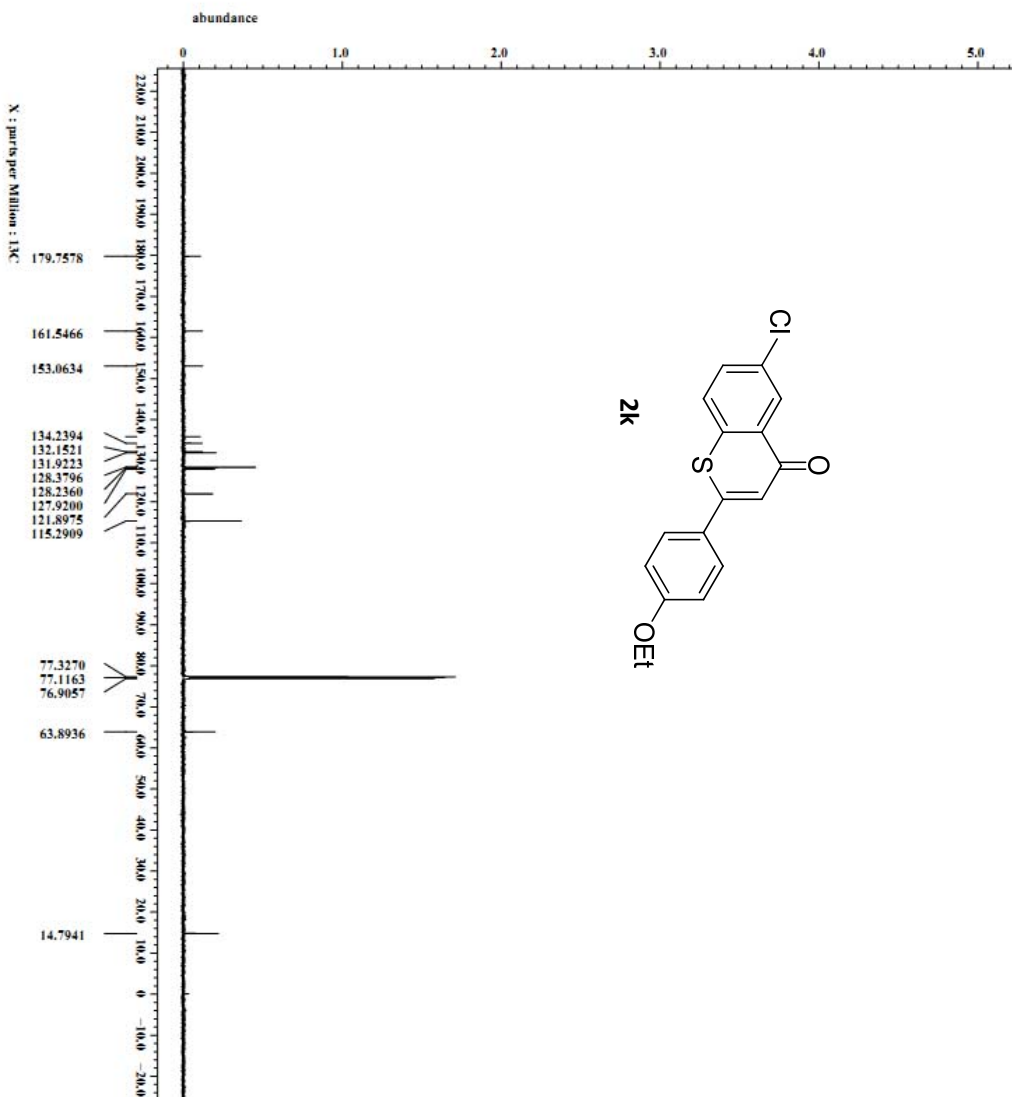




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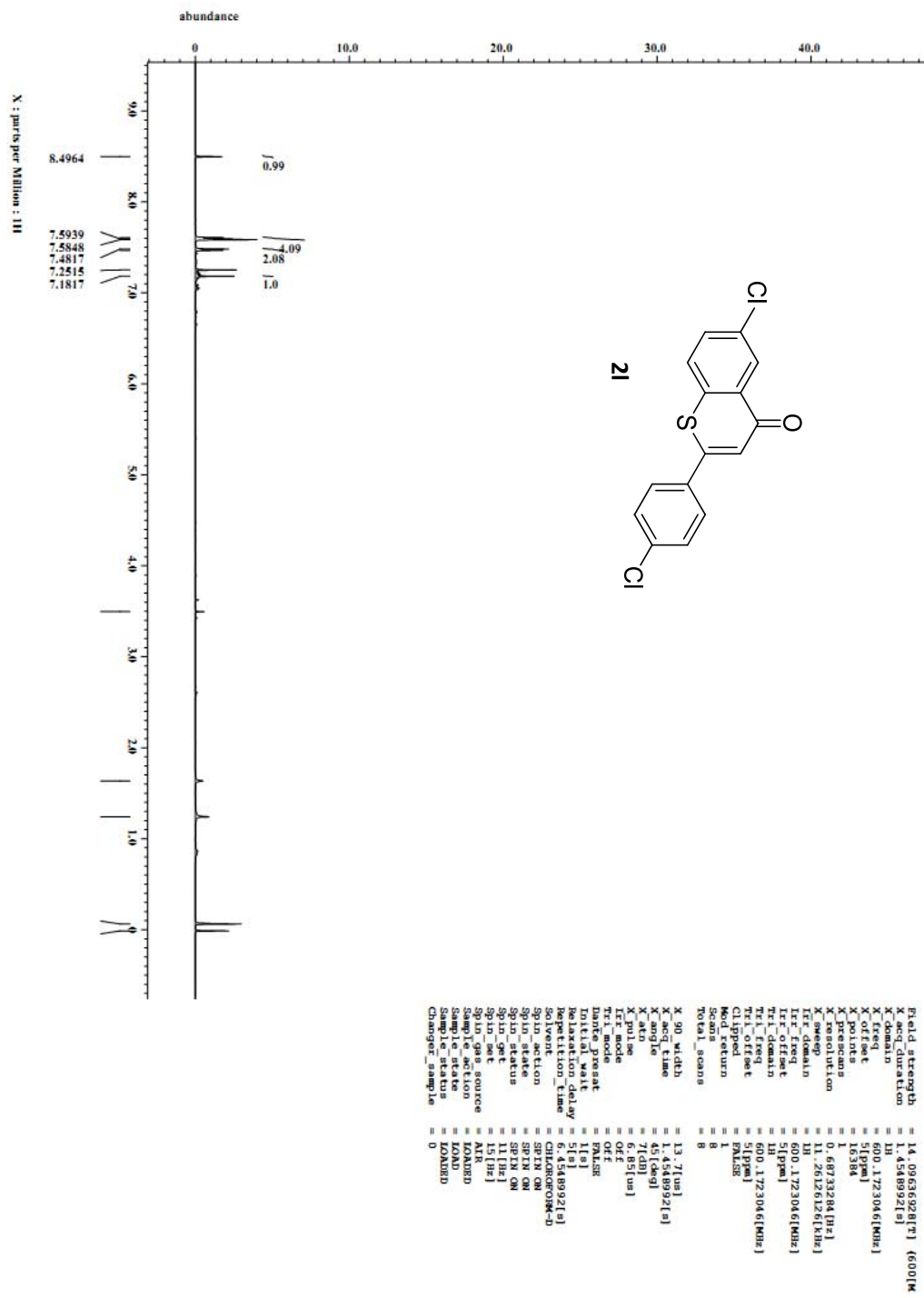
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X_chan = 13
X_freq = 150.91343030 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 4.44196100 [Hz]
X_sweep = 47.34848485 [kHz]
Ir_domain = 600.1723046 [MHz]
Ir_offset = 51 [ppm]
Clipped = FALSE
No_return = 263
Total_scans = 263
X_90_width = 13.25 [us]
X_180_width = 0.76320106 [us]
X_angle = 30 [deg]
X_atn = 10.66 [dB]
X_pulse = 4.4166667 [us]
Ir_atn_dec = 19.68 [dB]
Ir_atn_inc = 19.68 [dB]
Ir_noise = MUTE
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_delay = 2 [s]
Repetition_delay = 2.69206016 [s]
Solvent = CHLOROFORM-D
Spin_action = SPTN ON
Spin_echo = SPTN ON
Spin_echoes = 30
Spin_get = 16 [Hz]
Spin_set = 15 [Hz]
Spin_gas_source = AIR
Sample_action = LOCKED
Sample_status = LOCKED
Change_sample = 0
    
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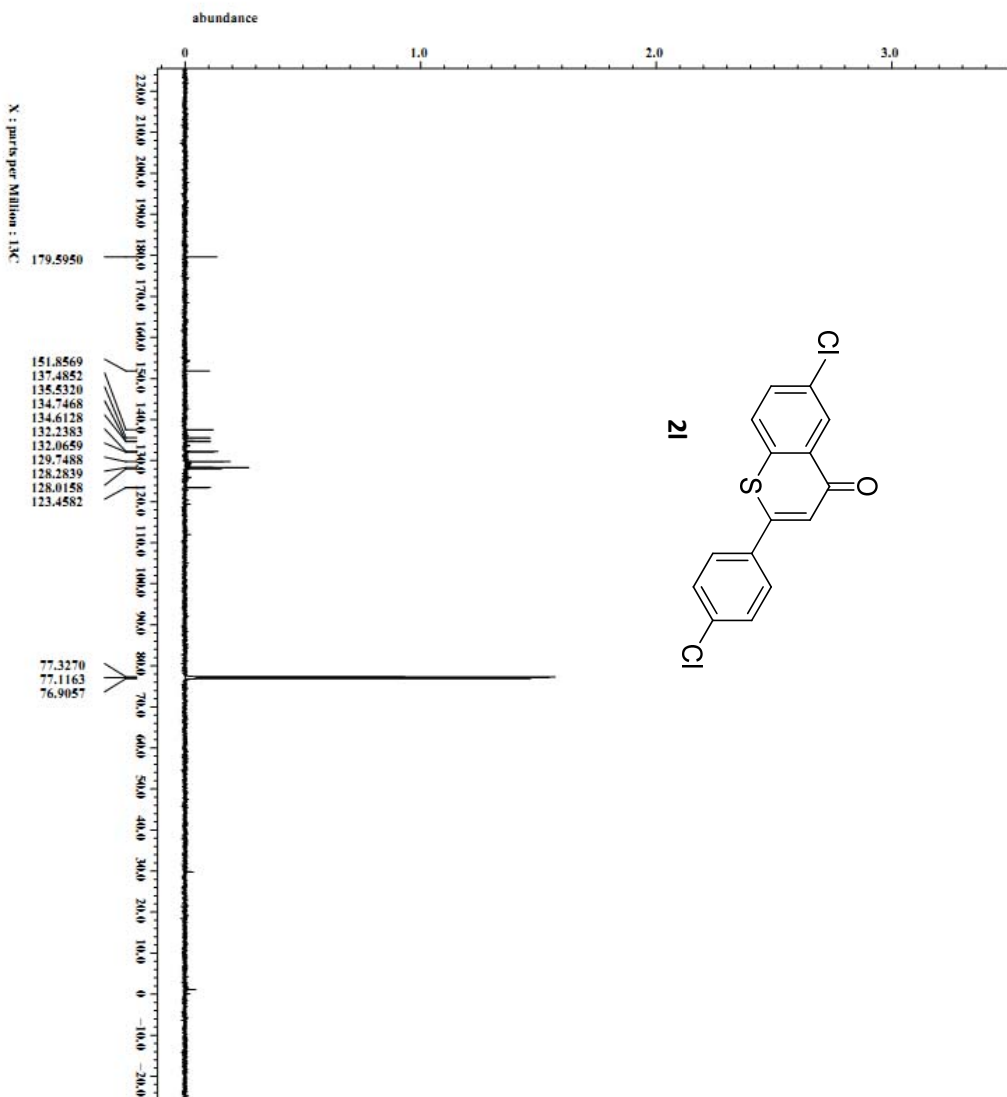




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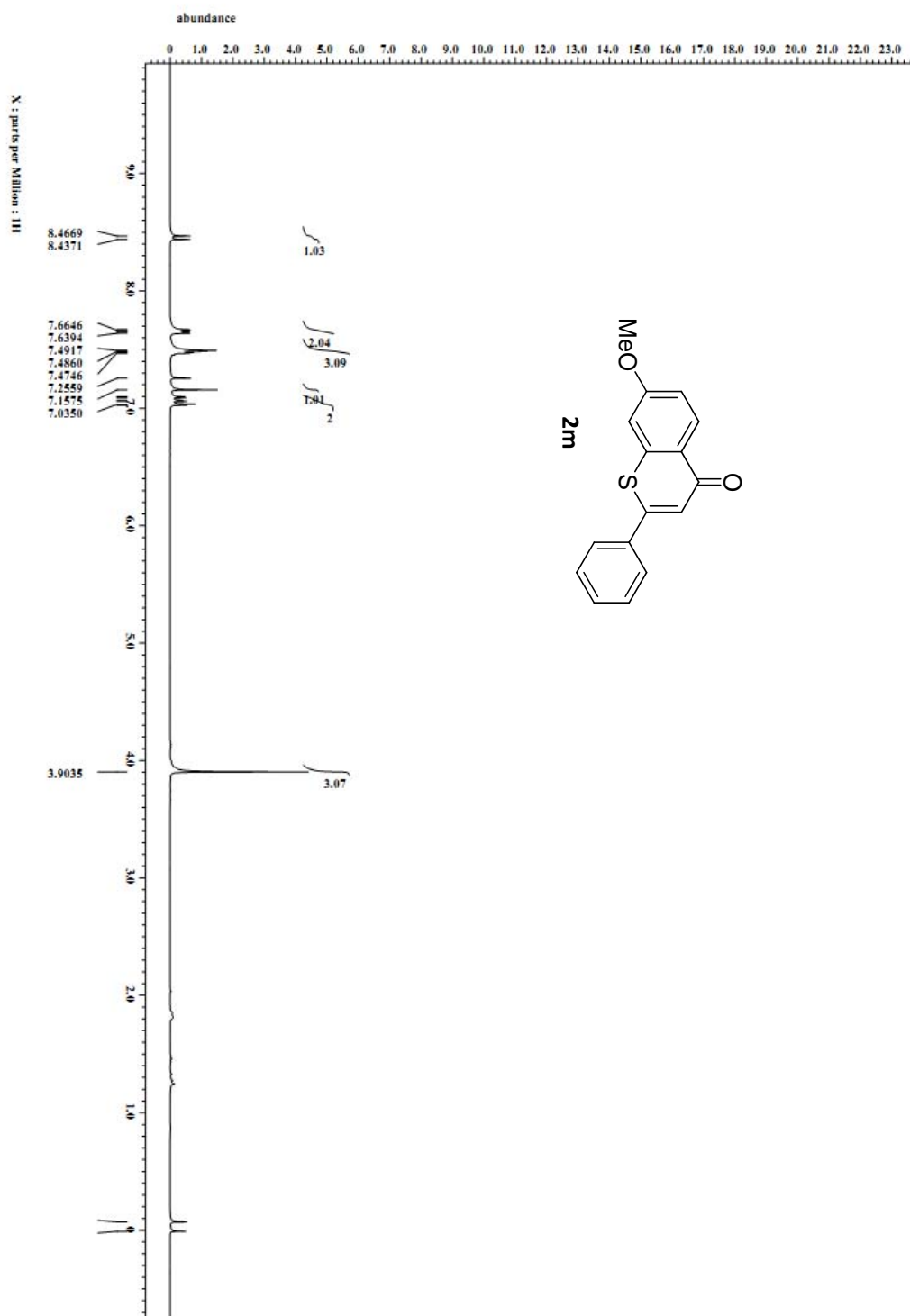
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X_freq = 150.91343030 [MHz]
X_ofset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 4.44496100 [Hz]
X_sweep = 47.34848485 [kHz]
Ir_domain = 600.1723046 [MHz]
Ir_ofset = 51 [ppm]
Clipped = FALSE
No_return = 355
Total_scans = 355
X_90_width = 13.25 [us]
X_delay = 0.69206016 [s]
X_angle = 30 [deg]
X_atn = 10.66 [dB]
X_pulse = 4.4166667 [us]
Ir_atn_dec = 19.68 [dB]
Ir_on_time = 19.68 [us]
Ir_noise = MUTE [dB]
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_delay = 2 [s]
Repetition_delay = 2.69206016 [s]
Repetition_time = 2.69206016 [s]
Solvent = CHLOROFORM-D
Spin_action = SPTX ON
Spin_delay = 30 [us]
Spin_echo = SPTX ON
Spin_echo_delay = 15 [us]
Spin_set = 15 [Hz]
Spin_gas_source = AIR
Sample_action = LOCKED
Sample_status = LOCKED
Changer_sample = 0
    
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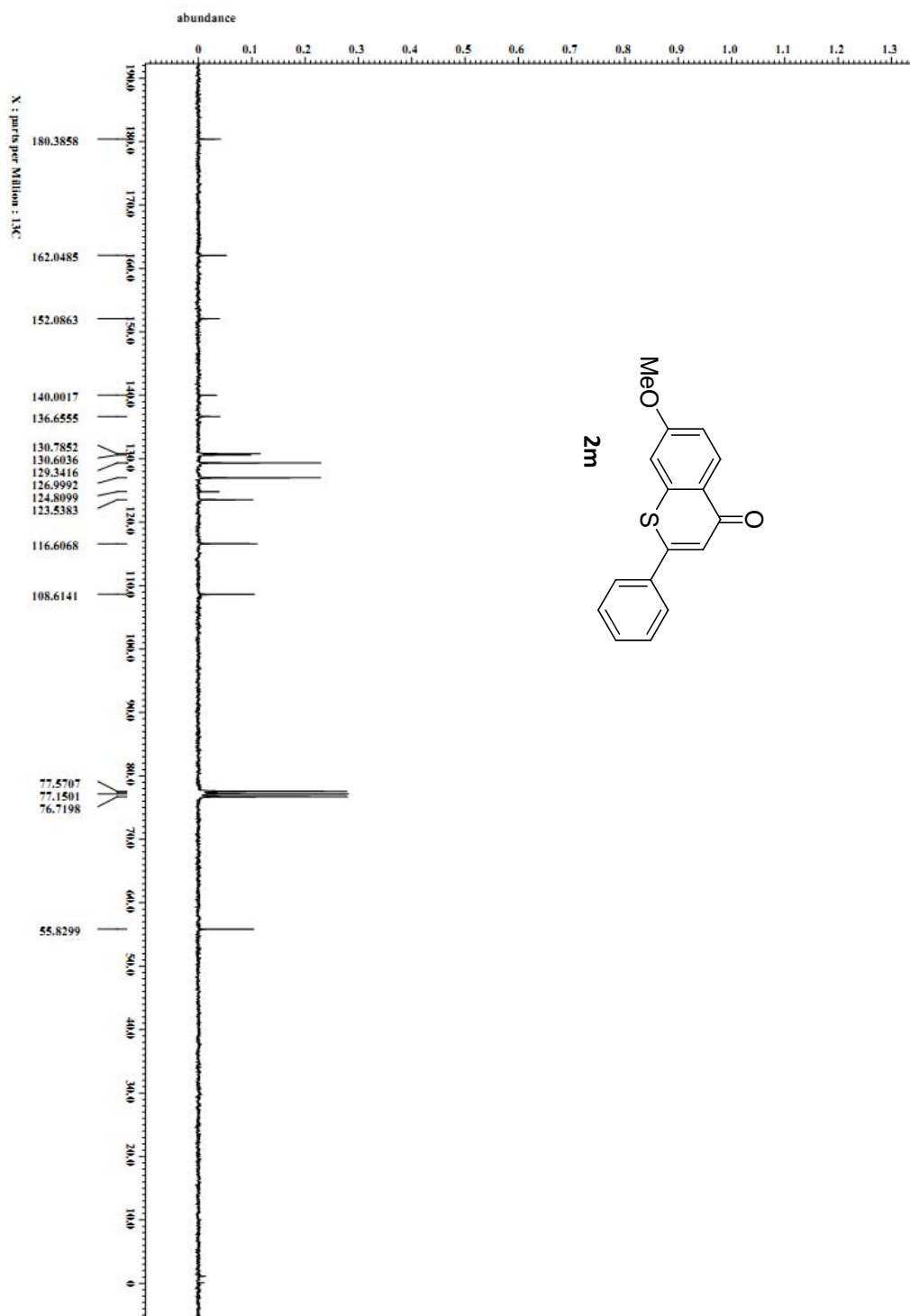


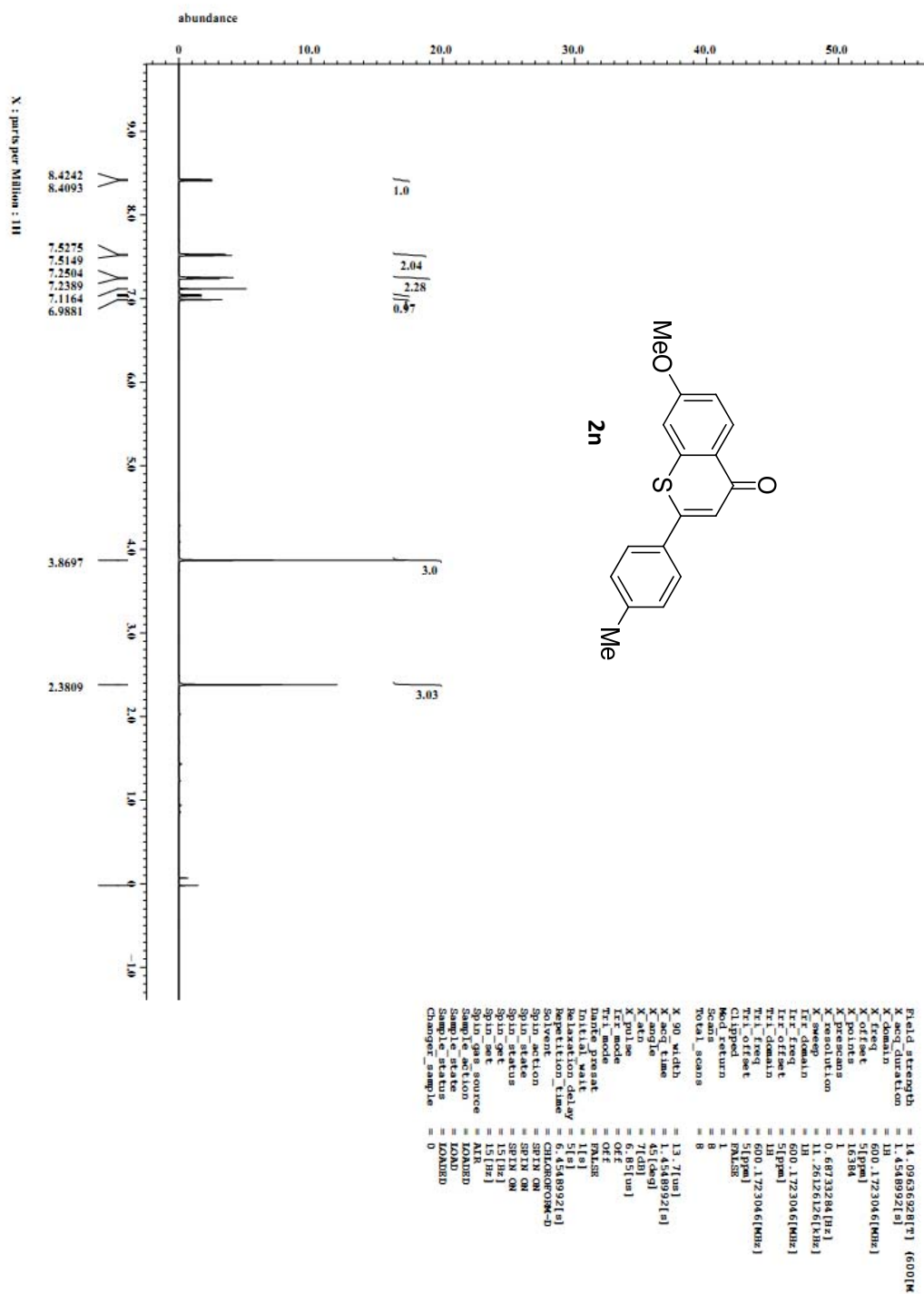


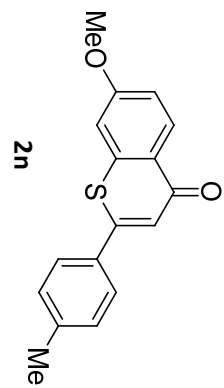
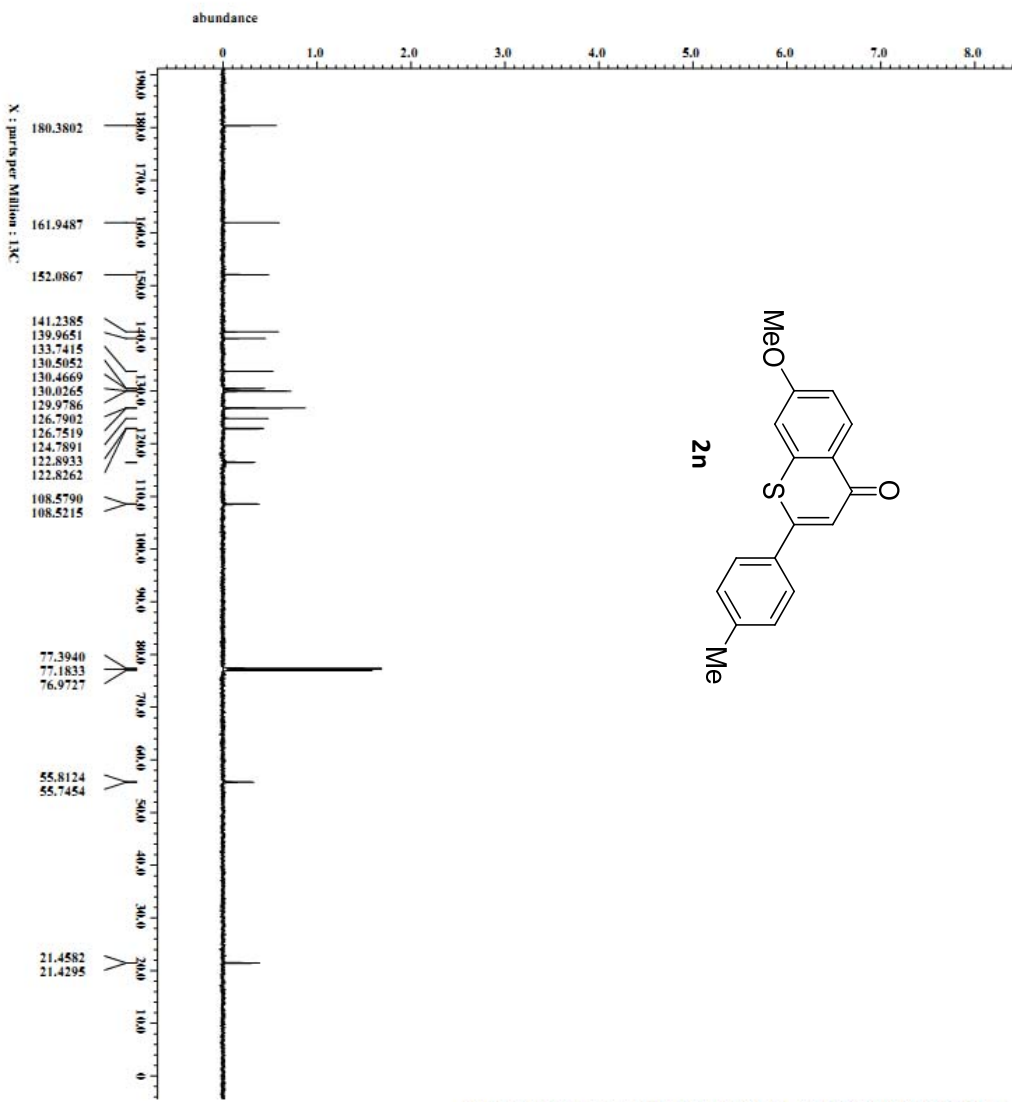
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Field_strength = 14.09636928171 (6001M
X_acq_duration = 0.69206016[s]
X_scan = 13
X_freq = 150.91343030 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 4.44196100 [Hz]
X_resolution = 47.34848485 [kHz]
Ir_domain = 600.17230461 [kHz]
Ir_offset = 51 [ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 442
X_90_width = 13.25 [us]
X_acq_time = 0.69206016 [s]
X_angle = 30 [deg]
X_atn = 10.66 [dB]
X_pulse = 4.4166667 [us]
Ir_ad_noise = 19.68 [dB]
Ir_noise = WALTZ
Decoupling = TRUE
Inletial_wait = 1[s]
Noe_time = 2[s]
Relaxation_delay = 2.69206016 [s]
Repetition_time = 2.69206016 [s]
Solvent = CDCl3(CROCI3-D)
Spin_action = SPIN ON
Spin_delay = 17 [Hz]
Spin_get = 15 [Hz]
Spin_set = 15 [Hz]
Spin_gate_source = AIRBURD
Sample_delay = 10.00 [s]
Sample_status = LOABD
Charger_sample = 0
    
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Field_strength = 14.09636928171 (6001M
X_acq_duration = 0.69206016[s]
X_chan = 13
X_freq = 150.91343030 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 4.44496100 [Hz]
X_sweep = 47.34848485 [kHz]
Ir_domain = 600.1723046 [kHz]
Ir_offset = 51 [ppm]
Clipped = FALSE
Mv_return = 91
Scans = 91
Total_scans = 91
X_90_width = 13.29 [us]
X_pulse = 0.69206016 [s]
X_angle = 30 [deg]
X_atn = 10.66 [dB]
X_pulse = 4.4166667 [us]
Ir_atn_dec = 19.68 [dB]
Ir_atn_inc = 19.68 [dB]
Ir_noise = NALYZE [dB]
Decoupling = TRUE
Initial_wait = 1 [s]
Koe_time = TRUE
Koe_delay = 2 [s]
Repetition_delay = 2 [s]
Repetition_time = 2.69206016 [s]
Solvent = CHLOROFORM-D
Spin_action = SPIN ON
Spin_delay = 30 [ms]
Spin_echo = SPIN ON
Spin_echo = 14 [Hz]
Spin_set = 15 [Hz]
Spin_gas_source = AIR
Sample_action = LOCKED
Sample_status = LOCKED
Charger_sample = 0
    
```

