

Supporting Information

Scalable Synthesis and Cancer Cell Cytotoxicity of Rooperol and Analogues.

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¹ Dept. of Chemistry & Biochemistry, Texas State University, San Marcos, TX 78666

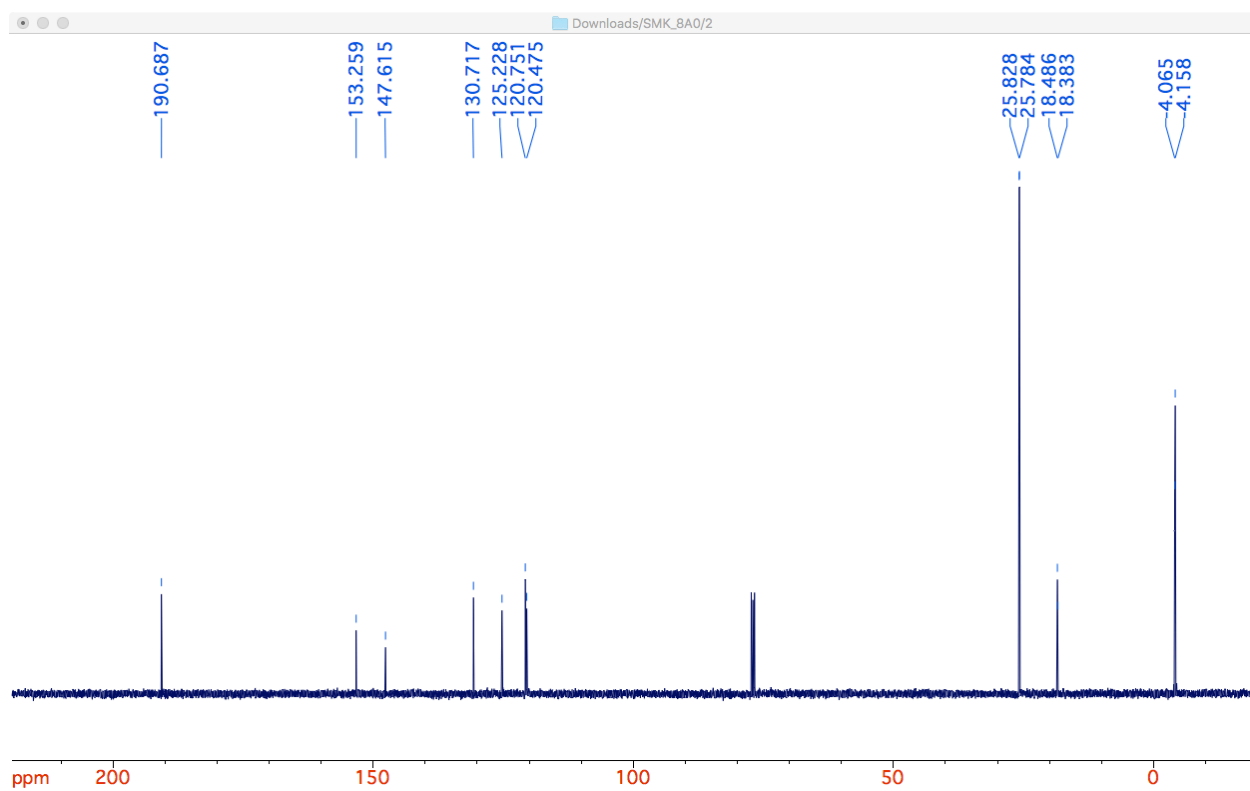
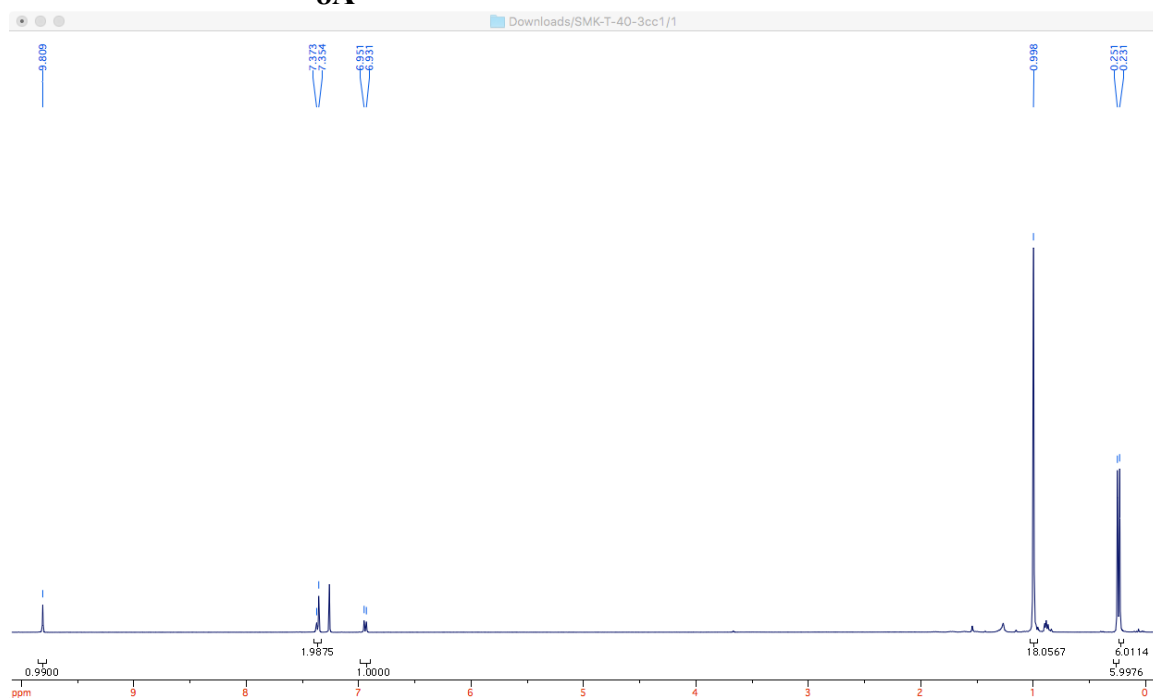
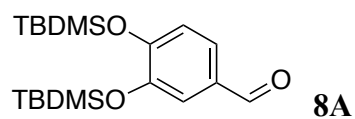
² Division of Chemical Biology and Medicinal Chemistry, University of Texas at Austin, Austin, TX, 78712

³ Materials Science, Engineering, and Commercialization Program, Texas State University, San Marcos, TX, 78666

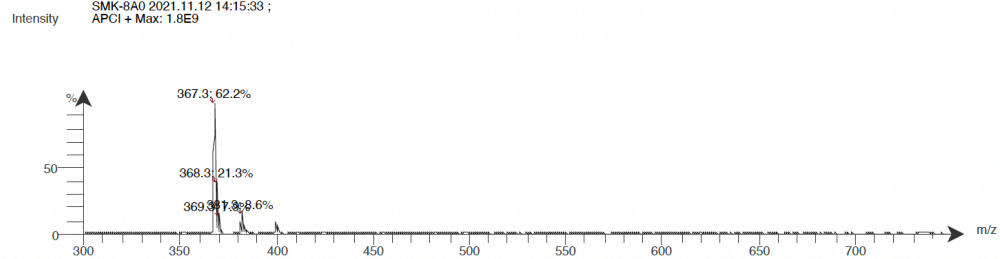
‡ Deceased August 27, 2018

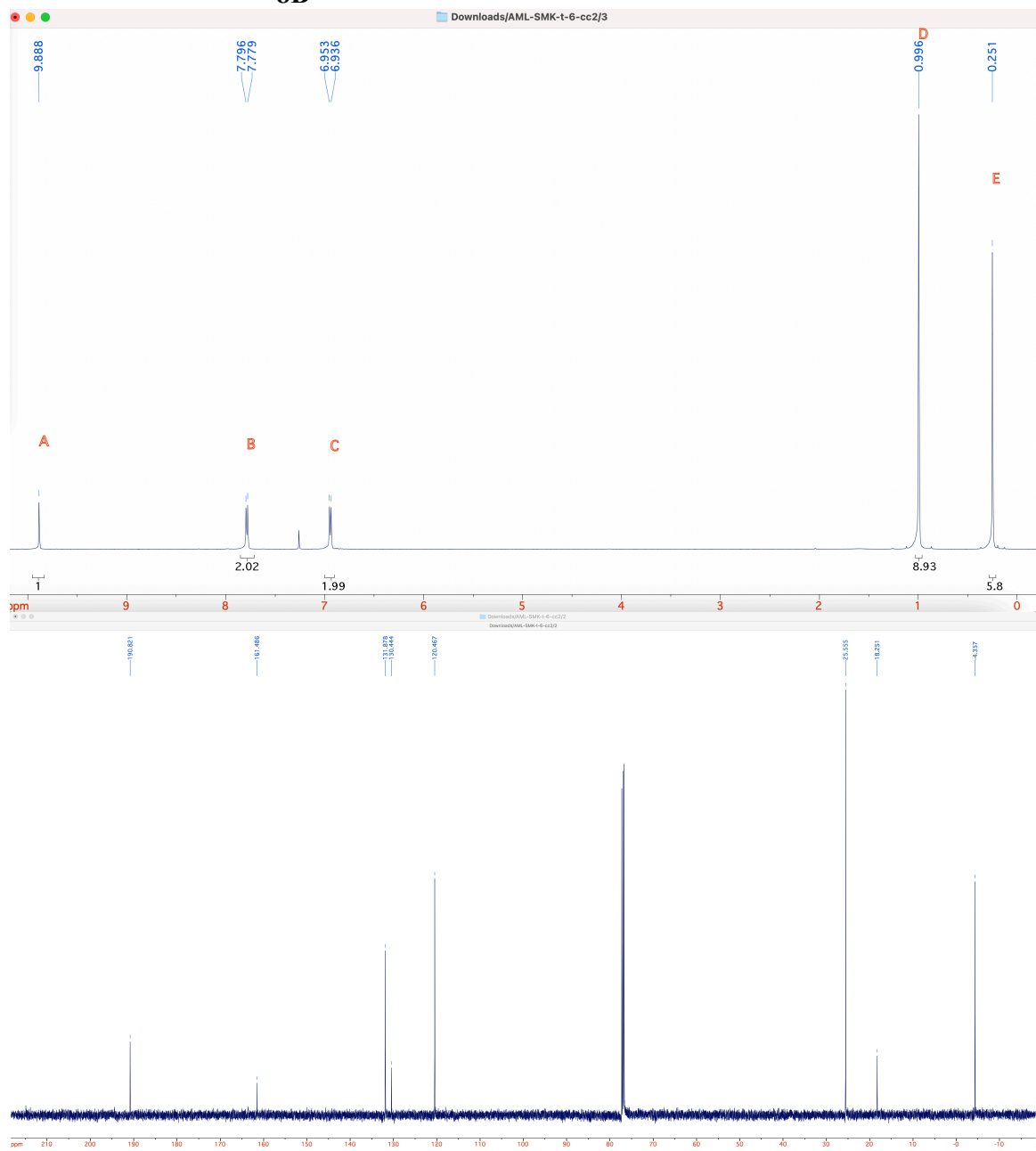
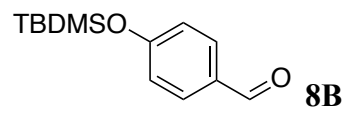
§ These authors made equal contributions to the work.

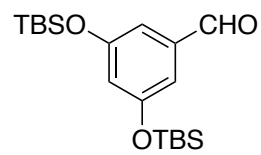
* Correspondence: smk89@txstate.edu; Tel.: +1 5122452056



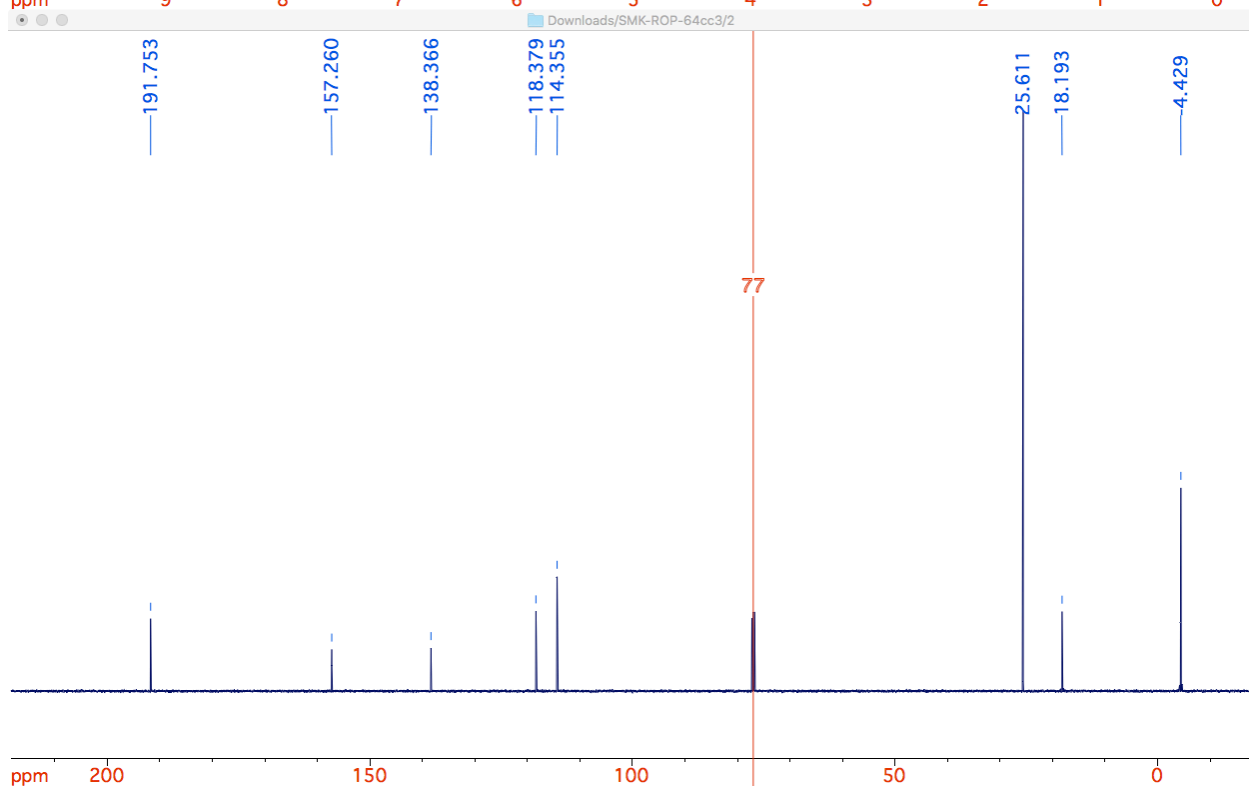
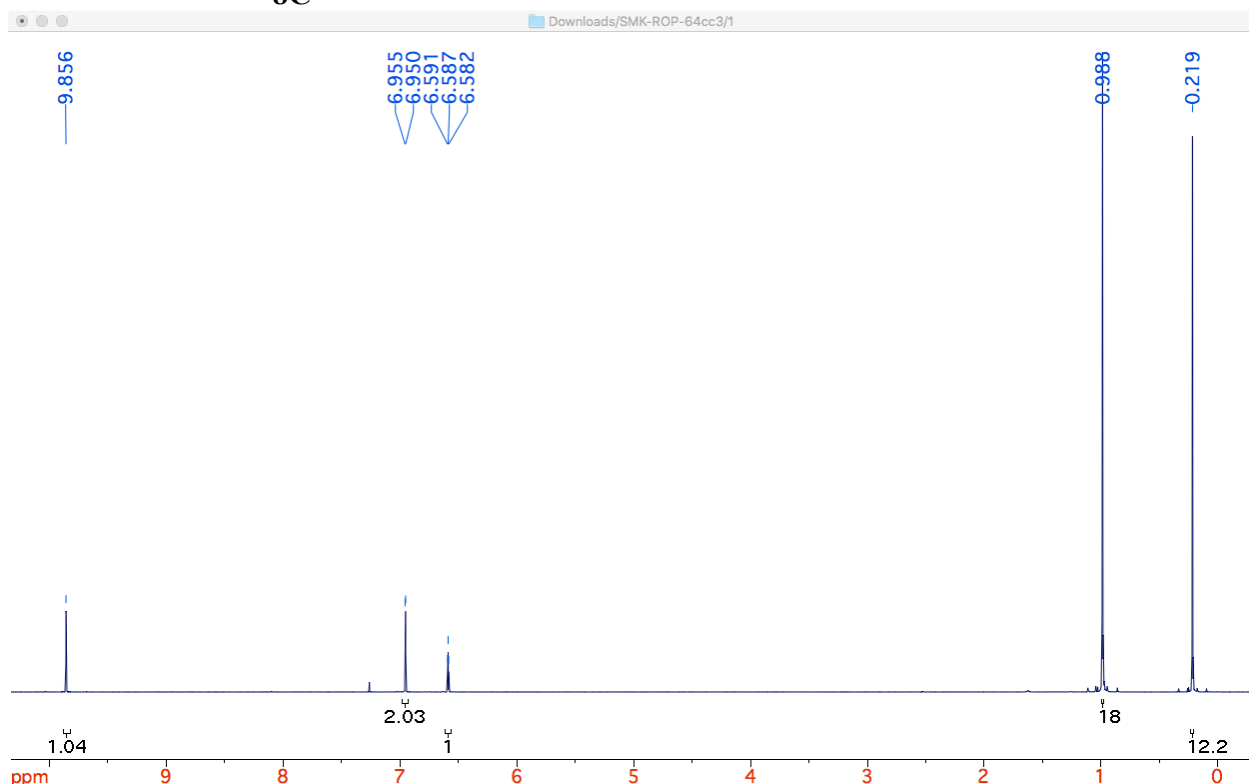
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APCI + Max: 1.8E9



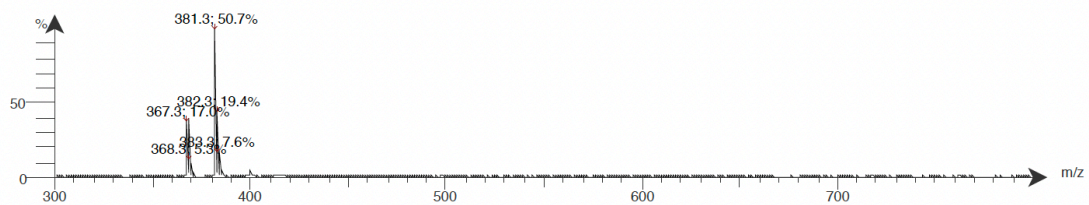


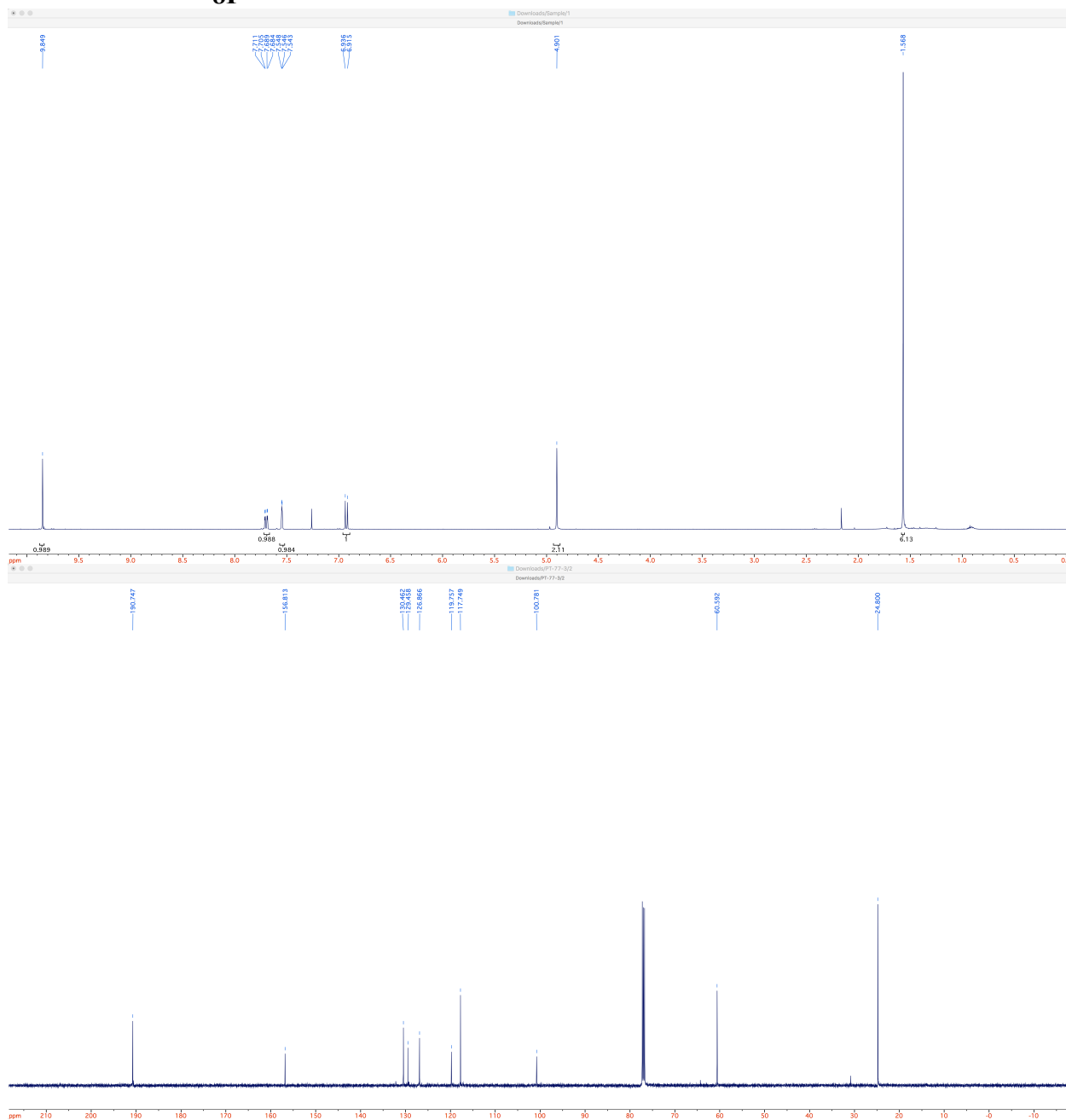


8C

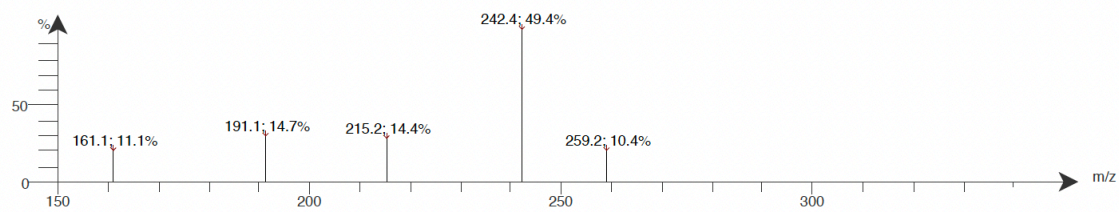


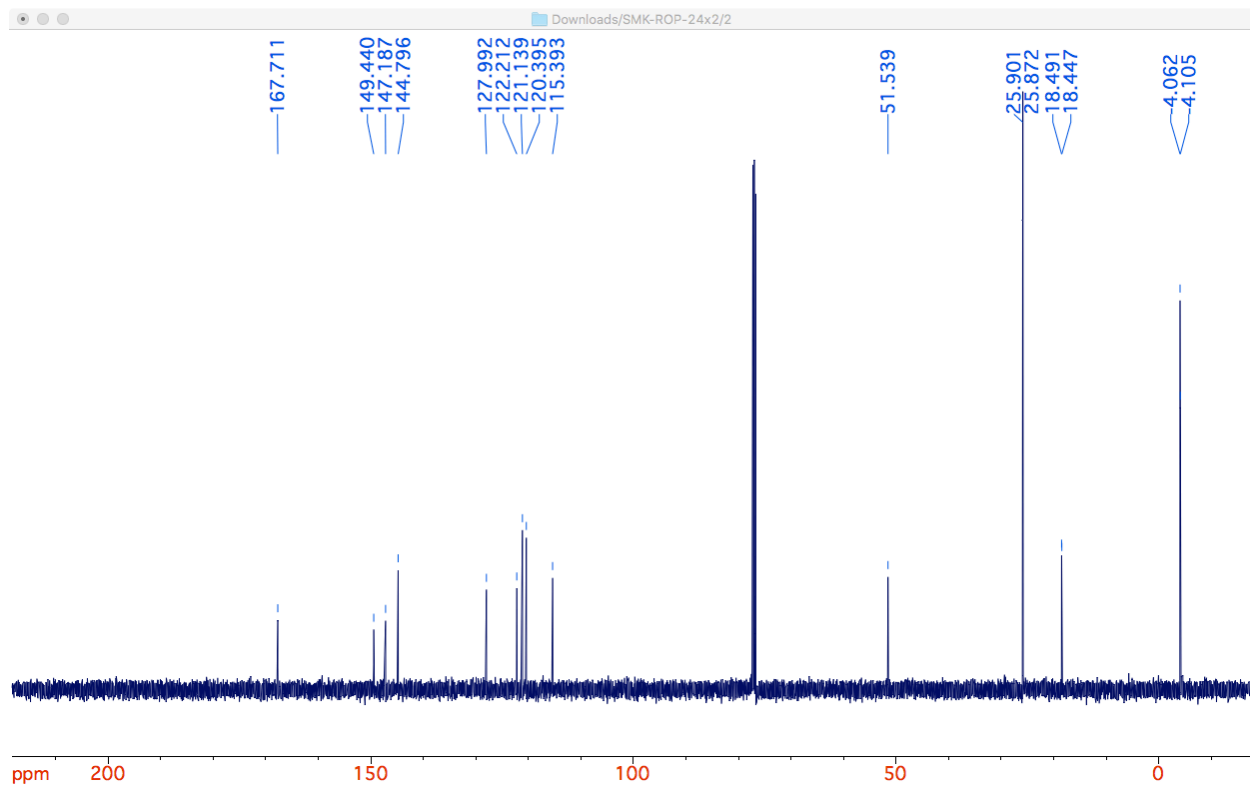
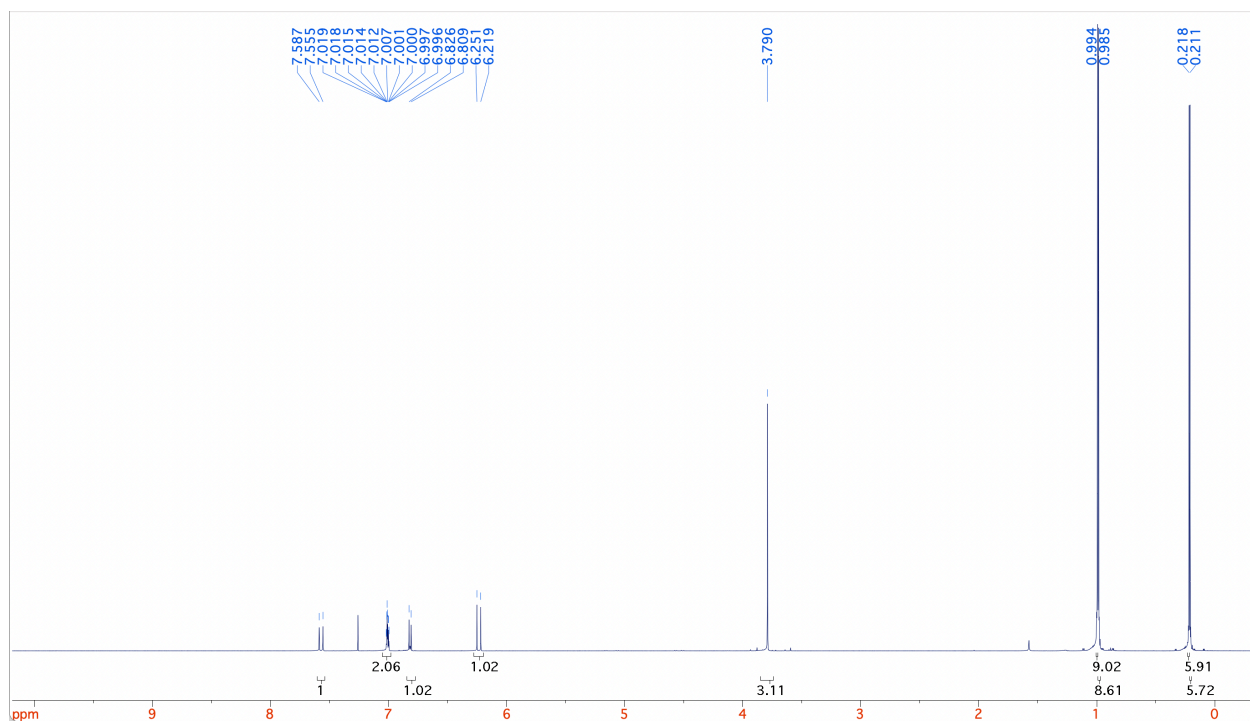
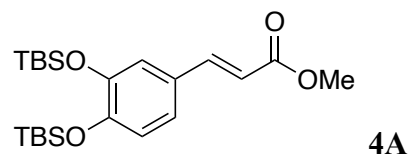
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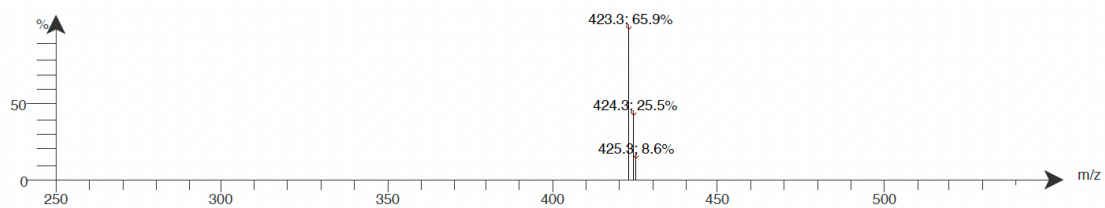


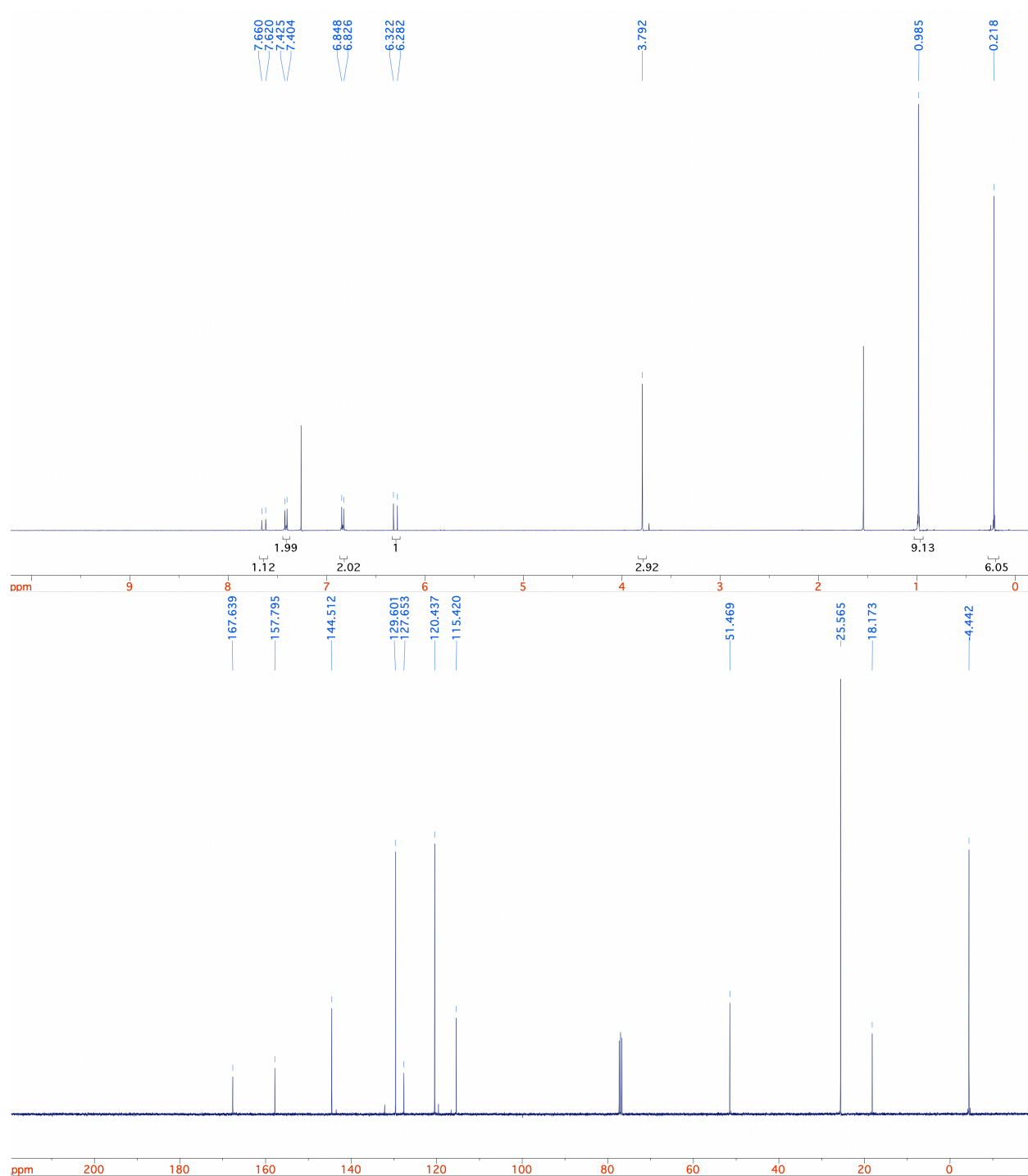
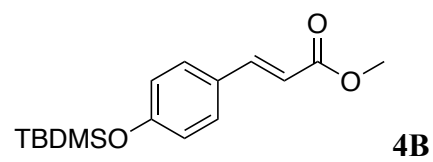
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PT-83-4_8C4_inj3.datx 2021.10.29 11:46:57 ;
ESI + Max: 2E8



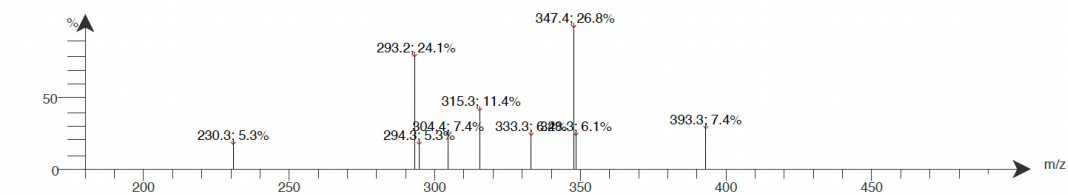


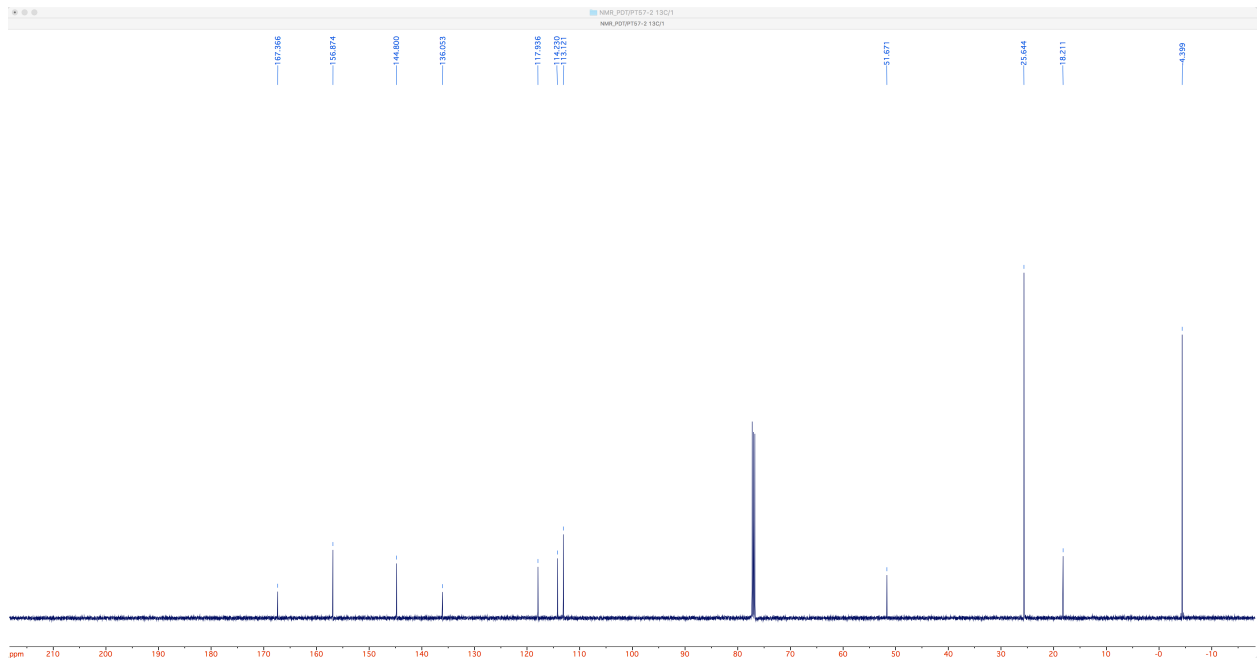
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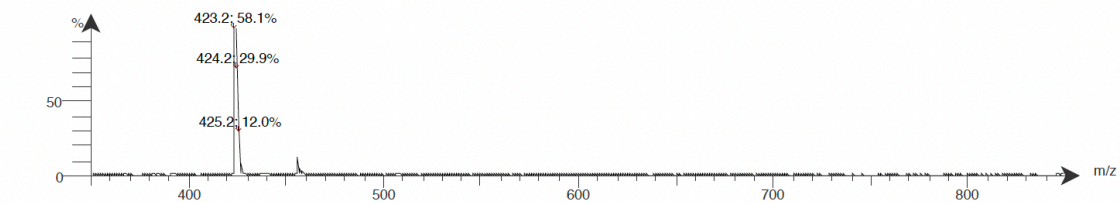


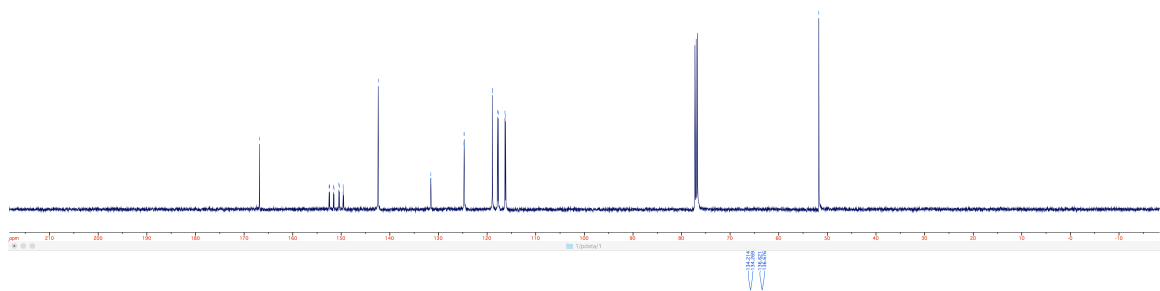
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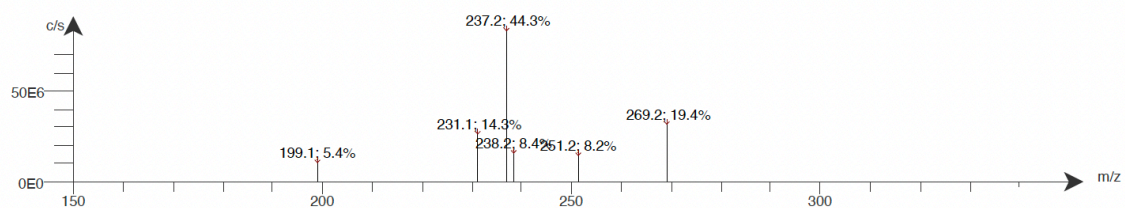


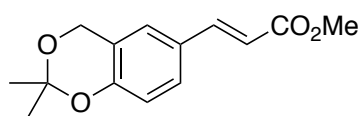
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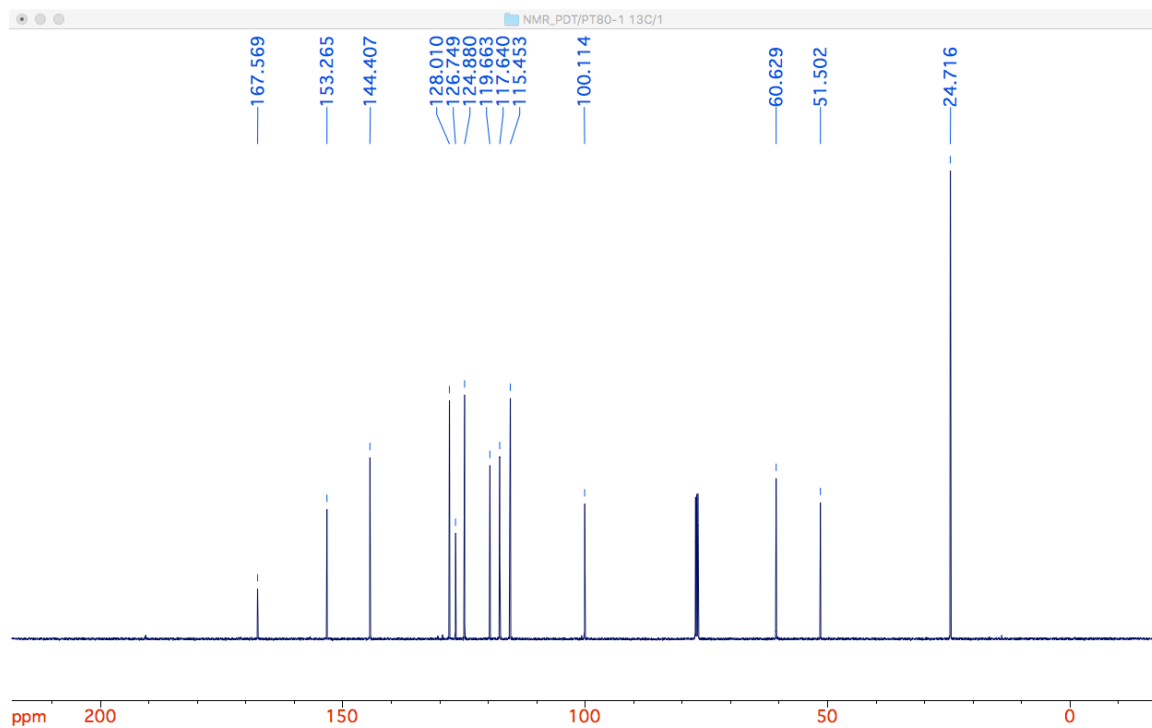
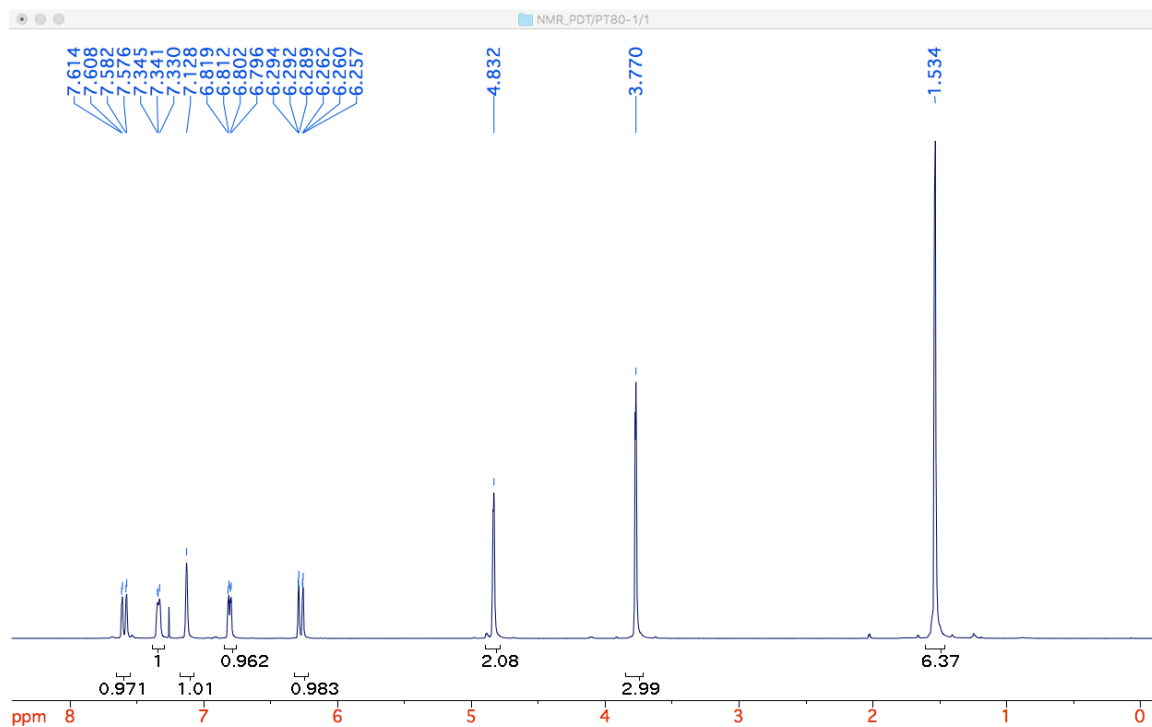


Background RT 0.90 - 1.03 (25 scans)
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Intensity APCI +

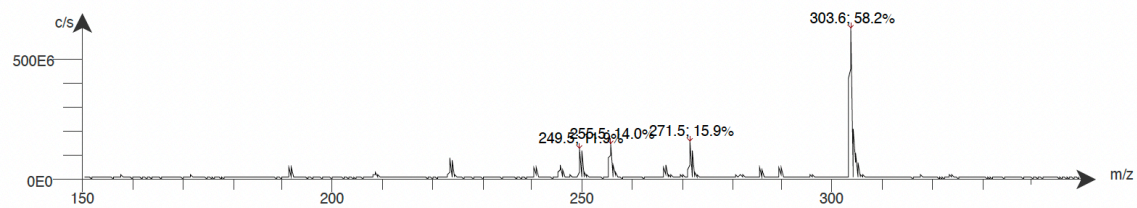


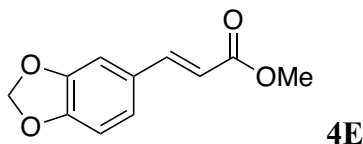


4F



Background RT 1.05 - 1.21 (29 scans)
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ESI +





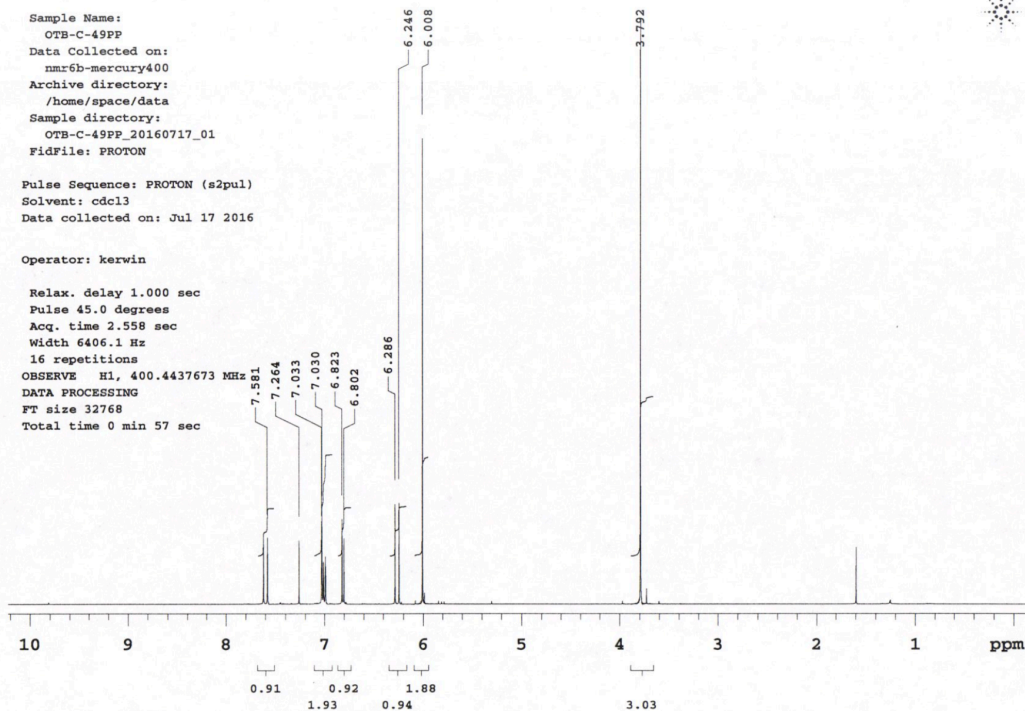
OTB-C-49PF//1H; CDC13//17JUL2016

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Archive directory:
/home/space/data
Sample directory:
OTB-C-49PF_20160717_01
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 17 2016

Operator: kerwin

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.558 sec
Width 6406.1 Hz
16 repetitions
OBSERVE H1, 400.4437673 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 57 sec



Agilent Technologies

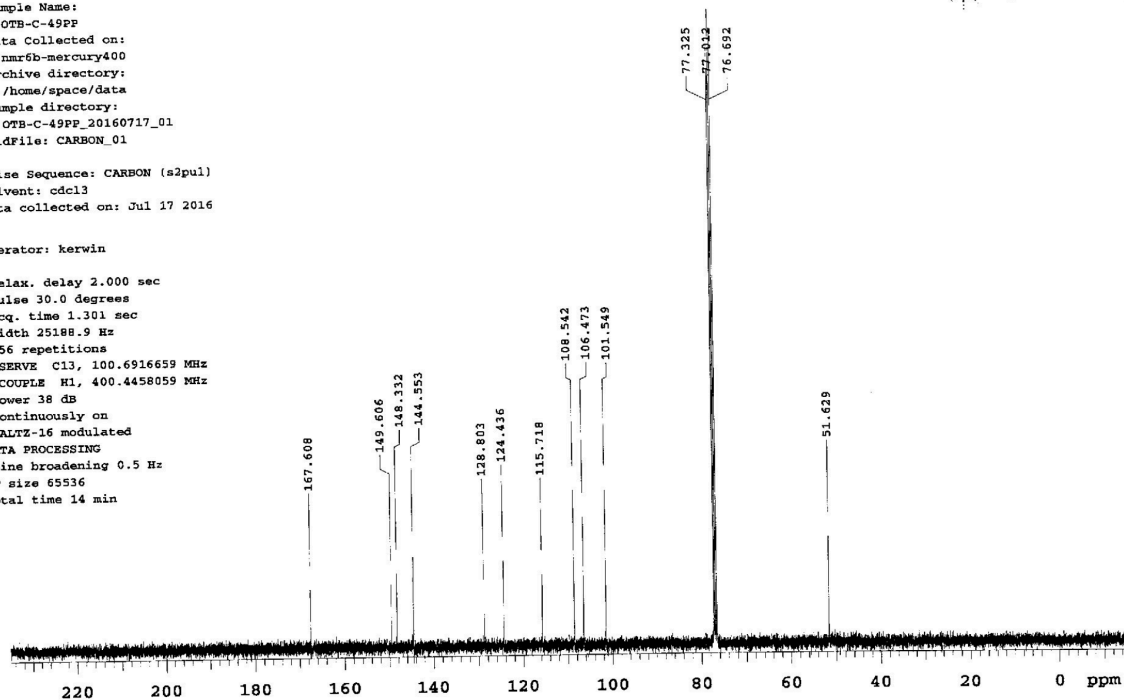
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Solvent: cdcl3
Data collected on: Jul 17 2016

Operator: kerwin

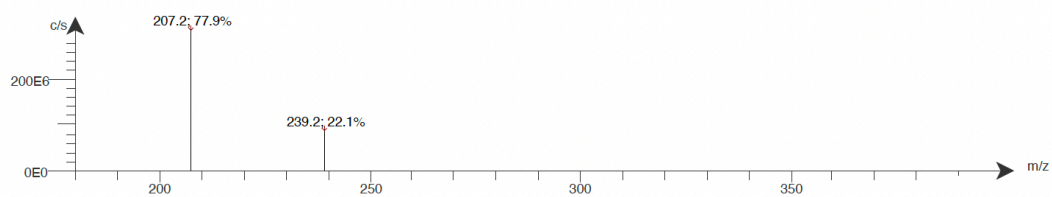
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256 repetitions
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Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
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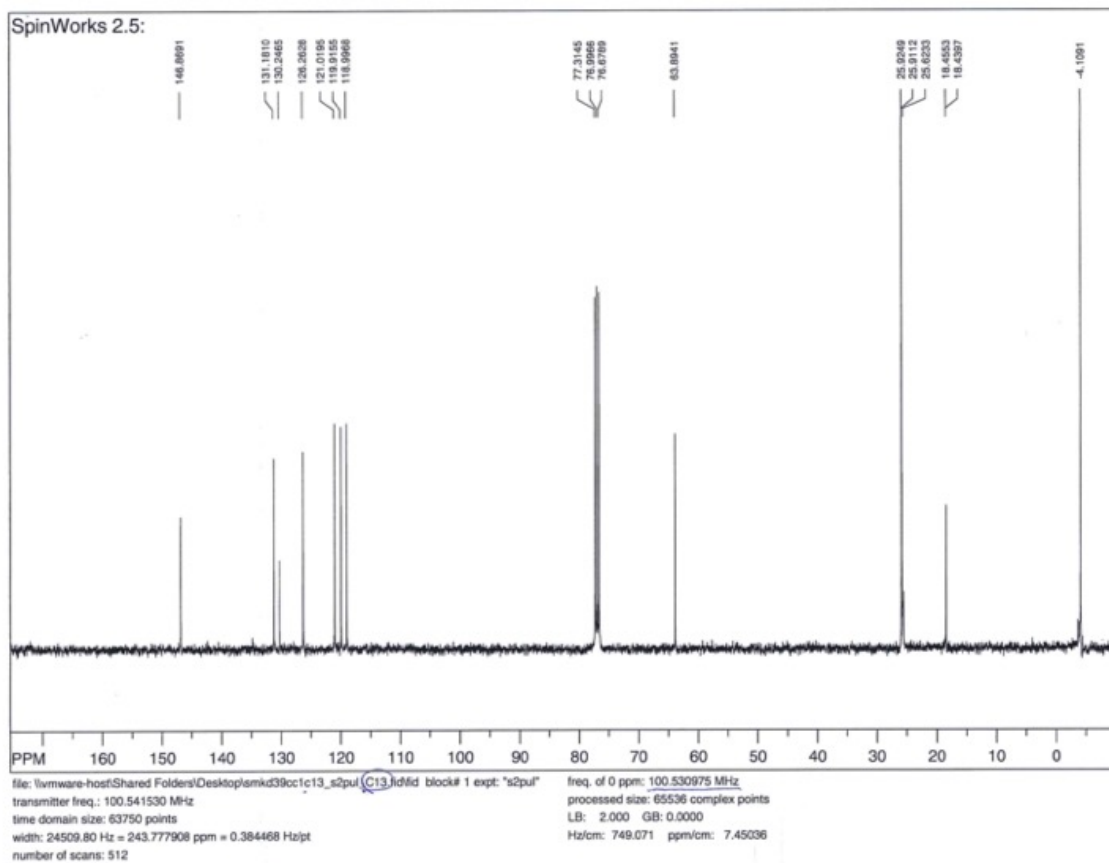
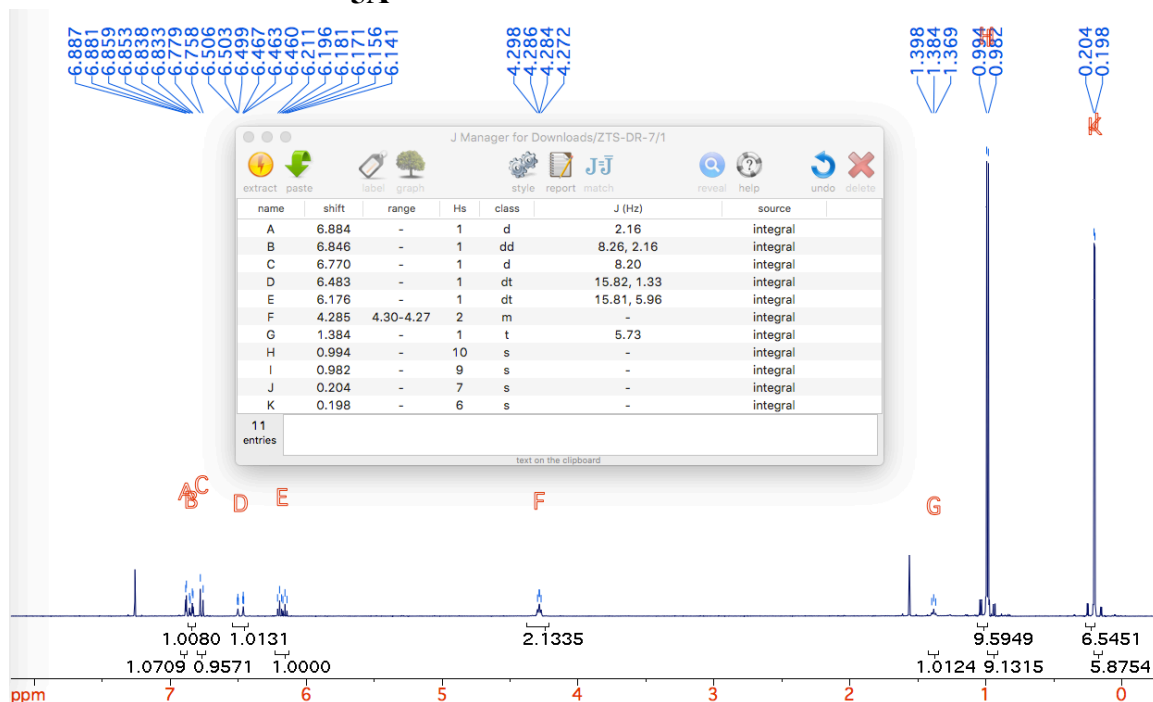
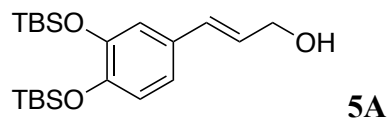


Agilent Technologies

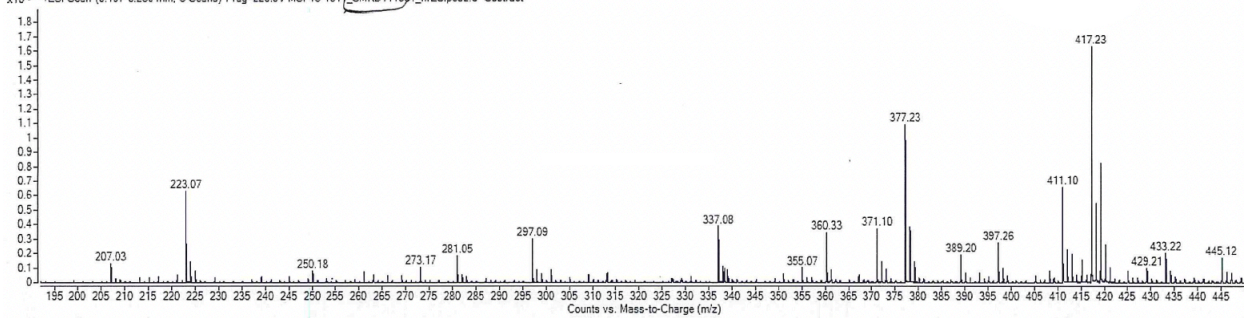
Intensity

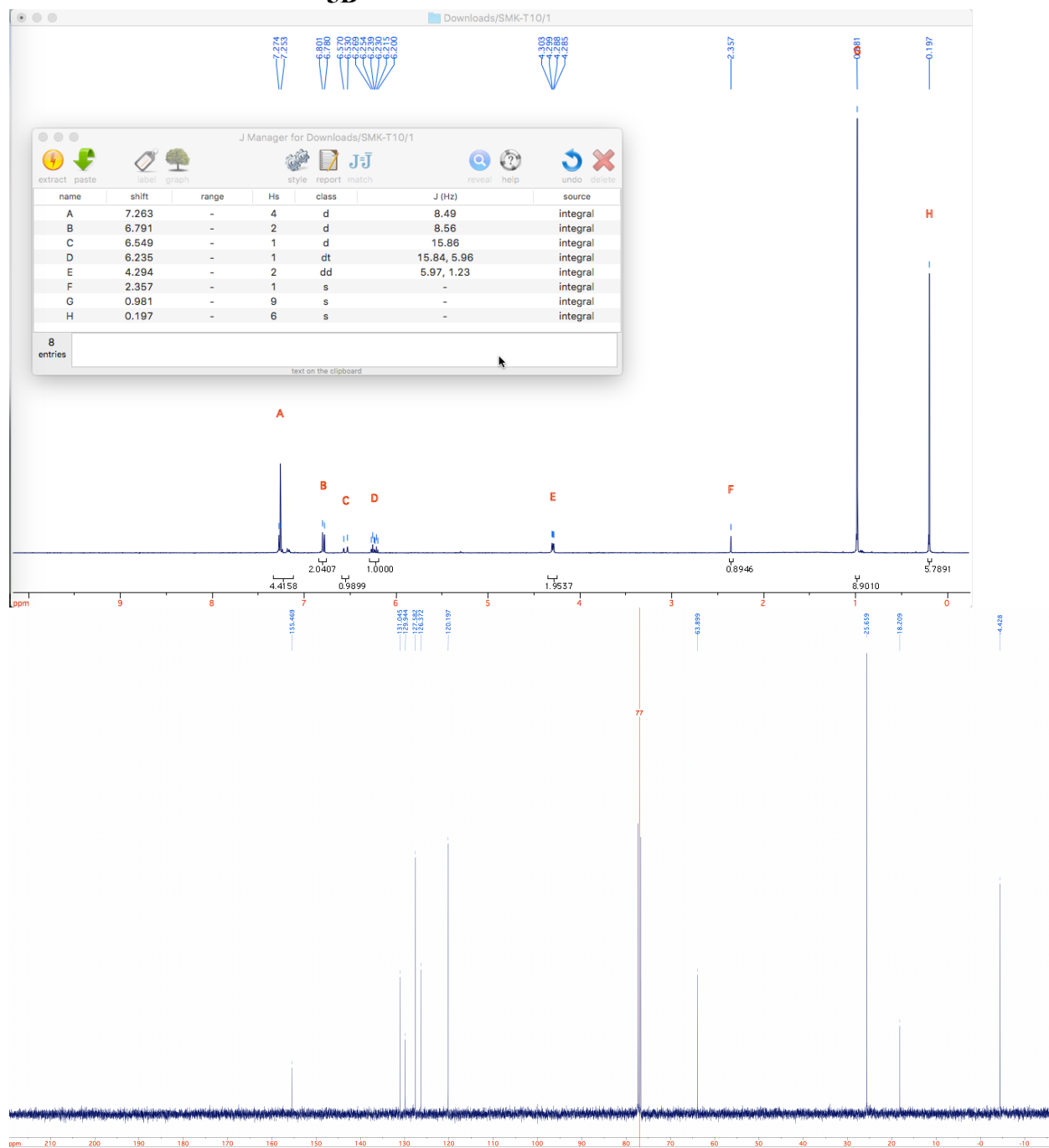
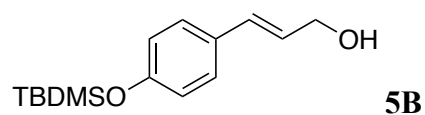
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ESI +



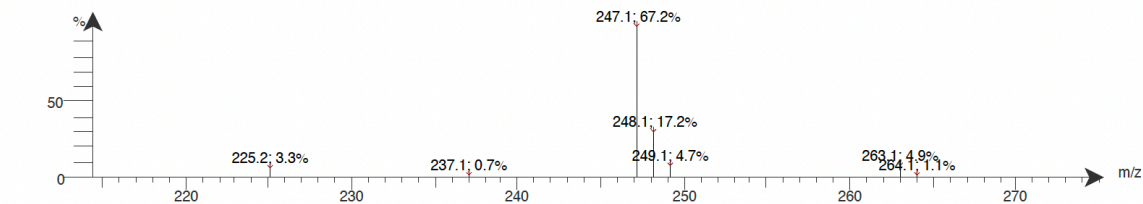


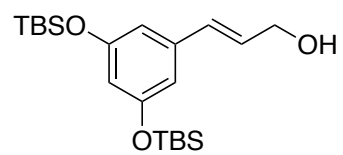
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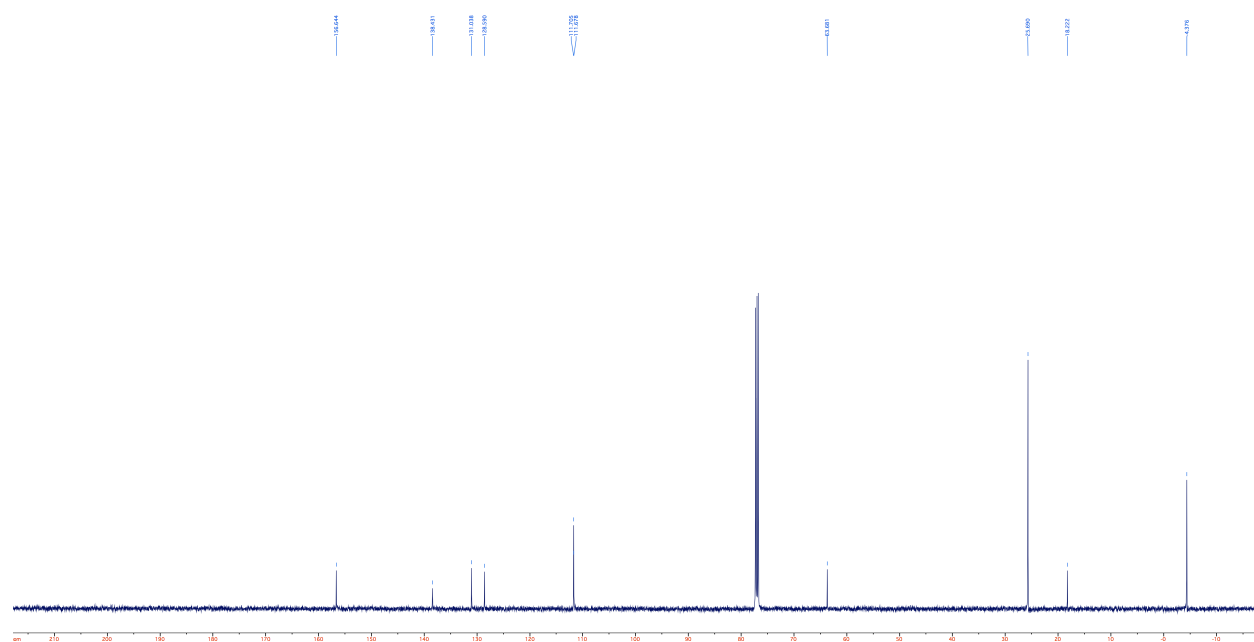
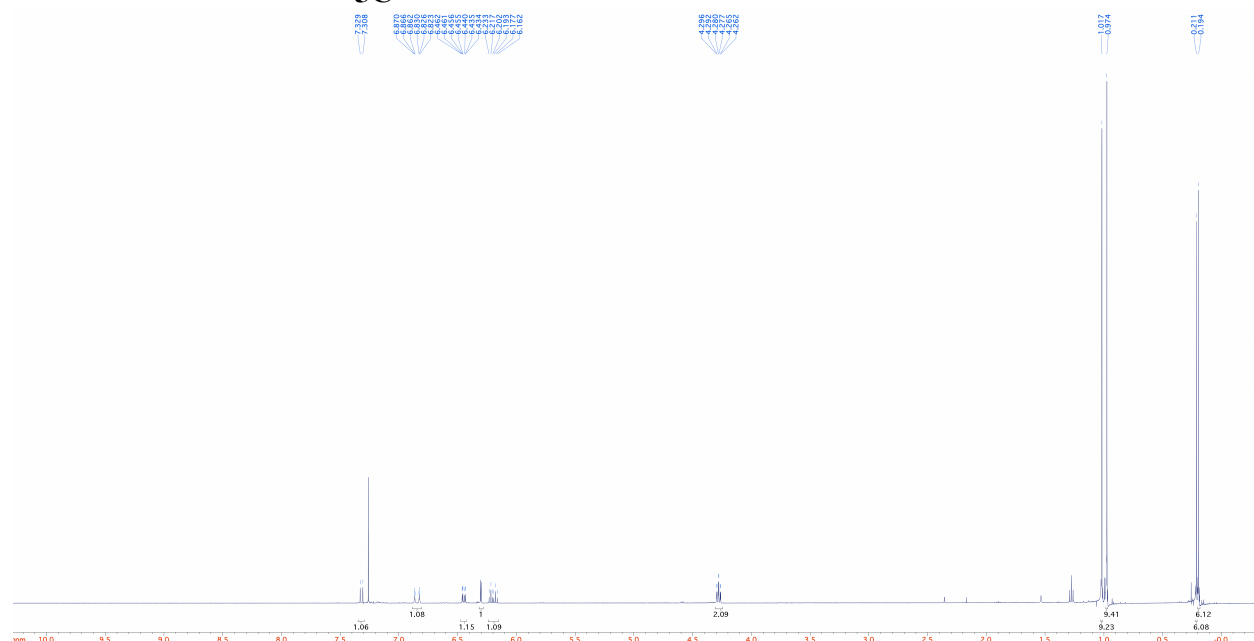


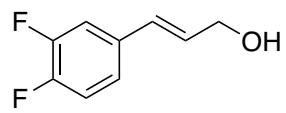
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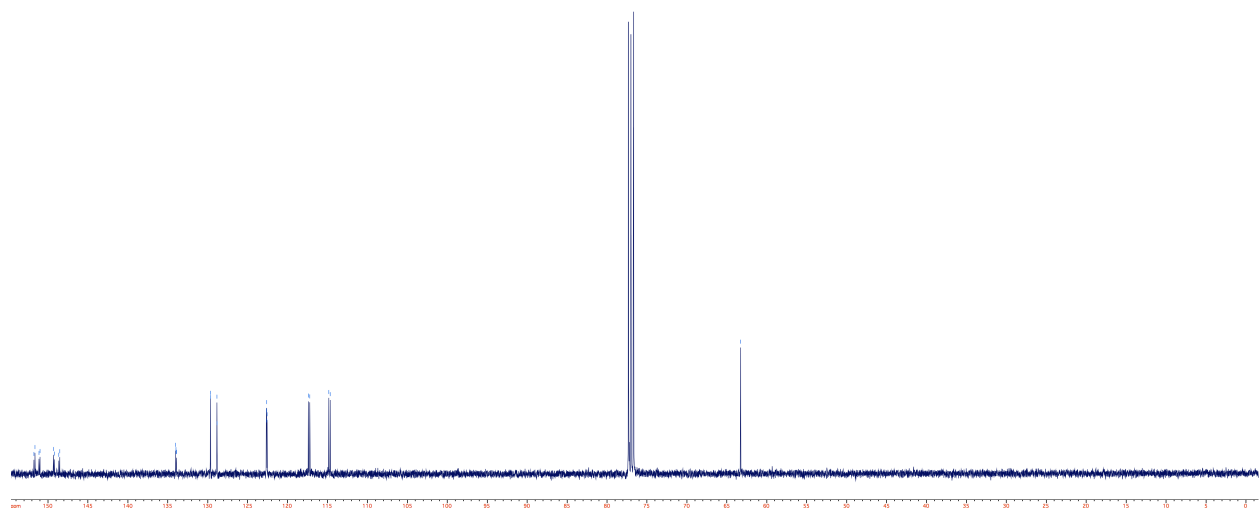
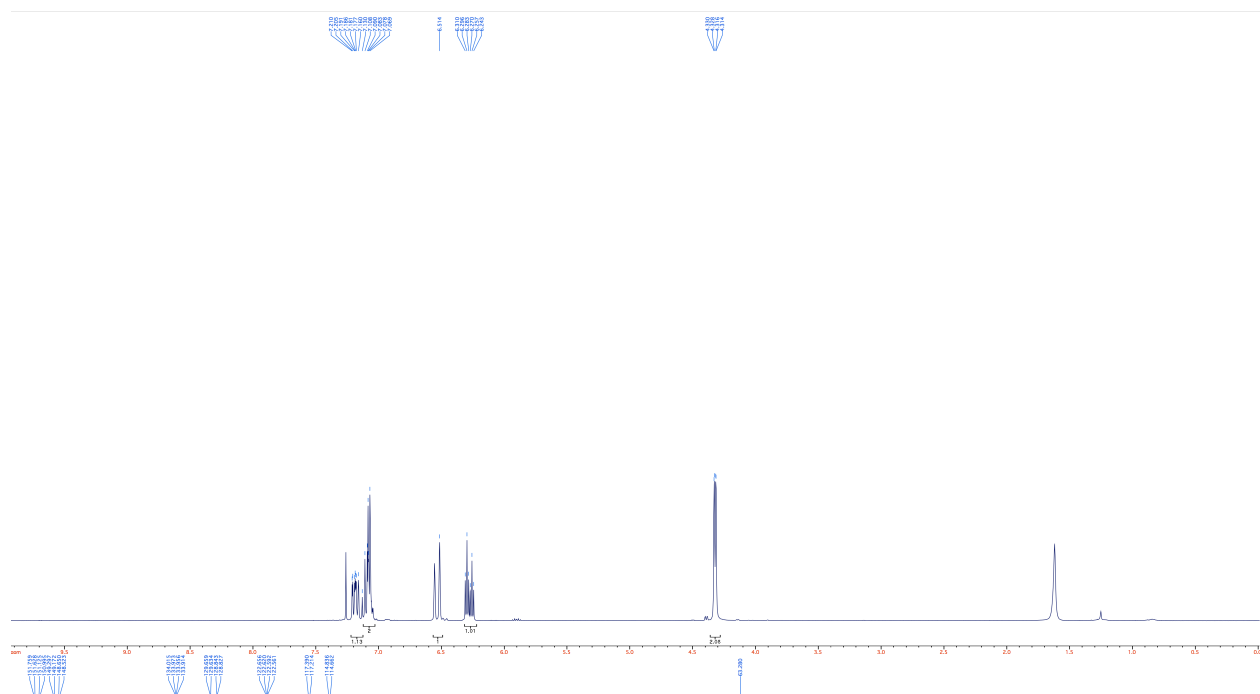


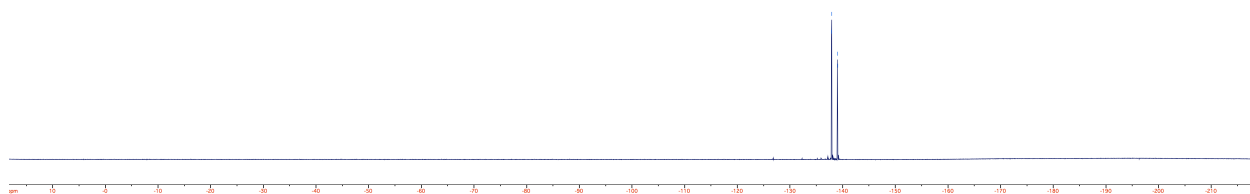
5C



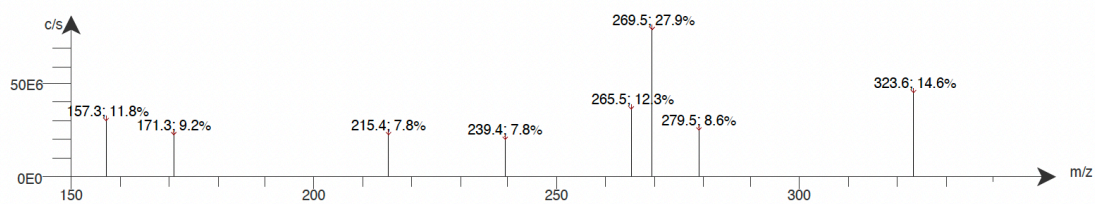


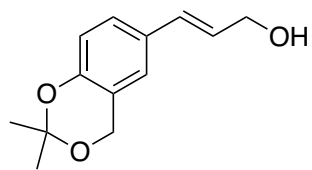
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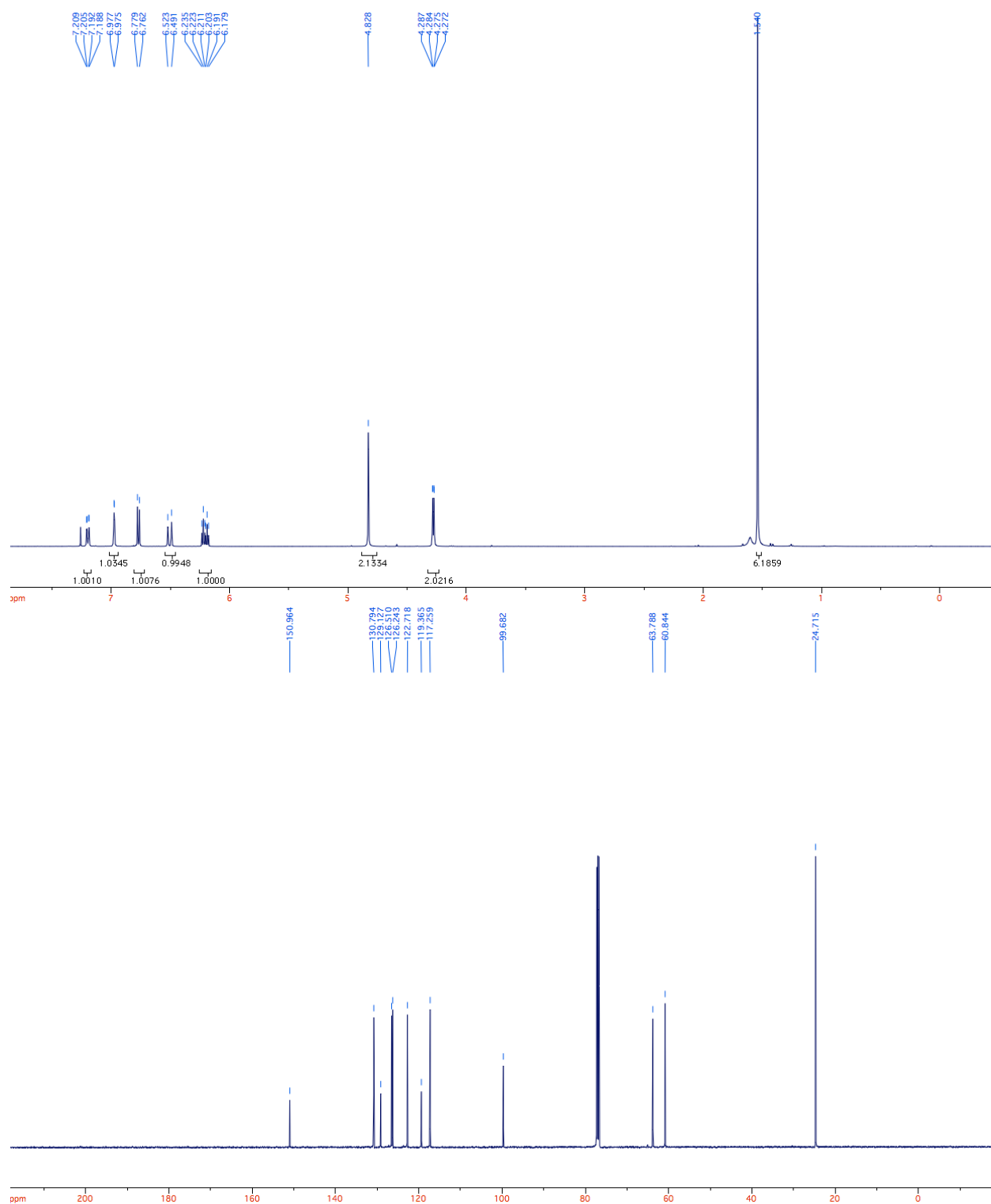


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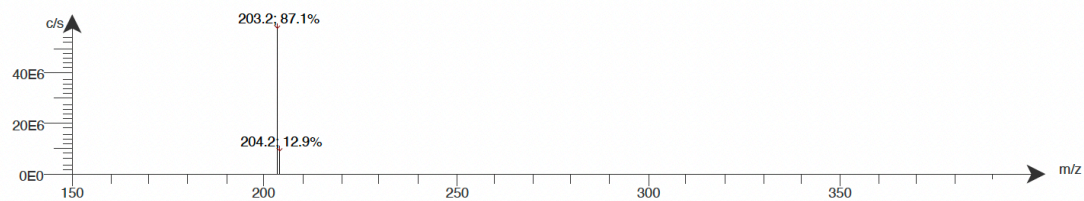


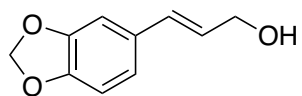


5F

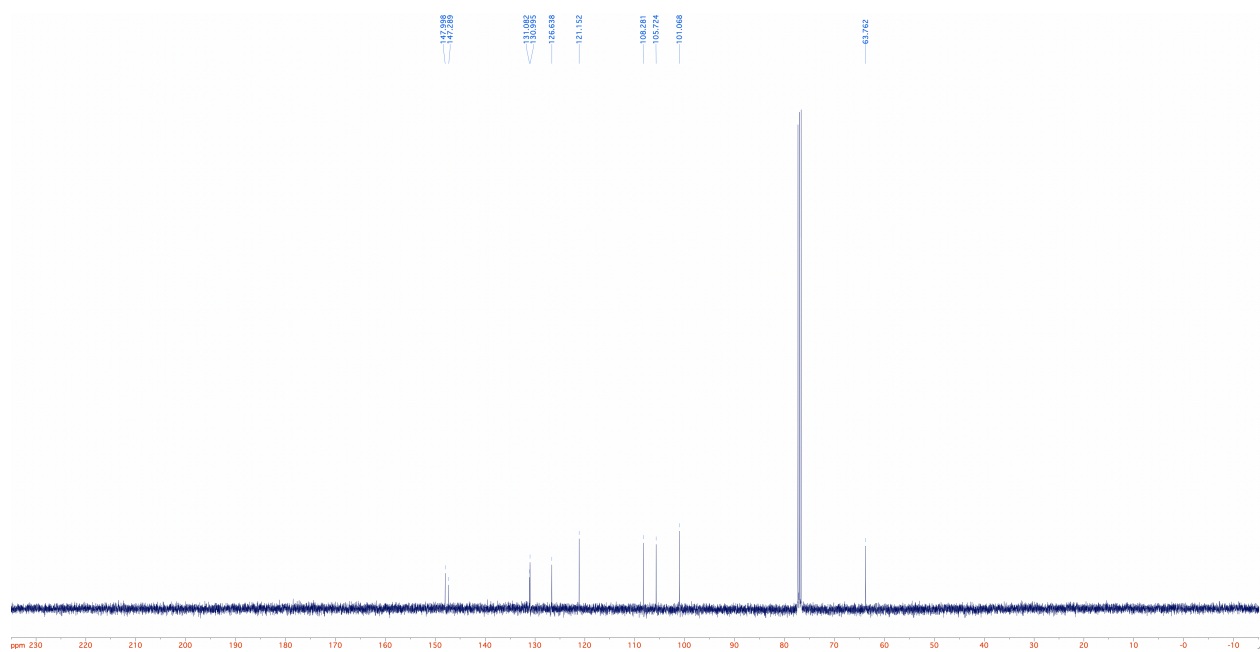
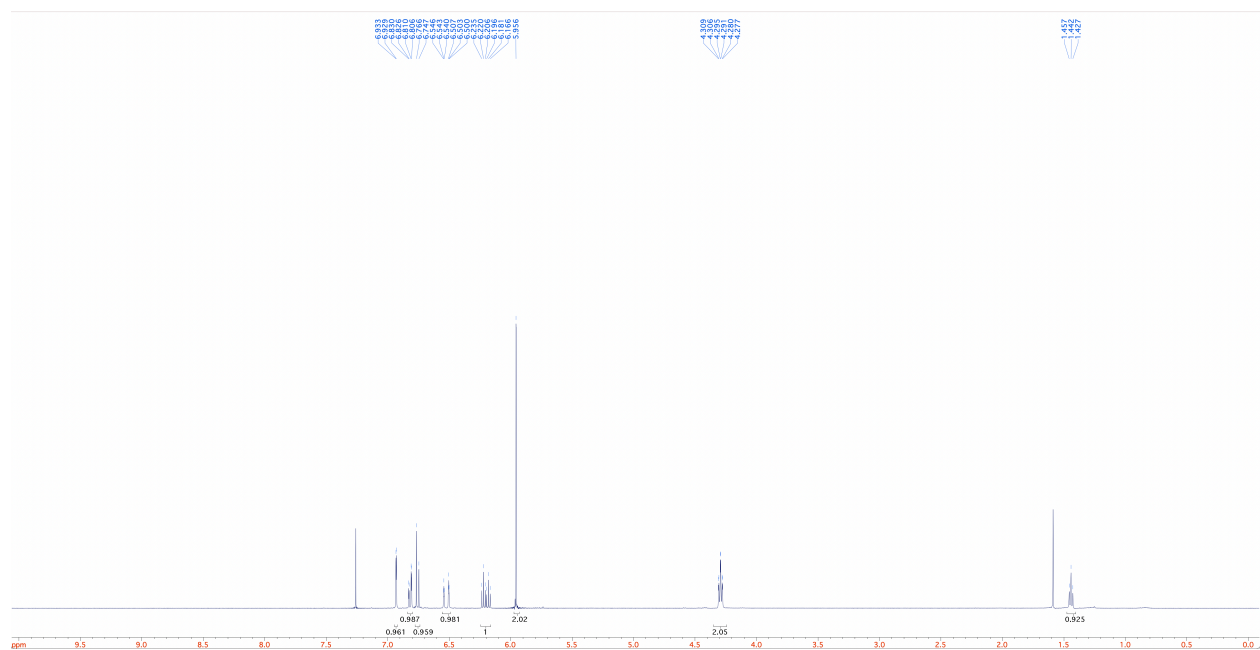


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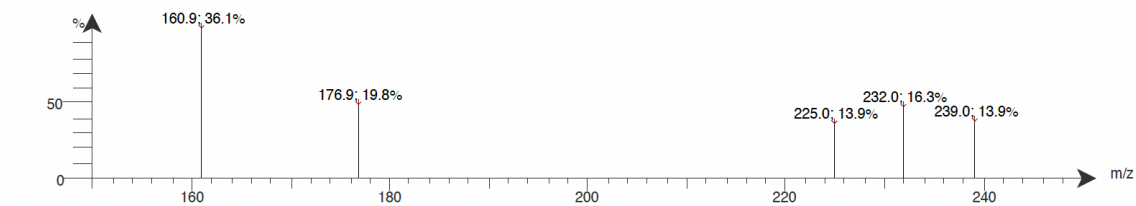


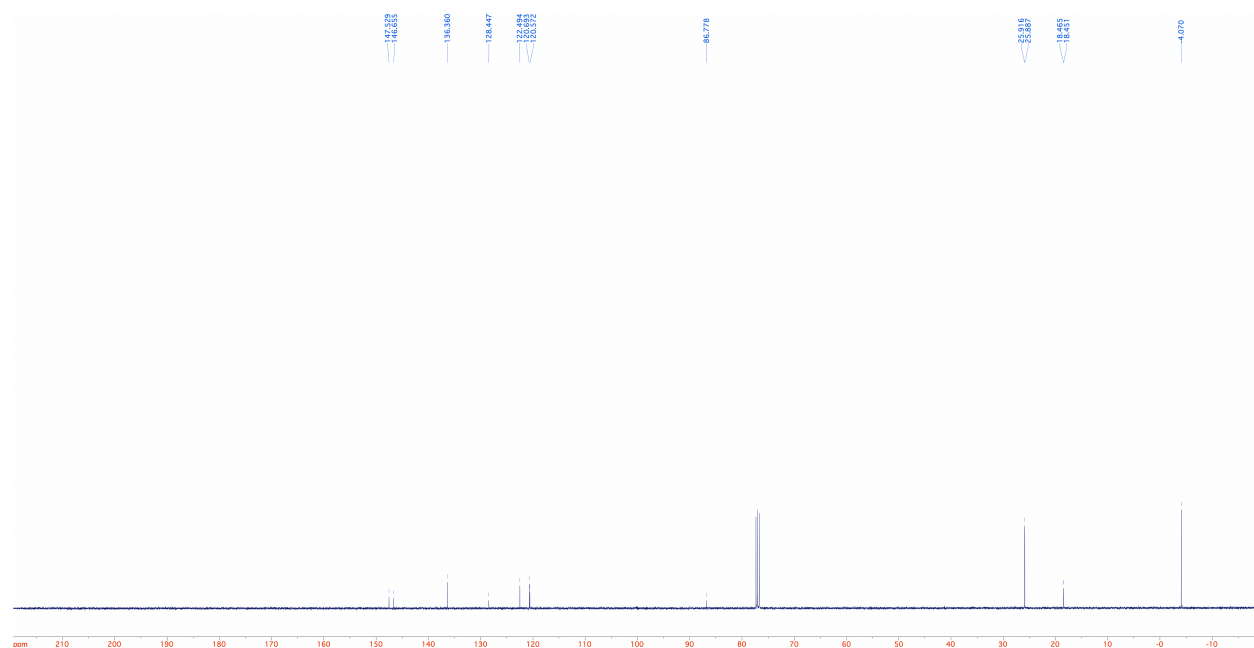
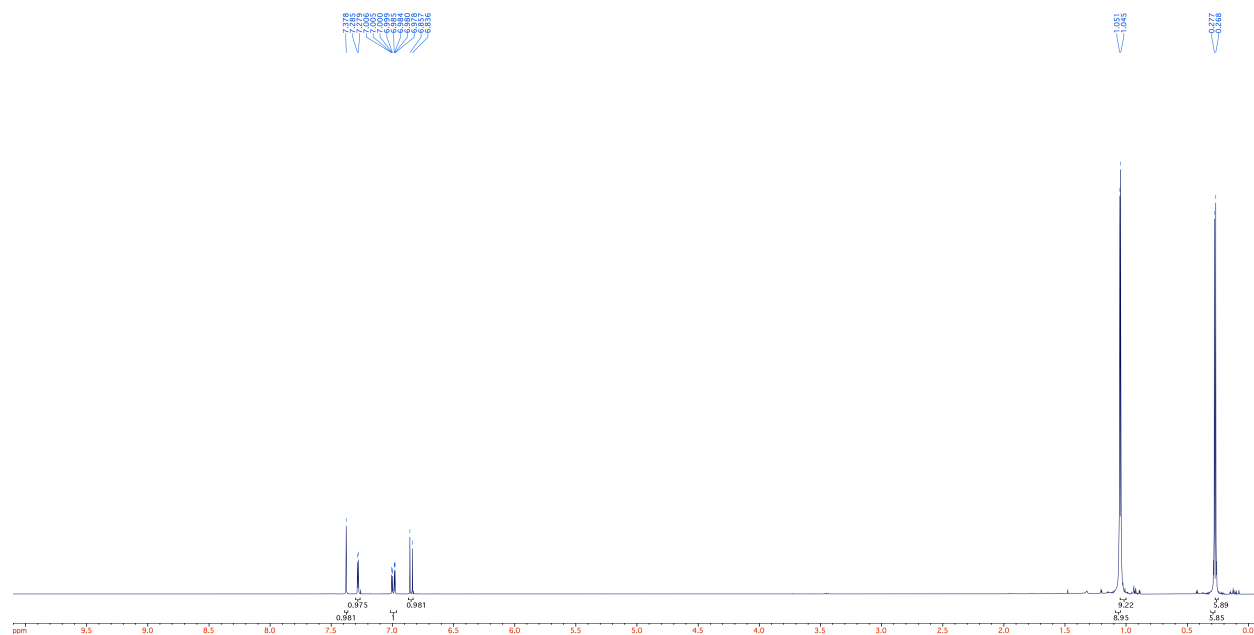
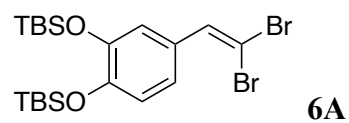


5E

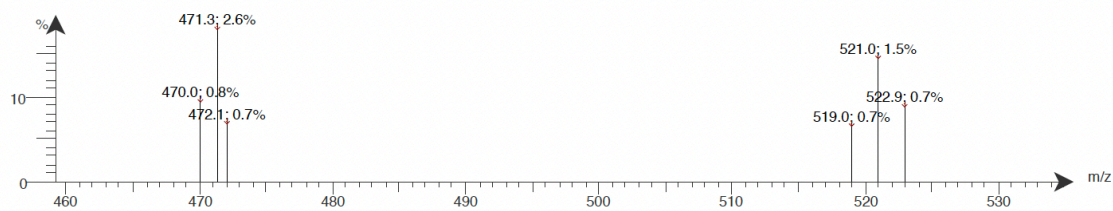


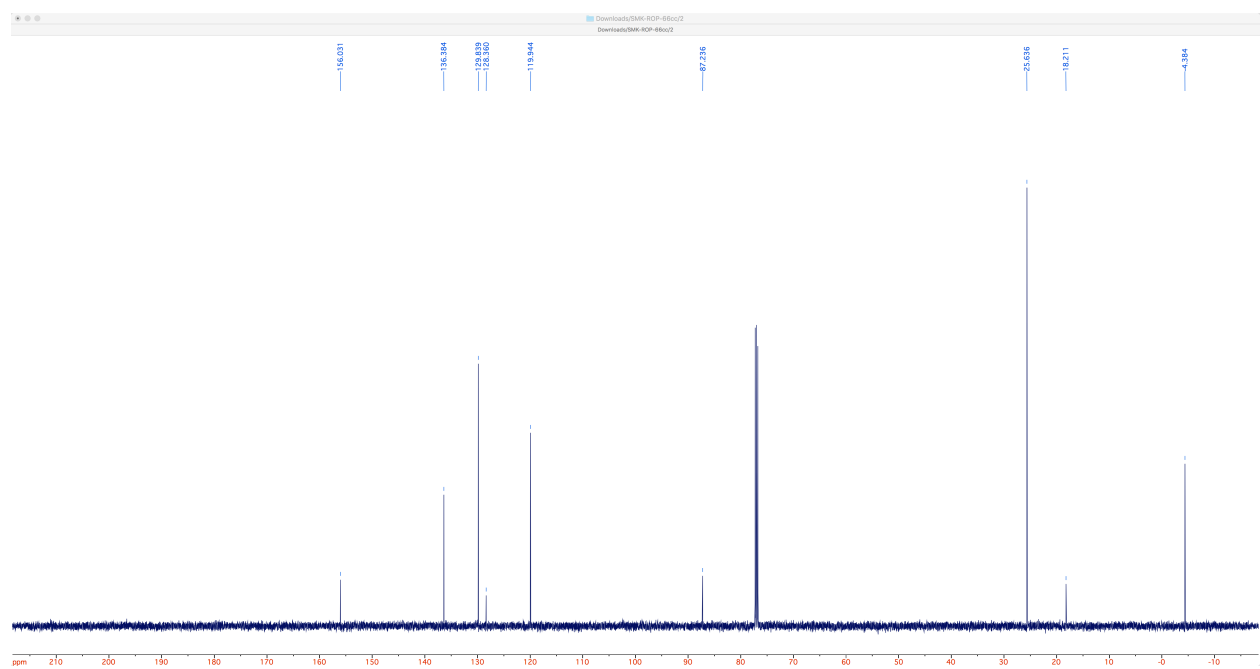
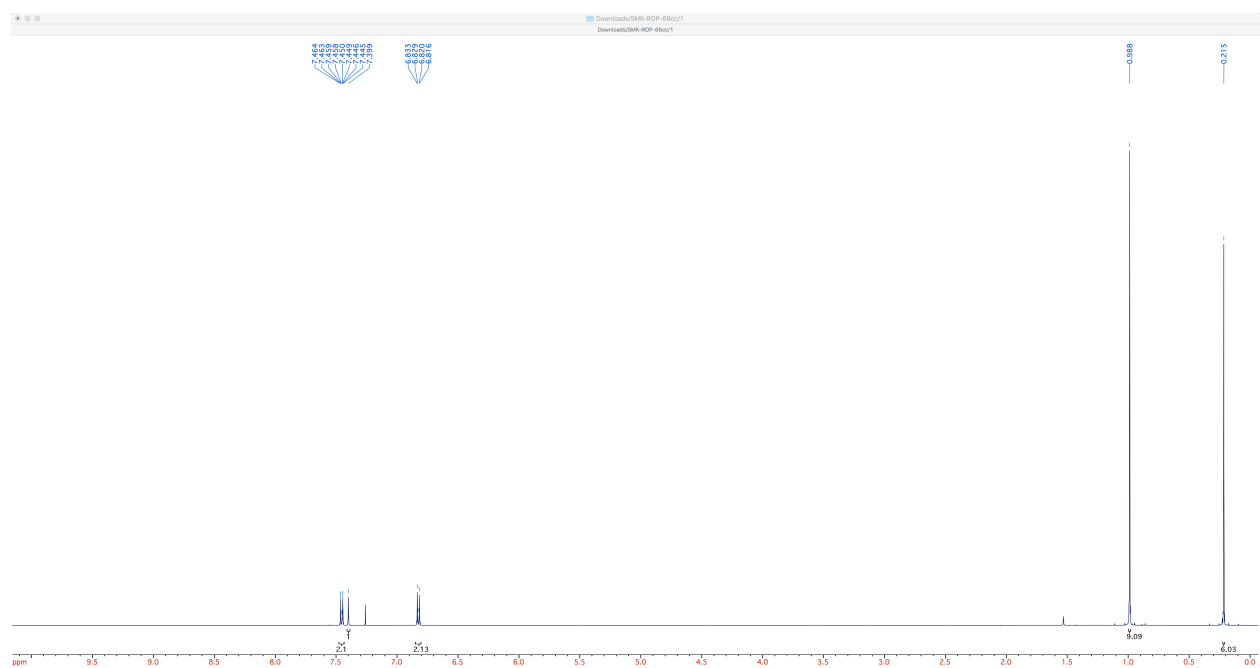
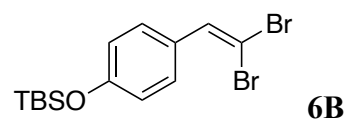
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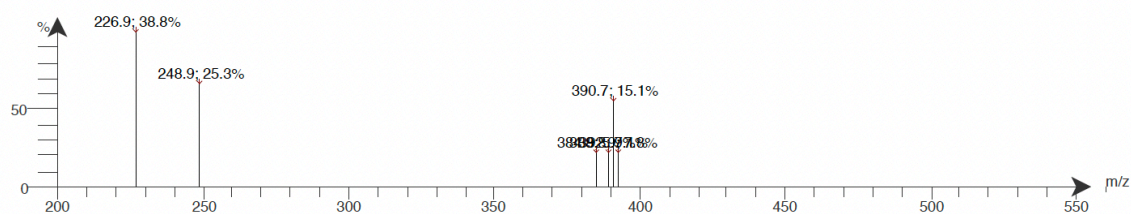


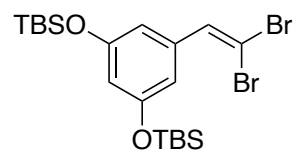
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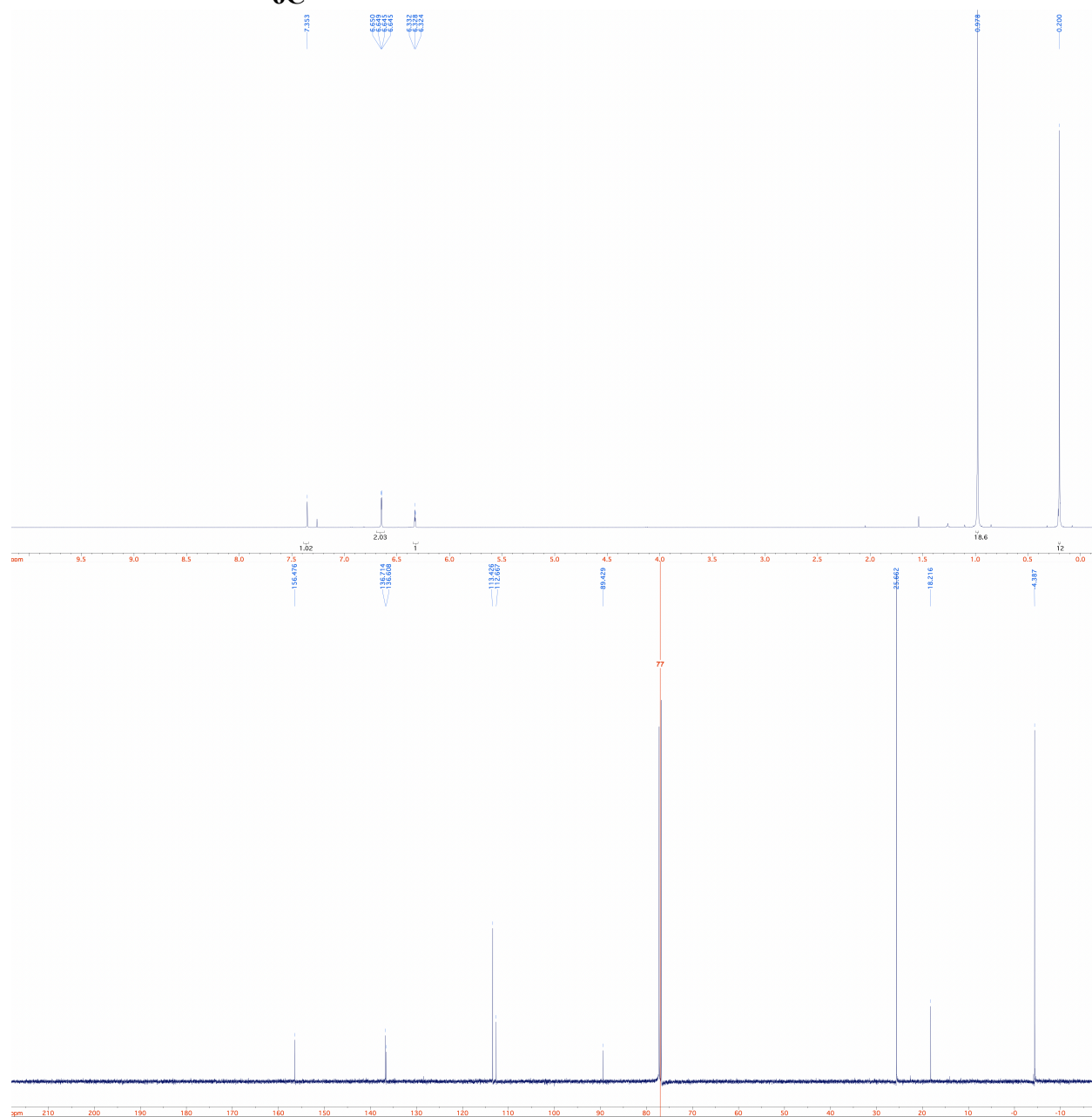


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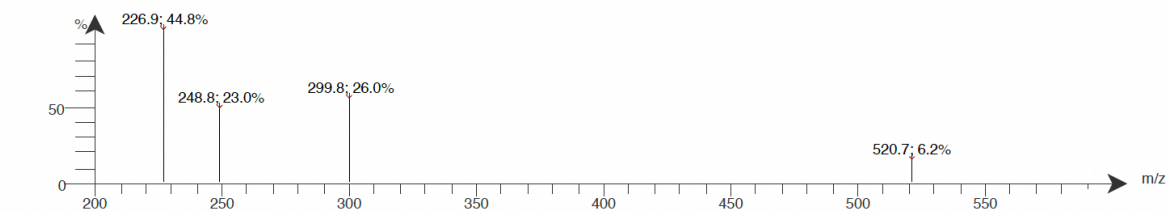


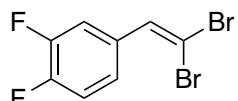


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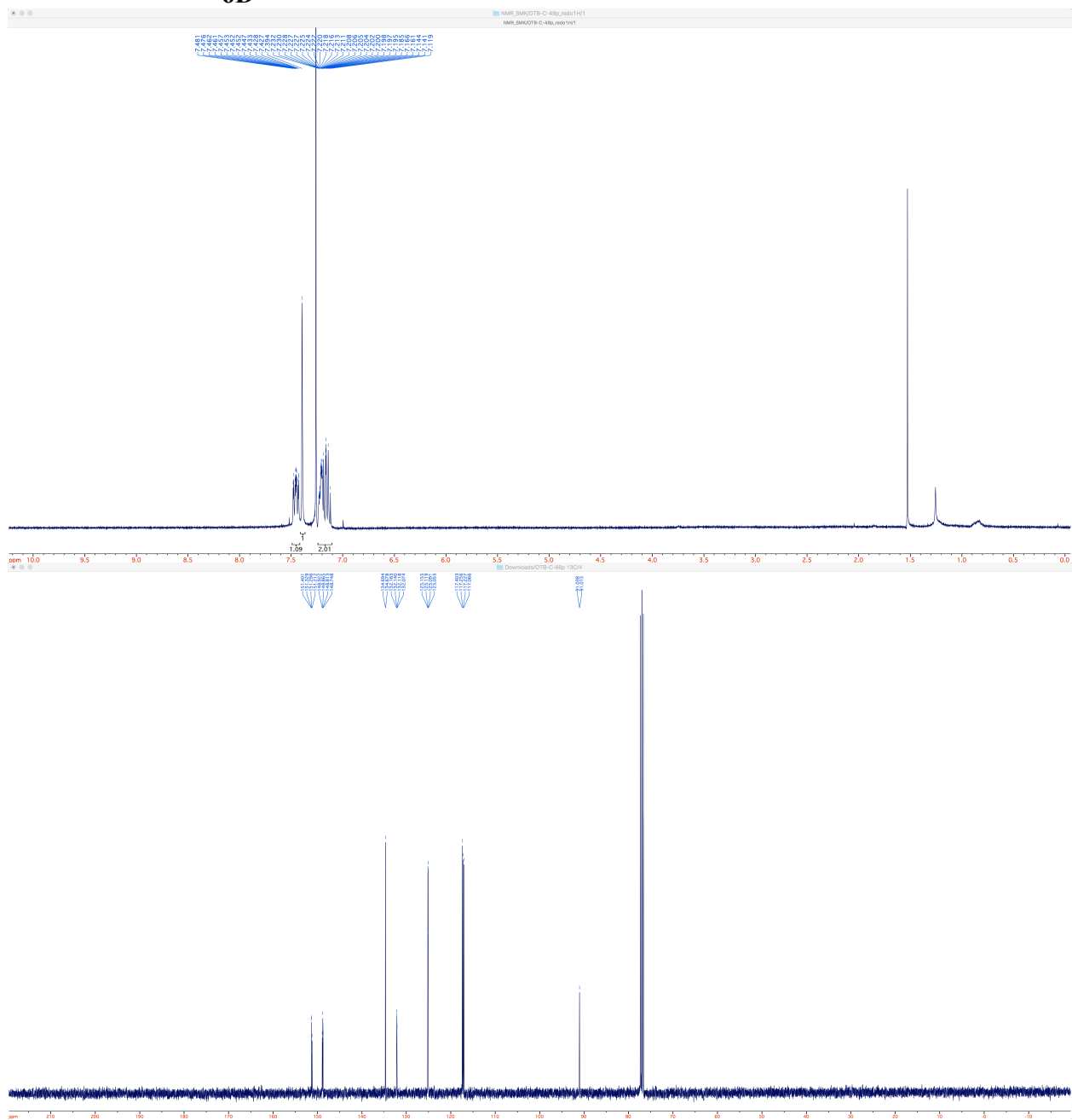


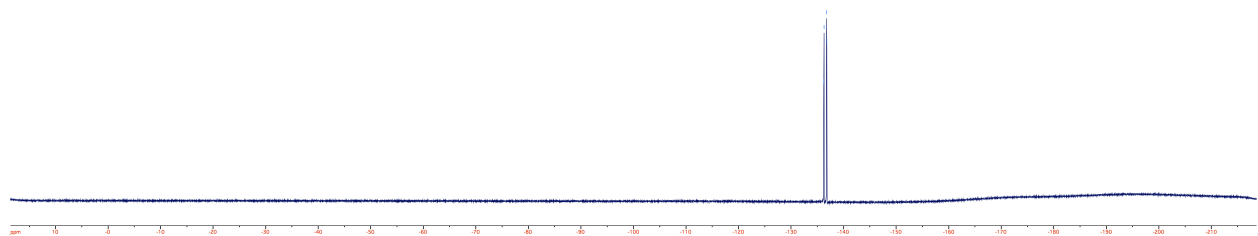
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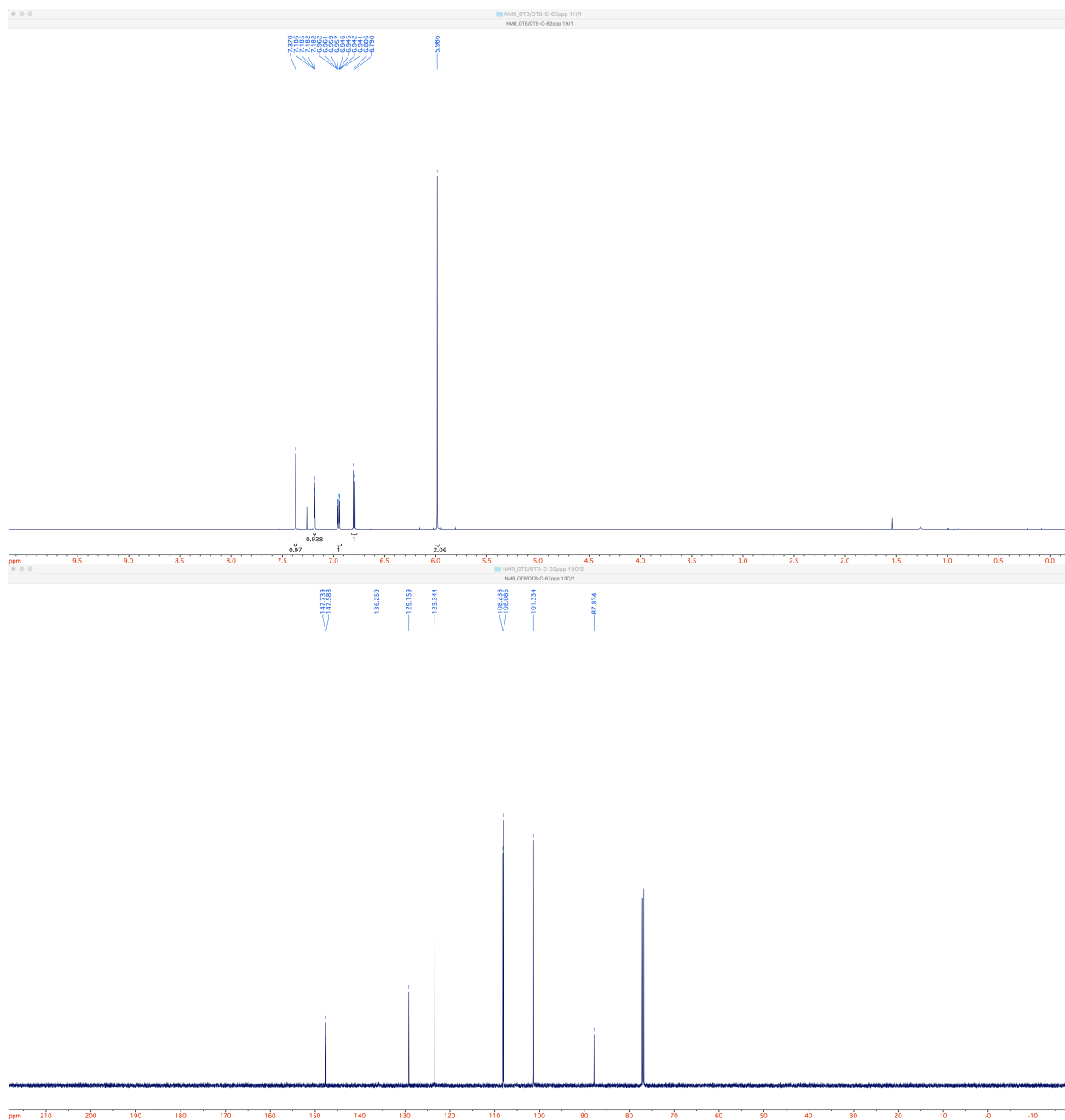
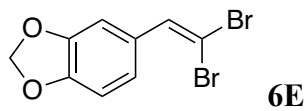




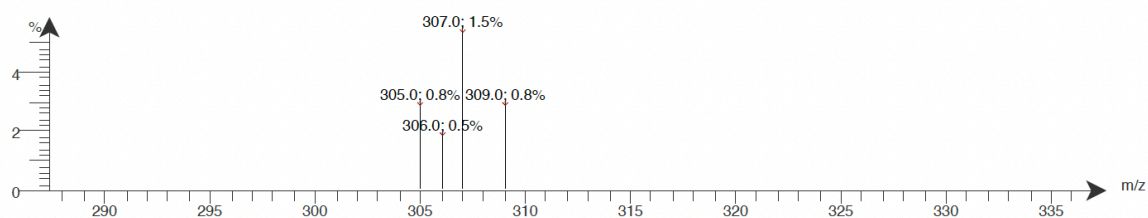
6D

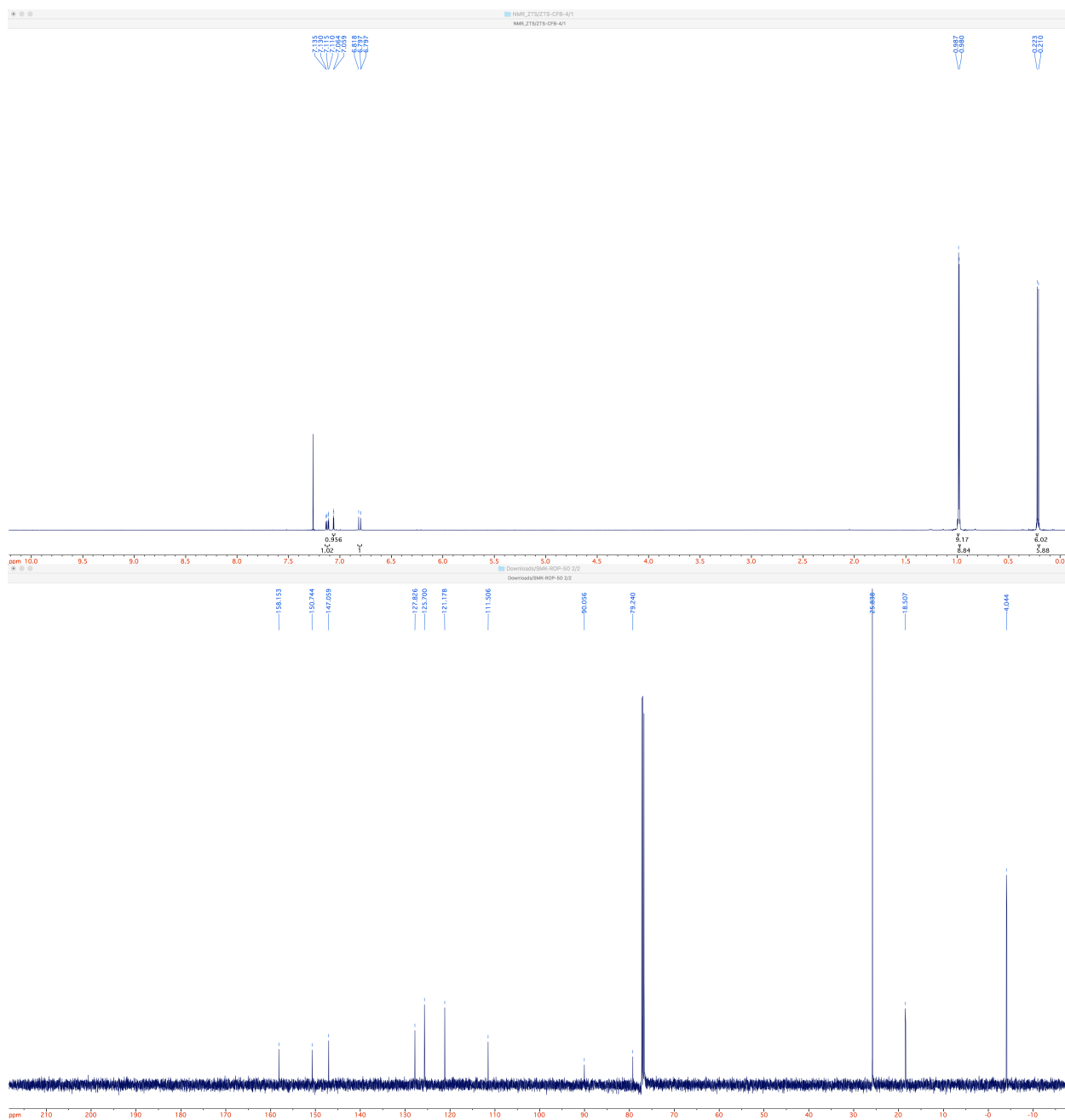
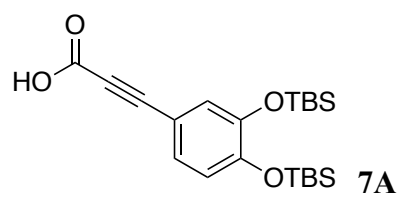




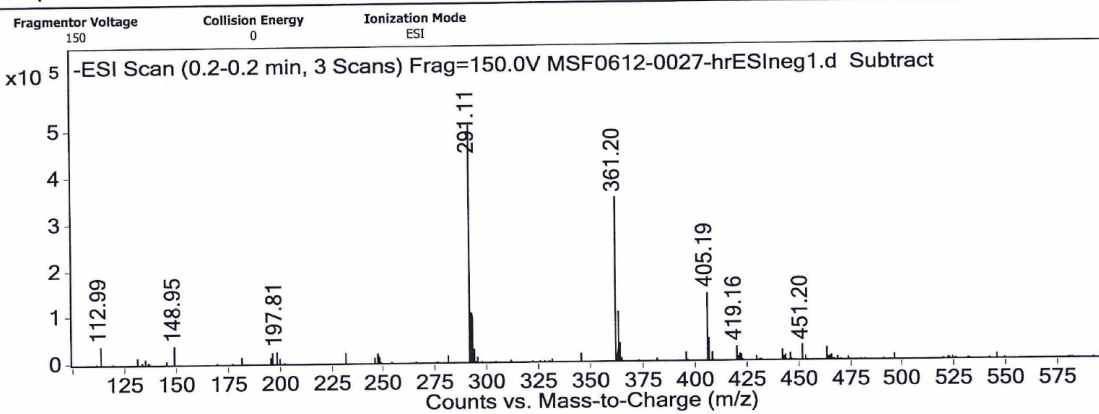


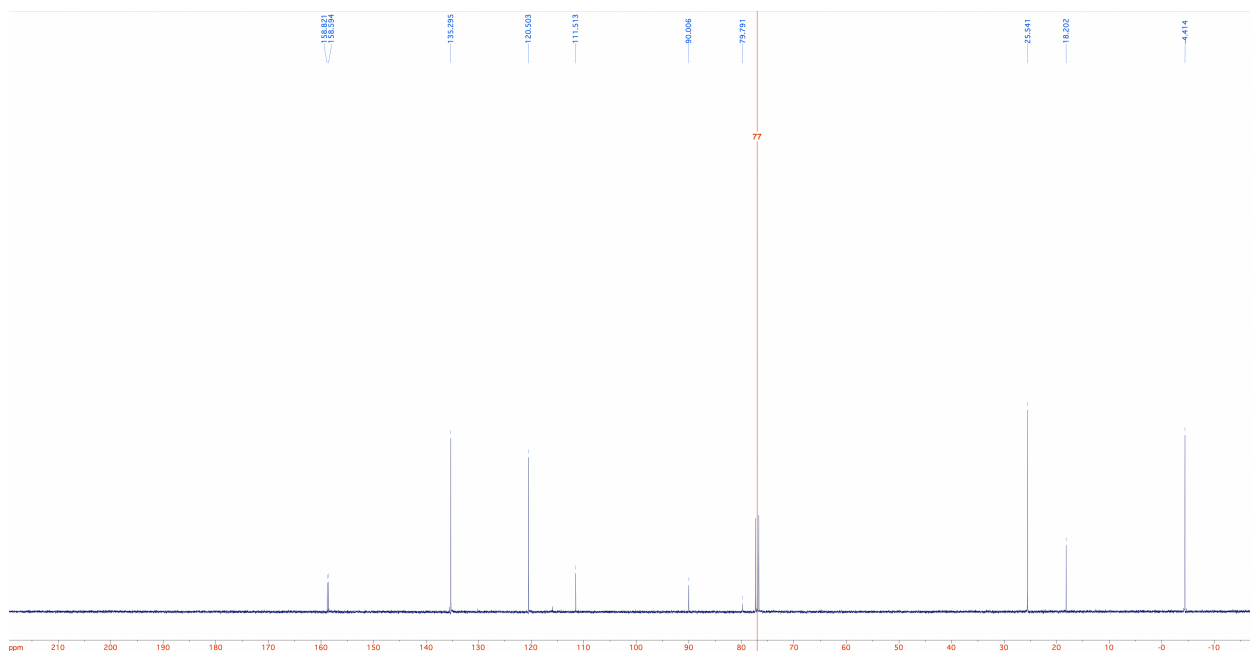
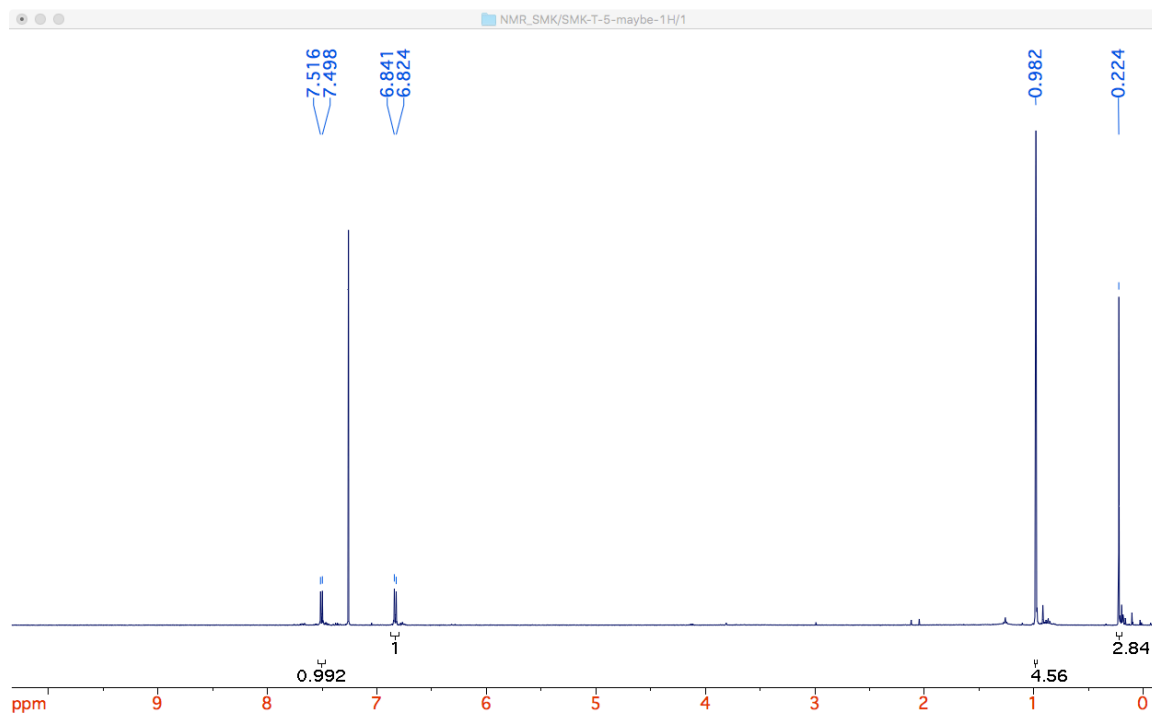
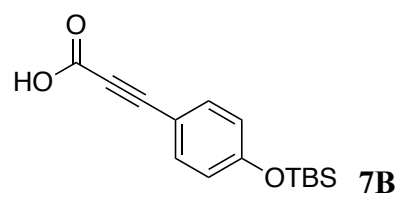
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Intensity APCI + Max: 1E7



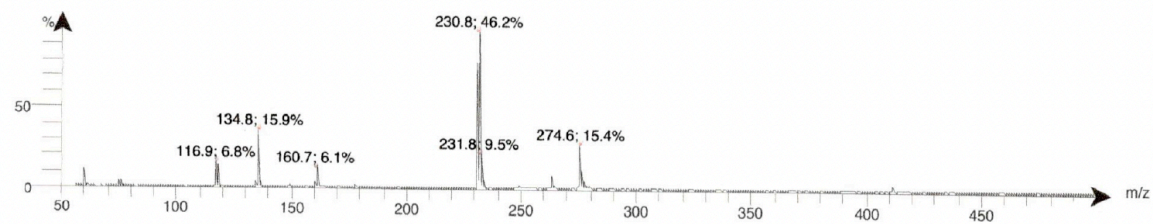


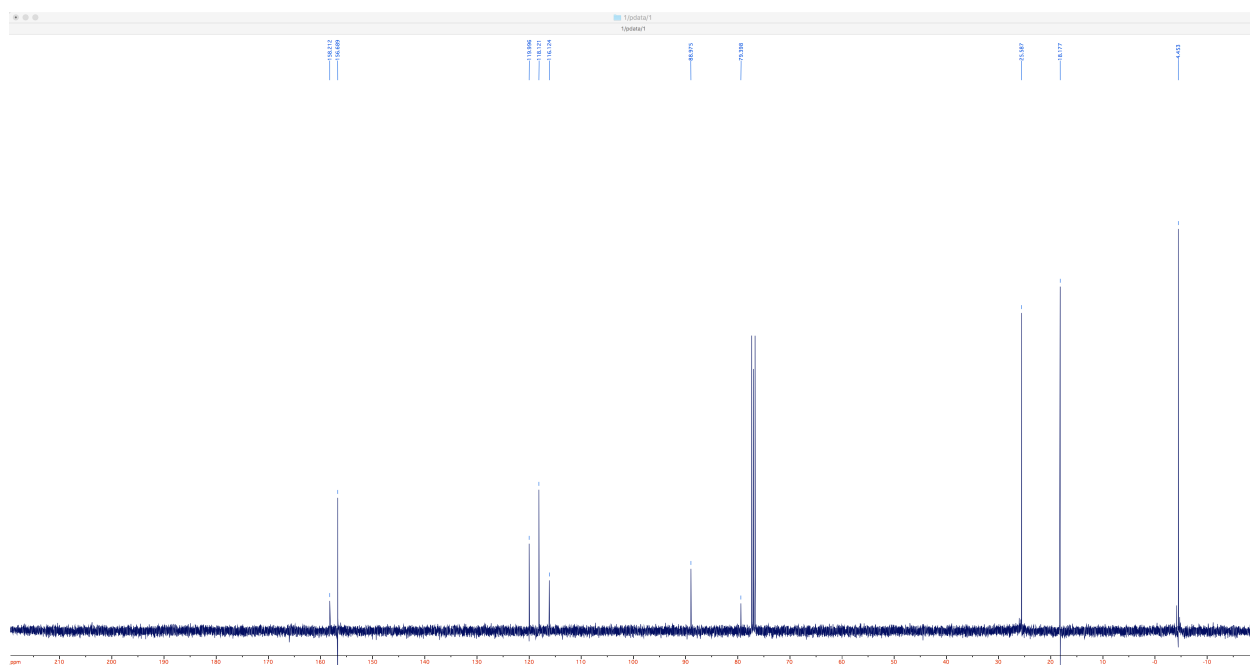
User Spectra



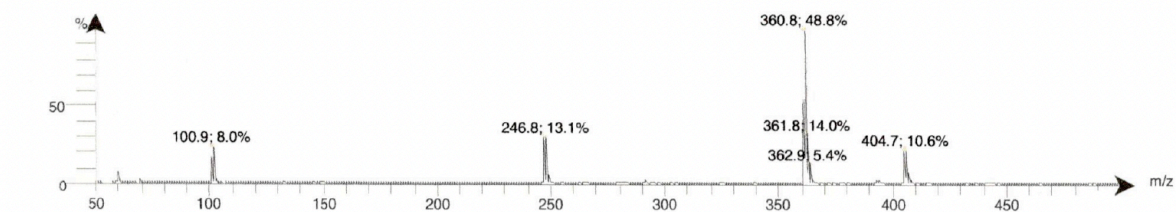


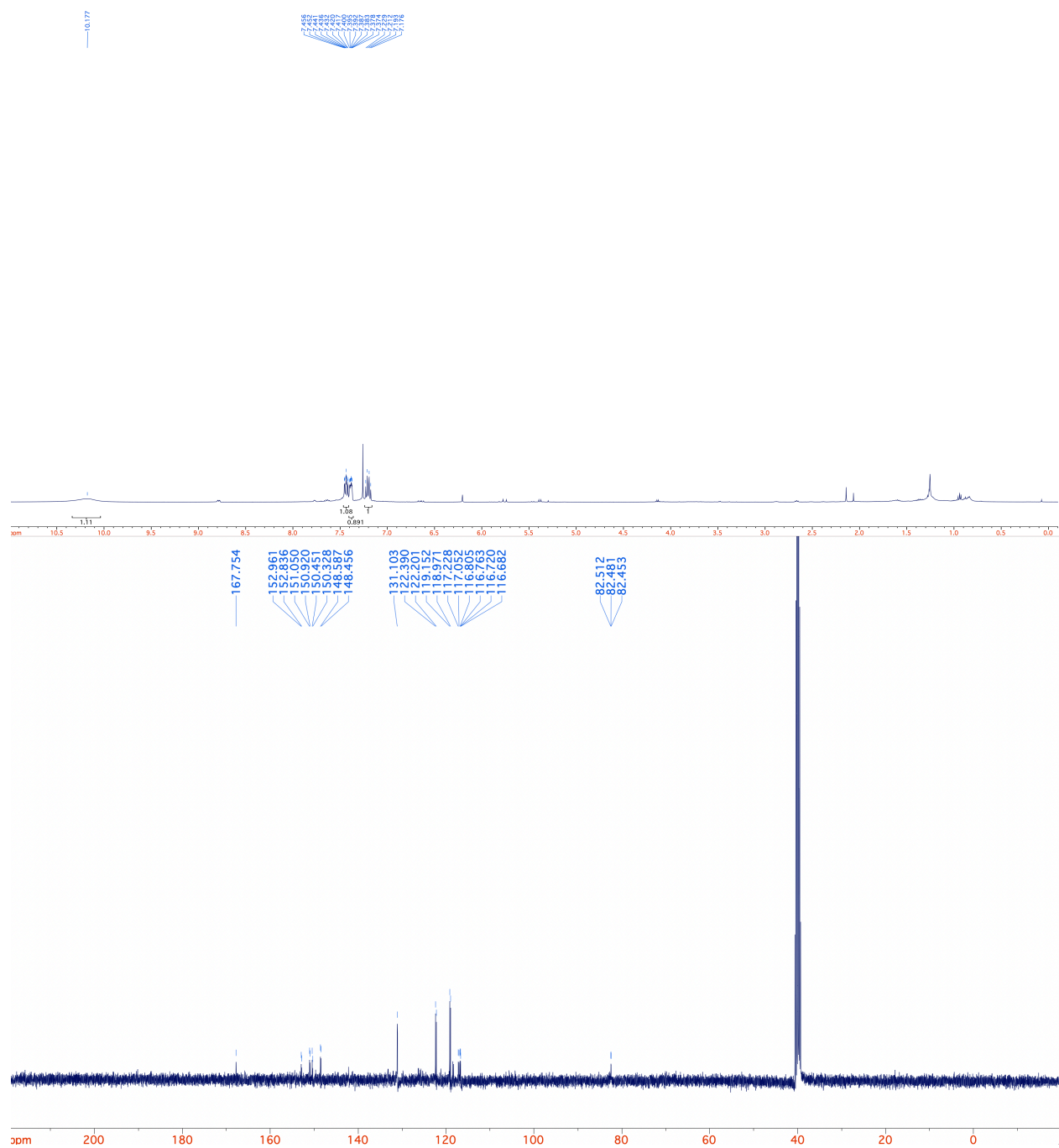
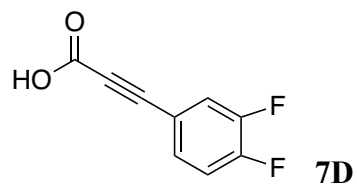
Background RT 0.97 - 1.13 {13 scans}
SMK-T-5_inj1.datx 2021.07.27 15:27:19 ;
ESI - Max: 3E8



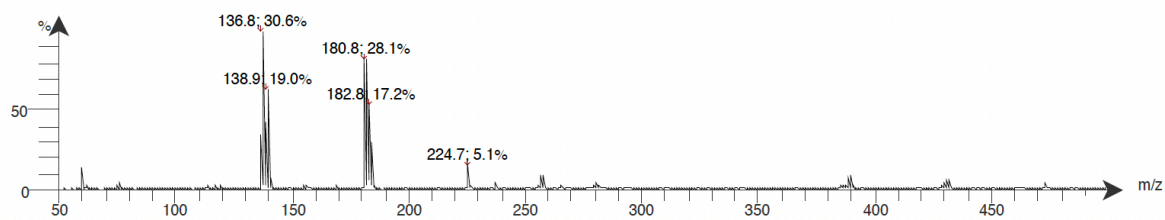


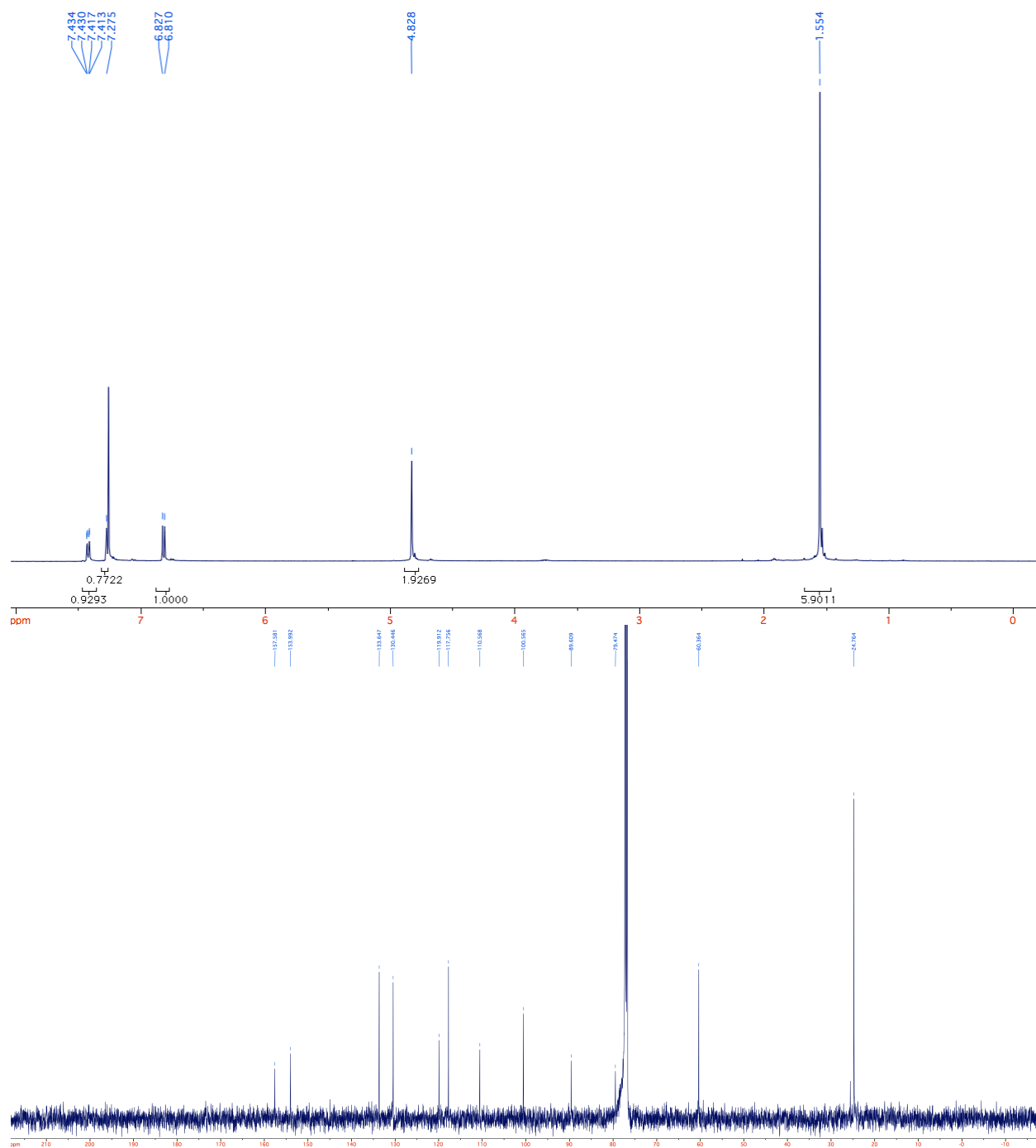
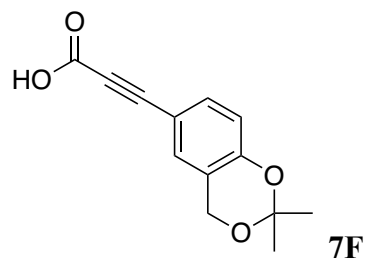
Background RT 1.63 - 1.91 (22 scans)
KeMIS-180A_inj1.datx 2021.07.26 15:46:12 ;
ESI - Max: 2.7E8



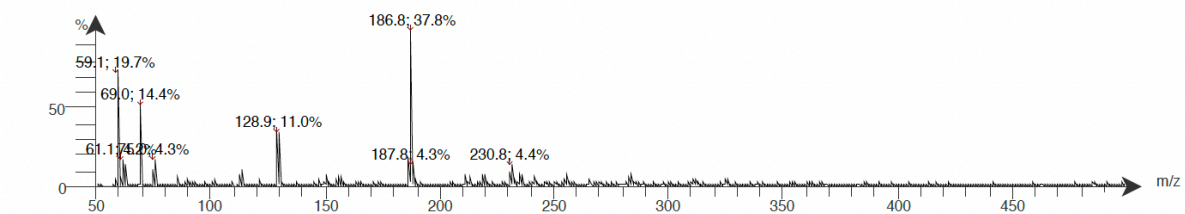


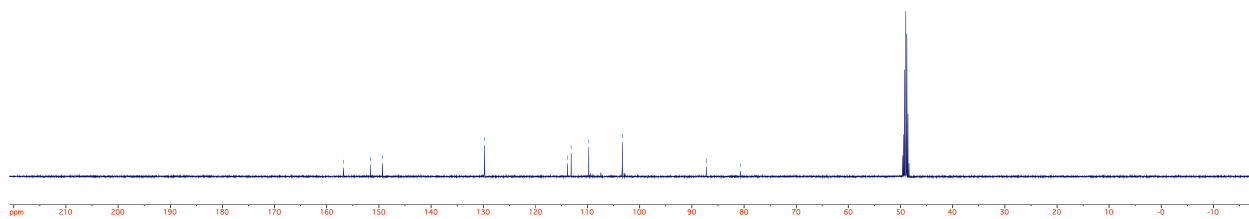
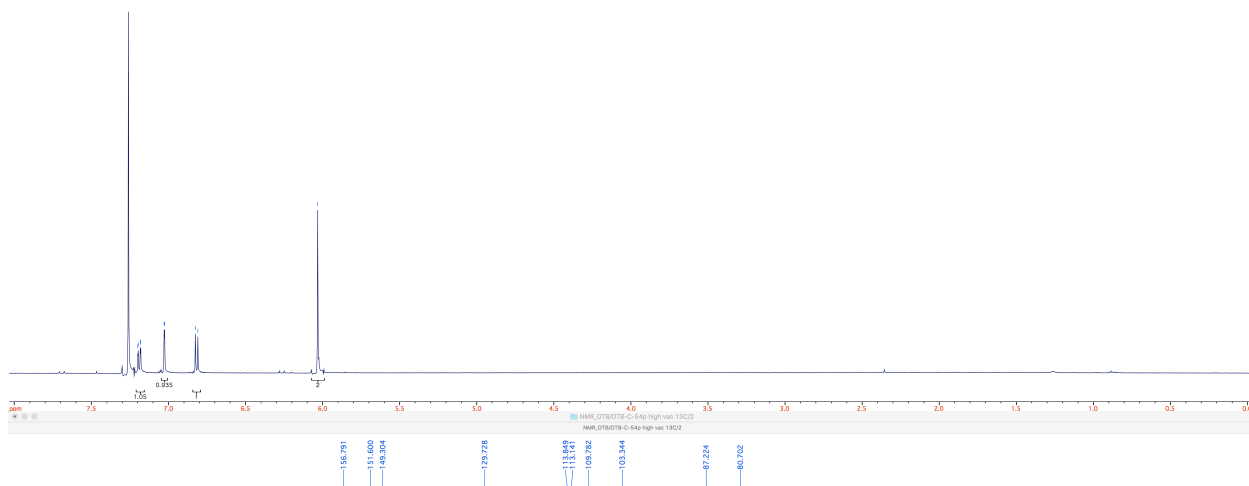
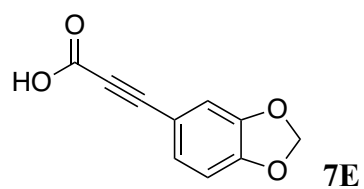
Background RT 1.09 - 1.25 (13 scans)
OTB-C-71_inj1.datx 2021.08.03 16:04:08 ;
ESI - Max: 1.9E8



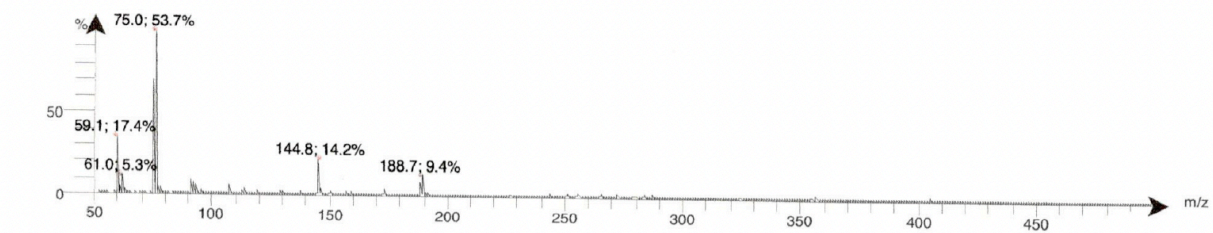


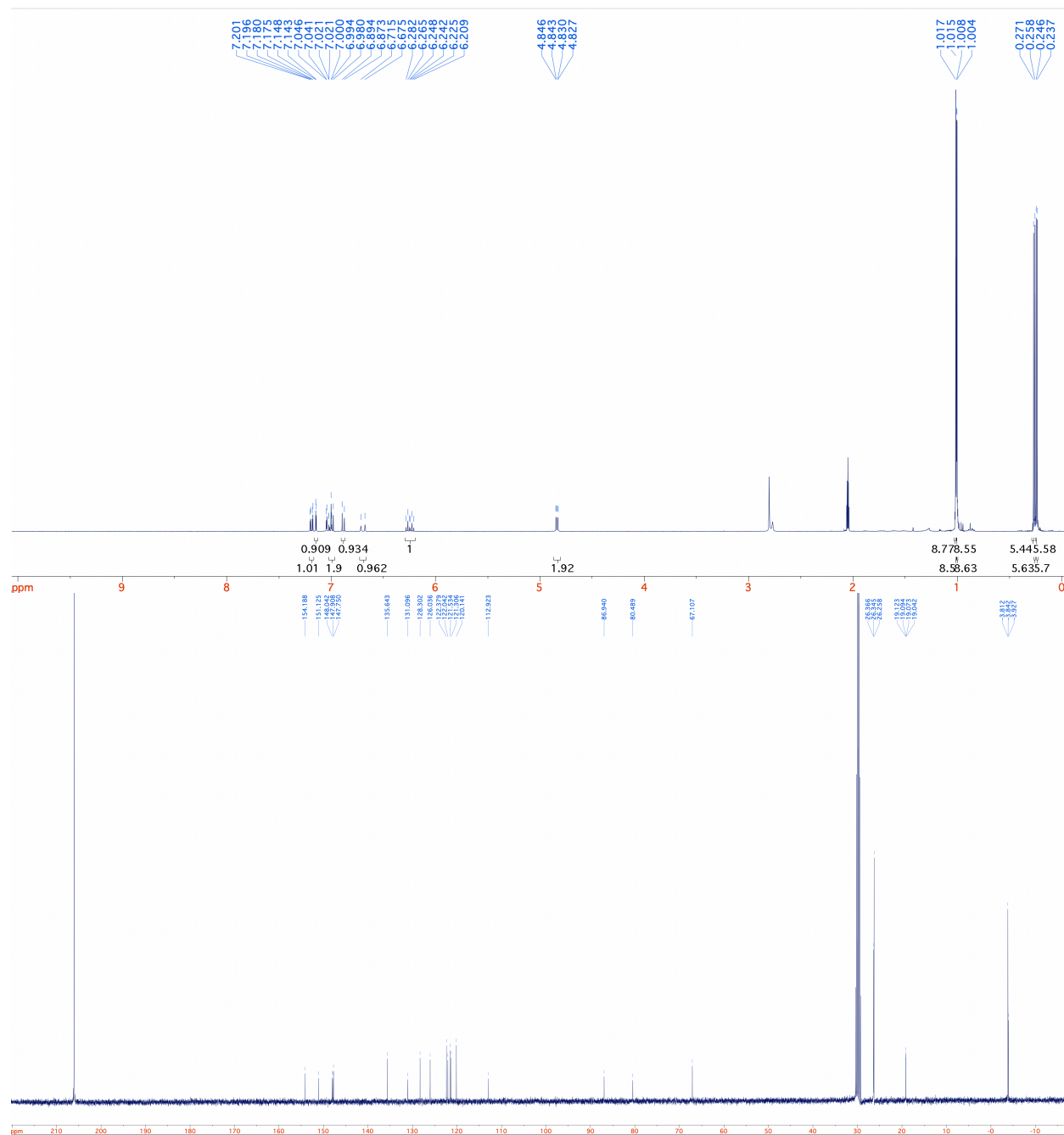
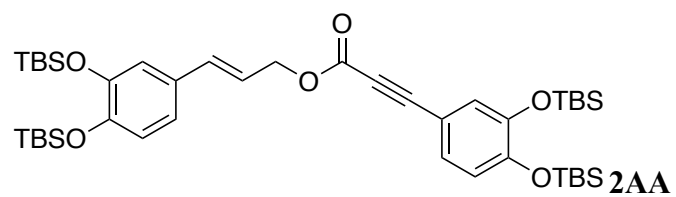
Background RT 0.97 - 1.14 (14 scans)
SMK-PT-94X1_inj1.datx 2021.07.26 17:33:03 ;
ESI - Max: 3.6E7





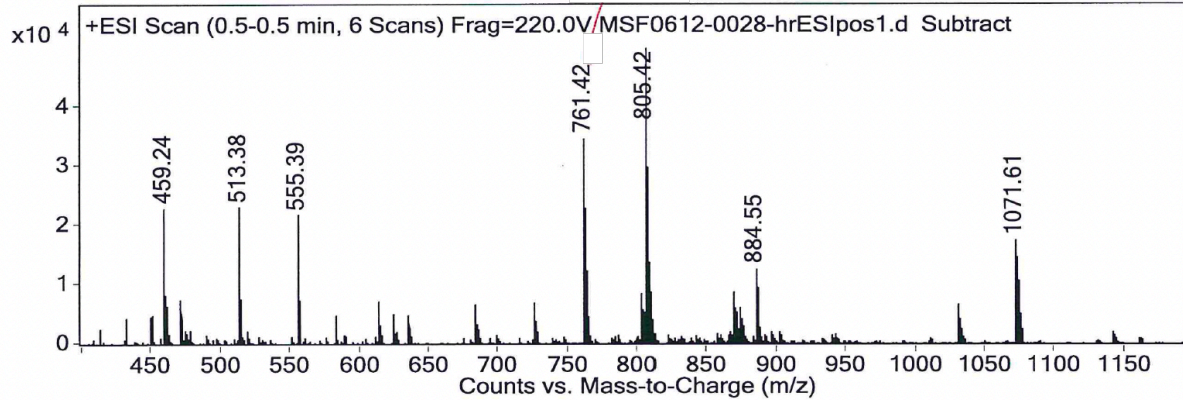
Background RT 0.80 - 0.94 (12 scans)
OTB-C-54_inj4.datx 2021.08.05 12:47:15 ;
ESI - Max: 7.7E7

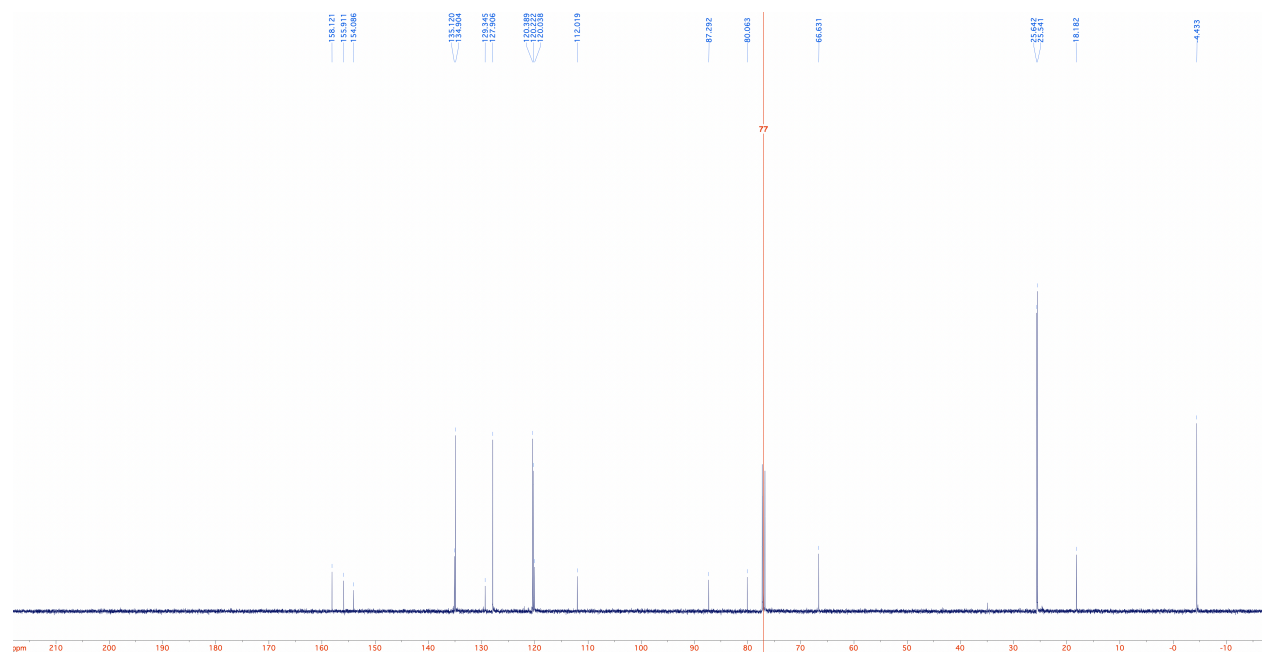
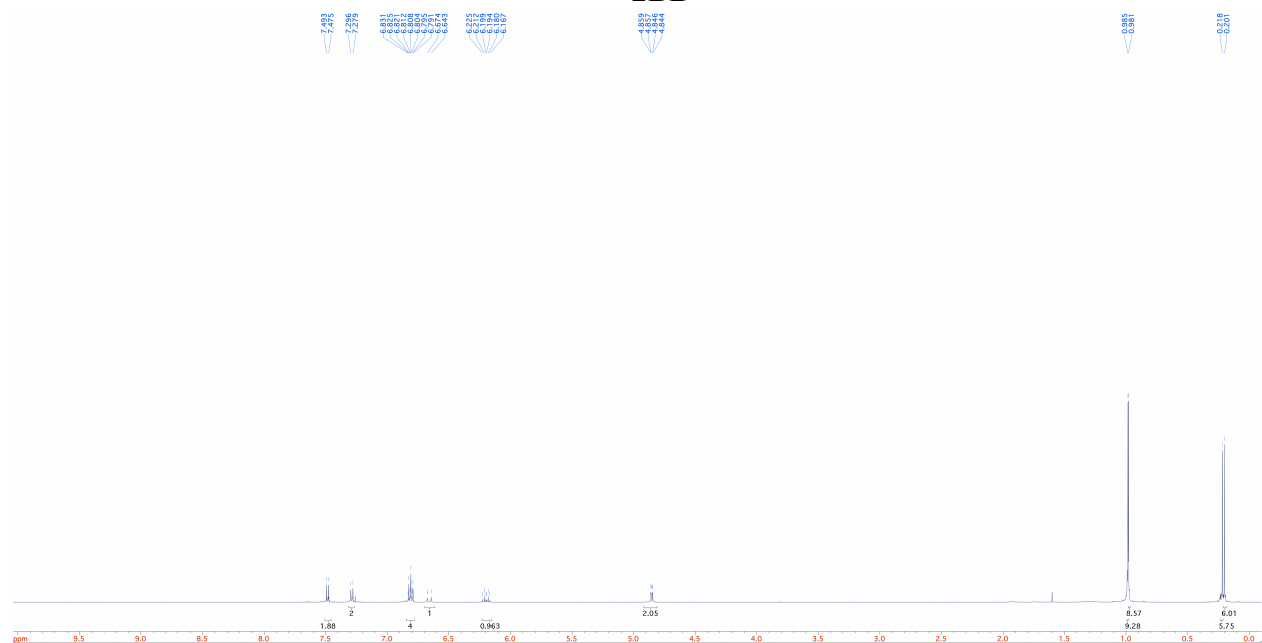
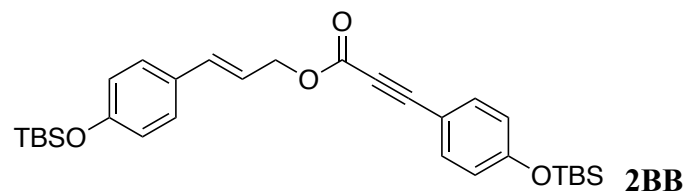




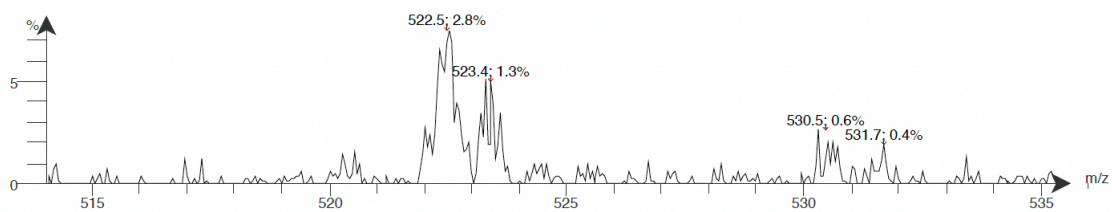
User Spectra

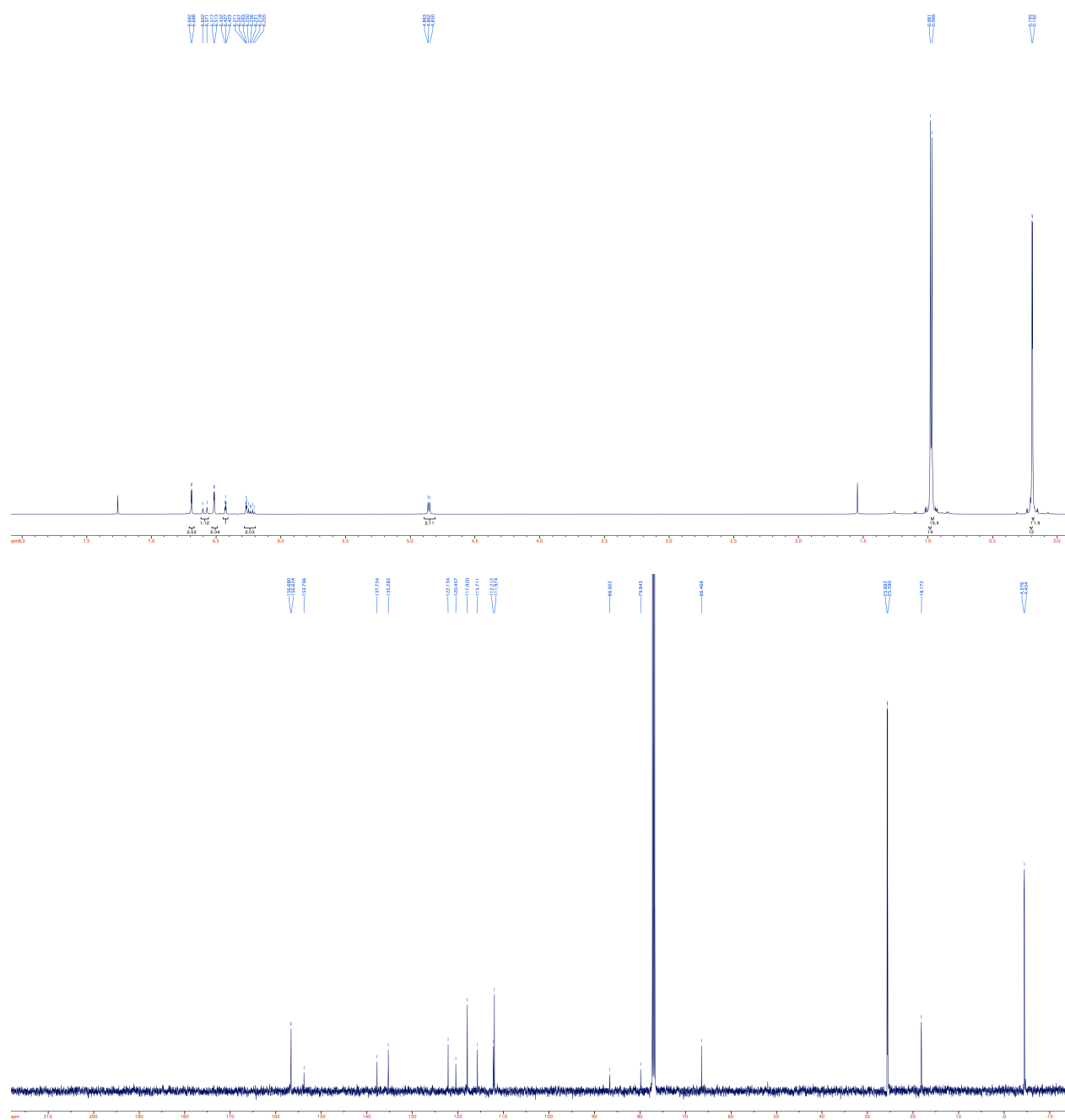
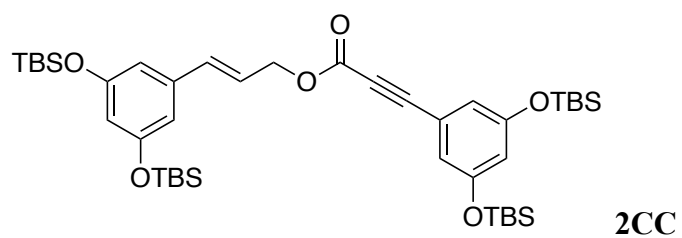
Fragmentor Voltage 220 Collision Energy 0 Ionization Mode ESI





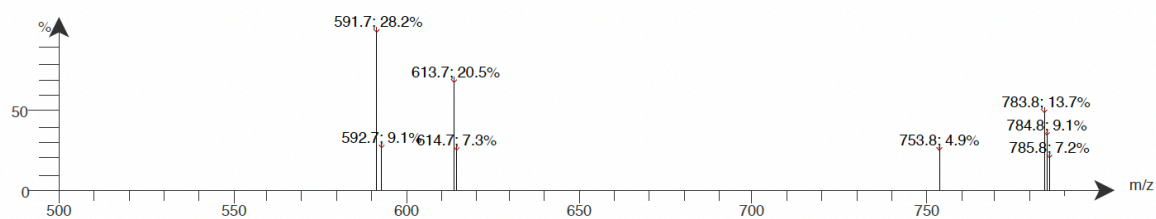
Background RT 0.88 - 0.99 (14 scans)
SMK-T60_ESIpos_inj2.datx 2021.12.08 12:13:24 ;
ESI + Max: 3E6

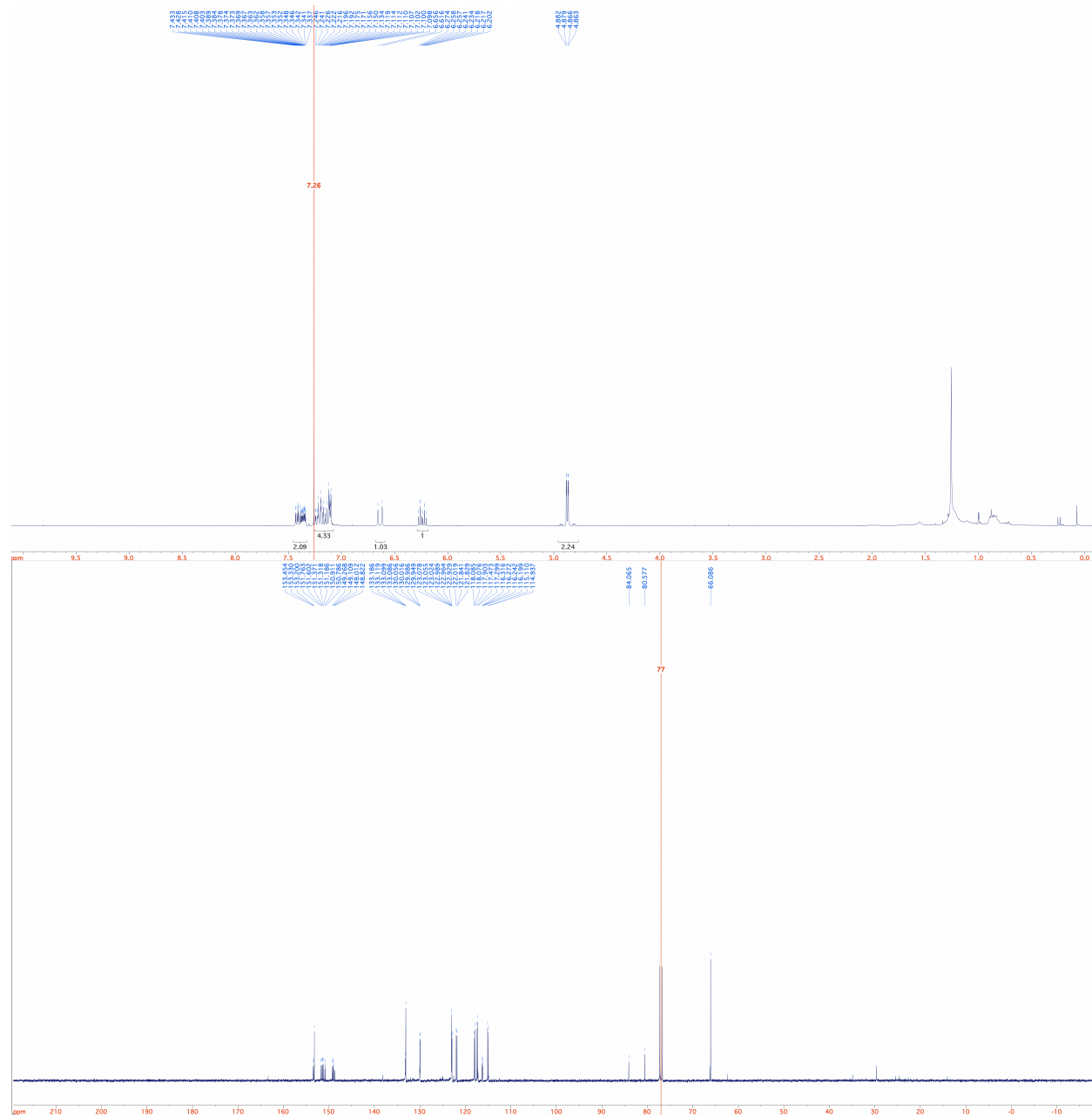
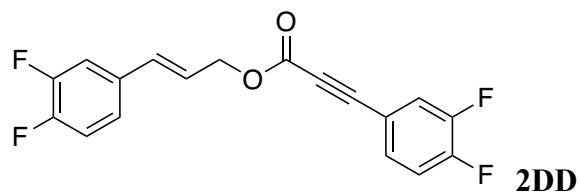


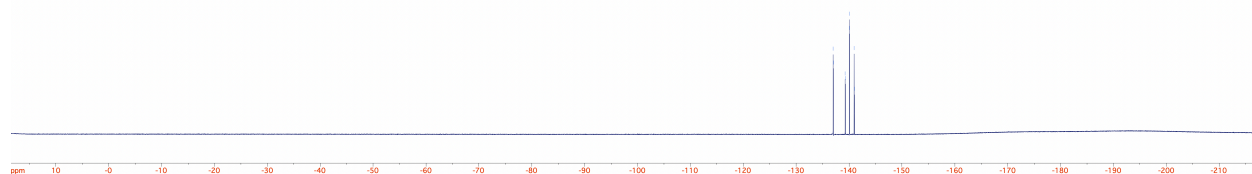


Intensity

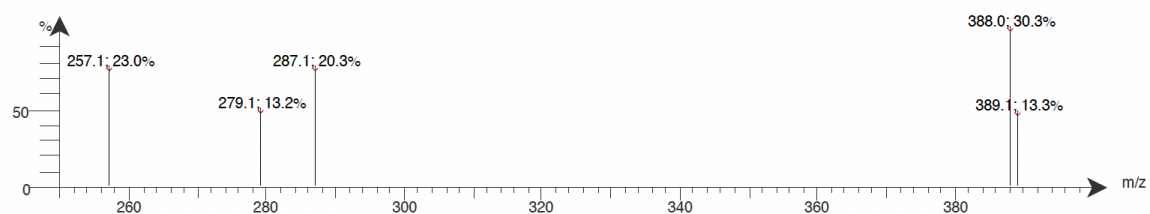
Background RT 0.87 - 1.12 {31 scans}
SMK-T-82cc2_ESIpos_inj1.datx 2021.12.09 10:38:29 ;
ESI + Max: 4.2E6

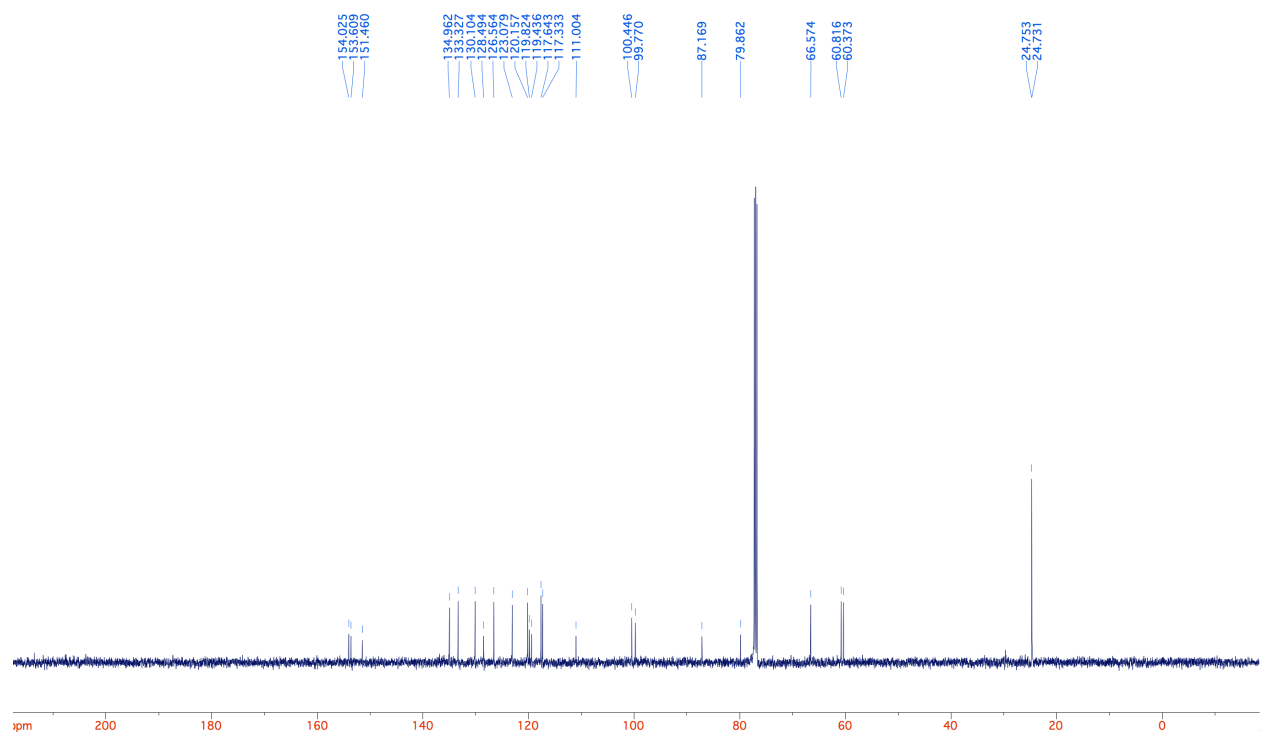
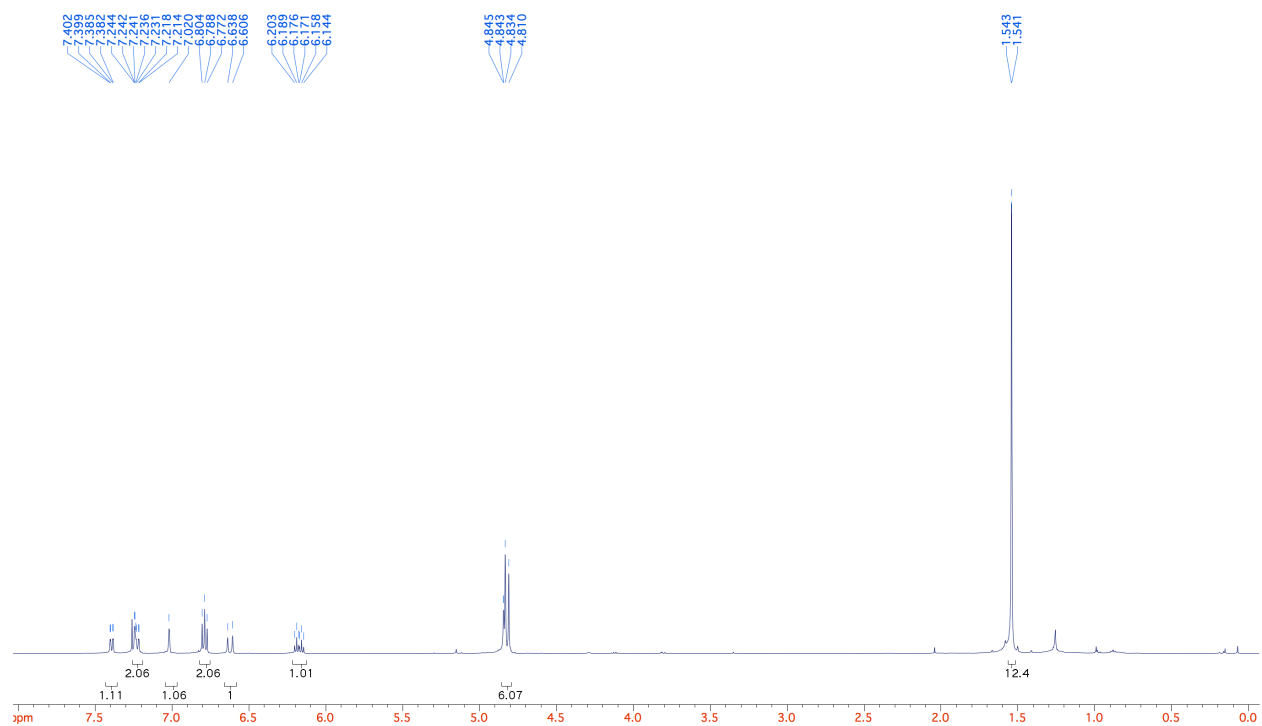
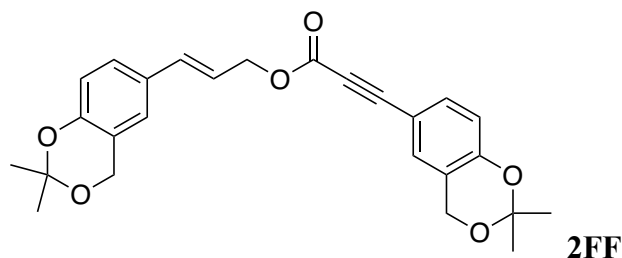




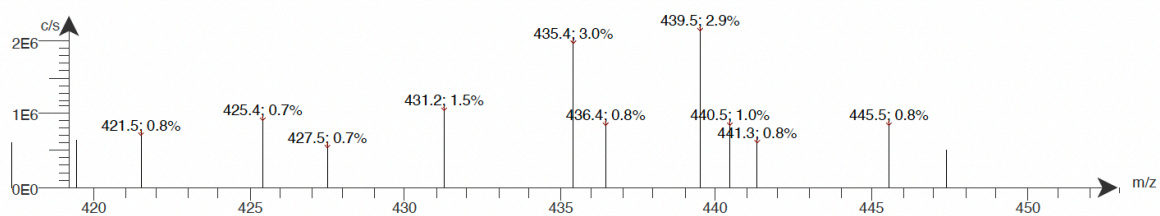


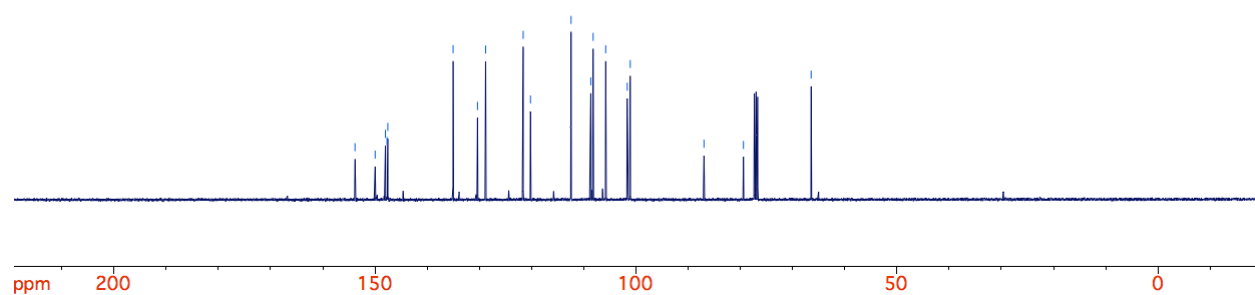
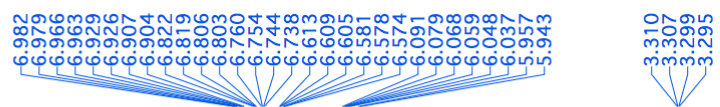
Background RT 0.75 - 1.01 (64 scans)
SMK-2B4B4_APCIpos_inj3.datx 2021.12.07 18:41:32 ;
APCI + Max: 2.8E6



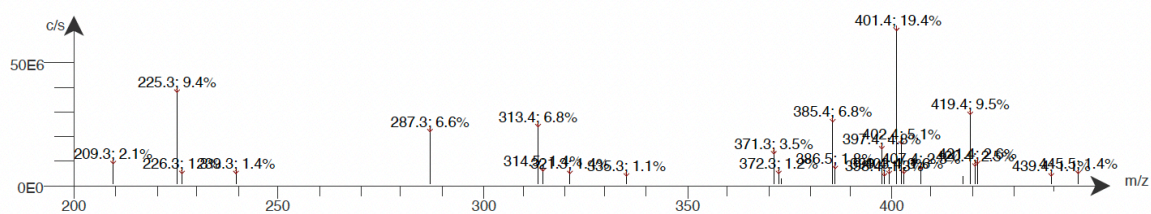


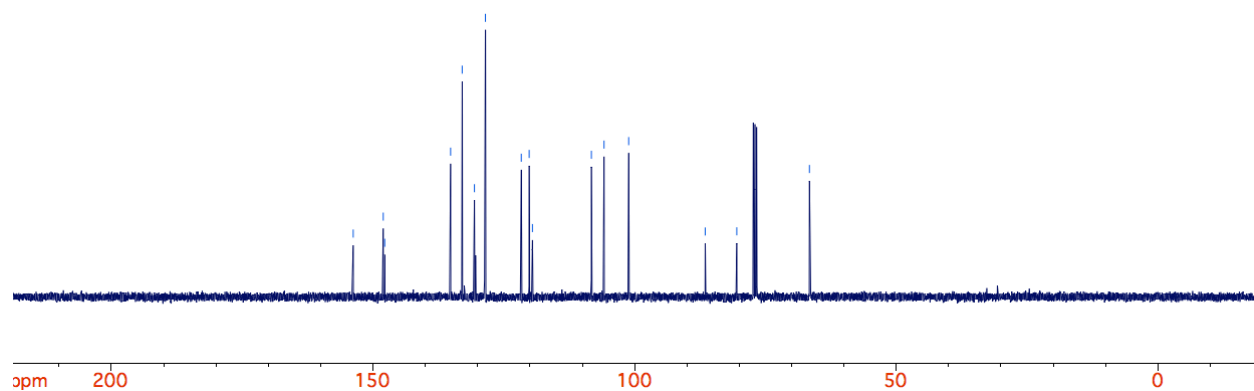
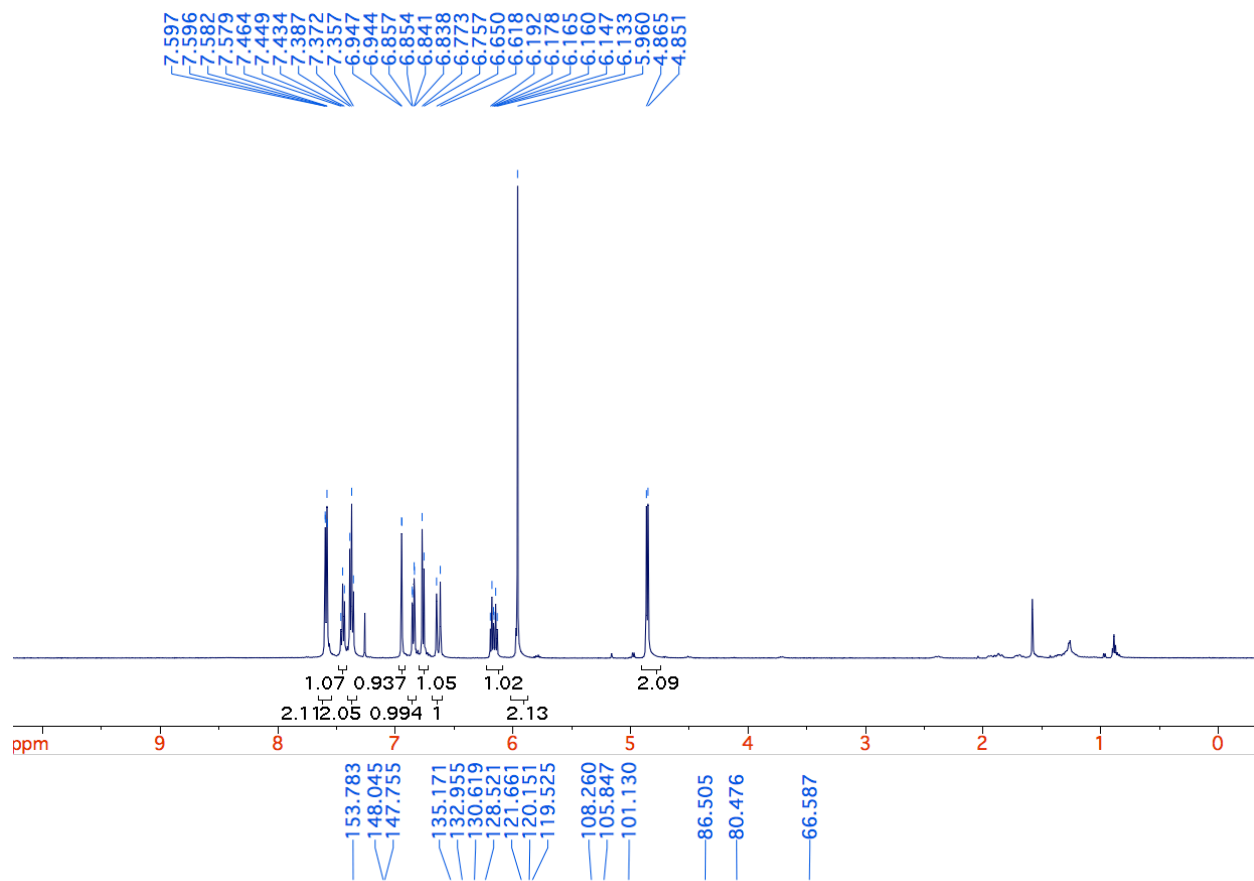
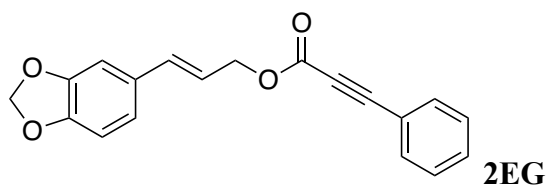
Intensity
Background RT 0.90 - 1.03 (25 scans)
SMK-T-88_ESIpos_inj1.datx 2021.12.09 11:20:47 ;
ESI +



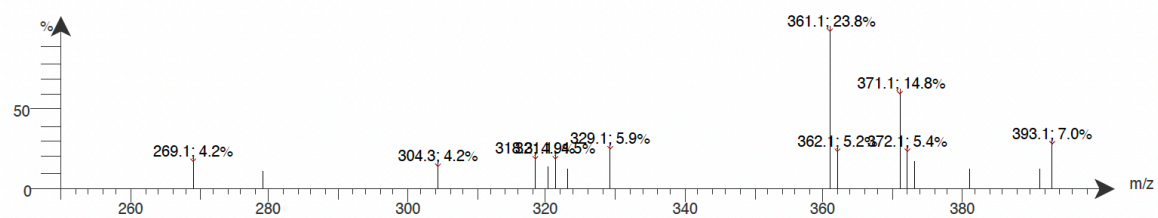


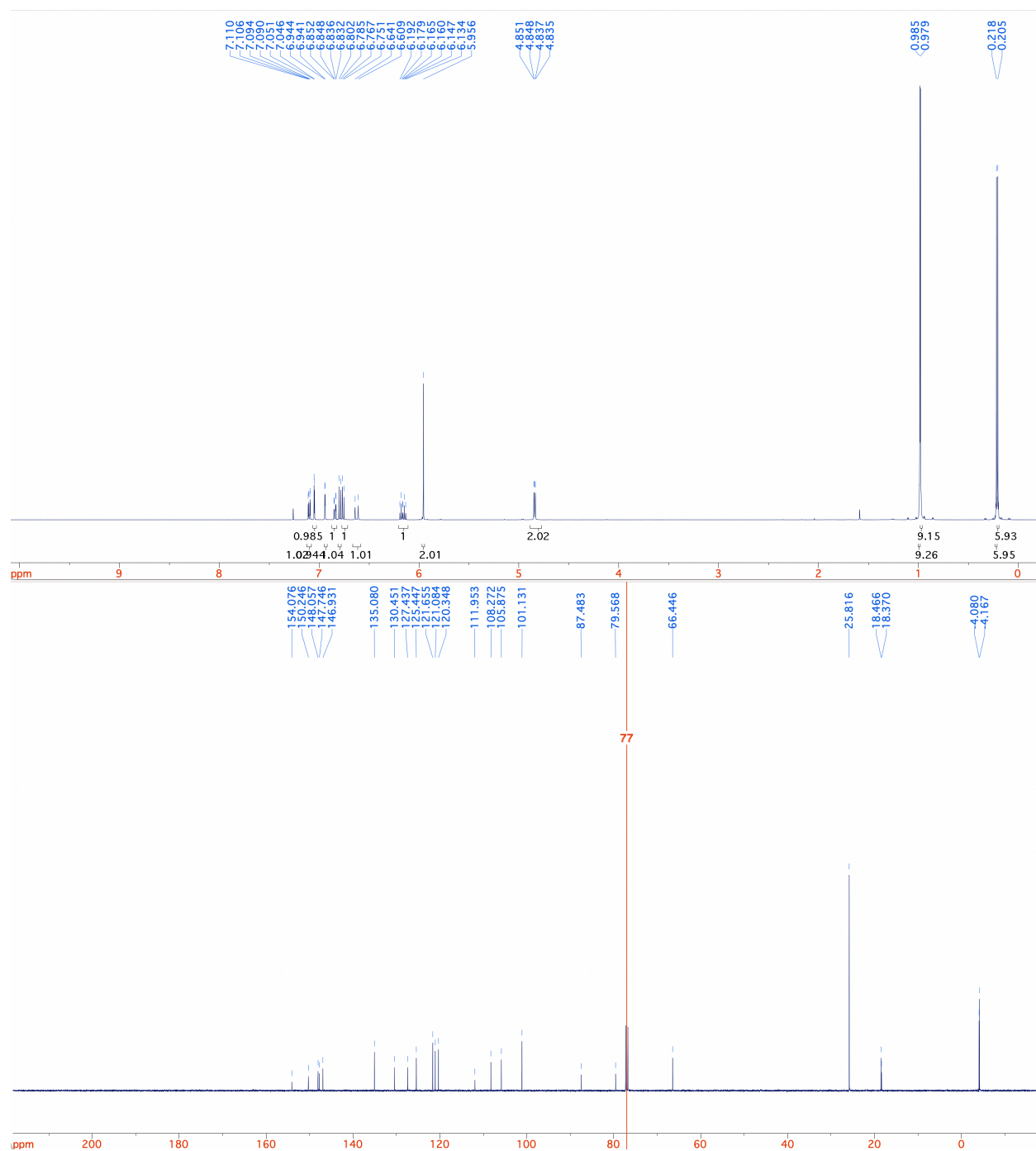
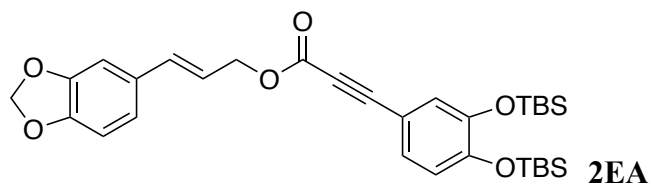
Background RT 1.07 - 1.32 {36 scans}
OTB-C81p_ESIpos_inj2.datx 2021.12.09 14:21:13 ;
ESI +



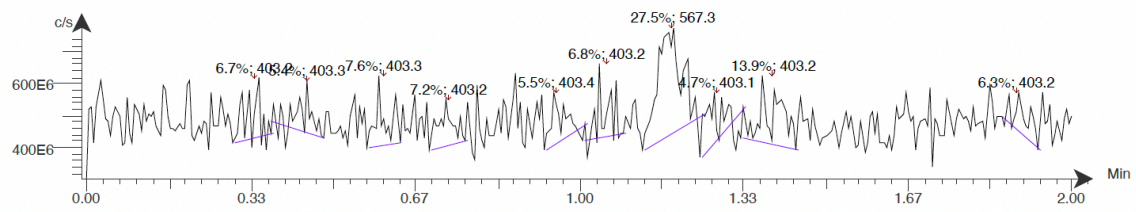


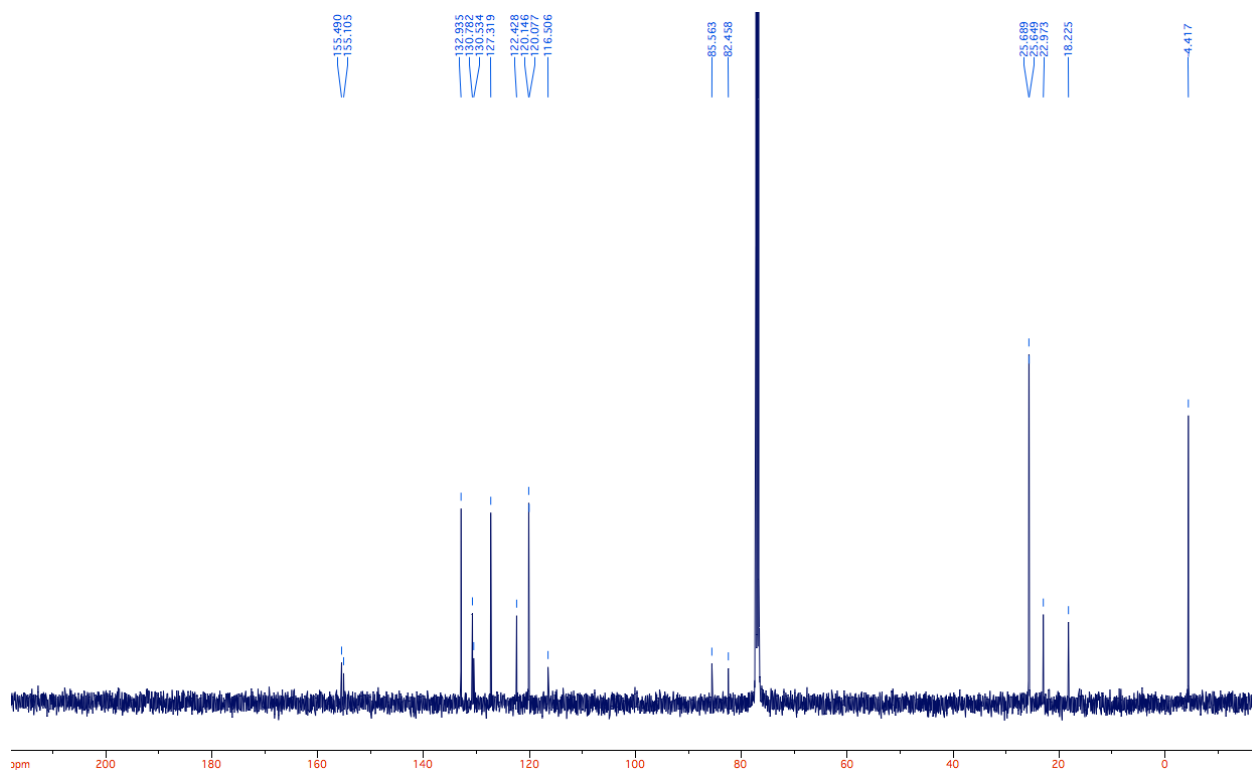
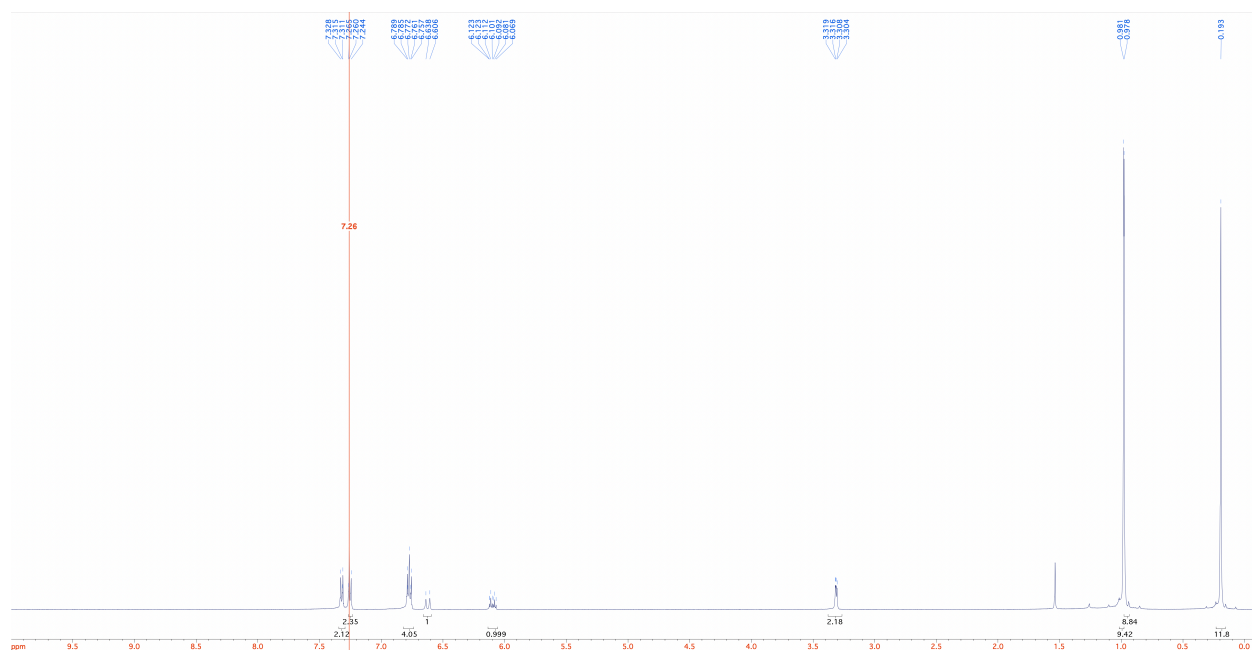
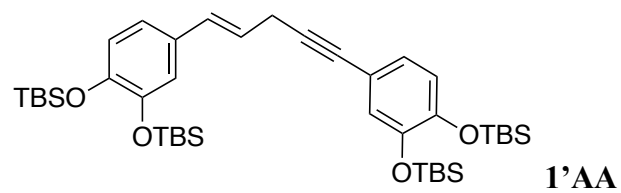
Background RT 1.07 - 1.28 (51 scans)
ZTS-PDC-5_ESIpos_inj2.datx 2021.12.13 16:53:07 ;
ESI + Max: 4.2E7



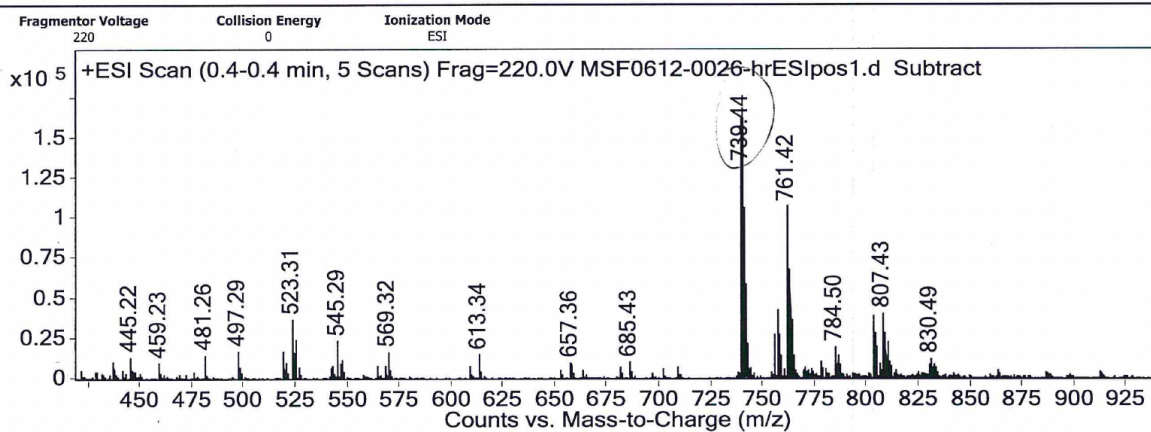


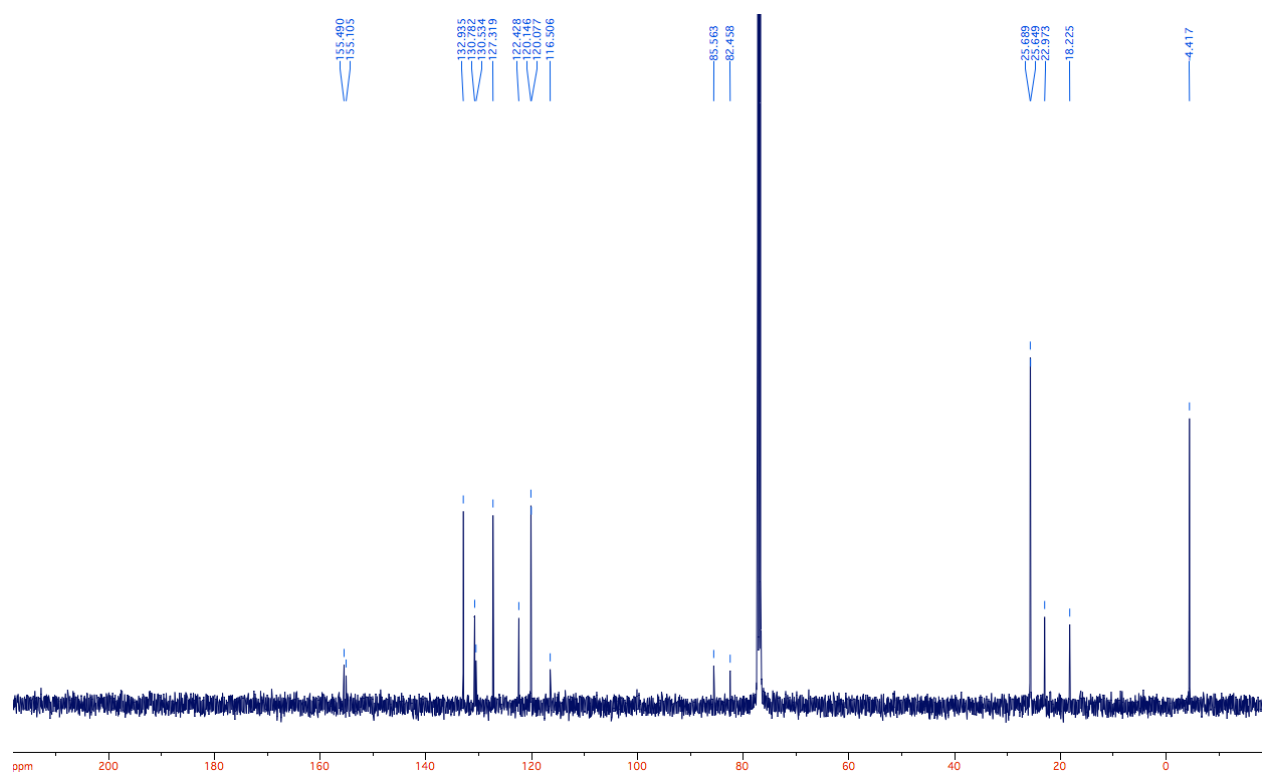
TIC
SMK-T-58_ESIpos_inj2.datx 2021.12.09 10:27:08 ;
Intensity ESI +



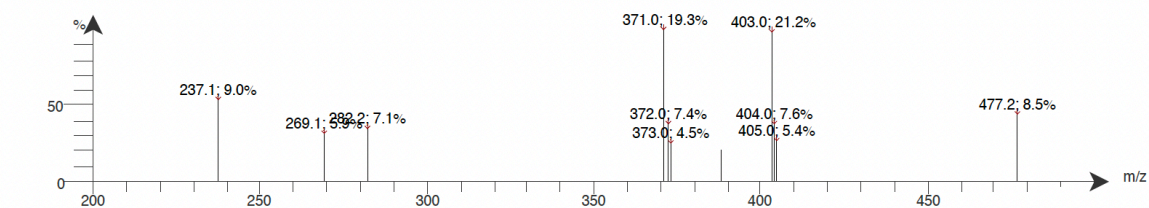


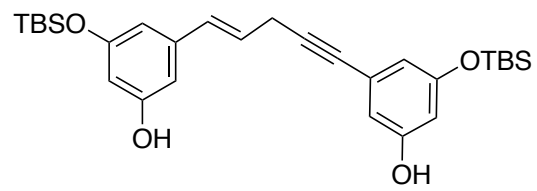
User Spectra



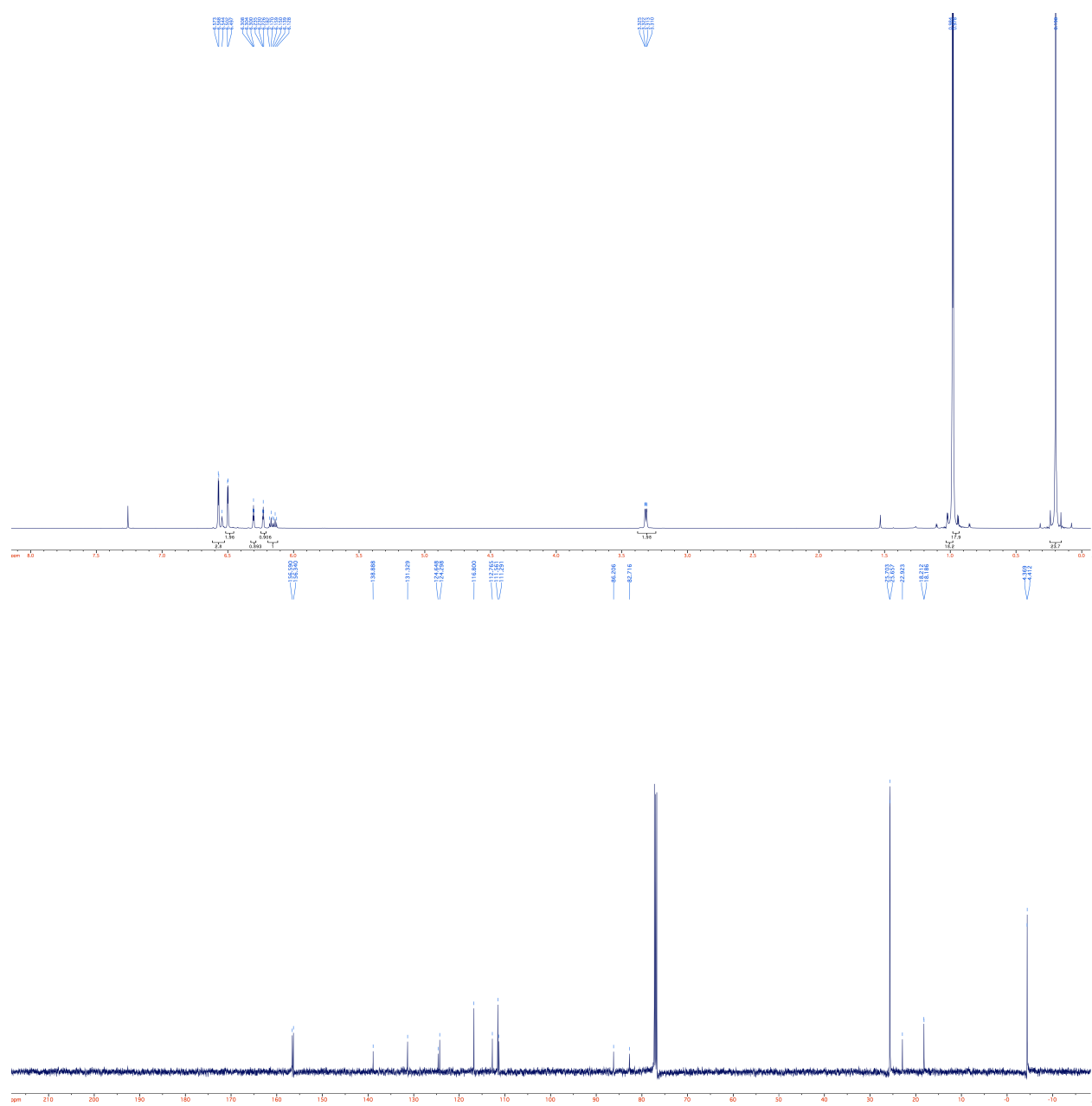


Background RT 0.90 - 1.09 (24 scans)
SMK-T-81_APCIpos_inj1.datx 2021.12.07 18:08:47 ;
APCI + Max: 4.5E7

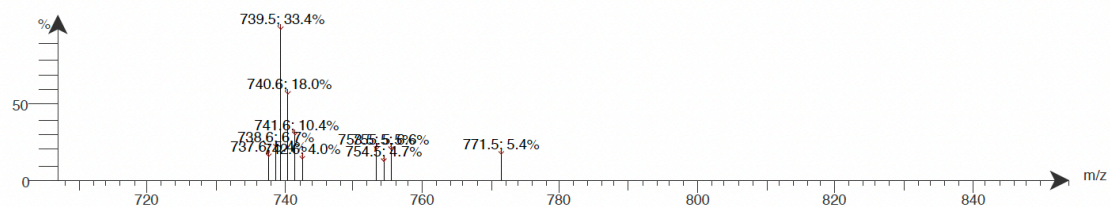


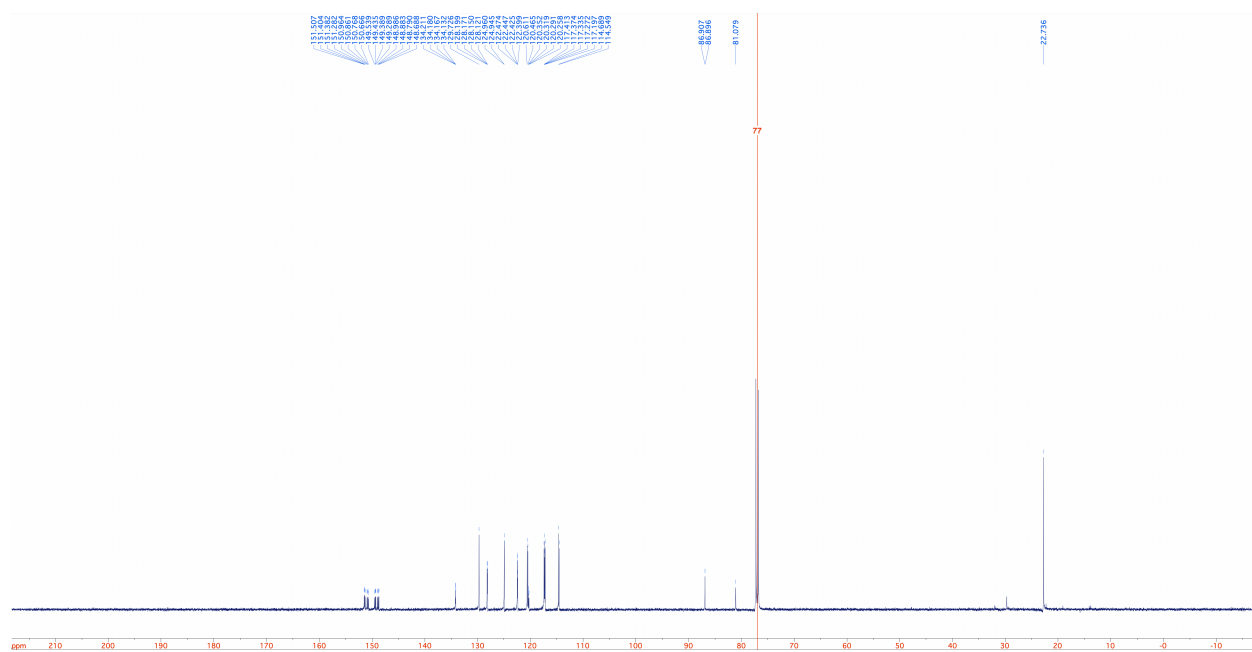
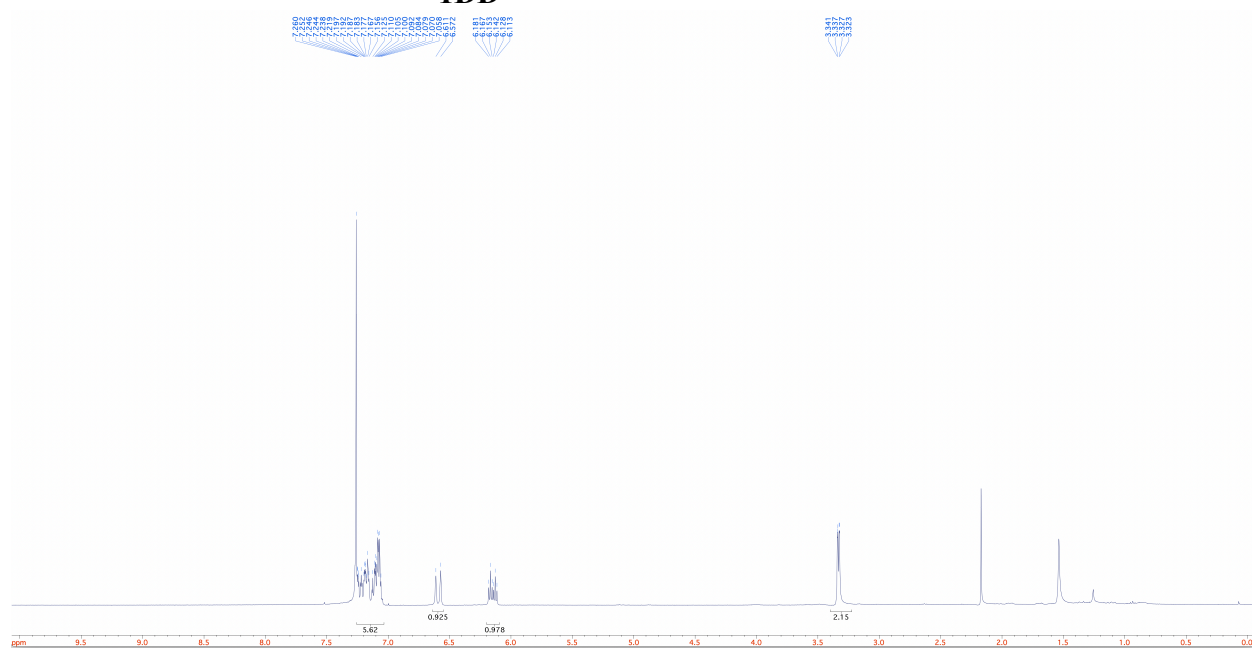
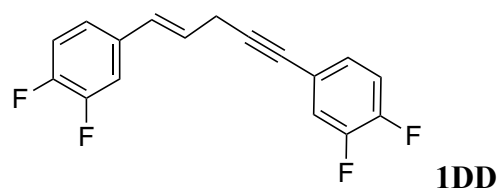


1'CC

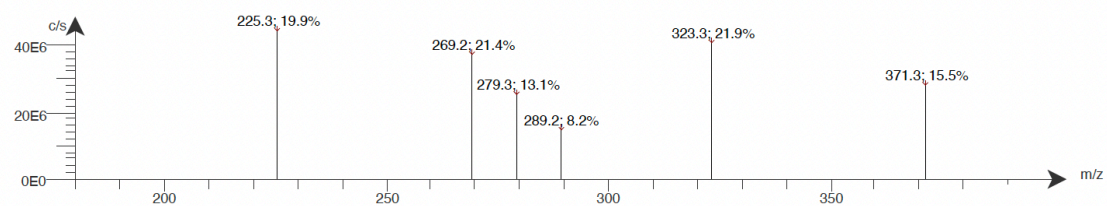


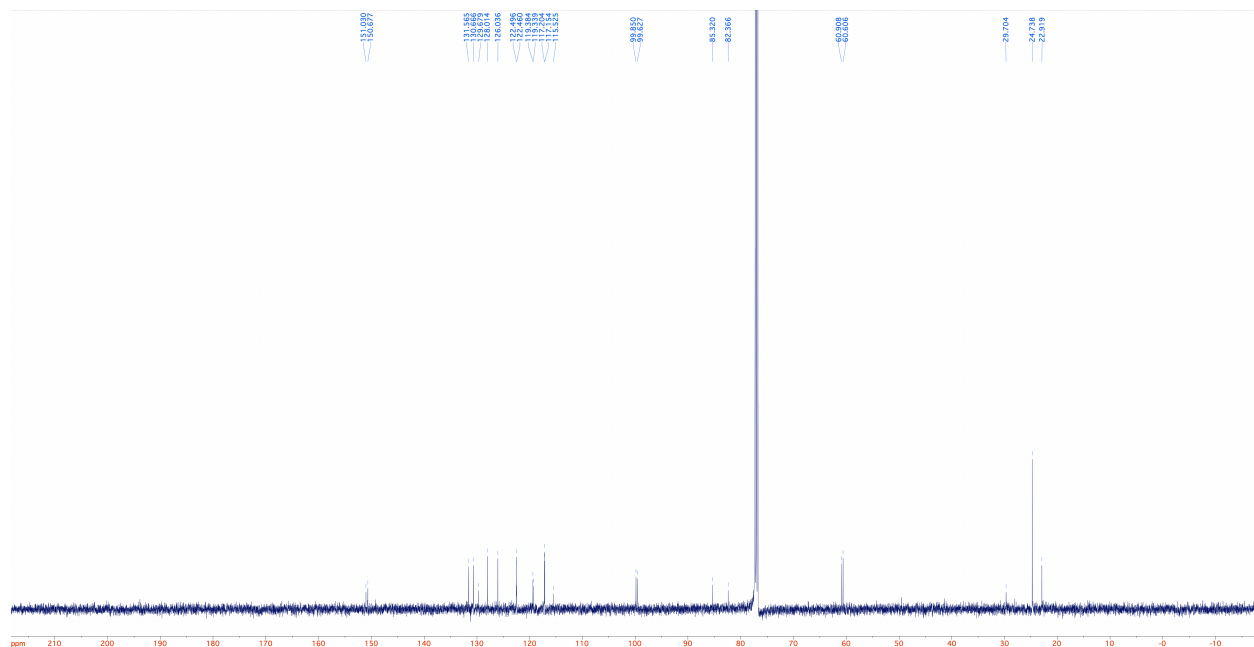
Background RT 1.12 - 1.28 {15 scans}
SMK-T-83cc3_3A4A4_APCI_inj1.datx 2021.11.30 14:21:32 ;
Intensity APCI + Max: 2.7E7



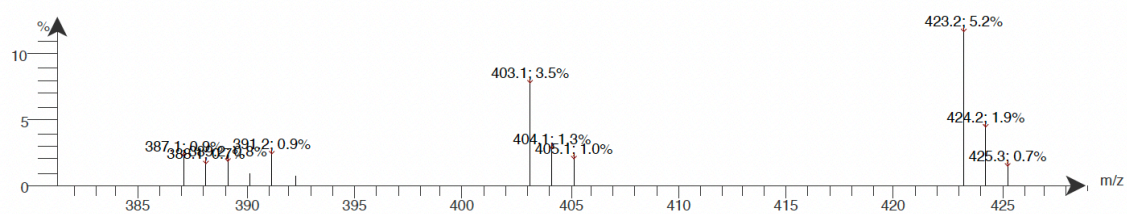


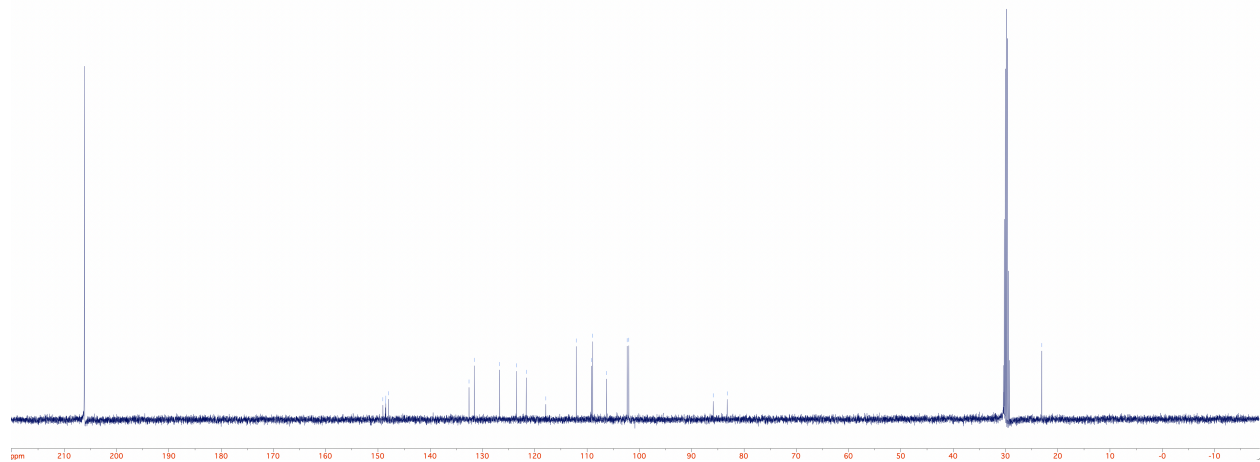
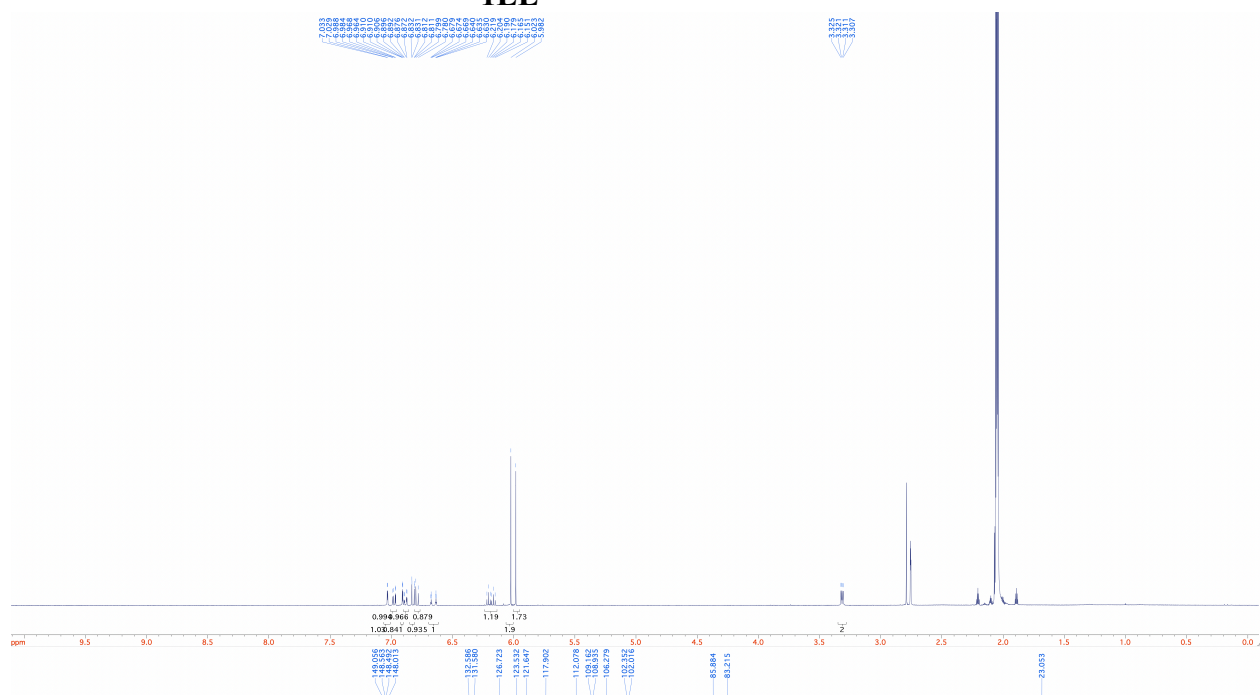
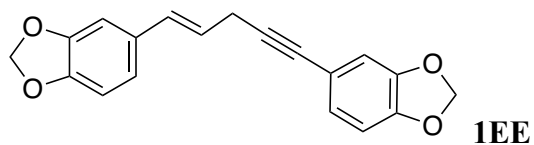
Background RT 1.56 - 1.73 {28 scans}
SMK-ROPB4B4_ESIpos_inj2.dabx 2021.12.09 12:14:17 ;
ESI +



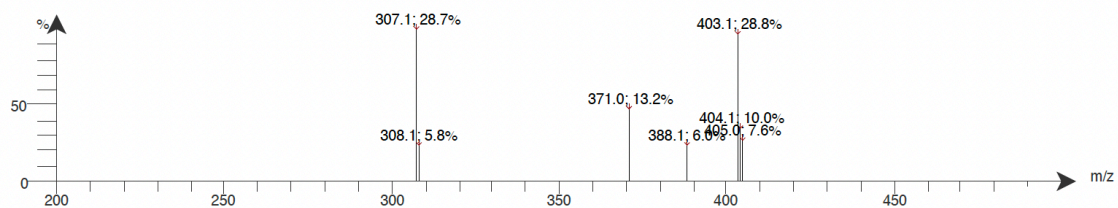


Background RT 0.93 - 1.16 (29 scans)
SMK-T-93_3C3C3_APCI_inj3.datx 2021.11.30 19:06:18 ;
Intensity APCI + Max: 2.5E7



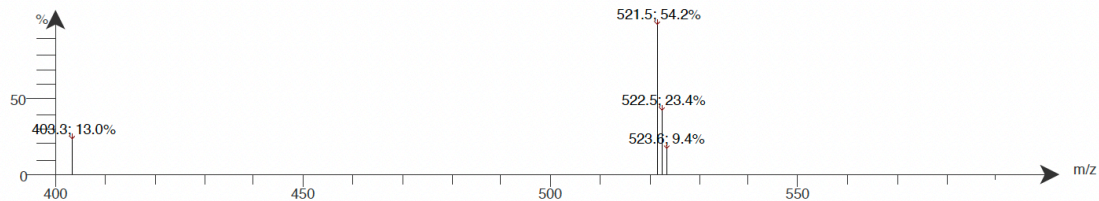


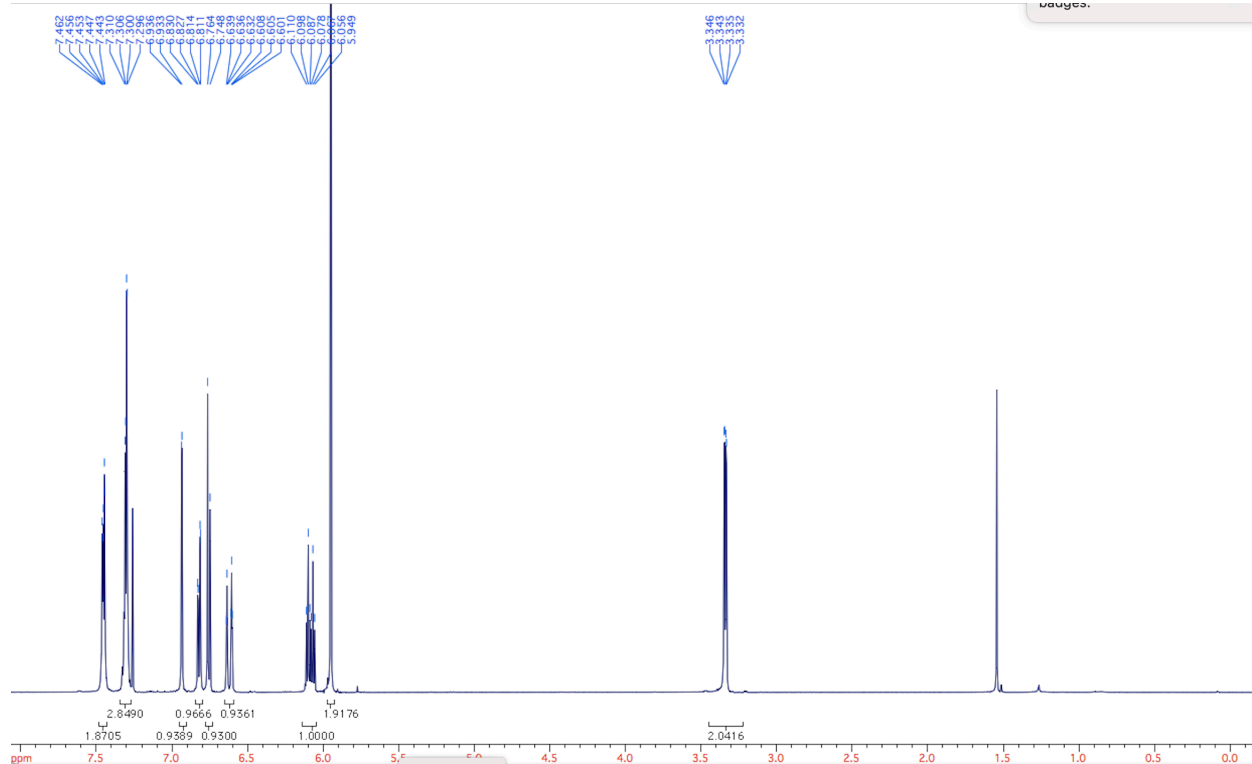
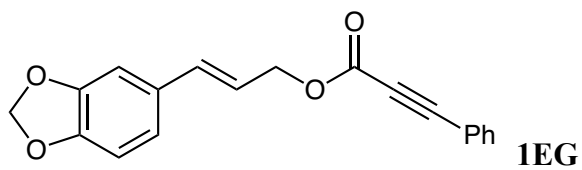
Background RT 1.09 - 1.24 (19 scans)
 OTB-C-92_APCipos_inj1.datx 2021.12.07 18:03:18 ;
 APCI + Max: 3.9E7



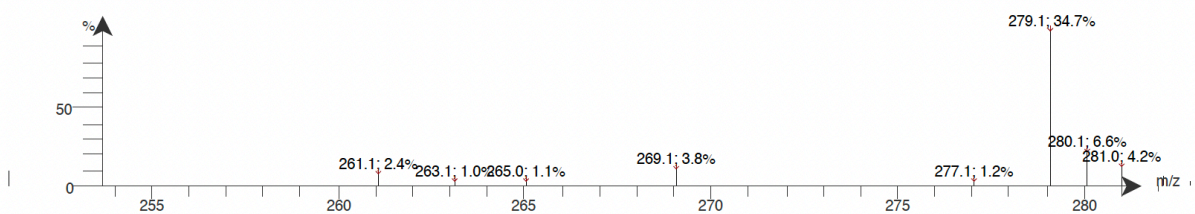


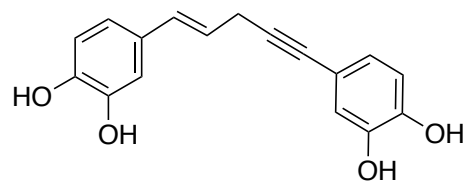
ESI + Max: 5.8E7





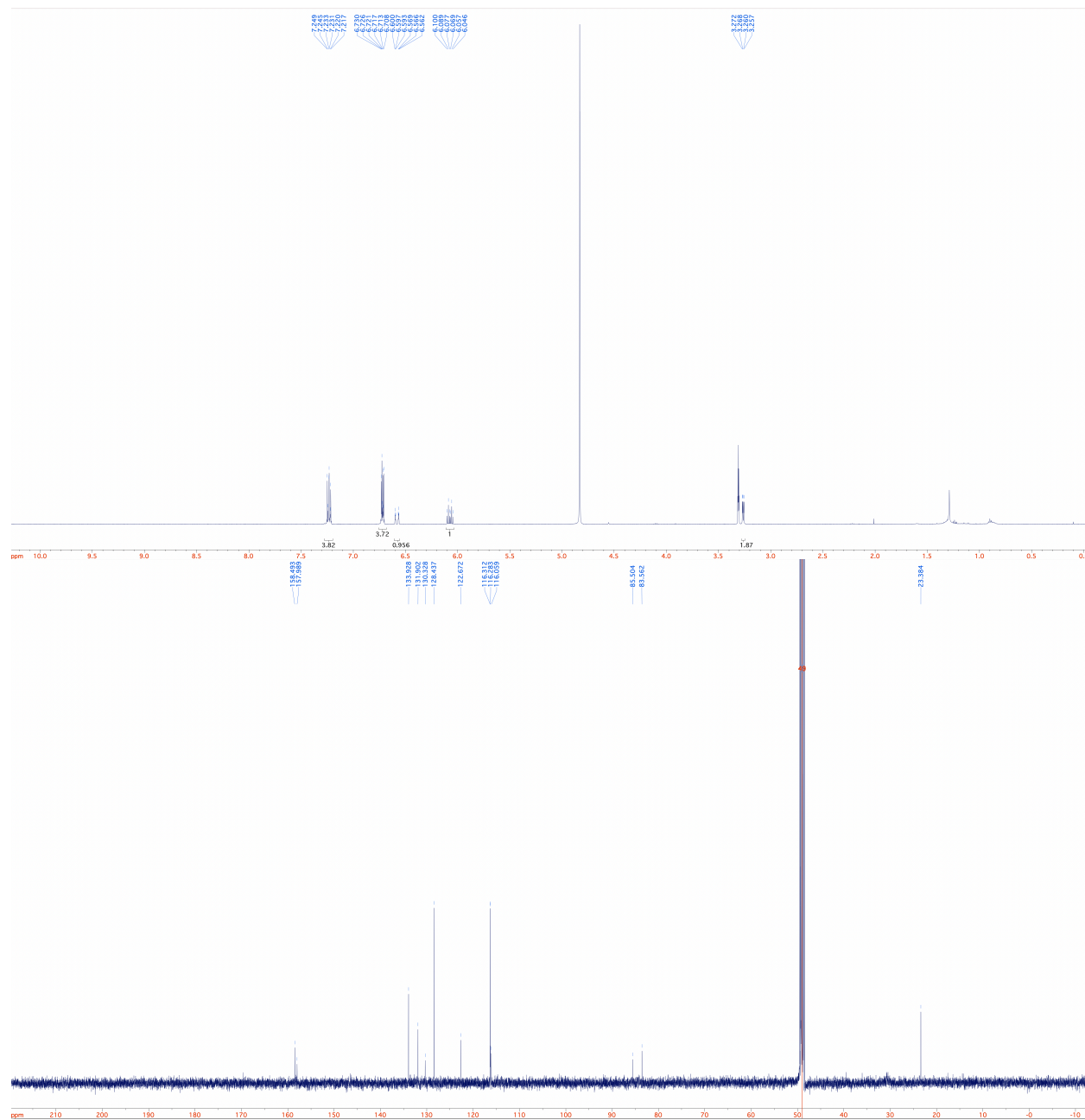
Background RT 1.06 - 1.26 (60 scans)
ZTS-PDC-16_ESIpos_inj1.datx 2021.12.13 17:36:59 ;
ESI + Max: 3.9E7

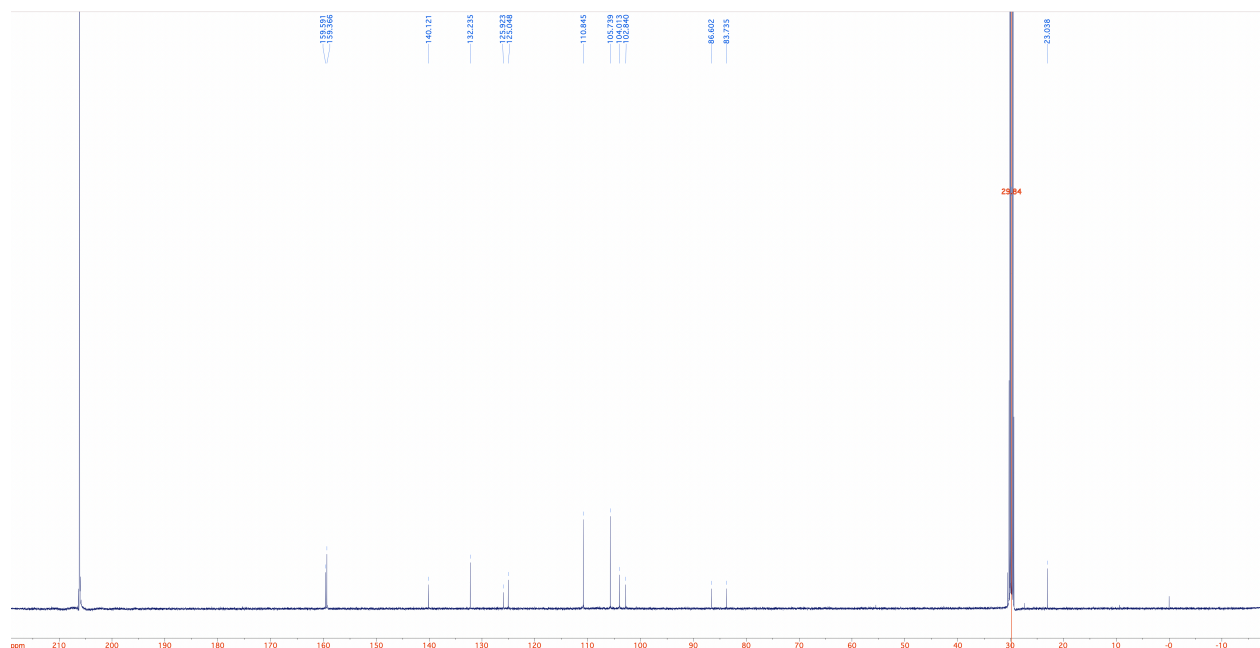
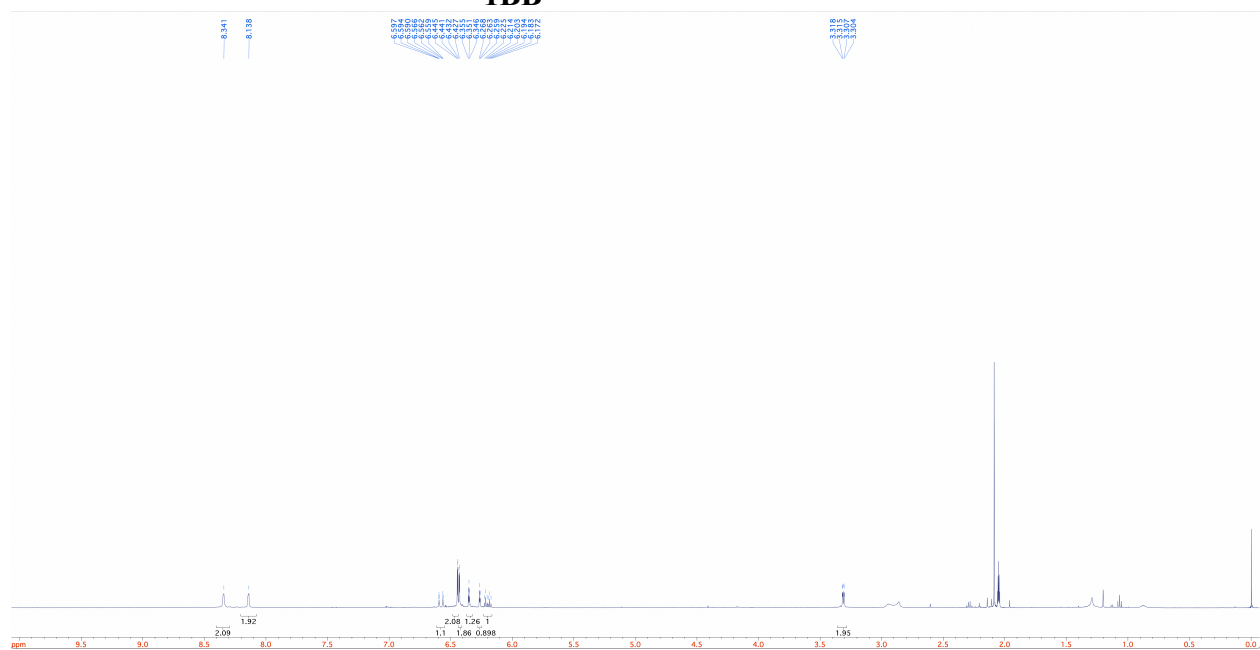
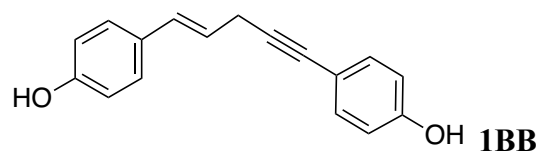




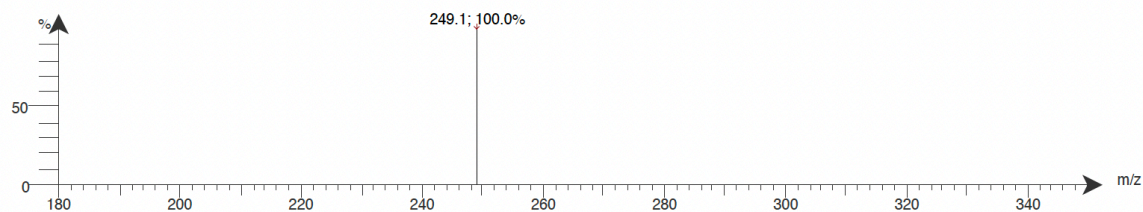
rooperol

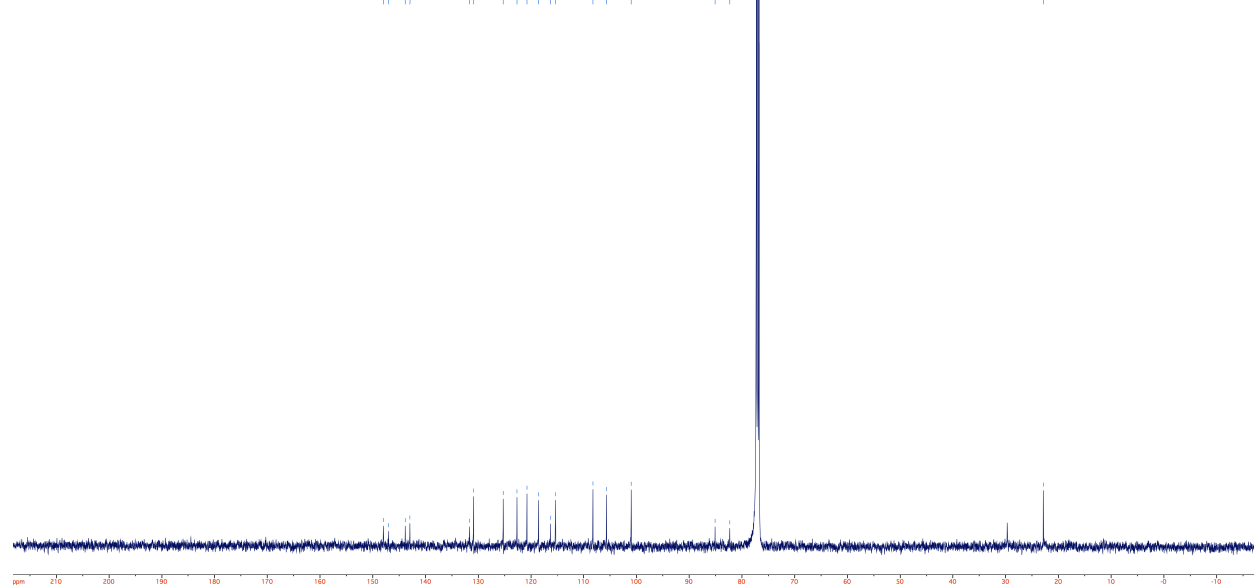
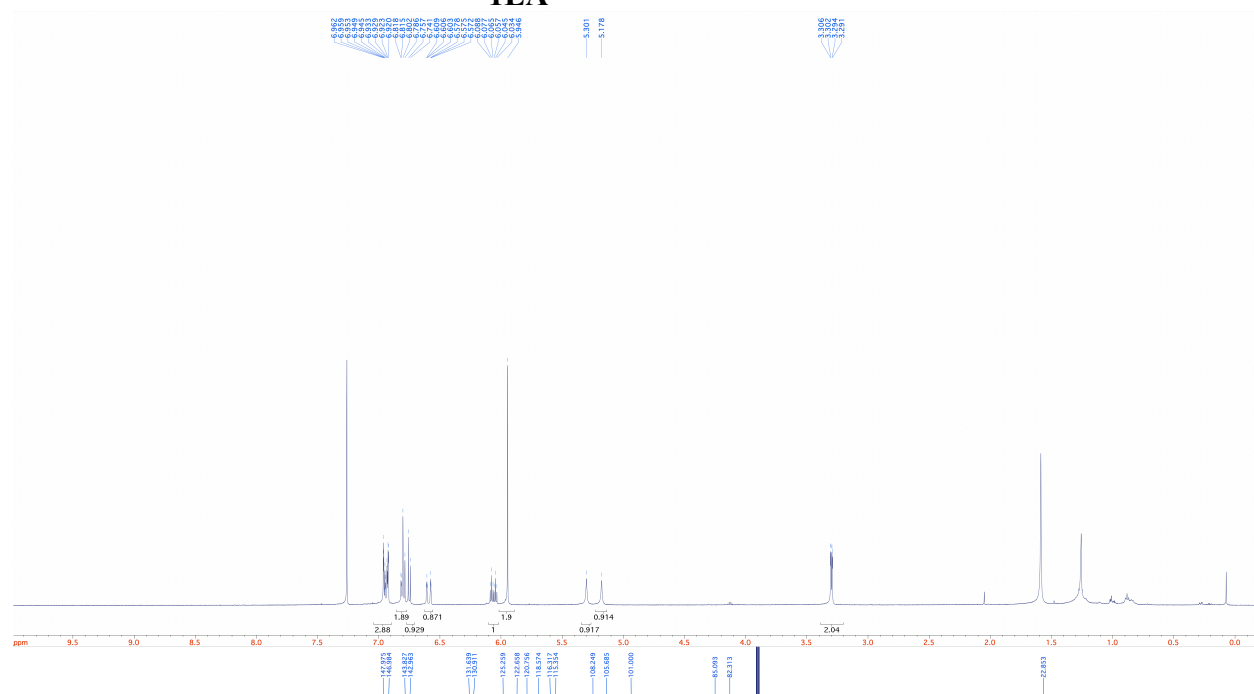
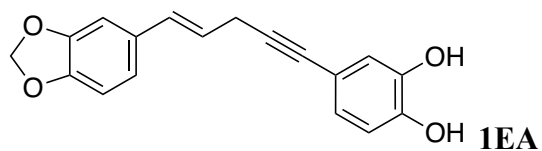
1AA



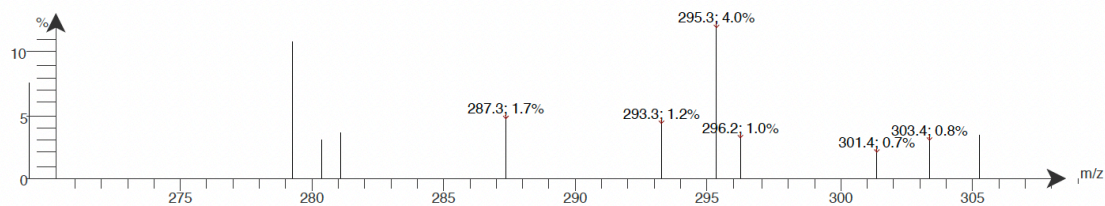


Spectrum RT 1.10 - 1.26 (35 scans) - Background Subtracted 1.09 - 1.10
 SMK-T-101ESIneg_inj4.datx 2021.12.13 16:19:35 ;
 ESI - Max: 1.2E7





Background RT 0.83 - 1.03 {37 scans}
 SMK-T-97cc1_ESIpos_inj1.datx 2021.12.09 10:52:42 ;
 ESI + Max: 3.6E6



Supplemental Figure 1. Dose-dependent cytotoxicity of rooperol and analogs in cancer cell lines. Cells were treated with a serial of dilutions of each compound in three replicates in 96-well plates for 96 h, and cell viability was measured using MTT assay. Shown in each figure is dose-dependent response of the indicated cells to the indicated compound, with the dotted line signifying the IC_{50} .

