

Discovery of Ligands for a Novel Target, the Human Telomerase RNA, Based on Flexible-Target Virtual Screening and NMR

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Supplemental material

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1) Mass spectroscopy purity table

Structure #	Zinc Number	LC/MS MH+ Calc.	LC/MS MH+ Found
1	3830842	415	415
2	3831167	310	310
3	1681039	281	281
4	1728888	305	305
5	1659950	363	363
6	1755302	364	364
7	1755784	319	319
8	3831302	214	214
9	1578896	186	186
10	1736291	350	350
11	1530657	375	375
12	28449	215	215
13	57106	228	228
14	484	331	331
15	57320	304	304
16	3872807	421	421
17	1766827	548	274*
18	3830747	481	481
19	1666894	370	370
20	1653191	370	370
21	1729641	352	352
22	1755462	379	379
23	1621260	356	356
24	1724568	370	370
25	1704090	504	252*
26	1631690	425	425
27	1695616	285	285
28	1596778	370	370
29	1641916	347	347
30	1692893	507	507
31	608154	412	412
32	3830916	357	357
33	1665554	395	395
34	1684589	482	482
35	1678484	481	481
36	4707118	526	526
37	538503	408	408
38	3831528	447	447
39	5010740	384	384
40	5386677	330	330
41	5439641	600	600

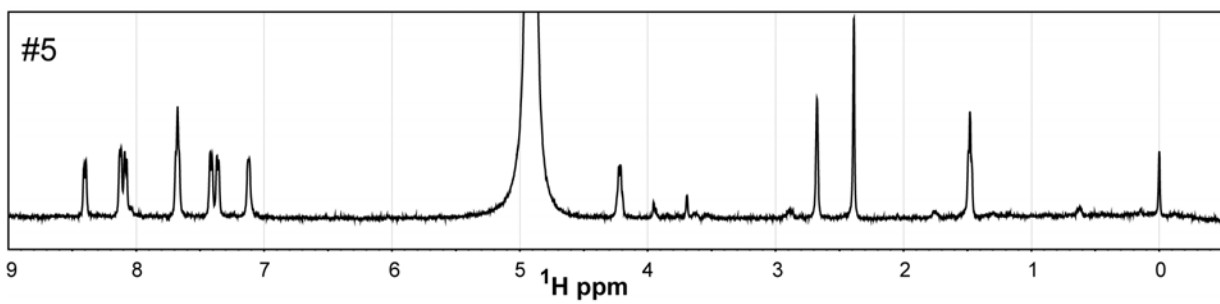
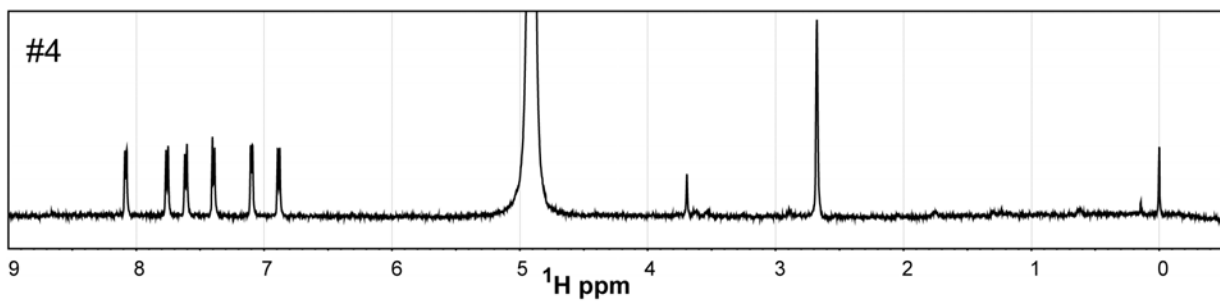
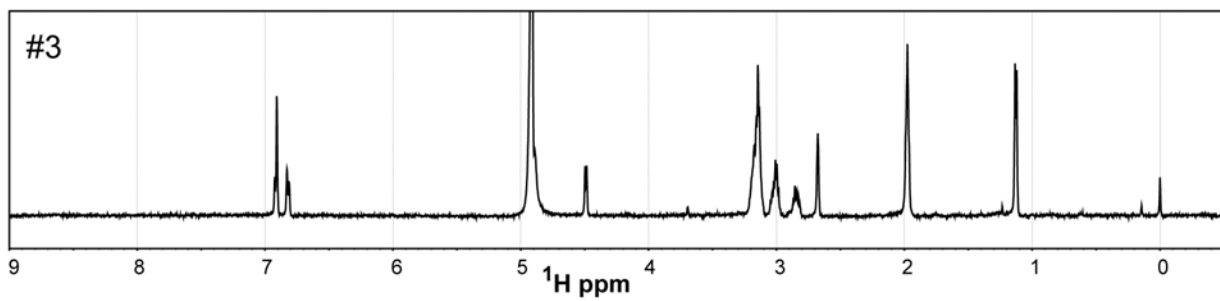
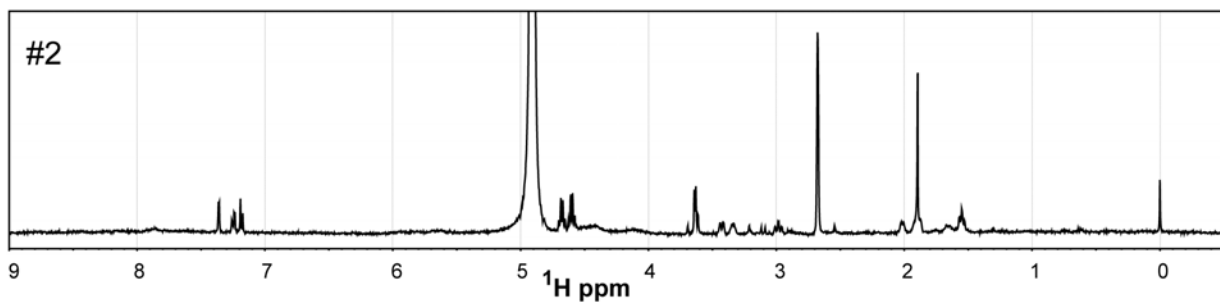
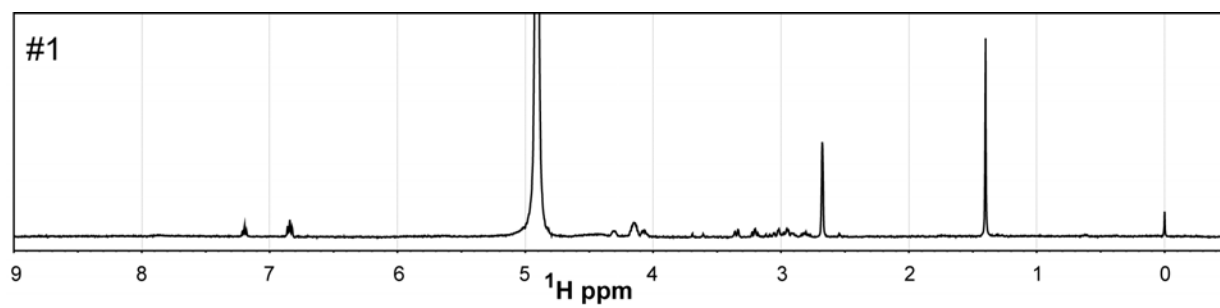
42	5496932	614	614
43	3954210	596	596
44	4198846	652	326*
45	1601558	297	297
46	1530748	384	384
47	1655587	319	319
48	1566281	293	293
49	509	266	266
50	3831586	295	295
51	27696	319	319
52	1678385	366	366
53	1137	316	316
54	1701768	240	223**
55	57146	255	255

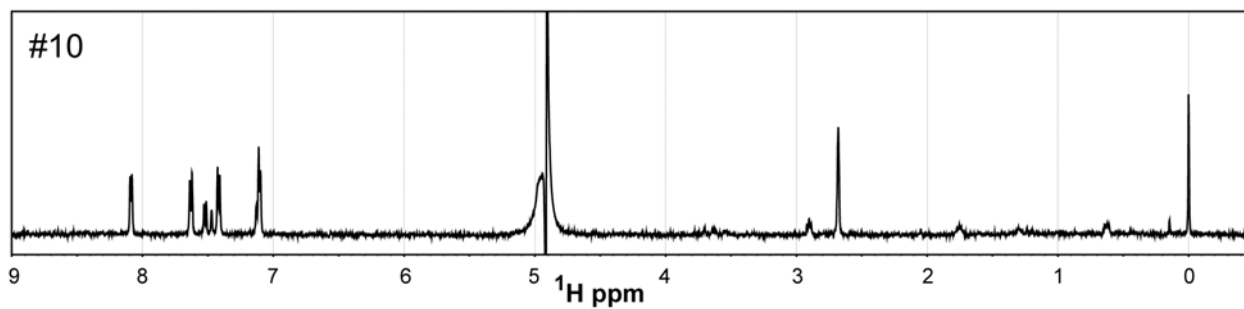
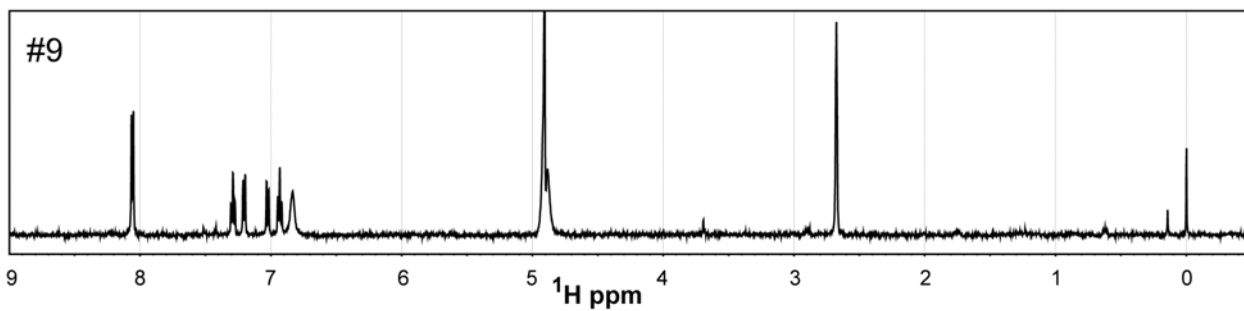
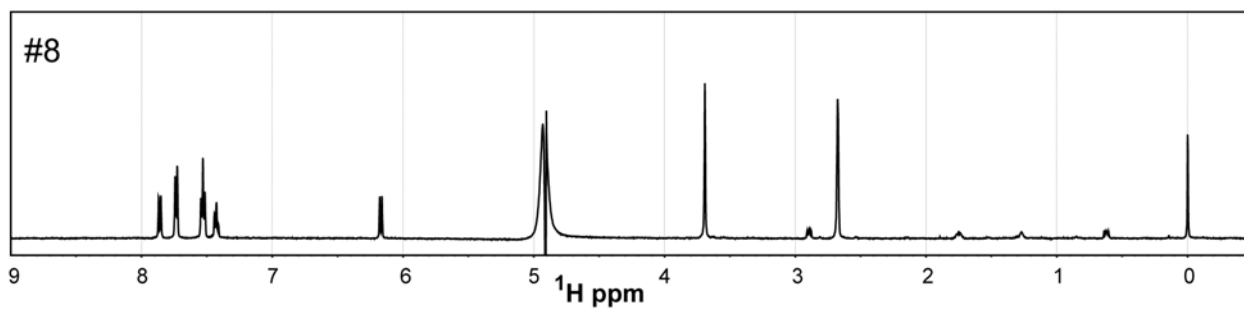
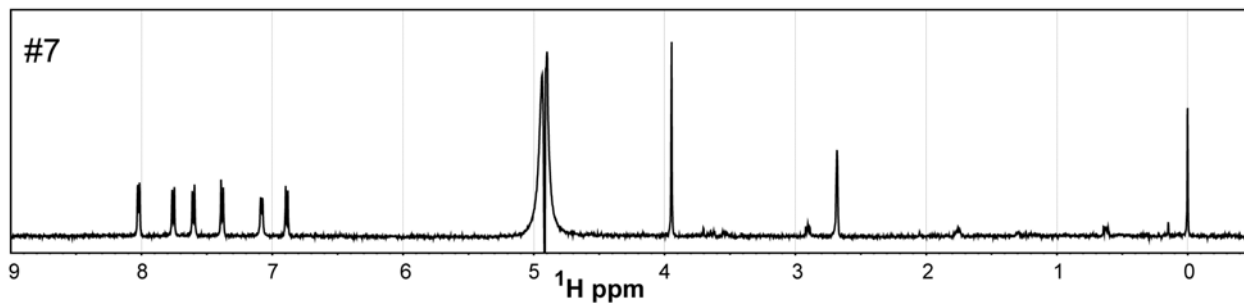
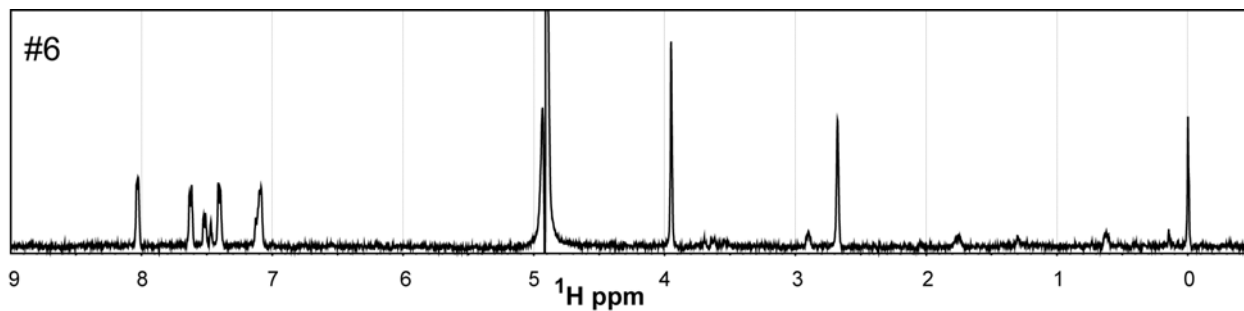
* Double charge – 2 quaternary nitrogens.

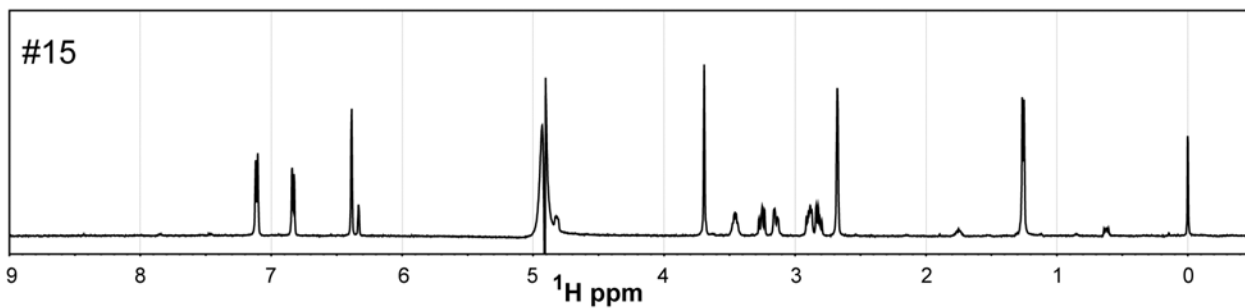
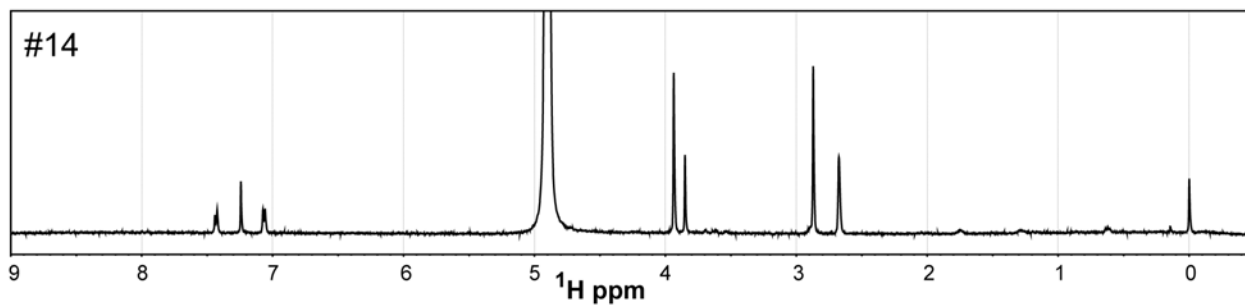
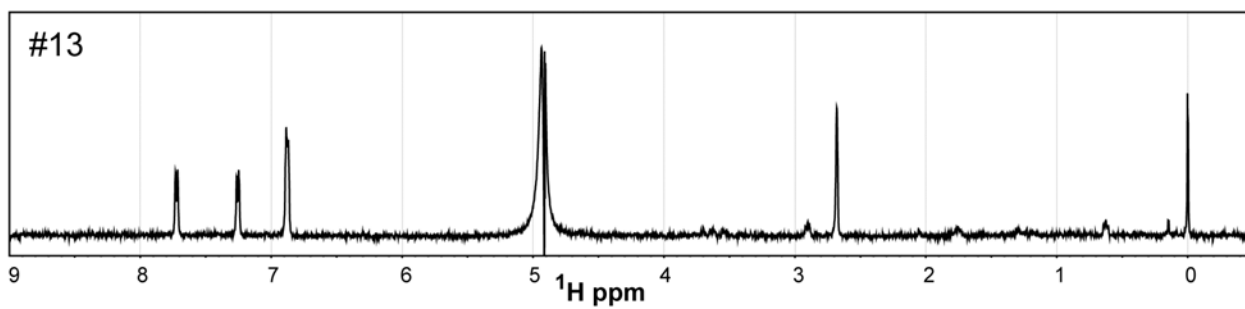
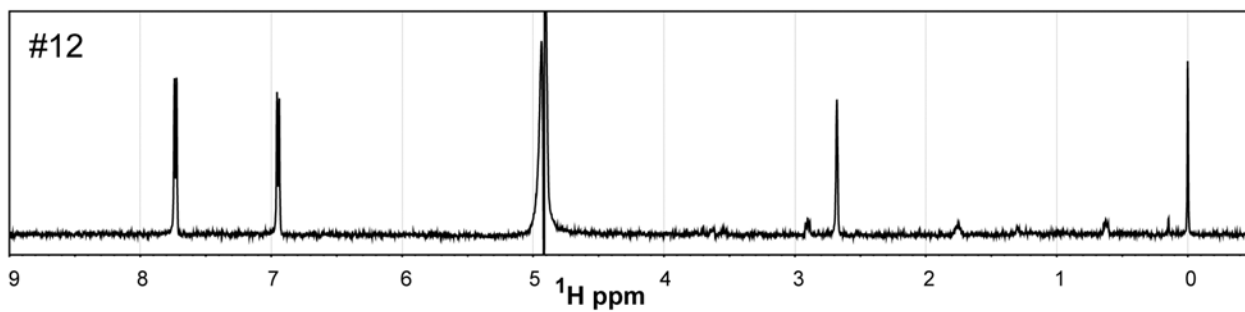
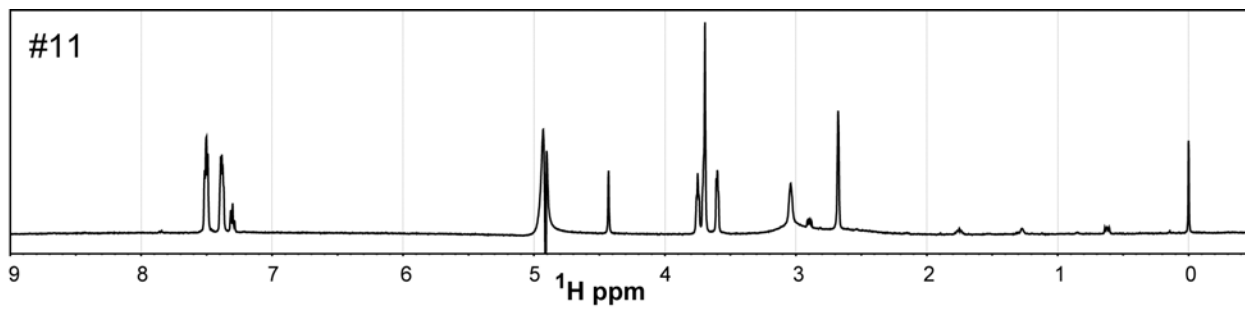
** MH⁺ with loss of water.

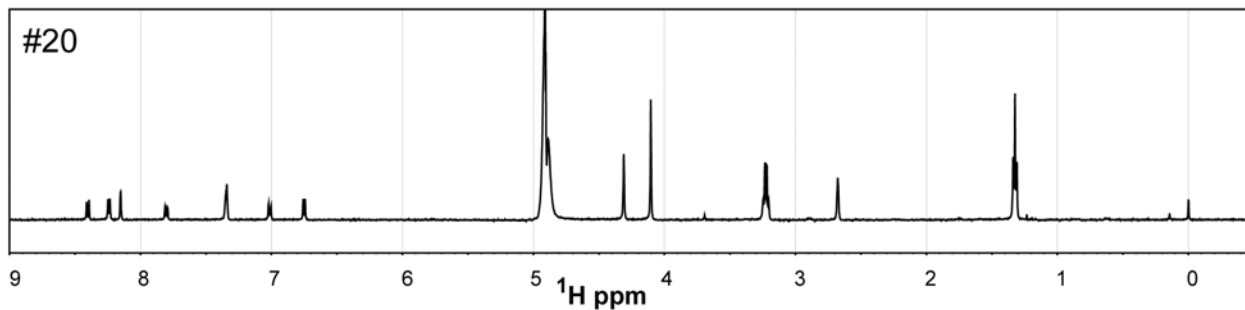
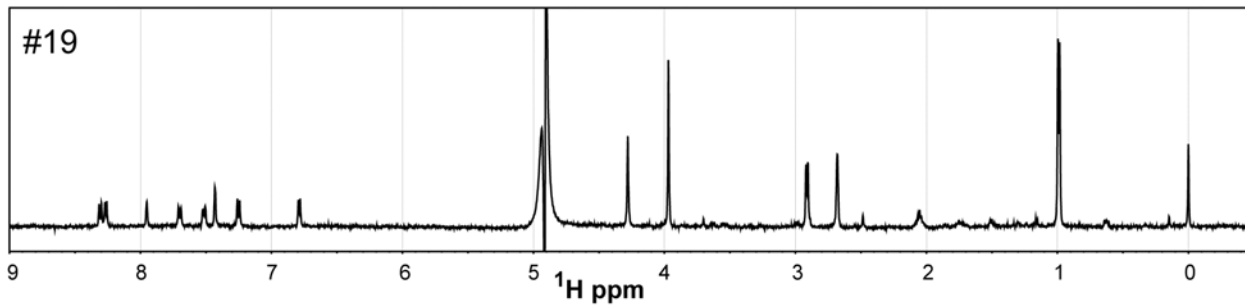
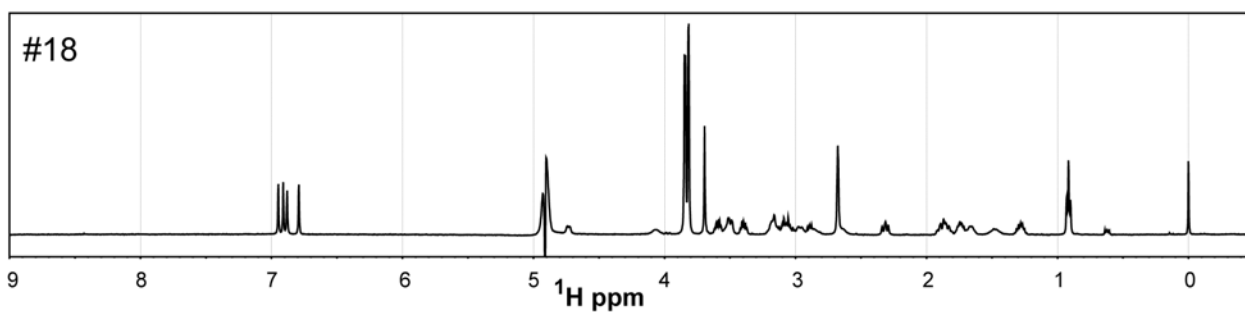
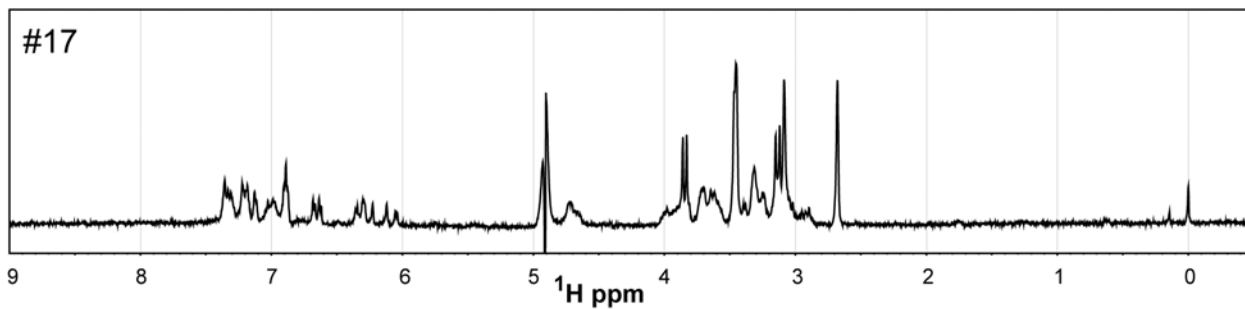
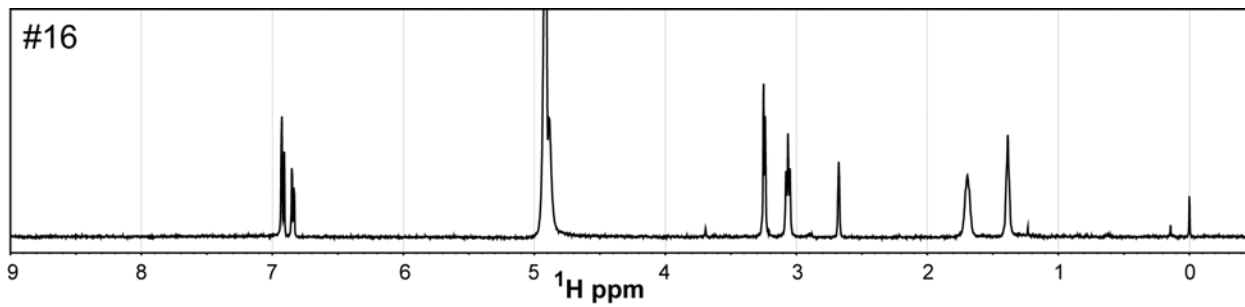
No validated assays were used. All compounds were greater than 95% purity as estimated by LC-MS and NMR

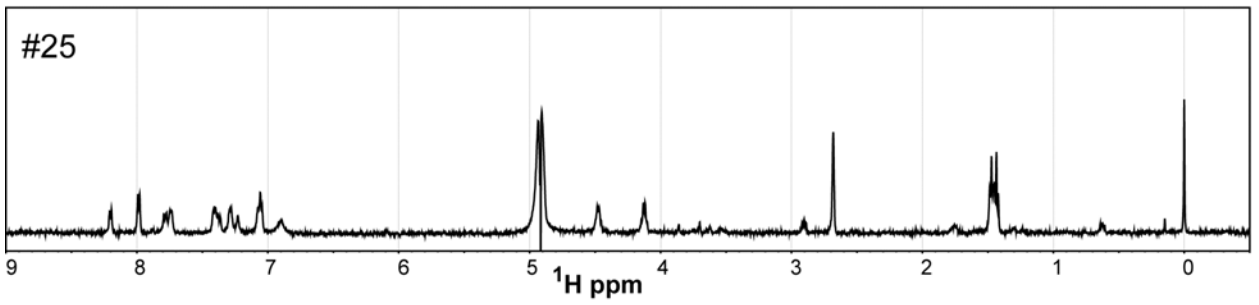
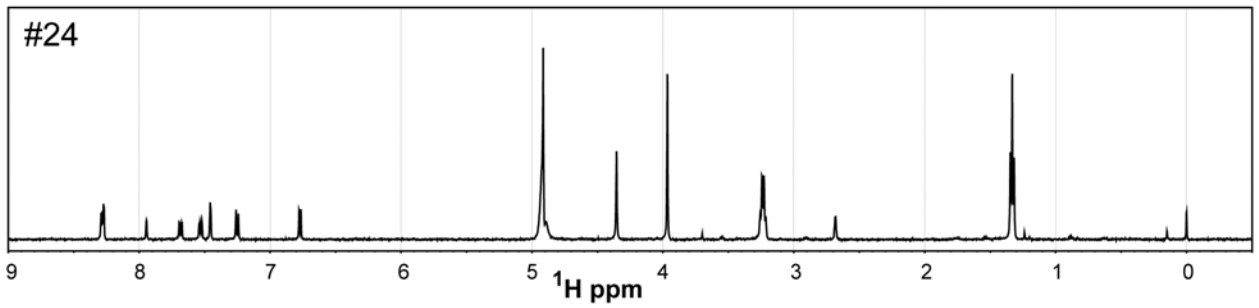
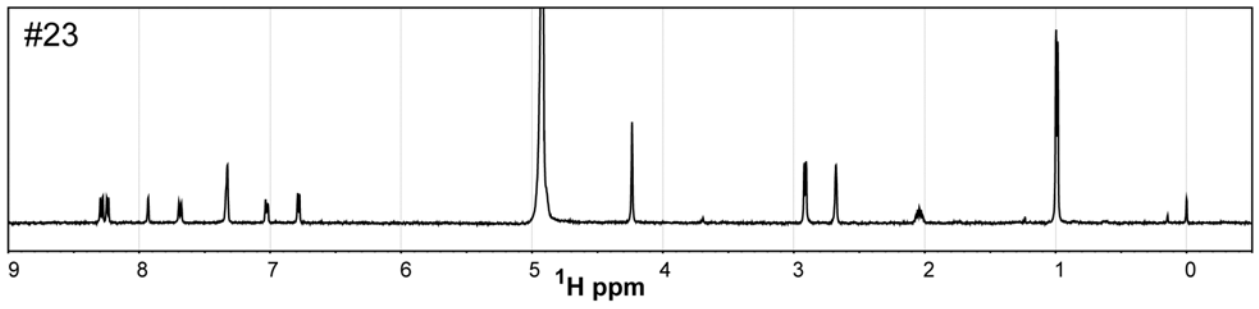
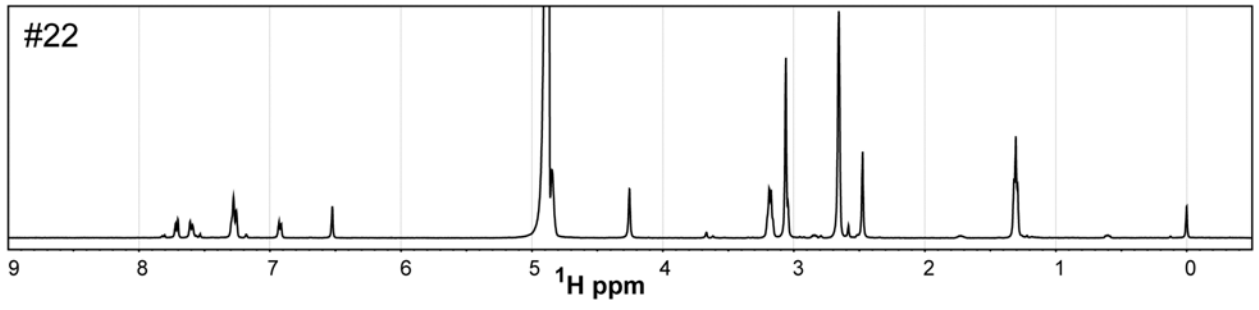
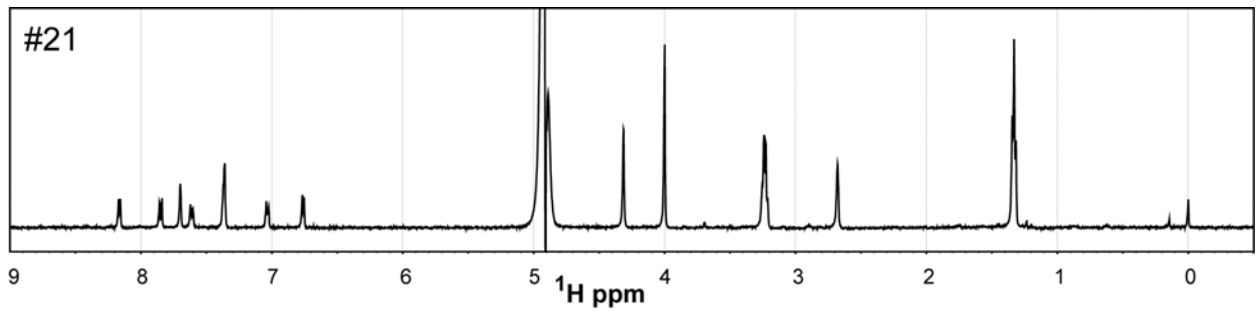
2) 1D NMR traces

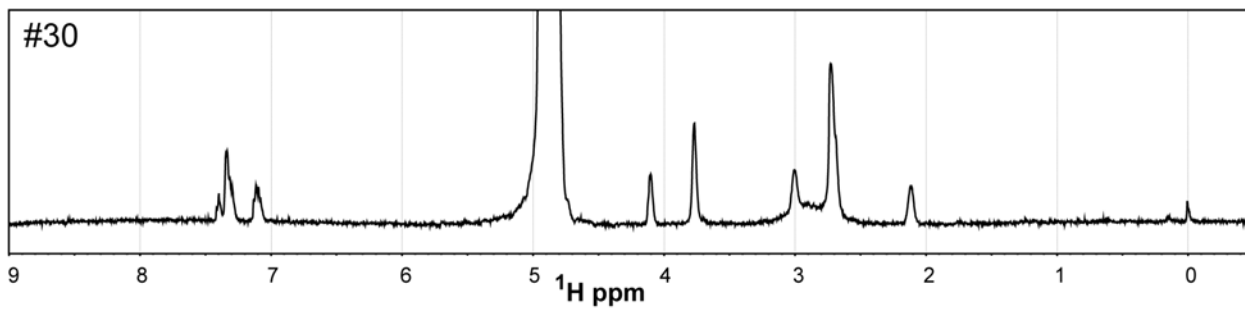
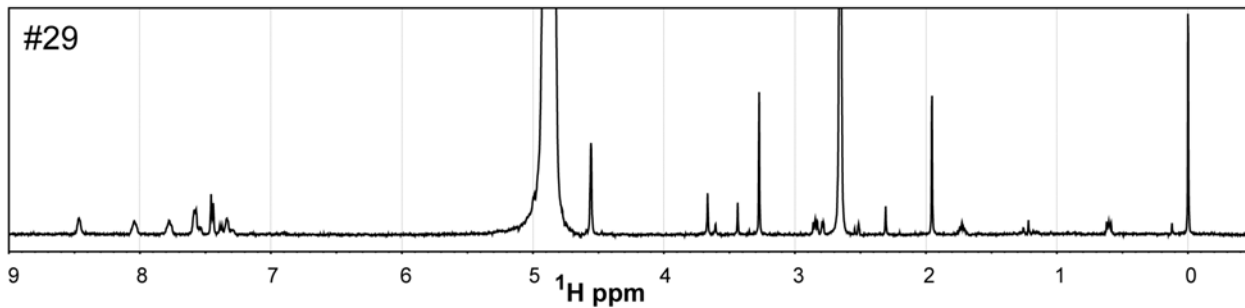
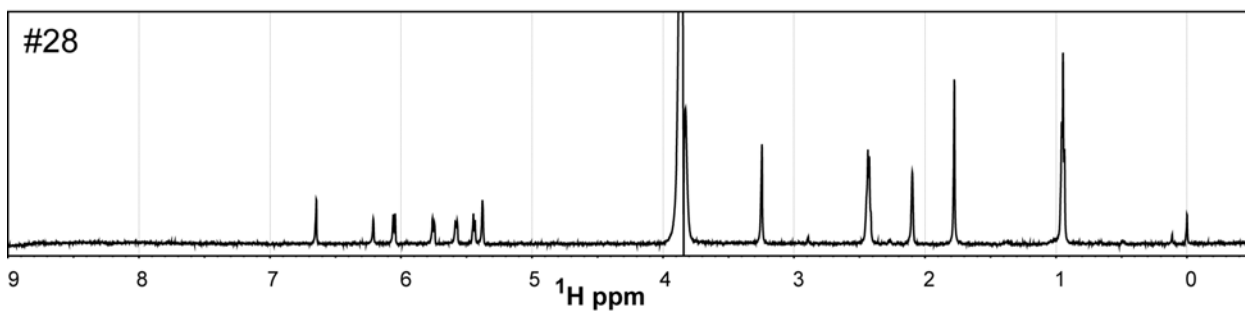
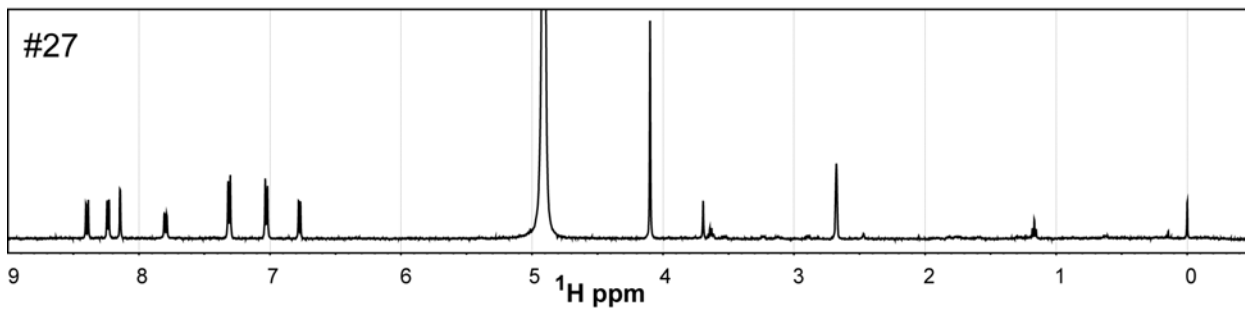
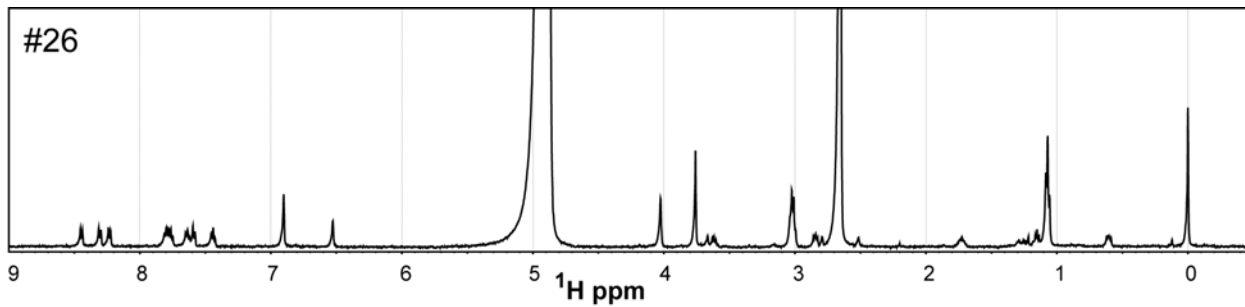


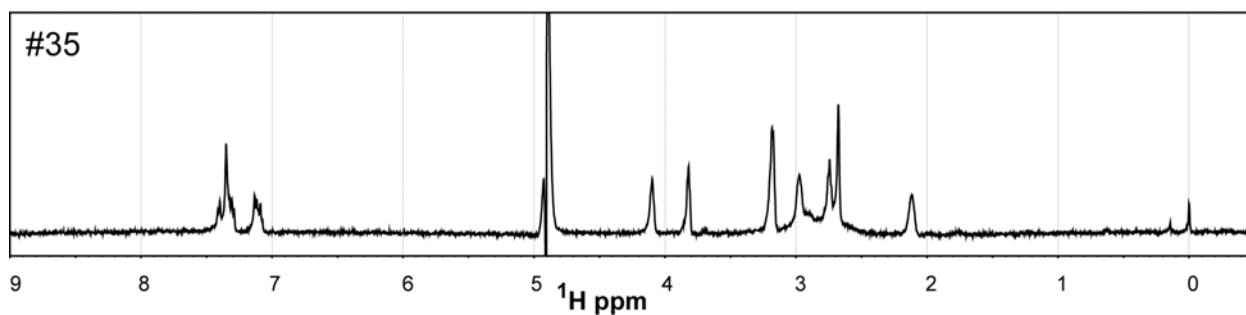
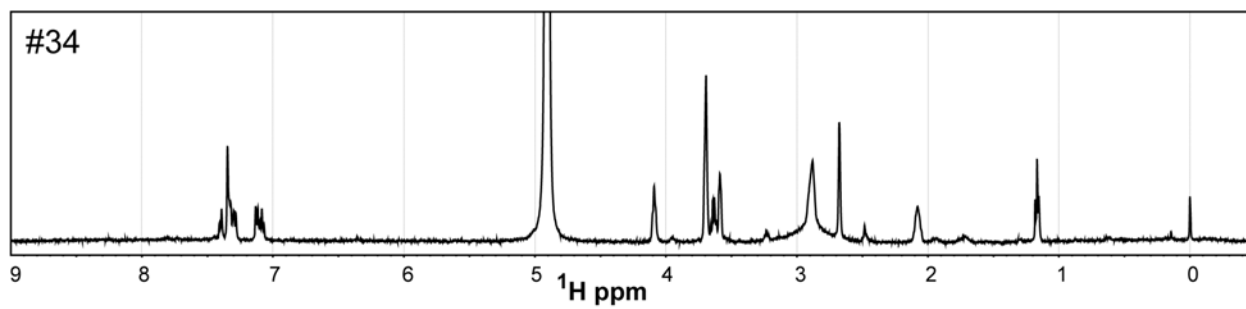
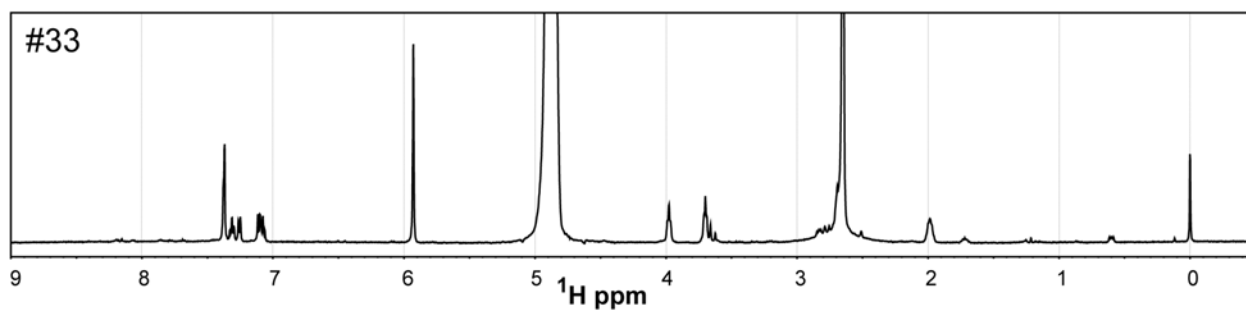
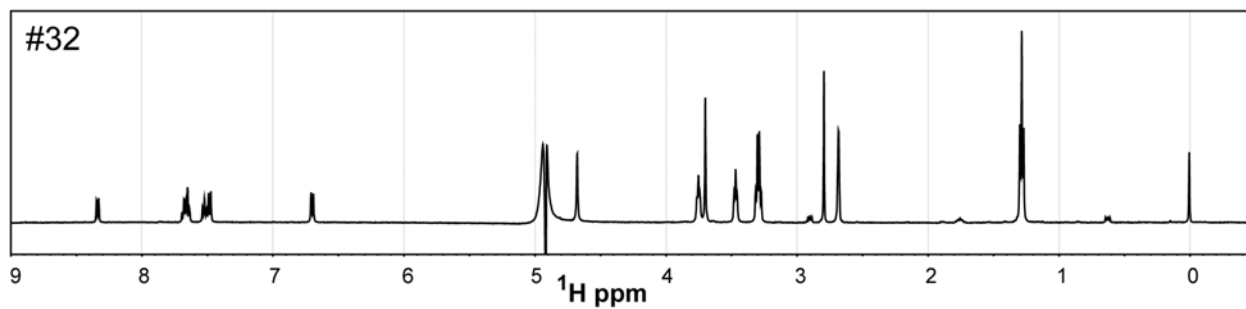
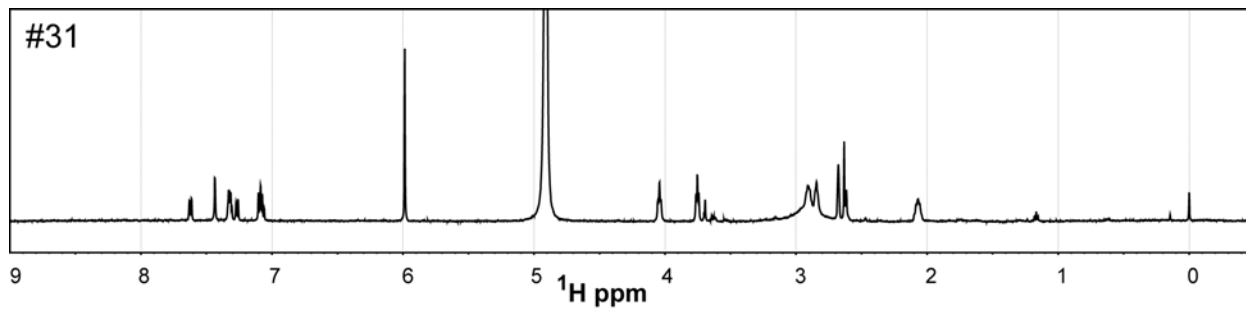


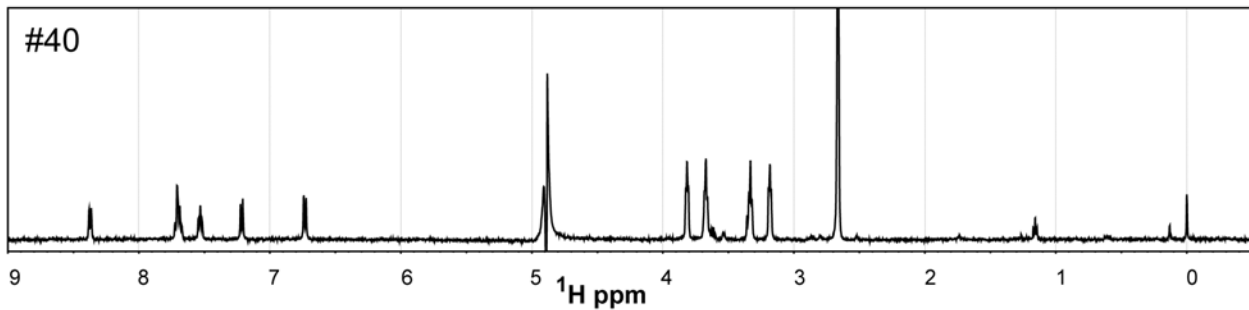
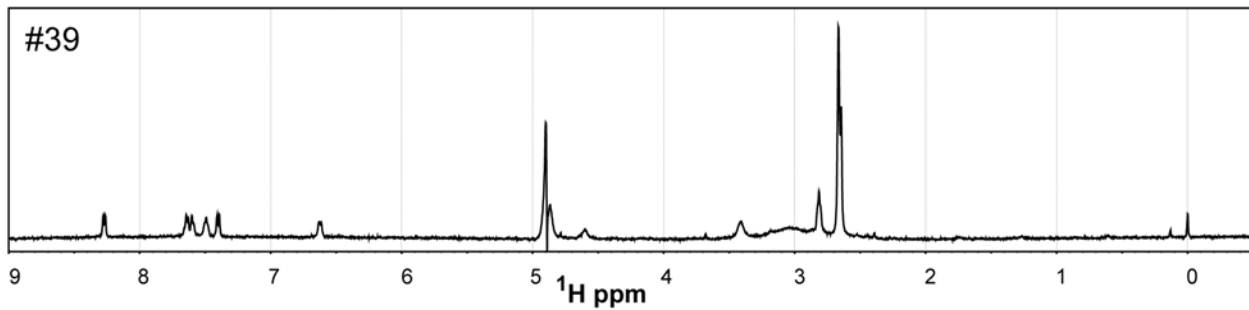
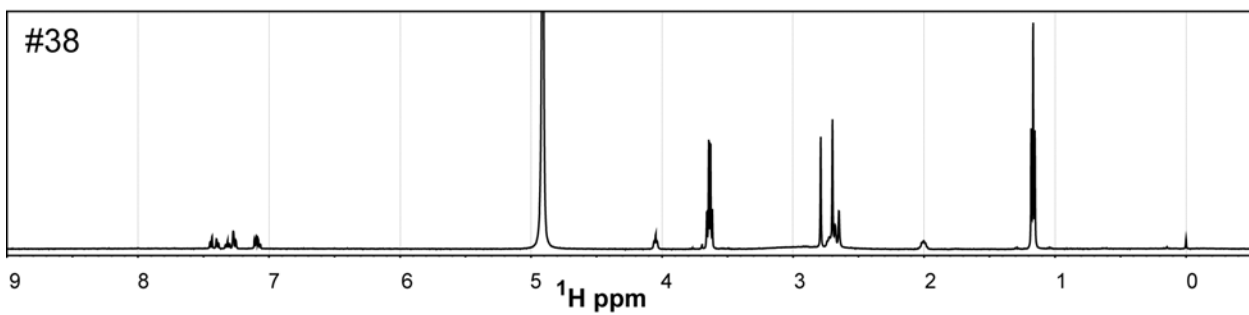
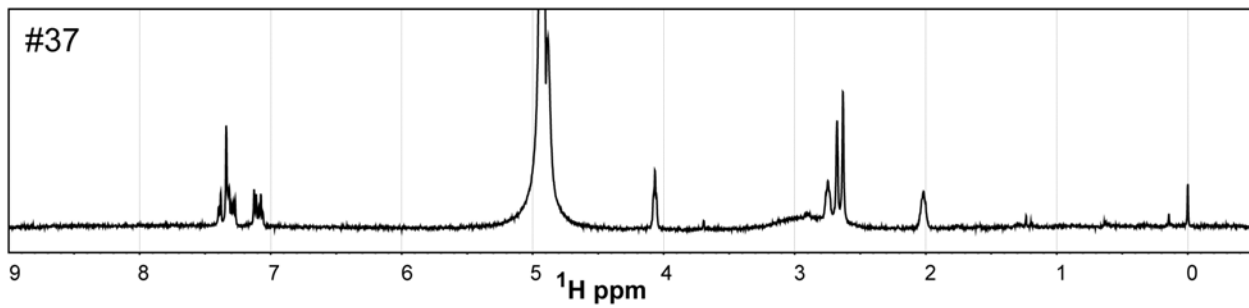
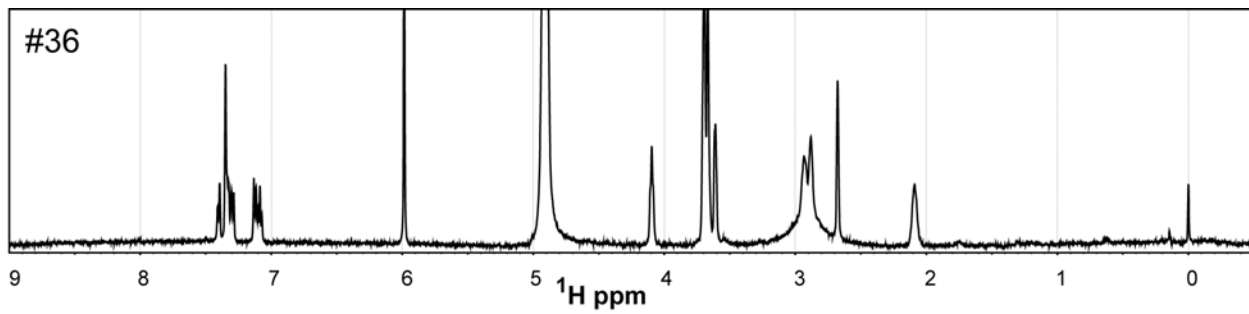


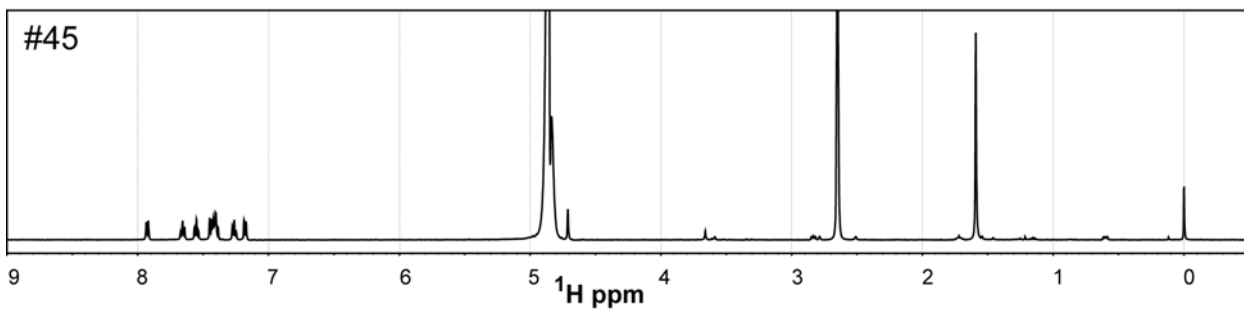
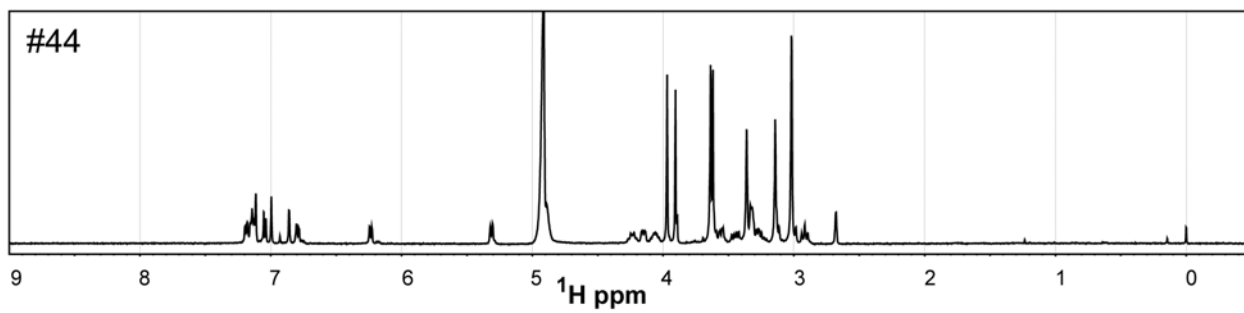
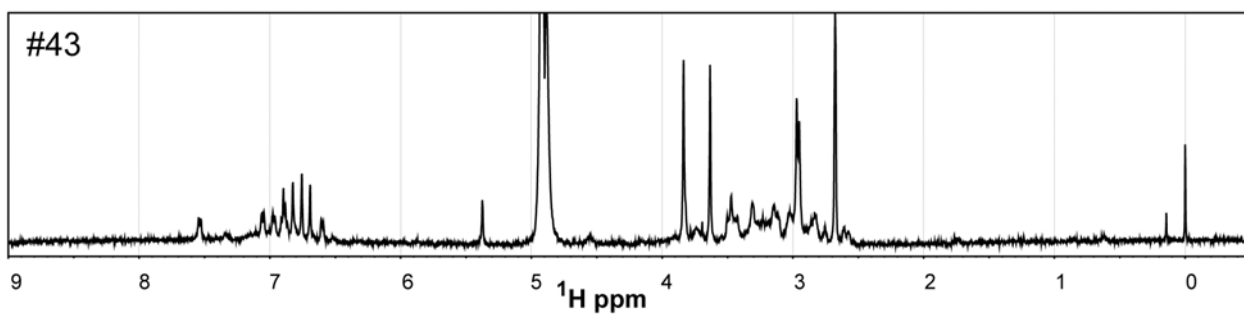
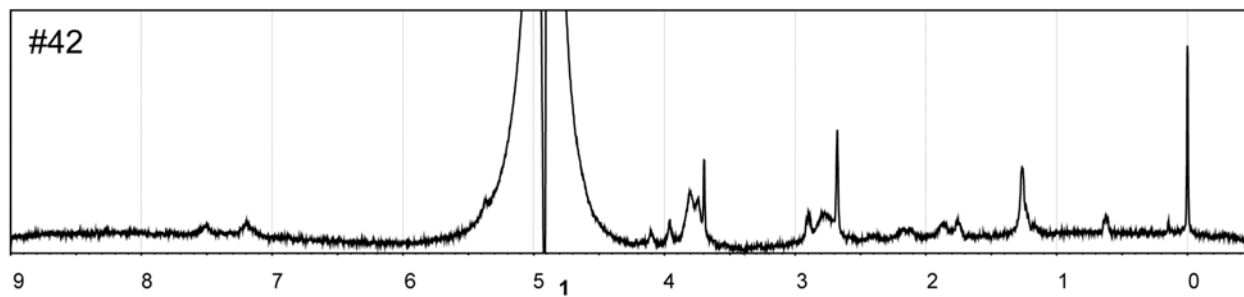
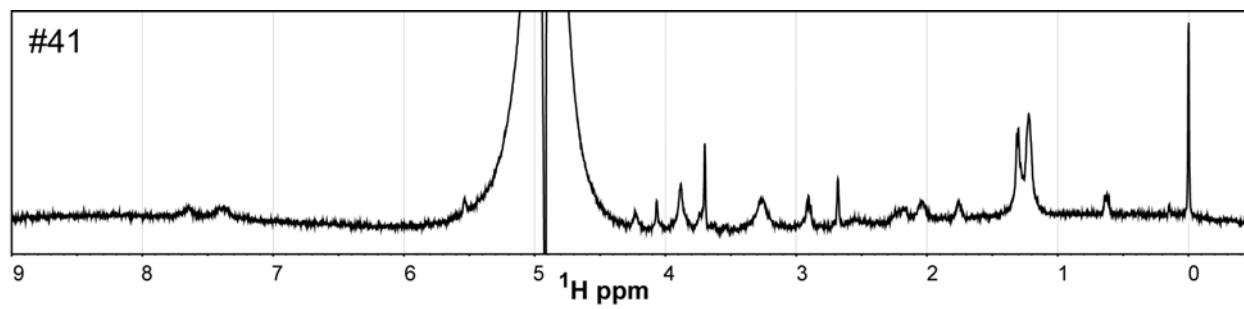


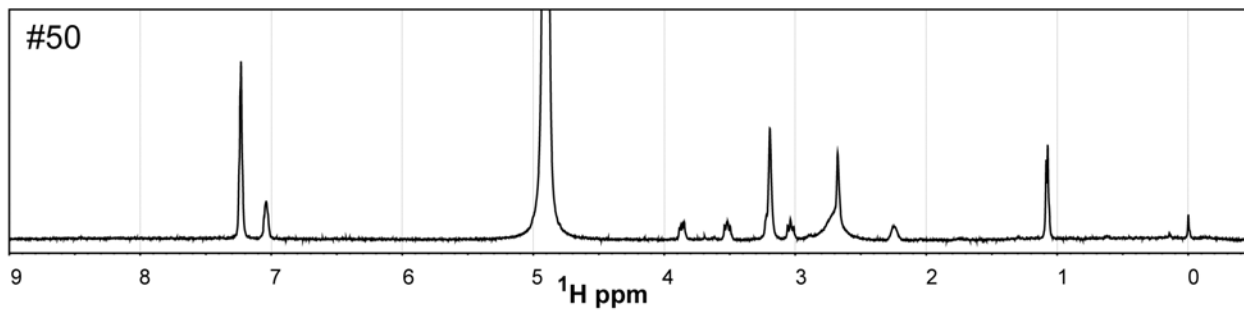
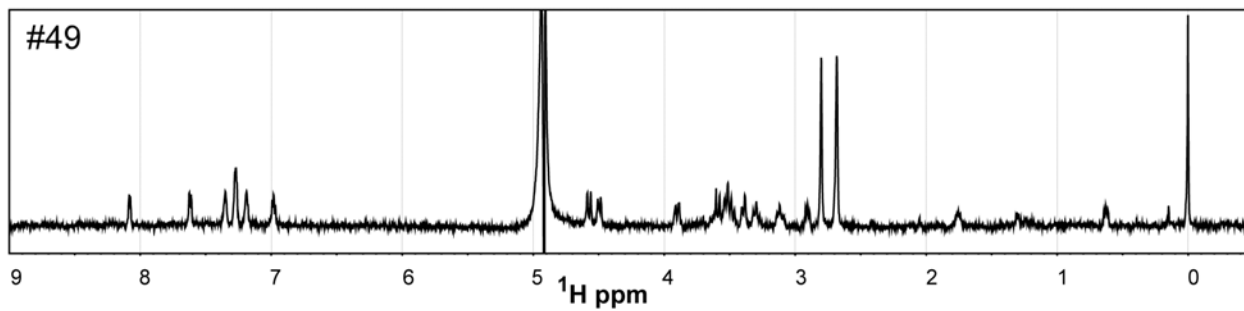
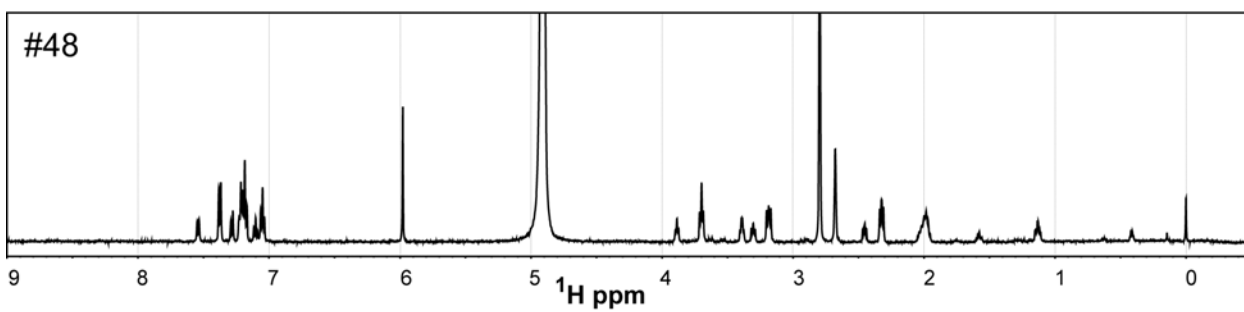
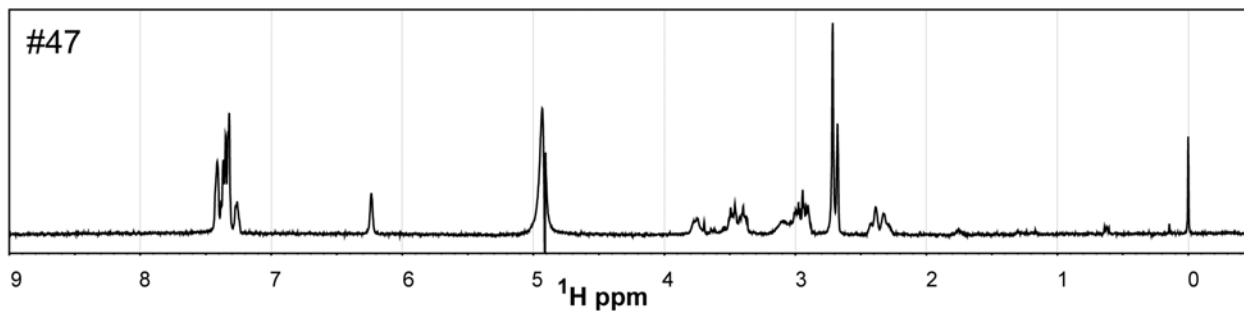
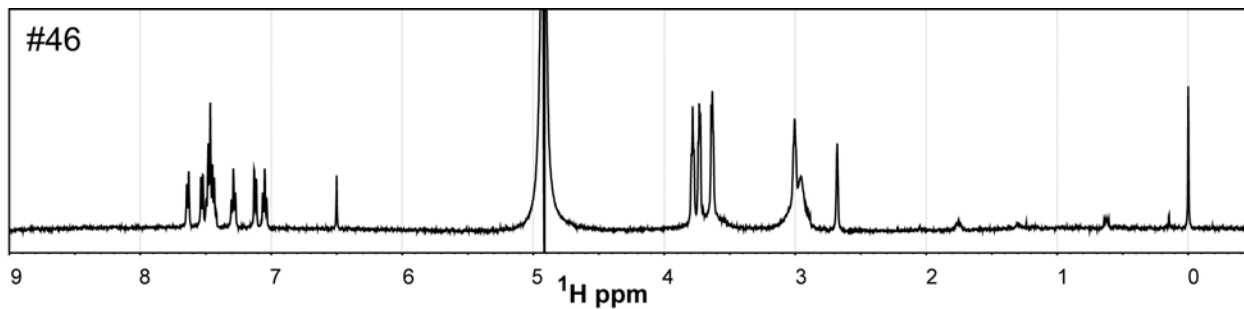


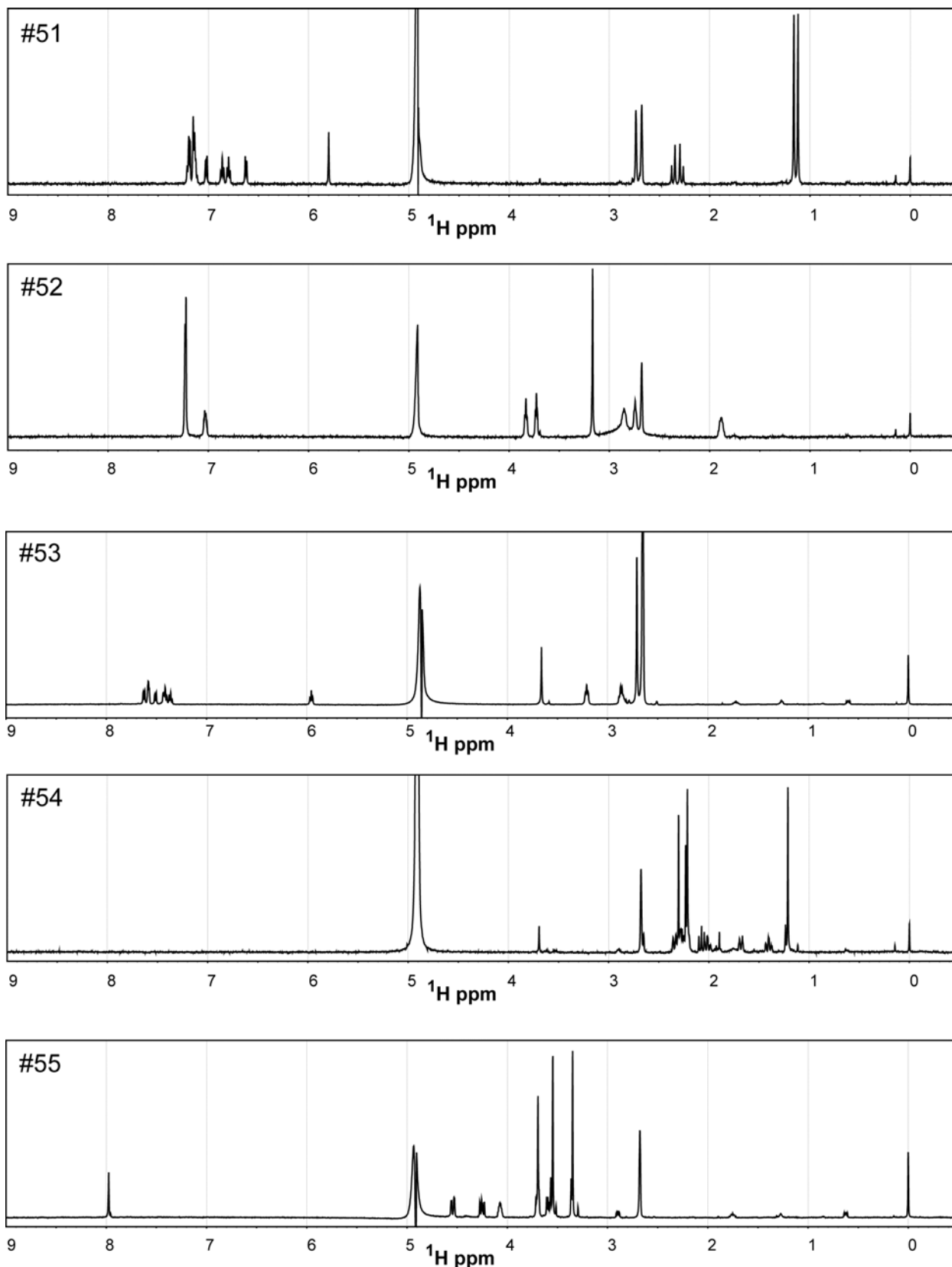












1D ^1H NMR spectra of the compounds were acquired on a 500 MHz Bruker DRX spectrometer equipped with a Cryoprobe as described in the main text. The number in each box corresponds to the compound number in Fig. 3. In addition to the compound, all samples contained TSP (resonating at 0 ppm) and DMSO- d_6 (2.68 ppm). Also, some samples contained maleate (6 ppm), methanesulfonate (2.63 ppm), or cyclohexane (1.4 ppm).

3) Mass Spectrometry

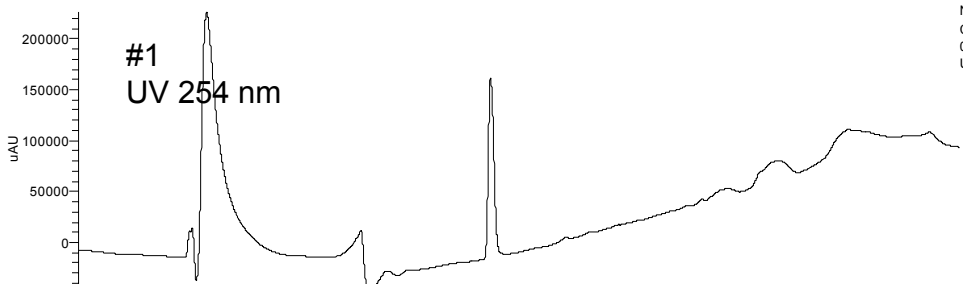
3.1) LC-MS/MS protocols

LC-MS/MS analyses were conducted using an Agilent 1100 HPLC (Agilent Technologies, Palo Alto, CA) equipped with a binary pump, a variable wavelength UV detector set to 254nm, a degasser, and column heater kept at 25C. Chromatographic resolution was achieved with a Phenomenex Luna, 5 μ , C18(2), 150 x 2.0nm, (Phenomenex, Torrance, CA). Mobile phases consisted of 0.1% aqueous formic acid (solvent-A) and acetonitrile with 0.08% formic acid (solvent-B) run at a constant flow rate of 1mL/min. The solvent gradient was initially set at 0% solvent-B and increased linearly to 100% solvent-B over 10min, kept at 100% solvent-B for an additional 3 min, then immediately dropped to 0% solvent-B over 0.1 min where it was held constant at 0% solvent-B for 4 min before the next sample injection (10 μ L). A Thermo Fisher TSQ Quantum Discovery Max mass spectrometer (Thermo Fisher Scientific, Waltham, MA), linked to a CTC HTS PAL Autosampler (Leap Technologies, Carrboro, NC) was used in the present studies. Electrospray ionization was employed with the needle potential held at 4.5 kV. MS/MS conditions used were 2mTorr argon collision gas and 30 eV collision potential. Positive ion mode full scan (100 to 800 Da), was conducted with scan time 0.73 seconds and source collision energy of 10 V. Xcalibur software (version 2.0, San Jose, CA) was used to acquire all data. Compounds of interest were dissolved with a mixture of acetonitrile and distilled water (1/1, v/v) to provide a concentration of 25 μ M for LC-MS and LC-MS/MS analysis. Sample size was 10 μ L. The data for each compound show the UV chromatogram, the extracted ion chromatogram (XIC) for the m/z range 100 to 800, and the XIC for the protonated molecular ion of the compound on one page. Then on the next page is the tandem mass spectrum of the compound.

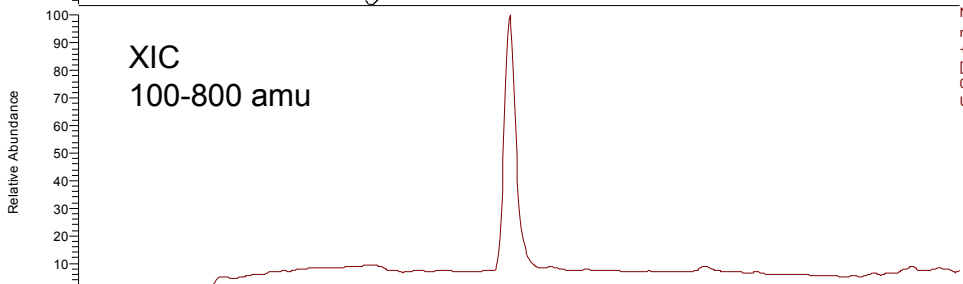
Notes: The last two slides for blank acetonitrile/water LC-MS analysis. This is the same solution that was used to make the 25 μ M test solutions for each compound. The two blanks are from analysis done with one old and one new HPLC column (same make and model). Four structures (#3, 16, 25 & 36) needed to be re-analyzed. The conditions for these four compounds were as follows: analytical LC-MS ESI (Alliance HT Waters 2795 HPLC, Waters ZQ mass analyser) with a UV 254 photodiode array detector (Waters 9996 photodiode array detector), was carried out using Xterra MS C18 stationary phase (column: 5 μ m; 4.6 x 50 mm) at 1 ml/min. Solvent gradient was used: water:acetonitrile(0.05% trifluoroacetic acid) 95:5 to 0:100 over 4.5 min.

3.2) LC-MS/MS Data

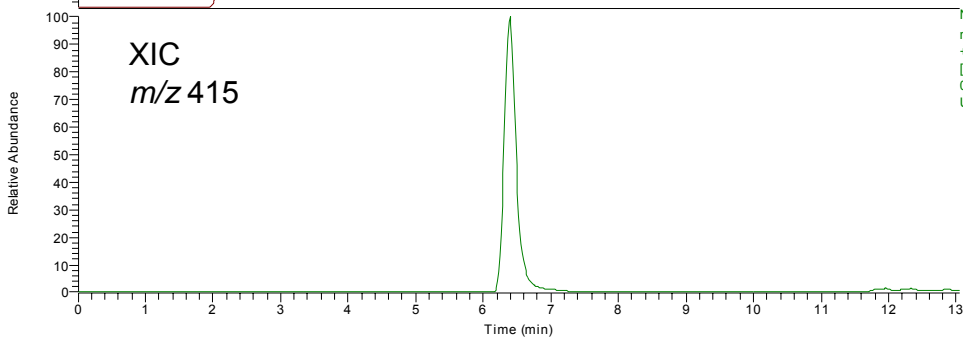
RT: 0.00 - 13.04 SM: 15G



NL: 2.26E5
Channel A UV
08_22_2008_UCSF_P
URITY_A01

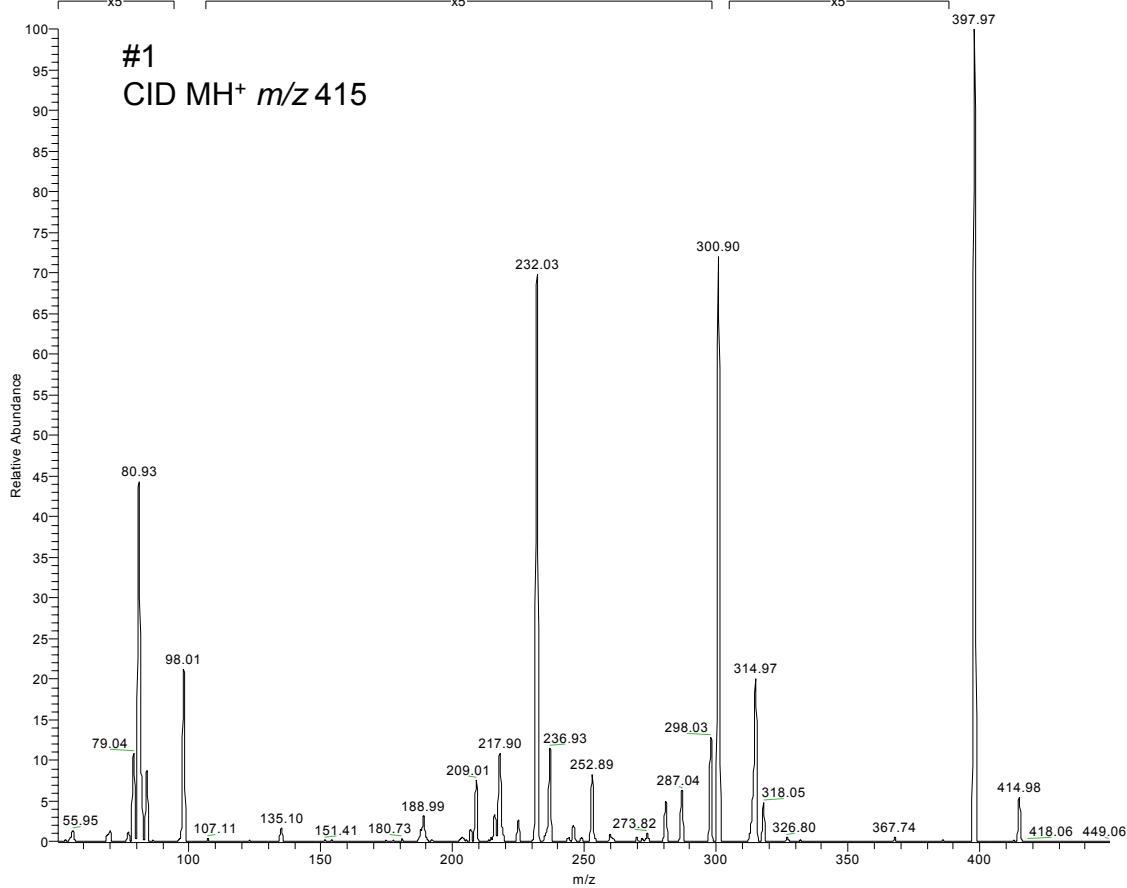


NL: 5.16E8
m/z= 100.00-800.00 F:
+ p sid=-10.00 Q1MS
[50.00-1200.00] MS
08_22_2008_UCSF_P
URITY_A01

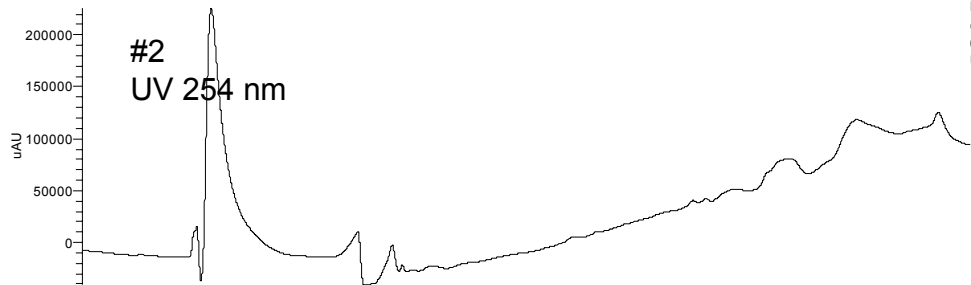


NL: 3.72E8
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+ p sid=-10.00 Q1MS
[50.00-1200.00] MS
08_22_2008_UCSF_P
URITY_A01

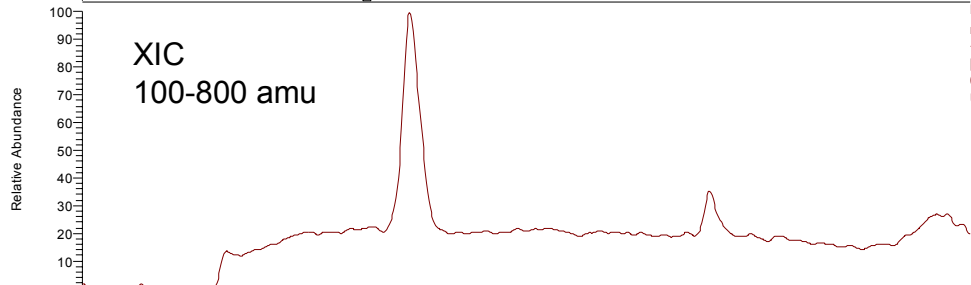
08_22_2008_UCSF_PURITY_A01_080824185156 #424-447 RT: 6.28-6.62 AV: 24 SB: 2 0.01, 0.01 SM: 15G NL: 1.71E7
F: + p sid=-10.00 Full ms2 415.10@-30.00 [50.00-700.00]



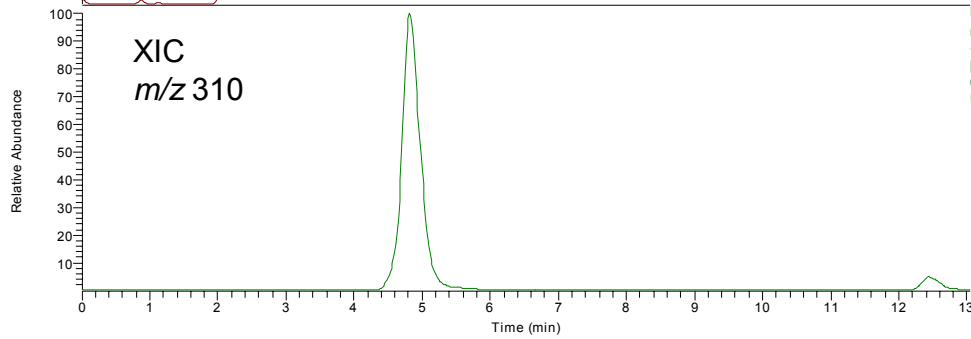
RT: 0.00 - 13.04 SM: 15G



NL: 2.25E5
Channel A UV
08_22_2008_UCSF_P
URITY_A02

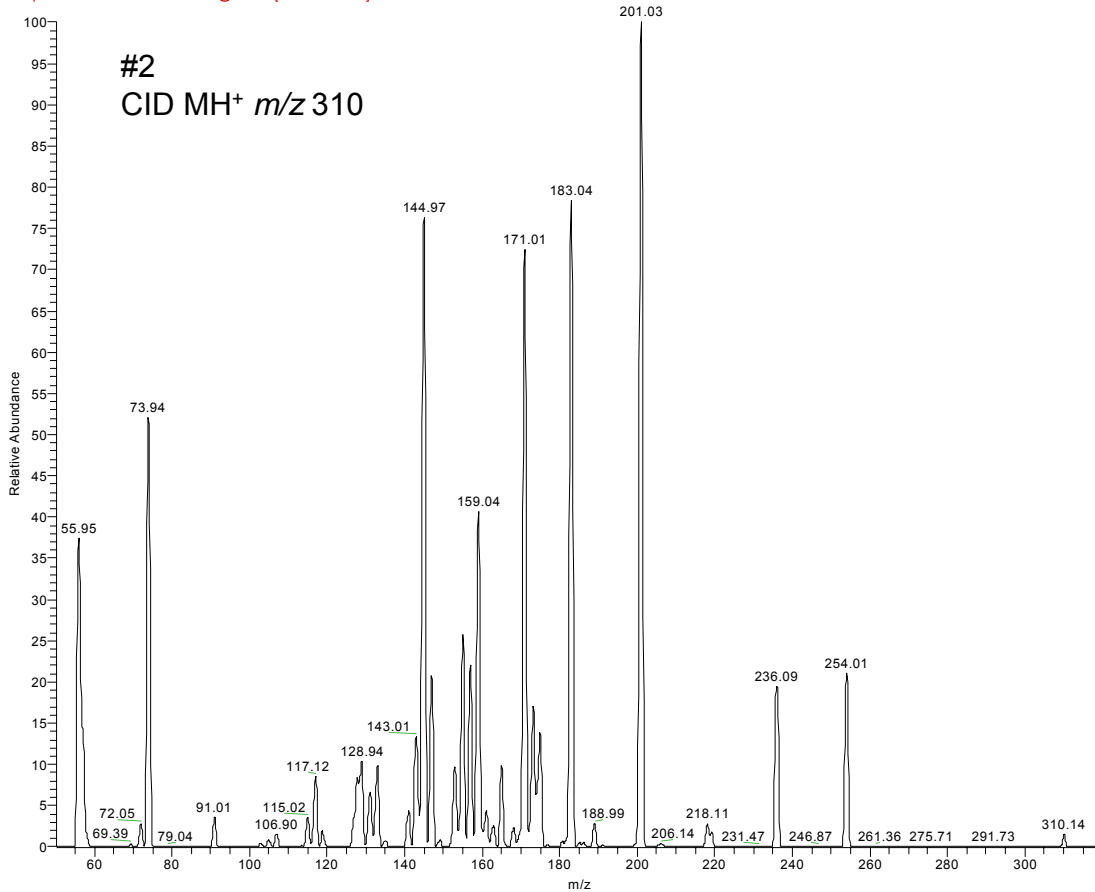


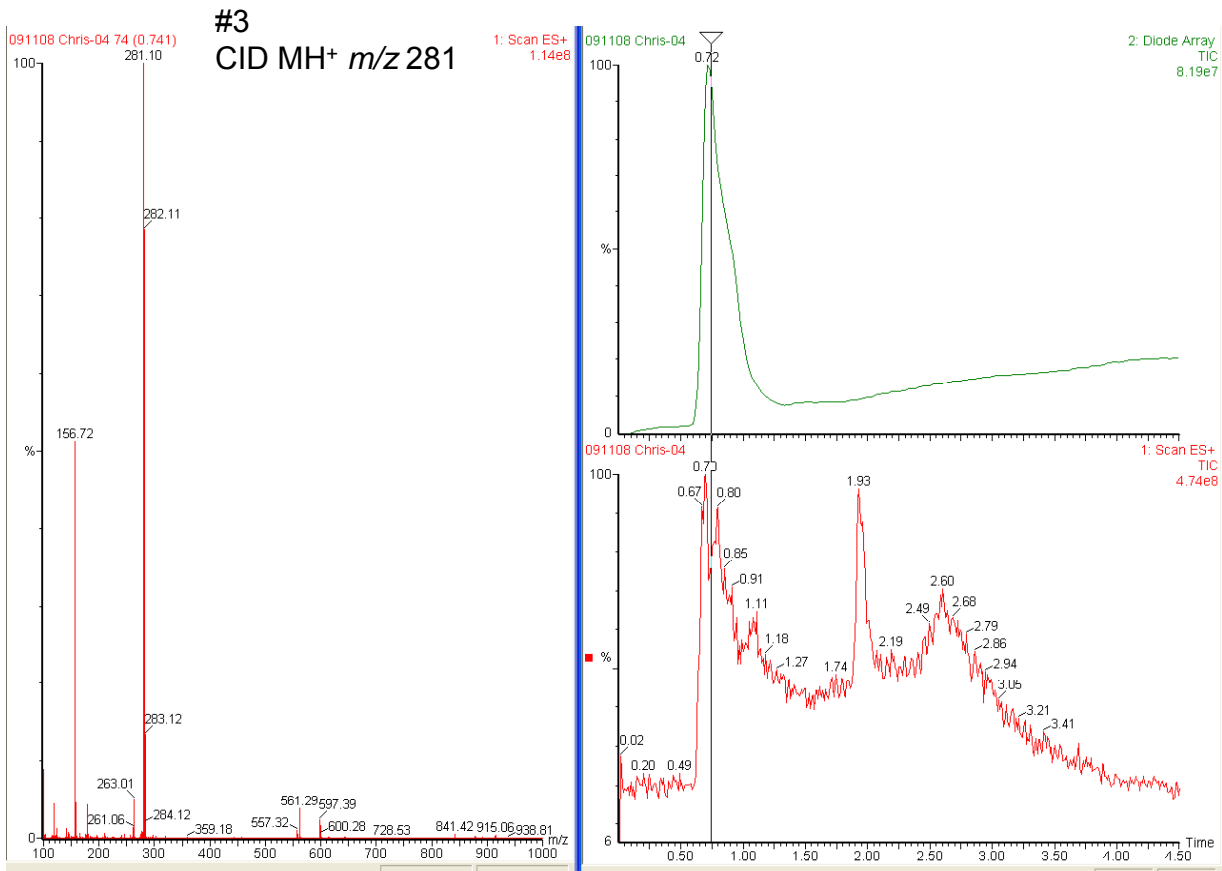
NL: 1.86E8
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[50.00-1200.00] MS
08_22_2008_UCSF_P
URITY_A02



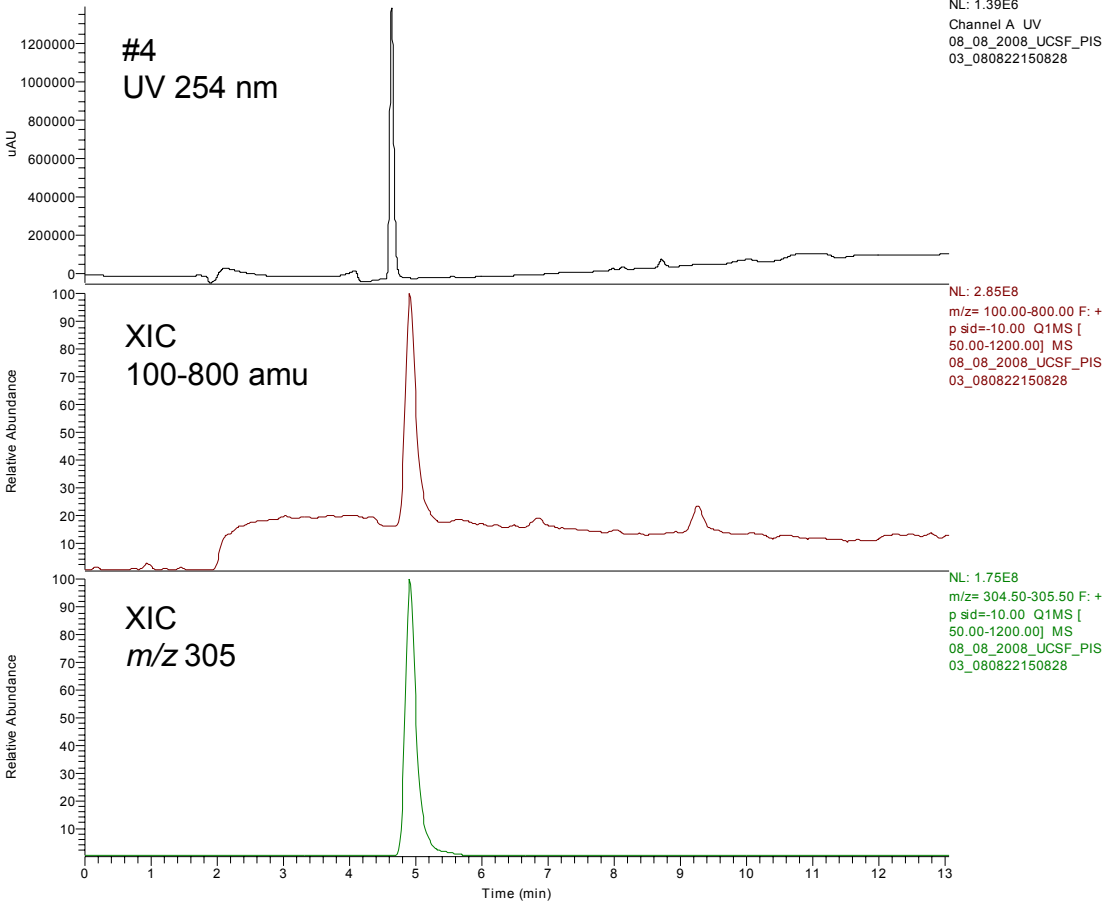
NL: 1.11E8
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+ p sid=-10.00 Q1MS
[50.00-1200.00] MS
08_22_2008_UCSF_P
URITY_A02

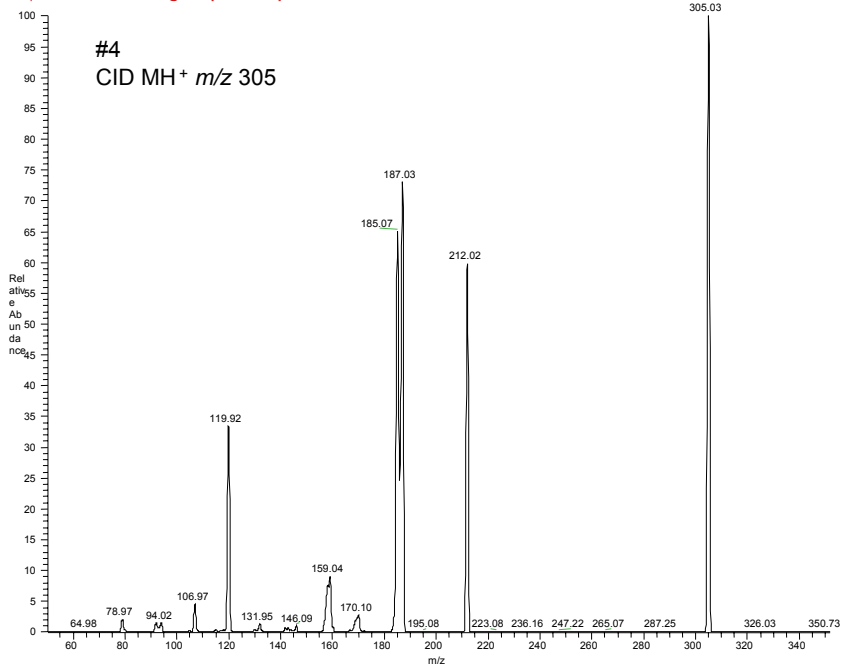
08_22_2008_UCSF_PURITY_A02_080824190943 #317-344 RT: 4.69-5.09 AV: 28 SB: 2 17.00, 17.00 SM: 15G NL: 1.44E6
F: + p sid=-10.00 Full ms2 310.10@-30.00 [50.00-700.00]



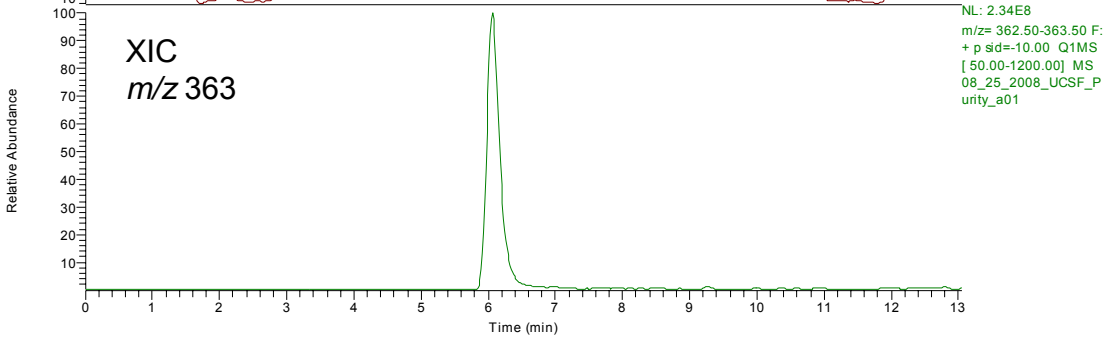
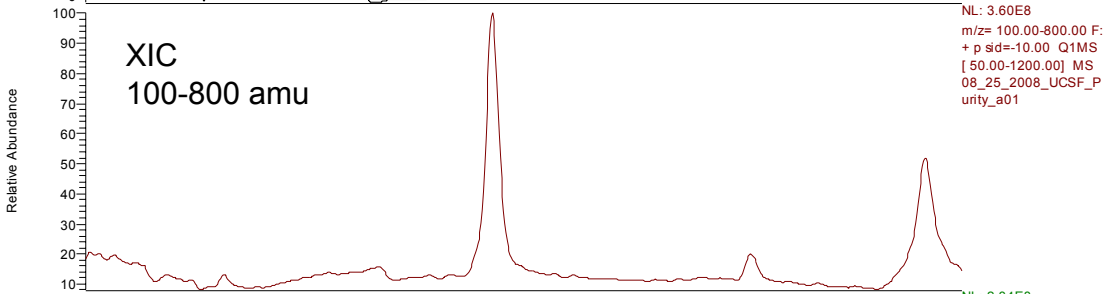
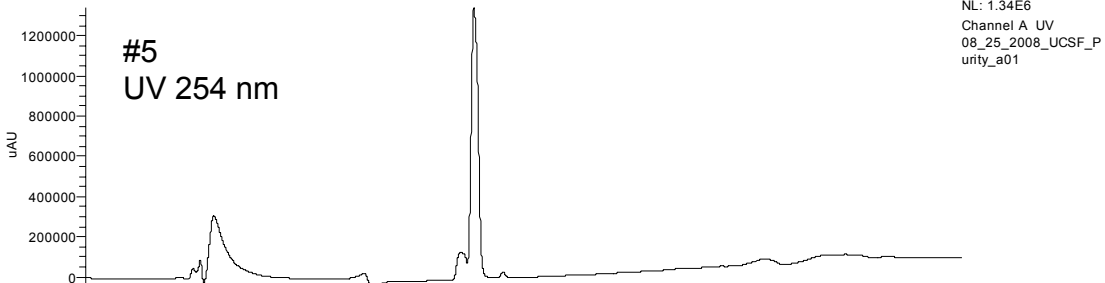


RT: 0.00 - 13.04 SM: 15G

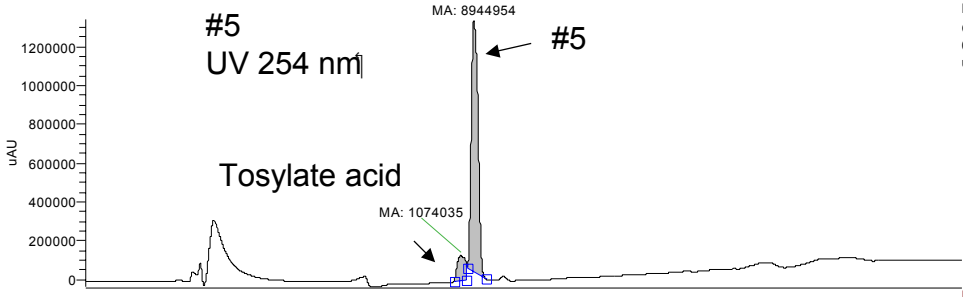




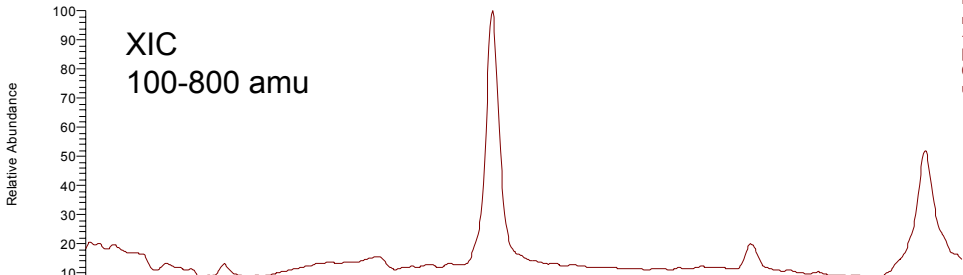
RT: 0.00 - 13.04 SM: 15G



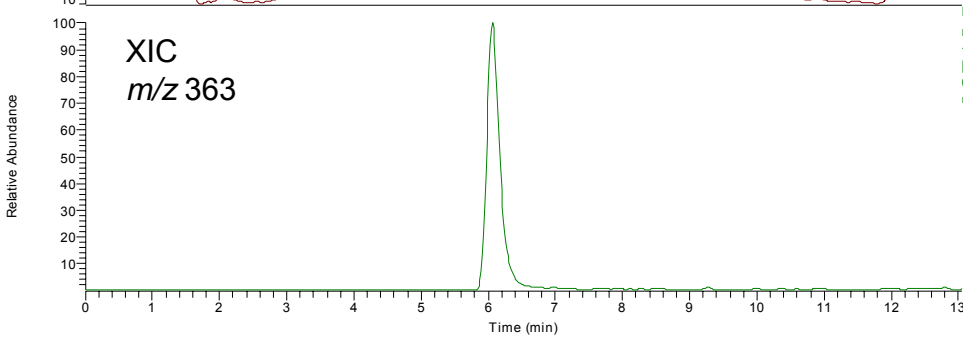
RT: 0.00 - 13.04 SM: 15G



NL: 1.34E6
Channel A UV
08_25_2008_UCSF_P
unity_a01

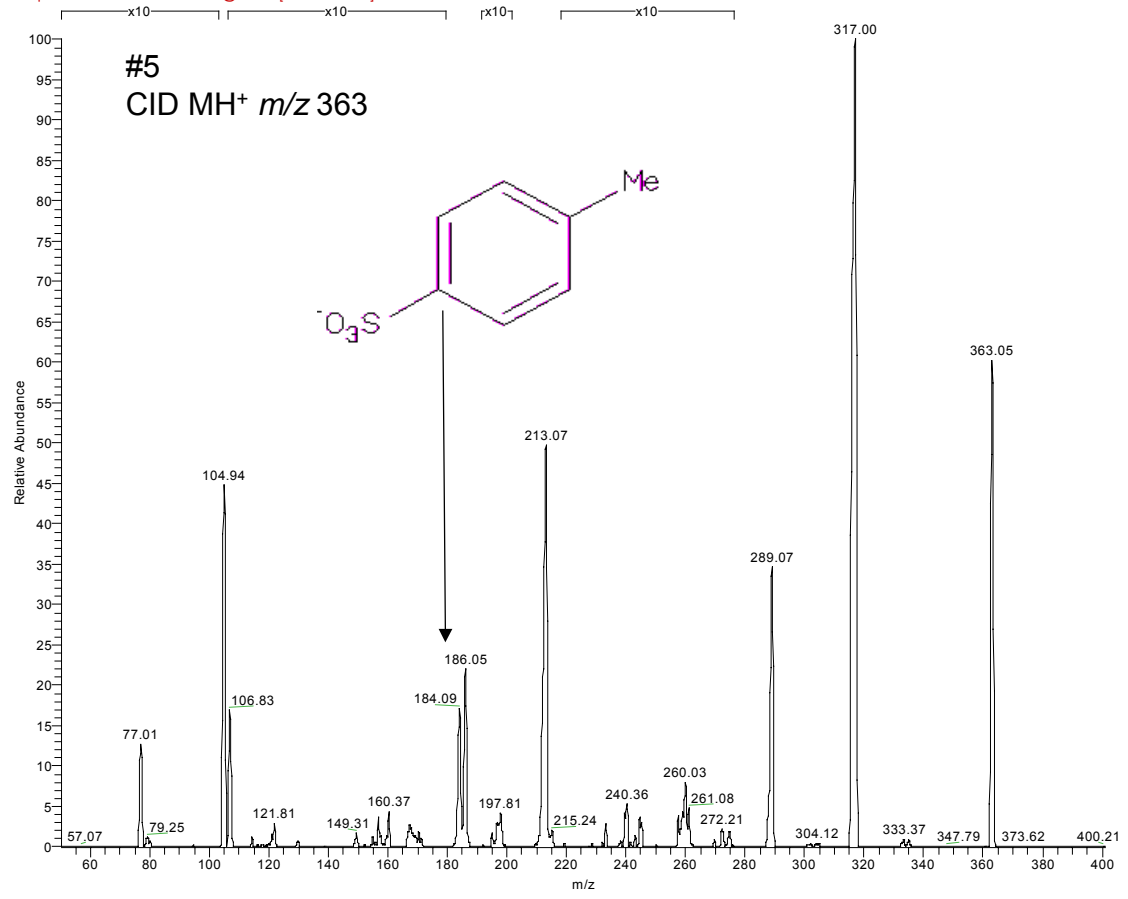


NL: 3.60E8
m/z= 100.00-800.00 F:
+ p sid=-10.00 Q1MS
[50.00-1200.00] MS
08_25_2008_UCSF_P
unity_a01

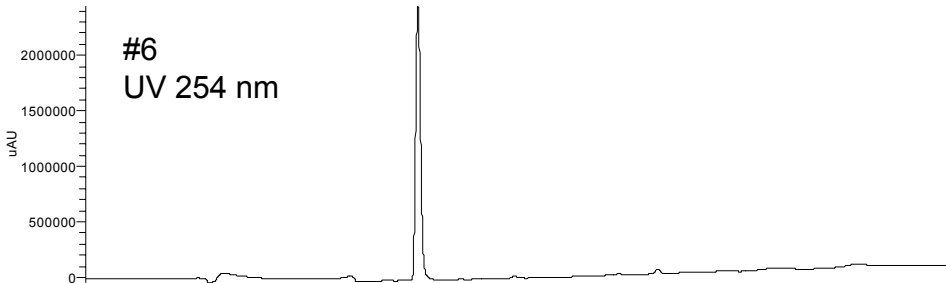


NL: 2.34E8
m/z= 362.50-363.50 F:
+ p sid=-10.00 Q1MS
[50.00-1200.00] MS
08_25_2008_UCSF_P
unity_a01

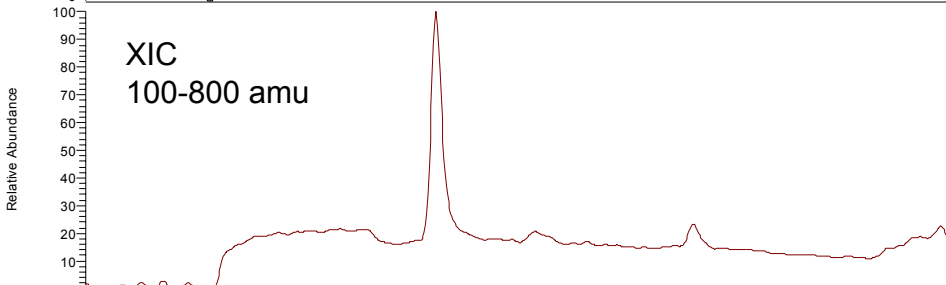
08_22_2008_UCSF_PURITY_A05_080824194517 #412-432 RT: 6.10-6.40 AV: 21 SB: 2 17.00 , 17.00 SM: 15G NL: 3.77E6
F: + p sid=-10.00 Full ms2 363.10@-30.00 [50.00-700.00]



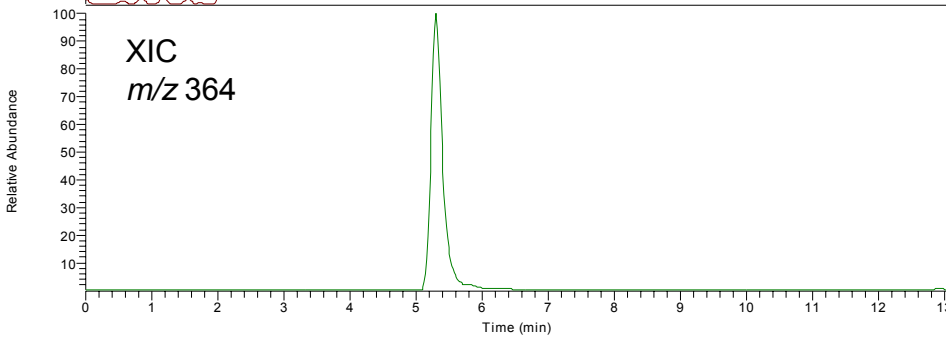
RT: 0.00 - 13.04 SM: 15G



NL: 2.44E6
Channel A UV
08_08_2008_UCSF_PIS
05_080822154359



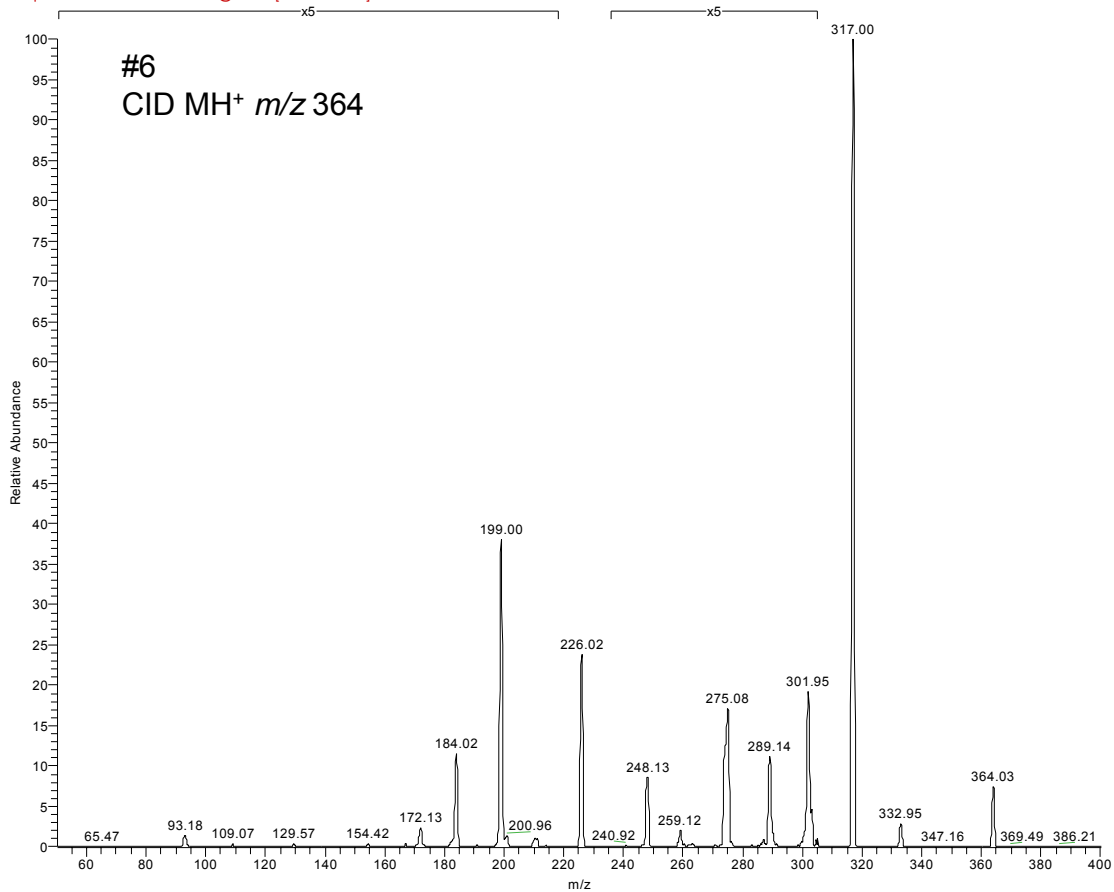
NL: 2.52E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
05_080822154359



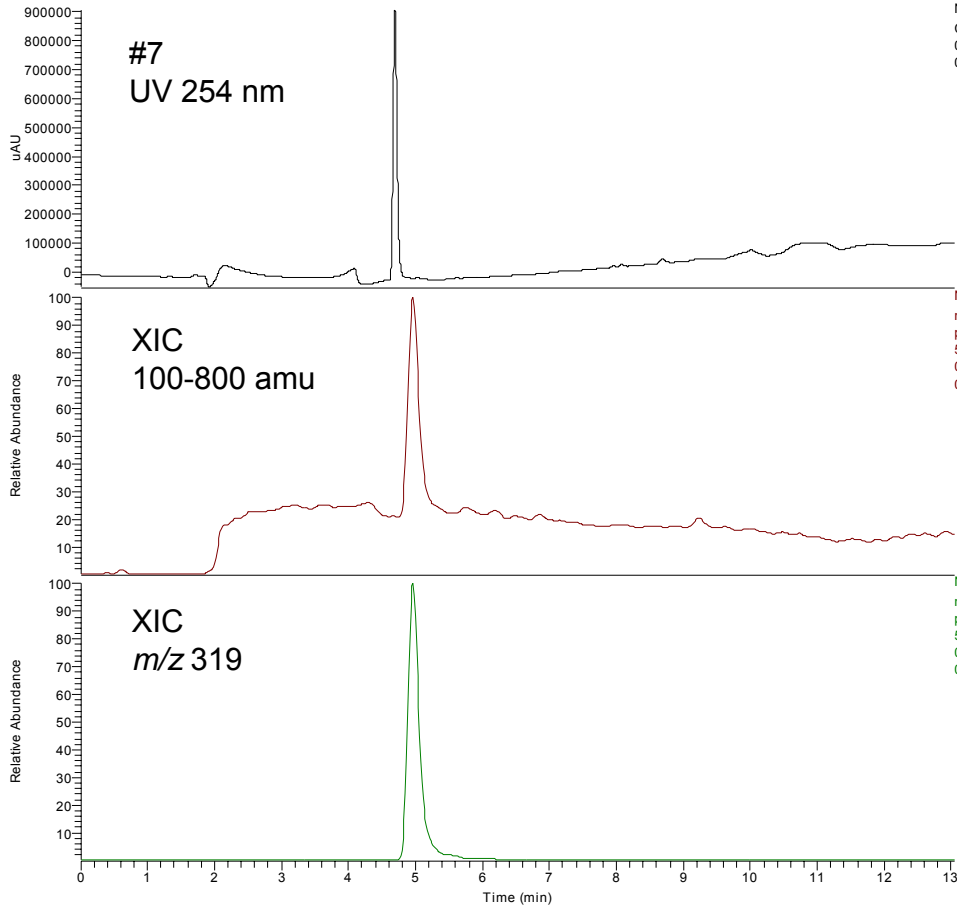
NL: 1.61E8
m/z= 363.50-364.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
05_080822154359

08_08_2008_UCSF_PIS05_080821163810 #347-364 RT: 5.14-5.39 AV: 18 SB: 2 16.99, 16.99 SM: 15G NL: 2.46E7

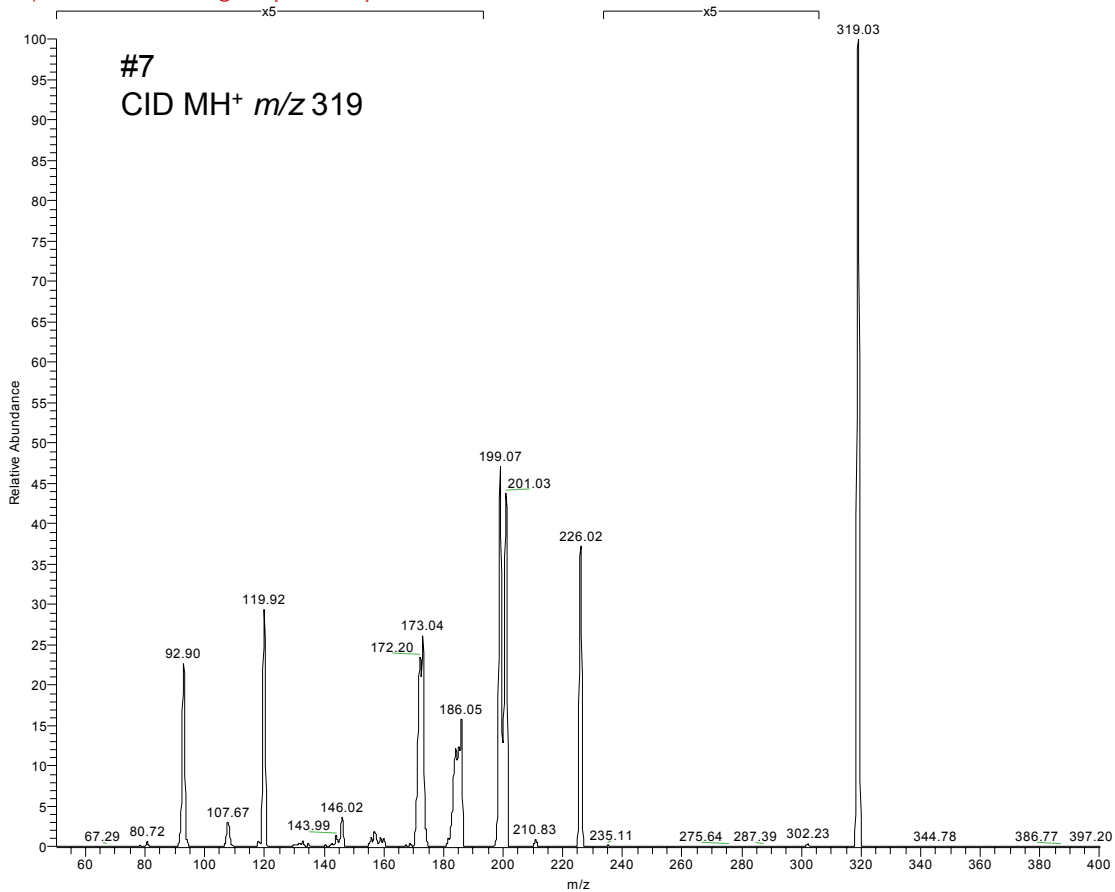
F: + p sid=-10.00 Full m/z 364.10@-30.00 [50.00-700.00]



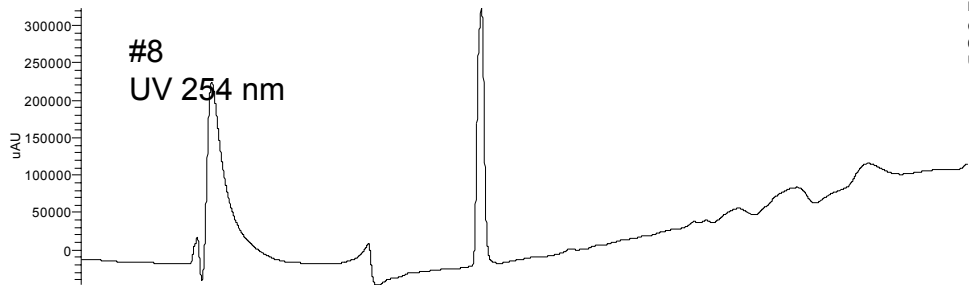
RT: 0.00 - 13.04 SM: 15G



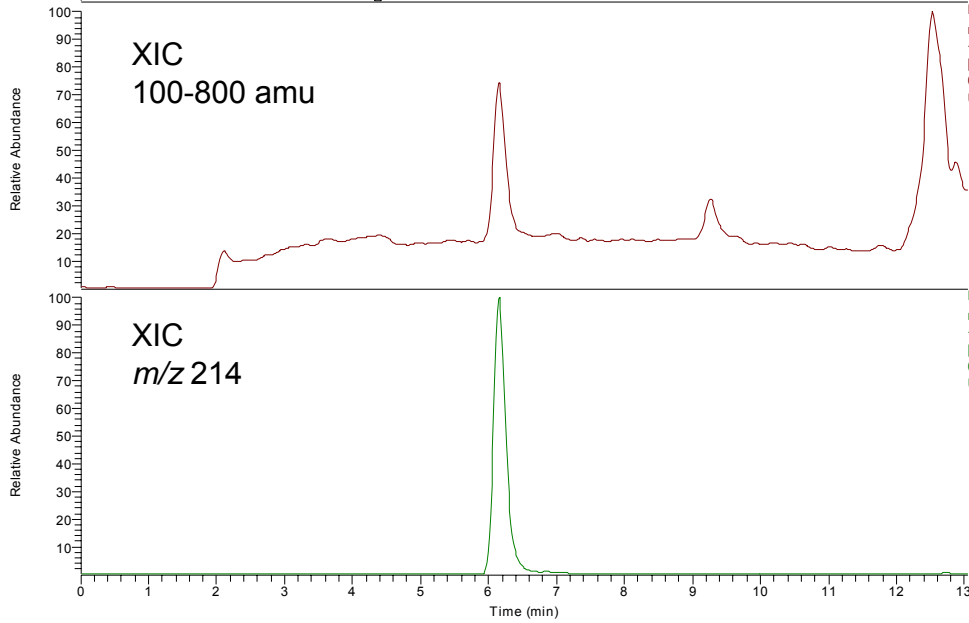
08_08_2008_UCSF_PIS06_080821165558 #324-339 RT: 4.80-5.02 AV: 16 SB: 2 16.99, 16.99 SM: 15G NL: 8.70E6
F: + p sid=-10.00 Full ms2 319.10@-30.00 [50.00-700.00]



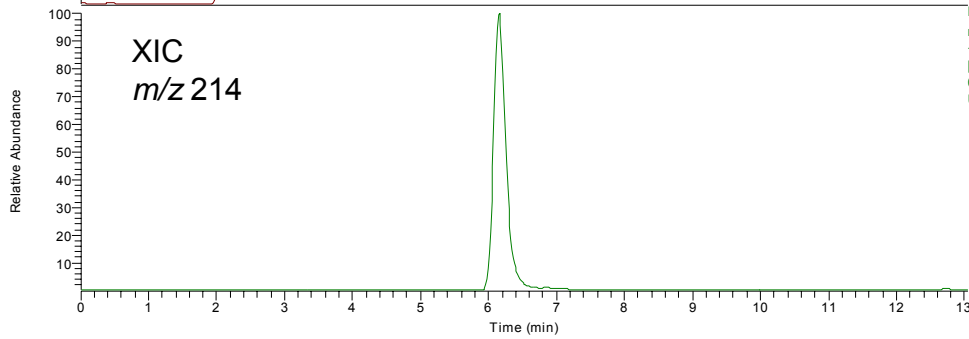
RT: 0.00 - 13.04 SM: 15G



NL: 3.22E5
Channel A_UV
08_22_2008_UCSF_P
URITY_A06

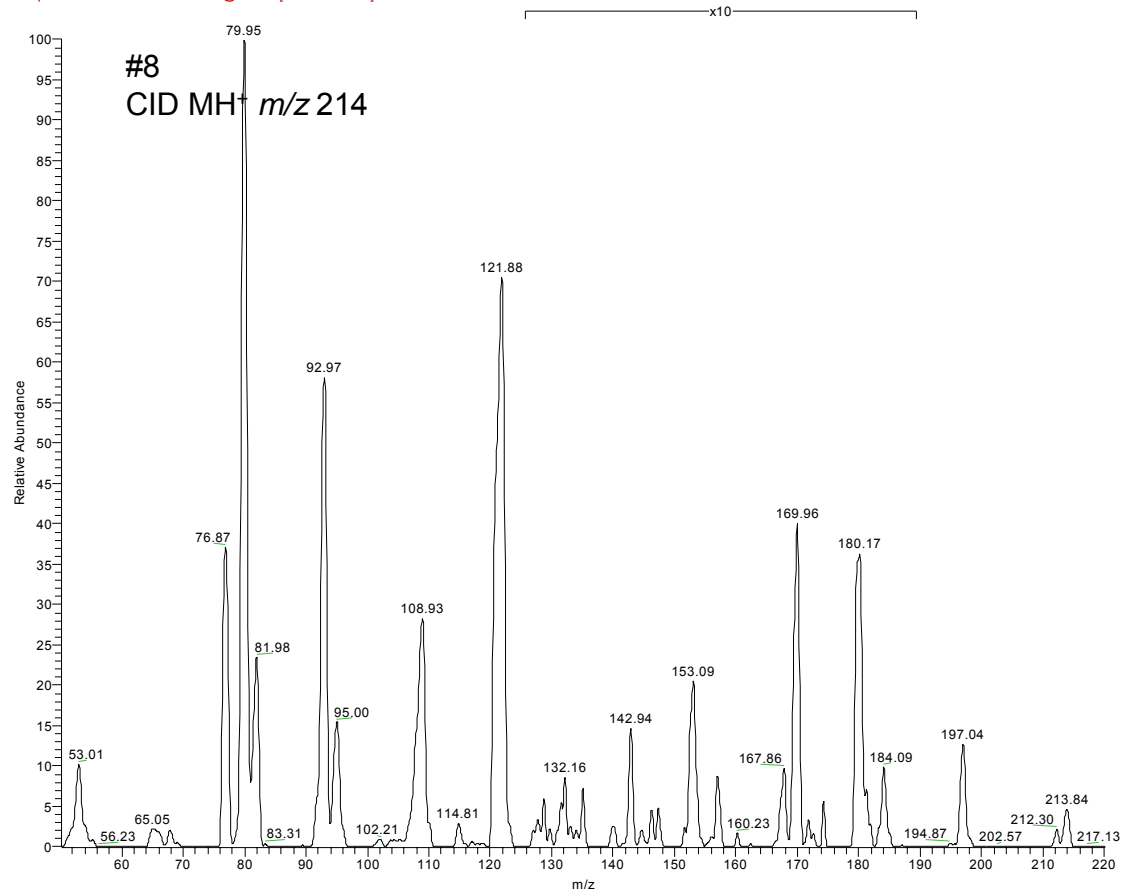


NL: 2.13E8
m/z= 100.00-800.00 F:
+ p sd=-10.00 Q1MS
[50.00-1200.00] MS
08_22_2008_UCSF_P
URITY_A06

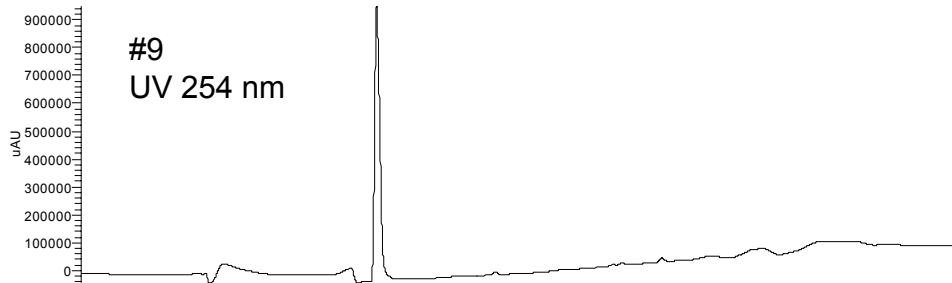


NL: 9.20E7
m/z= 213.50-214.50 F:
+ p sd=-10.00 Q1MS
[50.00-1200.00] MS
08_22_2008_UCSF_P
URITY_A06

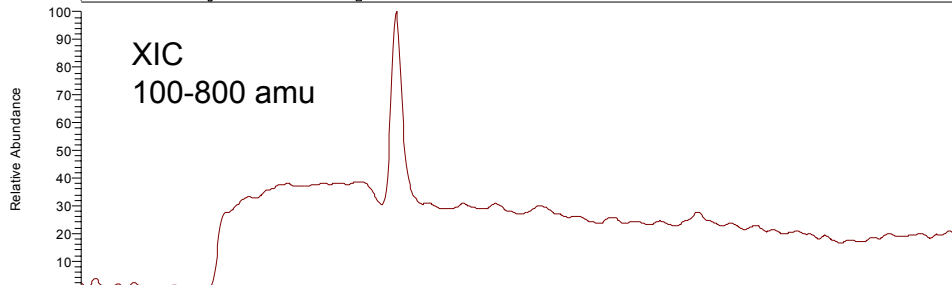
08_22_2008_UCSF_PURITY_A06_080824200302 #404-421 RT: 5.98-6.24 AV: 18 SB: 2 17.00, 17.00 SM: 15G NL: 1.91E6
F: + p sd=-10.00 Full ms2 214.10@-30.00 [50.00-700.00]



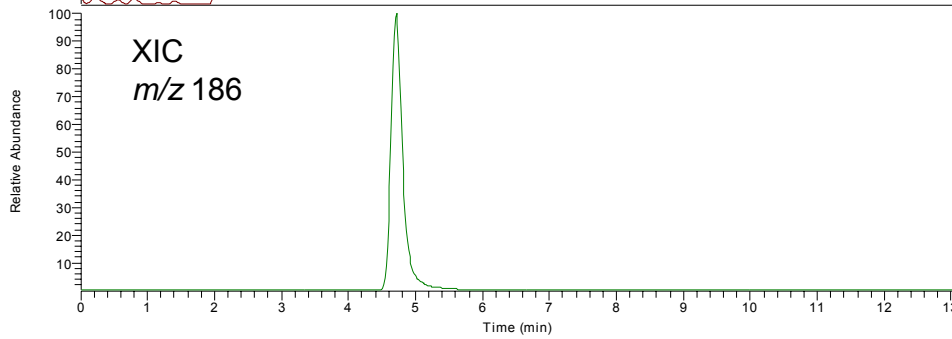
RT: 0.00 - 13.04 SM: 15G



NL: 9.47E5
Channel A UV
08_08_2008_UCSF_PIS
07_080822161927

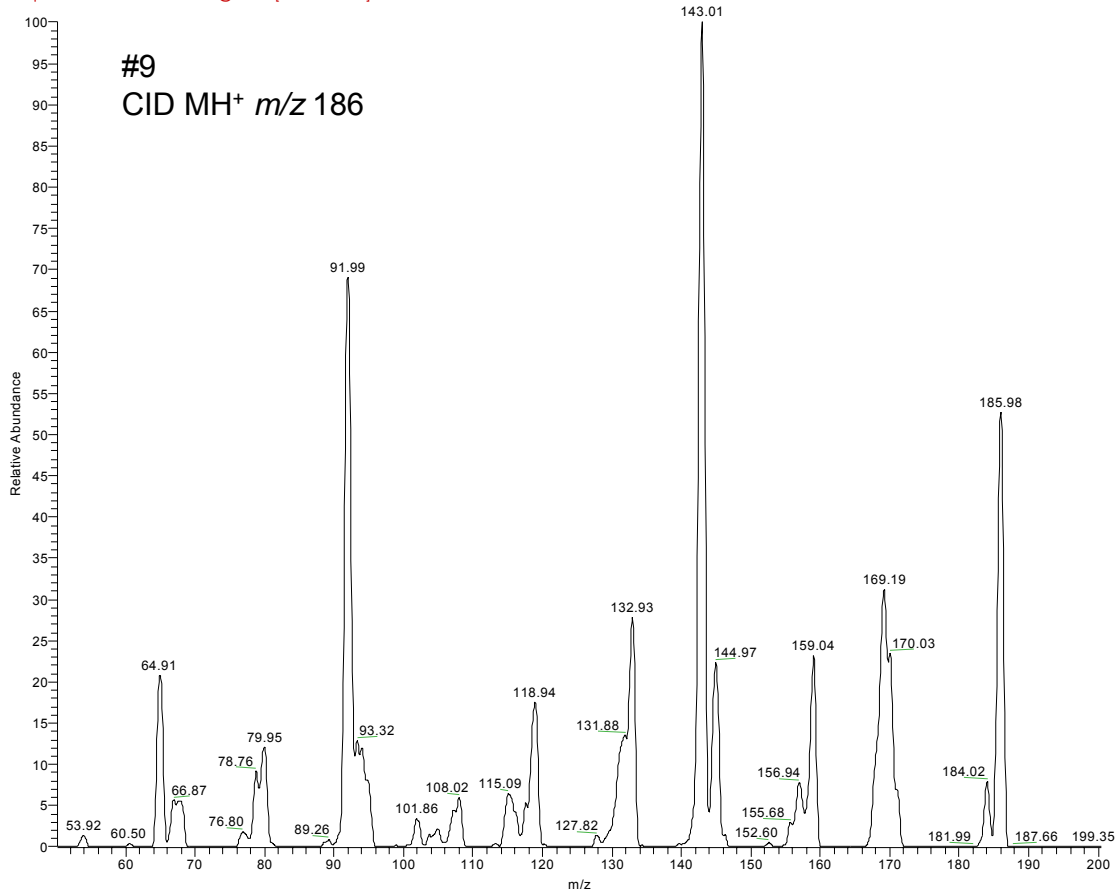


NL: 1.56E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
07_080822161927

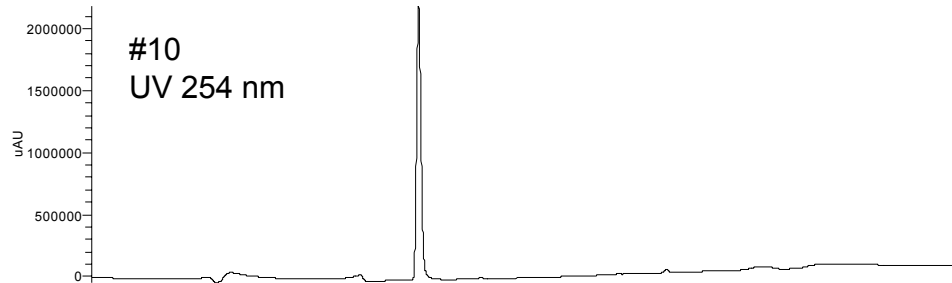


NL: 9.40E7
m/z= 185.50-186.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
07_080822161927

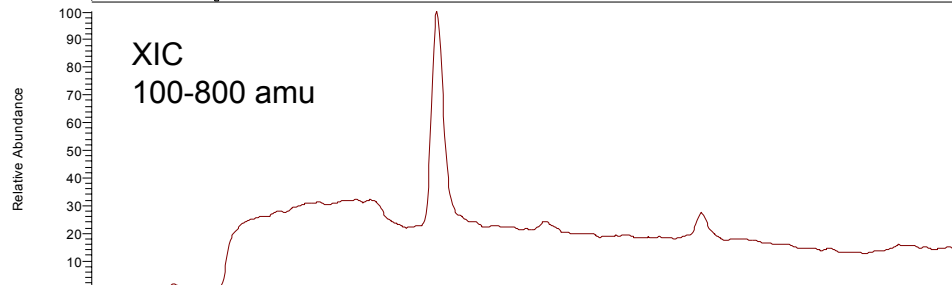
08_08_2008_UCSF_PIS07_080821171342 #307-318 RT: 4.54-4.71 AV: 12 SB: 2 17.00, 17.00 SM: 15G NL: 2.44E6
F: + p sid=-10.00 Full ms2 186.10@-30.00 [50.00-700.00]



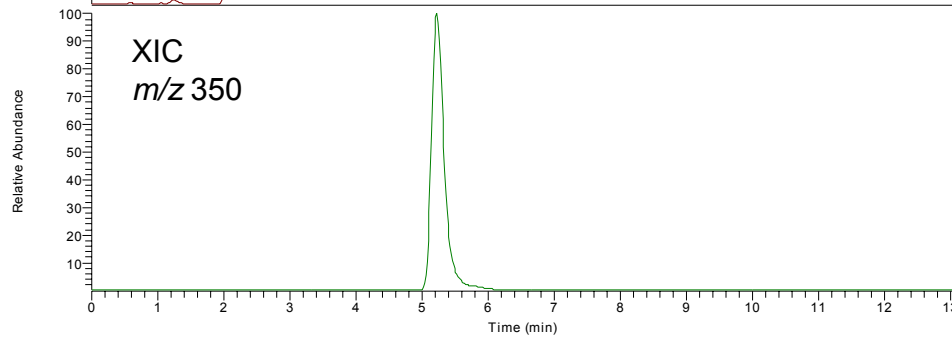
RT: 0.00 - 13.04 SM: 15G



NL: 2.18E6
Channel A UV
08_08_2008_UCSF_PIS
08_080822163713



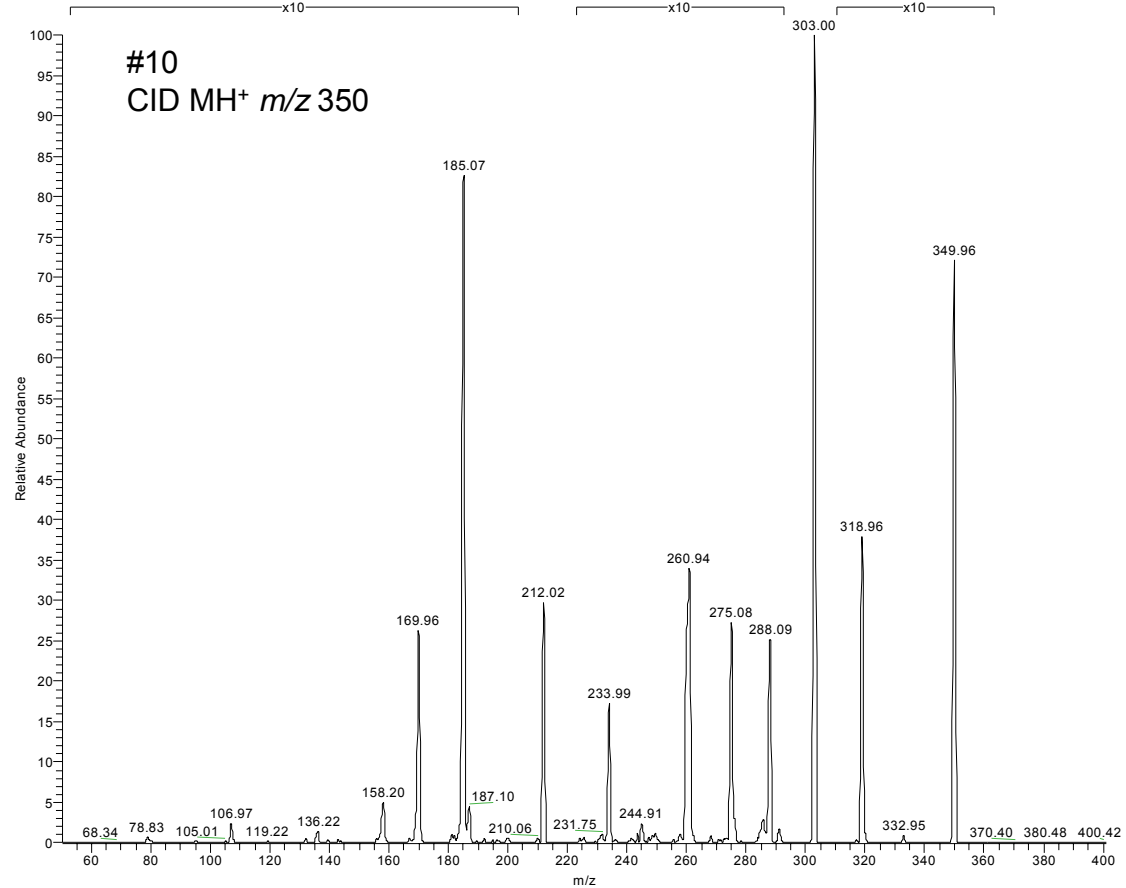
NL: 2.04E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
08_080822163713



NL: 1.20E8
m/z= 349.50-350.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
08_080822163713

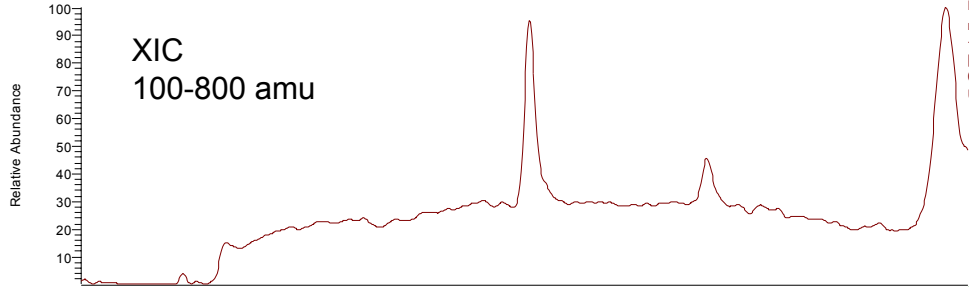
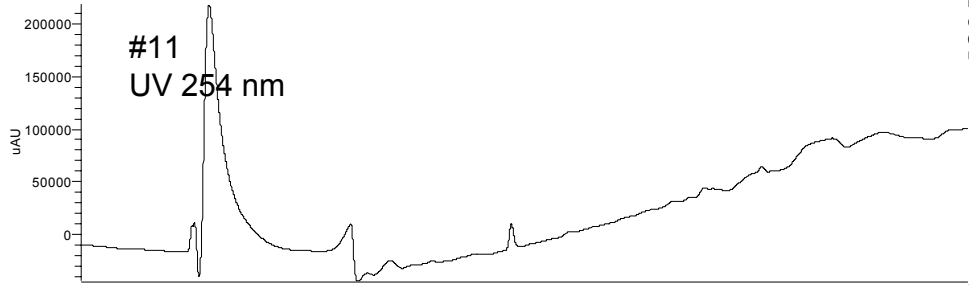
08_08_2008_UCSF_PIS08_080821173129 #338-358 RT: 5.00-5.30 AV: 21 SB: 2 17.00, 17.00 SM: 15G NL: 1.71E7

F: + p sid=-10.00 Full m/z 350.10@-30.00 [50.00-700.00]

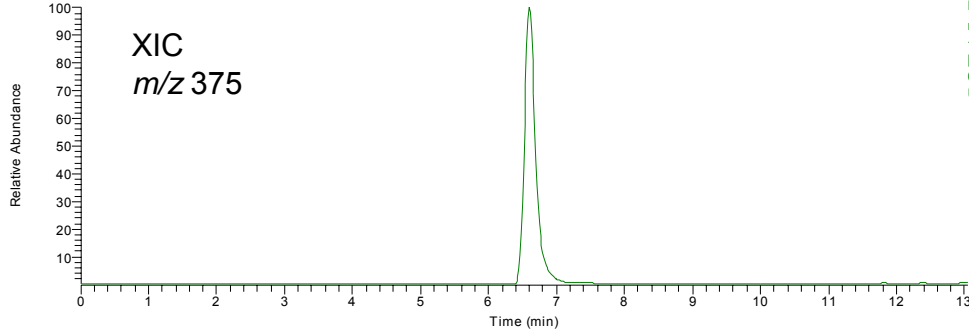


RT: 0.00 - 13.04 SM: 15G

NL: 2.18E5
Channel A_UV
08_22_2008_UCSF_P
URITY_A07

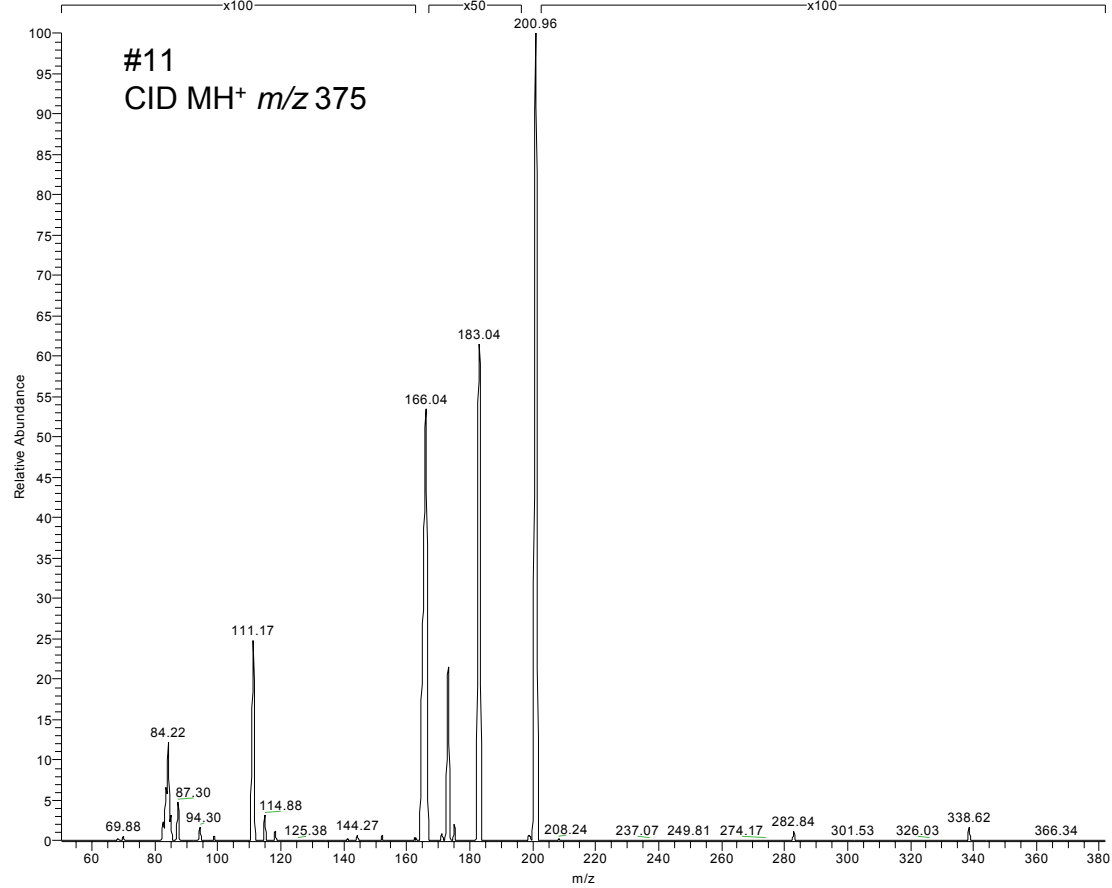


NL: 1.65E8
m/z= 100.00-800.00 F:
+ p sd=-10.00 Q1MS
[50.00-1200.00] MS
08_22_2008_UCSF_P
URITY_A07

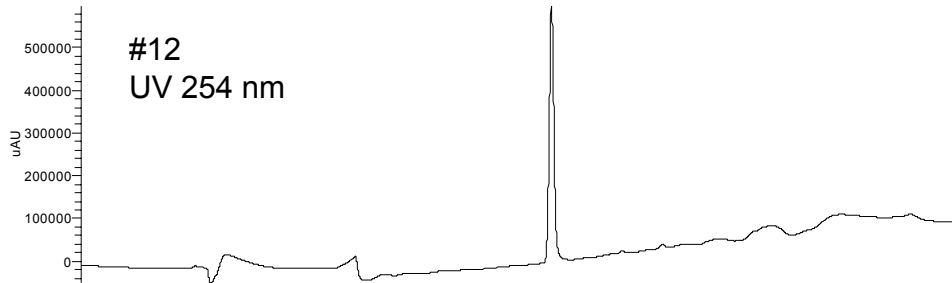


NL: 5.54E7
m/z= 374.50-375.50 F:
+ p sd=-10.00 Q1MS
[50.00-1200.00] MS
08_22_2008_UCSF_P
URITY_A07

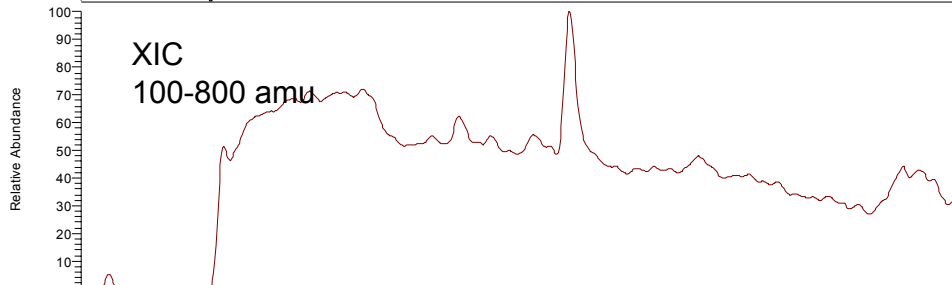
08_22_2008_UCSF_PURITY_A07_080824202046 #444-455 RT: 6.58-6.74 AV: 12 SB: 2 16.99, 16.99 SM: 15G NL: 9.20E6
F: + p sd=-10.00 Full m/z 375.10@-30.00 [50.00-700.00]



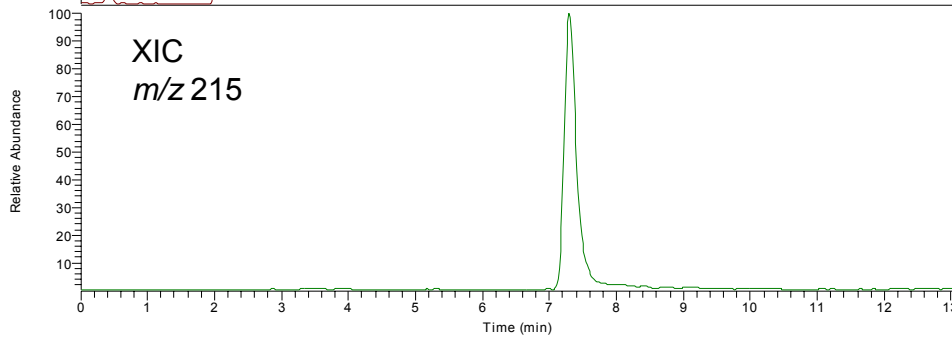
RT: 0.00 - 13.04 SM: 15G



NL: 5.96E5
Channel A UV
08_08_2008_UCSF_PIS
09_080822165500

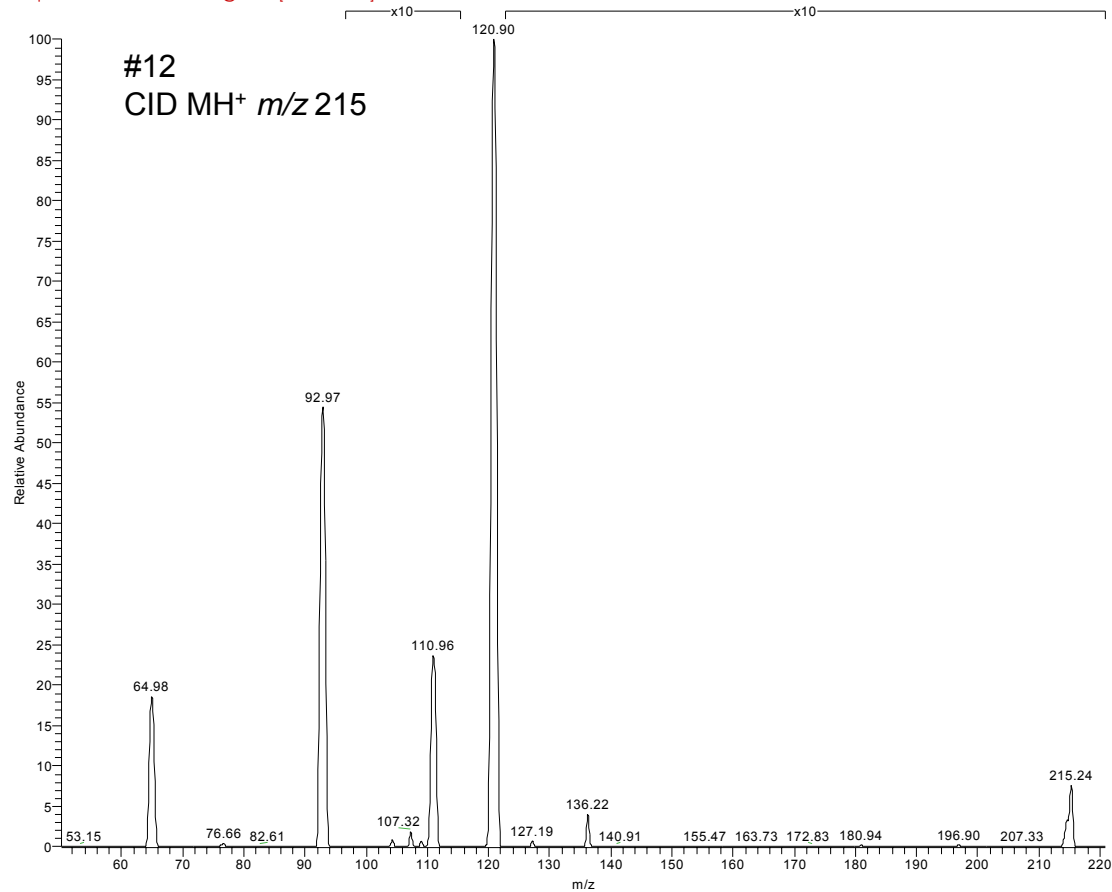


NL: 8.97E7
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
09_080822165500

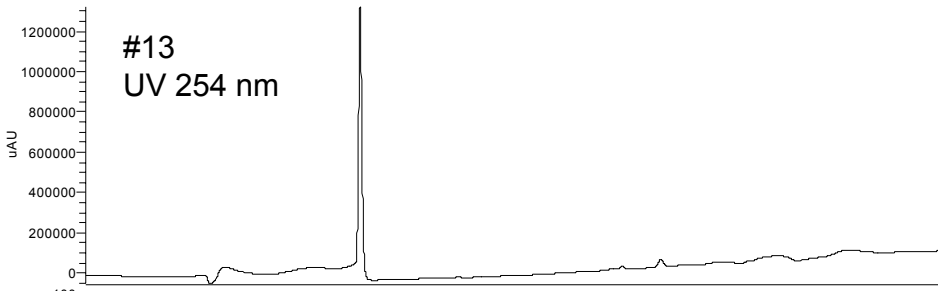


NL: 3.60E7
m/z= 214.50-215.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
09_080822165500

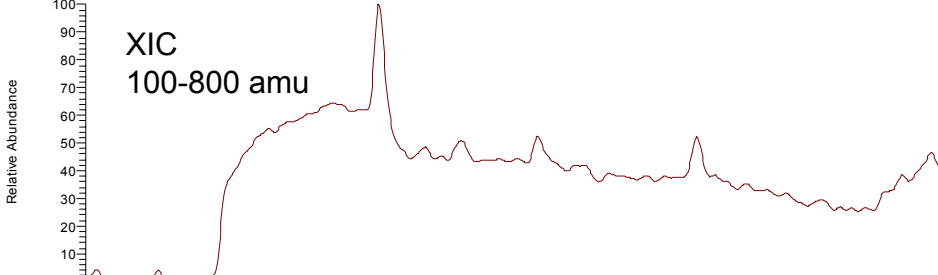
08_08_2008_UCSF_PIS09_080821174913 #482-499 RT: 7.14-7.39 AV: 18 SB: 2 17.00, 17.00 SM: 15G NL: 1.77E6
F: + p sid=-10.00 Full m/z 215.10@-30.00 [50.00-700.00]



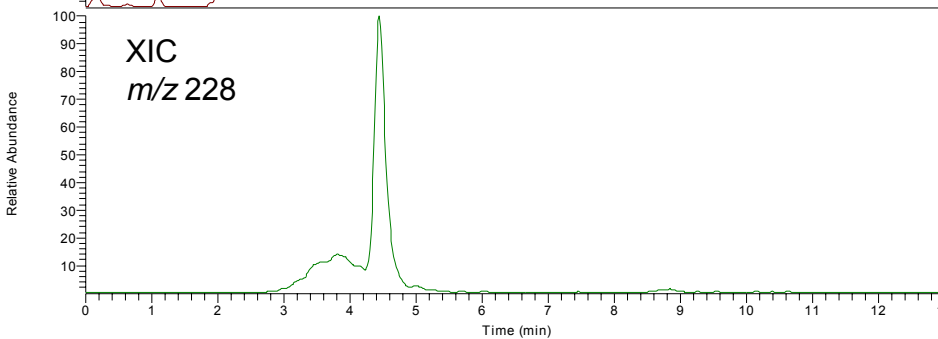
RT: 0.00 - 13.04 SM: 15G



NL: 1.32E6
Channel A UV
08_08_2008_UCSF_PIS
13_080822171247



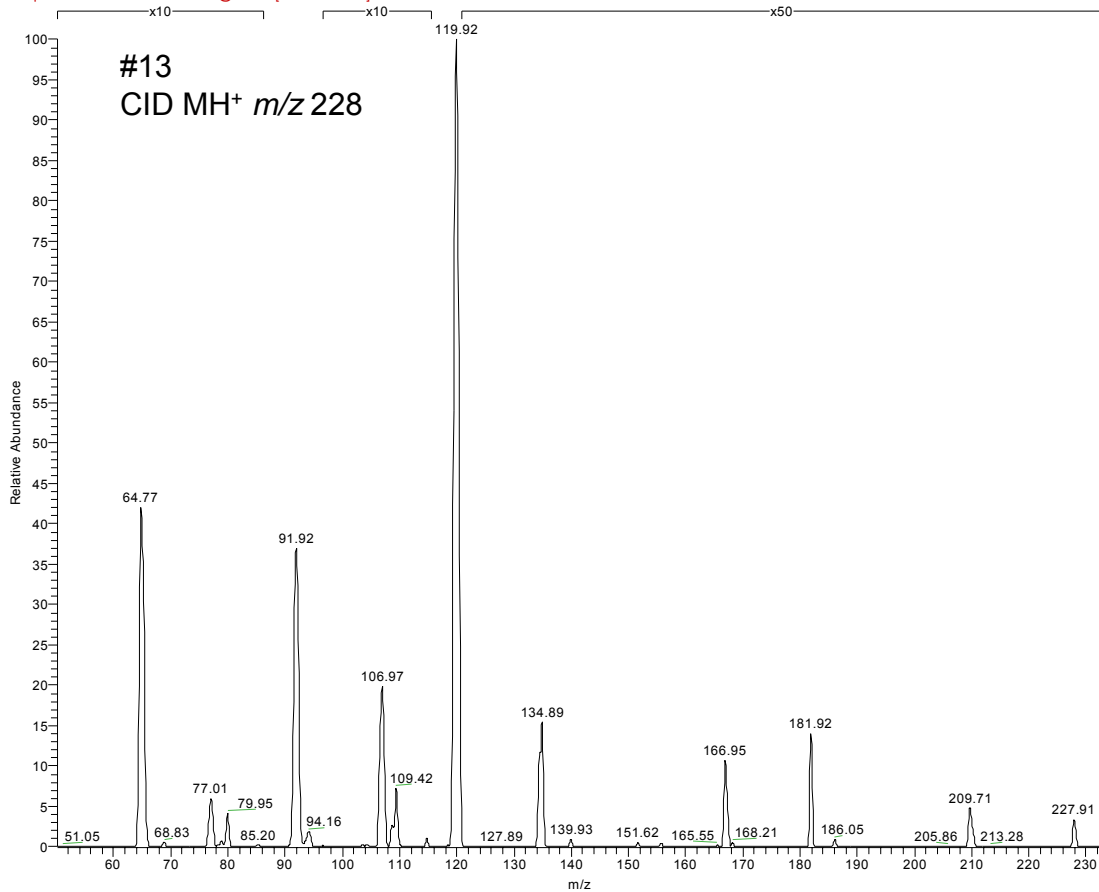
NL: 1.06E8
m/z= 100.00-800.00 F: +
p sld=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
13_080822171247



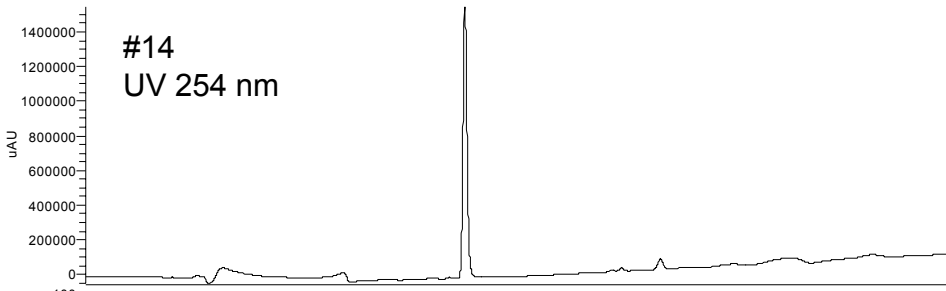
NL: 3.48E7
m/z= 227.50-228.50 F: +
p sld=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
13_080822171247

08_08_2008_UCSF_PIS13_080821180657 #283-292 RT: 4.19-4.32 AV: 10 SB: 2 16.99, 16.99 SM: 15G NL: 2.59E6

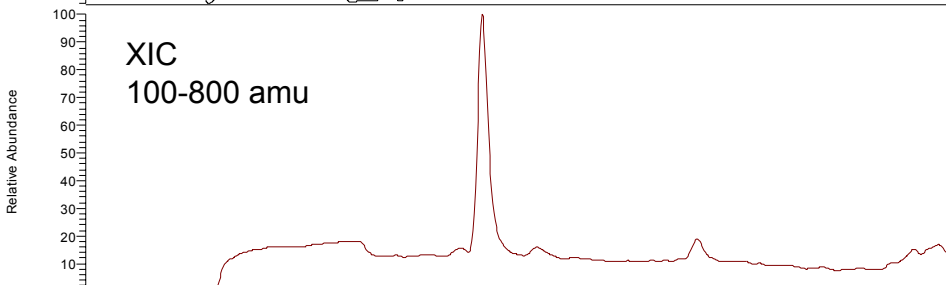
F: + p sld=-10.00 Full ms2 228.10@-30.00 [50.00-700.00]



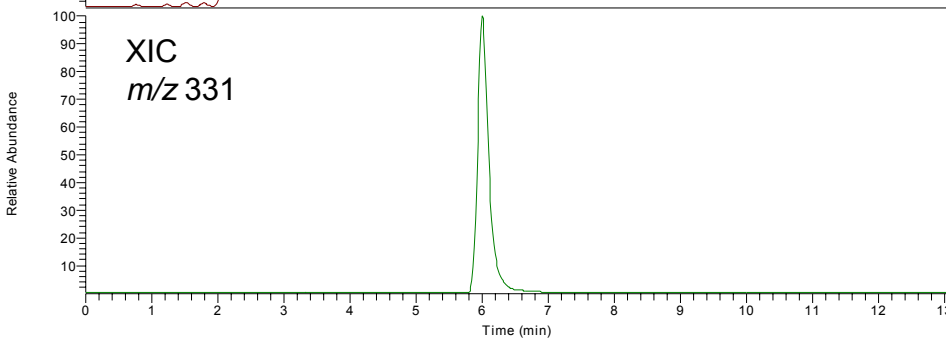
RT: 0.00 - 13.04 SM: 15G



NL: 1.54E6
Channel A UV
08_08_2008_UCSF_PIS
14_080822173034



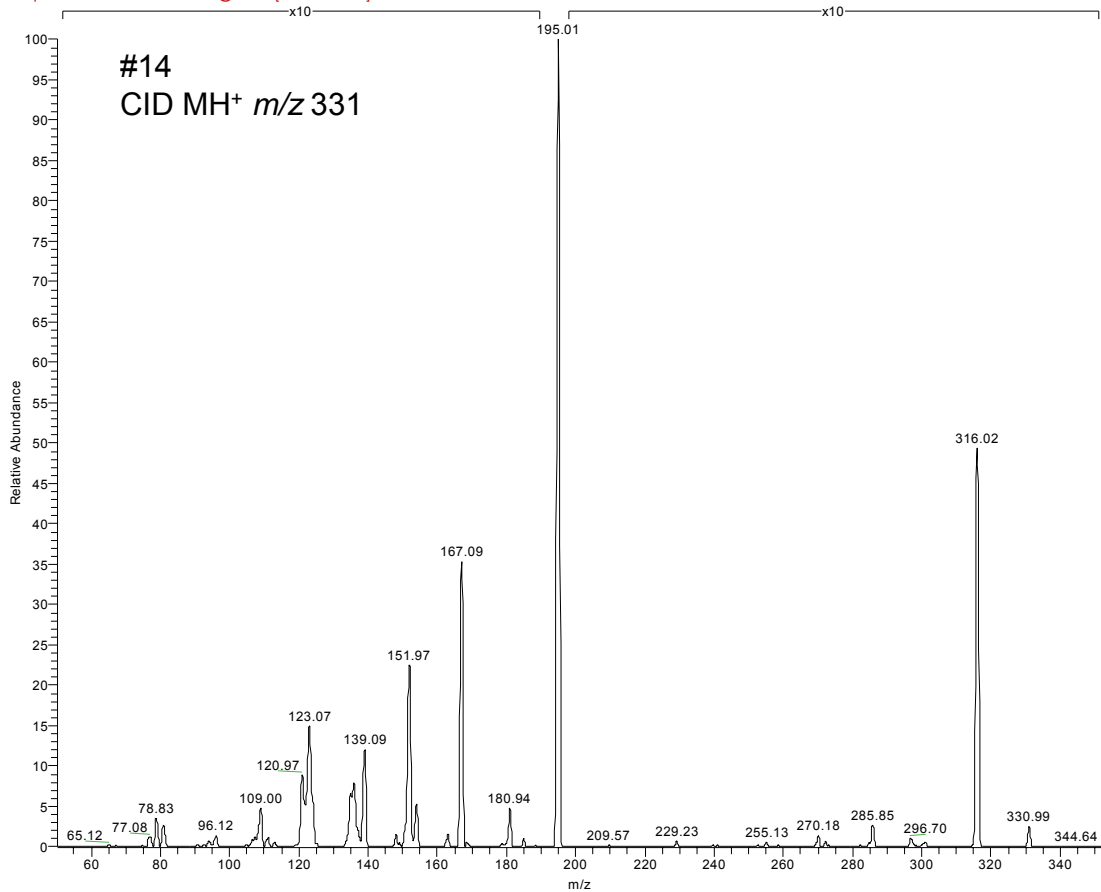
NL: 3.42E8
m/z= 100.00-800.00 F: +
p sld=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
14_080822173034



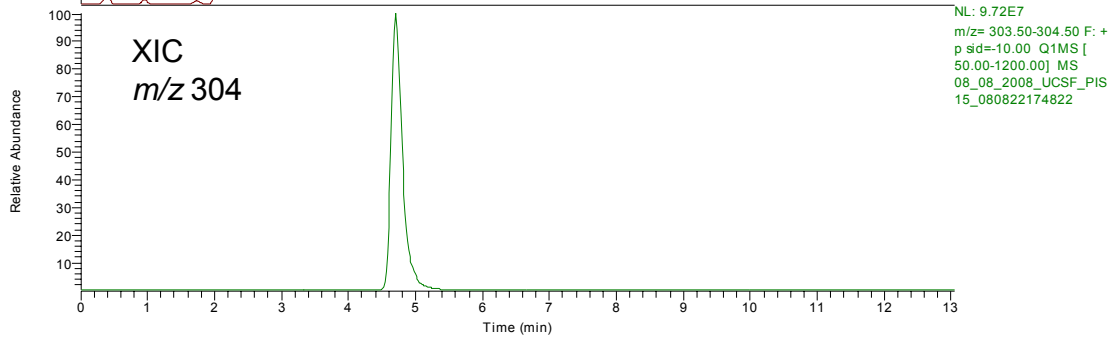
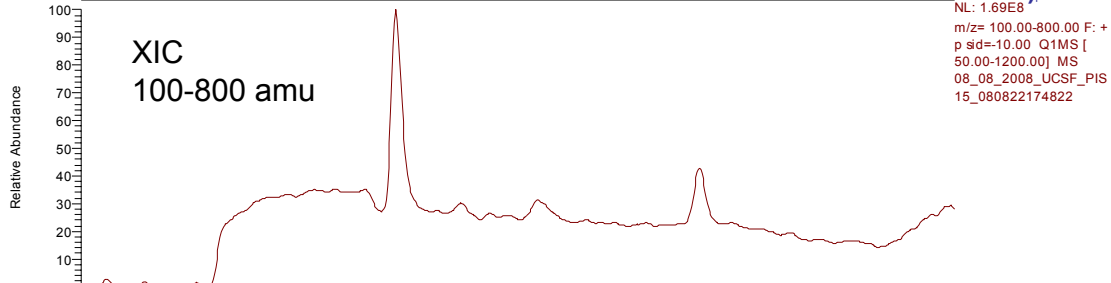
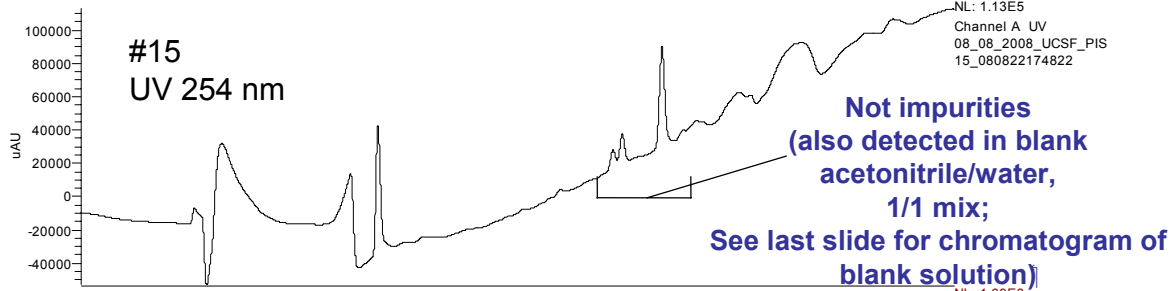
NL: 2.12E8
m/z= 330.50-331.50 F: +
p sld=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
14_080822173034

08_08_2008_UCSF_PIS14_080821182445 #396-413 RT: 5.86-6.12 AV: 18 SB: 2 17.00, 17.00 SM: 15G NL: 3.20E7

F: + p sld=-10.00 Full ms2 331.10@-30.00 [50.00-700.00]

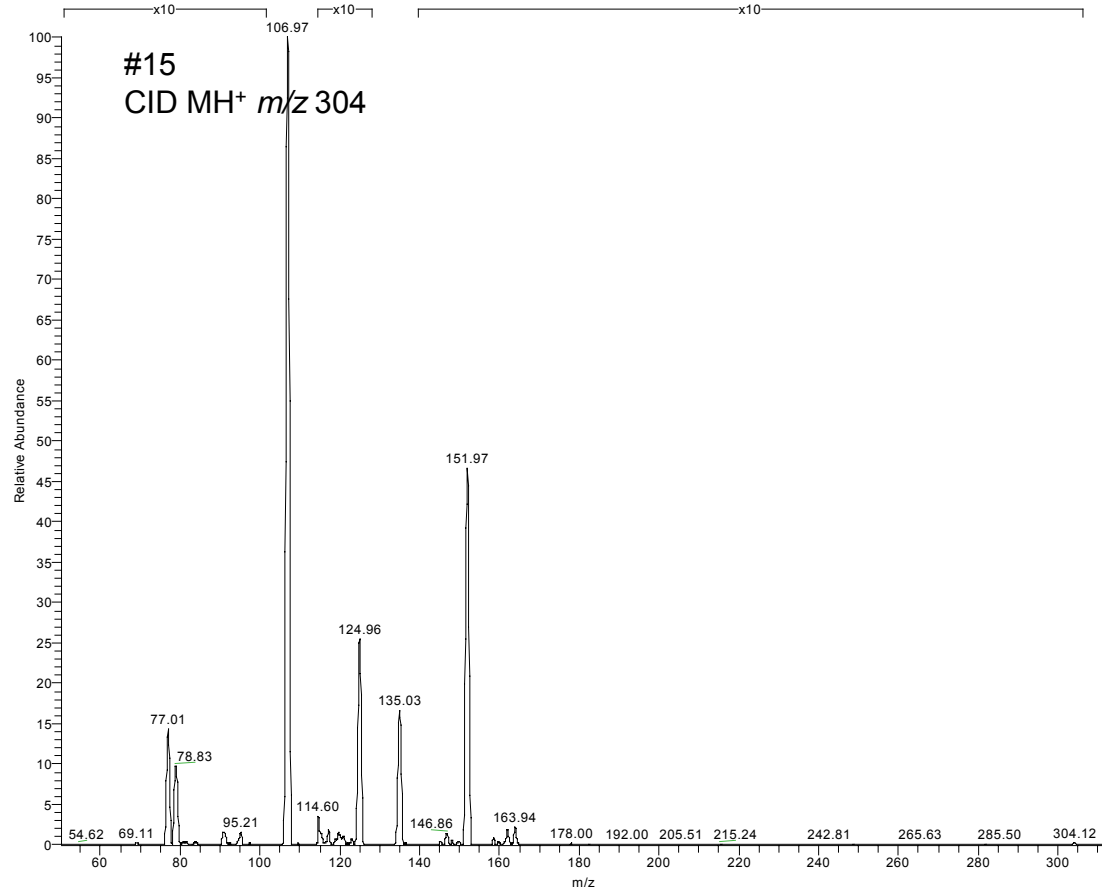


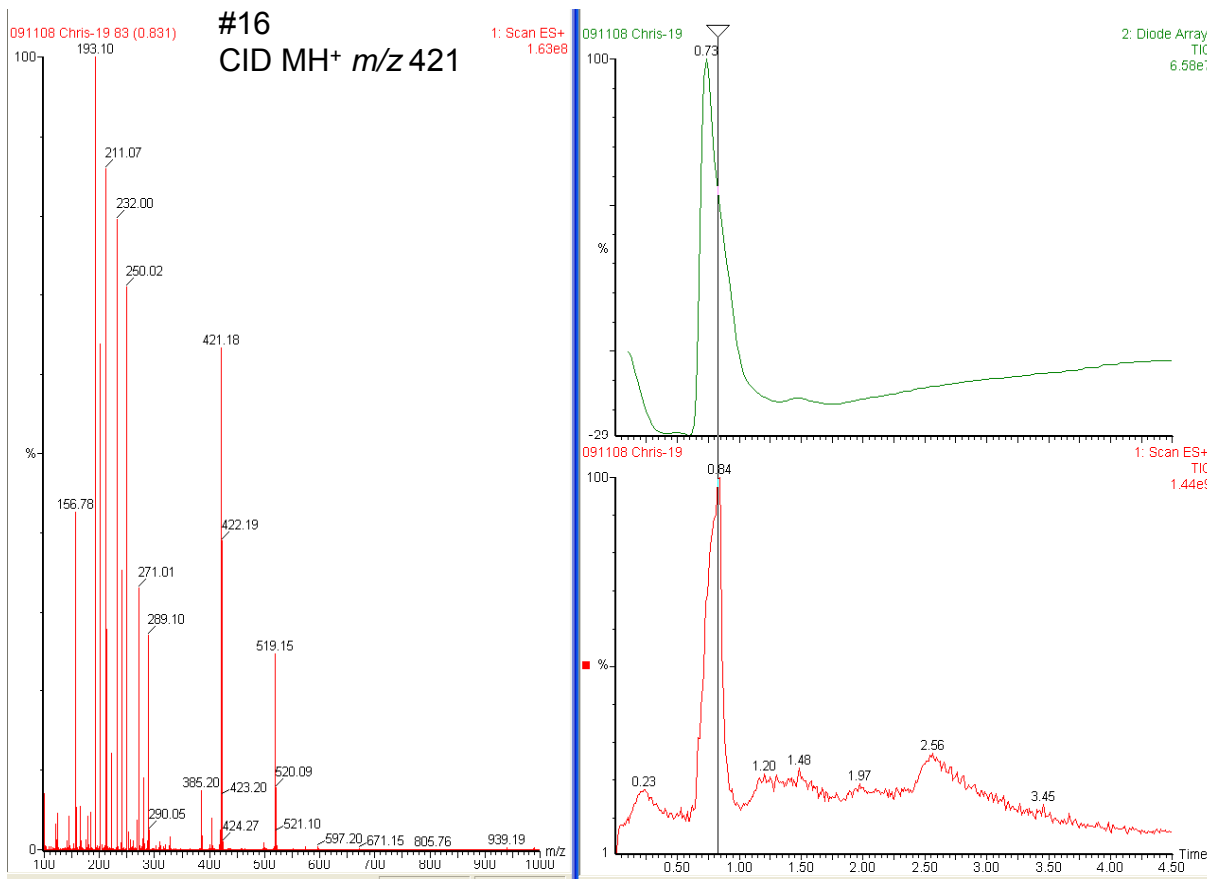
RT: 0.00 - 13.04 SM: 15G



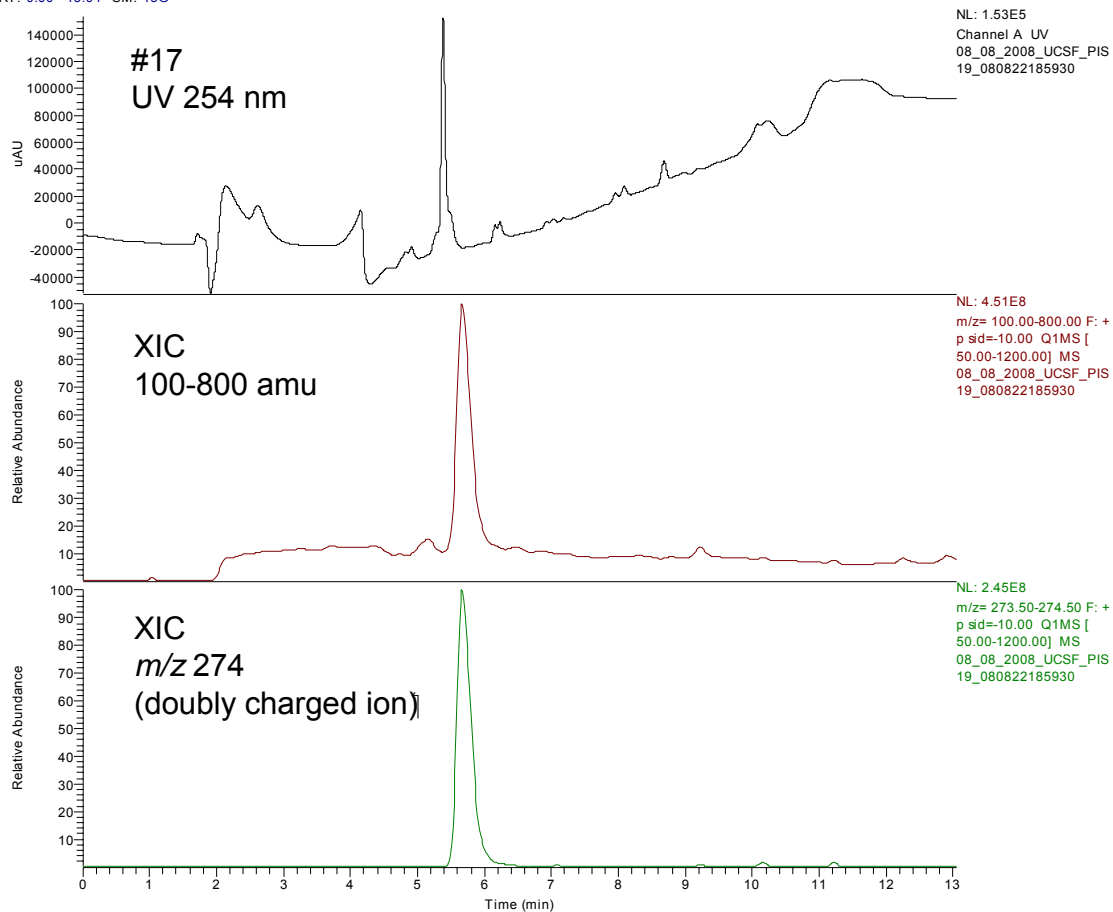
08_08_2008_UCSF_PIS15_080821184233 #307-330 RT: 4.54-4.89 AV: 24 SB: 2 17.00, 17.00 SM: 15G NL: 5.50E6

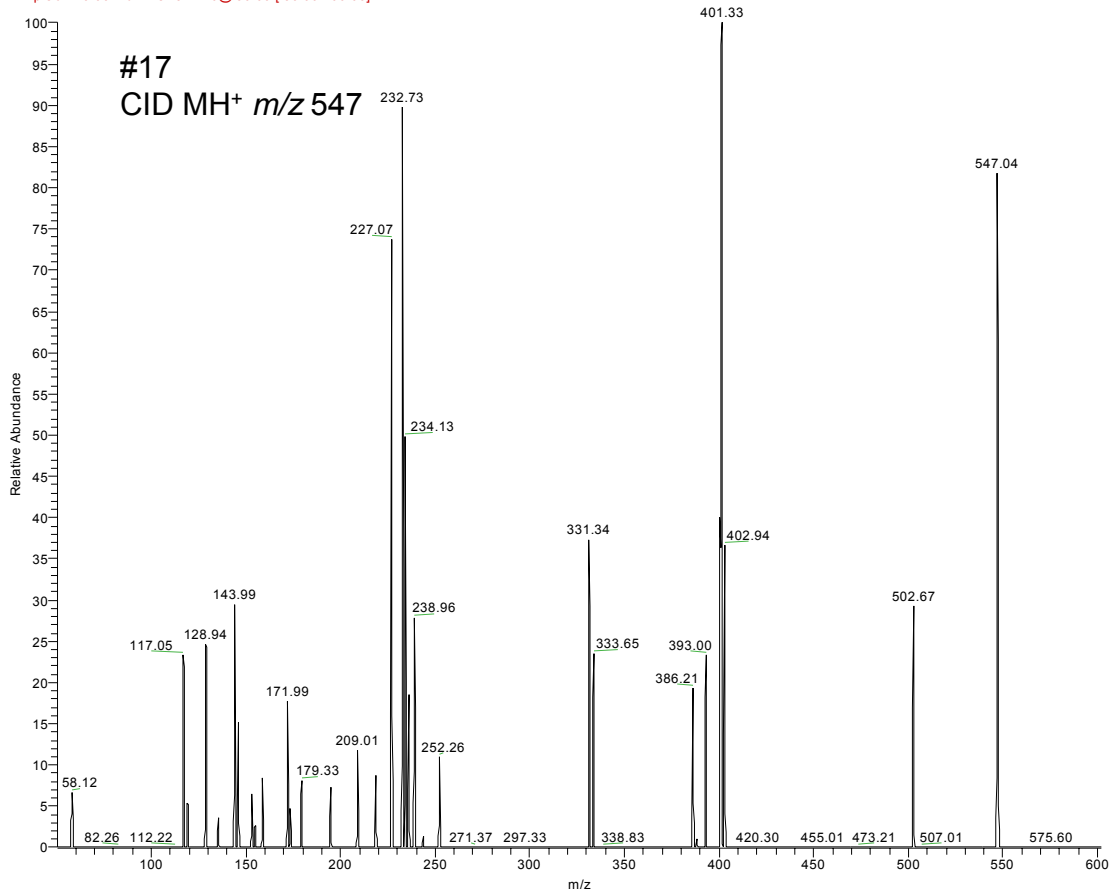
F: + p sid=-10.00 Full ms2 304.10@-30.00 [50.00-700.00]



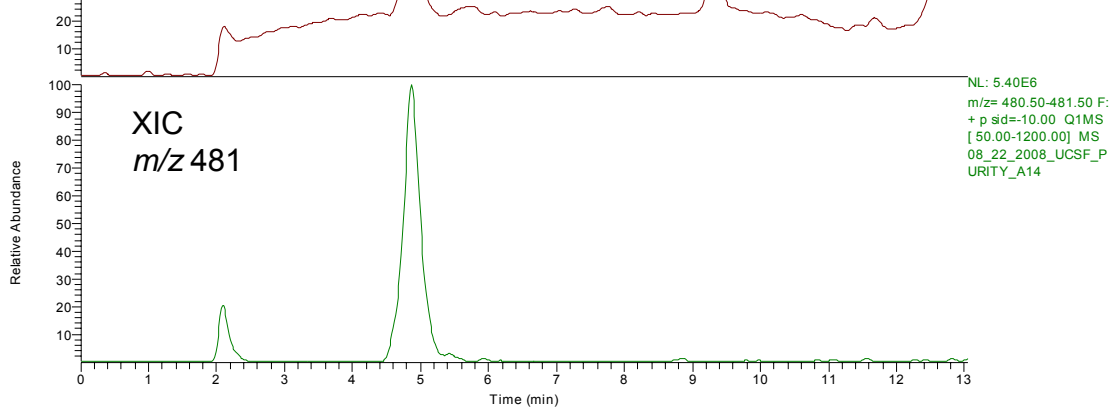
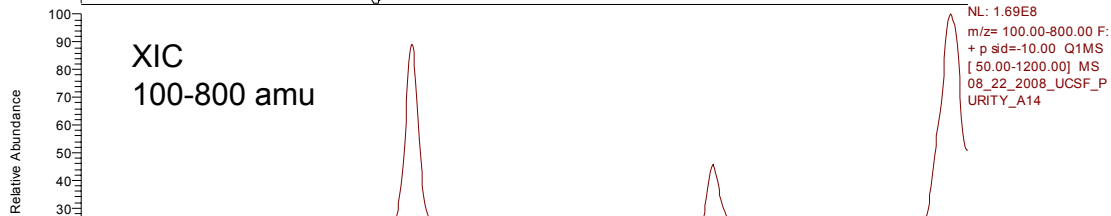
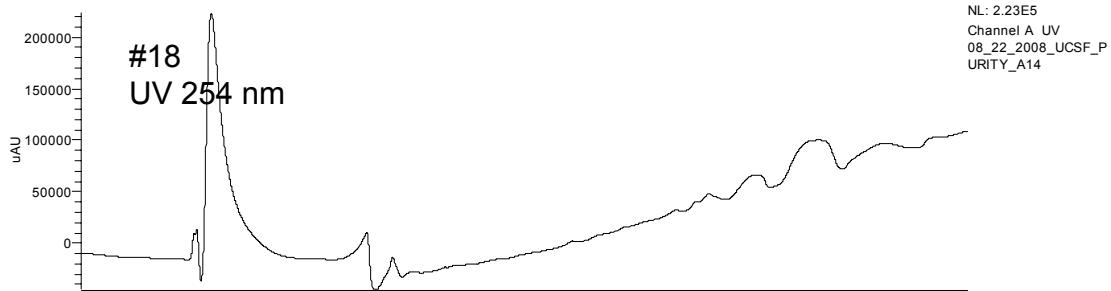


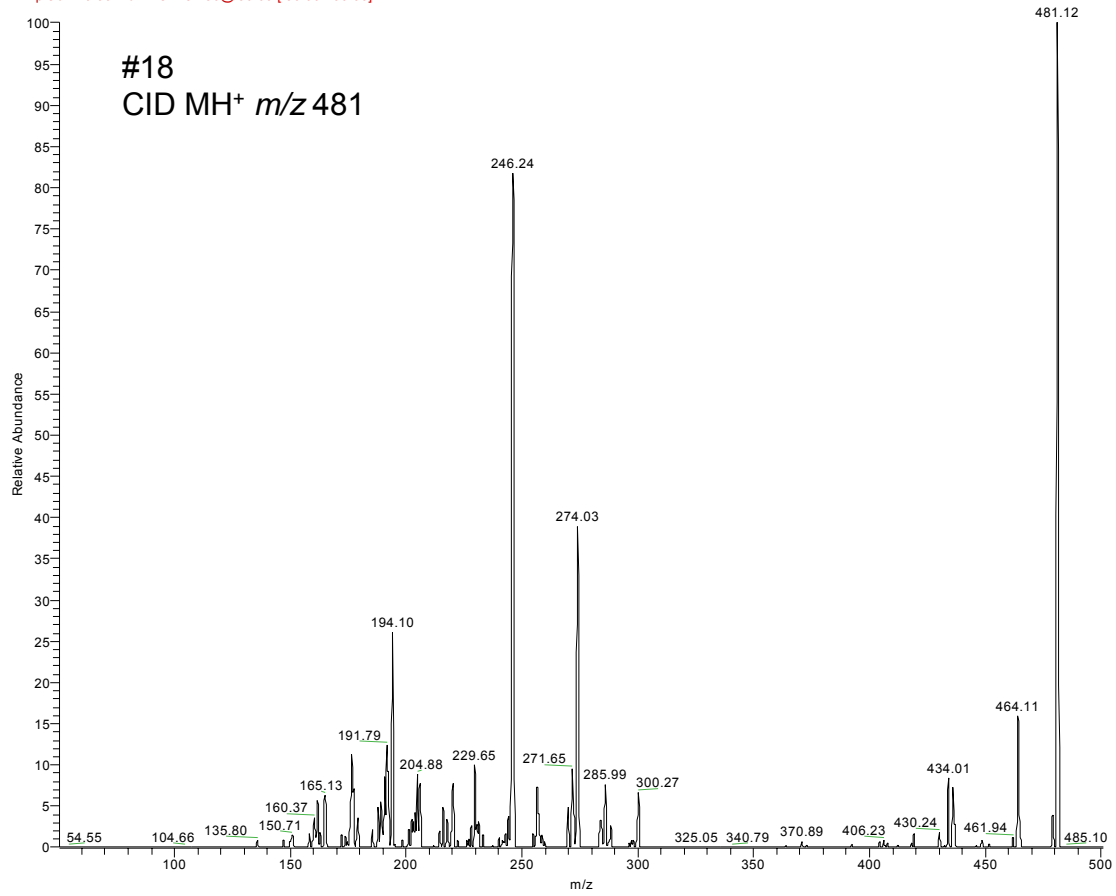
RT: 0.00 - 13.04 SM: 15G



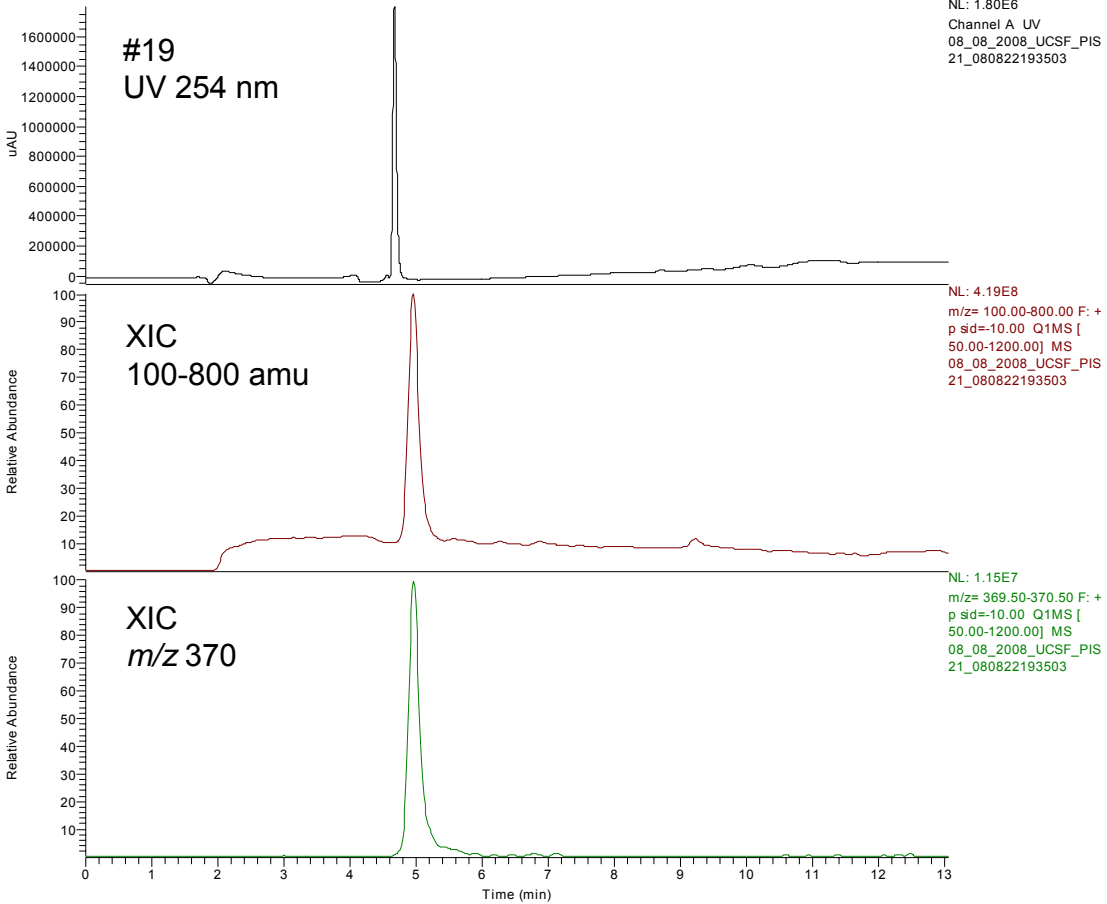


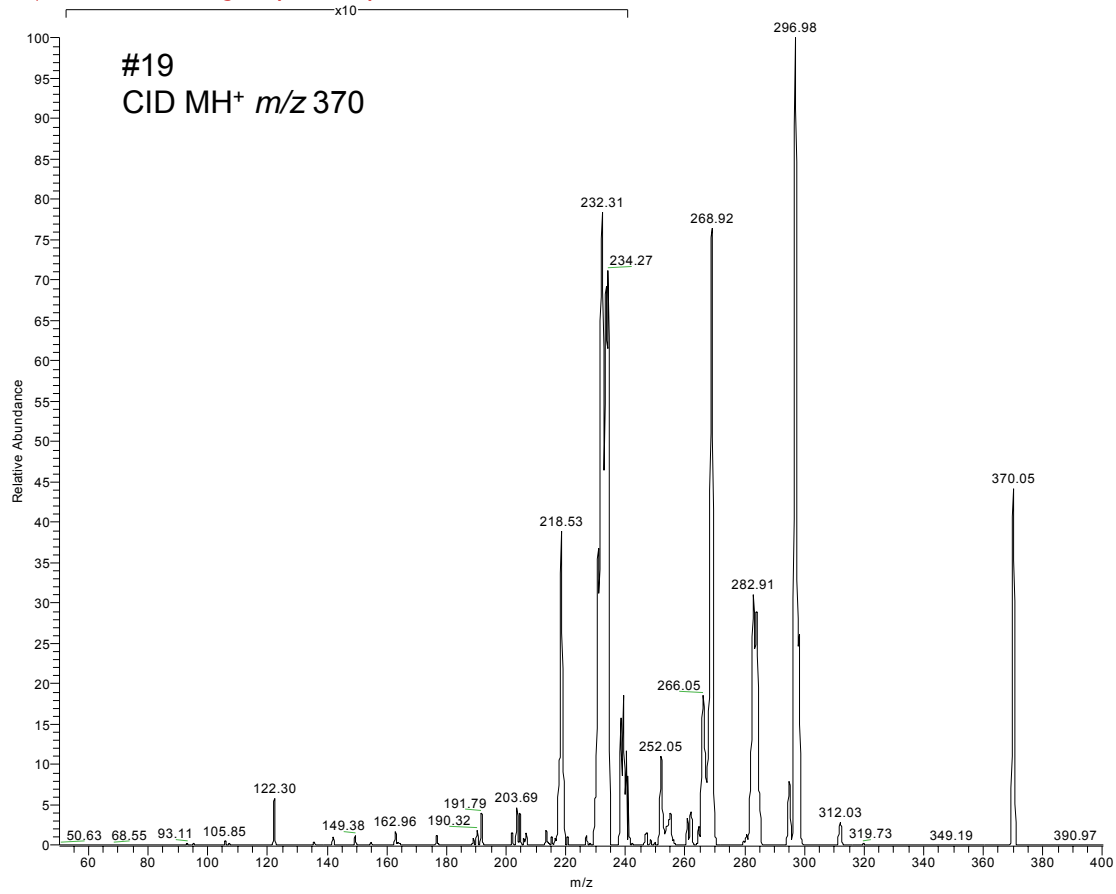
RT: 0.00 - 13.04 SM: 15G



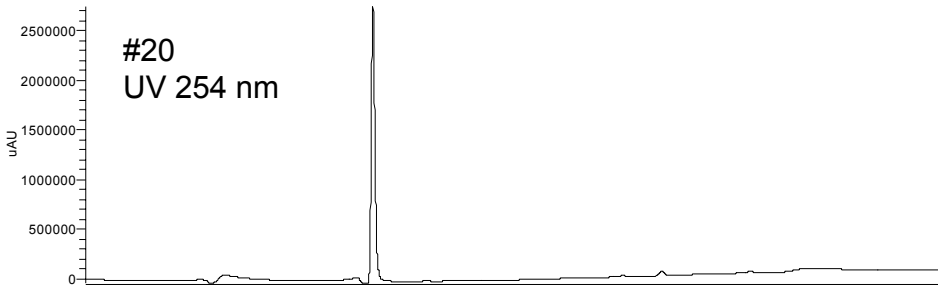


RT: 0.00 - 13.04 SM: 15G

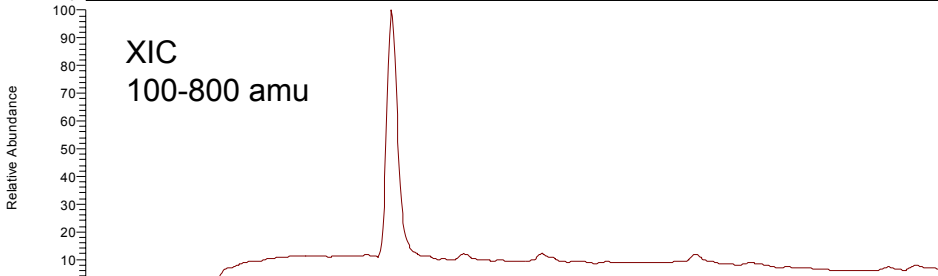




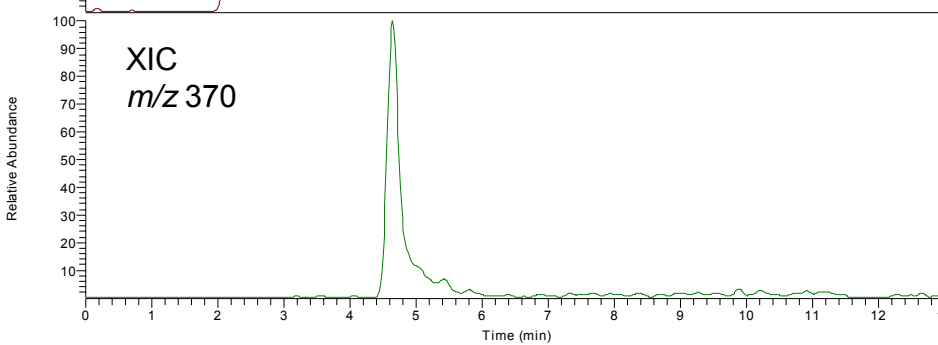
RT: 0.00 - 13.04 SM: 15G



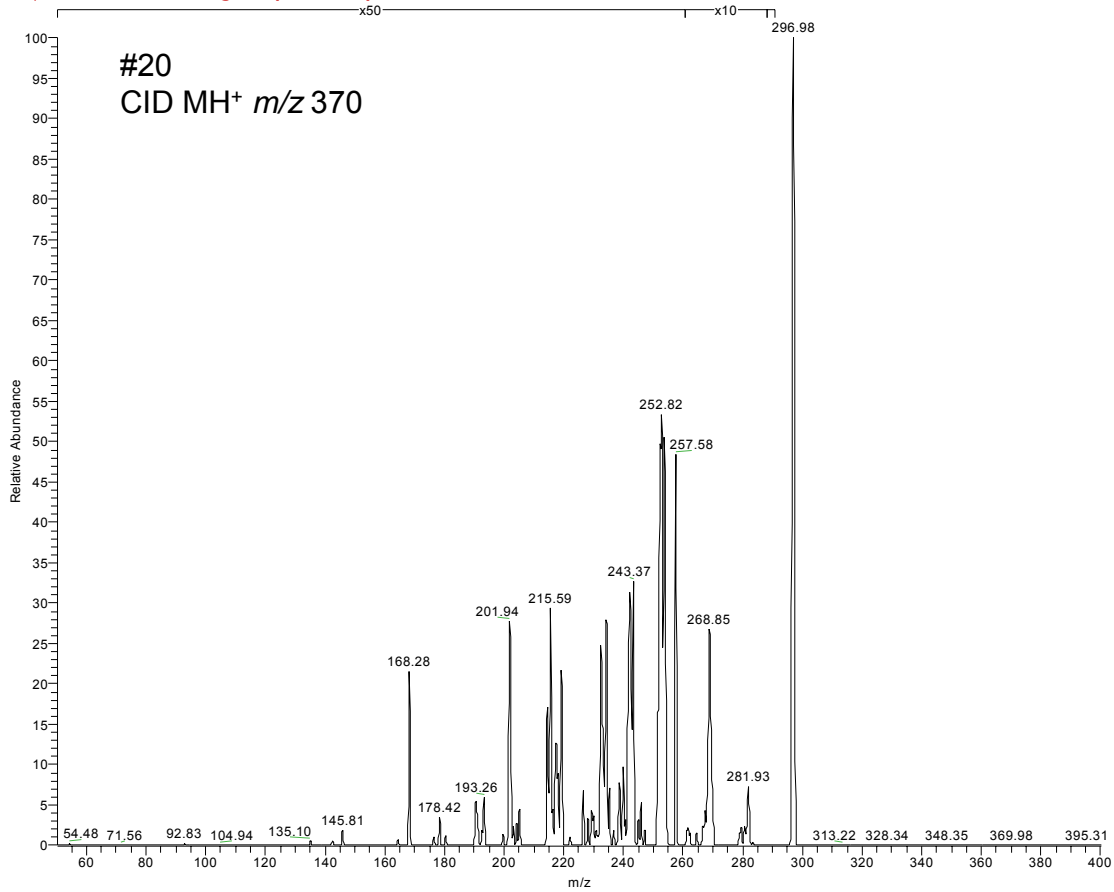
NL: 2.74E6
Channel A UV
08_08_2008_UCSF_PIS
25_080822195247



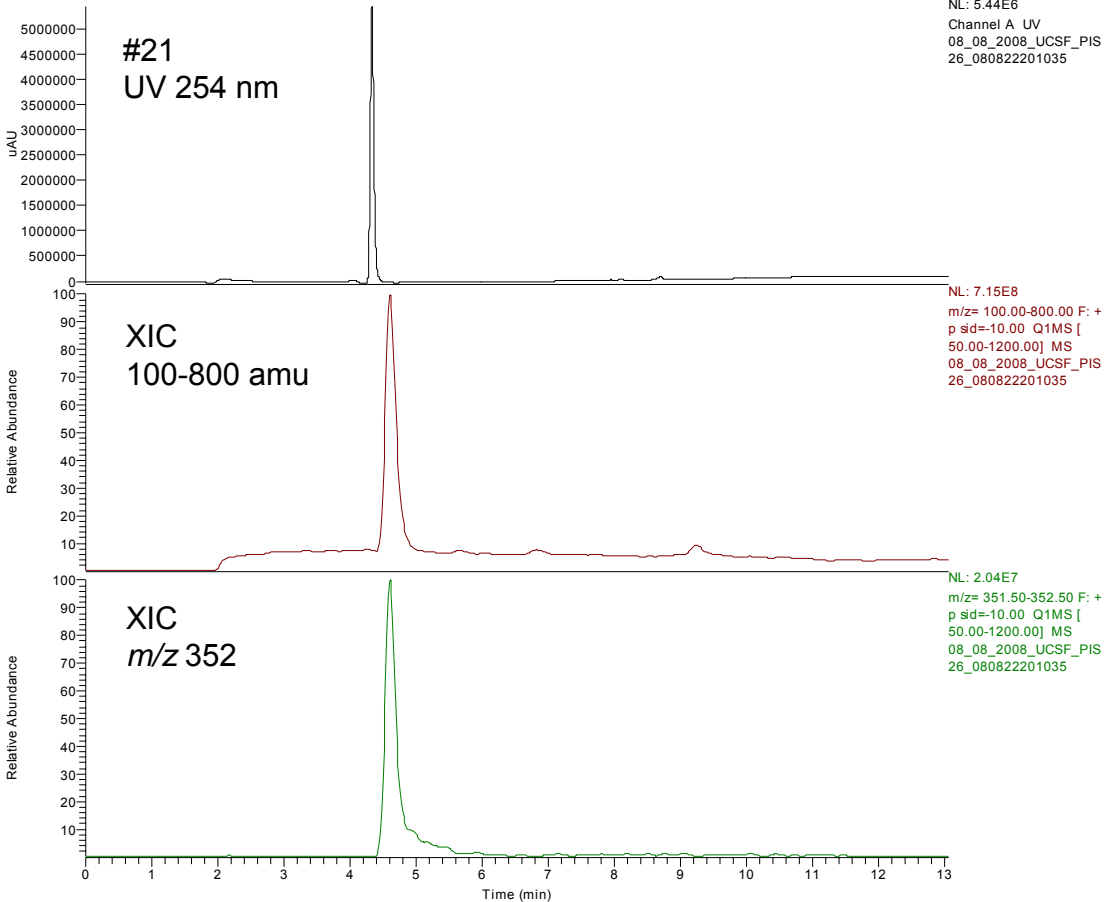
NL: 4.47E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
25_080822195247

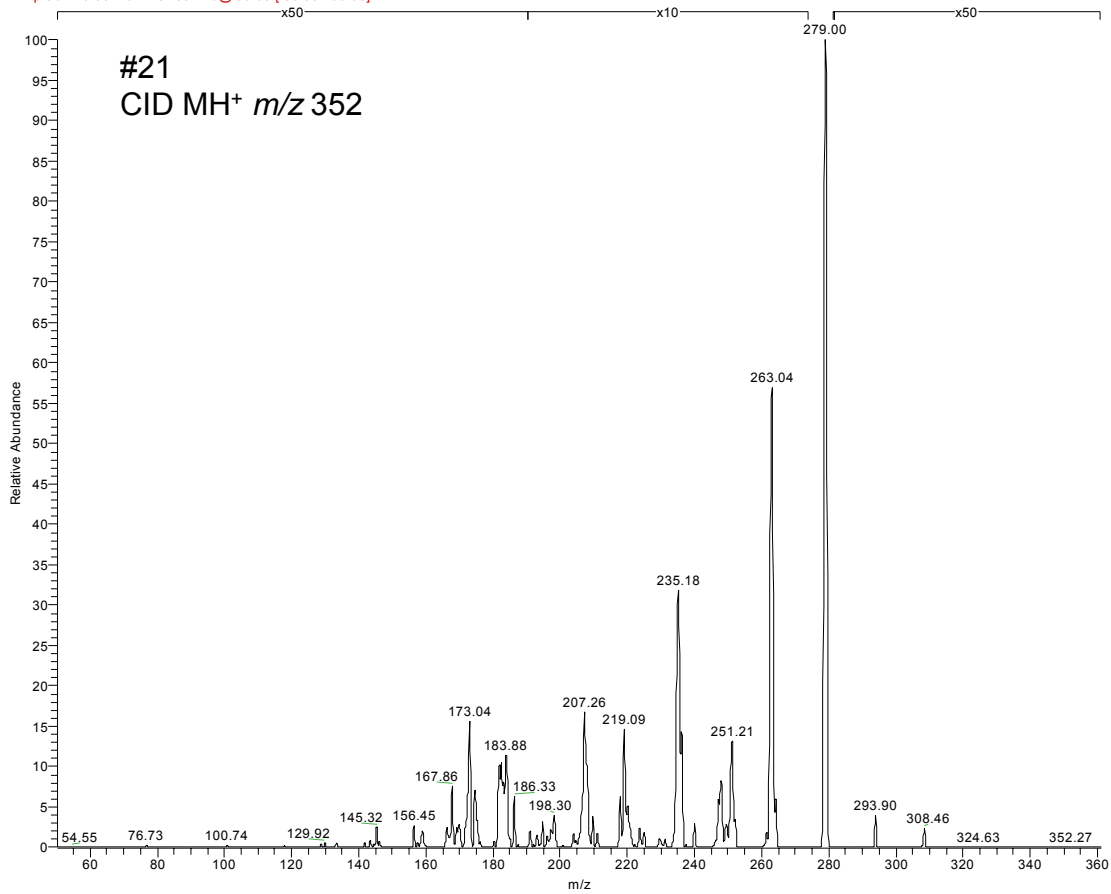


NL: 8.22E6
m/z= 369.50-370.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
25_080822195247

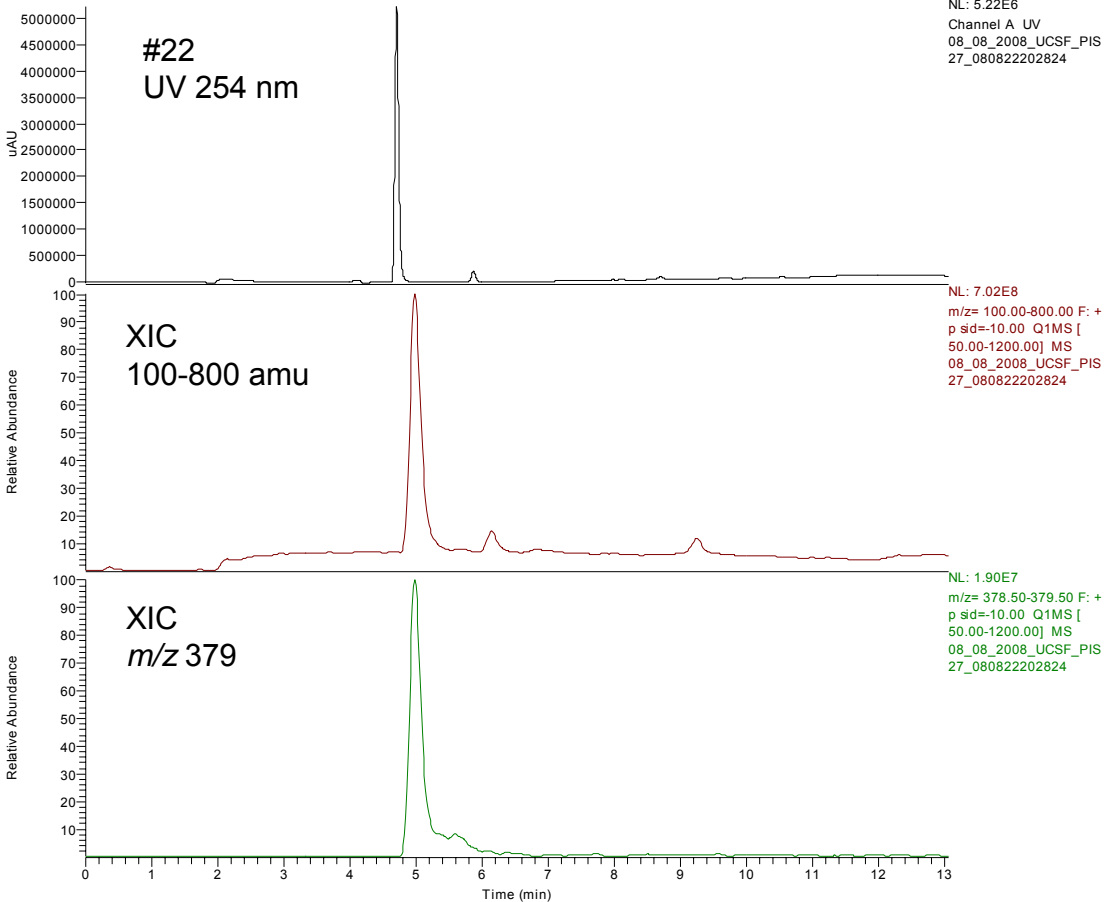


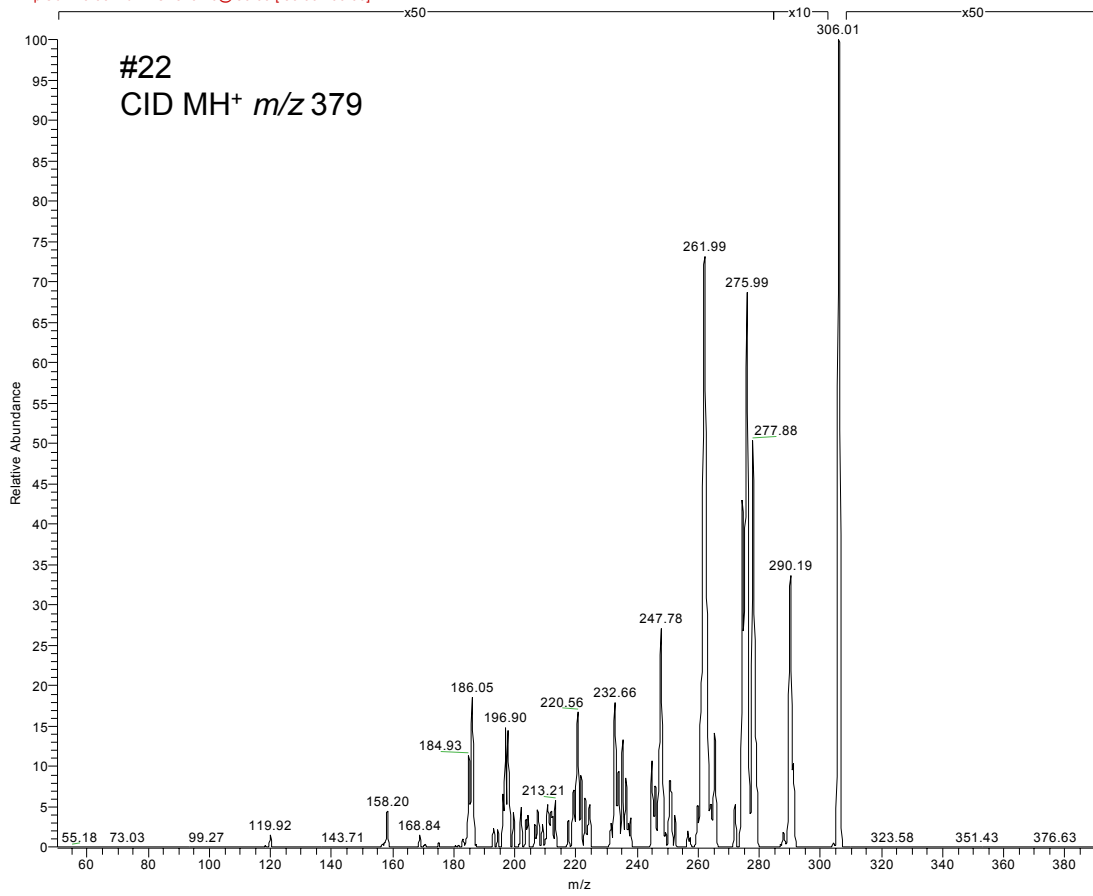
RT: 0.00 - 13.04 SM: 15G





RT: 0.00 - 13.04 SM: 15G

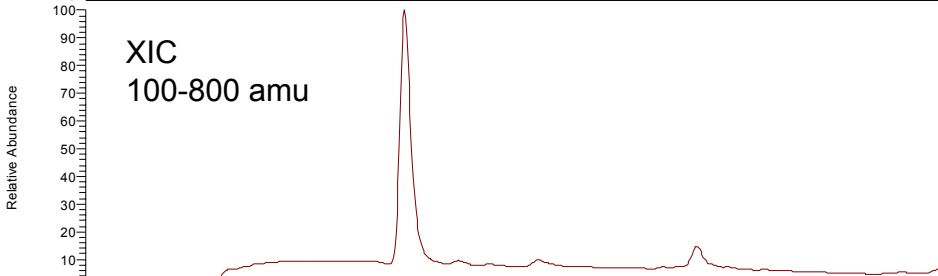




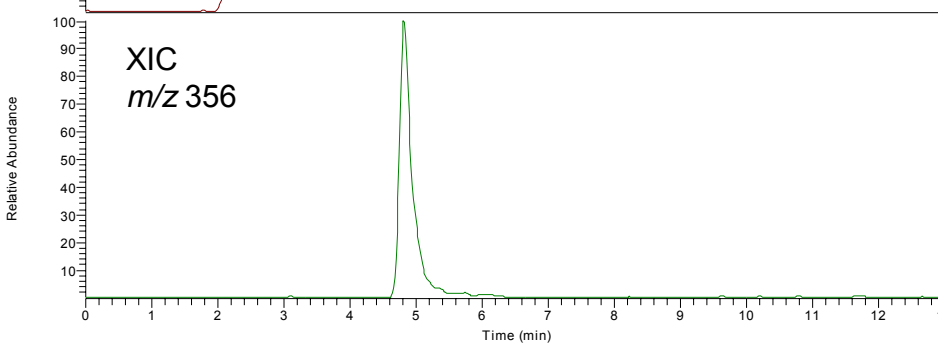
RT: 0.00 - 13.04 SM: 15G



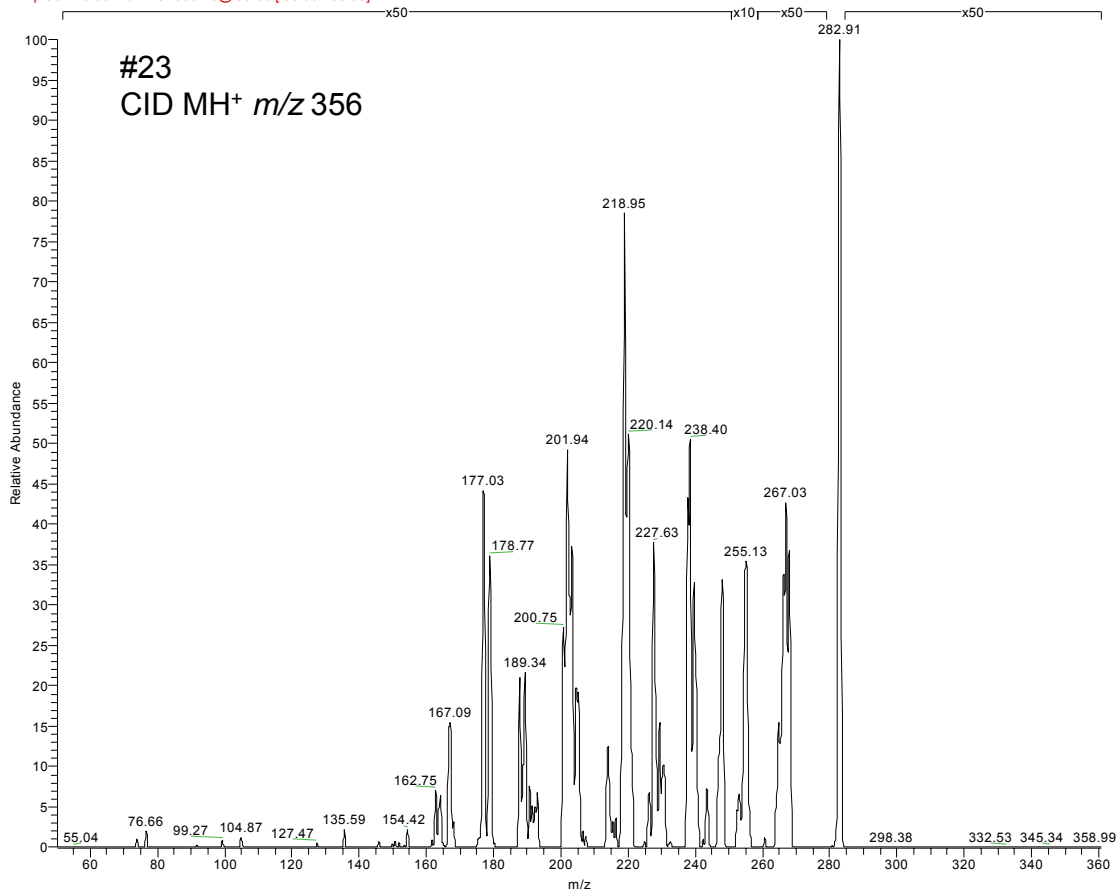
NL: 2.81E6
Channel A UV
08_08_2008_UCSF_PIS
28_080822204608



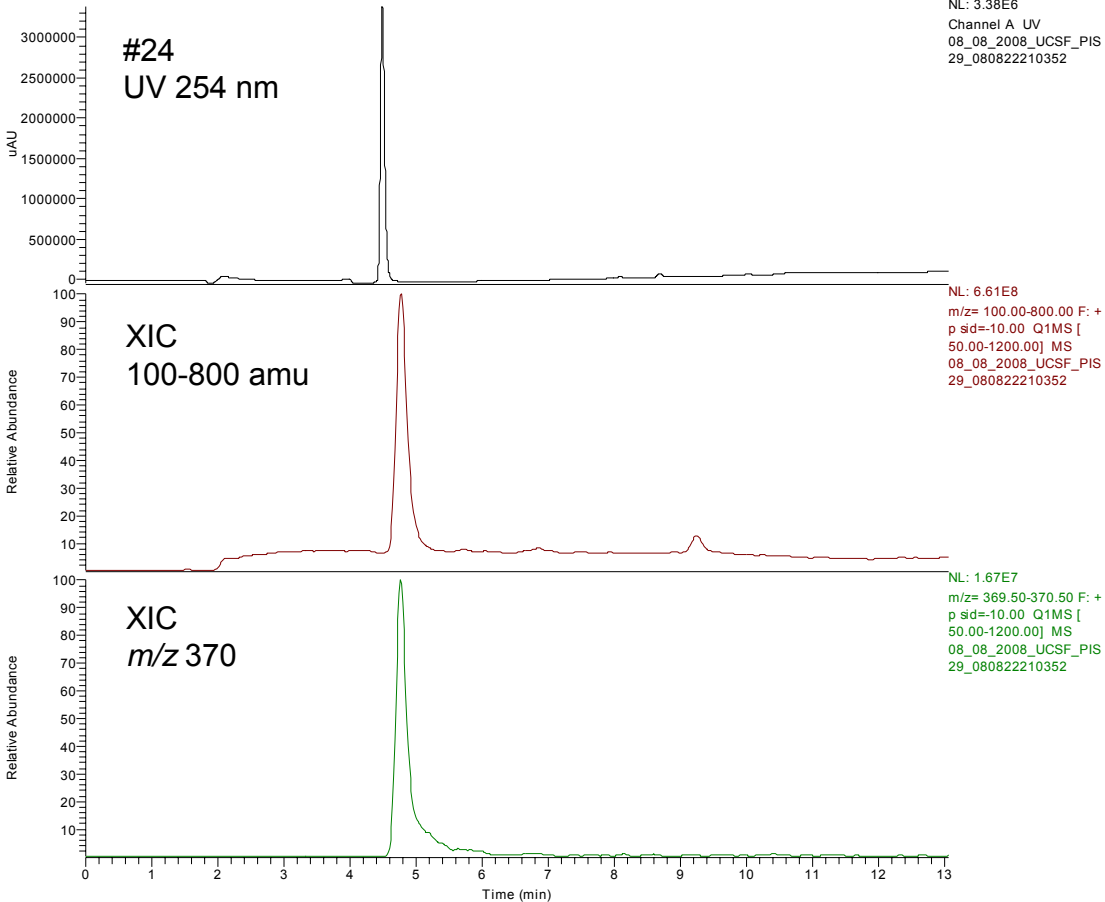
NL: 5.67E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
28_080822204608

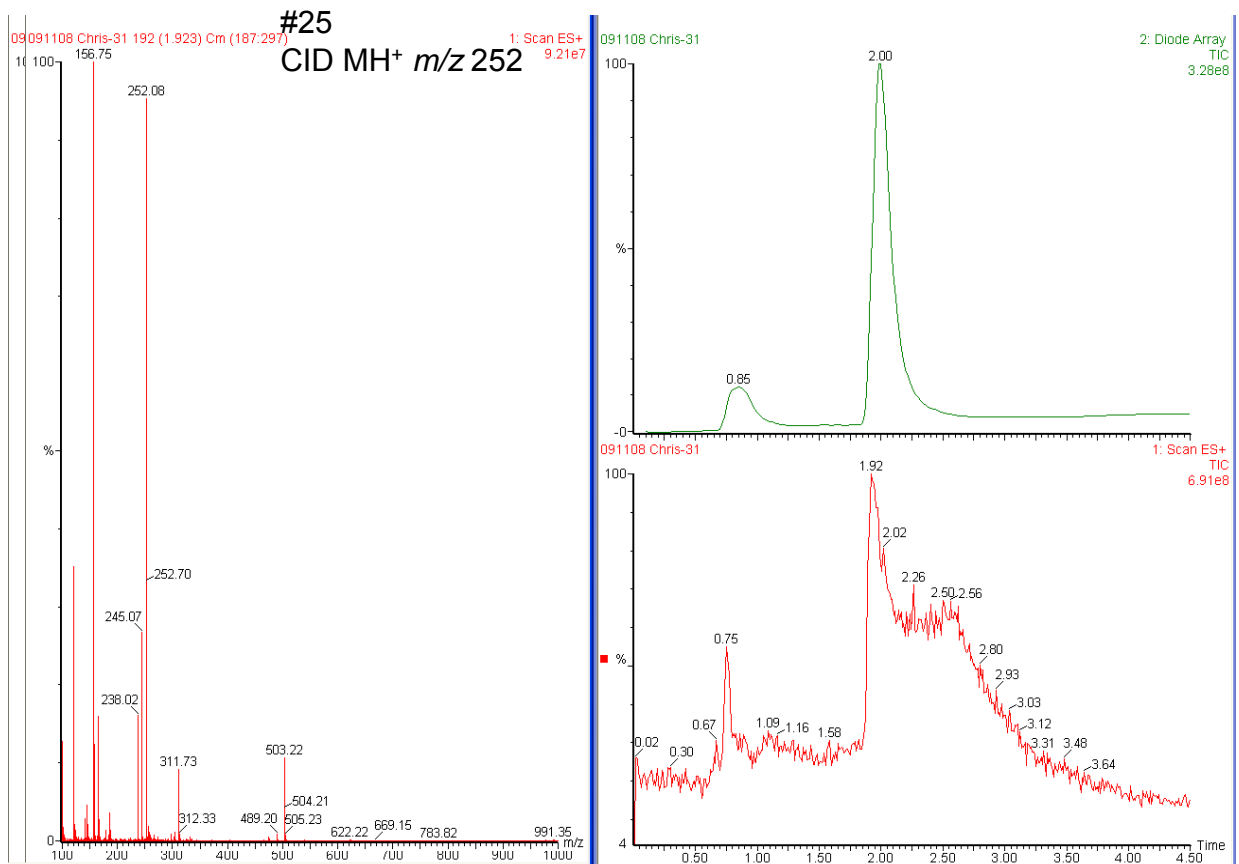
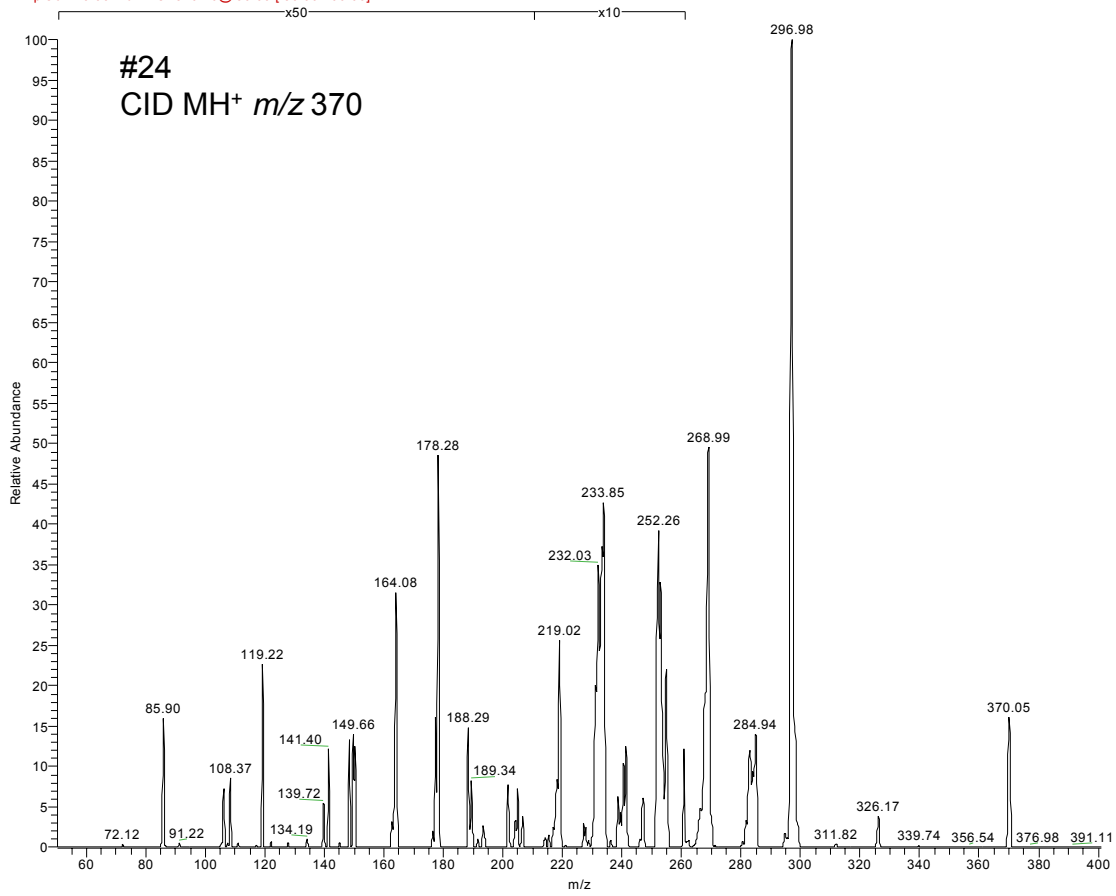


NL: 1.74E7
m/z= 355.50-356.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
28_080822204608

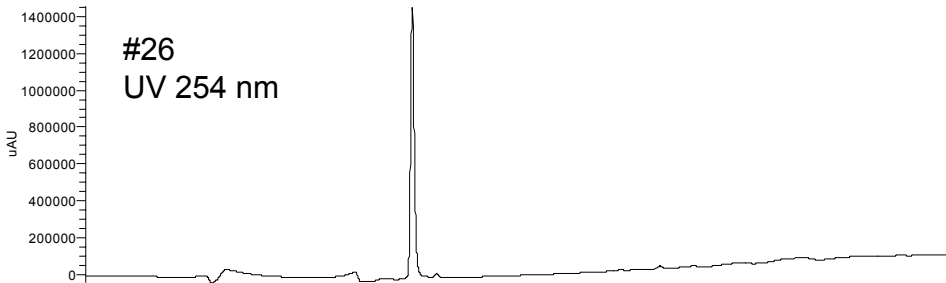


RT: 0.00 - 13.04 SM: 15G

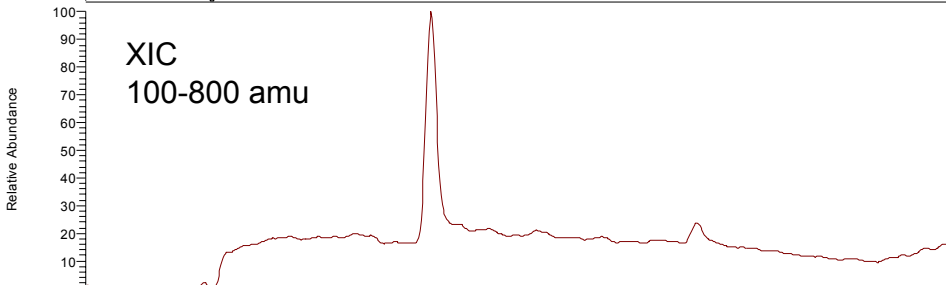




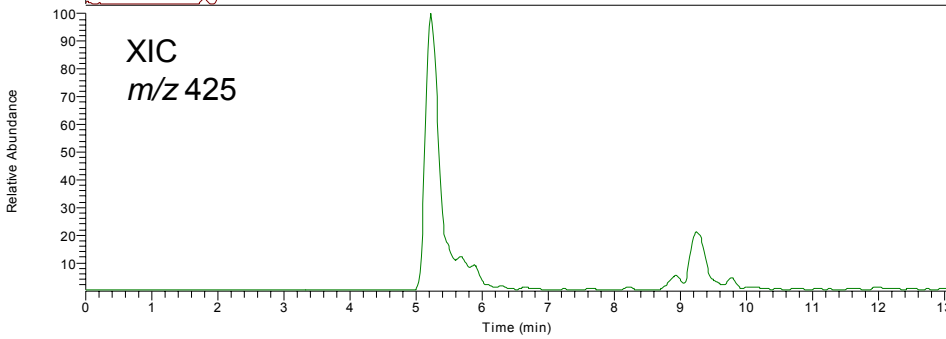
RT: 0.00 - 13.04 SM: 15G



NL: 1.45E6
Channel A UV
08_08_2008_UCSF_PIS
32_080822215713

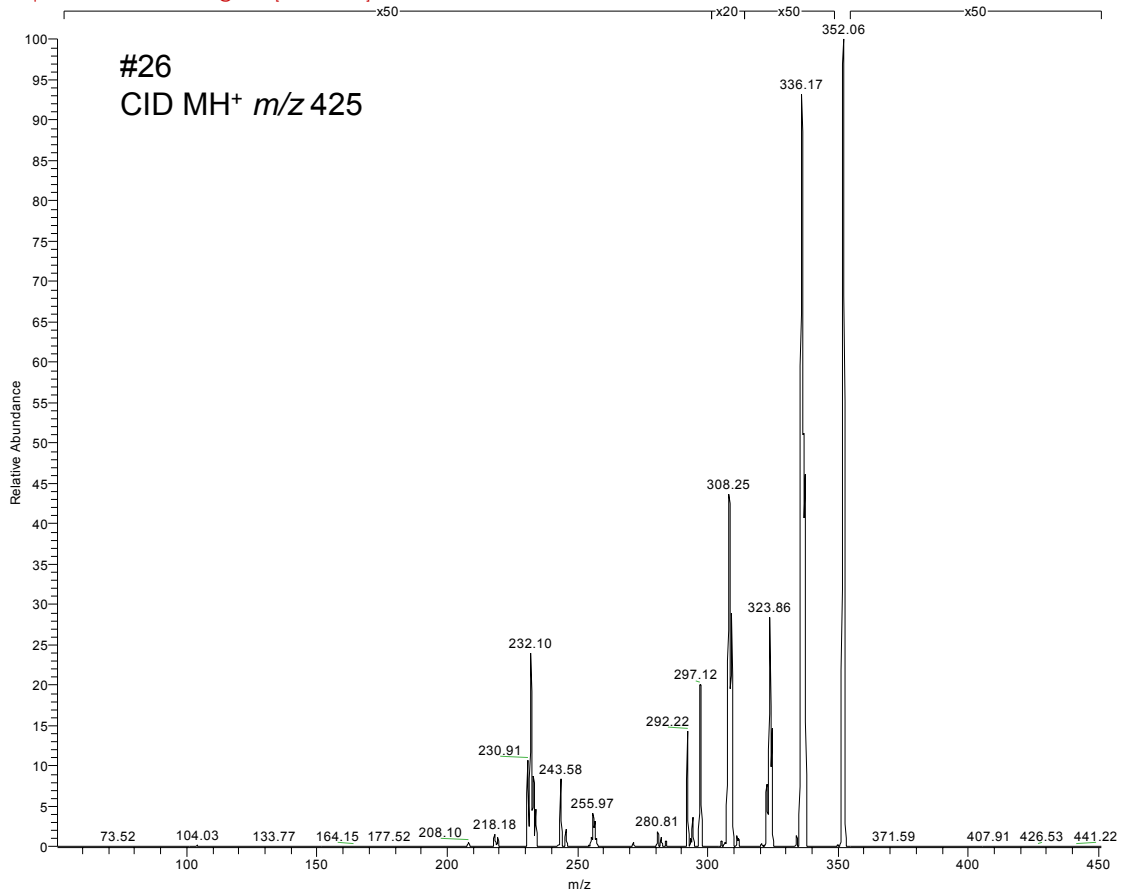


NL: 2.78E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
32_080822215713

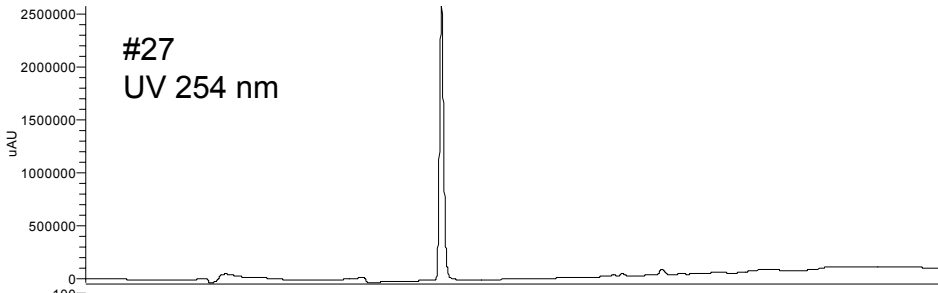


NL: 5.22E6
m/z= 424.50-425.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
32_080822215713

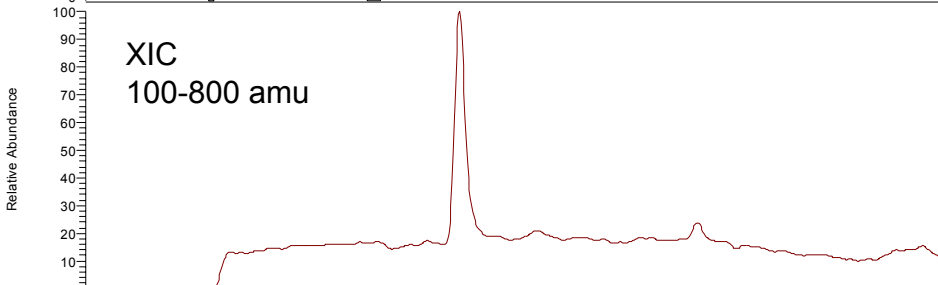
08_08_2008_UCSF_PIS32_080821225118 #345-357 RT: 5.11-5.29 AV: 13 SB: 520 0.84-4.37, 5.87-10.02 SM: 15G NL: 1.94E6
F: + p sid=-10.00 Full ms2 425.10@-30.00 [50.00-700.00]



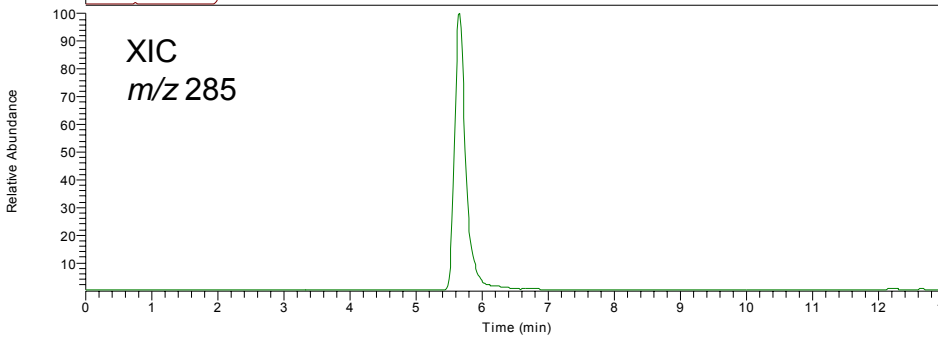
RT: 0.00 - 13.04 SM: 15G



NL: 2.57E6
Channel A UV
08_08_2008_UCSF_PIS
37_080822223243

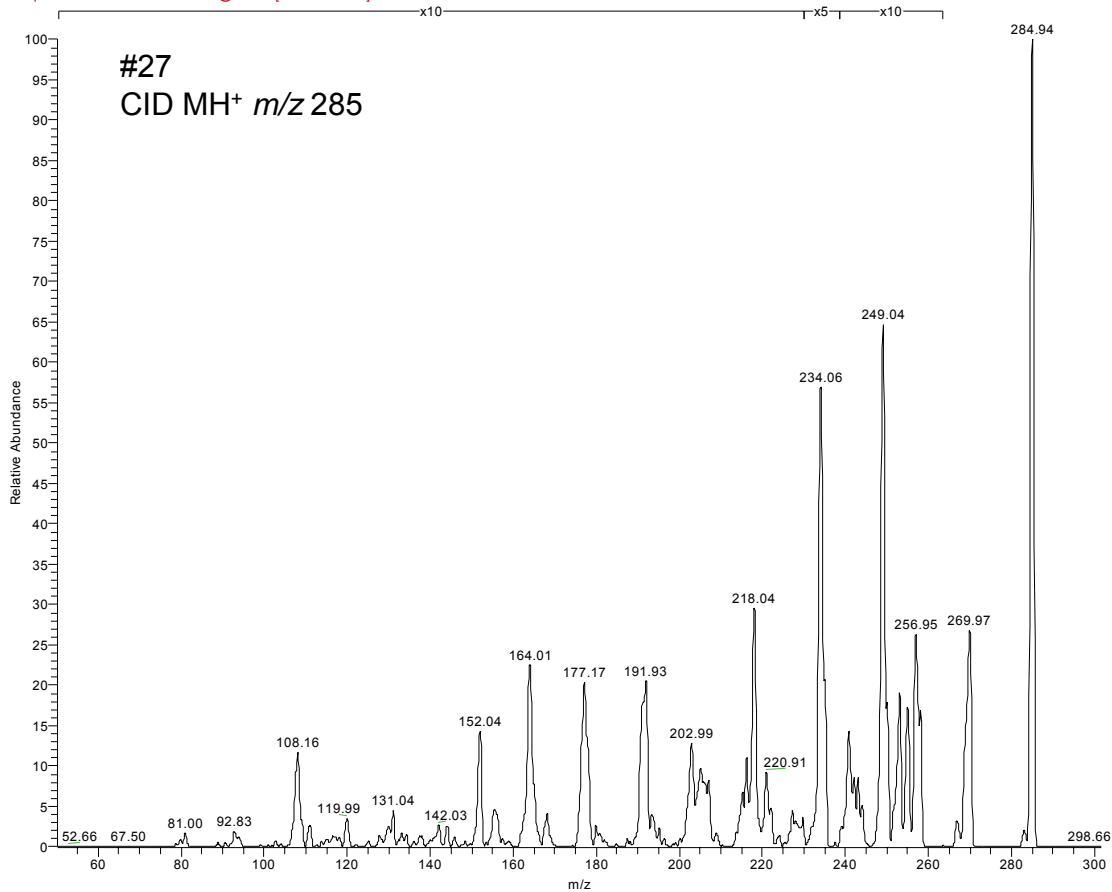


NL: 3.32E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
37_080822223243

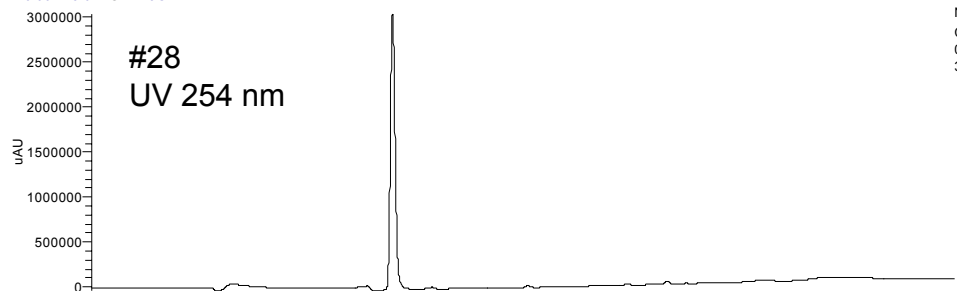


NL: 1.67E8
m/z= 284.50-285.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
37_080822223243

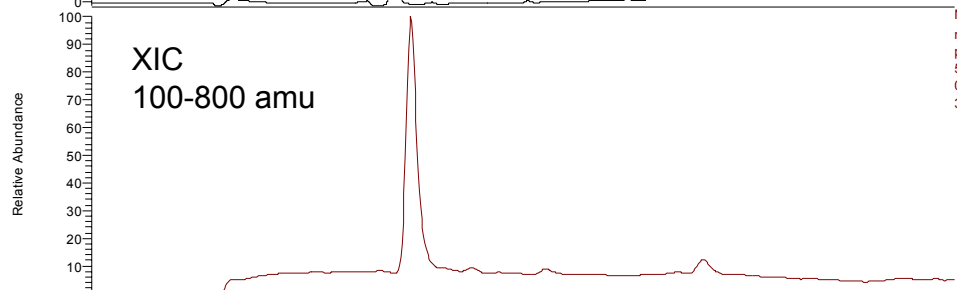
08_08_2008_UCSF_PIS37_080821232653 #371-394 RT: 5.50-5.84 AV: 24 SB: 520 0.84-4.37, 5.87-10.02 SM: 15G NL: 9.71E6
F: + p sid=-10.00 Full ms2 285.10@-30.00 [50.00-700.00]



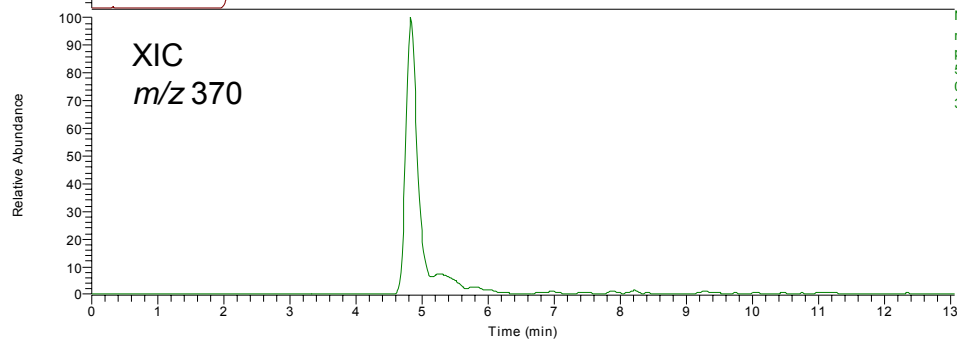
RT: 0.00 - 13.04 SM: 15G



NL: 3.03E6
Channel A UV
08_08_2008_UCSF_PIS
31_080822213928

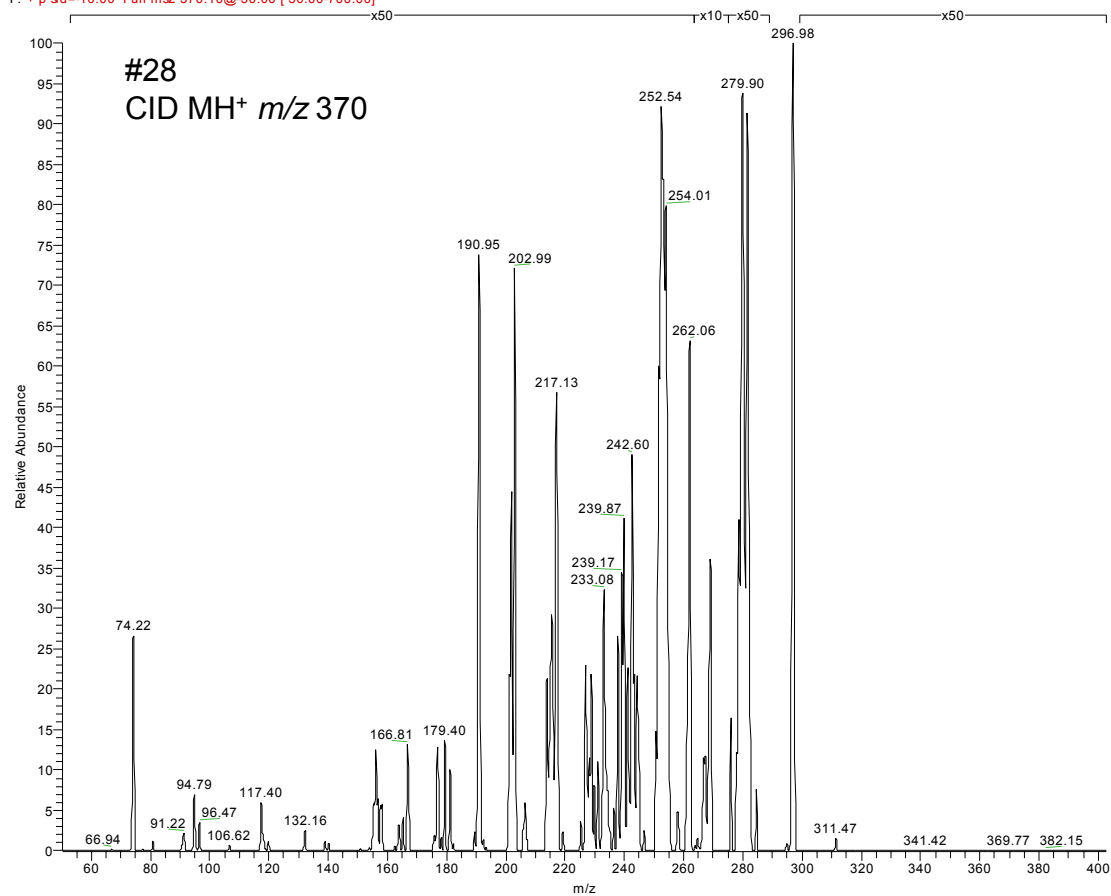


NL: 6.38E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
31_080822213928

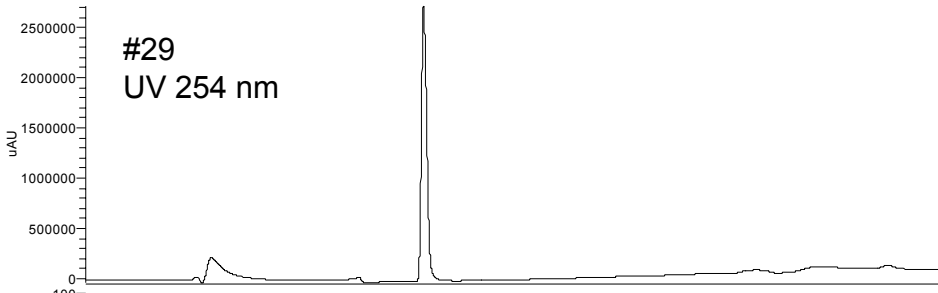


NL: 1.51E7
m/z= 369.50-370.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
31_080822213928

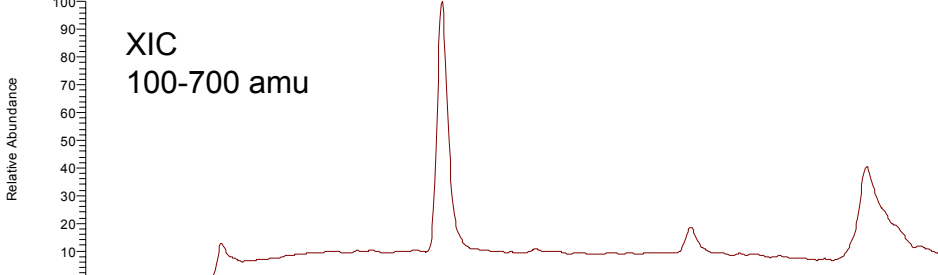
08_08_2008_UCSF_PIS31_080821223330 #310-325 RT: 4.59-4.81 AV: 16 SB: 520 0.84-4.37, 5.86-10.02 SM: 15G NL: 3.12E6
F: + p sid=-10.00 Full ms2 370.10@-30.00 [50.00-700.00]



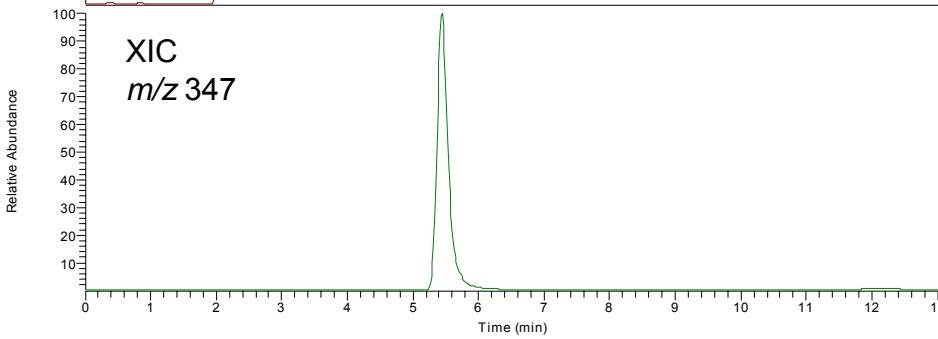
RT: 0.00 - 13.04 SM: 15G



NL: 2.71E6
Channel A UV
08_22_2008_UCSF_PURI
TY_A17_080824155413

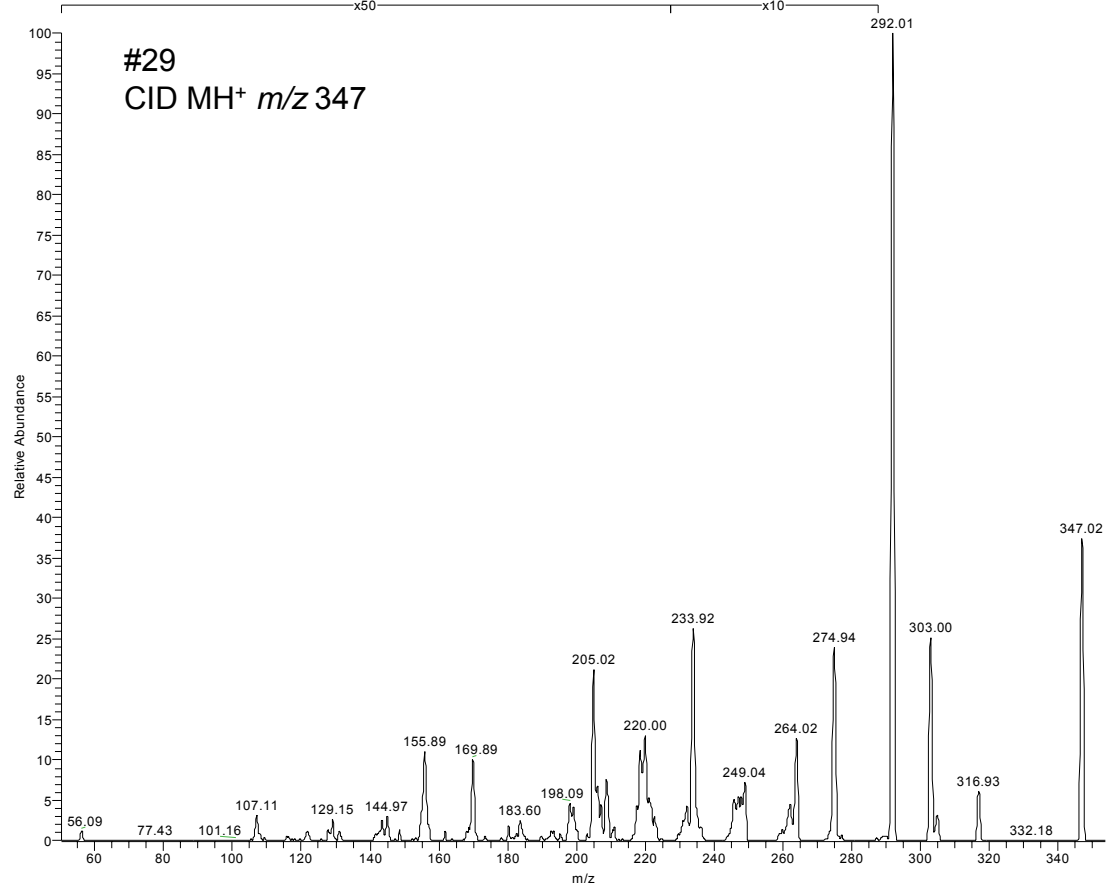


NL: 4.62E8
m/z= 100.00-800.00 F: +
p sd=-10.00 Q1MS [
50.00-1200.00] MS
08_22_2008_UCSF_PURI
TY_A17_080824155413

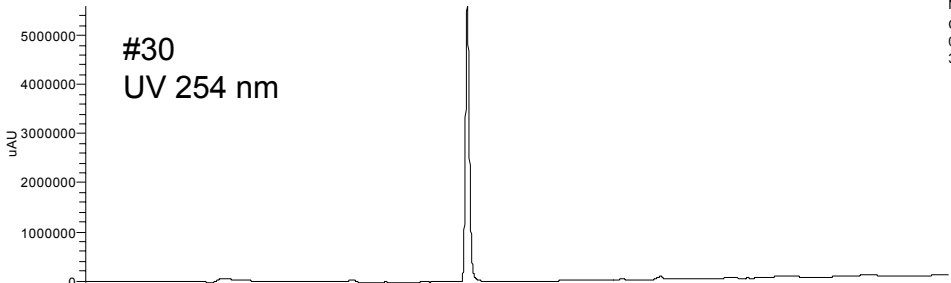


NL: 3.15E8
m/z= 346.50-347.50 F: +
p sd=-10.00 Q1MS [
50.00-1200.00] MS
08_22_2008_UCSF_PURI
TY_A17_080824155413

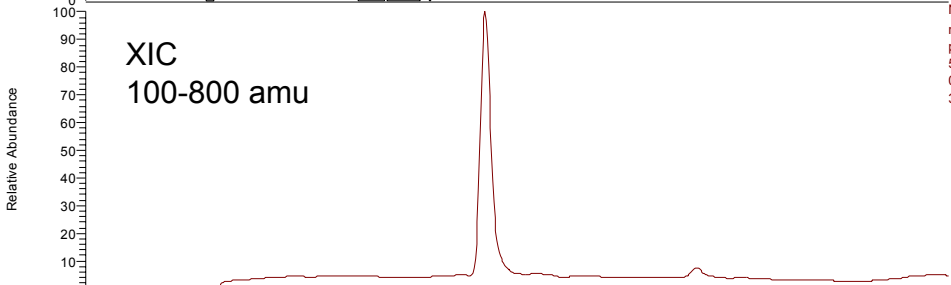
08_22_2008_UCSF_PURITY_A17_080824230046 #359-383 RT: 5.32-5.67 AV: 25 SB: 2 0.01, 0.01 SM: 15G NL: 2.76E7
F: + p sd=-10.00 Full ms2 347.10@-30.00 [50.00-700.00]



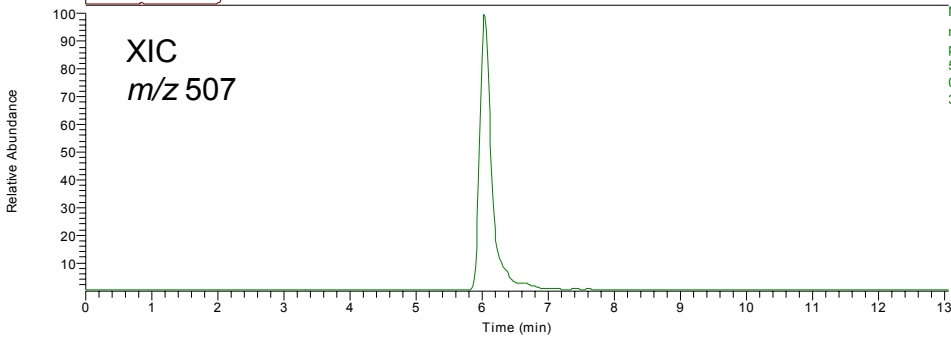
RT: 0.00 - 13.04 SM: 15G



NL: 5.59E6
Channel A UV
08_08_2008_UCSF_PIS
39_080822230814

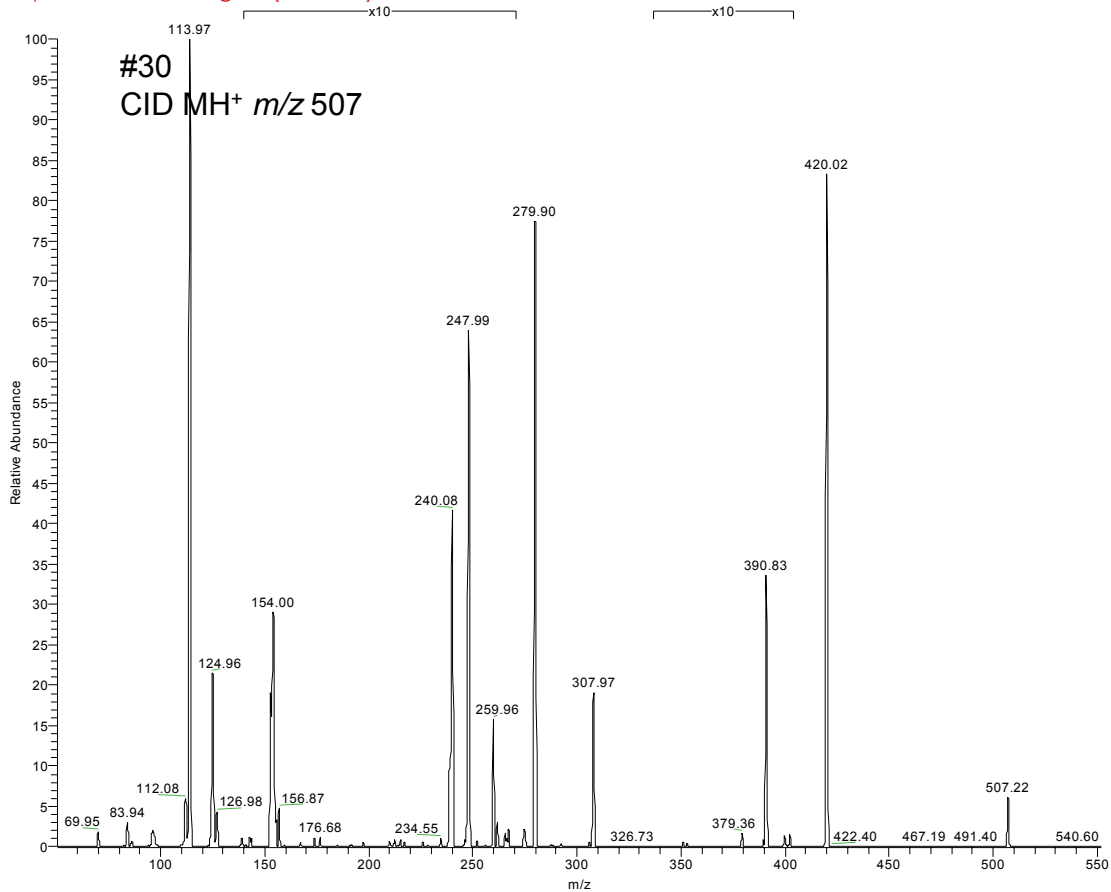


NL: 1.04E9
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
39_080822230814

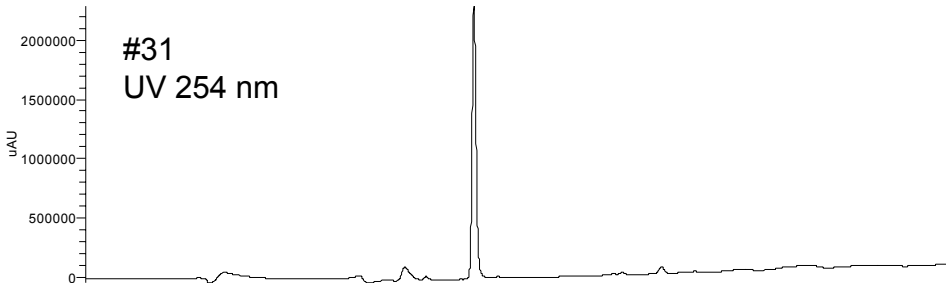


NL: 7.80E7
m/z= 506.50-507.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
39_080822230814

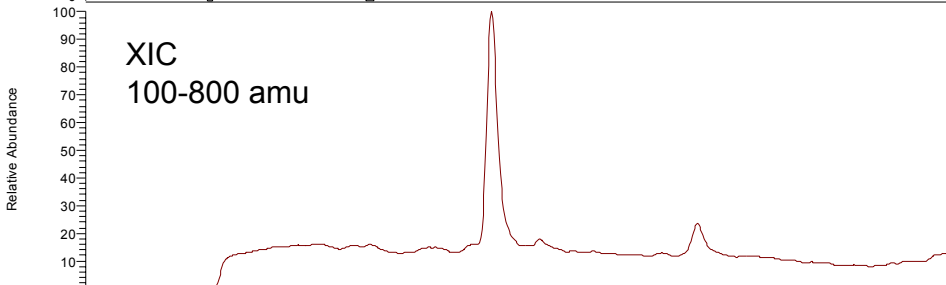
08_08_2008_UCSF_PIS39_08082200225 #397-413 RT: 5.88-6.12 AV: 17 SB: 520 0.84-4.37, 5.86-10.02 SM: 15G NL: 3.06E6
F: + p sid=-10.00 Full ms2 507.10@-30.00 [50.00-700.00]



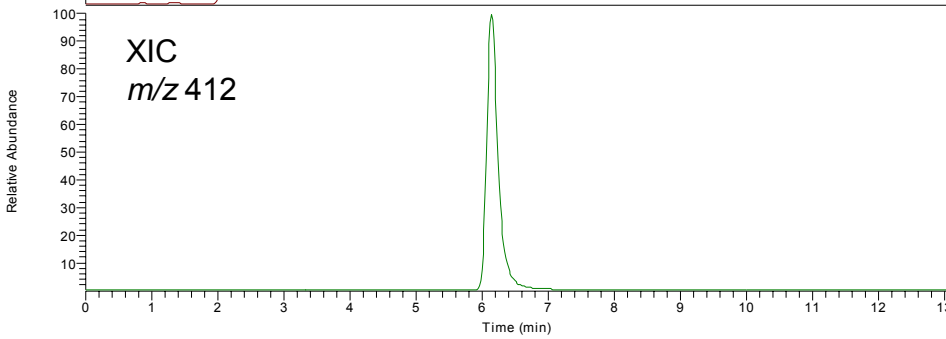
RT: 0.00 - 13.04 SM: 15G



NL: 2.28E6
Channel A UV
08_08_2008_UCSF_PIS
40_080822232600

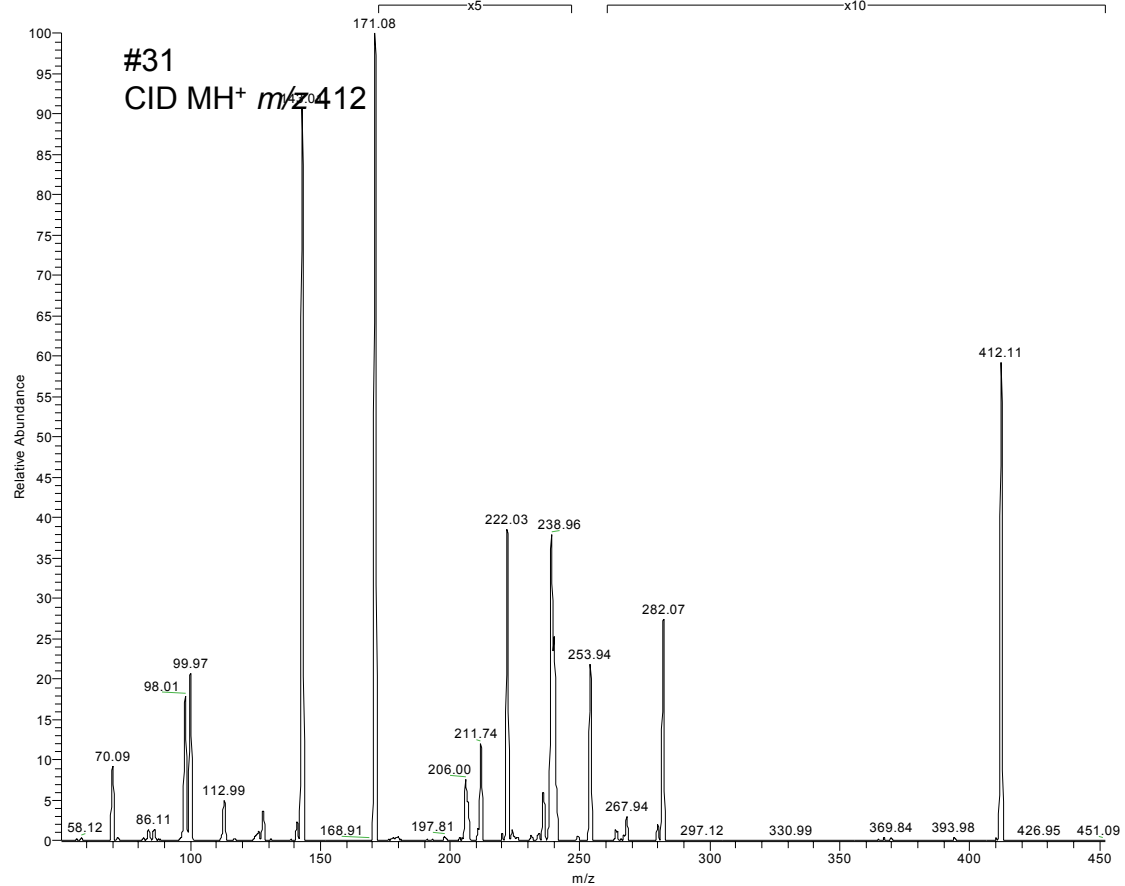


NL: 3.21E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
40_080822232600

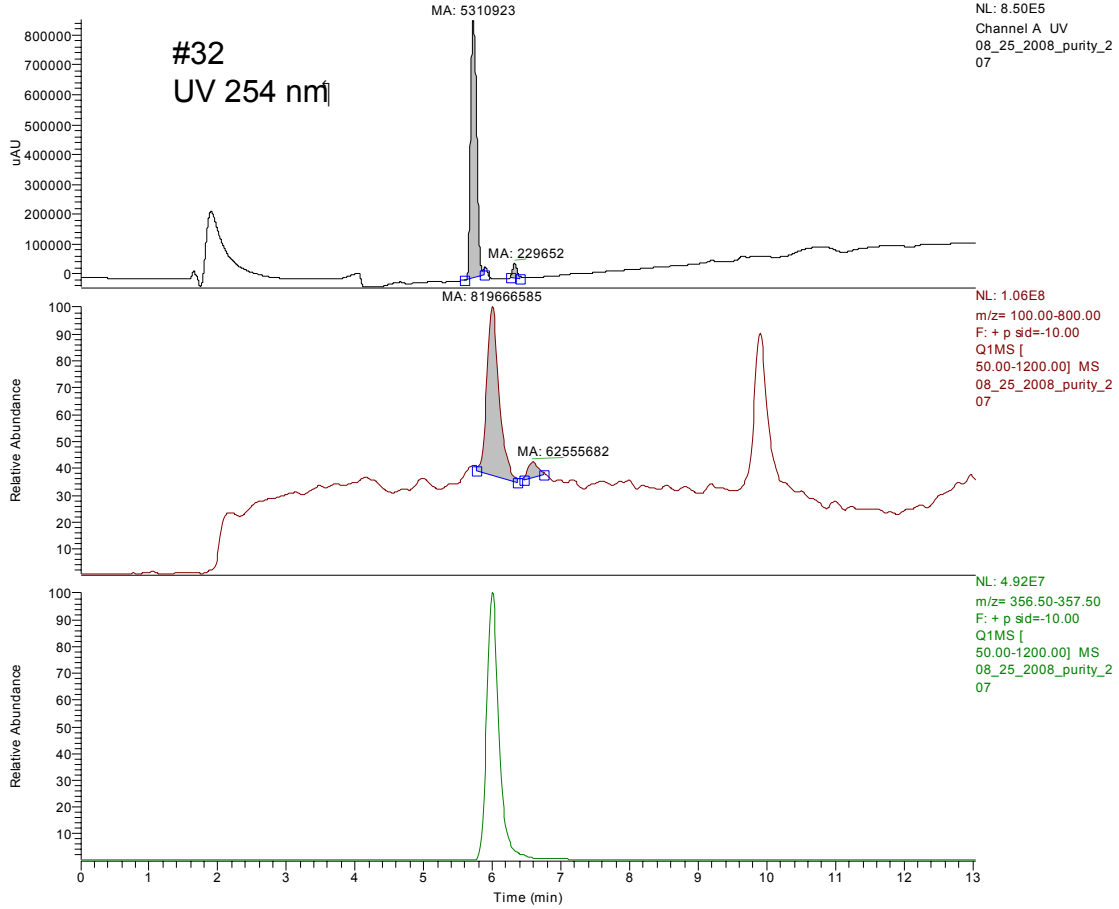


NL: 1.86E8
m/z= 411.50-412.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
40_080822232600

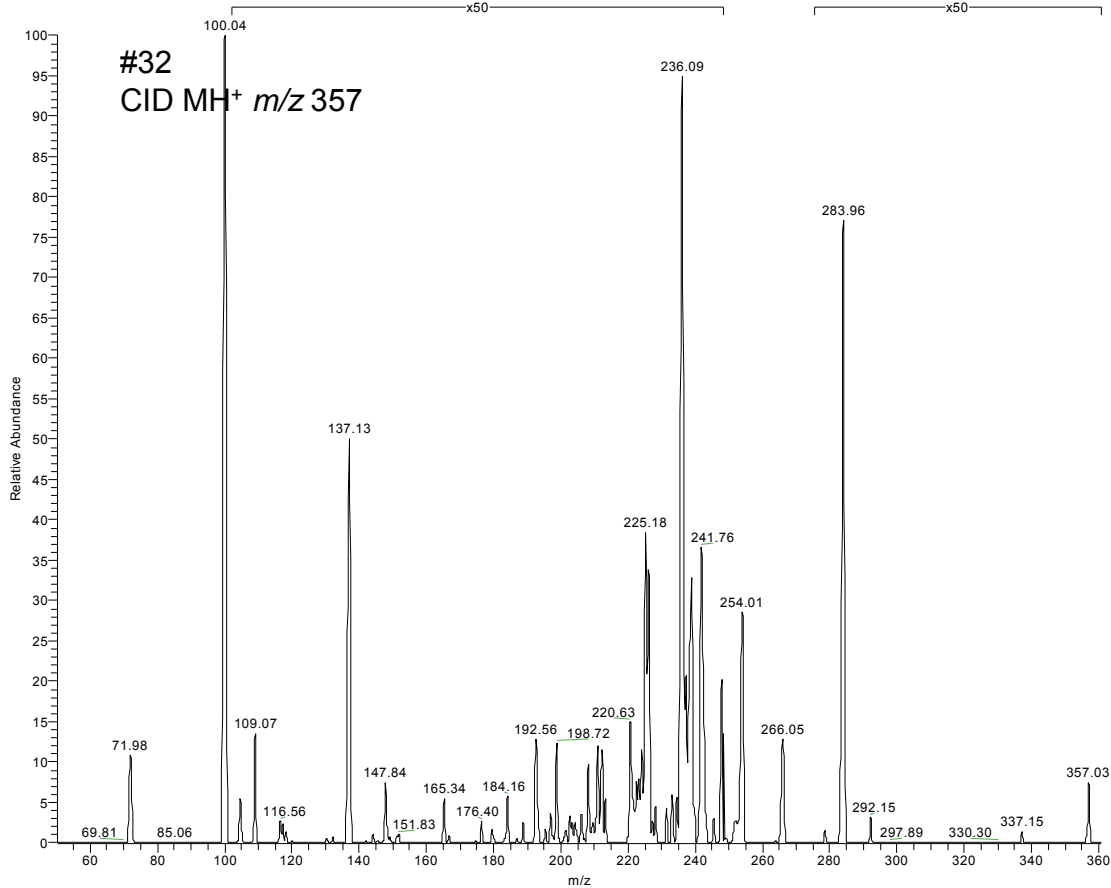
08_08_2008_UCSF_PIS40_080822002013 #400-416 RT: 5.92-6.16 AV: 17 SB: 520 0.84-4.37, 5.86-10.01 SM: 15G NL: 8.31E6
F: + p sid=-10.00 Full ms2 412.10@-30.00 [50.00-700.00]



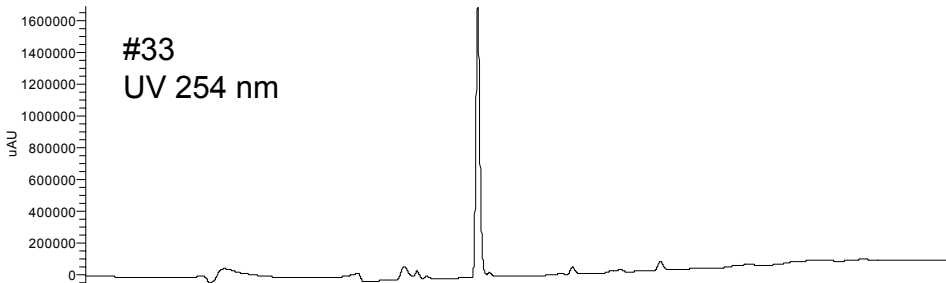
RT: 0.00 - 13.04 SM: 15G



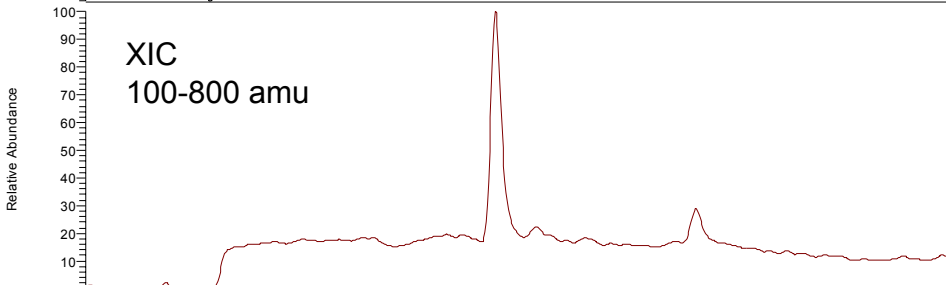
08_22_2008_UCSF_PURITY_A18_080824231833 #394-411 RT: 5.84-6.09 AV: 18 SB: 2 0.01, 0.01 SM: 15G NL: 4.24E6
F: + p sd=-10.00 Full ms2 357.10@-30.00 [50.00-700.00]



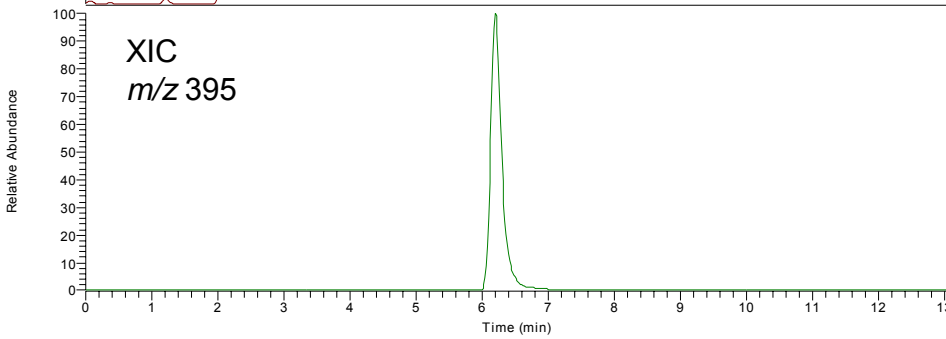
RT: 0.00 - 13.04 SM: 15G



NL: 1.69E6
Channel A UV
08_08_2008_UCSF_PIS
51_080823014810

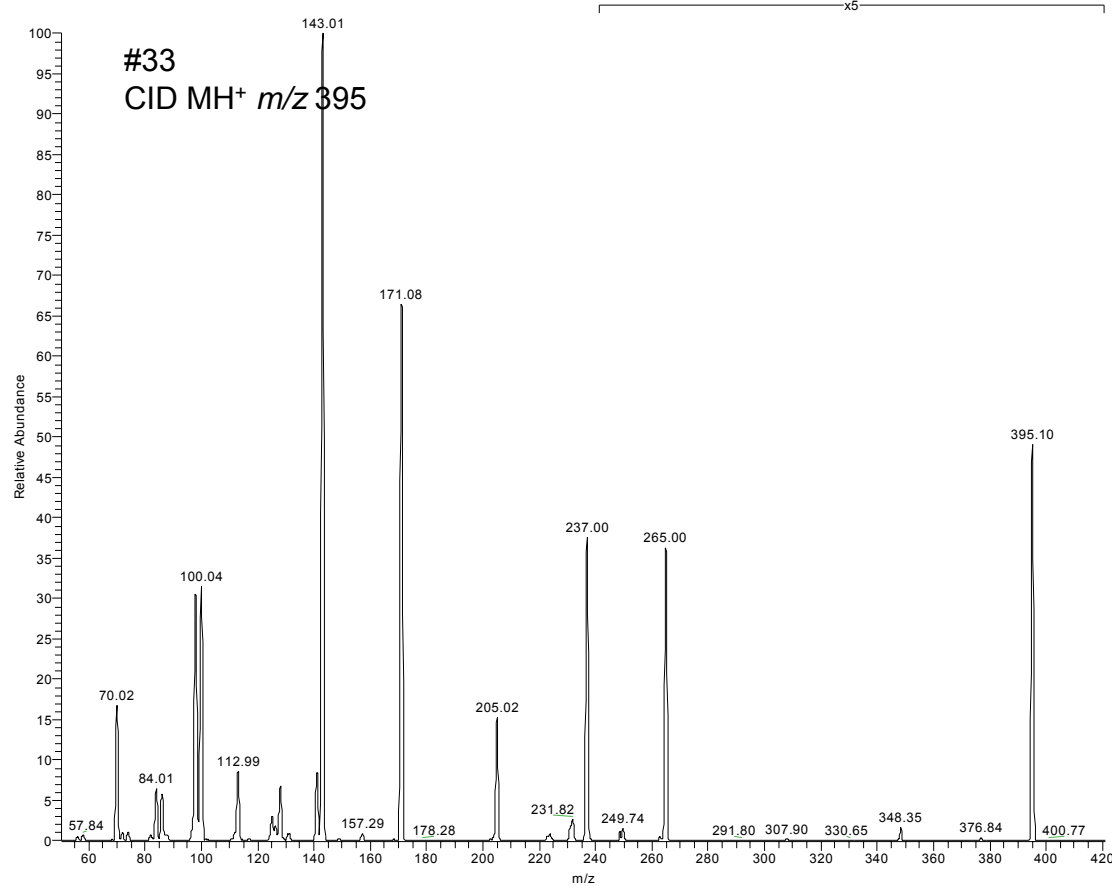


NL: 2.58E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
51_080823014810

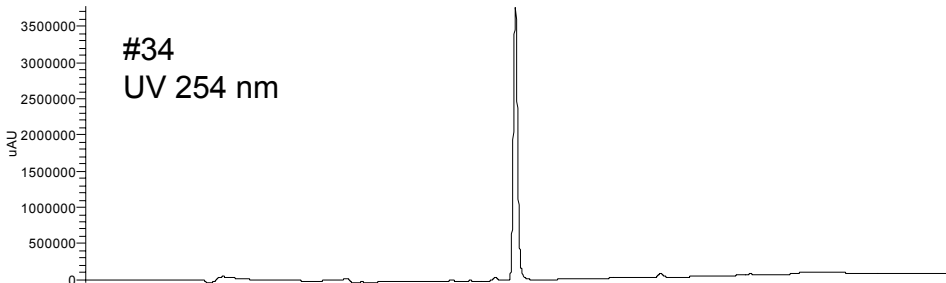


NL: 1.56E8
m/z= 394.50-395.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
51_080823014810

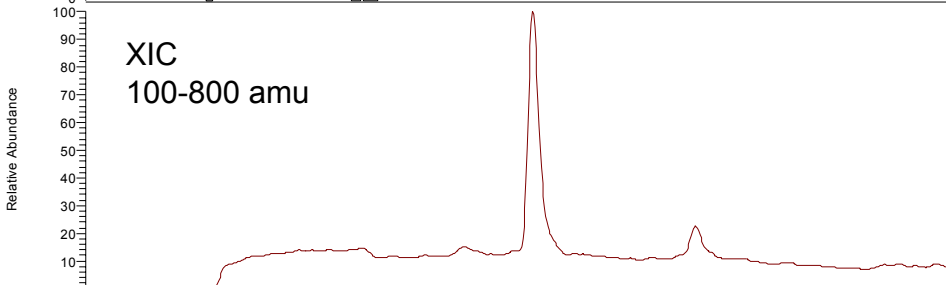
08_08_2008_UCSF_PIS51_080822024217 #410-428 RT: 6.07-6.34 AV: 19 SB: 520 0.84-4.37, 5.87-10.02 SM: 15G NL: 4.11E6
F: + p sid=-10.00 Full ms2 395.10@-30.00 [50.00-700.00]



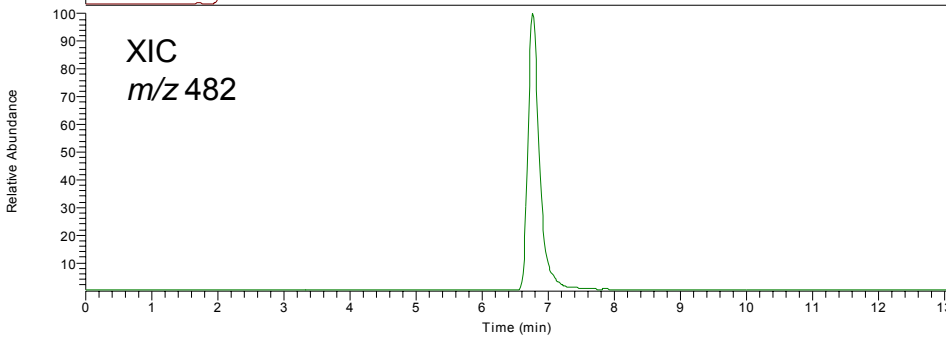
RT: 0.00 - 13.04 SM: 15G



NL: 3.77E6
Channel A UV
08_08_2008_UCSF_PIS
41_080822234348

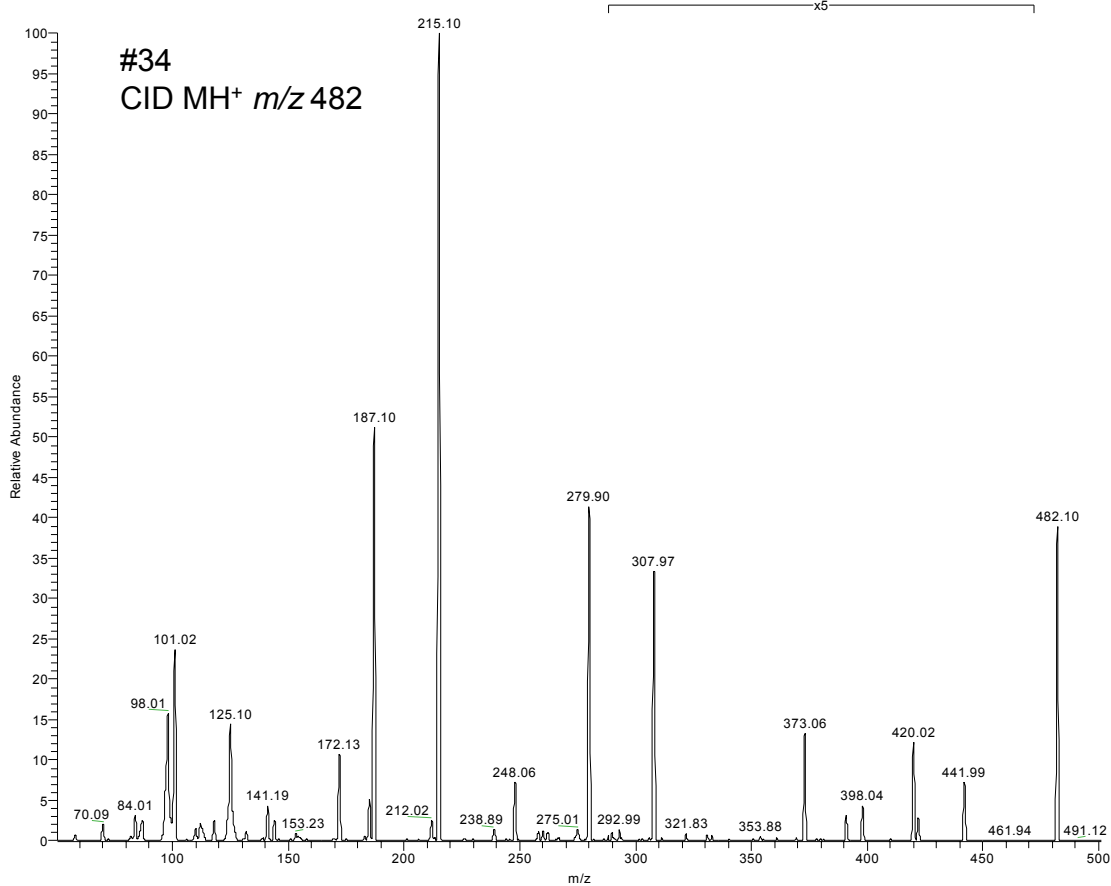


NL: 3.63E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
41_080822234348

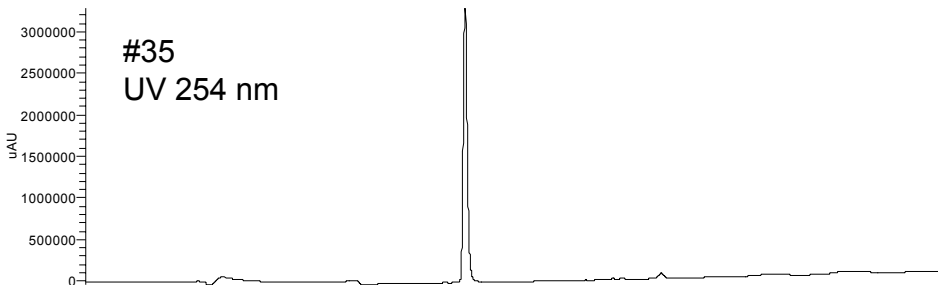


NL: 2.12E8
m/z= 481.50-482.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
41_080822234348

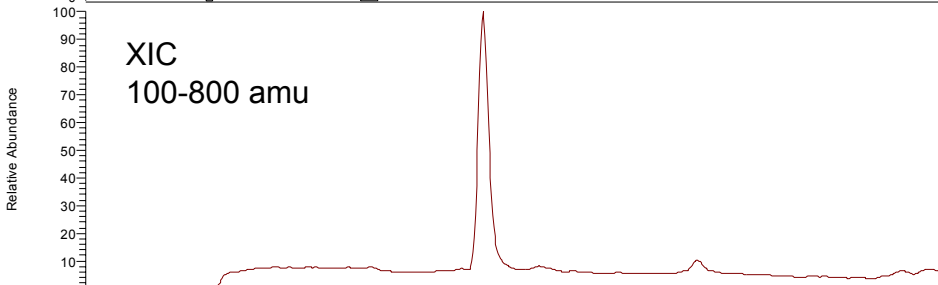
08_08_2008_UCSF_PIS41_080822003801 #442-465 RT: 6.55-6.89 AV: 24 SB: 520 0.84-4.37 , 5.87-10.02 SM: 15G NL: 6.16E6
F: + p sid=-10.00 Full ms2 482.10@-30.00 [50.00-700.00]



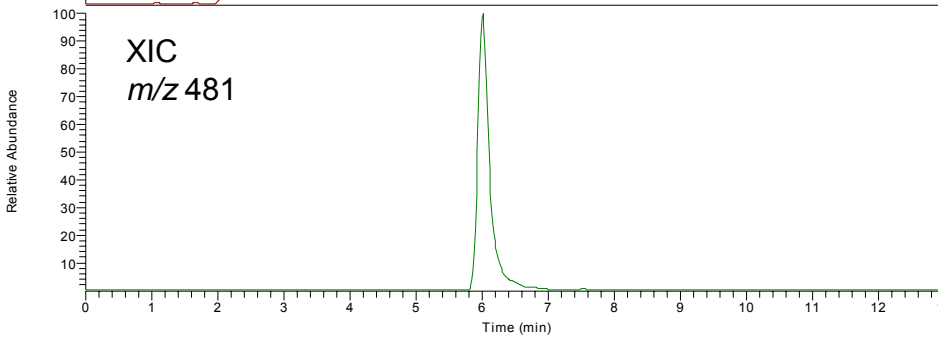
RT: 0.00 - 13.04 SM: 15G



NL: 3.28E6
Channel A UV
08_08_2008_UCSF_PIS
43_080823001918

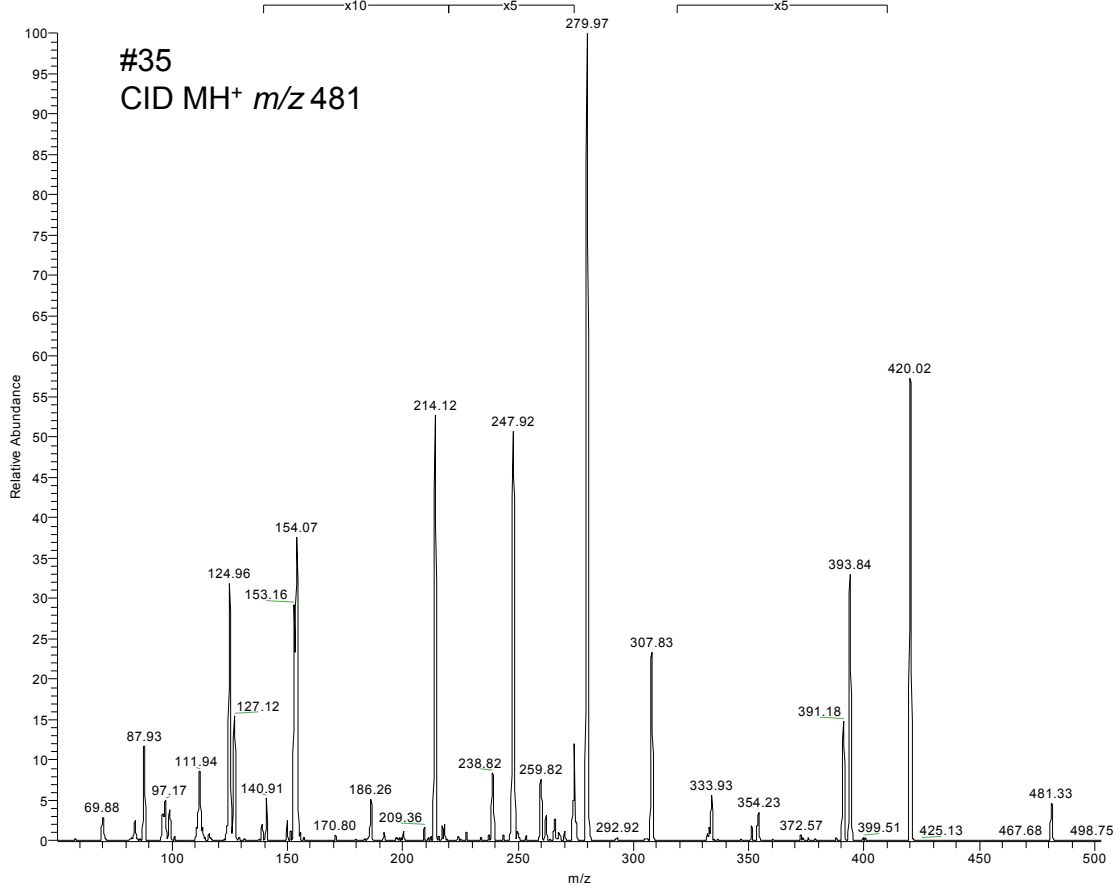


NL: 6.75E8
m/z= 100.00-800.00 F: +
p sd=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
43_080823001918



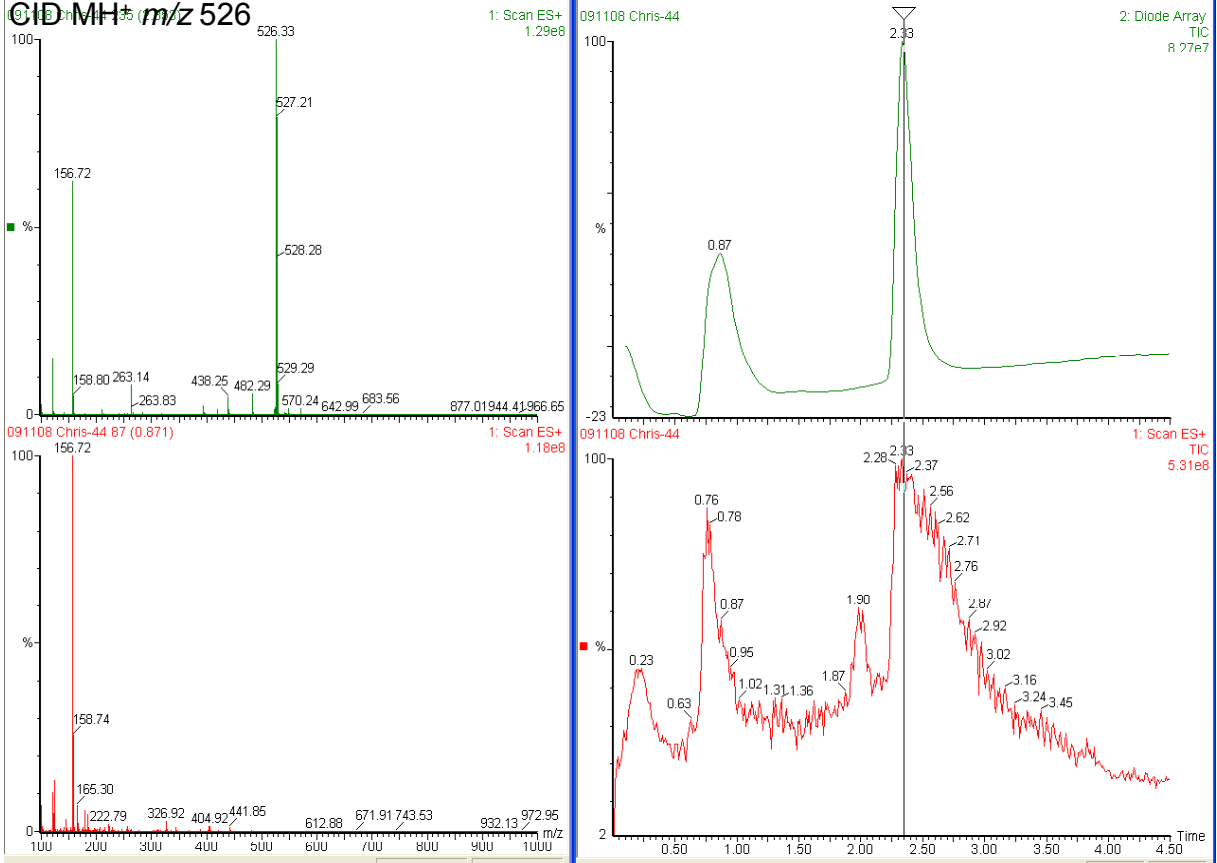
NL: 3.83E7
m/z= 480.50-481.50 F: +
p sd=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
43_080823001918

08_08_2008_UCSF_PIS43_080822011326 #396-414 RT: 5.87-6.13 AV: 19 SB: 520 0.84-4.37, 5.87-10.02 SM: 15G NL: 1.73E6
F: + p sd=-10.00 Full ms2 481.10@-30.00 [50.00-700.00]

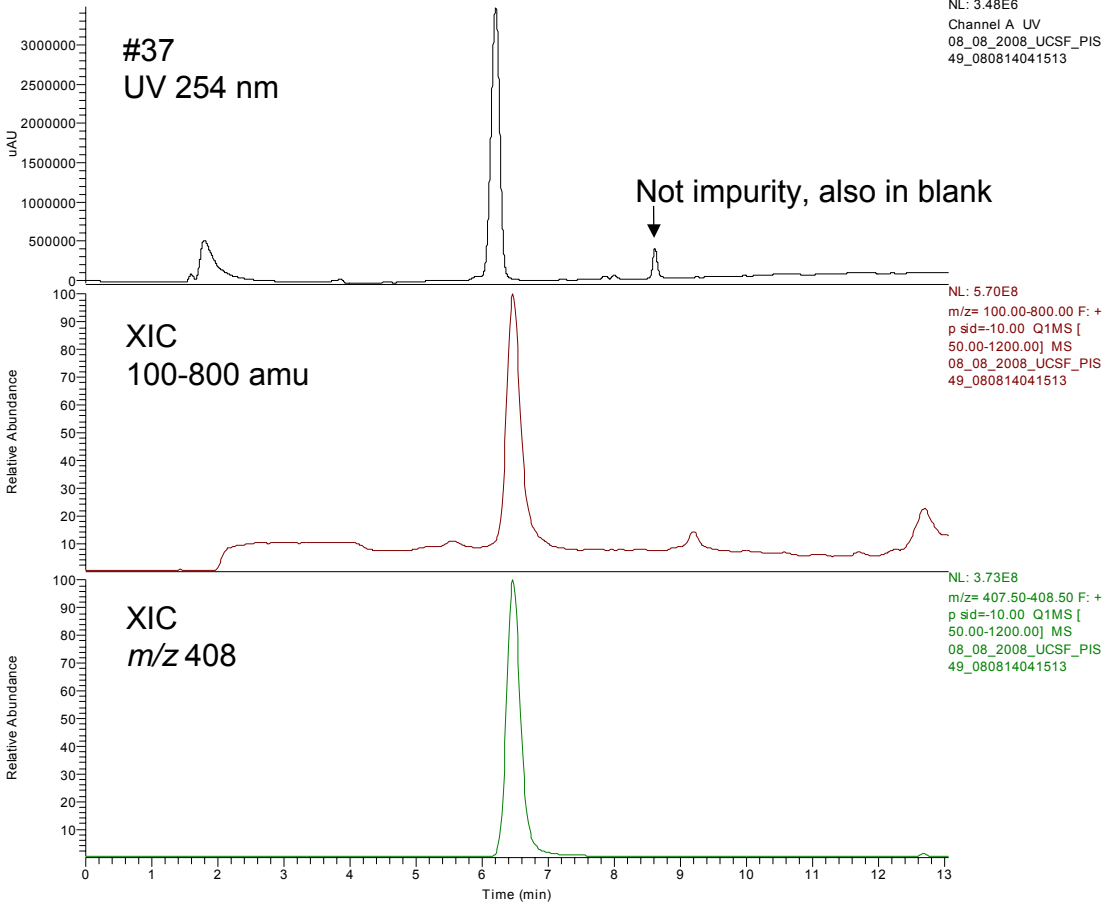


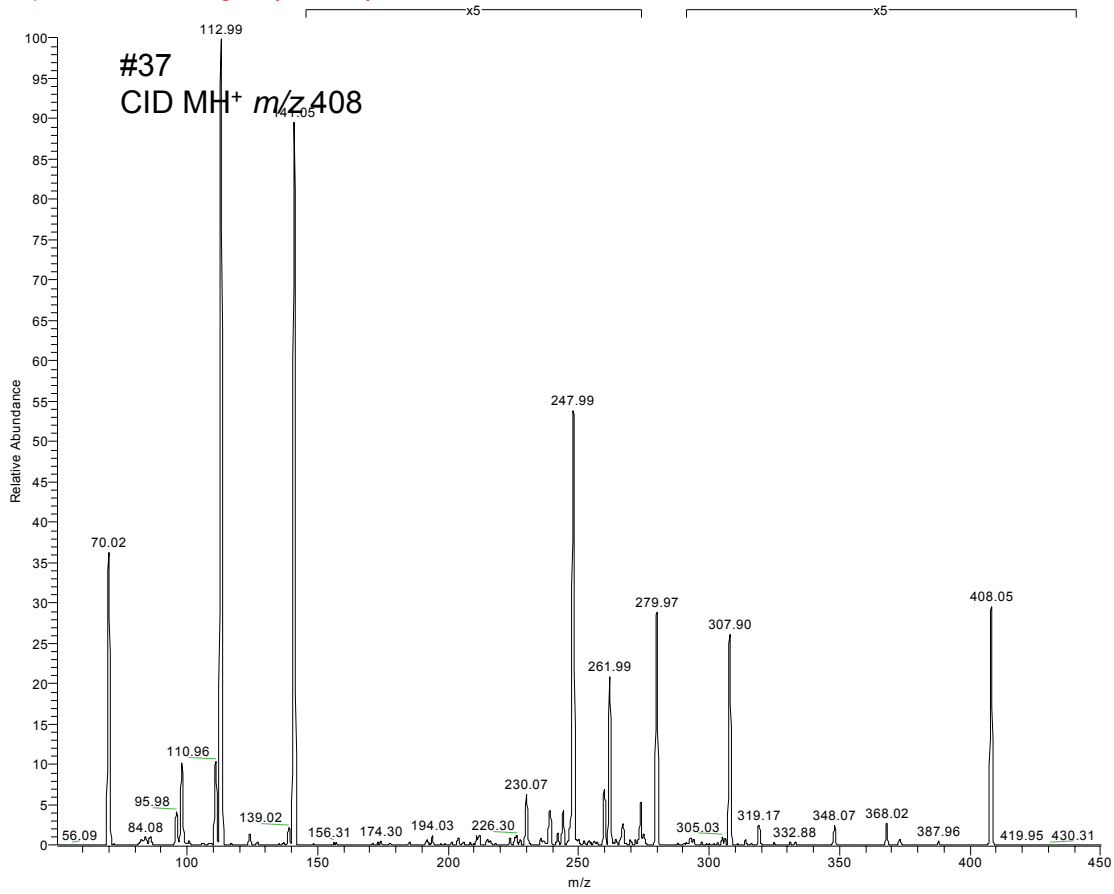
#36

GID MH+ m/z 526

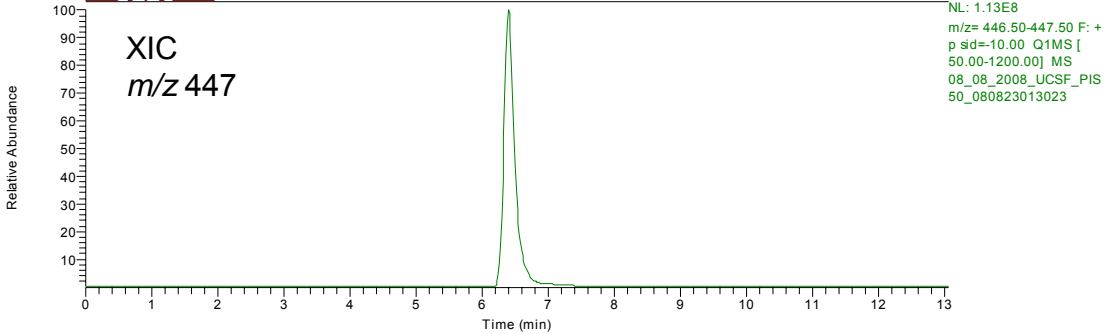
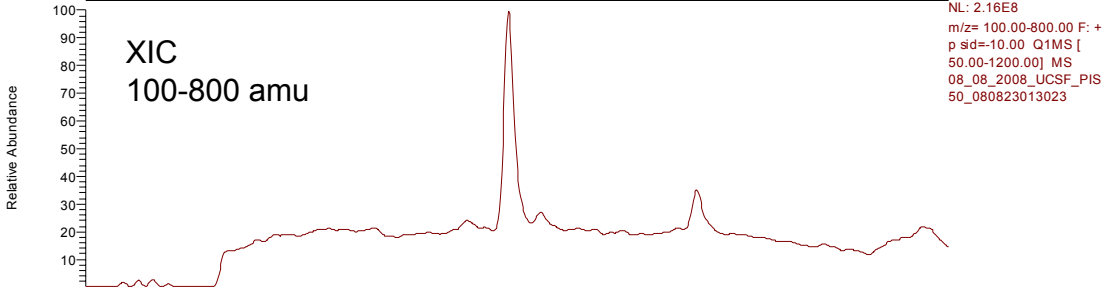
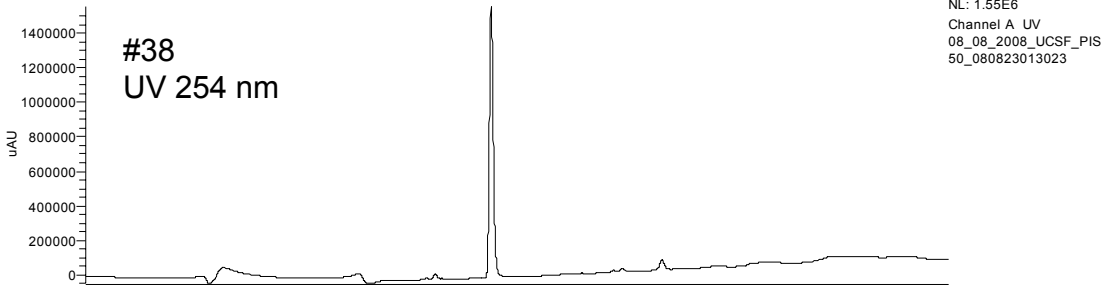


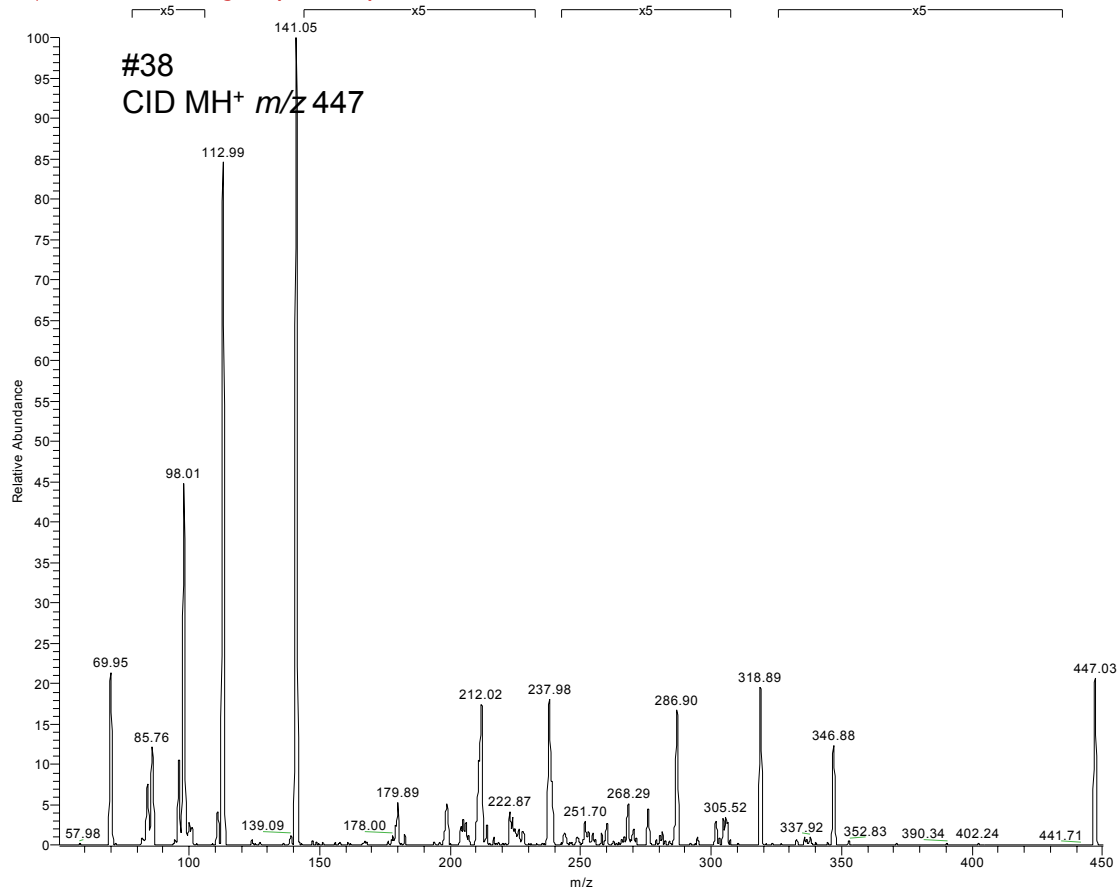
RT: 0.00 - 13.04 SM: 15G



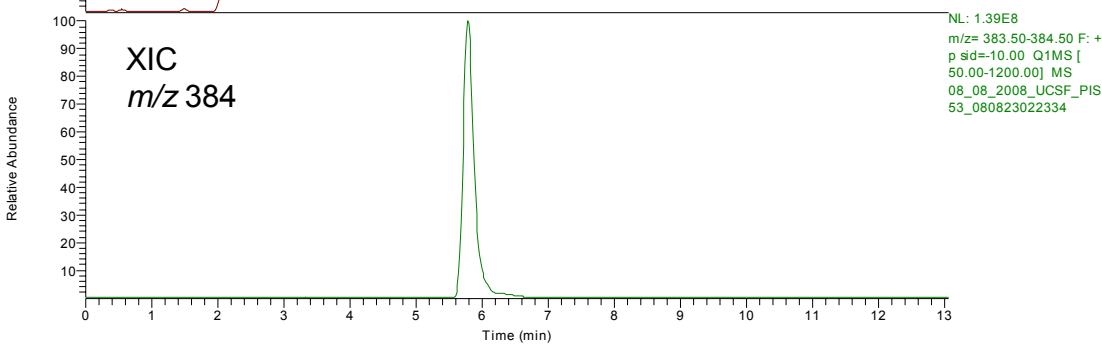
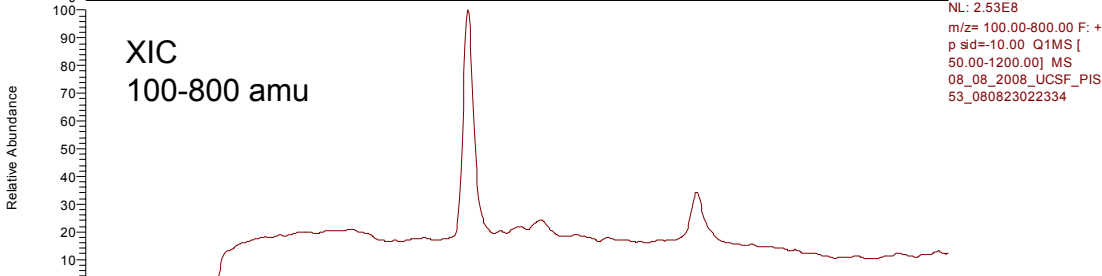
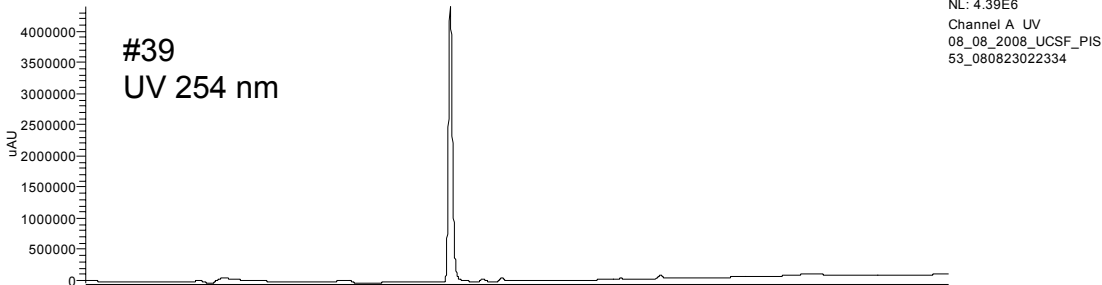


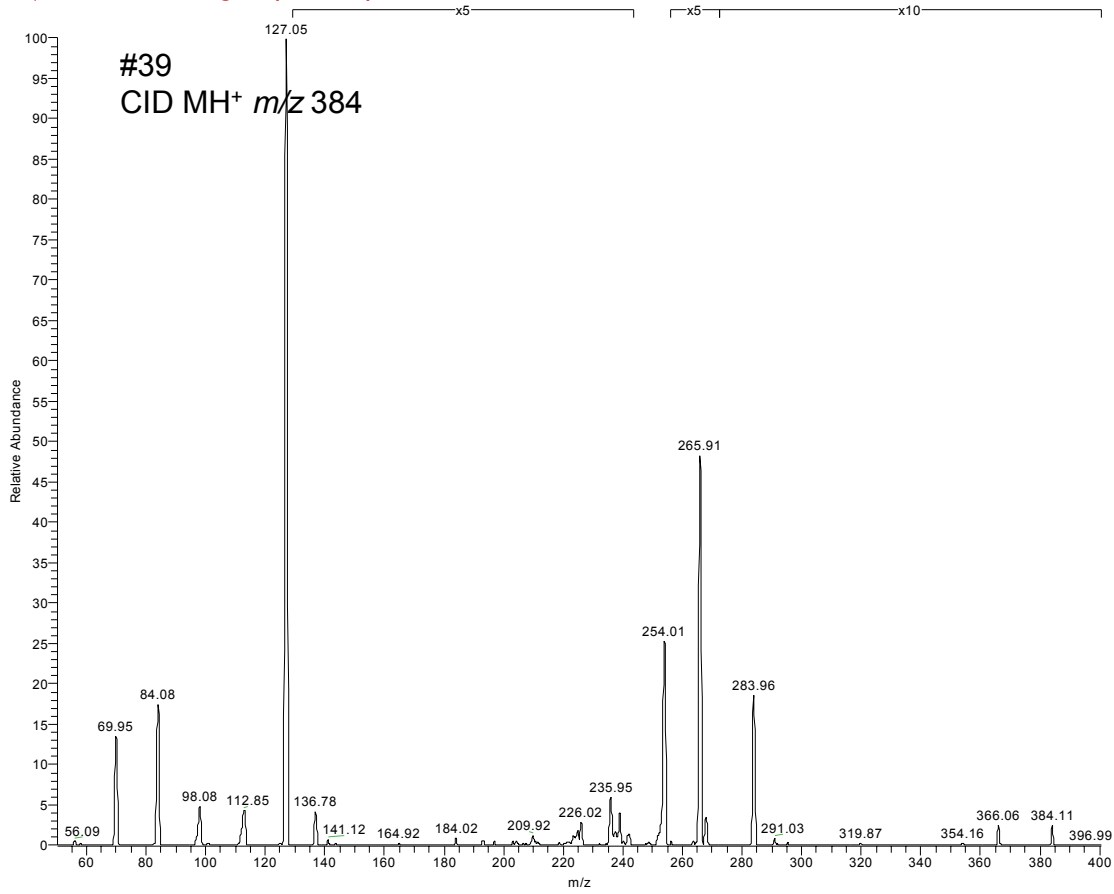
RT: 0.00 - 13.04 SM: 15G



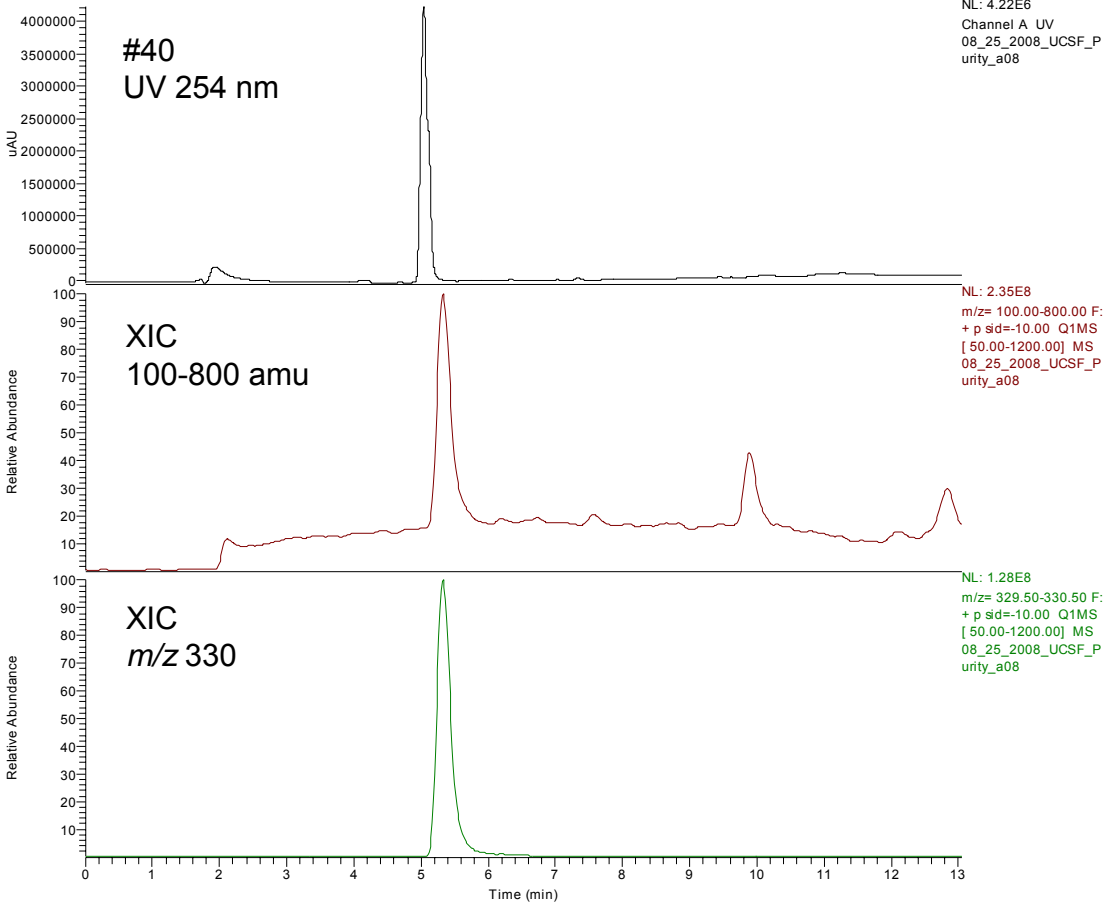


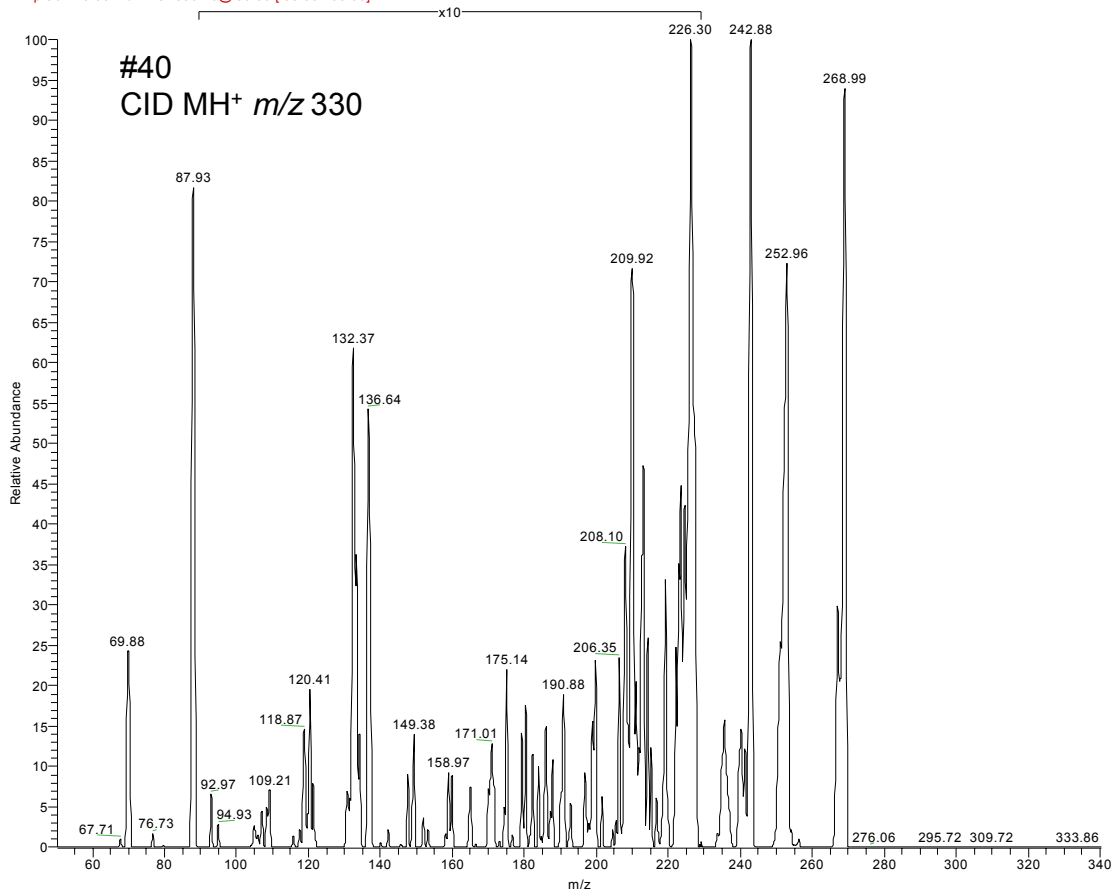
RT: 0.00 - 13.04 SM: 15G



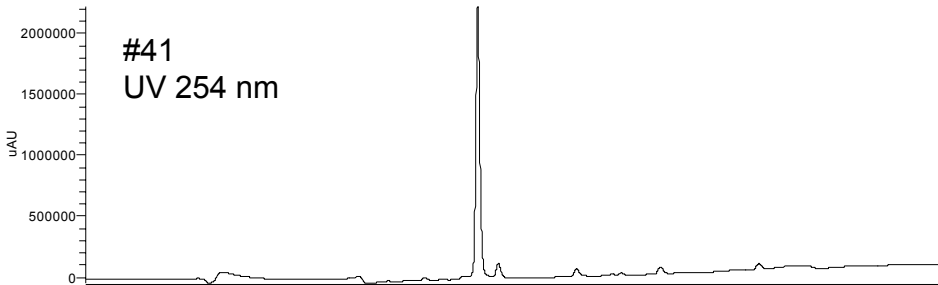


RT: 0.00 - 13.04 SM: 15G

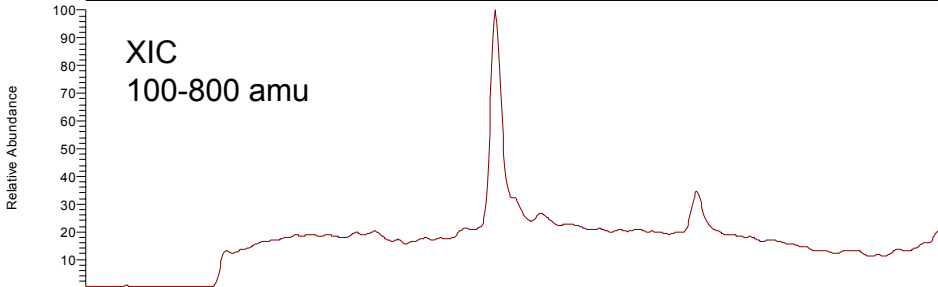




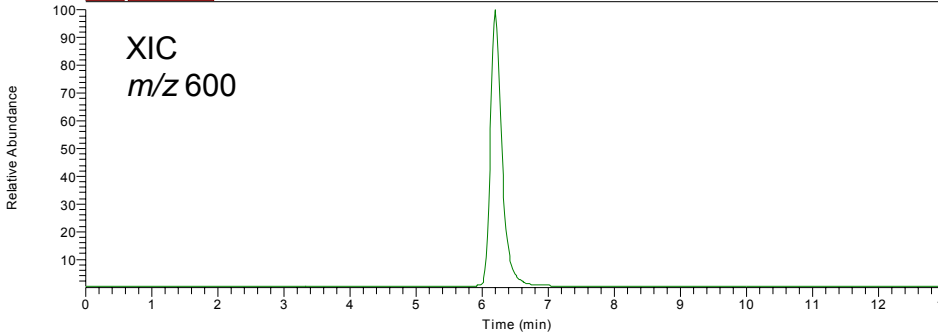
RT: 0.00 - 13.04 SM: 15G



NL: 2.22E6
Channel A UV
08_08_2008_UCSF_PIS
55_080823025901

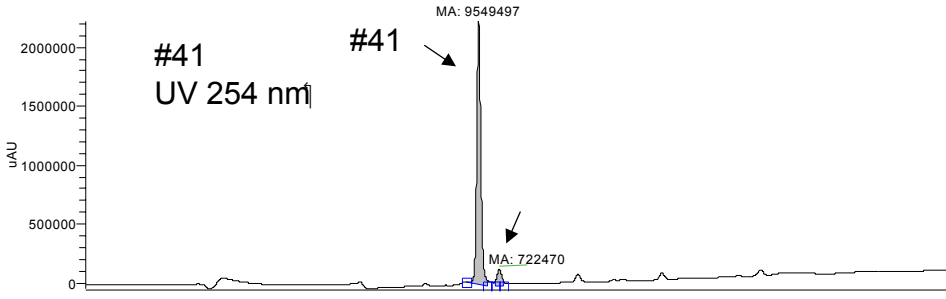


NL: 2.57E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
55_080823025901

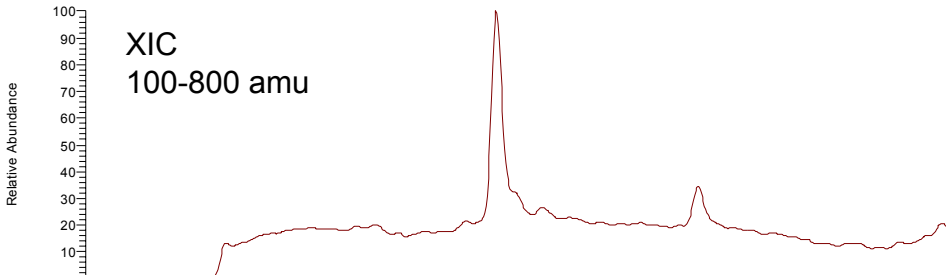


NL: 1.21E8
m/z= 599.50-600.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
55_080823025901

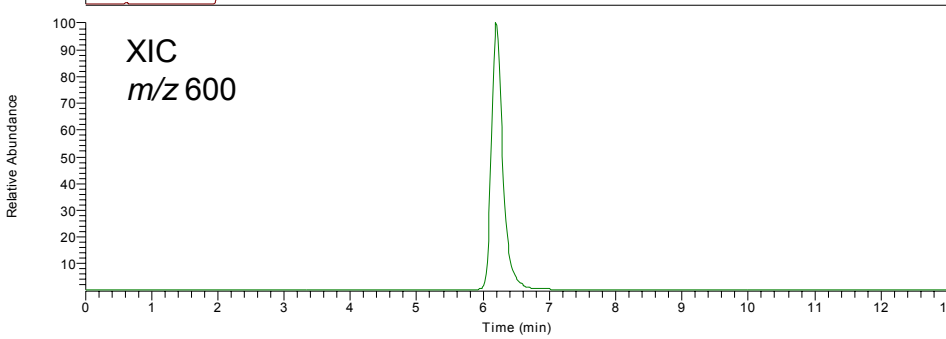
RT: 0.00 - 13.01 SM: 15G



NL: 2.22E6
Channel A UV
08_08_2008_UCSF_PIS
55_080823025901

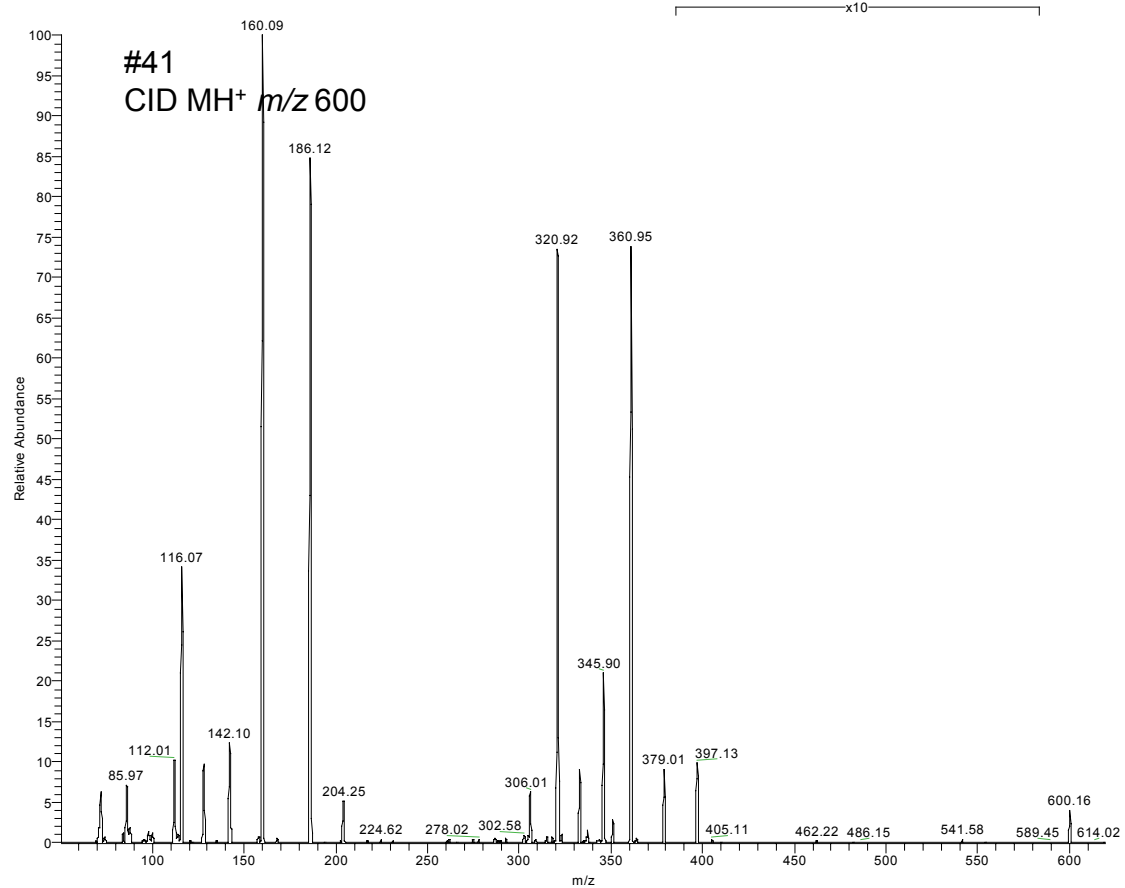


NL: 2.57E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
55_080823025901

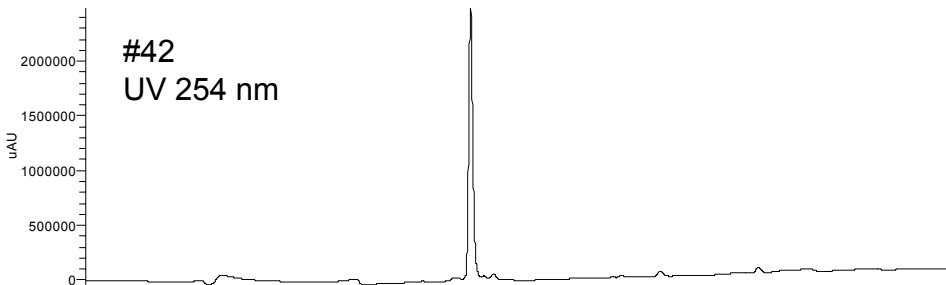


NL: 1.21E8
m/z= 599.50-600.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
55_080823025901

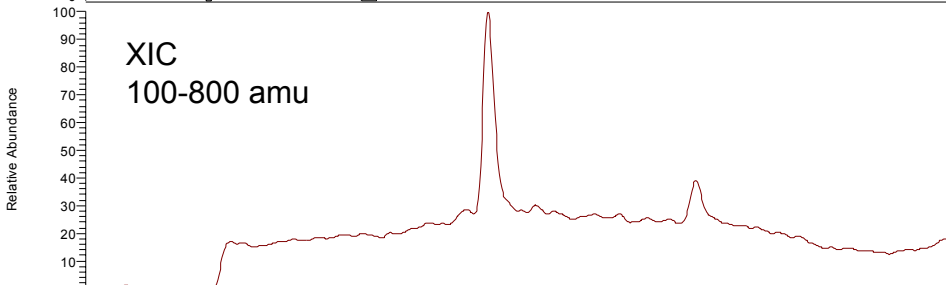
08_08_2008_UCSF_PIS55_080822035324 #404-420 RT: 5.98-6.22 AV: 17 SB: 520 0.84-4.37, 5.87-10.02 SM: 15G NL: 3.07E6
F: + p sid=-10.00 Full ms2 600.10@-30.00 [50.00-700.00]



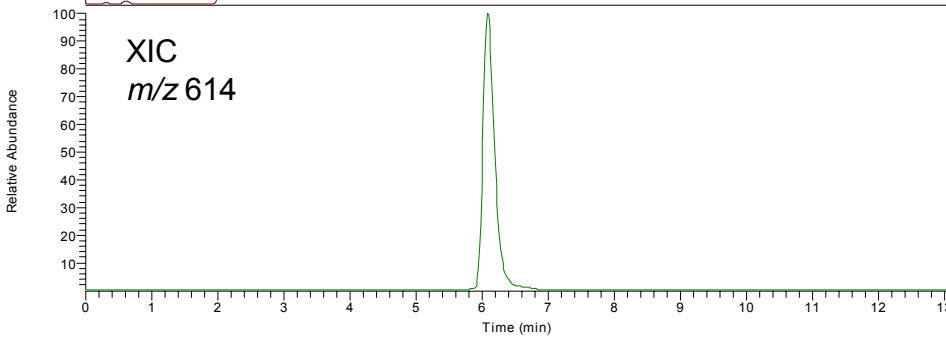
RT: 0.00 - 13.04 SM: 15G



NL: 2.48E6
Channel A UV
08_08_2008_UCSF_PIS
56_080823031649

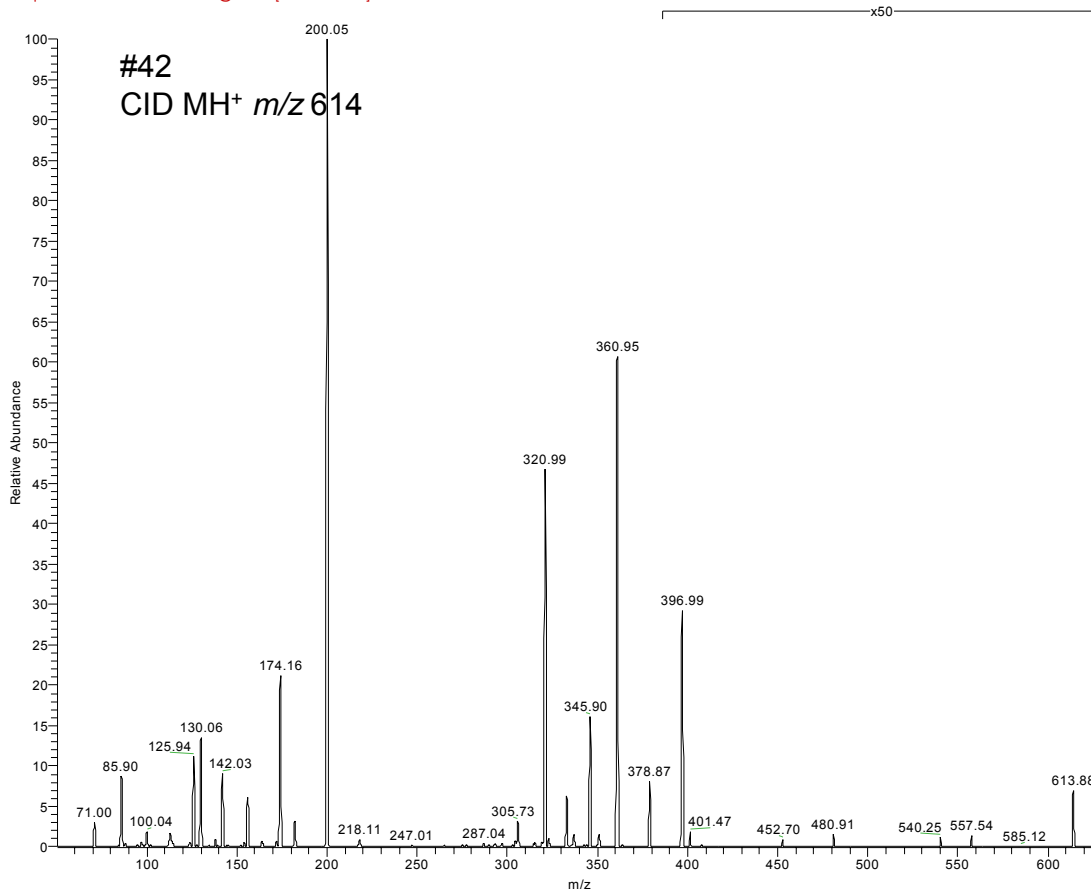


NL: 2.50E8
m/z= 100.00-800.00 F: +
p sd=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
56_080823031649

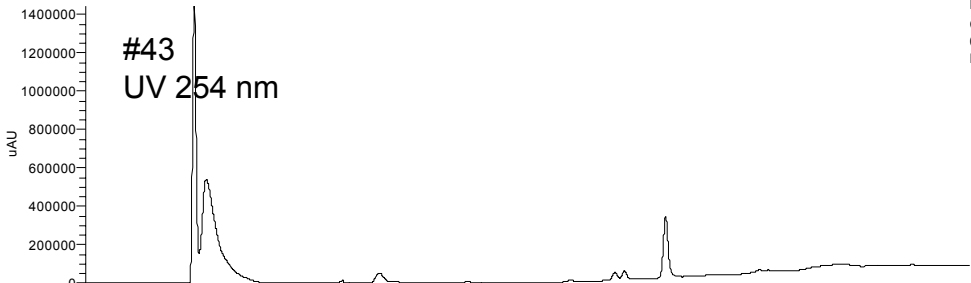


NL: 1.13E8
m/z= 613.50-614.50 F: +
p sd=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
56_080823031649

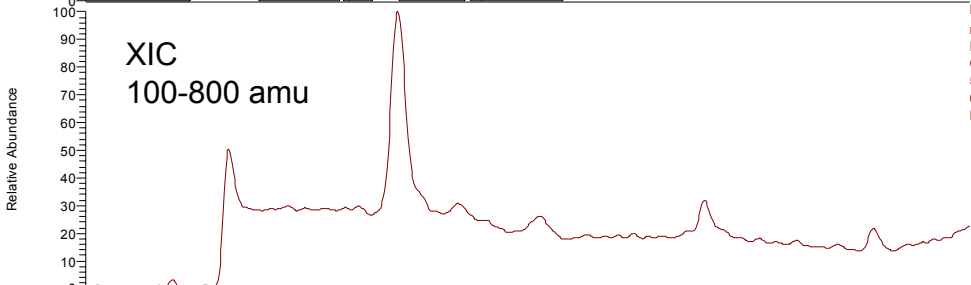
08_08_2008_UCSF_PIS56_080822041108 #398-424 RT: 5.89-6.28 AV: 27 SB: 520 0.84-4.37, 5.86-10.02 SM: 15G NL: 2.95E6
F: + p sd=-10.00 Full ms2 614.10@-30.00 [50.00-700.00]



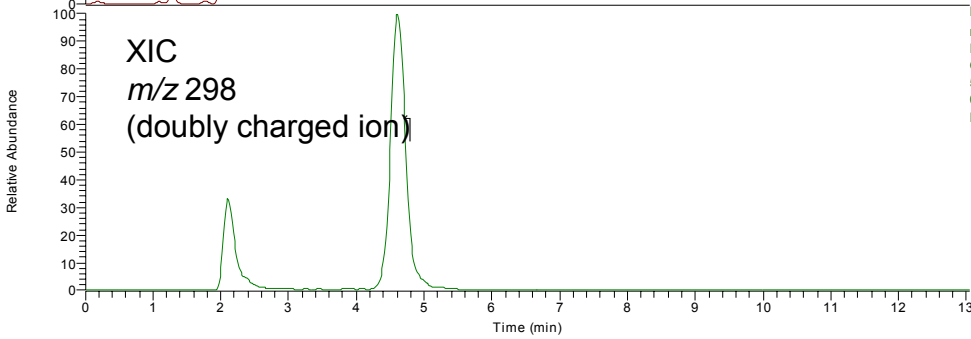
RT: 0.00 - 13.04 SM: 15G



NL: 1.44E6
Channel A UV
08_08_2008_UCSF_
PIS61

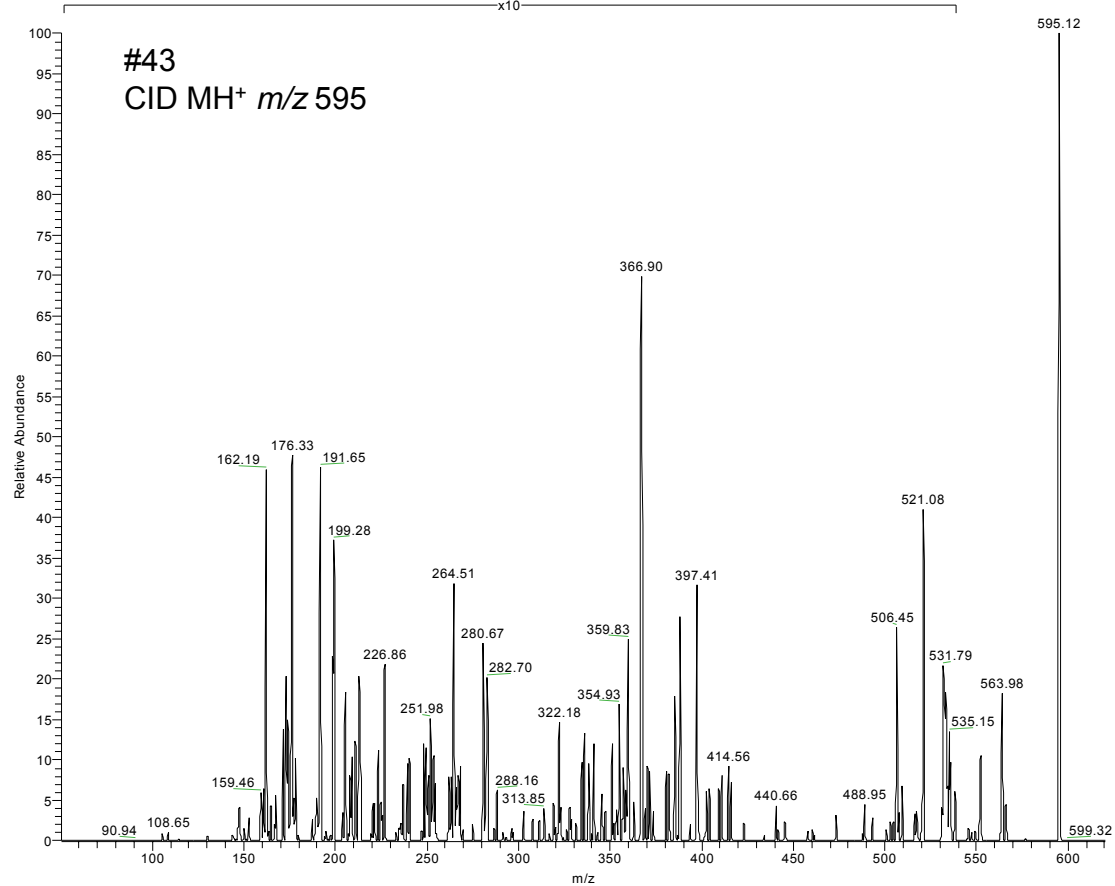


NL: 2.21E8
m/z= 100.00-800.00
F: + p sd=-10.00
Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_
PIS61

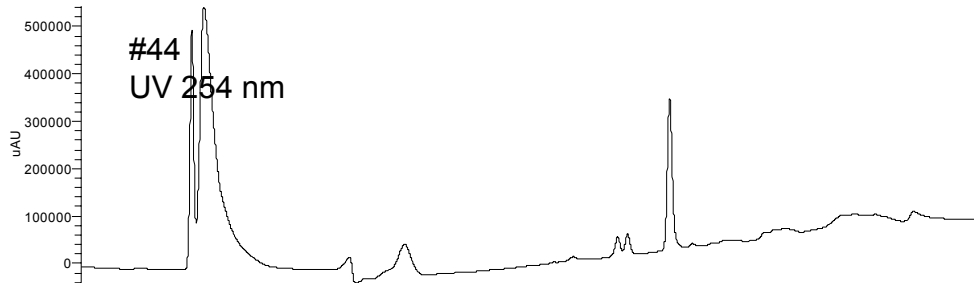


NL: 8.96E7
m/z= 297.50-298.50
F: + p sd=-10.00
Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_
PIS61

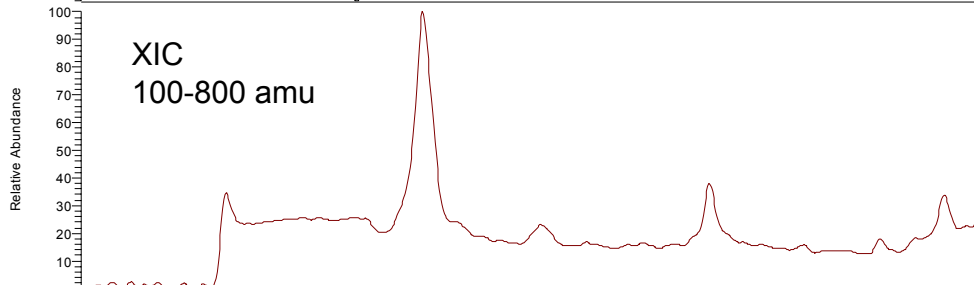
08_08_2008_UCSF_PIS61_080822044641 #324-343 RT: 4.80-5.08 AV: 20 SB: 520 0.84-4.37, 5.86-10.02 SM: 15G NL: 3.56E5
F: + p sd=-10.00 Full ms2 595.10@-30.00 [50.00-700.00]



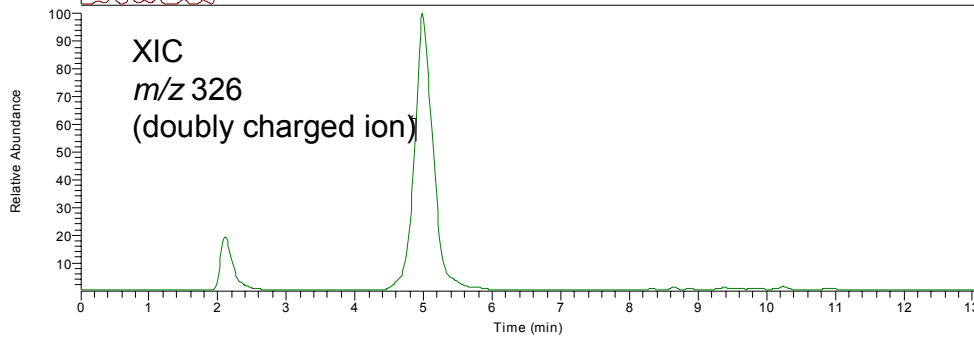
RT: 0.00 - 13.04 SM: 15G



NL: 5.42E5
Channel A UV
08_08_2008_UCSF_
PIS62

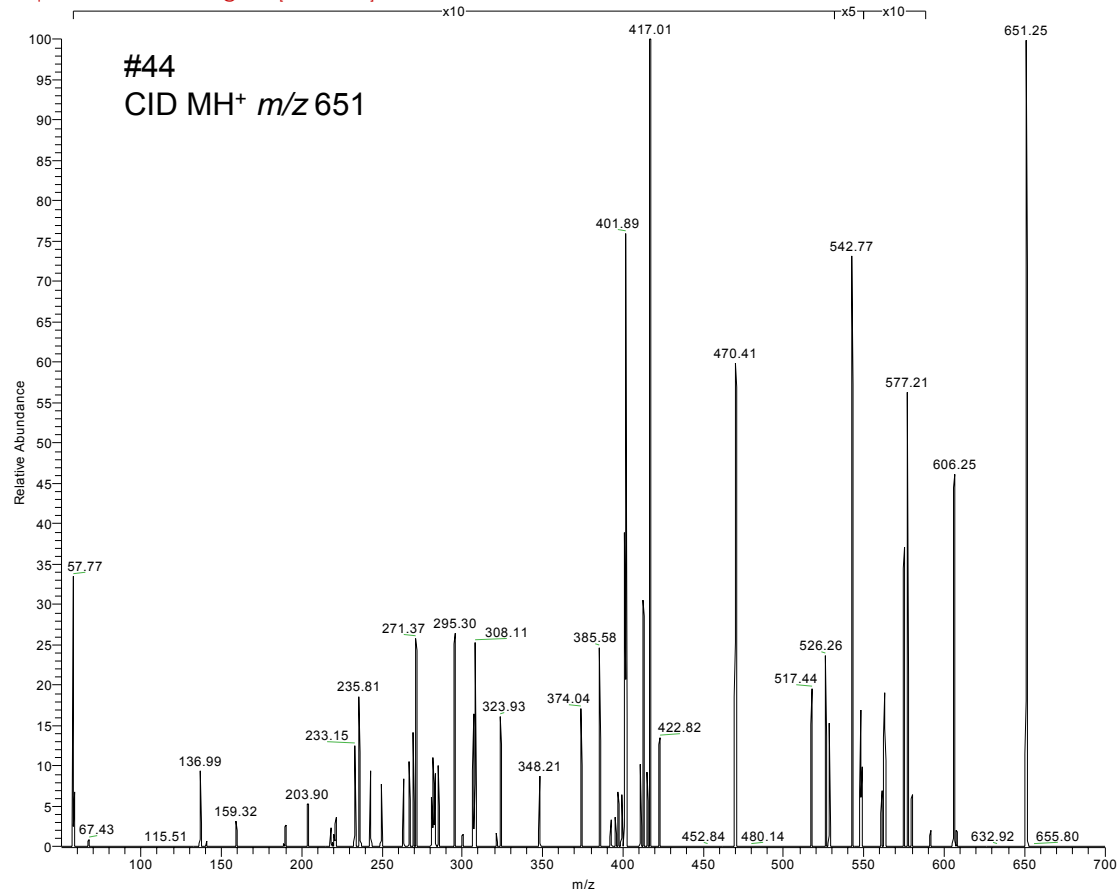


NL: 2.55E8
m/z= 100.00-800.00
F: + p sd=-10.00
Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_
PIS62

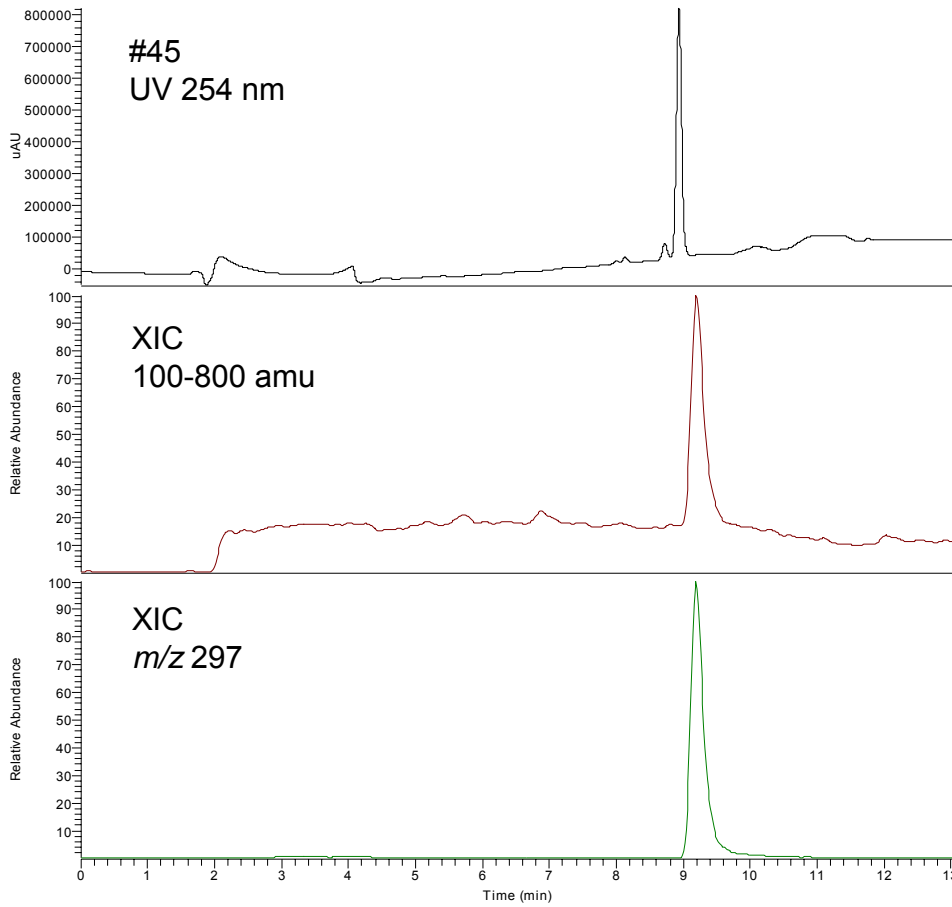


NL: 1.25E8
m/z= 325.50-326.50
F: + p sd=-10.00
Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_
PIS62

08_08_2008_UCSF_PIS62_080822050425 #349-363 RT: 5.17-5.38 AV: 15 SB: 520.0 8.4-4.37, 5.87-10.02 SM: 15G NL: 8.04E4
F: + p sd=-10.00 Full ms2 651.10@-30.00 [50.00-700.00]



RT: 0.00 - 13.04 SM: 15G

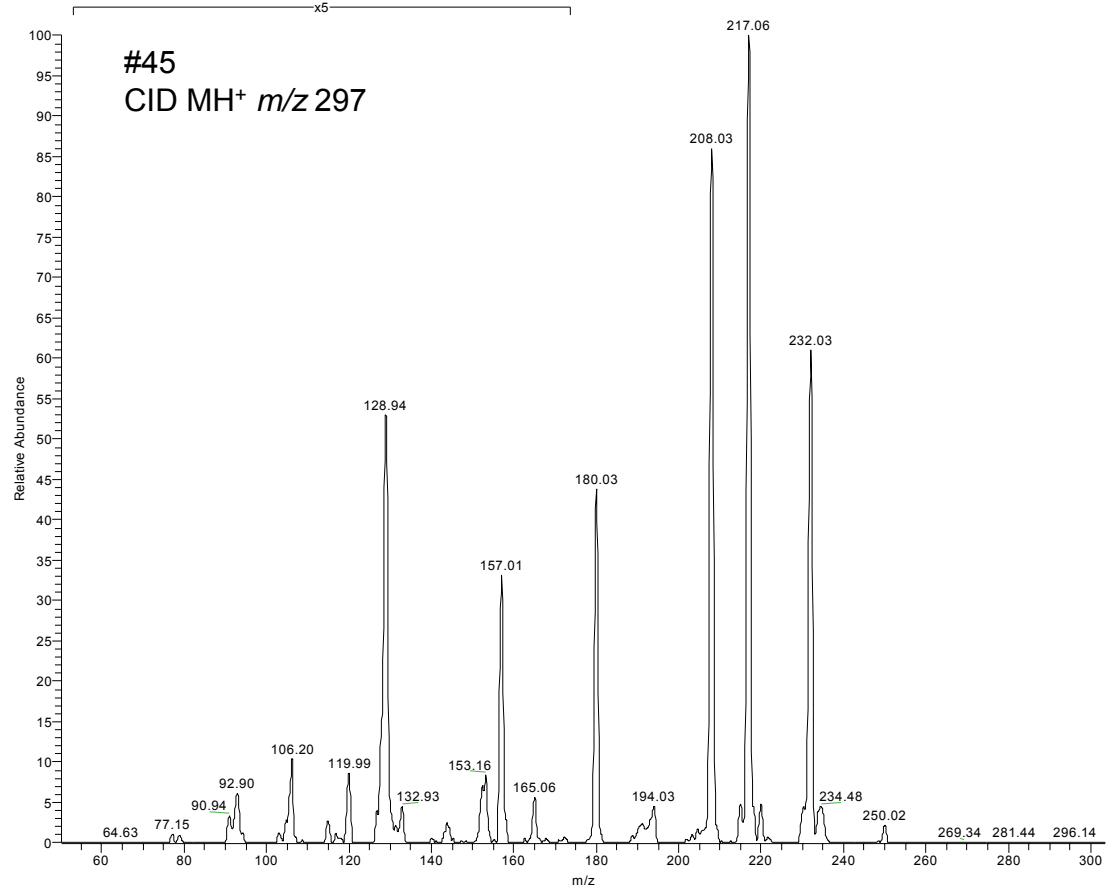


NL: 8.20E5
Channel A UV
08_08_2008_UCSF_PIS
63_080823042750

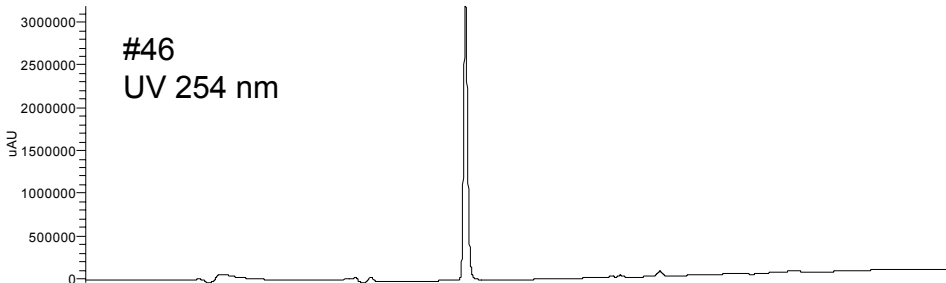
NL: 2.93E8
 m/z = 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
63_080823042750

NL: 1.05E8
 m/z = 296.50-297.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
63_080823042750

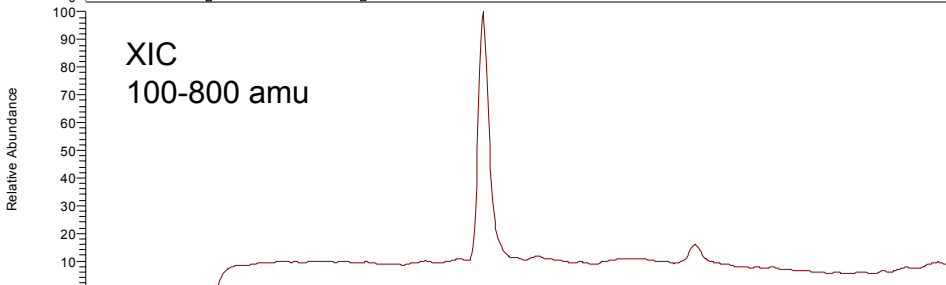
08_08_2008_UCSF_PIS63_080822052209 #609-623 RT: 9.02-9.23 AV: 15 SB: 520 0.84-4.37, 5.87-10.02 SM: 15G NL: 5.50E6
F: + p sid=-10.00 Full ms2 297.10@-30.00 [50.00-700.00]



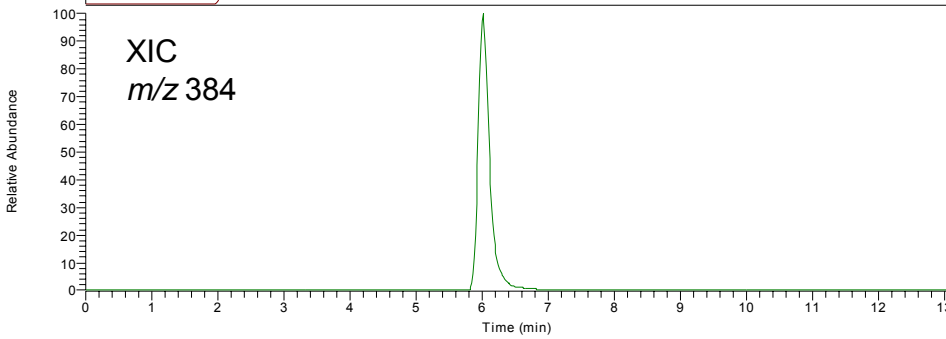
RT: 0.00 - 13.04 SM: 15G



NL: 3.18E6
Channel A UV
08_08_2008_UCSF_PIS
65_080823050320

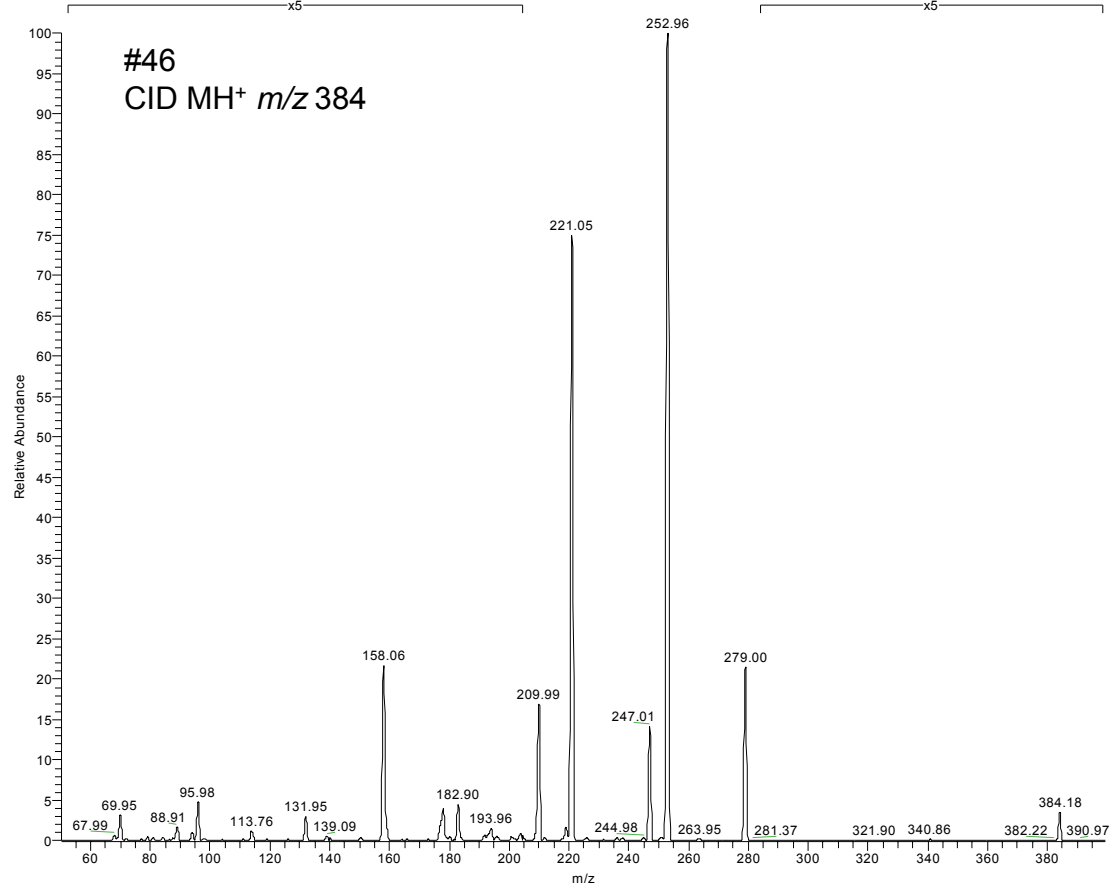


NL: 5.44E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
65_080823050320

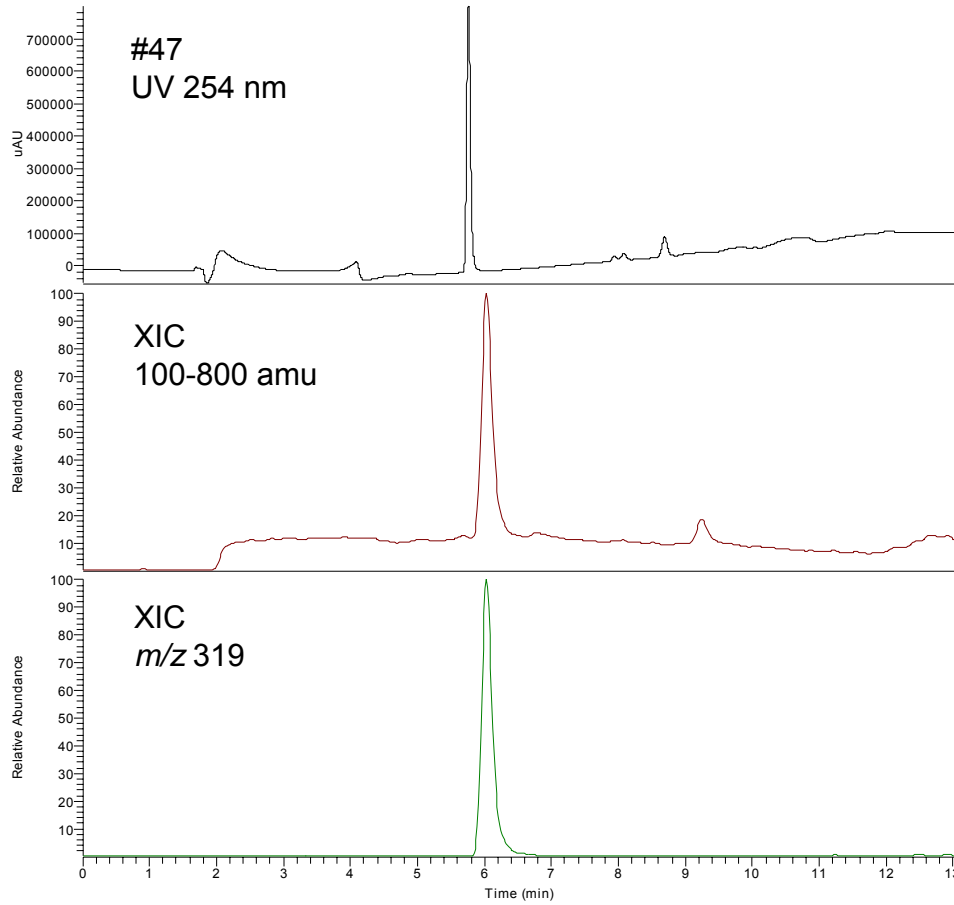


NL: 3.35E8
m/z= 383.50-384.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
65_080823050320

08_08_2008_UCSF_PIS65_080822055742 #396-416 RT: 5.86-6.16 AV: 21 SB: 520 0.84-4.37, 5.86-10.02 SM: 15G NL: 2.10E7
F: + p sid=-10.00 Full ms2 384.10@-30.00 [50.00-700.00]



RT: 0.00 - 13.04 SM: 15G

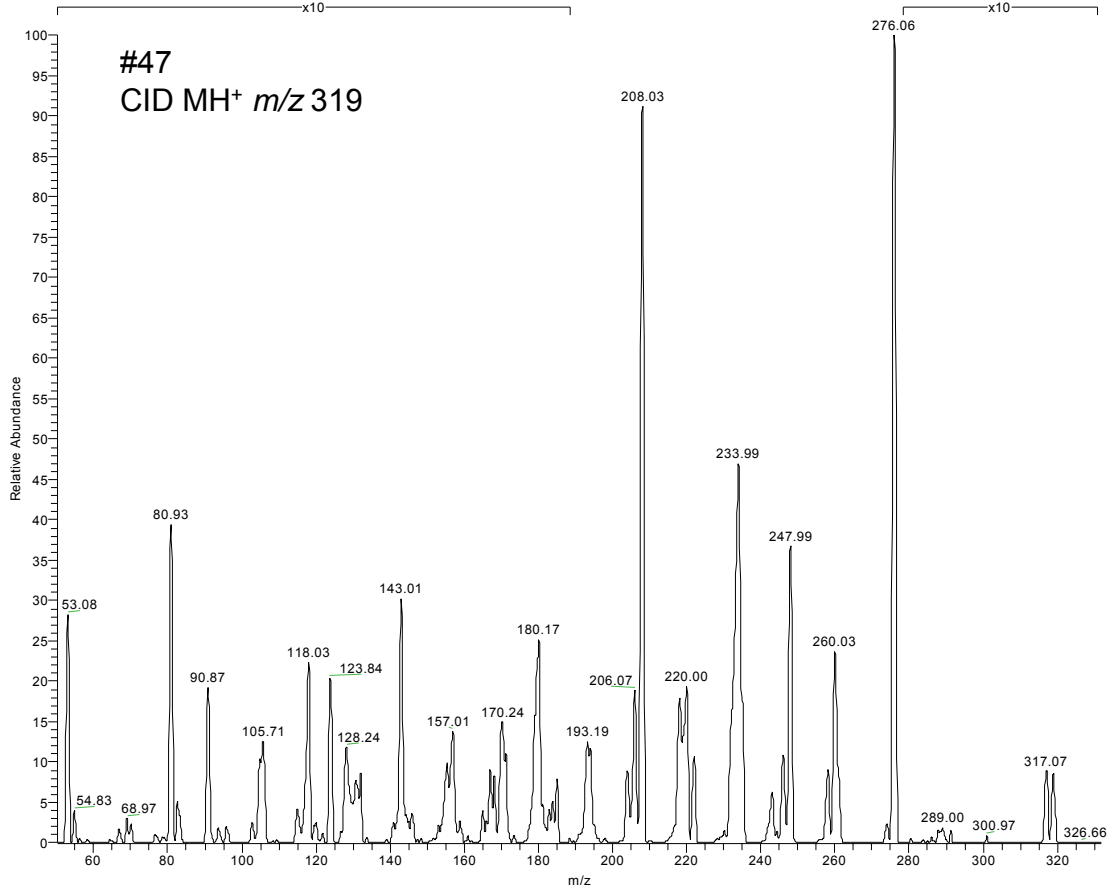


NL: 7.98E5
Channel A UV
08_08_2008_UCSF_PIS
66_080823052108

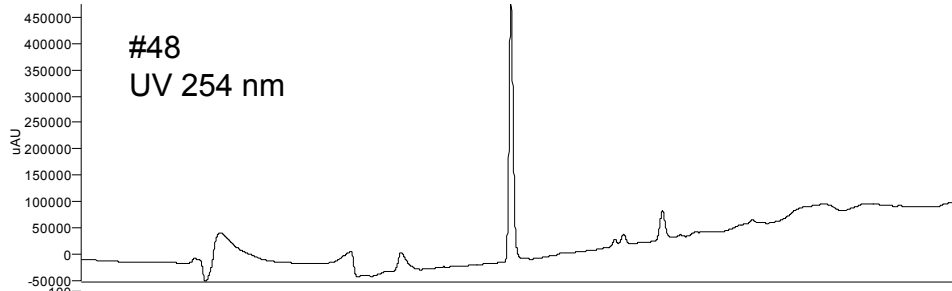
NL: 4.47E8
 $m/z=$ 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
66_080823052108

NL: 2.53E8
 $m/z=$ 318.50-319.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
66_080823052108

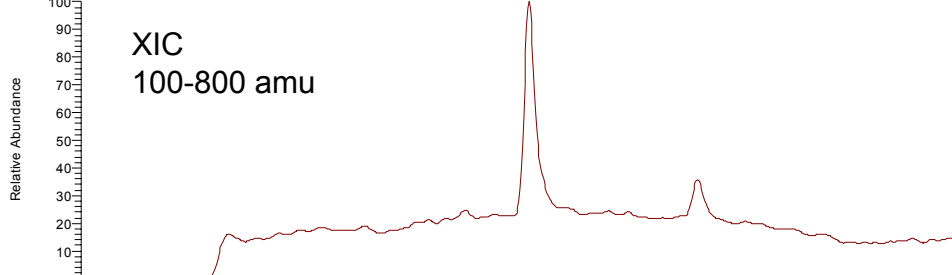
08_08_2008_UCSF_PIS66_080823182301 #404-421 RT: 5.98-6.24 AV: 18 SB: 2 17.00, 17.00 SM: 15G NL: 6.51E6
F: + p sid=-10.00 Full ms2 319.10@-30.00 [50.00-700.00]



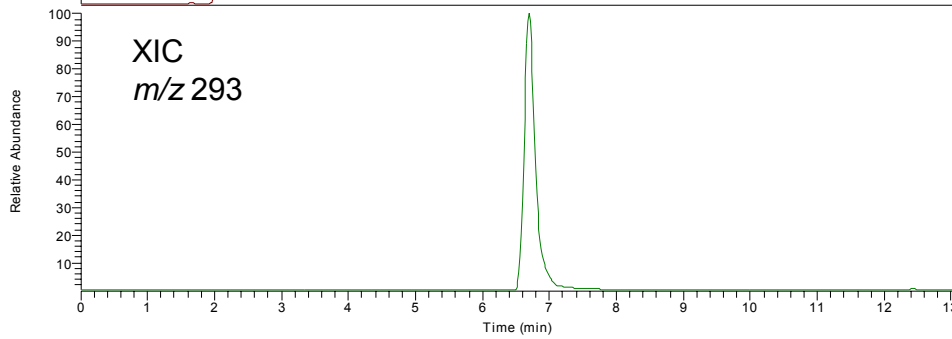
RT: 0.00 - 13.04 SM: 15G



NL: 4.73E5
Channel A UV
08_08_2008_UCSF_PIS
67_080823053855

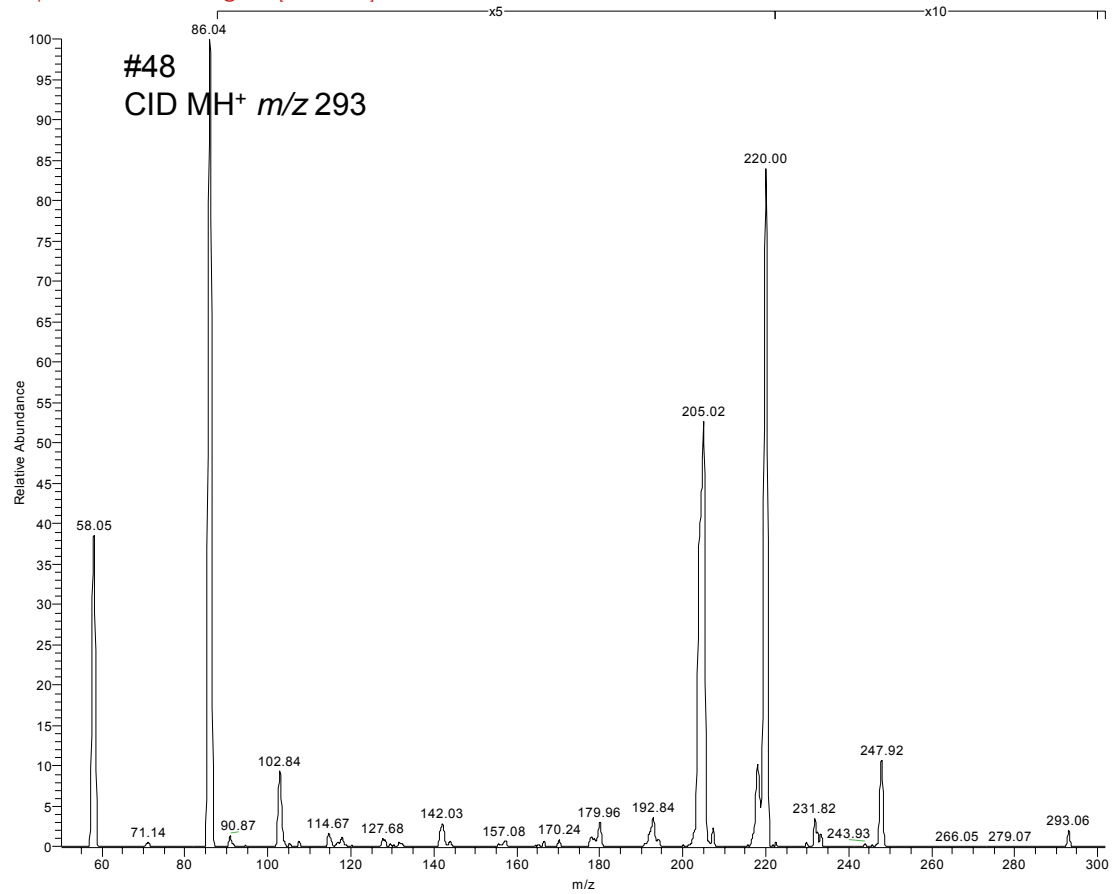


NL: 2.67E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
67_080823053855

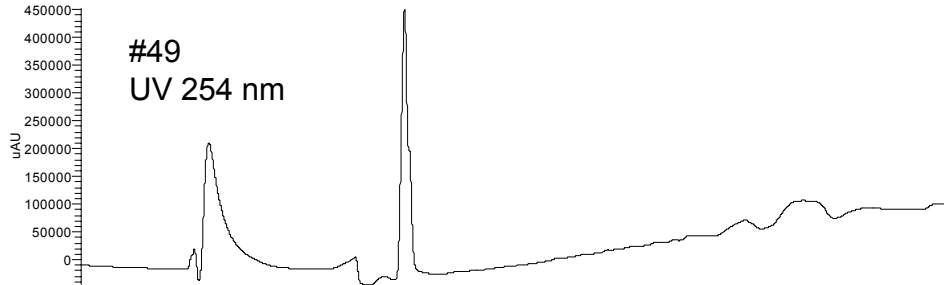


NL: 1.61E8
m/z= 292.50-293.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
67_080823053855

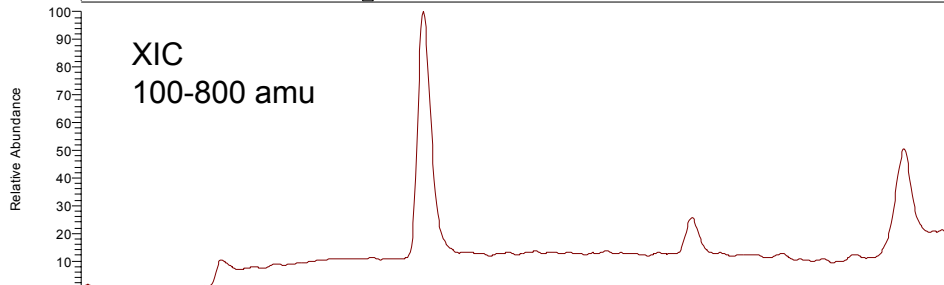
08_08_2008_UCSF_PIS67_080822063314 #438-452 RT: 6.49-6.70 AV: 15 SB: 520 0.84-4.37, 5.86-10.02 SM: 15G NL: 5.75E6
F: + p sid=-10.00 Full ms2 293.10@-30.00 [50.00-700.00]



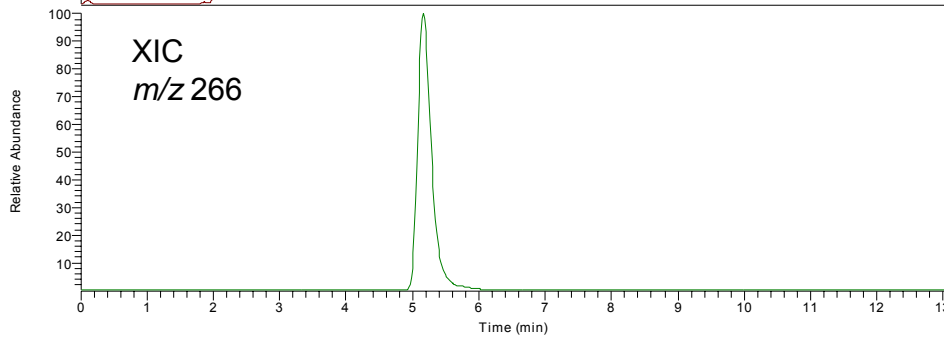
RT: 0.00 - 13.04 SM: 15G



NL: 4.52E5
Channel A UV
08_22_2008_UCSF_PURI
TY_A23_080824174059

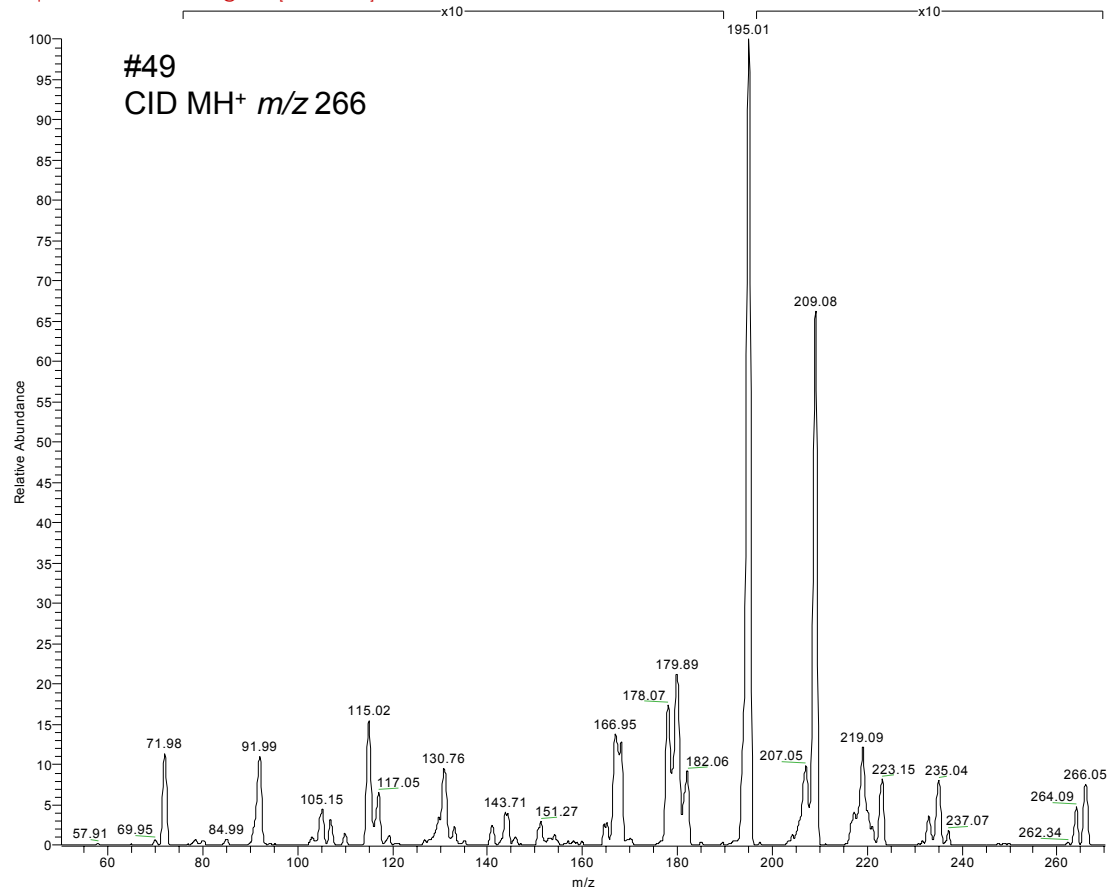


NL: 3.25E8
m/z= 100.00-800.00 F: +
p sd=-10.00 Q1MS [
50.00-1200.00] MS
08_22_2008_UCSF_PURI
TY_A23_080824174059

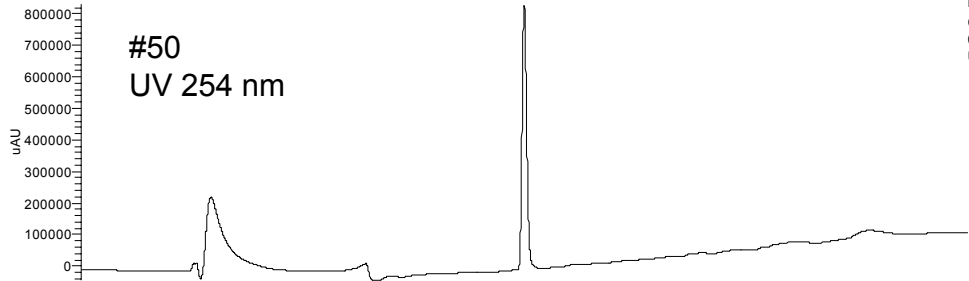


NL: 1.97E8
m/z= 265.50-266.50 F: +
p sd=-10.00 Q1MS [
50.00-1200.00] MS
08_22_2008_UCSF_PURI
TY_A23_080824174059

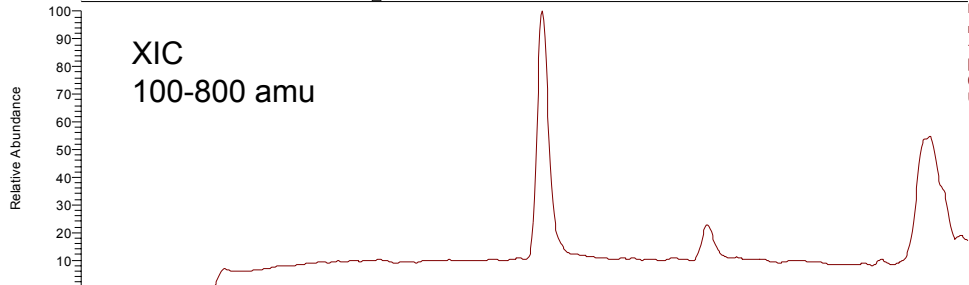
08_22_2008_UCSF_PURITY_A23_080825004726 #338-358 RT: 5.01-5.30 AV: 21 SB: 2 0.01, 0.01 SM: 15G NL: 1.88E7
F: + p sd=-10.00 Full ms2 266.10@-30.00 [50.00-700.00]



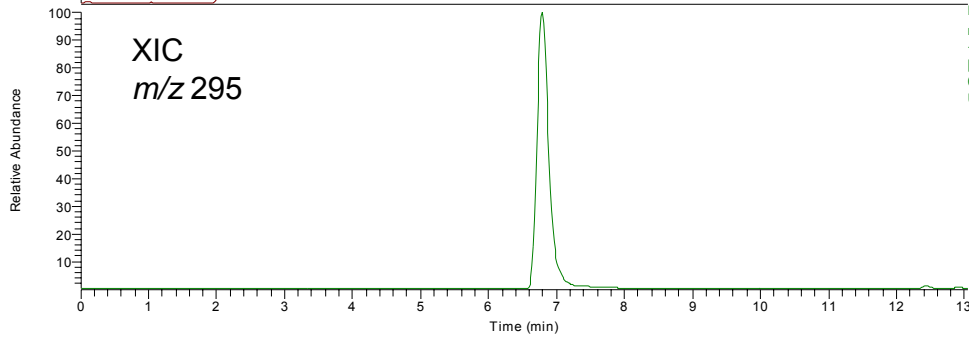
RT: 0.00 - 13.04 SM: 15G



NL: 8.29E5
Channel A UV
08_22_2008_UCSF_P
URITY_A24

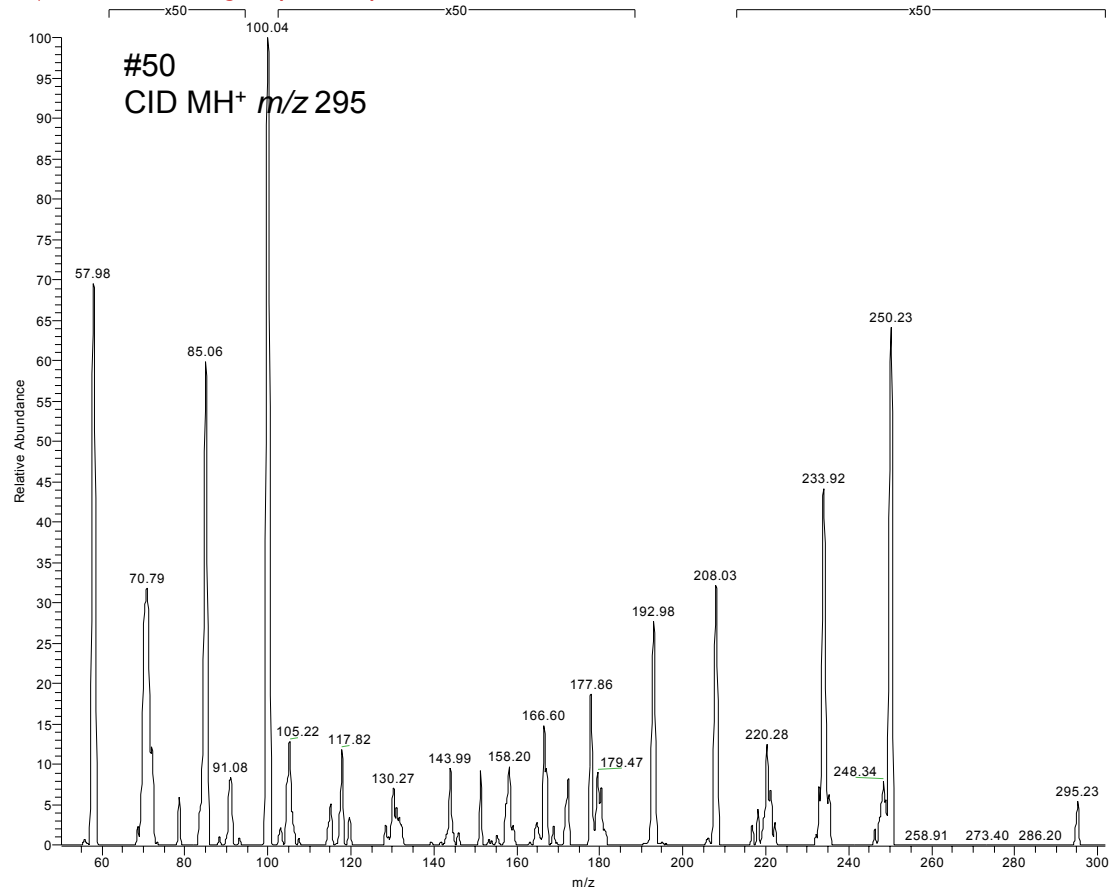


NL: 3.45E8
m/z= 100.00-800.00 F:
+ p sid=-10.00 Q1MS
[50.00-1200.00] MS
08_22_2008_UCSF_P
URITY_A24

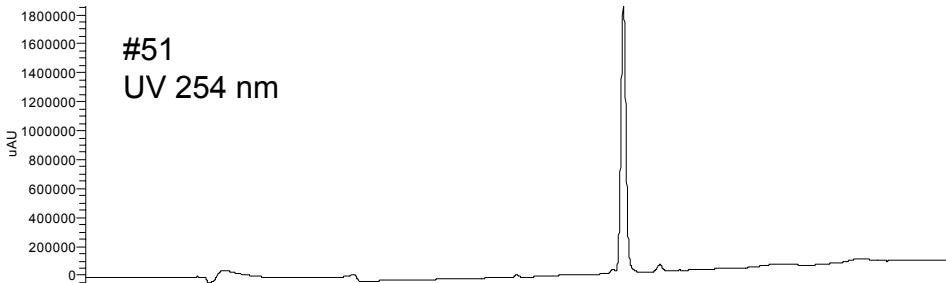


NL: 2.24E8
m/z= 294.50-295.50 F:
+ p sid=-10.00 Q1MS
[50.00-1200.00] MS
08_22_2008_UCSF_P
URITY_A24

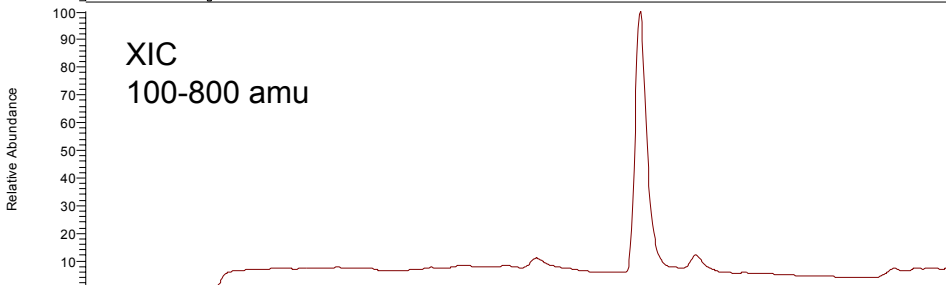
08_22_2008_UCSF_PURITY_A24_080825010514 #444-469 RT: 6.58-6.95 AV: 26 SB: 2 0.01, 0.01 SM: 15G NL: 4.46E6
F: + p sid=-10.00 Full m/z 295.20@-30.00 [50.00-700.00]



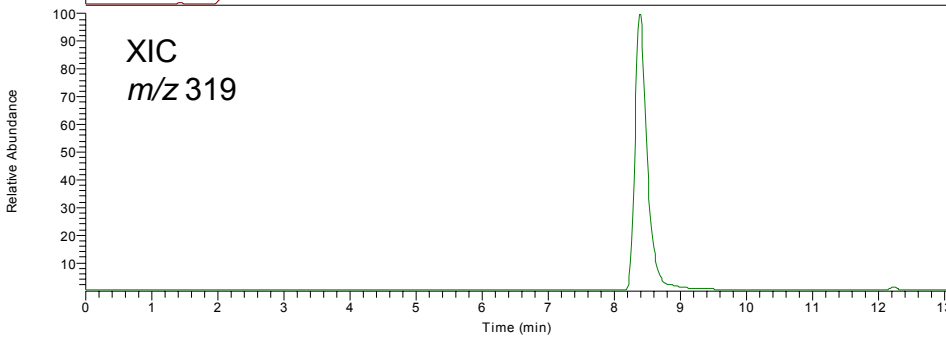
RT: 0.00 - 13.04 SM: 15G



NL: 1.86E6
Channel A UV
08_08_2008_UCSF_PIS
69_080823061425

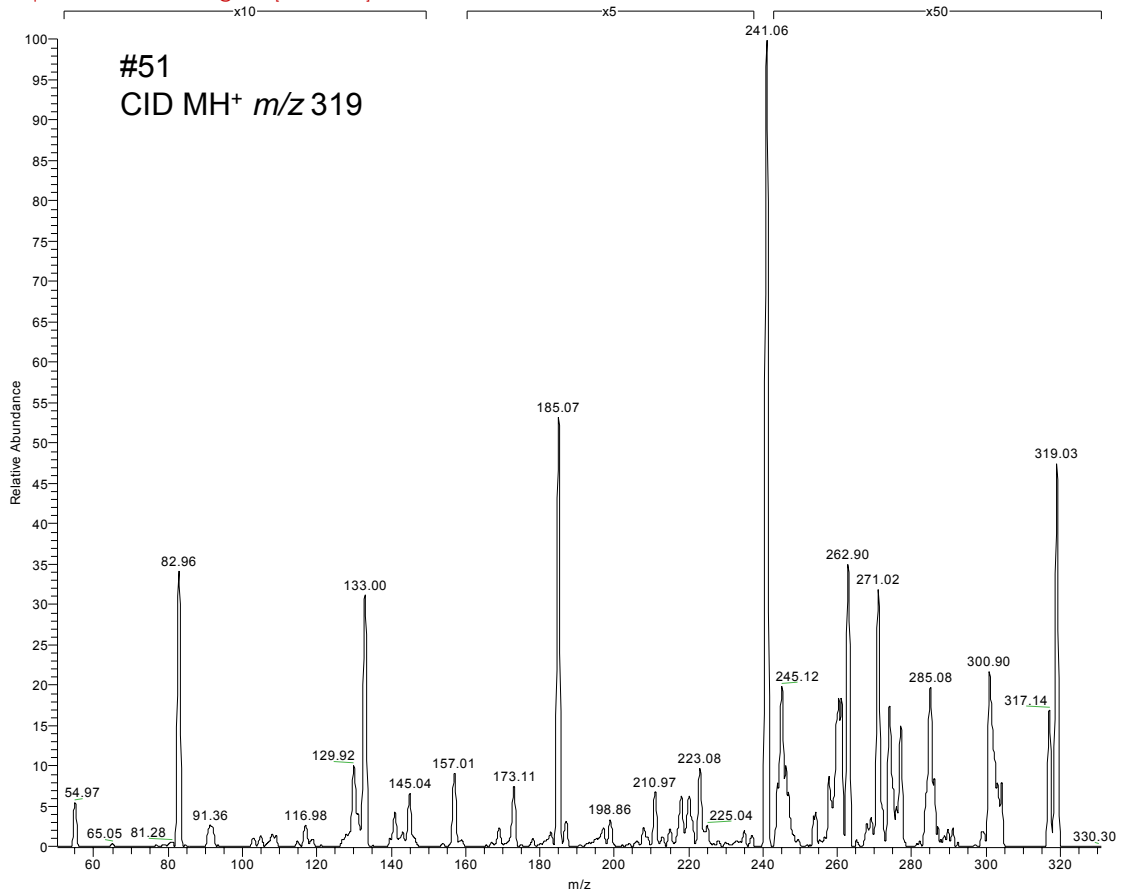


NL: 6.90E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
69_080823061425

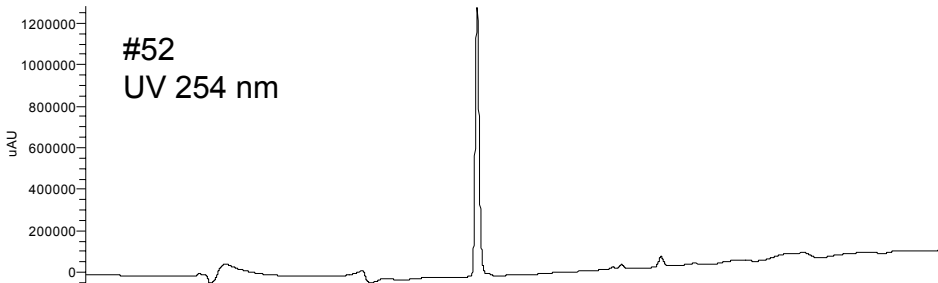


NL: 4.78E8
m/z= 318.50-319.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
69_080823061425

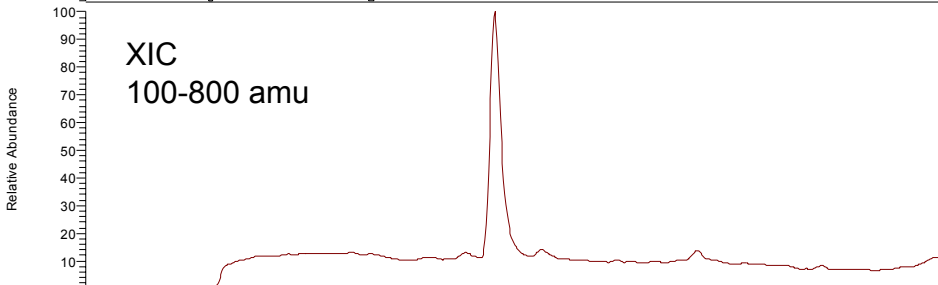
08_08_2008_UCSF_PIS69_080822070847 #556-570 RT: 8.24-8.45 AV: 15 SB: 520 0.84-4.37, 5.87-10.02 SM: 15G NL: 5.28E7
F: + p sid=-10.00 Full ms2 319.10@-30.00 [50.00-700.00]



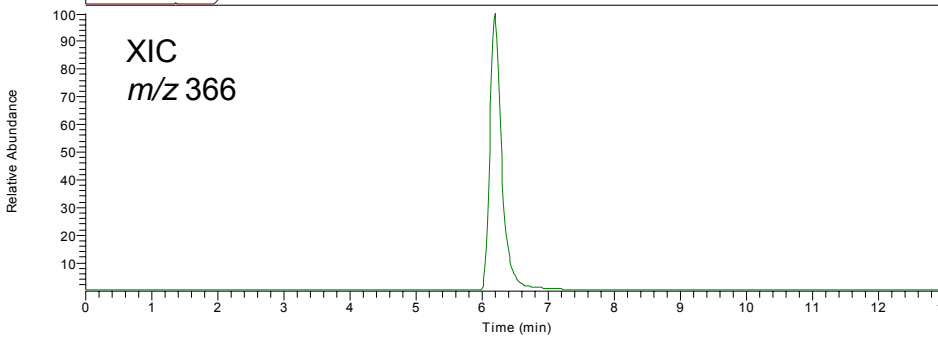
RT: 0.00 - 13.04 SM: 15G



NL: 1.28E6
Channel A UV
08_08_2008_UCSF_PIS
73_080823063213

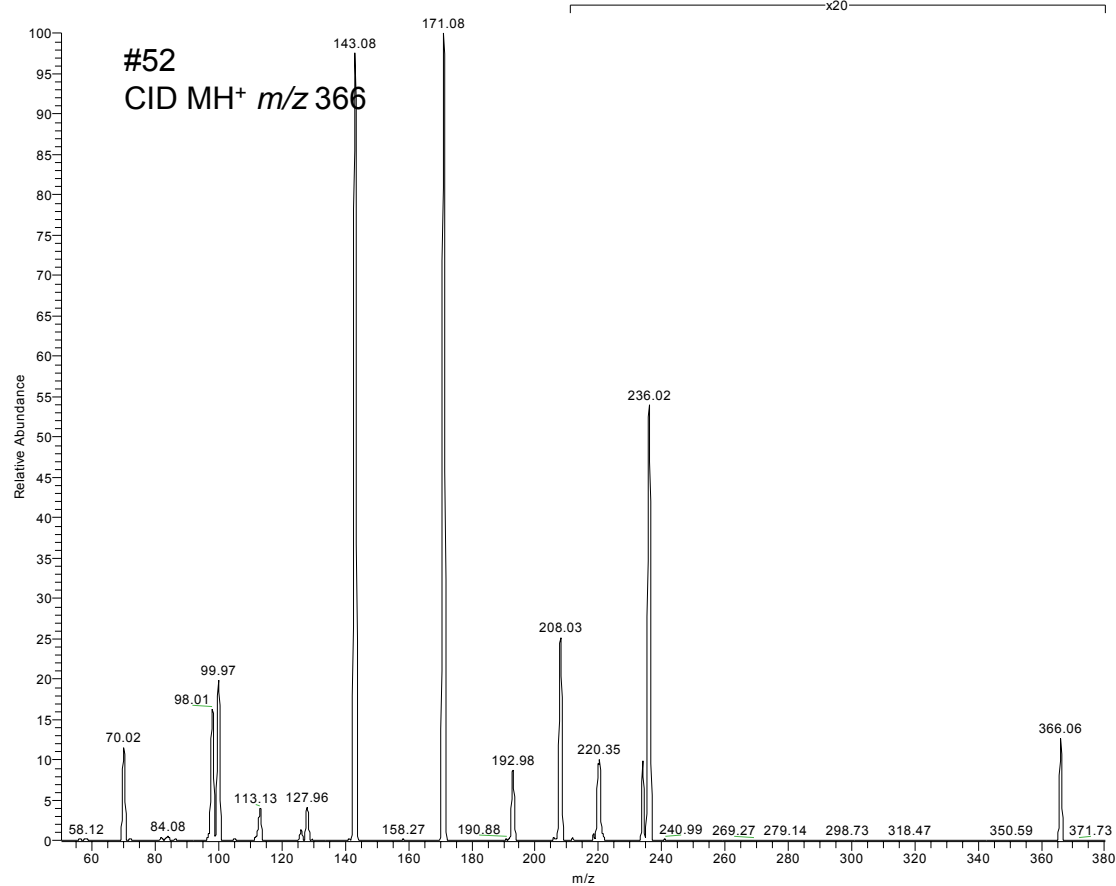


NL: 4.05E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
73_080823063213

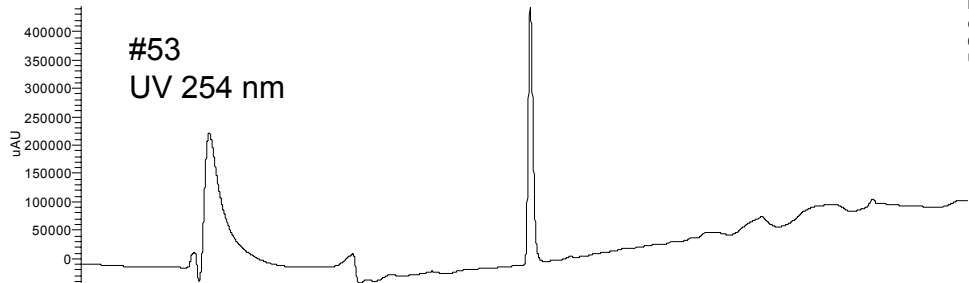


NL: 1.83E8
m/z= 365.50-366.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
73_080823063213

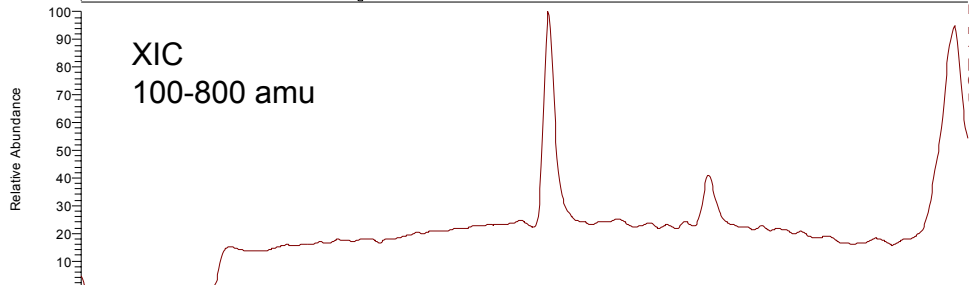
08_08_2008_UCSF_PIS73_080822072629 #400-416 RT: 5.92-6.16 AV: 17 SB: 520 0.84-4.37, 5.86-10.01 SM: 15G NL: 8.85E6
F: + p sid=-10.00 Full ms2 366.10@-30.00 [50.00-700.00]



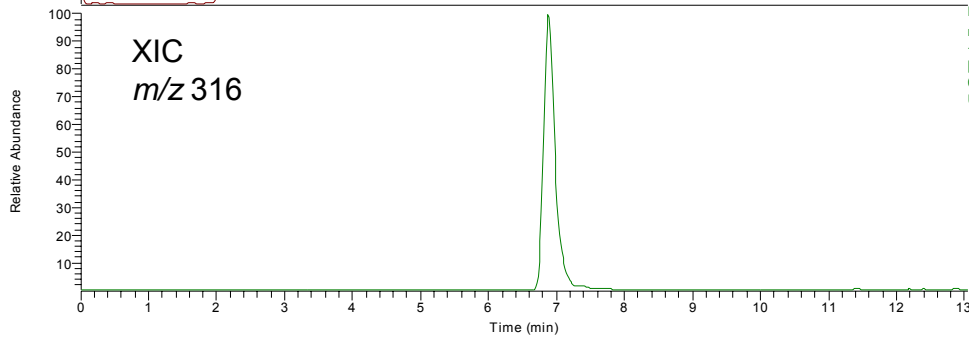
RT: 0.00 - 13.04 SM: 15G



NL: 4.44E5
Channel A_UV
08_22_2008_UCSF_P
URITY_A25

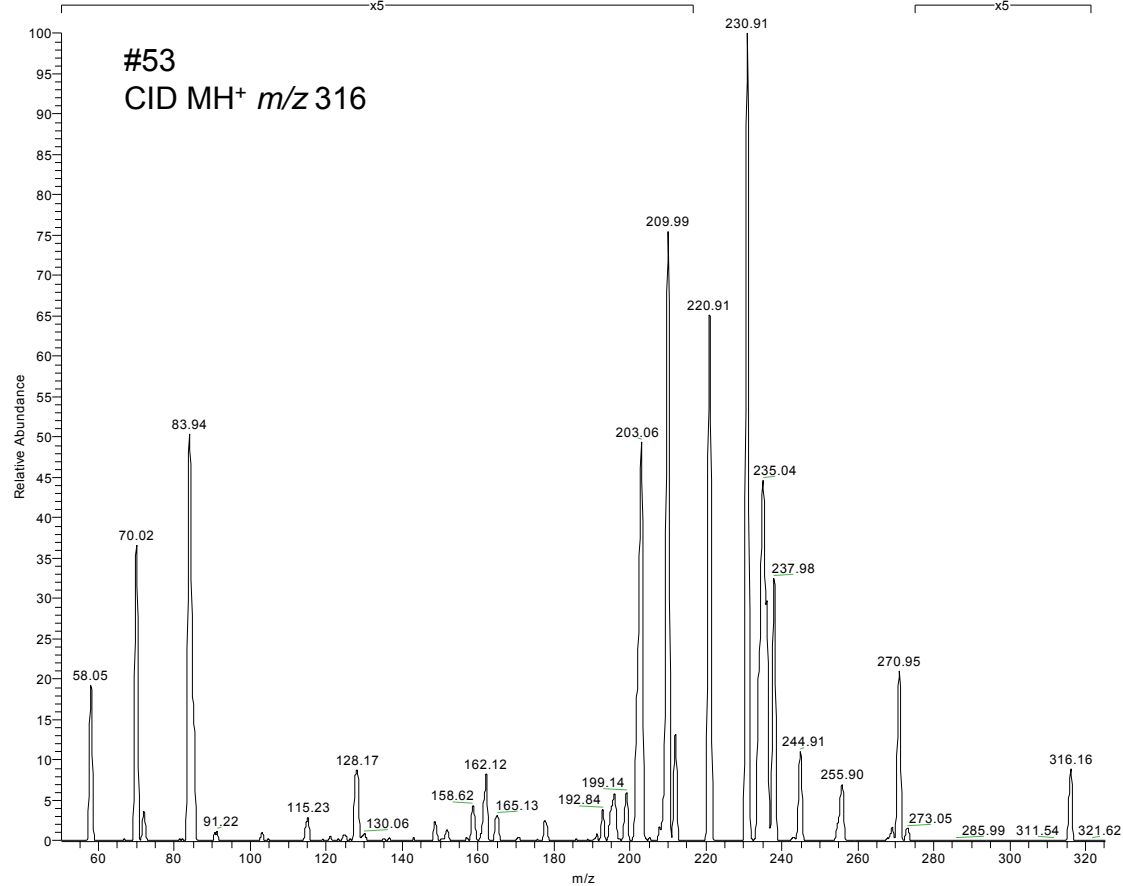


NL: 2.10E8
m/z= 100.00-800.00 F:
+ p sd=-10.00 Q1MS
[50.00-1200.00] MS
08_22_2008_UCSF_P
URITY_A25

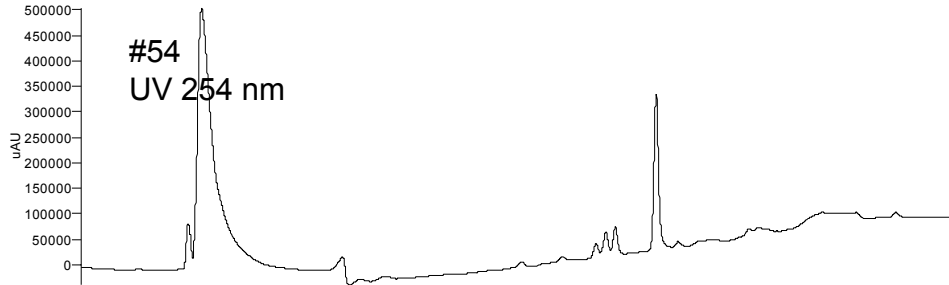


NL: 8.78E7
m/z= 315.50-316.50 F:
+ p sd=-10.00 Q1MS
[50.00-1200.00] MS
08_22_2008_UCSF_P
URITY_A25

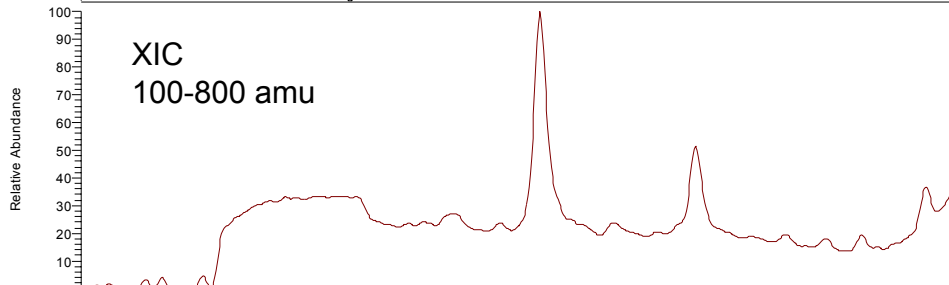
08_22_2008_UCSF_PURITY_A25_080825012302 #453-476 RT: 6.71-7.05 AV: 24 SB: 2 0.01 , 0.01 SM: 15G NL: 2.78E6
F: + p sd=-10.00 Full m/z 316.10@-30.00 [50.00-700.00]



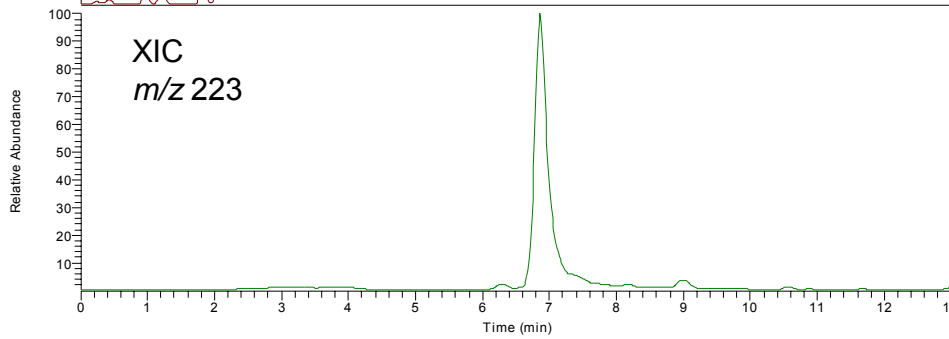
RT: 0.00 - 13.04 SM: 15G



NL: 5.02E5
Channel A UV
08_08_2008_UCSF_PIS
75_080814101059

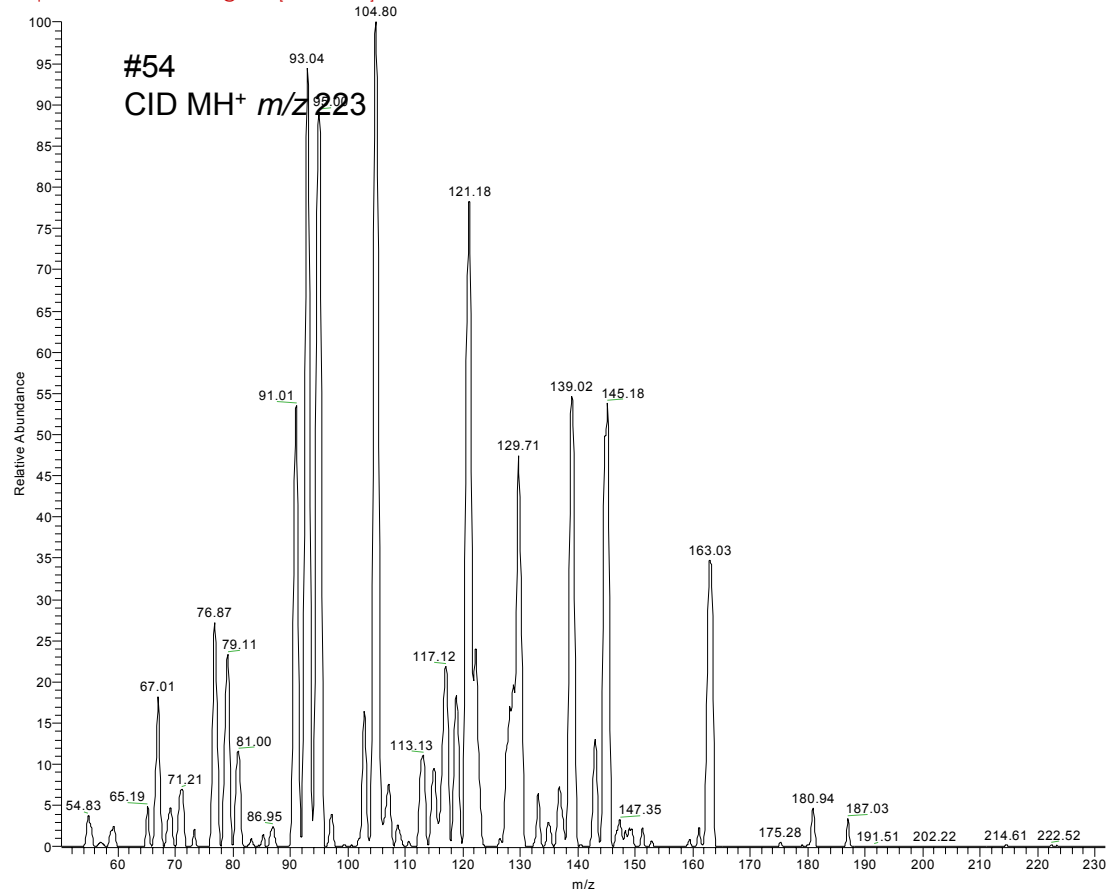


NL: 2.20E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
75_080814101059

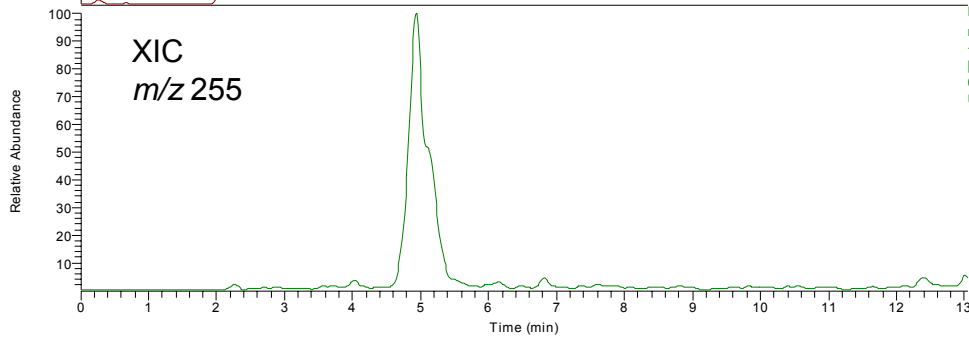
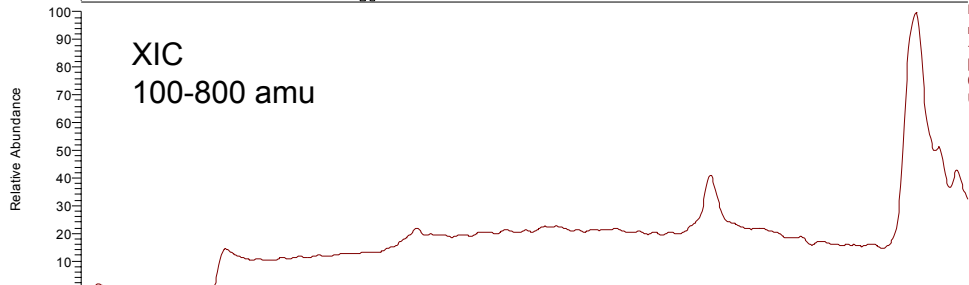


NL: 9.37E7
m/z= 222.50-223.50 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
75_080814101059

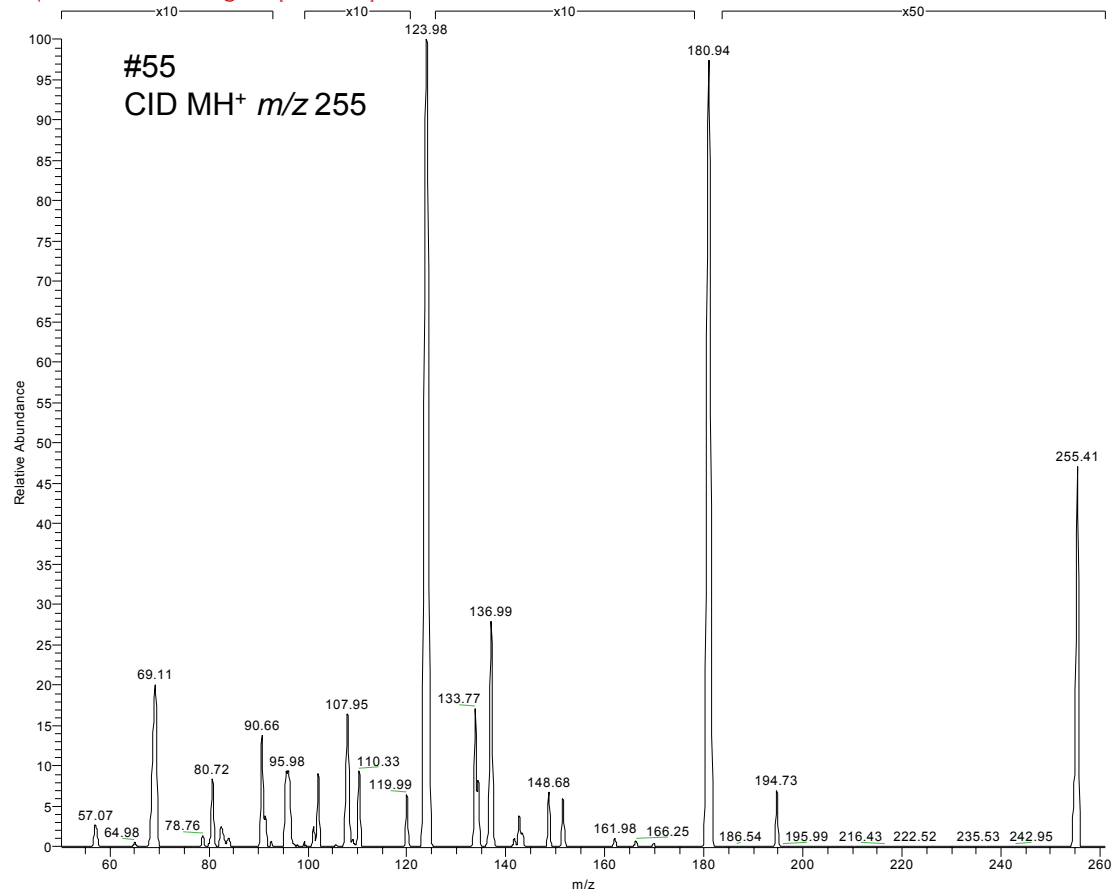
08_08_2008_UCSF_PIS75_080822080205 #464-483 RT: 6.87-7.16 AV: 20 SB: 520 0.84-4.37, 5.87-10.02 SM: 15G NL: 1.76E5
F: + p sid=-10.00 Full ms2 223.10@-30.00 [50.00-700.00]



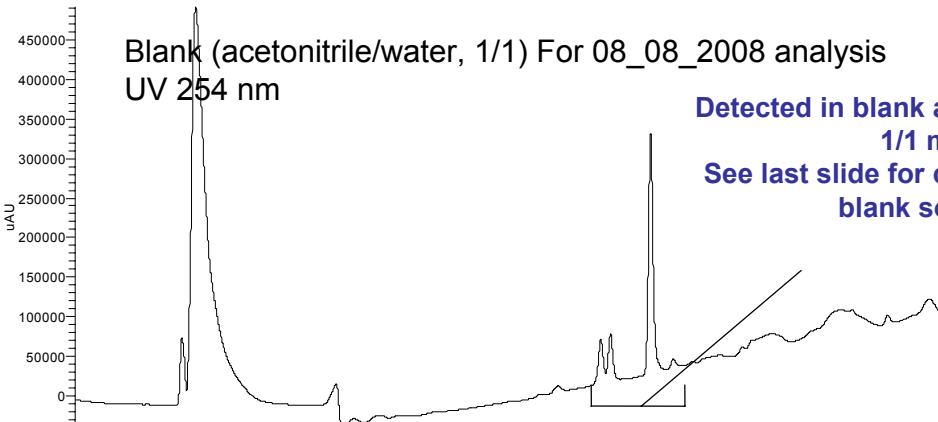
RT: 0.00 - 13.04 SM: 15G



08_22_2008_UCSF_PURITY_A28_080825114636 #321-340 RT: 4.75-5.03 AV: 20 SB: 2 17.00, 17.00 SM: 15G NL: 3.72E5
F: + p sd=-10.00 Full ms2 255.10@-30.00 [50.00-700.00]



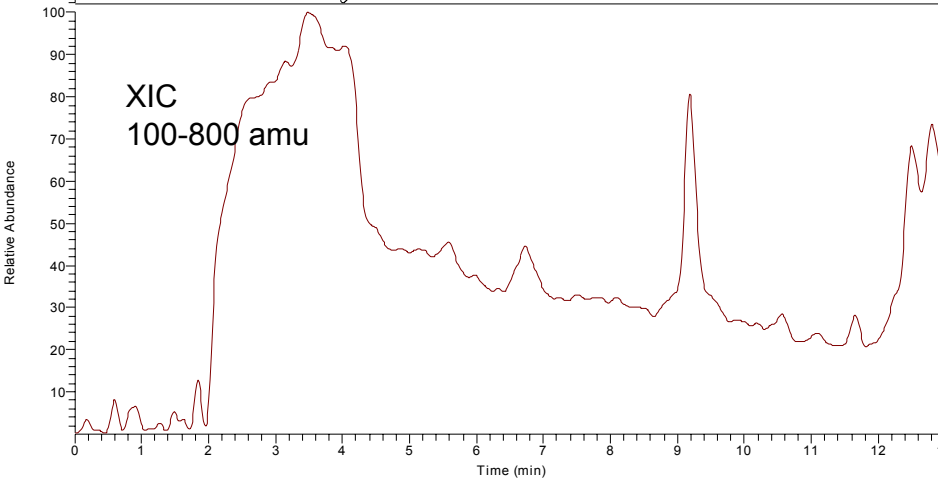
RT: 0.00 - 13.04 SM: 15G



Blank (acetonitrile/water, 1/1) For 08_08_2008 analysis
UV 254 nm

NL: 4.91E5
Channel A UV
08_08_2008_UCSF_PIS
77_080814104636

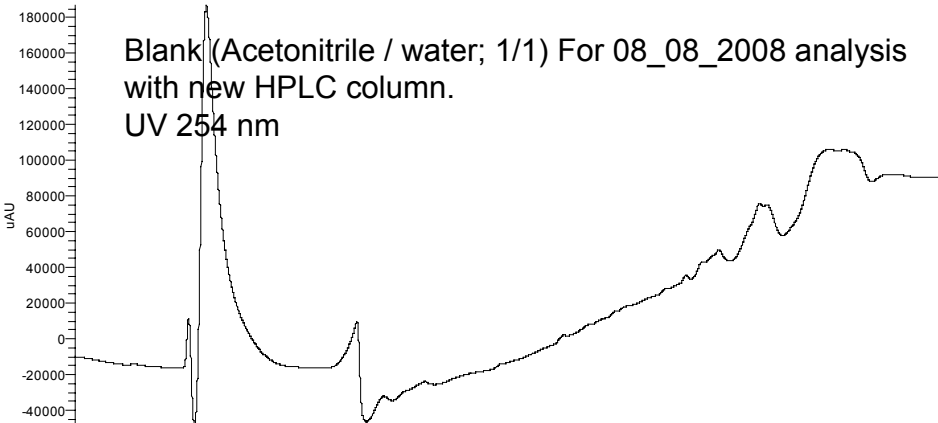
Detected in blank acetonitrile/water,
1/1 mix;
See last slide for chromatogram of
blank solution



XIC
100-800 amu

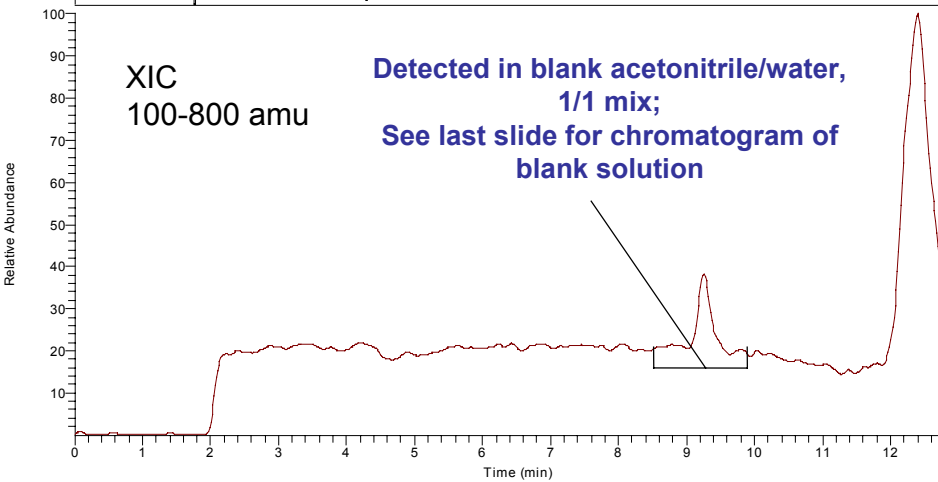
NL: 1.70E8
m/z= 100.00-800.00 F: +
p sid=-10.00 Q1MS [
50.00-1200.00] MS
08_08_2008_UCSF_PIS
77_080814104636

RT: 0.00 - 13.04 SM: 15G



Blank (Acetonitrile / water; 1/1) For 08_08_2008 analysis
with new HPLC column.
UV 254 nm

NL: 1.86E5
Channel A UV
08_22_2008_UCSF_P
URITY_A30



XIC
100-800 amu

Detected in blank acetonitrile/water,
1/1 mix;
See last slide for chromatogram of
blank solution

NL: 2.05E8
m/z= 100.00-800.00 F:
+ p sid=-10.00 Q1MS
[50.00-1200.00] MS
08_22_2008_UCSF_P
URITY_A30