LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096312.D
Acq On : 30 Jun 2017 00:43
Operator : SJ/MA
Sample : I3882-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G56-0-1.5

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.781	283	288	291	rBV	20196	27970	2.15%	0.237%
2	4.322	377	380	387	rVB	56663	68885	5.28%	0.584%
3	4.951	484	487	495	rVB	362607	380334	29.17%	3.222%
4	5.375	550	559	563	rBV	531303	463095	35.52%	3.924%
5	6.392	728	732	738	rBV	806082	655299	50.26%	5.552%
6	6.534	752	756	760	rBV	635592	529859	40.64%	4.489%
7	6.769	793	796	800	rBV	1146855	1019765	78.21%	8.640%
8	6.834	804	807	813	rVB2	16712	17298	1.33%	0.147%
9	6.928	819	823	826	rBV	594510	477064	36.59%	4.042%
10	7.322	883	890	894	rBV	439078	373753	28.67%	3.167%
11	8.051	1010	1014	1017	rBV	1480713	1303821	100.00%	11.047%
12	8.075	1017	1018	1020	rVB	35686	17160	1.32%	0.145%
13	8.492	1084	1089	1093	rBV2	21951	27856	2.14%	0.236%
14	8.657	1113	1117	1120	rBV	34793	32787	2.51%	0.278%
15	8.763	1131	1135	1139	rVB2	29022	29589	2.27%	0.251%
16	8.863	1149	1152	1157	rVB2	19734	16967	1.30%	0.144%
17	9.086	1188	1190	1193	rVB2	20180	16879	1.29%	0.143%
18	9.128	1193	1197	1200	rBV	811650	623868	47.85%	5.286%
19	9.222	1209	1213	1220	rBV2	45903	55442	4.25%	0.470%
20	9.392	1238	1242	1248	rVB6	13436	25994	1.99%	0.220%
21	9.469	1252	1255	1257	rBV2	20159	17834	1.37%	0.151%
22	9.522	1261	1264	1266	rBV	78378	67648	5.19%	0.573%
23	9.692	1291	1293	1297	rVB3	14612	17813	1.37%	0.151%
24	9.751	1301	1303	1306	rVB	45322	32705	2.51%	0.277%
25	9.804	1307	1312	1316	rBV	1195283	1091756	83.74%	9.250%
26	10.010	1344	1347	1350	rVB2	29489	23127	1.77%	0.196%
27	10.075	1355	1358	1362	rVB4	15995	14374	1.10%	0.122%
28	10.127	1362	1367	1369	rBV4	10234	14176	1.09%	0.120%
29	10.216	1378	1382	1385	rBV3	12625	17480	1.34%	0.148%
30	10.251	1385	1388	1390	rVB	47555	39676	3.04%	0.336%
31	10.469	1422	1425	1430	rVV2	27715	31948	2.45%	0.271%
32	10.504	1430	1431	1437	rVB4	11919	17297	1.33%	0.147%
33	10.586	1442	1445	1449	rBV3	49565	40333	3.09%	0.342%
34	10.722	1465	1468	1469	rBV	64404	54450	4.18%	0.461%

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.733	1469	1470	1474	rVB	48452	41071	3.15%	0.348%
36	11.086	1528	1530	1536	rVB4	12332	14793	1.13%	0.125%
37	11.169	1541	1544	1547	rVV2	47845	49181	3.77%	0.417%
38	11.198	1547	1549	1554	rVB	32349	29742	2.28%	0.252%
39	11.286	1560	1564	1566	rBV	1064690	884040	67.80%	7.490%
40	11.310	1566	1568	1571	rVV	127731	96400	7.39%	0.817%
41	11.357	1572	1576	1579	rVB2	48527	48905	3.75%	0.414%
42	11.510	1600	1602	1606	rVB3	12264	14761	1.13%	0.125%
43	11.551	1606	1609	1612	rBV5	13145	17344	1.33%	0.147%
44	11.592	1614	1616	1619	rBV	34791	29621	2.27%	0.251%
45	11.786	1646	1649	1651	rBV2	23005	22628	1.74%	0.192%
46	11.816	1651	1654	1656	rVB	52160	40142	3.08%	0.340%
47	11.898	1664	1668	1670	rBV2	33265	40532	3.11%	0.343%
48	11.998	1683	1685	1687	rVB	21955	17917	1.37%	0.152%
49	12.080	1697	1699	1701	rBV2	19942	15452	1.19%	0.131%
50	12.339	1740	1743	1745	rBV3	39362	40751	3.13%	0.345%
51	12.386	1749	1751	1754	rVB2	31823	27546	2.11%	0.233%
52	12.492	1766	1769	1772	rBV	196054	163515	12.54%	1.385%
53	12.721	1803	1808	1811	rBV	182532	185667	14.24%	1.573%
54	12.763	1813	1815	1816	rVB	26902	17001	1.30%	0.144%
55	12.868	1830	1833	1836	rBV	551012	475933	36.50%	4.032%
56	13.115	1872	1875	1878	rVB	51050	46753	3.59%	0.396%
57	13.351	1912	1915	1921	rVB	123011	117692	9.03%	0.997%
58	13.457	1931	1933	1936	rVB3	46103	34985	2.68%	0.296%
59	13.768	1984	1986	1991	rVB2	81032	98570	7.56%	0.835%
60	13.915	2007	2011	2014	rBV	1028650	1006870	77.22%	8.531%
61	15.345	2250	2254	2258	rVB	505133	580684	44.54%	4.920%

Sum of corrected areas: 11802798

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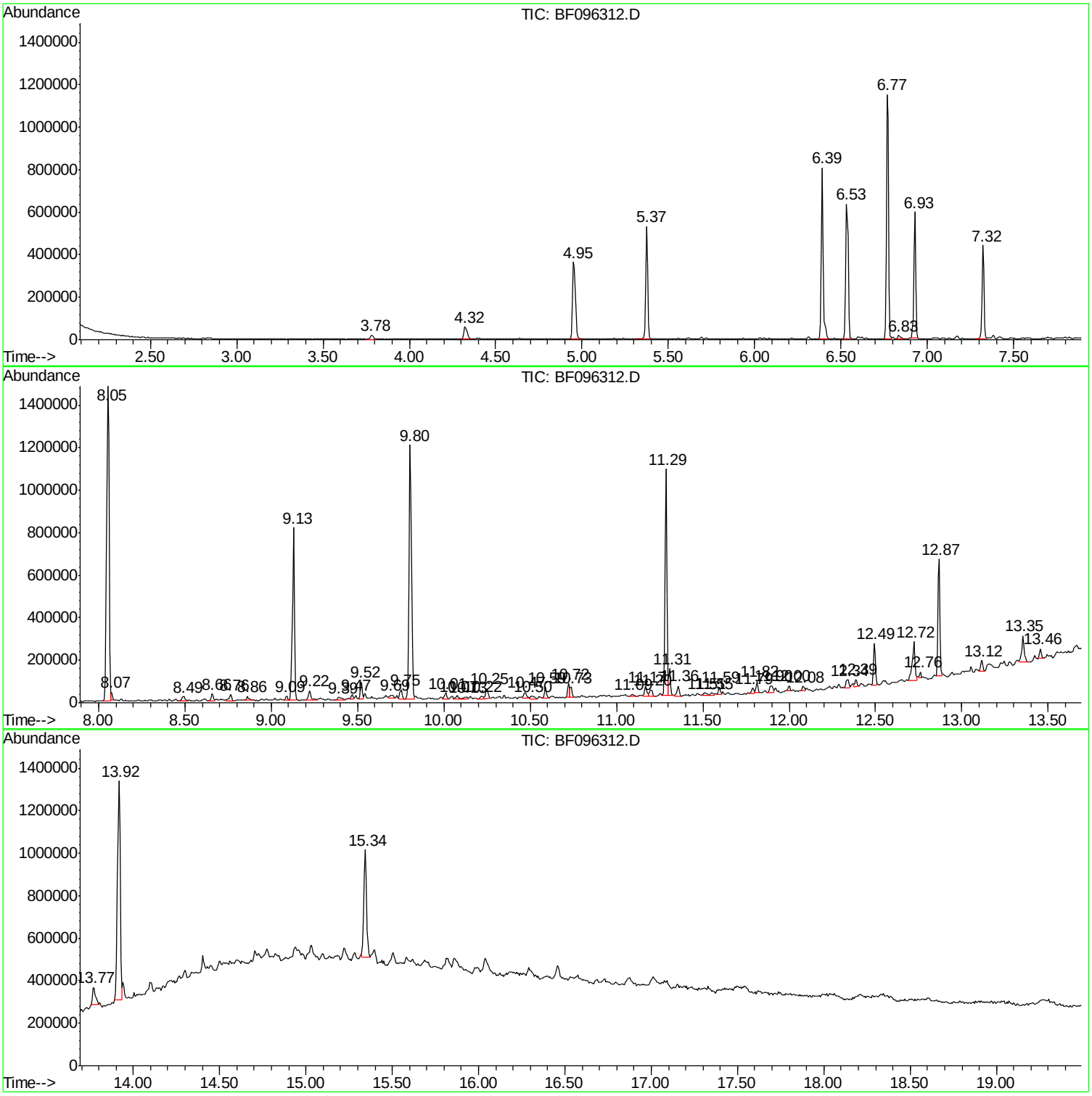
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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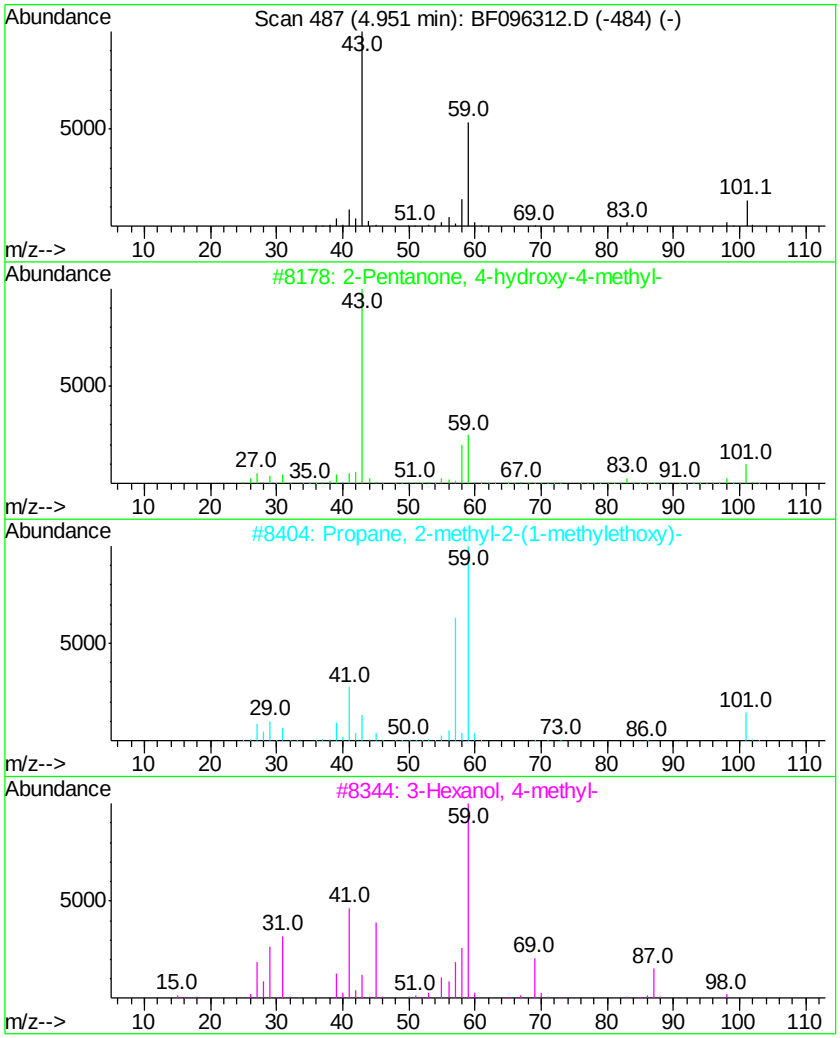
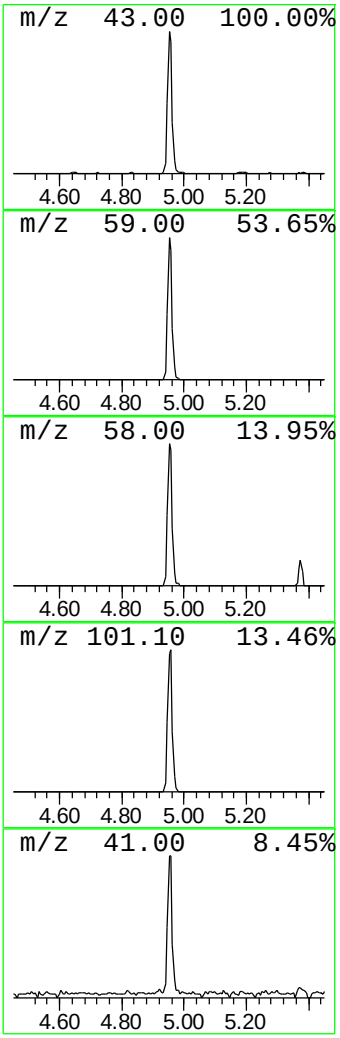
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	7.46 ng	380334	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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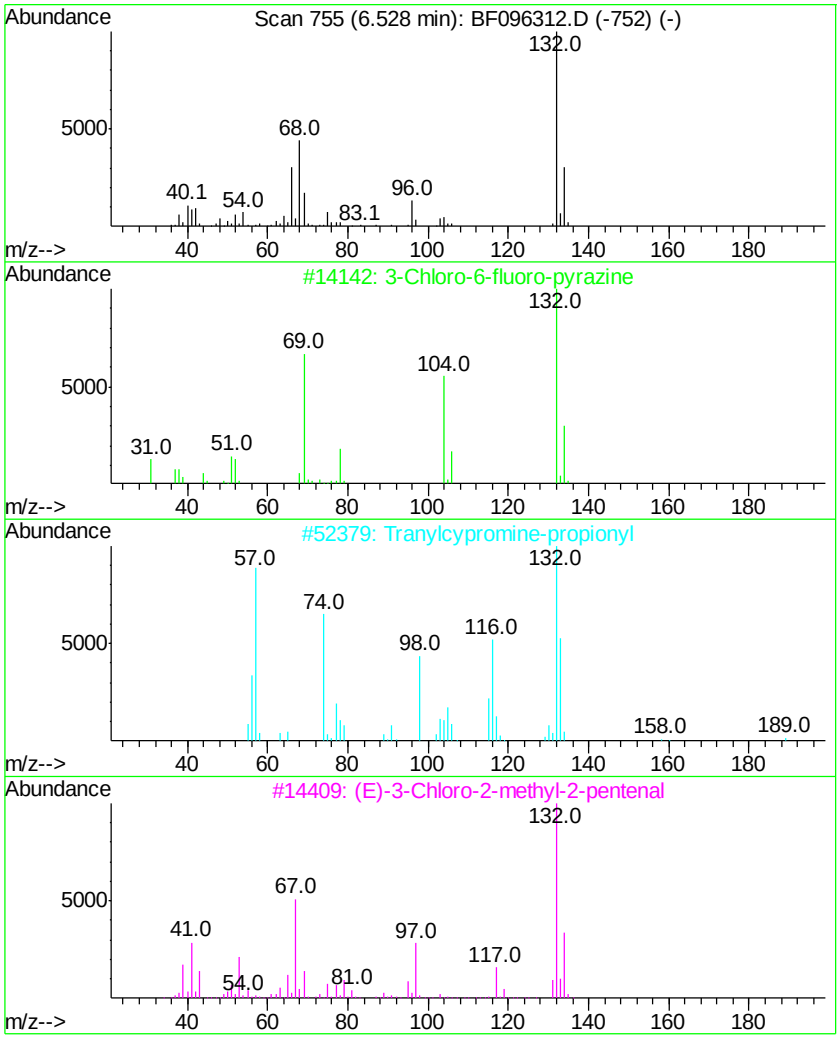
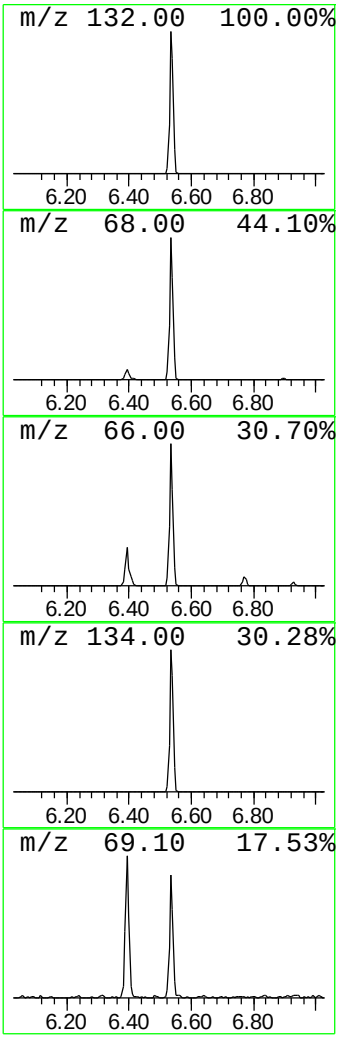
****

Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	10.39 ng	529859	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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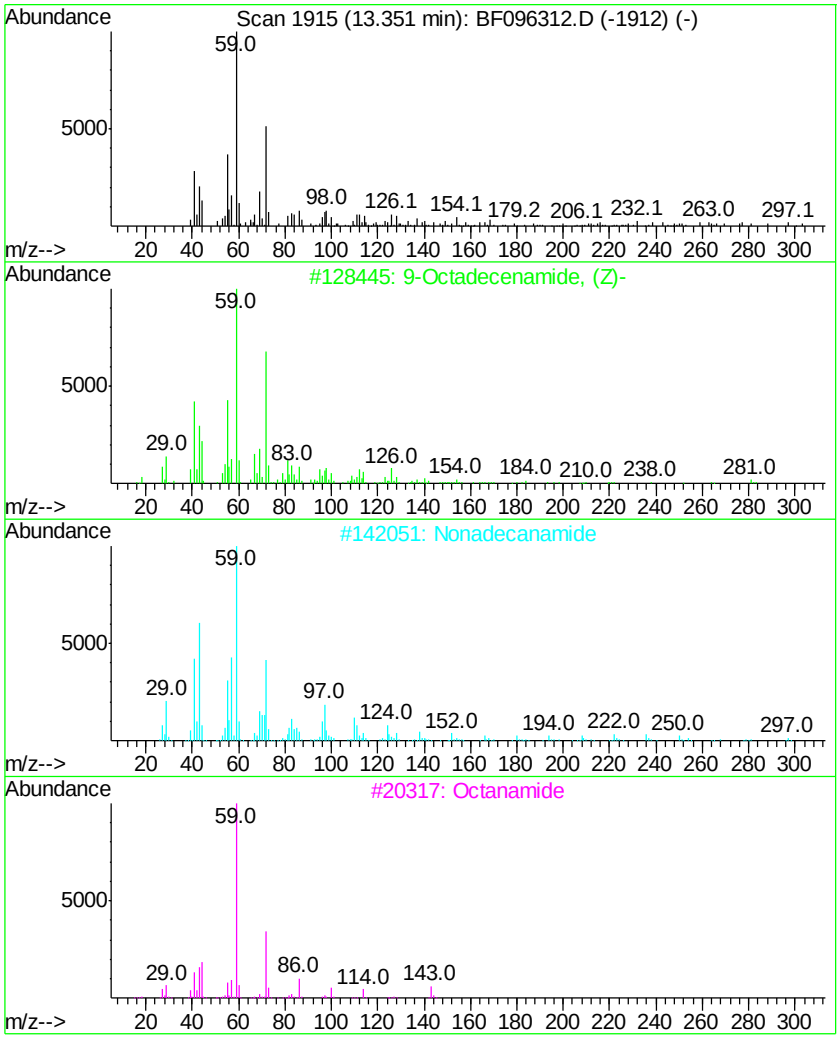
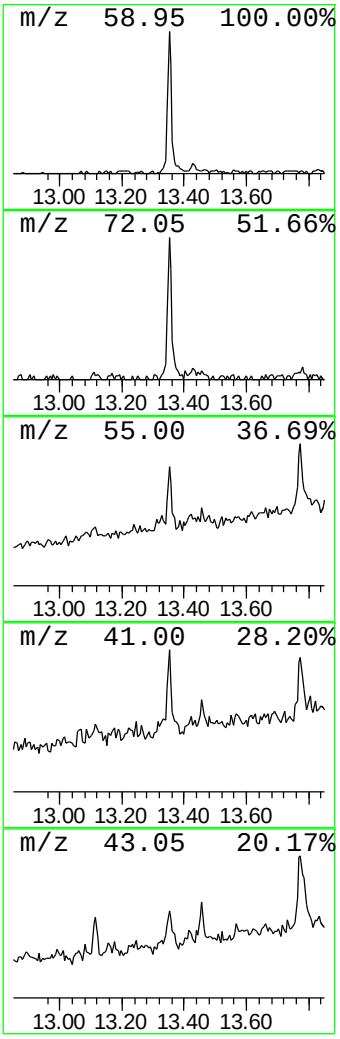
****

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	2.34 ng	117692	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2	Nonadecanamide	297	C19H39NO	058185-32-3	78
3	Octanamide	143	C8H17NO	000629-01-6	64
4	Acetic acid, bromo-, methyl ester	152	C3H5BrO2	000096-32-2	64
5	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59





Tentatively Identified Compound (LSC) summary

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TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.95	7.5	ng	380334	1	6.77	1019770	20.0
unknown6.53	6.53	10.4	ng	529859	1	6.77	1019770	20.0
9-Octadecenamide,...	13.35	2.3	ng	117692	5	13.92	1006870	20.0