

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
 Data File : BF098707.D
 Acq On : 22 Sep 2017 20:21
 Operator : SJ/JU
 Sample : I5330-01 5X
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HD-01-092017

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

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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	5.140	515	519	528	rVB	112488	108694	8.06%	0.861%
2	5.534	582	586	589	rBV	695800	649310	48.18%	5.145%
3	6.534	752	756	763	rBV	858261	677740	50.29%	5.370%
4	6.687	778	782	786	rBV	832833	692639	51.39%	5.488%
5	6.928	819	823	826	rBV	1117895	918549	68.16%	7.278%
6	7.081	845	849	852	rBV	532714	408679	30.32%	3.238%
7	7.481	913	917	920	rBV	504117	385355	28.59%	3.053%
8	8.210	1036	1041	1044	rBV	1493162	1256101	93.20%	9.952%
9	9.280	1217	1223	1226	rBV	758468	619655	45.98%	4.910%
10	9.563	1262	1271	1276	rBV	18128	32099	2.38%	0.254%
11	9.669	1286	1289	1293	rBV	106575	82714	6.14%	0.655%
12	9.963	1335	1339	1343	rVB	1632446	1347733	100.00%	10.678%
13	10.351	1398	1405	1409	rBV7	16714	39747	2.95%	0.315%
14	10.386	1409	1411	1414	rVB	28956	22019	1.63%	0.174%
15	10.745	1468	1472	1478	rVB	538988	423446	31.42%	3.355%
16	10.857	1488	1491	1499	rBV	32468	38727	2.87%	0.307%
17	11.304	1565	1567	1570	rBV	20817	17421	1.29%	0.138%
18	11.451	1588	1592	1595	rBV	1530860	1299121	96.39%	10.293%
19	11.833	1654	1657	1660	rBV	52287	39426	2.93%	0.312%
20	11.963	1674	1679	1683	rBV2	54460	71191	5.28%	0.564%
21	12.521	1771	1774	1775	rBV	161966	135840	10.08%	1.076%
22	12.539	1775	1777	1783	rVB2	133930	115269	8.55%	0.913%
23	12.621	1789	1791	1794	rBV2	22409	20714	1.54%	0.164%
24	12.657	1794	1797	1804	rVV2	55706	68208	5.06%	0.540%
25	12.745	1809	1812	1820	rBV6	33653	51364	3.81%	0.407%
26	12.886	1834	1836	1841	rVB2	44389	53045	3.94%	0.420%
27	13.027	1857	1860	1864	rBV	713659	593366	44.03%	4.701%
28	13.104	1870	1873	1875	rBV4	12576	17161	1.27%	0.136%
29	13.563	1948	1951	1954	rBV2	35015	33279	2.47%	0.264%
30	13.598	1954	1957	1961	rVV	35187	36819	2.73%	0.292%
31	13.915	2008	2011	2015	rBV2	51680	69866	5.18%	0.554%
32	13.951	2015	2017	2023	rVB	38849	37044	2.75%	0.294%
33	14.086	2036	2040	2043	rBV	1087622	937003	69.52%	7.424%
34	14.545	2116	2118	2123	rVB	35263	33923	2.52%	0.269%

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35	14.939	2182	2185	2189	rVB	168144	166856	12.38%	1.322%
36	15.210	2228	2231	2234	rBV	47535	48936	3.63%	0.388%
37	15.580	2289	2294	2304	rVB	789115	1072136	79.55%	8.495%

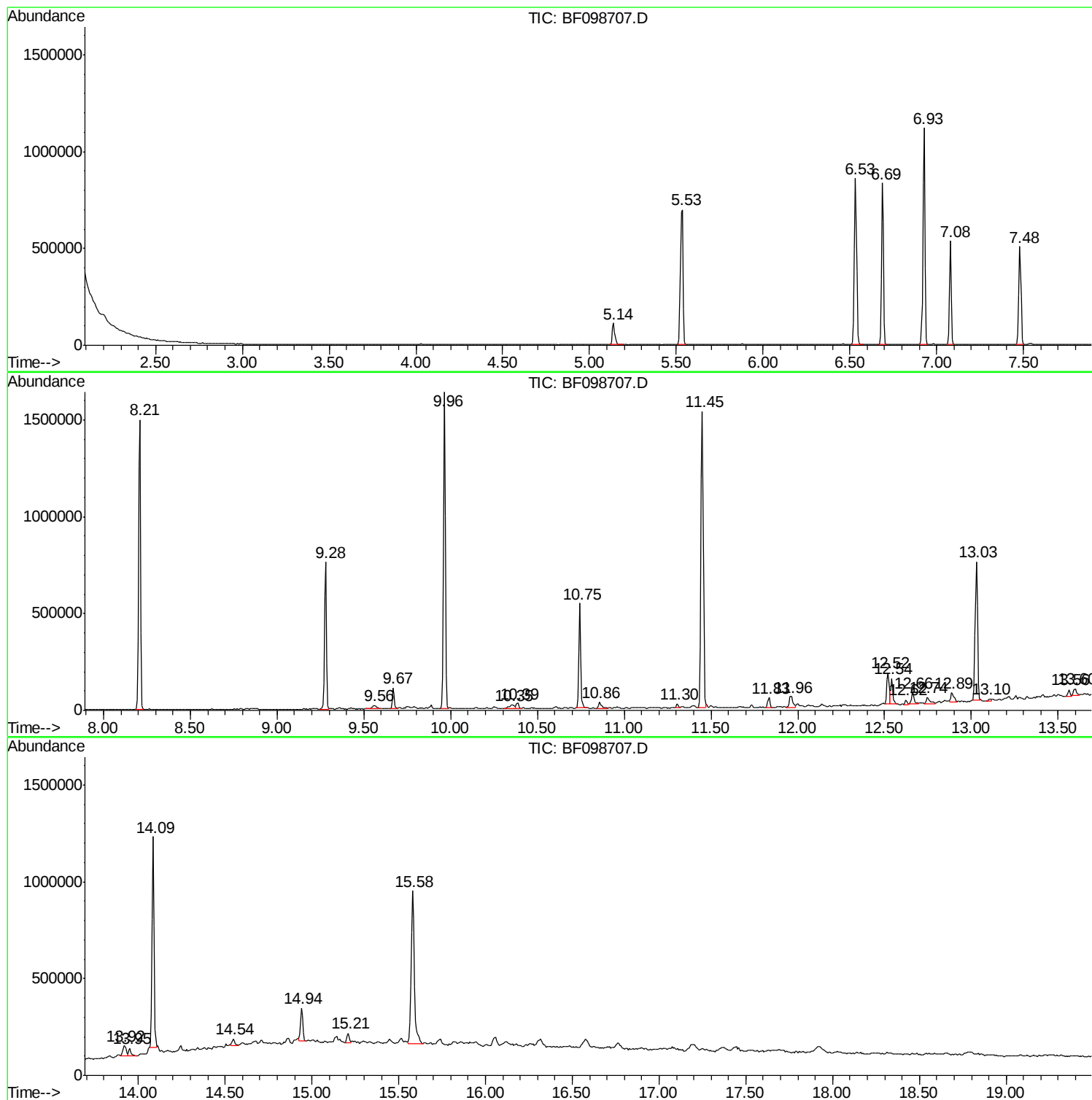
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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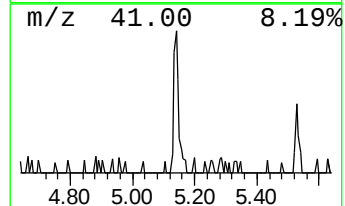
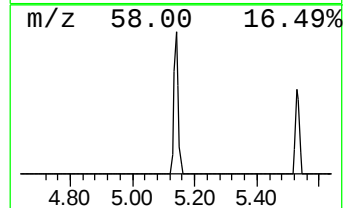
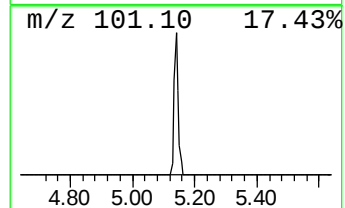
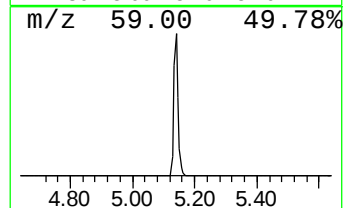
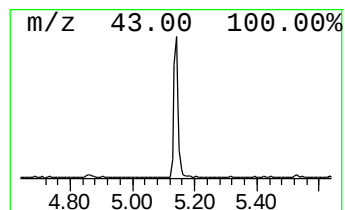
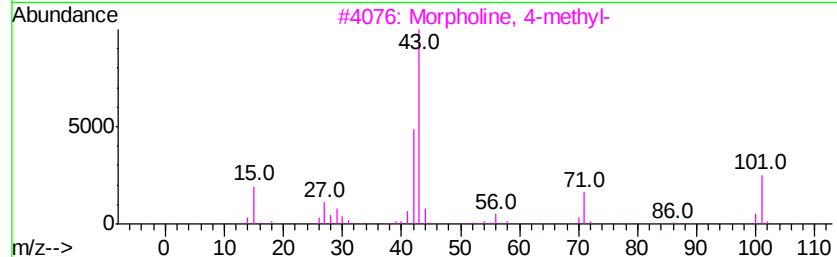
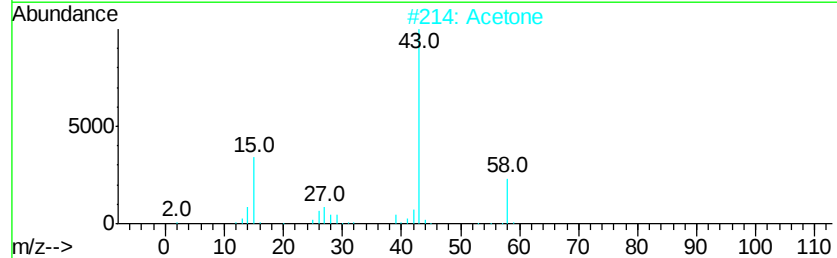
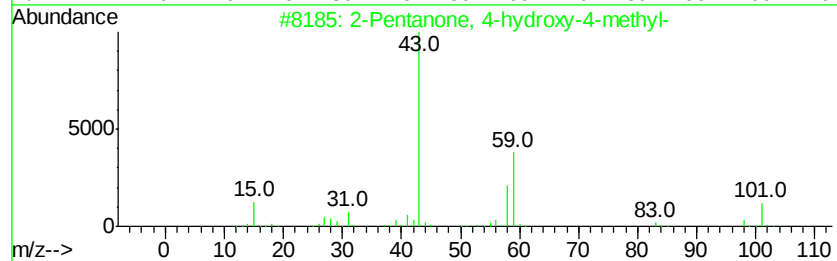
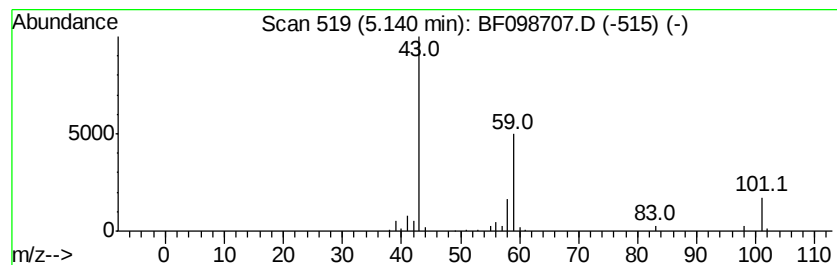
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	2.37 ng	108694	1,4-Dichlorobenzene-d4	6.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetone	58	C3H6O	000067-64-1	9
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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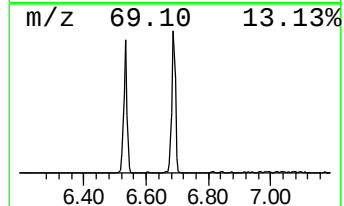
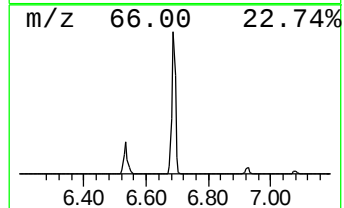
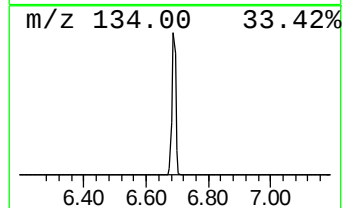
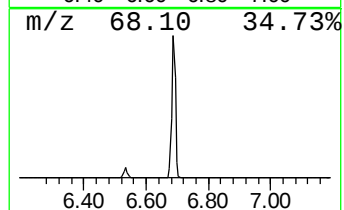
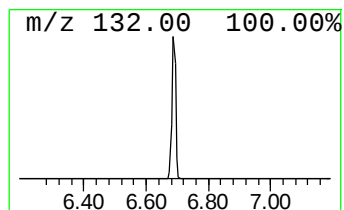
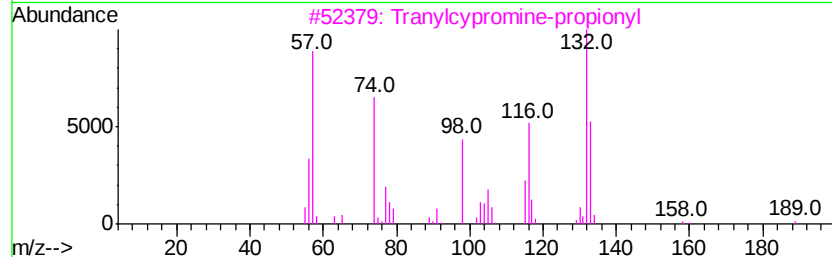
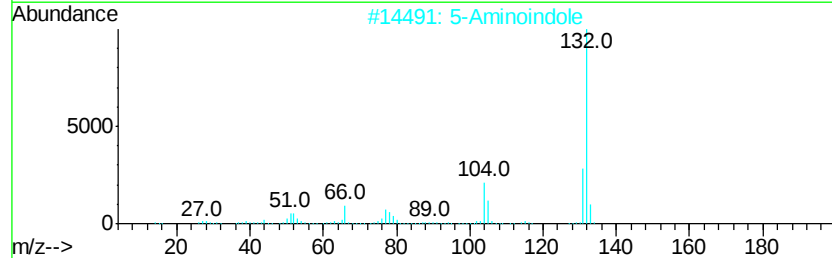
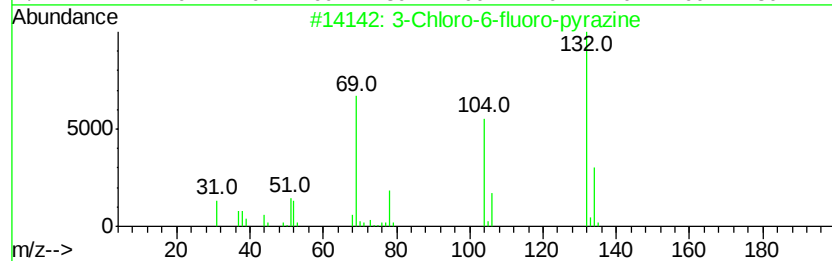
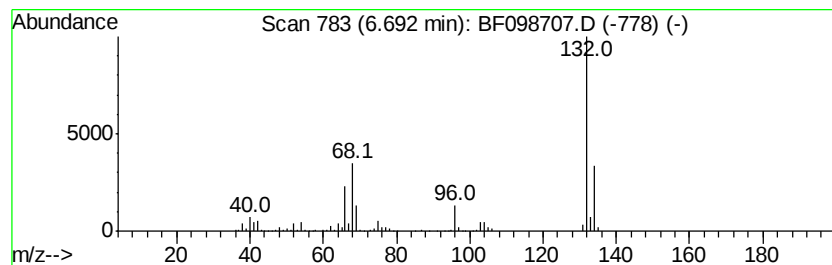
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Peak Number 2 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	15.08 ng	692639	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		2H-Cyclopentadlpvridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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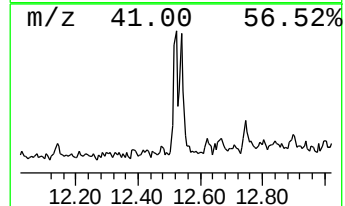
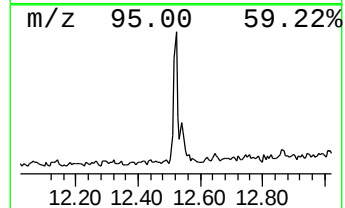
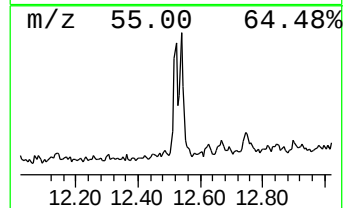
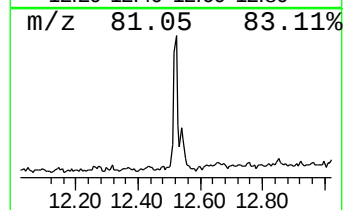
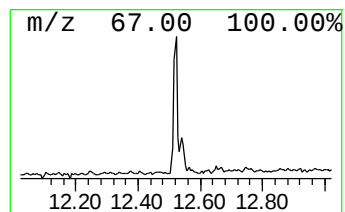
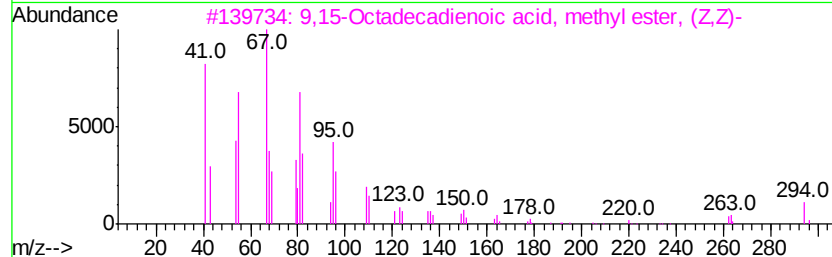
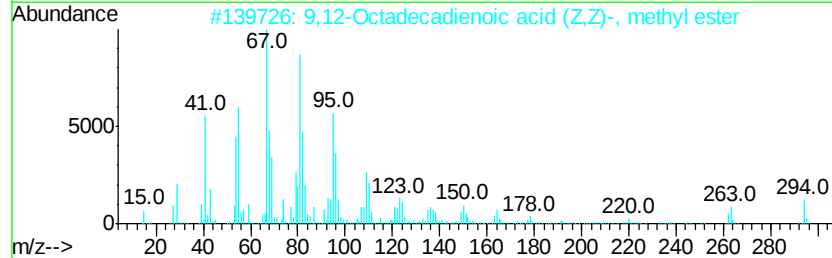
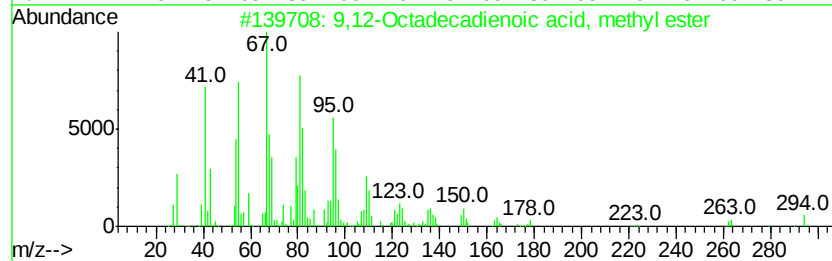
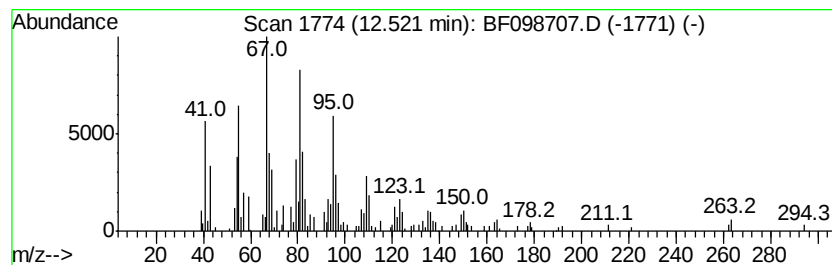
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Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	2.09 ng	135840	Phenanthrene-d10	11.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
3		9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	96
4		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	96
5		Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	95



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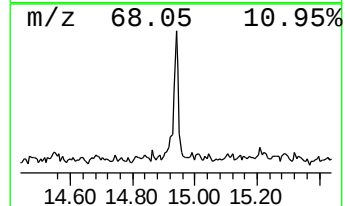
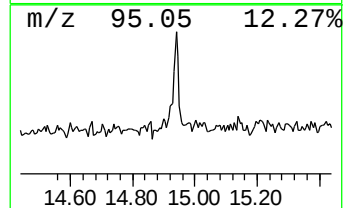
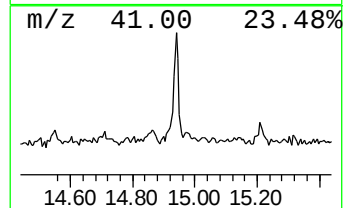
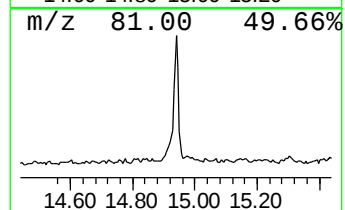
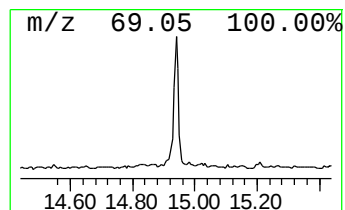
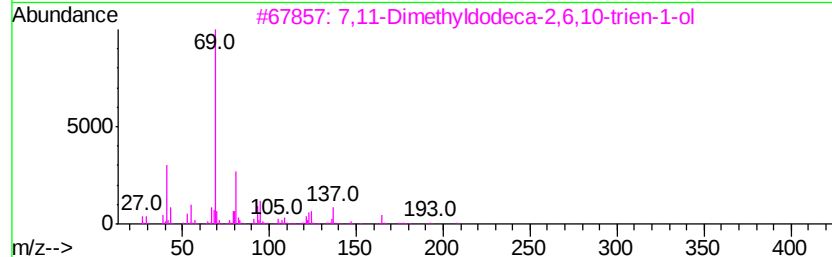
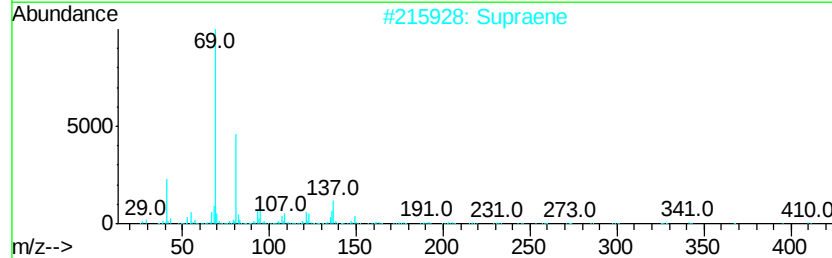
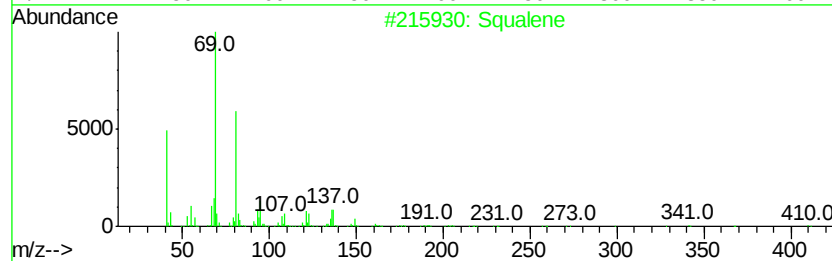
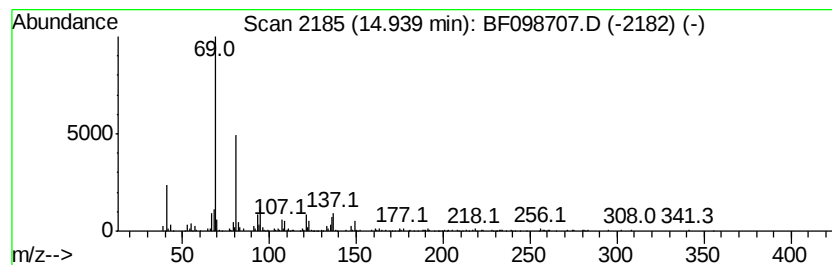
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Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	3.11 ng	166856	Perylene-d12	15.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	83
4		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
5		Farnesol isomer a	222	C15H26O	1000108-92-4	72



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	2.4	ng	108694	1	6.93	918549	20.0
unknown6.69	6.69	15.1	ng	692639	1	6.93	918549	20.0
9,12-Octadecadien...	12.52	2.1	ng	135840	4	11.45	1299120	20.0
Squalene	14.94	3.1	ng	166856	6	15.58	1072140	20.0