

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081718\
 Data File : BF108243.D
 Acq On : 17 Aug 2018 15:15
 Operator : JU/SJ
 Sample : J4500-13 2X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-7

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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	5.243	490	494	503	rBV	334020	340850	19.48%	1.698%
2	5.637	557	561	564	rBV	1737283	1514317	86.55%	7.545%
3	6.625	725	729	742	rBV	1623949	1599603	91.43%	7.970%
4	6.784	752	756	759	rBV	1812457	1597955	91.33%	7.961%
5	7.013	792	795	799	rBV	1063895	886276	50.66%	4.416%
6	7.172	818	822	825	rBV	1528660	1237289	70.72%	6.165%
7	7.572	886	890	894	rBV	1203973	995941	56.92%	4.962%
8	8.301	1010	1014	1017	rBV	1171599	1079828	61.72%	5.380%
9	9.366	1192	1195	1199	rBV	1907693	1749589	100.00%	8.717%
10	9.760	1259	1262	1269	rVB	126812	101910	5.82%	0.508%
11	10.060	1309	1313	1324	rBV	1339245	1166382	66.67%	5.811%
12	10.848	1443	1447	1456	rBV	1074397	982998	56.18%	4.898%
13	11.554	1563	1567	1570	rBV	1368476	1132259	64.72%	5.641%
14	11.577	1570	1571	1575	rVB	65415	38279	2.19%	0.191%
15	12.771	1771	1774	1778	rBV	127725	107584	6.15%	0.536%
16	13.007	1807	1814	1819	rBV	121672	138245	7.90%	0.689%
17	13.136	1832	1836	1840	rBV	1877894	1701320	97.24%	8.476%
18	13.383	1874	1878	1883	rBV5	16729	27624	1.58%	0.138%
19	13.695	1927	1931	1934	rBV3	13886	18278	1.04%	0.091%
20	13.824	1949	1953	1955	rBV	35921	45679	2.61%	0.228%
21	14.054	1989	1992	2000	rBV4	46794	90048	5.15%	0.449%
22	14.160	2008	2010	2013	rBV	22781	18435	1.05%	0.092%
23	14.207	2013	2018	2021	rVV	1290584	1279346	73.12%	6.374%
24	14.236	2021	2023	2031	rVB	121643	125259	7.16%	0.624%
25	14.624	2086	2089	2091	rBV2	66347	66761	3.82%	0.333%
26	14.977	2146	2149	2153	rVB2	42019	45317	2.59%	0.226%
27	15.030	2155	2158	2160	rVV2	67653	90266	5.16%	0.450%
28	15.060	2160	2163	2168	rVB	141484	154955	8.86%	0.772%
29	15.295	2200	2203	2207	rBV	66573	100222	5.73%	0.499%
30	15.489	2233	2236	2244	rVB2	49500	79119	4.52%	0.394%
31	15.630	2257	2260	2267	rVB	47779	72054	4.12%	0.359%
32	15.695	2268	2271	2277	rVV	50725	77985	4.46%	0.389%
33	15.771	2278	2284	2298	rVB	881191	1295587	74.05%	6.455%
34	16.230	2359	2362	2369	rVB	71237	113507	6.49%	0.566%

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Integration Parameters: rteint.p
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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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

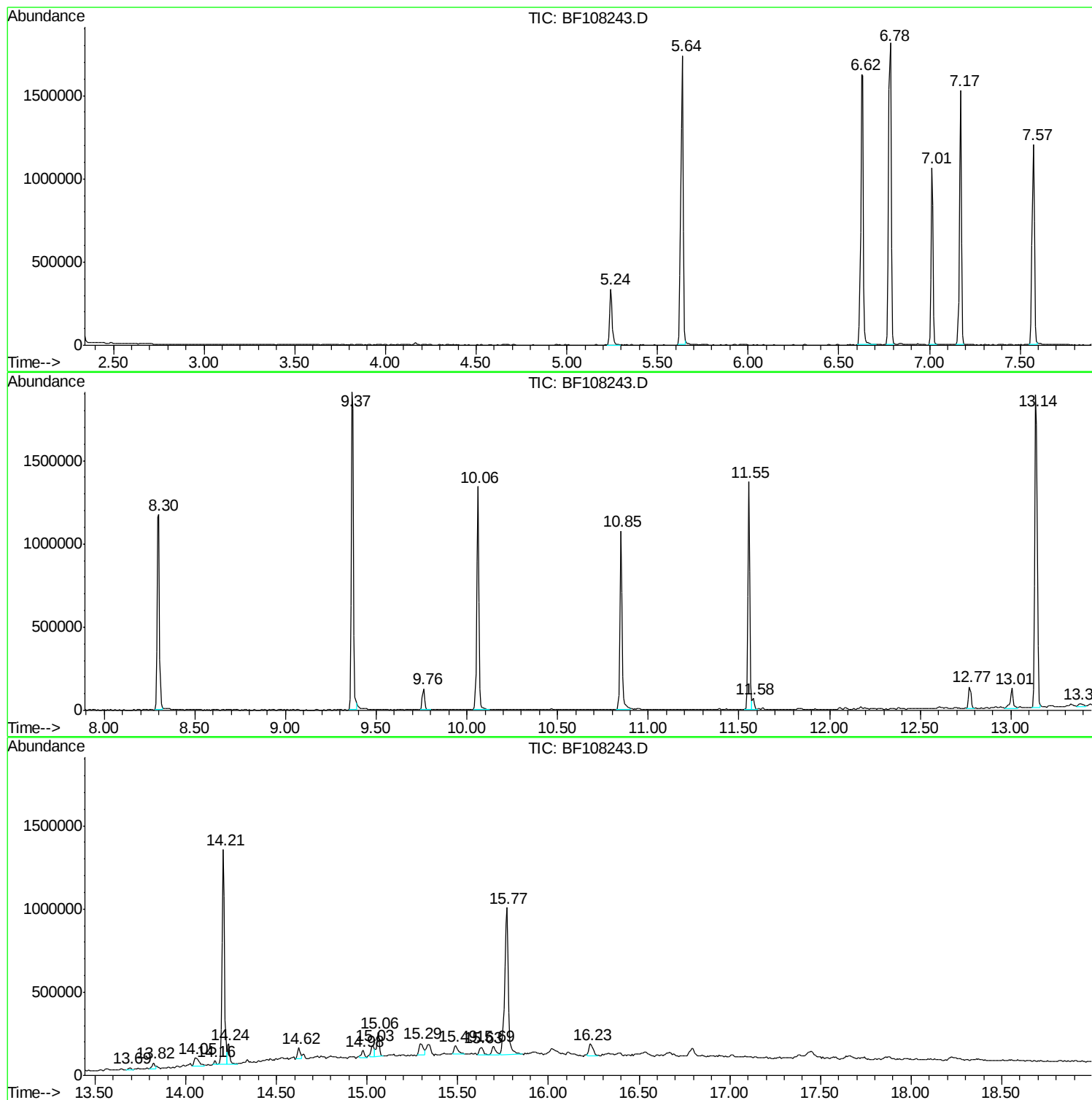
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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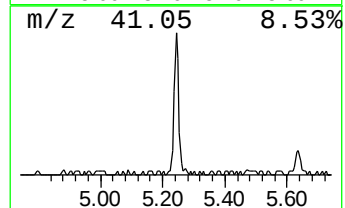
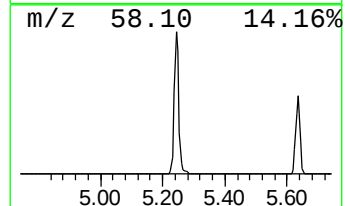
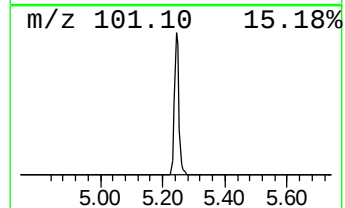
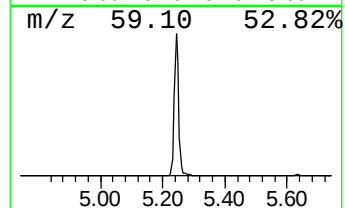
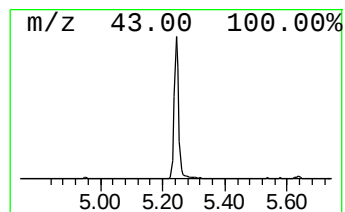
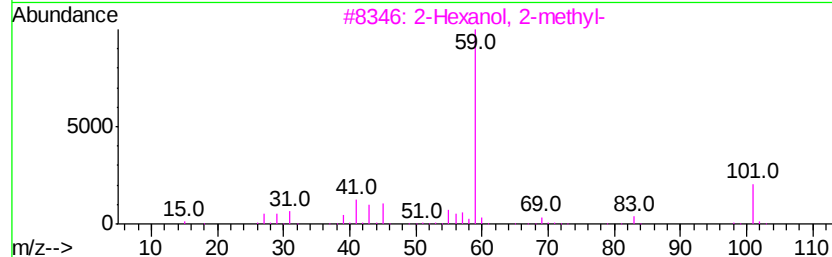
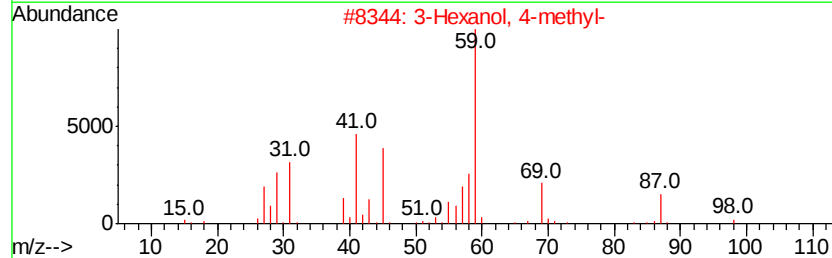
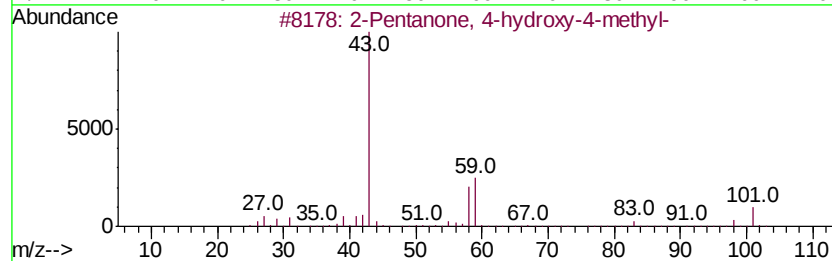
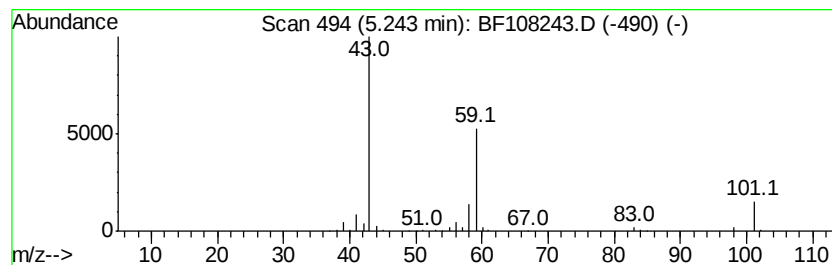
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	7.69 ng	340850	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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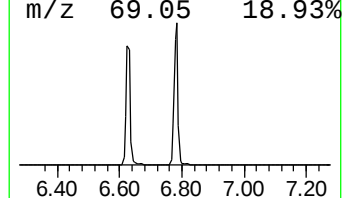
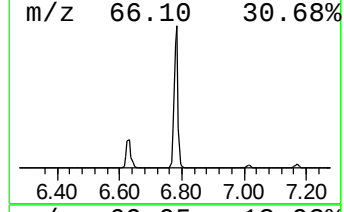
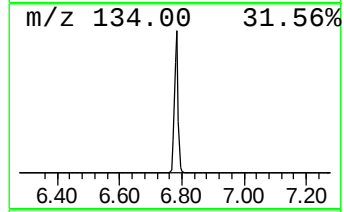
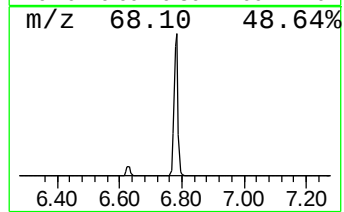
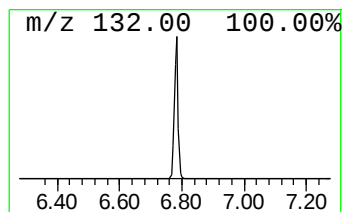
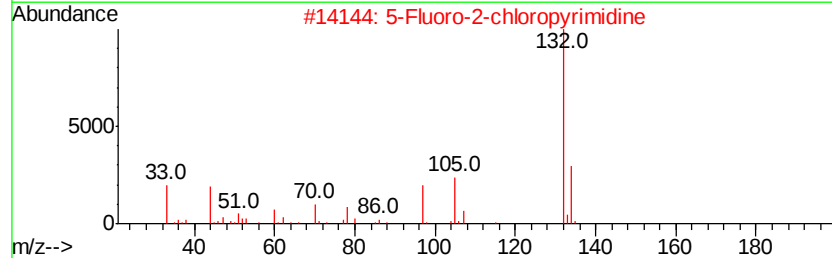
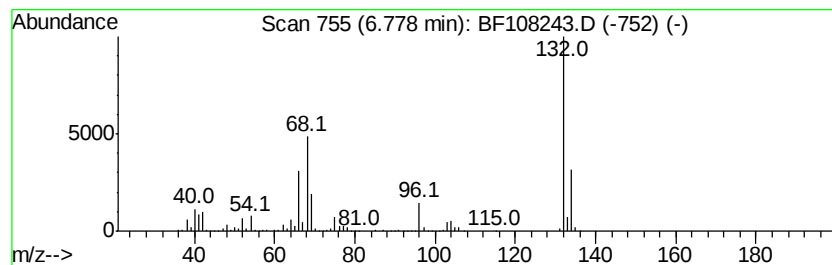
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	36.06 ng	1597960	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16	
3	Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10	
4	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9	
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9	



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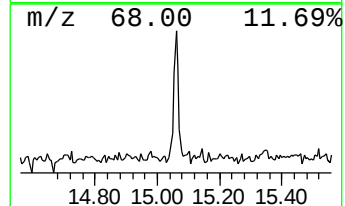
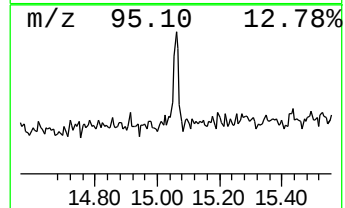
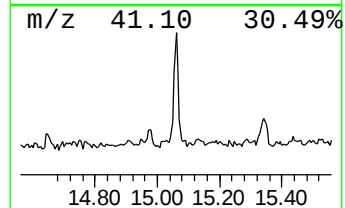
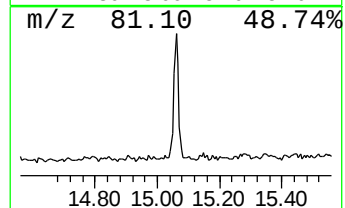
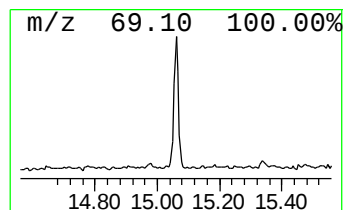
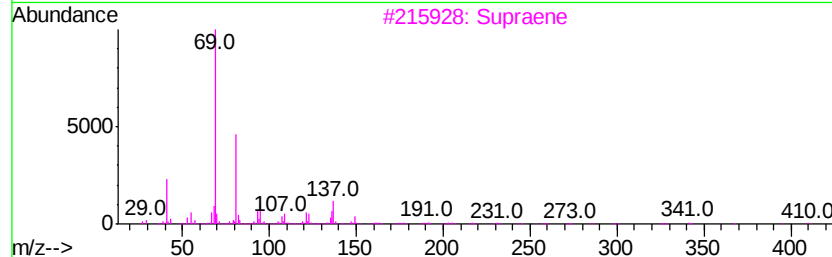
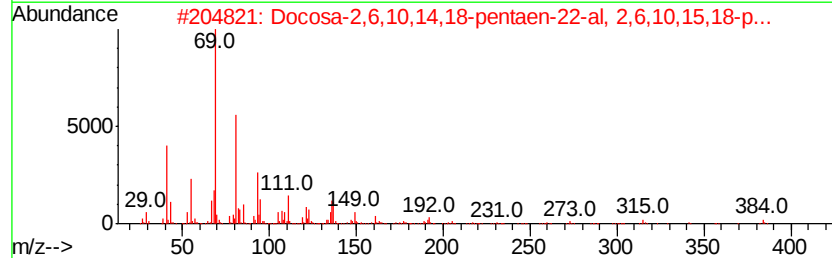
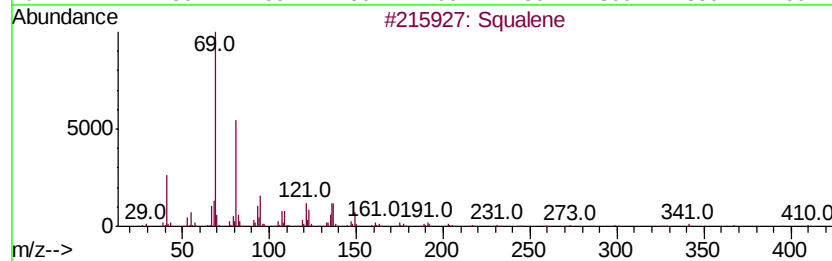
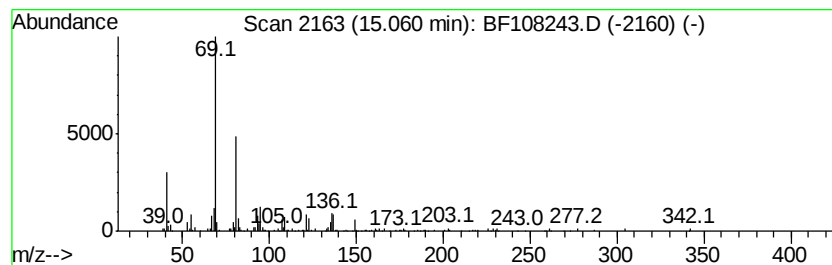
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	2.39 ng	154955	Perylene-d12	15.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	90
2		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
3		Supraene	410	C30H50	007683-64-9	80
4		trans-Farnesol	222	C15H26O	000106-28-5	72
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.24	7.7	ng	340850	1	7.01	886276	20.0
unknown6.78	6.78	36.1	ng	1597960	1	7.01	886276	20.0
Squalene	15.06	2.4	ng	154955	6	15.77	1295590	20.0