

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091718\
 Data File : BF109078.D
 Acq On : 18 Sep 2018 5:50
 Operator : JU/SJ
 Sample : J4907-05
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CBH-128(2)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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	4.901	432	436	449	rVB	159052	179132	4.69%	0.727%
2	5.325	504	508	511	rBV	1343357	1178098	30.84%	4.783%
3	6.348	678	682	689	rBV	986254	769513	20.14%	3.124%
4	6.490	701	706	709	rBV	2326509	2145646	56.16%	8.711%
5	6.719	742	745	749	rBV	1028859	790462	20.69%	3.209%
6	6.878	768	772	775	rBV	3295402	2836727	74.25%	11.517%
7	7.284	835	841	844	rBV	2512670	2394690	62.68%	9.722%
8	8.001	959	963	966	rBV	1173579	895471	23.44%	3.636%
9	9.078	1142	1146	1149	rBV	4198692	3820376	100.00%	15.510%
10	9.466	1209	1212	1216	rBV	252805	214183	5.61%	0.870%
11	9.748	1257	1260	1264	rBV	1067476	909111	23.80%	3.691%
12	10.530	1389	1393	1406	rBV	1616902	1586202	41.52%	6.440%
13	11.225	1508	1511	1515	rBV	1021459	892209	23.35%	3.622%
14	11.536	1559	1564	1568	rVB2	47992	64214	1.68%	0.261%
15	11.766	1600	1603	1607	rBV2	43421	40614	1.06%	0.165%
16	12.689	1757	1760	1769	rVB	70237	77135	2.02%	0.313%
17	12.813	1776	1781	1784	rBV	3970151	3742194	97.95%	15.193%
18	13.395	1876	1880	1882	rBV	47593	44120	1.15%	0.179%
19	13.724	1932	1936	1945	rVB	42767	63638	1.67%	0.258%
20	13.848	1954	1957	1961	rBV	952436	922297	24.14%	3.744%
21	14.707	2099	2103	2107	rVB	210175	199582	5.22%	0.810%
22	14.954	2142	2145	2150	rVB	42479	47145	1.23%	0.191%
23	15.254	2191	2196	2201	rBV	602136	678505	17.76%	2.755%
24	15.307	2202	2205	2210	rVB	39840	46474	1.22%	0.189%
25	15.712	2270	2274	2278	rVB2	33664	44536	1.17%	0.181%
26	17.330	2544	2549	2553	rBV6	24732	48628	1.27%	0.197%

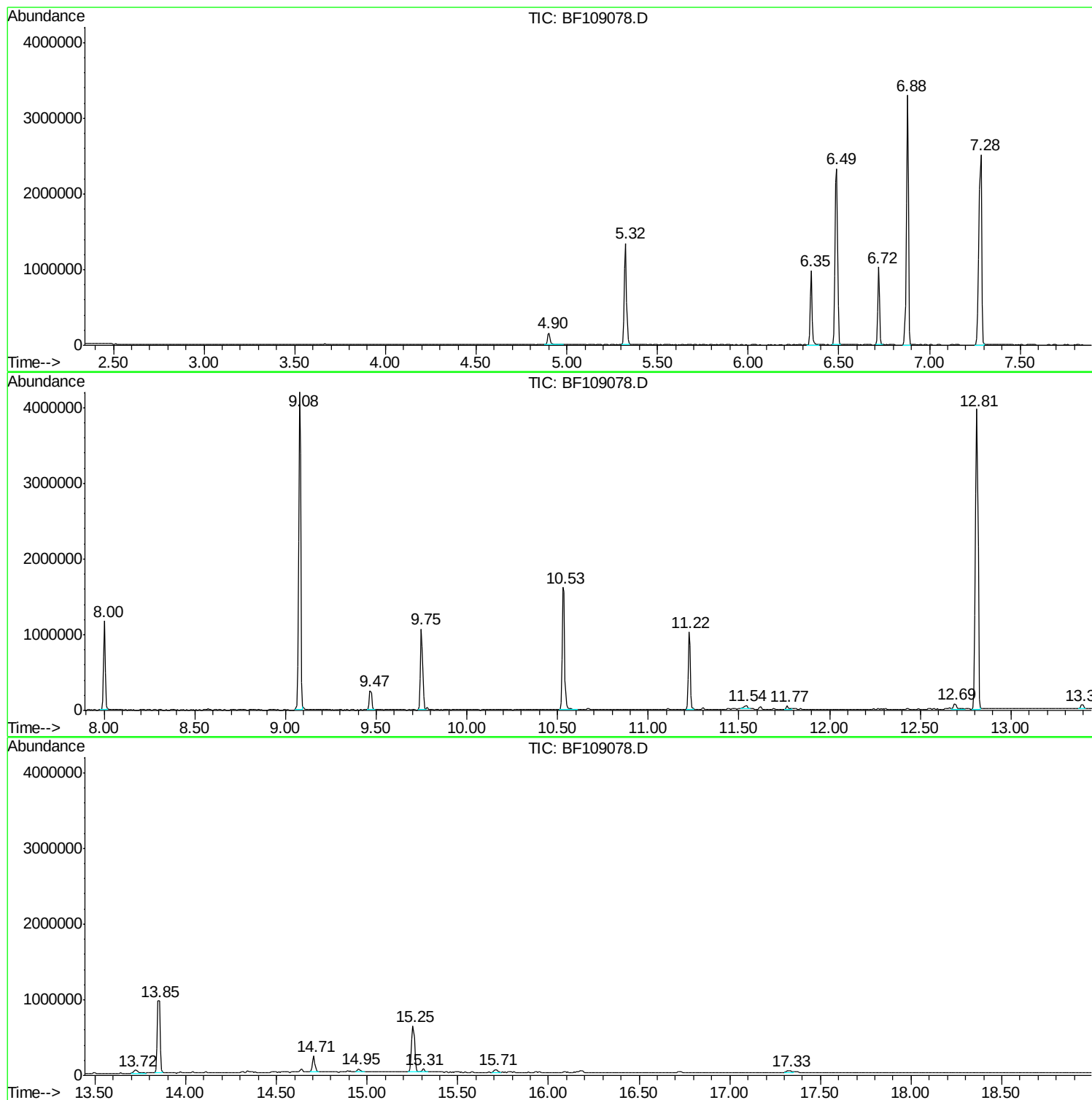
Sum of corrected areas: 24630902

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



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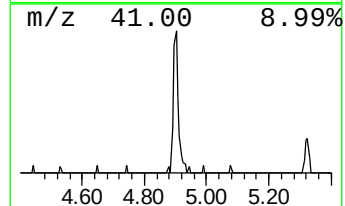
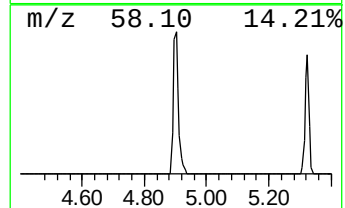
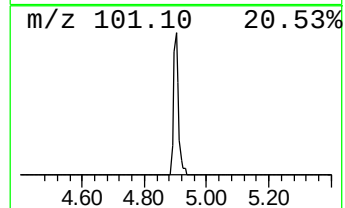
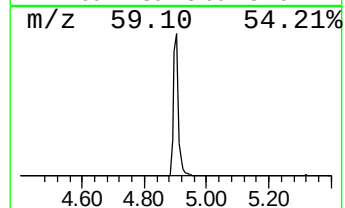
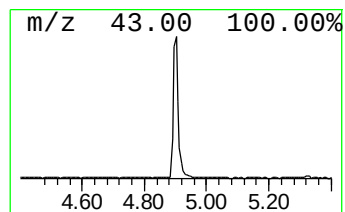
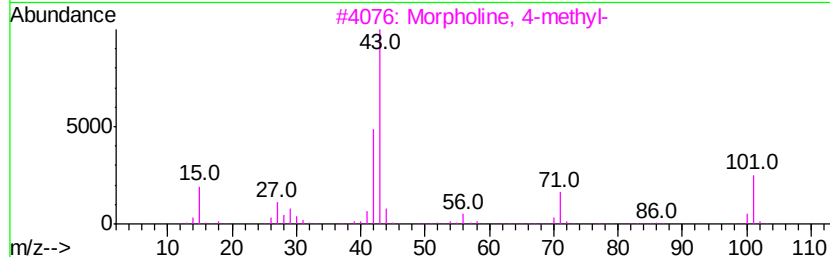
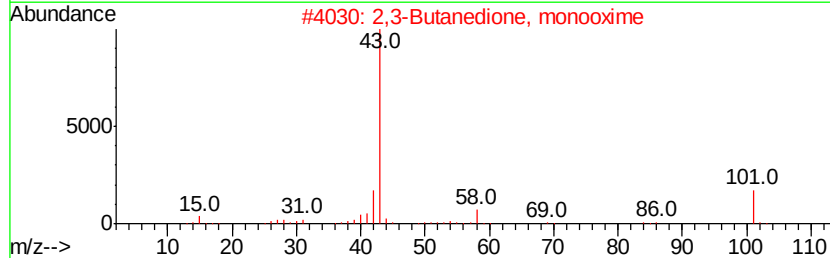
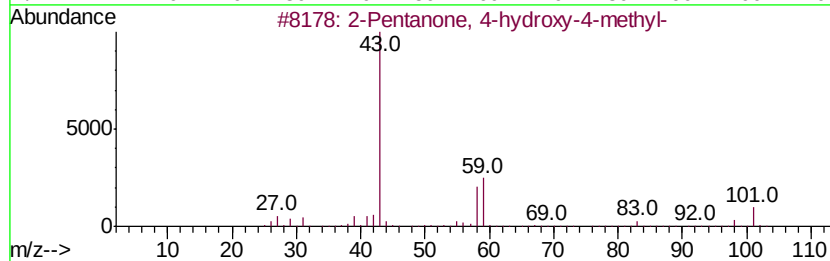
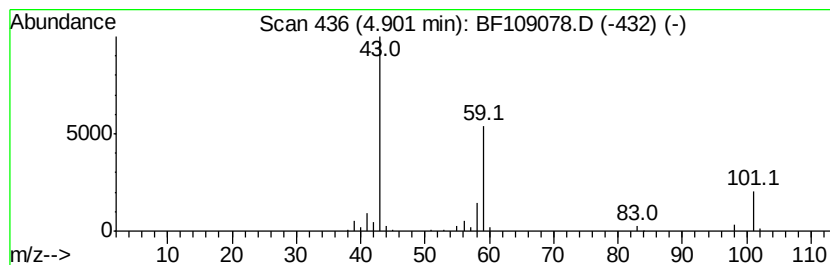
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.90	4.53 ng	179132	1,4-Dichlorobenzene-d4	6.72	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9



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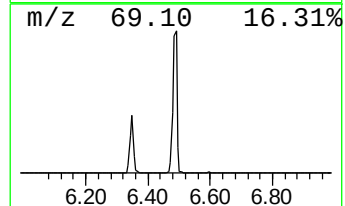
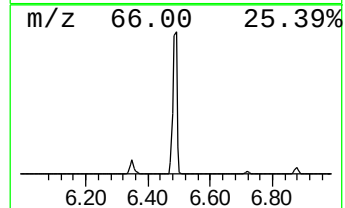
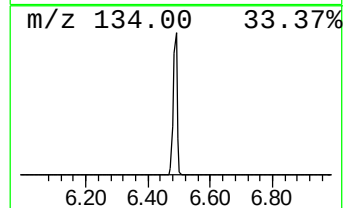
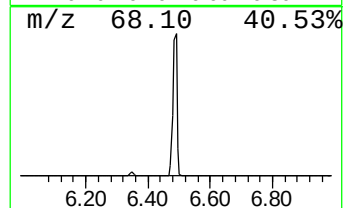
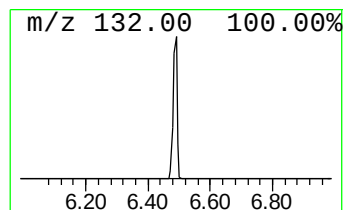
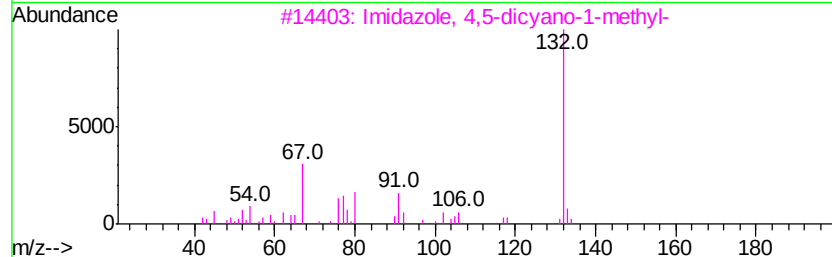
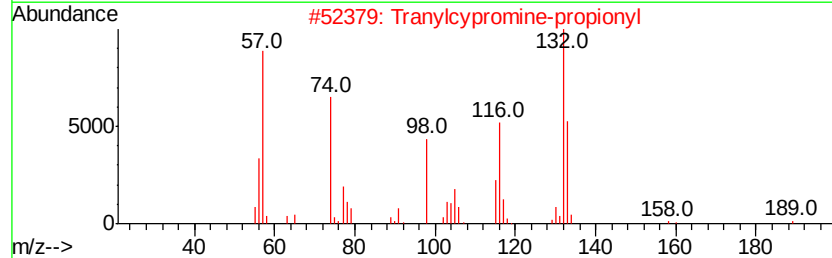
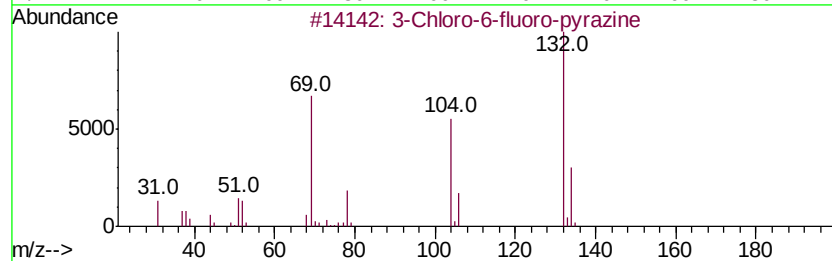
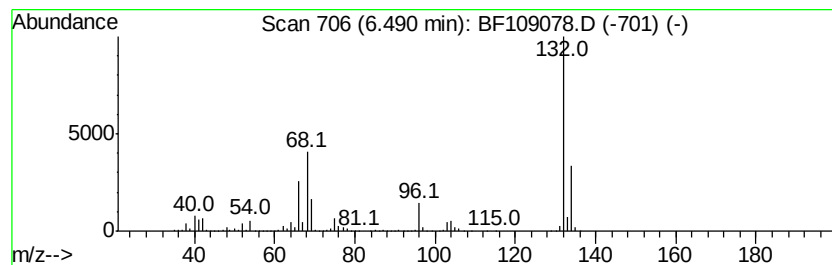
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Peak Number 2 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	54.29 ng	2145650	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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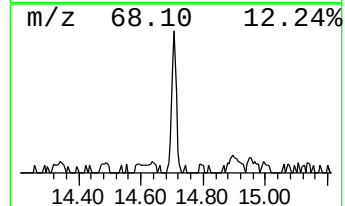
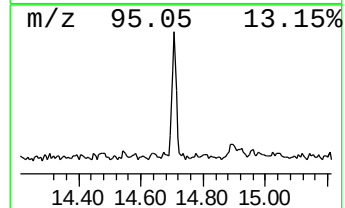
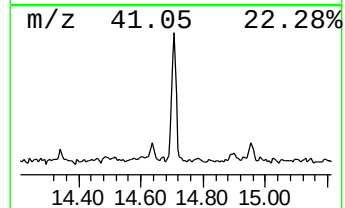
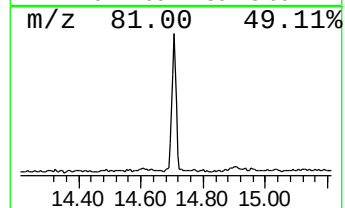
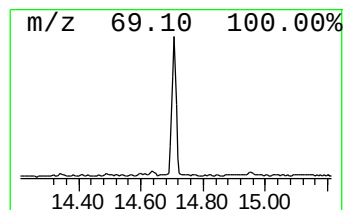
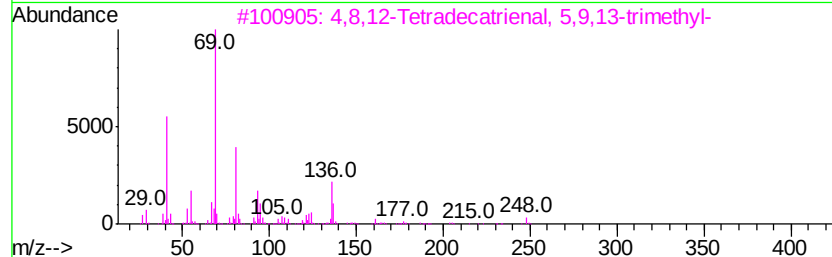
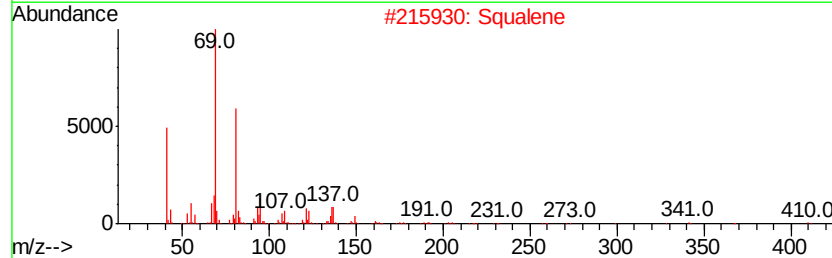
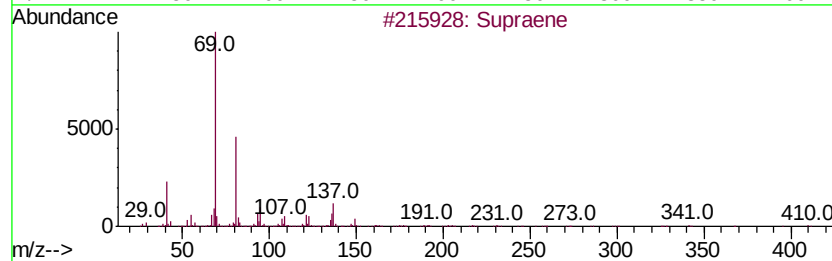
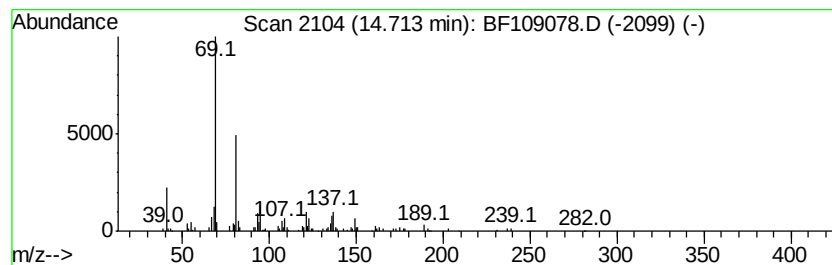
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Peak Number 4 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	5.88 ng	199582	Perylene-d12	15.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	91
2	Squalene		410	C30H50	000111-02-4	91
3	4,8,12-Tetradecatrienal, 5,9,13-...		248	C17H28O	066408-55-7	72
4	1,5-Heptadiene, 3,3,6-trimethyl-		138	C10H18	035387-63-4	52
5	Docosa-2,6,10,14,18-pentaen-22-a...		384	C27H44O	1000163-04-7	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	4.5	ng	179132	1	6.72	790462	20.0
unknown6.49	6.49	54.3	ng	2145650	1	6.72	790462	20.0
Supraene	14.71	5.9	ng	199582	6	15.25	678505	20.0