

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072718\
 Data File : BF107782.D
 Acq On : 28 Jul 2018 8:16
 Operator : JU/SJ
 Sample : J4184-08
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1B

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-BF072018.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	5.196	482	486	494	rBV	215721	256309	5.88%	0.850%
2	5.596	551	554	583	rBV	1093540	1937714	44.43%	6.423%
3	6.601	721	725	744	rBV	514455	1248257	28.62%	4.137%
4	6.737	744	748	771	rVV	2748798	3573311	81.93%	11.844%
5	6.960	783	786	793	rBV	495235	762030	17.47%	2.526%
6	7.119	809	813	845	rVB	2707604	3439608	78.86%	11.401%
7	7.531	879	883	905	rBV	1521744	2571965	58.97%	8.525%
8	7.678	906	908	919	rVB3	41265	71858	1.65%	0.238%
9	8.242	1000	1004	1023	rBV	802666	1114407	25.55%	3.694%
10	9.313	1182	1186	1202	rBV	3590134	4361428	100.00%	14.456%
11	9.707	1249	1253	1256	rBV	188541	181760	4.17%	0.602%
12	10.001	1299	1303	1312	rBV	964947	1000161	22.93%	3.315%
13	10.795	1434	1438	1467	rBV	1745528	2448791	56.15%	8.117%
14	11.495	1553	1557	1565	rBV	703703	912220	20.92%	3.024%
15	11.695	1587	1591	1596	rVB7	24695	44349	1.02%	0.147%
16	13.077	1822	1826	1841	rBV	3134567	3621517	83.04%	12.004%
17	13.954	1972	1975	1981	rVB	86827	90117	2.07%	0.299%
18	14.148	2004	2008	2025	rBV	891261	1198604	27.48%	3.973%
19	14.577	2078	2081	2086	rBV2	43763	59192	1.36%	0.196%
20	14.895	2132	2135	2141	rVB	76019	82316	1.89%	0.273%
21	14.977	2145	2149	2153	rVV	89587	88501	2.03%	0.293%
22	15.248	2192	2195	2200	rVB	71239	82682	1.90%	0.274%
23	15.677	2264	2268	2282	rVB	476572	839971	19.26%	2.784%
24	16.107	2337	2341	2346	rBV2	62786	102043	2.34%	0.338%
25	16.642	2428	2432	2442	rVB3	44047	81358	1.87%	0.270%

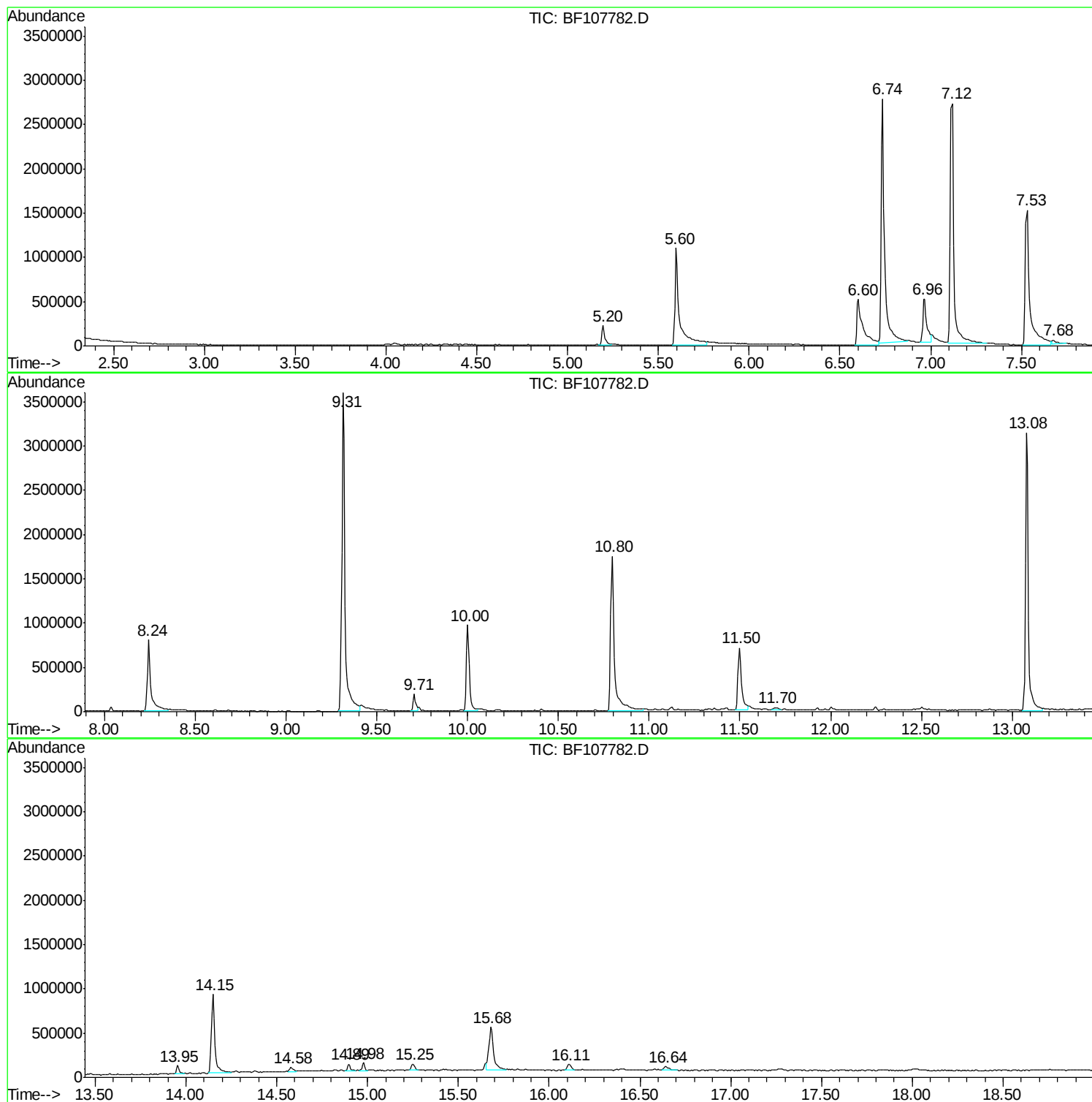
Sum of corrected areas: 30170469

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



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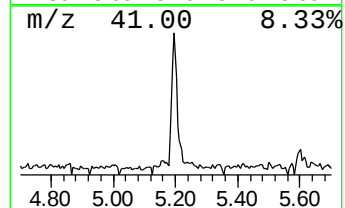
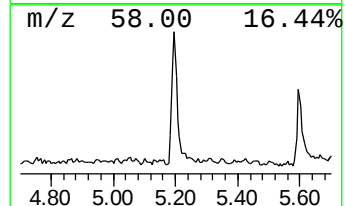
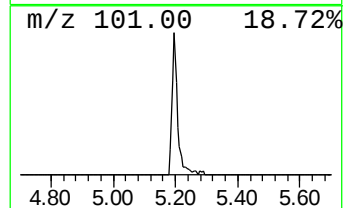
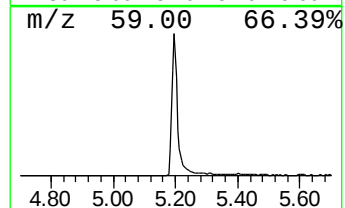
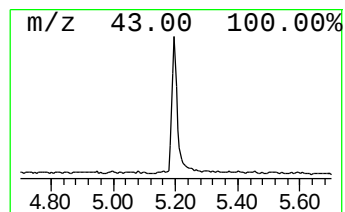
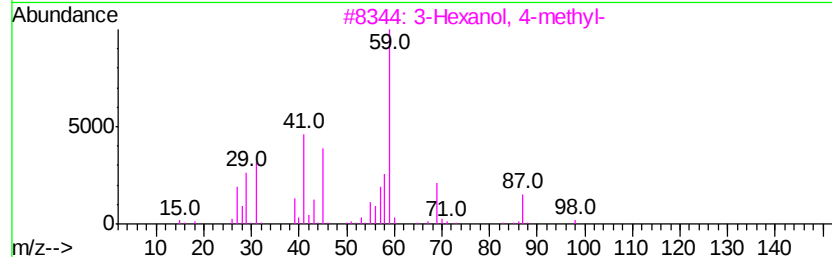
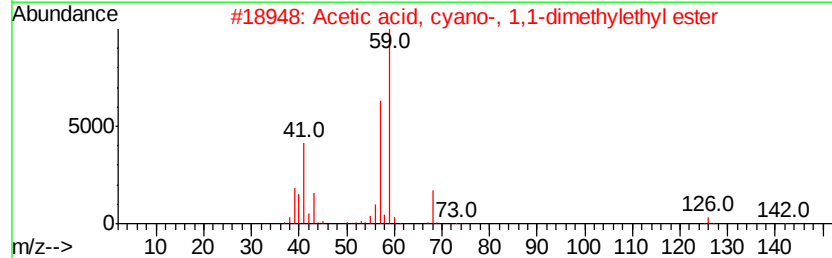
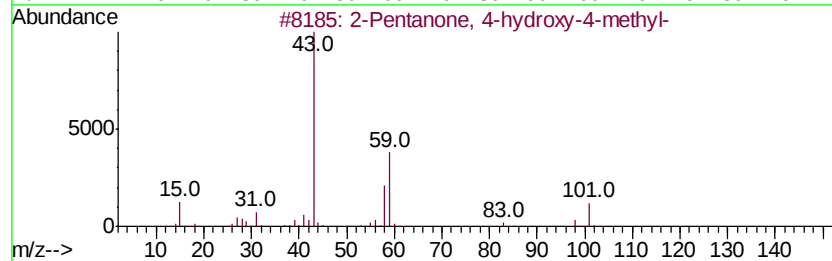
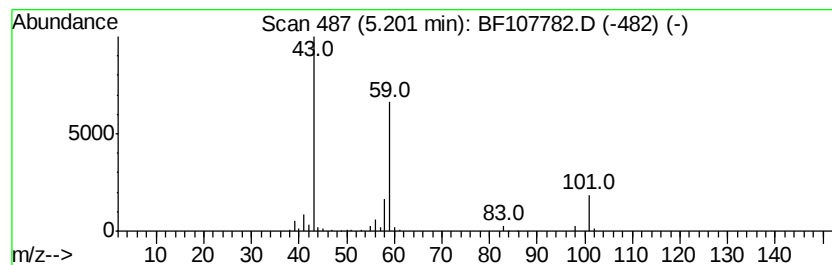
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.20	6.73 ng	256309	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	37
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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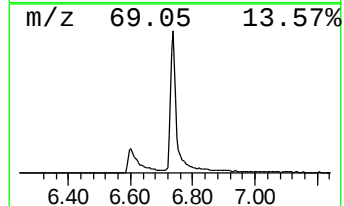
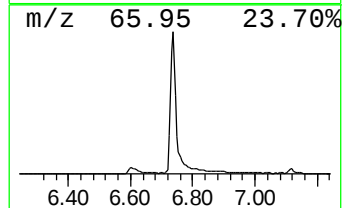
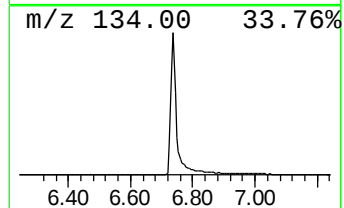
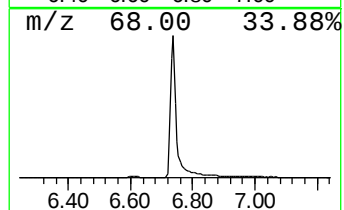
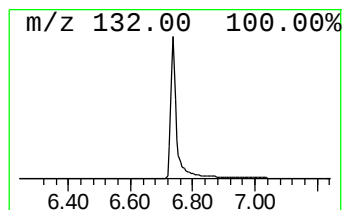
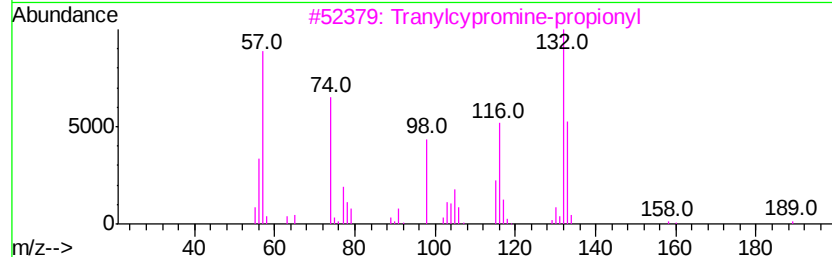
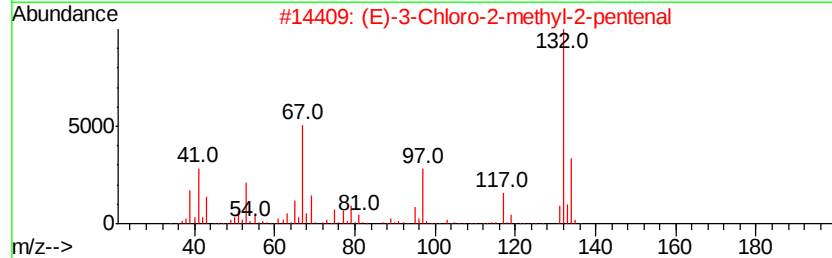
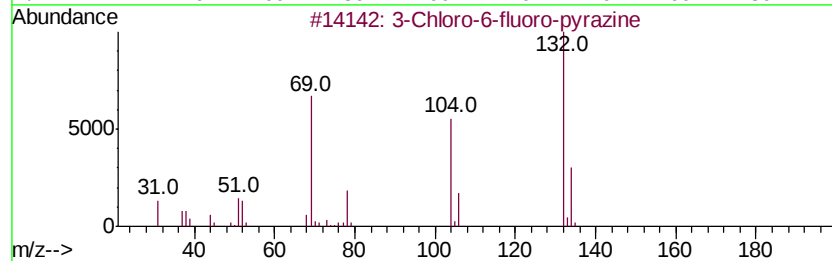
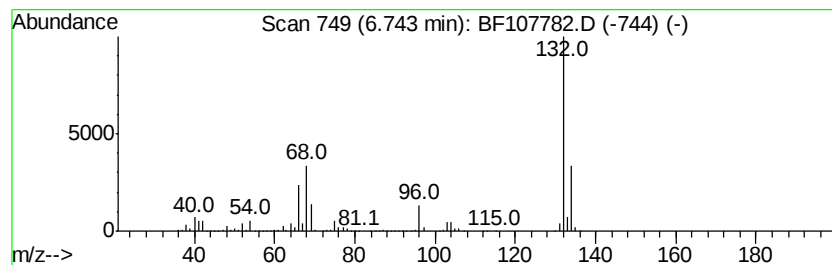
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	93.78 ng	3573310	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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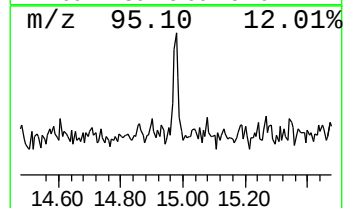
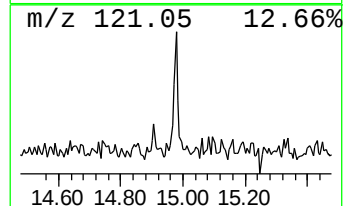
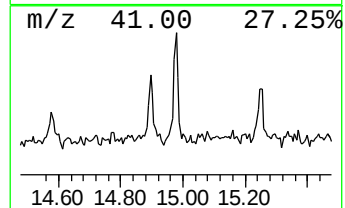
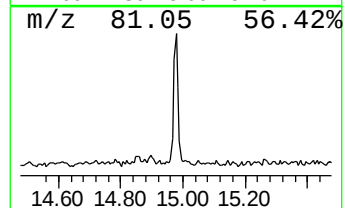
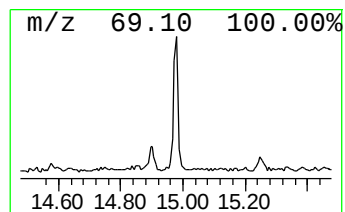
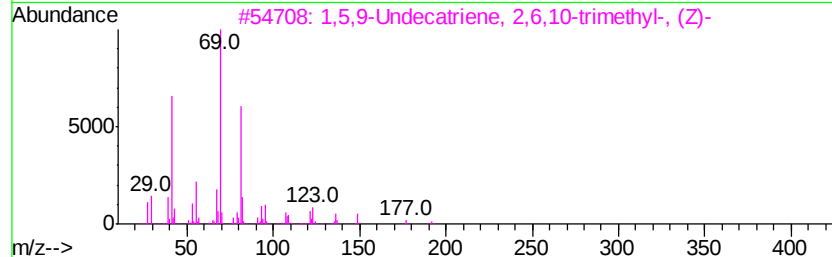
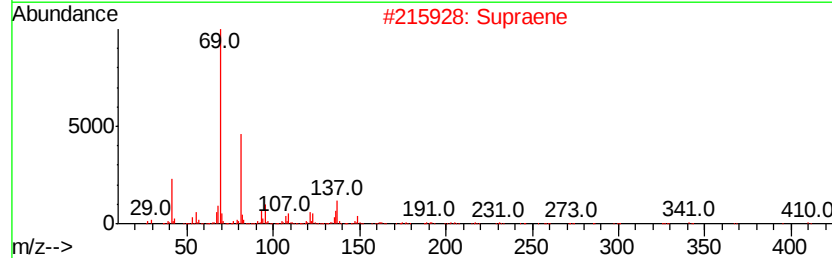
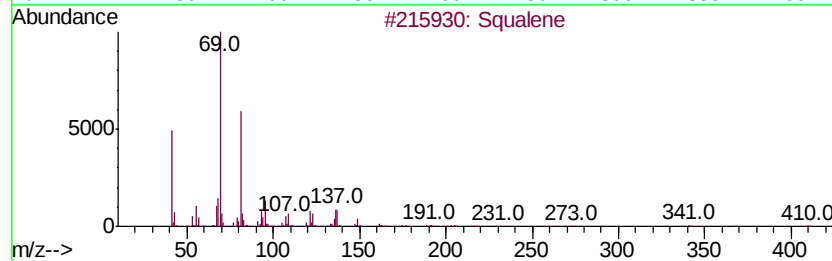
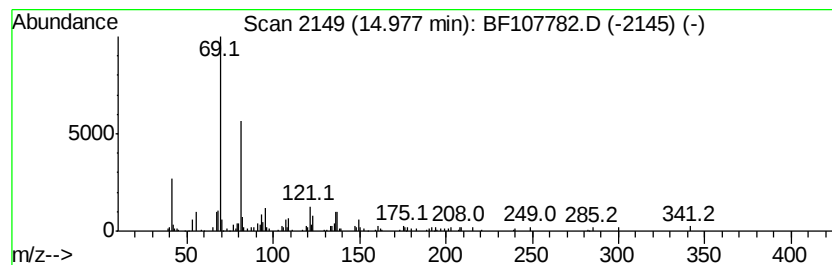
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Peak Number 4 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.11 ng	88501	Perylene-d12	15.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene		410	C30H50	000111-02-4	90
2	Supraene		410	C30H50	007683-64-9	74
3	1,5,9-Undecatriene, 2,6,10-trime...		192	C14H24	062951-96-6	72
4	1,5-Heptadiene, 3,3,6-trimethyl-		138	C10H18	035387-63-4	52
5	2,6-Octadiene, 4-methyl-		124	C9H16	074498-94-5	50



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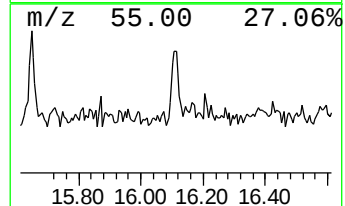
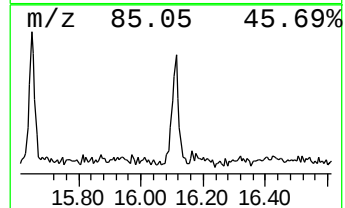
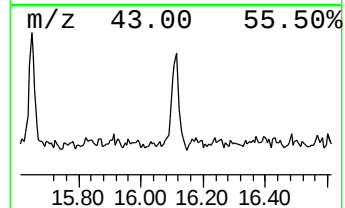
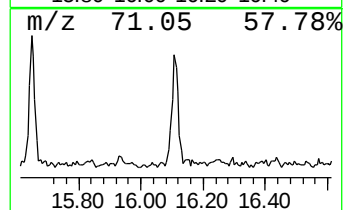
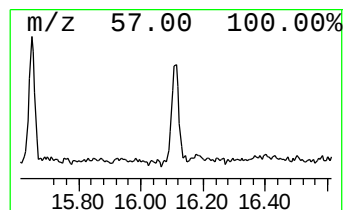
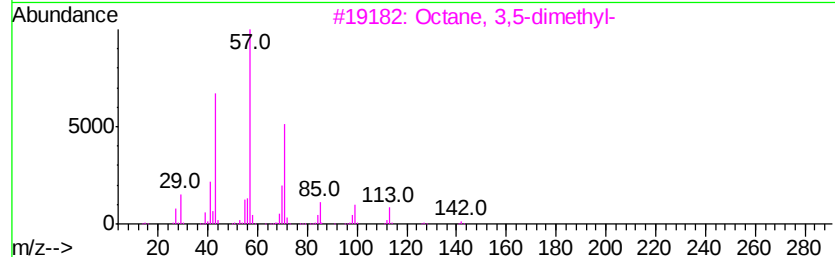
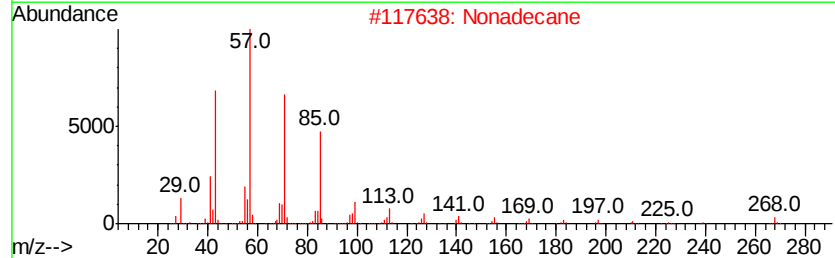
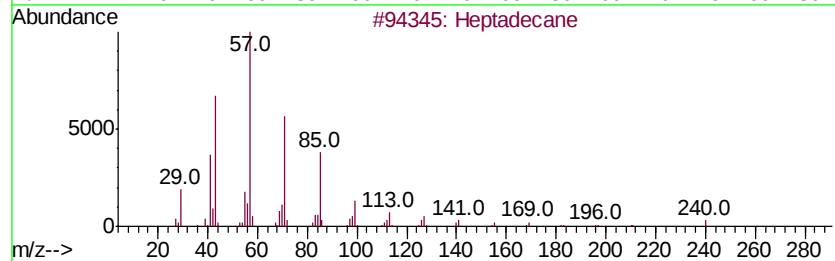
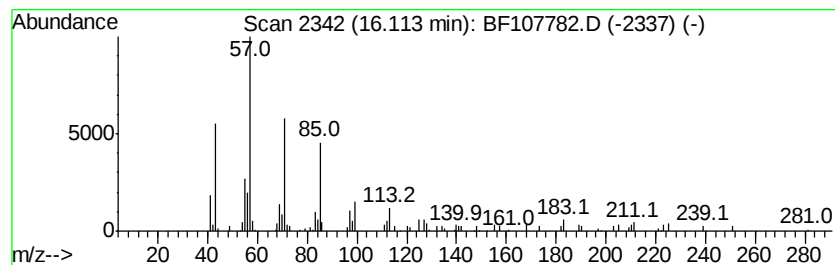
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Peak Number 5 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	2.43 ng	102043	Perylene-d12	15.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	64
2	Nonadecane		268	C19H40	000629-92-5	58
3	Octane, 3,5-dimethyl-		142	C10H22	015869-93-9	58
4	Hexacosane		366	C26H54	000630-01-3	58
5	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	6.7	ng	256309	1	6.97	762030	20.0
unknown6.74	6.74	93.8	ng	3573310	1	6.97	762030	20.0
Squalene	14.98	2.1	ng	88501	6	15.68	839971	20.0
Heptadecane	16.11	2.4	ng	102043	6	15.68	839971	20.0