

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081718\
 Data File : BF108244.D
 Acq On : 17 Aug 2018 15:42
 Operator : JU/SJ
 Sample : J4500-05
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-2

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	5.254	491	496	506	rVB	635539	712259	21.99%	2.417%
2	5.642	557	562	565	rBV	2788544	2566687	79.25%	8.711%
3	6.631	725	730	740	rBV	2797883	3033931	93.67%	10.297%
4	6.784	752	756	759	rBV	3326876	2896804	89.44%	9.832%
5	7.013	792	795	799	rBV	1106252	937418	28.94%	3.182%
6	7.172	818	822	825	rBV	2781294	2301782	71.07%	7.812%
7	7.578	886	891	894	rBV	2048419	1896473	58.55%	6.436%
8	8.301	1010	1014	1017	rBV	1273596	1163754	35.93%	3.950%
9	9.372	1192	1196	1199	rBV	3895655	3238921	100.00%	10.993%
10	9.760	1259	1262	1267	rBV	244495	190285	5.87%	0.646%
11	10.060	1309	1313	1325	rVB	1527898	1299451	40.12%	4.410%
12	10.854	1444	1448	1458	rBV	1597861	1627439	50.25%	5.523%
13	11.554	1563	1567	1571	rBV	1431043	1267926	39.15%	4.303%
14	12.771	1771	1774	1779	rVB	43445	39678	1.23%	0.135%
15	13.007	1808	1814	1820	rBV	47677	62336	1.92%	0.212%
16	13.142	1833	1837	1840	rBV	3424938	2943884	90.89%	9.991%
17	14.054	1989	1992	2002	rBV3	76130	163035	5.03%	0.553%
18	14.212	2014	2019	2022	rBV	1186052	1197982	36.99%	4.066%
19	14.401	2048	2051	2054	rBV	49530	40514	1.25%	0.138%
20	14.648	2091	2093	2097	rBV2	42938	48859	1.51%	0.166%
21	14.977	2146	2149	2154	rVB	51690	52736	1.63%	0.179%
22	15.065	2160	2164	2168	rVB	255297	281531	8.69%	0.955%
23	15.342	2208	2211	2216	rVB2	63447	83070	2.56%	0.282%
24	15.771	2278	2284	2293	rVB2	836529	1230949	38.00%	4.178%
25	16.236	2360	2363	2369	rVB	70788	108695	3.36%	0.369%
26	16.795	2455	2458	2464	rVB2	43569	78084	2.41%	0.265%

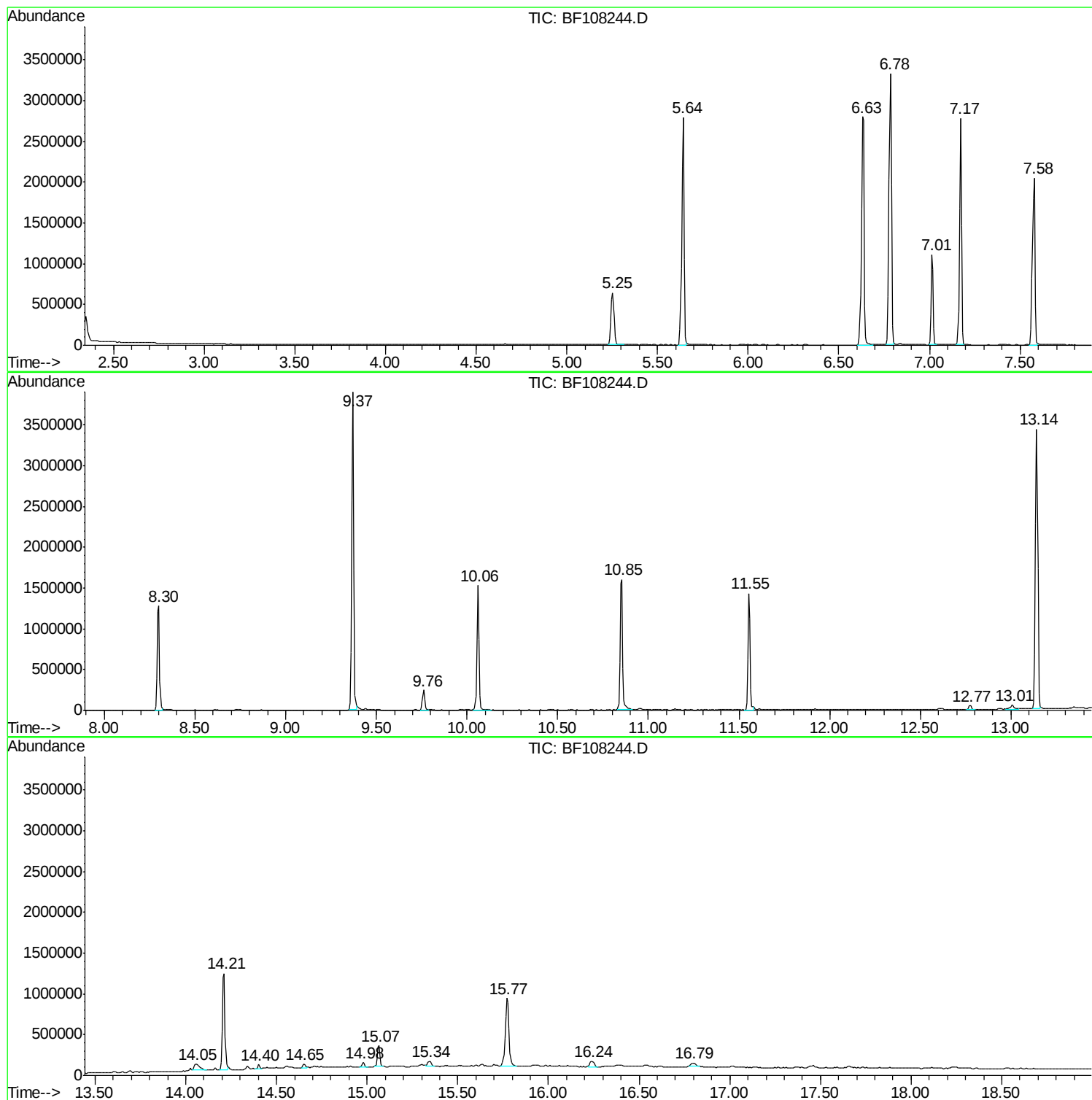
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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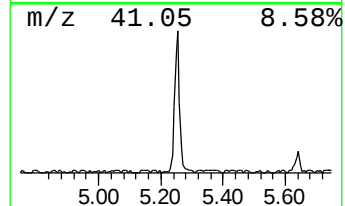
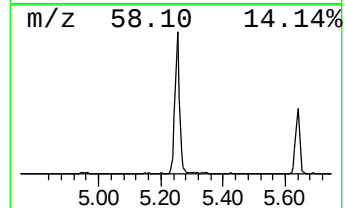
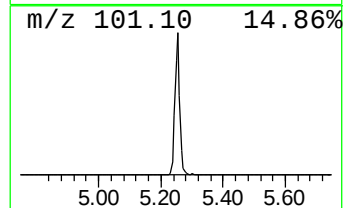
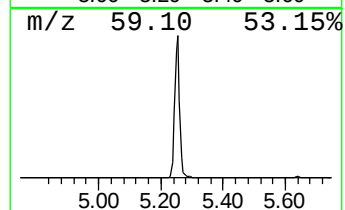
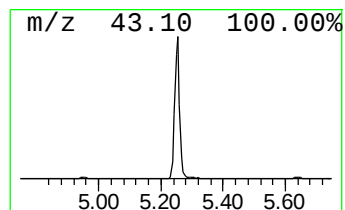
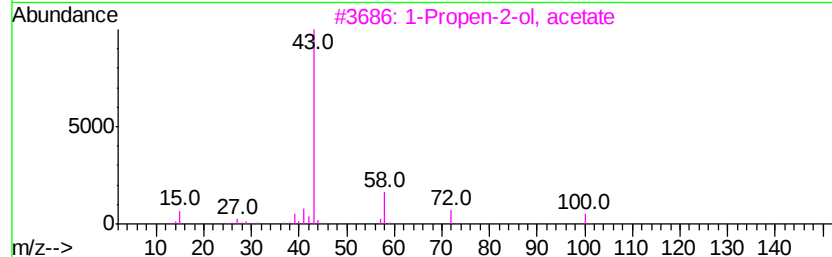
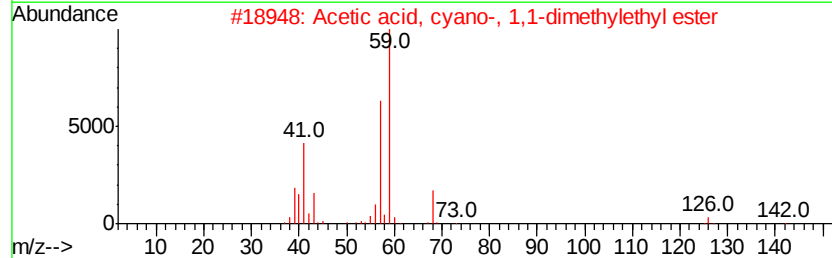
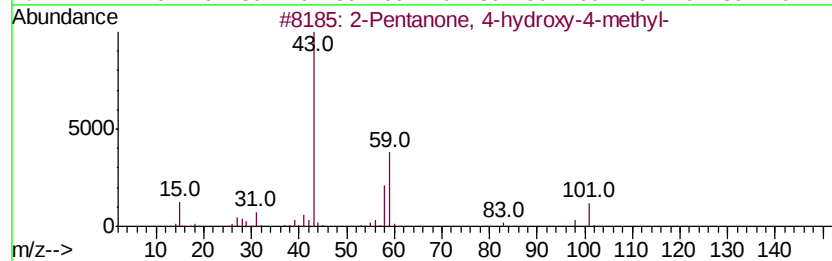
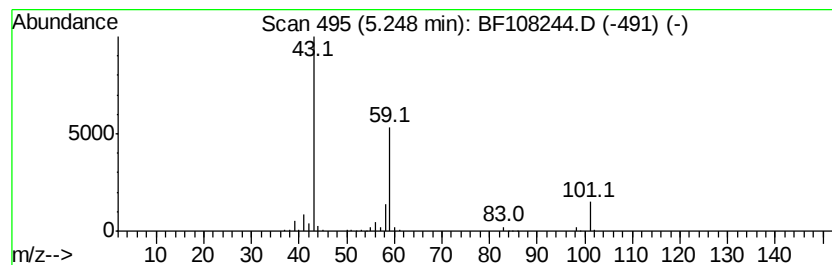
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.25	15.20 ng	712259	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		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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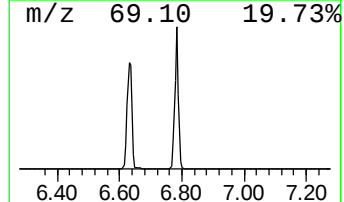
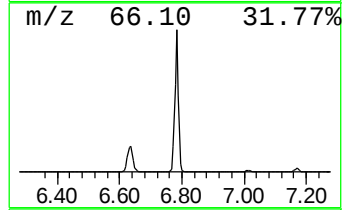
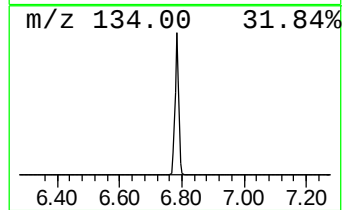
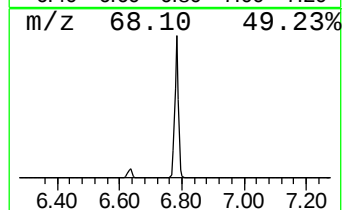
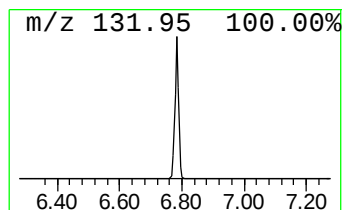
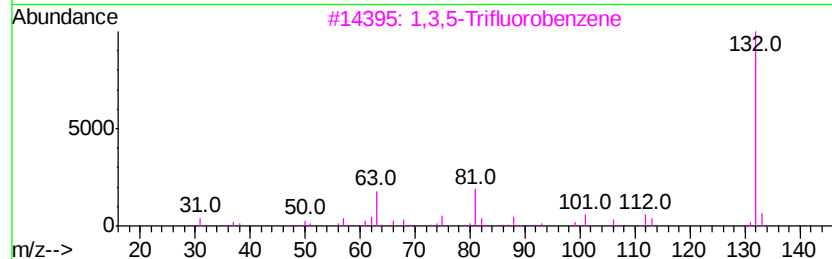
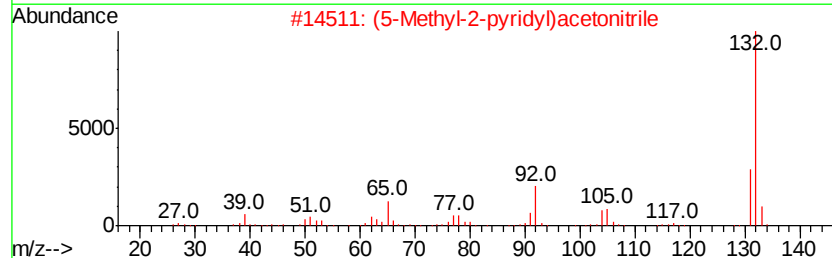
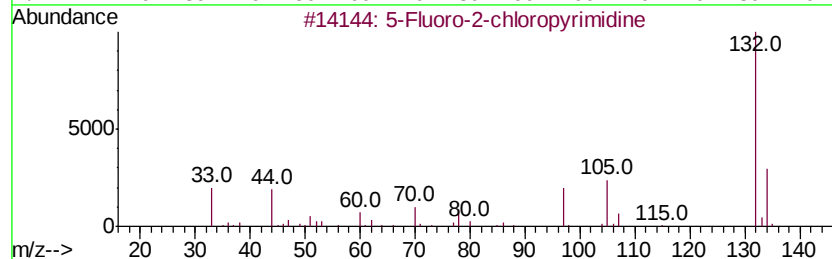
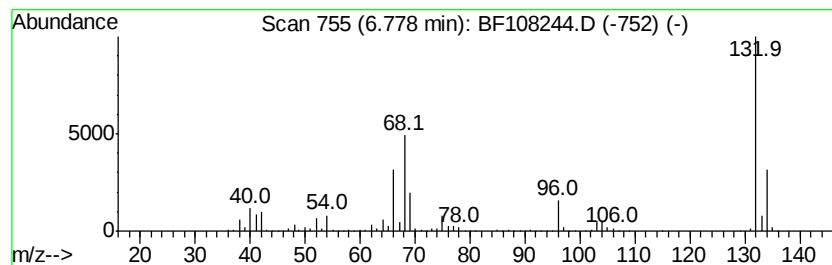
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Peak Number 2 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	61.80 ng	2896800	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Xenon	132	Xe	007440-63-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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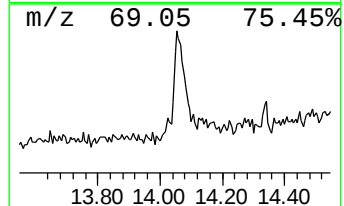
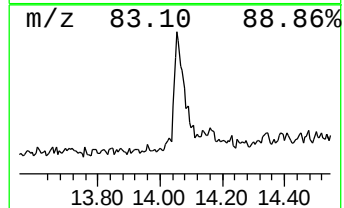
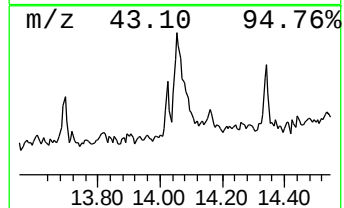
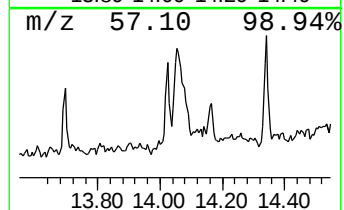
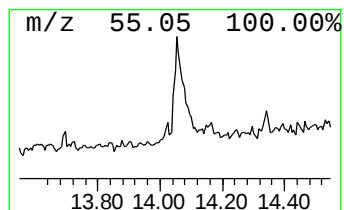
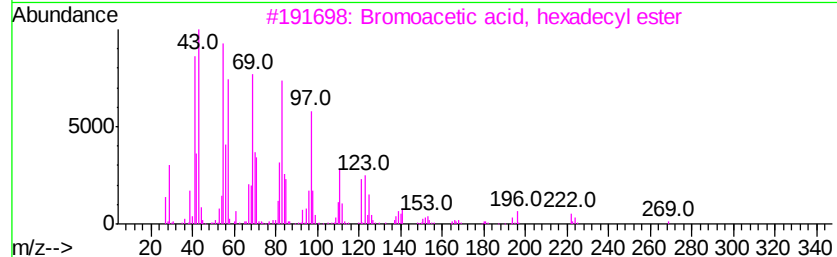
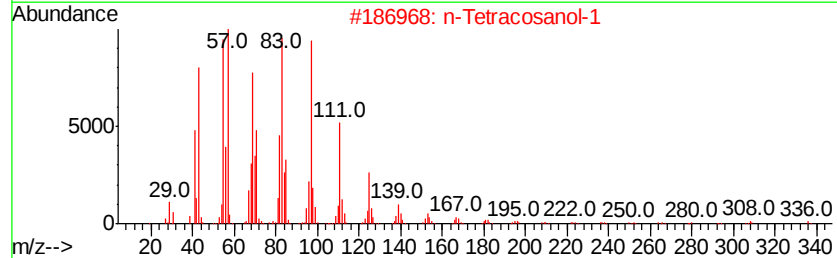
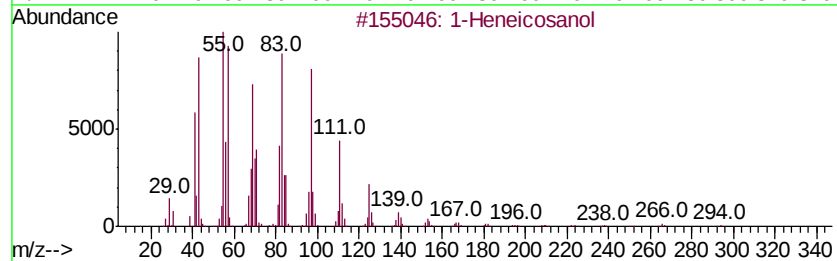
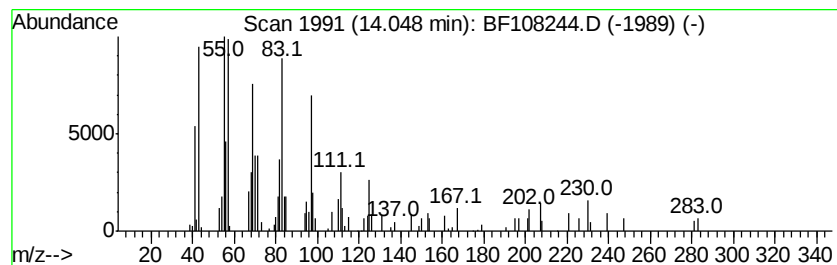
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Peak Number 4 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.05	2.72 ng	163035	Chrysene-d12	14.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	91
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	90
3		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
4		Behenic alcohol	326	C22H46O	000661-19-8	87
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	81



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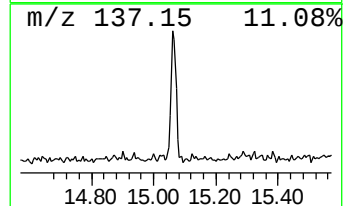
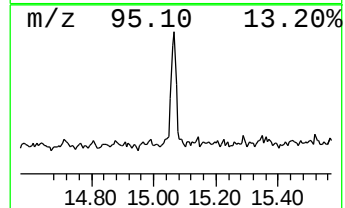
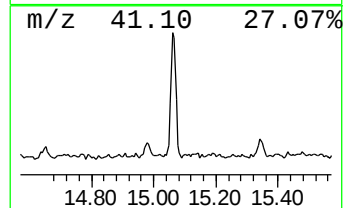
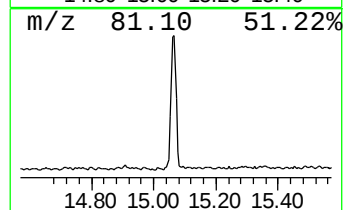
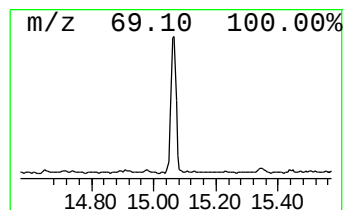
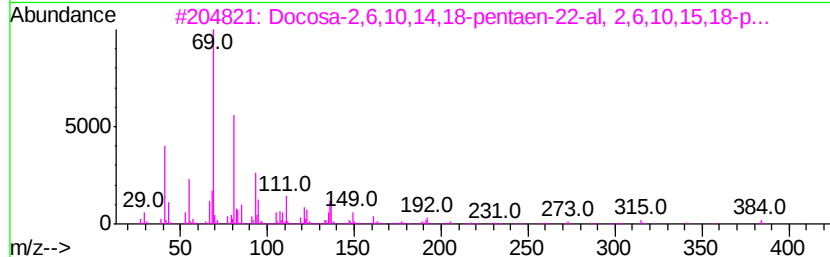
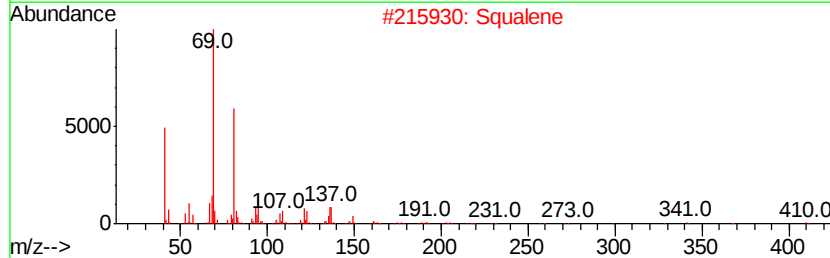
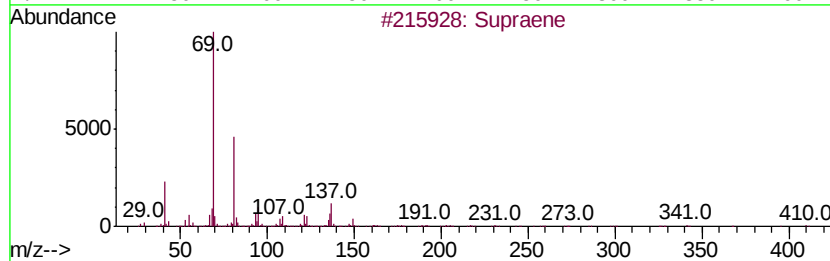
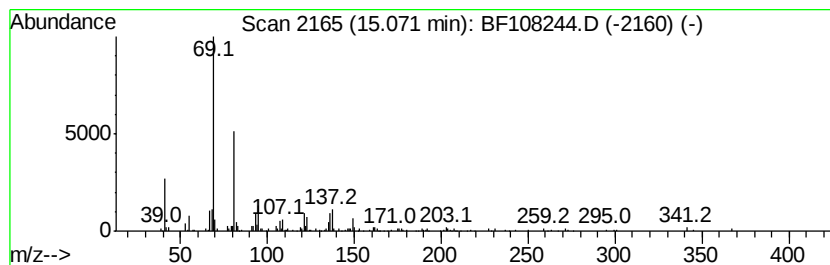
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Peak Number 5 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	4.57 ng	281531	Perylene-d12	15.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.25	15.2	ng	712259	1	7.01	937418	20.0
unknown6.78	6.78	61.8	ng	2896800	1	7.01	937418	20.0
1-Heneicosanol	14.05	2.7	ng	163035	5	14.21	1197980	20.0
Supraene	15.07	4.6	ng	281531	6	15.77	1230950	20.0