

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032318\
 Data File : BF103906.D
 Acq On : 24 Mar 2018 3:33
 Operator : JU/SJ
 Sample : J2014-04
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 032018-TIDO-F-U-S

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-BF031518.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	2.299	31	36	44	rVB	358647	449536	12.02%	2.014%
2	5.198	526	529	539	rVB	143908	139630	3.73%	0.626%
3	5.592	592	596	609	rBV	1256149	1107366	29.61%	4.962%
4	6.587	761	765	768	rBV	890003	734439	19.64%	3.291%
5	6.616	768	770	781	rVB	100944	92579	2.48%	0.415%
6	6.739	787	791	795	rBV	2158692	1981315	52.99%	8.878%
7	6.975	827	831	834	rBV	945389	738298	19.74%	3.308%
8	7.134	853	858	861	rBV	3076544	2704264	72.32%	12.118%
9	7.539	921	927	930	rBV	2197411	2078821	55.59%	9.315%
10	8.257	1045	1049	1052	rBV	1190335	938217	25.09%	4.204%
11	9.333	1227	1232	1235	rBV	4076428	3739286	100.00%	16.755%
12	9.722	1293	1298	1305	rBV	69016	72970	1.95%	0.327%
13	9.927	1330	1333	1337	rBV	56233	43435	1.16%	0.195%
14	10.016	1345	1348	1355	rVB2	1130748	958461	25.63%	4.295%
15	10.427	1416	1418	1421	rVB	62629	47425	1.27%	0.213%
16	10.674	1458	1460	1463	rVB	63031	46205	1.24%	0.207%
17	10.810	1479	1483	1496	rBV	1281535	1318238	35.25%	5.907%
18	10.904	1496	1499	1508	rVB	54869	56757	1.52%	0.254%
19	11.510	1598	1602	1609	rBV	986229	825512	22.08%	3.699%
20	13.098	1867	1872	1875	rBV	2963529	2798851	74.85%	12.541%
21	13.974	2019	2021	2033	rVB	111012	127162	3.40%	0.570%
22	14.163	2049	2053	2057	rBV	770043	708520	18.95%	3.175%
23	15.015	2195	2198	2203	rBV	54721	58032	1.55%	0.260%
24	15.709	2311	2316	2323	rVB	412174	551627	14.75%	2.472%

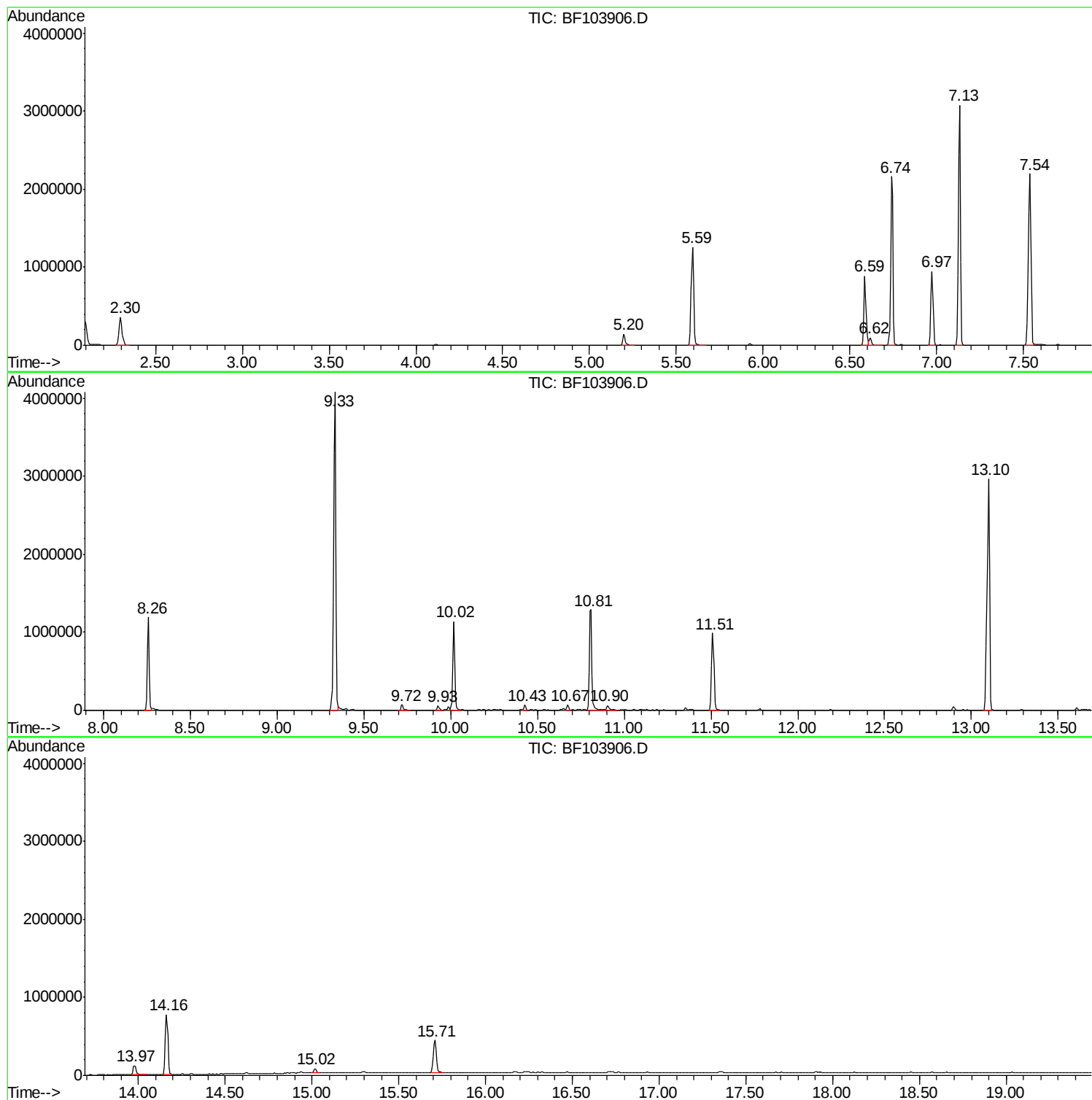
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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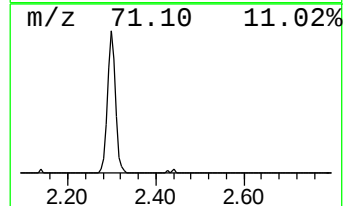
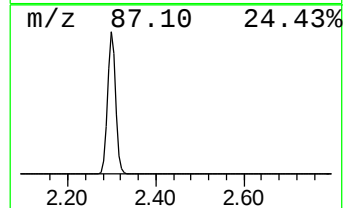
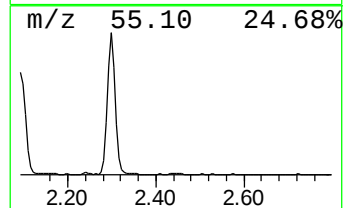
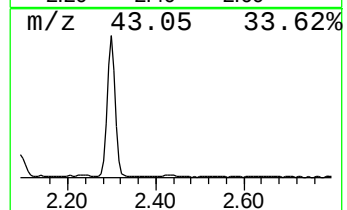
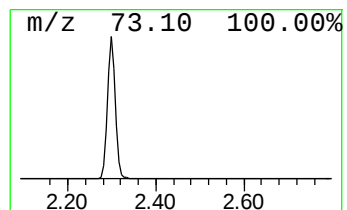
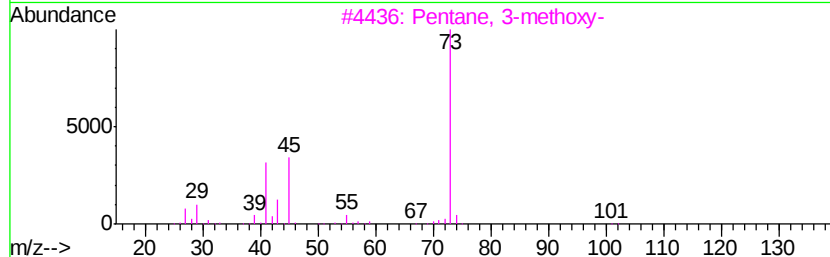
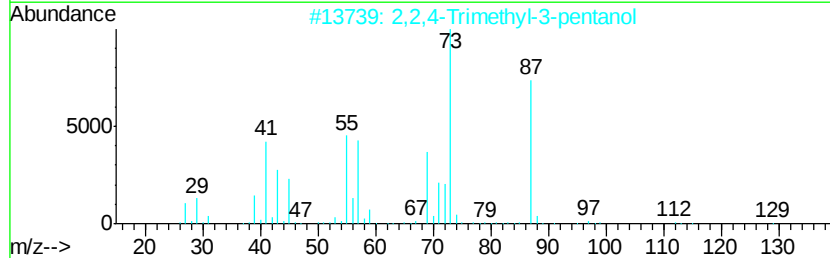
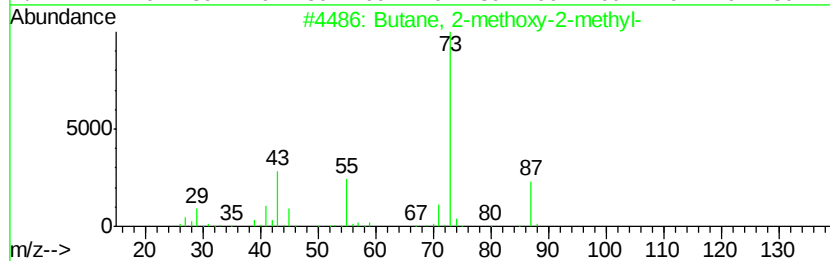
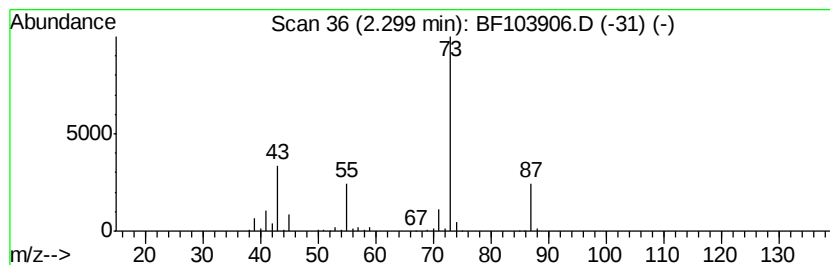
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.30	12.18 ng	449536	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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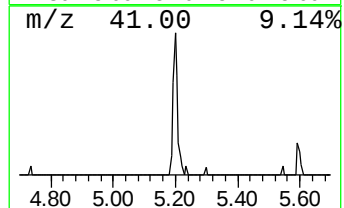
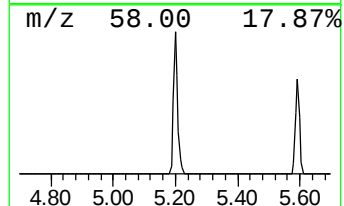
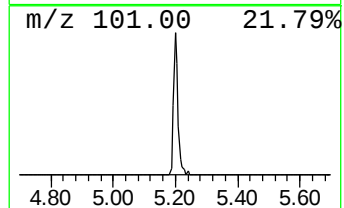
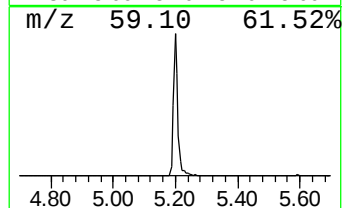
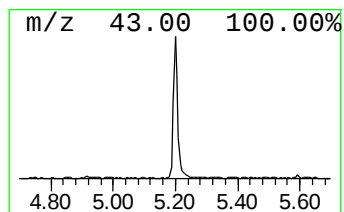
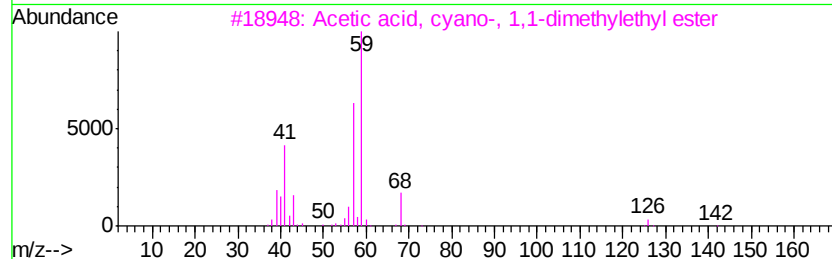
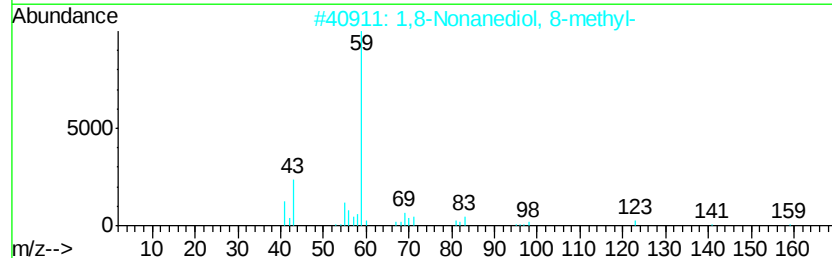
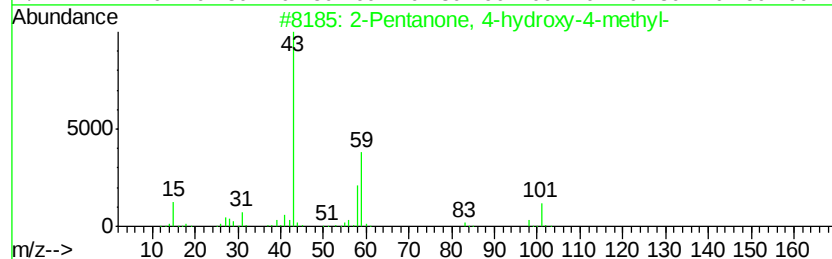
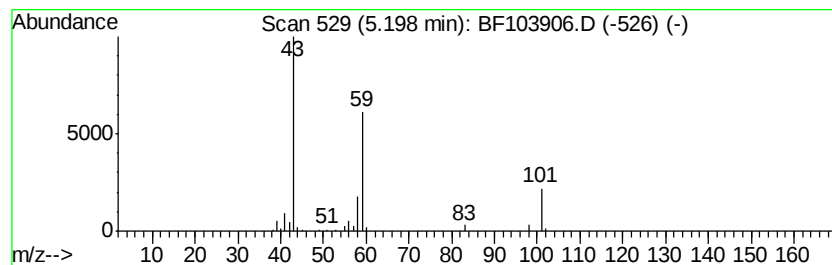
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	3.78 ng	139630	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			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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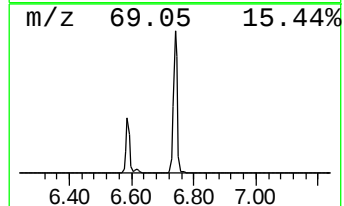
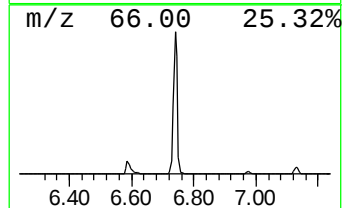
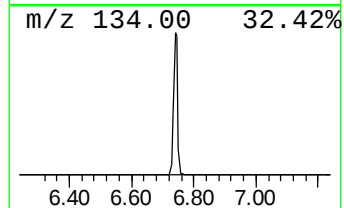
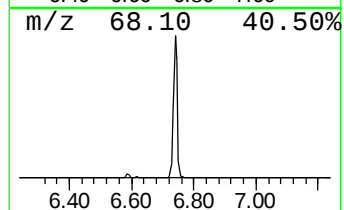
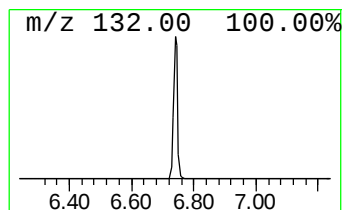
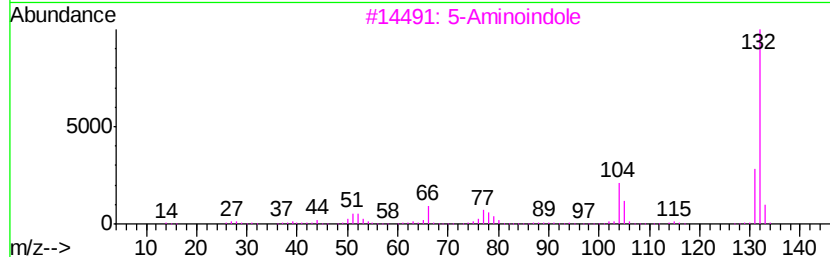
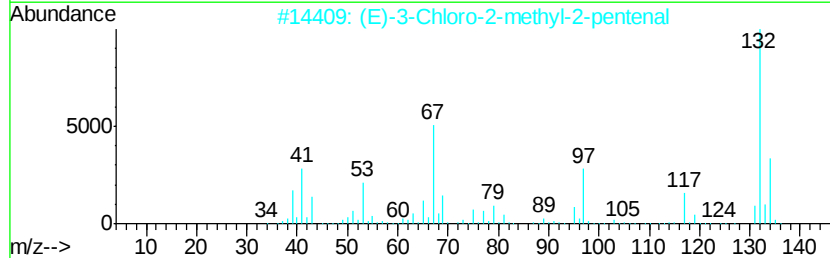
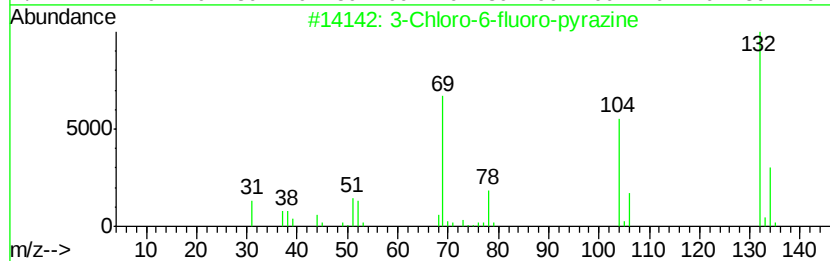
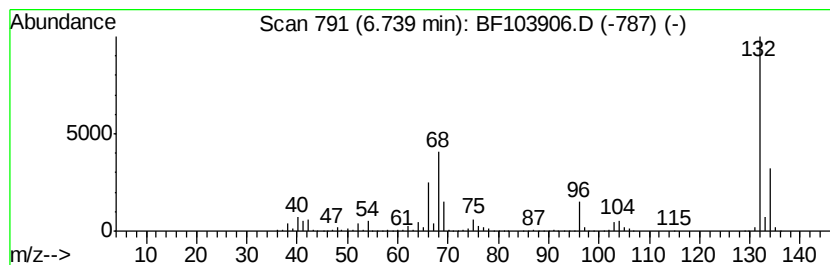
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Peak Number 3 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	53.67 ng	1981320	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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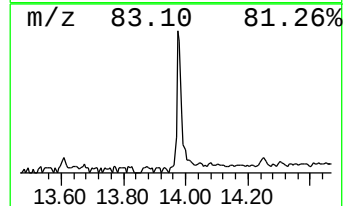
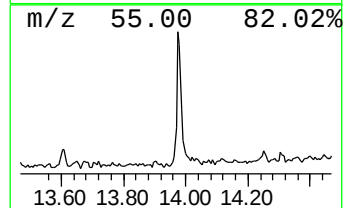
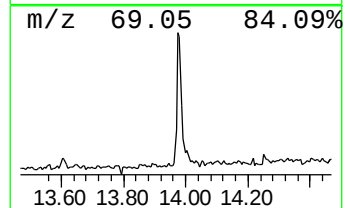
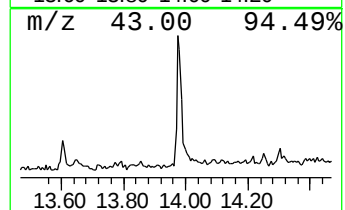
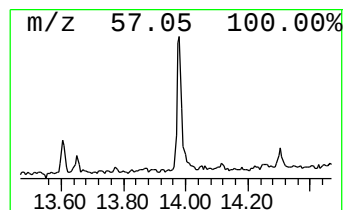
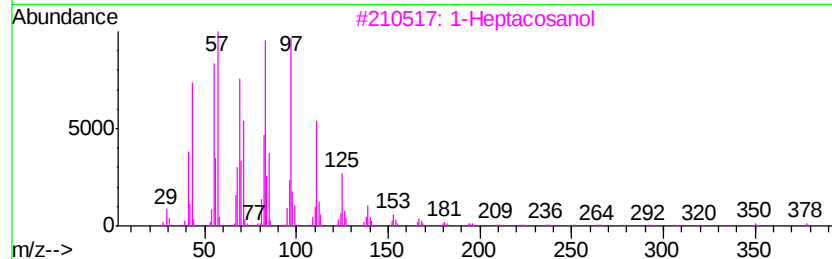
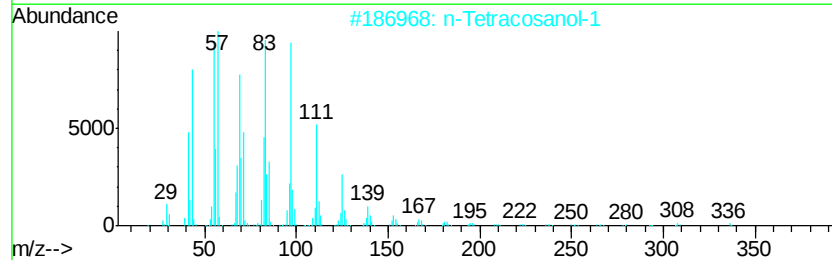
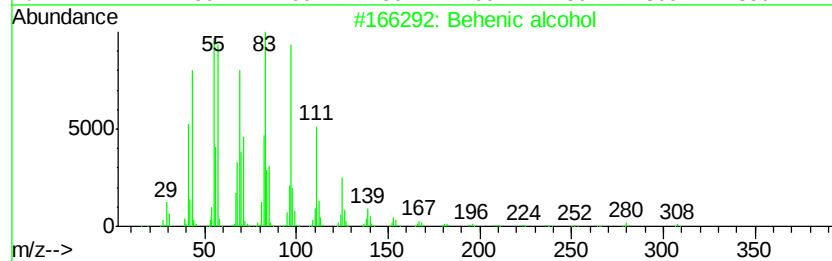
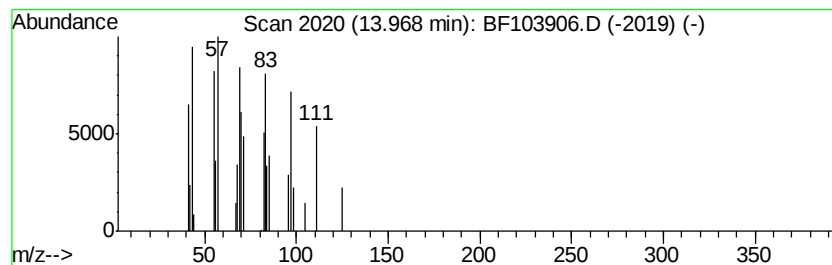
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Peak Number 5 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.97	3.59 ng	127162	Chrysene-d12	14.16	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90



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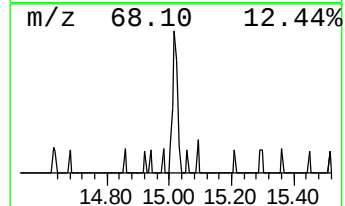
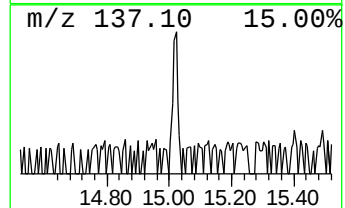
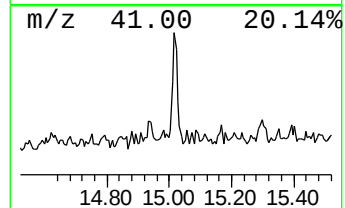
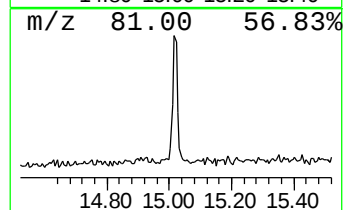
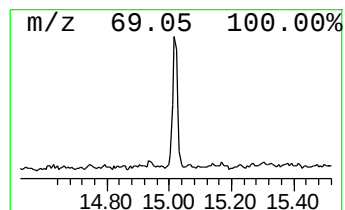
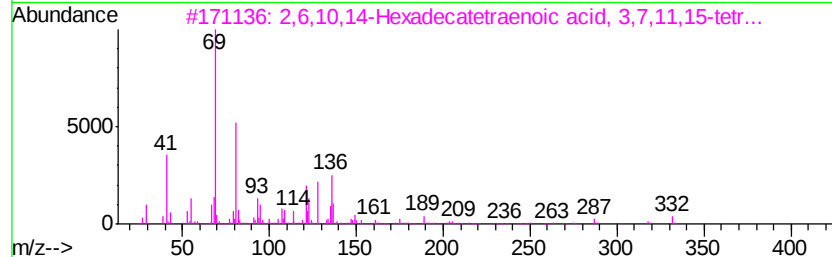
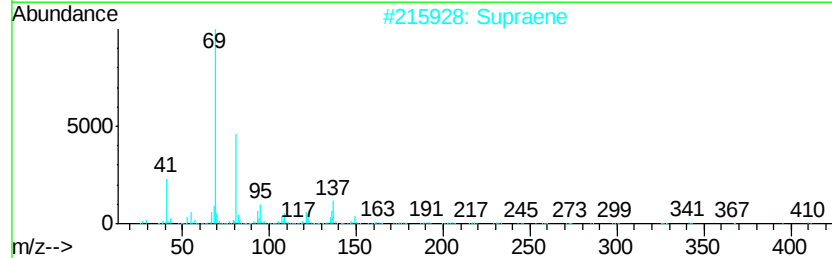
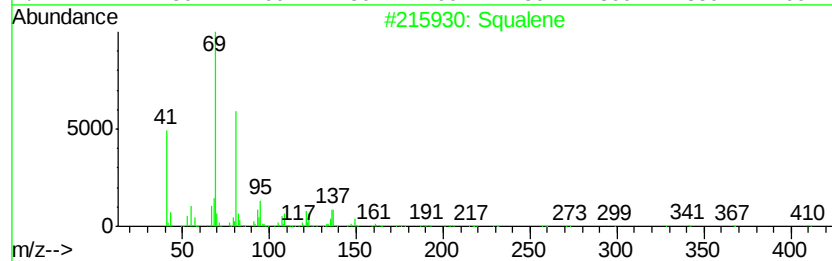
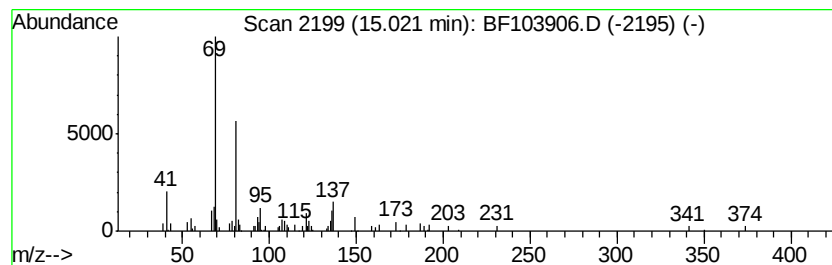
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Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	2.10 ng	58032	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	90
3		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78
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	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.30	12.2	ng	449536	1	6.97	738298	20.0
2-Pentanone, 4-hy...	5.20	3.8	ng	139630	1	6.97	738298	20.0
unknown6.74	6.74	53.7	ng	1981320	1	6.97	738298	20.0
Behenic alcohol	13.97	3.6	ng	127162	5	14.16	708520	20.0
Squalene	15.02	2.1	ng	58032	6	15.71	551627	20.0