

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111116\
 Data File : BF091156.D
 Acq On : 11 Nov 2016 22:35
 Operator : UM/SJ
 Sample : H5628-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-COMP

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:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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	1.744	3	5	54	rVB	3278226	8898557	100.00%	19.349%
2	4.784	268	271	283	rBV	860701	1249729	14.04%	2.717%
3	5.230	308	310	313	rBV	2557216	3463527	38.92%	7.531%
4	6.304	401	404	406	rBV	3376116	3941254	44.29%	8.570%
5	6.407	411	413	416	rBV	2736779	3777408	42.45%	8.214%
6	6.636	431	433	439	rBV	597065	929447	10.44%	2.021%
7	6.796	445	447	450	rBV	3244440	2924251	32.86%	6.359%
8	7.207	481	483	486	rBV	1529521	2200790	24.73%	4.785%
9	7.927	544	546	558	rBV	1359551	1311244	14.74%	2.851%
10	9.013	638	641	643	rBV	3294497	3887583	43.69%	8.453%
11	9.413	674	676	678	rBV	152651	195767	2.20%	0.426%
12	9.676	697	699	702	rBV	1519577	1331277	14.96%	2.895%
13	10.465	766	768	771	rBV	2235937	2222250	24.97%	4.832%
14	10.591	777	779	784	rVB	84751	106797	1.20%	0.232%
15	11.151	826	828	833	rBV2	901506	1387554	15.59%	3.017%
16	11.768	880	882	888	rVB	74957	117837	1.32%	0.256%
17	12.362	932	934	938	rBV	433205	437689	4.92%	0.952%
18	12.591	951	954	956	rBV	394366	462100	5.19%	1.005%
19	12.739	964	967	970	rBV	3684828	3555686	39.96%	7.732%
20	13.642	1044	1046	1051	rVB2	187850	207482	2.33%	0.451%
21	13.779	1055	1058	1065	rBV	1020438	1504806	16.91%	3.272%
22	14.625	1130	1132	1141	rVB	162176	264266	2.97%	0.575%
23	14.785	1143	1146	1151	rVB	120117	253465	2.85%	0.551%
24	15.048	1166	1169	1172	rVB	68741	105317	1.18%	0.229%
25	15.105	1172	1174	1176	rVB	84273	117449	1.32%	0.255%
26	15.151	1176	1178	1186	rVB	680029	861898	9.69%	1.874%
27	16.431	1287	1290	1293	rBV2	45281	97250	1.09%	0.211%
28	16.808	1320	1323	1335	rVB	44867	176384	1.98%	0.384%

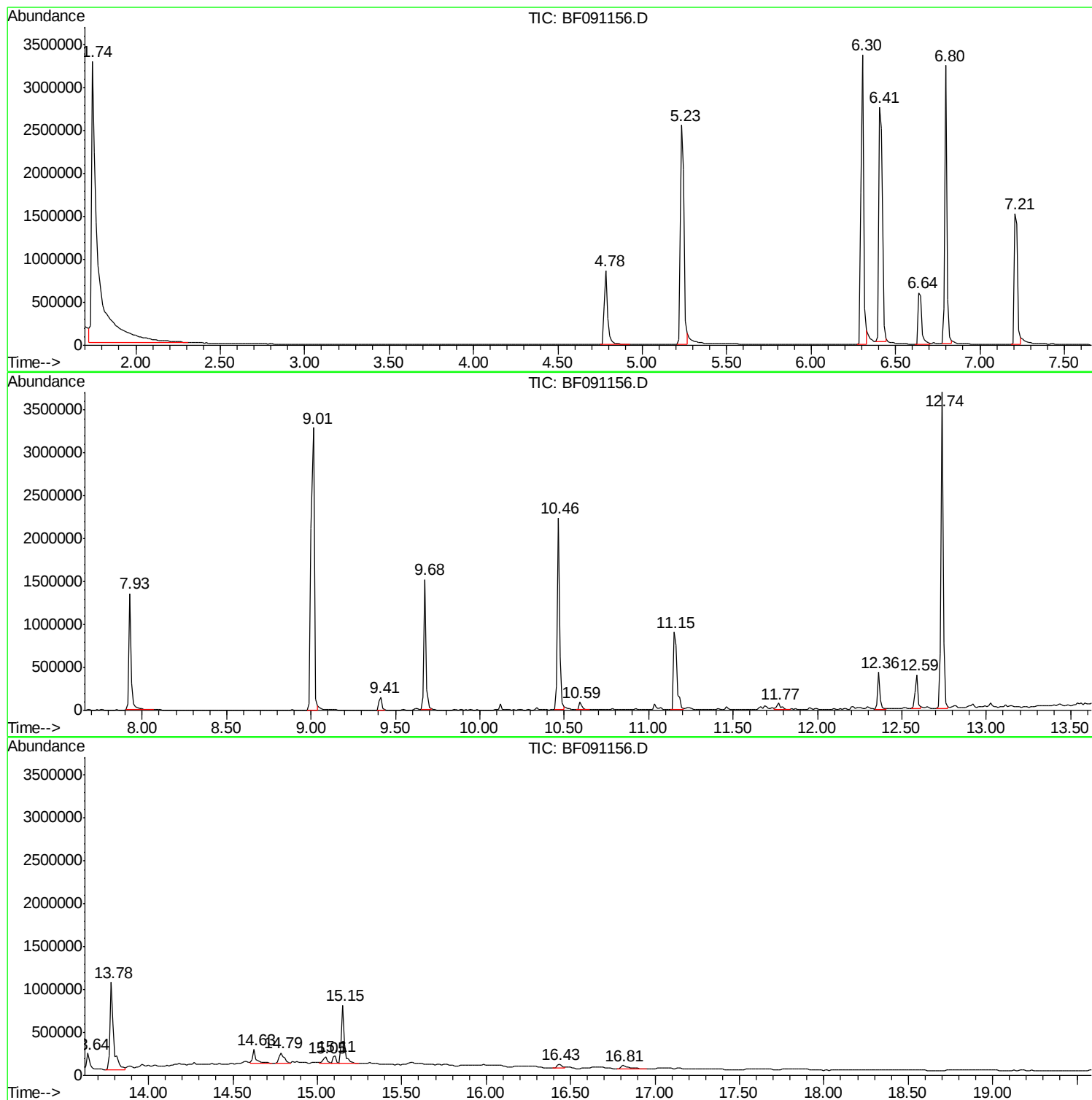
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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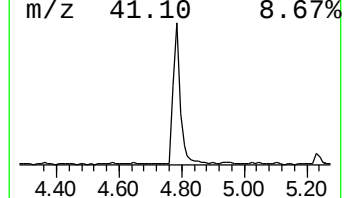
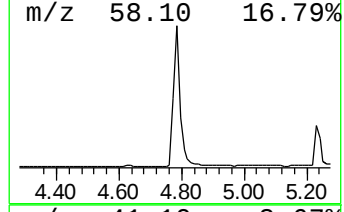
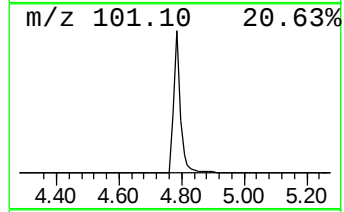
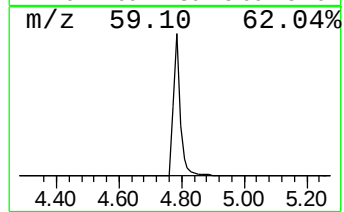
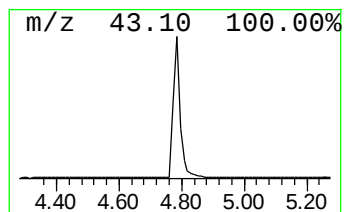
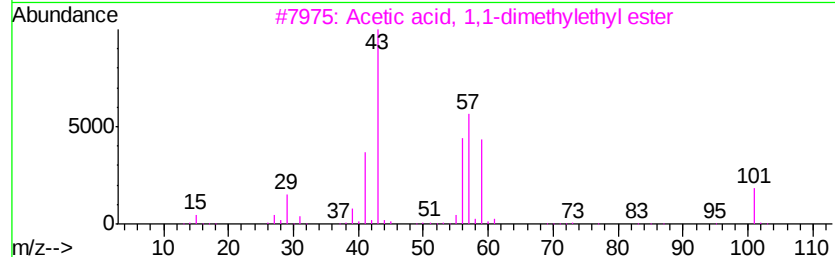
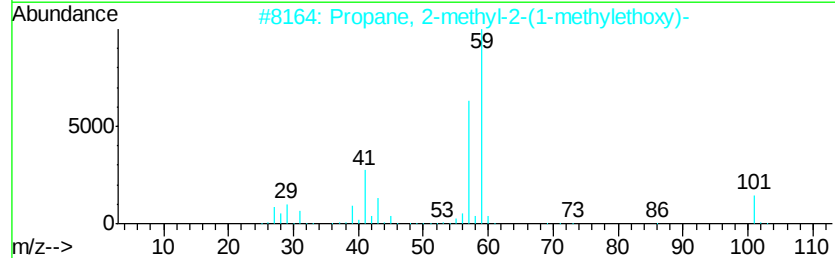
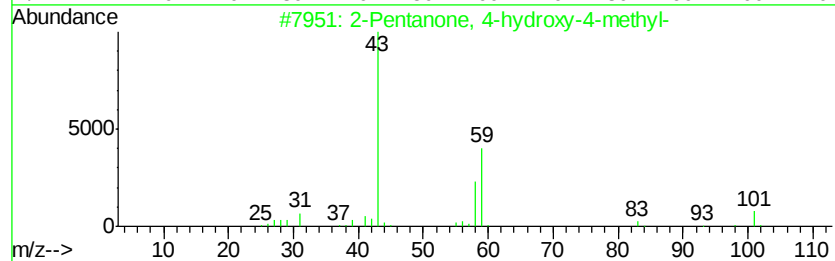
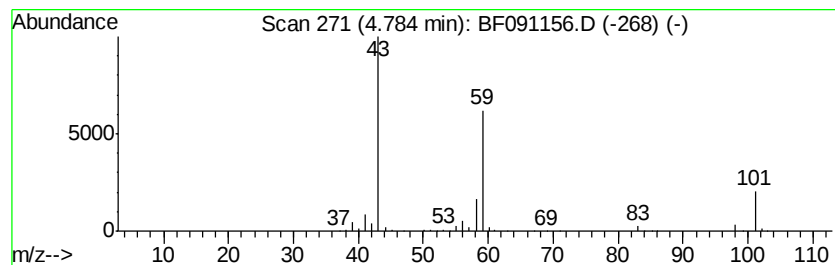
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	26.89 ng	1249730	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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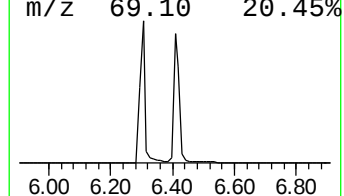
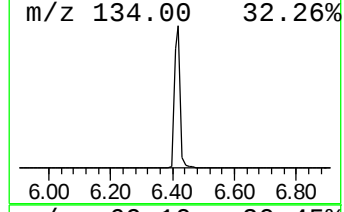
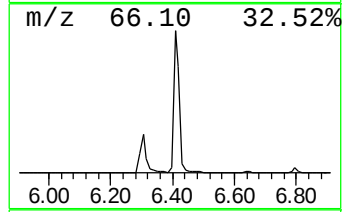
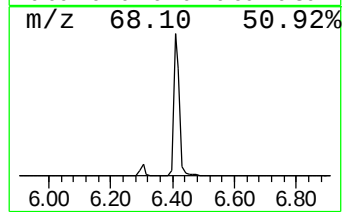
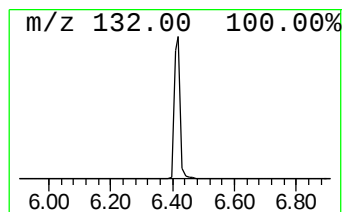
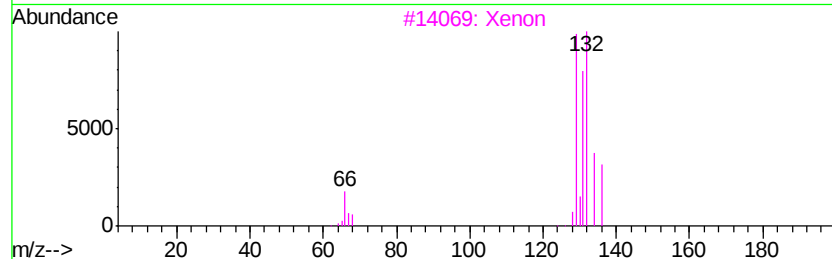
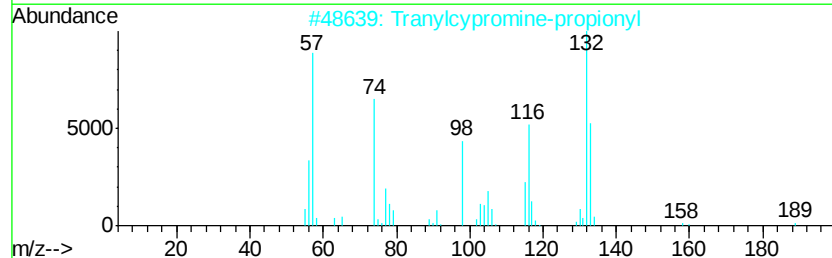
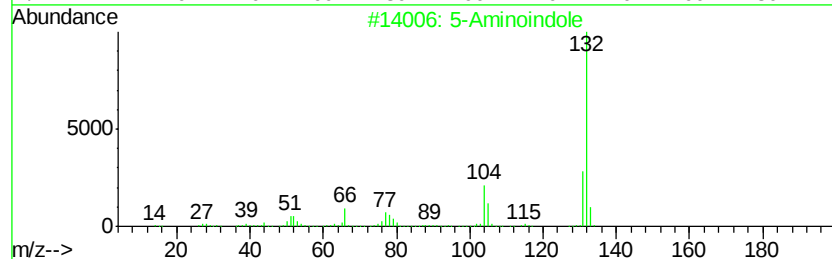
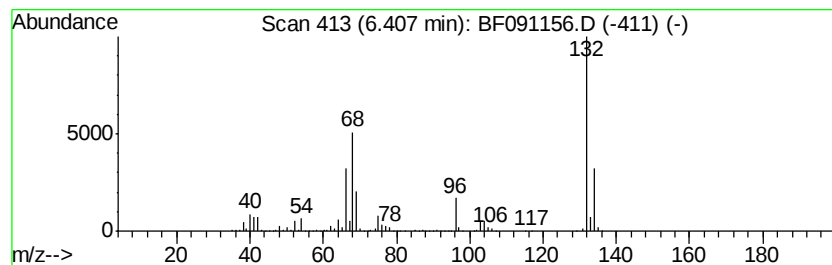
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Peak Number 3 unknown6.41 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	81.28 ng	3777410	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	22
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Xenon	132	Xe	007440-63-3	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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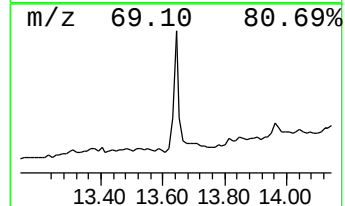
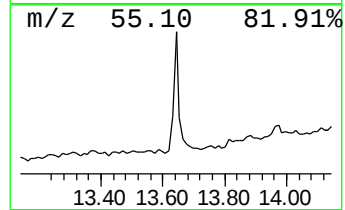
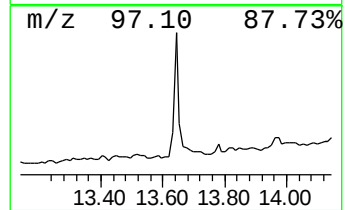
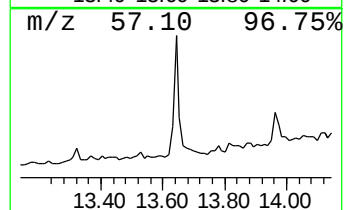
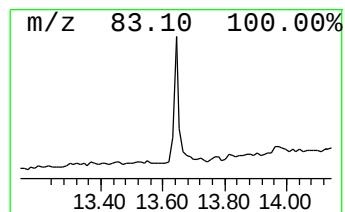
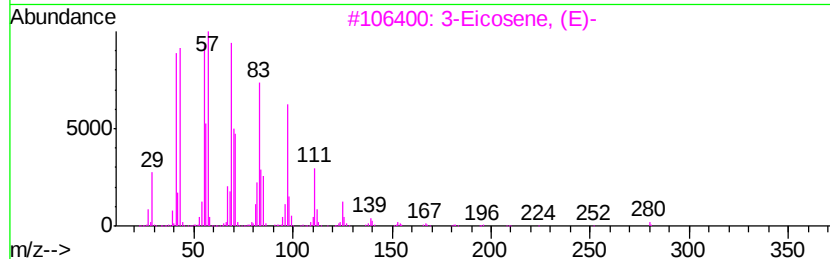
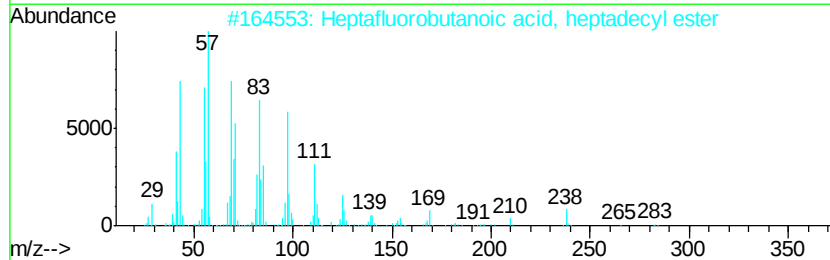
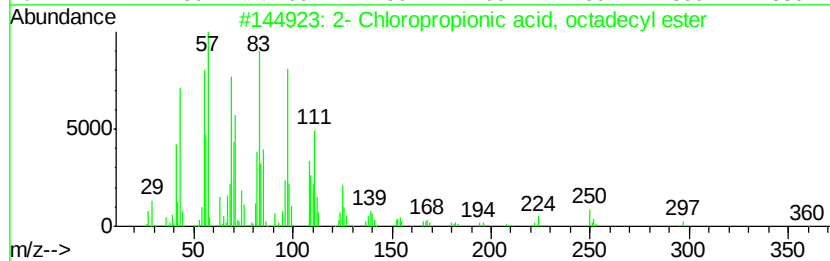
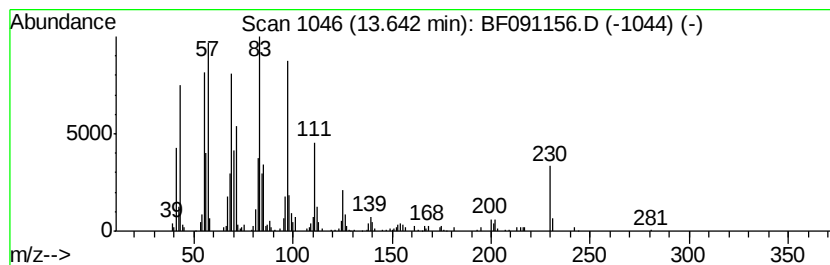
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Peak Number 5 2- Chloropropionic acid, oc... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	2.76 ng	207482	Chrysene-d12	13.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
2		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90



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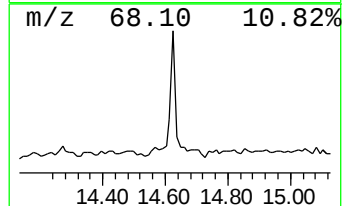
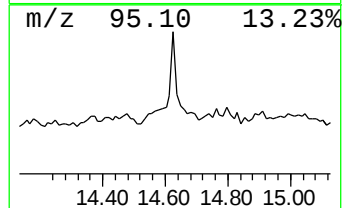
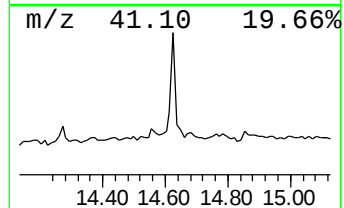
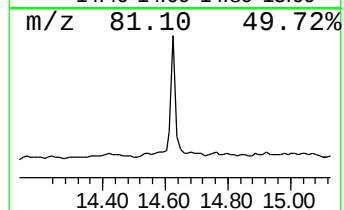
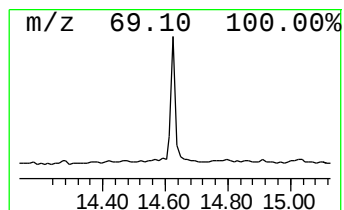
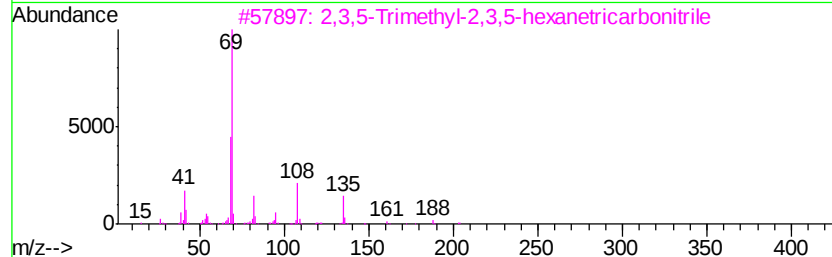
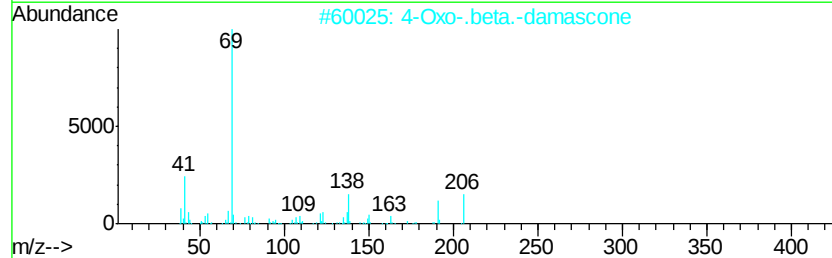
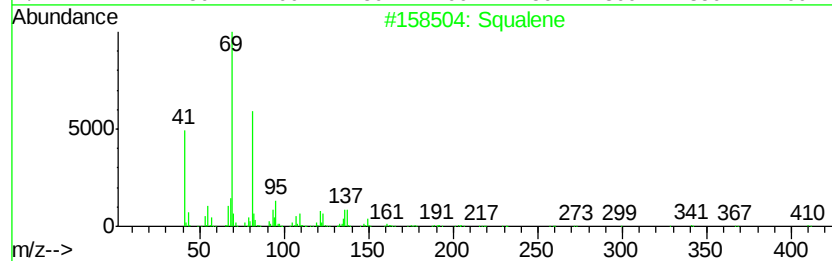
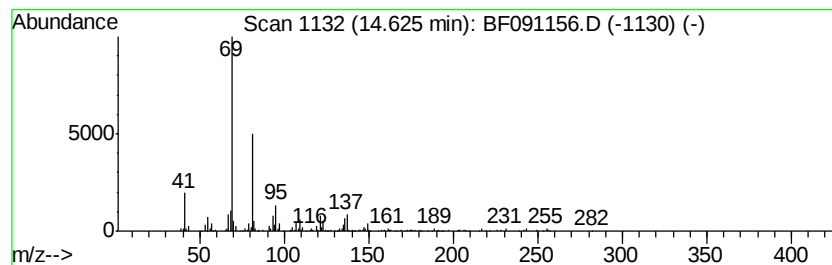
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Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	6.13 ng	264266	Perylene-d12	15.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		4-Oxo-.beta.-damascone	206	C13H18O2	053398-08-6	72
3		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	59
4		2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	53
5		1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.78	26.9	ng	1249730	1	6.65	929447	20.0
unknown6.41	6.41	81.3	ng	3777410	1	6.65	929447	20.0
2- Chloropropioni...	13.64	2.8	ng	207482	5	13.78	1504810	20.0
Squalene	14.63	6.1	ng	264266	6	15.15	861898	20.0