

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021617\
 Data File : BF092996.D
 Acq On : 16 Feb 2017 22:15
 Operator : SJ/MA
 Sample : I1869-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TILCON-NO-57

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-BF013017.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	5.024	254	257	266	rBV	887895	1124323	30.82%	3.397%
2	5.459	292	295	297	rBV	2468304	3138269	86.03%	9.481%
3	6.499	383	386	388	rBV	2816149	3354399	91.95%	10.134%
4	6.624	394	397	399	rBV	3212896	2930703	80.34%	8.854%
5	6.853	415	417	420	rBV	913874	845666	23.18%	2.555%
6	7.013	428	431	433	rBV	2701207	2414652	66.19%	7.295%
7	7.424	464	467	469	rBV	2004510	2095426	57.44%	6.330%
8	7.539	474	477	483	rVV	28599	56805	1.56%	0.172%
9	8.145	527	530	532	rBV	925144	1084126	29.72%	3.275%
10	9.219	621	624	626	rBV	3457456	3647930	100.00%	11.020%
11	9.333	632	634	636	rVB	58860	51553	1.41%	0.156%
12	9.607	656	658	661	rBV	857361	850947	23.33%	2.571%
13	9.893	680	683	685	rVB	1453835	1285383	35.24%	3.883%
14	10.328	716	721	722	rBV2	41458	79592	2.18%	0.240%
15	10.545	736	740	743	rBV	21842	43638	1.20%	0.132%
16	10.682	749	752	754	rBV	1943121	2023409	55.47%	6.113%
17	10.796	760	762	769	rVB	91786	112080	3.07%	0.339%
18	11.242	799	801	803	rBV	66292	65388	1.79%	0.198%
19	11.379	810	813	815	rBV	1089294	1251227	34.30%	3.780%
20	11.608	830	833	837	rBV	120624	241000	6.61%	0.728%
21	11.665	837	838	841	rVB	40009	38709	1.06%	0.117%
22	12.156	879	881	882	rBV	48936	43963	1.21%	0.133%
23	12.419	902	904	913	rBV	188475	319465	8.76%	0.965%
24	12.956	948	951	954	rBV	2740384	3225743	88.43%	9.745%
25	13.859	1028	1030	1037	rBV	45251	91886	2.52%	0.278%
26	14.008	1040	1043	1045	rBV	1306056	1185224	32.49%	3.581%
27	14.774	1108	1110	1114	rVB	36793	39259	1.08%	0.119%
28	14.842	1114	1116	1118	rBV	167258	166457	4.56%	0.503%
29	15.094	1136	1138	1141	rVB	42935	45928	1.26%	0.139%
30	15.437	1165	1168	1177	rBV	792406	1017458	27.89%	3.074%
31	15.871	1203	1206	1210	rVB	45880	62416	1.71%	0.189%
32	16.351	1245	1248	1253	rVB	38837	72204	1.98%	0.218%
33	16.911	1293	1297	1302	rBV	22996	51098	1.40%	0.154%
34	17.563	1351	1354	1358	rVB3	17975	45333	1.24%	0.137%

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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-BF013017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

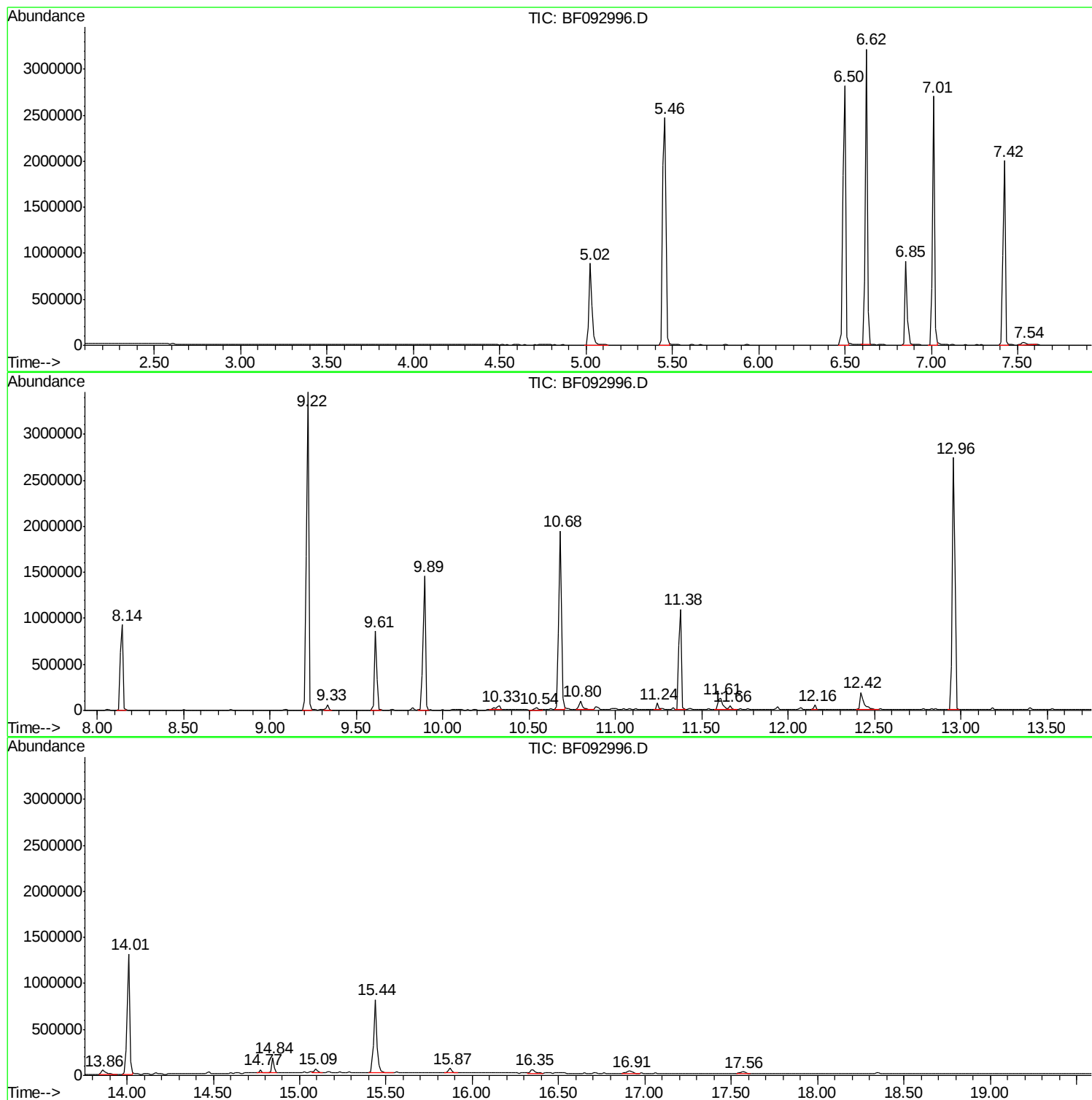
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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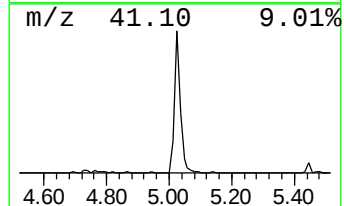
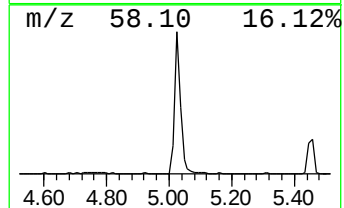
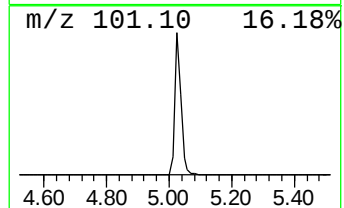
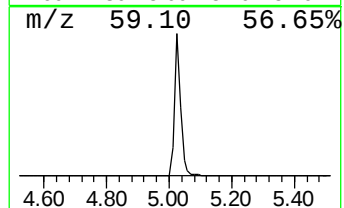
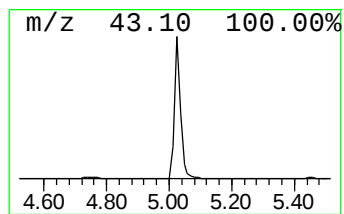
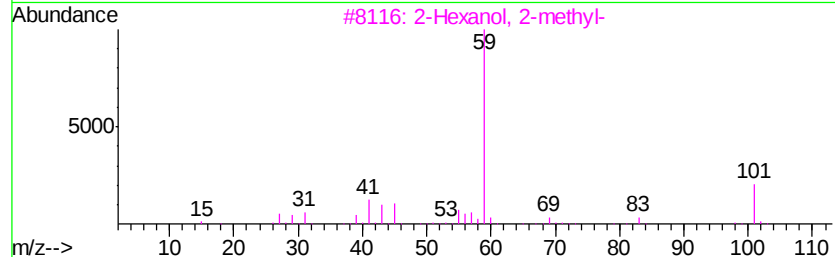
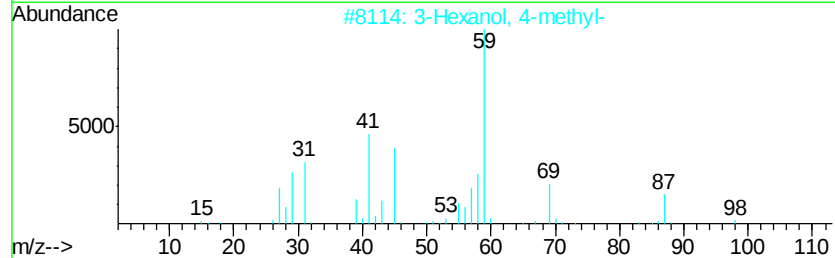
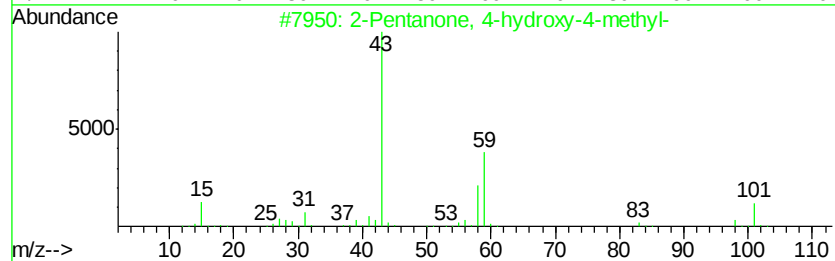
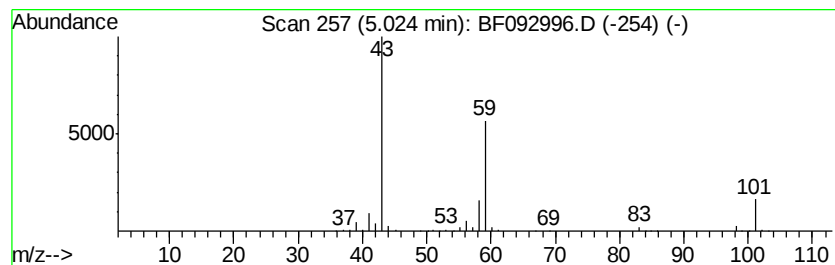
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	26.59 ng	1124320	1,4-Dichlorobenzene-d4	6.85

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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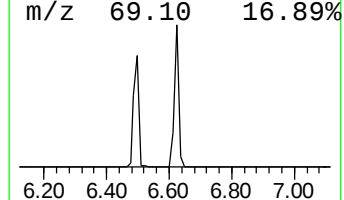
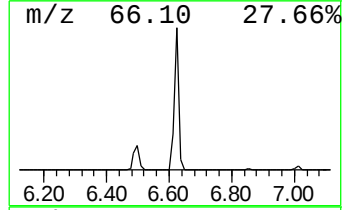
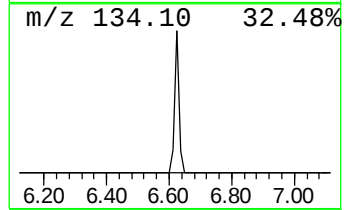
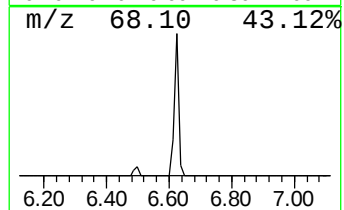
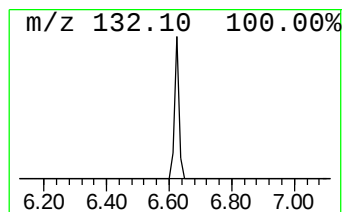
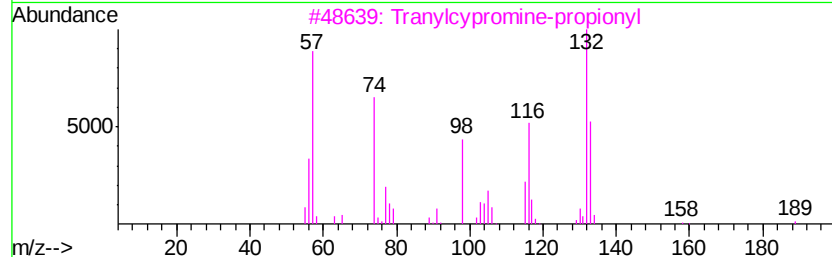
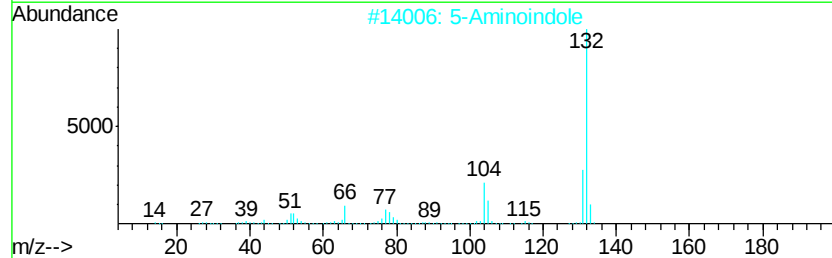
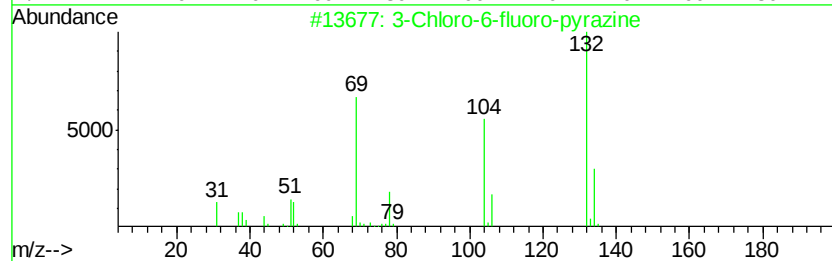
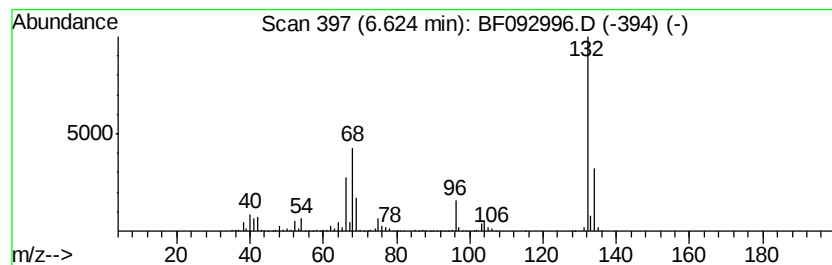
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Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	69.31 ng	2930700	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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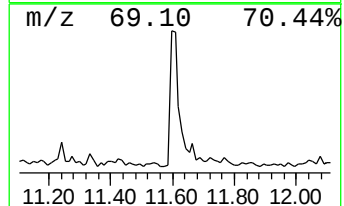
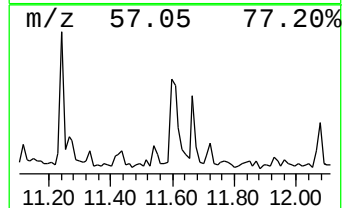
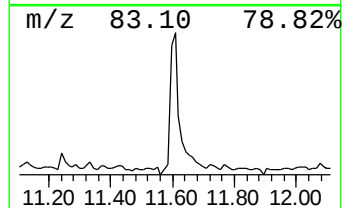
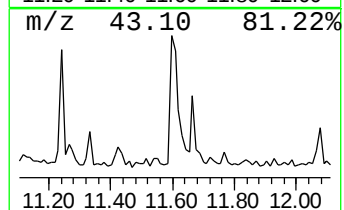
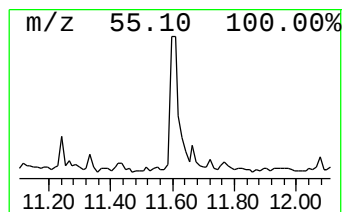
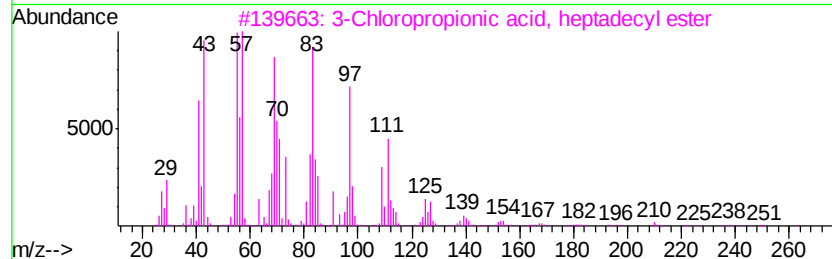
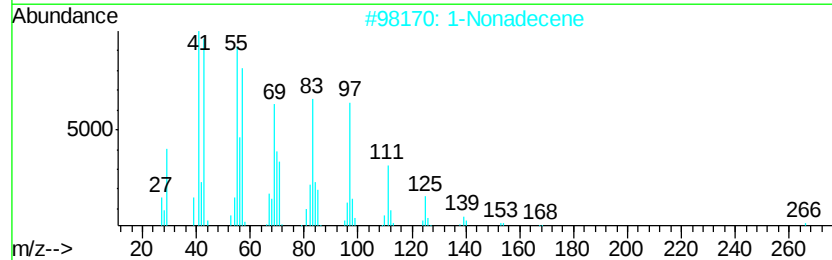
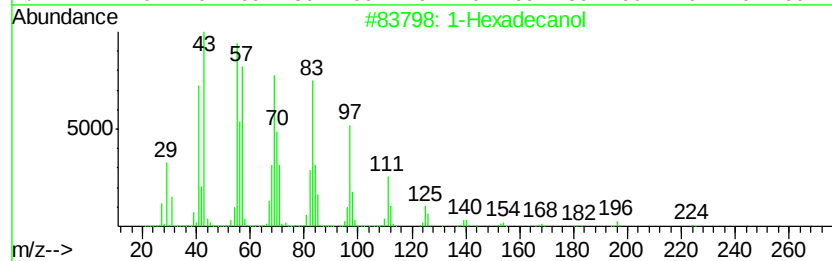
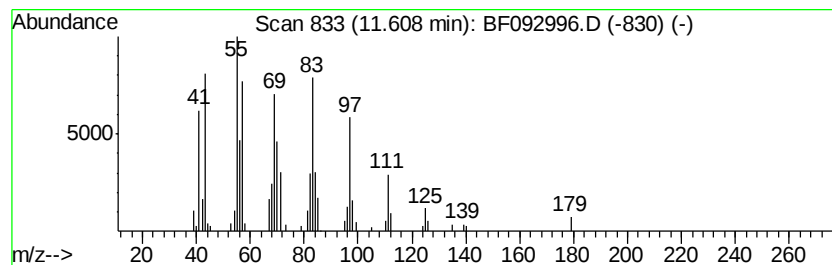
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Peak Number 4 1-Hexadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.61	3.85 ng	241000	Phenanthrene-d10	11.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	95
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
4	1-Heptadecanol	256	C17H36O	001454-85-9	91
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91



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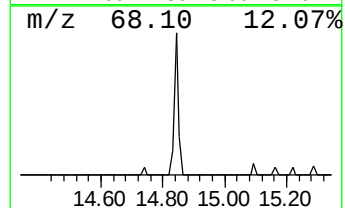
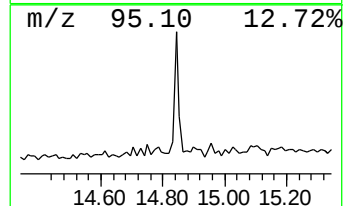
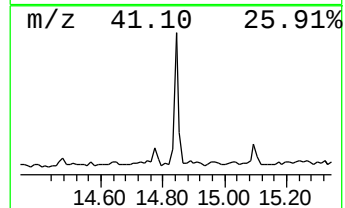
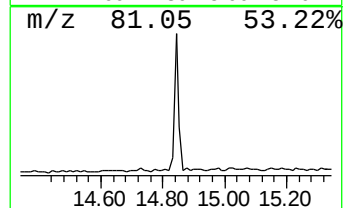
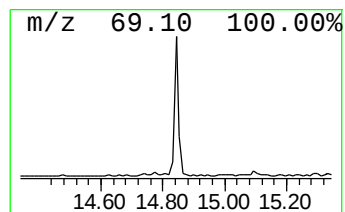
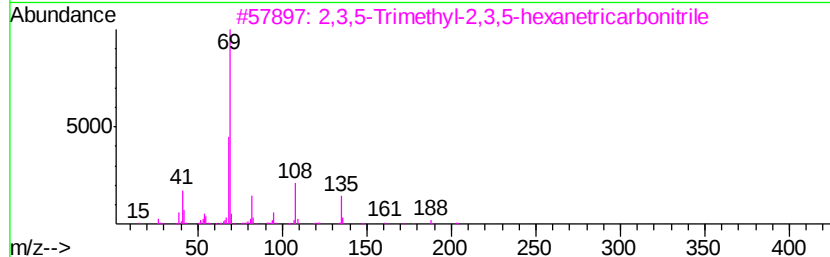
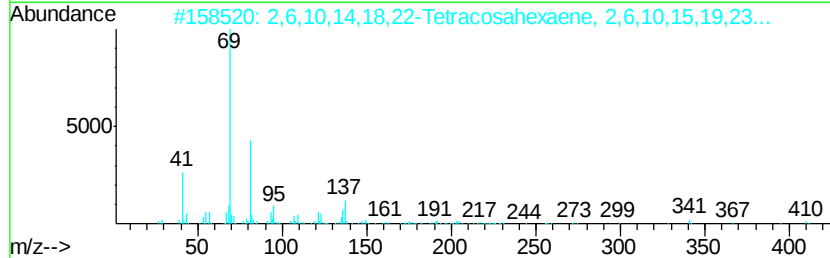
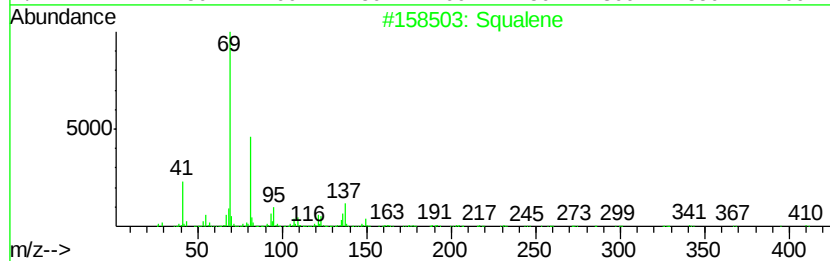
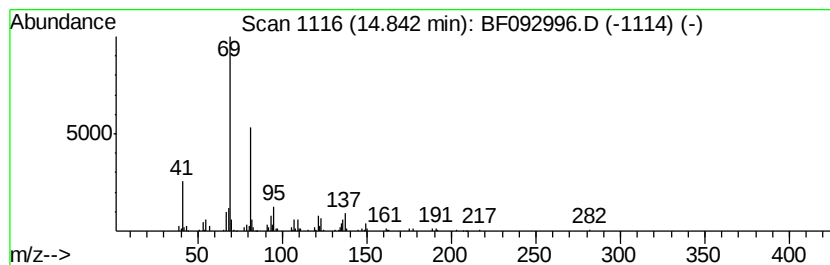
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	3.27 ng	166457	Perylene-d12	15.44
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	007683-64-9 91
2	2,6,10,14,18,22-Tetracosahexaene...		410 C30H50	000111-02-4 91
3	2,3,5-Trimethyl-2,3,5-hexanetric...		203 C12H17N3	003974-79-6 59
4	1,5-Heptadiene, 3,3,6-trimethyl-		138 C10H18	035387-63-4 58
5	Methanone, dicyclopropyl-		110 C7H10O	001121-37-5 50



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	26.6	ng	1124320	1	6.85	845666	20.0
unknown6.62	6.62	69.3	ng	2930700	1	6.85	845666	20.0
1-Hexadecanol	11.61	3.9	ng	241000	4	11.38	1251230	20.0
Squalene	14.84	3.3	ng	166457	6	15.44	1017460	20.0