

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021517\
 Data File : BF092958.D
 Acq On : 15 Feb 2017 18:36
 Operator : SJ/MA
 Sample : I1794-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 22A-9-11

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

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.047	256	259	270	rBV	1207425	1896163	39.25%	4.545%
2	5.470	293	296	299	rBV	3291766	4439842	91.90%	10.641%
3	6.510	384	387	390	rBV	3364401	4376627	90.59%	10.490%
4	6.647	396	399	401	rBV	3430518	4600499	95.23%	11.026%
5	6.876	416	419	421	rBV	709891	862169	17.85%	2.066%
6	7.024	430	432	435	rBV	2655441	3287041	68.04%	7.878%
7	7.436	465	468	471	rBV	2026744	3020615	62.52%	7.240%
8	8.156	529	531	533	rBV	1435831	1215269	25.15%	2.913%
9	9.230	622	625	628	rBV	4159167	4449133	92.09%	10.663%
10	9.619	657	659	661	rBV	195319	246863	5.11%	0.592%
11	9.825	674	677	682	rVV	85680	168064	3.48%	0.403%
12	9.905	682	684	687	rVB	1594833	1372462	28.41%	3.289%
13	10.339	720	722	723	rVB	90236	82406	1.71%	0.198%
14	10.693	750	753	756	rBV	2083257	2339611	48.43%	5.607%
15	10.808	761	763	770	rVB	137999	164080	3.40%	0.393%
16	11.253	800	802	804	rBV	82008	81219	1.68%	0.195%
17	11.391	811	814	816	rBV	1570401	1449516	30.00%	3.474%
18	12.979	950	953	955	rBV	4396044	4831143	100.00%	11.579%
19	13.859	1028	1030	1039	rBV	155126	229215	4.74%	0.549%
20	14.019	1042	1044	1047	rVB	1281490	1320586	27.33%	3.165%
21	15.460	1167	1170	1176	rBV	926030	1240795	25.68%	2.974%
22	16.374	1247	1250	1257	rBV2	21497	49742	1.03%	0.119%

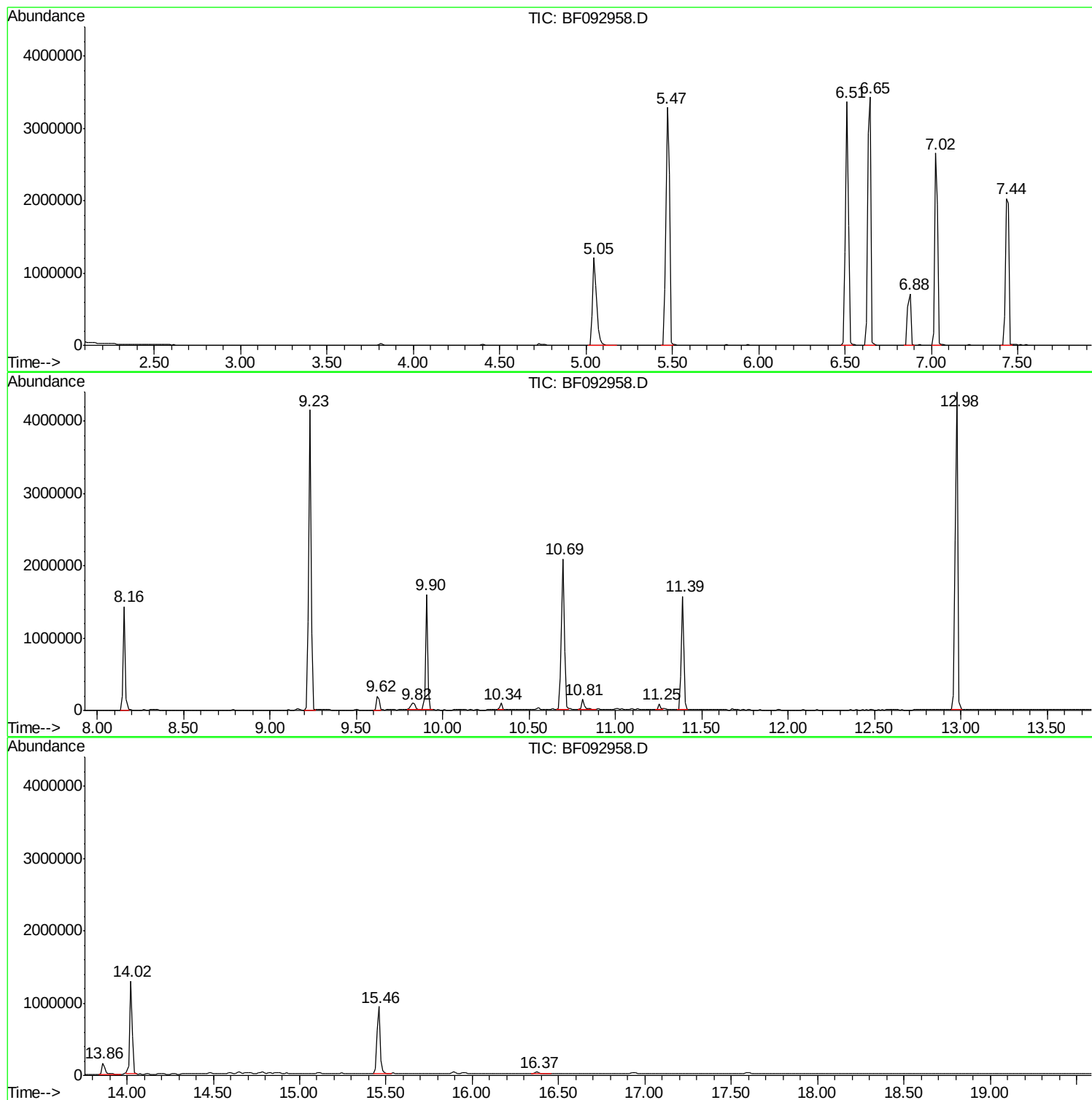
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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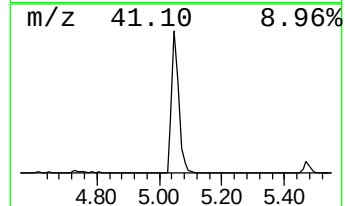
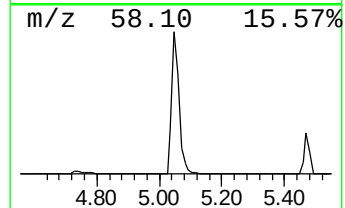
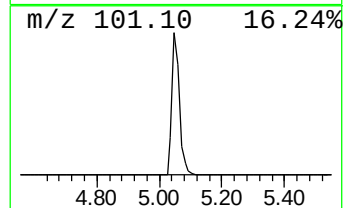
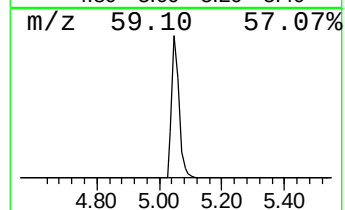
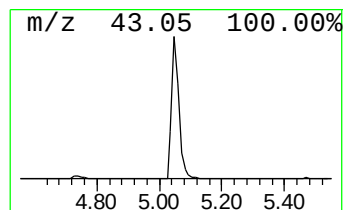
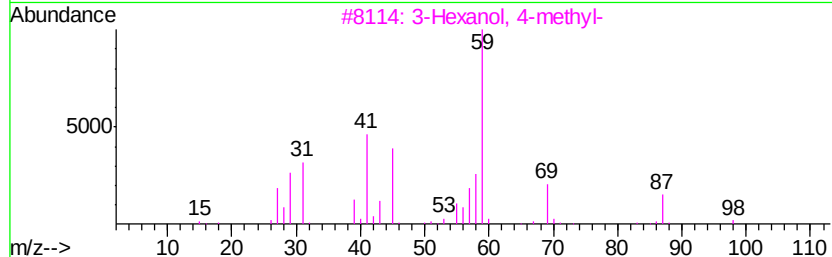
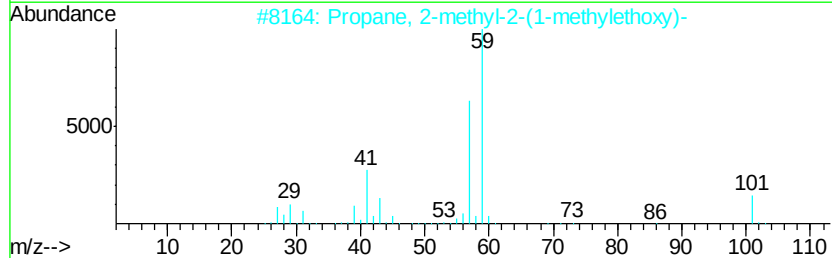
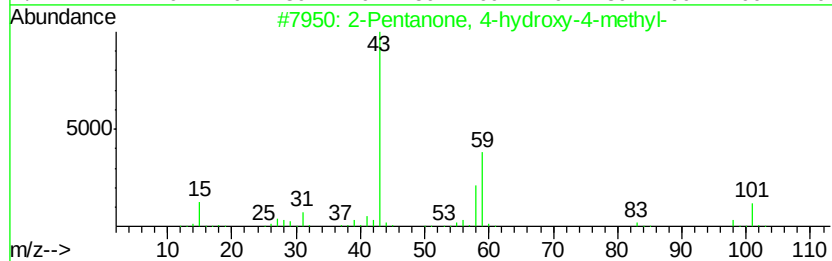
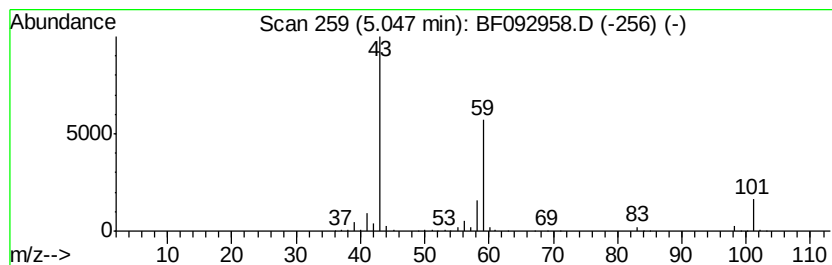
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	43.99 ng	1896160	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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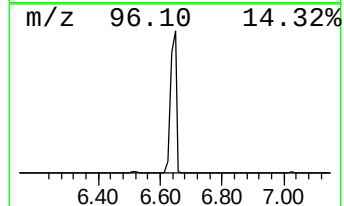
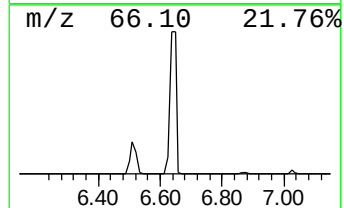
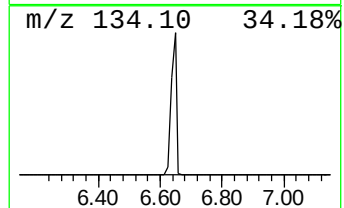
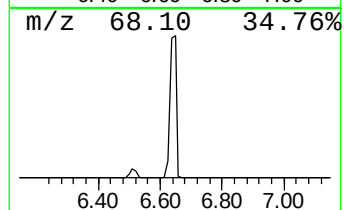
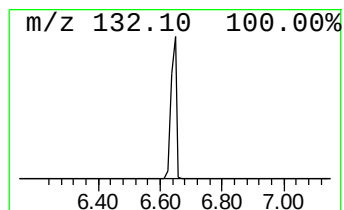
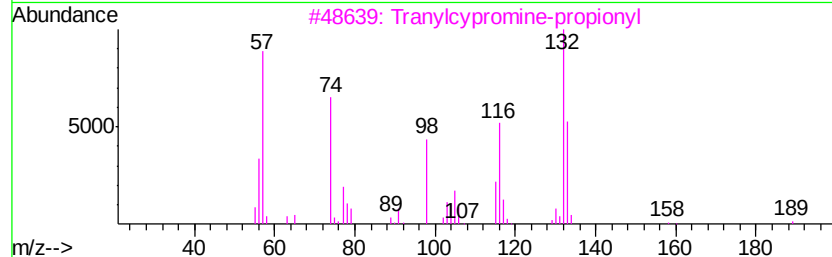
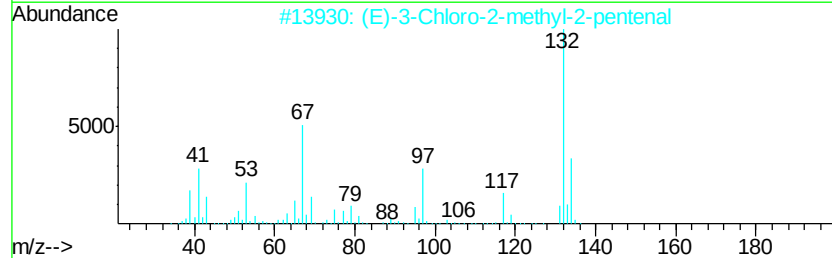
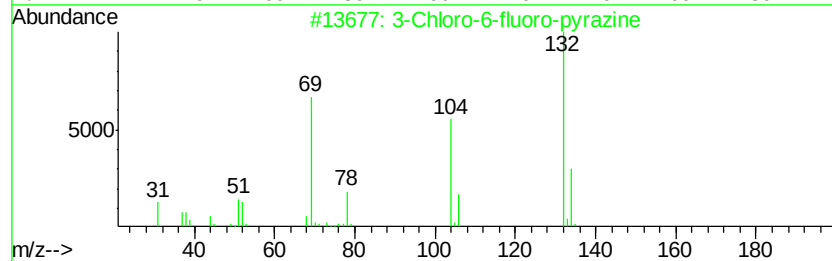
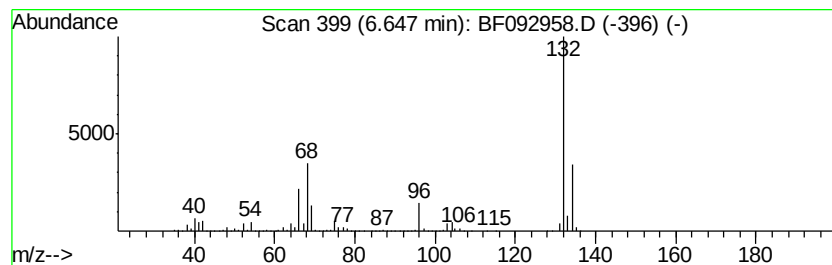
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Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	106.72 ng	4600500	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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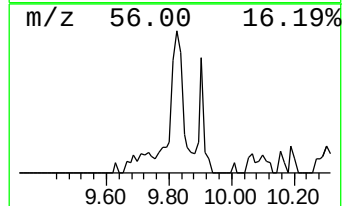
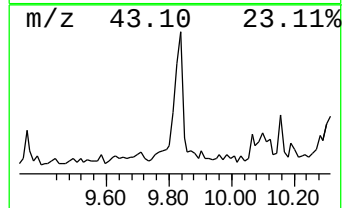
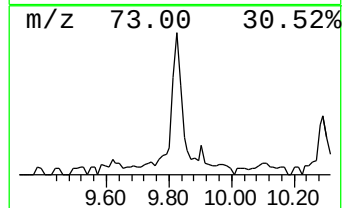
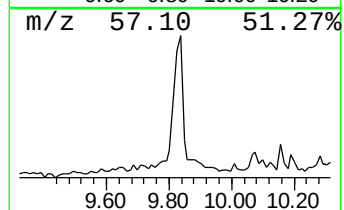
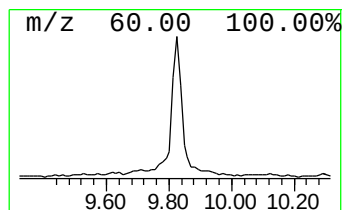
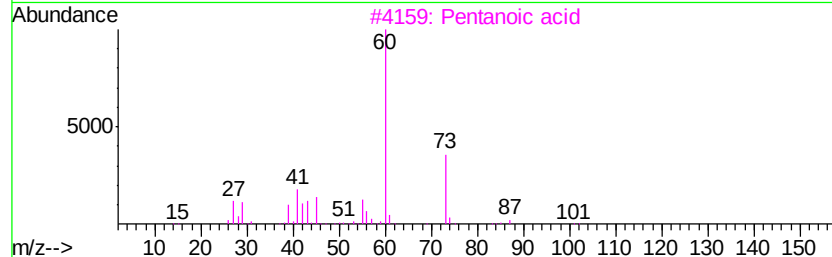
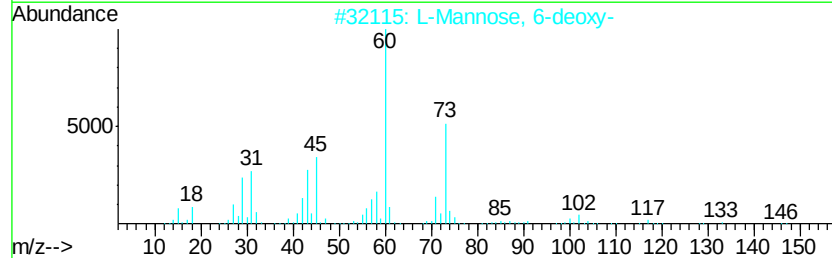
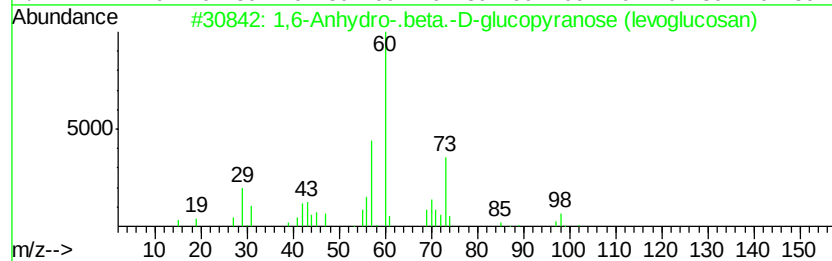
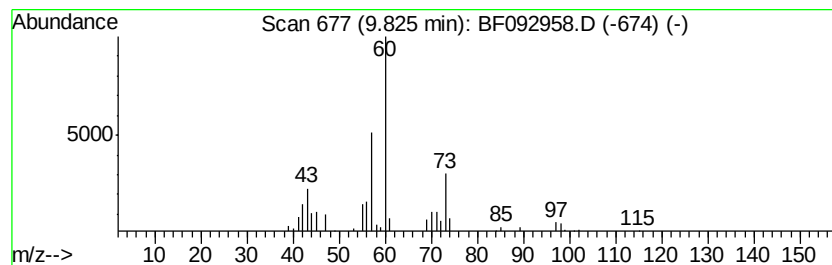
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Peak Number 4 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	2.45 ng	168064	Acenaphthene-d10	9.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	78
2		L-Mannose, 6-deoxy-	164	C6H12O5	003615-41-6	50
3		Pentanoic acid	102	C5H10O2	000109-52-4	50
4		Heptanoic acid	130	C7H14O2	000111-14-8	50
5		.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	42



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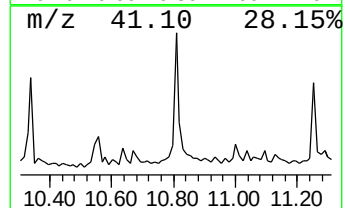
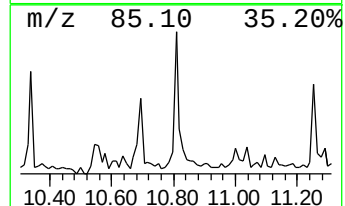
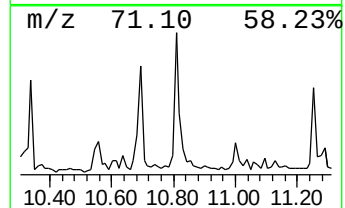
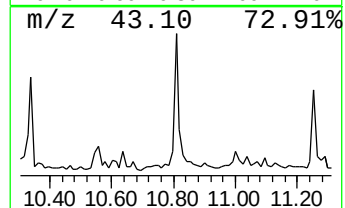
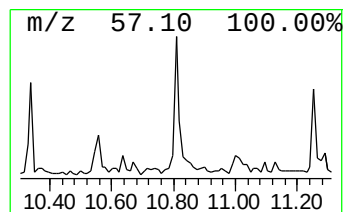
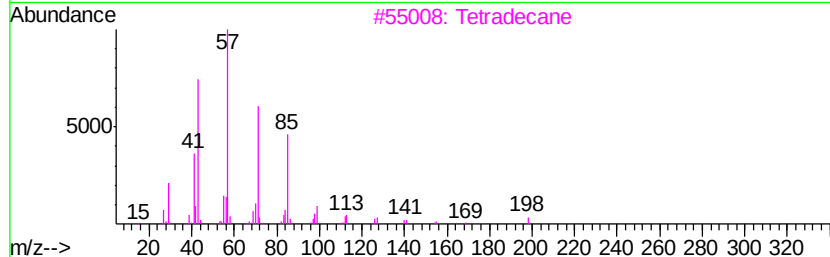
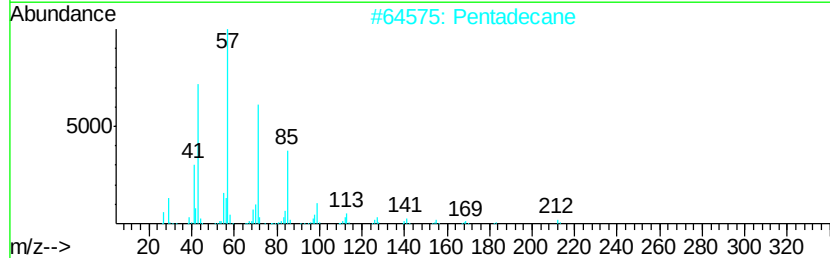
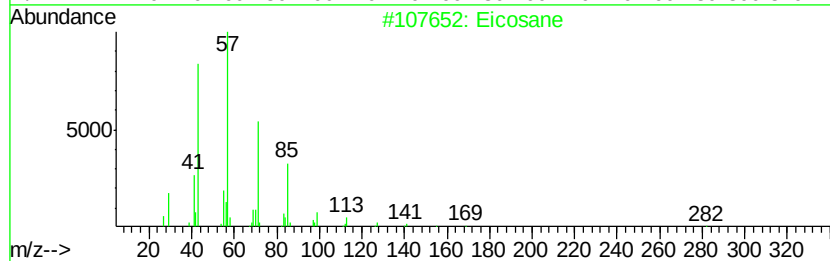
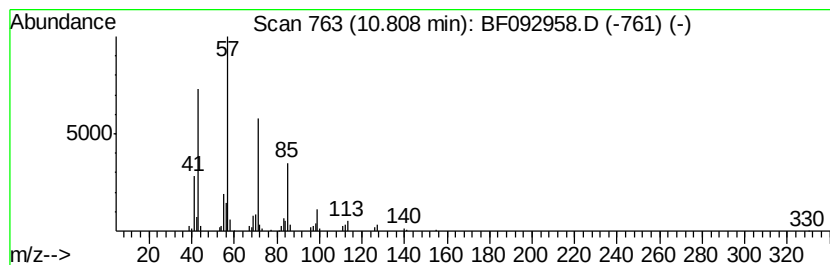
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Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	2.26 ng	164080	Phenanthrene-d10	11.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	91
2	Pentadecane	212 C15H32	000629-62-9	90
3	Tetradecane	198 C14H30	000629-59-4	90
4	Heptadecane	240 C17H36	000629-78-7	90
5	Hexadecane	226 C16H34	000544-76-3	90



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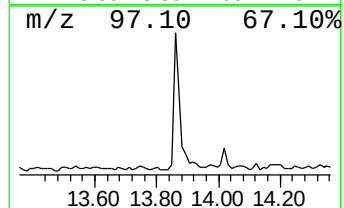
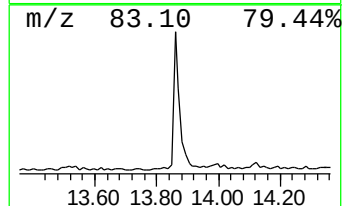
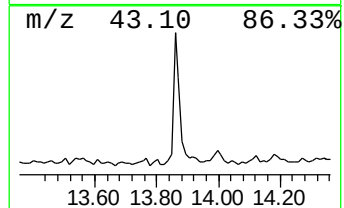
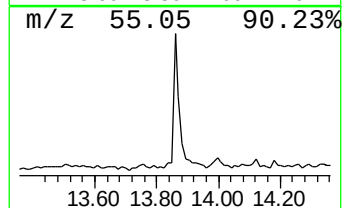
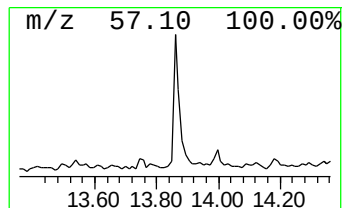
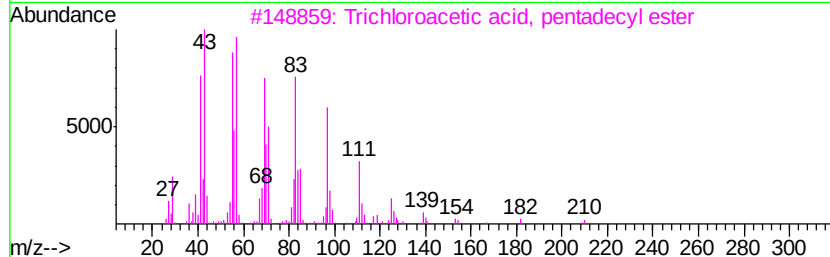
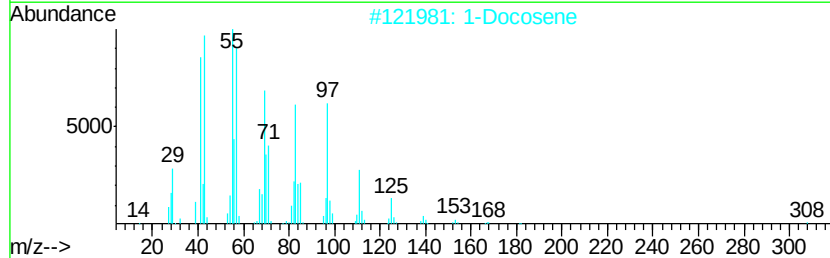
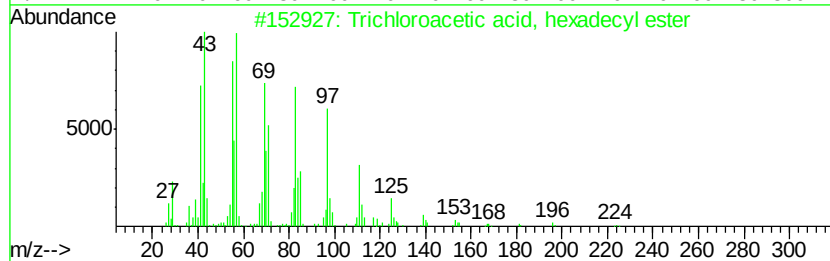
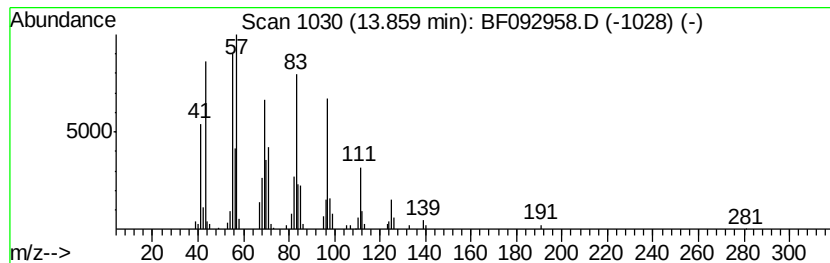
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trichloroacetic acid, hexadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	3.47 ng	229215	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		1-Docosene	308	C22H44	001599-67-3	94
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
5		Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	44.0	ng	1896160	1	6.88	862169	20.0
unknown6.65	6.65	106.7	ng	4600500	1	6.88	862169	20.0
1,6-Anhydro-.beta...	9.82	2.5	ng	168064	3	9.90	1372460	20.0
Eicosane	10.81	2.3	ng	164080	4	11.39	1449520	20.0
Trichloroacetic a...	13.86	3.5	ng	229215	5	14.02	1320590	20.0