

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
 Data File : BF092749.D
 Acq On : 2 Feb 2017 21:43
 Operator : SJ/MA
 Sample : I1650-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-28-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-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	3.938	158	162	165	rBV	70387	111453	2.37%	0.286%
2	5.127	263	266	280	rVB	1676539	2523885	53.66%	6.473%
3	5.550	300	303	306	rBV	3954839	4682393	99.55%	12.008%
4	6.579	390	393	396	rBV	3484224	4296069	91.34%	11.018%
5	6.704	401	404	407	rBV	3371495	4249703	90.35%	10.899%
6	6.933	422	424	427	rBV	999903	860680	18.30%	2.207%
7	7.093	435	438	441	rBV	3550930	3297410	70.11%	8.456%
8	7.505	471	474	476	rBV	2589951	2704268	57.49%	6.935%
9	8.225	534	537	540	rBV	1177849	1080102	22.96%	2.770%
10	9.310	628	632	634	rBV	3610642	4703488	100.00%	12.062%
11	9.699	663	666	668	rBV	265741	280429	5.96%	0.719%
12	9.985	688	691	693	rBV	1021831	1156076	24.58%	2.965%
13	10.408	724	728	729	rBV	87739	87230	1.85%	0.224%
14	10.773	757	760	762	rBV	2102744	2327497	49.48%	5.969%
15	10.876	767	769	774	rVB	130720	149829	3.19%	0.384%
16	11.322	806	808	809	rBV	94127	78608	1.67%	0.202%
17	11.459	818	820	823	rBV	1015783	1020196	21.69%	2.616%
18	13.048	956	959	961	rBV	3357036	3246915	69.03%	8.327%
19	13.939	1035	1037	1042	rBV	65025	108518	2.31%	0.278%
20	14.099	1048	1051	1053	rBV	864264	856316	18.21%	2.196%
21	14.934	1122	1124	1127	rBV	67186	93924	2.00%	0.241%
22	15.562	1176	1179	1183	rBV	698226	1004887	21.36%	2.577%
23	16.500	1259	1261	1268	rVB4	27007	73206	1.56%	0.188%

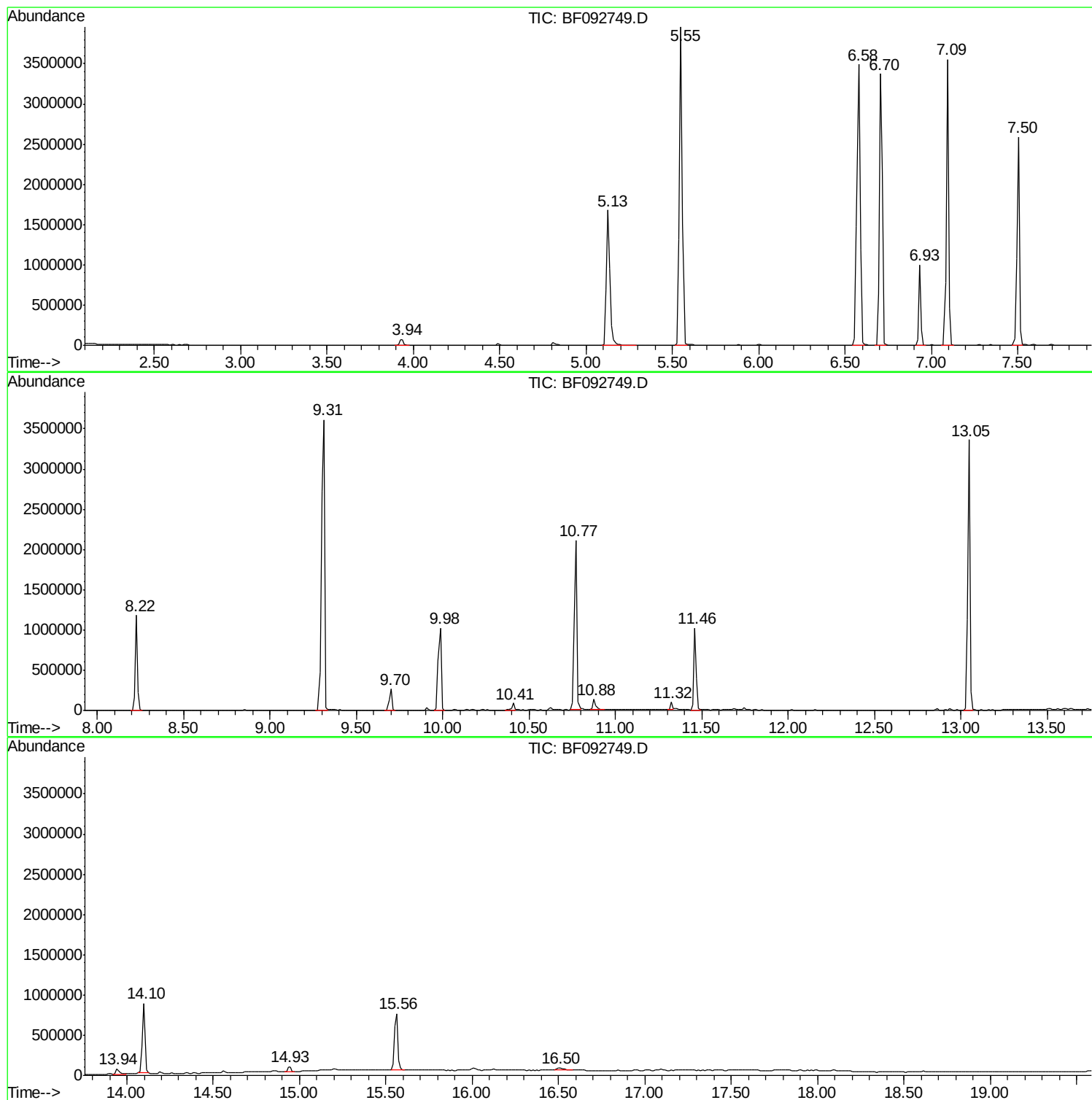
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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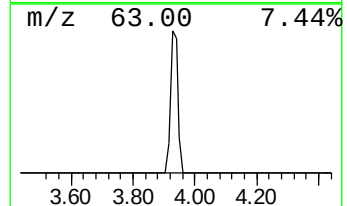
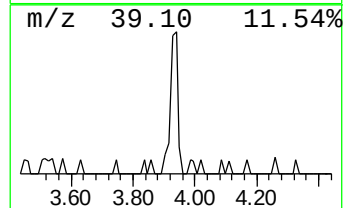
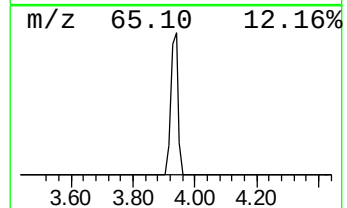
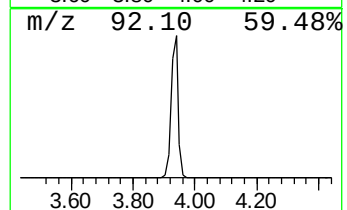
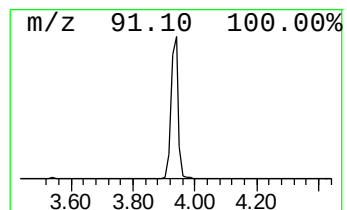
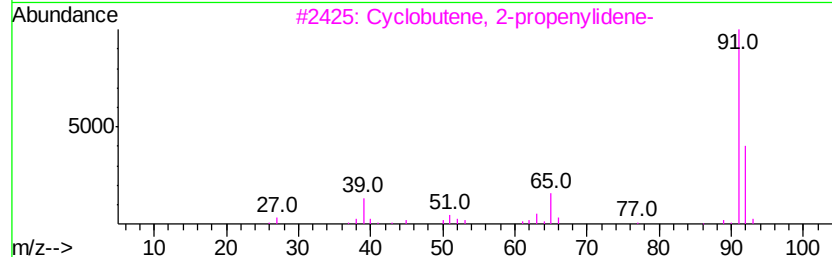
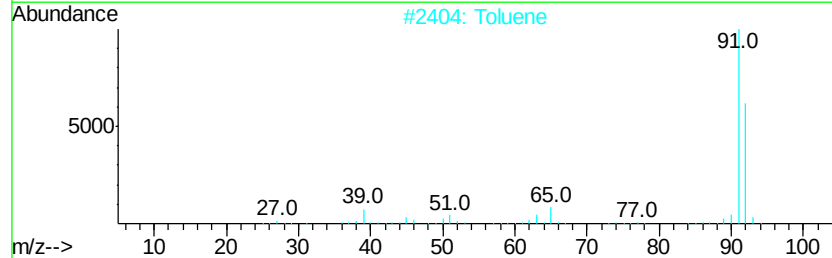
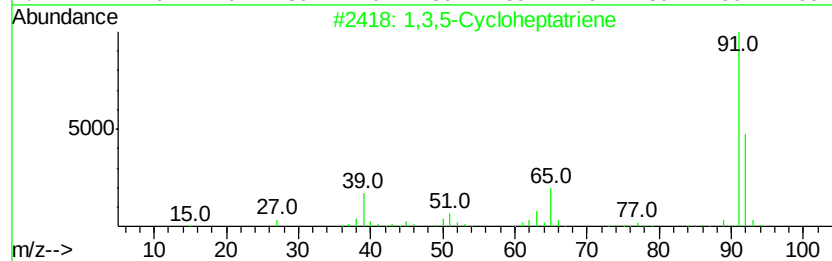
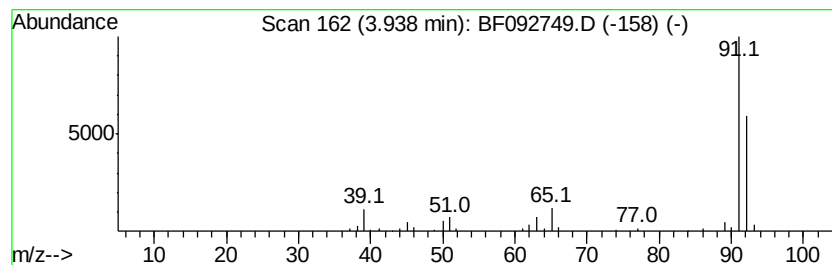
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3,5-Cycloheptatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.94	2.59 ng	111453	1,4-Dichlorobenzene-d4	6.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	91
2			Toluene	92	C7H8	000108-88-3	87
3			Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	72
4			Tetracyclo[3.2.0.0(2,7).0(4,6)]h...	92	C7H8	000278-06-8	64
5			2,5-Norbornadiene	92	C7H8	000121-46-0	64



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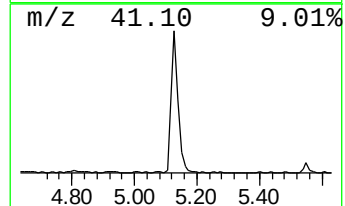
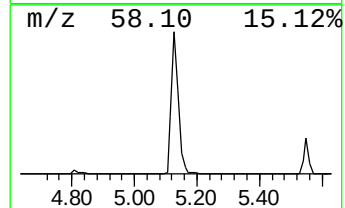
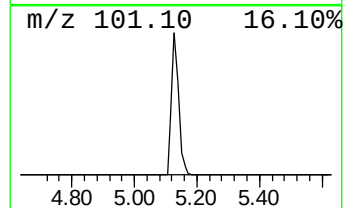
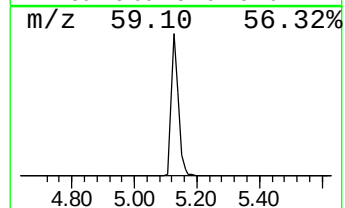
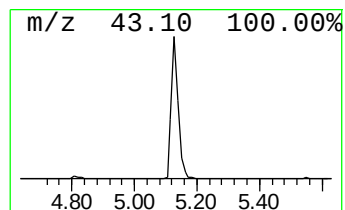
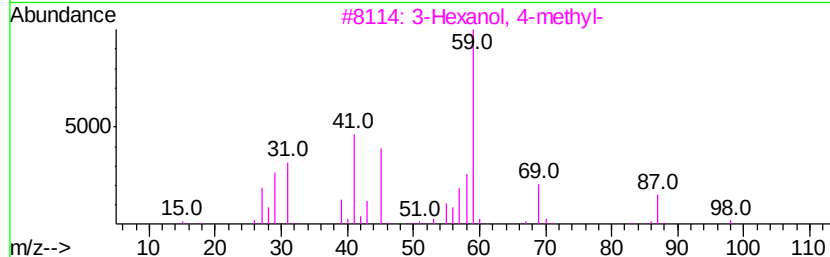
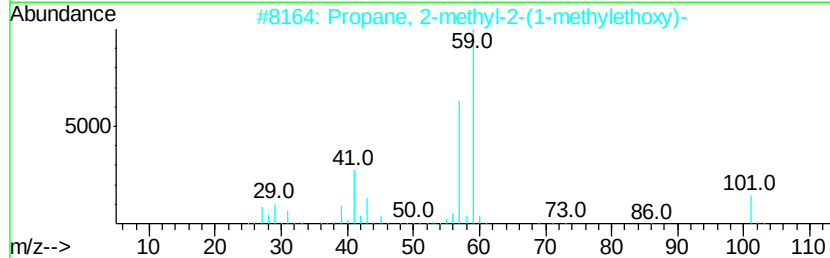
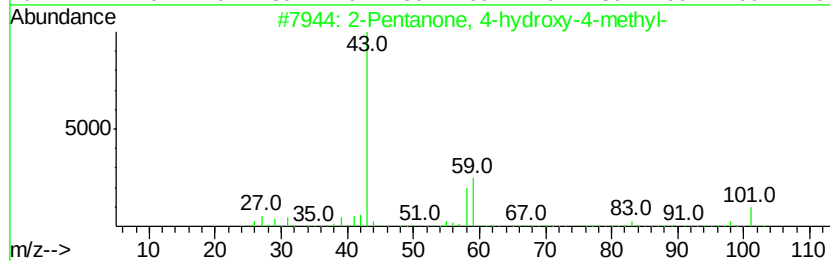
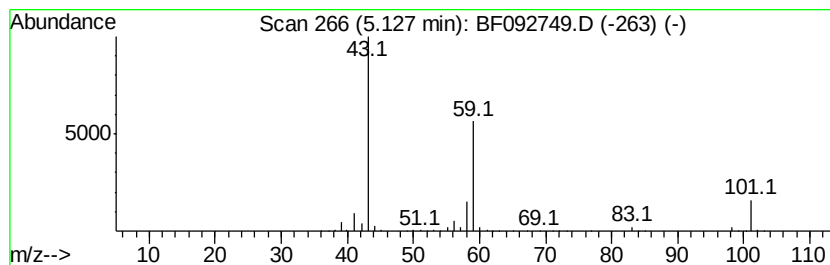
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	58.65 ng	2523890	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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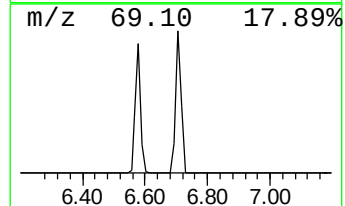
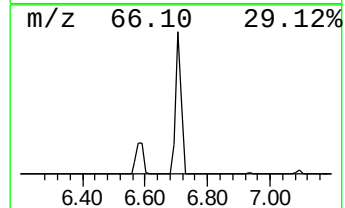
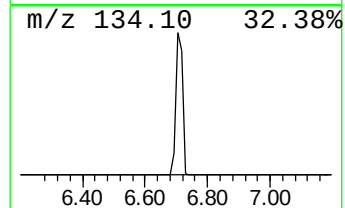
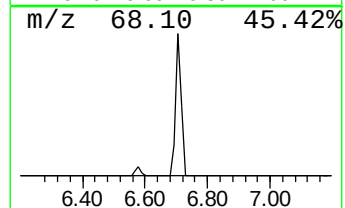
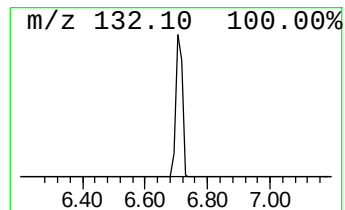
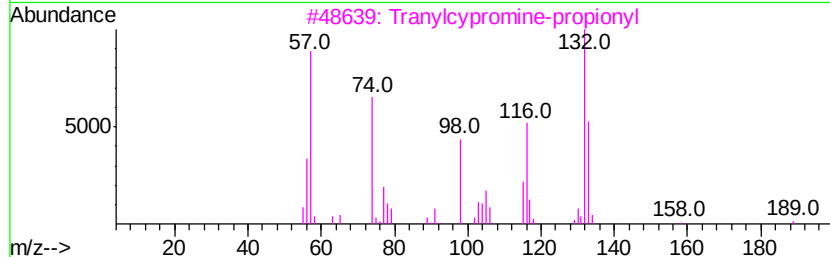
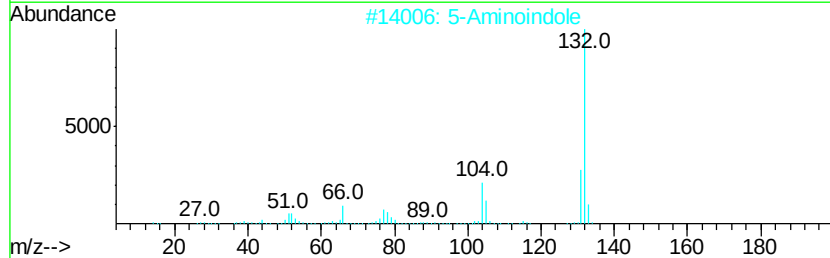
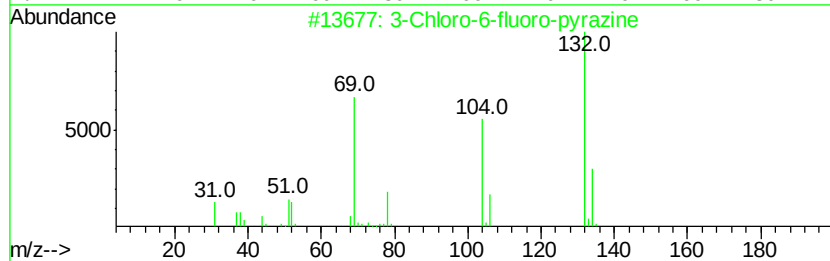
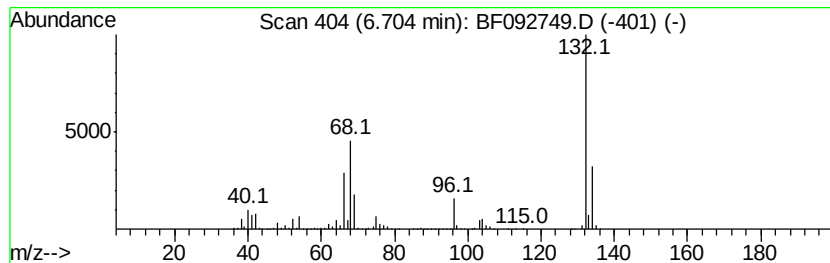
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Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	98.75 ng	4249700	1,4-Dichlorobenzene-d4	6.93

Hit#	of	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	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10	
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9	
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9	



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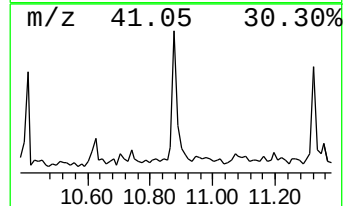
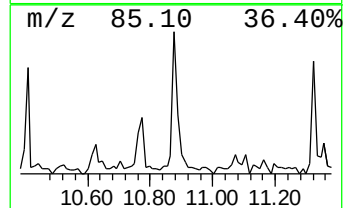
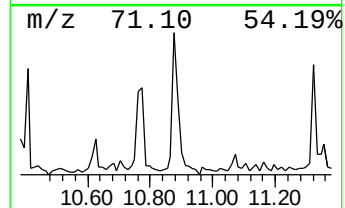
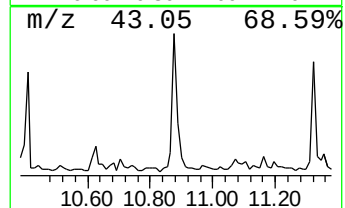
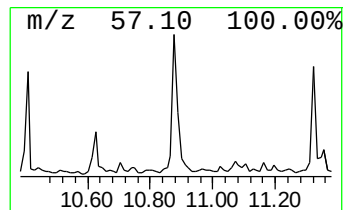
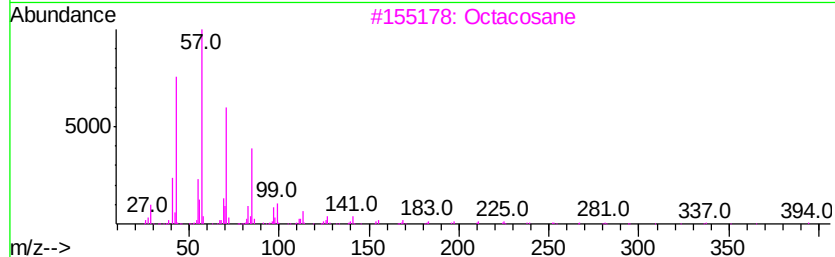
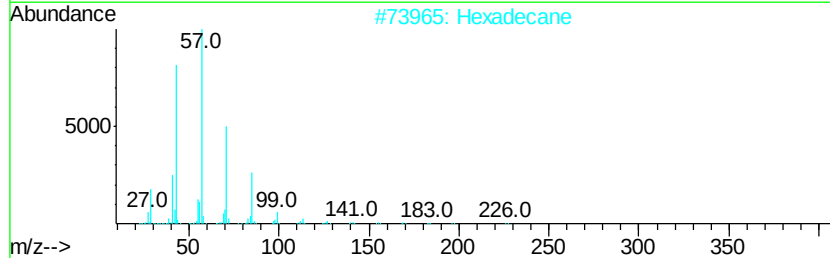
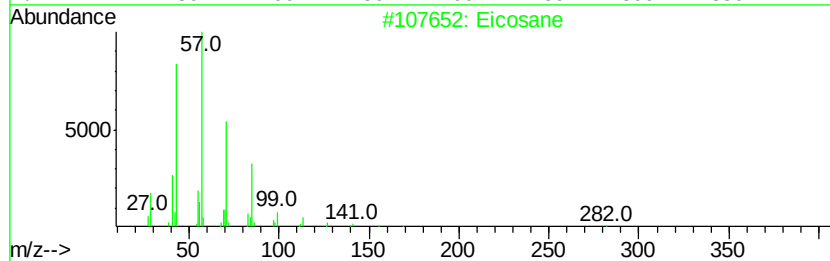
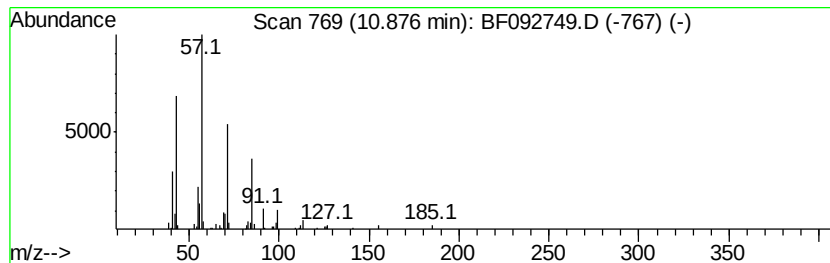
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	2.94 ng	149829	Phenanthrene-d10	11.46
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	87
2	Hexadecane	226 C16H34	000544-76-3	86
3	Octacosane	394 C28H58	000630-02-4	80
4	Heptacosane	380 C27H56	000593-49-7	78
5	Tetracosane	338 C24H50	000646-31-1	72



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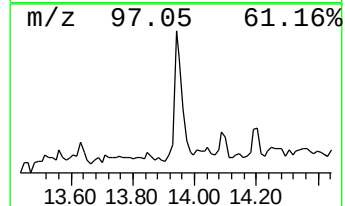
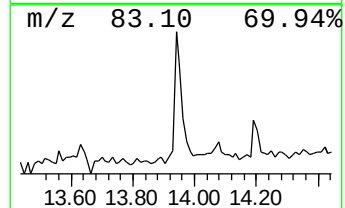
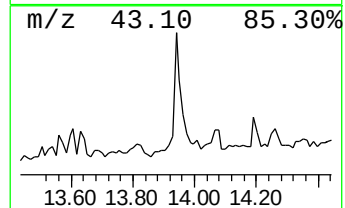
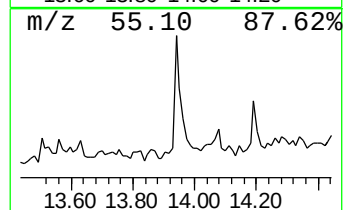
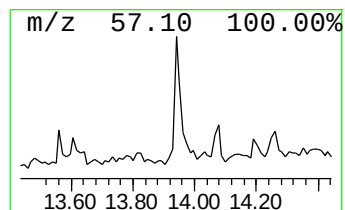
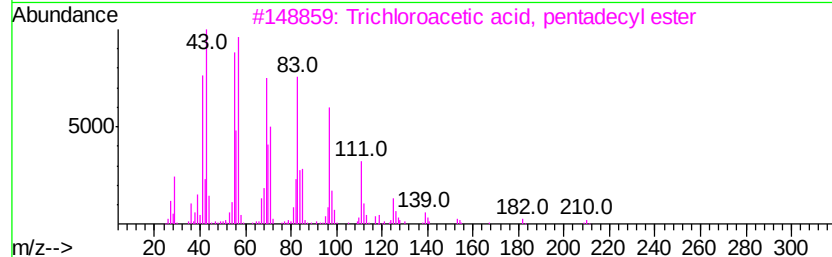
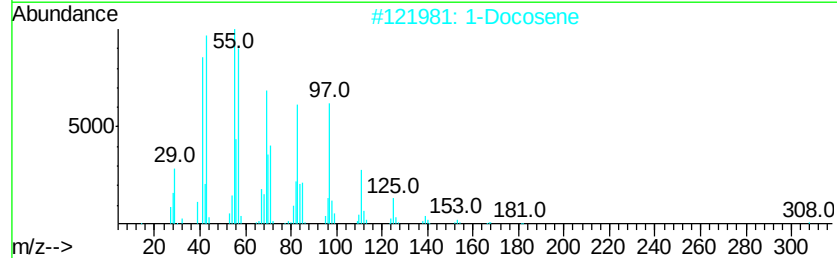
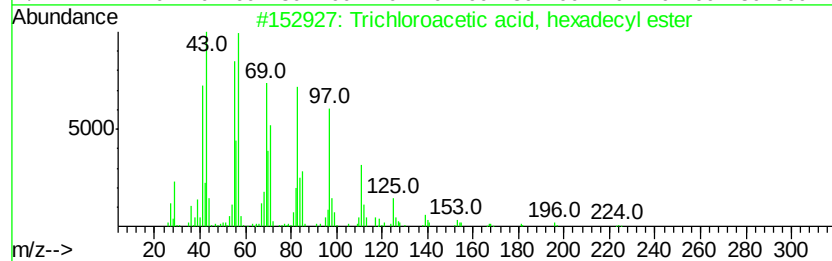
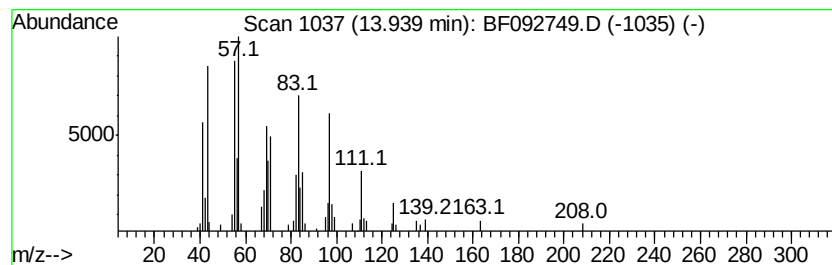
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	2.53 ng	108518	Chrysene-d12	14.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2		1-Docosene	308	C22H44	001599-67-3	93
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3,5-Cycloheptat...	3.94	2.6	ng	111453	1	6.93	860680	20.0
2-Pentanone, 4-hy...	5.13	58.6	ng	2523890	1	6.93	860680	20.0
unknown6.70	6.70	98.8	ng	4249700	1	6.93	860680	20.0
Eicosane	10.88	2.9	ng	149829	4	11.46	1020200	20.0
Trichloroacetic a...	13.94	2.5	ng	108518	5	14.10	856316	20.0