

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
 Data File : BF093368.D
 Acq On : 3 Mar 2017 19:39
 Operator : SJ/MA
 Sample : I2079-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-1

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	4.933	247	249	258	rBV	338066	495934	9.04%	1.315%
2	5.379	286	288	303	rBV	2475253	2604918	47.51%	6.906%
3	6.430	378	380	388	rBV	1759304	1872499	34.15%	4.964%
4	6.556	388	391	393	rBV	3439575	3801119	69.32%	10.077%
5	6.784	409	411	413	rBV	1083195	1089526	19.87%	2.888%
6	6.933	422	424	427	rBV	2394267	3374317	61.54%	8.946%
7	7.356	458	461	464	rBV	2755199	2885716	52.63%	7.650%
8	8.076	521	524	526	rBV	1234462	1523003	27.78%	4.038%
9	9.150	614	618	620	rBV	4509076	5483207	100.00%	14.537%
10	9.539	650	652	655	rBV	406314	414846	7.57%	1.100%
11	9.756	668	671	674	rBV2	57820	108092	1.97%	0.287%
12	9.825	674	677	679	rVV	1422762	1755410	32.01%	4.654%
13	10.225	710	712	713	rBV	56714	80759	1.47%	0.214%
14	10.248	713	714	716	rVB	192987	146327	2.67%	0.388%
15	10.465	730	733	736	rBV	61744	91684	1.67%	0.243%
16	10.613	743	746	748	rBV	2524182	2651302	48.35%	7.029%
17	10.716	753	755	760	rVB	212716	287563	5.24%	0.762%
18	11.162	792	794	800	rVB2	147642	232653	4.24%	0.617%
19	11.299	804	806	809	rVV	1495191	1711589	31.22%	4.538%
20	11.356	809	811	814	rVB2	30074	56603	1.03%	0.150%
21	11.596	829	832	834	rBV	141518	156364	2.85%	0.415%
22	11.996	864	867	869	rVB	82868	76895	1.40%	0.204%
23	12.888	942	945	948	rBV	3859712	3965812	72.33%	10.514%
24	13.779	1020	1023	1027	rBV	166208	207364	3.78%	0.550%
25	13.939	1035	1037	1040	rVB	1502125	1449472	26.43%	3.843%
26	15.357	1158	1161	1164	rBV	889927	1131829	20.64%	3.001%
27	16.214	1233	1236	1240	rBV2	32464	64858	1.18%	0.172%

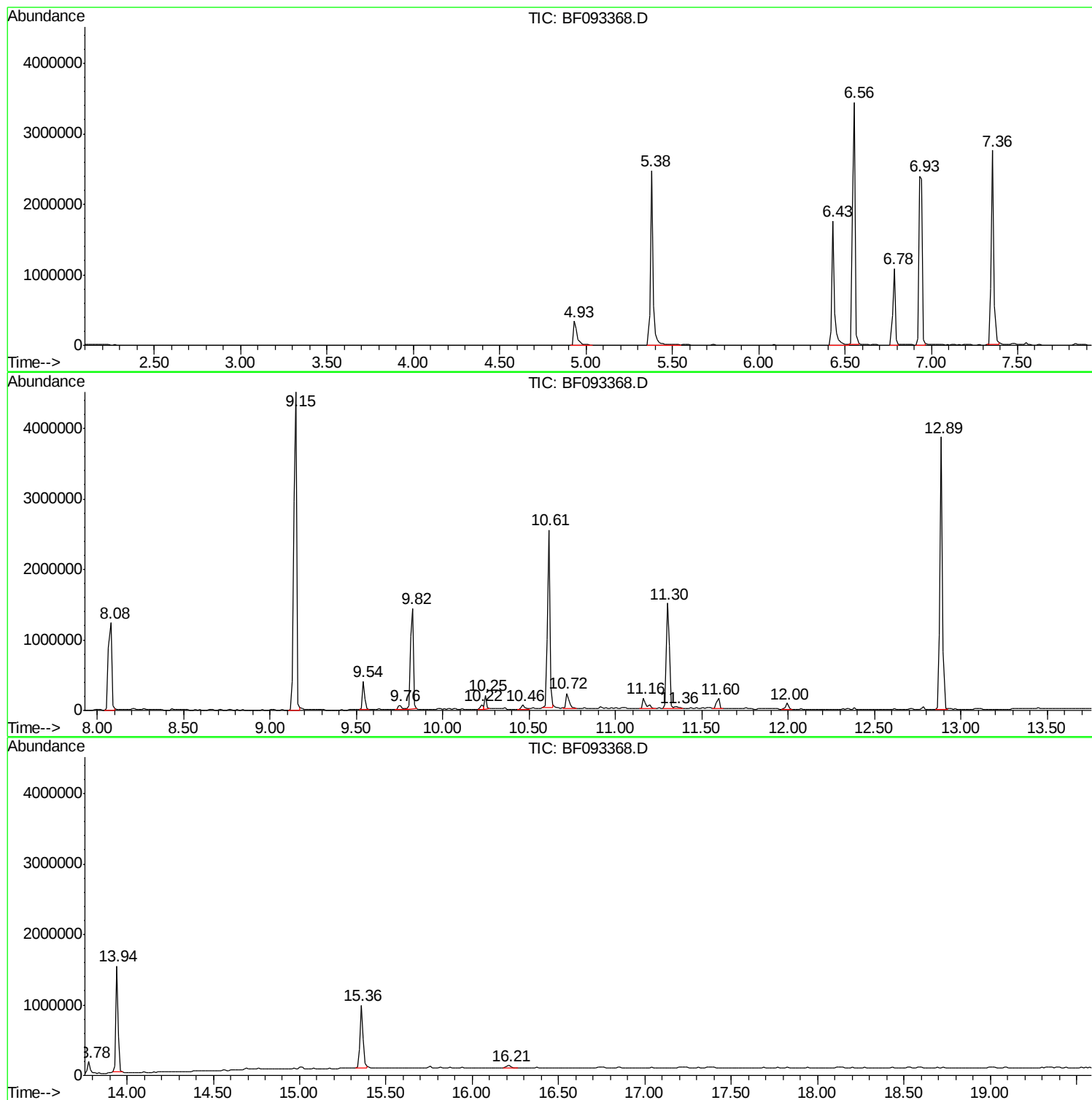
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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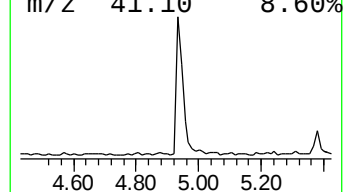
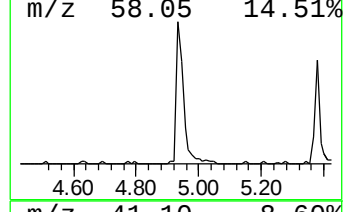
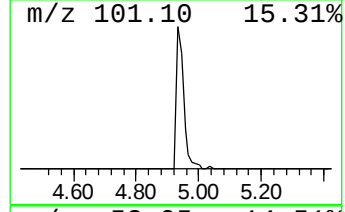
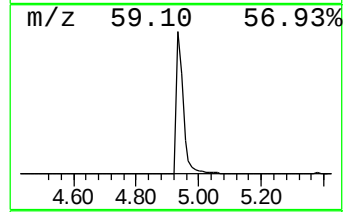
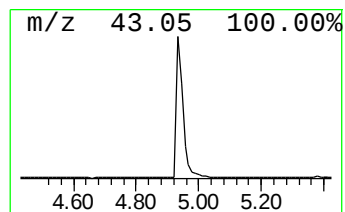
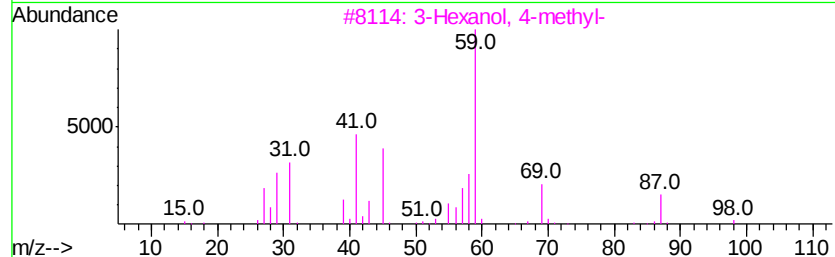
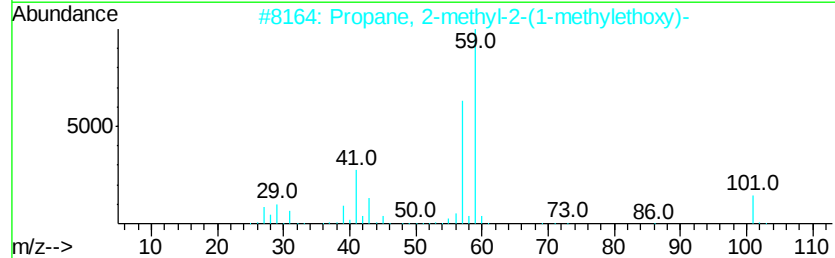
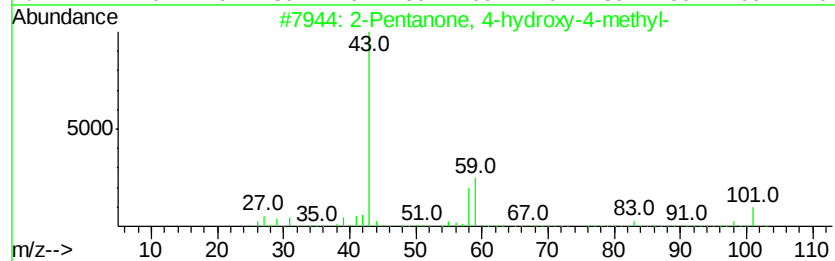
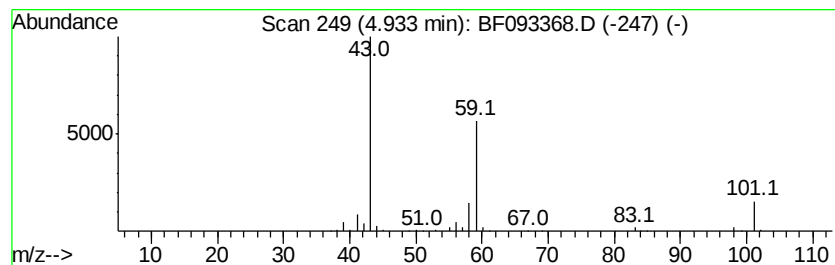
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	9.10 ng	495934	1,4-Dichlorobenzene-d4	6.78

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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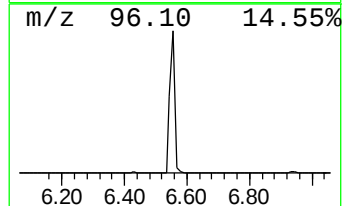
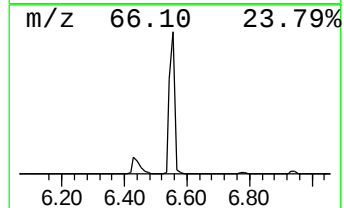
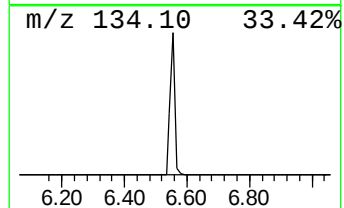
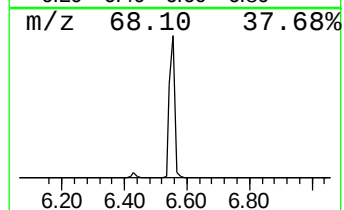
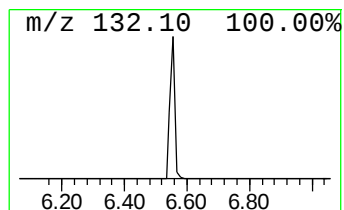
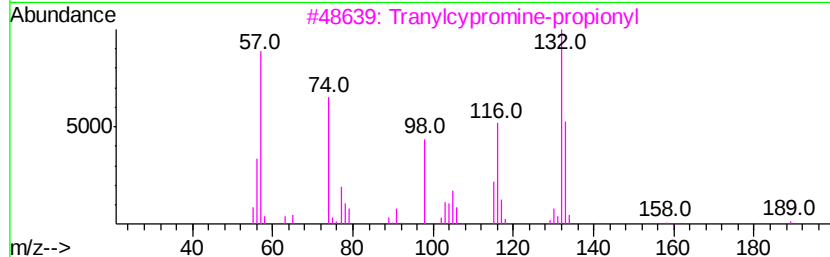
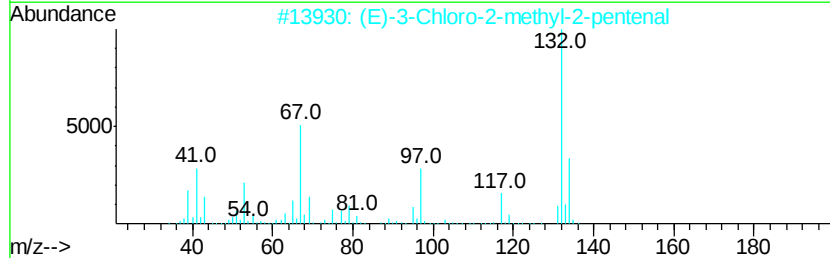
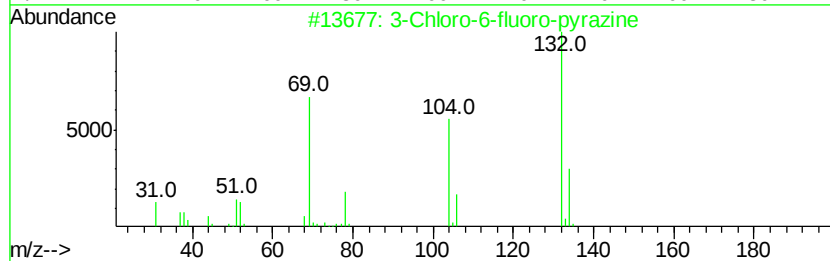
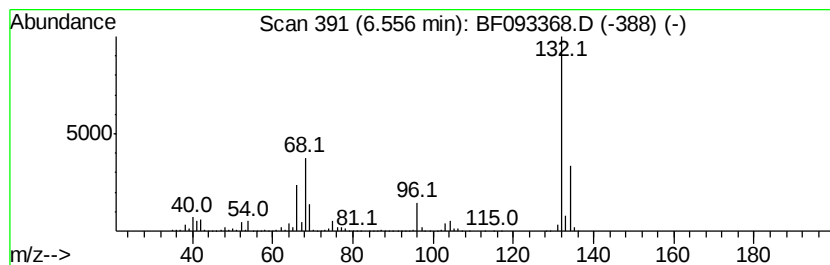
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	69.78 ng	3801120	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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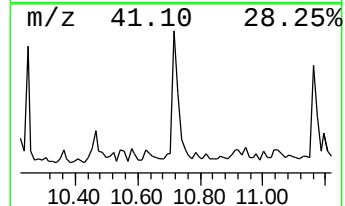
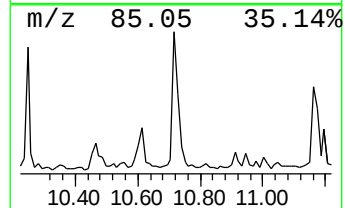
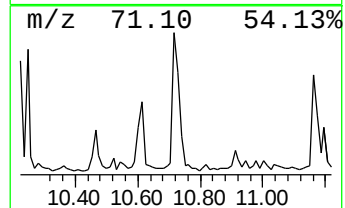
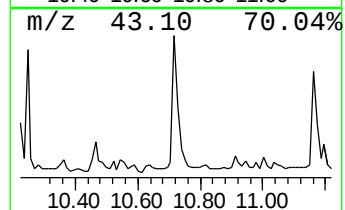
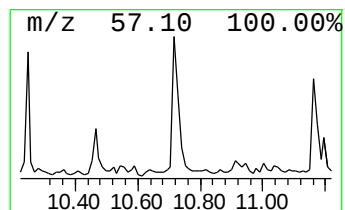
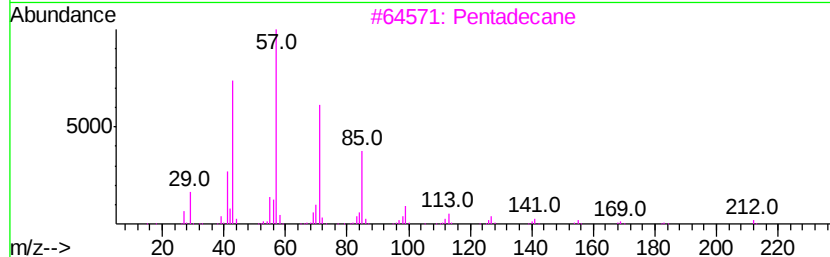
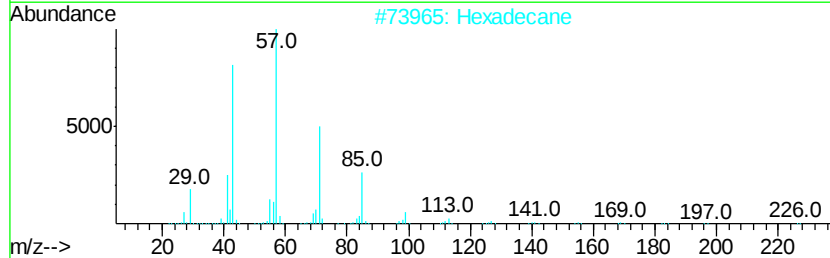
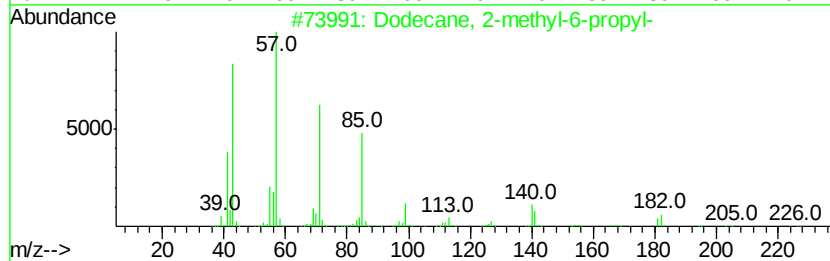
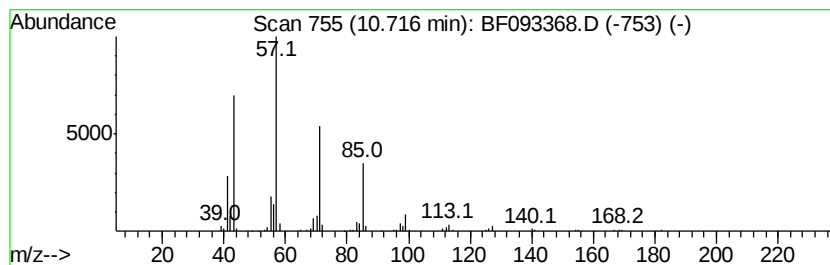
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Dodecane, 2-methyl-6-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	3.36 ng	287563	Phenanthrene-d10	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86	
2	Hexadecane	226	C16H34	000544-76-3	86	
3	Pentadecane	212	C15H32	000629-62-9	78	
4	Nonane, 5-butyl-	184	C13H28	017312-63-9	72	
5	Dodecane, 3-methyl-	184	C13H28	017312-57-1	72	



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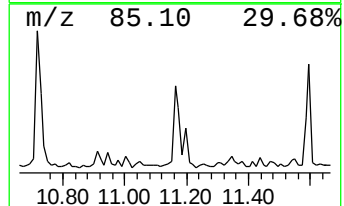
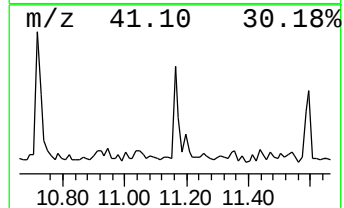
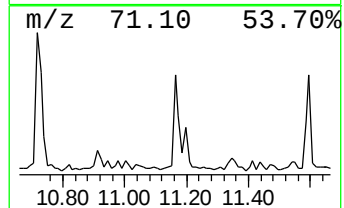
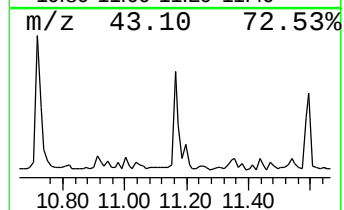
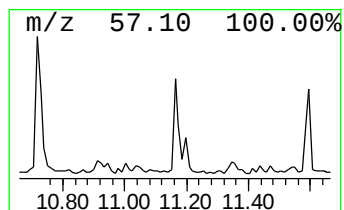
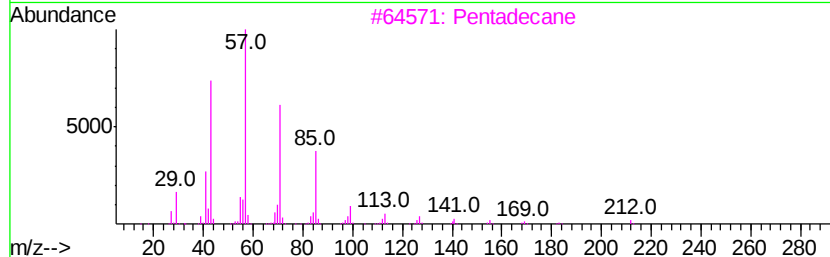
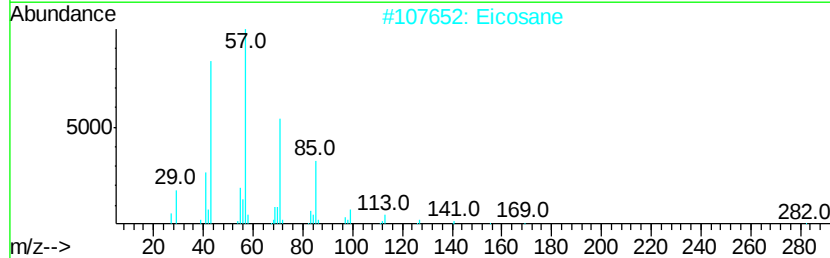
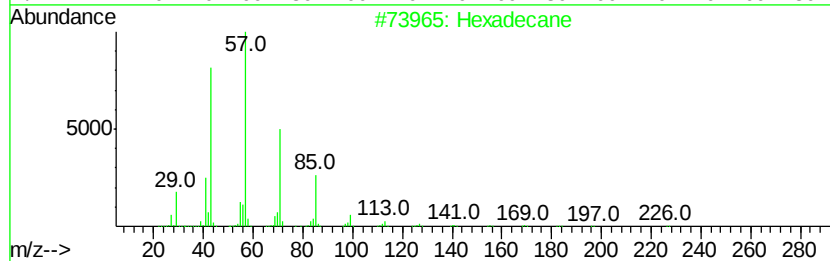
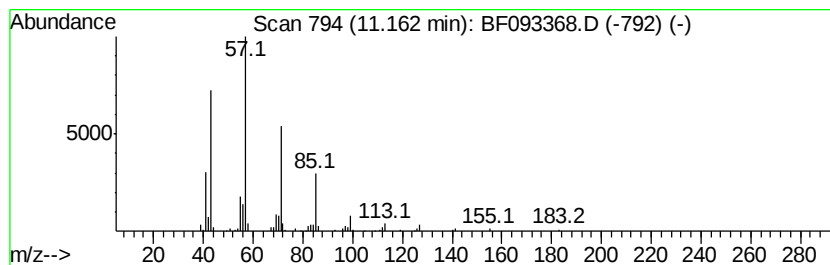
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Peak Number 5 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.16	2.72 ng	232653	Phenanthrene-d10	11.30	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Pentadecane	212	C15H32	000629-62-9	90
4	Octacosane	394	C28H58	000630-02-4	83
5	Octadecane	254	C18H38	000593-45-3	83



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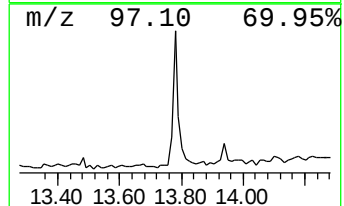
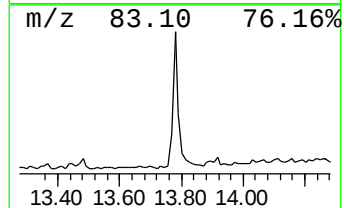
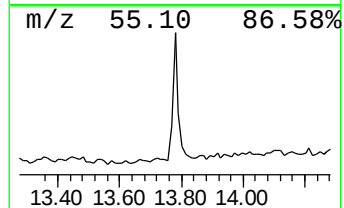
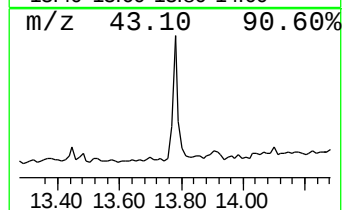
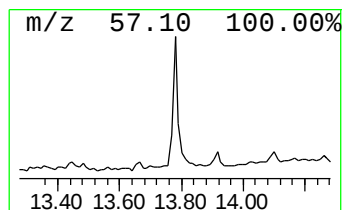
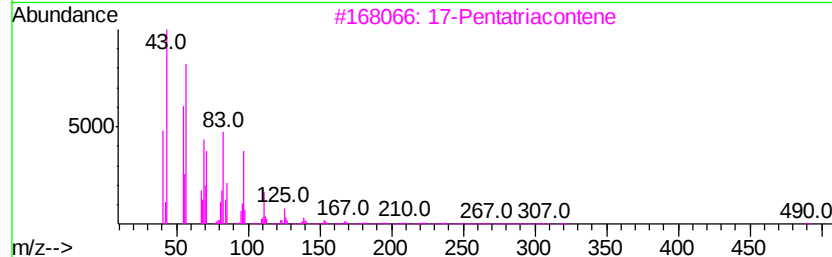
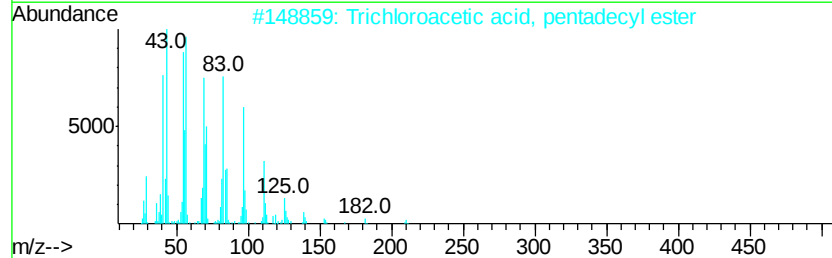
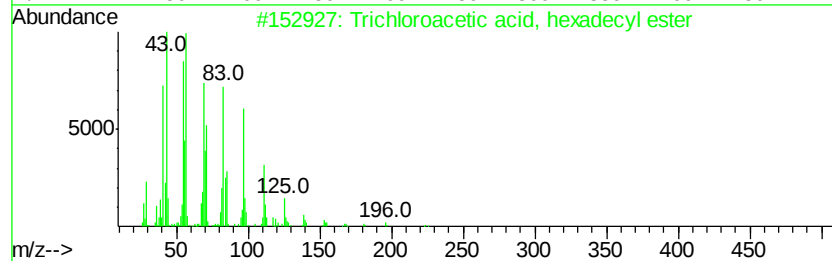
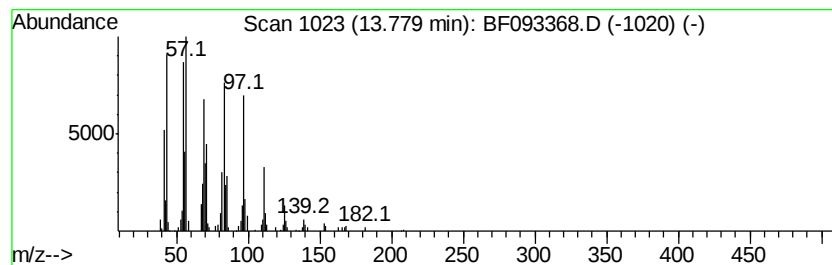
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	2.86 ng	207364	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	91
4		Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	91
5		11-Tricosene	322	C23H46	052078-56-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	9.1 ng		495934	1	6.78	1089530	20.0
unknown6.56	6.56	69.8 ng		3801120	1	6.78	1089530	20.0
Dodecane, 2-methy...	10.72	3.4 ng		287563	4	11.30	1711590	20.0
Hexadecane	11.16	2.7 ng		232653	4	11.30	1711590	20.0
Trichloroacetic a...	13.78	2.9 ng		207364	5	13.94	1449470	20.0