

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041516\
 Data File : BF086259.D
 Acq On : 16 Apr 2016 12:06
 Operator : UM/SJ
 Sample : H2471-03
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CDM3H3

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-BF041516.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	2.167	5	7	36	rVB3	281366	876656	13.79%	1.566%
2	5.093	260	263	269	rBV	235478	345621	5.44%	0.618%
3	5.493	295	298	300	rBV	5318951	6032752	94.88%	10.779%
4	6.521	384	388	390	rBV	5074509	6358491	100.00%	11.361%
5	6.659	397	400	402	rBV	5643369	5752898	90.48%	10.279%
6	6.887	418	420	423	rBV	1535899	1660974	26.12%	2.968%
7	7.047	431	434	436	rBV	4782346	4312171	67.82%	7.705%
8	7.459	467	470	472	rBV	3458378	4285144	67.39%	7.656%
9	7.527	474	476	479	rVB	42941	63696	1.00%	0.114%
10	8.179	530	533	535	rBV	2586778	2337881	36.77%	4.177%
11	9.253	624	627	630	rBV	5472889	5707132	89.76%	10.197%
12	9.642	659	661	663	rBV	548857	690434	10.86%	1.234%
13	9.870	679	681	683	rBV	212491	176138	2.77%	0.315%
14	9.927	684	686	689	rVB	2307784	2389576	37.58%	4.270%
15	10.373	722	725	726	rVB	200983	273941	4.31%	0.489%
16	10.590	740	744	747	rBV	109510	189966	2.99%	0.339%
17	10.716	752	755	758	rBV	3327563	3416303	53.73%	6.104%
18	10.842	764	766	771	rVB	373121	417603	6.57%	0.746%
19	11.036	781	783	785	rBV	44846	72290	1.14%	0.129%
20	11.288	803	805	806	rBV	204539	161213	2.54%	0.288%
21	11.413	814	816	818	rBV	2745232	2354959	37.04%	4.208%
22	11.939	860	862	867	rVB	63809	77483	1.22%	0.138%
23	13.002	952	955	957	rBV	4765945	4875815	76.68%	8.712%
24	13.905	1031	1034	1038	rBV	167507	278287	4.38%	0.497%
25	14.042	1044	1046	1049	rBV	1627036	1539450	24.21%	2.751%
26	15.482	1169	1172	1175	rBV	1015397	1320691	20.77%	2.360%

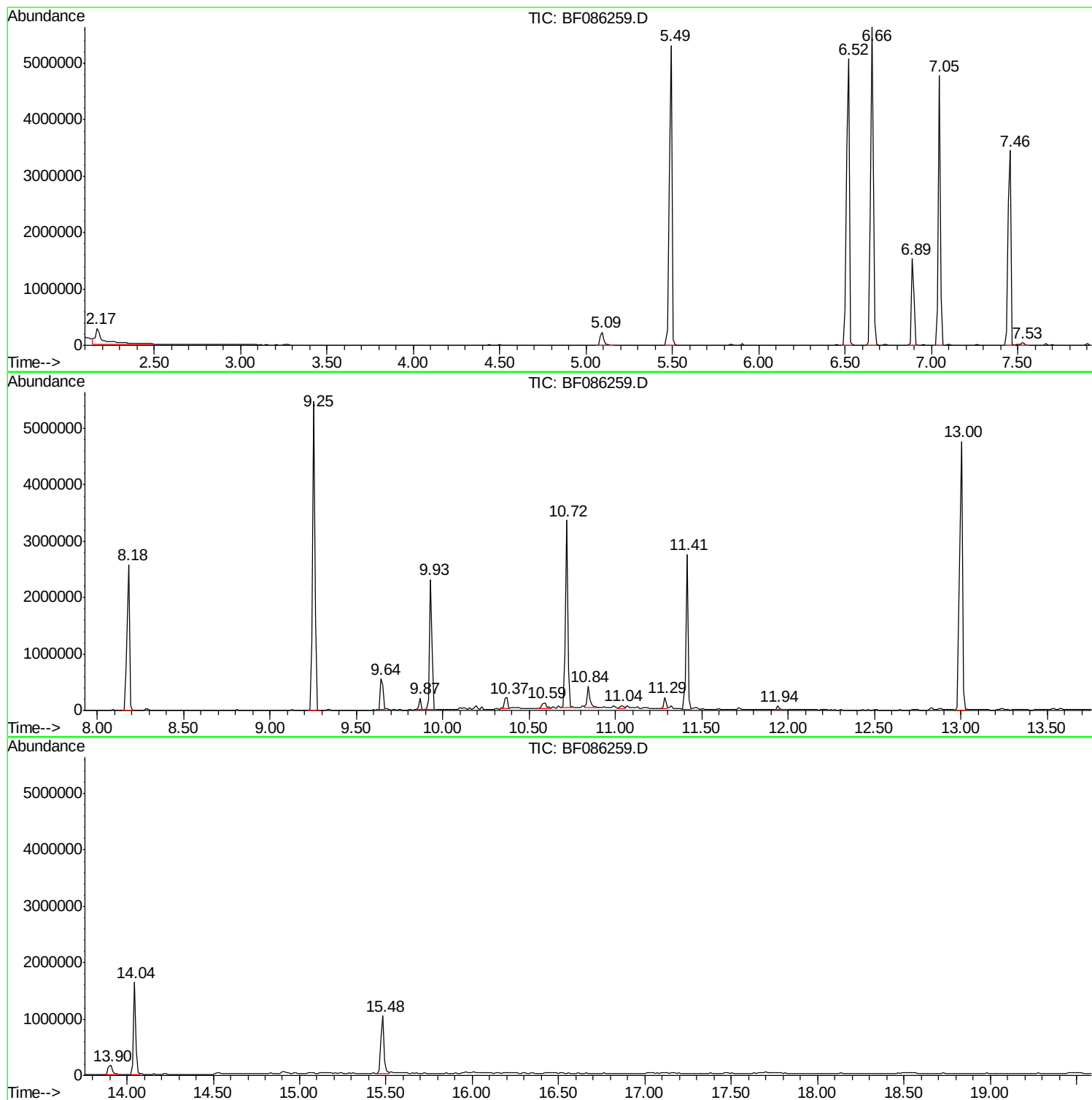
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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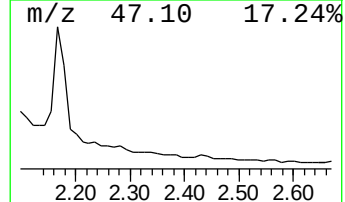
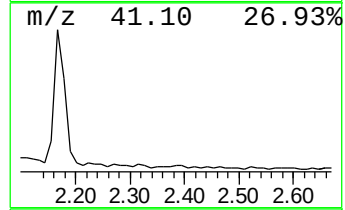
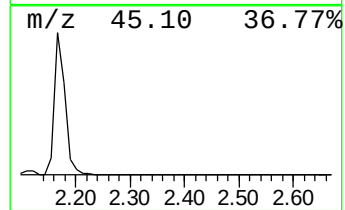
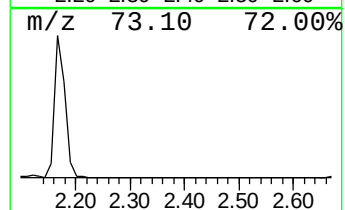
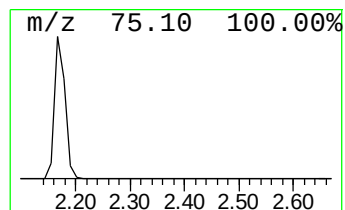
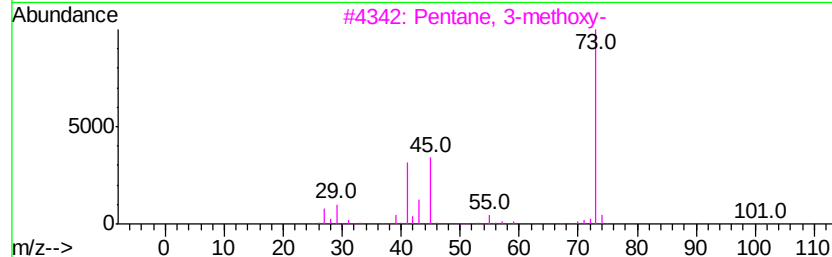
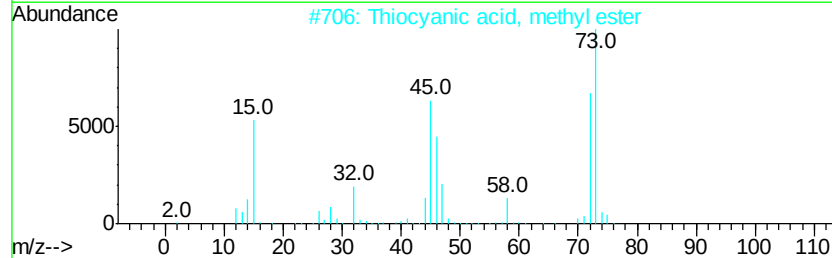
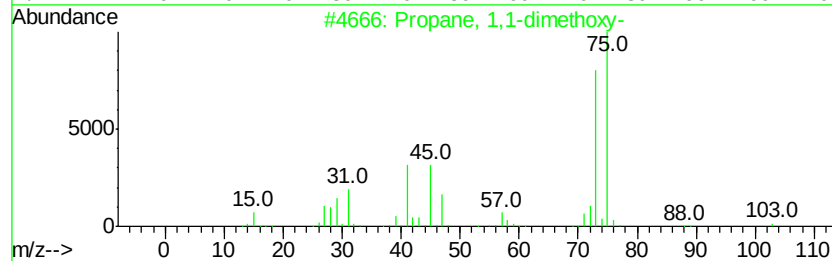
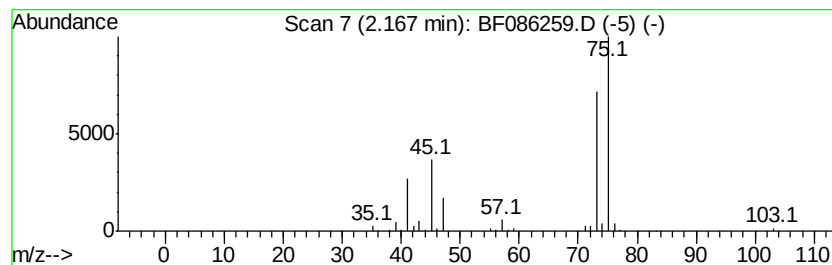
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	10.56 ng	876656	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	14
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
4			2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9
5			Ethane, 2-chloro-1,1-dimethoxy-	124	C4H9ClO2	000097-97-2	9



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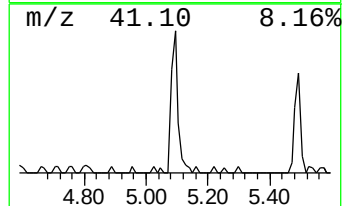
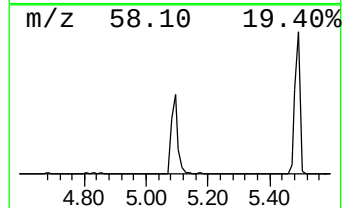
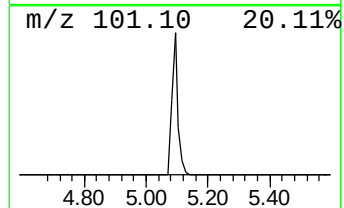
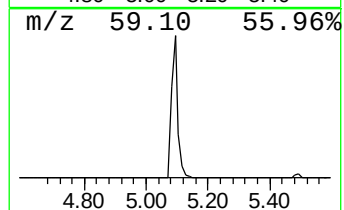
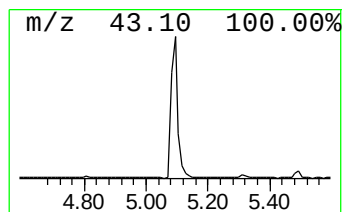
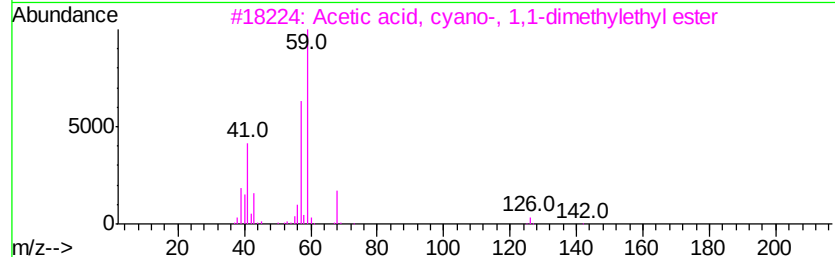
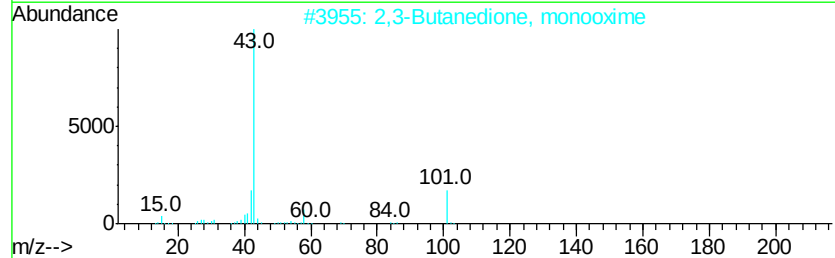
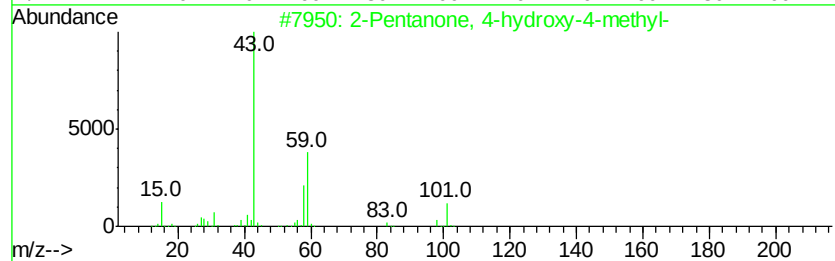
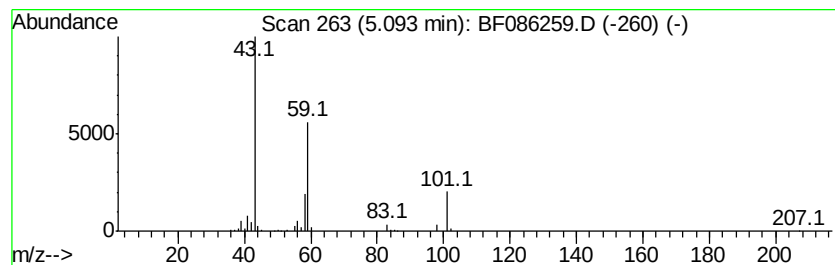
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.09	4.16 ng	345621	1,4-Dichlorobenzene-d4	6.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	12
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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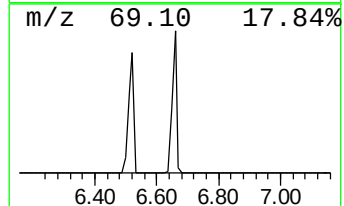
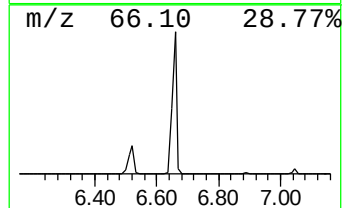
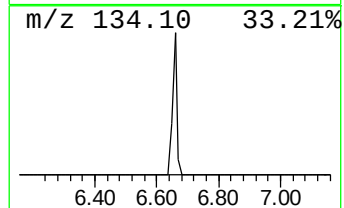
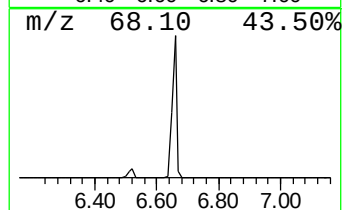
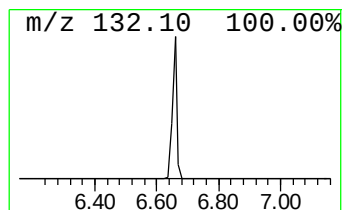
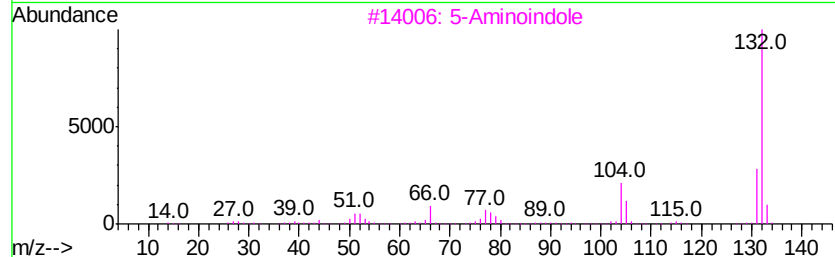
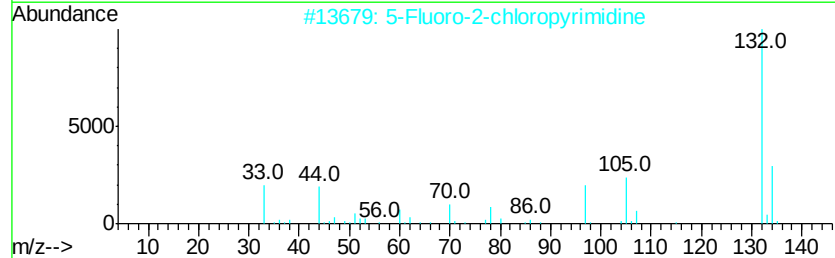
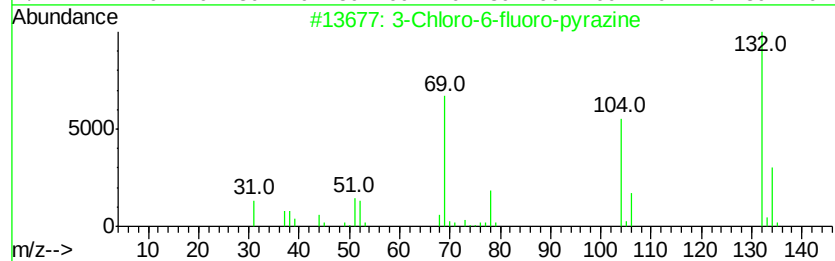
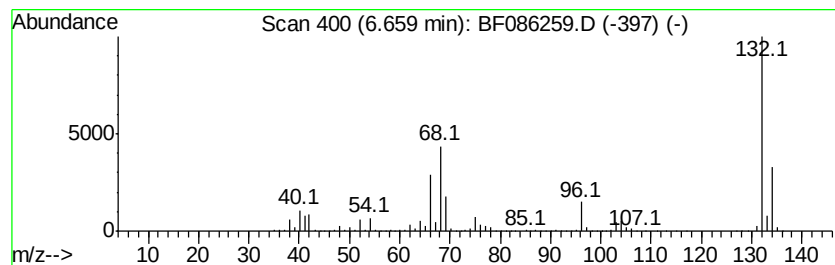
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Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	69.27 ng	5752900	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole			132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl			189	C12H15NO	1000123-86-3	10
5	Imidazole, 4,5-dicyano-1-methyl-			132	C6H4N4	019485-35-9	9



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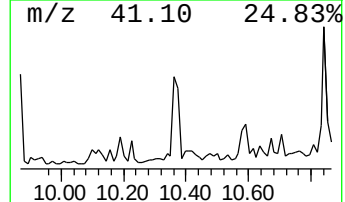
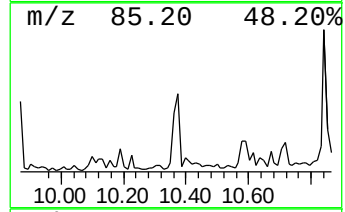
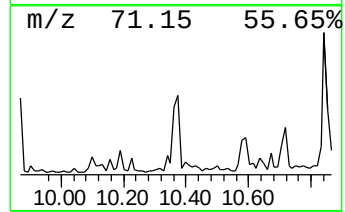
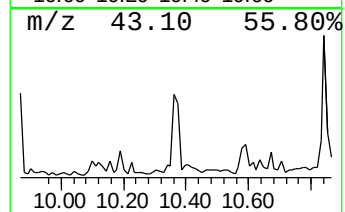
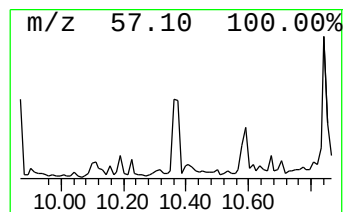
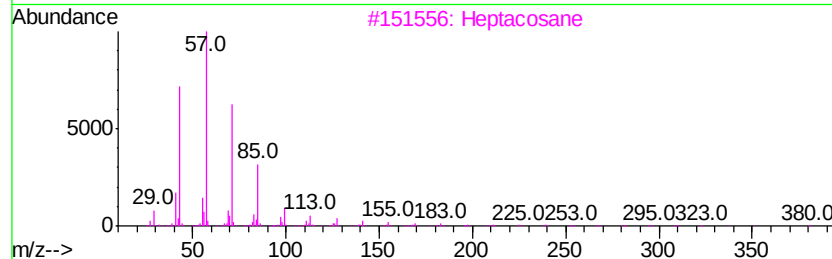
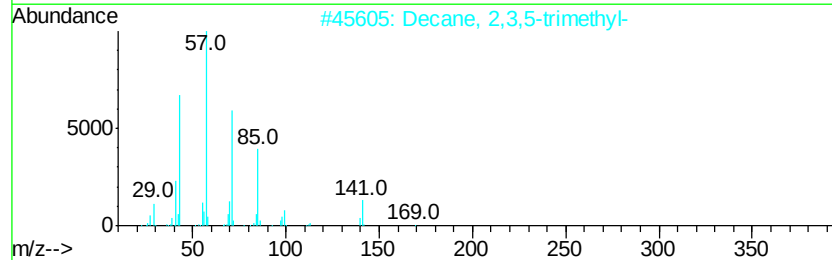
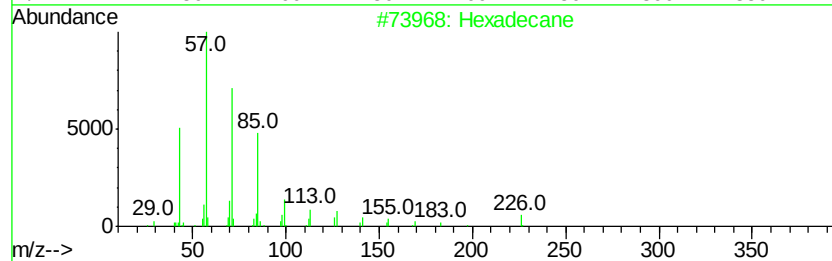
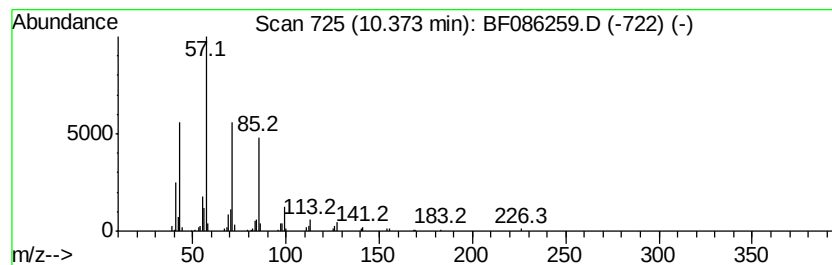
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.37	2.29 ng	273941	Acenaphthene-d10		9.93
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	94
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
3	Heptacosane	380	C27H56	000593-49-7	72
4	Bacchotricuneatin c	342	C20H22O5	066563-30-2	64
5	Tetradecane	198	C14H30	000629-59-4	58



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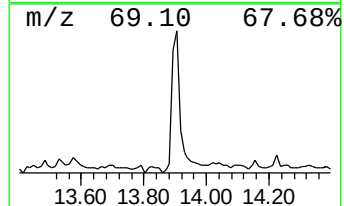
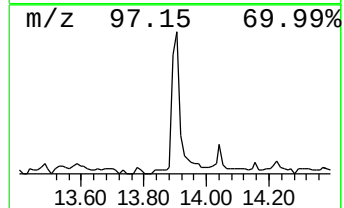
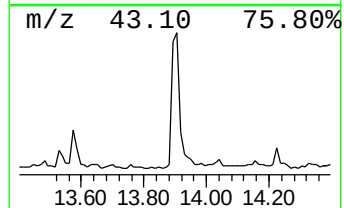
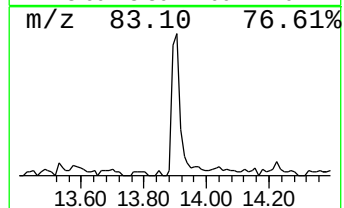
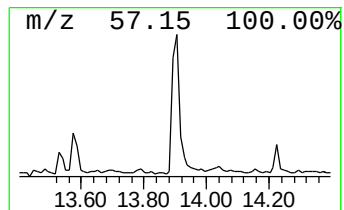
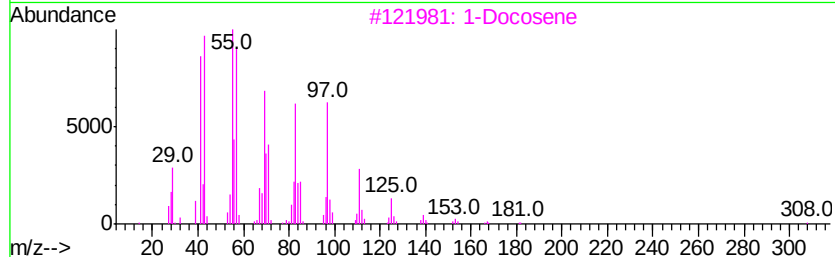
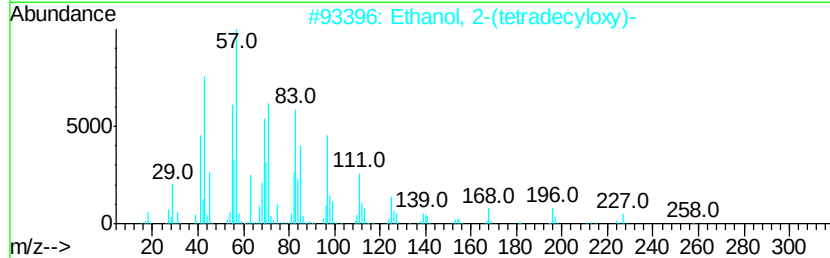
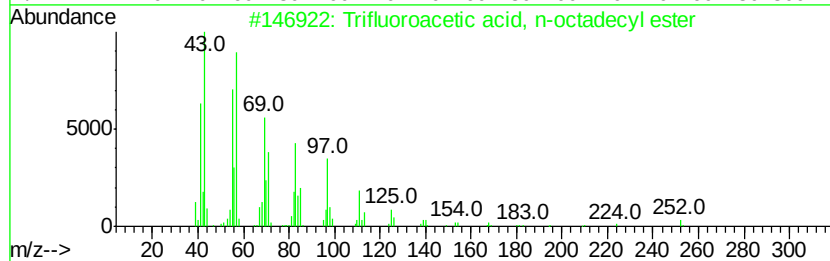
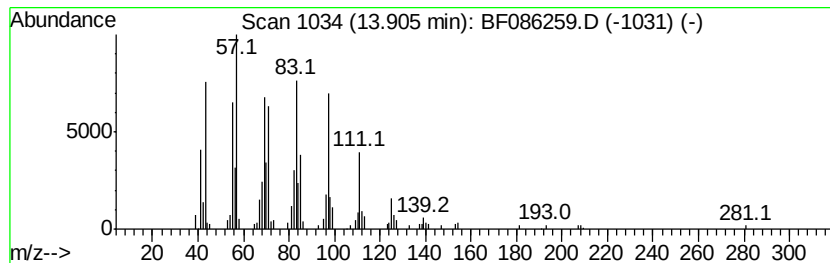
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 Trifluoroacetic acid, n-oct... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	3.62 ng	278287	Chrysene-d12	14.04

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	91
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
3		1-Docosene	308	C22H44	001599-67-3	90
4		17-Pentatriacontene	491	C35H70	006971-40-0	87
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.17	10.6	ng	876656	1	6.89	1660970	20.0
2-Pentanone, 4-hy...	5.09	4.2	ng	345621	1	6.89	1660970	20.0
unknown6.66	6.66	69.3	ng	5752900	1	6.89	1660970	20.0
Hexadecane	10.37	2.3	ng	273941	3	9.93	2389580	20.0
Trifluoroacetic a...	13.90	3.6	ng	278287	5	14.04	1539450	20.0