

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
 Data File : BF093803.D
 Acq On : 21 Mar 2017 17:32
 Operator : SJ/MA
 Sample : I2314-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FIELD DUPLICATE

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-BF032017.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	2.092	15	18	26	rVB2	87608	120405	2.69%	0.304%
2	4.996	269	272	277	rBV	659689	1008941	22.52%	2.548%
3	5.430	307	310	312	rBV	3648322	3867384	86.32%	9.769%
4	5.830	343	345	347	rVB	87431	74056	1.65%	0.187%
5	6.459	397	400	402	rBV	3708095	4021034	89.75%	10.157%
6	6.596	409	412	414	rBV	3757272	4102009	91.56%	10.361%
7	6.824	430	432	434	rBV	1353177	1100054	24.55%	2.779%
8	6.984	443	446	448	rBV	3440387	3116824	69.57%	7.873%
9	7.384	478	481	483	rBV	2550751	2425444	54.14%	6.126%
10	8.104	542	544	547	rBV	1110086	1493085	33.33%	3.771%
11	9.190	636	639	641	rBV	4449567	4480254	100.00%	11.317%
12	9.579	671	673	675	rBV	683788	549340	12.26%	1.388%
13	9.865	695	698	700	rBV	1720584	1697383	37.89%	4.287%
14	10.276	732	734	736	rBV	37051	53685	1.20%	0.136%
15	10.310	736	737	738	rVB	83207	57111	1.27%	0.144%
16	10.642	763	766	769	rVV2	2051819	2324740	51.89%	5.872%
17	10.779	776	778	783	rVB	133521	149325	3.33%	0.377%
18	11.225	815	817	819	rBV	127879	117159	2.62%	0.296%
19	11.339	824	827	829	rVV	1906241	1599300	35.70%	4.040%
20	11.648	852	854	857	rBV	93571	95762	2.14%	0.242%
21	11.876	872	874	876	rBV	81071	83251	1.86%	0.210%
22	12.928	963	966	968	rBV	3338370	3541040	79.04%	8.944%
23	13.831	1042	1045	1051	rBV	83383	132655	2.96%	0.335%
24	13.968	1054	1057	1059	rBV	1082890	1179241	26.32%	2.979%
25	14.825	1129	1132	1135	rBV	59216	60539	1.35%	0.153%
26	15.374	1177	1180	1183	rBV	723982	906365	20.23%	2.289%
27	16.871	1289	1311	1312	rBV7	142545	1233383	27.53%	3.115%

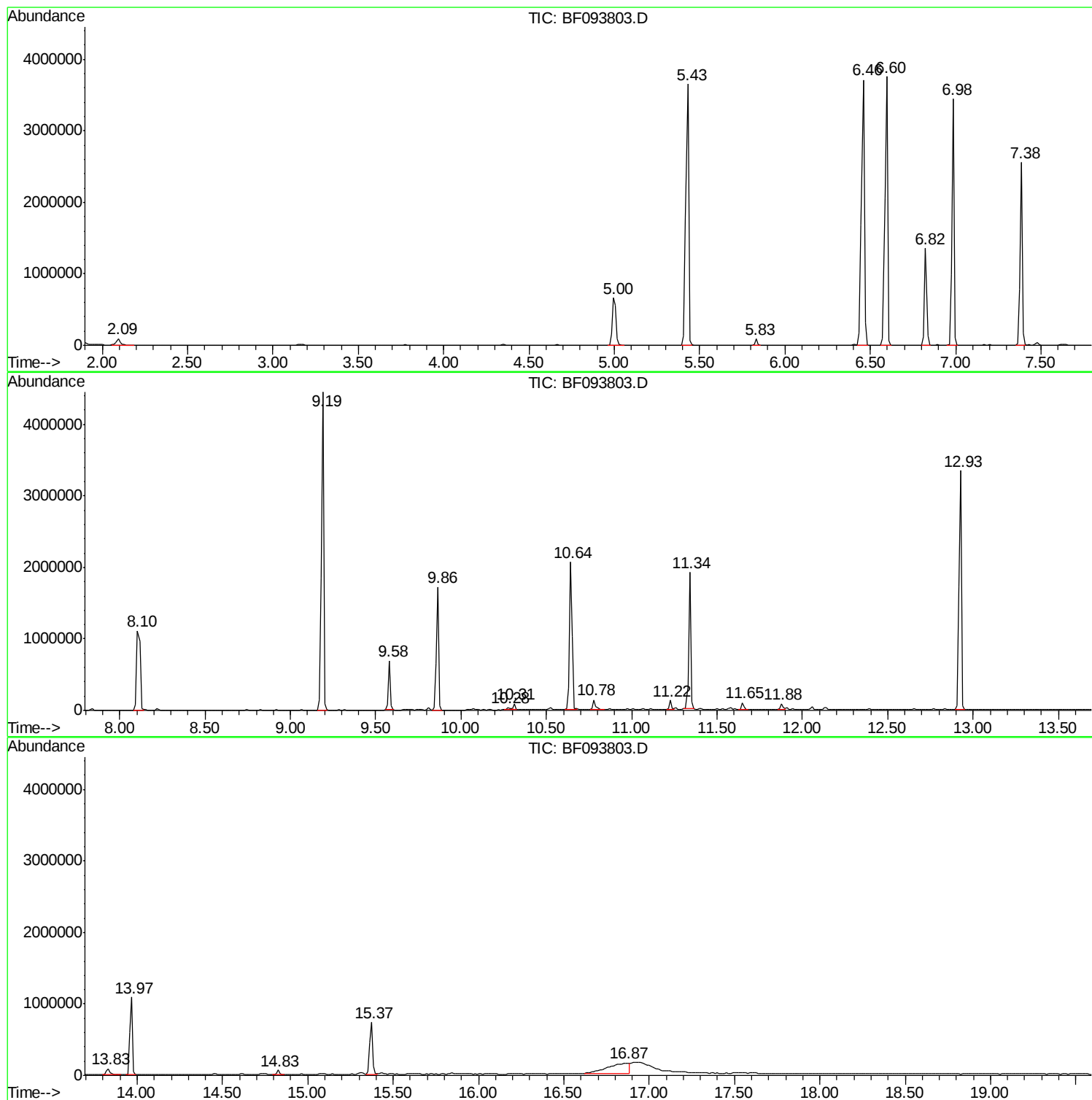
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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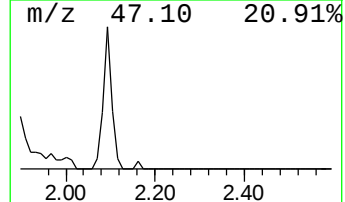
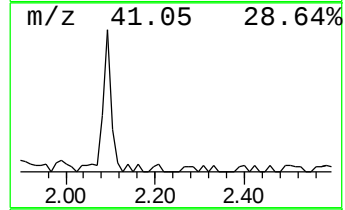
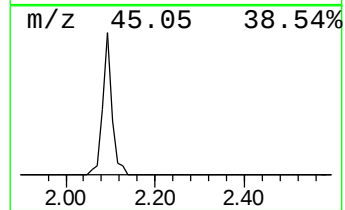
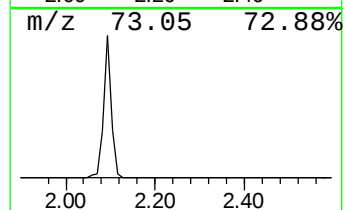
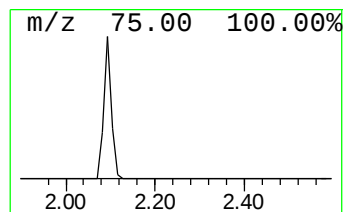
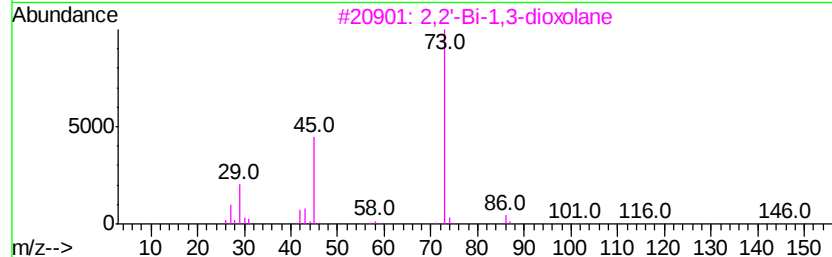
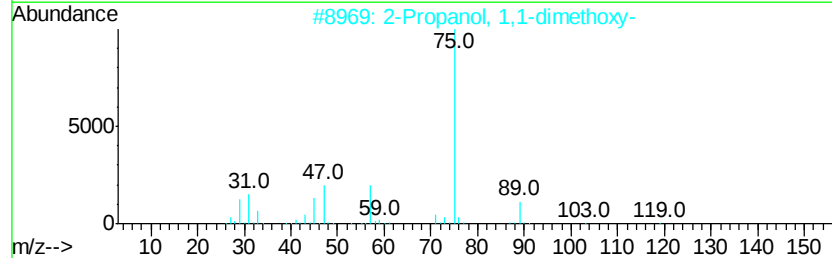
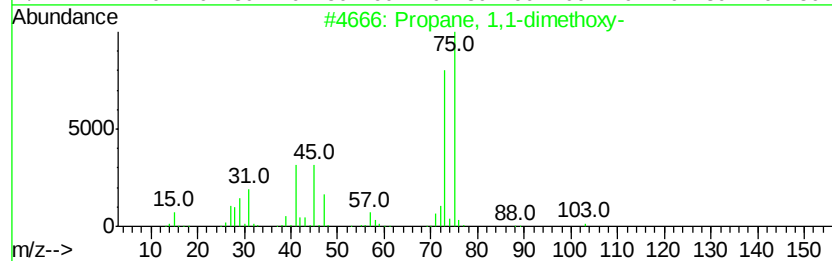
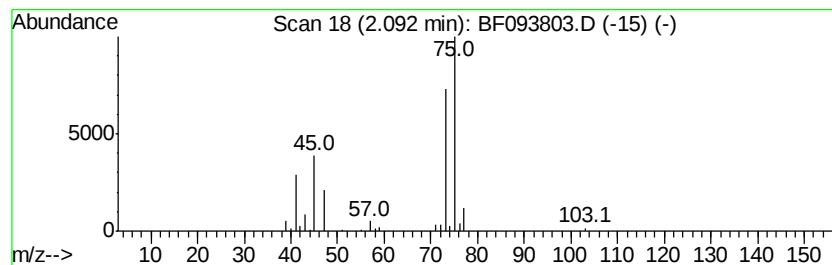
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.09	2.19 ng	120405	1,4-Dichlorobenzene-d4	6.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2		2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	33
3		2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9
4		Ethane, 2-chloro-1,1-dimethoxy-	124	C4H9ClO2	000097-97-2	9
5		1,1,3-Trimethoxypropane	134	C6H14O3	014315-97-0	9



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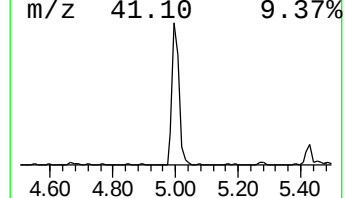
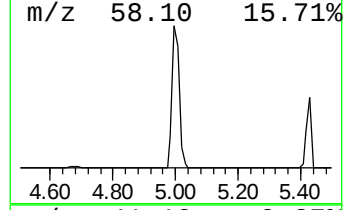
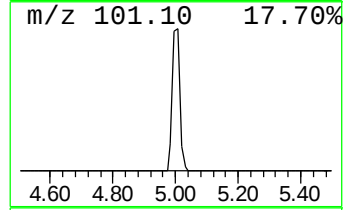
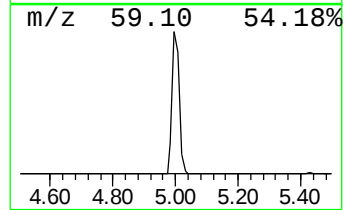
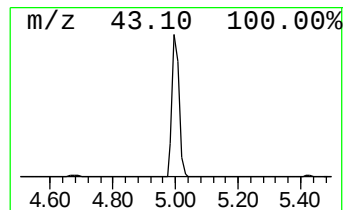
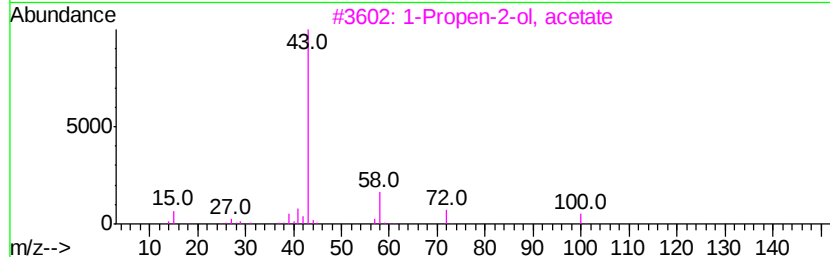
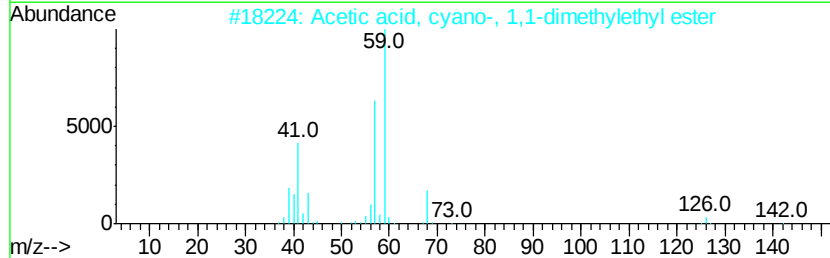
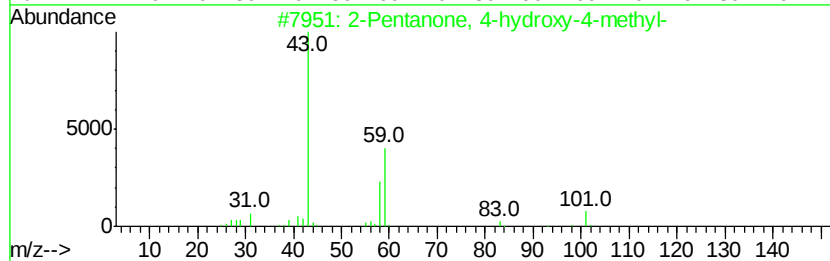
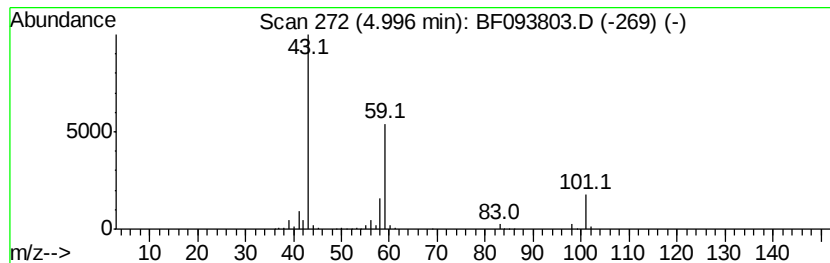
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	18.34 ng	1008940	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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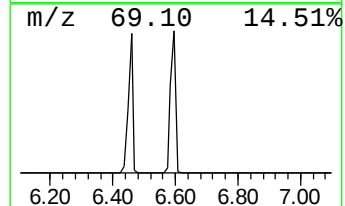
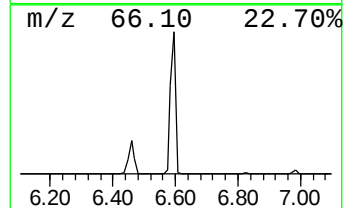
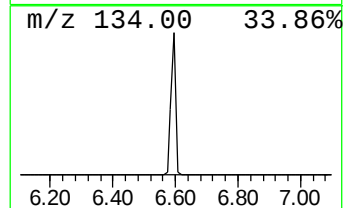
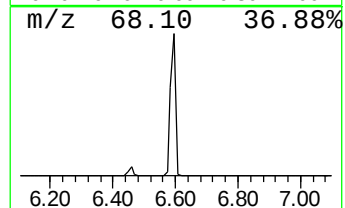
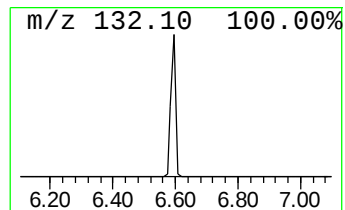
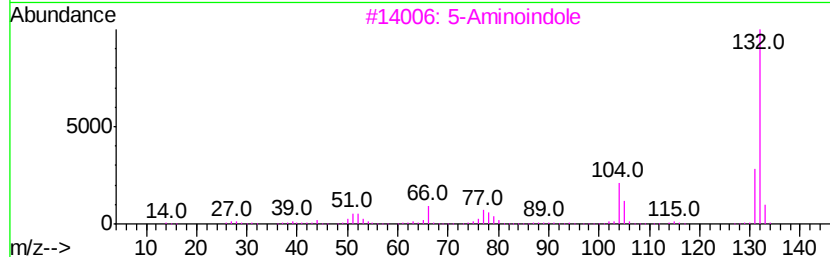
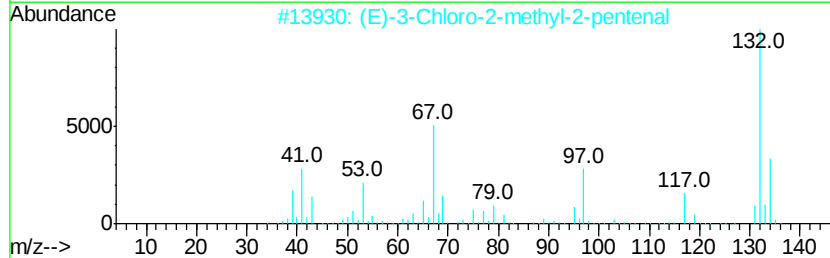
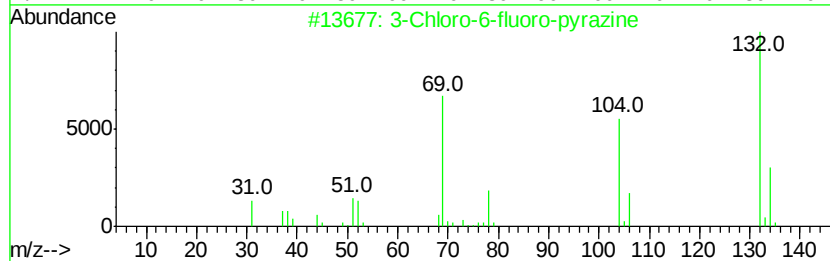
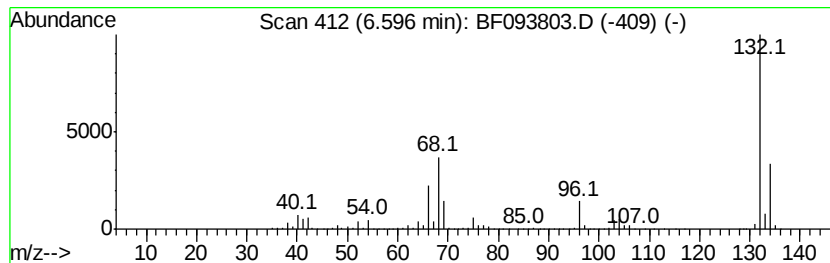
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Peak Number 3 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	74.58 ng	4102010	1,4-Dichlorobenzene-d4	6.82

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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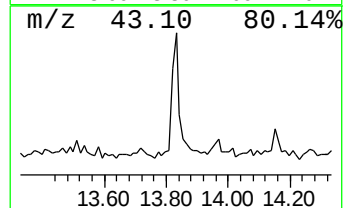
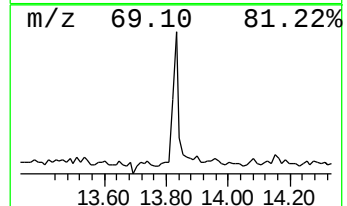
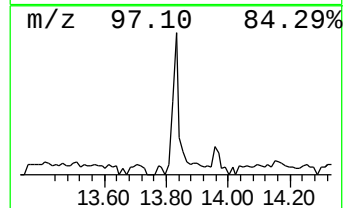
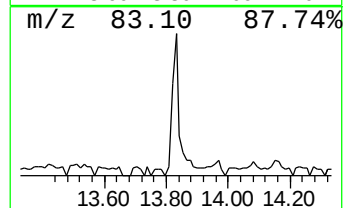
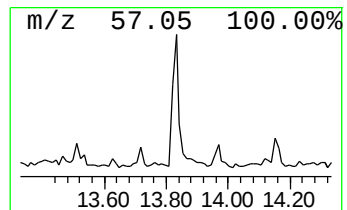
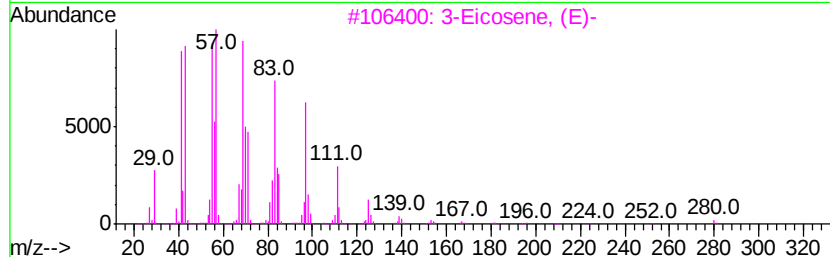
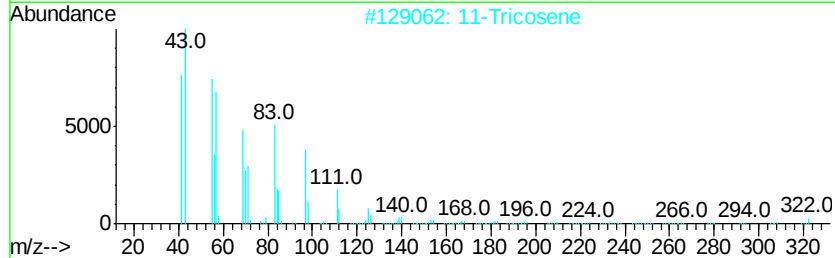
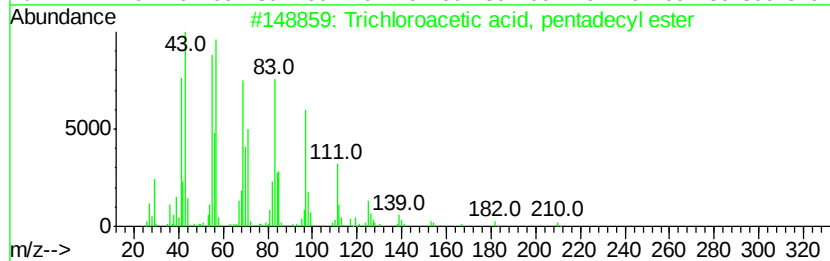
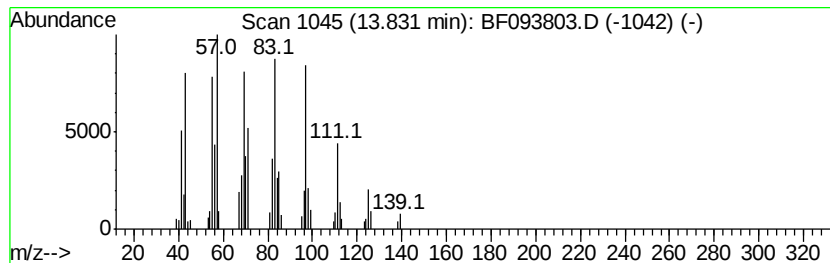
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Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.25 ng	132655	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2		11-Tricosene	322	C23H46	052078-56-5	91
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		1-Hexadecanol	242	C16H34O	036653-82-4	86
5		Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	83



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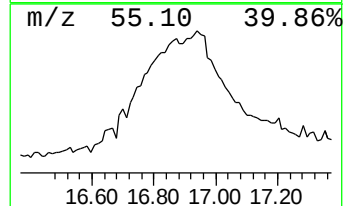
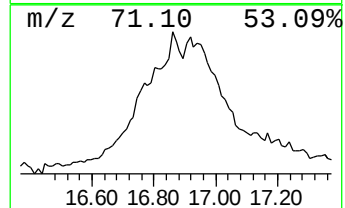
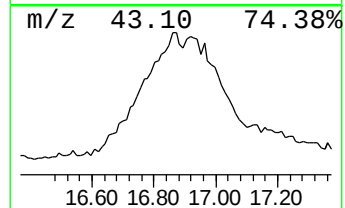
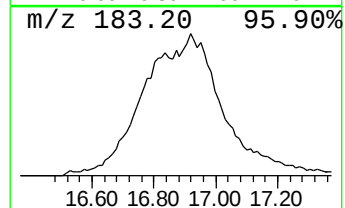
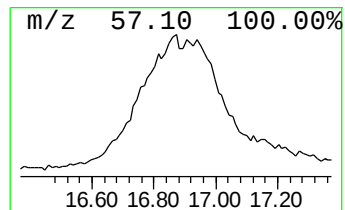
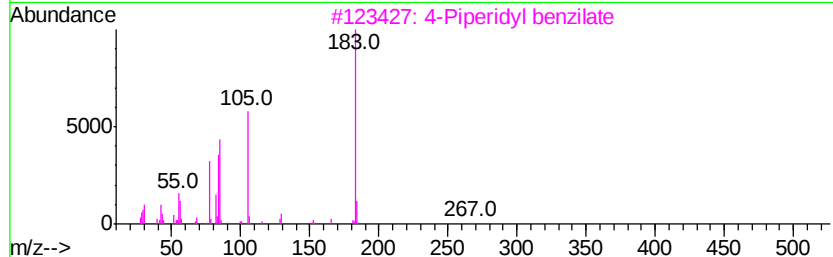
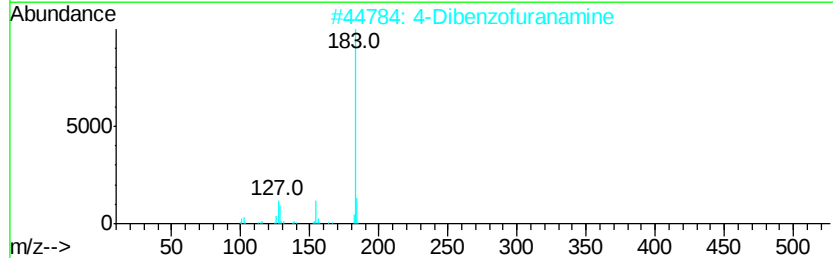
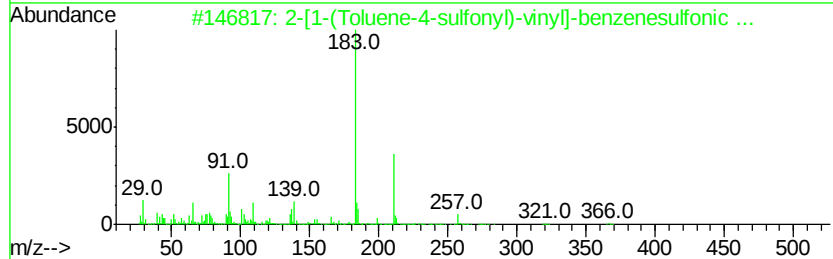
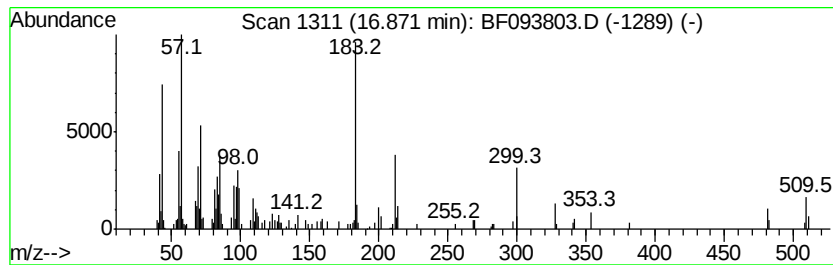
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 unknown16.87 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.87	27.22 ng	1233380	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	2	[1-(Toluene-4-sulfonyl)-vinyl]...	366	C17H18O5S2	1000193-97-5	40
2	4	Dibenzofuranamine	183	C12H9NO	050548-43-1	38
3	4	Piperidyl benzilate	311	C19H21NO3	025811-48-7	35
4	5,8	Methano-4H-3,1-benzoxazine-2...	183	C9H13NOS	1000142-76-8	35
5	1	Naphthalenecarbonitrile, 2-met...	183	C12H9NO	016000-39-8	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.09	2.2	ng	120405	1	6.82	1100050	20.0
2-Pentanone, 4-hy...	5.00	18.3	ng	1008940	1	6.82	1100050	20.0
unknown6.60	6.60	74.6	ng	4102010	1	6.82	1100050	20.0
Trichloroacetic a...	13.83	2.3	ng	132655	5	13.97	1179240	20.0
unknown16.87	16.87	27.2	ng	1233380	6	15.37	906365	20.0