

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
 Data File : BF088977.D
 Acq On : 14 Jul 2016 00:35
 Operator : UM/SJ
 Sample : H3946-13
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P7-B5(0-6)C

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-BF063016.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	1.667	5	7	13	rVV	126201	184325	9.87%	1.138%
2	1.781	16	17	26	rVV	952954	1510094	80.85%	9.327%
3	1.895	26	27	57	rVB2	53200	226789	12.14%	1.401%
4	4.844	283	285	291	rBB	198090	334110	17.89%	2.064%
5	5.290	322	324	327	rBV	1043362	1525651	81.68%	9.423%
6	5.690	357	359	361	rBB	26800	23224	1.24%	0.143%
7	6.353	413	417	419	rBV	1060277	1619642	86.72%	10.004%
8	6.467	424	427	429	rBV	1729574	1699484	90.99%	10.497%
9	6.696	445	447	449	rBB	470862	411687	22.04%	2.543%
10	6.856	458	461	463	rBB	1042496	1266849	67.83%	7.825%
11	7.267	493	497	499	rBV	725012	1024731	54.86%	6.329%
12	7.976	557	559	562	rBV	521126	490136	26.24%	3.027%
13	9.062	651	654	656	rBV	2065192	1867737	100.00%	11.536%
14	9.450	686	688	690	rBB	249775	243895	13.06%	1.506%
15	9.725	710	712	715	rBB2	464052	485529	26.00%	2.999%
16	10.513	779	781	784	rBV	925237	835193	44.72%	5.159%
17	10.650	791	793	797	rBV	15104	26975	1.44%	0.167%
18	11.096	830	832	833	rBV	21562	26959	1.44%	0.167%
19	11.199	839	841	844	rVB	403119	395588	21.18%	2.443%
20	12.788	978	980	982	rBV	1257786	1101269	58.96%	6.802%
21	13.542	1045	1046	1048	rBV	13604	22401	1.20%	0.138%
22	13.588	1048	1050	1051	rVV	26483	27178	1.46%	0.168%
23	13.611	1051	1052	1054	rVB	20914	27079	1.45%	0.167%
24	13.691	1057	1059	1063	rBV2	44787	64282	3.44%	0.397%
25	13.828	1068	1071	1073	rBV	417596	372211	19.93%	2.299%
26	14.319	1111	1114	1118	rBV3	8452	20591	1.10%	0.127%
27	14.411	1118	1122	1126	rBV	11165	32741	1.75%	0.202%
28	15.200	1188	1191	1194	rBV	296057	323999	17.35%	2.001%

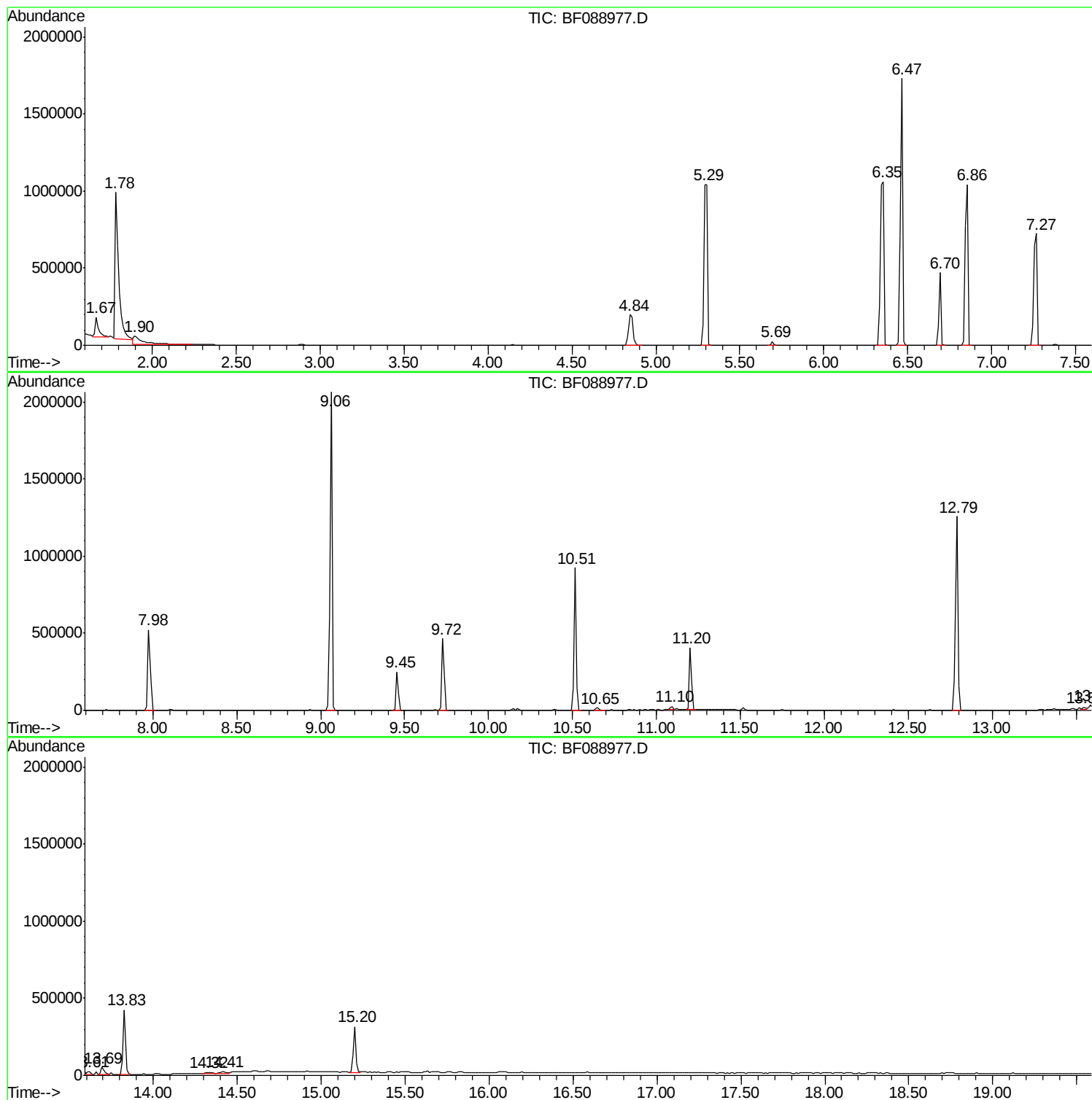
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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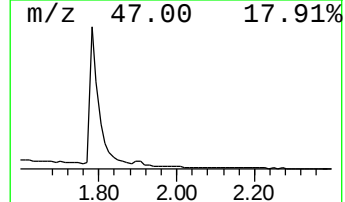
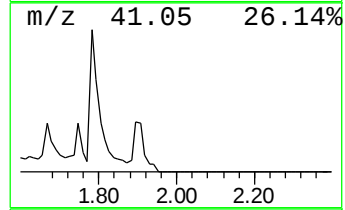
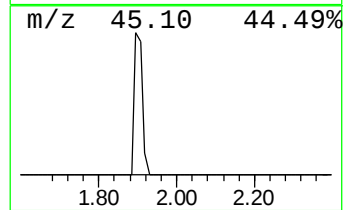
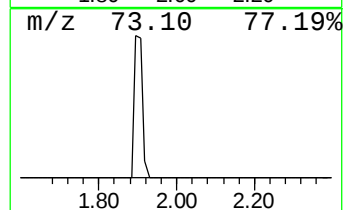
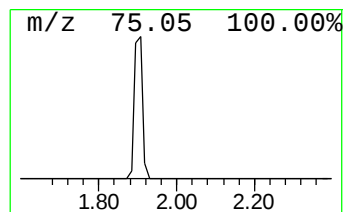
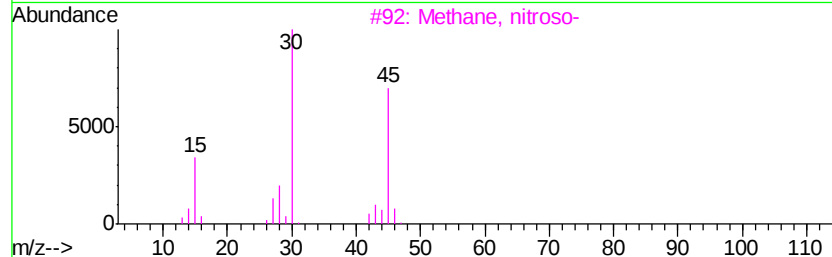
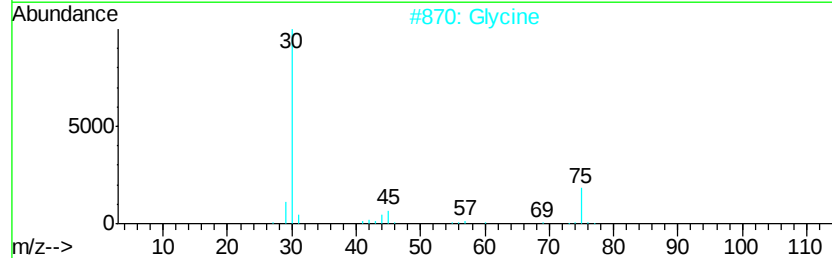
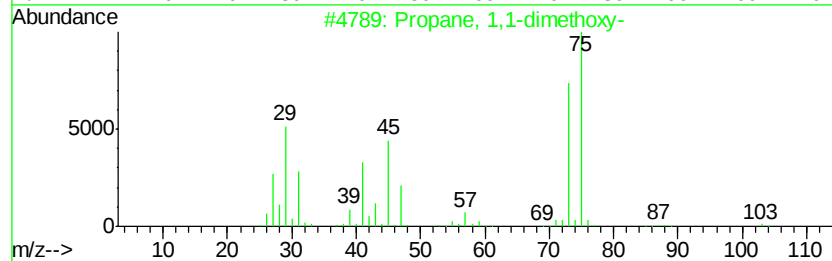
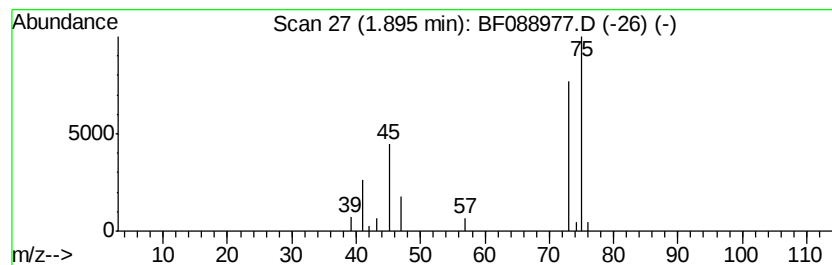
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.90	11.02 ng	226789	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2		Glycine	75	C2H5NO2	000056-40-6	7
3		Methane, nitroso-	45	CH3NO	000865-40-7	4
4		Silanol, trimethyl-	90	C3H10OSi	001066-40-6	4
5		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	4



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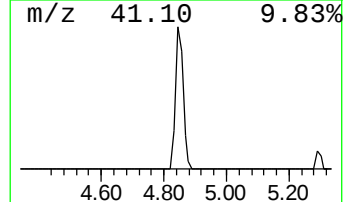
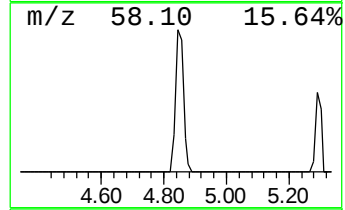
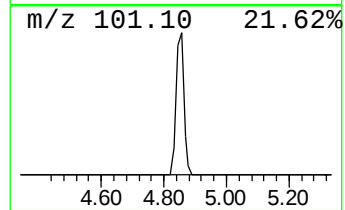
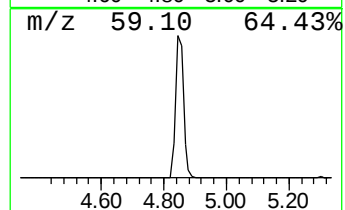
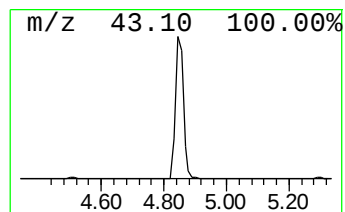
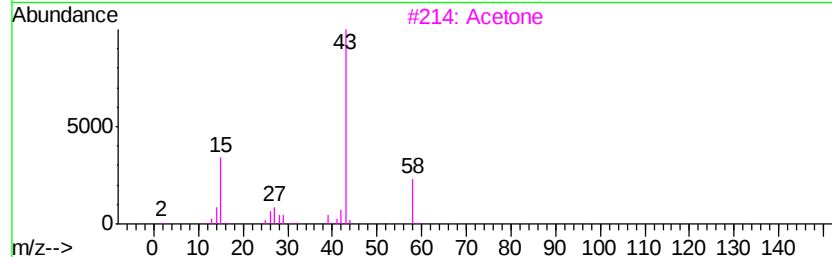
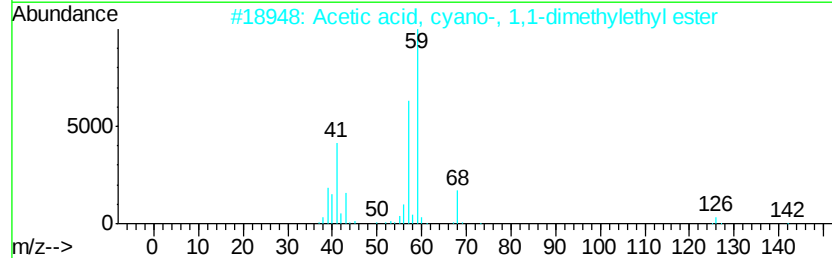
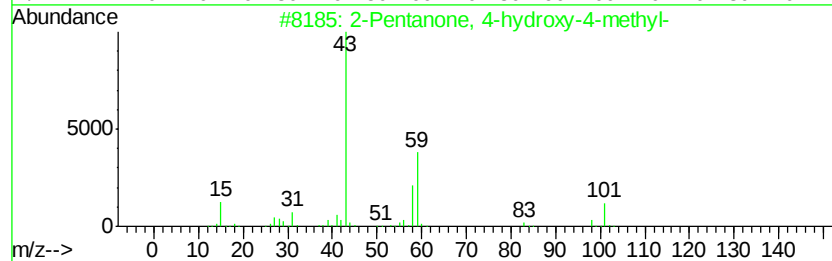
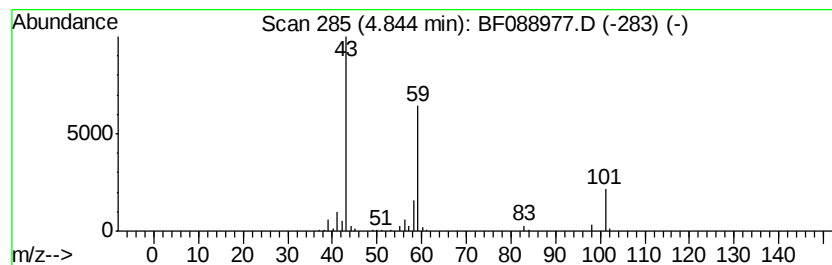
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	16.23 ng	334110	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Acetone	58	C3H6O	000067-64-1	10
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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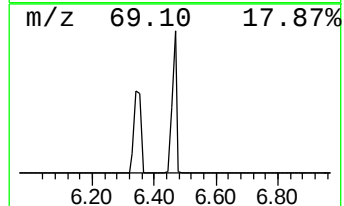
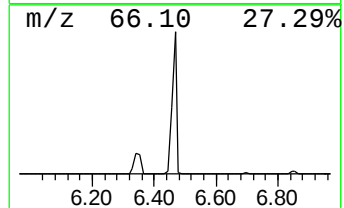
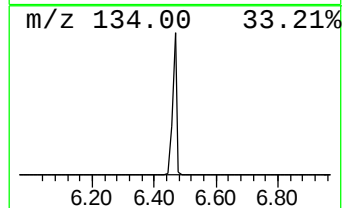
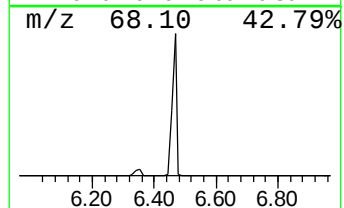
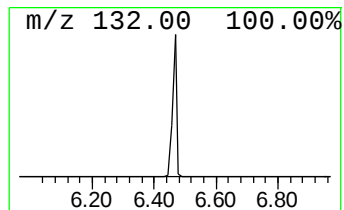
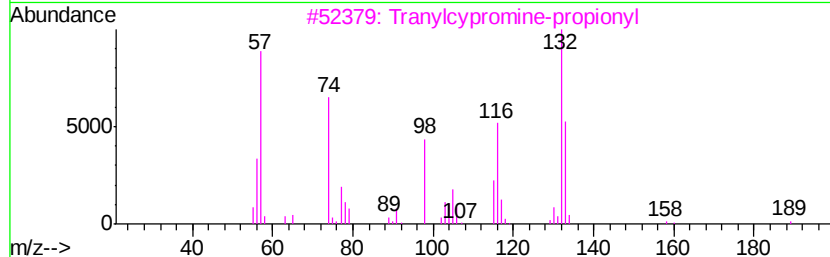
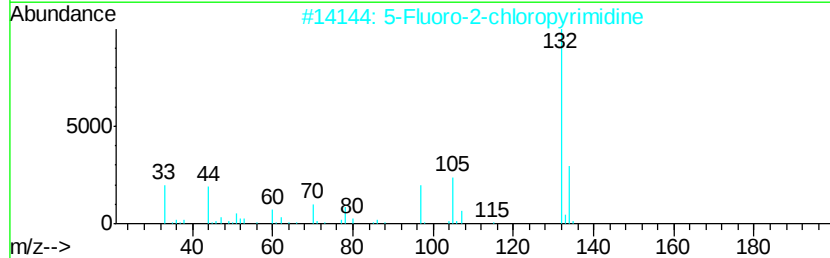
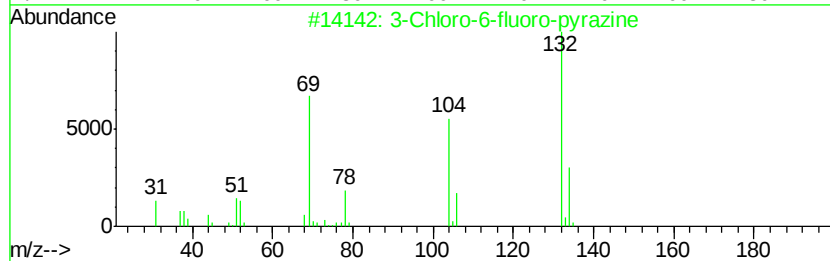
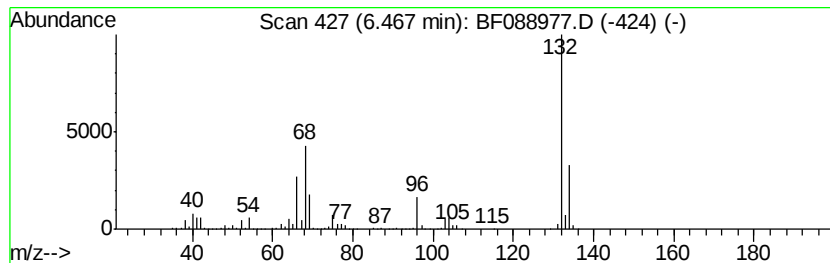
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Peak Number 5 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	82.56 ng	1699480	1,4-Dichlorobenzene-d4	6.70

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



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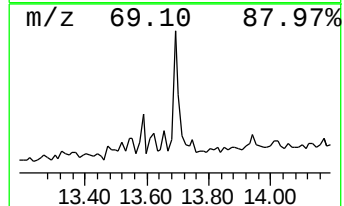
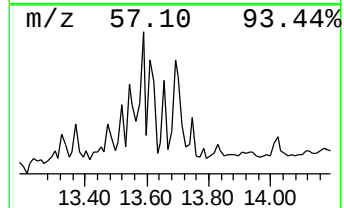
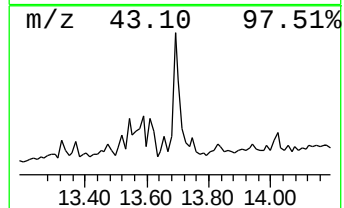
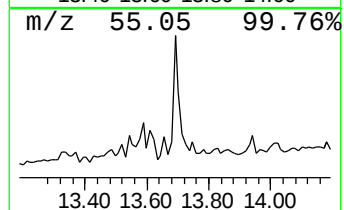
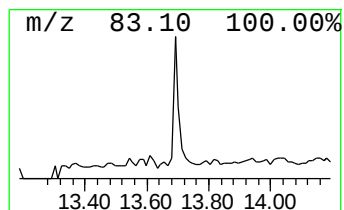
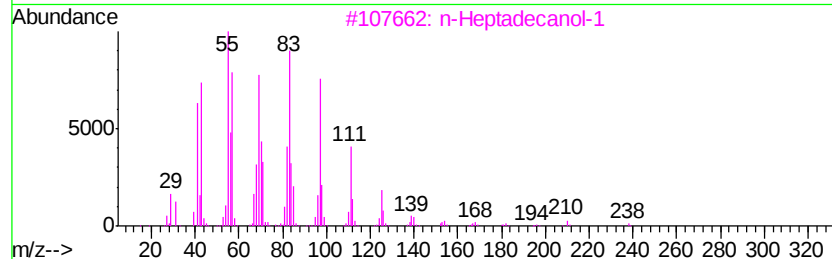
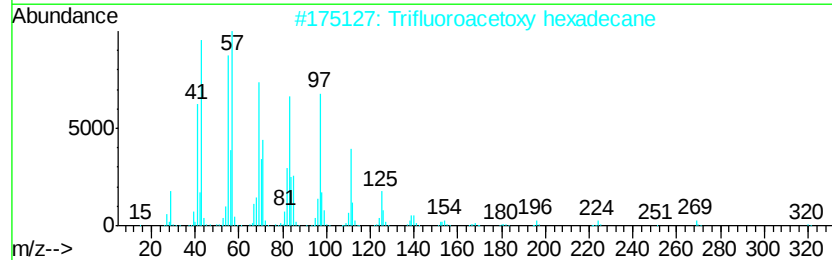
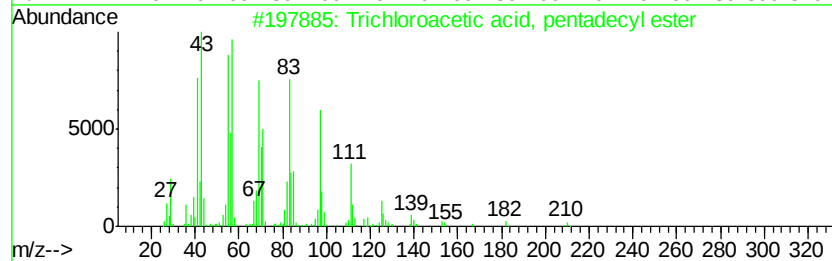
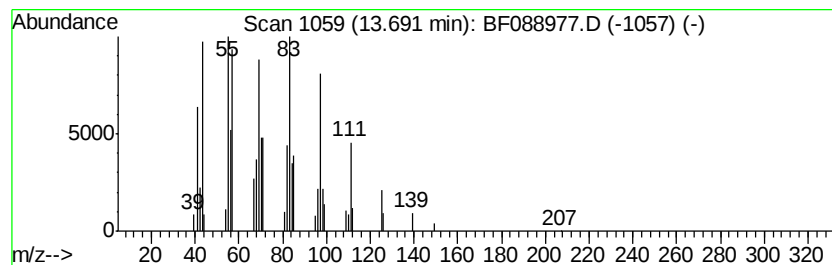
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Peak Number 7 Trichloroacetic acid, penta... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	3.45 ng	64282	Chrysene-d12	13.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3			n-Heptadecanol-1	256	C17H36O	001454-85-9	90
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.90	11.0	ng	226789	1	6.70	411687	20.0
2-Pentanone, 4-hy...	4.84	16.2	ng	334110	1	6.70	411687	20.0
unknown6.47	6.47	82.6	ng	1699480	1	6.70	411687	20.0
Trichloroacetic a...	13.69	3.5	ng	64282	5	13.83	372211	20.0