

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031315\
 Data File : BF077744.D
 Acq On : 13 Mar 2015 17:19
 Operator : TP/IZ
 Sample : G1517-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW5

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-BF031115.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	1.458	46	50	53	rVB	303665	486075	25.58%	3.628%
2	1.618	61	64	67	rBV	278287	331314	17.44%	2.473%
3	1.710	71	72	77	rVB3	20070	29173	1.54%	0.218%
4	1.790	77	79	88	rBV	28536	45593	2.40%	0.340%
5	4.933	352	354	359	rBV	43030	50221	2.64%	0.375%
6	5.459	397	400	402	rBV	462954	566000	29.79%	4.224%
7	6.739	509	512	514	rBV	278610	349270	18.38%	2.607%
8	6.876	522	524	527	rBV	1176676	1131174	59.53%	8.442%
9	7.173	547	550	552	rBV	230136	316822	16.67%	2.364%
10	7.356	563	566	568	rBV	1200409	1148336	60.43%	8.570%
11	7.859	608	610	613	rBV	870803	814861	42.88%	6.081%
12	8.739	685	687	690	rBV	380939	444896	23.41%	3.320%
13	9.448	747	749	752	rVB	28655	28180	1.48%	0.210%
14	9.779	774	778	782	rVB3	9799	23684	1.25%	0.177%
15	10.088	803	805	808	rBV	2062623	1842595	96.97%	13.751%
16	10.259	816	820	822	rBV	14795	23542	1.24%	0.176%
17	10.591	847	849	852	rBV3	13481	29790	1.57%	0.222%
18	10.637	852	853	856	rVB3	14239	22129	1.16%	0.165%
19	10.911	874	877	879	rBV	593669	553146	29.11%	4.128%
20	10.945	879	880	884	rVB2	16975	25146	1.32%	0.188%
21	11.242	903	906	911	rVB2	10561	21655	1.14%	0.162%
22	11.677	941	944	945	rBV	20263	32104	1.69%	0.240%
23	11.814	954	956	958	rVB	41988	38780	2.04%	0.289%
24	11.894	960	963	965	rBV	898541	1079710	56.82%	8.058%
25	12.317	998	1000	1001	rBV	15194	22206	1.17%	0.166%
26	12.751	1035	1038	1040	rBV	585536	587619	30.92%	4.385%
27	13.505	1102	1104	1109	rVB5	11868	23678	1.25%	0.177%
28	14.328	1173	1176	1178	rVB	37020	43590	2.29%	0.325%
29	14.740	1210	1212	1215	rBV	1635106	1900231	100.00%	14.182%
30	15.917	1312	1315	1322	rBV	79410	130031	6.84%	0.970%
31	16.020	1322	1324	1327	rBV	459476	638759	33.61%	4.767%
32	17.734	1471	1474	1477	rBV	511337	619040	32.58%	4.620%

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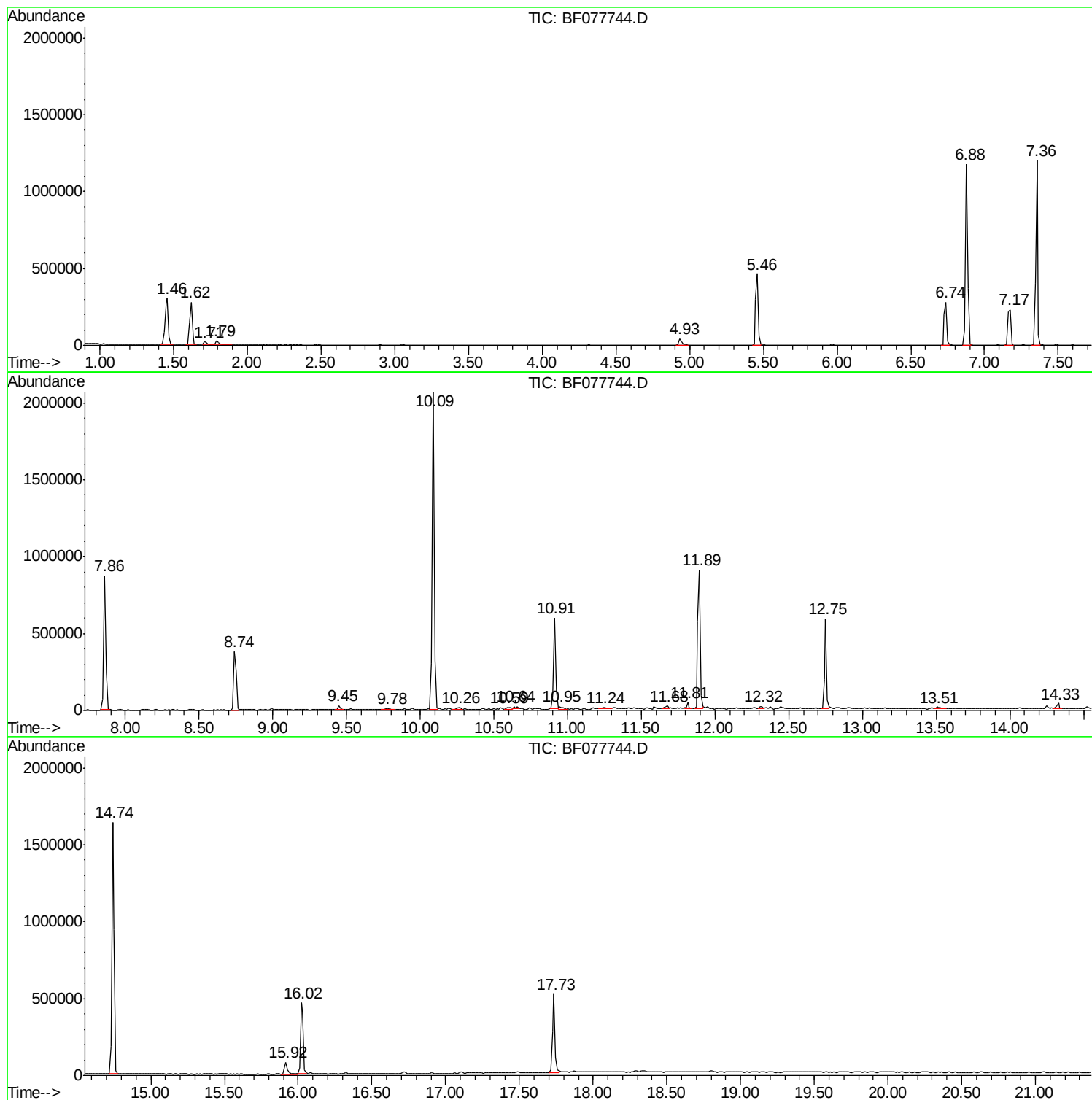
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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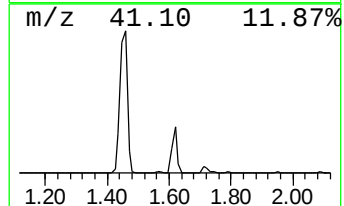
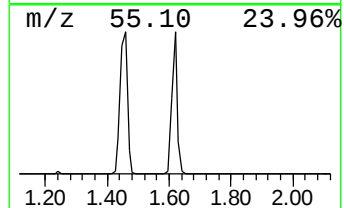
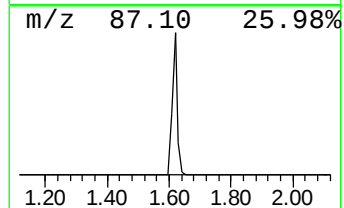
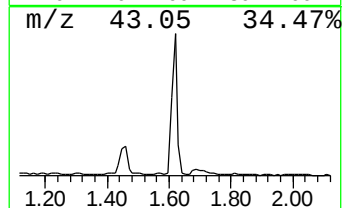
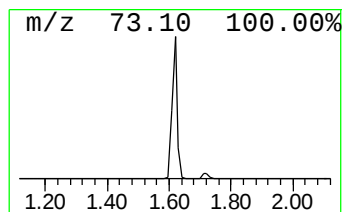
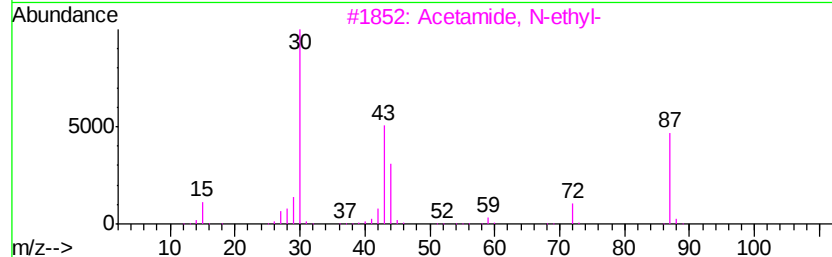
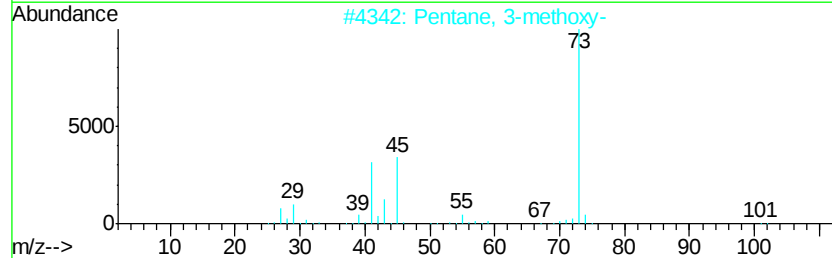
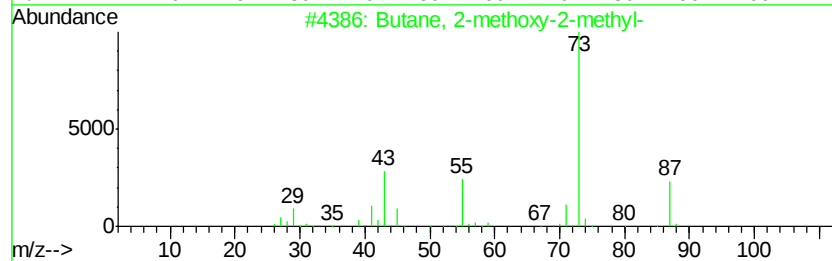
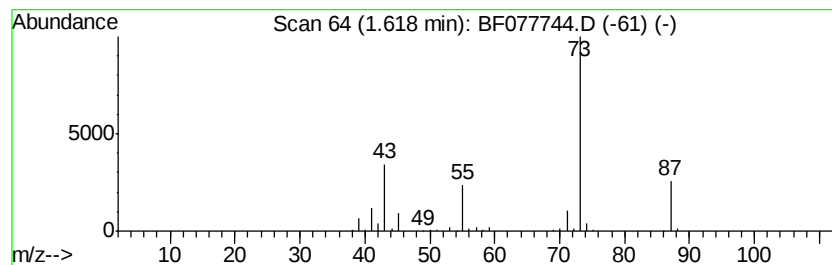
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.62	20.91 ng	331314	1,4-Dichlorobenzene-d4	7.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
4		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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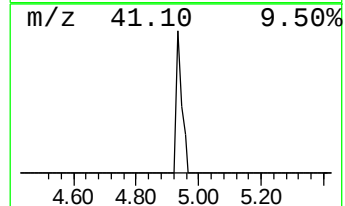
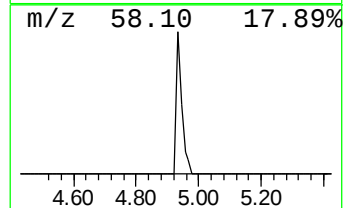
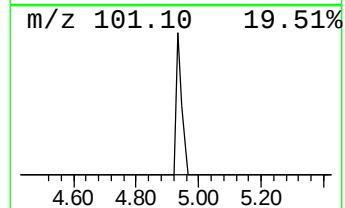
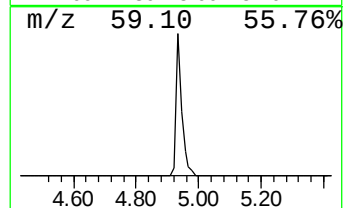
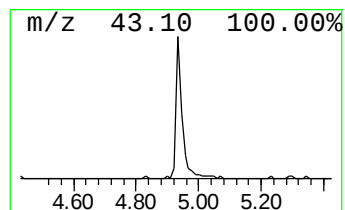
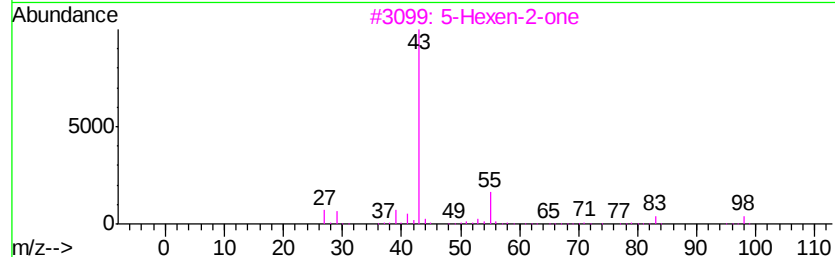
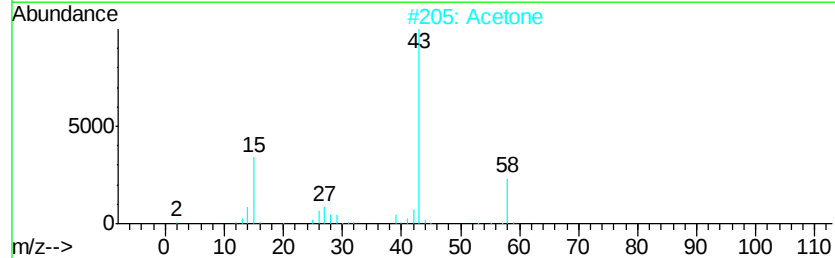
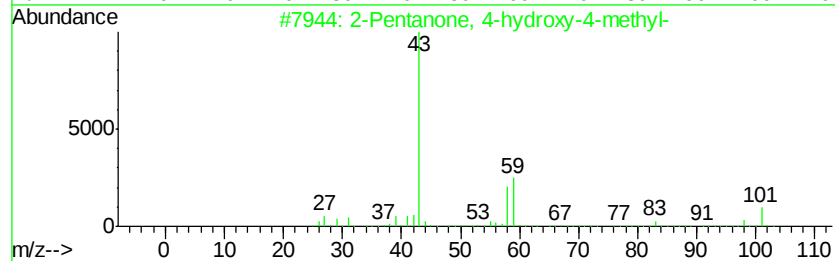
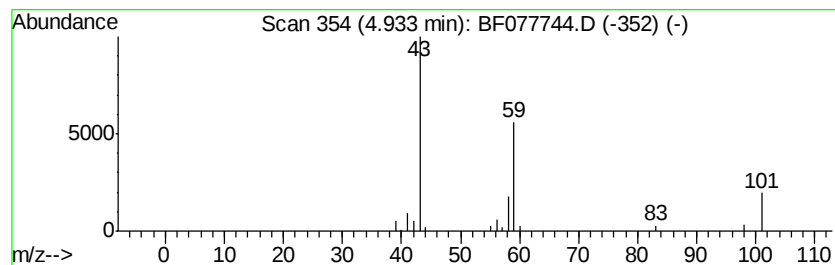
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	3.17 ng	50221	1,4-Dichlorobenzene-d4	7.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetone	58	C3H6O	000067-64-1	9
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9
5	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9



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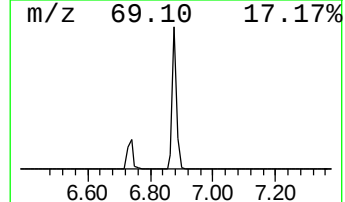
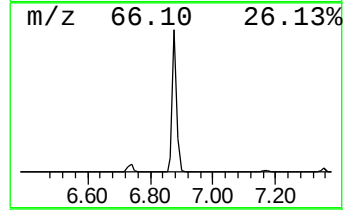
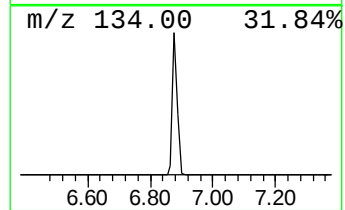
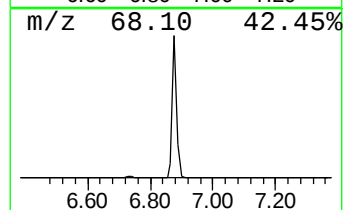
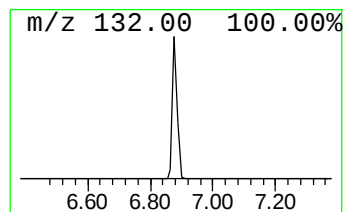
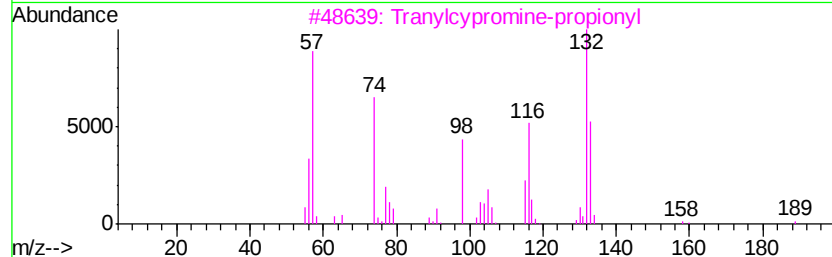
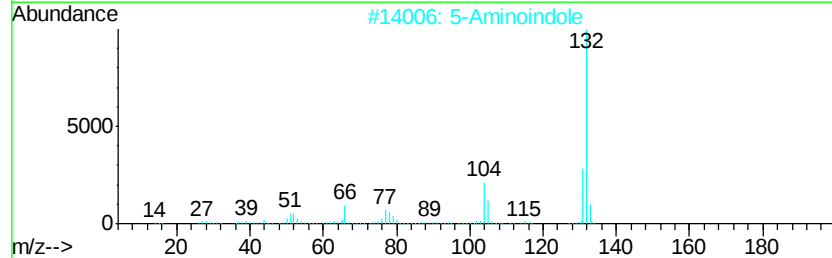
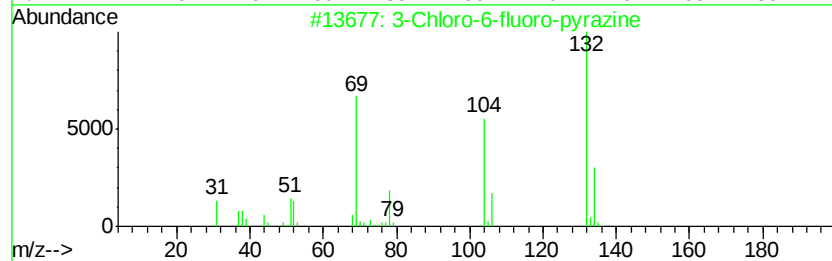
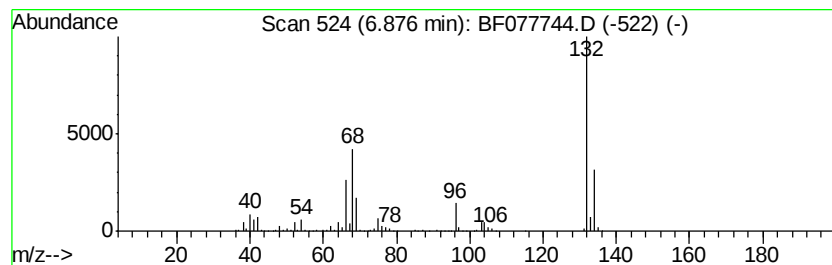
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Peak Number 5 unknown6.88 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.88	71.41 ng	1131170	1,4-Dichlorobenzene-d4	7.17

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10	
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9	
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9	



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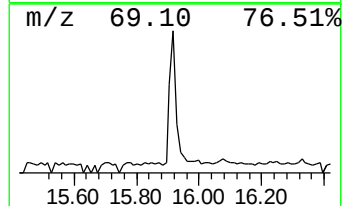
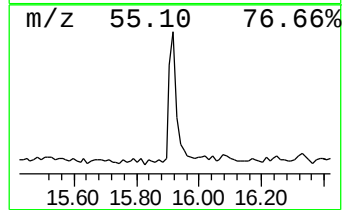
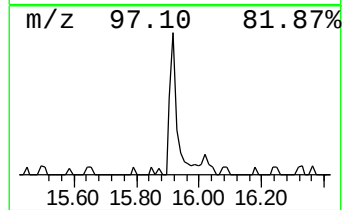
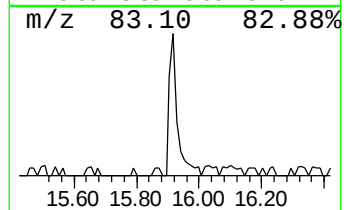
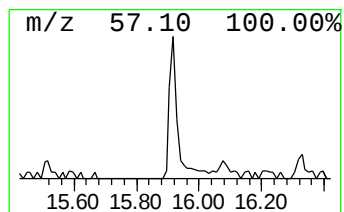
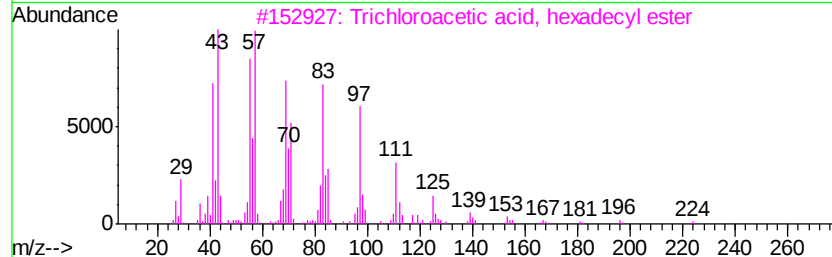
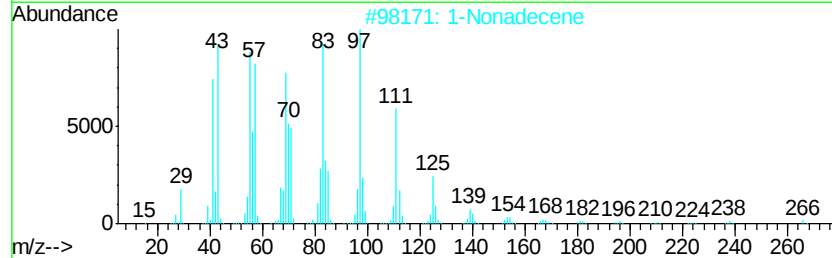
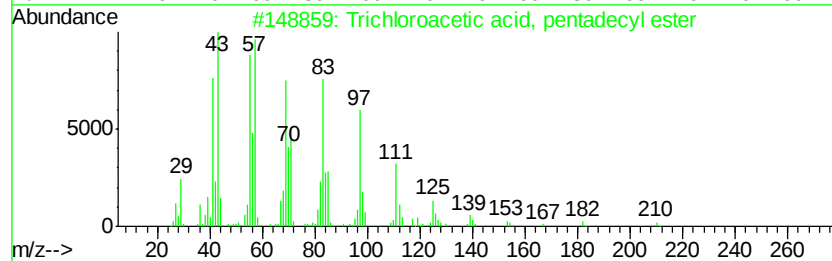
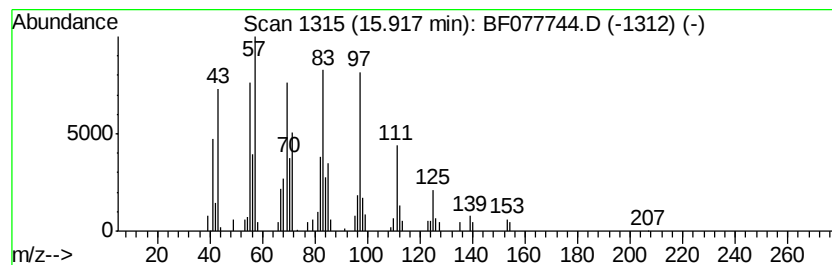
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	4.07 ng	130031	Chrysene-d12	16.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2		1-Nonadecene	266	C19H38	018435-45-5	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	1.62	20.9	ng	331314	1	7.17	316822	20.0
2-Pentanone, 4-hy...	4.93	3.2	ng	50221	1	7.17	316822	20.0
unknown6.88	6.88	71.4	ng	1131170	1	7.17	316822	20.0
Trichloroacetic a...	15.92	4.1	ng	130031	5	16.03	638759	20.0