

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
 Data File : BG016380.D
 Acq On : 14 Apr 2015 4:18
 Operator : TP/IZ
 Sample : G1849-09
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-04-COMP

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_G\METHODS\8270-BG040615.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	2.773	8	14	23	rVV	126340	255718	7.56%	1.082%
2	2.850	23	27	33	rVB	122009	168241	4.97%	0.712%
3	4.789	351	357	364	rBV	172568	240515	7.11%	1.018%
4	5.265	431	438	453	rBV	1506536	2098121	62.01%	8.876%
5	6.863	703	710	722	rBV	1463521	2261970	66.86%	9.569%
6	7.209	762	769	782	rBV	1466874	2298014	67.92%	9.722%
7	7.673	842	848	855	rVB	282915	422954	12.50%	1.789%
8	7.997	894	903	910	rBV	1034094	1648436	48.72%	6.974%
9	8.831	1036	1045	1057	rBV	822522	1345342	39.76%	5.692%
10	10.458	1315	1322	1332	rBV	380217	626169	18.51%	2.649%
11	12.938	1736	1744	1754	rBV	1874869	2754890	81.42%	11.655%
12	13.772	1881	1886	1895	rVB	150112	211069	6.24%	0.893%
13	14.313	1972	1978	1988	rBV2	528384	798147	23.59%	3.377%
14	15.805	2226	2232	2246	rBV	1328258	1855410	54.84%	7.849%
15	17.057	2439	2445	2454	rBV2	705620	960126	28.38%	4.062%
16	17.956	2594	2598	2604	rBV3	21279	34214	1.01%	0.145%
17	19.689	2887	2893	2901	rBV	2569115	3383363	100.00%	14.313%
18	20.946	3102	3107	3118	rBV3	76754	136832	4.04%	0.579%
19	21.234	3151	3156	3164	rBV	904990	1082624	32.00%	4.580%
20	23.467	3529	3536	3550	rVB	555800	1055576	31.20%	4.466%

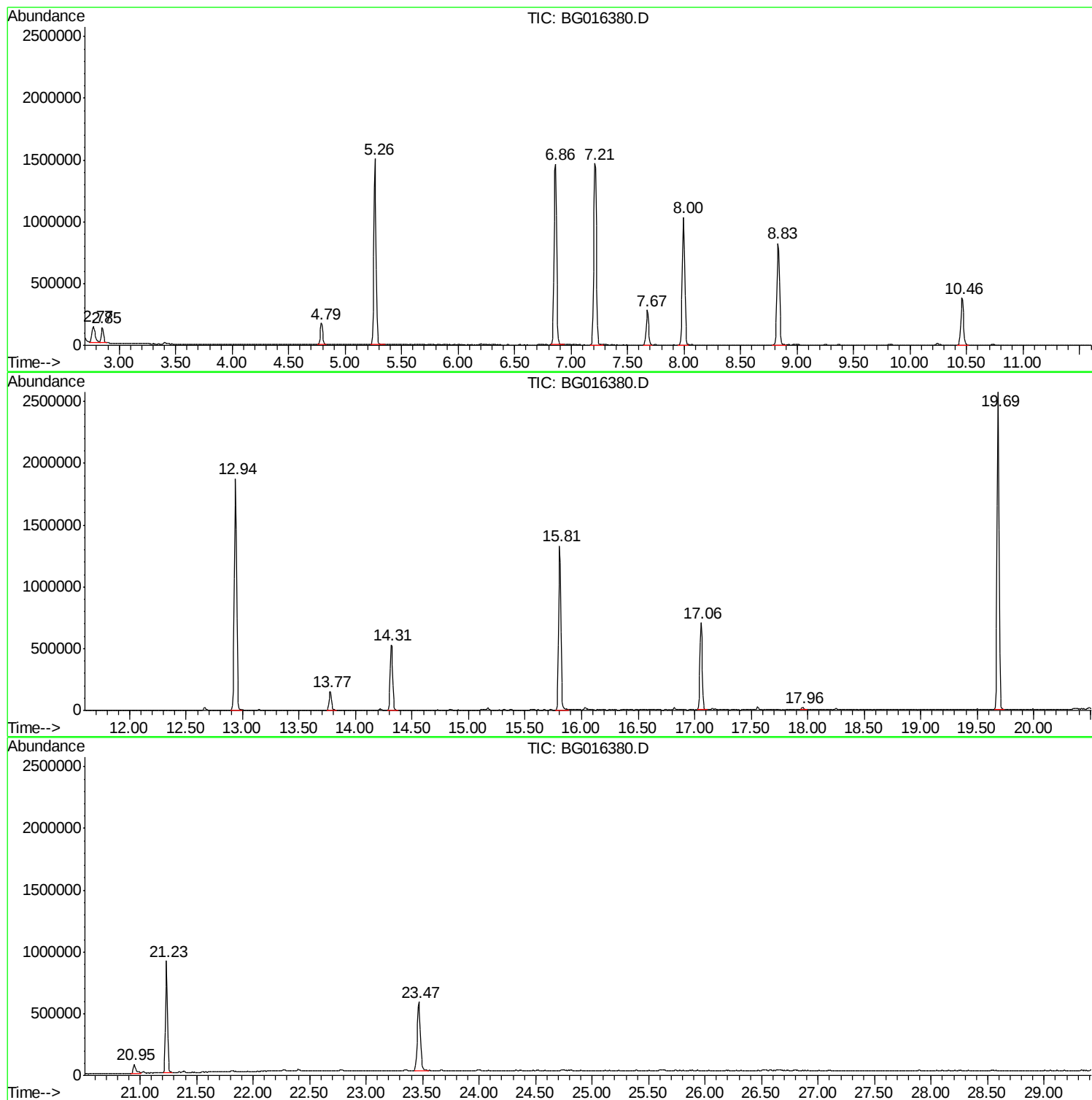
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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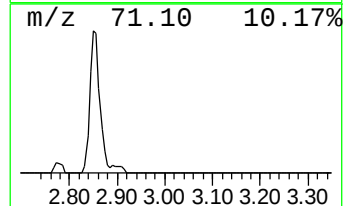
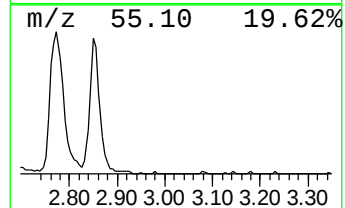
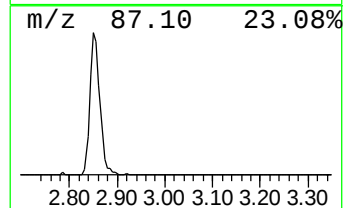
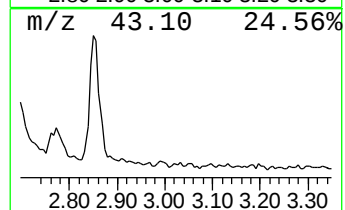
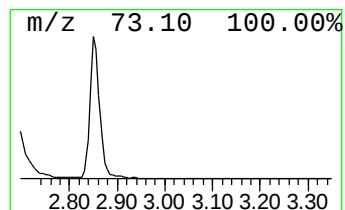
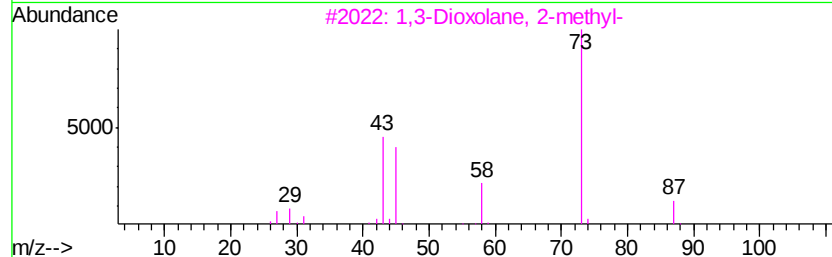
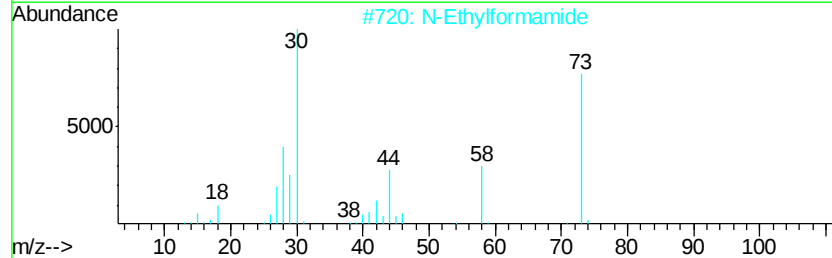
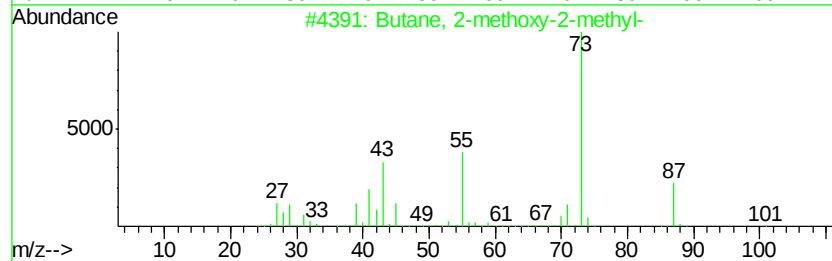
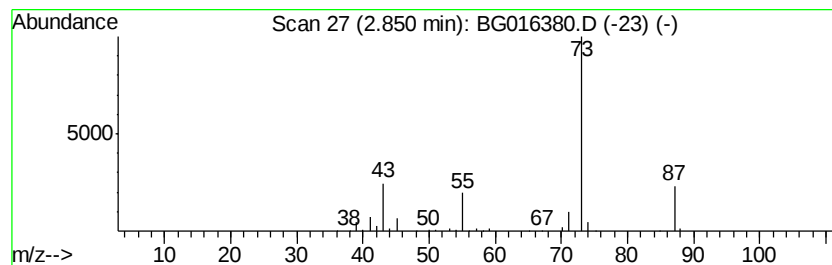
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.85	7.96 ng	168241	1,4-Dichlorobenzene-d4	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	7
5		1,3-Dioxolane	74	C3H6O2	000646-06-0	4



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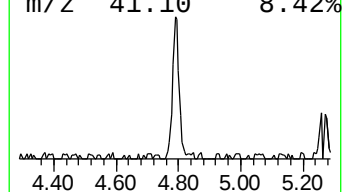
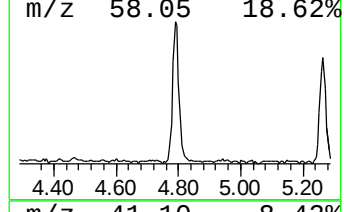
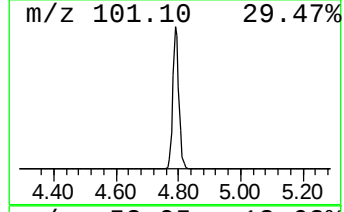
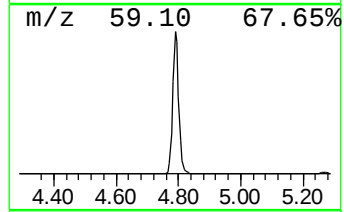
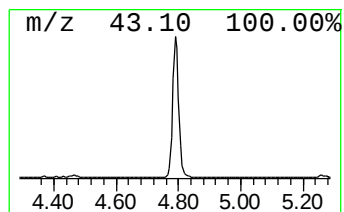
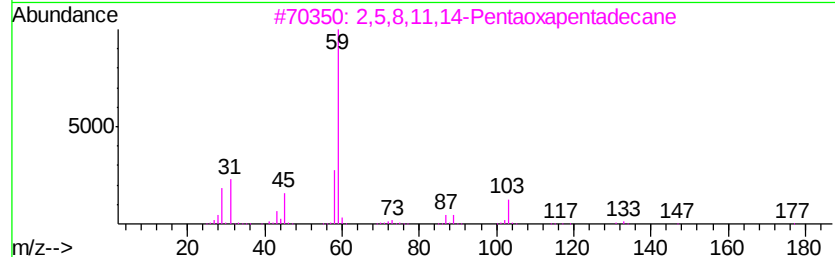
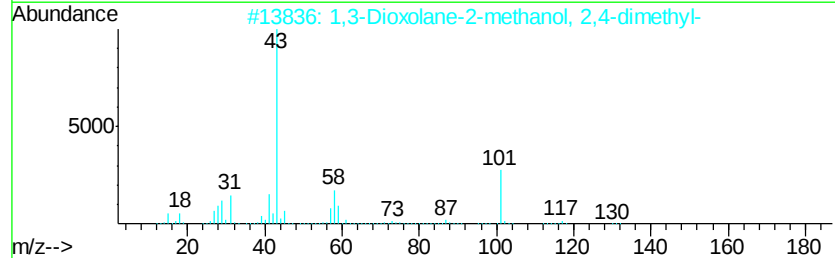
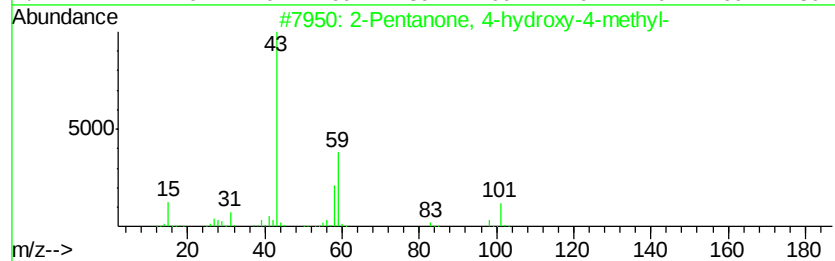
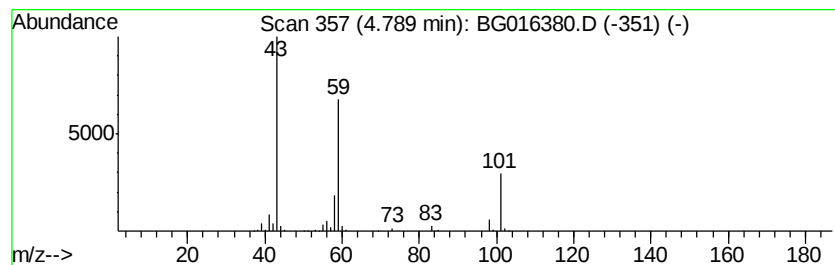
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	11.37 ng	240515	1,4-Dichlorobenzene-d4	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
3		2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	25
4		2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	23
5		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23



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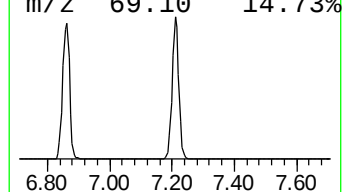
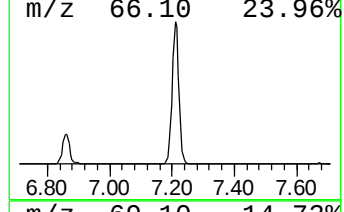
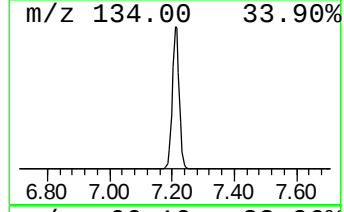
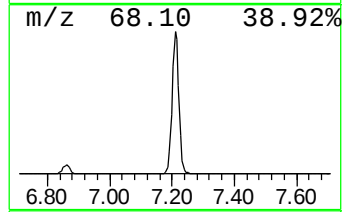
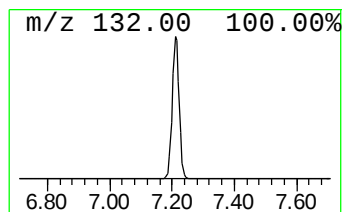
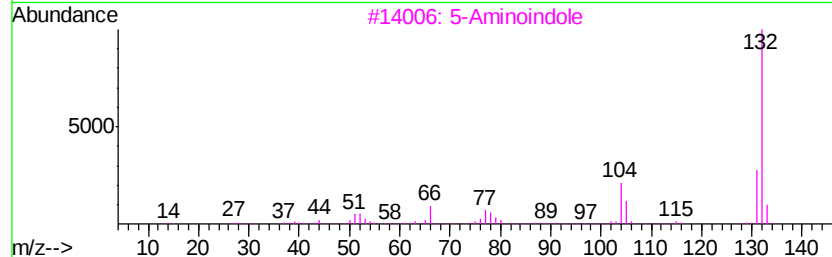
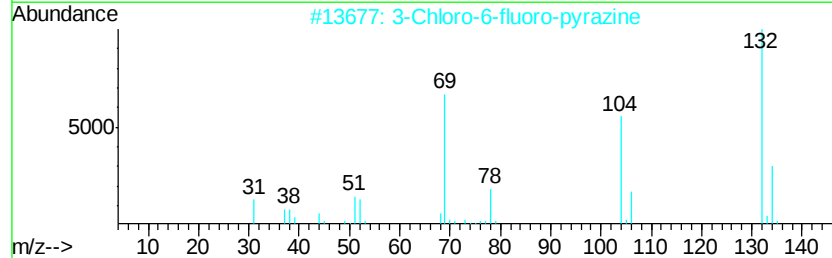
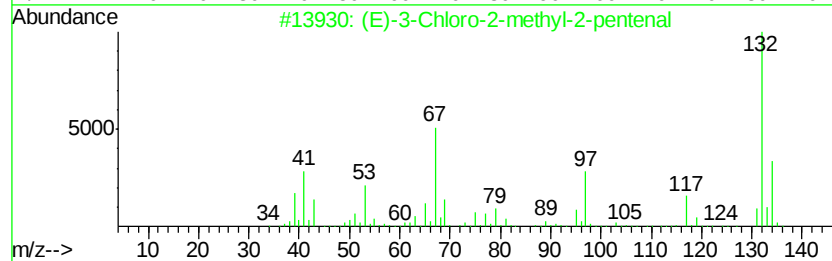
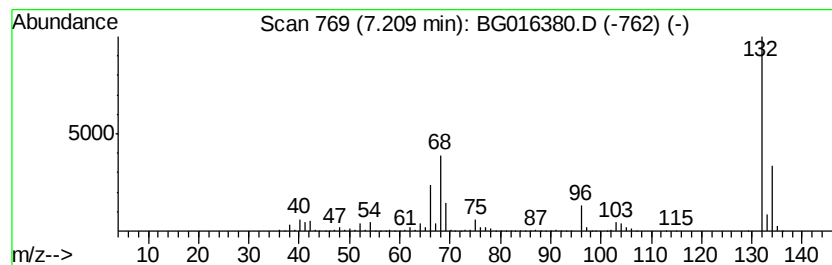
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Peak Number 4 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	108.67 ng	2298010	1,4-Dichlorobenzene-d4	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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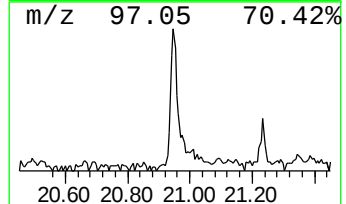
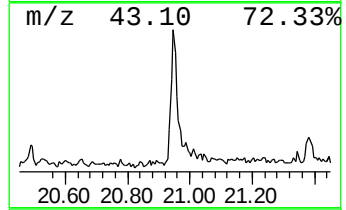
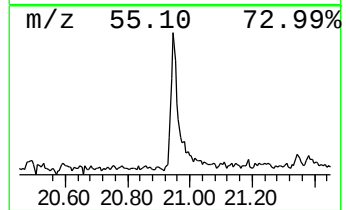
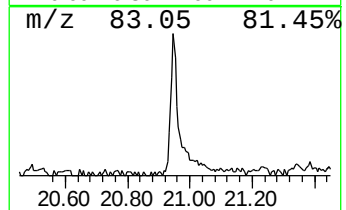
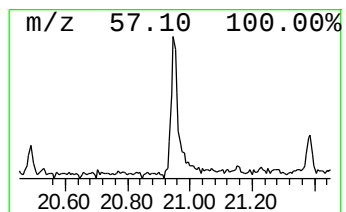
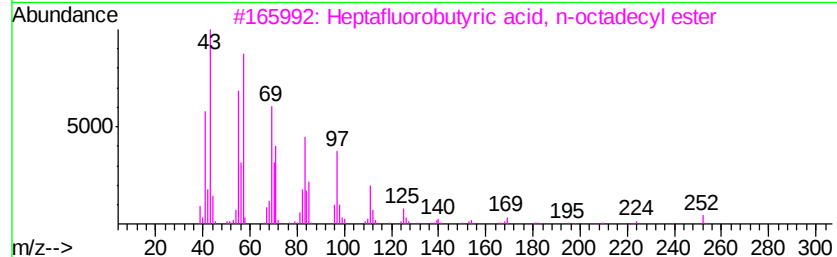
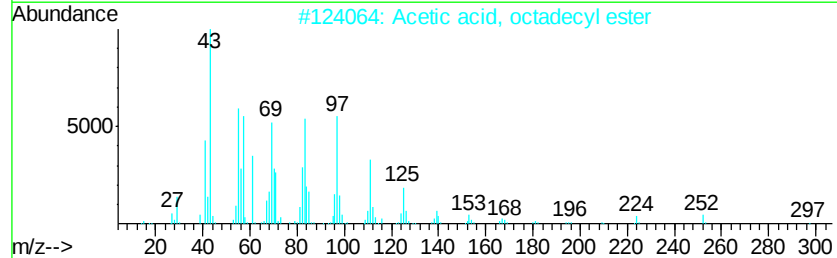
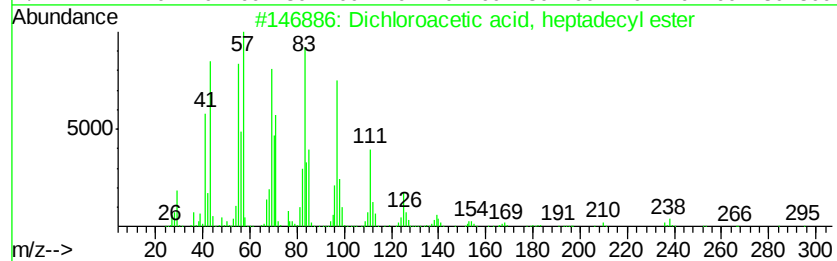
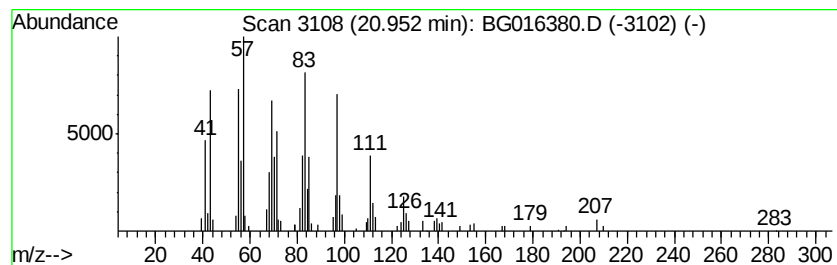
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Dichloroacetic acid, heptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.95	2.53 ng	136832	Chrysene-d12	21.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	91
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	90
5	1-Nonadecene	266	C19H38	018435-45-5	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.85	8.0	ng	168241	1	7.67	422954	20.0
2-Pentanone, 4-hy...	4.79	11.4	ng	240515	1	7.67	422954	20.0
unknown7.21	7.21	108.7	ng	2298010	1	7.67	422954	20.0
Dichloroacetic ac...	20.95	2.5	ng	136832	5	21.23	1082620	20.0