

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092617\
 Data File : BF098850.D
 Acq On : 26 Sep 2017 23:38
 Operator : SJ/JU
 Sample : I5427-06
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 092217-SIDI-F-U-S

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-BF092317.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	2.193	14	18	35	rVB	328399	546798	12.15%	2.059%
2	5.128	514	517	526	rVB	230571	233593	5.19%	0.879%
3	5.522	580	584	588	rBV	1415667	1339913	29.78%	5.045%
4	6.528	751	755	758	rBV	1206014	912040	20.27%	3.434%
5	6.681	776	781	784	rBV	2778152	2390570	53.14%	9.001%
6	6.910	817	820	824	rVB	970245	844053	18.76%	3.178%
7	7.069	843	847	851	rBV	3218214	3075381	68.36%	11.579%
8	7.475	911	916	919	rBV	2336009	2546551	56.60%	9.588%
9	8.192	1034	1038	1042	rBV	1313728	1143136	25.41%	4.304%
10	9.269	1216	1221	1225	rBV	4338683	4498988	100.00%	16.939%
11	9.657	1284	1287	1290	rBV	171269	125331	2.79%	0.472%
12	9.951	1333	1337	1341	rBV	1448777	1212387	26.95%	4.565%
13	10.739	1466	1471	1474	rBV	1848872	1608727	35.76%	6.057%
14	11.439	1586	1590	1593	rBV	1282615	1100669	24.46%	4.144%
15	13.021	1854	1859	1862	rBV	3378819	3359309	74.67%	12.648%
16	13.904	2005	2009	2014	rBV	79201	78195	1.74%	0.294%
17	14.074	2034	2038	2042	rVB	963135	780709	17.35%	2.939%
18	15.568	2286	2292	2301	rVB	585659	763604	16.97%	2.875%

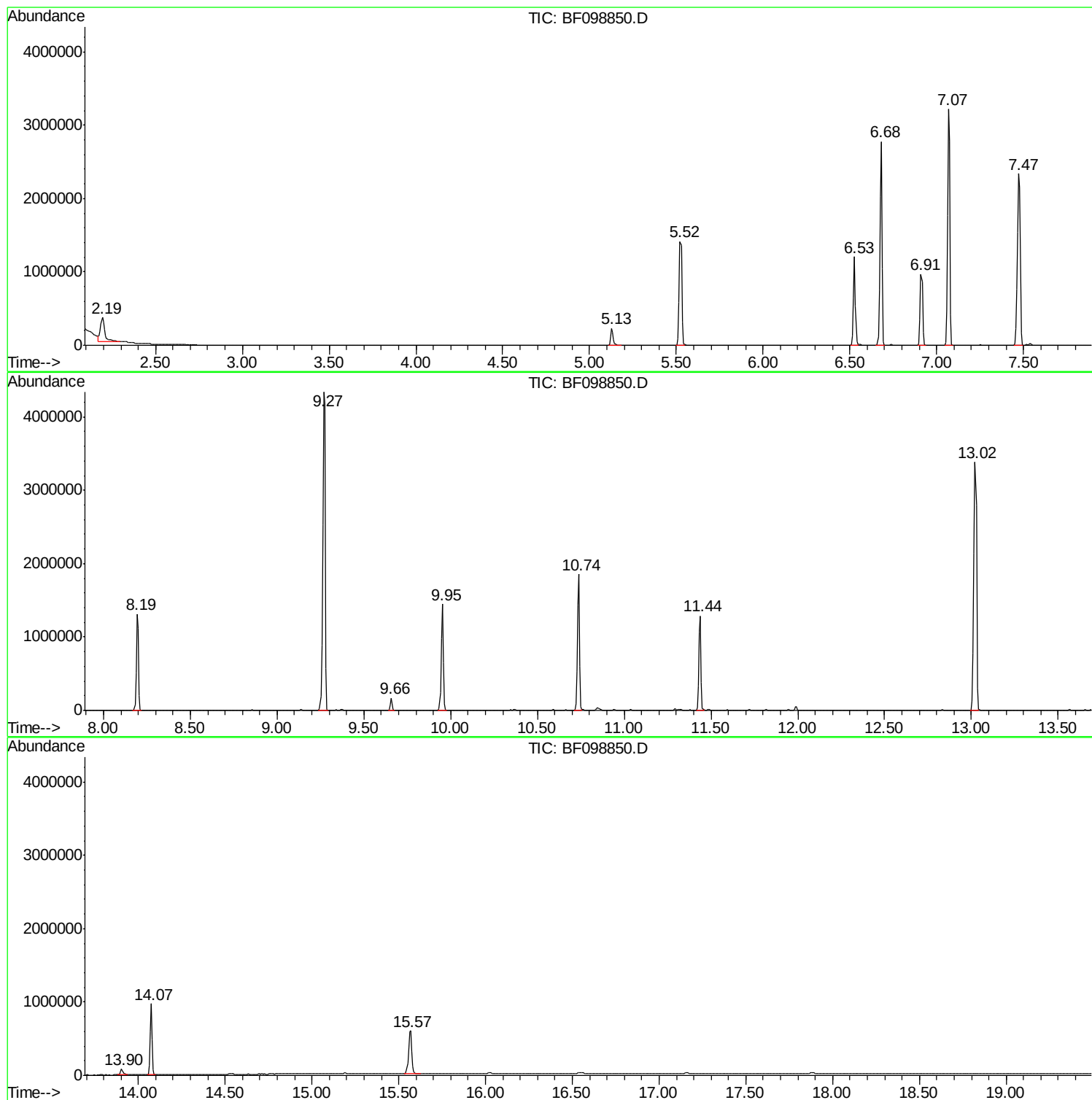
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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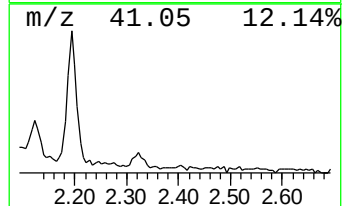
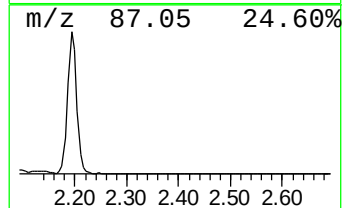
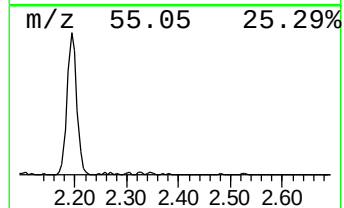
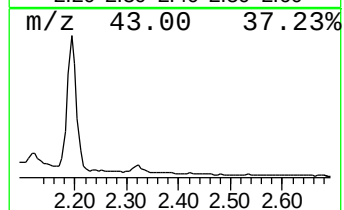
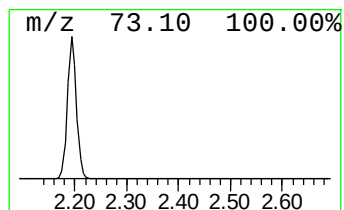
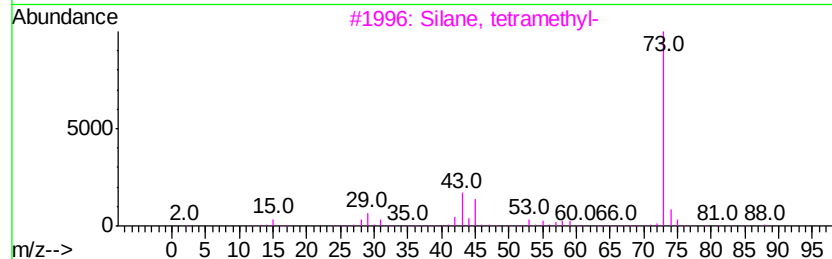
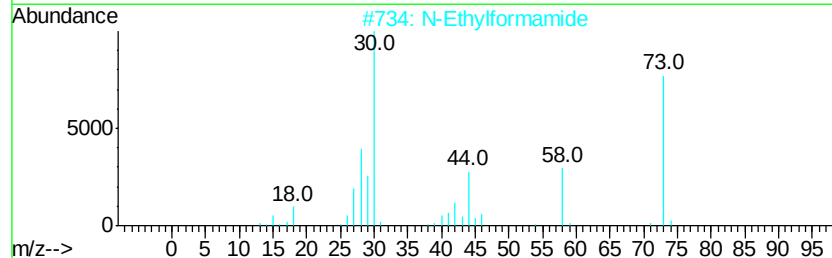
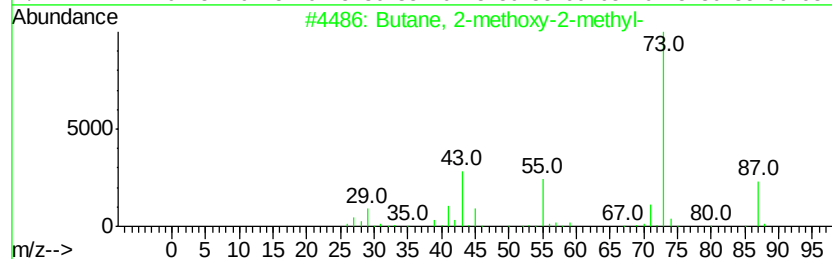
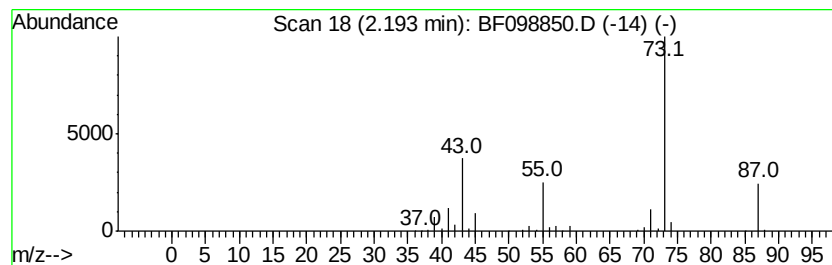
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.19	12.96 ng	546798	1,4-Dichlorobenzene-d4	6.91	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9



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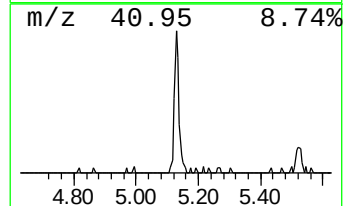
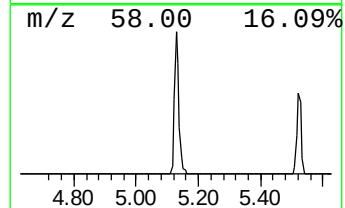
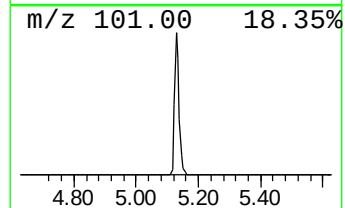
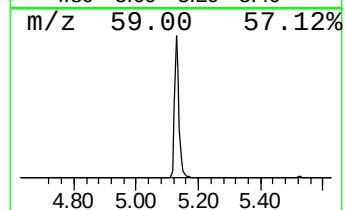
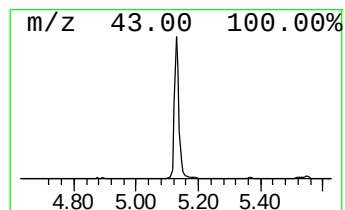
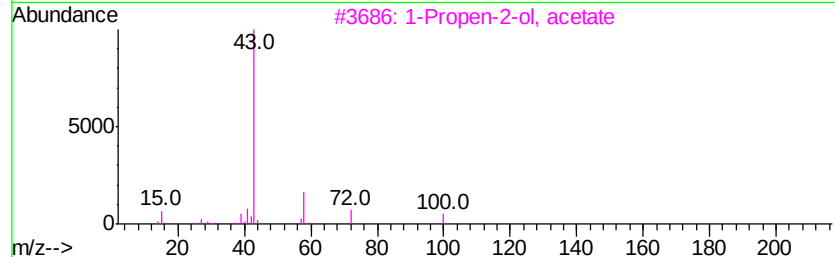
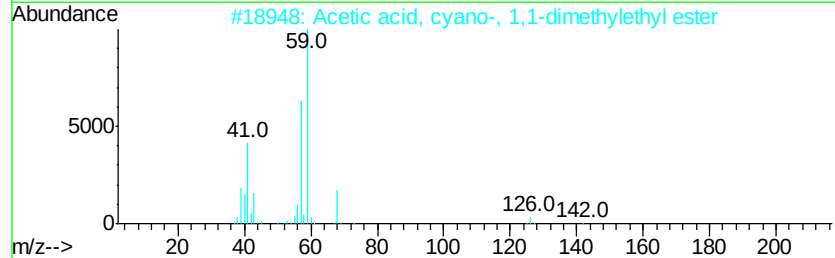
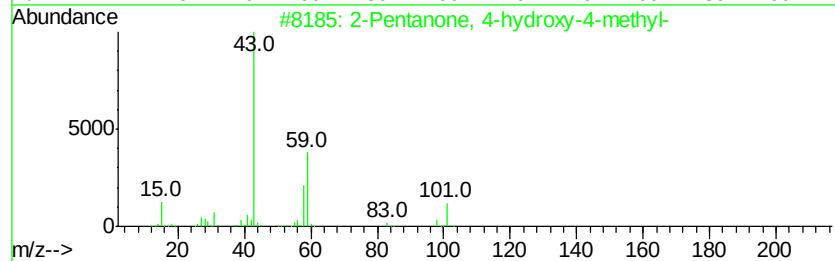
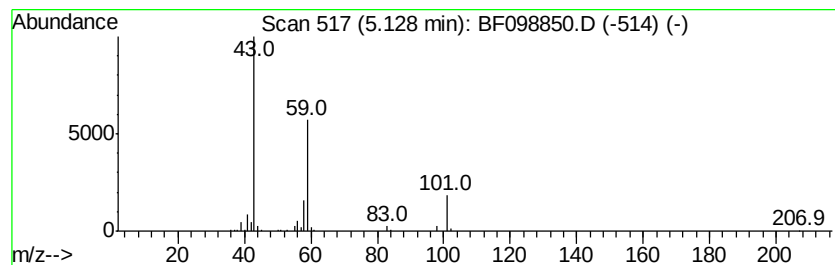
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	5.54 ng	233593	1,4-Dichlorobenzene-d4	6.91

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
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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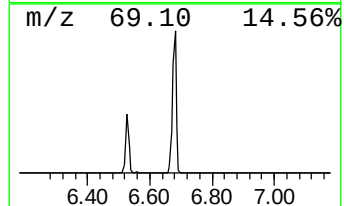
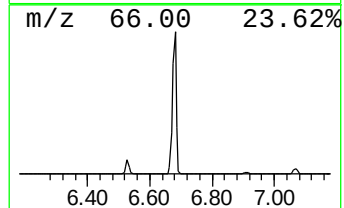
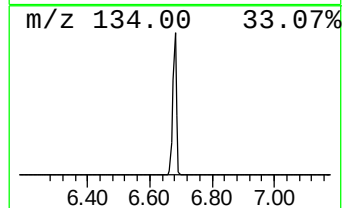
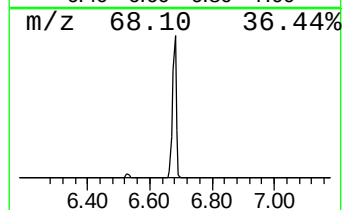
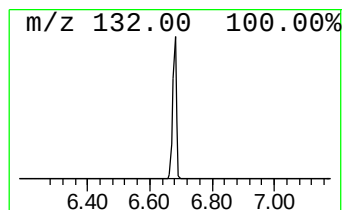
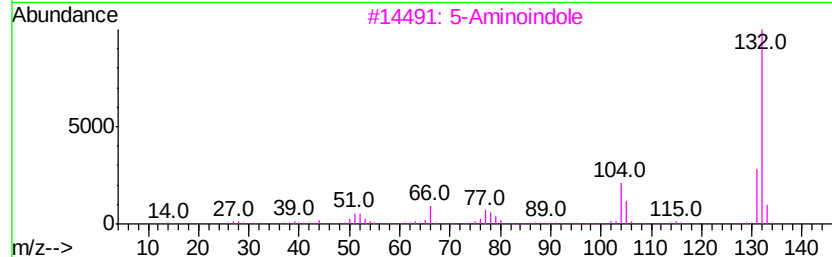
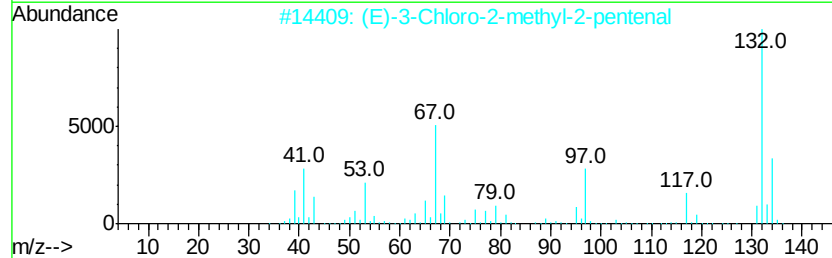
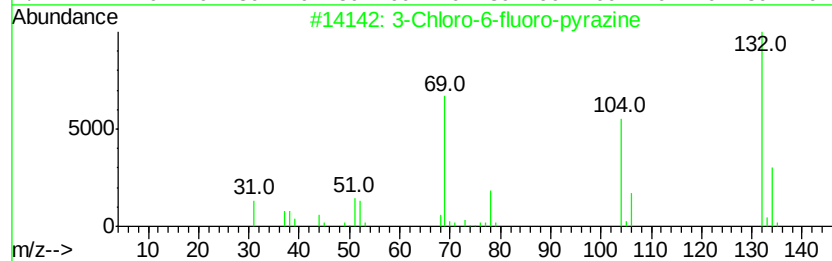
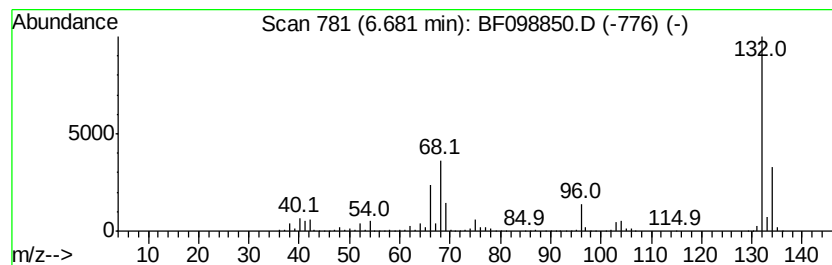
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Peak Number 3 unknown6.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	56.65 ng	2390570	1,4-Dichlorobenzene-d4	6.91

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3		Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	5		Aminoindole	132	C8H8N2	005192-03-0	12
4	4		Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1		Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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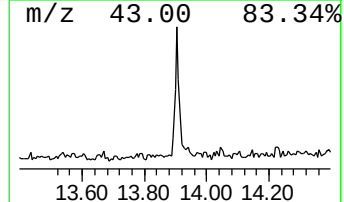
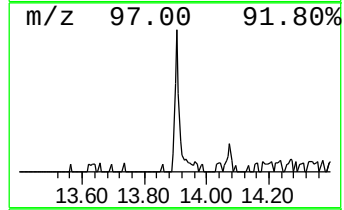
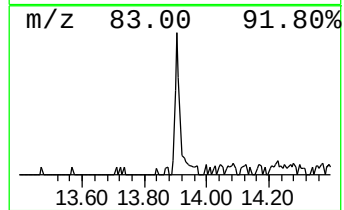
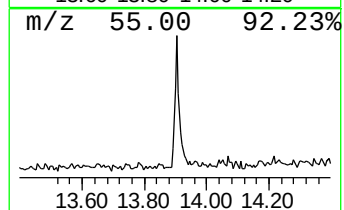
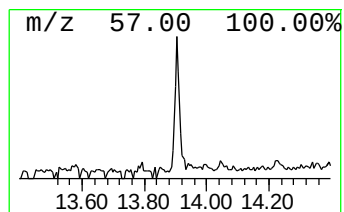
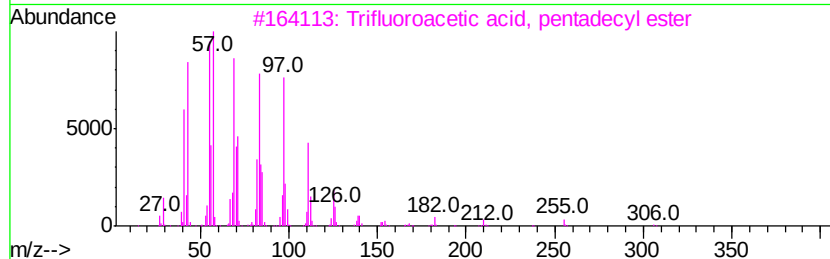
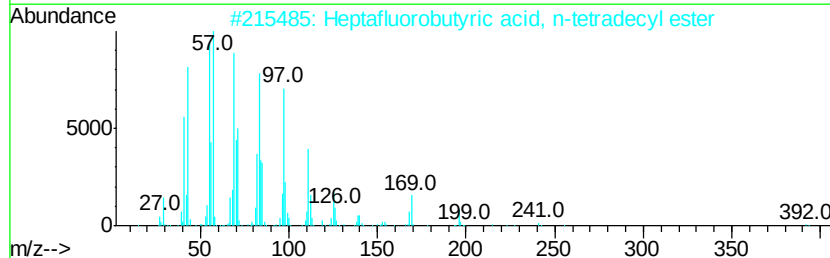
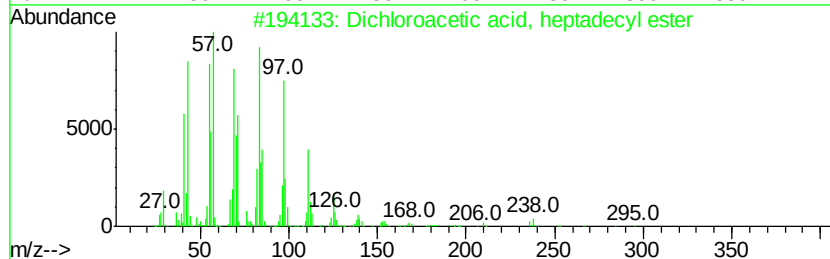
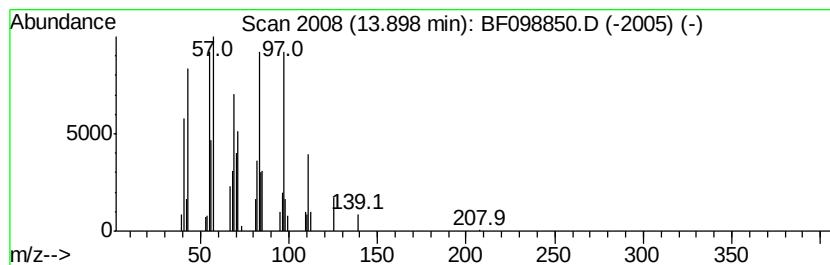
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Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	2.00 ng	78195	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4		2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	94
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.19	13.0	ng	546798	1	6.91	844053	20.0
2-Pentanone, 4-hy...	5.13	5.5	ng	233593	1	6.91	844053	20.0
unknown6.68	6.68	56.6	ng	2390570	1	6.91	844053	20.0
Dichloroacetic ac...	13.90	2.0	ng	78195	5	14.07	780709	20.0