

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040618\
 Data File : BG033661.D
 Acq On : 7 Apr 2018 11:47
 Operator : SJ/JU
 Sample : J2225-06
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 040218-DBRI-F-U-B

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-BG031918.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	3.475	27	32	42	rBV	151620	290058	7.47%	1.923%
2	3.564	42	47	57	rVB	111704	182201	4.69%	1.208%
3	5.767	417	422	432	rBV2	39875	66911	1.72%	0.444%
4	6.284	504	510	528	rBV	139844	329966	8.49%	2.187%
5	7.970	792	797	811	rBV2	85152	240392	6.19%	1.594%
6	8.376	858	866	885	rBV	328802	737386	18.98%	4.888%
7	8.863	942	949	957	rBV2	80901	187742	4.83%	1.245%
8	9.192	997	1005	1023	rBV2	469926	966669	24.88%	6.408%
9	10.062	1146	1153	1178	rBV	393948	948529	24.41%	6.288%
10	11.742	1432	1439	1453	rBV	145550	331438	8.53%	2.197%
11	14.104	1834	1841	1855	rBV	1403586	2367498	60.93%	15.694%
12	14.897	1970	1976	1980	rBV	45832	71154	1.83%	0.472%
13	15.479	2068	2075	2086	rBV2	330585	573907	14.77%	3.804%
14	16.243	2200	2205	2209	rVB	35643	45345	1.17%	0.301%
15	16.948	2319	2325	2341	rBV	759274	1308634	33.68%	8.675%
16	17.095	2346	2350	2359	rVB2	34005	58138	1.50%	0.385%
17	18.205	2533	2539	2553	rBV	429167	750064	19.30%	4.972%
18	20.726	2962	2968	2989	rBV	2720347	3885537	100.00%	25.757%
19	22.077	3192	3198	3203	rBV2	46047	94012	2.42%	0.623%
20	22.553	3270	3279	3291	rBV2	404456	858305	22.09%	5.690%
21	24.422	3588	3597	3602	rBV4	16854	39769	1.02%	0.264%
22	26.319	3906	3920	3934	rBV2	214323	751823	19.35%	4.984%

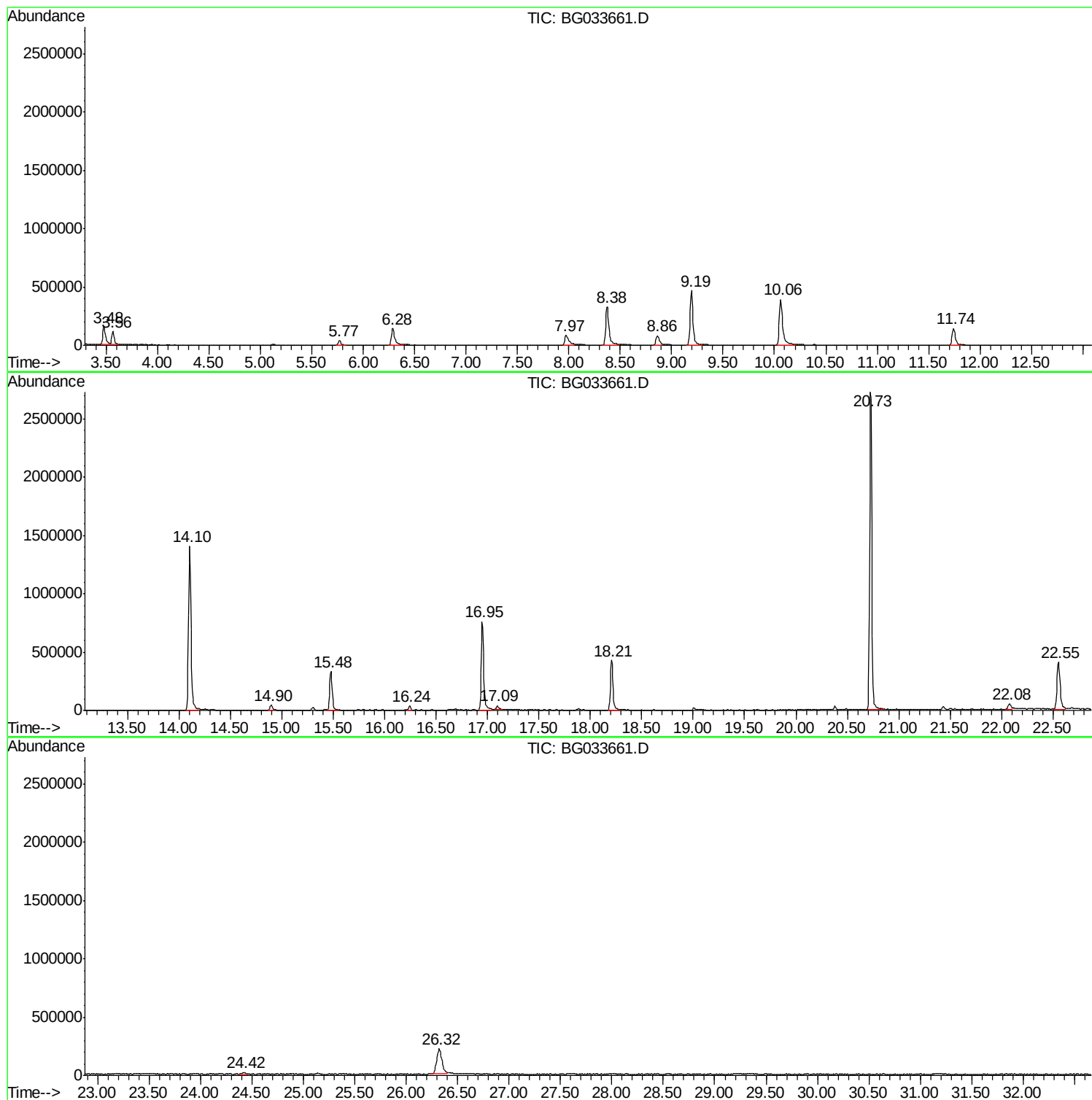
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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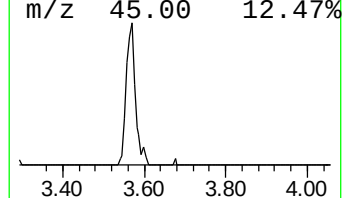
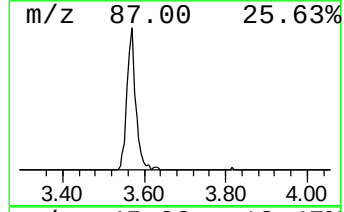
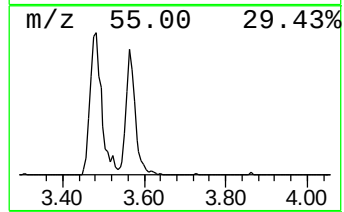
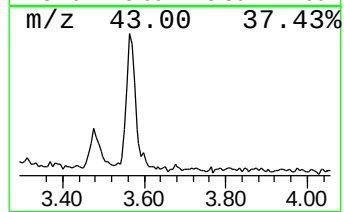
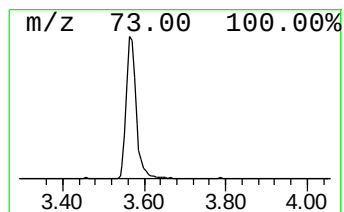
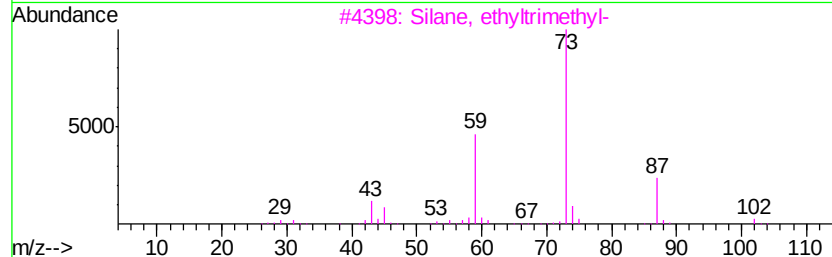
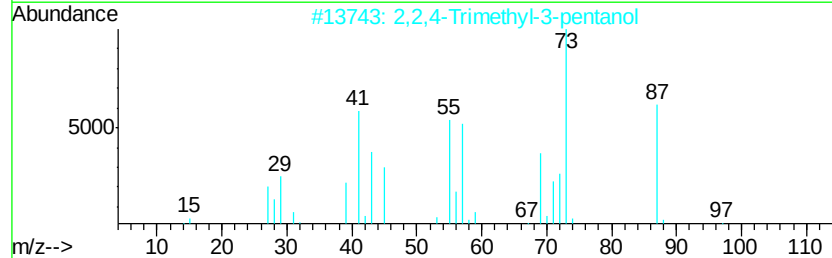
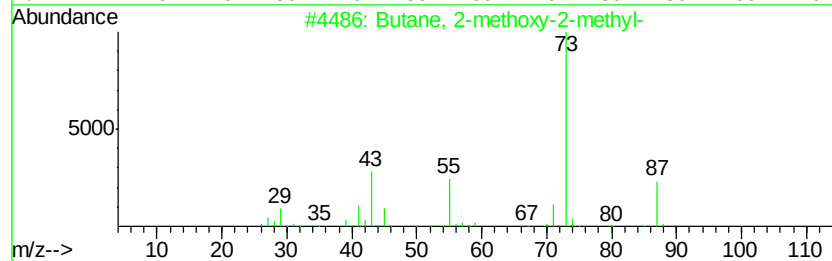
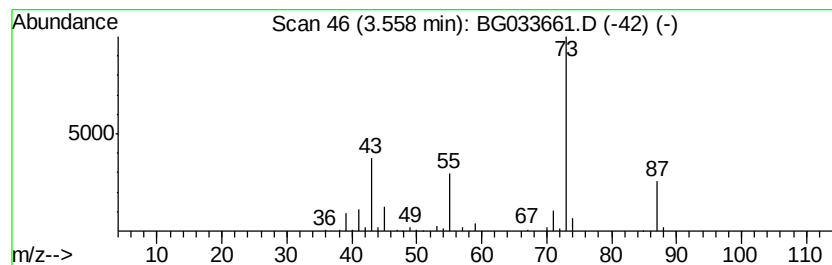
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.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.
3.56	19.41 ng	182201	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
5		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25



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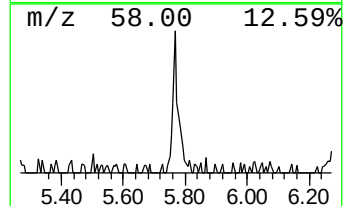
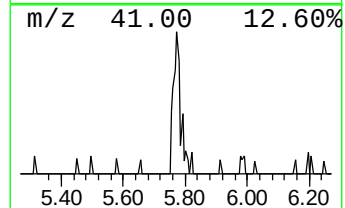
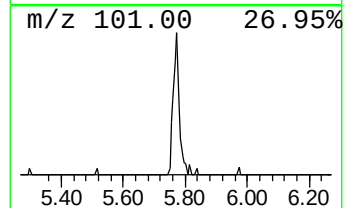
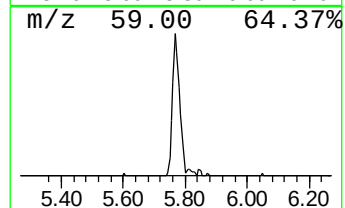
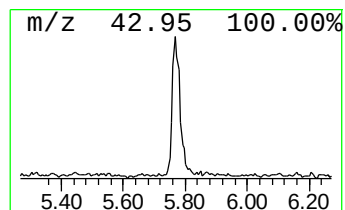
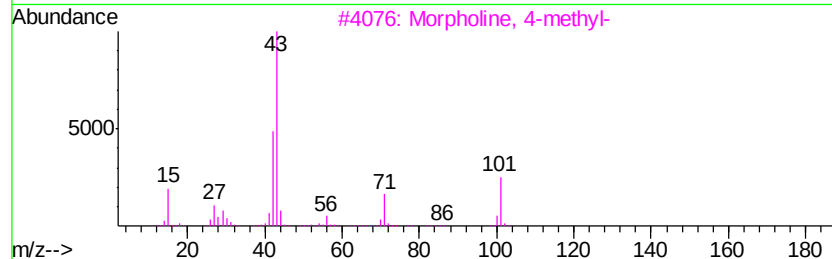
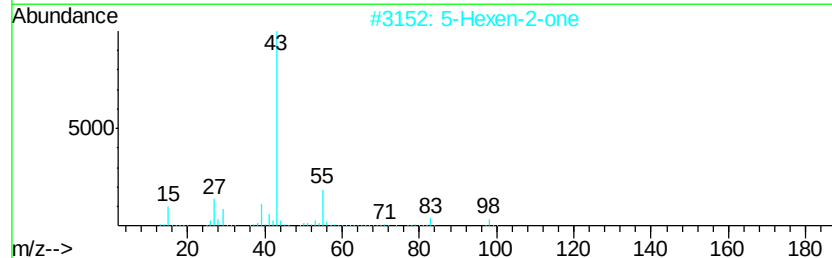
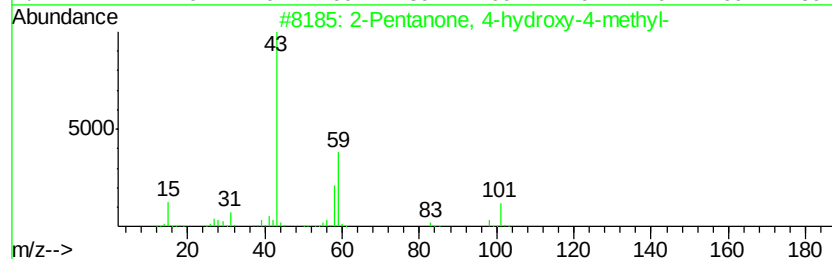
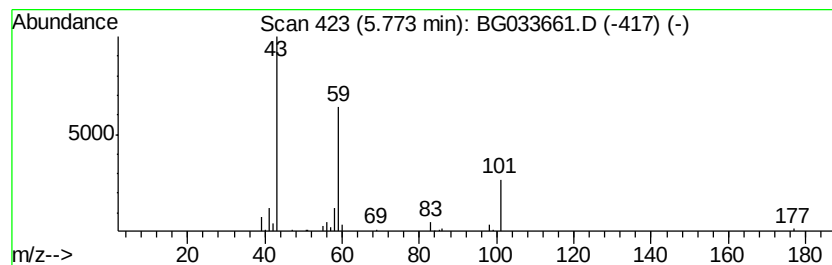
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	7.13 ng	66911	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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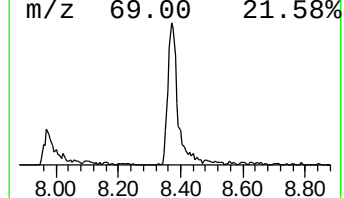
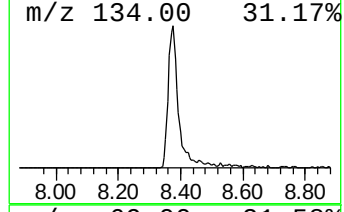
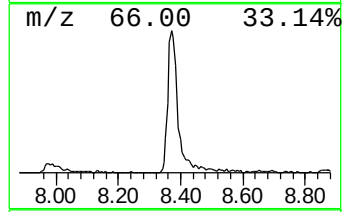
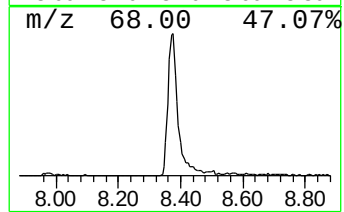
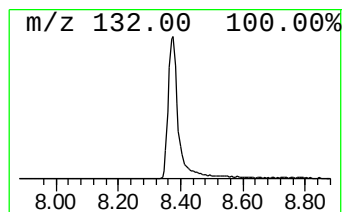
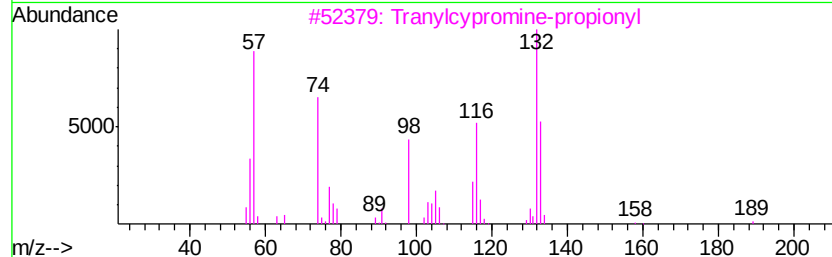
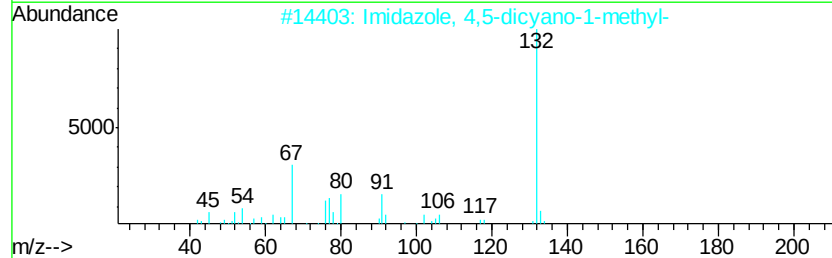
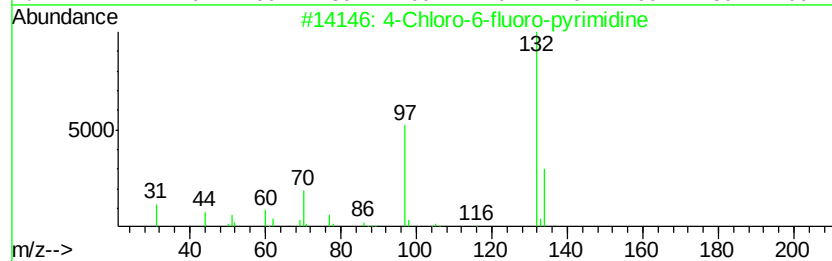
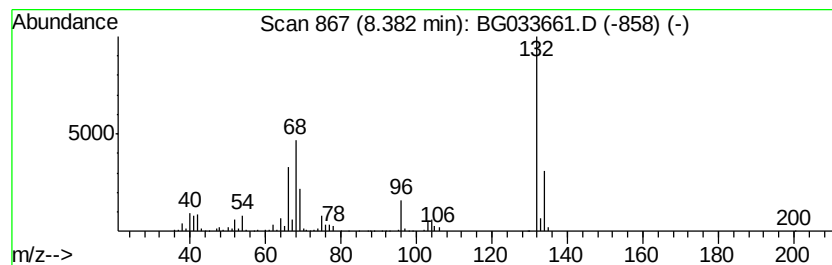
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Peak Number 4 unknown8.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.38	78.55 ng	737386	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12



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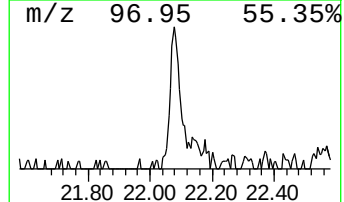
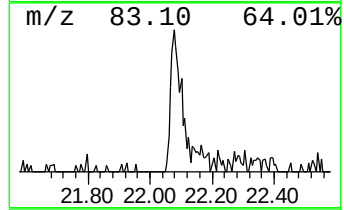
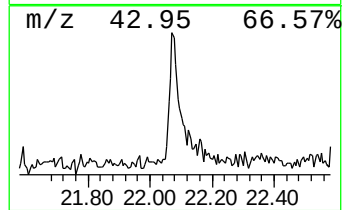
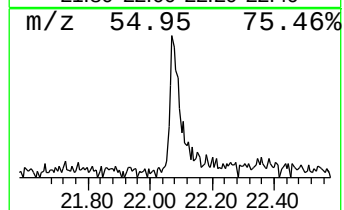
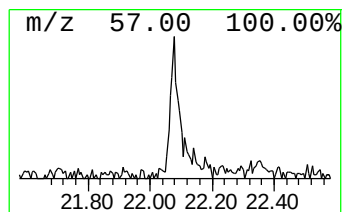
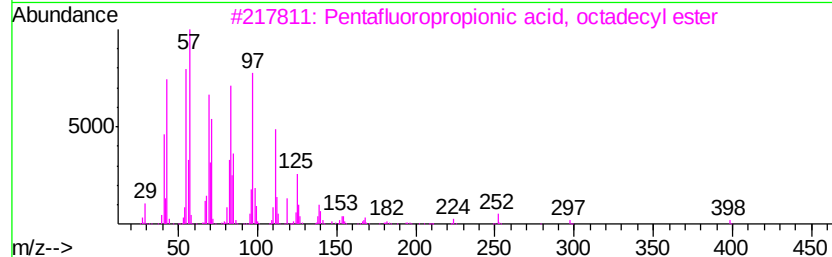
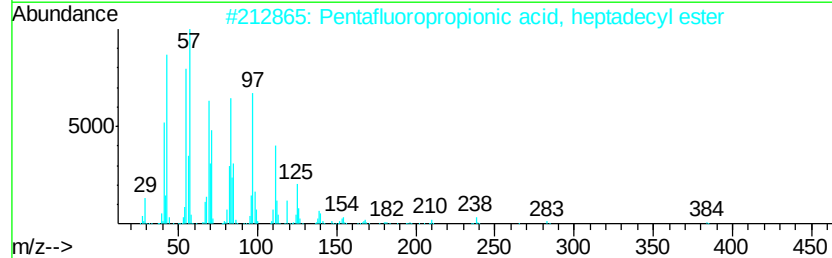
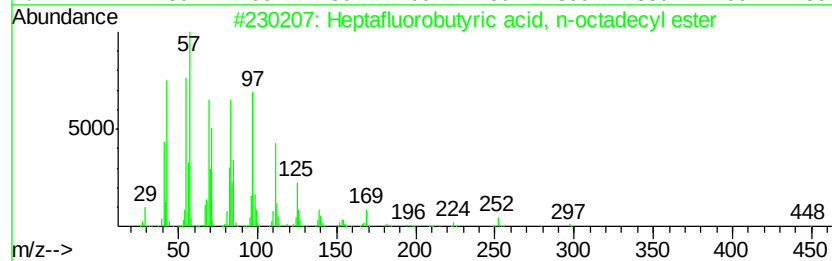
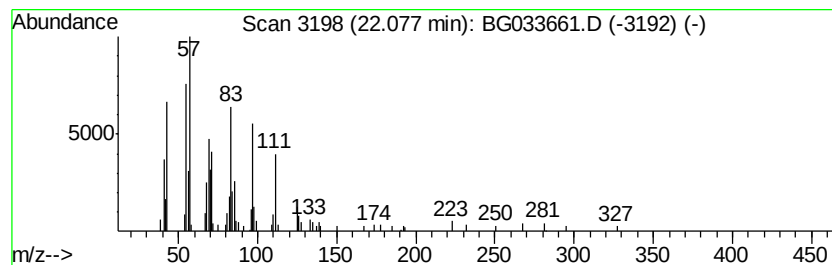
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Peak Number 6 Heptafluorobutyric acid, n-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
22.08	2.19 ng	94012	Chrysene-d12	22.55		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	91
2		Pentafluoropropionic acid, heptadecyl ester	402	C20H35F5O2	959218-78-1	91
3		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	91
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87
5		Trichloroacetic acid, pentadecyl ester	372	C17H31Cl3O2	074339-53-0	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.56	19.4	ng	182201	1	8.86	187742	20.0
2-Pentanone, 4-hy...	5.77	7.1	ng	66911	1	8.86	187742	20.0
unknown8.38	8.38	78.5	ng	737386	1	8.86	187742	20.0
Heptafluorobutyri...	22.08	2.2	ng	94012	5	22.55	858305	20.0