

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040418\
 Data File : BG033566.D
 Acq On : 4 Apr 2018 18:59
 Operator : SJ/JU
 Sample : J2177-15
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 032818-SIDI-E-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	3.479	26	32	42	rBV	137688	273406	6.77%	1.774%
2	3.567	42	47	58	rVB	108861	184337	4.56%	1.196%
3	5.776	416	423	429	rBV	30252	49893	1.24%	0.324%
4	6.293	505	511	533	rBV	143769	355821	8.81%	2.309%
5	7.979	792	798	817	rBV	96287	274539	6.80%	1.782%
6	8.373	858	865	878	rBV	319888	705115	17.46%	4.576%
7	8.866	940	949	963	rBV	78452	194264	4.81%	1.261%
8	9.195	997	1005	1022	rBV	482985	988469	24.47%	6.415%
9	10.065	1145	1153	1174	rBV	376115	927029	22.95%	6.016%
10	11.745	1432	1439	1452	rBV	128698	297471	7.37%	1.930%
11	14.107	1834	1841	1859	rBV	1411167	2428684	60.13%	15.761%
12	15.476	2069	2074	2087	rVB2	298934	537617	13.31%	3.489%
13	16.951	2318	2325	2338	rBV2	843959	1470186	36.40%	9.541%
14	18.208	2531	2539	2549	rBV	441934	766937	18.99%	4.977%
15	19.007	2668	2675	2684	rBV5	23670	46329	1.15%	0.301%
16	20.382	2905	2909	2913	rVB	47025	57276	1.42%	0.372%
17	20.729	2962	2968	2979	rBV	2919560	4038745	100.00%	26.210%
18	21.434	3084	3088	3095	rVB3	32819	42851	1.06%	0.278%
19	22.069	3191	3196	3207	rBV6	46826	102176	2.53%	0.663%
20	22.556	3271	3279	3292	rBV2	432840	871837	21.59%	5.658%
21	26.322	3908	3920	3936	rBV3	214264	796050	19.71%	5.166%

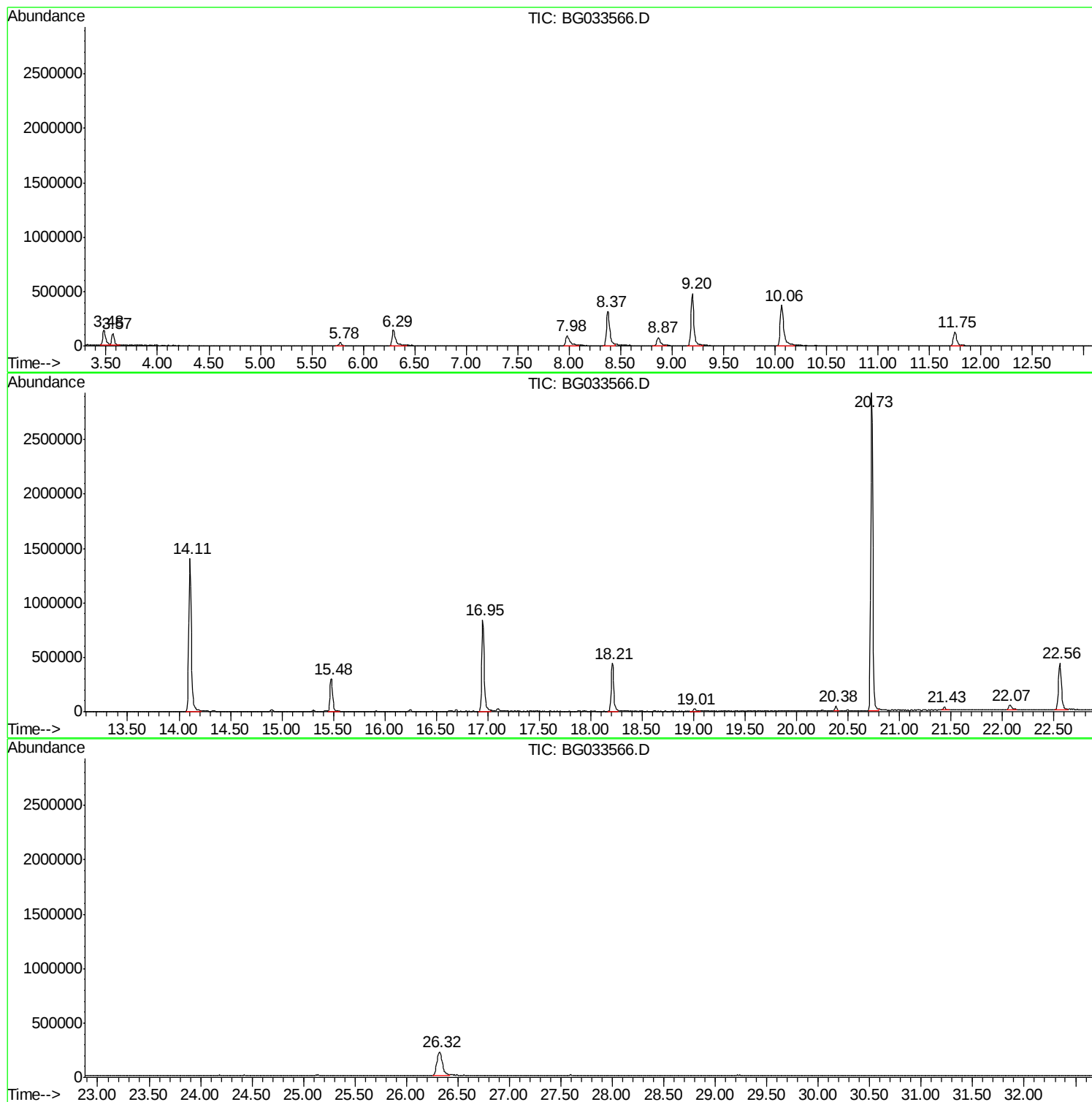
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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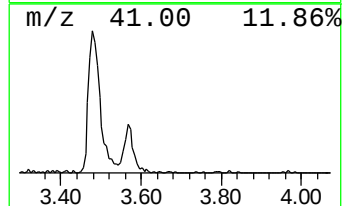
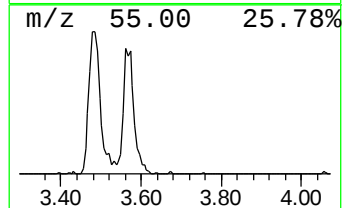
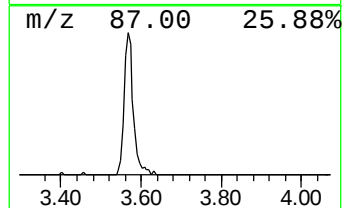
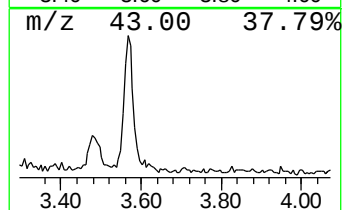
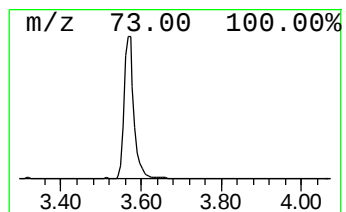
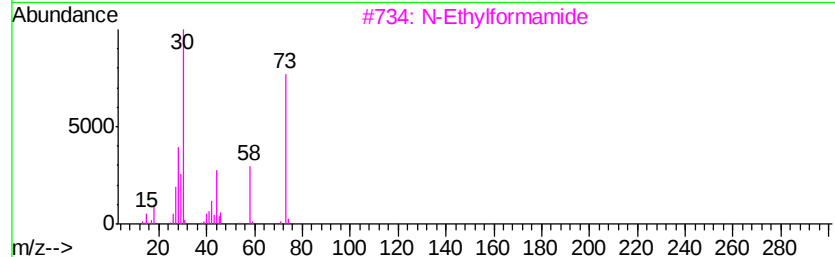
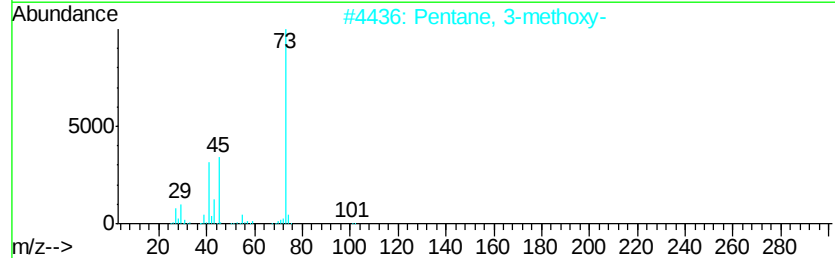
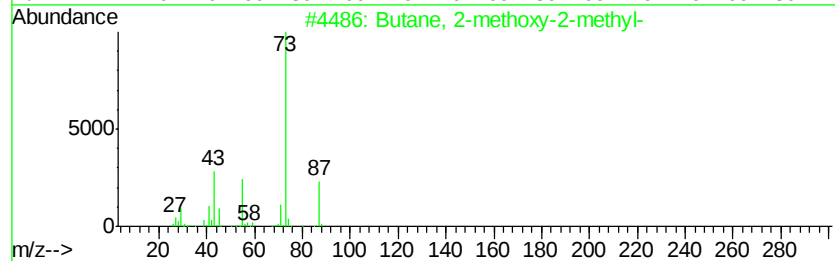
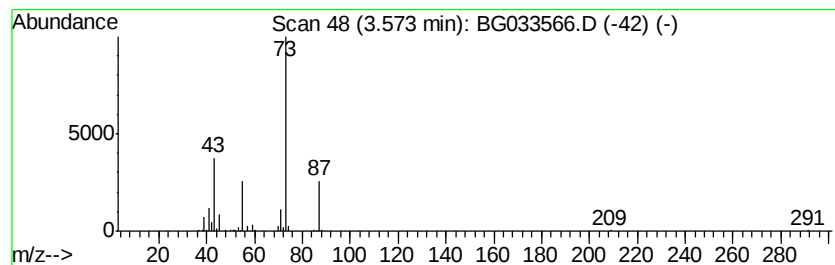
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	18.98 ng	184337	1,4-Dichlorobenzene-d4	8.87

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	12
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
5		Butanoic acid, 2-hydroxy-2-methyl-	132	C6H12O3	032793-34-3	9



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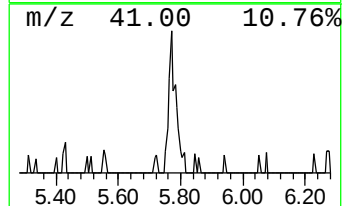
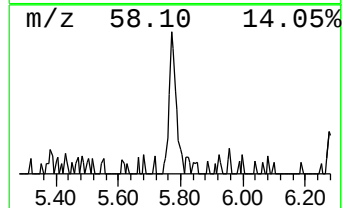
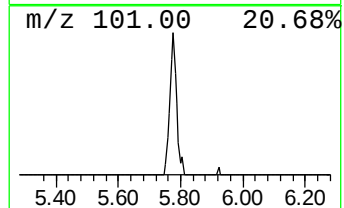
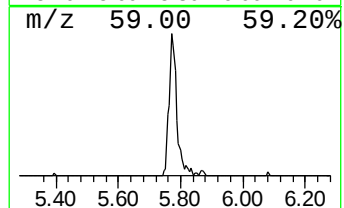
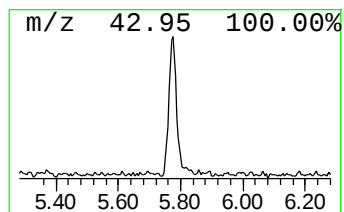
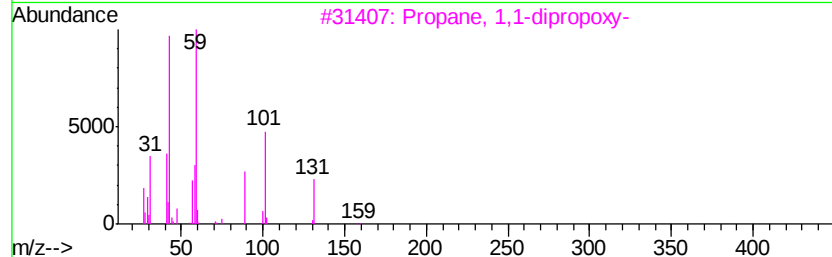
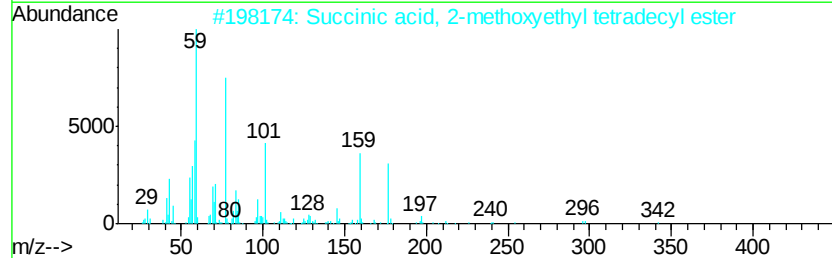
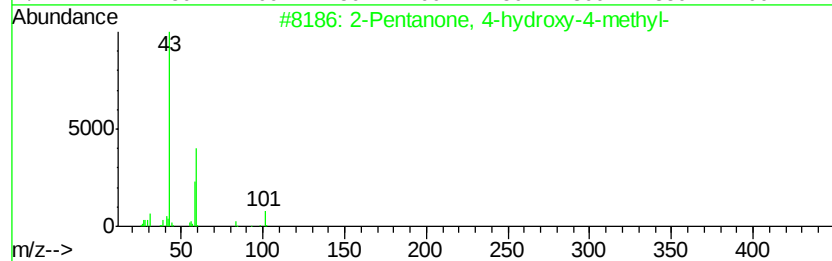
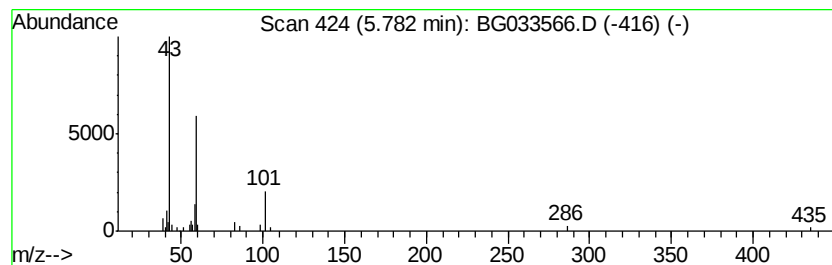
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.78	5.14 ng	49893	1,4-Dichlorobenzene-d4	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Succinic acid, 2-methoxyethyl tetradecyl ester	372	C21H40O5	1000325-81-3	36
3		Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	36
4		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9



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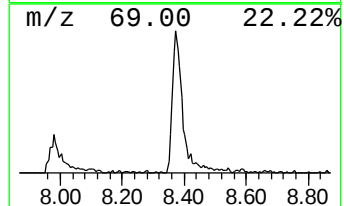
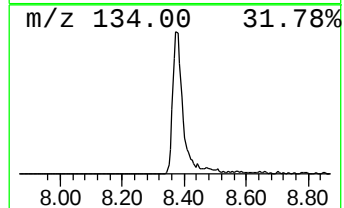
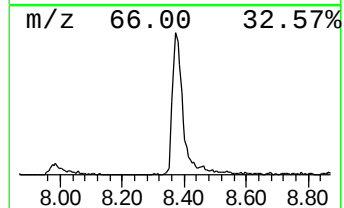
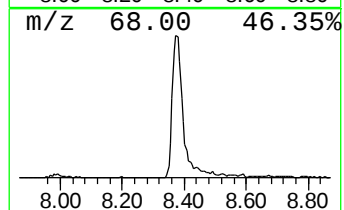
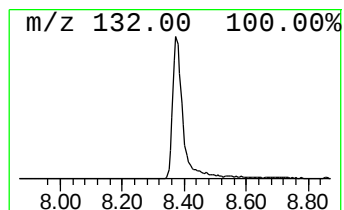
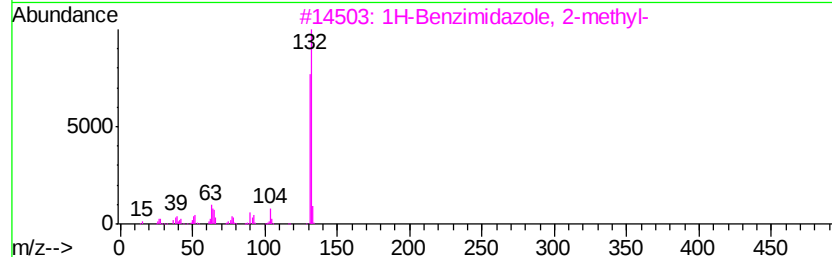
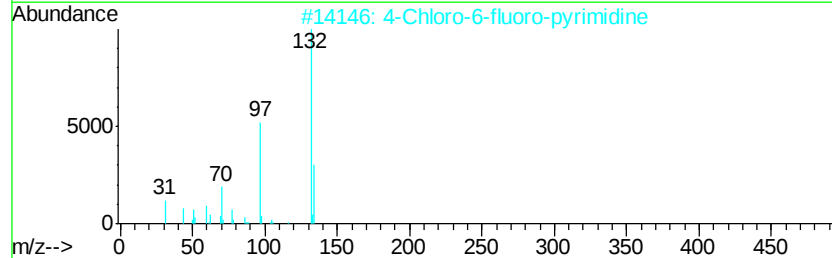
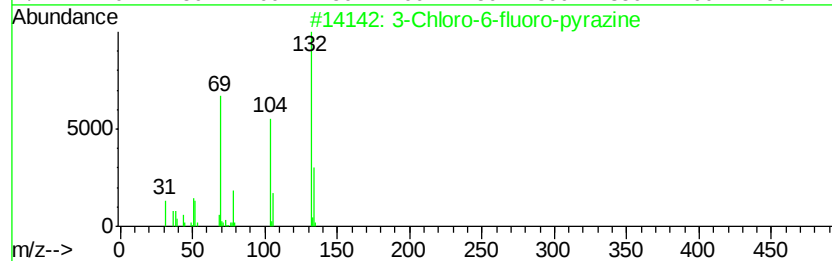
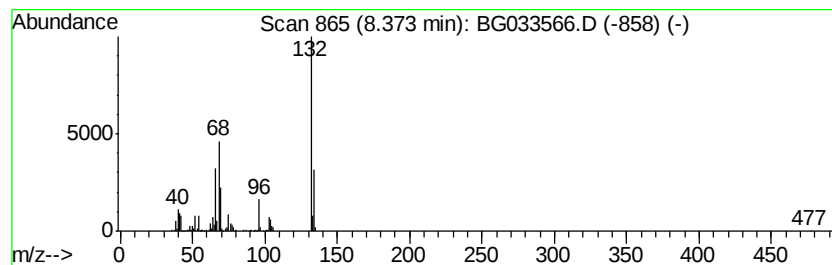
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Peak Number 4 unknown8.37 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.37	72.59 ng	705115	1,4-Dichlorobenzene-d4	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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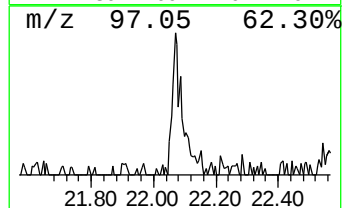
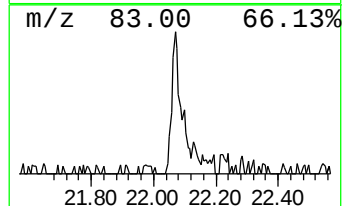
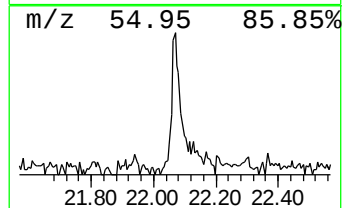
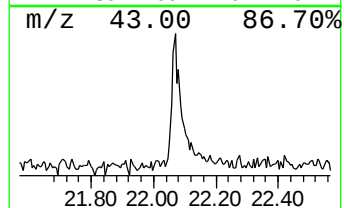
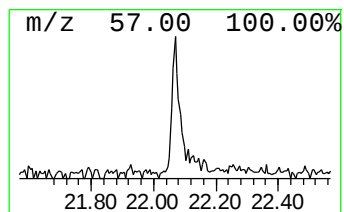
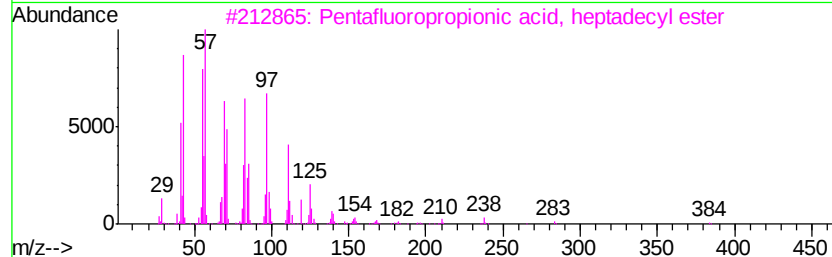
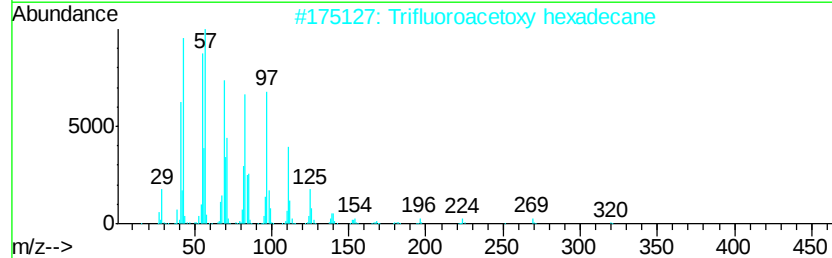
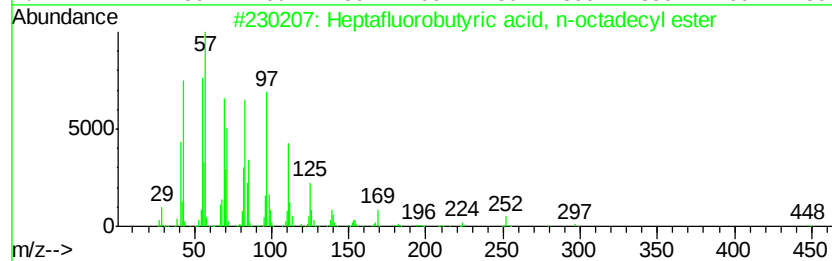
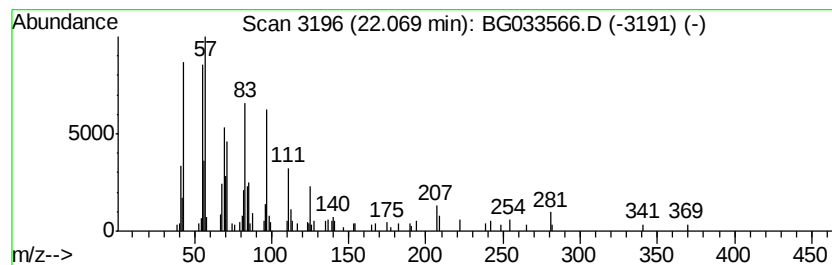
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Peak Number 6 Heptafluorobutyric acid, n-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	2.34 ng	102176	Chrysene-d12	22.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	90
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
3		Pentafluoropropionic acid, heptadecyl ester	402	C20H35F5O2	959218-78-1	87
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.57	19.0	ng	184337	1	8.87	194264	20.0
2-Pentanone, 4-hy...	5.78	5.1	ng	49893	1	8.87	194264	20.0
unknown8.37	8.37	72.6	ng	705115	1	8.87	194264	20.0
Heptafluorobutyri...	22.07	2.3	ng	102176	5	22.56	871837	20.0