

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
 Data File : BG024661.D
 Acq On : 4 Nov 2016 00:19
 Operator : UM/SJ
 Sample : H5502-02
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-79-9.5-10.0

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_G\METHODS\8270-BG102516.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	3.122	43	48	70	rVB	8011936	13758010	100.00%	23.537%
2	5.331	418	424	433	rBV	439136	721044	5.24%	1.234%
3	5.795	495	503	513	rBV	2001188	3366736	24.47%	5.760%
4	7.405	769	777	787	rVB	2088617	3733498	27.14%	6.387%
5	7.793	835	843	851	rBV	2028036	3485327	25.33%	5.963%
6	8.269	915	924	933	rBV	347256	649126	4.72%	1.111%
7	8.592	971	979	986	rBV	1424129	2537193	18.44%	4.341%
8	9.444	1115	1124	1132	rBV	1237751	2325964	16.91%	3.979%
9	11.095	1397	1405	1412	rVB	472066	864955	6.29%	1.480%
10	13.510	1805	1816	1824	rBV	2930340	4749264	34.52%	8.125%
11	14.321	1945	1954	1961	rBV	573533	853261	6.20%	1.460%
12	14.885	2043	2050	2058	rBV	784588	1270846	9.24%	2.174%
13	16.365	2294	2302	2312	rBV	3009811	4812318	34.98%	8.233%
14	17.623	2506	2516	2524	rBV2	1094582	1759976	12.79%	3.011%
15	18.469	2655	2660	2668	rBV3	109851	171264	1.24%	0.293%
16	20.208	2948	2956	2964	rBV	5859195	8296541	60.30%	14.194%
17	21.500	3170	3176	3189	rBV3	162340	343317	2.50%	0.587%
18	21.918	3238	3247	3256	rBV	1443908	2394975	17.41%	4.097%
19	25.349	3820	3831	3843	rVB3	750499	2359114	17.15%	4.036%

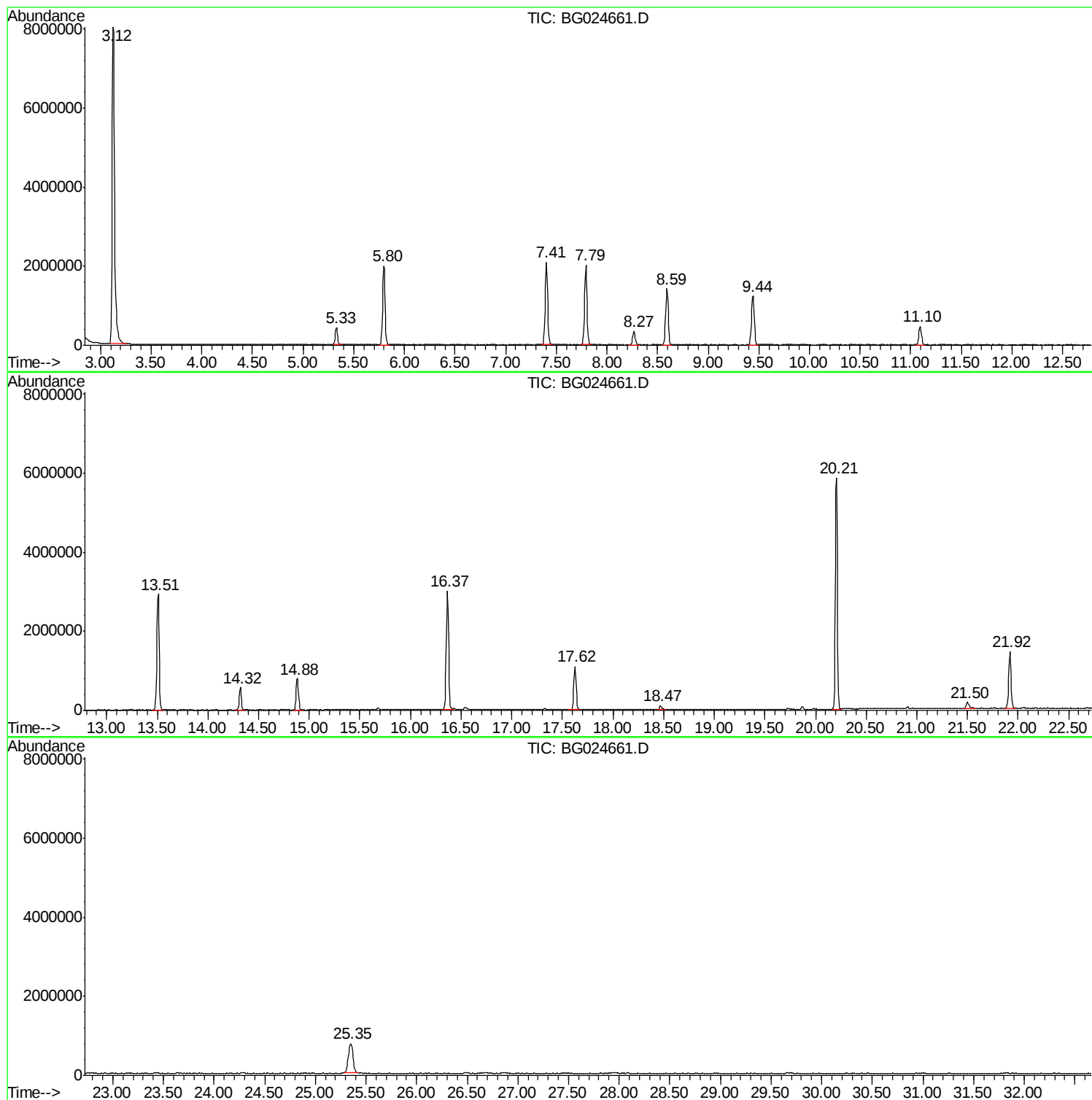
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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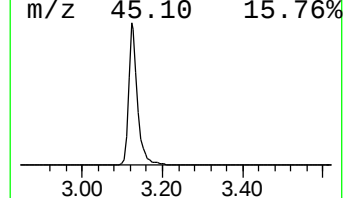
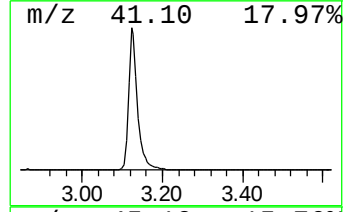
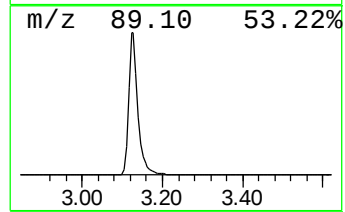
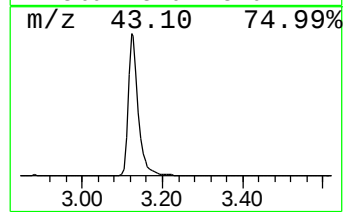
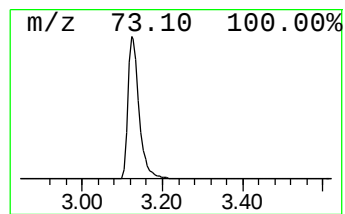
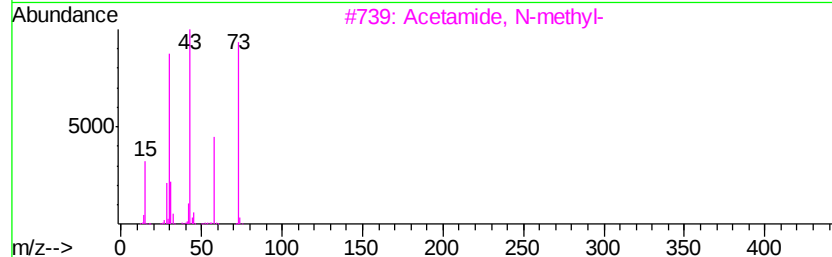
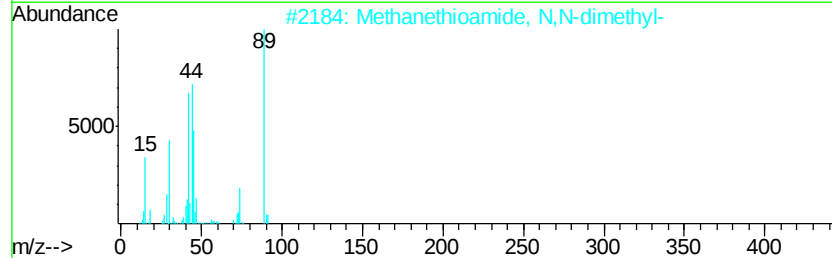
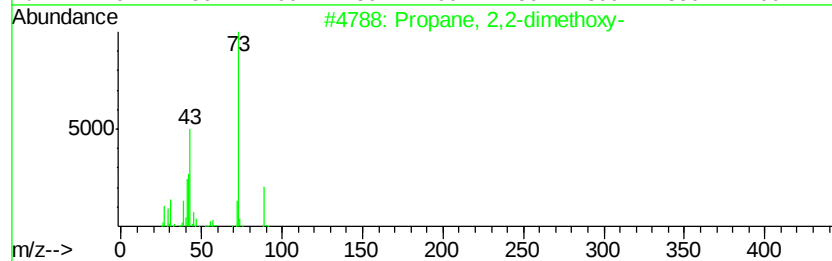
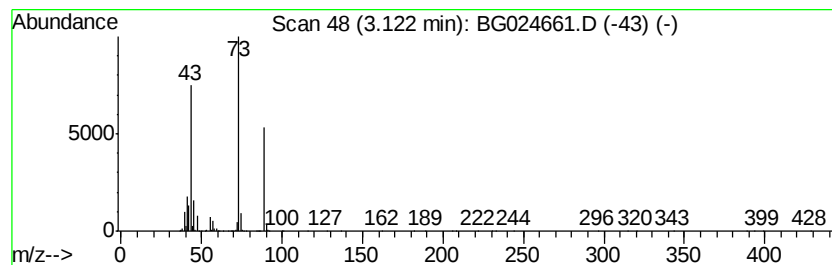
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	423.89 ng	13758000	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2		Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	32
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
5		1-Propene-1-thiol	74	C3H6S	000925-89-3	9



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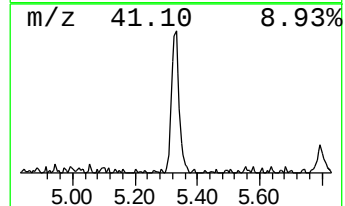
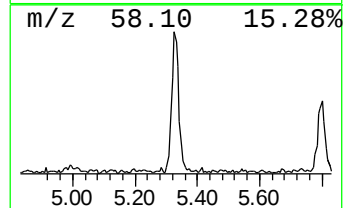
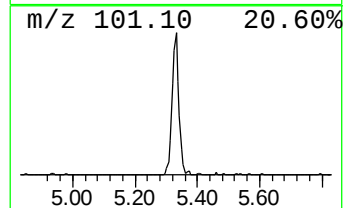
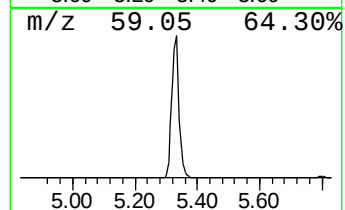
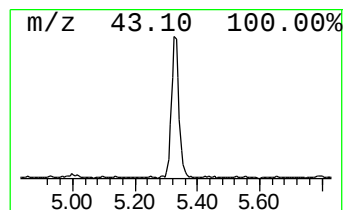
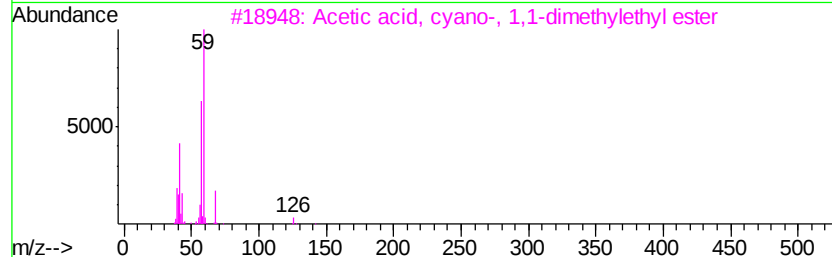
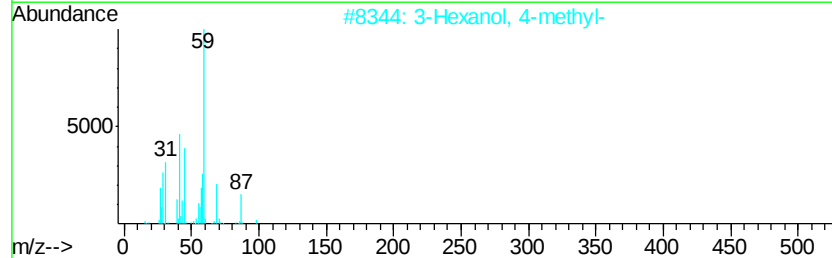
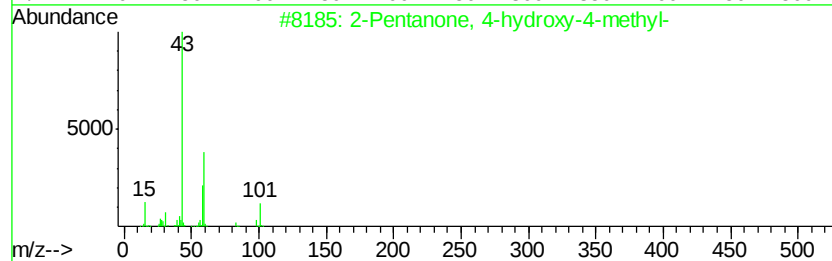
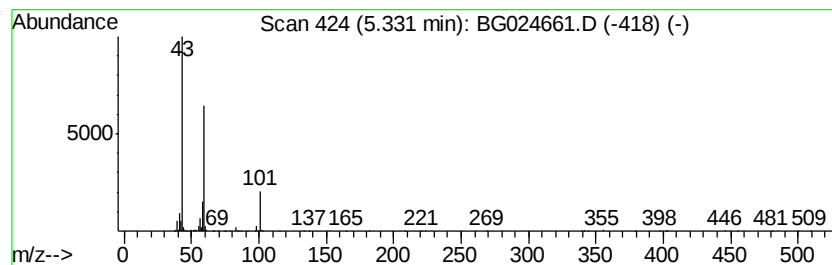
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	22.22 ng	721044	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
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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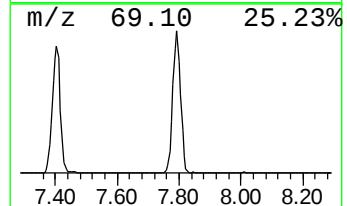
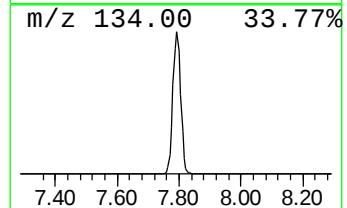
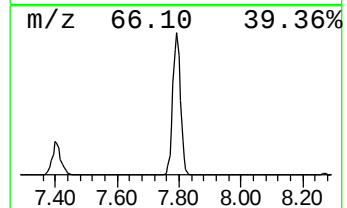
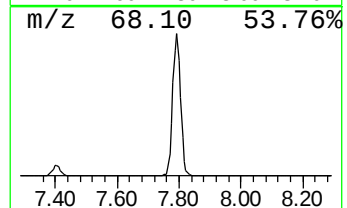
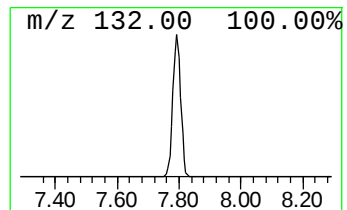
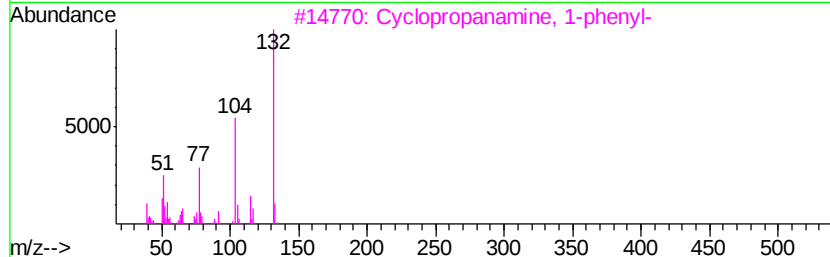
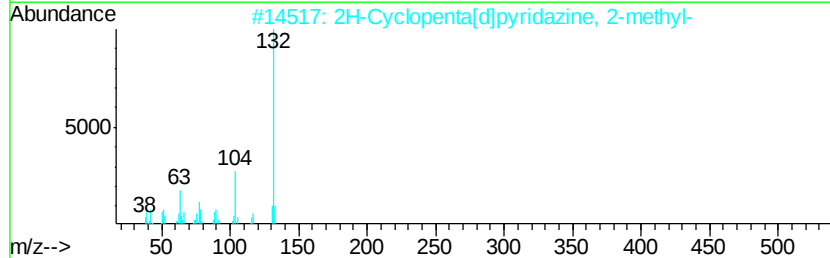
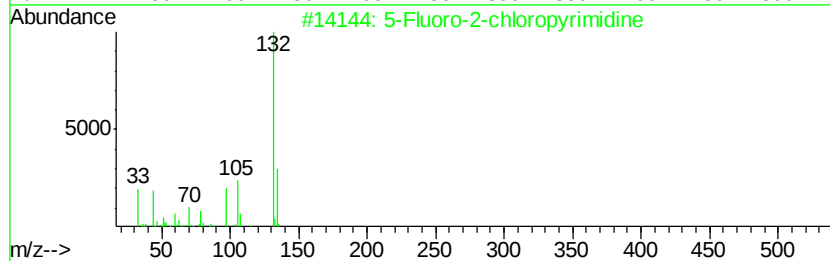
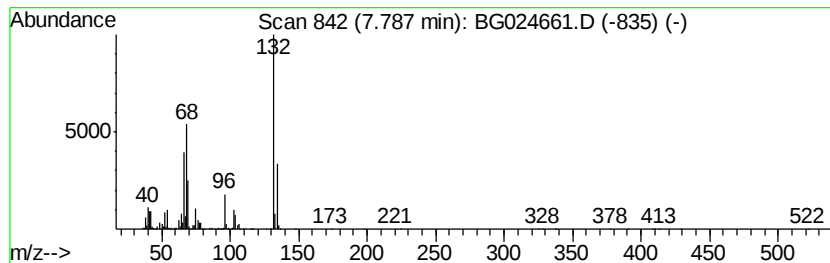
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Peak Number 3 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	107.39 ng	3485330	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
2		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	14
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14



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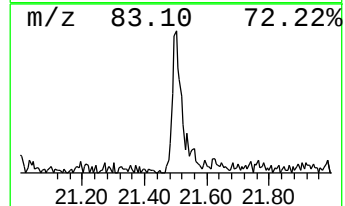
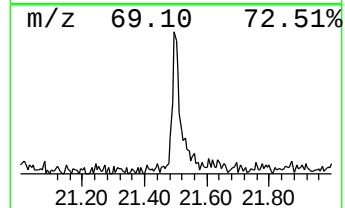
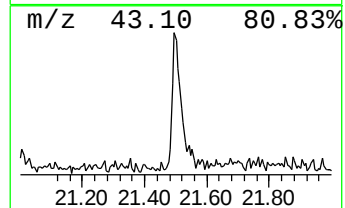
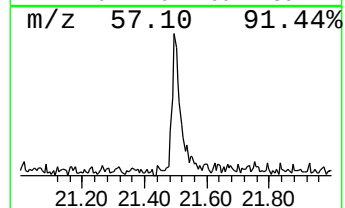
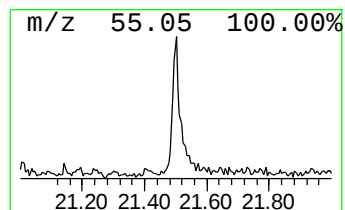
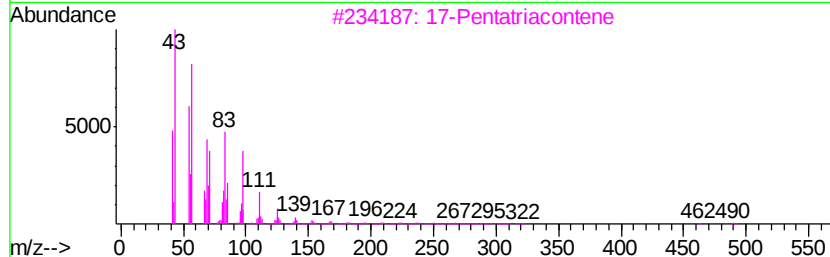
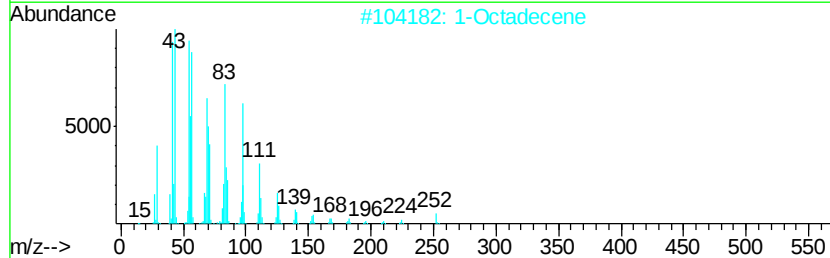
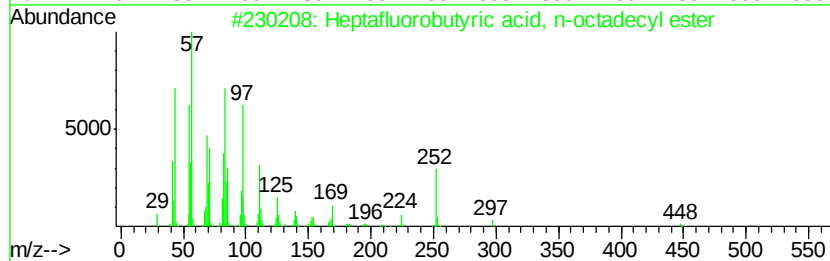
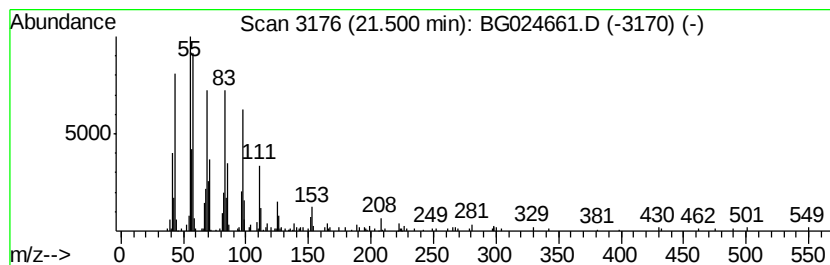
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Peak Number 5 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	2.87 ng	343317	Chrysene-d12	21.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
2		1-Octadecene	252	C18H36	000112-88-9	90
3		17-Pentatriacontene	491	C35H70	006971-40-0	90
4		Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	87
5		Cyclooctacosane	392	C28H56	000297-24-5	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	3.12	423.9	ng	13758000	1	8.27	649126	20.0
2-Pentanone, 4-hy...	5.33	22.2	ng	721044	1	8.27	649126	20.0
unknown7.79	7.79	107.4	ng	3485330	1	8.27	649126	20.0
Heptafluorobutyri...	21.50	2.9	ng	343317	5	21.92	2394980	20.0