

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024679.D
Acq On : 4 Nov 2016 12:44
Operator : UM/SJ
Sample : H5502-22
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-89-17.5-18.0

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-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	3.126	43	49	69	rVB	7505086	12583763	100.00%	21.943%
2	5.330	417	424	433	rBV	415560	675912	5.37%	1.179%
3	5.800	497	504	514	rVB	1923685	3231372	25.68%	5.635%
4	7.404	769	777	788	rBV	1988583	3597745	28.59%	6.274%
5	7.791	833	843	851	rBV	1893238	3353951	26.65%	5.849%
6	8.267	918	924	934	rVB	399267	702599	5.58%	1.225%
7	8.590	971	979	987	rVB	1334111	2427944	19.29%	4.234%
8	9.442	1116	1124	1134	rVB	1226162	2243893	17.83%	3.913%
9	11.093	1394	1405	1411	rBV	508994	937839	7.45%	1.635%
10	13.508	1806	1816	1823	rBV	2828358	4437740	35.27%	7.738%
11	14.319	1948	1954	1960	rVB	654961	985329	7.83%	1.718%
12	14.883	2043	2050	2057	rVB	858511	1340547	10.65%	2.338%
13	16.364	2295	2302	2312	rBV	3020713	4748660	37.74%	8.281%
14	17.621	2508	2516	2524	rBV2	1214938	1932538	15.36%	3.370%
15	18.467	2654	2660	2668	rBV3	96773	158302	1.26%	0.276%
16	19.865	2895	2898	2904	rVB2	157811	201031	1.60%	0.351%
17	20.206	2949	2956	2961	rBV	5829469	7900428	62.78%	13.777%
18	20.905	3071	3075	3081	rBV3	116511	141984	1.13%	0.248%
19	21.493	3170	3175	3184	rBV2	262163	467421	3.71%	0.815%
20	21.922	3241	3248	3257	rVB	1526713	2685926	21.34%	4.684%
21	25.353	3820	3832	3845	rVB2	835883	2591923	20.60%	4.520%

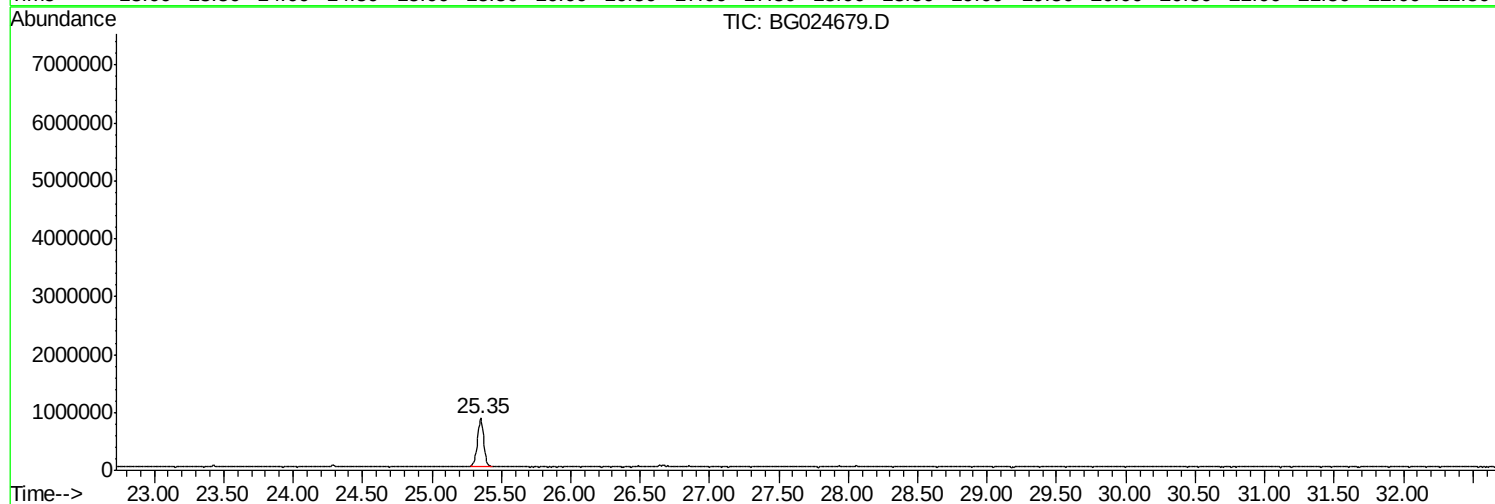
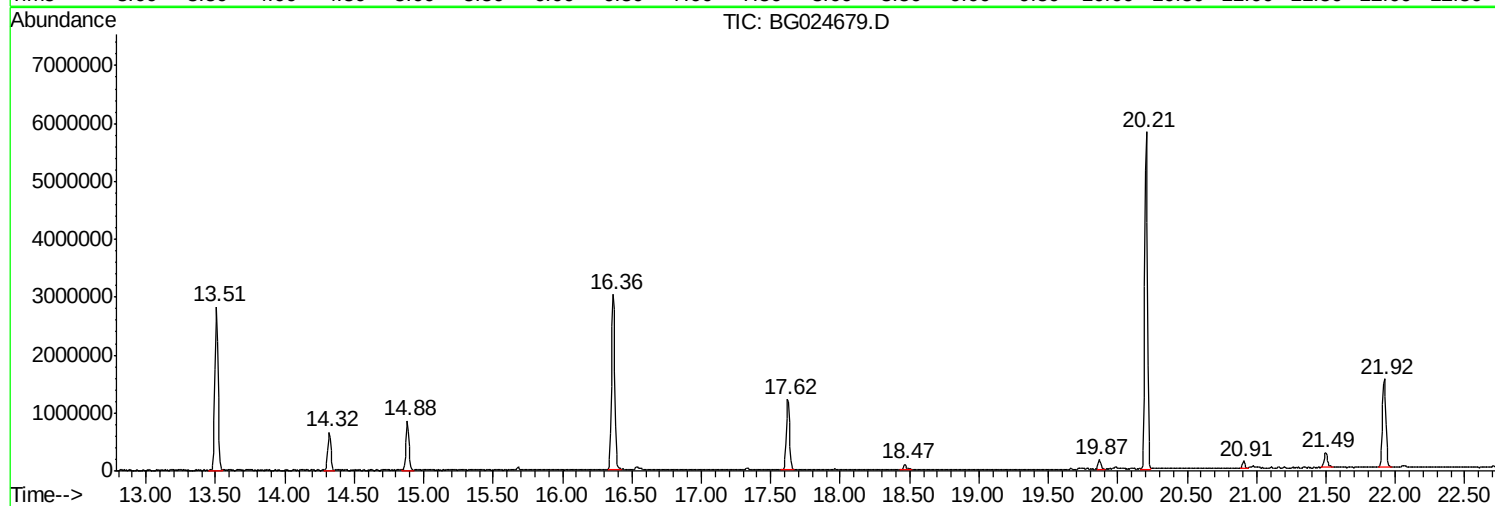
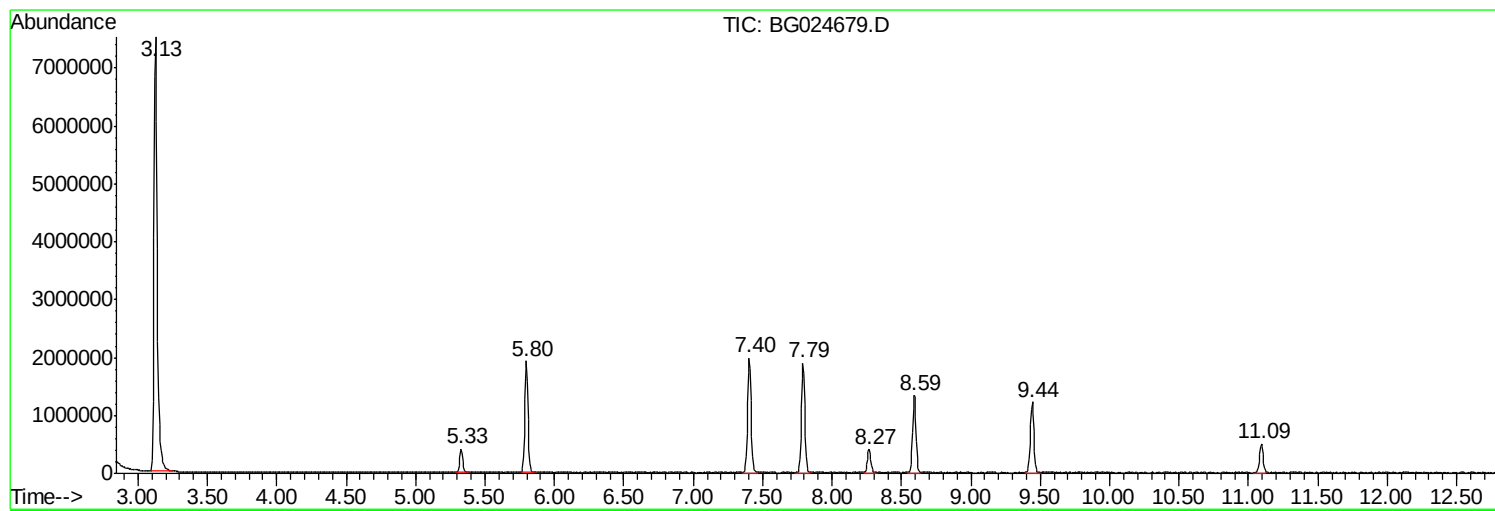
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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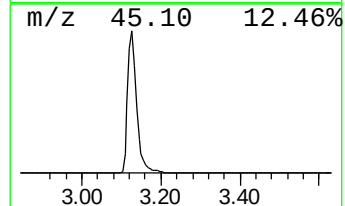
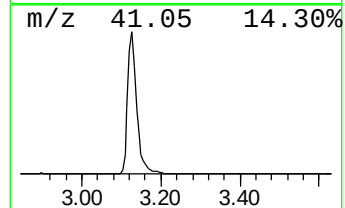
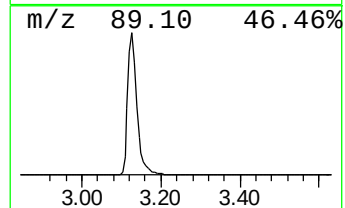
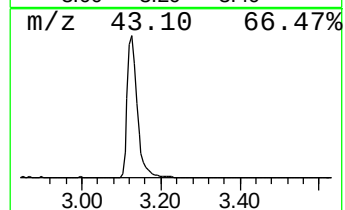
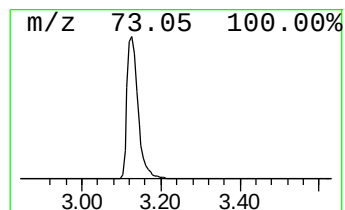
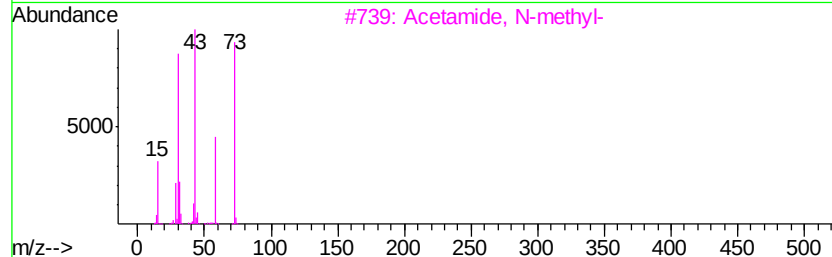
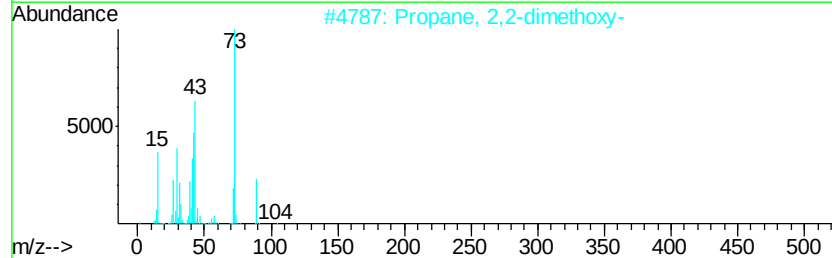
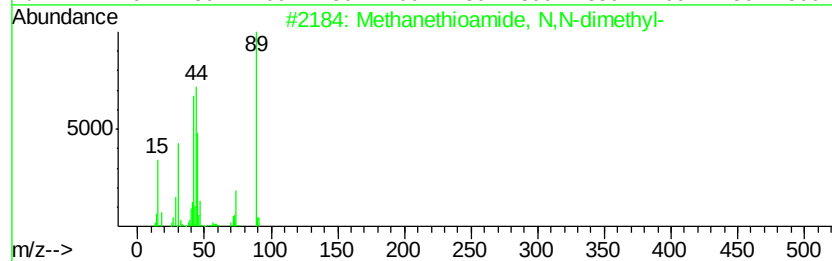
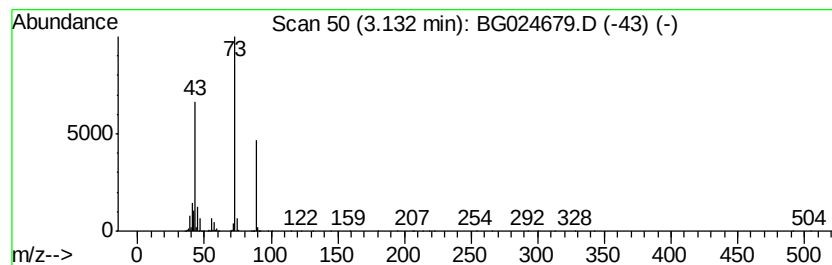
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	358.21 ng	12583800	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	42
2		Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	28
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	12
4		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
5		Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	9



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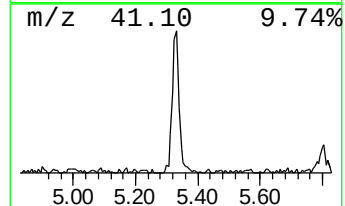
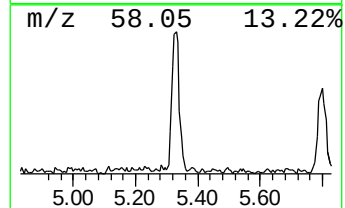
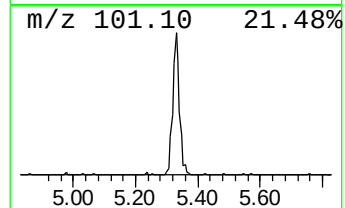
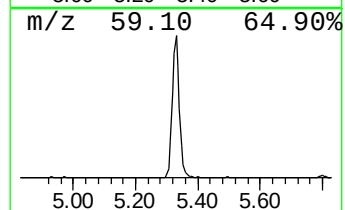
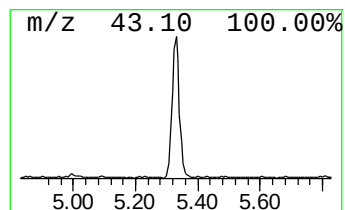
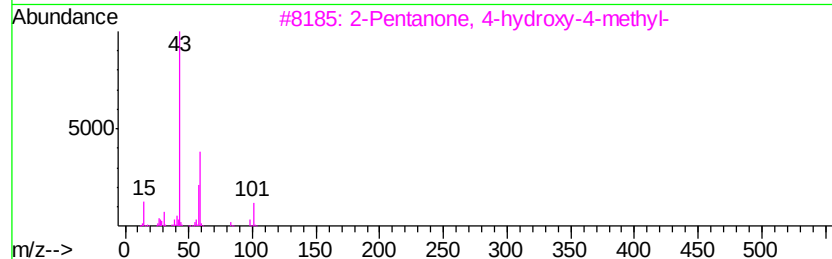
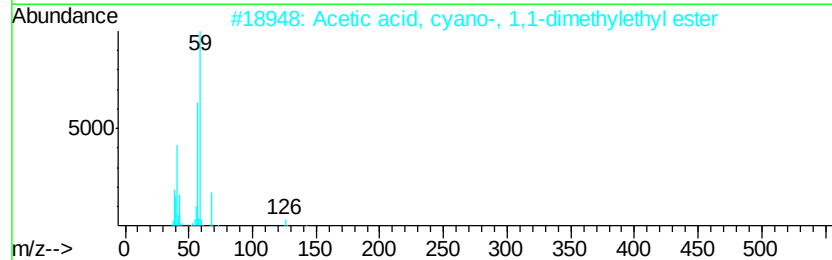
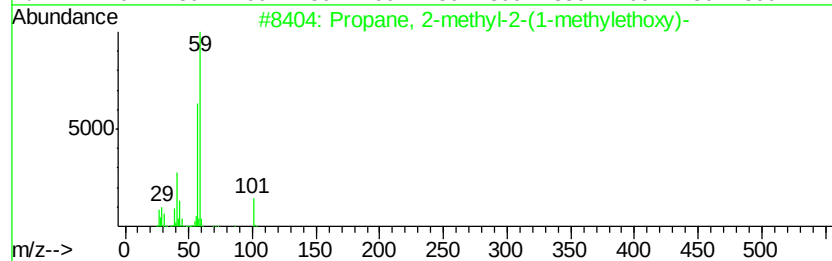
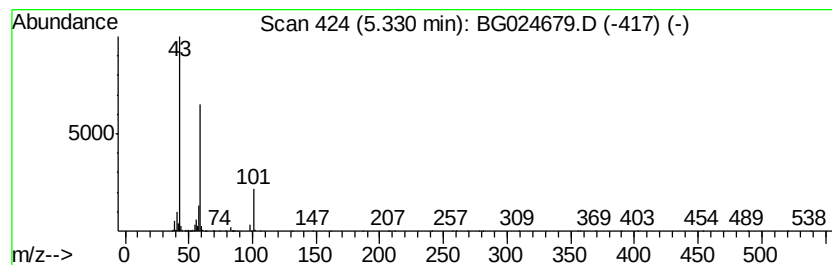
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propane, 2-methyl-2-(1-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	19.24 ng	675912	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5		4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	12



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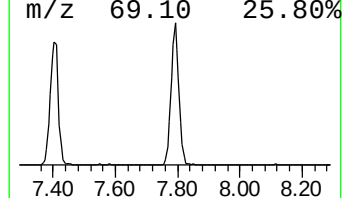
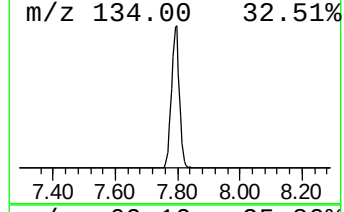
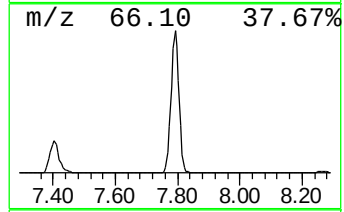
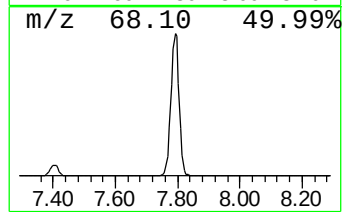
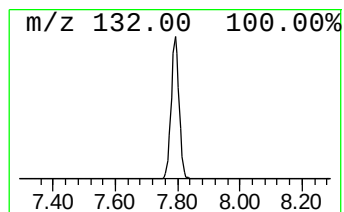
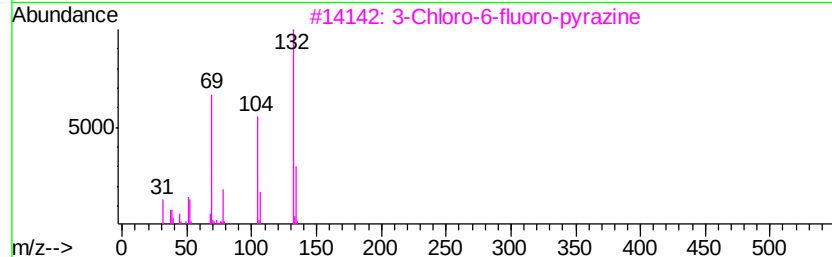
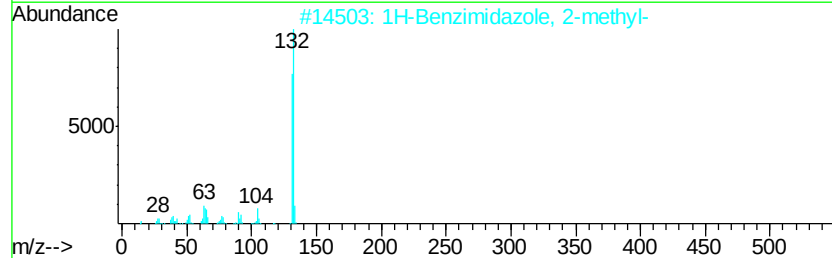
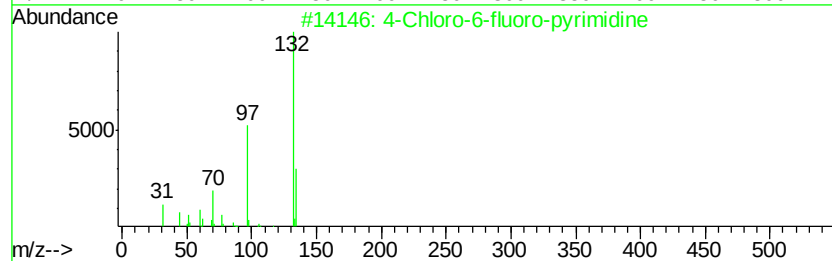
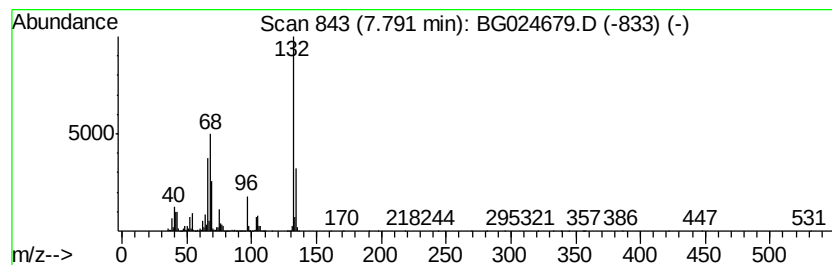
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Peak Number 3 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	95.47 ng	3353950	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14



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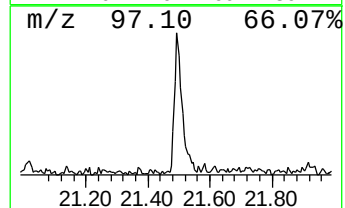
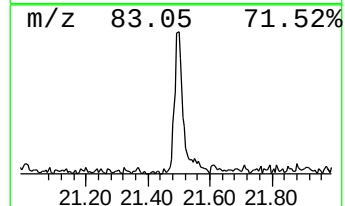
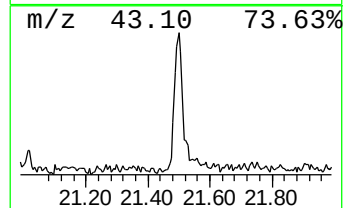
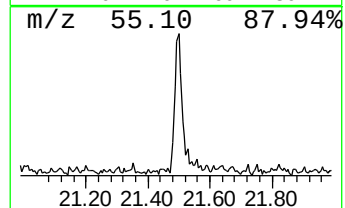
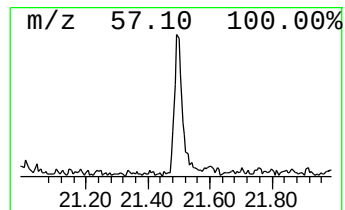
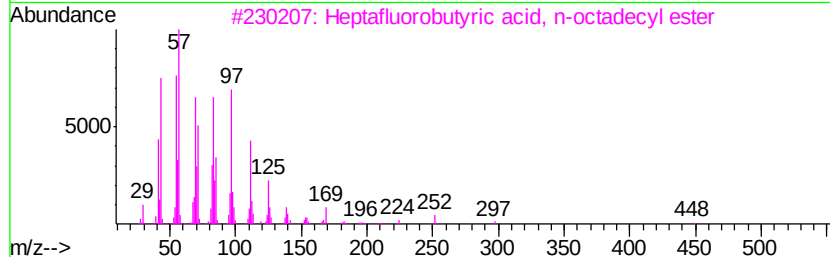
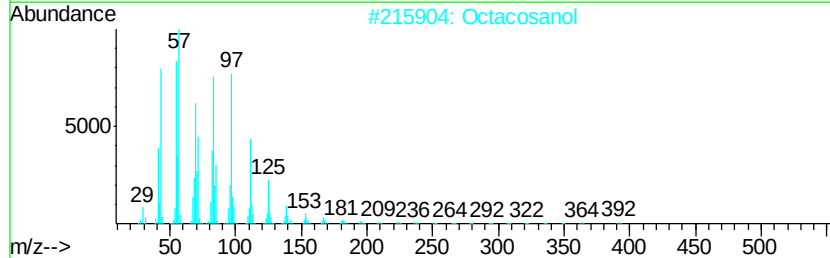
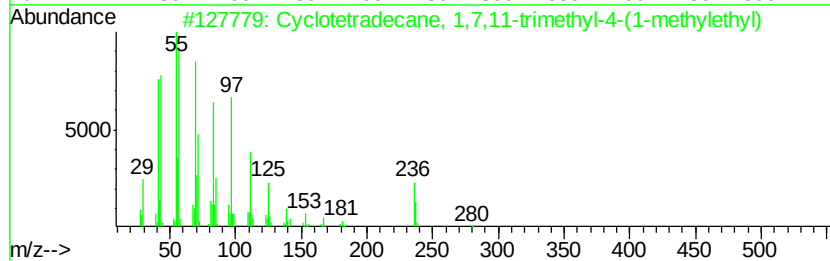
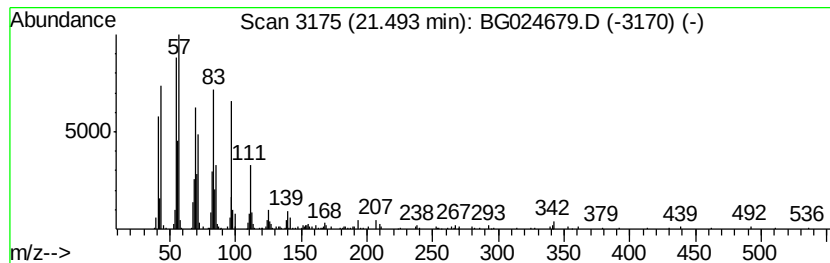
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclotetradecane, 1,7,11-tr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.49	3.48 ng	467421	Chrysene-d12	21.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane, 1,7,11-trimeth...	280	C20H40	001786-12-5	93
2	Octacosanol	410	C28H58O	000557-61-9	91
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5	Octadecane, 1-(ethenyl)-	296	C20H40O	000930-02-9	89



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Propane, 2-methyl...	5.33	19.2	ng	675912	1	8.27	702599	20.0
unknown7.79	7.79	95.5	ng	3353950	1	8.27	702599	20.0
Cyclotetradecane,...	21.49	3.5	ng	467421	5	21.92	2685930	20.0