

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071416\
 Data File : BG023105.D
 Acq On : 14 Jul 2016 17:32
 Operator : UM/SJ
 Sample : H3996-25
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 D8-B1(5-11)C

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-BG070816.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	3.040	29	34	53	rBV	6600893	10158450	100.00%	14.959%
2	5.226	399	406	412	rBV	257654	399875	3.94%	0.589%
3	5.702	478	487	498	rBV	2233767	3650184	35.93%	5.375%
4	7.311	753	761	772	rBV	2616782	4636201	45.64%	6.827%
5	7.687	815	825	835	rBV	2328796	4151123	40.86%	6.113%
6	8.152	898	904	912	rVV2	445906	774233	7.62%	1.140%
7	8.481	953	960	967	rVB	1579410	2766155	27.23%	4.073%
8	9.327	1096	1104	1115	rBV	1640736	2940961	28.95%	4.331%
9	10.984	1378	1386	1394	rBV	691995	1293524	12.73%	1.905%
10	13.416	1792	1800	1813	rBV	4211380	6925430	68.17%	10.198%
11	14.239	1934	1940	1947	rBV	814158	1203860	11.85%	1.773%
12	14.803	2028	2036	2045	rBV2	1326223	2212625	21.78%	3.258%
13	16.289	2282	2289	2303	rBV	4293726	6845456	67.39%	10.081%
14	17.276	2453	2457	2461	rBV	117613	140837	1.39%	0.207%
15	17.552	2497	2504	2514	rBV	1735154	2743333	27.01%	4.040%
16	18.016	2579	2583	2589	rVB2	105289	127858	1.26%	0.188%
17	18.416	2646	2651	2656	rBV2	244716	346357	3.41%	0.510%
18	19.679	2861	2866	2871	rBV7	65971	113613	1.12%	0.167%
19	19.903	2901	2904	2908	rVB3	92303	103065	1.01%	0.152%
20	20.155	2941	2947	2953	rBV	7276338	9423878	92.77%	13.878%
21	20.431	2992	2994	2999	rVB2	105773	120596	1.19%	0.178%
22	21.465	3165	3170	3180	rBV6	116455	284891	2.80%	0.420%
23	21.712	3208	3212	3218	rVB	209913	286789	2.82%	0.422%
24	21.859	3229	3237	3245	rBV	1763507	3064820	30.17%	4.513%
25	23.375	3489	3495	3506	rVB4	179568	362269	3.57%	0.533%
26	25.237	3800	3812	3824	rBV2	899570	2831083	27.87%	4.169%

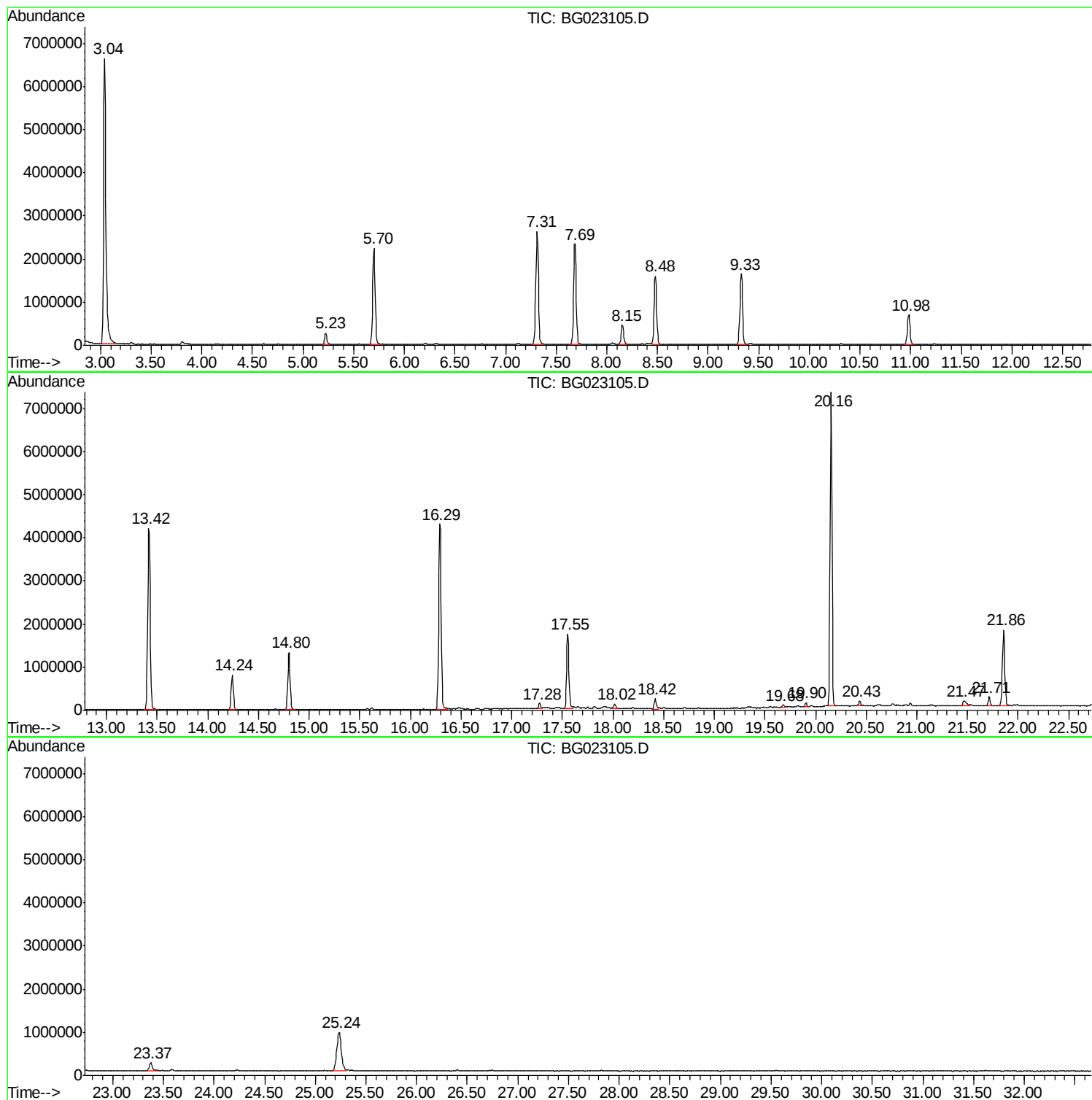
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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ClientSampleId :
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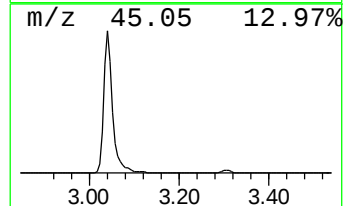
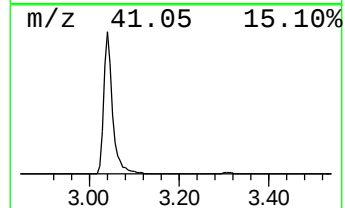
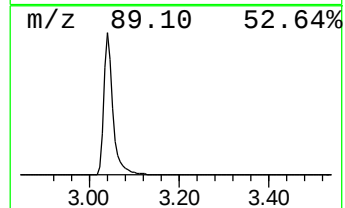
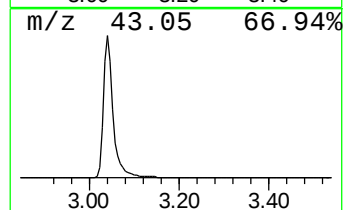
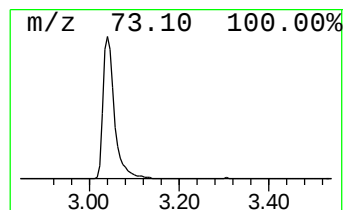
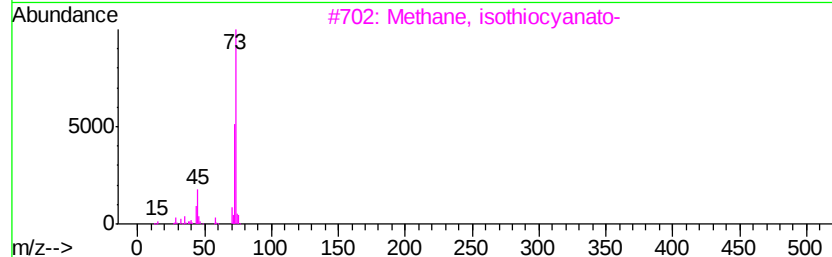
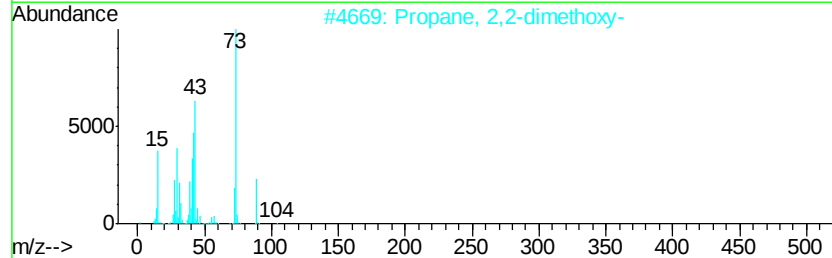
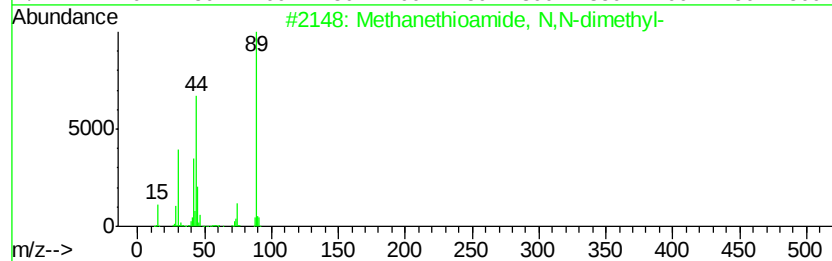
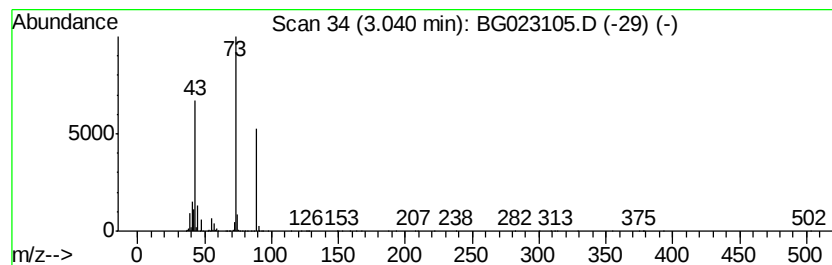
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	262.41 ng	10158500	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	47
2		Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	25
3		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9



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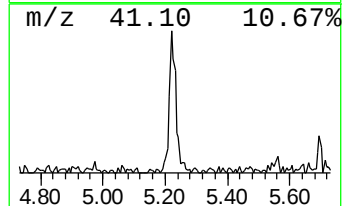
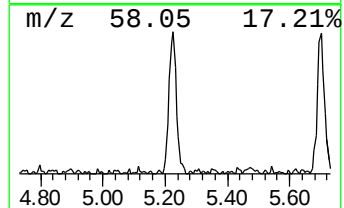
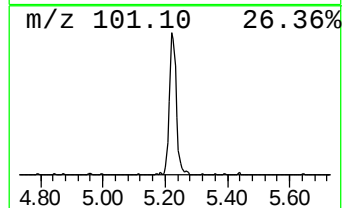
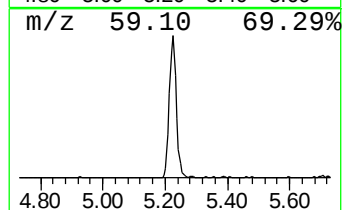
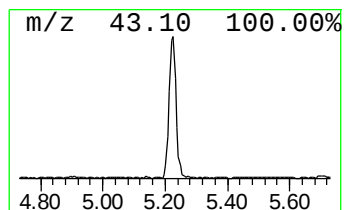
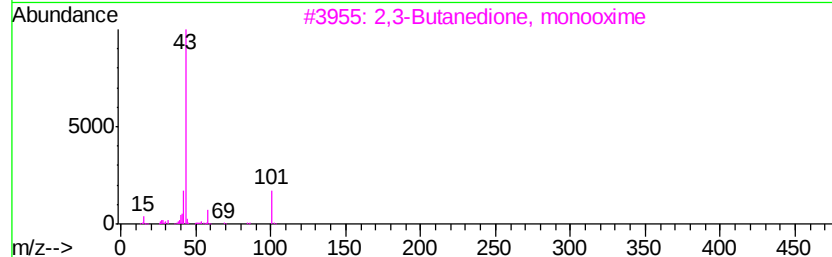
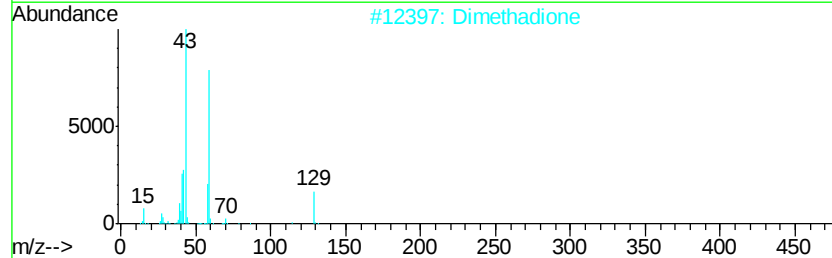
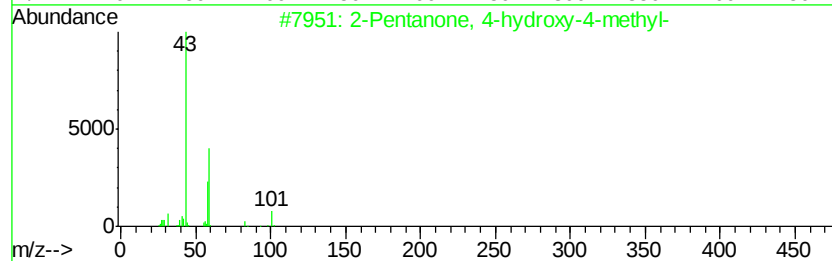
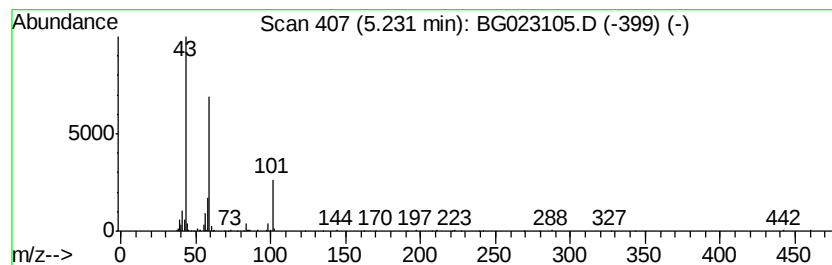
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	10.33 ng	399875	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Dimethadione	129	C5H7NO3	000695-53-4	33
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	25
5		Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	17



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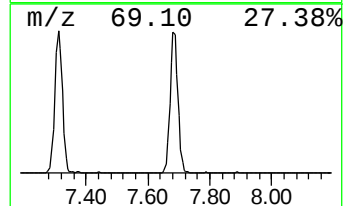
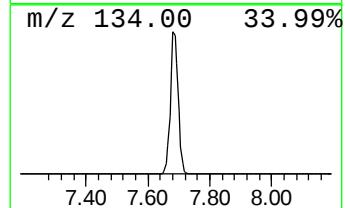
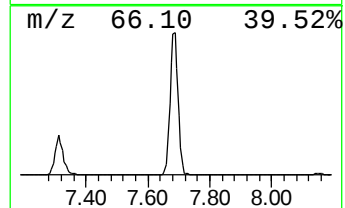
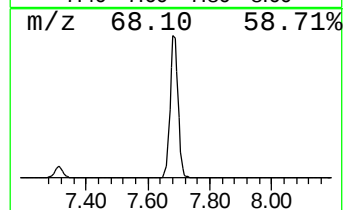
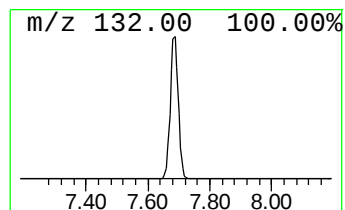
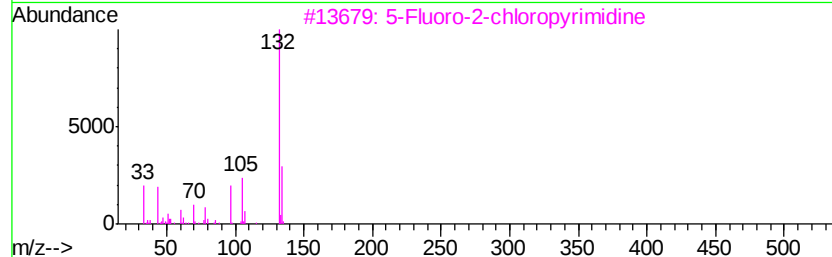
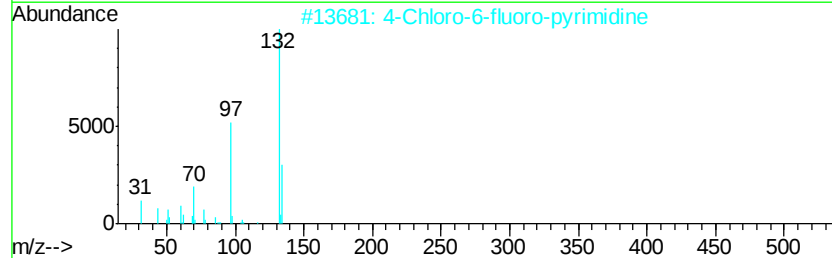
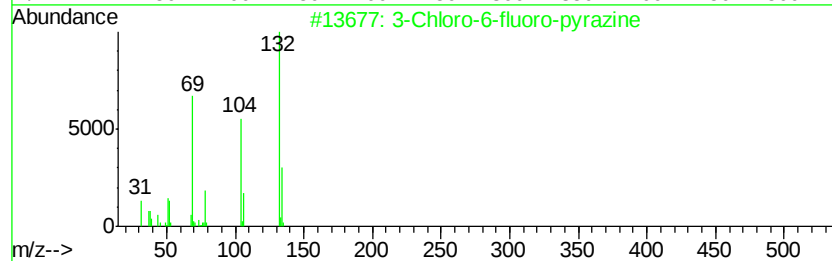
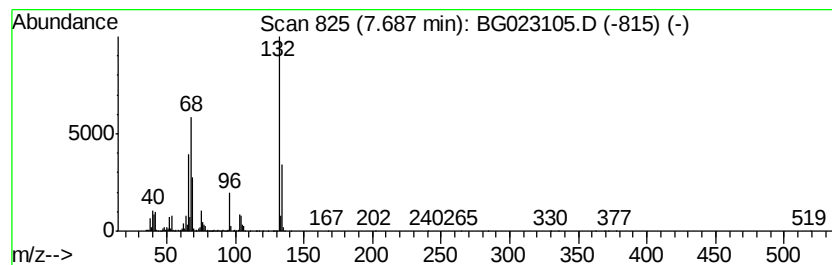
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Peak Number 3 unknown7.69 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	107.23 ng	4151120	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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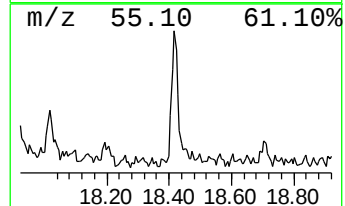
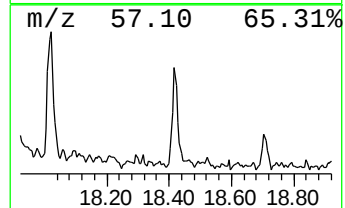
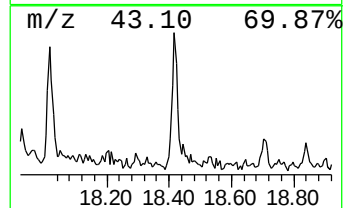
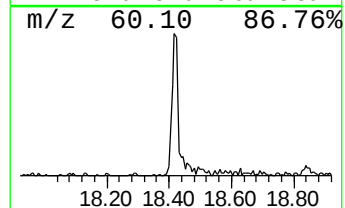
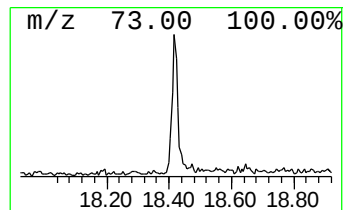
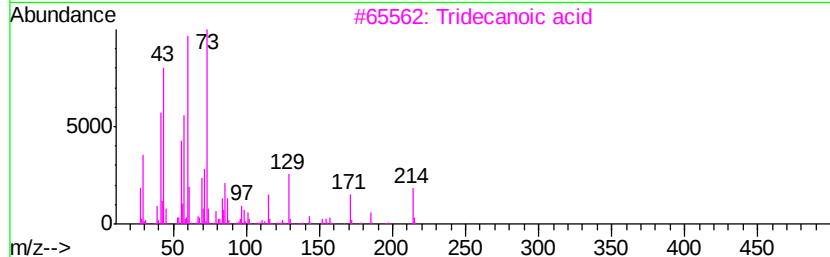
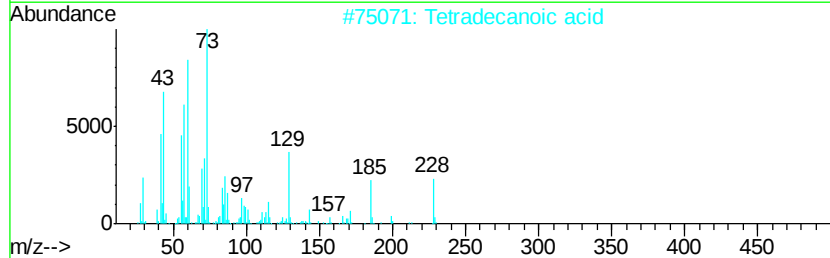
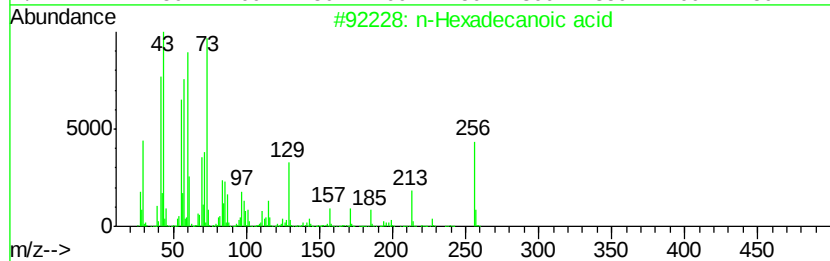
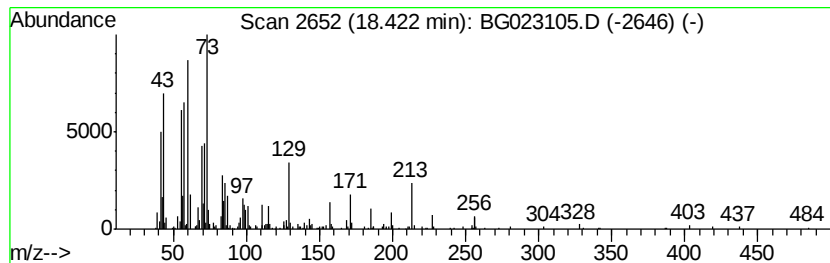
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.42	2.53 ng	346357	Phenanthrene-d10	17.55	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	.alpha.-d-6,3-Furanose, methyl-....	192	C7H12O6	1000149-62-6	59



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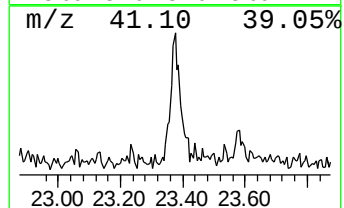
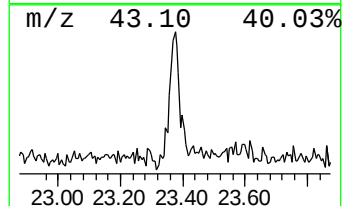
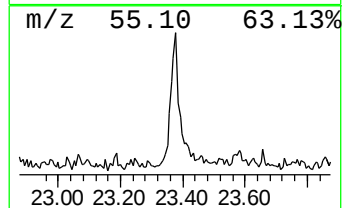
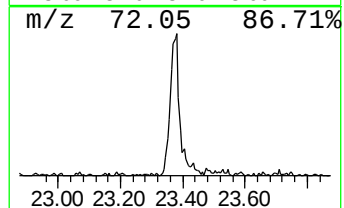
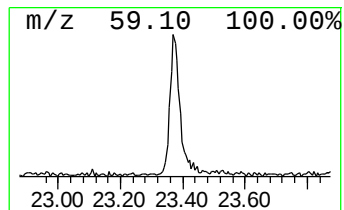
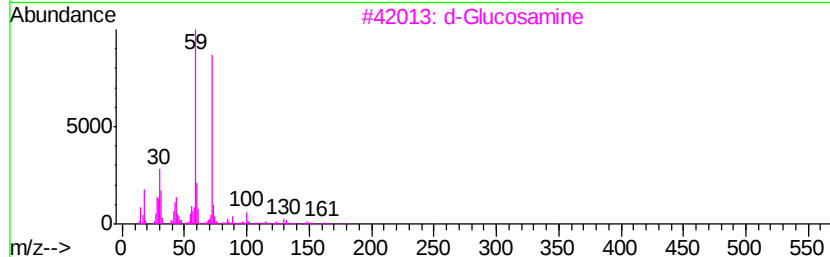
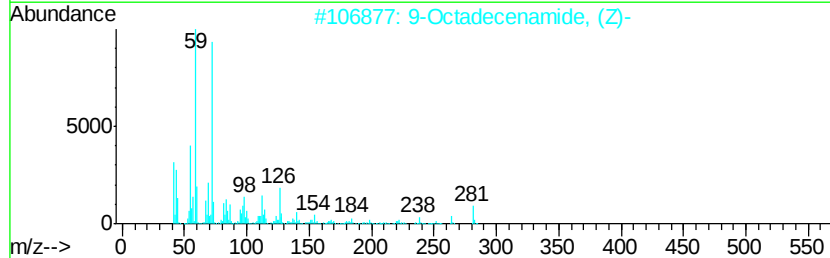
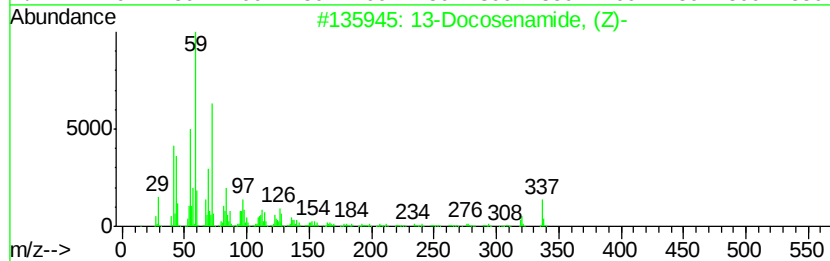
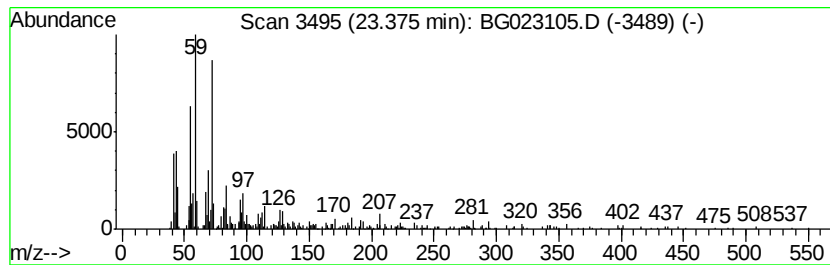
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.37	2.36 ng	362269	Chrysene-d12	21.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	86
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
3		d-Glucosamine	179	C6H13NO5	000090-77-7	72
4		3-Cyclohexylpropionamide	155	C9H17NO	004361-29-9	47
5		Dodecanamide	199	C12H25NO	001120-16-7	46



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.04	3.04	262.4	ng	10158500	1	8.16	774233	20.0
2-Pentanone, 4-hy...	5.23	10.3	ng	399875	1	8.16	774233	20.0
unknown7.69	7.69	107.2	ng	4151120	1	8.16	774233	20.0
n-Hexadecanoic acid	18.42	2.5	ng	346357	4	17.55	2743330	20.0
13-Docosenamide, ...	23.37	2.4	ng	362269	5	21.86	3064820	20.0