

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
 Data File : BG016445.D
 Acq On : 16 Apr 2015 6:01
 Operator : TP/IZ
 Sample : G1829-15
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FB

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-BG040615.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	2.758	7	12	21	rBV	346018	574245	12.28%	2.290%
2	2.840	21	26	38	rVB	388772	525015	11.23%	2.094%
3	4.779	350	356	363	rBV2	50195	74469	1.59%	0.297%
4	5.255	431	437	445	rBV	612375	876901	18.75%	3.497%
5	6.853	703	709	721	rVB	389044	586983	12.55%	2.341%
6	7.206	761	769	777	rBV	1253597	1944916	41.60%	7.756%
7	7.664	841	847	855	rBV	296260	451703	9.66%	1.801%
8	7.981	892	901	909	rBV	1091837	1751212	37.45%	6.983%
9	8.822	1037	1044	1052	rBV	904048	1460869	31.24%	5.825%
10	10.449	1315	1321	1328	rVB	423301	703952	15.06%	2.807%
11	12.928	1736	1743	1751	rBV	2404350	3460239	74.00%	13.798%
12	14.309	1972	1978	1989	rVB2	659601	979837	20.96%	3.907%
13	14.738	2047	2051	2058	rBV	53901	77589	1.66%	0.309%
14	15.802	2225	2232	2246	rBV	1700653	2444987	52.29%	9.750%
15	16.953	2423	2428	2438	rBV2	23585	47520	1.02%	0.189%
16	17.047	2438	2444	2453	rBV2	869181	1232383	26.36%	4.914%
17	17.946	2594	2597	2606	rBV4	36399	63156	1.35%	0.252%
18	18.469	2681	2686	2697	rBV	167214	239968	5.13%	0.957%
19	19.233	2812	2816	2821	rBV2	37654	62932	1.35%	0.251%
20	19.679	2885	2892	2897	rBV	3716002	4675725	100.00%	18.645%
21	20.384	3008	3012	3017	rBV5	45102	55283	1.18%	0.220%
22	20.731	3067	3071	3076	rBV	214732	227663	4.87%	0.908%
23	21.230	3150	3156	3161	rBV	967967	1262920	27.01%	5.036%
24	21.753	3243	3245	3251	rVB4	58312	88482	1.89%	0.353%
25	23.457	3528	3535	3544	rBV	664831	1208429	25.84%	4.819%

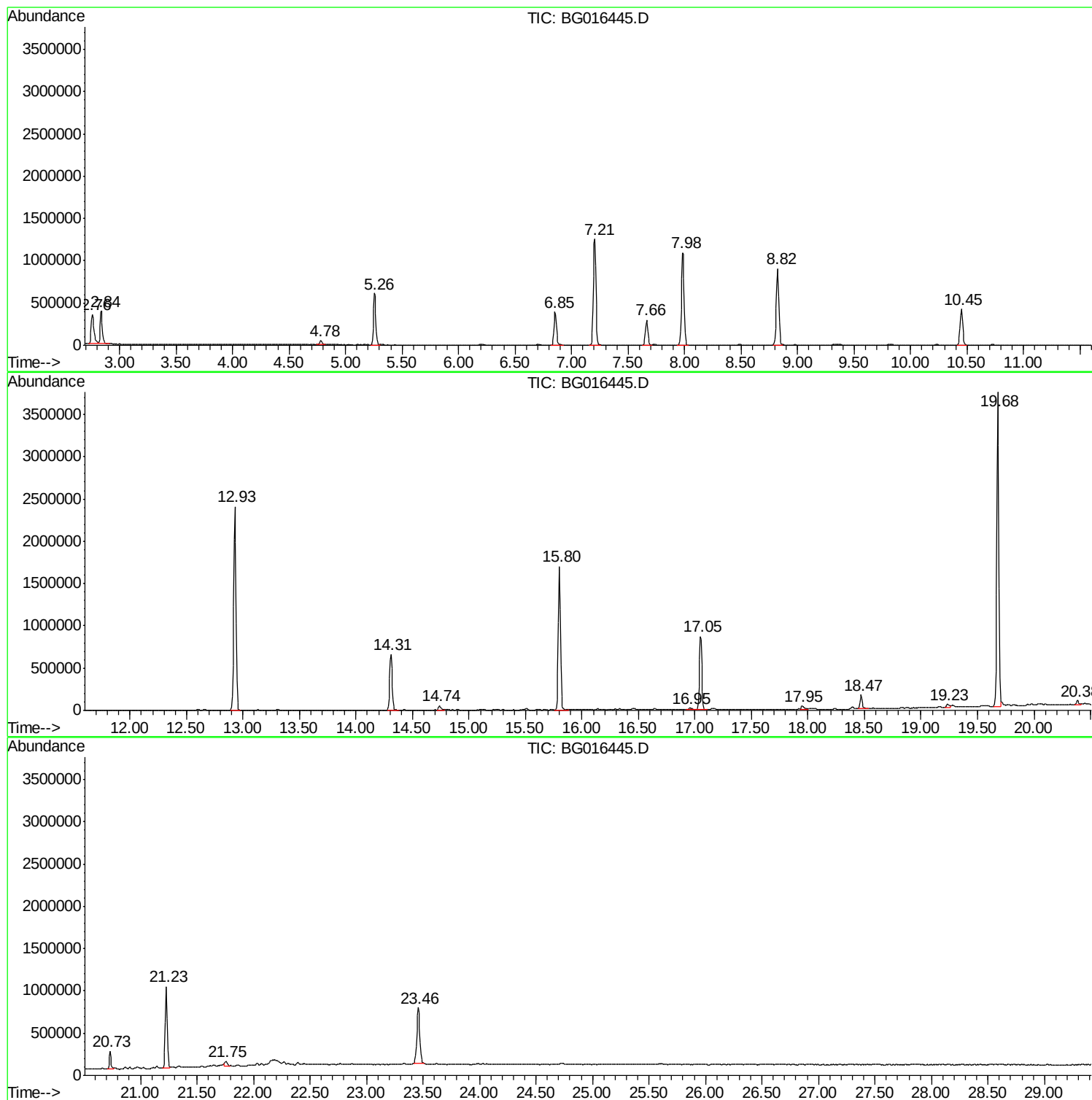
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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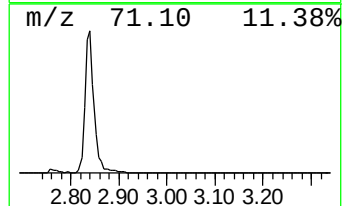
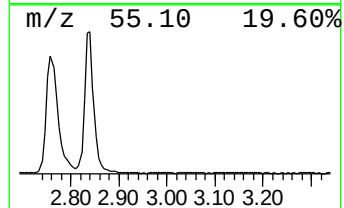
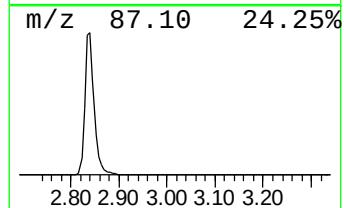
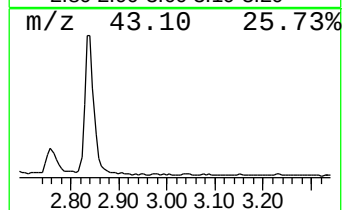
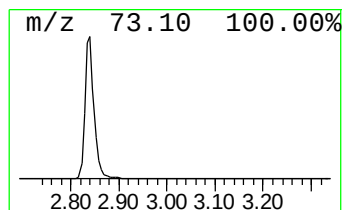
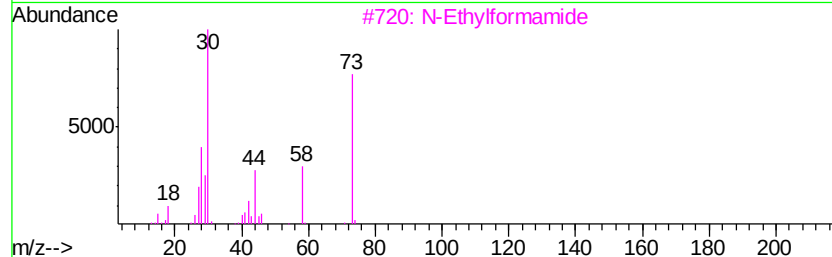
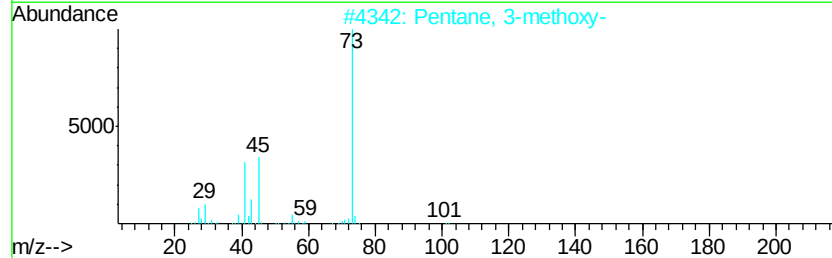
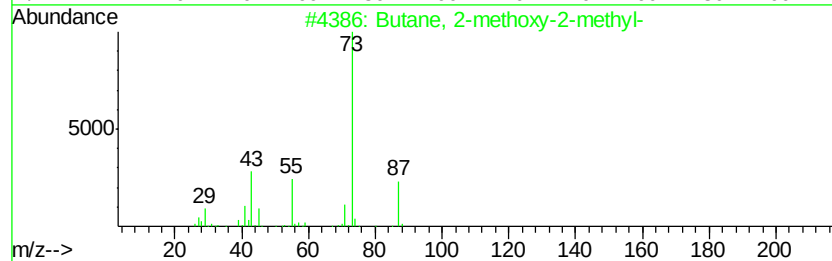
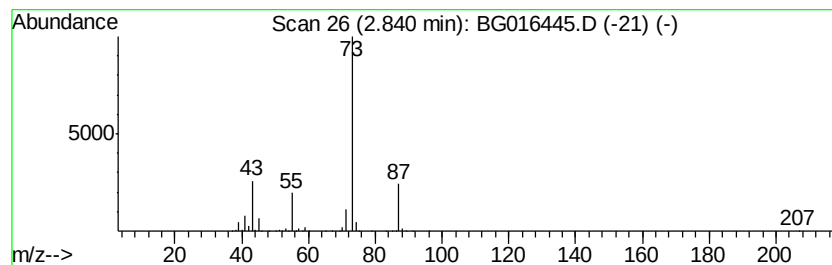
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
2.84	23.25 ng	525015	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7



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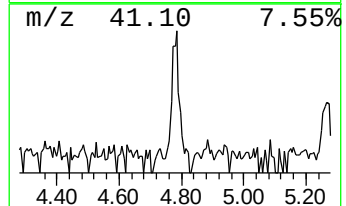
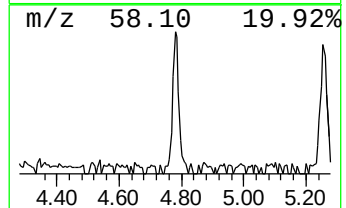
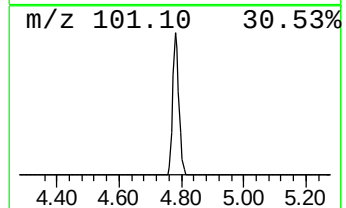
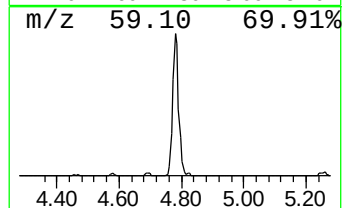
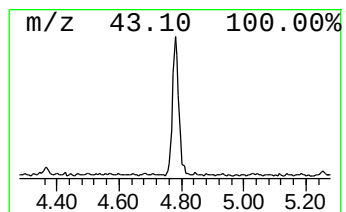
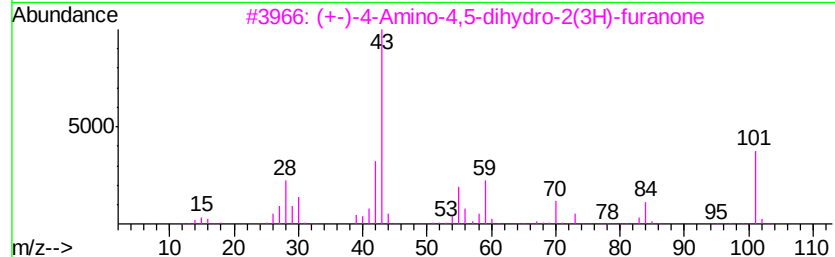
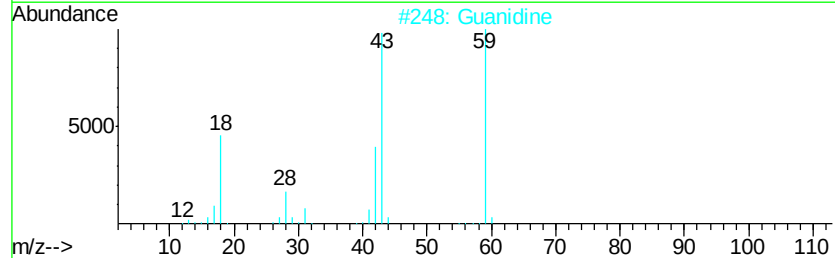
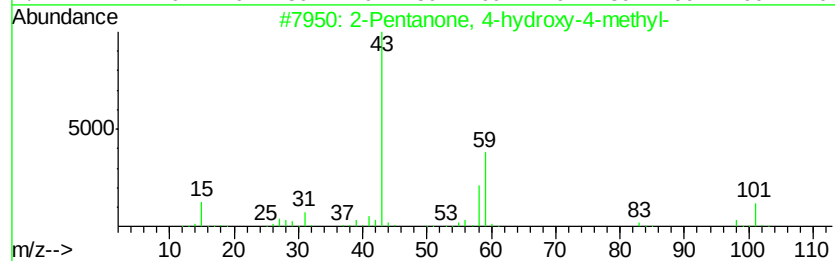
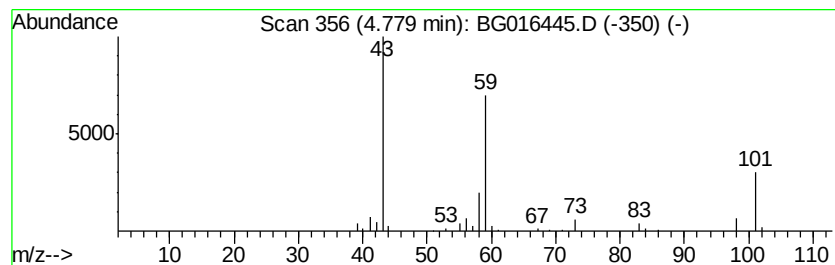
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	3.30 ng	74469	1,4-Dichlorobenzene-d4	7.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42	
2	Guanidine	59	CH5N3	000113-00-8	38	
3	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	37	
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	27	
5	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	25	



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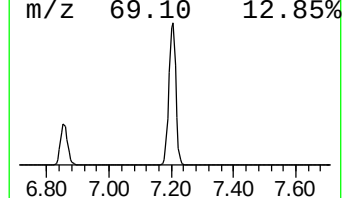
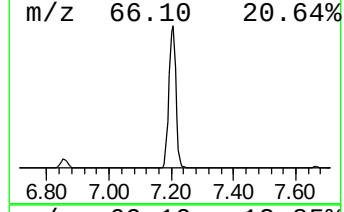
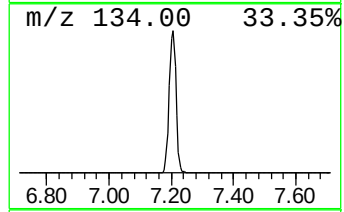
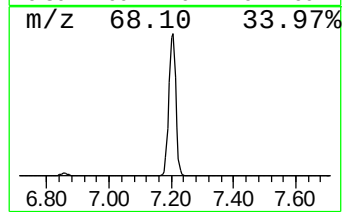
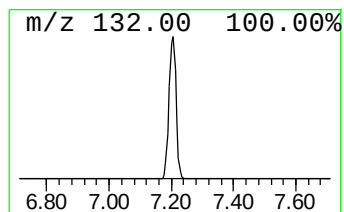
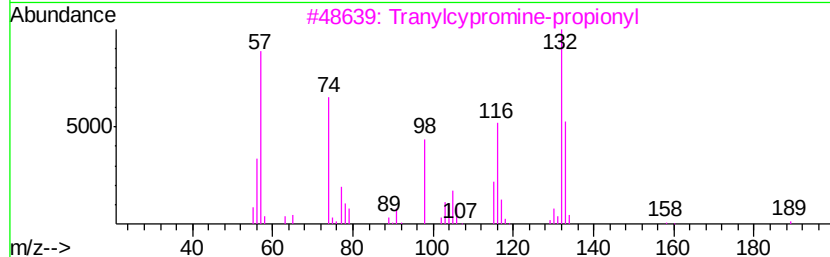
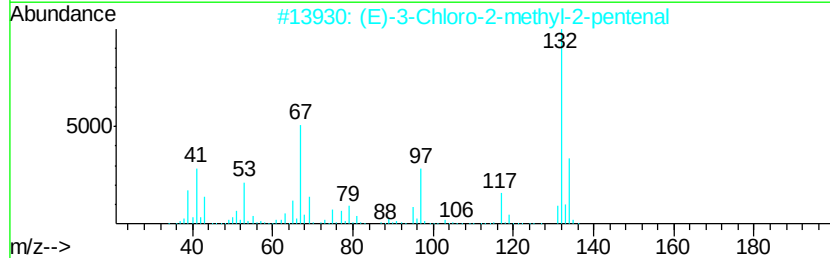
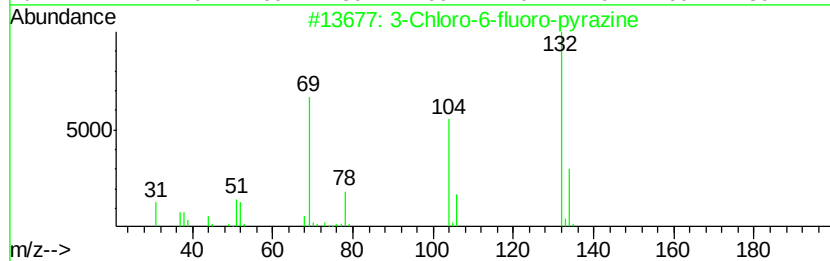
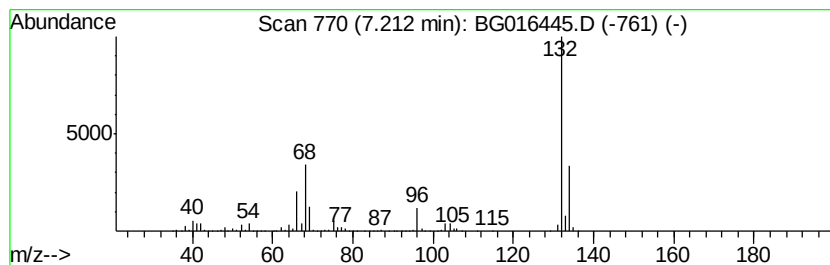
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TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	86.11 ng	1944920	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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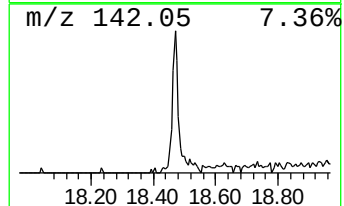
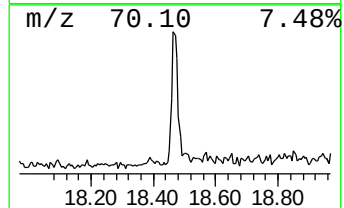
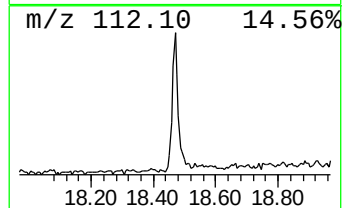
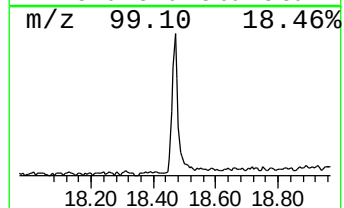
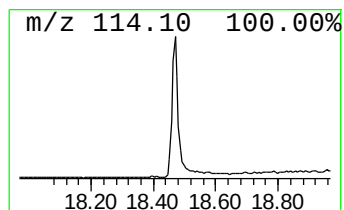
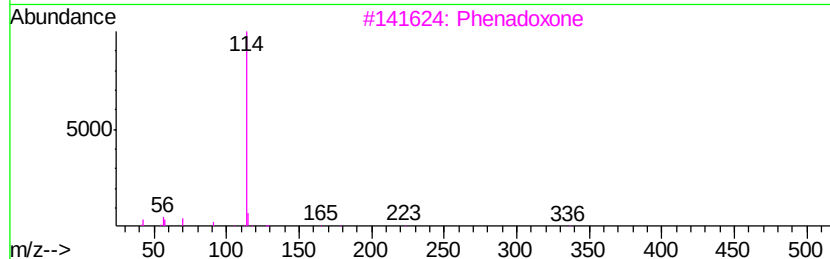
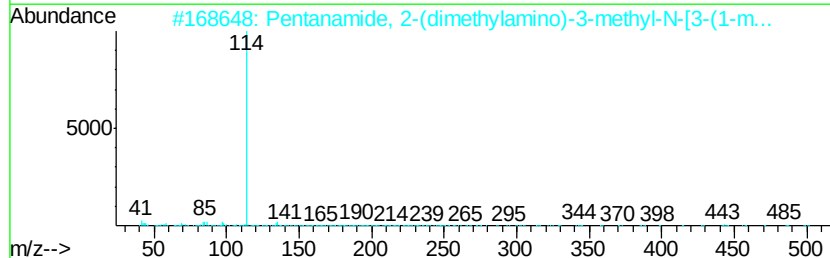
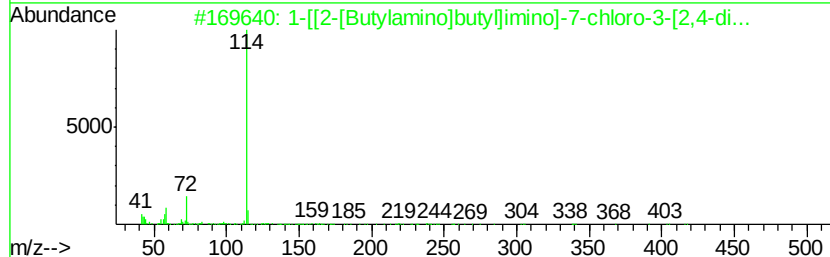
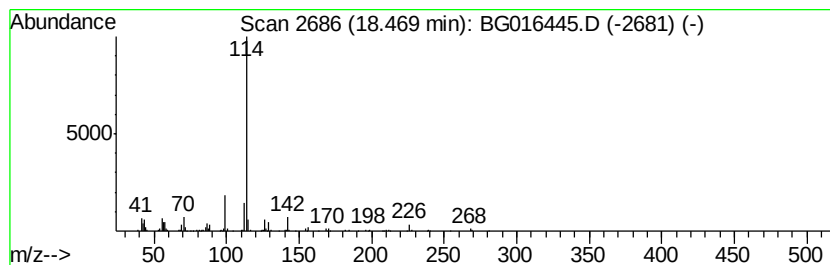
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-[[2-[Butylamino]butyl]imi... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.47	3.89 ng	239968	Phenanthrene-d10	17.05	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-[[2-[Butylamino]butyl]imino]-7...	517	C27H30Cl3N3O	144155-60-2	50
2	Pentanamide, 2-(dimethylamino)-3...	500	C28H44N4O4	025350-22-5	38
3	Phenadoxone	351	C23H29N02	000467-84-5	38
4	2H-[1,2,3]Triazole, 4-nitro-	114	C2H2N4O2	014544-45-7	38
5	Pentanamide, 2-(dimethylamino)-4...	631	C36H49N5O5	038496-01-4	38



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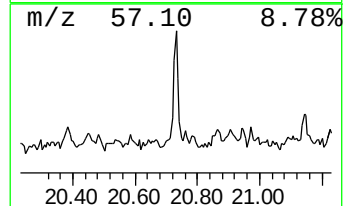
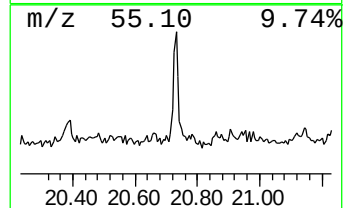
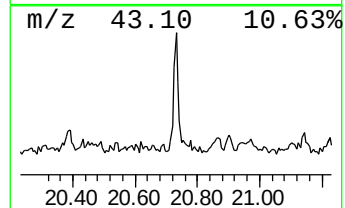
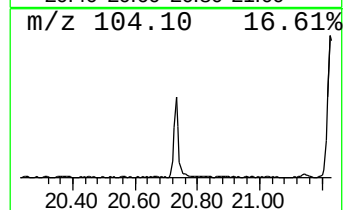
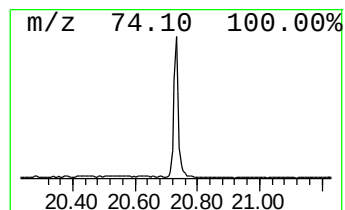
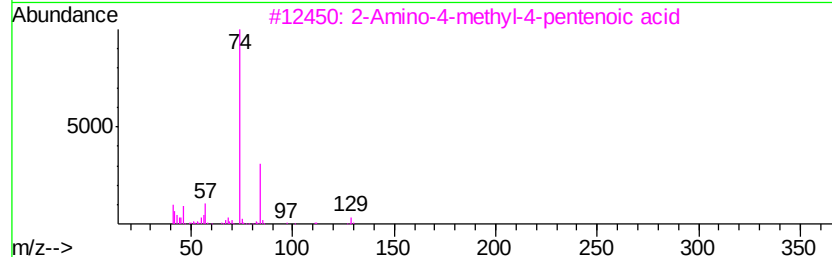
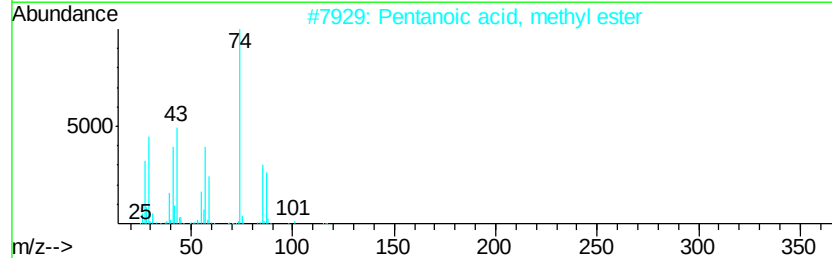
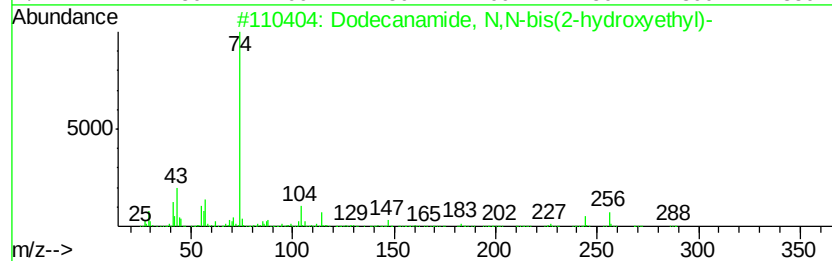
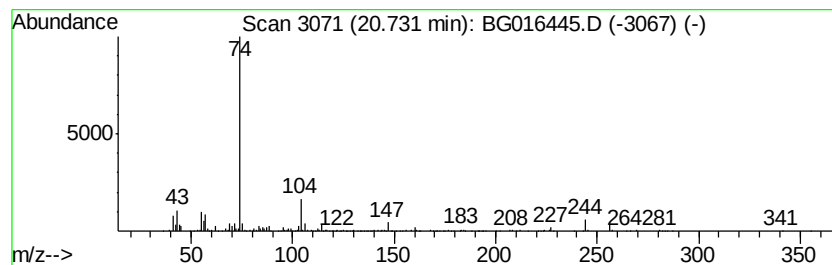
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 Dodecanamide, N,N-bis(2-hyd... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.73	3.61 ng	227663	Chrysene-d12	21.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecanamide, N,N-bis(2-hydroxye...	287	C16H33N03	000120-40-1	90
2		Pentanoic acid, methyl ester	116	C6H12O2	000624-24-8	33
3		2-Amino-4-methyl-4-pentenoic acid	129	C6H11N02	1000133-00-5	33
4		Butanoic acid, 3-methyl-, methyl...	116	C6H12O2	000556-24-1	33
5		Diethanolamine	105	C4H11N02	000111-42-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.84	23.3	ng	525015	1	7.66	451703	20.0
2-Pentanone, 4-hy...	4.78	3.3	ng	74469	1	7.66	451703	20.0
unknown7.21	7.21	86.1	ng	1944920	1	7.66	451703	20.0
1-[[2-[Butylamino...	18.47	3.9	ng	239968	4	17.05	1232380	20.0
Dodecanamide, N,N...	20.73	3.6	ng	227663	5	21.23	1262920	20.0