

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052015\
 Data File : BG017225.D
 Acq On : 20 May 2015 21:14
 Operator : TP/IZ
 Sample : G2299-09
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EB-2015.05.17

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-BG051315.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	2.781	11	16	25	rBV	104144	182545	5.20%	1.157%
2	2.863	25	30	41	rVB	434031	617533	17.58%	3.915%
3	4.802	355	360	366	rVB	45394	65830	1.87%	0.417%
4	5.289	437	443	453	rVB	331092	479435	13.65%	3.039%
5	6.893	709	716	724	rVB	196912	305472	8.69%	1.936%
6	7.234	767	774	782	rBV	695776	1043008	29.69%	6.612%
7	7.693	846	852	859	rVB	176080	269625	7.67%	1.709%
8	8.010	900	906	913	rBV	607460	958718	27.29%	6.078%
9	8.850	1043	1049	1058	rBV	545959	895017	25.47%	5.674%
10	10.483	1321	1327	1334	rVB	217617	360893	10.27%	2.288%
11	12.969	1740	1750	1758	rBV	1281931	1893527	53.89%	12.003%
12	13.351	1810	1815	1822	rVB	49765	72996	2.08%	0.463%
13	14.349	1978	1985	1990	rBV2	340794	514677	14.65%	3.263%
14	14.391	1990	1992	1996	rVB	30181	35654	1.01%	0.226%
15	15.442	2164	2171	2176	rVB2	31143	41951	1.19%	0.266%
16	15.560	2182	2191	2196	rBV	284980	406281	11.56%	2.575%
17	15.848	2232	2240	2249	rBV	1234238	1794277	51.07%	11.374%
18	17.099	2447	2453	2461	rBV	504550	700710	19.94%	4.442%
19	19.731	2895	2901	2907	rBV	2816483	3513506	100.00%	22.273%
20	21.282	3160	3165	3171	rBV	694153	815192	23.20%	5.168%
21	23.545	3542	3550	3562	rBV	415758	808015	23.00%	5.122%

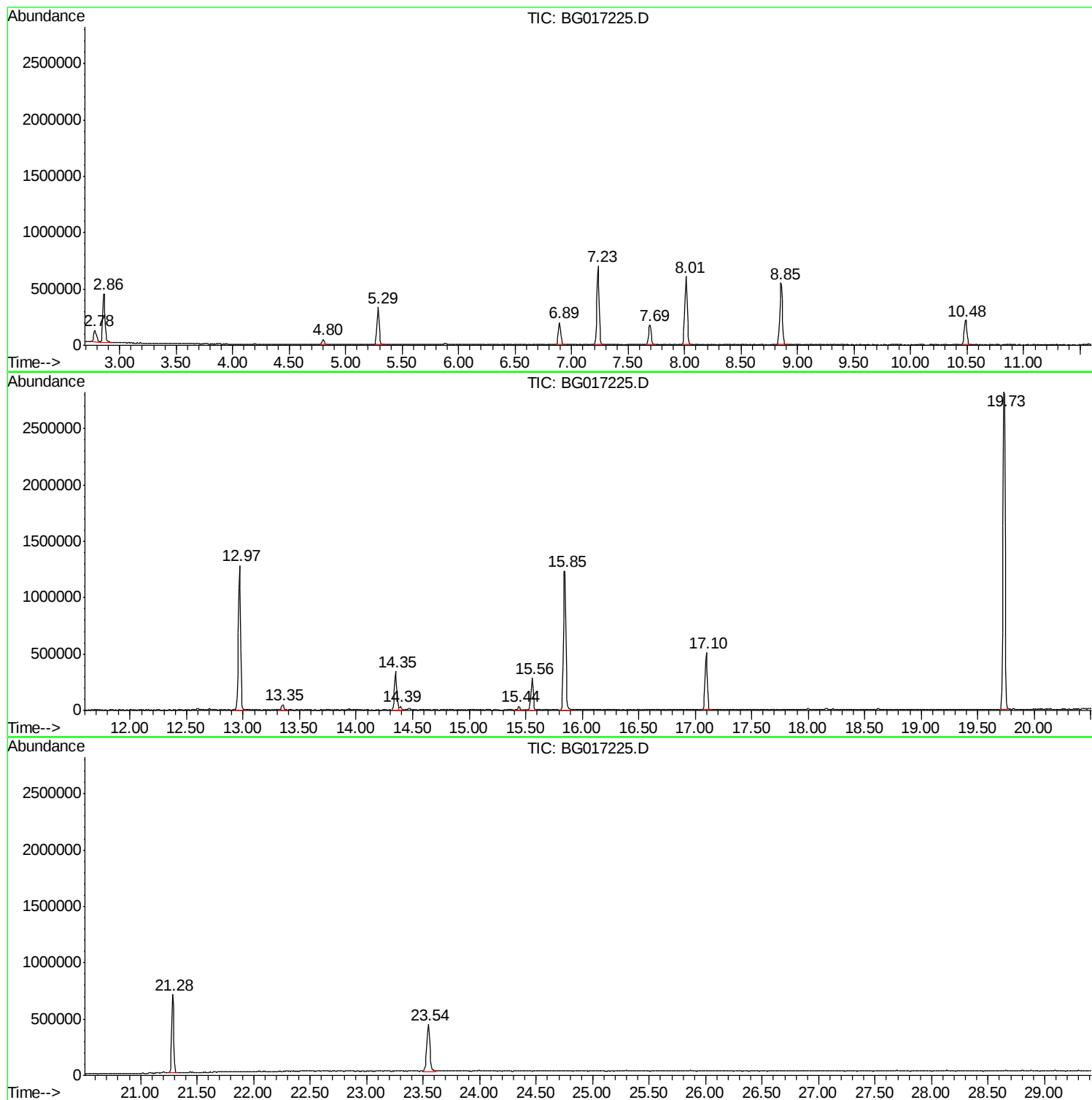
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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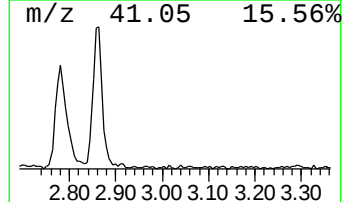
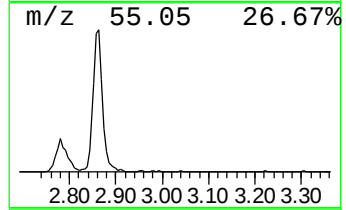
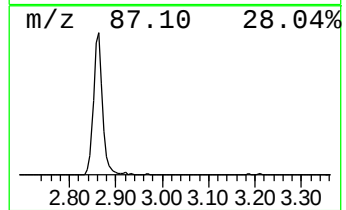
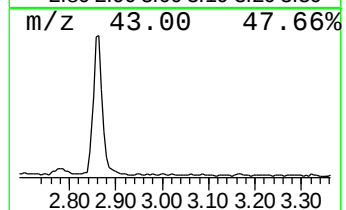
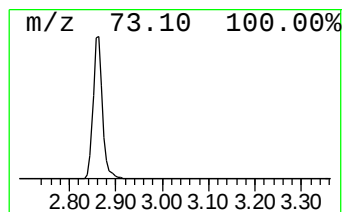
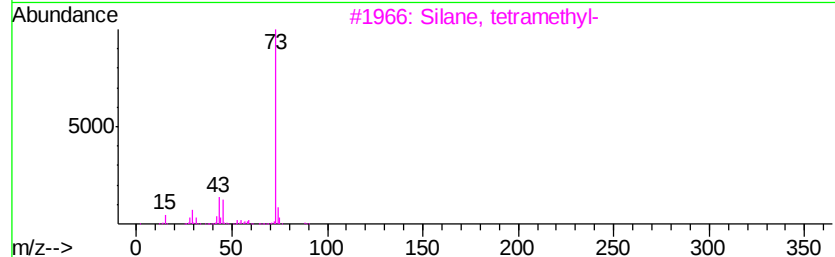
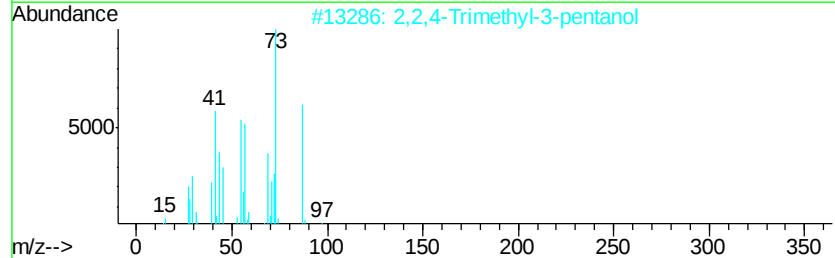
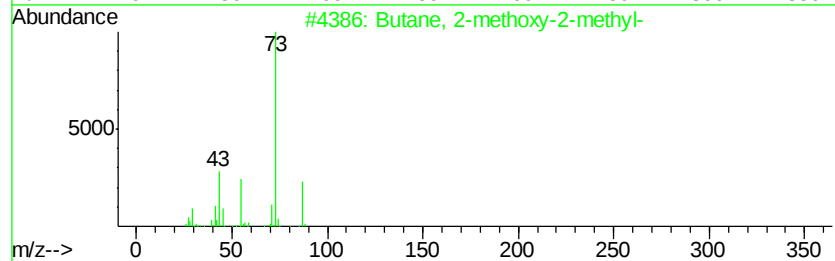
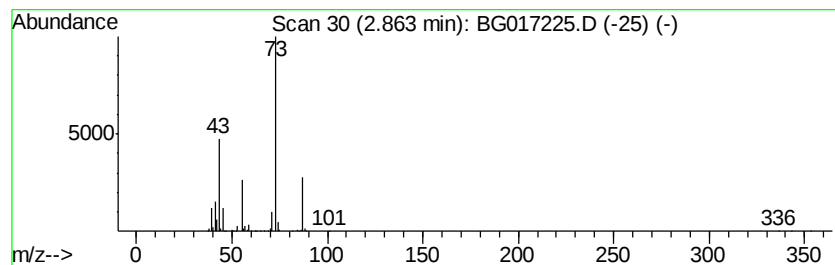
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.86	45.81 ng	617533	1,4-Dichlorobenzene-d4	7.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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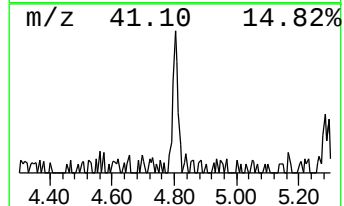
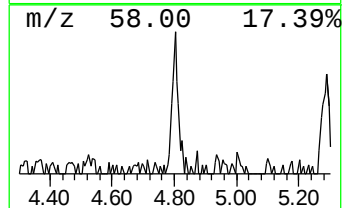
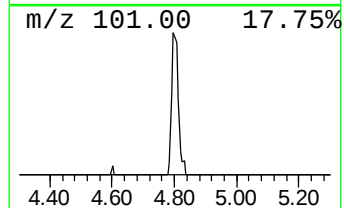
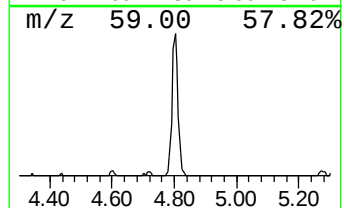
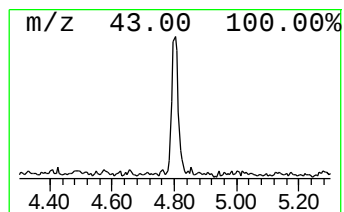
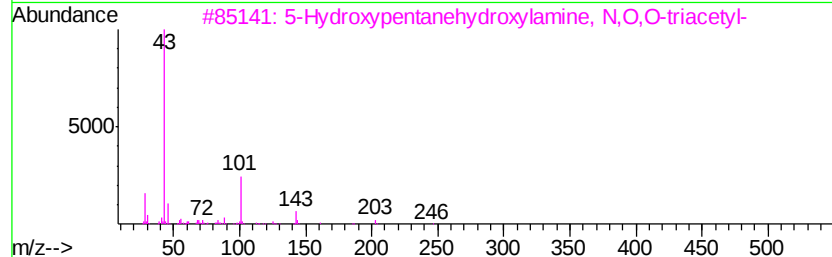
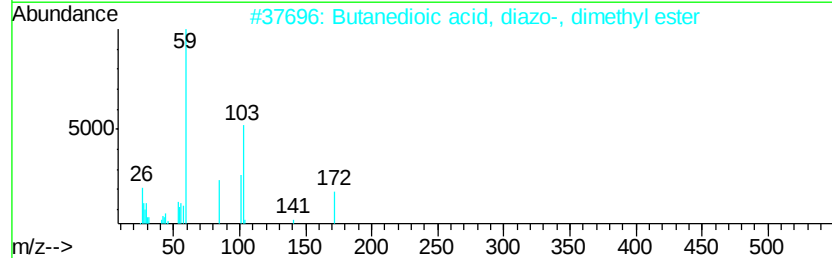
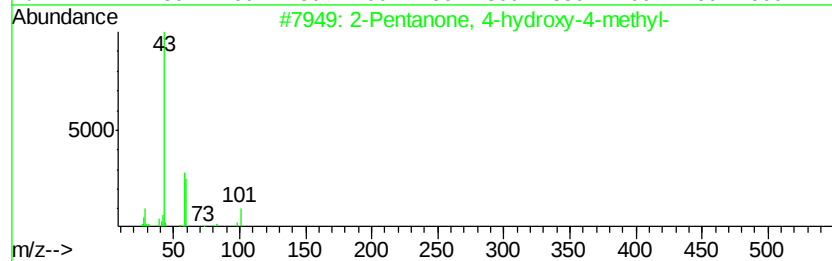
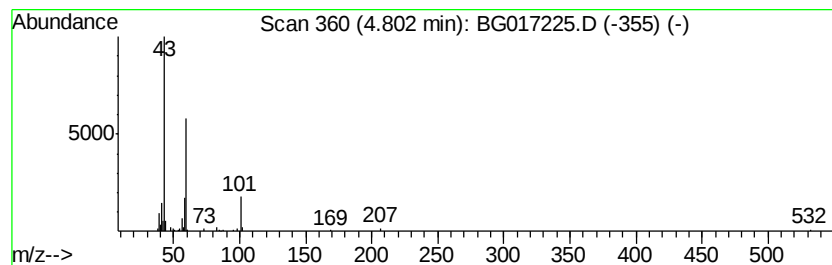
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	4.88 ng	65830	1,4-Dichlorobenzene-d4	7.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	25	
2	Butanedioic acid, diazo-, dimeth...	172	C6H8N2O4	055514-36-8	23	
3	5-Hydroxypentanehydroxylamine, N...	245	C11H19NO5	104556-13-0	10	
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	10	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	



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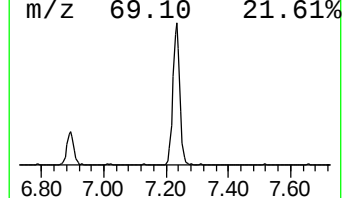
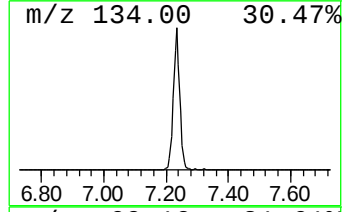
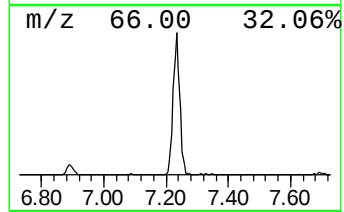
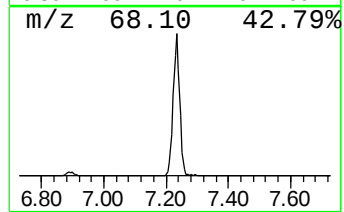
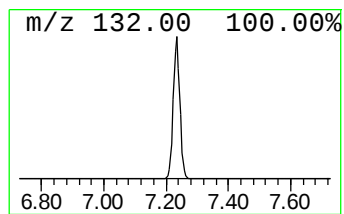
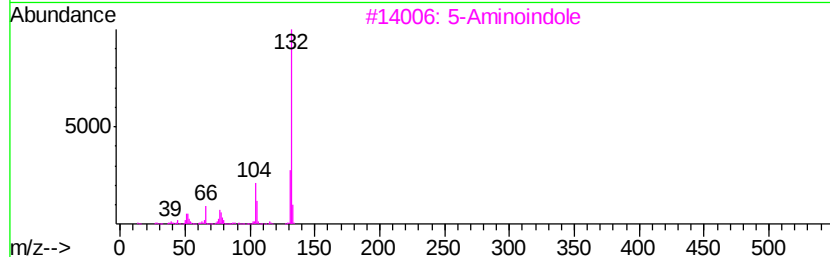
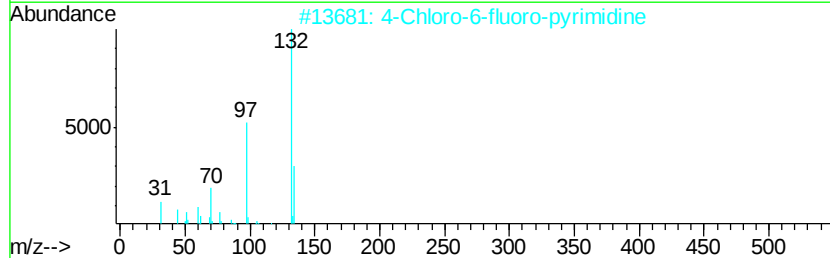
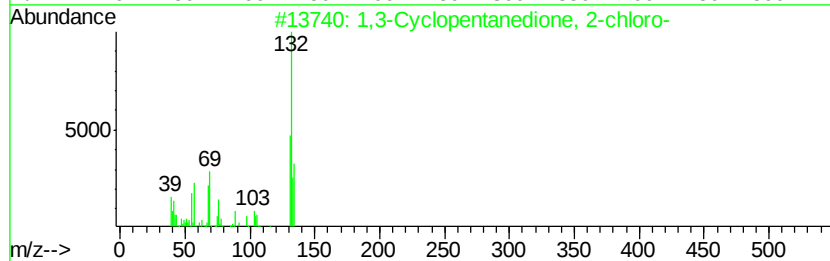
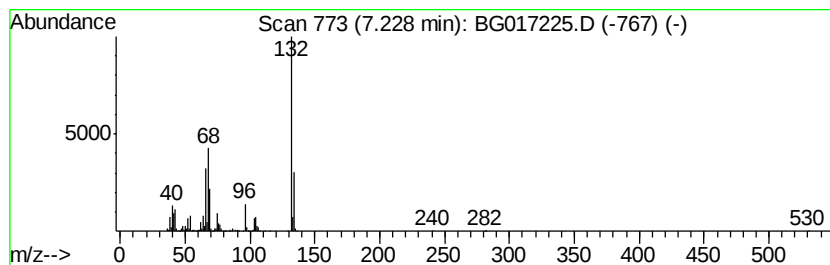
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Peak Number 4 unknown7.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	77.37 ng	1043010	1,4-Dichlorobenzene-d4	7.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	35
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	16



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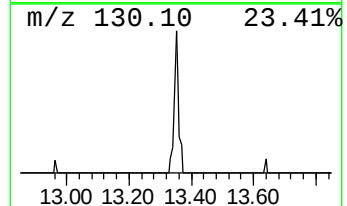
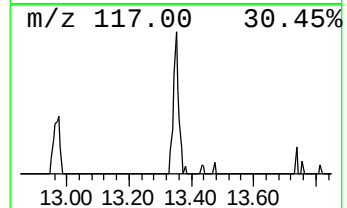
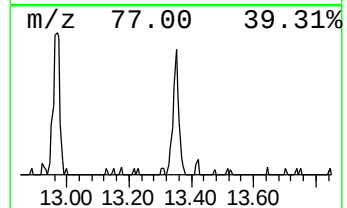
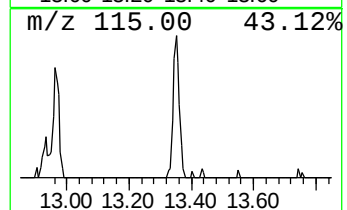
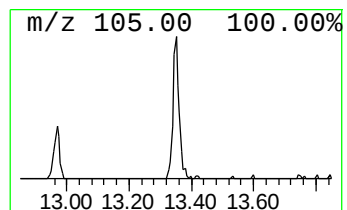
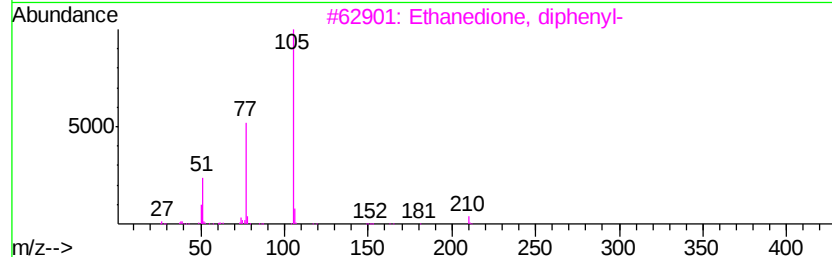
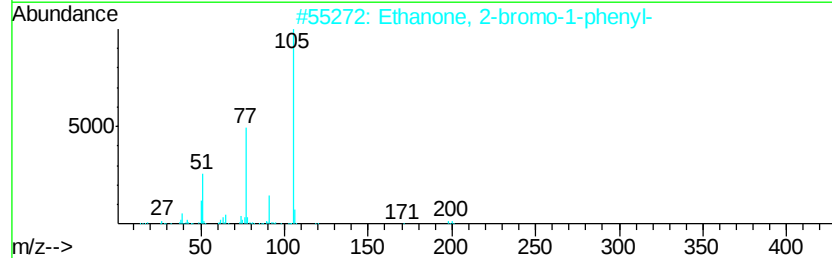
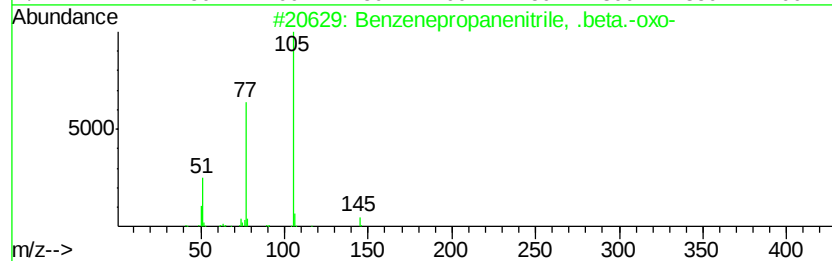
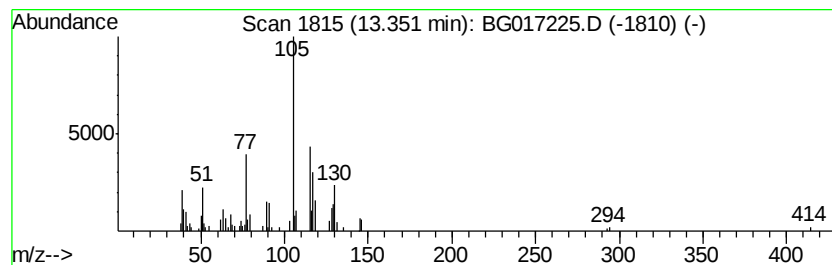
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 unknown13.35 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	2.84 ng	72996	Acenaphthene-d10	14.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	11
2		Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	000070-11-1	11
3		Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	10
4		Benzoyl chloride	140	C7H5ClO	000098-88-4	10
5		2(3H)-Furanone, 3-[(4-nitropheny...	293	C17H11NO4	054833-77-1	10



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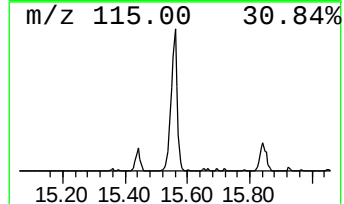
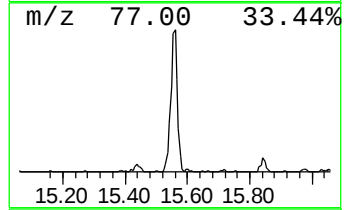
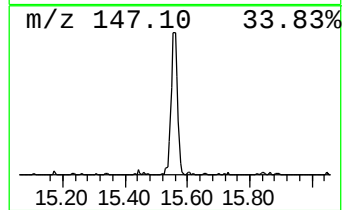
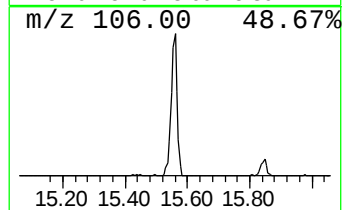
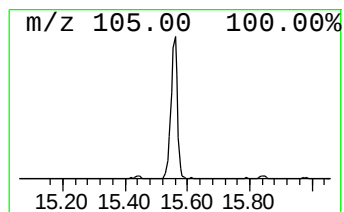
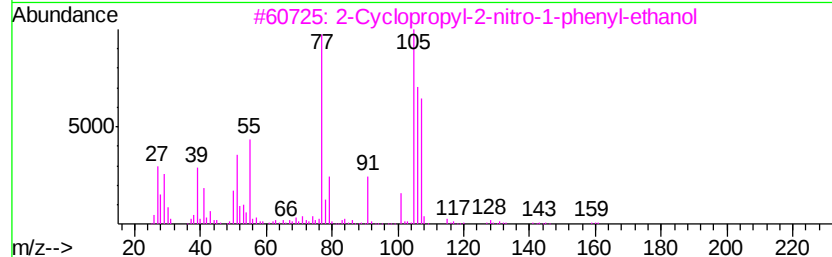
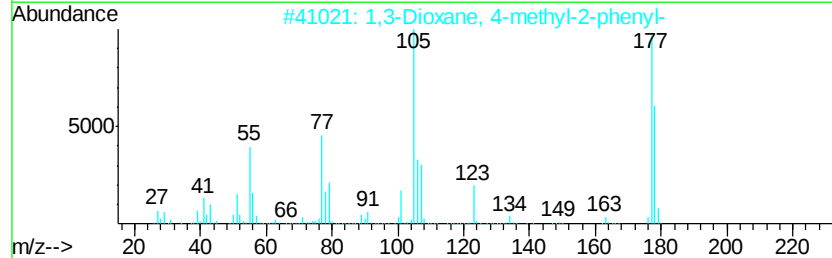
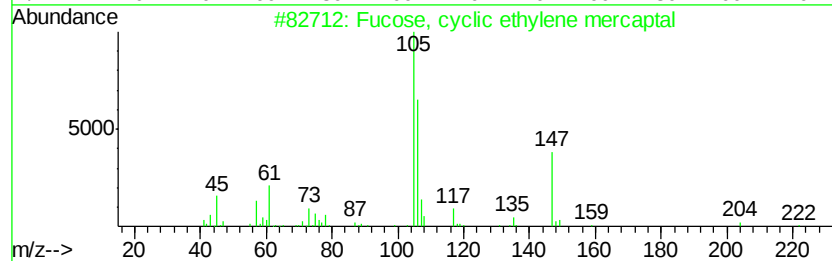
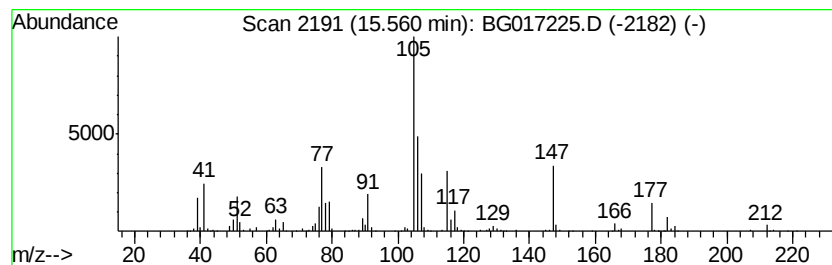
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 unknown15.56 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	15.79 ng	406281	Acenaphthene-d10	14.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Fucose, cyclic ethylene mercaptal	240	C8H16O4S2	003650-70-2	43
2		1,3-Dioxane, 4-methyl-2-phenyl-	178	C11H14O2	000774-44-7	38
3		2-Cyclopropyl-2-nitro-1-phenyl-e...	207	C11H13NO3	1000194-91-5	35
4		Chloromethyl 3-chlorobutanoate	170	C5H8Cl2O2	080418-48-0	35
5		3-Pyridinecarbonitrile, 1,4-dihy...	106	C6H6N2	023974-91-6	27



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.86	45.8	ng	617533	1	7.69	269625	20.0
2-Pentanone, 4-hy...	4.80	4.9	ng	65830	1	7.69	269625	20.0
unknown7.23	7.23	77.4	ng	1043010	1	7.69	269625	20.0
unknown13.35	13.35	2.8	ng	72996	3	14.35	514677	20.0
unknown15.56	15.56	15.8	ng	406281	3	14.35	514677	20.0