

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
 Data File : BF076951.D
 Acq On : 20 Jan 2015 5:44
 Operator : IZ / TP
 Sample : G1080-07
 Misc : W
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TE-PMW-43

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_F\METHODS\8270-BF011415.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	1.464	30	33	42	rVB	24135	51753	3.66%	0.559%
2	4.104	262	264	275	rVB	40639	87875	6.21%	0.949%
3	5.041	343	346	355	rBV	218533	432819	30.57%	4.673%
4	7.373	548	550	556	rBV	116494	249242	17.60%	2.691%
5	7.476	556	559	567	rVB	497547	929566	65.65%	10.036%
6	7.967	599	602	607	rVB	124095	207789	14.68%	2.243%
7	8.299	627	631	634	rBV	530341	892166	63.01%	9.632%
8	9.270	712	716	719	rBV	483910	718697	50.76%	7.759%
9	10.882	853	857	860	rBV	199048	293755	20.75%	3.172%
10	13.534	1085	1089	1092	rBV	962158	1415844	100.00%	15.286%
11	15.008	1215	1218	1222	rBV	211380	318372	22.49%	3.437%
12	16.677	1361	1364	1367	rBV	646301	854574	60.36%	9.226%
13	17.774	1458	1460	1463	rBV	286538	328076	23.17%	3.542%
14	18.757	1544	1546	1550	rBV2	16474	19668	1.39%	0.212%
15	20.003	1652	1655	1658	rBV	1266408	1393441	98.42%	15.044%
16	21.146	1752	1755	1757	rBV	39385	59970	4.24%	0.647%
17	21.180	1757	1758	1760	rVB	82700	79560	5.62%	0.859%
18	21.272	1760	1766	1769	rBV	342341	436937	30.86%	4.717%
19	21.397	1775	1777	1780	rVB	18128	25362	1.79%	0.274%
20	22.037	1830	1833	1836	rBV5	8585	16587	1.17%	0.179%
21	22.483	1869	1872	1873	rBV3	12573	16046	1.13%	0.173%
22	22.769	1895	1897	1902	rVB4	7702	15963	1.13%	0.172%
23	22.917	1907	1910	1913	rVB	244318	315561	22.29%	3.407%
24	23.420	1951	1954	1956	rBV3	6585	14716	1.04%	0.159%
25	23.512	1956	1962	1965	rVV5	12630	46102	3.26%	0.498%
26	23.855	1988	1992	1995	rVB4	9377	25528	1.80%	0.276%
27	24.460	2040	2045	2048	rBV6	5896	16277	1.15%	0.176%

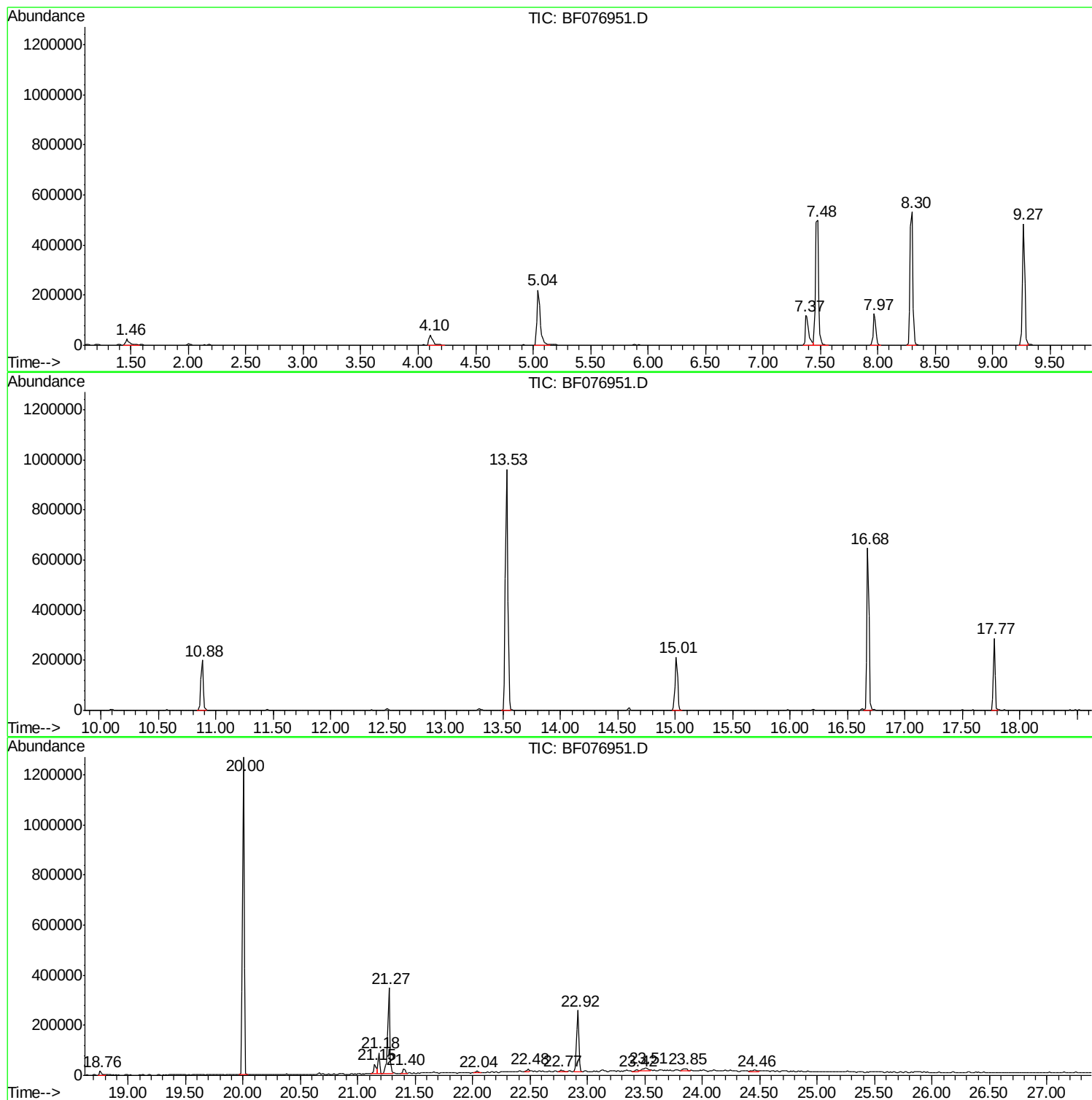
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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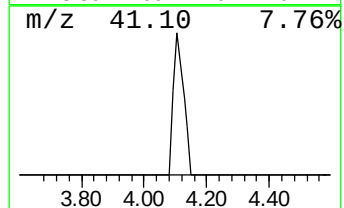
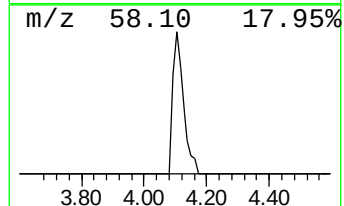
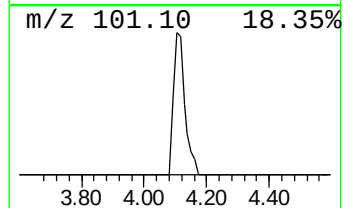
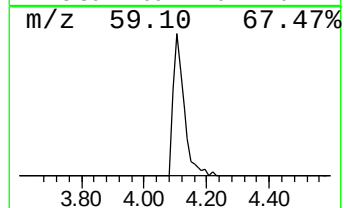
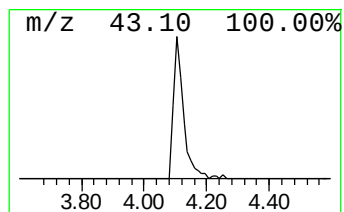
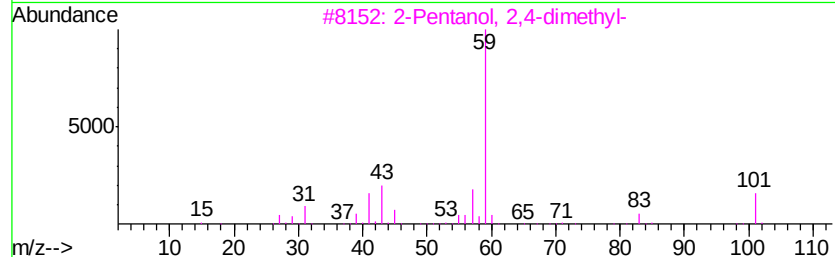
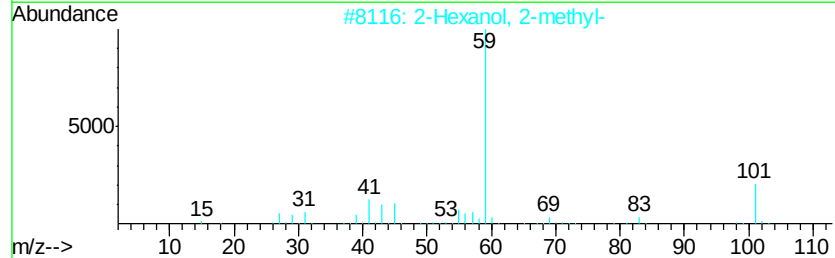
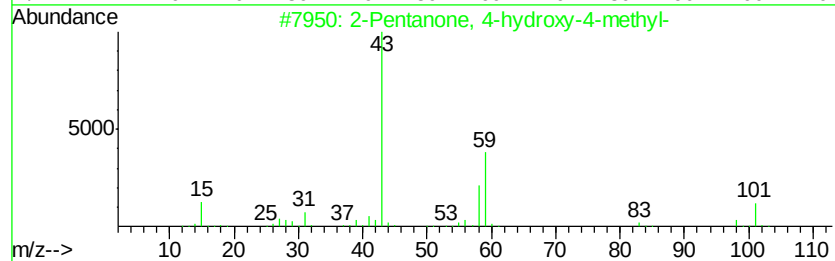
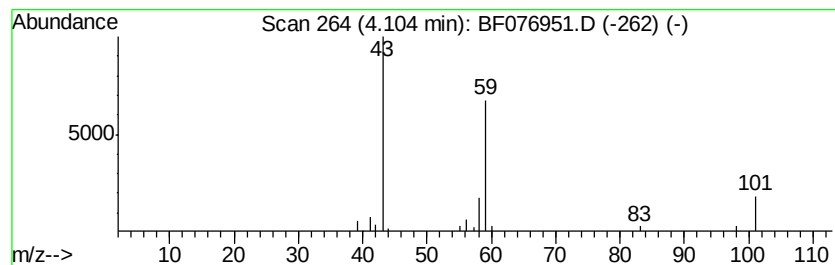
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.10	8.46 ng	87875	1,4-Dichlorobenzene-d4	7.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Guanidine	59	CH5N3	000113-00-8	9



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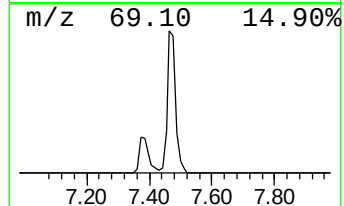
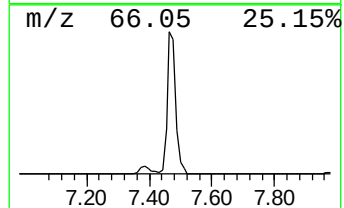
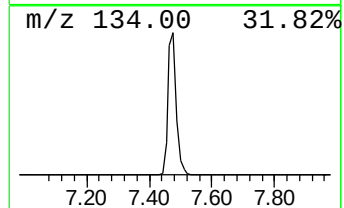
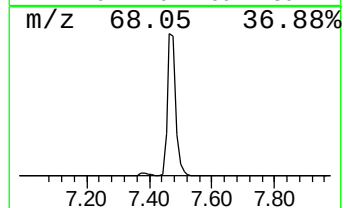
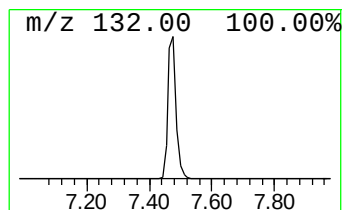
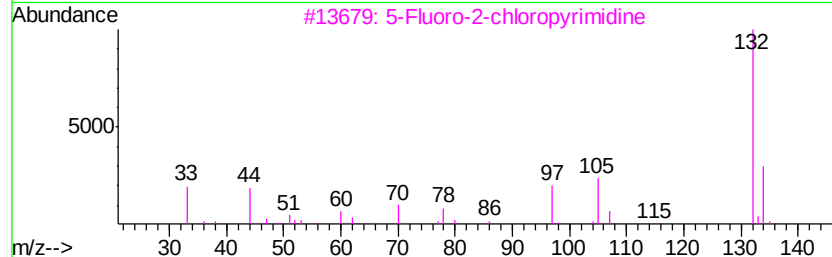
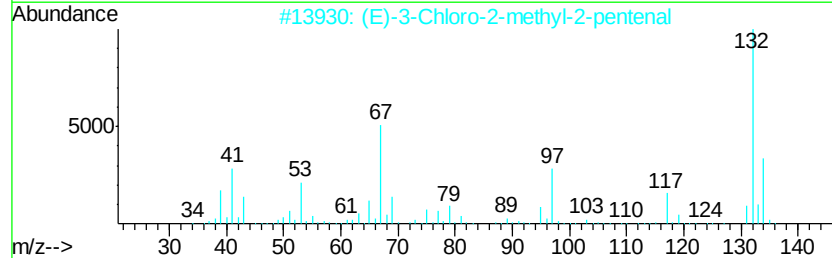
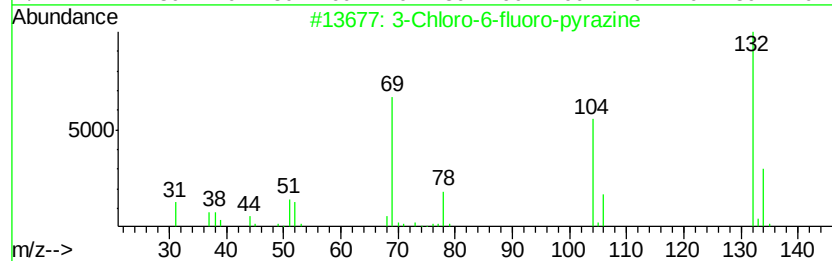
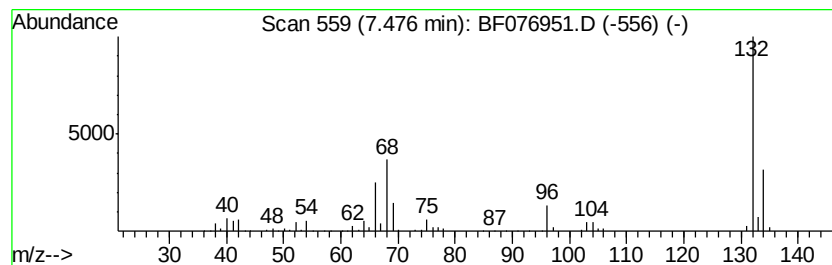
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	89.47 ng	929566	1,4-Dichlorobenzene-d4	7.97

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	17
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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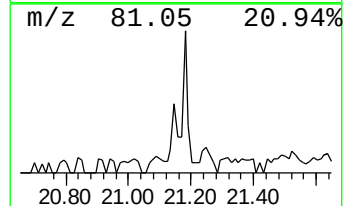
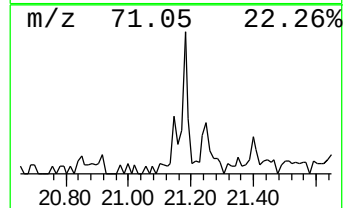
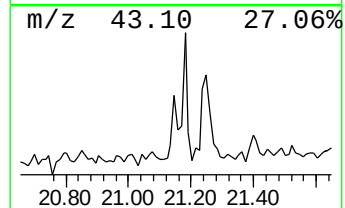
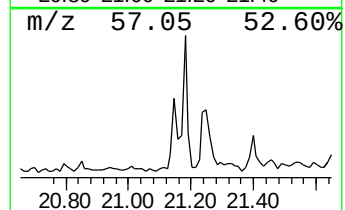
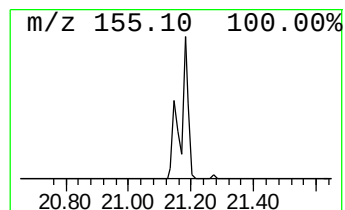
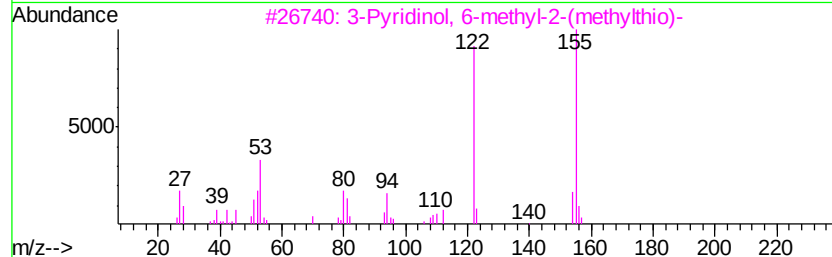
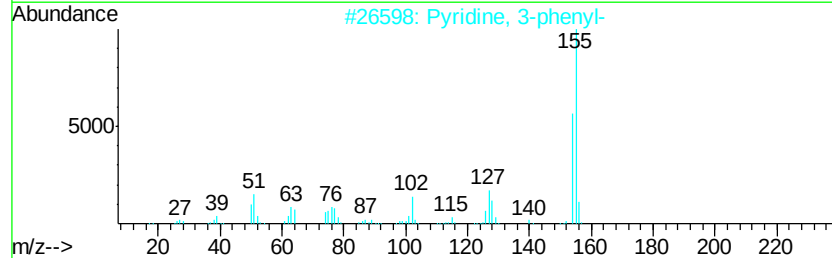
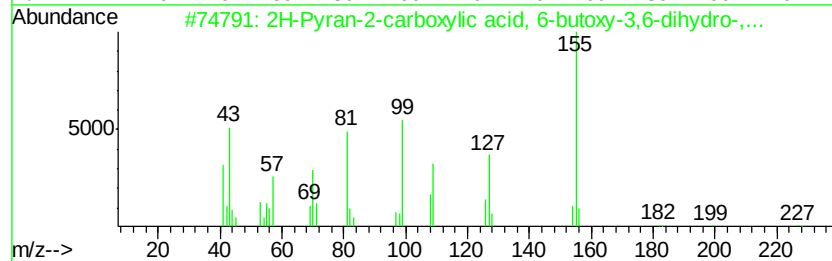
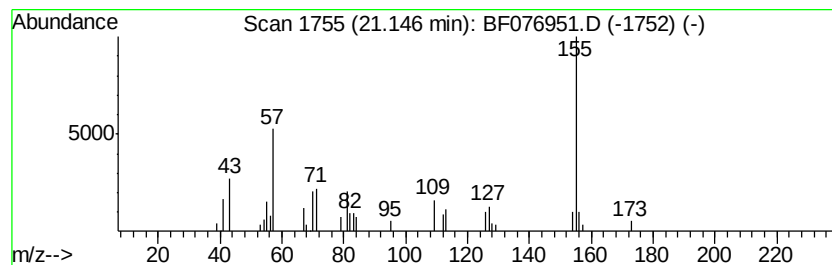
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Peak Number 5 2H-Pyran-2-carboxylic acid,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.15	2.75 ng	59970	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Pyran-2-carboxylic acid, 6-bu...	228	C12H20O4	026457-97-6	59
2		Pyridine, 3-phenyl-	155	C11H9N	001008-88-4	47
3		3-Pyridinol, 6-methyl-2-(methylt...	155	C7H9NOS	023003-25-0	38
4		Imidazole, 4-amino-5-ethoxycarbo...	155	C6H9N3O2	021190-16-9	38
5		Octahydropyrano[3,2-b]pyridin-6-one	155	C8H13NO2	1000193-43-8	38



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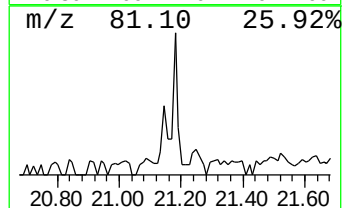
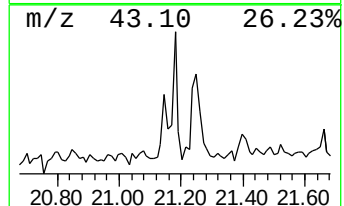
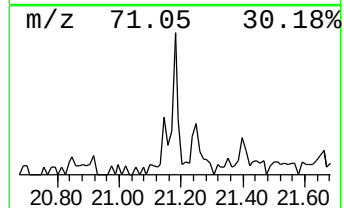
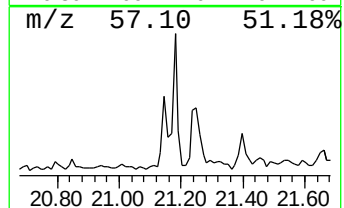
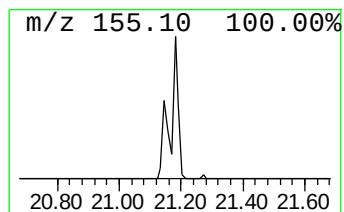
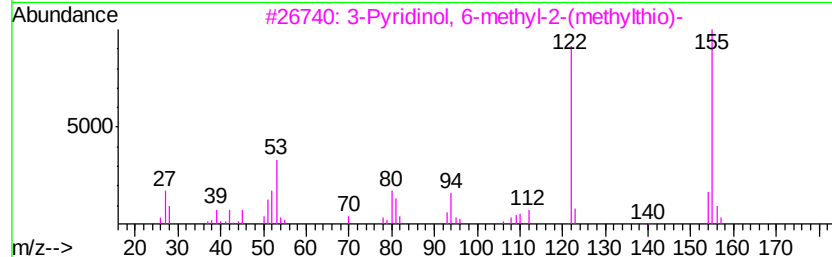
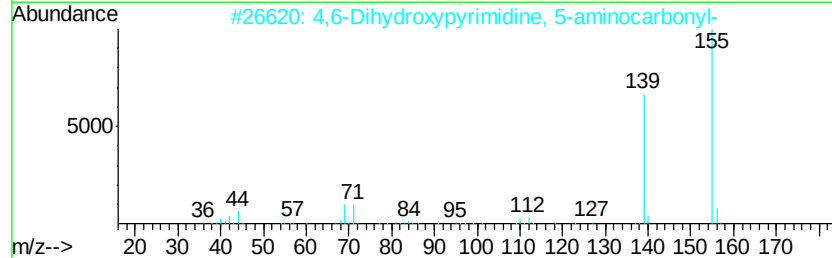
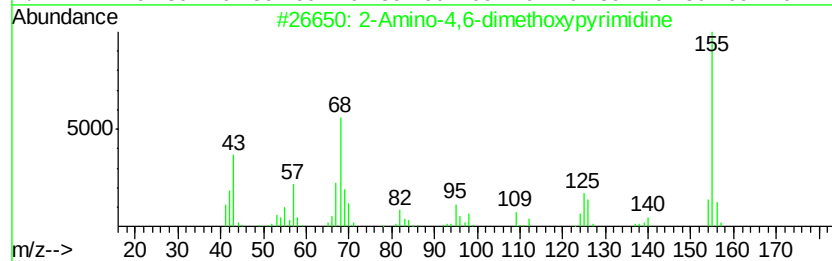
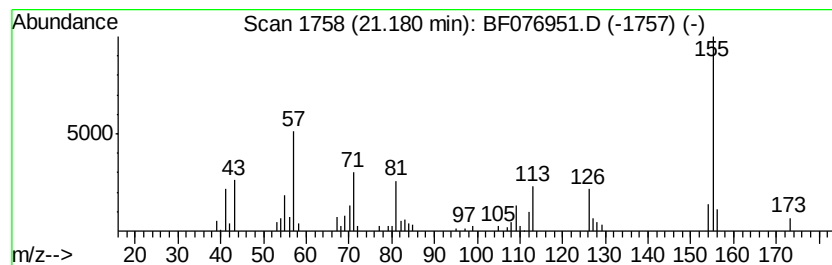
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 unknown21.18 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.18	3.64 ng	79560	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Amino-4,6-dimethoxypyrimidine	155	C6H9N3O2	036315-01-2	40
2		4,6-Dihydroxypyrimidine, 5-amino...	155	C5H5N3O3	001074-97-1	38
3		3-Pyridinol, 6-methyl-2-(methylt...	155	C7H9NOS	023003-25-0	38
4		Benzaldehyde, 4-chloro-2-nitro-	185	C7H4ClNO3	005551-11-1	35
5		Pyridine, 3-phenyl-	155	C11H9N	001008-88-4	32



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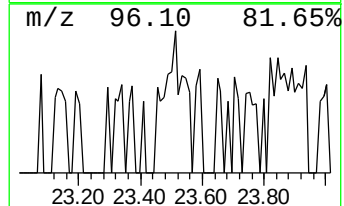
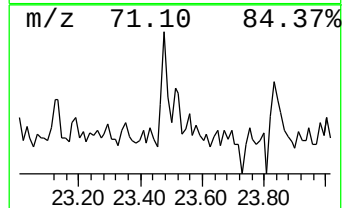
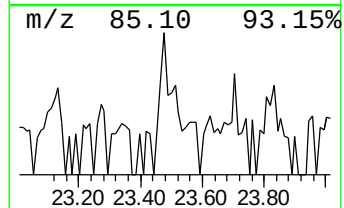
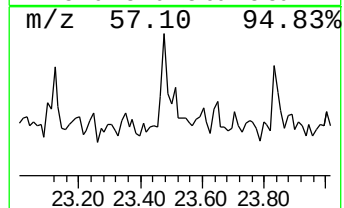
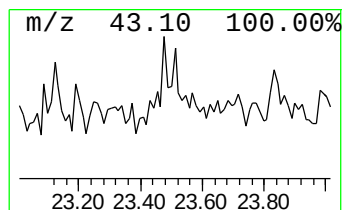
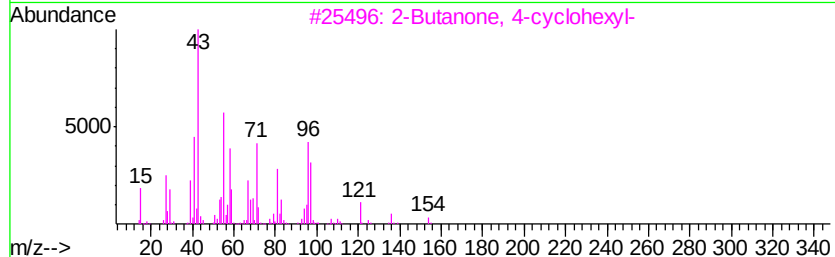
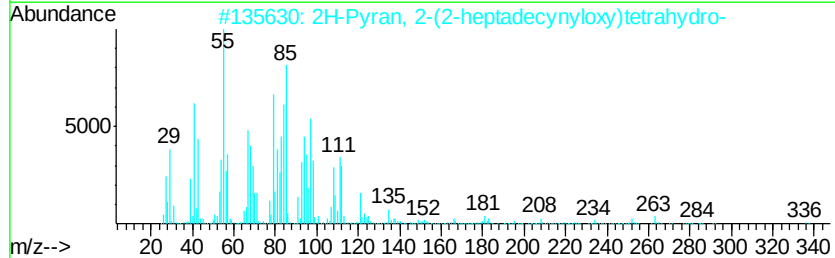
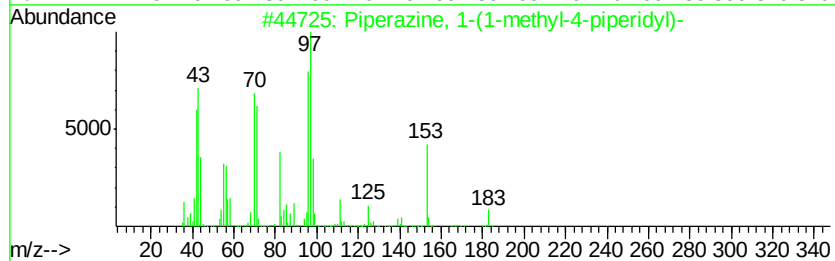
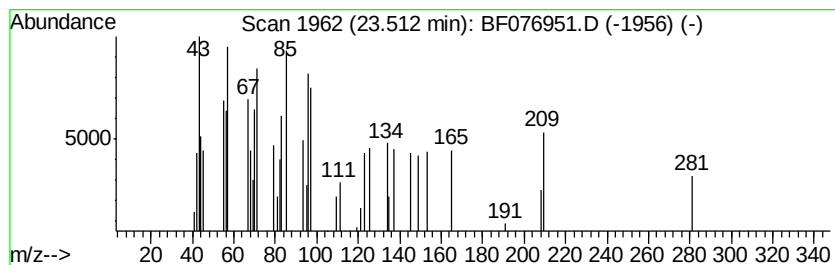
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Peak Number 7 unknown23.51 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.51	2.92 ng	46102	Perylene-d12	22.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Piperazine, 1-(1-methyl-4-piperi...	183	C10H21N3	023995-88-2	27
2	2H-Pyran, 2-(2-heptadecynvloxy)t...	336	C22H40O2	069502-96-1	22
3	2-Butanone, 4-cvclohexyl-	154	C10H18O	002316-85-0	14
4	Undecanoic acid, 4,8-dimethyl-10...	242	C14H26O3	005024-24-8	14
5	3-Cyclopentylpropionic acid, 1-(...	238	C15H26O2	1000293-36-9	14



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.10	8.5	ng	87875	1	7.97	207789	20.0
unknown7.48	7.48	89.5	ng	929566	1	7.97	207789	20.0
2H-Pyran-2-carbox...	21.15	2.8	ng	59970	5	21.27	436937	20.0
unknown21.18	21.18	3.6	ng	79560	5	21.27	436937	20.0
unknown23.51	23.51	2.9	ng	46102	6	22.92	315561	20.0