

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032317\
 Data File : BF093889.D
 Acq On : 23 Mar 2017 19:59
 Operator : SJ/MA
 Sample : I2371-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S8-0665

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-BF032217.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	2.051	23	28	38	rVB3	45870	75745	1.42%	0.226%
2	4.110	373	378	382	rBV	309683	330963	6.20%	0.985%
3	4.498	439	444	447	rBV	2167052	2038297	38.15%	6.069%
4	4.898	506	512	514	rBV	74700	66518	1.25%	0.198%
5	5.551	619	623	628	rVB	1397703	1438686	26.93%	4.284%
6	5.716	645	651	654	rBV	3538477	3665507	68.61%	10.914%
7	5.975	690	695	698	rBV	1025455	938535	17.57%	2.794%
8	6.122	716	720	721	rBV	142340	117477	2.20%	0.350%
9	6.157	721	726	729	rVB	3417843	3592210	67.24%	10.696%
10	6.622	798	805	808	rBV	2573309	3070008	57.47%	9.141%
11	6.998	865	869	875	rVB	169287	171899	3.22%	0.512%
12	7.133	888	892	895	rBV	144657	151898	2.84%	0.452%
13	7.475	945	950	954	rBV	1231424	1260569	23.60%	3.753%
14	8.504	1122	1125	1128	rVB3	91148	86157	1.61%	0.257%
15	8.804	1170	1176	1180	rBV	4445281	5342256	100.00%	15.907%
16	9.239	1247	1250	1256	rBV2	65034	67288	1.26%	0.200%
17	9.298	1256	1260	1266	rVB	61320	65603	1.23%	0.195%
18	9.622	1309	1315	1319	rVB2	1326448	1375491	25.75%	4.096%
19	10.598	1474	1481	1484	rBV	2223662	2661099	49.81%	7.923%
20	11.445	1621	1625	1629	rBV	1227686	1252787	23.45%	3.730%
21	12.168	1745	1748	1752	rBV	88375	92225	1.73%	0.275%
22	13.145	1911	1914	1921	rVB4	50458	59816	1.12%	0.178%
23	13.433	1957	1963	1966	rBV	3468058	3975393	74.41%	11.837%
24	14.698	2174	2178	2186	rBV	837636	931723	17.44%	2.774%
25	16.339	2452	2457	2463	rBV	653129	757167	14.17%	2.254%

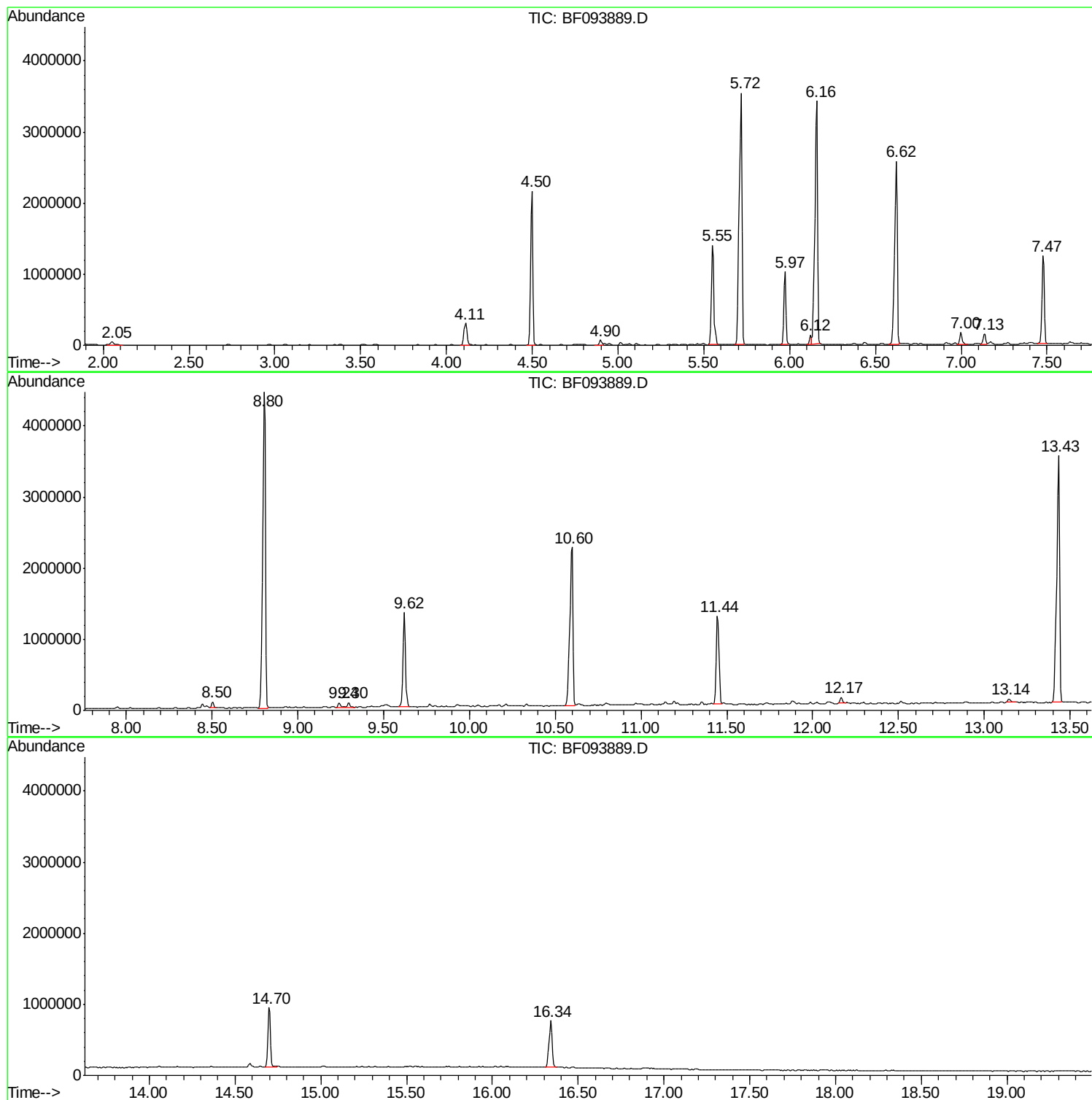
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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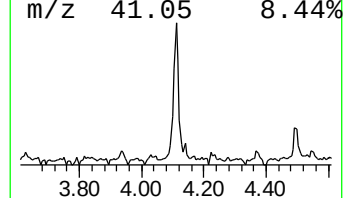
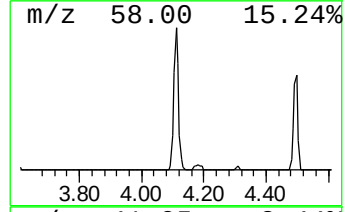
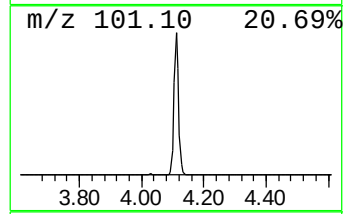
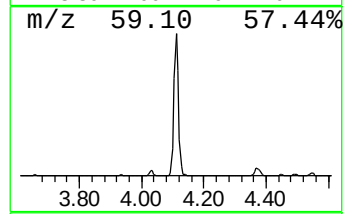
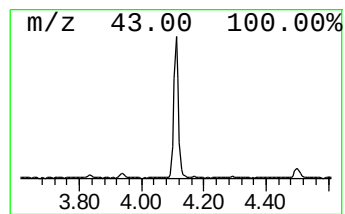
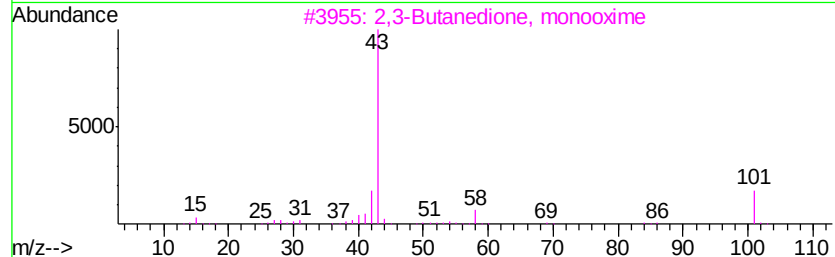
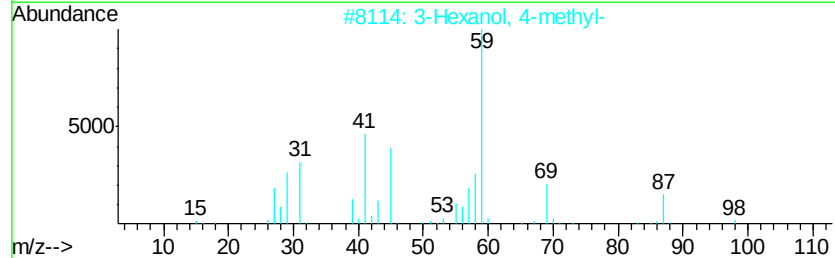
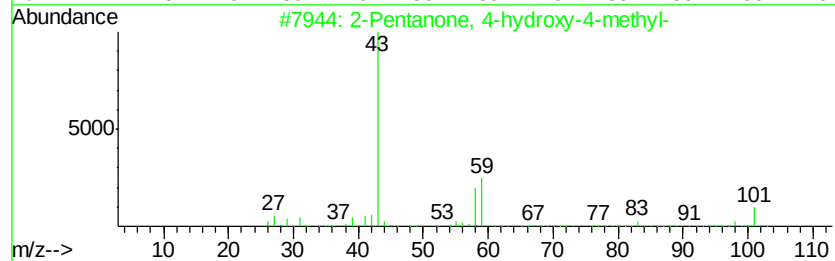
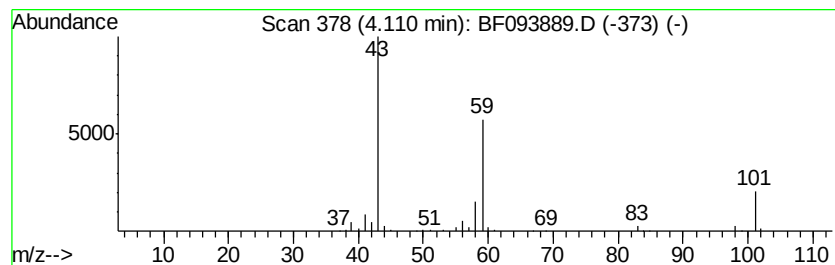
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.11	7.05 ng	330963	1,4-Dichlorobenzene-d4	5.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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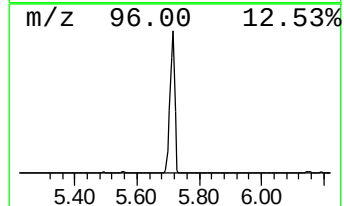
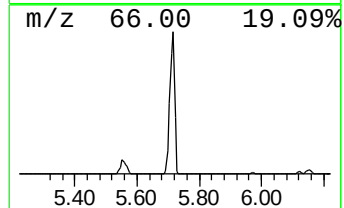
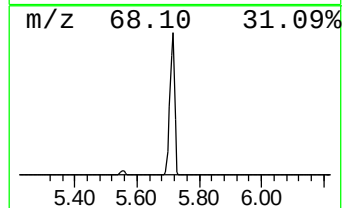
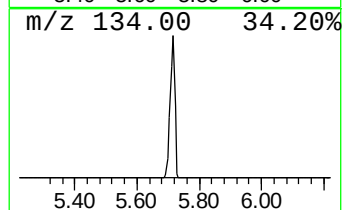
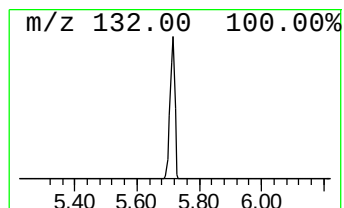
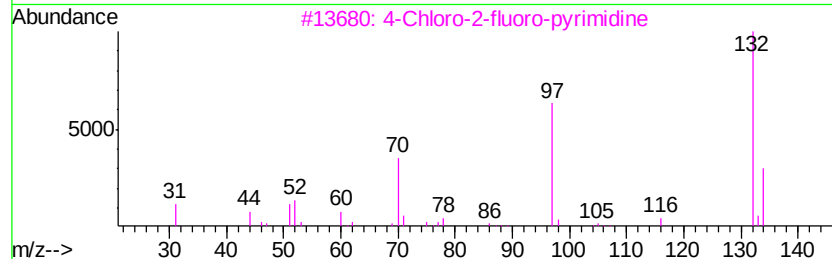
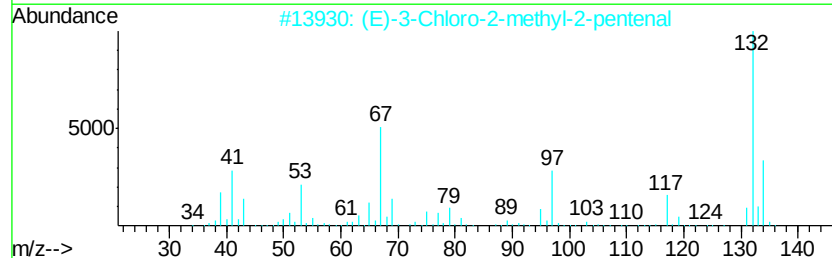
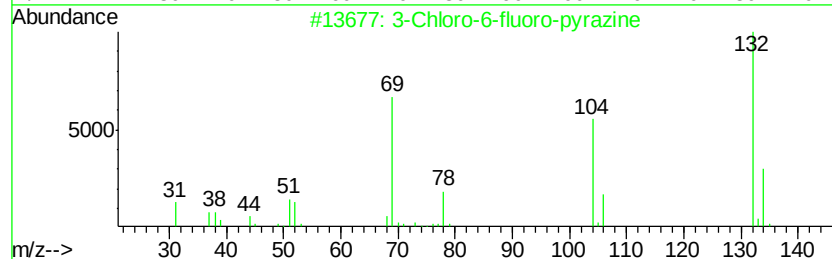
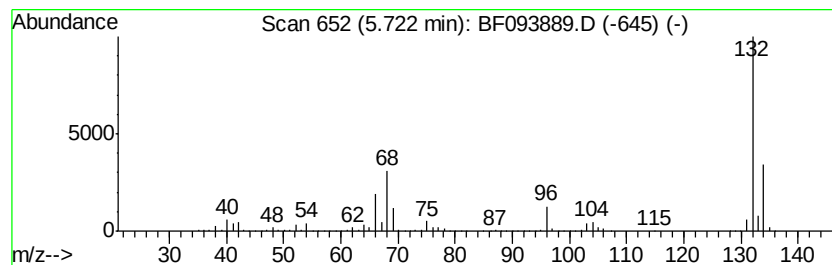
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	78.11 ng	3665510	1,4-Dichlorobenzene-d4	5.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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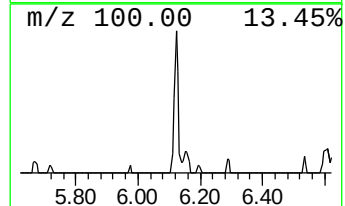
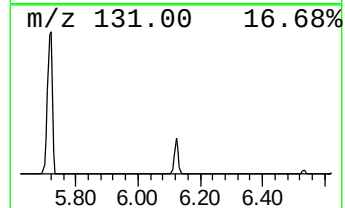
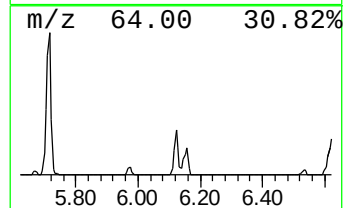
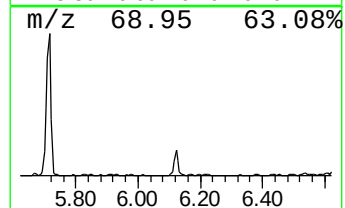
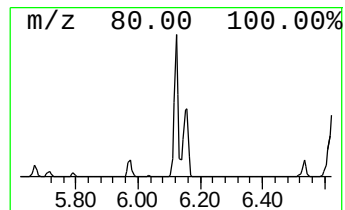
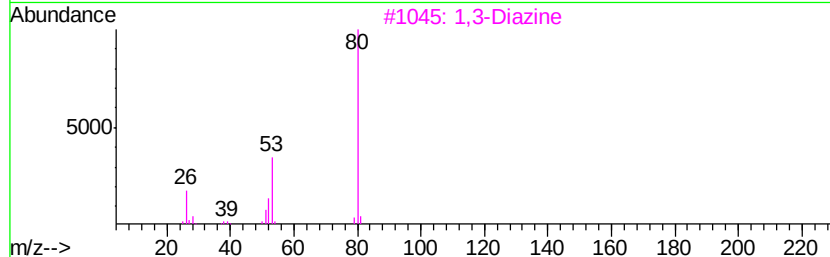
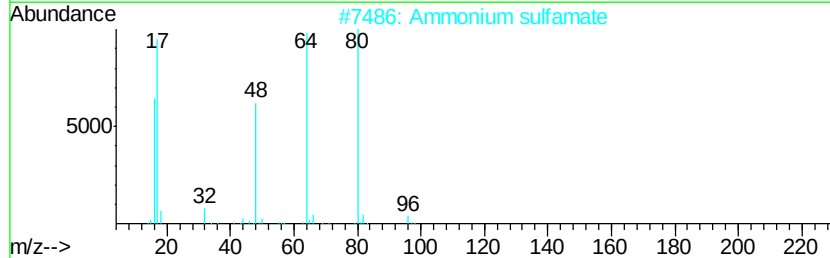
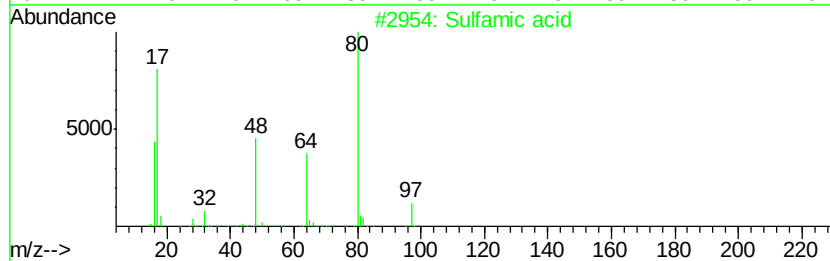
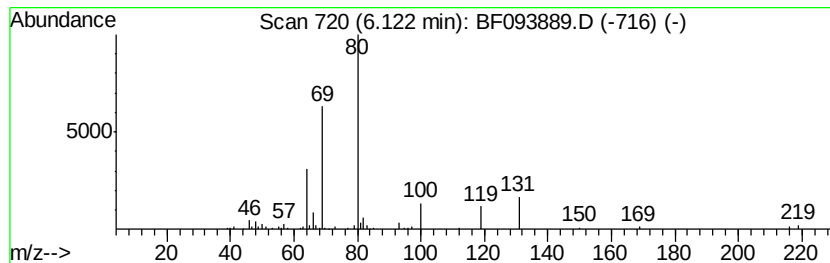
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Peak Number 3 unknown6.12 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.12	2.50 ng	117477	1,4-Dichlorobenzene-d4	5.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfamic acid	97	H3N03S	005329-14-6	40
2		Ammonium sulfamate	114	H6N203S	007773-06-0	9
3		1,3-Diazine	80	C4H4N2	000289-95-2	7
4		Ethene, 1-chloro-2-fluoro-	80	C2H2ClF	000460-16-2	7
5		Boron, (methanamine)tris(trifluo...	249	C4H5BF9N	128353-61-7	4



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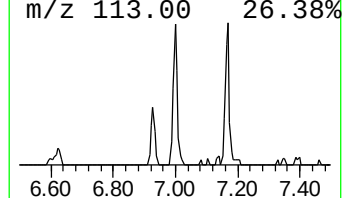
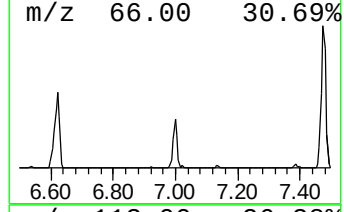
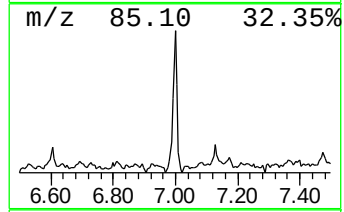
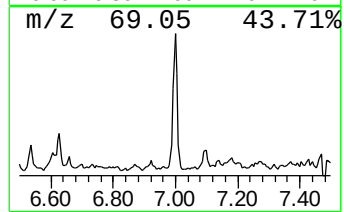
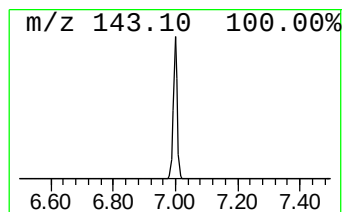
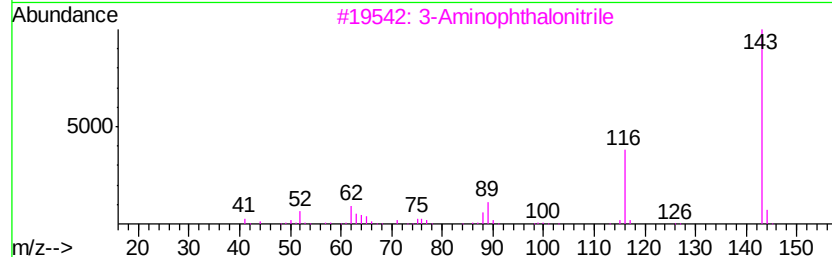
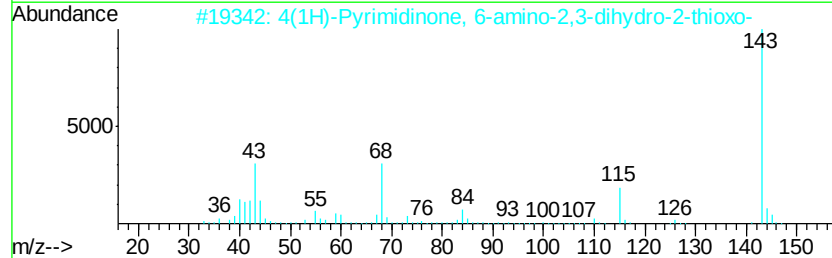
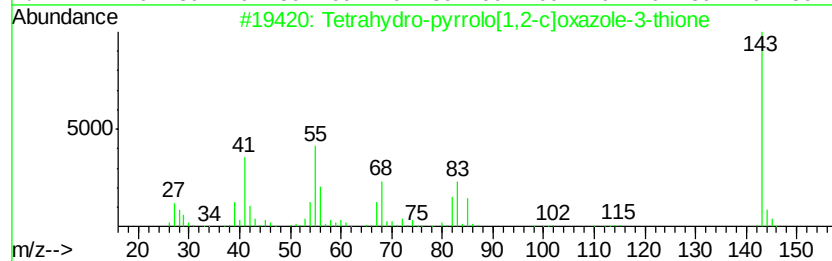
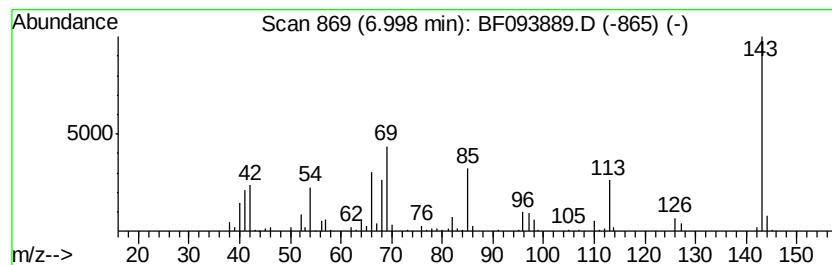
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown7.00 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.00	2.73 ng	171899	Napthalene-d8	7.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetrahydro-pyrrolo[1,2-c]oxazole...	143	C6H9NOS	1000190-53-6	17
2		4(1H)-Pyrimidinone, 6-amino-2,3-...	143	C4H5N3OS	001004-40-6	16
3		3-Aminophthalonitrile	143	C8H5N3	058632-96-5	10
4		4-Amino-6-hydroxy-2-mercaptopyri...	143	C4H5N3OS	065802-56-4	9
5		Isoquinoline, 1-methyl-	143	C10H9N	001721-93-3	9



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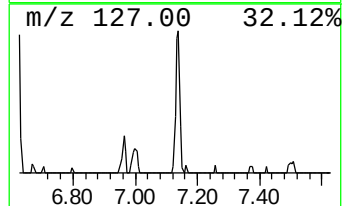
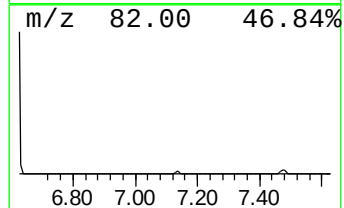
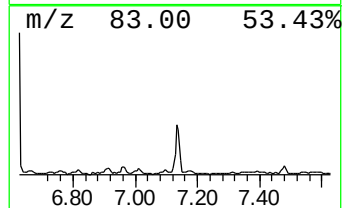
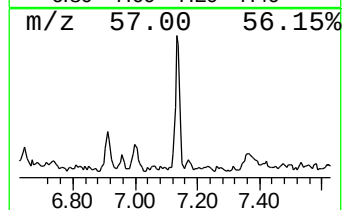
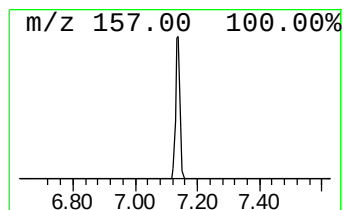
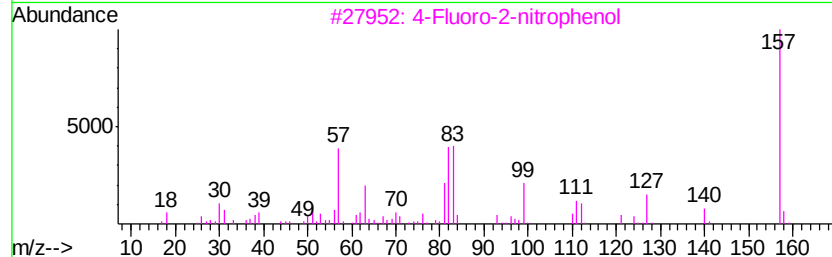
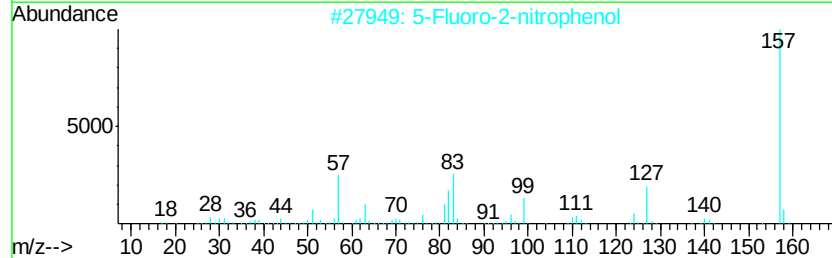
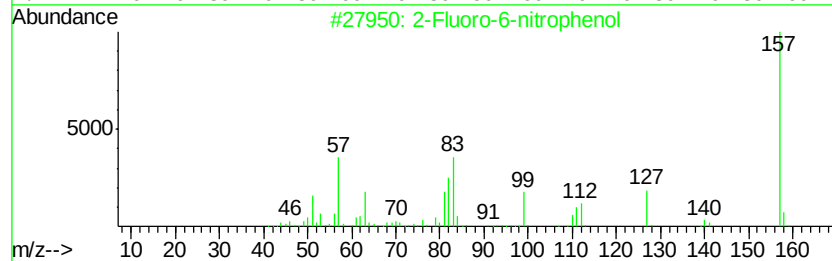
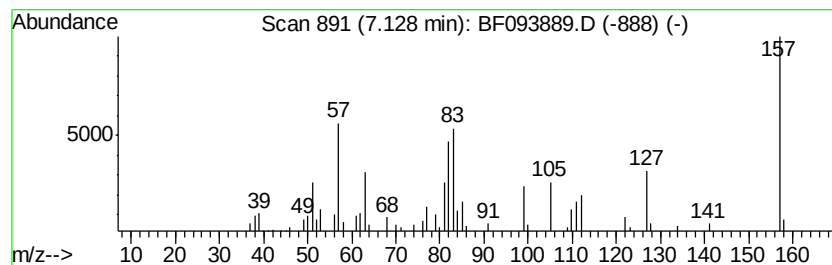
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Peak Number 6 2-Fluoro-6-nitrophenol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.13	2.41 ng	151898	Napthalene-d8	7.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Fluoro-6-nitrophenol	157	C6H4FN03	001526-17-6	96
2		5-Fluoro-2-nitrophenol	157	C6H4FN03	000446-36-6	76
3		4-Fluoro-2-nitrophenol	157	C6H4FN03	000394-33-2	64
4		2-Fluoro-4-nitrophenol	157	C6H4FN03	000403-19-0	49
5		Phenol, 2-fluoro-4-nitro-, aceta...	199	C8H6FN04	1000125-98-6	47



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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
2-Pentanone, 4-hy...	4.11	7.0	ng	330963	1	5.97	938535	20.0
unknown5.72	5.72	78.1	ng	3665510	1	5.97	938535	20.0
unknown6.12	6.12	2.5	ng	117477	1	5.97	938535	20.0
unknown7.00	7.00	2.7	ng	171899	2	7.47	1260570	20.0
2-Fluoro-6-nitrop...	7.13	2.4	ng	151898	2	7.47	1260570	20.0