

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050515\
 Data File : BF078940.D
 Acq On : 5 May 2015 14:56
 Operator : TP/IZ
 Sample : G2032-08
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B4(5-7)

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-BF043015.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	1.507	26	28	31	rVB	3488211	4381021	100.00%	18.443%
2	1.655	38	41	44	rVB	175306	306492	7.00%	1.290%
3	1.770	50	51	55	rBV	297369	407120	9.29%	1.714%
4	1.838	55	57	61	rVB	159851	227010	5.18%	0.956%
5	1.907	61	63	102	rVB	1674704	4276039	97.60%	18.001%
6	5.164	346	348	354	rVB	123767	181900	4.15%	0.766%
7	5.656	388	391	393	rBV	833692	1130798	25.81%	4.760%
8	6.902	497	500	502	rBV	1441250	1240518	28.32%	5.222%
9	7.062	512	514	517	rBV	1304724	1223890	27.94%	5.152%
10	7.359	537	540	542	rBV	440803	436923	9.97%	1.839%
11	7.542	554	556	558	rVB	1134784	984355	22.47%	4.144%
12	8.045	597	600	602	rBV	884127	758148	17.31%	3.192%
13	8.936	675	678	680	rBV	525828	597624	13.64%	2.516%
14	10.273	793	795	798	rBV	1355314	1516003	34.60%	6.382%
15	10.776	837	839	842	rBV	88166	96482	2.20%	0.406%
16	11.108	866	868	871	rBV	724547	678609	15.49%	2.857%
17	12.091	951	954	956	rBV	722664	867287	19.80%	3.651%
18	12.948	1027	1029	1032	rBV	528796	734831	16.77%	3.093%
19	14.811	1190	1192	1195	rBV	37427	47571	1.09%	0.200%
20	14.948	1201	1204	1207	rBV	1860096	1849753	42.22%	7.787%
21	16.137	1305	1308	1316	rBV2	66974	133215	3.04%	0.561%
22	16.263	1316	1319	1322	rBV	796490	826878	18.87%	3.481%
23	18.080	1475	1478	1481	rBV	645314	851915	19.45%	3.586%

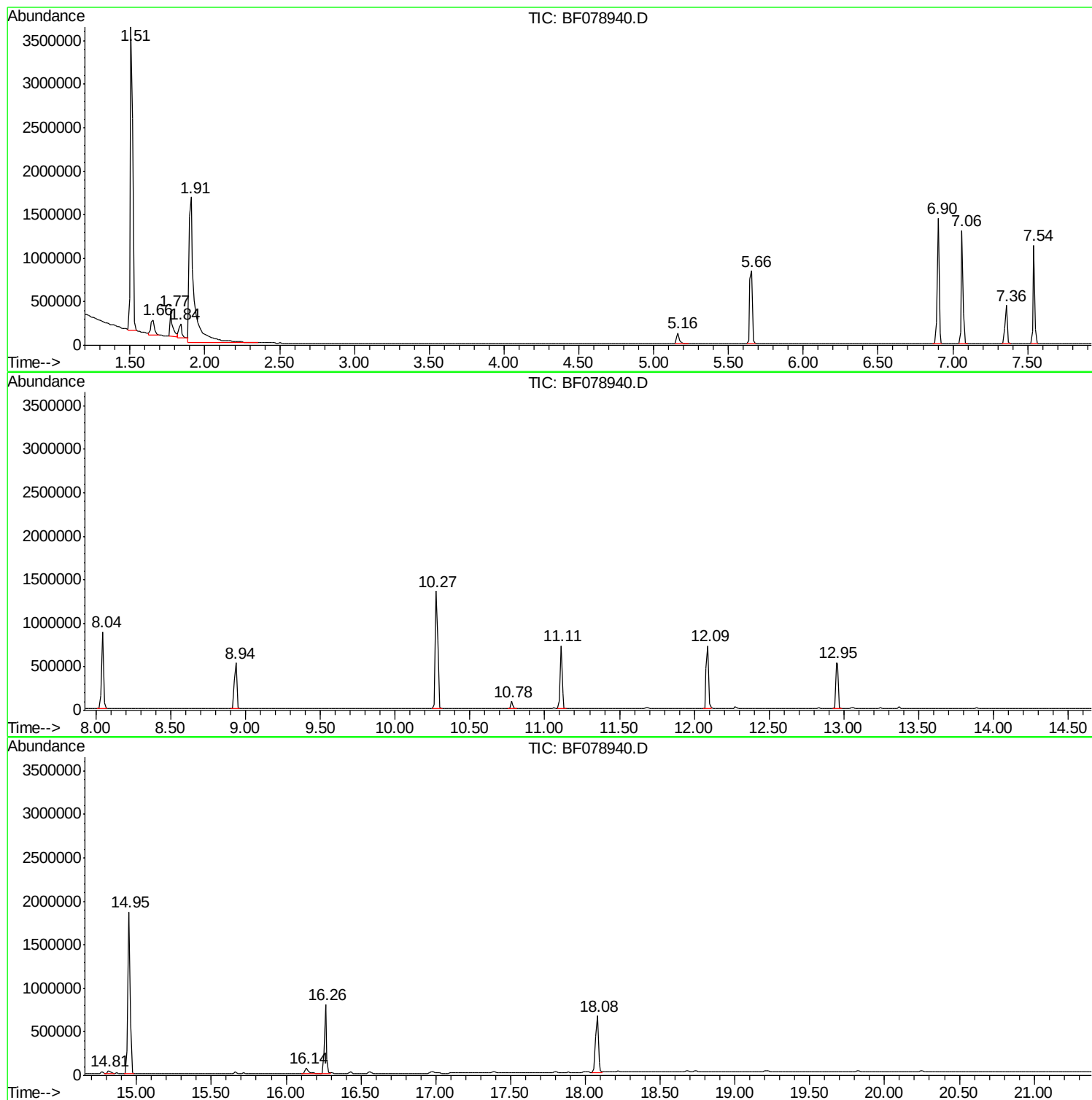
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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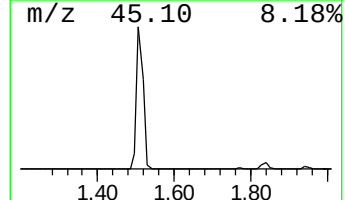
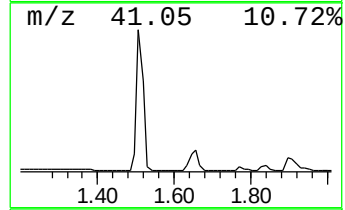
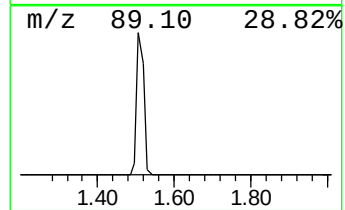
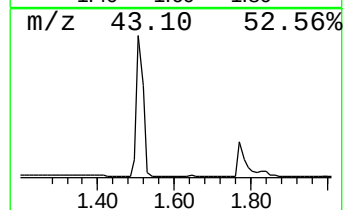
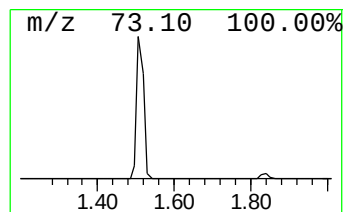
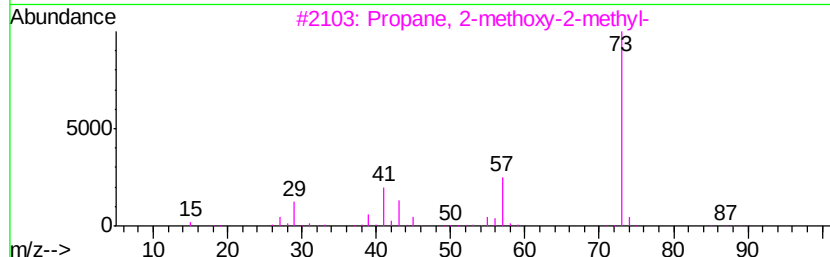
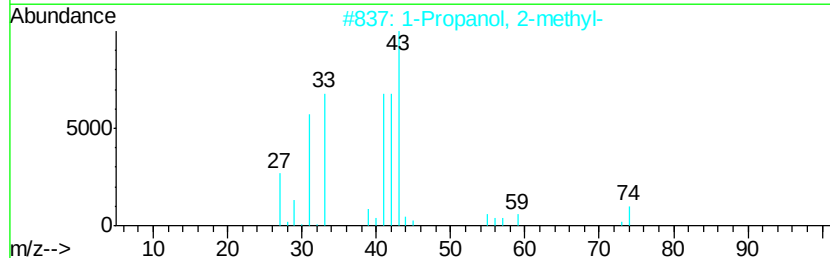
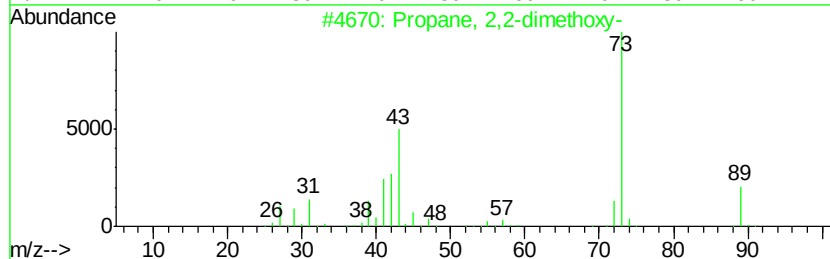
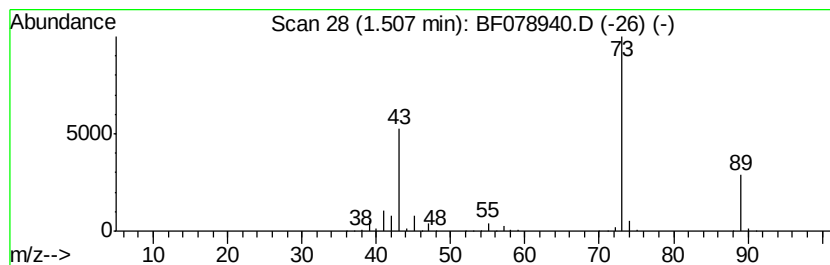
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.51	200.54 ng	4381020	1,4-Dichlorobenzene-d4	7.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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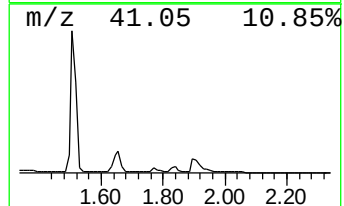
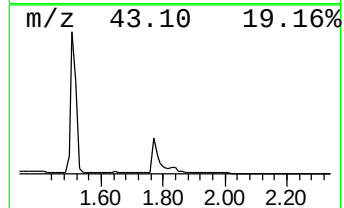
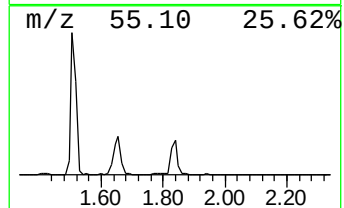
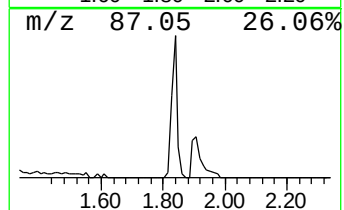
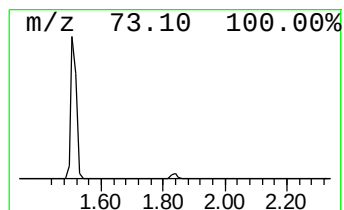
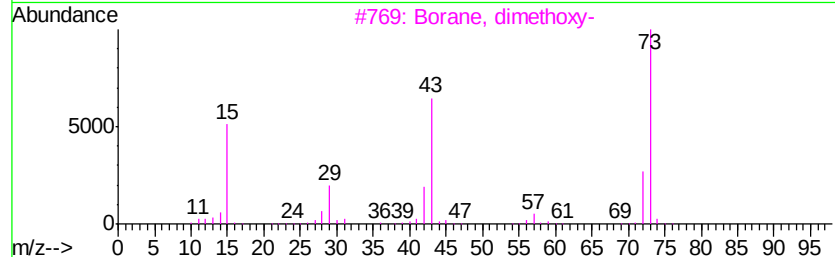
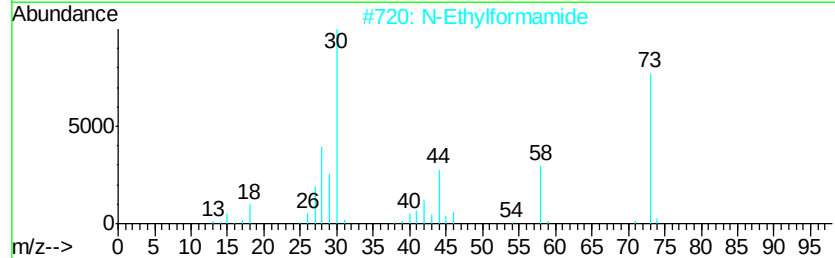
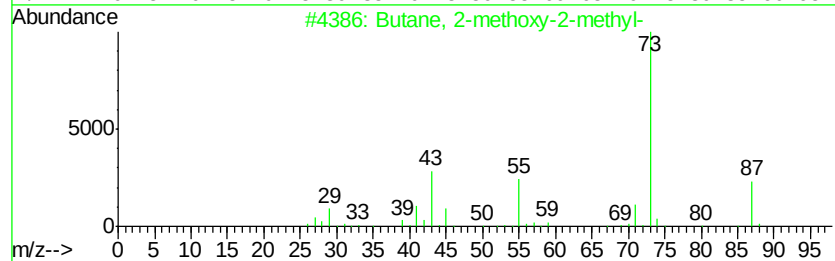
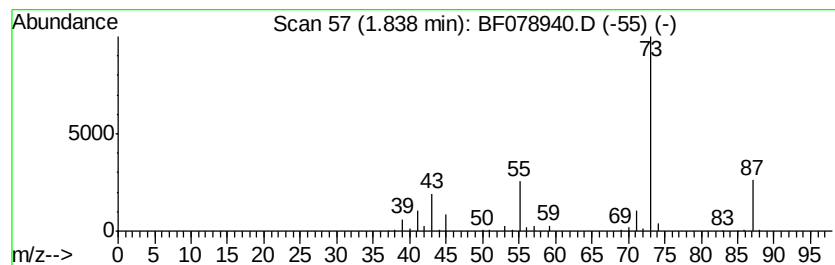
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.84	10.39 ng	227010	1,4-Dichlorobenzene-d4	7.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
4		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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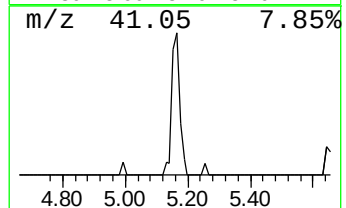
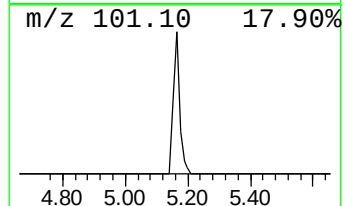
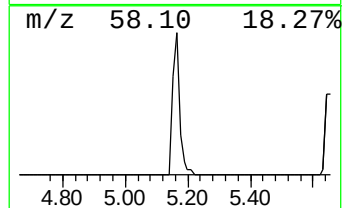
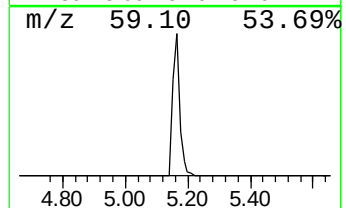
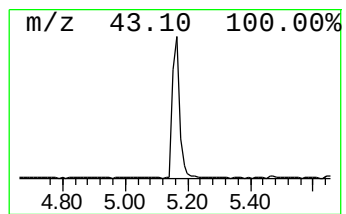
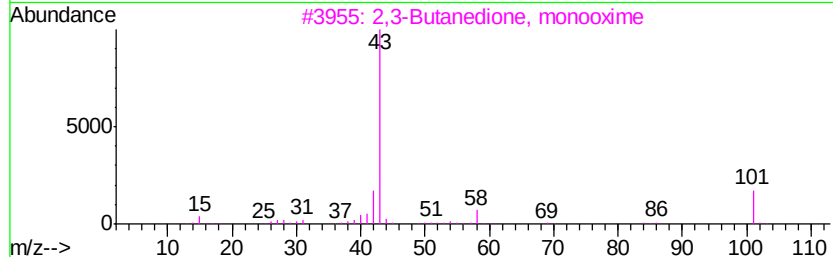
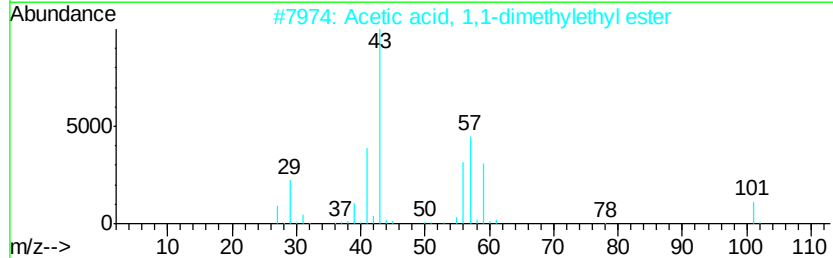
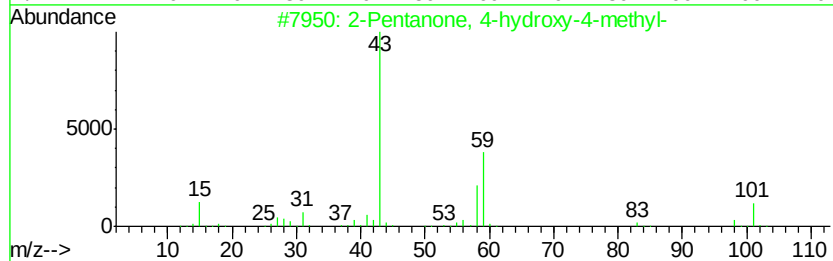
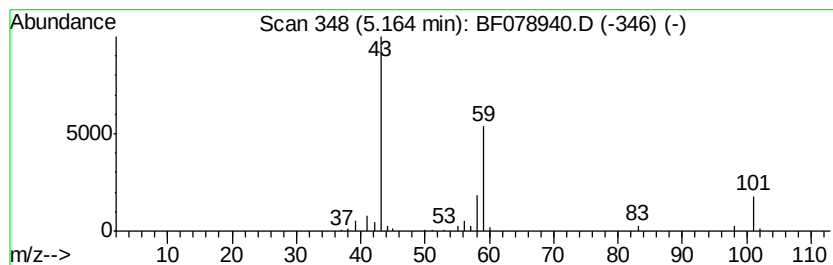
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Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	8.33 ng	181900	1,4-Dichlorobenzene-d4	7.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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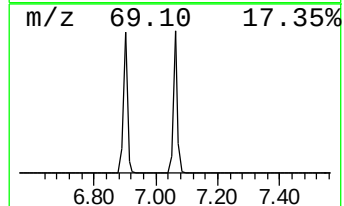
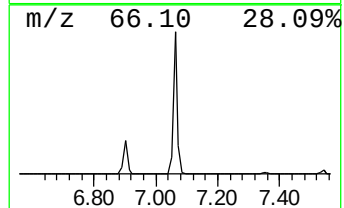
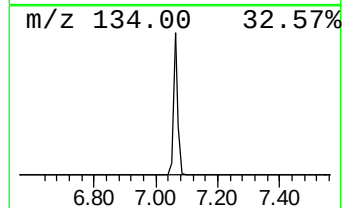
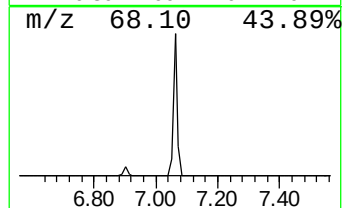
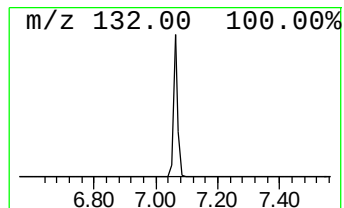
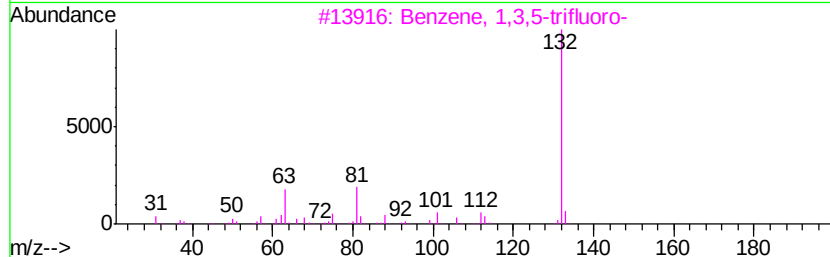
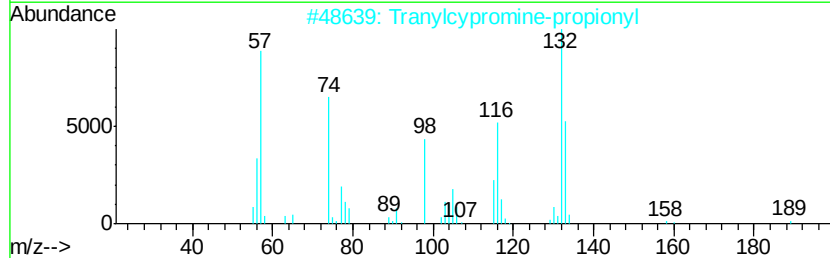
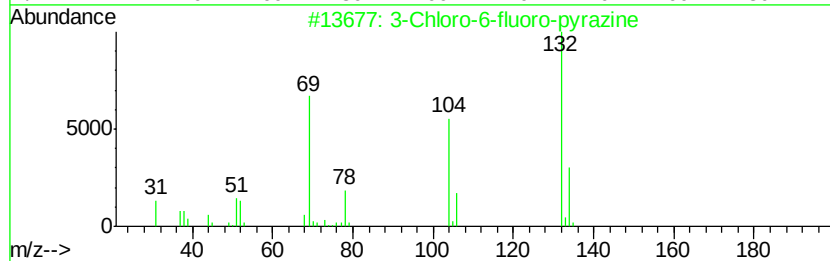
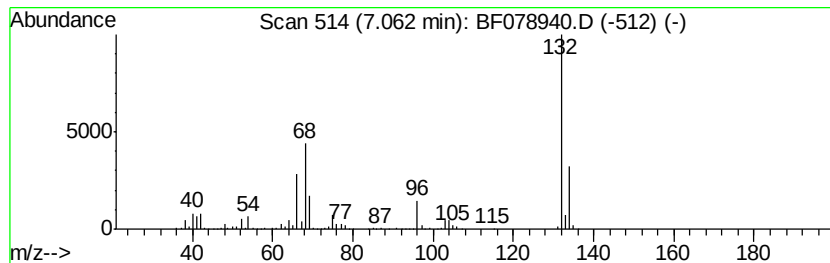
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TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown7.06 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	56.02 ng	1223890	1,4-Dichlorobenzene-d4	7.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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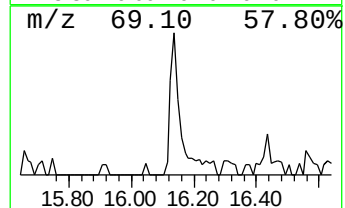
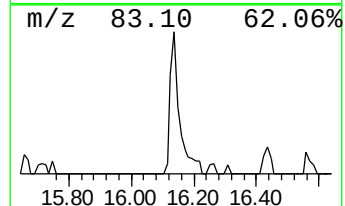
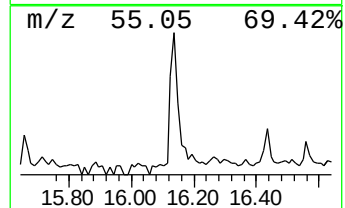
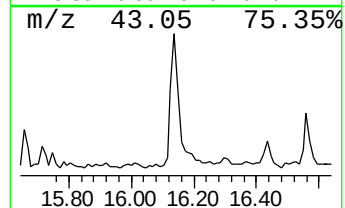
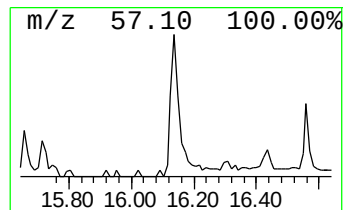
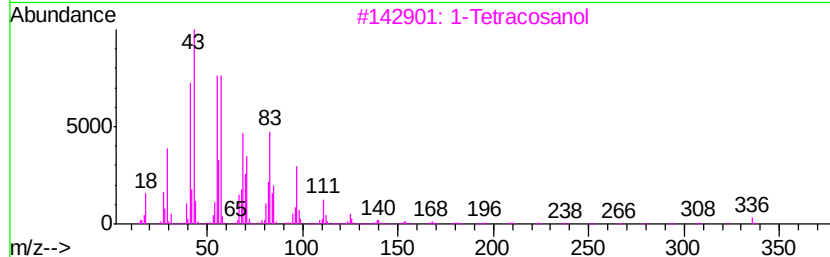
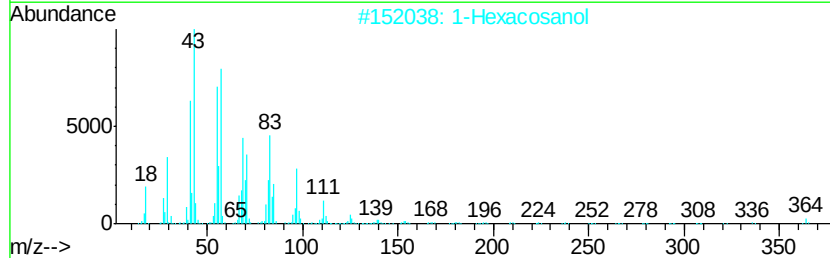
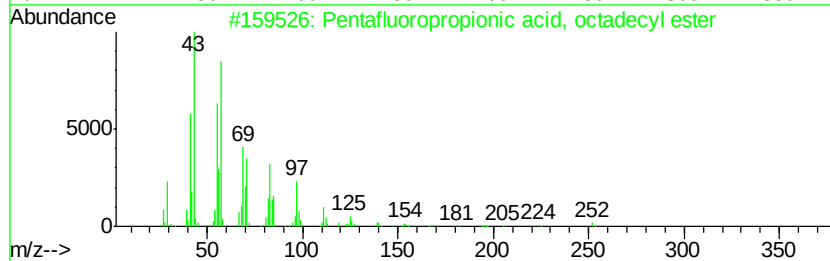
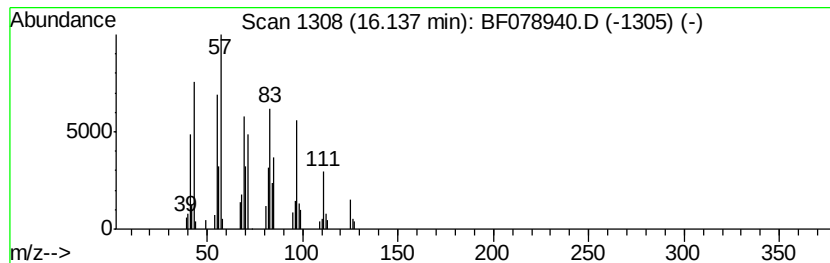
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Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	3.22 ng	133215	Chrysene-d12	16.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
2		1-Hexacosanol	382	C26H54O	000506-52-5	90
3		1-Tetracosanol	354	C24H50O	000506-51-4	81
4		Octadecane, 1-(ethenvloxy)-	296	C20H40O	000930-02-9	64
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	64



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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
Propane, 2,2-dime...	1.51	200.5	ng	4381020	1	7.36	436923	20.0
Butane, 2-methoxy...	1.84	10.4	ng	227010	1	7.36	436923	20.0
2-Pentanone, 4-hy...	5.16	8.3	ng	181900	1	7.36	436923	20.0
unknown7.06	7.06	56.0	ng	1223890	1	7.36	436923	20.0
Pentafluoropropio...	16.14	3.2	ng	133215	5	16.26	826878	20.0