

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051415\
 Data File : BF079242.D
 Acq On : 14 May 2015 19:56
 Operator : TP/IZ
 Sample : G2246-05
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-16

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	1.358	13	15	18	rVB	2868359	3862197	74.09%	16.016%
2	1.495	23	27	39	rVB	297156	767424	14.72%	3.182%
3	1.667	39	42	43	rBV	110590	149111	2.86%	0.618%
4	1.690	43	44	53	rVB	576917	907577	17.41%	3.764%
5	1.816	53	55	96	rVB	2473370	5212537	100.00%	21.615%
6	4.993	331	333	339	rVB	219781	277463	5.32%	1.151%
7	5.507	376	378	381	rBV	1075169	1155188	22.16%	4.790%
8	6.787	487	490	492	rBV	1181796	1261808	24.21%	5.232%
9	6.925	500	502	505	rBV	1175721	1267210	24.31%	5.255%
10	7.222	525	528	530	rBV	235905	296738	5.69%	1.231%
11	7.405	542	544	546	rBV	1078539	987258	18.94%	4.094%
12	7.908	586	588	591	rBV	855584	749982	14.39%	3.110%
13	8.788	663	665	668	rBV	325075	403381	7.74%	1.673%
14	10.136	781	783	786	rBV	1448253	1480358	28.40%	6.139%
15	10.971	854	856	858	rVB	421789	456965	8.77%	1.895%
16	11.942	939	941	944	rBV2	715672	983934	18.88%	4.080%
17	12.811	1014	1017	1019	rBV	510421	478834	9.19%	1.986%
18	14.320	1147	1149	1151	rBV	49736	54065	1.04%	0.224%
19	14.594	1171	1173	1175	rBV	52108	56718	1.09%	0.235%
20	14.811	1189	1192	1194	rBV	1459258	1701710	32.65%	7.057%
21	15.988	1292	1295	1301	rBV2	115246	176914	3.39%	0.734%
22	16.114	1303	1306	1308	rVV	559525	615853	11.81%	2.554%
23	16.148	1308	1309	1314	rVB2	37561	53939	1.03%	0.224%
24	17.451	1421	1423	1425	rBV	33555	63017	1.21%	0.261%
25	17.931	1462	1465	1471	rBV	443011	640649	12.29%	2.657%
26	19.360	1587	1590	1595	rBV2	19253	54016	1.04%	0.224%

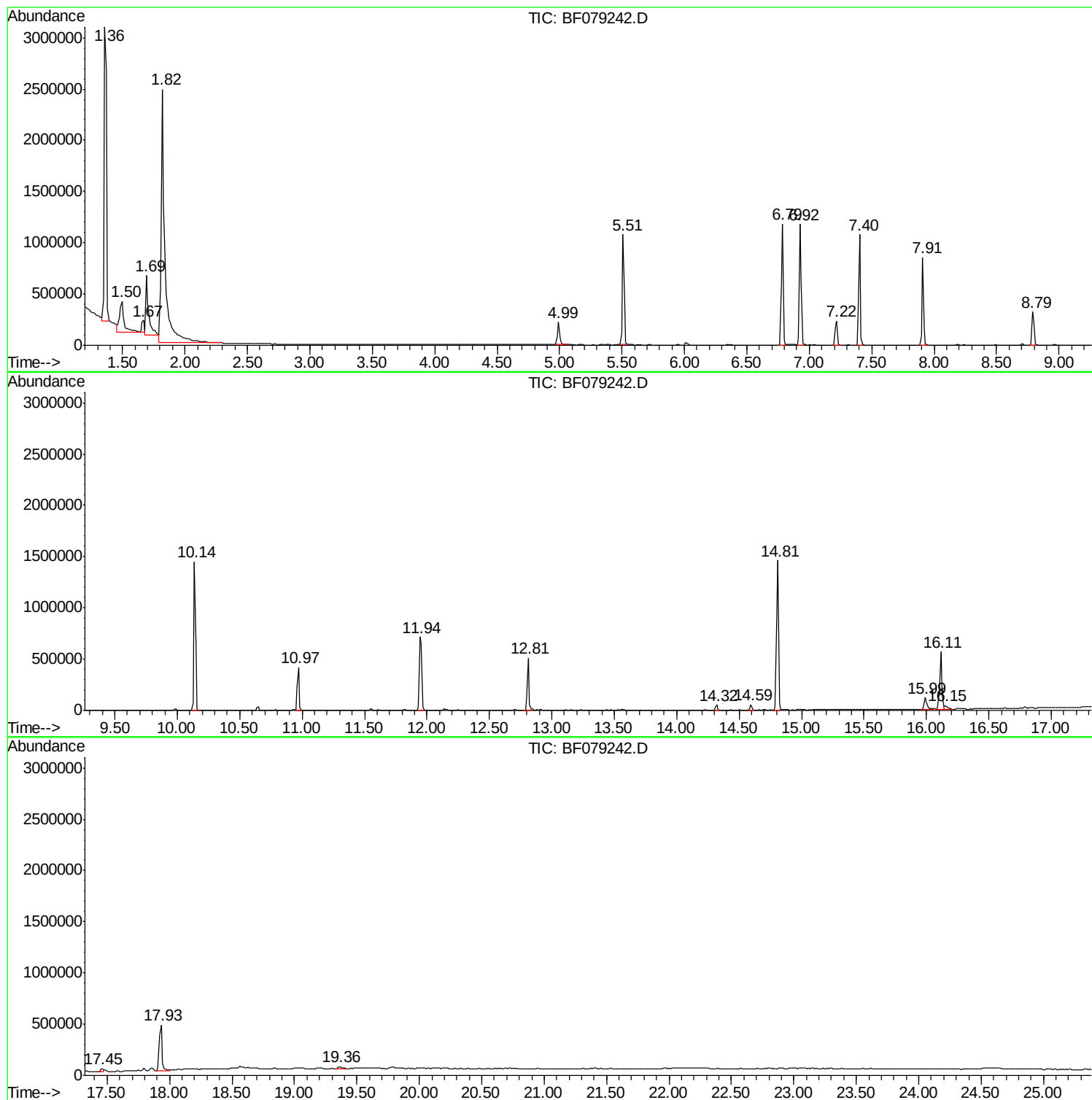
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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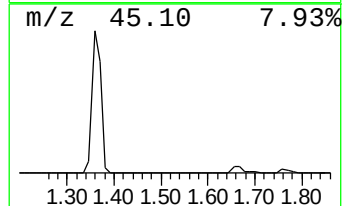
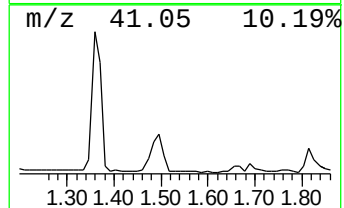
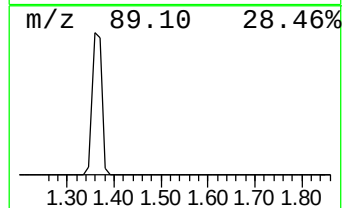
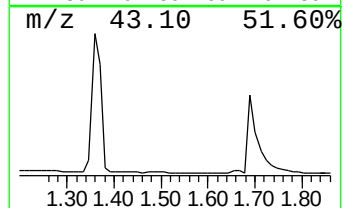
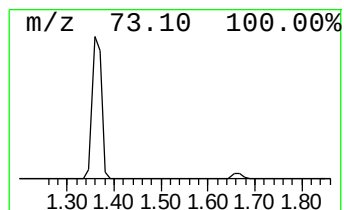
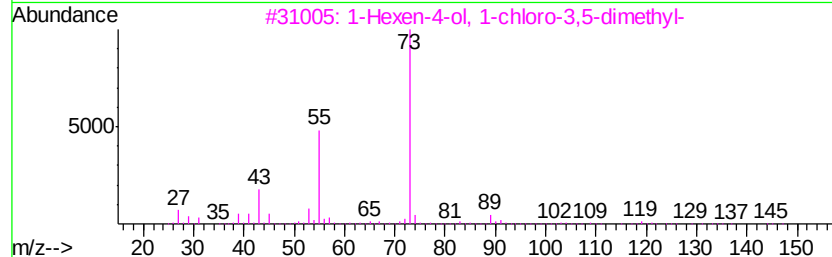
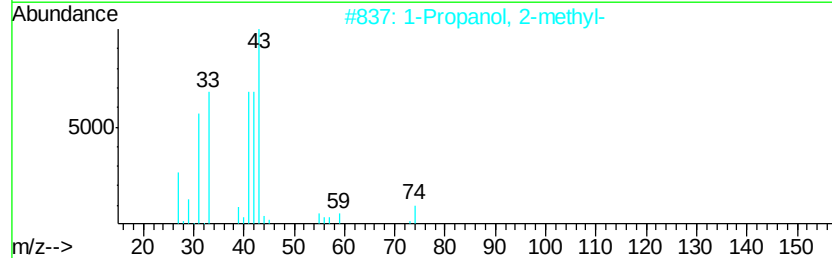
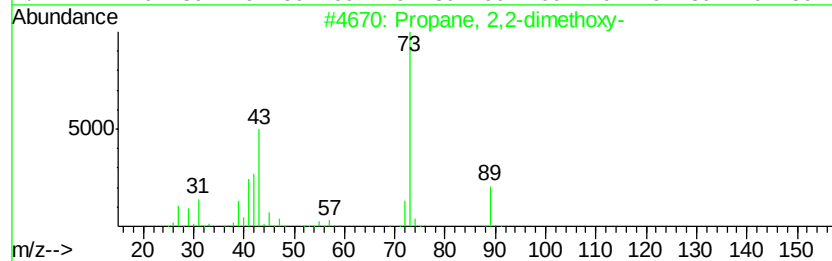
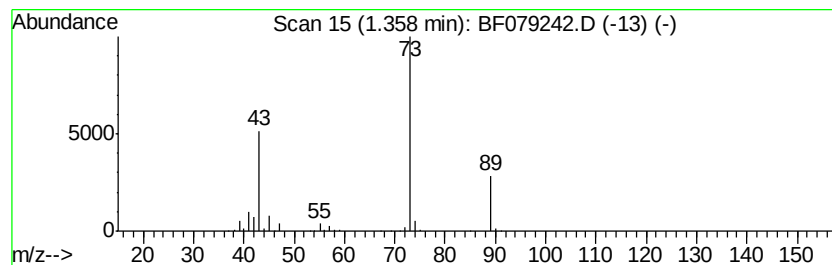
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.36	260.31 ng	3862200	1,4-Dichlorobenzene-d4	7.22

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		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9



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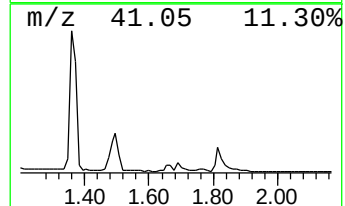
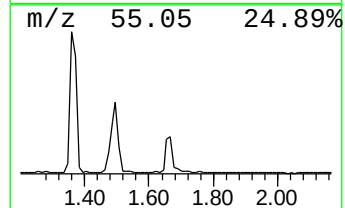
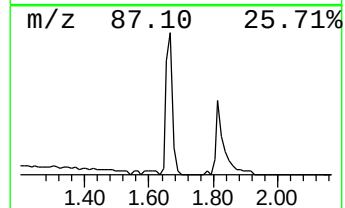
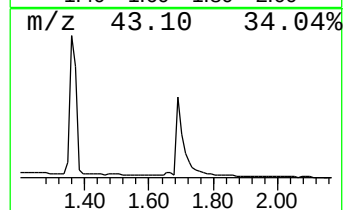
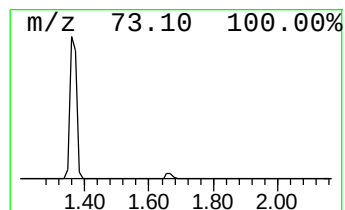
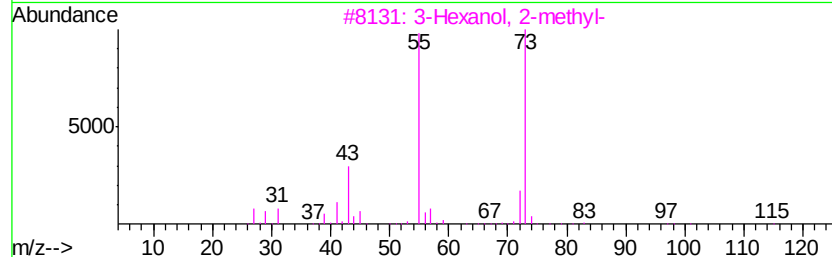
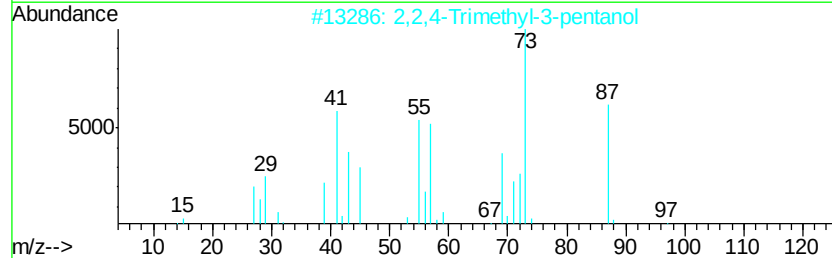
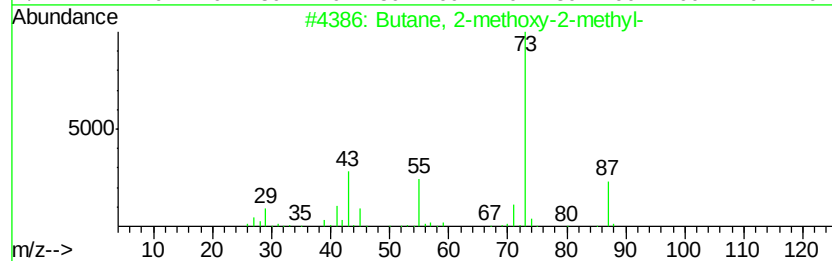
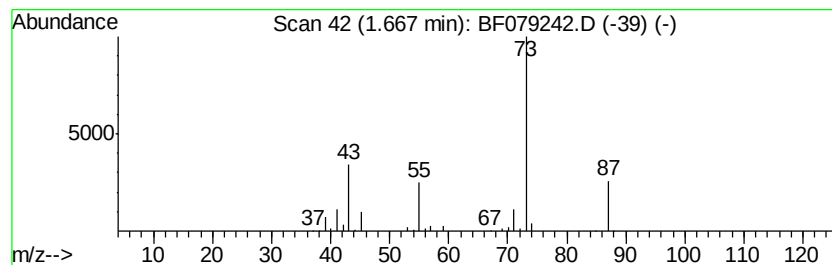
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	10.05 ng	149111	1,4-Dichlorobenzene-d4	7.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	23
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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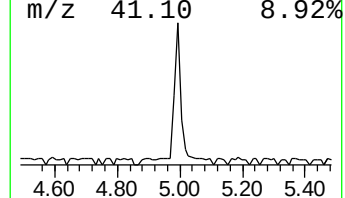
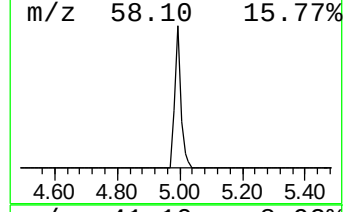
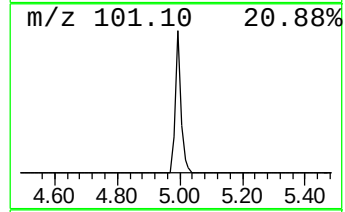
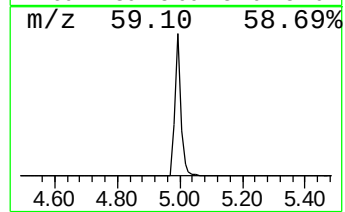
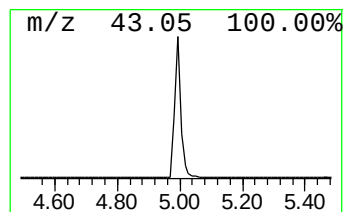
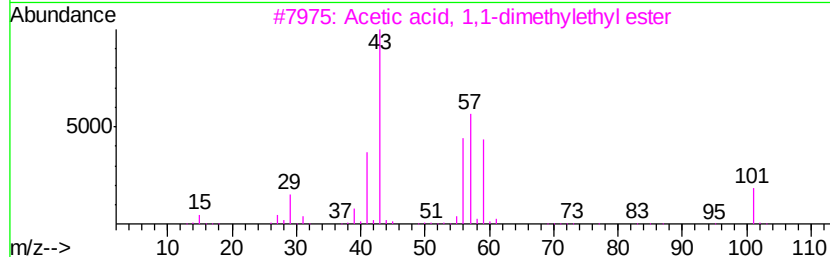
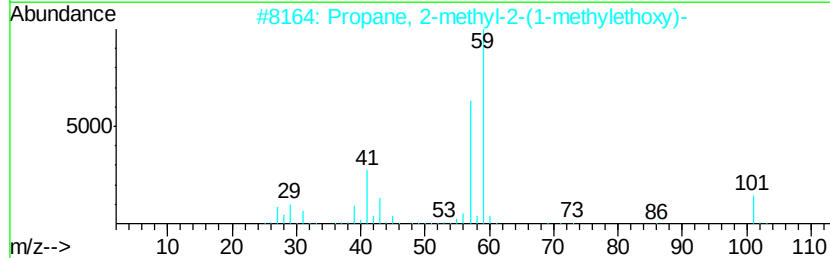
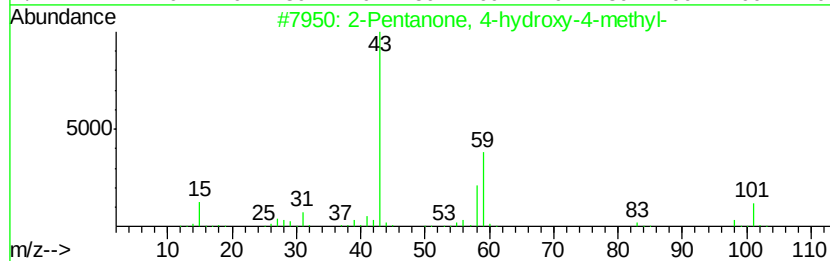
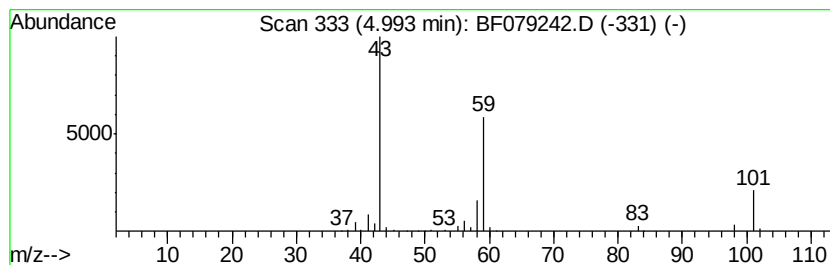
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	18.70 ng	277463	1,4-Dichlorobenzene-d4	7.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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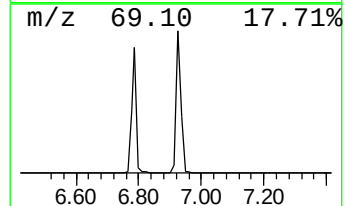
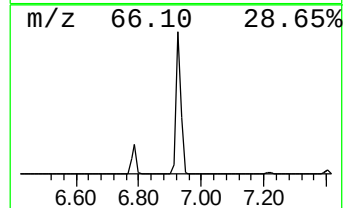
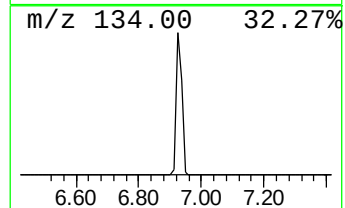
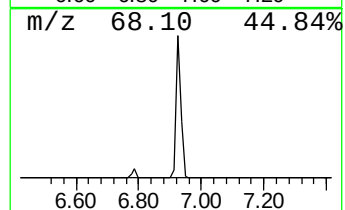
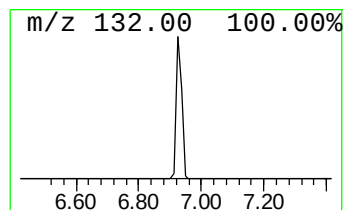
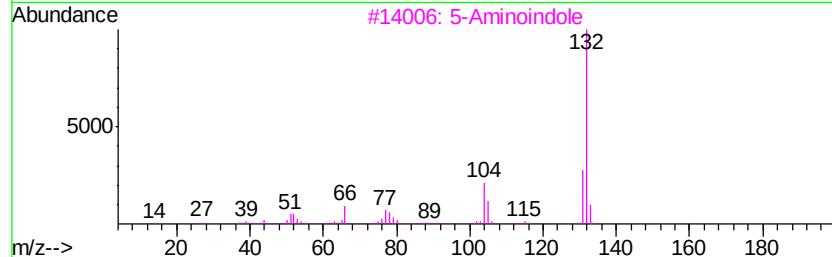
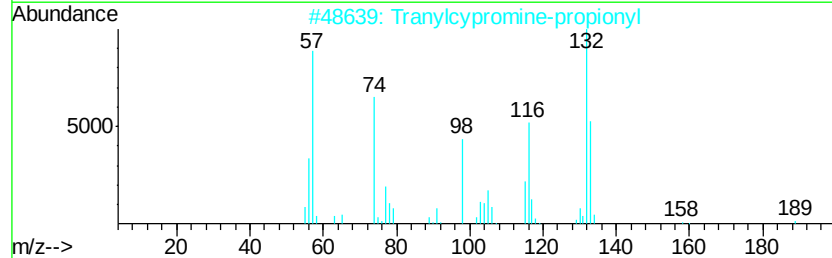
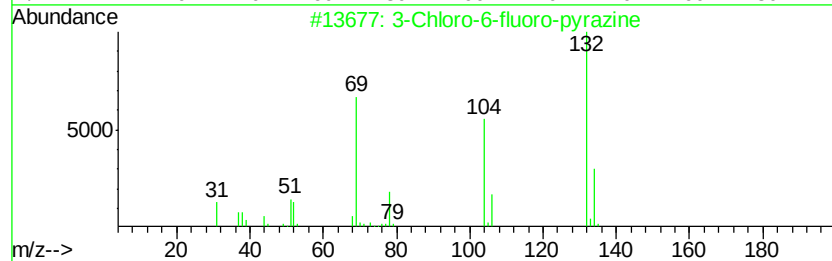
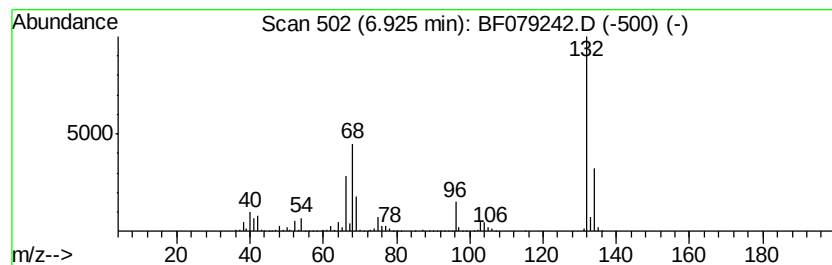
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 unknown6.92 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.92	85.41 ng	1267210	1,4-Dichlorobenzene-d4	7.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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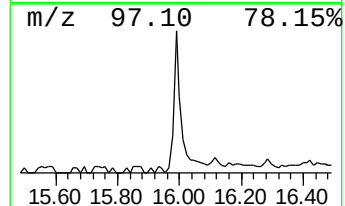
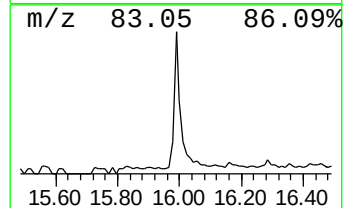
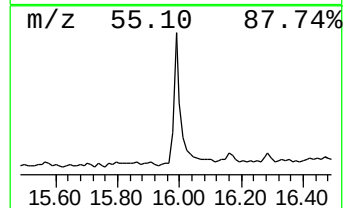
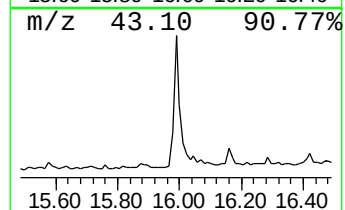
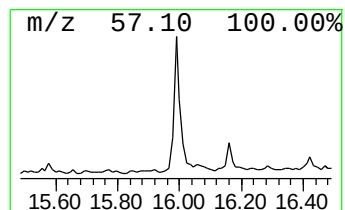
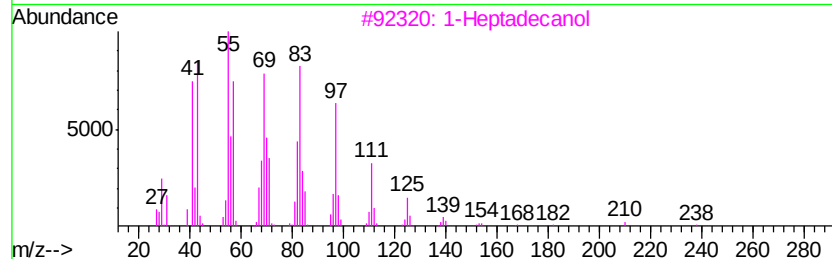
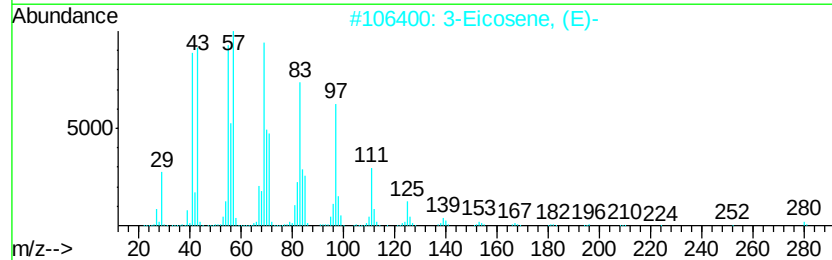
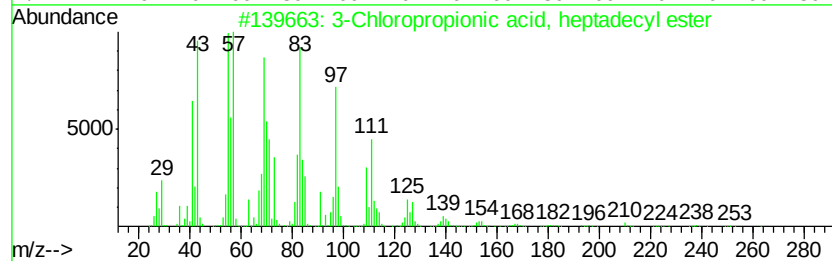
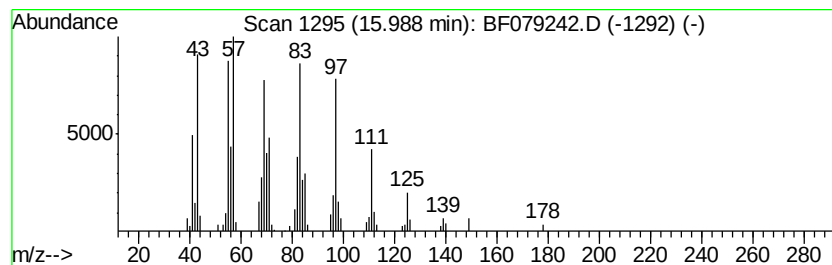
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 3-Chloropropionic acid, hep... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	5.75 ng	176914	Chrysene-d12	16.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	90
3		1-Heptadecanol	256	C17H36O	001454-85-9	87
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.36	260.3	ng	3862200	1	7.22	296738	20.0
Butane, 2-methoxy...	1.67	10.1	ng	149111	1	7.22	296738	20.0
2-Pentanone, 4-hy...	4.99	18.7	ng	277463	1	7.22	296738	20.0
unknown6.92	6.92	85.4	ng	1267210	1	7.22	296738	20.0
3-Chloropropionic...	15.99	5.8	ng	176914	5	16.11	615853	20.0