

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050815\
Data File : BF079099.D
Acq On : 10 May 2015 00:13
Operator : TP/IZ
Sample : G2152-08
Misc :
ALS Vial : 58 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-050515

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_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	1.484	23	26	29	rVB	4769615	5268212	88.10%	18.007%
2	1.621	35	38	41	rVB	195995	316563	5.29%	1.082%
3	1.747	47	49	52	rBV	313692	425760	7.12%	1.455%
4	1.793	52	53	58	rVV	177593	276473	4.62%	0.945%
5	1.873	58	60	100	rVB	2955369	5979813	100.00%	20.439%
6	5.119	343	344	351	rVB	76766	99781	1.67%	0.341%
7	5.622	385	388	391	rBV	1511002	1497970	25.05%	5.120%
8	6.879	495	498	500	rBV	1808205	1607245	26.88%	5.494%
9	7.027	509	511	514	rBV	1562636	1606476	26.86%	5.491%
10	7.325	534	537	539	rBV	388661	536105	8.97%	1.832%
11	7.508	550	553	555	rBV	1348706	1253463	20.96%	4.284%
12	8.010	594	597	599	rBV	1147259	1012708	16.94%	3.461%
13	8.890	672	674	676	rBV	629333	752641	12.59%	2.573%
14	10.239	790	792	795	rBV	2153431	1931500	32.30%	6.602%
15	10.742	834	836	839	rVB	71620	67402	1.13%	0.230%
16	11.074	862	865	867	rBV	806764	825803	13.81%	2.823%
17	12.057	948	951	953	rBV2	866104	1136559	19.01%	3.885%
18	12.914	1024	1026	1029	rBV	756481	805231	13.47%	2.752%
19	14.914	1198	1201	1204	rBV	1996240	1932794	32.32%	6.606%
20	16.080	1300	1303	1312	rBV	159415	237673	3.97%	0.812%
21	16.206	1312	1314	1317	rBV	707303	831026	13.90%	2.840%
22	17.943	1463	1466	1469	rBV	692509	855746	14.31%	2.925%

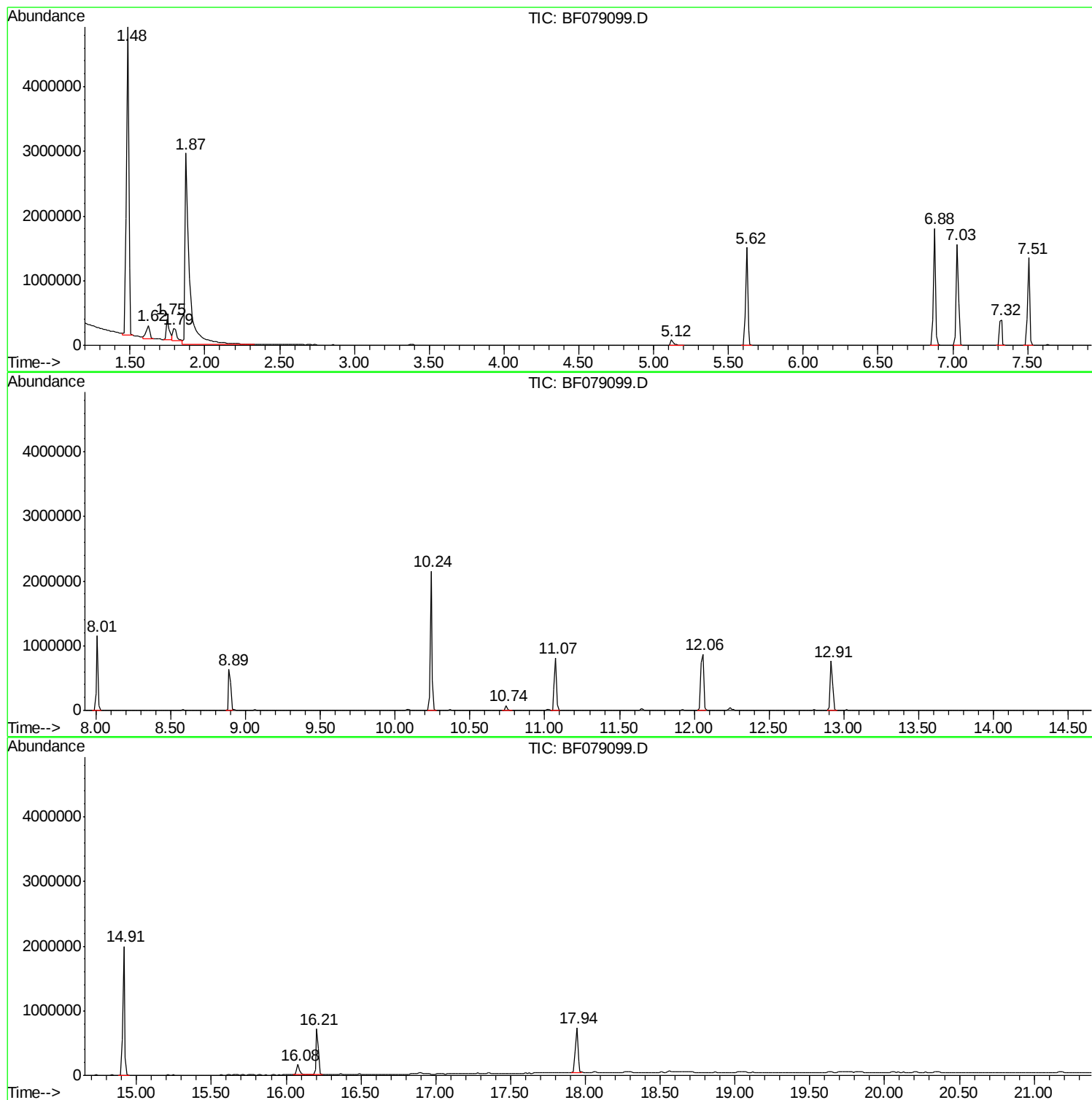
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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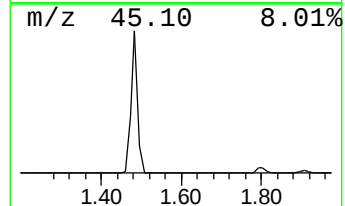
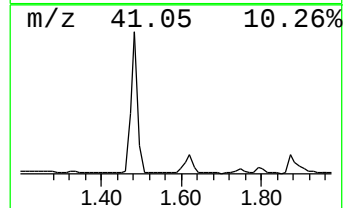
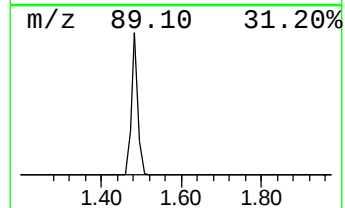
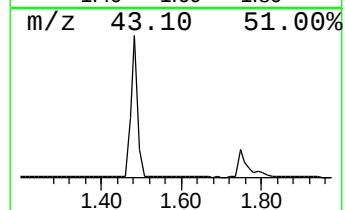
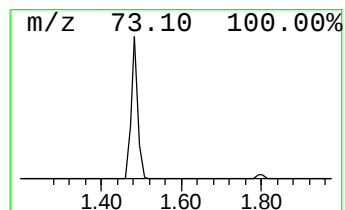
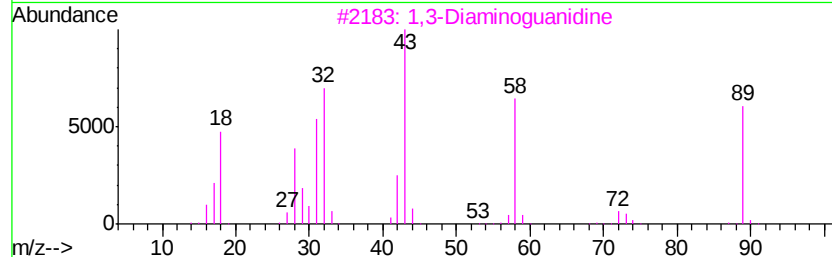
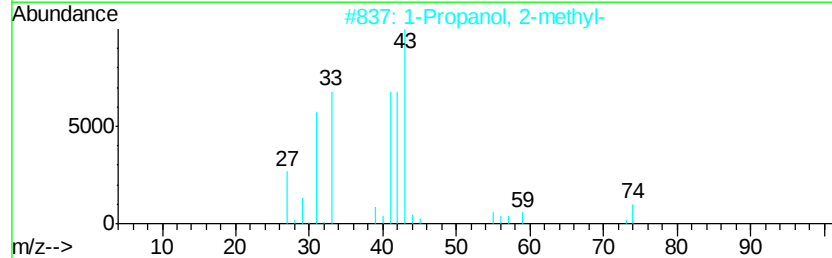
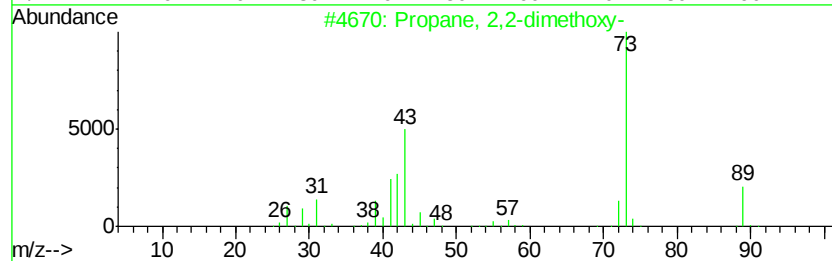
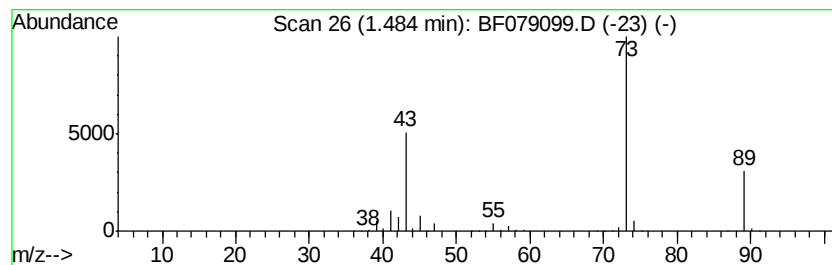
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown1.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	196.54 ng	5268210	1,4-Dichlorobenzene-d4	7.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3		1,3-Diaminoquanidine	89	CH7N5	004364-78-7	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9



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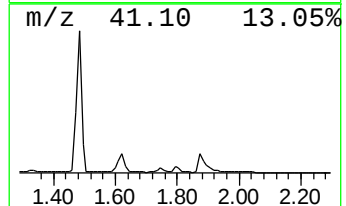
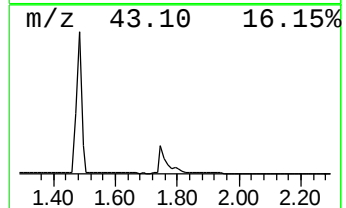
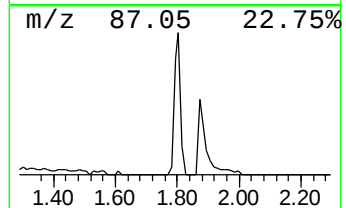
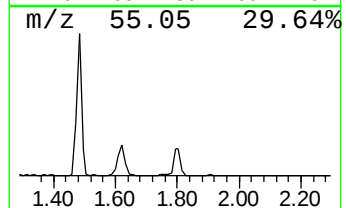
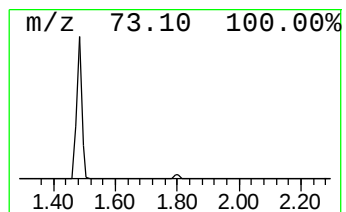
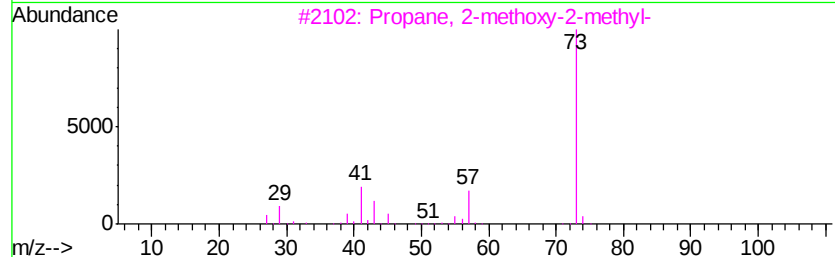
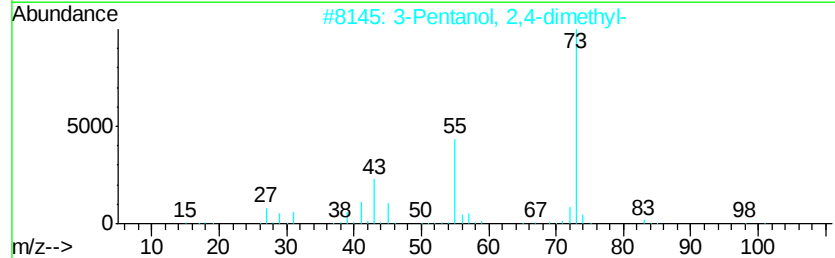
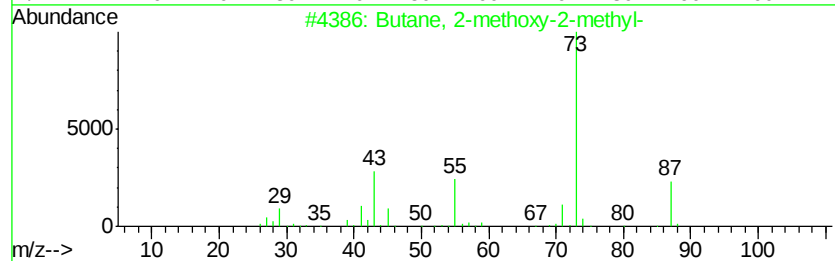
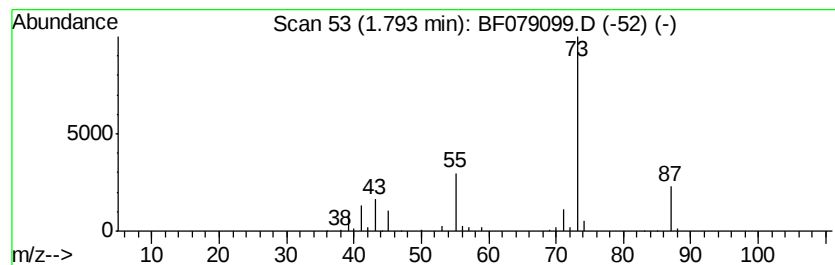
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	10.31 ng	276473	1,4-Dichlorobenzene-d4	7.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
3			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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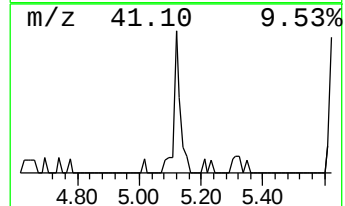
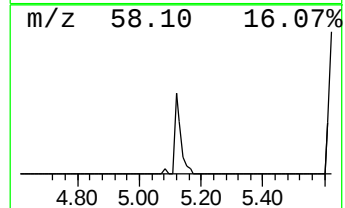
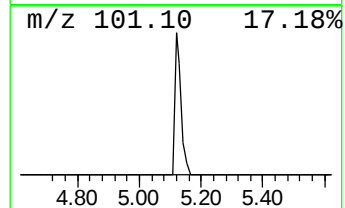
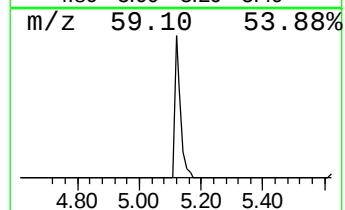
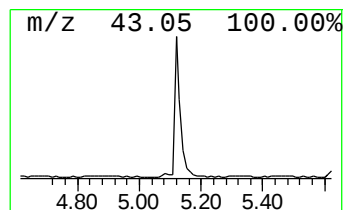
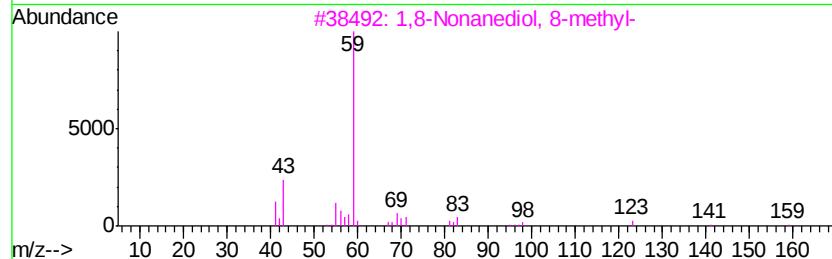
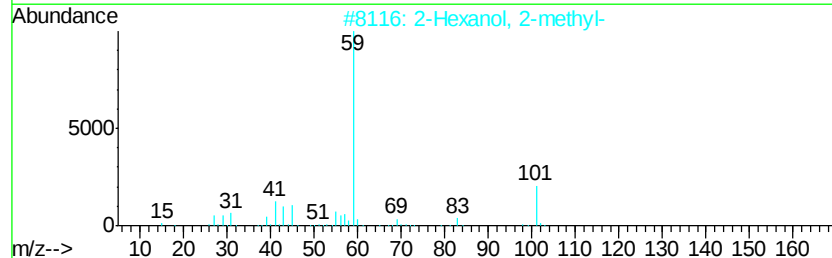
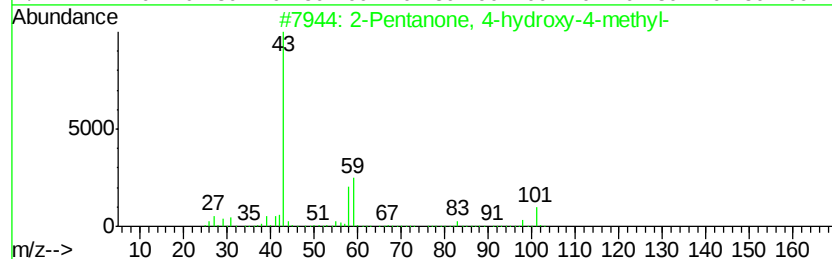
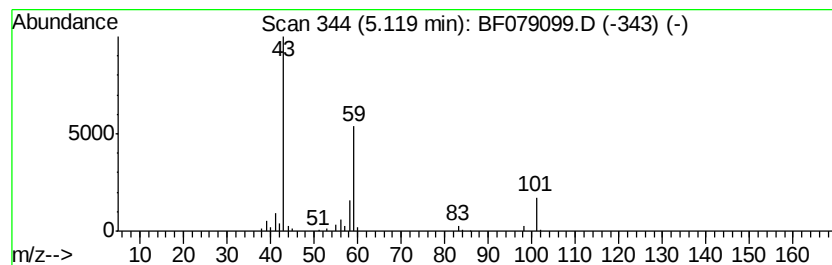
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Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.72 ng	99781	1,4-Dichlorobenzene-d4	7.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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Misc :
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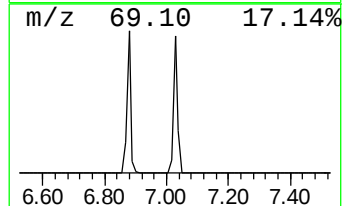
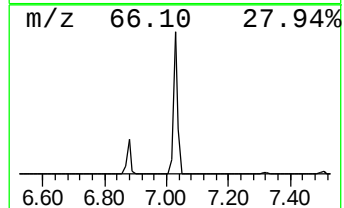
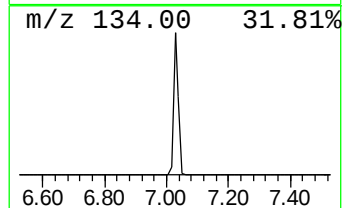
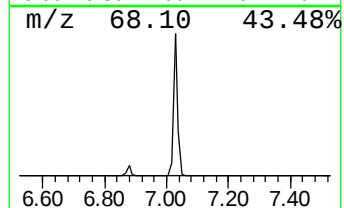
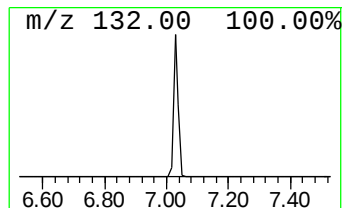
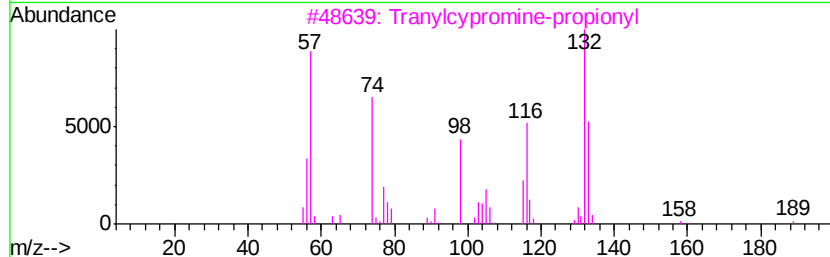
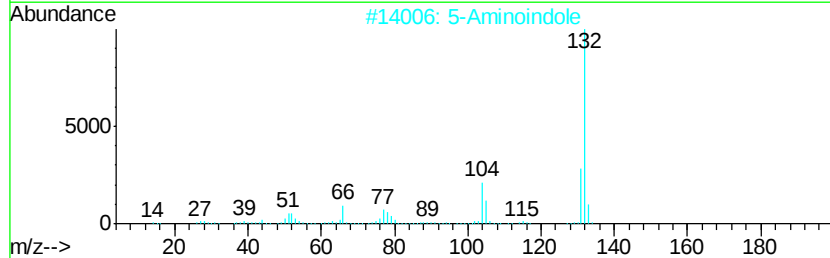
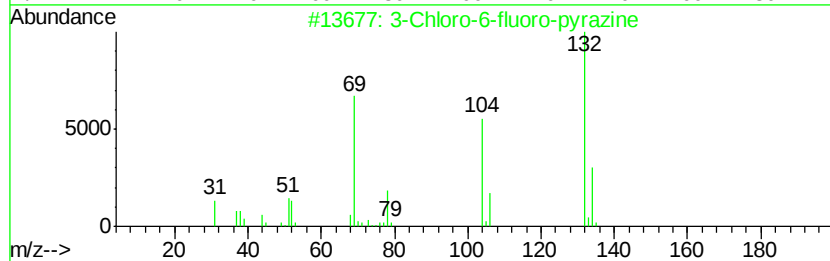
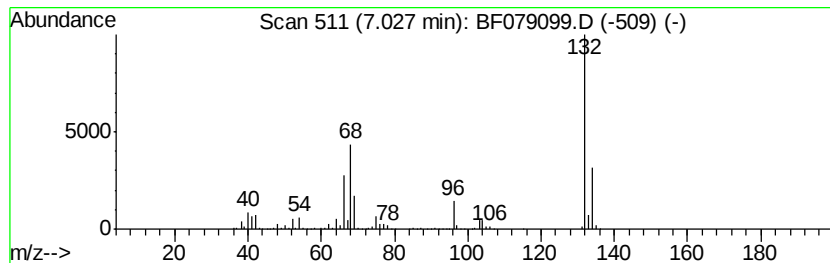
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Peak Number 7 unknown7.03 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	59.93 ng	1606480	1,4-Dichlorobenzene-d4	7.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5	Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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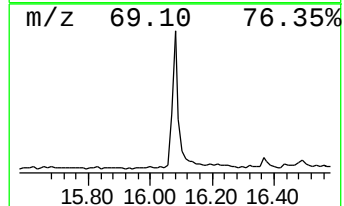
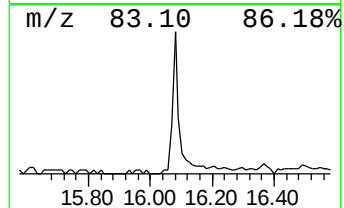
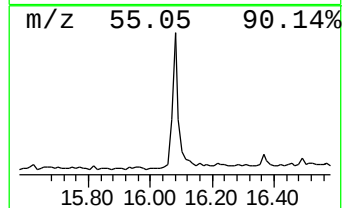
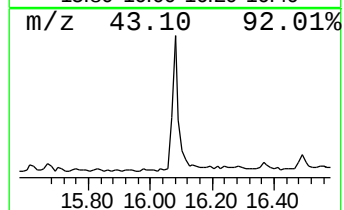
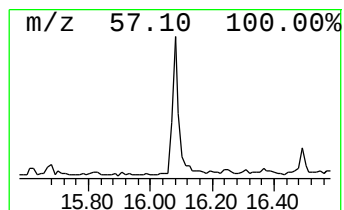
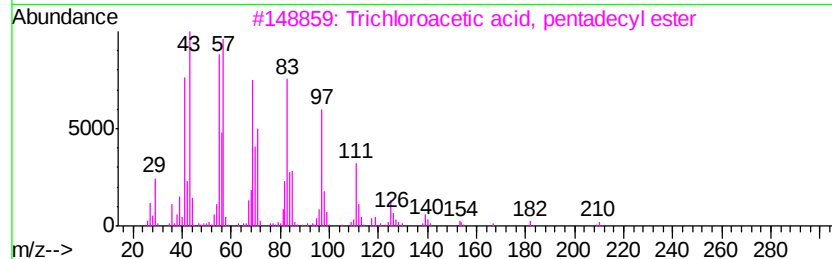
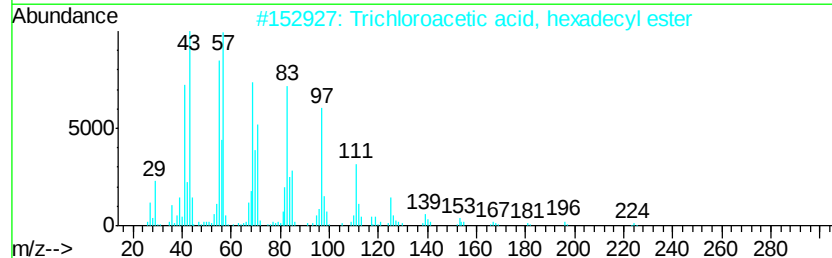
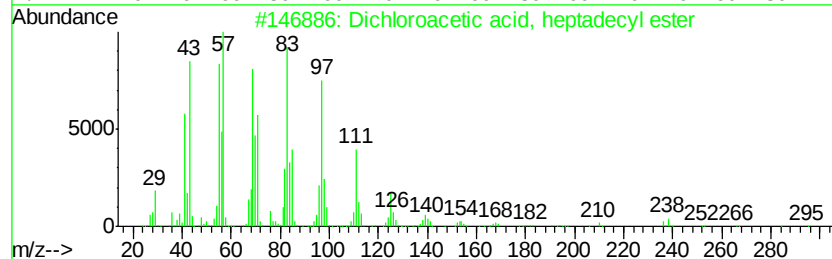
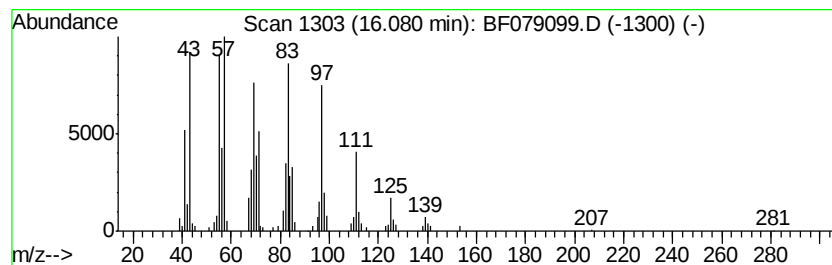
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Dichloroacetic acid, heptad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	5.72 ng	237673	Chrysene-d12	16.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.48	1.48	196.5	ng	5268210	1	7.32	536105	20.0
Butane, 2-methoxy...	1.79	10.3	ng	276473	1	7.32	536105	20.0
2-Pentanone, 4-hy...	5.12	3.7	ng	99781	1	7.32	536105	20.0
unknown7.03	7.03	59.9	ng	1606480	1	7.32	536105	20.0
Dichloroacetic ac...	16.08	5.7	ng	237673	5	16.21	831026	20.0