

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051115\
 Data File : BF079147.D
 Acq On : 12 May 2015 8:04
 Operator : TP/IZ
 Sample : G2176-08
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PS-29(5-10)

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	1.438	20	22	25	rVB	4254554	4890729	100.00%	22.151%
2	1.575	31	34	37	rVB	161164	244512	5.00%	1.107%
3	1.747	47	49	57	rVV2	213714	460124	9.41%	2.084%
4	1.861	57	59	91	rVB	1163083	2113585	43.22%	9.573%
5	5.096	340	342	350	rVB	58021	70934	1.45%	0.321%
6	5.599	384	386	389	rBV	1179238	1278442	26.14%	5.790%
7	6.867	494	497	499	rBV	1494789	1420282	29.04%	6.433%
8	7.016	507	510	512	rBV	1274204	1418930	29.01%	6.427%
9	7.302	532	535	537	rBV	258416	282725	5.78%	1.281%
10	7.485	549	551	553	rBV	1192028	1050198	21.47%	4.757%
11	7.988	593	595	598	rBV	938832	827034	16.91%	3.746%
12	8.879	670	673	675	rBV	322943	394779	8.07%	1.788%
13	10.216	788	790	793	rBV	1448858	1629654	33.32%	7.381%
14	10.719	833	834	837	rBV	49931	63956	1.31%	0.290%
15	11.051	861	863	866	rVB	511833	470258	9.62%	2.130%
16	12.034	946	949	951	rBV	1202339	1186530	24.26%	5.374%
17	12.891	1022	1024	1026	rBV	420461	514330	10.52%	2.329%
18	14.400	1154	1156	1159	rVB	45201	56716	1.16%	0.257%
19	14.685	1178	1181	1182	rBV	59338	65107	1.33%	0.295%
20	14.891	1197	1199	1202	rBV	1846396	1982843	40.54%	8.981%
21	16.057	1299	1301	1308	rVB	149550	235632	4.82%	1.067%
22	16.183	1310	1312	1315	rBV	448642	715763	14.64%	3.242%
23	17.931	1462	1465	1469	rBV	506166	705953	14.43%	3.197%

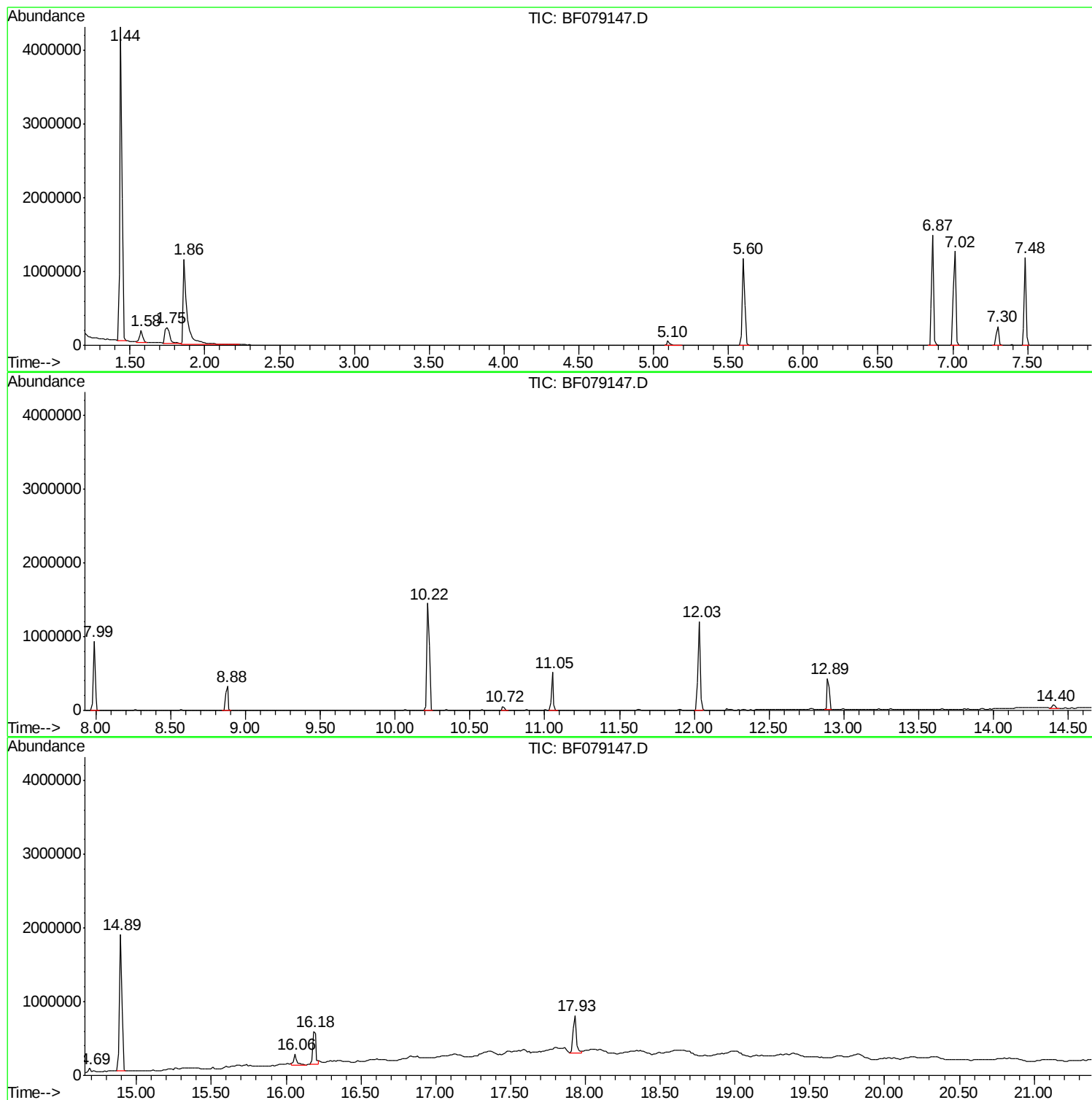
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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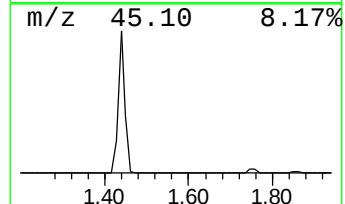
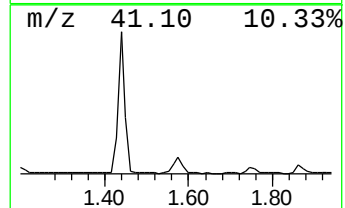
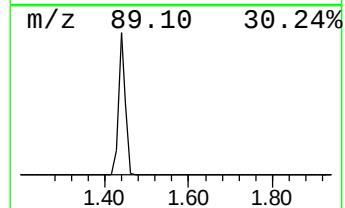
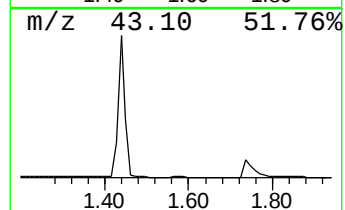
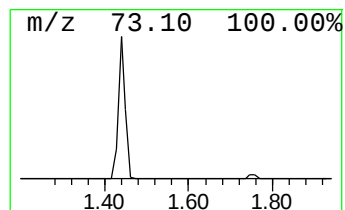
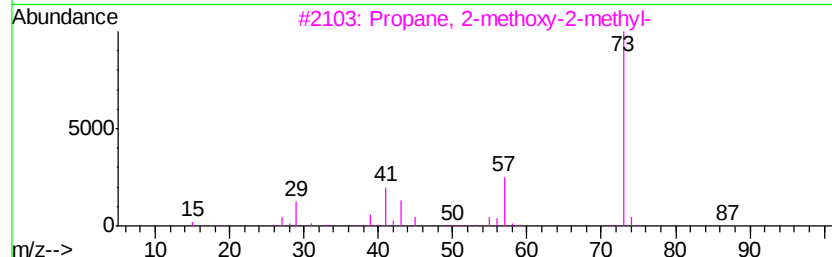
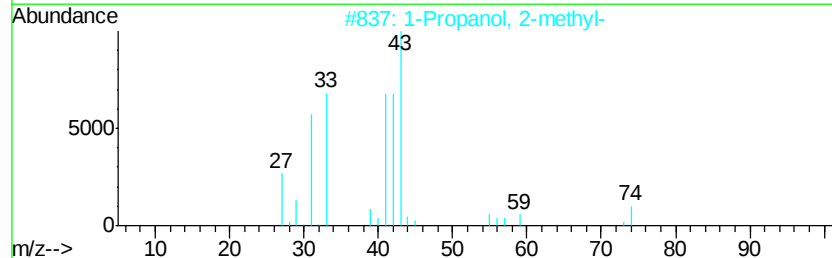
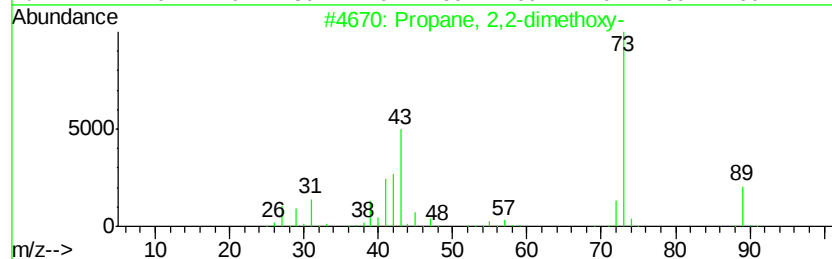
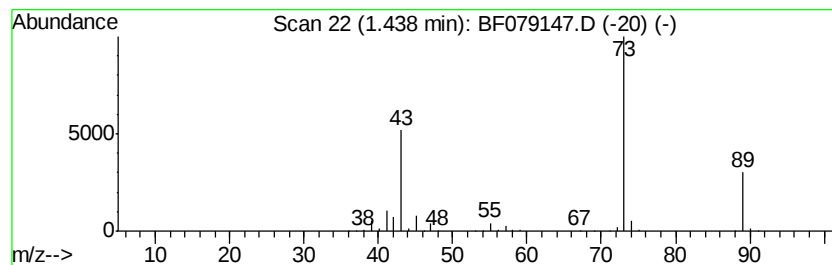
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
1.44	345.97 ng	4890730	1,4-Dichlorobenzene-d4	7.30

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		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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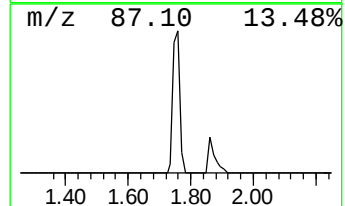
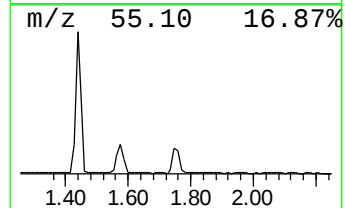
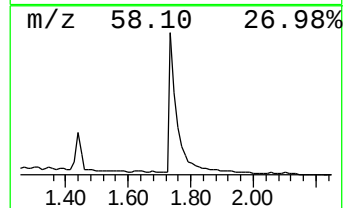
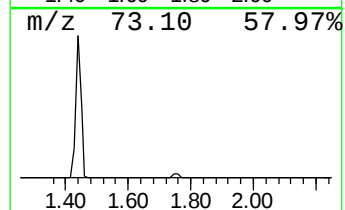
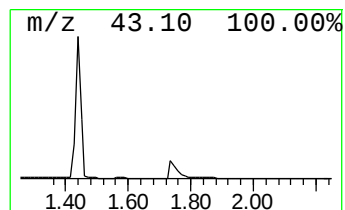
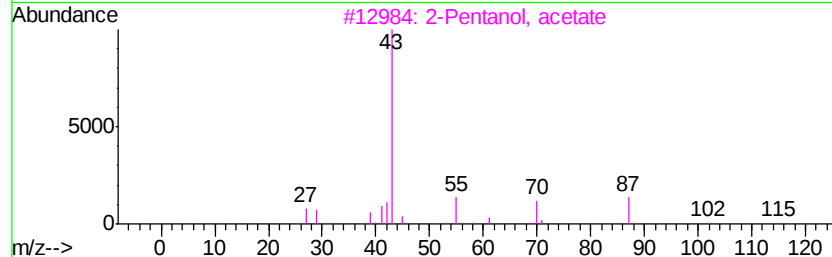
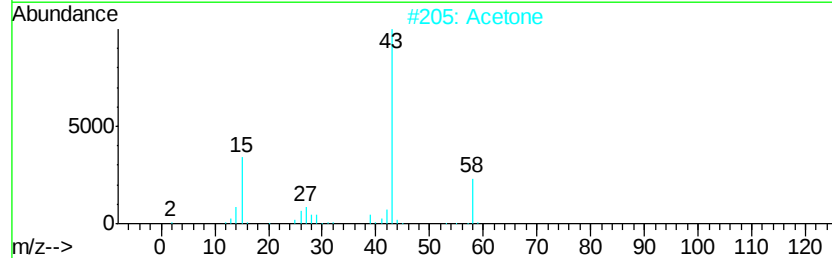
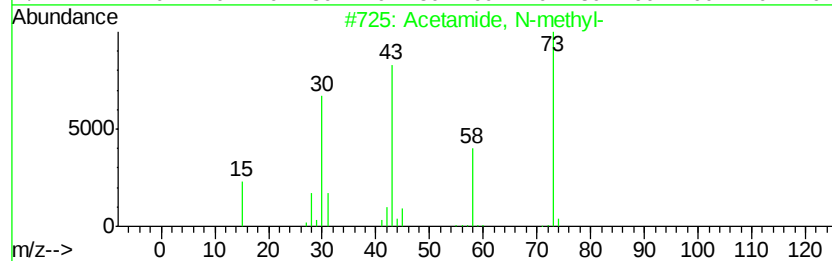
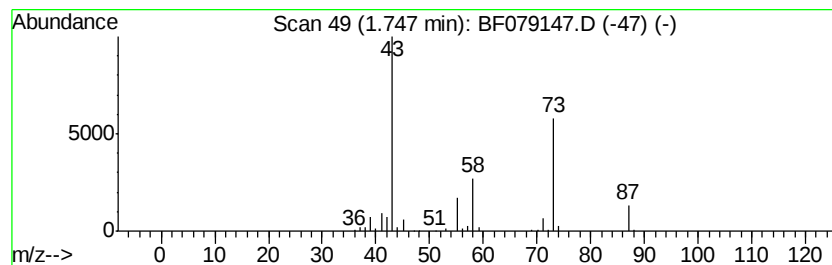
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown1.75 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.75	32.55 ng	460124	1,4-Dichlorobenzene-d4	7.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	47
2		Acetone	58	C3H6O	000067-64-1	37
3		2-Pentanol, acetate	130	C7H14O2	000626-38-0	37
4		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	35
5		2-Butanol, 3-methyl-, acetate	130	C7H14O2	005343-96-4	17



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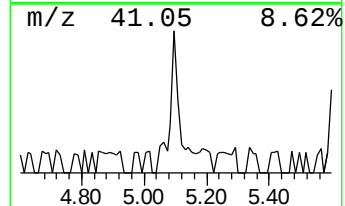
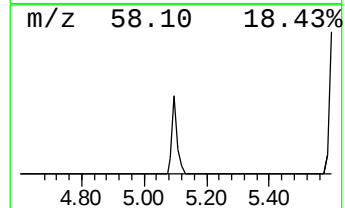
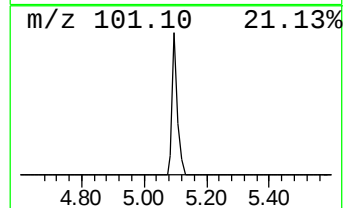
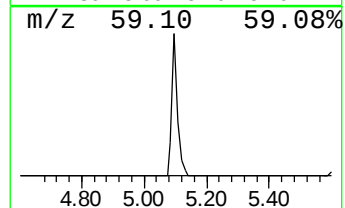
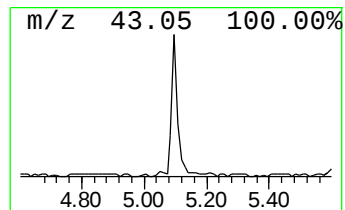
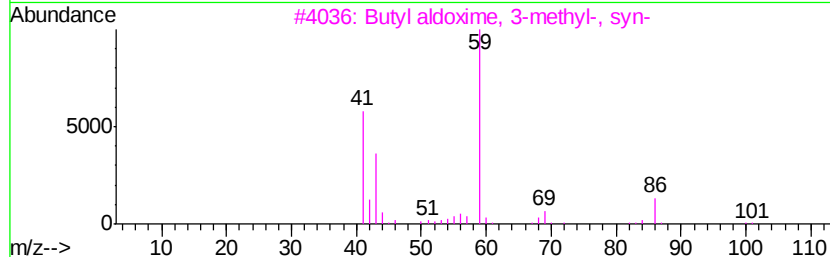
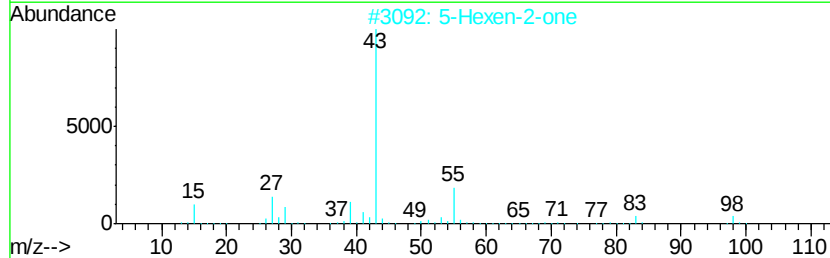
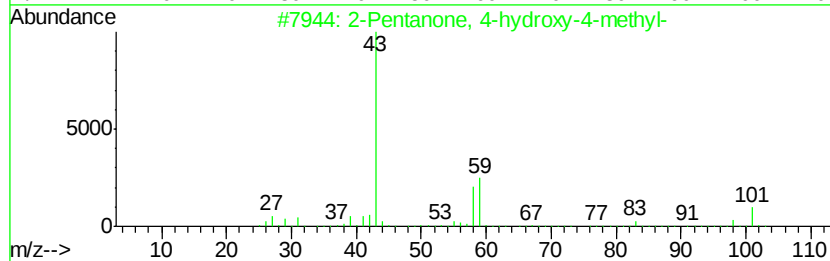
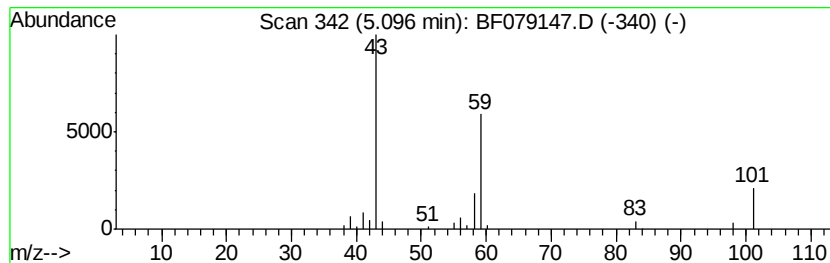
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TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	5.02 ng	70934	1,4-Dichlorobenzene-d4	7.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		5-Hexen-2-one	98	C6H10O	000109-49-9	22
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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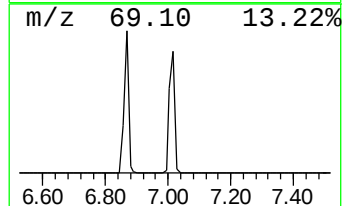
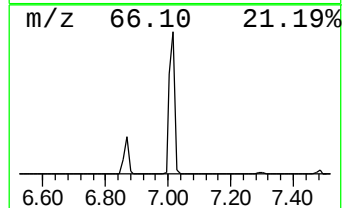
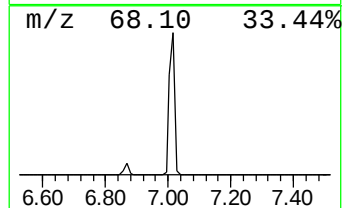
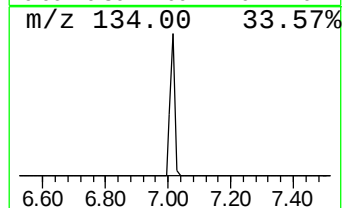
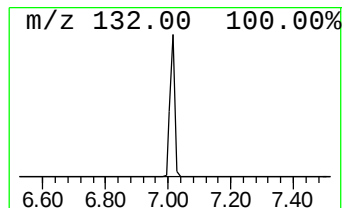
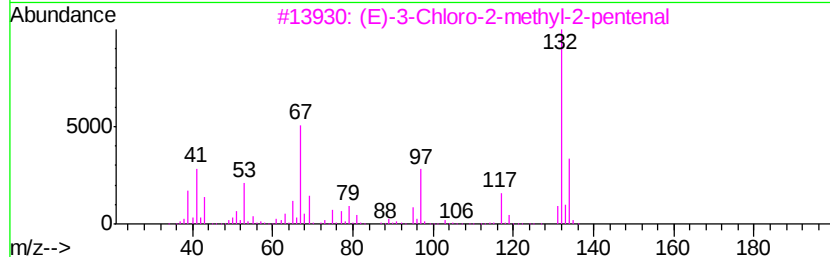
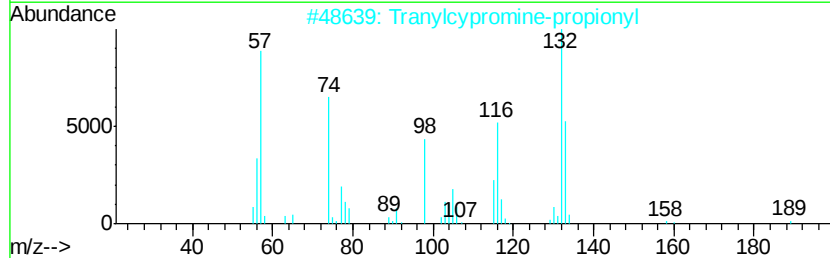
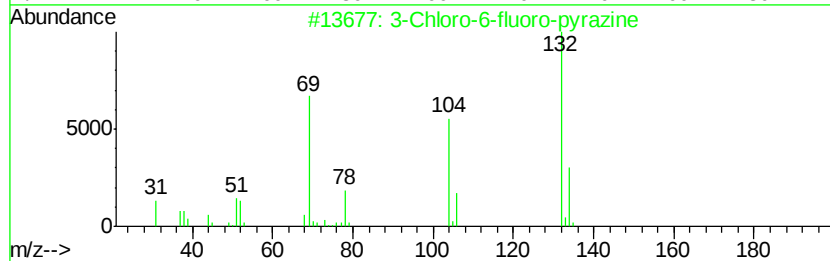
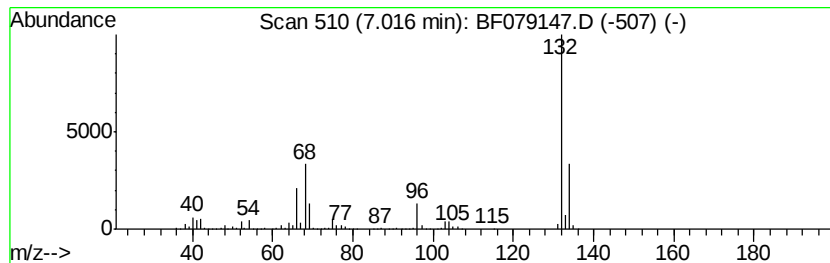
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Peak Number 6 unknown7.02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	100.38 ng	1418930	1,4-Dichlorobenzene-d4	7.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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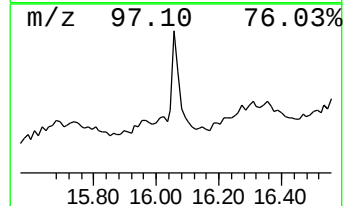
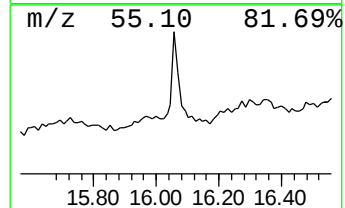
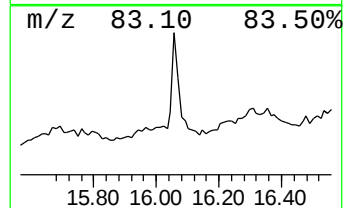
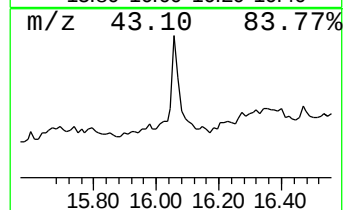
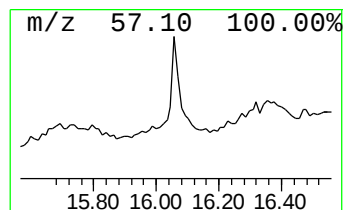
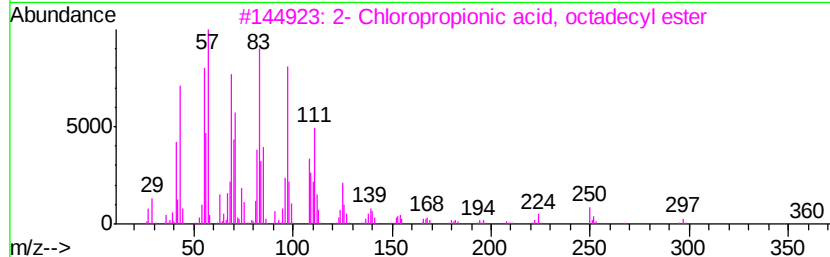
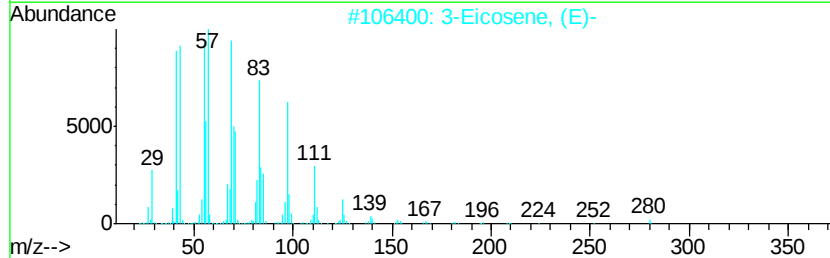
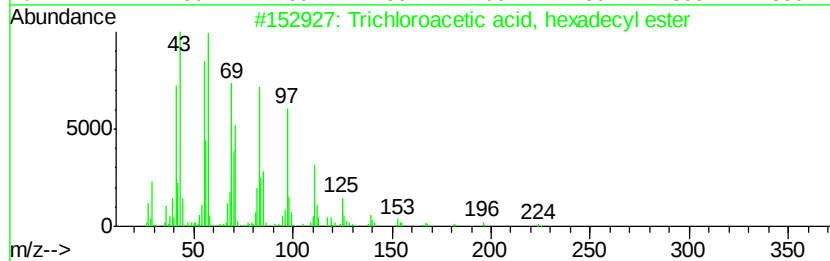
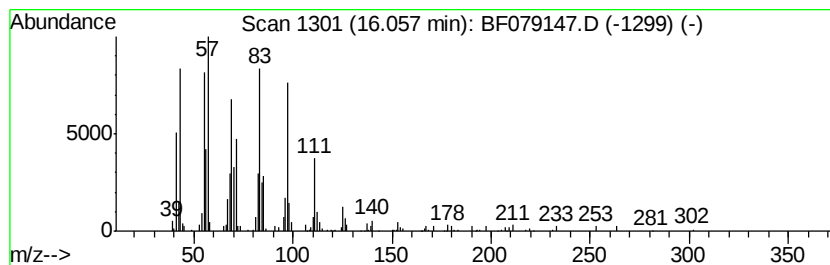
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	6.58 ng	235632	Chrysene-d12	16.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
5		1-Heneicosyl formate	340	C22H44O2	077899-03-7	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.44	346.0	ng	4890730	1	7.30	282725	20.0
unknown1.75	1.75	32.5	ng	460124	1	7.30	282725	20.0
2-Pentanone, 4-hy...	5.10	5.0	ng	70934	1	7.30	282725	20.0
unknown7.02	7.02	100.4	ng	1418930	1	7.30	282725	20.0
Trichloroacetic a...	16.06	6.6	ng	235632	5	16.19	715763	20.0