

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031815\
 Data File : BF077819.D
 Acq On : 19 Mar 2015 4:16
 Operator : TP/IZ
 Sample : G1544-01
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-8(3-5)

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-BF031115.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	1.321	35	38	41	rBV	4609381	5450276	100.00%	34.713%
2	1.447	44	49	51	rBV	69507	130489	2.39%	0.831%
3	1.607	61	63	66	rBV	56788	82373	1.51%	0.525%
4	4.933	352	354	362	rVB	118520	145100	2.66%	0.924%
5	5.459	398	400	403	rBV	801800	889627	16.32%	5.666%
6	6.750	510	513	515	rBV	756191	906975	16.64%	5.777%
7	6.876	522	524	527	rBV	988393	964784	17.70%	6.145%
8	7.162	547	549	552	rBV	239968	208892	3.83%	1.330%
9	7.345	563	565	568	rBV	737274	751262	13.78%	4.785%
10	7.859	607	610	612	rBV	638439	587200	10.77%	3.740%
11	8.739	685	687	689	rBV	348628	295970	5.43%	1.885%
12	10.088	802	805	807	rBV	1230923	1164530	21.37%	7.417%
13	10.911	875	877	879	rBV	345406	335875	6.16%	2.139%
14	11.894	960	963	965	rBV	568037	725487	13.31%	4.621%
15	12.751	1035	1038	1040	rBV	351968	361605	6.63%	2.303%
16	14.751	1210	1213	1215	rBV	993696	1381714	25.35%	8.800%
17	15.928	1313	1316	1319	rBV	135629	192271	3.53%	1.225%
18	16.043	1323	1326	1328	rVV	312712	447666	8.21%	2.851%
19	16.100	1329	1331	1333	rVB	196181	236885	4.35%	1.509%
20	17.814	1478	1481	1484	rBV	367182	441852	8.11%	2.814%

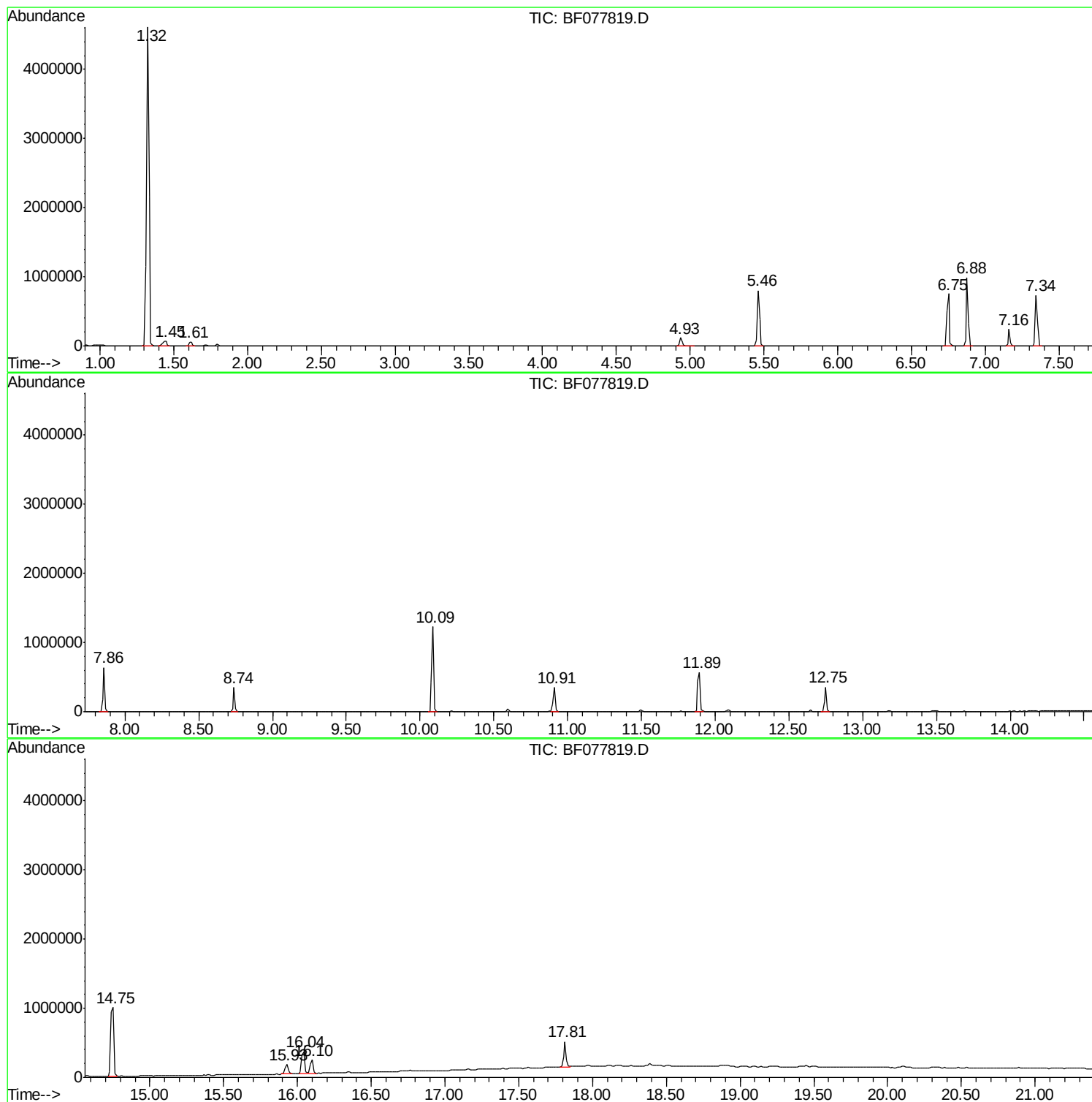
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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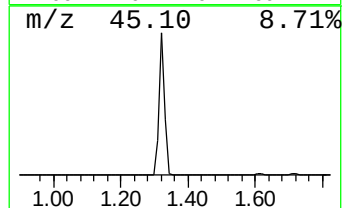
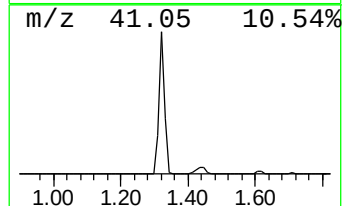
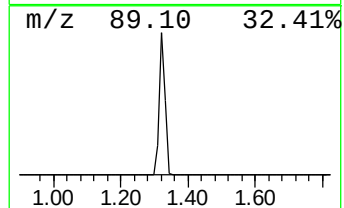
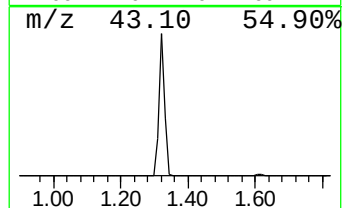
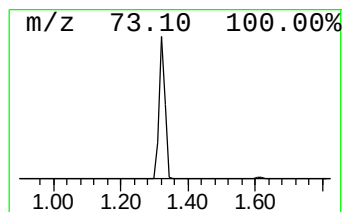
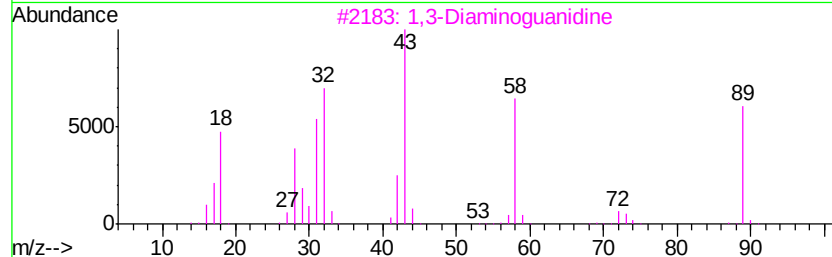
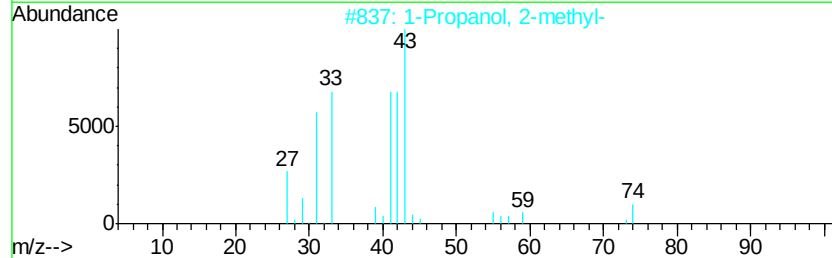
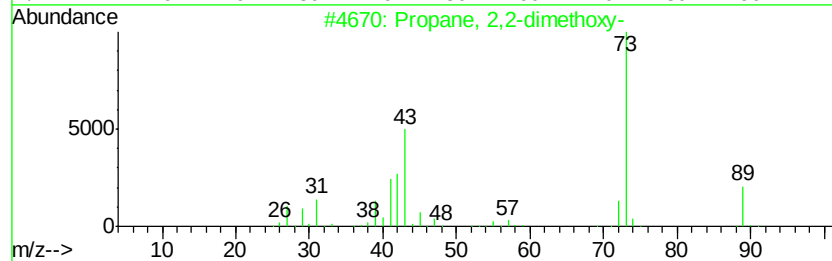
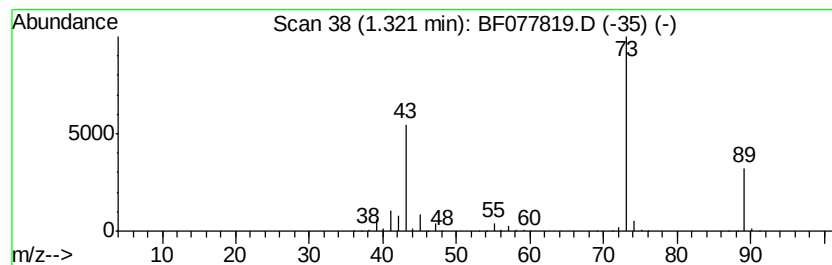
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.32	521.83 ng	5450280	1,4-Dichlorobenzene-d4	7.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9



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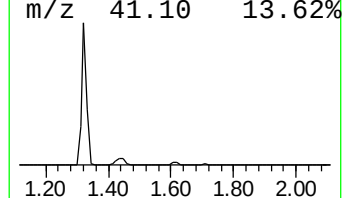
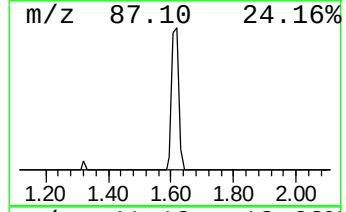
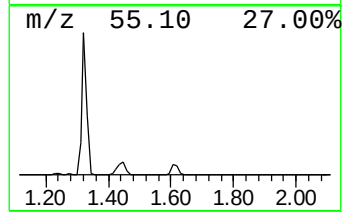
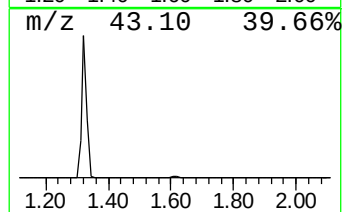
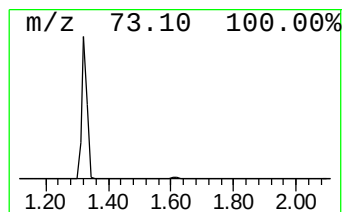
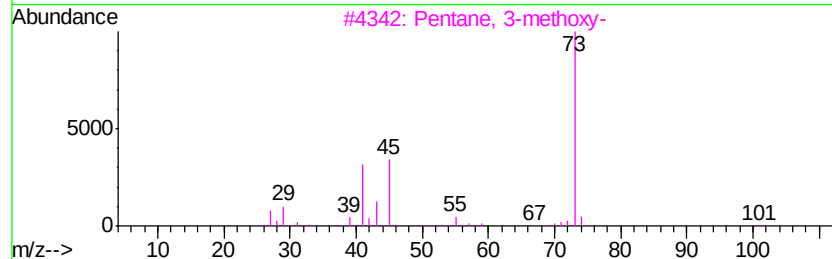
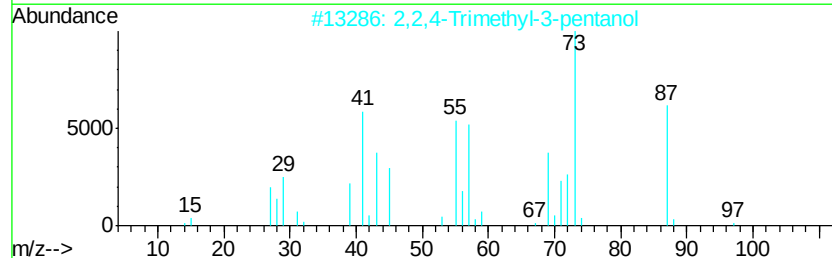
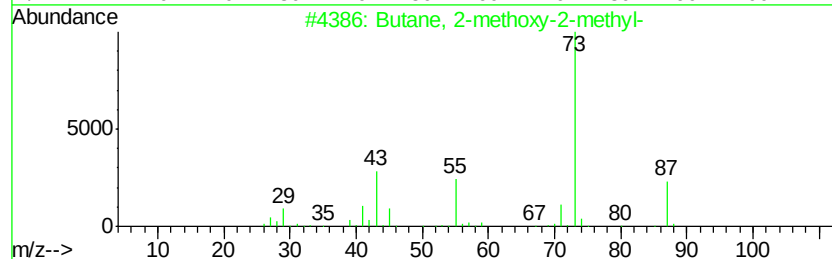
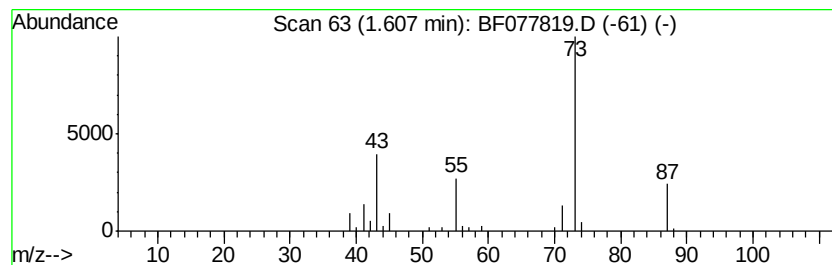
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Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.61	7.89 ng	82373	1,4-Dichlorobenzene-d4	7.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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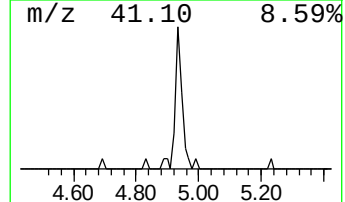
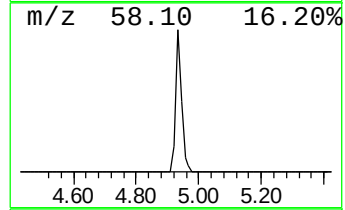
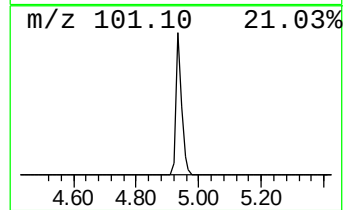
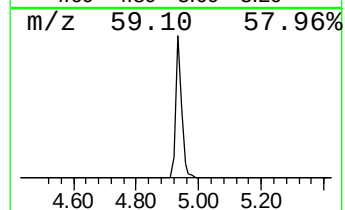
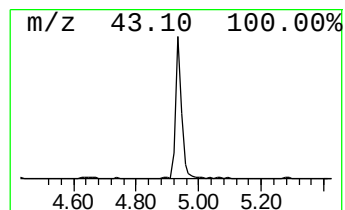
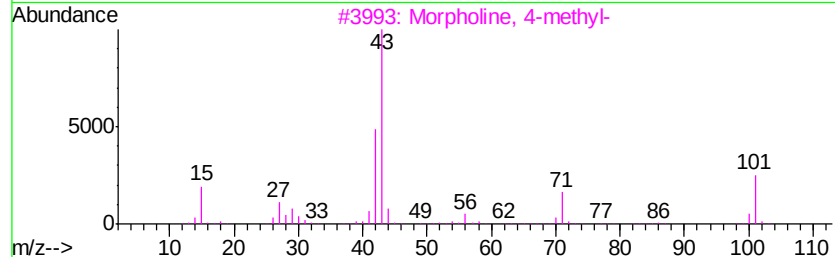
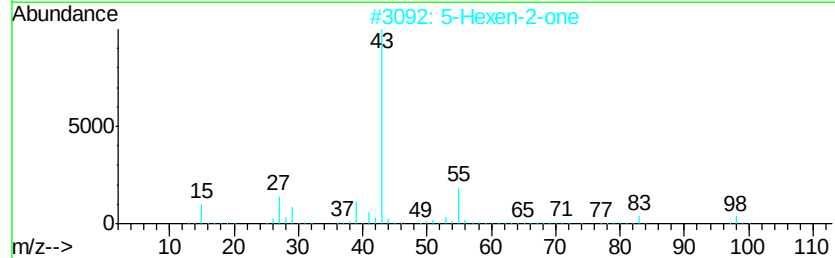
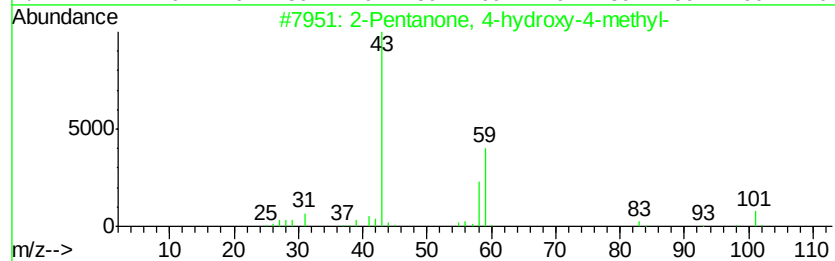
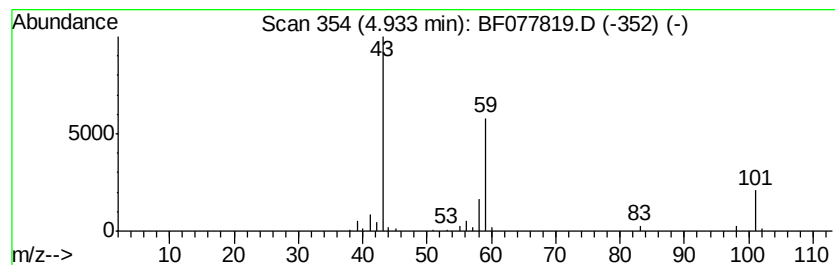
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	13.89 ng	145100	1,4-Dichlorobenzene-d4	7.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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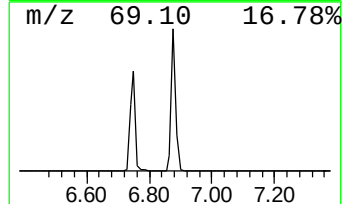
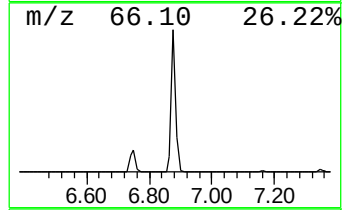
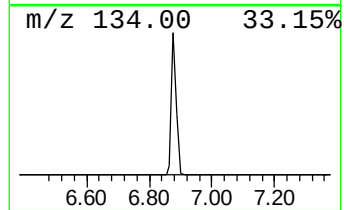
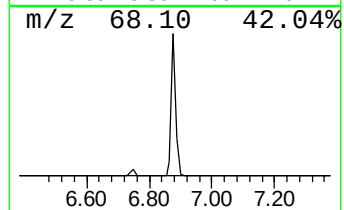
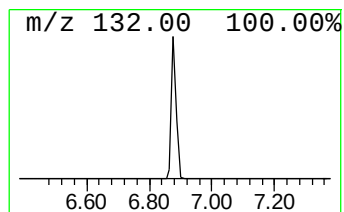
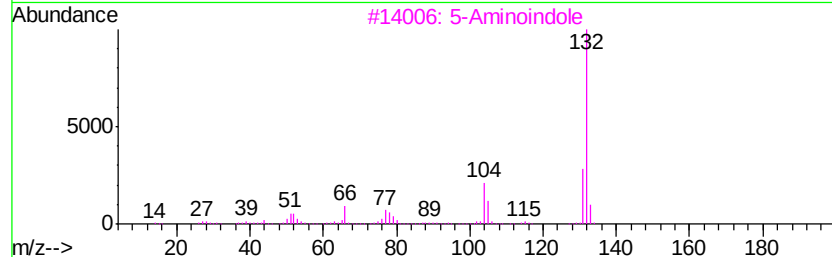
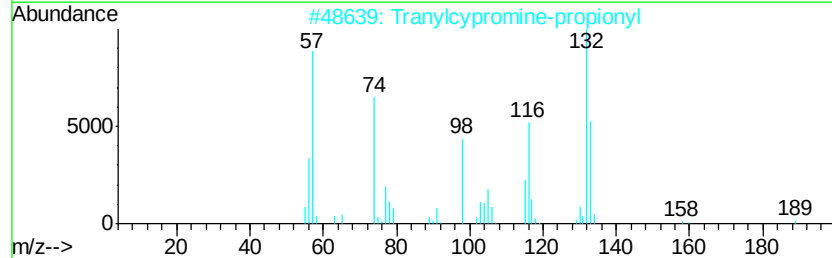
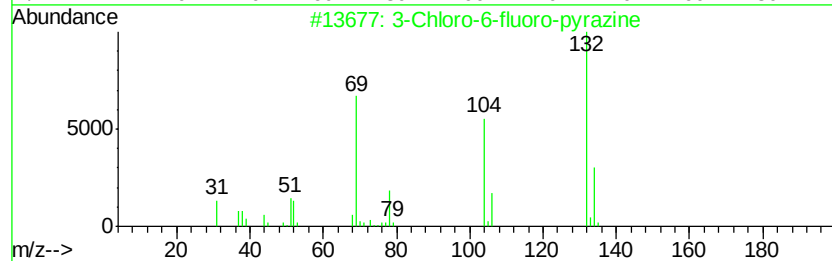
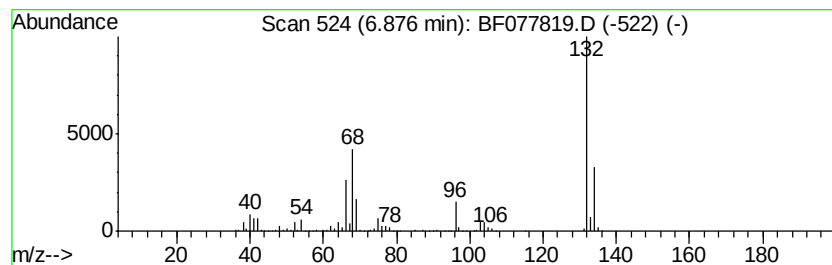
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Peak Number 5 unknown6.88 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.88	92.37 ng	964784	1,4-Dichlorobenzene-d4	7.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
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-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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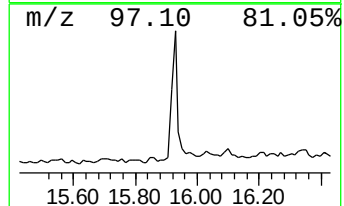
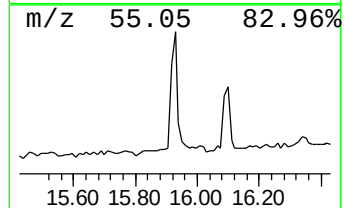
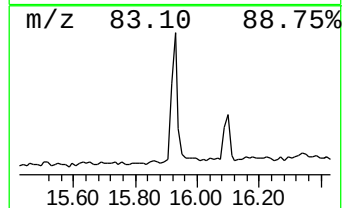
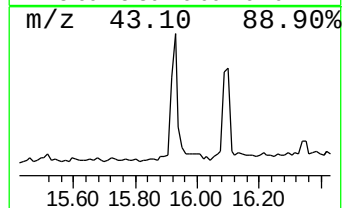
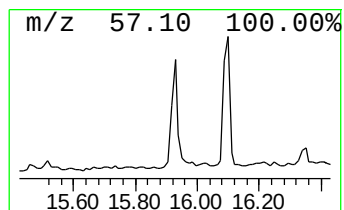
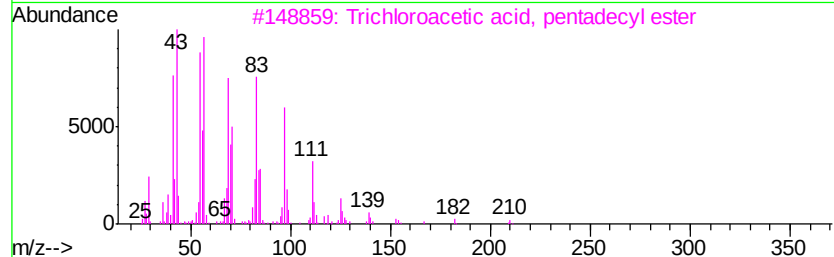
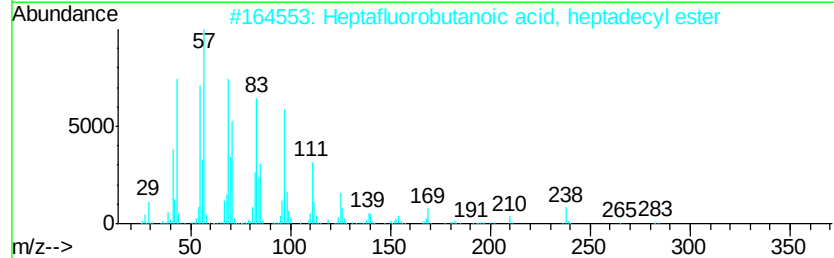
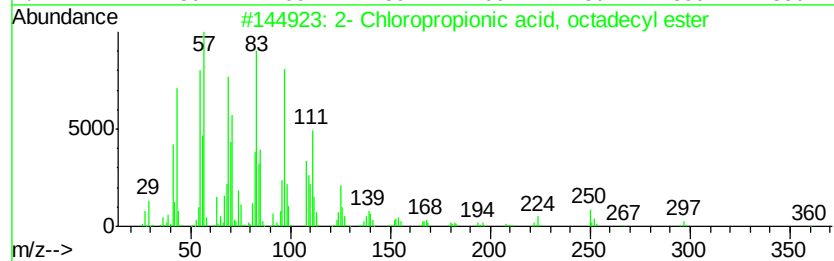
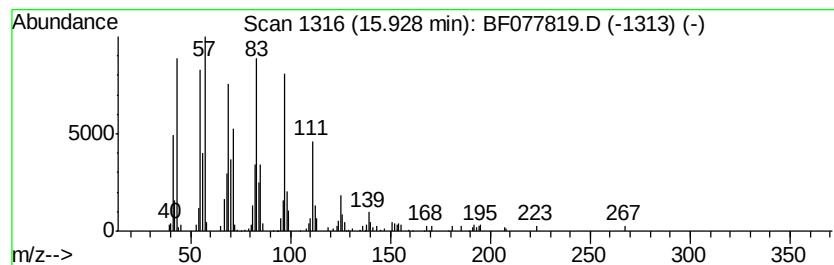
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Peak Number 7 2- Chloropropionic acid, oc... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	8.59 ng	192271	Chrysene-d12	16.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
2		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5		17-Pentatriacontene	491	C35H70	006971-40-0	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.32	1.32	521.8	ng	5450280	1	7.16	208892	20.0
Butane, 2-methoxy...	1.61	7.9	ng	82373	1	7.16	208892	20.0
2-Pentanone, 4-hy...	4.93	13.9	ng	145100	1	7.16	208892	20.0
unknown6.88	6.88	92.4	ng	964784	1	7.16	208892	20.0
2- Chloropropioni...	15.93	8.6	ng	192271	5	16.04	447666	20.0