

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070516\
 Data File : BF088702.D
 Acq On : 5 Jul 2016 14:47
 Operator : UM/SJ
 Sample : PB91664BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB91664BL

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-BF063016.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	1.678	3	8	10	rVB	3313807	4397150	100.00%	14.096%
2	1.713	10	11	20	rVV	377676	524867	11.94%	1.683%
3	1.838	20	22	39	rVB	1252896	1951612	44.38%	6.256%
4	2.056	39	41	65	rVB3	48630	175336	3.99%	0.562%
5	4.959	292	295	299	rBV	124790	169228	3.85%	0.542%
6	5.382	329	332	334	rBV	2154132	2427869	55.21%	7.783%
7	6.410	419	422	424	rBV	1987457	2030466	46.18%	6.509%
8	6.547	431	434	436	rBV	2037377	2471537	56.21%	7.923%
9	6.776	452	454	456	rBV	839044	711973	16.19%	2.282%
10	6.936	465	468	470	rVB	1633858	1916142	43.58%	6.143%
11	7.336	500	503	505	rBV	1362491	1401155	31.87%	4.492%
12	8.056	564	566	569	rVB	939929	924731	21.03%	2.964%
13	9.142	657	661	663	rBV	1958432	2950479	67.10%	9.458%
14	9.805	716	719	722	rBB	1068018	1063424	24.18%	3.409%
15	10.594	785	788	791	rBV	1811946	1827763	41.57%	5.859%
16	11.291	846	849	851	rBV	998014	1241276	28.23%	3.979%
17	12.868	984	987	990	rBV	2409067	2979134	67.75%	9.550%
18	13.908	1076	1078	1081	rBV	1220579	1091074	24.81%	3.498%
19	15.303	1197	1200	1202	rBV	752347	939292	21.36%	3.011%

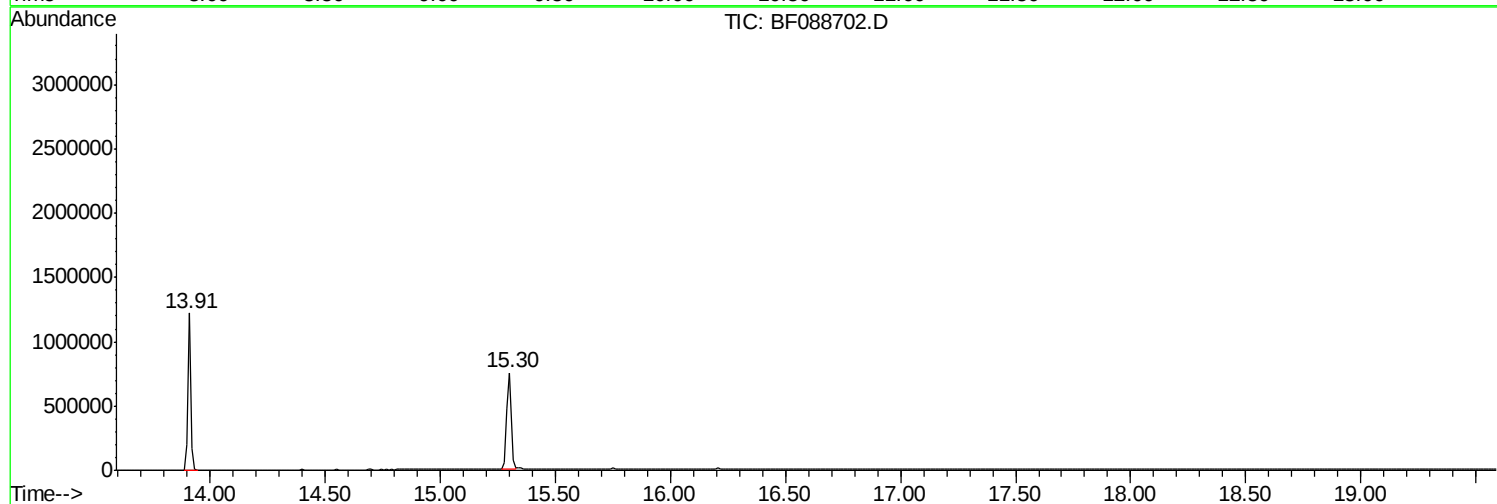
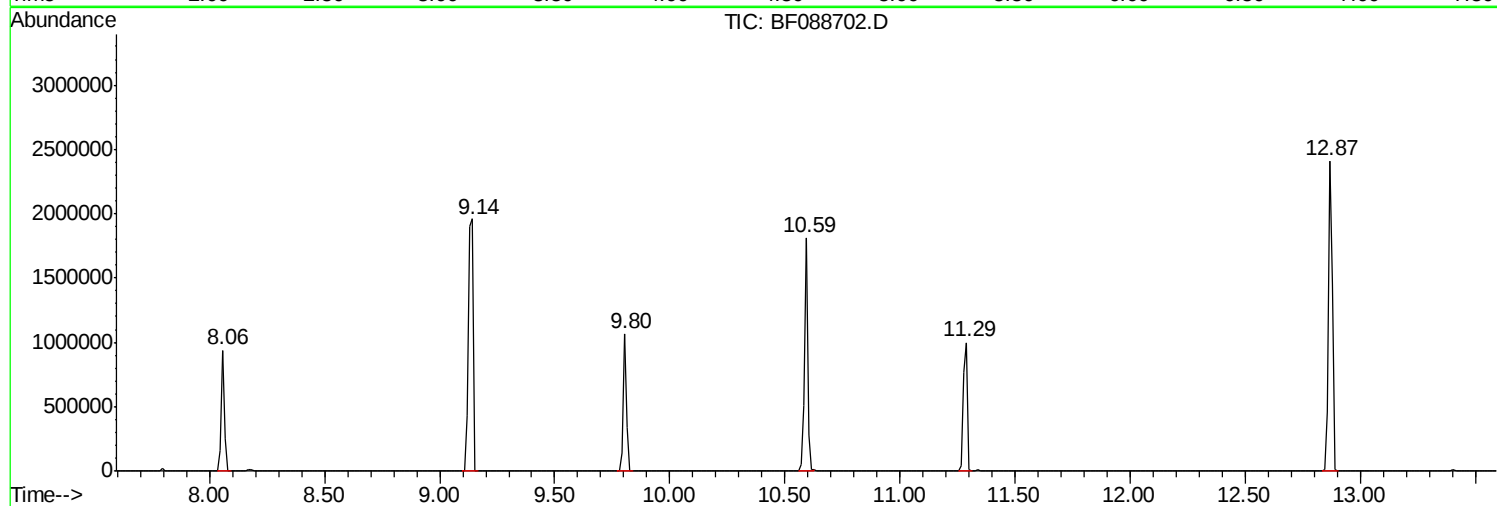
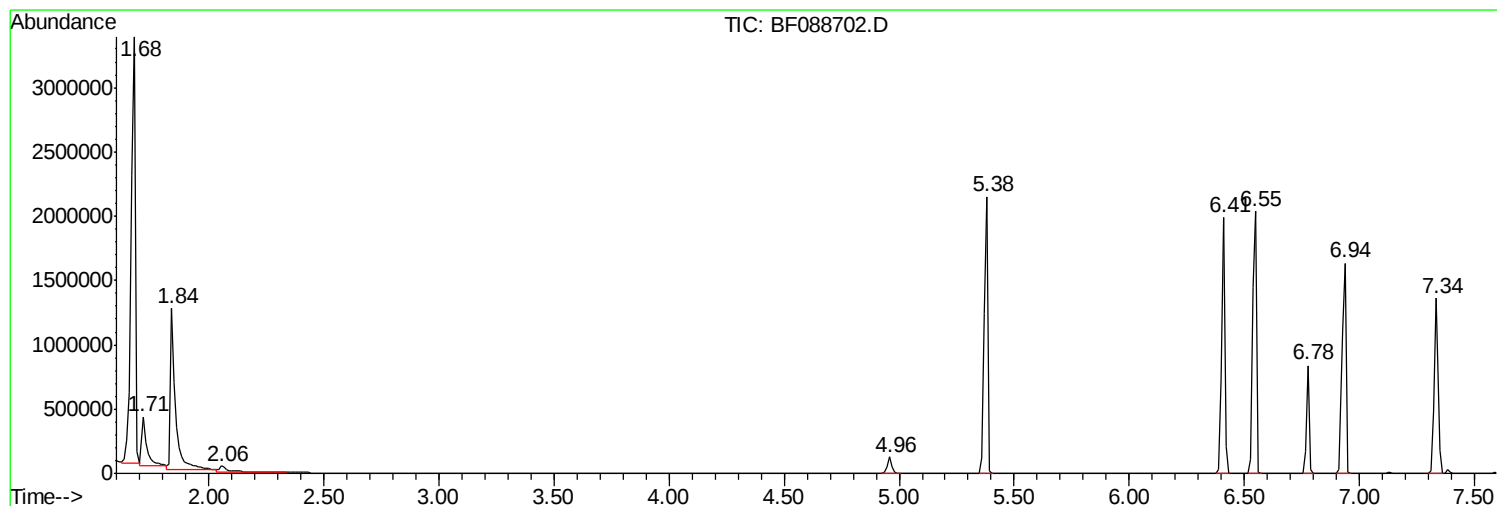
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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Operator : UM/SJ
Sample : PB91664BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PB91664BL

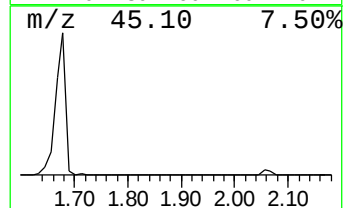
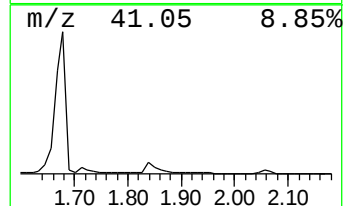
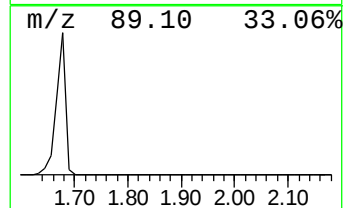
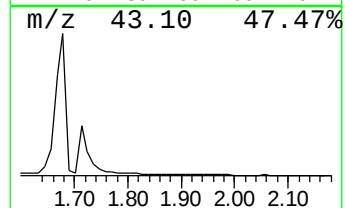
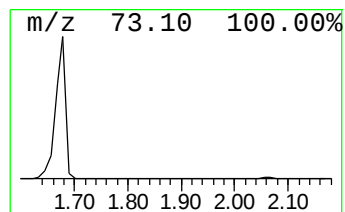
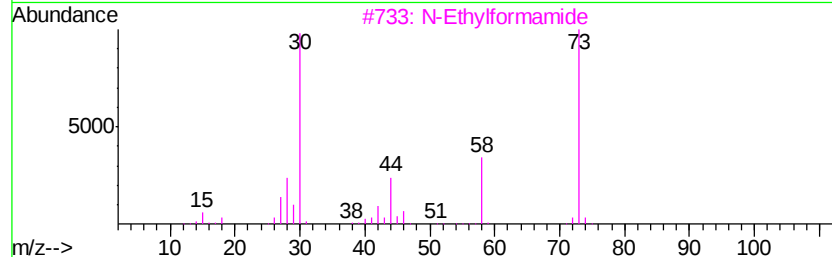
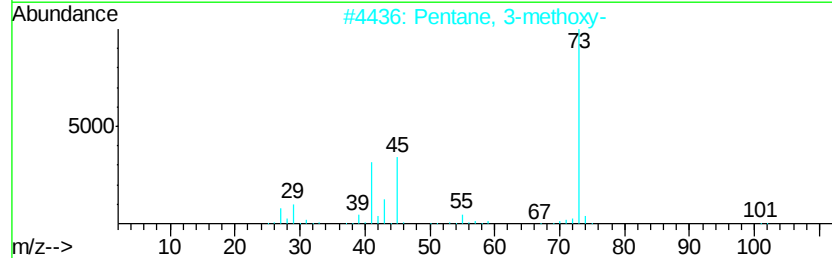
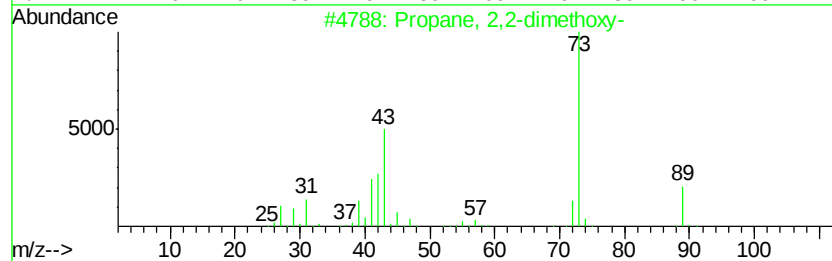
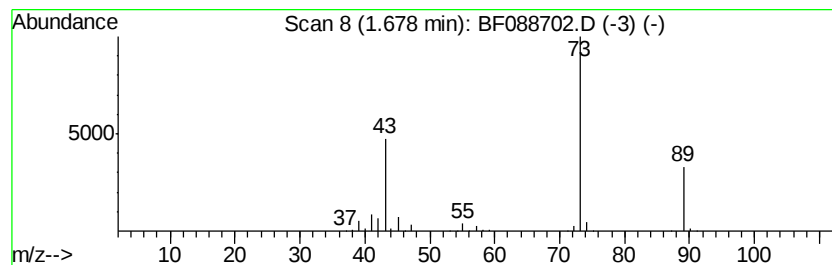
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.68	123.52 ng	4397150	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		N-Ethylformamide	73	C3H7NO	000627-45-2	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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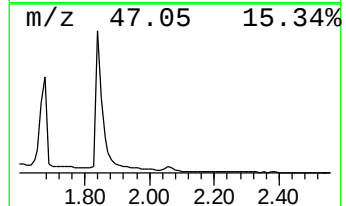
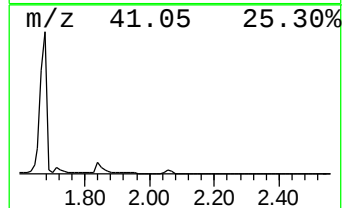
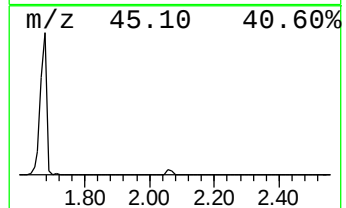
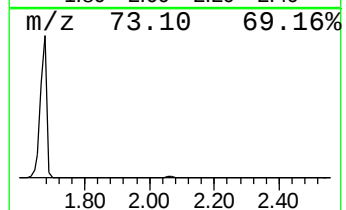
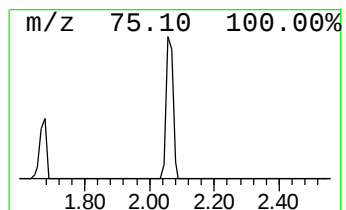
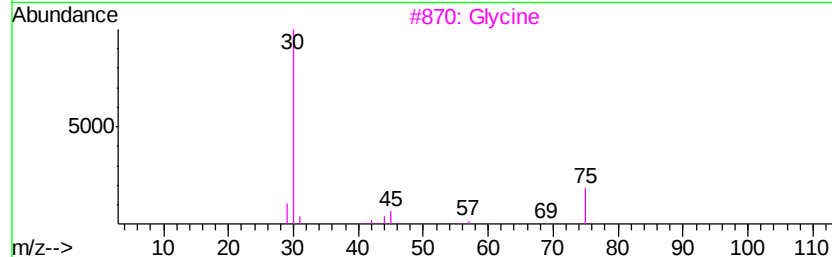
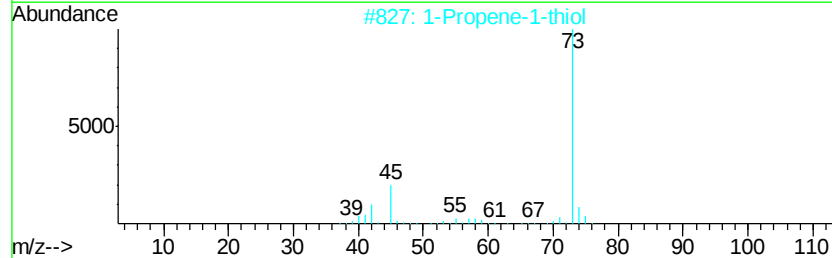
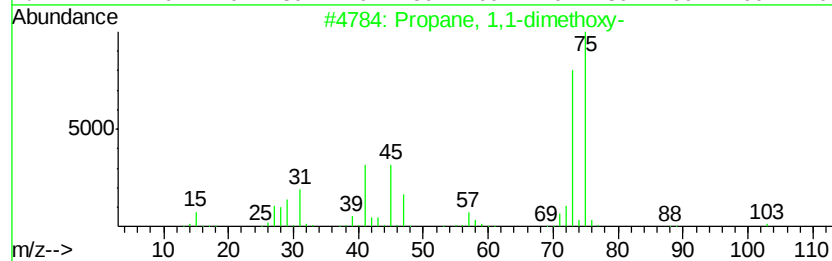
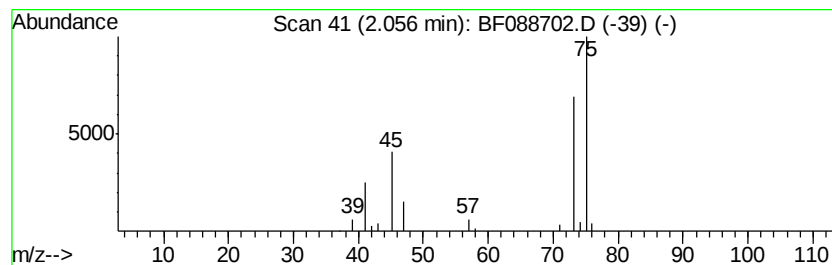
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.06	4.93 ng	175336	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2			1-Propene-1-thiol	74	C3H6S	000925-89-3	7
3			Glycine	75	C2H5NO2	000056-40-6	5
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	4
5			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	4



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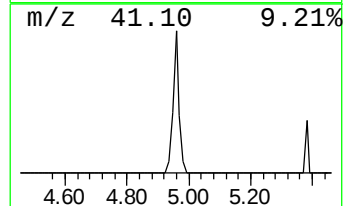
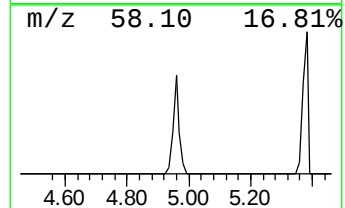
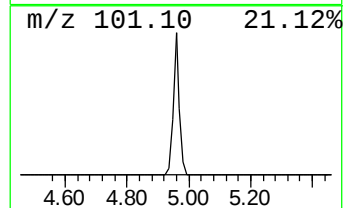
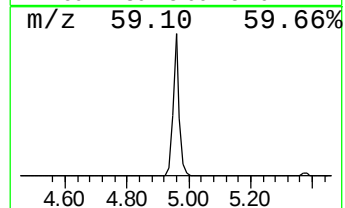
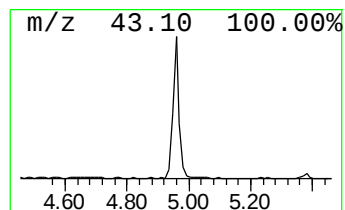
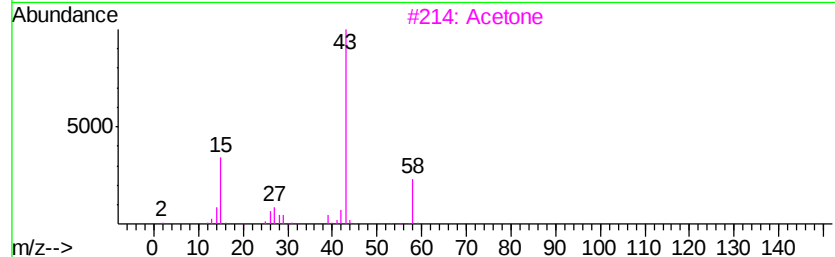
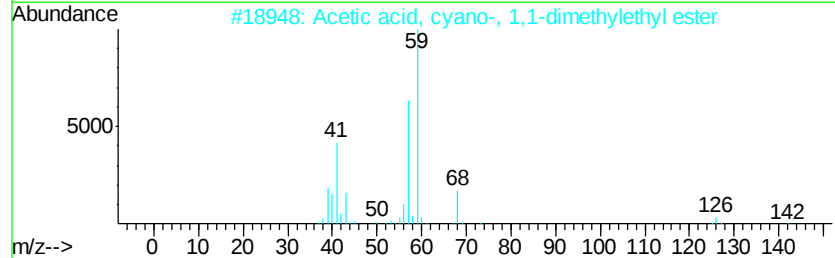
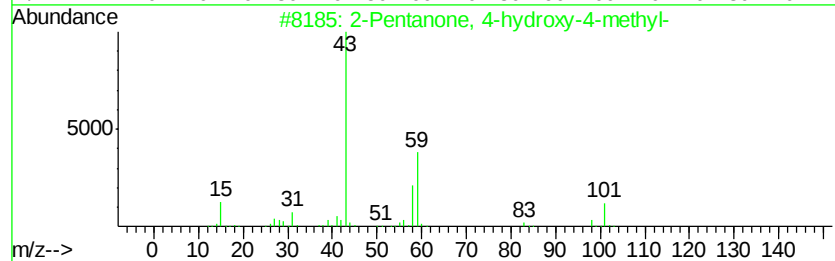
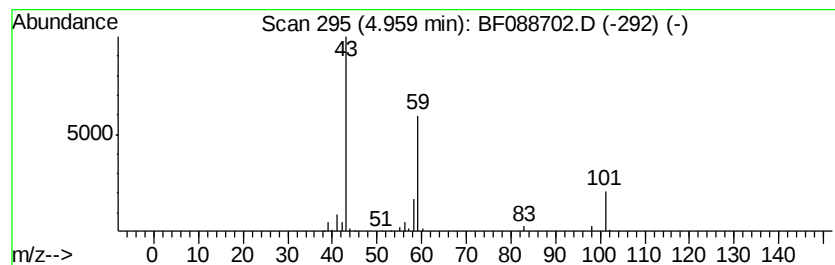
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	4.75 ng	169228	1,4-Dichlorobenzene-d4	6.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Acetone	58	C3H6O	000067-64-1	10
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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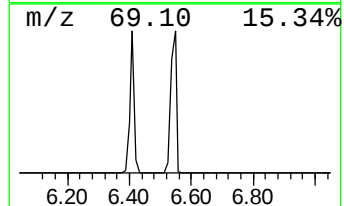
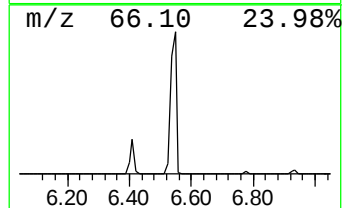
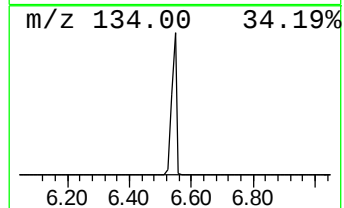
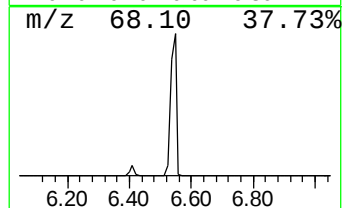
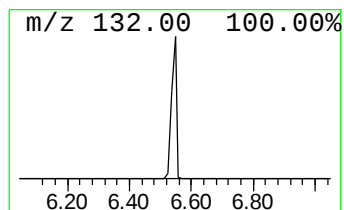
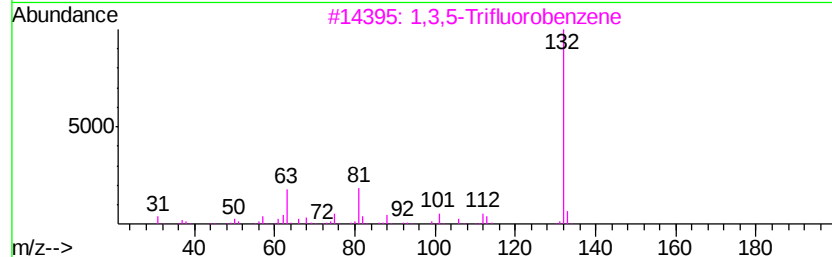
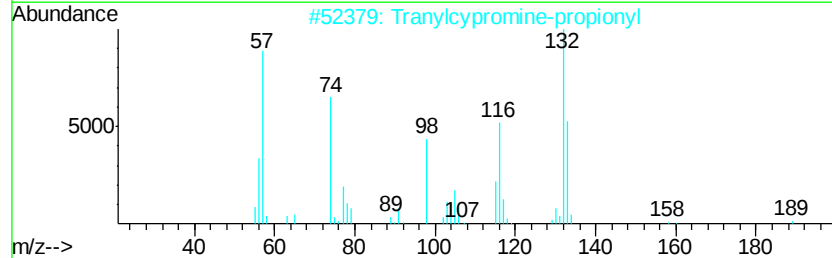
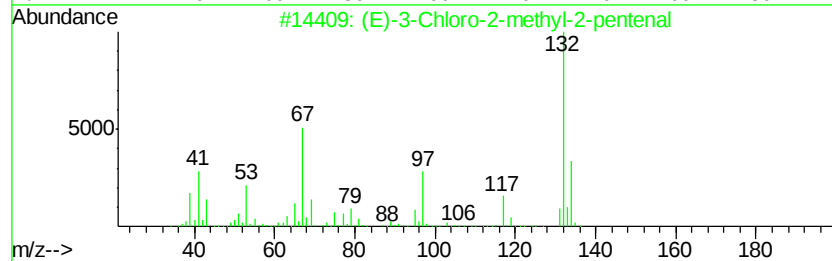
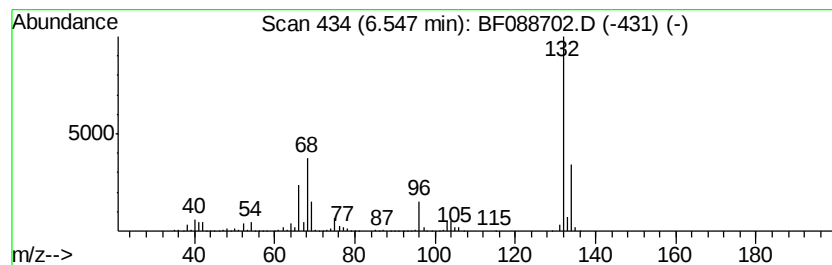
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TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown6.55 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	69.43 ng	2471540	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Propane, 1,1-dime...	2.06	4.9	ng	175336	1	6.78	711973	20.0
2-Pentanone, 4-hy...	4.96	4.8	ng	169228	1	6.78	711973	20.0
unknown6.55	6.55	69.4	ng	2471540	1	6.78	711973	20.0