

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041416\
 Data File : BG021678.D
 Acq On : 15 Apr 2016 8:45
 Operator : UM/SJ
 Sample : PB89734BL
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB89734BL

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_G\METHODS\8270-BG041316.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	3.108	40	46	55	rVB	92224	130329	5.95%	1.141%
2	3.372	85	91	99	rBV	24642	33447	1.53%	0.293%
3	5.300	412	419	426	rBV	49728	79448	3.63%	0.696%
4	5.764	490	498	507	rBV	488645	800077	36.55%	7.007%
5	7.368	760	771	780	rBV	517031	921542	42.10%	8.071%
6	7.744	826	835	844	rBV	485764	850291	38.84%	7.447%
7	8.214	909	915	922	rVB	102971	180835	8.26%	1.584%
8	8.543	963	971	978	rVB	329514	588243	26.87%	5.152%
9	9.383	1104	1114	1123	rBV	299275	539446	24.64%	4.725%
10	11.034	1386	1395	1402	rBV	155641	284596	13.00%	2.493%
11	13.449	1799	1806	1813	rBV	877066	1395930	63.77%	12.226%
12	14.824	2032	2040	2050	rBV2	278777	460256	21.03%	4.031%
13	16.298	2284	2291	2302	rBV	675616	1047015	47.83%	9.170%
14	17.556	2498	2505	2512	rBV2	371323	562963	25.72%	4.931%
15	20.141	2939	2945	2954	rVB	1695936	2188976	100.00%	19.172%
16	21.827	3225	3232	3242	rVB	395843	685310	31.31%	6.002%
17	25.153	3787	3798	3814	rBV4	206205	668912	30.56%	5.859%

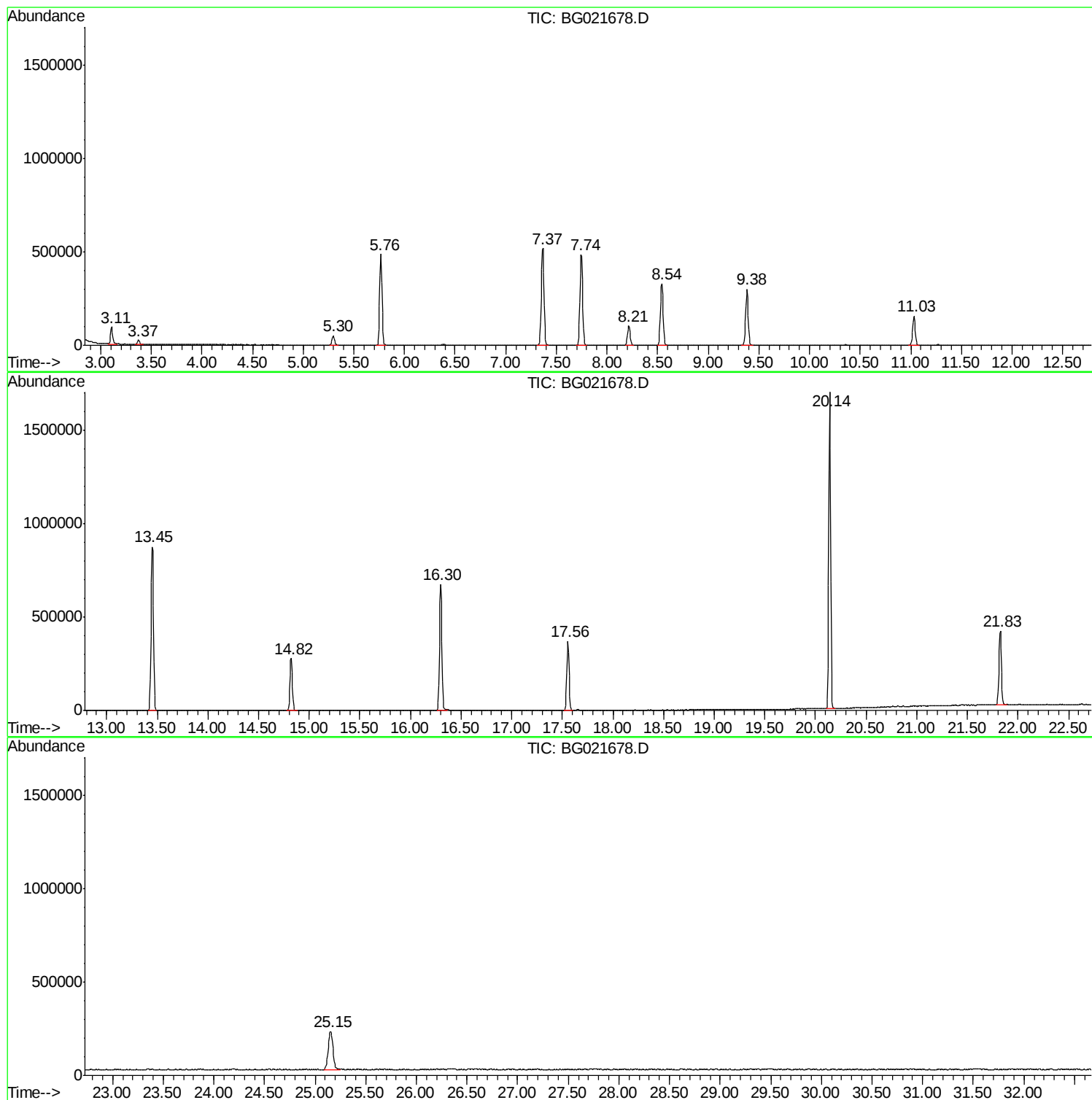
Sum of corrected areas: 11417616

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



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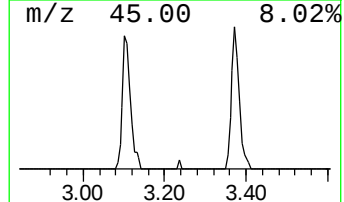
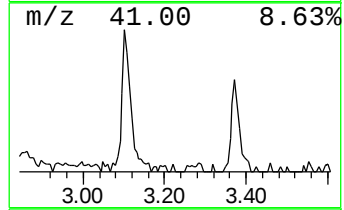
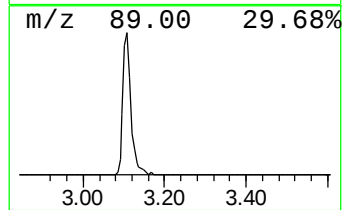
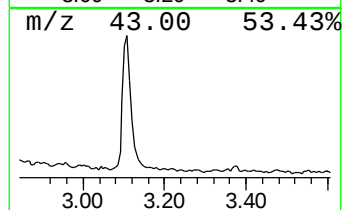
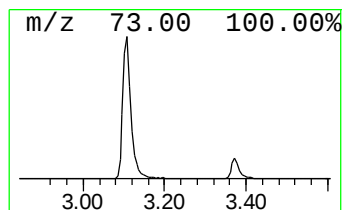
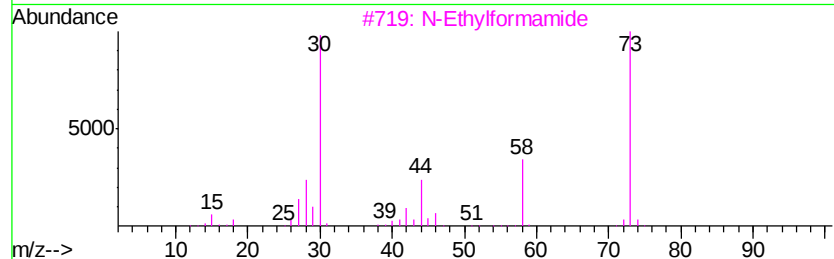
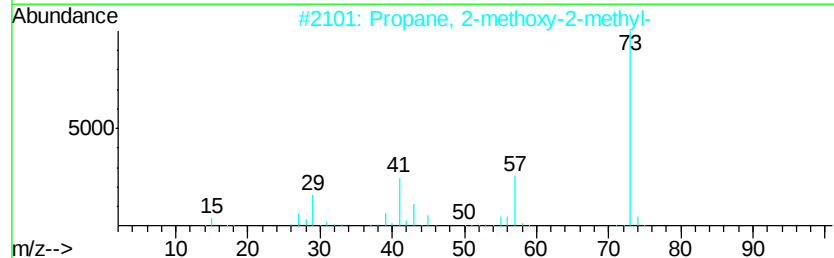
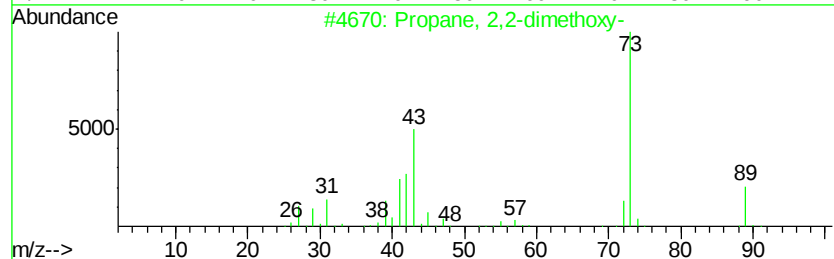
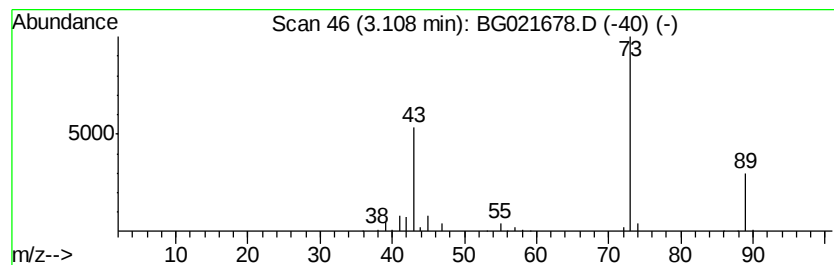
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.11	14.41 ng	130329	1,4-Dichlorobenzene-d4	8.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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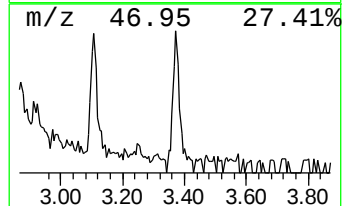
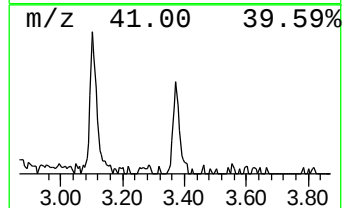
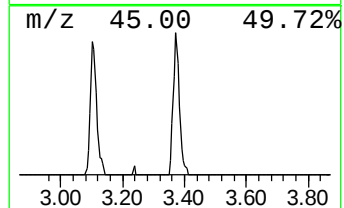
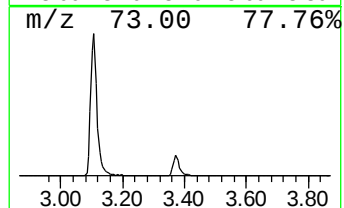
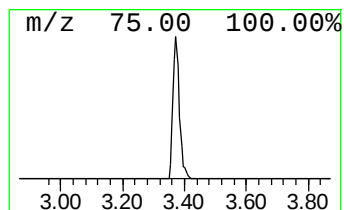
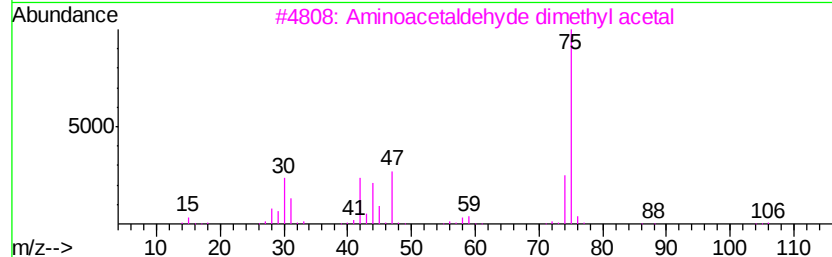
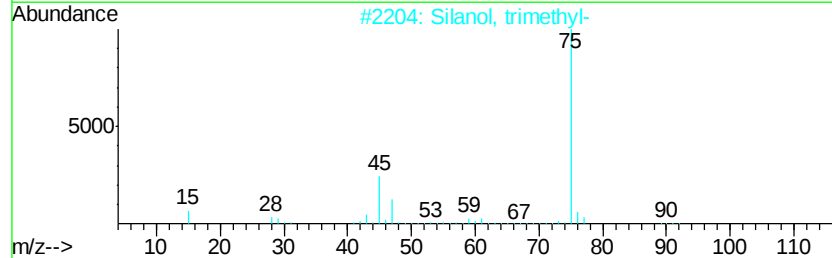
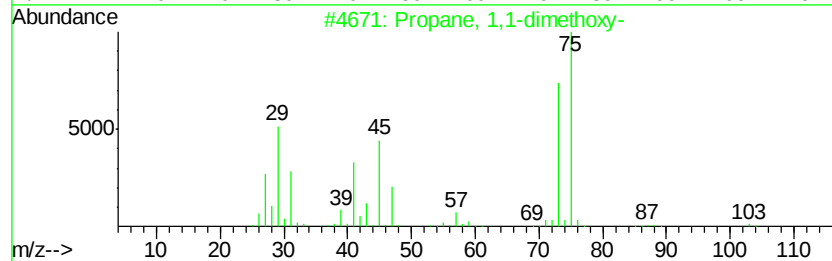
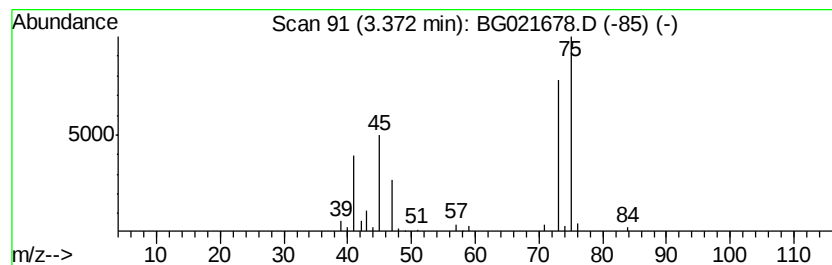
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.37	3.70 ng	33447	1,4-Dichlorobenzene-d4	8.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2		Silanol, trimethyl-	90	C3H10OSi	001066-40-6	39
3		Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5		Formamide, N-methylthio	75	C2H5NS	018952-41-5	7



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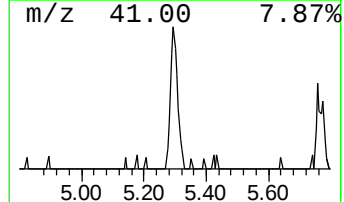
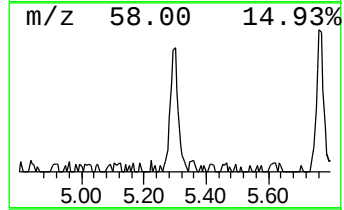
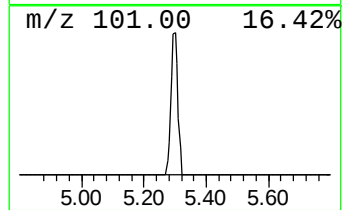
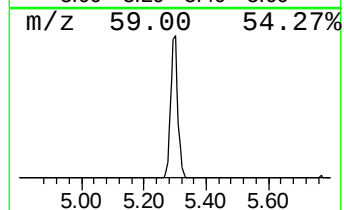
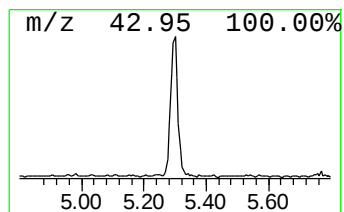
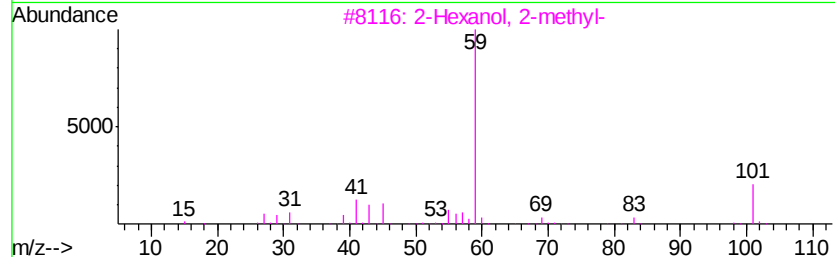
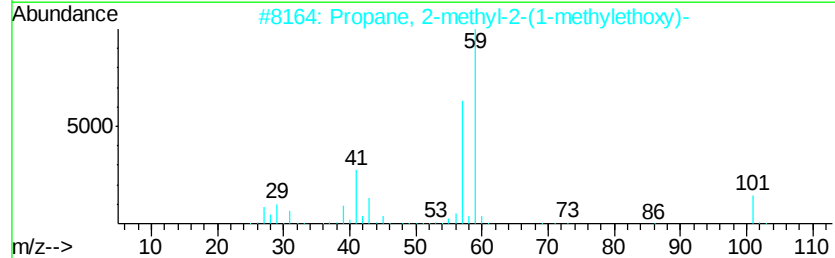
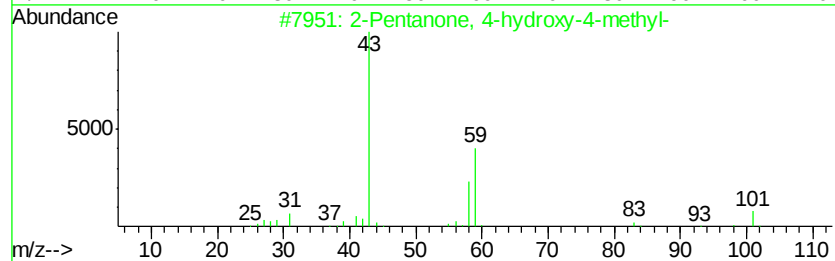
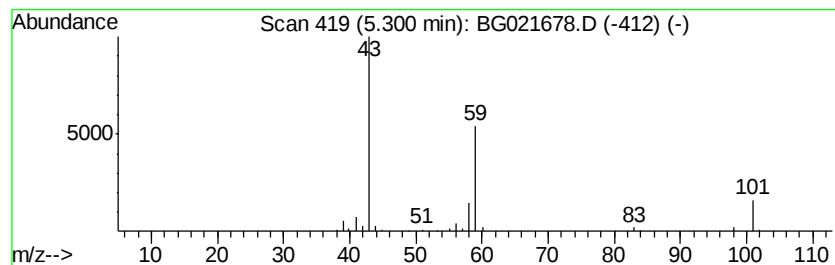
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.30	8.79 ng	79448	1,4-Dichlorobenzene-d4	8.22

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol	102	C6H14O	000623-37-0	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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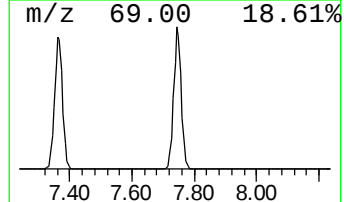
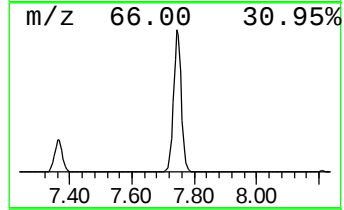
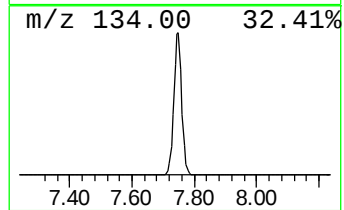
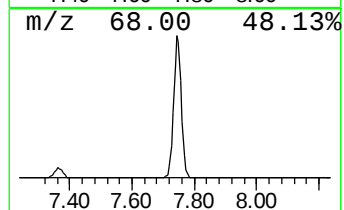
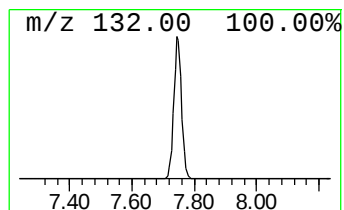
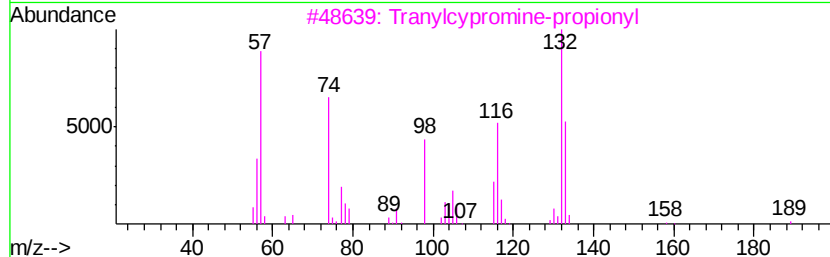
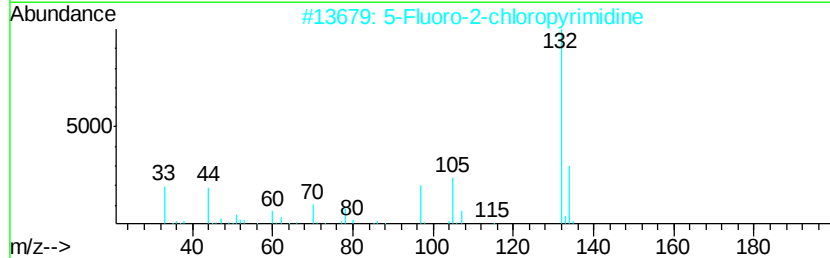
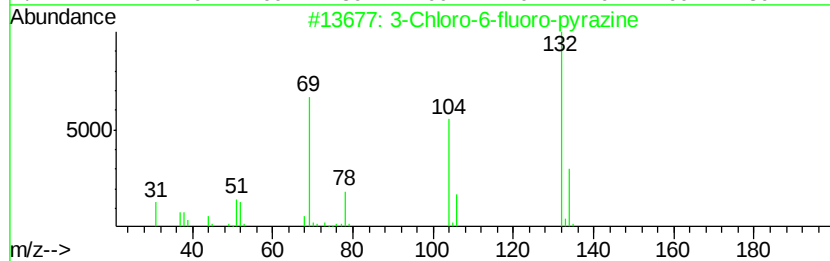
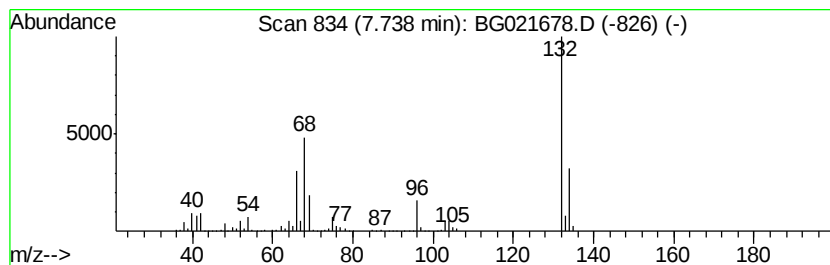
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Peak Number 4 unknown7.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.74	94.04 ng	850291	1,4-Dichlorobenzene-d4	8.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	3.11	14.4	ng	130329	1	8.22	180835	20.0
Propane, 1,1-dime...	3.37	3.7	ng	33447	1	8.22	180835	20.0
2-Pentanone, 4-hy...	5.30	8.8	ng	79448	1	8.22	180835	20.0
unknown7.74	7.74	94.0	ng	850291	1	8.22	180835	20.0