

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032817\
 Data File : BF094002.D
 Acq On : 28 Mar 2017 19:40
 Operator : SJ/MA
 Sample : PB97860BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB97860BL

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-BF032217.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	3.546	278	282	288	rVB	256191	254411	5.15%	0.740%
2	4.087	367	374	381	rBV	1516117	1987052	40.24%	5.783%
3	4.469	434	439	442	rBV	2818157	2769613	56.09%	8.060%
4	4.857	501	505	510	rBB	128104	112504	2.28%	0.327%
5	5.528	613	619	622	rBV	2641831	2768142	56.06%	8.056%
6	5.669	638	643	647	rBV	2691994	2927033	59.27%	8.518%
7	5.928	682	687	690	rBV	980494	930604	18.85%	2.708%
8	6.104	712	717	721	rBV	3015603	3290589	66.64%	9.576%
9	6.575	791	797	800	rBV	2187371	2685136	54.38%	7.814%
10	7.428	937	942	946	rBV	1232593	1265648	25.63%	3.683%
11	8.757	1160	1168	1171	rBV	3990860	4938134	100.00%	14.371%
12	9.569	1300	1306	1313	rVB2	1289157	1391853	28.19%	4.051%
13	10.545	1465	1472	1475	rBV	1656372	1897780	38.43%	5.523%
14	11.392	1610	1616	1620	rBV	1337747	1306940	26.47%	3.803%
15	13.375	1947	1953	1957	rBV	3329427	4176079	84.57%	12.153%
16	14.639	2164	2168	2174	rBV	856550	936408	18.96%	2.725%
17	16.274	2441	2446	2452	rBV	588648	723724	14.66%	2.106%

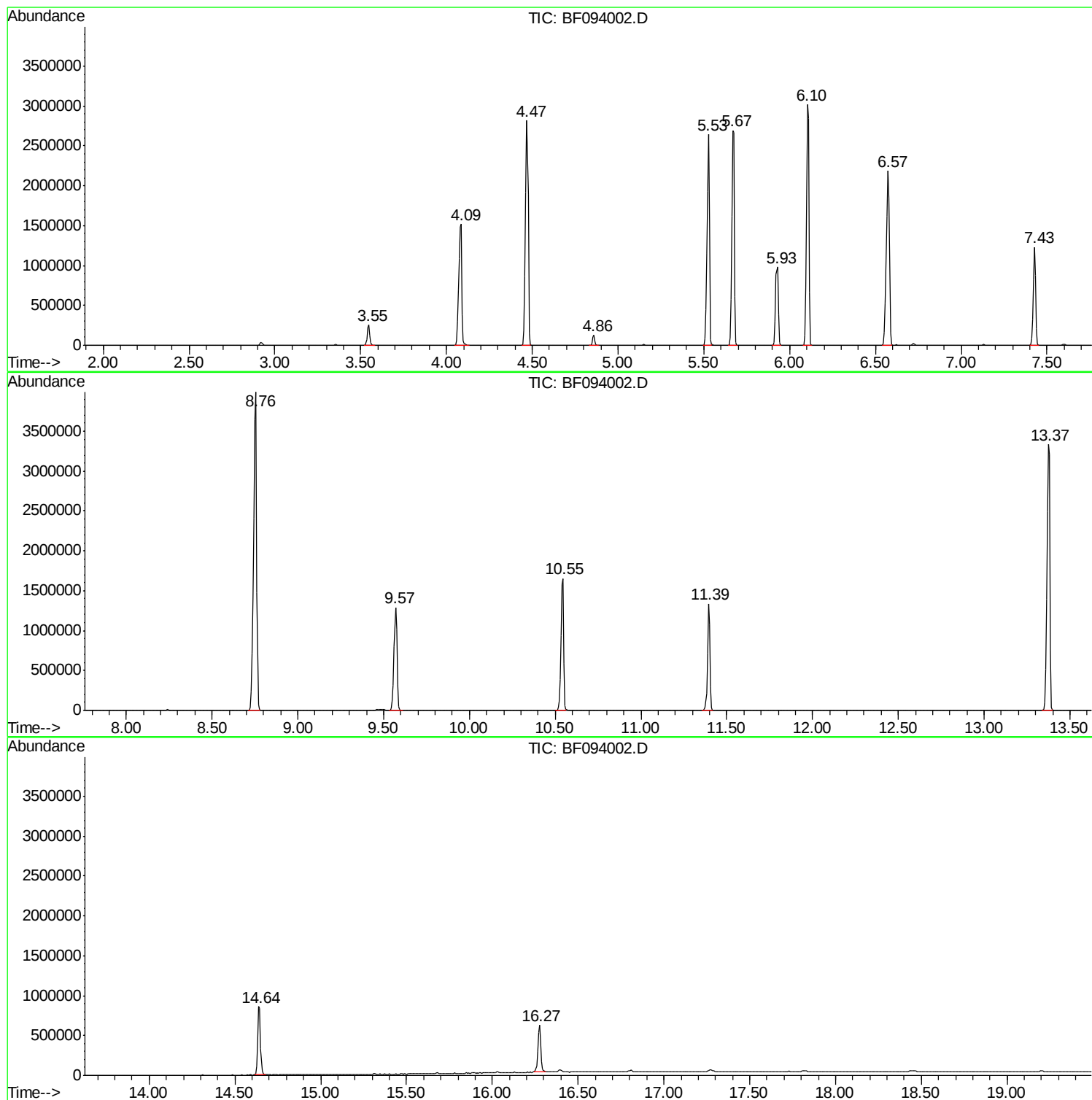
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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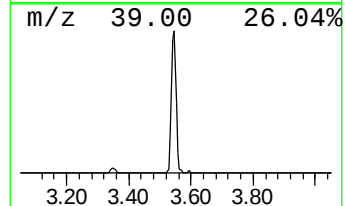
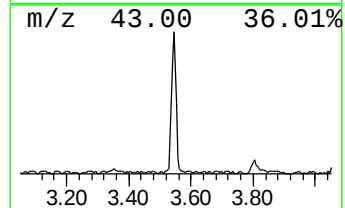
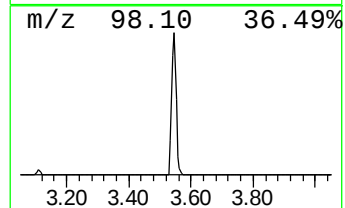
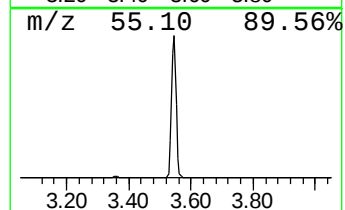
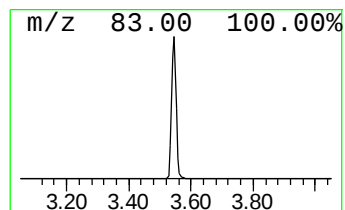
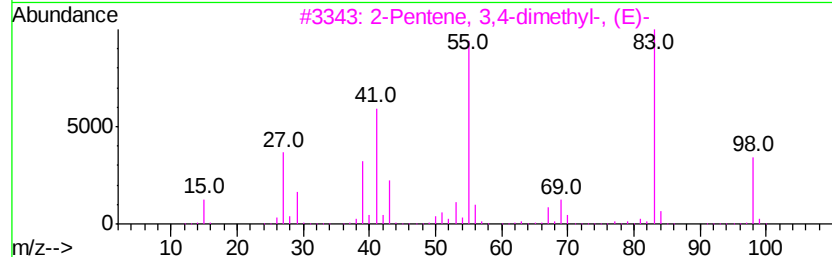
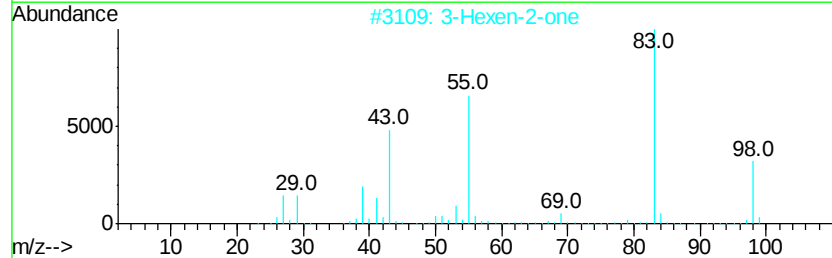
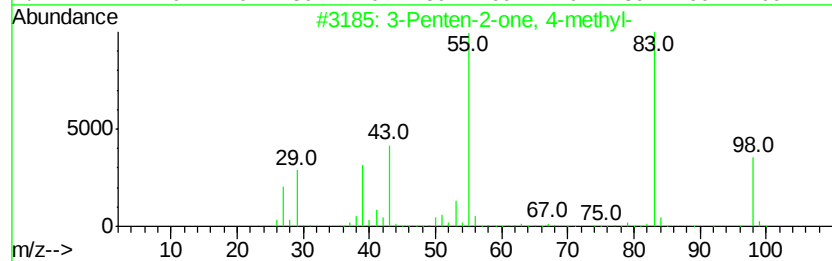
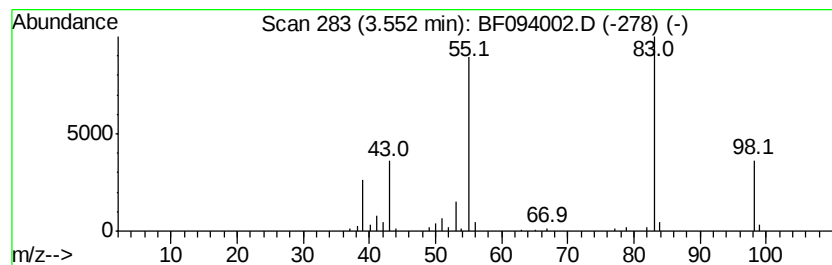
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.55	5.47 ng	254411	1,4-Dichlorobenzene-d4	5.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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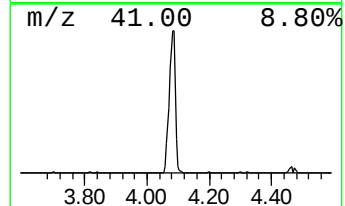
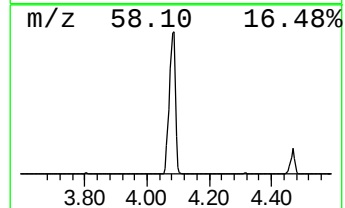
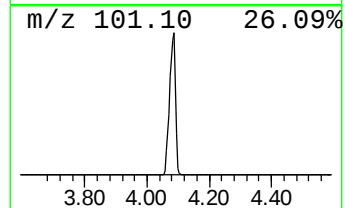
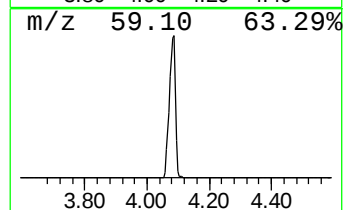
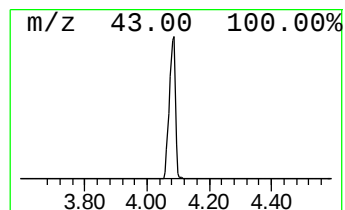
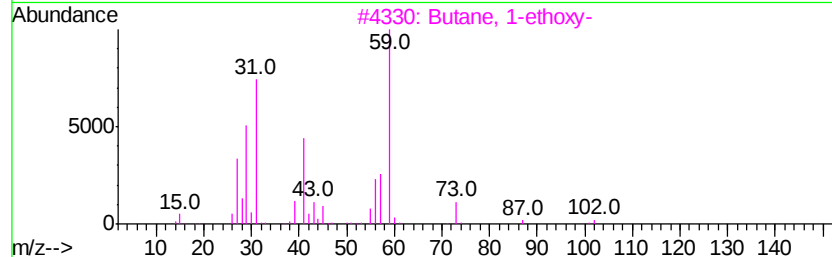
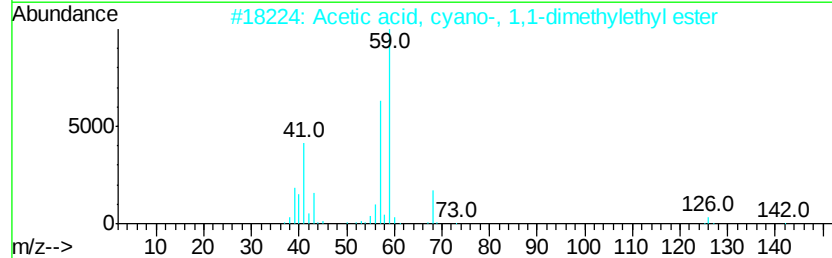
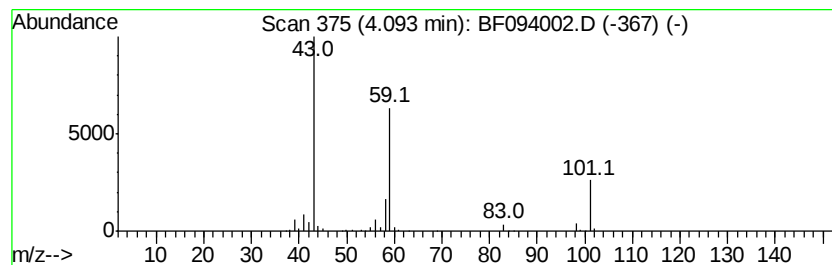
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.09	42.70 ng	1987050	1,4-Dichlorobenzene-d4	5.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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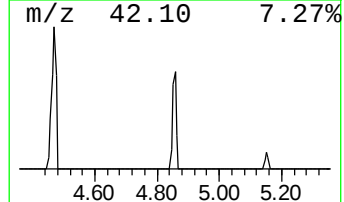
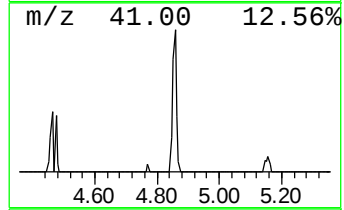
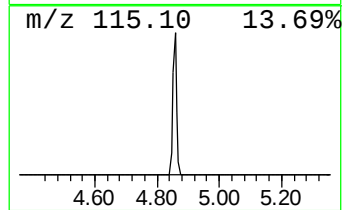
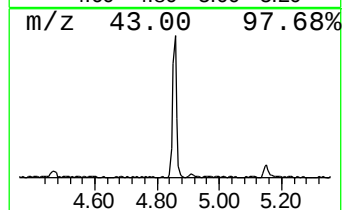
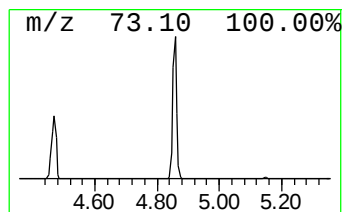
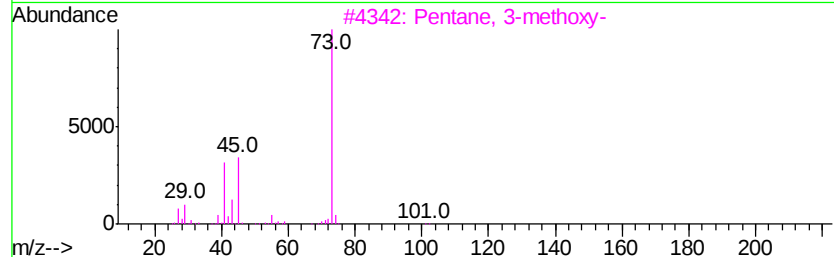
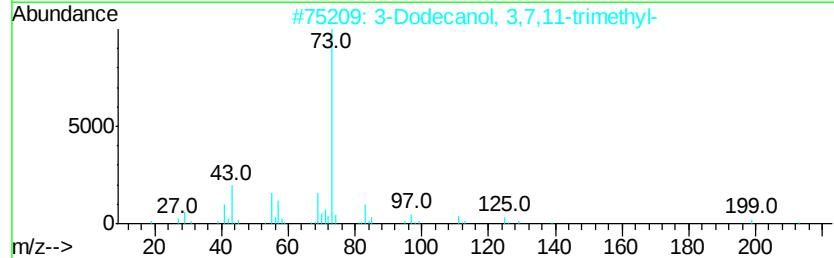
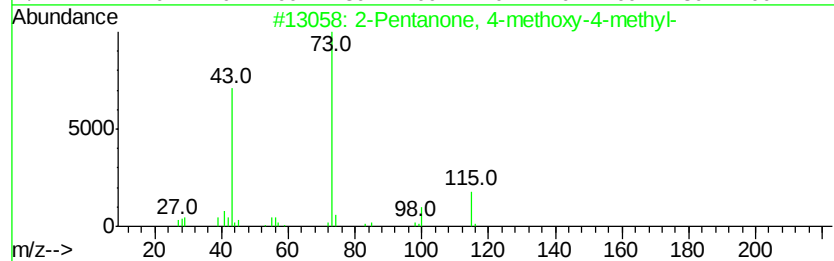
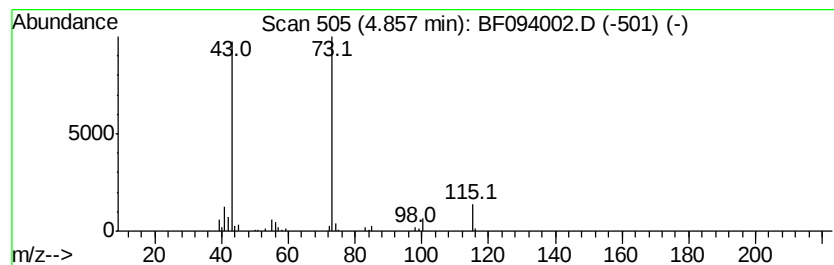
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	2.42 ng	112504	1,4-Dichlorobenzene-d4	5.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83	
2	3-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	007278-65-1	17	
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12	
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	12	
5	N-Ethylformamide	73	C3H7NO	000627-45-2	12	



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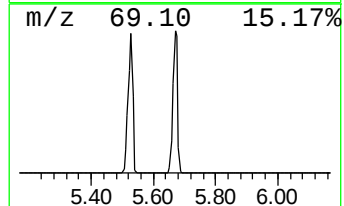
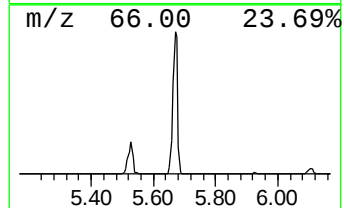
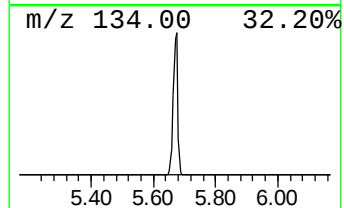
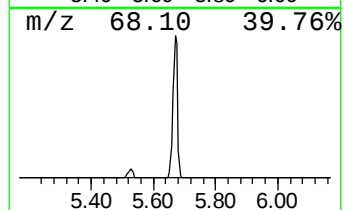
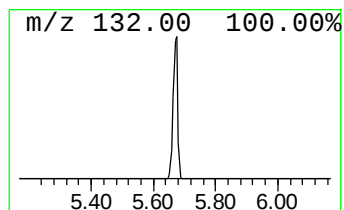
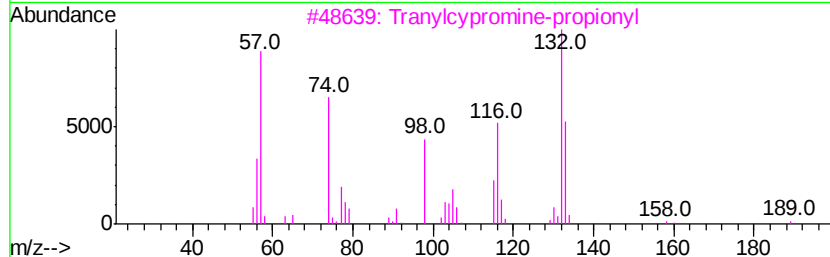
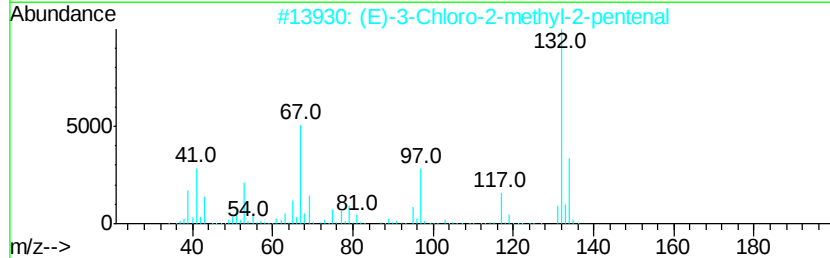
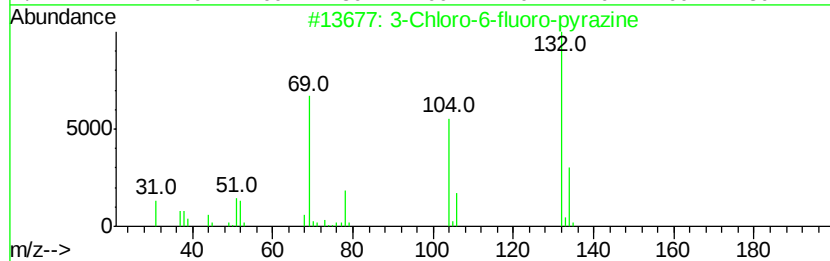
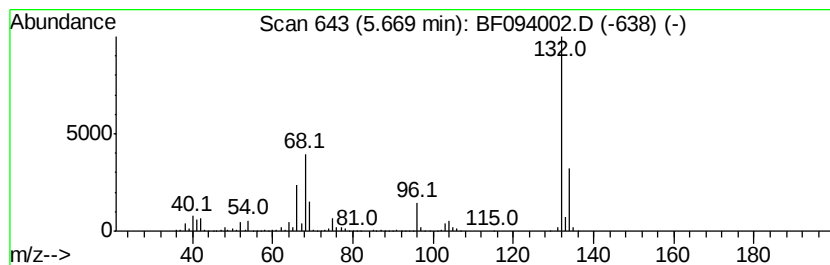
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Peak Number 4 unknown5.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.67	62.91 ng	2927030	1,4-Dichlorobenzene-d4	5.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	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
3-Penten-2-one, 4...	3.55	5.5	ng	254411	1	5.93	930604	20.0
2-Pentanone, 4-hy...	4.09	42.7	ng	1987050	1	5.93	930604	20.0
2-Pentanone, 4-me...	4.86	2.4	ng	112504	1	5.93	930604	20.0
unknown5.67	5.67	62.9	ng	2927030	1	5.93	930604	20.0