

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020116\
 Data File : BF084727.D
 Acq On : 1 Feb 2016 23:36
 Operator : SJ/IZ
 Sample : PB88098BL
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB88098BL

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-BF020116.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	4.167	180	182	191	rVB	469680	674922	11.22%	1.429%
2	4.876	240	244	251	rBV	2396530	3734585	62.07%	7.908%
3	5.310	279	282	285	rBV	4180222	4304330	71.54%	9.115%
4	5.710	315	317	320	rBV	278289	235582	3.92%	0.499%
5	6.361	371	374	376	rBV	4463555	4648634	77.26%	9.844%
6	6.476	382	384	387	rBV	3822876	4323920	71.86%	9.156%
7	6.704	402	404	407	rBV	1030677	1036212	17.22%	2.194%
8	6.864	415	418	421	rBV	3902655	3462940	57.55%	7.333%
9	7.276	451	454	457	rBV	2675789	2726740	45.32%	5.774%
10	7.996	514	517	519	rBV	1638343	1452300	24.14%	3.075%
11	9.082	608	612	614	rBV	4230457	5531417	91.93%	11.713%
12	9.745	667	670	673	rBV	1590086	1542741	25.64%	3.267%
13	10.533	736	739	742	rBV	3094674	3312773	55.06%	7.015%
14	11.230	797	800	802	rBV	1298858	1580531	26.27%	3.347%
15	12.819	936	939	941	rBV	5396711	6016988	100.00%	12.741%
16	13.859	1027	1030	1032	rBV	1380129	1510709	25.11%	3.199%
17	15.242	1148	1151	1153	rBV	790213	1128394	18.75%	2.389%

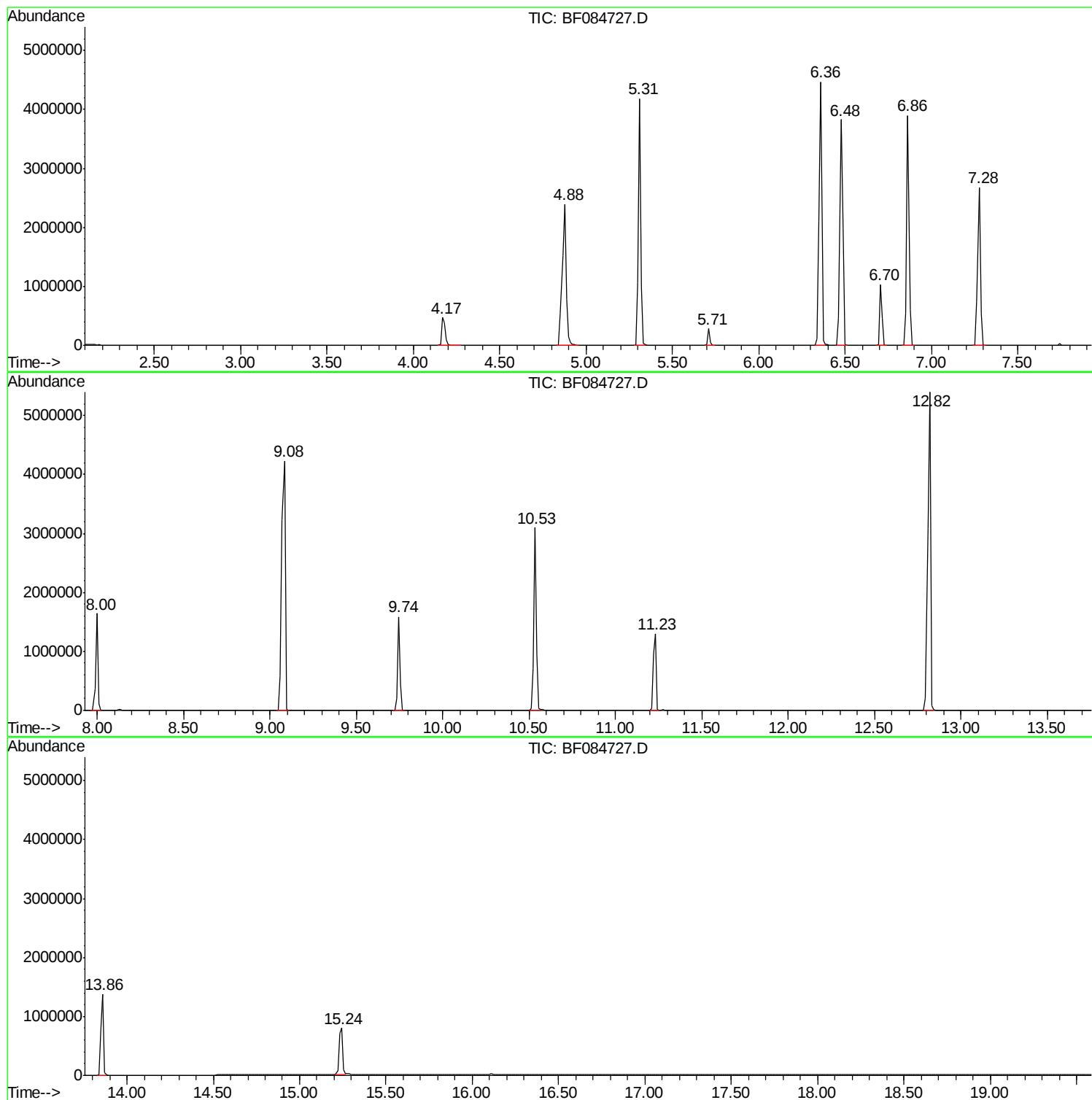
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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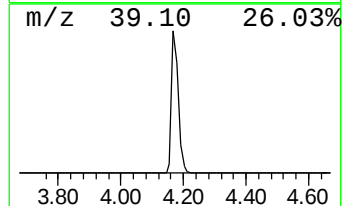
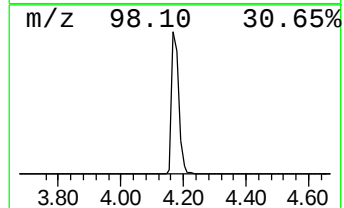
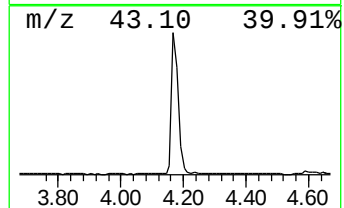
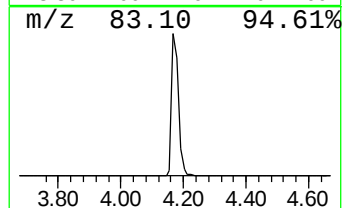
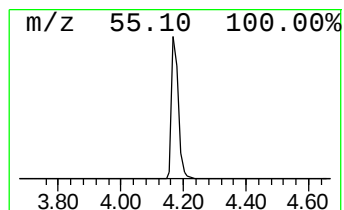
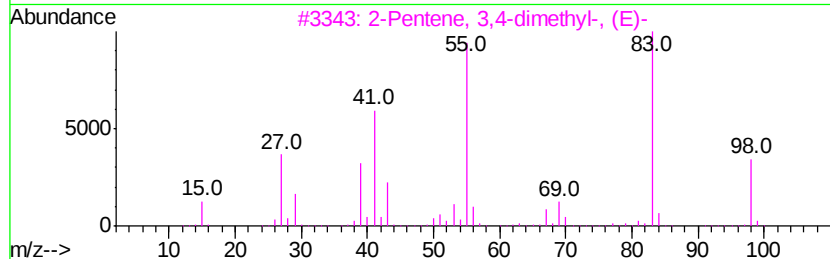
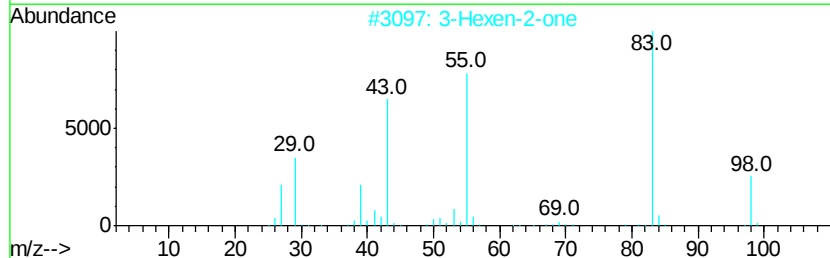
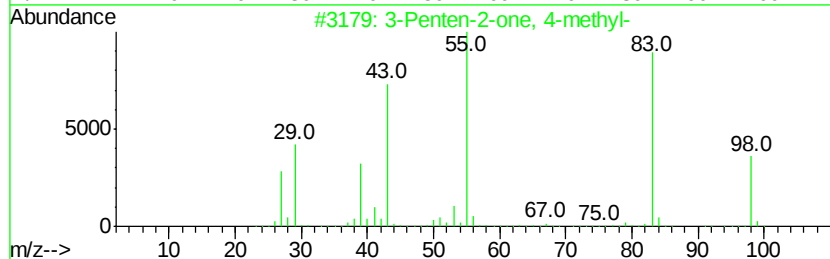
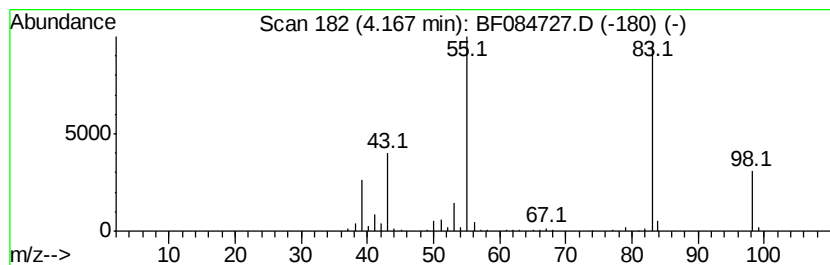
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.17	13.03 ng	674922	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



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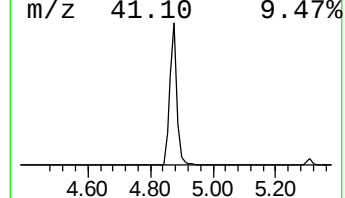
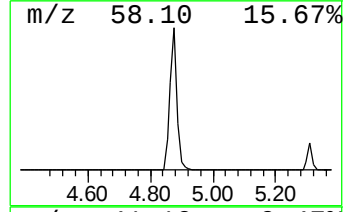
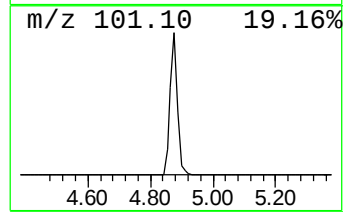
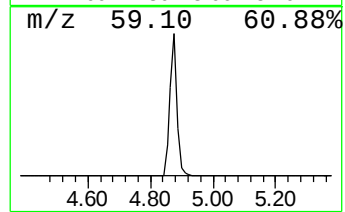
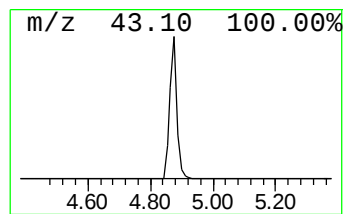
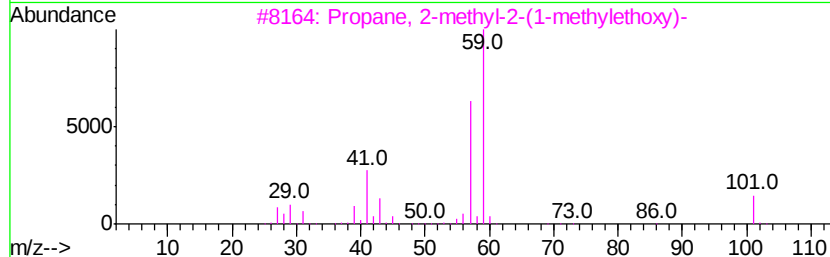
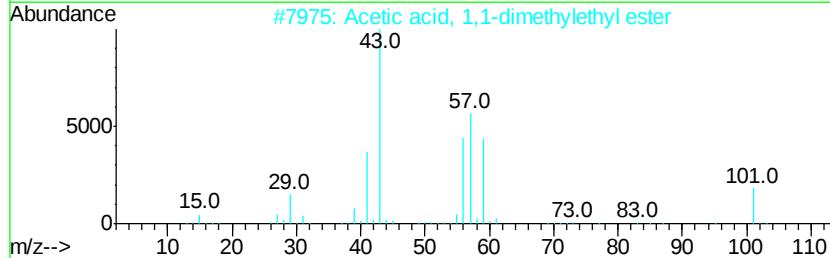
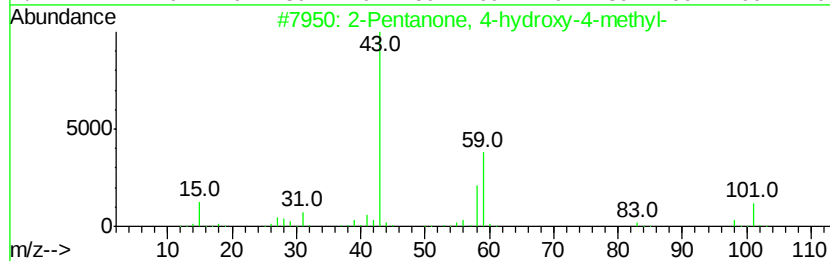
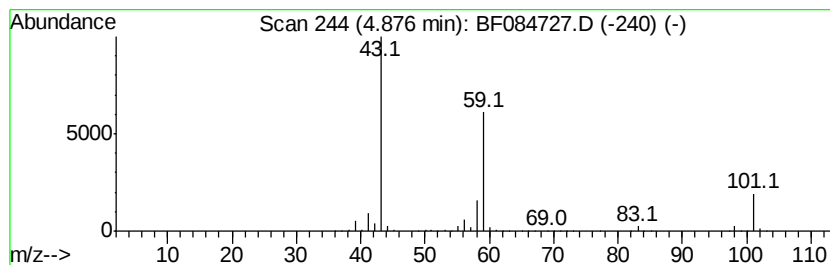
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	72.08 ng	3734590	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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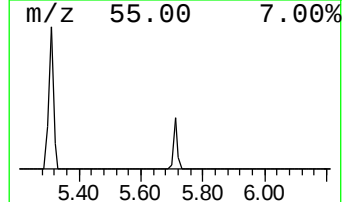
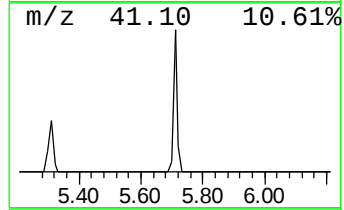
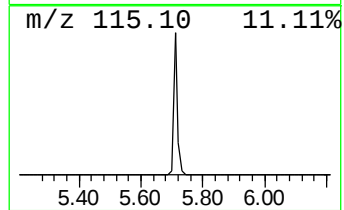
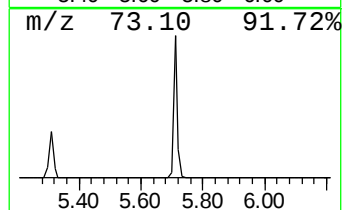
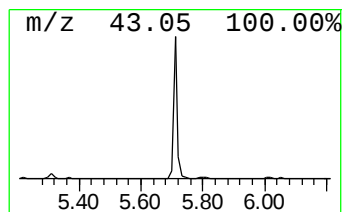
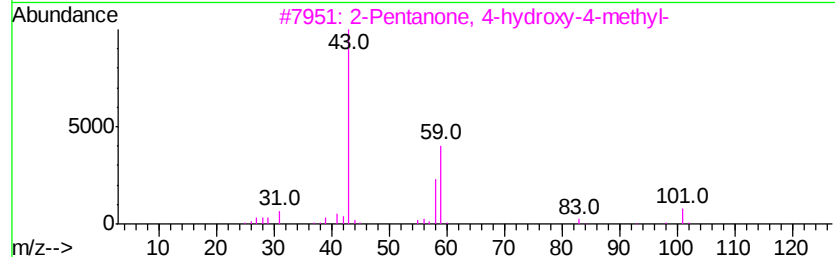
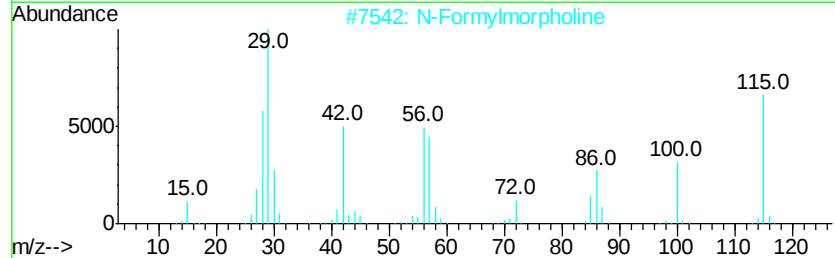
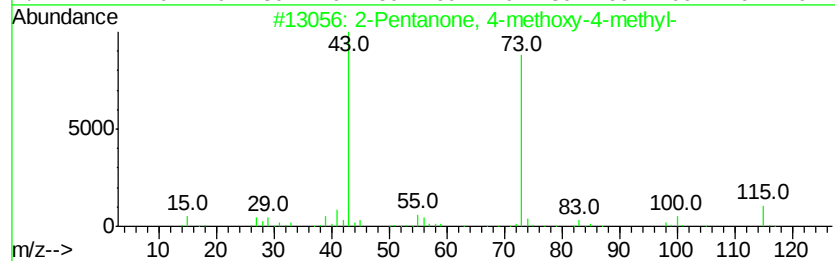
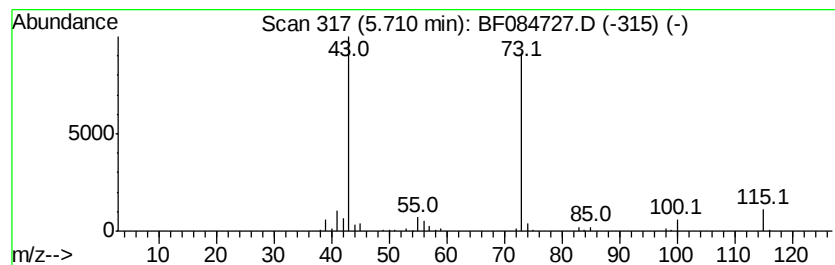
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.71	4.55 ng	235582	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
3		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	10
4		Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9
5		Hexane, 2-methyl-	100	C7H16	000591-76-4	9



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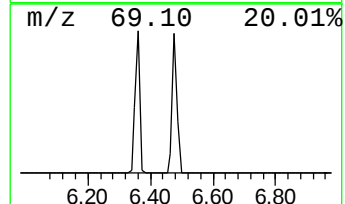
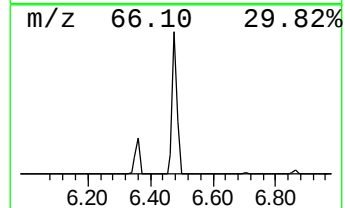
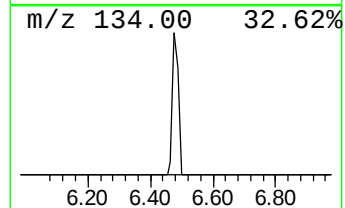
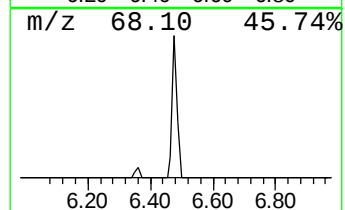
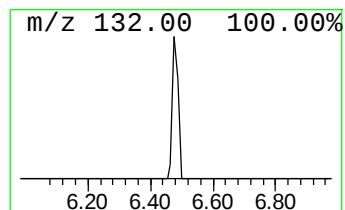
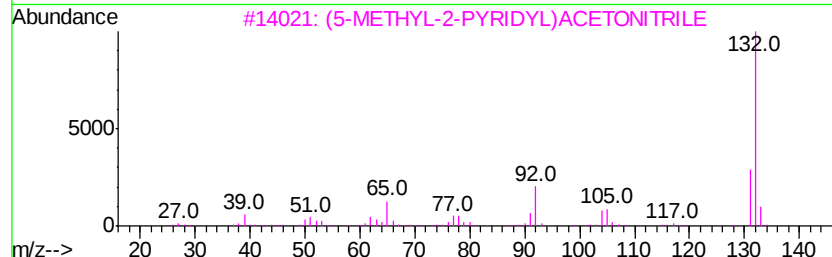
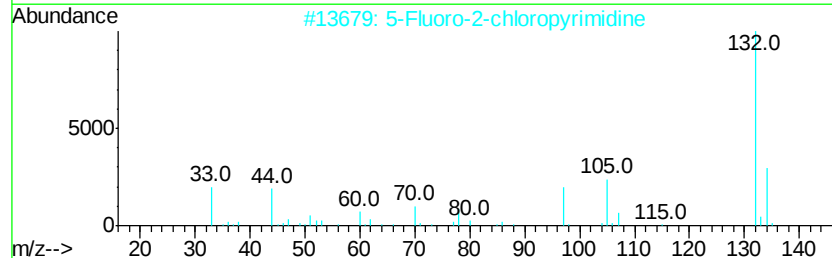
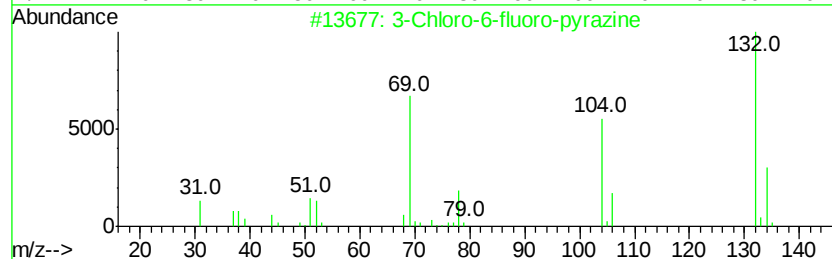
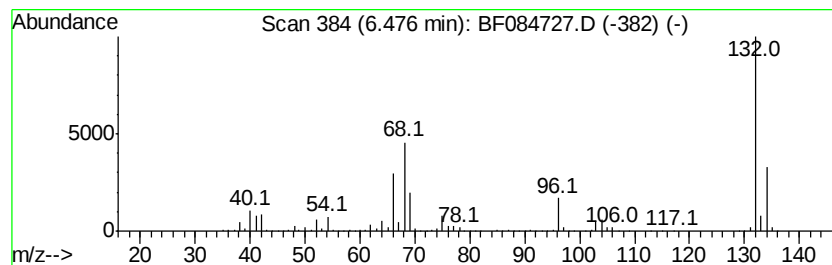
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Peak Number 4 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	83.46 ng	4323920	1,4-Dichlorobenzene-d4	6.70

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		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.17	13.0	ng	674922	1	6.70	1036210	20.0
2-Pentanone, 4-hy...	4.88	72.1	ng	3734590	1	6.70	1036210	20.0
2-Pentanone, 4-me...	5.71	4.5	ng	235582	1	6.70	1036210	20.0
unknown6.48	6.48	83.5	ng	4323920	1	6.70	1036210	20.0