

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032717\
 Data File : BF093975.D
 Acq On : 28 Mar 2017 6:34
 Operator : SJ/MA
 Sample : PB97833BL
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB97833BL

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-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	2.934	174	178	183	rBV	281706	292340	6.14%	0.775%
2	3.569	280	286	289	rBV	3453760	4097000	86.07%	10.866%
3	4.093	369	375	378	rBV	1797148	2273005	47.75%	6.028%
4	4.216	393	396	404	rBV	50932	53416	1.12%	0.142%
5	4.475	435	440	444	rBV	2722321	2820662	59.26%	7.481%
6	4.863	503	506	512	rVB	101985	88049	1.85%	0.234%
7	5.534	614	620	623	rBV	2645629	2819365	59.23%	7.477%
8	5.681	640	645	648	rBV	2959785	2969449	62.38%	7.875%
9	5.934	684	688	692	rBV	996967	966189	20.30%	2.562%
10	6.116	714	719	723	rBV	3194099	3308500	69.51%	8.775%
11	6.587	792	799	802	rBV	2328857	2682358	56.35%	7.114%
12	7.439	939	944	948	rBV	1342817	1300238	27.32%	3.448%
13	8.769	1163	1170	1173	rBV	4291249	4759994	100.00%	12.624%
14	9.586	1302	1309	1313	rBV	1304515	1348520	28.33%	3.576%
15	10.557	1467	1474	1477	rBV	1554242	1628468	34.21%	4.319%
16	11.410	1609	1619	1623	rBV	1196147	1186289	24.92%	3.146%
17	13.392	1948	1956	1959	rBV	3042898	3508678	73.71%	9.306%
18	14.657	2167	2171	2177	rVB	821520	837898	17.60%	2.222%
19	16.292	2444	2449	2455	rBV	647987	764852	16.07%	2.029%

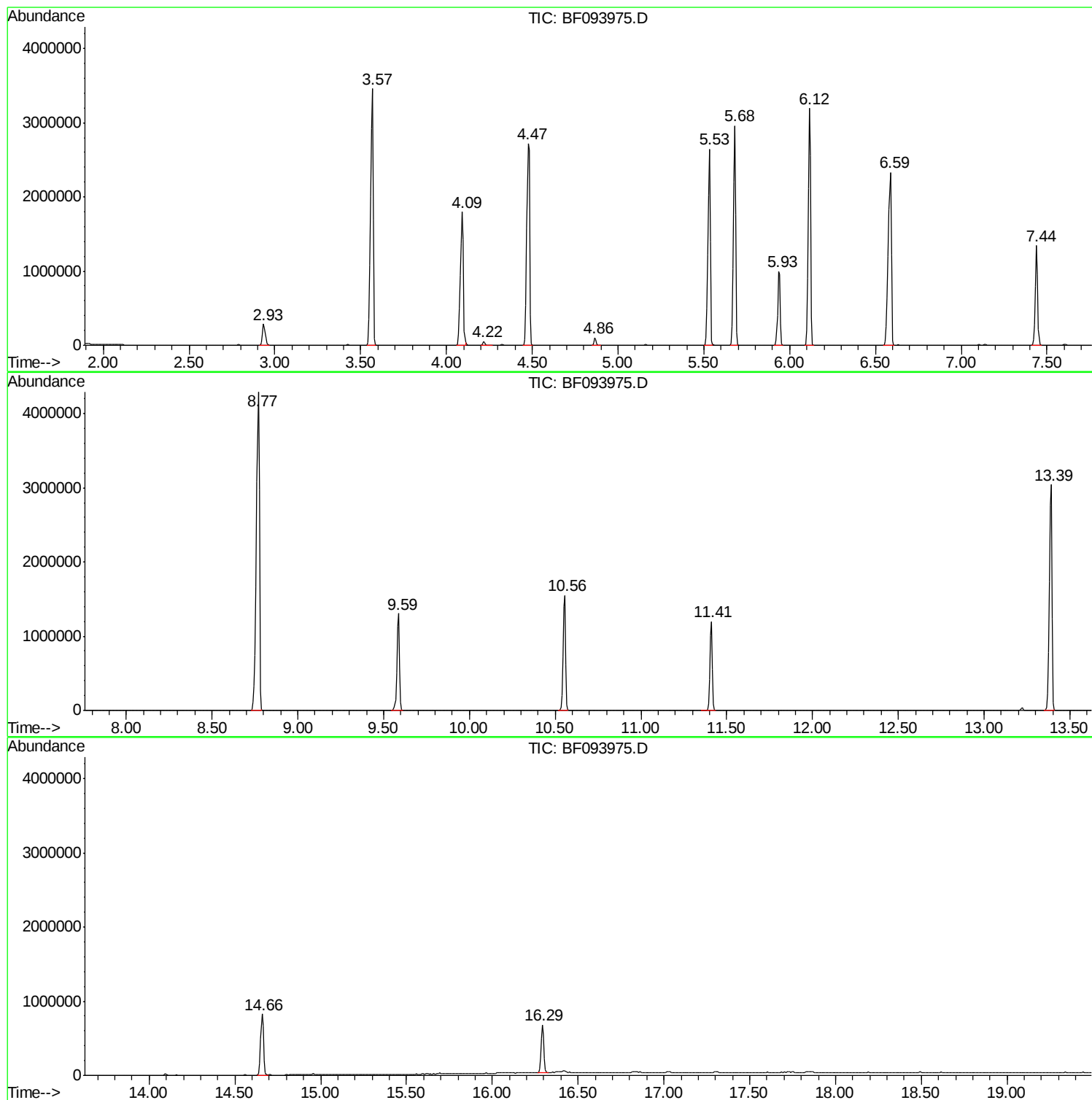
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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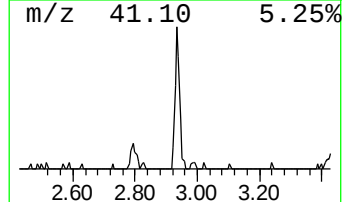
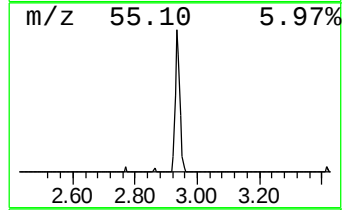
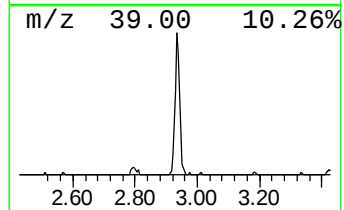
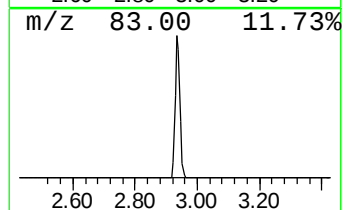
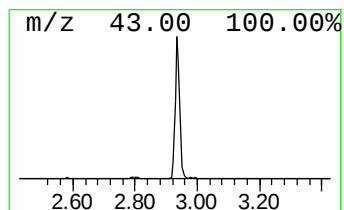
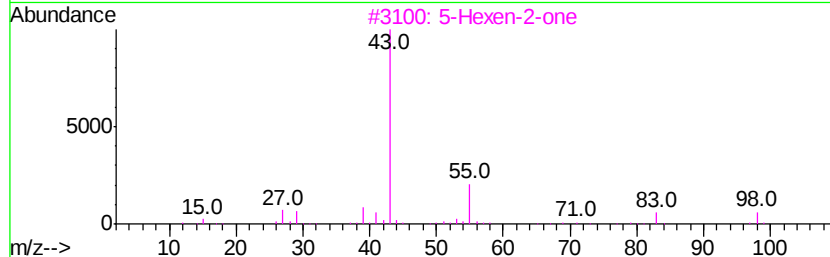
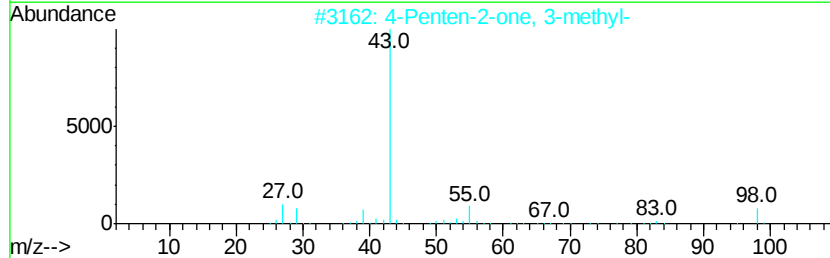
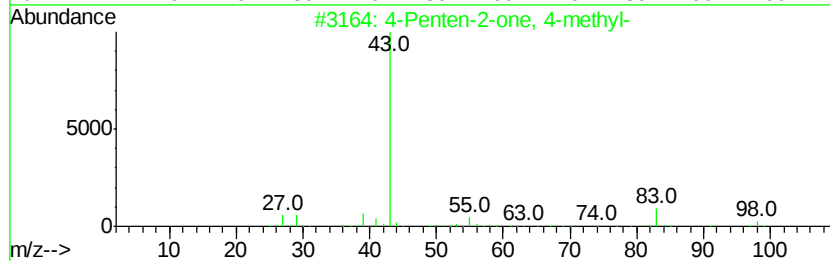
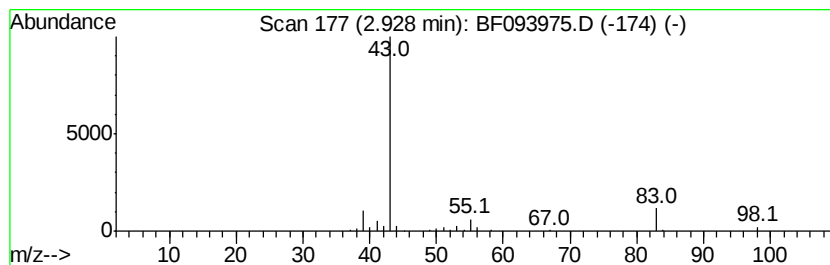
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	6.05 ng	292340	1,4-Dichlorobenzene-d4	5.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	50
3		5-Hexen-2-one	98	C6H10O	000109-49-9	36
4		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	12
5		4-Hexen-2-one	98	C6H10O	025659-22-7	9



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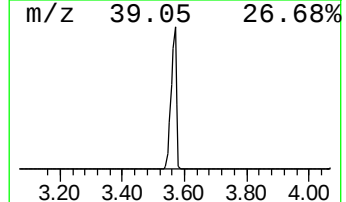
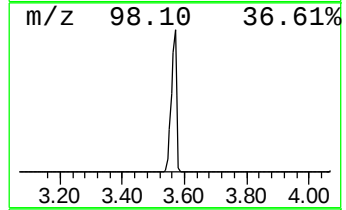
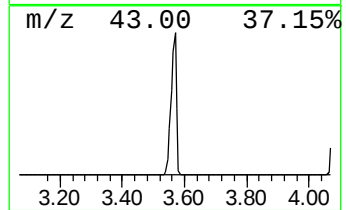
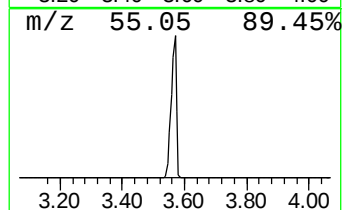
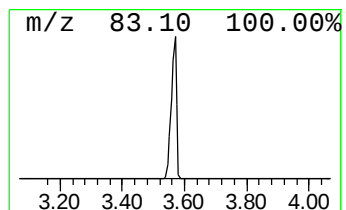
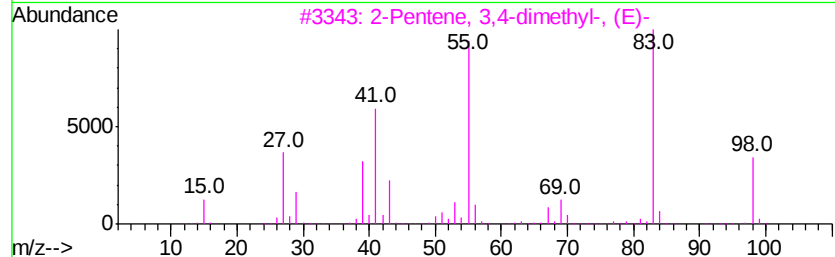
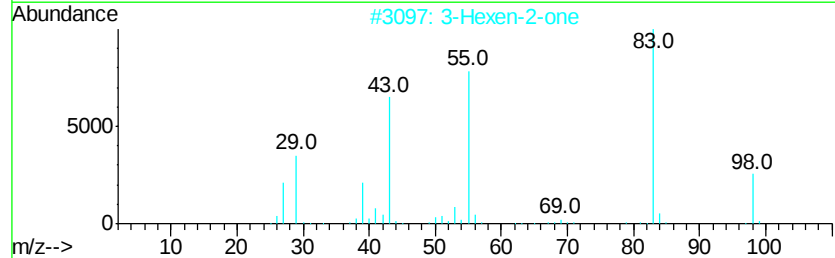
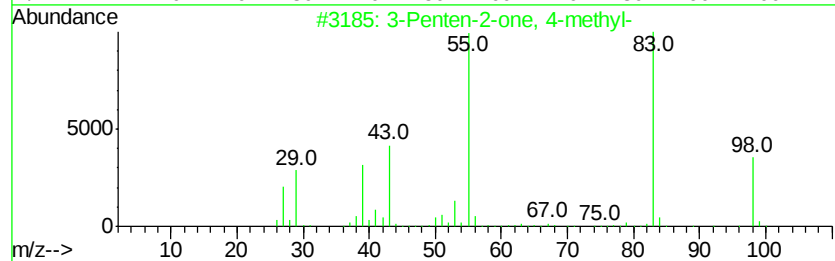
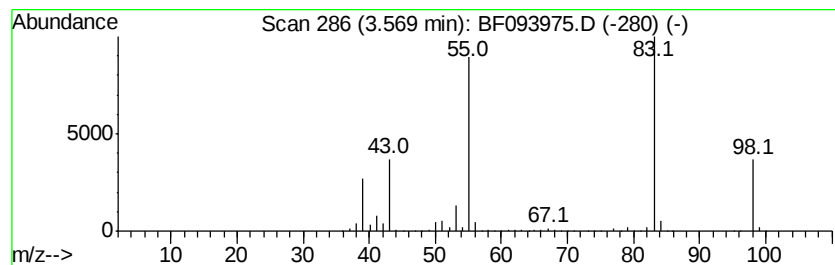
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	84.81 ng	4097000	1,4-Dichlorobenzene-d4	5.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
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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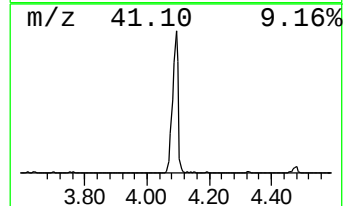
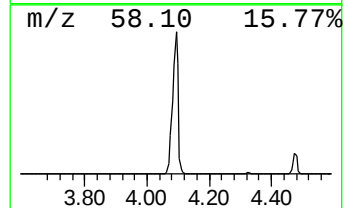
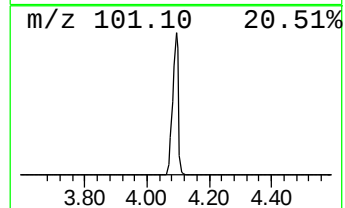
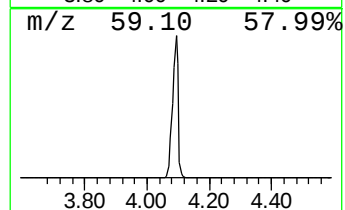
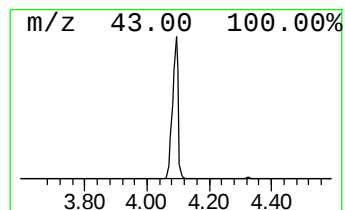
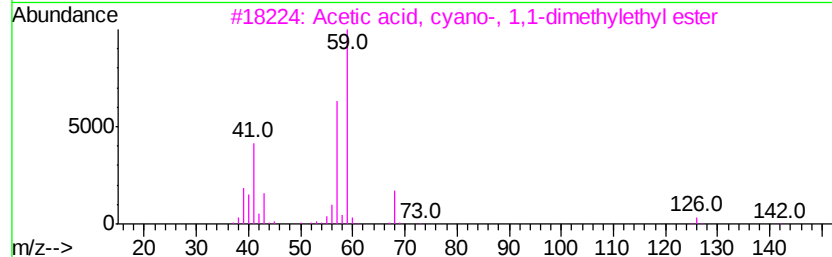
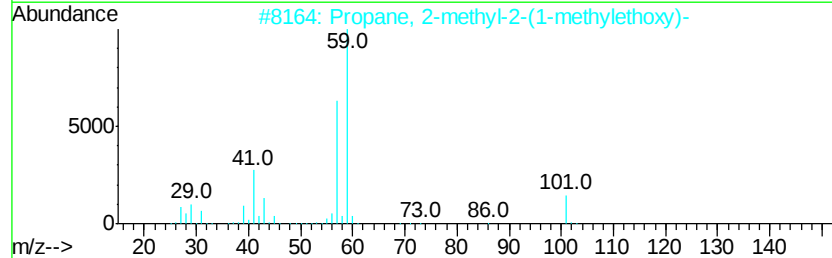
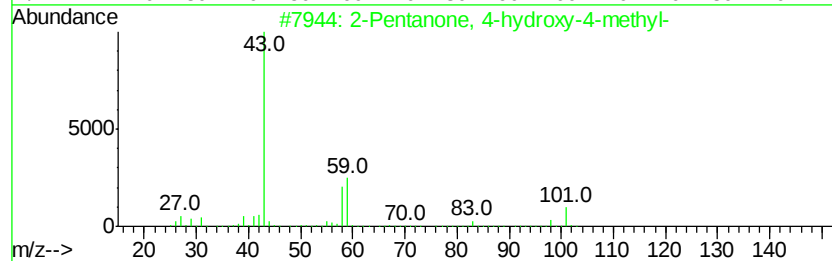
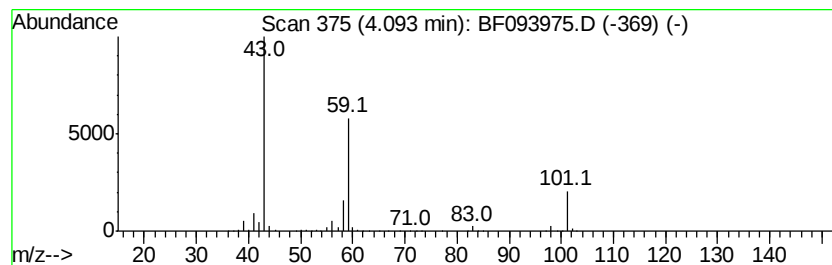
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.09	47.05 ng	2273010	1,4-Dichlorobenzene-d4	5.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		1,2-Butanediol, (+/-)-	90	C4H10O2	026171-83-5	9



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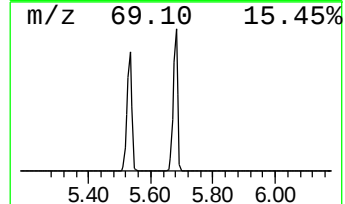
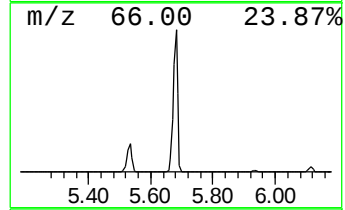
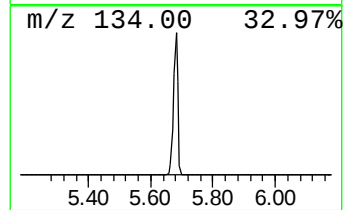
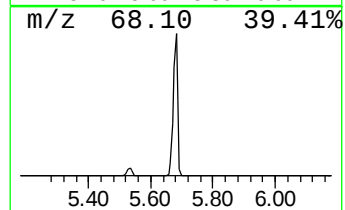
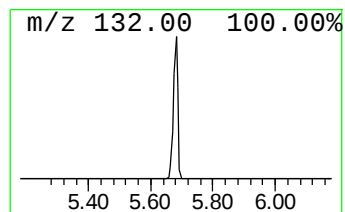
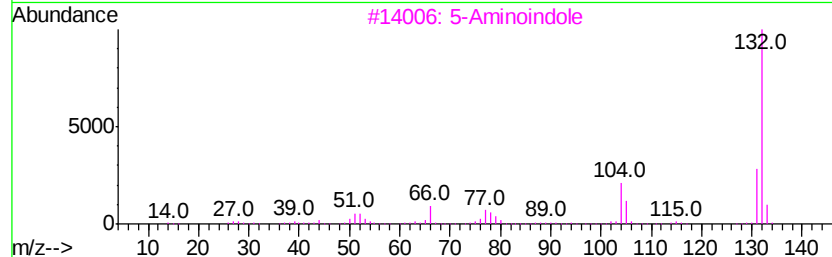
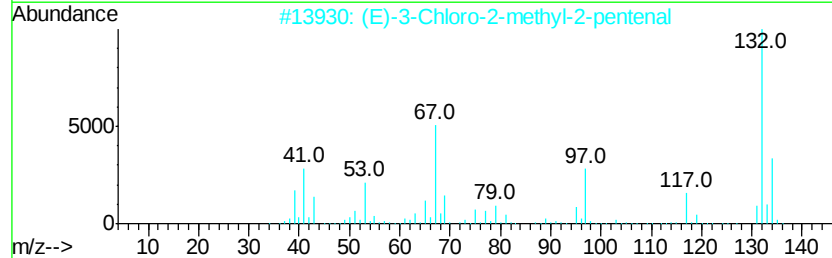
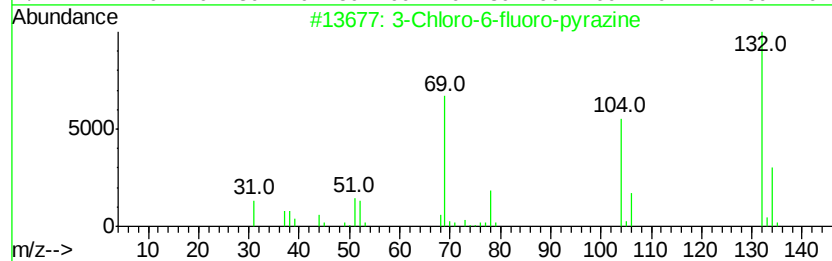
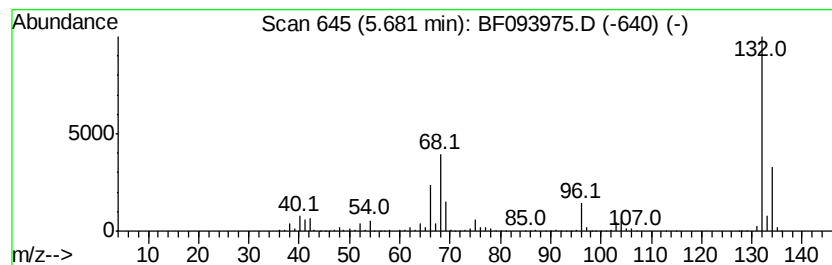
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Peak Number 4 unknown5.68 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.68	61.47 ng	2969450	1,4-Dichlorobenzene-d4	5.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	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
4-Penten-2-one, 4...	2.93	6.0	ng	292340	1	5.94	966189	20.0
3-Penten-2-one, 4...	3.57	84.8	ng	4097000	1	5.94	966189	20.0
2-Pentanone, 4-hy...	4.09	47.0	ng	2273010	1	5.94	966189	20.0
unknown5.68	5.68	61.5	ng	2969450	1	5.94	966189	20.0