

Data Path : Z:\HPCHEM1\BNA_F\Data\BF042117\
 Data File : BF094566.D
 Acq On : 21 Apr 2017 16:55
 Operator : SJ/MA
 Sample : I2783-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C-10

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-BF041717.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	2.696	124	129	139	rBV	438409	509601	2.75%	1.262%
2	3.407	235	250	253	rBV	6182801	18529545	100.00%	45.895%
3	3.943	329	341	344	rBV	3295507	8142091	43.94%	20.167%
4	5.760	646	650	655	rBV	645702	565705	3.05%	1.401%
5	5.937	676	680	683	rBV	1774012	1591720	8.59%	3.942%
6	6.131	709	713	718	rBV	293554	287386	1.55%	0.712%
7	6.407	755	760	763	rBV	1299998	1193610	6.44%	2.956%
8	7.254	900	904	907	rBV	900749	807177	4.36%	1.999%
9	8.578	1124	1129	1132	rBV	2428737	2402520	12.97%	5.951%
10	9.078	1210	1214	1218	rBV	211173	227378	1.23%	0.563%
11	9.383	1260	1266	1271	rBV2	868604	969182	5.23%	2.401%
12	11.207	1572	1576	1578	rBV	854184	853596	4.61%	2.114%
13	11.230	1578	1580	1586	rVB	238405	223379	1.21%	0.553%
14	12.695	1825	1829	1834	rBV	230303	243343	1.31%	0.603%
15	12.966	1872	1875	1879	rVB	201021	208443	1.12%	0.516%
16	13.183	1907	1912	1916	rBV	2003926	2110106	11.39%	5.226%
17	14.454	2122	2128	2131	rBV	642347	813716	4.39%	2.015%
18	16.077	2400	2404	2411	rBV	615259	695259	3.75%	1.722%

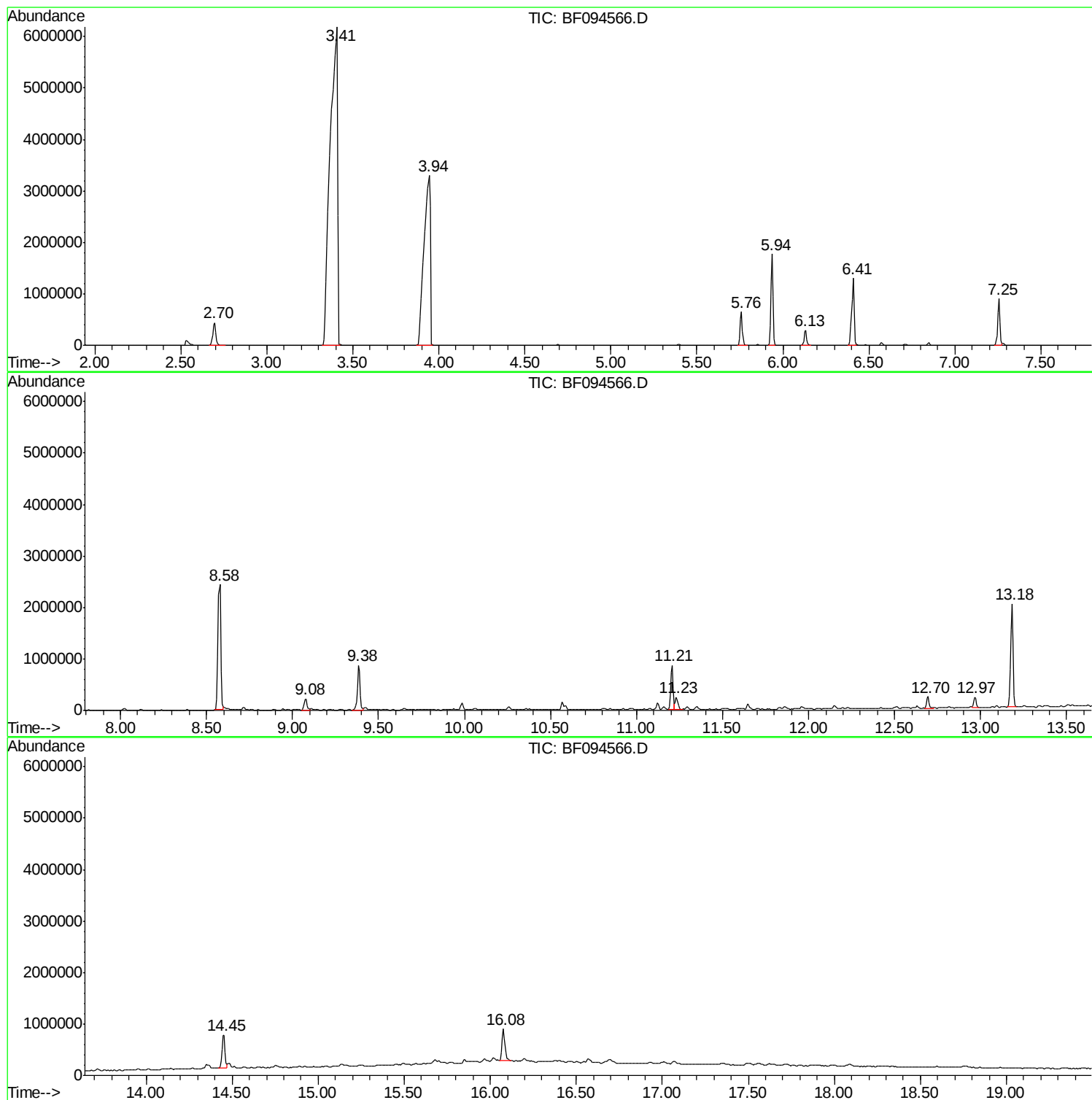
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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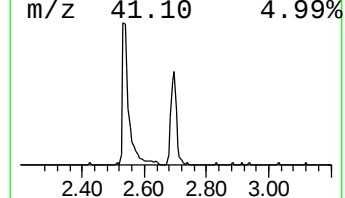
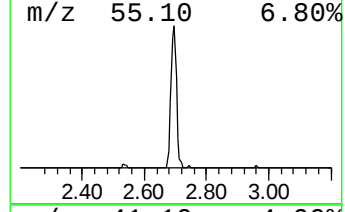
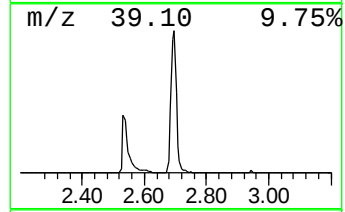
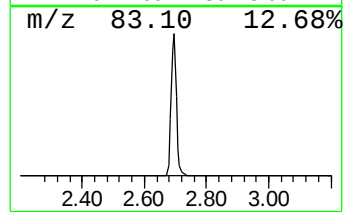
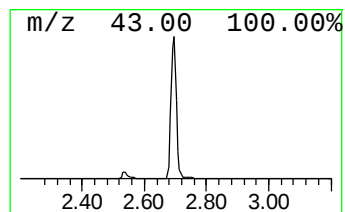
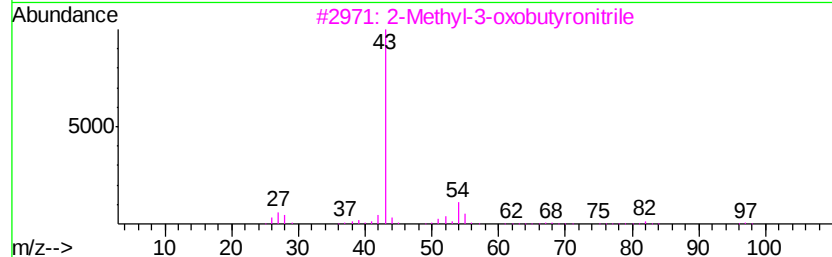
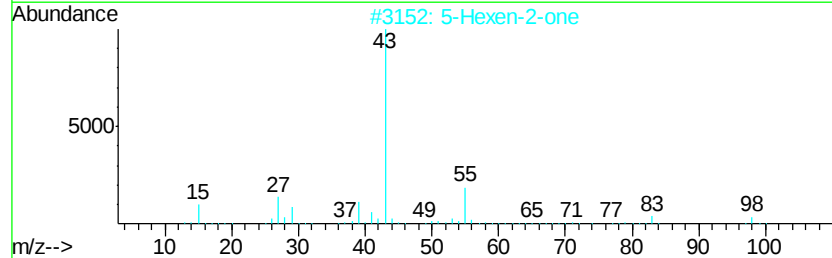
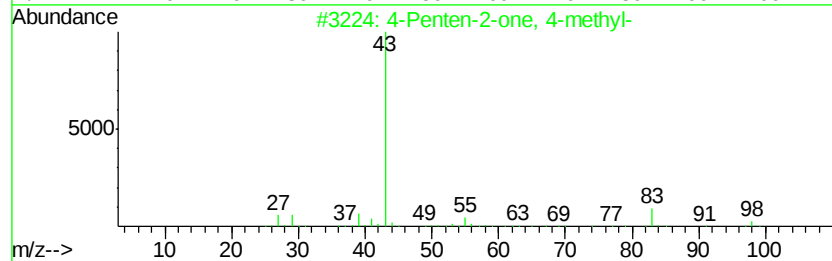
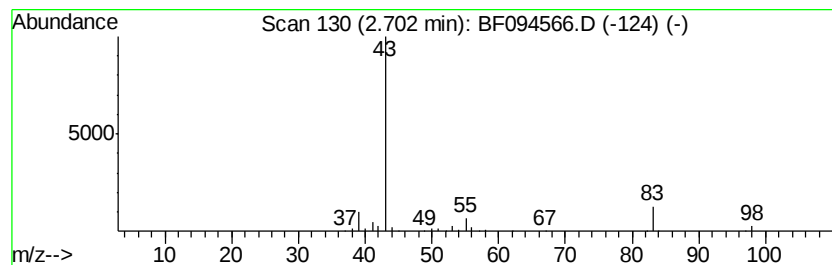
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.70	18.02 ng	509601	1,4-Dichlorobenzene-d4	5.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2		5-Hexen-2-one	98	C6H10O	000109-49-9	35
3		2-Methyl-3-oxobutyronitrile	97	C5H7NO	004468-47-7	9
4		2-Pentanone, 5-hydroxy-	102	C5H10O2	001071-73-4	9
5		Pent-3-enylamine	85	C5H11N	087156-70-5	9



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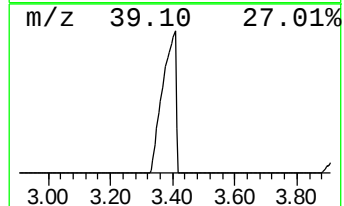
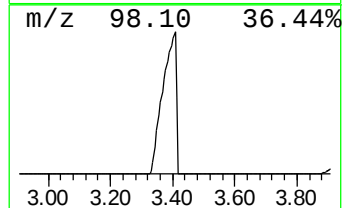
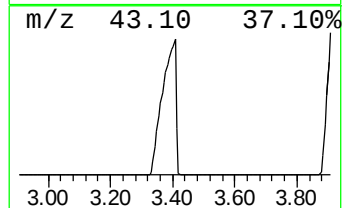
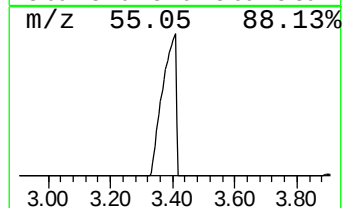
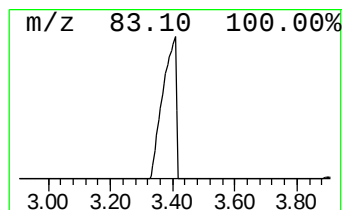
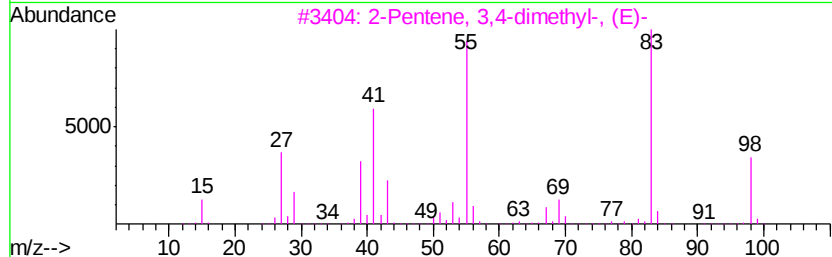
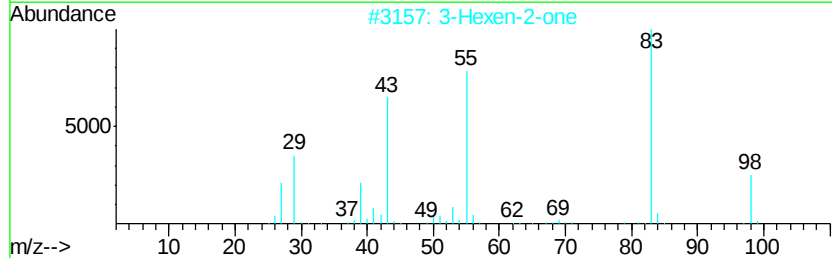
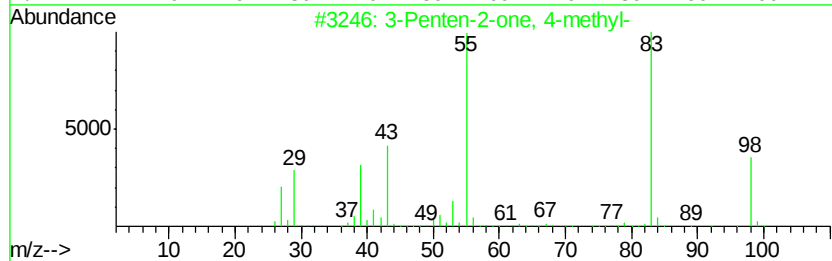
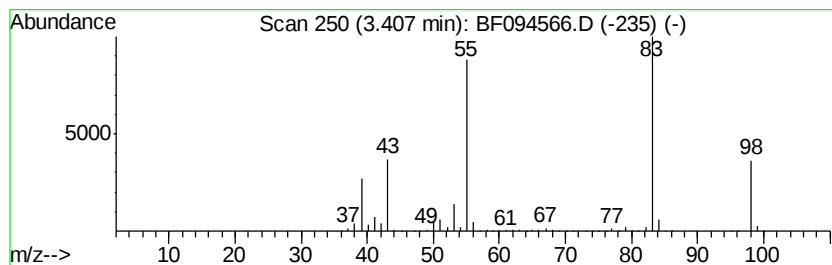
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.41	655.10 ng	18529500	1,4-Dichlorobenzene-d4	5.76

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, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86



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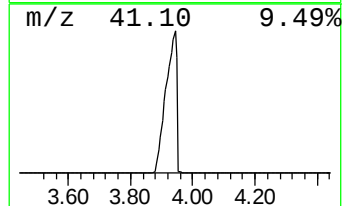
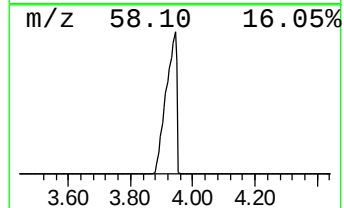
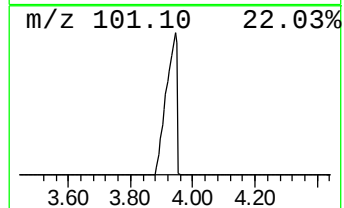
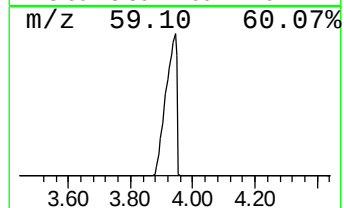
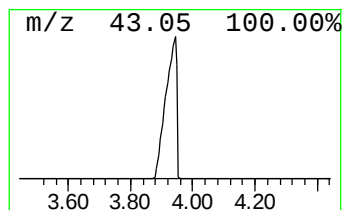
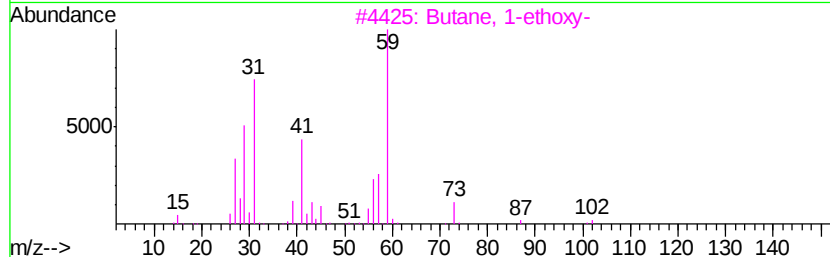
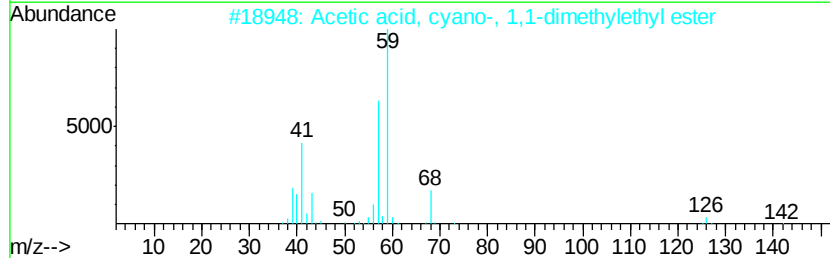
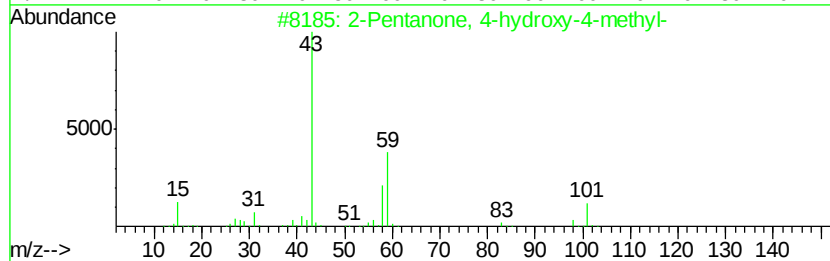
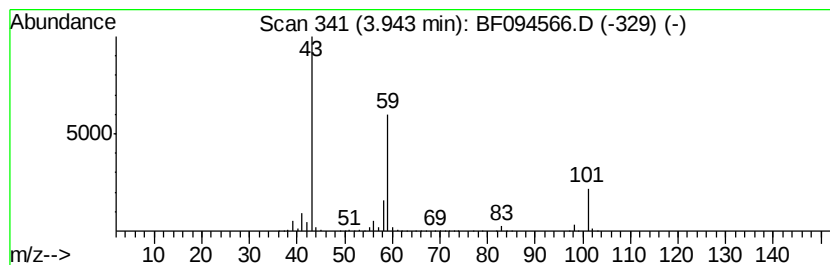
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.94	287.86 ng	8142090	1,4-Dichlorobenzene-d4	5.76

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	25
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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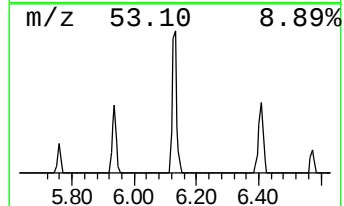
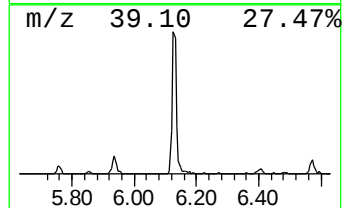
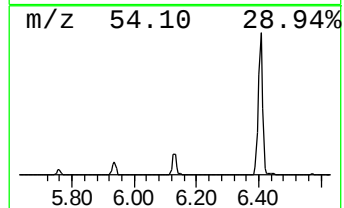
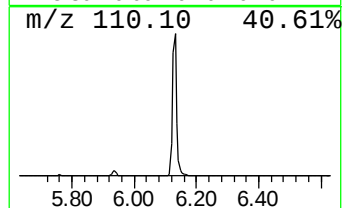
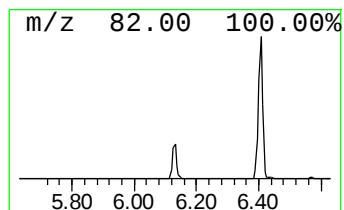
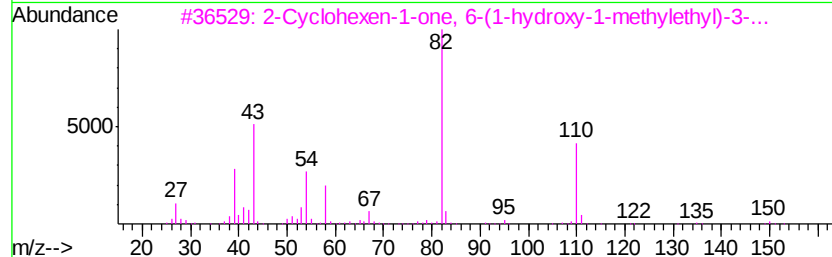
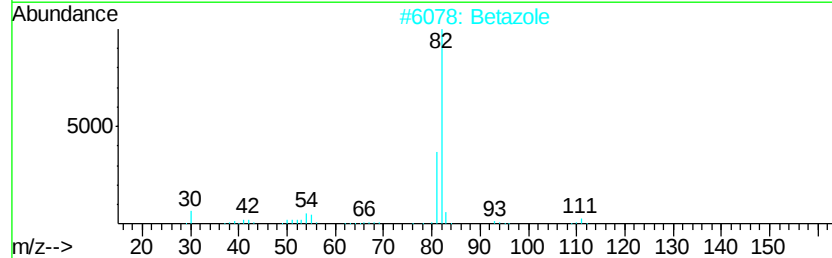
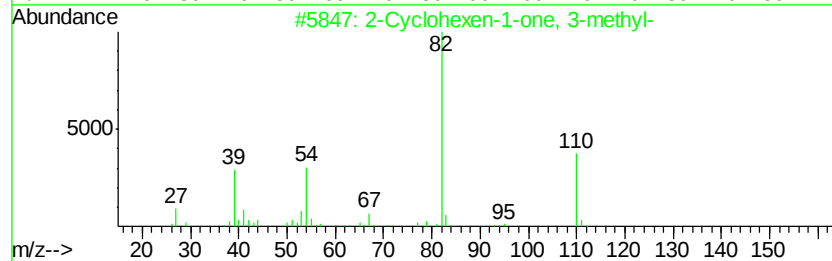
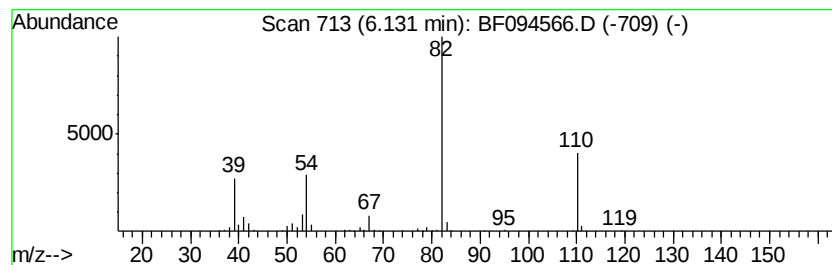
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Peak Number 5 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.13	10.16 ng	287386	1,4-Dichlorobenzene-d4	5.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2		Betazole	111	C5H9N3	000105-20-4	47
3		2-Cyclohexen-1-one, 6-(1-hydroxyv...	168	C10H16O2	087791-00-2	43
4		1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	40
5		Furan, 2-methyl-	82	C5H6O	000534-22-5	33



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one, 4...	2.70	18.0	ng	509601	1	5.76	565705	20.0
3-Penten-2-one, 4...	3.41	655.1	ng	18529500	1	5.76	565705	20.0
2-Pentanone, 4-hy...	3.94	287.9	ng	8142090	1	5.76	565705	20.0
2-Cyclohexen-1-on...	6.13	10.2	ng	287386	1	5.76	565705	20.0