

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061716\
 Data File : BF088098.D
 Acq On : 17 Jun 2016 17:39
 Operator : UM/SJ
 Sample : H3558-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP-05

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-BF060716.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	1.667	6	7	16	rVB	242300	410099	10.16%	1.835%
2	1.793	16	18	75	rVB	1566237	4035765	100.00%	18.060%
3	4.136	220	223	236	rVB	425040	562567	13.94%	2.517%
4	4.833	282	284	287	rBV	447608	670102	16.60%	2.999%
5	5.279	321	323	334	rVB	695726	637126	15.79%	2.851%
6	5.690	357	359	362	rBV	124632	105235	2.61%	0.471%
7	6.330	413	415	421	rBV	446482	413790	10.25%	1.852%
8	6.456	424	426	429	rBV	1081981	1121644	27.79%	5.019%
9	6.696	445	447	449	rBV	656656	582558	14.43%	2.607%
10	6.856	458	461	463	rVB	1242364	1699197	42.10%	7.604%
11	7.267	494	497	499	rBV	1379181	1516698	37.58%	6.787%
12	7.976	557	559	562	rBV	716364	786500	19.49%	3.520%
13	9.062	651	654	656	rBV	2604163	2606106	64.58%	11.662%
14	9.462	683	689	690	rBV	35271	48297	1.20%	0.216%
15	9.736	710	713	715	rVV	688819	943821	23.39%	4.224%
16	10.159	747	750	753	rVB2	157829	180155	4.46%	0.806%
17	10.513	779	781	784	rBV	968235	1018508	25.24%	4.558%
18	10.639	791	792	797	rBV	34320	46030	1.14%	0.206%
19	11.211	840	842	844	rBV	1133288	976413	24.19%	4.369%
20	12.799	978	981	983	rBV	2303584	2561169	63.46%	11.461%
21	13.839	1069	1072	1075	rBV	880920	810844	20.09%	3.628%
22	15.222	1190	1193	1196	rBV	533717	614226	15.22%	2.749%

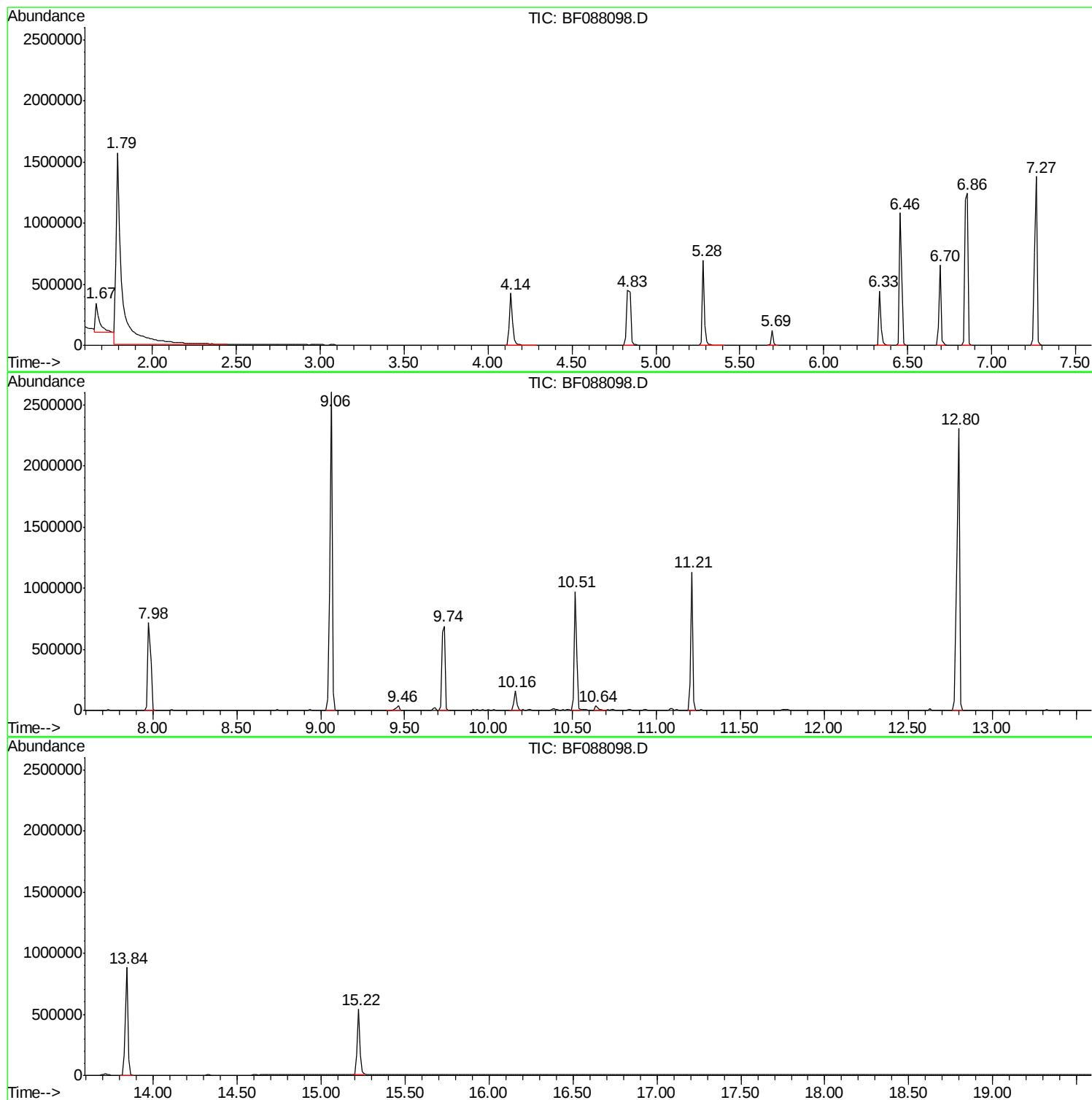
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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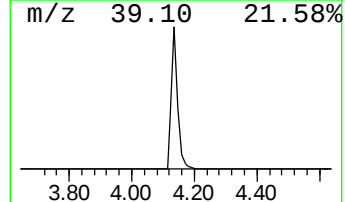
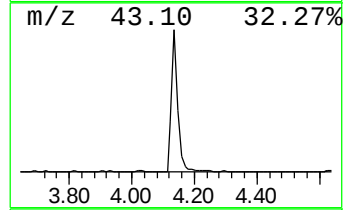
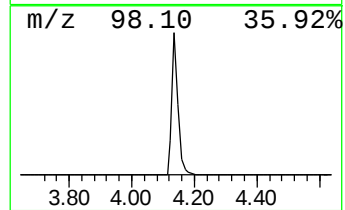
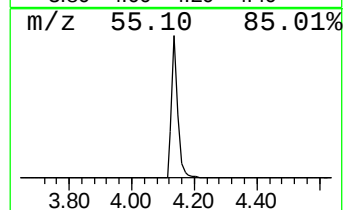
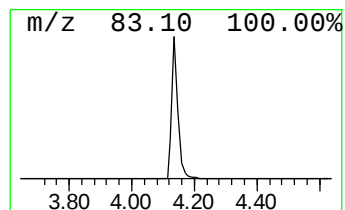
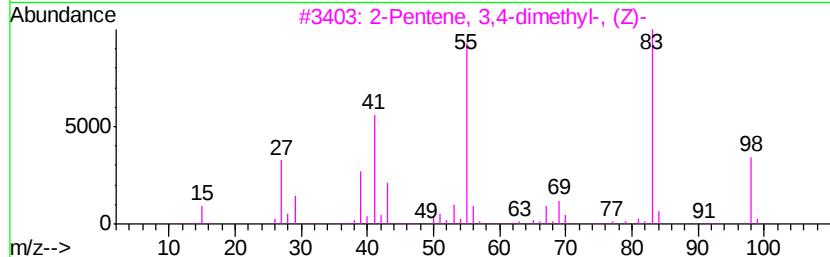
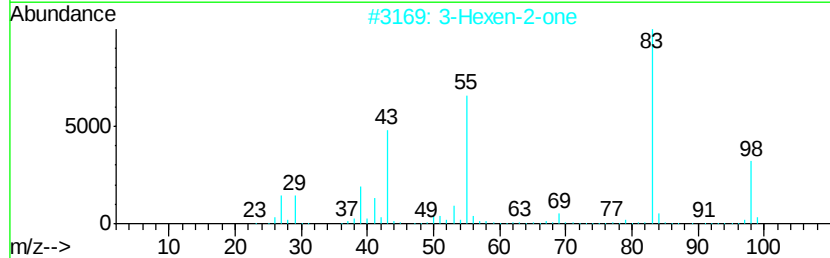
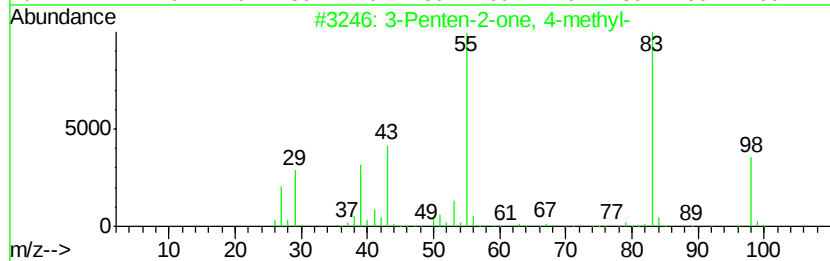
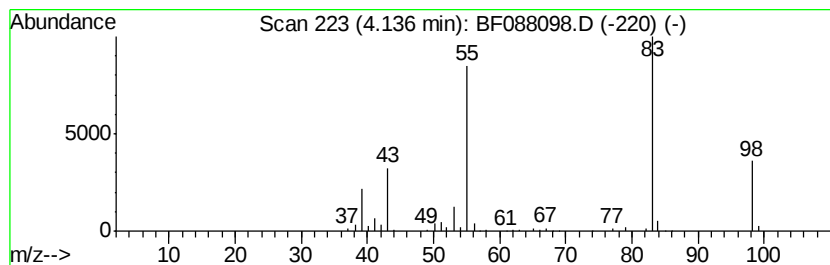
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.14	19.31 ng	562567	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-, (Z)-	98	C7H14	004914-91-4	86
4		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5		Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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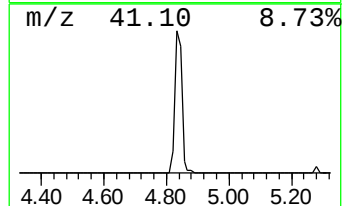
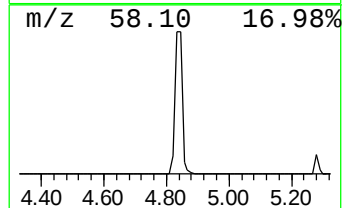
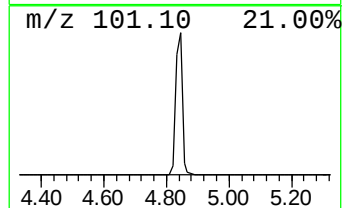
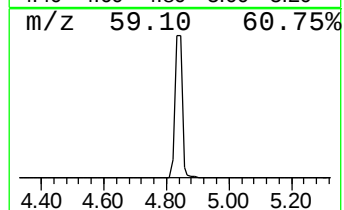
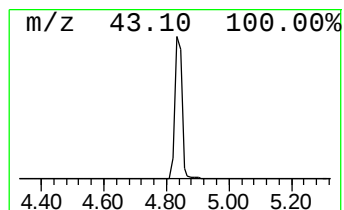
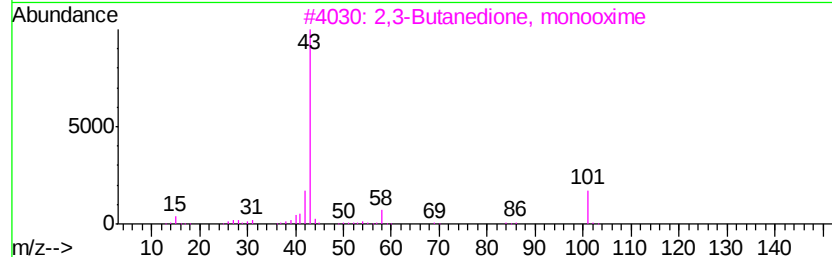
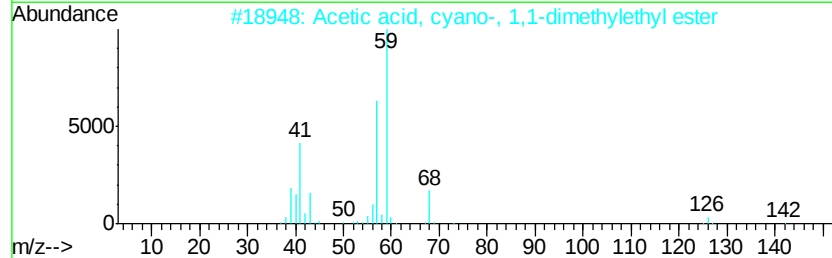
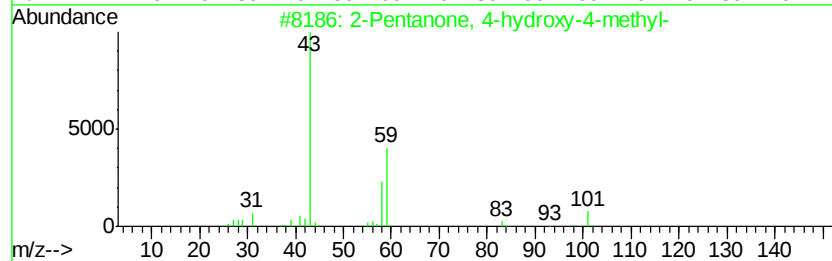
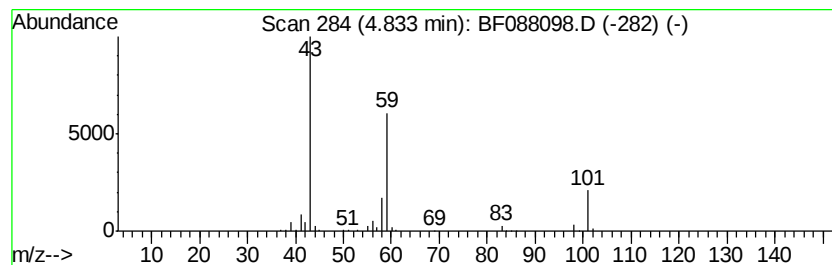
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	23.01 ng	670102	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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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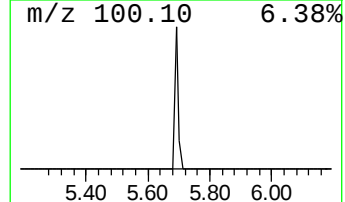
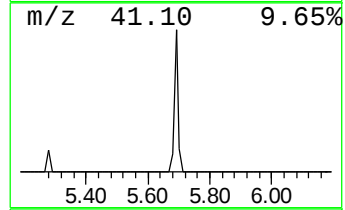
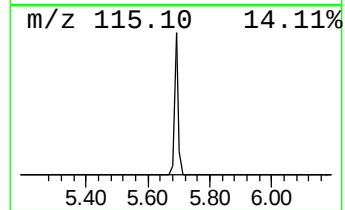
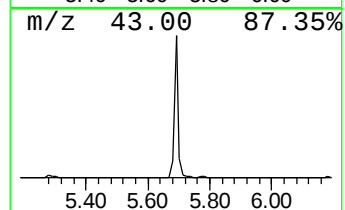
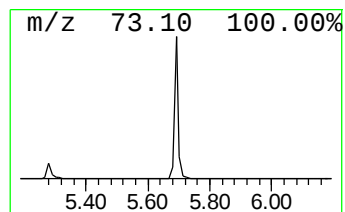
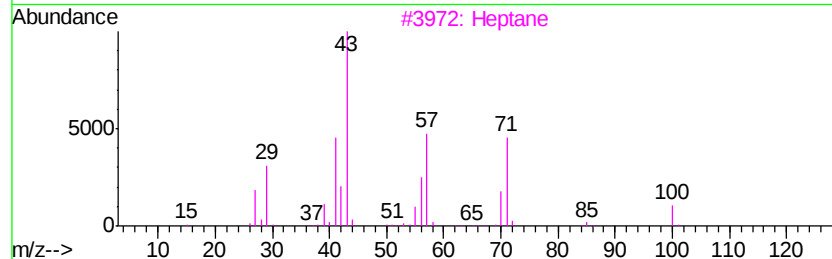
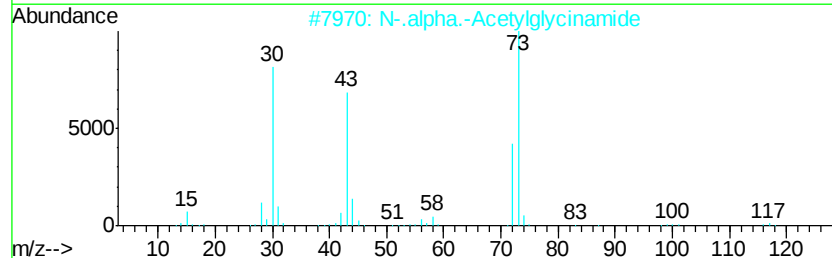
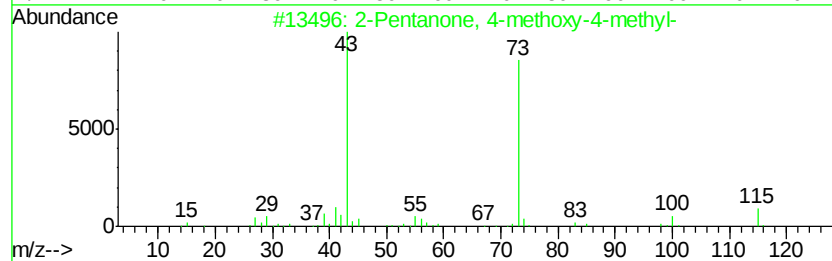
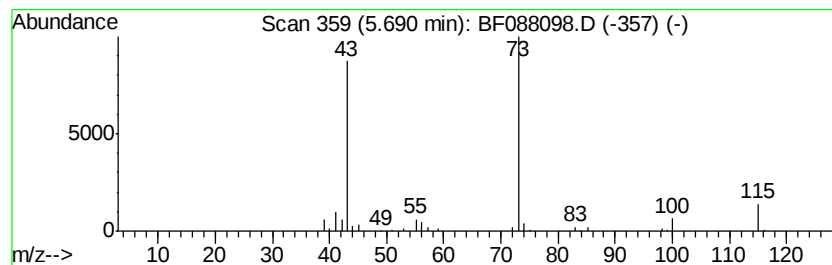
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Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.69	3.61 ng	105235	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-.alpha.-Acetylglutcinamide	116	C4H8N2O2	002620-63-5	28
3		Heptane	100	C7H16	000142-82-5	16
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		N-Formylmorpholine	115	C5H9NO2	004394-85-8	9



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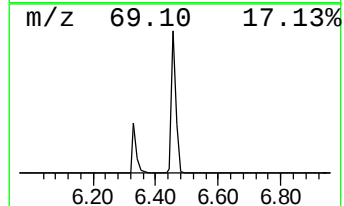
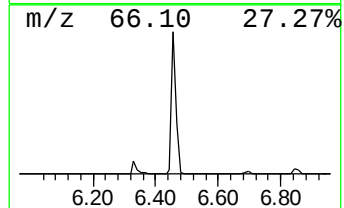
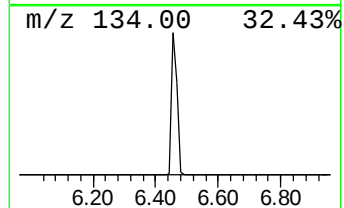
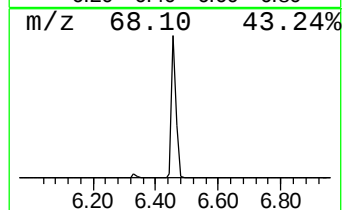
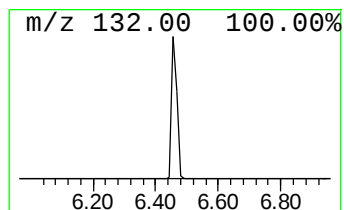
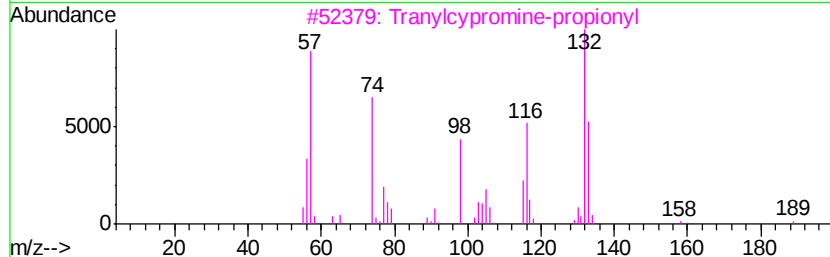
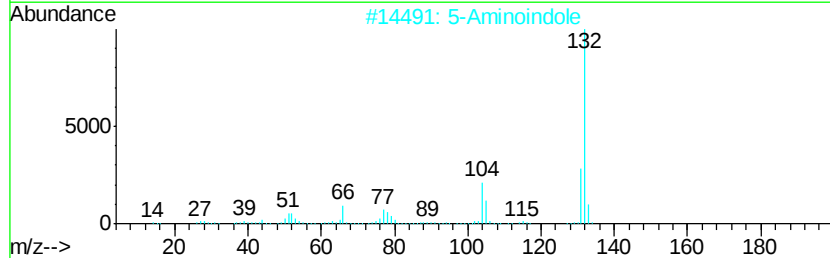
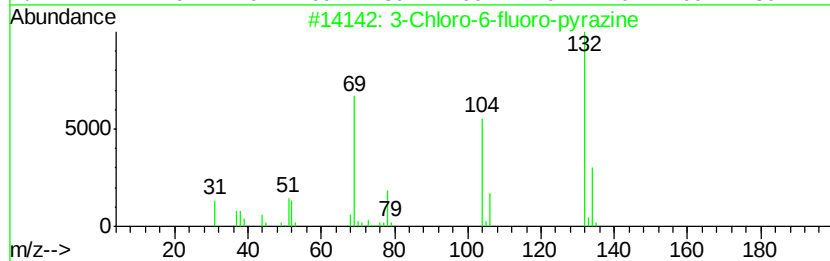
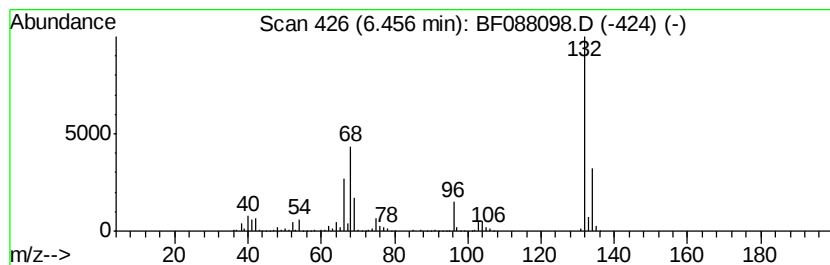
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Peak Number 6 unknown6.46 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	38.51 ng	1121640	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.14	19.3	ng	562567	1	6.70	582558	20.0
2-Pentanone, 4-hy...	4.83	23.0	ng	670102	1	6.70	582558	20.0
2-Pentanone, 4-me...	5.69	3.6	ng	105235	1	6.70	582558	20.0
unknown6.46	6.46	38.5	ng	1121640	1	6.70	582558	20.0