

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
 Data File : BG055849.D
 Acq On : 30 Nov 2022 19:53
 Operator : CG/JU
 Sample : N5809-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 HOWE-DRUM-A-1129

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:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055849.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.662	228	234	245	rBV	25134	52712	3.43%	0.585%
2	5.279	331	339	349	rVB	399683	639369	41.58%	7.097%
3	5.761	414	421	440	rBV	561624	1041173	67.71%	11.558%
4	6.372	517	525	531	rBV	33478	57789	3.76%	0.641%
5	7.383	687	697	709	rBV	588801	1093526	71.12%	12.139%
6	7.512	712	719	727	rBV	102000	197224	12.83%	2.189%
7	8.223	830	840	847	rBV	157716	276216	17.96%	3.066%
8	9.398	1031	1040	1051	rBV	211530	388824	25.29%	4.316%
9	11.055	1313	1322	1329	rBV	201362	375014	24.39%	4.163%
10	13.470	1727	1733	1740	rVB	904137	1421861	92.47%	15.783%
11	14.850	1962	1968	1974	rVB	308452	484566	31.51%	5.379%
12	16.337	2215	2221	2229	rBV	602875	1080065	70.24%	11.989%
13	17.594	2432	2435	2439	rVB	287949	362574	23.58%	4.025%
14	20.185	2873	2876	2881	rVB	1204728	1537657	100.00%	17.069%

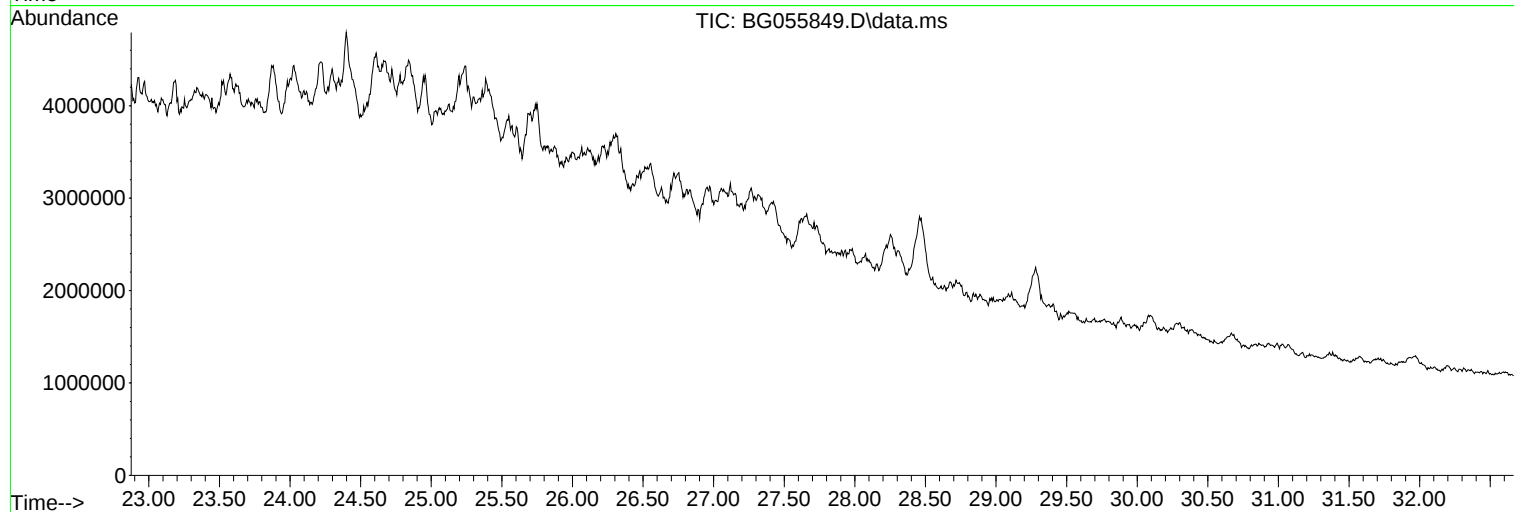
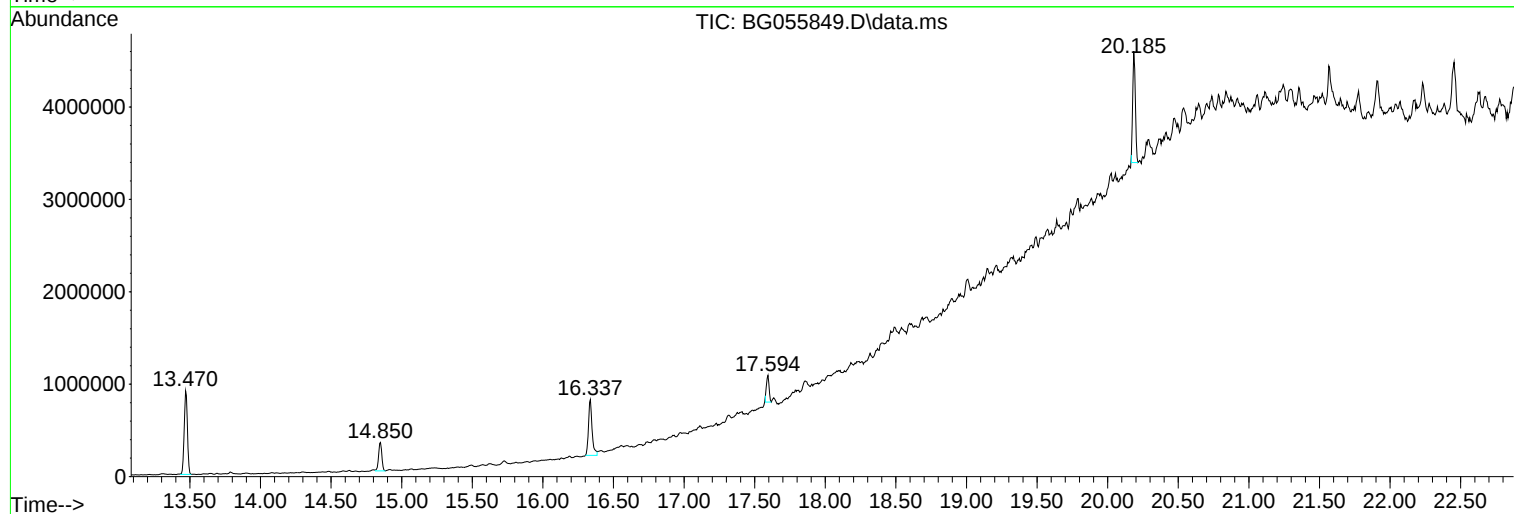
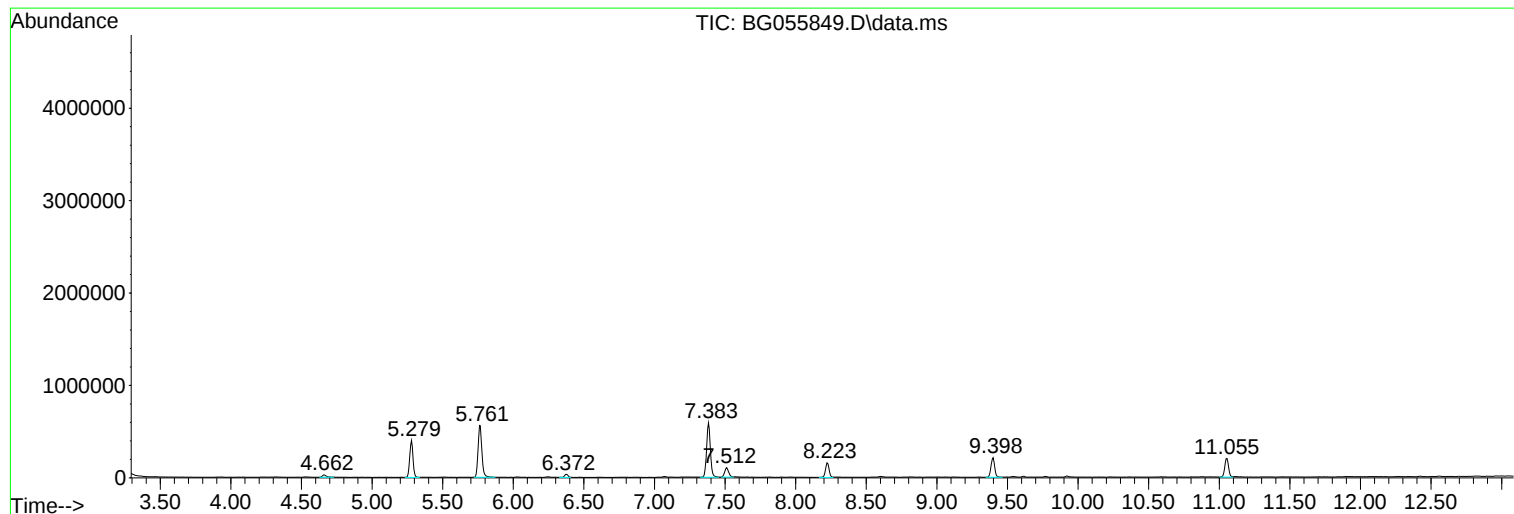
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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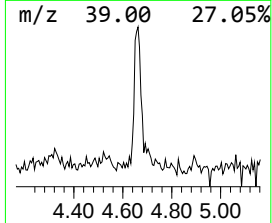
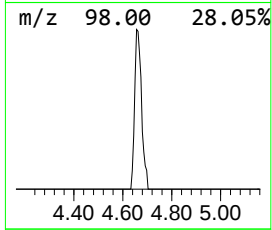
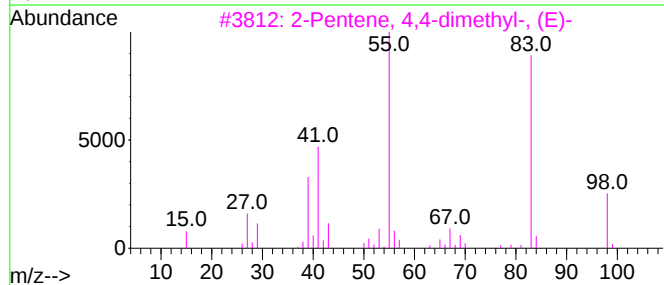
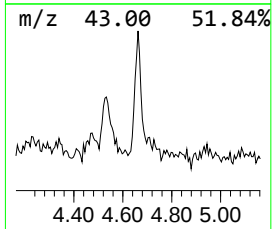
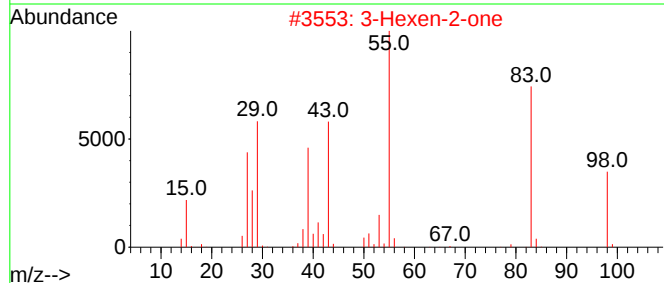
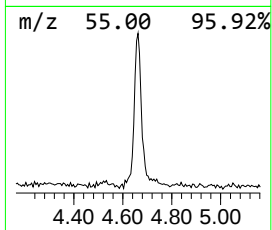
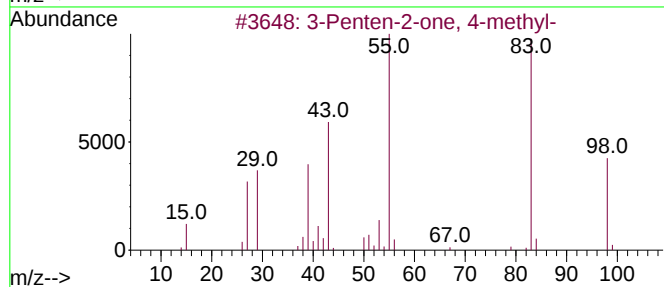
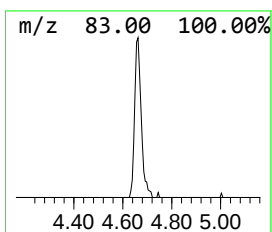
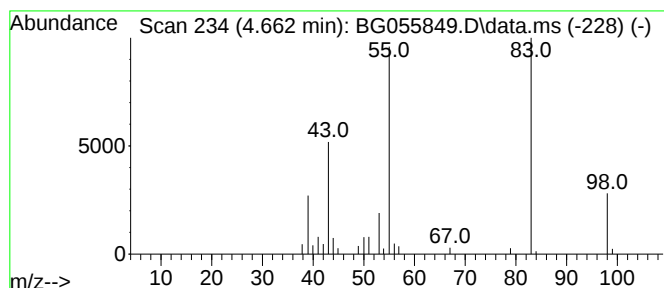
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
4.662	3.82 ng	52712	1,4-Dichlorobenzene-d4	8.223

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
2		3-Hexen-2-one	98	C6H10O	000763-93-9	86
3		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5		Cyclohexane, methyl-	98	C7H14	000108-87-2	72



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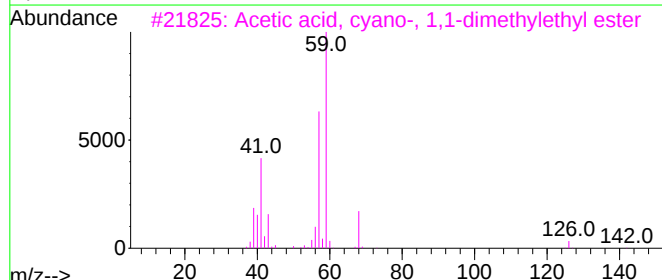
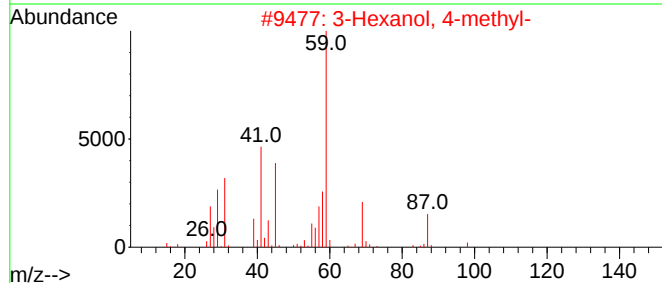
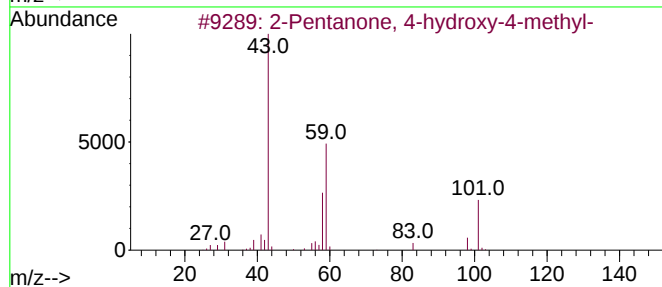
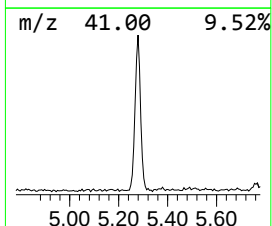
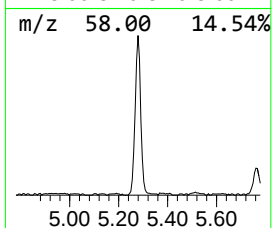
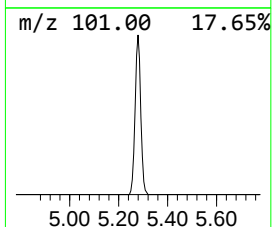
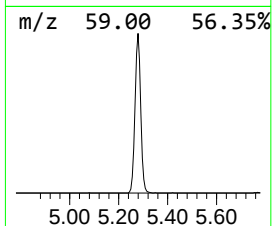
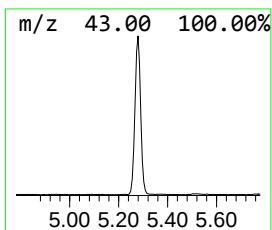
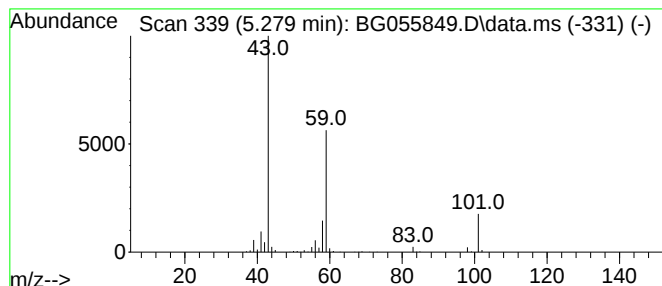
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.279	46.29 ng	639369	1,4-Dichlorobenzene-d4	8.223

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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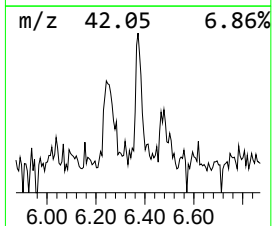
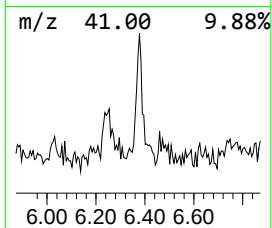
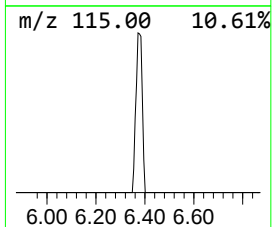
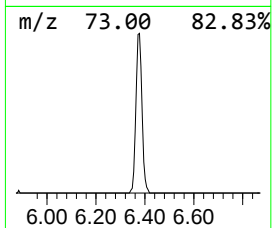
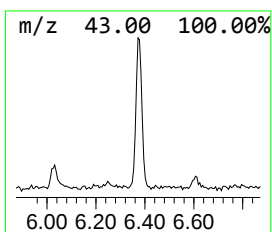
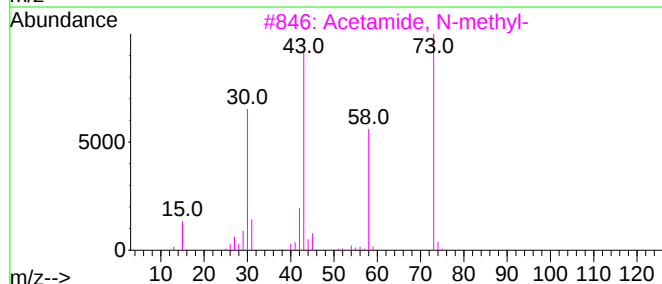
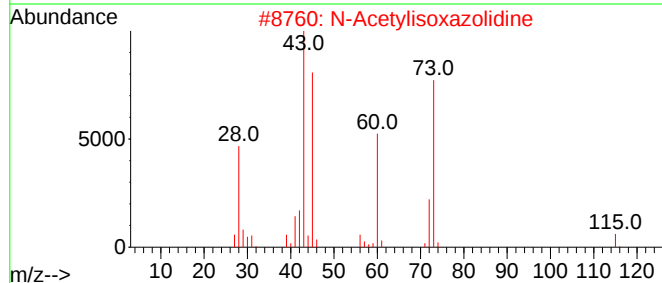
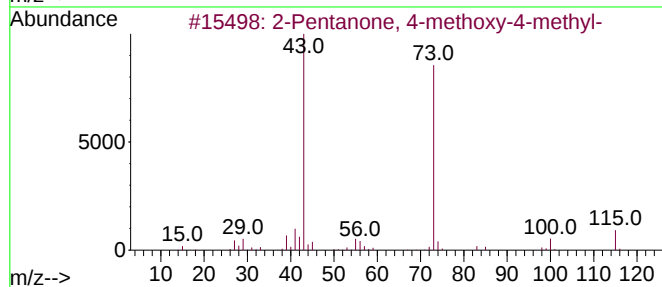
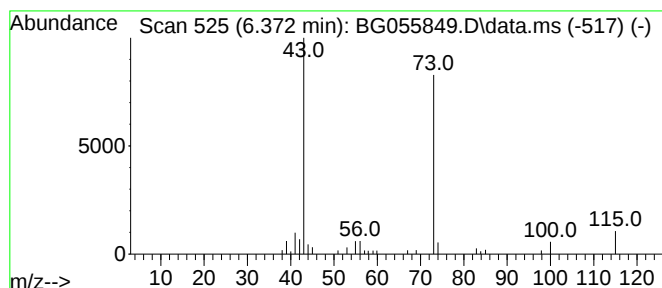
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.372	4.18 ng	57789	1,4-Dichlorobenzene-d4	8.223

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	86
2		N-Acetylisoaxazolidine	115	C5H9NO2	115615-36-6	53
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	40
4		Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	37
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	22



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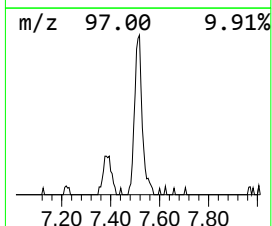
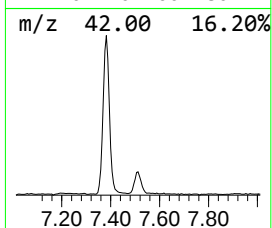
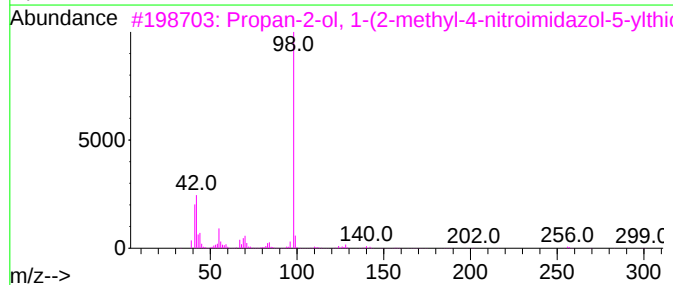
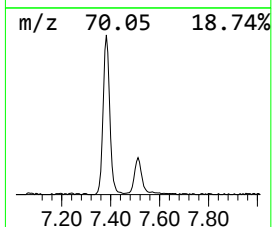
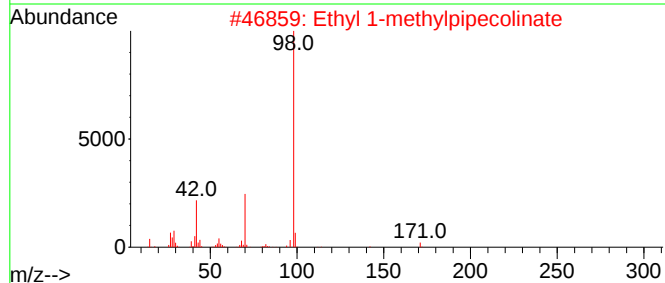
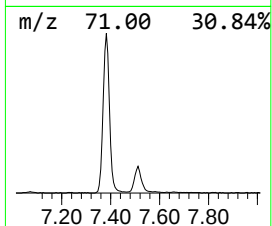
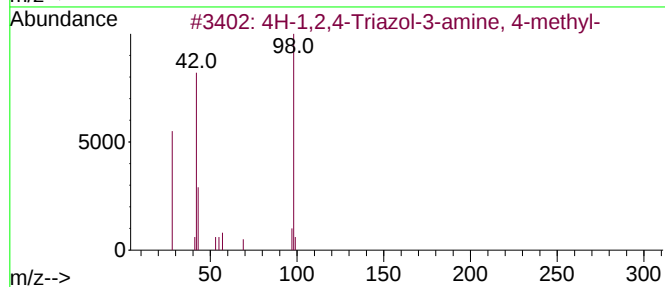
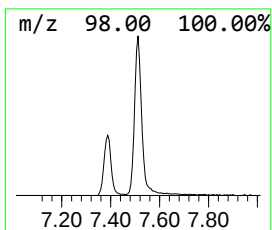
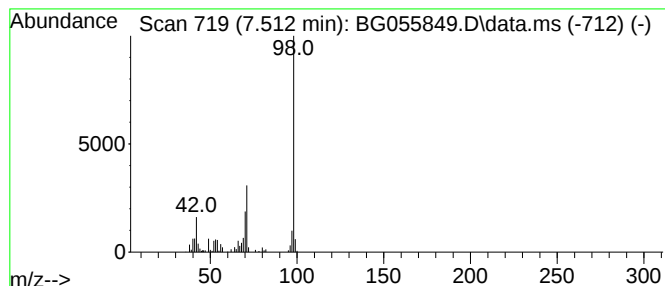
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Peak Number 4 4H-1,2,4-Triazol-3-amine, 4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.512	14.28 ng	197224	1,4-Dichlorobenzene-d4	8.223

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-1,2,4-Triazol-3-amine, 4-methyl-	98	C3H6N4	016681-76-8	53
2			Ethyl 1-methylpipercolinate	171	C9H17NO2	030727-18-5	53
3			Propan-2-ol, 1-(2-methyl-4-nitro...	300	C12H20N4O3S	306326-24-9	53
4			(R)-(1-Ethyl-2-pyrrolidinyl)meth...	128	C7H16N2	022795-97-7	53
5			1-(4-Amino-furazan-3-yl)-5-piper...	321	C13H19N7O3	311314-85-9	53



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.662	3.8	ng	52712	1	8.223	276216	20.0
2-Pentanone, 4-...	5.279	46.3	ng	639369	1	8.223	276216	20.0
2-Pentanone, 4-...	6.372	4.2	ng	57789	1	8.223	276216	20.0
4H-1,2,4-Triazo...	7.512	14.3	ng	197224	1	8.223	276216	20.0