

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
 Data File : BG055850.D
 Acq On : 30 Nov 2022 20:35
 Operator : CG/JU
 Sample : N5806-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMP-1

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: BG055850.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.658	228	233	240	rBV	24523	46205	2.72%	0.531%
2	5.280	331	339	349	rBV	292309	470918	27.71%	5.416%
3	5.768	414	422	446	rBV	486831	976637	57.47%	11.232%
4	6.379	519	526	534	rBV	28471	47800	2.81%	0.550%
5	7.384	689	697	712	rBV	540328	1025231	60.33%	11.791%
6	7.513	712	719	728	rVB	144196	278168	16.37%	3.199%
7	8.224	833	840	847	rVB	150420	255514	15.03%	2.939%
8	9.399	1030	1040	1053	rVB	180555	321832	18.94%	3.701%
9	9.616	1071	1077	1088	rVB	17878	33393	1.96%	0.384%
10	11.056	1314	1322	1329	rBV	203156	361553	21.27%	4.158%
11	13.471	1727	1733	1744	rVB	855056	1373595	80.82%	15.797%
12	13.647	1757	1763	1767	rBV3	13620	25777	1.52%	0.296%
13	14.852	1962	1968	1974	rVB	302295	474556	27.92%	5.458%
14	16.338	2215	2221	2234	rBV	403719	761003	44.78%	8.752%
15	17.589	2429	2434	2439	rBV	348153	543689	31.99%	6.253%
16	20.175	2870	2874	2880	rVB	1337427	1699508	100.00%	19.545%

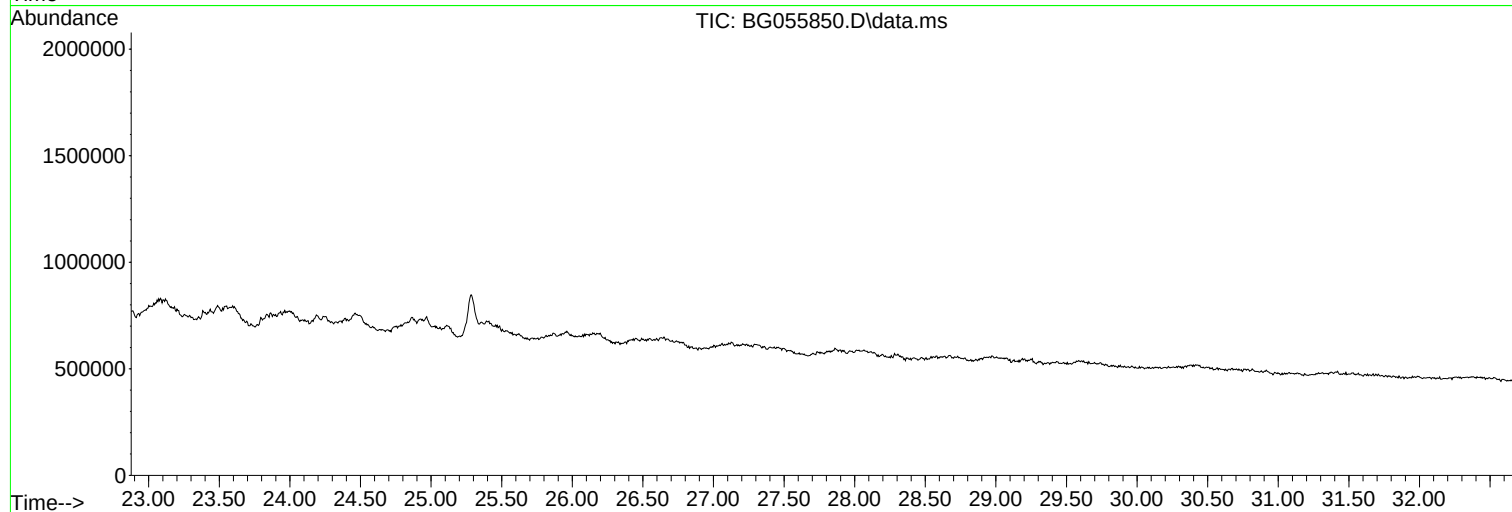
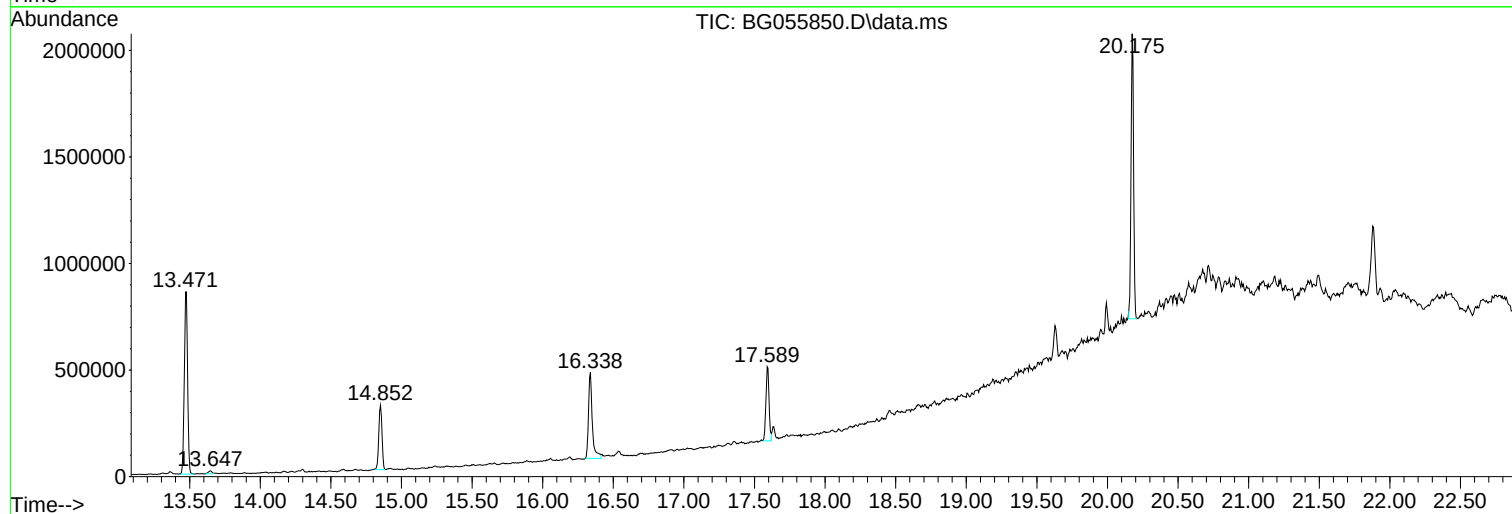
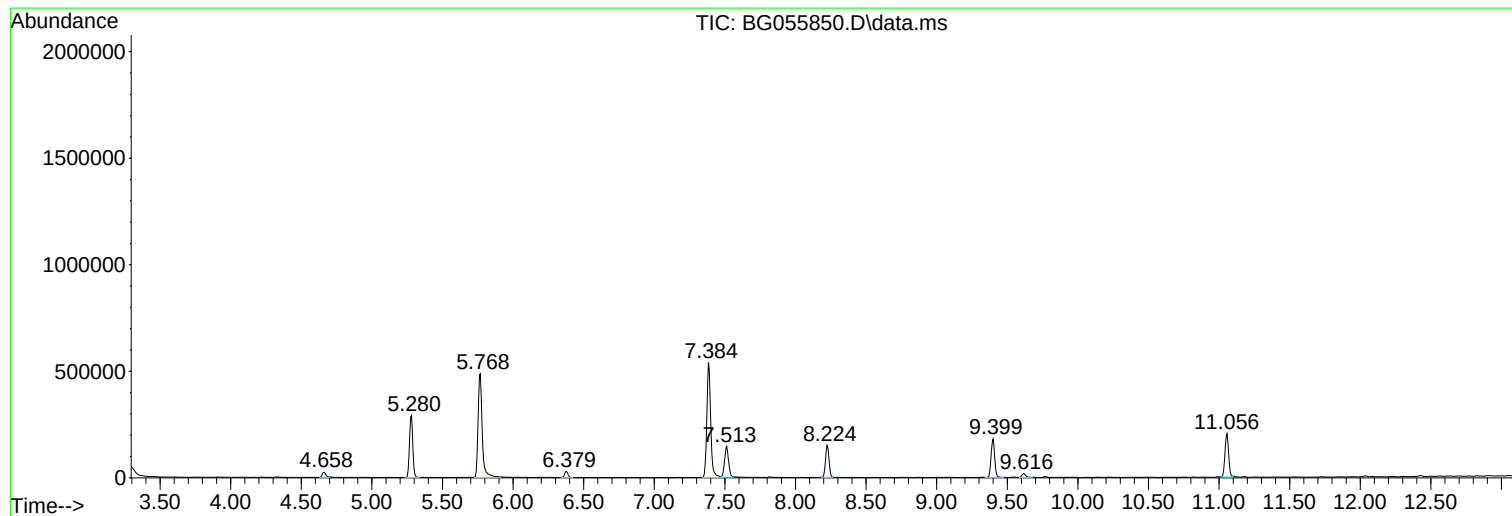
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
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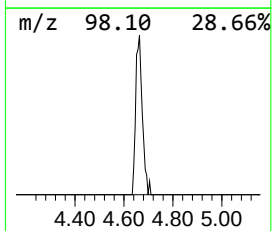
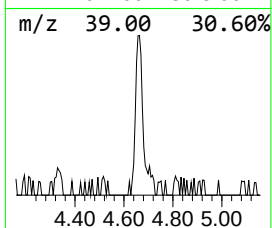
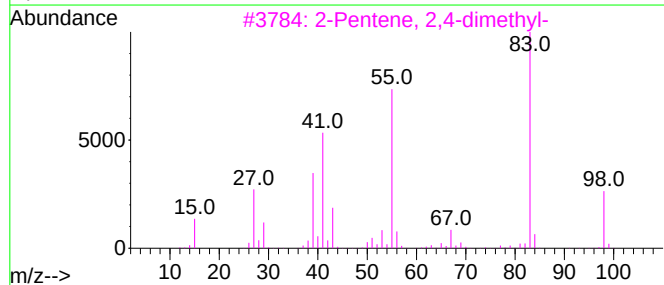
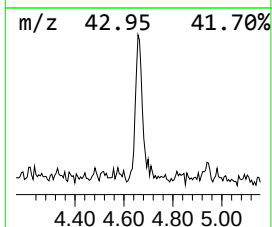
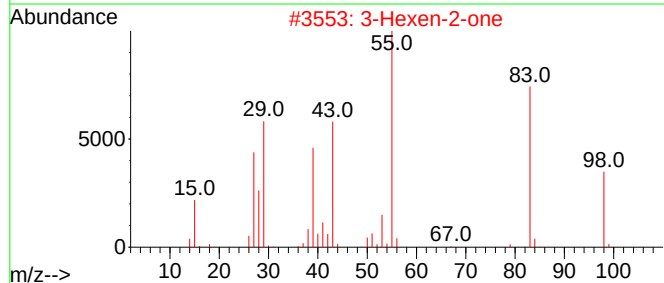
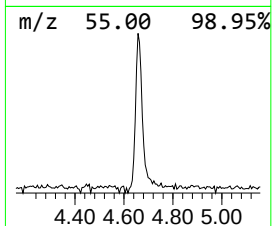
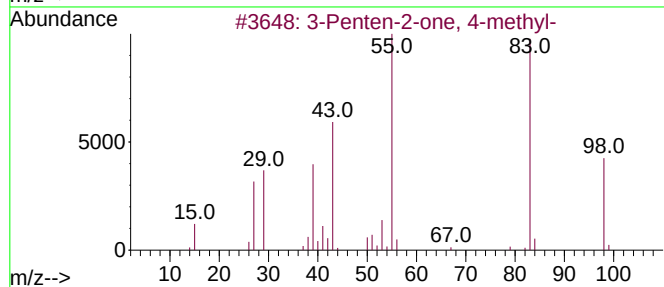
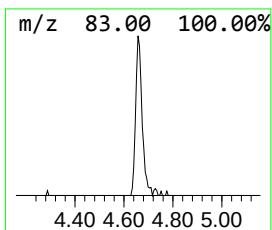
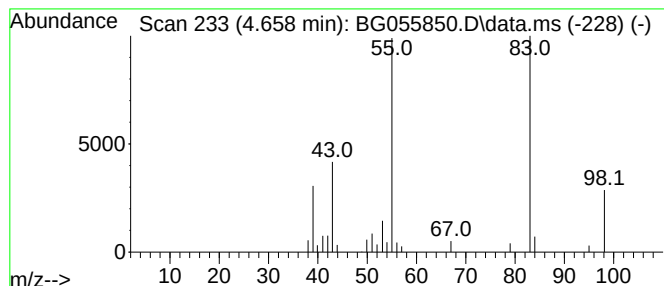
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.658	3.62 ng	46205	1,4-Dichlorobenzene-d4	8.224

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	87
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80
5		2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	72



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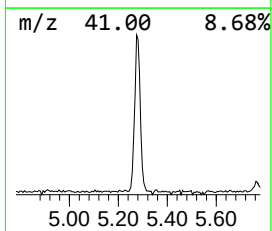
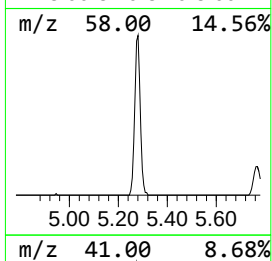
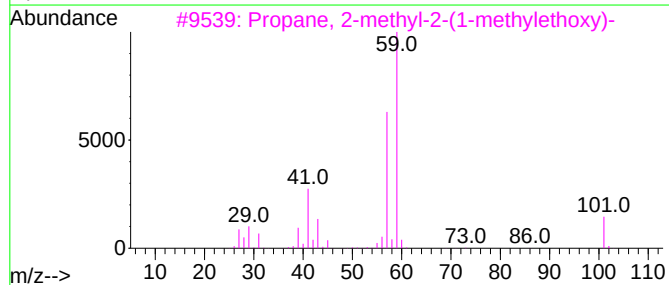
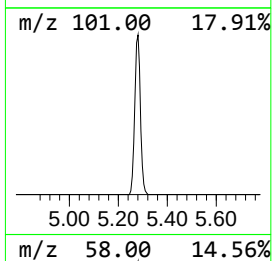
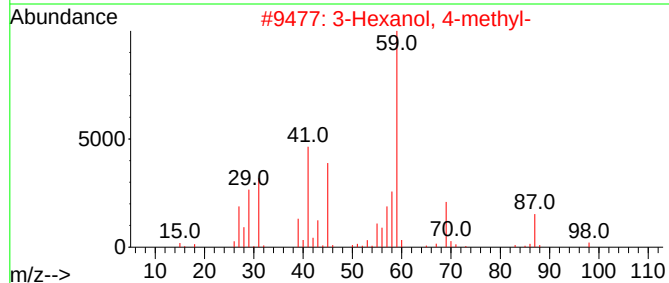
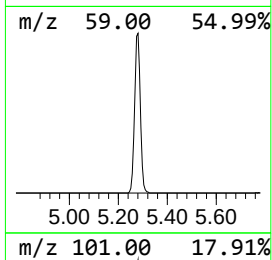
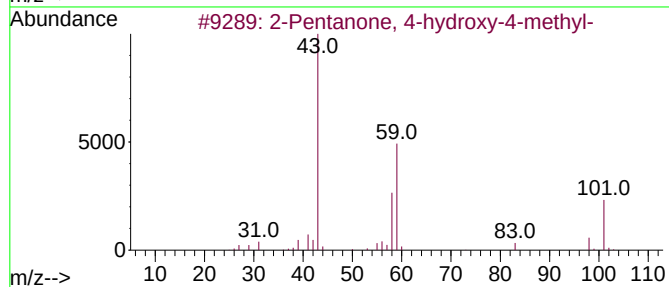
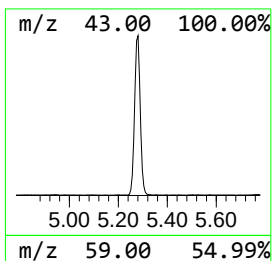
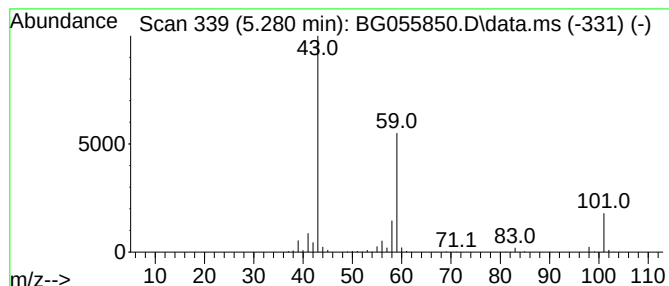
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.280	36.86 ng	470918	1,4-Dichlorobenzene-d4			8.224
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
3	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	33
4	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	28
5	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	28



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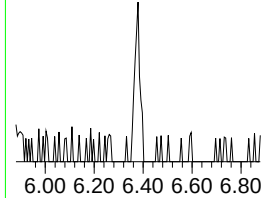
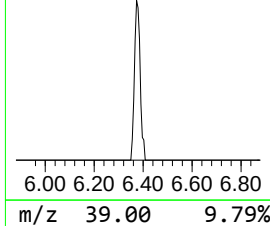
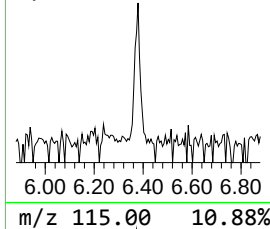
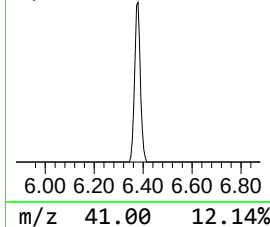
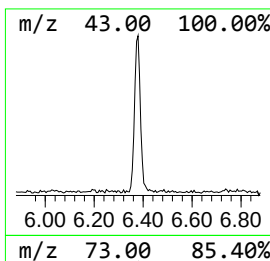
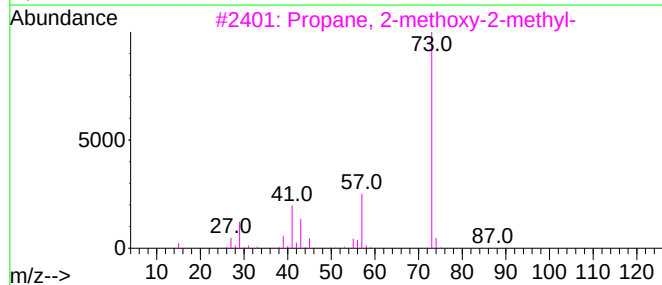
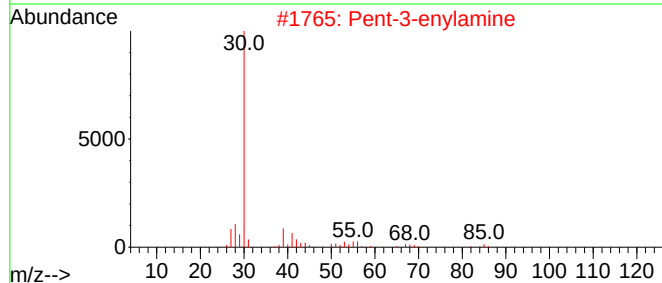
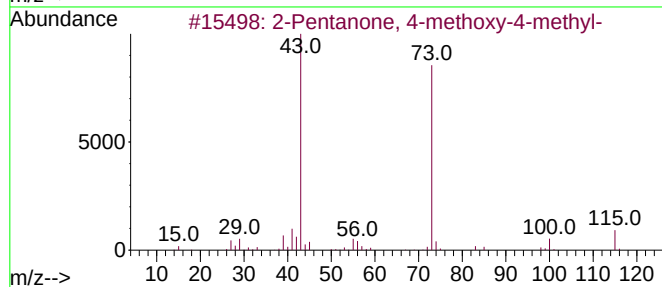
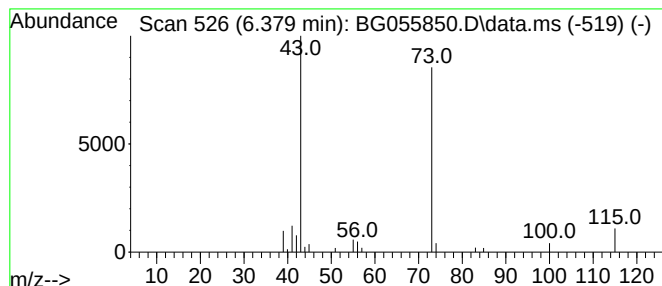
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.379	3.74 ng	47800	1,4-Dichlorobenzene-d4	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			Pent-3-enylamine	85	C5H11N	087156-70-5	9
3			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5			Guanidine, methyl-	73	C2H7N3	000471-29-4	7



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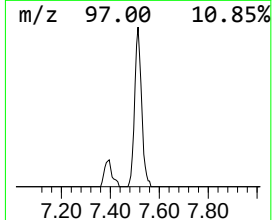
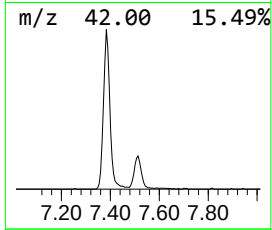
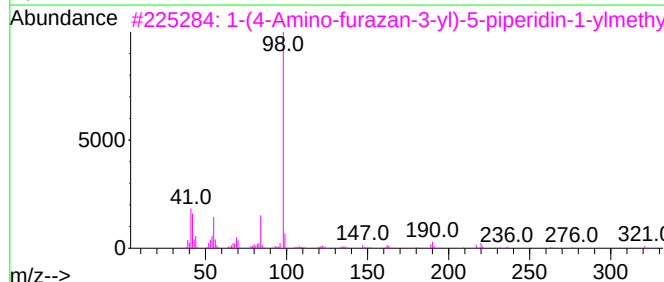
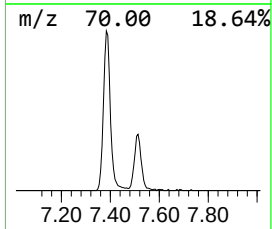
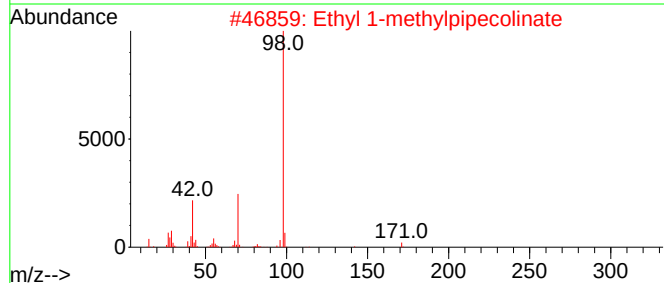
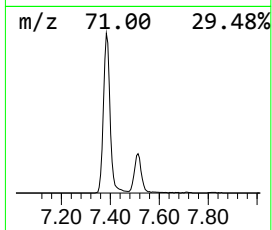
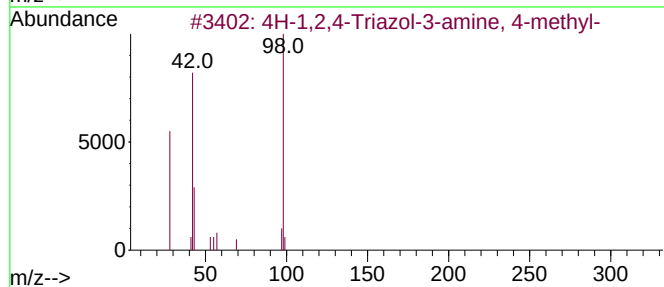
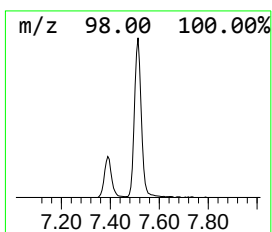
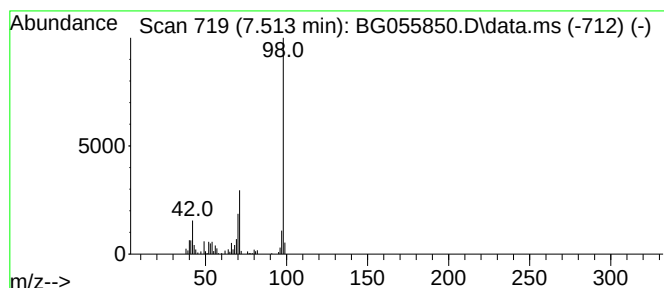
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.513	21.77 ng	278168	1,4-Dichlorobenzene-d4	8.224

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			1-(4-Amino-furazan-3-yl)-5-piper...	321	C13H19N7O3	311314-85-9	50
4			Benzen-d5-amine	98	C6H2D5N	004165-61-1	50
5			Pyrido[2,3-d]pyrimidine-2,4(1H,3...	385	C16H21Cl2N5O2	1000265-65-2	47



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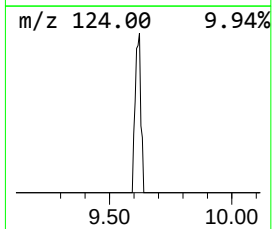
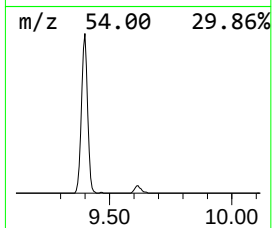
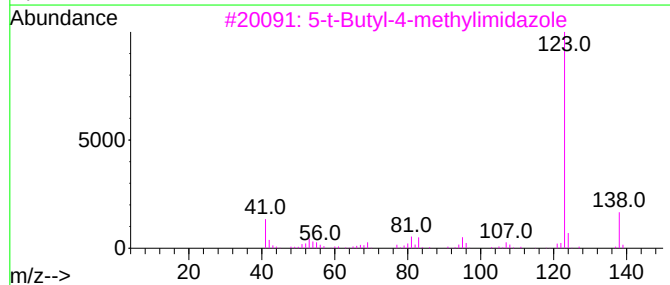
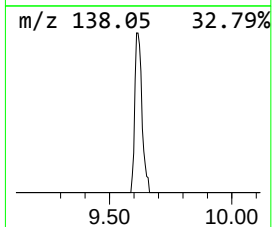
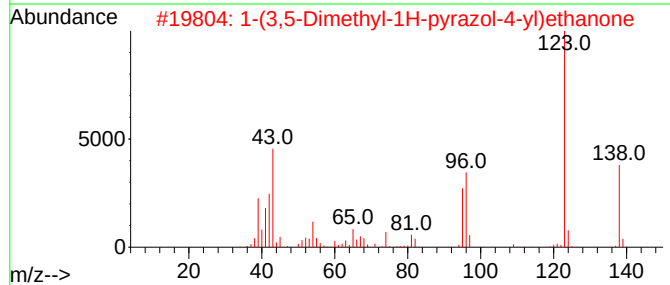
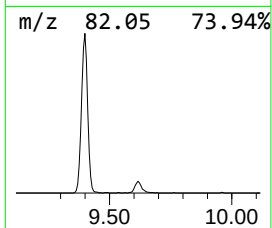
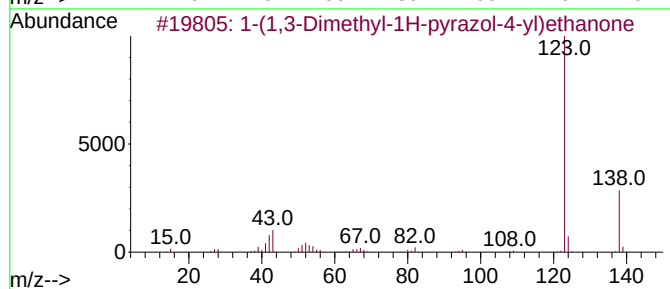
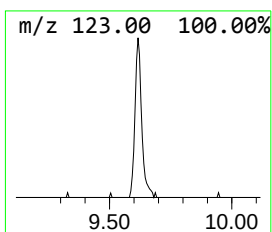
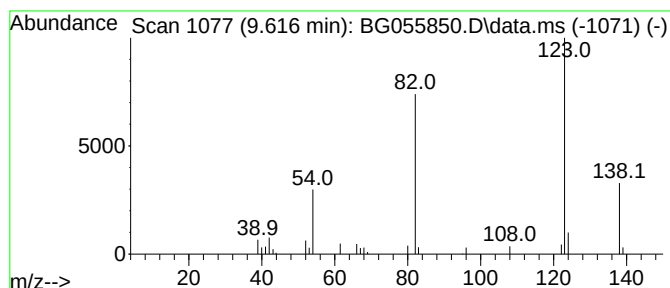
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown9.616 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.616	2.61 ng	33393	1,4-Dichlorobenzene-d4	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(1,3-Dimethyl-1H-pyrazol-4-yl)...	138	C7H10N2O	052773-23-6	43		
2	1-(3,5-Dimethyl-1H-pyrazol-4-yl)...	138	C7H10N2O	001123-48-4	43		
3	5-t-Butyl-4-methylimidazole	138	C8H14N2	146979-50-2	38		
4	p-Hydroxyphenyl methyl carbinol	138	C8H10O2	002380-91-8	38		
5	1-(2,4-Dimethyl-furan-3-yl)-etha...	138	C8H10O2	032933-07-6	38		



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.658	3.6	ng	46205	1	8.224	255514	20.0
2-Pentanone, 4-...	5.280	36.9	ng	470918	1	8.224	255514	20.0
2-Pentanone, 4-...	6.379	3.7	ng	47800	1	8.224	255514	20.0
4H-1,2,4-Triazo...	7.513	21.8	ng	278168	1	8.224	255514	20.0
unknown9.616	9.616	2.6	ng	33393	1	8.224	255514	20.0