

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
 Data File : BG055963.D
 Acq On : 14 Dec 2022 17:25
 Operator : CG/JU
 Sample : N6001-16
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-15

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-BG121322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055963.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.326	3	6	12	rVB2	3333	4874	1.07%	0.217%
2	3.403	14	19	30	rVB	79622	108174	23.72%	4.818%
3	5.882	435	441	447	rBB	38951	60182	13.20%	2.681%
4	7.492	709	715	721	rBB	26930	42546	9.33%	1.895%
5	8.367	859	864	870	rBB	15704	25386	5.57%	1.131%
6	9.543	1057	1064	1070	rBB	59857	102259	22.42%	4.555%
7	11.205	1340	1347	1353	rBB	21894	36789	8.07%	1.639%
8	13.608	1749	1756	1763	rBB	248595	361018	79.16%	16.080%
9	14.895	1970	1975	1983	rBV	16809	24604	5.39%	1.096%
10	14.977	1983	1989	1996	rVB	47180	69961	15.34%	3.116%
11	15.365	2049	2055	2064	rBV2	45090	69118	15.15%	3.079%
12	16.452	2233	2240	2250	rVB	287317	428577	93.97%	19.089%
13	16.693	2274	2281	2287	rBV	4316	6245	1.37%	0.278%
14	17.715	2447	2455	2461	rBV	75842	113478	24.88%	5.054%
15	19.607	2771	2777	2783	rVB	5795	8270	1.81%	0.368%
16	20.289	2887	2893	2900	rBV	366816	456088	100.00%	20.314%
17	21.758	3137	3143	3147	rBV4	3845	4712	1.03%	0.210%
18	22.022	3180	3188	3196	rVB	88454	150115	32.91%	6.686%
19	22.815	3316	3323	3329	rBV2	8636	15150	3.32%	0.675%
20	25.512	3772	3782	3792	rBV2	53468	157591	34.55%	7.019%

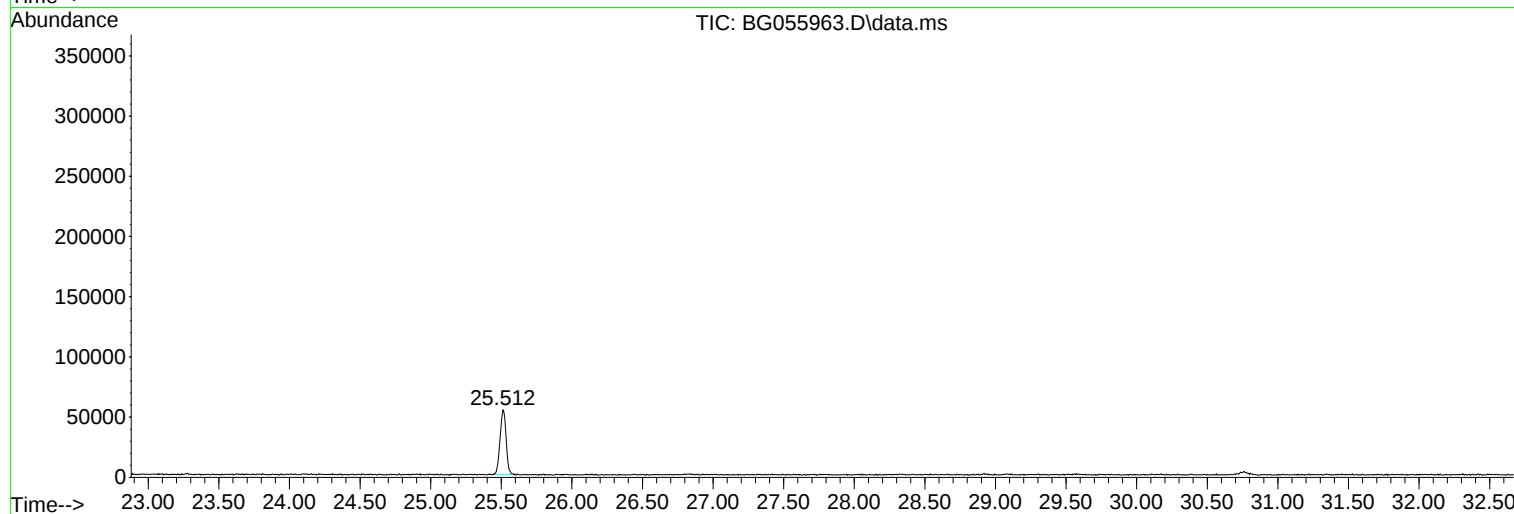
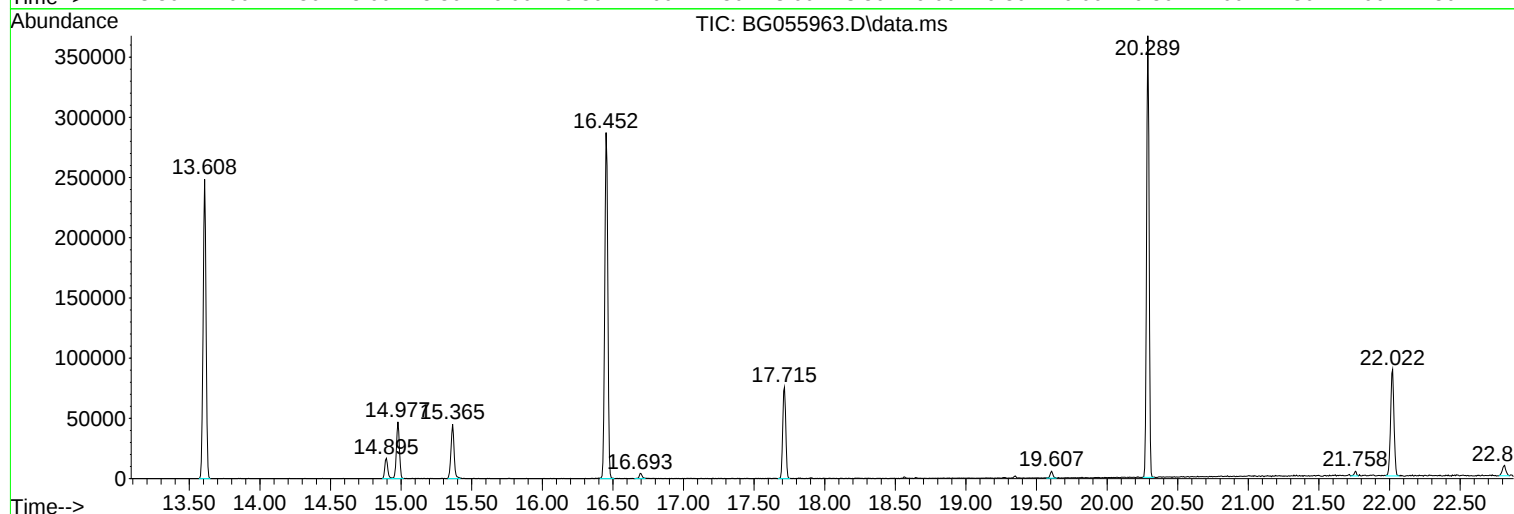
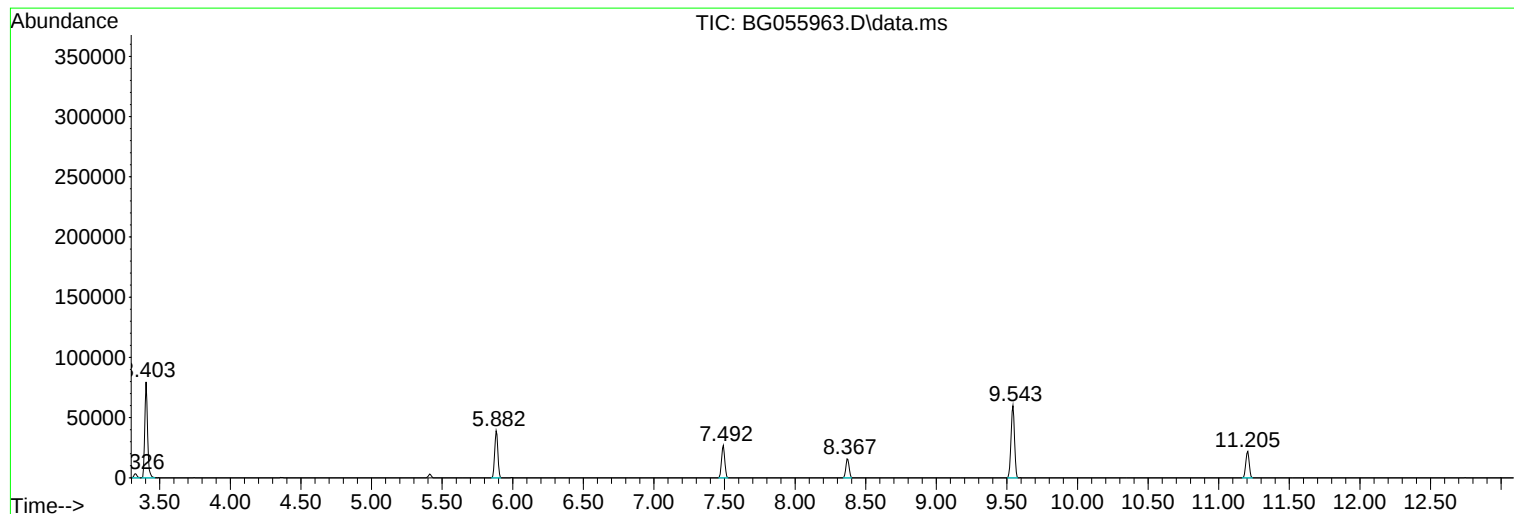
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG/JU
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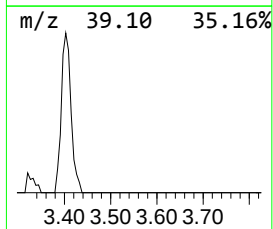
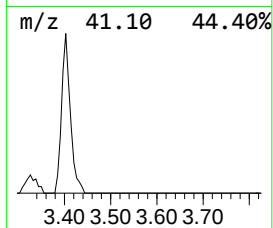
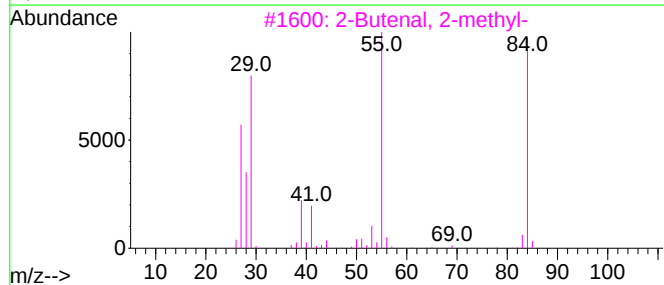
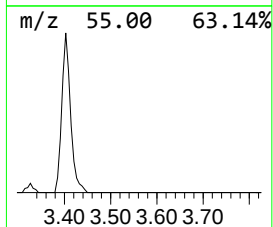
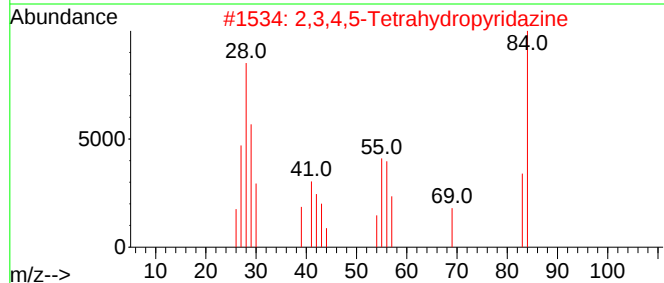
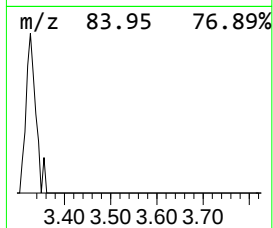
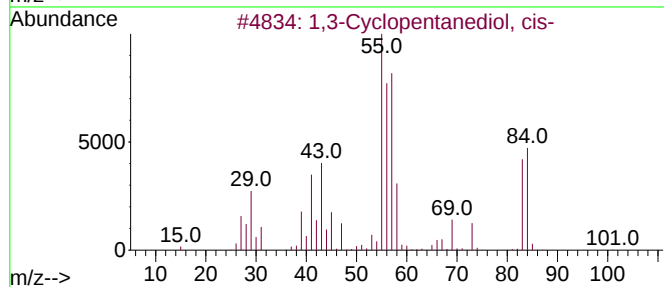
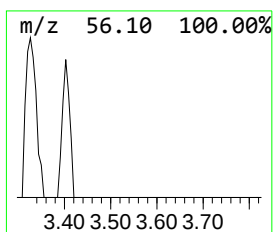
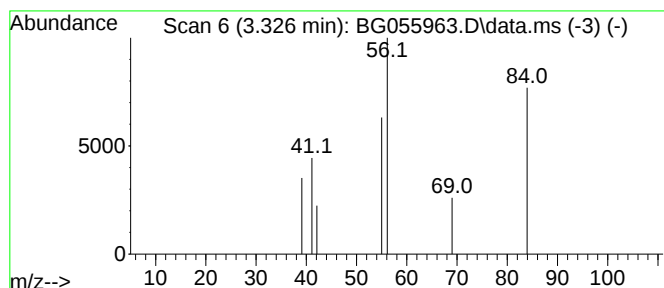
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.326 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.326	3.84 ng	4874	1,4-Dichlorobenzene-d4	8.373

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Cyclopentanediol, cis-	102	C5H10O2	016326-97-9	9
2		2,3,4,5-Tetrahydropyridazine	84	C4H8N2	000694-06-4	4
3		2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	4
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	4
5		2-Propenal	56	C3H4O	000107-02-8	4



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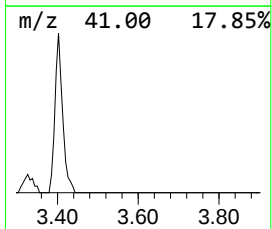
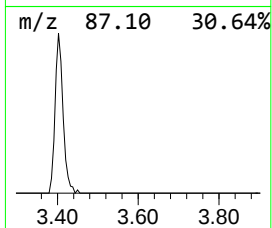
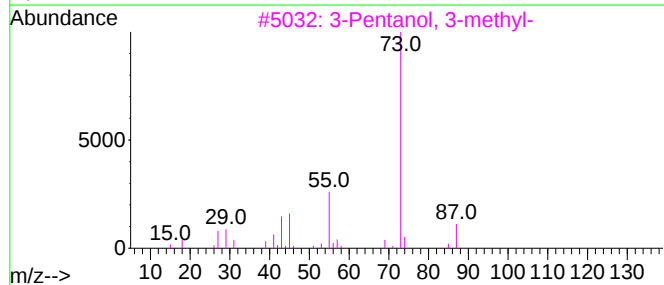
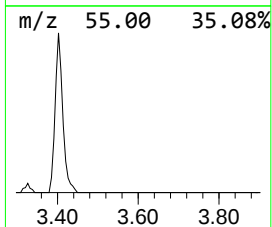
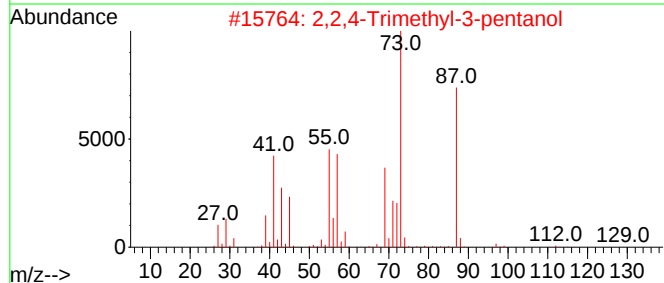
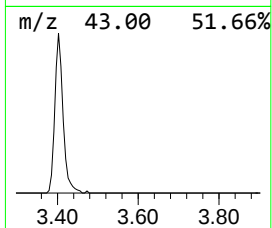
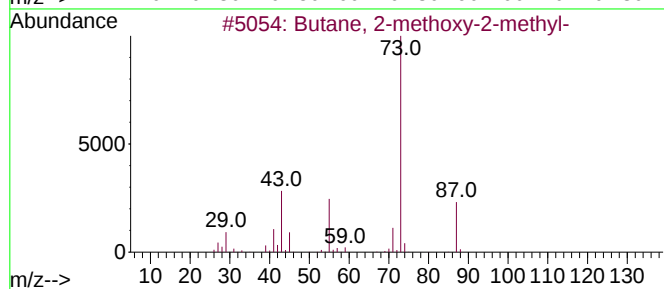
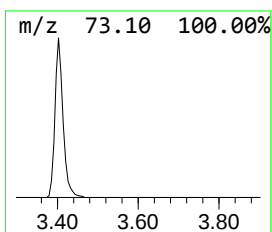
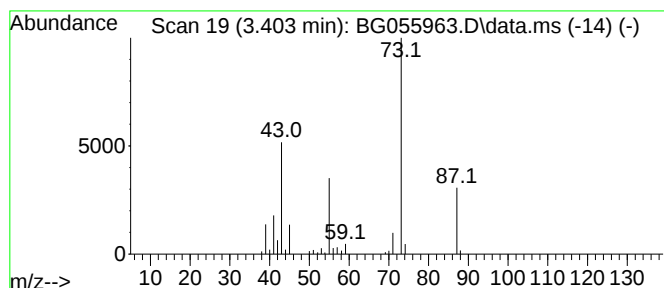
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.403	85.22 ng	108174	1,4-Dichlorobenzene-d4	8.373

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25



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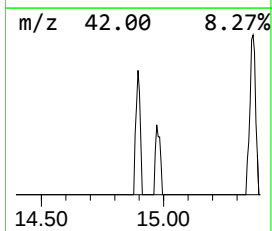
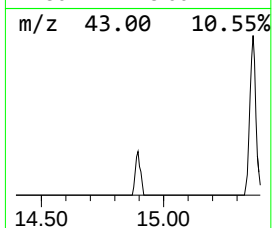
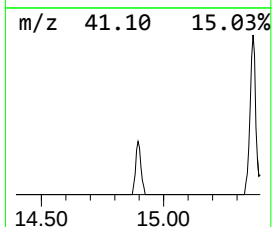
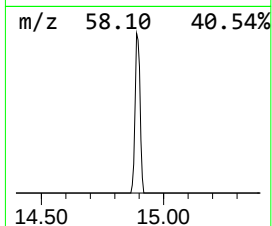
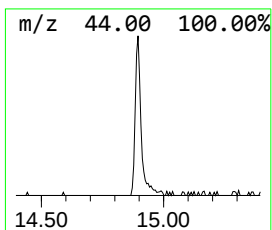
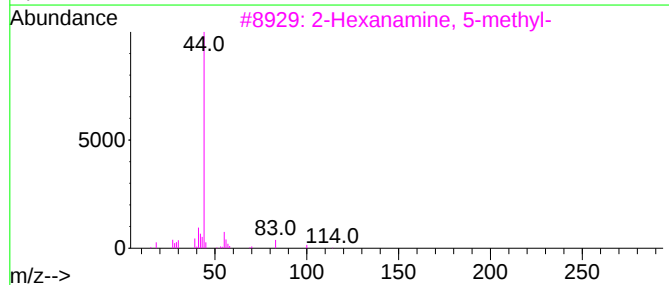
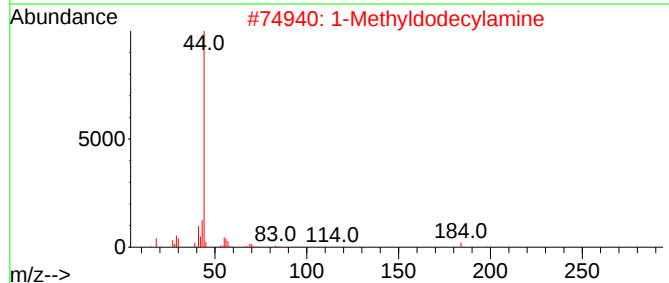
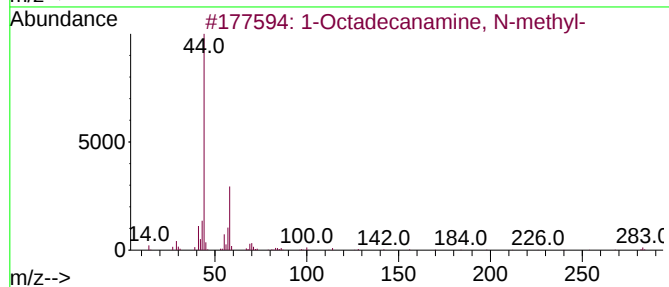
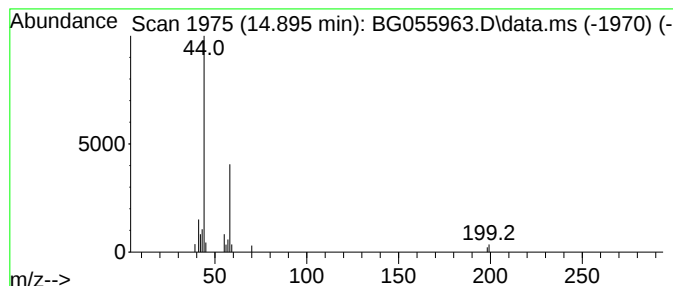
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Octadecanamine, N-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.895	7.03 ng	24604	Acenaphthene-d10	14.977

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	64
2			1-Methyldodecylamine	199	C13H29N	013205-57-7	28
3			2-Hexanamine, 5-methyl-	115	C7H17N	028292-43-5	28
4			2-Propanamine	59	C3H9N	000075-31-0	9
5			(+)-2-Aminoheptane	115	C7H17N	006240-90-0	9



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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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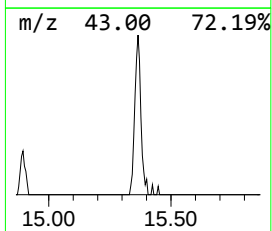
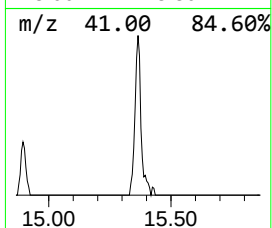
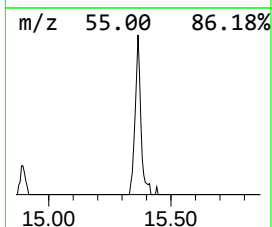
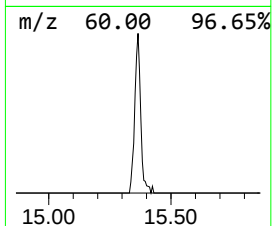
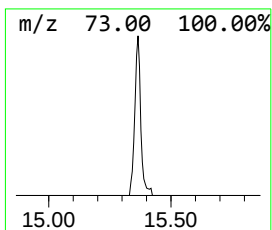
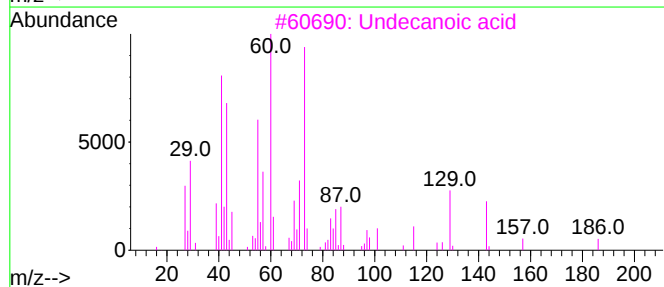
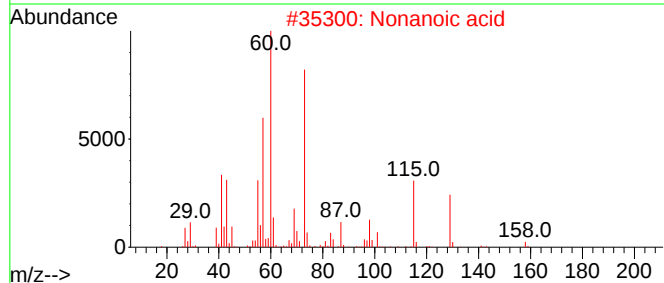
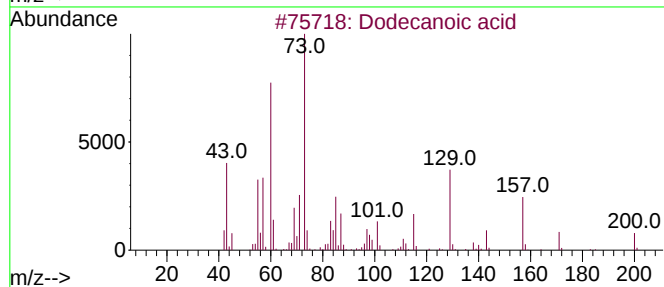
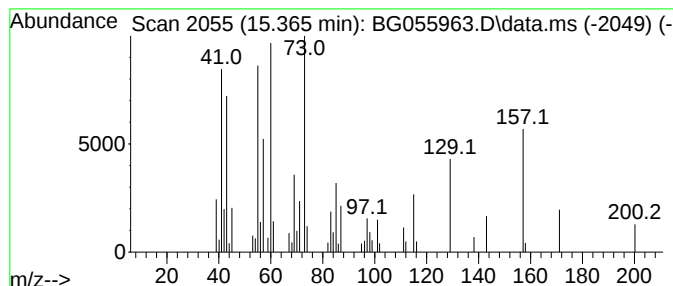
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Dodecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.365	19.76 ng	69118	Acenaphthene-d10	14.977

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	96
2			Nonanoic acid	158	C9H18O2	000112-05-0	49
3			Undecanoic acid	186	C11H22O2	000112-37-8	46
4			n-Decanoic acid	172	C10H20O2	000334-48-5	43
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	38



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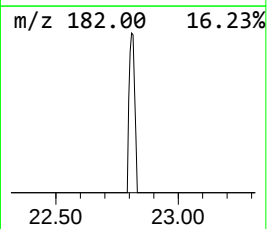
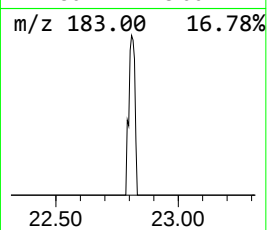
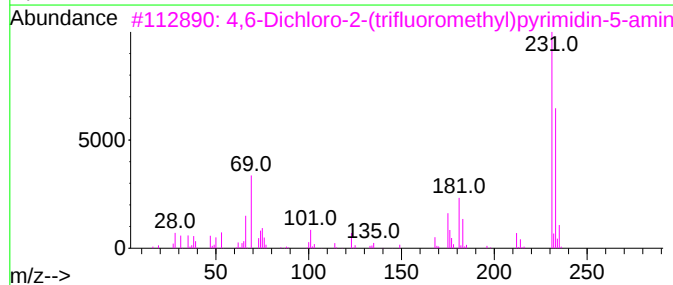
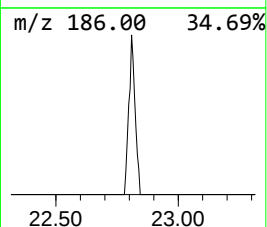
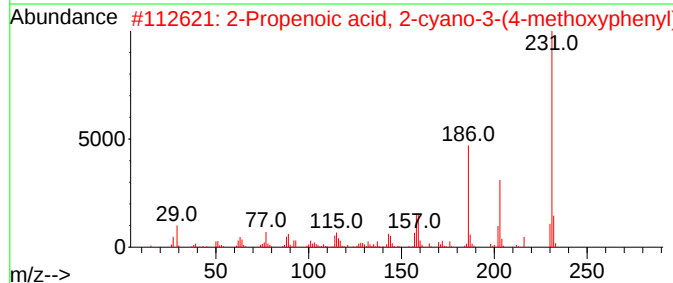
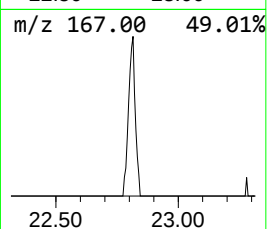
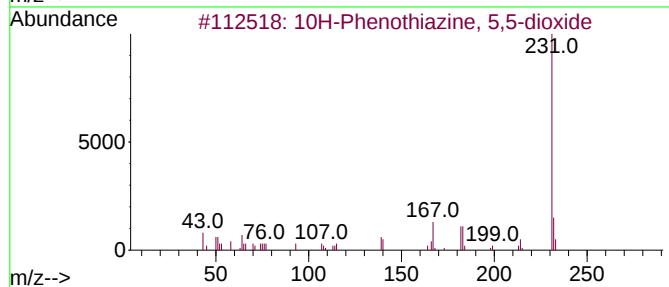
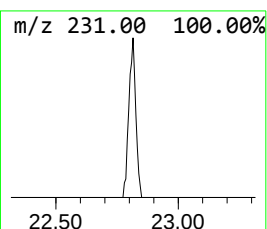
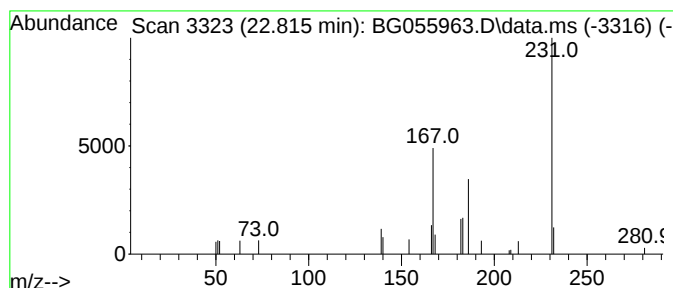
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown22.815 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.815	2.02 ng	15150	Chrysene-d12	22.022

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		10H-Phenothiazine, 5,5-dioxide	231	C12H9NO2S	001209-66-1	43
2		2-Propenoic acid, 2-cyano-3-(4-methoxyphenyl)	231	C13H13NO3	002286-29-5	37
3		4,6-Dichloro-2-(trifluoromethyl)pyrimidin-5-amine	231	C5H2Cl2F3N3	002344-17-4	37
4		Furan-2-carbaldehyde, 5-(4-methoxyphenyl)	231	C12H9NO4	1000302-96-8	37
5		10H-Phenothiazine, 10-acetyl-, 5,5-dioxide	273	C14H11NO3S	001220-99-1	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.326	3.326	3.8	ng	4874	1	8.373	25386	20.0
Butane, 2-metho...	3.403	85.2	ng	108174	1	8.373	25386	20.0
1-Octadecanamin...	14.895	7.0	ng	24604	3	14.977	69961	20.0
Dodecanoic acid	15.365	19.8	ng	69118	3	14.977	69961	20.0
unknown22.815	22.815	2.0	ng	15150	5	22.022	150115	20.0