

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122022\
 Data File : BG056028.D
 Acq On : 20 Dec 2022 13:39
 Operator : CG/JU
 Sample : N6037-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RB-19-(2.3-4.3)

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: BG056028.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.393	12	18	29	rBB	23582	36511	4.24%	0.930%
2	5.408	356	361	368	rBB	19457	28872	3.35%	0.735%
3	5.884	436	442	450	rBB	153972	243800	28.29%	6.209%
4	7.500	710	717	724	rBB	161547	270782	31.42%	6.896%
5	8.370	859	865	871	rBB	37461	59897	6.95%	1.525%
6	9.539	1057	1064	1071	rBB	96893	175048	20.31%	4.458%
7	11.201	1340	1347	1354	rBV	51426	87560	10.16%	2.230%
8	13.605	1749	1756	1763	rVB	358127	534608	62.03%	13.616%
9	14.974	1983	1989	1996	rBB	89080	134907	15.65%	3.436%
10	16.313	2211	2217	2222	rBV	11664	16251	1.89%	0.414%
11	16.448	2232	2240	2248	rBV	350612	539414	62.58%	13.738%
12	17.712	2449	2455	2459	rBV	113141	172058	19.96%	4.382%
13	17.753	2459	2462	2467	rVB	23488	31283	3.63%	0.797%
14	18.558	2594	2599	2607	rBV4	29662	46543	5.40%	1.185%
15	18.628	2607	2611	2615	rVB3	5843	10054	1.17%	0.256%
16	18.769	2629	2635	2639	rBV6	5175	10958	1.27%	0.279%
17	19.104	2689	2692	2698	rVB6	5673	9732	1.13%	0.248%
18	19.304	2720	2726	2731	rBV6	5179	11774	1.37%	0.300%
19	19.486	2752	2757	2759	rVB6	7895	12910	1.50%	0.329%
20	19.615	2774	2779	2780	rBV5	6989	8793	1.02%	0.224%
21	19.739	2795	2800	2805	rBV	53335	74557	8.65%	1.899%
22	19.809	2808	2812	2816	rBV7	11789	19918	2.31%	0.507%
23	19.891	2822	2826	2829	rBV5	8670	14125	1.64%	0.360%
24	20.073	2853	2857	2858	rBV2	7617	10816	1.25%	0.275%
25	20.103	2858	2862	2867	rVB	51710	75923	8.81%	1.934%
26	20.285	2887	2893	2898	rBV	661824	861909	100.00%	21.952%
27	22.012	3181	3187	3193	rBV3	115579	229104	26.58%	5.835%
28	25.508	3774	3782	3792	rBV3	65812	198280	23.00%	5.050%

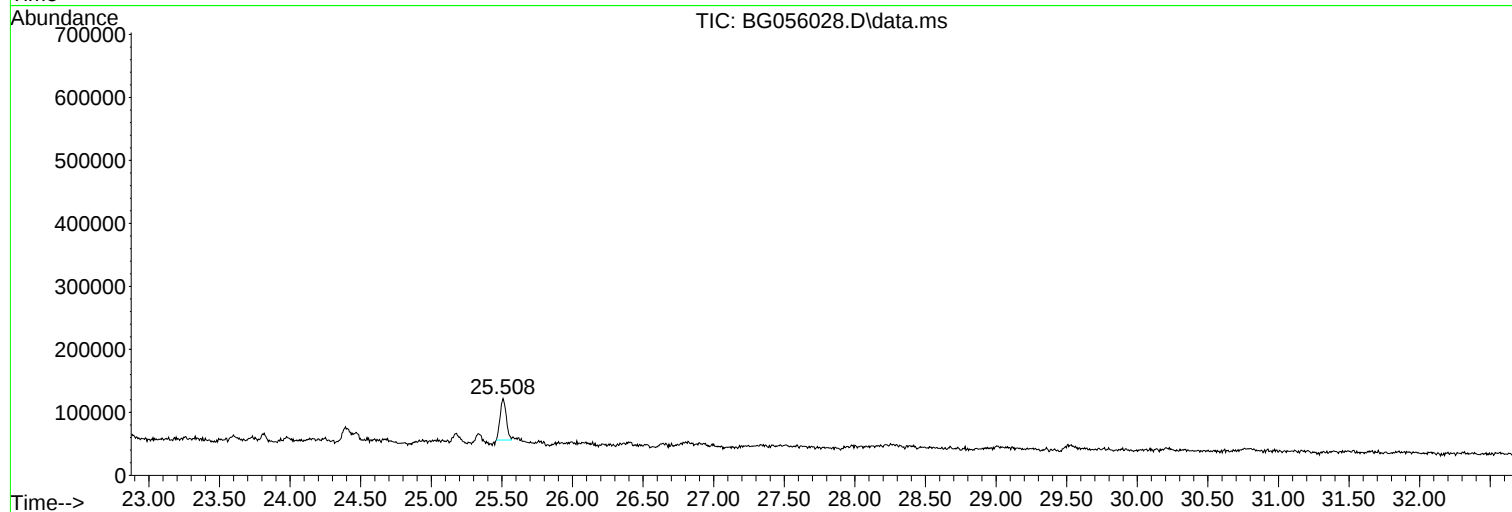
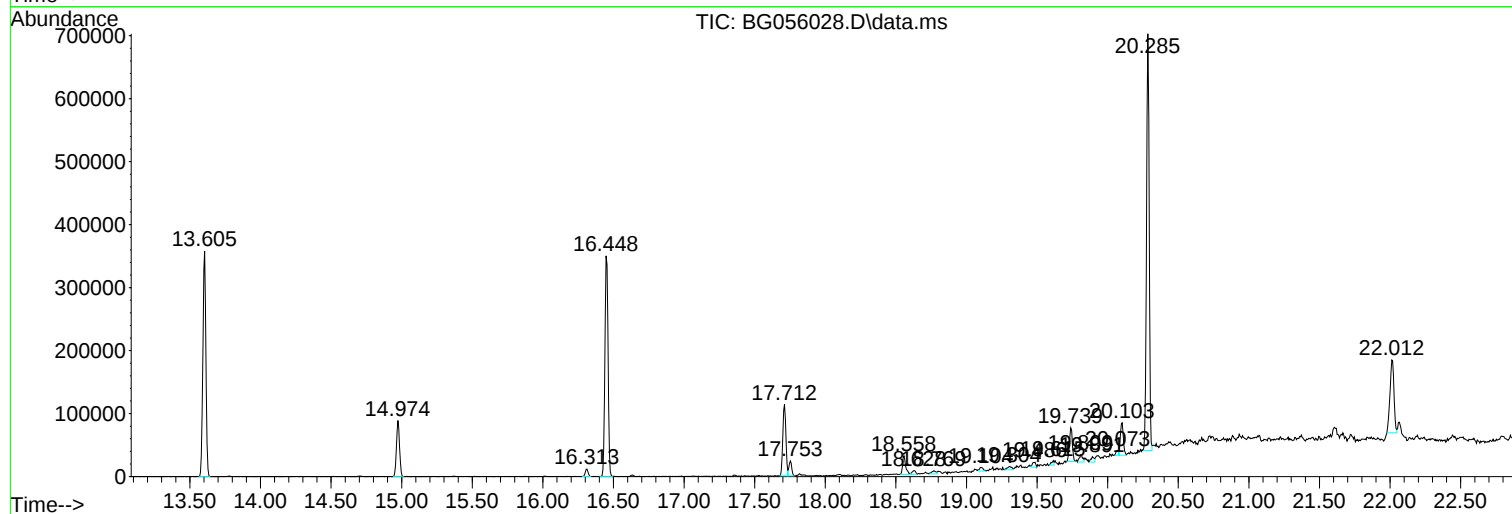
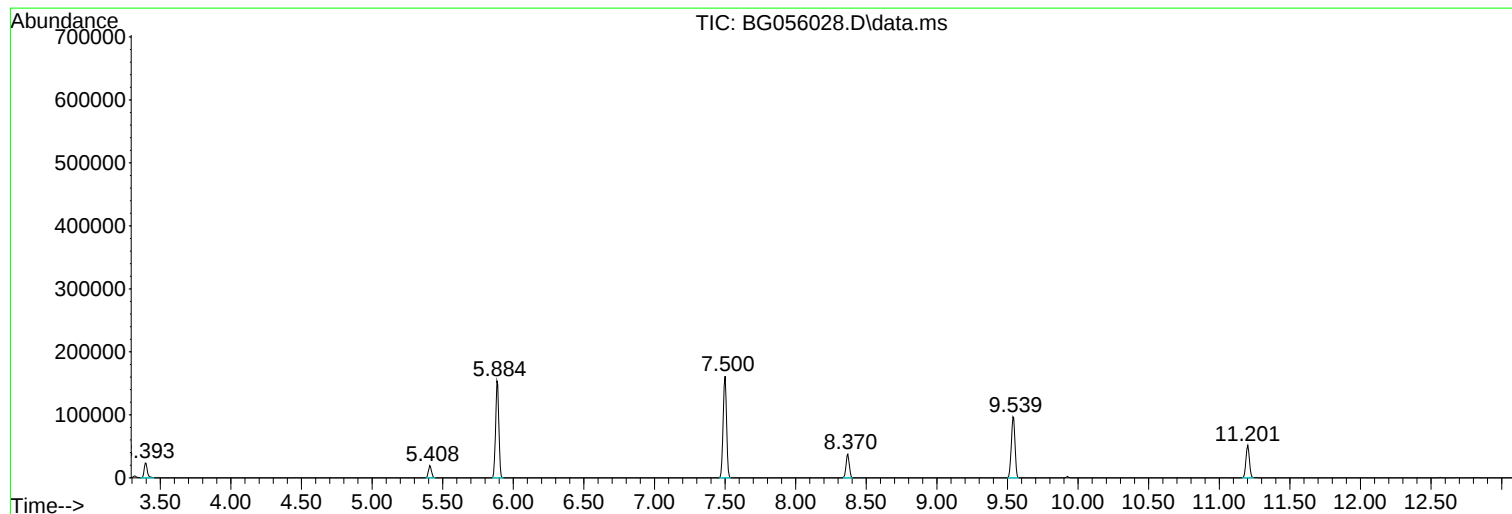
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Sample : N6037-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-19-(2.3-4.3)

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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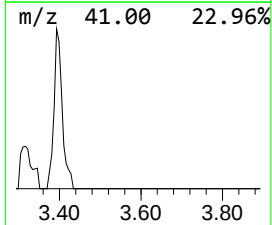
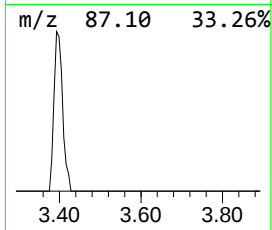
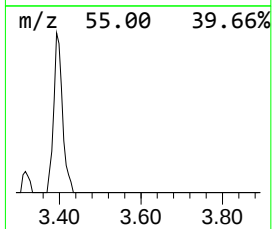
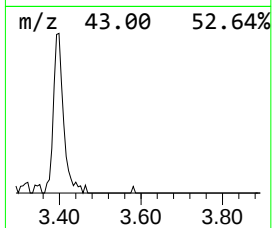
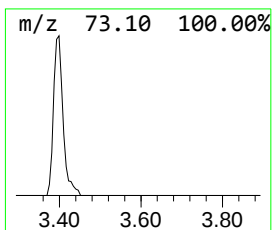
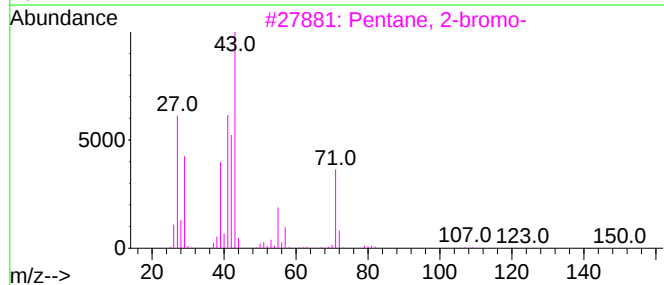
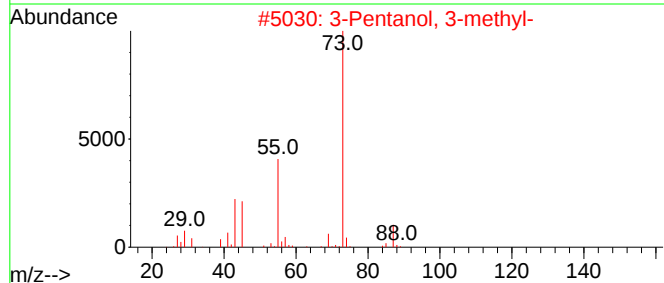
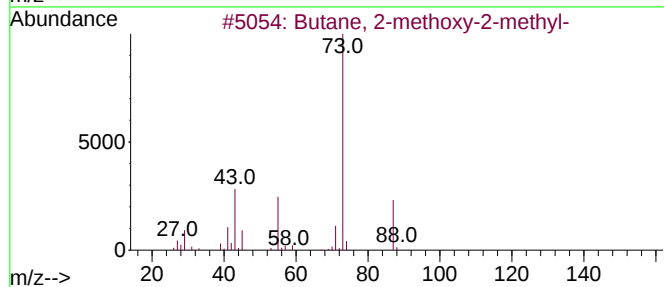
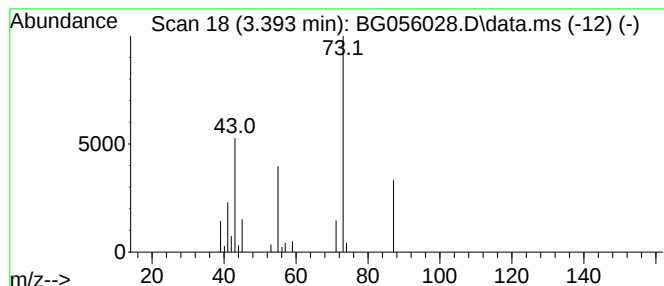
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.393	12.19 ng	36511	1,4-Dichlorobenzene-d4	8.370

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	28
3			Pentane, 2-bromo-	150	C5H11Br	000107-81-3	9
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
5			1-Hepten-4-ol	114	C7H14O	003521-91-3	9



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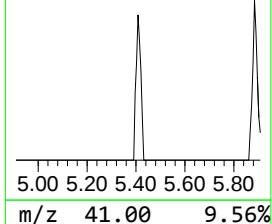
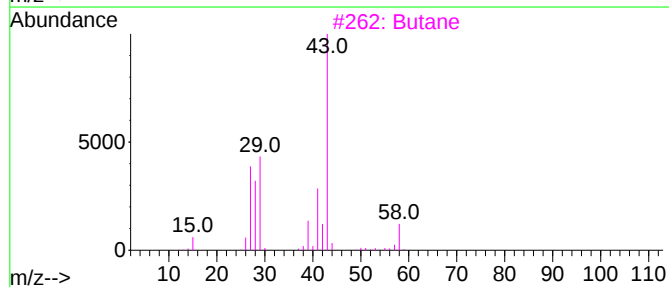
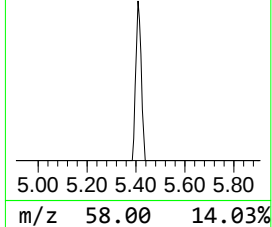
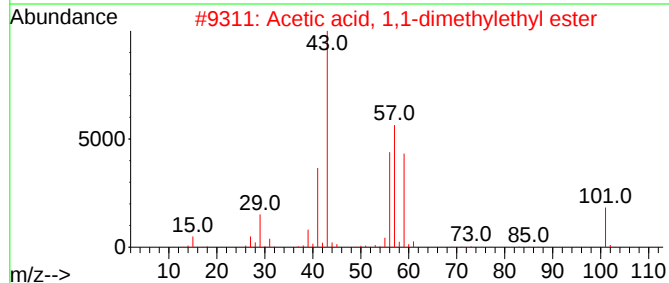
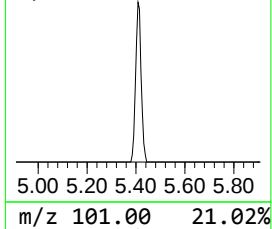
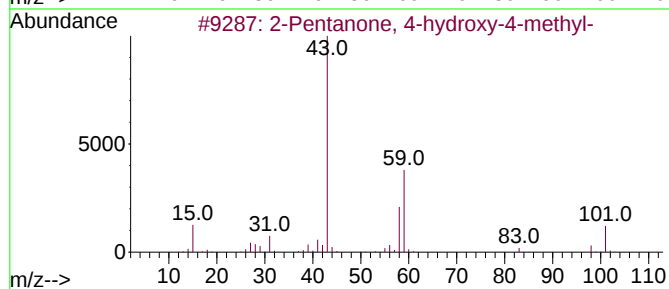
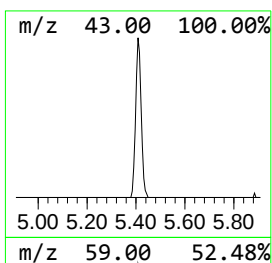
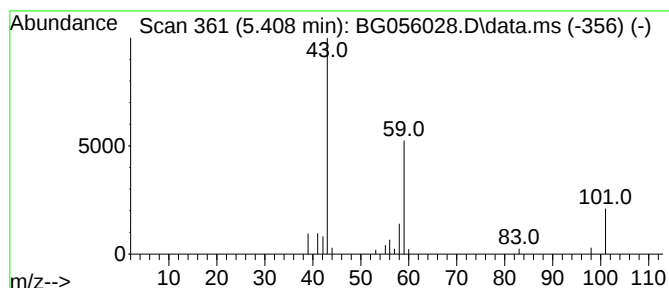
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.408	9.64 ng	28872	1,4-Dichlorobenzene-d4	8.370

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Butane	58	C4H10	000106-97-8	10
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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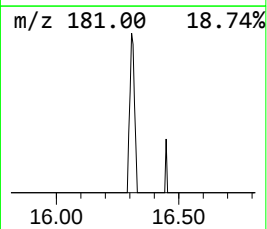
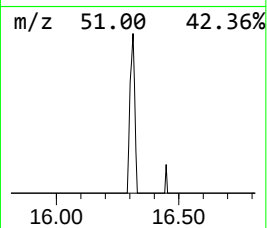
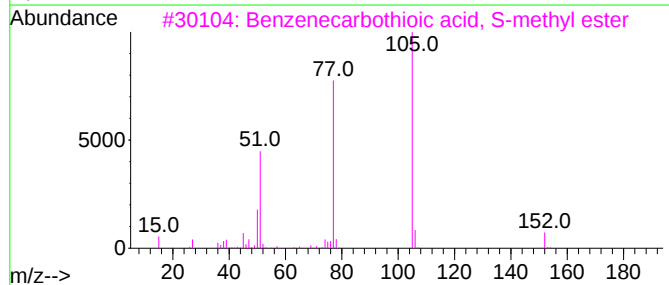
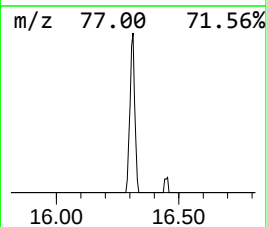
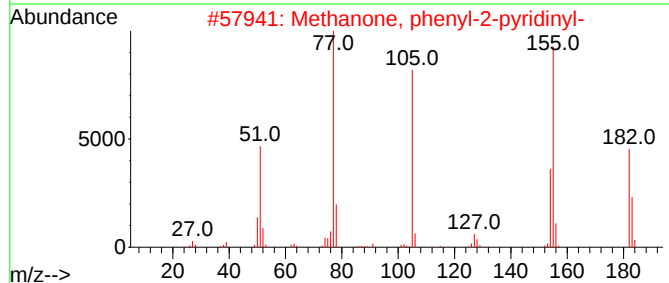
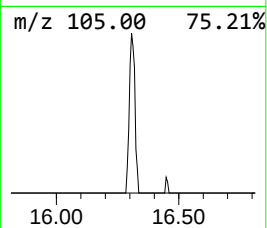
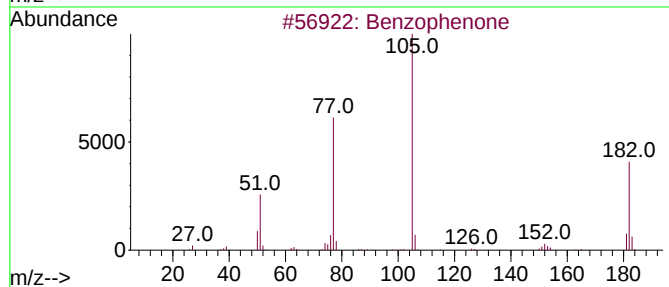
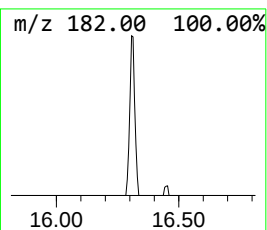
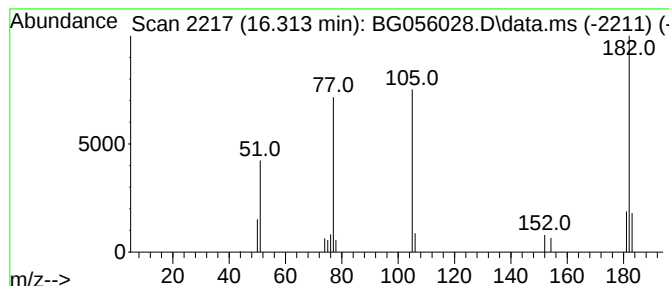
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.313	2.41 ng	16251	Acenaphthene-d10	14.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	94
2			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	47
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	43
4			1,2-Propanedione, 1-phenyl-, 2-o...	163	C9H9NO2	000119-51-7	38
5			3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	38



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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-19-(2.3-4.3)

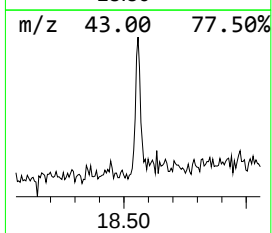
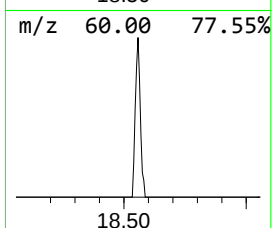
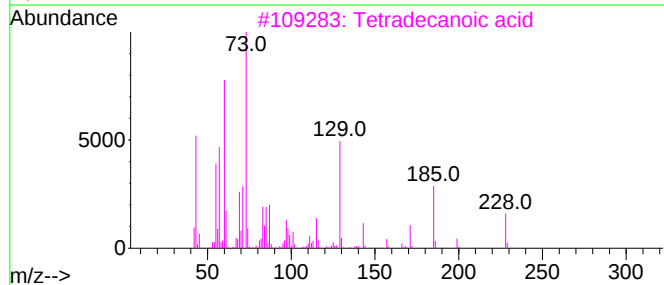
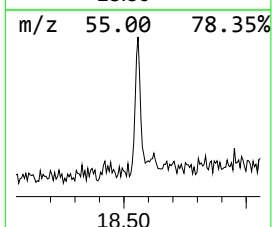
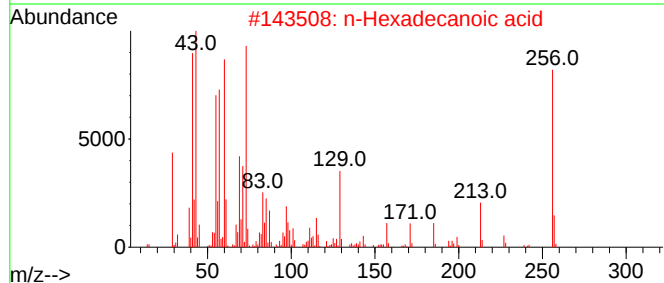
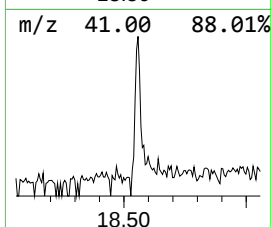
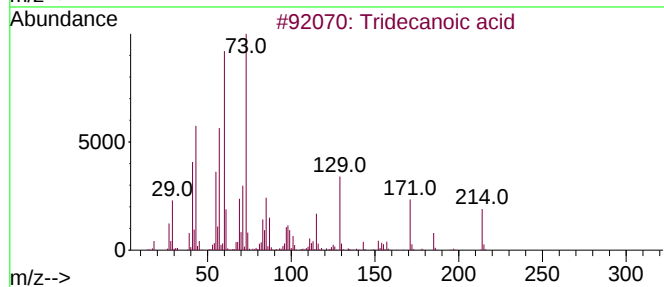
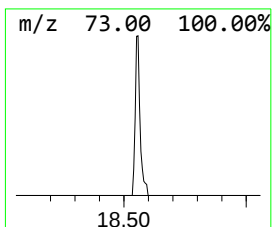
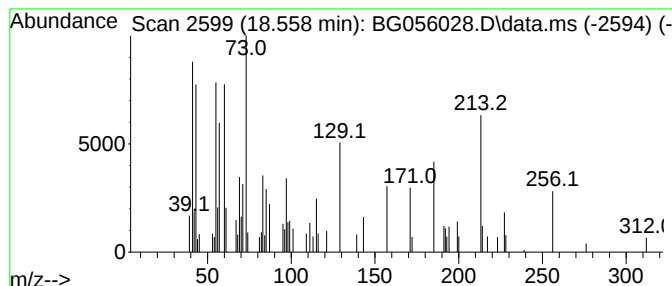
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.558	5.41 ng	46543	Phenanthrene-d10	17.712

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	70
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	47
4			Dodecanoic acid	200	C12H24O2	000143-07-7	42
5			n-Decanoic acid	172	C10H20O2	000334-48-5	38



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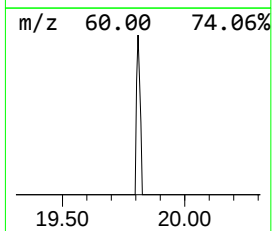
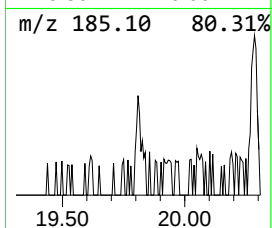
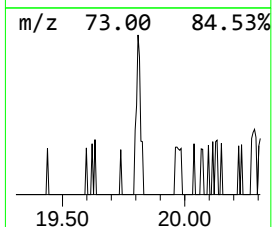
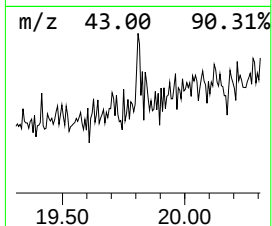
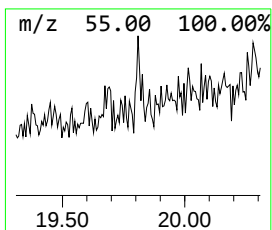
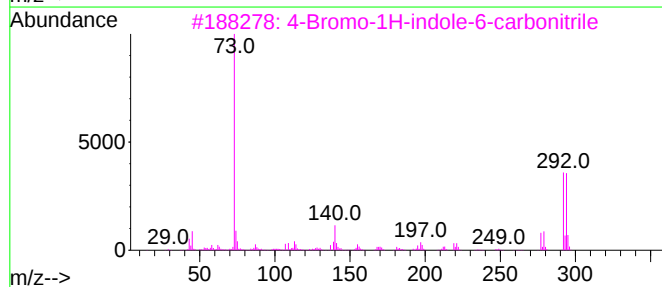
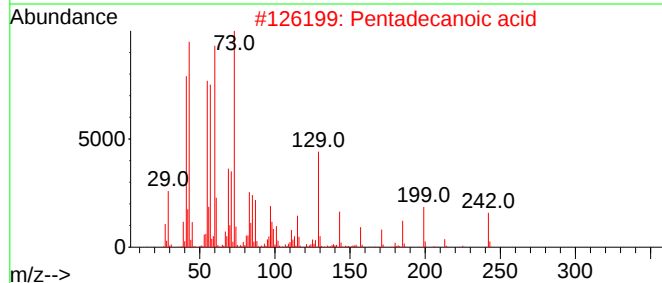
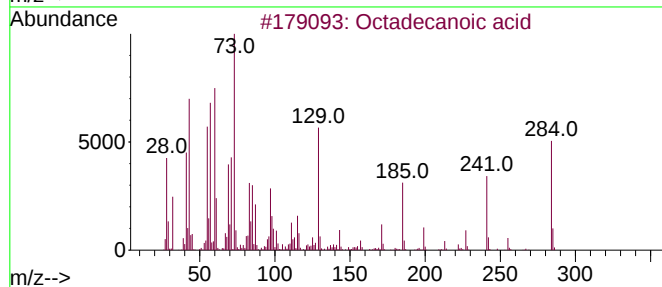
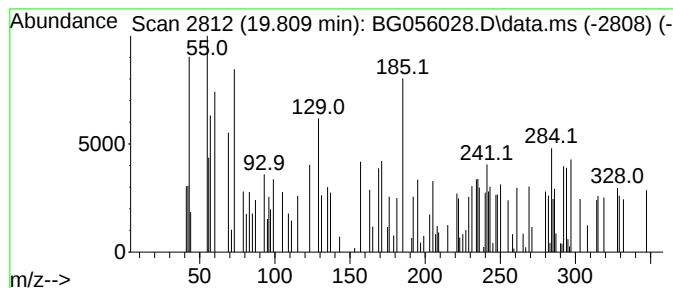
Instrument :
BNA_G
ClientSampleId :
RB-19-(2.3-4.3)

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 5 unknown19.809 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.809	2.32 ng	19918	Phenanthrene-d10		17.712	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	12
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	11
3	4-Bromo-1H-indole-6-carbonitrile		292	C12H13BrN2Si	1000501-02-6	11
4	3-Bromo-4-cyanindole, TMS		292	C12H13BrN2Si	1000508-62-4	11
5	Sebacic acid, 4-cyanophenyl hexy...		387	C23H33NO4	1000354-44-5	10



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.393	12.2	ng	36511	1	8.370	59897	20.0
2-Pentanone, 4-...	5.408	9.6	ng	28872	1	8.370	59897	20.0
Benzophenone	16.313	2.4	ng	16251	3	14.974	134907	20.0
Tridecanoic acid	18.558	5.4	ng	46543	4	17.712	172058	20.0
unknown19.809	19.809	2.3	ng	19918	4	17.712	172058	20.0