

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061623\
 Data File : BG057750.D
 Acq On : 17 Jun 2023 1:46
 Operator : CG/JU
 Sample : 03178-02
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-2A

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-BG061323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057750.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.117	3	5	23	rVB	416753	578558	20.74%	3.093%
2	5.038	326	332	338	rBV	26957	39341	1.41%	0.210%
3	5.503	404	411	422	rVB	340827	523543	18.76%	2.798%
4	5.603	422	428	433	rBV	20974	31342	1.12%	0.168%
5	7.083	673	680	692	rVB	231480	382031	13.69%	2.042%
6	7.929	817	824	833	rBV	185102	310325	11.12%	1.659%
7	9.093	1015	1022	1030	rVB	452652	788837	28.27%	4.217%
8	10.732	1294	1301	1308	rBV	287202	511407	18.33%	2.734%
9	13.188	1712	1719	1726	rBV	1166378	1829535	65.57%	9.779%
10	14.563	1947	1953	1963	rBV	523908	807997	28.96%	4.319%
11	15.920	2179	2184	2189	rVB	30894	44178	1.58%	0.236%
12	16.049	2199	2206	2213	rBV	1127315	1687000	60.46%	9.017%
13	17.306	2413	2420	2428	rBV	712487	1077343	38.61%	5.759%
14	18.200	2566	2572	2579	rBV	84923	128854	4.62%	0.689%
15	19.475	2784	2789	2795	rBV	55295	85033	3.05%	0.455%
16	19.927	2860	2866	2873	rBV	2121939	2790215	100.00%	14.914%
17	21.220	3082	3086	3094	rVV3	59719	103625	3.71%	0.554%
18	21.296	3095	3099	3109	rVB	57596	90424	3.24%	0.483%
19	21.560	3138	3144	3157	rVB2	663288	1109487	39.76%	5.930%
20	21.766	3176	3179	3186	rVB2	23465	34089	1.22%	0.182%
21	22.348	3272	3278	3289	rVB5	50874	133998	4.80%	0.716%
22	23.047	3393	3397	3405	rVB2	23087	42376	1.52%	0.227%
23	23.205	3417	3424	3434	rBV2	96602	221436	7.94%	1.184%
24	23.840	3528	3532	3538	rVB2	25297	52061	1.87%	0.278%
25	24.245	3594	3601	3611	rVB2	146876	365112	13.09%	1.952%
26	24.721	3672	3682	3701	rVB	427327	1319917	47.31%	7.055%
27	25.526	3808	3819	3833	rVB2	178384	588133	21.08%	3.144%
28	25.891	3874	3881	3892	rVB2	30254	86911	3.11%	0.465%
29	27.118	4076	4090	4104	rBV3	185183	846924	30.35%	4.527%
30	28.852	4373	4385	4398	rVB8	18121	82977	2.97%	0.444%
31	29.134	4415	4433	4463	rBV3	172784	1018256	36.49%	5.443%
32	31.695	4846	4869	4895	rBV4	123703	997015	35.73%	5.329%

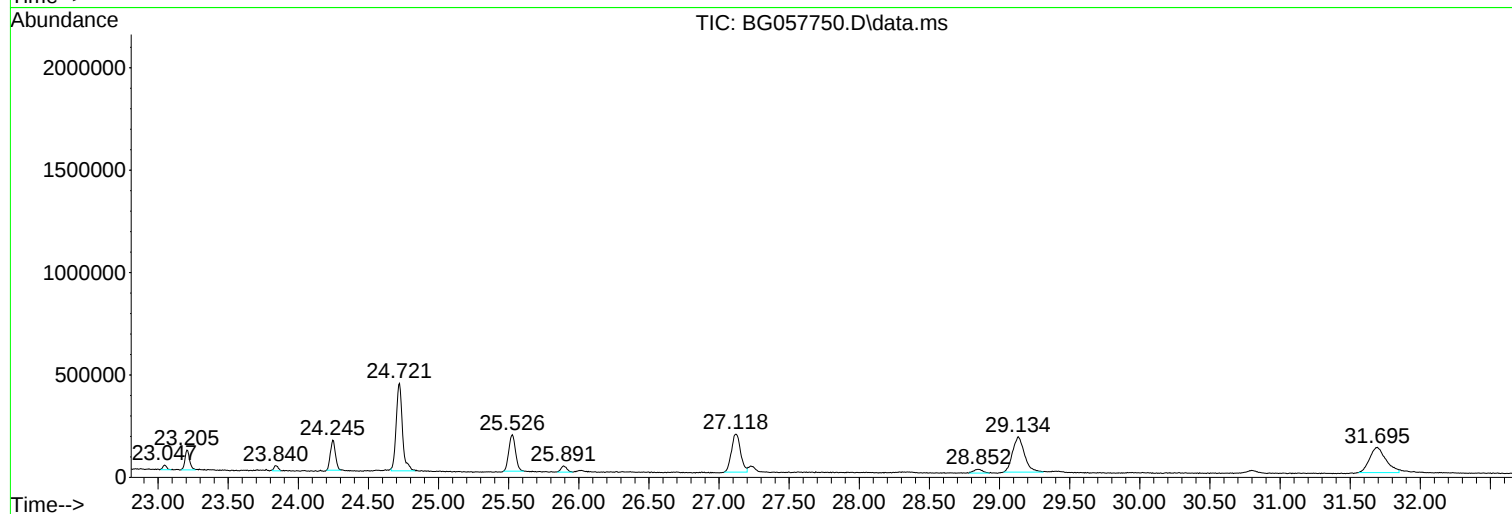
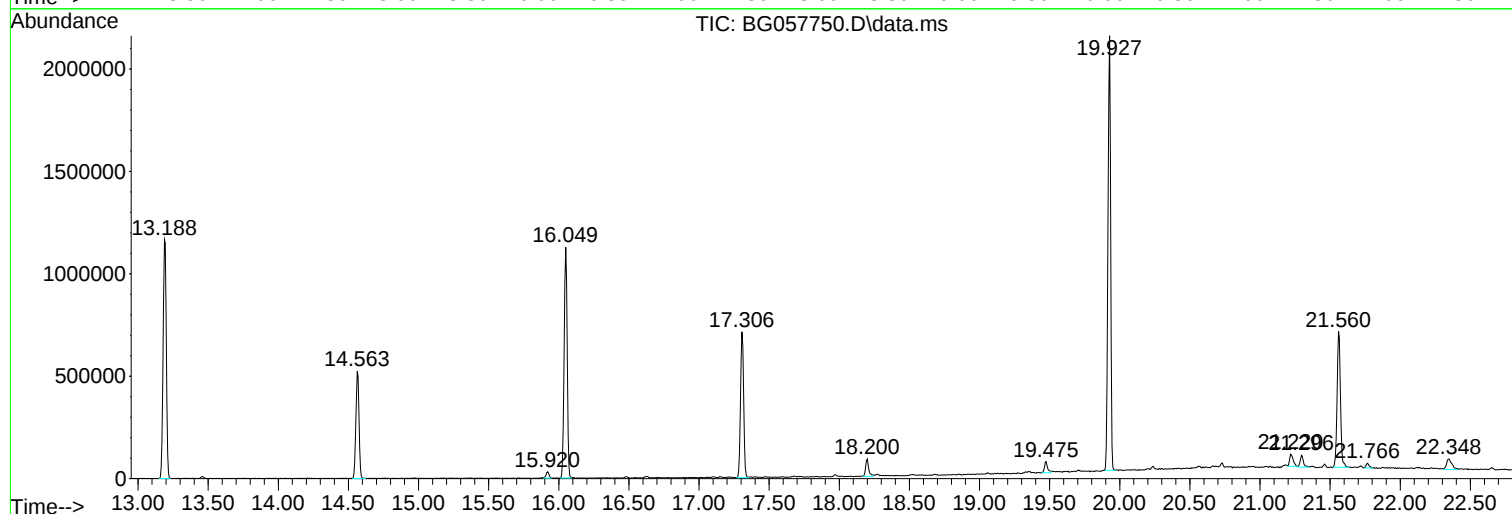
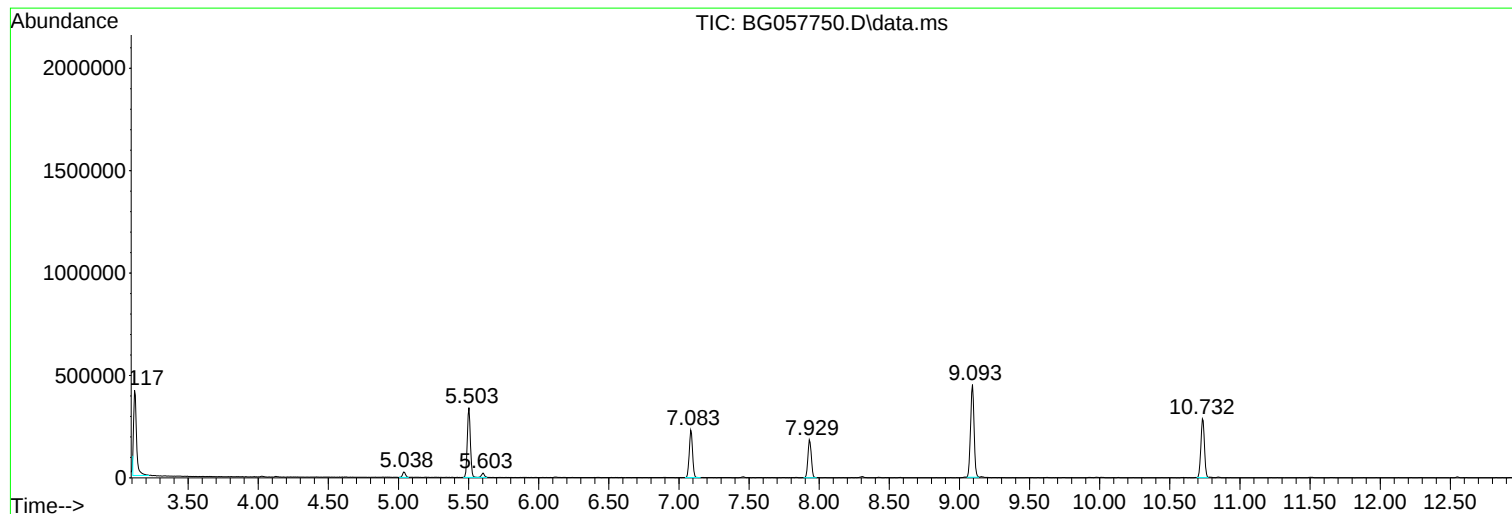
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Instrument :
BNA_G
ClientSampleId :
MW-2A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.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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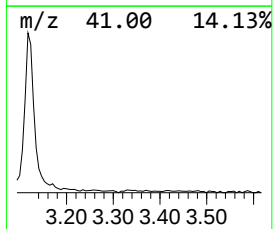
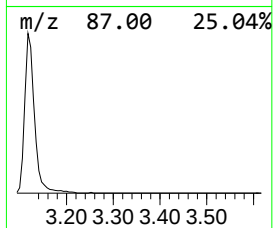
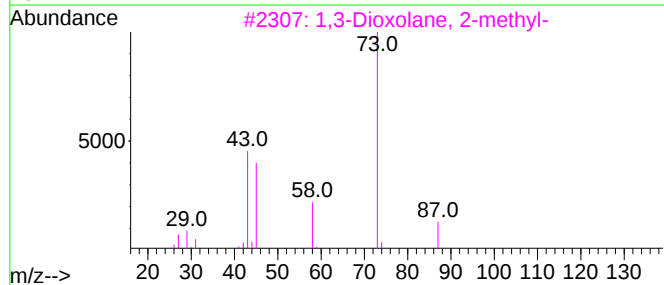
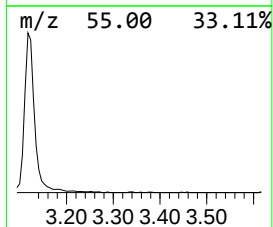
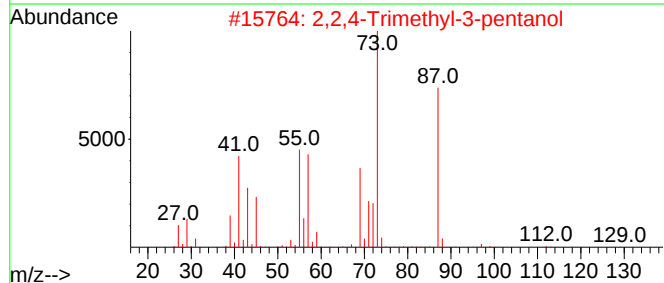
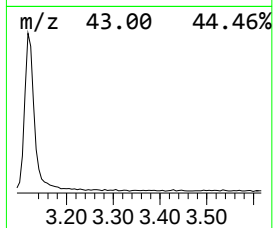
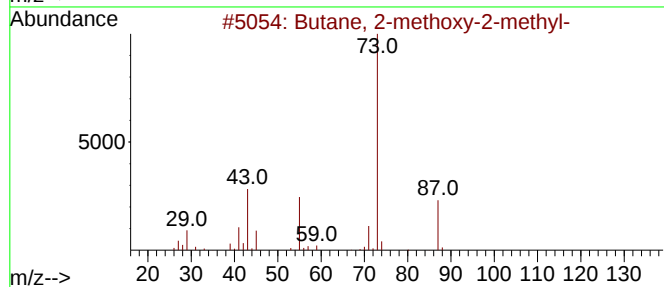
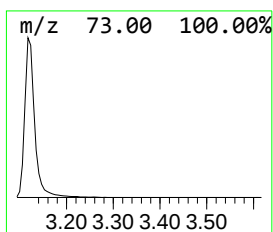
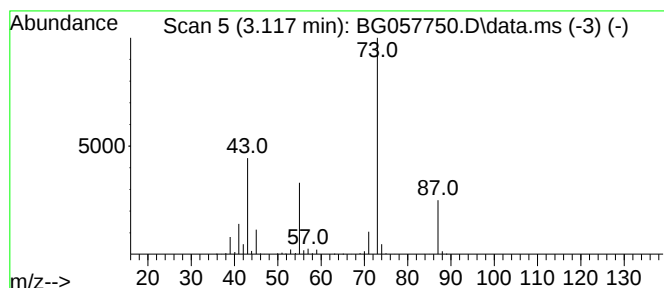
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.117	37.29 ng	578558	1,4-Dichlorobenzene-d4	7.929

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



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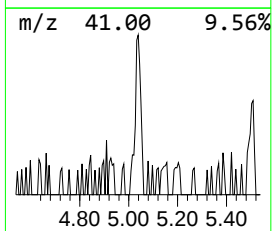
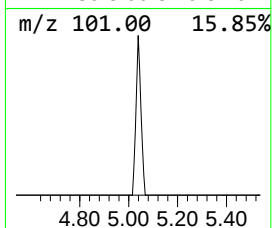
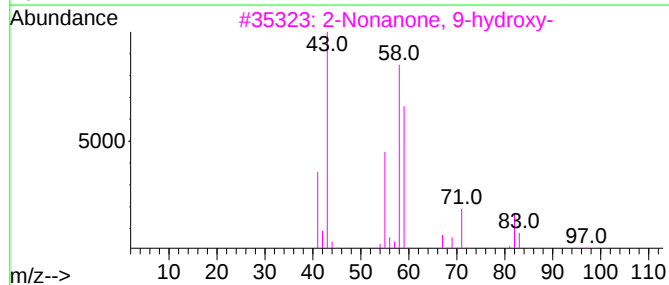
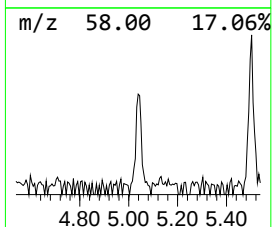
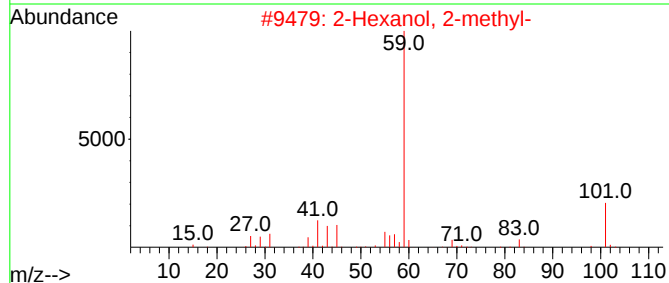
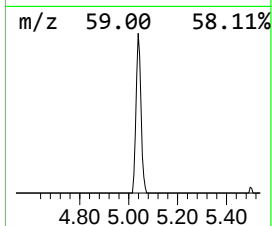
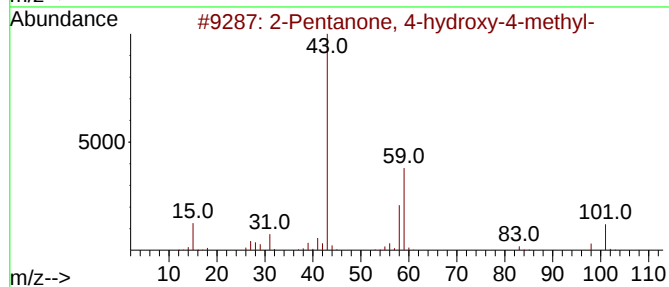
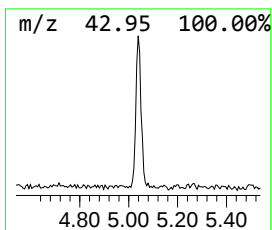
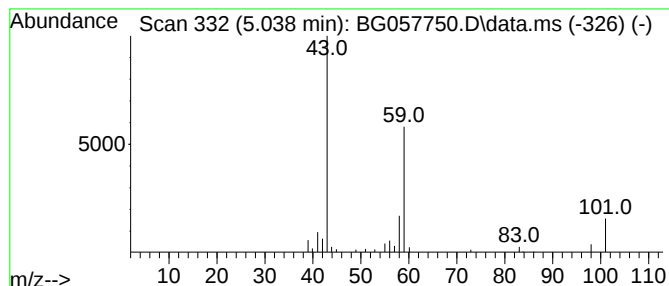
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.038	2.54 ng	39341	1,4-Dichlorobenzene-d4	7.929

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	47
3		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
4		Ethanol, pentamethyl-	116	C7H16O	000594-83-2	28
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25



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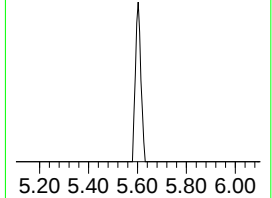
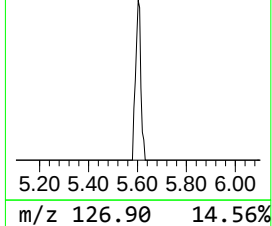
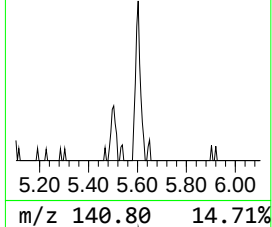
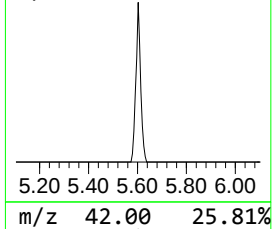
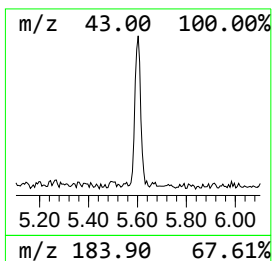
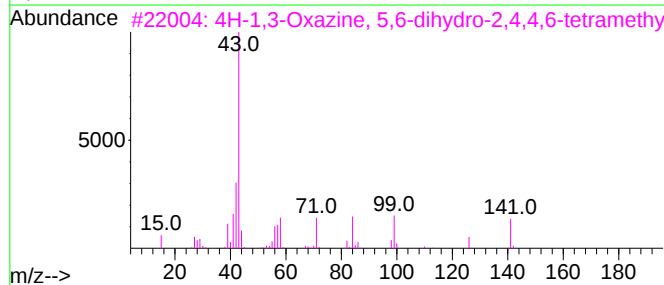
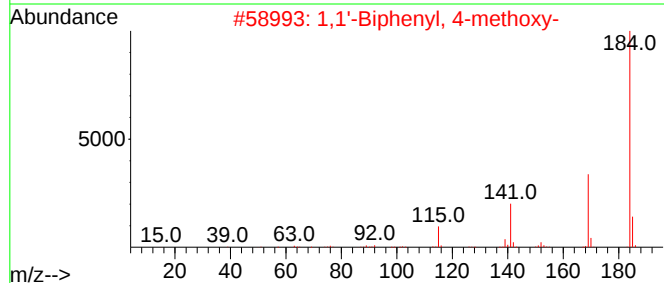
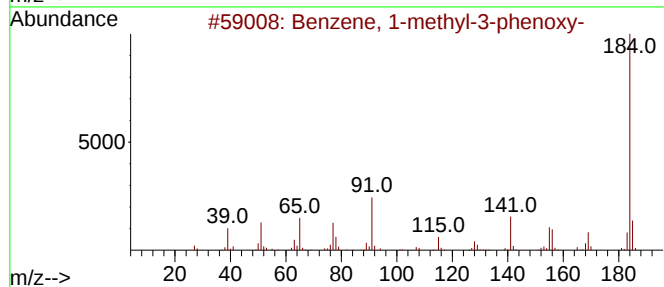
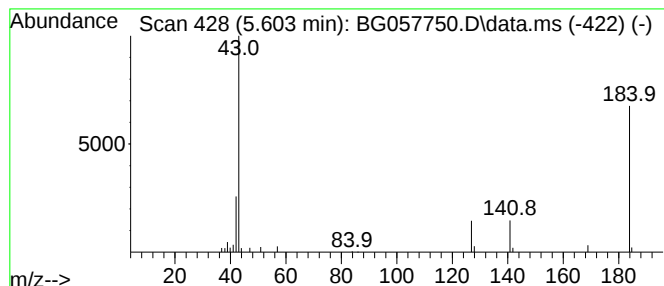
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.603 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.603	2.02 ng	31342	1,4-Dichlorobenzene-d4	7.929	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-phenoxy-	184	C13H12O	003586-14-9	9
2	1,1'-Biphenyl, 4-methoxy-	184	C13H12O	000613-37-6	9
3	4H-1,3-Oxazine, 5,6-dihydro-2,4,...	141	C8H15NO	026939-18-4	9
4	1,1'-Biphenyl, 2-methoxy-	184	C13H12O	000086-26-0	9
5	2H-1,3-Oxazine-2,4(3H)-dione, 3,...	141	C6H7NO3	1000327-48-4	9



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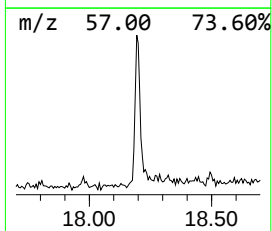
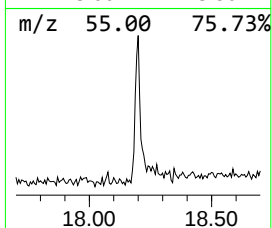
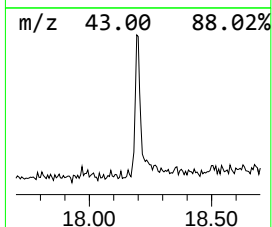
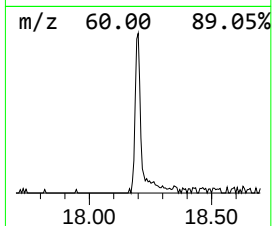
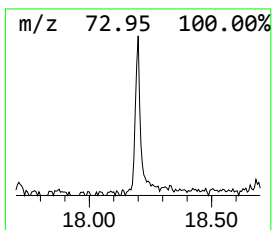
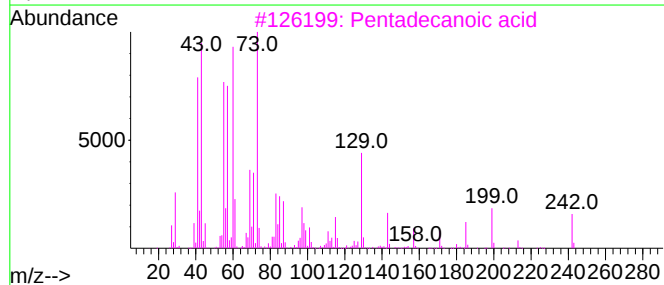
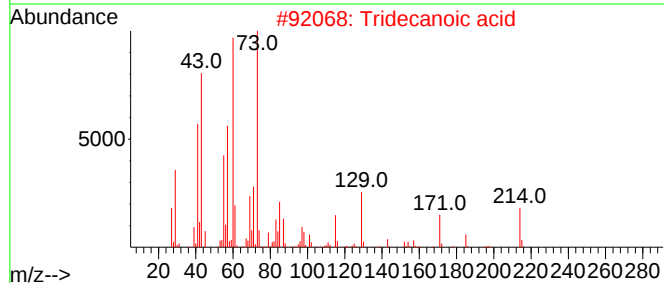
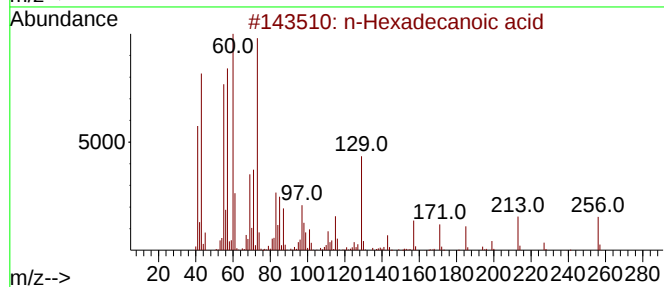
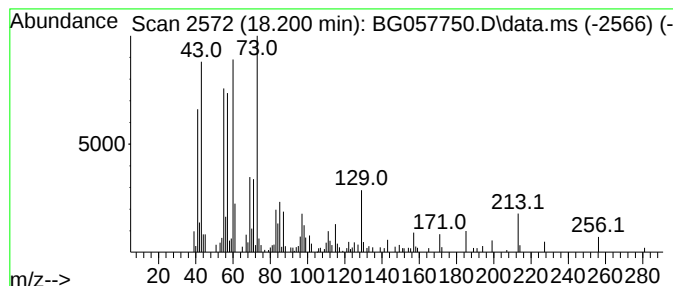
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.200	2.39 ng	128854	Phenanthrene-d10	17.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



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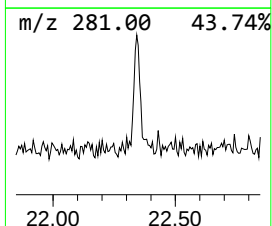
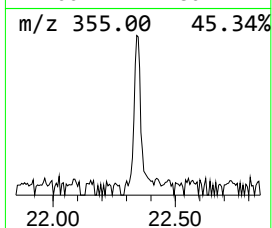
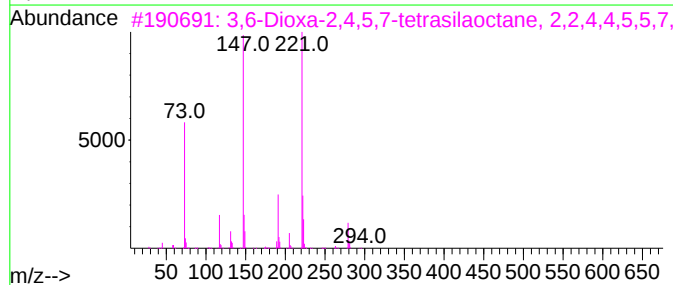
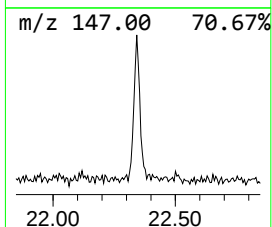
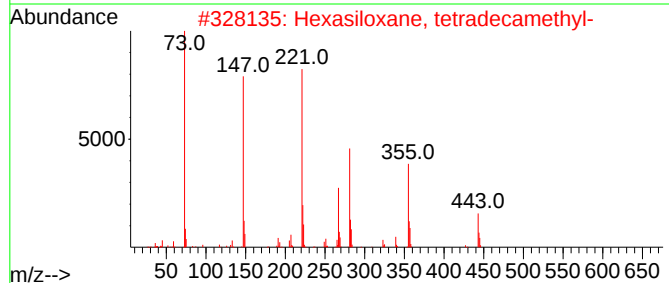
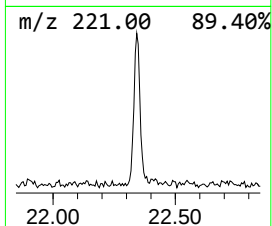
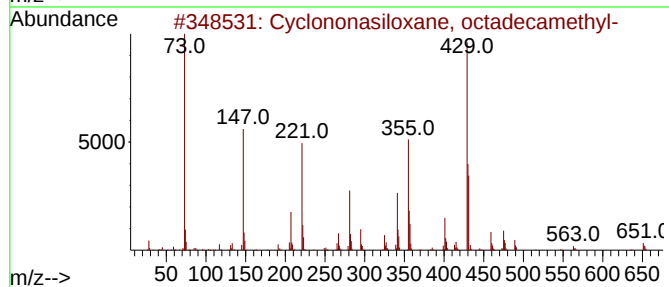
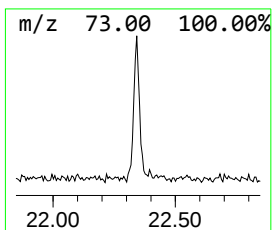
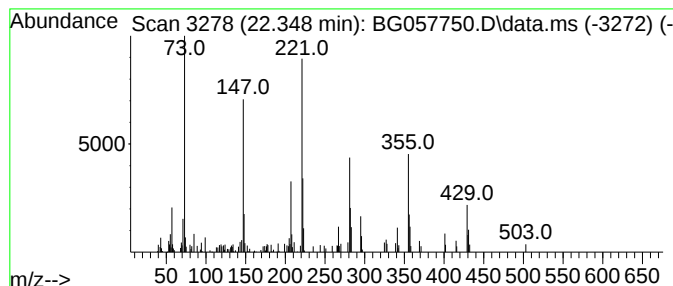
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Peak Number 5 Cyclononasiloxane, octadeca... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.348	2.42 ng	133998	Chrysene-d12		21.560	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-		666	C18H54O9Si9	000556-71-8	72
2	Hexasiloxane, tetradecamethyl-		458	C14H42O5Si6	000107-52-8	45
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...		294	C10H30O2Si4	004342-25-0	25
4	N-Benzyl-N-ethyl-p-isopropylbenz...		281	C19H23NO	015089-22-2	18
5	3,5-di-tert-Butyl-4-hydroxybenzy...		236	C15H24O2	000088-26-6	12



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ClientSampleId :
MW-2A

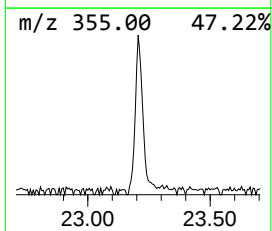
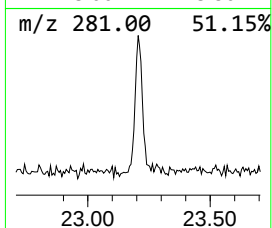
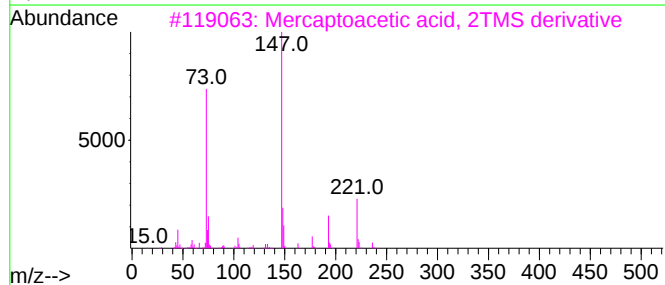
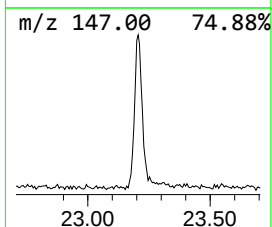
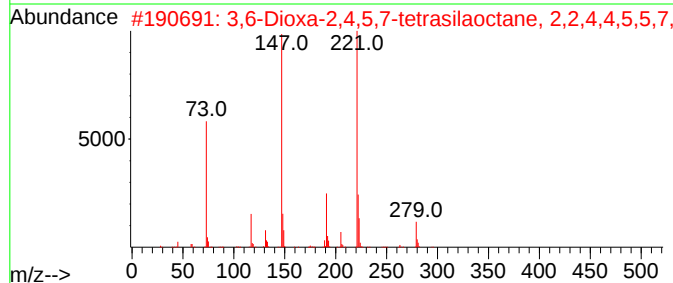
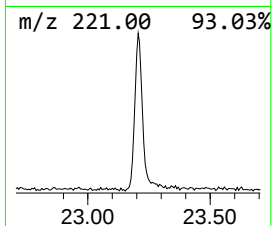
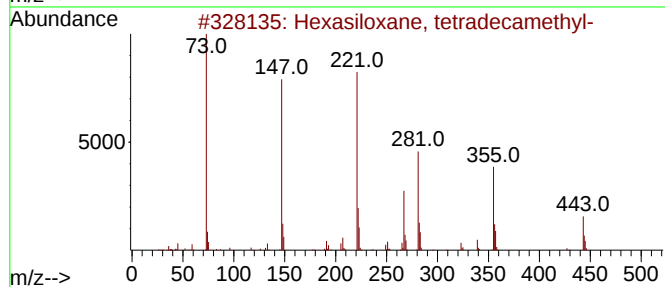
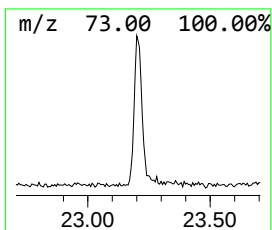
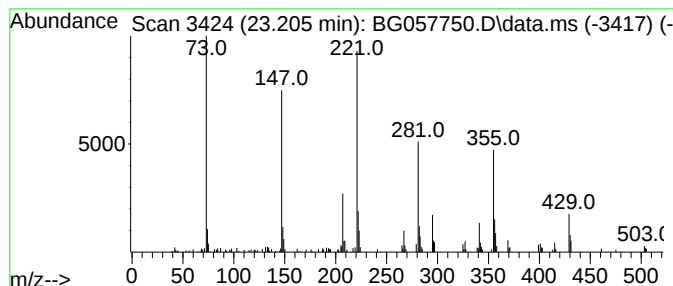
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexasiloxane, tetradecamethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.205	3.36 ng	221436	Perylene-d12	24.721

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	86
2		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
3		Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	38
4		1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	38
5		3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061623\
Data File : BG057750.D
Acq On : 17 Jun 2023 1:46
Operator : CG/JU
Sample : 03178-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2A

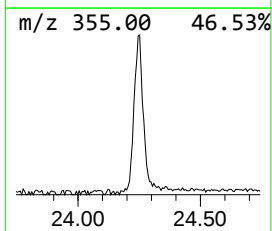
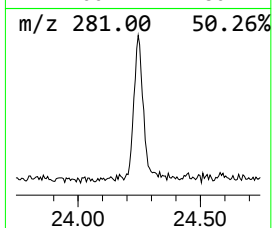
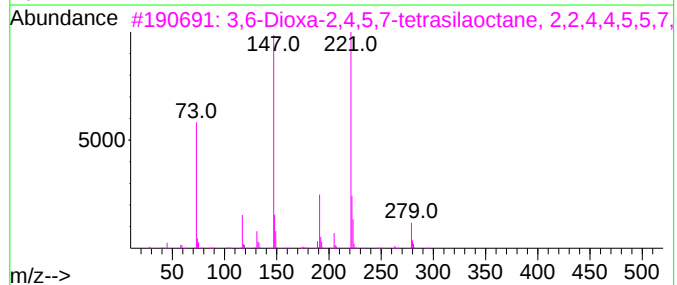
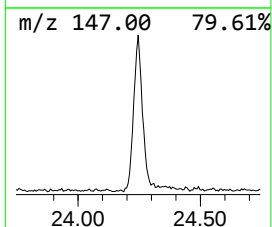
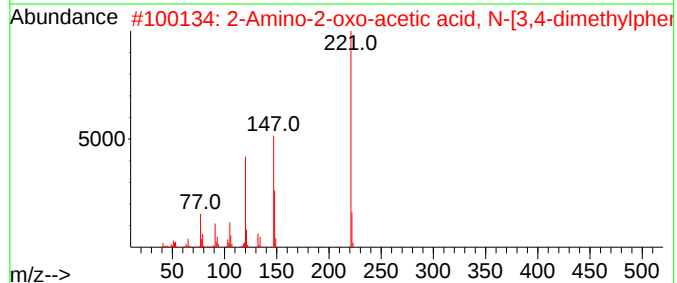
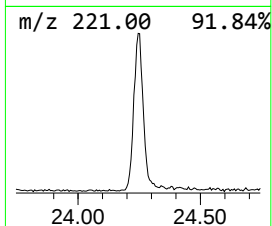
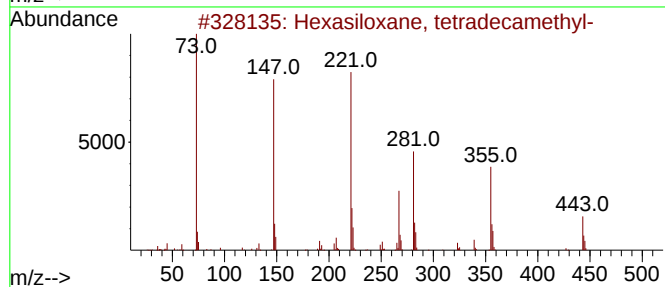
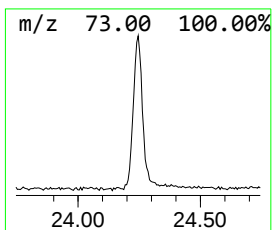
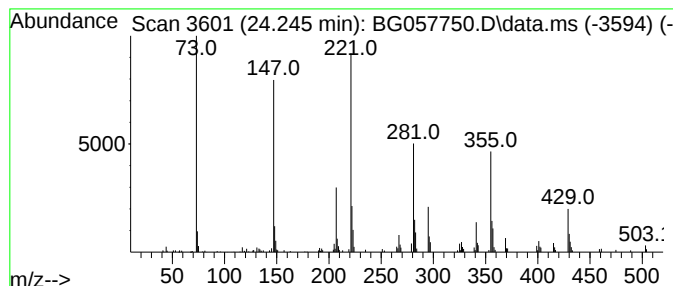
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown24.245 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.245	5.53 ng	365112	Perylene-d12	24.721

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	74
2			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	37
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
4			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22
5			3-Oxobutan-2-yl trimethylsilyl p...	308	C15H20O5Si	1000373-49-5	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061623\
Data File : BG057750.D
Acq On : 17 Jun 2023 1:46
Operator : CG/JU
Sample : 03178-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2A

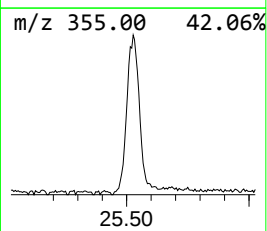
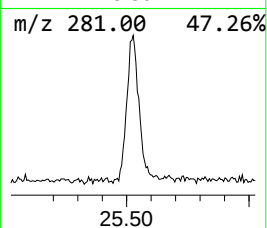
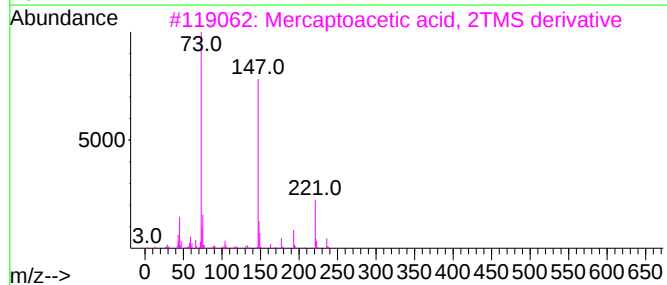
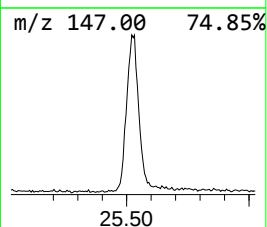
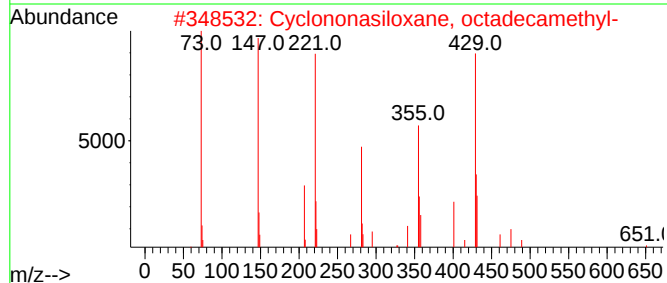
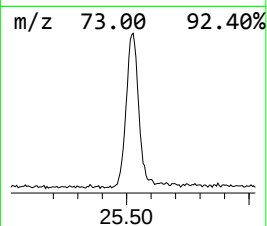
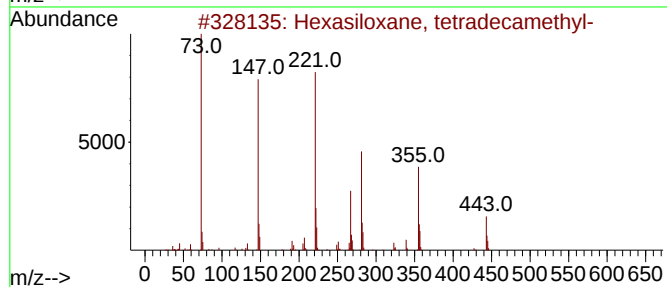
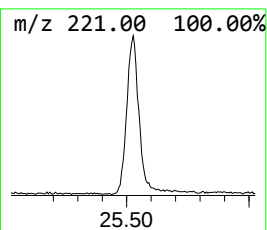
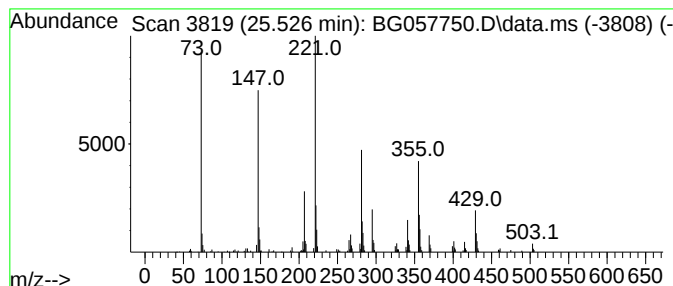
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown25.526 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.526	8.91 ng	588133	Perylene-d12	24.721

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	62
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	38
3			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37
4			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	37
5			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061623\
Data File : BG057750.D
Acq On : 17 Jun 2023 1:46
Operator : CG/JU
Sample : 03178-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2A

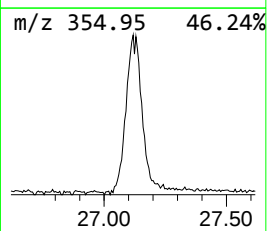
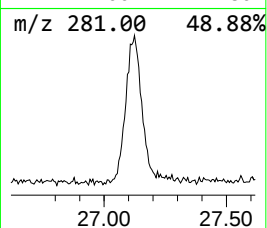
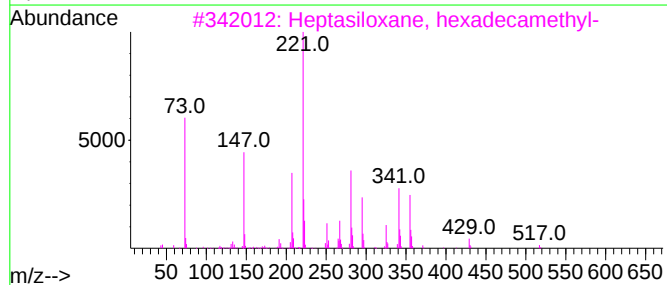
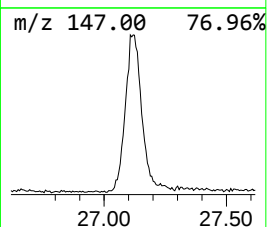
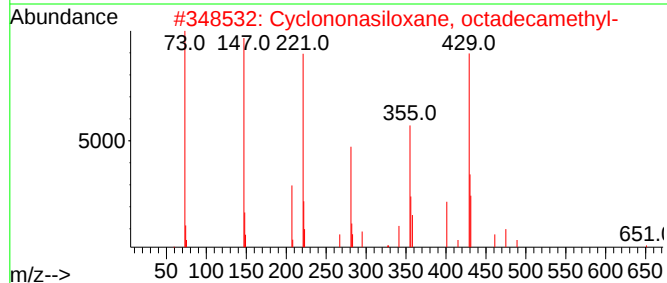
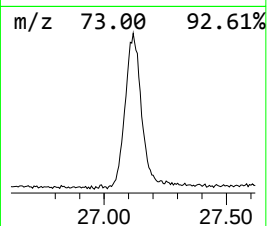
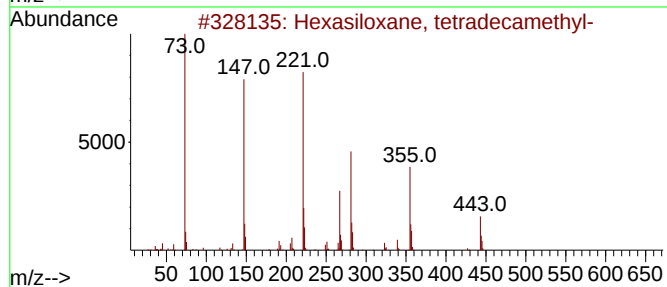
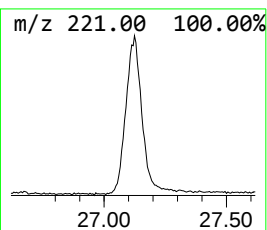
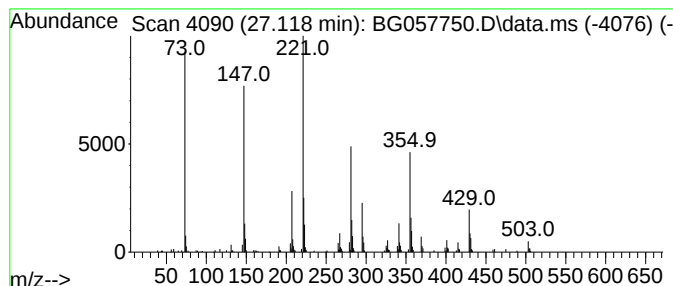
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown27.119 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.119	12.83 ng	846924	Perylene-d12	24.721

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	81
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	80
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	42
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37
5			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061623\
Data File : BG057750.D
Acq On : 17 Jun 2023 1:46
Operator : CG/JU
Sample : 03178-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2A

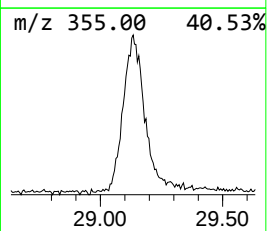
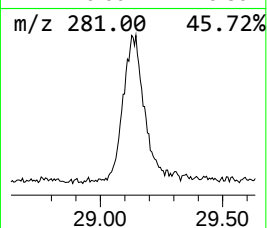
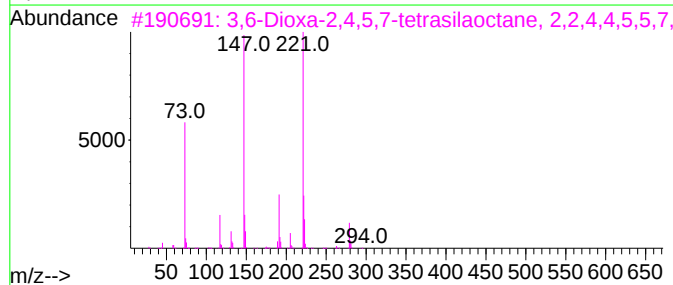
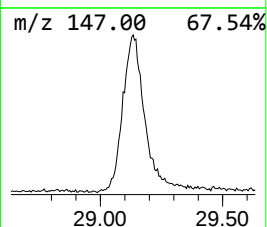
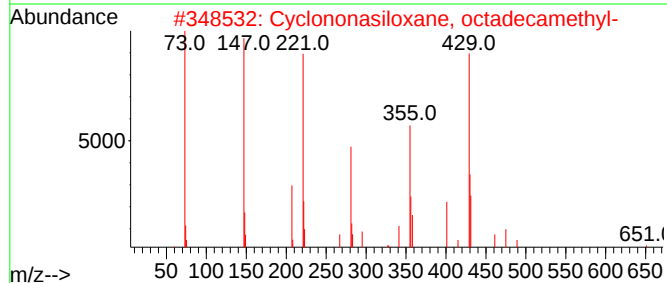
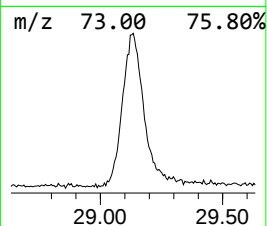
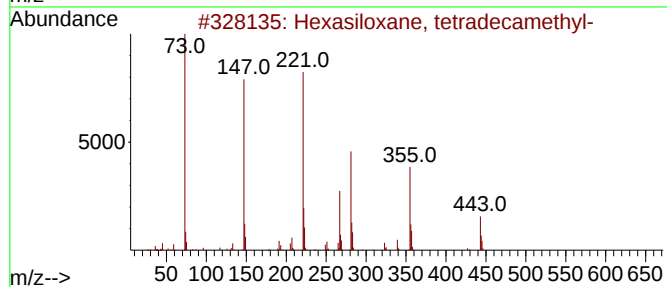
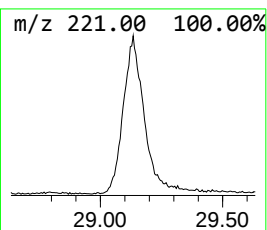
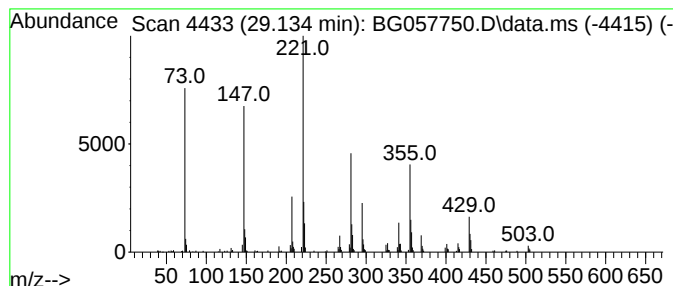
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown29.134 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.134	15.43 ng	1018260	Perylene-d12	24.721

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	46
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	42
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
4			2,6-Dimethyl-3,4-bis(trimethylsi...	311	C15H29N02Si2	1000079-52-1	37
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061623\
Data File : BG057750.D
Acq On : 17 Jun 2023 1:46
Operator : CG/JU
Sample : 03178-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2A

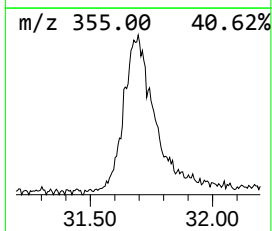
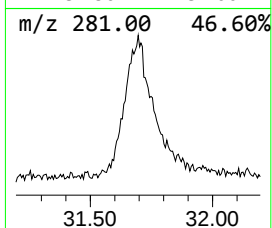
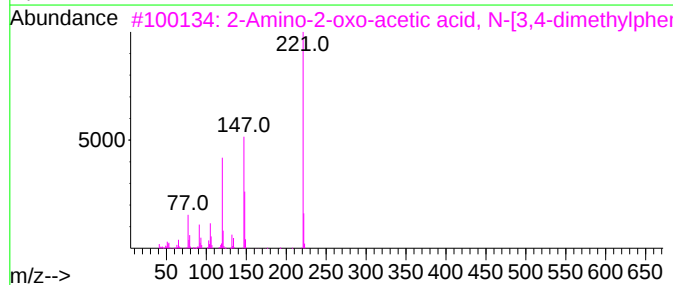
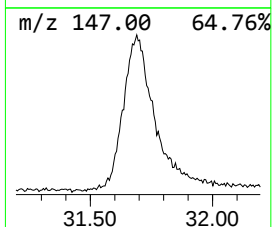
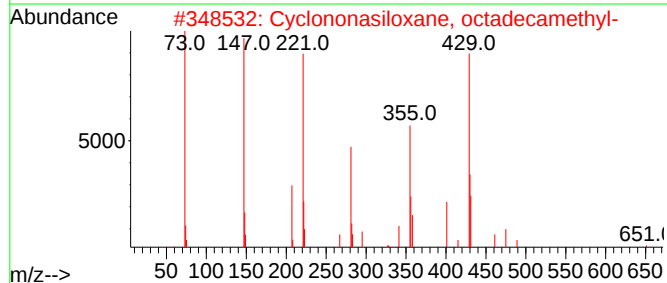
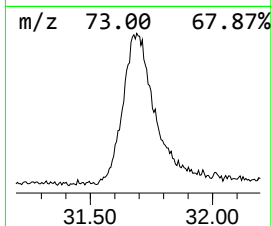
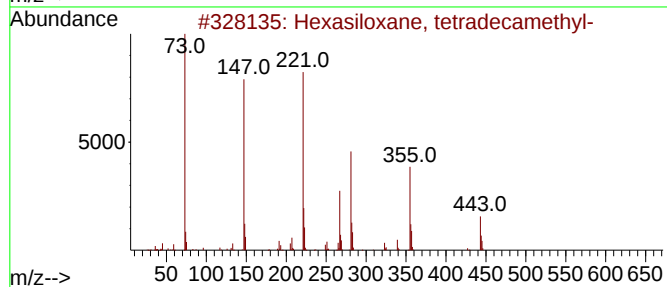
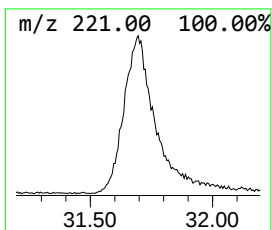
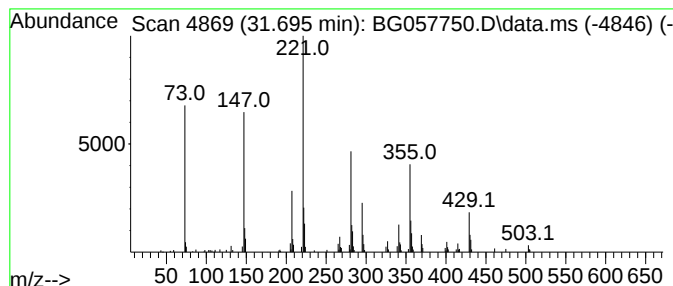
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown31.695 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.695	15.11 ng	997015	Perylene-d12	24.721

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	53
2		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	47
3		2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	37
4		3,6-Dioxo-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
5		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061623\
Data File : BG057750.D
Acq On : 17 Jun 2023 1:46
Operator : CG/JU
Sample : 03178-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
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
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2-Pentanone, 4-...	5.038	2.5	ng	39341	1	7.929	310325	20.0
unknown5.603	5.603	2.0	ng	31342	1	7.929	310325	20.0
n-Hexadecanoic ...	18.200	2.4	ng	128854	4	17.307	1077340	20.0
Cyclononasiloxa...	22.348	2.4	ng	133998	5	21.560	1109490	20.0
Hexasiloxane, t...	23.205	3.4	ng	221436	6	24.721	1319920	20.0
unknown24.245	24.245	5.5	ng	365112	6	24.721	1319920	20.0
unknown25.526	25.526	8.9	ng	588133	6	24.721	1319920	20.0
unknown27.119	27.119	12.8	ng	846924	6	24.721	1319920	20.0
unknown29.134	29.134	15.4	ng	1018260	6	24.721	1319920	20.0
unknown31.695	31.695	15.1	ng	997015	6	24.721	1319920	20.0