

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042524\
 Data File : BG061039.D
 Acq On : 25 Apr 2024 15:58
 Operator : MA/JU
 Sample : P2261-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RO-RBR200059

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-BG042024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061039.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.170	25	31	39	rVB2	34202	65253	3.39%	0.608%
2	3.687	114	119	128	rBV	58628	92004	4.78%	0.857%
3	5.537	426	434	441	rBV	572949	907905	47.12%	8.453%
4	6.942	662	673	680	rBV4	10226	25960	1.35%	0.242%
5	7.118	695	703	712	rBV	517112	896372	46.52%	8.346%
6	7.940	835	843	850	rBV	103696	176224	9.15%	1.641%
7	9.098	1033	1040	1047	rVB	333098	572486	29.71%	5.330%
8	10.737	1310	1319	1325	rBV	135922	246520	12.79%	2.295%
9	11.472	1438	1444	1449	rBV2	23274	39608	2.06%	0.369%
10	13.193	1730	1737	1745	rBV	840428	1278131	66.34%	11.900%
11	14.568	1961	1971	1978	rBV	222581	348010	18.06%	3.240%
12	14.774	1998	2006	2007	rBV	157056	183849	9.54%	1.712%
13	16.060	2219	2225	2233	rBV	906176	1355789	70.37%	12.623%
14	16.319	2259	2269	2274	rBV8	18557	48694	2.53%	0.453%
15	16.401	2280	2283	2289	rBV4	11708	20907	1.09%	0.195%
16	16.466	2290	2294	2299	rVV6	13186	23826	1.24%	0.222%
17	16.530	2299	2305	2309	rVV8	11097	21561	1.12%	0.201%
18	16.789	2344	2349	2353	rBV5	11022	20655	1.07%	0.192%
19	17.136	2406	2408	2413	rVB4	14474	20469	1.06%	0.191%
20	17.318	2433	2439	2444	rBV	284795	429218	22.28%	3.996%
21	17.359	2444	2446	2453	rVB	34202	43138	2.24%	0.402%
22	17.453	2458	2462	2466	rVB	14193	24298	1.26%	0.226%
23	18.217	2588	2592	2601	rVB3	67345	115816	6.01%	1.078%
24	18.387	2619	2621	2626	rVB	20863	26567	1.38%	0.247%
25	18.610	2657	2659	2666	rVB8	14875	22884	1.19%	0.213%
26	18.804	2687	2692	2695	rBV6	31579	50193	2.61%	0.467%
27	19.374	2784	2789	2794	rBV	160073	224042	11.63%	2.086%
28	19.433	2796	2799	2803	rVV3	40791	46685	2.42%	0.435%
29	19.733	2842	2850	2858	rBV	179474	322436	16.73%	3.002%
30	19.938	2880	2885	2897	rVB	1455307	1926753	100.00%	17.939%
31	20.156	2919	2922	2926	rVB	39683	44089	2.29%	0.410%
32	20.232	2932	2935	2939	rVB2	35313	46348	2.41%	0.432%
33	21.254	3105	3109	3115	rVB4	60145	105521	5.48%	0.982%
34	21.577	3157	3164	3169	rBV2	326446	650141	33.74%	6.053%
35	24.709	3690	3697	3705	rBV2	109255	318340	16.52%	2.964%

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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-BG042024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

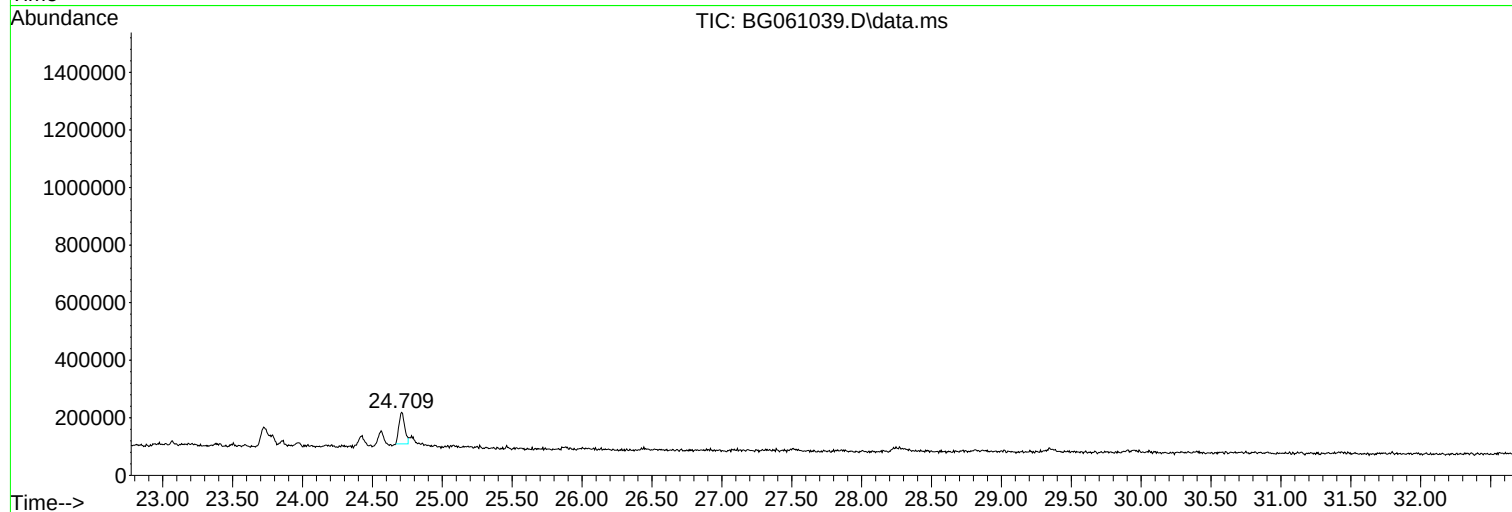
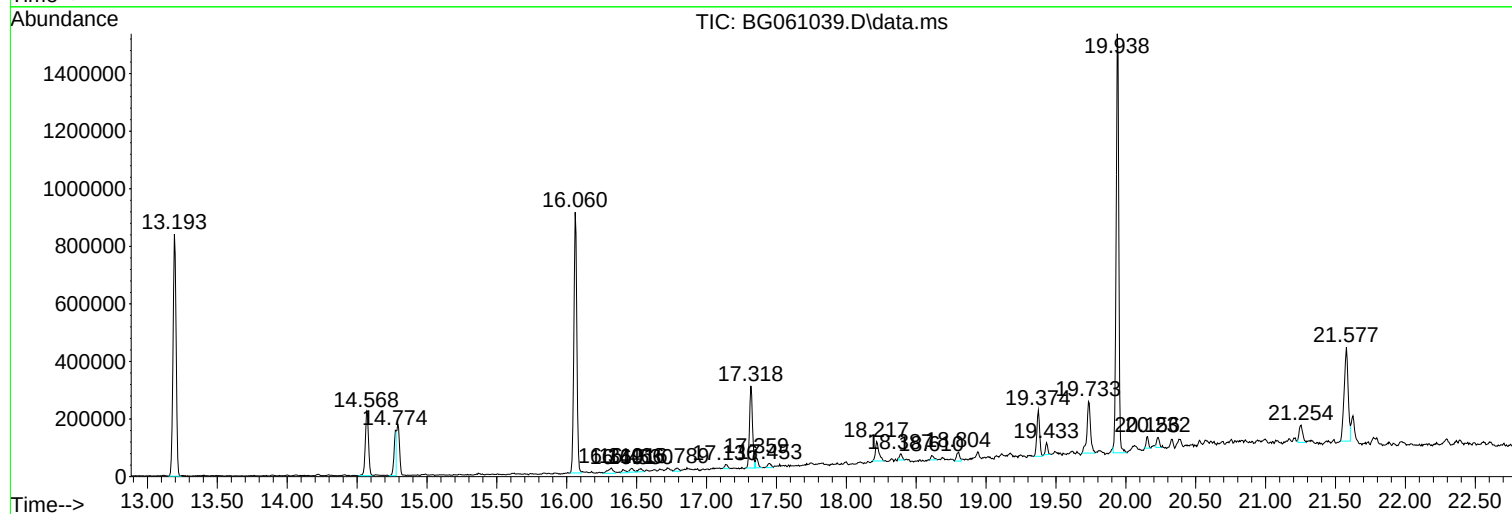
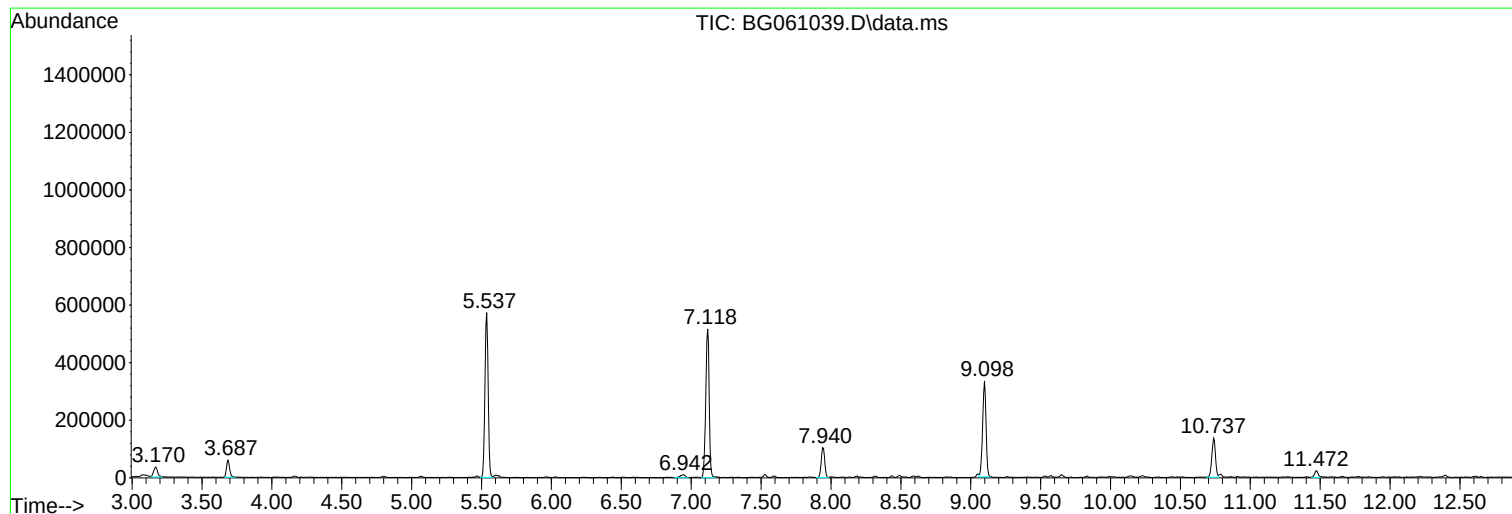
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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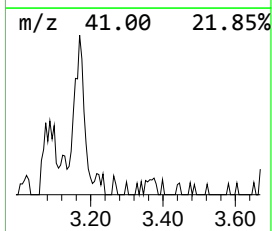
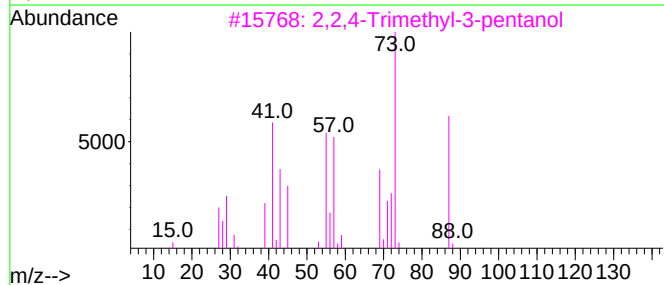
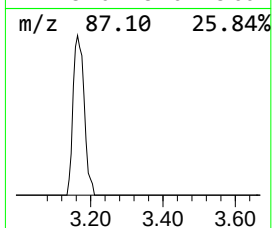
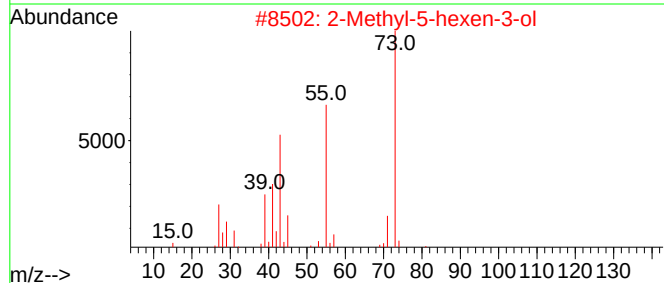
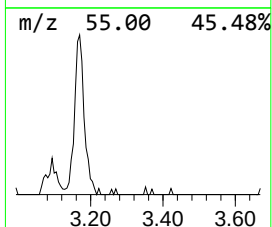
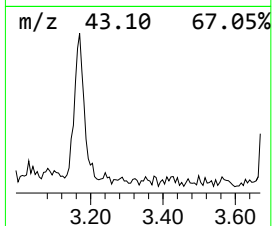
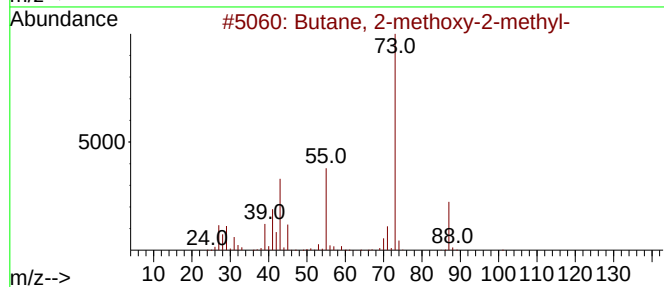
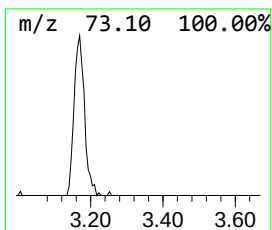
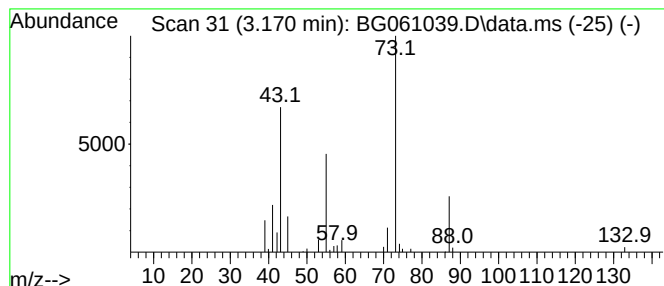
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.170	7.41 ng	65253	1,4-Dichlorobenzene-d4	7.946

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	40
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	33
4			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	25
5			Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	23



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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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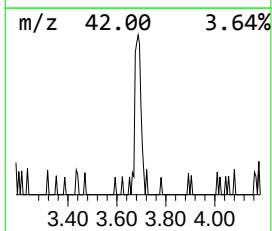
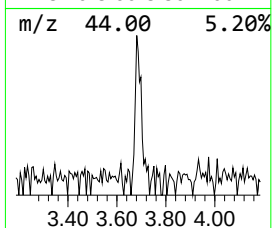
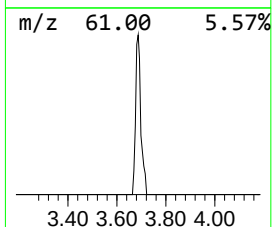
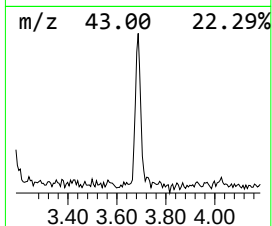
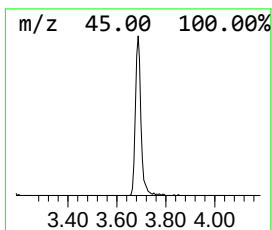
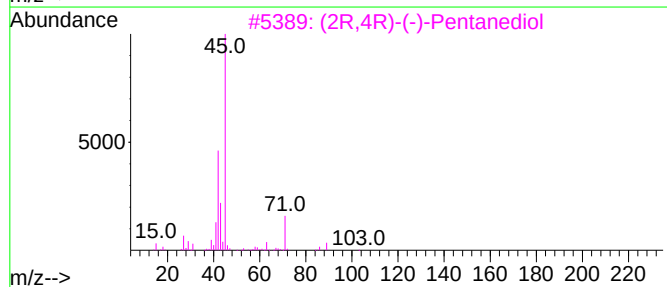
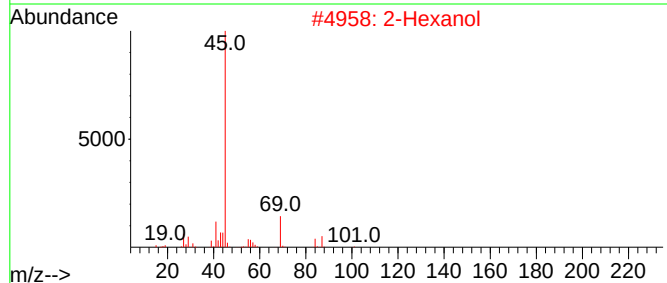
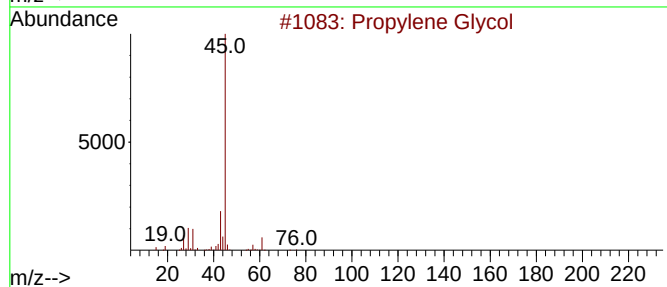
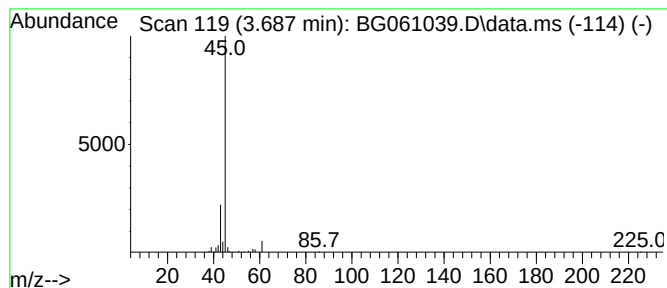
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.687 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.687	10.44 ng	92004	1,4-Dichlorobenzene-d4	7.946

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	9
2			2-Hexanol	102	C6H14O	000626-93-7	9
3			(2R,4R)-(-)-Pentanediol	104	C5H12O2	042075-32-1	9
4			Hydrazine, (2-methoxyethyl)-	90	C3H10N2O	003044-15-3	9
5			2,4-Pentanediol	104	C5H12O2	000625-69-4	9



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ALS Vial : 9 Sample Multiplier: 1

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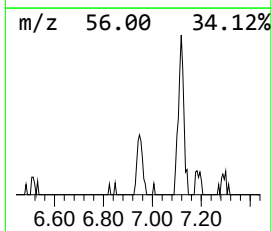
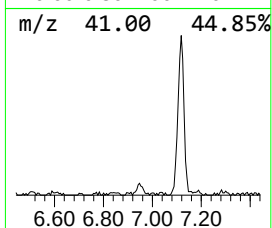
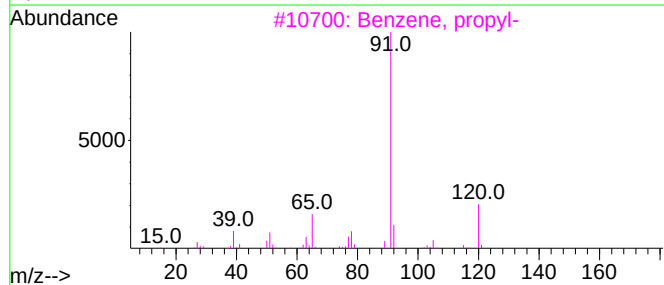
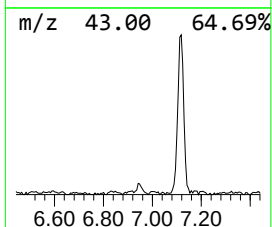
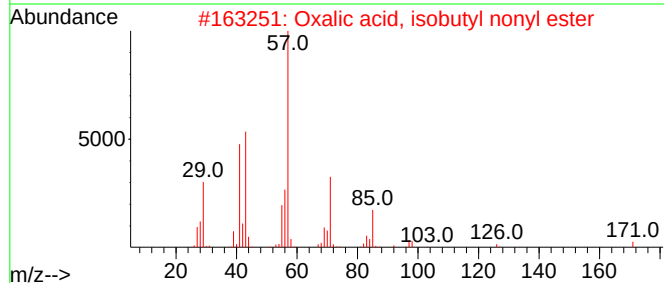
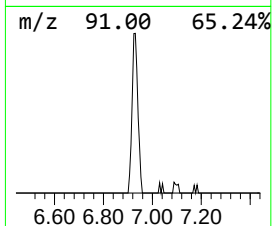
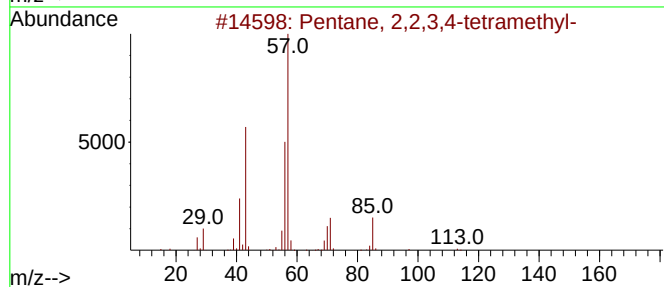
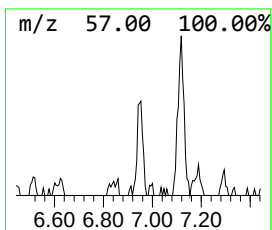
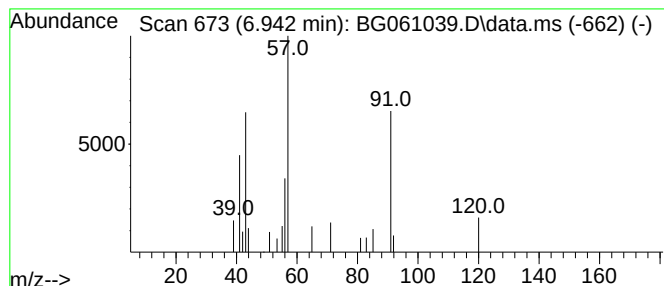
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.942 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.942	2.95 ng	25960	1,4-Dichlorobenzene-d4	7.946

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	37
2			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	32
3			Benzene, propyl-	120	C9H12	000103-65-1	27
4			Octane, 2,5,6-trimethyl-	156	C11H24	062016-14-2	23
5			2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	23



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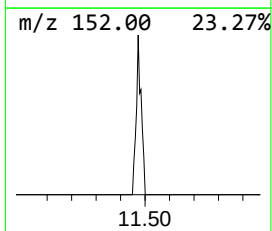
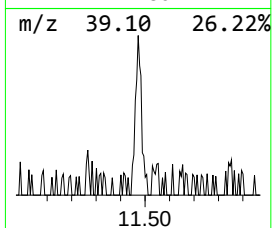
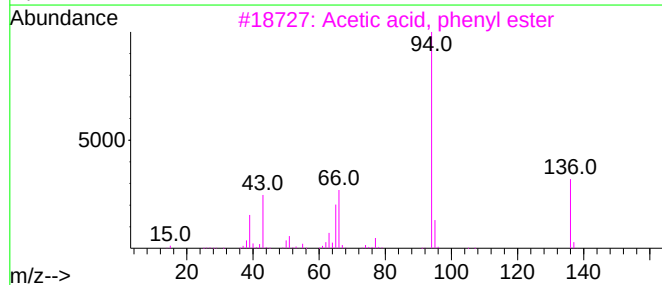
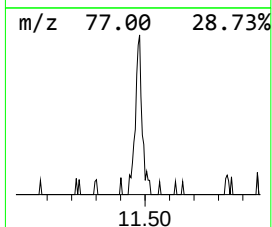
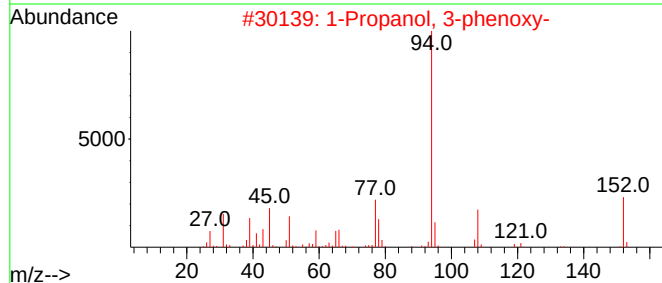
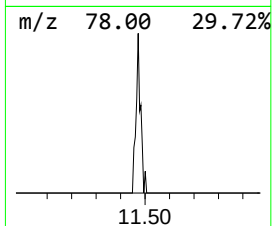
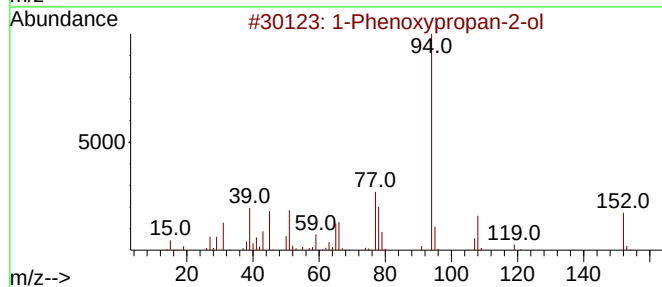
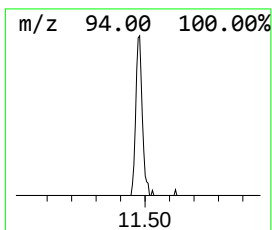
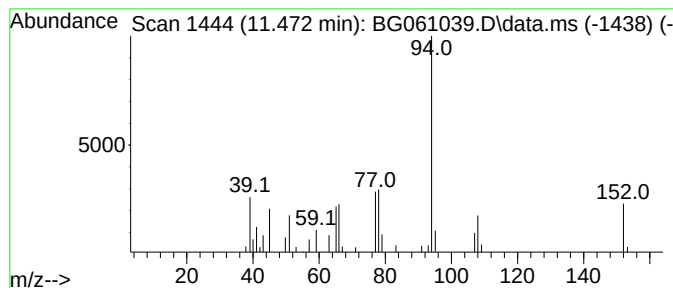
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.472	3.21 ng	39608	Naphthalene-d8	10.737

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	70
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	60
3			Acetic acid, phenyl ester	136	C8H8O2	000122-79-2	53
4			Butanoic acid, 4-phenoxy-	180	C10H12O3	006303-58-8	53
5			Phenol	94	C6H6O	000108-95-2	52



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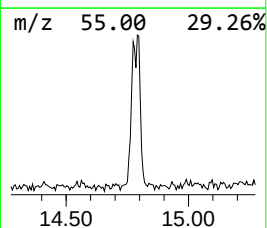
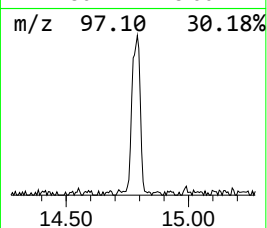
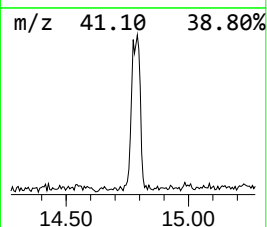
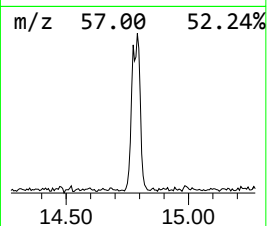
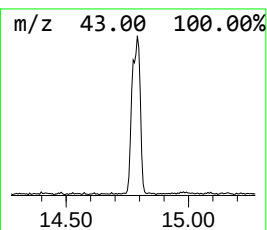
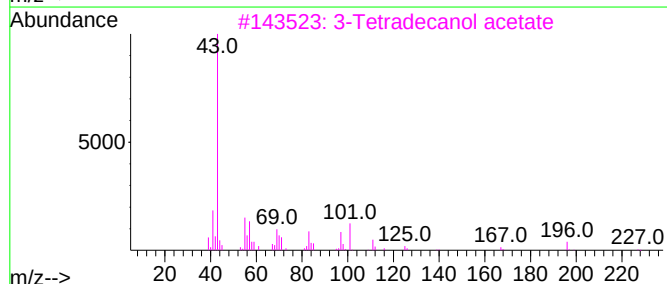
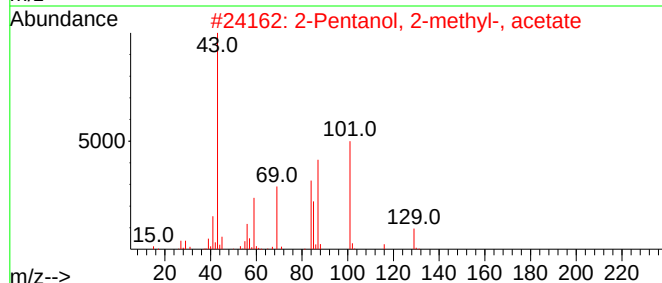
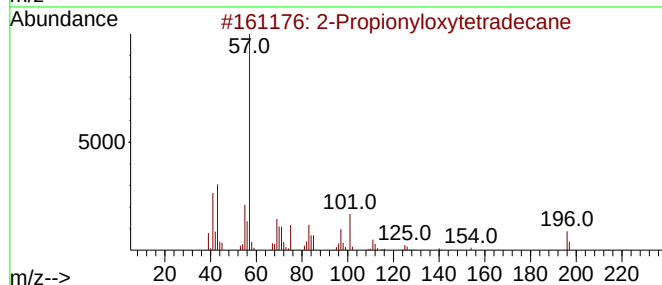
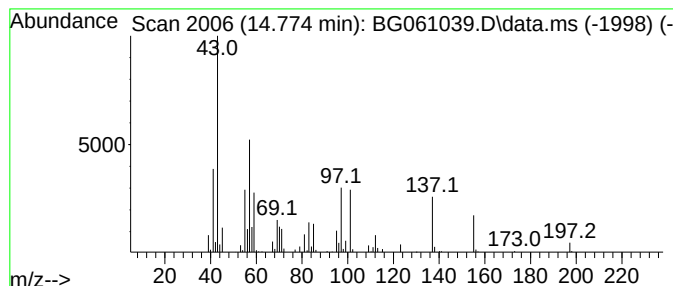
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown14.774 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.774	10.57 ng	183849	Acenaphthene-d10	14.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propionyloxytetradecane		270	C17H34O2	1000245-62-7	14	
2	2-Pentanol, 2-methyl-, acetate		144	C8H16O2	034859-98-8	14	
3	3-Tetradecanol acetate		256	C16H32O2	051354-23-5	12	
4	Pentadecane, 1-bromo-		290	C15H31Br	000629-72-1	10	
5	5-Ethyl-3-nonanol		172	C11H24O	019780-71-3	10	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042524\
Data File : BG061039.D
Acq On : 25 Apr 2024 15:58
Operator : MA/JU
Sample : P2261-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-RBR200059

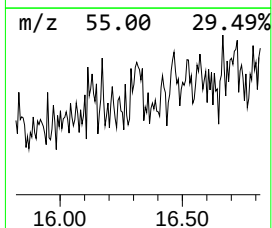
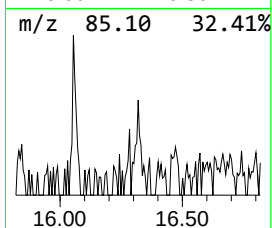
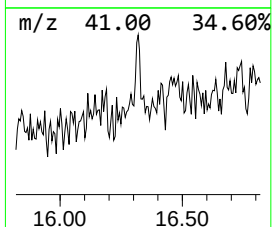
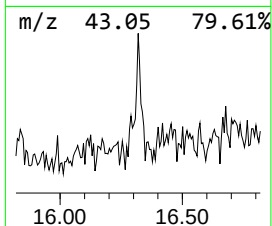
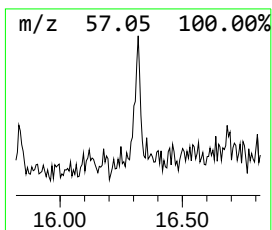
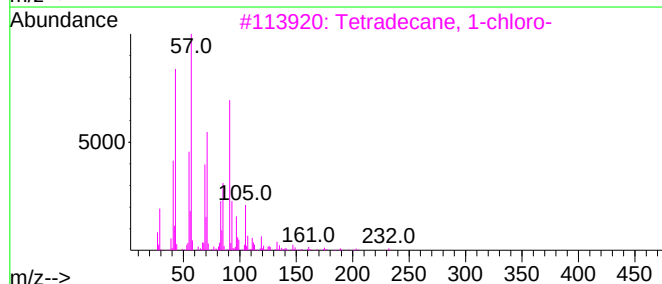
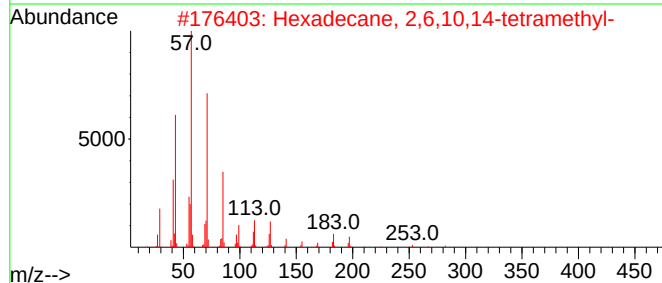
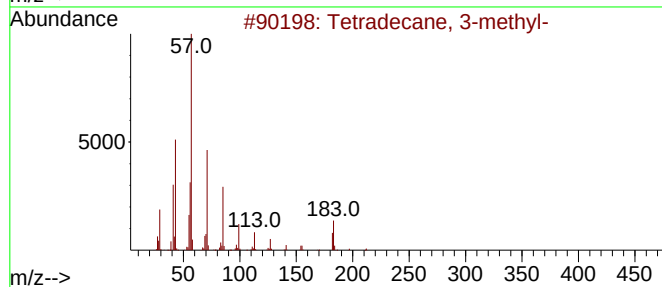
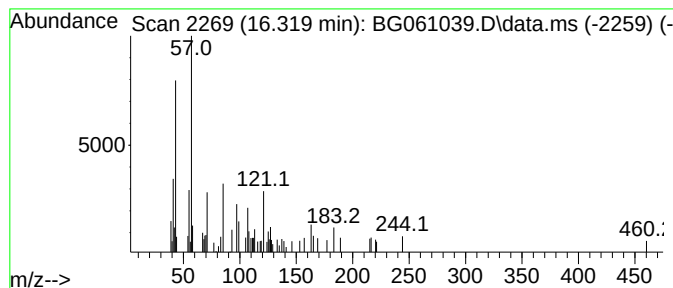
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown16.319 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.319	2.27 ng	48694	Phenanthrene-d10	17.318

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane, 3-methyl-	212	C15H32	018435-22-8	22
2		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	22
3		Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	16
4		Octadecane, 2-methyl-	268	C19H40	001560-88-9	14
5		Pentadecane, 2-methyl-	226	C16H34	001560-93-6	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042524\
Data File : BG061039.D
Acq On : 25 Apr 2024 15:58
Operator : MA/JU
Sample : P2261-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RO-RBR200059

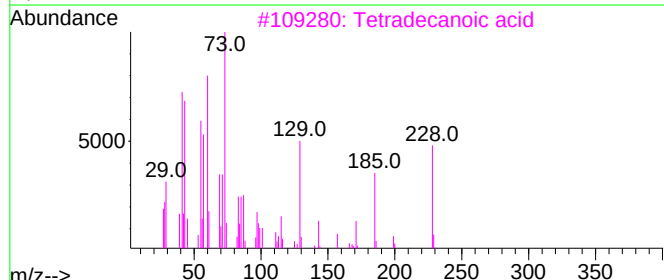
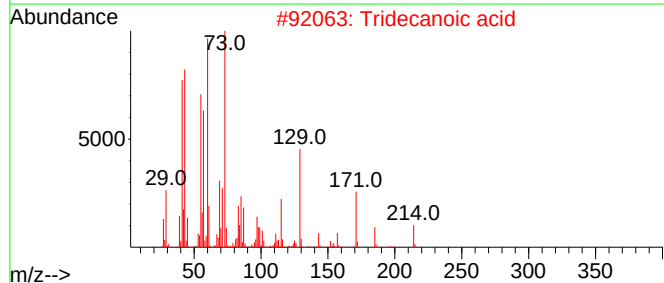
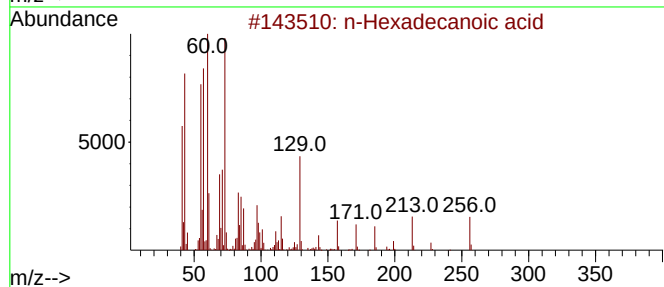
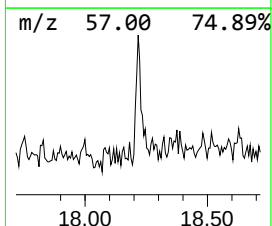
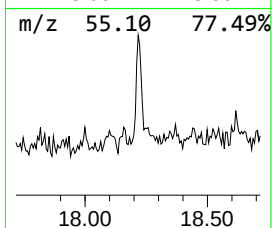
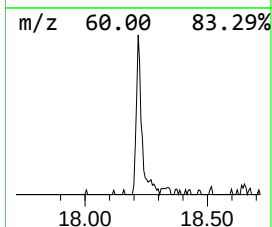
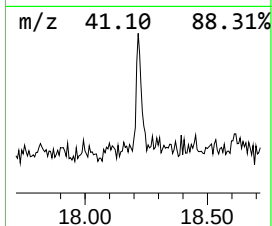
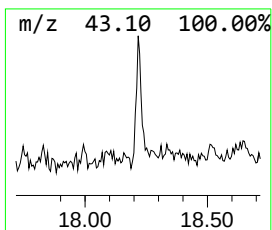
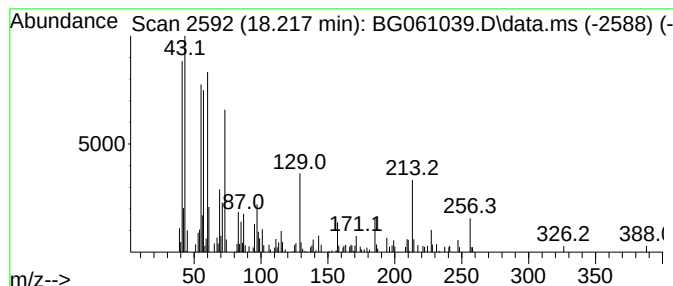
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.217	5.40 ng	115816	Phenanthrene-d10	17.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	58
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	56
4			n-Decanoic acid	172	C10H20O2	000334-48-5	50
5			Undecanoic acid	186	C11H22O2	000112-37-8	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042524\
Data File : BG061039.D
Acq On : 25 Apr 2024 15:58
Operator : MA/JU
Sample : P2261-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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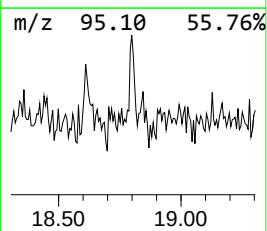
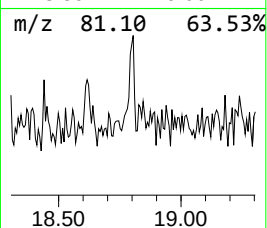
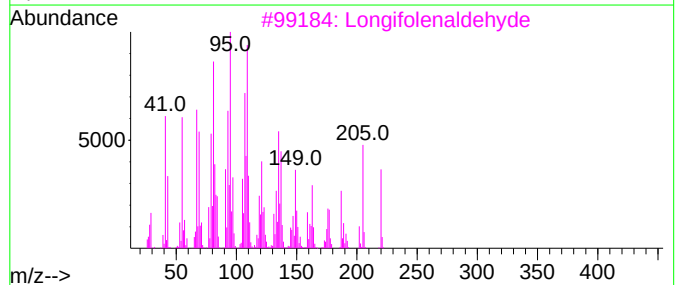
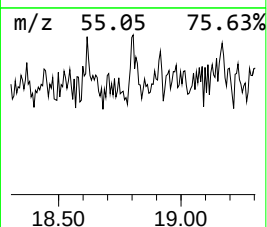
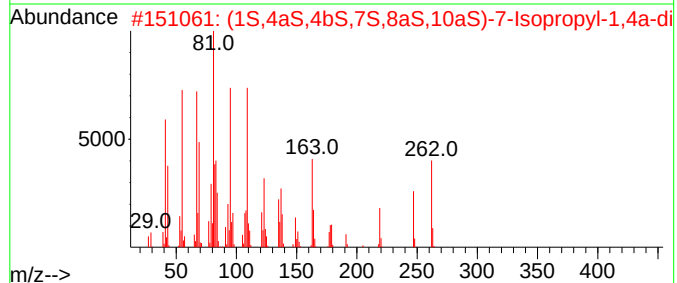
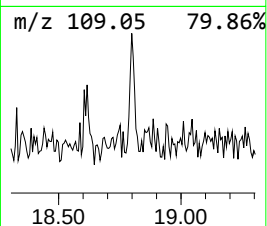
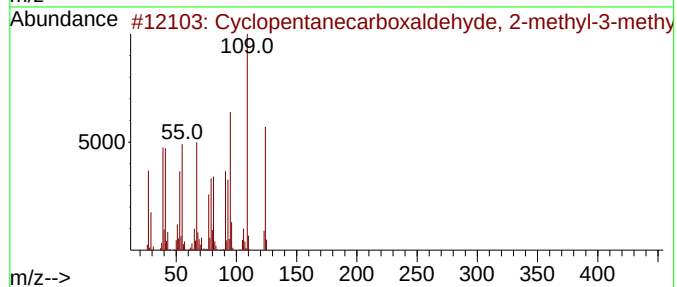
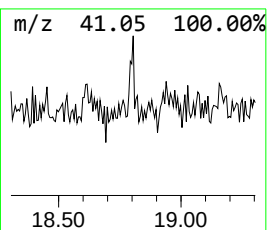
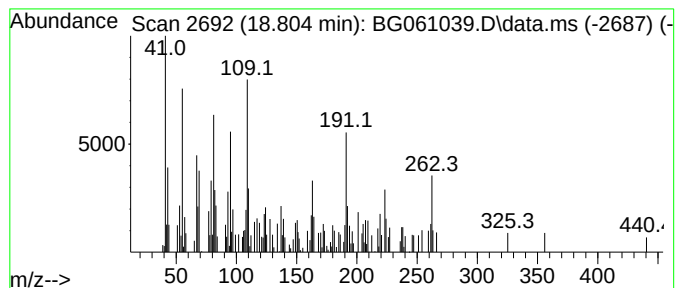
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclopentanecarboxaldehyde,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.804	2.34 ng	50193	Phenanthrene-d10	17.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanecarboxaldehyde, 2-me...	124	C8H12O	1000154-24-0	84
2			(1S,4aS,4bS,7S,8aS,10aS)-7-Isopr...	262	C19H34	002221-95-6	53
3			Longifolenaldehyde	220	C15H24O	019890-84-7	35
4			Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	25
5			4-Fluorobenzylamine, N-(2-fluoro...	219	C13H11F2N	1000310-47-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042524\
Data File : BG061039.D
Acq On : 25 Apr 2024 15:58
Operator : MA/JU
Sample : P2261-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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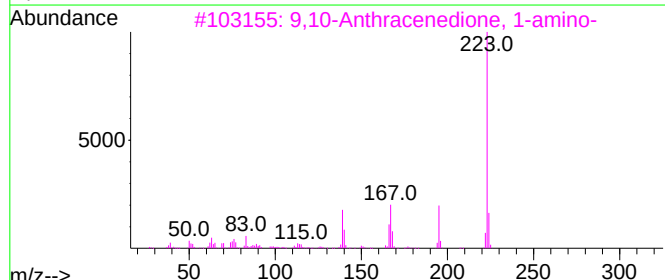
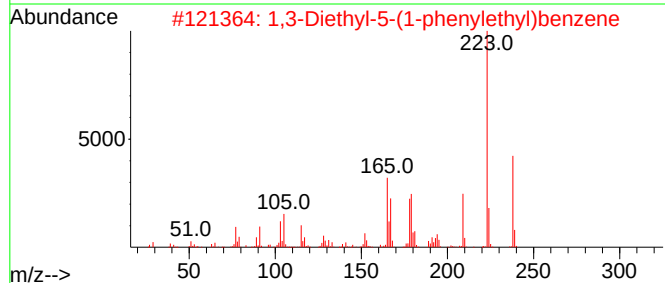
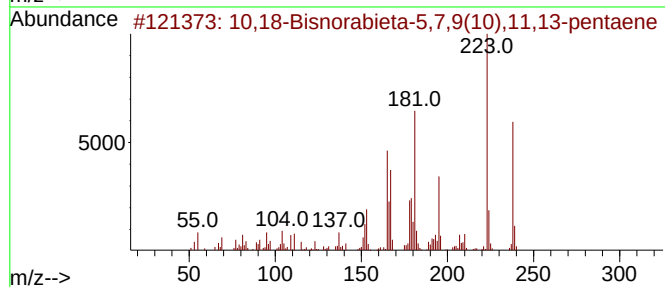
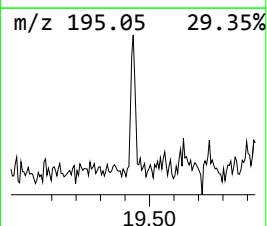
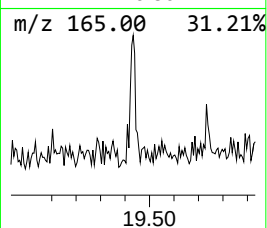
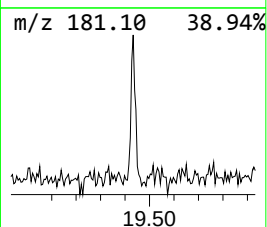
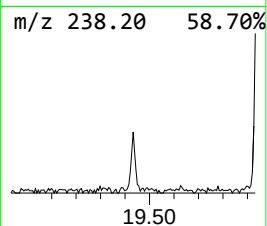
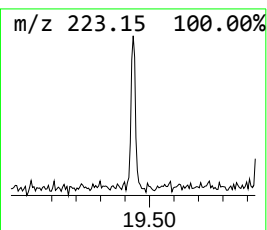
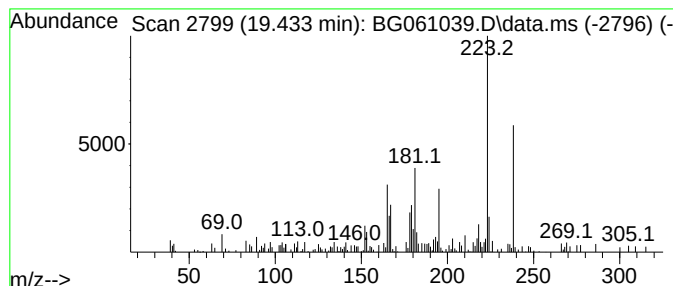
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.433	2.18 ng	46685	Phenanthrene-d10	17.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	93		
2	1,3-Diethyl-5-(1-phenylethyl)ben...	238	C18H22	1000482-32-6	89		
3	9,10-Anthracenedione, 1-amino-	223	C14H9NO2	000082-45-1	43		
4	3,3'-Diacetylbiphenyl	238	C16H14O2	094113-07-2	43		
5	9-Acridinecarboxylic acid	223	C14H9NO2	005336-90-3	43		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042524\
Data File : BG061039.D
Acq On : 25 Apr 2024 15:58
Operator : MA/JU
Sample : P2261-01
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ALS Vial : 9 Sample Multiplier: 1

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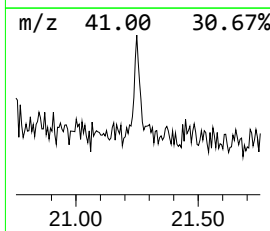
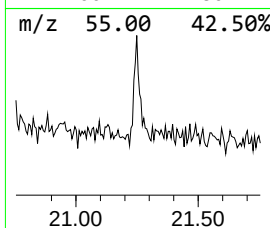
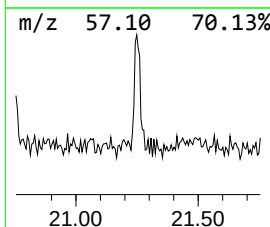
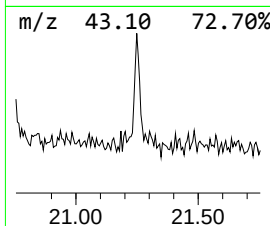
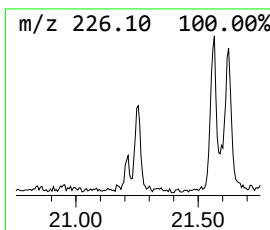
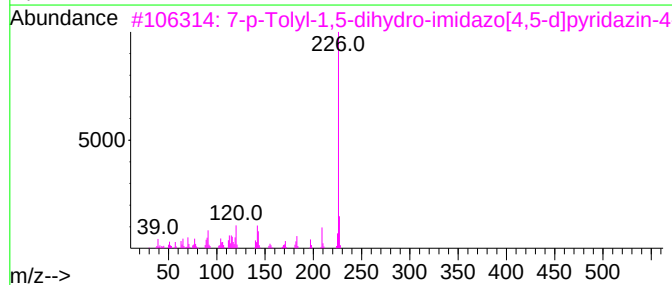
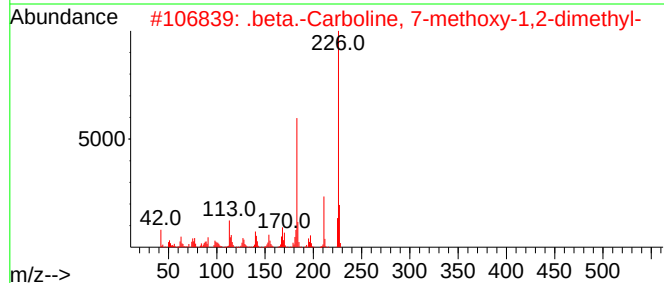
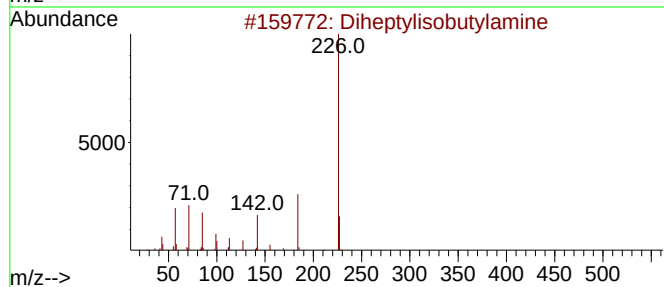
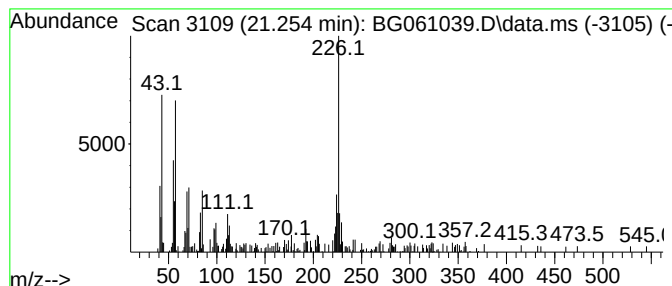
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown21.254 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.254	3.25 ng	105521	Chrysene-d12	21.577

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diheptylisobutylamine	269	C18H39N	1000310-32-0	47
2			.beta.-Carboline, 7-methoxy-1,2-...	226	C14H14N2O	006519-18-2	45
3			7-p-Tolyl-1,5-dihydro-imidazo[4,...	226	C12H10N4O	1000317-75-5	43
4			Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	1000300-57-6	43
5			Propenone, 3-(5-chloro-2-benzoth...	349	C16H9ClFNOS2	277325-89-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042524\
Data File : BG061039.D
Acq On : 25 Apr 2024 15:58
Operator : MA/JU
Sample : P2261-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.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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unknown3.687	3.687	10.4	ng	92004	1	7.946	176224	20.0
unknown6.942	6.942	3.0	ng	25960	1	7.946	176224	20.0
1-Phenoxypropan...	11.472	3.2	ng	39608	2	10.737	246520	20.0
unknown14.774	14.774	10.6	ng	183849	3	14.568	348010	20.0
unknown16.319	16.319	2.3	ng	48694	4	17.318	429218	20.0
n-Hexadecanoic ...	18.217	5.4	ng	115816	4	17.318	429218	20.0
Cyclopentanecar...	18.804	2.3	ng	50193	4	17.318	429218	20.0
10,18-Bisnorabi...	19.433	2.2	ng	46685	4	17.318	429218	20.0
unknown21.254	21.254	3.3	ng	105521	5	21.577	650141	20.0