

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041723\
 Data File : BG057121.D
 Acq On : 17 Apr 2023 21:54
 Operator : CG/JU
 Sample : 02357-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P2-S2-230413

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-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057121.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.472	154	159	165	rBB	11696	17063	2.01%	0.374%
2	5.423	315	321	328	rBB	41394	62529	7.36%	1.372%
3	5.911	397	404	411	rBB	143590	229222	26.99%	5.028%
4	7.532	673	680	687	rBV	168550	280872	33.07%	6.161%
5	8.396	821	827	833	rBB	36584	59398	6.99%	1.303%
6	9.154	951	956	961	rBB	6113	8793	1.04%	0.193%
7	9.577	1021	1028	1035	rBB	95164	167541	19.73%	3.675%
8	11.239	1303	1311	1324	rBB	50653	91503	10.77%	2.007%
9	13.636	1713	1719	1726	rBB	263146	387051	45.57%	8.490%
10	15.010	1947	1953	1961	rBB	92467	140301	16.52%	3.078%
11	16.344	2176	2180	2187	rBV2	9962	14592	1.72%	0.320%
12	16.491	2199	2205	2214	rBV	253955	379024	44.62%	8.314%
13	16.567	2214	2218	2228	rVB3	13190	20149	2.37%	0.442%
14	17.748	2413	2419	2424	rBV	116314	183442	21.60%	4.024%
15	17.795	2424	2427	2432	rVB	33784	45233	5.33%	0.992%
16	17.883	2435	2442	2448	rBV3	9455	15055	1.77%	0.330%
17	18.588	2558	2562	2565	rBV2	20415	26401	3.11%	0.579%
18	18.664	2571	2575	2581	rVB3	8715	12899	1.52%	0.283%
19	18.817	2594	2601	2604	rBV6	9048	18487	2.18%	0.406%
20	18.999	2627	2632	2639	rVB5	11285	16094	1.89%	0.353%
21	19.780	2759	2765	2770	rBV	78895	108333	12.75%	2.376%
22	19.927	2784	2790	2794	rBV2	9871	19171	2.26%	0.421%
23	20.098	2815	2819	2822	rBV3	17358	26966	3.17%	0.592%
24	20.139	2822	2826	2833	rVB	92512	133735	15.74%	2.934%
25	20.321	2851	2857	2862	rVB	649198	849381	100.00%	18.632%
26	20.462	2872	2881	2886	rBV9	11786	32777	3.86%	0.719%
27	20.626	2904	2909	2913	rVB	22086	37024	4.36%	0.812%
28	20.720	2921	2925	2930	rBV2	22185	35096	4.13%	0.770%
29	20.979	2966	2969	2975	rVB8	8233	14045	1.65%	0.308%
30	21.625	3074	3079	3090	rVB3	48861	100568	11.84%	2.206%
31	21.719	3092	3095	3099	rVB4	9644	13533	1.59%	0.297%
32	21.854	3114	3118	3121	rBV5	11549	17365	2.04%	0.381%
33	21.889	3122	3124	3128	rVV2	6565	9049	1.07%	0.198%
34	22.066	3145	3154	3159	rBV2	173099	390687	46.00%	8.570%
35	22.118	3159	3163	3167	rVB	38916	63426	7.47%	1.391%
36	22.212	3176	3179	3185	rVB7	11081	17767	2.09%	0.390%

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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-BG033023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.865	3284	3290	3295	rBV8	10262	23426	2.76%	0.514%
38	24.474	3555	3564	3566	rBV2	28554	71624	8.43%	1.571%
39	25.267	3692	3699	3705	rBV3	14665	41464	4.88%	0.910%
40	25.426	3719	3726	3738	rBV2	25829	76048	8.95%	1.668%
41	25.596	3745	3755	3766	rBV2	86902	273364	32.18%	5.996%
42	26.794	3955	3959	3967	rVB5	11669	28289	3.33%	0.621%

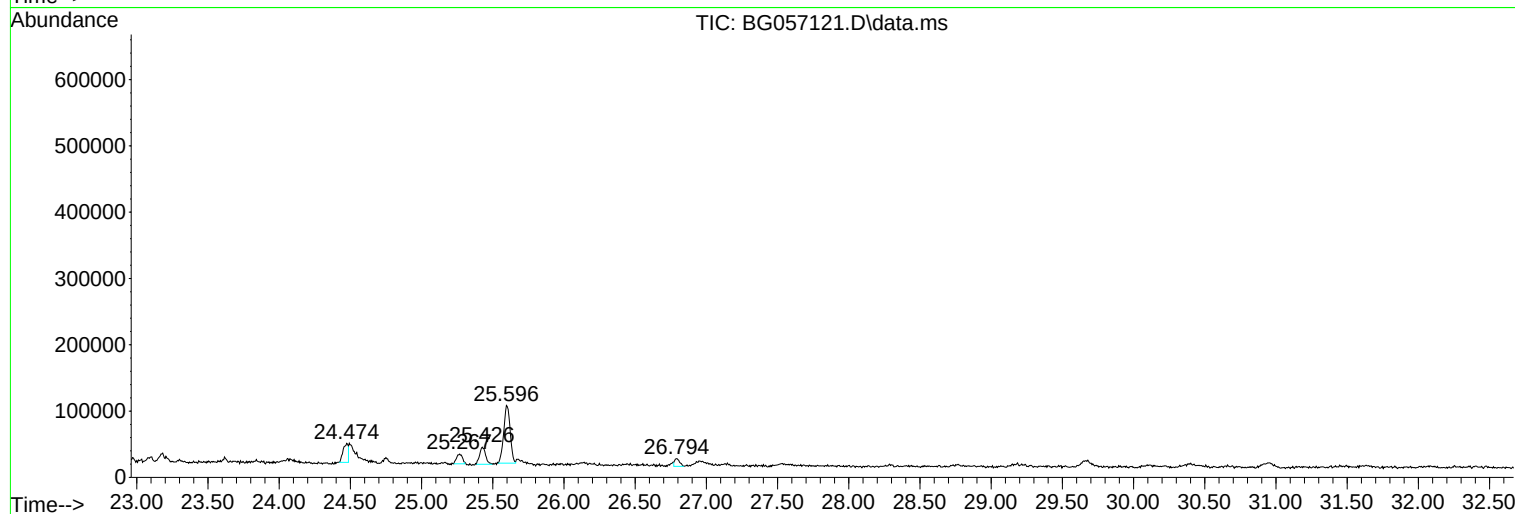
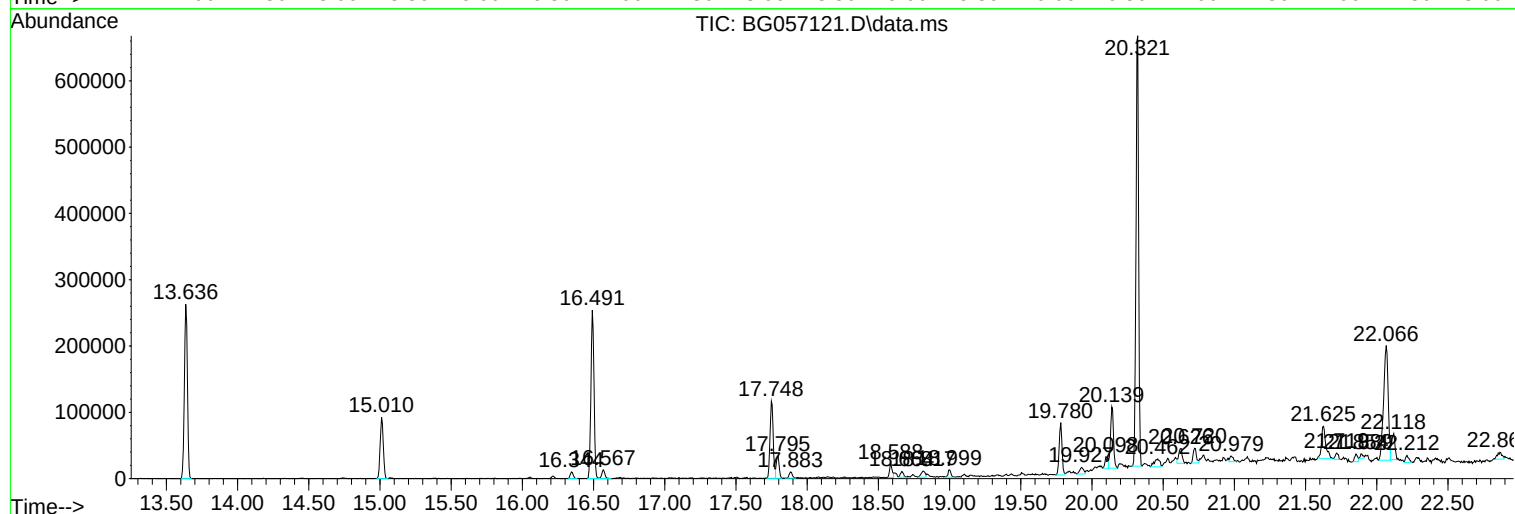
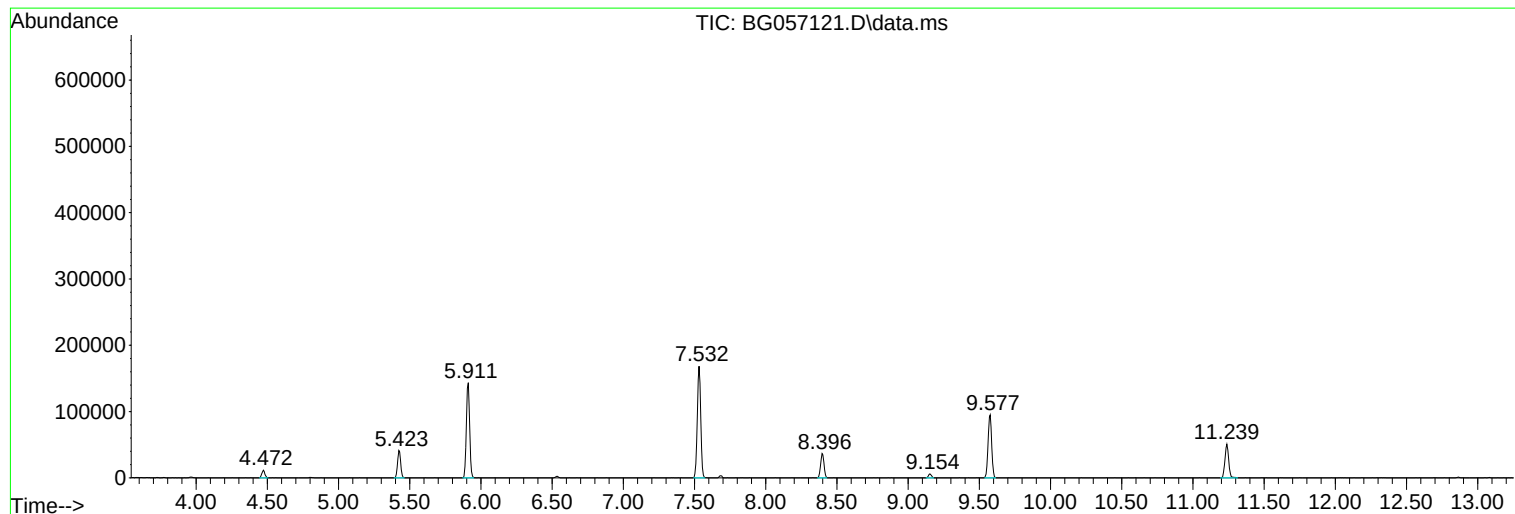
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : 02357-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P2-S2-230413

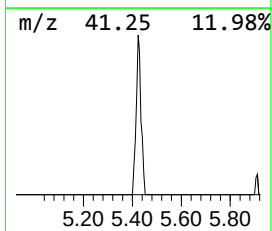
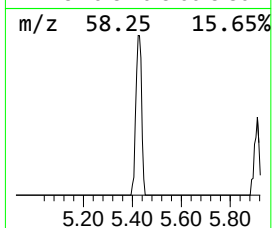
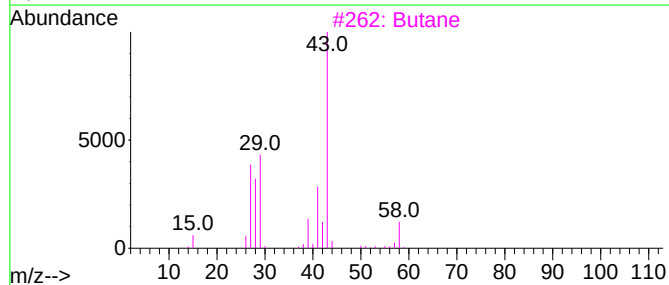
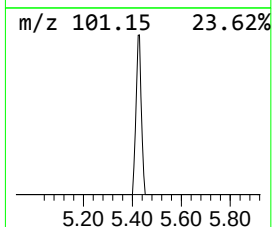
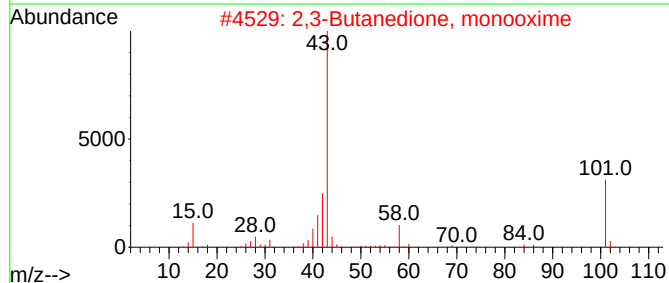
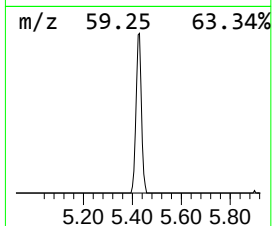
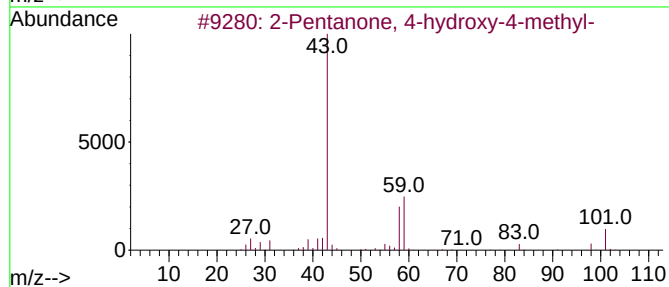
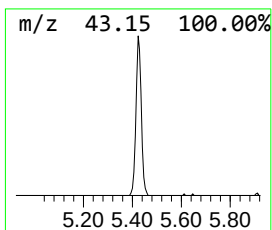
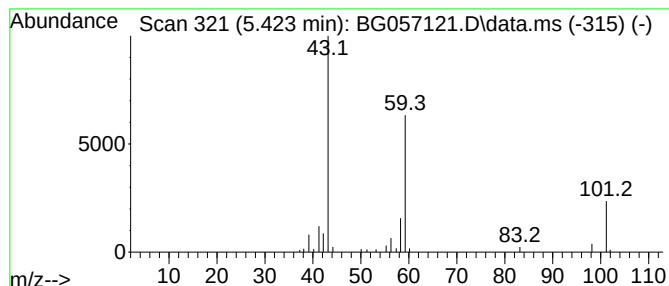
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.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.
5.423	21.05 ng	62529	1,4-Dichlorobenzene-d4	8.396

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Butane	58	C4H10	000106-97-8	10
4		Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	10
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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Misc :
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Instrument :
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ClientSampleId :
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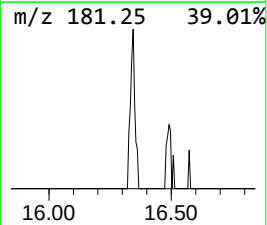
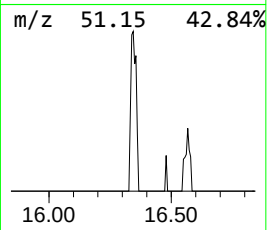
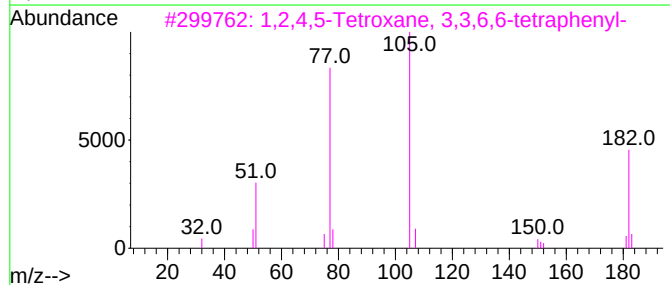
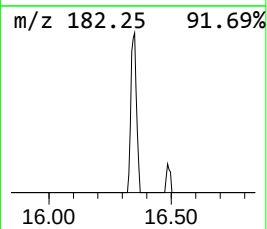
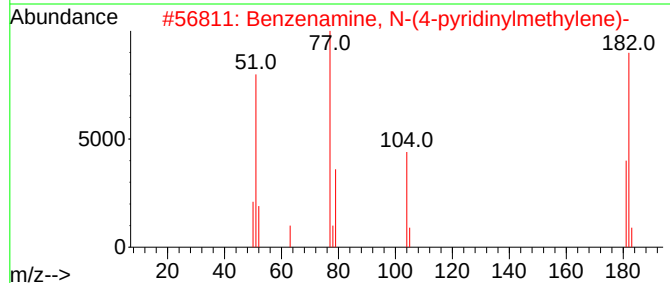
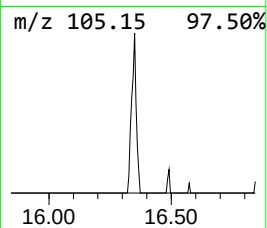
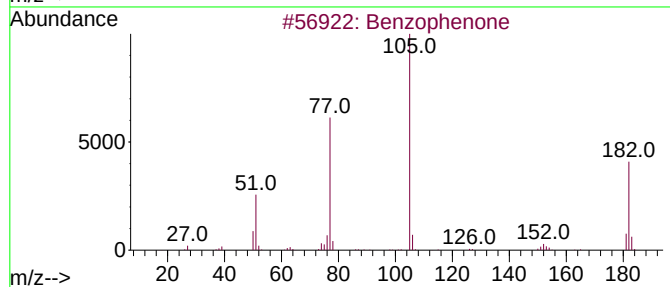
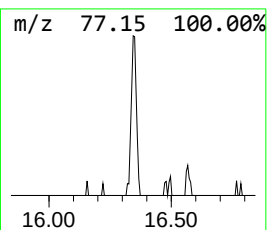
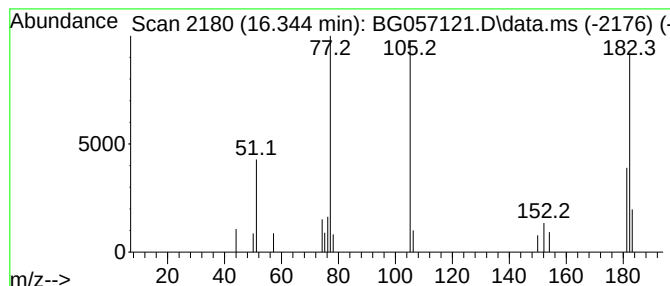
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.344	2.08 ng	14592	Acenaphthene-d10	15.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	59
2			Benzenamine, N-(4-pyridinylmethy...	182	C12H10N2	027768-46-3	50
3			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	47
4			4,4'-Dimethylbiphenyl	182	C14H14	000613-33-2	38
5			Benzhydrazide, N2-(2-methoxy-5-n...	299	C15H13N3O4	349572-84-5	38



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Misc :
ALS Vial : 12 Sample Multiplier: 1

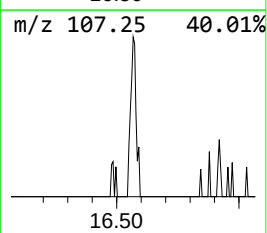
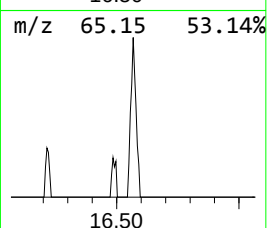
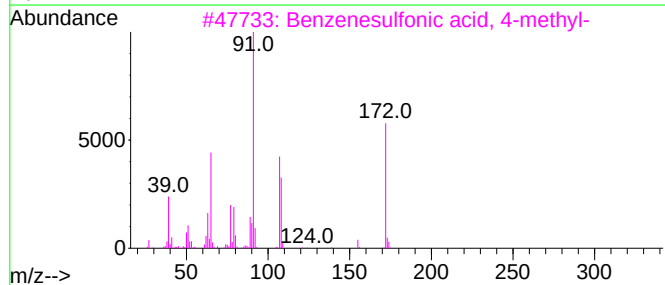
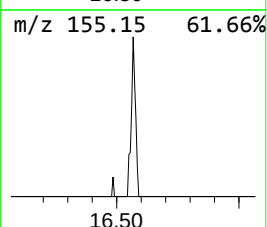
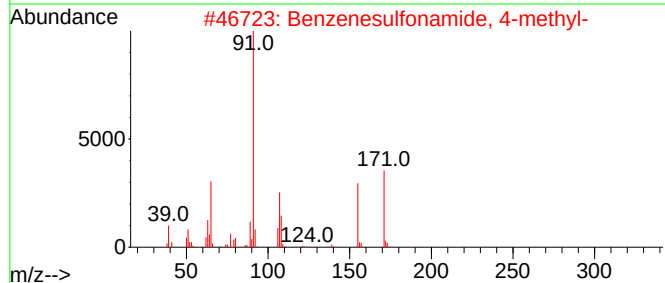
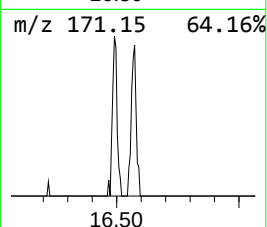
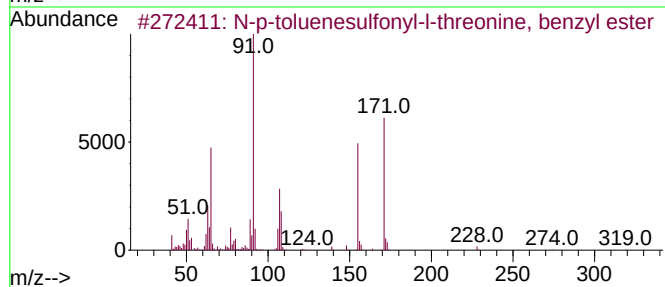
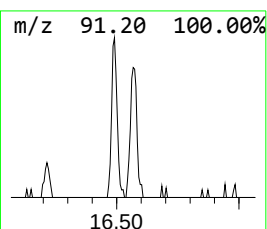
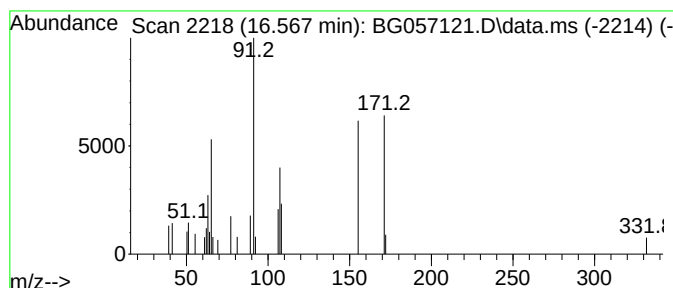
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 N-p-toluenesulfonyl-l-threo... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.567	2.20 ng	20149	Phenanthrene-d10		17.748	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	N-p-toluenesulfonyl-l-threonine,...		363	C18H21NO5S	1000130-34-4	91
2	Benzenesulfonamide, 4-methyl-		171	C7H9NO2S	000070-55-3	90
3	Benzenesulfonic acid, 4-methyl-		172	C7H8O3S	000104-15-4	62
4	2,4-Octadiyne		106	C8H10	002809-71-4	49
5	Benzene, 1-methyl-4-nitro-		137	C7H7NO2	000099-99-0	47



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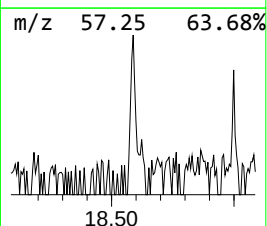
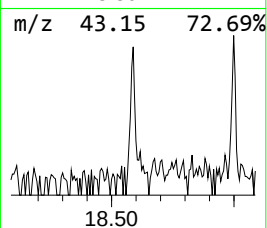
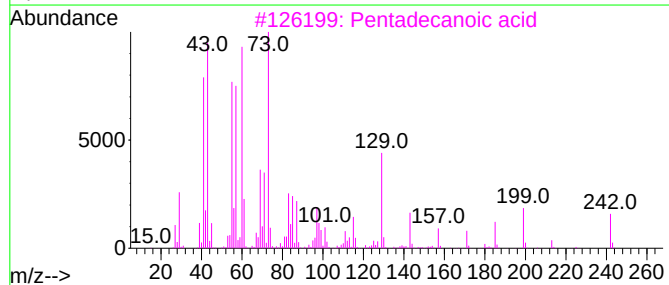
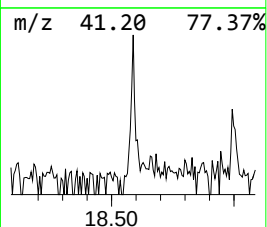
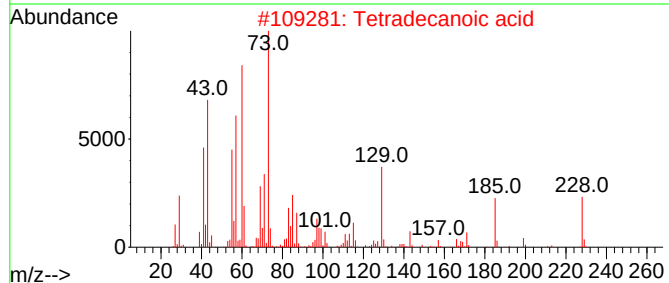
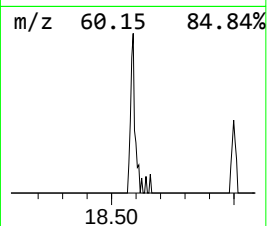
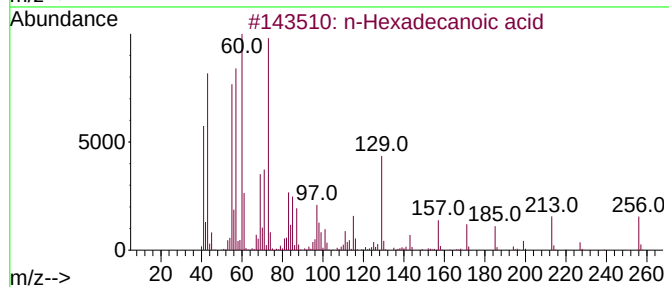
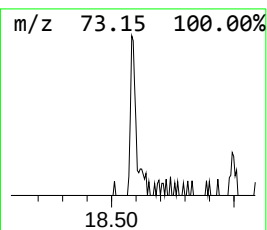
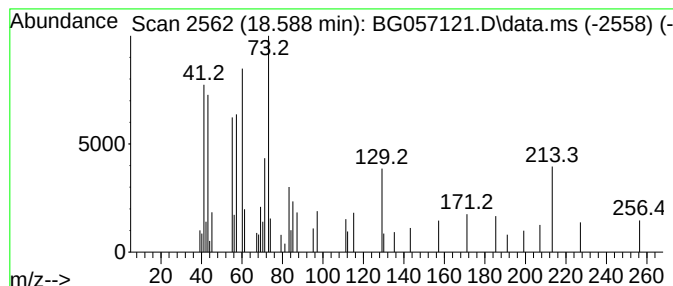
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.588	2.88 ng	26401	Phenanthrene-d10	17.748

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4			Tridecanoic acid	214	C13H26O2	000638-53-9	52
5			Dodecanoic acid	200	C12H24O2	000143-07-7	52



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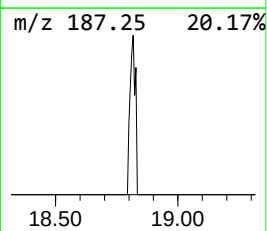
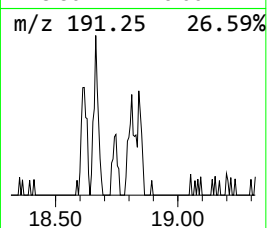
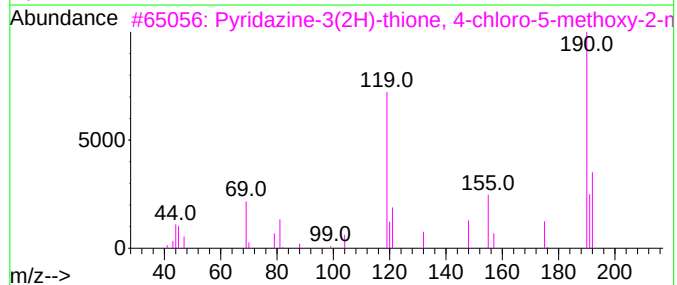
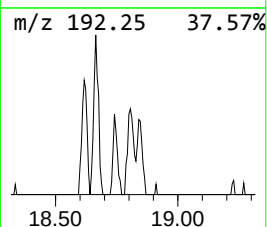
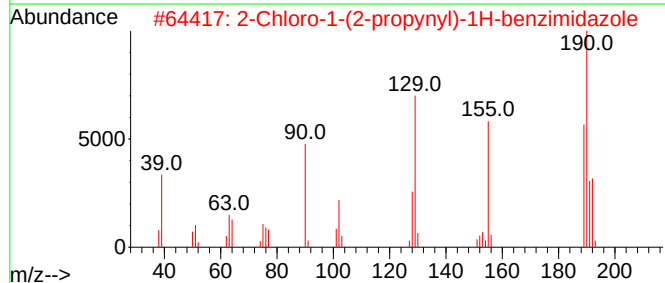
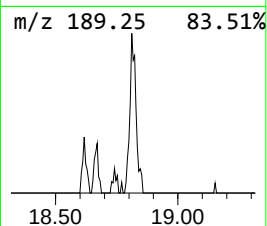
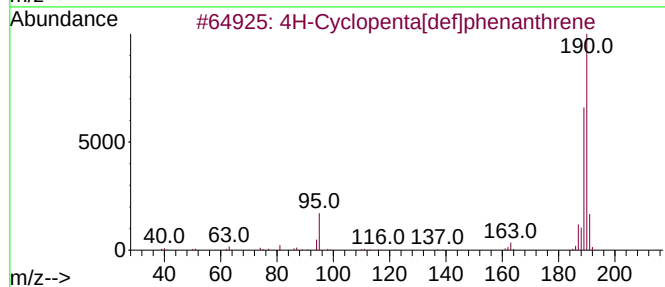
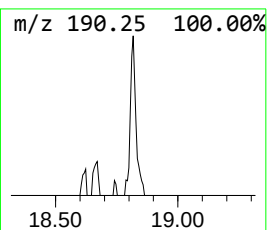
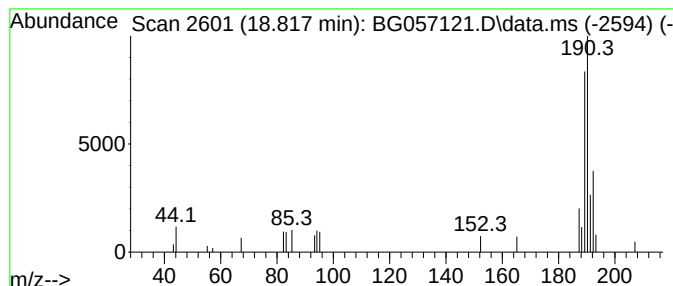
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.817	2.02 ng	18487	Phenanthrene-d10	17.748

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2			2-Chloro-1-(2-propynyl)-1H-benzi...	190	C10H7ClN2	080276-19-3	47
3			Pyridazine-3(2H)-thione, 4-chlor...	190	C6H7ClN2OS	072038-53-0	35
4			1,1'-Biphenyl, 4,4'-difluoro-	190	C12H8F2	000398-23-2	32
5			2,2'-Difluorobiphenyl	190	C12H8F2	000388-82-9	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041723\
Data File : BG057121.D
Acq On : 17 Apr 2023 21:54
Operator : CG/JU
Sample : 02357-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P2-S2-230413

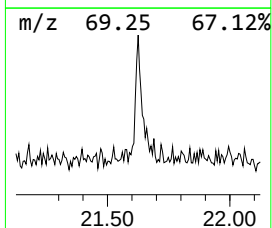
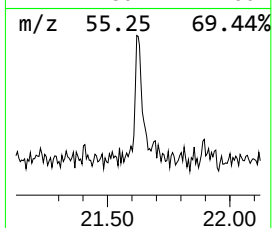
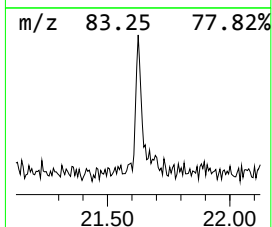
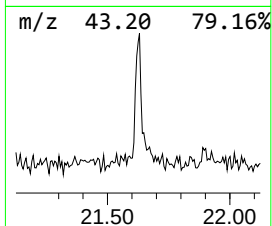
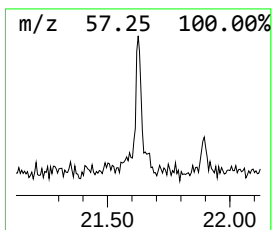
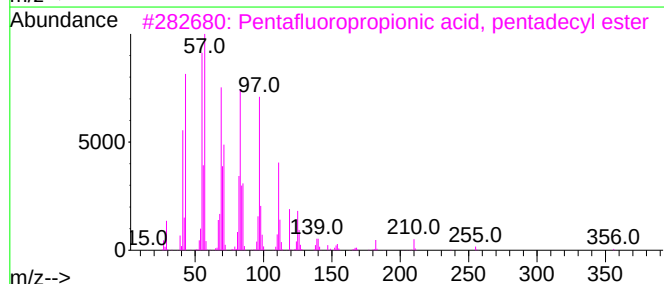
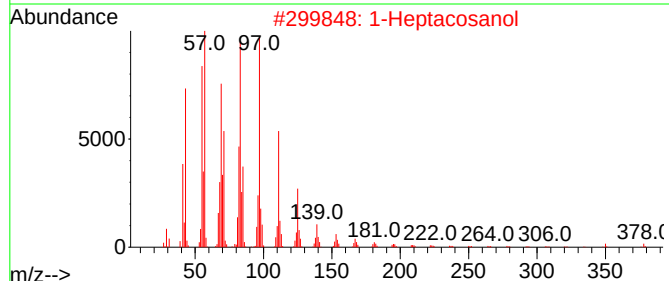
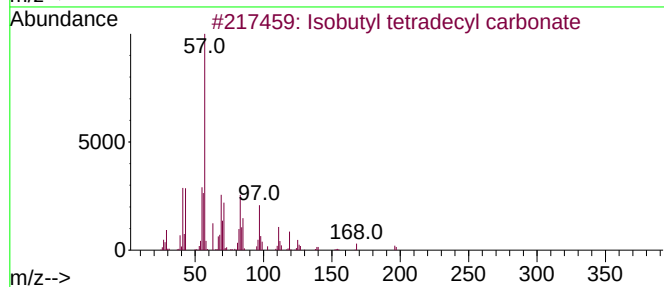
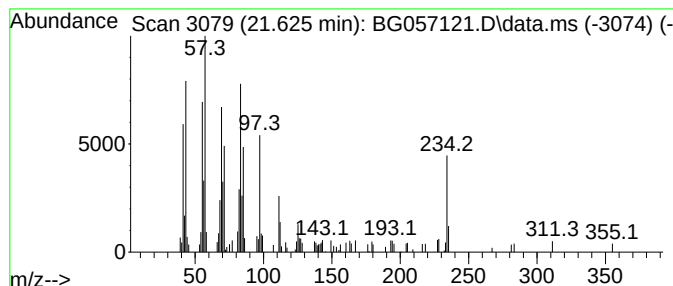
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Isobutyl tetradecyl carbonate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.625	5.15 ng	100568	Chrysene-d12	22.066

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	74
2		1-Heptacosanol	396	C27H56O	002004-39-9	70
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	62
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	62
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041723\
Data File : BG057121.D
Acq On : 17 Apr 2023 21:54
Operator : CG/JU
Sample : 02357-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P2-S2-230413

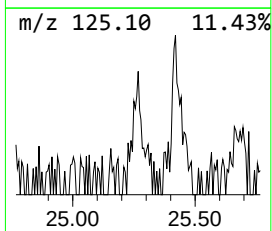
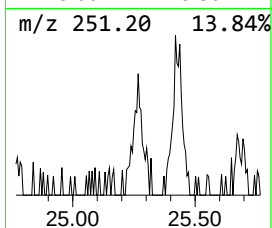
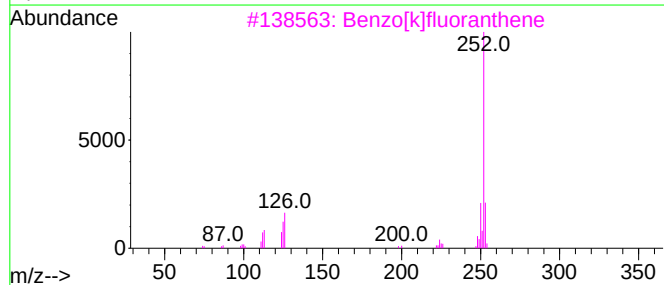
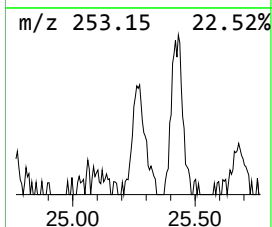
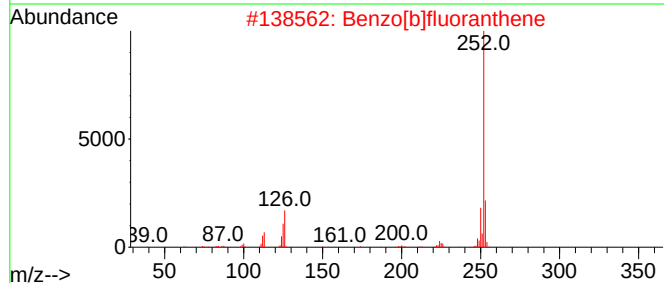
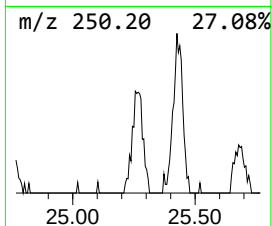
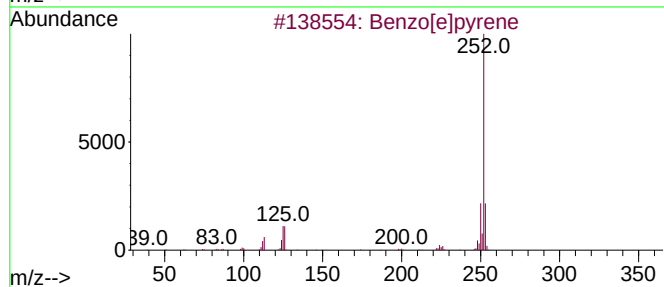
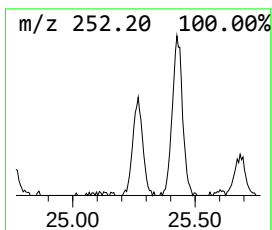
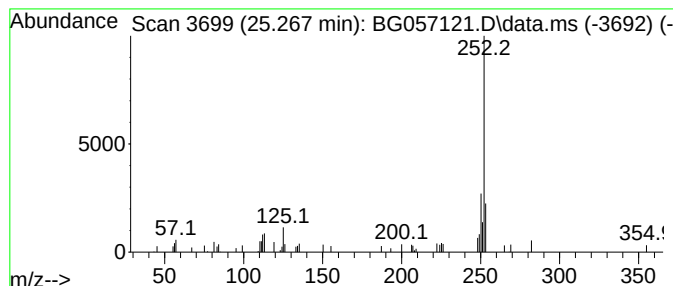
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.267	3.03 ng	41464	Perylene-d12	25.596

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	81
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	74
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	74
4			Benzo[a]pyrene	252	C20H12	000050-32-8	72
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041723\
Data File : BG057121.D
Acq On : 17 Apr 2023 21:54
Operator : CG/JU
Sample : 02357-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P2-S2-230413

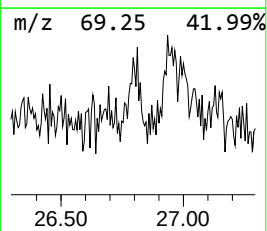
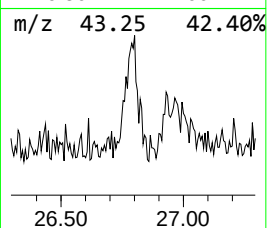
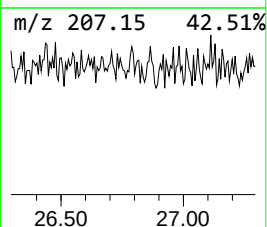
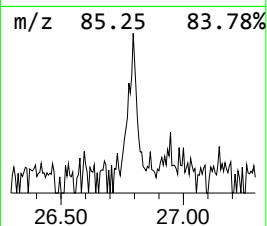
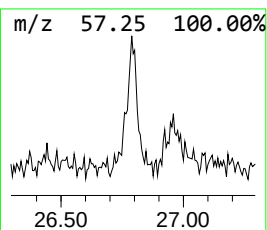
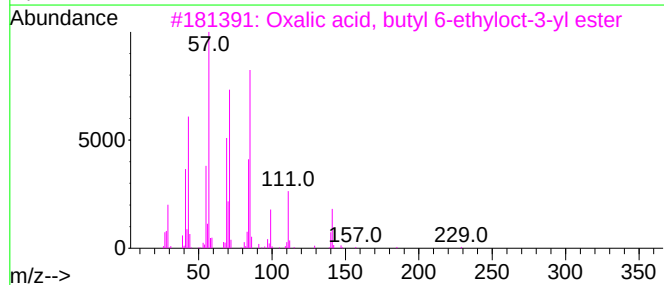
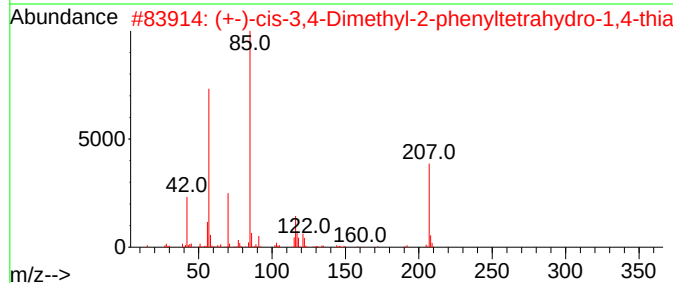
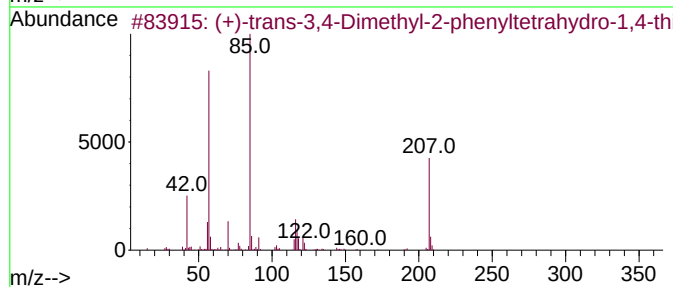
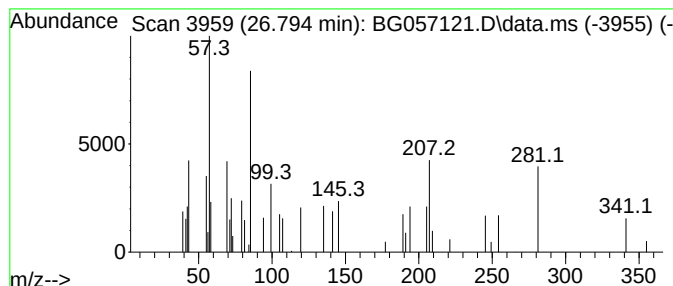
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown26.794 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.794	2.07 ng	28289	Perylene-d12	25.596

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-trans-3,4-Dimethyl-2-phenylt...	207	C12H17NS	1000244-64-9	35		
2	(+)-cis-3,4-Dimethyl-2-phenylt...	207	C12H17NS	092772-63-9	35		
3	Oxalic acid, butyl 6-ethyloct-3-...	286	C16H30O4	1000309-34-2	10		
4	Phendimetrazine	191	C12H17NO	000634-03-7	9		
5	N',N'-Dimethyl-N-[2,2,3,3-tetrac...	336	C17H16N6O2	1000326-98-2	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041723\
Data File : BG057121.D
Acq On : 17 Apr 2023 21:54
Operator : CG/JU
Sample : 02357-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P2-S2-230413

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.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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Benzophenone	16.344	2.1	ng	14592	3	15.010	140301	20.0
N-p-toluenesulf...	16.567	2.2	ng	20149	4	17.748	183442	20.0
n-Hexadecanoic ...	18.588	2.9	ng	26401	4	17.748	183442	20.0
4H-Cyclopenta[d...	18.817	2.0	ng	18487	4	17.748	183442	20.0
Isobutyl tetrad...	21.625	5.2	ng	100568	5	22.066	390687	20.0
Benzo[e]pyrene	25.267	3.0	ng	41464	6	25.596	273364	20.0
unknown26.794	26.794	2.1	ng	28289	6	25.596	273364	20.0