

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053023\
 Data File : BG057613.D
 Acq On : 30 May 2023 19:33
 Operator : CG/JU
 Sample : 02953-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PNNL-RH-524-1

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-BG052723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057613.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.371	306	312	320	rBV	32825	50389	3.32%	0.564%
2	5.859	388	395	408	rBV	318035	538860	35.49%	6.035%
3	7.486	664	672	691	rBV	347191	618148	40.71%	6.923%
4	8.338	811	817	825	rBV	87842	147120	9.69%	1.648%
5	9.519	1011	1018	1029	rBV	210134	380332	25.05%	4.259%
6	11.175	1293	1300	1307	rBV	122765	216930	14.29%	2.429%
7	13.578	1702	1709	1719	rBV	663553	986803	64.99%	11.051%
8	14.952	1933	1943	1950	rBV	202869	323940	21.34%	3.628%
9	16.292	2165	2171	2178	rVB2	30868	44186	2.91%	0.495%
10	16.439	2190	2196	2209	rBV	491309	762233	50.20%	8.536%
11	17.690	2401	2409	2414	rBV	257977	425404	28.02%	4.764%
12	17.737	2414	2417	2424	rVB	110026	154871	10.20%	1.734%
13	17.825	2427	2432	2439	rBV	24850	39734	2.62%	0.445%
14	18.530	2548	2552	2556	rBV3	31393	55943	3.68%	0.626%
15	18.606	2562	2565	2571	rVB	28882	39923	2.63%	0.447%
16	18.694	2575	2580	2583	rBV3	9836	16612	1.09%	0.186%
17	18.759	2583	2591	2595	rVV2	27401	59300	3.91%	0.664%
18	18.788	2595	2596	2603	rVB4	15167	17470	1.15%	0.196%
19	19.047	2635	2640	2645	rBV	16803	25503	1.68%	0.286%
20	19.100	2645	2649	2653	rVB5	10056	15366	1.01%	0.172%
21	19.458	2706	2710	2714	rVB	10703	15469	1.02%	0.173%
22	19.611	2734	2736	2742	rVB3	11887	16382	1.08%	0.183%
23	19.728	2749	2756	2761	rBV	252793	362806	23.90%	4.063%
24	20.051	2805	2811	2813	rBV3	41689	70847	4.67%	0.793%
25	20.087	2813	2817	2823	rVV	238243	336245	22.15%	3.766%
26	20.151	2824	2828	2832	rVB	14754	24494	1.61%	0.274%
27	20.263	2841	2847	2852	rBV	1163618	1518287	100.00%	17.003%
28	20.404	2866	2871	2876	rVB4	16730	36395	2.40%	0.408%
29	20.568	2889	2899	2906	rVB	34292	83445	5.50%	0.934%
30	20.662	2912	2915	2919	rBV	26511	41721	2.75%	0.467%
31	20.868	2948	2950	2953	rBV	16888	16439	1.08%	0.184%
32	20.915	2956	2958	2965	rVB	17009	26560	1.75%	0.297%
33	21.355	3031	3033	3038	rVB3	20829	27627	1.82%	0.309%
34	21.555	3063	3067	3071	rBV3	38789	65592	4.32%	0.735%
35	21.655	3080	3084	3090	rBV3	16081	28989	1.91%	0.325%
36	21.996	3133	3142	3147	rBV2	255861	630451	41.52%	7.060%

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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-BG052723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.043	3147	3150	3157	rVB	91387	144232	9.50%	1.615%
38	22.207	3175	3178	3185	rVB2	19575	36802	2.42%	0.412%
39	24.369	3540	3546	3554	rBV	66375	190812	12.57%	2.137%
40	25.479	3730	3735	3746	rVB2	122292	336801	22.18%	3.772%

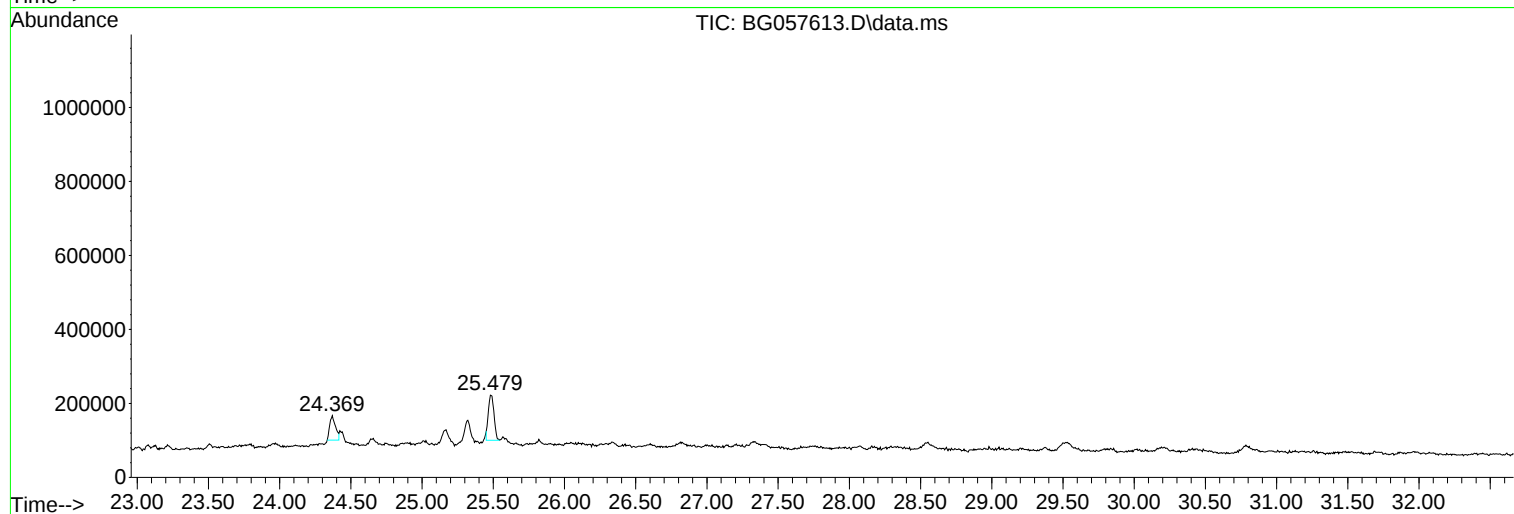
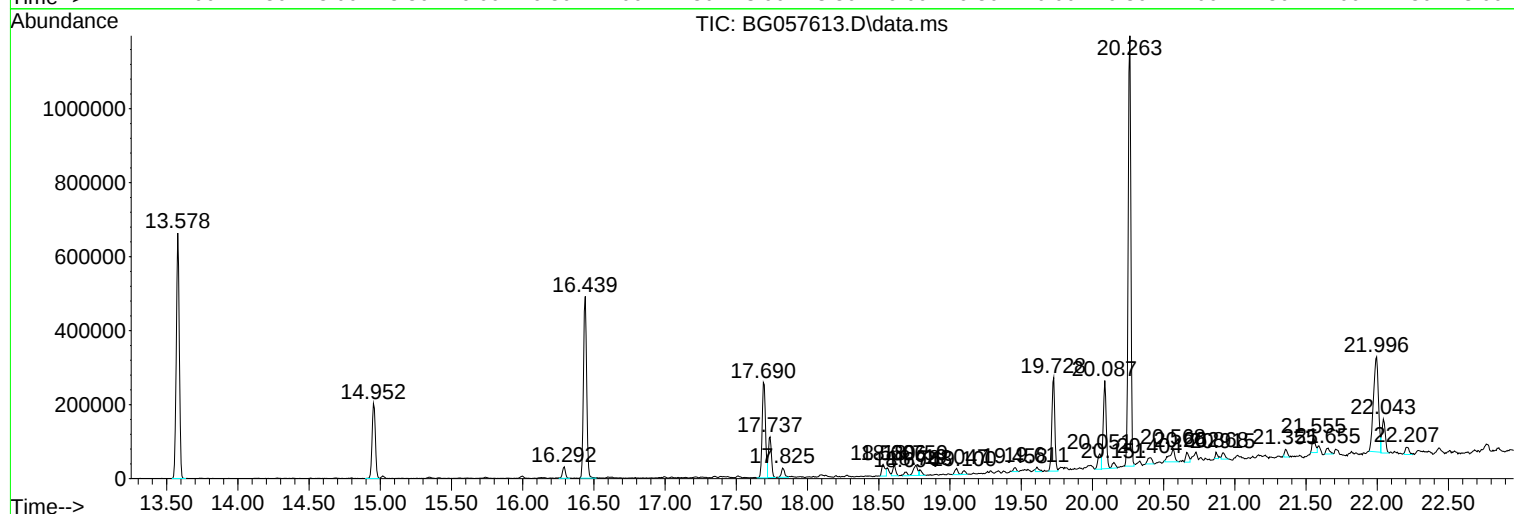
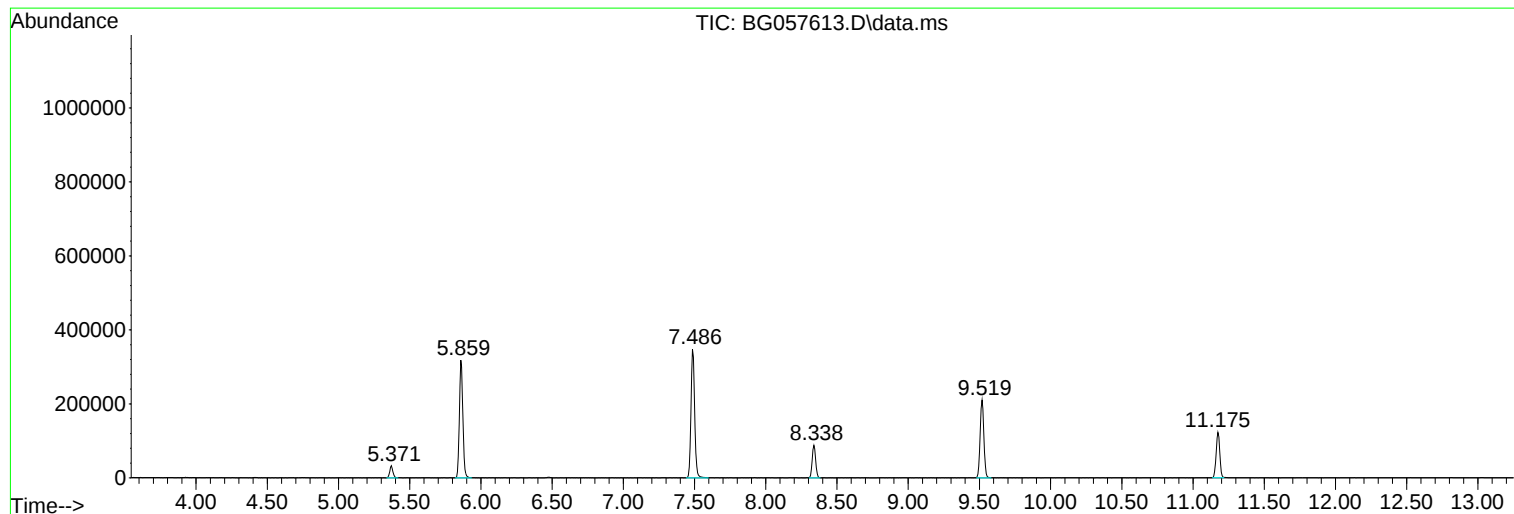
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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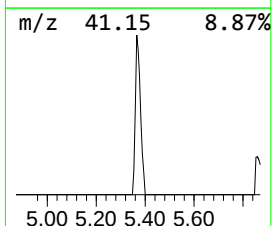
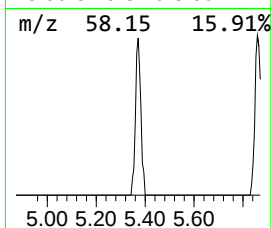
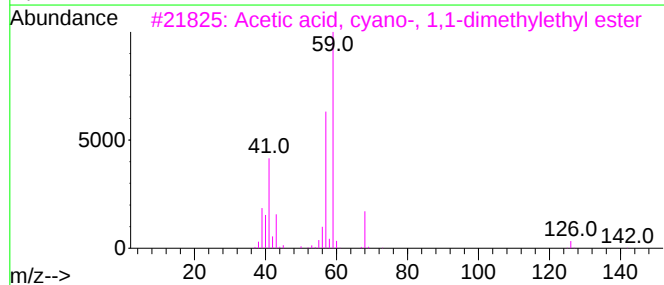
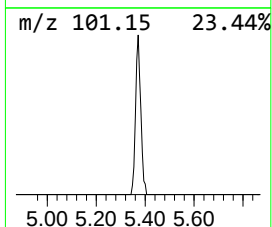
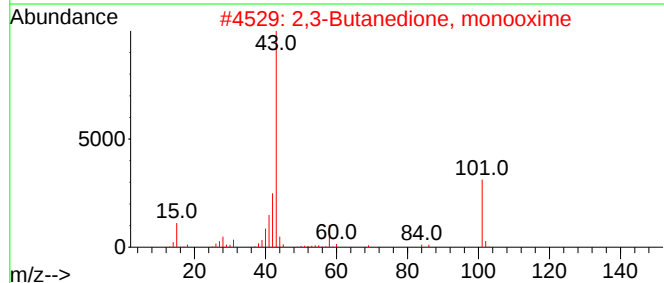
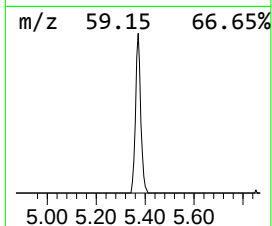
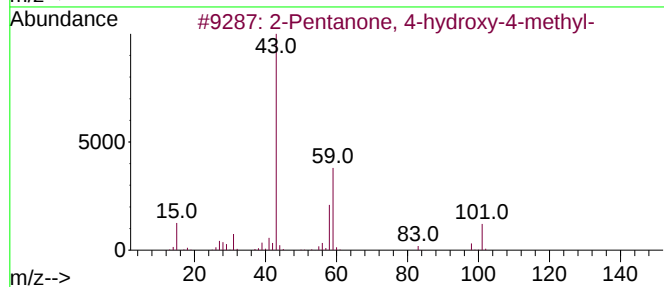
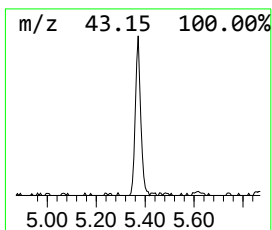
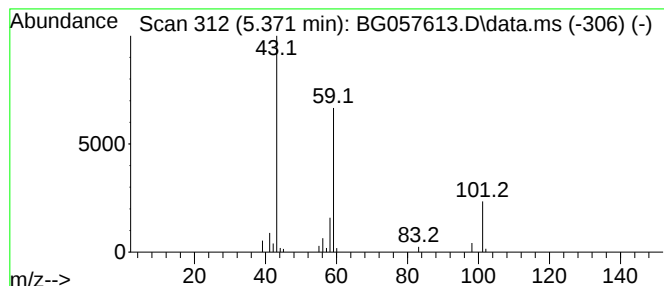
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.371	6.85 ng	50389	1,4-Dichlorobenzene-d4	8.338

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Guanidine	59	CH5N3	000113-00-8	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PNNL-RH-524-1

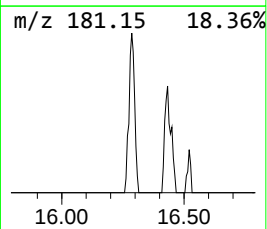
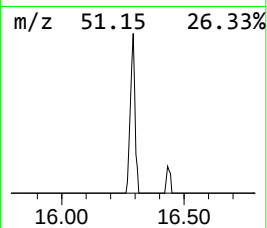
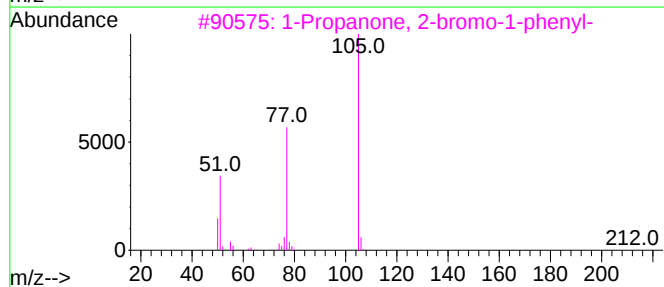
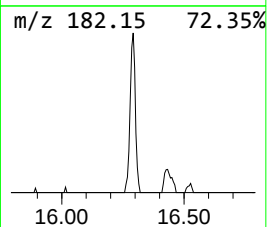
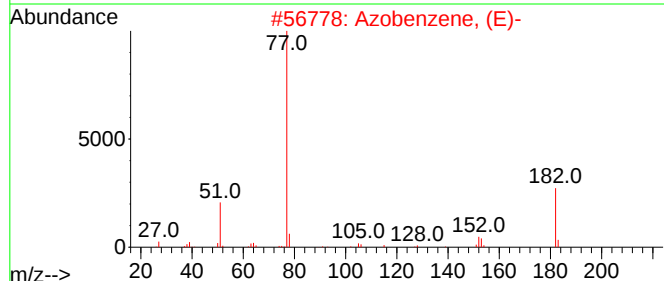
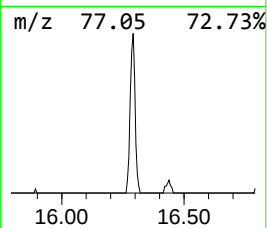
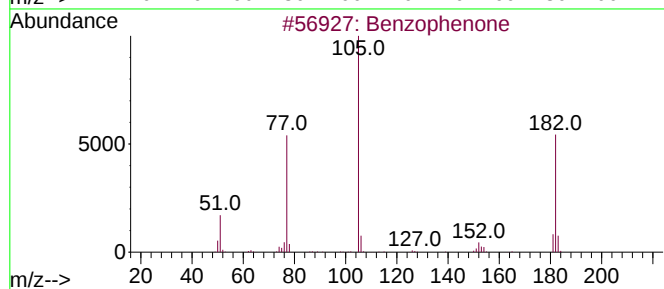
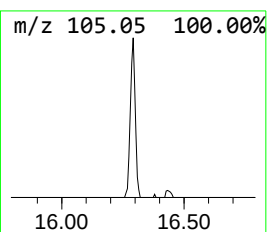
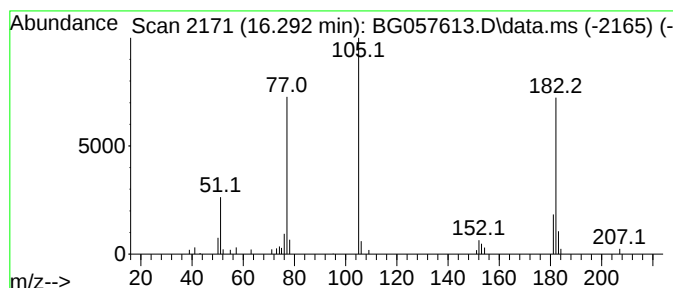
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.292	2.73 ng	44186	Acenaphthene-d10	14.952

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			Azobenzene, (E)-	182	C12H10N2	017082-12-1	53
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	43
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	38
5			2,3-Dihydro-1-oxo-1H-phenalene	182	C13H10O	000518-85-4	38



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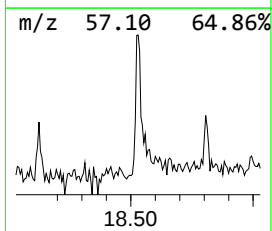
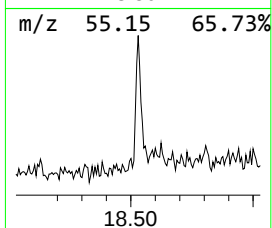
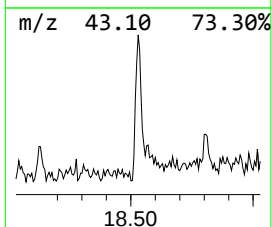
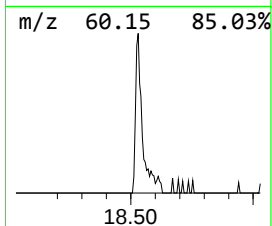
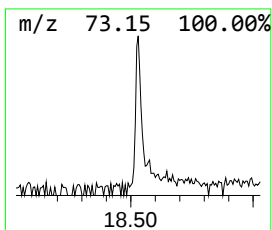
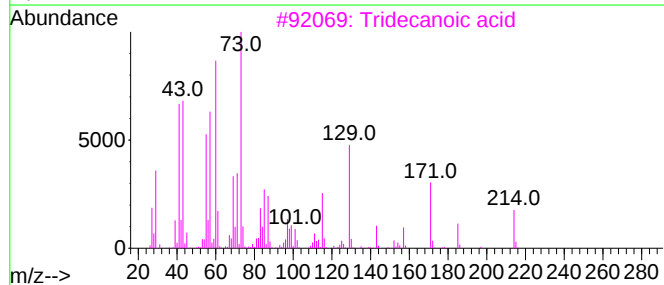
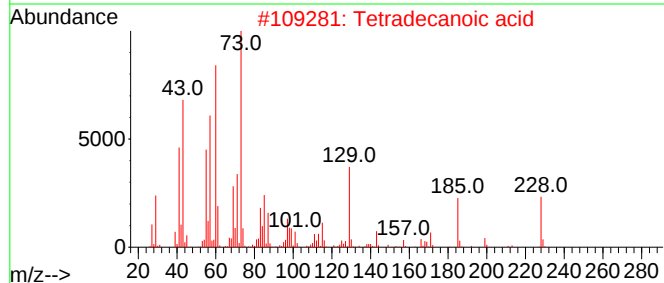
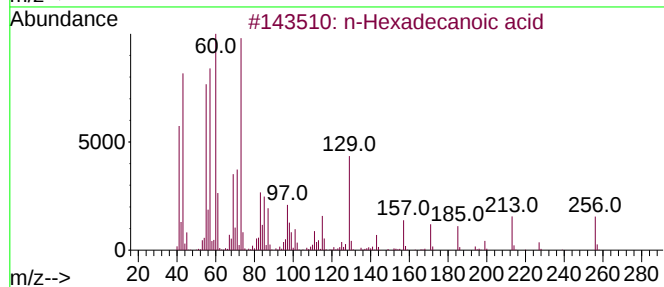
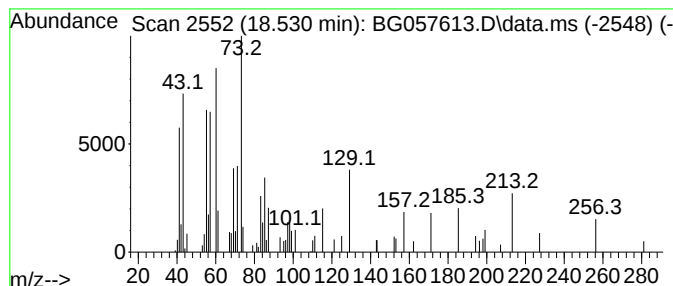
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.530	2.63 ng	55943	Phenanthrene-d10	17.690

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3			Tridecanoic acid	214	C13H26O2	000638-53-9	80
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53



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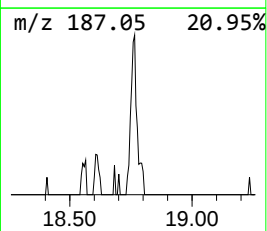
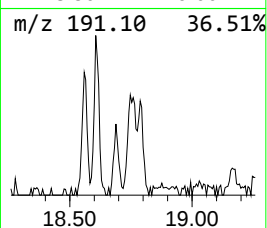
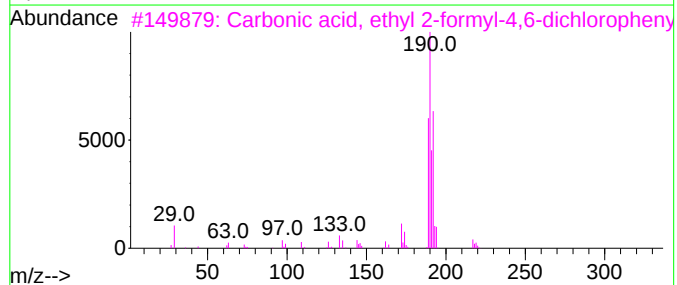
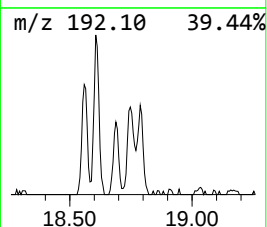
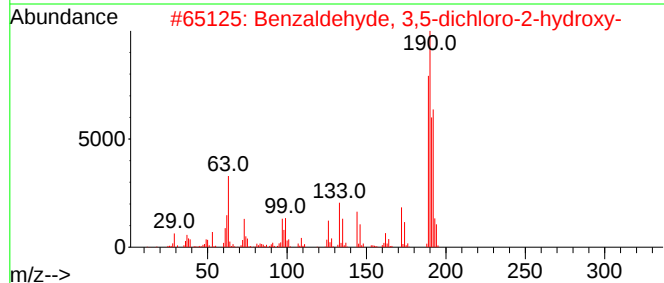
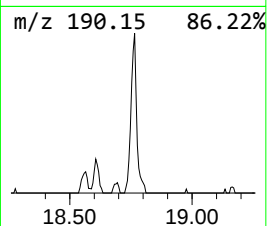
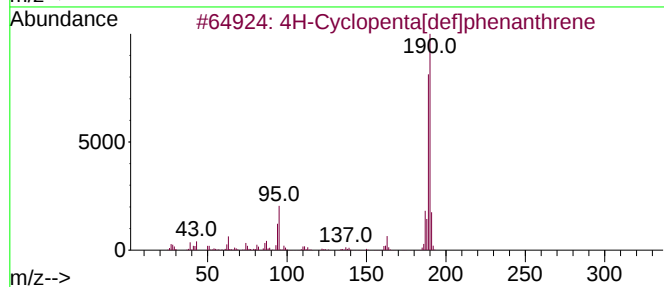
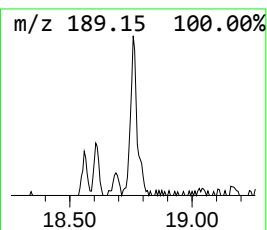
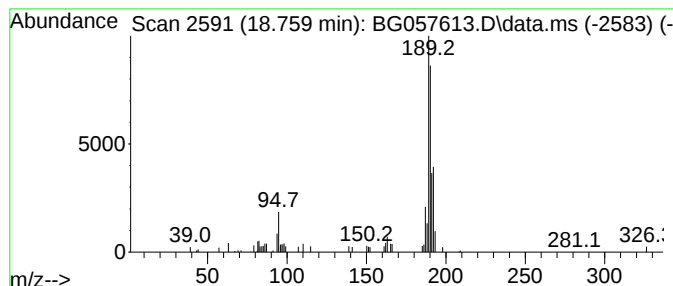
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.759	2.79 ng	59300	Phenanthrene-d10	17.690

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2			Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	52
3			Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	47
4			3-(Trifluoromethoxy)benzaldehyde	190	C8H5F3O2	052771-21-8	38
5			Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	38



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PNNL-RH-524-1

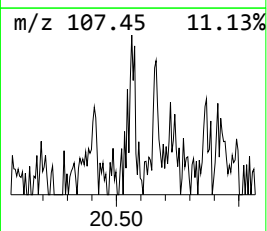
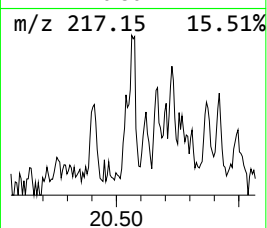
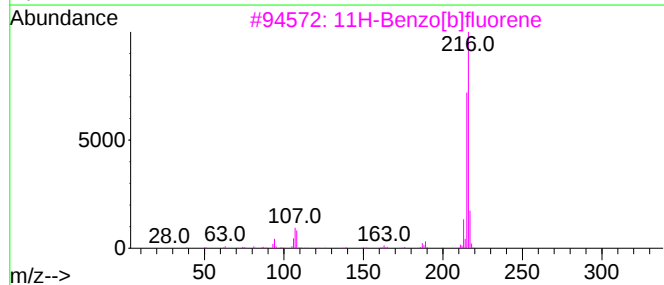
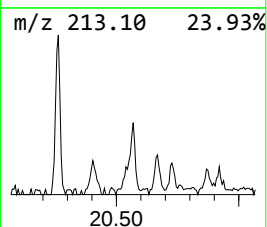
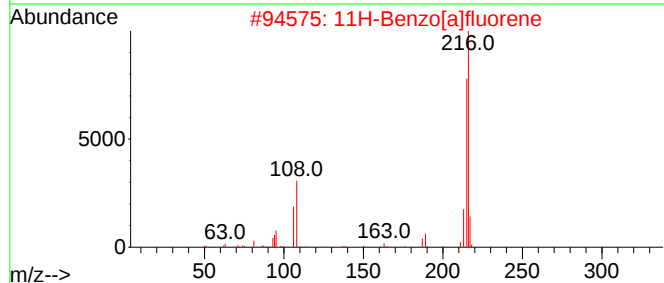
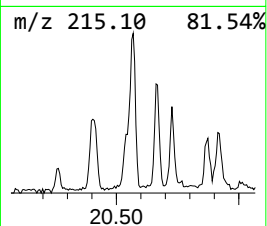
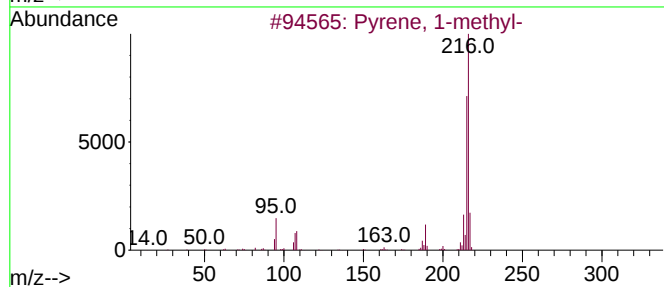
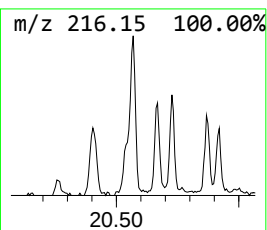
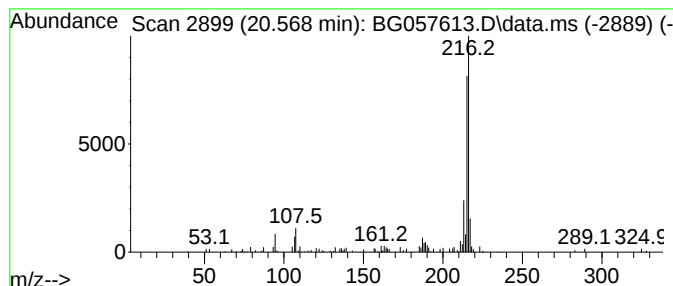
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pyrene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.568	2.65 ng	83445	Chrysene-d12	21.996

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
4			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	83
5			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053023\
Data File : BG057613.D
Acq On : 30 May 2023 19:33
Operator : CG/JU
Sample : 02953-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PNNL-RH-524-1

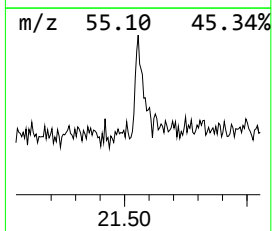
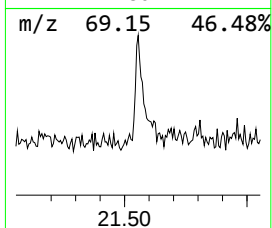
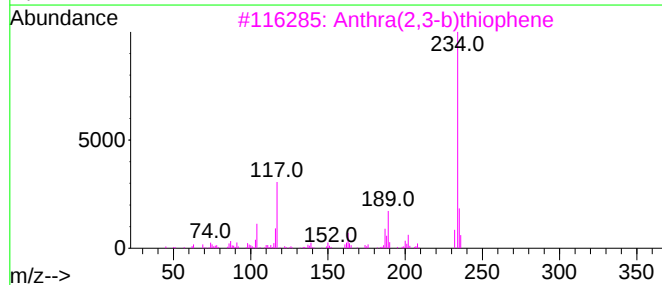
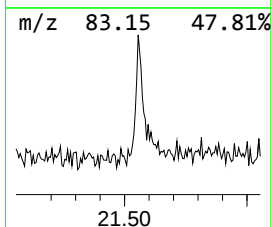
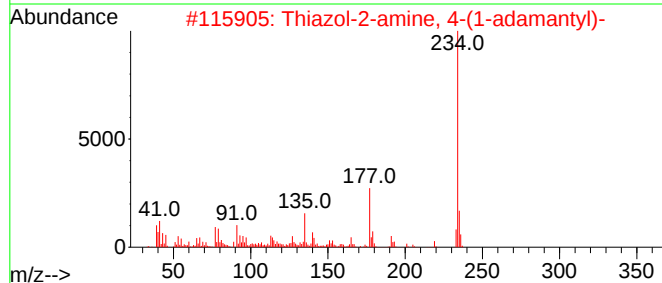
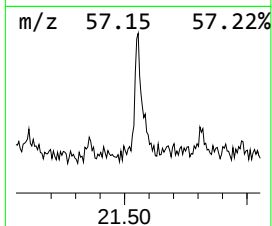
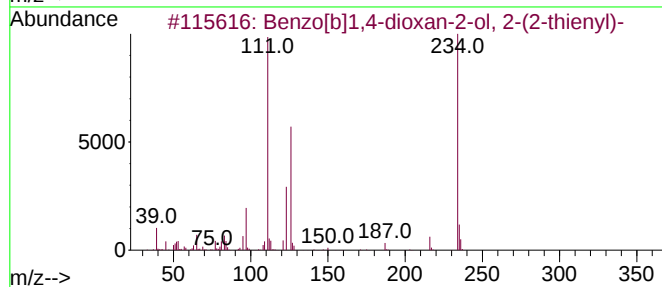
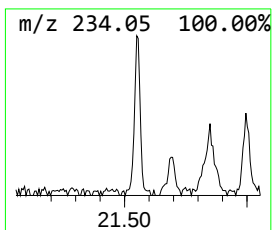
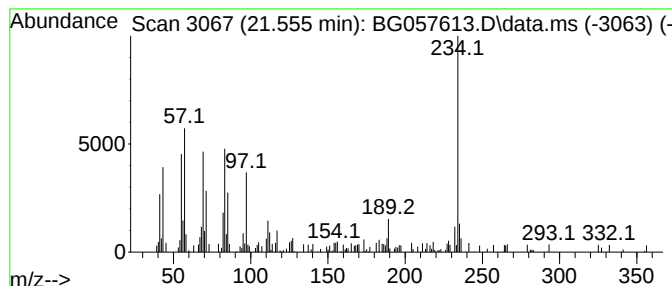
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[b]1,4-dioxan-2-ol, 2-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.555	2.08 ng	65592	Chrysene-d12	21.996

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]1,4-dioxan-2-ol, 2-(2-th...	234	C12H10O3S	312614-85-0	50
2			Thiazol-2-amine, 4-(1-adamantyl)-	234	C13H18N2S	019735-74-1	43
3			Anthra(2,3-b)thiophene	234	C16H10S	022108-55-0	43
4			[1,1'-Biphenyl]-4-sulfonic acid	234	C12H10O3S	002113-68-0	38
5			1-Nonadecene	266	C19H38	018435-45-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053023\
Data File : BG057613.D
Acq On : 30 May 2023 19:33
Operator : CG/JU
Sample : 02953-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PNNL-RH-524-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.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
2-Pentanone, 4-...	5.371	6.8	ng	50389	1	8.338	147120	20.0
Benzophenone	16.292	2.7	ng	44186	3	14.952	323940	20.0
n-Hexadecanoic ...	18.530	2.6	ng	55943	4	17.690	425404	20.0
4H-Cyclopenta[d...]	18.759	2.8	ng	59300	4	17.690	425404	20.0
Pyrene, 1-methyl-	20.568	2.6	ng	83445	5	21.996	630451	20.0
Benzo[b]1,4-dio...	21.555	2.1	ng	65592	5	21.996	630451	20.0