

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011123\
 Data File : BG056260.D
 Acq On : 11 Jan 2023 21:27
 Operator : CG/JU
 Sample : 01064-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S4-01

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056260.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.330	3	7	13	rBV	131435	186782	7.81%	1.476%
2	5.351	343	351	360	rBV	106877	169764	7.10%	1.342%
3	5.833	424	433	444	rVB	433003	704908	29.47%	5.571%
4	7.449	700	708	720	rBV	455320	778419	32.54%	6.152%
5	8.313	848	855	864	rVB	118365	203469	8.51%	1.608%
6	9.488	1046	1055	1063	rBB	255596	457038	19.11%	3.612%
7	11.144	1328	1337	1345	rBV	158832	285095	11.92%	2.253%
8	13.553	1739	1747	1757	rBV	967795	1446711	60.48%	11.434%
9	14.928	1971	1981	1988	rBV	310083	487975	20.40%	3.857%
10	16.262	2202	2208	2215	rVB	87395	122182	5.11%	0.966%
11	16.403	2225	2232	2240	rBV	760111	1141928	47.74%	9.025%
12	17.660	2440	2446	2451	rBV	458063	676132	28.26%	5.344%
13	17.701	2451	2453	2459	rVB	65547	86064	3.60%	0.680%
14	18.506	2585	2590	2593	rBV2	66335	105251	4.40%	0.832%
15	18.577	2598	2602	2609	rVB	48632	72492	3.03%	0.573%
16	18.718	2619	2626	2630	rBV3	36851	66439	2.78%	0.525%
17	18.759	2630	2633	2638	rVB2	25450	34861	1.46%	0.276%
18	19.012	2673	2676	2680	rBV3	21072	29383	1.23%	0.232%
19	19.065	2680	2685	2694	rVB4	12296	29324	1.23%	0.232%
20	19.306	2722	2726	2729	rBV	22095	25580	1.07%	0.202%
21	19.429	2742	2747	2751	rBV2	44154	69657	2.91%	0.551%
22	19.482	2751	2756	2760	rBV3	15796	27902	1.17%	0.221%
23	19.564	2766	2770	2776	rBV3	15054	31860	1.33%	0.252%
24	19.693	2786	2792	2797	rVB	89402	127763	5.34%	1.010%
25	19.764	2797	2804	2806	rBV7	18131	36443	1.52%	0.288%
26	20.052	2844	2853	2860	rVB	155250	241691	10.10%	1.910%
27	20.122	2860	2865	2871	rBV4	20985	41704	1.74%	0.330%
28	20.234	2879	2884	2890	rBV	1800480	2392169	100.00%	18.906%
29	20.381	2901	2909	2915	rVB3	23056	55610	2.32%	0.440%
30	20.522	2926	2933	2934	rBV7	19588	36319	1.52%	0.287%
31	20.639	2947	2953	2957	rVB4	16150	25574	1.07%	0.202%
32	20.692	2957	2962	2967	rBV	35868	60709	2.54%	0.480%
33	20.839	2983	2987	2991	rBV	34146	50597	2.12%	0.400%
34	20.880	2991	2994	2998	rVV	21216	28563	1.19%	0.226%
35	21.315	3063	3068	3075	rVB3	20730	39449	1.65%	0.312%
36	21.538	3099	3106	3114	rVB6	66909	133979	5.60%	1.059%

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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-BG122722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.955	3168	3177	3183	rBV2	454202	891999	37.29%	7.050%
38	22.002	3183	3185	3192	rVB	54281	72821	3.04%	0.576%
39	22.114	3198	3204	3210	rBV7	16971	37005	1.55%	0.292%
40	22.725	3298	3308	3314	rBV2	21718	61158	2.56%	0.483%
41	23.712	3471	3476	3484	rVB7	23777	52944	2.21%	0.418%
42	24.294	3570	3575	3583	rBV4	18855	55478	2.32%	0.438%
43	25.063	3701	3706	3717	rVB2	26266	81131	3.39%	0.641%
44	25.228	3726	3734	3742	rVB2	30385	91670	3.83%	0.725%
45	25.392	3751	3762	3773	rBV	256854	798838	33.39%	6.314%

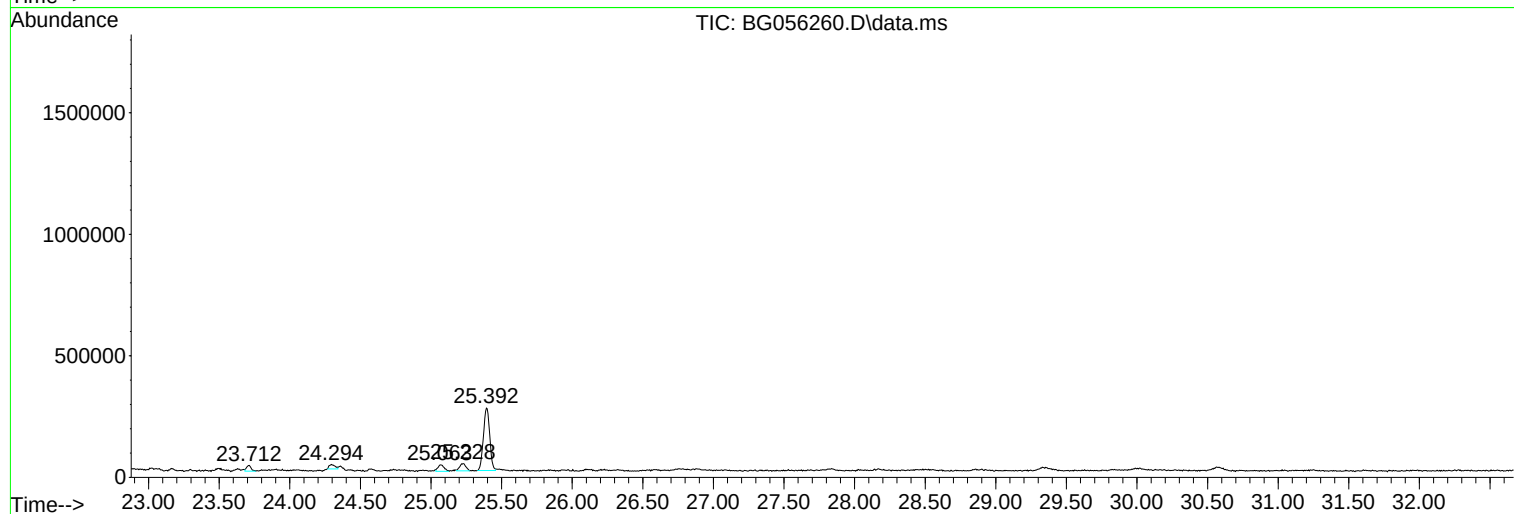
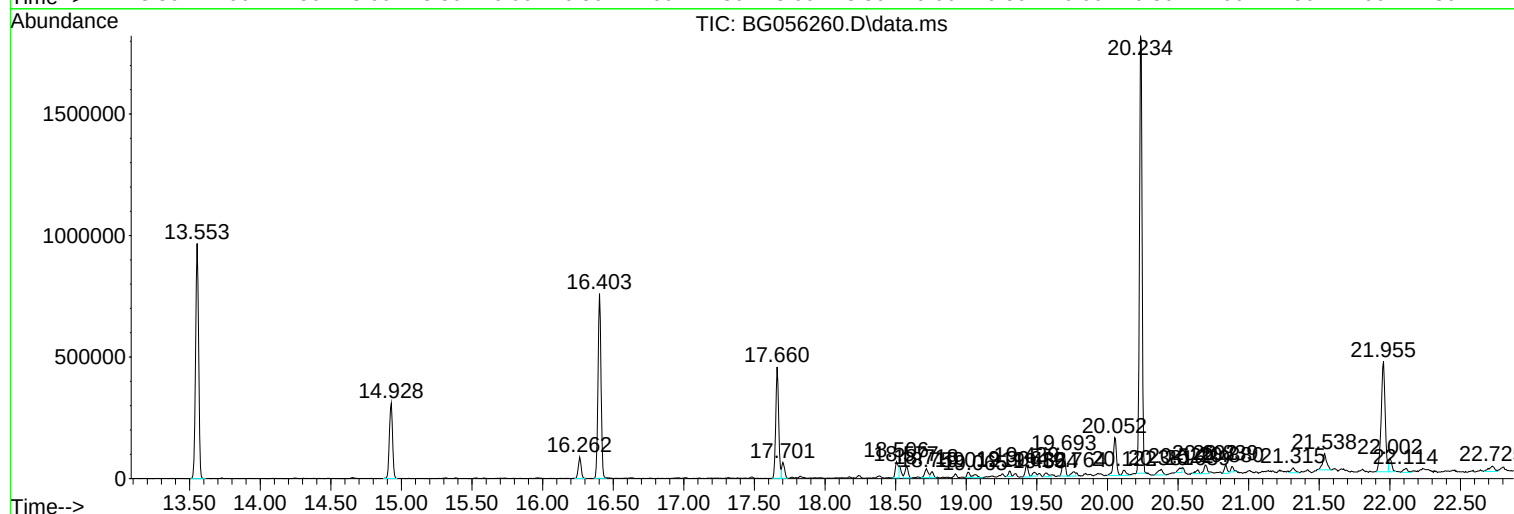
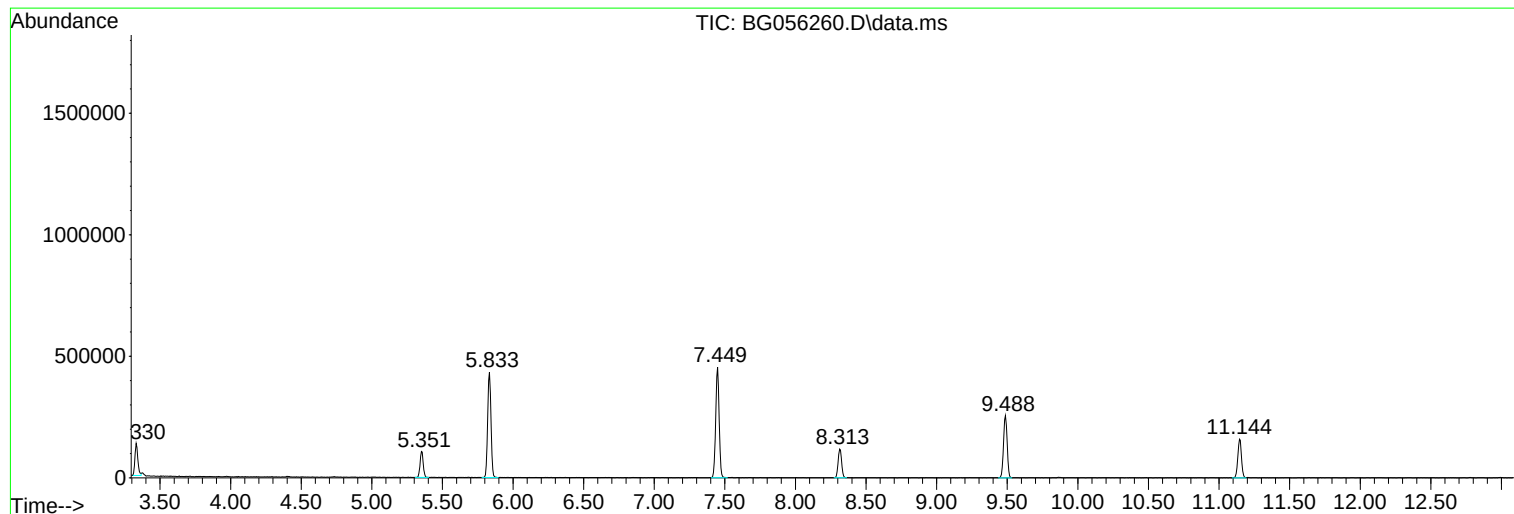
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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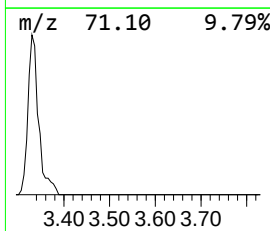
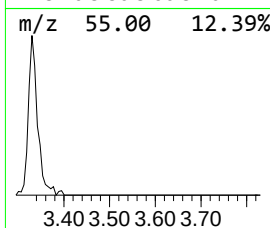
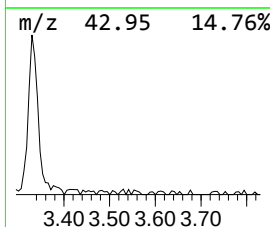
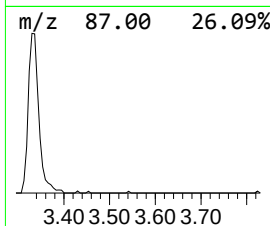
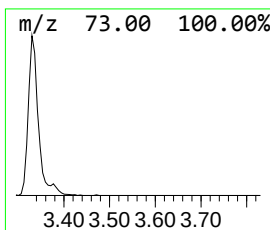
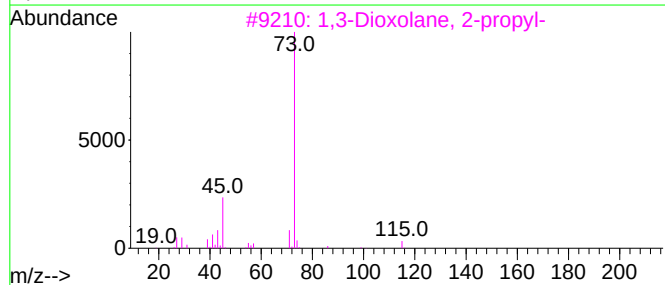
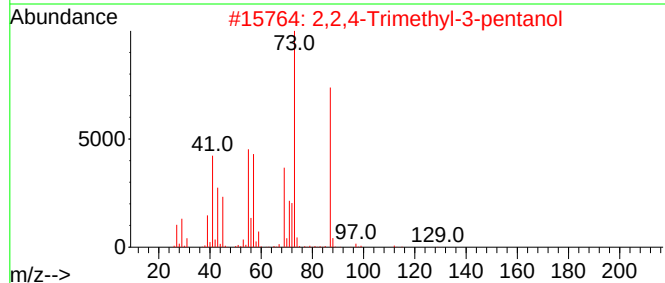
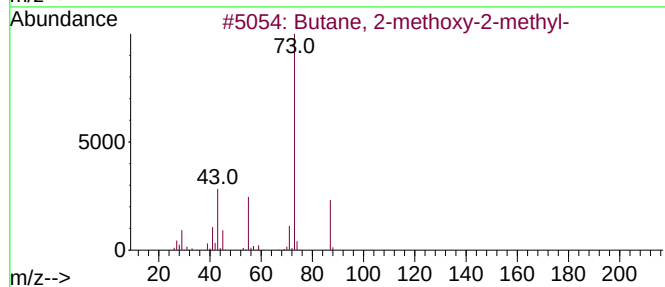
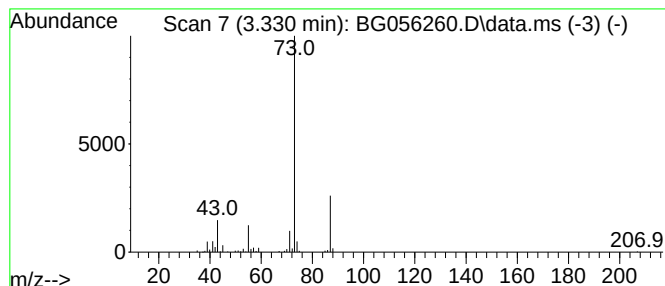
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.330	18.36 ng	186782	1,4-Dichlorobenzene-d4	8.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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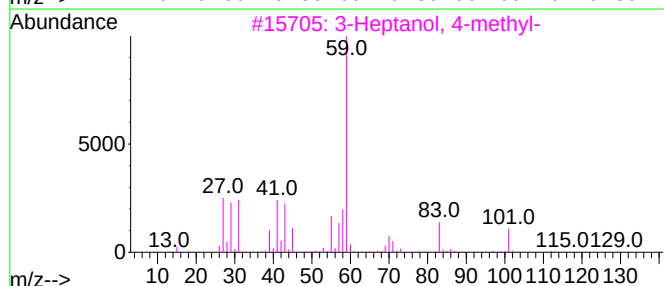
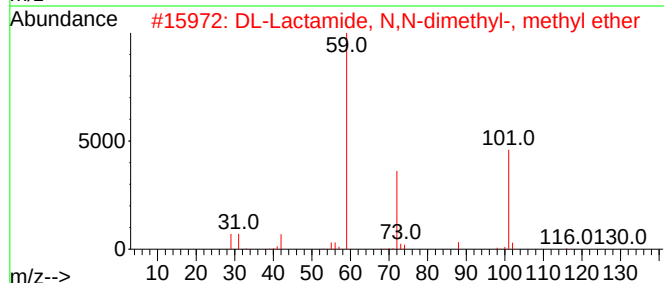
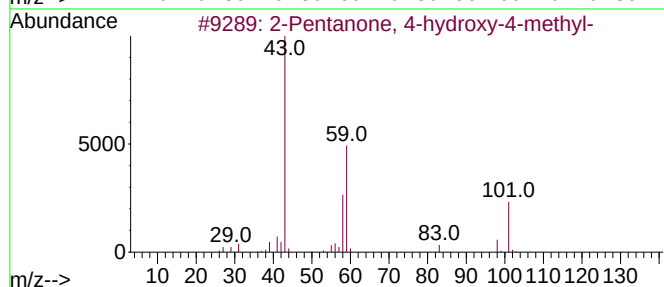
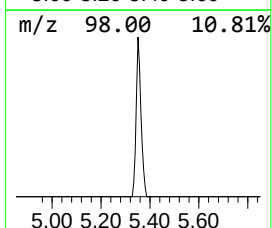
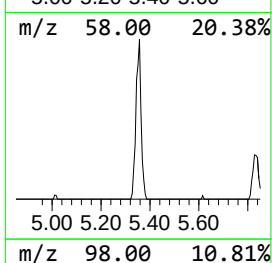
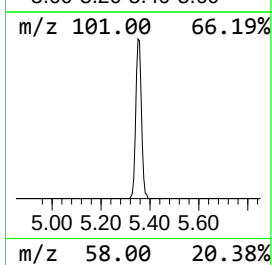
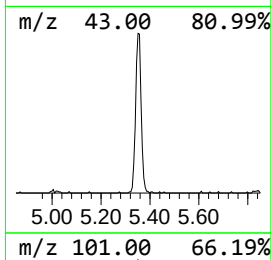
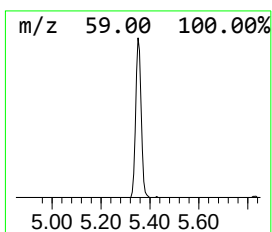
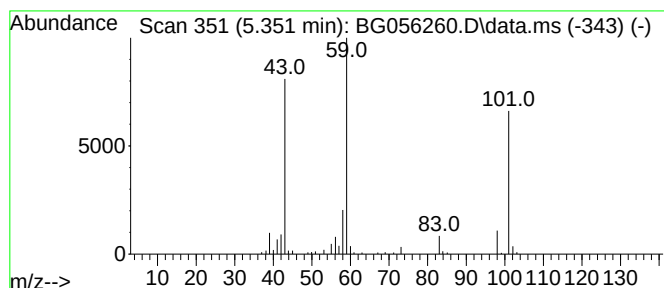
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.351	16.69 ng	169764	1,4-Dichlorobenzene-d4	8.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	40
3			3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	38
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32



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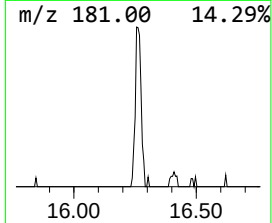
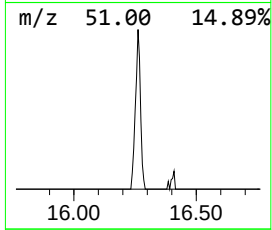
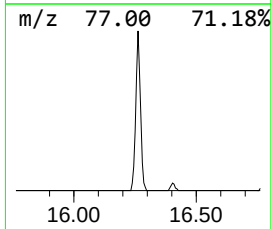
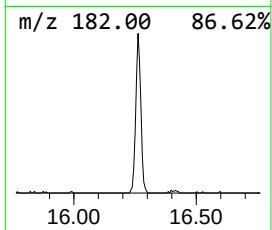
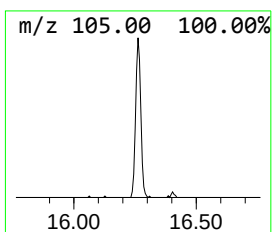
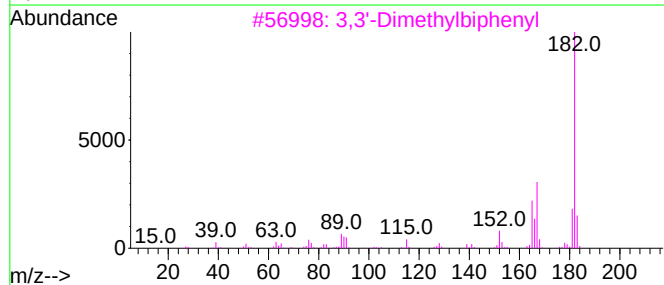
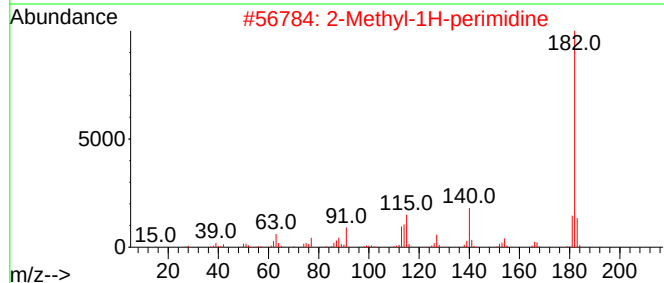
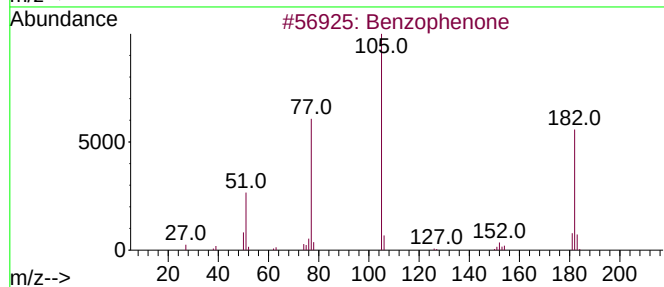
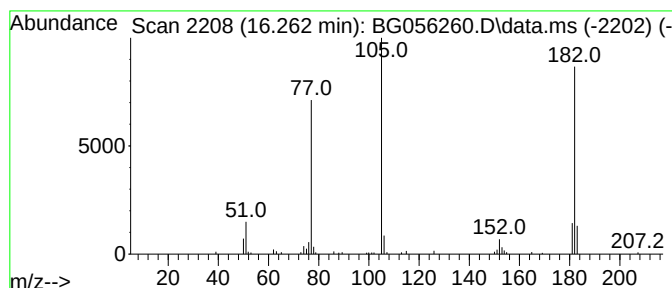
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.262	5.01 ng	122182	Acenaphthene-d10	14.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	90
2			2-Methyl-1H-perimidine	182	C12H10N2	005157-10-8	46
3			3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	43
4			3-Mercaptobenzoic acid, S-methyl...	182	C9H10O2S	090721-40-7	43
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	27



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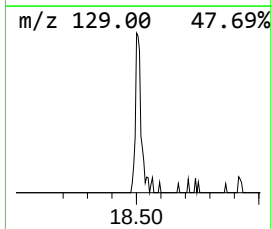
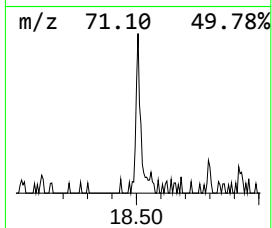
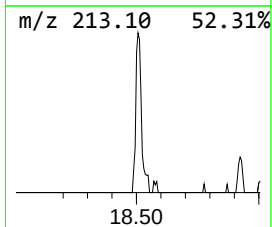
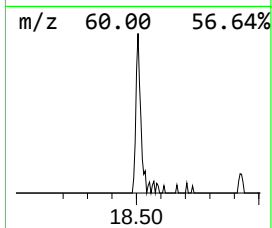
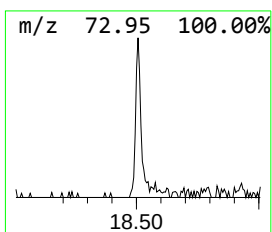
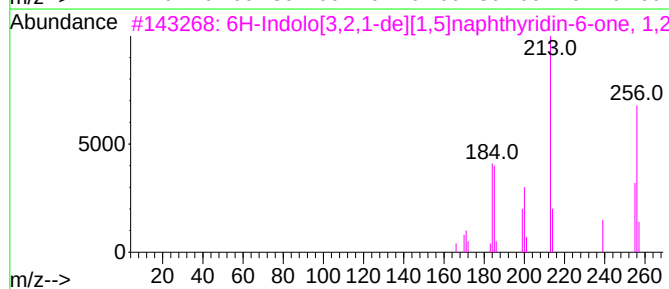
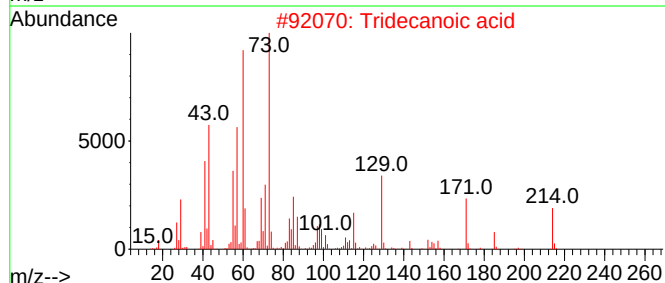
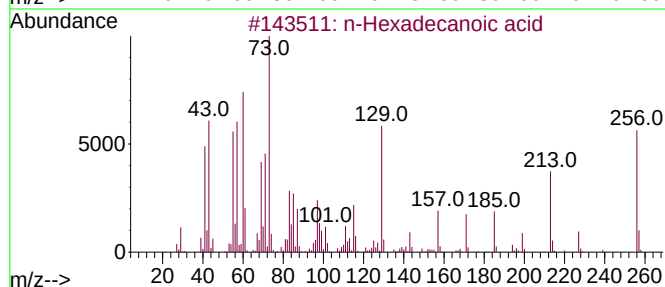
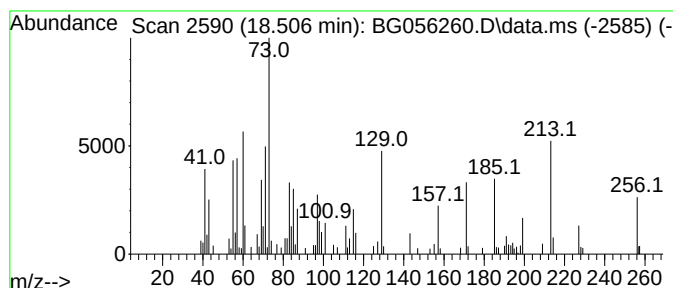
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.506	3.11 ng	105251	Phenanthrene-d10	17.660

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			6H-Indolo[3,2,1-de][1,5]naphthyr...	256	C15H16N2O2	050630-67-6	59
4			Dodecanoic acid	200	C12H24O2	000143-07-7	47
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	38



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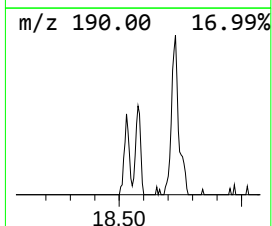
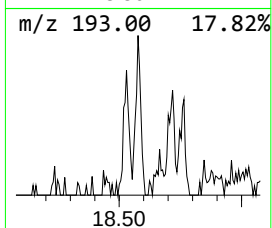
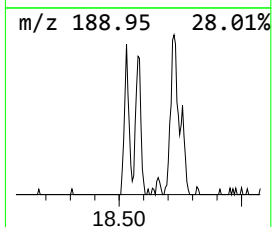
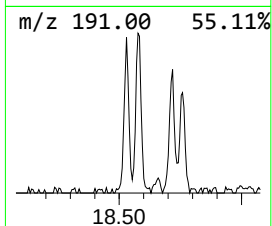
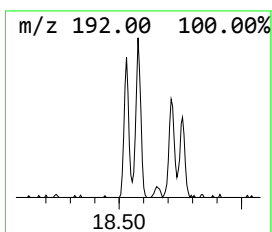
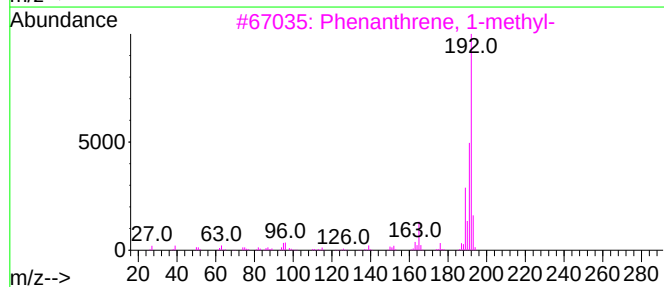
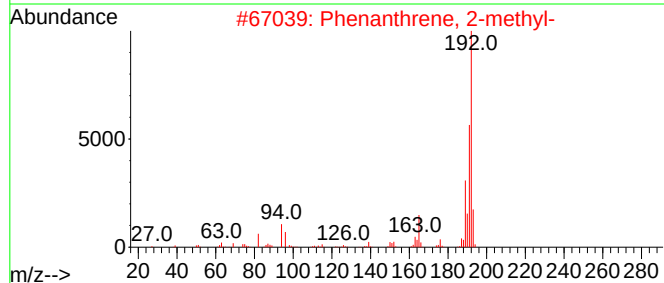
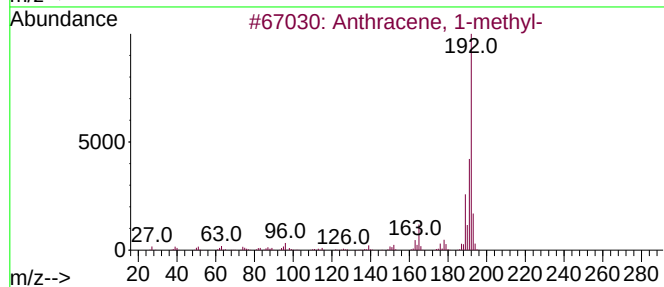
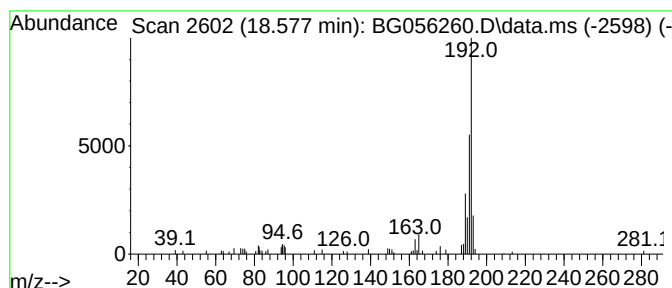
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Anthracene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.577	2.14 ng	72492	Phenanthrene-d10	17.660

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 1-methyl-	192	C15H12	000610-48-0	92
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
4			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	87
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011123\
Data File : BG056260.D
Acq On : 11 Jan 2023 21:27
Operator : CG/JU
Sample : 01064-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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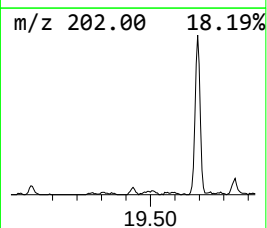
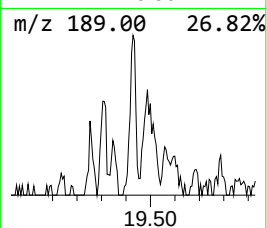
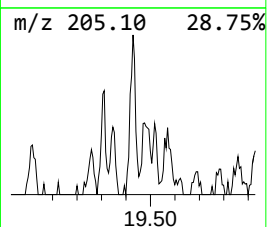
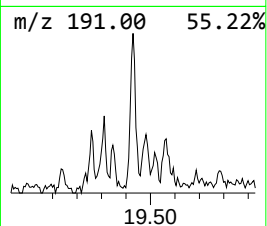
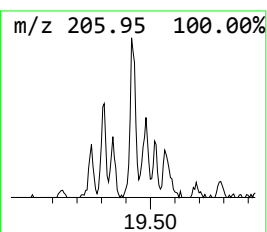
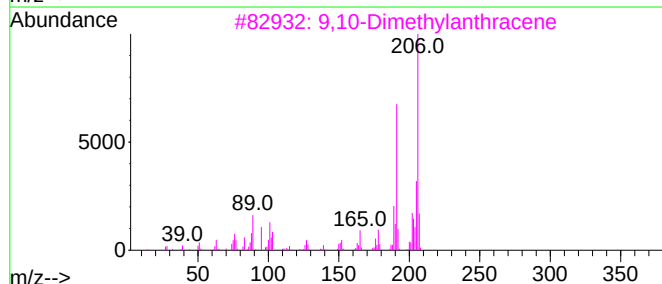
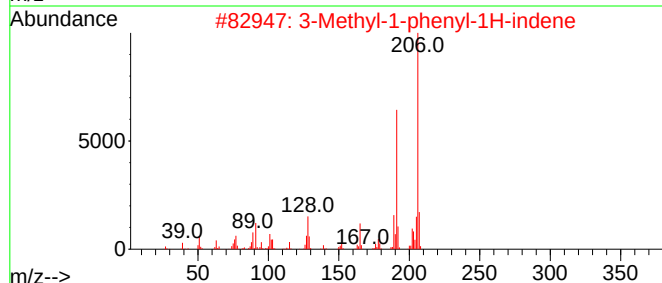
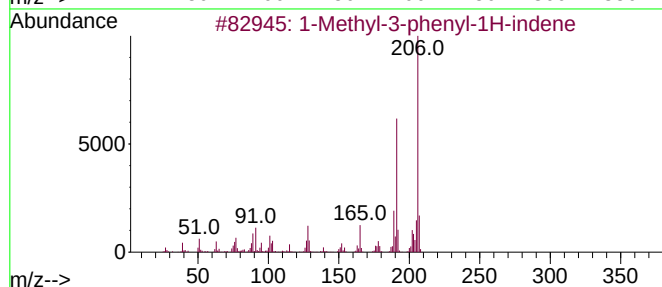
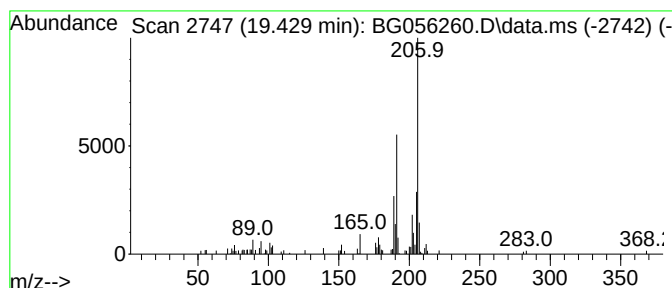
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Methyl-3-phenyl-1H-indene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.429	2.06 ng	69657	Phenanthrene-d10	17.660

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-3-phenyl-1H-indene	206	C16H14	022360-62-9	94
2			3-Methyl-1-phenyl-1H-indene	206	C16H14	022360-63-0	93
3			9,10-Dimethylantracene	206	C16H14	000781-43-1	93
4			Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	87
5			Phenanthrene, 4,5-dimethyl-	206	C16H14	003674-69-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011123\
Data File : BG056260.D
Acq On : 11 Jan 2023 21:27
Operator : CG/JU
Sample : 01064-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S4-01

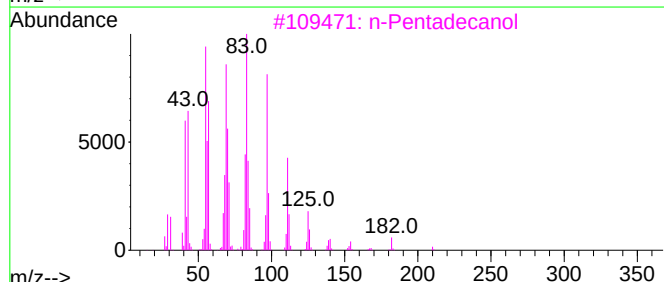
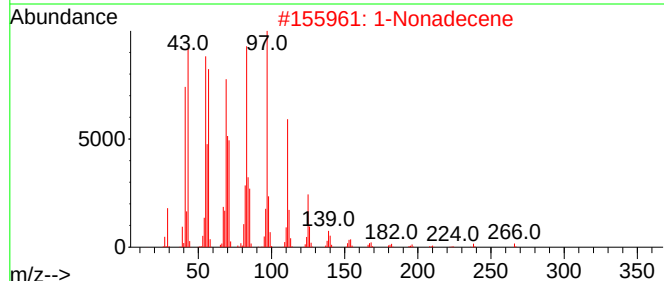
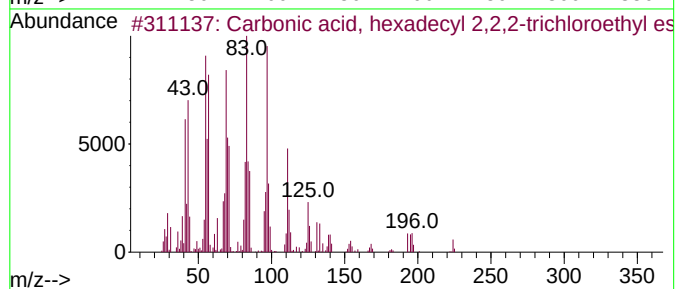
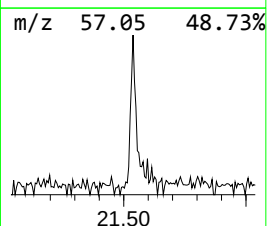
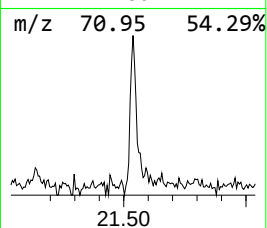
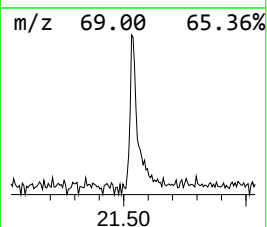
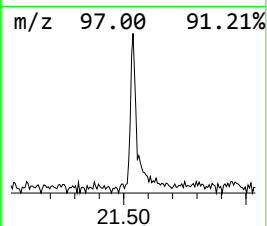
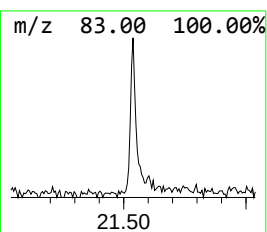
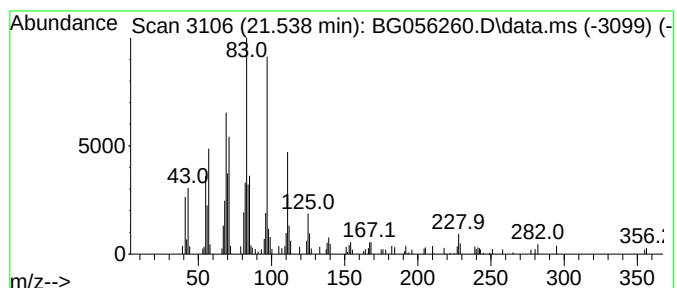
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Carbonic acid, hexadecyl 2,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.538	3.00 ng	133979	Chrysene-d12	21.955

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	80
2			1-Nonadecene	266	C19H38	018435-45-5	80
3			n-Pentadecanol	228	C15H32O	000629-76-5	64
4			1-Hexacosanol	382	C26H54O	000506-52-5	38
5			Methyl tetracosyl ether	368	C25H52O	1000406-29-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011123\
Data File : BG056260.D
Acq On : 11 Jan 2023 21:27
Operator : CG/JU
Sample : 01064-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S4-01

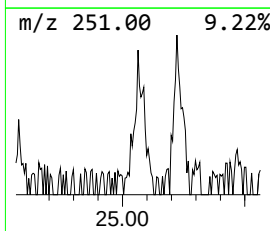
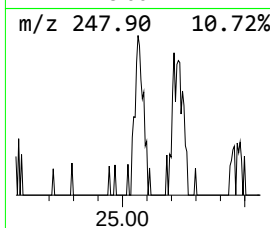
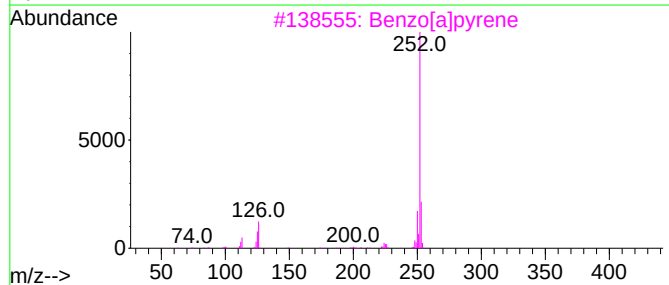
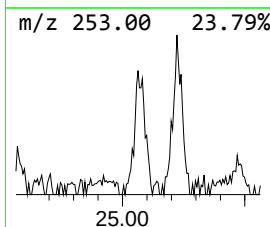
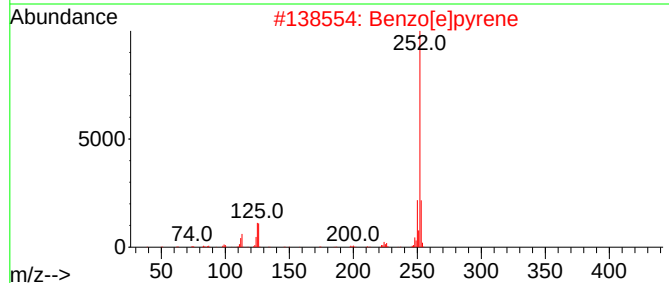
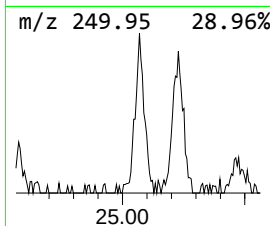
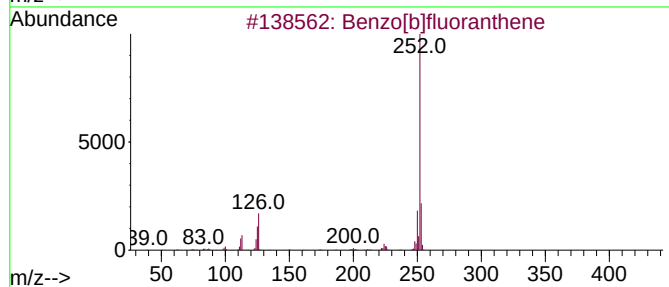
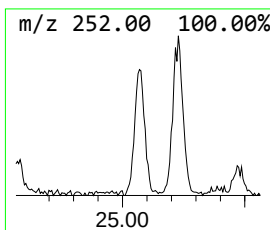
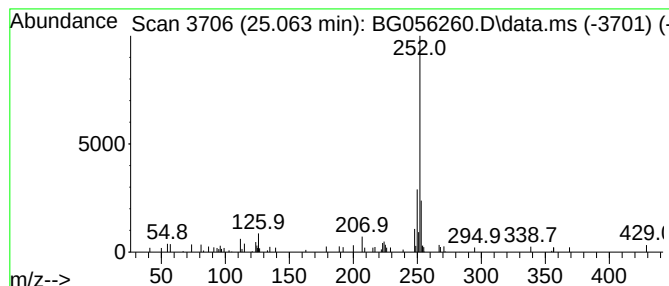
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.064	2.03 ng	81131	Perylene-d12	25.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	76
2			Benzo[e]pyrene	252	C20H12	000192-97-2	76
3			Benzo[a]pyrene	252	C20H12	000050-32-8	68
4			Chromium, (.eta.5-2,4-cyclopenta...	252	C15H20Cr	135162-31-1	64
5			Benzo[b]naphtho[2,3-d]thiophene,...	252	C17H16S	024964-04-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011123\
Data File : BG056260.D
Acq On : 11 Jan 2023 21:27
Operator : CG/JU
Sample : 01064-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S4-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.330	18.4	ng	186782	1	8.318	203469	20.0
2-Pentanone, 4-...	5.351	16.7	ng	169764	1	8.318	203469	20.0
Benzophenone	16.262	5.0	ng	122182	3	14.928	487975	20.0
n-Hexadecanoic ...	18.506	3.1	ng	105251	4	17.660	676132	20.0
Anthracene, 1-m...	18.577	2.1	ng	72492	4	17.660	676132	20.0
1-Methyl-3-phen...	19.429	2.1	ng	69657	4	17.660	676132	20.0
Carbonic acid, ...	21.538	3.0	ng	133979	5	21.955	891999	20.0
Benzo[e]pyrene	25.064	2.0	ng	81131	6	25.392	798838	20.0