

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040523\
 Data File : BG057004.D
 Acq On : 6 Apr 2023 00:07
 Operator : CG/JU
 Sample : 02126-05 5X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RS-E

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: BG057004.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.441	319	324	331	rBV2	16070	26514	6.89%	0.956%
2	5.922	400	406	414	rBB	45139	74856	19.45%	2.698%
3	7.544	674	682	690	rBB	48903	85636	22.25%	3.087%
4	8.413	822	830	836	rBV2	69138	116495	30.26%	4.199%
5	9.588	1023	1030	1038	rVB	28952	51507	13.38%	1.856%
6	11.256	1306	1314	1320	rBV	91839	164345	42.69%	5.924%
7	13.653	1716	1722	1729	rVB	82569	126548	32.87%	4.561%
8	14.752	1905	1909	1915	rBV2	2463	4799	1.25%	0.173%
9	15.028	1949	1956	1962	rVB	153926	239355	62.18%	8.627%
10	15.086	1962	1966	1973	rVB2	3800	6044	1.57%	0.218%
11	16.068	2126	2133	2137	rBV3	5363	9931	2.58%	0.358%
12	16.502	2200	2207	2215	rBV	64798	100808	26.19%	3.633%
13	17.278	2334	2339	2341	rBV4	4050	5585	1.45%	0.201%
14	17.583	2387	2391	2394	rBV3	4716	6182	1.61%	0.223%
15	17.765	2416	2422	2426	rBV	188527	279460	72.59%	10.073%
16	17.806	2426	2429	2435	rVB	51998	77664	20.17%	2.799%
17	17.900	2439	2445	2450	rBV2	13401	22706	5.90%	0.818%
18	18.159	2486	2489	2491	rBV4	4778	4451	1.16%	0.160%
19	18.270	2505	2508	2512	rBV4	3913	6246	1.62%	0.225%
20	18.341	2517	2520	2526	rVB4	4197	8264	2.15%	0.298%
21	18.541	2552	2554	2557	rBV4	3308	4291	1.11%	0.155%
22	18.605	2561	2565	2567	rVV4	12929	18263	4.74%	0.658%
23	18.635	2567	2570	2573	rVV2	19086	29001	7.53%	1.045%
24	18.682	2574	2578	2583	rVB	23593	35072	9.11%	1.264%
25	18.758	2589	2591	2597	rVB2	9065	10776	2.80%	0.388%
26	18.823	2597	2602	2607	rBV2	24144	55428	14.40%	1.998%
27	18.917	2617	2618	2620	rBV2	5479	4178	1.09%	0.151%
28	19.016	2632	2635	2639	rVB5	6495	9681	2.51%	0.349%
29	19.058	2639	2642	2643	rBV3	5807	5250	1.36%	0.189%
30	19.116	2649	2652	2655	rBV	10849	12406	3.22%	0.447%
31	19.163	2657	2660	2663	rVB6	6300	8050	2.09%	0.290%
32	19.357	2687	2693	2697	rBV9	6734	14128	3.67%	0.509%
33	19.410	2698	2702	2705	rBV6	6627	8730	2.27%	0.315%
34	19.434	2705	2706	2708	rBV2	5665	5055	1.31%	0.182%
35	19.528	2719	2722	2728	rVB3	18297	20805	5.40%	0.750%
36	19.592	2728	2733	2735	rBV5	8878	14737	3.83%	0.531%

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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	19.674	2742	2747	2750	rBV4	18353	32048	8.33%	1.155%
38	19.798	2762	2768	2773	rBV	153014	228693	59.41%	8.243%
39	20.121	2819	2823	2825	rBV2	27097	42977	11.16%	1.549%
40	20.156	2825	2829	2835	rVB	166582	234026	60.79%	8.435%
41	20.332	2855	2859	2864	rVB	142926	178480	46.36%	6.433%
42	22.089	3150	3158	3163	rBV2	156623	384960	100.00%	13.875%

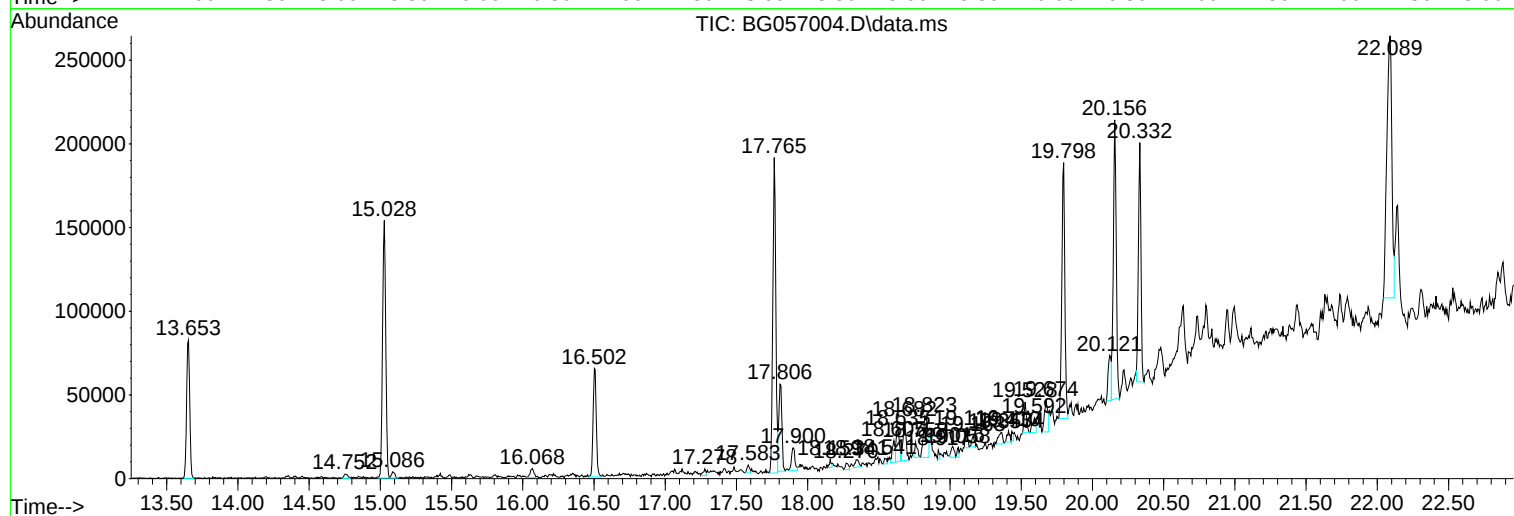
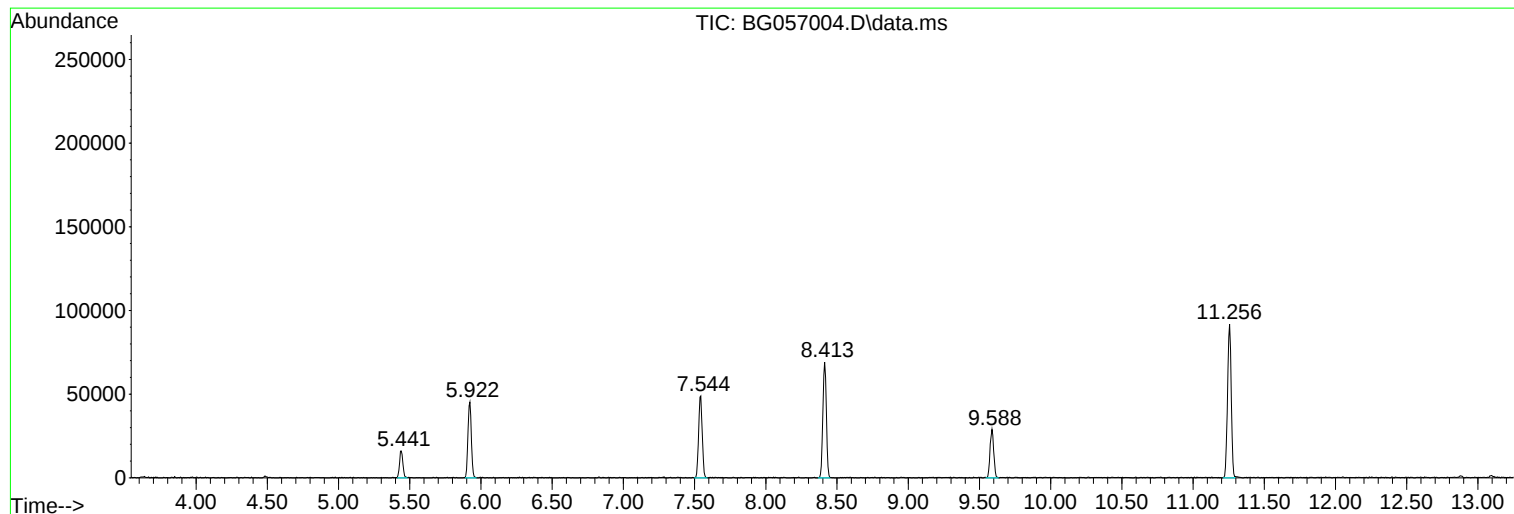
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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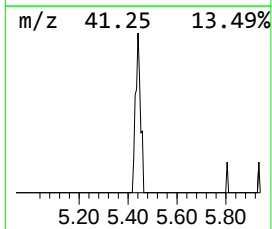
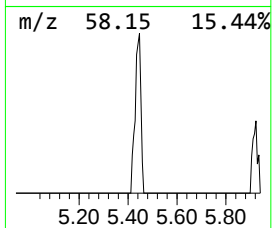
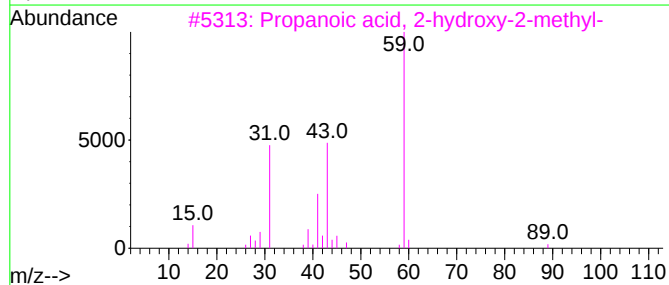
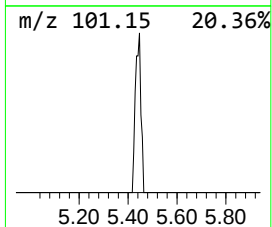
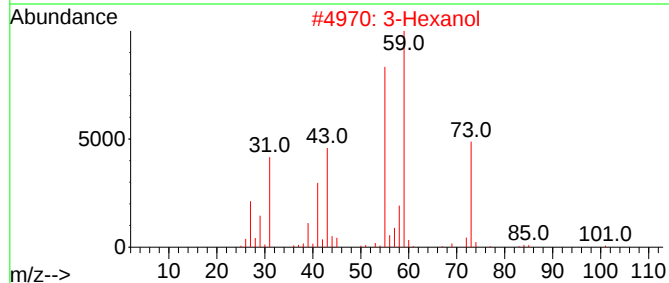
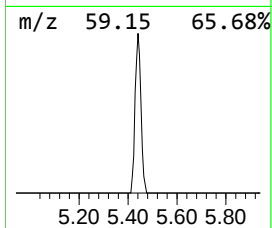
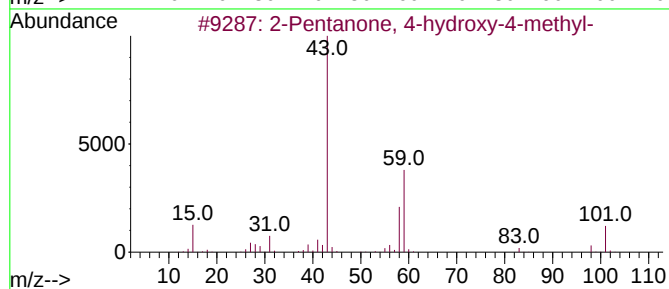
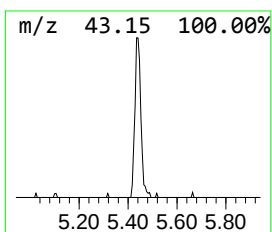
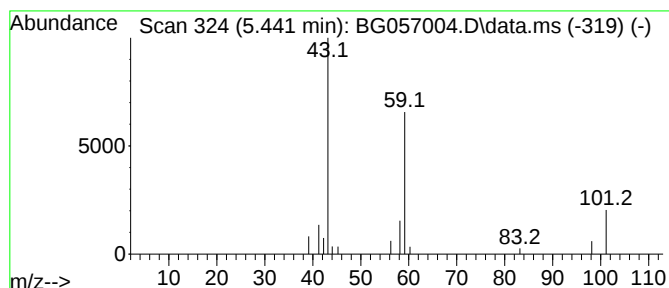
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.441	4.55 ng	26514	1,4-Dichlorobenzene-d4	8.413

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	3-Hexanol	102	C6H14O	000623-37-0	28		
3	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	17		
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9		
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9		



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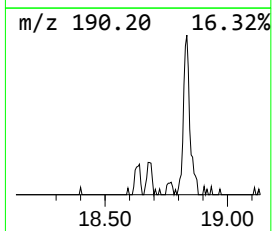
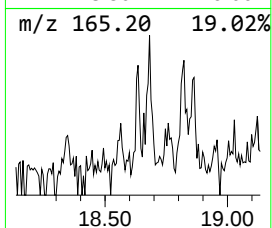
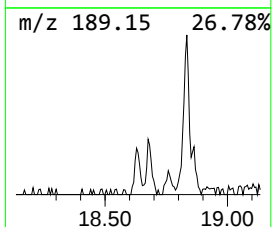
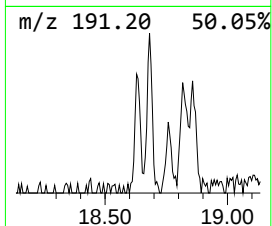
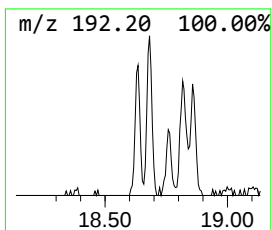
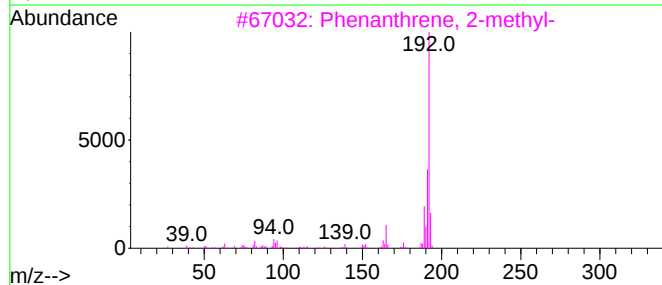
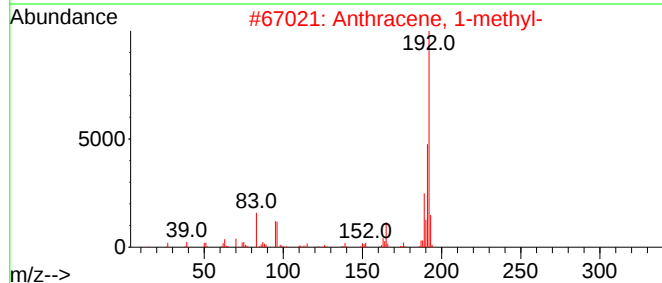
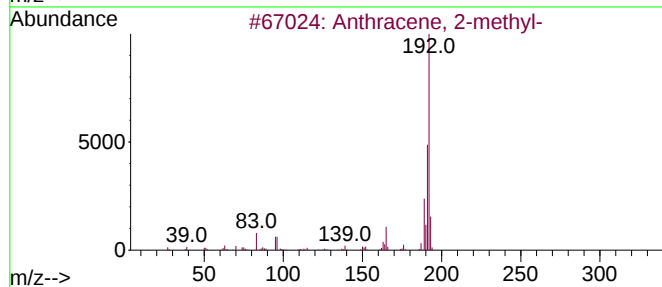
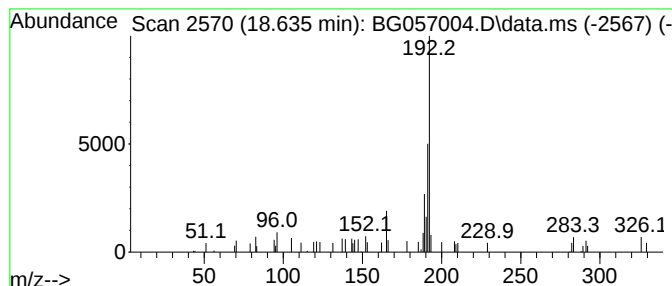
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Anthracene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.635	2.08 ng	29001	Phenanthrene-d10	17.765

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 2-methyl-	192	C15H12	000613-12-7	53
2			Anthracene, 1-methyl-	192	C15H12	000610-48-0	53
3			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	53
4			Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	53
5			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	53



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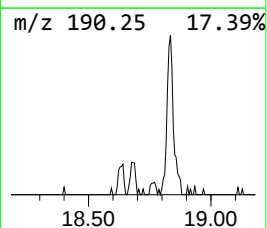
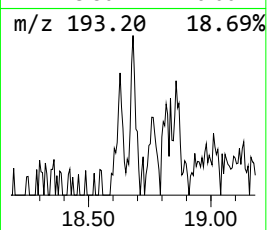
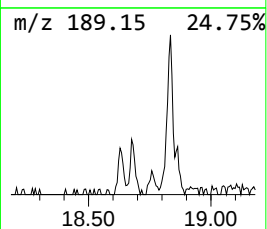
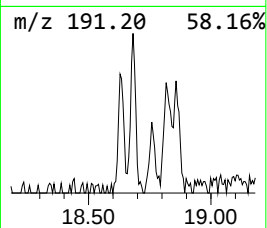
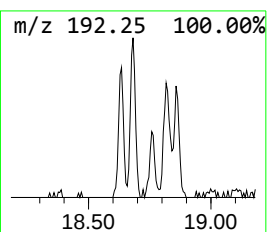
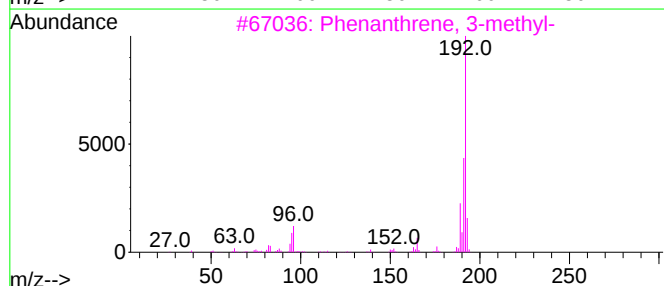
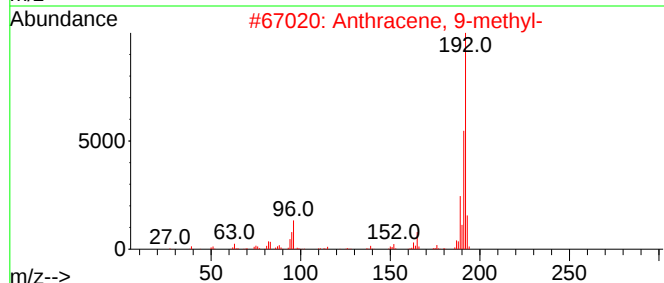
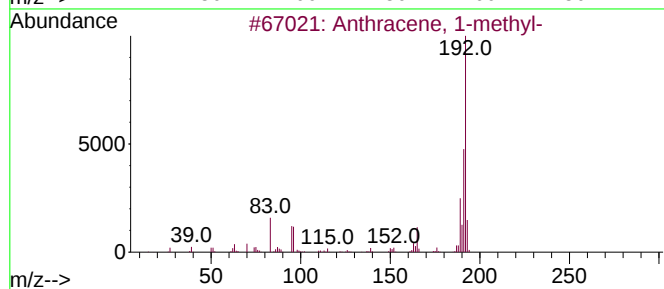
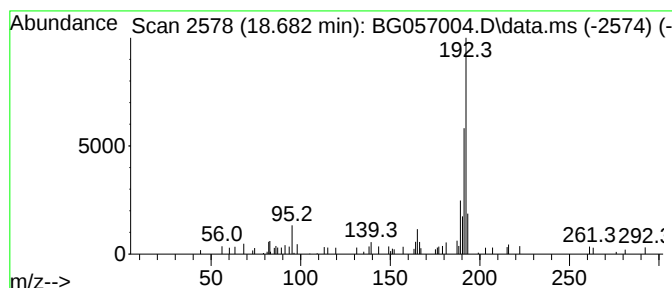
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Anthracene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.682	2.51 ng	35072	Phenanthrene-d10	17.765

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
2			Anthracene, 9-methyl-	192	C15H12	000779-02-2	81
3			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	81
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	81
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	81



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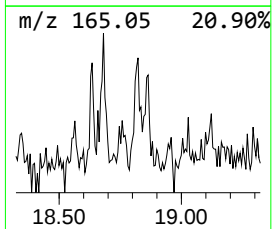
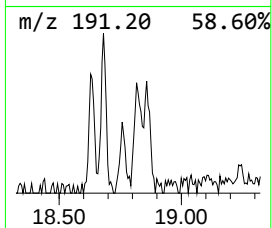
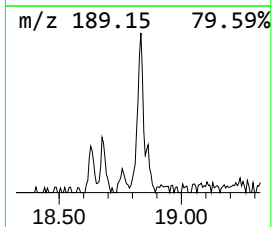
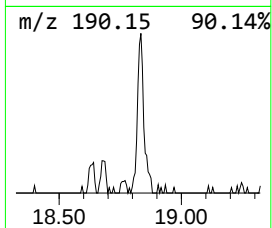
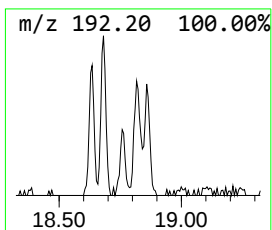
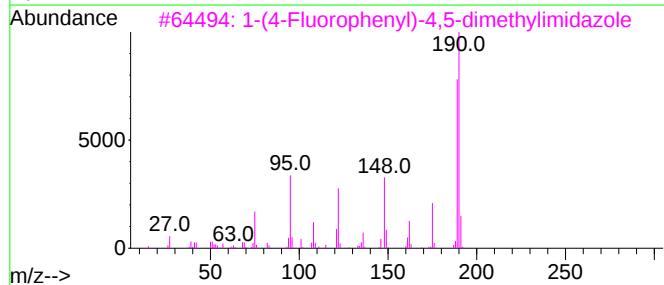
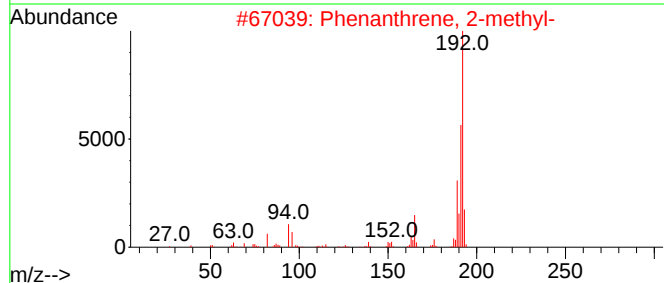
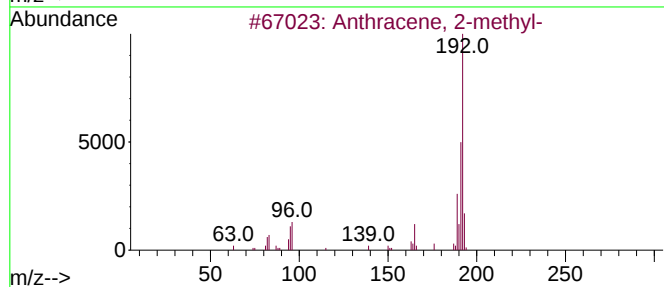
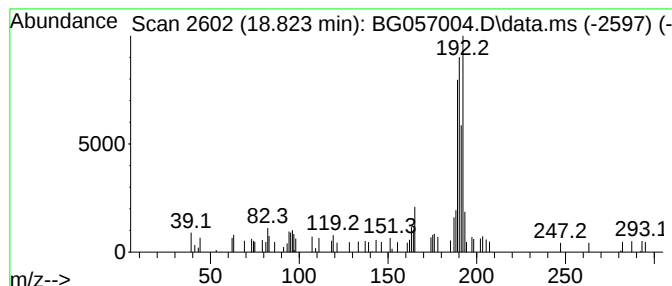
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown18.823 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.823	3.97 ng	55428	Phenanthrene-d10	17.765
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		Anthracene, 2-methyl-	192 C15H12	000613-12-7 46
2		Phenanthrene, 2-methyl-	192 C15H12	002531-84-2 46
3		1-(4-Fluorophenyl)-4,5-dimethyl-...	190 C11H11FN2	1000443-18-7 43
4		Anthracene, 9-methyl-	192 C15H12	000779-02-2 42
5		3-(Bromomethyl)-1-isopropylpyrro...	205 C8H16BrN	1000489-23-8 38



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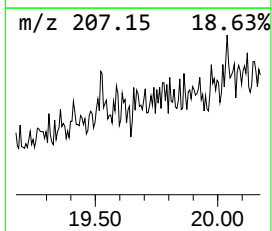
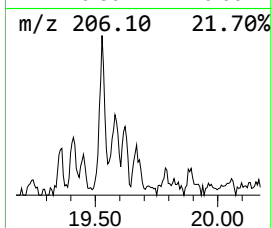
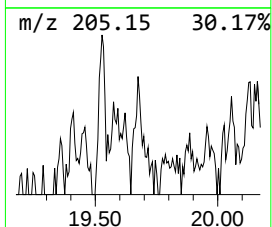
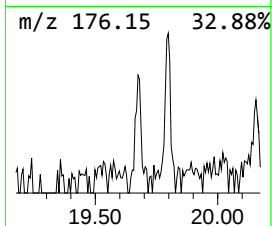
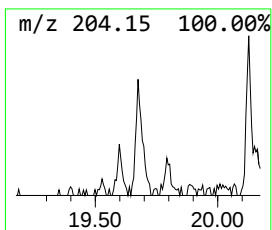
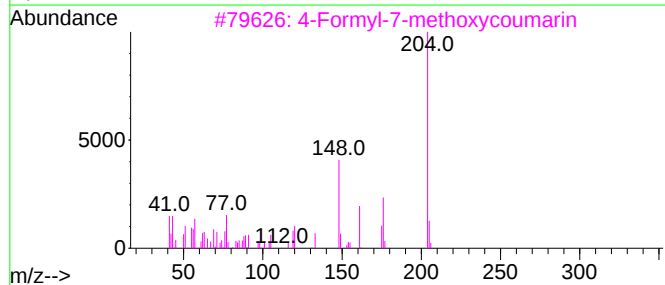
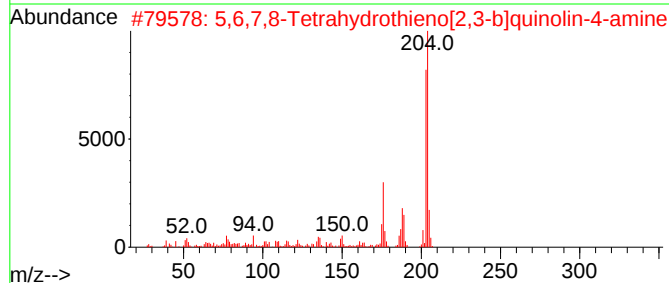
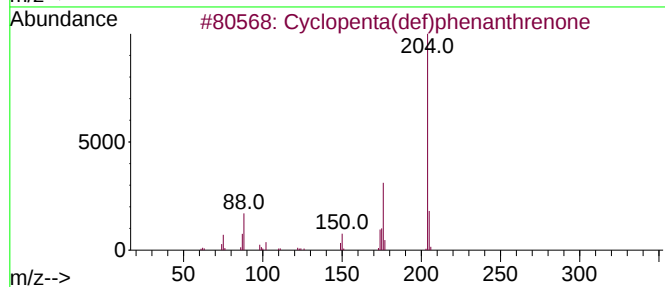
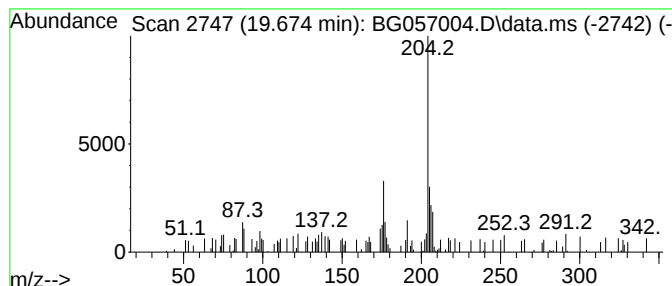
Instrument :
BNA_G
ClientSampleId :
RS-E

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 Cyclopenta(def)phenanthrenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.674	2.29 ng	32048	Phenanthrene-d10	17.765	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	52
2	5,6,7,8-Tetrahydrothieno[2,3-b]q...	204	C11H12N2S	122914-50-5	52
3	4-Formyl-7-methoxycoumarin	204	C11H8O4	1000429-03-0	50
4	[1,1'-Biphenyl]-4-ol, 4'-chloro-	204	C12H9ClO	028034-99-3	50
5	2-butanone, 4-[4-(diethylamino)p...	219	C14H21NO	1000400-76-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040523\
Data File : BG057004.D
Acq On : 6 Apr 2023 00:07
Operator : CG/JU
Sample : 02126-05 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RS-E

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.441	4.5	ng	26514	1	8.413	116495	20.0
Anthracene, 2-m...	18.635	2.1	ng	29001	4	17.765	279460	20.0
Anthracene, 1-m...	18.682	2.5	ng	35072	4	17.765	279460	20.0
unknown18.823	18.823	4.0	ng	55428	4	17.765	279460	20.0
Cyclopenta(def)...	19.674	2.3	ng	32048	4	17.765	279460	20.0