LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058526.D
Acq On : 28 Jul 2023 20:23
Operator : MA/JU
Sample : 03580-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-2

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-BG072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058526.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.388	384	391	411	rBV	645858	1068048	49.20%	5.752%
2	6.986	655	663	678	rBV	616410	1103808	50.85%	5.944%
3	7.815	797	804	815	rBV	193907	331810	15.29%	1.787%
4	8.978	994	1002	1015	rBV	359617	663804	30.58%	3.575%
5	10.617	1274	1281	1297	rBV	250096	479156	22.07%	2.580%
6	13.079	1693	1700	1716	rBV	972157	1526582	70.32%	8.221%
7	13.919	1838	1843	1849	rVB	23361	36021	1.66%	0.194%
8	14.460	1928	1935	1942	rBV	429367	668252	30.78%	3.599%
9	14.525	1942	1946	1953	rVB3	15252	24810	1.14%	0.134%
10	15.512	2108	2114	2123	rBV2	12718	22130	1.02%	0.119%
11	15.952	2182	2189	2204	rBV	703912	1175995	54.17%	6.333%
12	16.957	2353	2360	2363	rBV3	19594	28184	1.30%	0.152%
13	17.204	2396	2402	2406	rBV	515161	796411	36.69%	4.289%
14	17.245	2406	2409	2416	rVV	252932	370808	17.08%	1.997%
15	17.339	2419	2425	2430	rVB	56601	89131	4.11%	0.480%
16	17.615	2466	2472	2476	rBV	15641	32514	1.50%	0.175%
17	18.091	2546	2553	2557	rBV3	79493	155013	7.14%	0.835%
18	18.126	2557	2559	2567	rVB	51536	71345	3.29%	0.384%
19	18.273	2579	2584	2588	rBV2	57863	101656	4.68%	0.547%
20	18.579	2632	2636	2640	rBV	25616	37024	1.71%	0.199%
21	18.626	2640	2644	2650	rVB3	14763	23901	1.10%	0.129%
22	18.996	2703	2707	2713	rBV4	27314	53247	2.45%	0.287%
23	19.137	2727	2731	2740	rBV4	22270	46303	2.13%	0.249%
24	19.260	2746	2752	2759	rBV	563774	801569	36.93%	4.317%
25	19.372	2765	2771	2774	rBV7	20652	36815	1.70%	0.198%
26	19.507	2790	2794	2798	rVB	18737	24686	1.14%	0.133%
27	19.624	2803	2814	2822	rBV	528601	892588	41.12%	4.807%
28	19.701	2822	2827	2833	rVB4	23749	44275	2.04%	0.238%
29	19.824	2839	2848	2853	rBV	1620177	2170777	100.00%	11.690%
30	19.948	2863	2869	2876	rBV5	34636	87022	4.01%	0.469%
31	20.083	2887	2892	2893	rBV4	31402	44527	2.05%	0.240%
32	20.118	2894	2898	2903	rVB	75185	117767	5.43%	0.634%
33	20.218	2910	2915	2919	rBV	38887	55861	2.57%	0.301%
34	20.277	2919	2925	2928	rVV3	47632	79775	3.67%	0.430%
35	20.412	2945	2948	2952	rBV	29317	34714	1.60%	0.187%
36	20.459	2952	2956	2961	rBV2	34294	47330	2.18%	0.255%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058526.D
Acq On : 28 Jul 2023 20:23
Operator : MA/JU
Sample : 03580-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-2

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-BG072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.864	3022	3025	3032	rVB	39319	56674	2.61%	0.305%
38	21.046	3049	3056	3059	rBV3	43990	89001	4.10%	0.479%
39	21.082	3059	3062	3066	rVV2	45079	72124	3.32%	0.388%
40	21.129	3067	3070	3075	rVV2	39143	71310	3.28%	0.384%
41	21.187	3076	3080	3085	rVB2	30631	55329	2.55%	0.298%
42	21.446	3115	3124	3128	rBV2	573214	1304791	60.11%	7.027%
43	21.487	3128	3131	3144	rVB	244220	395515	18.22%	2.130%
44	21.634	3151	3156	3163	rBV2	55012	97207	4.48%	0.523%
45	21.839	3186	3191	3197	rVB3	24358	50464	2.32%	0.272%
46	22.204	3250	3253	3262	rVB2	37442	71246	3.28%	0.384%
47	23.032	3390	3394	3400	rVB2	69838	124620	5.74%	0.671%
48	23.543	3473	3481	3488	rBV	170738	563218	25.95%	3.033%
49	24.225	3591	3597	3610	rVB	118357	314730	14.50%	1.695%
50	24.366	3614	3621	3634	rVB	161169	436971	20.13%	2.353%
51	24.513	3637	3646	3655	rBV	347355	980011	45.15%	5.278%
52	28.003	4232	4240	4257	rVB5	68162	318111	14.65%	1.713%
53	29.090	4415	4425	4437	rVB3	56974	224355	10.34%	1.208%

Sum of corrected areas: 18569336

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
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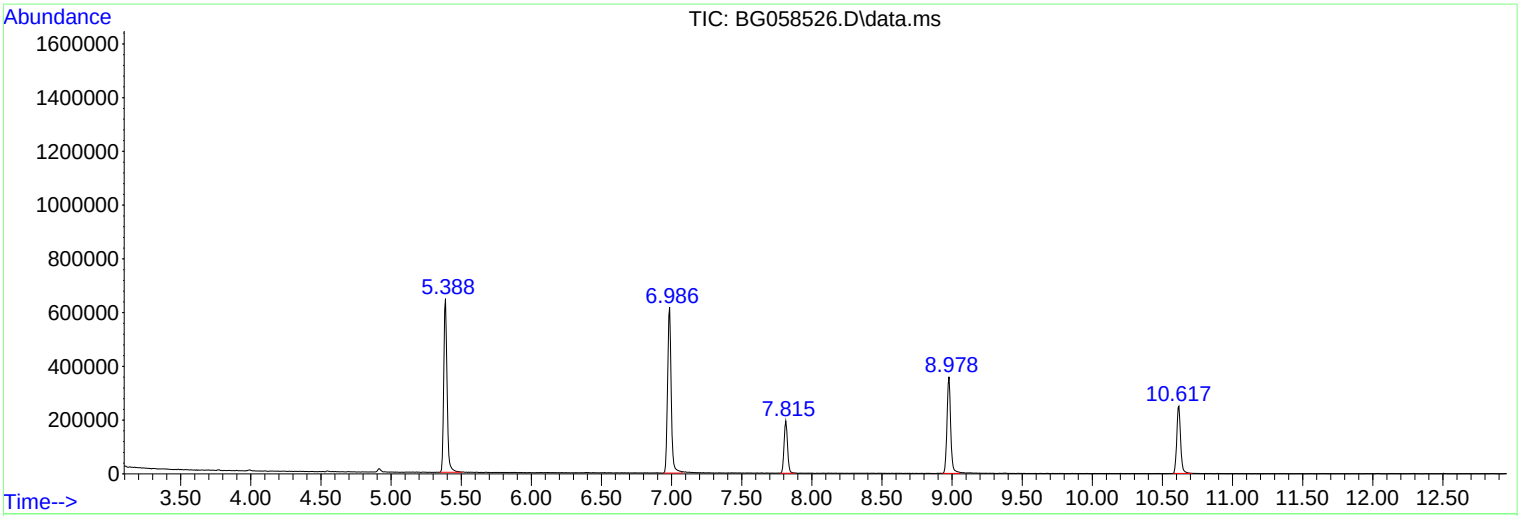
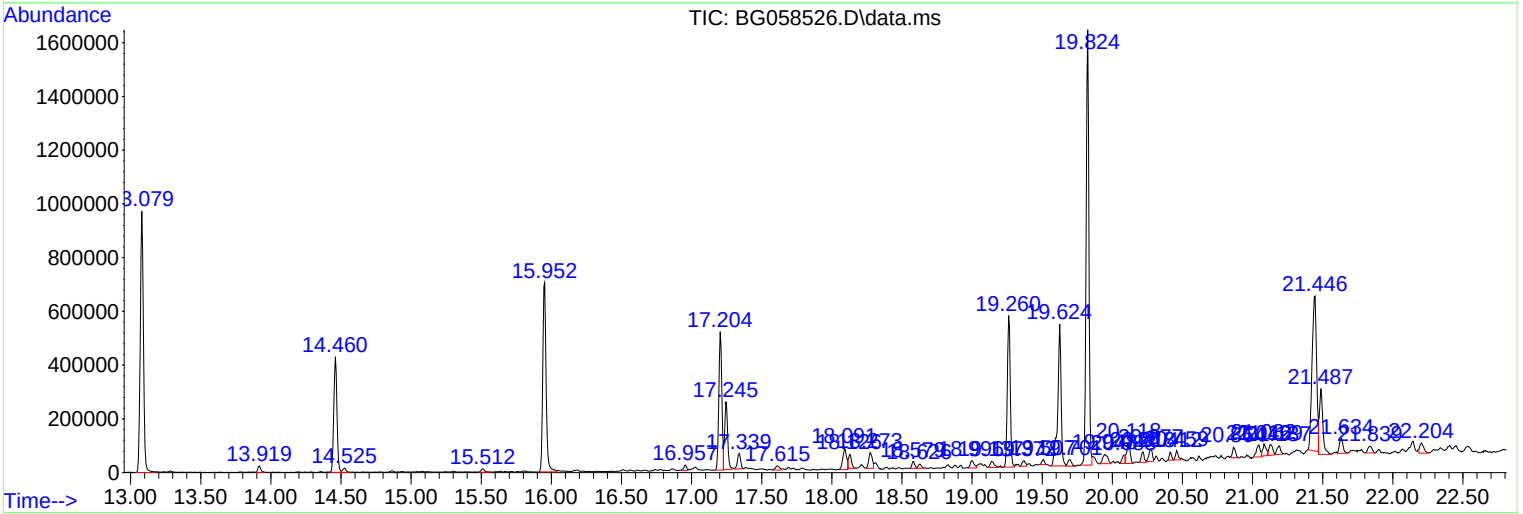
Operator : MA/JU
Sample : 03580-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

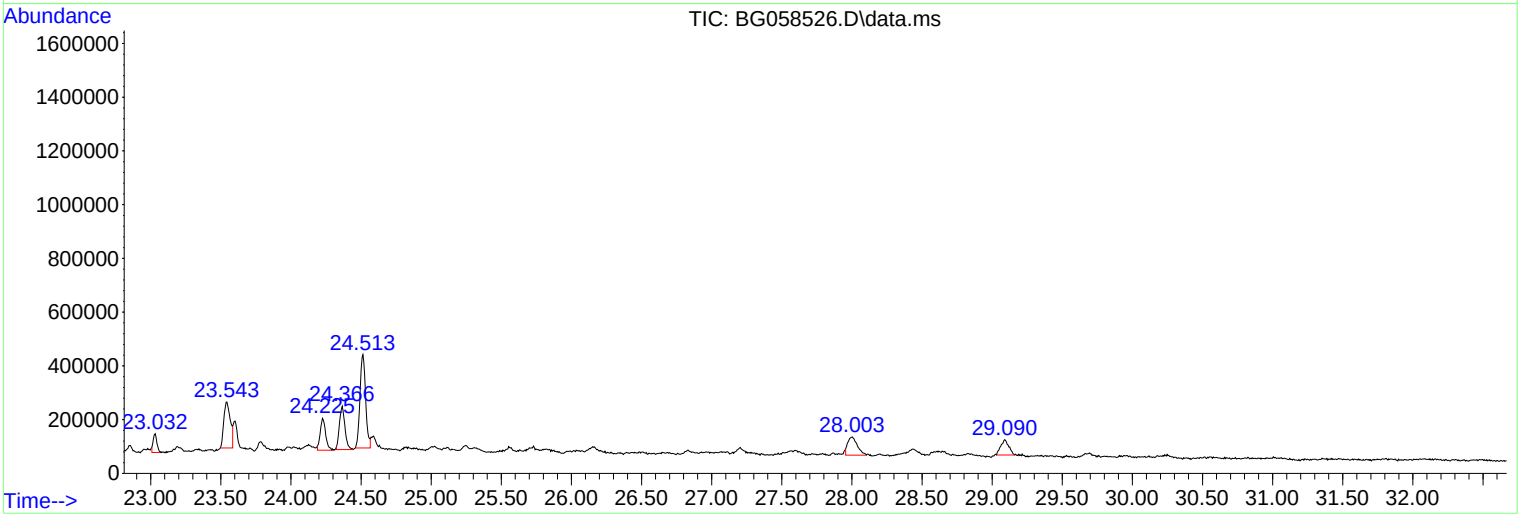
Instrument :
BNA_G
ClientSampleId :
SAMPLE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058526.D
Acq On : 28 Jul 2023 20:23
Operator : MA/JU
Sample : 03580-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

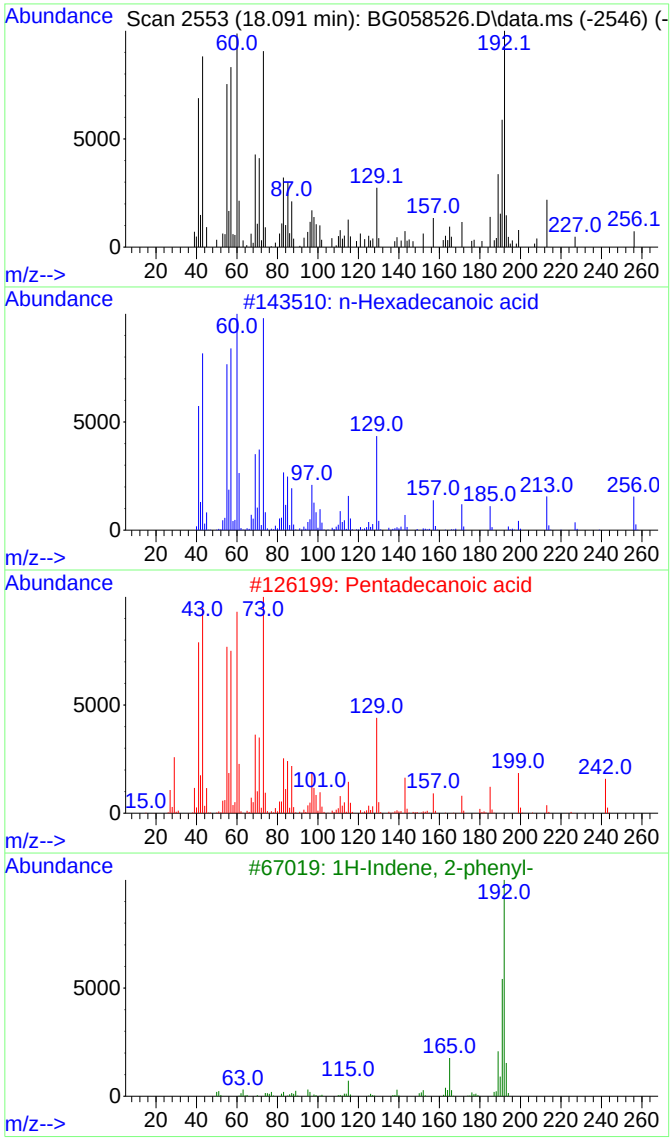
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

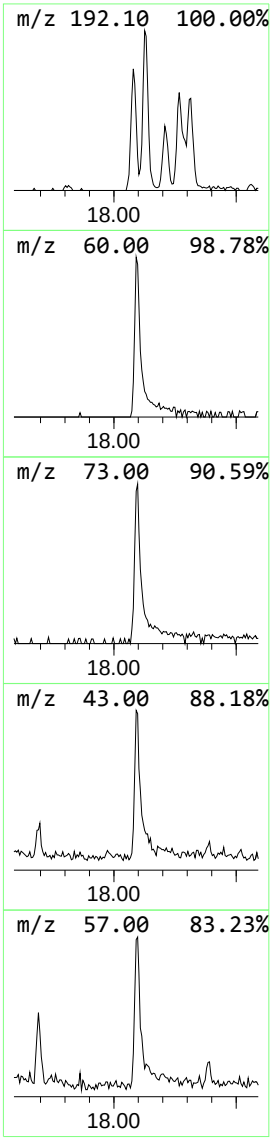
****

Peak Number 1 unknown18.091 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.091	3.89 ng	155013	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	45
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	43
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	35
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	35
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058526.D
Acq On : 28 Jul 2023 20:23
Operator : MA/JU
Sample : 03580-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-2

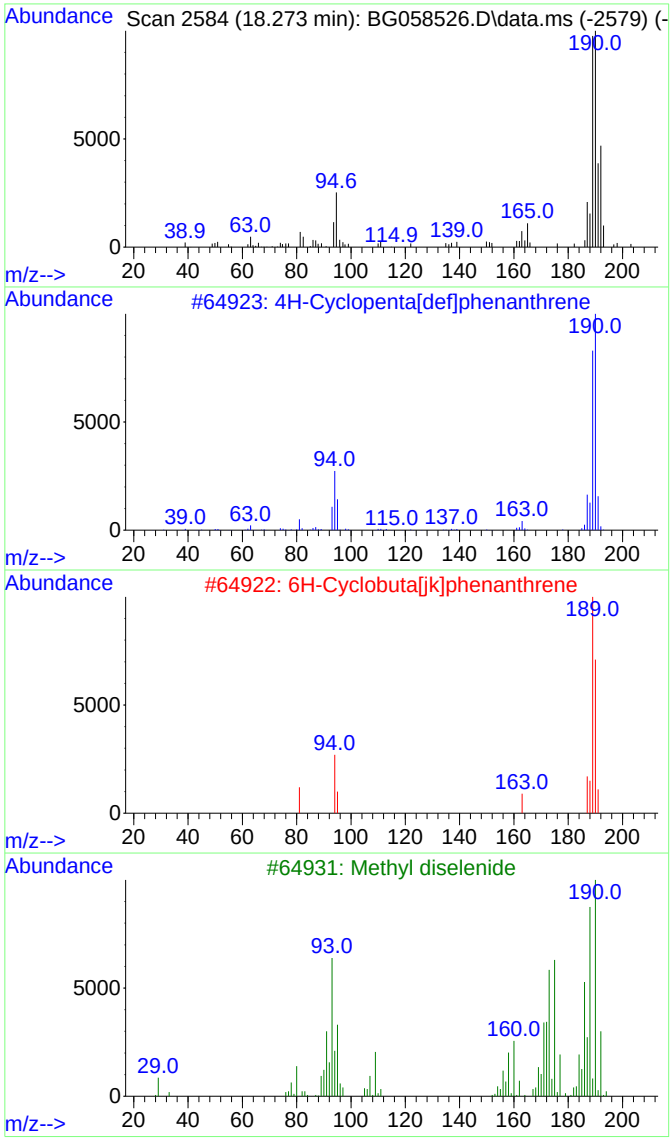
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

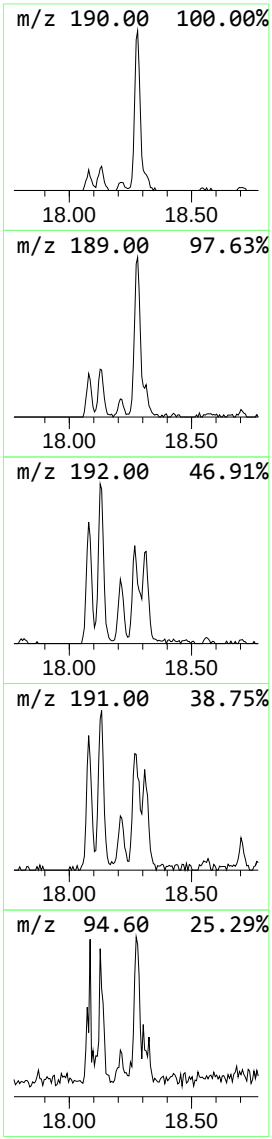
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.273	2.55 ng	101656	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	Methyl diselenide	190	C2H6Se2	007101-31-7	27
4	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058526.D
Acq On : 28 Jul 2023 20:23
Operator : MA/JU
Sample : 03580-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

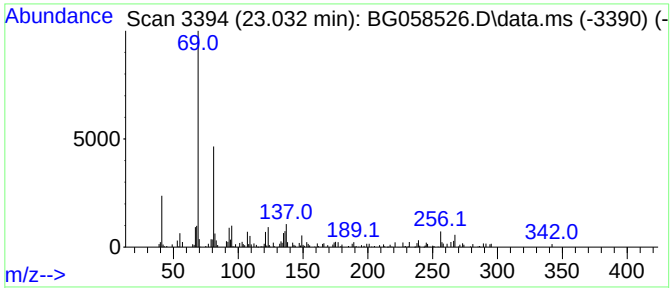
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

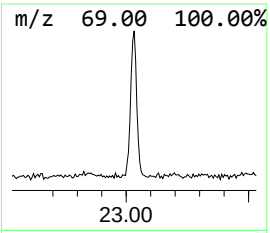
****

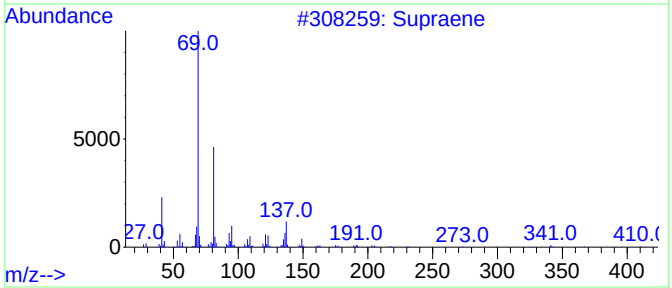
Peak Number 3 Supraene Concentration Rank 4

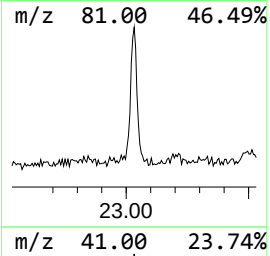
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.032	2.54 ng	124620	Perylene-d12	24.513

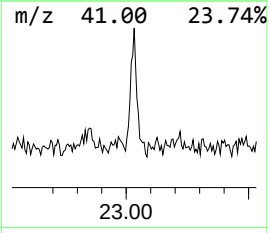
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	83
2	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
3	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	72
4	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	64
5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64

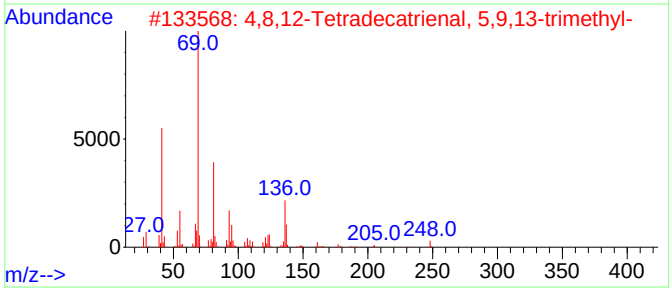


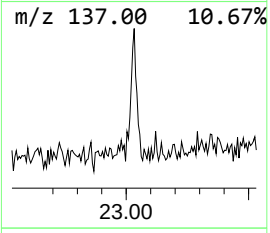


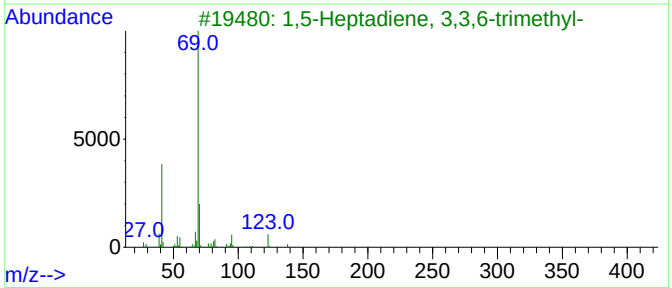


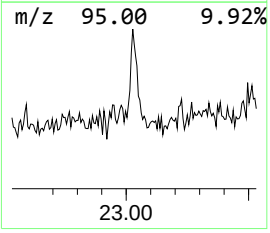












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058526.D
Acq On : 28 Jul 2023 20:23
Operator : MA/JU
Sample : 03580-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

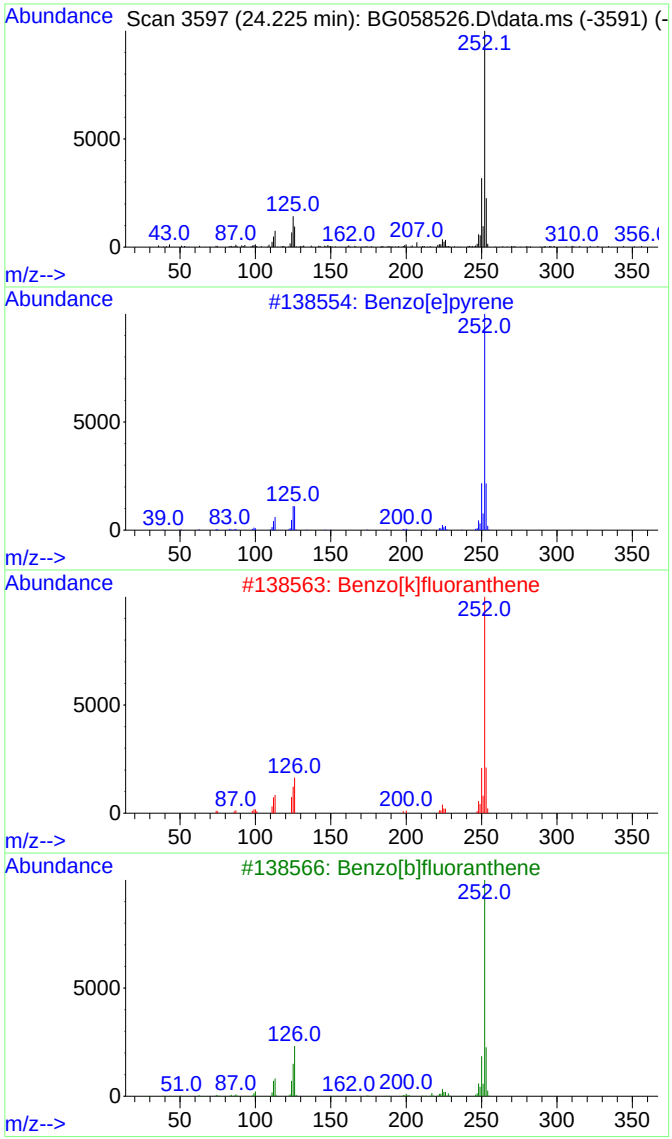
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

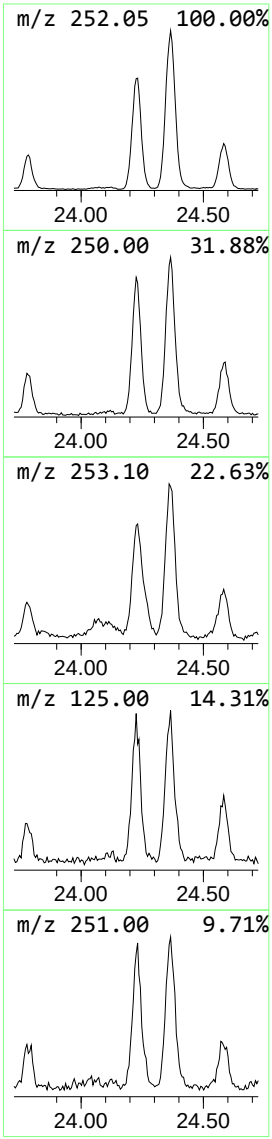
****

Peak Number 4 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.225	6.42 ng	314730	Perylene-d12	24.513

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Perylene	252	C20H12	000198-55-0	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058526.D
Acq On : 28 Jul 2023 20:23
Operator : MA/JU
Sample : 03580-03 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SAMPLE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown18.091	18.091	3.9	ng	155013	4	17.204	796411	20.0
4H-Cyclopenta[d...	18.273	2.5	ng	101656	4	17.204	796411	20.0
Supraene	23.032	2.5	ng	124620	6	24.513	980011	20.0
Benzo[e]pyrene	24.225	6.4	ng	314730	6	24.513	980011	20.0