LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053062.D
Acq On : 6 Apr 2022 19:44
Operator : CG/JU
Sample : N2237-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-0401

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-BG031522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053062.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.691	384	392	401	rBV	438643	718057	48.44%	5.808%
2	7.288	655	664	674	rBV	474688	848852	57.26%	6.866%
3	8.128	800	807	813	rBV	129133	223990	15.11%	1.812%
4	9.286	995	1004	1013	rBV	324590	597536	40.31%	4.834%
5	10.936	1277	1285	1292	rBV	178628	324253	21.87%	2.623%
6	13.374	1692	1700	1707	rBV	759308	1191482	80.37%	9.638%
7	13.956	1795	1799	1805	rBV3	13324	18566	1.25%	0.150%
8	14.749	1926	1934	1941	rBV	297316	472820	31.89%	3.825%
9	14.808	1941	1944	1952	rVB3	9405	14959	1.01%	0.121%
10	15.789	2107	2111	2118	rBV	16269	26567	1.79%	0.215%
11	16.229	2178	2186	2197	rBV	645514	1014543	68.44%	8.207%
12	17.146	2336	2342	2348	rVB3	12055	20287	1.37%	0.164%
13	17.234	2348	2357	2363	rBV5	13214	34913	2.36%	0.282%
14	17.492	2394	2401	2405	rBV	370696	605335	40.83%	4.897%
15	17.533	2405	2408	2416	rVV	208250	291514	19.66%	2.358%
16	17.622	2419	2423	2428	rVV	34130	54511	3.68%	0.441%
17	17.892	2460	2469	2473	rBV3	21313	41490	2.80%	0.336%
18	18.250	2525	2530	2533	rBV5	11814	17480	1.18%	0.141%
19	18.309	2533	2540	2544	rVV7	15433	24952	1.68%	0.202%
20	18.368	2545	2550	2554	rVV2	109757	156677	10.57%	1.267%
21	18.415	2554	2558	2565	rVB	53801	85522	5.77%	0.692%
22	18.497	2568	2572	2577	rVB3	12824	19198	1.30%	0.155%
23	18.561	2577	2583	2586	rBV3	42069	78147	5.27%	0.632%
24	18.661	2597	2600	2605	rBV5	17830	24261	1.64%	0.196%
25	18.791	2619	2622	2626	rVB5	16004	18771	1.27%	0.152%
26	18.855	2630	2633	2637	rVV2	27170	37704	2.54%	0.305%
27	18.896	2637	2640	2647	rVB4	29279	42973	2.90%	0.348%
28	19.284	2700	2706	2710	rBV3	32397	54392	3.67%	0.440%
29	19.413	2723	2728	2733	rBV2	34219	51692	3.49%	0.418%
30	19.537	2743	2749	2755	rVB	357894	523800	35.33%	4.237%
31	19.636	2762	2766	2769	rBV6	36208	47506	3.20%	0.384%
32	19.866	2801	2805	2807	rBV	69396	100358	6.77%	0.812%
33	19.901	2807	2811	2818	rVB	301676	444370	29.98%	3.595%
34	19.965	2818	2822	2826	rVB2	21767	30589	2.06%	0.247%
35	20.089	2837	2843	2849	rBV	1076664	1482459	100.00%	11.992%
36	20.224	2860	2866	2872	rBV7	26512	68201	4.60%	0.552%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053062.D
Acq On : 6 Apr 2022 19:44
Operator : CG/JU
Sample : N2237-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-0401

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-BG031522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.388	2891	2894	2900	rVB3	64308	90193	6.08%	0.730%
38	20.488	2907	2911	2915	rBV3	32945	45273	3.05%	0.366%
39	21.158	3021	3025	3030	rVB	40417	54720	3.69%	0.443%
40	21.393	3061	3065	3070	rBV4	74128	122529	8.27%	0.991%
41	21.775	3122	3130	3135	rBV2	368579	833454	56.22%	6.742%
42	21.822	3135	3138	3148	rVB	127323	219297	14.79%	1.774%
43	24.025	3507	3513	3520	rBV	92287	276522	18.65%	2.237%
44	24.771	3636	3640	3651	rVB2	60764	153791	10.37%	1.244%
45	24.918	3660	3665	3675	rVB	72653	201891	13.62%	1.633%
46	25.088	3684	3694	3702	rBV2	187200	555888	37.50%	4.497%

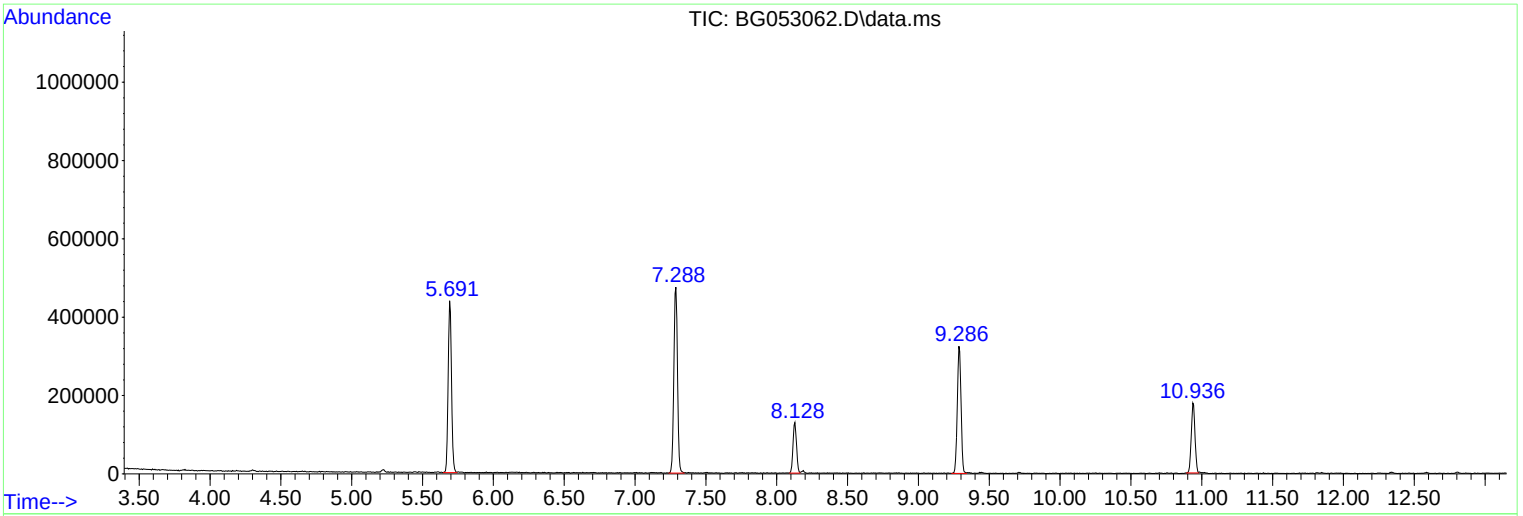
Sum of corrected areas: 12362285

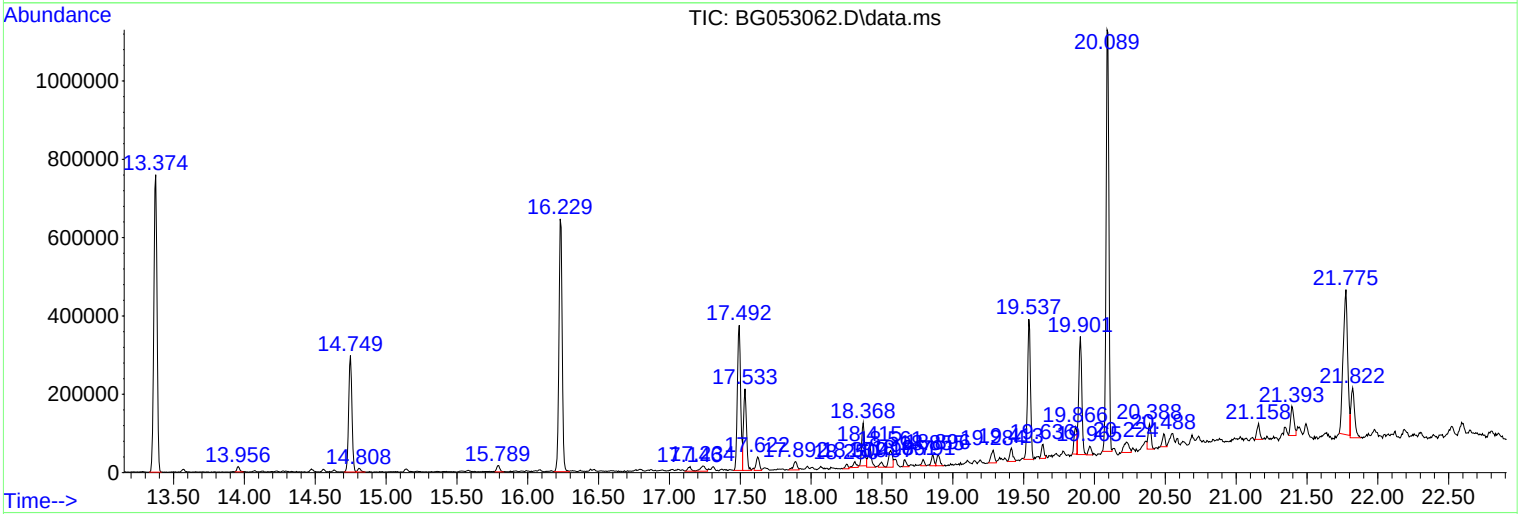
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053062.D
Acq On : 6 Apr 2022 19:44
Operator : CG/JU
Sample : N2237-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

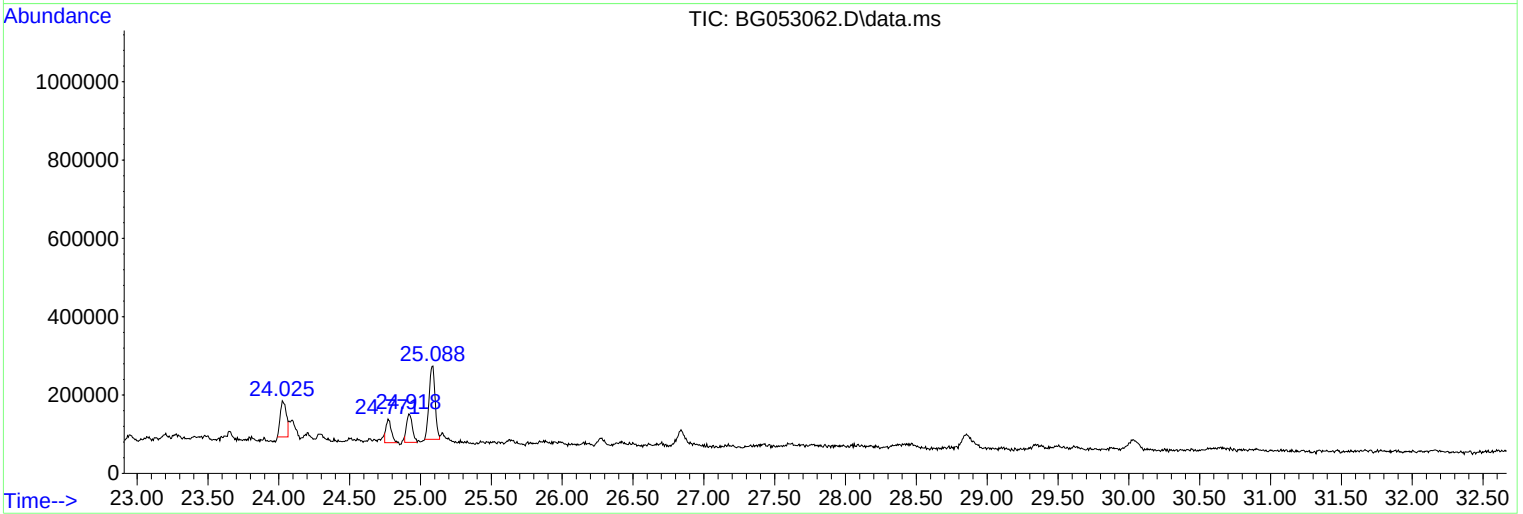
Instrument :
BNA_G
ClientSampleId :
DUP-0401

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.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\BG040622\
Data File : BG053062.D
Acq On : 6 Apr 2022 19:44
Operator : CG/JU
Sample : N2237-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-0401

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

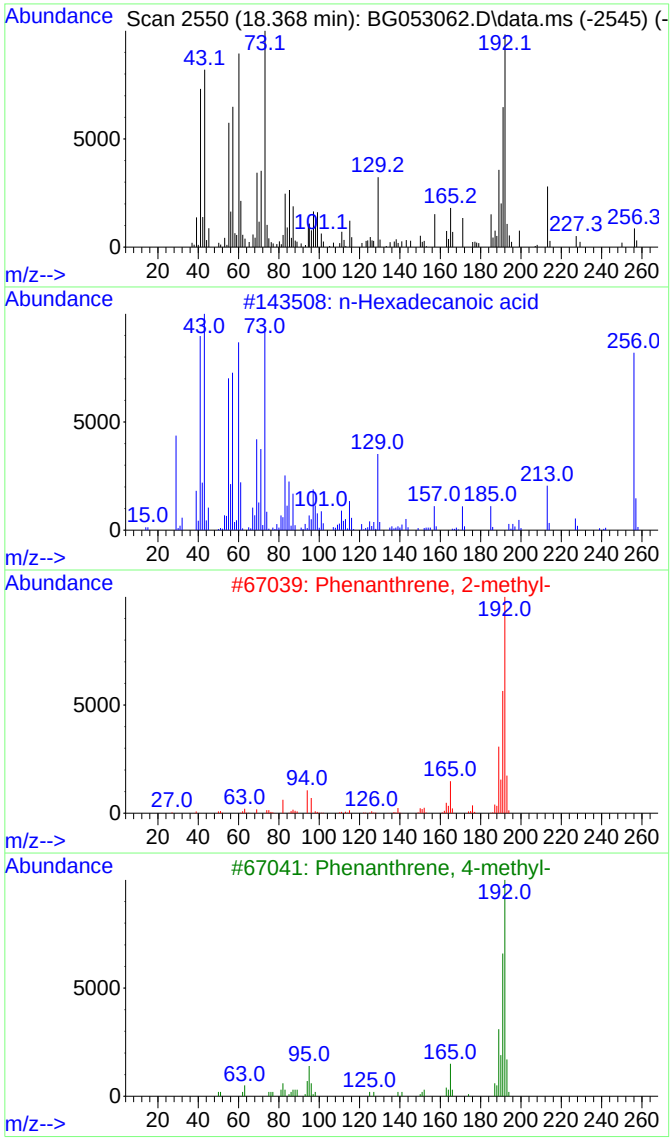
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

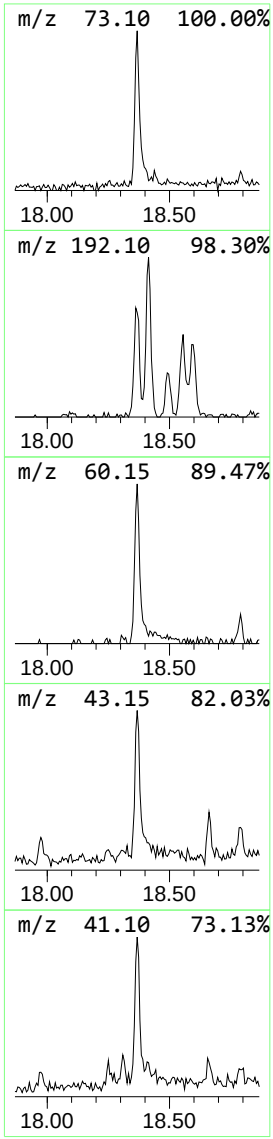
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.368	5.18 ng	156677	Phenanthrene-d10	17.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	55
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	51
4	Tridecanoic acid	214	C13H26O2	000638-53-9	46
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	41





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053062.D
Acq On : 6 Apr 2022 19:44
Operator : CG/JU
Sample : N2237-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-0401

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

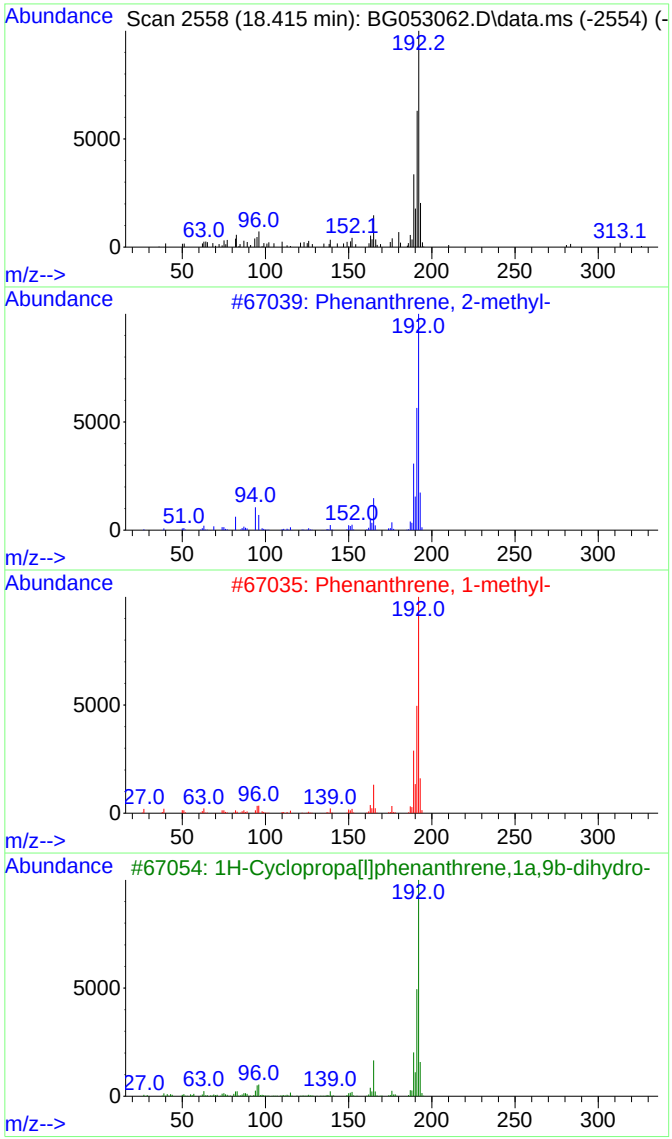
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

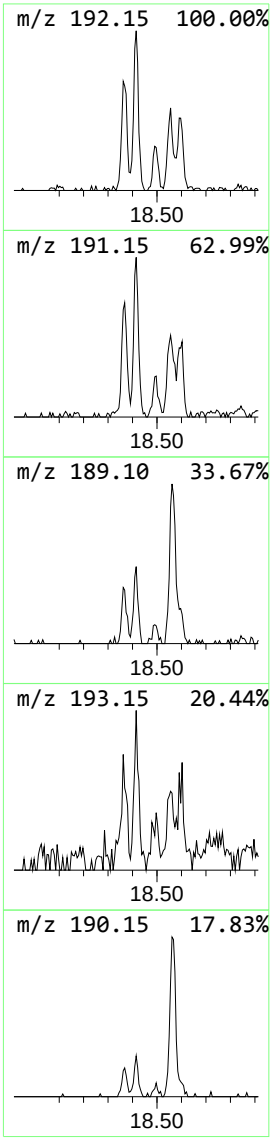
****

Peak Number 2 Phenanthrene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.415	2.83 ng	85522	Phenanthrene-d10	17.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	94
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053062.D
Acq On : 6 Apr 2022 19:44
Operator : CG/JU
Sample : N2237-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-0401

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

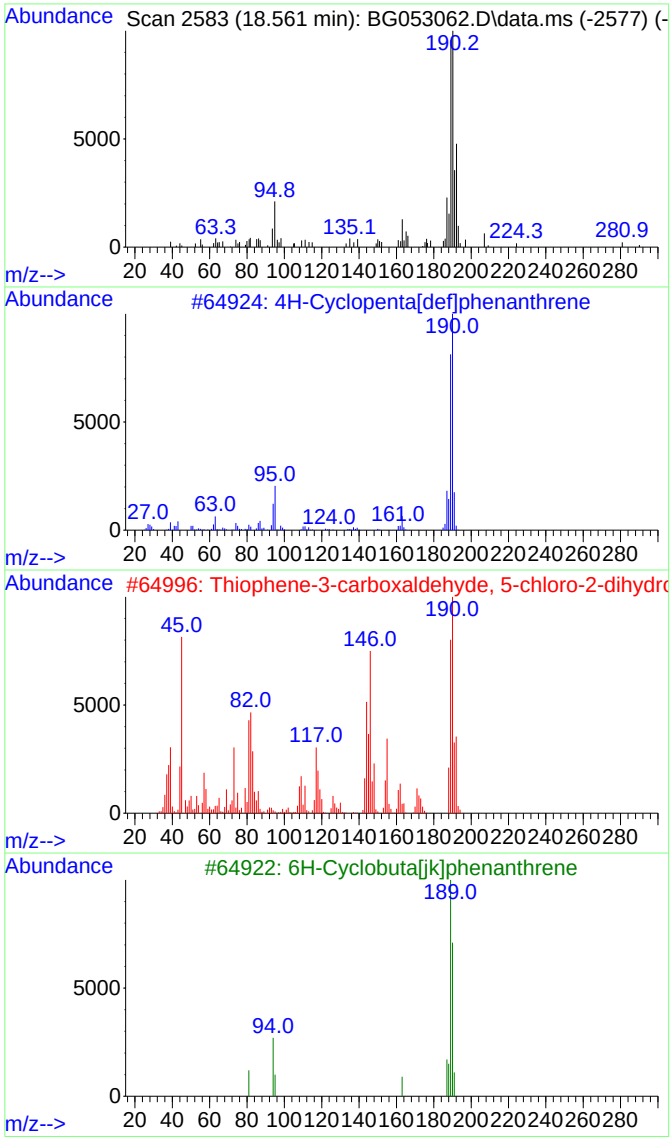
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

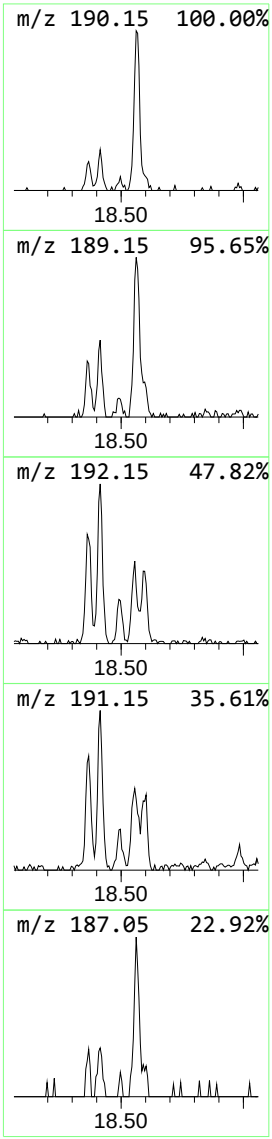
****

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.561	2.58 ng	78147	Phenanthrene-d10	17.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	64
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	45
4	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	40
5	4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053062.D
Acq On : 6 Apr 2022 19:44
Operator : CG/JU
Sample : N2237-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-0401

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

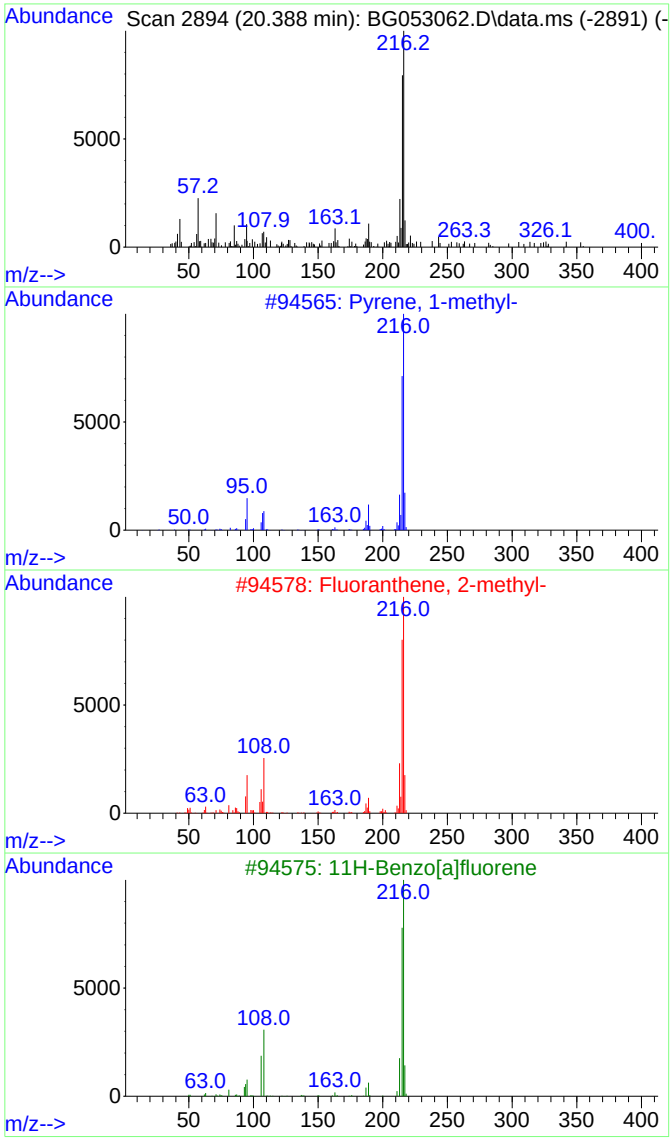
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

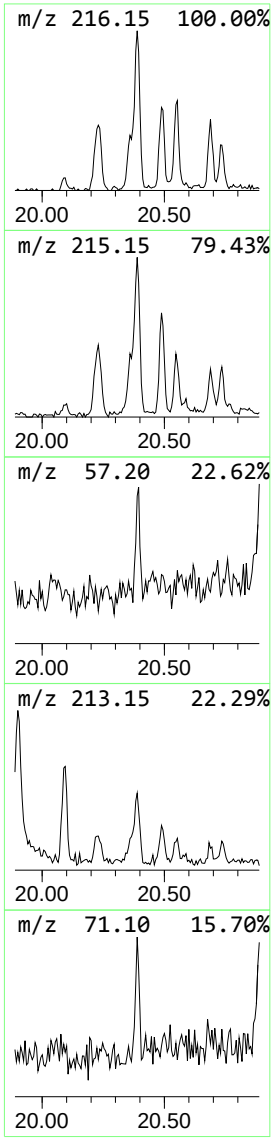
****

Peak Number 4 Pyrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.388	2.16 ng	90193	Chrysene-d12	21.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	92
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	83
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	81
5	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053062.D
Acq On : 6 Apr 2022 19:44
Operator : CG/JU
Sample : N2237-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-0401

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

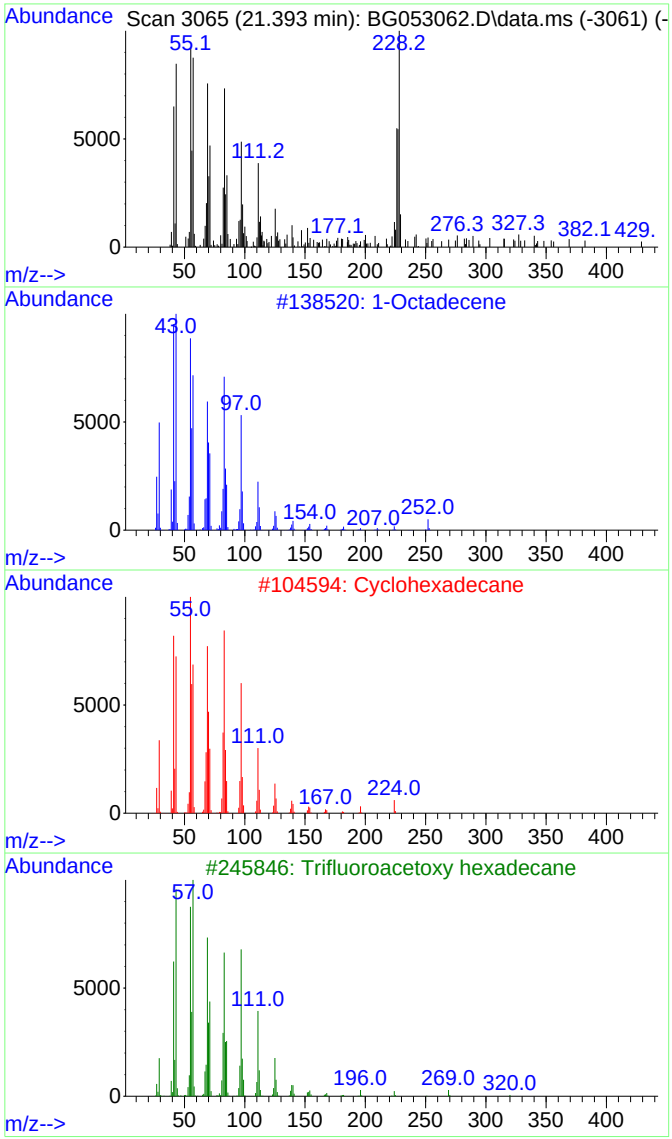
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

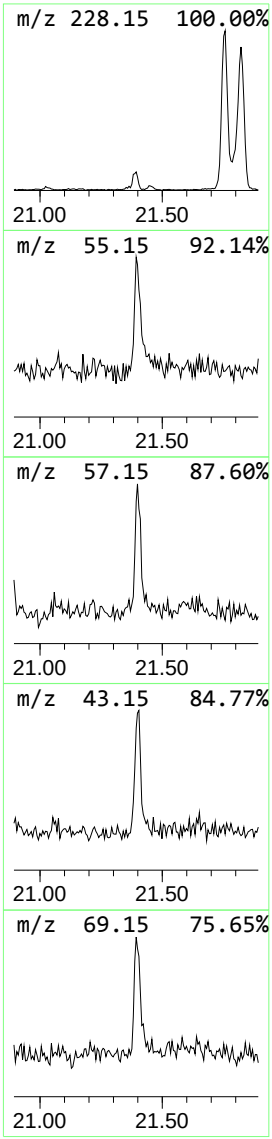
****

Peak Number 5 1-Octadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.393	2.94 ng	122529	Chrysene-d12	21.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	72
2	Cyclohexadecane	224	C16H32	000295-65-8	70
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	64
4	Z-8-Hexadecene	224	C16H32	1000130-87-5	58
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	55





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Sample : N2237-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-0401

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

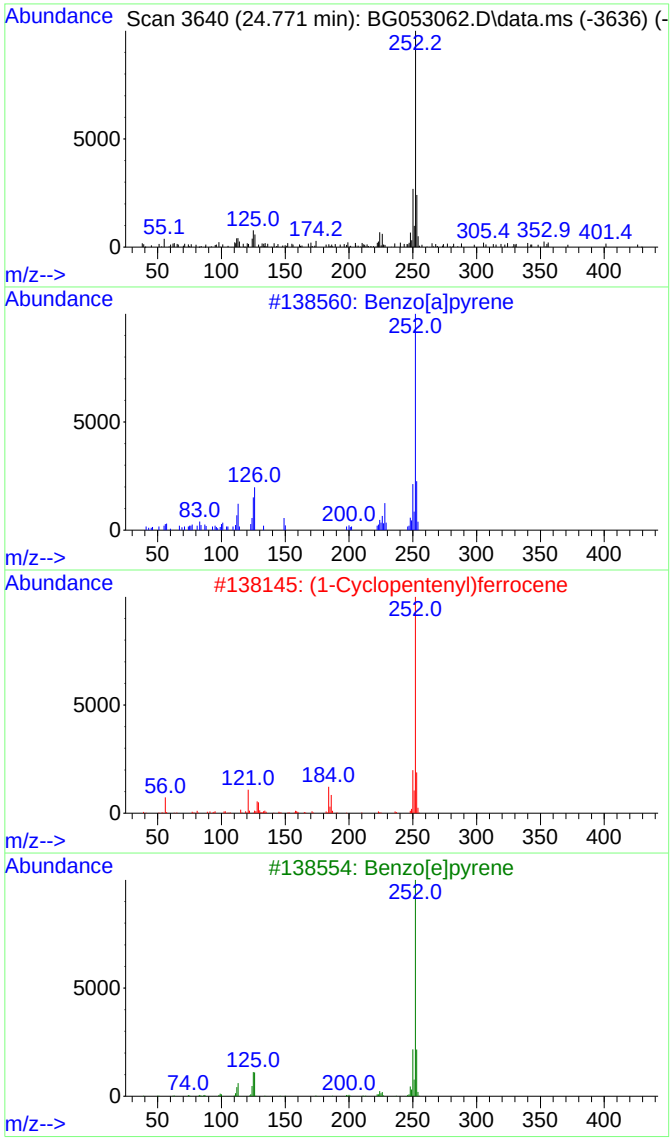
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

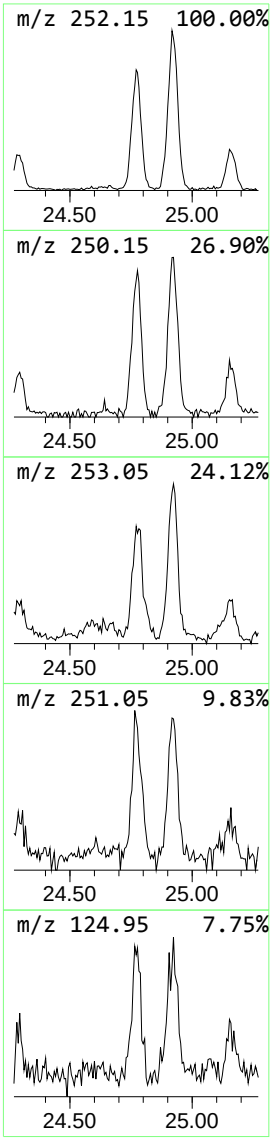
****

Peak Number 6 (1-Cyclopentenyl)ferrocene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.771	5.53 ng	153791	Perylene-d12	25.082

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	89
2	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	86
3	Benzo[e]pyrene	252	C20H12	000192-97-2	76
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	74
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053062.D
Acq On : 6 Apr 2022 19:44
Operator : CG/JU
Sample : N2237-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-0401

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.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
n-Hexadecanoic ...	18.368	5.2	ng	156677	4	17.492	605335	20.0
Phenanthrene, 2...	18.415	2.8	ng	85522	4	17.492	605335	20.0
4H-Cyclopenta[d...	18.561	2.6	ng	78147	4	17.492	605335	20.0
Pyrene, 1-methyl-	20.388	2.2	ng	90193	5	21.775	833454	20.0
1-Octadecene	21.393	2.9	ng	122529	5	21.775	833454	20.0
(1-Cyclopenteny...	24.771	5.5	ng	153791	6	25.082	555888	20.0