LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048612.D
Acq On : 6 Apr 2021 20:27
Operator : CG/JU
Sample : M1933-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BENNETT_BH_05_1-1.5

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-BG033021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048612.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.640	384	392	402	rVB	284678	453752	38.89%	5.242%
2	7.244	658	665	676	rBV	300236	516161	44.24%	5.963%
3	8.090	802	809	816	rVB	103736	172311	14.77%	1.991%
4	9.259	1000	1008	1016	rBV	196665	343136	29.41%	3.964%
5	10.916	1281	1290	1297	rBV	134587	234082	20.06%	2.704%
6	13.366	1700	1707	1714	rBV	474789	726576	62.27%	8.393%
7	14.189	1843	1847	1852	rBV2	14282	21287	1.82%	0.246%
8	14.741	1935	1941	1948	rBV2	203248	329210	28.22%	3.803%
9	14.812	1948	1953	1959	rVB2	6557	12215	1.05%	0.141%
10	16.234	2188	2195	2204	rBV2	407289	630463	54.04%	7.283%
11	17.497	2402	2410	2414	rBV	263029	406525	34.84%	4.696%
12	17.538	2414	2417	2425	rVV	131575	197046	16.89%	2.276%
13	17.632	2427	2433	2439	rVB	21878	39994	3.43%	0.462%
14	17.902	2475	2479	2484	rVB	17203	23733	2.03%	0.274%
15	18.378	2555	2560	2564	rBV3	61419	88840	7.61%	1.026%
16	18.419	2564	2567	2573	rVV3	23534	41103	3.52%	0.475%
17	18.507	2576	2582	2584	rVV7	8654	13682	1.17%	0.158%
18	18.578	2587	2594	2597	rVV2	23108	46609	3.99%	0.538%
19	18.607	2597	2599	2604	rVB3	11993	14401	1.23%	0.166%
20	18.872	2638	2644	2647	rBV3	10402	15324	1.31%	0.177%
21	18.913	2647	2651	2656	rVB5	11148	17041	1.46%	0.197%
22	19.289	2710	2715	2720	rBV8	9961	15867	1.36%	0.183%
23	19.424	2733	2738	2743	rVB7	12575	18336	1.57%	0.212%
24	19.553	2754	2760	2765	rBV	235341	327724	28.09%	3.786%
25	19.647	2772	2776	2780	rBV5	19051	24089	2.06%	0.278%
26	19.876	2811	2815	2817	rBV2	31223	45303	3.88%	0.523%
27	19.912	2817	2821	2829	rVV	174518	265087	22.72%	3.062%
28	19.988	2829	2834	2837	rVB4	9859	14125	1.21%	0.163%
29	20.105	2847	2854	2860	rBV	882398	1166762	100.00%	13.478%
30	20.235	2869	2876	2881	rBV7	14660	34504	2.96%	0.399%
31	20.405	2893	2905	2909	rVB	40555	78384	6.72%	0.905%
32	20.505	2918	2922	2926	rBV	24874	32770	2.81%	0.379%
33	20.564	2926	2932	2936	rVB5	18659	32547	2.79%	0.376%
34	20.705	2953	2956	2959	rBV4	12733	18402	1.58%	0.213%
35	20.746	2960	2963	2967	rVB5	13528	17390	1.49%	0.201%
36	21.169	3032	3035	3043	rVB4	16488	25676	2.20%	0.297%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048612.D
Acq On : 6 Apr 2021 20:27
Operator : CG/JU
Sample : M1933-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BENNETT_BH_05_1-1.5

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-BG033021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.369	3063	3069	3072	rBV4	13530	25860	2.22%	0.299%
38	21.416	3072	3077	3080	rBV4	68493	96544	8.27%	1.115%
39	21.516	3090	3094	3101	rVB2	24538	40541	3.47%	0.468%
40	21.798	3133	3142	3147	rBV2	308669	690247	59.16%	7.974%
41	21.845	3147	3150	3156	rVB	91563	137838	11.81%	1.592%
42	21.997	3173	3176	3182	rBV8	10361	15210	1.30%	0.176%
43	22.215	3207	3213	3217	rBV5	18858	33172	2.84%	0.383%
44	22.550	3266	3270	3277	rVB6	15821	28533	2.45%	0.330%
45	22.626	3279	3283	3290	rVB8	17130	35336	3.03%	0.408%
46	22.873	3323	3325	3332	rVB8	9456	16446	1.41%	0.190%
47	22.984	3341	3344	3349	rVB7	9790	16323	1.40%	0.189%
48	23.701	3462	3466	3474	rVB8	25273	46830	4.01%	0.541%
49	24.083	3521	3531	3539	rBV2	55372	217173	18.61%	2.509%
50	24.330	3570	3573	3581	rVB7	10235	23980	2.06%	0.277%
51	24.823	3649	3657	3665	rBV3	33539	98370	8.43%	1.136%
52	24.970	3674	3682	3691	rBV2	49363	137612	11.79%	1.590%
53	25.141	3701	3711	3720	rBV	167558	476273	40.82%	5.502%
54	28.954	4349	4360	4362	rBV10	21383	59885	5.13%	0.692%

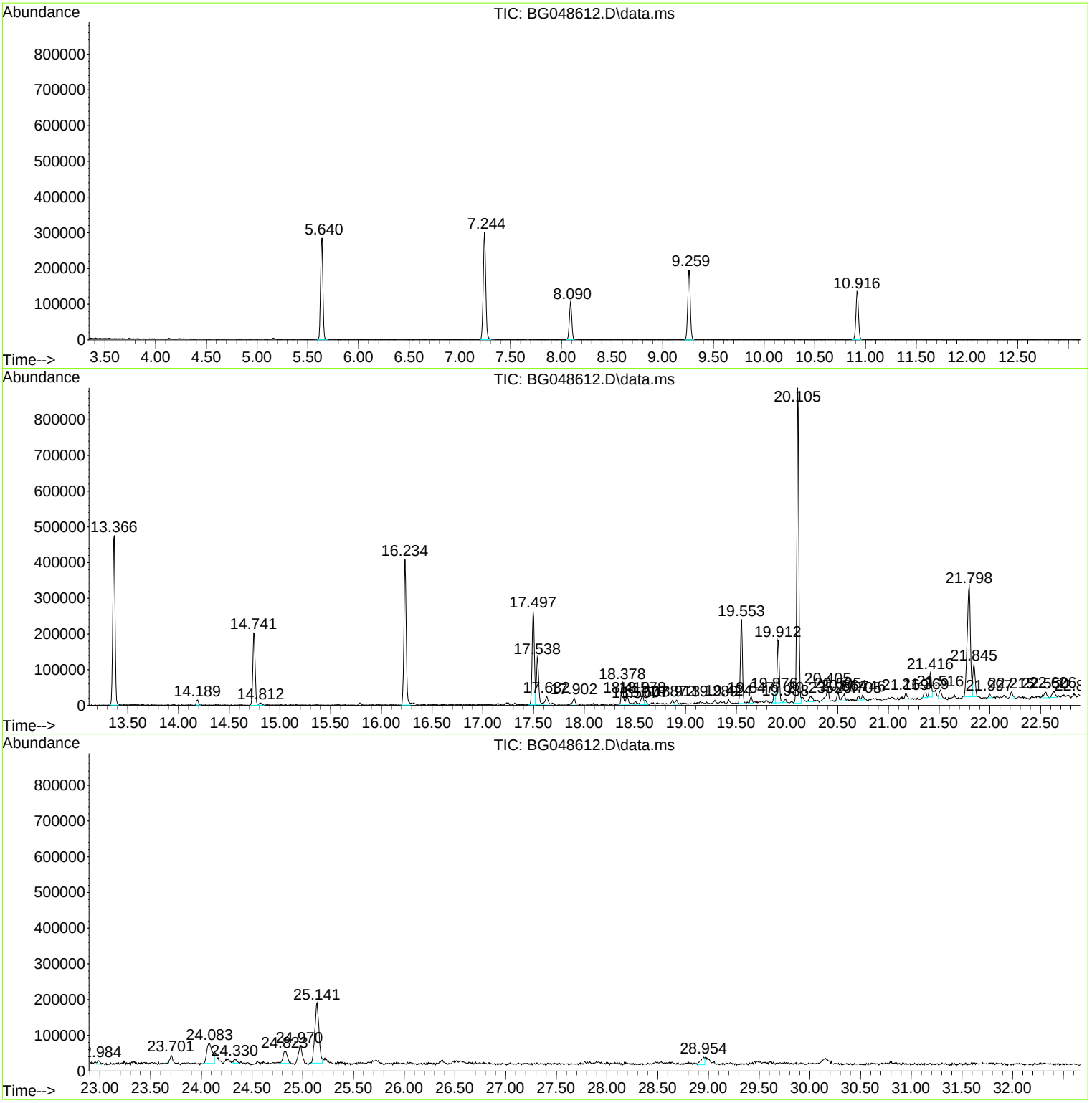
Sum of corrected areas: 8656630

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048612.D
Acq On : 6 Apr 2021 20:27
Operator : CG/JU
Sample : M1933-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_1-1.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048612.D
Acq On : 6 Apr 2021 20:27
Operator : CG/JU
Sample : M1933-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BENNETT_BH_05_1-1.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

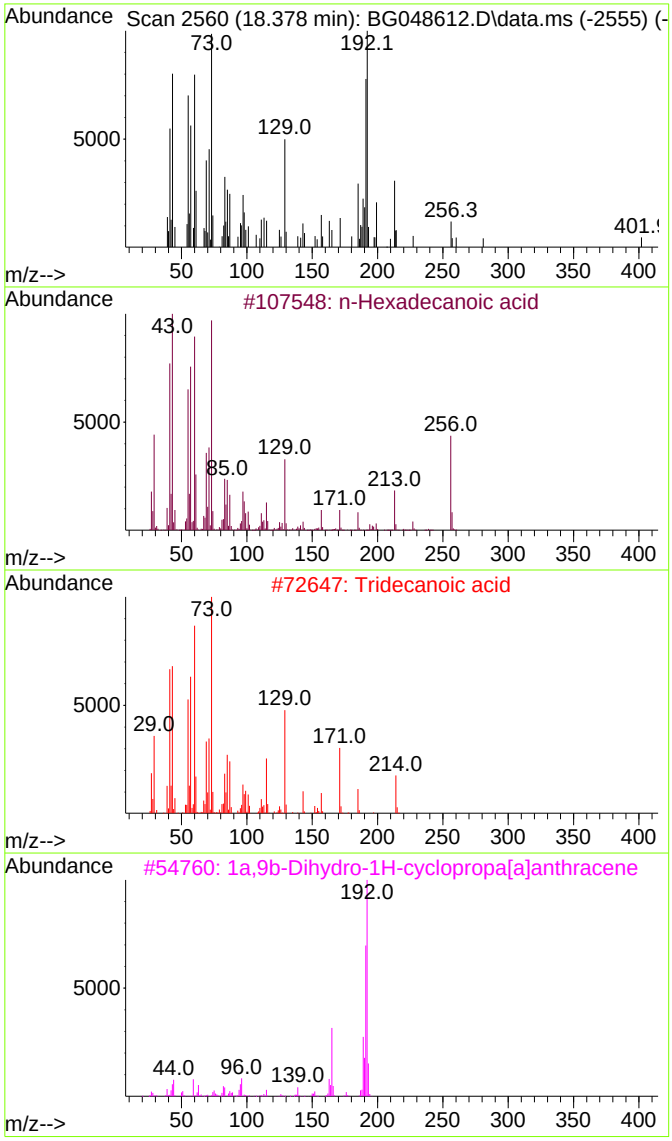
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

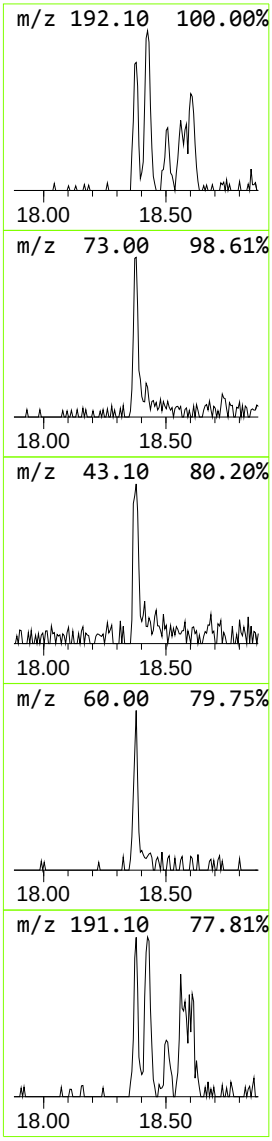
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.378	4.37 ng	88840	Phenanthrene-d10	17.497

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	47
3	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	38
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	38
5	Octadecanoic acid	284	C18H36O2	000057-11-4	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048612.D
Acq On : 6 Apr 2021 20:27
Operator : CG/JU
Sample : M1933-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_1-1.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

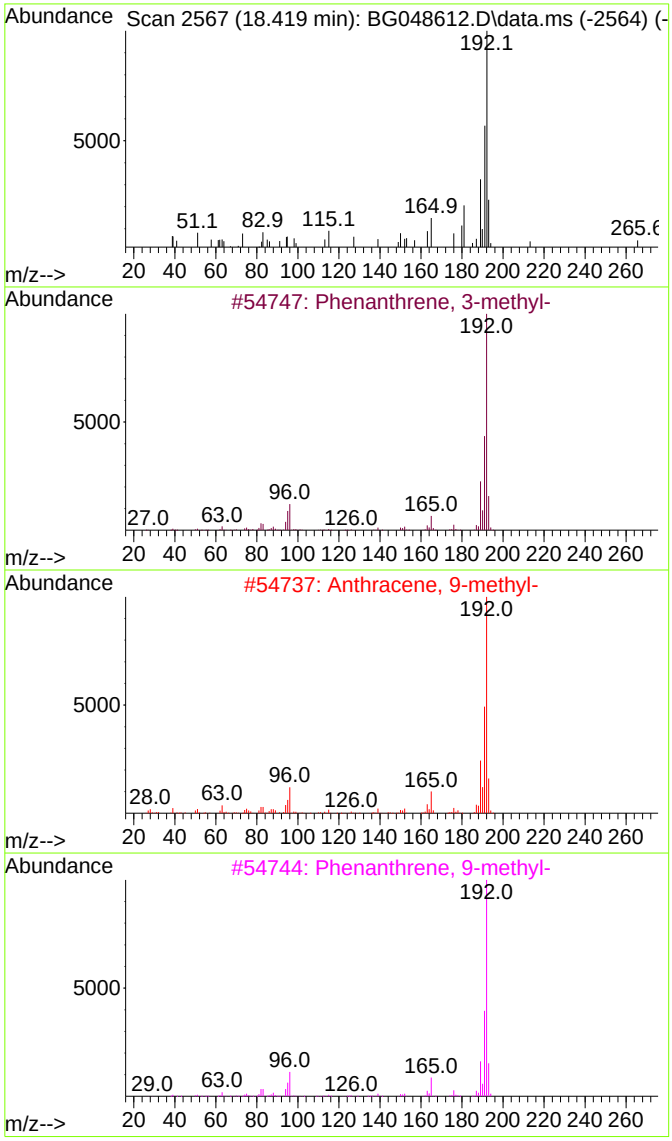
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

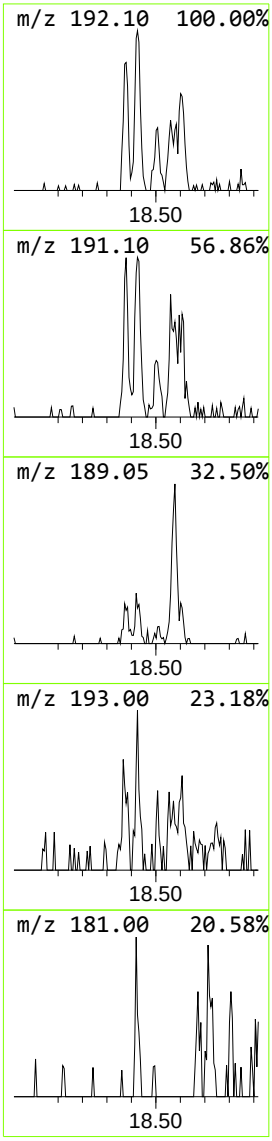
****

Peak Number 2 Phenanthrene, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.419	2.02 ng	41103	Phenanthrene-d10	17.497

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	70
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	62
3	Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	58
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	58
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048612.D
Acq On : 6 Apr 2021 20:27
Operator : CG/JU
Sample : M1933-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_1-1.5

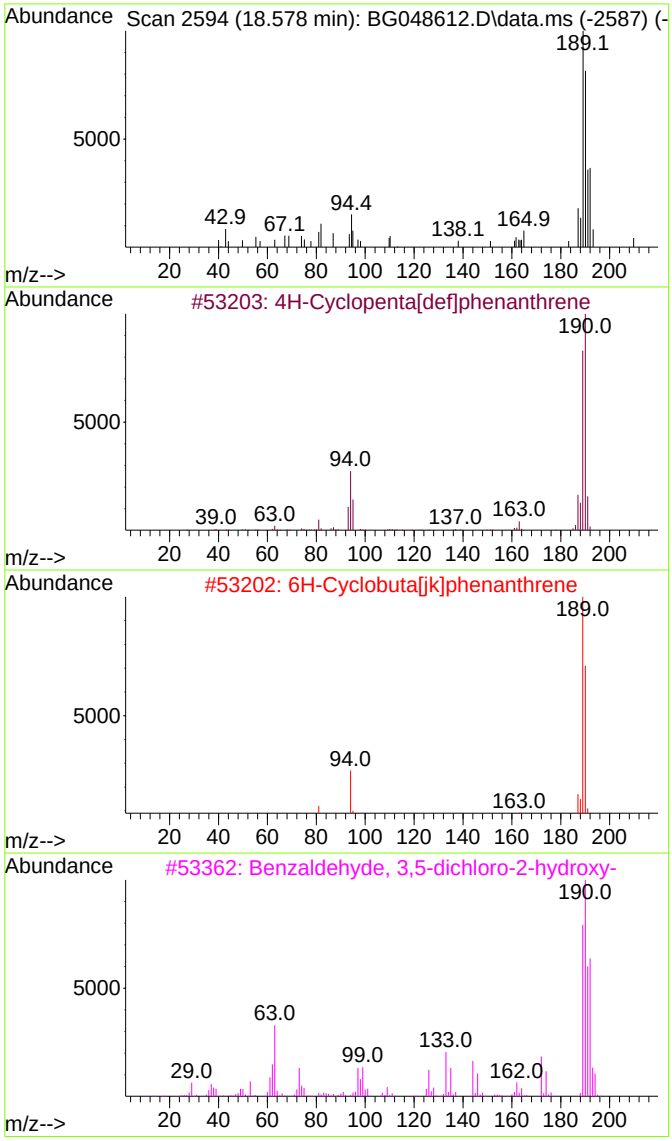
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

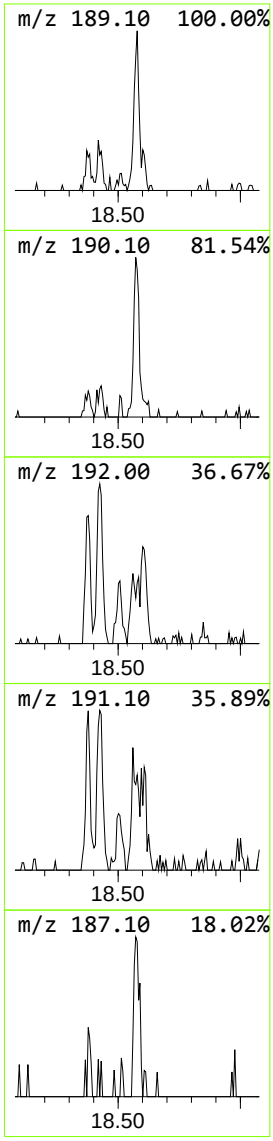
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.578	2.29 ng	46609	Phenanthrene-d10	17.497

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	72
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	52
4	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27
5	1-Aminocyclopentanecarboxylic ac...	403	C21H38ClNO4	1000329-17-3	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048612.D
Acq On : 6 Apr 2021 20:27
Operator : CG/JU
Sample : M1933-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_1-1.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

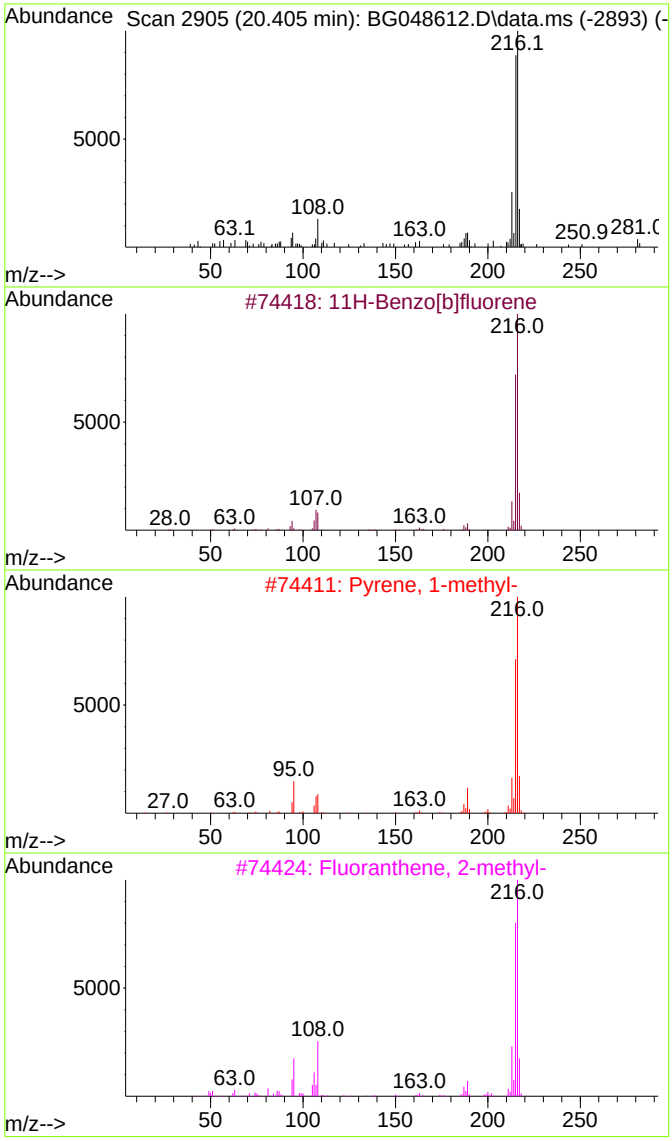
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

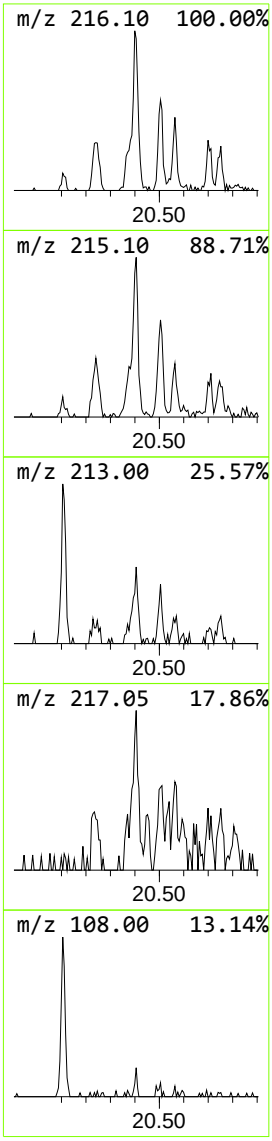
****

Peak Number 4 11H-Benzo[b]fluorene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.405	2.27 ng	78384	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	83
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	74
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	74
5	4-Trifluoromethylcinnamic acid	216	C10H7F3O2	002062-26-2	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048612.D
Acq On : 6 Apr 2021 20:27
Operator : CG/JU
Sample : M1933-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_1-1.5

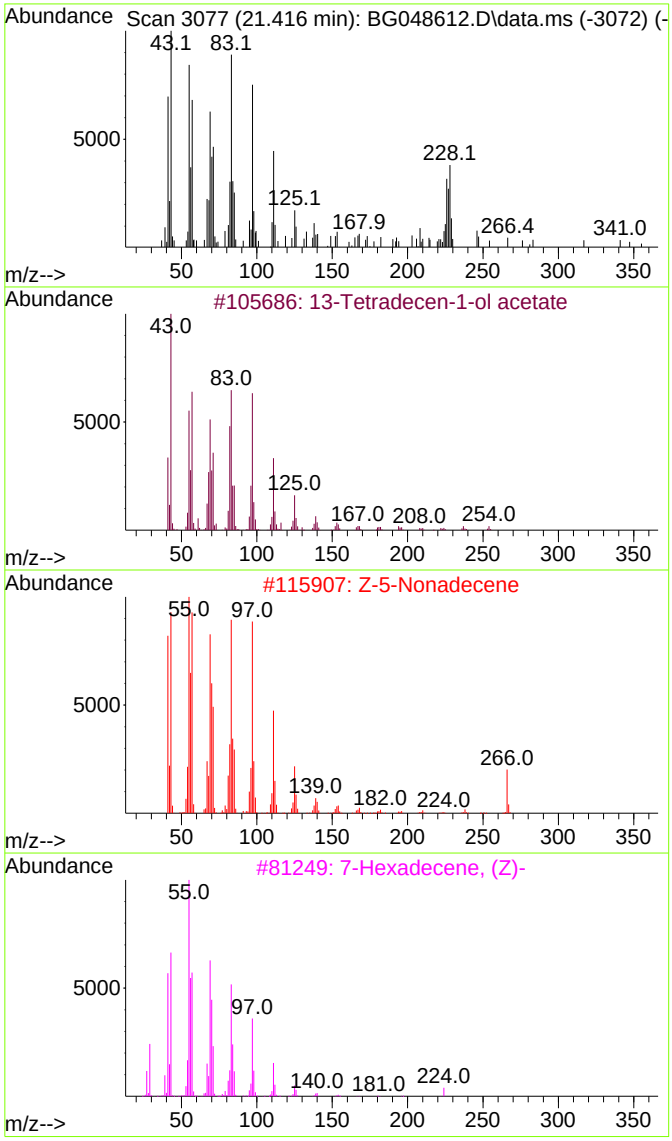
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

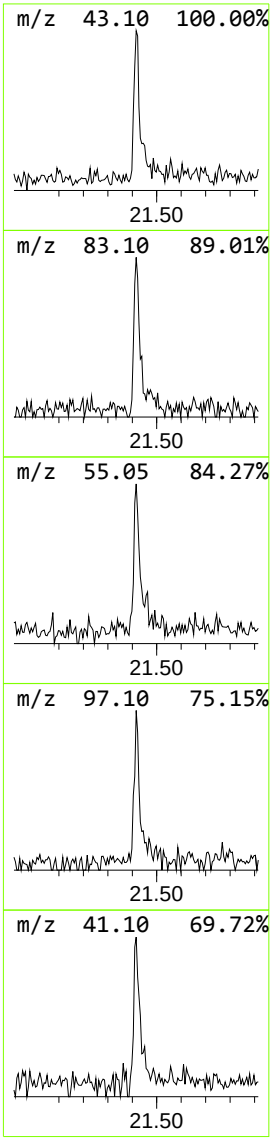
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 13-Tetradecen-1-ol acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	2.80 ng	96544	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	93
2	Z-5-Nonadecene	266	C19H38	1000131-11-8	90
3	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	90
4	1-Nonadecene	266	C19H38	018435-45-5	89
5	Cetene	224	C16H32	000629-73-2	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048612.D
Acq On : 6 Apr 2021 20:27
Operator : CG/JU
Sample : M1933-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_1-1.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

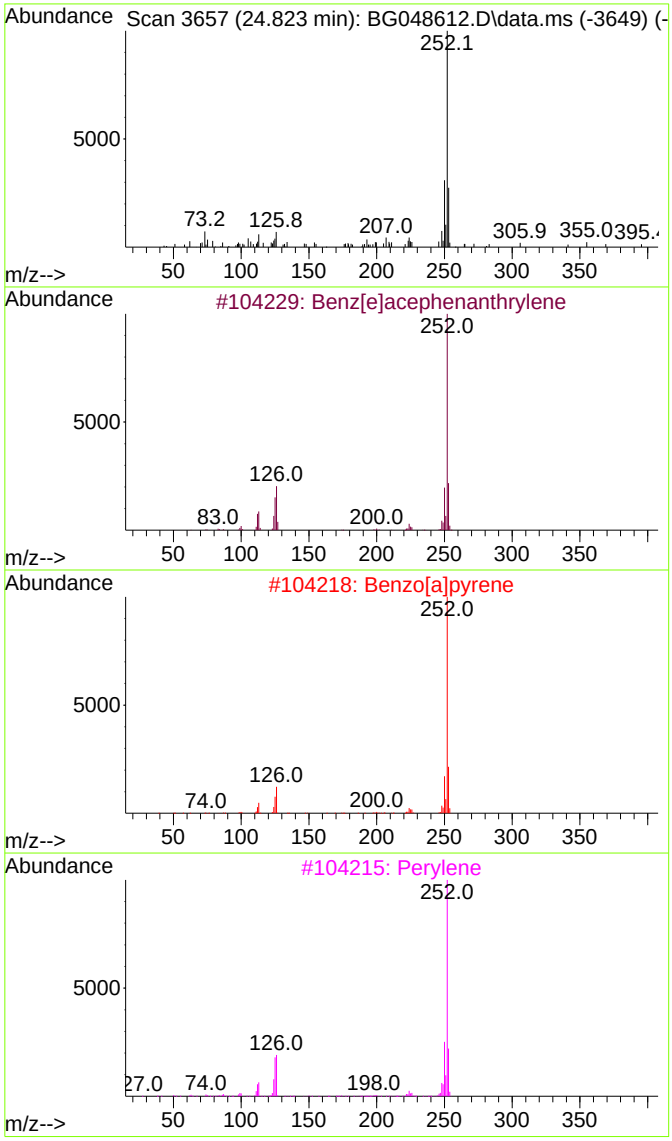
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

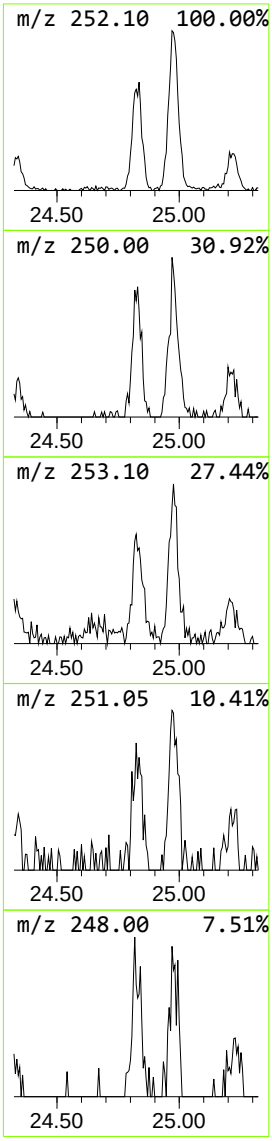
****

Peak Number 6 Perylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.823	4.13 ng	98370	Perylene-d12	25.141

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	81
2	Benzo[a]pyrene	252	C20H12	000050-32-8	76
3	Perylene	252	C20H12	000198-55-0	76
4	Benzo[e]pyrene	252	C20H12	000192-97-2	68
5	1-Phenyl-3-(4-methoxyphenyl)-2-p...	252	C16H16N2O	003314-43-0	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048612.D
Acq On : 6 Apr 2021 20:27
Operator : CG/JU
Sample : M1933-16
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BENNETT_BH_05_1-1.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	18.378	4.4	ng	88840	4	17.497	406525	20.0
Phenanthrene, 3...	18.419	2.0	ng	41103	4	17.497	406525	20.0
4H-Cyclopenta[d...	18.578	2.3	ng	46609	4	17.497	406525	20.0
11H-Benzo[b]flu...	20.405	2.3	ng	78384	5	21.798	690247	20.0
13-Tetradecen-1...	21.416	2.8	ng	96544	5	21.798	690247	20.0
Perylene	24.823	4.1	ng	98370	6	25.141	476273	20.0