LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054290.D
Acq On : 14 Jul 2022 21:52
Operator : CG/JU
Sample : N3688-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-12016

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-BG071222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054290.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.609	370	378	388	rBV	224379	383597	23.05%	3.876%
2	7.207	643	650	664	rBB	238437	423525	25.45%	4.279%
3	8.035	785	791	799	rBV	57406	100717	6.05%	1.018%
4	9.199	980	989	1000	rBB	146033	272107	16.35%	2.749%
5	10.844	1262	1269	1280	rBB	76886	141218	8.49%	1.427%
6	13.288	1678	1685	1695	rBV	504047	794716	47.76%	8.029%
7	14.669	1913	1920	1926	rBB	146147	233375	14.02%	2.358%
8	16.155	2166	2173	2187	rBV	491646	794492	47.74%	8.027%
9	17.412	2380	2387	2391	rBV	215253	344308	20.69%	3.479%
10	17.448	2391	2393	2400	rVB	70896	100650	6.05%	1.017%
11	18.288	2529	2536	2540	rBV	22988	39302	2.36%	0.397%
12	18.335	2540	2544	2552	rVB	27919	43864	2.64%	0.443%
13	18.476	2562	2568	2572	rBV3	28100	55015	3.31%	0.556%
14	18.511	2572	2574	2582	rVB2	17651	26866	1.61%	0.271%
15	18.781	2614	2620	2623	rBV	14516	23123	1.39%	0.234%
16	18.823	2623	2627	2635	rVB4	17222	28768	1.73%	0.291%
17	19.199	2685	2691	2695	rBV	23797	39920	2.40%	0.403%
18	19.340	2711	2715	2724	rBV4	14817	29122	1.75%	0.294%
19	19.463	2729	2736	2742	rBV	227840	343175	20.62%	3.467%
20	19.616	2757	2762	2766	rBV	16175	24137	1.45%	0.244%
21	19.786	2786	2791	2793	rBV	31768	46423	2.79%	0.469%
22	19.821	2793	2797	2805	rVB	201833	306046	18.39%	3.092%
23	19.892	2805	2809	2814	rVB2	14145	20715	1.24%	0.209%
24	20.015	2816	2830	2836	rBV	1175532	1664081	100.00%	16.813%
25	20.145	2846	2852	2858	rBV6	21404	53584	3.22%	0.541%
26	20.280	2870	2875	2876	rBV4	18414	23239	1.40%	0.235%
27	20.315	2877	2881	2886	rVB	42884	66609	4.00%	0.673%
28	20.415	2889	2898	2902	rBV	25104	45820	2.75%	0.463%
29	20.474	2902	2908	2912	rBV2	28348	44524	2.68%	0.450%
30	20.609	2927	2931	2935	rBV	21175	30354	1.82%	0.307%
31	20.656	2935	2939	2943	rVB	18292	26636	1.60%	0.269%
32	20.767	2954	2958	2963	rVB3	20947	26289	1.58%	0.266%
33	21.079	3006	3011	3017	rVB	26576	40415	2.43%	0.408%
34	21.261	3034	3042	3046	rBV3	26386	57878	3.48%	0.585%
35	21.308	3046	3050	3054	rVV3	46674	83791	5.04%	0.847%
36	21.355	3054	3058	3063	rVV4	24389	51568	3.10%	0.521%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054290.D
Acq On : 14 Jul 2022 21:52
Operator : CG/JU
Sample : N3688-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-12016

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-BG071222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.408	3063	3067	3076	rVB2	29691	56948	3.42%	0.575%
38	21.678	3103	3113	3118	rBV2	317786	742421	44.61%	7.501%
39	21.725	3118	3121	3132	rVB	115572	208811	12.55%	2.110%
40	21.878	3143	3147	3151	rBV4	10674	18714	1.12%	0.189%
41	21.948	3154	3159	3163	rBV	15920	29157	1.75%	0.295%
42	22.095	3176	3184	3190	rBV3	20187	61922	3.72%	0.626%
43	22.407	3229	3237	3243	rBV	26166	62963	3.78%	0.636%
44	22.489	3245	3251	3256	rVV3	19131	44132	2.65%	0.446%
45	22.577	3262	3266	3270	rVB4	19097	32554	1.96%	0.329%
46	22.695	3279	3286	3287	rBV4	27442	54738	3.29%	0.553%
47	22.847	3308	3312	3317	rBV3	32309	62606	3.76%	0.633%
48	23.076	3347	3351	3355	rBV4	16796	30443	1.83%	0.308%
49	23.282	3381	3386	3390	rBV2	22093	42562	2.56%	0.430%
50	23.499	3419	3423	3426	rBV5	11382	21741	1.31%	0.220%
51	23.887	3481	3489	3497	rBV	91867	291521	17.52%	2.945%
52	24.152	3527	3534	3541	rVB2	15496	42164	2.53%	0.426%
53	24.616	3605	3613	3624	rVB	54872	163440	9.82%	1.651%
54	24.763	3628	3638	3649	rVB	70110	208692	12.54%	2.108%
55	24.921	3654	3665	3674	rBV2	157091	477811	28.71%	4.827%
56	25.685	3791	3795	3807	rVB10	11511	38138	2.29%	0.385%
57	26.067	3854	3860	3864	rBV7	10544	24182	1.45%	0.244%
58	28.611	4280	4293	4310	rVB2	34834	166935	10.03%	1.687%
59	29.087	4366	4374	4381	rBV5	8114	26388	1.59%	0.267%
60	29.581	4447	4458	4460	rBV10	11356	31603	1.90%	0.319%
61	29.757	4475	4488	4505	rBV	27246	127155	7.64%	1.285%

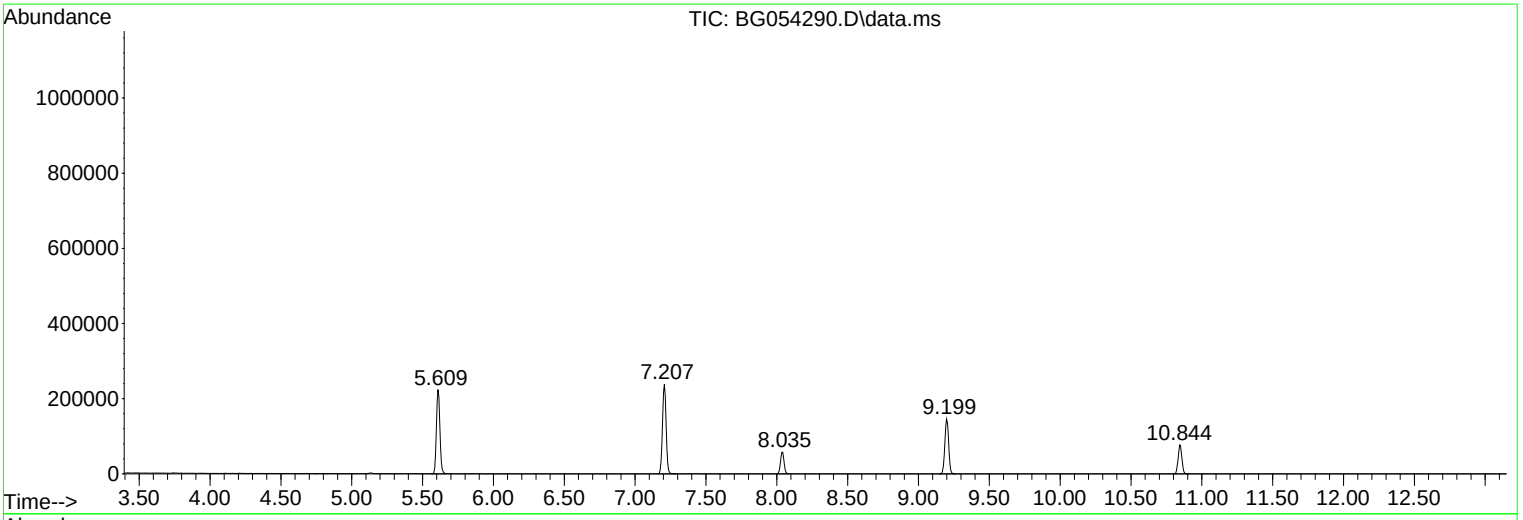
Sum of corrected areas: 9897710

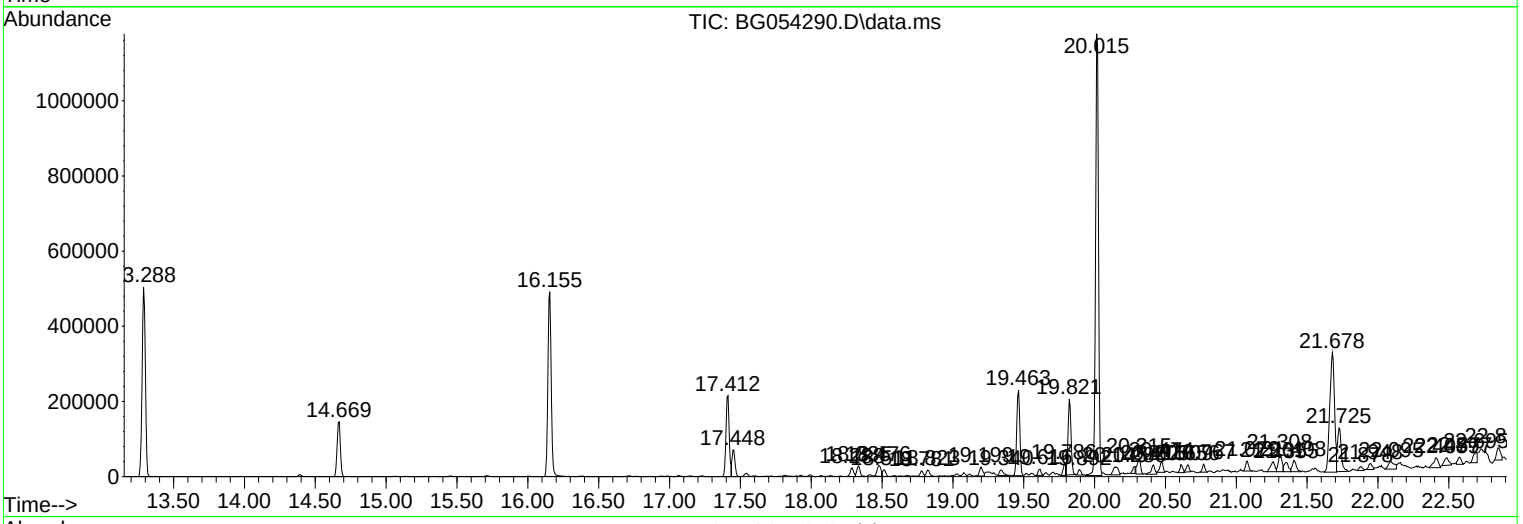
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054290.D
Acq On : 14 Jul 2022 21:52
Operator : CG/JU
Sample : N3688-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

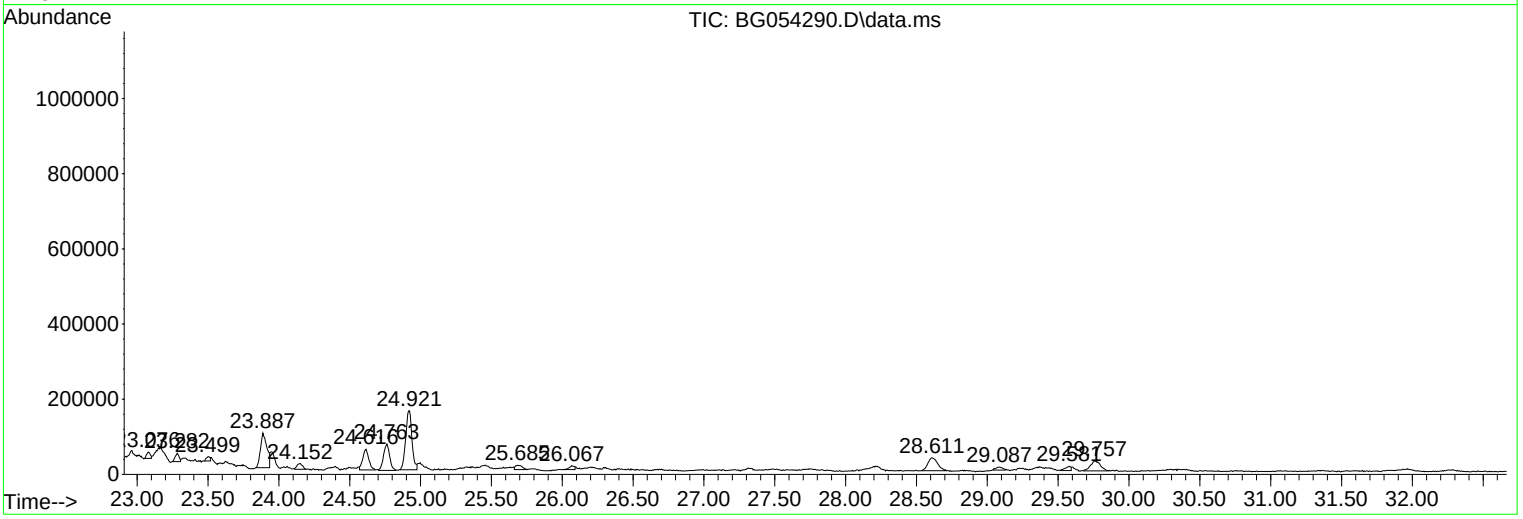
Instrument :
BNA_G
ClientSampleId :
72-12016

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.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\BG071422\
Data File : BG054290.D
Acq On : 14 Jul 2022 21:52
Operator : CG/JU
Sample : N3688-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-12016

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

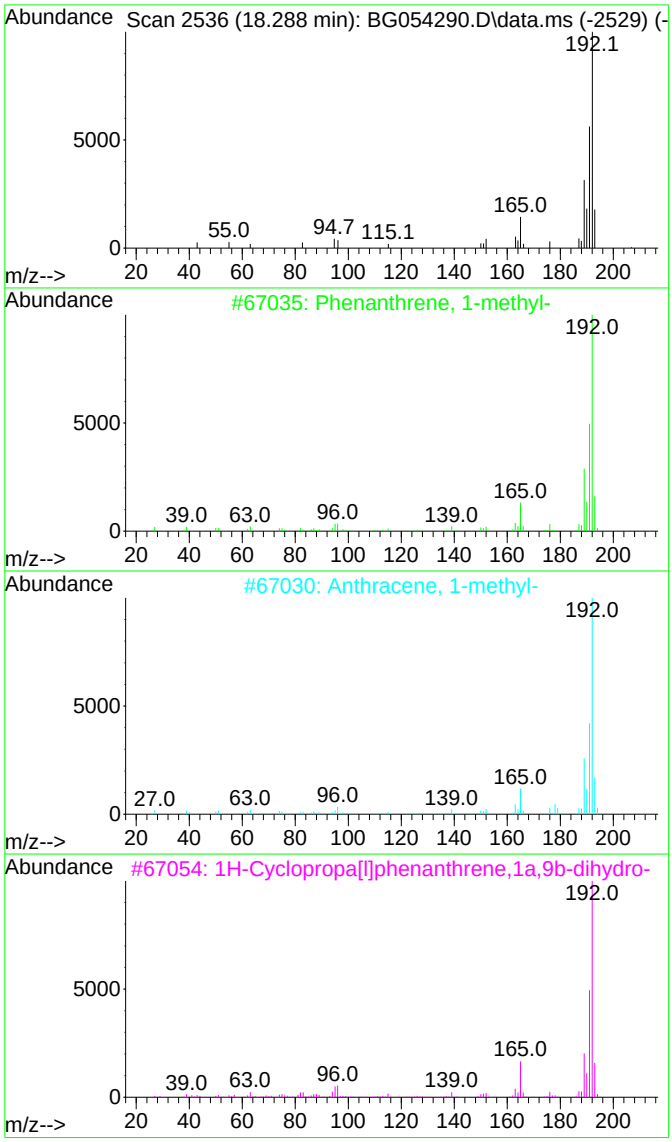
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

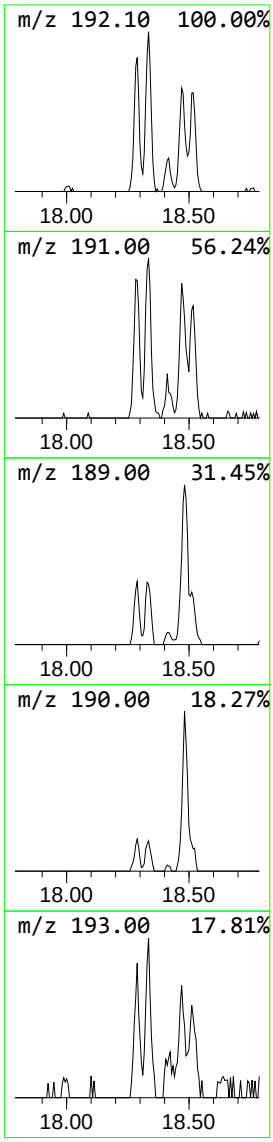
****

Peak Number 1 Phenanthrene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.288	2.28 ng	39302	Phenanthrene-d10	17.413

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054290.D
Acq On : 14 Jul 2022 21:52
Operator : CG/JU
Sample : N3688-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-12016

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

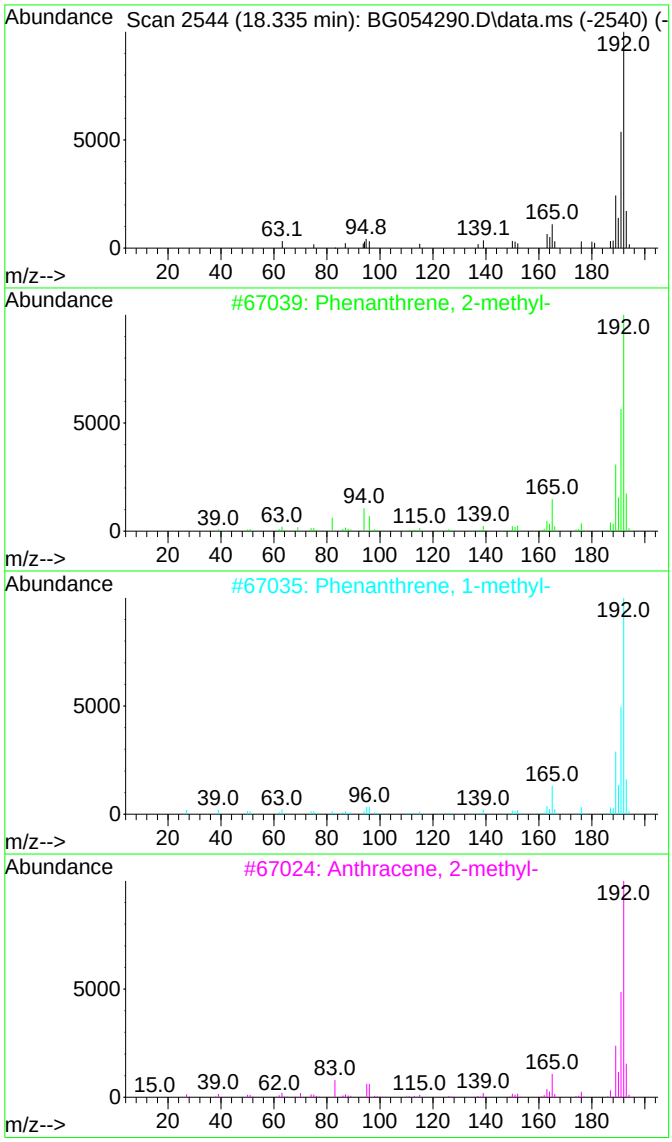
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

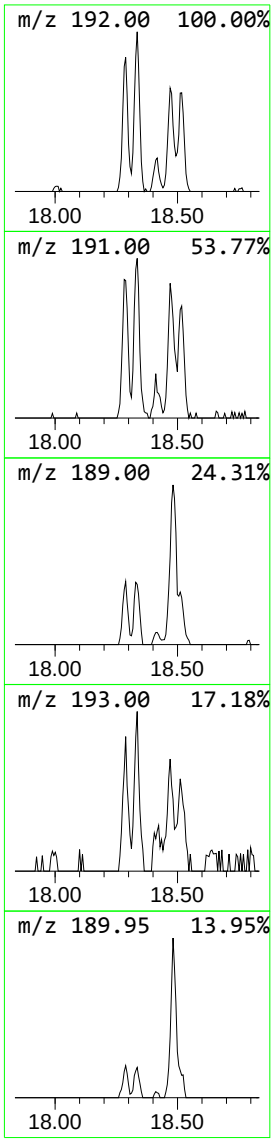
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.335	2.55 ng	43864	Phenanthrene-d10	17.413

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054290.D
Acq On : 14 Jul 2022 21:52
Operator : CG/JU
Sample : N3688-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-12016

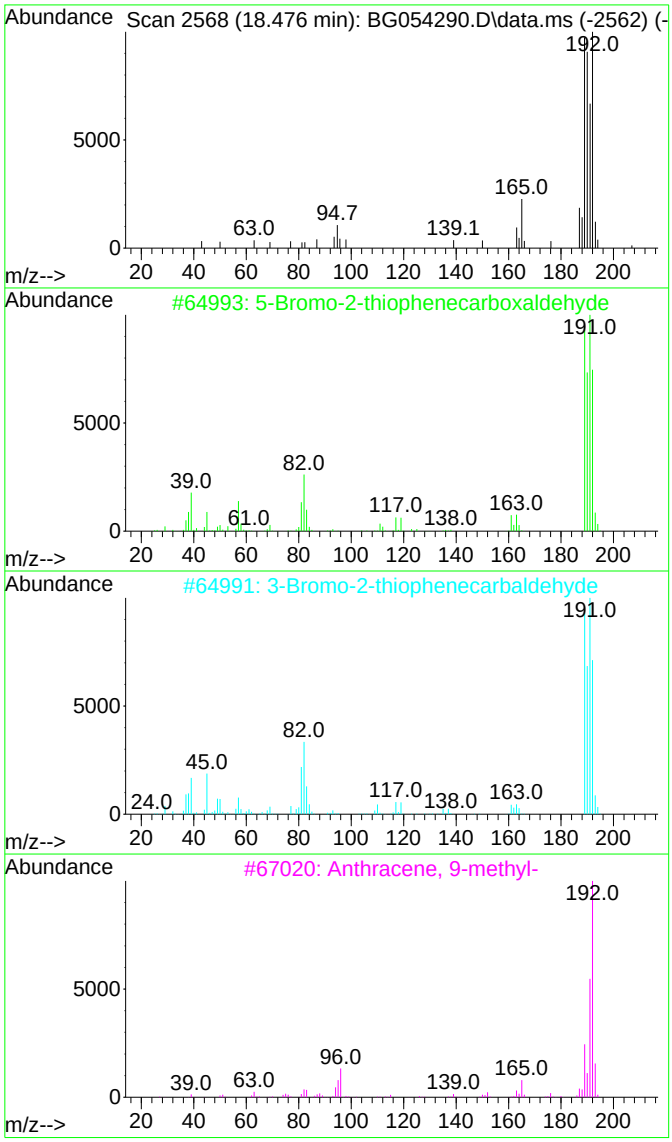
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

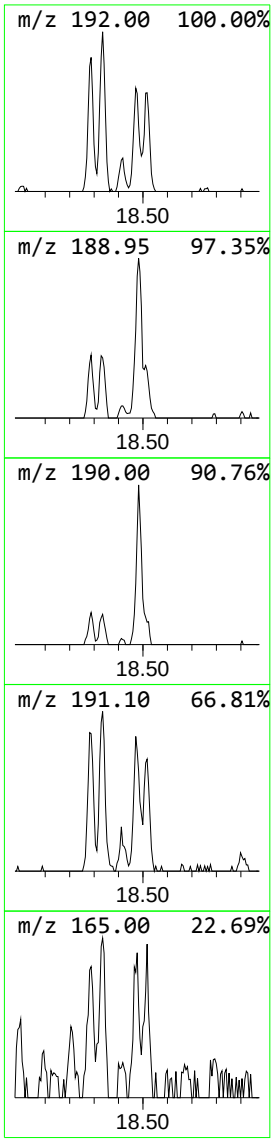
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 5-Bromo-2-thiophenecarboxal... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.476	3.20 ng	55015	Phenanthrene-d10	17.413

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	64
2	3-Bromo-2-thiophenecarbaldehyde	190	C5H3BrOS	000930-96-1	64
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	50
4	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	46
5	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054290.D
Acq On : 14 Jul 2022 21:52
Operator : CG/JU
Sample : N3688-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-12016

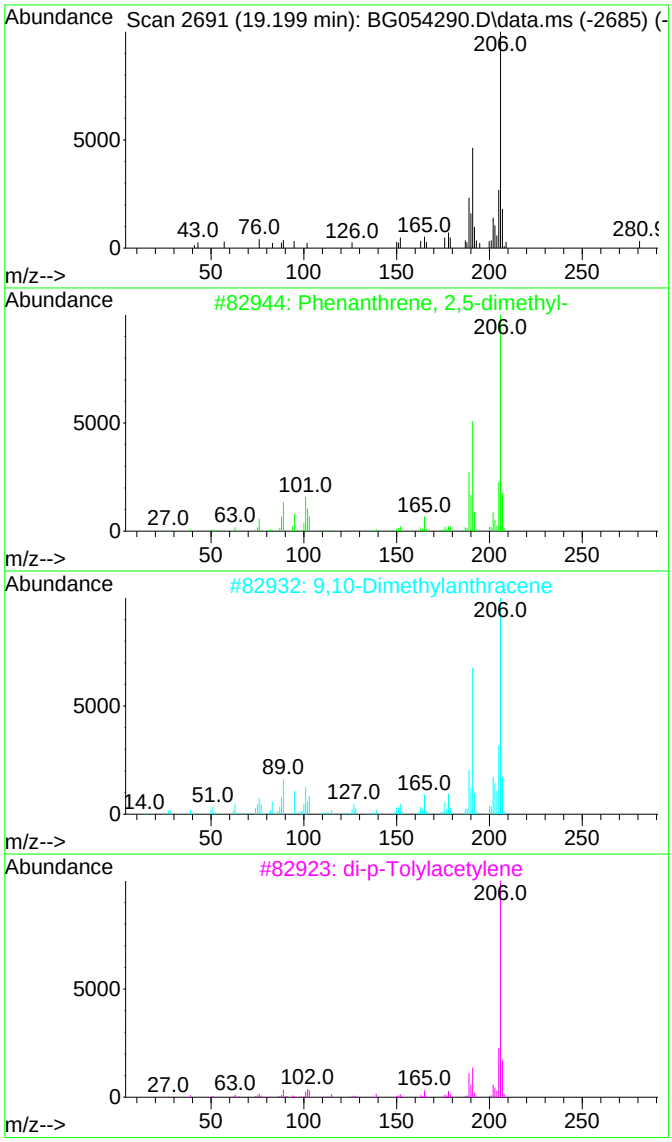
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

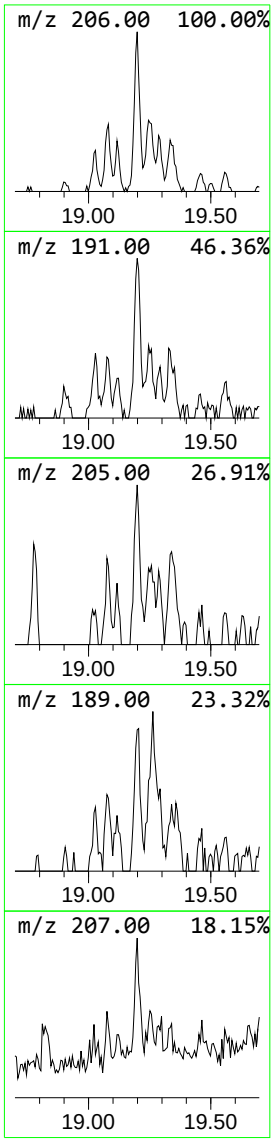
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenanthrene, 2,5-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.199	2.32 ng	39920	Phenanthrene-d10	17.413

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	91
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	91
3	di-p-Tolylacetylene	206	C16H14	002789-88-0	91
4	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	90
5	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054290.D
Acq On : 14 Jul 2022 21:52
Operator : CG/JU
Sample : N3688-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-12016

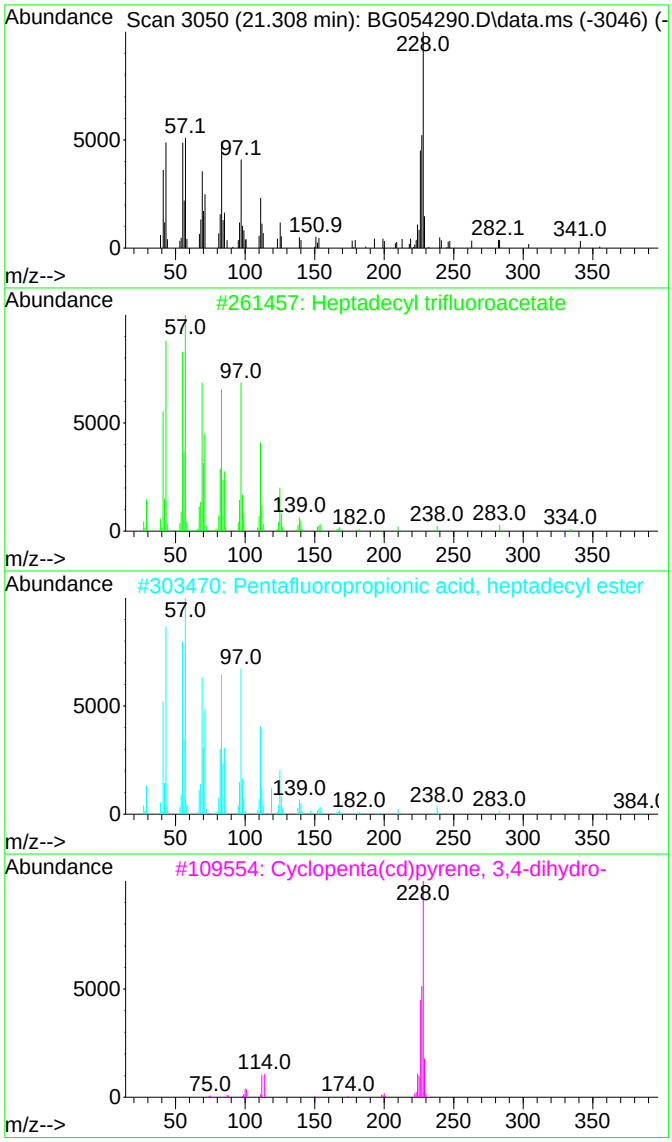
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

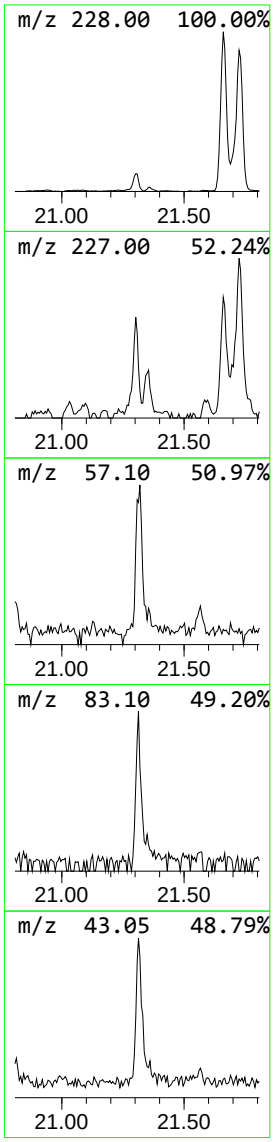
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.308	2.26 ng	83791	Chrysene-d12	21.684

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	72
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	70
3	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	46
4	Benzo[c]phenanthrene	228	C18H12	000195-19-7	46
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054290.D
Acq On : 14 Jul 2022 21:52
Operator : CG/JU
Sample : N3688-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-12016

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

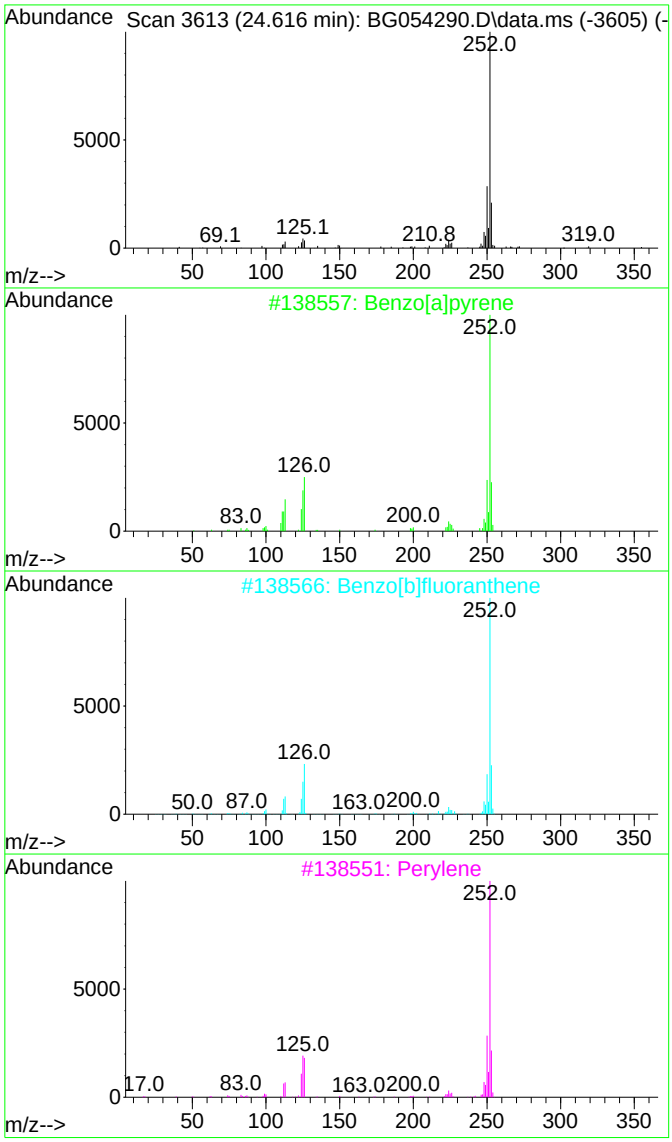
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

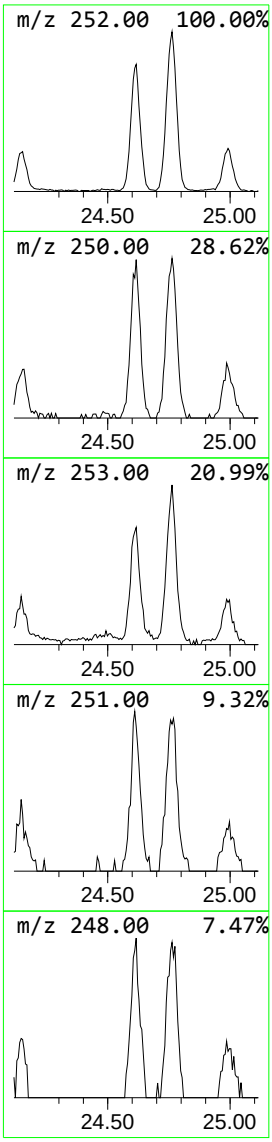
****

Peak Number 6 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.616	6.84 ng	163440	Perylene-d12	24.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	90
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
3	Perylene	252	C20H12	000198-55-0	81
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	81
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054290.D
Acq On : 14 Jul 2022 21:52
Operator : CG/JU
Sample : N3688-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-12016

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.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
Phenanthrene, 1...	18.288	2.3	ng	39302	4	17.413	344308	20.0
Phenanthrene, 2...	18.335	2.5	ng	43864	4	17.413	344308	20.0
5-Bromo-2-thiop...	18.476	3.2	ng	55015	4	17.413	344308	20.0
Phenanthrene, 2...	19.199	2.3	ng	39920	4	17.413	344308	20.0
Heptadecyl trif...	21.308	2.3	ng	83791	5	21.684	742421	20.0
Perylene	24.616	6.8	ng	163440	6	24.916	477811	20.0