LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058864.D
Acq On : 26 Aug 2023 00:56
Operator : MA/JU
Sample : 04110-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DUP-1(X-X)

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-BG081823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058864.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.511	236	242	252	rBV2	26640	48958	6.29%	0.720%
2	5.380	383	390	399	rBV	232649	381772	49.07%	5.616%
3	6.978	653	662	675	rBV	232223	411268	52.86%	6.050%
4	7.801	792	802	811	rBV	70097	122517	15.75%	1.802%
5	8.970	994	1001	1018	rBV	141551	266130	34.21%	3.915%
6	10.603	1269	1279	1287	rBV	88749	171715	22.07%	2.526%
7	12.278	1554	1564	1572	rBB3	4254	8296	1.07%	0.122%
8	12.489	1593	1600	1607	rBB3	4537	8246	1.06%	0.121%
9	13.071	1693	1699	1715	rVB	325648	516163	66.35%	7.593%
10	13.271	1728	1733	1739	rVB2	5685	9803	1.26%	0.144%
11	14.182	1882	1888	1897	rBV2	7425	14224	1.83%	0.209%
12	14.452	1928	1934	1942	rBV	143684	226858	29.16%	3.337%
13	14.851	1996	2002	2010	rVB4	4142	8036	1.03%	0.118%
14	15.492	2107	2111	2120	rBV4	4253	8837	1.14%	0.130%
15	15.944	2181	2188	2200	rBV	293446	461216	59.28%	6.785%
16	16.173	2220	2227	2232	rBV3	12398	24826	3.19%	0.365%
17	16.737	2316	2323	2326	rBV3	4052	7883	1.01%	0.116%
18	16.943	2352	2358	2362	rBV3	9422	14441	1.86%	0.212%
19	17.196	2394	2401	2406	rBV	192293	296772	38.15%	4.366%
20	17.243	2406	2409	2415	rVV	46617	63152	8.12%	0.929%
21	17.337	2419	2425	2429	rVB	9257	14957	1.92%	0.220%
22	17.607	2467	2471	2480	rBV6	4907	11187	1.44%	0.165%
23	17.683	2480	2484	2487	rVB3	8900	10606	1.36%	0.156%
24	18.083	2546	2552	2556	rBV4	44330	75870	9.75%	1.116%
25	18.124	2556	2559	2567	rVB	24023	37442	4.81%	0.551%
26	18.265	2578	2583	2588	rBV4	19570	39094	5.03%	0.575%
27	18.312	2588	2591	2597	rVB2	10900	15594	2.00%	0.229%
28	18.371	2597	2601	2608	rBV4	8039	12394	1.59%	0.182%
29	18.571	2631	2635	2640	rBV2	10437	16058	2.06%	0.236%
30	18.629	2640	2645	2649	rVB7	8772	13208	1.70%	0.194%
31	18.870	2683	2686	2690	rVV2	7383	10959	1.41%	0.161%
32	18.905	2690	2692	2697	rVB4	7050	7954	1.02%	0.117%
33	18.988	2702	2706	2712	rVV3	21864	43555	5.60%	0.641%
34	19.046	2712	2716	2720	rVV7	11426	21195	2.72%	0.312%
35	19.082	2720	2722	2727	rVV3	7413	9694	1.25%	0.143%
36	19.140	2727	2732	2738	rVB5	11675	21834	2.81%	0.321%

LSC Area Percent Report

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Acq On : 26 Aug 2023 00:56
Operator : MA/JU
Sample : 04110-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-1(X-X)

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-BG081823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.252	2745	2751	2759	rBV	122692	176381	22.67%	2.595%
38	19.358	2765	2769	2773	rBV5	10836	16156	2.08%	0.238%
39	19.405	2773	2777	2782	rVV2	13249	17965	2.31%	0.264%
40	19.534	2795	2799	2803	rVB7	6051	9370	1.20%	0.138%
41	19.587	2803	2808	2809	rBV	25219	30835	3.96%	0.454%
42	19.616	2809	2813	2822	rVB	115656	175085	22.50%	2.576%
43	19.693	2822	2826	2834	rVB5	13459	23176	2.98%	0.341%
44	19.816	2837	2847	2852	rBV	599516	777989	100.00%	11.445%
45	19.940	2862	2868	2877	rBV6	13918	40863	5.25%	0.601%
46	20.081	2886	2892	2893	rBV3	17156	24992	3.21%	0.368%
47	20.110	2893	2897	2902	rVB2	42623	60606	7.79%	0.892%
48	20.210	2910	2914	2919	rBV	22586	29778	3.83%	0.438%
49	20.269	2919	2924	2928	rVB4	20966	36527	4.70%	0.537%
50	20.410	2944	2948	2952	rBV2	14664	21981	2.83%	0.323%
51	20.451	2952	2955	2960	rVB3	13070	17042	2.19%	0.251%
52	20.603	2979	2981	2986	rBV3	12335	16680	2.14%	0.245%
53	20.703	2994	2998	3000	rBV4	6354	8987	1.16%	0.132%
54	20.727	3000	3002	3006	rVB5	8244	8791	1.13%	0.129%
55	20.821	3013	3018	3021	rBV6	10563	18496	2.38%	0.272%
56	20.862	3021	3025	3030	rVB	18159	32313	4.15%	0.475%
57	21.038	3051	3055	3058	rBV4	12007	19689	2.53%	0.290%
58	21.085	3059	3063	3068	rBV2	54467	79869	10.27%	1.175%
59	21.179	3074	3079	3087	rVB4	29208	65584	8.43%	0.965%
60	21.438	3115	3123	3128	rBV2	244948	502276	64.56%	7.389%
61	21.485	3128	3131	3142	rVB	71582	113311	14.56%	1.667%
62	21.608	3150	3152	3159	rVB5	10107	19280	2.48%	0.284%
63	21.696	3164	3167	3175	rVB4	14686	22262	2.86%	0.327%
64	21.837	3185	3191	3194	rBV5	8516	15668	2.01%	0.230%
65	22.137	3233	3242	3246	rBV2	19602	42721	5.49%	0.628%
66	22.184	3246	3250	3251	rBV4	10907	12038	1.55%	0.177%
67	22.395	3282	3286	3291	rBV4	12029	18696	2.40%	0.275%
68	22.836	3355	3361	3367	rBV8	7413	15956	2.05%	0.235%
69	23.018	3388	3392	3394	rVB5	7206	10086	1.30%	0.148%
70	23.535	3470	3480	3486	rBV	54632	166610	21.42%	2.451%
71	23.782	3515	3522	3527	rBV2	13788	34481	4.43%	0.507%
72	24.217	3588	3596	3607	rVB	32368	94787	12.18%	1.394%
73	24.358	3612	3620	3632	rVB2	47620	134609	17.30%	1.980%
74	24.499	3634	3644	3652	rBV	134660	370001	47.56%	5.443%
75	25.515	3812	3817	3818	rBV5	5861	8643	1.11%	0.127%
76	27.983	4227	4237	4238	rBV2	17038	41317	5.31%	0.608%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
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Acq On : 26 Aug 2023 00:56
Operator : MA/JU
Sample : 04110-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-1(X-X)

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-BG081823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	29.064	4410	4421	4422	rBV3	13342	33247	4.27%	0.489%

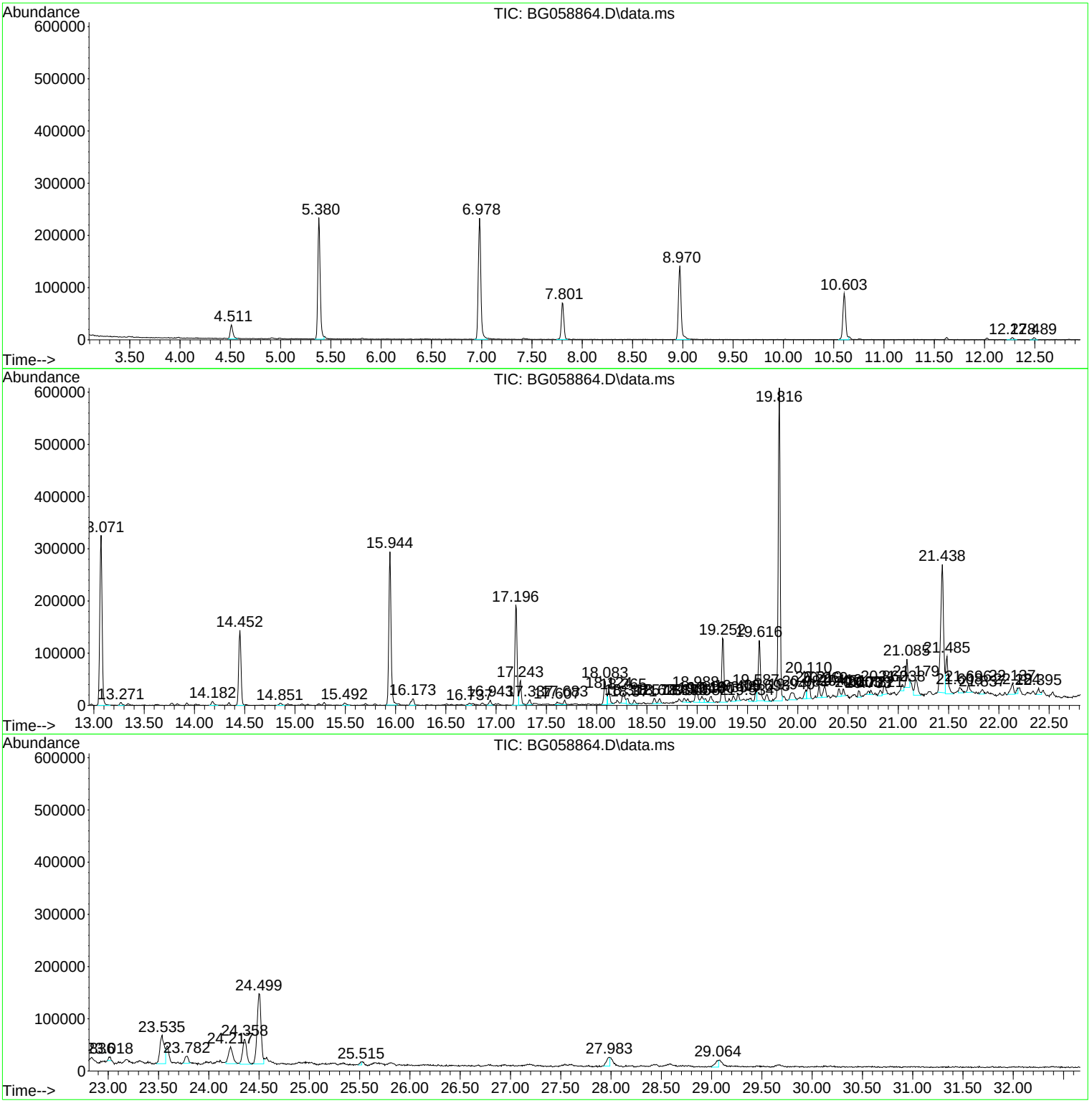
Sum of corrected areas: 6797858

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058864.D
Acq On : 26 Aug 2023 00:56
Operator : MA/JU
Sample : 04110-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-1(X-X)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.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\BG082523\
Data File : BG058864.D
Acq On : 26 Aug 2023 00:56
Operator : MA/JU
Sample : 04110-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-1(X-X)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

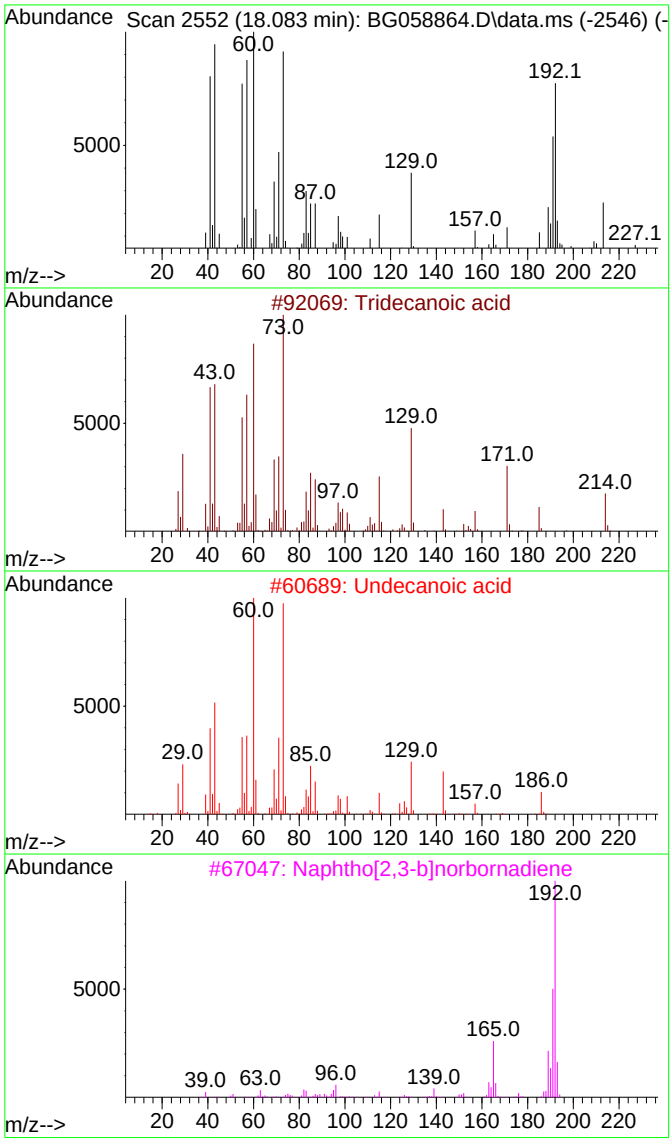
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

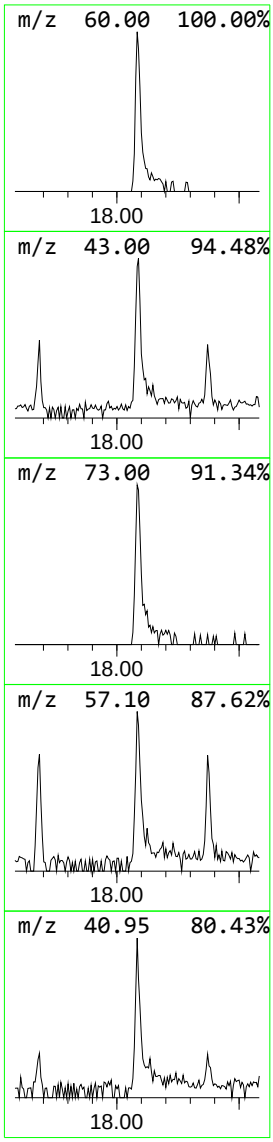
****

Peak Number 2 unknown18.083 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.083	5.11 ng	75870	Phenanthrene-d10	17.196

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	46
2	Undecanoic acid	186	C11H22O2	000112-37-8	38
3	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	18
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	18
5	Nonanoic acid	158	C9H18O2	000112-05-0	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058864.D
Acq On : 26 Aug 2023 00:56
Operator : MA/JU
Sample : 04110-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-1(X-X)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

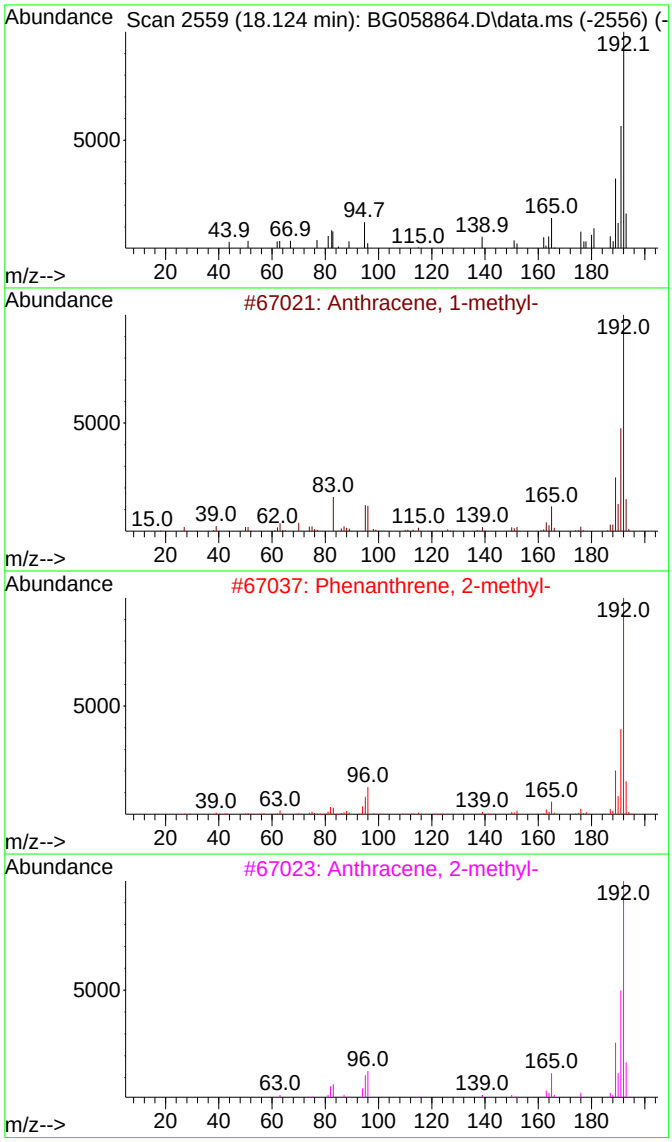
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

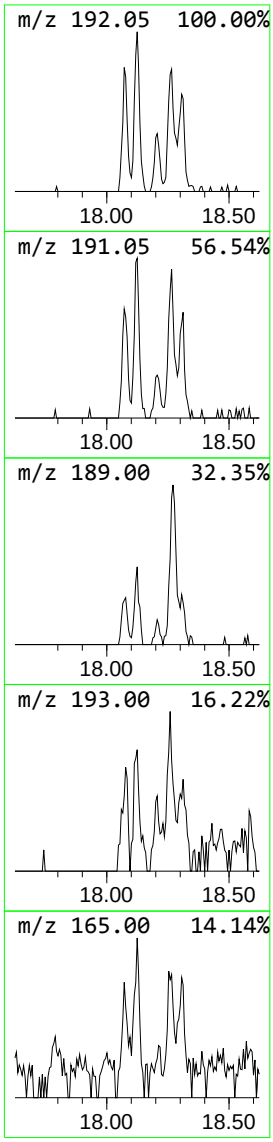
****

Peak Number 3 Anthracene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.124	2.52 ng	37442	Phenanthrene-d10	17.196

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	87
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	87
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	87
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	87
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058864.D
Acq On : 26 Aug 2023 00:56
Operator : MA/JU
Sample : 04110-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-1(X-X)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.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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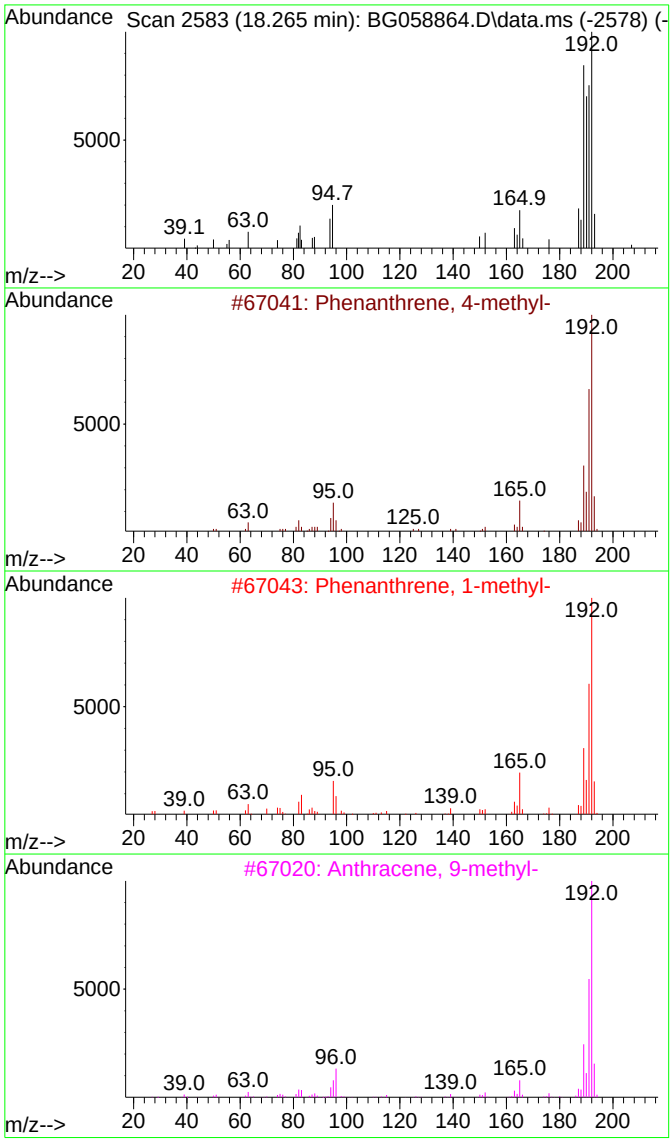
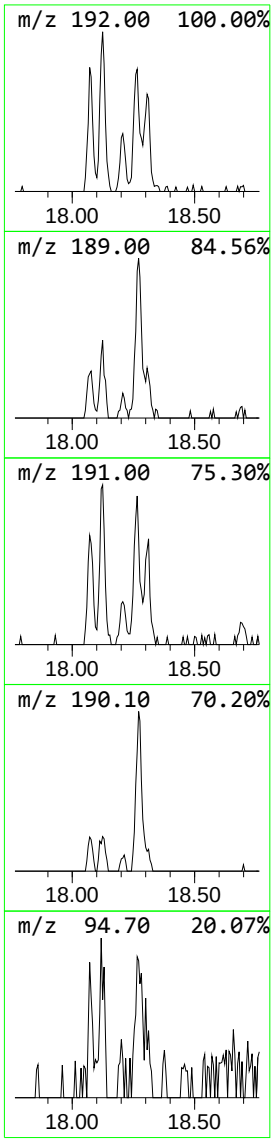
Peak Number 4 Phenanthrene, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.265	2.63 ng	39094	Phenanthrene-d10	17.196

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	60
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	60
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	60
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	55
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058864.D
Acq On : 26 Aug 2023 00:56
Operator : MA/JU
Sample : 04110-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-1(X-X)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.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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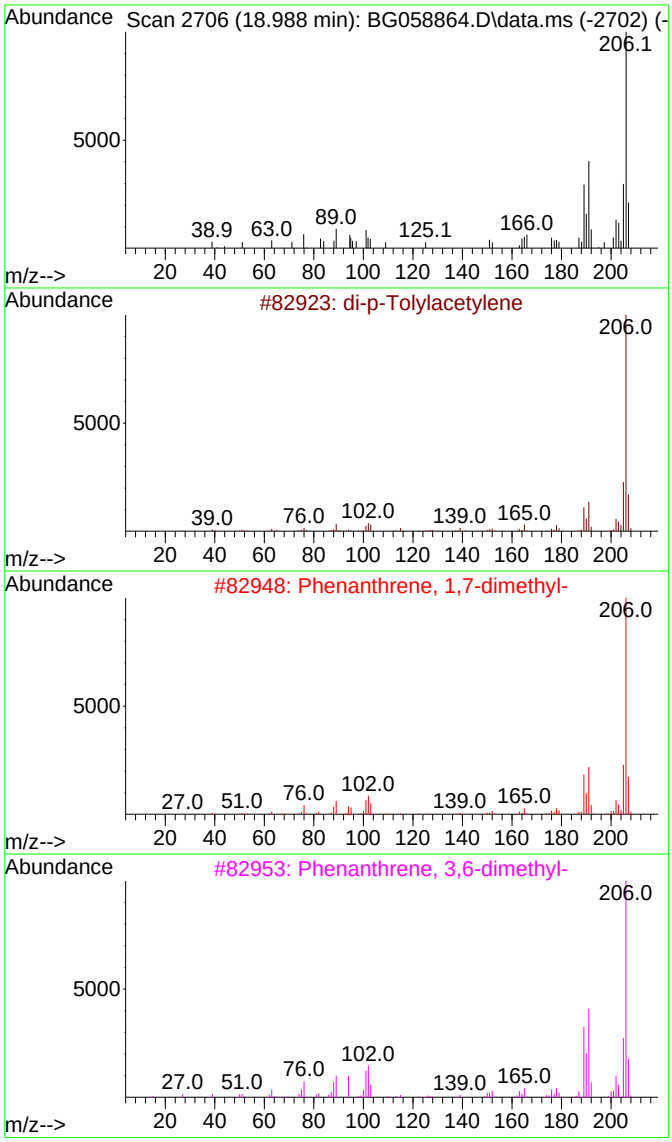
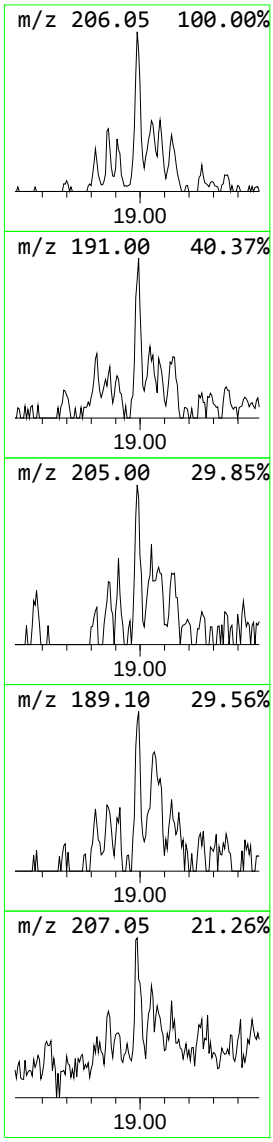
Peak Number 5 di-p-Tolylacetylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.988	2.94 ng	43555	Phenanthrene-d10	17.196

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	di-p-Tolylacetylene	206	C16H14	002789-88-0	94
2	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	93
3	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	91
4	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	90
5	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058864.D
Acq On : 26 Aug 2023 00:56
Operator : MA/JU
Sample : 04110-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-1(X-X)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

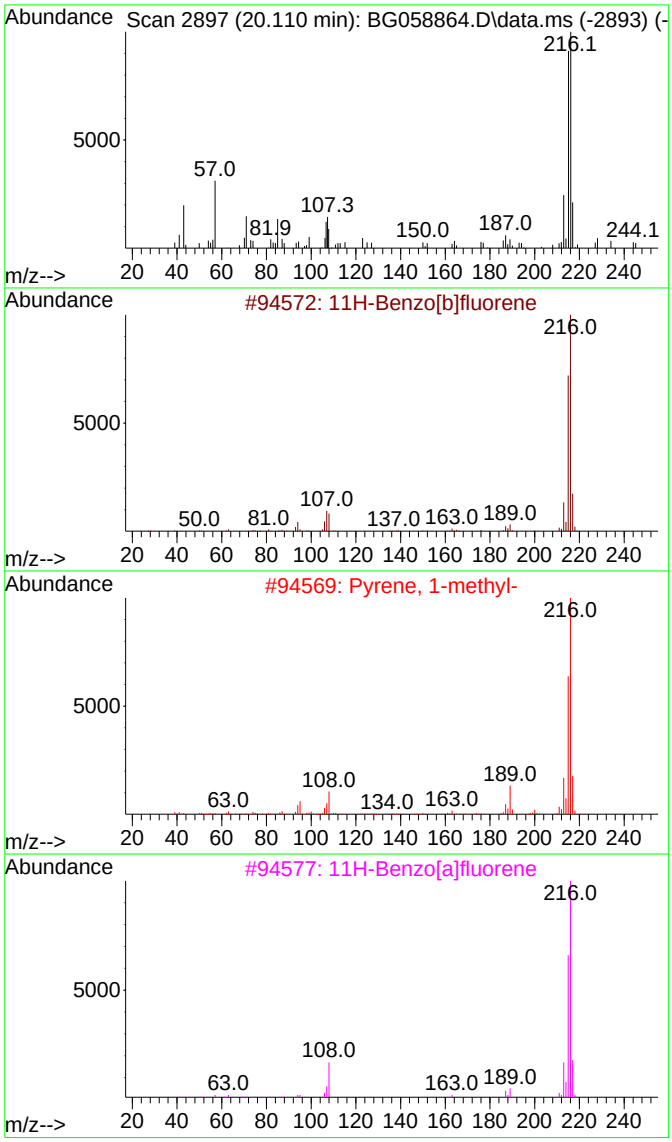
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

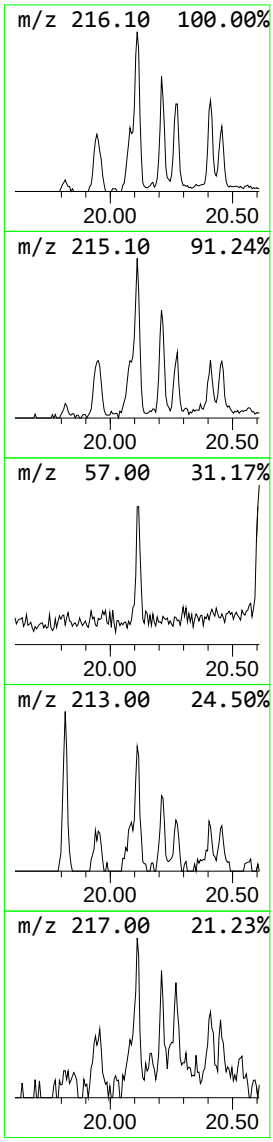
****

Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.110	2.41 ng	60606	Chrysene-d12	21.438

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	81
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	64
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	64
4	6H-Thiazolo[5,4-e]indole, 2,7,8-...	216	C12H12N2S	1000338-32-0	59
5	1,3,5-Triazine-2,4,6-triamine, N...	216	C10H12N6	046731-79-7	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058864.D
Acq On : 26 Aug 2023 00:56
Operator : MA/JU
Sample : 04110-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-1(X-X)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

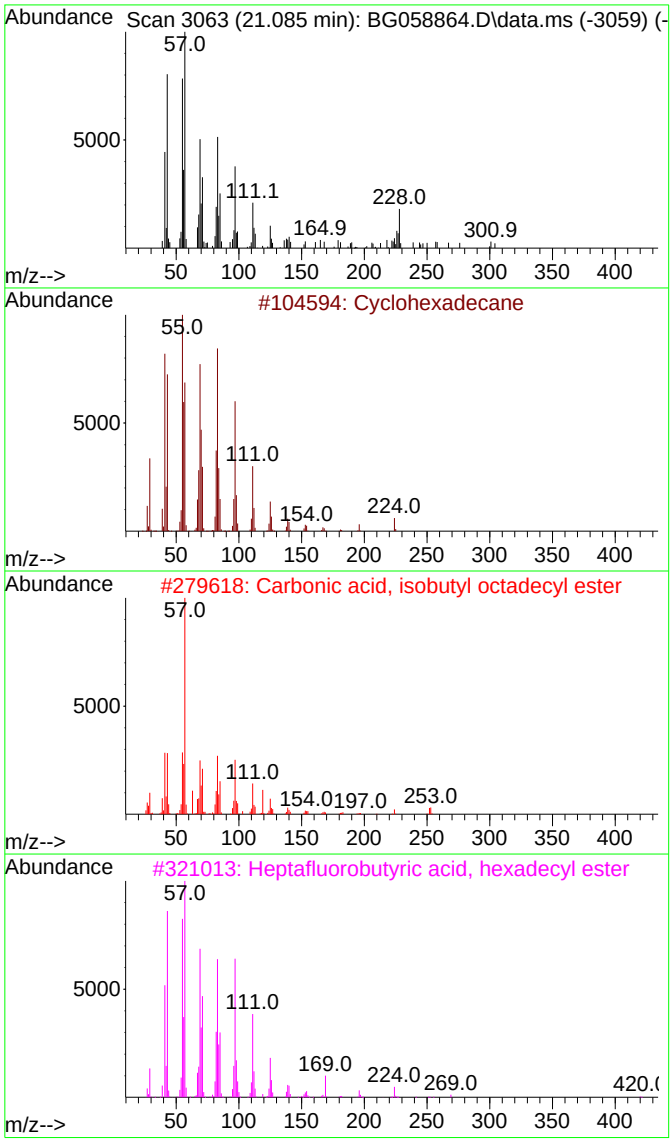
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

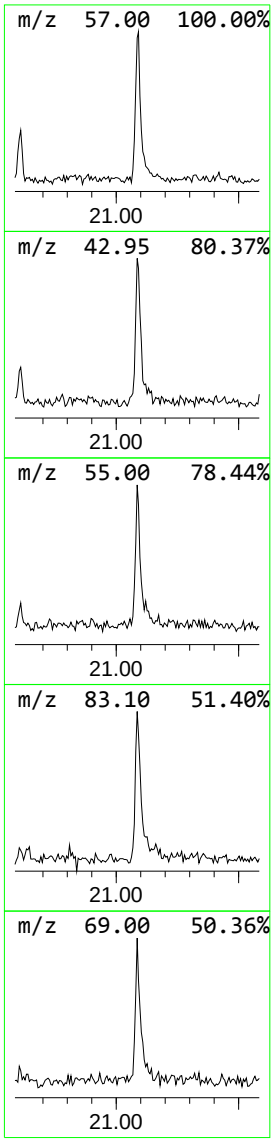
****

Peak Number 7 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.085	3.18 ng	79869	Chrysene-d12	21.438

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	95
2	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	90
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	86
4	1-Hexadecanethiol	258	C16H34S	002917-26-2	76
5	Cetene	224	C16H32	000629-73-2	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058864.D
Acq On : 26 Aug 2023 00:56
Operator : MA/JU
Sample : 04110-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-1(X-X)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

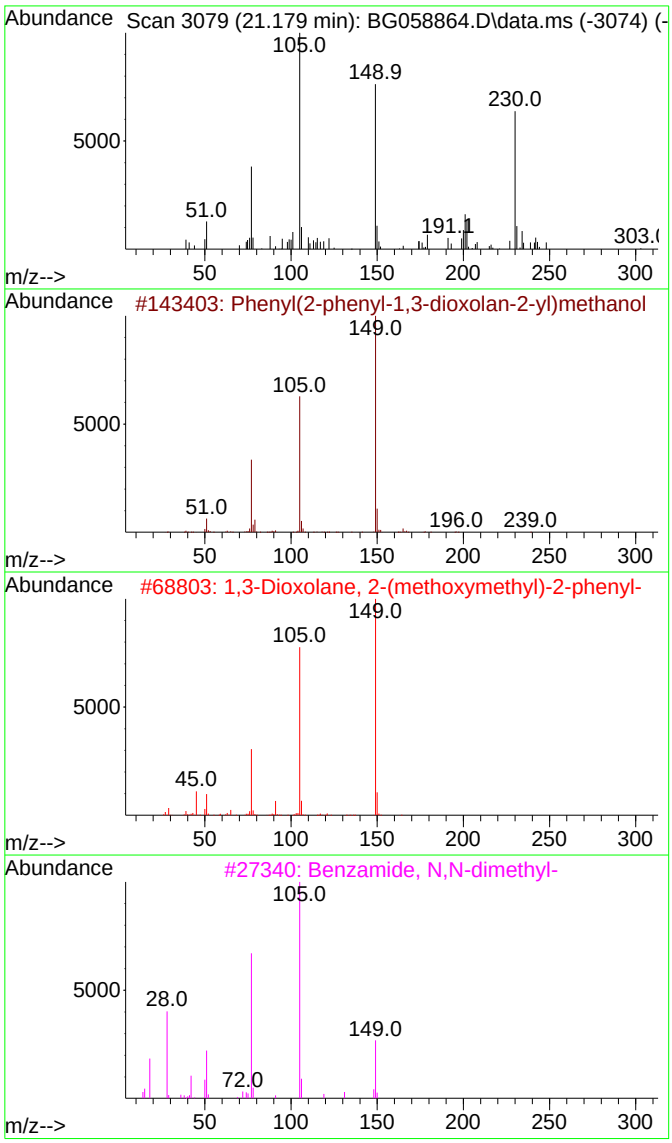
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

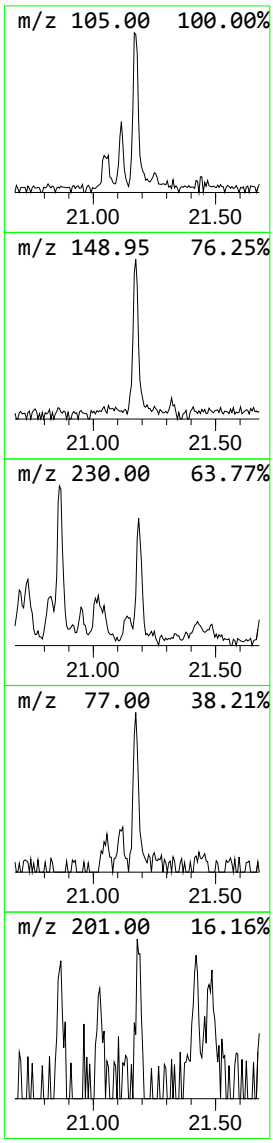
****

Peak Number 8 Phenyl(2-phenyl-1,3-dioxola... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.179	2.61 ng	65584	Chrysene-d12	21.438

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	50
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	50
3	Benzamide, N,N-dimethyl-	149	C9H11NO	000611-74-5	50
4	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	50
5	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058864.D
Acq On : 26 Aug 2023 00:56
Operator : MA/JU
Sample : 04110-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-1(X-X)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

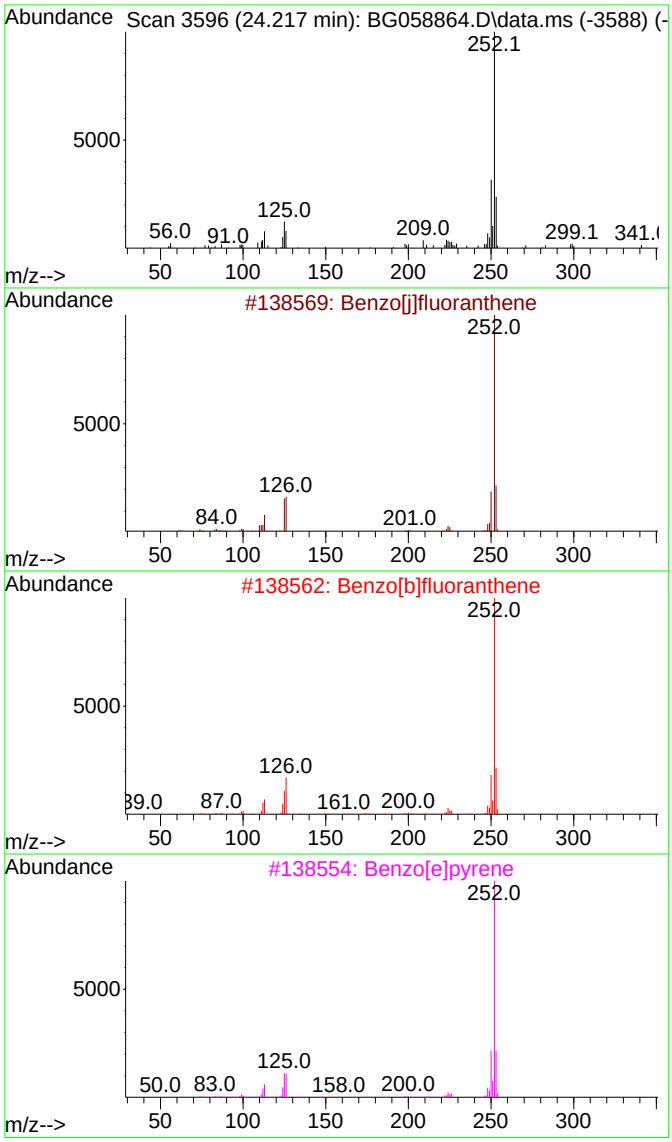
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

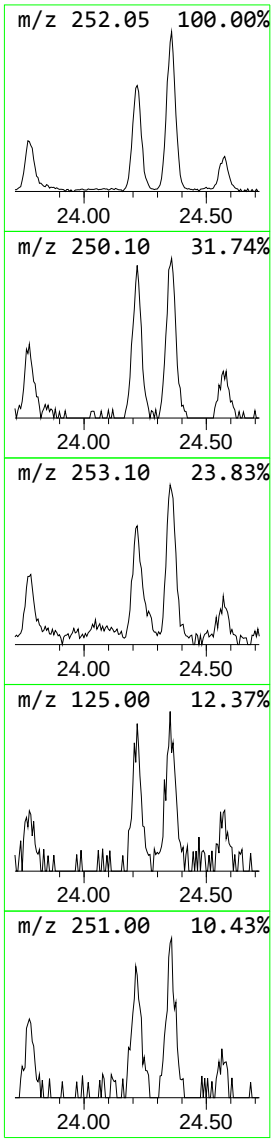
****

Peak Number 9 Benzo[j]fluoranthene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.217	5.12 ng	94787	Perylene-d12	24.499

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3	Benzo[e]pyrene	252	C20H12	000192-97-2	91
4	Benzo[a]pyrene	252	C20H12	000050-32-8	91
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058864.D
Acq On : 26 Aug 2023 00:56
Operator : MA/JU
Sample : 04110-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-1(X-X)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.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
unknown18.083	18.083	5.1	ng	75870	4	17.196	296772	20.0
Anthracene, 1-m...	18.124	2.5	ng	37442	4	17.196	296772	20.0
Phenanthrene, 4...	18.265	2.6	ng	39094	4	17.196	296772	20.0
di-p-Tolylacety...	18.988	2.9	ng	43555	4	17.196	296772	20.0
11H-Benzo[b]flu...	20.110	2.4	ng	60606	5	21.438	502276	20.0
Cyclohexadecane	21.085	3.2	ng	79869	5	21.438	502276	20.0
Phenyl(2-phenyl...	21.179	2.6	ng	65584	5	21.438	502276	20.0
Benzo[j]fluoran...	24.217	5.1	ng	94787	6	24.499	370001	20.0