LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031122\
Data File : BG052649.D
Acq On : 11 Mar 2022 16:19
Operator : CG/JU
Sample : N1864-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MB-B1-030922-0-2

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-BG030922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG052649.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.205	304	309	316	rVB2	10151	15962	1.06%	0.142%
2	5.699	386	393	405	rBV	344734	568495	37.77%	5.045%
3	7.320	661	669	681	rBV	387193	668114	44.39%	5.928%
4	8.166	804	813	820	rBV	105954	178632	11.87%	1.585%
5	9.341	1005	1013	1021	rBV	249390	438090	29.10%	3.887%
6	11.003	1289	1296	1304	rBV	140459	257659	17.12%	2.286%
7	13.441	1704	1711	1719	rBV	711154	1090134	72.42%	9.673%
8	14.821	1937	1946	1952	rBV	260541	387259	25.73%	3.436%
9	14.886	1952	1957	1964	rVB	16822	25133	1.67%	0.223%
10	15.867	2119	2124	2130	rBV4	15765	25917	1.72%	0.230%
11	16.308	2193	2199	2209	rBV	541526	840148	55.82%	7.455%
12	17.224	2349	2355	2360	rBV3	13915	23015	1.53%	0.204%
13	17.300	2362	2368	2375	rVV6	6926	15768	1.05%	0.140%
14	17.389	2379	2383	2389	rVB2	12451	19173	1.27%	0.170%
15	17.571	2408	2414	2418	rBV	322039	489626	32.53%	4.345%
16	17.612	2418	2421	2427	rVV	254531	363387	24.14%	3.224%
17	17.706	2429	2437	2442	rVB	34174	56325	3.74%	0.500%
18	17.970	2476	2482	2487	rBV3	22098	37084	2.46%	0.329%
19	18.164	2509	2515	2519	rVB4	8227	16017	1.06%	0.142%
20	18.446	2557	2563	2568	rBV	54795	96502	6.41%	0.856%
21	18.499	2568	2572	2579	rVV	62475	96620	6.42%	0.857%
22	18.575	2579	2585	2591	rVV2	14069	23918	1.59%	0.212%
23	18.646	2591	2597	2600	rBV2	49691	101570	6.75%	0.901%
24	18.675	2600	2602	2607	rVB	30392	40586	2.70%	0.360%
25	18.939	2642	2647	2651	rBV	28719	43259	2.87%	0.384%
26	18.986	2651	2655	2664	rVB	38245	57387	3.81%	0.509%
27	19.180	2684	2688	2694	rBV5	15208	24506	1.63%	0.217%
28	19.357	2713	2718	2723	rBV	30945	51128	3.40%	0.454%
29	19.421	2723	2729	2732	rVV4	8753	18935	1.26%	0.168%
30	19.503	2737	2743	2749	rBV3	24424	50410	3.35%	0.447%
31	19.621	2755	2763	2769	rBV	416837	579670	38.51%	5.144%
32	19.715	2775	2779	2783	rVB5	14721	23074	1.53%	0.205%
33	19.815	2792	2796	2798	rBV3	12822	17587	1.17%	0.156%
34	19.868	2801	2805	2812	rVB4	14141	32315	2.15%	0.287%
35	19.950	2814	2819	2820	rVV	64276	86062	5.72%	0.764%
36	19.985	2820	2825	2831	rVV	324737	488239	32.44%	4.332%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031122\
Data File : BG052649.D
Acq On : 11 Mar 2022 16:19
Operator : CG/JU
Sample : N1864-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MB-B1-030922-0-2

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-BG030922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.050	2832	2836	2841	rVB3	28480	40174	2.67%	0.356%
38	20.167	2850	2856	2862	rBV	1198665	1505215	100.00%	13.356%
39	20.302	2873	2879	2886	rBV6	33421	81336	5.40%	0.722%
40	20.473	2897	2908	2912	rVB	47686	114392	7.60%	1.015%
41	20.567	2921	2924	2927	rBV	21820	28395	1.89%	0.252%
42	20.631	2929	2935	2938	rVV2	33237	53940	3.58%	0.479%
43	20.813	2963	2966	2971	rBV2	23376	29483	1.96%	0.262%
44	21.248	3036	3040	3046	rVB2	42632	68384	4.54%	0.607%
45	21.483	3076	3080	3086	rVB2	63879	96388	6.40%	0.855%
46	21.595	3096	3099	3106	rVB	38643	65433	4.35%	0.581%
47	21.877	3139	3147	3152	rBV2	293507	726015	48.23%	6.442%
48	21.924	3152	3155	3167	rVB	137426	251694	16.72%	2.233%
49	24.215	3538	3545	3553	rBV2	87564	290623	19.31%	2.579%
50	25.143	3699	3703	3713	rVB2	73634	177286	11.78%	1.573%
51	25.307	3723	3731	3741	rBV2	134576	393108	26.12%	3.488%

Sum of corrected areas: 11269572

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031122\
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Operator : CG/JU
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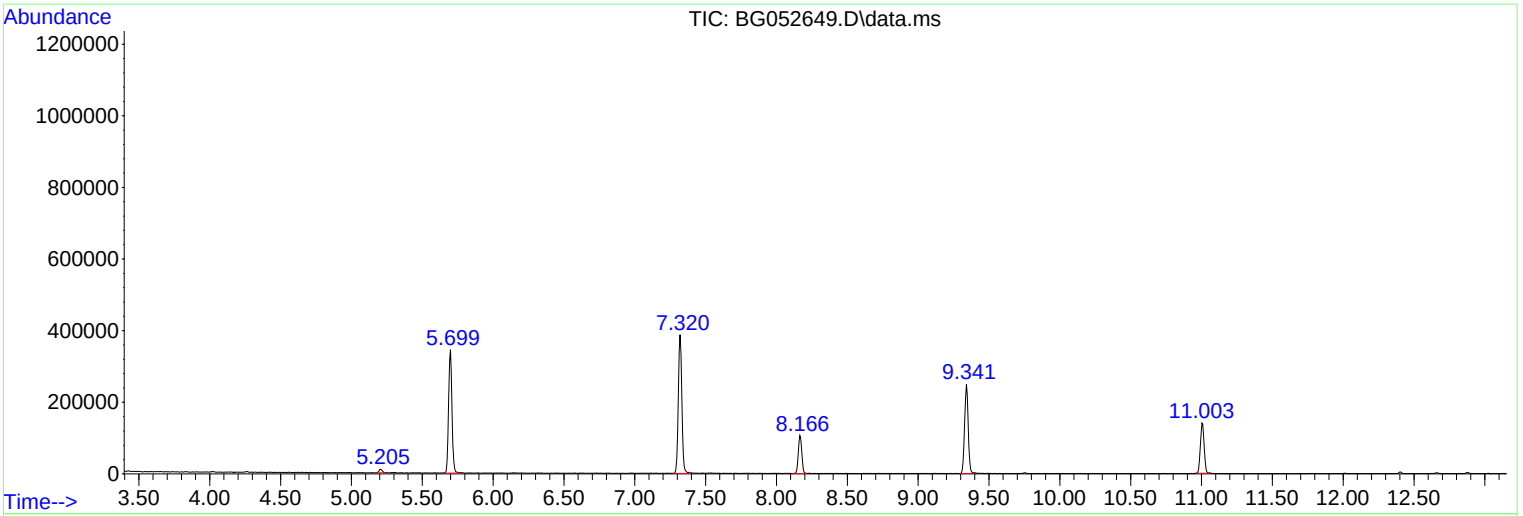
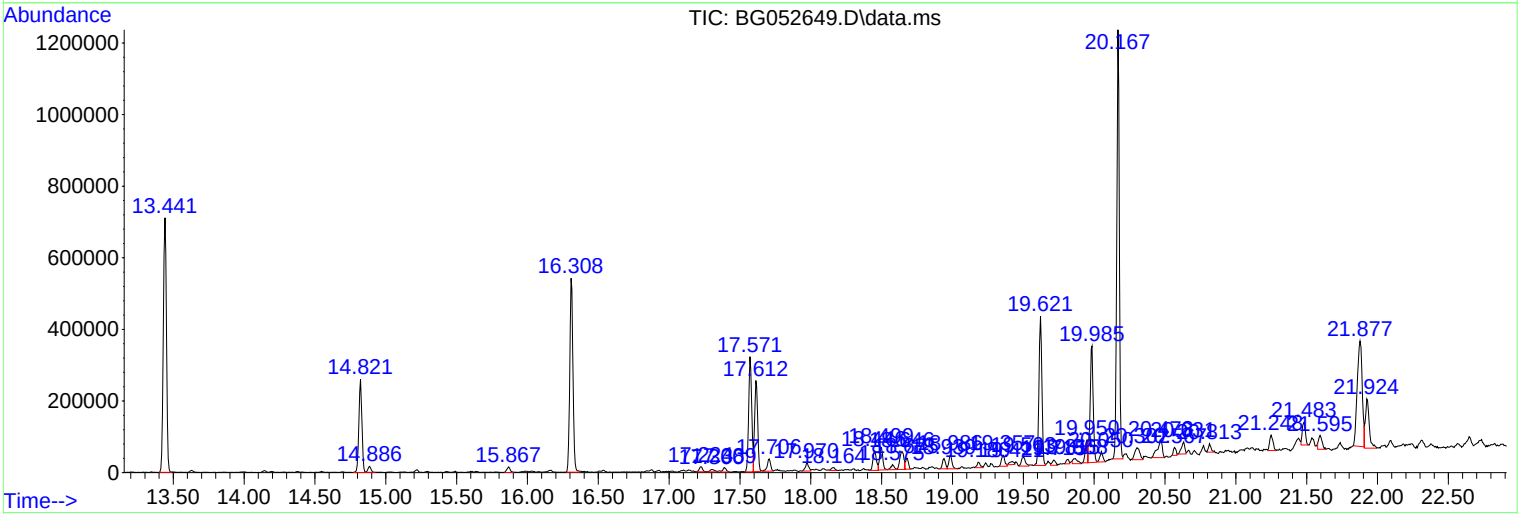
Misc :
ALS Vial : 5 Sample Multiplier: 1

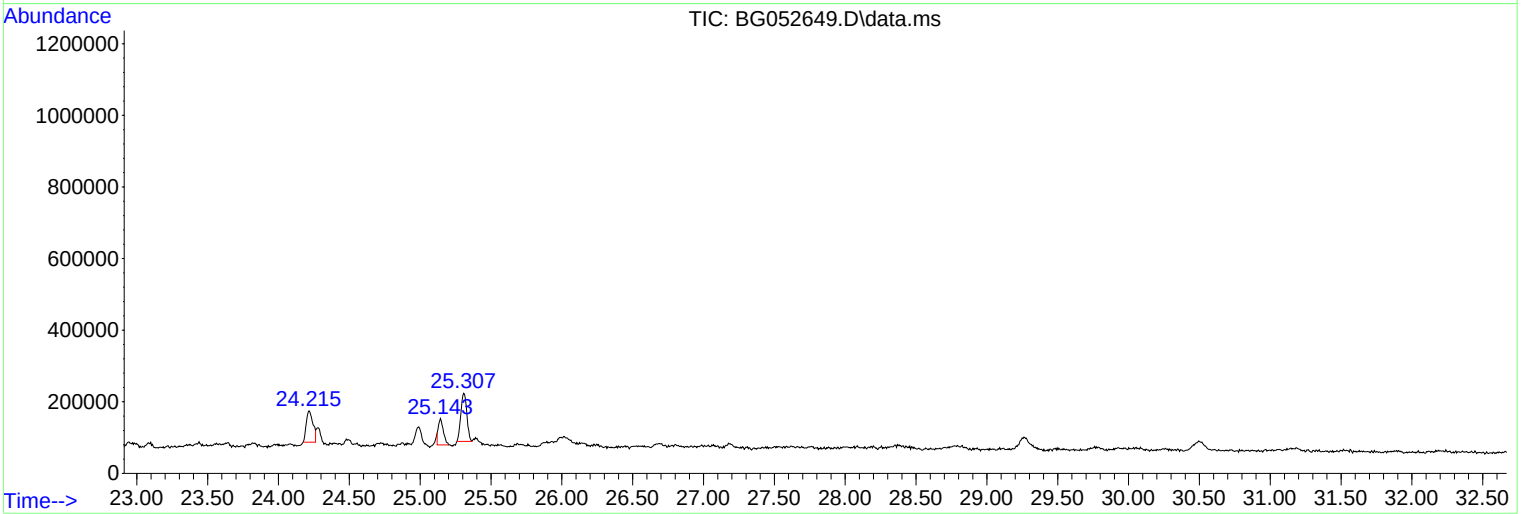
Instrument :
BNA_G
ClientSampleId :
MB-B1-030922-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030922.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\BG031122\
Data File : BG052649.D
Acq On : 11 Mar 2022 16:19
Operator : CG/JU
Sample : N1864-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MB-B1-030922-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

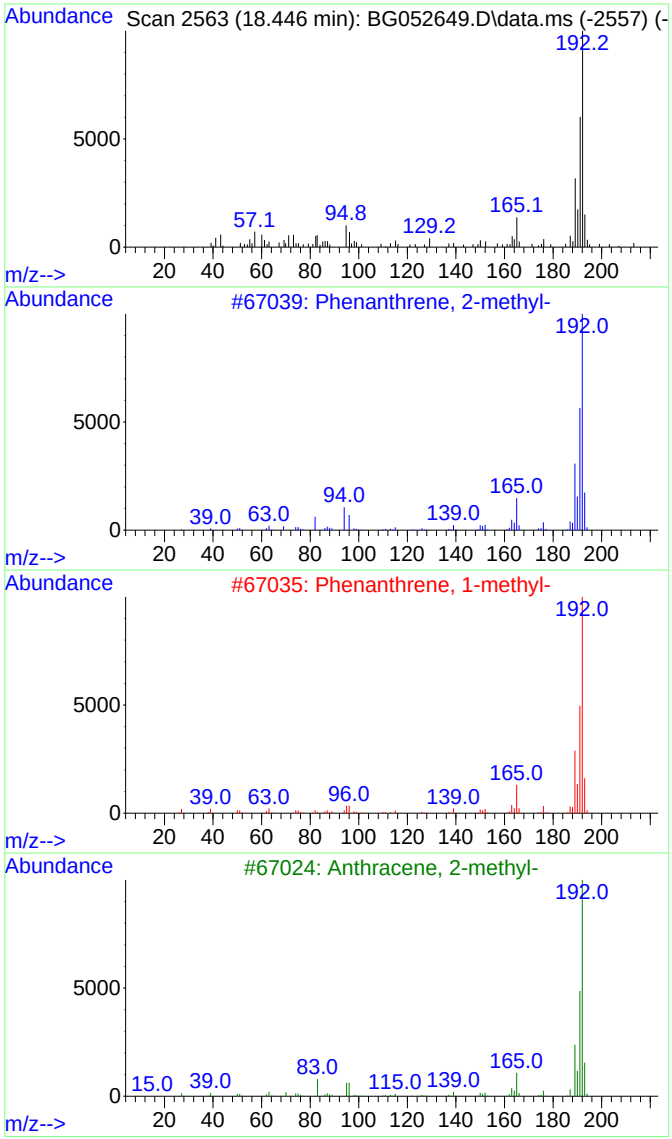
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

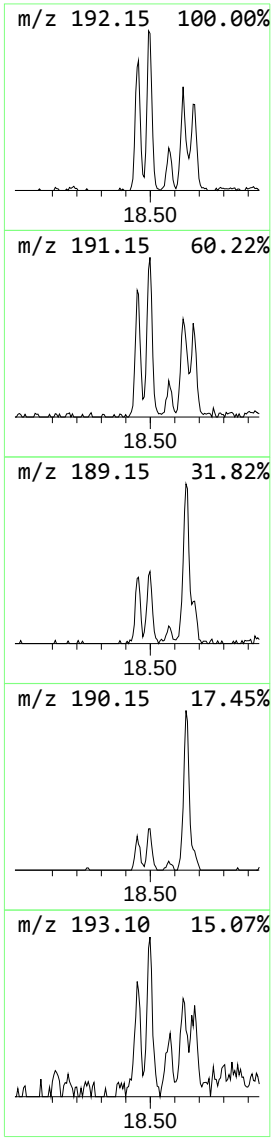
****

Peak Number 1 Phenanthrene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.446	3.94 ng	96502	Phenanthrene-d10	17.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
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	93
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031122\
Data File : BG052649.D
Acq On : 11 Mar 2022 16:19
Operator : CG/JU
Sample : N1864-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MB-B1-030922-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

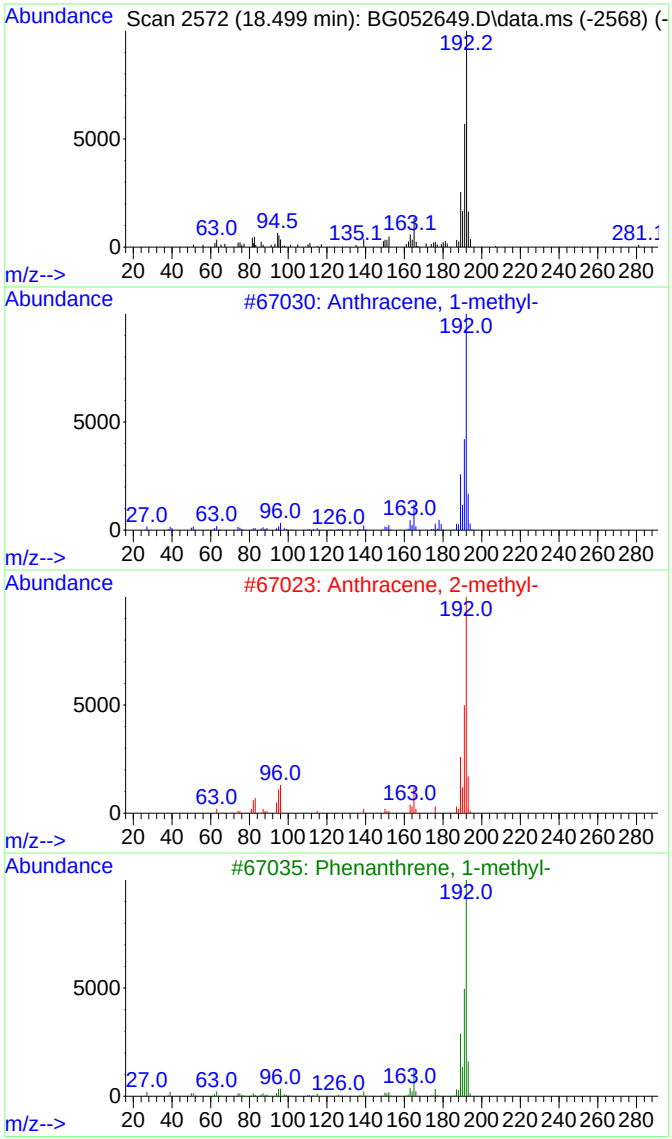
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

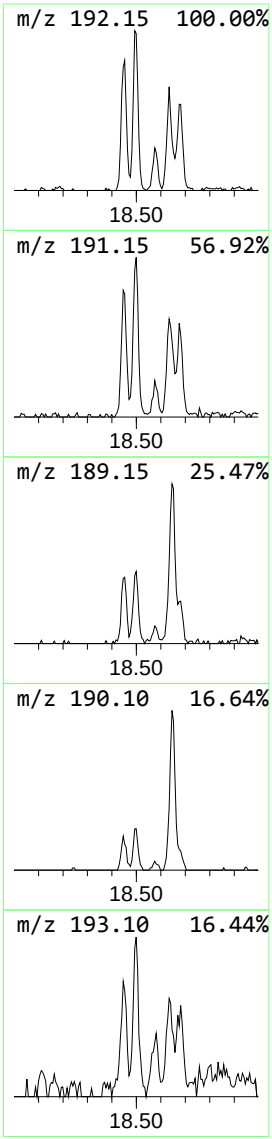
****

Peak Number 2 Anthracene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.499	3.95 ng	96620	Phenanthrene-d10	17.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	91
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031122\
Data File : BG052649.D
Acq On : 11 Mar 2022 16:19
Operator : CG/JU
Sample : N1864-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MB-B1-030922-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

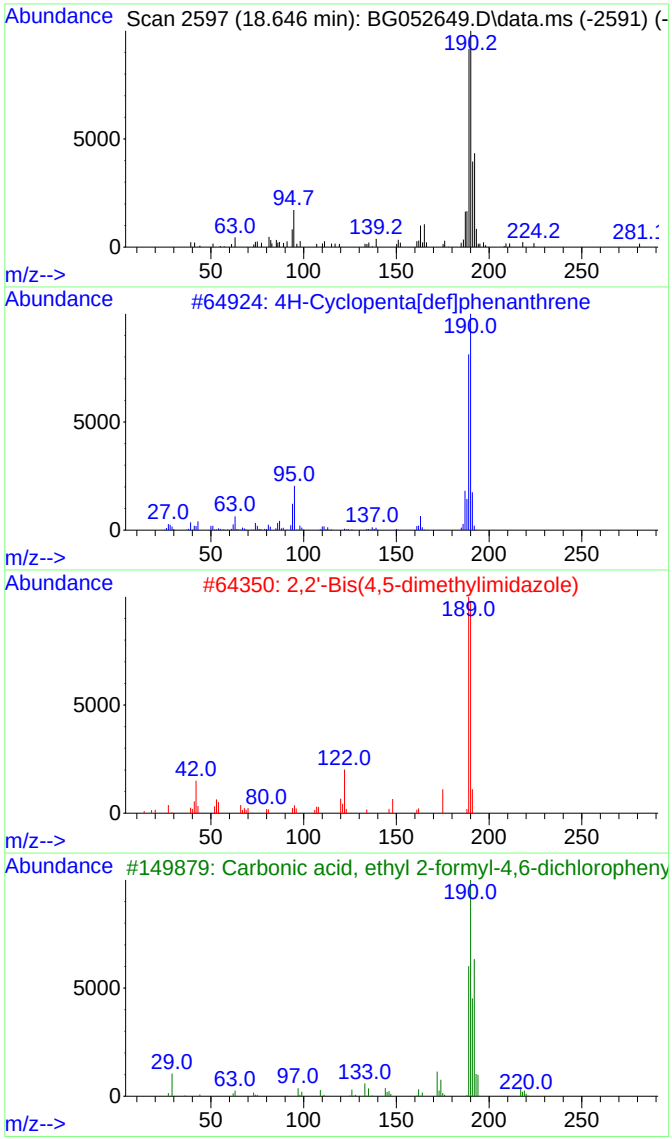
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

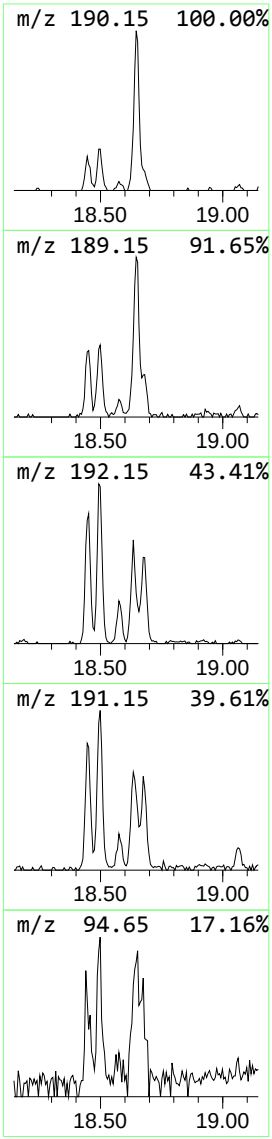
****

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.646	4.15 ng	101570	Phenanthrene-d10	17.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	47
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40
4	Pyrimidine, 6-oxo-4-(3-fluorophe...	190	C10H7FN2O	085979-55-1	37
5	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031122\
Data File : BG052649.D
Acq On : 11 Mar 2022 16:19
Operator : CG/JU
Sample : N1864-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MB-B1-030922-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

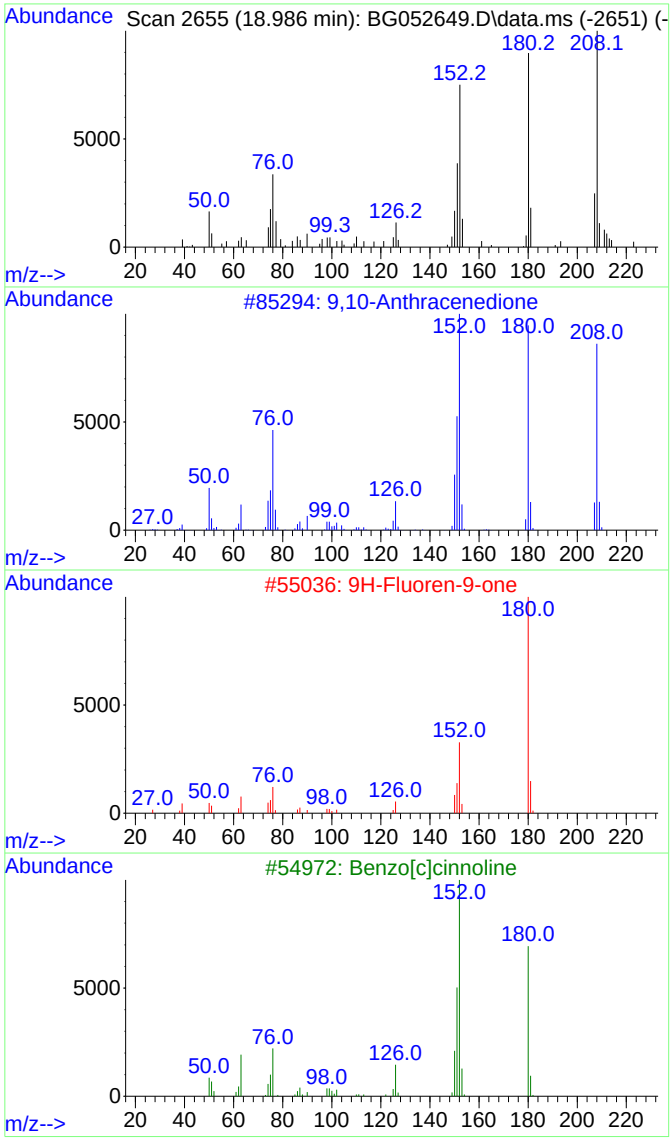
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

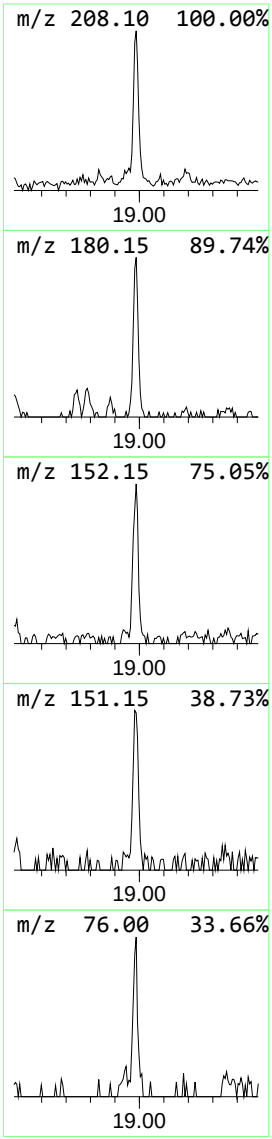
****

Peak Number 4 9,10-Anthracenedione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.986	2.34 ng	57387	Phenanthrene-d10	17.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	97
2	9H-Fluoren-9-one	180	C13H8O	000486-25-9	78
3	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	64
4	1H-Phenalen-1-one	180	C13H8O	000548-39-0	60
5	1,4-Anthracenedione	208	C14H8O2	000635-12-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031122\
Data File : BG052649.D
Acq On : 11 Mar 2022 16:19
Operator : CG/JU
Sample : N1864-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MB-B1-030922-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

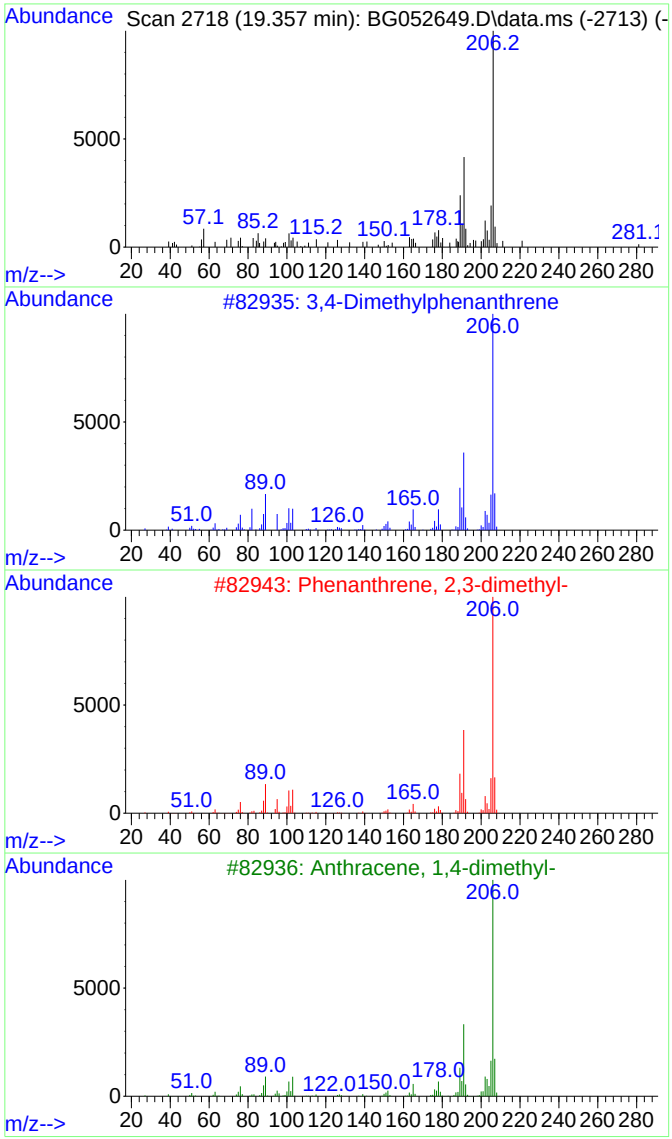
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

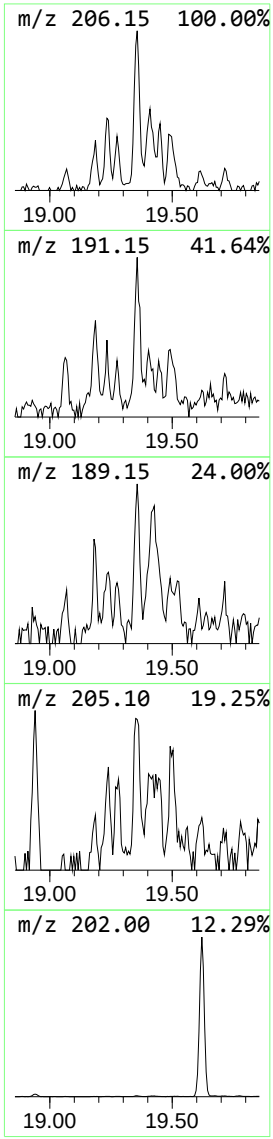
****

Peak Number 5 3,4-Dimethylphenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.357	2.09 ng	51128	Phenanthrene-d10	17.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	91
2	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	83
3	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	81
4	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	81
5	9,10-Dimethylanthracene	206	C16H14	000781-43-1	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031122\
Data File : BG052649.D
Acq On : 11 Mar 2022 16:19
Operator : CG/JU
Sample : N1864-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MB-B1-030922-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030922.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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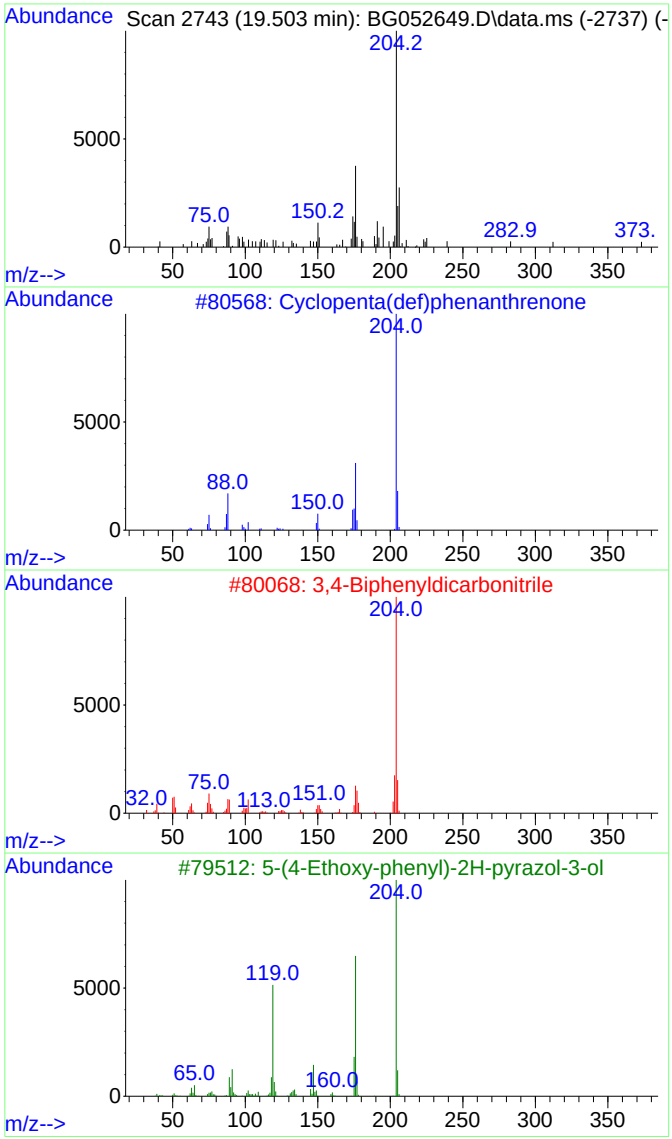
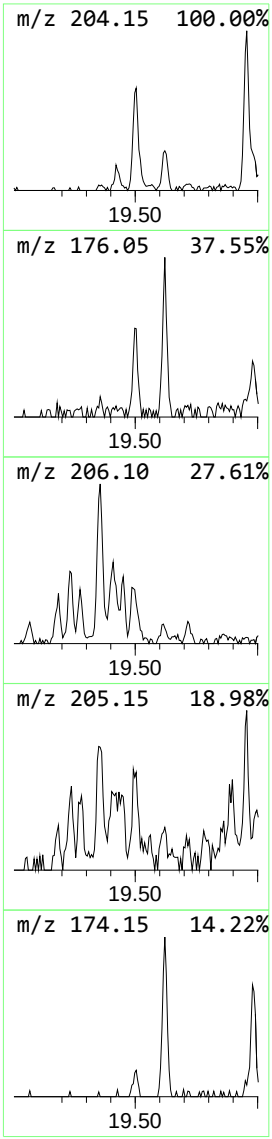
Peak Number 6 Cyclopenta(def)phenanthrenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.503	2.06 ng	50410	Phenanthrene-d10	17.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	89
2	3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	53
3	5-(4-Ethoxy-phenyl)-2H-pyrazol-3-ol	204	C11H12N2O2	1000278-26-8	49
4	Benzene, 1-chloro-4-phenoxy-	204	C12H9ClO	007005-72-3	47
5	L-Rhamnose, (R,R,S,S)-, 4TMS der...	452	C18H44O5Si4	108392-01-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031122\
Data File : BG052649.D
Acq On : 11 Mar 2022 16:19
Operator : CG/JU
Sample : N1864-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MB-B1-030922-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030922.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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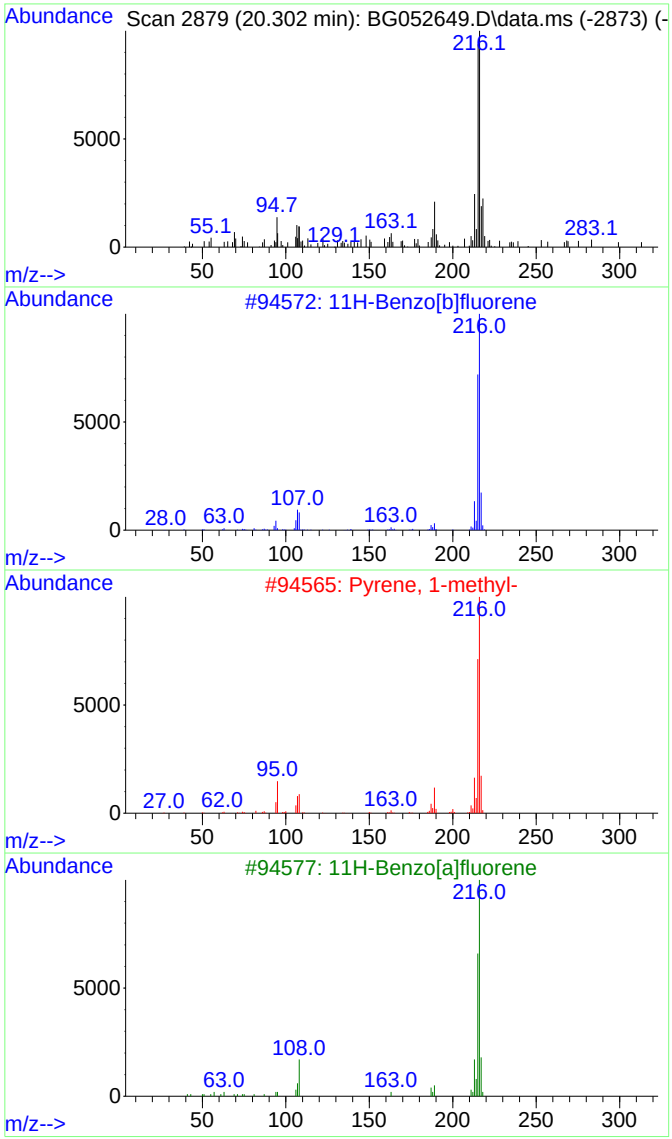
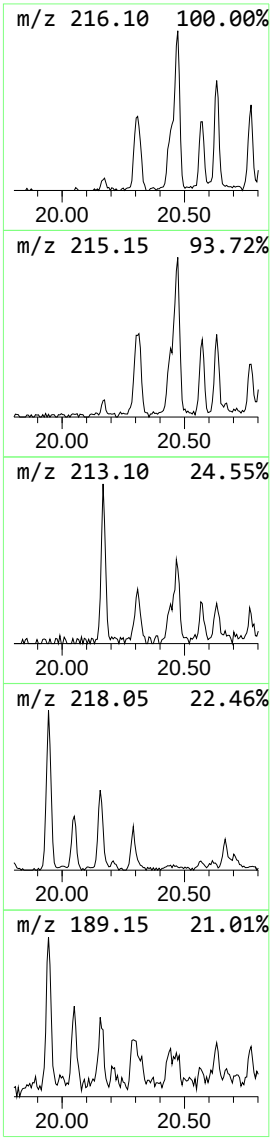
Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.302	2.24 ng	81336	Chrysene-d12	21.883

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	76
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	74
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031122\
Data File : BG052649.D
Acq On : 11 Mar 2022 16:19
Operator : CG/JU
Sample : N1864-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MB-B1-030922-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030922.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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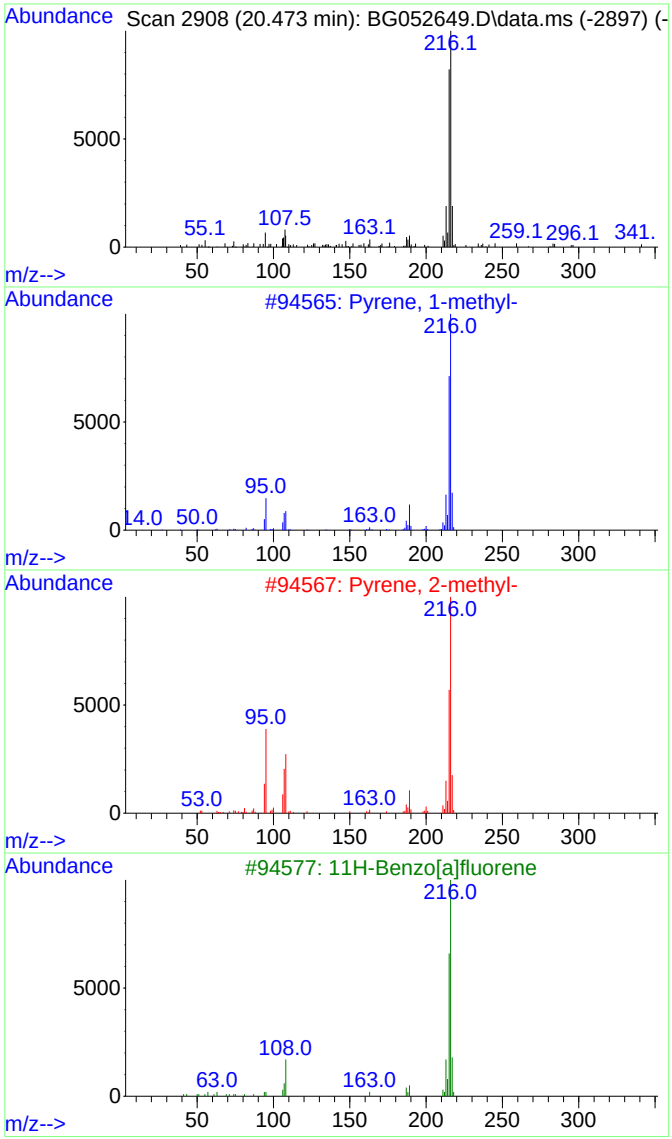
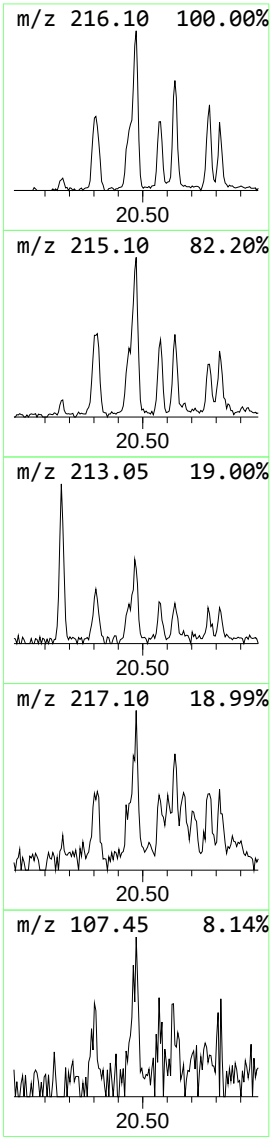
Peak Number 8 Pyrene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.473	3.15 ng	114392	Chrysene-d12	21.883

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2	Pyrene, 2-methyl-	216	C17H12	003442-78-2	91
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
5	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031122\
Data File : BG052649.D
Acq On : 11 Mar 2022 16:19
Operator : CG/JU
Sample : N1864-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MB-B1-030922-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030922.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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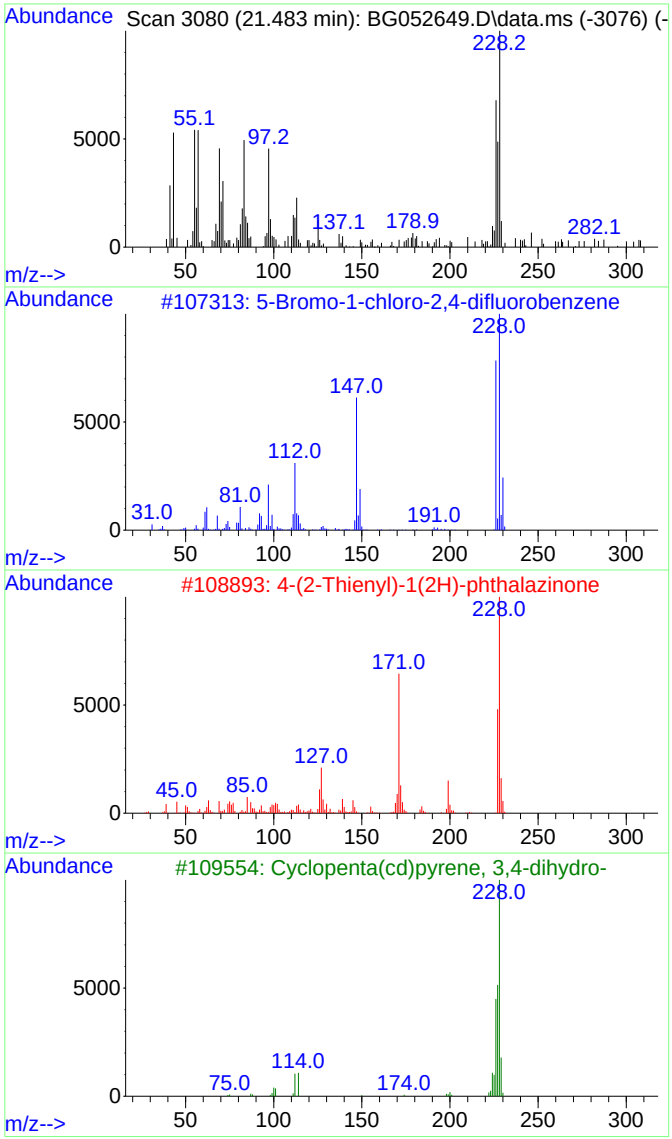
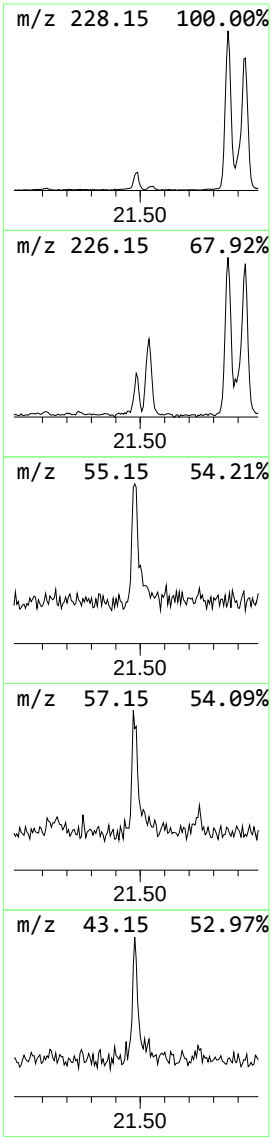
Peak Number 9 unknown21.483 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.483	2.66 ng	96388	Chrysene-d12	21.883

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-1-chloro-2,4-difluoroben...	226	C6H2BrClF2	914636-89-8	35
2	4-(2-Thienyl)-1(2H)-phthalazinone	228	C12H8N2OS	137382-45-7	30
3	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	30
4	Triphenylene	228	C18H12	000217-59-4	27
5	1(2H)-Phenanthrenone, 3,4,9,10-t...	228	C15H16O2	014427-61-3	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031122\
Data File : BG052649.D
Acq On : 11 Mar 2022 16:19
Operator : CG/JU
Sample : N1864-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MB-B1-030922-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030922.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, 2...	18.446	3.9	ng	96502	4	17.571	489626	20.0
Anthracene, 1-m...	18.499	4.0	ng	96620	4	17.571	489626	20.0
4H-Cyclopenta[d...	18.646	4.2	ng	101570	4	17.571	489626	20.0
9,10-Anthracene...	18.986	2.3	ng	57387	4	17.571	489626	20.0
3,4-Dimethylphe...	19.357	2.1	ng	51128	4	17.571	489626	20.0
Cyclopenta(def)...	19.503	2.1	ng	50410	4	17.571	489626	20.0
11H-Benzo[b]flu...	20.302	2.2	ng	81336	5	21.883	726015	20.0
Pyrene, 1-methyl-	20.473	3.1	ng	114392	5	21.883	726015	20.0
unknown21.483	21.483	2.7	ng	96388	5	21.883	726015	20.0