LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054842.D
Acq On : 2 Sep 2022 16:10
Operator : CG/JU
Sample : N4464-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-1

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-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054842.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.209	321	327	336	rBV	91786	143907	8.29%	0.828%
2	5.685	401	408	423	rBV	457549	749373	43.15%	4.314%
3	7.295	672	682	697	rBV	467872	839456	48.34%	4.832%
4	8.147	818	827	834	rBV	128003	216613	12.47%	1.247%
5	8.911	952	957	966	rBV	9598	17810	1.03%	0.103%
6	9.316	1019	1026	1039	rBV	271785	513683	29.58%	2.957%
7	10.973	1301	1308	1315	rBV	182814	331408	19.08%	1.908%
8	13.399	1713	1721	1733	rBV	777684	1264374	72.81%	7.278%
9	14.510	1903	1910	1918	rBV	9764	22940	1.32%	0.132%
10	14.780	1947	1956	1963	rBV	301956	494391	28.47%	2.846%
11	16.267	2202	2209	2222	rBV	582217	956361	55.07%	5.505%
12	16.478	2242	2245	2254	rVB7	14344	26441	1.52%	0.152%
13	17.177	2358	2364	2371	rBV3	10069	19194	1.11%	0.110%
14	17.248	2371	2376	2381	rBV3	12131	19484	1.12%	0.112%
15	17.342	2388	2392	2399	rVB2	10220	17502	1.01%	0.101%
16	17.524	2416	2423	2427	rBV	381380	592506	34.12%	3.411%
17	17.565	2427	2430	2437	rVB	167959	253032	14.57%	1.457%
18	17.659	2438	2446	2450	rBV	27317	45930	2.64%	0.264%
19	17.882	2479	2484	2488	rBV	27926	43957	2.53%	0.253%
20	17.929	2488	2492	2499	rVB	19693	36659	2.11%	0.211%
21	18.399	2567	2572	2575	rBV	35088	52287	3.01%	0.301%
22	18.446	2576	2580	2586	rVB4	46485	79058	4.55%	0.455%
23	18.593	2598	2605	2609	rBV3	64050	129618	7.46%	0.746%
24	18.629	2609	2611	2616	rVB	29997	38215	2.20%	0.220%
25	18.893	2651	2656	2659	rBV2	31865	48596	2.80%	0.280%
26	18.934	2659	2663	2669	rVB3	40392	64448	3.71%	0.371%
27	19.134	2689	2697	2702	rBV4	21658	41919	2.41%	0.241%
28	19.222	2709	2712	2721	rVB4	11685	22658	1.30%	0.130%
29	19.304	2721	2726	2731	rBV	53695	90525	5.21%	0.521%
30	19.369	2732	2737	2740	rBV3	13743	25675	1.48%	0.148%
31	19.451	2746	2751	2763	rBV3	34556	78891	4.54%	0.454%
32	19.575	2766	2772	2778	rVV	558670	804771	46.34%	4.632%
33	19.669	2785	2788	2791	rVB2	13939	17885	1.03%	0.103%
34	19.815	2809	2813	2820	rVB2	24413	50028	2.88%	0.288%
35	19.898	2822	2827	2829	rVV2	76886	124520	7.17%	0.717%
36	19.933	2829	2833	2840	rVV	535218	817786	47.09%	4.707%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054842.D
Acq On : 2 Sep 2022 16:10
Operator : CG/JU
Sample : N4464-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-1

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-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.998	2841	2844	2849	rVB2	34021	50969	2.94%	0.293%
38	20.121	2859	2865	2871	rBV	1298094	1736563	100.00%	9.996%
39	20.262	2882	2889	2894	rBV3	47757	107620	6.20%	0.619%
40	20.391	2906	2911	2912	rBV5	36072	56204	3.24%	0.324%
41	20.421	2912	2916	2921	rVB2	85724	142555	8.21%	0.821%
42	20.520	2929	2933	2937	rBV	54451	63382	3.65%	0.365%
43	20.579	2937	2943	2947	rBV2	57292	105924	6.10%	0.610%
44	20.720	2963	2967	2971	rBV	57011	84210	4.85%	0.485%
45	20.767	2971	2975	2978	rVV	42343	56307	3.24%	0.324%
46	21.190	3044	3047	3054	rVB	55795	91160	5.25%	0.525%
47	21.384	3077	3080	3083	rVV	36199	43134	2.48%	0.248%
48	21.425	3083	3087	3092	rVV2	114425	159607	9.19%	0.919%
49	21.478	3092	3096	3101	rVV2	48513	75786	4.36%	0.436%
50	21.537	3103	3106	3114	rVB	51092	84036	4.84%	0.484%
51	21.678	3126	3130	3136	rVB2	40526	64648	3.72%	0.372%
52	21.813	3145	3153	3158	rBV2	445122	1154259	66.47%	6.644%
53	21.866	3158	3162	3174	rVB	262427	489953	28.21%	2.820%
54	22.025	3185	3189	3196	rVB	41996	67740	3.90%	0.390%
55	23.329	3406	3411	3426	rVB3	116245	281068	16.19%	1.618%
56	24.110	3536	3544	3552	rBV	223537	770315	44.36%	4.434%
57	24.874	3666	3674	3686	rVB	162708	485961	27.98%	2.797%
58	25.027	3691	3700	3714	rVB	190830	581682	33.50%	3.348%
59	25.186	3718	3727	3736	rBV3	221650	669747	38.57%	3.855%
60	29.069	4377	4388	4408	rVB4	93558	499400	28.76%	2.875%
61	30.280	4583	4594	4611	rVB3	75634	358165	20.62%	2.062%

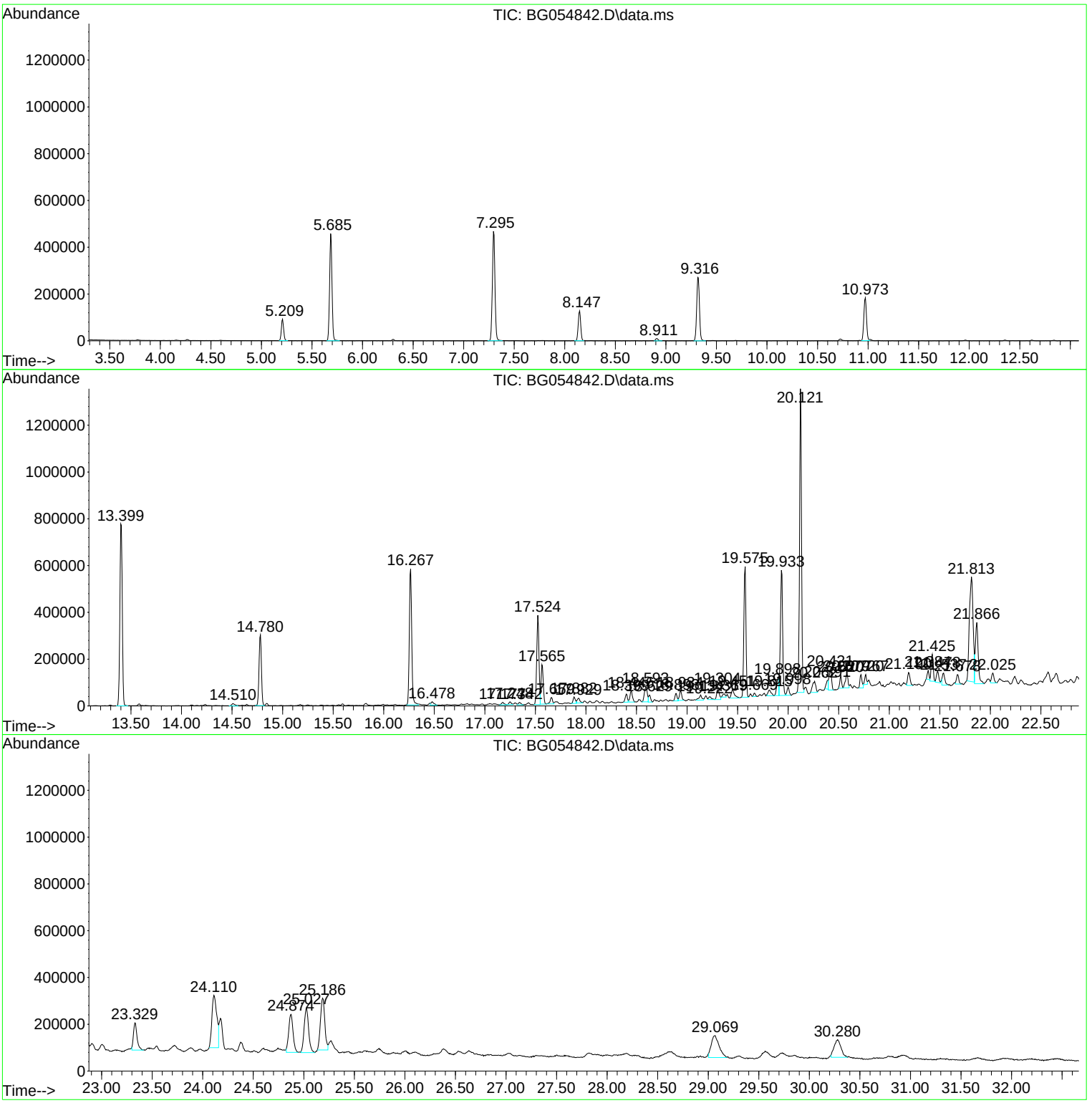
Sum of corrected areas: 17372296

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054842.D
Acq On : 2 Sep 2022 16:10
Operator : CG/JU
Sample : N4464-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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\BG090222\
Data File : BG054842.D
Acq On : 2 Sep 2022 16:10
Operator : CG/JU
Sample : N4464-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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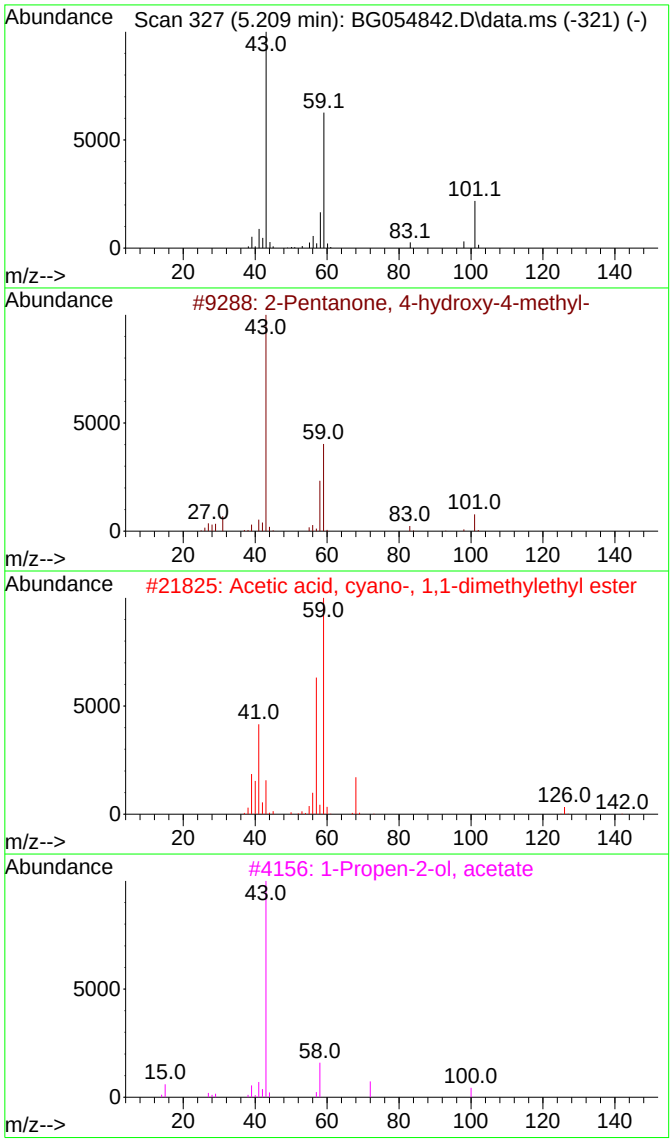
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

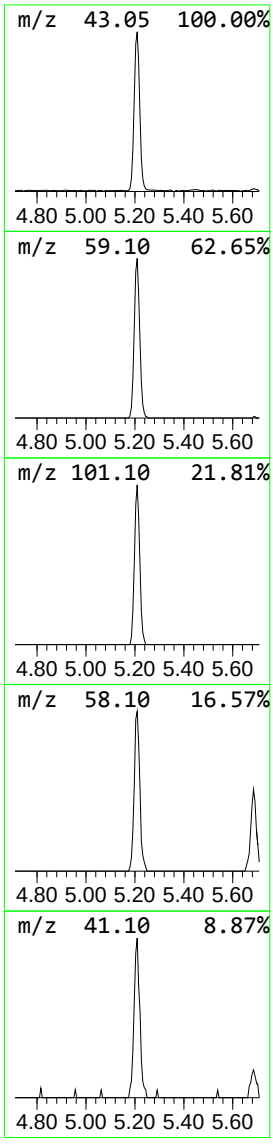
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.209	13.29 ng	143907	1,4-Dichlorobenzene-d4	8.147

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054842.D
Acq On : 2 Sep 2022 16:10
Operator : CG/JU
Sample : N4464-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

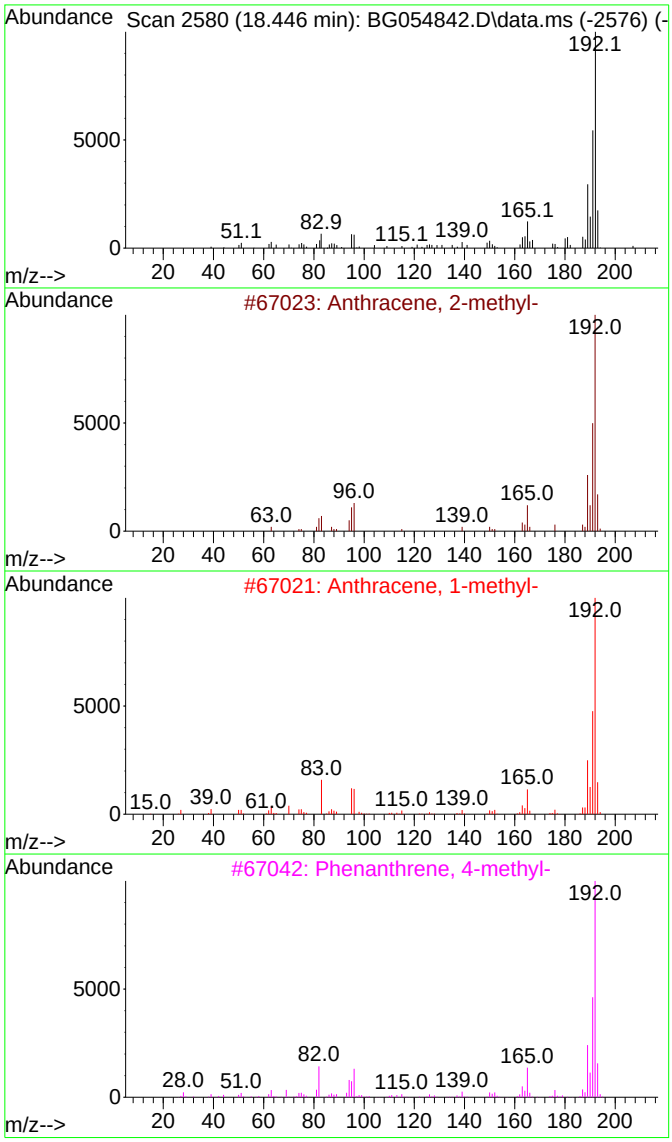
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

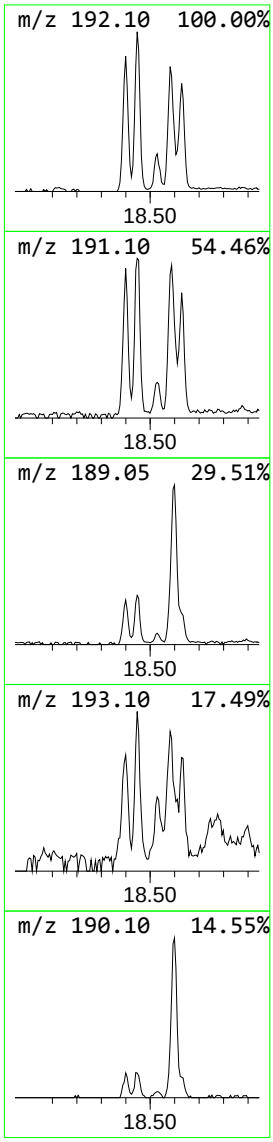
****

Peak Number 2 Anthracene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.446	2.67 ng	79058	Phenanthrene-d10	17.524

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	91
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054842.D
Acq On : 2 Sep 2022 16:10
Operator : CG/JU
Sample : N4464-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

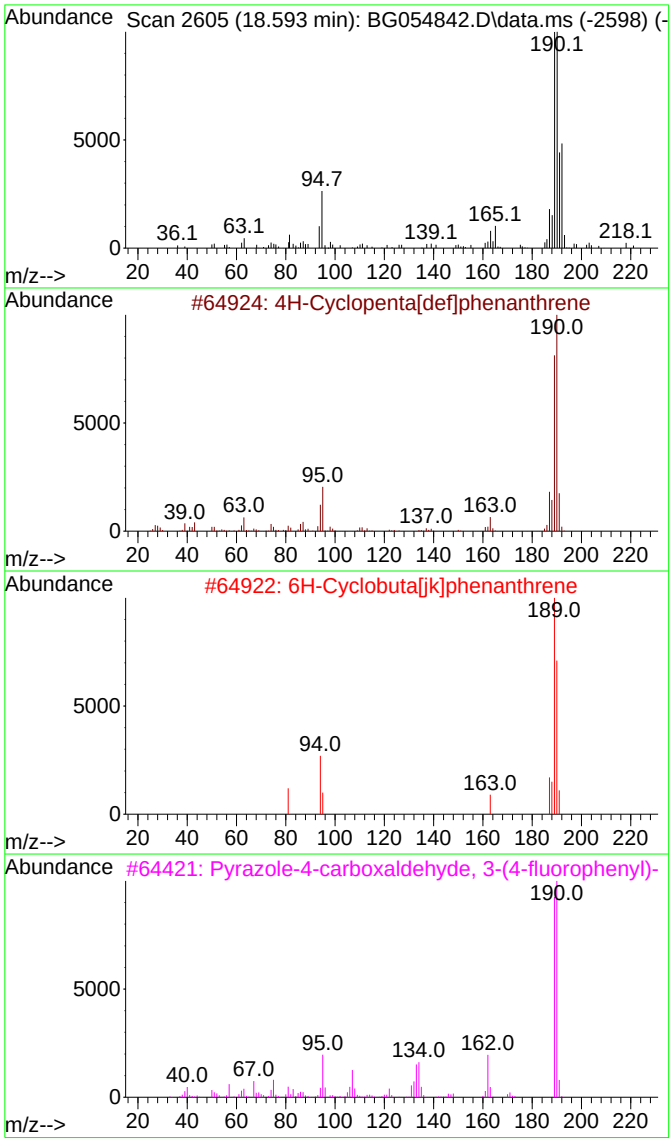
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

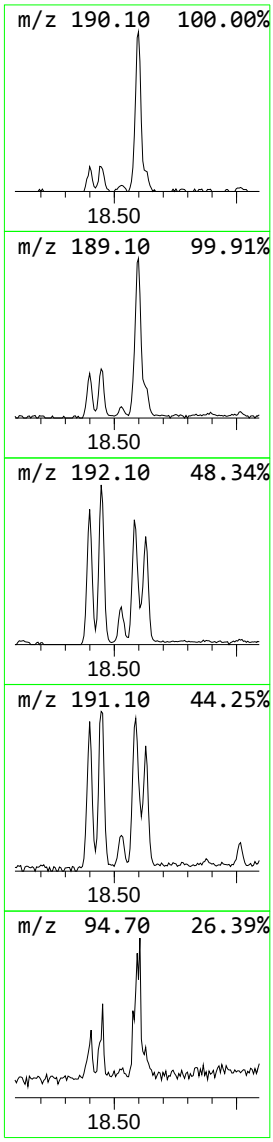
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.593	4.38 ng	129618	Phenanthrene-d10	17.524

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	49
4	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	40
5	Carbonic acid, butyl 2-formyl-4,...	290	C12H12Cl2O4	1000331-42-2	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054842.D
Acq On : 2 Sep 2022 16:10
Operator : CG/JU
Sample : N4464-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

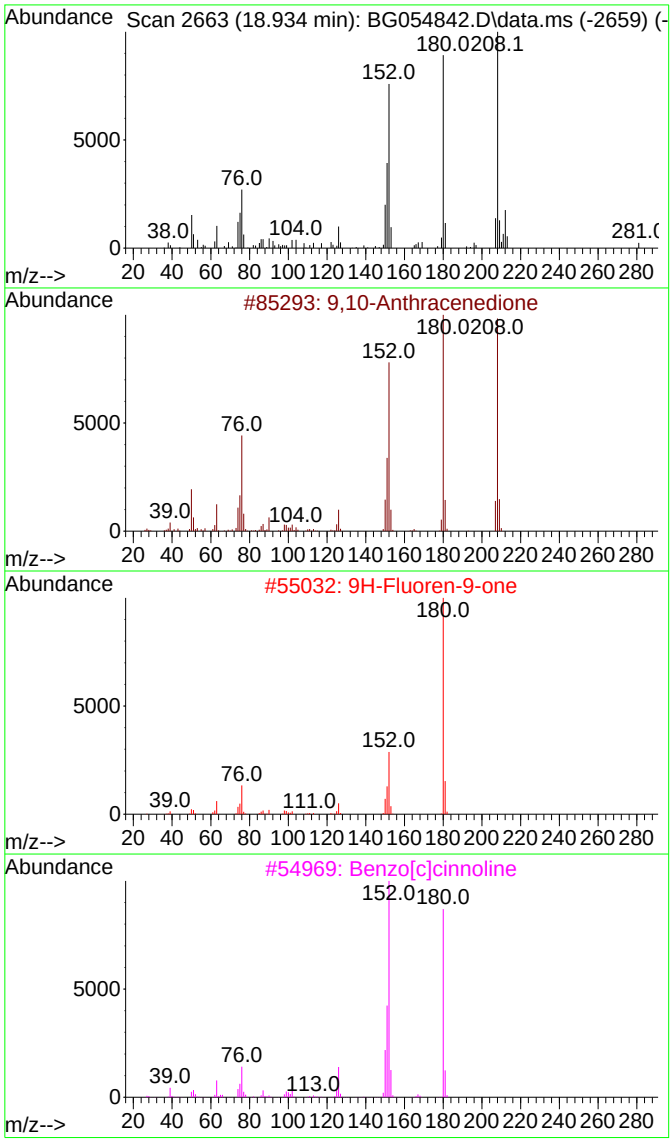
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

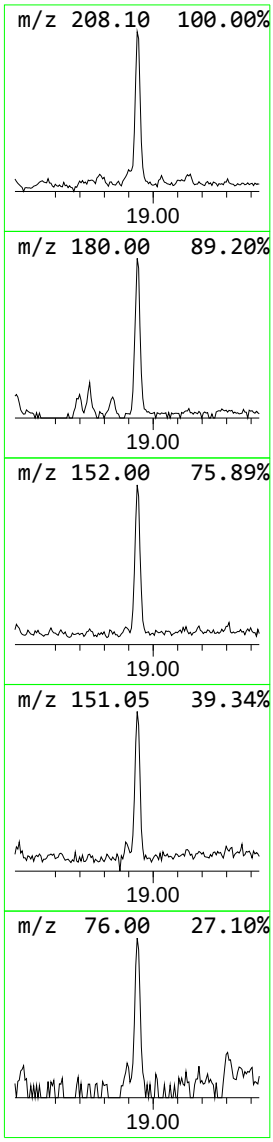
****

Peak Number 4 9,10-Anthracenedione Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.934	2.18 ng	64448	Phenanthrene-d10	17.524

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	95
2	9H-Fluoren-9-one	180	C13H8O	000486-25-9	70
3	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	64
4	9,10-Phenanthrenedione	208	C14H8O2	000084-11-7	49
5	1,4-Anthracenedione	208	C14H8O2	000635-12-1	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054842.D
Acq On : 2 Sep 2022 16:10
Operator : CG/JU
Sample : N4464-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

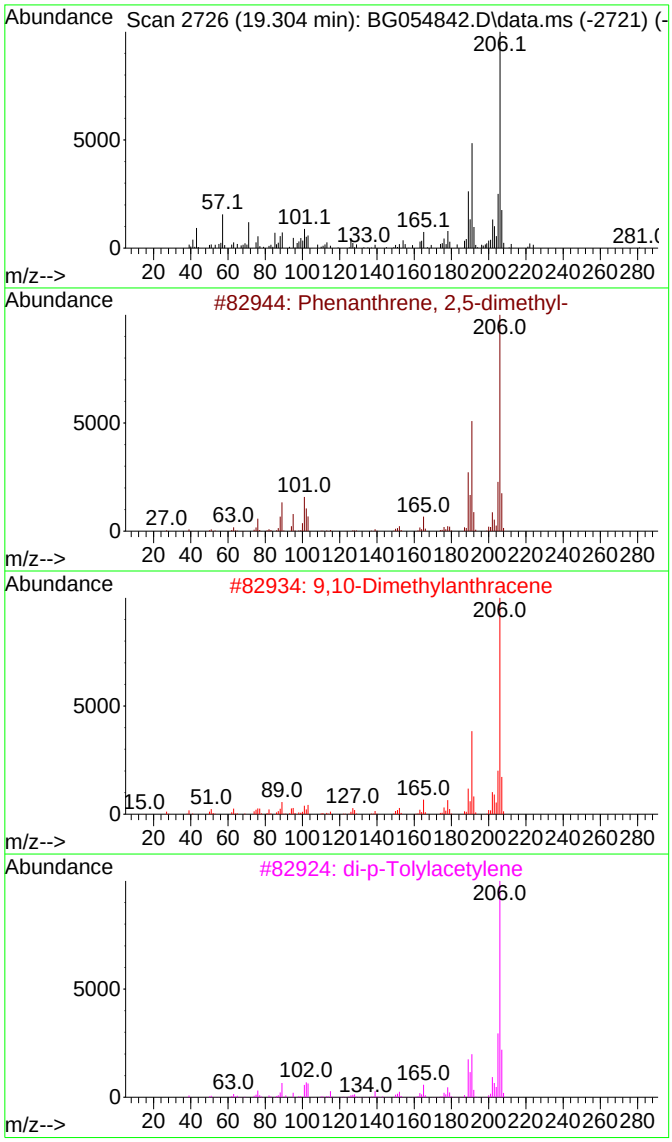
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

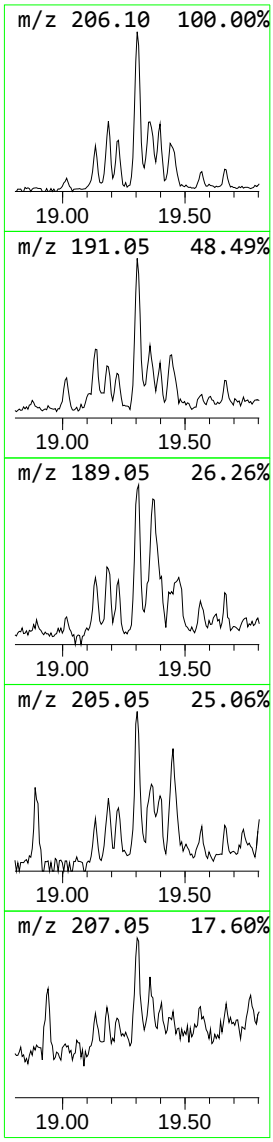
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.304	3.06 ng	90525	Phenanthrene-d10	17.524

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	96
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	96
3	di-p-Tolylacetylene	206	C16H14	002789-88-0	93
4	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	93
5	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054842.D
Acq On : 2 Sep 2022 16:10
Operator : CG/JU
Sample : N4464-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

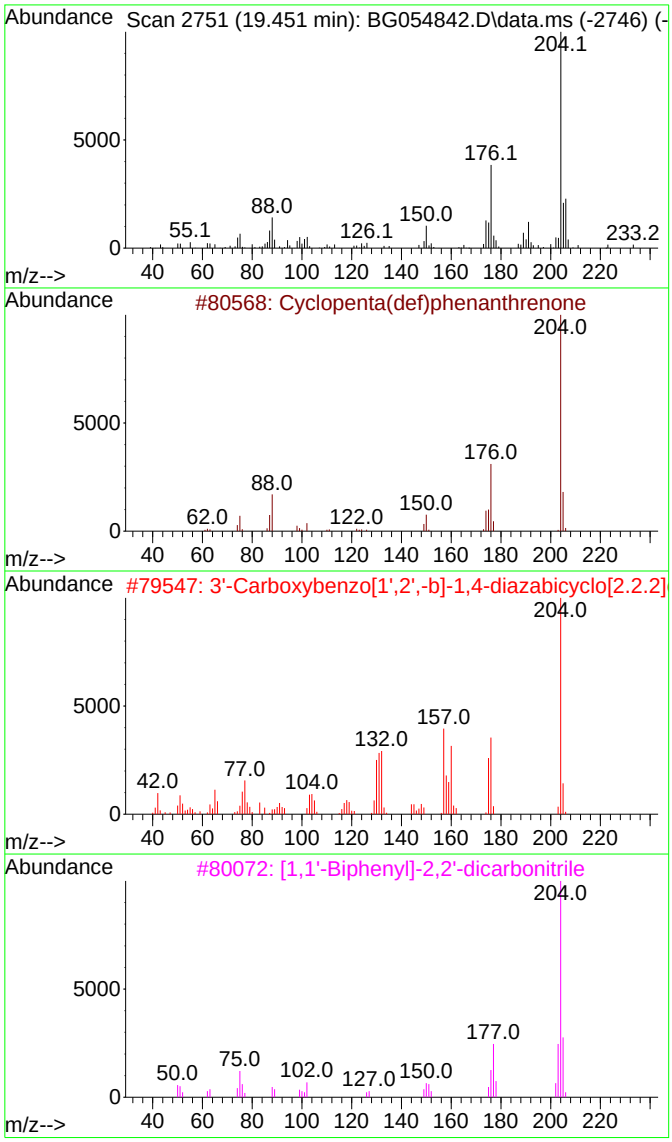
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

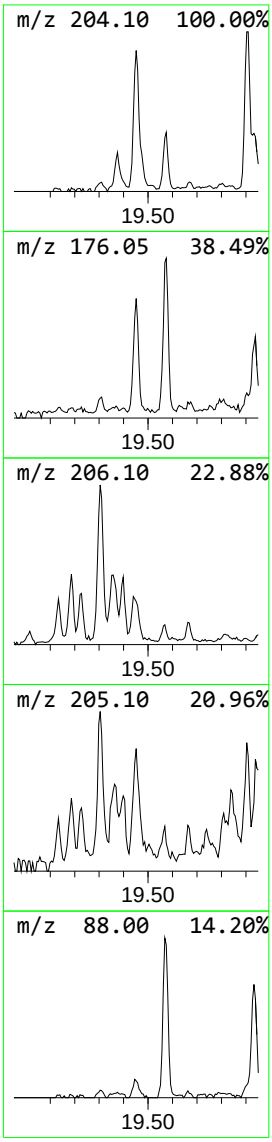
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopenta(def)phenanthrenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	2.66 ng	78891	Phenanthrene-d10	17.524

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	95
2	3'-Carboxybenzo[1',2',-b]-1,4-di...	204	C11H12N2O2	138023-41-3	50
3	[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	49
4	6-Chloro-4-hydroxyquinoline-3-ca...	204	C10H5ClN2O	1000435-79-8	45
5	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054842.D
Acq On : 2 Sep 2022 16:10
Operator : CG/JU
Sample : N4464-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

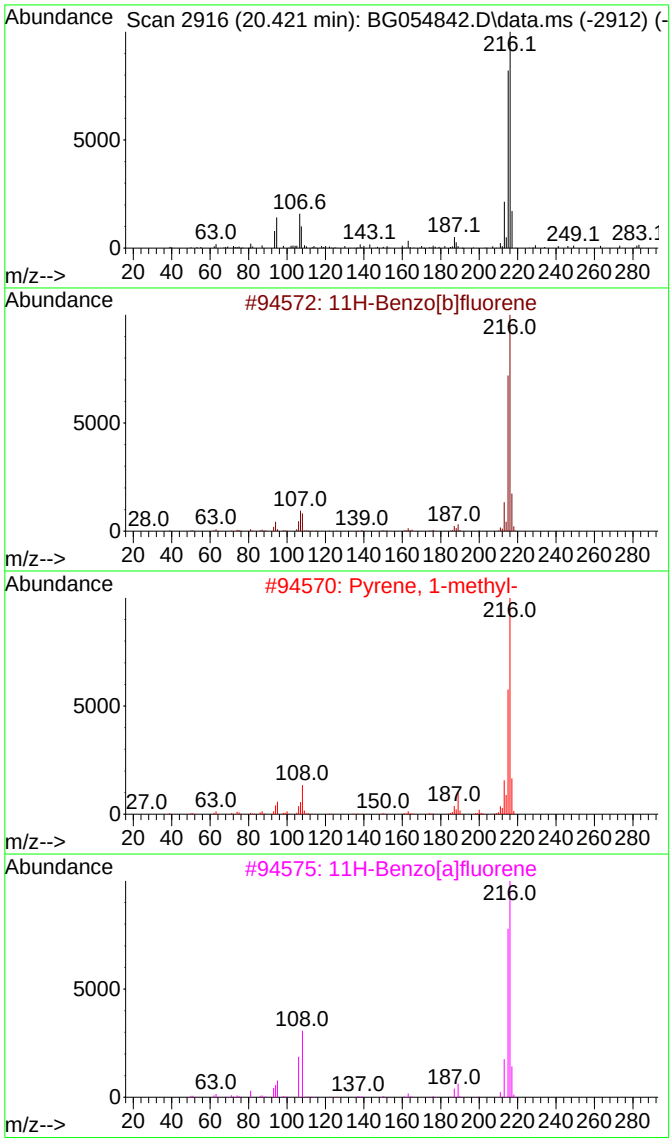
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

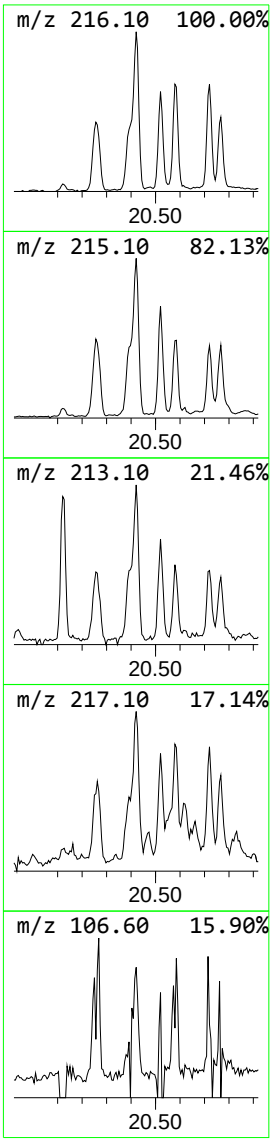
****

Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.421	2.47 ng	142555	Chrysene-d12	21.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	86
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	83
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	83
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054842.D
Acq On : 2 Sep 2022 16:10
Operator : CG/JU
Sample : N4464-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

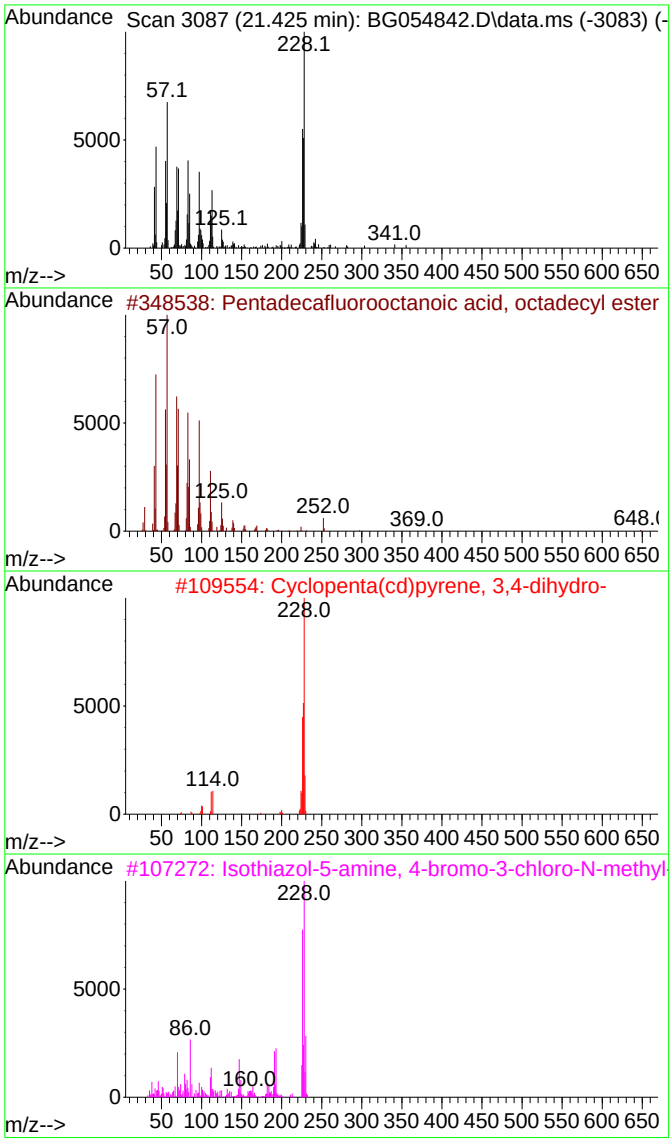
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

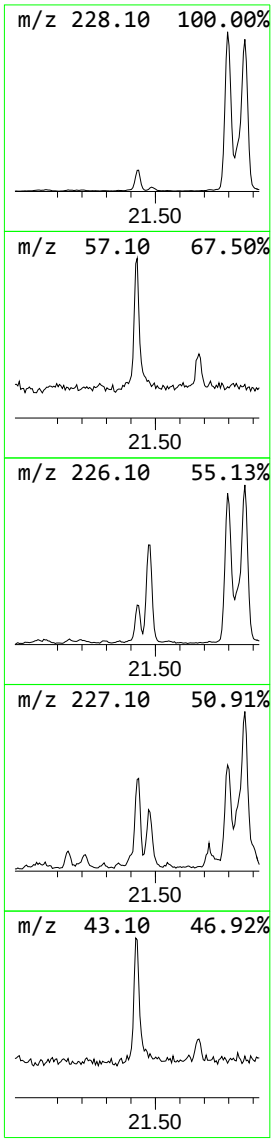
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Pentadecafluorooctanoic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.425	2.77 ng	159607	Chrysene-d12	21.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	62
2	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	53
3	Isothiazol-5-amine, 4-bromo-3-ch...	226	C4H4BrClN2S	1000272-59-9	43
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	25
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054842.D
Acq On : 2 Sep 2022 16:10
Operator : CG/JU
Sample : N4464-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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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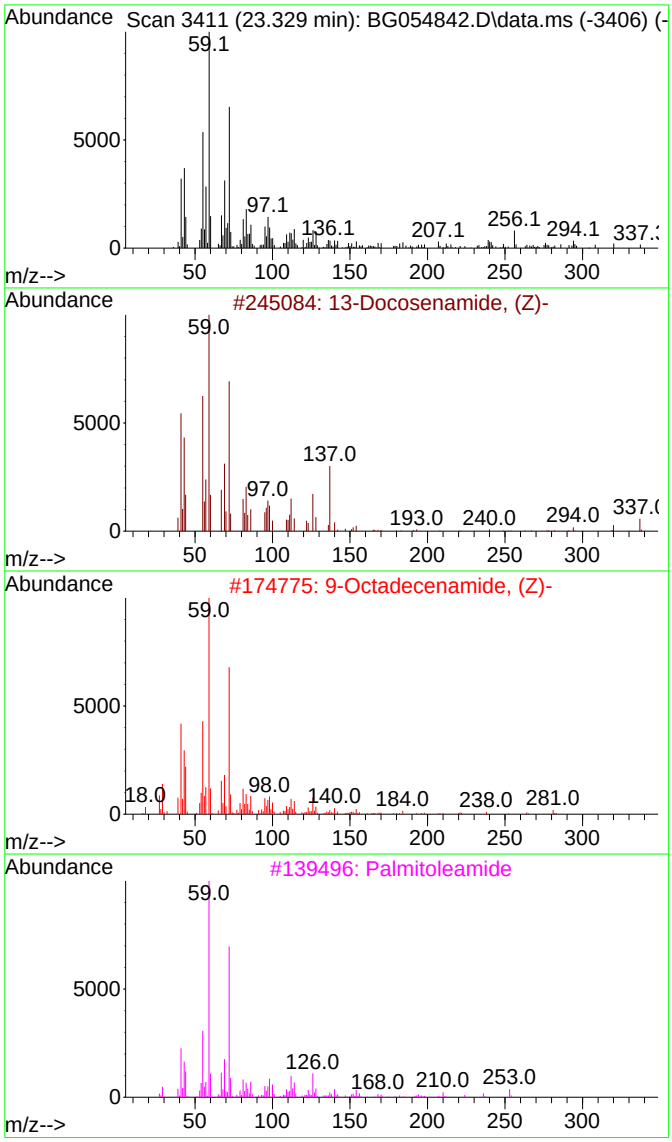
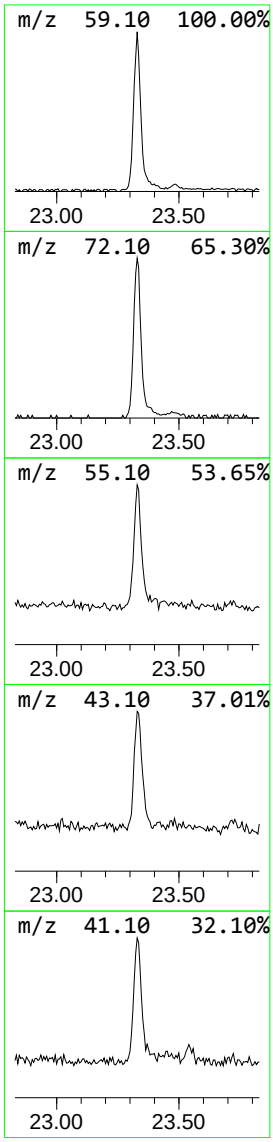
Peak Number 9 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.329	4.87 ng	281068	Chrysene-d12	21.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3	Palmitoleamide	253	C16H31NO	106010-22-4	64
4	d-Glucosamine	179	C6H13NO5	000090-77-7	53
5	Nonanamide	157	C9H19NO	001120-07-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054842.D
Acq On : 2 Sep 2022 16:10
Operator : CG/JU
Sample : N4464-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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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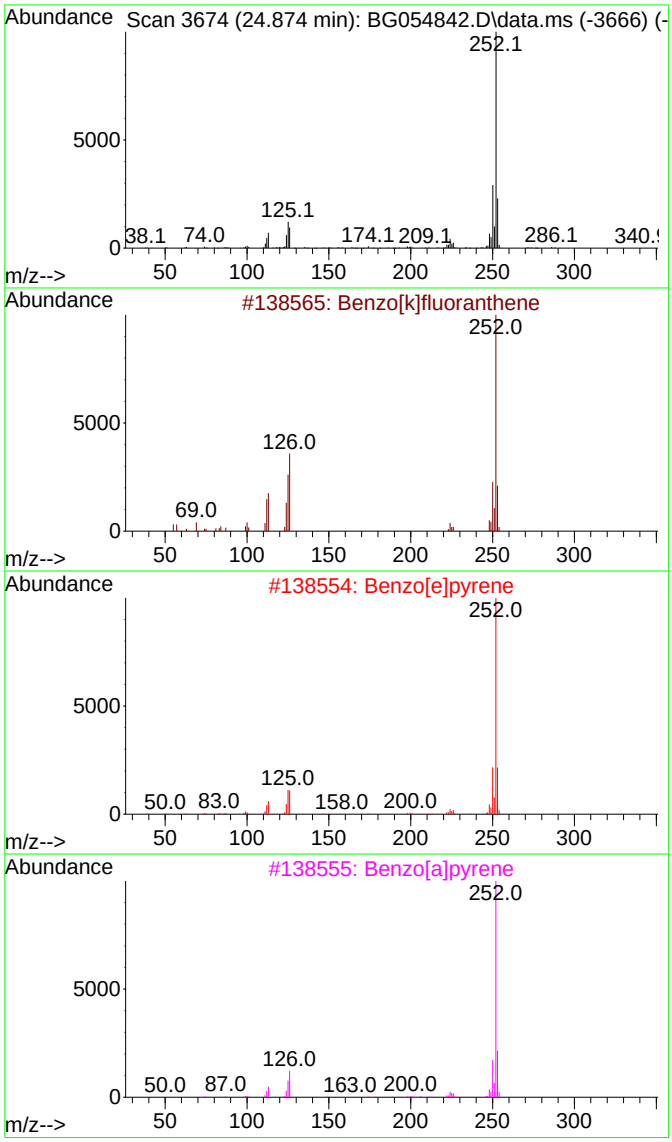
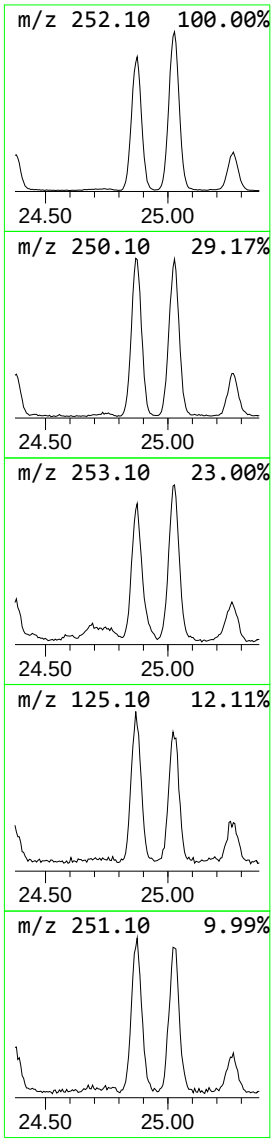
Peak Number 10 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.874	14.51 ng	485961	Perylene-d12	25.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
2	Benzo[e]pyrene	252	C20H12	000192-97-2	94
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054842.D
Acq On : 2 Sep 2022 16:10
Operator : CG/JU
Sample : N4464-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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
2-Pentanone, 4-...	5.209	13.3	ng	143907	1	8.147	216613	20.0
Anthracene, 2-m...	18.446	2.7	ng	79058	4	17.524	592506	20.0
4H-Cyclopenta[d...	18.593	4.4	ng	129618	4	17.524	592506	20.0
9,10-Anthracene...	18.934	2.2	ng	64448	4	17.524	592506	20.0
Phenanthrene, 2...	19.304	3.1	ng	90525	4	17.524	592506	20.0
Cyclopenta(def)...	19.451	2.7	ng	78891	4	17.524	592506	20.0
11H-Benzo[b]flu...	20.421	2.5	ng	142555	5	21.819	1154260	20.0
Pentadecafluoro...	21.425	2.8	ng	159607	5	21.819	1154260	20.0
13-Docosenamide...	23.329	4.9	ng	281068	5	21.819	1154260	20.0
Benzo[e]pyrene	24.874	14.5	ng	485961	6	25.186	669747	20.0