LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
Data File : BG055987.D
Acq On : 15 Dec 2022 21:55
Operator : CG/JU
Sample : N6069-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PT-2-121422

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-BG121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055987.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.411	17	21	28	rBB2	3272	5229	2.00%	0.288%
2	5.420	359	363	368	rBB2	2293	3265	1.25%	0.180%
3	5.896	438	444	451	rBB	22051	34727	13.28%	1.913%
4	7.506	712	718	724	rBB	24960	41673	15.93%	2.296%
5	8.381	861	867	874	rBB	36142	58154	22.23%	3.203%
6	9.550	1060	1066	1072	rBB	14765	24671	9.43%	1.359%
7	11.219	1342	1350	1356	rBV	46433	80792	30.89%	4.450%
8	13.616	1752	1758	1764	rBB	47876	69923	26.73%	3.852%
9	14.310	1872	1876	1880	rBB	2130	2809	1.07%	0.155%
10	14.991	1986	1992	1998	rVV	76270	120079	45.91%	6.615%
11	15.050	1998	2002	2007	rVB2	6046	8528	3.26%	0.470%
12	15.379	2053	2058	2064	rVB2	4175	6447	2.46%	0.355%
13	16.025	2163	2168	2176	rBB2	9189	15740	6.02%	0.867%
14	16.319	2214	2218	2223	rVB3	2782	4242	1.62%	0.234%
15	16.466	2237	2243	2250	rVB	54936	85452	32.67%	4.707%
16	16.683	2277	2280	2285	rVB4	2052	3531	1.35%	0.195%
17	17.024	2331	2338	2342	rBV2	3292	5715	2.18%	0.315%
18	17.071	2342	2346	2349	rBV4	2545	3287	1.26%	0.181%
19	17.371	2391	2397	2402	rBV6	4069	6956	2.66%	0.383%
20	17.447	2405	2410	2414	rVV4	2768	4038	1.54%	0.222%
21	17.541	2422	2426	2433	rVB2	4962	9029	3.45%	0.497%
22	17.723	2452	2457	2461	rBV	99198	153760	58.78%	8.470%
23	17.770	2461	2465	2471	rVB	60155	88363	33.78%	4.868%
24	17.858	2475	2480	2484	rVV	16104	21109	8.07%	1.163%
25	17.911	2485	2489	2494	rVB5	3149	4584	1.75%	0.253%
26	18.117	2521	2524	2530	rBV2	5548	8544	3.27%	0.471%
27	18.240	2541	2545	2549	rBV2	3334	4312	1.65%	0.238%
28	18.311	2552	2557	2560	rVB3	4134	6798	2.60%	0.374%
29	18.446	2575	2580	2585	rBV6	3979	9217	3.52%	0.508%
30	18.593	2597	2605	2610	rBV5	12556	33266	12.72%	1.832%
31	18.646	2610	2614	2617	rVV	15229	20525	7.85%	1.131%
32	18.722	2622	2627	2632	rBV	7265	14967	5.72%	0.824%
33	18.787	2632	2638	2642	rBV2	23345	45594	17.43%	2.512%
34	18.822	2642	2644	2648	rVB3	9525	11330	4.33%	0.624%
35	19.034	2675	2680	2683	rBV6	5130	8789	3.36%	0.484%
36	19.081	2685	2688	2691	rVB	11026	13101	5.01%	0.722%

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Misc :
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Instrument :
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ClientSampleId :
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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-BG121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.110	2691	2693	2694	rBV2	5133	4362	1.67%	0.240%
38	19.374	2735	2738	2742	rBV5	7331	10644	4.07%	0.586%
39	19.410	2742	2744	2746	rBV3	7354	7584	2.90%	0.418%
40	19.492	2754	2758	2762	rBV2	15404	21824	8.34%	1.202%
41	19.756	2798	2803	2808	rBV	128427	189086	72.29%	10.416%
42	20.120	2860	2865	2871	rVB	112146	169050	64.63%	9.312%
43	20.297	2891	2895	2900	rBV	85243	112701	43.09%	6.208%
44	22.036	3184	3191	3197	rBV2	101478	261565	100.00%	14.408%

Sum of corrected areas: 1815362

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Instrument :
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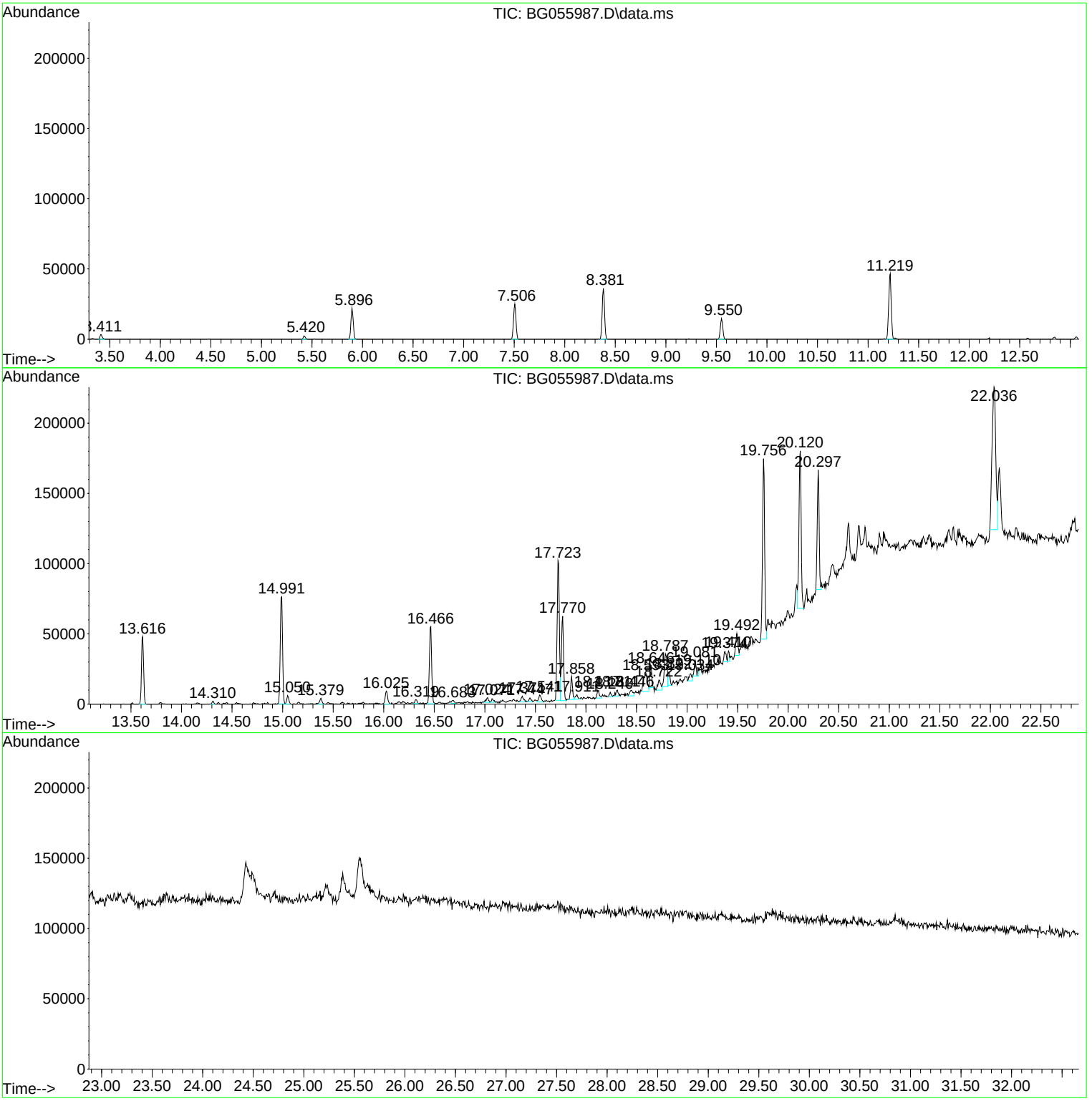
ClientSampleId :
PT-2-121422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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\BG121522\
Data File : BG055987.D
Acq On : 15 Dec 2022 21:55
Operator : CG/JU
Sample : N6069-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PT-2-121422

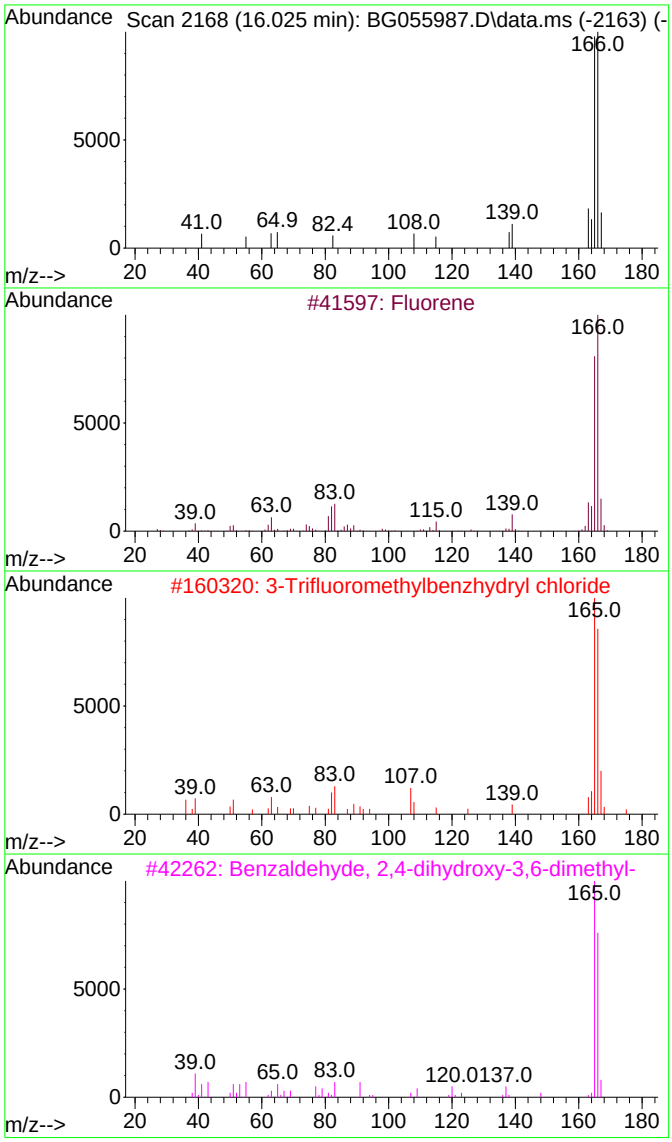
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

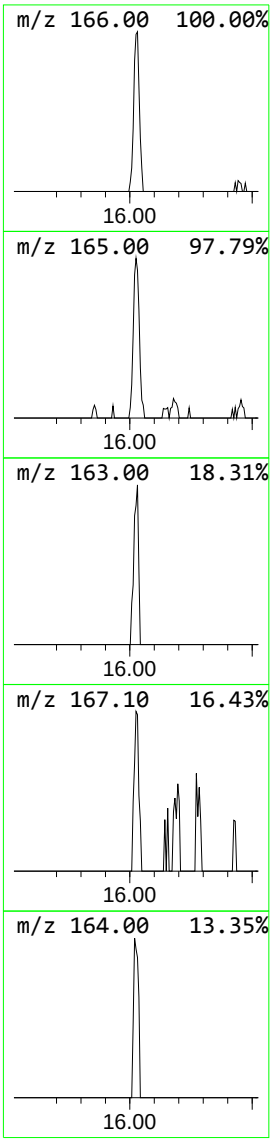
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 3-Trifluoromethylbenzhydryl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.025	2.62 ng	15740	Acenaphthene-d10	14.991

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluorene	166	C13H10	000086-73-7	90
2	3-Trifluoromethylbenzhydryl chlo...	270	C14H10ClF3	067240-79-3	56
3	Benzaldehyde, 2,4-dihydroxy-3,6-...	166	C9H10O3	034883-14-2	50
4	1,4-Oxathiino[3,2-b]pyridine, 6-...	165	C8H7NOS	056114-39-7	37
5	4-Hydroxy-m-tolyl thiocyanate	165	C8H7NOS	003774-53-6	37





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Data File : BG055987.D
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Instrument :
BNA_G
ClientSampleId :
PT-2-121422

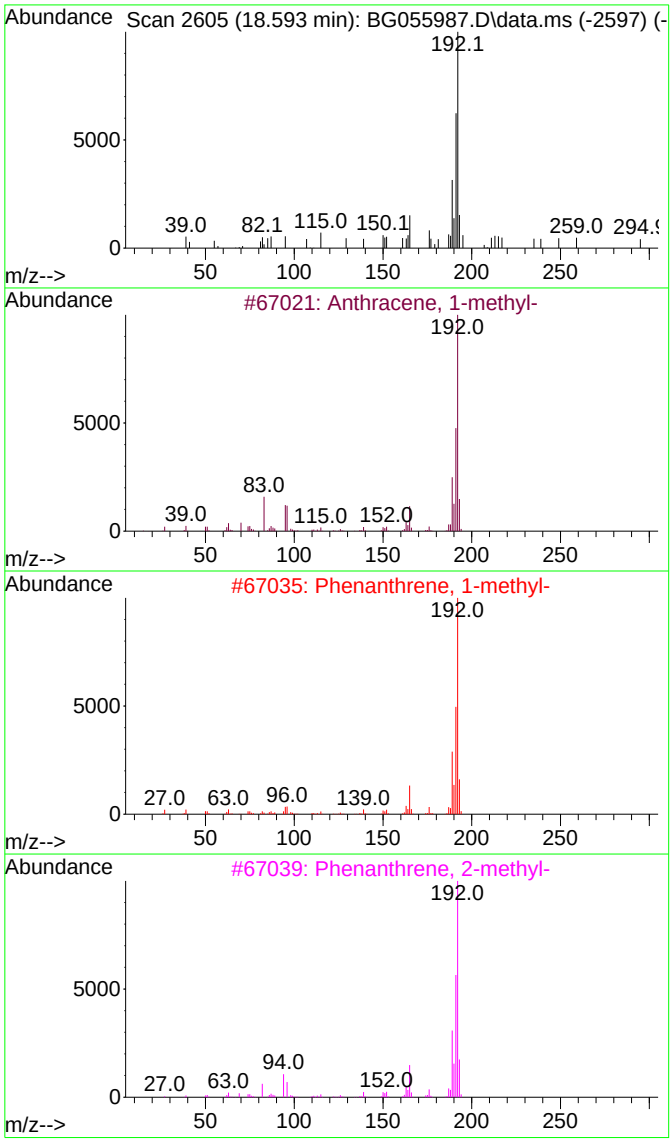
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

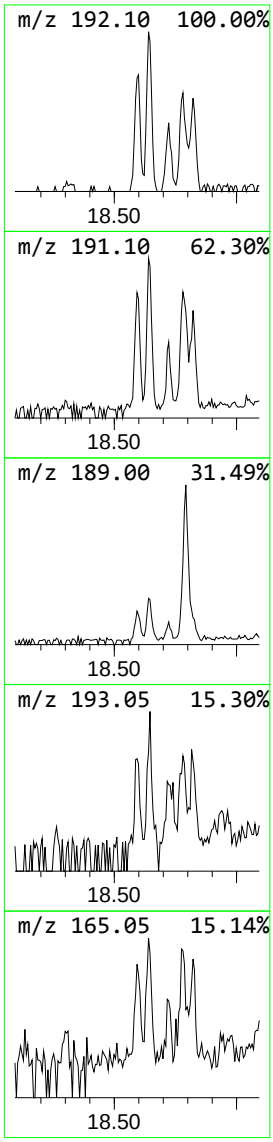
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.593	4.33 ng	33266	Phenanthrene-d10	17.723

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	81
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	81
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	81
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	81
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
Data File : BG055987.D
Acq On : 15 Dec 2022 21:55
Operator : CG/JU
Sample : N6069-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PT-2-121422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

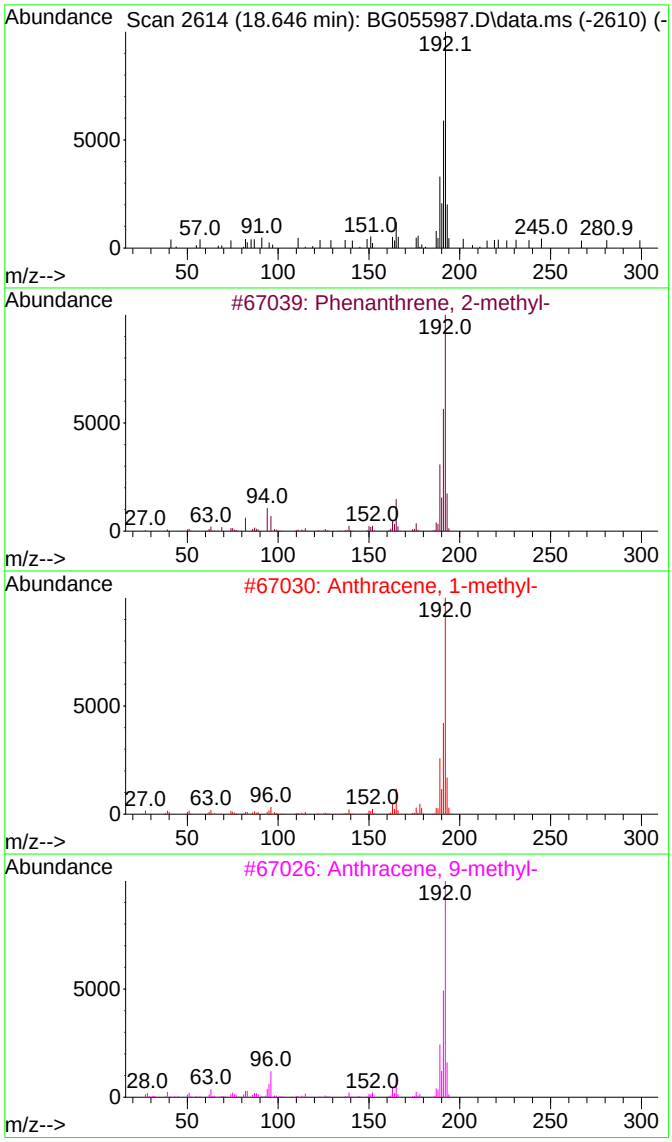
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

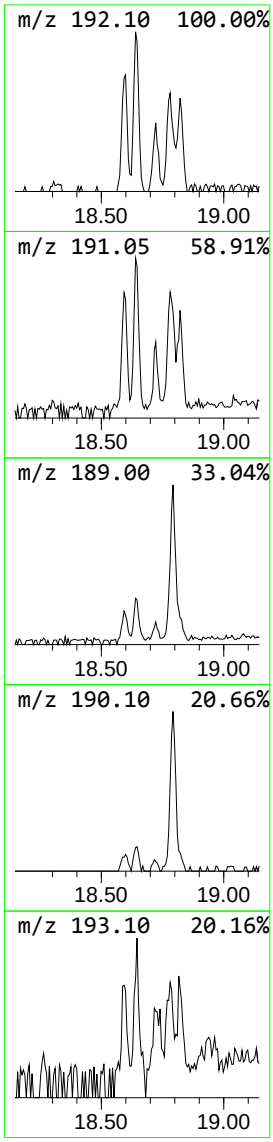
****

Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.646	2.67 ng	20525	Phenanthrene-d10	17.723

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	76
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	76
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	76
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	68
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
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Acq On : 15 Dec 2022 21:55
Operator : CG/JU
Sample : N6069-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PT-2-121422

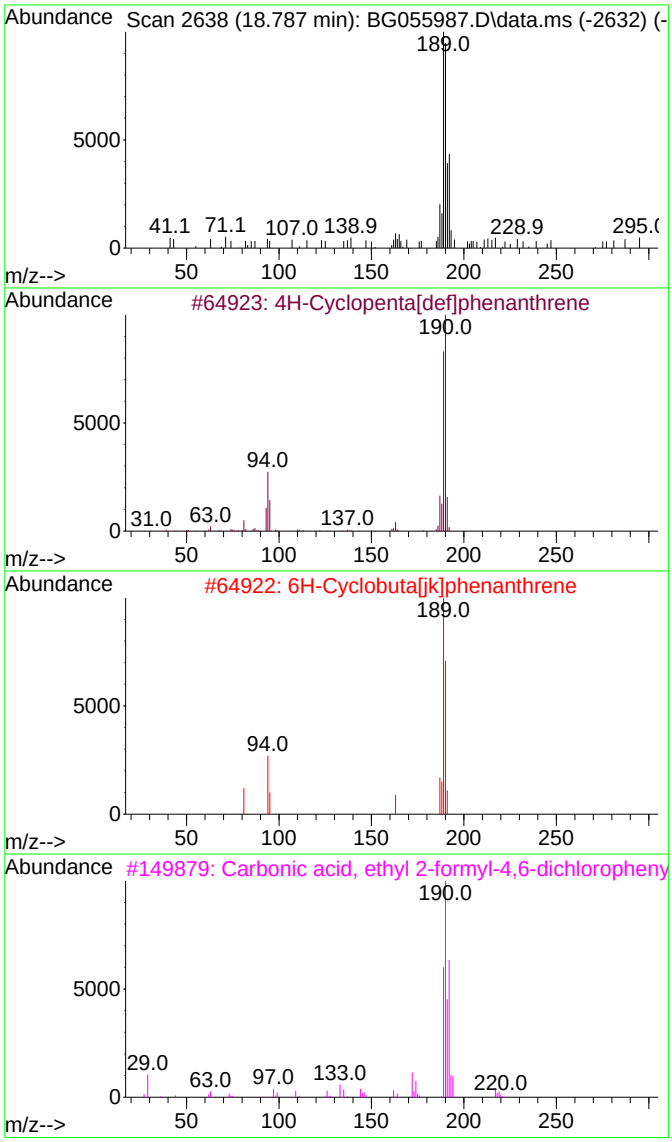
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

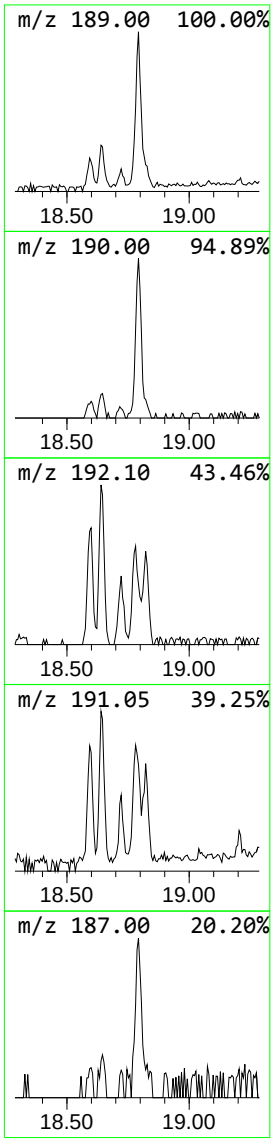
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.787	5.93 ng	45594	Phenanthrene-d10	17.723

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	47
5	Methyl diselenide	190	C2H6Se2	007101-31-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
Data File : BG055987.D
Acq On : 15 Dec 2022 21:55
Operator : CG/JU
Sample : N6069-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PT-2-121422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

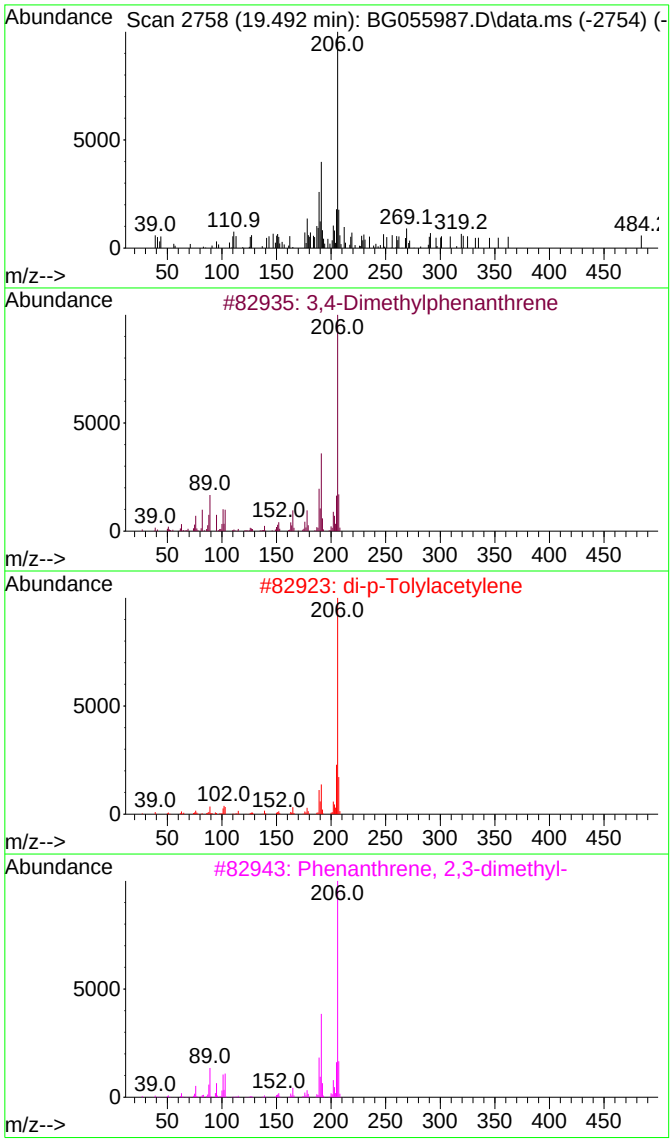
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

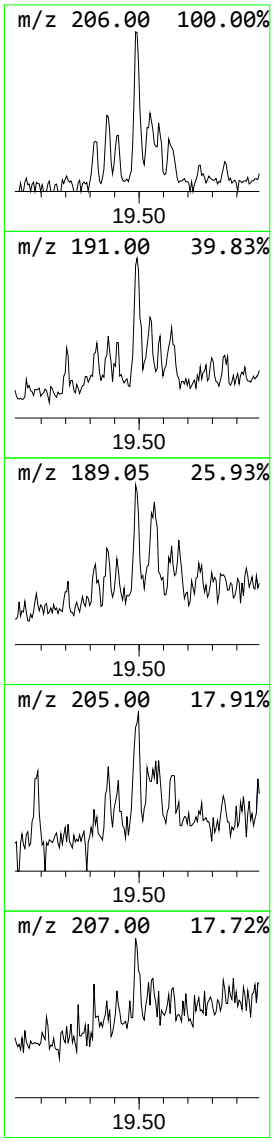
****

Peak Number 5 3,4-Dimethylphenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.492	2.84 ng	21824	Phenanthrene-d10	17.723

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	94
2	di-p-Tolylacetylene	206	C16H14	002789-88-0	89
3	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	76
4	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	76
5	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
Data File : BG055987.D
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Operator : CG/JU
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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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
3-Trifluorometh...	16.025	2.6	ng	15740	3	14.991	120079	20.0
Anthracene, 1-m...	18.593	4.3	ng	33266	4	17.723	153760	20.0
Phenanthrene, 2...	18.646	2.7	ng	20525	4	17.723	153760	20.0
4H-Cyclopenta[d...	18.787	5.9	ng	45594	4	17.723	153760	20.0
3,4-Dimethylphe...	19.492	2.8	ng	21824	4	17.723	153760	20.0