LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020723\
Data File : BG056574.D
Acq On : 7 Feb 2023 19:25
Operator : CG/JU
Sample : 01460-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OR-2-020623

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-BG012723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056574.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.304	333	343	349	rBV	99379	151799	8.46%	1.109%
2	5.792	420	426	438	rBV	384719	632327	35.26%	4.619%
3	7.419	696	703	716	rBV	388634	665155	37.09%	4.859%
4	8.271	841	848	856	rBB	127019	214683	11.97%	1.568%
5	9.446	1039	1048	1058	rBB	235958	414276	23.10%	3.026%
6	11.103	1322	1330	1336	rBV	169129	302518	16.87%	2.210%
7	13.512	1733	1740	1749	rBV	859861	1288494	71.85%	9.413%
8	13.682	1763	1769	1774	rBV3	10700	18080	1.01%	0.132%
9	14.211	1854	1859	1863	rBV3	10504	18310	1.02%	0.134%
10	14.746	1944	1950	1955	rVB2	14794	21063	1.17%	0.154%
11	14.893	1968	1975	1981	rVB	294691	466686	26.02%	3.409%
12	14.951	1981	1985	1990	rBV2	15681	21549	1.20%	0.157%
13	15.280	2036	2041	2046	rVB3	13821	25275	1.41%	0.185%
14	15.351	2048	2053	2062	rBV5	11854	20430	1.14%	0.149%
15	15.686	2105	2110	2115	rVB3	18958	29042	1.62%	0.212%
16	15.927	2145	2151	2162	rBV2	22918	43320	2.42%	0.316%
17	16.091	2175	2179	2182	rVB4	12086	18025	1.01%	0.132%
18	16.226	2192	2202	2207	rVB2	26016	55048	3.07%	0.402%
19	16.373	2221	2227	2235	rBV	560347	842615	46.99%	6.155%
20	16.544	2251	2256	2259	rBV2	15900	24607	1.37%	0.180%
21	16.926	2318	2321	2326	rVB7	11982	20138	1.12%	0.147%
22	17.343	2387	2392	2397	rBV6	14239	27776	1.55%	0.203%
23	17.448	2406	2410	2416	rVB2	17107	25517	1.42%	0.186%
24	17.631	2434	2441	2444	rBV	364816	564780	31.49%	4.126%
25	17.672	2444	2448	2454	rVV	304175	440348	24.55%	3.217%
26	17.760	2458	2463	2470	rVV	83559	128025	7.14%	0.935%
27	18.077	2513	2517	2523	rVB5	16003	26050	1.45%	0.190%
28	18.136	2523	2527	2530	rBV	15350	19854	1.11%	0.145%
29	18.500	2582	2589	2593	rBV	56279	115244	6.43%	0.842%
30	18.547	2593	2597	2603	rVB	81152	113145	6.31%	0.827%
31	18.624	2606	2610	2615	rBV	33638	51880	2.89%	0.379%
32	18.694	2616	2622	2626	rBV2	70339	158536	8.84%	1.158%
33	18.982	2668	2671	2675	rBV	47517	59690	3.33%	0.436%
34	19.276	2718	2721	2725	rBV	22999	32825	1.83%	0.240%
35	19.317	2725	2728	2732	rVB2	20450	25855	1.44%	0.189%
36	19.399	2735	2742	2747	rBV2	54387	129241	7.21%	0.944%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020723\
Data File : BG056574.D
Acq On : 7 Feb 2023 19:25
Operator : CG/JU
Sample : 01460-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-2-020623

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-BG012723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.546	2762	2767	2770	rBV4	33053	57113	3.18%	0.417%
38	19.664	2781	2787	2792	rBV	584474	865966	48.29%	6.326%
39	19.993	2838	2843	2845	rBV2	90871	159662	8.90%	1.166%
40	20.028	2845	2849	2855	rVV	531284	747852	41.70%	5.463%
41	20.087	2856	2859	2865	rVB	41017	58855	3.28%	0.430%
42	20.204	2874	2879	2884	rVB	1398497	1793314	100.00%	13.100%
43	20.610	2945	2948	2950	rBV	38383	40246	2.24%	0.294%
44	20.809	2979	2982	2986	rBV	38140	54300	3.03%	0.397%
45	21.914	3162	3170	3176	rBV3	426291	1144665	63.83%	8.362%
46	21.967	3176	3179	3187	rVB	227977	370345	20.65%	2.705%
47	22.125	3204	3206	3214	rVB	41633	66118	3.69%	0.483%
48	24.252	3564	3568	3576	rBV2	109151	237893	13.27%	1.738%
49	25.181	3721	3726	3736	rVB	143526	400985	22.36%	2.929%
50	25.345	3748	3754	3763	rVB2	178513	479531	26.74%	3.503%

Sum of corrected areas: 13689051

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ALS Vial : 12 Sample Multiplier: 1

Instrument :
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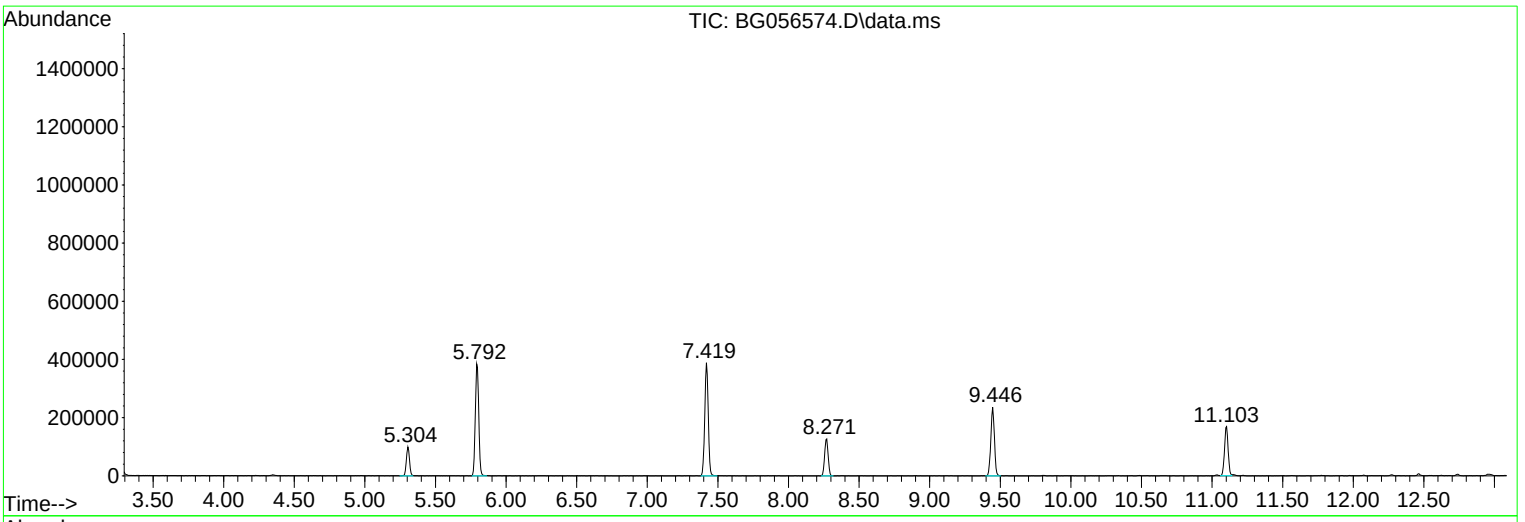
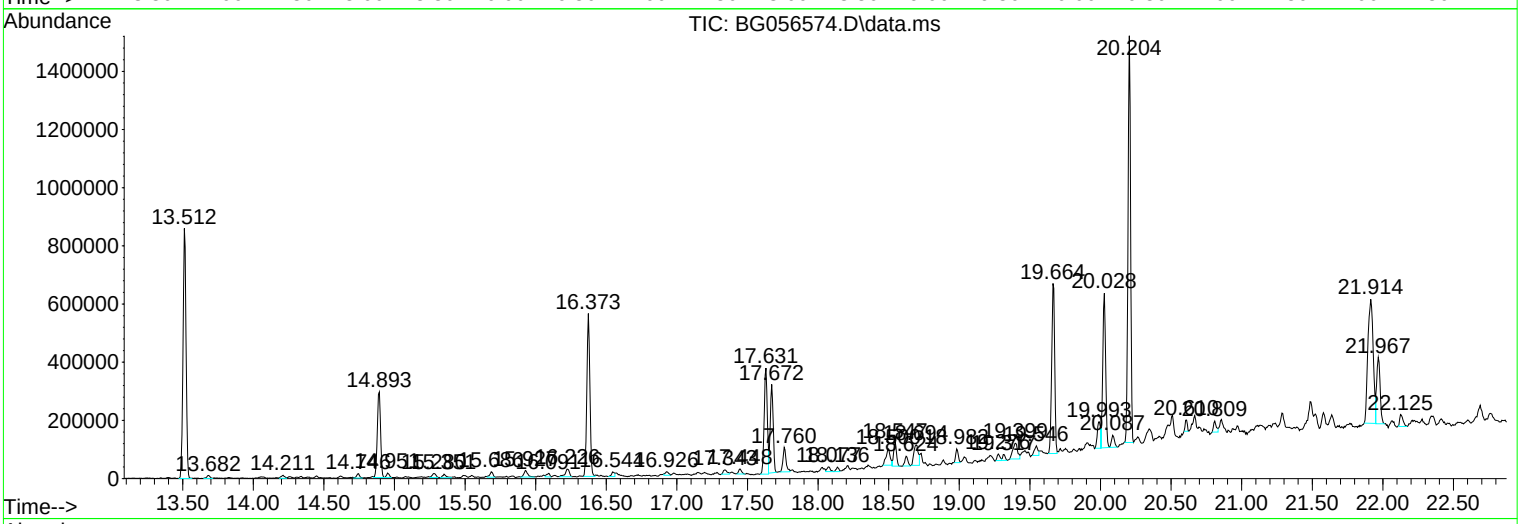
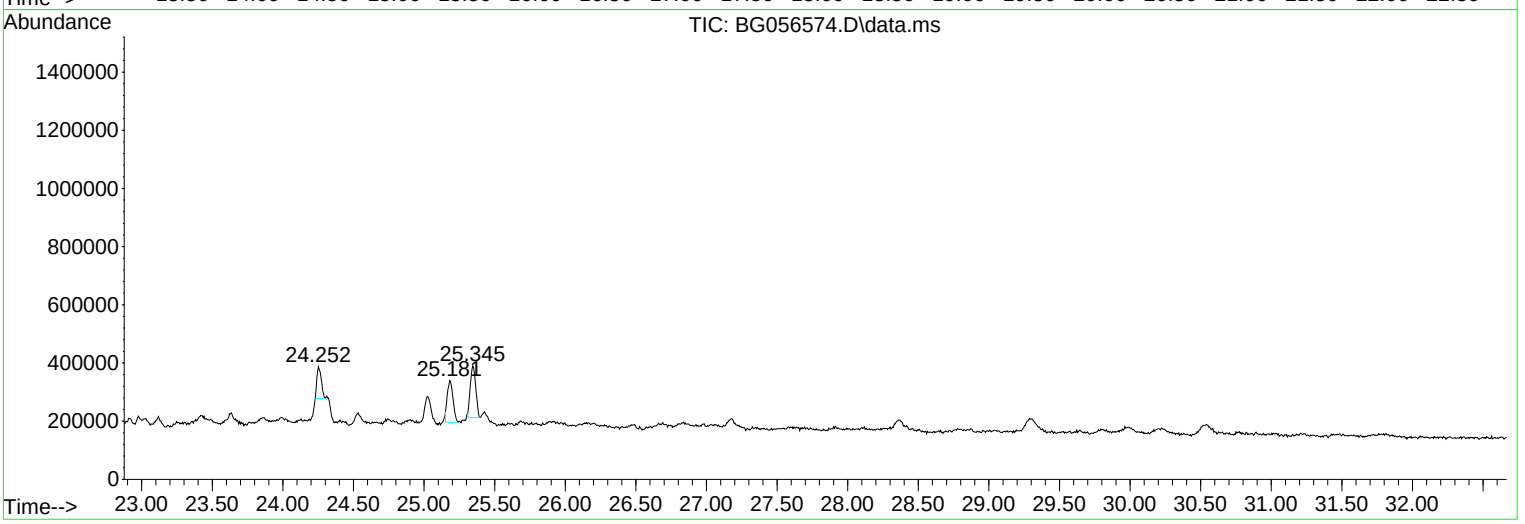
ClientSampleId :
OR-2-020623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.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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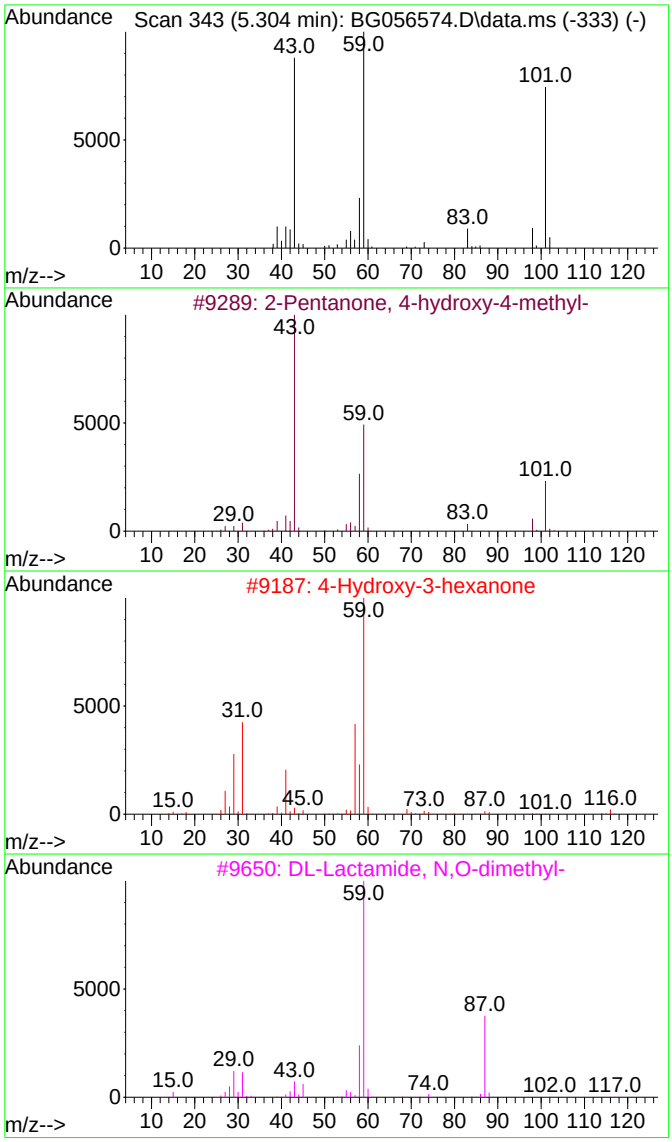
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

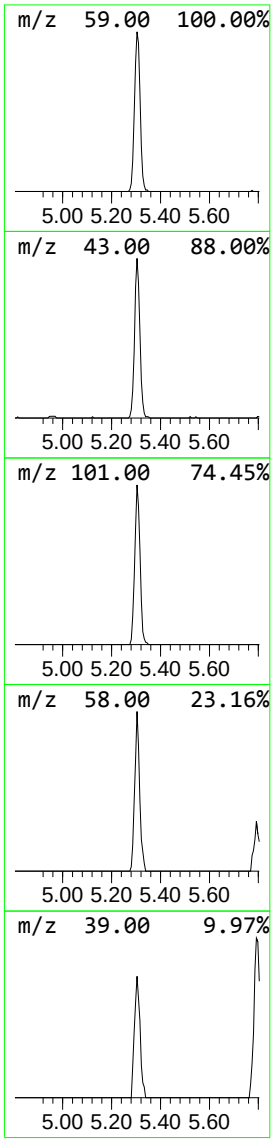
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.304	14.14 ng	151799	1,4-Dichlorobenzene-d4	8.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17
3	DL-Lactamide, N,O-dimethyl-	117	C5H11NO2	1000452-56-3	17
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	16
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16





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Data File : BG056574.D
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Operator : CG/JU
Sample : 01460-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-2-020623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

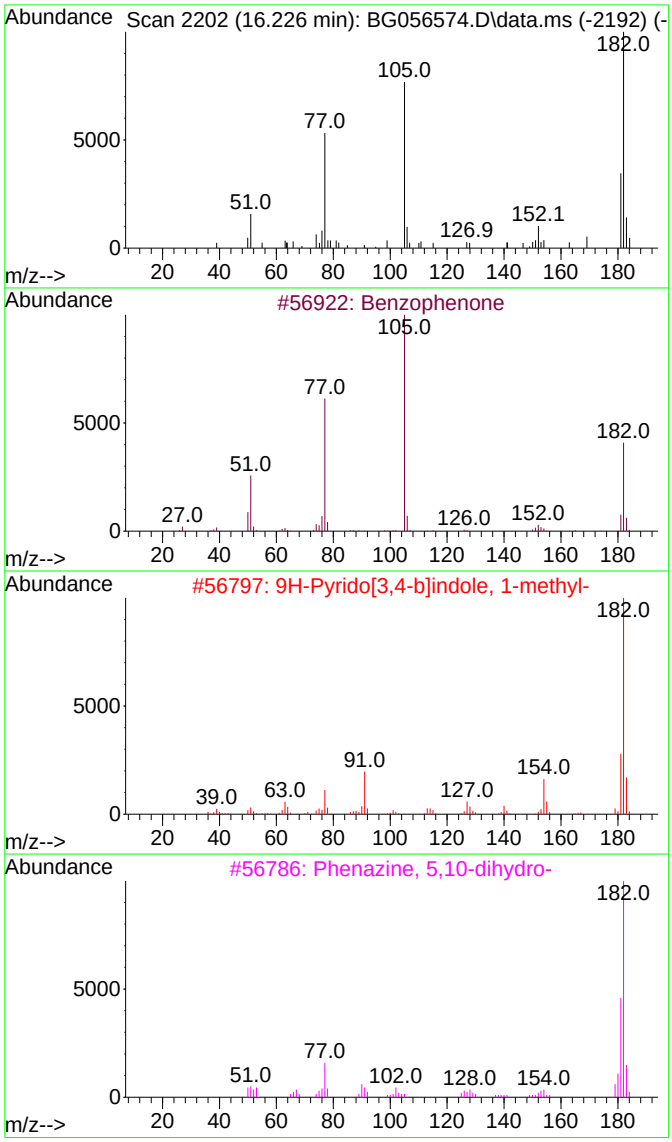
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

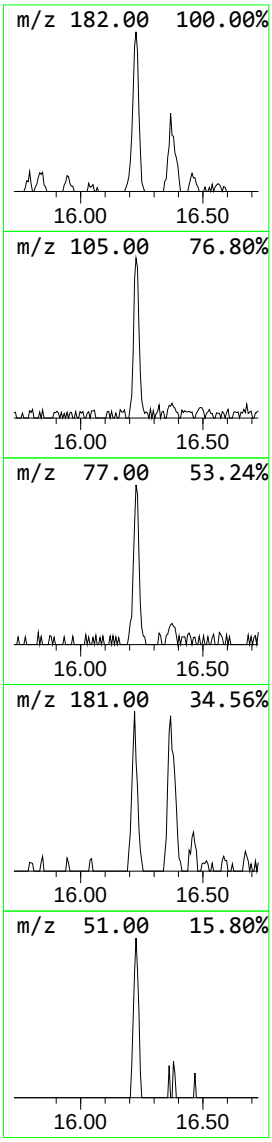
****

Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.226	2.36 ng	55048	Acenaphthene-d10	14.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	87
2	9H-Pyrido[3,4-b]indole, 1-methyl-	182	C12H10N2	000486-84-0	59
3	Phenazine, 5,10-dihydro-	182	C12H10N2	000613-32-1	49
4	Azobenzene	182	C12H10N2	000103-33-3	47
5	3-Aminocarbazole	182	C12H10N2	006377-12-4	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020723\
Data File : BG056574.D
Acq On : 7 Feb 2023 19:25
Operator : CG/JU
Sample : 01460-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-2-020623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

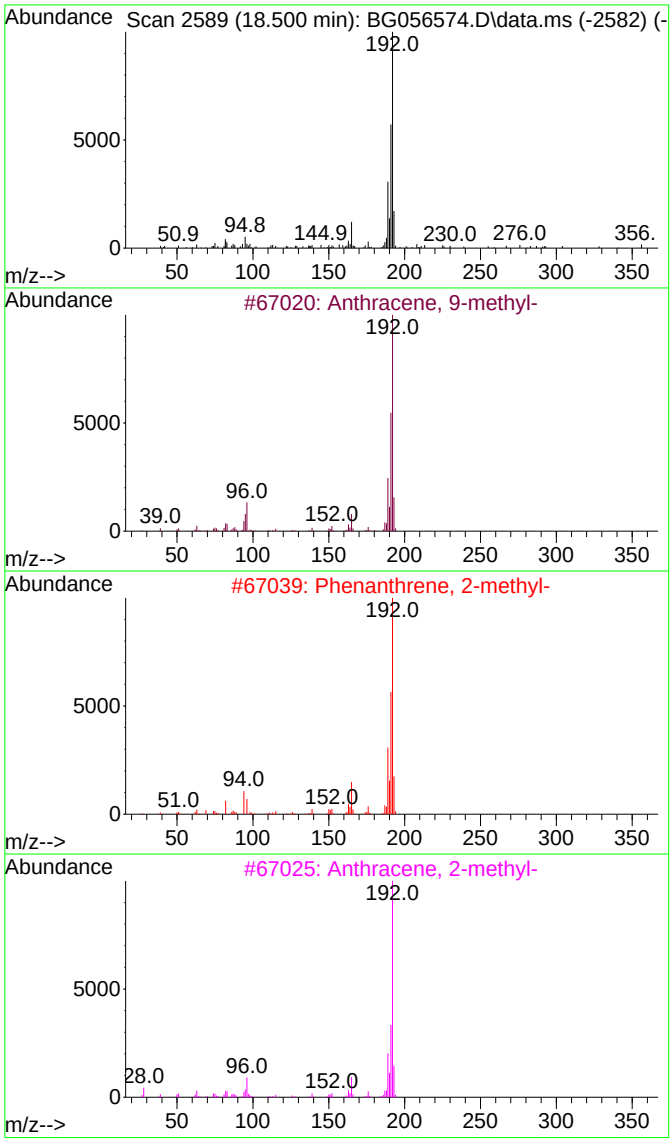
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

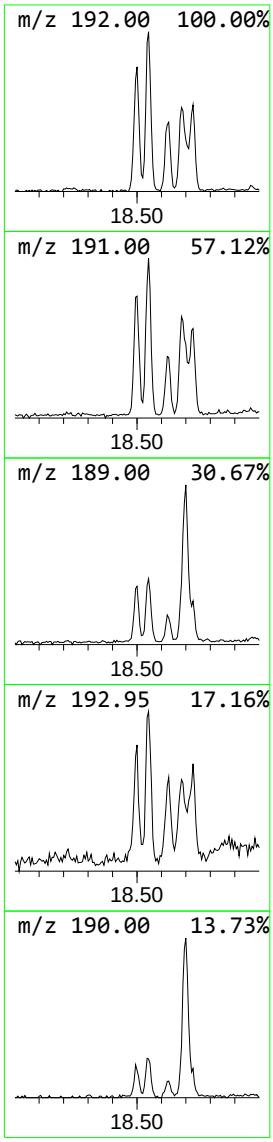
****

Peak Number 3 Anthracene, 9-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.500	4.08 ng	115244	Phenanthrene-d10	17.631

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	87
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
4	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	83
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020723\
Data File : BG056574.D
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-2-020623

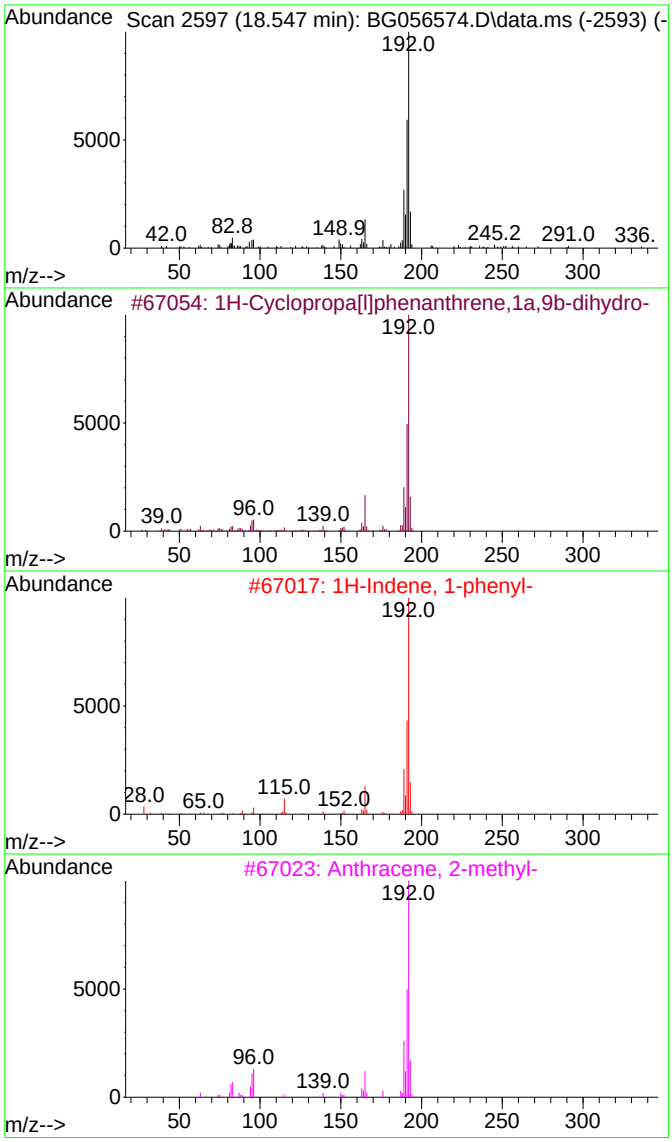
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

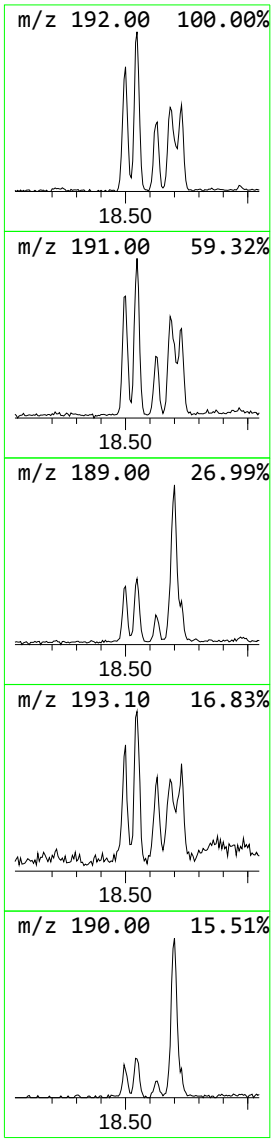
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1H-Cyclopropa[l]phenanthren... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.547	4.01 ng	113145	Phenanthrene-d10	17.631

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95
2	1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	94
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91





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Instrument :
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ClientSampleId :
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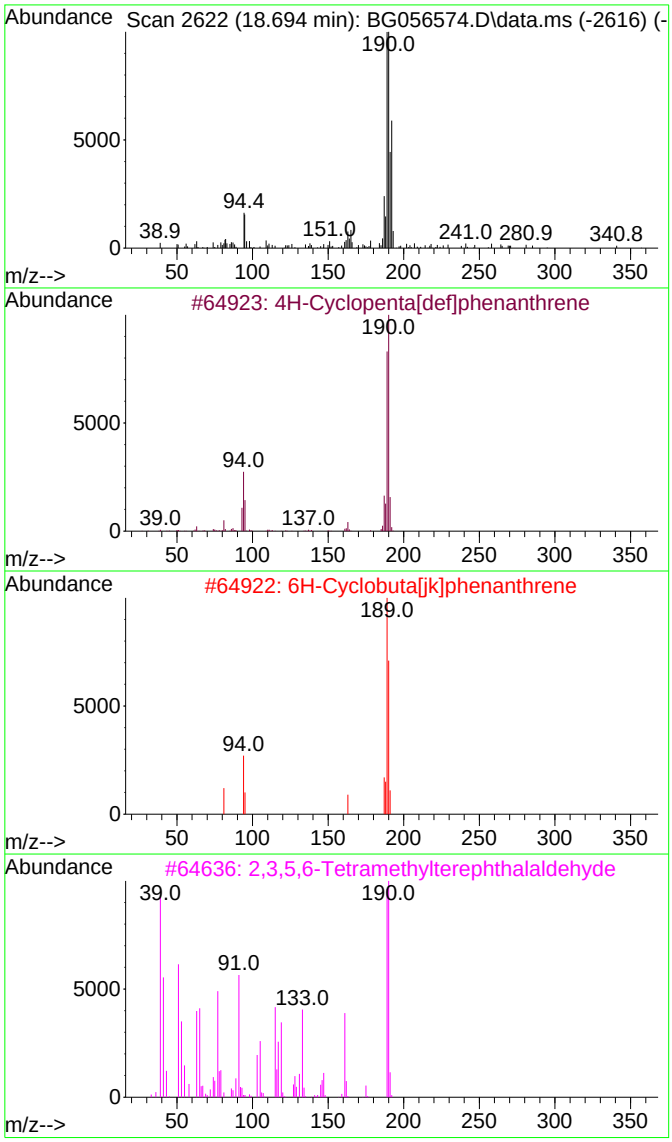
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

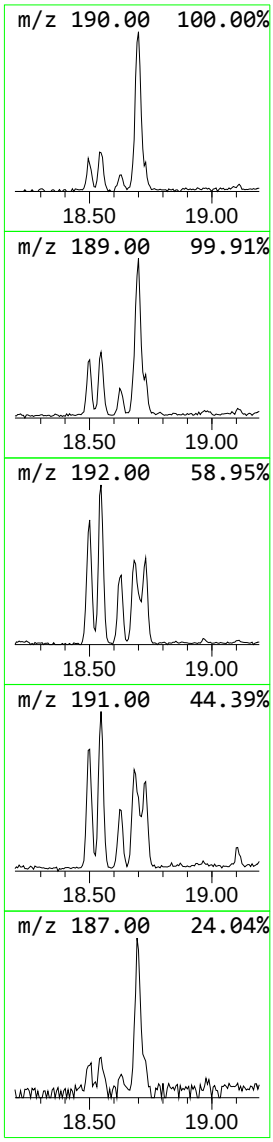
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.694	5.61 ng	158536	Phenanthrene-d10	17.631

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	53
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	43
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40
5	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	37





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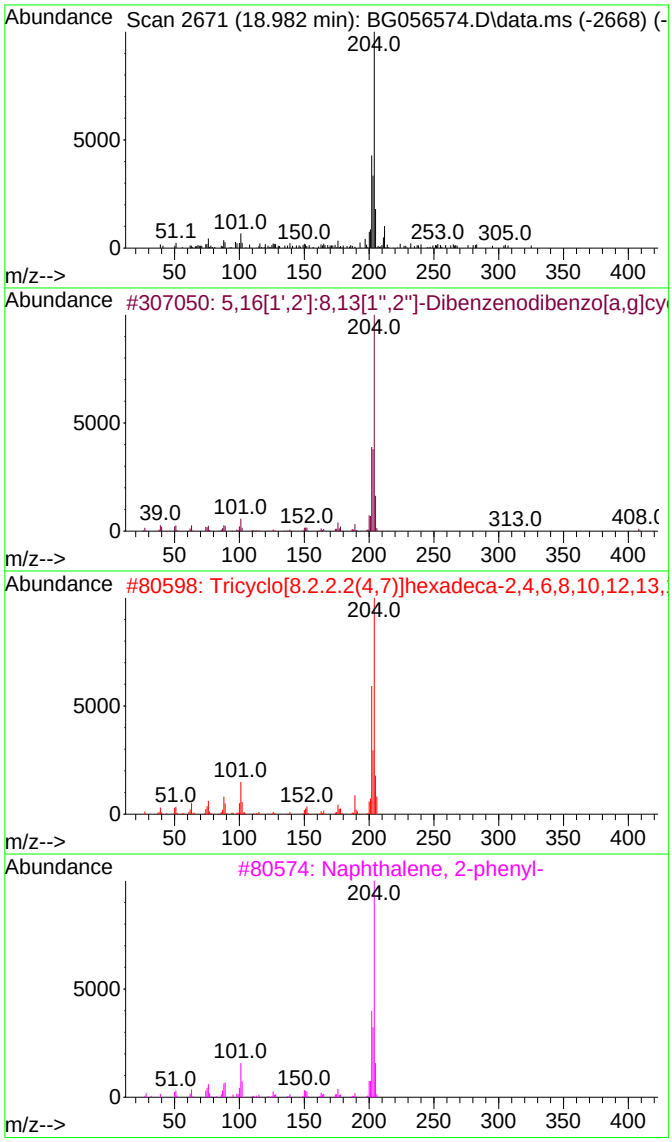
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

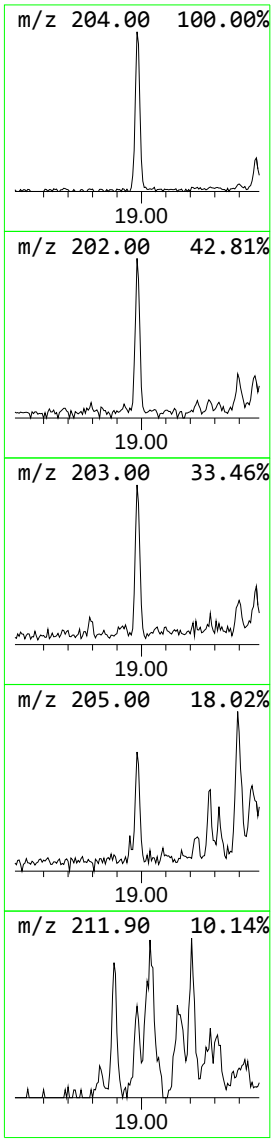
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 5,16[1',2']:8,13[1'',2'']-D... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.982	2.11 ng	59690	Phenanthrene-d10	17.631

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	83
2	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	60
3	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	53
4	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	49
5	9-Acridinecarbonitrile	204	C14H8N2	005326-19-2	47





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Data File : BG056574.D
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Operator : CG/JU
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Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

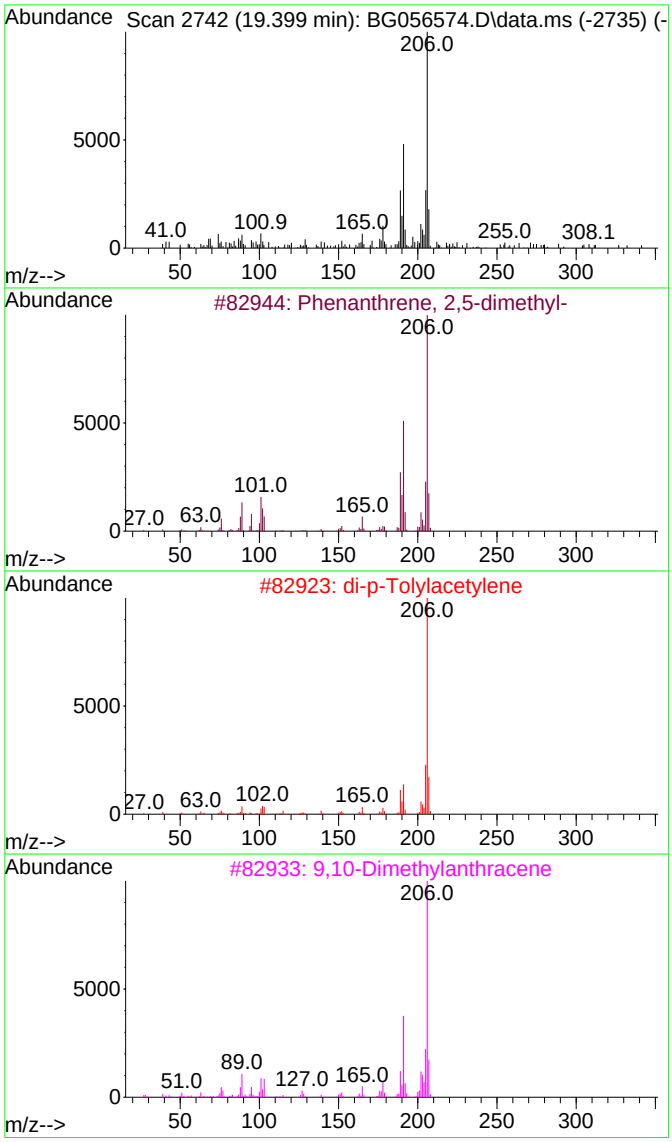
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

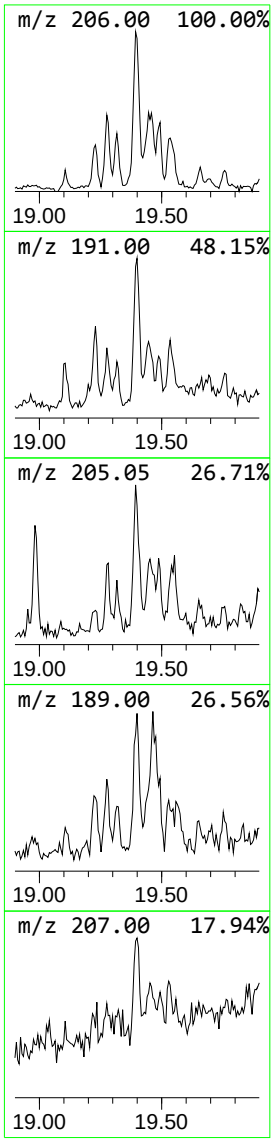
****

Peak Number 7 Phenanthrene, 2,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.399	4.58 ng	129241	Phenanthrene-d10	17.631

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
2	di-p-Tolylacetylene	206	C16H14	002789-88-0	93
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	91
4	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	90
5	Naphthalene, 1,2-dihydro-4-phenyl-	206	C16H14	007469-40-1	87





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Data File : BG056574.D
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ClientSampleId :
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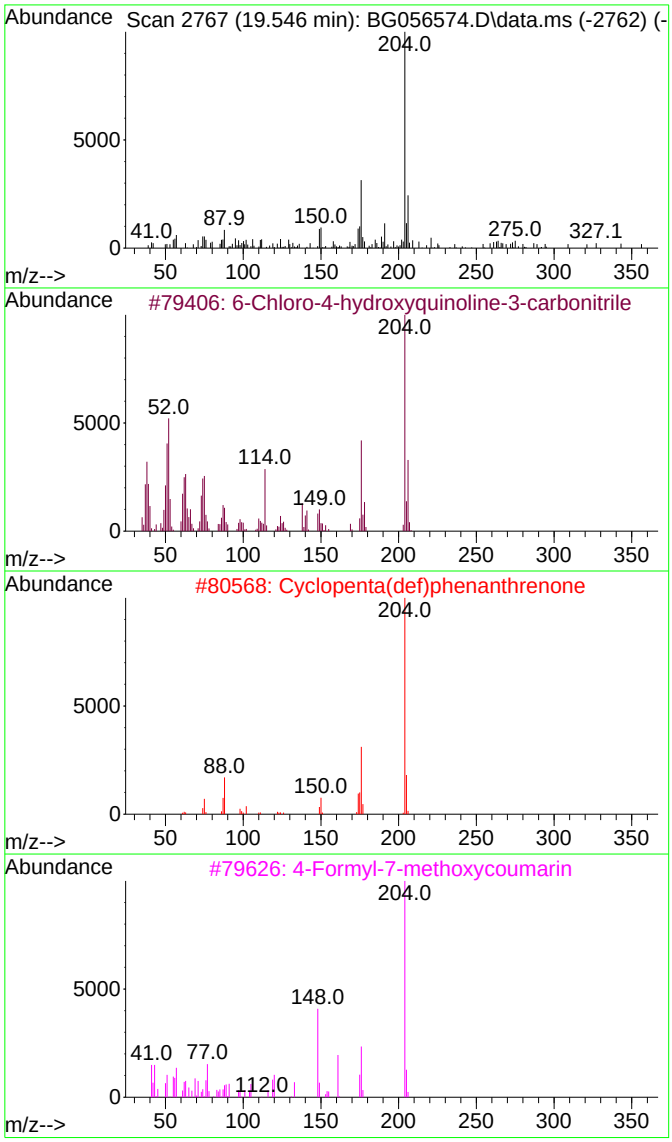
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

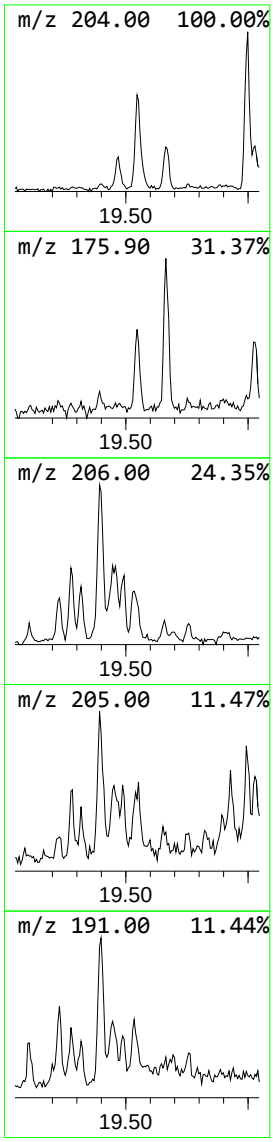
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 6-Chloro-4-hydroxyquinoline... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.546	2.02 ng	57113	Phenanthrene-d10	17.631

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Chloro-4-hydroxyquinoline-3-ca...	204	C10H5ClN2O	1000435-79-8	64
2	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	62
3	4-Formyl-7-methoxycoumarin	204	C11H8O4	1000429-03-0	58
4	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	53
5	Tetrathiafulvalene	204	C6H4S4	031366-25-3	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020723\
Data File : BG056574.D
Acq On : 7 Feb 2023 19:25
Operator : CG/JU
Sample : 01460-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-2-020623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.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-...	5.304	14.1	ng	151799	1	8.271	214683	20.0
Benzophenone	16.226	2.4	ng	55048	3	14.887	466686	20.0
Anthracene, 9-m...	18.500	4.1	ng	115244	4	17.631	564780	20.0
1H-Cyclopropa[l...	18.547	4.0	ng	113145	4	17.631	564780	20.0
4H-Cyclopenta[d...	18.694	5.6	ng	158536	4	17.631	564780	20.0
5,16[1',2']:8,1...	18.982	2.1	ng	59690	4	17.631	564780	20.0
Phenanthrene, 2...	19.399	4.6	ng	129241	4	17.631	564780	20.0
6-Chloro-4-hydr...	19.546	2.0	ng	57113	4	17.631	564780	20.0