LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050705.D
Acq On : 23 Oct 2021 1:48
Operator : CG/JU
Sample : M4297-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TR-04-10202021

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-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050705.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.796	385	393	403	rBV	367867	670365	35.24%	3.868%
2	7.400	658	666	675	rBV	391567	734142	38.59%	4.236%
3	8.258	805	812	824	rVB	198597	363721	19.12%	2.099%
4	9.427	1003	1011	1021	rBV	254771	477943	25.12%	2.758%
5	10.826	1241	1249	1260	rBV	36913	81042	4.26%	0.468%
6	11.078	1285	1292	1299	rBV	277566	525312	27.61%	3.031%
7	11.131	1299	1301	1308	rVB	13681	19797	1.04%	0.114%
8	13.493	1694	1703	1711	rBV	600133	958056	50.36%	5.529%
9	14.604	1885	1892	1899	rBV4	12126	25971	1.37%	0.150%
10	14.874	1927	1938	1944	rBV	415839	665116	34.96%	3.838%
11	14.938	1944	1949	1955	rVB	39311	64415	3.39%	0.372%
12	15.267	2001	2005	2012	rVB2	24375	44312	2.33%	0.256%
13	15.914	2108	2115	2121	rBV2	60804	105789	5.56%	0.610%
14	16.208	2160	2165	2172	rVB2	16547	31265	1.64%	0.180%
15	16.354	2184	2190	2199	rBV	370391	636004	33.43%	3.670%
16	16.548	2218	2223	2227	rBV4	17468	34269	1.80%	0.198%
17	16.913	2280	2285	2291	rVB4	11474	22046	1.16%	0.127%
18	17.118	2315	2320	2327	rBV4	39277	67613	3.55%	0.390%
19	17.183	2328	2331	2340	rVB4	12200	26273	1.38%	0.152%
20	17.271	2340	2346	2351	rBV	49124	86377	4.54%	0.498%
21	17.336	2353	2357	2362	rBV6	14771	22640	1.19%	0.131%
22	17.436	2370	2374	2382	rVB2	42257	66396	3.49%	0.383%
23	17.618	2399	2405	2409	rBV	430242	722086	37.95%	4.167%
24	17.659	2409	2412	2419	rVV	732330	1112555	58.48%	6.420%
25	17.753	2419	2428	2432	rVV	80333	138897	7.30%	0.802%
26	17.812	2434	2438	2442	rVB2	15551	25663	1.35%	0.148%
27	18.017	2466	2473	2480	rVB2	101827	176836	9.29%	1.020%
28	18.129	2488	2492	2498	rBV3	23812	36132	1.90%	0.209%
29	18.252	2510	2513	2518	rBV3	17860	23449	1.23%	0.135%
30	18.487	2549	2553	2557	rBV	73593	107431	5.65%	0.620%
31	18.540	2557	2562	2566	rVB	101630	153341	8.06%	0.885%
32	18.622	2572	2576	2579	rVB2	19156	27034	1.42%	0.156%
33	18.687	2581	2587	2592	rBV2	145254	306857	16.13%	1.771%
34	18.975	2632	2636	2640	rBV	69823	100661	5.29%	0.581%
35	19.022	2640	2644	2653	rVB	204120	309263	16.26%	1.785%
36	19.380	2701	2705	2707	rBV2	91518	123466	6.49%	0.712%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050705.D
Acq On : 23 Oct 2021 1:48
Operator : CG/JU
Sample : M4297-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TR-04-10202021

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-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.539	2728	2732	2737	rBV2	63985	95585	5.02%	0.552%
38	19.662	2747	2753	2759	rBV	1285549	1902535	100.00%	10.979%
39	19.985	2803	2808	2810	rBV2	160576	254843	13.39%	1.471%
40	20.021	2810	2814	2821	rVV	1043383	1567694	82.40%	9.047%
41	20.079	2822	2824	2829	rVB2	46335	63637	3.34%	0.367%
42	20.203	2840	2845	2850	rBV	772508	1033717	54.33%	5.965%
43	20.503	2893	2896	2901	rVB	139225	218724	11.50%	1.262%
44	20.608	2910	2914	2917	rBV2	97720	131265	6.90%	0.757%
45	21.907	3129	3135	3142	rBV3	508764	1425549	74.93%	8.226%
46	21.971	3142	3146	3158	rVB	425337	824808	43.35%	4.760%
47	24.263	3528	3536	3543	rBV	196841	718102	37.74%	4.144%

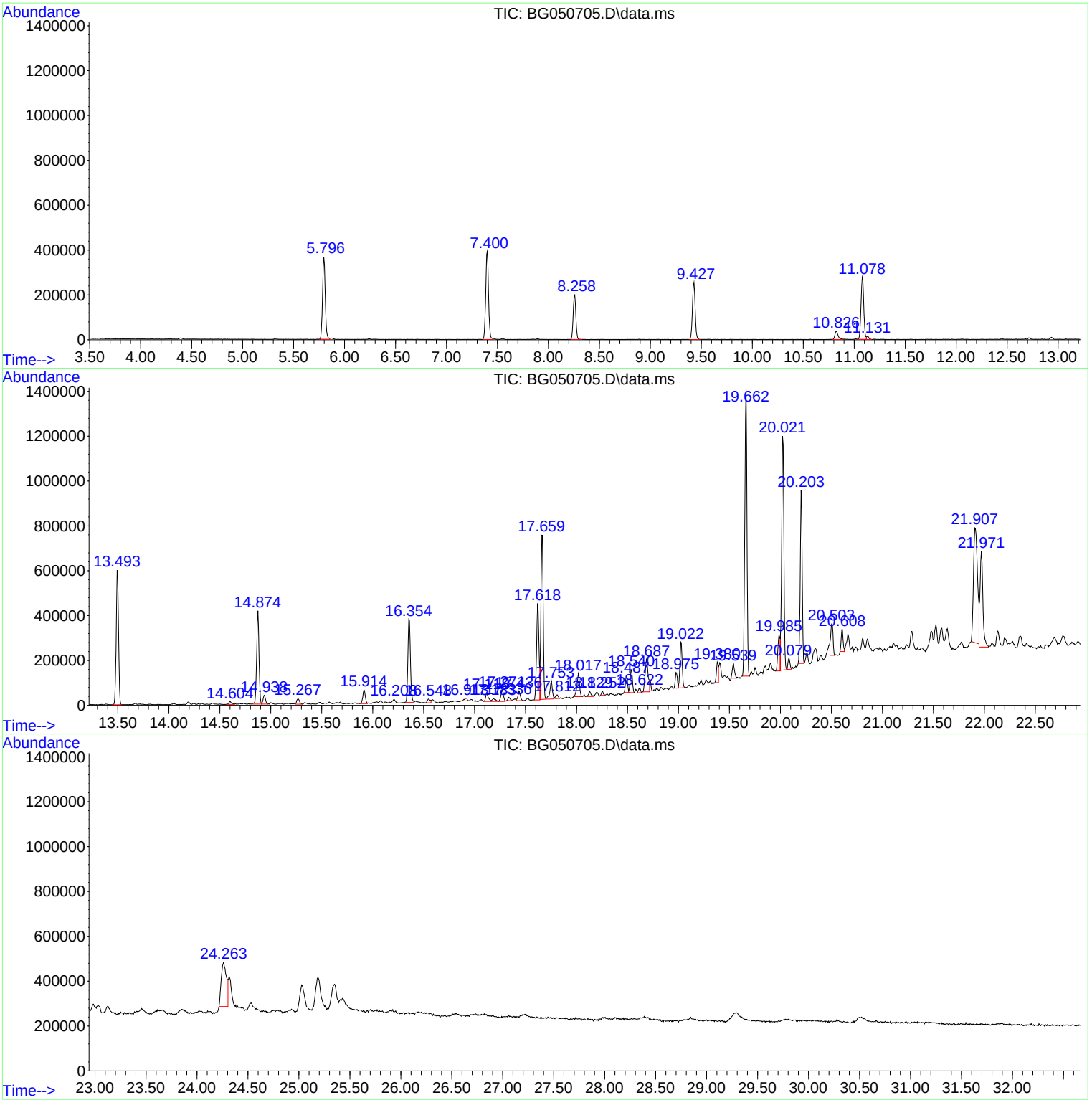
Sum of corrected areas: 17328994

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050705.D
Acq On : 23 Oct 2021 1:48
Operator : CG/JU
Sample : M4297-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-10202021

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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\BG102221\
Data File : BG050705.D
Acq On : 23 Oct 2021 1:48
Operator : CG/JU
Sample : M4297-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TR-04-10202021

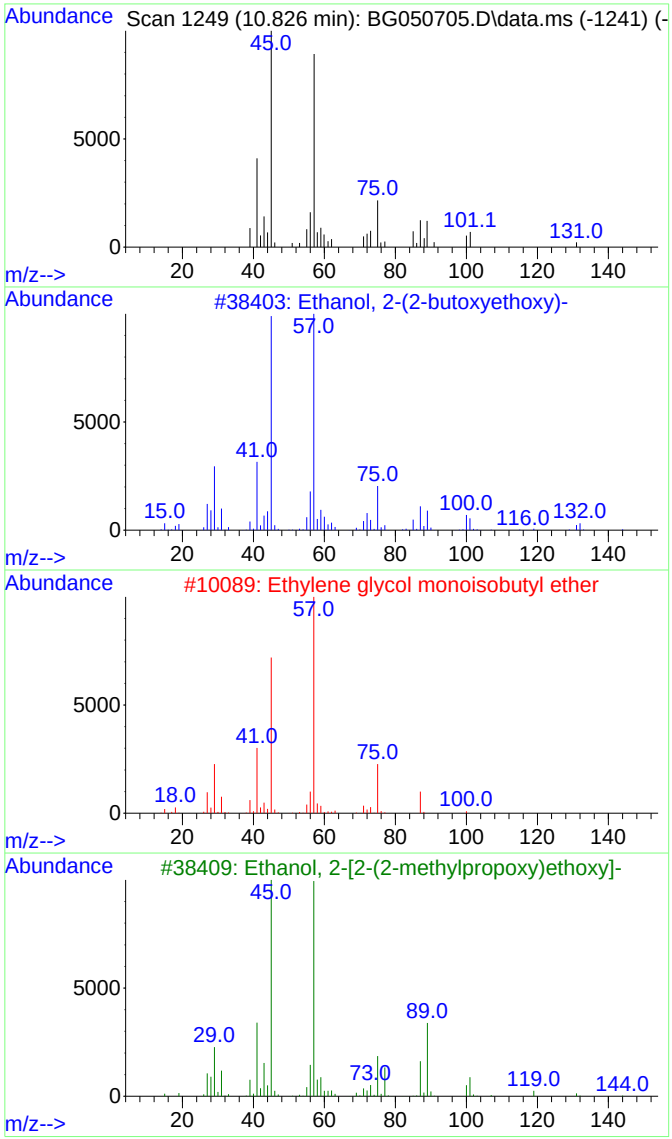
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

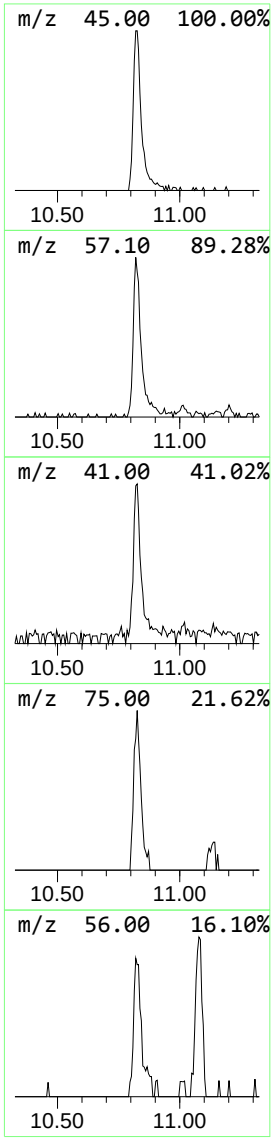
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.826	3.09 ng	81042	Naphthalene-d8	11.078

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050705.D
Acq On : 23 Oct 2021 1:48
Operator : CG/JU
Sample : M4297-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-10202021

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

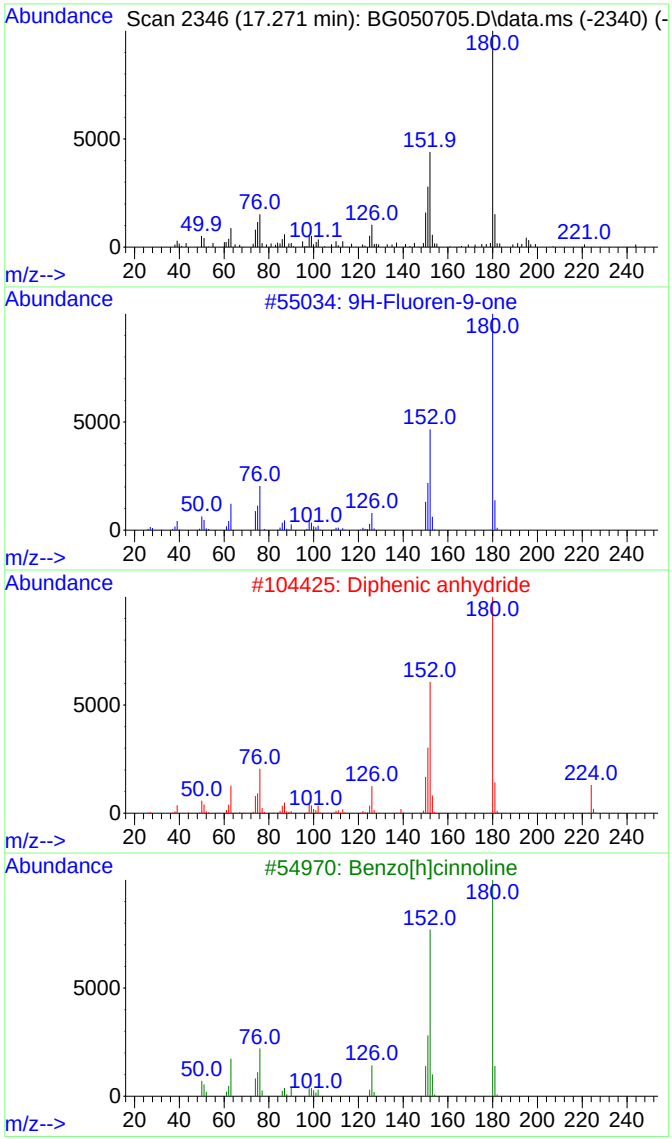
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

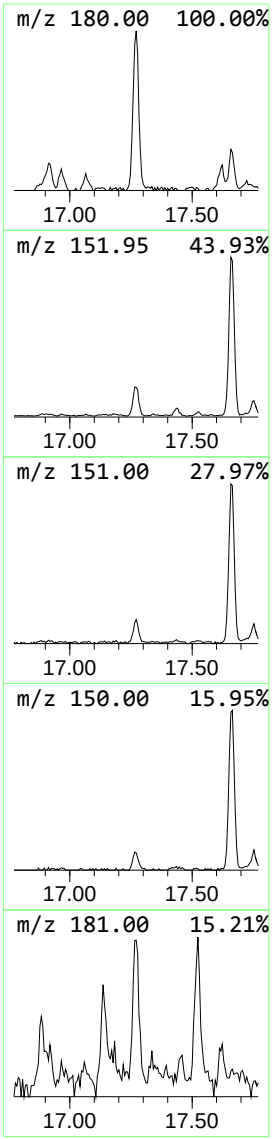
****

Peak Number 2 9H-Fluoren-9-one Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.271	2.39 ng	86377	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluoren-9-one	180	C13H8O	000486-25-9	97
2	Diphenic anhydride	224	C14H8O3	006050-13-1	91
3	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	87
4	9,10-Phenanthrenedione	208	C14H8O2	000084-11-7	83
5	1H-Phenalen-1-one	180	C13H8O	000548-39-0	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050705.D
Acq On : 23 Oct 2021 1:48
Operator : CG/JU
Sample : M4297-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-10202021

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

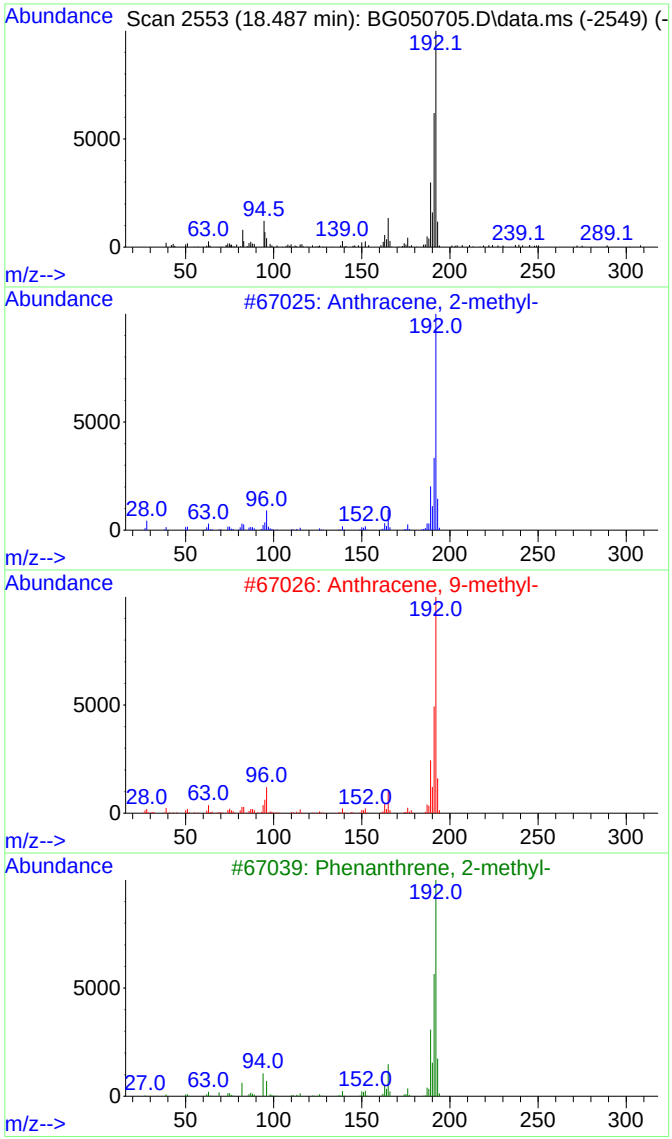
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

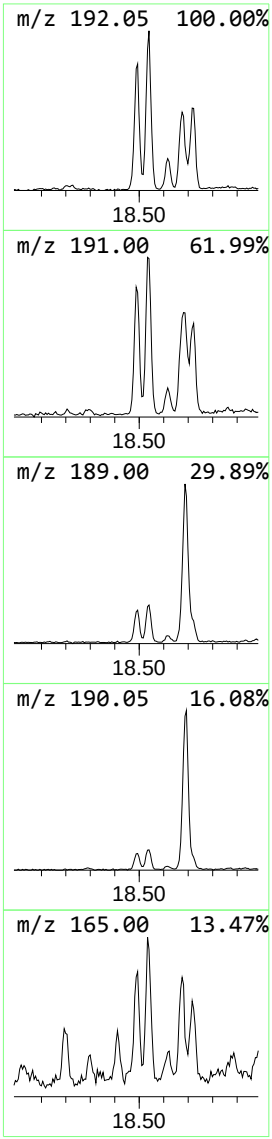
****

Peak Number 3 Anthracene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.487	2.98 ng	107431	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	90
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	90
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050705.D
Acq On : 23 Oct 2021 1:48
Operator : CG/JU
Sample : M4297-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TR-04-10202021

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

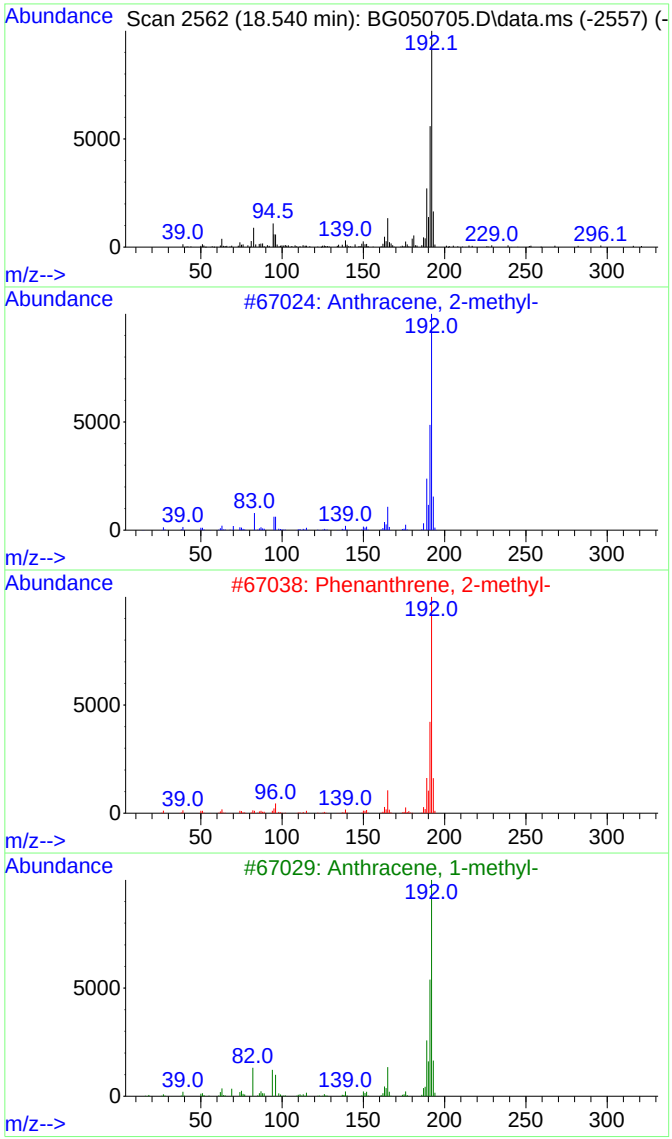
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

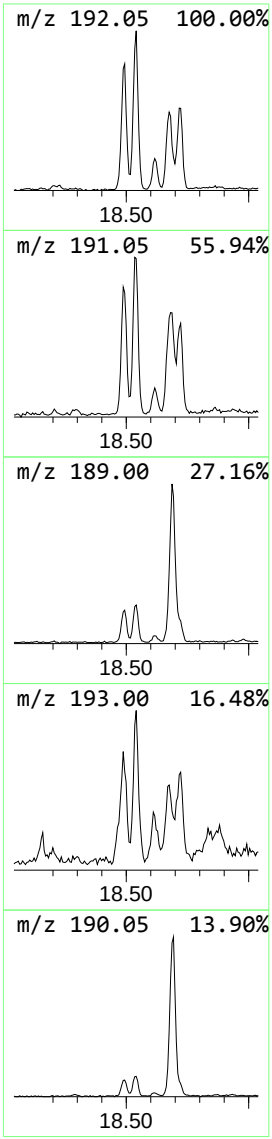
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.540	4.25 ng	153341	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050705.D
Acq On : 23 Oct 2021 1:48
Operator : CG/JU
Sample : M4297-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TR-04-10202021

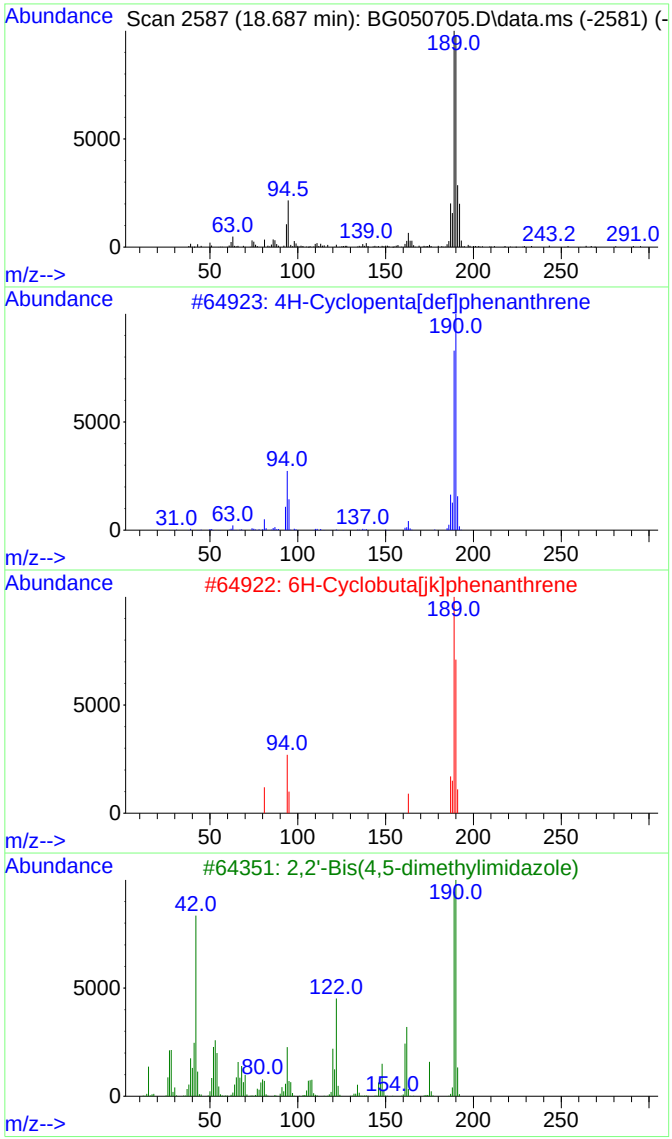
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

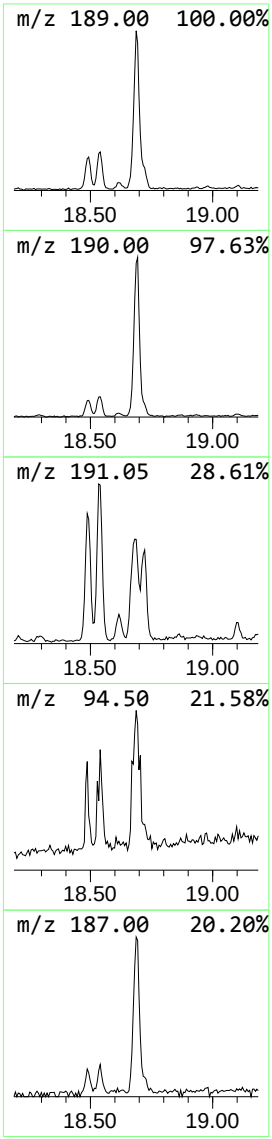
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.687	8.50 ng	306857	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	90
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
4	2-Naphthaldehyde, 1,2,3,4-tetrah...	190	C12H14O2	002472-02-8	18
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050705.D
Acq On : 23 Oct 2021 1:48
Operator : CG/JU
Sample : M4297-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TR-04-10202021

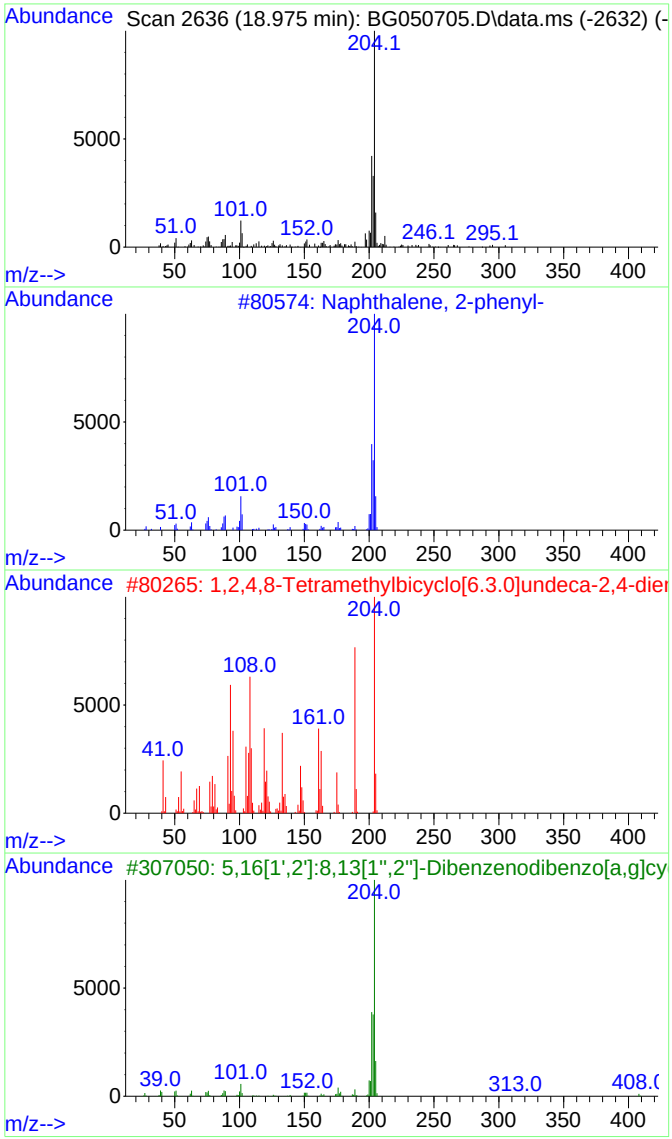
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

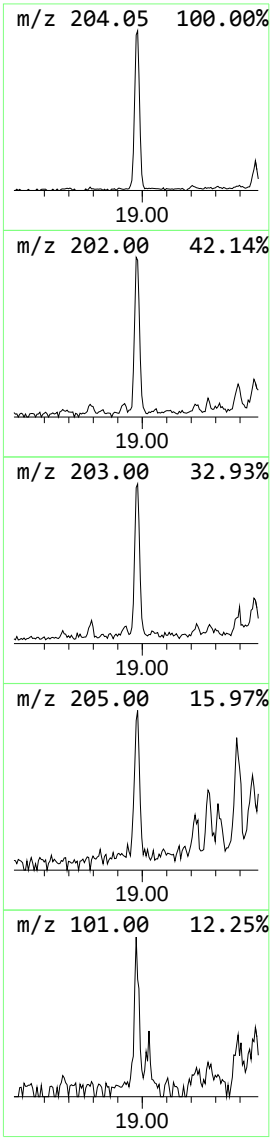
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 2-phenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.975	2.79 ng	100661	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	91
2	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	86
3	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	83
4	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	64
5	Benzene, 1,1'-(1-buten-3-yne-1,4...	204	C16H12	013141-45-2	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050705.D
Acq On : 23 Oct 2021 1:48
Operator : CG/JU
Sample : M4297-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TR-04-10202021

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

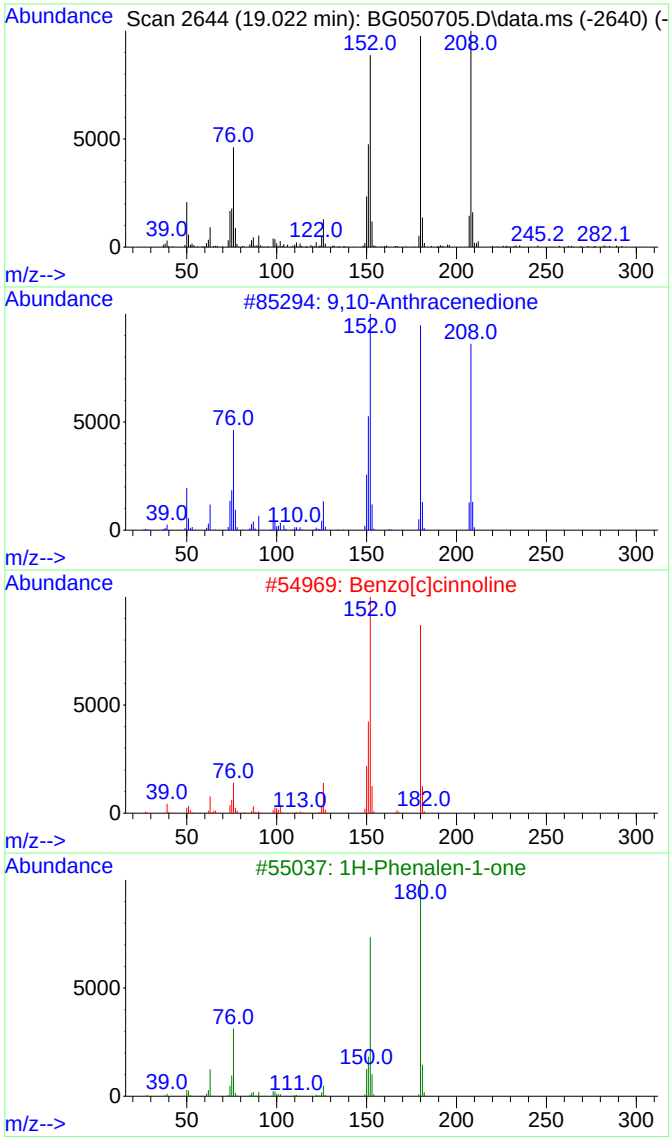
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

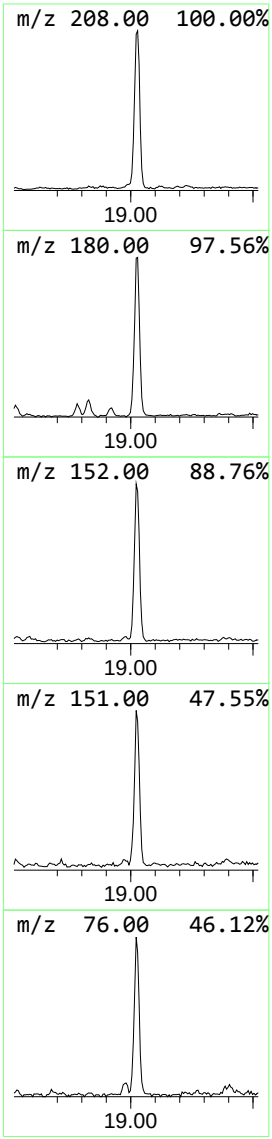
****

Peak Number 7 9,10-Anthracenedione Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.022	8.57 ng	309263	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	99
2	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	91
3	1H-Phenalen-1-one	180	C13H8O	000548-39-0	83
4	9,10-Phenanthrenedione	208	C14H8O2	000084-11-7	60
5	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050705.D
Acq On : 23 Oct 2021 1:48
Operator : CG/JU
Sample : M4297-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TR-04-10202021

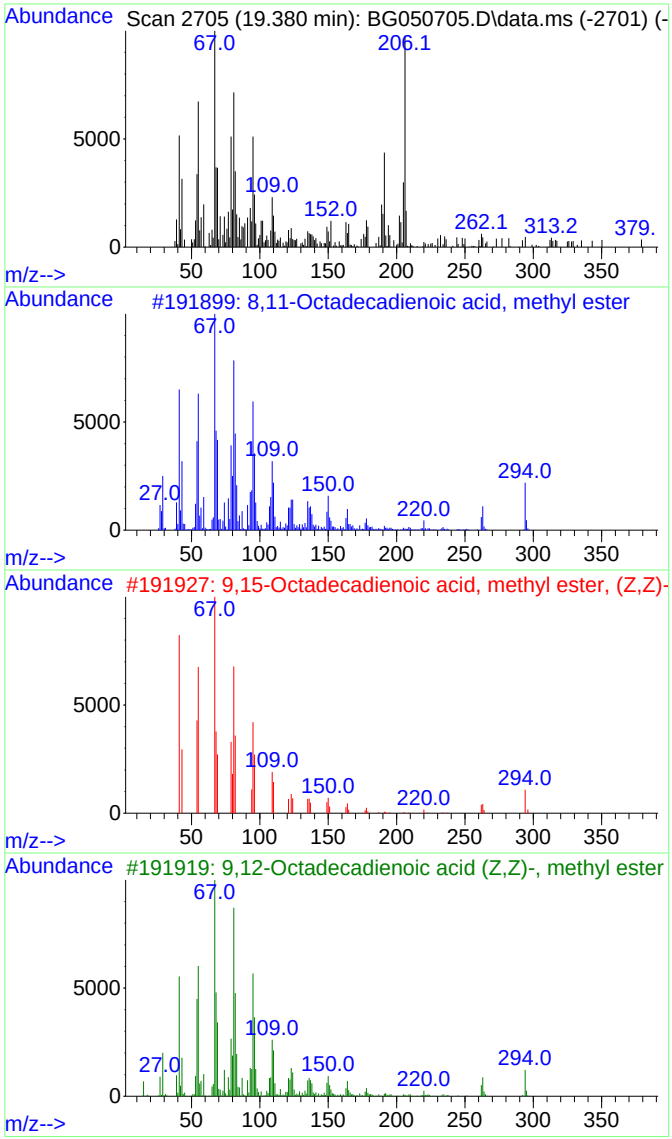
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

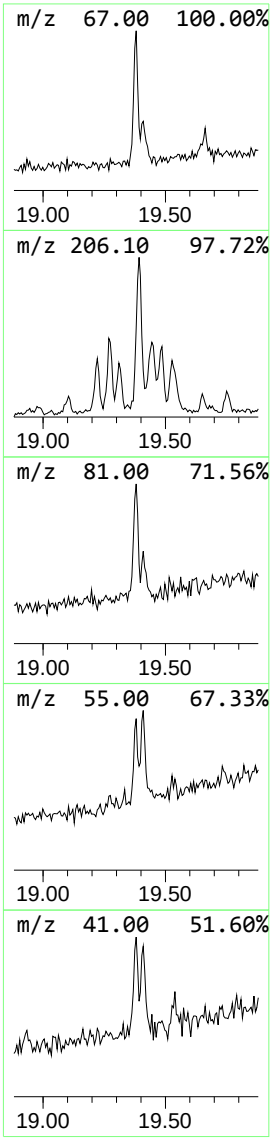
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 8,11-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.380	3.42 ng	123466	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	96
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	95
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	86
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	86
5	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	86





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Data File : BG050705.D
Acq On : 23 Oct 2021 1:48
Operator : CG/JU
Sample : M4297-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TR-04-10202021

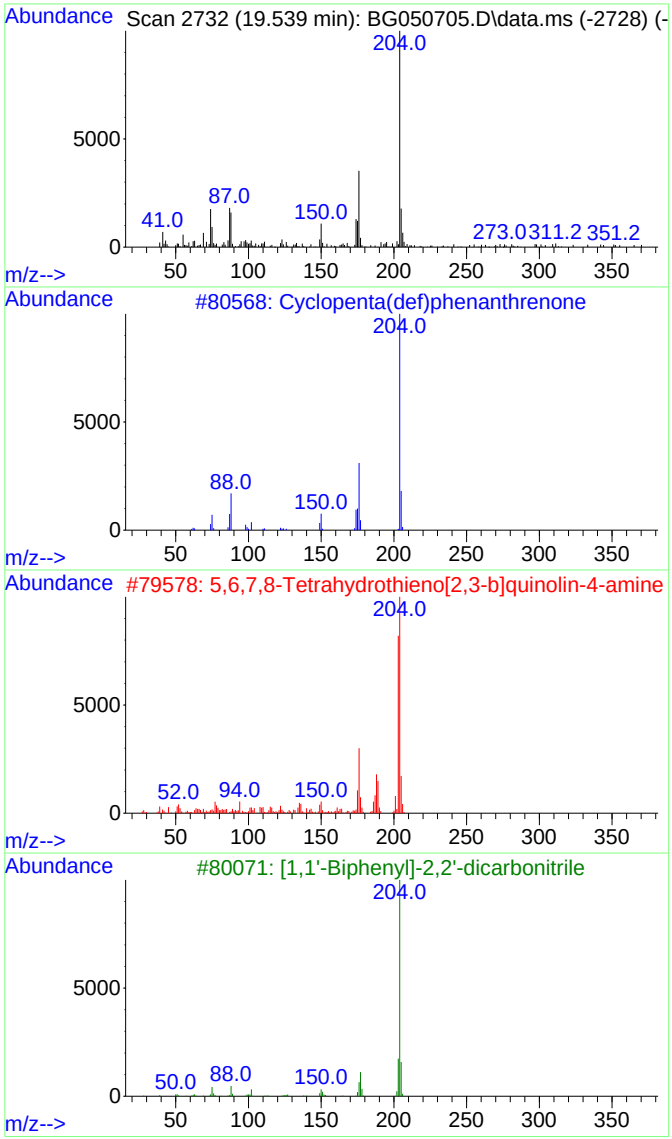
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

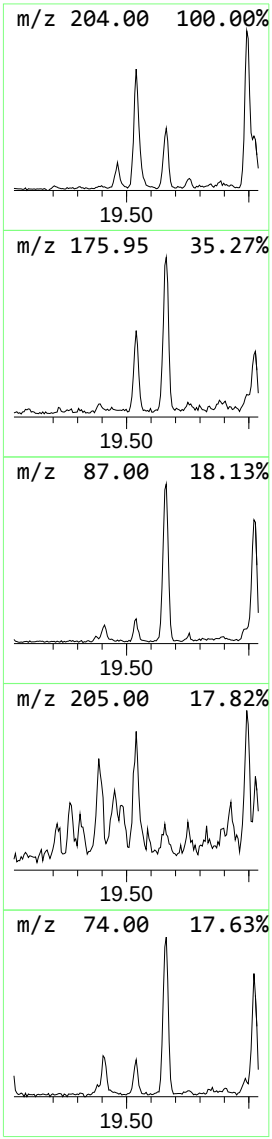
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclopenta(def)phenanthrenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.539	2.65 ng	95585	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	97
2	5,6,7,8-Tetrahydrothieno[2,3-b]q...	204	C11H12N2S	122914-50-5	59
3	[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	53
4	3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	50
5	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050705.D
Acq On : 23 Oct 2021 1:48
Operator : CG/JU
Sample : M4297-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TR-04-10202021

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

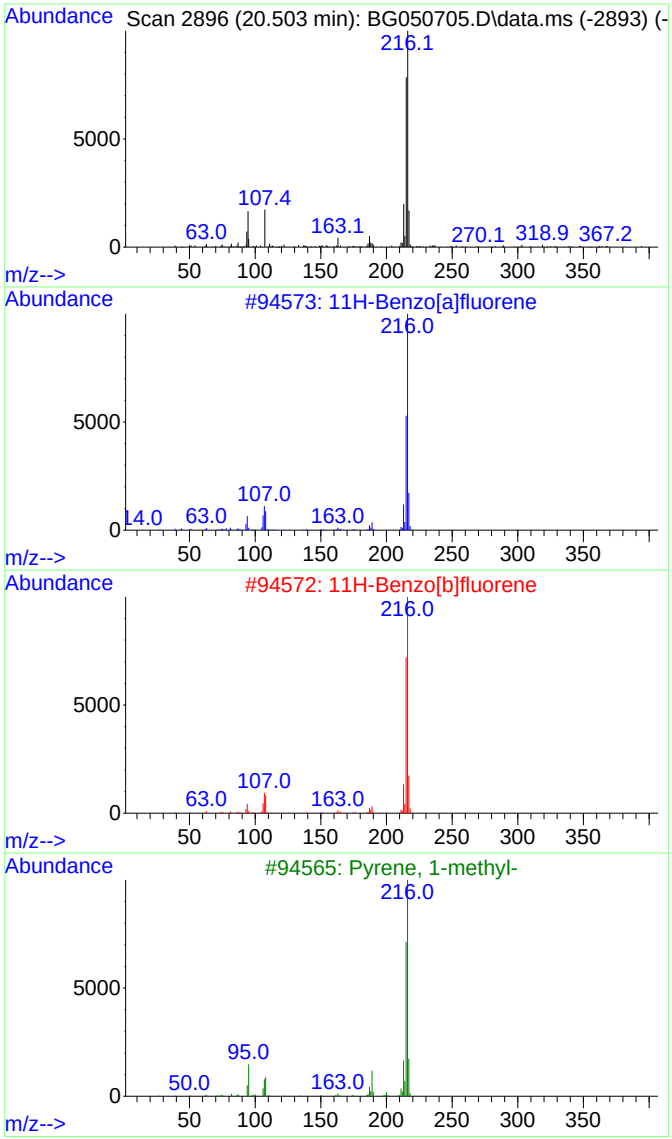
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

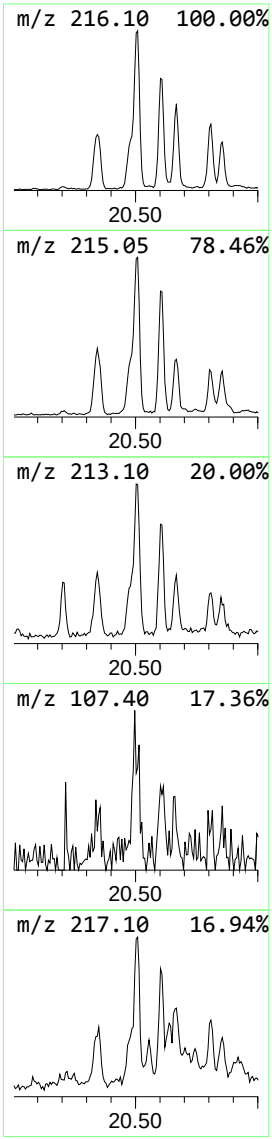
****

Peak Number 10 11H-Benzo[a]fluorene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.503	3.07 ng	218724	Chrysene-d12	21.924

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	86
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	86
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	78
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050705.D
Acq On : 23 Oct 2021 1:48
Operator : CG/JU
Sample : M4297-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TR-04-10202021

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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
Ethanol, 2-(2-b...	10.826	3.1	ng	81042	2	11.078	525312	20.0
9H-Fluoren-9-one	17.271	2.4	ng	86377	4	17.618	722086	20.0
Anthracene, 2-m...	18.487	3.0	ng	107431	4	17.618	722086	20.0
Phenanthrene, 2...	18.540	4.3	ng	153341	4	17.618	722086	20.0
4H-Cyclopenta[d...	18.687	8.5	ng	306857	4	17.618	722086	20.0
Naphthalene, 2-...	18.975	2.8	ng	100661	4	17.618	722086	20.0
9,10-Anthracene...	19.022	8.6	ng	309263	4	17.618	722086	20.0
8,11-Octadecadi...	19.380	3.4	ng	123466	4	17.618	722086	20.0
Cyclopenta(def)...	19.539	2.6	ng	95585	4	17.618	722086	20.0
11H-Benzo[a]flu...	20.503	3.1	ng	218724	5	21.924	1425550	20.0