LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050697.D
Acq On : 22 Oct 2021 20:20
Operator : CG/JU
Sample : M4285-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-GB-(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-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050697.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.792	385	392	407	rBV	577471	1000540	66.28%	7.113%
2	7.396	656	665	683	rVB	597032	1085656	71.91%	7.718%
3	8.253	804	811	818	rBV	195009	335088	22.20%	2.382%
4	9.423	1001	1010	1023	rVB	372454	687559	45.54%	4.888%
5	10.821	1238	1248	1264	rBV	183796	348779	23.10%	2.479%
6	11.074	1283	1291	1298	rBV	264190	481967	31.93%	3.426%
7	13.494	1691	1703	1711	rBV	852571	1341635	88.87%	9.537%
8	13.741	1738	1745	1752	rVB	26167	42855	2.84%	0.305%
9	14.869	1928	1937	1944	rBV	390327	624739	41.38%	4.441%
10	14.934	1944	1948	1954	rVB	28378	42967	2.85%	0.305%
11	15.263	1999	2004	2009	rBV4	9882	15682	1.04%	0.111%
12	15.909	2109	2114	2122	rBV3	17805	28866	1.91%	0.205%
13	16.356	2183	2190	2208	rBV	476673	899836	59.60%	6.397%
14	17.266	2339	2345	2351	rBV2	14875	25016	1.66%	0.178%
15	17.431	2369	2373	2379	rVB2	13274	23624	1.56%	0.168%
16	17.613	2397	2404	2408	rBV	431108	684907	45.37%	4.869%
17	17.654	2408	2411	2418	rVV	224545	335312	22.21%	2.384%
18	17.748	2418	2427	2432	rVV	42187	77258	5.12%	0.549%
19	18.013	2462	2472	2479	rBV2	26278	60110	3.98%	0.427%
20	18.248	2508	2512	2517	rBV2	34481	40741	2.70%	0.290%
21	18.483	2548	2552	2556	rBV	31070	43187	2.86%	0.307%
22	18.530	2556	2560	2566	rVB	43856	71311	4.72%	0.507%
23	18.612	2570	2574	2579	rVB	14219	21600	1.43%	0.154%
24	18.682	2579	2586	2589	rBV3	48031	99994	6.62%	0.711%
25	18.976	2631	2636	2639	rBV	26587	37446	2.48%	0.266%
26	19.017	2639	2643	2650	rVB2	34296	51453	3.41%	0.366%
27	19.405	2701	2709	2713	rBV4	61856	109998	7.29%	0.782%
28	19.534	2725	2731	2737	rBV4	38136	75885	5.03%	0.539%
29	19.652	2745	2751	2757	rBV	418503	615225	40.75%	4.373%
30	19.981	2803	2807	2809	rBV2	54909	88422	5.86%	0.629%
31	20.016	2809	2813	2820	rVB	348666	501986	33.25%	3.569%
32	20.204	2839	2845	2850	rBV	1103747	1509679	100.00%	10.732%
33	20.598	2909	2912	2916	rBV	38408	54505	3.61%	0.387%
34	21.279	3025	3028	3032	rVB	28576	40102	2.66%	0.285%
35	21.514	3065	3068	3075	rBV3	62830	96892	6.42%	0.689%
36	21.767	3108	3111	3115	rVB2	36181	47813	3.17%	0.340%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050697.D
Acq On : 22 Oct 2021 20:20
Operator : CG/JU
Sample : M4285-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-GB-(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-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.914	3127	3136	3141	rBV2	391678	967280	64.07%	6.876%
38	21.961	3141	3144	3155	rVB	146479	251366	16.65%	1.787%
39	24.235	3525	3531	3539	rBV	98787	321915	21.32%	2.288%
40	25.169	3683	3690	3701	rVB	91458	270575	17.92%	1.923%
41	25.327	3709	3717	3727	rBV2	198593	607345	40.23%	4.317%

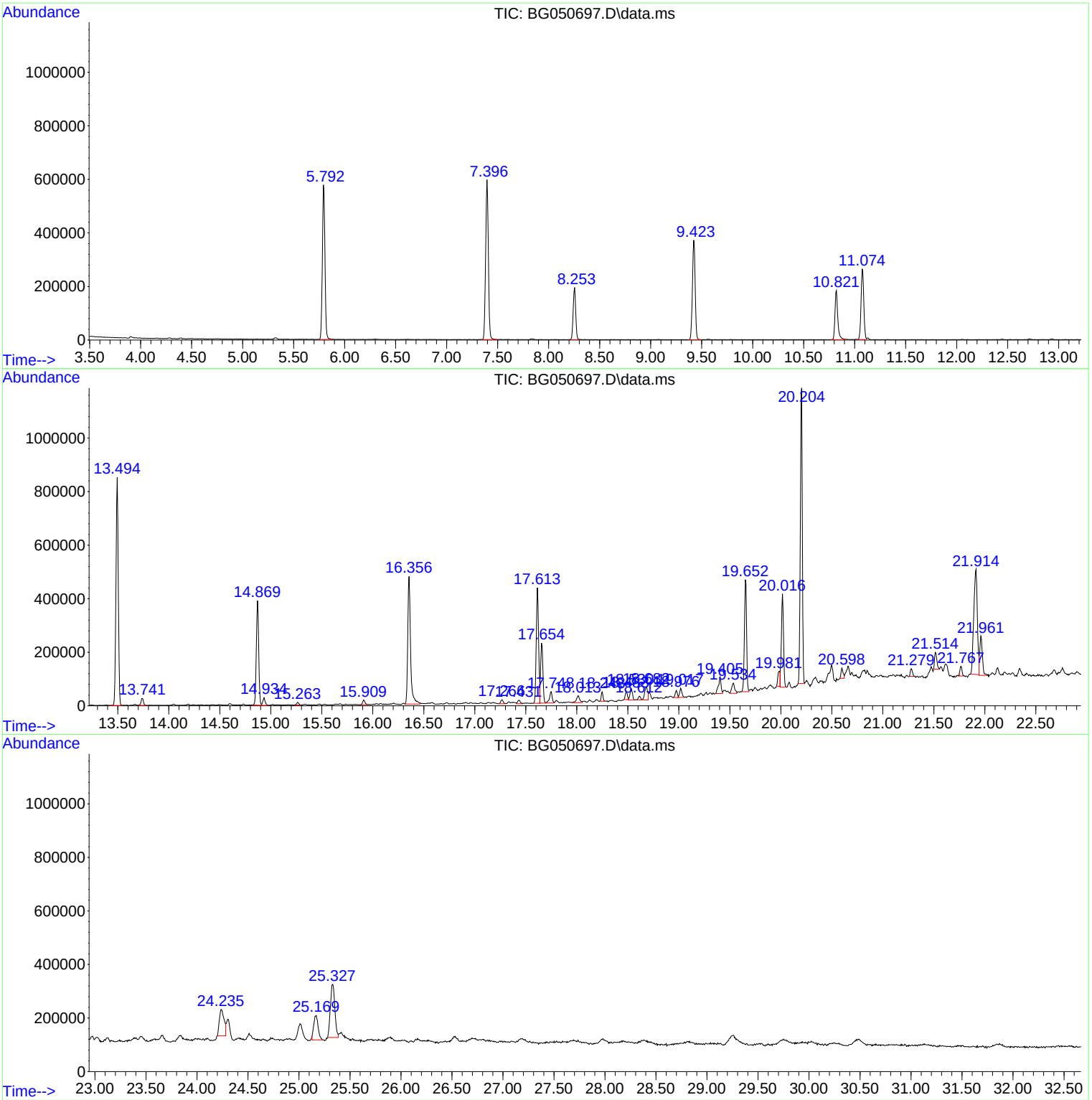
Sum of corrected areas: 14067116

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050697.D
Acq On : 22 Oct 2021 20:20
Operator : CG/JU
Sample : M4285-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-GB-(1)

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 : BG050697.D
Acq On : 22 Oct 2021 20:20
Operator : CG/JU
Sample : M4285-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-GB-(1)

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

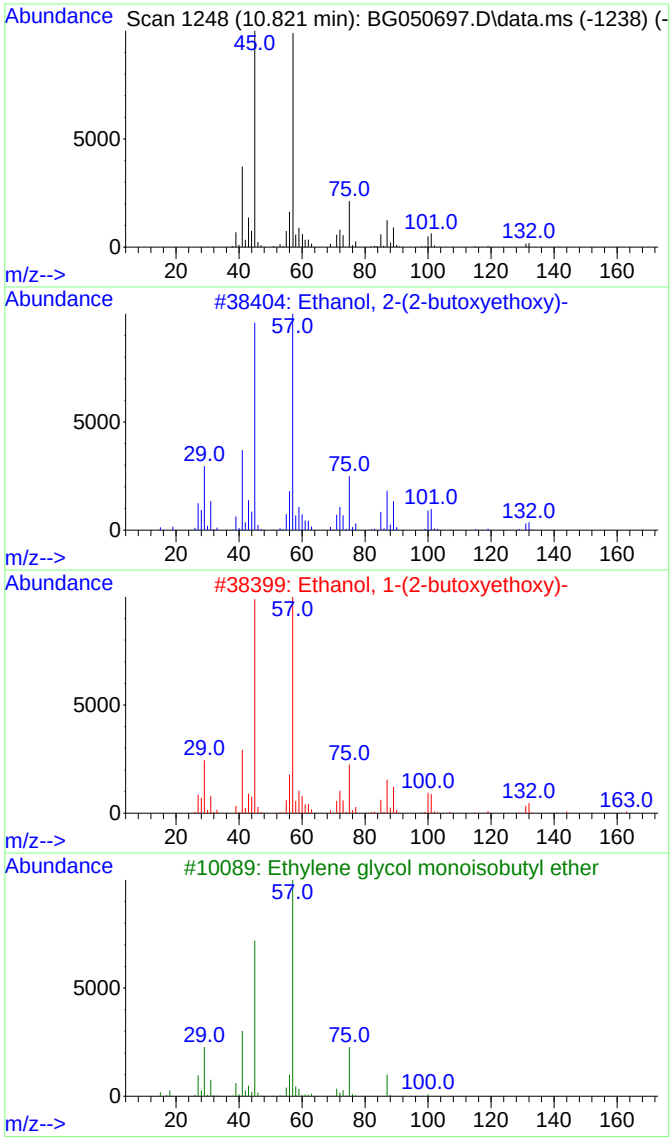
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

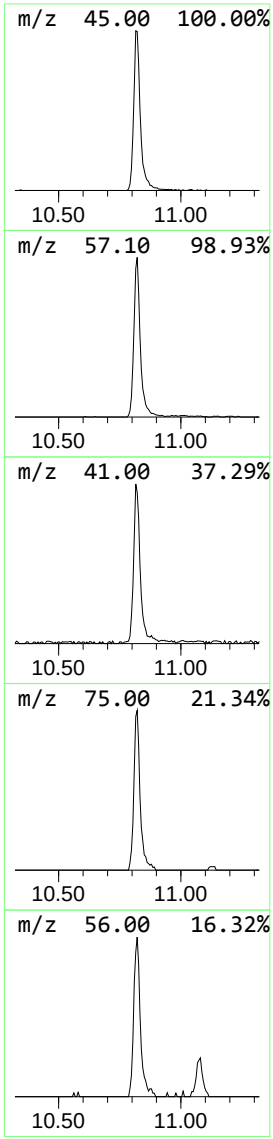
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.821	14.47 ng	348779	Naphthalene-d8	11.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050697.D
Acq On : 22 Oct 2021 20:20
Operator : CG/JU
Sample : M4285-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-GB-(1)

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

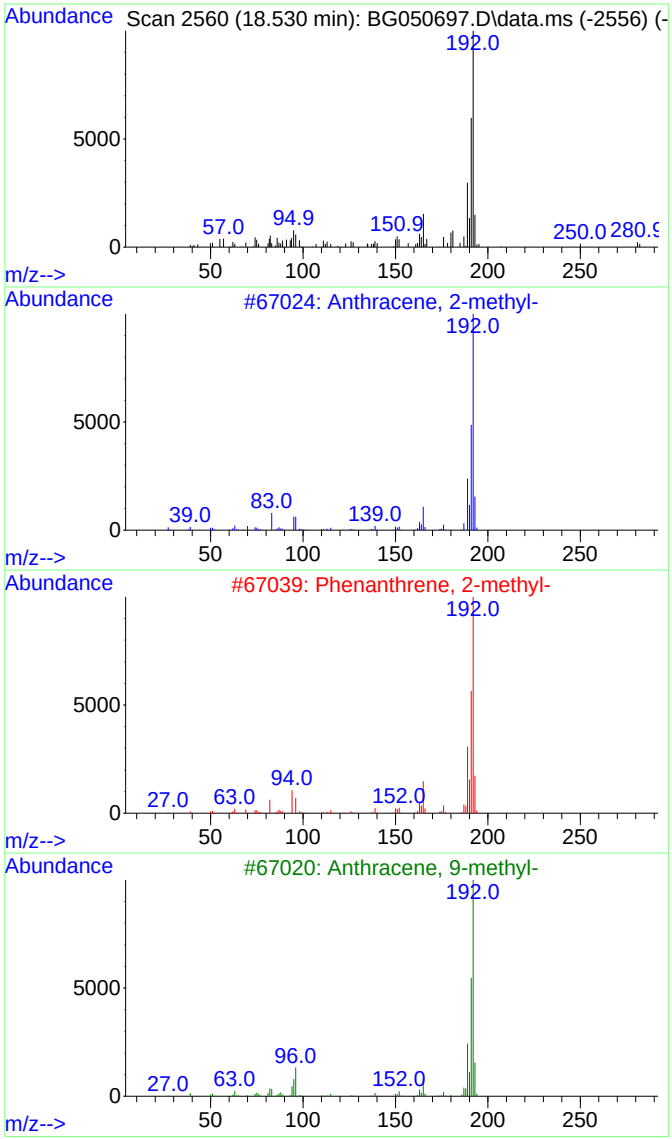
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

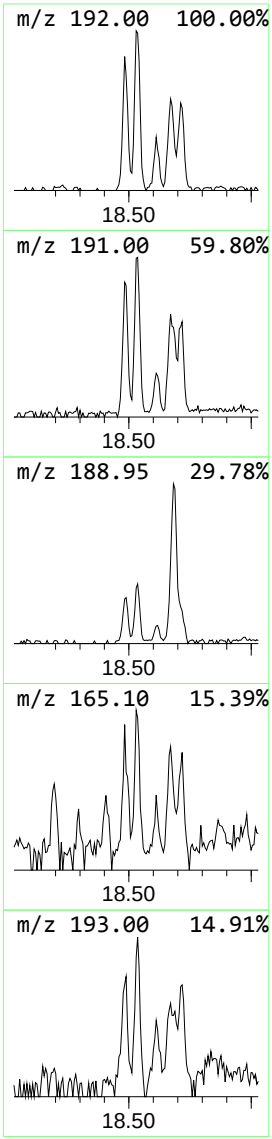
****

Peak Number 3 Anthracene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.530	2.08 ng	71311	Phenanthrene-d10	17.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050697.D
Acq On : 22 Oct 2021 20:20
Operator : CG/JU
Sample : M4285-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-GB-(1)

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

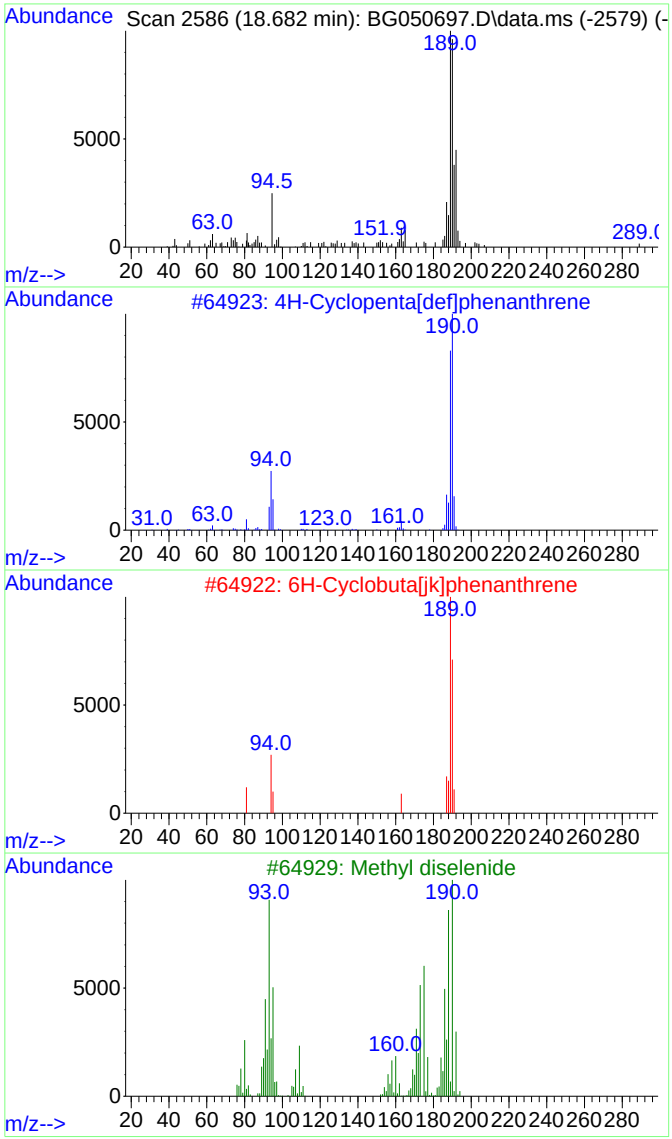
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

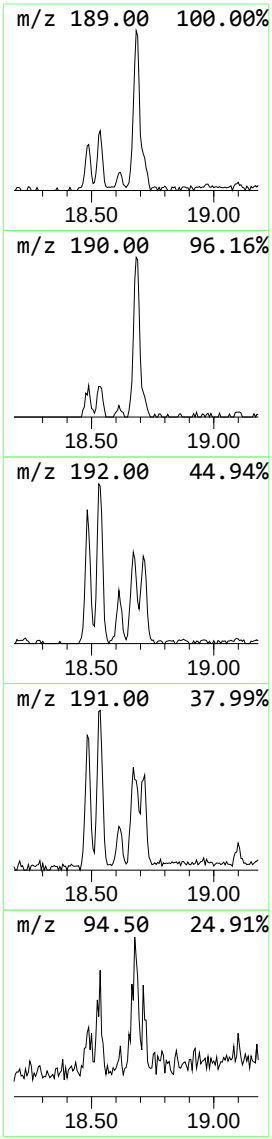
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.682	2.92 ng	99994	Phenanthrene-d10	17.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	72
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	Methyl diselenide	190	C2H6Se2	007101-31-7	49
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050697.D
Acq On : 22 Oct 2021 20:20
Operator : CG/JU
Sample : M4285-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-GB-(1)

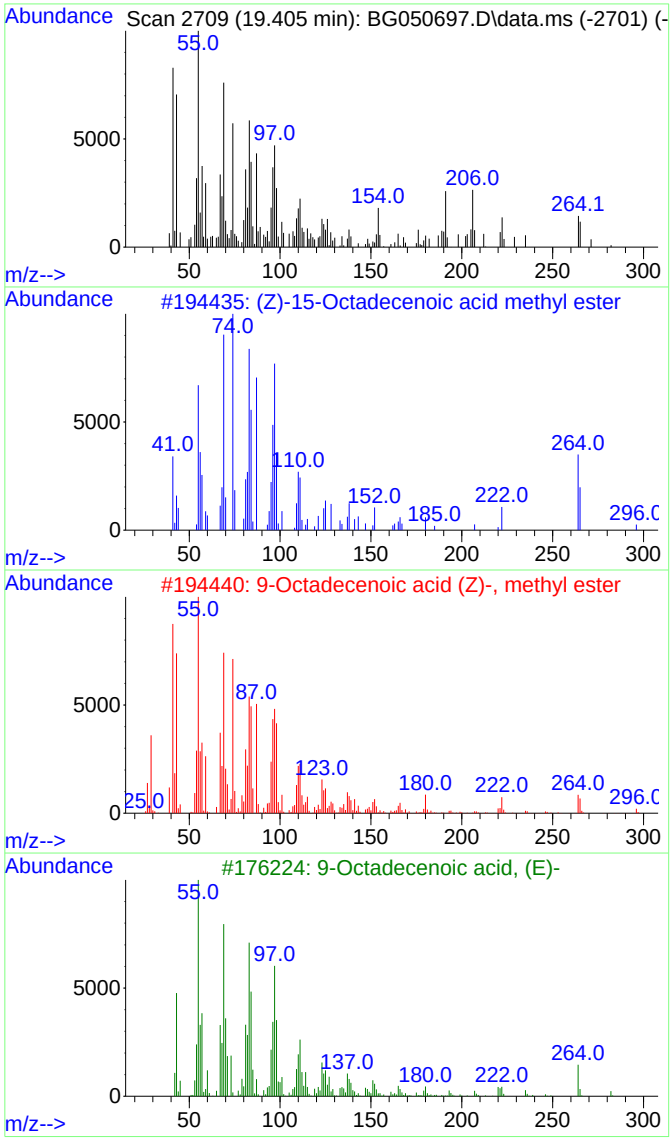
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

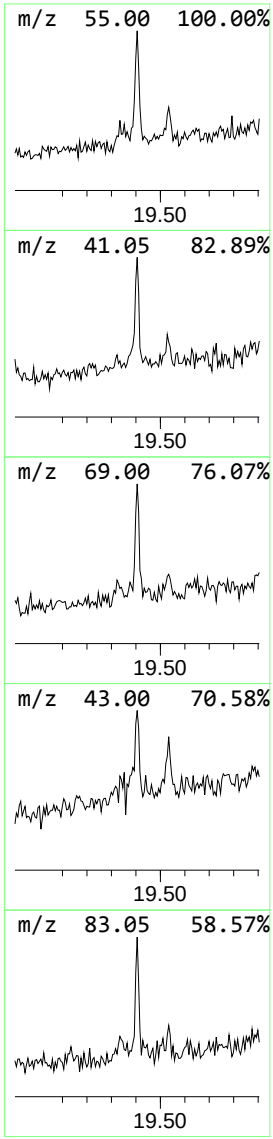
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (Z)-15-Octadecenoic acid me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.405	3.21 ng	109998	Phenanthrene-d10	17.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	90
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	81
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	64
4	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	55
5	13-Methyltetradec-9-enoic acid m...	254	C16H30O2	1010365-89-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050697.D
Acq On : 22 Oct 2021 20:20
Operator : CG/JU
Sample : M4285-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-GB-(1)

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

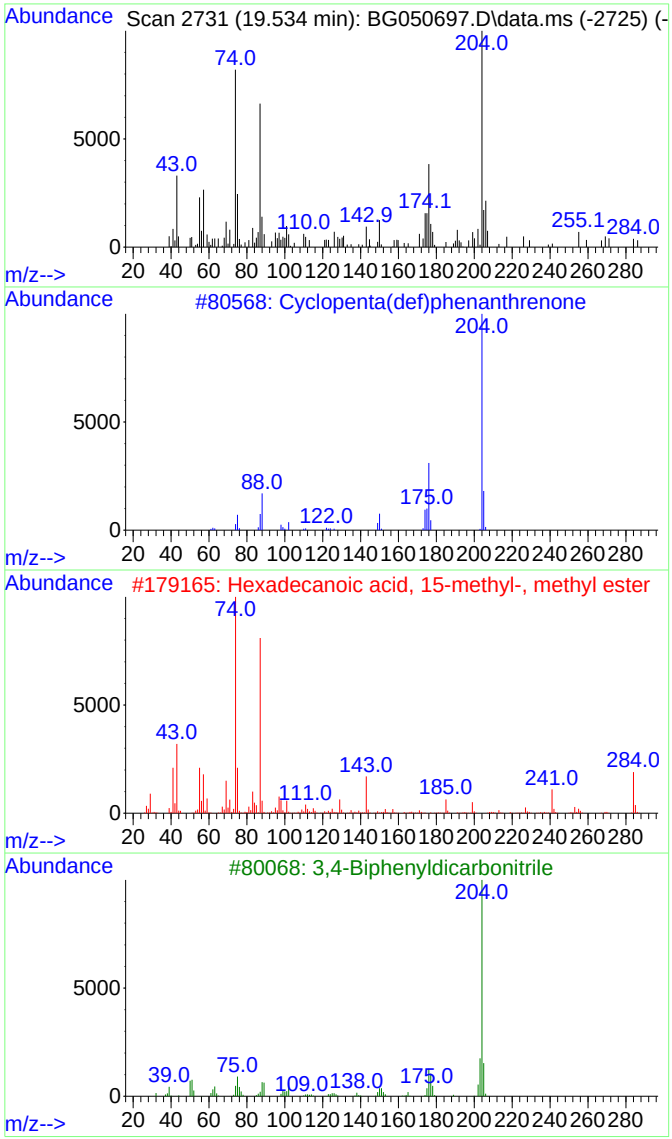
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

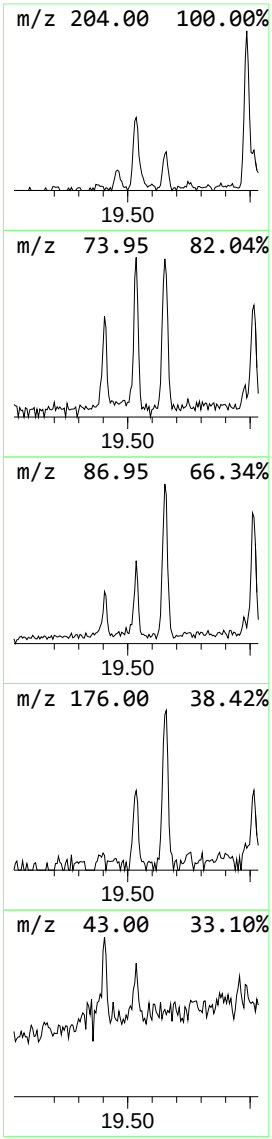
****

Peak Number 6 Cyclopenta(def)phenanthrenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.534	2.22 ng	75885	Phenanthrene-d10	17.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	55
2	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	42
3	3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	30
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	27
5	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050697.D
Acq On : 22 Oct 2021 20:20
Operator : CG/JU
Sample : M4285-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-GB-(1)

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

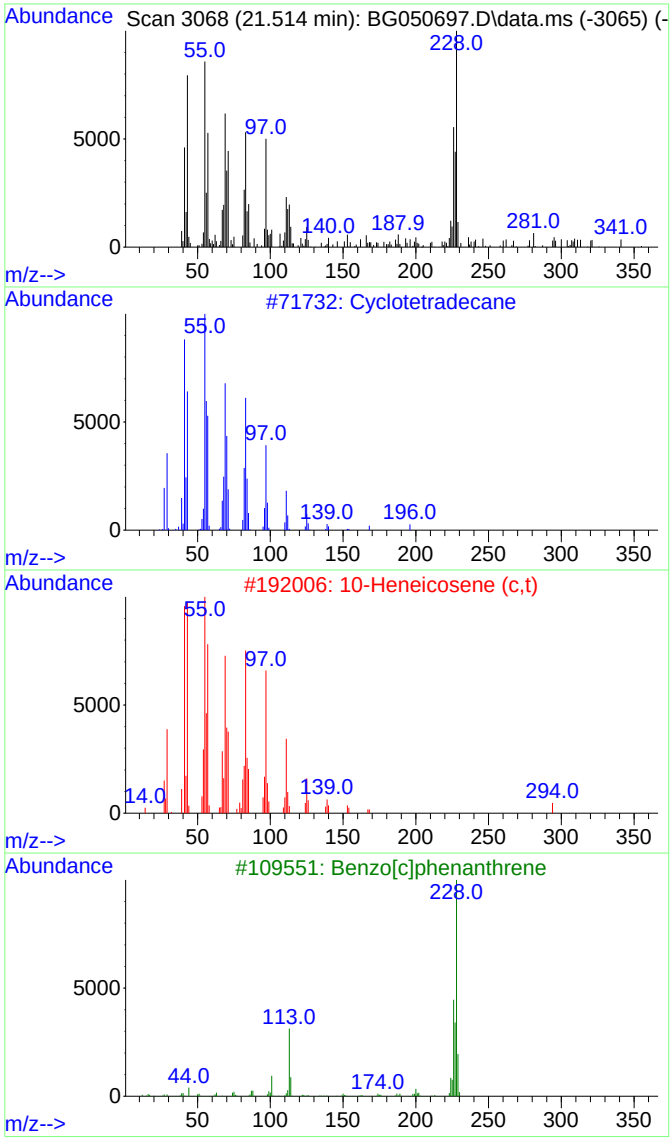
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

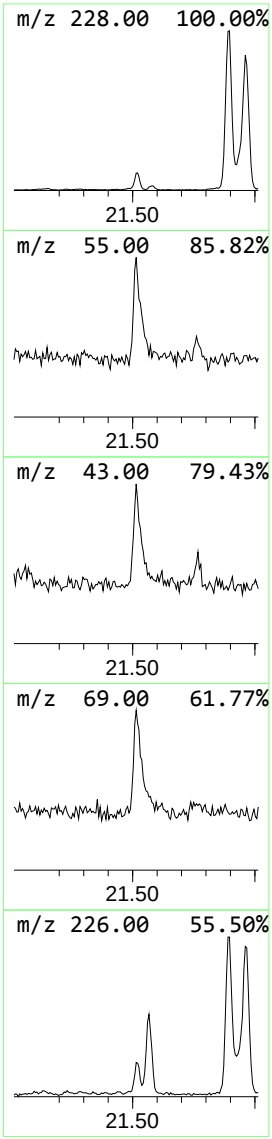
****

Peak Number 7 unknown21.514 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.514	2.00 ng	96892	Chrysene-d12	21.914

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	45
2	10-Heneicosene (c,t)	294	C21H42	095008-11-0	44
3	Benzo[c]phenanthrene	228	C18H12	000195-19-7	38
4	1-Heptadecene	238	C17H34	006765-39-5	30
5	1-Eicosanol	298	C20H42O	000629-96-9	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050697.D
Acq On : 22 Oct 2021 20:20
Operator : CG/JU
Sample : M4285-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-GB-(1)

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...	10.821	14.5	ng	348779	2	11.074	481967	20.0
Anthracene, 2-m...	18.530	2.1	ng	71311	4	17.613	684907	20.0
4H-Cyclopenta[d...	18.682	2.9	ng	99994	4	17.613	684907	20.0
(Z)-15-Octadece...	19.405	3.2	ng	109998	4	17.613	684907	20.0
Cyclopenta(def)...	19.534	2.2	ng	75885	4	17.613	684907	20.0
unknown21.514	21.514	2.0	ng	96892	5	21.914	967280	20.0