LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048474.D
Acq On : 23 Mar 2021 17:50
Operator : CG/JU
Sample : M1746-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-4

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-BG031821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048474.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.179	308	313	319	rVB	31224	46089	1.48%	0.189%
2	5.650	386	393	407	rVB	649700	1033394	33.19%	4.241%
3	7.254	656	666	676	rBV	677593	1179562	37.89%	4.841%
4	8.105	800	811	818	rBV	148612	250489	8.05%	1.028%
5	9.269	999	1009	1020	rBV	436813	767149	24.64%	3.149%
6	10.926	1283	1291	1297	rBV	198602	354526	11.39%	1.455%
7	13.364	1699	1706	1713	rBV	1155534	1705725	54.79%	7.001%
8	14.187	1840	1846	1853	rBV	22609	31166	1.00%	0.128%
9	14.745	1931	1941	1947	rBV	359553	554493	17.81%	2.276%
10	14.809	1947	1952	1959	rVB	122376	199366	6.40%	0.818%
11	15.138	2003	2008	2015	rVB	47534	76925	2.47%	0.316%
12	15.791	2113	2119	2128	rVB	78783	124298	3.99%	0.510%
13	16.231	2187	2194	2201	rBV	1175615	1758663	56.49%	7.218%
14	17.312	2373	2378	2384	rVB	42428	66382	2.13%	0.272%
15	17.494	2403	2409	2412	rBV	492274	735838	23.64%	3.020%
16	17.536	2412	2416	2422	rVV	769460	1136842	36.52%	4.666%
17	17.624	2422	2431	2438	rVB	176807	295873	9.50%	1.214%
18	17.894	2469	2477	2483	rBV2	84948	142635	4.58%	0.585%
19	18.370	2552	2558	2562	rBV2	167560	230031	7.39%	0.944%
20	18.417	2562	2566	2571	rVB	77335	112361	3.61%	0.461%
21	18.499	2575	2580	2586	rVB2	24668	39362	1.26%	0.162%
22	18.570	2586	2592	2596	rBV2	106566	191331	6.15%	0.785%
23	18.869	2638	2643	2646	rBV	48095	77587	2.49%	0.318%
24	18.905	2646	2649	2653	rVB2	55957	72825	2.34%	0.299%
25	19.281	2708	2713	2718	rBV4	22096	36416	1.17%	0.149%
26	19.416	2733	2736	2746	rVB3	23954	37904	1.22%	0.156%
27	19.545	2752	2758	2764	rBV	1139732	1585079	50.91%	6.506%
28	19.639	2770	2774	2779	rVB2	49439	60985	1.96%	0.250%
29	19.786	2795	2799	2806	rVB3	42463	77185	2.48%	0.317%
30	19.874	2808	2814	2816	rBV2	202464	314914	10.12%	1.292%
31	19.909	2816	2820	2826	rVV	842557	1206193	38.74%	4.951%
32	19.974	2828	2831	2837	rVB3	35041	47592	1.53%	0.195%
33	20.103	2843	2853	2858	rBV	2268412	3113200	100.00%	12.777%
34	20.144	2858	2860	2865	rVB2	37803	47229	1.52%	0.194%
35	20.221	2868	2873	2875	rBV2	42892	68544	2.20%	0.281%
36	20.279	2880	2883	2888	rVB2	27902	37409	1.20%	0.154%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048474.D
Acq On : 23 Mar 2021 17:50
Operator : CG/JU
Sample : M1746-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-4

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-BG031821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.397	2888	2903	2907	rBV	120246	257279	8.26%	1.056%
38	20.497	2915	2920	2924	rBV	98035	143109	4.60%	0.587%
39	20.556	2924	2930	2933	rVV3	50371	94230	3.03%	0.387%
40	20.591	2933	2936	2940	rVB2	55003	68251	2.19%	0.280%
41	20.691	2950	2953	2957	rBV	26298	42301	1.36%	0.174%
42	21.161	3029	3033	3039	rVB2	41955	71242	2.29%	0.292%
43	21.355	3060	3066	3070	rBV	68064	113493	3.65%	0.466%
44	21.413	3070	3076	3079	rBV2	93248	202143	6.49%	0.830%
45	21.502	3087	3091	3098	rVB3	71532	117510	3.77%	0.482%
46	21.778	3130	3138	3144	rBV3	590743	1566934	50.33%	6.431%
47	21.831	3144	3147	3155	rVB	359353	572653	18.39%	2.350%
48	21.989	3169	3174	3181	rBV2	87768	147584	4.74%	0.606%
49	22.124	3194	3197	3203	rVB	34619	60391	1.94%	0.248%
50	22.195	3206	3209	3217	rVB2	58487	112167	3.60%	0.460%
51	22.530	3263	3266	3272	rVB2	36759	71343	2.29%	0.293%
52	22.818	3312	3315	3318	rBV5	28399	35012	1.12%	0.144%
53	22.859	3319	3322	3330	rVB7	36592	76513	2.46%	0.314%
54	24.051	3517	3525	3534	rBV2	252864	864484	27.77%	3.548%
55	24.804	3646	3653	3665	rVB	137071	396786	12.75%	1.629%
56	24.956	3670	3679	3693	rVB2	205293	601034	19.31%	2.467%
57	25.115	3696	3706	3714	rBV2	251823	794793	25.53%	3.262%
58	28.899	4344	4350	4351	rBV	64844	90374	2.90%	0.371%
59	30.103	4550	4555	4556	rBV3	34744	49573	1.59%	0.203%

Sum of corrected areas: 24364761

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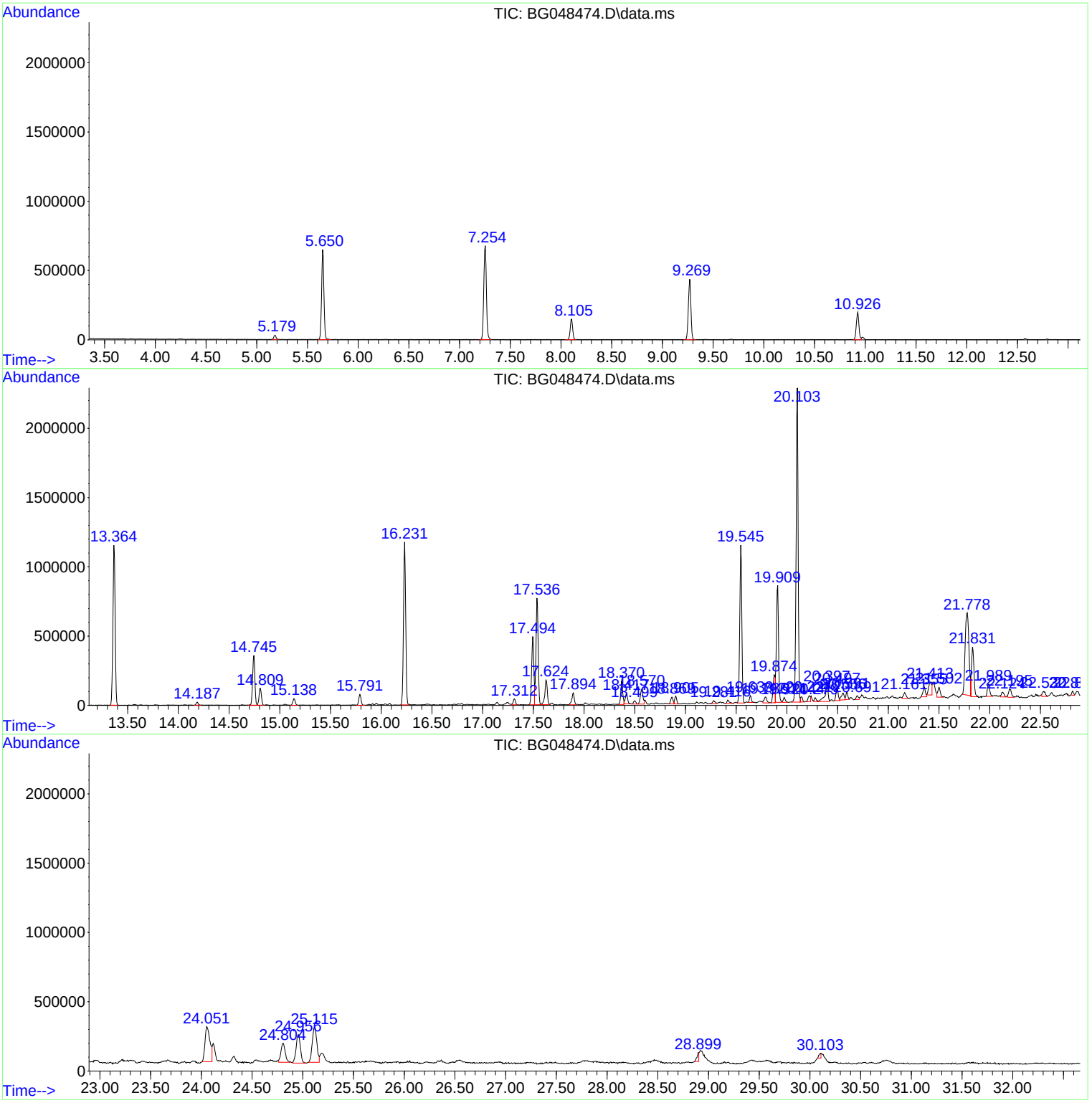
Instrument :
BNA_G
ClientSampleId :
COMP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048474.D
Acq On : 23 Mar 2021 17:50
Operator : CG/JU
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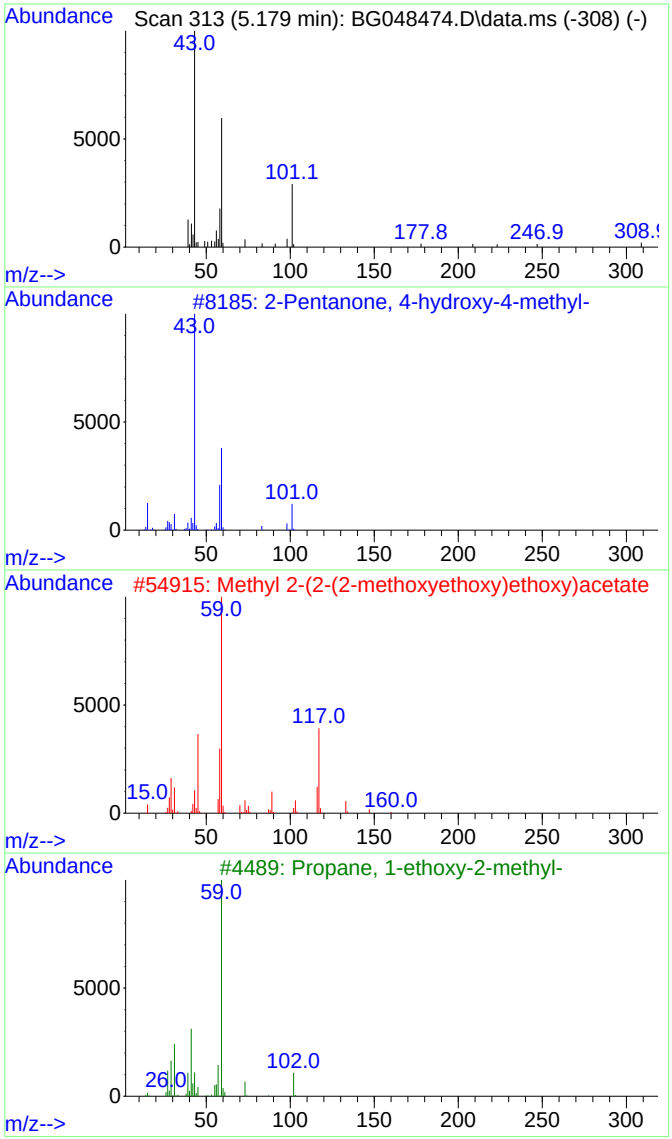
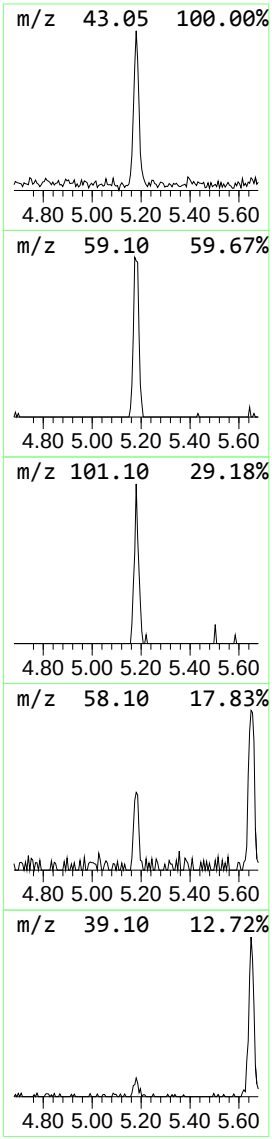
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.179	3.68 ng	46089	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	Methyl 2-(2-(2-methoxyethoxy)eth...	192	C8H16O5	1000366-88-2	23
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	16
4	3-Pentanol	88	C5H12O	000584-02-1	12
5	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	12





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Data File : BG048474.D
Acq On : 23 Mar 2021 17:50
Operator : CG/JU
Sample : M1746-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

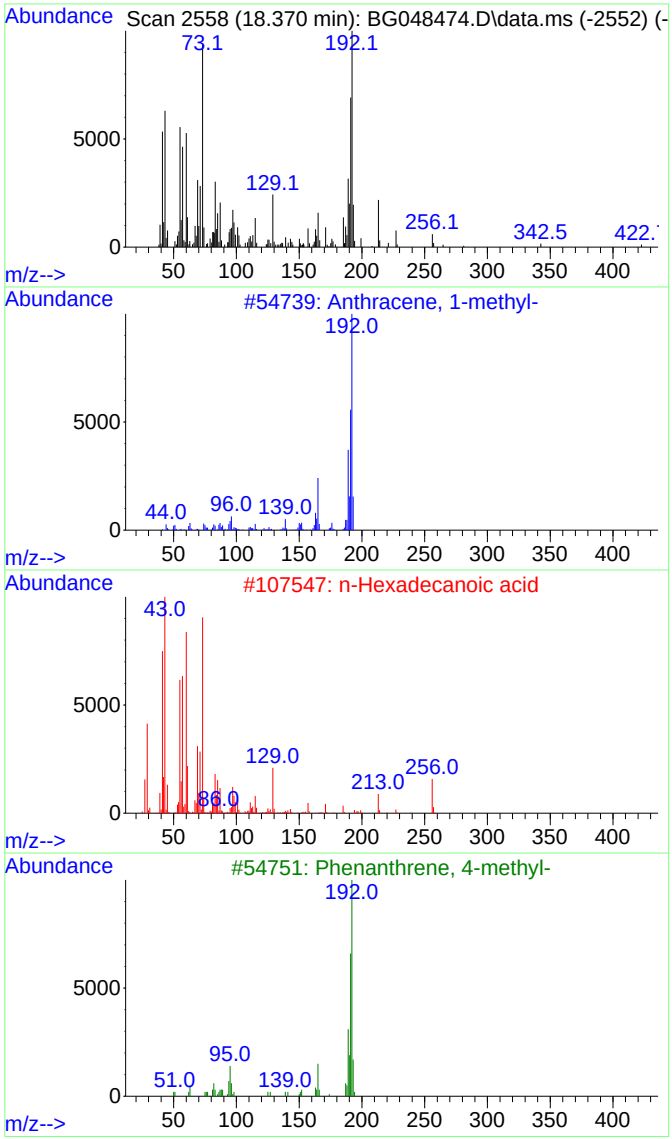
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

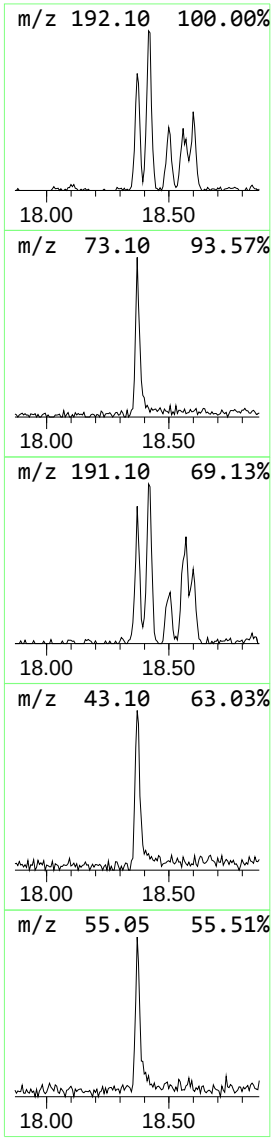
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.370	6.25 ng	230031	Phenanthrene-d10	17.494

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	86
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	60
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	50
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048474.D
Acq On : 23 Mar 2021 17:50
Operator : CG/JU
Sample : M1746-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

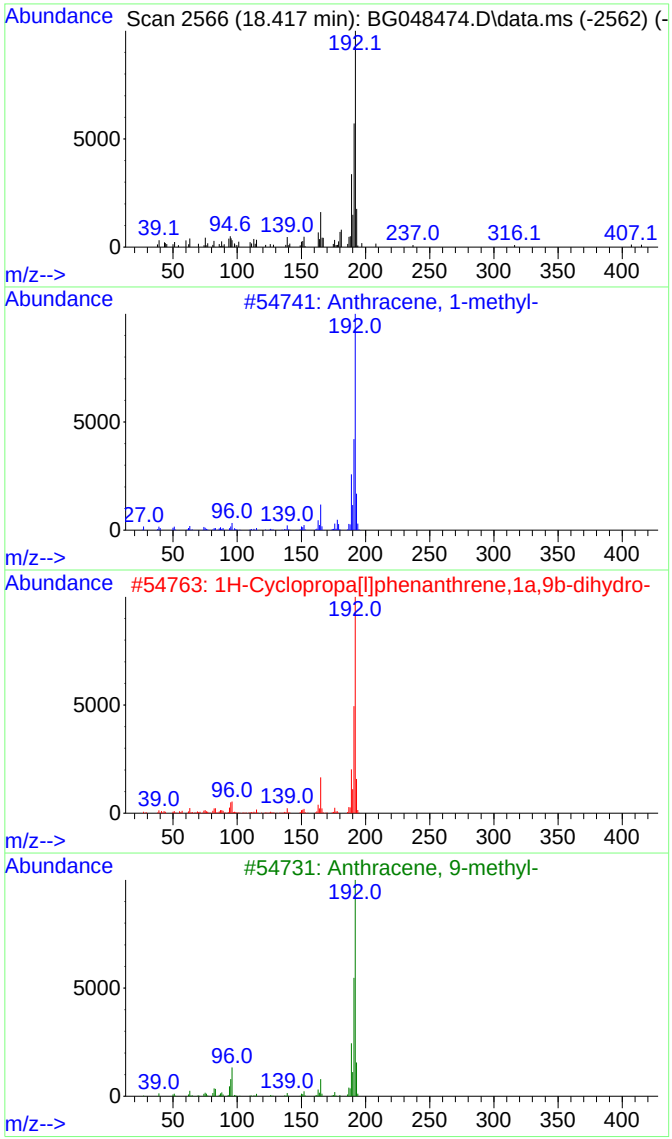
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

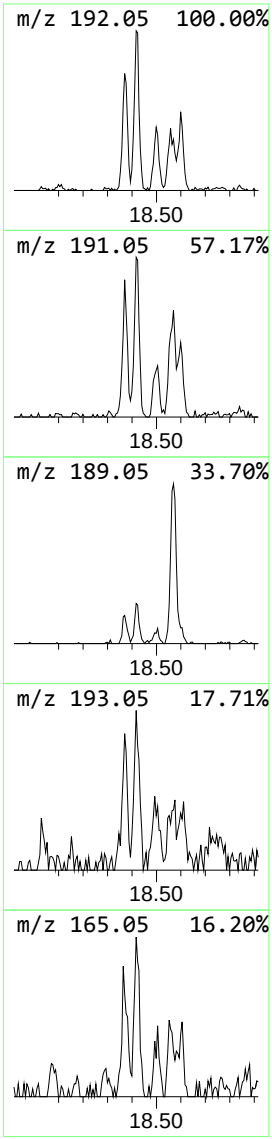
****

Peak Number 3 Anthracene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.417	3.05 ng	112361	Phenanthrene-d10	17.494

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	91
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
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Acq On : 23 Mar 2021 17:50
Operator : CG/JU
Sample : M1746-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-4

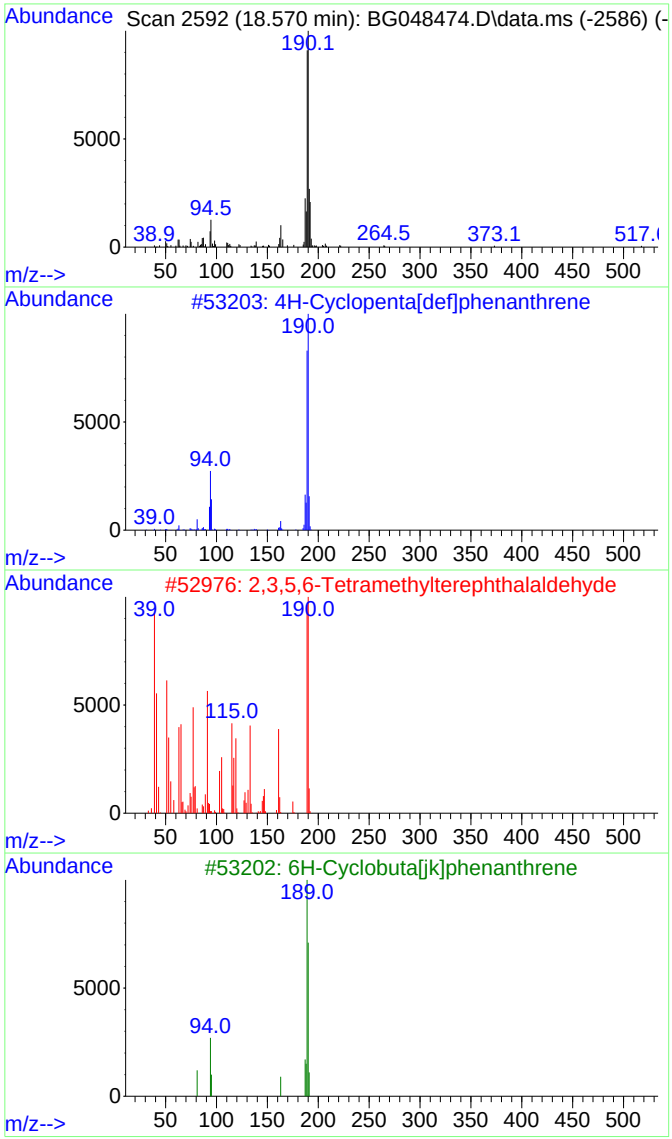
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

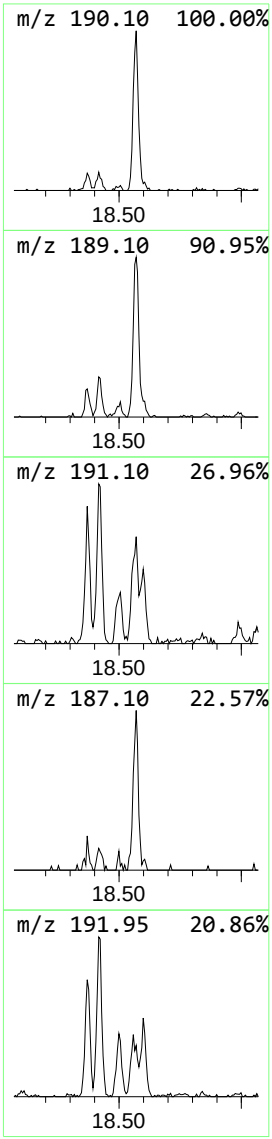
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.570	5.20 ng	191331	Phenanthrene-d10	17.494

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	37
4	Phenantro[9,10-b]furazano[3,4-c]...	272	C16H8N4O	024294-86-8	12
5	Megastigmatrienone	190	C13H18O	038818-55-2	12





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

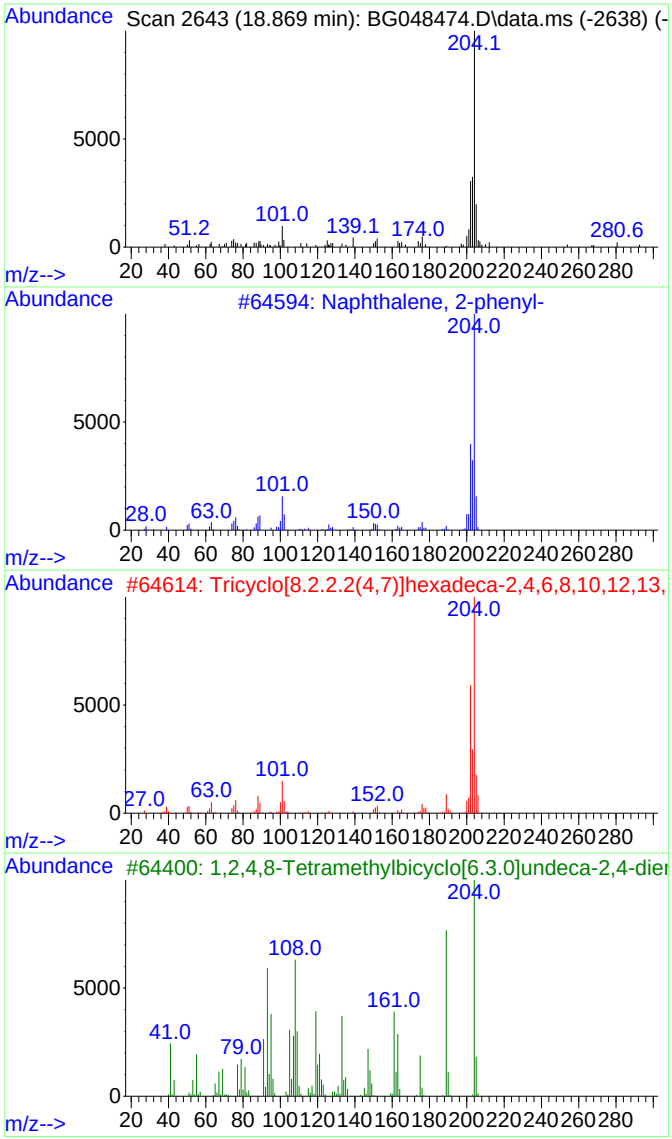
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

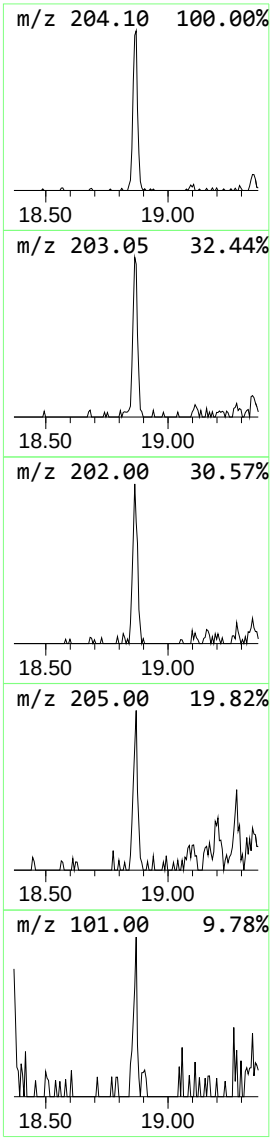
****

Peak Number 5 Naphthalene, 2-phenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.869	2.11 ng	77587	Phenanthrene-d10	17.494

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	81
2	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	72
3	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	60
4	3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	59
5	[1,1'-Biphenyl]-2-ol, 5-chloro-	204	C12H9ClO	000607-12-5	58





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

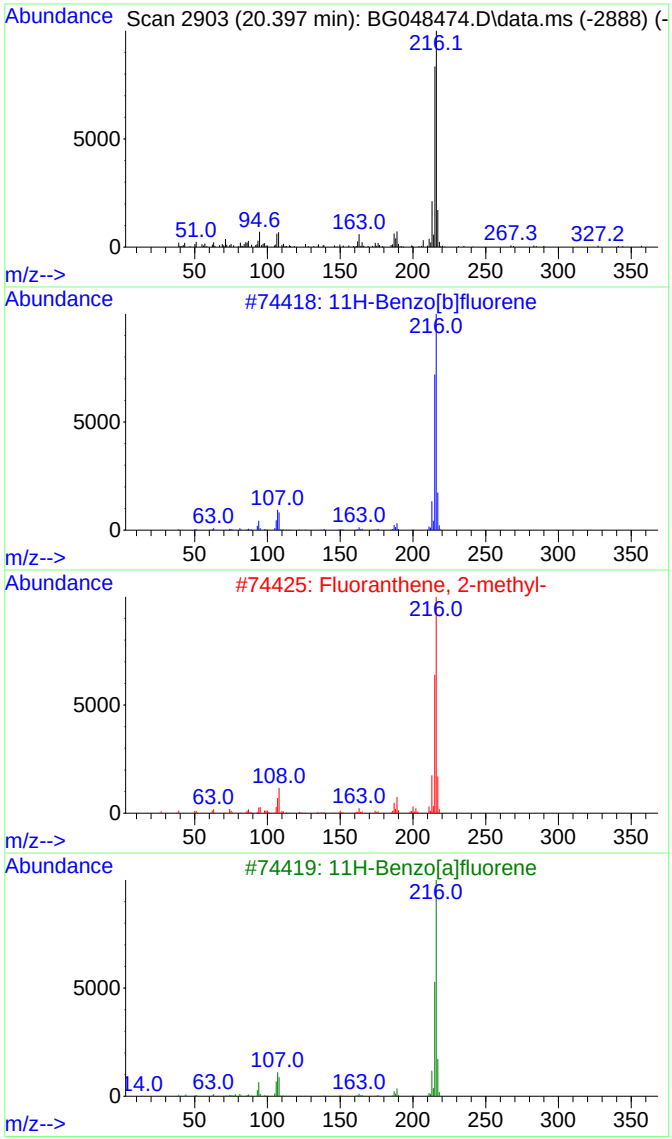
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

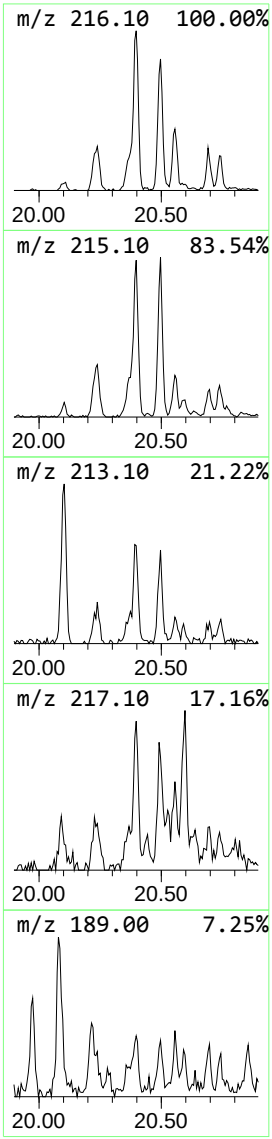
****

Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.397	3.28 ng	257279	Chrysene-d12	21.784

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	96
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	96
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	83





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Sample : M1746-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

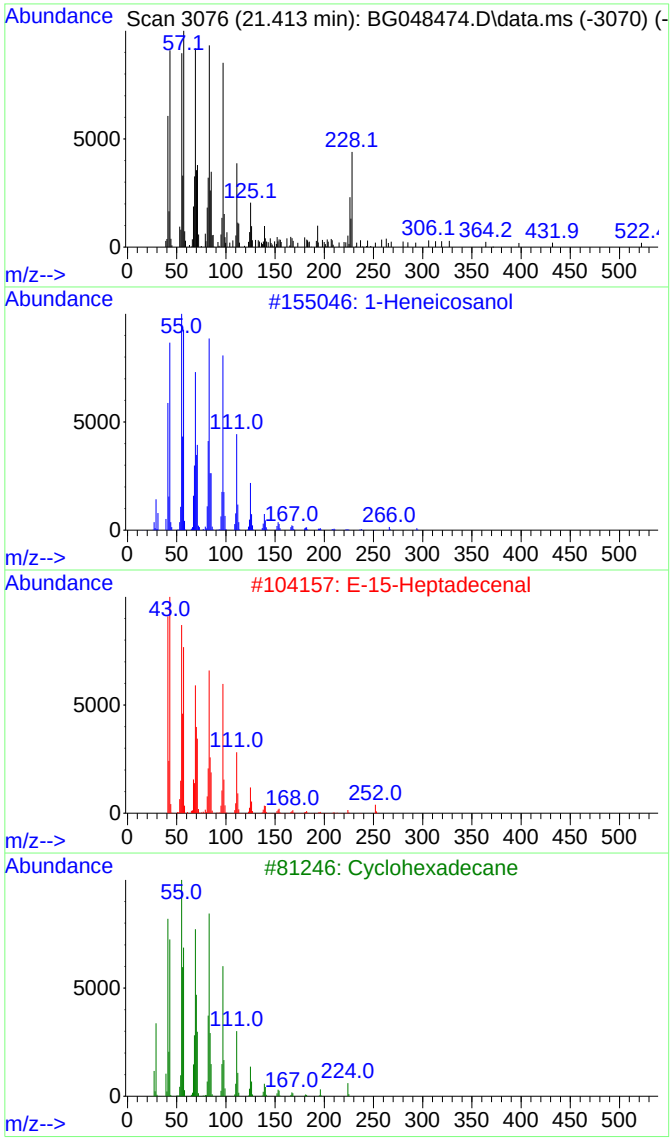
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

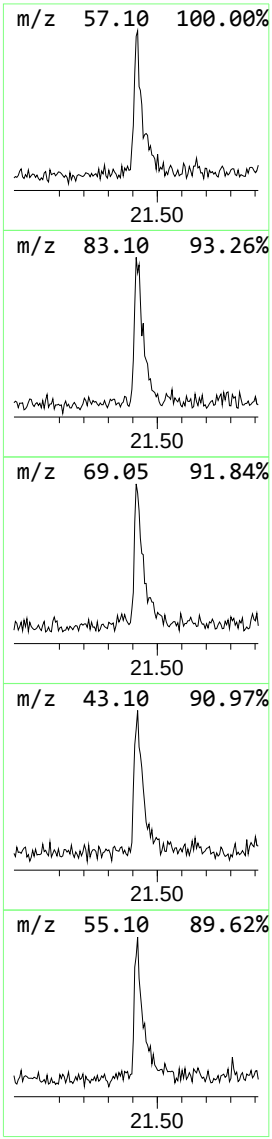
****

Peak Number 7 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.413	2.58 ng	202143	Chrysene-d12	21.784

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	90
3	Cyclohexadecane	224	C16H32	000295-65-8	86
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	70
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048474.D
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Operator : CG/JU
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.179	3.7	ng	46089	1	8.105	250489	20.0
n-Hexadecanoic ...	18.370	6.3	ng	230031	4	17.494	735838	20.0
Anthracene, 1-m...	18.417	3.0	ng	112361	4	17.494	735838	20.0
4H-Cyclopenta[d...	18.570	5.2	ng	191331	4	17.494	735838	20.0
Naphthalene, 2-...	18.869	2.1	ng	77587	4	17.494	735838	20.0
11H-Benzo[b]flu...	20.397	3.3	ng	257279	5	21.784	1566930	20.0
1-Heneicosanol	21.413	2.6	ng	202143	5	21.784	1566930	20.0