LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052326.D
Acq On : 8 Feb 2022 19:28
Operator : CG/JU
Sample : N1401-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PSC-124055

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-BG020722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG052326.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.329	138	143	154	rBV2	8633	16759	1.10%	0.131%
2	5.275	298	304	312	rBV	18717	29473	1.94%	0.231%
3	5.757	378	386	397	rBV	538741	874006	57.39%	6.840%
4	7.378	653	662	674	rBV	562142	1017540	66.82%	7.963%
5	8.230	797	807	813	rBV	129645	219402	14.41%	1.717%
6	9.399	997	1006	1022	rVB	361358	668352	43.89%	5.230%
7	10.815	1239	1247	1253	rBV2	13992	26224	1.72%	0.205%
8	11.067	1282	1290	1296	rBV	181680	326120	21.42%	2.552%
9	11.120	1296	1299	1306	rVB	12399	19024	1.25%	0.149%
10	13.494	1695	1703	1711	rBV	810718	1267679	83.24%	9.921%
11	13.682	1730	1735	1744	rBV5	6449	17521	1.15%	0.137%
12	14.198	1816	1823	1828	rBV3	10952	19491	1.28%	0.153%
13	14.874	1926	1938	1944	rBV	290014	457585	30.05%	3.581%
14	14.939	1944	1949	1956	rVB2	26823	41332	2.71%	0.323%
15	15.268	1999	2005	2012	rVB2	24472	36459	2.39%	0.285%
16	15.655	2064	2071	2075	rBV3	11328	23314	1.53%	0.182%
17	15.920	2110	2116	2122	rBV2	36184	57557	3.78%	0.450%
18	16.360	2185	2191	2202	rBV	755787	1181928	77.61%	9.250%
19	16.584	2227	2229	2235	rVB5	9733	16342	1.07%	0.128%
20	17.347	2356	2359	2365	rBV6	12263	18340	1.20%	0.144%
21	17.441	2372	2375	2380	rVB	15586	19871	1.30%	0.156%
22	17.512	2383	2387	2391	rVB4	13077	18696	1.23%	0.146%
23	17.623	2399	2406	2410	rBV	348216	530957	34.87%	4.155%
24	17.670	2410	2414	2421	rVV	209899	316513	20.78%	2.477%
25	17.758	2421	2429	2434	rVV	64661	98386	6.46%	0.770%
26	18.023	2469	2474	2479	rBV	19051	31785	2.09%	0.249%
27	18.269	2512	2516	2521	rBV4	13036	16699	1.10%	0.131%
28	18.499	2547	2555	2559	rBV2	40773	70784	4.65%	0.554%
29	18.551	2559	2564	2570	rVB	45243	74035	4.86%	0.579%
30	18.628	2573	2577	2582	rVV2	17225	27330	1.79%	0.214%
31	18.698	2582	2589	2593	rVV2	58650	121894	8.00%	0.954%
32	18.728	2593	2594	2599	rVB2	26825	25104	1.65%	0.196%
33	18.986	2633	2638	2642	rBV	27623	40470	2.66%	0.317%
34	19.039	2643	2647	2652	rVB8	11975	19064	1.25%	0.149%
35	19.233	2676	2680	2683	rBV6	13324	19549	1.28%	0.153%
36	19.403	2704	2709	2715	rBV2	28487	47862	3.14%	0.375%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052326.D
Acq On : 8 Feb 2022 19:28
Operator : CG/JU
Sample : N1401-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124055

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-BG020722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.468	2715	2720	2728	rVB6	14935	32409	2.13%	0.254%
38	19.544	2729	2733	2737	rBV6	11190	18068	1.19%	0.141%
39	19.673	2746	2755	2760	rBV	319378	491128	32.25%	3.844%
40	19.720	2760	2763	2767	rVV6	11753	17679	1.16%	0.138%
41	19.762	2767	2770	2774	rVB5	11950	17421	1.14%	0.136%
42	19.903	2792	2794	2803	rVB2	14198	26683	1.75%	0.209%
43	19.997	2805	2810	2811	rVV	54077	73533	4.83%	0.575%
44	20.032	2812	2816	2823	rVV	270329	403512	26.50%	3.158%
45	20.096	2823	2827	2833	rVB3	18644	31168	2.05%	0.244%
46	20.220	2841	2848	2853	rBV	1170518	1522846	100.00%	11.918%
47	20.261	2853	2855	2862	rVB4	11288	17924	1.18%	0.140%
48	20.349	2865	2870	2872	rBV5	22399	38657	2.54%	0.303%
49	20.519	2889	2899	2904	rVB3	62217	128751	8.45%	1.008%
50	20.619	2912	2916	2920	rBV2	49678	66059	4.34%	0.517%
51	20.678	2920	2926	2930	rVV3	26271	48028	3.15%	0.376%
52	20.860	2955	2957	2962	rBV5	14278	17885	1.17%	0.140%
53	21.007	2978	2982	2986	rVB2	21011	29952	1.97%	0.234%
54	21.500	3063	3066	3069	rBV	14093	15338	1.01%	0.120%
55	21.536	3069	3072	3078	rVB2	67423	93688	6.15%	0.733%
56	21.800	3112	3117	3121	rVB	59333	93742	6.16%	0.734%
57	21.941	3132	3141	3146	rBV3	303684	744773	48.91%	5.828%
58	21.994	3146	3150	3161	rVB	106059	197465	12.97%	1.545%
59	22.376	3211	3215	3224	rVB7	16260	33294	2.19%	0.261%
60	22.775	3280	3283	3284	rBV3	18282	19024	1.25%	0.149%
61	24.308	3536	3544	3551	rBV	61939	207859	13.65%	1.627%
62	25.254	3698	3705	3716	rVB	46279	147199	9.67%	1.152%
63	25.419	3724	3733	3744	rBV2	124298	430593	28.28%	3.370%

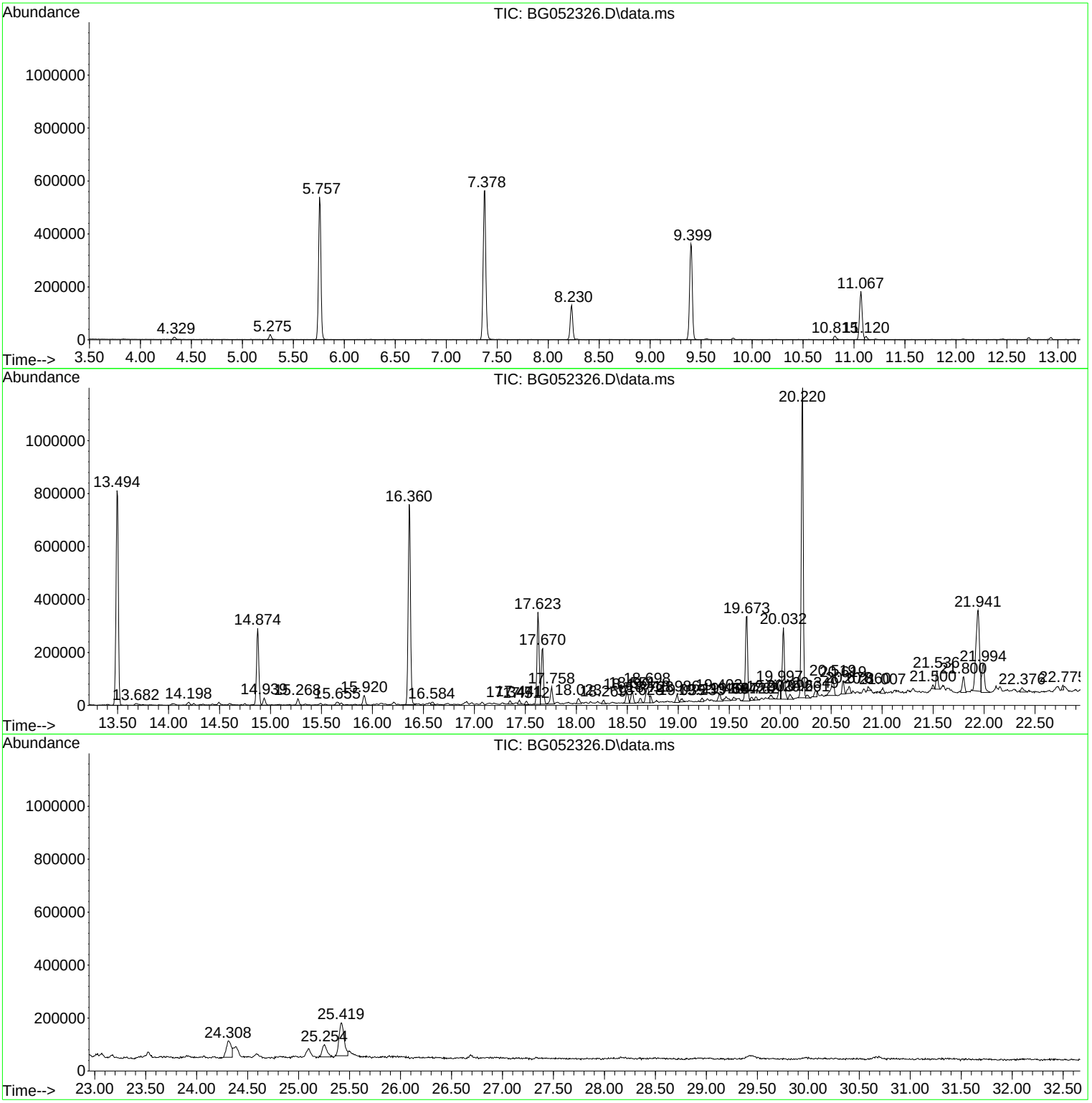
Sum of corrected areas: 12778125

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052326.D
Acq On : 8 Feb 2022 19:28
Operator : CG/JU
Sample : N1401-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124055

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.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\BG020822\
Data File : BG052326.D
Acq On : 8 Feb 2022 19:28
Operator : CG/JU
Sample : N1401-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124055

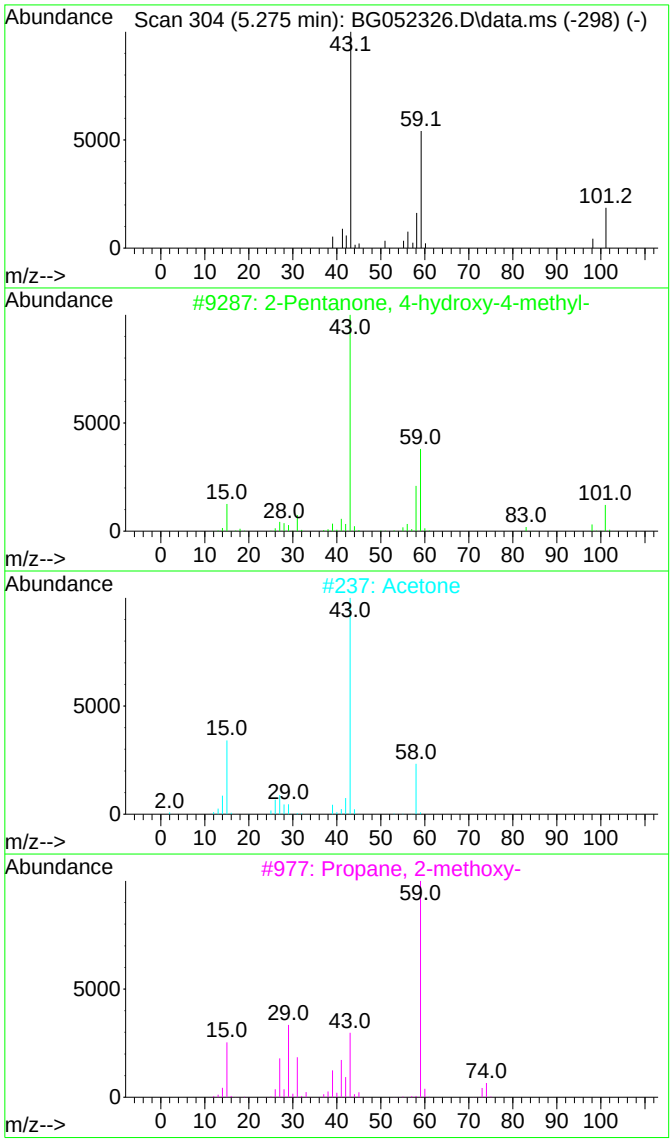
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

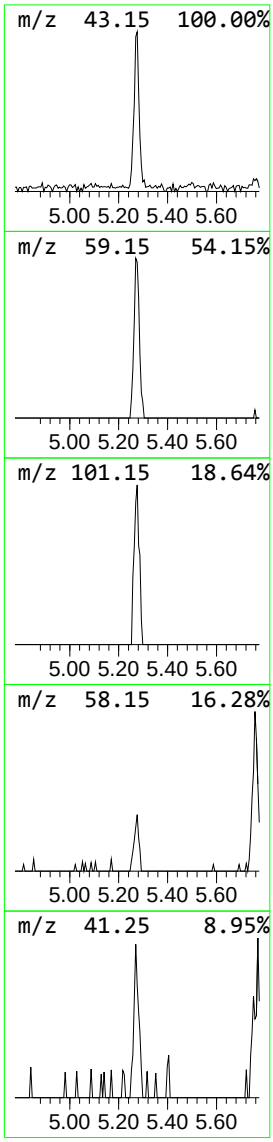
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.275	2.69 ng	29473	1,4-Dichlorobenzene-d4	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetone	58	C3H6O	000067-64-1	9
3	Propane, 2-methoxy-	74	C4H10O	000598-53-8	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052326.D
Acq On : 8 Feb 2022 19:28
Operator : CG/JU
Sample : N1401-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124055

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

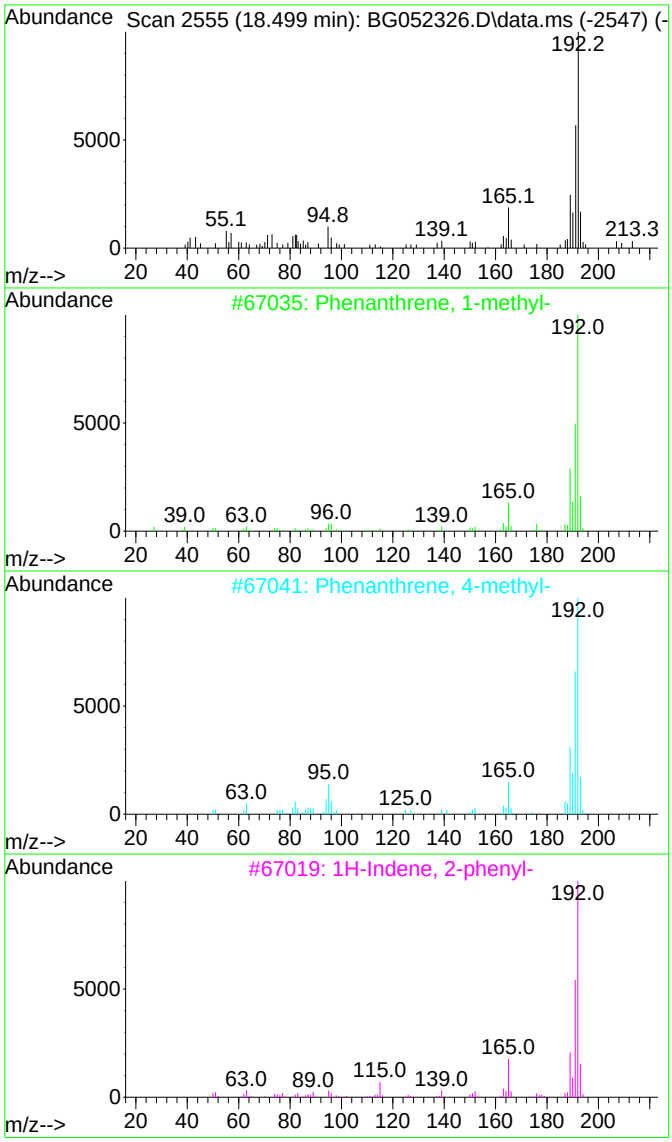
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

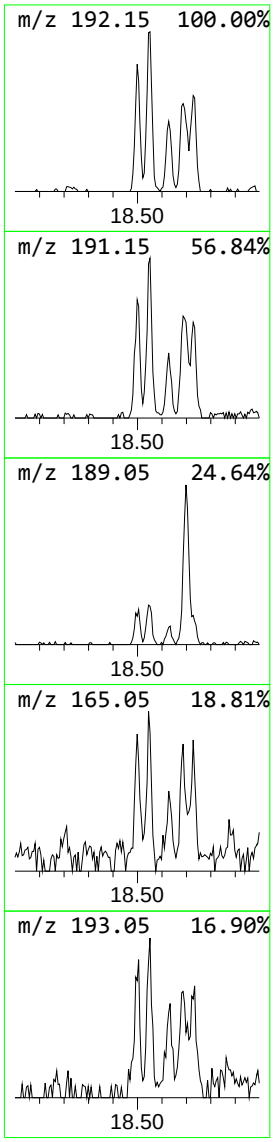
****

Peak Number 2 Phenanthrene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.499	2.67 ng	70784	Phenanthrene-d10	17.623

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	94
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	94
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052326.D
Acq On : 8 Feb 2022 19:28
Operator : CG/JU
Sample : N1401-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124055

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

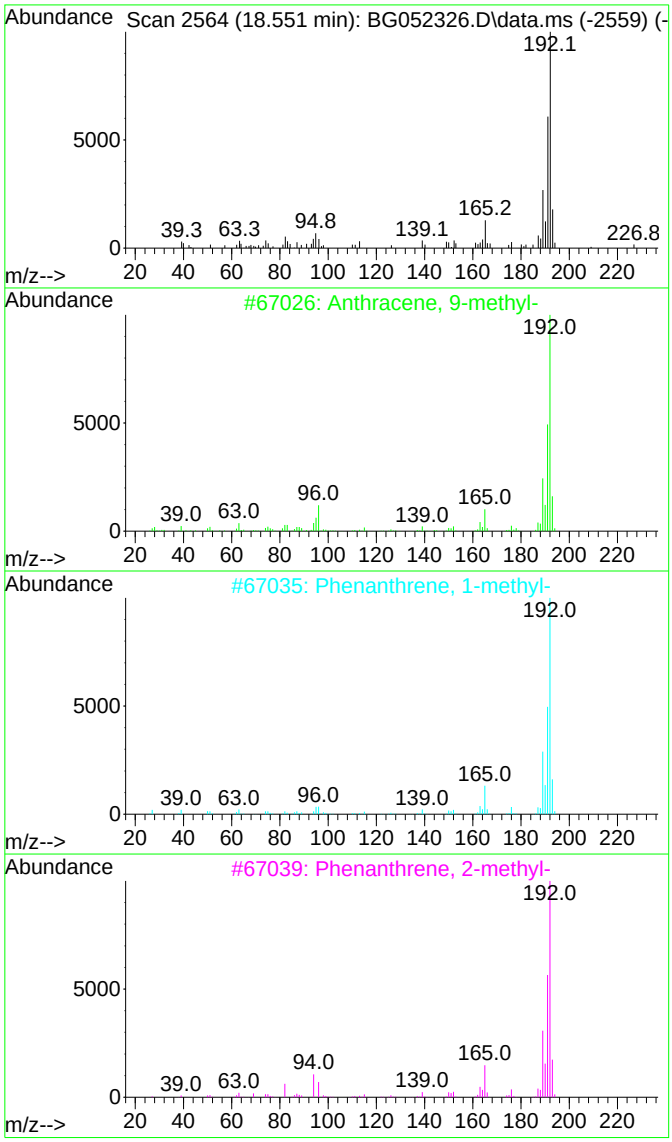
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

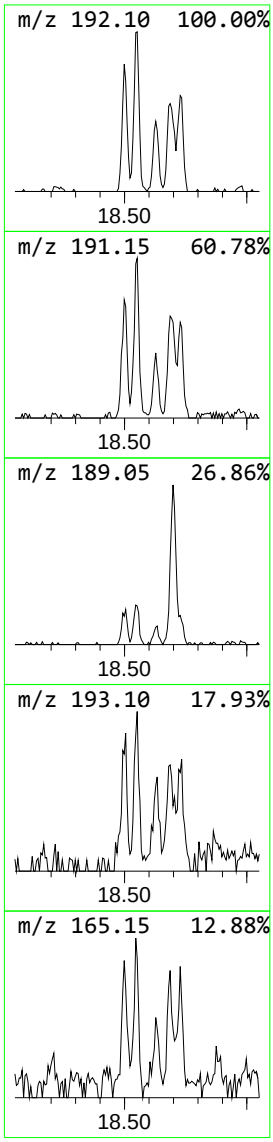
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.551	2.79 ng	74035	Phenanthrene-d10	17.623

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052326.D
Acq On : 8 Feb 2022 19:28
Operator : CG/JU
Sample : N1401-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124055

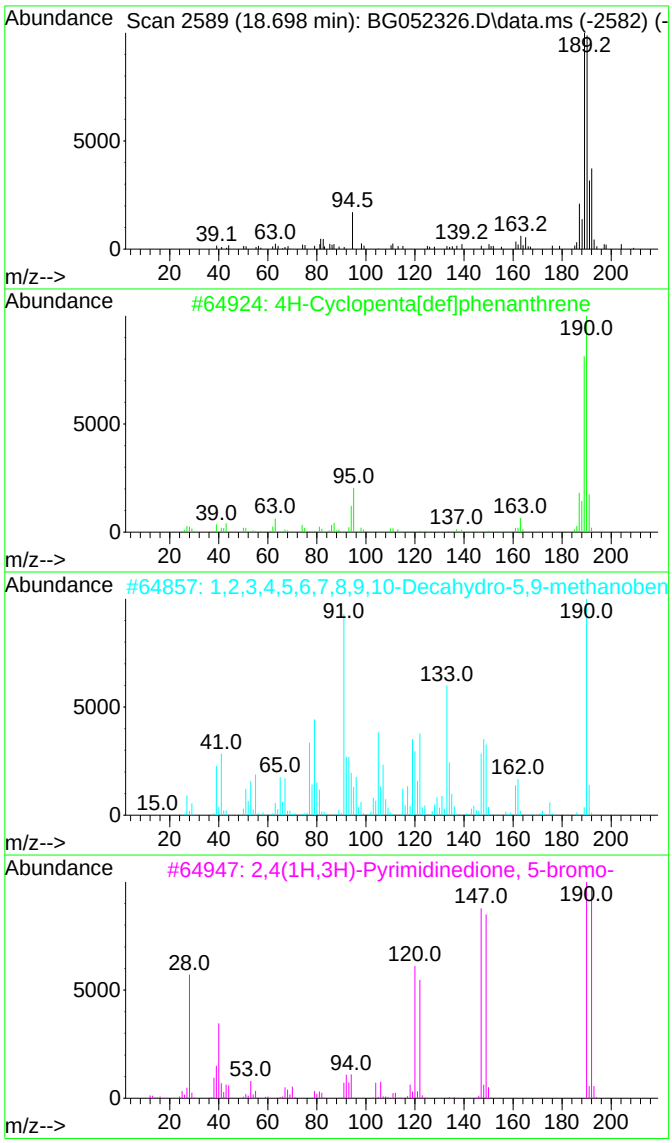
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

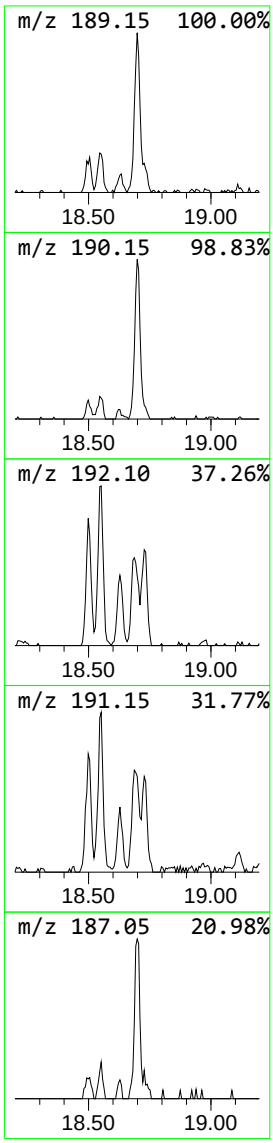
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.698	4.59 ng	121894	Phenanthrene-d10	17.623

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	89
2	1,2,3,4,5,6,7,8,9,10-Decahydro-5...	190	C13H18O	1000497-99-6	27
3	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25
4	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25
5	1-Aminocyclopentanecarboxylic ac...	445	C24H44ClNO4	1000329-17-5	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052326.D
Acq On : 8 Feb 2022 19:28
Operator : CG/JU
Sample : N1401-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124055

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

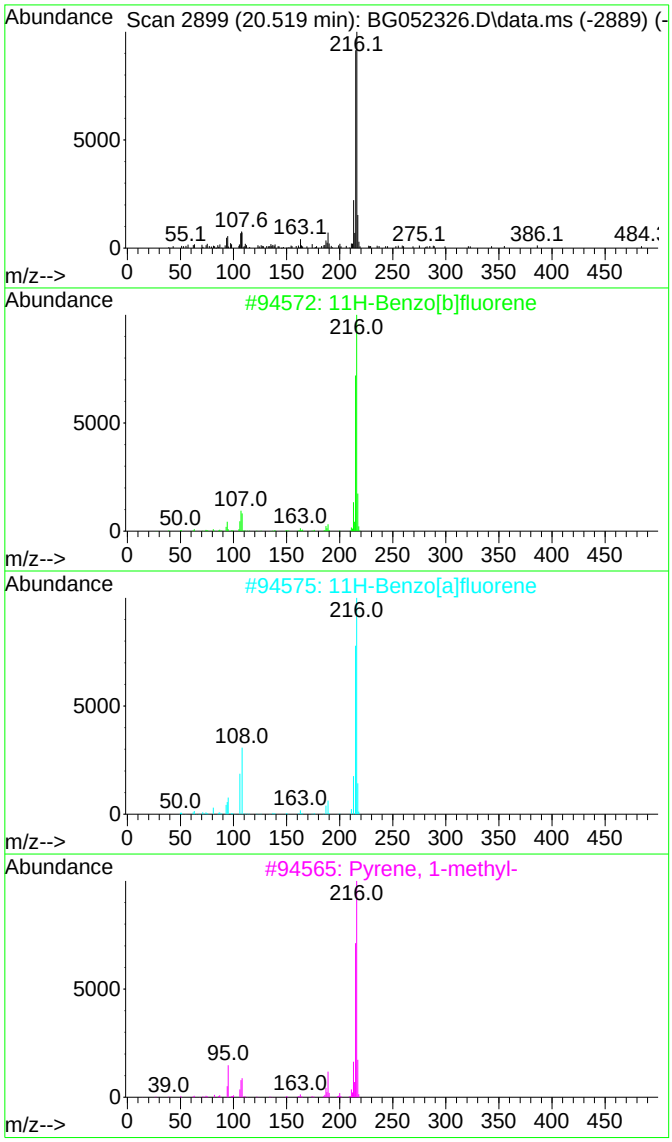
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

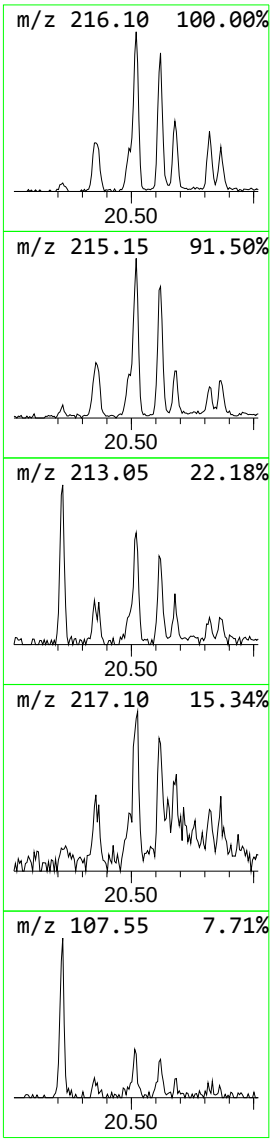
****

Peak Number 5 11H-Benzo[b]fluorene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.519	3.46 ng	128751	Chrysene-d12	21.941

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	86
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	72
5	Benzoic acid, 3-(3,5-dimethyl-1-...	216	C12H12N2O2	312531-88-7	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052326.D
Acq On : 8 Feb 2022 19:28
Operator : CG/JU
Sample : N1401-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124055

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

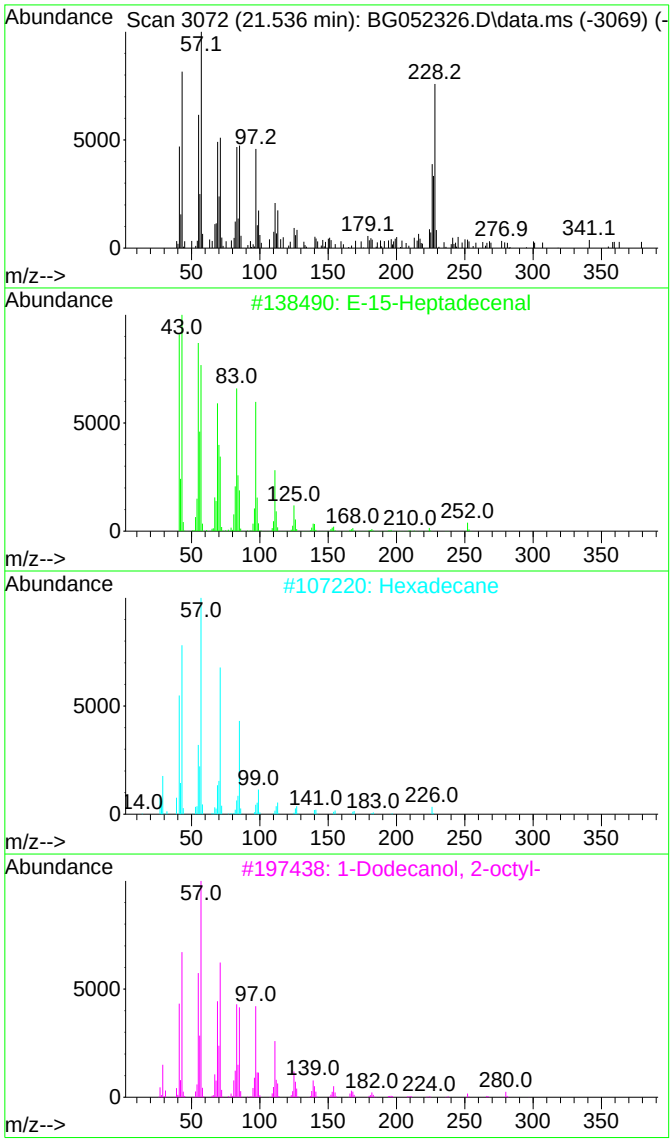
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

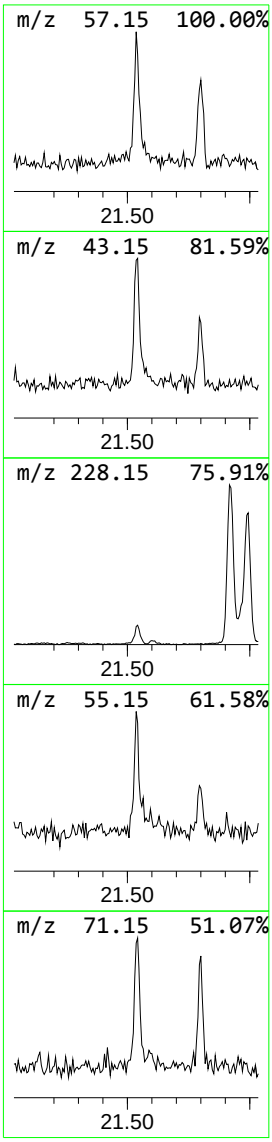
****

Peak Number 6 E-15-Heptadecenal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.536	2.52 ng	93688	Chrysene-d12	21.941

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	93
2	Hexadecane	226	C16H34	000544-76-3	74
3	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	55
4	Carbonic acid, decyl hexadecyl e...	426	C27H54O3	1000383-16-5	46
5	1-Heptacosanol	396	C27H56O	002004-39-9	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052326.D
Acq On : 8 Feb 2022 19:28
Operator : CG/JU
Sample : N1401-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124055

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.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-...	5.275	2.7	ng	29473	1	8.230	219402	20.0
Phenanthrene, 1...	18.499	2.7	ng	70784	4	17.623	530957	20.0
Anthracene, 9-m...	18.551	2.8	ng	74035	4	17.623	530957	20.0
4H-Cyclopenta[d...	18.698	4.6	ng	121894	4	17.623	530957	20.0
11H-Benzo[b]flu...	20.519	3.5	ng	128751	5	21.941	744773	20.0
E-15-Heptadecenal	21.536	2.5	ng	93688	5	21.941	744773	20.0