LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047234.D
Acq On : 16 Aug 2024 14:31
Operator : RC/JU
Sample : P3582-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-855-J-SO-4-4.5-081224

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_M\Methods\8270-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047234.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.269	61	65	74	rBV	71392	104208	2.19%	0.171%
2	4.575	282	287	293	rVB	120367	160226	3.37%	0.263%
3	5.016	356	362	374	rBV	1920565	2625956	55.25%	4.304%
4	6.575	620	627	642	rBV	1668445	2625041	55.23%	4.302%
5	7.363	754	761	772	rBV	1074886	1608068	33.83%	2.636%
6	8.510	948	956	964	rBV	1038781	1728181	36.36%	2.832%
7	10.116	1216	1229	1245	rBV	1243713	2020325	42.51%	3.311%
8	10.881	1353	1359	1370	rBV	87948	197415	4.15%	0.324%
9	12.628	1649	1656	1668	rBV	2313094	3382414	71.17%	5.544%
10	14.022	1886	1893	1899	rBV	1600724	2307896	48.56%	3.783%
11	14.086	1899	1904	1914	rVB	100913	173862	3.66%	0.285%
12	14.263	1927	1934	1935	rBV5	40584	66236	1.39%	0.109%
13	14.428	1958	1962	1967	rBV	32321	48902	1.03%	0.080%
14	14.492	1968	1973	1981	rBV6	31756	67871	1.43%	0.111%
15	15.080	2068	2073	2080	rVB2	90919	139455	2.93%	0.229%
16	15.380	2120	2124	2135	rVB	26447	53001	1.12%	0.087%
17	15.528	2143	2149	2160	rBV	1664864	2362469	49.71%	3.872%
18	16.233	2264	2269	2276	rVB7	34915	68258	1.44%	0.112%
19	16.539	2314	2321	2325	rBV3	78324	136048	2.86%	0.223%
20	16.598	2328	2331	2337	rVB	55077	83598	1.76%	0.137%
21	16.780	2357	2362	2366	rBV	1619363	2373136	49.93%	3.889%
22	16.827	2366	2370	2376	rVV	976359	1350867	28.42%	2.214%
23	16.916	2380	2385	2393	rVB	356444	492970	10.37%	0.808%
24	16.986	2393	2397	2404	rBV5	27879	57201	1.20%	0.094%
25	17.663	2507	2512	2516	rBV	97131	144255	3.04%	0.236%
26	17.721	2516	2522	2530	rVV2	1048362	1722594	36.24%	2.823%
27	17.786	2531	2533	2539	rVV2	138230	250833	5.28%	0.411%
28	17.857	2540	2545	2549	rVV	332006	563057	11.85%	0.923%
29	17.892	2549	2551	2557	rVB	84785	104009	2.19%	0.170%
30	18.174	2594	2599	2603	rBV	112834	159473	3.36%	0.261%
31	18.216	2603	2606	2610	rVB3	36136	47898	1.01%	0.079%
32	18.263	2610	2614	2618	rBV	84466	129109	2.72%	0.212%
33	18.421	2638	2641	2647	rVB3	34087	48547	1.02%	0.080%
34	18.598	2666	2671	2676	rBV2	70886	137726	2.90%	0.226%
35	18.663	2678	2682	2685	rBV2	45809	63494	1.34%	0.104%
36	18.739	2691	2695	2704	rBV2	74944	132009	2.78%	0.216%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047234.D
Acq On : 16 Aug 2024 14:31
Operator : RC/JU
Sample : P3582-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-855-J-SO-4-4.5-081224

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_M\Methods\8270-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.863	2710	2716	2721	rBV	3101230	4030429	84.80%	6.606%
38	19.021	2739	2743	2753	rBV	442306	786890	16.56%	1.290%
39	19.104	2754	2757	2763	rVB	93262	155635	3.27%	0.255%
40	19.227	2769	2778	2783	rBV	2501891	3981725	83.78%	6.526%
41	19.415	2806	2810	2812	rBV	148228	187410	3.94%	0.307%
42	19.451	2812	2816	2826	rVB	3058809	3747623	78.85%	6.142%
43	19.568	2830	2836	2842	rVV4	119018	286975	6.04%	0.470%
44	19.704	2854	2859	2860	rBV4	107493	157368	3.31%	0.258%
45	19.733	2860	2864	2869	rVB	418167	620754	13.06%	1.017%
46	19.839	2878	2882	2886	rBV2	415808	500779	10.54%	0.821%
47	19.892	2886	2891	2895	rBV2	198405	310287	6.53%	0.509%
48	20.033	2912	2915	2919	rVB	104896	118843	2.50%	0.195%
49	20.080	2919	2923	2927	rBV3	121739	185592	3.90%	0.304%
50	20.257	2950	2953	2956	rVB	107865	111500	2.35%	0.183%
51	20.657	3017	3021	3024	rBV	208064	278412	5.86%	0.456%
52	20.698	3025	3028	3030	rBV	179271	178957	3.77%	0.293%
53	20.733	3031	3034	3035	rBV	124612	141804	2.98%	0.232%
54	21.021	3076	3083	3087	rBV2	2381126	4752806	100.00%	7.790%
55	21.062	3087	3090	3102	rVB	1317237	1846585	38.85%	3.026%
56	21.192	3109	3112	3116	rVB	312260	373306	7.85%	0.612%
57	22.739	3369	3375	3387	rVB2	944968	1728708	36.37%	2.833%
58	22.880	3393	3399	3405	rBV	956287	2511050	52.83%	4.115%
59	23.474	3494	3500	3511	rVB	610390	1427875	30.04%	2.340%
60	23.592	3514	3520	3531	rVB	878156	2023554	42.58%	3.316%
61	23.721	3535	3542	3548	rBV	1275016	2833460	59.62%	4.644%

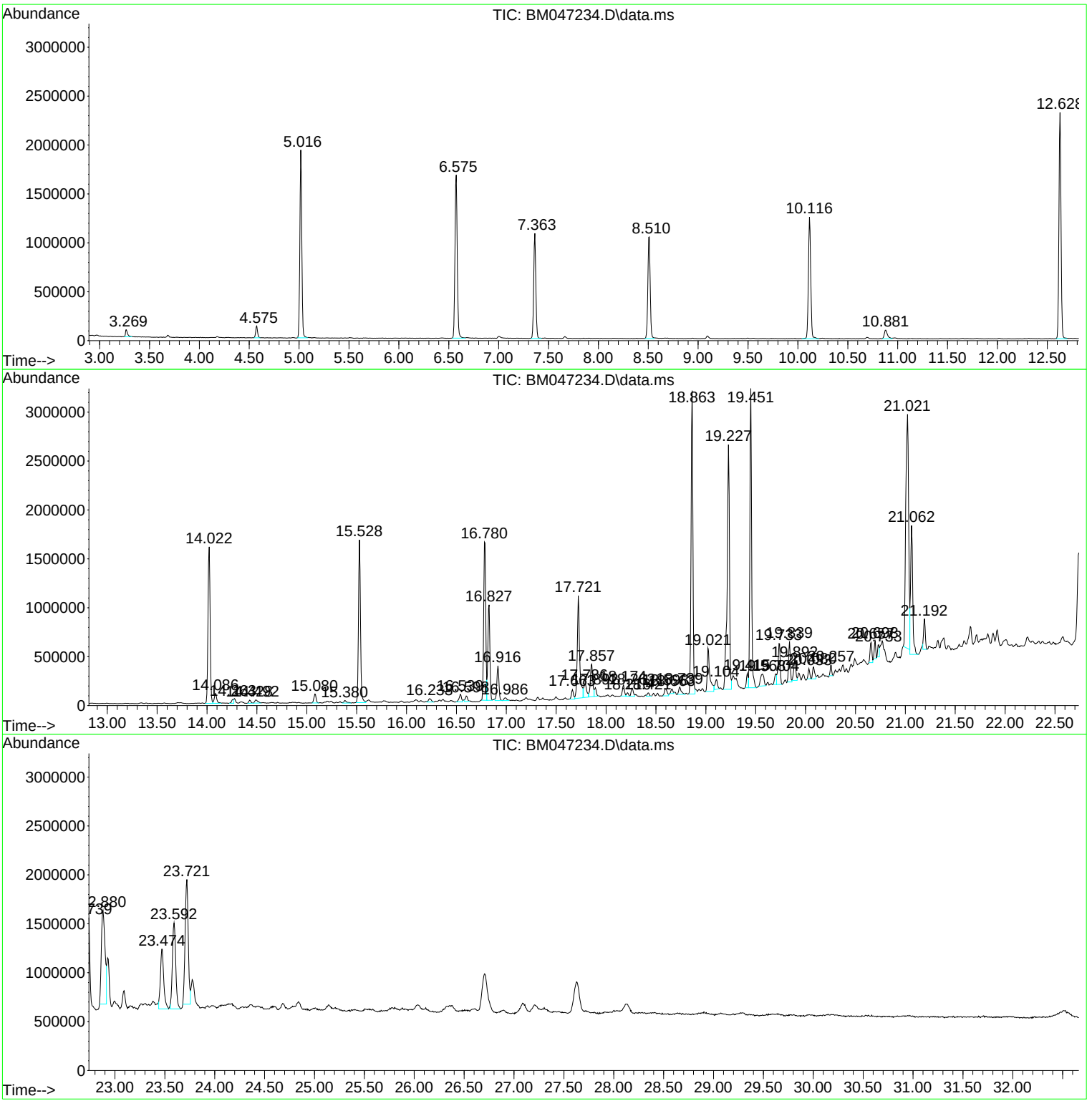
Sum of corrected areas: 61014935

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047234.D
Acq On : 16 Aug 2024 14:31
Operator : RC/JU
Sample : P3582-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-855-J-SO-4-4.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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_M\Data\BM081624\
Data File : BM047234.D
Acq On : 16 Aug 2024 14:31
Operator : RC/JU
Sample : P3582-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-855-J-SO-4-4.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

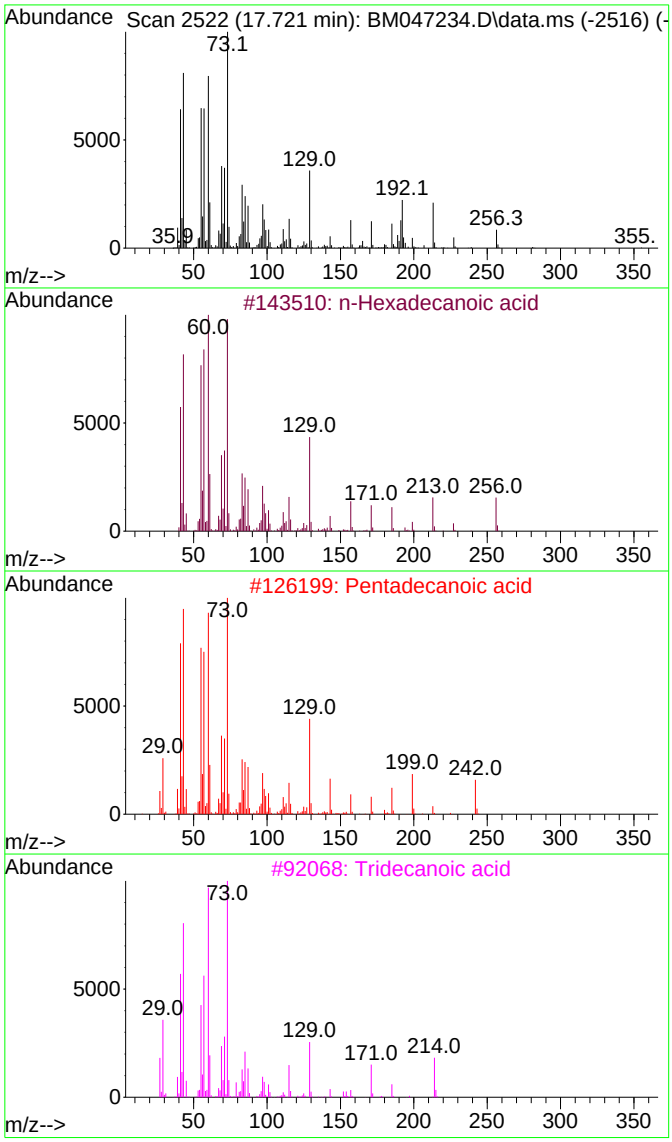
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

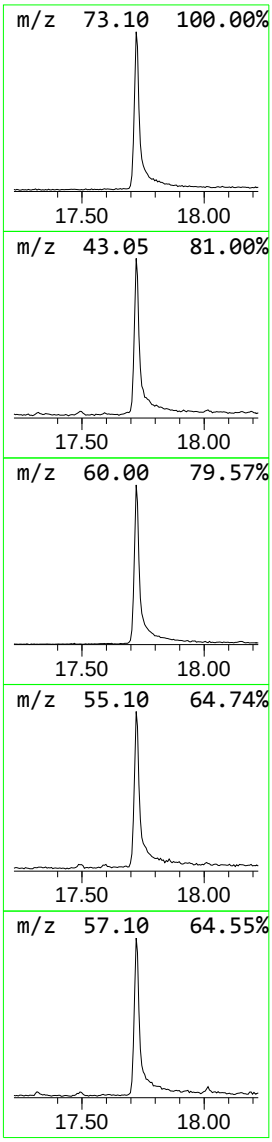
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.721	14.52 ng	1722590	Phenanthrene-d10	16.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047234.D
Acq On : 16 Aug 2024 14:31
Operator : RC/JU
Sample : P3582-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-855-J-SO-4-4.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

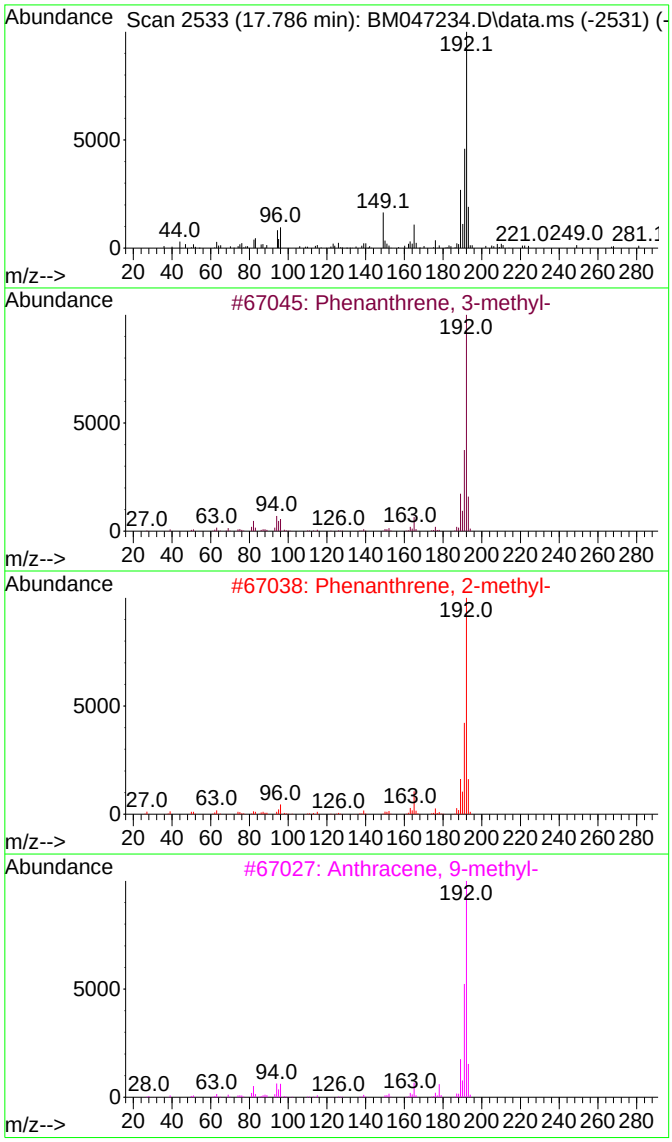
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

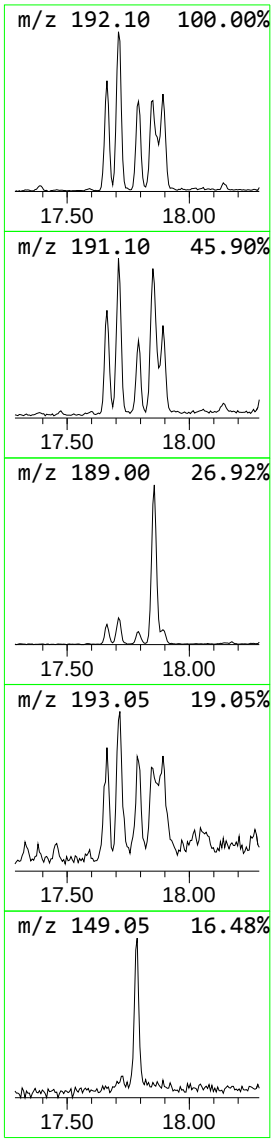
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.786	2.11 ng	250833	Phenanthrene-d10	16.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	93
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047234.D
Acq On : 16 Aug 2024 14:31
Operator : RC/JU
Sample : P3582-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-855-J-SO-4-4.5-081224

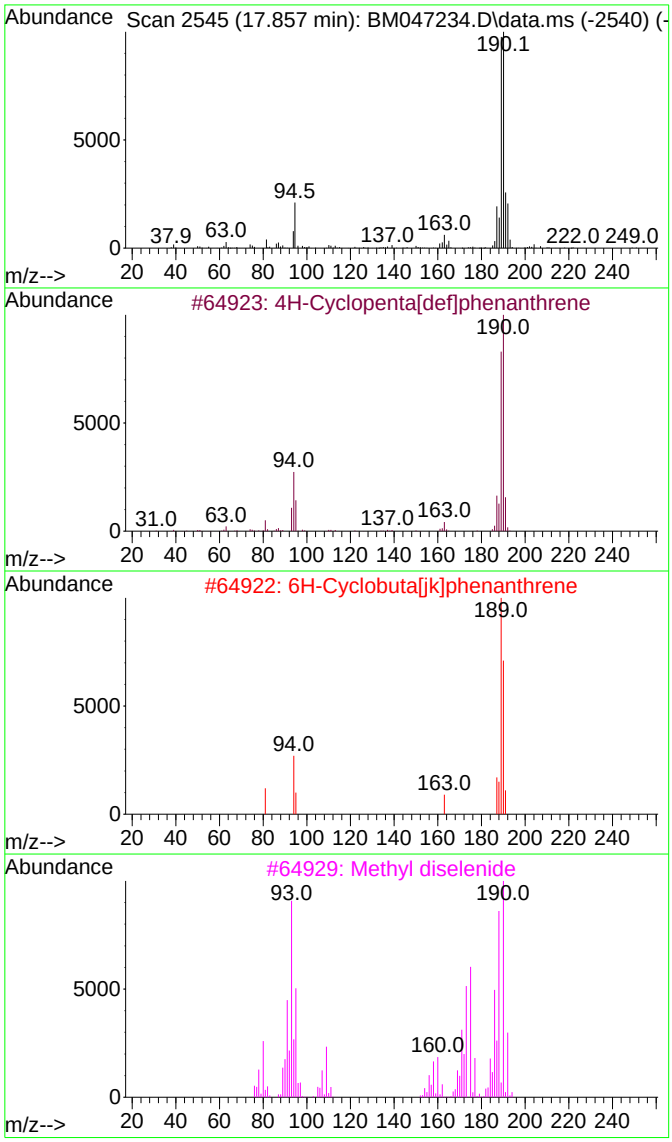
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

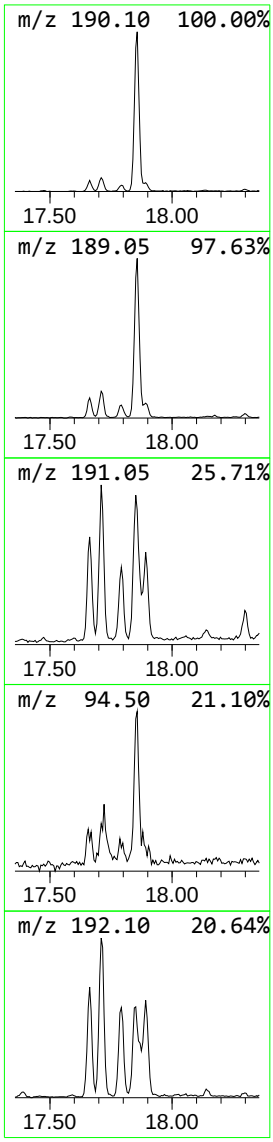
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.857	4.75 ng	563057	Phenanthrene-d10	16.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Methyl diselenide	190	C2H6Se2	007101-31-7	49
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047234.D
Acq On : 16 Aug 2024 14:31
Operator : RC/JU
Sample : P3582-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-855-J-SO-4-4.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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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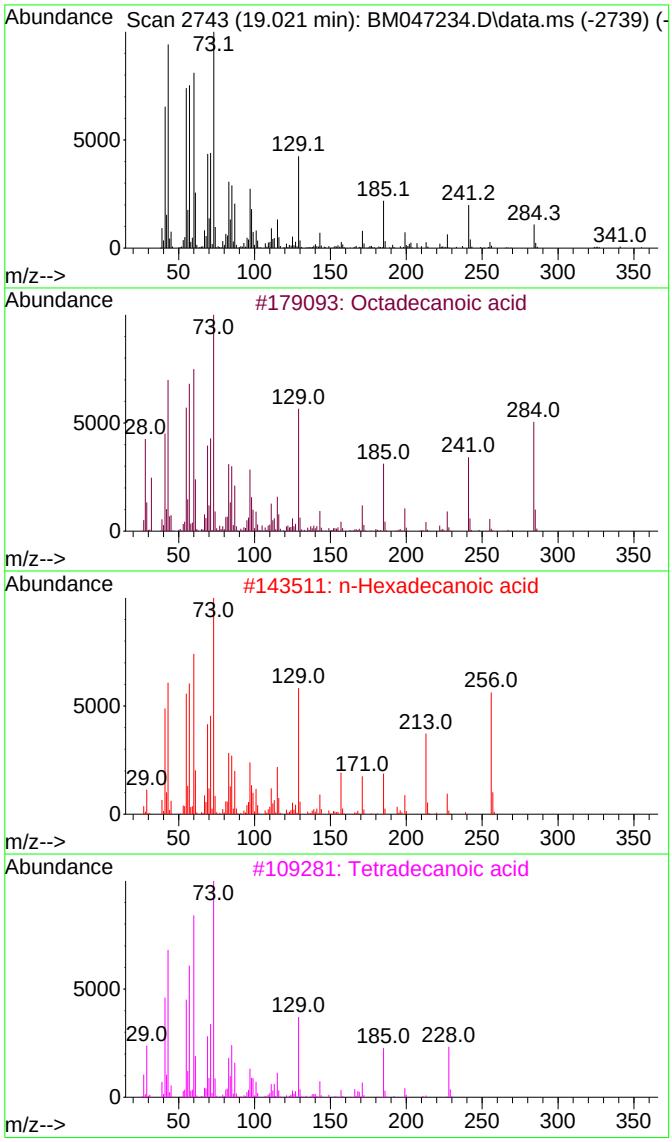
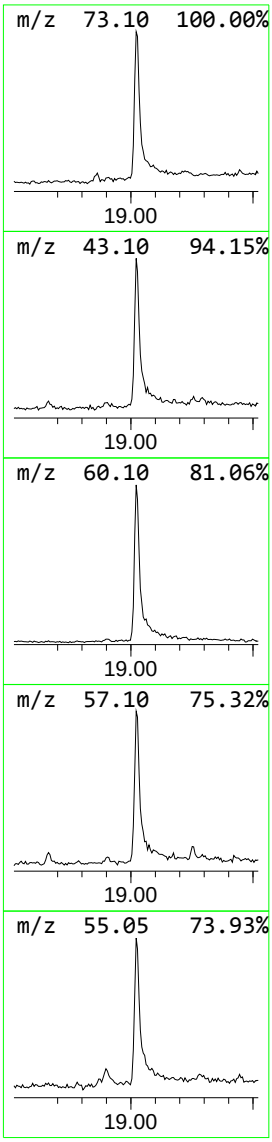
Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.021	3.31 ng	786890	Chrysene-d12	21.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047234.D
Acq On : 16 Aug 2024 14:31
Operator : RC/JU
Sample : P3582-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-855-J-SO-4-4.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

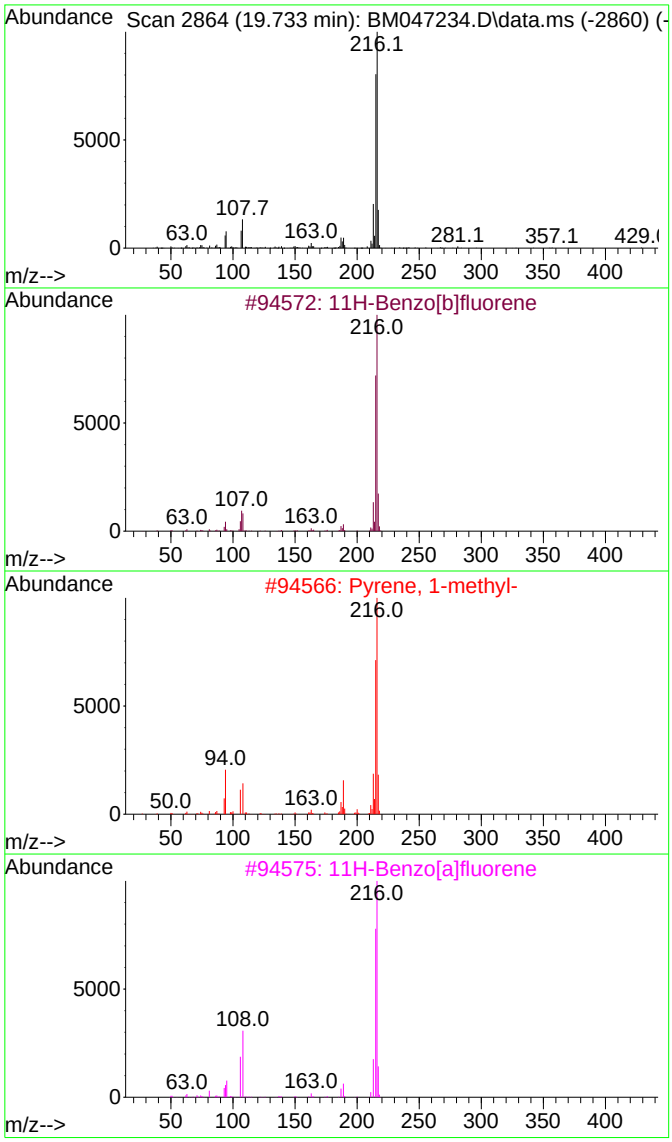
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

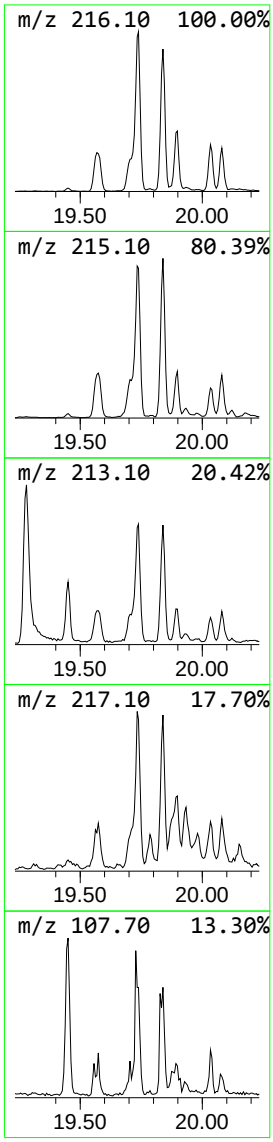
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.733	2.61 ng	620754	Chrysene-d12	21.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	95
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	89
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047234.D
Acq On : 16 Aug 2024 14:31
Operator : RC/JU
Sample : P3582-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-855-J-SO-4-4.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

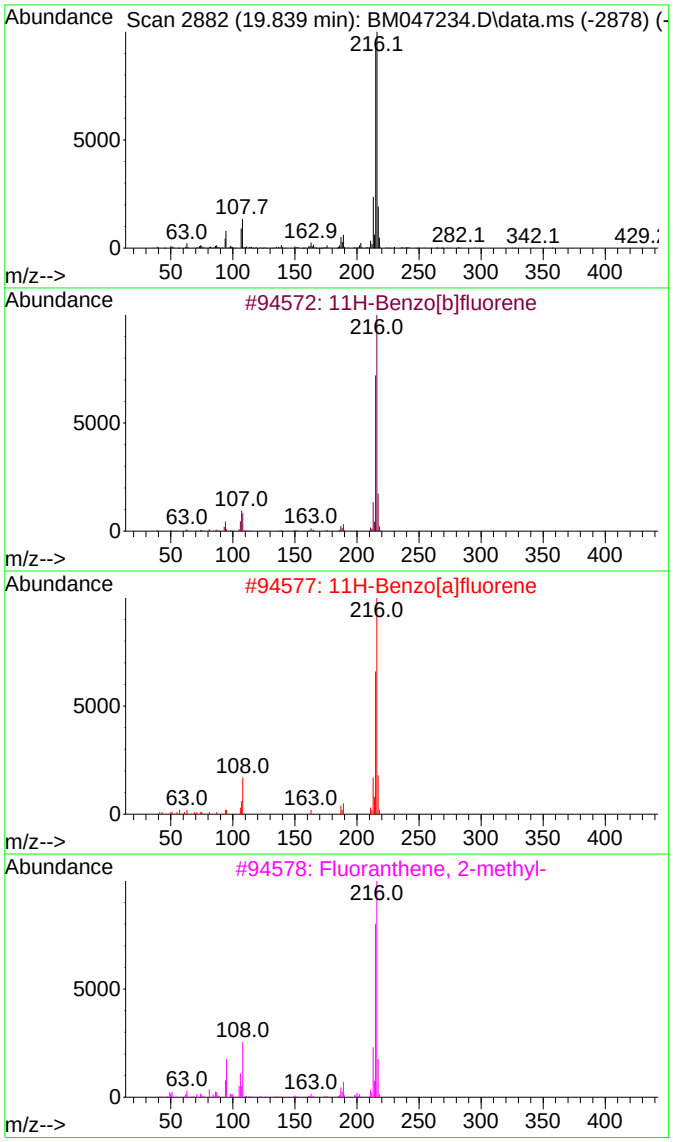
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

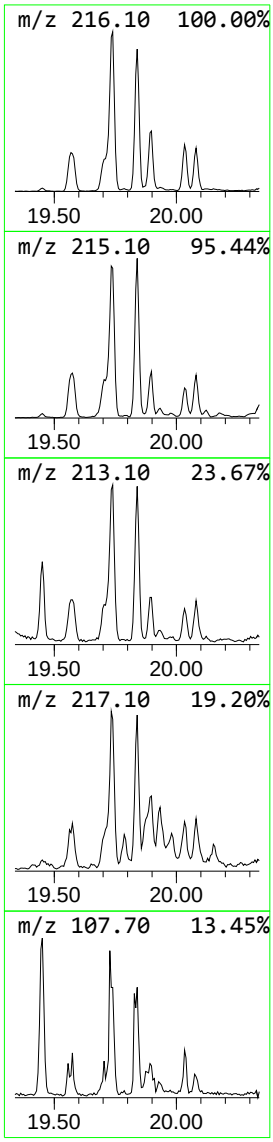
****

Peak Number 6 11H-Benzo[a]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.839	2.11 ng	500779	Chrysene-d12	21.021

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	92
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	76
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047234.D
Acq On : 16 Aug 2024 14:31
Operator : RC/JU
Sample : P3582-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-855-J-SO-4-4.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

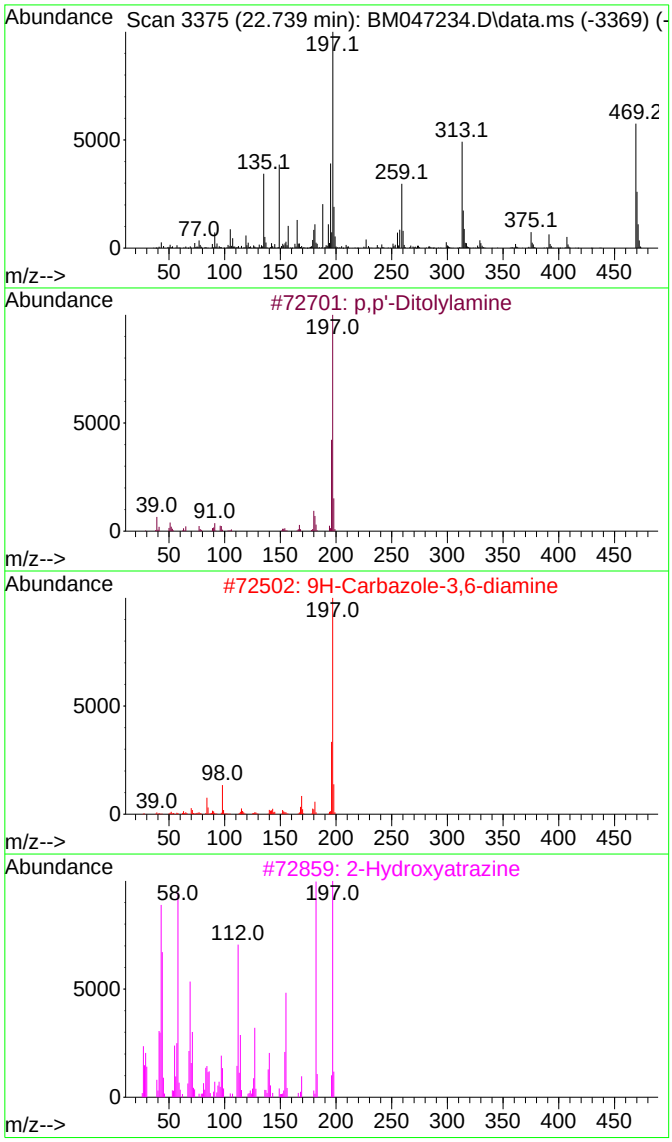
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

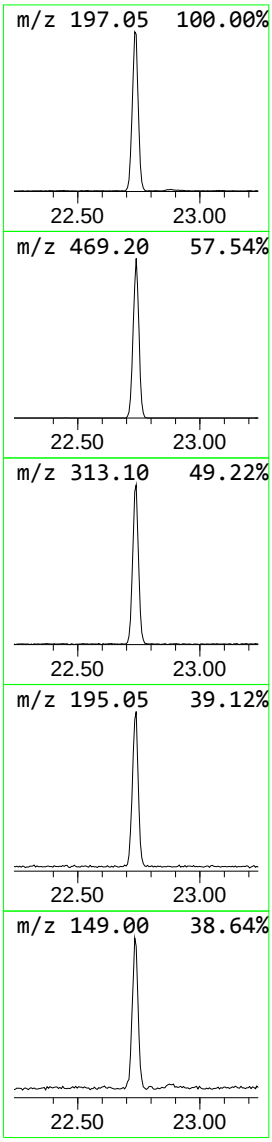
****

Peak Number 7 unknown22.739 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.739	12.20 ng	1728710	Perylene-d12	23.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p,p'-Ditolylamine	197	C14H15N	000620-93-9	18
2	9H-Carbazole-3,6-diamine	197	C12H11N3	000086-71-5	18
3	2-Hydroxyatrazine	197	C8H15N5O	002163-68-0	15
4	Glutaric acid, monoamide, N,N-di...	353	C22H27NO3	1000360-23-0	14
5	Benzene, 1,1',1''-[1-(bromomethy...	394	C23H23BrO	055373-93-8	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047234.D
Acq On : 16 Aug 2024 14:31
Operator : RC/JU
Sample : P3582-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-855-J-SO-4-4.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

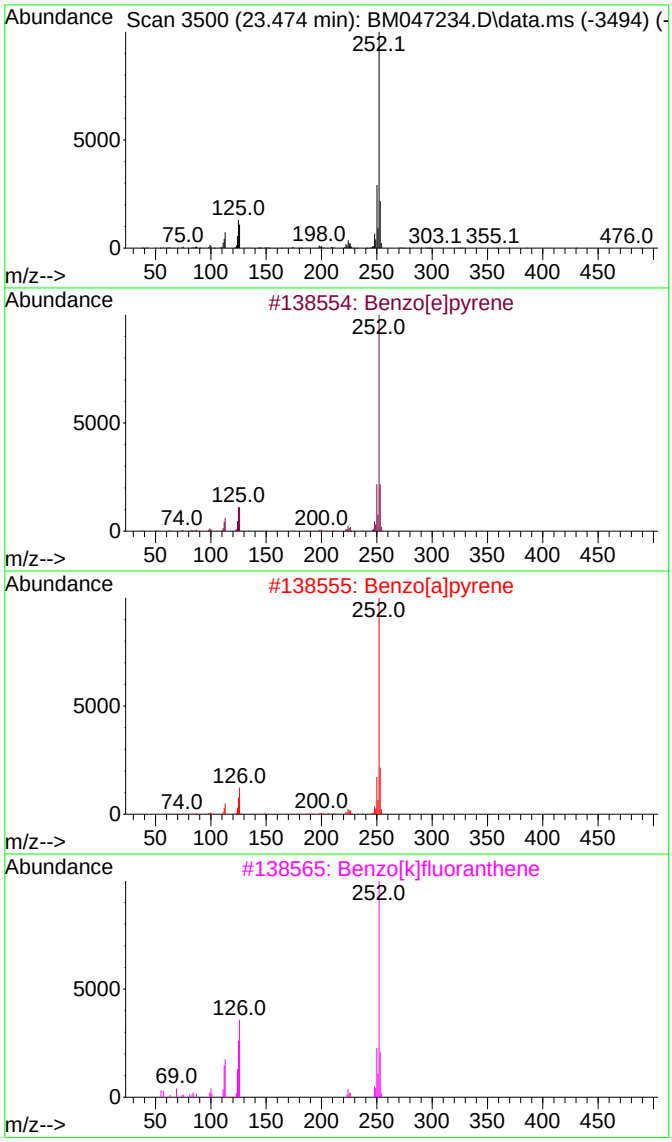
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

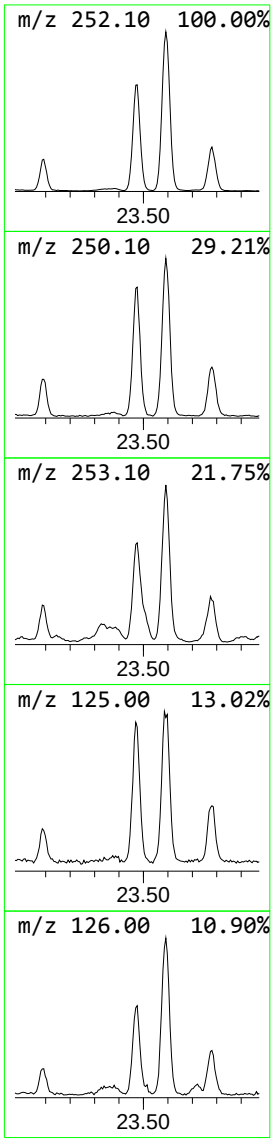
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.474	10.08 ng	1427880	Perylene-d12	23.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[a]pyrene	252	C20H12	000050-32-8	97
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4	Perylene	252	C20H12	000198-55-0	94
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047234.D
Acq On : 16 Aug 2024 14:31
Operator : RC/JU
Sample : P3582-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-855-J-SO-4-4.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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
n-Hexadecanoic ...	17.721	14.5	ng	1722590	4	16.786	2373140	20.0
Phenanthrene, 3...	17.786	2.1	ng	250833	4	16.786	2373140	20.0
4H-Cyclopenta[d...	17.857	4.8	ng	563057	4	16.786	2373140	20.0
Octadecanoic acid	19.021	3.3	ng	786890	5	21.021	4752810	20.0
11H-Benzo[b]flu...	19.733	2.6	ng	620754	5	21.021	4752810	20.0
11H-Benzo[a]flu...	19.839	2.1	ng	500779	5	21.021	4752810	20.0
unknown22.739	22.739	12.2	ng	1728710	6	23.721	2833460	20.0
Benzo[e]pyrene	23.474	10.1	ng	1427880	6	23.721	2833460	20.0