LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022421\
Data File : BM028886.D
Acq On : 24 Feb 2021 19:22
Operator : CG/JU
Sample : M1460-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : HD-01-022221

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-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028886.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.357	397	403	413	rBB	206027	290305	39.16%	5.919%
2	6.993	674	681	692	rBB	200290	318312	42.94%	6.490%
3	7.804	813	819	825	rBB	52222	77895	10.51%	1.588%
4	8.981	1012	1019	1028	rBB	121548	193942	26.16%	3.954%
5	10.604	1289	1295	1302	rVB	75062	119205	16.08%	2.431%
6	13.080	1710	1716	1723	rBB	319742	442728	59.72%	9.027%
7	13.927	1854	1860	1864	rBB2	5616	7742	1.04%	0.158%
8	14.351	1923	1932	1936	rVB2	7032	13078	1.76%	0.267%
9	14.463	1946	1951	1957	rVB	119978	169865	22.91%	3.463%
10	15.304	2090	2094	2098	rVB	6148	7935	1.07%	0.162%
11	15.957	2200	2205	2211	rBV	277314	376767	50.82%	7.682%
12	16.163	2235	2240	2248	rBV2	6679	10851	1.46%	0.221%
13	16.951	2368	2374	2378	rBV3	6247	7854	1.06%	0.160%
14	17.209	2412	2418	2422	rBV	152371	213384	28.78%	4.351%
15	17.251	2422	2425	2430	rVV	43076	53651	7.24%	1.094%
16	17.339	2433	2440	2445	rVB	13135	18139	2.45%	0.370%
17	17.868	2525	2530	2535	rVB	38850	43133	5.82%	0.879%
18	18.092	2561	2568	2571	rBV2	18174	30859	4.16%	0.629%
19	18.127	2571	2574	2578	rVB	10496	13736	1.85%	0.280%
20	18.274	2593	2599	2603	rBV3	14602	25820	3.48%	0.526%
21	18.580	2646	2651	2655	rVB	5194	7761	1.05%	0.158%
22	18.839	2689	2695	2699	rBV	11678	16895	2.28%	0.344%
23	19.009	2718	2724	2726	rBV	122943	152817	20.61%	3.116%
24	19.039	2726	2729	2740	rVB2	105276	140718	18.98%	2.869%
25	19.174	2748	2752	2755	rVB2	15194	17965	2.42%	0.366%
26	19.256	2758	2766	2771	rBV	140456	186044	25.09%	3.793%
27	19.592	2818	2823	2824	rBV3	26190	33126	4.47%	0.675%
28	19.621	2824	2828	2836	rVB	118898	158010	21.31%	3.222%
29	19.692	2836	2840	2845	rBV2	5416	8530	1.15%	0.174%
30	19.821	2854	2862	2867	rBV	607213	741359	100.00%	15.116%
31	19.939	2878	2882	2883	rBV	6445	8264	1.11%	0.168%
32	20.115	2901	2912	2917	rBV	27593	52679	7.11%	1.074%
33	20.209	2924	2928	2932	rBV	20597	25186	3.40%	0.514%
34	20.268	2933	2938	2942	rVV3	11354	18782	2.53%	0.383%
35	20.409	2959	2962	2966	rBV2	5948	8554	1.15%	0.174%
36	20.450	2966	2969	2973	rVV	6059	8647	1.17%	0.176%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022421\
Data File : BM028886.D
Acq On : 24 Feb 2021 19:22
Operator : CG/JU
Sample : M1460-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : HD-01-022221

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-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.609	2993	2996	3001	rBV3	7393	8940	1.21%	0.182%
38	20.856	3036	3038	3044	rVB2	6504	7489	1.01%	0.153%
39	21.021	3062	3066	3068	rBV	13059	16677	2.25%	0.340%
40	21.074	3070	3075	3079	rVV2	36607	53582	7.23%	1.093%
41	21.368	3118	3125	3129	rBV2	215380	356032	48.02%	7.259%
42	21.403	3129	3131	3136	rVB	66403	73547	9.92%	1.500%
43	22.921	3385	3389	3394	rBV	39074	78670	10.61%	1.604%
44	23.391	3466	3469	3474	rVB	20169	29575	3.99%	0.603%
45	23.486	3481	3485	3492	rVB	39415	70060	9.45%	1.428%
46	23.586	3496	3502	3507	rBV2	105001	189417	25.55%	3.862%

Sum of corrected areas: 4904527

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022421\
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Acq On : 24 Feb 2021 19:22
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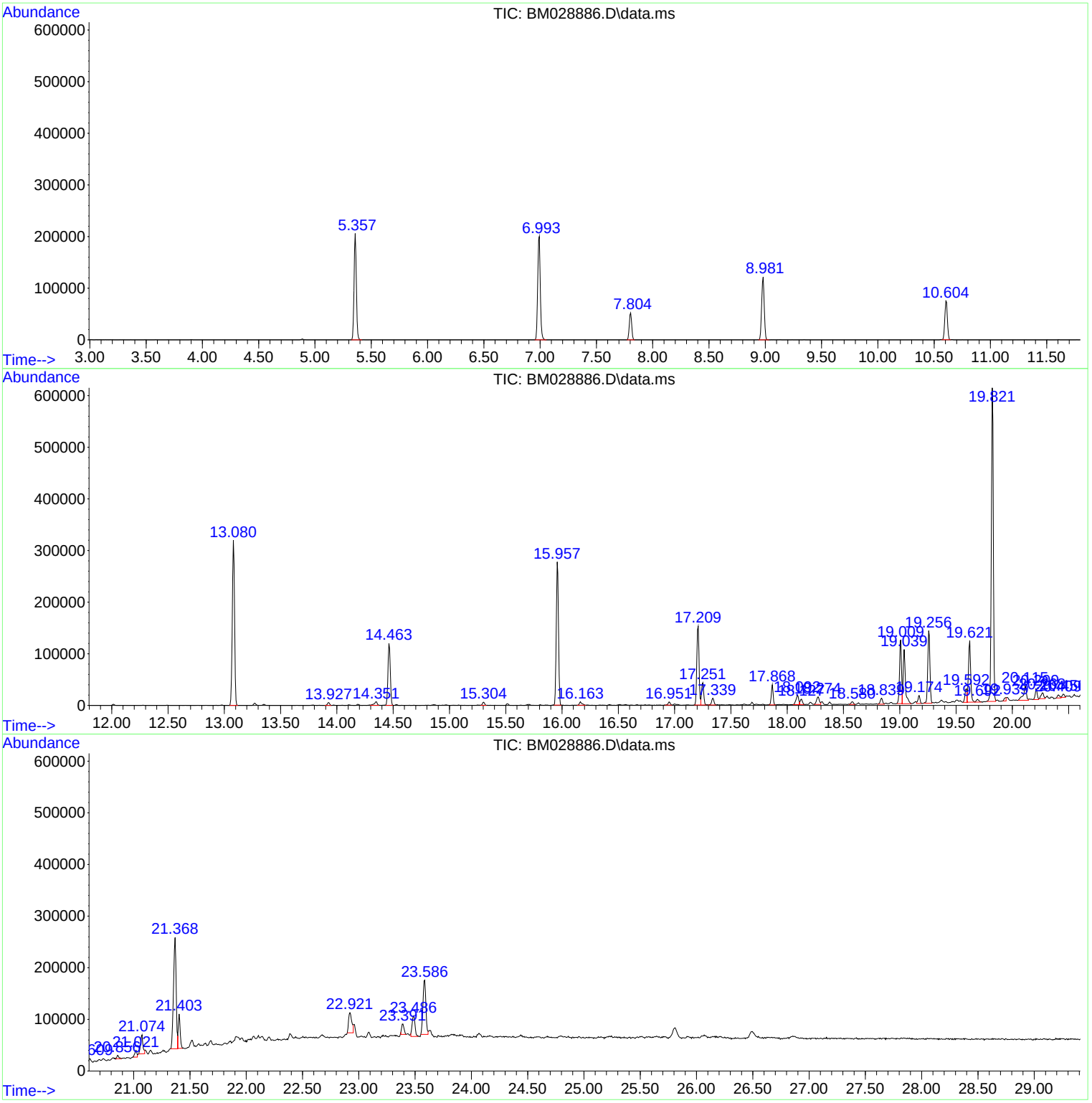
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HD-01-022221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.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_M\Data\BM022421\
Data File : BM028886.D
Acq On : 24 Feb 2021 19:22
Operator : CG/JU
Sample : M1460-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HD-01-022221

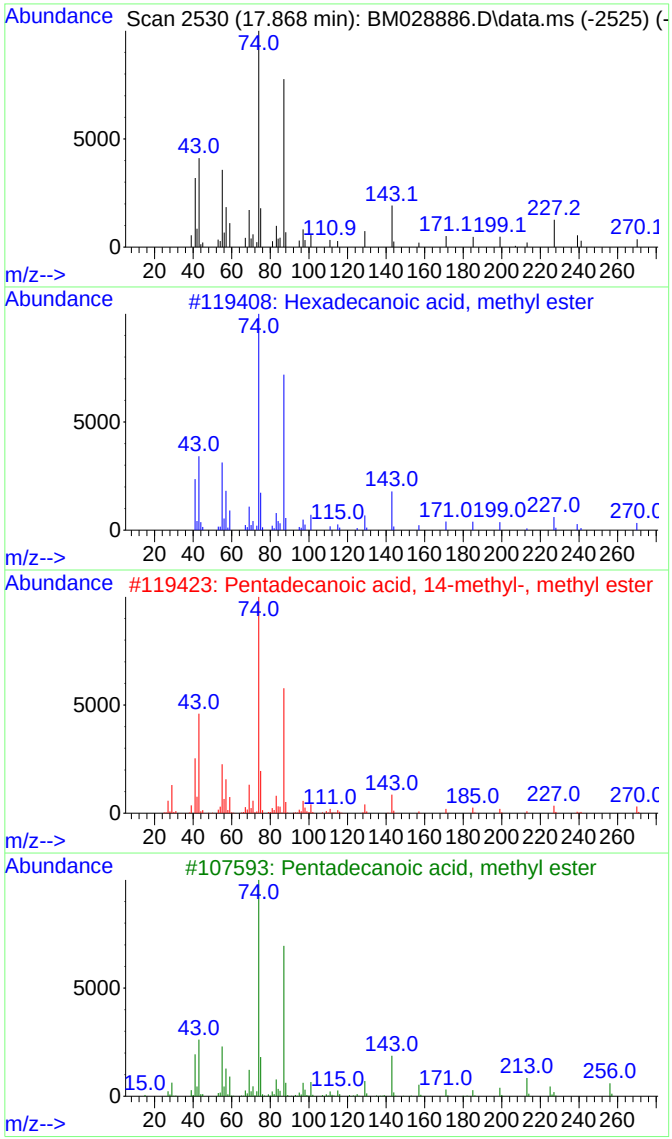
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

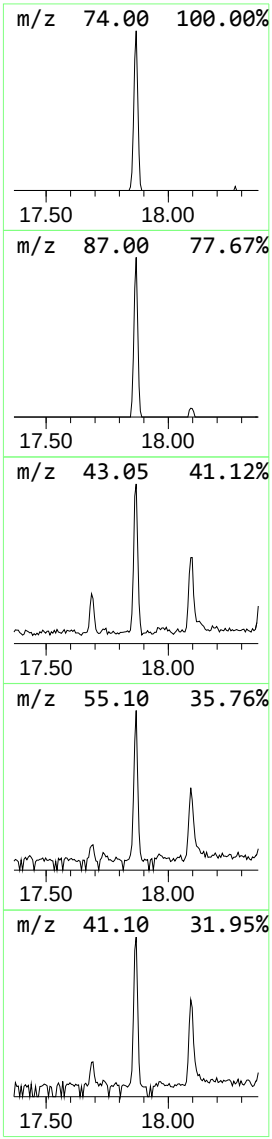
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.868	4.04 ng	43133	Phenanthrene-d10	17.209

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80
5	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022421\
Data File : BM028886.D
Acq On : 24 Feb 2021 19:22
Operator : CG/JU
Sample : M1460-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : HD-01-022221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

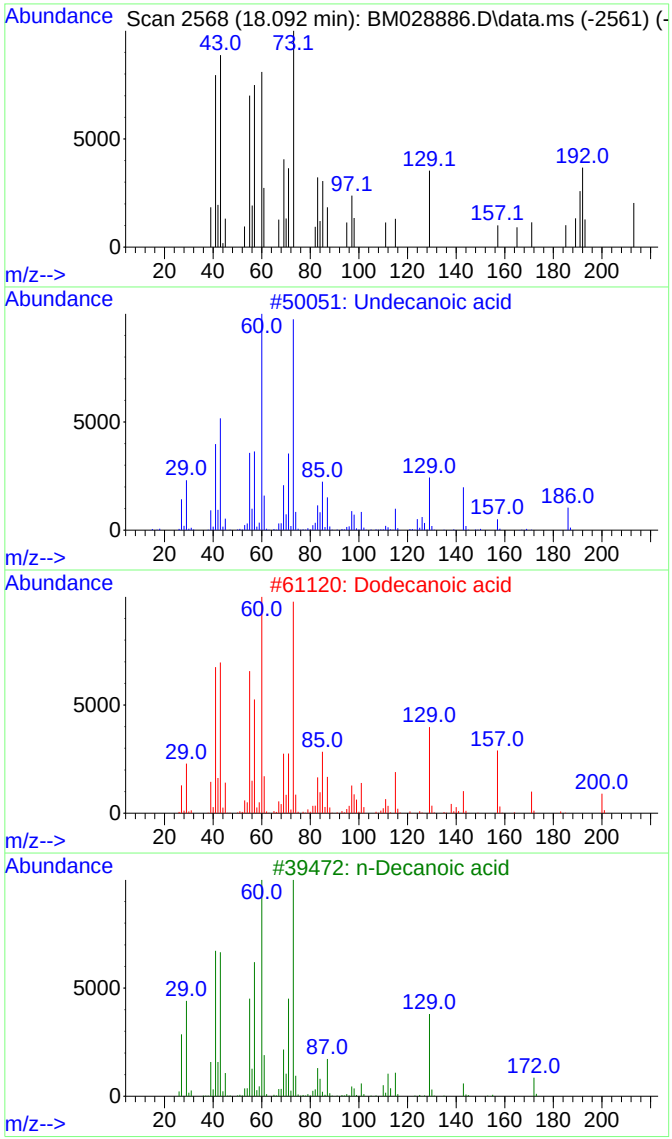
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

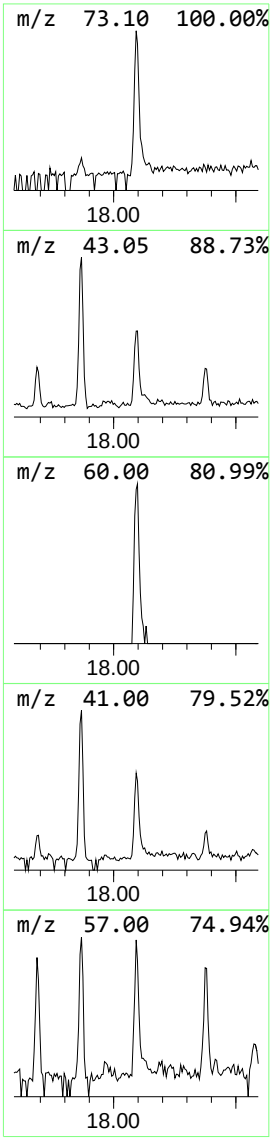
****

Peak Number 2 unknown18.092 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	2.89 ng	30859	Phenanthrene-d10	17.209

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	43
2	Dodecanoic acid	200	C12H24O2	000143-07-7	38
3	n-Decanoic acid	172	C10H20O2	000334-48-5	38
4	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	38
5	Maltose	342	C12H22O11	000069-79-4	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022421\
Data File : BM028886.D
Acq On : 24 Feb 2021 19:22
Operator : CG/JU
Sample : M1460-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : HD-01-022221

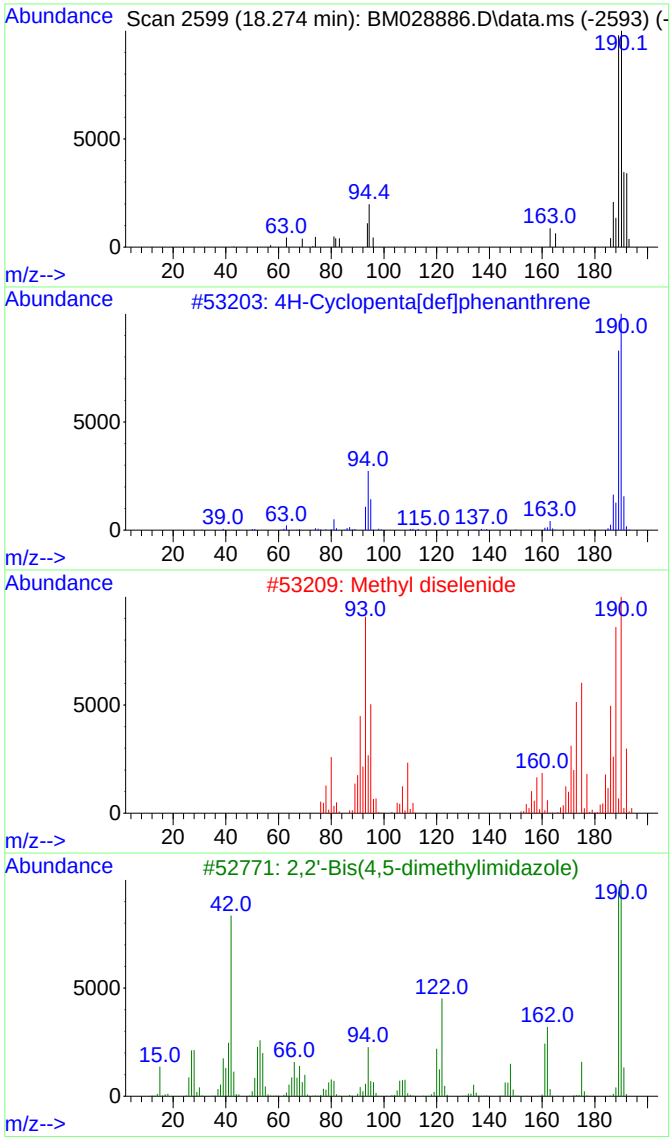
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

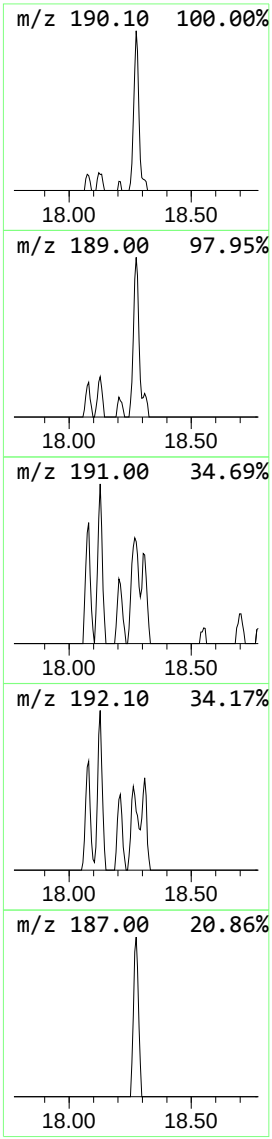
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.274	2.42 ng	25820	Phenanthrene-d10	17.209

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	Methyl diselenide	190	C2H6Se2	007101-31-7	49
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	33
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022421\
Data File : BM028886.D
Acq On : 24 Feb 2021 19:22
Operator : CG/JU
Sample : M1460-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : HD-01-022221

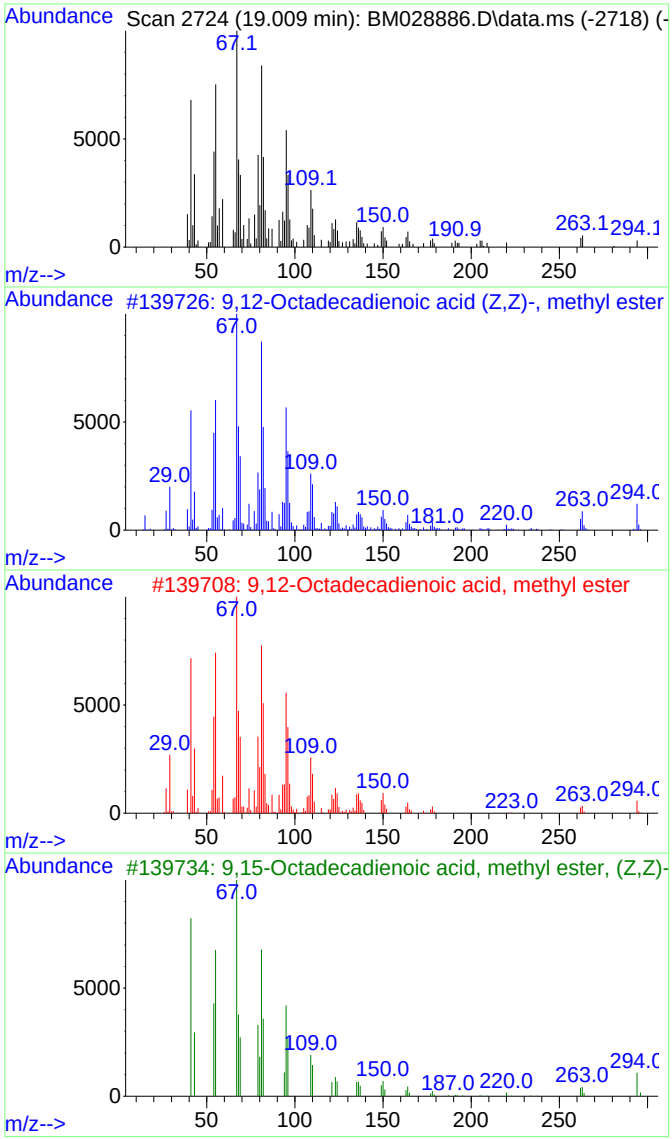
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

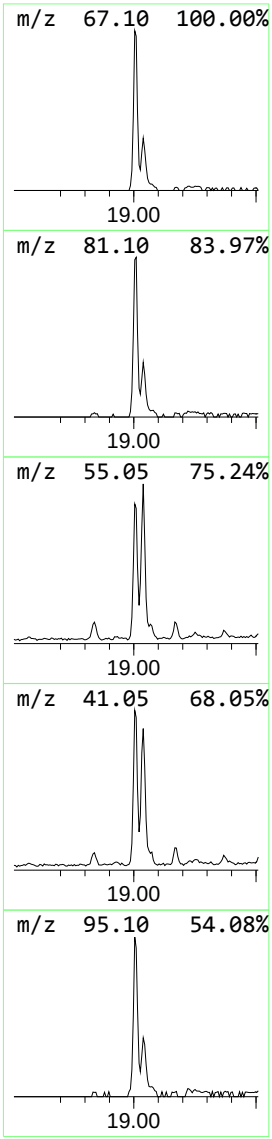
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.009	14.32 ng	152817	Phenanthrene-d10	17.209

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022421\
Data File : BM028886.D
Acq On : 24 Feb 2021 19:22
Operator : CG/JU
Sample : M1460-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : HD-01-022221

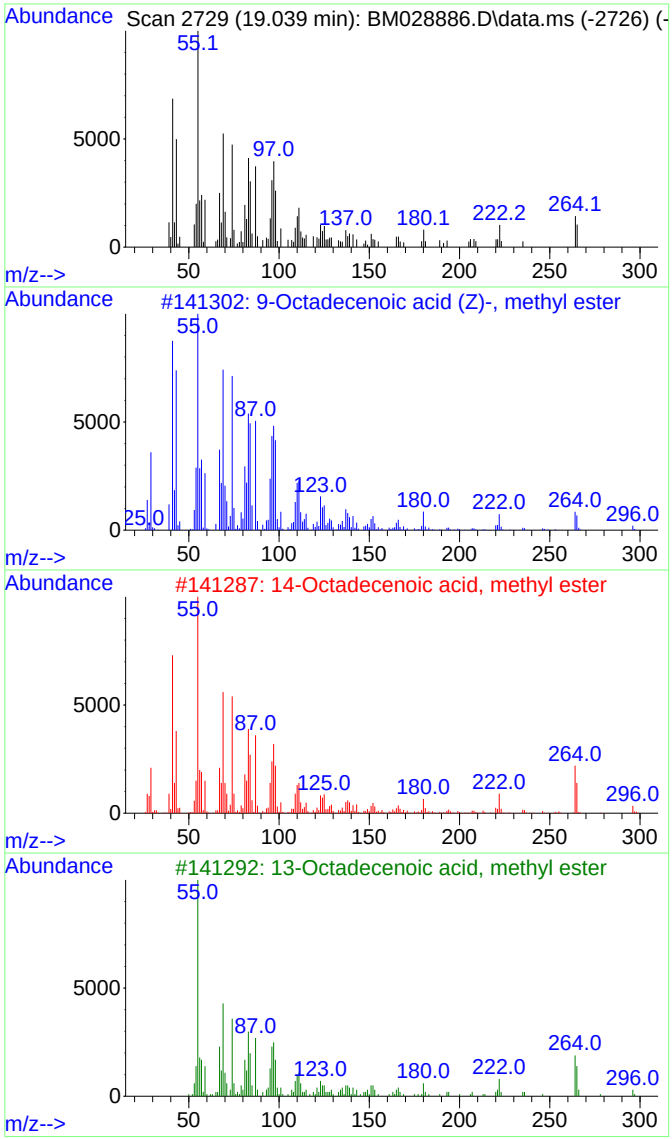
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

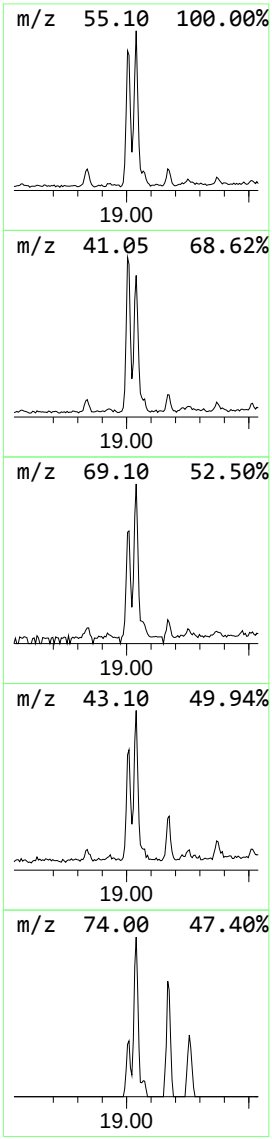
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.039	13.19 ng	140718	Phenanthrene-d10	17.209

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	90
5	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	87





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Sample : M1460-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : HD-01-022221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

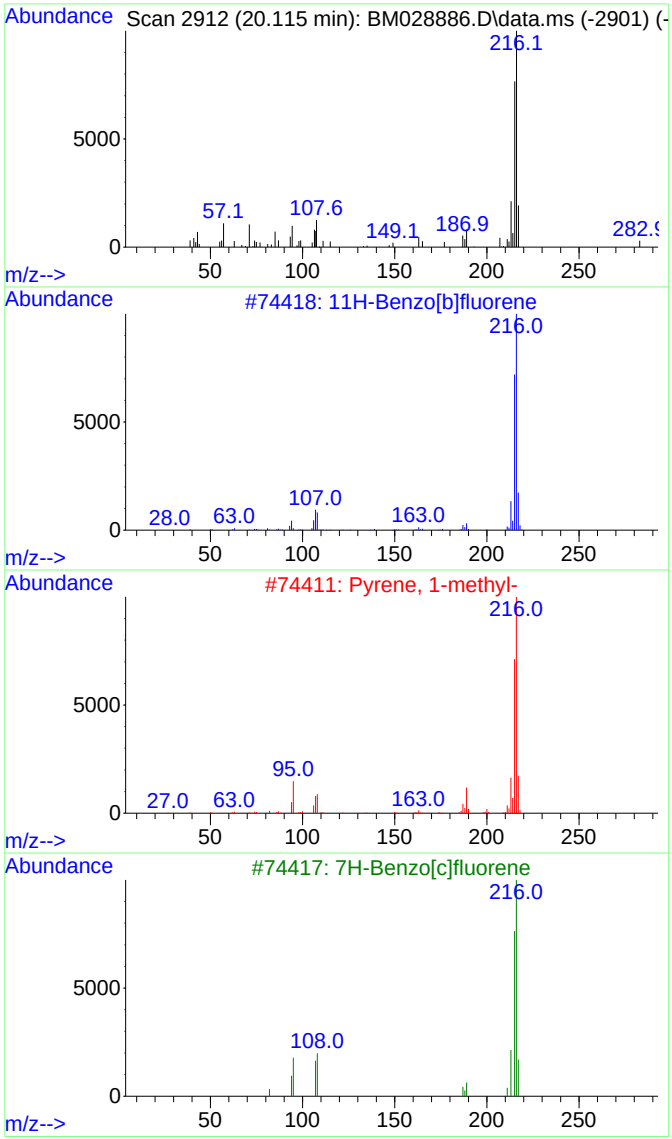
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

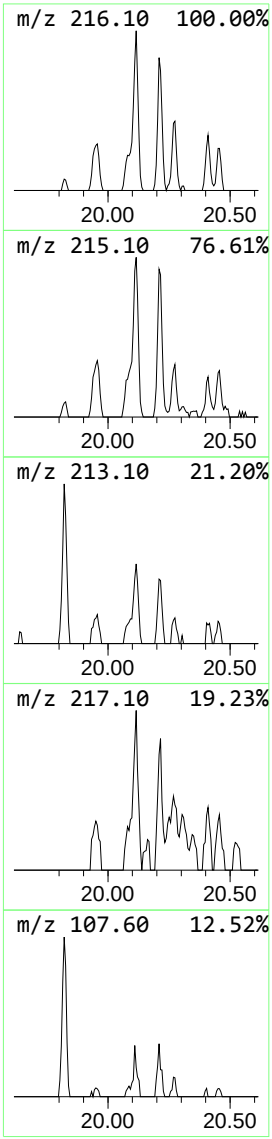
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.115	2.96 ng	52679	Chrysene-d12	21.368

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	90
3	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81





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Operator : CG/JU
Sample : M1460-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : HD-01-022221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

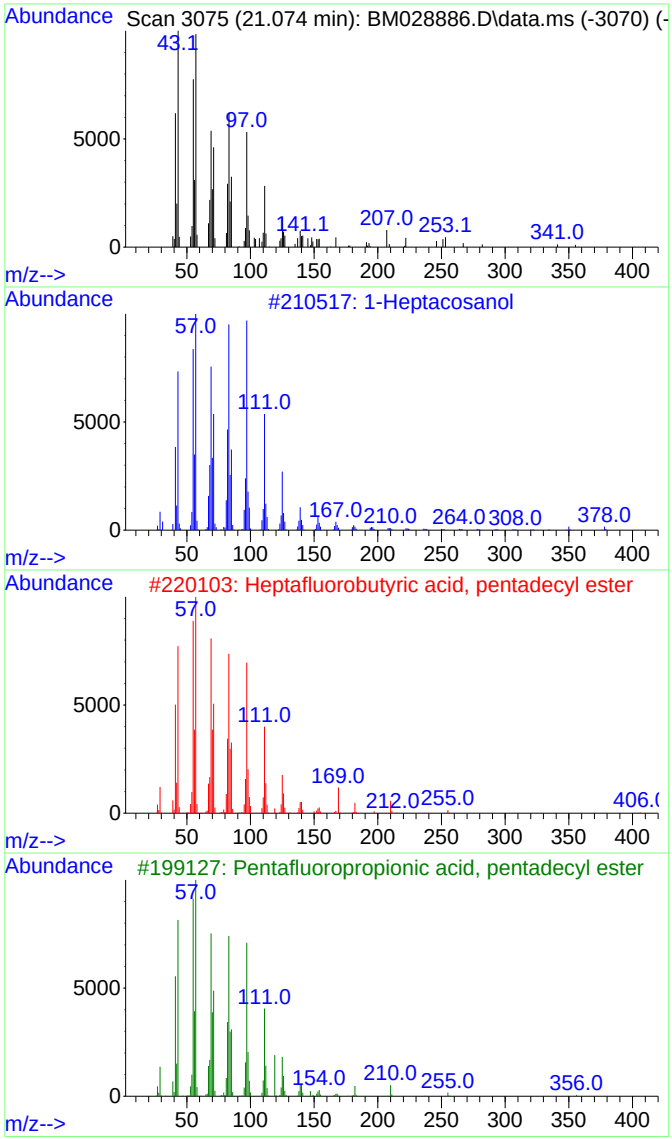
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

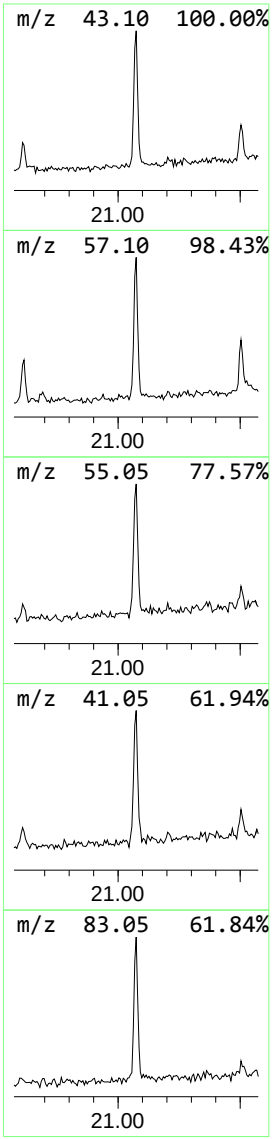
****

Peak Number 7 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	3.01 ng	53582	Chrysene-d12	21.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022421\
Data File : BM028886.D
Acq On : 24 Feb 2021 19:22
Operator : CG/JU
Sample : M1460-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : HD-01-022221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

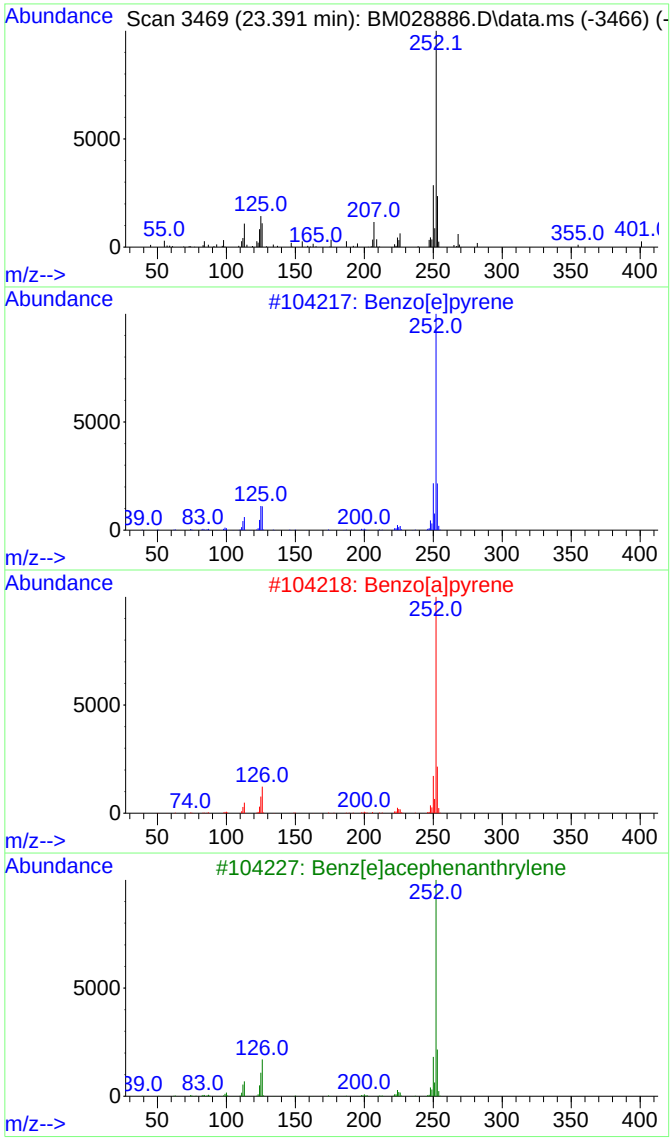
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

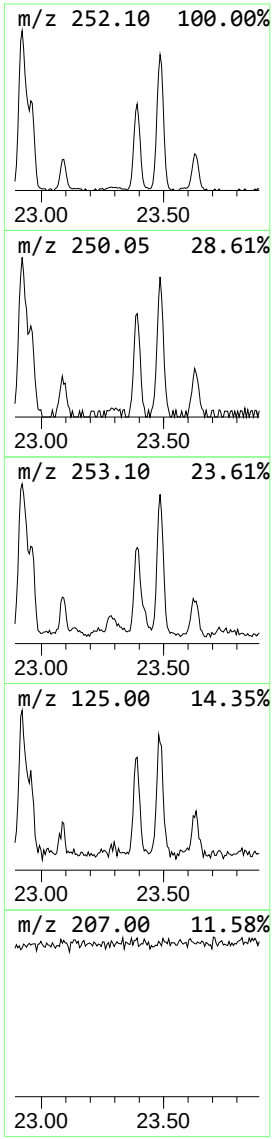
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.391	3.12 ng	29575	Perylene-d12	23.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[a]pyrene	252	C20H12	000050-32-8	93
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	89
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	86
5	Perylene	252	C20H12	000198-55-0	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022421\
Data File : BM028886.D
Acq On : 24 Feb 2021 19:22
Operator : CG/JU
Sample : M1460-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : HD-01-022221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.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
Hexadecanoic ac...	17.868	4.0	ng	43133	4	17.209	213384	20.0
unknown18.092	18.092	2.9	ng	30859	4	17.209	213384	20.0
4H-Cyclopenta[d...	18.274	2.4	ng	25820	4	17.209	213384	20.0
9,12-Octadecadi...	19.009	14.3	ng	152817	4	17.209	213384	20.0
9-Octadecenoic ...	19.039	13.2	ng	140718	4	17.209	213384	20.0
11H-Benzo[b]flu...	20.115	3.0	ng	52679	5	21.368	356032	20.0
1-Heptacosanol	21.074	3.0	ng	53582	5	21.368	356032	20.0
Benzo[e]pyrene	23.391	3.1	ng	29575	6	23.586	189417	20.0