LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020724\
Data File : BP019599.D
Acq On : 07 Feb 2024 18:07
Operator : MA/JU
Sample : P1366-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2-6-8

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_P\Methods\8270E-BP013124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019599.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.481	399	407	415	rBV	964047	1468555	33.45%	4.194%
2	7.075	669	678	693	rBV	1011449	1636441	37.28%	4.673%
3	7.905	811	819	826	rBV	293211	469202	10.69%	1.340%
4	9.069	1010	1017	1025	rBV	606232	1055710	24.05%	3.015%
5	10.705	1287	1295	1301	rBV	373658	653180	14.88%	1.865%
6	13.163	1706	1713	1726	rBV	1674255	2593318	59.08%	7.406%
7	14.257	1893	1899	1909	rBV	72039	114339	2.60%	0.327%
8	14.534	1939	1946	1953	rBV	614702	931716	21.23%	2.661%
9	16.028	2192	2200	2211	rBV	1515607	2224771	50.68%	6.353%
10	17.292	2408	2415	2419	rBV	777228	1181937	26.93%	3.375%
11	17.334	2419	2422	2429	rVV	305885	418393	9.53%	1.195%
12	17.422	2432	2437	2442	rVB	125269	186057	4.24%	0.531%
13	18.157	2558	2562	2564	rBV	47241	60065	1.37%	0.172%
14	18.192	2564	2568	2577	rVV2	261224	429242	9.78%	1.226%
15	18.286	2577	2584	2588	rVV2	42688	89582	2.04%	0.256%
16	18.345	2589	2594	2598	rVV2	97267	177710	4.05%	0.507%
17	18.381	2598	2600	2606	rVB	43070	51559	1.17%	0.147%
18	18.645	2642	2645	2649	rBV	38560	46794	1.07%	0.134%
19	18.686	2649	2652	2658	rVB4	29747	45257	1.03%	0.129%
20	19.045	2709	2713	2718	rBV2	55007	91962	2.09%	0.263%
21	19.104	2718	2723	2726	rBV4	30407	55135	1.26%	0.157%
22	19.181	2732	2736	2744	rBV2	45603	75611	1.72%	0.216%
23	19.298	2751	2756	2764	rBV	1035351	1459580	33.25%	4.168%
24	19.428	2775	2778	2786	rVB3	84994	149560	3.41%	0.427%
25	19.569	2798	2802	2806	rVB2	163405	201560	4.59%	0.576%
26	19.651	2812	2816	2825	rVB	949186	1304901	29.73%	3.726%
27	19.728	2825	2829	2835	rVB3	47359	78832	1.80%	0.225%
28	19.857	2843	2851	2863	rVB	3341474	4389707	100.00%	12.536%
29	19.969	2865	2870	2877	rBV5	75052	180972	4.12%	0.517%
30	20.104	2889	2893	2894	rBV3	51852	64736	1.47%	0.185%
31	20.139	2895	2899	2903	rVB	171416	232640	5.30%	0.664%
32	20.233	2912	2915	2919	rVB	117406	143151	3.26%	0.409%
33	20.292	2919	2925	2929	rBV2	99741	167791	3.82%	0.479%
34	20.428	2945	2948	2951	rVB	50808	55262	1.26%	0.158%
35	20.475	2953	2956	2960	rVB	48987	62423	1.42%	0.178%
36	20.622	2976	2981	2986	rBV	713780	901390	20.53%	2.574%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020724\
Data File : BP019599.D
Acq On : 07 Feb 2024 18:07
Operator : MA/JU
Sample : P1366-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2-6-8

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_P\Methods\8270E-BP013124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.869	3020	3023	3029	rVB	82489	111420	2.54%	0.318%
38	21.033	3049	3051	3054	rVB	98024	84110	1.92%	0.240%
39	21.069	3054	3057	3060	rBV	89215	93949	2.14%	0.268%
40	21.116	3060	3065	3069	rBV3	279815	415452	9.46%	1.186%
41	21.380	3103	3110	3114	rBV2	1232969	2516770	57.33%	7.187%
42	21.422	3114	3117	3126	rVB	625720	842060	19.18%	2.405%
43	21.539	3134	3137	3144	rBV2	134364	234432	5.34%	0.669%
44	23.063	3390	3396	3402	rBV	654331	1653294	37.66%	4.721%
45	23.245	3423	3427	3434	rVB	148909	253438	5.77%	0.724%
46	23.586	3479	3485	3495	rVB	392329	823607	18.76%	2.352%
47	23.686	3496	3502	3511	rBV	577995	1215285	27.68%	3.471%
48	23.798	3514	3521	3527	rBV	612215	1305459	29.74%	3.728%
49	26.310	3941	3948	3963	rVB2	331892	1085087	24.72%	3.099%
50	27.080	4072	4079	4100	rVB2	262276	933721	21.27%	2.666%

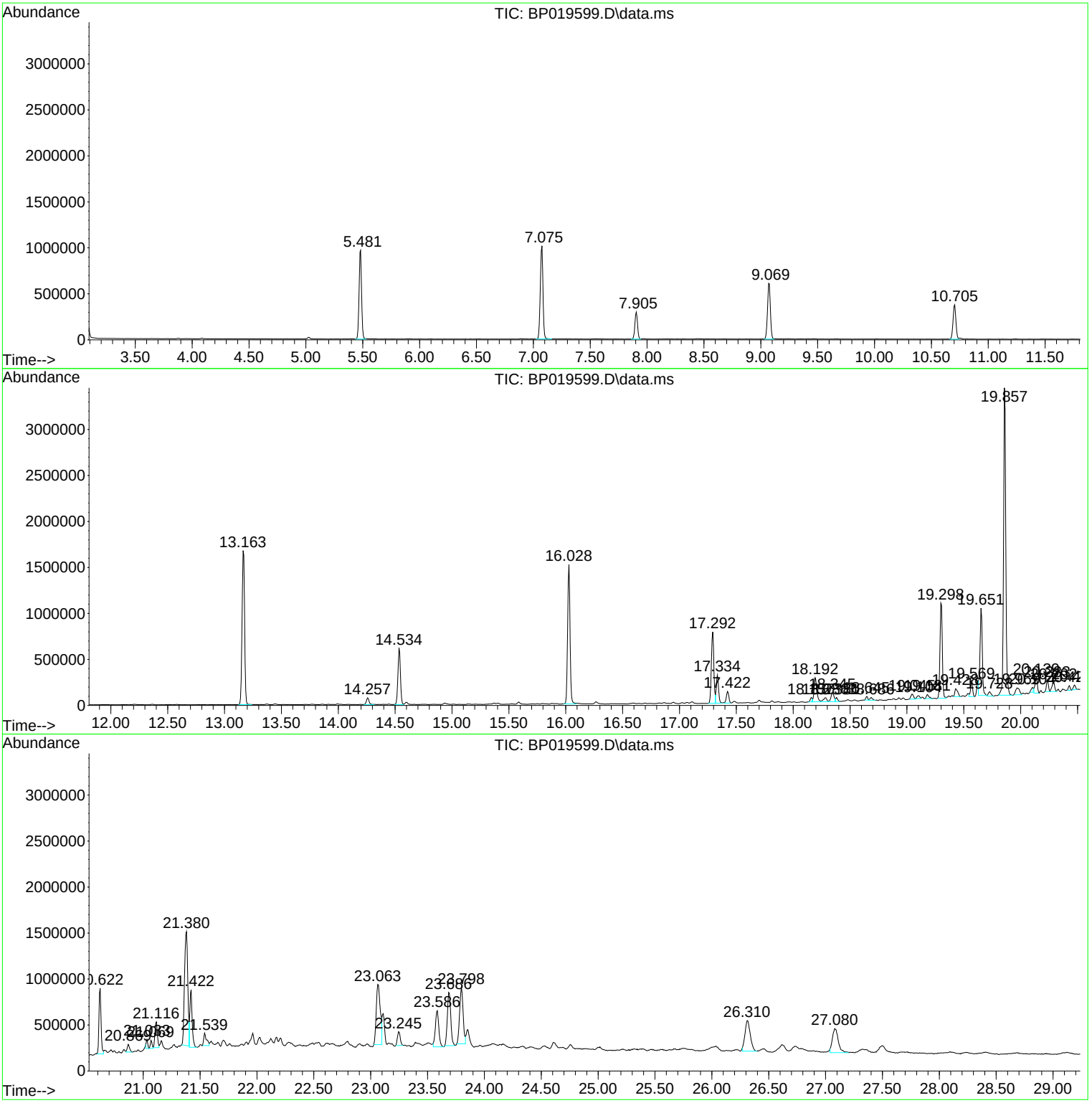
Sum of corrected areas: 35017125

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020724\
Data File : BP019599.D
Acq On : 07 Feb 2024 18:07
Operator : MA/JU
Sample : P1366-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2-6-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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_P\Data\BP020724\
Data File : BP019599.D
Acq On : 07 Feb 2024 18:07
Operator : MA/JU
Sample : P1366-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2-6-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

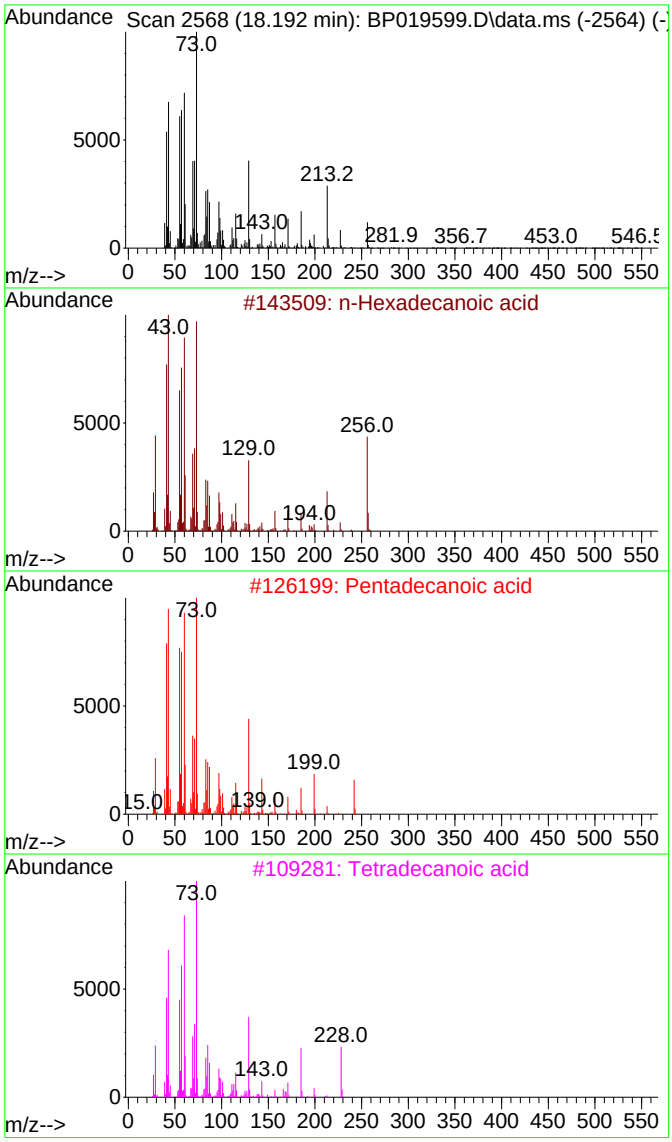
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

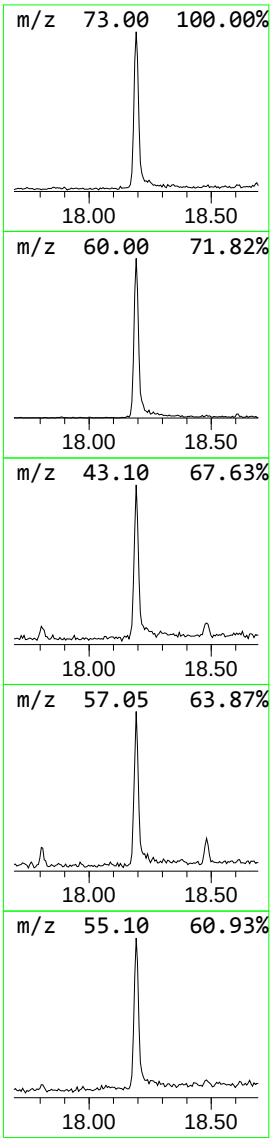
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	7.26 ng	429242	Phenanthrene-d10	17.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Octadecanoic acid	284	C18H36O2	000057-11-4	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020724\
Data File : BP019599.D
Acq On : 07 Feb 2024 18:07
Operator : MA/JU
Sample : P1366-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2-6-8

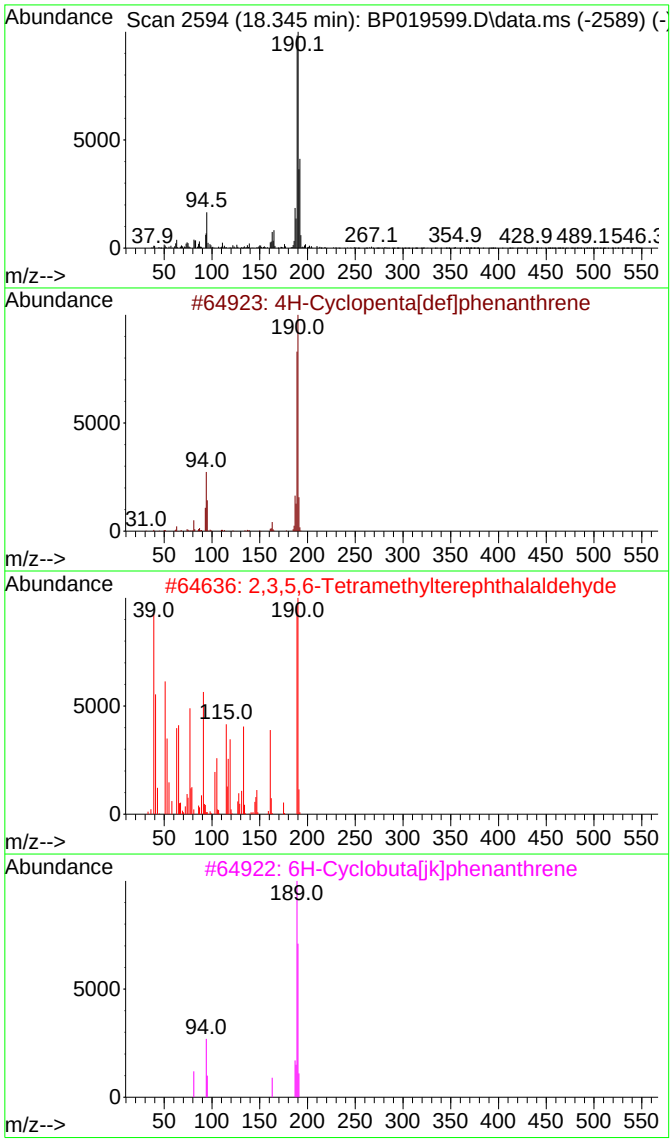
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

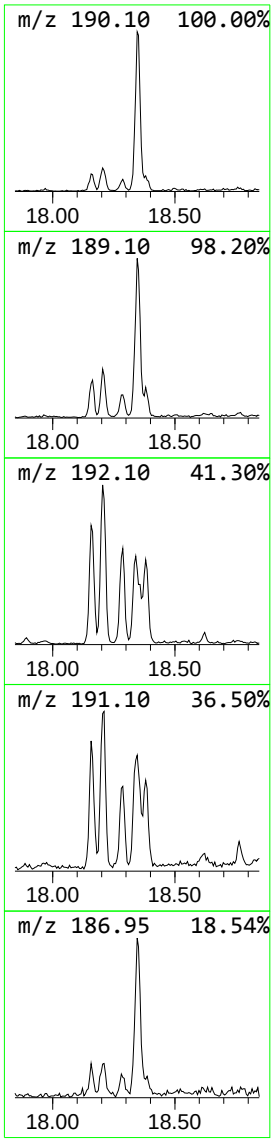
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.345	3.01 ng	177710	Phenanthrene-d10	17.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	47
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	45
4	Methyl diselenide	190	C2H6Se2	007101-31-7	43
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020724\
Data File : BP019599.D
Acq On : 07 Feb 2024 18:07
Operator : MA/JU
Sample : P1366-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2-6-8

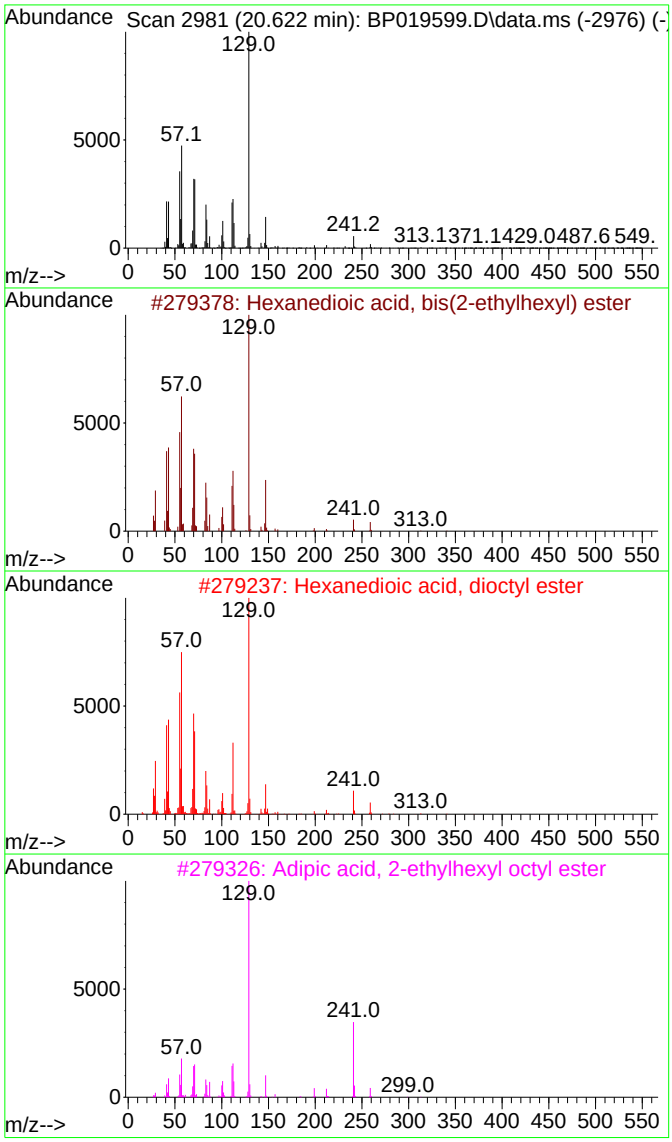
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

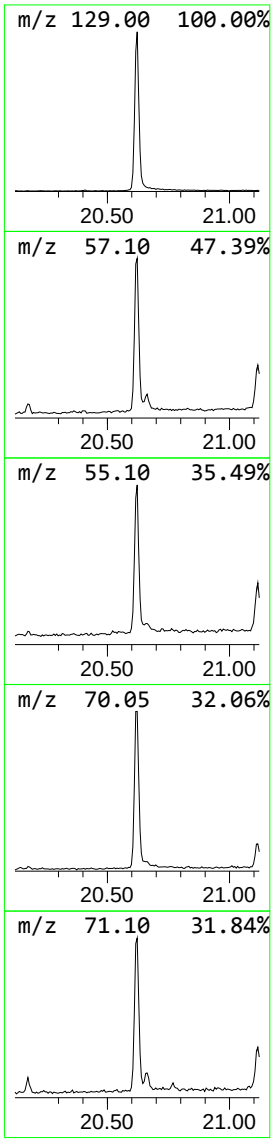
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexanedioic acid, bis(2-eth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.622	7.16 ng	901390	Chrysene-d12	21.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	94
2	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	92
3	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	91
4	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	53
5	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020724\
Data File : BP019599.D
Acq On : 07 Feb 2024 18:07
Operator : MA/JU
Sample : P1366-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2-6-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

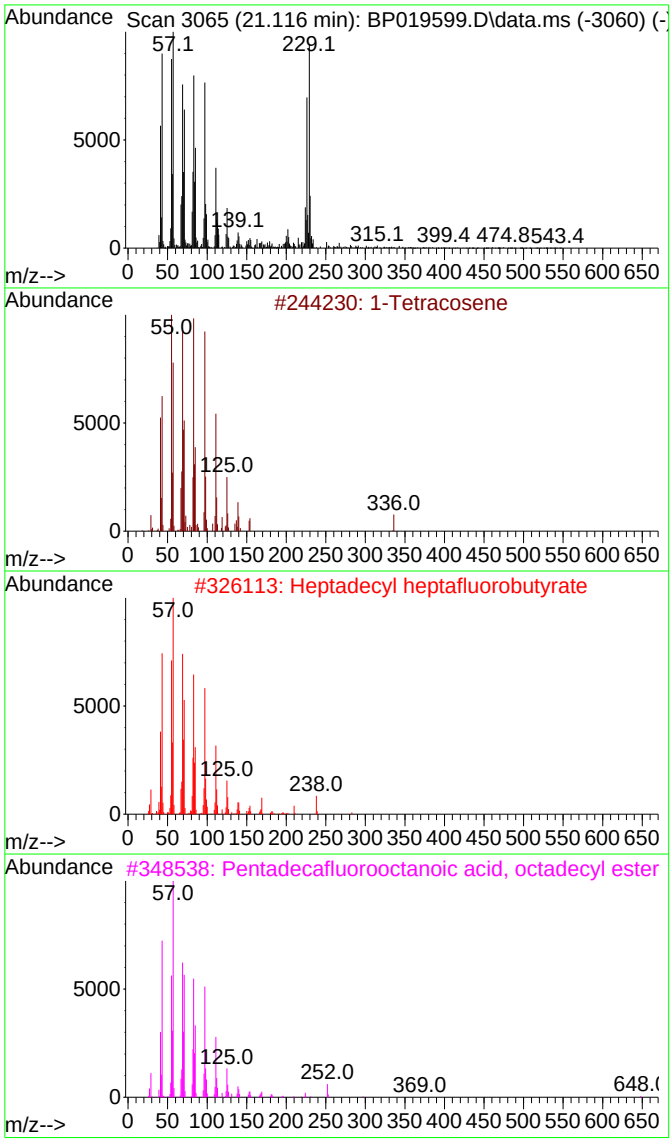
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

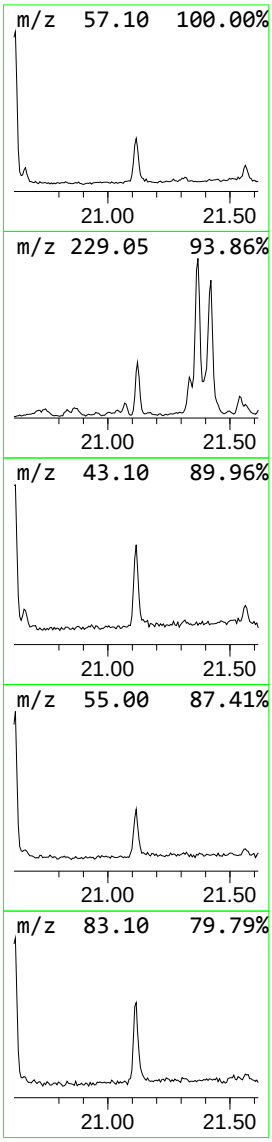
****

Peak Number 4 1-Tetracosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.116	3.30 ng	415452	Chrysene-d12	21.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	83
4	Cyclohexadecane	224	C16H32	000295-65-8	70
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020724\
Data File : BP019599.D
Acq On : 07 Feb 2024 18:07
Operator : MA/JU
Sample : P1366-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2-6-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

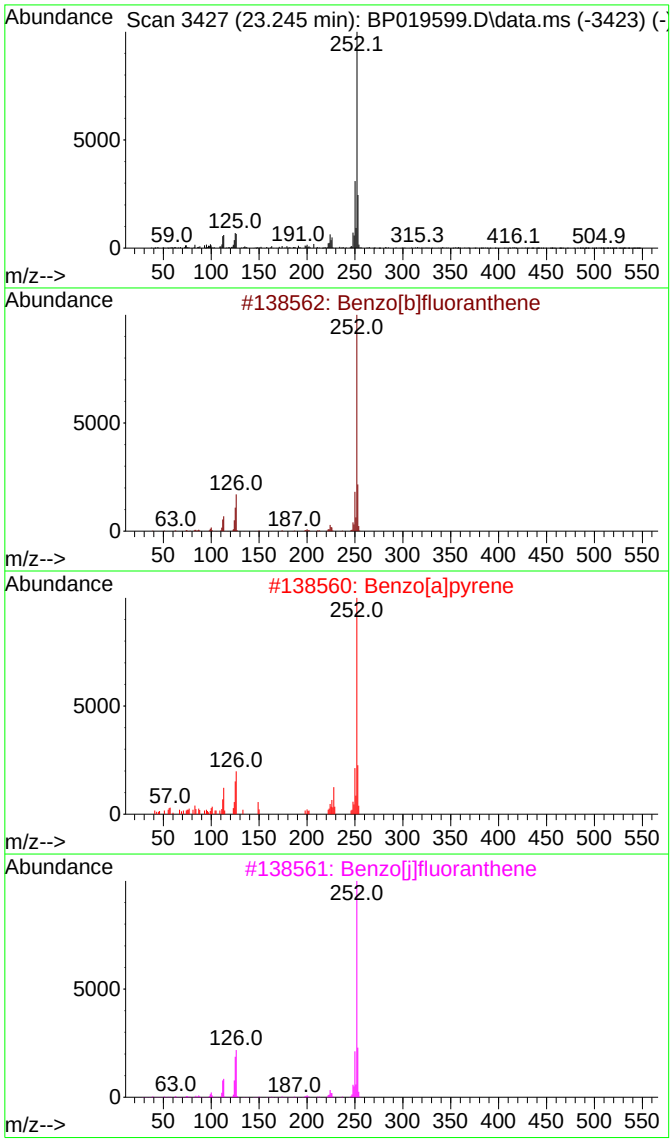
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

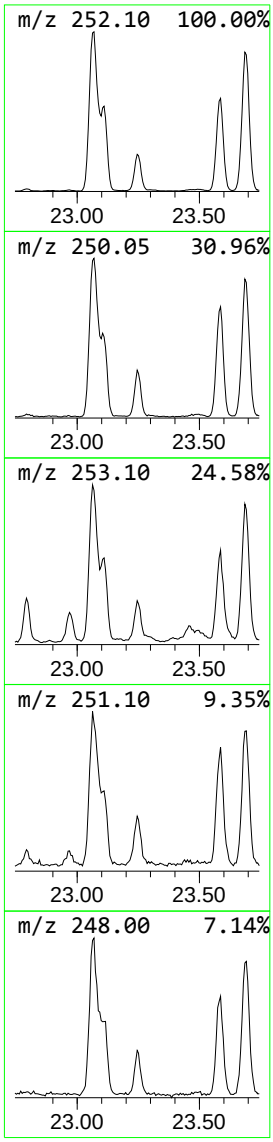
****

Peak Number 5 Benzo[j]fluoranthene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.245	3.88 ng	253438	Perylene-d12	23.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
2	Benzo[a]pyrene	252	C20H12	000050-32-8	76
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	76
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	76
5	Benzo[e]pyrene	252	C20H12	000192-97-2	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020724\
Data File : BP019599.D
Acq On : 07 Feb 2024 18:07
Operator : MA/JU
Sample : P1366-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2-6-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

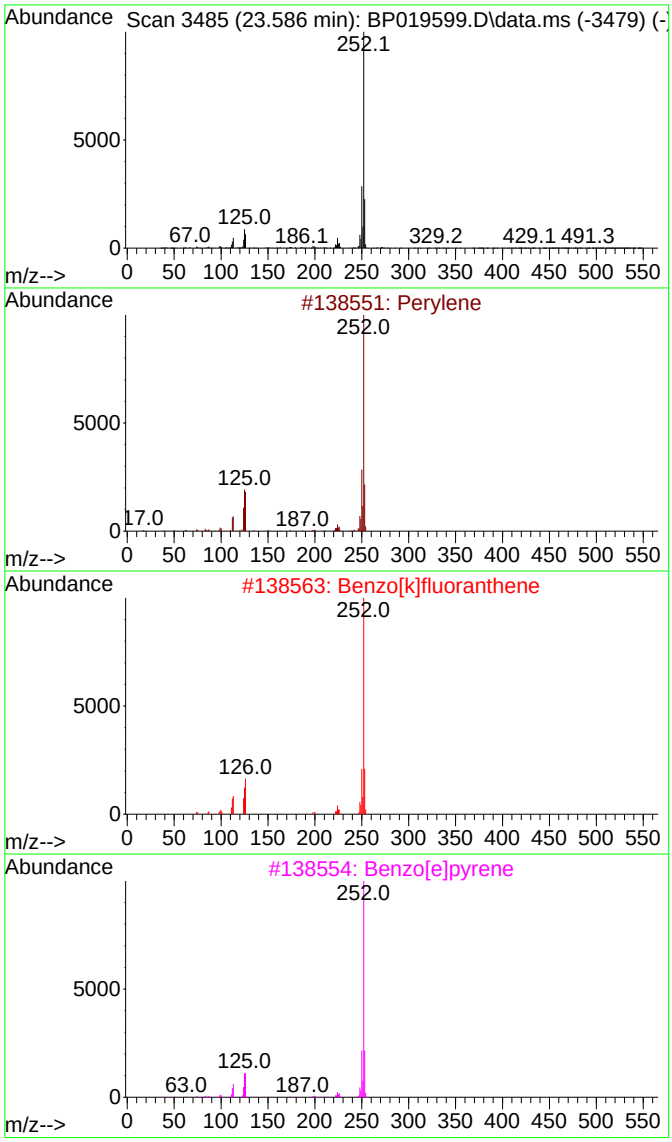
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

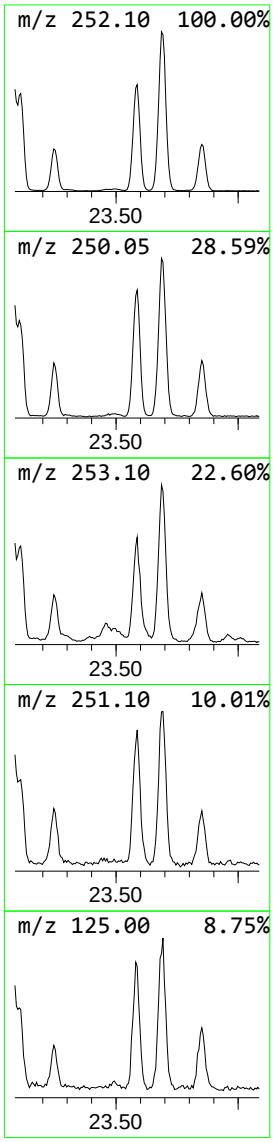
****

Peak Number 6 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.586	12.62 ng	823607	Perylene-d12	23.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	95
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3	Benzo[e]pyrene	252	C20H12	000192-97-2	94
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
5	Benzo[a]pyrene	252	C20H12	000050-32-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020724\
Data File : BP019599.D
Acq On : 07 Feb 2024 18:07
Operator : MA/JU
Sample : P1366-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2-6-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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 ...	18.192	7.3	ng	429242	4	17.292	1181940	20.0
4H-Cyclopenta[d...	18.345	3.0	ng	177710	4	17.292	1181940	20.0
Hexanedioic aci...	20.622	7.2	ng	901390	5	21.380	2516770	20.0
1-Tetracosene	21.116	3.3	ng	415452	5	21.380	2516770	20.0
Benzo[j]fluoran...	23.245	3.9	ng	253438	6	23.798	1305460	20.0
Perylene	23.586	12.6	ng	823607	6	23.798	1305460	20.0