LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005157.D
Acq On : 02 Apr 2021 13:56
Operator : CG/JU
Sample : M1836-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : B6-0-2

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-BP032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005157.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.846	294	299	306	rVB	50971	73016	5.58%	0.718%
2	5.299	370	376	384	rBV	456669	638996	48.86%	6.288%
3	6.881	635	645	657	rBV	457391	704912	53.90%	6.936%
4	7.699	777	784	793	rBV	108770	176741	13.51%	1.739%
5	8.863	974	982	990	rBV	262856	439349	33.59%	4.323%
6	10.493	1252	1259	1265	rBV	143914	244329	18.68%	2.404%
7	12.975	1672	1681	1691	rBV	638147	948931	72.55%	9.338%
8	13.816	1819	1824	1834	rBV	27807	41749	3.19%	0.411%
9	14.081	1864	1869	1874	rBV2	12838	19505	1.49%	0.192%
10	14.357	1907	1916	1922	rBV	225976	320931	24.54%	3.158%
11	14.422	1922	1927	1934	rVB2	12914	20763	1.59%	0.204%
12	14.763	1977	1985	1994	rBV	10580	18084	1.38%	0.178%
13	15.410	2090	2095	2100	rBV3	15029	22226	1.70%	0.219%
14	15.857	2164	2171	2180	rBV	459552	649056	49.63%	6.387%
15	16.775	2321	2327	2332	rVB2	9367	14936	1.14%	0.147%
16	16.934	2350	2354	2366	rVB	13054	22428	1.71%	0.221%
17	17.116	2379	2385	2389	rBV	254243	362677	27.73%	3.569%
18	17.163	2389	2393	2399	rVV	209245	294719	22.53%	2.900%
19	17.251	2403	2408	2414	rVV	45137	68286	5.22%	0.672%
20	17.528	2446	2455	2460	rBV3	15147	32314	2.47%	0.318%
21	17.992	2529	2534	2535	rBV2	28392	31917	2.44%	0.314%
22	18.022	2535	2539	2547	rVB2	107078	188095	14.38%	1.851%
23	18.116	2552	2555	2560	rVV	17722	24705	1.89%	0.243%
24	18.181	2560	2566	2570	rVV2	40091	73924	5.65%	0.727%
25	18.216	2570	2572	2577	rVB2	21826	25744	1.97%	0.253%
26	18.481	2612	2617	2620	rBV2	22435	30694	2.35%	0.302%
27	18.522	2620	2624	2629	rVB2	17798	24805	1.90%	0.244%
28	18.886	2681	2686	2691	rBV2	15521	26310	2.01%	0.259%
29	19.016	2705	2708	2717	rVB4	15834	25357	1.94%	0.250%
30	19.139	2723	2729	2737	rBV	326310	421395	32.22%	4.147%
31	19.257	2743	2749	2757	rBV6	38828	75195	5.75%	0.740%
32	19.463	2780	2784	2785	rBV	47834	54674	4.18%	0.538%
33	19.492	2785	2789	2797	rVV	277139	366865	28.05%	3.610%
34	19.563	2797	2801	2807	rVB3	17889	29320	2.24%	0.289%
35	19.692	2816	2823	2828	rBV	1024705	1307882	100.00%	12.870%
36	19.816	2838	2844	2850	rBV4	19103	42811	3.27%	0.421%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005157.D
Acq On : 02 Apr 2021 13:56
Operator : CG/JU
Sample : M1836-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : B6-0-2

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-BP032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.945	2861	2866	2867	rBV4	14476	22733	1.74%	0.224%
38	19.975	2867	2871	2877	rVB2	39149	61040	4.67%	0.601%
39	20.075	2884	2888	2891	rBV	20141	21623	1.65%	0.213%
40	20.133	2893	2898	2902	rVB2	27566	42799	3.27%	0.421%
41	20.269	2918	2921	2924	rVB	13715	15510	1.19%	0.153%
42	20.310	2925	2928	2932	rBV3	17377	21932	1.68%	0.216%
43	20.710	2992	2996	3000	rBV	24739	33783	2.58%	0.332%
44	20.904	3027	3029	3031	rBV2	19128	22984	1.76%	0.226%
45	20.933	3031	3034	3042	rVV4	143564	232890	17.81%	2.292%
46	20.998	3042	3045	3054	rVB	75717	98911	7.56%	0.973%
47	21.216	3076	3082	3086	rBV2	392080	643367	49.19%	6.331%
48	21.251	3086	3088	3098	rVB	137385	167309	12.79%	1.646%
49	21.369	3105	3108	3114	rVB4	24747	30980	2.37%	0.305%
50	22.810	3348	3353	3358	rBV	93399	203030	15.52%	1.998%
51	23.304	3432	3437	3444	rVB	59975	108960	8.33%	1.072%
52	23.398	3448	3453	3460	rVB	100190	177658	13.58%	1.748%
53	23.498	3464	3470	3476	rBV2	200273	393360	30.08%	3.871%

Sum of corrected areas: 10162510

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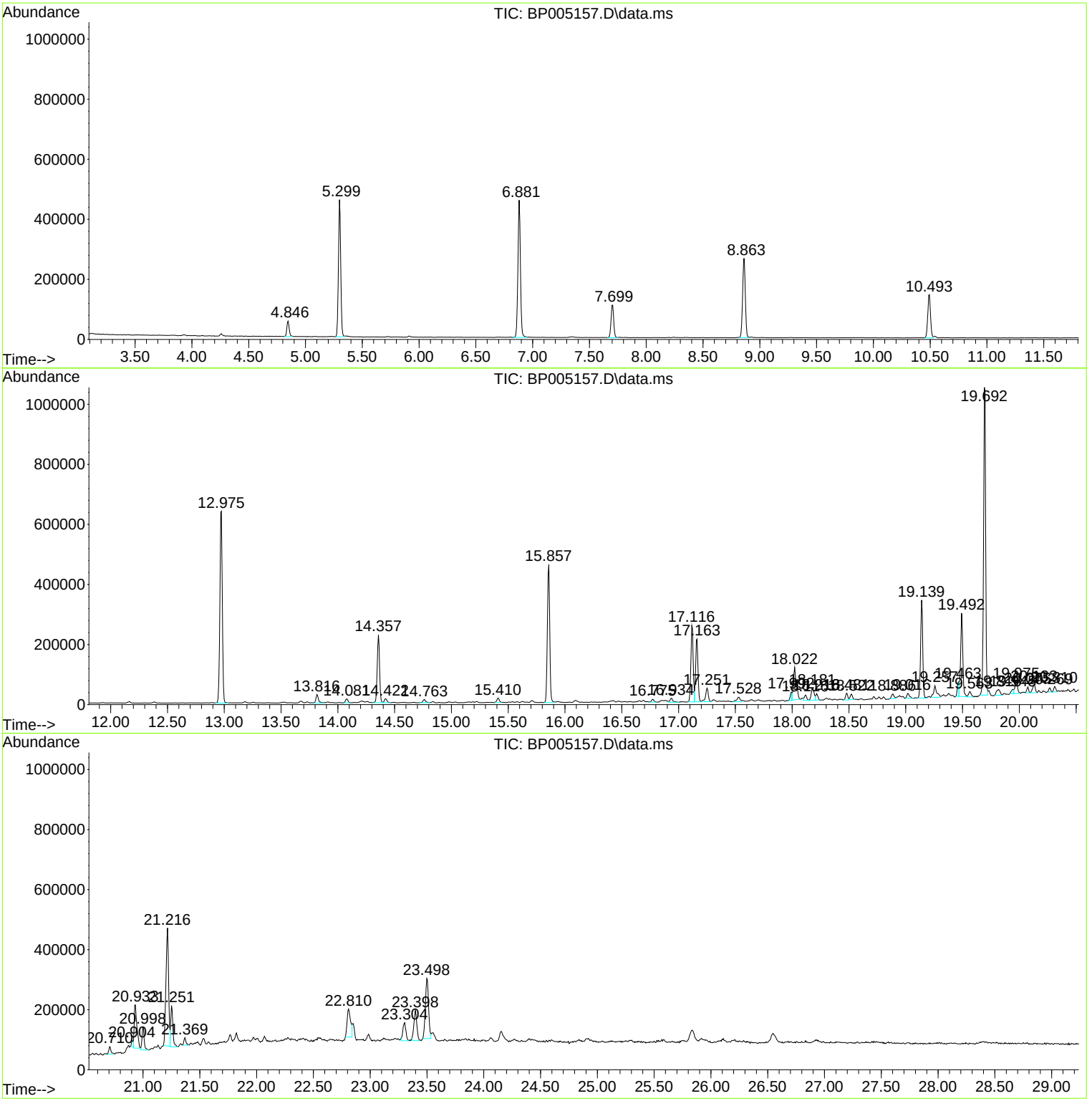
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B6-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.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_P\Data\BP040221\
Data File : BP005157.D
Acq On : 02 Apr 2021 13:56
Operator : CG/JU
Sample : M1836-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B6-0-2

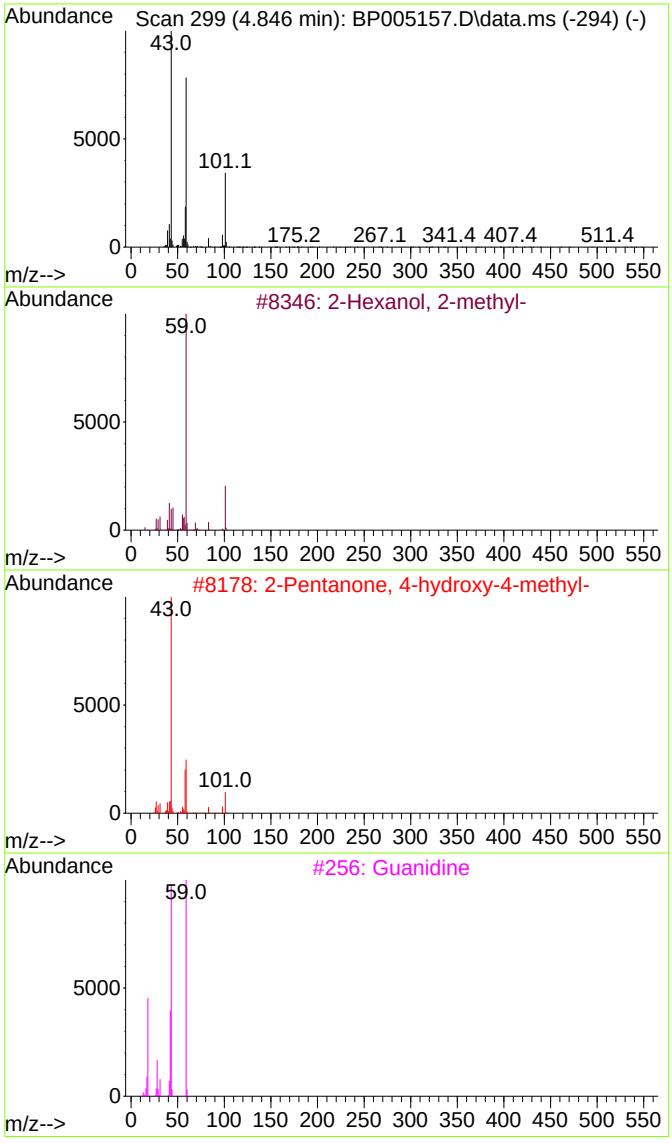
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

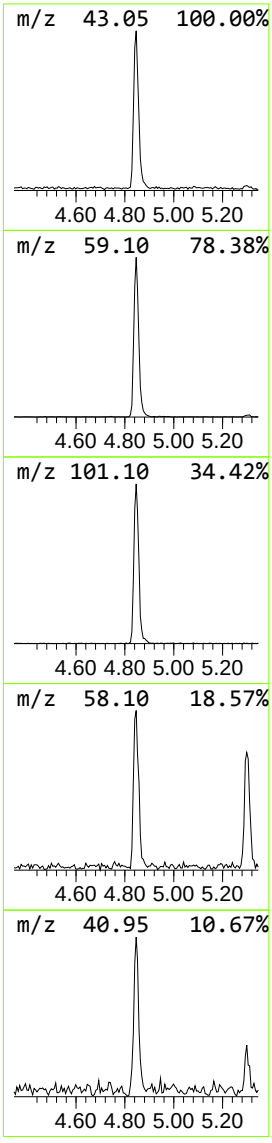
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Hexanol, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.846	8.26 ng	73016	1,4-Dichlorobenzene-d4	7.705

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	59
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	Guanidine	59	CH5N3	000113-00-8	50
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	43
5	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005157.D
Acq On : 02 Apr 2021 13:56
Operator : CG/JU
Sample : M1836-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B6-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

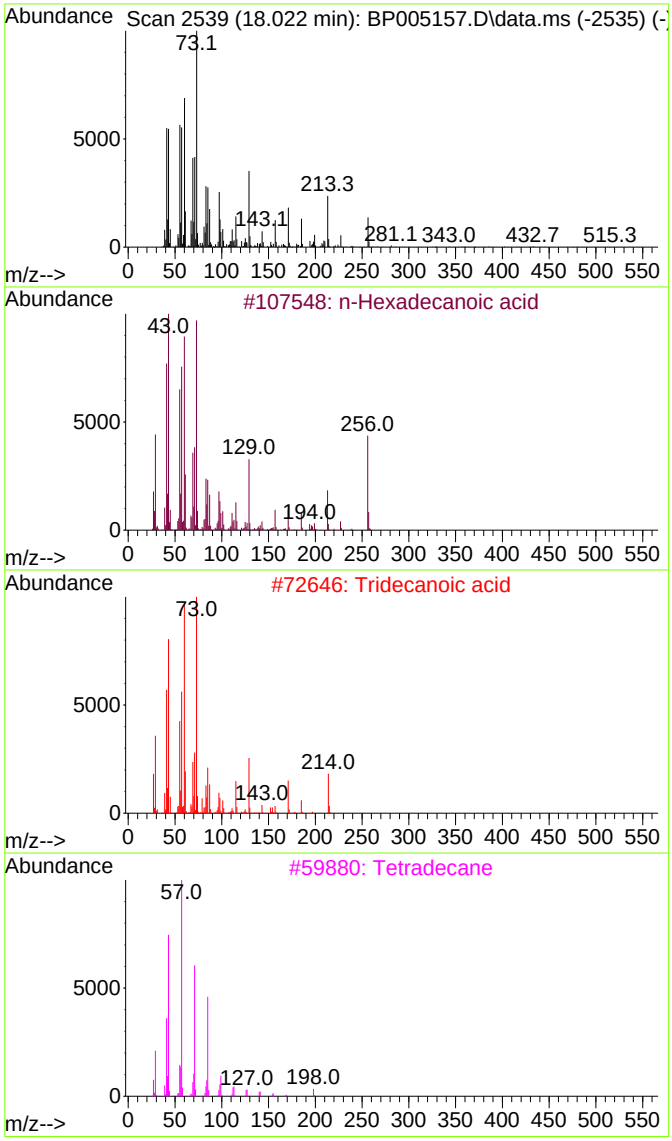
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

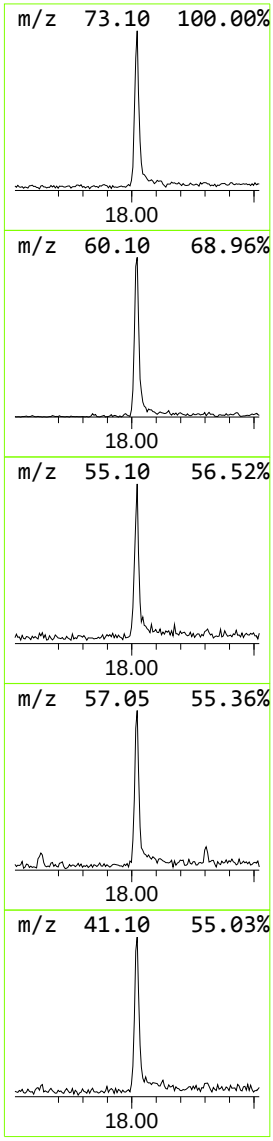
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.022	10.37 ng	188095	Phenanthrene-d10	17.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Tetradecane	198	C14H30	000629-59-4	68
4	Octadecanoic acid	284	C18H36O2	000057-11-4	58
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005157.D
Acq On : 02 Apr 2021 13:56
Operator : CG/JU
Sample : M1836-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B6-0-2

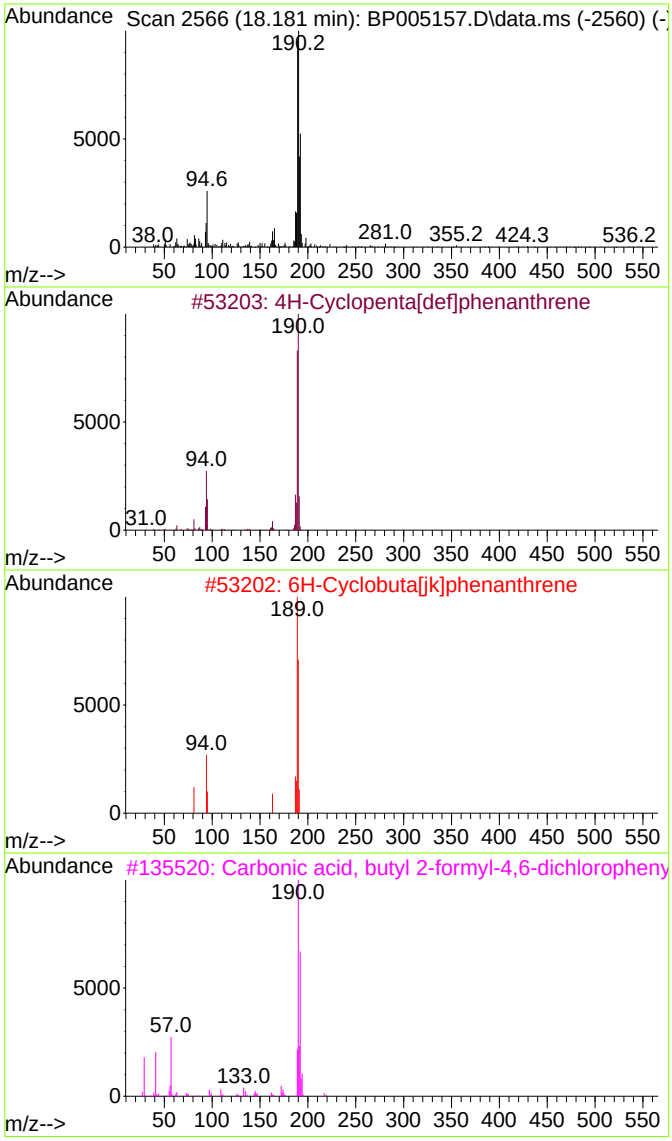
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

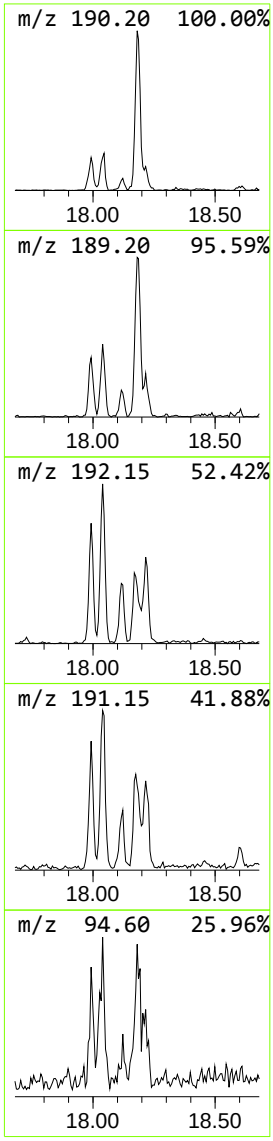
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.180	4.08 ng	73924	Phenanthrene-d10	17.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	Carbonic acid, butyl 2-formyl-4,...	290	C12H12Cl2O4	1000331-42-2	32
4	3,5-Dichlorobenzoic acid	190	C7H4Cl2O2	000051-36-5	27
5	Megastigmatrienone	190	C13H18O	038818-55-2	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005157.D
Acq On : 02 Apr 2021 13:56
Operator : CG/JU
Sample : M1836-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : B6-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

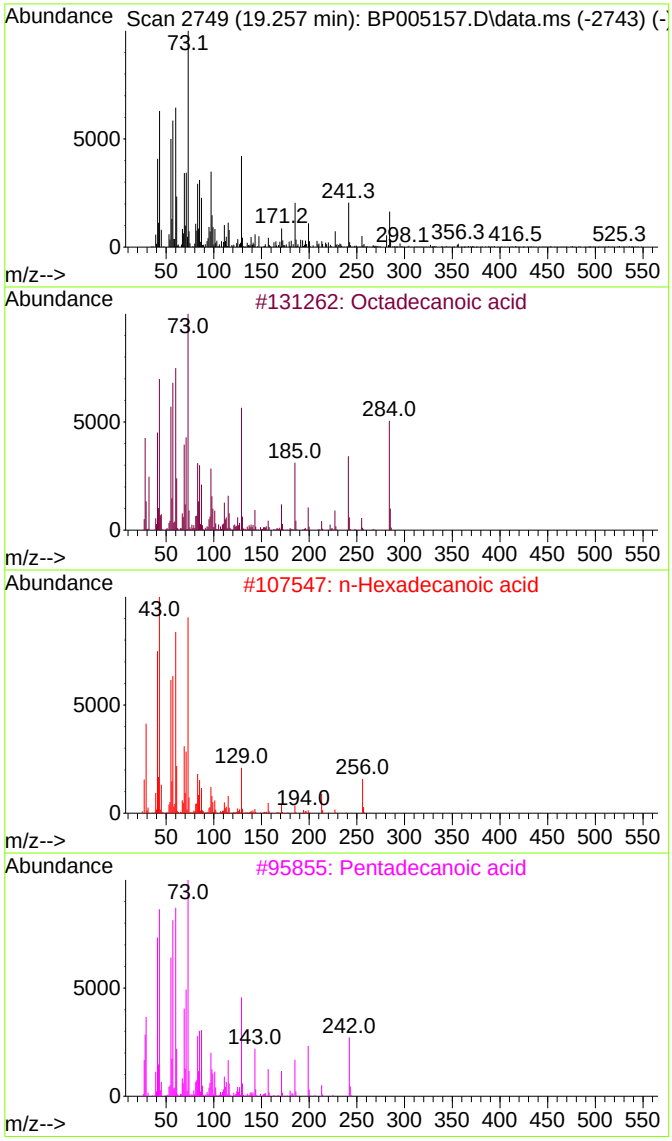
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

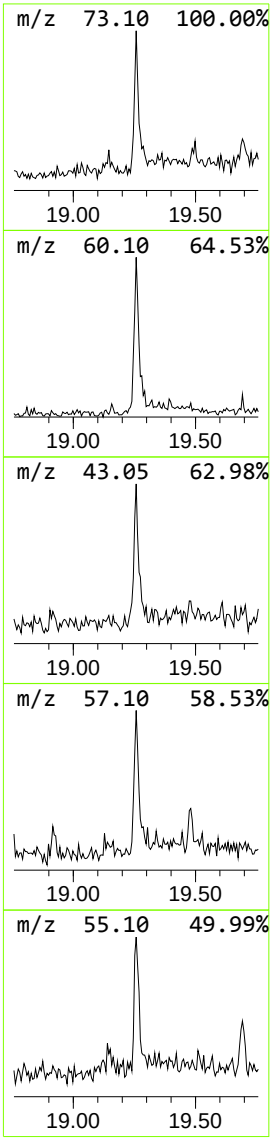
****

Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.257	2.34 ng	75195	Chrysene-d12	21.216

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	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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Data File : BP005157.D
Acq On : 02 Apr 2021 13:56
Operator : CG/JU
Sample : M1836-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : B6-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

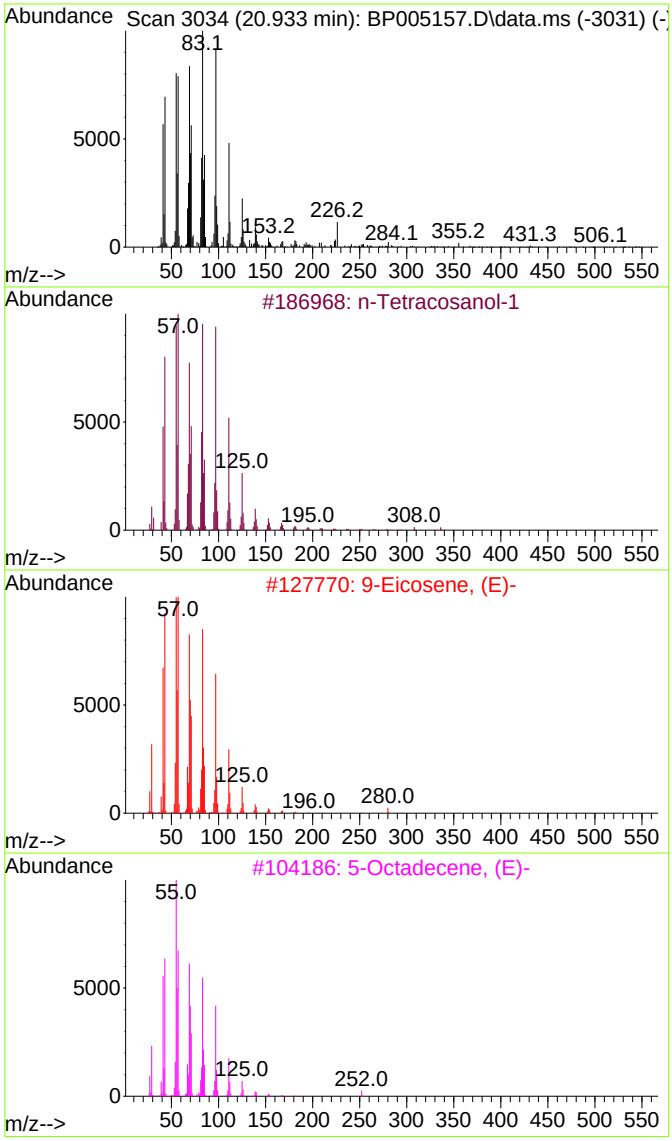
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

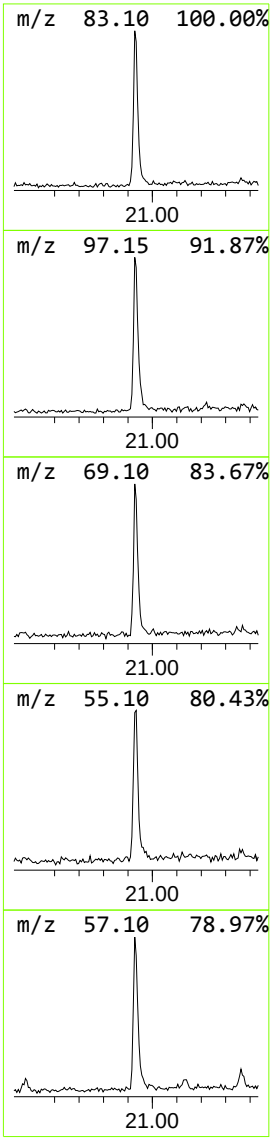
****

Peak Number 5 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.933	7.24 ng	232890	Chrysene-d12	21.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
5	1-Heneicosanol	312	C21H44O	015594-90-8	90





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Operator : CG/JU
Sample : M1836-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : B6-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

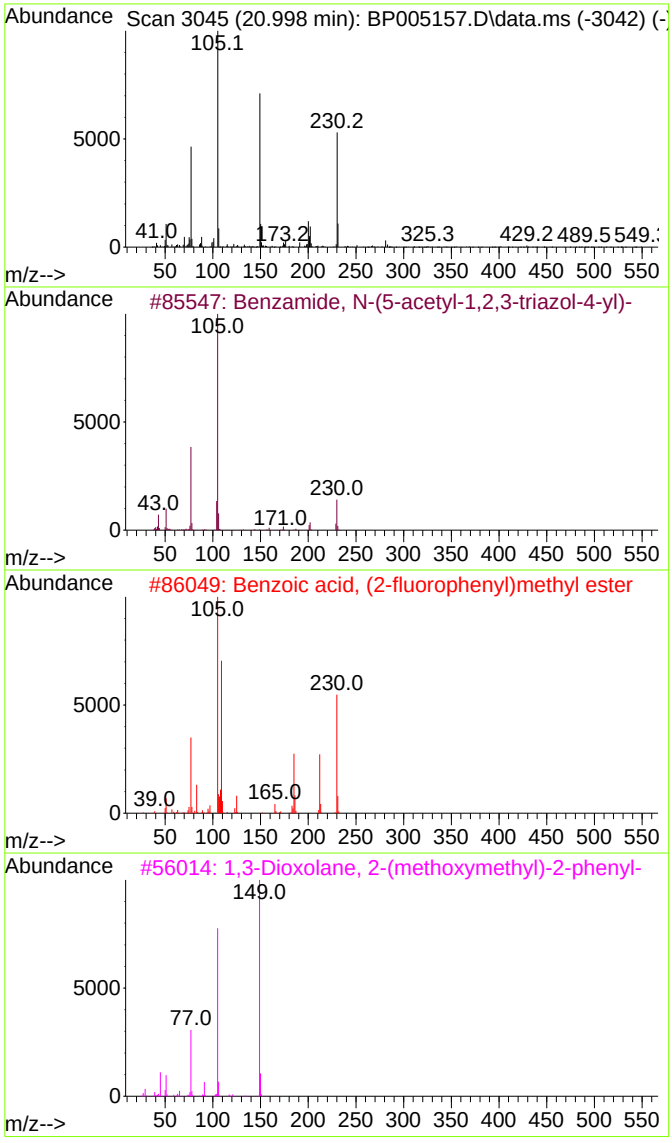
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

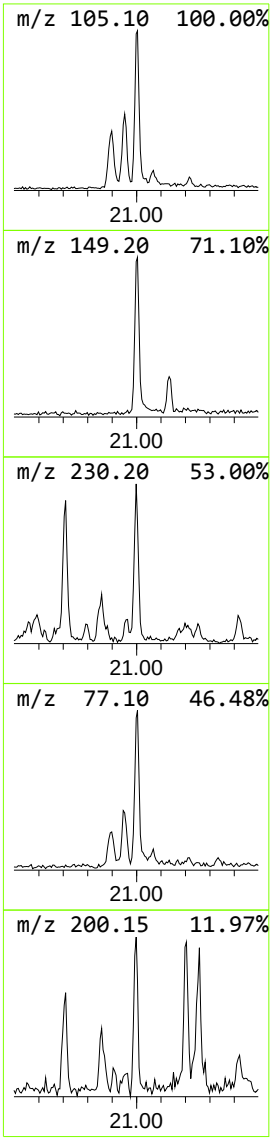
****

Peak Number 6 Benzamide, N-(5-acetyl-1,2,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.998	3.07 ng	98911	Chrysene-d12	21.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-(5-acetyl-1,2,3-tri...	230	C11H10N4O2	129959-33-7	52
2	Benzoic acid, (2-fluorophenyl)me...	230	C14H11FO2	1000368-73-8	47
3	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	47
4	Benzoic acid, (4-fluorophenyl)me...	230	C14H11FO2	1000368-73-1	46
5	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	35





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Operator : CG/JU
Sample : M1836-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B6-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

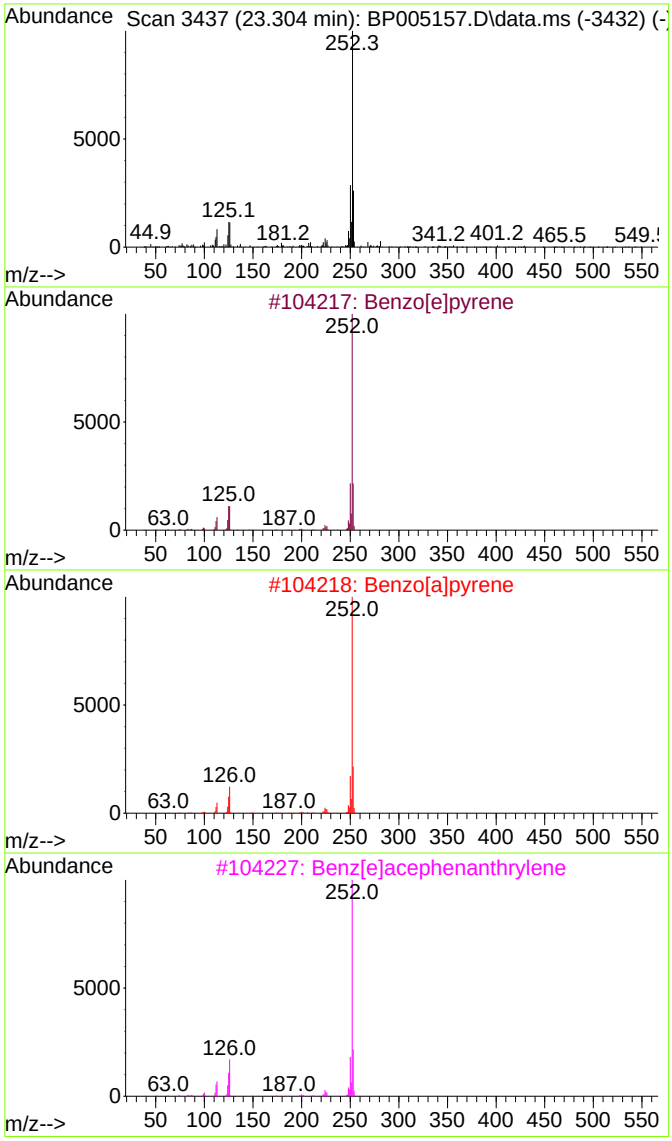
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

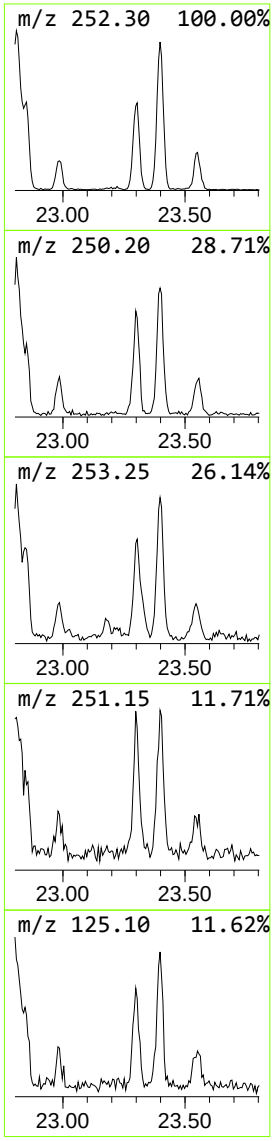
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.304	5.54 ng	108960	Perylene-d12	23.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
5	Perylene	252	C20H12	000198-55-0	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005157.D
Acq On : 02 Apr 2021 13:56
Operator : CG/JU
Sample : M1836-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : B6-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.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-Hexanol, 2-me...	4.846	8.3	ng	73016	1	7.705	176741	20.0
n-Hexadecanoic ...	18.022	10.4	ng	188095	4	17.116	362677	20.0
4H-Cyclopenta[d...	18.180	4.1	ng	73924	4	17.116	362677	20.0
Octadecanoic acid	19.257	2.3	ng	75195	5	21.216	643367	20.0
n-Tetracosanol-1	20.933	7.2	ng	232890	5	21.216	643367	20.0
Benzamide, N-(5...	20.998	3.1	ng	98911	5	21.216	643367	20.0
Benzo[e]pyrene	23.304	5.5	ng	108960	6	23.504	393360	20.0