LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004737.D
Acq On : 12 Feb 2021 19:13
Operator : CG/JU
Sample : M1389-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-1

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-BP020521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004737.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.358	362	369	378	rBV	940566	1314742	48.77%	5.748%
2	6.940	630	638	650	rBV	879401	1431442	53.10%	6.259%
3	7.769	772	779	786	rBV	201657	317796	11.79%	1.389%
4	8.922	968	975	986	rBV	531835	864564	32.07%	3.780%
5	10.563	1247	1254	1262	rBV	256926	426300	15.81%	1.864%
6	13.034	1667	1674	1682	rBV	1242153	1810231	67.15%	7.915%
7	13.869	1809	1816	1822	rBV	55753	83421	3.09%	0.365%
8	14.416	1902	1909	1915	rBV	411299	585114	21.70%	2.558%
9	15.469	2083	2088	2092	rVB2	19036	28527	1.06%	0.125%
10	15.910	2156	2163	2171	rBV	1111164	1595928	59.20%	6.978%
11	17.169	2371	2377	2381	rBV	494614	714701	26.51%	3.125%
12	17.210	2381	2384	2391	rVV	418397	557314	20.67%	2.437%
13	17.298	2391	2399	2405	rVV	37364	68938	2.56%	0.301%
14	17.575	2437	2446	2451	rBV	69811	109275	4.05%	0.478%
15	18.069	2521	2530	2541	rBV2	173181	340707	12.64%	1.490%
16	18.228	2551	2557	2561	rBV3	62232	99775	3.70%	0.436%
17	18.263	2561	2563	2570	rVB	22029	28159	1.04%	0.123%
18	18.528	2603	2608	2610	rBV	32428	42795	1.59%	0.187%
19	18.563	2610	2614	2620	rVB	110197	138431	5.13%	0.605%
20	19.063	2695	2699	2707	rVB2	29570	42785	1.59%	0.187%
21	19.186	2712	2720	2726	rBV	937870	1239704	45.99%	5.420%
22	19.298	2733	2739	2747	rBV4	64707	103873	3.85%	0.454%
23	19.533	2775	2779	2787	rVB	703697	943462	35.00%	4.125%
24	19.604	2787	2791	2796	rVB2	29176	42311	1.57%	0.185%
25	19.739	2805	2814	2826	rVB	2110216	2695851	100.00%	11.787%
26	19.851	2828	2833	2839	rBV3	34332	80555	2.99%	0.352%
27	20.016	2858	2861	2867	rVB	92588	120380	4.47%	0.526%
28	20.116	2873	2878	2882	rBV2	70545	93251	3.46%	0.408%
29	20.169	2882	2887	2891	rVV2	44229	75922	2.82%	0.332%
30	20.210	2891	2894	2898	rVB	27611	33253	1.23%	0.145%
31	20.310	2907	2911	2914	rBV2	22717	28630	1.06%	0.125%
32	20.351	2915	2918	2922	rVV2	23791	31013	1.15%	0.136%
33	20.745	2981	2985	2990	rVB	58413	77141	2.86%	0.337%
34	20.910	3007	3013	3016	rBV2	88865	129358	4.80%	0.566%
35	20.945	3016	3019	3020	rVV2	57477	58347	2.16%	0.255%
36	20.969	3020	3023	3030	rVV4	193966	363440	13.48%	1.589%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004737.D
Acq On : 12 Feb 2021 19:13
Operator : CG/JU
Sample : M1389-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-1

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-BP020521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.033	3031	3034	3041	rVB2	88503	118988	4.41%	0.520%
38	21.145	3050	3053	3060	rVB3	20806	28980	1.07%	0.127%
39	21.257	3065	3072	3075	rVV2	749435	1429178	53.01%	6.249%
40	21.292	3075	3078	3087	rVB	430570	535508	19.86%	2.341%
41	21.410	3094	3098	3103	rBV	70118	87091	3.23%	0.381%
42	21.569	3121	3125	3130	rBV2	65589	100218	3.72%	0.438%
43	21.869	3172	3176	3181	rVB2	63486	92206	3.42%	0.403%
44	22.116	3213	3218	3224	rBV2	247420	338904	12.57%	1.482%
45	22.469	3275	3278	3287	rVB	95694	146370	5.43%	0.640%
46	22.863	3339	3345	3351	rBV	373648	856551	31.77%	3.745%
47	23.363	3424	3430	3439	rVB	203357	398240	14.77%	1.741%
48	23.457	3441	3446	3454	rVB	251453	478794	17.76%	2.093%
49	23.563	3457	3464	3470	rBV2	415597	829591	30.77%	3.627%
50	25.927	3859	3866	3874	rVB2	141408	405709	15.05%	1.774%
51	26.657	3982	3990	3999	rVB2	101152	307882	11.42%	1.346%

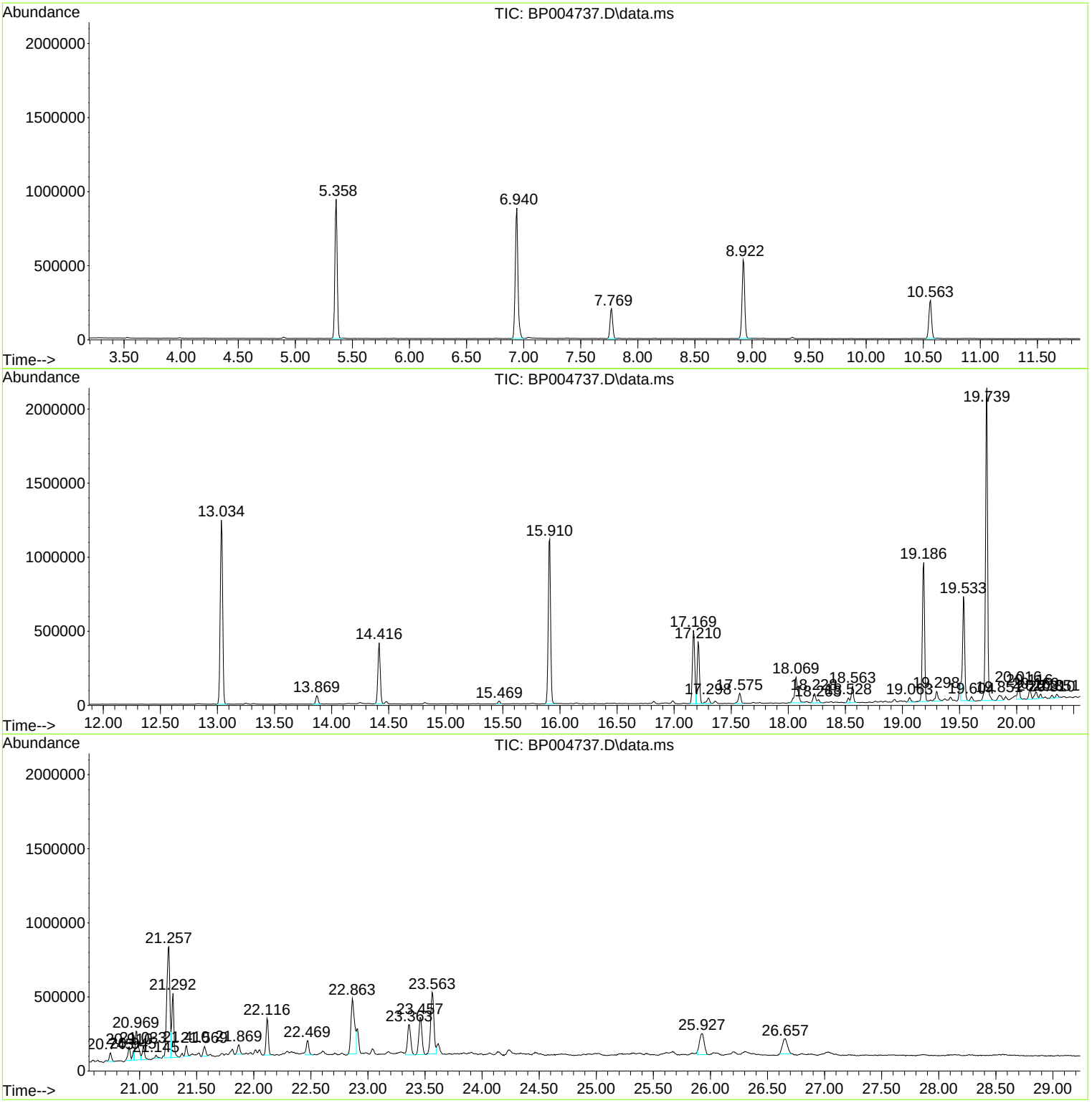
Sum of corrected areas: 22871646

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004737.D
Acq On : 12 Feb 2021 19:13
Operator : CG/JU
Sample : M1389-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.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\BP021221\
Data File : BP004737.D
Acq On : 12 Feb 2021 19:13
Operator : CG/JU
Sample : M1389-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

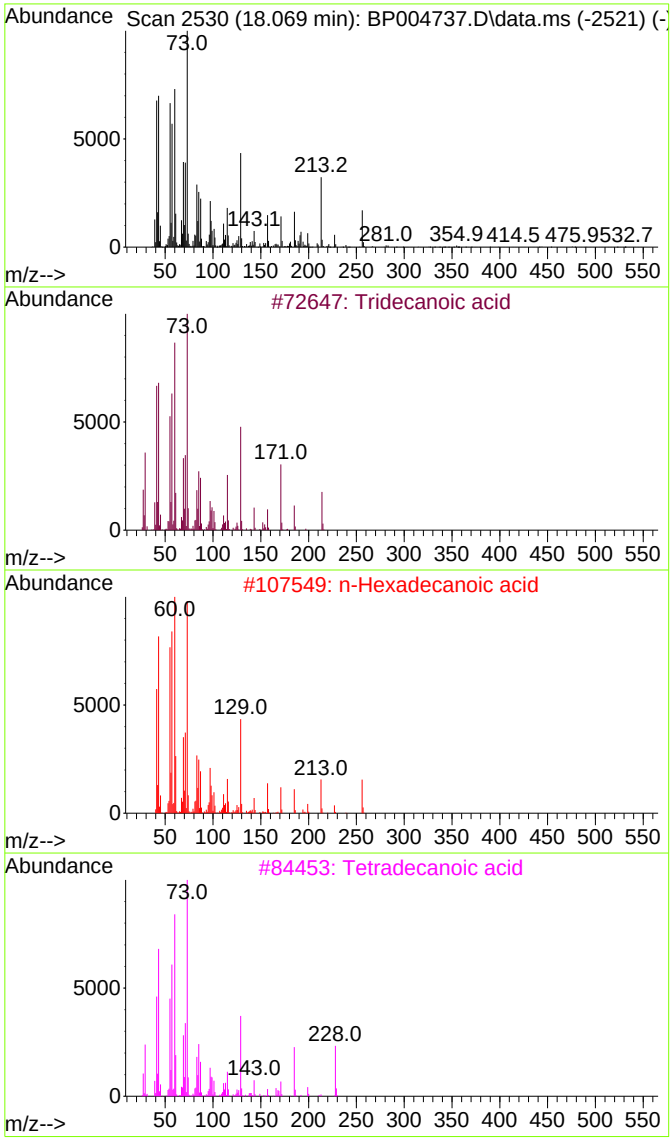
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

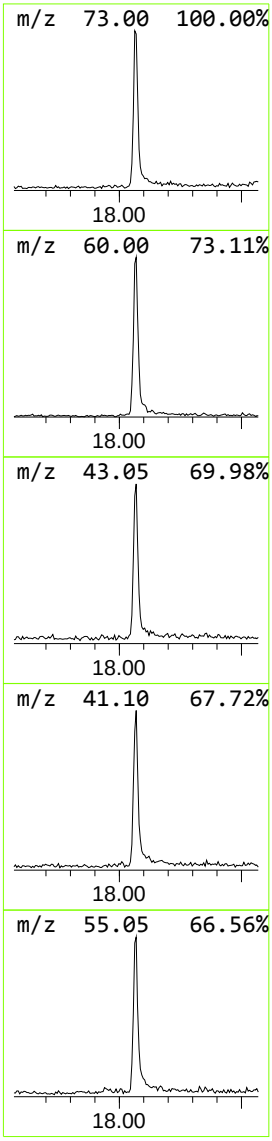
****

Peak Number 1 Tridecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.069	9.53 ng	340707	Phenanthrene-d10	17.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004737.D
Acq On : 12 Feb 2021 19:13
Operator : CG/JU
Sample : M1389-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-1

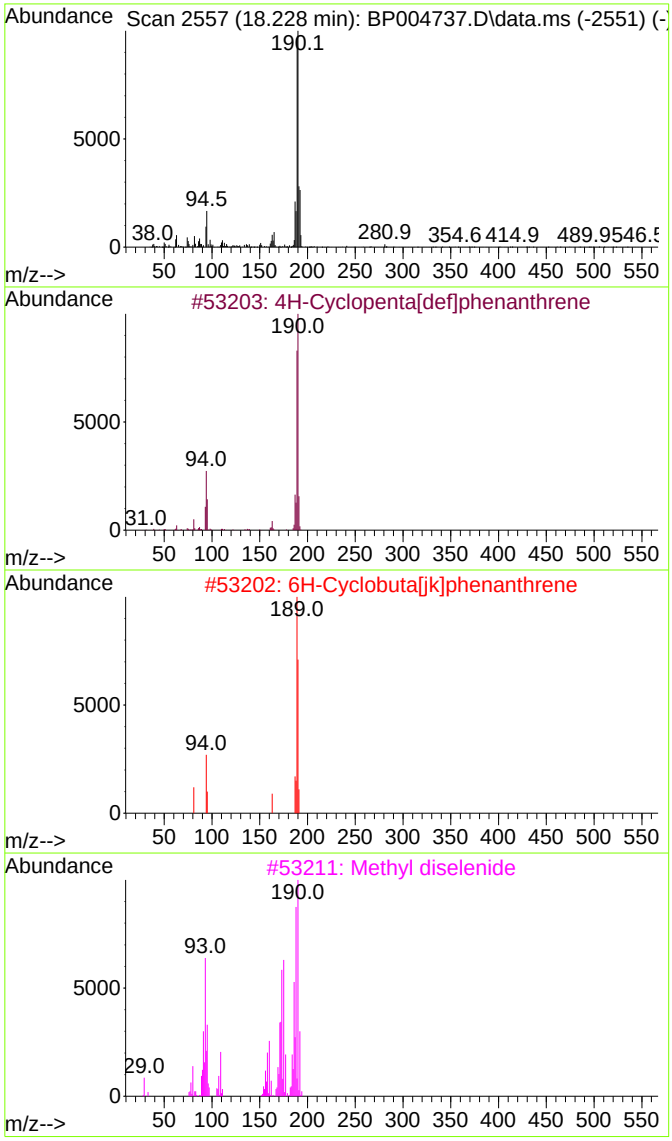
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

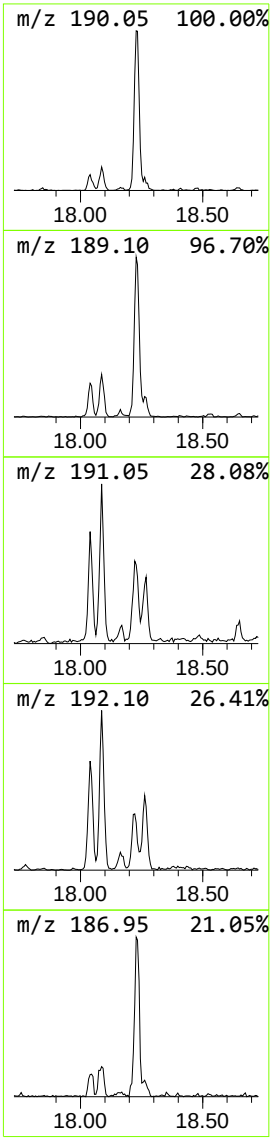
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.228	2.79 ng	99775	Phenanthrene-d10	17.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	Methyl diselenide	190	C2H6Se2	007101-31-7	43
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
5	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004737.D
Acq On : 12 Feb 2021 19:13
Operator : CG/JU
Sample : M1389-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

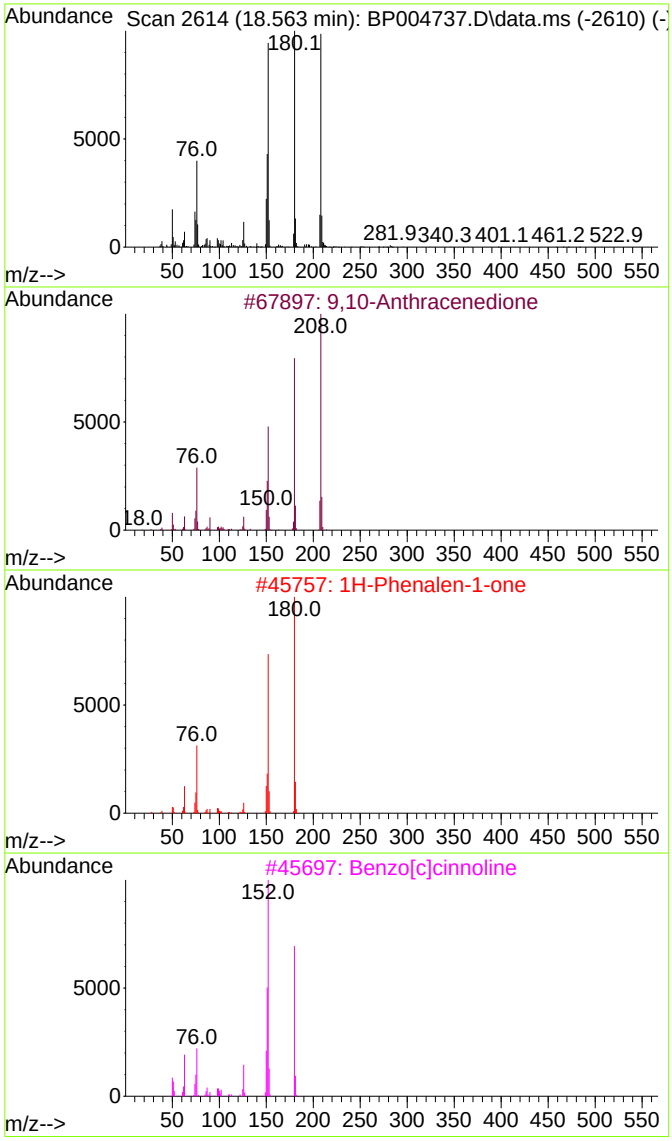
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

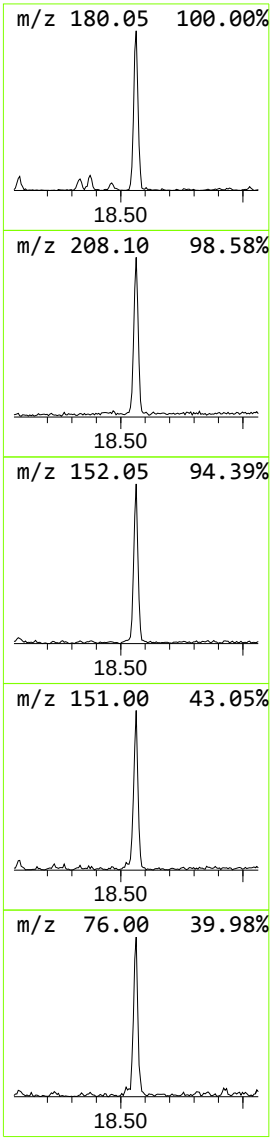
****

Peak Number 3 9,10-Anthracenedione Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.563	3.87 ng	138431	Phenanthrene-d10	17.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	95
2	1H-Phenalen-1-one	180	C13H8O	000548-39-0	83
3	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	83
4	9H-Fluoren-9-one	180	C13H8O	000486-25-9	70
5	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004737.D
Acq On : 12 Feb 2021 19:13
Operator : CG/JU
Sample : M1389-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

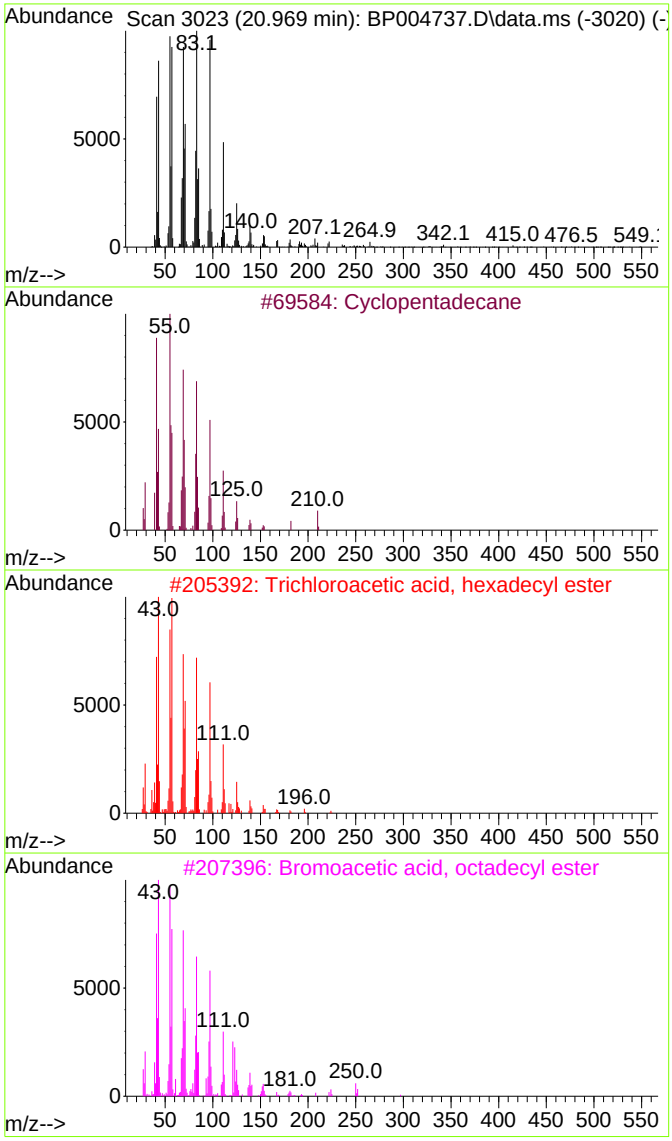
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

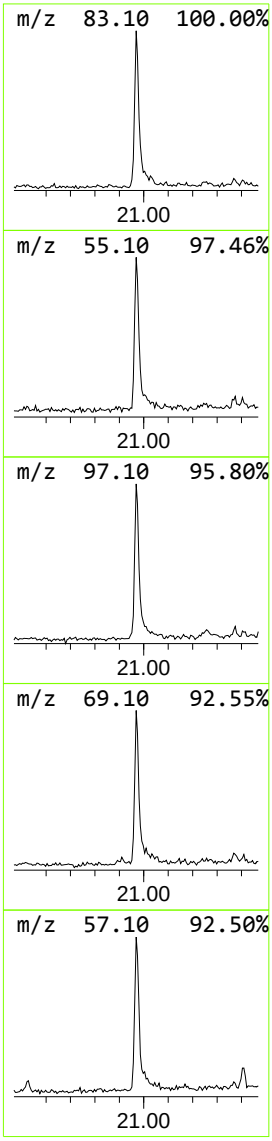
****

Peak Number 4 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.969	5.09 ng	363440	Chrysene-d12	21.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	93
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004737.D
Acq On : 12 Feb 2021 19:13
Operator : CG/JU
Sample : M1389-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-1

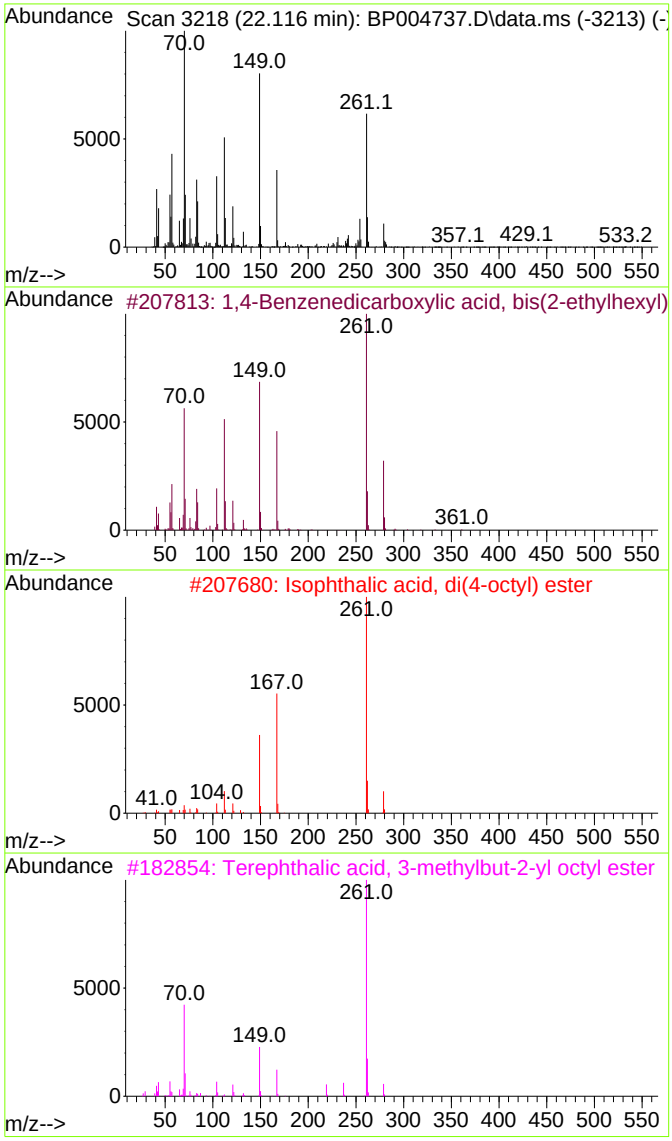
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

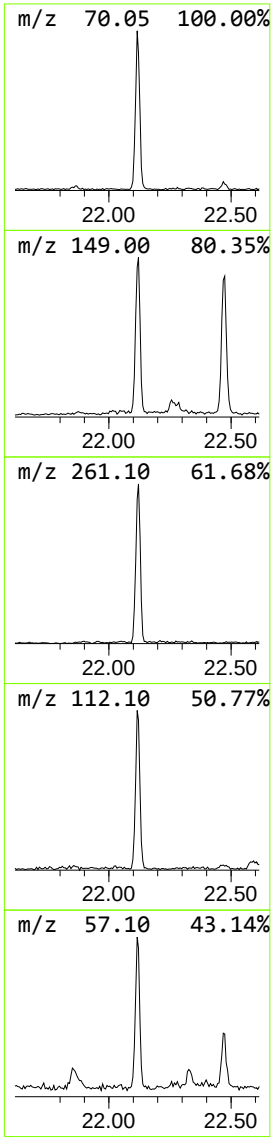
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.116	4.74 ng	338904	Chrysene-d12	21.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	74
2	Isophthalic acid, di(4-octyl) ester	390	C24H38O4	1000344-04-3	64
3	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	47
4	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	43
5	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004737.D
Acq On : 12 Feb 2021 19:13
Operator : CG/JU
Sample : M1389-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-1

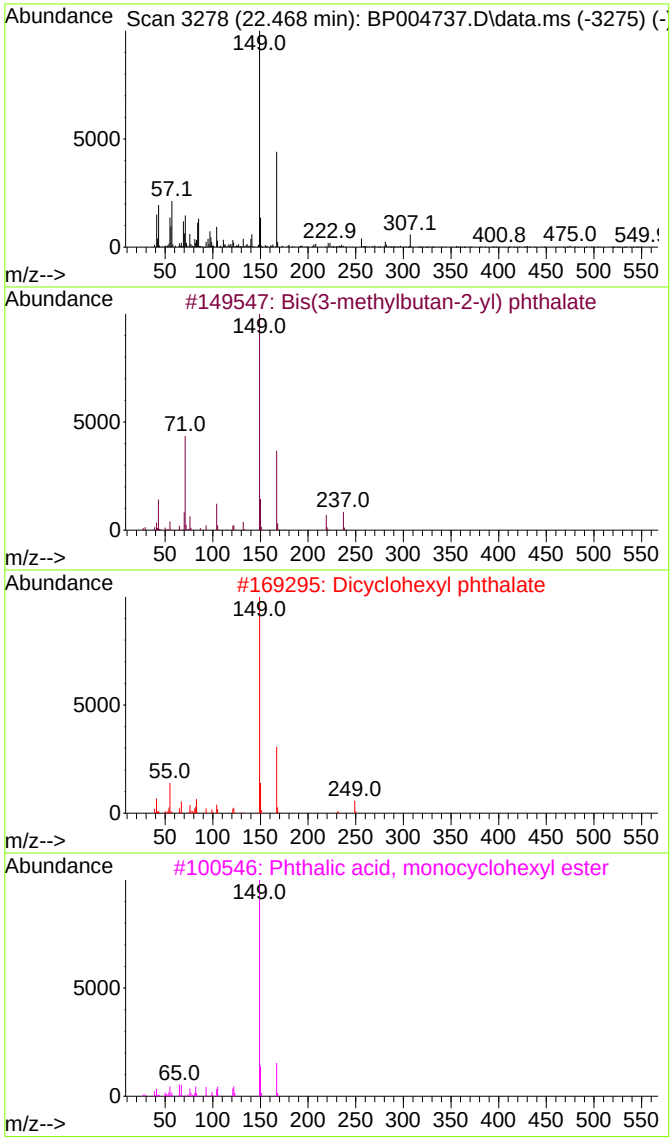
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

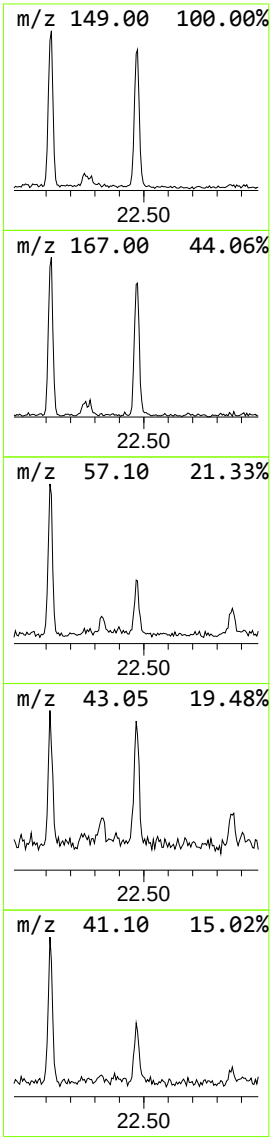
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Bis(3-methylbutan-2-yl) pht... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.468	3.53 ng	146370	Perylene-d12	23.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(3-methylbutan-2-yl) phthalate	306	C18H26O4	1000373-65-6	53
2	Dicyclohexyl phthalate	330	C20H26O4	000084-61-7	50
3	Phthalic acid, monocyclohexyl ester	248	C14H16O4	007517-36-4	50
4	Phthalic acid, octyl propyl ester	320	C19H28O4	1000309-10-8	49
5	Phthalic acid, 5-methylhex-2-yl ...	446	C28H46O4	1000371-08-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004737.D
Acq On : 12 Feb 2021 19:13
Operator : CG/JU
Sample : M1389-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

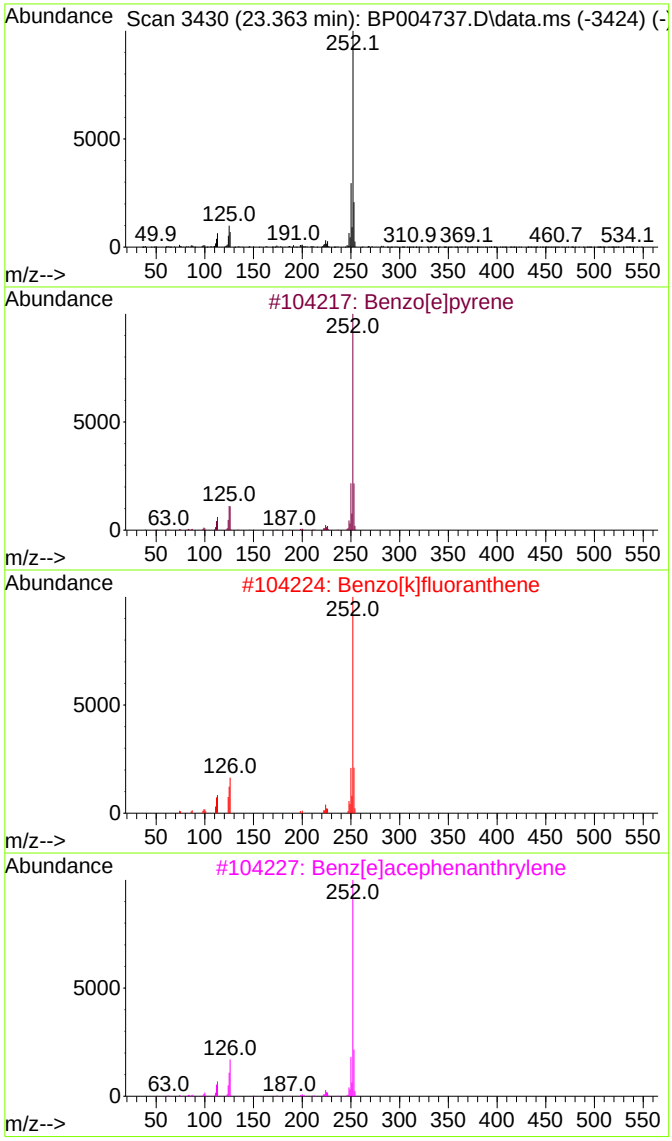
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

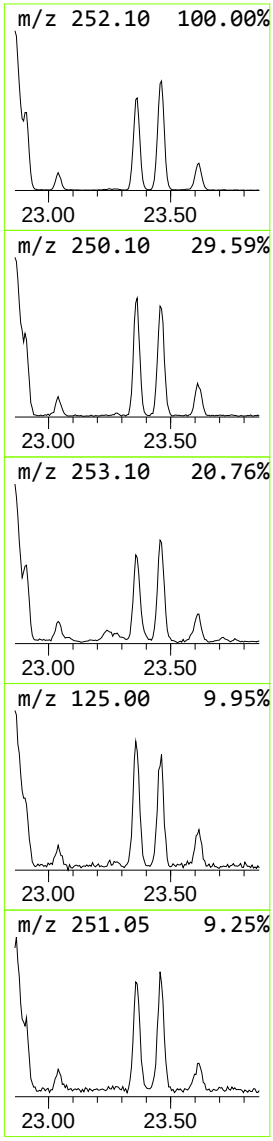
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.363	9.60 ng	398240	Perylene-d12	23.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Perylene	252	C20H12	000198-55-0	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004737.D
Acq On : 12 Feb 2021 19:13
Operator : CG/JU
Sample : M1389-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.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
Tridecanoic acid	18.069	9.5	ng	340707	4	17.169	714701	20.0
4H-Cyclopenta[d...	18.228	2.8	ng	99775	4	17.169	714701	20.0
9,10-Anthracene...	18.563	3.9	ng	138431	4	17.169	714701	20.0
Cyclopentadecane	20.969	5.1	ng	363440	5	21.257	1429180	20.0
1,4-Benzenedica...	22.116	4.7	ng	338904	5	21.257	1429180	20.0
Bis(3-methylbut...	22.468	3.5	ng	146370	6	23.563	829591	20.0
Benzo[e]pyrene	23.363	9.6	ng	398240	6	23.563	829591	20.0