LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005206.D
Acq On : 06 Apr 2021 20:33
Operator : CG/JU
Sample : M1924-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NB-07-040221

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: BP005206.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.293	368	375	384	rBV	309963	437621	30.33%	4.814%
2	6.875	637	644	656	rVB	284246	460053	31.88%	5.061%
3	7.693	776	783	791	rVB	87602	133593	9.26%	1.470%
4	8.852	972	980	991	rBV	169827	283957	19.68%	3.124%
5	10.481	1250	1257	1264	rBV	105163	176162	12.21%	1.938%
6	12.963	1672	1679	1687	rBV	413181	588839	40.81%	6.477%
7	13.810	1817	1823	1830	rBV2	9379	18544	1.29%	0.204%
8	14.351	1908	1915	1921	rBV2	150303	229295	15.89%	2.522%
9	15.404	2089	2094	2099	rBV	12436	19415	1.35%	0.214%
10	15.851	2162	2170	2177	rBV	274915	396392	27.47%	4.360%
11	16.075	2204	2208	2216	rBV8	7065	16428	1.14%	0.181%
12	17.110	2377	2384	2388	rBV	193943	267707	18.55%	2.945%
13	17.157	2388	2392	2397	rVB	59928	88035	6.10%	0.968%
14	17.245	2402	2407	2412	rVB	21790	31500	2.18%	0.346%
15	17.792	2495	2500	2506	rBV	385123	431340	29.89%	4.745%
16	17.986	2528	2533	2534	rBV	22648	26921	1.87%	0.296%
17	18.010	2534	2537	2547	rVB2	68808	126819	8.79%	1.395%
18	18.169	2559	2564	2569	rBV3	25645	49016	3.40%	0.539%
19	18.210	2569	2571	2576	rVB	14450	15682	1.09%	0.173%
20	18.475	2610	2616	2621	rBV4	9267	14575	1.01%	0.160%
21	18.898	2680	2688	2691	rBV	1177389	1442873	100.00%	15.872%
22	18.933	2691	2694	2703	rVV2	933351	1160921	80.46%	12.770%
23	19.057	2711	2715	2720	rVB	186983	217541	15.08%	2.393%
24	19.133	2720	2728	2736	rBV	139209	226400	15.69%	2.490%
25	19.251	2742	2748	2751	rBV5	22231	36596	2.54%	0.403%
26	19.486	2780	2788	2796	rVB	116174	181284	12.56%	1.994%
27	19.686	2817	2822	2833	rVB	733078	865528	59.99%	9.521%
28	19.969	2861	2870	2875	rBV2	26261	55898	3.87%	0.615%
29	20.016	2876	2878	2884	rVB7	14538	20714	1.44%	0.228%
30	20.069	2884	2887	2890	rVB2	19454	21623	1.50%	0.238%
31	20.128	2893	2897	2900	rBV	37912	43291	3.00%	0.476%
32	20.163	2900	2903	2909	rVB6	24468	35780	2.48%	0.394%
33	20.222	2909	2913	2917	rBV6	24485	33660	2.33%	0.370%
34	20.257	2917	2919	2922	rBV	14436	16191	1.12%	0.178%
35	20.428	2944	2948	2952	rVB7	16604	23718	1.64%	0.261%
36	20.927	3029	3033	3040	rVB3	71614	106691	7.39%	1.174%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005206.D
Acq On : 06 Apr 2021 20:33
Operator : CG/JU
Sample : M1924-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NB-07-040221

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	21.051	3051	3054	3058	rBV4	14965	22023	1.53%	0.242%
38	21.210	3075	3081	3085	rBV2	274982	410866	28.48%	4.520%
39	21.245	3085	3087	3092	rVB	53258	58636	4.06%	0.645%
40	23.486	3463	3468	3474	rVB2	166301	298830	20.71%	3.287%

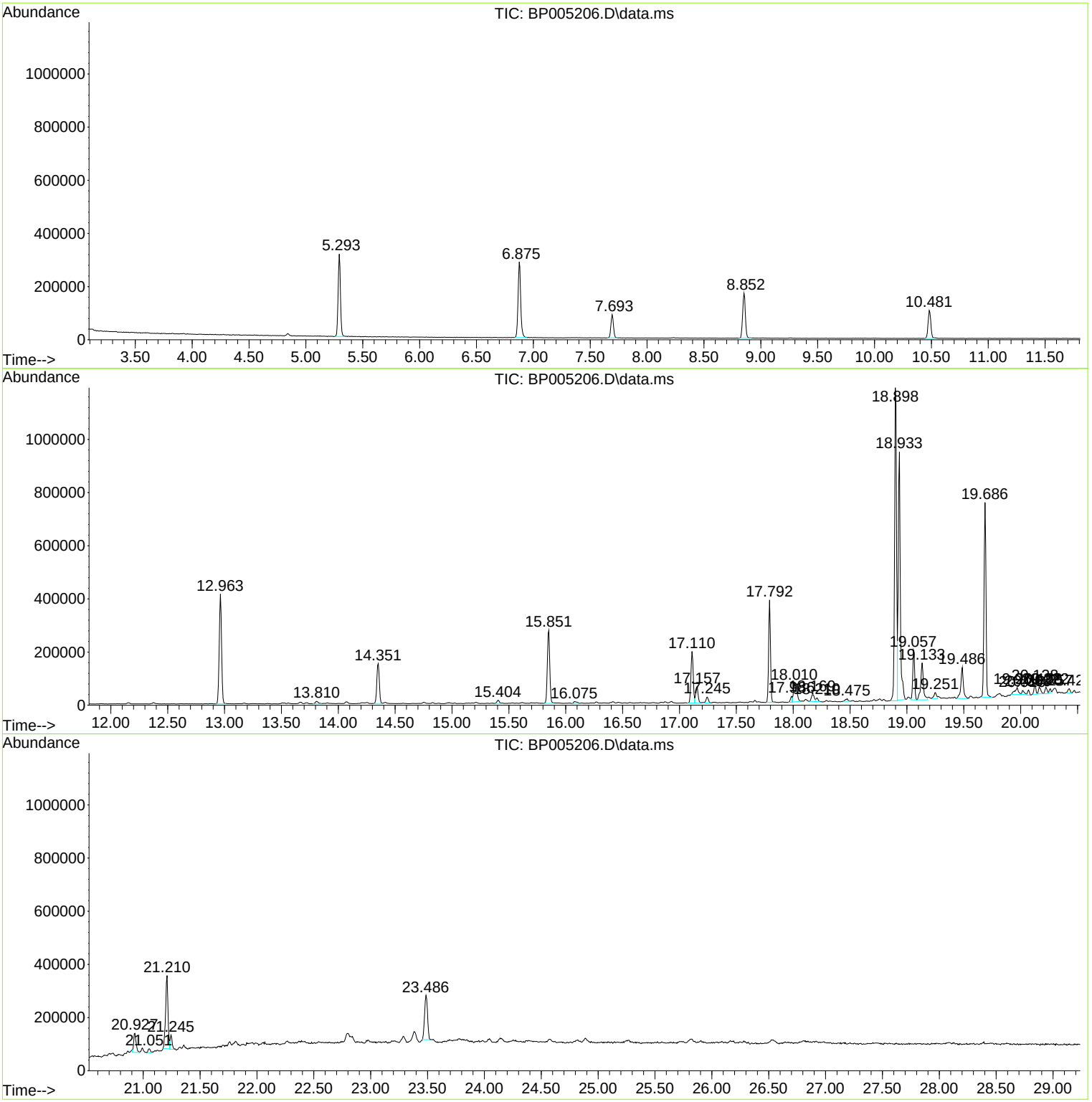
Sum of corrected areas: 9090958

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005206.D
Acq On : 06 Apr 2021 20:33
Operator : CG/JU
Sample : M1924-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NB-07-040221

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\BP040621\
Data File : BP005206.D
Acq On : 06 Apr 2021 20:33
Operator : CG/JU
Sample : M1924-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NB-07-040221

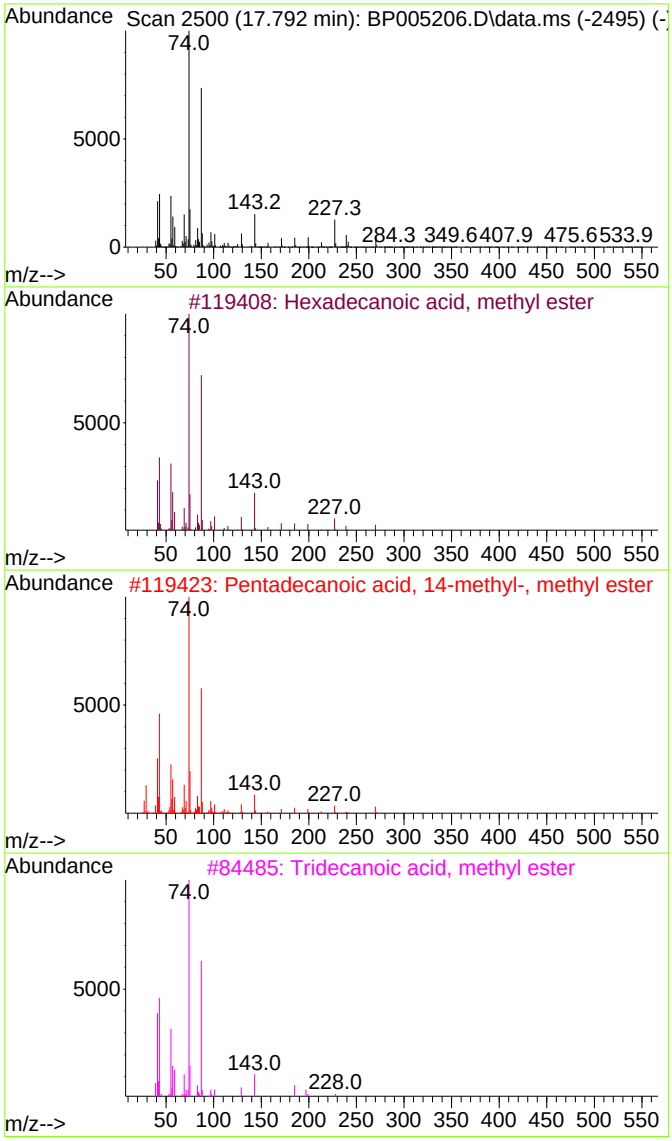
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

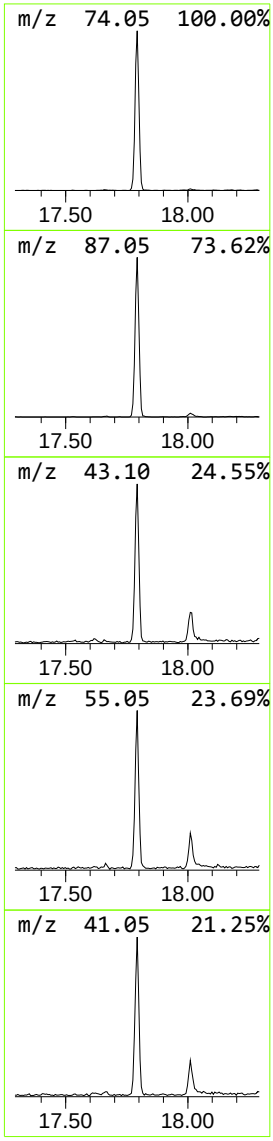
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.792	32.22 ng	431340	Phenanthrene-d10	17.110

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	96
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005206.D
Acq On : 06 Apr 2021 20:33
Operator : CG/JU
Sample : M1924-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NB-07-040221

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

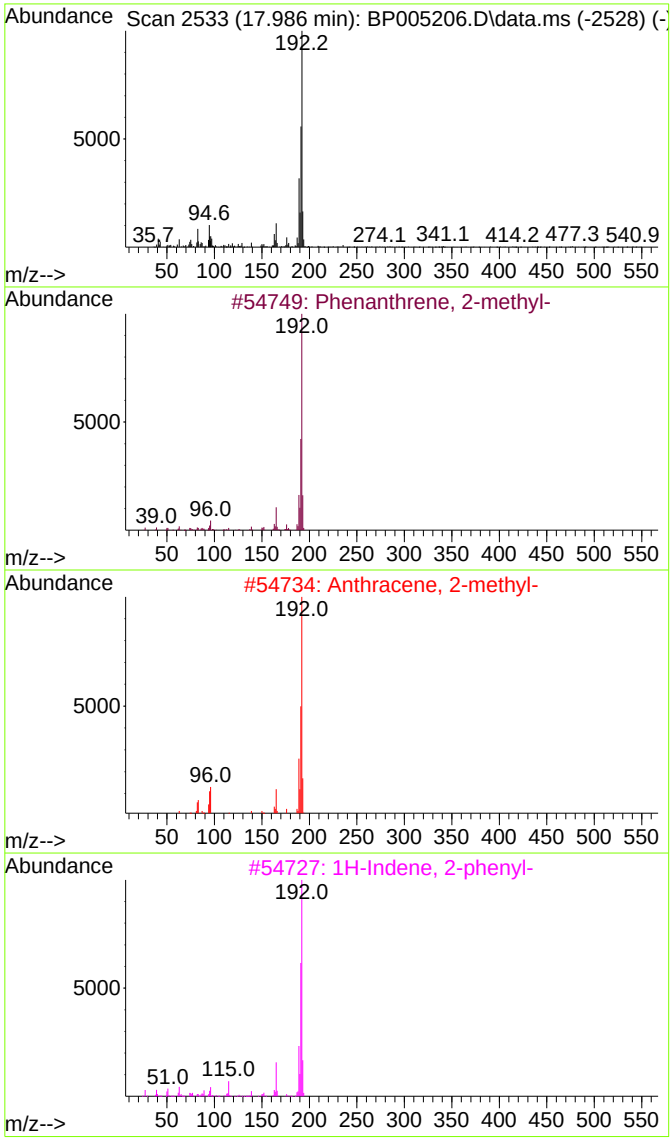
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

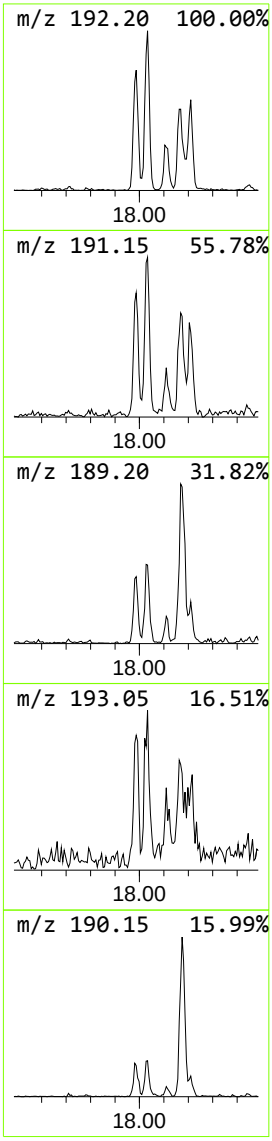
****

Peak Number 2 Phenanthrene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.986	2.01 ng	26921	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	81
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	81
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005206.D
Acq On : 06 Apr 2021 20:33
Operator : CG/JU
Sample : M1924-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NB-07-040221

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

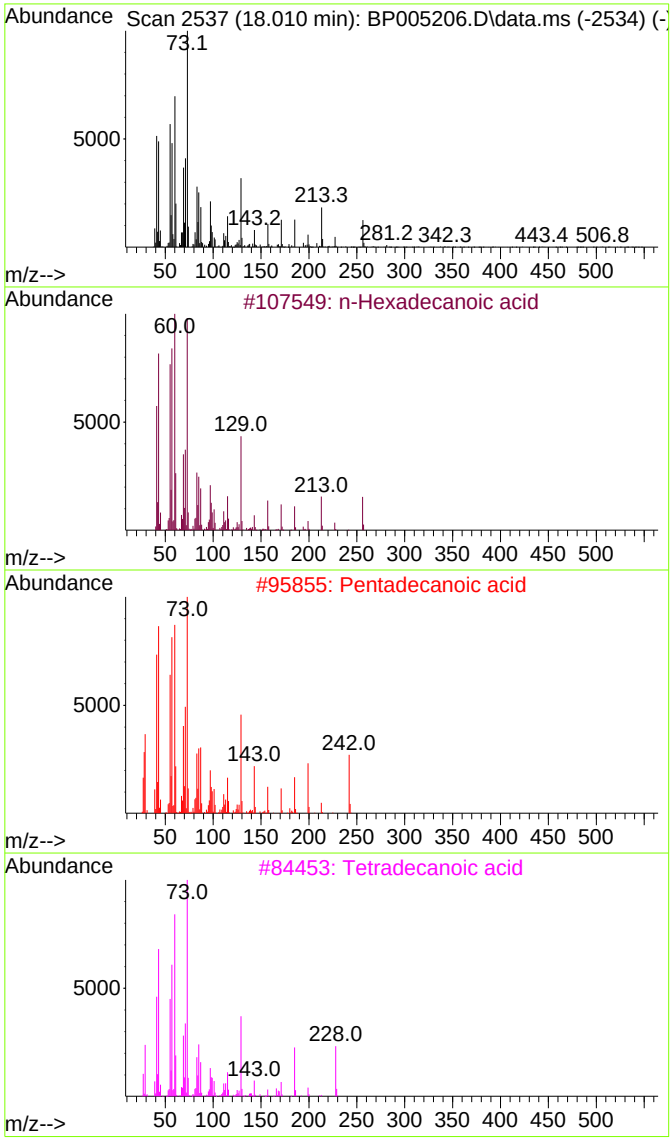
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

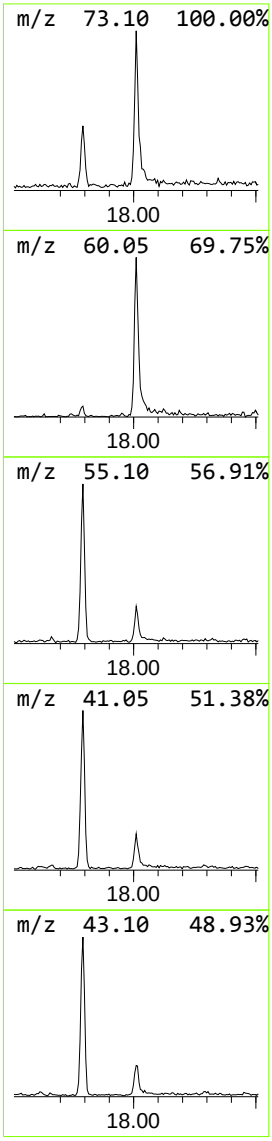
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.010	9.47 ng	126819	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	Octadecanoic acid	284	C18H36O2	000057-11-4	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005206.D
Acq On : 06 Apr 2021 20:33
Operator : CG/JU
Sample : M1924-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NB-07-040221

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

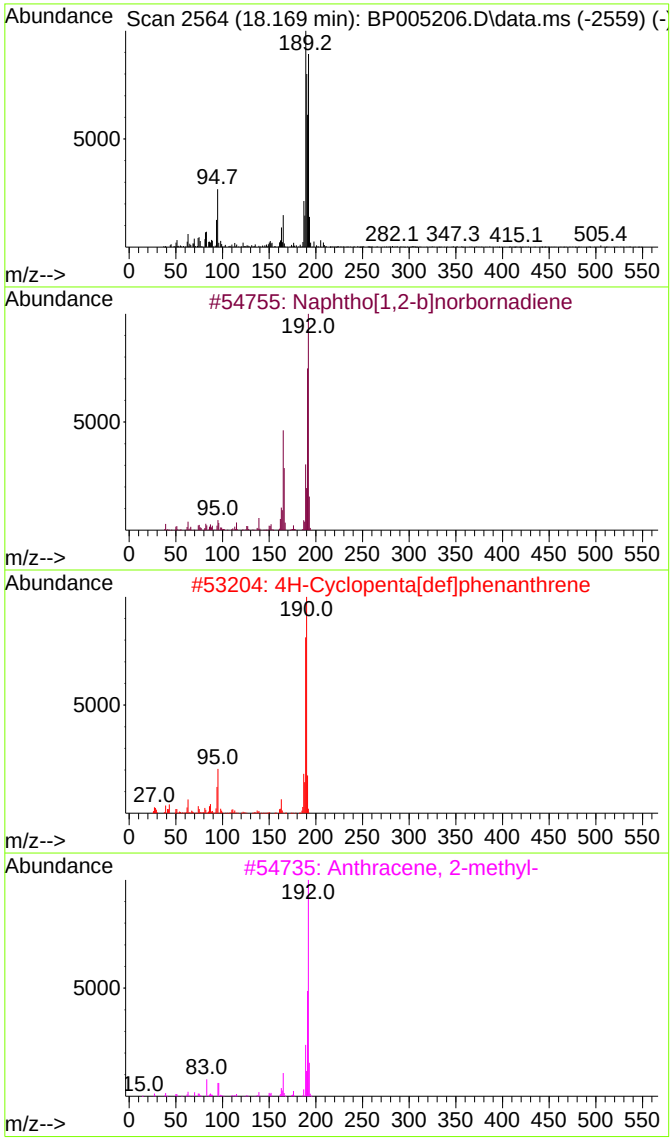
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

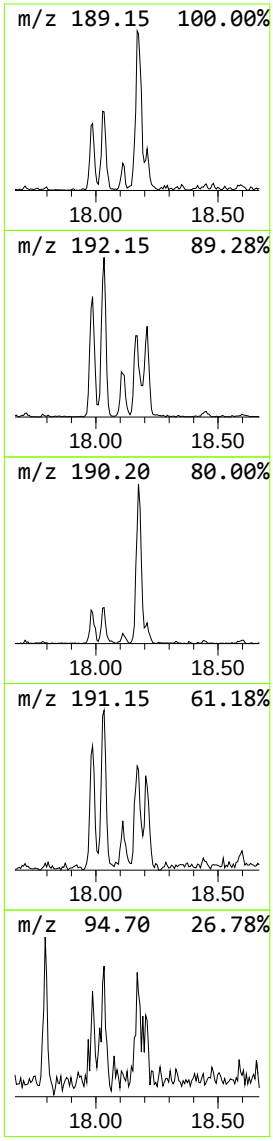
****

Peak Number 4 unknown18.169 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.169	3.66 ng	49016	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	46
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	35
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	30
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	30
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005206.D
Acq On : 06 Apr 2021 20:33
Operator : CG/JU
Sample : M1924-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NB-07-040221

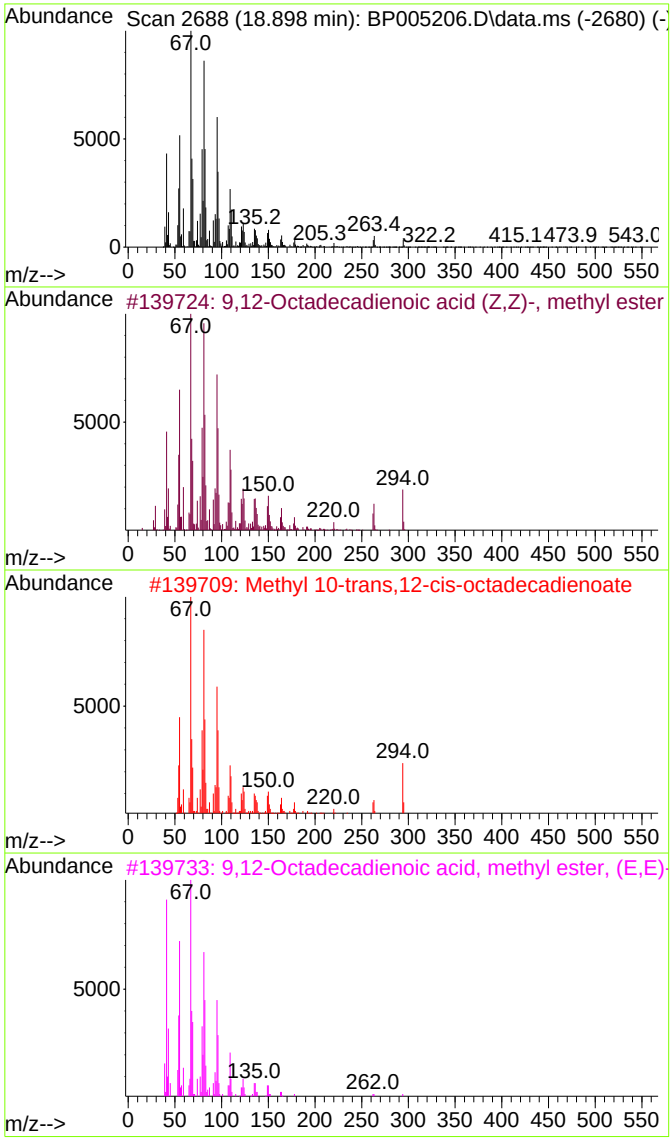
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

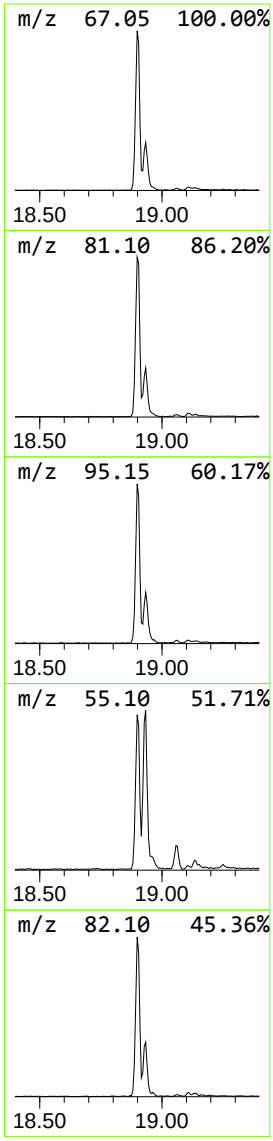
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.898	107.80 ng	1442870	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	95
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	95
4	cis-7-Dodecen-1-yl acetate	226	C14H26O2	014959-86-5	94
5	12,15-Octadecadienoic acid, meth...	294	C19H34O2	057156-97-5	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005206.D
Acq On : 06 Apr 2021 20:33
Operator : CG/JU
Sample : M1924-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NB-07-040221

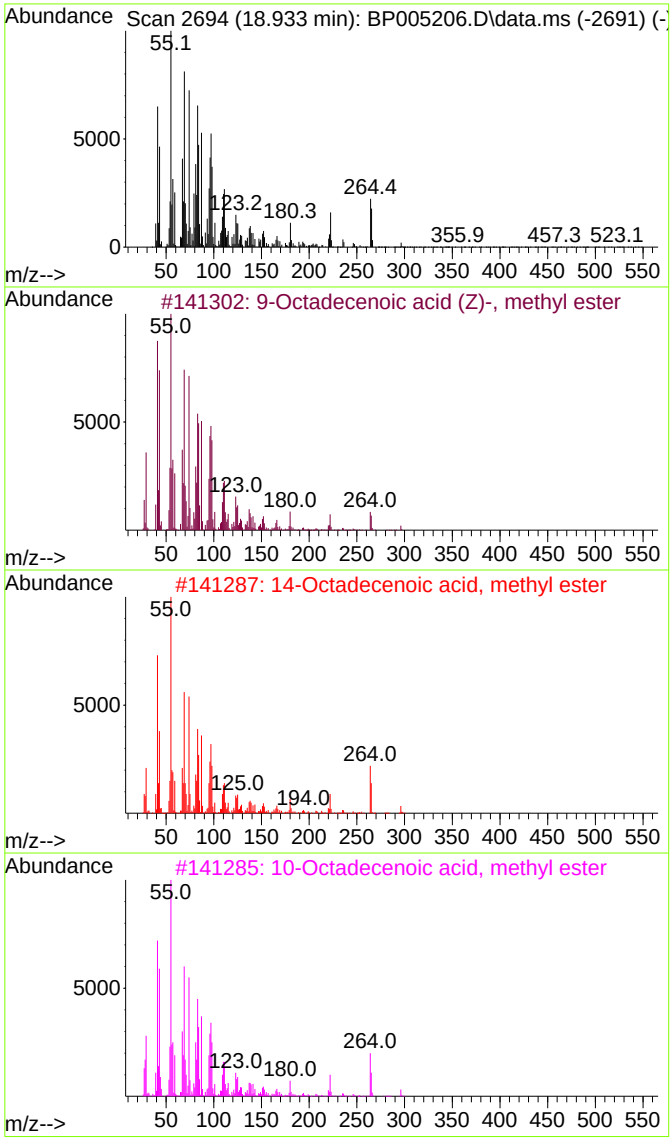
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

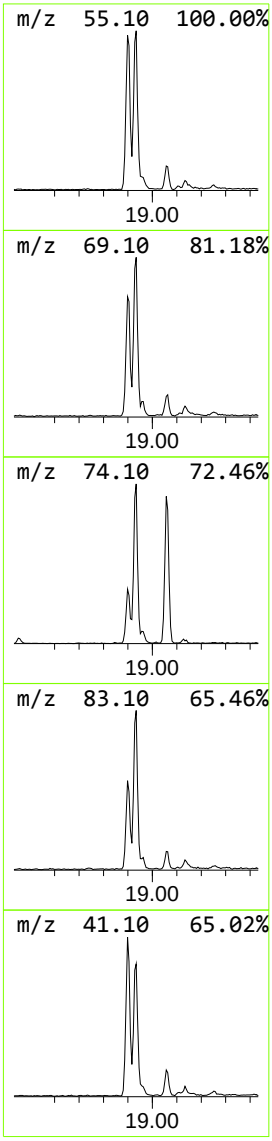
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.933	86.73 ng	1160920	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005206.D
Acq On : 06 Apr 2021 20:33
Operator : CG/JU
Sample : M1924-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NB-07-040221

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

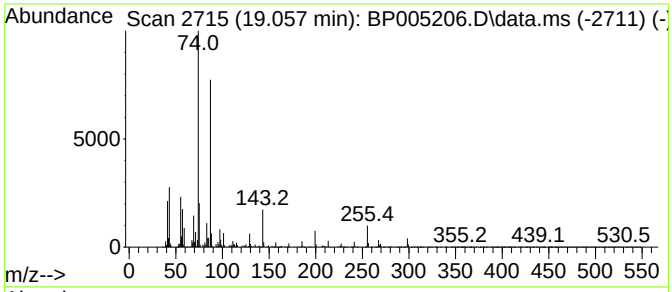
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

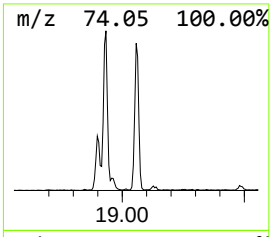
****

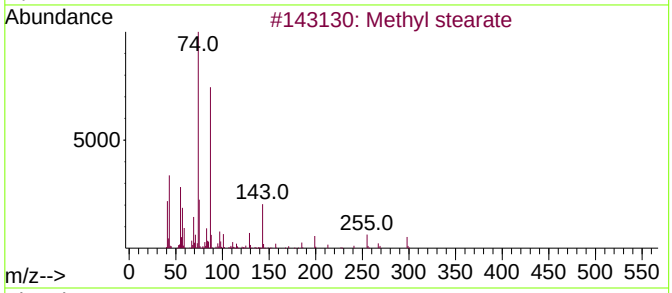
Peak Number 7 Methyl stearate Concentration Rank 4

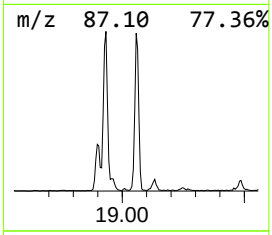
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.057	16.25 ng	217541	Phenanthrene-d10	17.110

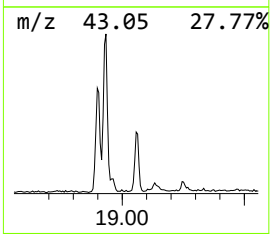
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	99
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
4	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	90
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87

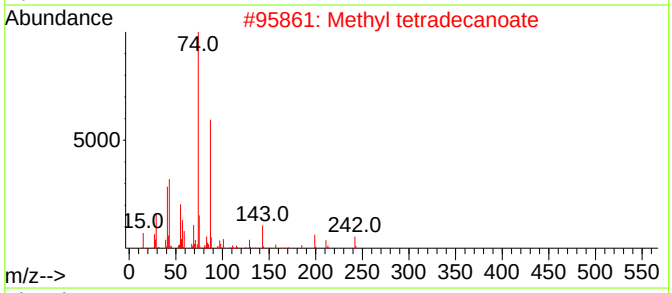


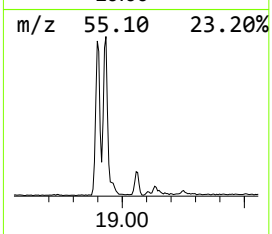


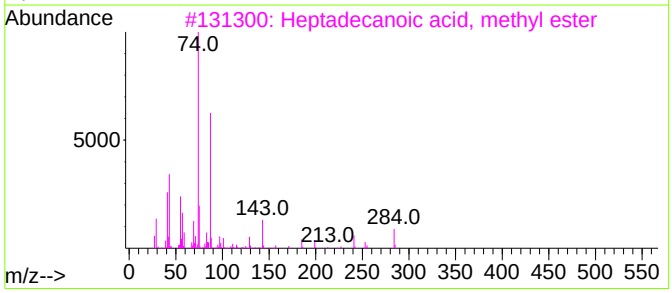


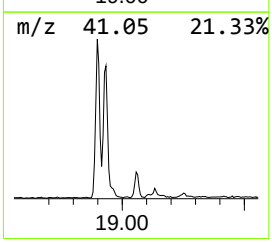












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005206.D
Acq On : 06 Apr 2021 20:33
Operator : CG/JU
Sample : M1924-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NB-07-040221

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

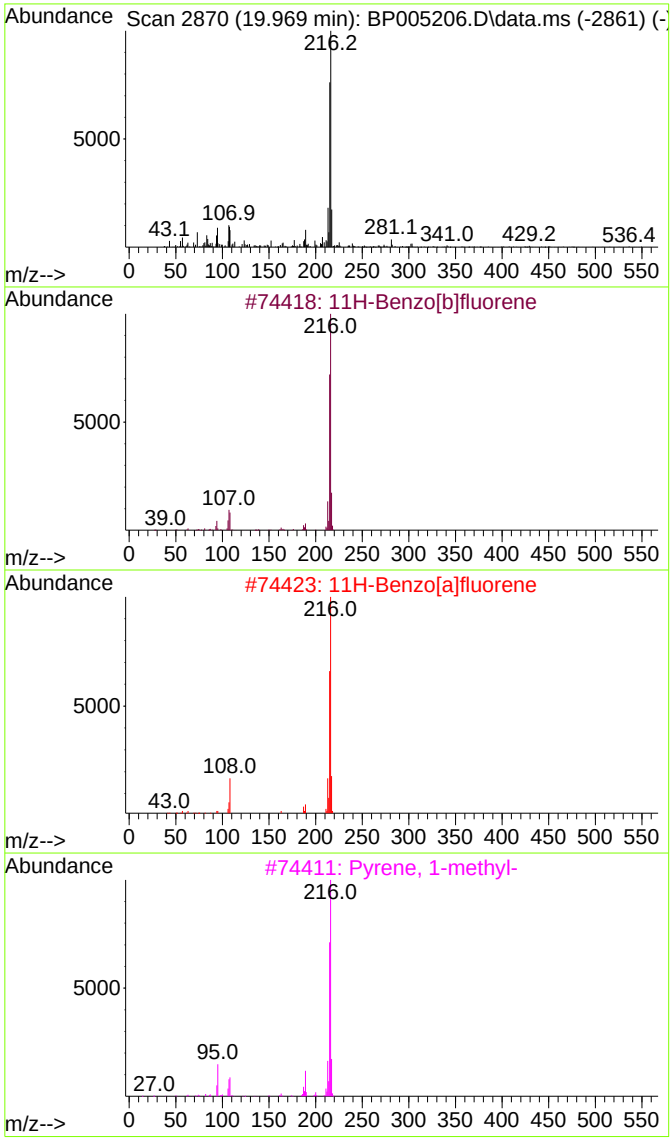
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

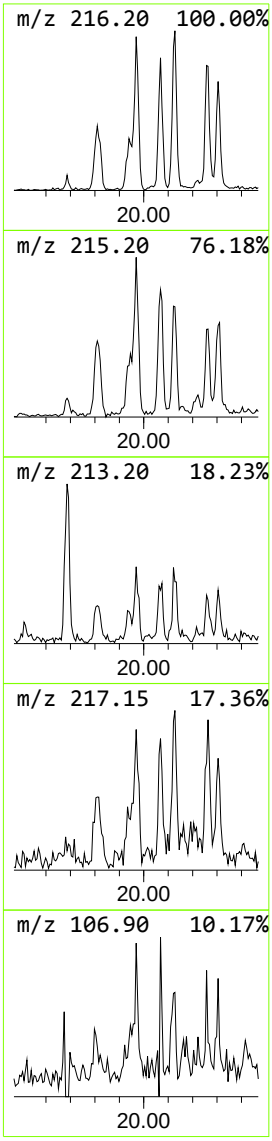
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.969	2.72 ng	55898	Chrysene-d12	21.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	80
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005206.D
Acq On : 06 Apr 2021 20:33
Operator : CG/JU
Sample : M1924-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NB-07-040221

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

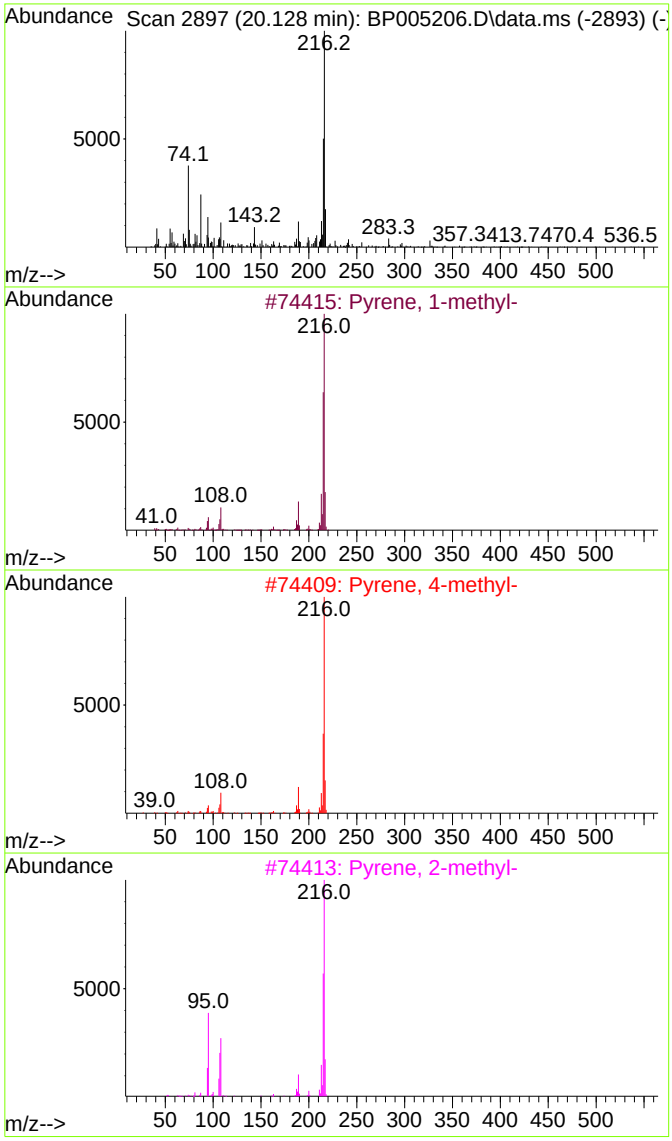
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

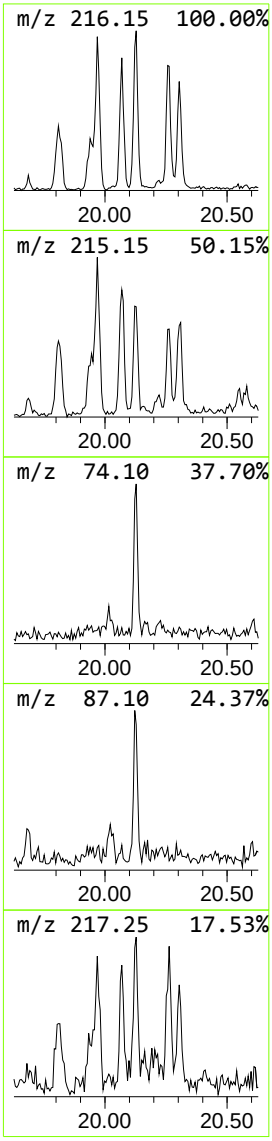
****

Peak Number 9 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.128	2.11 ng	43291	Chrysene-d12	21.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	96
2	Pyrene, 4-methyl-	216	C17H12	003353-12-6	95
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	90
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	68
5	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005206.D
Acq On : 06 Apr 2021 20:33
Operator : CG/JU
Sample : M1924-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NB-07-040221

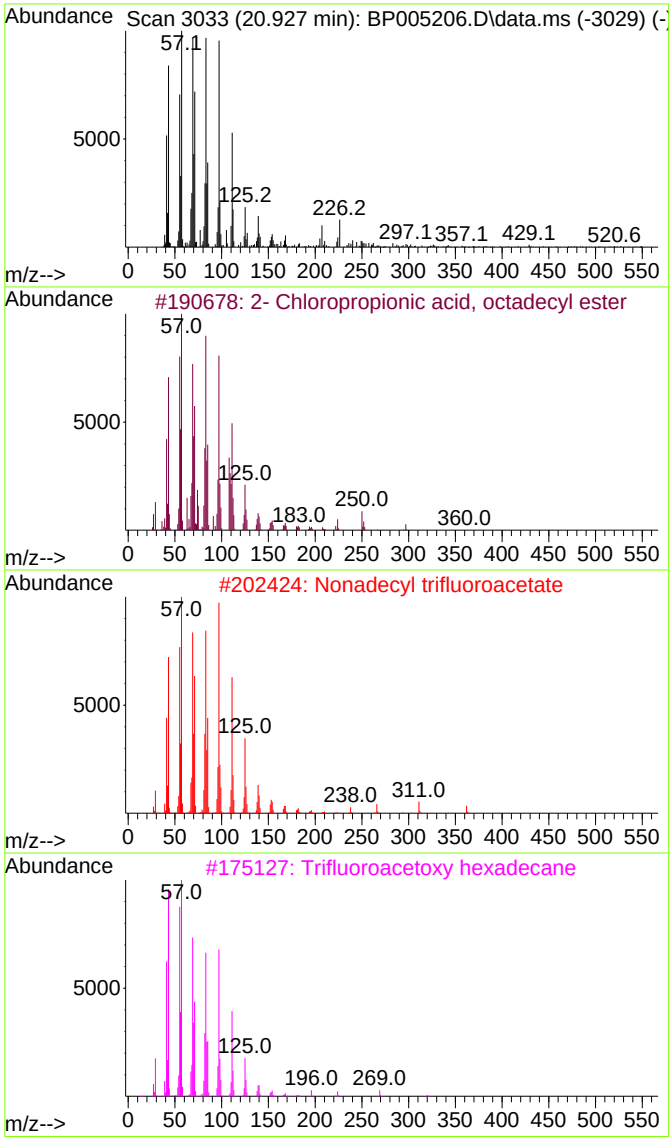
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

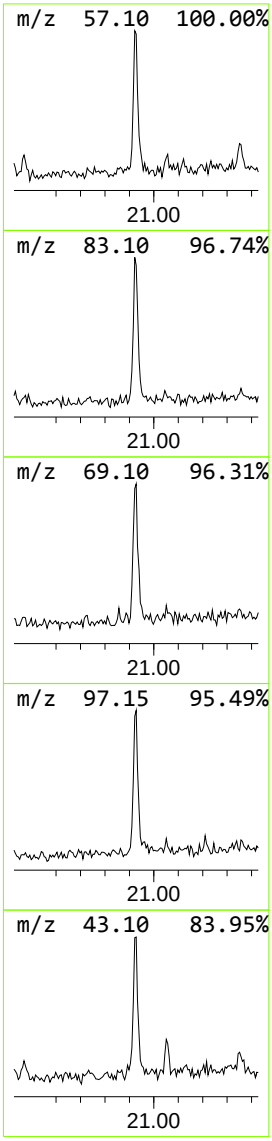
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2- Chloropropionic acid, oc... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.927	5.19 ng	106691	Chrysene-d12	21.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
2	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040621\
Data File : BP005206.D
Acq On : 06 Apr 2021 20:33
Operator : CG/JU
Sample : M1924-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NB-07-040221

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
Hexadecanoic ac...	17.792	32.2	ng	431340	4	17.110	267707	20.0
Phenanthrene, 2...	17.986	2.0	ng	26921	4	17.110	267707	20.0
n-Hexadecanoic ...	18.010	9.5	ng	126819	4	17.110	267707	20.0
unknown18.169	18.169	3.7	ng	49016	4	17.110	267707	20.0
9,12-Octadecadi...	18.898	107.8	ng	1442870	4	17.110	267707	20.0
9-Octadecenoic ...	18.933	86.7	ng	1160920	4	17.110	267707	20.0
Methyl stearate	19.057	16.3	ng	217541	4	17.110	267707	20.0
11H-Benzo[b]flu...	19.969	2.7	ng	55898	5	21.210	410866	20.0
Pyrene, 1-methyl-	20.128	2.1	ng	43291	5	21.210	410866	20.0
2- Chloropropio...	20.927	5.2	ng	106691	5	21.210	410866	20.0