LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091421\
Data File : BF125493.D
Acq On : 15 Sep 2021 1:27
Operator : JU/CG
Sample : M3725-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HR-01-091321

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_F\METHODS\8270-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125493.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	12	rVB	262918	313115	1.31%	0.489%
2	5.493	575	579	593	rBV	494630	533919	2.23%	0.834%
3	6.145	687	690	694	rBV	333783	312535	1.30%	0.488%
4	6.504	748	751	760	rBV	569303	577529	2.41%	0.902%
5	6.875	810	814	817	rBV	1033991	848951	3.54%	1.326%
6	7.434	906	909	917	rBV	464845	403858	1.68%	0.631%
7	7.916	985	991	1002	rBV	142404	276355	1.15%	0.432%
8	8.157	1028	1032	1035	rBV	1333636	1031263	4.30%	1.611%
9	9.228	1211	1214	1220	rBV	830118	704939	2.94%	1.101%
10	9.916	1327	1331	1334	rBV	1179229	1010555	4.21%	1.579%
11	10.704	1462	1465	1471	rBV2	276906	283883	1.18%	0.443%
12	11.404	1580	1584	1586	rBV	1053127	893777	3.73%	1.396%
13	11.427	1586	1588	1591	rVV	1360770	1015528	4.23%	1.586%
14	11.480	1591	1597	1600	rVB	242137	241194	1.01%	0.377%
15	11.798	1646	1651	1654	rBV	6269705	6261883	26.11%	9.782%
16	11.945	1671	1676	1681	rBV2	1510643	2004118	8.36%	3.131%
17	12.016	1686	1688	1696	rVB3	204389	345818	1.44%	0.540%
18	12.504	1758	1771	1773	rBV	11021577	23983593	100.00%	37.466%
19	12.527	1773	1775	1779	rVV2	10941009	10159434	42.36%	15.870%
20	12.586	1782	1785	1788	rVB	4060910	3373851	14.07%	5.270%
21	12.622	1788	1791	1794	rBV	1138331	948229	3.95%	1.481%
22	12.722	1804	1808	1811	rBV	1737072	1754313	7.31%	2.740%
23	12.851	1825	1830	1834	rVB2	856856	952146	3.97%	1.487%
24	12.992	1848	1854	1857	rBV	686346	679573	2.83%	1.062%
25	13.180	1878	1886	1889	rBV	178399	321790	1.34%	0.503%
26	13.227	1892	1894	1900	rVB2	295163	334556	1.39%	0.523%
27	13.310	1905	1908	1912	rVB	458092	416995	1.74%	0.651%
28	13.974	2018	2021	2026	rBV	466206	399750	1.67%	0.624%
29	14.051	2029	2034	2036	rVV2	1042496	1314922	5.48%	2.054%
30	14.074	2036	2038	2041	rVB	458369	369545	1.54%	0.577%
31	15.104	2209	2213	2216	rBV	325469	503007	2.10%	0.786%
32	15.410	2262	2265	2271	rVB	214987	280469	1.17%	0.438%
33	15.474	2272	2276	2282	rVB	296945	352804	1.47%	0.551%
34	15.539	2282	2287	2291	rBV	608555	810747	3.38%	1.266%

Sum of corrected areas: 64014944

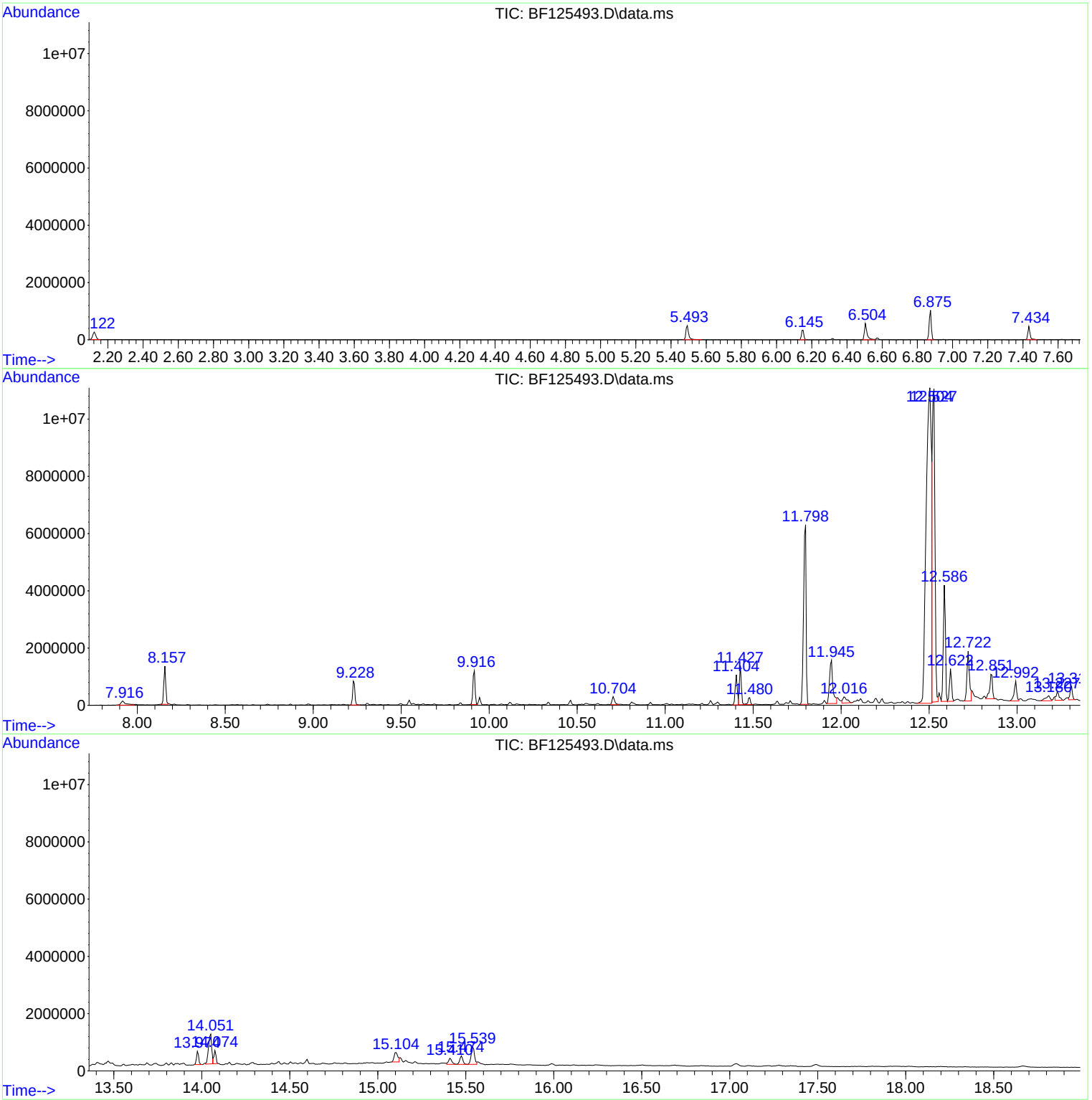
Instrument :
BNA_F
ClientSampleId :
HR-01-091321

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091421\
Data File : BF125493.D
Acq On : 15 Sep 2021 1:27
Operator : JU/CG
Sample : M3725-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-01-091321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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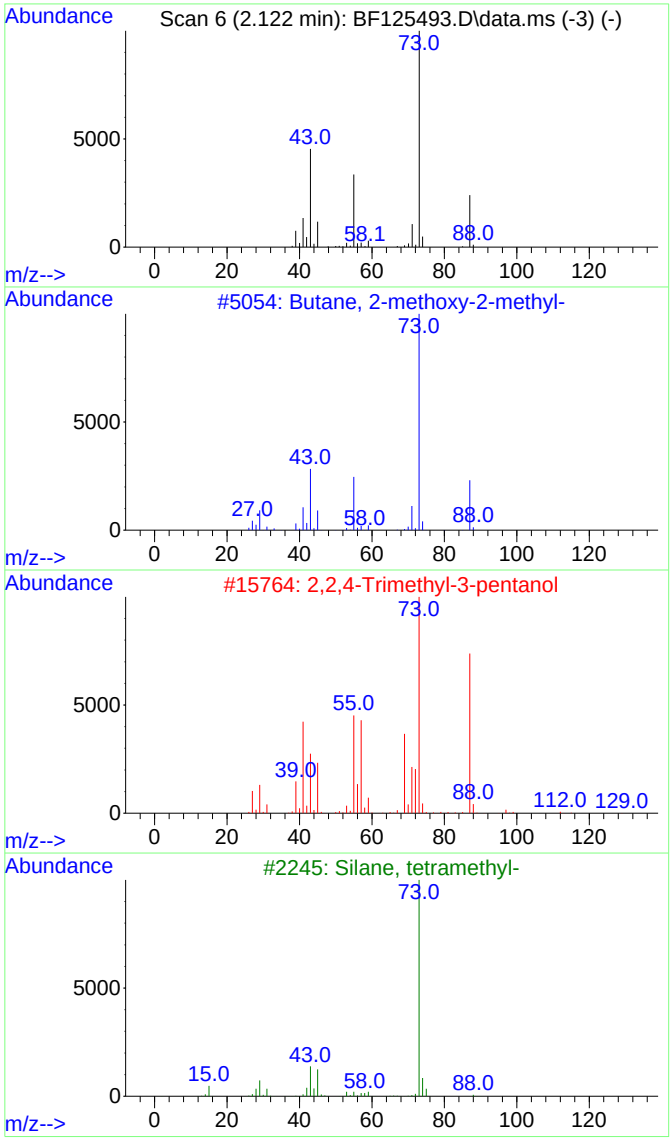
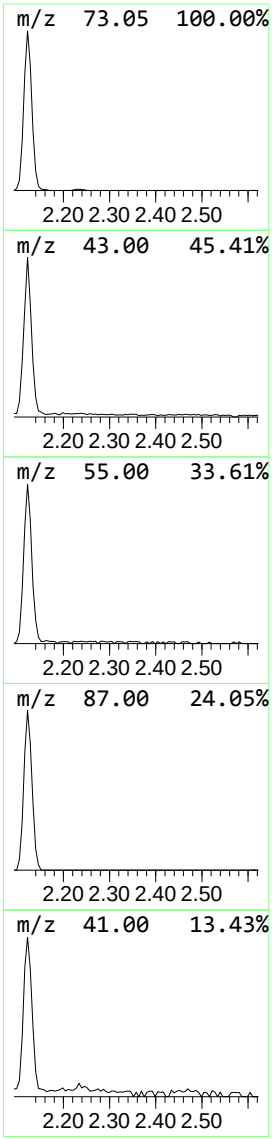
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	7.38 ng	313115	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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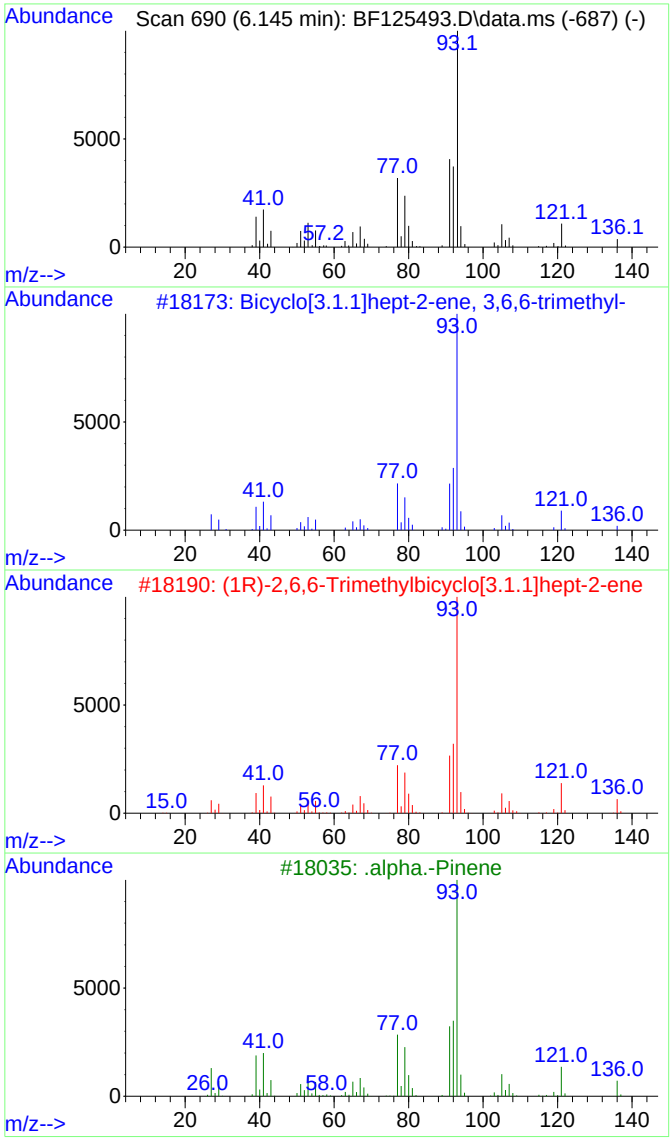
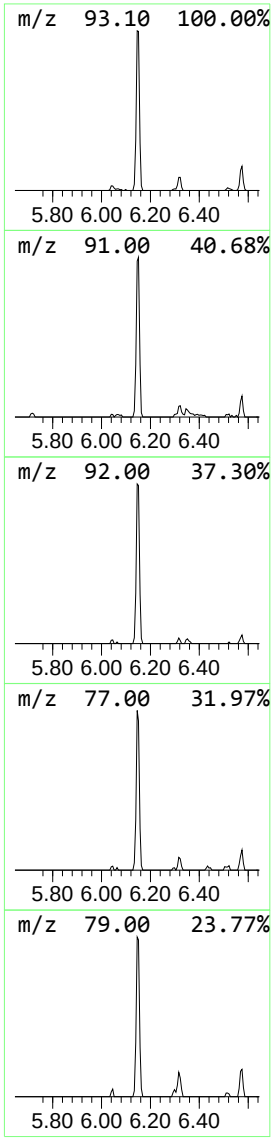
****
Peak Number 2 Bicyclo[3.1.1]hept-2-ene, 3... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.145	7.36 ng	312535	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	94
2	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	94
3	.alpha.-Pinene	136	C10H16	000080-56-8	91
4	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
5	3,5-Methanocyclopentapyrazole, 3...	164	C10H16N2	087143-58-6	90





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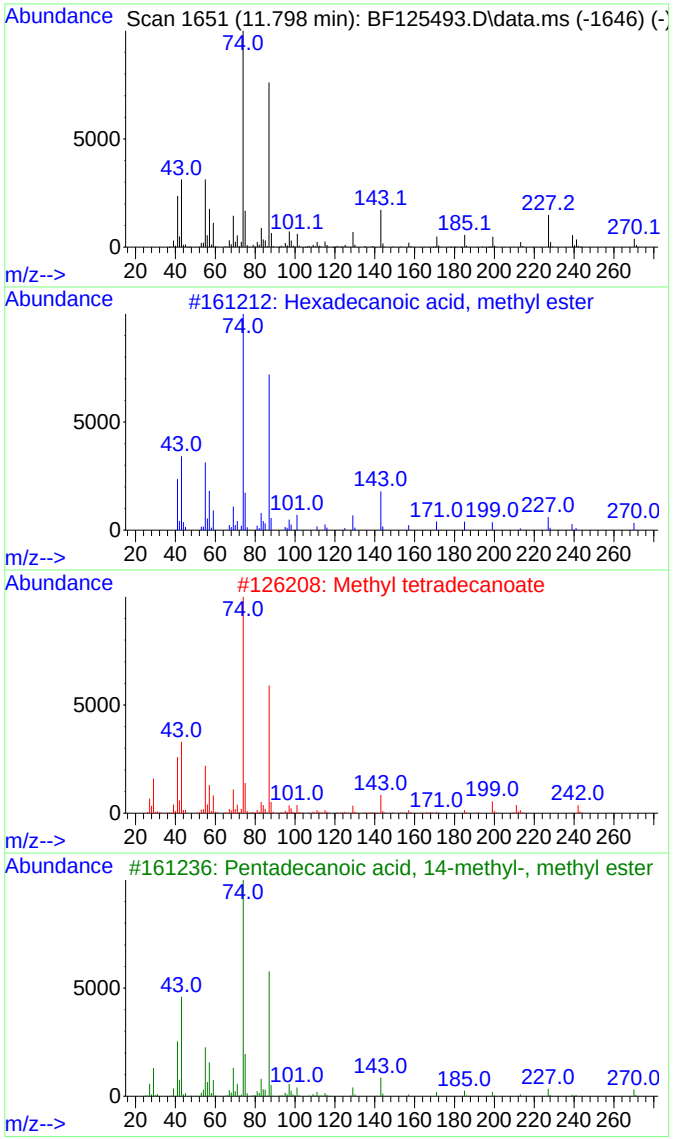
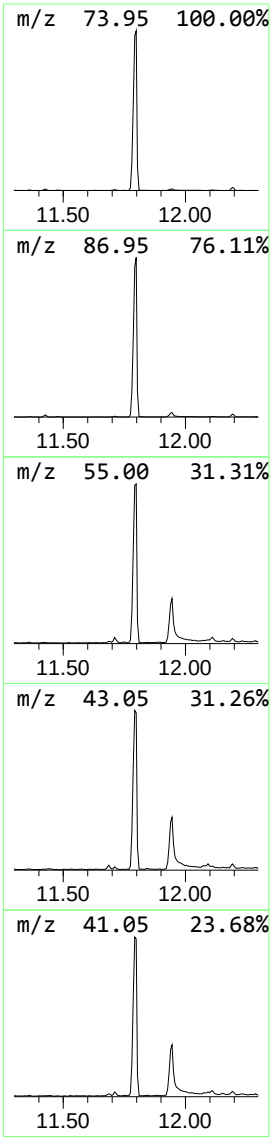
****
Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.798	140.12 ng	6261880	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	81





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Sample : M3725-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-01-091321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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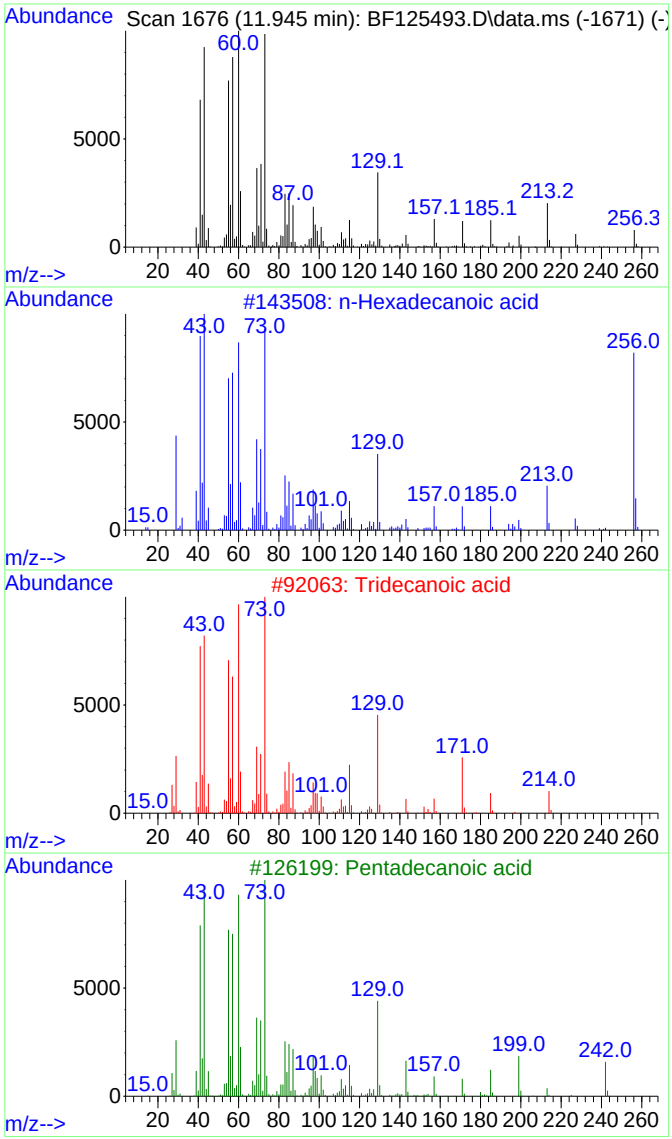
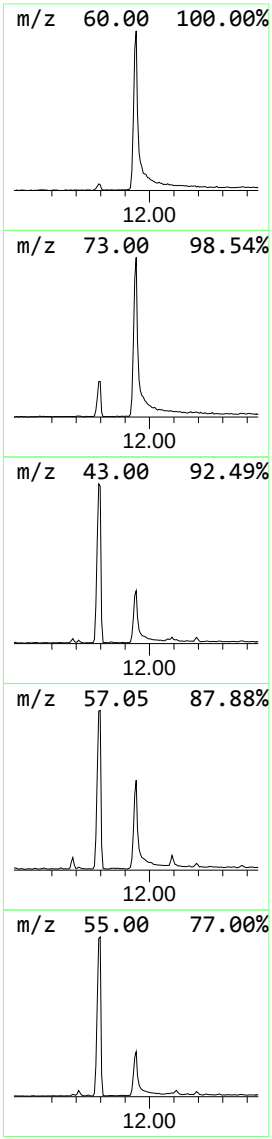
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	44.85 ng	2004120	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	70





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Sample : M3725-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-01-091321

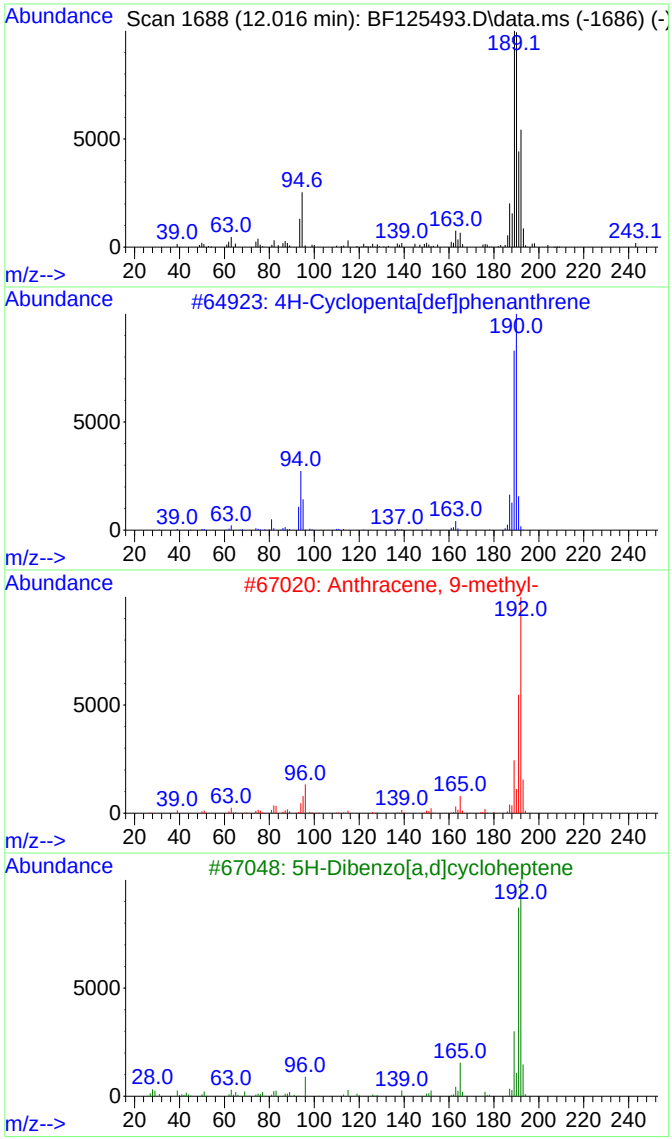
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

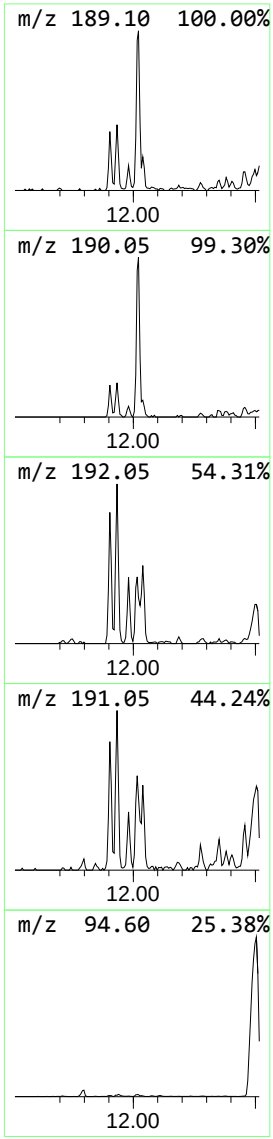
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.016	7.74 ng	345818	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	18
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	18
4	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	14
5	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	14





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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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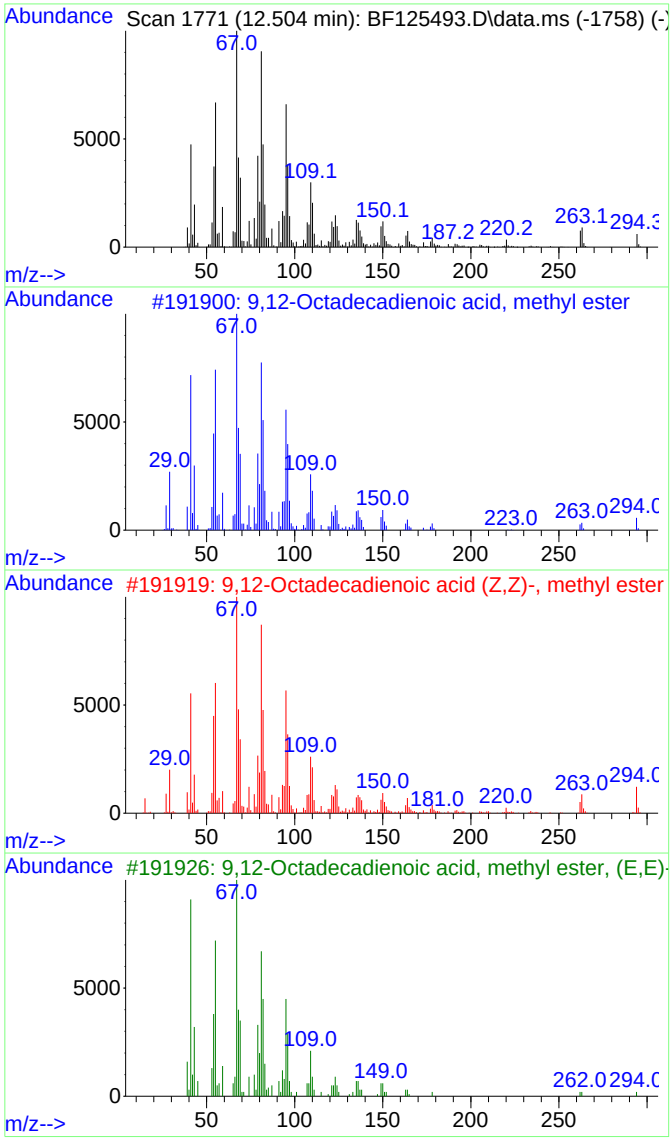
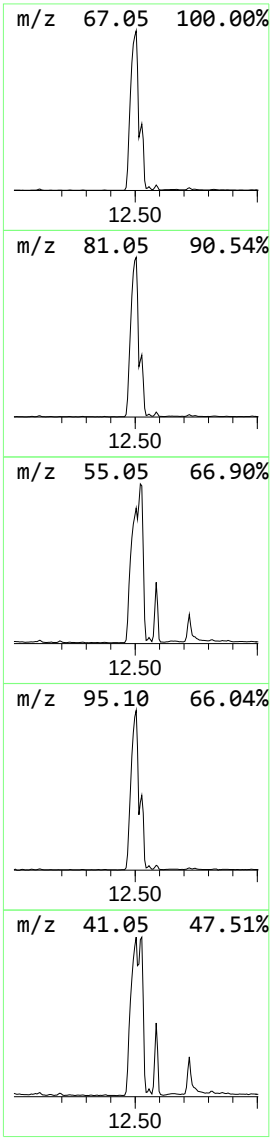
****
Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.504	536.68 ng	23983600	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99





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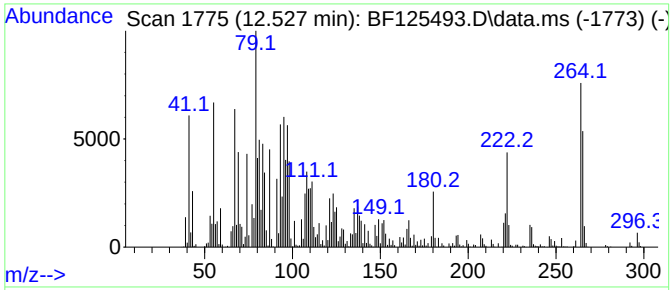
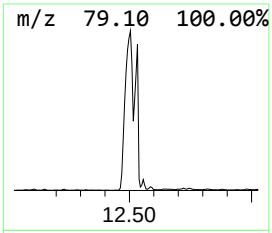
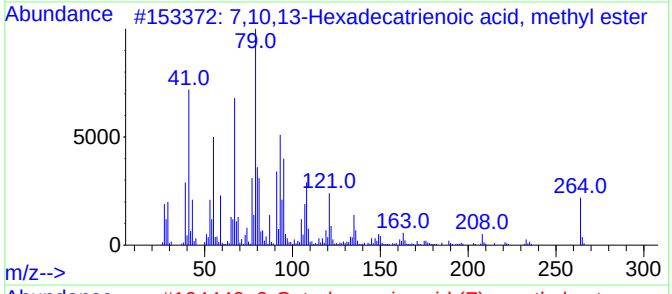
****
Peak Number 7 7,10,13-Hexadecatrienoic ac... Concentration Rank 2

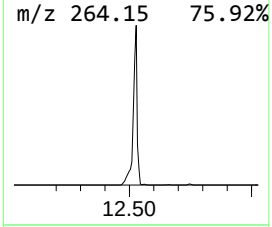
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	227.34 ng	10159400	Phenanthrene-d10	11.404

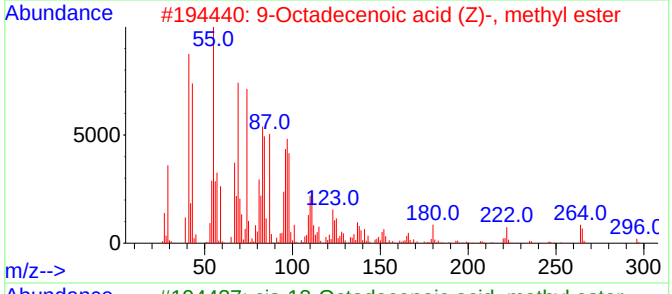
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,10,13-Hexadecatrienoic acid, m...	264	C17H28O2	056554-30-4	70
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	70
3	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	66
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	60
5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	56

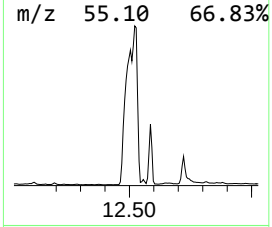


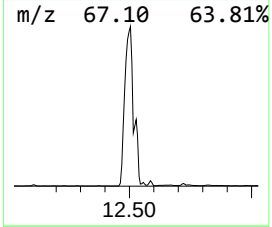


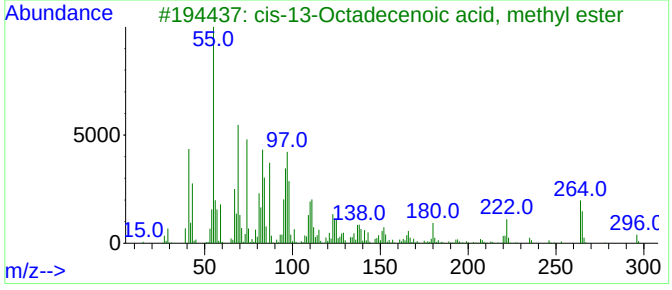


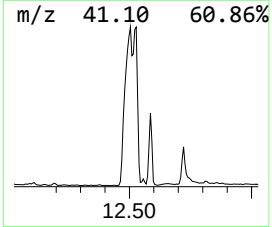












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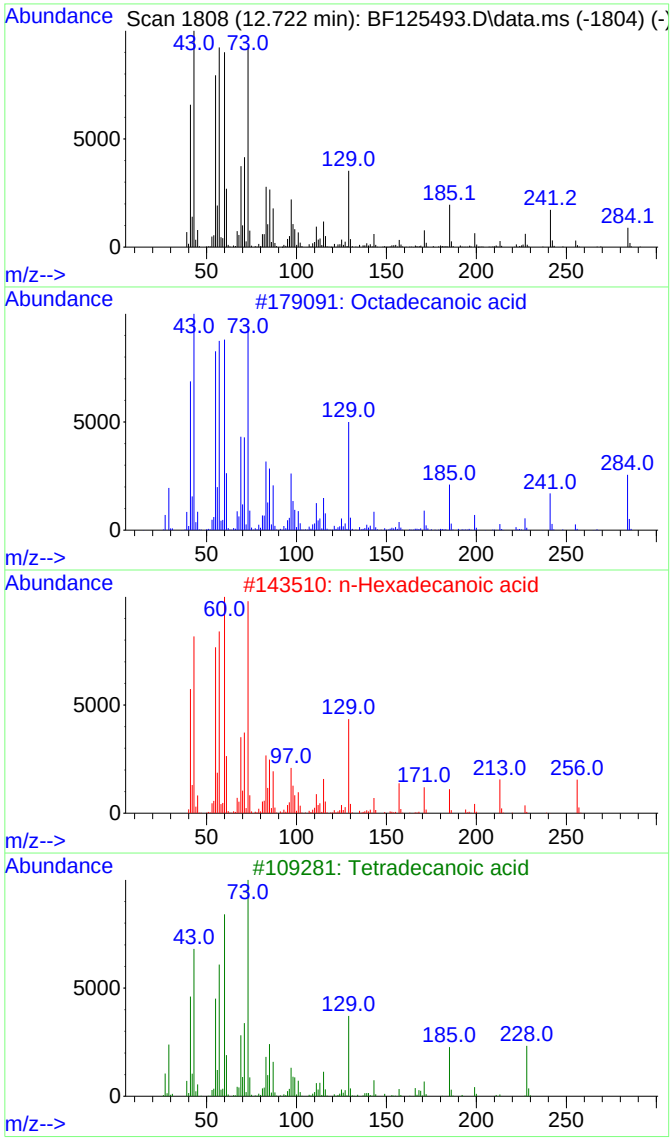
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

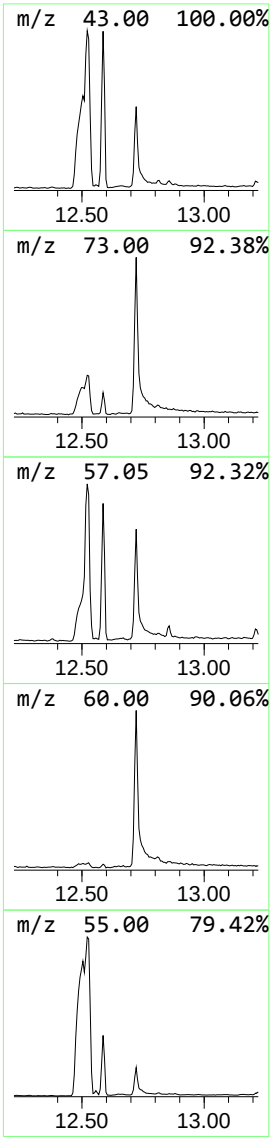
****

Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	39.26 ng	1754310	Phenanthrene-d10	11.404

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	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78





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Data File : BF125493.D
Acq On : 15 Sep 2021 1:27
Operator : JU/CG
Sample : M3725-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-01-091321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

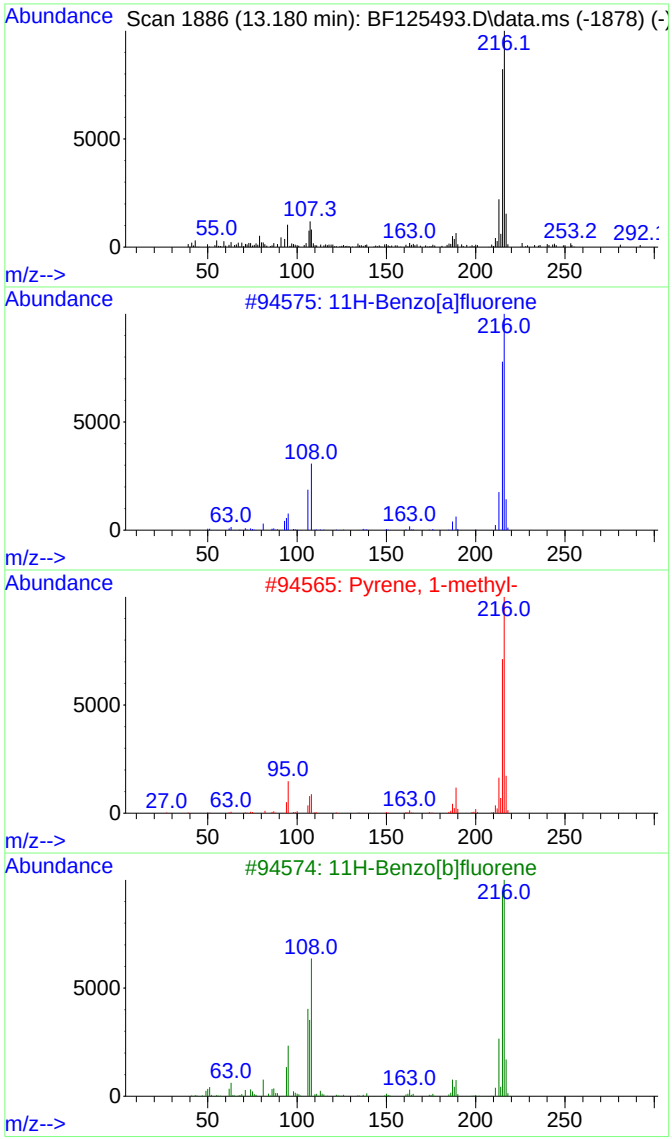
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

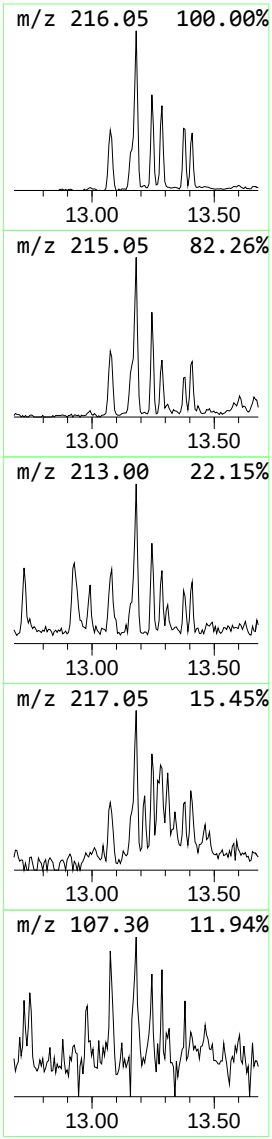
****

Peak Number 9 11H-Benzo[a]fluorene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.180	4.89 ng	321790	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	81
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	76
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72





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Data File : BF125493.D
Acq On : 15 Sep 2021 1:27
Operator : JU/CG
Sample : M3725-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-01-091321

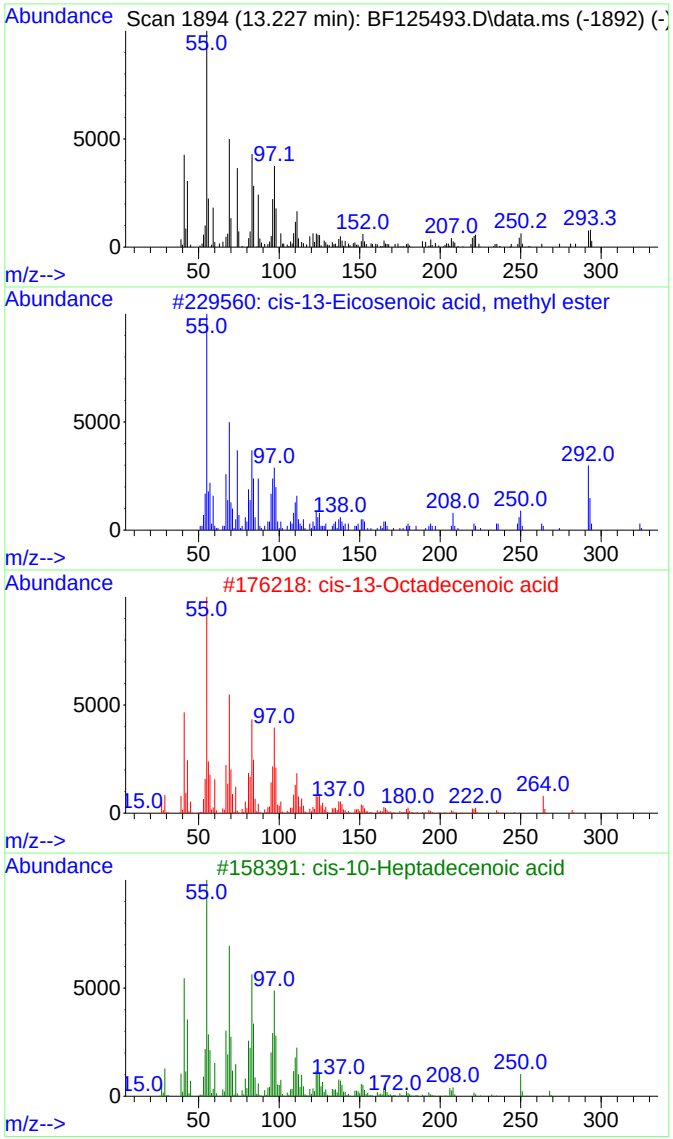
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

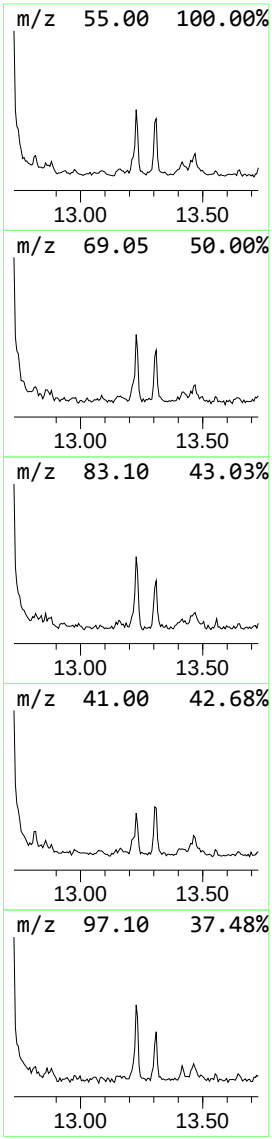
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 cis-13-Eicosenoic acid, met... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.227	5.09 ng	334556	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	83
2	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	58
3	cis-10-Heptadecenoic acid	268	C17H32O2	029743-97-3	53
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	52
5	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	50





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Data File : BF125493.D
Acq On : 15 Sep 2021 1:27
Operator : JU/CG
Sample : M3725-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-01-091321

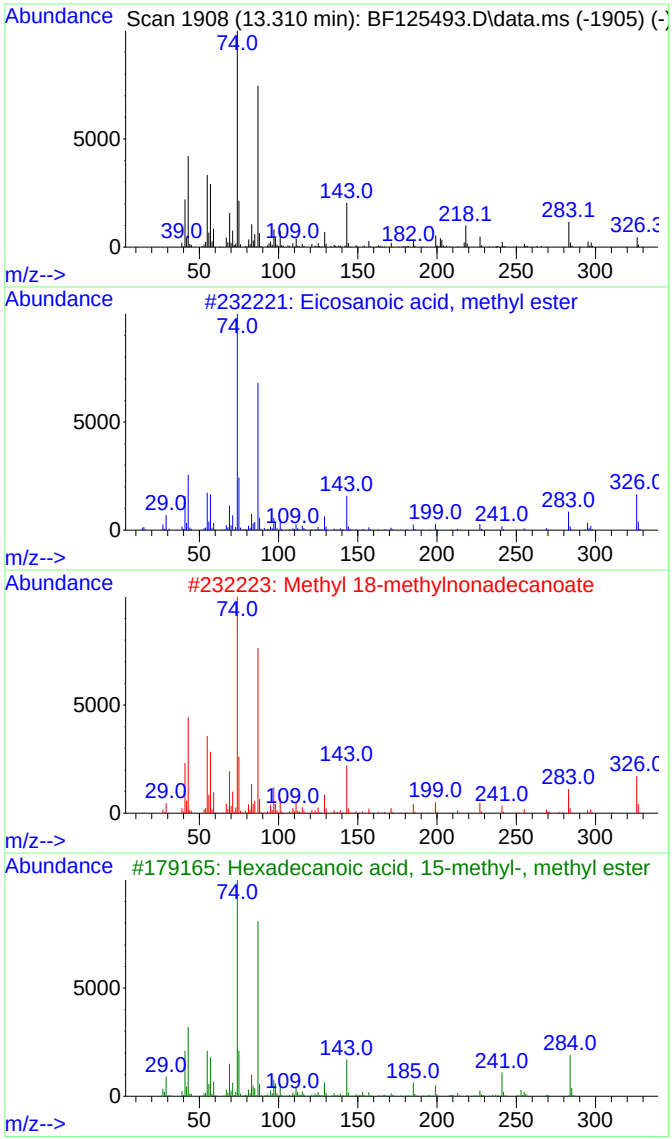
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

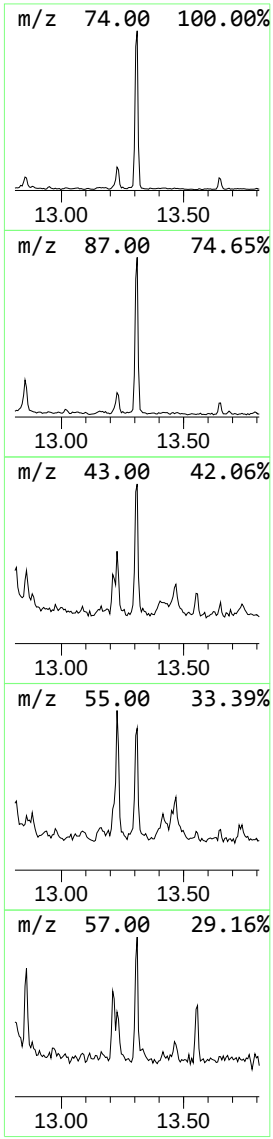
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Eicosanoic acid, methyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.310	6.34 ng	416995	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	98
2	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	97
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
5	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	87





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Data File : BF125493.D
Acq On : 15 Sep 2021 1:27
Operator : JU/CG
Sample : M3725-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-01-091321

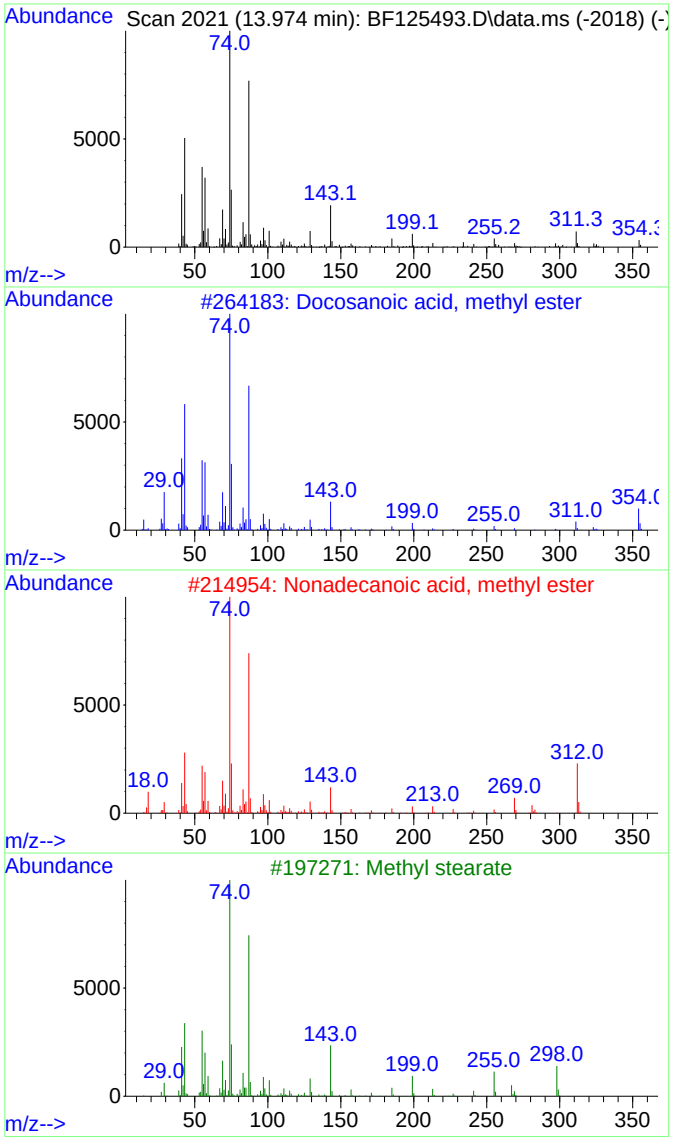
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

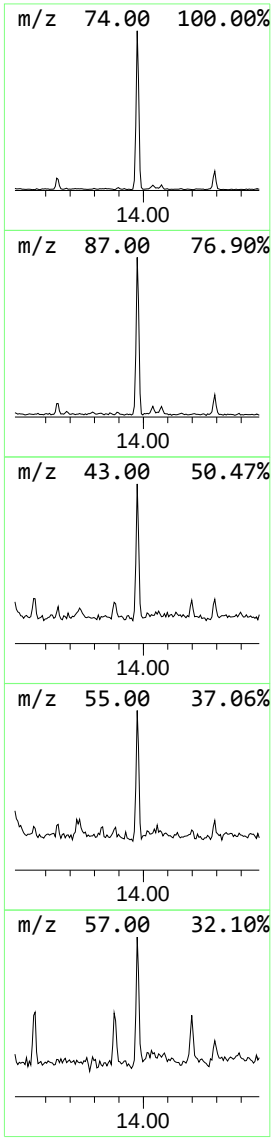
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Docosanoic acid, methyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	6.08 ng	399750	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	99
2	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	95
3	Methyl stearate	298	C19H38O2	000112-61-8	90
4	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	90
5	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091421\
Data File : BF125493.D
Acq On : 15 Sep 2021 1:27
Operator : JU/CG
Sample : M3725-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HR-01-091321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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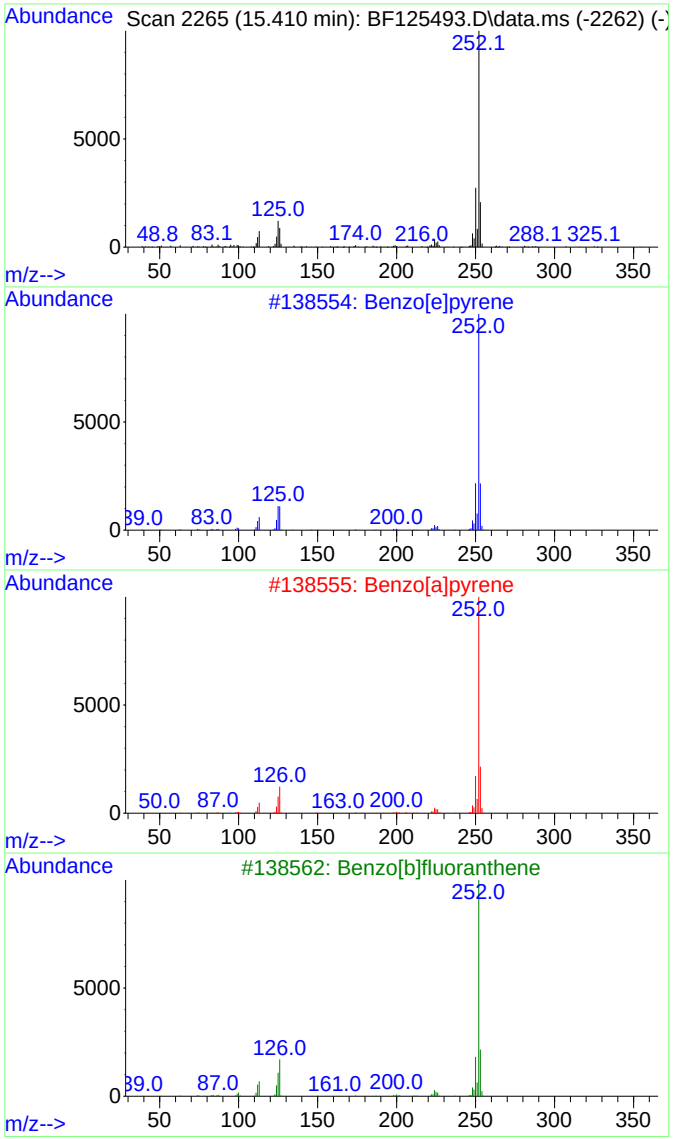
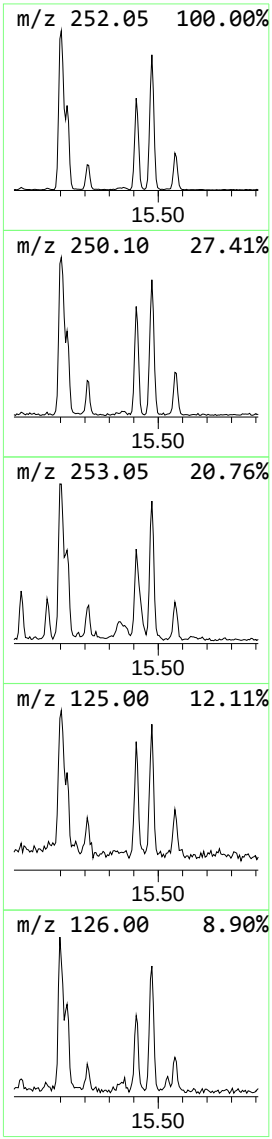
Peak Number 13 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	6.92 ng	280469	Perylene-d12	15.539

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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091421\
Data File : BF125493.D
Acq On : 15 Sep 2021 1:27
Operator : JU/CG
Sample : M3725-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HR-01-091321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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
Butane, 2-metho...	2.122	7.4	ng	313115	1	6.875	848951	20.0
Bicyclo[3.1.1]h...	6.145	7.4	ng	312535	1	6.875	848951	20.0
Hexadecanoic ac...	11.798	140.1	ng	6261880	4	11.404	893777	20.0
n-Hexadecanoic ...	11.945	44.9	ng	2004120	4	11.404	893777	20.0
4H-Cyclopenta[d...	12.016	7.7	ng	345818	4	11.404	893777	20.0
9,12-Octadecadi...	12.504	536.7	ng	23983600	4	11.404	893777	20.0
7,10,13-Hexadec...	12.527	227.3	ng	10159400	4	11.404	893777	20.0
Octadecanoic acid	12.722	39.3	ng	1754310	4	11.404	893777	20.0
11H-Benzo[a]flu...	13.180	4.9	ng	321790	5	14.051	1314920	20.0
cis-13-Eicoseno...	13.227	5.1	ng	334556	5	14.051	1314920	20.0
Eicosanoic acid...	13.310	6.3	ng	416995	5	14.051	1314920	20.0
Docosanoic acid...	13.974	6.1	ng	399750	5	14.051	1314920	20.0
Benzo[e]pyrene	15.410	6.9	ng	280469	6	15.539	810747	20.0