LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062122\
Data File : BF128921.D
Acq On : 22 Jun 2022 02:44
Operator : CG\JU
Sample : N3414-01 10X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-062022

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-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128921.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.393	525	528	537	rBV	126032	130677	6.72%	1.209%
2	6.416	699	702	714	rBV	128098	132114	6.80%	1.223%
3	6.751	756	759	763	rBV	793474	641947	33.04%	5.941%
4	7.316	852	855	863	rBV	111471	87910	4.52%	0.814%
5	8.040	973	978	981	rBV	868236	750891	38.64%	6.949%
6	9.110	1157	1160	1164	rVB	209677	153998	7.92%	1.425%
7	9.651	1249	1252	1255	rBV	77188	61157	3.15%	0.566%
8	9.792	1272	1276	1279	rVB	907701	711616	36.62%	6.586%
9	10.339	1366	1369	1375	rVB2	25870	30917	1.59%	0.286%
10	10.581	1407	1410	1413	rVB2	69434	58703	3.02%	0.543%
11	10.704	1427	1431	1435	rBV5	20144	27285	1.40%	0.253%
12	10.886	1458	1462	1465	rBV2	21470	24802	1.28%	0.230%
13	11.175	1508	1511	1517	rVB2	21975	25310	1.30%	0.234%
14	11.280	1525	1529	1531	rBV	749623	686706	35.34%	6.355%
15	11.298	1531	1532	1535	rVV	169920	131659	6.78%	1.218%
16	11.351	1539	1541	1544	rVB	55149	46743	2.41%	0.433%
17	11.516	1565	1569	1574	rBV3	14264	27567	1.42%	0.255%
18	11.610	1581	1585	1589	rVB2	20285	24247	1.25%	0.224%
19	11.669	1592	1595	1598	rBV	628130	507714	26.13%	4.699%
20	11.780	1611	1614	1616	rBV	66235	57029	2.93%	0.528%
21	11.810	1616	1619	1623	rVV	82166	72813	3.75%	0.674%
22	11.857	1624	1627	1629	rVV	27282	28637	1.47%	0.265%
23	11.892	1629	1633	1635	rVV2	95546	106343	5.47%	0.984%
24	11.916	1635	1637	1641	rVB	48697	42344	2.18%	0.392%
25	12.075	1661	1664	1667	rBV	41663	39874	2.05%	0.369%
26	12.104	1667	1669	1673	rVB4	27265	24621	1.27%	0.228%
27	12.257	1692	1695	1697	rBV	31365	26014	1.34%	0.241%
28	12.327	1704	1707	1709	rBV	66980	67887	3.49%	0.628%
29	12.357	1709	1712	1714	rVV	2267174	1943221	100.00%	17.984%
30	12.380	1714	1716	1722	rVB	1303213	1120823	57.68%	10.373%
31	12.463	1727	1730	1732	rVV	308156	232768	11.98%	2.154%
32	12.492	1732	1735	1739	rVB	400706	317664	16.35%	2.940%
33	12.539	1740	1743	1744	rVV2	29102	28983	1.49%	0.268%
34	12.586	1748	1751	1754	rVB	43927	40324	2.08%	0.373%
35	12.722	1771	1774	1777	rVB	350237	268073	13.80%	2.481%
36	12.780	1781	1784	1787	rVB2	33684	38113	1.96%	0.353%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062122\
Data File : BF128921.D
Acq On : 22 Jun 2022 02:44
Operator : CG\JU
Sample : N3414-01 10X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-062022

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-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.863	1795	1798	1800	rBV	142502	112826	5.81%	1.044%
38	12.939	1808	1811	1818	rBV5	38914	66139	3.40%	0.612%
39	13.051	1823	1830	1834	rVV	99301	141420	7.28%	1.309%
40	13.116	1839	1841	1844	rVB	59127	46896	2.41%	0.434%
41	13.157	1844	1848	1851	rBV2	70222	84762	4.36%	0.784%
42	13.245	1861	1863	1866	rVB	35524	28537	1.47%	0.264%
43	13.280	1866	1869	1870	rBV	40332	39870	2.05%	0.369%
44	13.921	1973	1978	1981	rBV2	679373	753070	38.75%	6.970%
45	13.945	1981	1982	1989	rVB	162647	128479	6.61%	1.189%
46	14.951	2150	2153	2161	rBV	117503	198889	10.24%	1.841%
47	15.304	2210	2213	2217	rVB	107505	121818	6.27%	1.127%
48	15.368	2220	2224	2228	rVV	299183	364866	18.78%	3.377%

Sum of corrected areas: 10805066

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062122\
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Acq On : 22 Jun 2022 02:44
Operator : CG\JU
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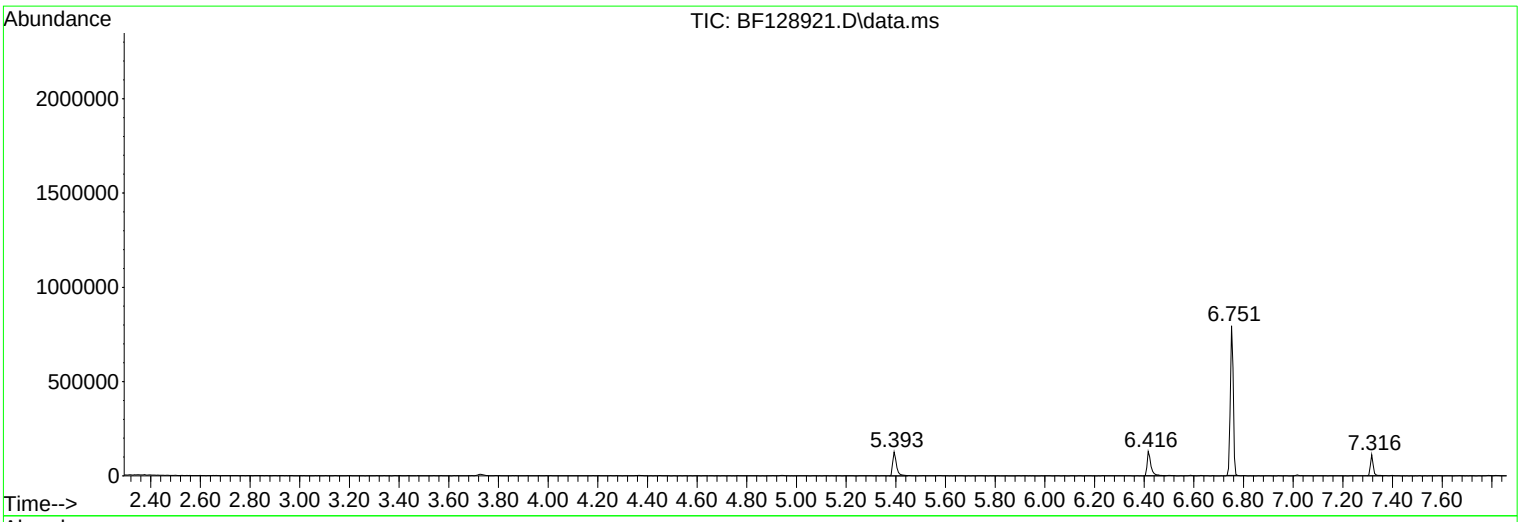
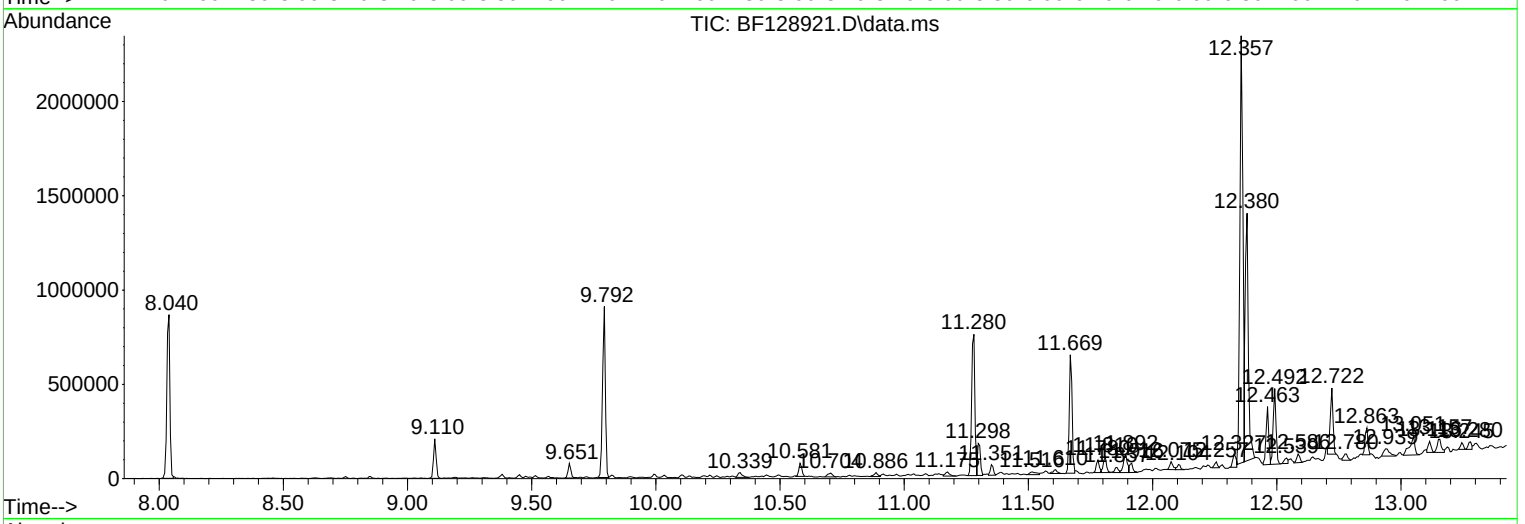
Misc :
ALS Vial : 22 Sample Multiplier: 1

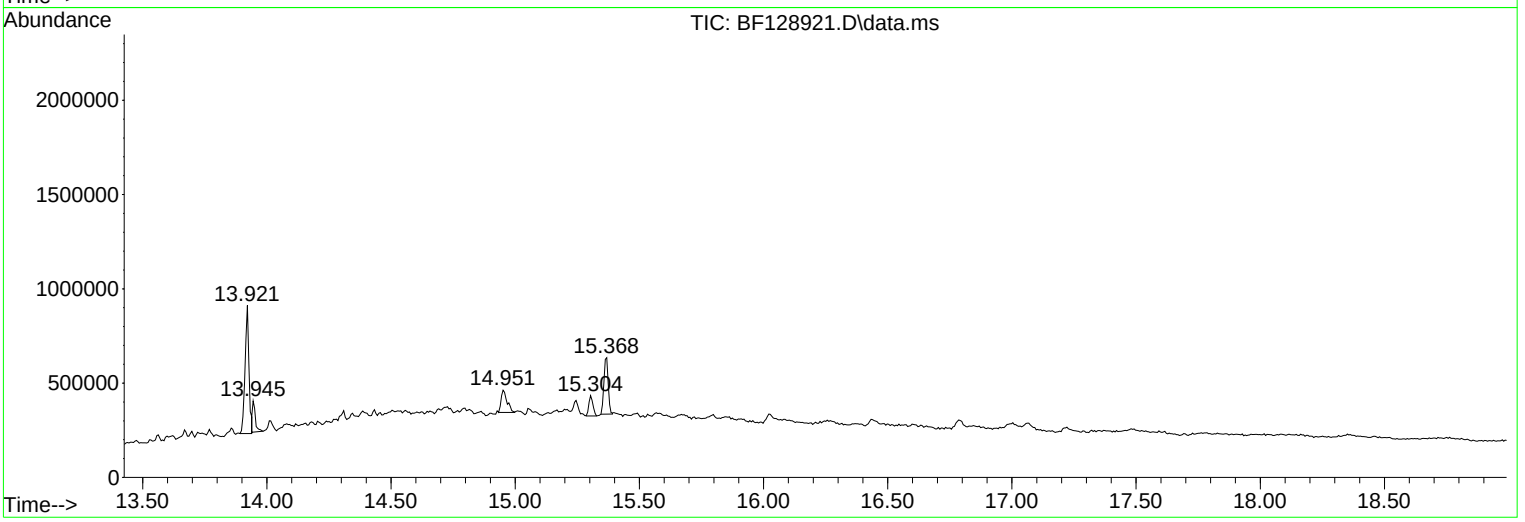
Instrument :
BNA_F
ClientSampleId :
SU-04-062022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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_F\Data\BF062122\
Data File : BF128921.D
Acq On : 22 Jun 2022 02:44
Operator : CG\JU
Sample : N3414-01 10X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-062022

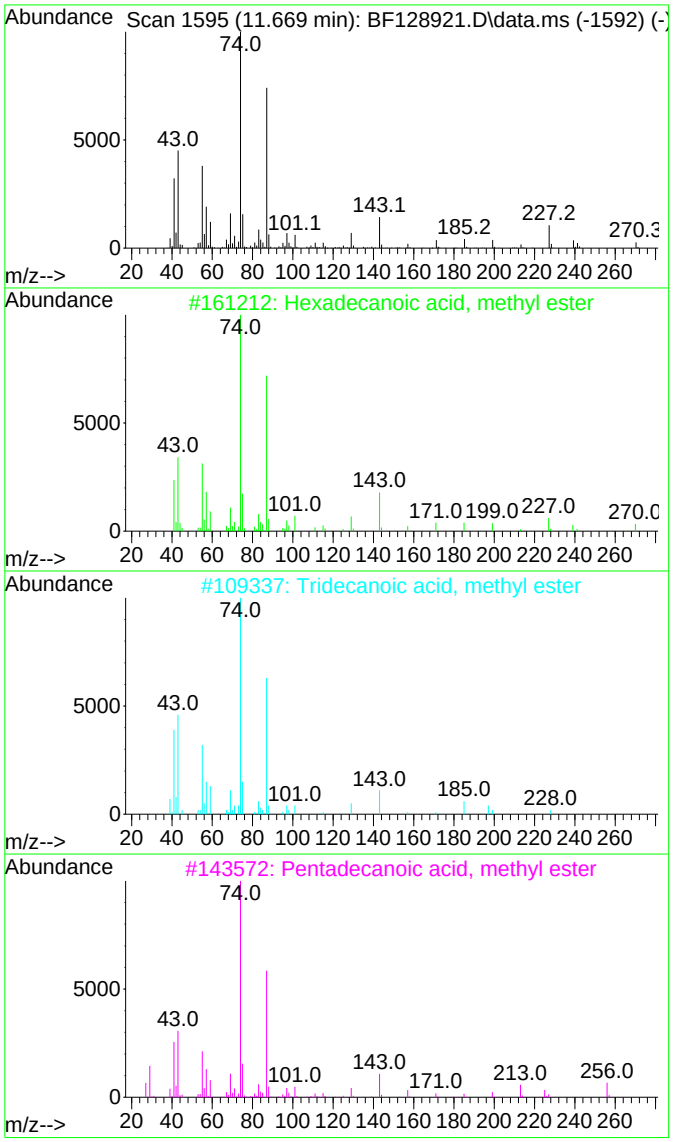
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

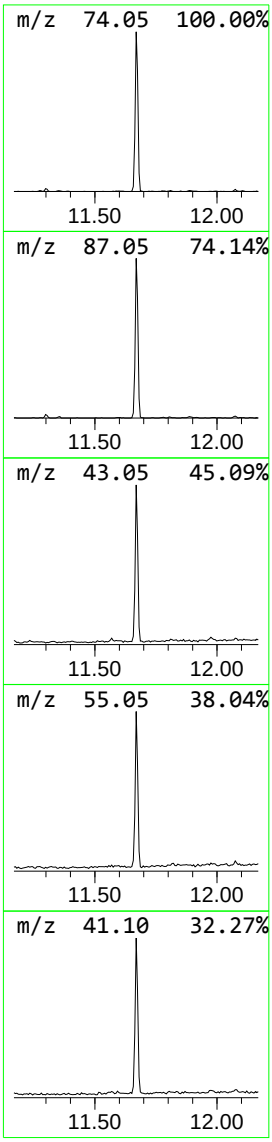
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.669	14.79 ng	507714	Phenanthrene-d10	11.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	99
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	83
5	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062122\
Data File : BF128921.D
Acq On : 22 Jun 2022 02:44
Operator : CG\JU
Sample : N3414-01 10X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-062022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

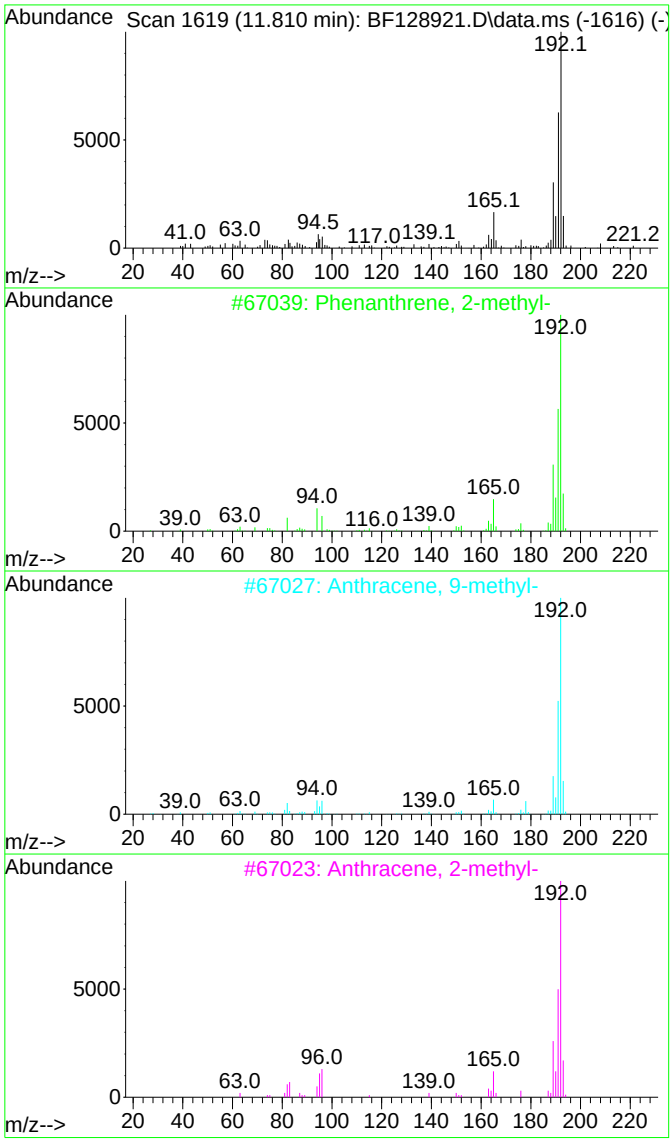
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

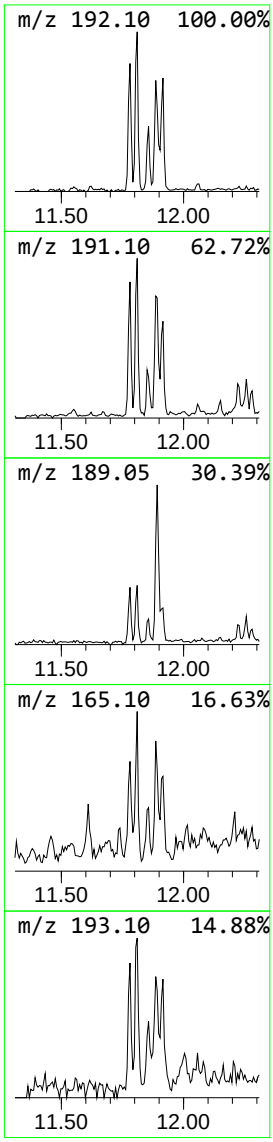
****

Peak Number 2 Phenanthrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	2.12 ng	72813	Phenanthrene-d10	11.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062122\
Data File : BF128921.D
Acq On : 22 Jun 2022 02:44
Operator : CG\JU
Sample : N3414-01 10X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-062022

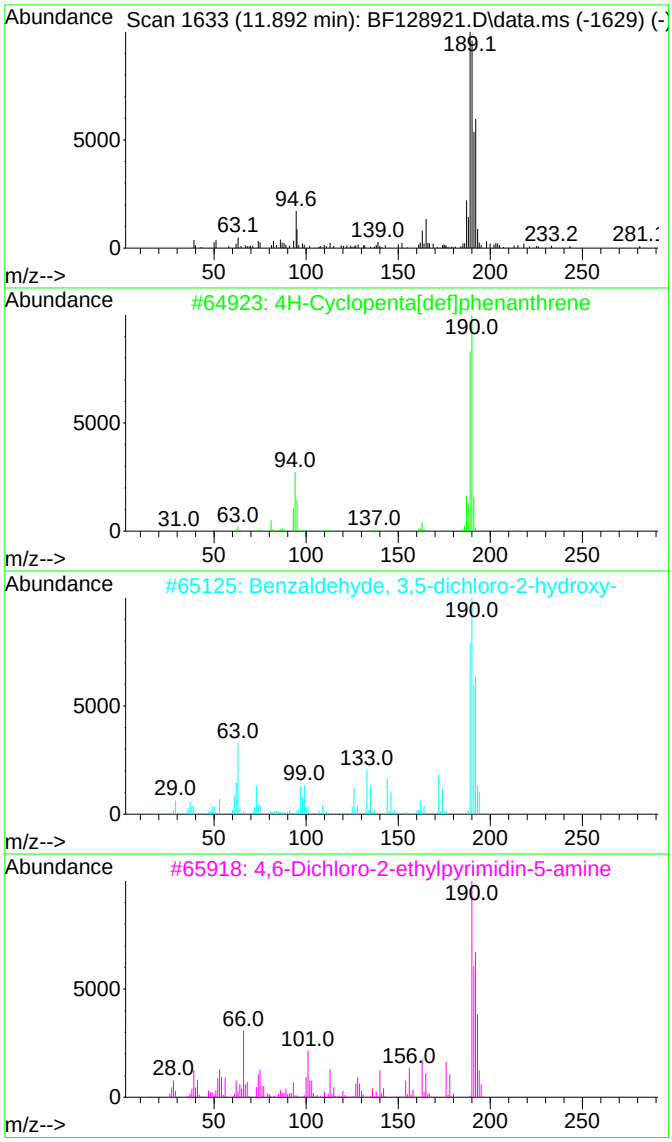
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

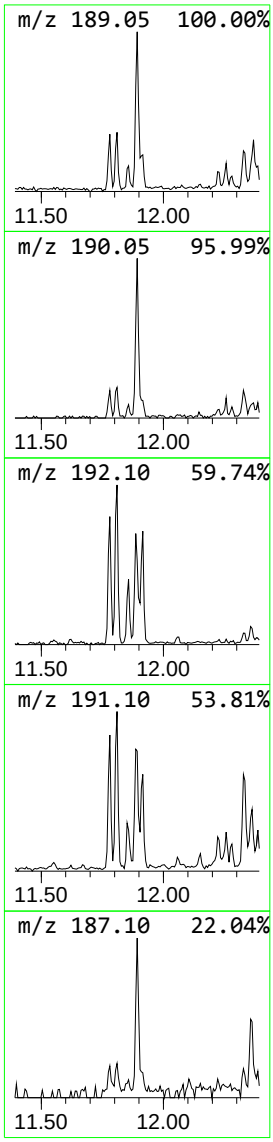
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	3.10 ng	106343	Phenanthrene-d10	11.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	62
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
3	4,6-Dichloro-2-ethylpyrimidin-5-...	191	C6H7Cl2N3	006237-96-3	43
4	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	35
5	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062122\
Data File : BF128921.D
Acq On : 22 Jun 2022 02:44
Operator : CG\JU
Sample : N3414-01 10X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-062022

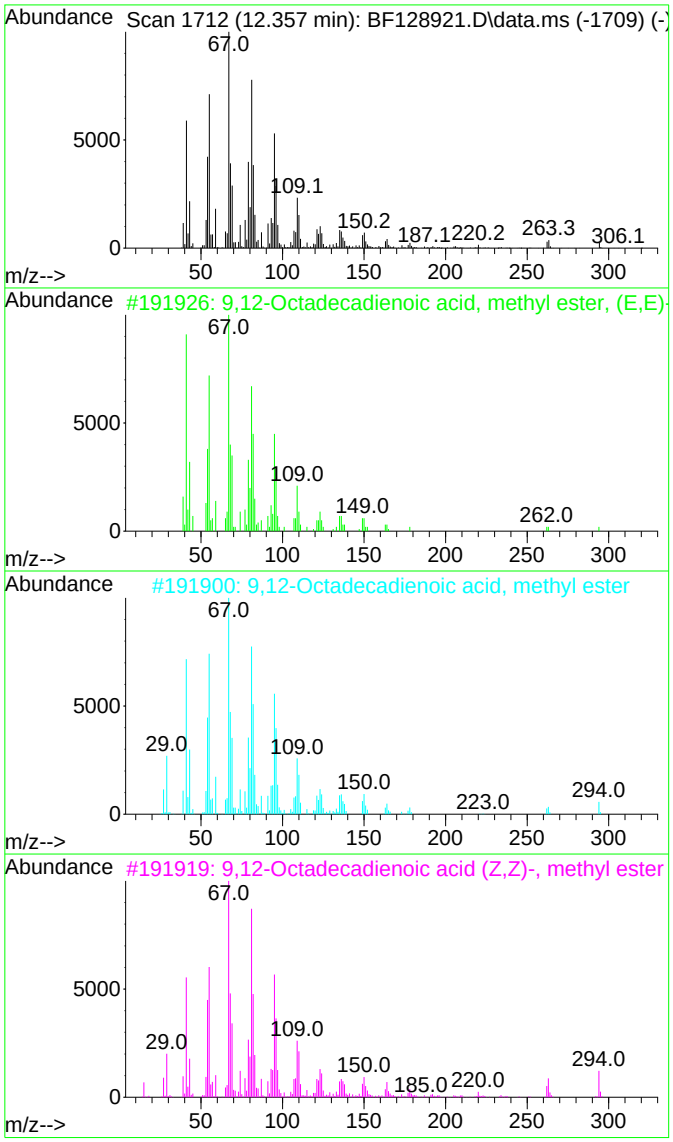
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

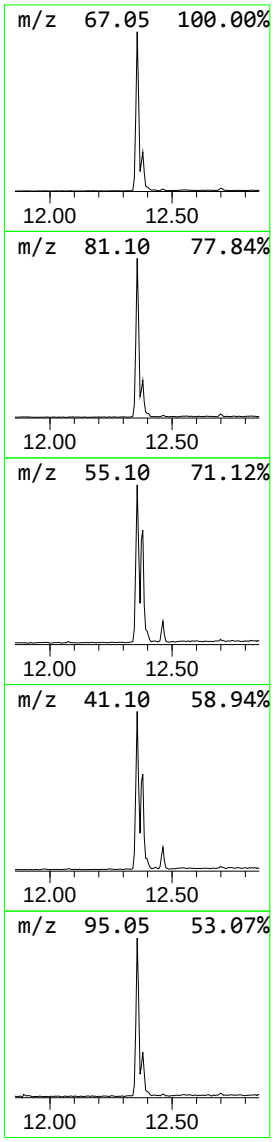
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.357	56.60 ng	1943220	Phenanthrene-d10	11.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062122\
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Acq On : 22 Jun 2022 02:44
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Instrument :
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ClientSampleId :
SU-04-062022

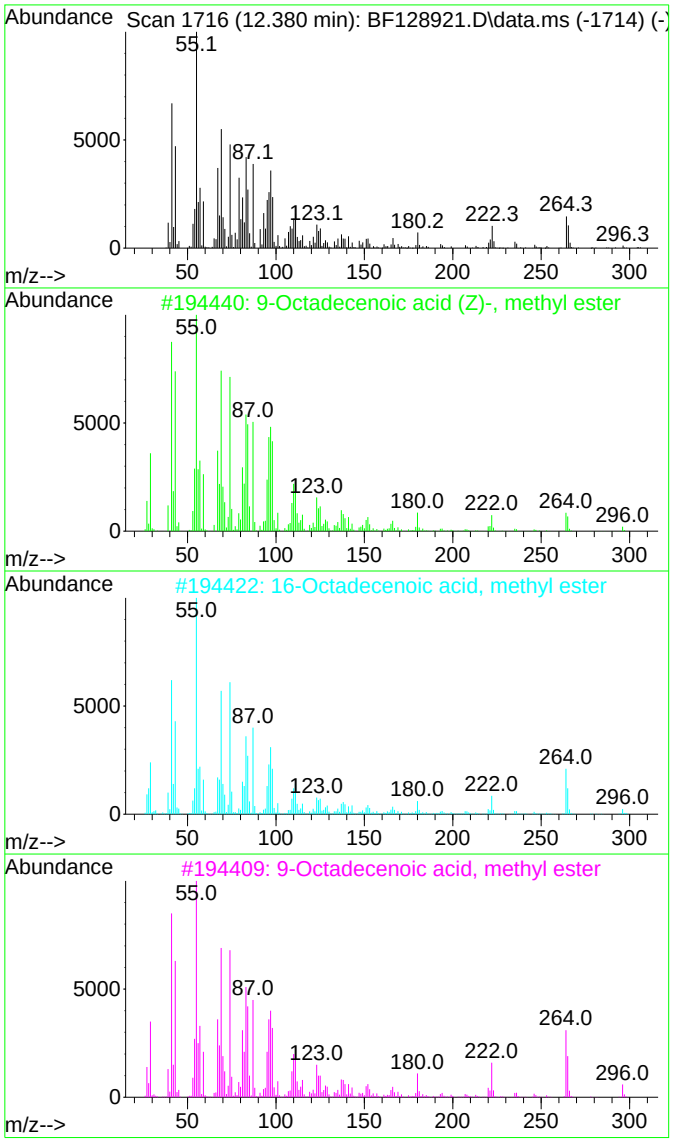
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

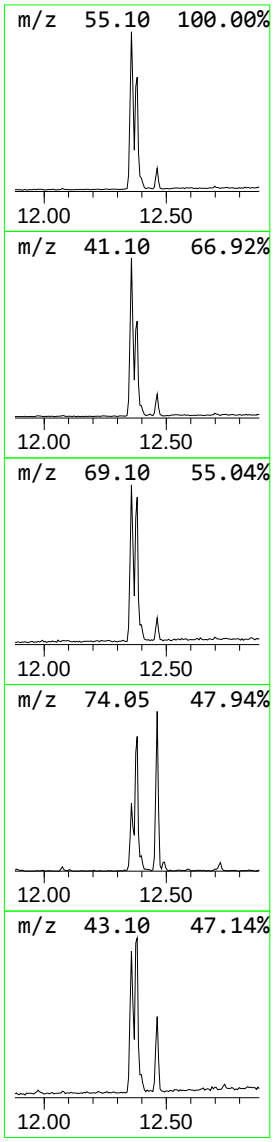
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.380	32.64 ng	1120820	Phenanthrene-d10	11.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	97
3	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	94
4	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	94
5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	94





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-062022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

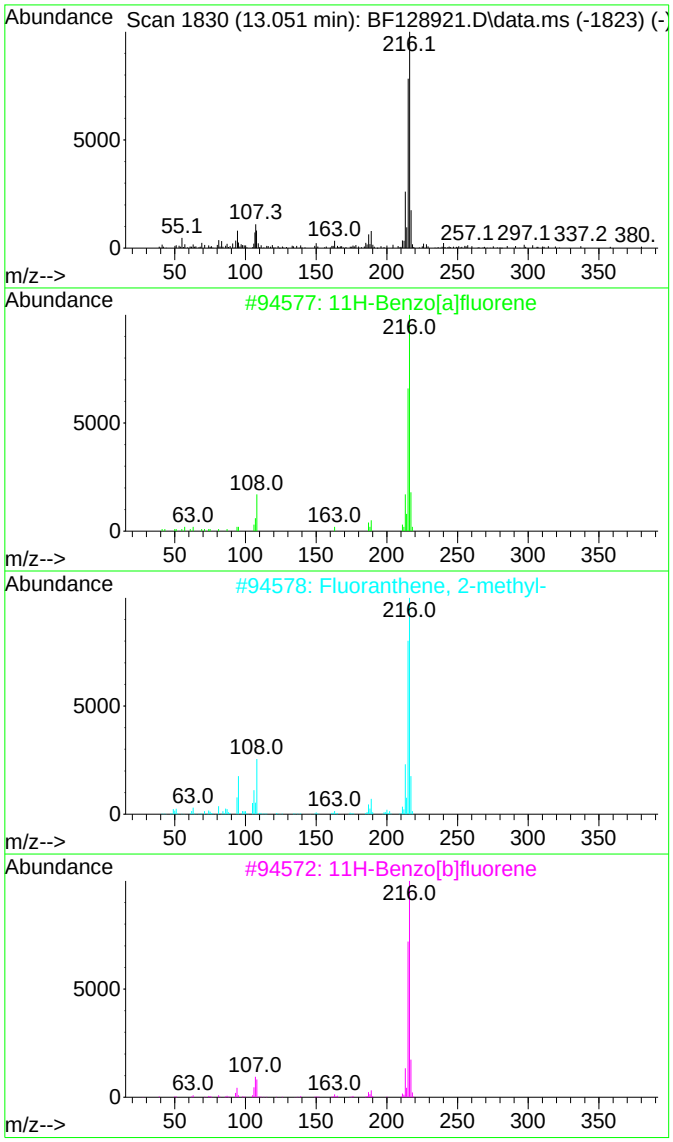
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

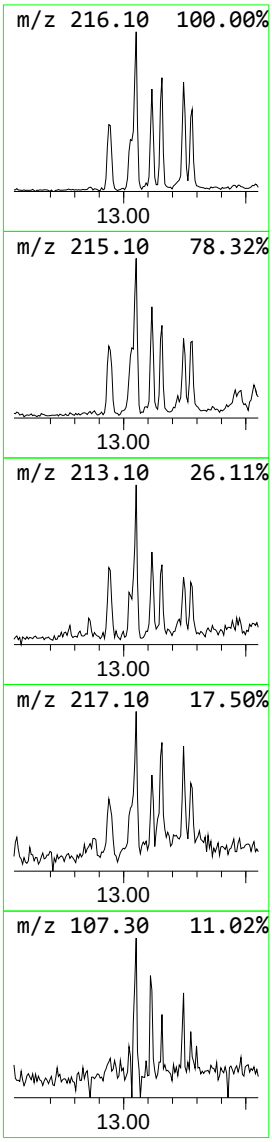
****

Peak Number 6 11H-Benzo[a]fluorene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.051	3.76 ng	141420	Chrysene-d12	13.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	81
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062122\
Data File : BF128921.D
Acq On : 22 Jun 2022 02:44
Operator : CG\JU
Sample : N3414-01 10X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-062022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

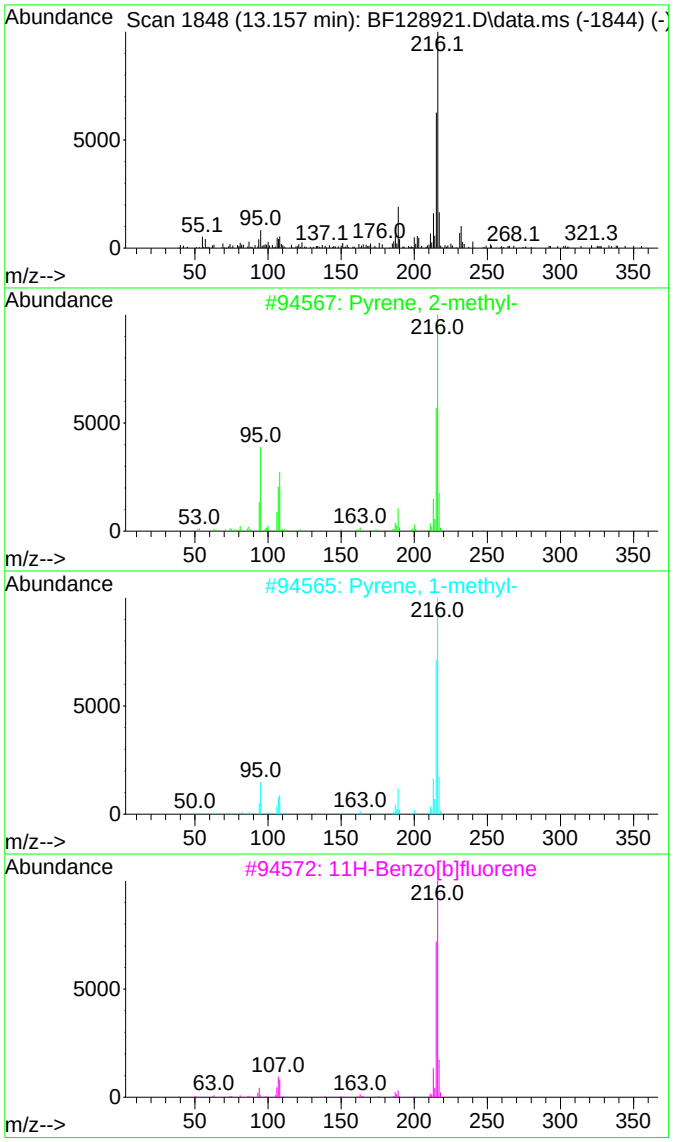
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

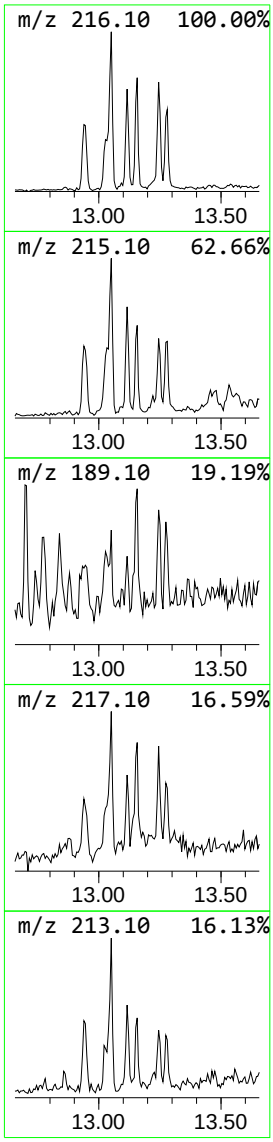
****

Peak Number 7 Pyrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.157	2.25 ng	84762	Chrysene-d12	13.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	87
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	83
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	74
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	74
5	Pyrene, 4-methyl-	216	C17H12	003353-12-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062122\
Data File : BF128921.D
Acq On : 22 Jun 2022 02:44
Operator : CG\JU
Sample : N3414-01 10X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-062022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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
Hexadecanoic ac...	11.669	14.8	ng	507714	4	11.281	686706	20.0
Phenanthrene, 2...	11.810	2.1	ng	72813	4	11.281	686706	20.0
4H-Cyclopenta[d...	11.892	3.1	ng	106343	4	11.281	686706	20.0
9,12-Octadecadi...	12.357	56.6	ng	1943220	4	11.281	686706	20.0
9-Octadecenoic ...	12.380	32.6	ng	1120820	4	11.281	686706	20.0
11H-Benzo[a]flu...	13.051	3.8	ng	141420	5	13.922	753070	20.0
Pyrene, 2-methyl-	13.157	2.3	ng	84762	5	13.922	753070	20.0