LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129420.D
Acq On : 28 Jul 2022 21:24
Operator : CG\JU
Sample : N3942-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11977

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129420.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.128	480	483	491	rVB	68934	85778	1.56%	0.197%
2	5.516	544	549	552	rBV	4918083	4607077	83.55%	10.607%
3	6.522	715	720	723	rBV	4493996	4722449	85.64%	10.872%
4	6.881	778	781	785	rVB	1556512	1242085	22.52%	2.860%
5	7.451	872	878	881	rBV	3061776	3126524	56.70%	7.198%
6	8.163	995	999	1002	rBV	1768435	1656508	30.04%	3.814%
7	8.875	1117	1120	1124	rVB	84323	69927	1.27%	0.161%
8	8.934	1127	1130	1134	rBV	133406	111362	2.02%	0.256%
9	9.245	1177	1183	1186	rBV	5778722	5514457	100.00%	12.696%
10	9.504	1222	1227	1232	rBV2	50951	70832	1.28%	0.163%
11	9.581	1236	1240	1242	rBV	72877	74587	1.35%	0.172%
12	9.786	1271	1275	1278	rVB	80435	72612	1.32%	0.167%
13	9.922	1292	1298	1301	rBV	2058216	1820538	33.01%	4.191%
14	9.957	1301	1304	1307	rVB	354193	282936	5.13%	0.651%
15	10.128	1329	1333	1336	rVB	140738	120988	2.19%	0.279%
16	10.469	1388	1391	1396	rVB	190775	179804	3.26%	0.414%
17	10.716	1429	1433	1436	rBV	3469435	3001299	54.43%	6.910%
18	10.828	1448	1452	1453	rBV2	60000	81413	1.48%	0.187%
19	11.022	1477	1485	1487	rBV5	40270	61715	1.12%	0.142%
20	11.216	1515	1518	1523	rBV2	58913	59263	1.07%	0.136%
21	11.416	1548	1552	1554	rBV	1652845	1507388	27.34%	3.470%
22	11.439	1554	1556	1559	rVV	597184	461353	8.37%	1.062%
23	11.486	1561	1564	1567	rVB	182135	145697	2.64%	0.335%
24	11.645	1584	1591	1596	rBV	63801	97924	1.78%	0.225%
25	11.916	1634	1637	1639	rBV	75940	72453	1.31%	0.167%
26	11.939	1639	1641	1645	rVB	92536	90974	1.65%	0.209%
27	12.028	1653	1656	1659	rBV2	160920	166901	3.03%	0.384%
28	12.463	1727	1730	1733	rBV2	42928	57288	1.04%	0.132%
29	12.551	1742	1745	1749	rBV	95285	91790	1.66%	0.211%
30	12.627	1755	1758	1762	rVB	918813	783222	14.20%	1.803%
31	12.857	1791	1797	1803	rBV	854825	921300	16.71%	2.121%
32	12.998	1815	1821	1825	rBV	3986755	3713463	67.34%	8.549%
33	13.075	1830	1834	1838	rBV3	73752	118007	2.14%	0.272%
34	13.186	1846	1853	1855	rBV3	124171	222941	4.04%	0.513%
35	13.251	1862	1864	1867	rBV	75641	61631	1.12%	0.142%
36	13.292	1867	1871	1873	rVV2	80391	92912	1.68%	0.214%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129420.D
Acq On : 28 Jul 2022 21:24
Operator : CG\JU
Sample : N3942-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11977

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.386	1884	1887	1889	rBV	69975	56580	1.03%	0.130%
38	13.674	1932	1936	1937	rBV4	42098	56594	1.03%	0.130%
39	13.698	1937	1940	1945	rVB2	75859	99623	1.81%	0.229%
40	13.857	1965	1967	1971	rBV2	84296	96896	1.76%	0.223%
41	13.904	1971	1975	1980	rVV3	158976	230332	4.18%	0.530%
42	14.027	1992	1996	1998	rBV	660866	622751	11.29%	1.434%
43	14.057	1998	2001	2004	rVV2	1244962	1519430	27.55%	3.498%
44	14.086	2004	2006	2014	rVB	391569	449138	8.14%	1.034%
45	14.316	2043	2045	2048	rBV3	39841	55210	1.00%	0.127%
46	14.445	2065	2067	2069	rVB2	98667	74005	1.34%	0.170%
47	14.480	2070	2073	2076	rVB2	65905	59970	1.09%	0.138%
48	14.539	2080	2083	2086	rVV2	73156	104873	1.90%	0.241%
49	14.569	2086	2088	2090	rVB	81032	63376	1.15%	0.146%
50	14.969	2154	2156	2160	rVB3	122311	122780	2.23%	0.283%
51	15.110	2176	2180	2184	rBV	672684	1060566	19.23%	2.442%
52	15.221	2196	2199	2211	rVB	192844	343945	6.24%	0.792%
53	15.421	2229	2233	2239	rVB	409703	493040	8.94%	1.135%
54	15.486	2240	2244	2250	rBV	370417	464608	8.43%	1.070%
55	15.551	2250	2255	2259	rBV	843014	1123485	20.37%	2.587%
56	15.763	2288	2291	2300	rVB6	58384	92185	1.67%	0.212%
57	15.998	2327	2331	2336	rVB	89569	131699	2.39%	0.303%
58	17.051	2505	2510	2518	rBV2	155792	320921	5.82%	0.739%
59	17.515	2584	2589	2597	rVB	112630	225653	4.09%	0.520%

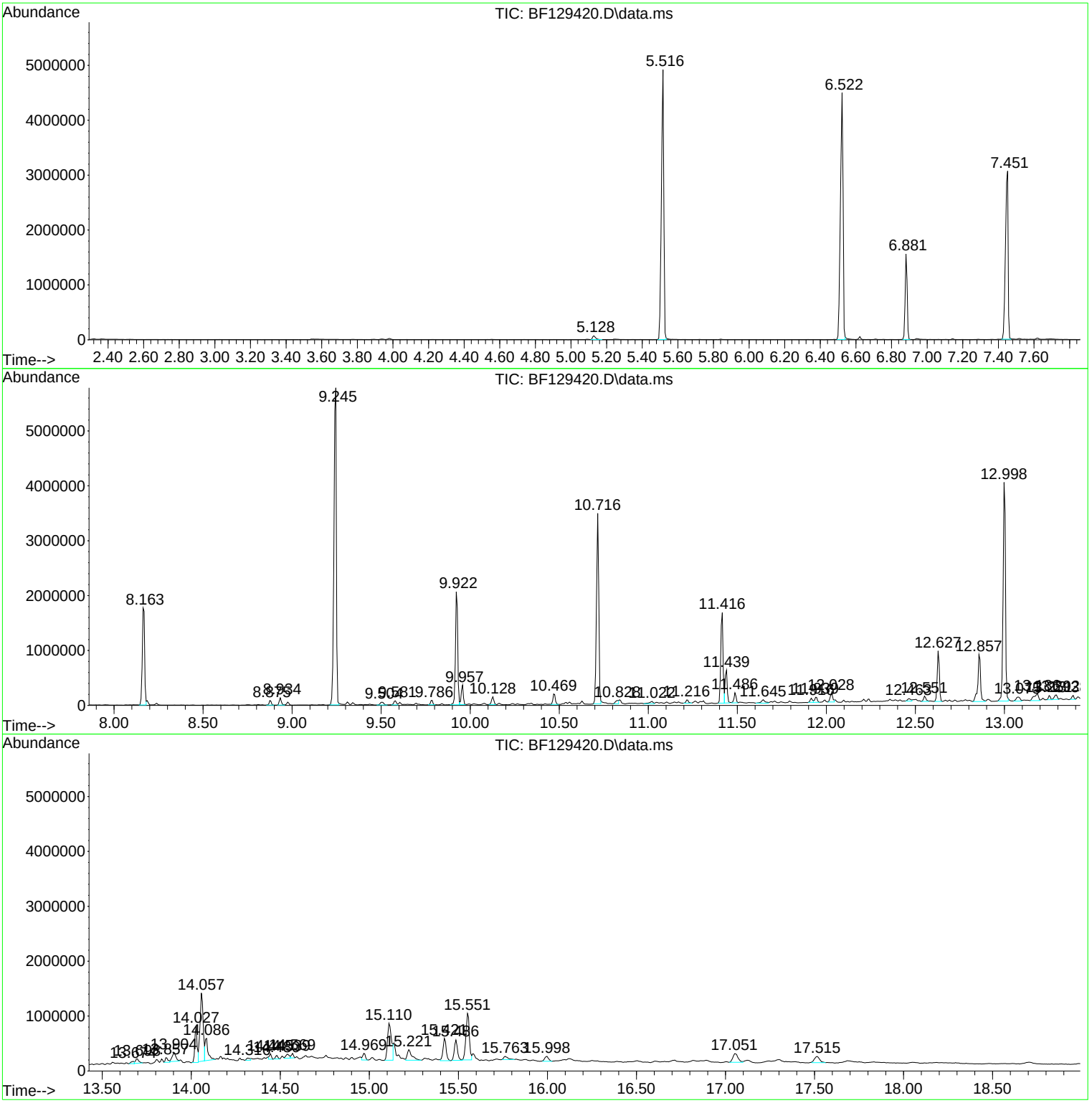
Sum of corrected areas: 43435058

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129420.D
Acq On : 28 Jul 2022 21:24
Operator : CG\JU
Sample : N3942-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11977

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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\BF072822\
Data File : BF129420.D
Acq On : 28 Jul 2022 21:24
Operator : CG\JU
Sample : N3942-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11977

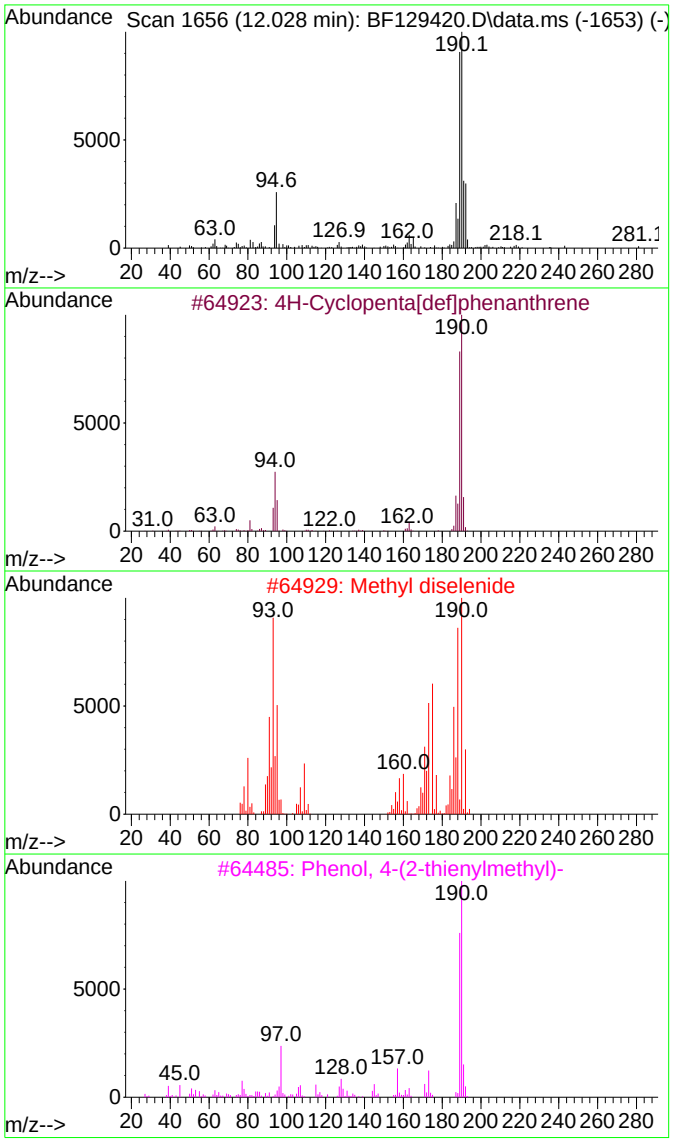
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

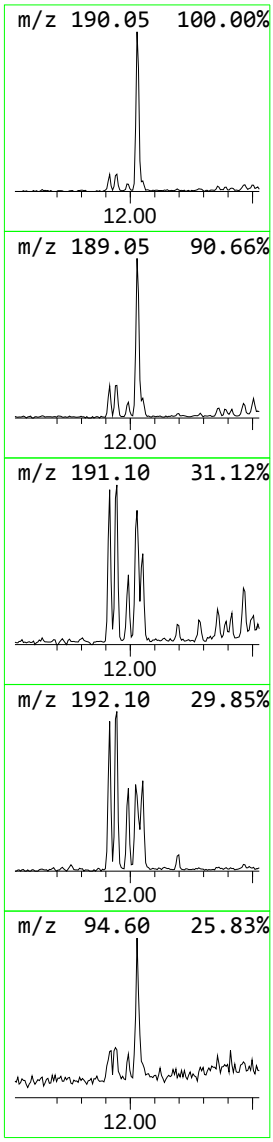
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.028	2.21 ng	166901	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	Methyl diselenide	190	C2H6Se2	007101-31-7	49
3	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	33
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	33
5	1-Aminocyclopentanecarboxylic ac...	361	C18H32ClNO4	1000329-17-0	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129420.D
Acq On : 28 Jul 2022 21:24
Operator : CG\JU
Sample : N3942-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11977

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

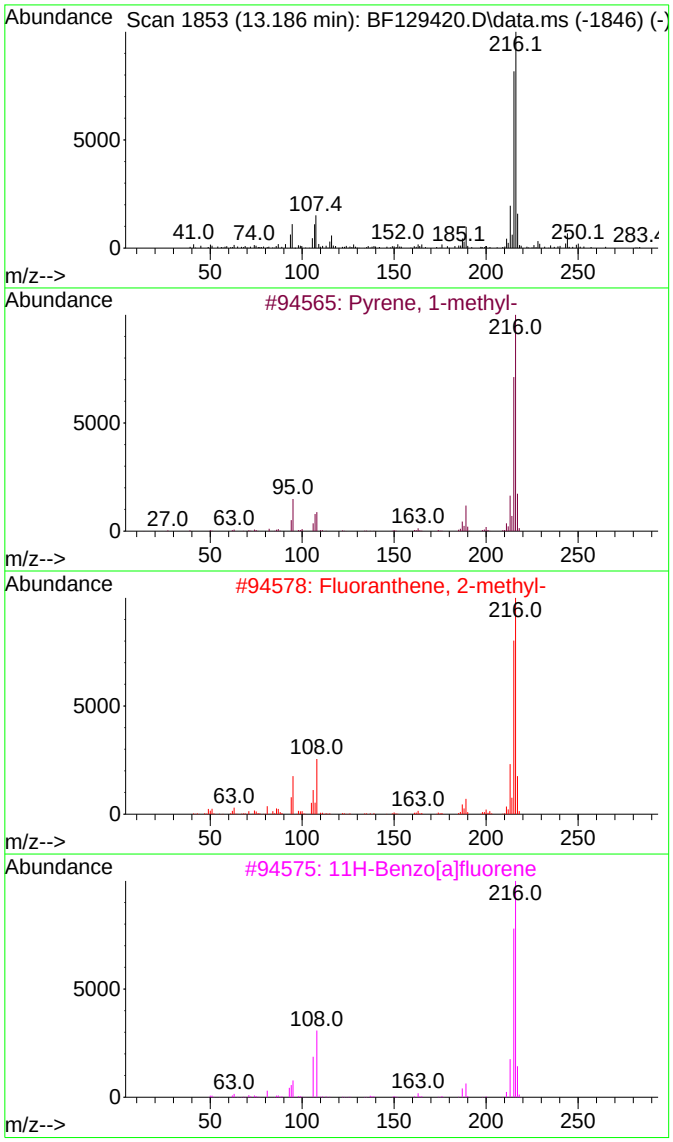
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

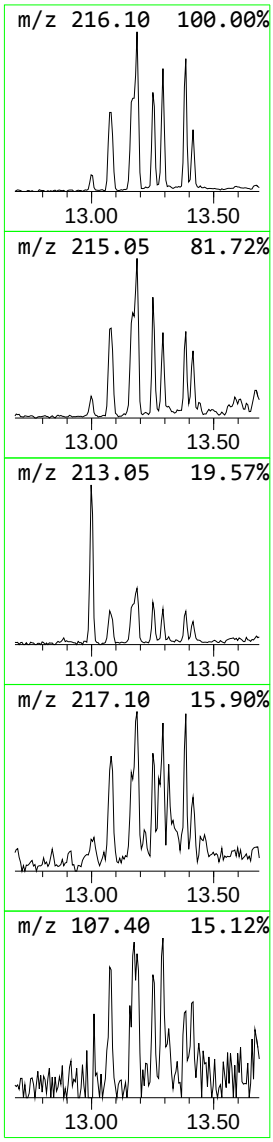
****

Peak Number 2 Pyrene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.186	2.93 ng	222941	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	95
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	94
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129420.D
Acq On : 28 Jul 2022 21:24
Operator : CG\JU
Sample : N3942-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11977

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

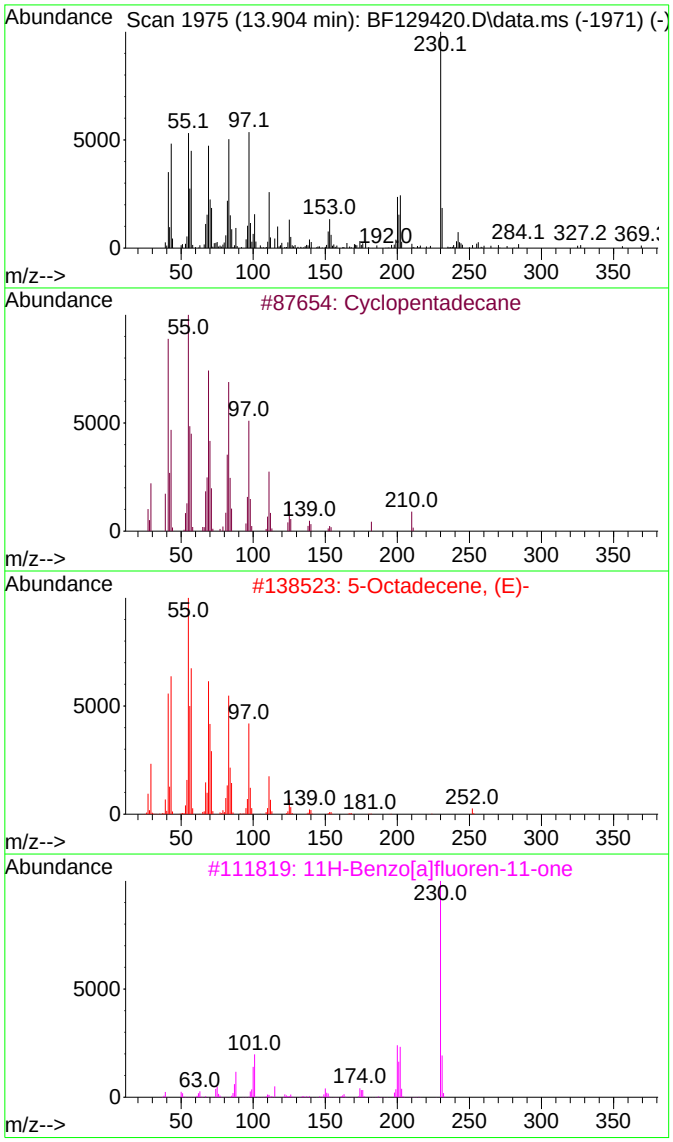
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

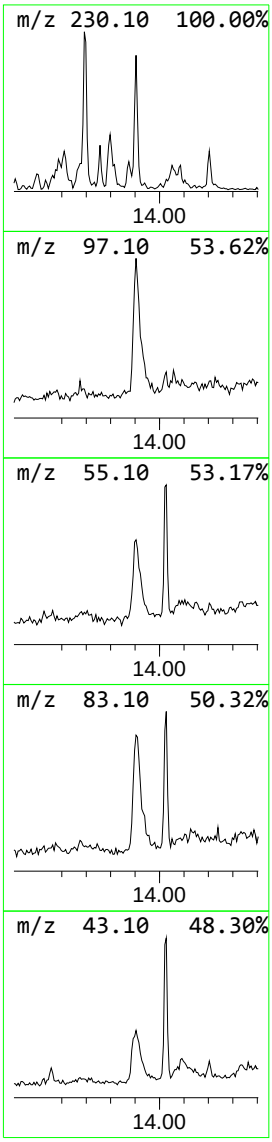
****

Peak Number 3 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.03 ng	230332	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	78
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	56
3	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	50
4	9-Octadecene, (E)-	252	C18H36	007206-25-9	45
5	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129420.D
Acq On : 28 Jul 2022 21:24
Operator : CG\JU
Sample : N3942-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11977

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

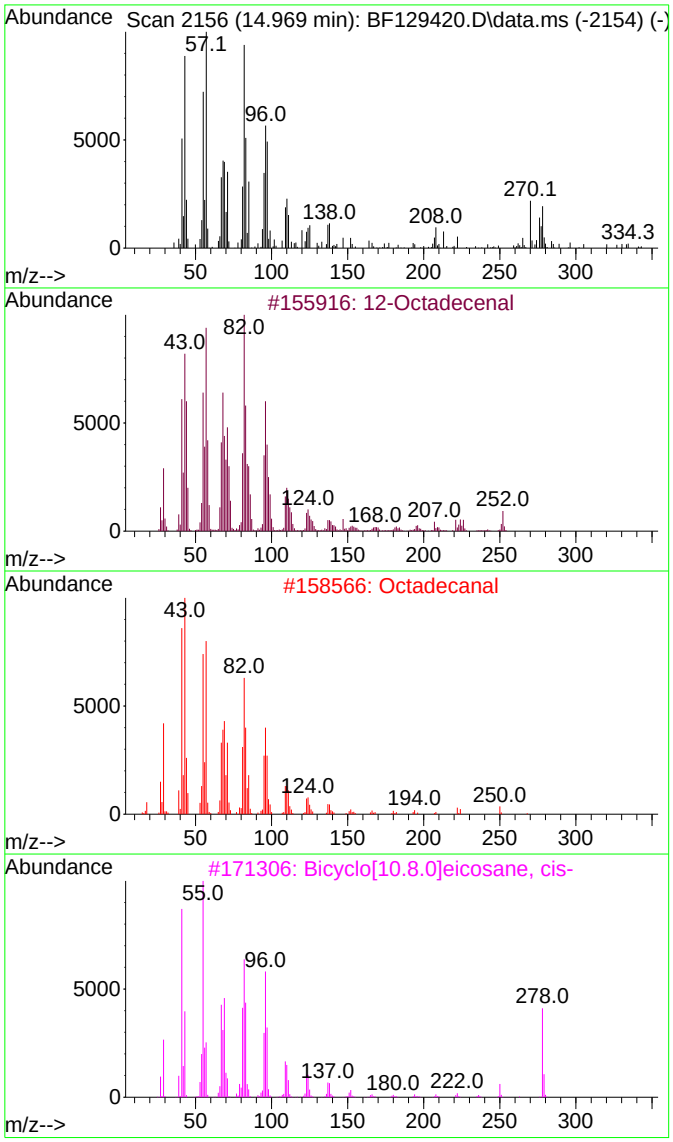
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

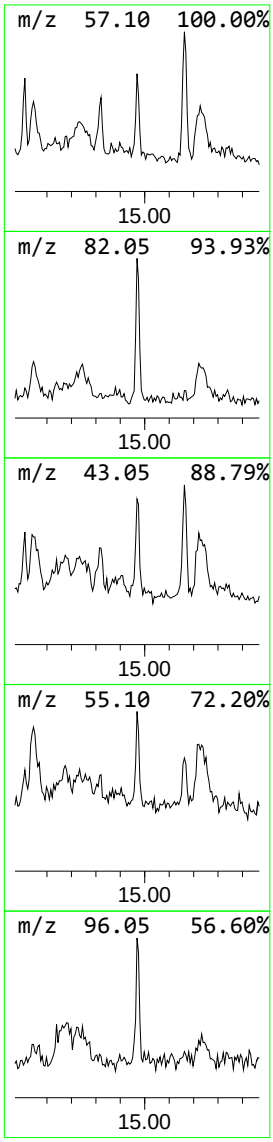
****

Peak Number 4 12-Octadecenal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.969	2.19 ng	122780	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Octadecenal	266	C18H34O	056554-91-7	64
2	Octadecanal	268	C18H36O	000638-66-4	64
3	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	60
4	Bicyclo[10.8.0]eicosane, (E)-	278	C20H38	1010155-85-0	58
5	1,15-Hexadecadiene	222	C16H30	021964-51-2	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129420.D
Acq On : 28 Jul 2022 21:24
Operator : CG\JU
Sample : N3942-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11977

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

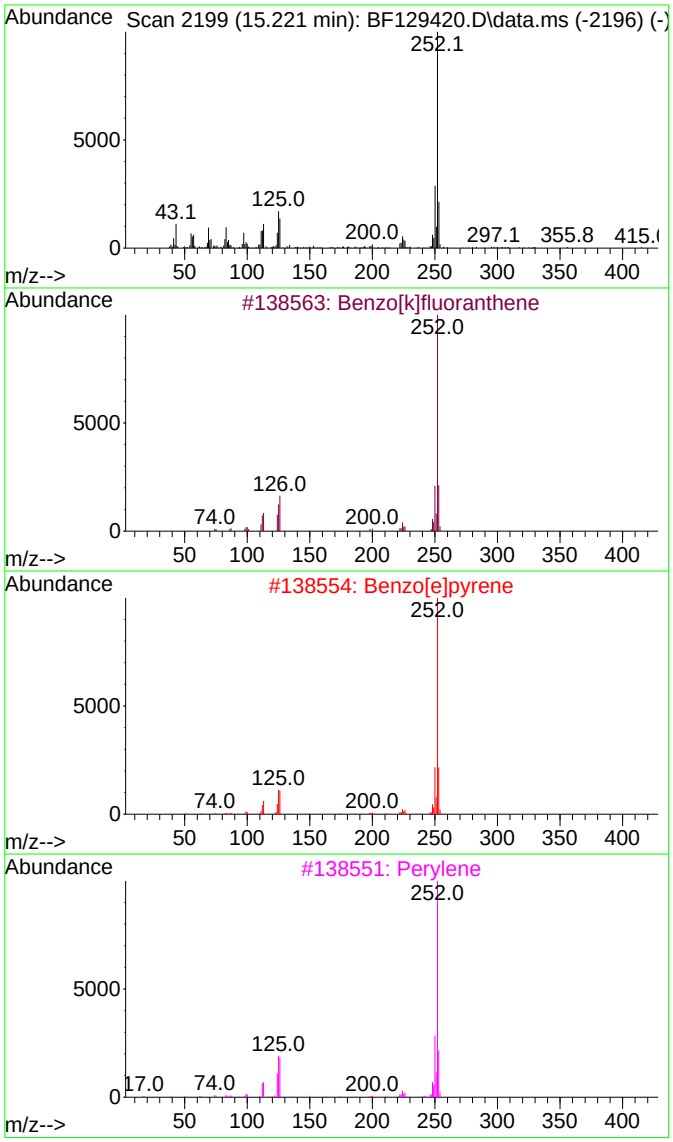
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

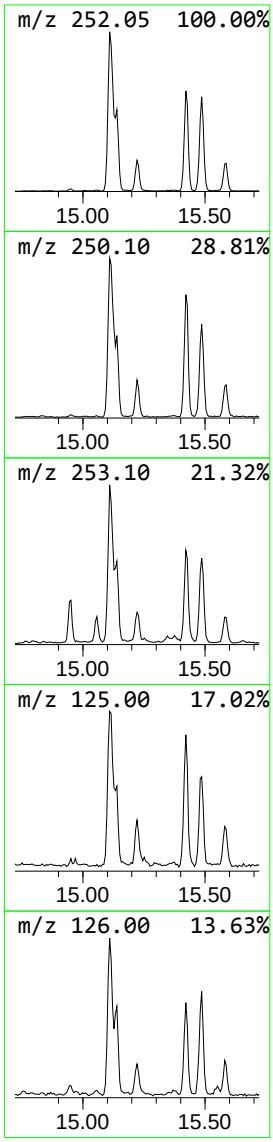
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.221	6.12 ng	343945	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
2	Benzo[e]pyrene	252	C20H12	000192-97-2	95
3	Perylene	252	C20H12	000198-55-0	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129420.D
Acq On : 28 Jul 2022 21:24
Operator : CG\JU
Sample : N3942-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11977

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

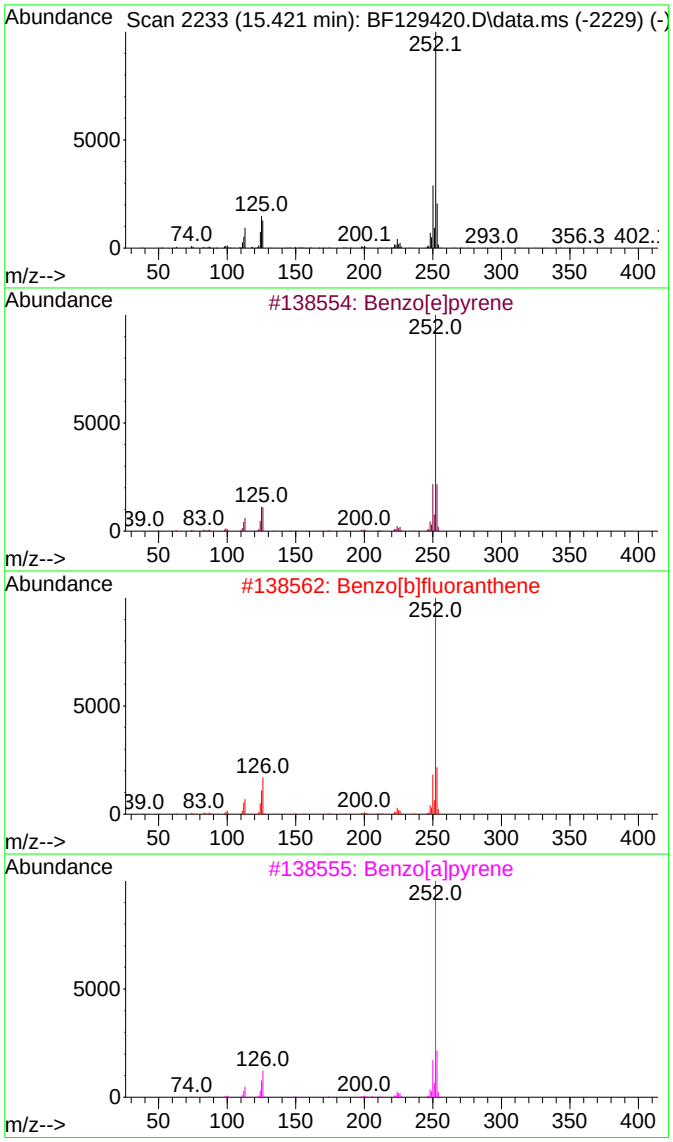
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

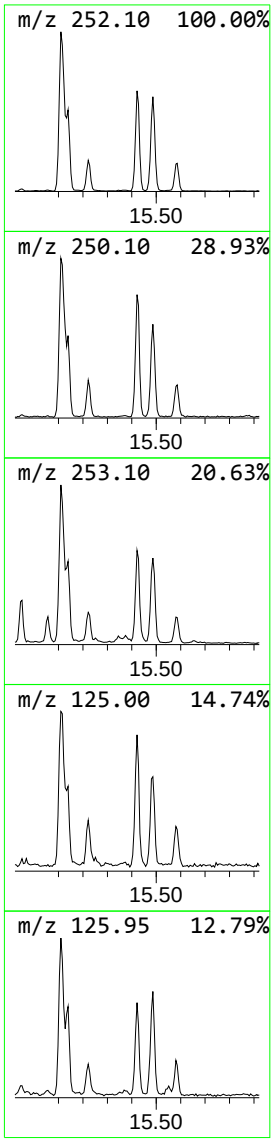
****

Peak Number 6 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.421	8.78 ng	493040	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
5	Perylene	252	C20H12	000198-55-0	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129420.D
Acq On : 28 Jul 2022 21:24
Operator : CG\JU
Sample : N3942-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11977

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

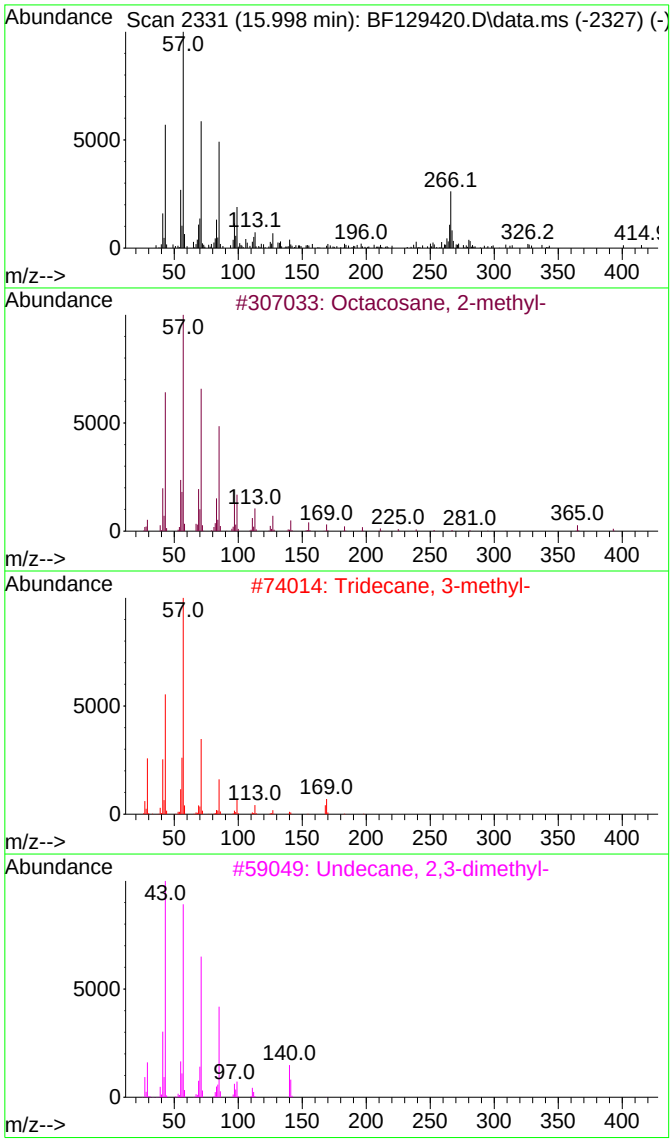
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

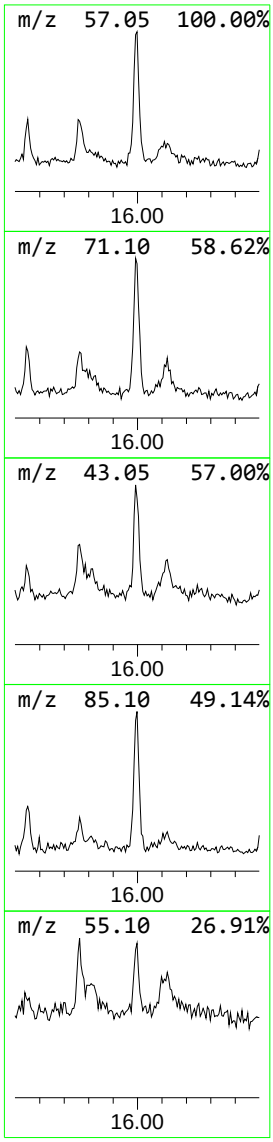
****

Peak Number 7 Octacosane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	2.34 ng	131699	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	52
2	Tridecane, 3-methyl-	198	C14H30	006418-41-3	50
3	Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	47
4	Nonadecane	268	C19H40	000629-92-5	46
5	Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129420.D
Acq On : 28 Jul 2022 21:24
Operator : CG\JU
Sample : N3942-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11977

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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
4H-Cyclopenta[d...	12.028	2.2	ng	166901	4	11.416	1507390	20.0
Pyrene, 1-methyl-	13.186	2.9	ng	222941	5	14.057	1519430	20.0
Cyclopentadecane	13.904	3.0	ng	230332	5	14.057	1519430	20.0
12-Octadecenal	14.969	2.2	ng	122780	6	15.551	1123490	20.0
Benzo[e]pyrene	15.221	6.1	ng	343945	6	15.551	1123490	20.0
Perylene	15.421	8.8	ng	493040	6	15.551	1123490	20.0
Octacosane, 2-m...	15.998	2.3	ng	131699	6	15.551	1123490	20.0