LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
Data File : BF123071.D
Acq On : 28 Jan 2021 21:18
Operator : JU/CG
Sample : M1253-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 124055

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-BF012721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123071.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	11	20	25	rBV	829074	1074801	13.07%	1.551%
2	5.128	514	517	524	rVB	73086	86524	1.05%	0.125%
3	5.510	577	582	585	rBV	5561132	5978980	72.69%	8.627%
4	6.516	747	753	757	rBV	5345440	6239891	75.86%	9.004%
5	6.893	813	817	820	rBV	1942167	1568498	19.07%	2.263%
6	7.451	907	912	915	rBV	4037700	4077320	49.57%	5.883%
7	8.175	1030	1035	1038	rBV	2413186	2101753	25.55%	3.033%
8	9.257	1213	1219	1222	rBV	7017373	7329969	89.11%	10.576%
9	9.645	1281	1285	1289	rBV	328882	271579	3.30%	0.392%
10	9.933	1326	1334	1338	rBV	2848209	2507928	30.49%	3.619%
11	10.728	1463	1469	1472	rBV	4958019	4905007	59.63%	7.077%
12	11.228	1551	1554	1558	rVB	106846	100155	1.22%	0.145%
13	11.286	1558	1564	1567	rBV5	36036	83246	1.01%	0.120%
14	11.322	1567	1570	1575	rVB	107960	101698	1.24%	0.147%
15	11.428	1583	1588	1590	rBV	2819421	2681374	32.60%	3.869%
16	11.451	1590	1592	1595	rVV	1480819	1194040	14.52%	1.723%
17	11.498	1595	1600	1603	rVB	203090	229783	2.79%	0.332%
18	11.651	1621	1626	1628	rBV2	123907	153451	1.87%	0.221%
19	11.927	1670	1673	1675	rBV	177839	149388	1.82%	0.216%
20	11.957	1675	1678	1682	rVV	983280	844647	10.27%	1.219%
21	12.039	1689	1692	1695	rBV	291694	317150	3.86%	0.458%
22	12.222	1718	1723	1725	rBV2	135269	176370	2.14%	0.254%
23	12.245	1725	1727	1731	rVB	131914	105705	1.29%	0.153%
24	12.480	1764	1767	1771	rBV	87799	101986	1.24%	0.147%
25	12.563	1778	1781	1786	rVB	223576	199195	2.42%	0.287%
26	12.645	1791	1795	1798	rBV	2525307	2210467	26.87%	3.189%
27	12.739	1808	1811	1814	rBV	245794	254257	3.09%	0.367%
28	12.874	1826	1834	1837	rBV	1819205	1950472	23.71%	2.814%
29	12.922	1839	1842	1846	rVB3	95973	110174	1.34%	0.159%
30	13.022	1852	1859	1862	rBV	7586716	8225422	100.00%	11.868%
31	13.186	1883	1887	1888	rBV3	102534	134383	1.63%	0.194%
32	13.204	1888	1890	1892	rVB	215849	175016	2.13%	0.253%
33	13.269	1896	1901	1904	rBV2	162894	222231	2.70%	0.321%
34	13.304	1904	1907	1910	rVB2	157024	166693	2.03%	0.241%
35	13.710	1973	1976	1981	rVB	196325	214243	2.60%	0.309%
36	13.821	1991	1995	1998	rBV2	135395	181766	2.21%	0.262%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
Data File : BF123071.D
Acq On : 28 Jan 2021 21:18
Operator : JU/CG
Sample : M1253-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 124055

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-BF012721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.874	2002	2004	2008	rVV2	111562	111916	1.36%	0.161%
38	13.927	2009	2013	2022	rVB3	935059	1573950	19.14%	2.271%
39	14.074	2030	2038	2041	rBV2	2491471	3219984	39.15%	4.646%
40	14.104	2041	2043	2049	rVB	490809	481548	5.85%	0.695%
41	14.498	2108	2110	2114	rVB3	93183	87196	1.06%	0.126%
42	14.557	2117	2120	2121	rVV2	118856	130776	1.59%	0.189%
43	14.586	2123	2125	2128	rVB2	223831	193823	2.36%	0.280%
44	14.668	2134	2139	2143	rVB3	248836	518703	6.31%	0.748%
45	14.716	2143	2147	2152	rBV	636570	812614	9.88%	1.173%
46	14.763	2152	2155	2161	rVB2	205538	313908	3.82%	0.453%
47	14.816	2161	2164	2166	rBV	130656	123001	1.50%	0.177%
48	14.904	2177	2179	2183	rVB	169076	148010	1.80%	0.214%
49	14.945	2183	2186	2187	rBV2	99652	101764	1.24%	0.147%
50	15.127	2213	2217	2220	rBV	497125	721634	8.77%	1.041%
51	15.210	2228	2231	2234	rBV3	144607	170046	2.07%	0.245%
52	15.433	2265	2269	2275	rVB	306833	394907	4.80%	0.570%
53	15.498	2276	2280	2285	rVB	305422	374579	4.55%	0.540%
54	15.563	2286	2291	2295	rVV	1457521	1808110	21.98%	2.609%
55	15.598	2295	2297	2303	rVB3	156632	214665	2.61%	0.310%
56	16.051	2370	2374	2380	rBV	173431	271222	3.30%	0.391%
57	16.133	2382	2388	2400	rVV8	100990	318821	3.88%	0.460%
58	16.880	2511	2515	2522	rVB5	55648	108362	1.32%	0.156%
59	17.051	2539	2544	2550	rBV2	113623	222247	2.70%	0.321%
60	17.192	2563	2568	2574	rBV	68149	132085	1.61%	0.191%
61	17.504	2616	2621	2630	rVB	99481	213458	2.60%	0.308%
62	18.362	2761	2767	2774	rBV3	47236	111899	1.36%	0.161%

Sum of corrected areas: 69304790

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Data File : BF123071.D
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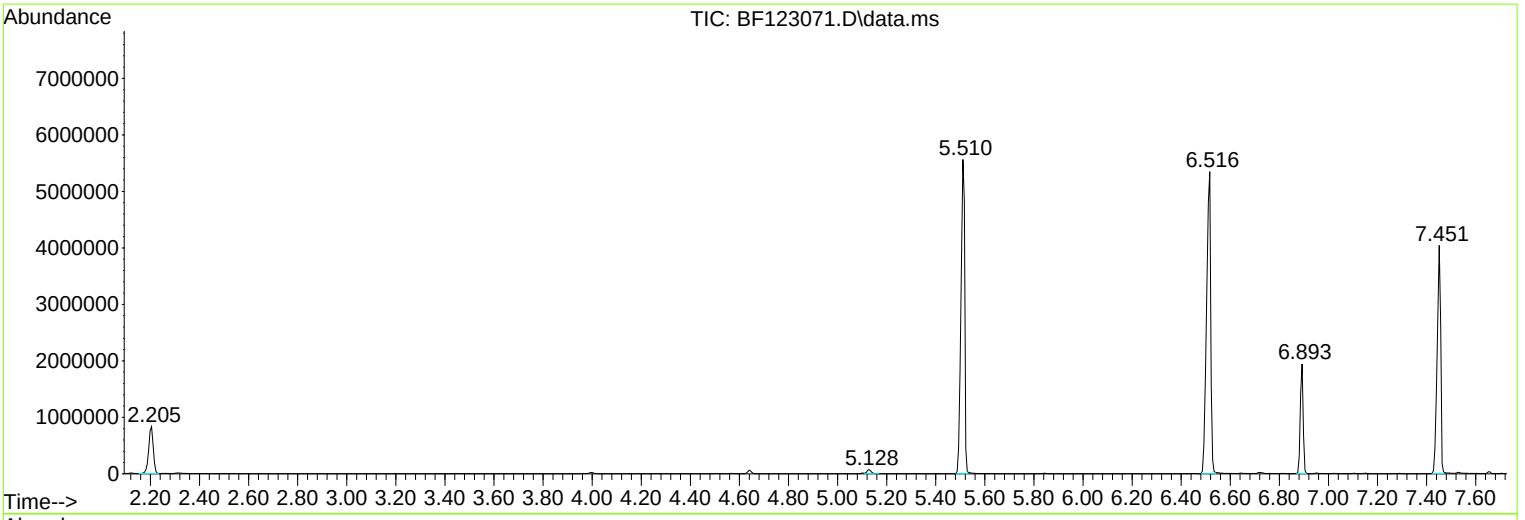
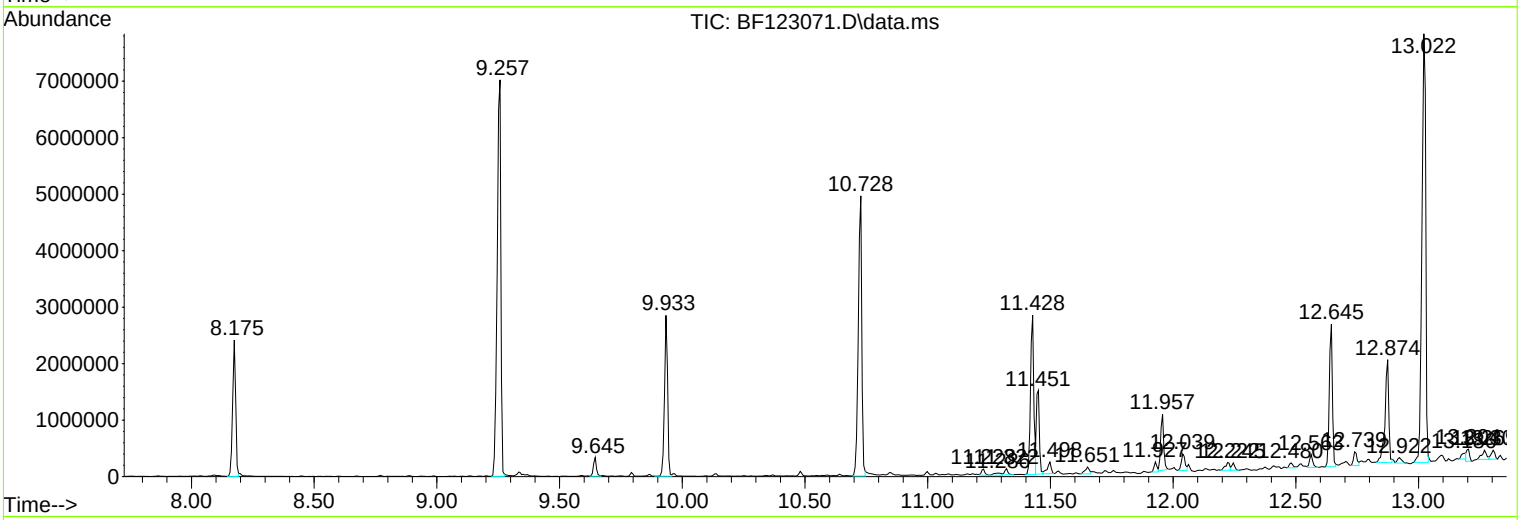
Misc :
ALS Vial : 19 Sample Multiplier: 1

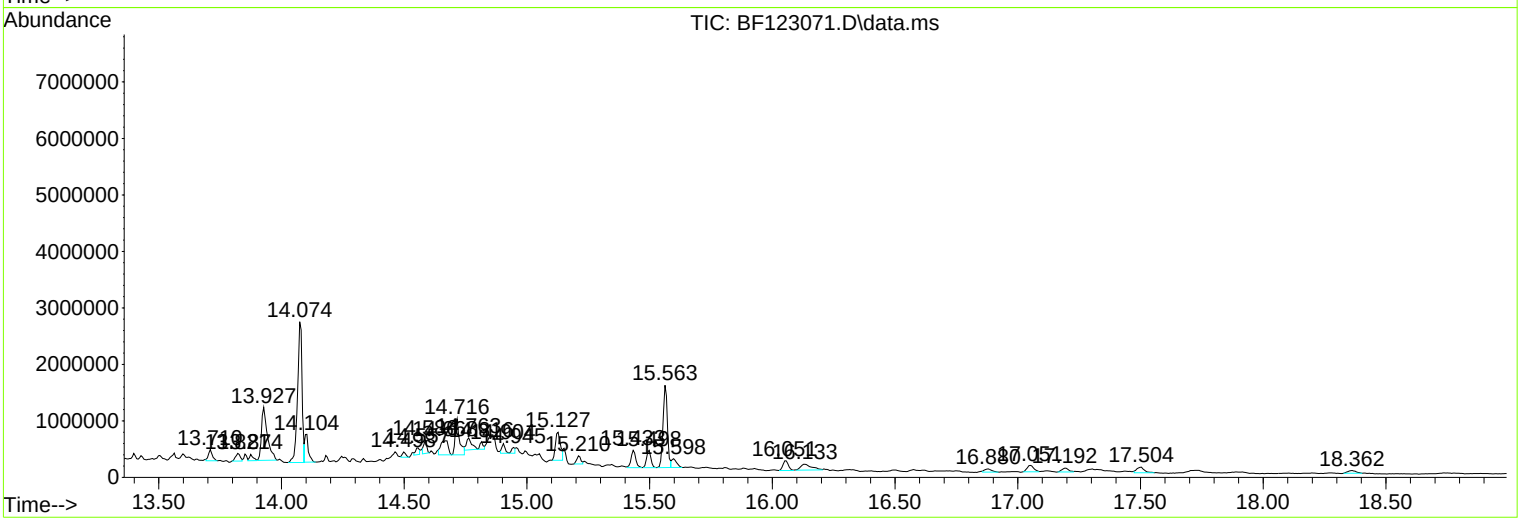
Instrument :
BNA_F
ClientSampleId :
124055

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Sample : M1253-01
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BNA_F
ClientSampleId :
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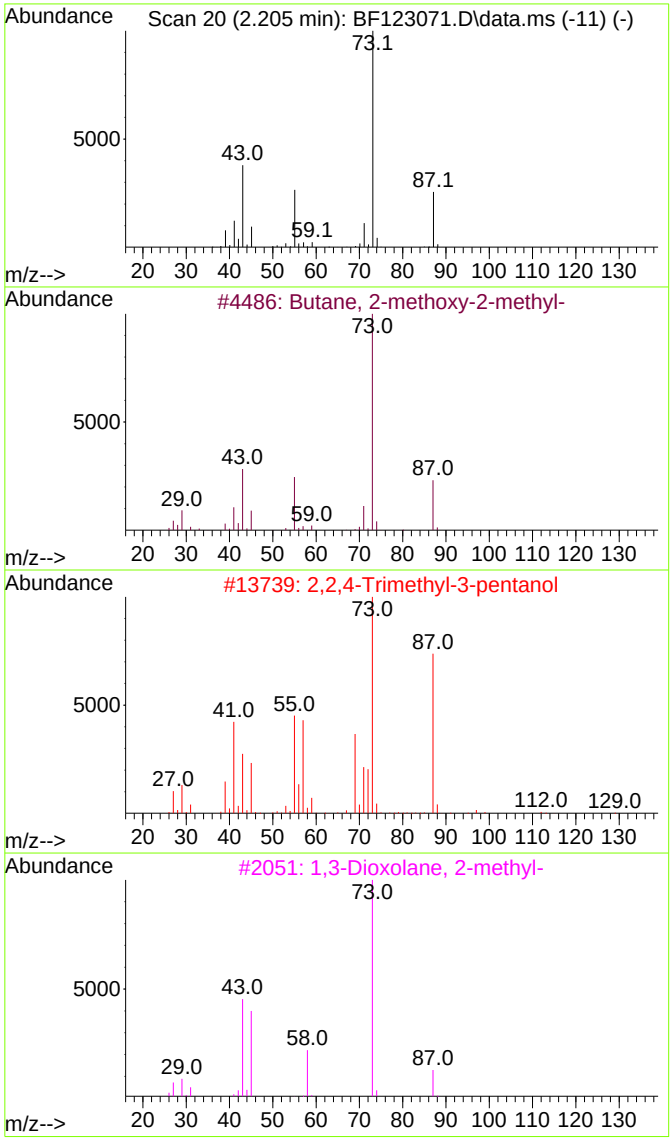
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

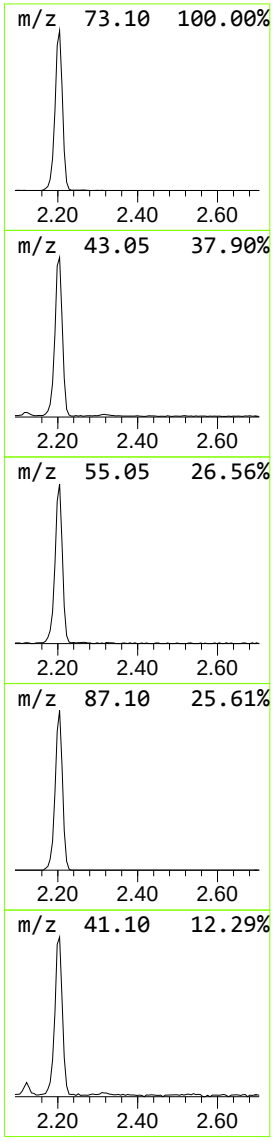
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	13.70 ng	1074800	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
Data File : BF123071.D
Acq On : 28 Jan 2021 21:18
Operator : JU/CG
Sample : M1253-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
124055

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

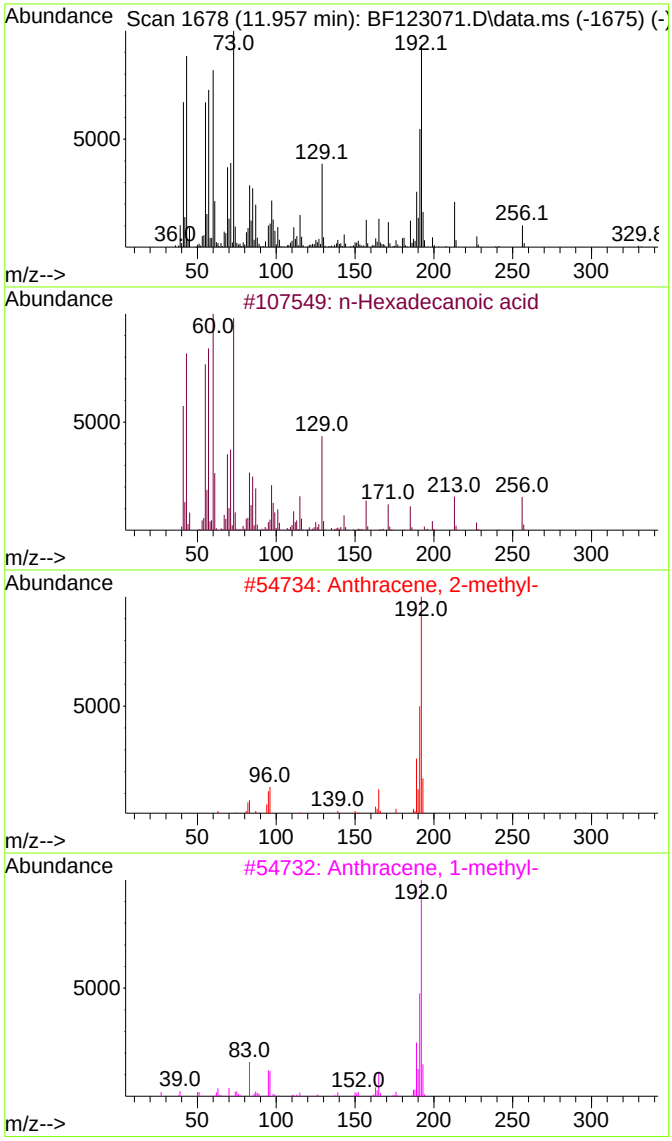
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

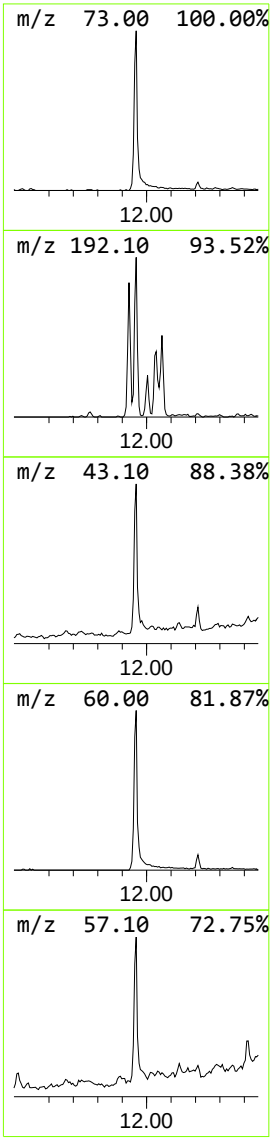
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	6.30 ng	844647	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91





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Acq On : 28 Jan 2021 21:18
Operator : JU/CG
Sample : M1253-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
124055

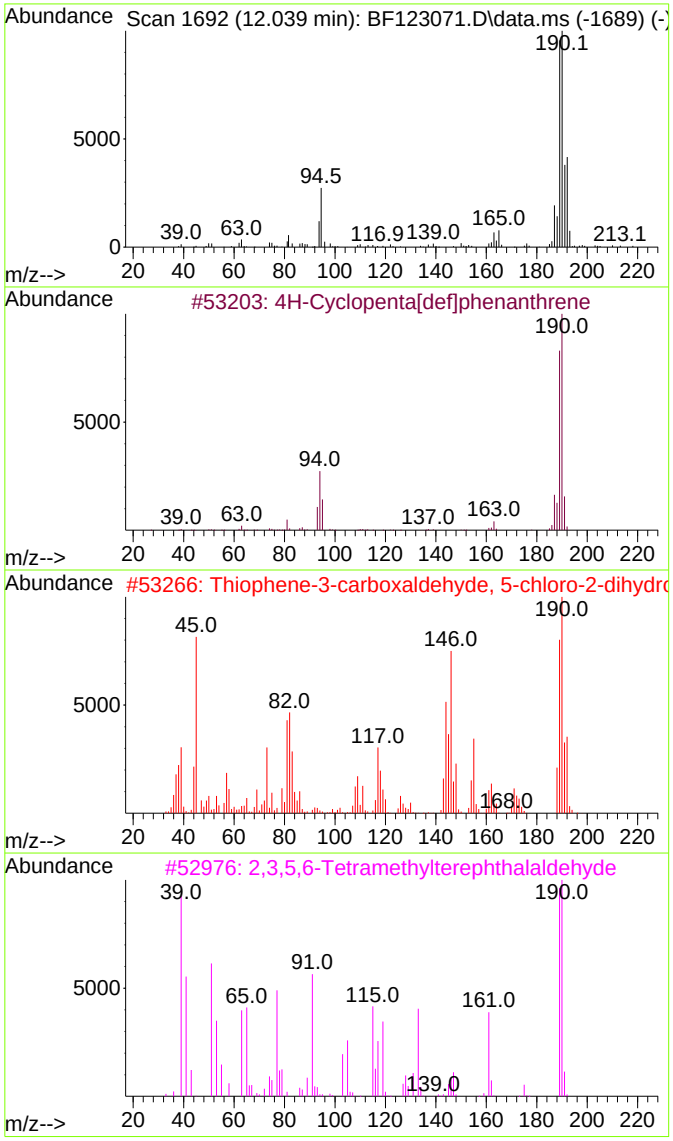
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

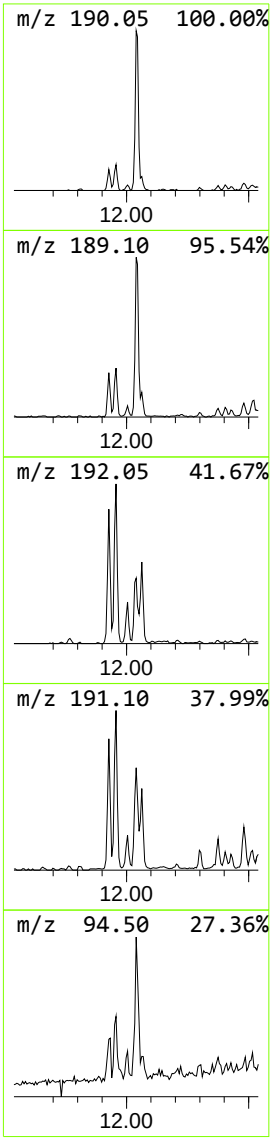
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.039	2.37 ng	317150	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	47
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	43
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	42
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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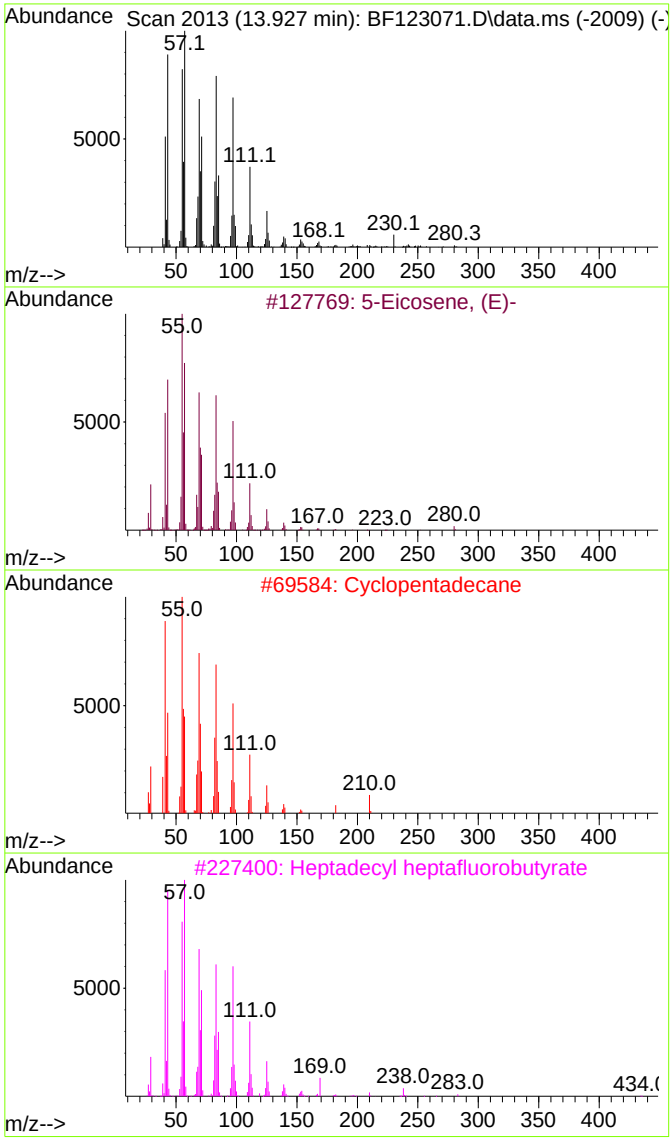
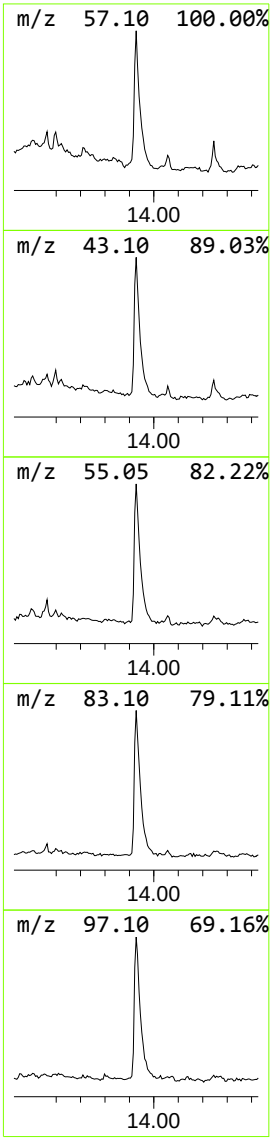
****

Peak Number 4 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	9.78 ng	1573950	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	Cyclopentadecane	210	C15H30	000295-48-7	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





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BNA_F
ClientSampleId :
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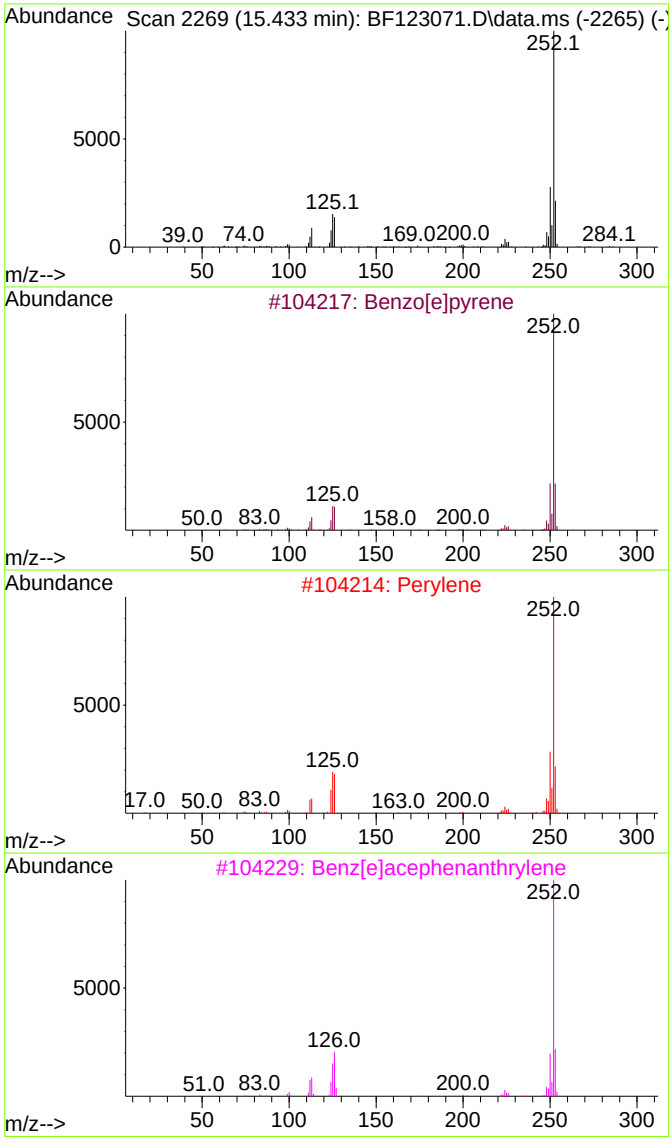
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

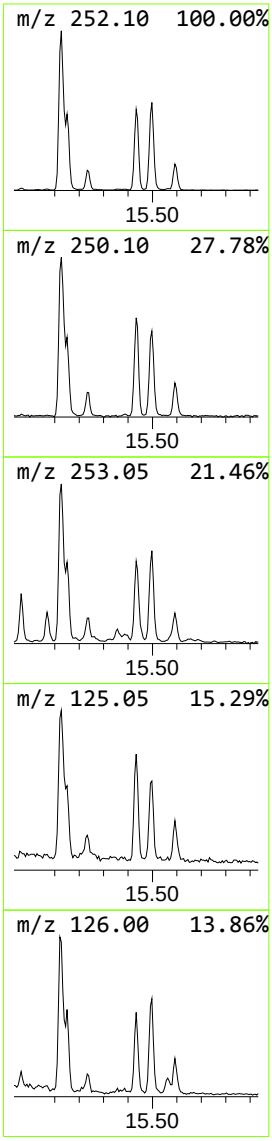
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.433	4.37 ng	394907	Perylene-d12	15.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Perylene	252	C20H12	000198-55-0	95
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
4	Benzo[a]pyrene	252	C20H12	000050-32-8	91
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





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Data File : BF123071.D
Acq On : 28 Jan 2021 21:18
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Sample : M1253-01
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ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 124055

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

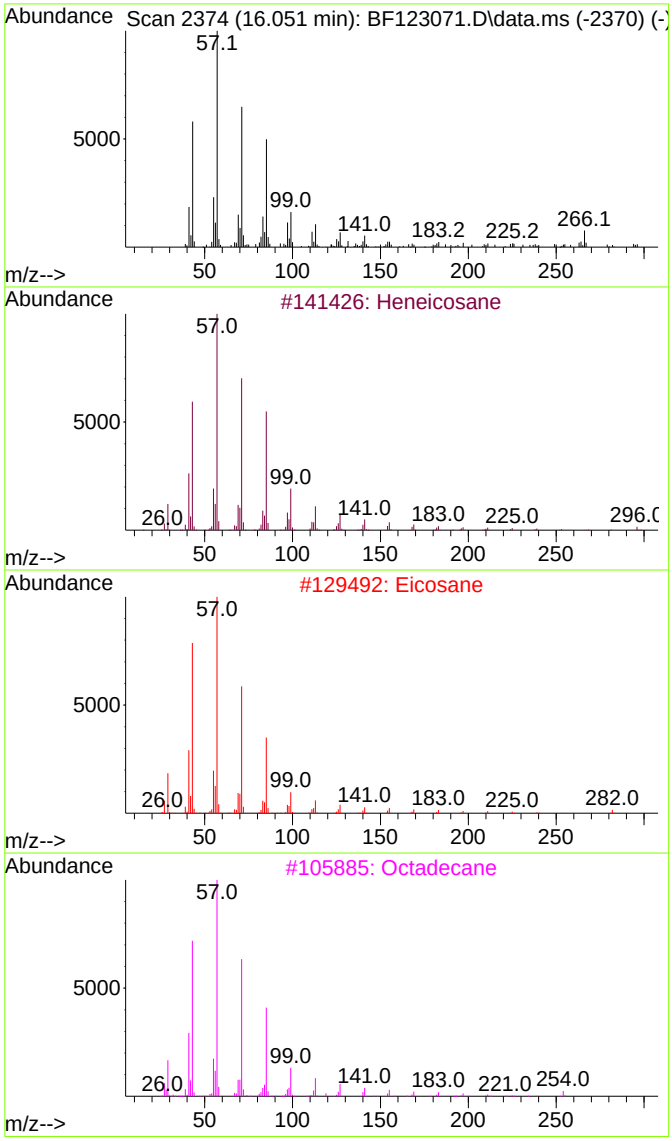
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

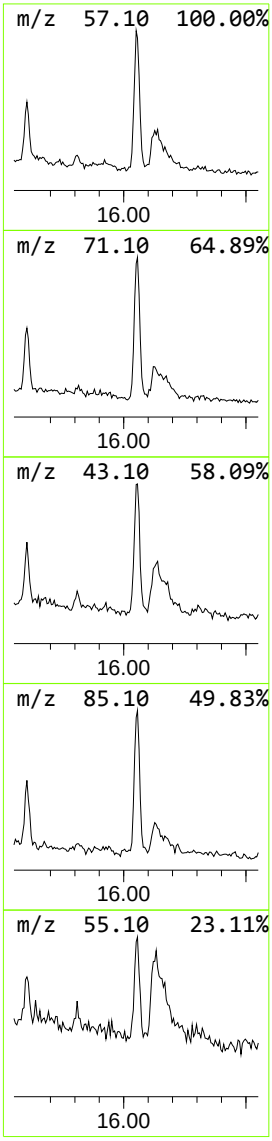
****

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.051	3.00 ng	271222	Perylene-d12	15.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Eicosane	282	C20H42	000112-95-8	93
3	Octadecane	254	C18H38	000593-45-3	91
4	Hentriacontane	437	C31H64	000630-04-6	90
5	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
Data File : BF123071.D
Acq On : 28 Jan 2021 21:18
Operator : JU/CG
Sample : M1253-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
124055

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

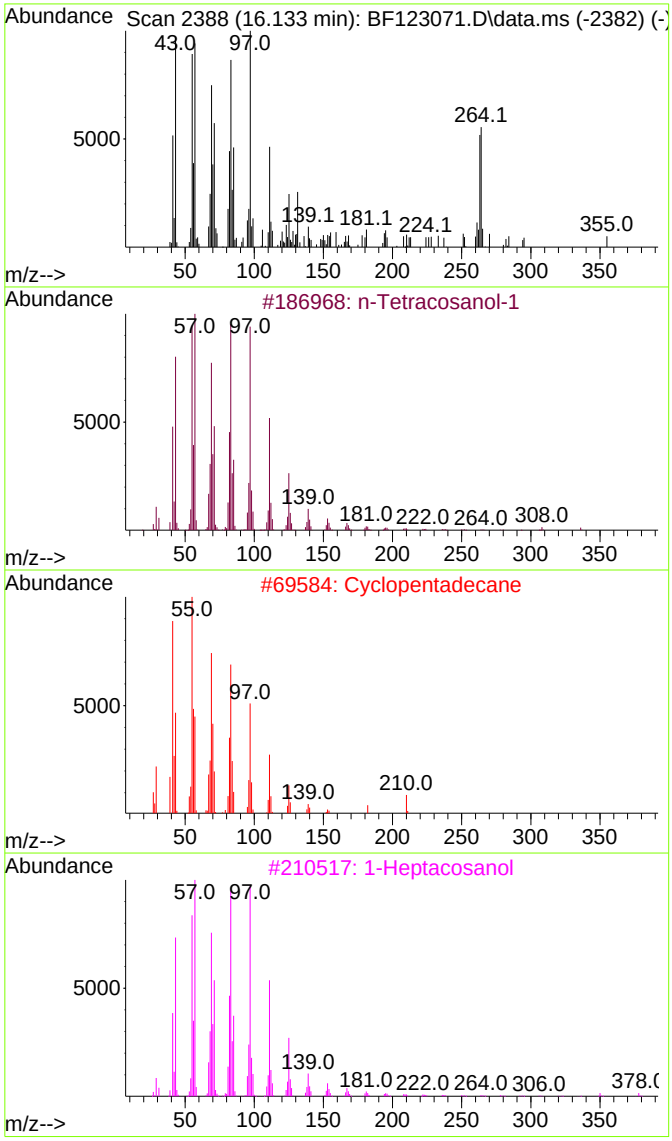
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

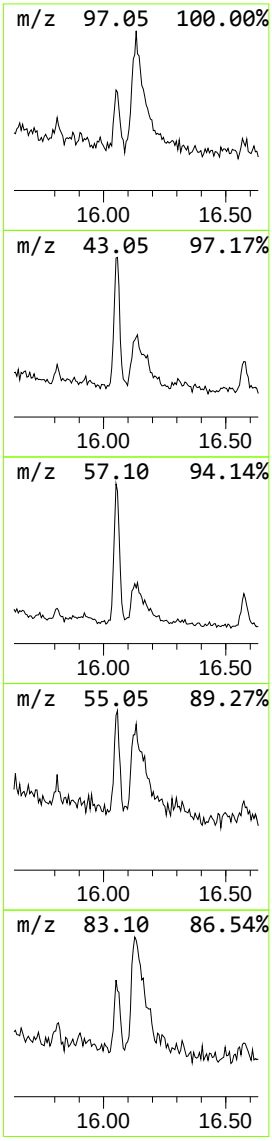
****

Peak Number 7 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.133	3.53 ng	318821	Perylene-d12	15.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	86
2	Cyclopentadecane	210	C15H30	000295-48-7	78
3	1-Heptacosanol	396	C27H56O	002004-39-9	70
4	Behenic alcohol	326	C22H46O	000661-19-8	70
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
Data File : BF123071.D
Acq On : 28 Jan 2021 21:18
Operator : JU/CG
Sample : M1253-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 124055

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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
Butane, 2-metho...	2.205	13.7	ng	1074800	1	6.893	1568500	20.0
n-Hexadecanoic ...	11.957	6.3	ng	844647	4	11.428	2681370	20.0
4H-Cyclopenta[d...	12.039	2.4	ng	317150	4	11.428	2681370	20.0
5-Eicosene, (E)-	13.927	9.8	ng	1573950	5	14.080	3219980	20.0
Benzo[e]pyrene	15.433	4.4	ng	394907	6	15.563	1808110	20.0
Heneicosane	16.051	3.0	ng	271222	6	15.563	1808110	20.0
n-Tetracosanol-1	16.133	3.5	ng	318821	6	15.563	1808110	20.0