LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123623.D
Acq On : 19 Apr 2021 15:30
Operator : JU/CG
Sample : M2051-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0124027

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-BF041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123623.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	13	rVB	2748263	3480921	57.13%	6.614%
2	3.363	214	217	226	rBV	29987	64945	1.07%	0.123%
3	3.934	310	314	319	rVB	57320	72812	1.20%	0.138%
4	5.081	505	509	516	rVB2	64873	76757	1.26%	0.146%
5	5.299	539	546	549	rBV3	69564	81022	1.33%	0.154%
6	5.451	569	572	574	rBV	71007	69321	1.14%	0.132%
7	5.487	574	578	582	rVB	6558130	5827411	95.65%	11.072%
8	6.498	745	750	756	rBV	6750363	6092604	100.00%	11.576%
9	6.687	779	782	784	rBV	215131	213727	3.51%	0.406%
10	6.863	808	812	815	rBV	1904014	1515244	24.87%	2.879%
11	7.422	902	907	910	rBV	4414968	3996068	65.59%	7.593%
12	8.145	1026	1030	1033	rBV	2378976	1962511	32.21%	3.729%
13	9.228	1208	1214	1217	rBV	5394202	5055723	82.98%	9.606%
14	9.339	1229	1233	1238	rVB	223895	213833	3.51%	0.406%
15	9.616	1277	1280	1283	rBV	650111	491331	8.06%	0.934%
16	9.904	1325	1329	1333	rBV	2356662	2020979	33.17%	3.840%
17	10.110	1360	1364	1367	rBV	76820	72817	1.20%	0.138%
18	10.698	1459	1464	1467	rBV	4560409	4258712	69.90%	8.092%
19	11.198	1546	1549	1554	rVB	75326	69130	1.13%	0.131%
20	11.292	1562	1565	1570	rVB2	62824	75395	1.24%	0.143%
21	11.392	1579	1582	1585	rBV	2415286	2249699	36.93%	4.275%
22	11.416	1585	1586	1590	rVV	891476	597721	9.81%	1.136%
23	11.469	1590	1595	1598	rVB2	142311	187426	3.08%	0.356%
24	11.622	1616	1621	1623	rBV2	112895	108842	1.79%	0.207%
25	11.898	1663	1668	1670	rBV	130920	127665	2.10%	0.243%
26	11.922	1670	1672	1677	rVV	404769	373436	6.13%	0.710%
27	12.010	1683	1687	1689	rBV2	130686	150040	2.46%	0.285%
28	12.027	1689	1690	1694	rVB	83056	65013	1.07%	0.124%
29	12.192	1715	1718	1720	rBV	99065	91669	1.50%	0.174%
30	12.216	1720	1722	1725	rVB	140473	108707	1.78%	0.207%
31	12.445	1758	1761	1764	rBV2	67791	69322	1.14%	0.132%
32	12.486	1764	1768	1773	rVV6	57610	90141	1.48%	0.171%
33	12.527	1773	1775	1781	rVB2	84774	96481	1.58%	0.183%
34	12.610	1785	1789	1793	rVB	1151492	921276	15.12%	1.750%
35	12.839	1822	1828	1831	rBV2	889597	877788	14.41%	1.668%
36	12.886	1834	1836	1844	rVB2	71732	78869	1.29%	0.150%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123623.D
Acq On : 19 Apr 2021 15:30
Operator : JU/CG
Sample : M2051-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0124027

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-BF041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.957	1844	1848	1849	rBV2	79380	74405	1.22%	0.141%
38	12.986	1849	1853	1856	rVV	5065480	4234985	69.51%	8.047%
39	13.057	1860	1865	1869	rBV2	65982	114085	1.87%	0.217%
40	13.145	1873	1880	1882	rBV6	73242	127366	2.09%	0.242%
41	13.163	1882	1883	1887	rVB	86936	75149	1.23%	0.143%
42	13.269	1897	1901	1905	rBV2	108019	123819	2.03%	0.235%
43	13.674	1967	1970	1975	rVB	113795	108995	1.79%	0.207%
44	13.780	1985	1988	1992	rBV3	51755	79763	1.31%	0.152%
45	13.880	2002	2005	2006	rBV3	78659	76028	1.25%	0.144%
46	13.910	2006	2010	2024	rVV4	247827	694926	11.41%	1.320%
47	14.039	2027	2032	2035	rVV2	1965198	2111766	34.66%	4.012%
48	14.063	2035	2036	2042	rVB	362375	290439	4.77%	0.552%
49	14.427	2095	2098	2100	rVB	73876	65919	1.08%	0.125%
50	15.086	2206	2210	2213	rBV	239349	351332	5.77%	0.668%
51	15.398	2259	2263	2268	rVB	130721	188286	3.09%	0.358%
52	15.457	2269	2273	2279	rVB	195180	243681	4.00%	0.463%
53	15.521	2279	2284	2288	rBV	1139917	1459781	23.96%	2.774%
54	17.004	2531	2536	2544	rVB2	96505	188060	3.09%	0.357%
55	17.445	2607	2611	2619	rVB2	61219	115573	1.90%	0.220%

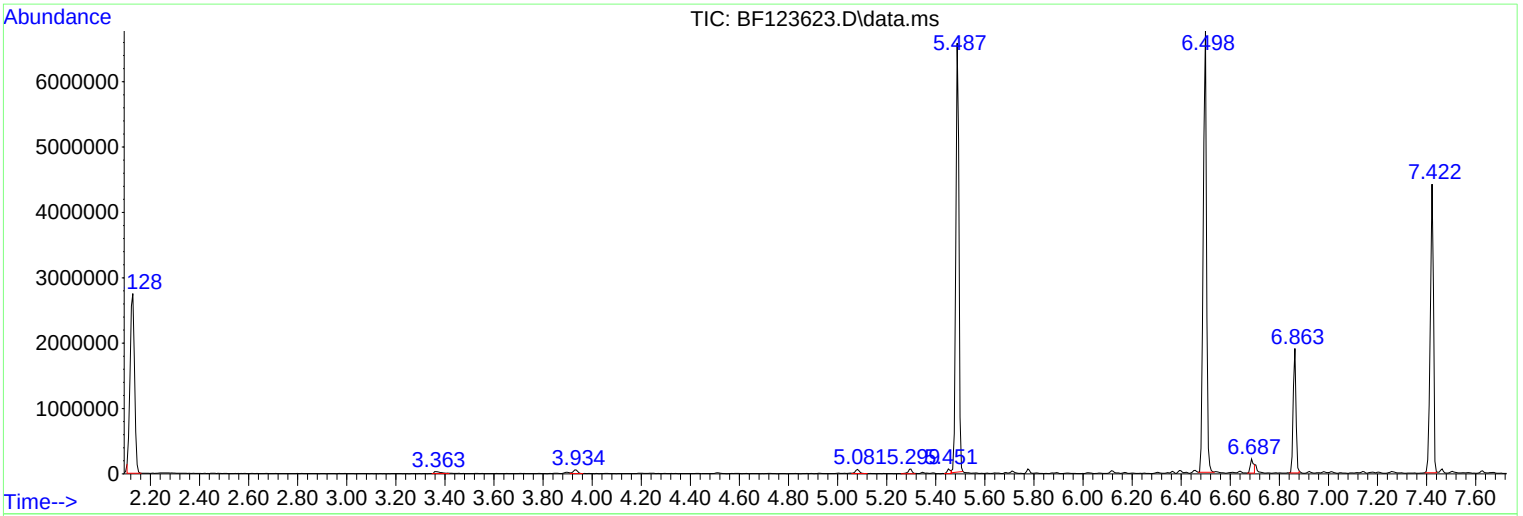
Sum of corrected areas: 52629716

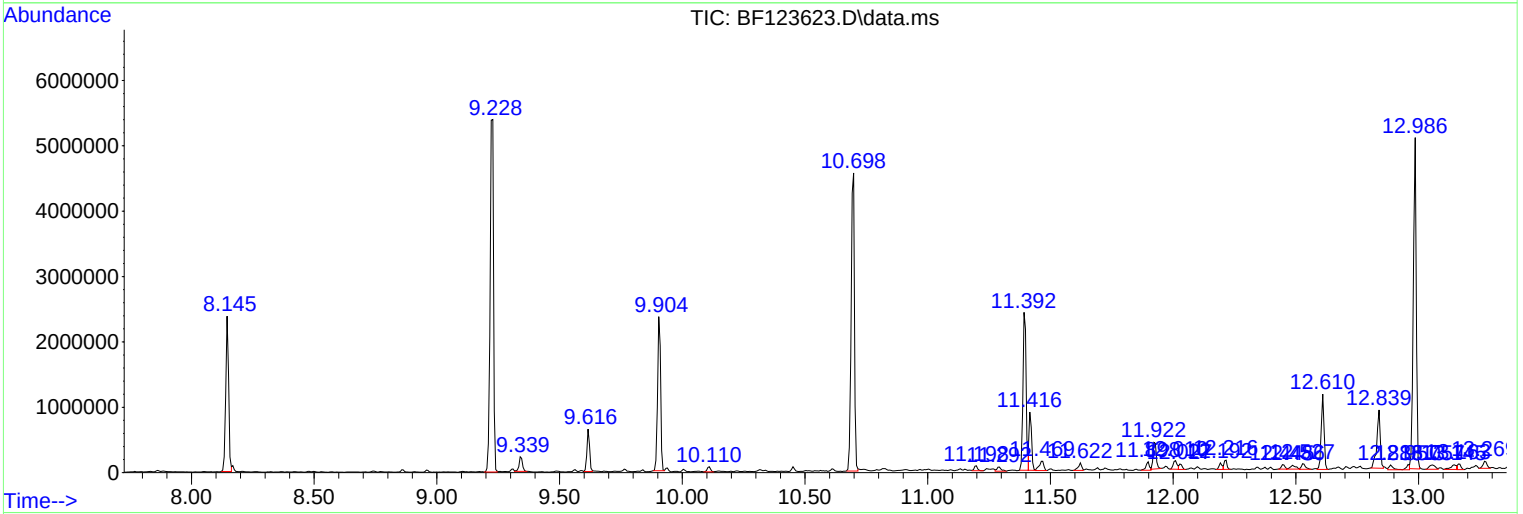
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123623.D
Acq On : 19 Apr 2021 15:30
Operator : JU/CG
Sample : M2051-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

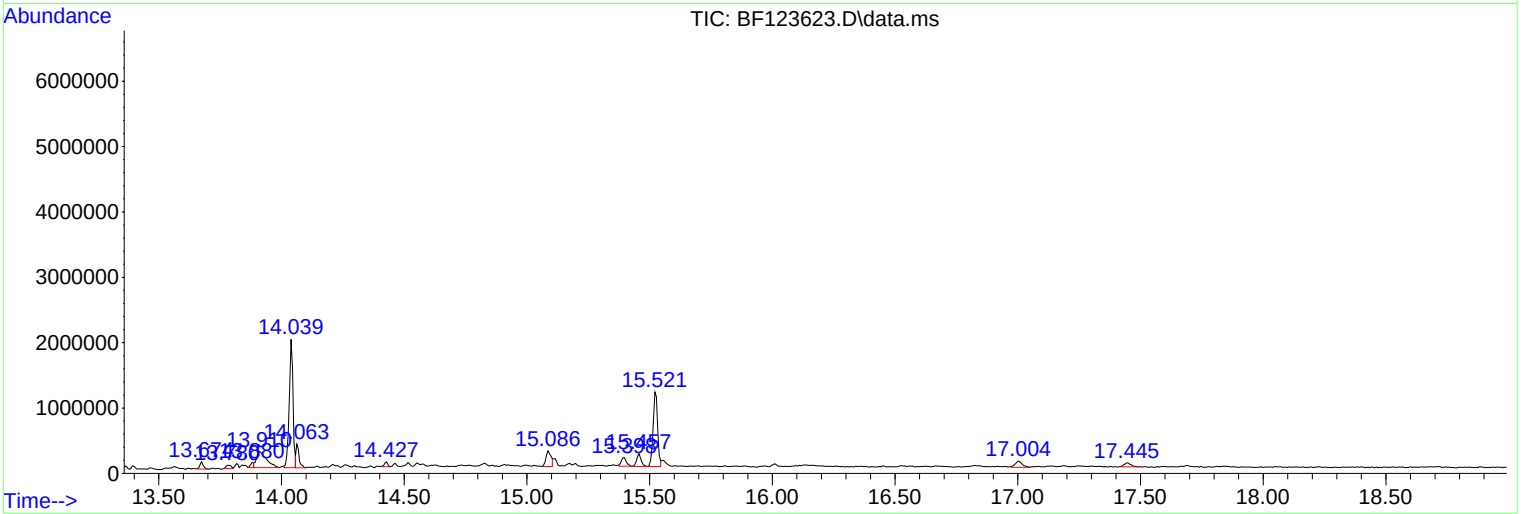
Instrument :
BNA_F
ClientSampleId :
0124027

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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_F\Data\BF041921\
Data File : BF123623.D
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Operator : JU/CG
Sample : M2051-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0124027

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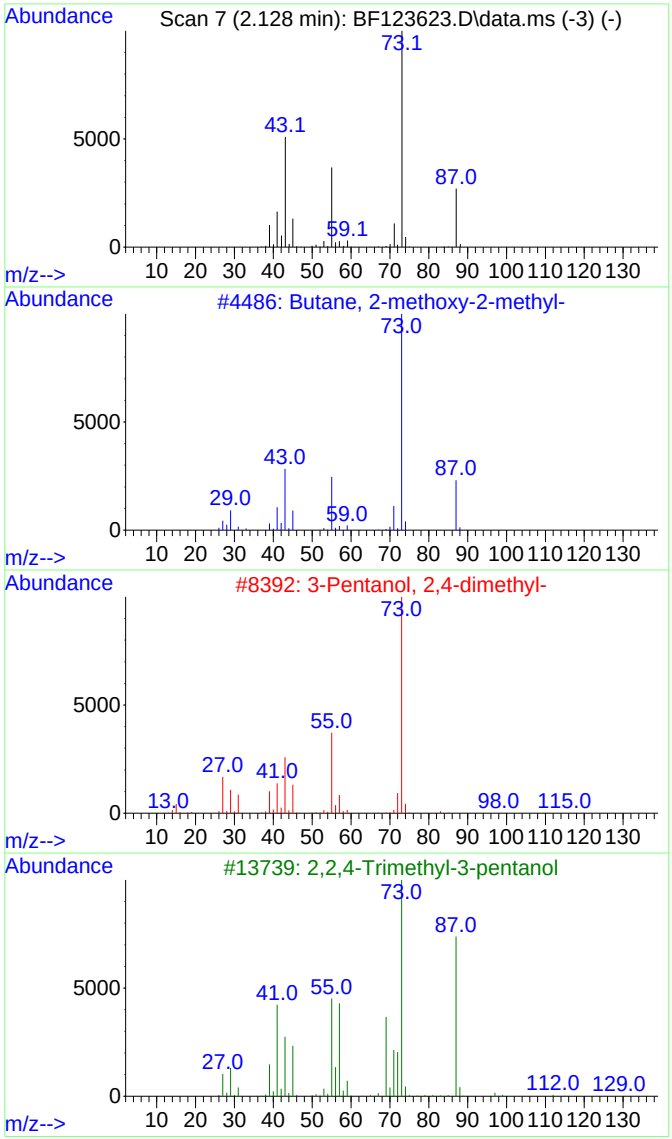
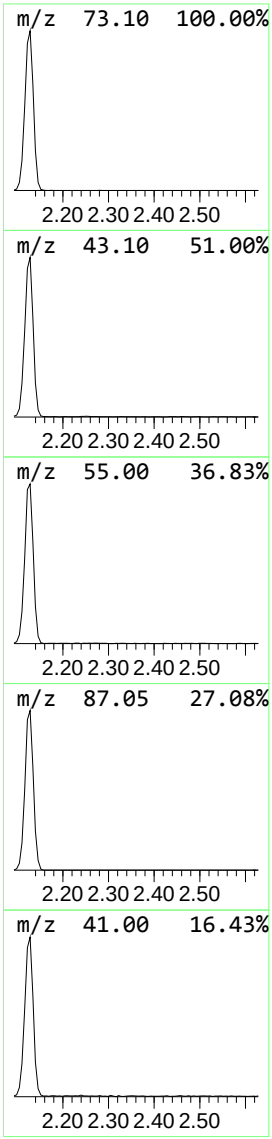
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	45.95 ng	3480920	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123623.D
Acq On : 19 Apr 2021 15:30
Operator : JU/CG
Sample : M2051-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0124027

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

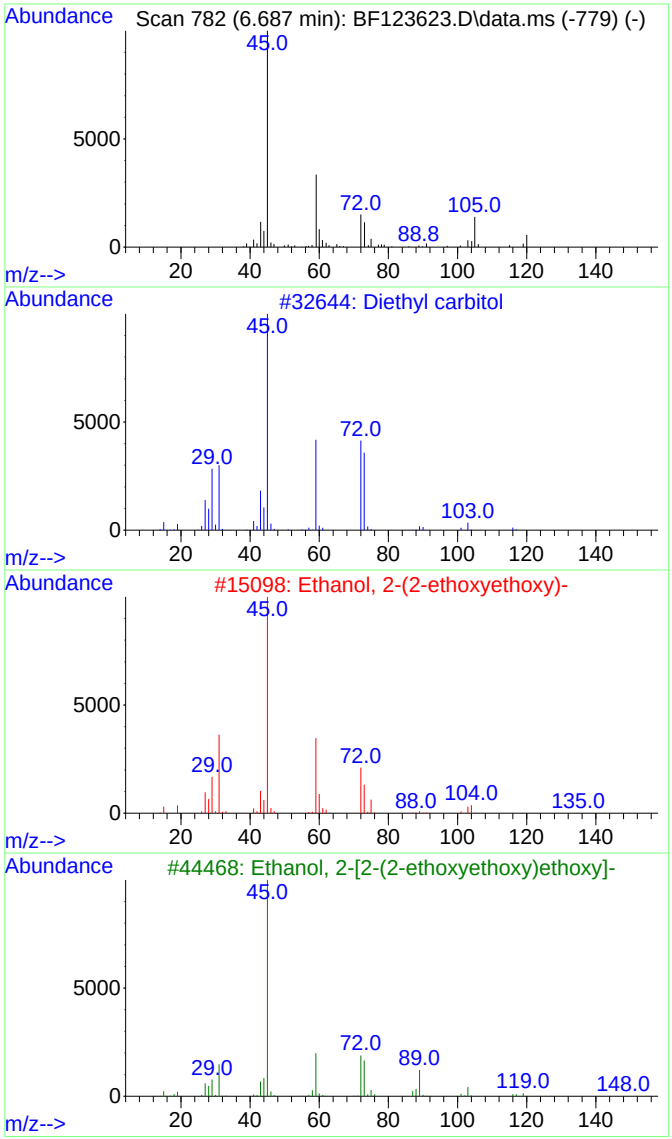
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

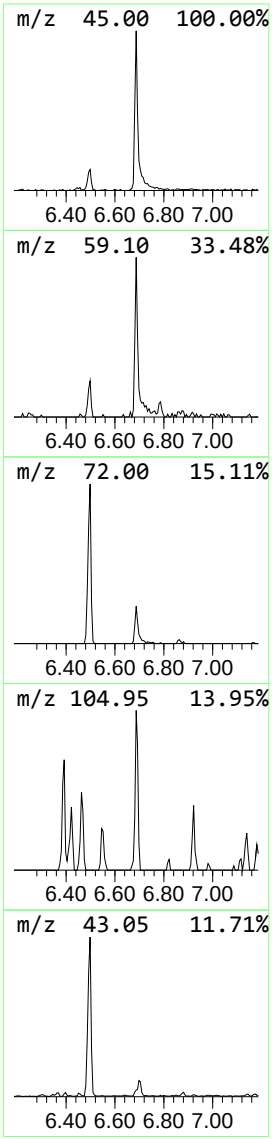
****

Peak Number 2 Diethyl carbitol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.687	2.82 ng	213727	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl carbitol	162	C8H18O3	000112-36-7	72
2	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	56
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	45
4	Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	37
5	Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123623.D
Acq On : 19 Apr 2021 15:30
Operator : JU/CG
Sample : M2051-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0124027

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

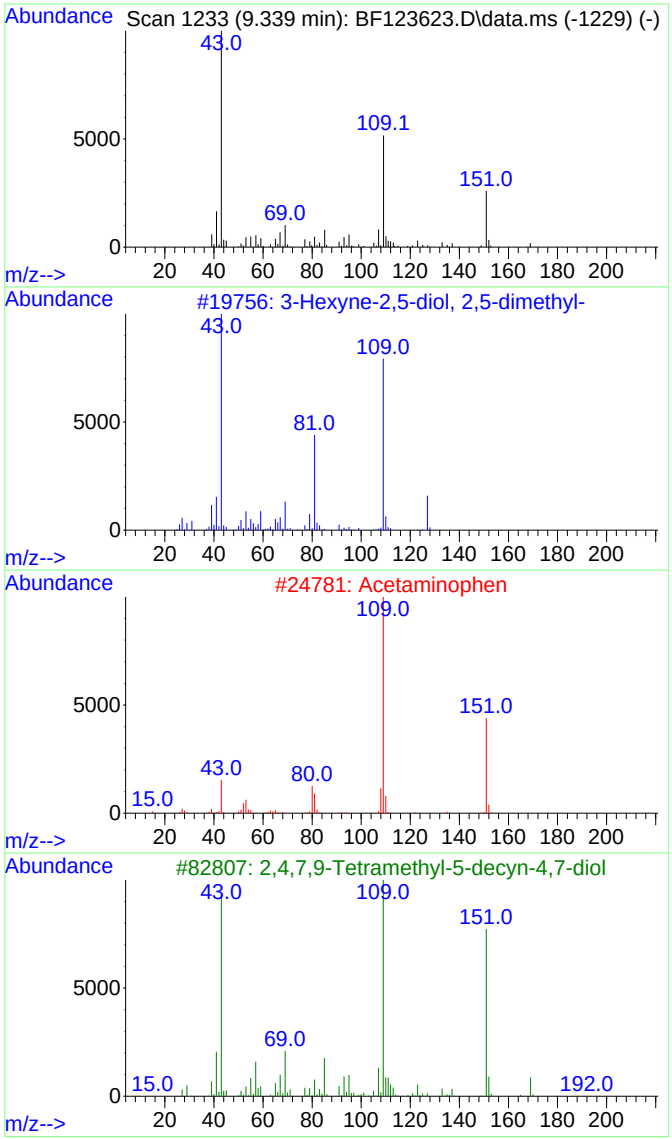
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

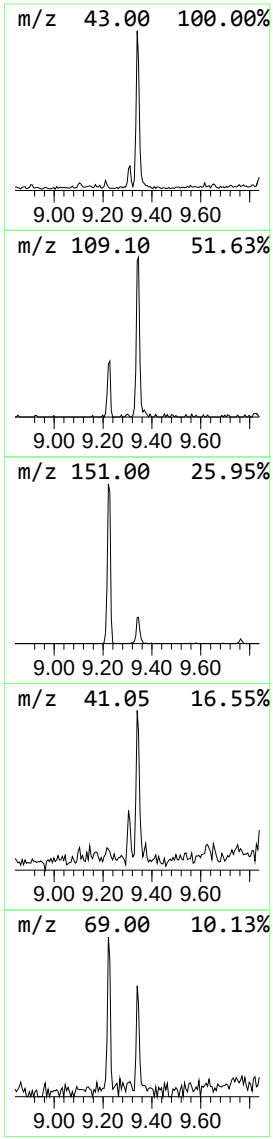
****

Peak Number 3 unknown9.33 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.339	2.12 ng	213833	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexyne-2,5-diol, 2,5-dimethyl-	142	C8H14O2	000142-30-3	47
2	Acetaminophen	151	C8H9NO2	000103-90-2	46
3	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	43
4	Metacetamol	151	C8H9NO2	000621-42-1	43
5	Cyclohexanol, 3,3,5-trimethyl-, ...	142	C9H18O	000767-54-4	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123623.D
Acq On : 19 Apr 2021 15:30
Operator : JU/CG
Sample : M2051-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0124027

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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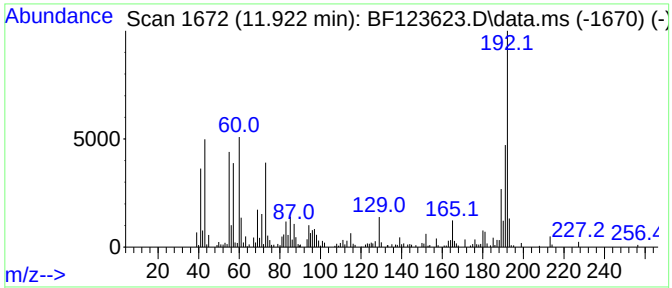
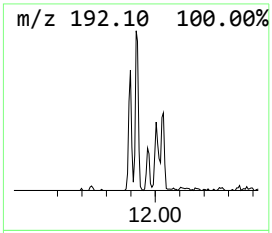
****

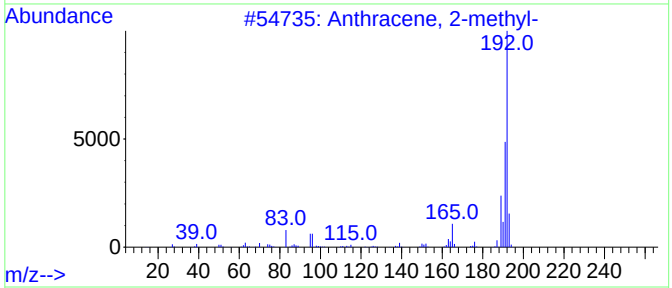
Peak Number 4 Anthracene, 2-methyl- Concentration Rank 3

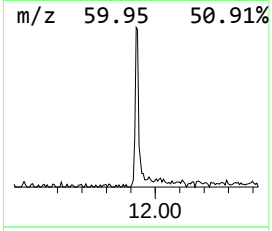
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.32 ng	373436	Phenanthrene-d10	11.392

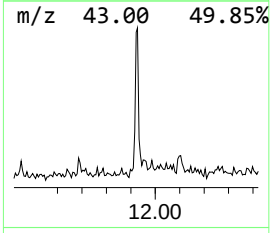
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	92
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
3	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	83
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	83
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	78

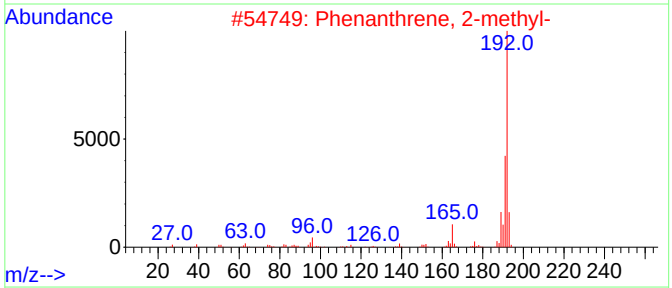


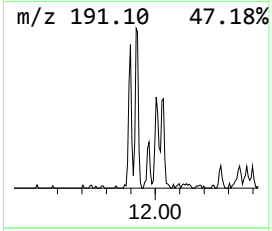


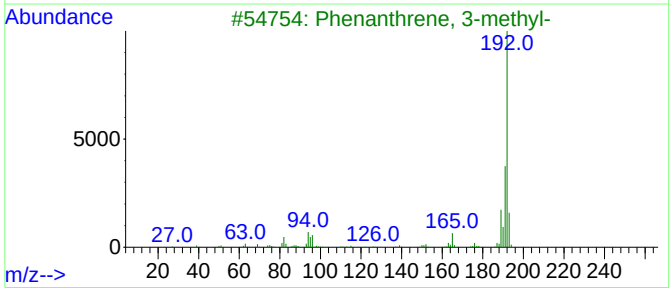


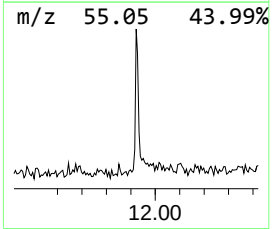












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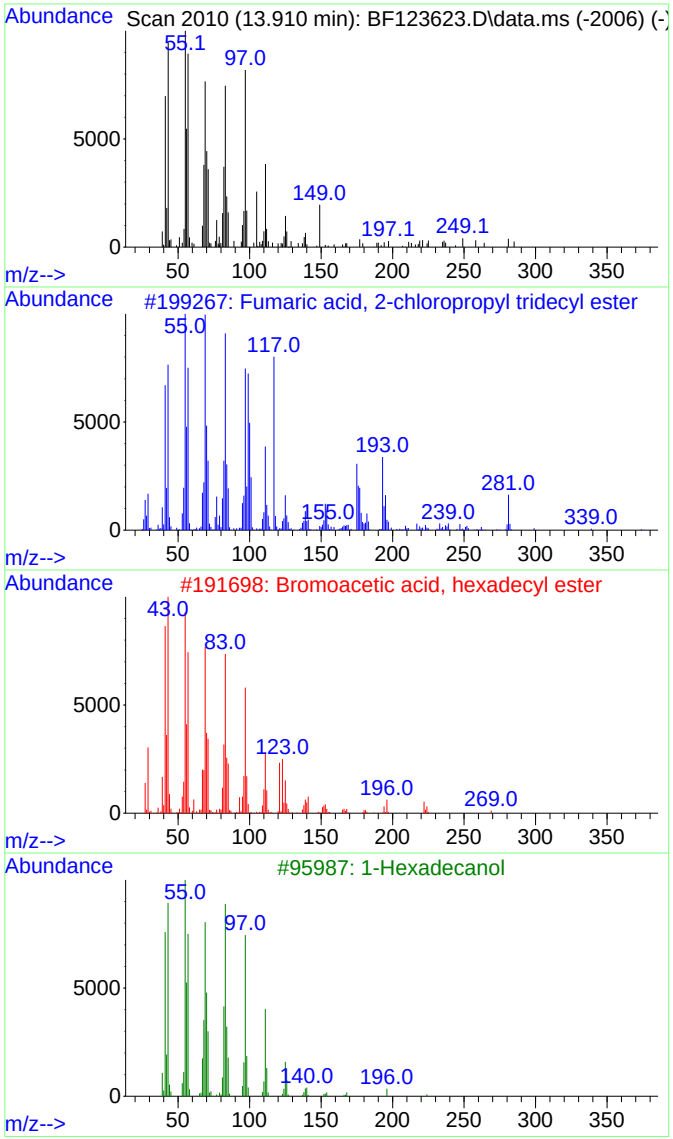
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

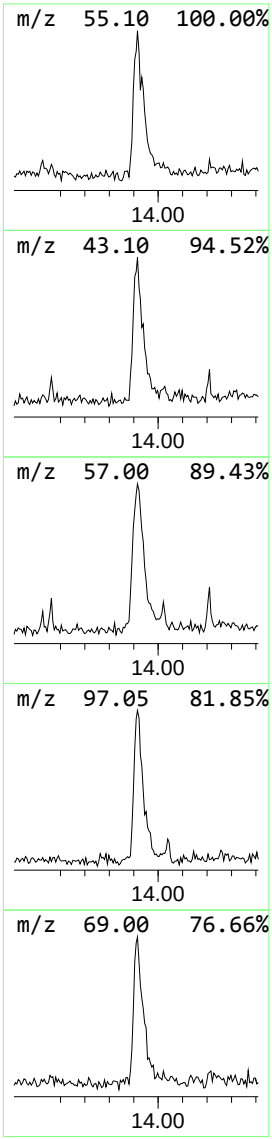
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Fumaric acid, 2-chloropropy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	6.58 ng	694926	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1000348-57-1	87
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	83
3	1-Hexadecanol	242	C16H34O	036653-82-4	83
4	1-Octadecanol	270	C18H38O	000112-92-5	81
5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123623.D
Acq On : 19 Apr 2021 15:30
Operator : JU/CG
Sample : M2051-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0124027

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

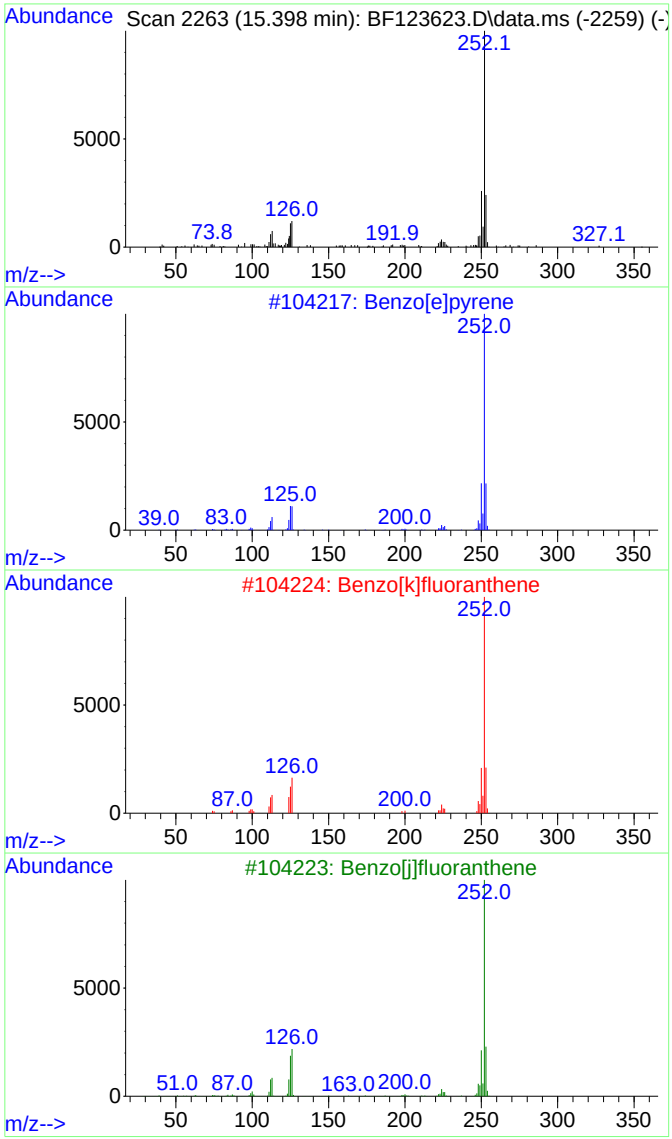
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

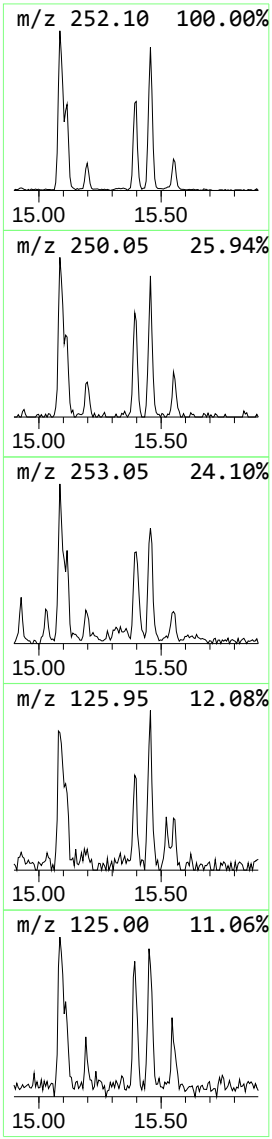
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	2.58 ng	188286	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4	Benzo[a]pyrene	252	C20H12	000050-32-8	95
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123623.D
Acq On : 19 Apr 2021 15:30
Operator : JU/CG
Sample : M2051-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0124027

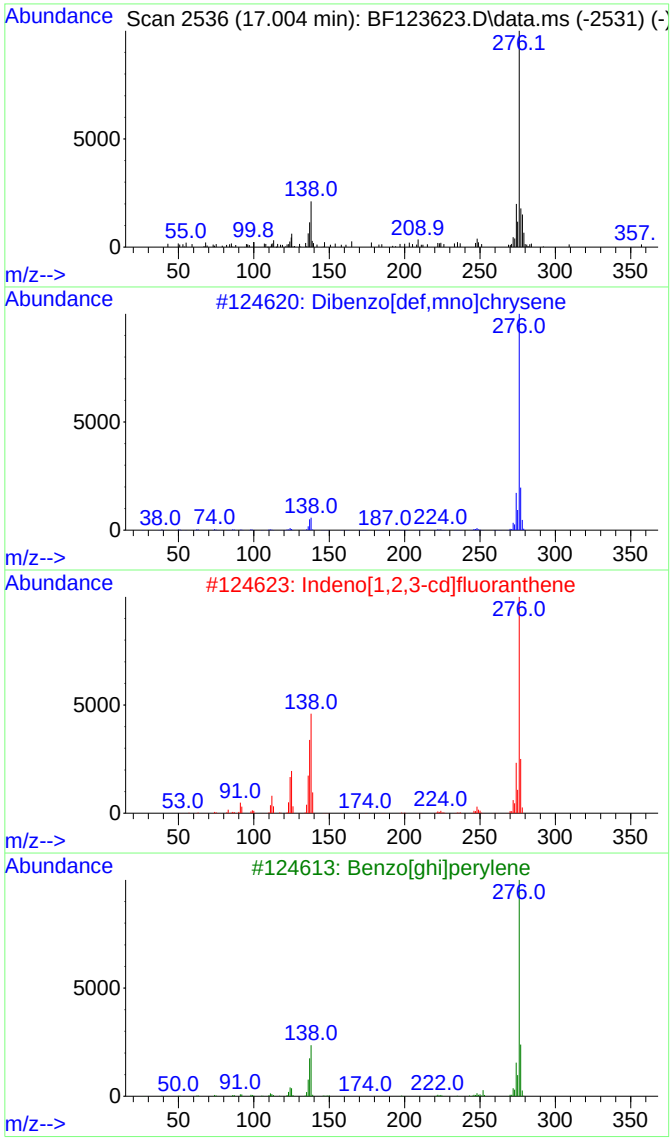
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

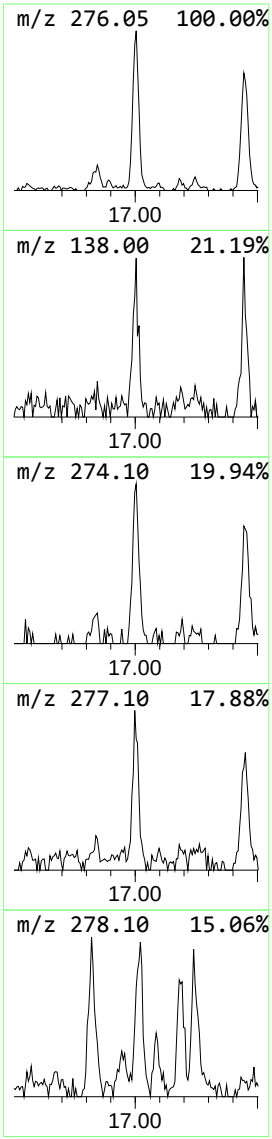
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Dibenzo[def,mno]chrysene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.004	2.58 ng	188060	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	81
2	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	76
3	Benzo[ghi]perylene	276	C22H12	000191-24-2	76
4	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	62
5	2-Thiophenecarbaldehyde, 5-[5-(t...	276	C13H8OS3	1000217-28-5	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123623.D
Acq On : 19 Apr 2021 15:30
Operator : JU/CG
Sample : M2051-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0124027

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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...	2.128	46.0	ng	3480920	1	6.863	1515240	20.0
Diethyl carbitol	6.687	2.8	ng	213727	1	6.863	1515240	20.0
unknown9.33	9.339	2.1	ng	213833	3	9.904	2020980	20.0
Anthracene, 2-m...	11.922	3.3	ng	373436	4	11.392	2249700	20.0
Fumaric acid, 2...	13.910	6.6	ng	694926	5	14.039	2111770	20.0
Benzo[e]pyrene	15.398	2.6	ng	188286	6	15.521	1459780	20.0
Dibenzo[def,mno...	17.004	2.6	ng	188060	6	15.521	1459780	20.0