LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050703.D
Acq On : 23 Oct 2021 00:26
Operator : CG/JU
Sample : M4311-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OR-2-102121

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_G\Methods\8270-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050703.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.798	386	393	408	rBV	240820	453788	40.85%	3.853%
2	7.396	657	665	675	rBV	265958	489248	44.04%	4.154%
3	8.254	804	811	823	rVB	202772	365246	32.88%	3.101%
4	9.423	1003	1010	1024	rVB	167462	326593	29.40%	2.773%
5	10.821	1242	1248	1258	rBV	21272	45876	4.13%	0.389%
6	11.080	1285	1292	1297	rVV	280366	518921	46.71%	4.406%
7	11.127	1297	1300	1307	rVB	39977	68960	6.21%	0.585%
8	12.449	1520	1525	1534	rVB3	10289	16246	1.46%	0.138%
9	12.719	1564	1571	1576	rVB	37000	61936	5.57%	0.526%
10	12.930	1597	1607	1614	rBV	32317	57790	5.20%	0.491%
11	13.389	1679	1685	1692	rVB7	8500	17414	1.57%	0.148%
12	13.495	1694	1703	1709	rBV	406922	640790	57.68%	5.440%
13	13.671	1726	1733	1737	rBV6	13285	25731	2.32%	0.218%
14	14.053	1787	1798	1804	rBV5	18347	51228	4.61%	0.435%
15	14.194	1815	1822	1827	rBV2	30171	59234	5.33%	0.503%
16	14.247	1827	1831	1835	rVB2	17255	26974	2.43%	0.229%
17	14.323	1841	1844	1848	rVB3	13022	15467	1.39%	0.131%
18	14.429	1857	1862	1866	rBV2	15985	27236	2.45%	0.231%
19	14.599	1885	1891	1900	rBV2	39997	87479	7.87%	0.743%
20	14.734	1911	1914	1918	rVB4	11370	13607	1.22%	0.116%
21	14.869	1928	1937	1943	rBV	387853	643193	57.89%	5.461%
22	14.934	1943	1948	1954	rVB	47001	75939	6.84%	0.645%
23	15.075	1966	1972	1979	rBV9	11742	26906	2.42%	0.228%
24	15.263	1997	2004	2012	rVB3	38650	76114	6.85%	0.646%
25	15.339	2012	2017	2021	rBV4	16357	31211	2.81%	0.265%
26	15.480	2033	2041	2045	rBV6	17582	39501	3.56%	0.335%
27	15.527	2045	2049	2053	rVB5	10284	16310	1.47%	0.138%
28	15.651	2063	2070	2073	rBV6	12902	31888	2.87%	0.271%
29	15.680	2073	2075	2080	rVB4	17947	24094	2.17%	0.205%
30	15.739	2080	2085	2088	rBV5	11208	19189	1.73%	0.163%
31	15.821	2096	2099	2104	rVB7	8861	12116	1.09%	0.103%
32	15.915	2109	2115	2124	rVB	74097	133926	12.05%	1.137%
33	16.074	2139	2142	2146	rVB6	13145	19454	1.75%	0.165%
34	16.203	2157	2164	2170	rVB6	11841	29929	2.69%	0.254%
35	16.356	2184	2190	2199	rBV	240545	407973	36.72%	3.464%
36	16.573	2218	2227	2237	rVB	18869	63138	5.68%	0.536%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050703.D
Acq On : 23 Oct 2021 00:26
Operator : CG/JU
Sample : M4311-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OR-2-102121

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_G\Methods\8270-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.714	2247	2251	2255	rBV6	8090	12311	1.11%	0.105%
38	16.920	2278	2286	2289	rBV4	20145	44791	4.03%	0.380%
39	17.067	2307	2311	2315	rVB6	15004	22895	2.06%	0.194%
40	17.337	2353	2357	2361	rBV4	19207	26468	2.38%	0.225%
41	17.437	2369	2374	2379	rVB2	35465	61398	5.53%	0.521%
42	17.619	2398	2405	2408	rBV	417386	678839	61.10%	5.763%
43	17.660	2408	2412	2418	rVB	394663	595561	53.61%	5.056%
44	17.748	2422	2427	2432	rVV	85001	127196	11.45%	1.080%
45	18.013	2468	2472	2479	rBV2	37552	73137	6.58%	0.621%
46	18.071	2480	2482	2487	rVB4	18195	24106	2.17%	0.205%
47	18.195	2500	2503	2509	rVB	29523	44372	3.99%	0.377%
48	18.489	2549	2553	2557	rBV	71944	112507	10.13%	0.955%
49	18.536	2557	2561	2567	rVB	101701	158868	14.30%	1.349%
50	18.618	2571	2575	2579	rBV	34741	51949	4.68%	0.441%
51	18.683	2580	2586	2590	rBV2	125127	257775	23.20%	2.188%
52	18.976	2632	2636	2640	rBV2	59746	80915	7.28%	0.687%
53	19.270	2683	2686	2690	rBV	28089	34443	3.10%	0.292%
54	19.388	2702	2706	2711	rBV2	91928	149640	13.47%	1.270%
55	19.658	2746	2752	2757	rBV	657651	938642	84.49%	7.969%
56	19.987	2805	2808	2809	rBV	54280	63363	5.70%	0.538%
57	20.022	2809	2814	2820	rVB	590111	905861	81.54%	7.691%
58	20.204	2840	2845	2849	rVB	509527	681779	61.37%	5.788%
59	20.604	2910	2913	2917	rVB2	82443	100689	9.06%	0.855%
60	21.914	3129	3136	3142	rBV2	411061	1110984	100.00%	9.432%
61	21.967	3143	3145	3157	rVB	247716	399585	35.97%	3.392%

Sum of corrected areas: 11778719

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
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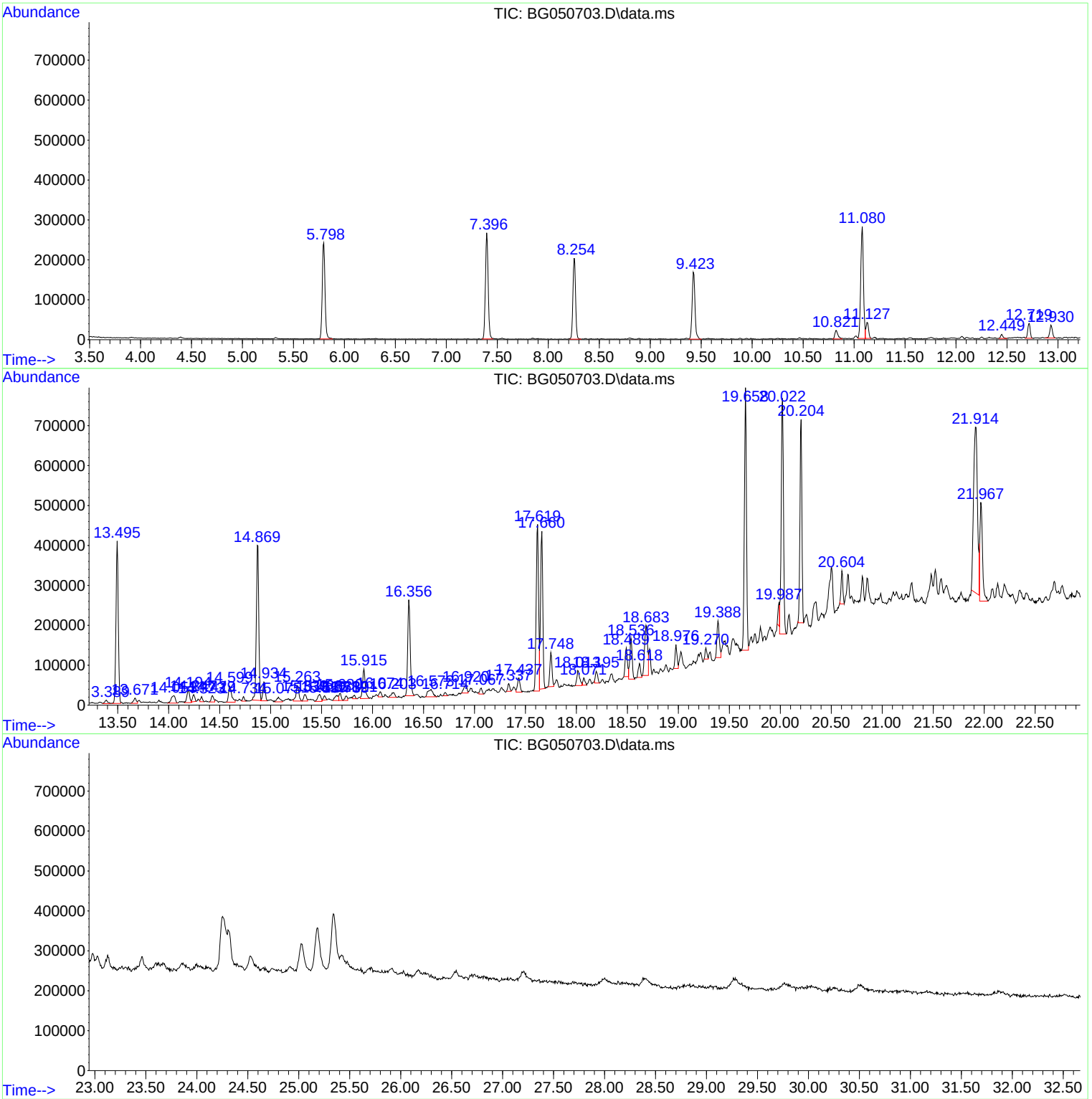
Acq On : 23 Oct 2021 00:26
Operator : CG/JU
Sample : M4311-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-2-102121

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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_G\Data\BG102221\
Data File : BG050703.D
Acq On : 23 Oct 2021 00:26
Operator : CG/JU
Sample : M4311-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OR-2-102121

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

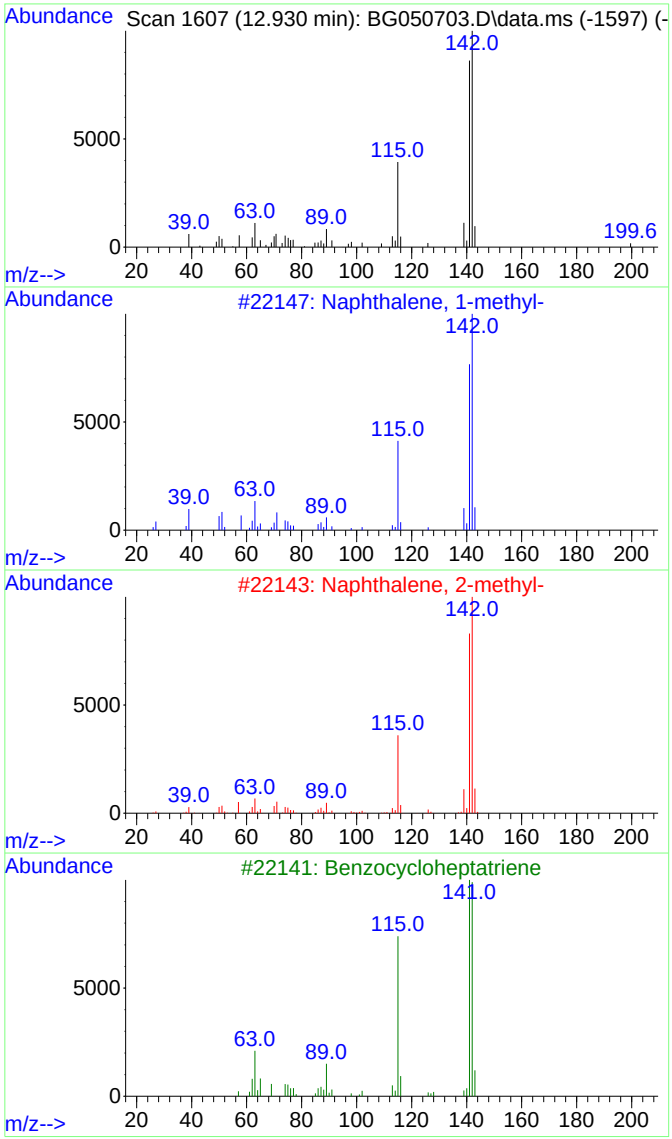
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

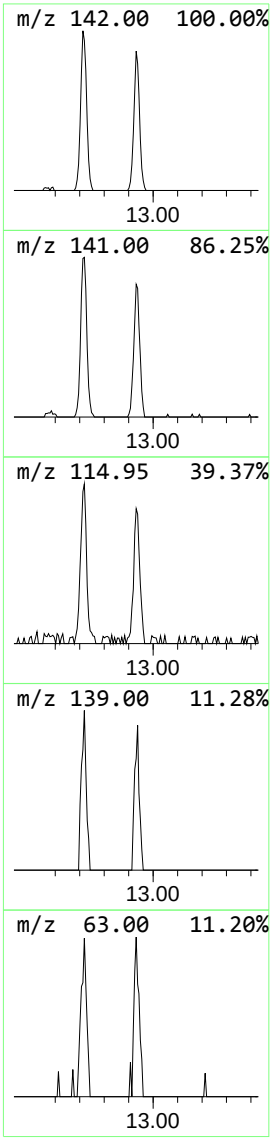
****

Peak Number 1 Benzocycloheptatriene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.931	2.23 ng	57790	Naphthalene-d8	11.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	97
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94
3	Benzocycloheptatriene	142	C11H10	000264-09-5	94
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050703.D
Acq On : 23 Oct 2021 00:26
Operator : CG/JU
Sample : M4311-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OR-2-102121

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

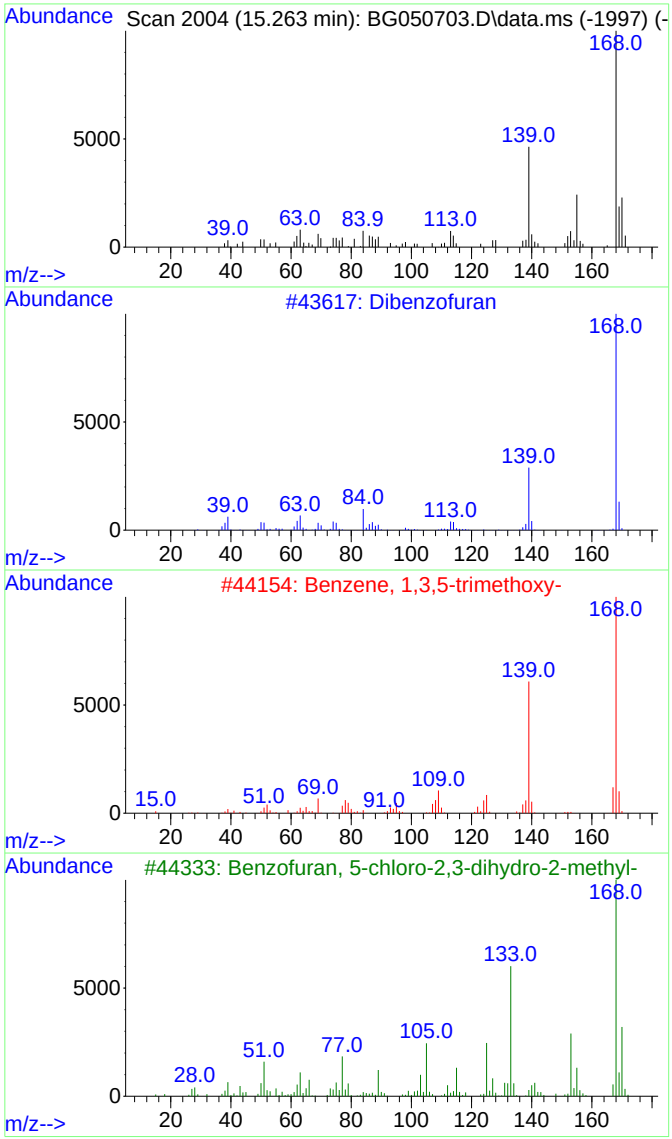
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

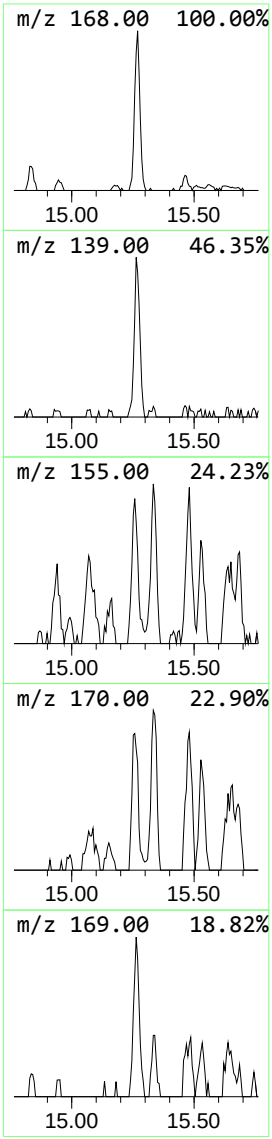
****

Peak Number 3 Benzene, 1,3,5-trimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.263	2.37 ng	76114	Acenaphthene-d10	14.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzofuran	168	C12H8O	000132-64-9	60
2	Benzene, 1,3,5-trimethoxy-	168	C9H12O3	000621-23-8	52
3	Benzofuran, 5-chloro-2,3-dihydro...	168	C9H9ClO	054410-96-7	38
4	5-Chloro-1,3-dihydro-2H-benzimid...	168	C7H5ClN2O	002034-23-3	37
5	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050703.D
Acq On : 23 Oct 2021 00:26
Operator : CG/JU
Sample : M4311-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-2-102121

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

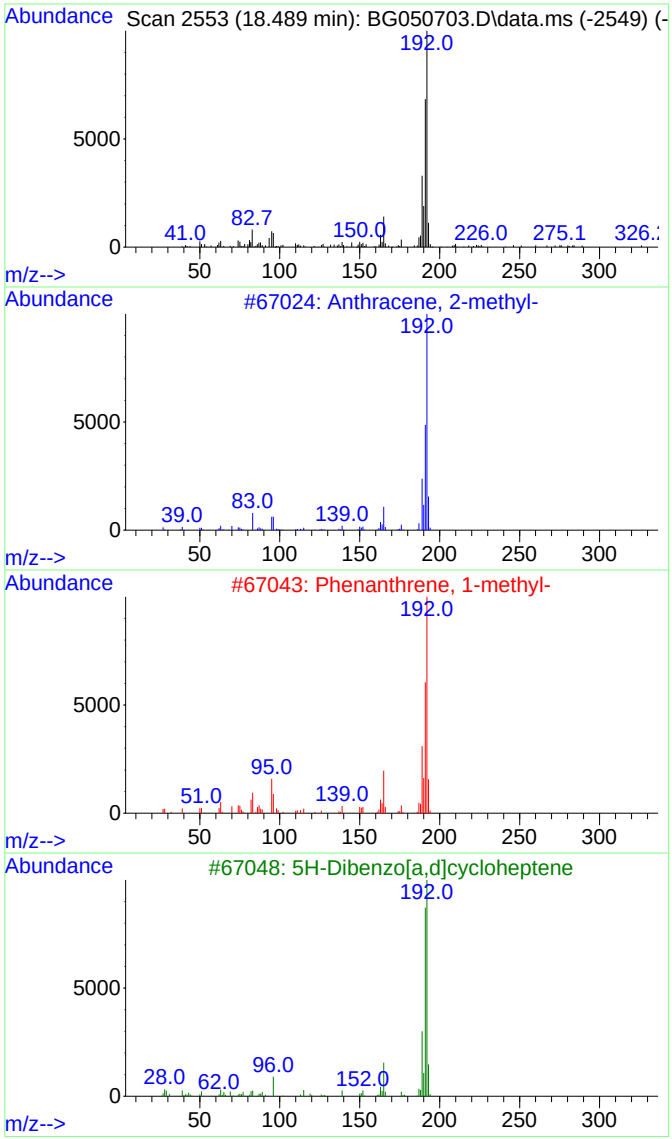
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

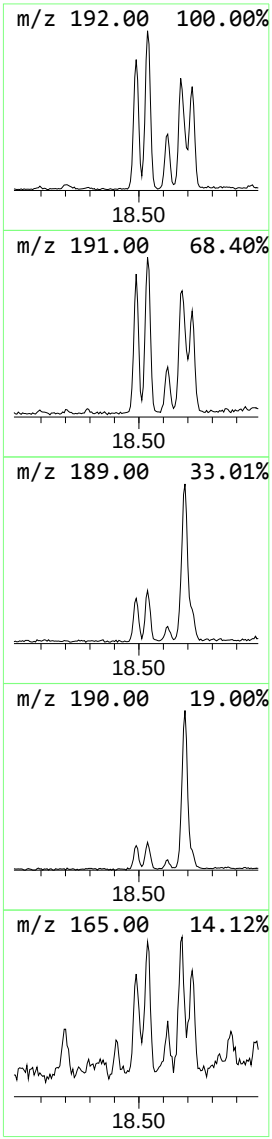
****

Peak Number 5 Anthracene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.489	3.31 ng	112507	Phenanthrene-d10	17.619

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	93
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	81
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050703.D
Acq On : 23 Oct 2021 00:26
Operator : CG/JU
Sample : M4311-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-2-102121

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

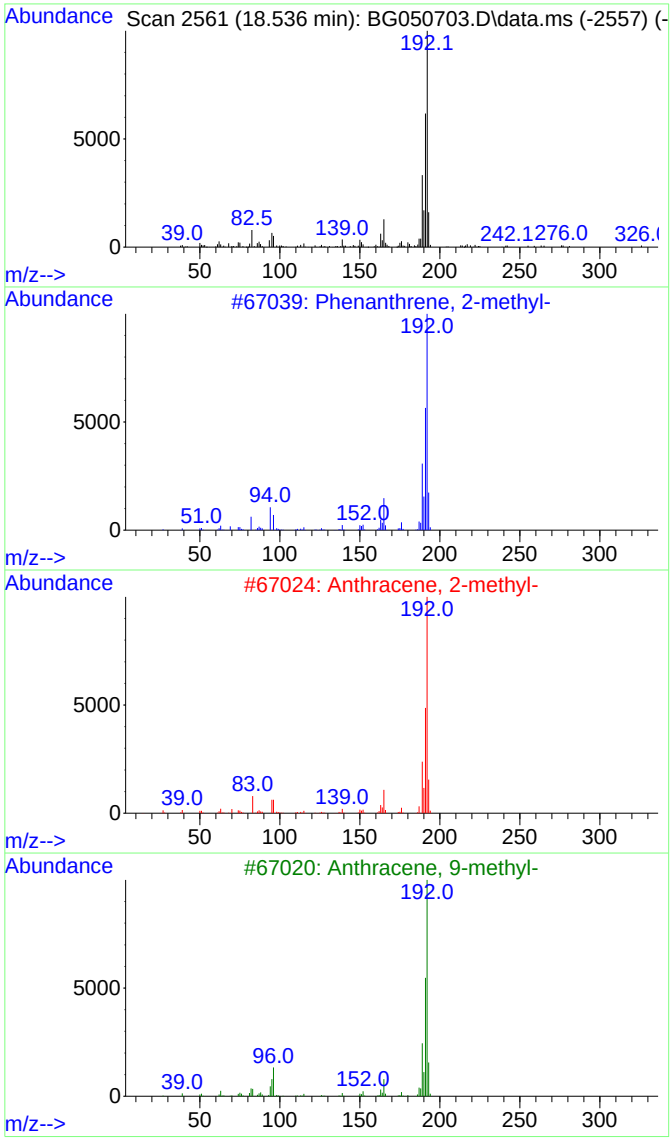
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

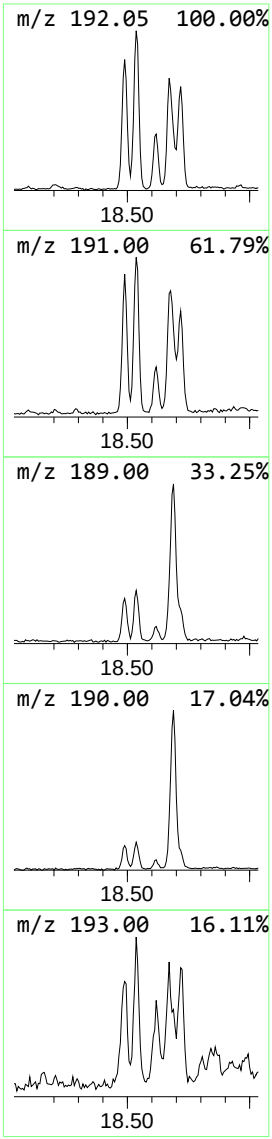
****

Peak Number 6 Phenanthrene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.536	4.68 ng	158868	Phenanthrene-d10	17.619

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050703.D
Acq On : 23 Oct 2021 00:26
Operator : CG/JU
Sample : M4311-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-2-102121

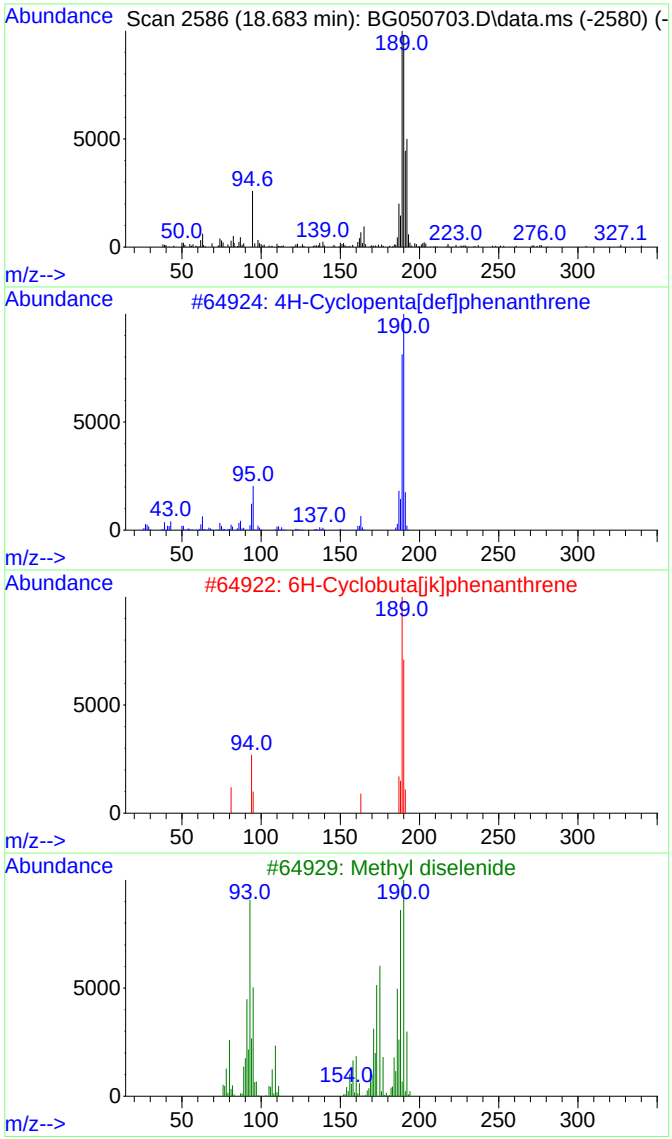
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

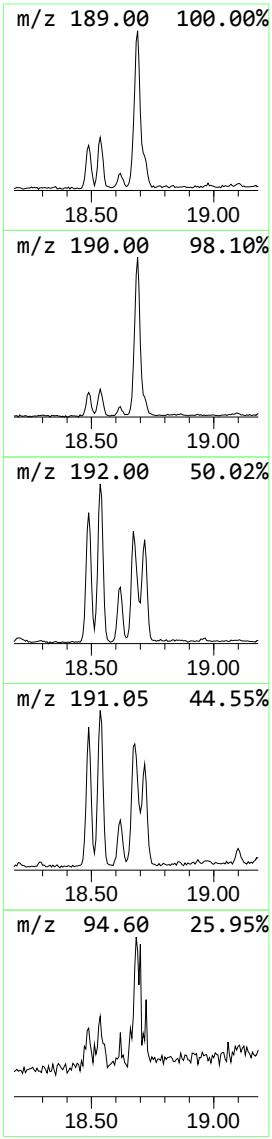
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.683	7.59 ng	257775	Phenanthrene-d10	17.619

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	Methyl diselenide	190	C2H6Se2	007101-31-7	45
4	4,6-Dichloro-2-ethylpyrimidin-5-...	191	C6H7Cl2N3	006237-96-3	43
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050703.D
Acq On : 23 Oct 2021 00:26
Operator : CG/JU
Sample : M4311-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-2-102121

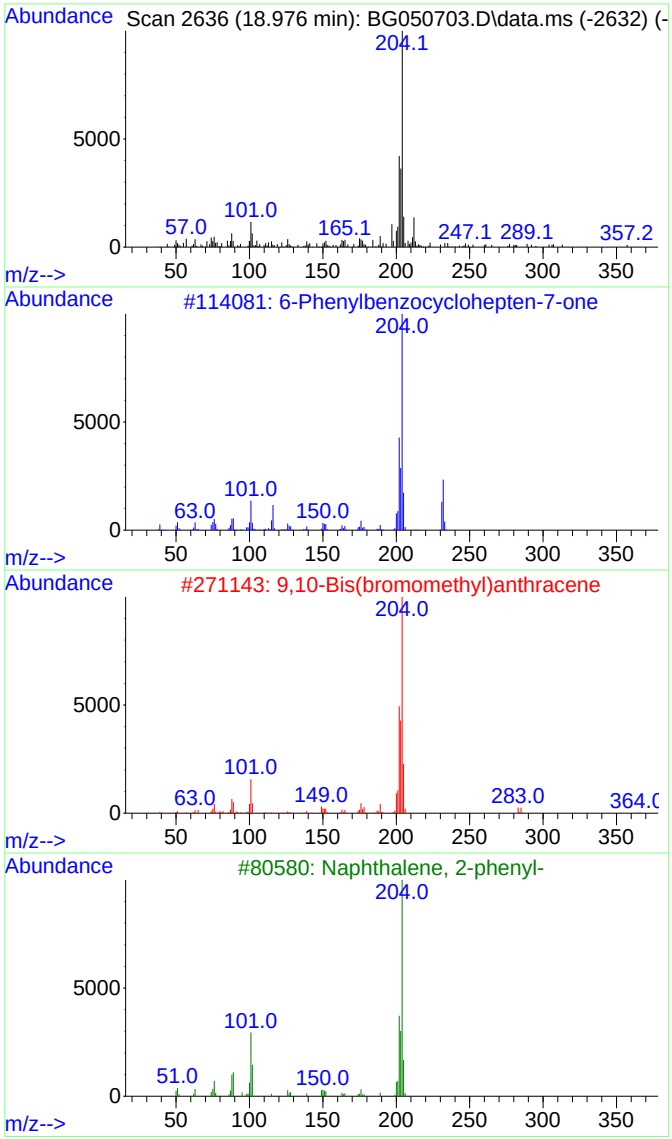
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

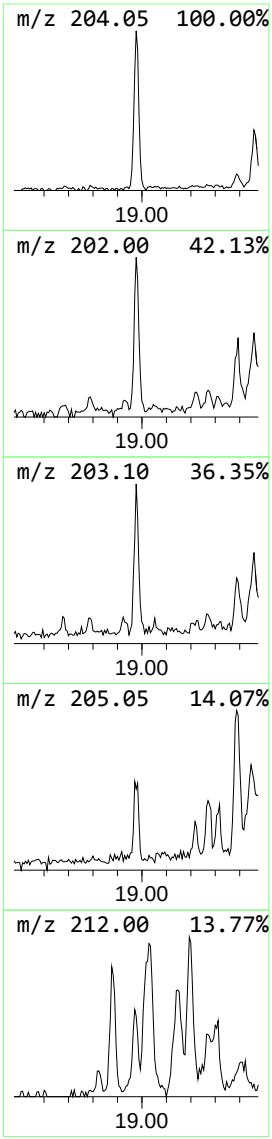
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 6-Phenylbenzocyclohepten-7-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.976	2.38 ng	80915	Phenanthrene-d10	17.619

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Phenylbenzocyclohepten-7-one	232	C17H12O	093327-56-1	72
2	9,10-Bis(bromomethyl)anthracene	362	C16H12Br2	034373-96-1	64
3	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	64
4	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	64
5	9,10-di(Chloromethyl)anthracene	274	C16H12Cl2	010387-13-0	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050703.D
Acq On : 23 Oct 2021 00:26
Operator : CG/JU
Sample : M4311-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-2-102121

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

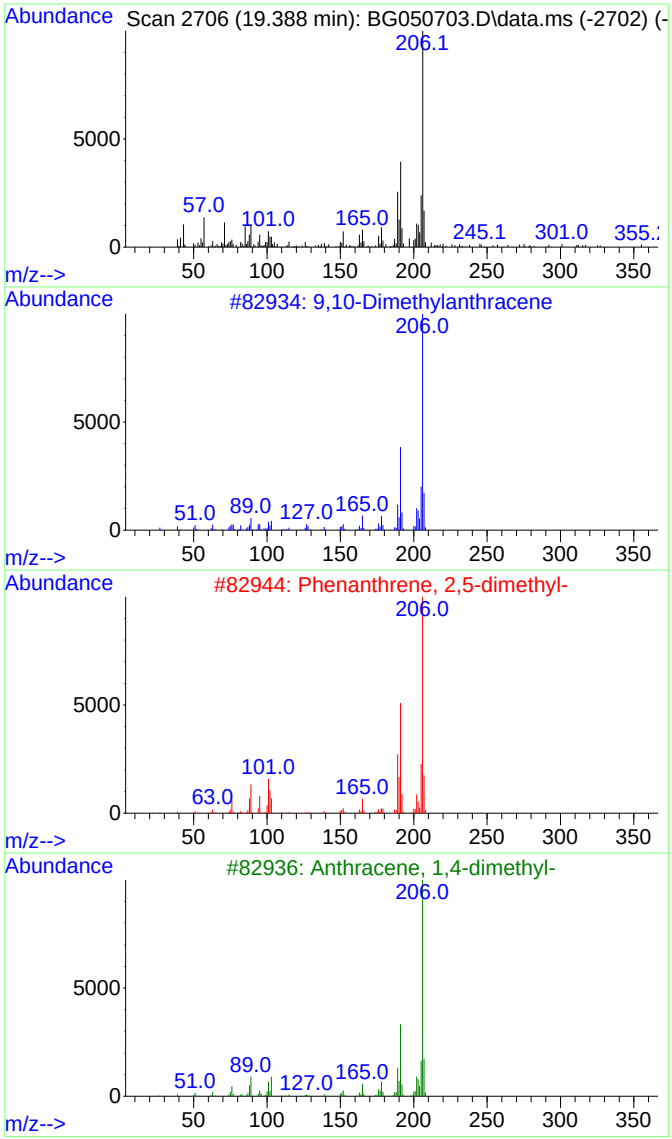
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

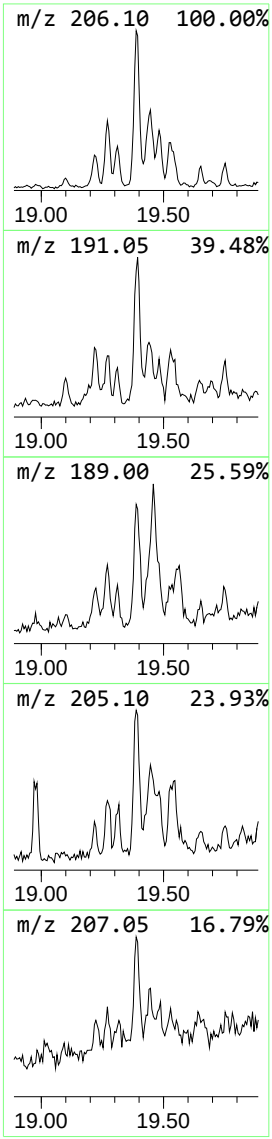
****

Peak Number 9 9,10-Dimethylanthracene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.388	4.41 ng	149640	Phenanthrene-d10	17.619

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylanthracene	206	C16H14	000781-43-1	98
2	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	95
3	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	93
4	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	93
5	di-p-Tolylacetylene	206	C16H14	002789-88-0	92





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050703.D
Acq On : 23 Oct 2021 00:26
Operator : CG/JU
Sample : M4311-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OR-2-102121

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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
Benzocyclohepta...	12.931	2.2	ng	57790	2	11.080	518921	20.0
Benzene, 1,3,5-...	15.263	2.4	ng	76114	3	14.875	643193	20.0
Anthracene, 2-m...	18.489	3.3	ng	112507	4	17.619	678839	20.0
Phenanthrene, 2...	18.536	4.7	ng	158868	4	17.619	678839	20.0
4H-Cyclopenta[d...	18.683	7.6	ng	257775	4	17.619	678839	20.0
6-Phenylbenzocy...	18.976	2.4	ng	80915	4	17.619	678839	20.0
9,10-Dimethylan...	19.388	4.4	ng	149640	4	17.619	678839	20.0