

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022223\
 Data File : BG056705.D
 Acq On : 22 Feb 2023 20:02
 Operator : CG/JU
 Sample : 01636-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 OR-02-022123

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-BG021523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056705.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.464	321	328	339	rVB	99272	166955	22.55%	2.522%
2	5.946	403	410	423	rBV	234218	412344	55.69%	6.229%
3	7.562	677	685	697	rVB	254168	460148	62.15%	6.952%
4	8.437	827	834	841	rVB	82329	142471	19.24%	2.152%
5	9.607	1026	1033	1044	rBV	164768	294477	39.77%	4.449%
6	11.275	1310	1317	1322	rBV	110040	201292	27.19%	3.041%
7	11.322	1322	1325	1333	rVB3	11351	18624	2.52%	0.281%
8	12.627	1542	1547	1554	rVB2	4408	8027	1.08%	0.121%
9	12.897	1587	1593	1597	rBV2	7015	11166	1.51%	0.169%
10	13.114	1624	1630	1635	rBV3	5478	8900	1.20%	0.134%
11	13.555	1699	1705	1709	rBV2	5847	7786	1.05%	0.118%
12	13.666	1717	1724	1731	rVB	413655	631769	85.33%	9.544%
13	13.837	1748	1753	1757	rBV3	12341	20071	2.71%	0.303%
14	14.219	1811	1818	1824	rBV4	4232	9738	1.32%	0.147%
15	14.360	1837	1842	1846	rBV4	6489	10459	1.41%	0.158%
16	14.413	1846	1851	1856	rBV8	5742	8072	1.09%	0.122%
17	14.595	1878	1882	1887	rVB7	5258	8918	1.20%	0.135%
18	14.771	1907	1912	1919	rBV6	5565	14399	1.94%	0.218%
19	14.894	1924	1933	1939	rVB2	14041	24846	3.36%	0.375%
20	15.035	1951	1957	1963	rVB	162608	264079	35.67%	3.989%
21	15.100	1963	1968	1973	rVB3	18812	28162	3.80%	0.425%
22	15.429	2019	2024	2030	rVB3	17775	30263	4.09%	0.457%
23	15.641	2055	2060	2064	rBV6	5750	11629	1.57%	0.176%
24	15.835	2087	2093	2098	rVB2	15499	25605	3.46%	0.387%
25	16.075	2128	2134	2139	rBV2	24795	41500	5.60%	0.627%
26	16.240	2158	2162	2166	rVB6	11090	16619	2.24%	0.251%
27	16.369	2179	2184	2192	rVB	73890	108182	14.61%	1.634%
28	16.516	2202	2209	2216	rBV	288403	458501	61.93%	6.927%
29	16.692	2235	2239	2241	rBV2	16914	20328	2.75%	0.307%
30	16.939	2275	2281	2283	rBV5	5312	9703	1.31%	0.147%
31	17.427	2359	2364	2368	rBV7	6322	9881	1.33%	0.149%
32	17.486	2370	2374	2380	rVV5	18333	25888	3.50%	0.391%
33	17.533	2380	2382	2387	rVV5	9622	12998	1.76%	0.196%
34	17.597	2387	2393	2399	rVB2	10198	18031	2.44%	0.272%
35	17.773	2417	2423	2427	rBV	189587	306618	41.41%	4.632%
36	17.815	2427	2430	2436	rVV	153971	223185	30.14%	3.372%

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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

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37	17.909	2440	2446	2451	rVV	40820	64289	8.68%	0.971%
38	18.167	2484	2490	2495	rBV2	15131	28841	3.90%	0.436%
39	18.226	2496	2500	2506	rVB	17149	23944	3.23%	0.362%
40	18.396	2526	2529	2533	rVB5	8229	8776	1.19%	0.133%
41	18.608	2561	2565	2568	rBV3	44832	69015	9.32%	1.043%
42	18.684	2575	2578	2583	rVB	29812	45140	6.10%	0.682%
43	18.766	2586	2592	2598	rBV3	15846	30948	4.18%	0.468%
44	18.837	2598	2604	2608	rBV2	38947	87370	11.80%	1.320%
45	18.902	2612	2615	2618	rVB3	16205	17274	2.33%	0.261%
46	19.031	2633	2637	2639	rBV5	14804	15755	2.13%	0.238%
47	19.125	2649	2653	2657	rBV	18163	28769	3.89%	0.435%
48	19.160	2657	2659	2666	rVB8	11420	23171	3.13%	0.350%
49	19.518	2716	2720	2727	rBV7	38569	93894	12.68%	1.418%
50	19.800	2763	2768	2773	rVB	293692	406792	54.94%	6.145%
51	20.124	2819	2823	2825	rBV2	41386	66192	8.94%	1.000%
52	20.159	2825	2829	2836	rVB	243386	365647	49.38%	5.524%
53	20.335	2854	2859	2864	rBV	570119	740411	100.00%	11.186%
54	22.086	3150	3157	3163	rBV2	163935	431511	58.28%	6.519%

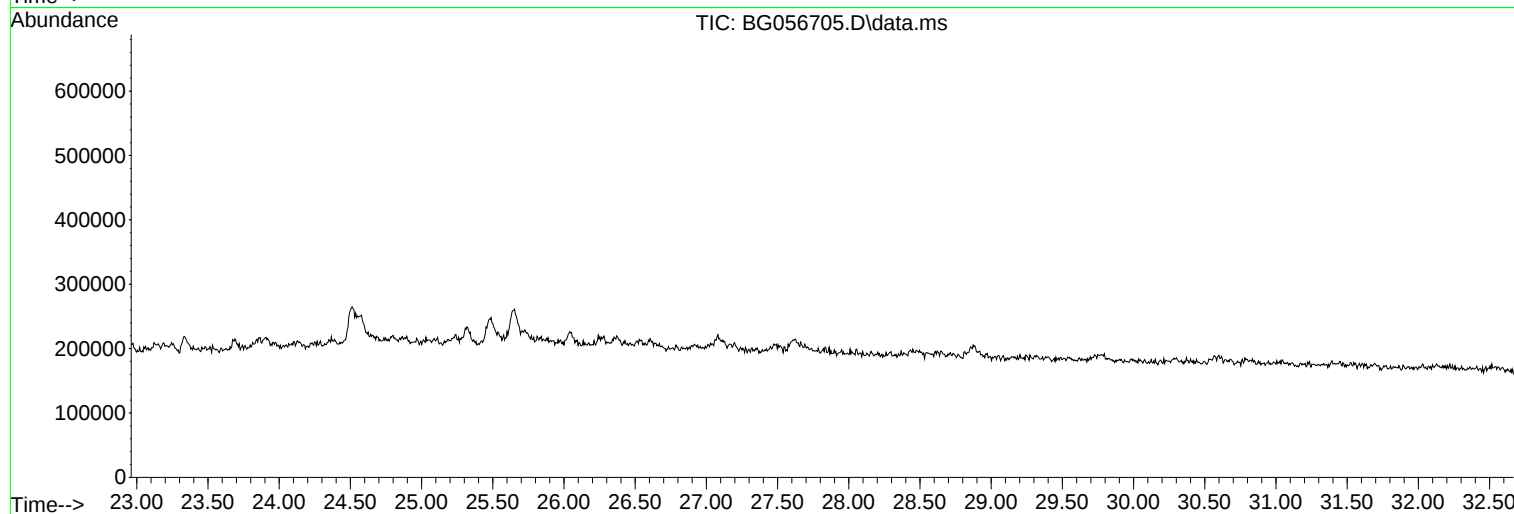
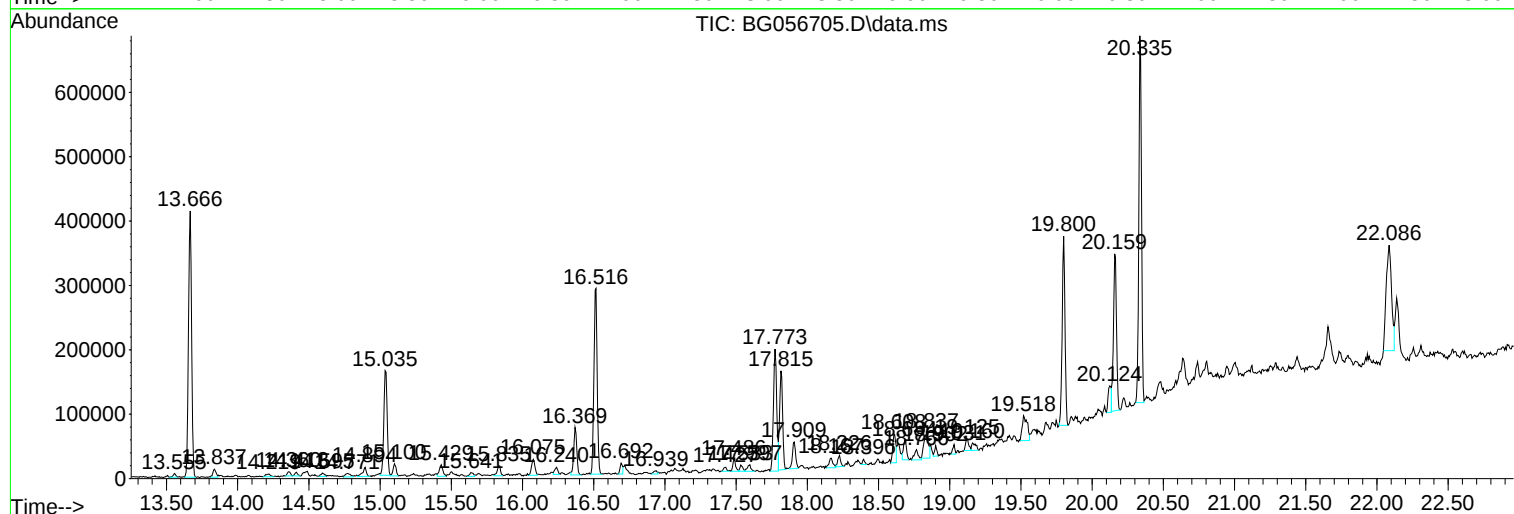
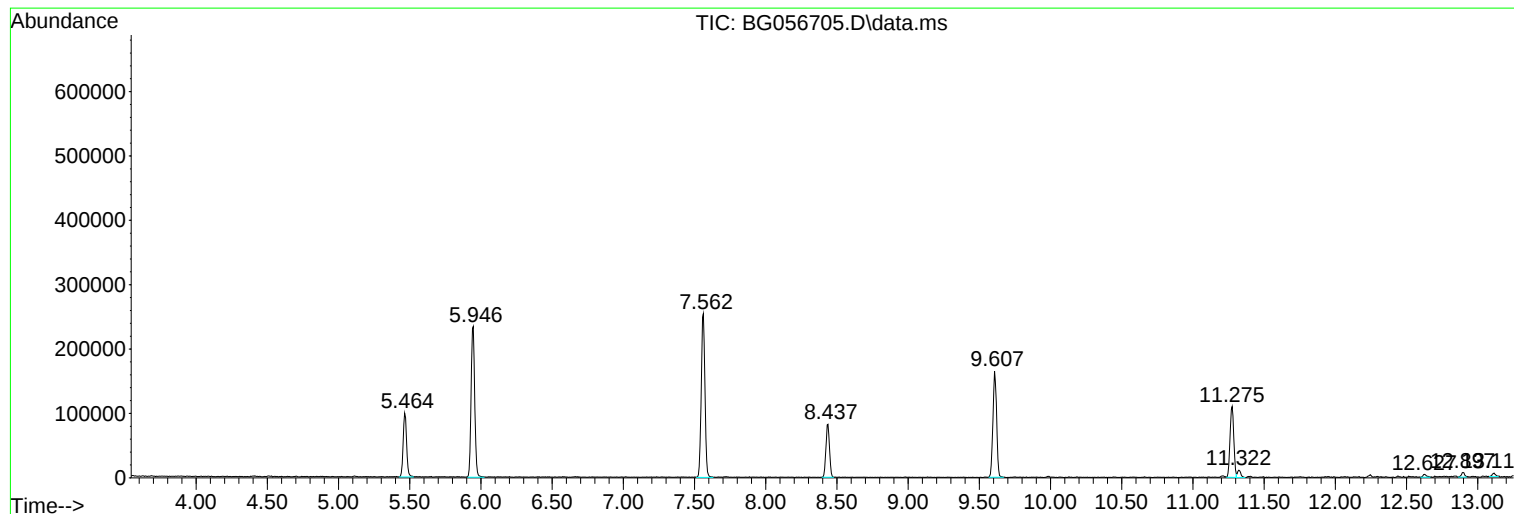
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG056705.D
Acq On : 22 Feb 2023 20:02
Operator : CG/JU
Sample : 01636-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

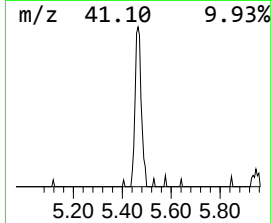
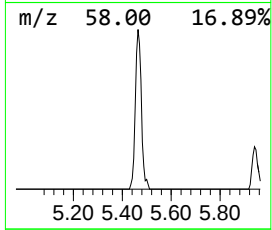
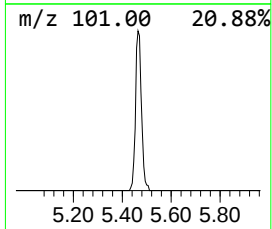
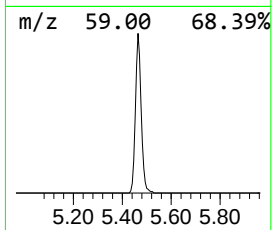
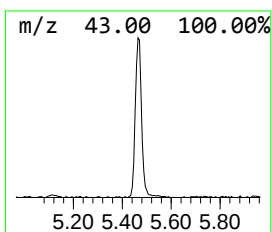
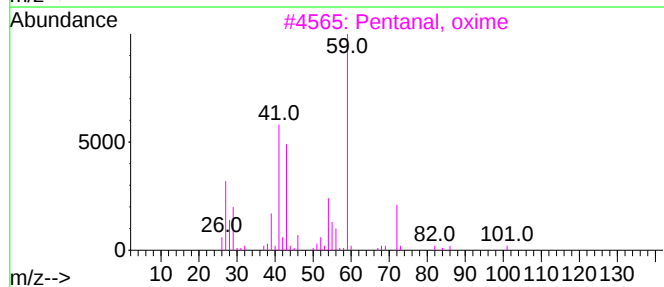
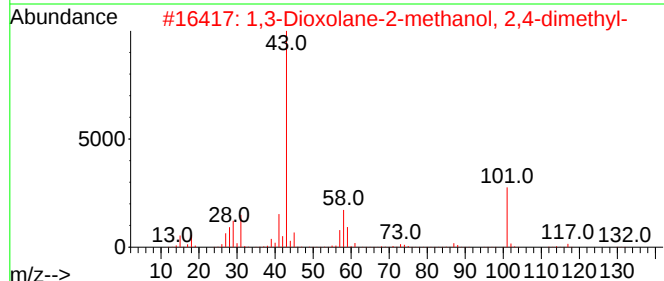
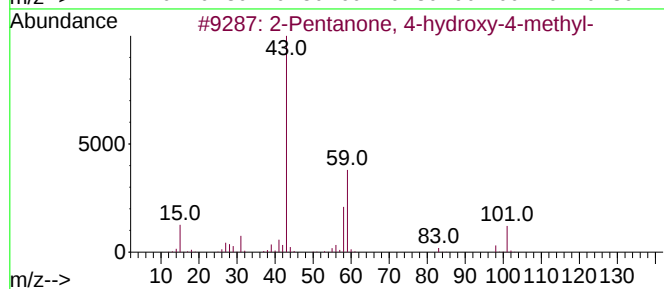
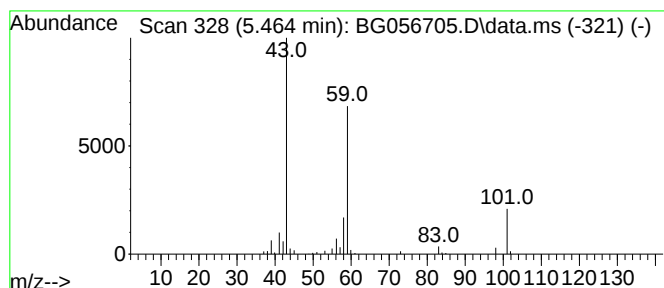
Instrument :
BNA_G
ClientSampleId :
OR-02-022123

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.464	23.44 ng	166955	1,4-Dichlorobenzene-d4	8.437	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
3	Pentanal, oxime	101	C5H11NO	000628-79-5	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
5	Guanidine	59	CH5N3	000113-00-8	9



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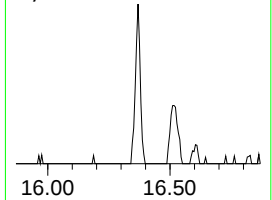
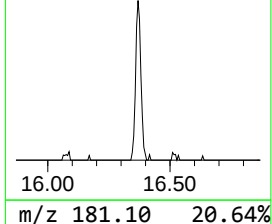
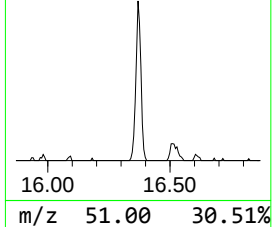
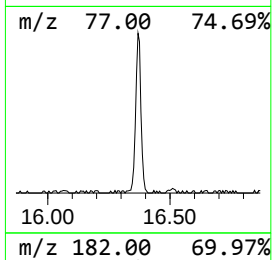
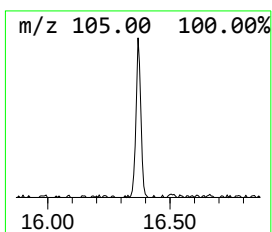
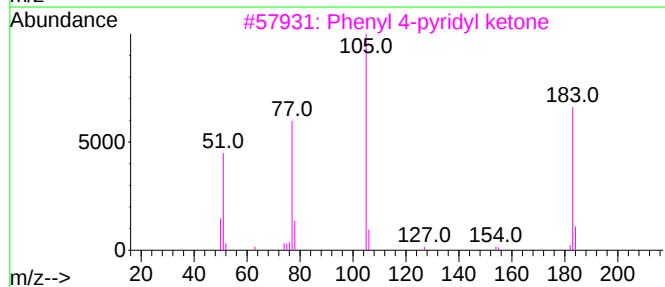
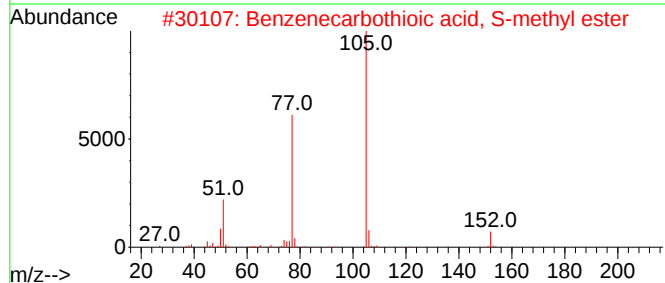
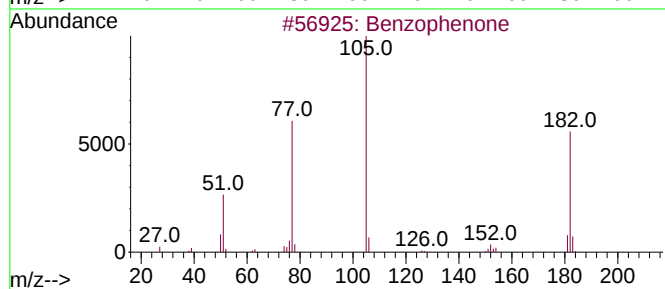
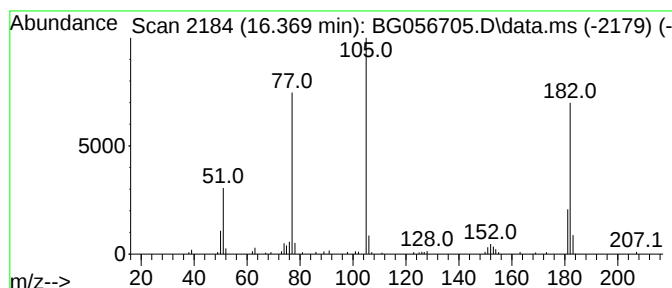
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.369	8.19 ng	108182	Acenaphthene-d10	15.036

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	64
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
4			Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	49
5			Benzoylformic acid	150	C8H6O3	000611-73-4	49



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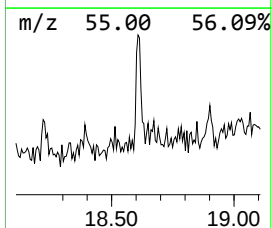
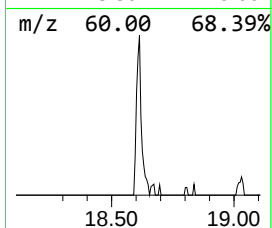
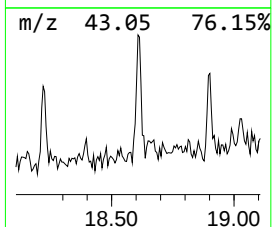
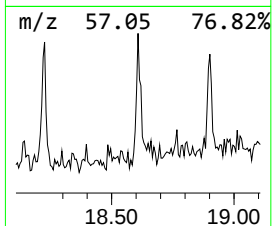
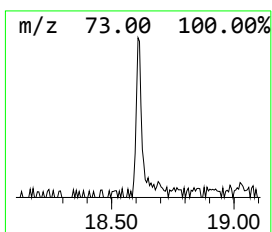
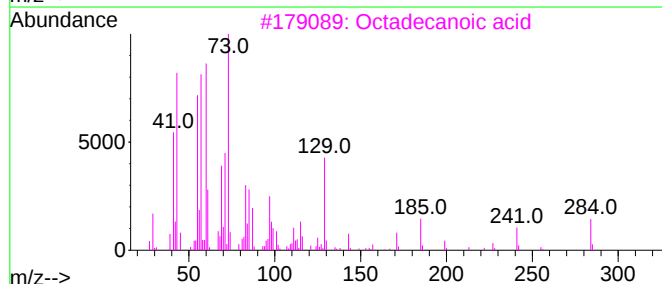
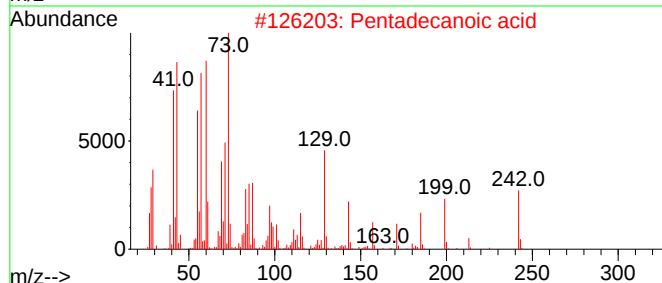
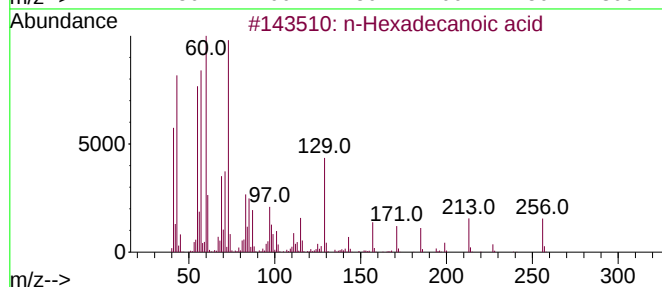
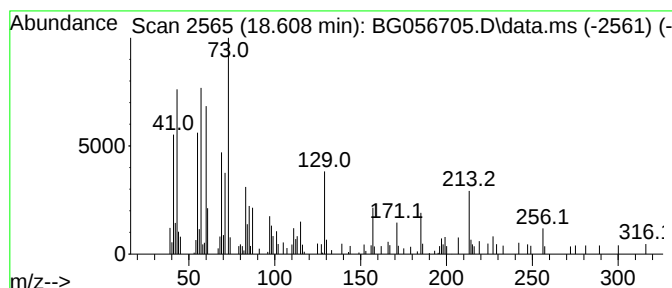
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.608	4.50 ng	69015	Phenanthrene-d10	17.773

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3			Octadecanoic acid	284	C18H36O2	000057-11-4	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



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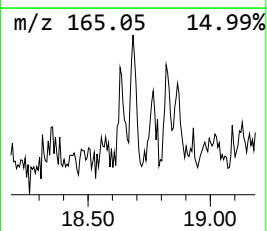
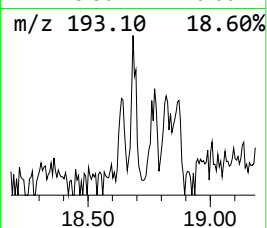
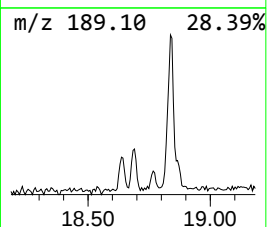
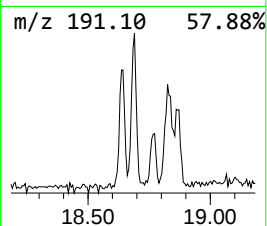
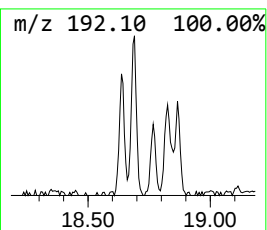
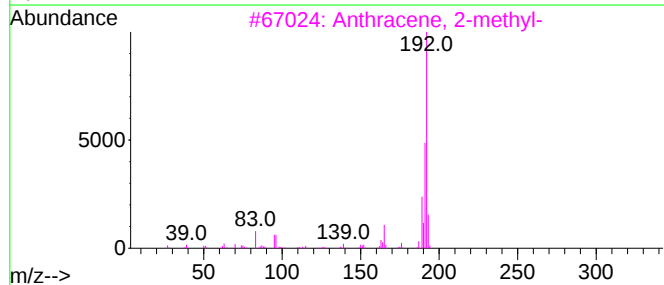
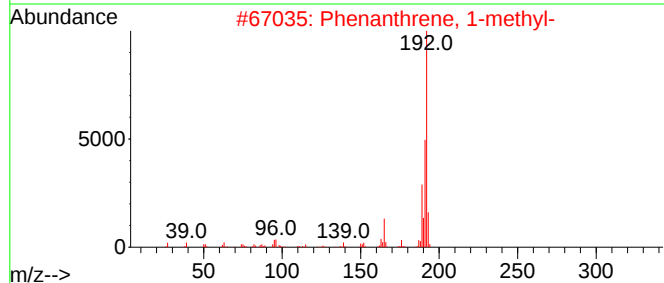
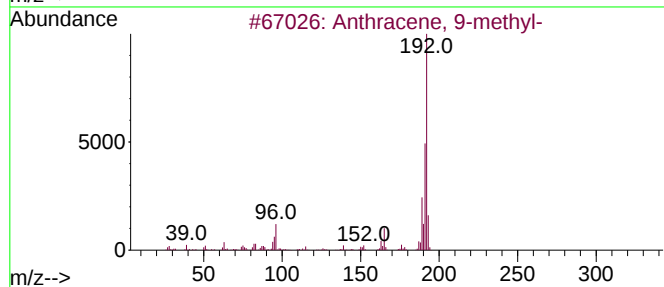
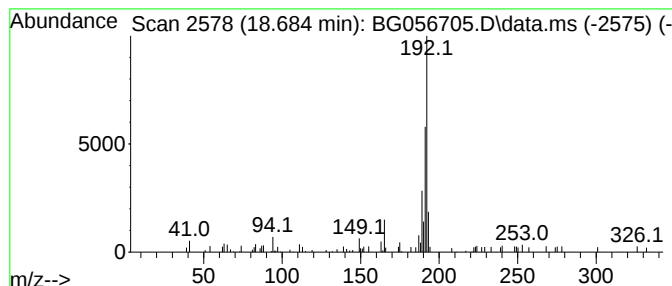
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Anthracene, 9-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.684	2.94 ng	45140	Phenanthrene-d10	17.773

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 9-methyl-	192	C15H12	000779-02-2	94
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
4			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	93
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93



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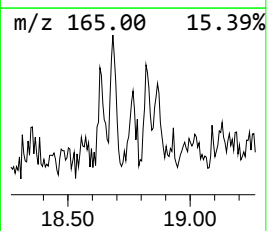
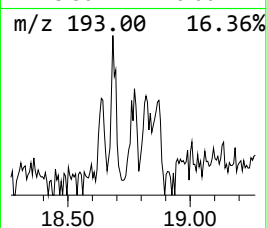
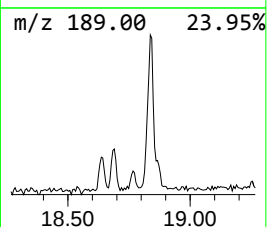
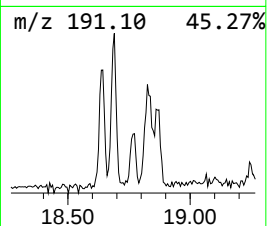
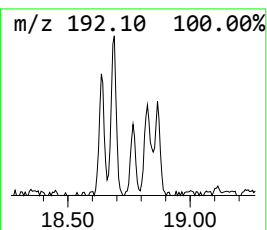
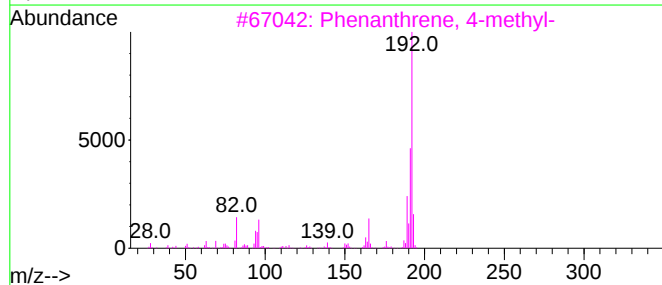
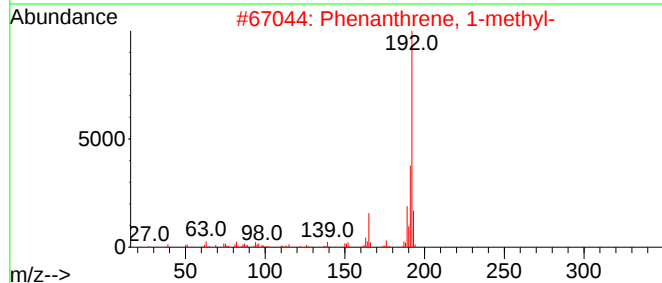
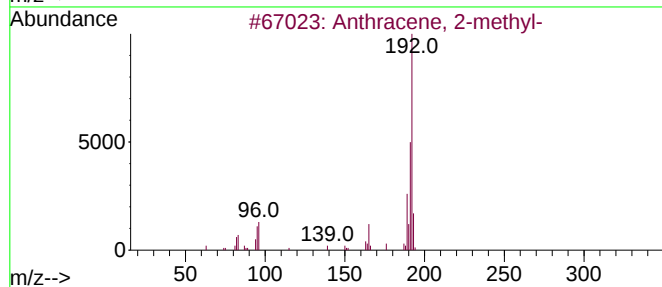
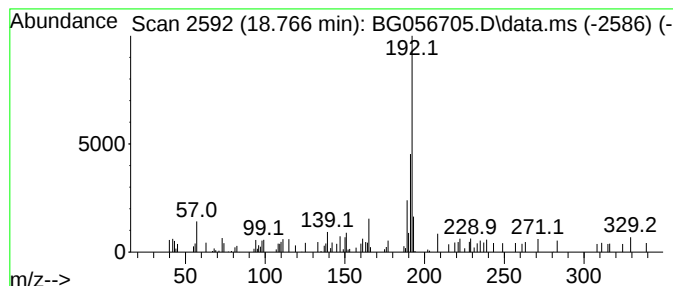
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Anthracene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.766	2.02 ng	30948	Phenanthrene-d10	17.773

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 2-methyl-	192	C15H12	000613-12-7	83
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	64
3			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	64
4			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	64
5			Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022223\
Data File : BG056705.D
Acq On : 22 Feb 2023 20:02
Operator : CG/JU
Sample : 01636-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

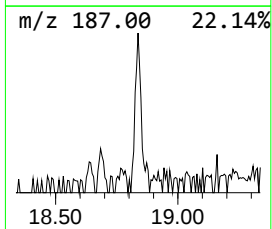
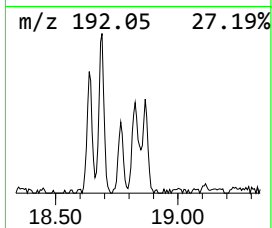
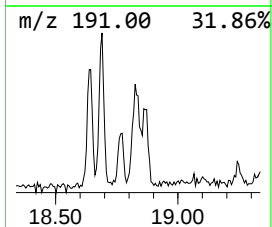
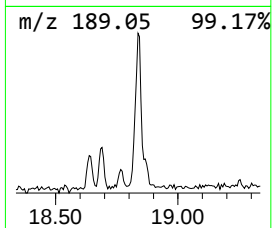
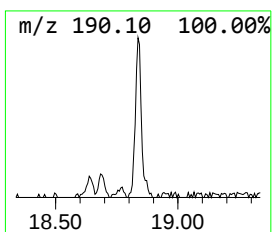
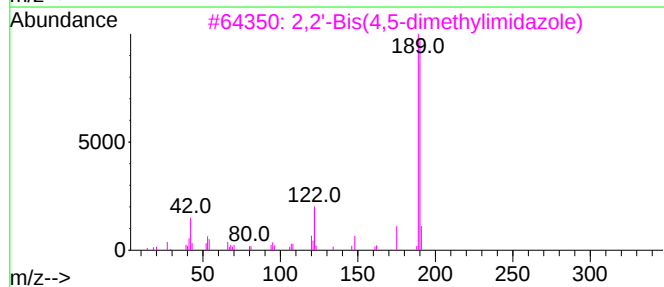
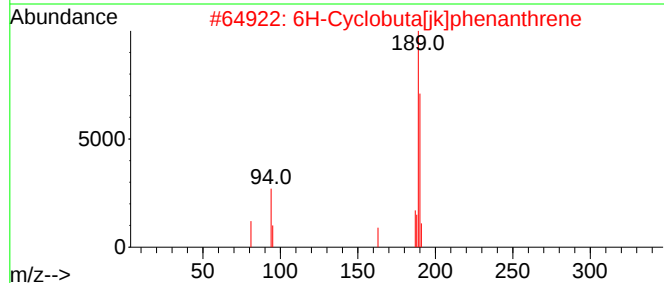
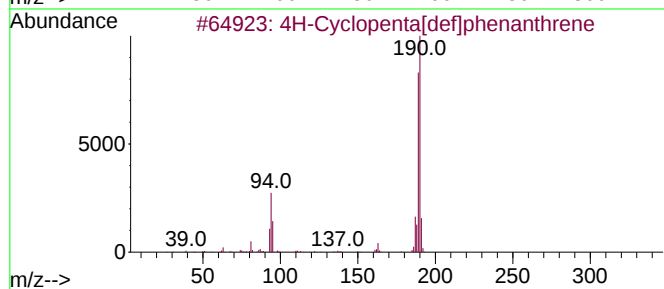
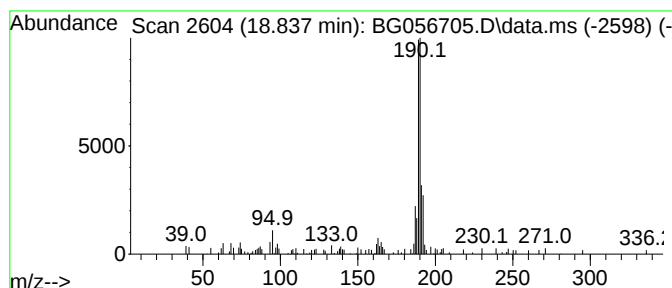
Instrument :
BNA_G
ClientSampleId :
OR-02-022123

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.837	5.70 ng	87370	Phenanthrene-d10	17.773	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	72
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	36
4	4-Oxo-2-(4-fluorophenyl)-3,4-dih...	190	C10H7FN2O	076128-79-5	27
5	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022223\
Data File : BG056705.D
Acq On : 22 Feb 2023 20:02
Operator : CG/JU
Sample : 01636-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-02-022123

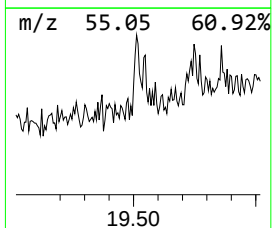
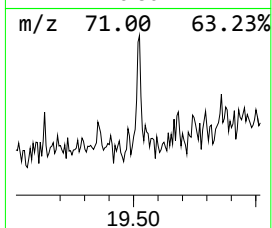
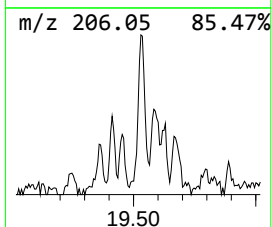
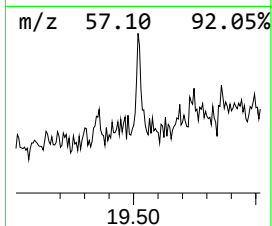
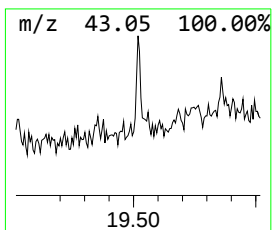
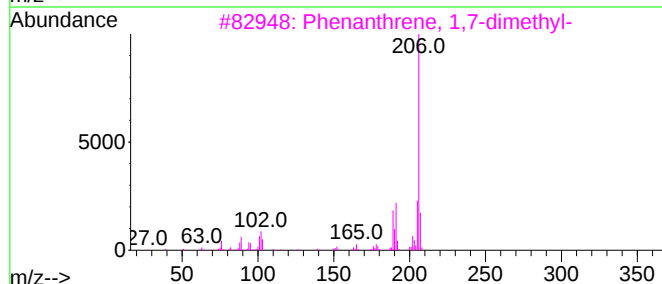
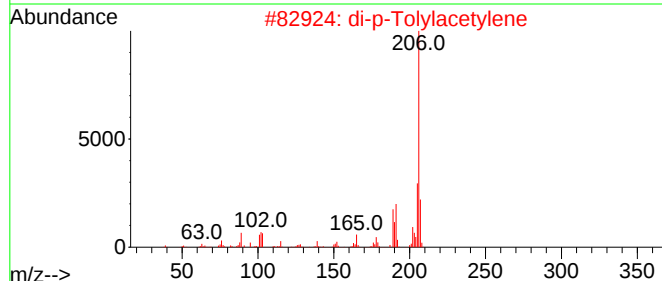
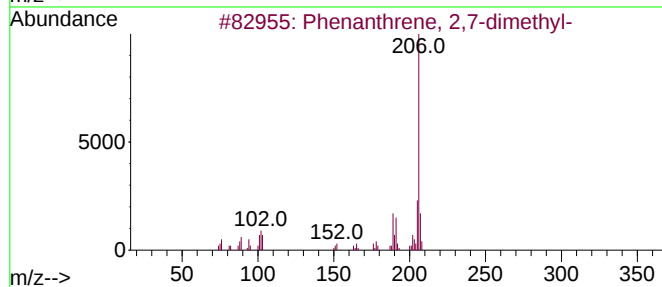
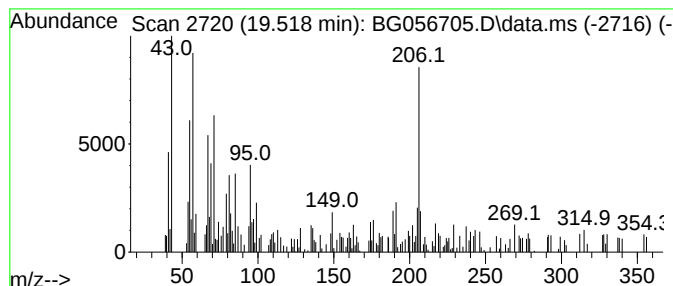
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phenanthrene, 2,7-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.518	6.12 ng	93894	Phenanthrene-d10	17.773

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	87
2			di-p-Tolylacetylene	206	C16H14	002789-88-0	86
3			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	78
4			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	60
5			Naphthalene, 1,2-dihydro-1-phenyl-	206	C16H14	016606-46-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022223\
Data File : BG056705.D
Acq On : 22 Feb 2023 20:02
Operator : CG/JU
Sample : 01636-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-02-022123

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.464	23.4	ng	166955	1	8.437	142471	20.0
Benzophenone	16.369	8.2	ng	108182	3	15.036	264079	20.0
n-Hexadecanoic ...	18.608	4.5	ng	69015	4	17.773	306618	20.0
Anthracene, 9-m...	18.684	2.9	ng	45140	4	17.773	306618	20.0
Anthracene, 2-m...	18.766	2.0	ng	30948	4	17.773	306618	20.0
4H-Cyclopenta[d...	18.837	5.7	ng	87370	4	17.773	306618	20.0
Phenanthrene, 2...	19.518	6.1	ng	93894	4	17.773	306618	20.0