

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062123\
 Data File : VX036273.D
 Acq On : 21 Jun 2023 16:08
 Operator : JC/MD
 Sample : 03331-31
 Misc : 20.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TOTAL-VOC-SB18-27-GRAB-10

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:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
 Title : SW846 8260

Signal : TIC: VX036273.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.398	48	51	57	rVB	14405	14288	1.25%	0.181%
2	1.636	77	90	96	rBV	18809	40961	3.57%	0.520%
3	2.715	259	267	275	rBV	68109	122456	10.68%	1.554%
4	2.947	296	305	311	rBV	7198	15522	1.35%	0.197%
5	5.385	694	705	717	rBV2	120710	348775	30.41%	4.426%
6	5.544	720	731	751	rVB	218023	625426	54.53%	7.937%
7	5.952	787	798	818	rBV	175151	473523	41.29%	6.009%
8	6.598	896	904	914	rVB3	5639	14429	1.26%	0.183%
9	6.757	920	930	945	rBV	345809	819501	71.45%	10.400%
10	8.647	1233	1240	1248	rBV	744129	1146891	100.00%	14.555%
11	8.720	1248	1252	1255	rBV	8982	12064	1.05%	0.153%
12	8.903	1276	1282	1290	rBV3	32454	58324	5.09%	0.740%
13	10.055	1465	1471	1486	rVB	687615	937601	81.75%	11.899%
14	10.195	1489	1494	1503	rVB	15689	23569	2.06%	0.299%
15	10.299	1503	1511	1517	rBV	34793	50559	4.41%	0.642%
16	10.640	1562	1567	1578	rVB2	26755	44720	3.90%	0.568%
17	10.963	1612	1620	1624	rBV2	18038	28785	2.51%	0.365%
18	11.085	1634	1640	1650	rBV	498450	703921	61.38%	8.933%
19	11.305	1672	1676	1679	rBV	11603	14673	1.28%	0.186%
20	11.378	1684	1688	1694	rVV2	23401	43216	3.77%	0.548%
21	11.451	1694	1700	1703	rVV	33338	53004	4.62%	0.673%
22	11.476	1703	1704	1715	rVV3	17235	22361	1.95%	0.284%
23	11.616	1718	1727	1734	rVB	13611	22037	1.92%	0.280%
24	11.756	1745	1750	1760	rVB	51716	71439	6.23%	0.907%
25	12.024	1788	1794	1801	rBV	712935	902484	78.69%	11.453%
26	12.085	1801	1804	1813	rVB	17263	25437	2.22%	0.323%
27	12.317	1838	1842	1849	rVB3	10737	19536	1.70%	0.248%
28	12.421	1855	1859	1863	rVB	9784	11639	1.01%	0.148%
29	12.963	1945	1948	1955	rVB2	7764	11493	1.00%	0.146%
30	13.774	2076	2081	2088	rBV	526408	652059	56.85%	8.275%
31	14.634	2215	2222	2233	rBV	189995	242074	21.11%	3.072%
32	14.780	2239	2246	2254	rVB	137541	177267	15.46%	2.250%
33	15.207	2307	2316	2320	rBV	13674	19762	1.72%	0.251%
34	15.475	2355	2360	2368	rVB2	17572	30361	2.65%	0.385%
35	15.615	2376	2383	2386	rBV	21627	35201	3.07%	0.447%
36	15.646	2386	2388	2394	rVB2	9636	13395	1.17%	0.170%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062123\
Data File : VX036273.D
Acq On : 21 Jun 2023 16:08
Operator : JC/MD
Sample : 03331-31
Misc : 20.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOTAL-VOC-SB18-27-GRAB-10

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:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Title : SW846 8260

37	15.835	2411	2419	2427	rVB6	4087	12050	1.05%	0.153%
38	16.328	2492	2500	2509	rVB2	9992	19110	1.67%	0.243%

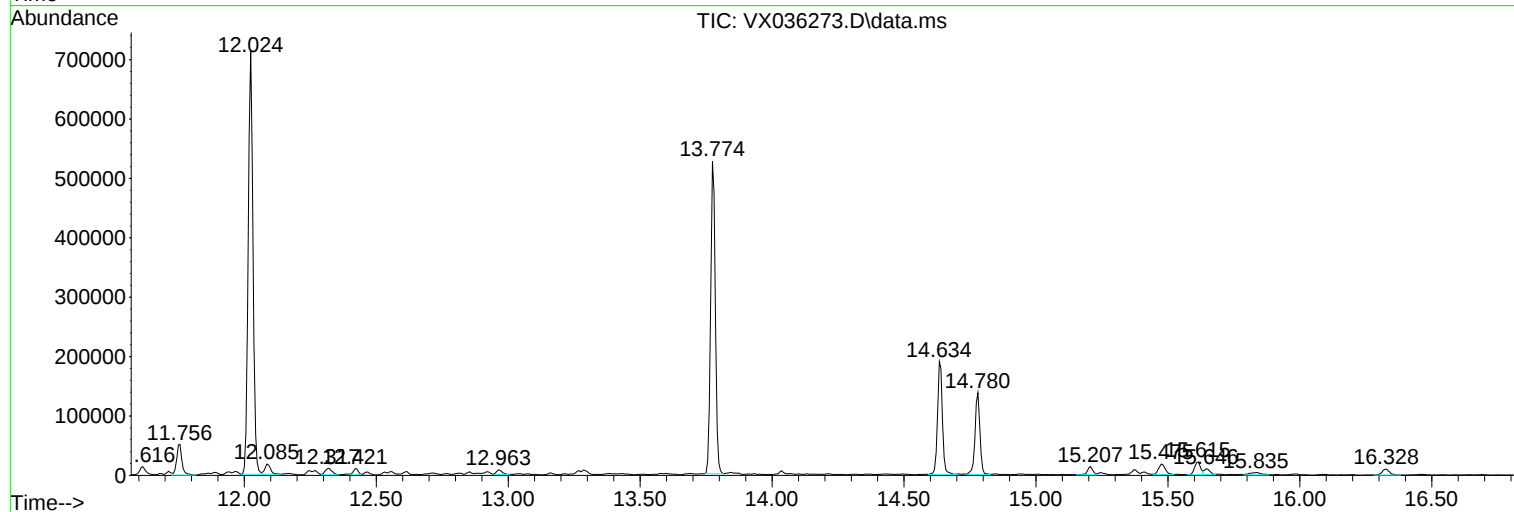
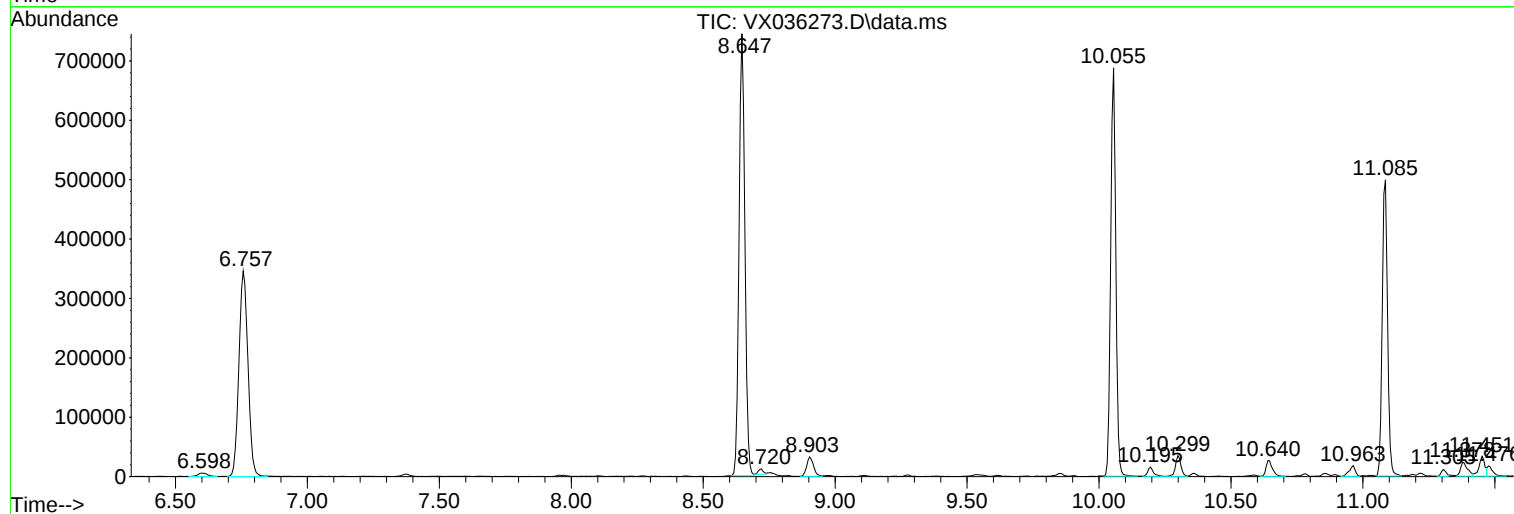
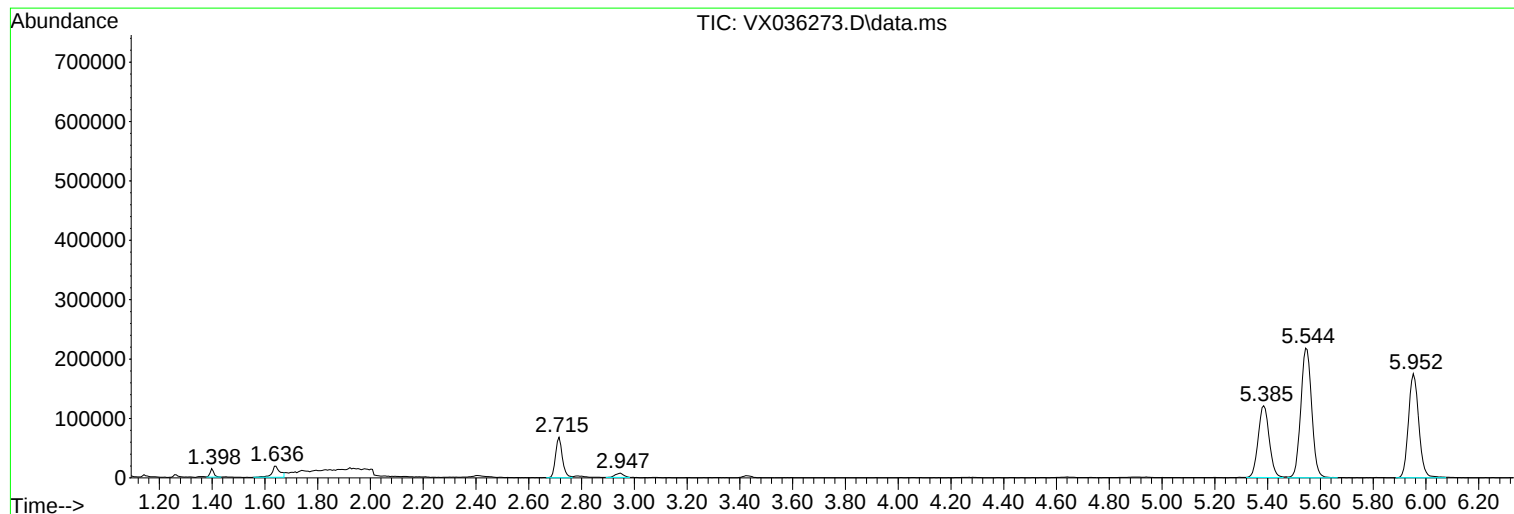
Sum of corrected areas: 7879913

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062123\
Data File : VX036273.D
Acq On : 21 Jun 2023 16:08
Operator : JC/MD
Sample : 03331-31
Misc : 20.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOTAL-VOC-SB18-27-GRAB-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062123\
Data File : VX036273.D
Acq On : 21 Jun 2023 16:08
Operator : JC/MD
Sample : 03331-31
Misc : 20.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOTAL-VOC-SB18-27-GRAB-10

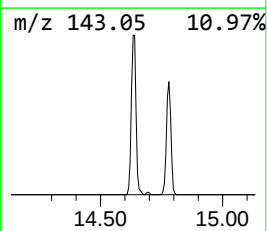
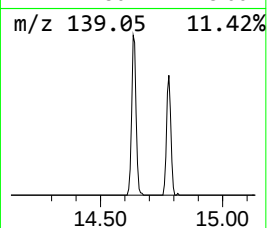
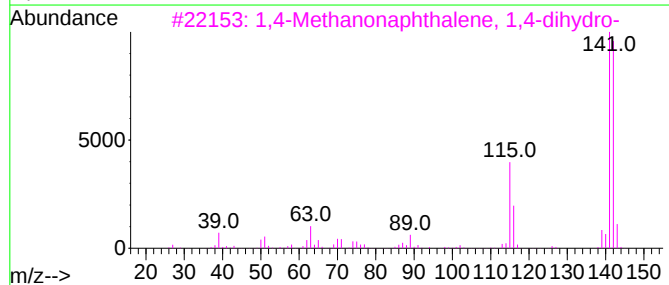
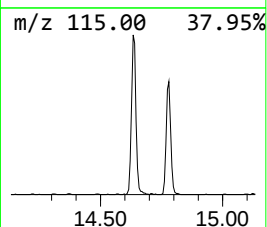
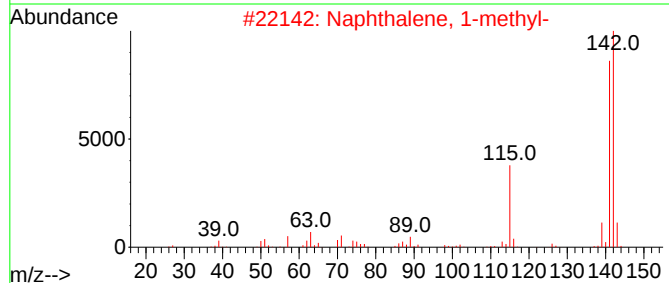
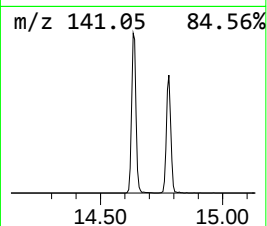
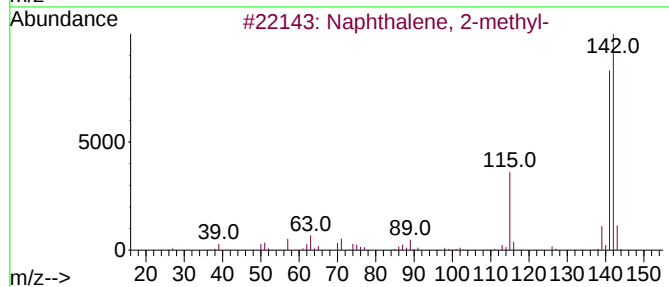
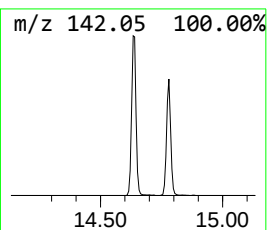
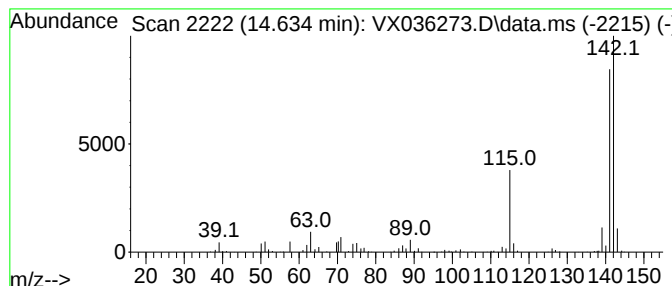
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

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

Peak Number 1 1,4-Methanonaphthalene, 1,4... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	13.41 ug/l	242074	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062123\
Data File : VX036273.D
Acq On : 21 Jun 2023 16:08
Operator : JC/MD
Sample : 03331-31
Misc : 20.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOTAL-VOC-SB18-27-GRAB-10

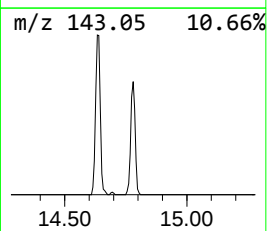
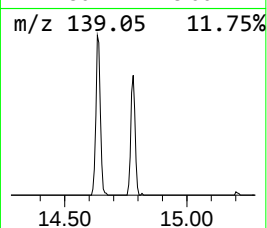
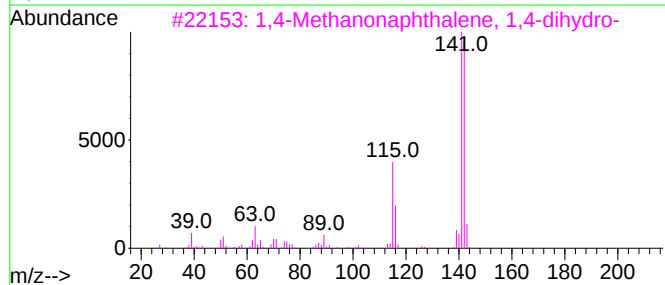
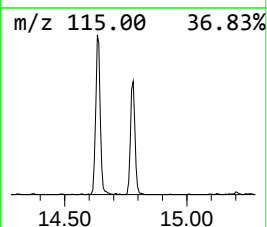
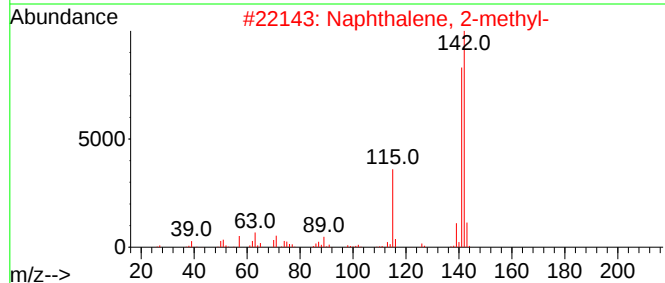
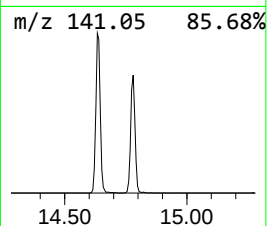
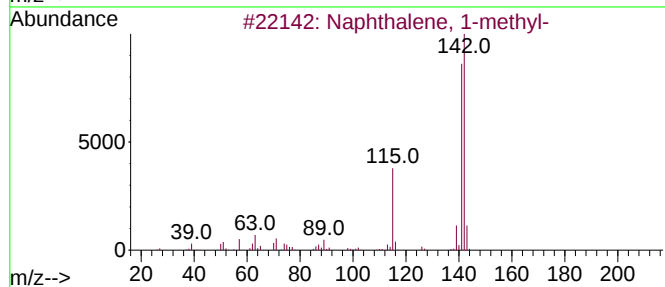
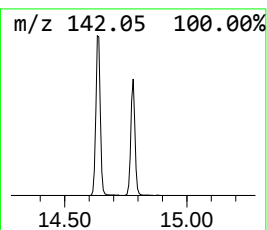
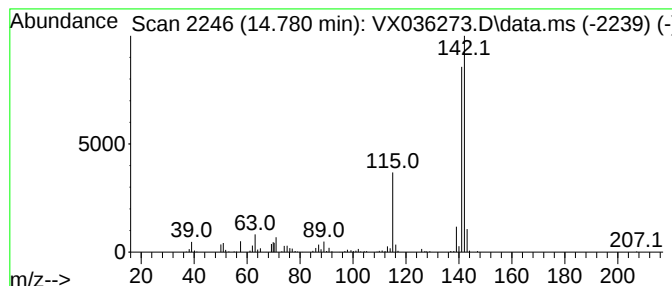
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	9.82 ug/l	177267	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062123\
Data File : VX036273.D
Acq On : 21 Jun 2023 16:08
Operator : JC/MD
Sample : 03331-31
Misc : 20.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOTAL-VOC-SB18-27-GRAB-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,4-Methanonaph...	14.634	13.4	ug/l	242074	4	12.024	902484	50.0
Benzocyclohepta...	14.780	9.8	ug/l	177267	4	12.024	902484	50.0