

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102925\
 Data File : VN088163.D
 Acq On : 29 Oct 2025 16:09
 Operator : JC\MD
 Sample : Q3472-12
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 COMP-5

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_N\methods\82N102325W.M
 Title : SW846 8260

Signal : TIC: VN088163.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.912	137	163	165	rBV6	60182	298086	3.40%	0.578%
2	7.194	879	891	902	rBV4	65818	206583	2.36%	0.401%
3	7.983	1013	1025	1039	rBV2	232191	664757	7.58%	1.290%
4	8.194	1042	1061	1072	rVV	3424059	8768121	100.00%	17.015%
5	8.300	1072	1079	1090	rVV	868392	2195078	25.03%	4.260%
6	8.418	1090	1099	1108	rVV	3671318	8616273	98.27%	16.721%
7	8.483	1108	1110	1117	rVV3	257932	520683	5.94%	1.010%
8	8.559	1117	1123	1133	rVV	246610	575904	6.57%	1.118%
9	8.688	1133	1145	1152	rVV3	564934	1596780	18.21%	3.099%
10	8.765	1152	1158	1163	rVV2	401499	920963	10.50%	1.787%
11	8.830	1163	1169	1180	rVV	423905	995423	11.35%	1.932%
12	8.941	1180	1188	1199	rVV	1057720	2126015	24.25%	4.126%
13	9.077	1201	1211	1227	rVB	534686	1128754	12.87%	2.190%
14	9.577	1283	1296	1307	rBV	129199	321972	3.67%	0.625%
15	10.541	1451	1460	1467	rBV	822074	1574075	17.95%	3.055%
16	10.606	1467	1471	1477	rVB2	53571	103386	1.18%	0.201%
17	10.718	1485	1490	1500	rVB2	52516	103668	1.18%	0.201%
18	11.618	1636	1643	1655	rVV6	70705	188975	2.16%	0.367%
19	11.724	1655	1661	1666	rVB	64775	103817	1.18%	0.201%
20	11.847	1674	1682	1693	rBV	686079	1313957	14.99%	2.550%
21	12.047	1707	1716	1727	rVV2	365967	854011	9.74%	1.657%
22	12.347	1760	1767	1769	rBV3	86168	158475	1.81%	0.308%
23	12.459	1781	1786	1791	rVB	108400	172483	1.97%	0.335%
24	12.576	1792	1806	1807	rBV5	93003	253129	2.89%	0.491%
25	12.747	1832	1835	1838	rBV3	67147	103907	1.19%	0.202%
26	12.776	1838	1840	1843	rVB	133866	129484	1.48%	0.251%
27	12.829	1843	1849	1859	rBV2	514714	1102760	12.58%	2.140%
28	13.006	1873	1879	1885	rBV5	65609	144947	1.65%	0.281%
29	13.076	1885	1891	1894	rVV3	164665	296456	3.38%	0.575%
30	13.135	1895	1901	1909	rVV	1034559	1973363	22.51%	3.829%
31	13.200	1909	1912	1918	rVB3	98569	164600	1.88%	0.319%
32	13.288	1923	1927	1929	rBV2	54845	93496	1.07%	0.181%
33	13.371	1937	1941	1946	rBV2	178584	256763	2.93%	0.498%
34	13.459	1952	1956	1966	rVB	316581	681027	7.77%	1.322%
35	13.653	1983	1989	1993	rBV3	256868	552731	6.30%	1.073%
36	13.694	1993	1996	1999	rVB2	123828	162119	1.85%	0.315%

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37	13.771	2004	2009	2016	rVV3	849708	1880056	21.44%	3.648%
38	13.829	2016	2019	2026	rVB2	183163	295452	3.37%	0.573%
39	13.959	2037	2041	2045	rBV2	181118	327904	3.74%	0.636%
40	14.082	2057	2062	2068	rBV	1142538	1979264	22.57%	3.841%
41	14.306	2096	2100	2104	rBV2	131624	202348	2.31%	0.393%
42	14.418	2114	2119	2124	rVB3	200130	334316	3.81%	0.649%
43	14.553	2138	2142	2145	rBV5	101441	181237	2.07%	0.352%
44	14.600	2145	2150	2154	rBV2	413747	659861	7.53%	1.281%
45	14.712	2165	2169	2172	rVB2	166470	222212	2.53%	0.431%
46	14.765	2173	2178	2183	rVB4	165076	330827	3.77%	0.642%
47	14.817	2183	2187	2190	rBV4	139004	237762	2.71%	0.461%
48	14.935	2198	2207	2214	rBV5	472254	1113974	12.70%	2.162%
49	15.023	2215	2222	2228	rBV5	344432	882102	10.06%	1.712%
50	15.188	2245	2250	2256	rVB	251084	492473	5.62%	0.956%
51	15.294	2263	2268	2273	rBV3	172105	301889	3.44%	0.586%
52	15.412	2282	2288	2295	rVB3	184163	427114	4.87%	0.829%
53	15.570	2311	2315	2318	rBV6	65339	113029	1.29%	0.219%
54	15.670	2328	2332	2336	rBV2	113979	172184	1.96%	0.334%
55	15.717	2337	2340	2344	rBV4	89436	133540	1.52%	0.259%
56	15.917	2366	2374	2381	rBV4	149328	398552	4.55%	0.773%
57	16.094	2398	2404	2405	rBV6	67917	126474	1.44%	0.245%
58	16.135	2406	2411	2421	rVB	303424	640804	7.31%	1.244%
59	16.464	2462	2467	2474	rBV4	107049	224664	2.56%	0.436%
60	16.676	2497	2503	2509	rBV3	126967	264648	3.02%	0.514%
61	16.747	2510	2515	2521	rBV3	69927	164927	1.88%	0.320%

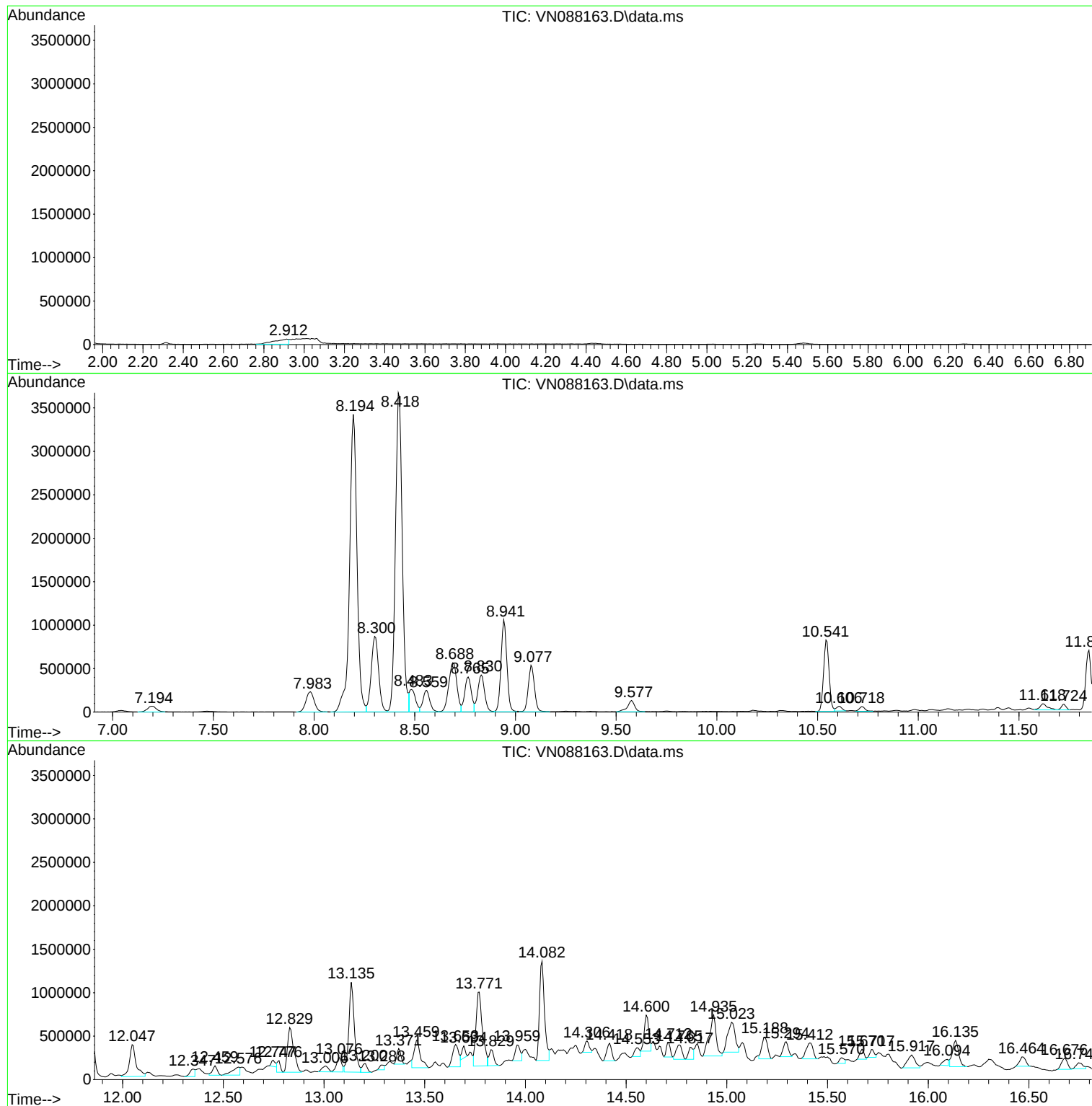
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
COMP-5

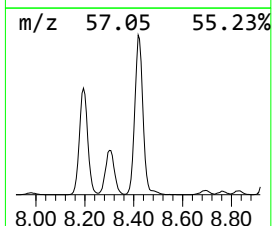
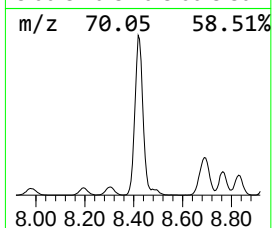
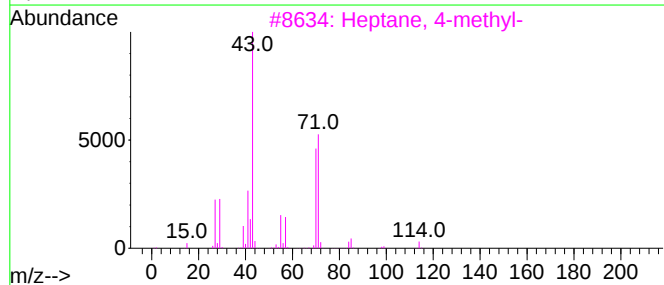
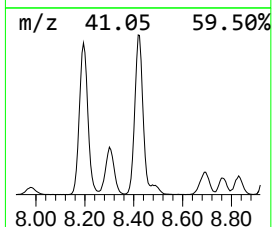
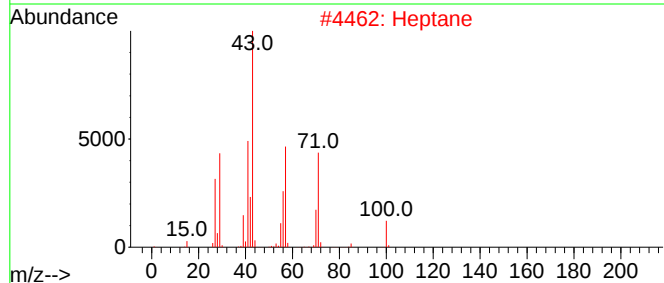
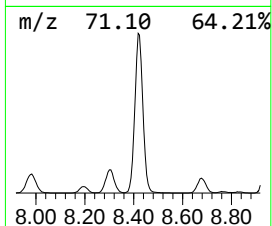
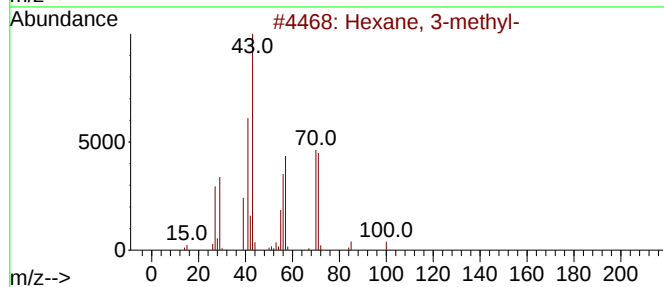
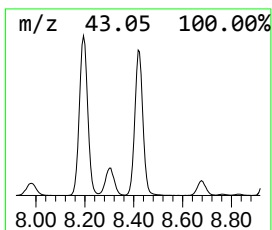
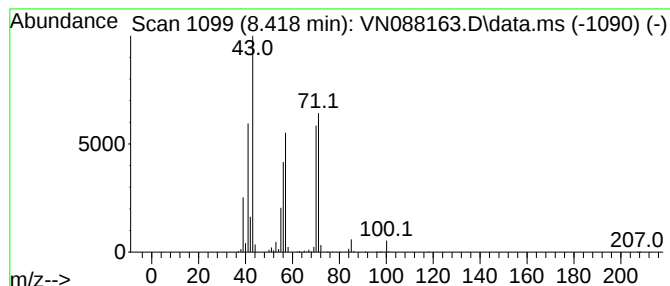
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.418	49.13 ug/l	8616270	Pentafluorobenzene	8.200

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2			Heptane	100	C7H16	000142-82-5	80
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	53
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53



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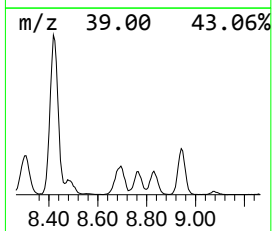
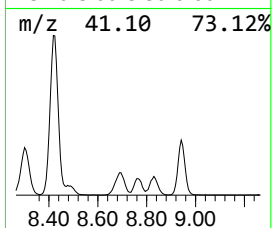
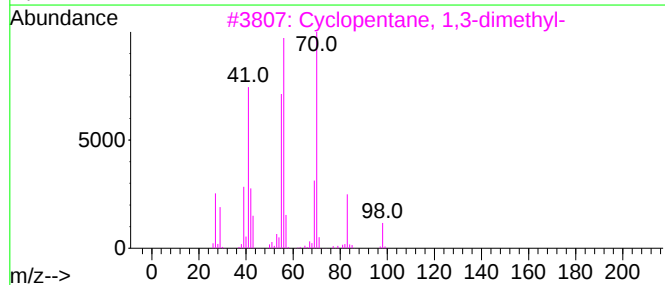
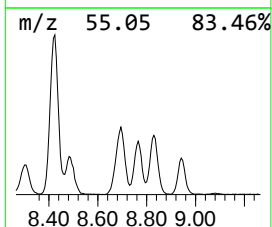
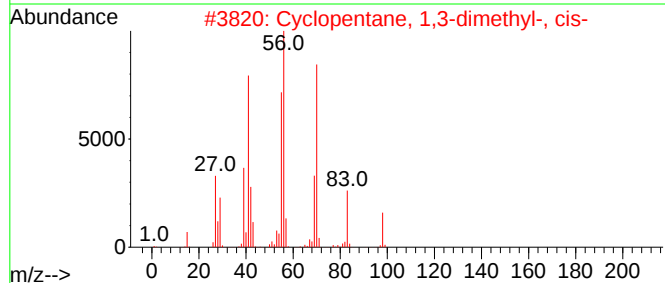
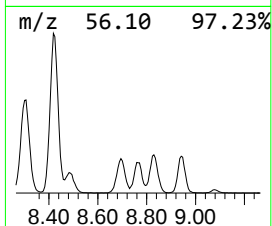
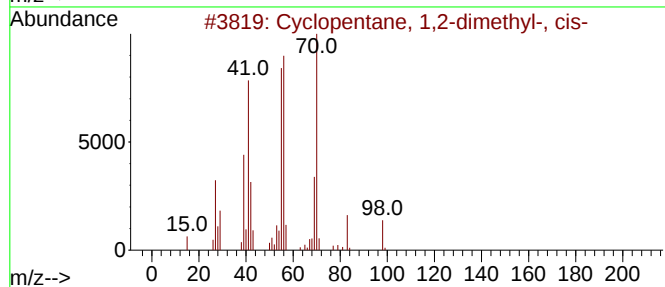
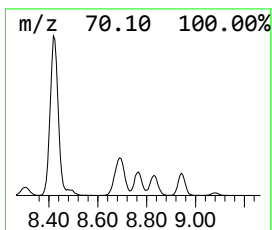
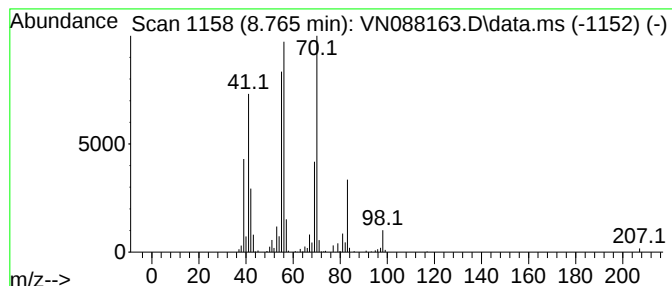
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, 1,2-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.765	40.80 ug/l	920963	1,4-Difluorobenzene	9.077

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	94
2			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	93
3			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	87
4			Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	81
5			Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	49



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
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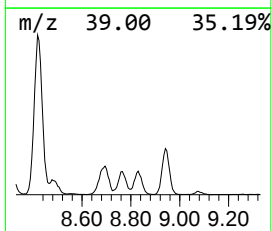
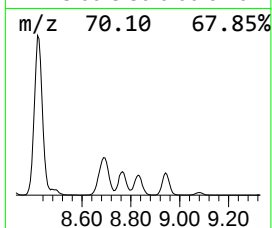
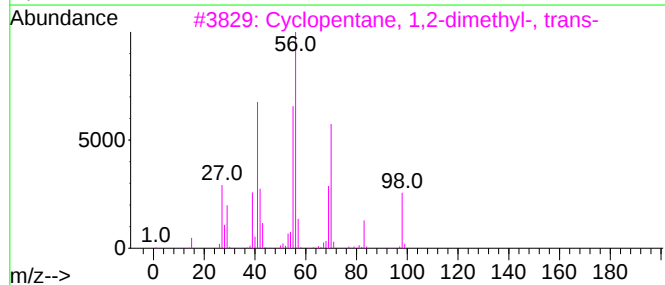
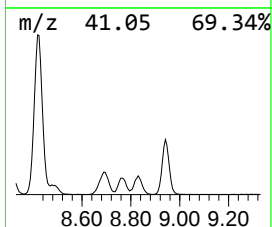
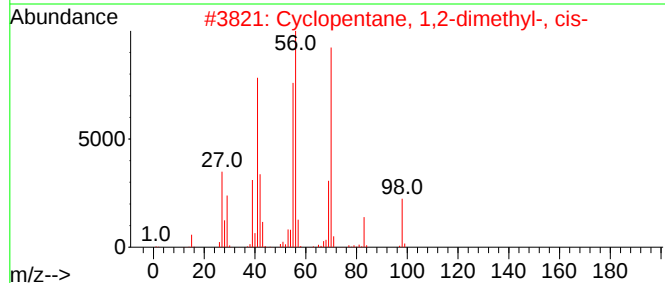
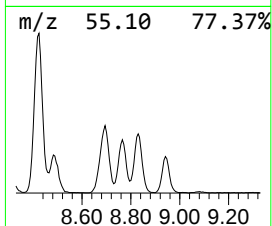
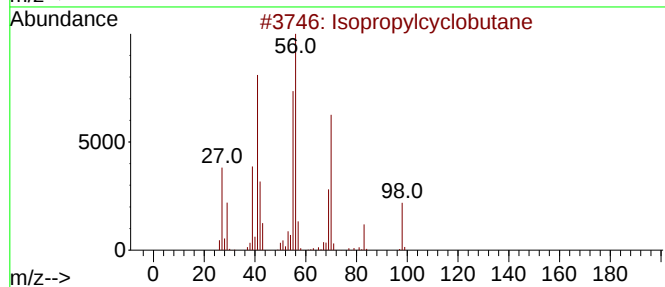
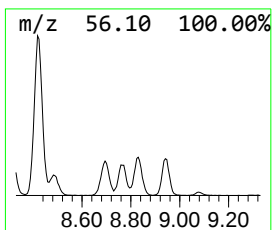
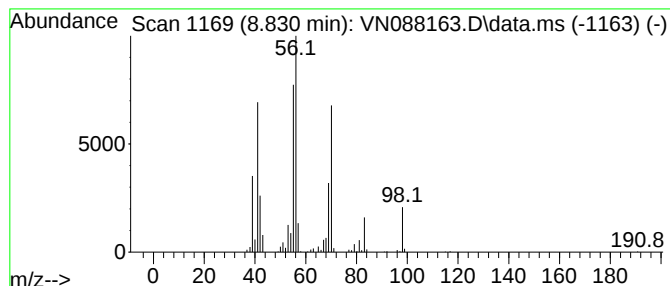
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Quant Title : SW846 8260

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

Peak Number 4 Isopropylcyclobutane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.830	44.09 ug/l	995423	1,4-Difluorobenzene	9.077

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropylcyclobutane	98	C7H14	000872-56-0	95
2			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	91
3			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	91
4			1-Heptene	98	C7H14	000592-76-7	80
5			Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	78



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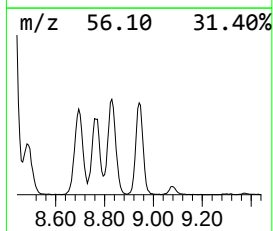
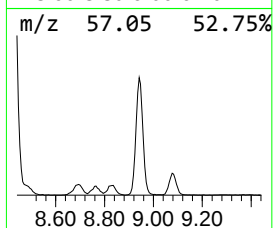
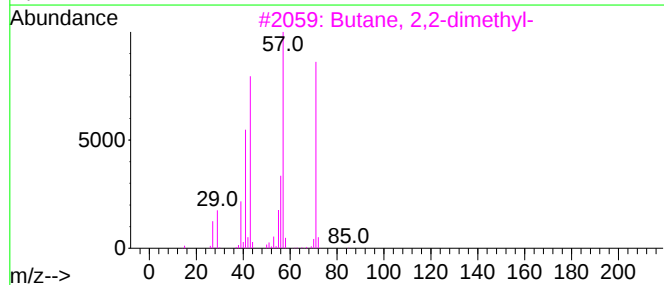
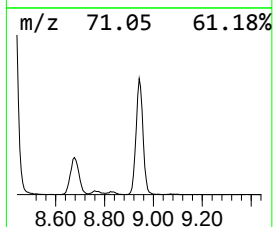
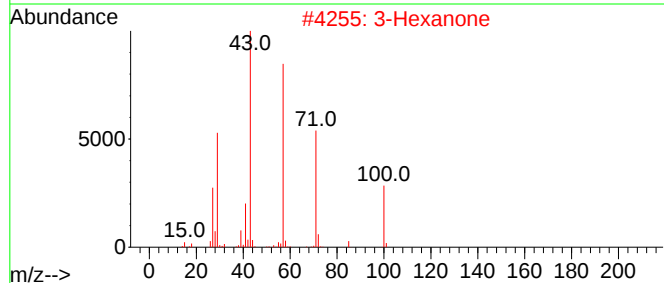
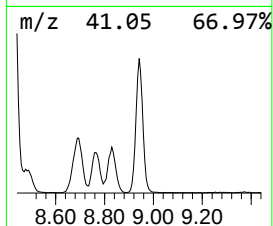
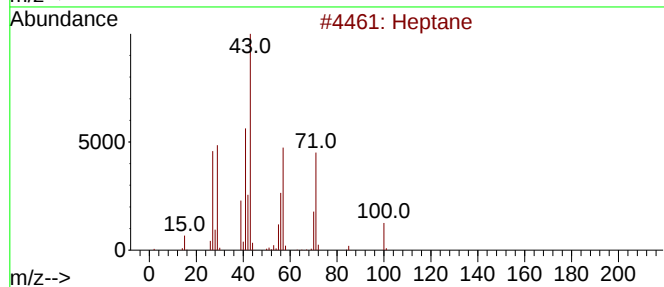
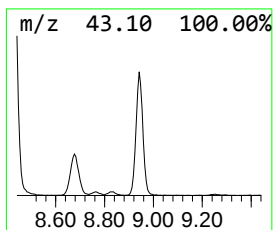
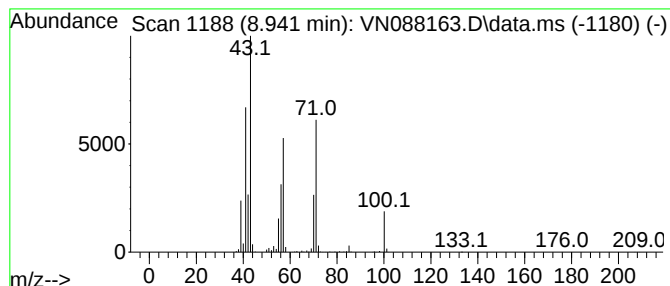
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Quant Title : SW846 8260

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

Peak Number 5 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.941	94.18 ug/l	2126020	1,4-Difluorobenzene	9.077

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			3-Hexanone	100	C6H12O	000589-38-8	46
3			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	43
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	42
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40



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ClientSampleId :
COMP-5

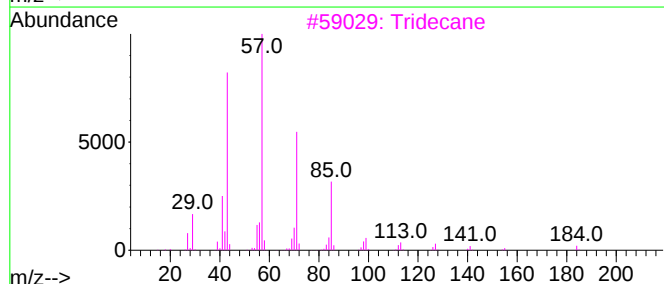
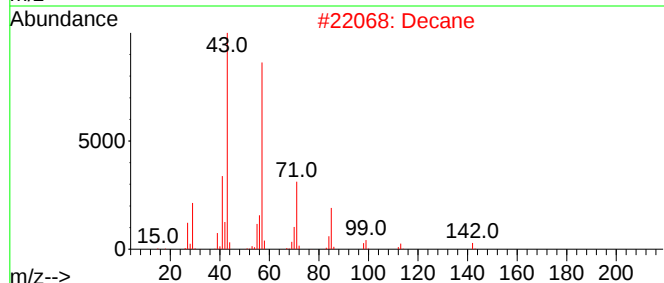
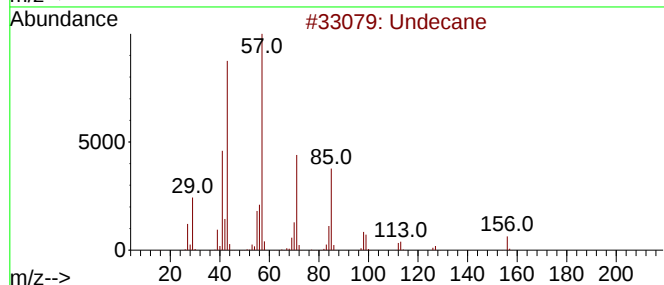
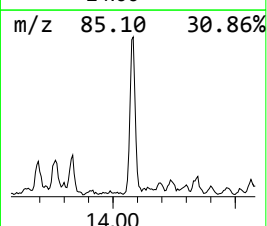
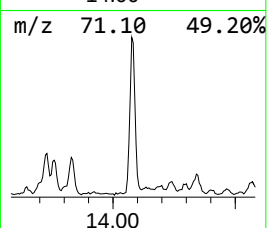
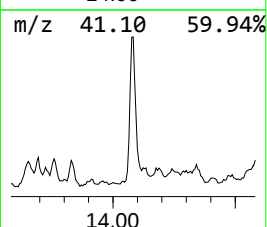
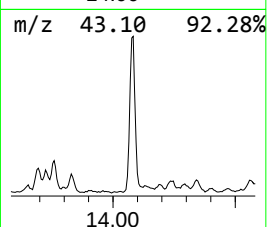
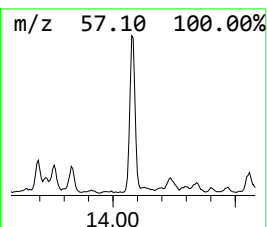
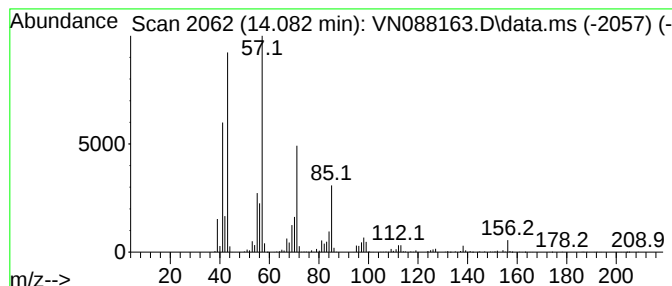
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Quant Title : SW846 8260

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

Peak Number 6 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.082	52.64 ug/l	1979260	1,4-Dichlorobenzene-d4	13.771

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	90
2	Decane			142	C10H22	000124-18-5	78
3	Tridecane			184	C13H28	000629-50-5	72
4	Hexadecane			226	C16H34	000544-76-3	59
5	Ether, hexyl pentyl			172	C11H24O	032357-83-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102925\
Data File : VN088163.D
Acq On : 29 Oct 2025 16:09
Operator : JC\MD
Sample : Q3472-12
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

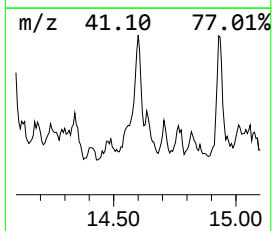
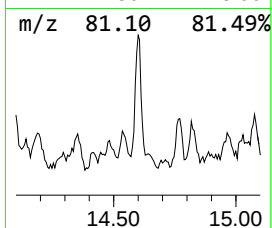
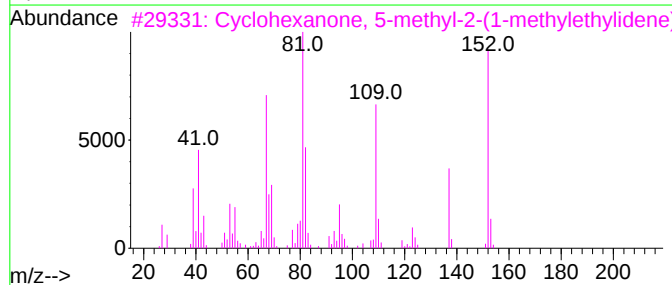
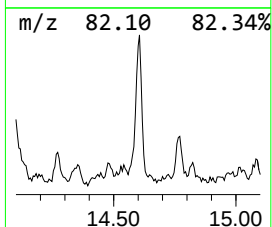
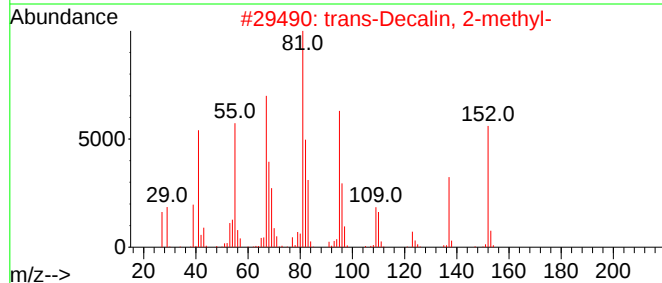
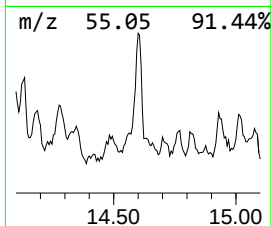
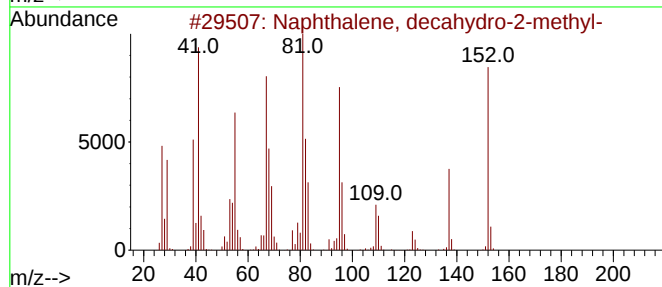
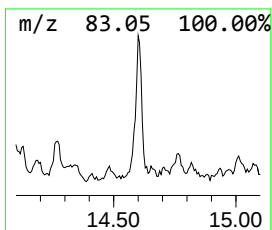
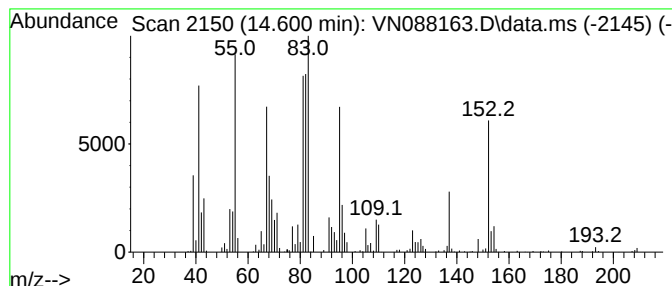
Instrument :
MSVOA_N
ClientSampleId :
COMP-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, decahydro-2-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.600	17.55 ug/l	659861	1,4-Dichlorobenzene-d4			13.771
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2-methyl-		152	C11H20	002958-76-1	97
2	trans-Decalin, 2-methyl-		152	C11H20	1000152-47-3	97
3	Cyclohexanone, 5-methyl-2-(1-met...		152	C10H16O	015932-80-6	50
4	Decalin, syn-1-methyl-, cis-		152	C11H20	1000158-89-1	49
5	1-Methyldecahydronaphthalene		152	C11H20	002958-75-0	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102925\
Data File : VN088163.D
Acq On : 29 Oct 2025 16:09
Operator : JC\MD
Sample : Q3472-12
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-5

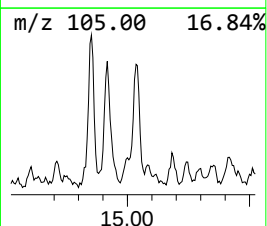
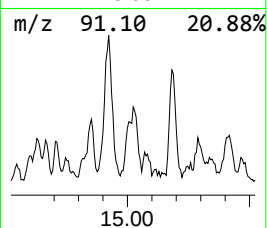
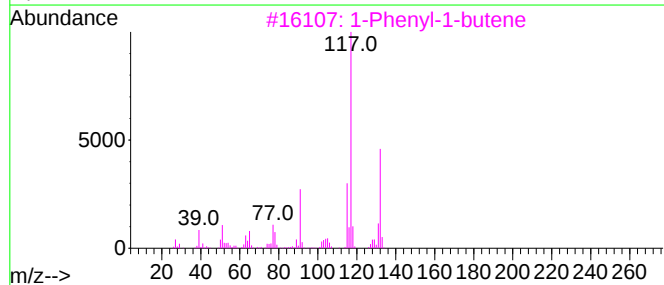
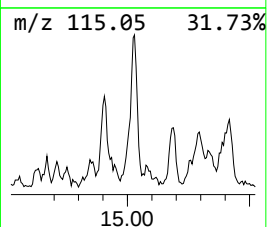
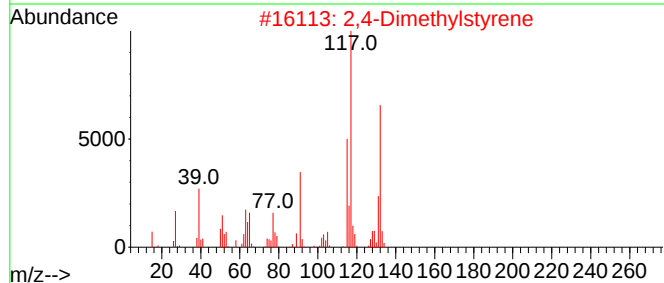
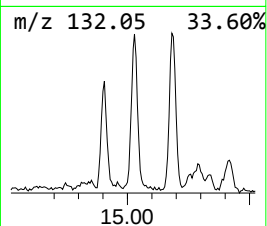
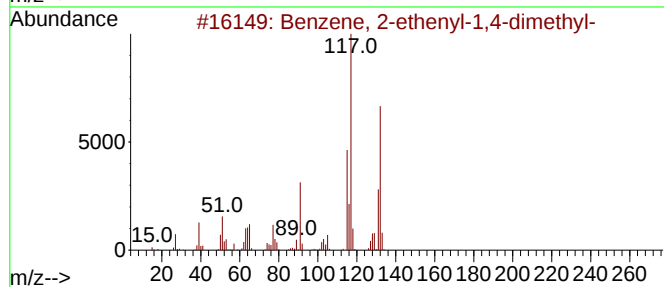
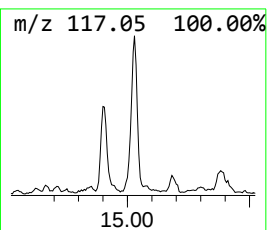
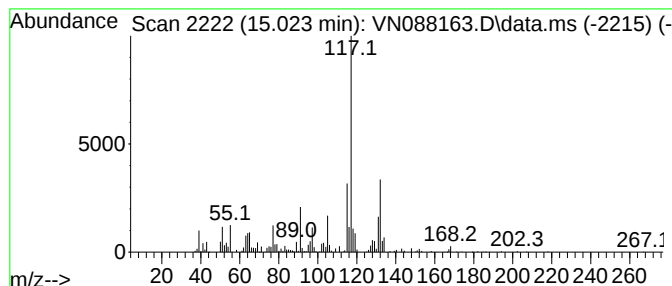
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.023	23.46 ug/l	882102	1,4-Dichlorobenzene-d4	13.771

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			2,4-Dimethylstyrene	132	C10H12	002234-20-0	93
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	93
4			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	92
5			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102925\
Data File : VN088163.D
Acq On : 29 Oct 2025 16:09
Operator : JC\MD
Sample : Q3472-12
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 3-methyl-	8.418	49.1	ug/l	8616270	1	8.200	8768120	50.0
Cyclopentane, 1...	8.765	40.8	ug/l	920963	2	9.077	1128750	50.0
Isopropylcyclob...	8.830	44.1	ug/l	995423	2	9.077	1128750	50.0
Heptane	8.941	94.2	ug/l	2126020	2	9.077	1128750	50.0
Undecane	14.082	52.6	ug/l	1979260	4	13.771	1880060	50.0
Naphthalene, de...	14.600	17.6	ug/l	659861	4	13.771	1880060	50.0
Benzene, 2-ethe...	15.023	23.5	ug/l	882102	4	13.771	1880060	50.0