

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX123119\
 Data File : VX014375.D
 Acq On : 31 Dec 2019 13:21
 Operator : JC/SP
 Sample : K6462-02
 Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 K500-2

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.070	26	30	44	rBV	446552	571808	24.08%	1.371%
2	1.265	58	62	68	rBV2	44351	67643	2.85%	0.162%
3	1.667	106	128	129	rBV2	85784	412962	17.39%	0.990%
4	3.009	340	348	354	rBV	22925	56715	2.39%	0.136%
5	5.490	744	755	770	rBV	229234	725925	30.57%	1.741%
6	5.648	771	781	797	rVB	463370	1336182	56.26%	3.204%
7	6.051	834	847	866	rBV	273661	796888	33.55%	1.911%
8	6.849	968	978	993	rBV	696246	1741629	73.33%	4.176%
9	8.709	1277	1283	1294	rVB	1480630	2375019	100.00%	5.695%
10	10.111	1508	1513	1520	rVV	1429194	1991898	83.87%	4.776%
11	10.233	1528	1533	1540	rBV5	19005	48187	2.03%	0.116%
12	10.367	1551	1555	1559	rVV3	44280	74435	3.13%	0.178%
13	10.410	1559	1562	1573	rVB4	29600	55882	2.35%	0.134%
14	10.635	1593	1599	1603	rBV4	67025	106434	4.48%	0.255%
15	10.696	1605	1609	1612	rBV	57666	80132	3.37%	0.192%
16	10.830	1623	1631	1635	rBV2	95480	144539	6.09%	0.347%
17	10.904	1640	1643	1647	rVV3	73936	123555	5.20%	0.296%
18	10.946	1647	1650	1654	rVV2	58155	82149	3.46%	0.197%
19	11.080	1664	1672	1675	rBV3	71225	130205	5.48%	0.312%
20	11.135	1675	1681	1687	rVV	1321048	1749108	73.65%	4.194%
21	11.239	1695	1698	1701	rVV2	95137	130958	5.51%	0.314%
22	11.269	1701	1703	1707	rVB2	80115	92450	3.89%	0.222%
23	11.385	1714	1722	1726	rBV6	43687	88266	3.72%	0.212%
24	11.440	1727	1731	1734	rVV5	47578	73951	3.11%	0.177%
25	11.483	1734	1738	1740	rVV2	133451	185586	7.81%	0.445%
26	11.525	1742	1745	1750	rVB2	264447	335338	14.12%	0.804%
27	11.678	1763	1770	1775	rBV4	125580	255308	10.75%	0.612%
28	11.733	1775	1779	1781	rBV2	86334	99269	4.18%	0.238%
29	11.763	1781	1784	1787	rVV	184538	189292	7.97%	0.454%
30	11.830	1787	1795	1800	rVB7	106027	300876	12.67%	0.721%
31	11.885	1800	1804	1806	rBV3	90651	119113	5.02%	0.286%
32	11.940	1809	1813	1818	rVB3	121588	188017	7.92%	0.451%
33	11.995	1818	1822	1824	rBV2	104510	133898	5.64%	0.321%
34	12.025	1824	1827	1829	rVB3	54092	52902	2.23%	0.127%

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Integration Parameters: RTEINT.P

Integrator: RTE
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 Sampling : 1
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35	12.074	1831	1835	1840	rVV	1597764	2079458	87.56%	4.986%
36	12.123	1840	1843	1845	rVV	128787	120552	5.08%	0.289%
37	12.153	1845	1848	1851	rVB3	138113	149801	6.31%	0.359%
38	12.196	1851	1855	1856	rBV4	48790	68316	2.88%	0.164%
39	12.220	1856	1859	1867	rVB2	236202	379315	15.97%	0.909%
40	12.300	1867	1872	1879	rBV6	108975	333744	14.05%	0.800%
41	12.367	1879	1883	1889	rVB2	363382	604085	25.43%	1.448%
42	12.470	1889	1900	1905	rBV	1017890	1422020	59.87%	3.410%
43	12.519	1905	1908	1914	rVB4	192410	347428	14.63%	0.833%
44	12.605	1916	1922	1924	rBV4	148940	282222	11.88%	0.677%
45	12.629	1924	1926	1933	rVB6	159720	318448	13.41%	0.764%
46	12.684	1933	1935	1939	rVB3	73606	85734	3.61%	0.206%
47	12.733	1939	1943	1947	rBV3	158072	241528	10.17%	0.579%
48	12.775	1947	1950	1953	rBV5	93113	136865	5.76%	0.328%
49	12.812	1953	1956	1959	rVV2	76805	90742	3.82%	0.218%
50	12.873	1962	1966	1971	rVB	575391	780335	32.86%	1.871%
51	12.940	1971	1977	1984	rBV5	299844	709991	29.89%	1.702%
52	12.995	1984	1986	1987	rBV	97853	90071	3.79%	0.216%
53	13.037	1987	1993	1997	rVB3	362945	643429	27.09%	1.543%
54	13.092	1998	2002	2005	rBV3	408568	482448	20.31%	1.157%
55	13.208	2016	2021	2023	rBV6	81246	155479	6.55%	0.373%
56	13.263	2028	2030	2032	rVV3	56009	48599	2.05%	0.117%
57	13.287	2032	2034	2035	rVV	64160	61195	2.58%	0.147%
58	13.318	2035	2039	2041	rVV	844006	959636	40.41%	2.301%
59	13.348	2041	2044	2049	rVB3	669908	893373	37.62%	2.142%
60	13.397	2049	2052	2054	rBV3	146743	183377	7.72%	0.440%
61	13.470	2060	2064	2073	rVB4	595200	1359281	57.23%	3.259%
62	13.550	2073	2077	2081	rBV4	234343	345132	14.53%	0.828%
63	13.641	2088	2092	2096	rBV4	250233	442316	18.62%	1.061%
64	13.726	2103	2106	2109	rBV4	224593	340509	14.34%	0.816%
65	13.763	2109	2112	2114	rVV3	218004	325388	13.70%	0.780%
66	13.787	2114	2116	2119	rVV2	212799	213251	8.98%	0.511%
67	13.854	2123	2127	2130	rBV2	372899	501378	21.11%	1.202%
68	13.891	2130	2133	2136	rBV4	137706	215994	9.09%	0.518%
69	13.976	2141	2147	2152	rVB6	299491	685896	28.88%	1.645%
70	14.031	2152	2156	2158	rBV3	113730	178320	7.51%	0.428%
71	14.086	2162	2165	2169	rVV	477047	548031	23.07%	1.314%

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Integration Parameters: RTEINT.P

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 Sampling : 1 Min Area: 3 % of largest Peak
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72	14.123	2169	2171	2174	rVV3	128723	162977	6.86%	0.391%
73	14.153	2174	2176	2180	rVB3	169043	194538	8.19%	0.466%
74	14.190	2180	2182	2184	rVB3	74006	54994	2.32%	0.132%
75	14.214	2184	2186	2190	rVB	124463	119315	5.02%	0.286%
76	14.269	2191	2195	2203	rBV5	426859	709397	29.87%	1.701%
77	14.373	2209	2212	2216	rBV2	214655	275654	11.61%	0.661%
78	14.427	2218	2221	2224	rVB	201884	222070	9.35%	0.532%
79	14.537	2234	2239	2247	rVB4	413024	923809	38.90%	2.215%
80	14.604	2247	2250	2251	rBV2	167648	169289	7.13%	0.406%
81	14.665	2257	2260	2267	rBV3	480260	786808	33.13%	1.887%
82	14.726	2267	2270	2274	rVB2	371925	481997	20.29%	1.156%
83	14.781	2276	2279	2280	rBV2	108953	118654	5.00%	0.284%
84	14.805	2280	2283	2287	rVB2	496338	542708	22.85%	1.301%
85	14.848	2287	2290	2292	rBV4	180190	232856	9.80%	0.558%
86	14.872	2292	2294	2296	rVV2	107386	115443	4.86%	0.277%
87	14.903	2296	2299	2305	rVB4	361571	507424	21.37%	1.217%
88	14.976	2305	2311	2316	rBV6	183525	514631	21.67%	1.234%
89	15.104	2327	2332	2336	rBV3	194979	334573	14.09%	0.802%
90	15.244	2350	2355	2362	rBV2	504631	957579	40.32%	2.296%
91	15.305	2362	2365	2368	rVV2	92360	111563	4.70%	0.267%
92	15.342	2368	2371	2374	rVB3	156136	194938	8.21%	0.467%
93	15.378	2374	2377	2382	rVB6	164401	297861	12.54%	0.714%
94	15.439	2383	2387	2391	rBV4	208396	346667	14.60%	0.831%
95	15.488	2391	2395	2398	rBV4	127909	219489	9.24%	0.526%
96	15.555	2401	2406	2410	rBV2	331398	523275	22.03%	1.255%
97	15.677	2422	2426	2430	rVB2	211814	329616	13.88%	0.790%
98	15.817	2446	2449	2453	rVB4	127068	169785	7.15%	0.407%
99	15.921	2462	2466	2468	rBV2	120432	187465	7.89%	0.449%
100	16.451	2550	2553	2559	rVB	99269	160616	6.76%	0.385%

Sum of corrected areas: 41706197

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ALS Vial : 7 Sample Multiplier: 1

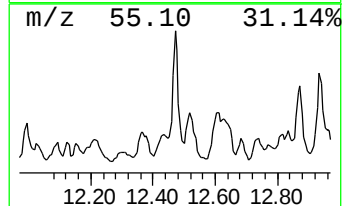
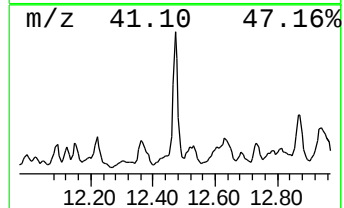
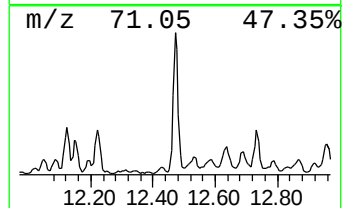
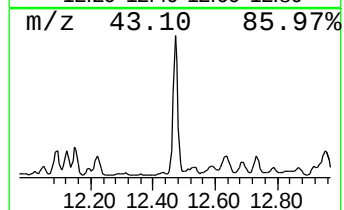
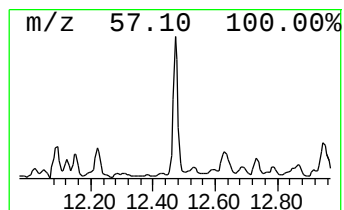
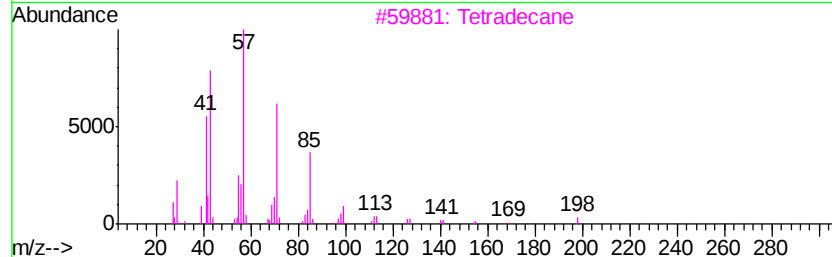
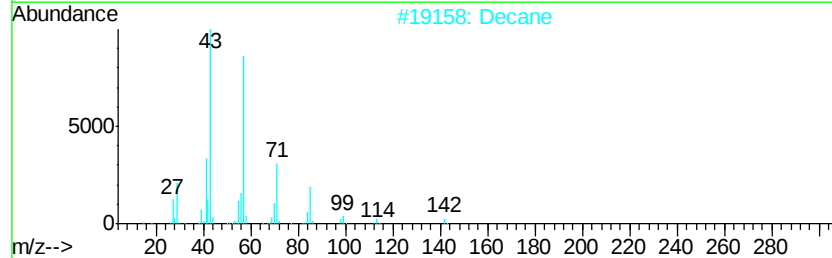
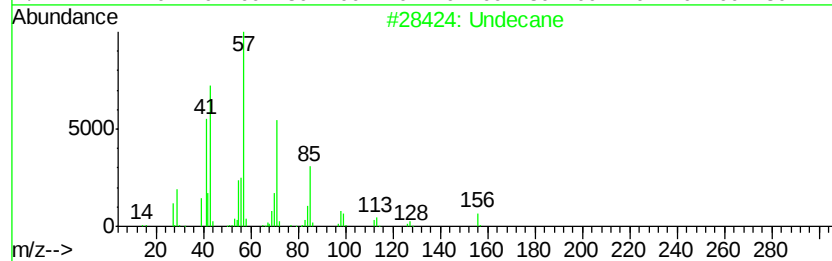
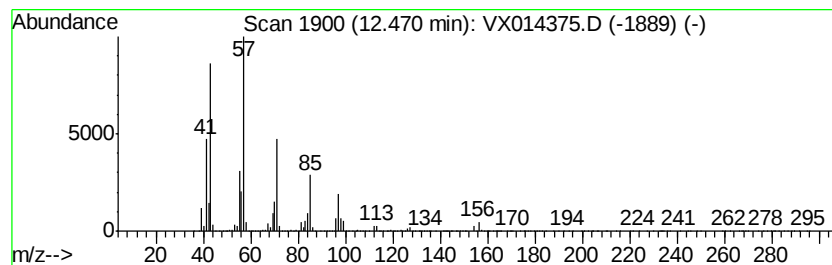
Instrument :
MSVOA_X
ClientSampled :
K500-2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 2 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	34.19 ug/l	1422020	1,4-Dichlorobenzene-d4	12.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Undecane	156 C11H24	001120-21-4	94
2	Decane	142 C10H22	000124-18-5	72
3	Tetradecane	198 C14H30	000629-59-4	64
4	Octane, 2,4,6-trimethyl-	156 C11H24	062016-37-9	58
5	Decane, 1-iodo-	268 C10H21I	002050-77-3	55



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ALS Vial : 7 Sample Multiplier: 1

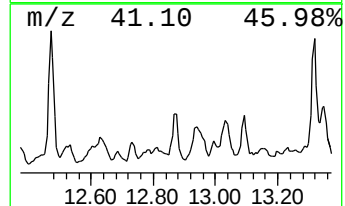
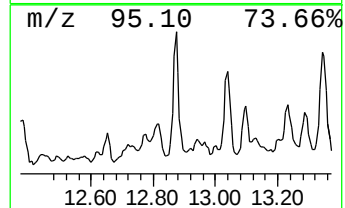
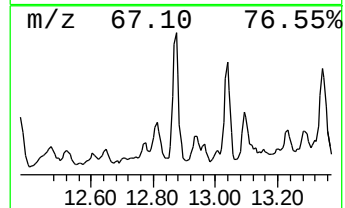
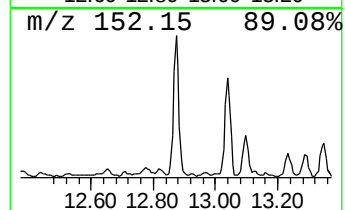
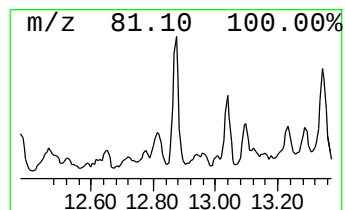
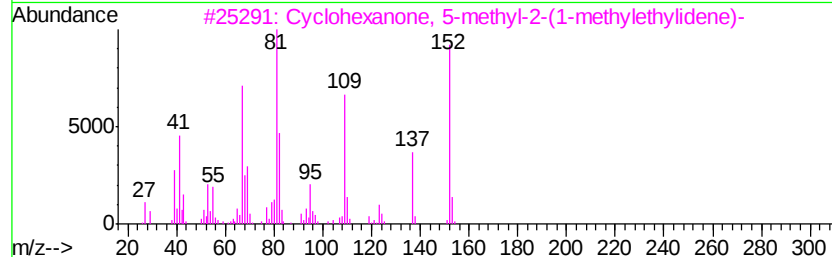
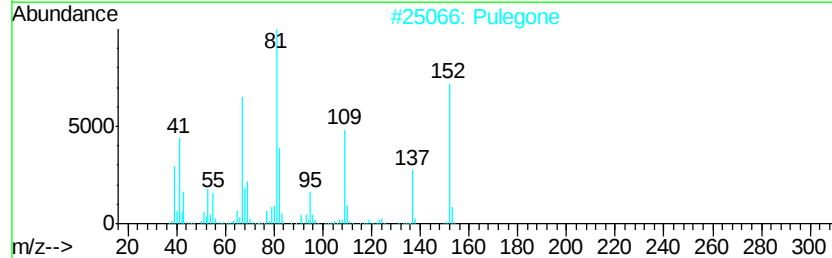
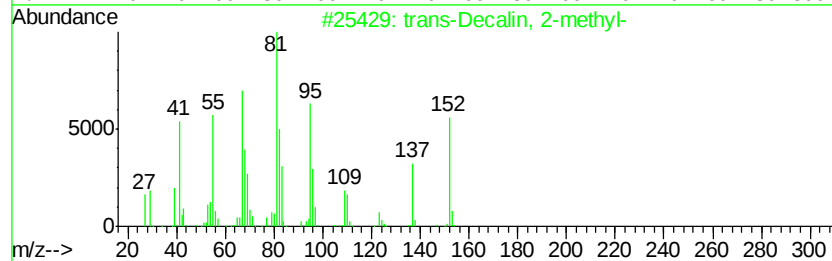
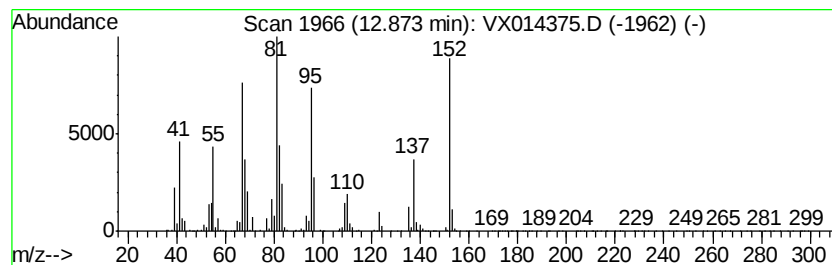
Instrument :
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Quant Title : SW846 8260

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

Peak Number 3 trans-Decalin, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	18.76 ug/l	780335	1,4-Dichlorobenzene-d4	12.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	trans-Decalin, 2-methyl-	152 C11H20	1000152-47-3	95
2	Pulegone	152 C10H16O	000089-82-7	68
3	Cyclohexanone, 5-methyl-2-(1-methyl-2-propenyl)-	152 C10H16O	015932-80-6	64
4	Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-	138 C10H18	018968-23-5	62
5	5-Hexadecyne	222 C16H30	071899-37-1	58



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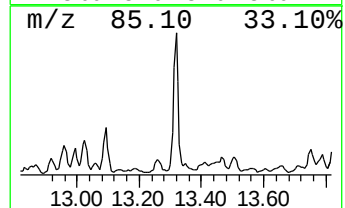
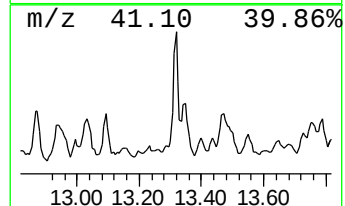
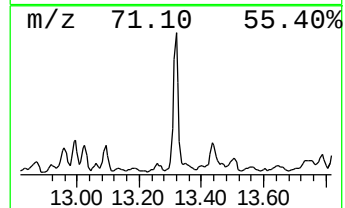
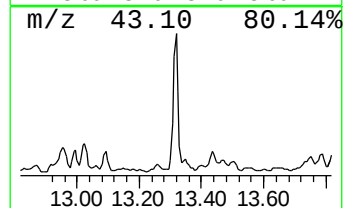
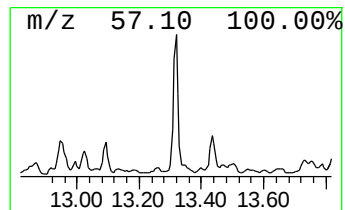
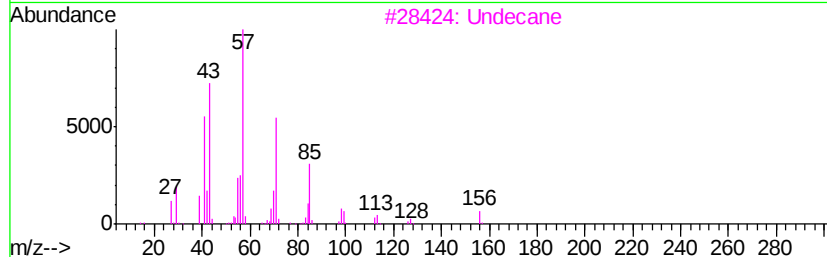
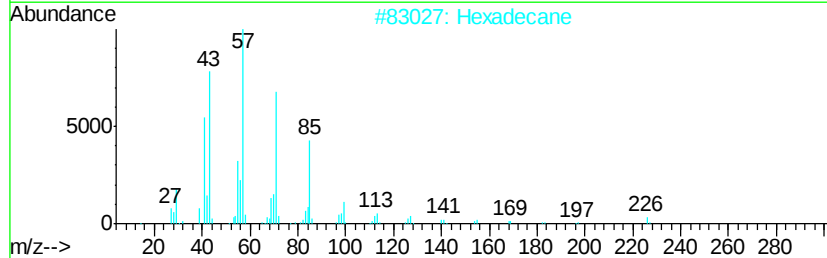
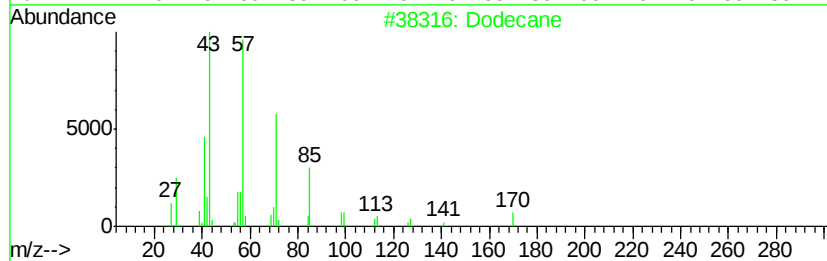
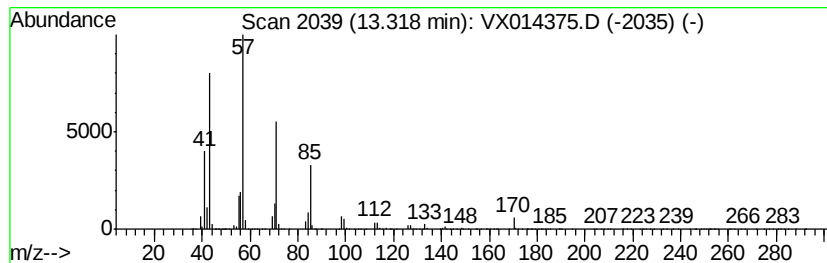
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 5 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	23.07 ug/l	959636	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane	170	C12H26	000112-40-3	94
2		Hexadecane	226	C16H34	000544-76-3	93
3		Undecane	156	C11H24	001120-21-4	90
4		Tridecane	184	C13H28	000629-50-5	83
5		Pentadecane	212	C15H32	000629-62-9	78



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Acq On : 31 Dec 2019 13:21
Operator : JC/SP
Sample : K6462-02
Misc : 5.05µl/10mL/100µL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
K500-2

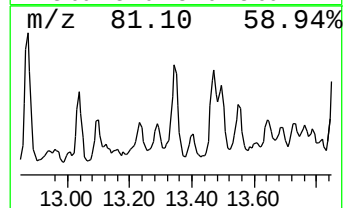
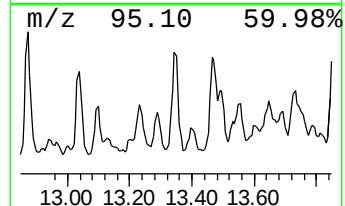
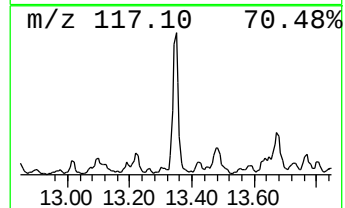
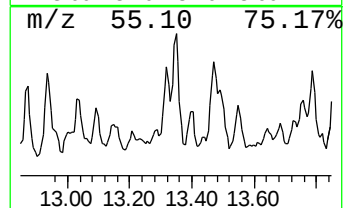
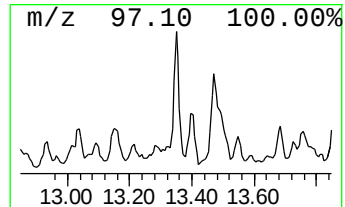
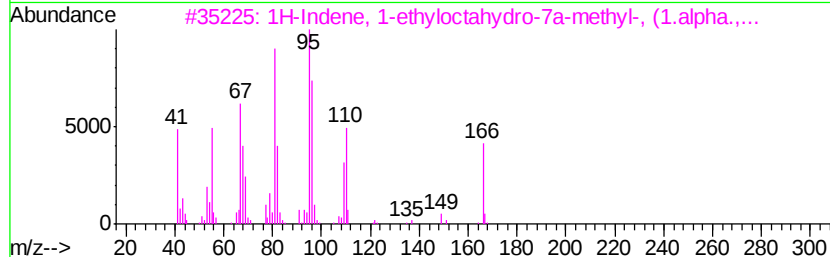
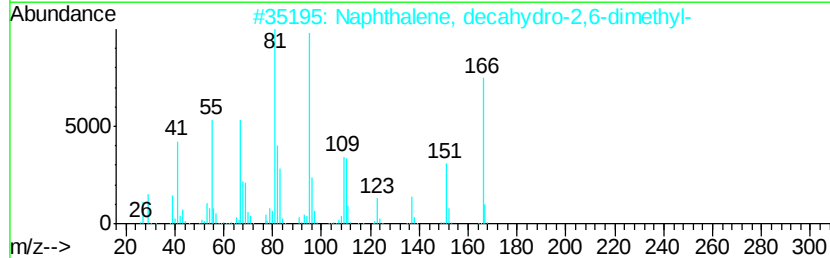
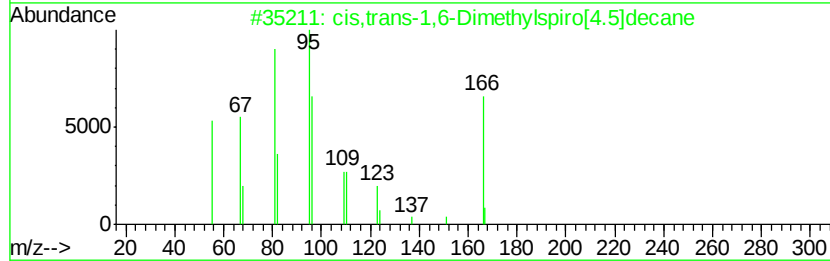
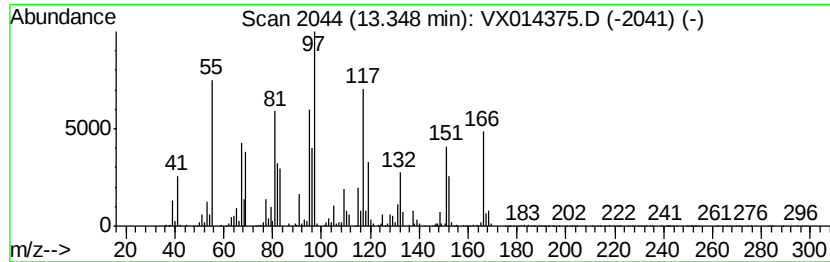
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Quant Title : SW846 8260

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

Peak Number 6 cis,trans-1,6-Dimethylspiro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	21.48 ug/l	893373	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	55
2		Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	48
3		1H-Indene, 1-ethyloctahydro-7a-m...	166	C12H22	056324-71-1	42
4		Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	054411-01-7	22
5		Carbonic acid, dithio-, S-methyl...	204	C9H16OS2	015288-12-7	22



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX123119\
Data File : VX014375.D
Acq On : 31 Dec 2019 13:21
Operator : JC/SP
Sample : K6462-02
Misc : 5.05µ/10mL/100µL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
K500-2

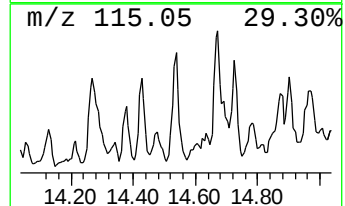
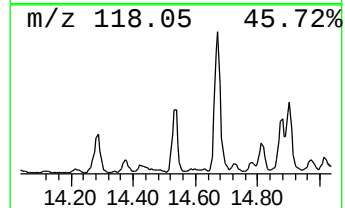
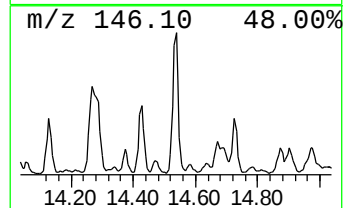
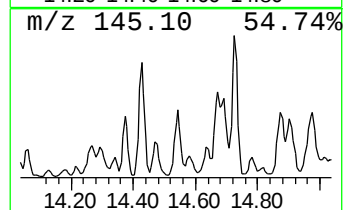
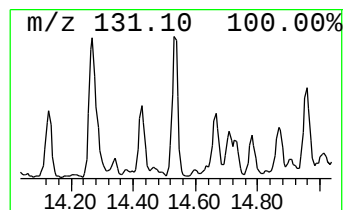
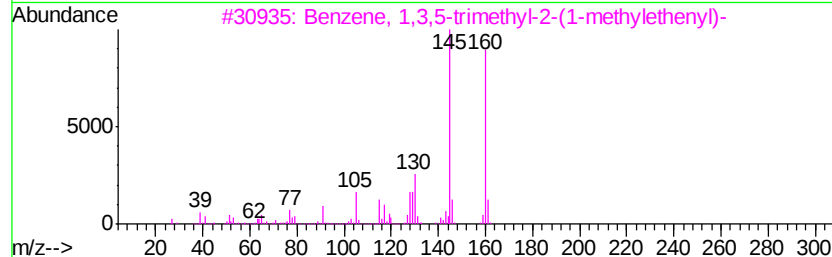
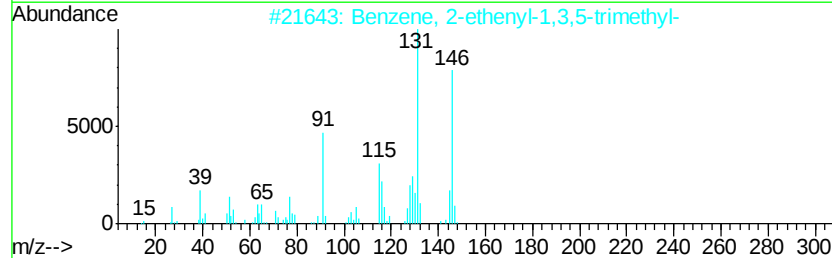
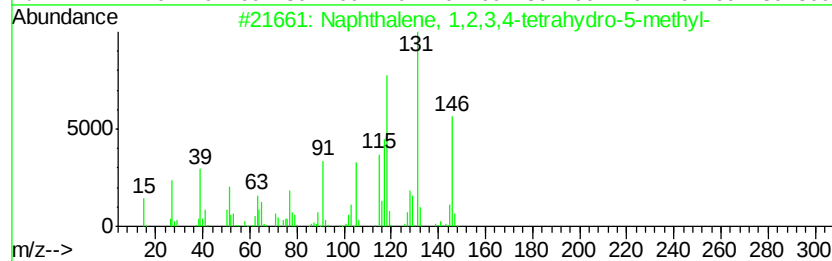
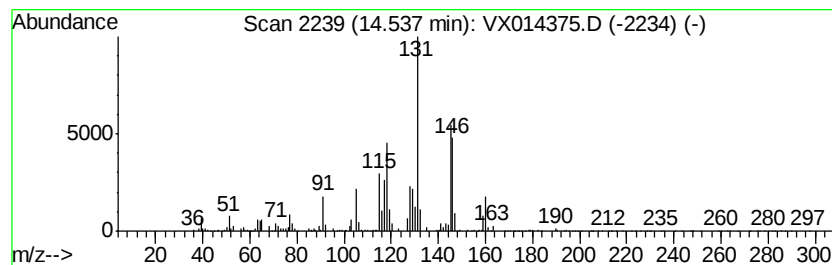
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,2,3,4-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	22.21 ug/l	923809	1,4-Dichlorobenzene-d4	12.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	81
2		Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	58
3		Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	55
4		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	55
5		2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX123119\
Data File : VX014375.D
Acq On : 31 Dec 2019 13:21
Operator : JC/SP
Sample : K6462-02
Misc : 5.05µL/10µL/100µL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
K500-2

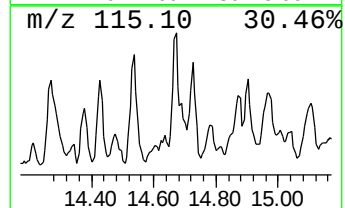
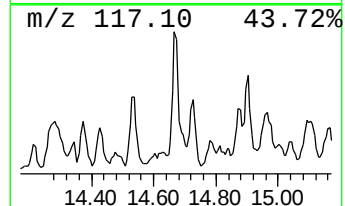
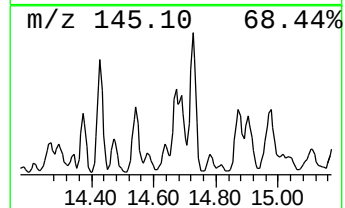
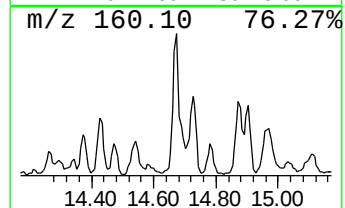
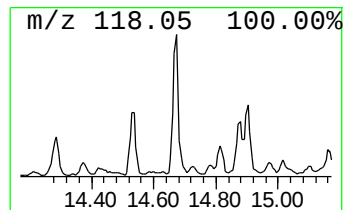
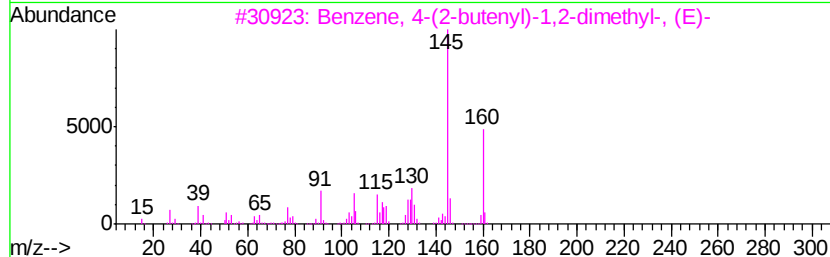
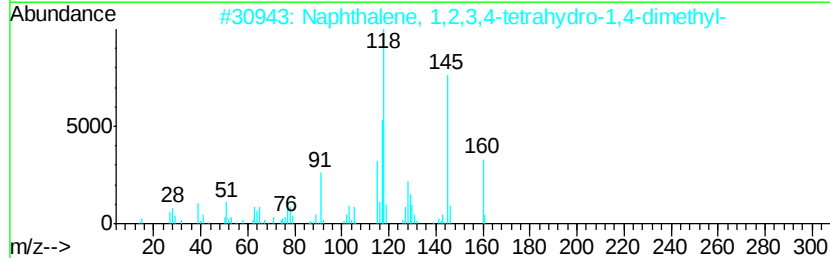
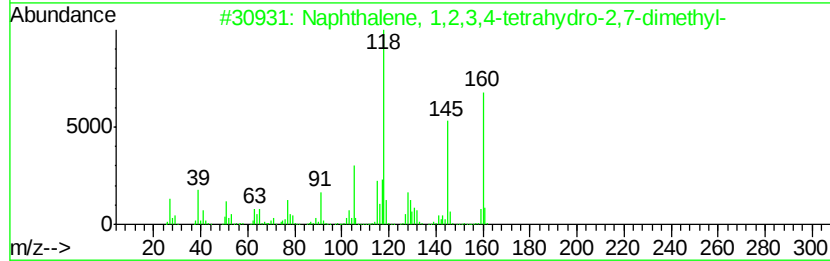
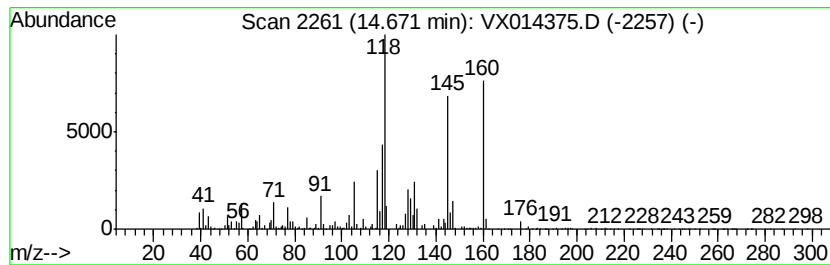
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	18.92 ug/l	786808	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	89
2		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	76
3		Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	60
4		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	58
5		Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	49



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX123119\
Data File : VX014375.D
Acq On : 31 Dec 2019 13:21
Operator : JC/SP
Sample : K6462-02
Misc : 5.05µL/100µL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
K500-2

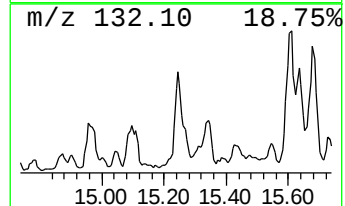
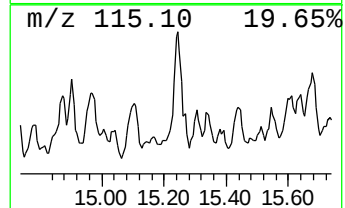
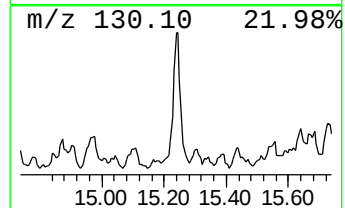
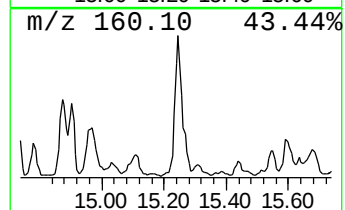
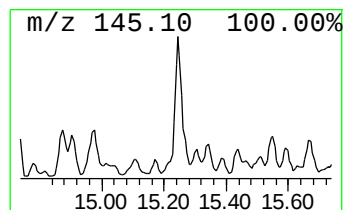
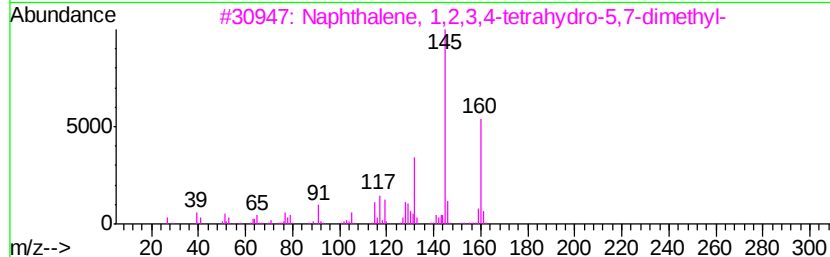
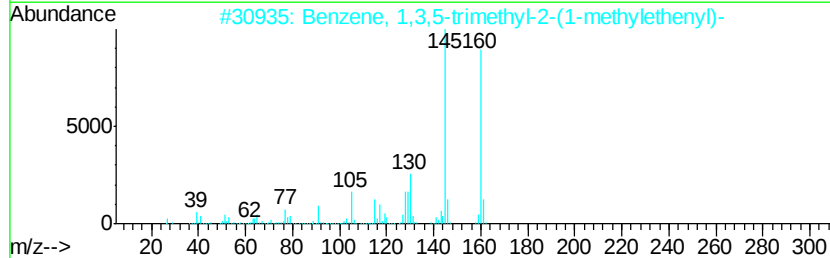
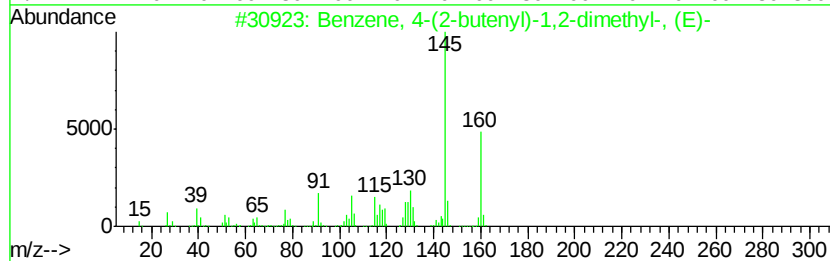
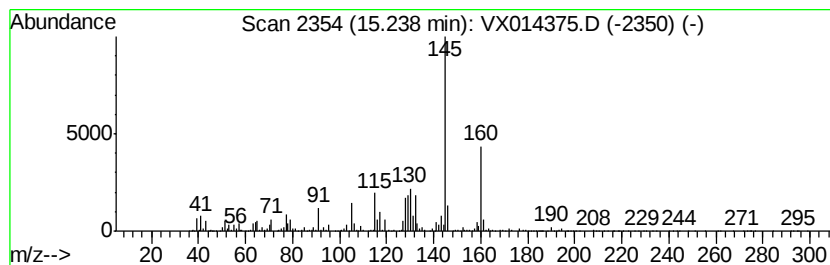
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 4-(2-butenyl)-1,2-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	23.02 ug/l	957579	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	94
2		Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	93
3		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	93
4		Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	91
5		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	91



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX123119\
Data File : VX014375.D
Acq On : 31 Dec 2019 13:21
Operator : JC/SP
Sample : K6462-02
Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
K500-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Undecane	12.47	34.2	ug/l	1422020	4	12.07	2079460	50.0
trans-Decalin, 2-...	12.87	18.8	ug/l	780335	4	12.07	2079460	50.0
Dodecane	13.32	23.1	ug/l	959636	4	12.07	2079460	50.0
cis,trans-1,6-Dim...	13.35	21.5	ug/l	893373	4	12.07	2079460	50.0
Naphthalene, 1,2,...	14.54	22.2	ug/l	923809	4	12.07	2079460	50.0
Naphthalene, 1,2,...	14.67	18.9	ug/l	786808	4	12.07	2079460	50.0
Benzene, 4-(2-but...	15.24	23.0	ug/l	957579	4	12.07	2079460	50.0