LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX122419\
Data File : VX014239.D
Acq On : 24 Dec 2019 12:55
Operator : JC/SP
Sample : K6401-01 40X
Misc : 4.72g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0B37

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\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	41	rBV	506228	630975	11.51%	1.223%
2	1.265	58	62	69	rBV	63973	86618	1.58%	0.168%
3	5.490	743	755	769	rBV	284991	829650	15.14%	1.608%
4	5.655	771	782	793	rVB	520582	1462936	26.69%	2.835%
5	6.051	838	847	858	rBV	330606	853981	15.58%	1.655%
6	6.850	968	978	989	rBV	821722	1890720	34.50%	3.665%
7	7.203	1030	1036	1046	rBV	141265	305387	5.57%	0.592%
8	8.709	1277	1283	1291	rVV	1759065	2589986	47.26%	5.020%
9	8.971	1319	1326	1332	rBV	61461	94882	1.73%	0.184%
10	9.550	1415	1421	1428	rBV2	36283	74576	1.36%	0.145%
11	9.873	1469	1474	1479	rBV4	43913	96929	1.77%	0.188%
12	9.959	1483	1488	1494	rVB	260955	388289	7.08%	0.753%
13	10.062	1499	1505	1508	rBV	230605	310027	5.66%	0.601%
14	10.111	1508	1513	1518	rVB	1602419	2194030	40.03%	4.253%
15	10.245	1529	1535	1541	rBV	1087188	1428370	26.06%	2.768%
16	10.349	1544	1552	1558	rVV	3500133	4986078	90.98%	9.664%
17	10.410	1558	1562	1574	rVB	1335701	1692085	30.87%	3.280%
18	10.587	1587	1591	1593	rBV2	39574	58984	1.08%	0.114%
19	10.636	1593	1599	1604	rVV2	333368	529648	9.66%	1.027%
20	10.697	1604	1609	1617	rVV	1413052	2291060	41.80%	4.441%
21	10.764	1617	1620	1623	rVV	131932	167424	3.05%	0.325%
22	10.831	1623	1631	1635	rVB	552773	768690	14.03%	1.490%
23	10.879	1635	1639	1640	rBV	88637	103701	1.89%	0.201%
24	10.910	1640	1644	1647	rVV	380497	573083	10.46%	1.111%
25	10.946	1647	1650	1655	rVB	180085	235431	4.30%	0.456%
26	11.007	1655	1660	1664	rVB3	80135	149543	2.73%	0.290%
27	11.081	1664	1672	1675	rBV2	344932	607422	11.08%	1.177%
28	11.135	1675	1681	1683	rVV2	1968826	2886447	52.67%	5.595%
29	11.154	1683	1684	1691	rVB	788500	844580	15.41%	1.637%
30	11.239	1691	1698	1701	rBV	765226	1042363	19.02%	2.020%
31	11.270	1701	1703	1707	rVV2	164365	193107	3.52%	0.374%
32	11.300	1707	1708	1713	rVB3	62908	62669	1.14%	0.121%
33	11.355	1713	1717	1720	rBV	110623	155571	2.84%	0.302%
34	11.428	1725	1729	1735	rVV	368145	651610	11.89%	1.263%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX122419\
Data File : VX014239.D
Acq On : 24 Dec 2019 12:55
Operator : JC/SP
Sample : K6401-01 40X
Misc : 4.72g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0B37

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\82X121319W.M
Title : SW846 8260

35	11.526	1735	1745	1751	rVB2	4165848	5480523	100.00%	10.622%
36	11.684	1763	1771	1775	rBV4	260552	571335	10.42%	1.107%
37	11.733	1775	1779	1781	rVV	285724	369162	6.74%	0.716%
38	11.763	1781	1784	1787	rVV	688320	807347	14.73%	1.565%
39	11.800	1787	1790	1800	rVB2	781718	1363512	24.88%	2.643%
40	11.885	1800	1804	1807	rBV	230139	326705	5.96%	0.633%
41	11.916	1807	1809	1810	rVV	132980	133970	2.44%	0.260%
42	11.940	1810	1813	1818	rVV	260847	374887	6.84%	0.727%
43	11.995	1818	1822	1824	rVV	334593	424229	7.74%	0.822%
44	12.019	1824	1826	1829	rVV	233905	285185	5.20%	0.553%
45	12.074	1829	1835	1840	rVV2	1780244	2875180	52.46%	5.573%
46	12.123	1840	1843	1845	rVV	466294	629093	11.48%	1.219%
47	12.147	1845	1847	1852	rVV	583582	718501	13.11%	1.393%
48	12.196	1852	1855	1856	rVV3	71575	89086	1.63%	0.173%
49	12.221	1856	1859	1867	rVB	480121	620254	11.32%	1.202%
50	12.318	1867	1875	1879	rBV2	259438	454919	8.30%	0.882%
51	12.367	1879	1883	1889	rVB3	364016	606703	11.07%	1.176%
52	12.471	1895	1900	1904	rBV	2080631	2340267	42.70%	4.536%
53	12.513	1904	1907	1914	rVB2	186888	296227	5.41%	0.574%
54	12.586	1914	1919	1920	rBV	130988	174925	3.19%	0.339%
55	12.605	1920	1922	1925	rVV2	154071	212423	3.88%	0.412%
56	12.660	1929	1931	1934	rVV	80439	89445	1.63%	0.173%
57	12.769	1946	1949	1955	rVB4	106891	191188	3.49%	0.371%
58	12.849	1957	1962	1963	rBV3	51867	74242	1.35%	0.144%
59	12.946	1973	1978	1984	rBV5	100731	263951	4.82%	0.512%
60	13.019	1987	1990	1994	rVB2	117763	151832	2.77%	0.294%
61	13.092	1996	2002	2005	rBV3	54926	80060	1.46%	0.155%
62	13.196	2015	2019	2026	rVB3	27452	60634	1.11%	0.118%
63	13.318	2033	2039	2042	rBV	159387	221704	4.05%	0.430%
64	13.477	2061	2065	2072	rVB4	35597	69470	1.27%	0.135%

Sum of corrected areas: 51593811

LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX122419\
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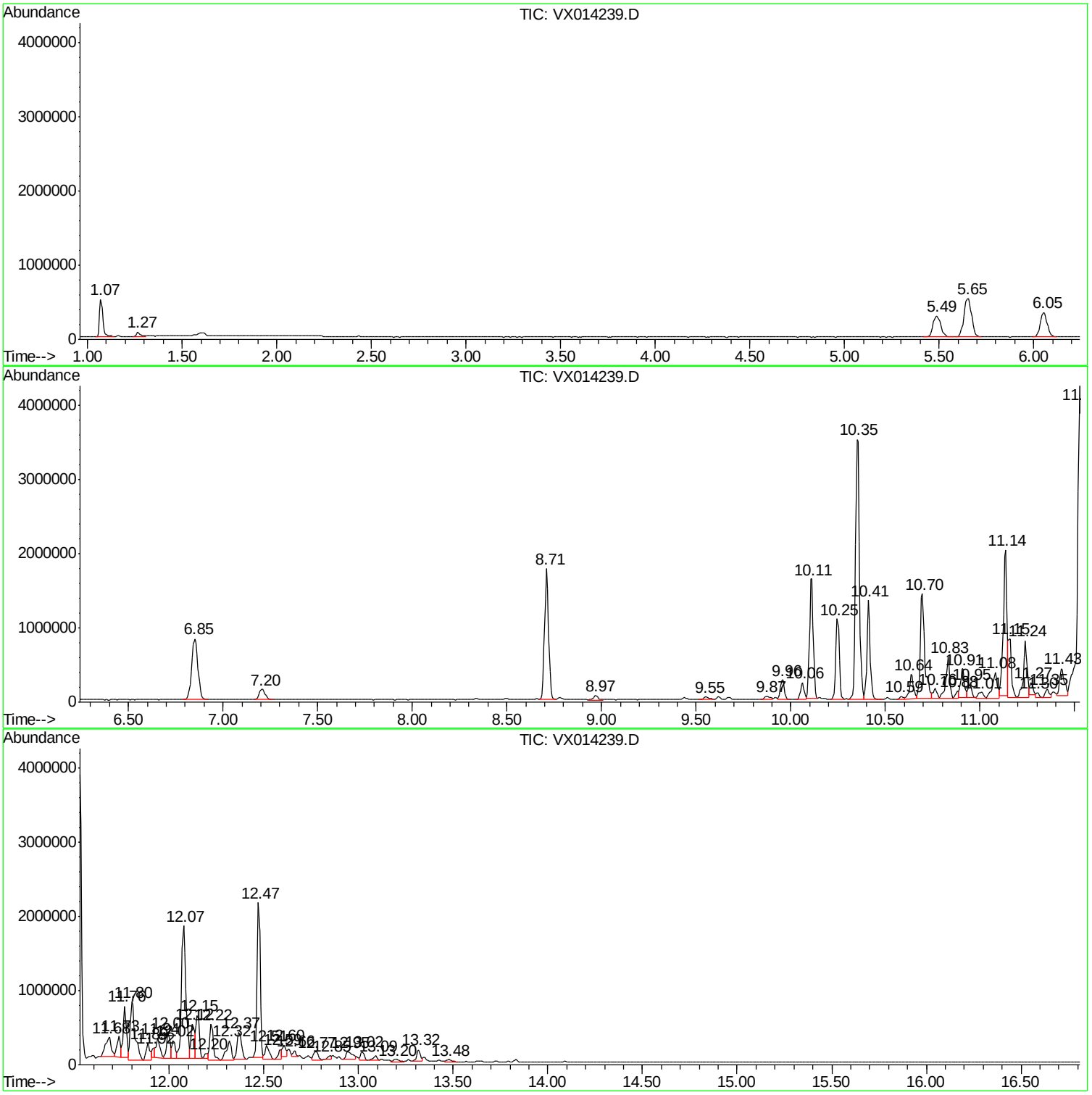
Acq On : 24 Dec 2019 12:55
Operator : JC/SP
Sample : K6401-01 40X
Misc : 4.72g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0B37

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX122419\
Data File : VX014239.D
Acq On : 24 Dec 2019 12:55
Operator : JC/SP
Sample : K6401-01 40X
Misc : 4.72g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0B37

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

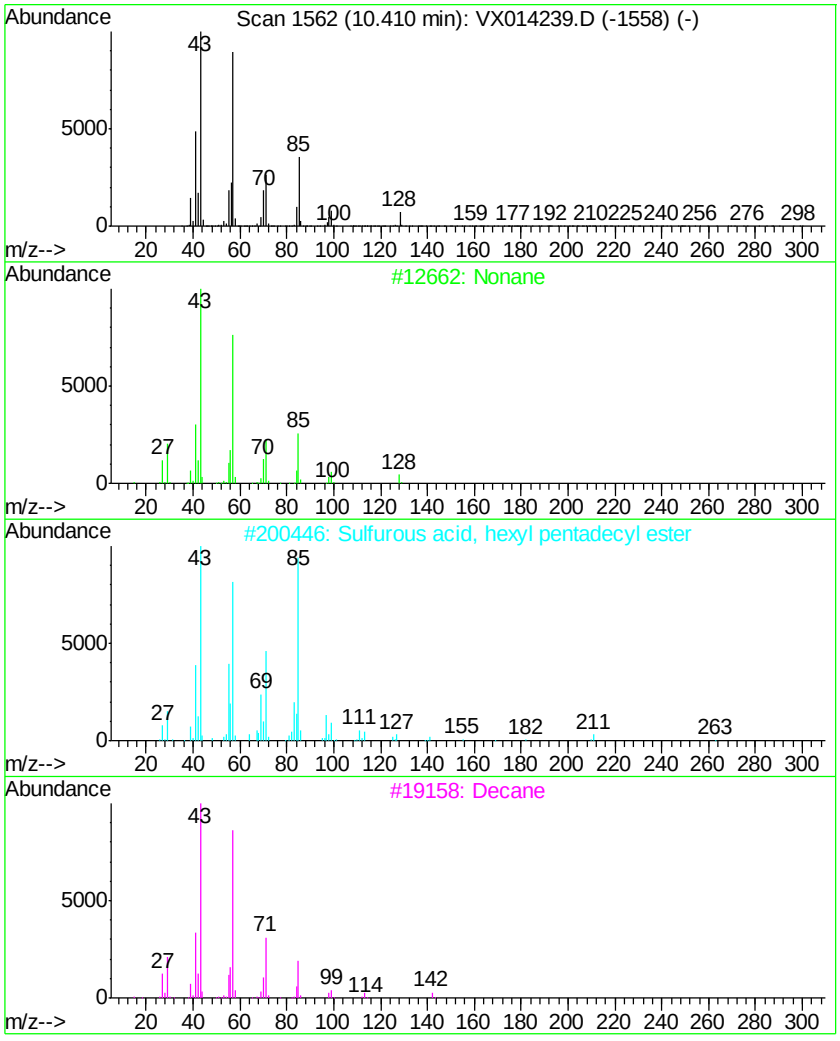
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

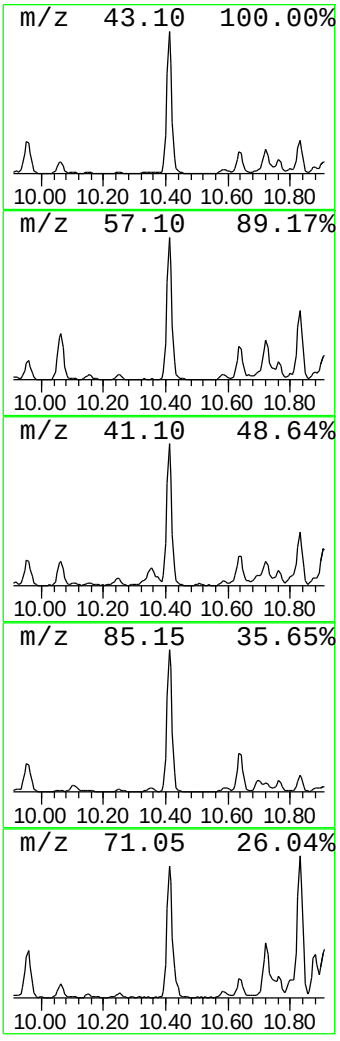
****

Peak Number 2 Nonane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	38.56 ug/l	1692090	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane	128	C9H20	000111-84-2	97
2	Sulfurous acid, hexyl pentadecyl...	376	C21H44O3S	1000309-13-7	72
3	Decane	142	C10H22	000124-18-5	64
4	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	53
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX122419\
Data File : VX014239.D
Acq On : 24 Dec 2019 12:55
Operator : JC/SP
Sample : K6401-01 40X
Misc : 4.72g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0B37

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

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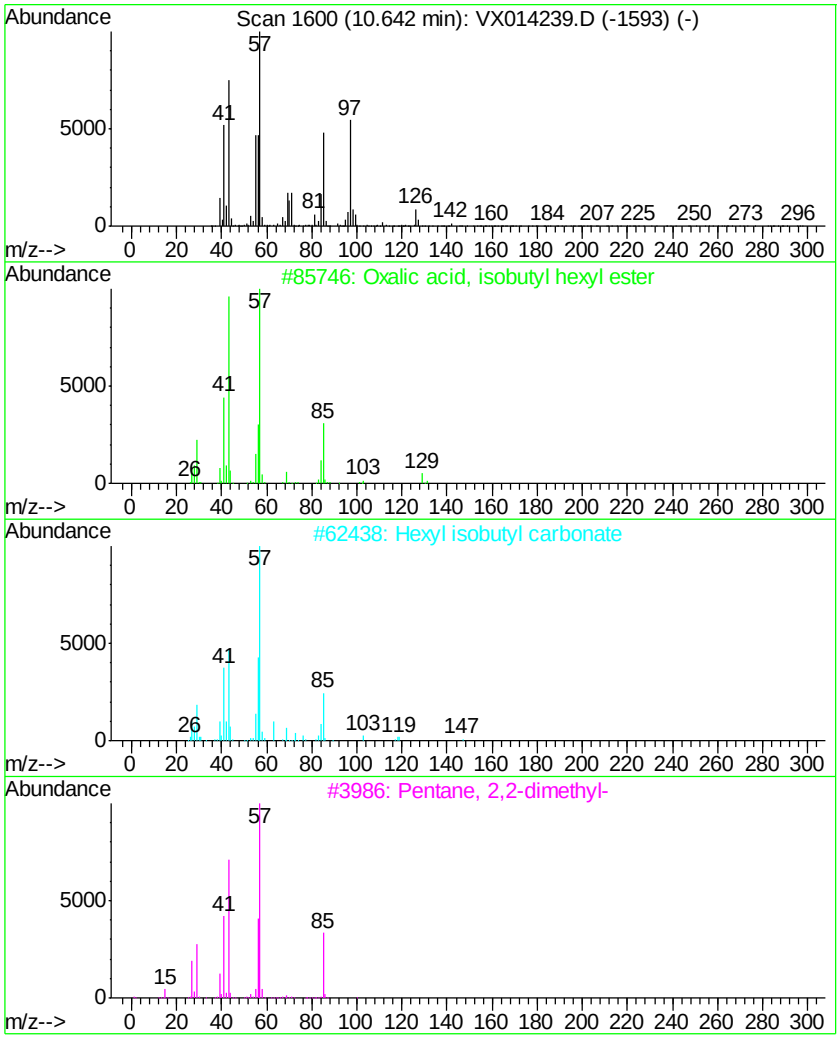
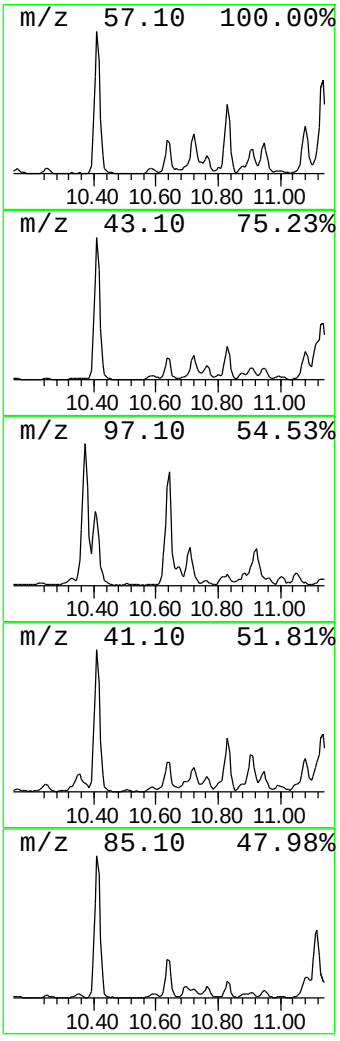
Peak Number 3 unknown10.64 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	12.07 ug/l	529648	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexyl ester	230	C12H22O4	1000309-37-1	47
2	Hexyl isobutyl carbonate	202	C11H22O3	959067-98-2	47
3	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	43
4	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	43
5	Heptane, 2,4,6-trimethyl-	142	C10H22	002613-61-8	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX122419\
Data File : VX014239.D
Acq On : 24 Dec 2019 12:55
Operator : JC/SP
Sample : K6401-01 40X
Misc : 4.72g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0B37

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

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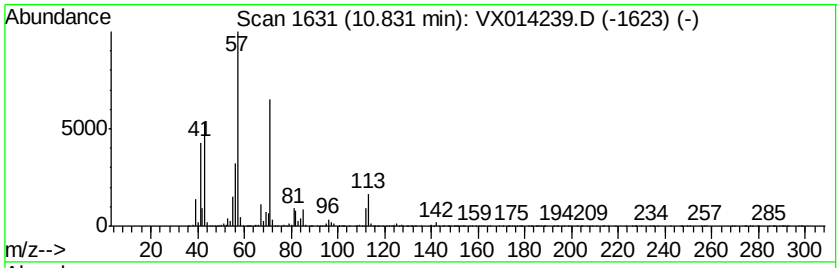
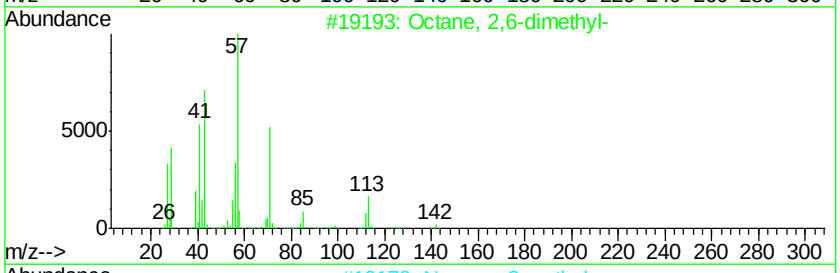
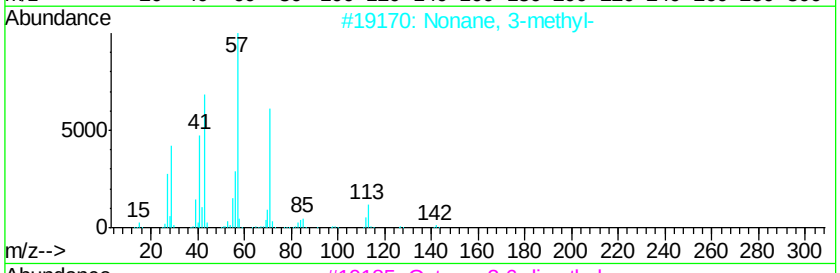
Peak Number 4 Octane, 2,6-dimethyl- Concentration Rank 5

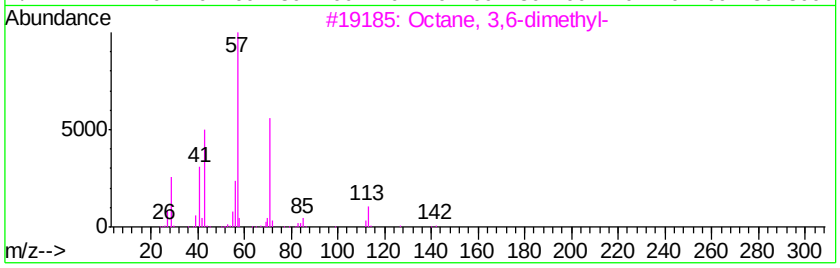
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	17.52 ug/l	768690	Chlorobenzene-d5	10.11

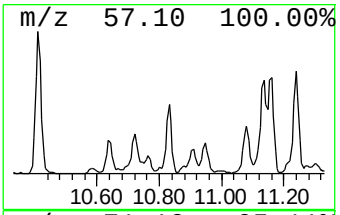
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	87
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	87
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	87
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	53
5	Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	50

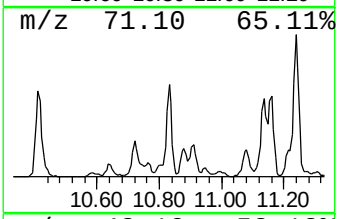


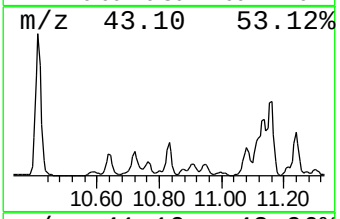


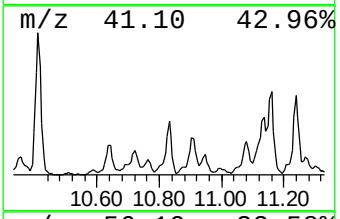


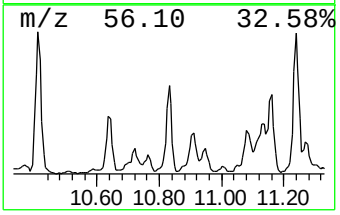












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Instrument : MSVOA_X
ClientSampleId : C0B37

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

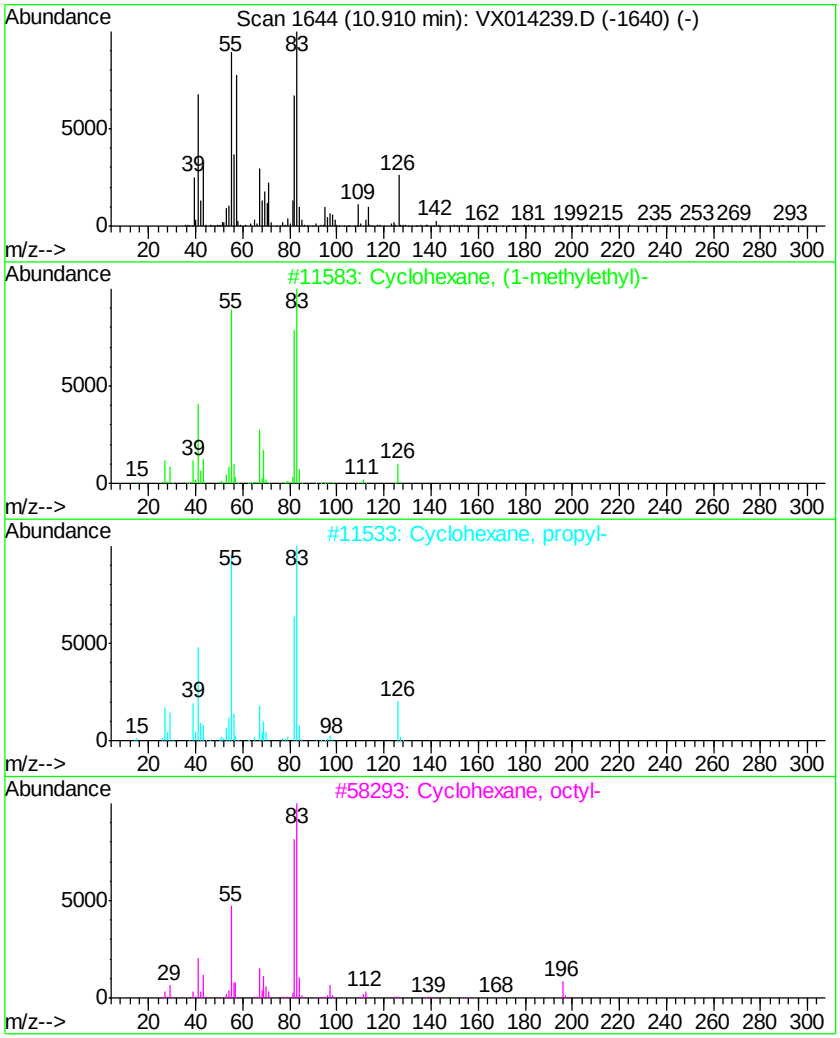
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

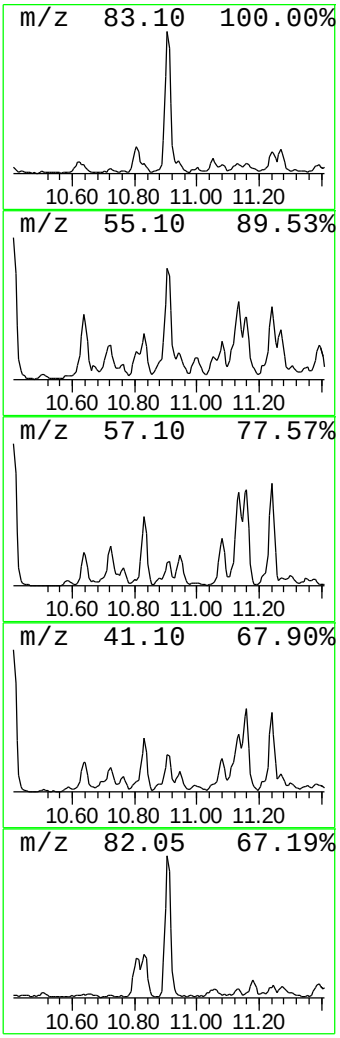
****

Peak Number 5 Cyclohexane, (1-methylethyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	13.06 ug/l	573083	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	70
2	Cyclohexane, propyl-	126	C9H18	001678-92-8	58
3	Cyclohexane, octyl-	196	C14H28	001795-15-9	50
4	Cyclohexane, butyl-	140	C10H20	001678-93-9	47
5	Cyclohexane, ethyl-	112	C8H16	001678-91-7	47





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ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0B37

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

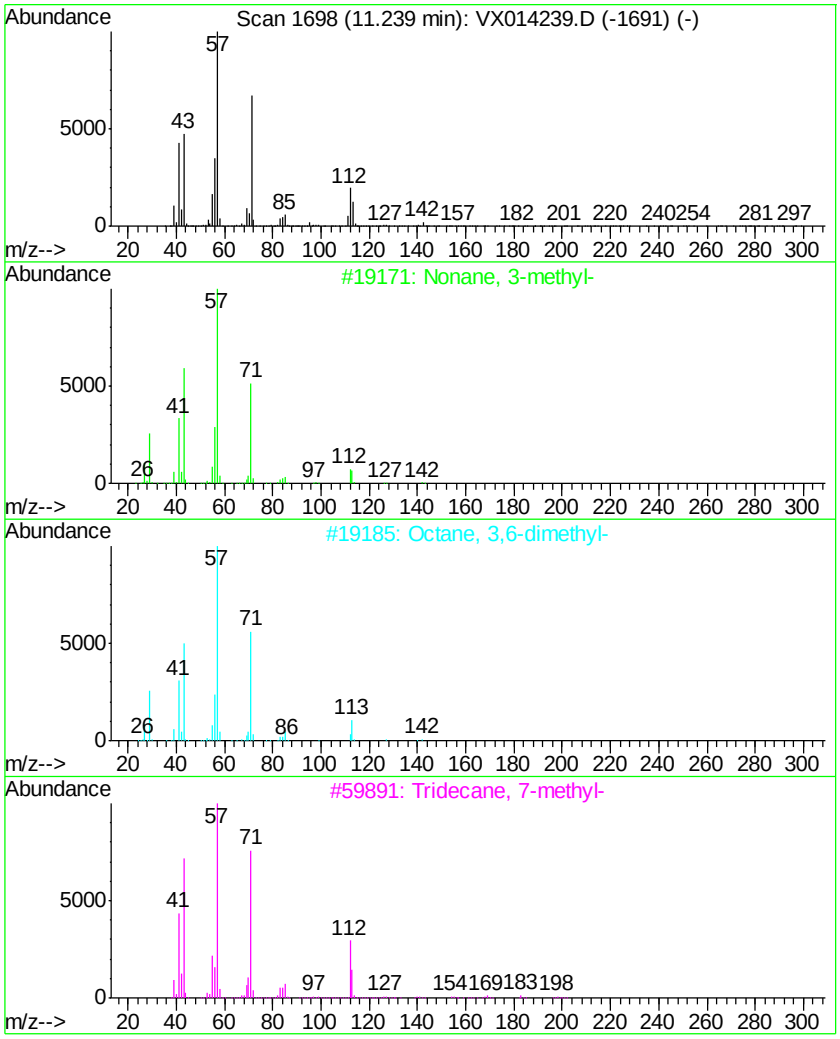
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

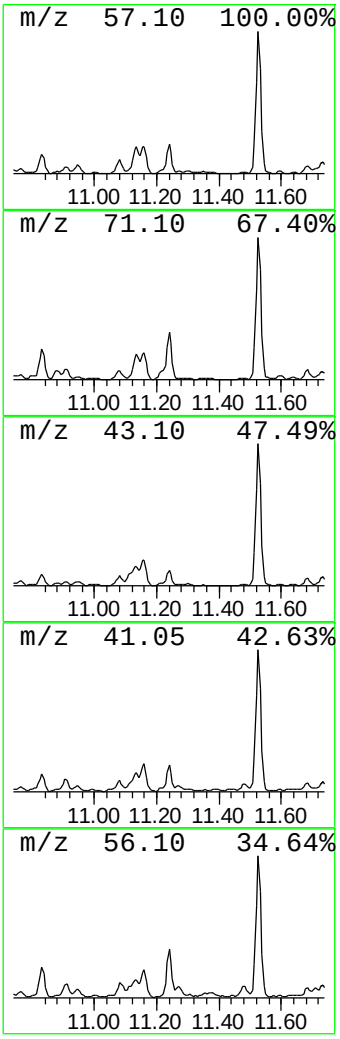
****

Peak Number 6 Nonane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	18.13 ug/l	1042360	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-	142	C10H22	005911-04-6	91
2	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	81
3	Tridecane, 7-methyl-	198	C14H30	026730-14-3	72
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX122419\
Data File : VX014239.D
Acq On : 24 Dec 2019 12:55
Operator : JC/SP
Sample : K6401-01 40X
Misc : 4.72g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0B37

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

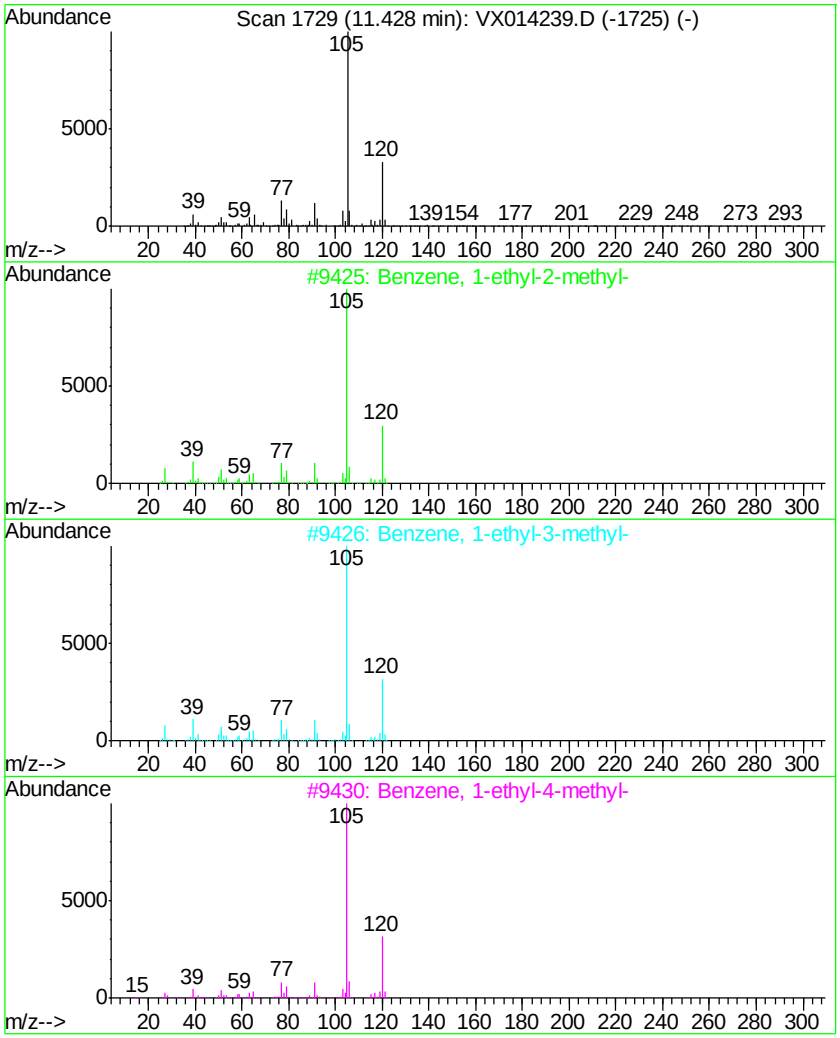
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

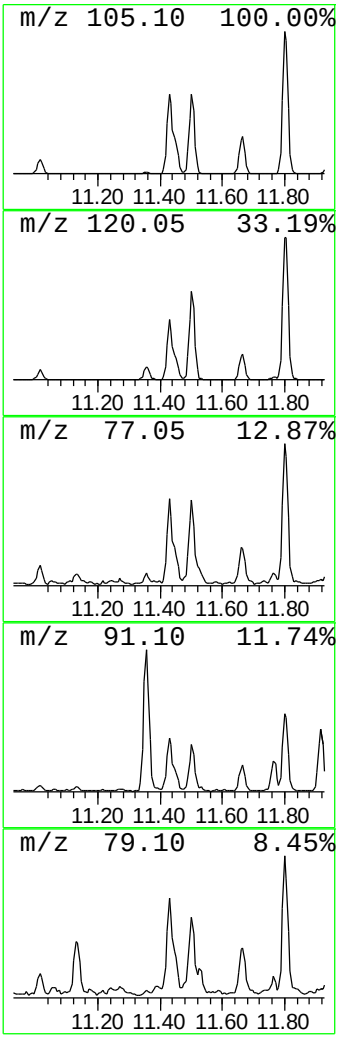
****

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	11.33 ug/l	651610	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX122419\
Data File : VX014239.D
Acq On : 24 Dec 2019 12:55
Operator : JC/SP
Sample : K6401-01 40X
Misc : 4.72g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0B37

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

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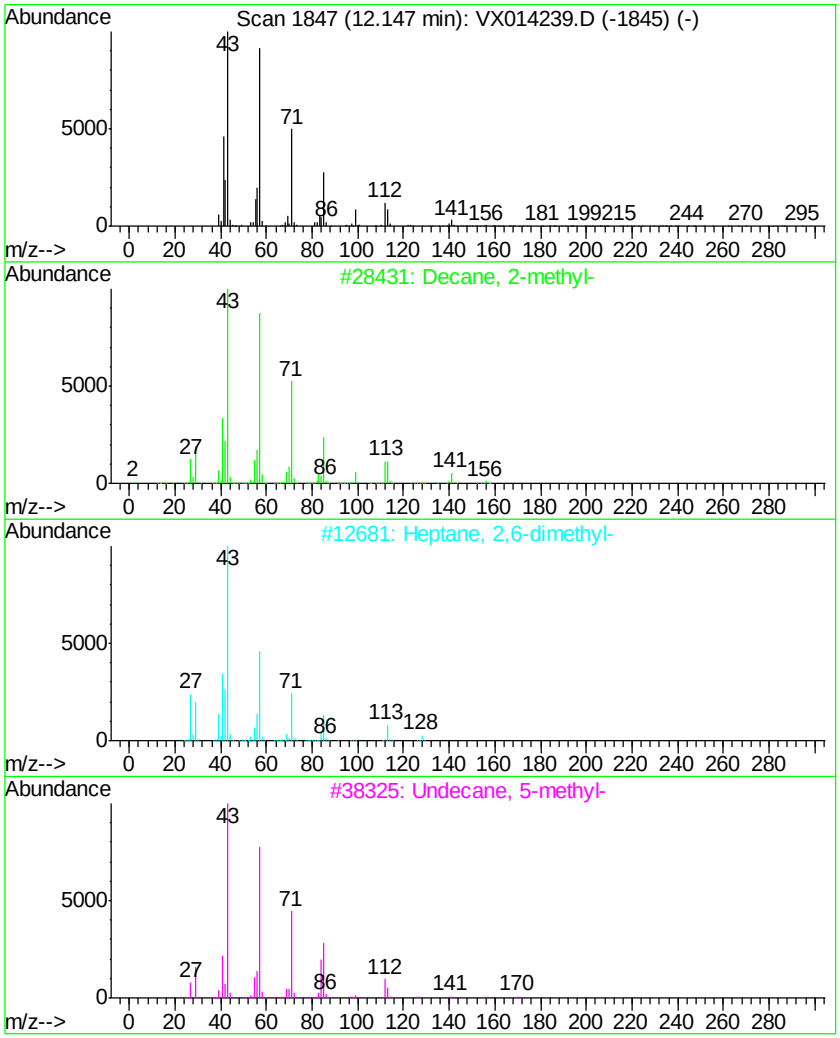
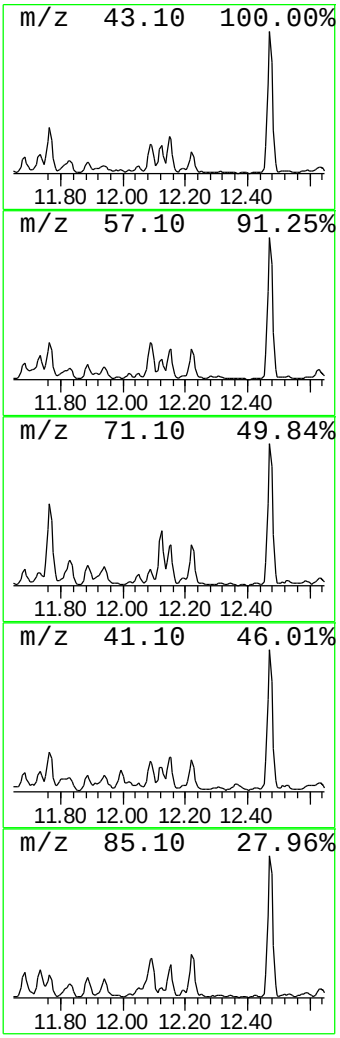
Peak Number 8 Decane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	12.49 ug/l	718501	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2-methyl-	156	C11H24	006975-98-0	94
2	Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	87
3	Undecane, 5-methyl-	170	C12H26	001632-70-8	64
4	Octane, 2-methyl-	128	C9H20	003221-61-2	59
5	Dodecane, 3-methyl-	184	C13H28	017312-57-1	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX122419\
Data File : VX014239.D
Acq On : 24 Dec 2019 12:55
Operator : JC/SP
Sample : K6401-01 40X
Misc : 4.72g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0B37

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

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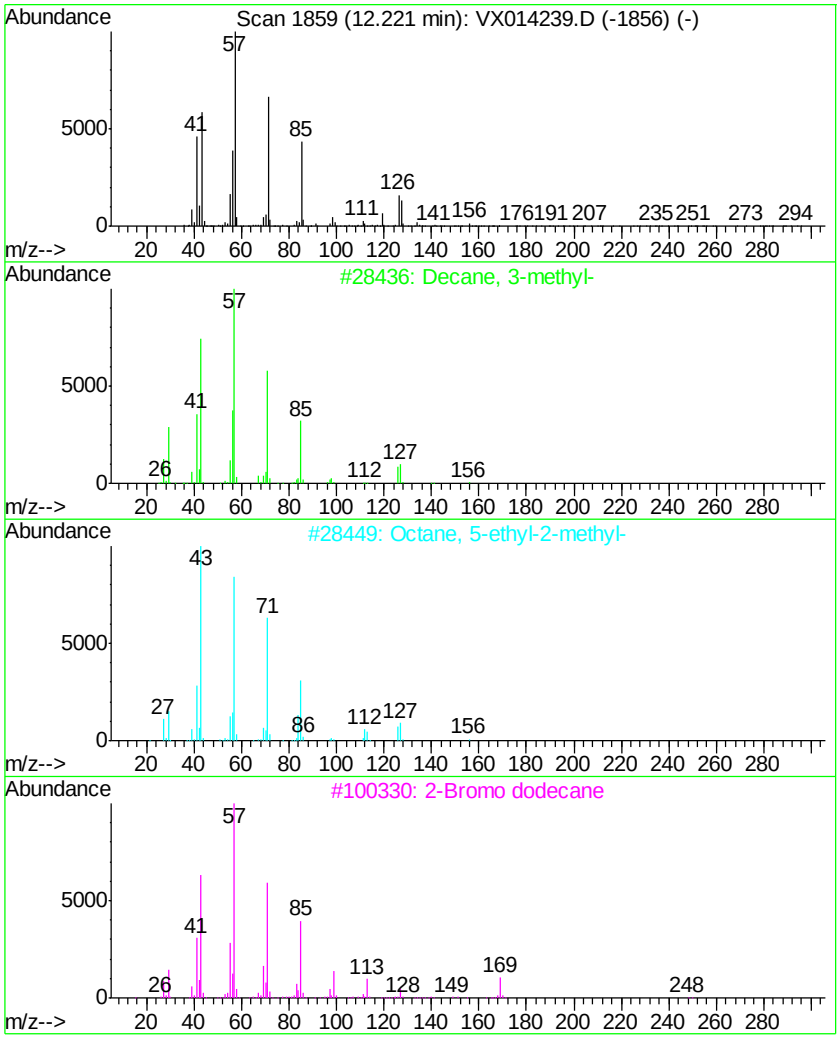
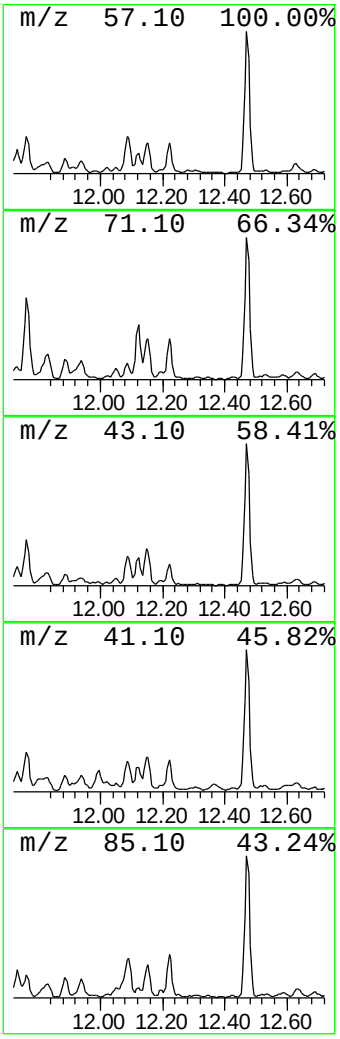
Peak Number 9 Decane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.22	10.79 ug/l	620254	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3-methyl-	156	C11H24	013151-34-3	91
2	Octane, 5-ethyl-2-methyl-	156	C11H24	062016-18-6	64
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	58
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	52
5	Oxalic acid, isobutyl hexyl ester	230	C12H22O4	1000309-37-1	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX122419\
Data File : VX014239.D
Acq On : 24 Dec 2019 12:55
Operator : JC/SP
Sample : K6401-01 40X
Misc : 4.72g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0B37

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

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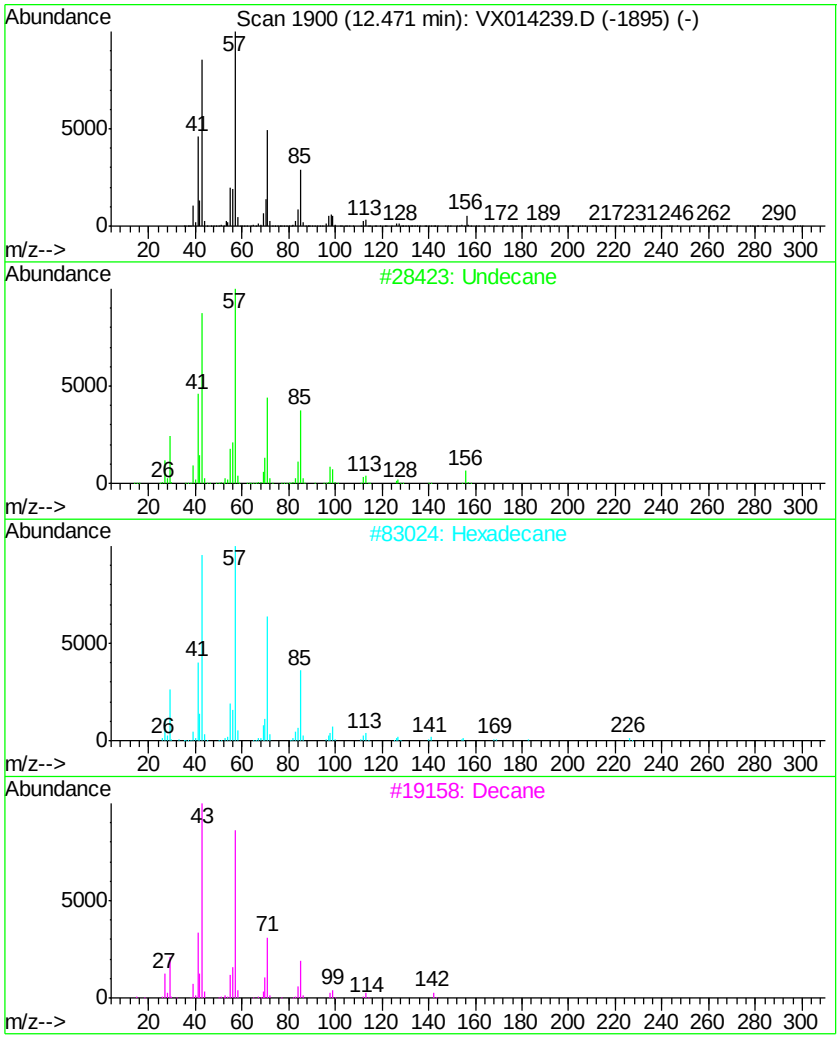
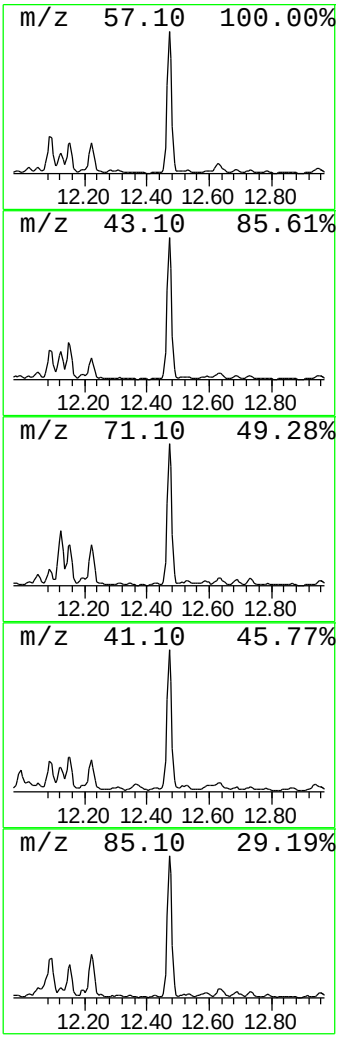
Peak Number 10 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	40.70 ug/l	2340270	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	94
2	Hexadecane	226	C16H34	000544-76-3	86
3	Decane	142	C10H22	000124-18-5	86
4	Tridecane	184	C13H28	000629-50-5	80
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX122419\
Data File : VX014239.D
Acq On : 24 Dec 2019 12:55
Operator : JC/SP
Sample : K6401-01 40X
Misc : 4.72g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0B37

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Nonane	10.41	38.6	ug/l	1692090	3	10.11	2194030	50.0
unknown10.64	10.64	12.1	ug/l	529648	3	10.11	2194030	50.0
Octane, 2,6-dimet...	10.83	17.5	ug/l	768690	3	10.11	2194030	50.0
Cyclohexane, (1-m...	10.91	13.1	ug/l	573083	3	10.11	2194030	50.0
Nonane, 3-methyl-	11.24	18.1	ug/l	1042360	4	12.07	2875180	50.0
Benzene, 1-ethyl-...	11.43	11.3	ug/l	651610	4	12.07	2875180	50.0
Decane, 2-methyl-	12.15	12.5	ug/l	718501	4	12.07	2875180	50.0
Decane, 3-methyl-	12.22	10.8	ug/l	620254	4	12.07	2875180	50.0
Undecane	12.47	40.7	ug/l	2340270	4	12.07	2875180	50.0