LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062718\
Data File : VX002945.D
Acq On : 27 Jun 2018 19:09
Operator : JC/MD
Sample : J3707-12 20X
Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WP021SB480-21-23-180622

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\82X062518W.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	1.075	76	80	91	rBV	532593	752727	20.24%	2.903%
2	4.604	646	659	677	rBV	376021	1061021	28.53%	4.091%
3	5.507	794	807	819	rBV	169994	489280	13.15%	1.887%
4	5.665	823	833	853	rVB	262039	751512	20.21%	2.898%
5	6.074	888	900	919	rBV	180599	481929	12.96%	1.858%
6	6.348	935	945	956	rVB2	14198	43681	1.17%	0.168%
7	6.702	996	1003	1013	rVB3	18305	46055	1.24%	0.178%
8	6.866	1019	1030	1050	rBV	367905	875011	23.53%	3.374%
9	7.464	1117	1128	1137	rBV2	28638	66350	1.78%	0.256%
10	8.720	1328	1334	1343	rVB	909564	1378920	37.07%	5.317%
11	8.976	1371	1376	1381	rBV	28164	39922	1.07%	0.154%
12	9.963	1534	1538	1544	rVB	61361	86177	2.32%	0.332%
13	10.067	1549	1555	1558	rBV	48456	67456	1.81%	0.260%
14	10.116	1558	1563	1569	rVV	798325	1034539	27.81%	3.989%
15	10.414	1608	1612	1623	rVB	384692	508765	13.68%	1.962%
16	10.646	1644	1650	1657	rBV3	86097	143206	3.85%	0.552%
17	10.725	1657	1663	1667	rVV3	68650	110890	2.98%	0.428%
18	10.768	1667	1670	1674	rVB	31795	40324	1.08%	0.155%
19	10.835	1674	1681	1686	rVB2	157133	244693	6.58%	0.944%
20	10.884	1686	1689	1690	rBV	40281	42905	1.15%	0.165%
21	10.914	1690	1694	1698	rVV2	152546	217400	5.85%	0.838%
22	10.951	1698	1700	1705	rVB2	63843	75351	2.03%	0.291%
23	11.018	1705	1711	1714	rVB2	26632	46536	1.25%	0.179%
24	11.085	1714	1722	1725	rBV2	144899	254449	6.84%	0.981%
25	11.140	1725	1731	1741	rVB2	1122582	1948678	52.39%	7.514%
26	11.219	1741	1744	1745	rBV	52077	49629	1.33%	0.191%
27	11.244	1745	1748	1752	rVV	328026	415551	11.17%	1.602%
28	11.280	1752	1754	1757	rVV4	55220	57982	1.56%	0.224%
29	11.359	1763	1767	1770	rBV	36505	50729	1.36%	0.196%
30	11.396	1770	1773	1777	rVB4	36463	48418	1.30%	0.187%
31	11.451	1777	1782	1785	rBV3	67349	105759	2.84%	0.408%
32	11.487	1785	1788	1791	rVV	121174	146879	3.95%	0.566%
33	11.536	1791	1796	1801	rVB	3116535	3719409	100.00%	14.342%
34	11.689	1814	1821	1825	rBV5	159634	269424	7.24%	1.039%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062718\
Data File : VX002945.D
Acq On : 27 Jun 2018 19:09
Operator : JC/MD
Sample : J3707-12 20X
Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WP021SB480-21-23-180622

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\82X062518W.M
Title : SW846 8260

35	11.737	1826	1829	1832	rVV	192773	277338	7.46%	1.069%
36	11.774	1832	1835	1838	rVV	536865	640447	17.22%	2.470%
37	11.835	1838	1845	1851	rVB5	166429	443605	11.93%	1.711%
38	11.896	1851	1855	1857	rBV	167157	226097	6.08%	0.872%
39	11.926	1857	1860	1861	rVV	153496	194484	5.23%	0.750%
40	11.945	1861	1863	1868	rVV2	197859	282864	7.61%	1.091%
41	11.999	1868	1872	1875	rVV	244176	334024	8.98%	1.288%
42	12.079	1879	1885	1891	rVV2	1051949	1825445	49.08%	7.039%
43	12.128	1891	1893	1895	rVV	262569	280001	7.53%	1.080%
44	12.158	1895	1898	1902	rVV	396960	461304	12.40%	1.779%
45	12.201	1902	1905	1906	rVV2	45803	50732	1.36%	0.196%
46	12.231	1906	1910	1918	rVB2	340726	453621	12.20%	1.749%
47	12.304	1918	1922	1928	rBV3	85118	140263	3.77%	0.541%
48	12.371	1928	1933	1940	rBV3	264259	502697	13.52%	1.938%
49	12.481	1946	1951	1955	rBV	1870379	2086749	56.10%	8.046%
50	12.524	1955	1958	1964	rVB2	107491	168837	4.54%	0.651%
51	12.591	1964	1969	1971	rBV	110799	150496	4.05%	0.580%
52	12.640	1974	1977	1979	rVV2	70465	98438	2.65%	0.380%
53	12.670	1979	1982	1985	rVB	171478	184263	4.95%	0.711%
54	12.780	1995	2000	2005	rVB3	145736	262368	7.05%	1.012%
55	12.853	2005	2012	2014	rVV2	71122	133184	3.58%	0.514%
56	12.902	2018	2020	2023	rVV2	57037	61322	1.65%	0.236%
57	12.951	2023	2028	2031	rVV4	92072	177998	4.79%	0.686%
58	12.981	2031	2033	2037	rVV2	113387	151726	4.08%	0.585%
59	13.024	2037	2040	2046	rVV3	132797	211033	5.67%	0.814%
60	13.097	2046	2052	2055	rVV3	51354	100505	2.70%	0.388%
61	13.219	2066	2072	2076	rVB3	31086	47058	1.27%	0.181%
62	13.322	2083	2089	2092	rBV2	150000	184253	4.95%	0.710%
63	13.353	2092	2094	2099	rVB4	37826	48414	1.30%	0.187%
64	13.487	2110	2116	2126	rVB7	35540	82589	2.22%	0.318%

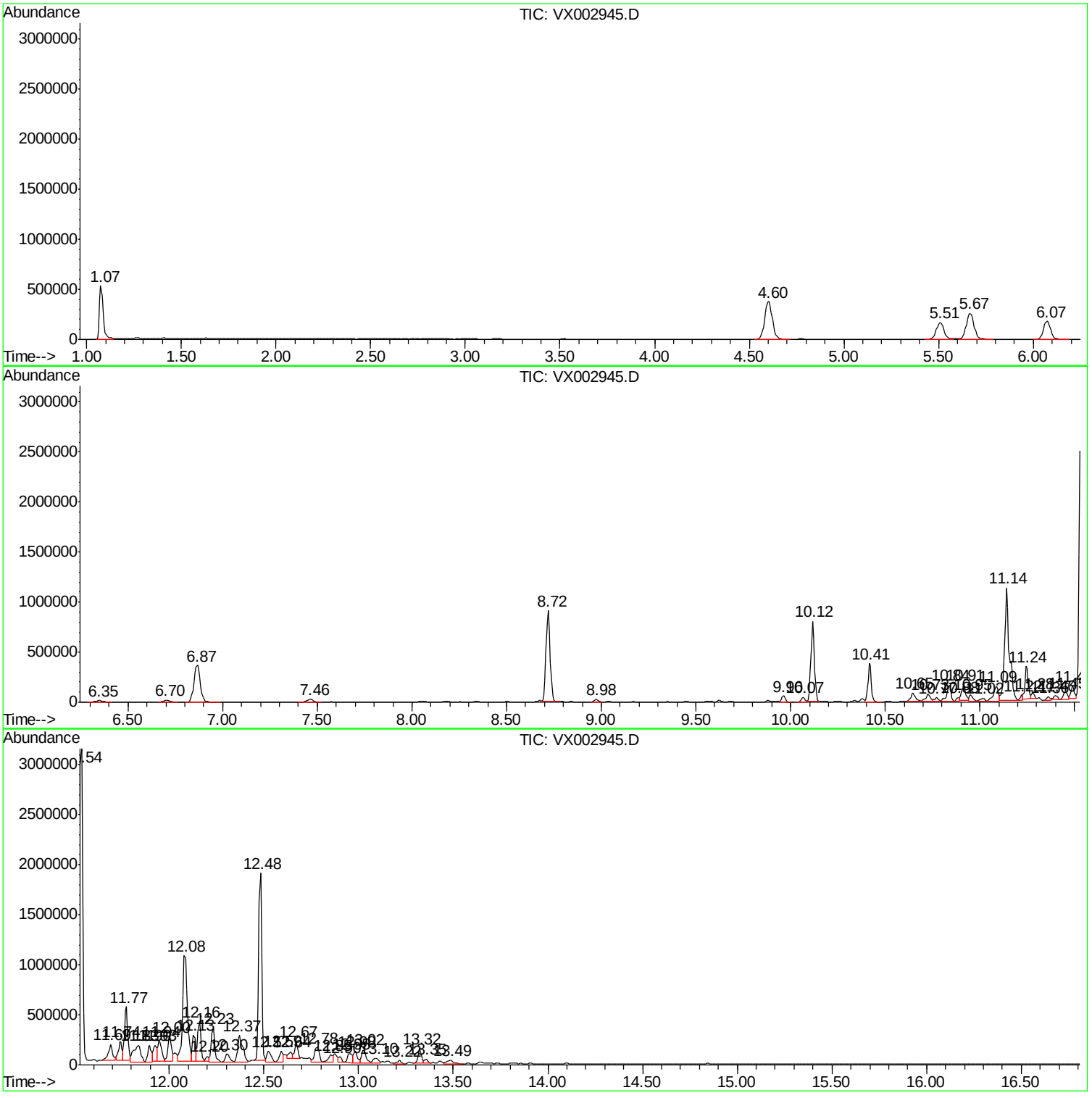
Sum of corrected areas: 25933712

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062718\
Data File : VX002945.D
Acq On : 27 Jun 2018 19:09
Operator : JC/MD
Sample : J3707-12 20X
Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WP021SB480-21-23-180622

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.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\VX062718\
Data File : VX002945.D
Acq On : 27 Jun 2018 19:09
Operator : JC/MD
Sample : J3707-12 20X
Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WP021SB480-21-23-180622

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

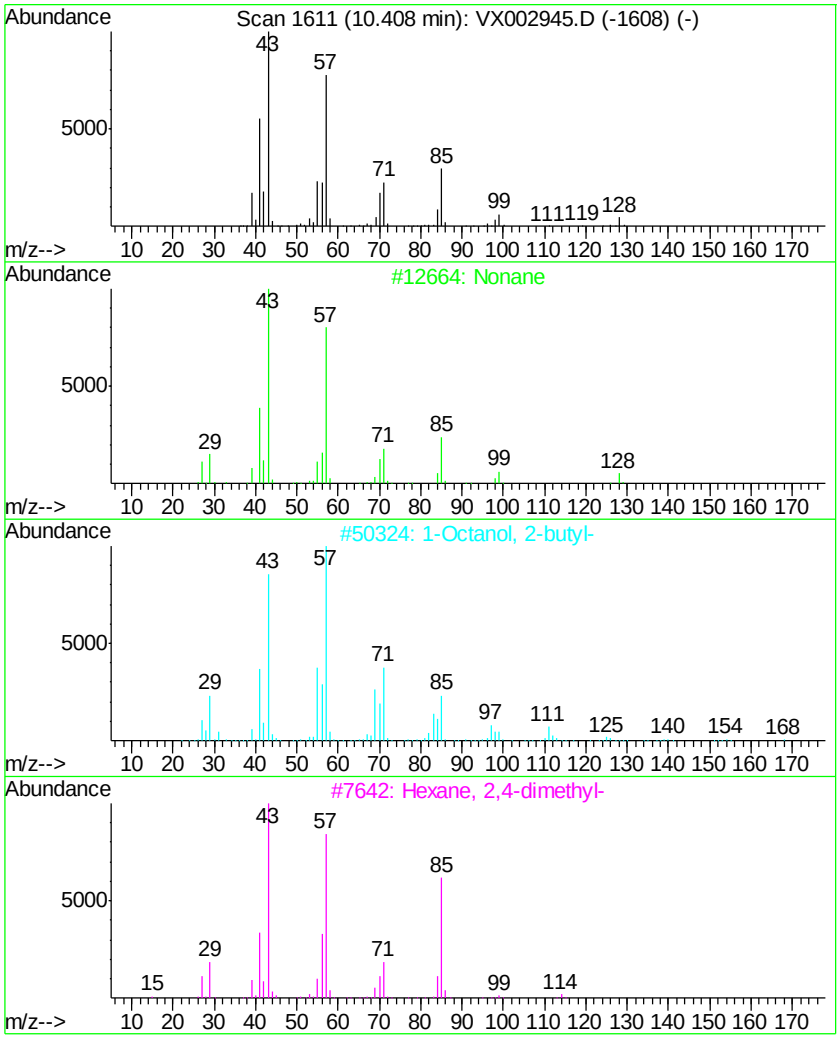
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

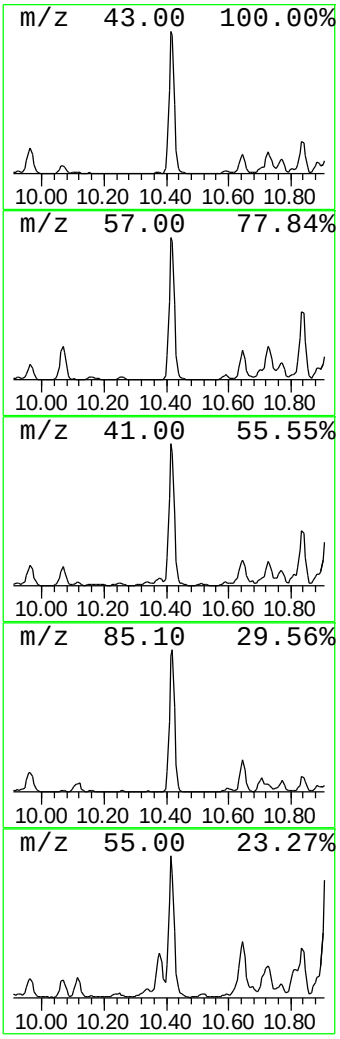
****

Peak Number 2 Nonane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	24.59 ug/l	508765	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane	128	C9H20	000111-84-2	91
2	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	72
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	59
4	Octane	114	C8H18	000111-65-9	59
5	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062718\
Data File : VX002945.D
Acq On : 27 Jun 2018 19:09
Operator : JC/MD
Sample : J3707-12 20X
Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WP021SB480-21-23-180622

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

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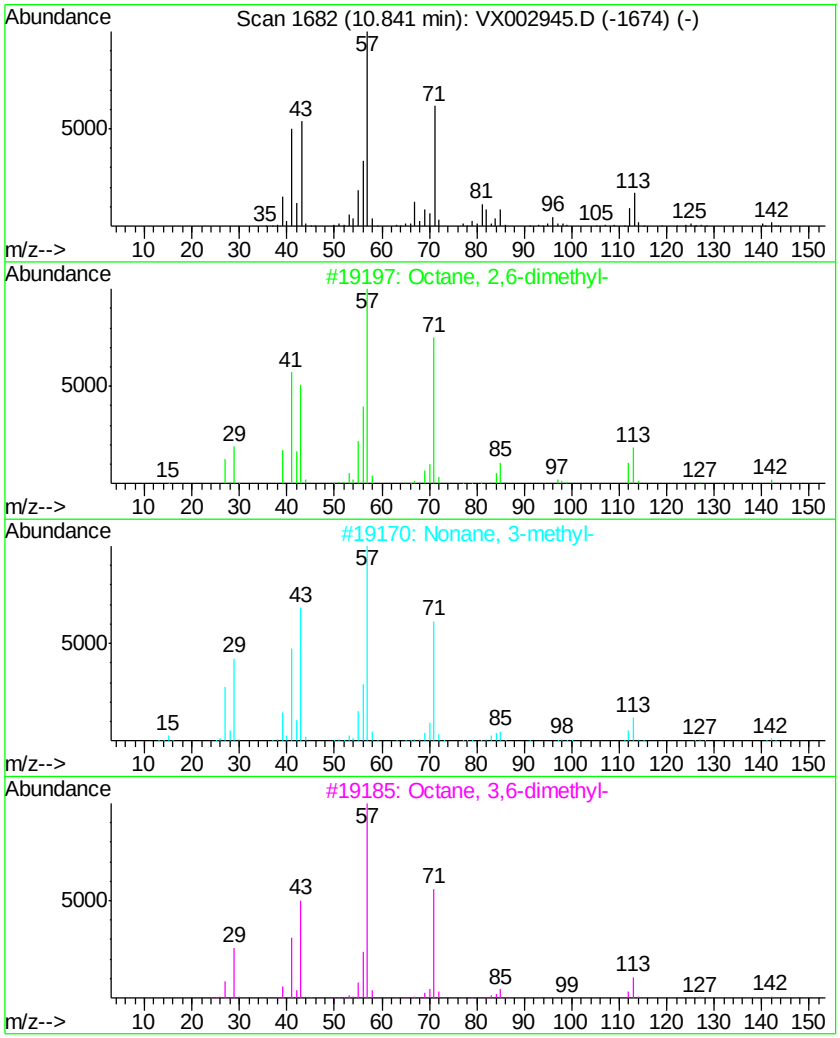
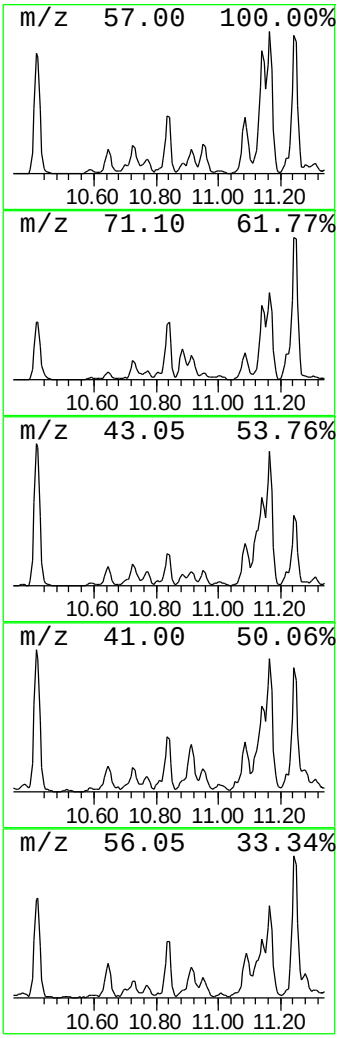
Peak Number 3 Octane, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	11.83 ug/l	244693	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
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 iso...	278	C14H30O3S	1000309-19-0	53
5	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062718\
Data File : VX002945.D
Acq On : 27 Jun 2018 19:09
Operator : JC/MD
Sample : J3707-12 20X
Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WP021SB480-21-23-180622

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

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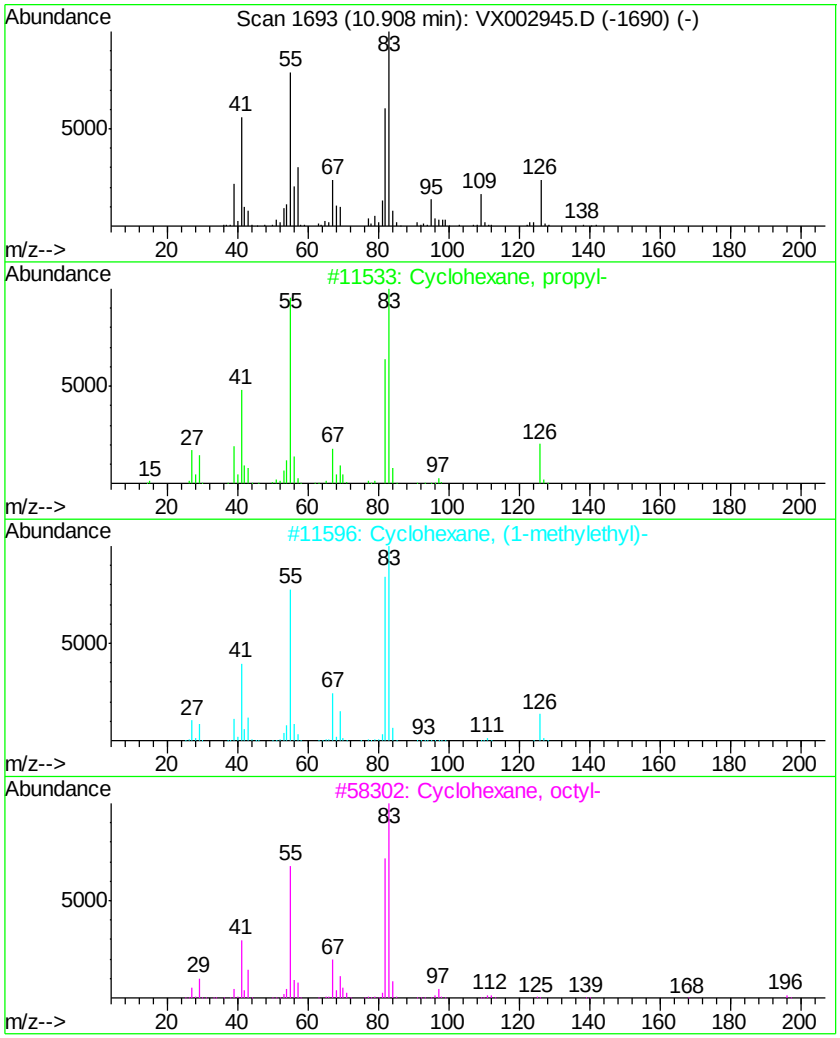
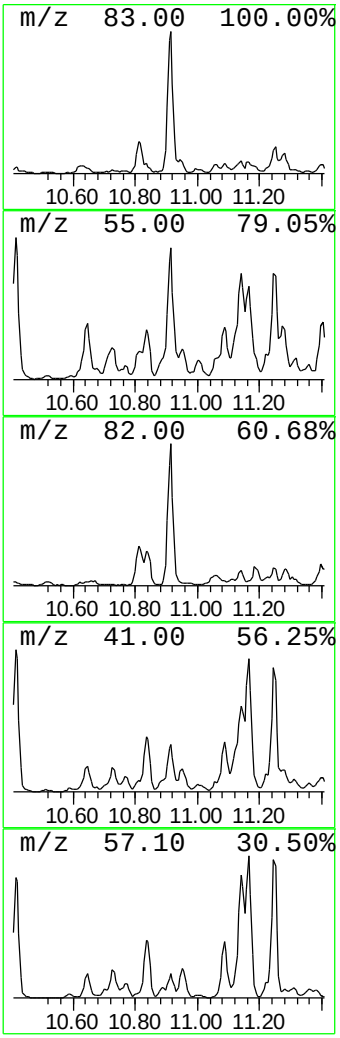
Peak Number 4 Cyclohexane, propyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	10.51 ug/l	217400	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	76
2	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	68
3	Cyclohexane, octyl-	196	C14H28	001795-15-9	53
4	Cyclohexane, butyl-	140	C10H20	001678-93-9	50
5	Trichloroacetic acid, 6-chlorohe...	280	C8H12Cl4O2	1000330-89-2	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062718\
Data File : VX002945.D
Acq On : 27 Jun 2018 19:09
Operator : JC/MD
Sample : J3707-12 20X
Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WP021SB480-21-23-180622

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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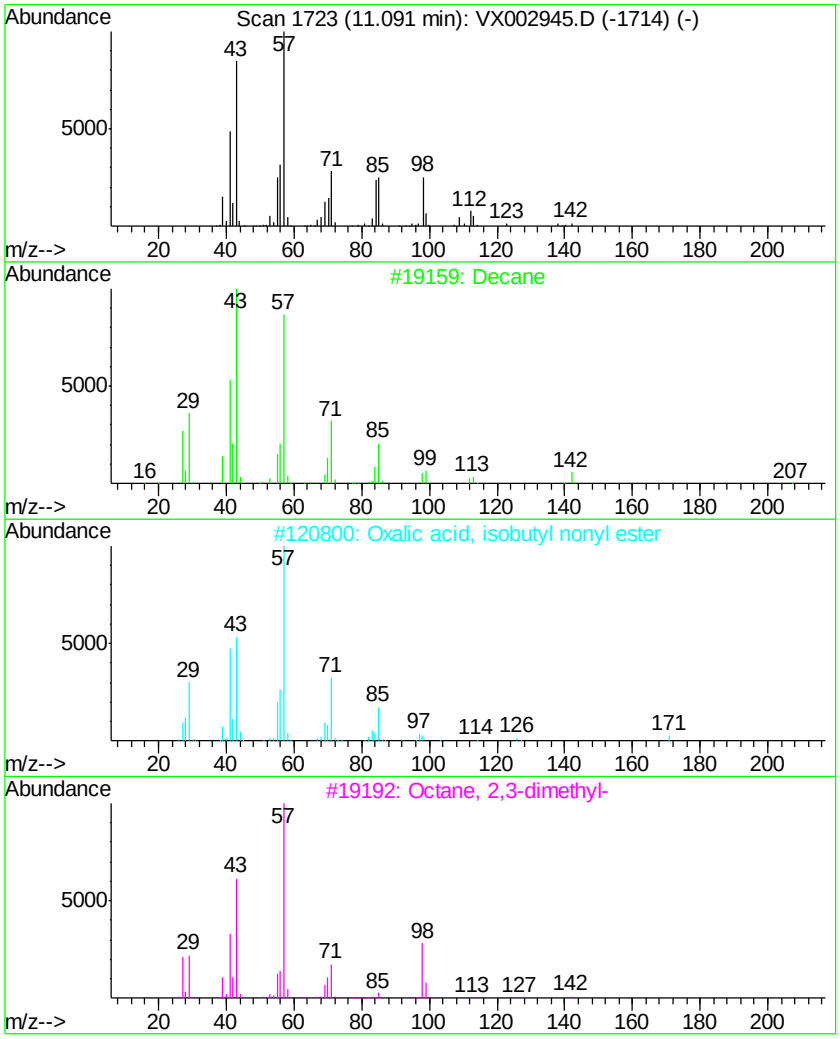
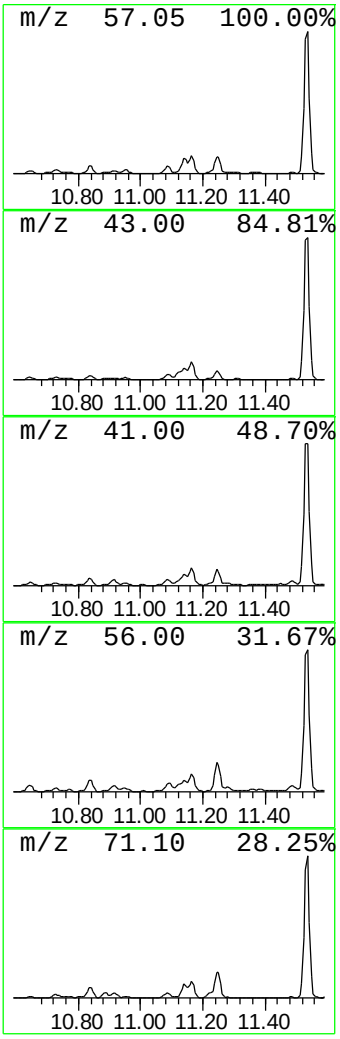
Peak Number 5 Decane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.09	12.30 ug/l	254449	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	50
2	Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1000309-37-4	50
3	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	47
4	Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	47
5	1-Azacyclononan-2-one	141	C8H15NO	000935-30-8	43





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062718\
Data File : VX002945.D
Acq On : 27 Jun 2018 19:09
Operator : JC/MD
Sample : J3707-12 20X
Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WP021SB480-21-23-180622

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

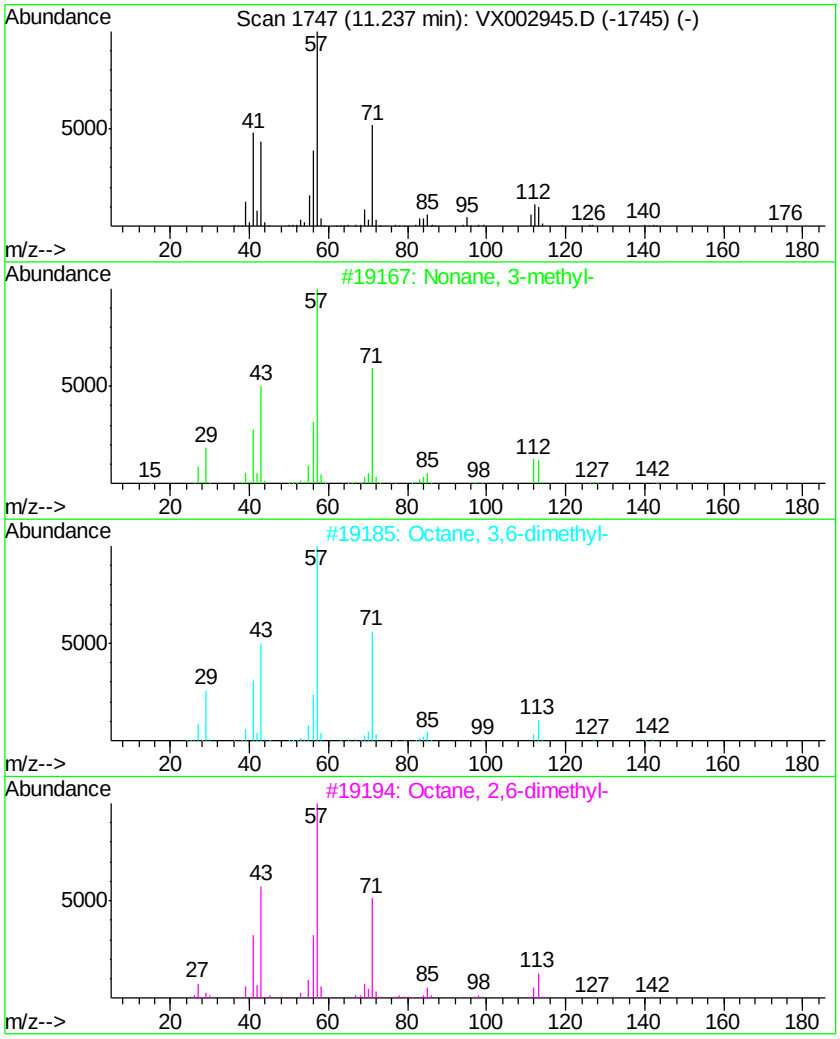
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

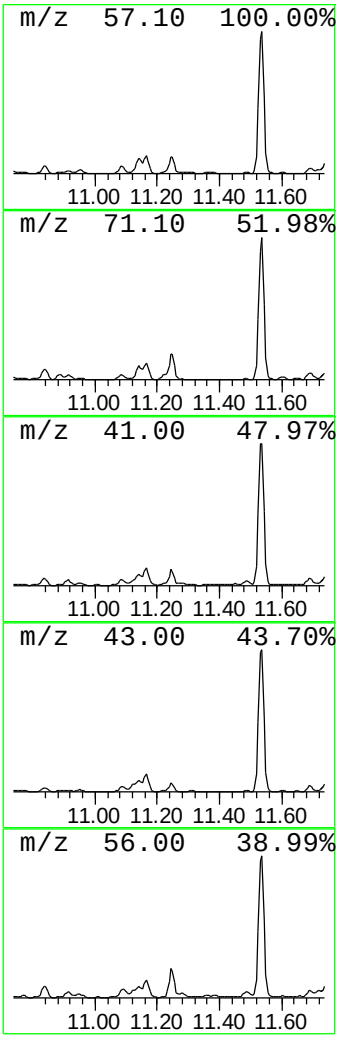
****

Peak Number 6 Nonane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	11.38 ug/l	415551	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-	142	C10H22	005911-04-6	94
2	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	74
3	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
4	Octane, 3-ethyl-	142	C10H22	005881-17-4	64
5	Tridecane, 7-methyl-	198	C14H30	026730-14-3	53





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062718\
Data File : VX002945.D
Acq On : 27 Jun 2018 19:09
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Sample : J3707-12 20X
Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WP021SB480-21-23-180622

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

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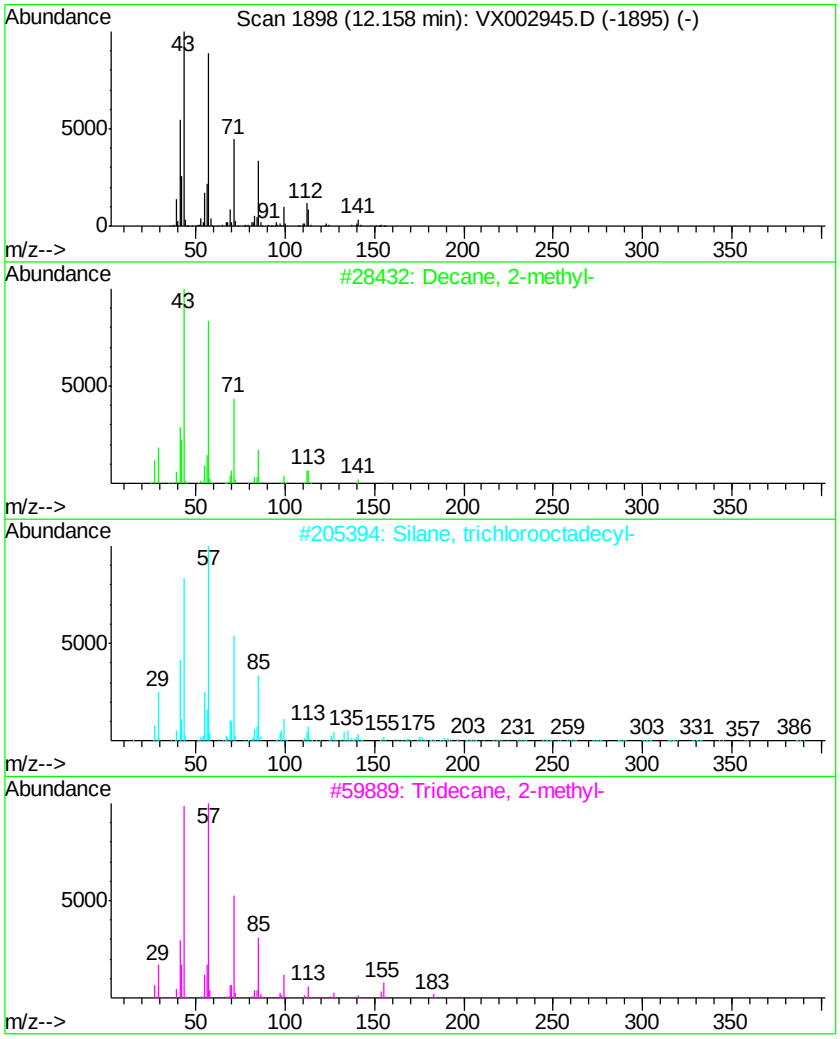
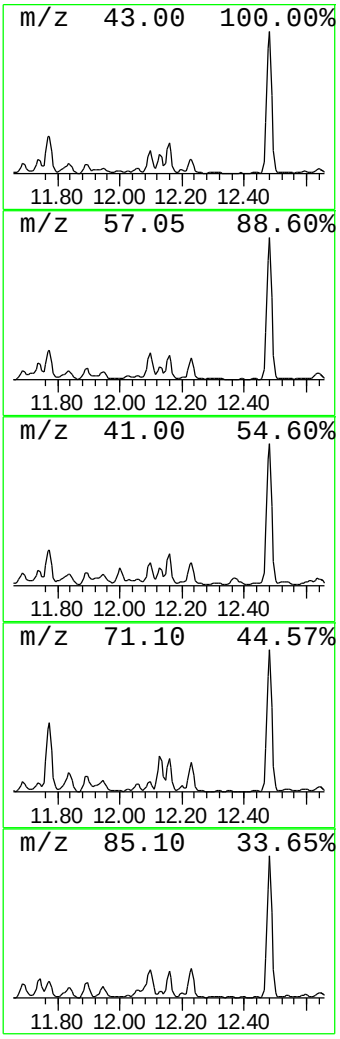
Peak Number 8 Decane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	12.64 ug/l	461304	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2-methyl-	156	C11H24	006975-98-0	72
2	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	64
3	Tridecane, 2-methyl-	198	C14H30	001560-96-9	64
4	Hexadecane	226	C16H34	000544-76-3	59
5	Heptadecane	240	C17H36	000629-78-7	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062718\
Data File : VX002945.D
Acq On : 27 Jun 2018 19:09
Operator : JC/MD
Sample : J3707-12 20X
Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WP021SB480-21-23-180622

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

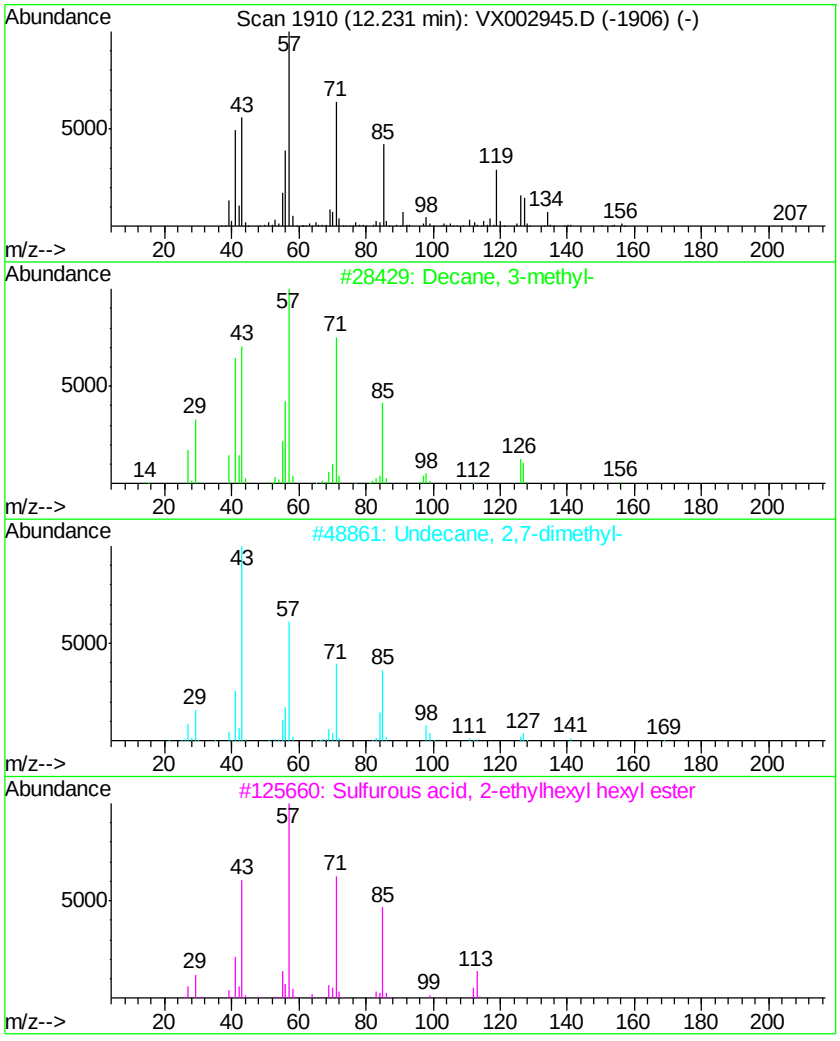
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

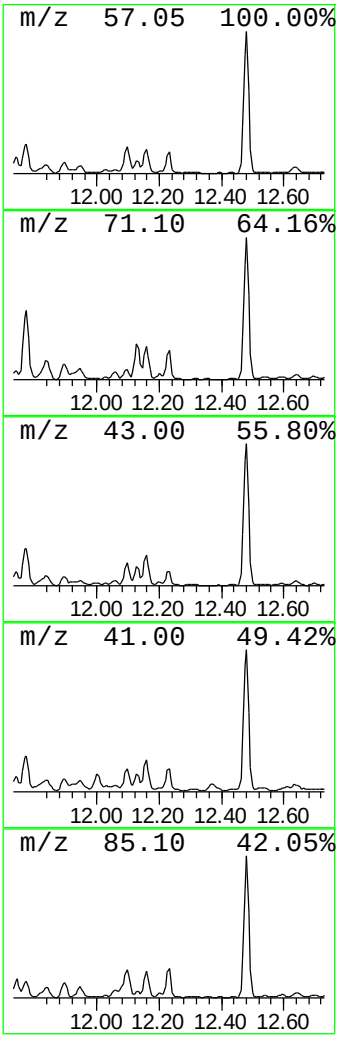
****

Peak Number 9 Decane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.23	12.42 ug/l	453621	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3-methyl-	156	C11H24	013151-34-3	87
2	Undecane, 2,7-dimethyl-	184	C13H28	017301-24-5	47
3	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	43
4	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	43
5	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062718\
Data File : VX002945.D
Acq On : 27 Jun 2018 19:09
Operator : JC/MD
Sample : J3707-12 20X
Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WP021SB480-21-23-180622

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

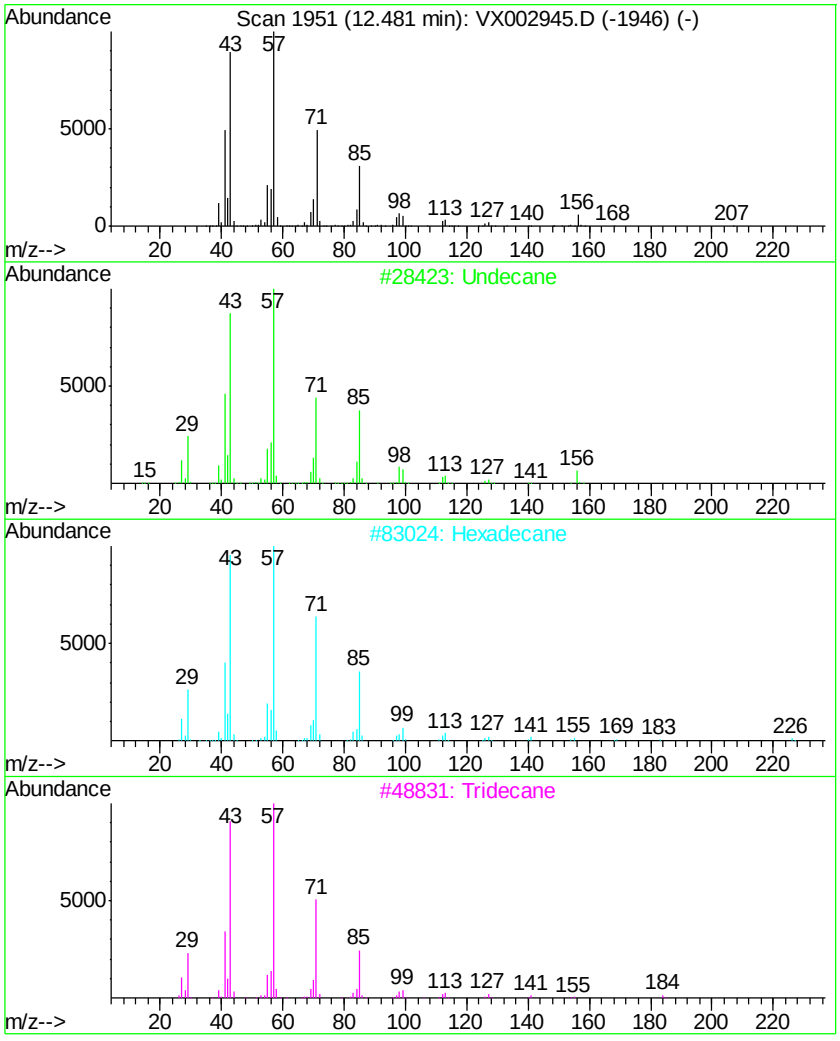
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

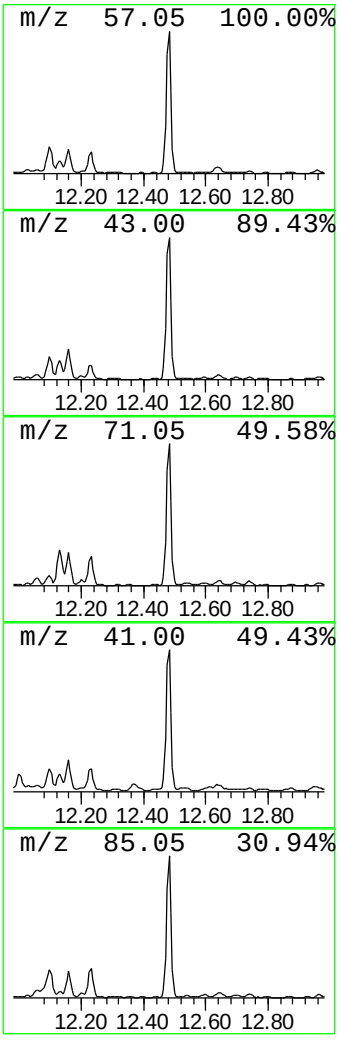
****

Peak Number 10 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	57.16 ug/l	2086750	1,4-Dichlorobenzene-d4	12.08

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	Tridecane	184	C13H28	000629-50-5	80
4	Decane	142	C10H22	000124-18-5	78
5	Tetradecane	198	C14H30	000629-59-4	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062718\
Data File : VX002945.D
Acq On : 27 Jun 2018 19:09
Operator : JC/MD
Sample : J3707-12 20X
Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WP021SB480-21-23-180622

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.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	24.6	ug/l	508765	3	10.12	1034540	50.0
Octane, 2,6-dimet...	10.84	11.8	ug/l	244693	3	10.12	1034540	50.0
Cyclohexane, propyl-	10.91	10.5	ug/l	217400	3	10.12	1034540	50.0
Decane	11.09	12.3	ug/l	254449	3	10.12	1034540	50.0
Nonane, 3-methyl-	11.24	11.4	ug/l	415551	4	12.08	1825450	50.0
Decane, 2-methyl-	12.16	12.6	ug/l	461304	4	12.08	1825450	50.0
Decane, 3-methyl-	12.23	12.4	ug/l	453621	4	12.08	1825450	50.0
Undecane	12.48	57.2	ug/l	2086750	4	12.08	1825450	50.0