LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX052319\
Data File : VX009867.D
Acq On : 23 May 2019 18:38
Operator : JC/SP
Sample : K2976-20 10X
Misc : 5.74g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : EP1-SB-SBR-3BR(17-20)

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\82X042919W.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	5.501	702	713	726	rBV	96535	281280	3.41%	0.305%
2	5.659	728	739	754	rVV	174232	501072	6.08%	0.543%
3	6.062	793	805	820	rBV	123381	325742	3.95%	0.353%
4	6.860	925	936	954	rBV	279958	678387	8.23%	0.735%
5	8.714	1235	1240	1256	rVB	613577	969758	11.77%	1.050%
6	9.037	1287	1293	1301	rVB	56468	98189	1.19%	0.106%
7	9.445	1350	1360	1369	rBV	123949	203898	2.47%	0.221%
8	9.561	1373	1379	1385	rBV2	129635	263911	3.20%	0.286%
9	9.622	1385	1389	1393	rVB2	60622	90218	1.09%	0.098%
10	9.677	1393	1398	1402	rBV	310759	480723	5.83%	0.521%
11	9.817	1414	1421	1425	rBV	61420	95617	1.16%	0.104%
12	9.890	1425	1433	1441	rVV4	407083	1056400	12.82%	1.144%
13	9.951	1441	1443	1448	rVB	166409	217288	2.64%	0.235%
14	10.061	1455	1461	1465	rBV	164781	280270	3.40%	0.304%
15	10.110	1465	1469	1474	rBV	607180	820252	9.95%	0.888%
16	10.171	1474	1479	1485	rVB6	99588	234349	2.84%	0.254%
17	10.238	1485	1490	1496	rBV2	282727	508875	6.18%	0.551%
18	10.335	1496	1506	1509	rBV2	666453	1389495	16.86%	1.505%
19	10.378	1509	1513	1516	rVV	1101474	1472145	17.87%	1.594%
20	10.408	1516	1518	1530	rVB	865209	1454666	17.65%	1.575%
21	10.512	1530	1535	1540	rBV	506135	761341	9.24%	0.825%
22	10.585	1540	1547	1549	rBV2	232449	321422	3.90%	0.348%
23	10.640	1549	1556	1564	rBV3	2219460	3863106	46.88%	4.184%
24	10.725	1564	1570	1574	rBV3	1320458	2146336	26.05%	2.325%
25	10.768	1574	1577	1580	rVB2	662870	832091	10.10%	0.901%
26	10.835	1580	1588	1592	rBV	5539354	8239891	100.00%	8.924%
27	10.914	1592	1601	1604	rBV	4094123	7039845	85.44%	7.624%
28	10.951	1604	1607	1612	rVB	2564199	3321999	40.32%	3.598%
29	11.006	1612	1616	1621	rVB3	749934	1294666	15.71%	1.402%
30	11.061	1621	1625	1626	rBV2	932258	1256128	15.24%	1.360%
31	11.085	1626	1629	1633	rVB2	1345900	1734083	21.04%	1.878%
32	11.134	1633	1637	1641	rVB3	950462	1601715	19.44%	1.735%
33	11.183	1641	1645	1648	rBV	665655	822758	9.99%	0.891%
34	11.219	1648	1651	1653	rBV	405877	475147	5.77%	0.515%

LSC Area Percent Report

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Instrument : MSVOA_X
ClientSampleId : EP1-SB-SBR-3BR(17-20)

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

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Title : SW846 8260

35	11.274	1653	1660	1669	rVB3	2754815	4793667	58.18%	5.192%
36	11.359	1670	1674	1676	rBV	484830	590922	7.17%	0.640%
37	11.396	1676	1680	1684	rBV2	836893	1343886	16.31%	1.455%
38	11.445	1684	1688	1691	rBV2	974989	1297579	15.75%	1.405%
39	11.487	1691	1695	1699	rBV	2471483	3075757	37.33%	3.331%
40	11.536	1699	1703	1707	rVB3	1432406	2328953	28.26%	2.522%
41	11.579	1707	1710	1715	rVB5	383369	539622	6.55%	0.584%
42	11.628	1715	1718	1720	rBV	372410	410909	4.99%	0.445%
43	11.682	1720	1727	1732	rVB4	1240712	2380178	28.89%	2.578%
44	11.737	1732	1736	1738	rBV2	997902	1236595	15.01%	1.339%
45	11.768	1738	1741	1744	rBV	3726809	3943279	47.86%	4.271%
46	11.804	1744	1747	1749	rBV2	493235	589472	7.15%	0.638%
47	11.890	1757	1761	1763	rBV2	786755	1044853	12.68%	1.132%
48	11.945	1763	1770	1775	rVV4	1874670	4257176	51.67%	4.611%
49	12.000	1775	1779	1782	rVV	2341761	3207613	38.93%	3.474%
50	12.030	1782	1784	1789	rVV3	727373	1190106	14.44%	1.289%
51	12.079	1789	1792	1797	rVV4	893566	1657827	20.12%	1.795%
52	12.128	1797	1800	1803	rVV4	447935	574160	6.97%	0.622%
53	12.164	1803	1806	1808	rVV3	206603	278680	3.38%	0.302%
54	12.213	1808	1814	1824	rVB6	437577	1463606	17.76%	1.585%
55	12.298	1824	1828	1833	rBV2	825861	1211080	14.70%	1.312%
56	12.365	1835	1839	1846	rBV2	1359751	2413220	29.29%	2.614%
57	12.469	1846	1856	1862	rBV3	441202	1273523	15.46%	1.379%
58	12.524	1862	1865	1870	rVB4	499941	876868	10.64%	0.950%
59	12.609	1870	1879	1881	rBV4	436898	878289	10.66%	0.951%
60	12.664	1885	1888	1892	rVB	546212	636361	7.72%	0.689%
61	12.737	1897	1900	1901	rBV	171484	192791	2.34%	0.209%
62	12.816	1910	1913	1918	rVB4	118282	157933	1.92%	0.171%
63	12.871	1918	1922	1929	rVB3	504374	824676	10.01%	0.893%
64	12.944	1929	1934	1937	rBV3	419578	708450	8.60%	0.767%
65	12.975	1937	1939	1943	rVV2	366228	398019	4.83%	0.431%
66	13.042	1943	1950	1953	rVV3	267547	363058	4.41%	0.393%
67	13.079	1953	1956	1963	rVB2	148314	268244	3.26%	0.291%
68	13.152	1963	1968	1972	rBV2	107111	183468	2.23%	0.199%
69	13.194	1972	1975	1978	rVB	80721	83704	1.02%	0.091%
70	13.347	1996	2000	2006	rVB4	213971	339296	4.12%	0.367%
71	13.426	2010	2013	2017	rVV2	55171	97560	1.18%	0.106%

LSC Area Percent Report

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Instrument : MSVOA_X
ClientSampleId : EP1-SB-SBR-3BR(17-20)

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Title : SW846 8260

72	13.469	2017	2020	2025	rVB4	58016	90678	1.10%	0.098%

Sum of corrected areas: 92335121

LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX052319\
Data File : VX009867.D
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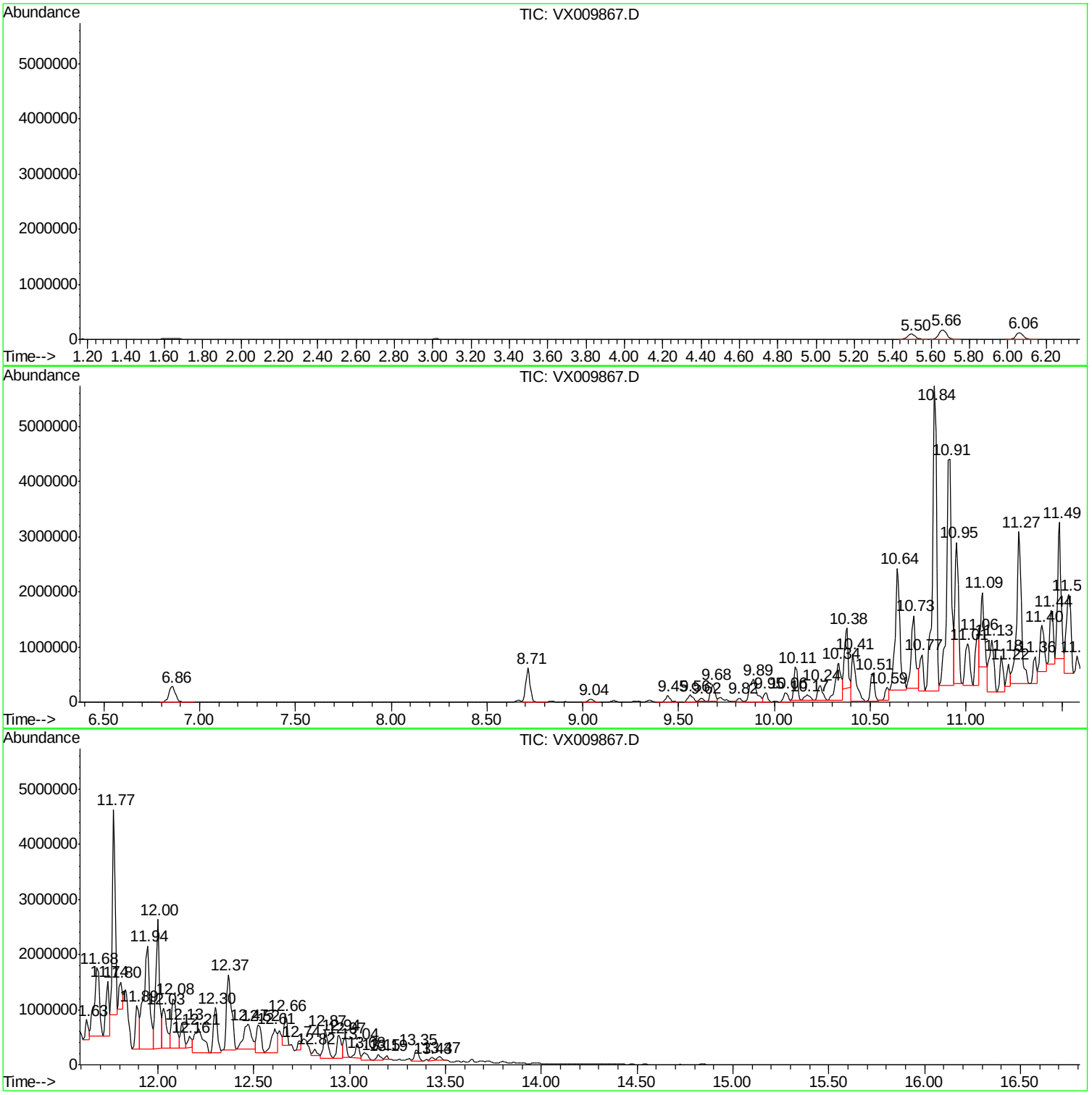
Operator : JC/SP
Sample : K2976-20 10X
Misc : 5.74g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EP1-SB-SBR-3BR(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.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\VX052319\
Data File : VX009867.D
Acq On : 23 May 2019 18:38
Operator : JC/SP
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Instrument : MSVOA_X
ClientSampleId : EP1-SB-SBR-3BR(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

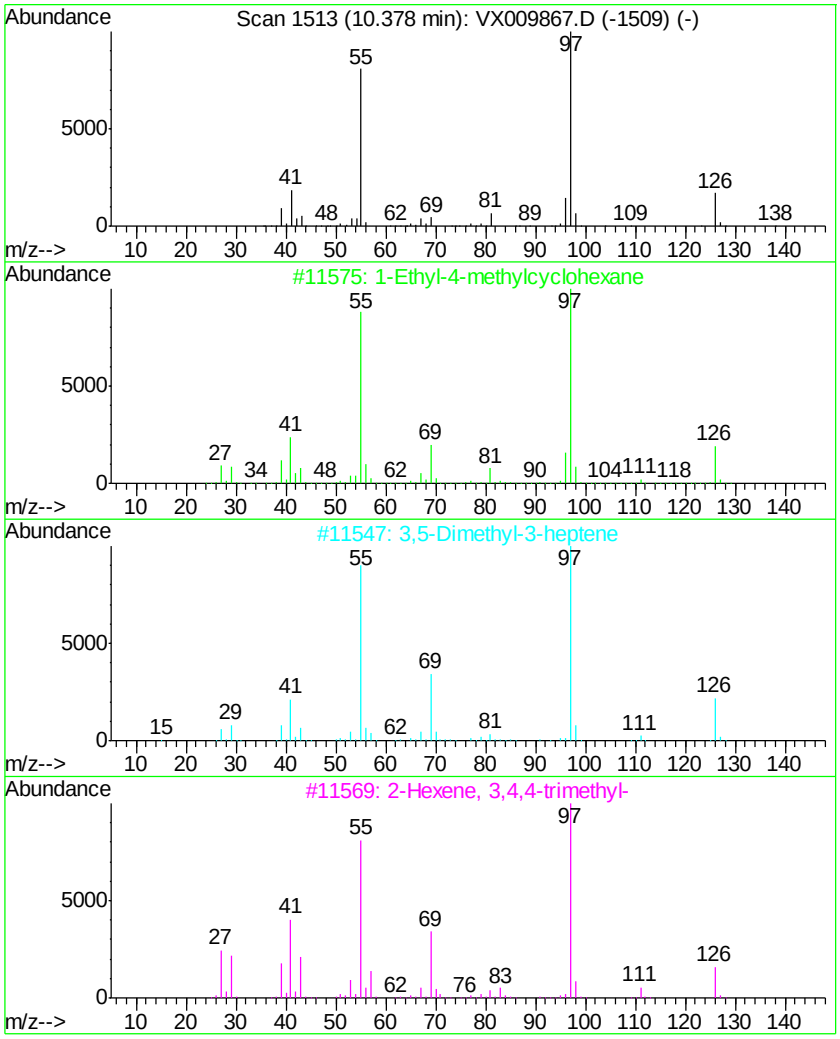
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

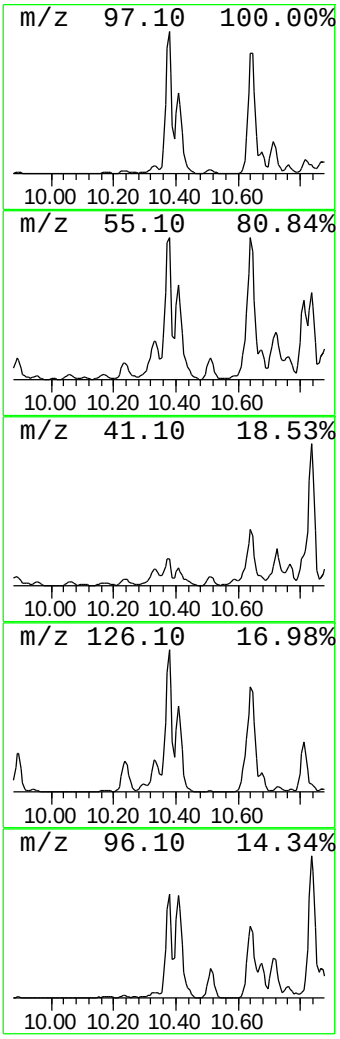
****

Peak Number 1 1-Ethyl-4-methylcyclohexane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	89.74 ug/l	1472150	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	91
2	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	80
3	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	64
4	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	64
5	Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	56





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX052319\
Data File : VX009867.D
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Operator : JC/SP
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ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : EP1-SB-SBR-3BR(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

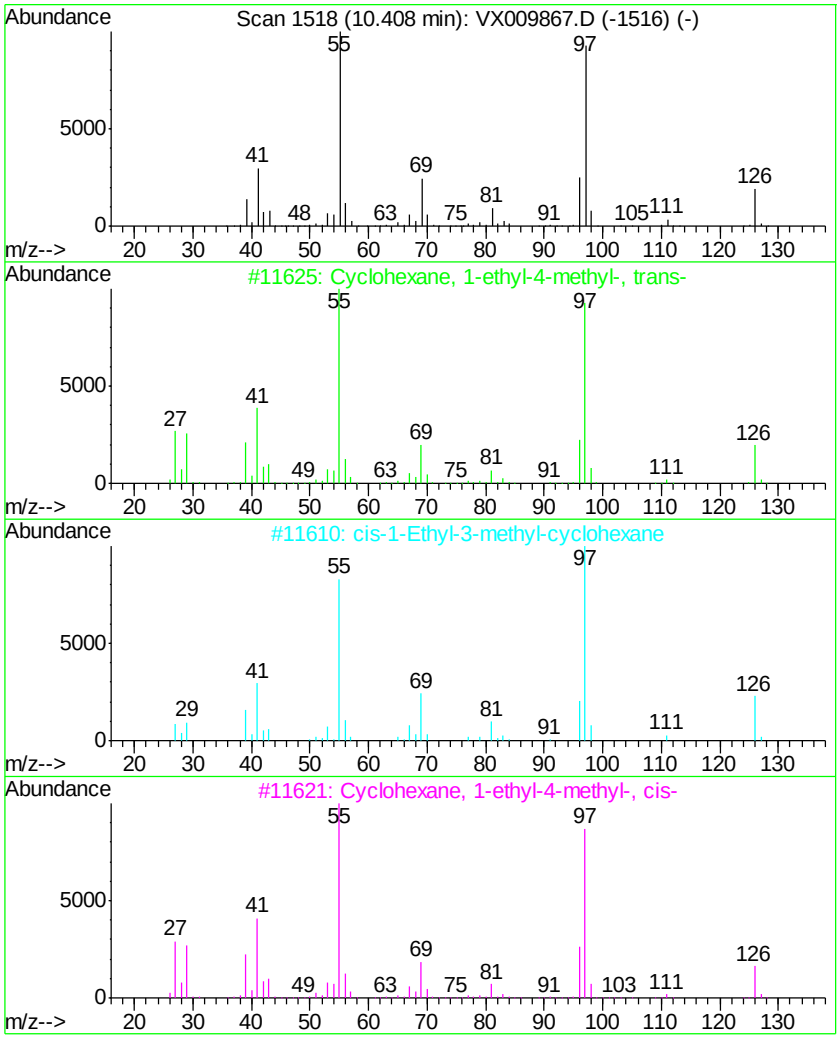
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

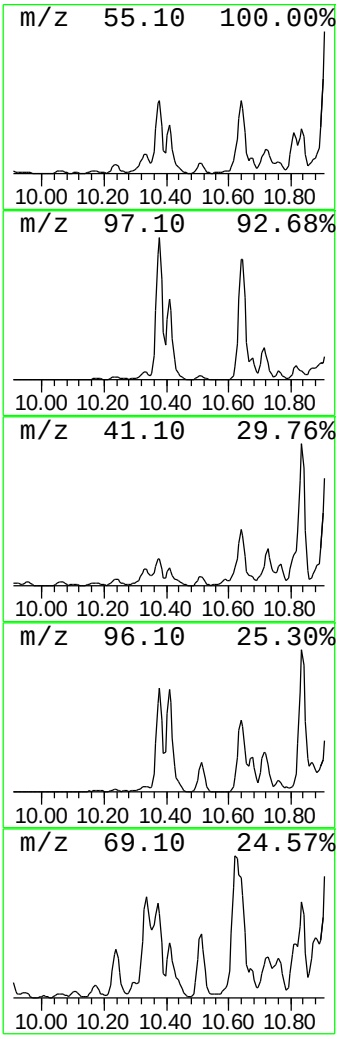
****

Peak Number 2 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	88.67 ug/l	1454670	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	94
2	cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	91
3	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	91
4	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	90
5	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	87





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX052319\
Data File : VX009867.D
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Sample : K2976-20 10X
Misc : 5.74g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : EP1-SB-SBR-3BR(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
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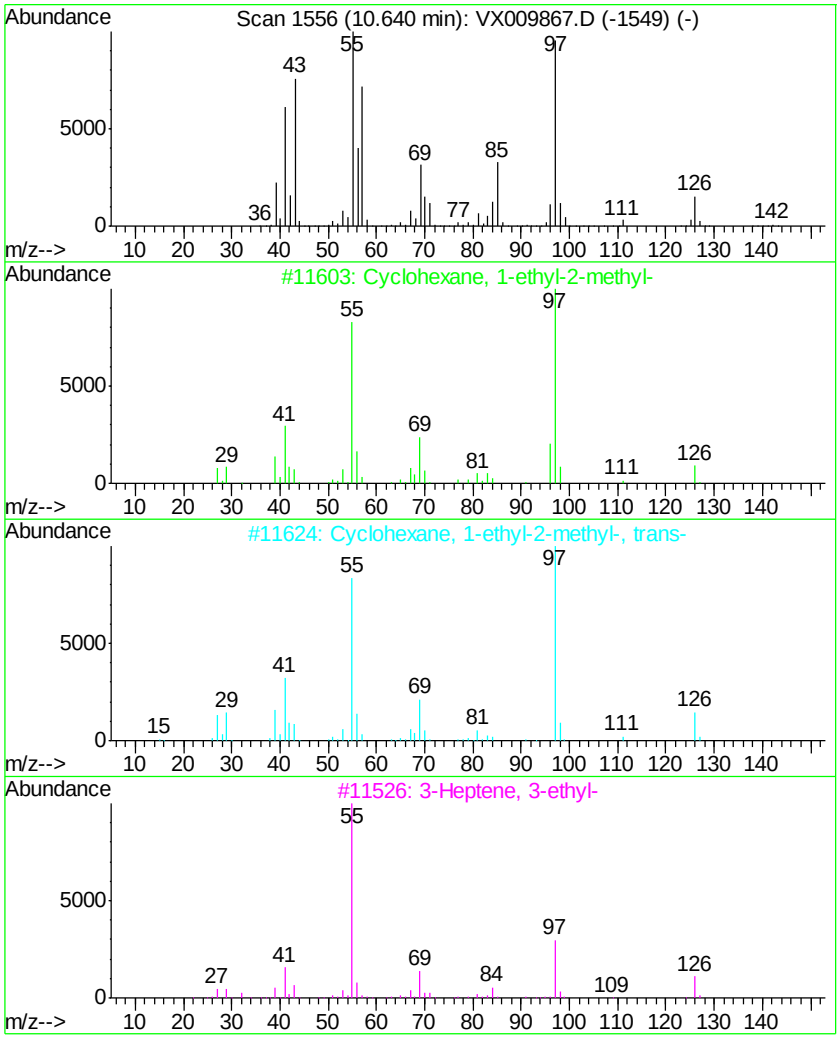
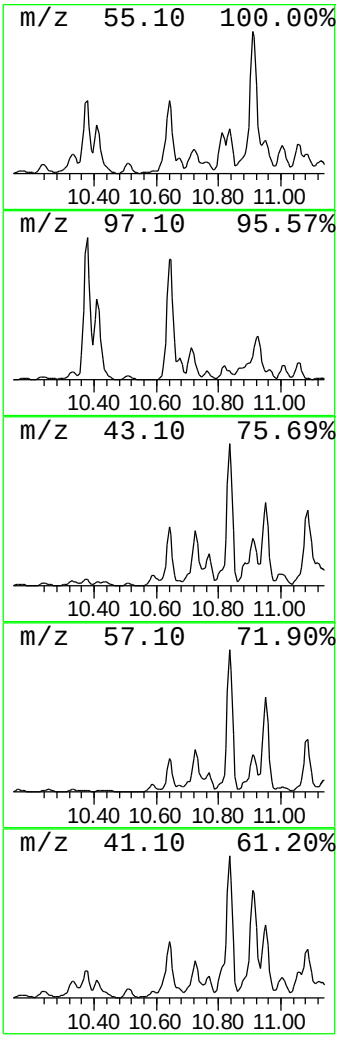
****

Peak Number 3 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	235.48 ug/l	3863110	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	60
2	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	53
3	3-Heptene, 3-ethyl-	126	C9H18	074764-46-8	52
4	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	49
5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	49





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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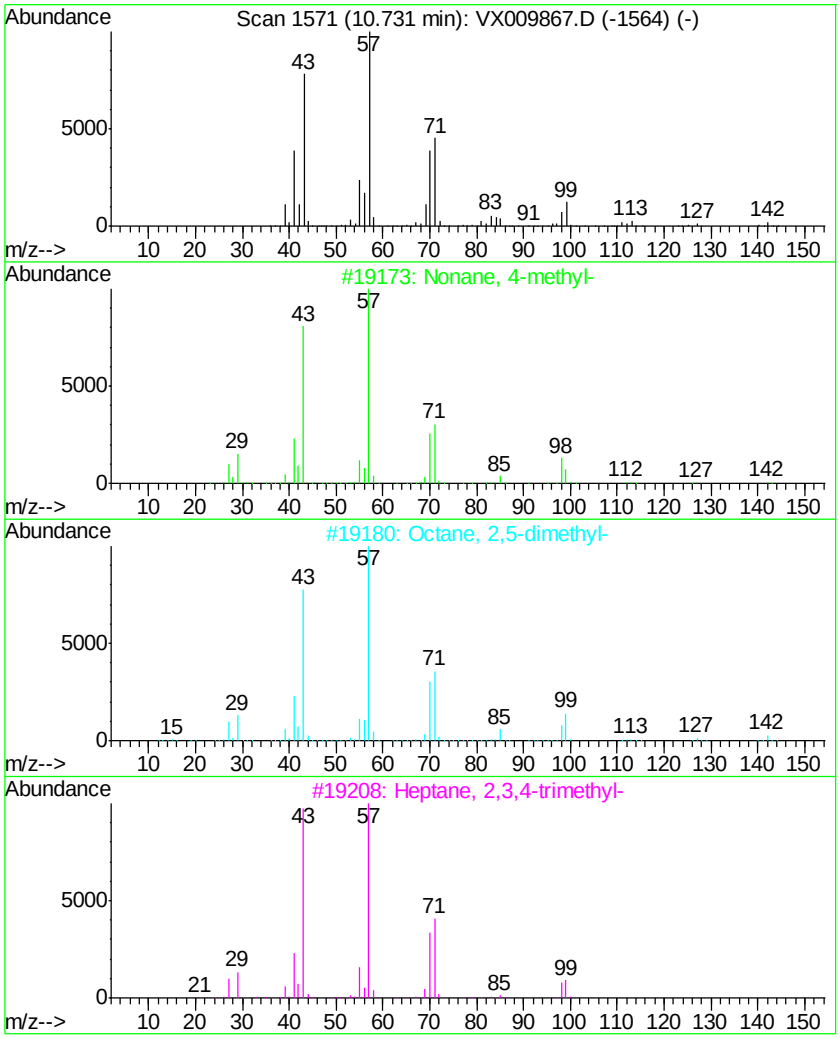
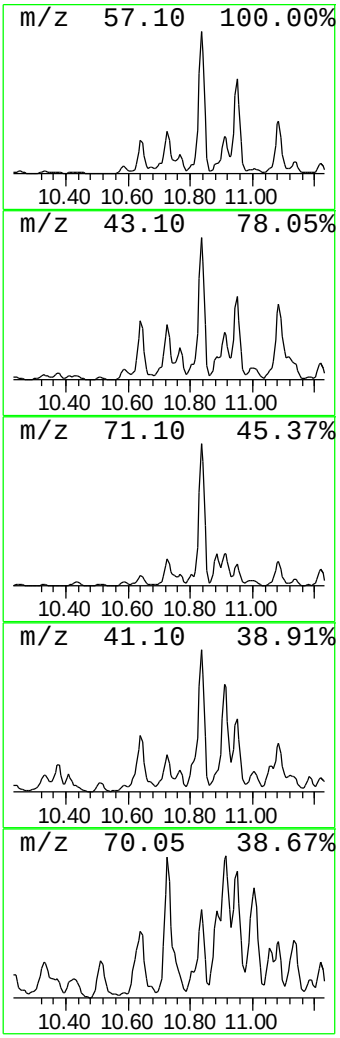
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	130.83 ug/l	2146340	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4-methyl-	142	C10H22	017301-94-9	87
2	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	74
3	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	72
4	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	72
5	Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	53





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Misc : 5.74g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : EP1-SB-SBR-3BR(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

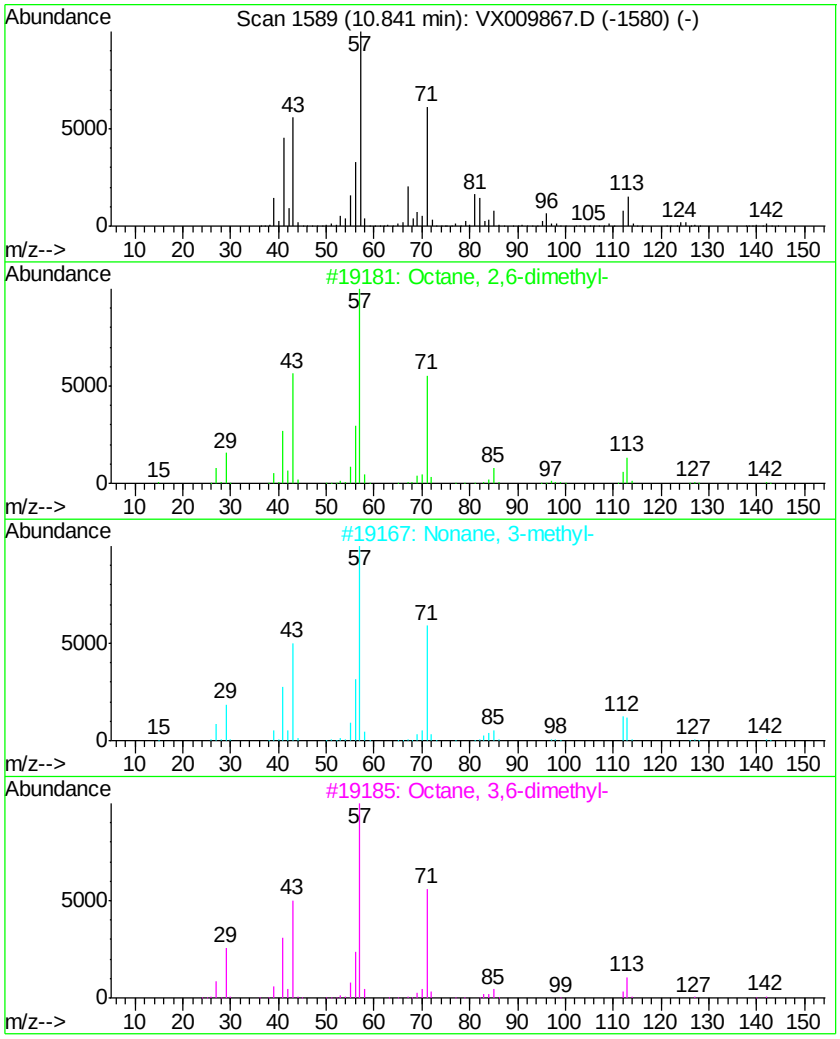
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

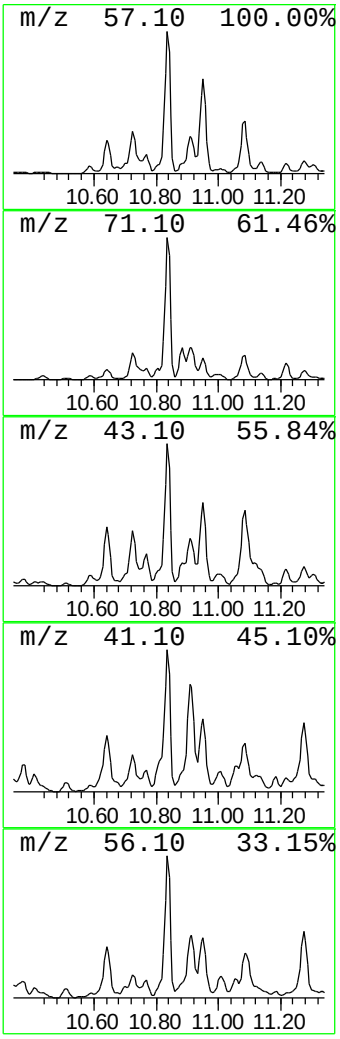
****

Peak Number 5 Octane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	502.28 ug/l	8239890	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	94
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	70
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	70
4	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	47
5	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	43





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Instrument : MSVOA_X
ClientSampleId : EP1-SB-SBR-3BR(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

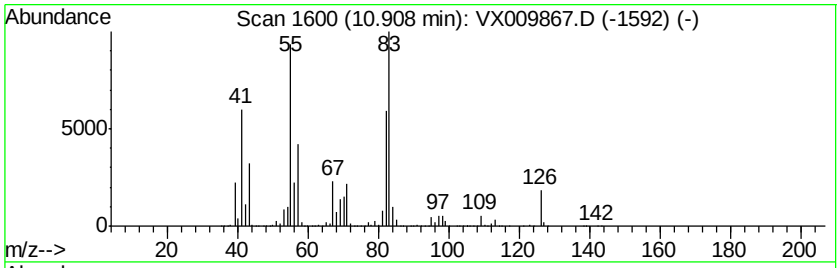
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

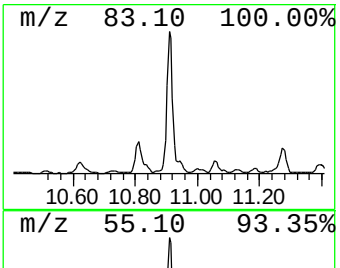
****

Peak Number 6 Cyclohexanone, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	429.13 ug/l	7039850	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 2,3-dimethyl-	126	C8H14O	013395-76-1	86
2	Cyclohexane, propyl-	126	C9H18	001678-92-8	76
3	Cyclohexane, octyl-	196	C14H28	001795-15-9	59
4	Cyclohexane, butyl-	140	C10H20	001678-93-9	59
5	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	58





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX052319\
Data File : VX009867.D
Acq On : 23 May 2019 18:38
Operator : JC/SP
Sample : K2976-20 10X
Misc : 5.74g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : EP1-SB-SBR-3BR(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

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

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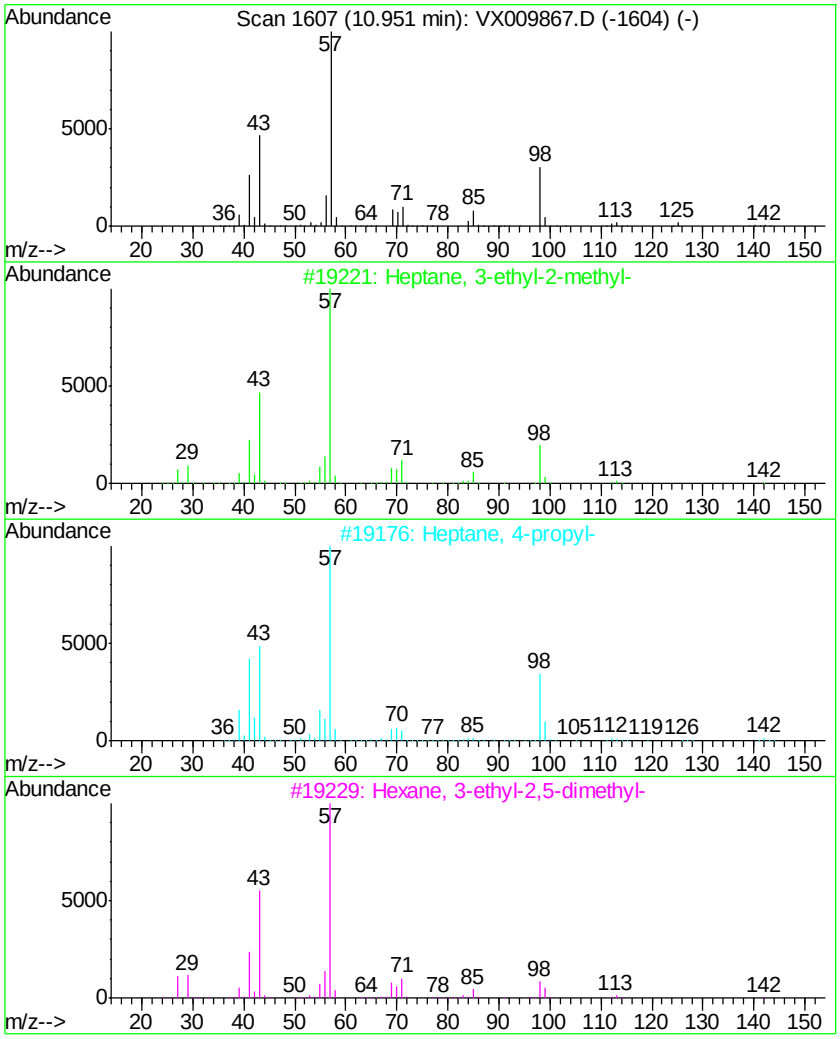
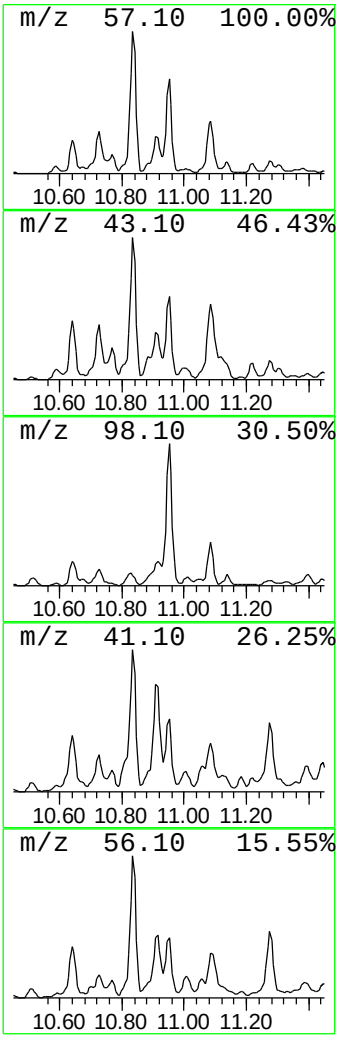
Peak Number 7 Heptane, 3-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	202.50 ug/l	3322000	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	90
2	Heptane, 4-propyl-	142	C10H22	003178-29-8	56
3	Hexane, 3-ethyl-2,5-dimethyl-	142	C10H22	052897-04-8	53
4	Undecane, 6-methyl-	170	C12H26	017302-33-9	50
5	Decane, 2,5-dimethyl-	170	C12H26	017312-50-4	40





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Data File : VX009867.D
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Instrument : MSVOA_X
ClientSampleId : EP1-SB-SBR-3BR(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

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

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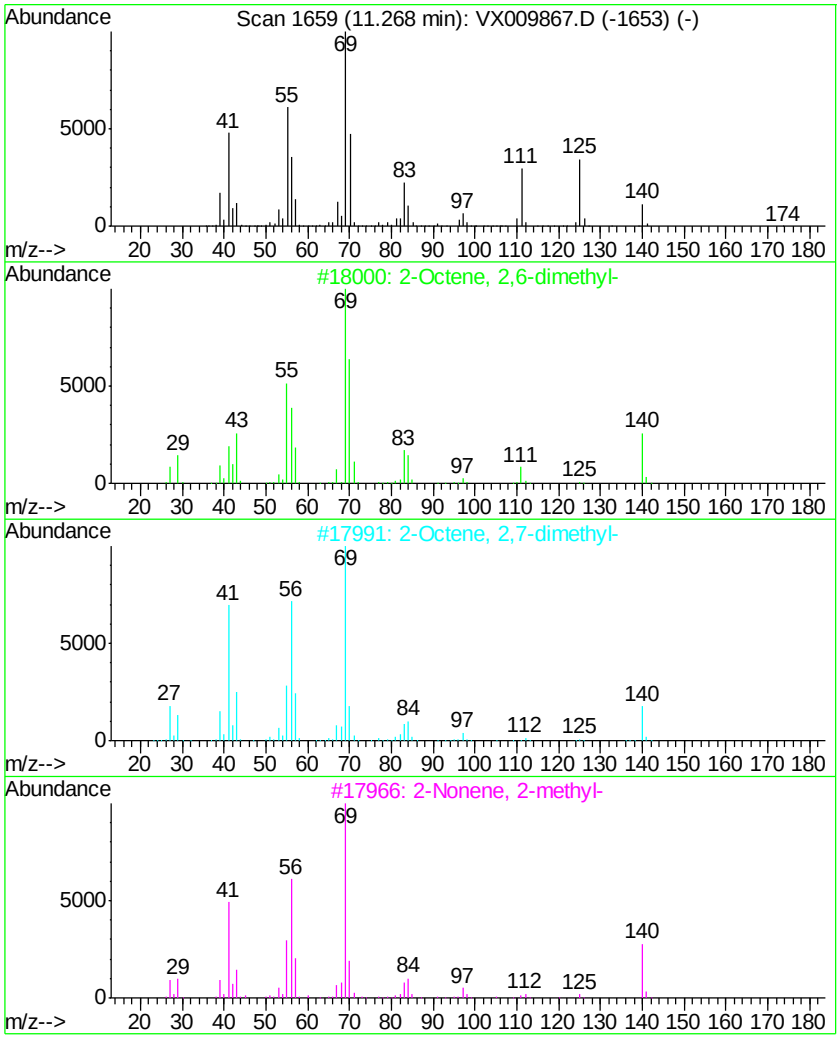
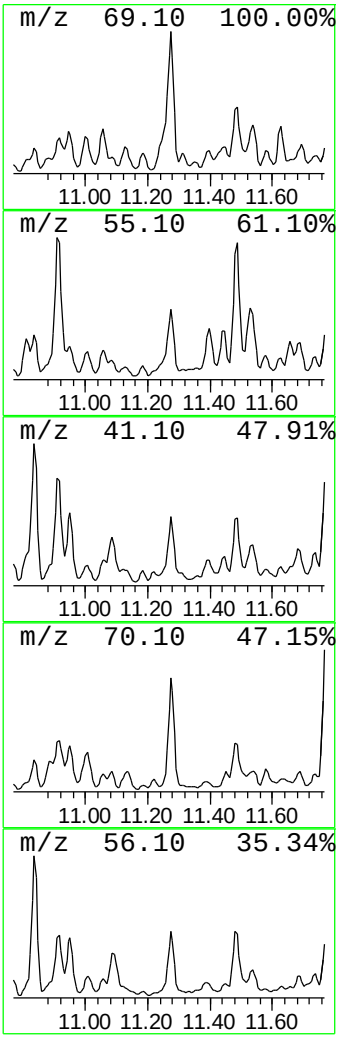
Peak Number 8 2-Octene, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.27	144.58 ug/l	4793670	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	64
2	2-Octene, 2,7-dimethyl-	140	C10H20	002050-81-9	49
3	2-Nonene, 2-methyl-	140	C10H20	002129-95-5	46
4	Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	46
5	3-Ethyl-4-octene	140	C10H20	019781-32-9	43





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Acq On : 23 May 2019 18:38
Operator : JC/SP
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Misc : 5.74g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : EP1-SB-SBR-3BR(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

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

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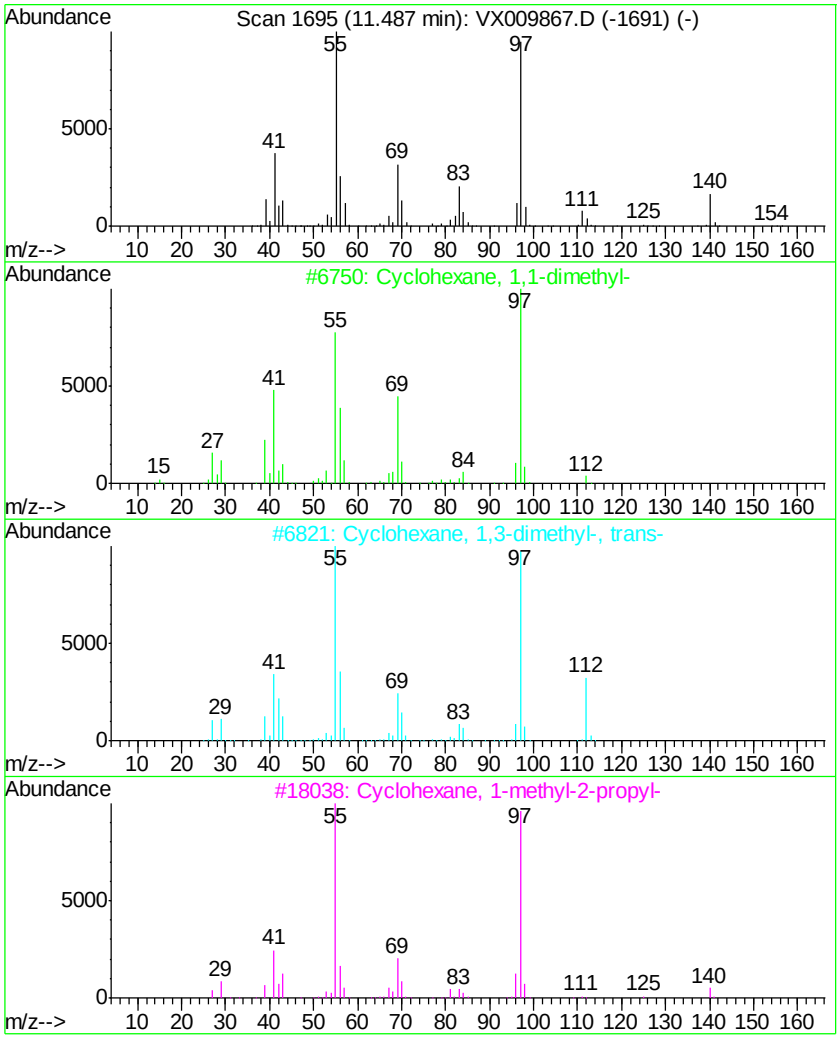
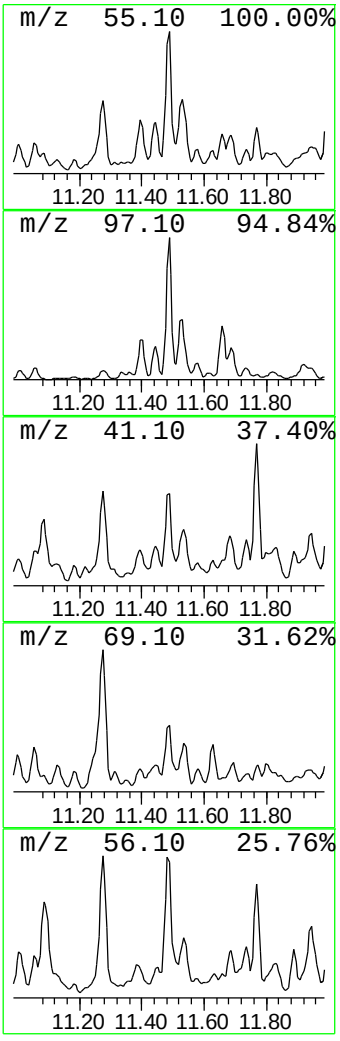
Peak Number 9 Cyclohexane, 1,1-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.49	92.76 ug/l	3075760	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	76
2	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	64
3	Cyclohexane, 1-methyl-2-propyl-	140	C10H20	004291-79-6	59
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	59
5	3-Hexene, 3-ethyl-2,5-dimethyl-	140	C10H20	062338-08-3	58





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Operator : JC/SP
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Misc : 5.74g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : EP1-SB-SBR-3BR(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

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

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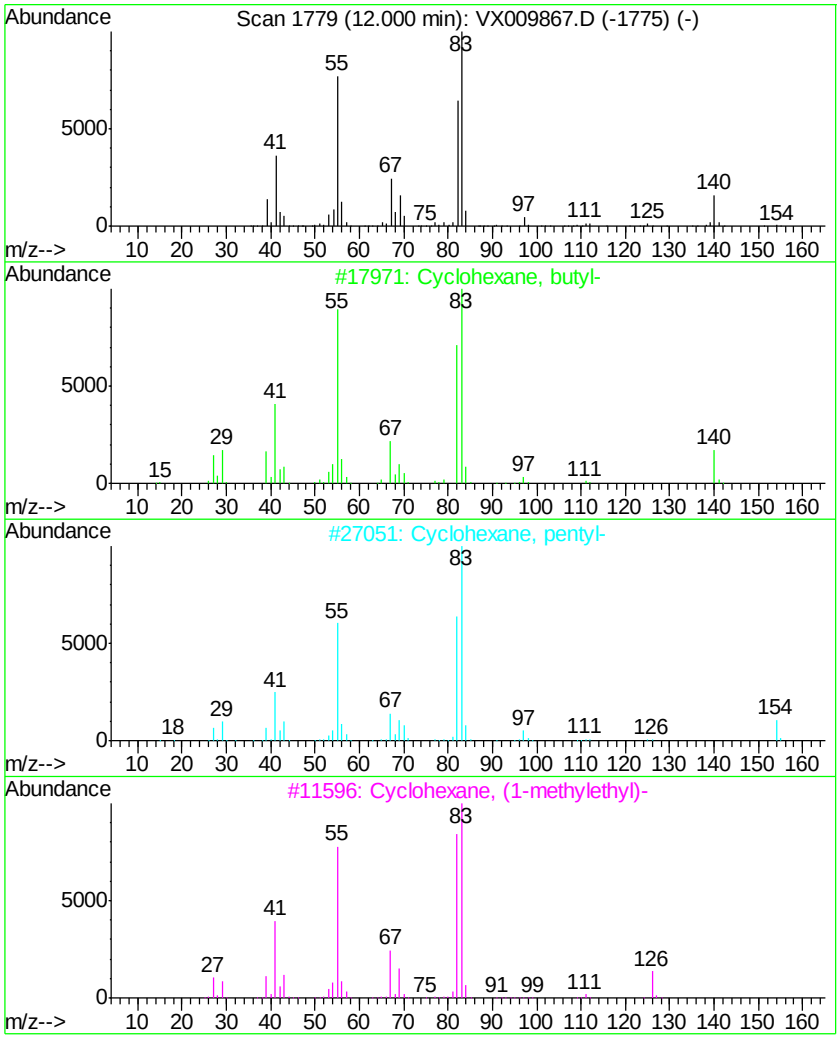
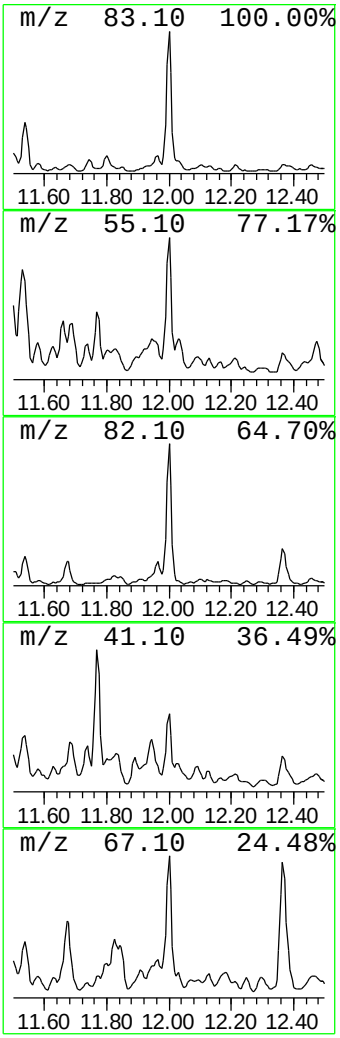
Peak Number 10 Cyclohexane, butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	96.74 ug/l	3207610	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, butyl-	140	C10H20	001678-93-9	97
2	Cyclohexane, pentyl-	154	C11H22	004292-92-6	87
3	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	86
4	Cyclohexane, octyl-	196	C14H28	001795-15-9	86
5	Cyclohexane, 1,1'-(1,4-butanediy...	222	C16H30	006165-44-2	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX052319\
Data File : VX009867.D
Acq On : 23 May 2019 18:38
Operator : JC/SP
Sample : K2976-20 10X
Misc : 5.74g/5mL/100uL/5.00mL/MSVOA_X/MEOH
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Instrument : MSVOA_X
ClientSampleId : EP1-SB-SBR-3BR(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.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
1-Ethyl-4-methylc...	10.38	89.7	ug/l	1472150	3	10.11	820252	50.0
Cyclohexane, 1-et...	10.41	88.7	ug/l	1454670	3	10.11	820252	50.0
Cyclohexane, 1-et...	10.64	235.5	ug/l	3863110	3	10.11	820252	50.0
Nonane, 4-methyl-	10.73	130.8	ug/l	2146340	3	10.11	820252	50.0
Octane, 2,6-dimet...	10.84	502.3	ug/l	8239890	3	10.11	820252	50.0
Cyclohexanone, 2,...	10.91	429.1	ug/l	7039850	3	10.11	820252	50.0
Heptane, 3-ethyl-...	10.95	202.5	ug/l	3322000	3	10.11	820252	50.0
2-Octene, 2,6-dim...	11.27	144.6	ug/l	4793670	4	12.08	1657830	50.0
Cyclohexane, 1,1-...	11.49	92.8	ug/l	3075760	4	12.08	1657830	50.0
Cyclohexane, butyl-	12.00	96.7	ug/l	3207610	4	12.08	1657830	50.0