LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034757.D
Acq On : 27 Mar 2023 18:08
Operator : JC/MD
Sample : 02052-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

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\82X031023W.M
Title : SW846 8260

Signal : TIC: VX034757.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.404	208	216	239	rVB	312402	726651	5.58%	1.621%
2	2.892	284	296	310	rVB	206353	521064	4.00%	1.163%
3	4.038	469	484	498	rBV	47320	145433	1.12%	0.325%
4	4.202	498	511	529	rBV	168532	544898	4.18%	1.216%
5	5.117	645	661	679	rBB2	251929	899730	6.90%	2.008%
6	5.385	694	705	712	rBV	162059	470046	3.61%	1.049%
7	5.501	712	724	735	rVV	3707667	11885388	91.20%	26.522%
8	5.611	735	742	760	rVV	1125871	3554552	27.27%	7.932%
9	5.818	762	776	790	rVV	4503345	13032459	100.00%	29.081%
10	5.952	790	798	813	rVB	204969	553793	4.25%	1.236%
11	6.178	819	835	842	rBV5	404029	1558267	11.96%	3.477%
12	6.251	842	847	855	rVV3	175342	472525	3.63%	1.054%
13	6.348	855	863	879	rVB2	218081	603336	4.63%	1.346%
14	6.604	893	905	921	rBV	473282	1149014	8.82%	2.564%
15	6.757	921	930	948	rVB	491201	1183082	9.08%	2.640%
16	7.372	1020	1031	1042	rBV	123387	299545	2.30%	0.668%
17	8.647	1234	1240	1246	rBV	1025333	1582045	12.14%	3.530%
18	8.720	1246	1252	1264	rVB	866354	1396866	10.72%	3.117%
19	10.055	1466	1471	1485	rVB	944035	1373102	10.54%	3.064%
20	11.085	1634	1640	1650	rVB	772552	1091730	8.38%	2.436%
21	11.280	1668	1672	1679	rBV2	89194	144449	1.11%	0.322%
22	11.481	1701	1705	1715	rVB3	66907	148626	1.14%	0.332%
23	12.024	1789	1794	1800	rBV	1014616	1311025	10.06%	2.925%
24	12.225	1823	1827	1837	rBV3	63628	166242	1.28%	0.371%

Sum of corrected areas: 44813868

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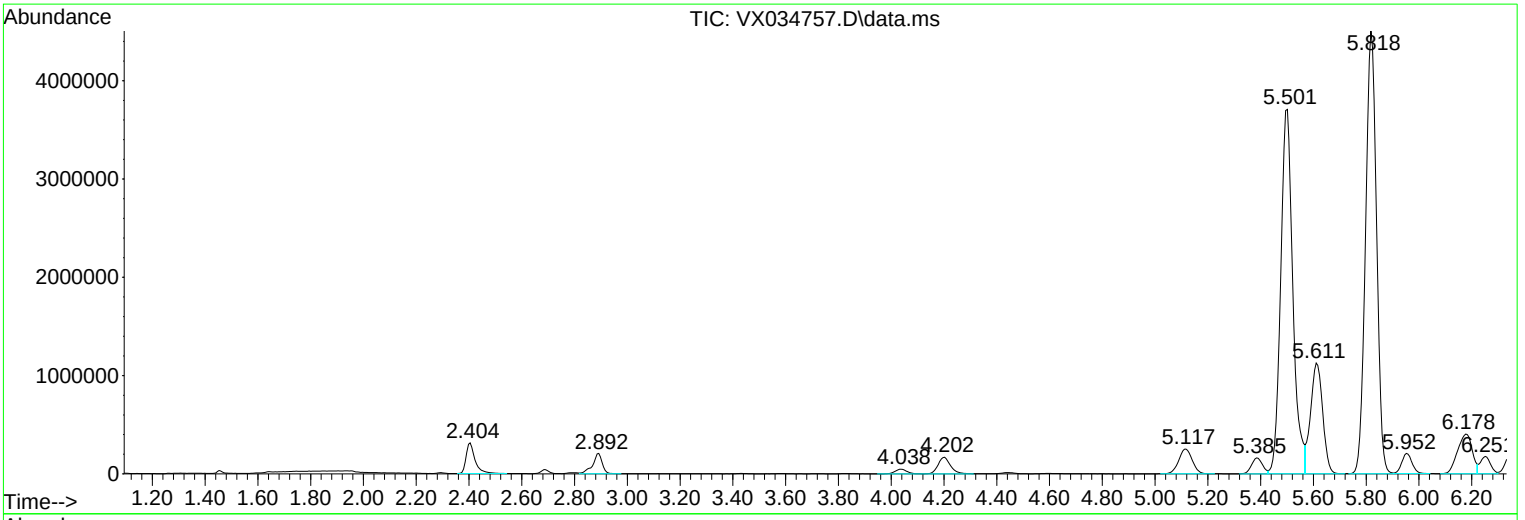
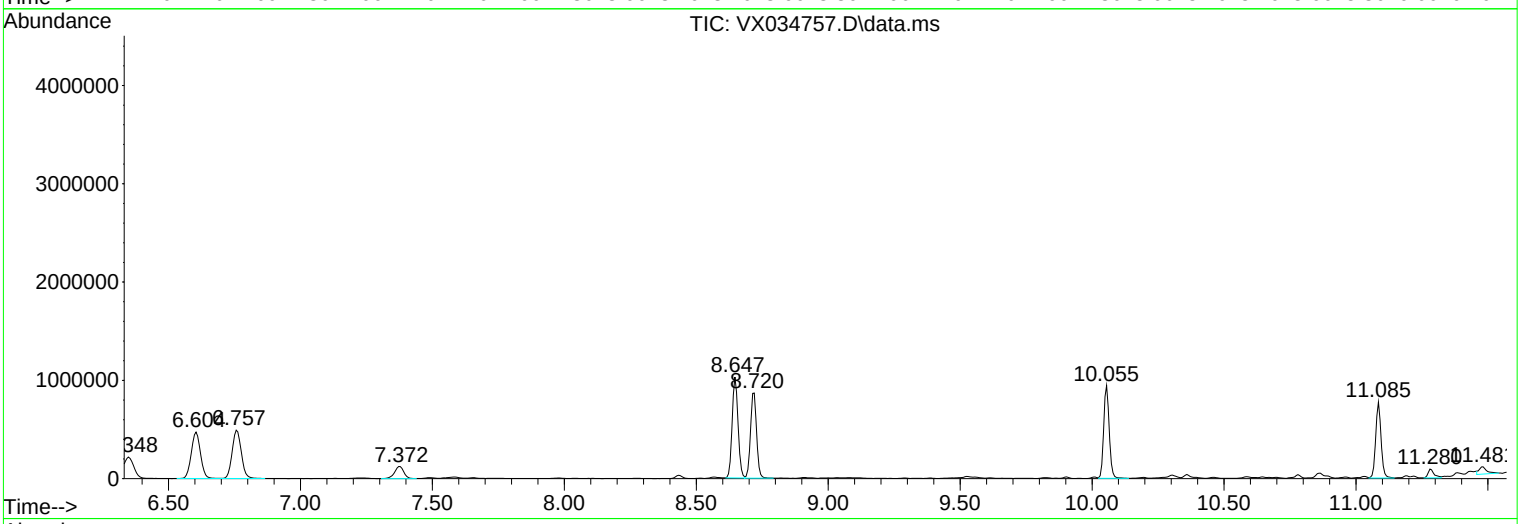
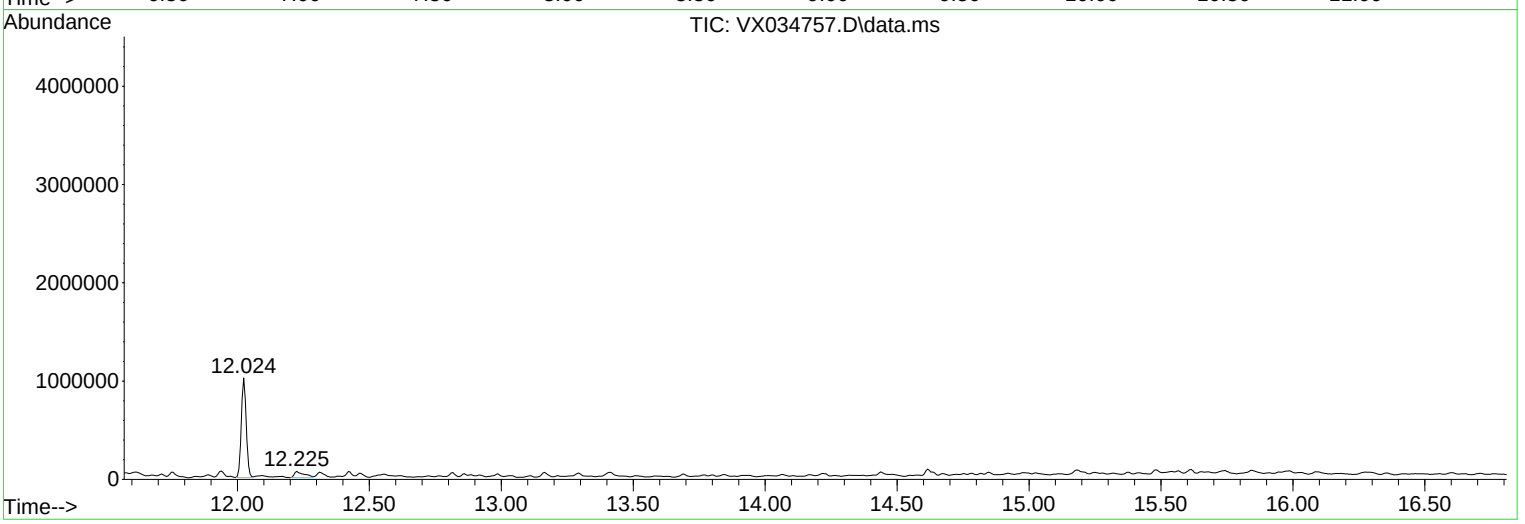
Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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







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Quant Title : SW846 8260

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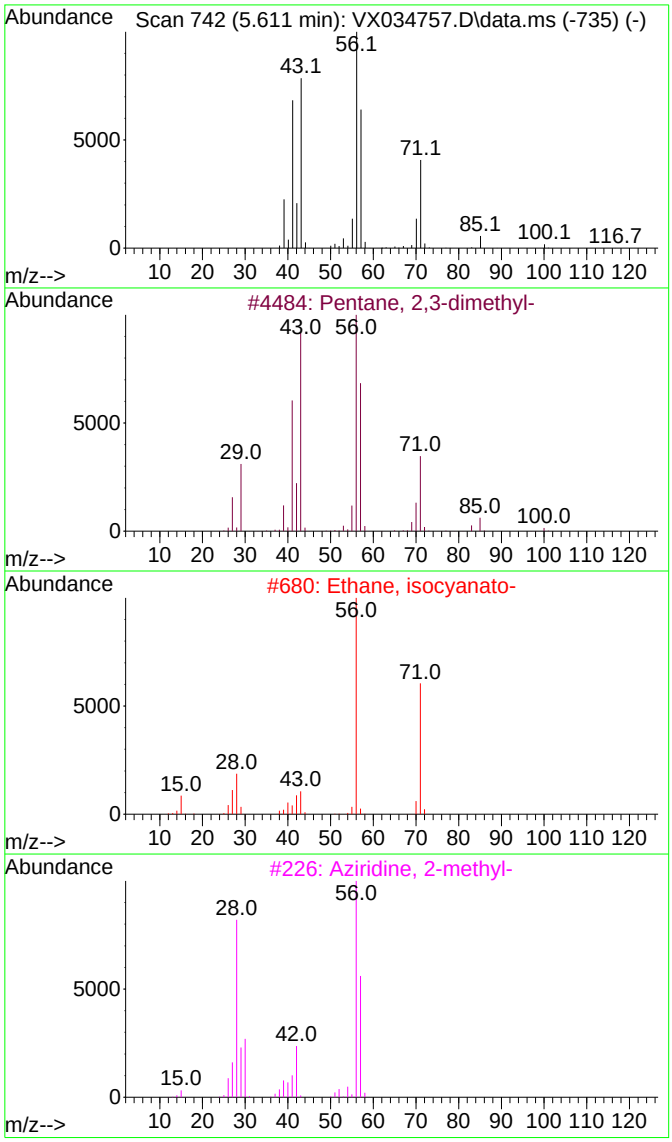
TIC Integration Parameters: LSCINT.P

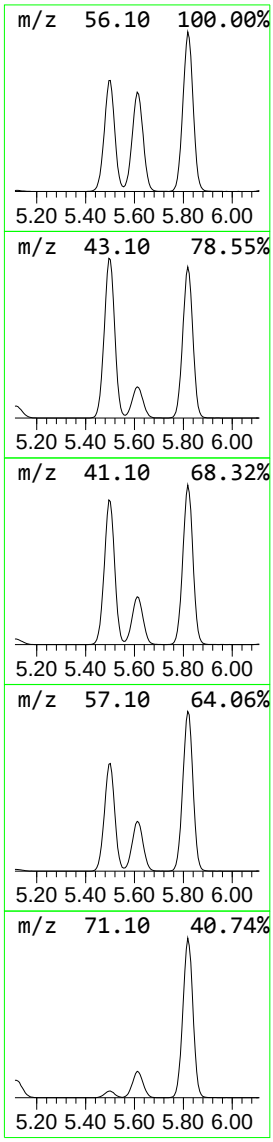
****

Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.611	14.95 ug/l	3554550	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Ethane, isocyanato-	71	C3H5NO	000109-90-0	42
3	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	37
4	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	37
5	Heptane	100	C7H16	000142-82-5	37





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Operator : JC/MD
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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

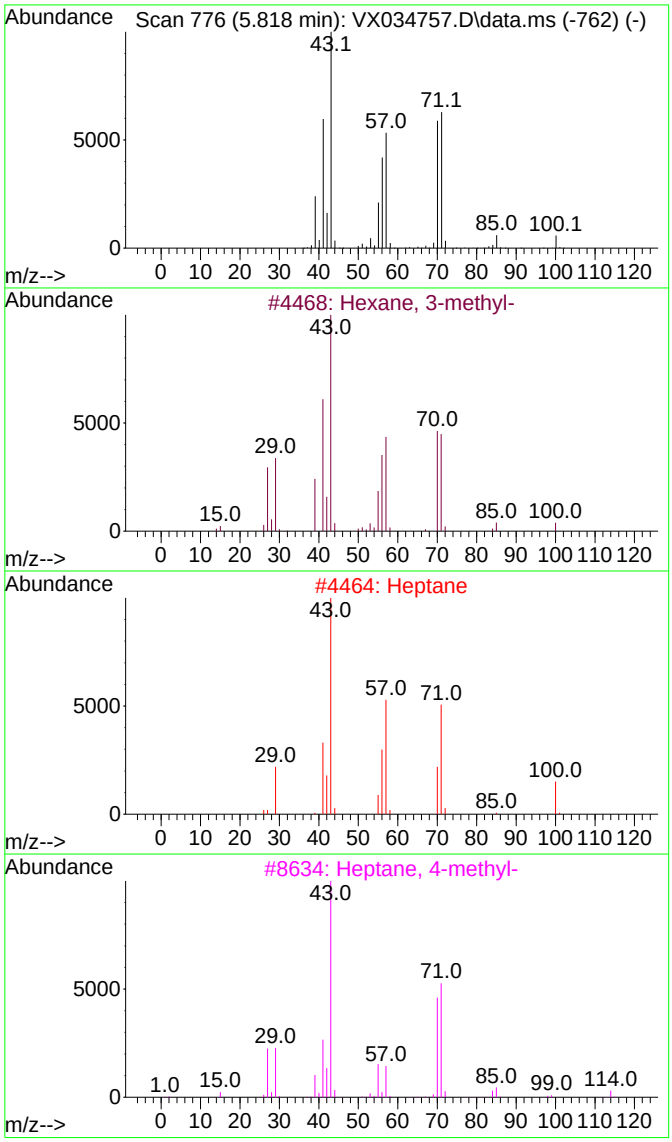
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

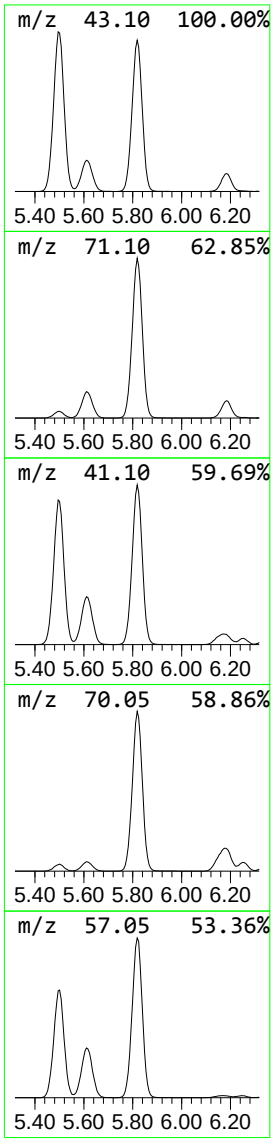
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.818	54.83 ug/l	13032500	Pentafluorobenzene	5.550

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	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5	Diisoamyl ether	158	C10H22O	000544-01-4	50





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Operator : JC/MD
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Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

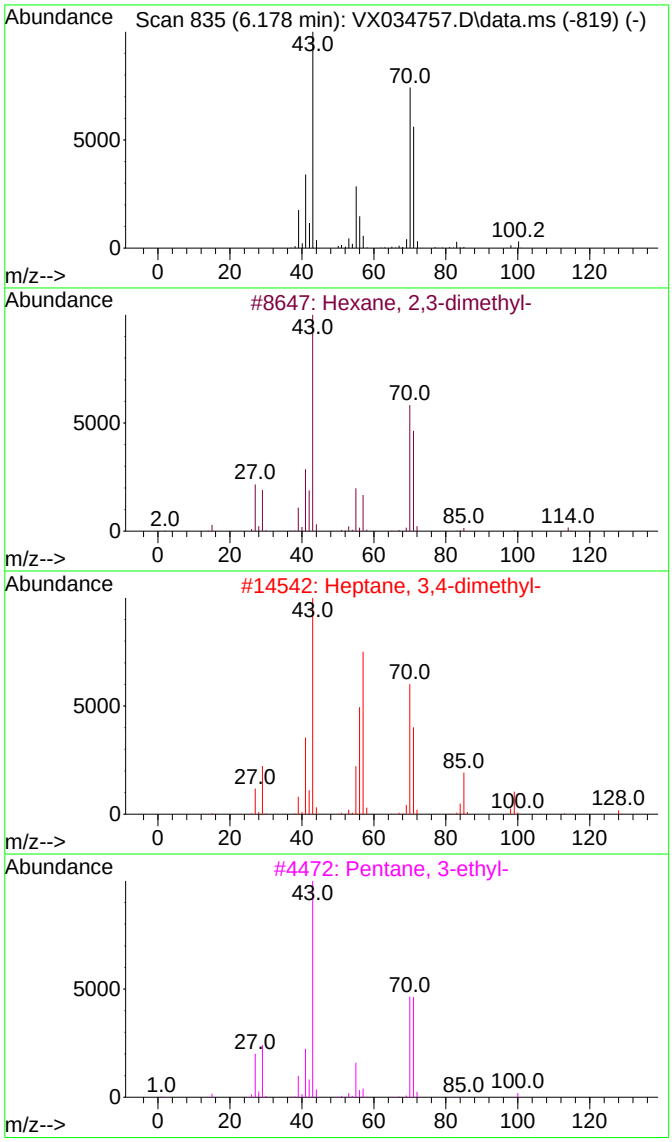
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

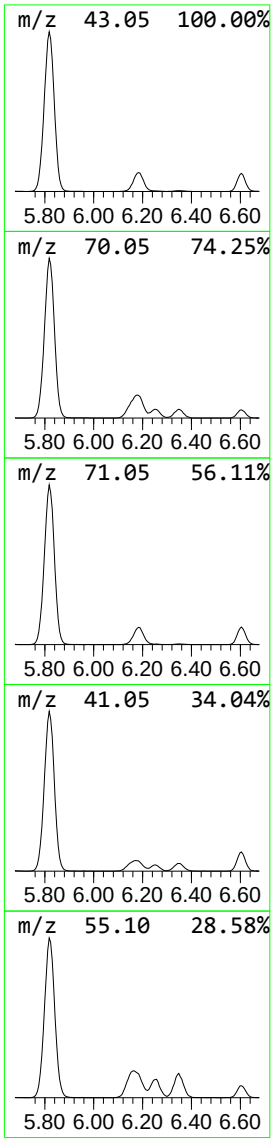
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexane, 2,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.178	65.86 ug/l	1558270	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	72
2	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	72
3	Pentane, 3-ethyl-	100	C7H16	000617-78-7	72
4	Propanoic acid, 2-methyl-, 3-met...	158	C9H18O2	002050-01-3	56
5	Octane, 4,5-dimethyl-	142	C10H22	015869-96-2	56





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Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

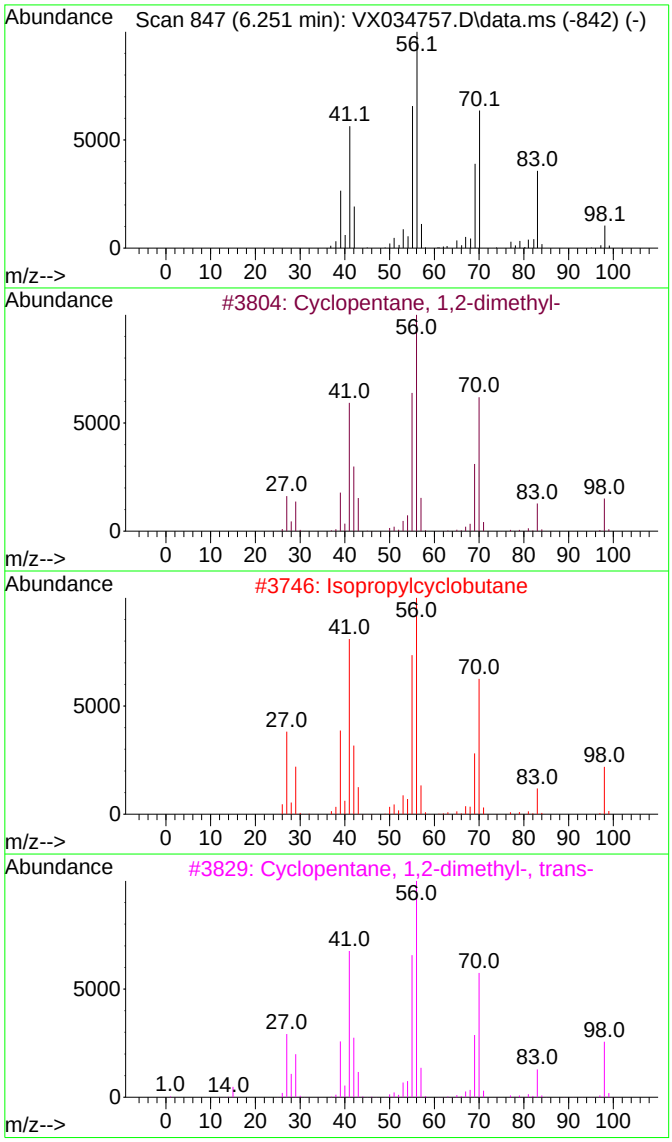
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

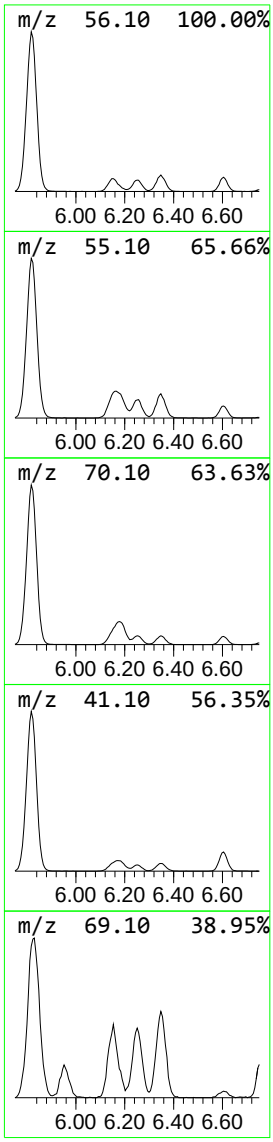
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, 1,2-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	19.97 ug/l	472525	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	86
2	Isopropylcyclobutane	98	C7H14	000872-56-0	83
3	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	78
4	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	70
5	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	70





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Data File : VX034757.D
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Operator : JC/MD
Sample : 02052-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

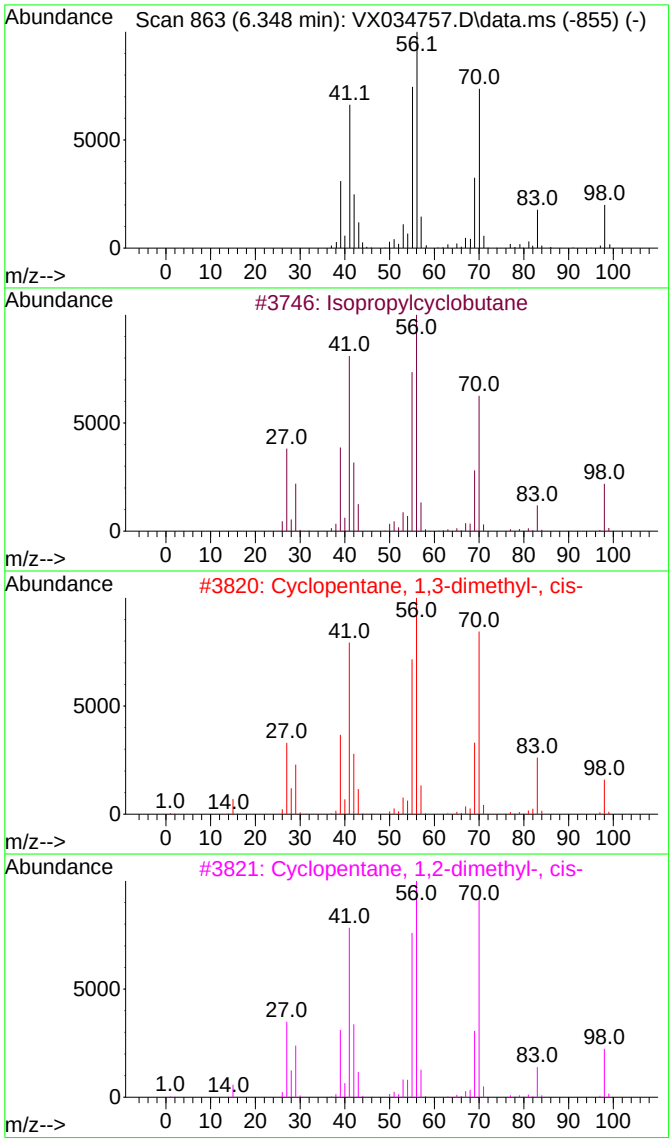
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

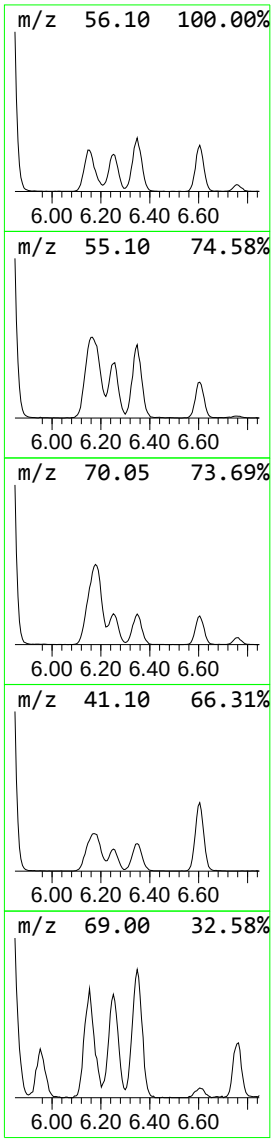
****

Peak Number 5 Isopropylcyclobutane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.348	25.50 ug/l	603336	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropylcyclobutane	98	C7H14	000872-56-0	97
2	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	93
3	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	91
4	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	91
5	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	91





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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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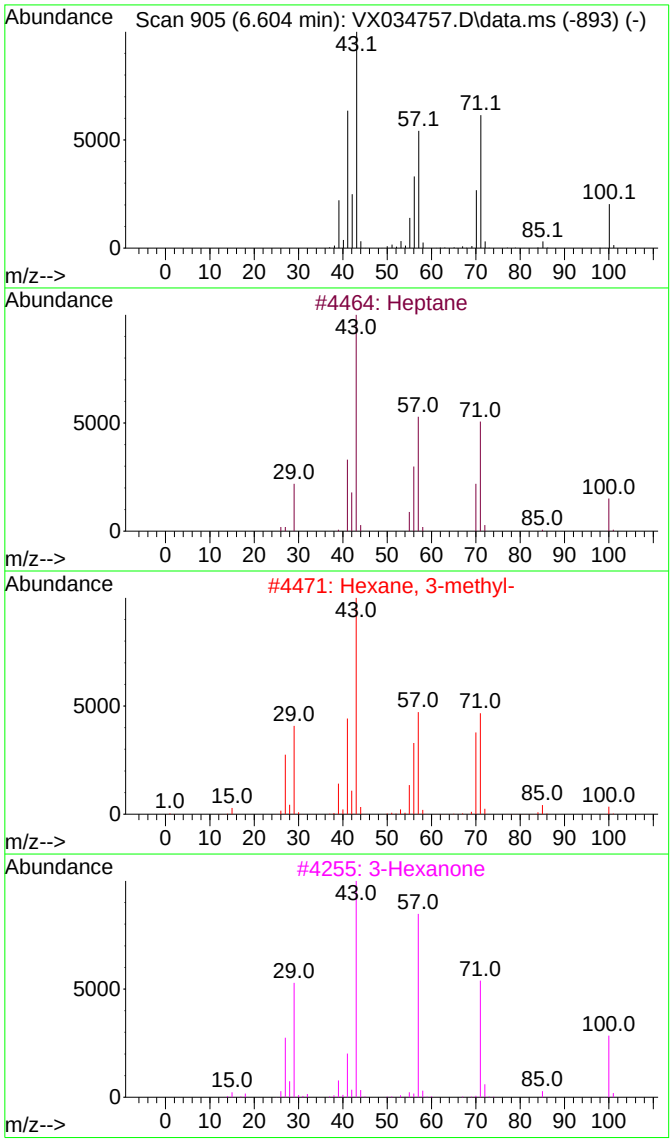
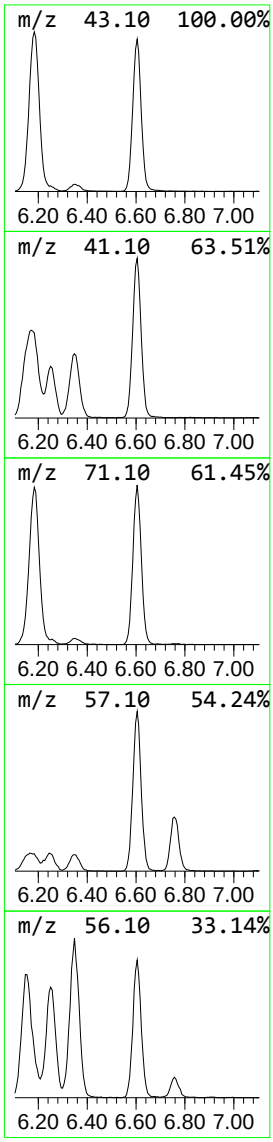
****

Peak Number 6 Heptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.604	48.56 ug/l	1149010	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	47
3	3-Hexanone	100	C6H12O	000589-38-8	46
4	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
5	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38





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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

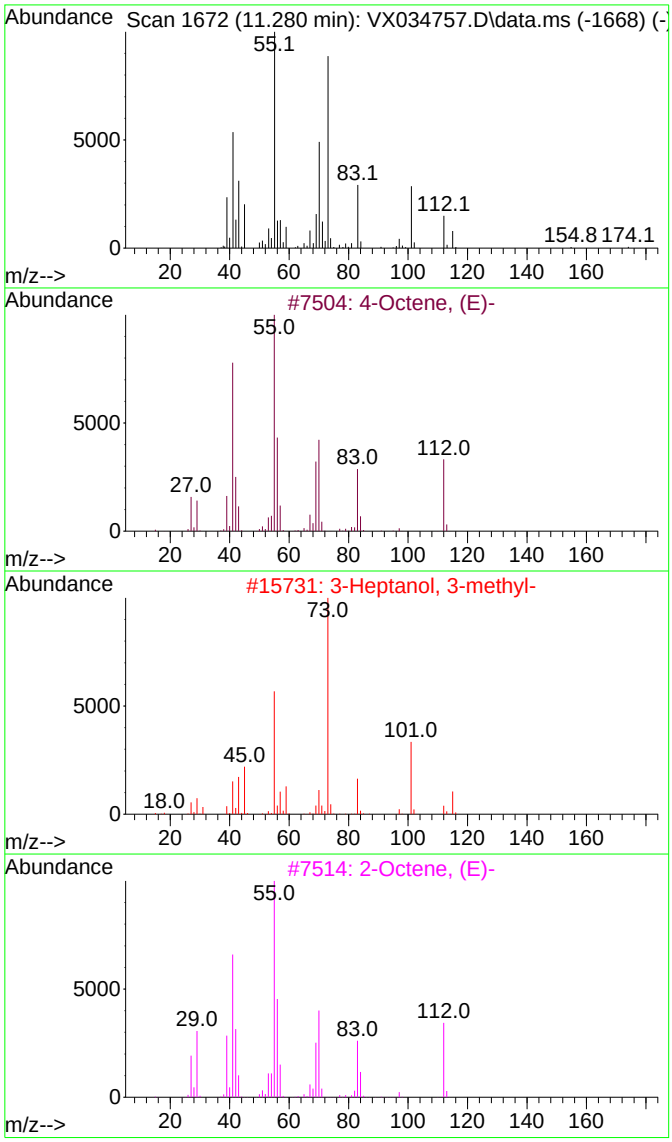
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

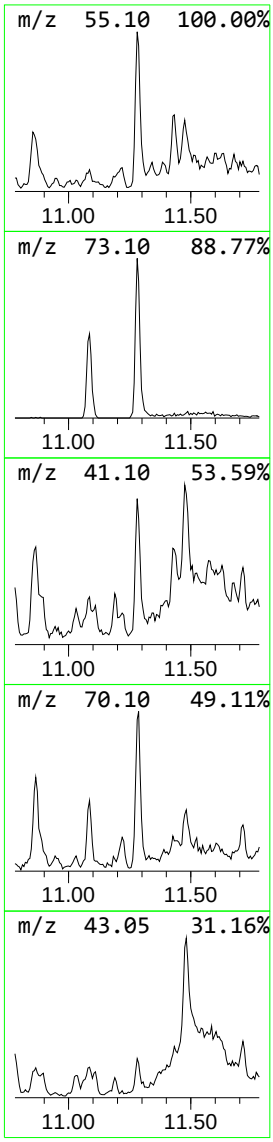
****

Peak Number 7 unknown11.280 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.280	5.51 ug/l	144449	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Octene, (E)-	112	C8H16	014850-23-8	43
2	3-Heptanol, 3-methyl-	130	C8H18O	005582-82-1	43
3	2-Octene, (E)-	112	C8H16	013389-42-9	43
4	3-Octene, (E)-	112	C8H16	014919-01-8	38
5	3-Octene, (Z)-	112	C8H16	014850-22-7	35





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TIC Library : C:\Database\NIST20.L
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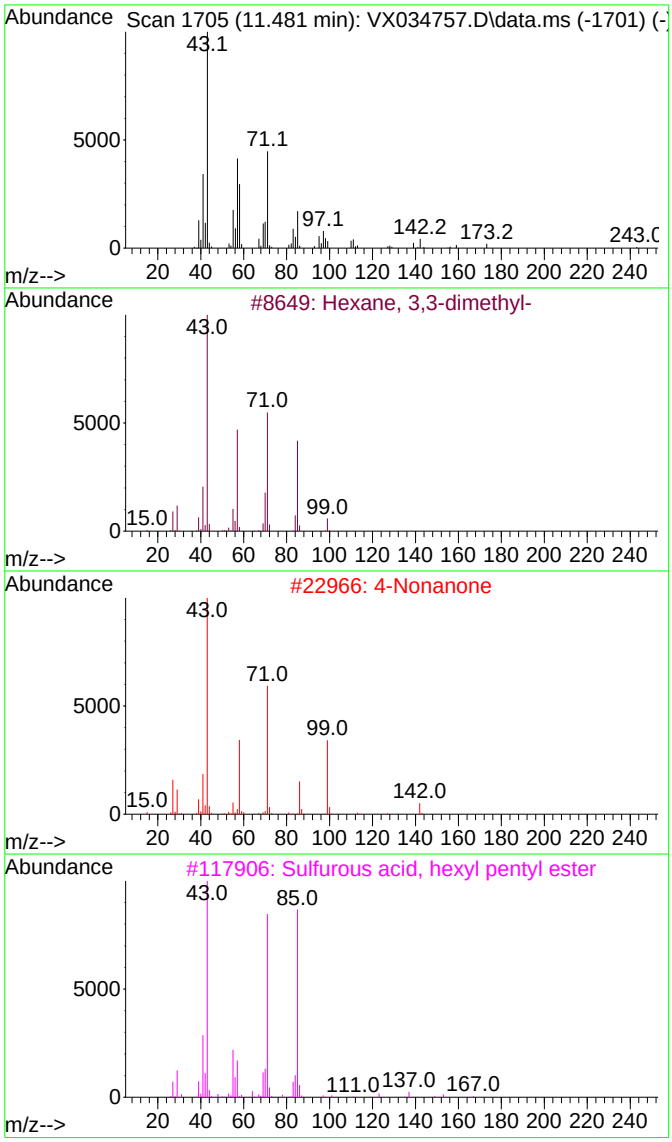
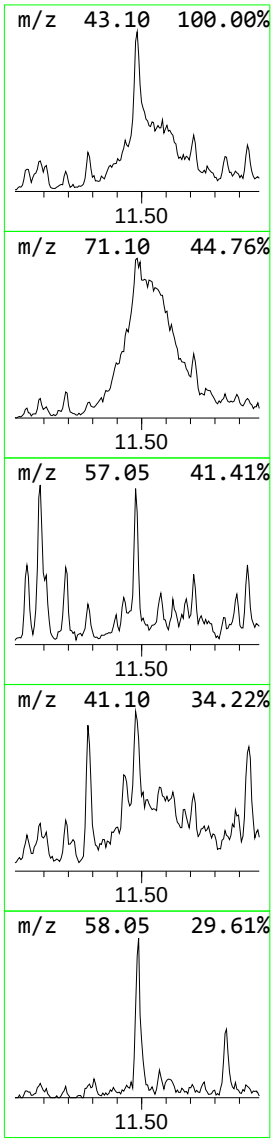
****
Peak Number 8 unknown11482 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.482	5.67 ug/l	148626	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	47
2	4-Nonanone	142	C9H18O	004485-09-0	47
3	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	43
4	Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	43
5	Decane	142	C10H22	000124-18-5	43





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Acq On : 27 Mar 2023 18:08
Operator : JC/MD
Sample : 02052-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

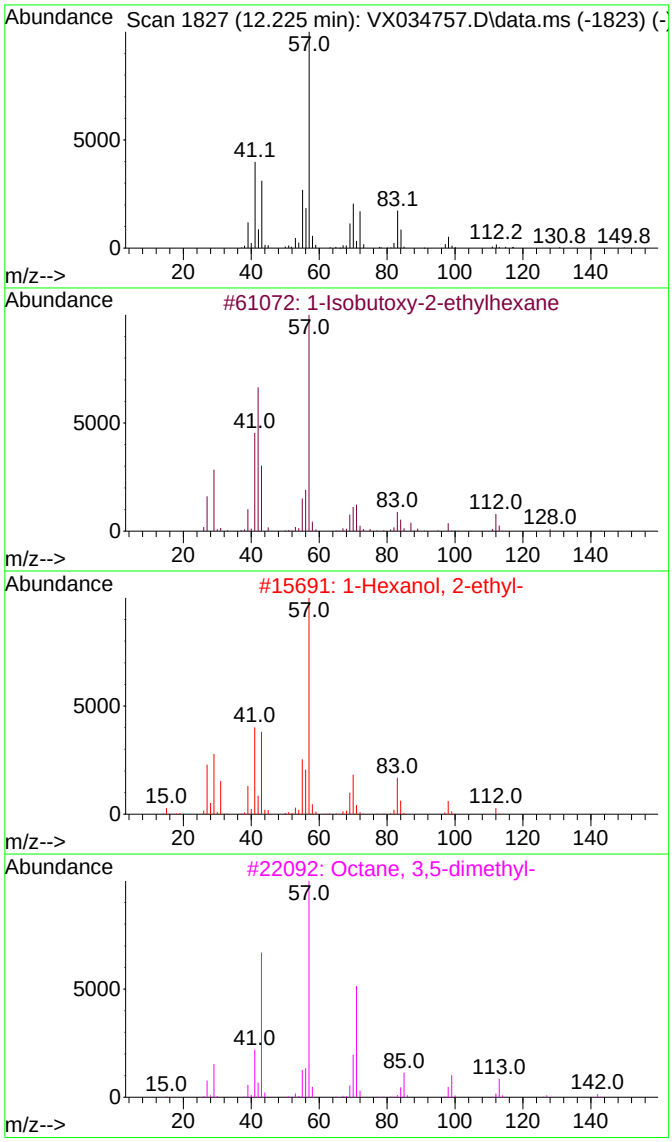
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

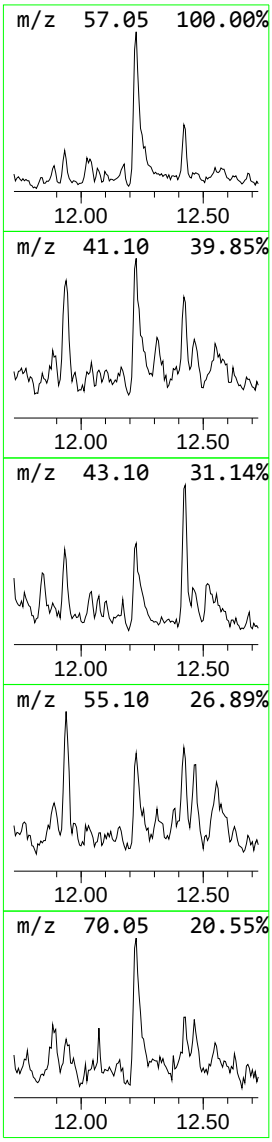
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Isobutoxy-2-ethylhexane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.225	6.34 ug/l	166242	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	78
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	59
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034757.D
Acq On : 27 Mar 2023 18:08
Operator : JC/MD
Sample : 02052-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Pentane, 2,3-di...	5.611	14.9	ug/l	3554550	1	5.550	11885400	50.0
Hexane, 3-methyl-	5.818	54.8	ug/l	13032500	1	5.550	11885400	50.0
Hexane, 2,3-dim...	6.178	65.9	ug/l	1558270	2	6.757	1183080	50.0
Cyclopentane, 1...	6.251	20.0	ug/l	472525	2	6.757	1183080	50.0
Isopropylcyclob...	6.348	25.5	ug/l	603336	2	6.757	1183080	50.0
Heptane	6.604	48.6	ug/l	1149010	2	6.757	1183080	50.0
unknown11.280	11.280	5.5	ug/l	144449	4	12.024	1311030	50.0
unknown11482	11.482	5.7	ug/l	148626	4	12.024	1311030	50.0
1-Isobutoxy-2-e...	12.225	6.3	ug/l	166242	4	12.024	1311030	50.0