LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034794.D
Acq On : 28 Mar 2023 15:41
Operator : JC/MD
Sample : 02052-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 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: VX034794.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	209	216	237	rBV	393922	958881	6.81%	1.948%
2	2.886	284	295	305	rVB	202461	476548	3.39%	0.968%
3	4.038	468	484	496	rBV2	49489	146836	1.04%	0.298%
4	4.196	496	510	531	rBV	173992	576018	4.09%	1.170%
5	5.111	644	660	681	rVB2	270124	978001	6.95%	1.987%
6	5.385	694	705	712	rBV	155491	453928	3.23%	0.922%
7	5.495	712	723	734	rVV	4003631	12687761	90.15%	25.772%
8	5.611	735	742	760	rVV	1259945	3903254	27.73%	7.928%
9	5.818	760	776	790	rVV	4847290	14074054	100.00%	28.588%
10	5.952	790	798	817	rVB	201409	540800	3.84%	1.099%
11	6.178	819	835	842	rBV5	445832	1722718	12.24%	3.499%
12	6.251	842	847	855	rVV2	191951	510295	3.63%	1.037%
13	6.349	855	863	876	rVB	235689	669477	4.76%	1.360%
14	6.605	894	905	921	rBV	593799	1446748	10.28%	2.939%
15	6.757	921	930	952	rVB	468475	1162785	8.26%	2.362%
16	7.373	1020	1031	1043	rBV2	140510	345106	2.45%	0.701%
17	8.647	1234	1240	1246	rVV	969876	1525083	10.84%	3.098%
18	8.714	1246	1251	1265	rVB	1129381	1775269	12.61%	3.606%
19	10.055	1466	1471	1487	rVB	905701	1317750	9.36%	2.677%
20	10.860	1595	1603	1614	rVB4	71867	183449	1.30%	0.373%
21	11.085	1634	1640	1651	rVB	701055	1075463	7.64%	2.185%
22	11.287	1668	1673	1680	rBV2	138846	218796	1.55%	0.444%
23	11.433	1693	1697	1701	rVV3	75370	154765	1.10%	0.314%
24	11.476	1701	1704	1715	rVB3	98538	183957	1.31%	0.374%
25	12.024	1789	1794	1800	rBV	959998	1239054	8.80%	2.517%
26	12.226	1823	1827	1837	rBV2	95041	245026	1.74%	0.498%
27	12.555	1872	1881	1889	rBV6	45086	149980	1.07%	0.305%
28	13.414	2016	2022	2030	rBV6	130415	209108	1.49%	0.425%
29	14.981	2274	2279	2280	rBV	104786	142598	1.01%	0.290%
30	15.024	2284	2286	2295	rVB3	121876	157232	1.12%	0.319%

Sum of corrected areas: 49230740

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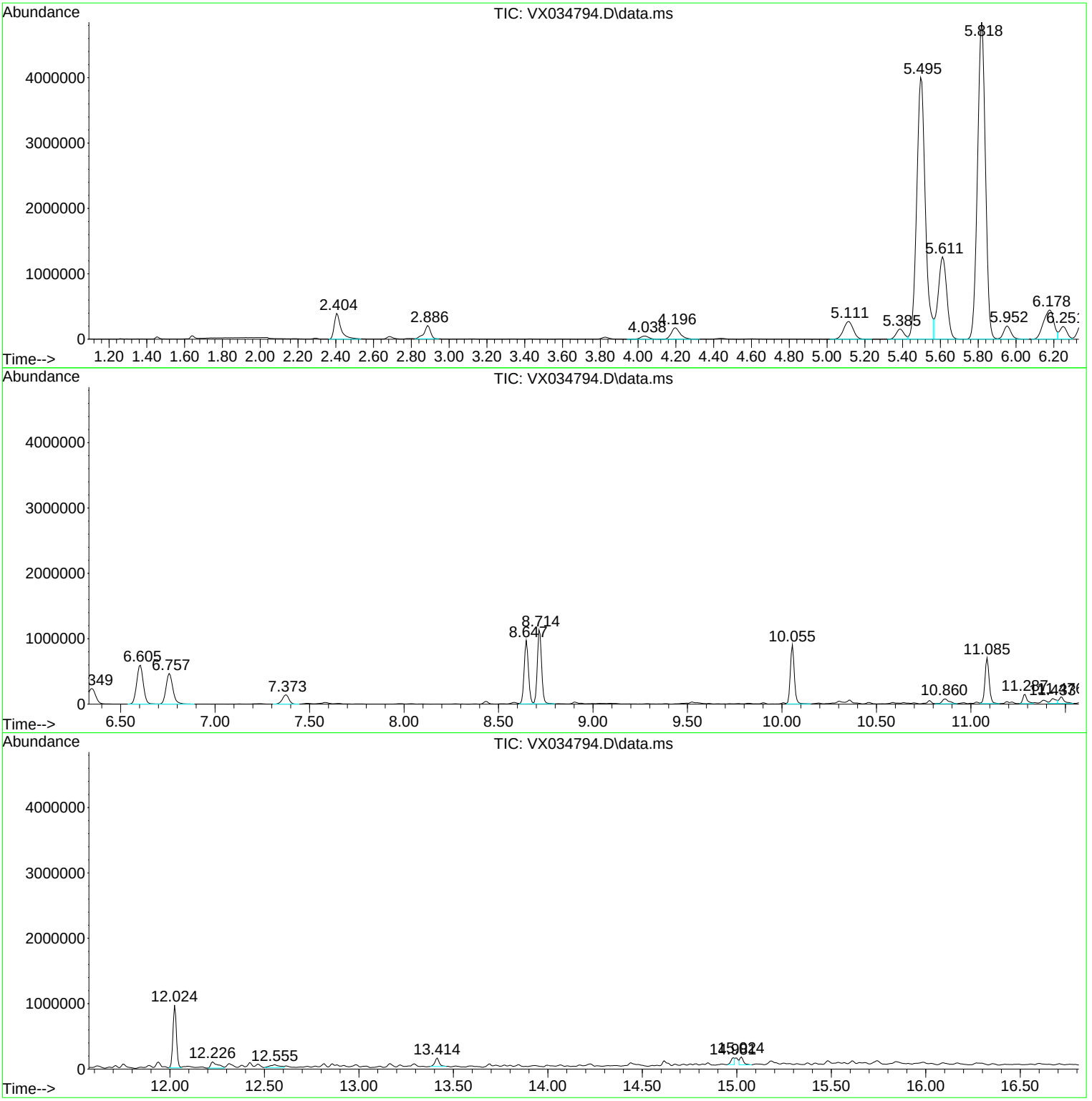
ALS Vial : 18 Sample Multiplier: 1

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



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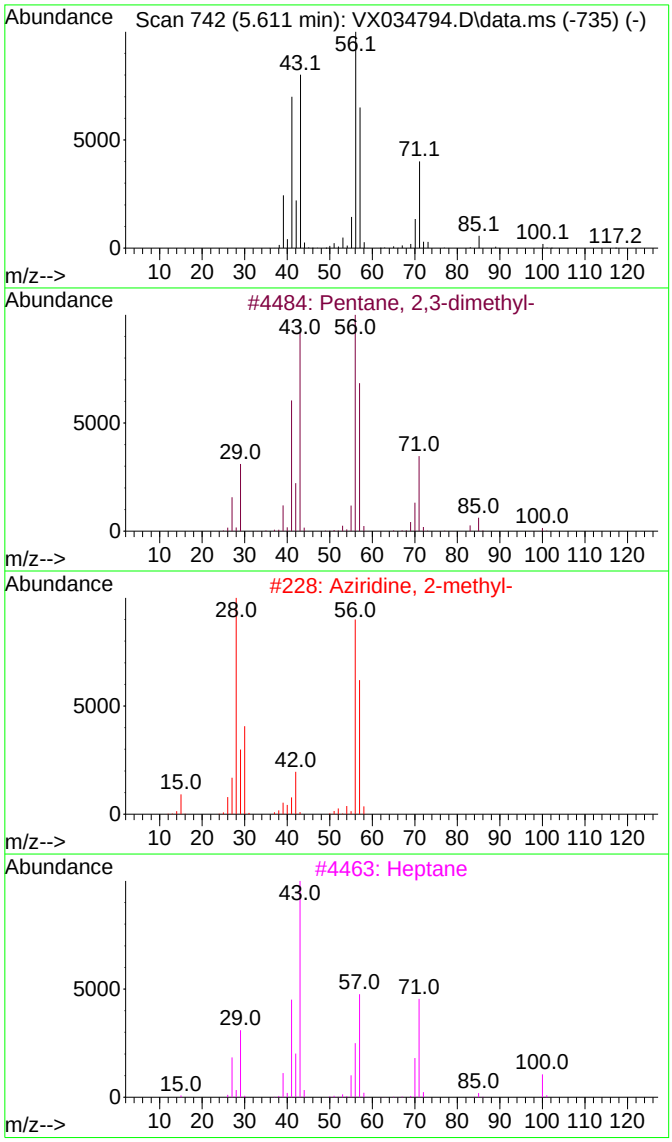
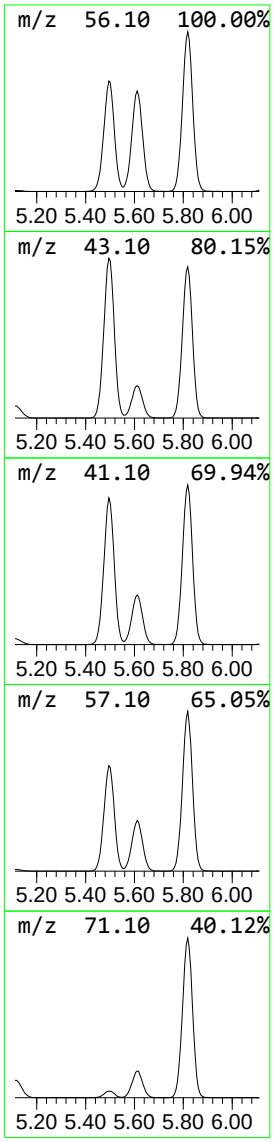
****
Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.611	15.38 ug/l	3903250	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	43
3	Heptane	100	C7H16	000142-82-5	37
4	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	37
5	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	32





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Data File : VX034794.D
Acq On : 28 Mar 2023 15:41
Operator : JC/MD
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

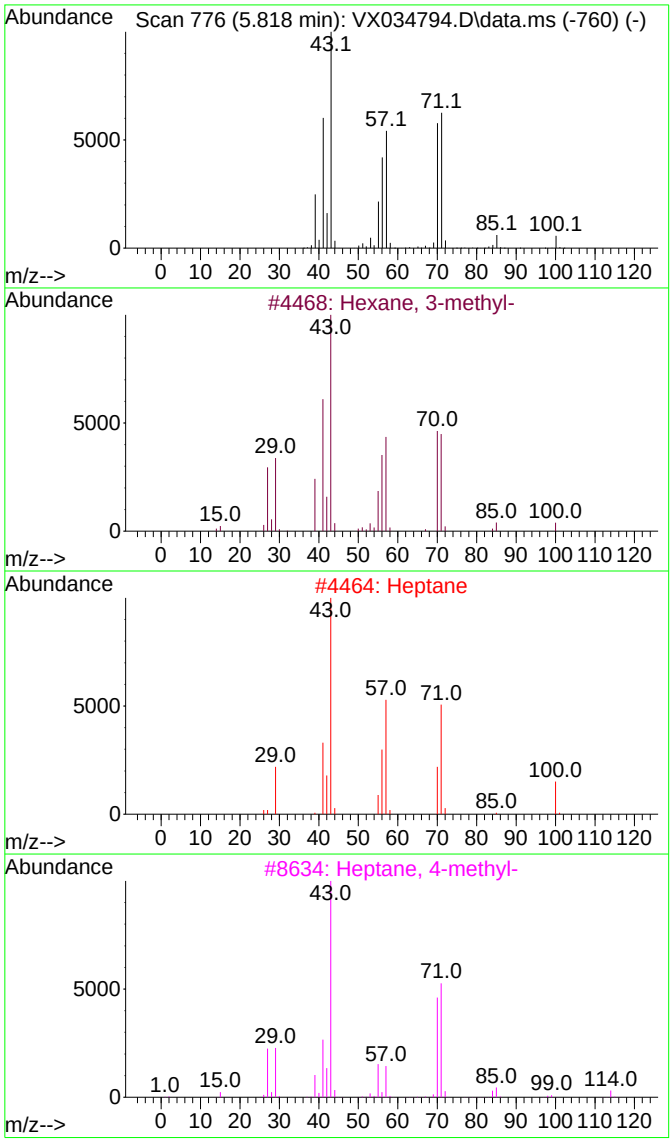
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

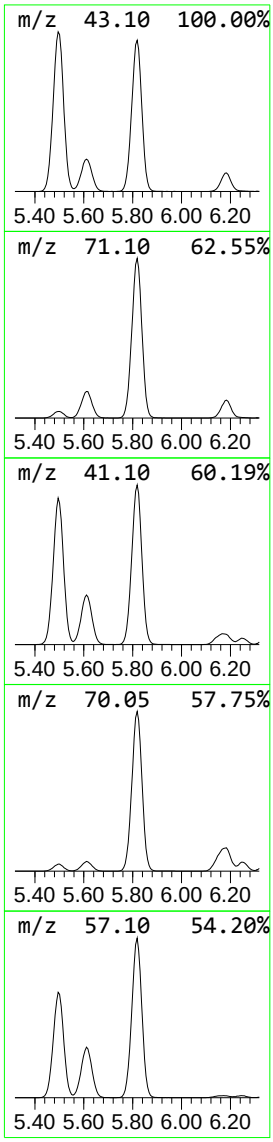
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.818	55.46 ug/l	14074100	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
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 : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

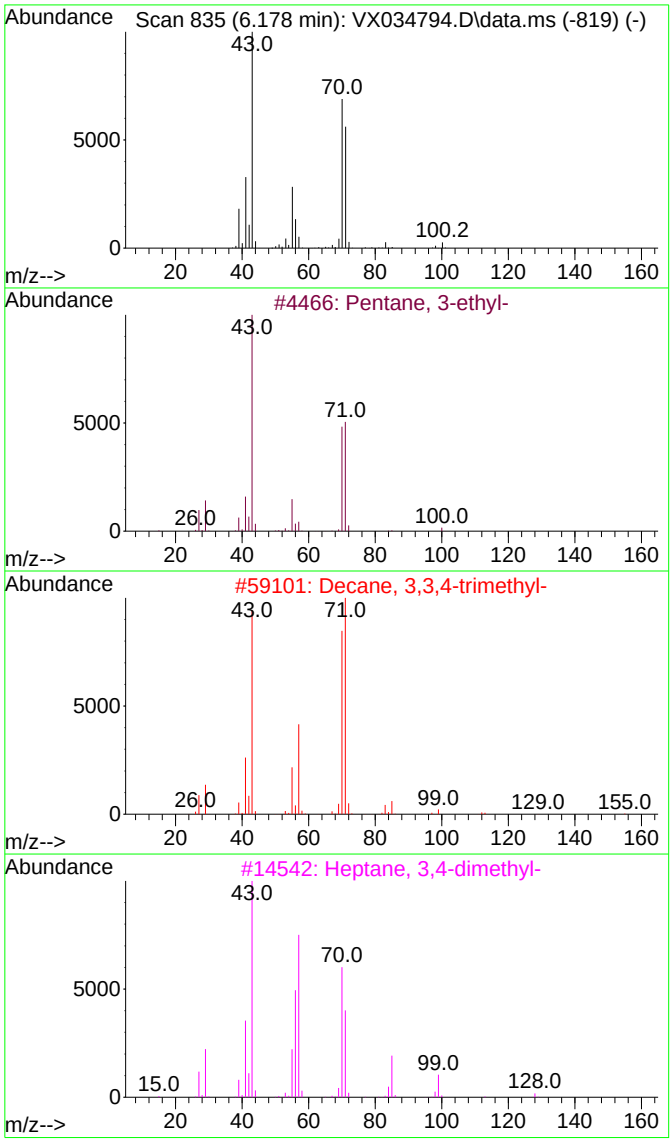
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

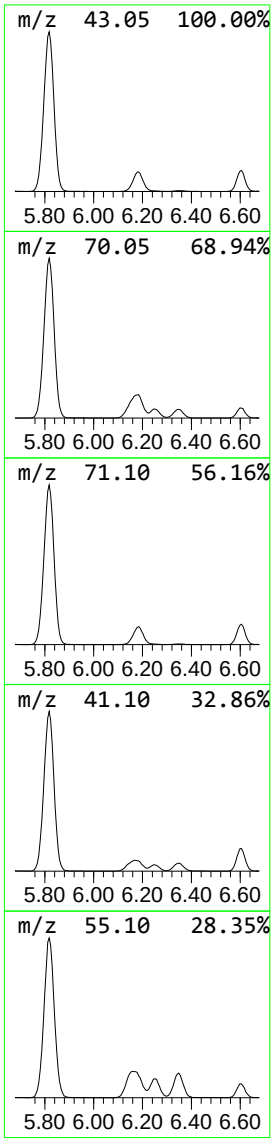
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 3-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.178	74.08 ug/l	1722720	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
2	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	72
3	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	72
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	72
5	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	64





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Operator : JC/MD
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Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

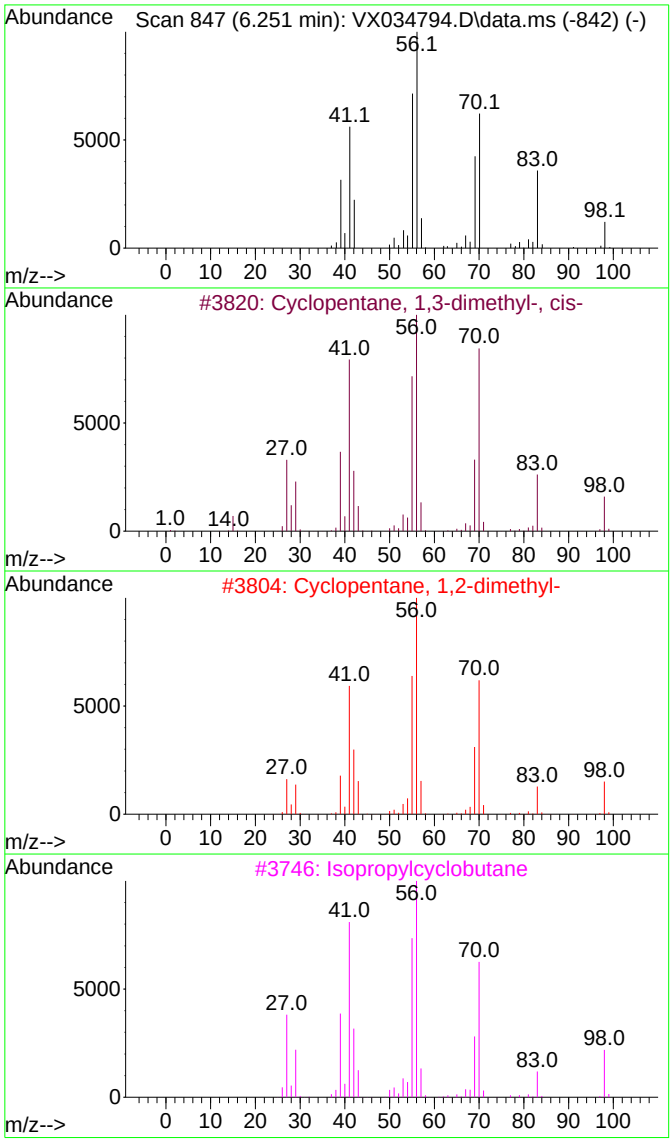
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

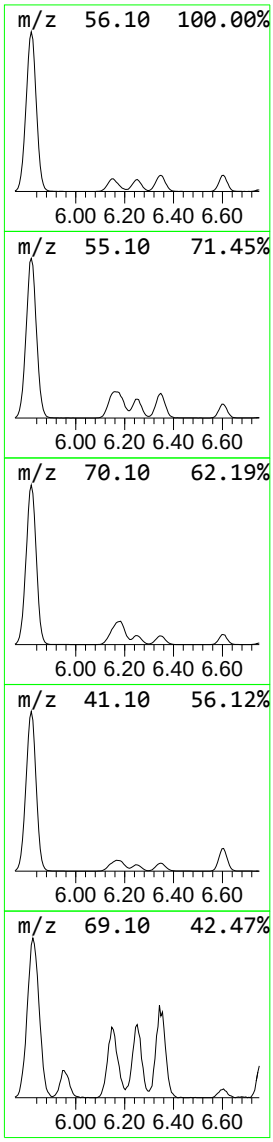
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, 1,3-dimethyl-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	21.94 ug/l	510295	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	90
2	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	87
3	Isopropylcyclobutane	98	C7H14	000872-56-0	86
4	Cycloheptane	98	C7H14	000291-64-5	83
5	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	80





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Operator : JC/MD
Sample : 02052-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

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

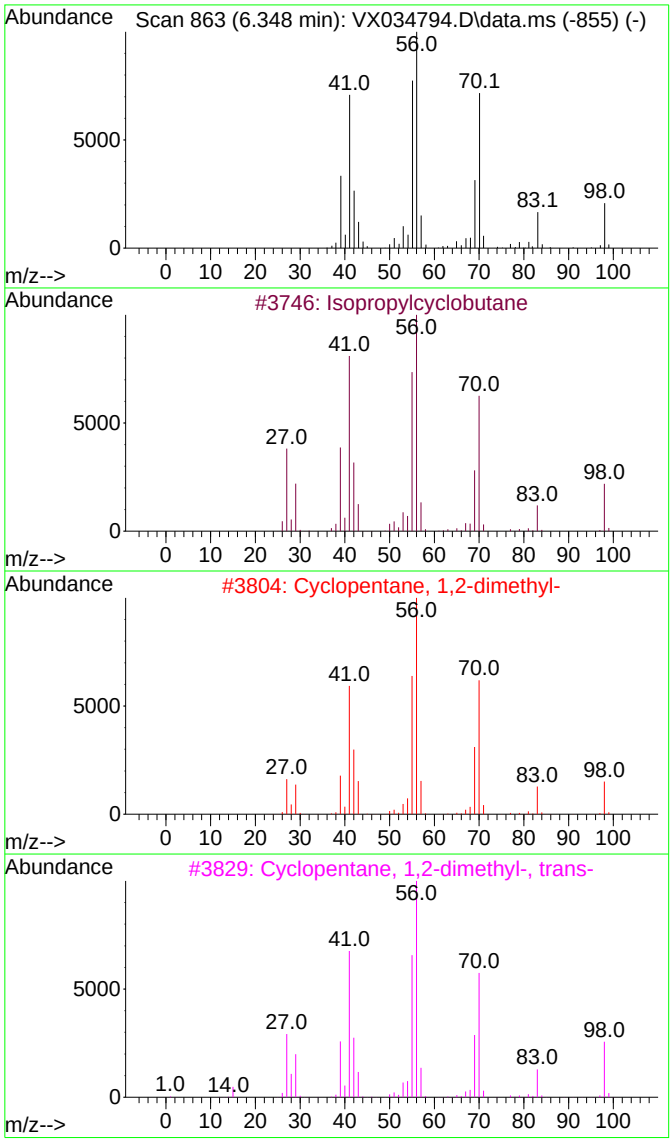
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

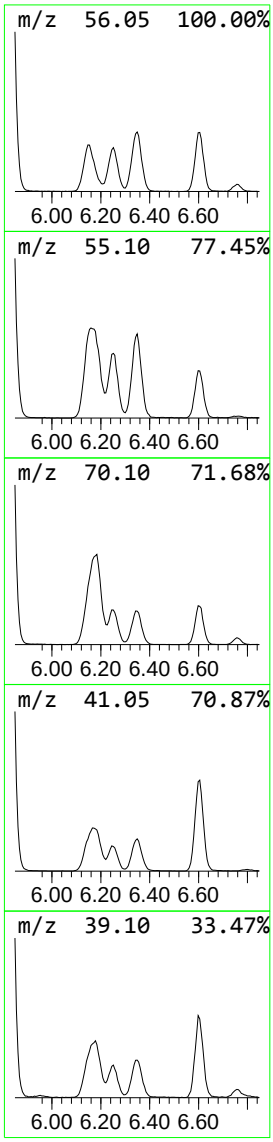
****

Peak Number 5 Isopropylcyclobutane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.348	28.79 ug/l	669477	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropylcyclobutane	98	C7H14	000872-56-0	97
2	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	91
3	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	91
4	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	91
5	1-Heptene	98	C7H14	000592-76-7	86





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

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

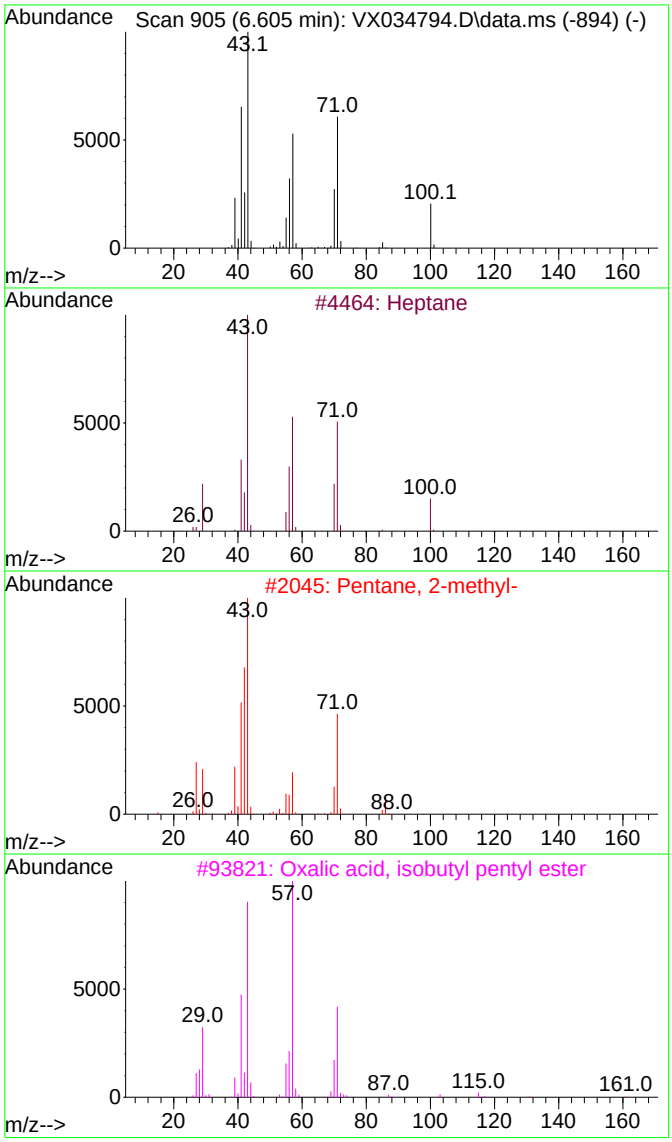
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

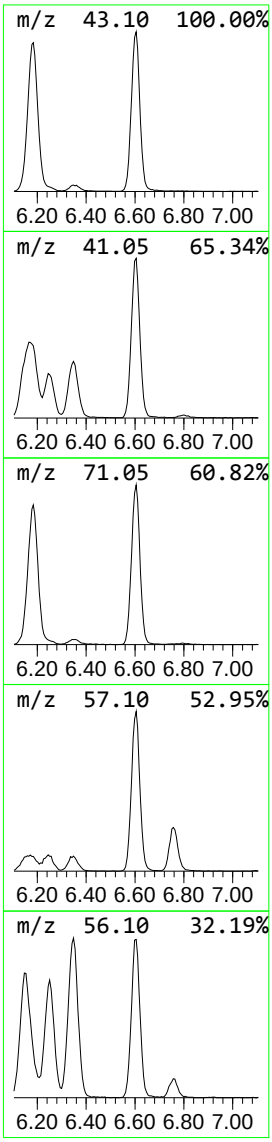
****

Peak Number 6 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.605	62.21 ug/l	1446750	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	43
3	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	42
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	40
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	38





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Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

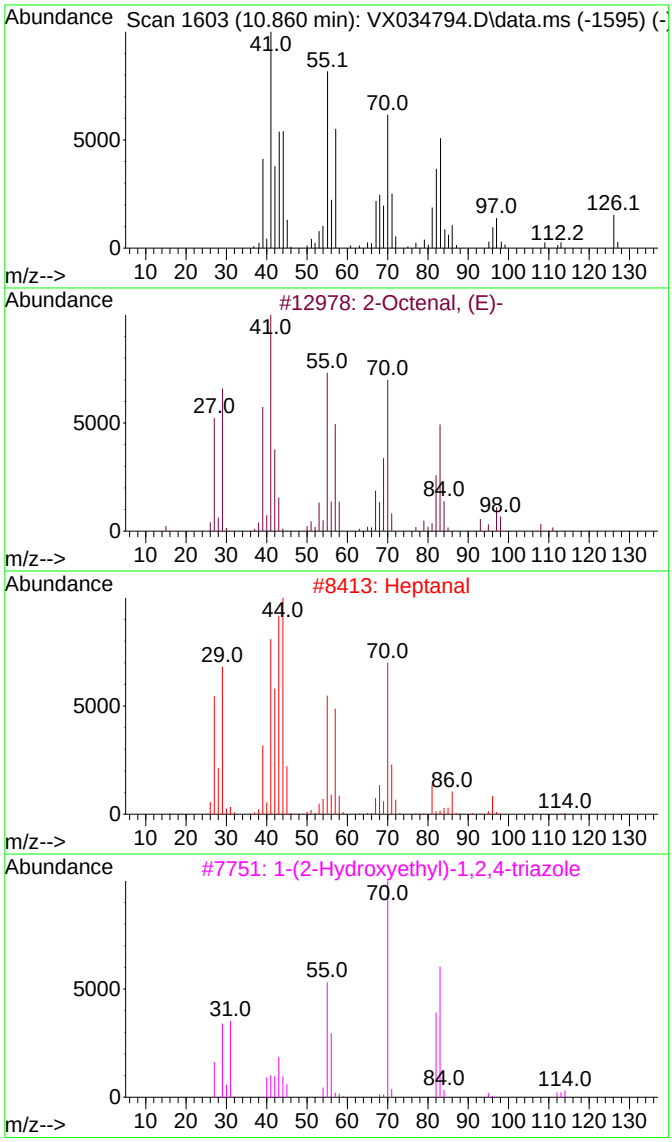
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

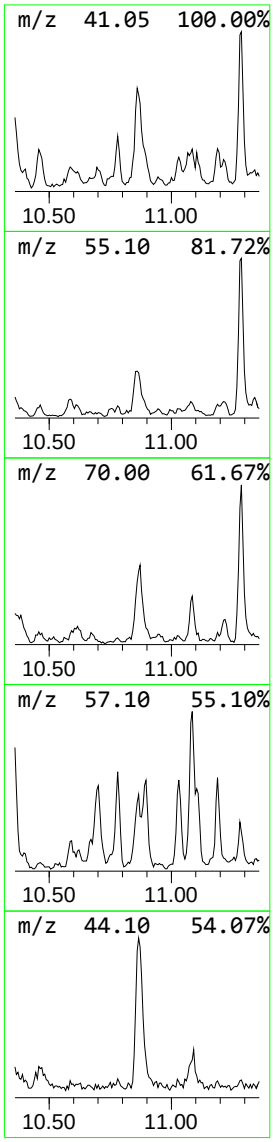
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 unknown10.860 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.860	6.96 ug/l	183449	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octenal, (E)-	126	C8H14O	002548-87-0	43
2	Heptanal	114	C7H14O	000111-71-7	43
3	1-(2-Hydroxyethyl)-1,2,4-triazole	113	C4H7N3O	003273-14-1	35
4	Cyclohexanone, 2,3-dimethyl-	126	C8H14O	013395-76-1	30
5	Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	30





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Quant Title : SW846 8260

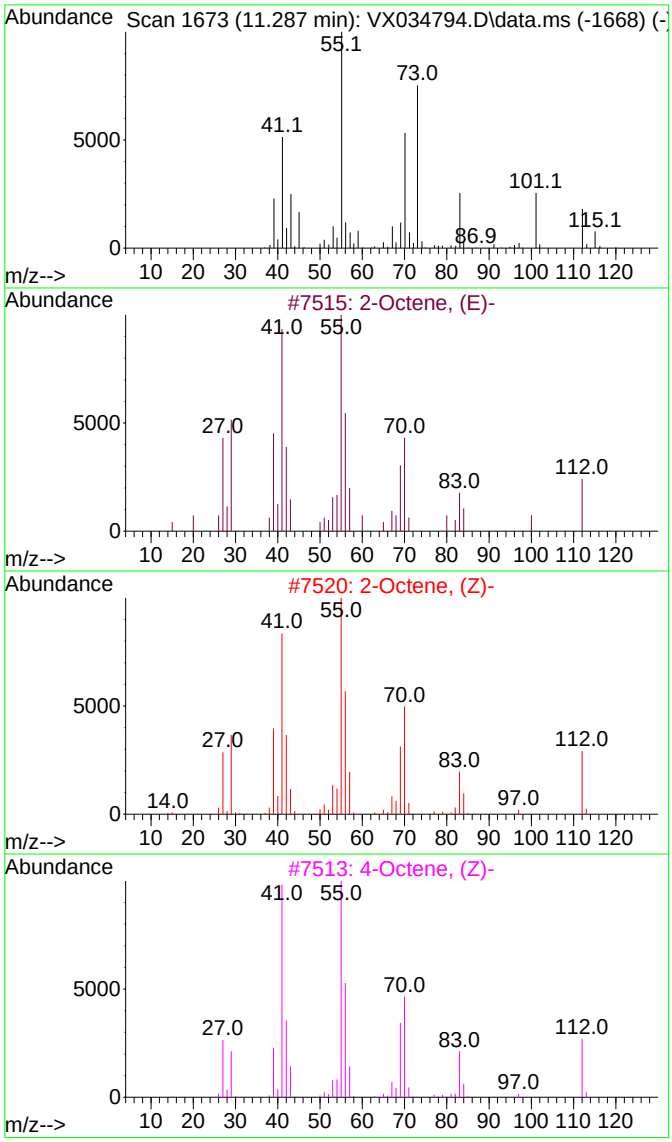
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

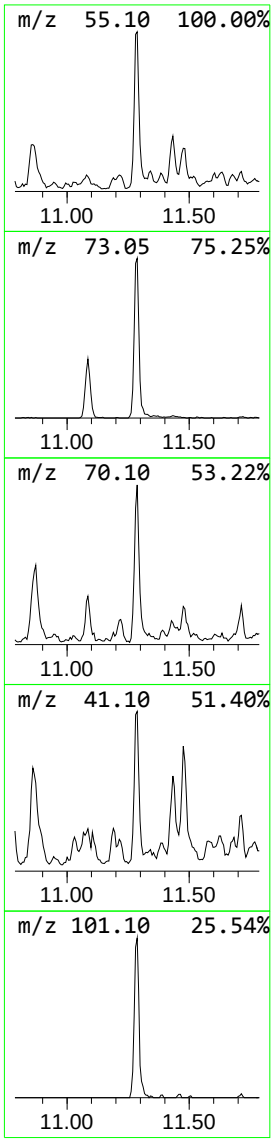
****

Peak Number 8 unknown11.287 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.287	8.83 ug/l	218796	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octene, (E)-	112	C8H16	013389-42-9	47
2	2-Octene, (Z)-	112	C8H16	007642-04-8	46
3	4-Octene, (Z)-	112	C8H16	007642-15-1	43
4	3-Ethyl-3-hexene	112	C8H16	016789-51-8	43
5	2-Heptene, 3-methyl-	112	C8H16	003404-75-9	43





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Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

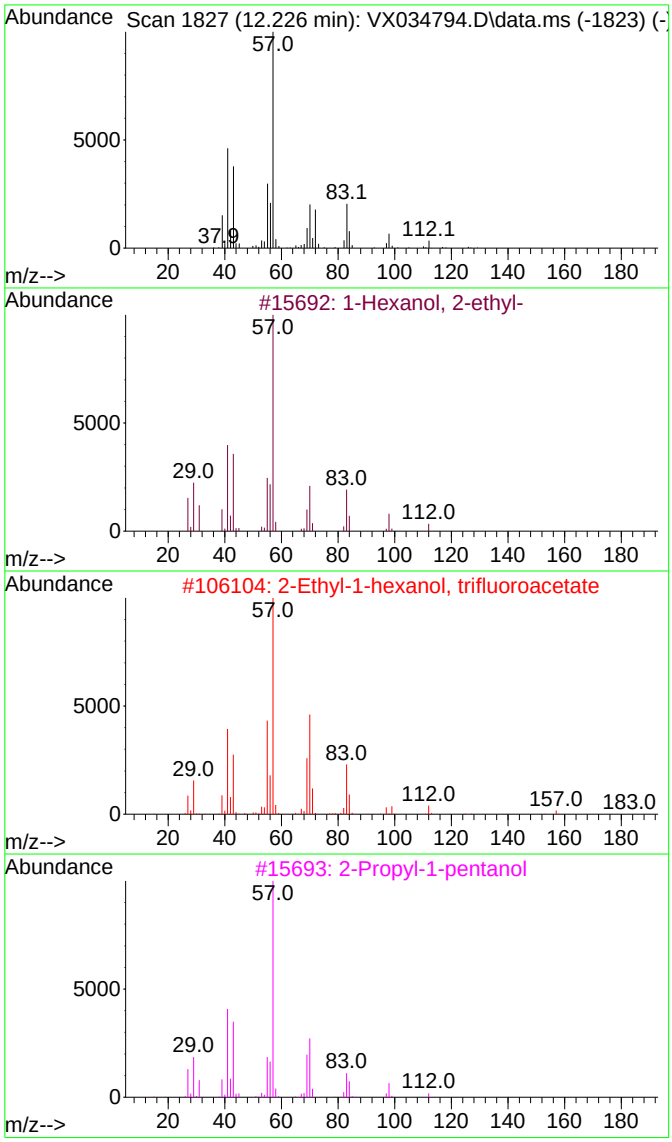
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

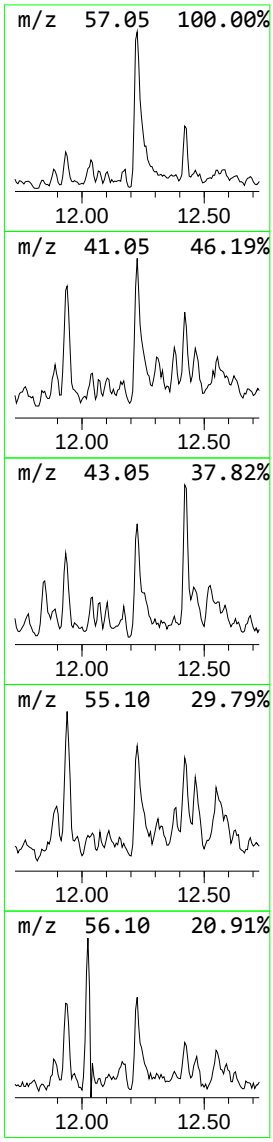
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.226	9.89 ug/l	245026	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2	2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	47
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	43
4	Carbonic acid, butyl heptyl ester	216	C12H24O3	1000314-63-4	43
5	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034794.D
Acq On : 28 Mar 2023 15:41
Operator : JC/MD
Sample : 02052-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1525

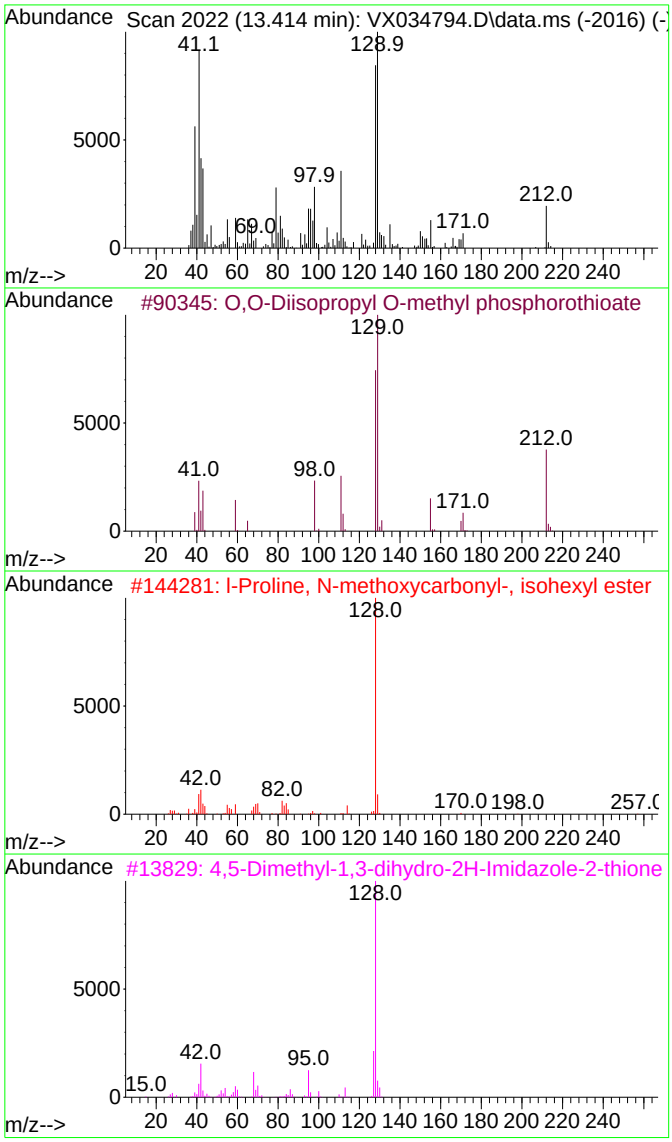
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

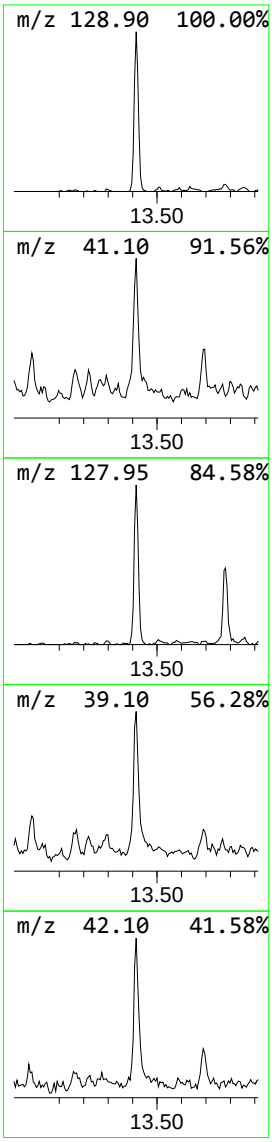
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 O,O-Diisopropyl O-methyl ph... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.414	8.44 ug/l	209108	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	O,O-Diisopropyl O-methyl phospho...	212	C7H17O3PS	1000306-07-1	90
2	l-Proline, N-methoxycarbonyl-, i...	257	C13H23NO4	1000314-40-2	35
3	4,5-Dimethyl-1,3-dihydro-2H-Imid...	128	C5H8N2S	001192-72-9	27
4	2,3-Furandione, dihydro-4,4-dime...	128	C6H8O3	013031-04-4	27
5	2-Heptenoic acid, pentadecyl ester	338	C22H42O2	1000406-10-0	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034794.D
Acq On : 28 Mar 2023 15:41
Operator : JC/MD
Sample : 02052-02
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 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	15.4	ug/l	3903250	1	5.544	12687800	50.0
Hexane, 3-methyl-	5.818	55.5	ug/l	14074100	1	5.544	12687800	50.0
Pentane, 3-ethyl-	6.178	74.1	ug/l	1722720	2	6.757	1162790	50.0
Cyclopentane, 1...	6.251	21.9	ug/l	510295	2	6.757	1162790	50.0
Isopropylcyclob...	6.348	28.8	ug/l	669477	2	6.757	1162790	50.0
Heptane	6.605	62.2	ug/l	1446750	2	6.757	1162790	50.0
unknown10.860	10.860	7.0	ug/l	183449	3	10.055	1317750	50.0
unknown11.287	11.287	8.8	ug/l	218796	4	12.024	1239050	50.0
1-Hexanol, 2-et...	12.226	9.9	ug/l	245026	4	12.024	1239050	50.0
O,O-Diisopropyl...	13.414	8.4	ug/l	209108	4	12.024	1239050	50.0