LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041272.D
Acq On : 29 Apr 2024 13:30
Operator : JC/MD
Sample : P2257-02
Misc : 1.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1356

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\82X042224W.M
Title : SW846 8260

Signal : TIC: VX041272.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.105	643	659	676	rBV2	124503	454971	1.68%	0.463%
2	5.489	711	722	733	rVV	3373412	10502658	38.87%	10.681%
3	5.605	733	741	761	rVV	1153725	3740350	13.84%	3.804%
4	5.818	761	776	791	rVV	6434211	18616406	68.89%	18.933%
5	5.952	791	798	817	rVV	96206	333104	1.23%	0.339%
6	6.178	819	835	842	rVV2	834853	2987654	11.06%	3.038%
7	6.245	842	846	854	rVV2	284991	707074	2.62%	0.719%
8	6.342	854	862	876	rVB	341323	953899	3.53%	0.970%
9	6.617	889	907	923	rBV	10871404	27022930	100.00%	27.482%
10	6.757	923	930	950	rVB	218337	574114	2.12%	0.584%
11	7.238	999	1009	1018	rBV	340845	776438	2.87%	0.790%
12	7.372	1018	1031	1042	rVV2	1255039	3209011	11.88%	3.264%
13	7.488	1042	1050	1055	rVV	320702	654507	2.42%	0.666%
14	7.555	1055	1061	1069	rVV	441664	937316	3.47%	0.953%
15	7.647	1069	1076	1087	rVV	541812	1086359	4.02%	1.105%
16	8.647	1234	1240	1247	rBV	433373	666428	2.47%	0.678%
17	10.055	1466	1471	1478	rVB	424929	583184	2.16%	0.593%
18	11.085	1634	1640	1650	rVB2	460446	784919	2.90%	0.798%
19	11.378	1684	1688	1694	rBV	208136	363440	1.34%	0.370%
20	11.475	1701	1704	1709	rVB	500128	584234	2.16%	0.594%
21	11.750	1746	1749	1759	rVB	337921	521158	1.93%	0.530%
22	11.890	1765	1772	1777	rVB2	214951	307996	1.14%	0.313%
23	12.024	1789	1794	1799	rBV	520432	740333	2.74%	0.753%
24	12.317	1838	1842	1850	rVB3	334893	592974	2.19%	0.603%
25	12.420	1850	1859	1863	rBV	401525	553922	2.05%	0.563%
26	12.963	1944	1948	1955	rVB2	175627	309347	1.14%	0.315%
27	13.164	1974	1981	1986	rBV3	173865	295690	1.09%	0.301%
28	13.268	1991	1998	1999	rVV3	201071	302681	1.12%	0.308%
29	13.292	1999	2002	2007	rVB2	330592	428409	1.59%	0.436%
30	13.420	2019	2023	2032	rVB	237709	392977	1.45%	0.400%
31	14.231	2149	2156	2164	rVB2	192622	337661	1.25%	0.343%
32	15.560	2368	2374	2381	rBV	12265411	18006308	66.63%	18.312%

Sum of corrected areas: 98328452

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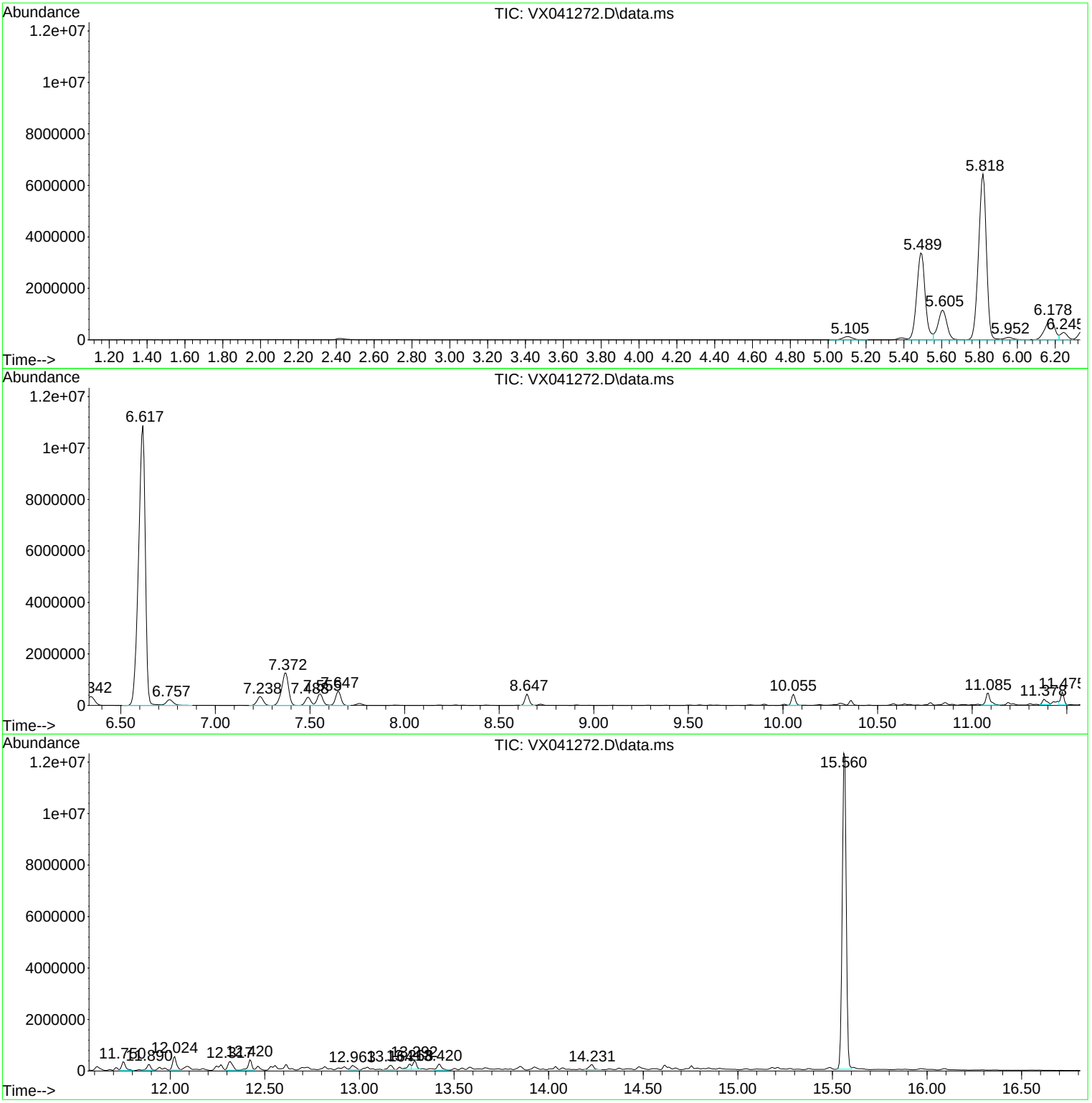
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1356

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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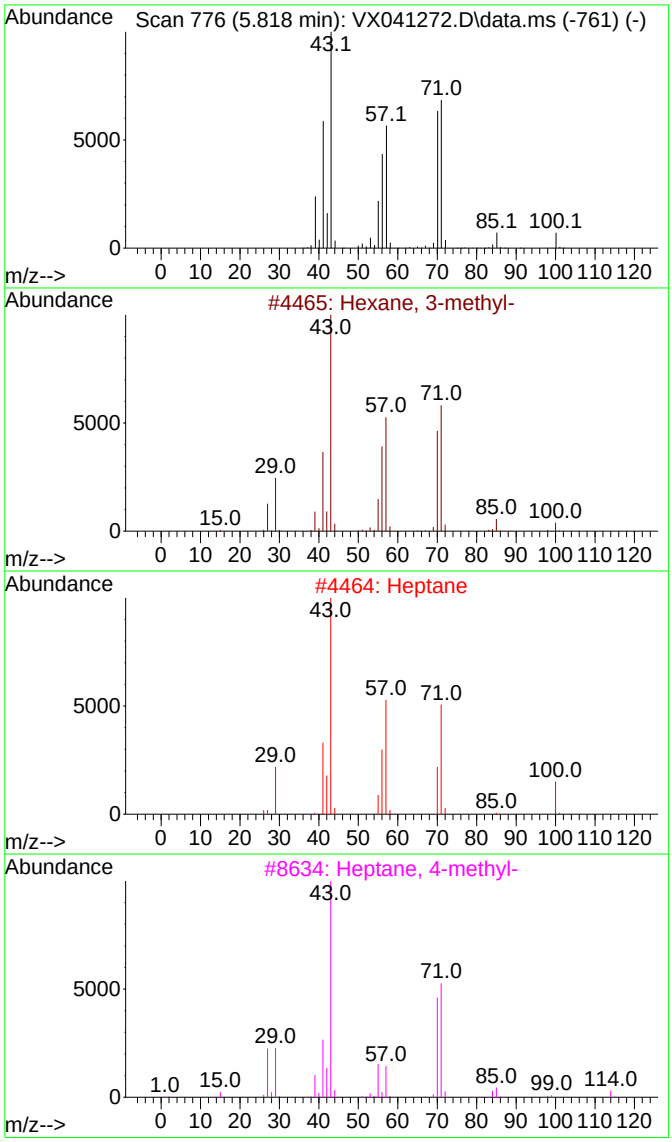
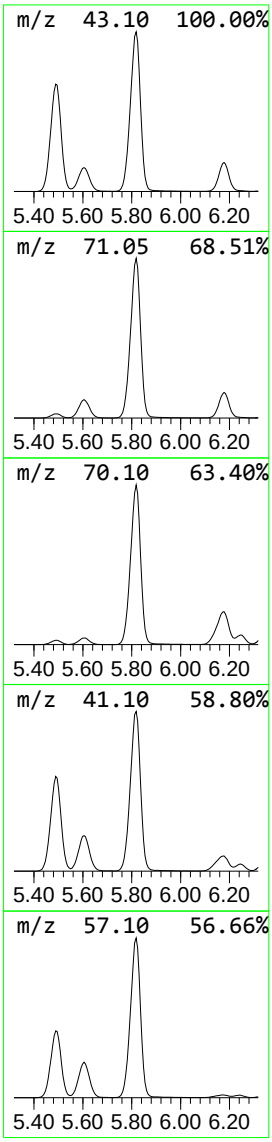
****
Peak Number 1 Hexane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.818	88.63 ug/l	18616400	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	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	53
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53





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Operator : JC/MD
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1356

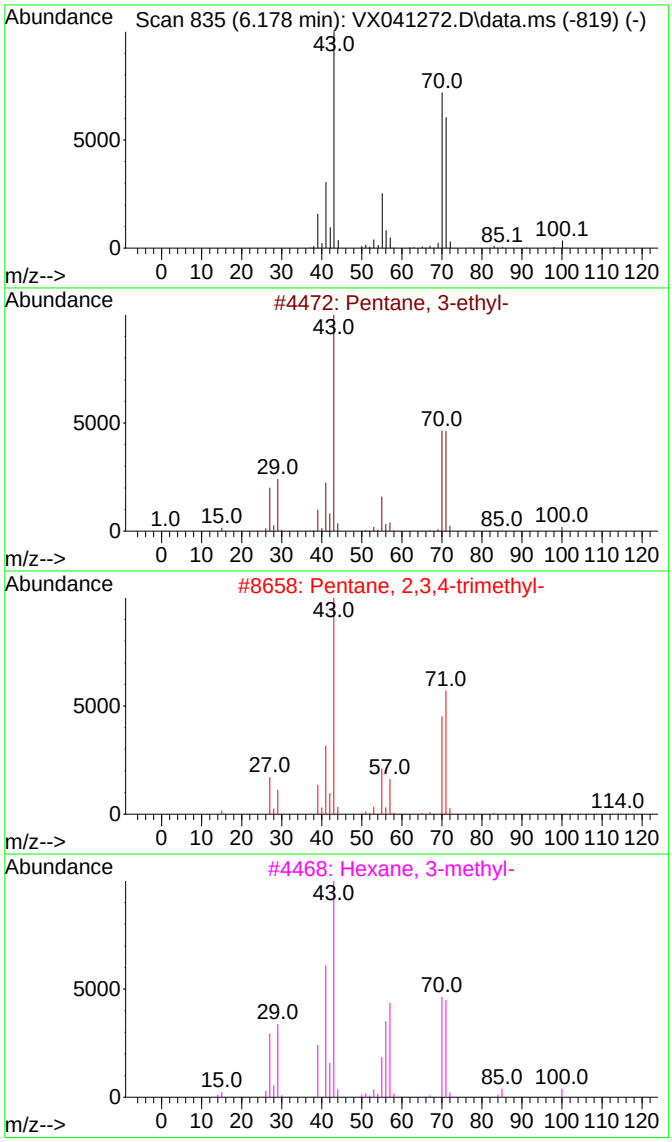
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

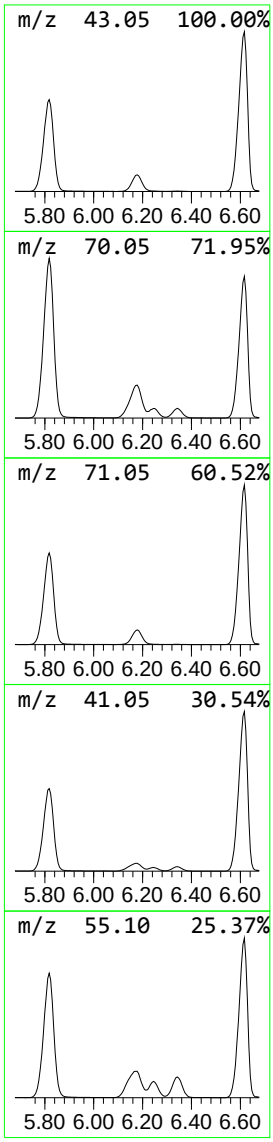
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane, 3-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.178	260.20 ug/l	2987650	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-ethyl-	100	C7H16	000617-78-7	80
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	78
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	64
4	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	64
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64





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Data File : VX041272.D
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Operator : JC/MD
Sample : P2257-02
Misc : 1.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1356

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

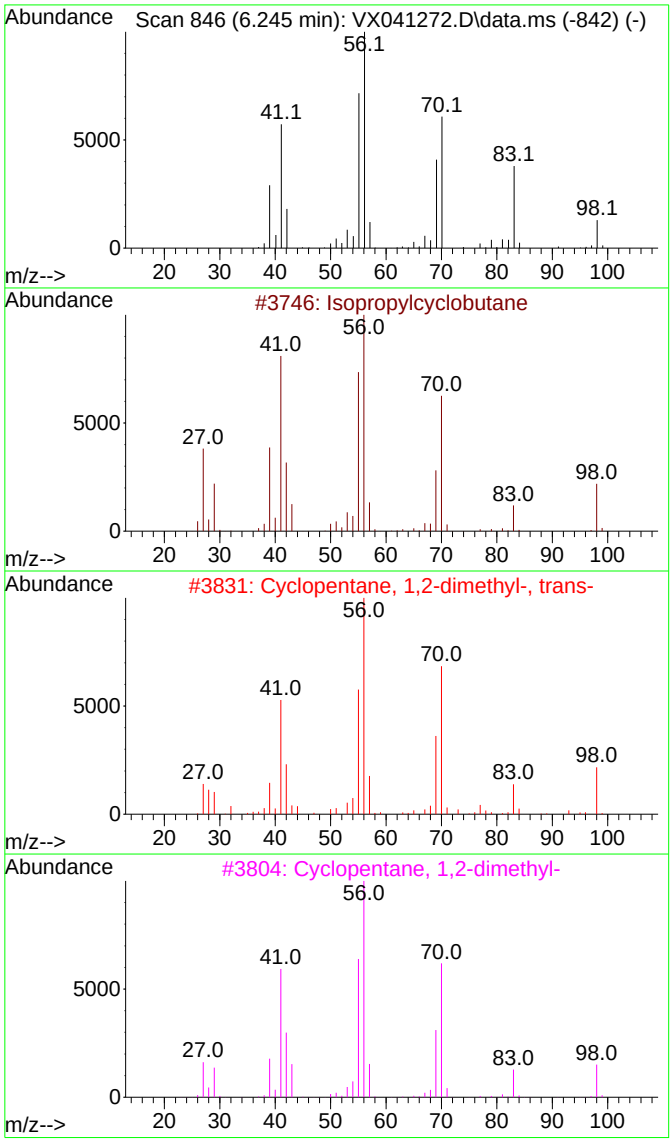
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

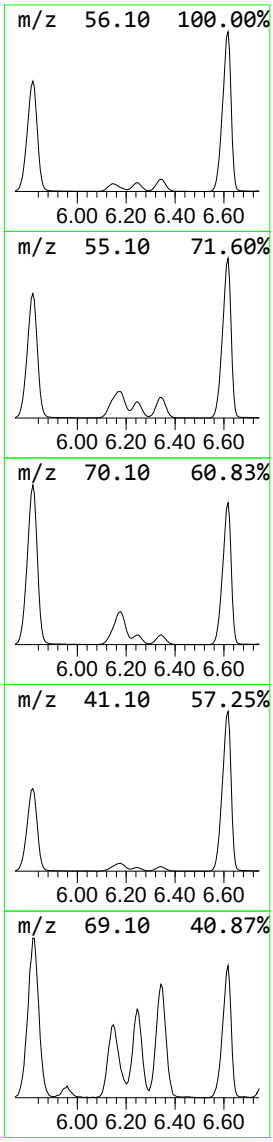
****

Peak Number 3 Isopropylcyclobutane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.245	61.58 ug/l	707074	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropylcyclobutane	98	C7H14	000872-56-0	87
2	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	80
3	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	80
4	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	64
5	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	62





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Data File : VX041272.D
Acq On : 29 Apr 2024 13:30
Operator : JC/MD
Sample : P2257-02
Misc : 1.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1356

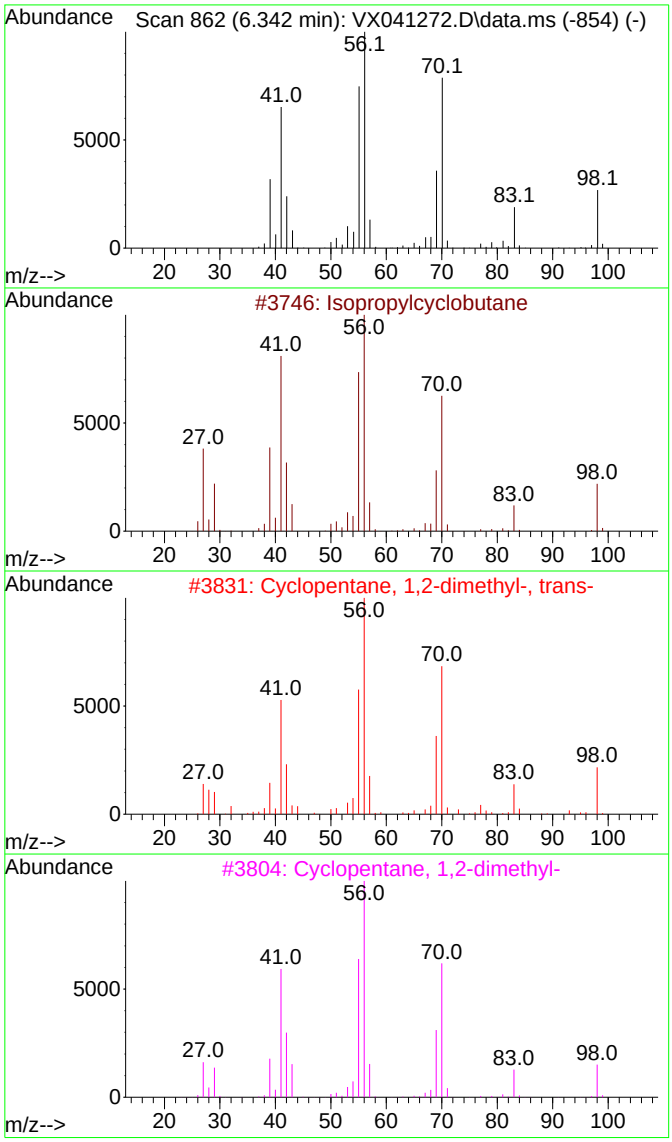
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

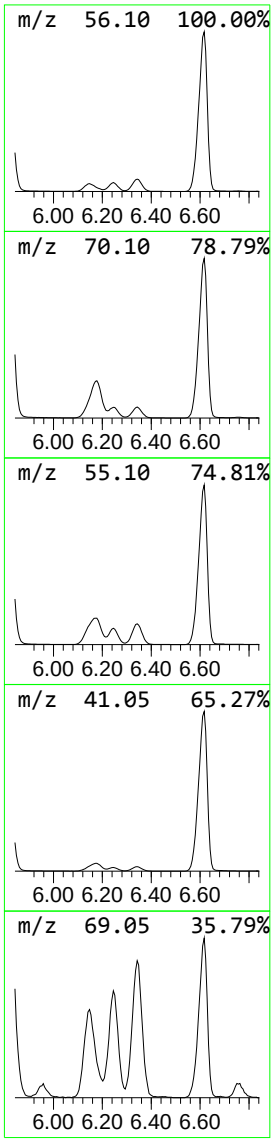
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, 1,2-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.342	83.08 ug/l	953899	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropylcyclobutane	98	C7H14	000872-56-0	94
2	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	91
3	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	90
4	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	86
5	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	86





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Acq On : 29 Apr 2024 13:30
Operator : JC/MD
Sample : P2257-02
Misc : 1.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1356

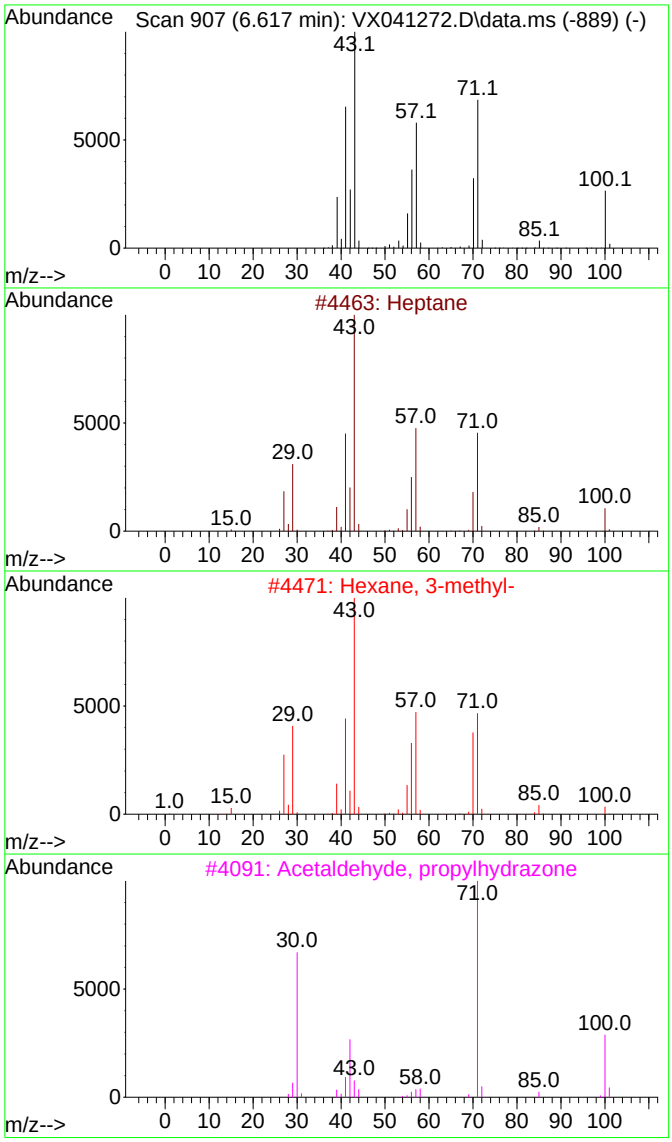
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

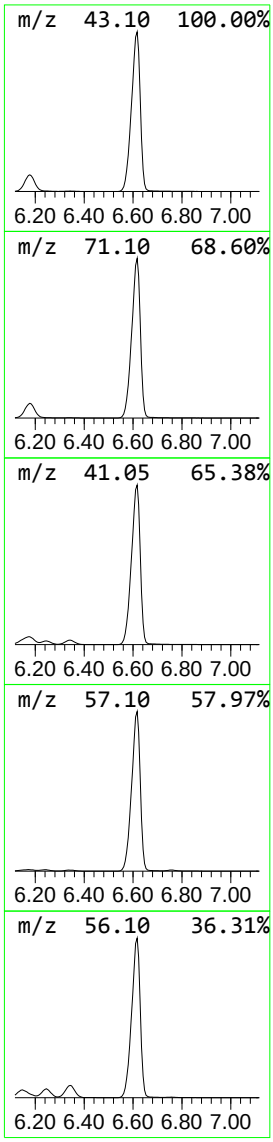
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.617	2353.45 ug/l	27022900	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	59
3	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	47
4	3-Hexanone	100	C6H12O	000589-38-8	38
5	Oxirane, butyl-	100	C6H12O	001436-34-6	38





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Instrument :
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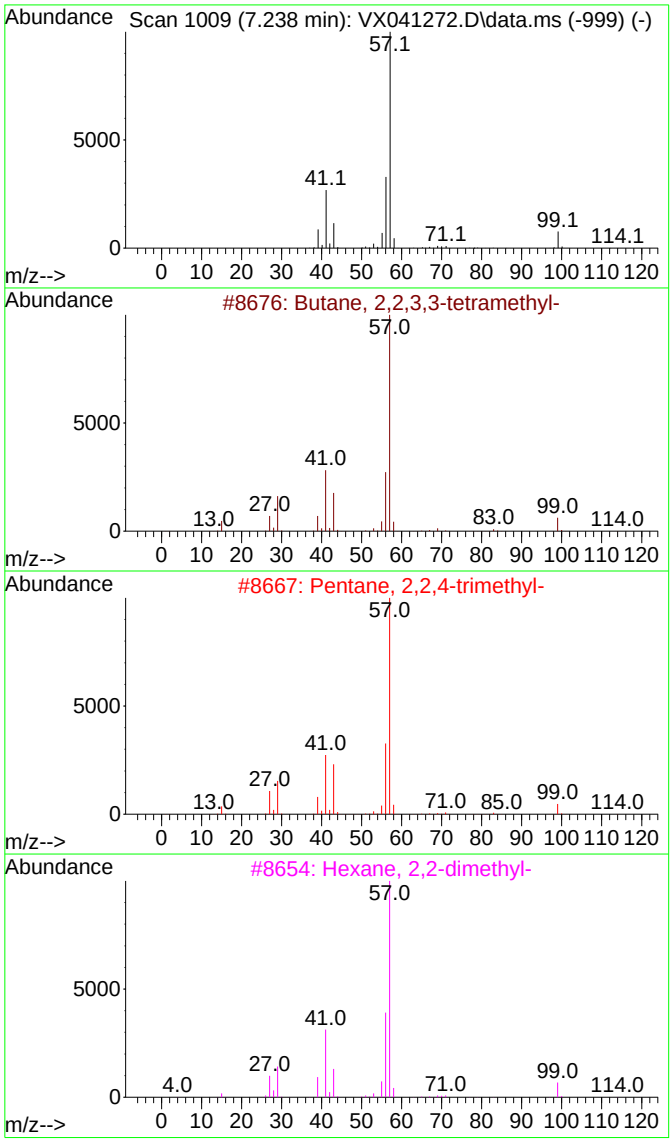
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

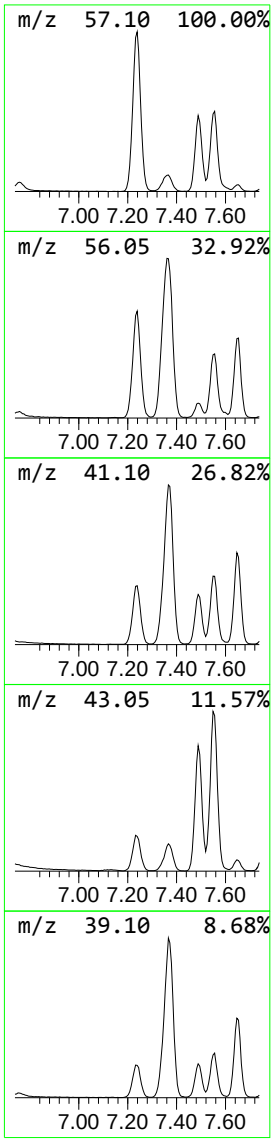
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butane, 2,2,3,3-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.238	67.62 ug/l	776438	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	72
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64





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TIC Library : C:\Database\NIST20.L
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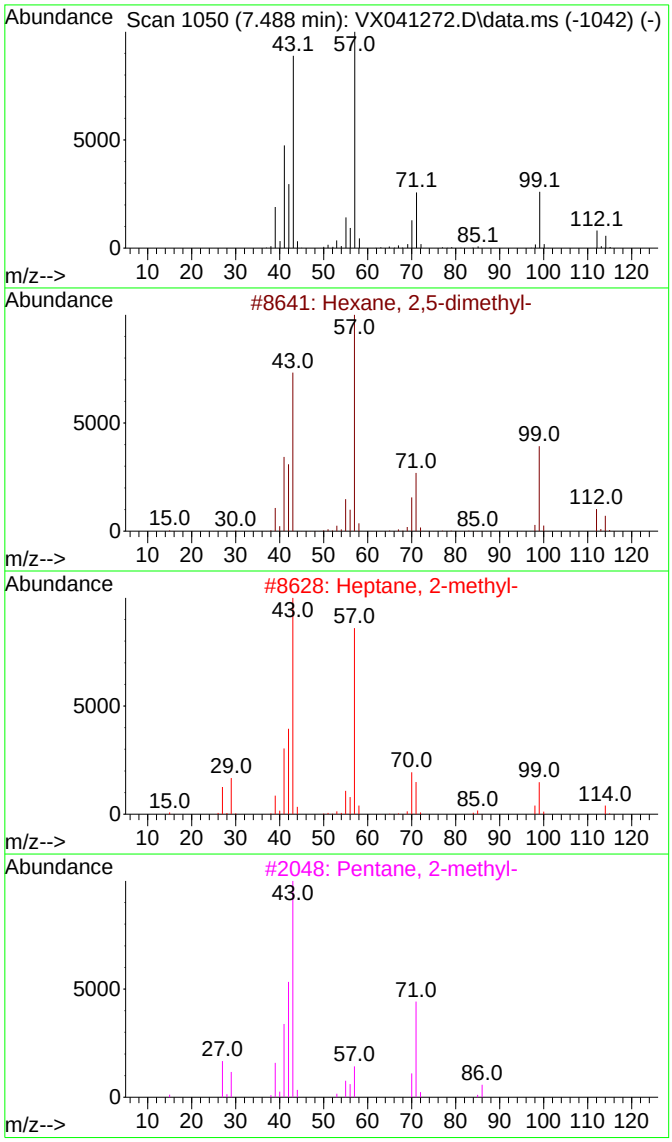
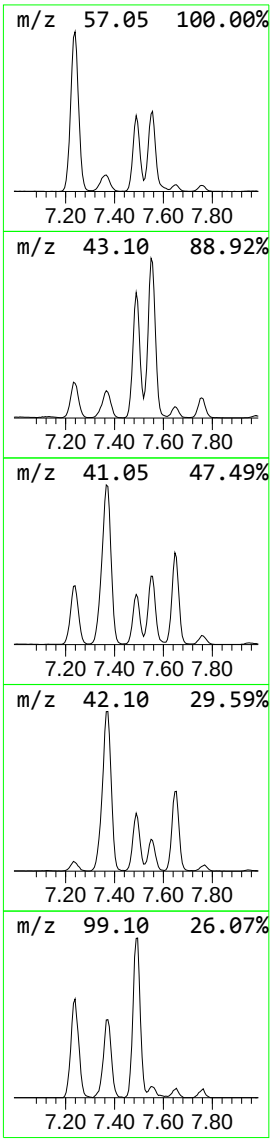
****
Peak Number 7 Hexane, 2,5-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.488	57.00 ug/l	654507	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	94
2	Heptane, 2-methyl-	114	C8H18	000592-27-8	83
3	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
4	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	43
5	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	43





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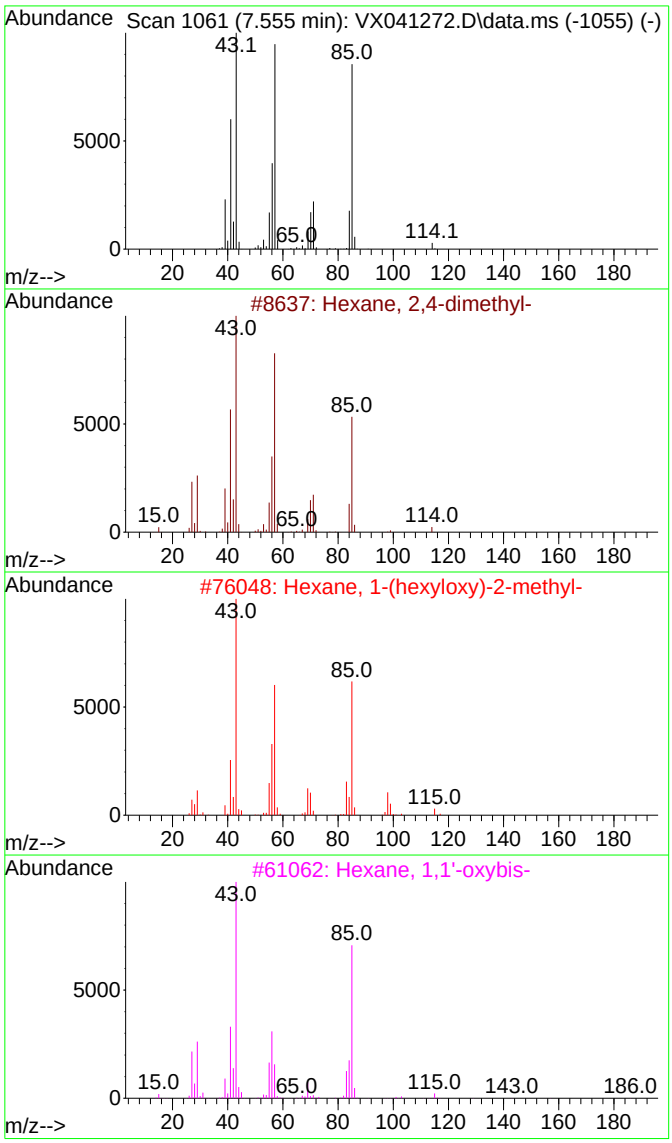
Quant Title : SW846 8260

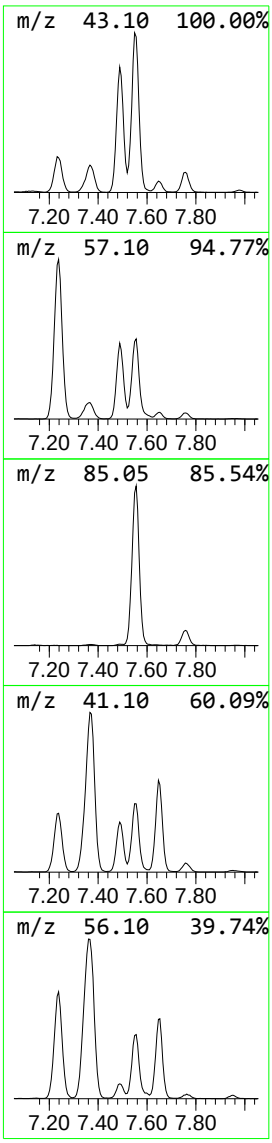
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Hexane, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.555	81.63 ug/l	937316	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	95
2	Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	78
3	Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	64
4	Sulfurous acid, butyl hexyl ester	222	C10H22O3S	1000309-17-3	59
5	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	53





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Data File : VX041272.D
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Sample : P2257-02
Misc : 1.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
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Instrument :
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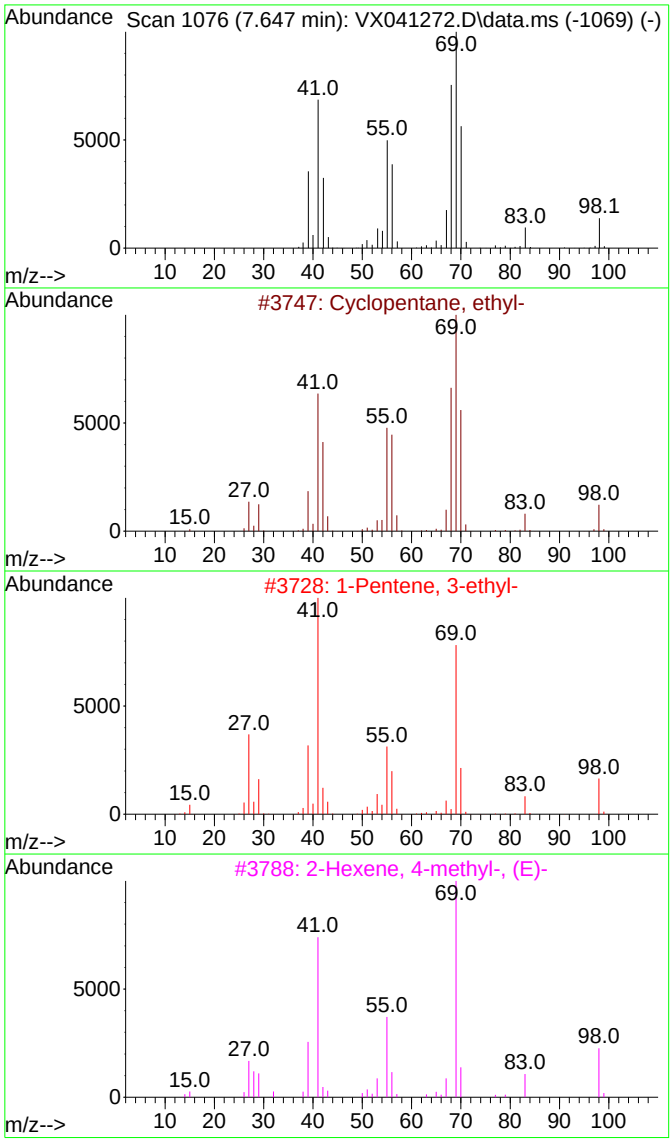
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

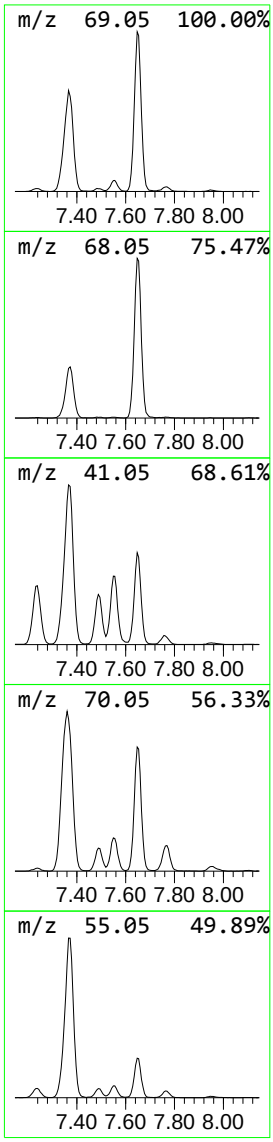
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclopentane, ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.647	94.61 ug/l	1086360	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, ethyl-	98	C7H14	001640-89-7	95
2	1-Pentene, 3-ethyl-	98	C7H14	004038-04-4	43
3	2-Hexene, 4-methyl-, (E)-	98	C7H14	003683-22-5	38
4	Butanedinitrile, 2,3-diamino-2,3...	138	C6H10N4	082929-43-9	38
5	3-Hexene, 3-methyl-, (E)-	98	C7H14	003899-36-3	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041272.D
Acq On : 29 Apr 2024 13:30
Operator : JC/MD
Sample : P2257-02
Misc : 1.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1356

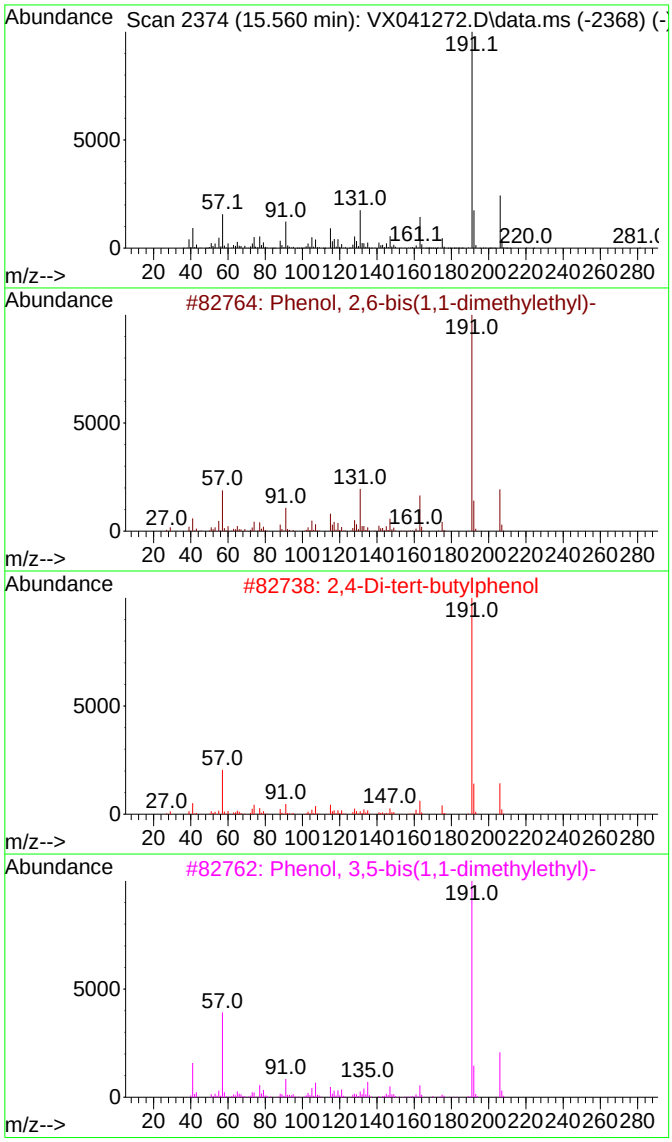
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

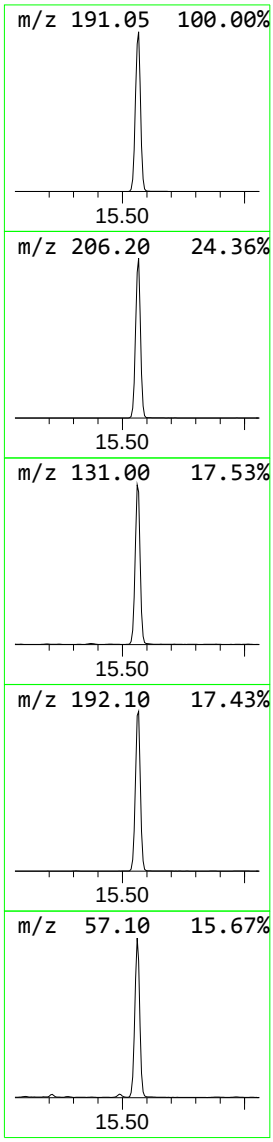
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	1216.10 ug/l	18006300	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	97
2	2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	90
3	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	81
4	Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	81
5	2H-Indeno[1,2-b]furan-2-one, 3,3...	206	C13H18O2	1000196-74-3	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
Data File : VX041272.D
Acq On : 29 Apr 2024 13:30
Operator : JC/MD
Sample : P2257-02
Misc : 1.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1356

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.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
Hexane, 3-methyl-	5.818	88.6	ug/l	18616400	1	5.544	10502700	50.0
Pentane, 3-ethyl-	6.178	260.2	ug/l	2987650	2	6.757	574114	50.0
Isopropylcyclob...	6.245	61.6	ug/l	707074	2	6.757	574114	50.0
Cyclopentane, 1...	6.342	83.1	ug/l	953899	2	6.757	574114	50.0
Heptane	6.617	2353.4	ug/l	27022900	2	6.757	574114	50.0
Butane, 2,2,3,3...	7.238	67.6	ug/l	776438	2	6.757	574114	50.0
Hexane, 2,5-dim...	7.488	57.0	ug/l	654507	2	6.757	574114	50.0
Hexane, 2,4-dim...	7.555	81.6	ug/l	937316	2	6.757	574114	50.0
Cyclopentane, e...	7.647	94.6	ug/l	1086360	2	6.757	574114	50.0
Phenol, 2,6-bis...	15.560	1216.1	ug/l	18006300	4	12.024	740333	50.0