LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031225.D
Acq On : 08 Sep 2022 20:35
Operator : JC/MD
Sample : N4505-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-109

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\82X090722W.M
Title : SW846 8260

Signal : TIC: VX031225.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.385	206	213	230	rBV	3962115	6631976	100.00%	40.875%
2	2.550	233	240	257	rVB	89985	213133	3.21%	1.314%
3	2.971	298	309	321	rBV	58122	142537	2.15%	0.878%
4	4.233	505	516	528	rBV2	37405	103715	1.56%	0.639%
5	4.562	560	570	585	rBV	119021	326499	4.92%	2.012%
6	5.385	694	705	722	rBV2	67021	196088	2.96%	1.209%
7	5.556	722	733	747	rBV2	79206	224605	3.39%	1.384%
8	5.958	790	799	807	rBV	77195	201854	3.04%	1.244%
9	6.043	807	813	821	rVB3	35526	91424	1.38%	0.563%
10	6.763	921	931	942	rBV	123396	333888	5.03%	2.058%
11	7.458	1038	1045	1052	rBV	47158	87086	1.31%	0.537%
12	8.653	1234	1241	1246	rBV	339654	526669	7.94%	3.246%
13	8.720	1246	1252	1259	rVV	1996034	3091124	46.61%	19.051%
14	10.000	1455	1462	1467	rBV2	41285	101299	1.53%	0.624%
15	10.055	1467	1471	1484	rVB	243003	332233	5.01%	2.048%
16	10.195	1489	1494	1500	rBV	80597	110040	1.66%	0.678%
17	10.299	1506	1511	1519	rVB	312685	439080	6.62%	2.706%
18	10.445	1531	1535	1540	rVB	66123	85539	1.29%	0.527%
19	10.646	1561	1568	1572	rBV	134102	203205	3.06%	1.252%
20	11.079	1634	1639	1645	rBV	292752	389631	5.88%	2.401%
21	11.573	1714	1720	1725	rBV	672457	830578	12.52%	5.119%
22	11.829	1753	1762	1767	rBV	199445	283867	4.28%	1.750%
23	11.890	1767	1772	1780	rVB3	49062	83897	1.27%	0.517%
24	12.024	1790	1794	1802	rVB	242211	313226	4.72%	1.930%
25	12.219	1822	1826	1839	rBV	206085	392716	5.92%	2.420%
26	13.146	1973	1978	1982	rBV	136589	187067	2.82%	1.153%
27	13.219	1986	1990	2001	rVB2	43694	81422	1.23%	0.502%
28	13.731	2067	2074	2078	rBV2	107248	150527	2.27%	0.928%
29	13.780	2078	2082	2085	rBV	53603	70232	1.06%	0.433%

Sum of corrected areas: 16225157

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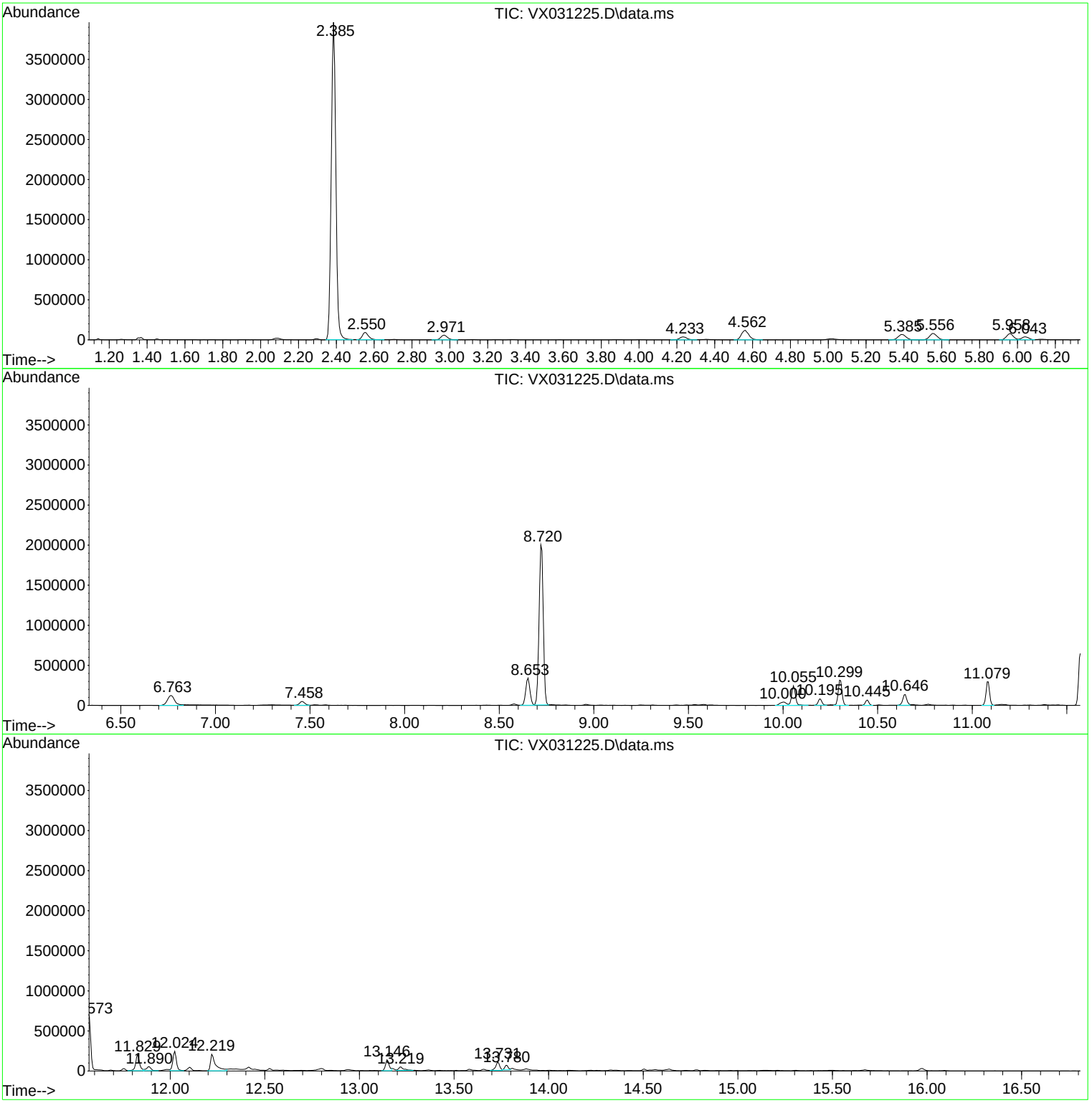
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-109

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

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



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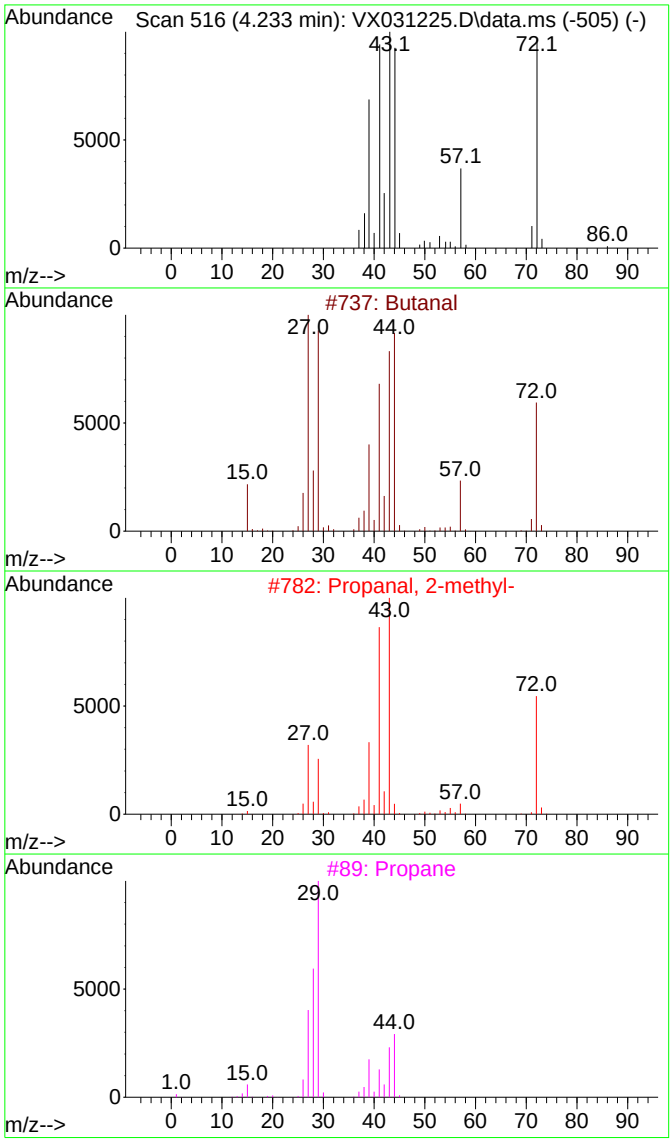
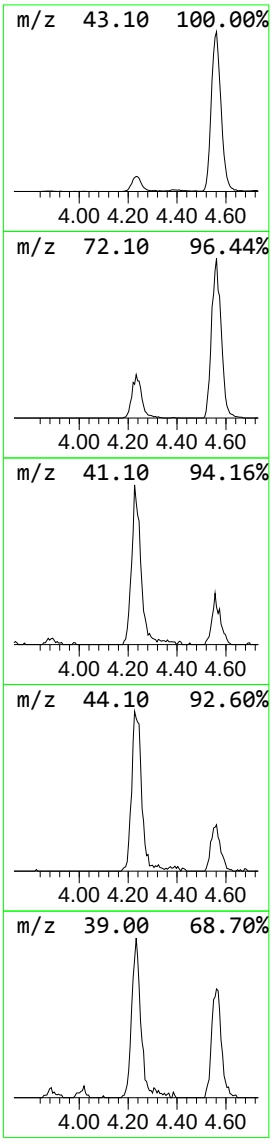
****

Peak Number 1 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	23.09 ug/l	103715	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	62
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3	Propane	44	C3H8	000074-98-6	38
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32
5	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	25





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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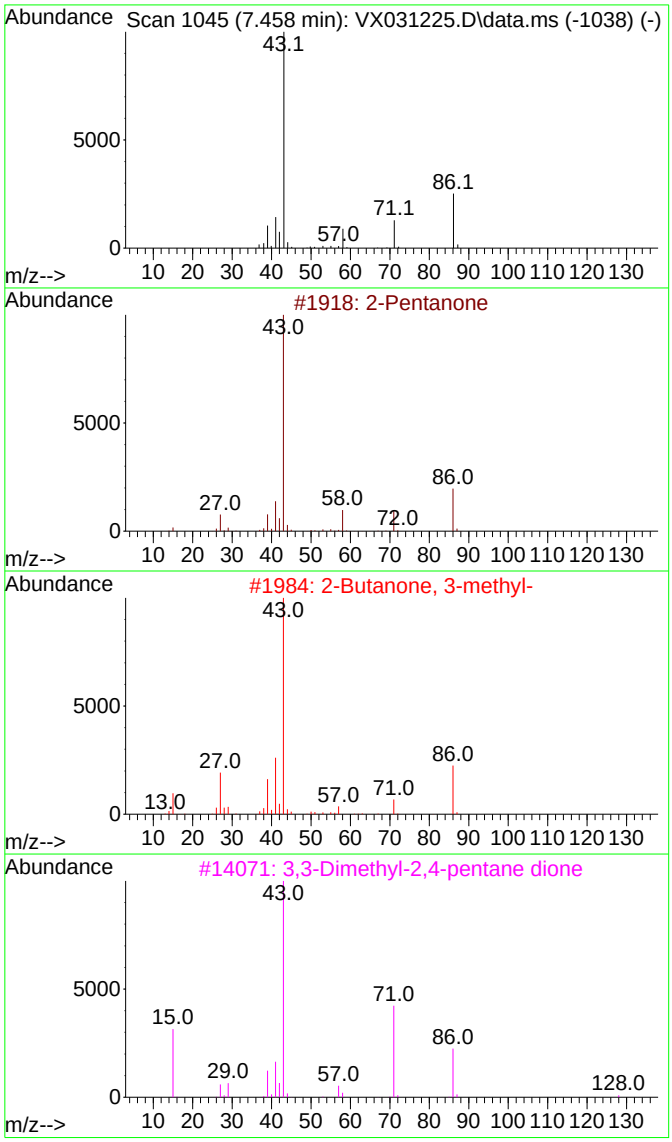
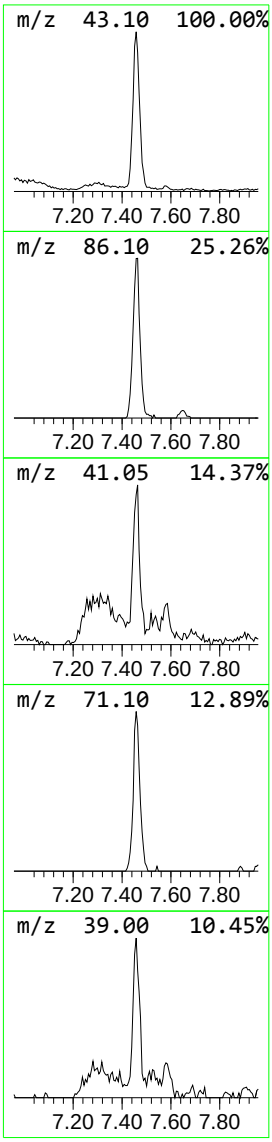
****
Peak Number 2 2-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.458	13.04 ug/l	87086	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	86
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	36
4	Propane, 2-(ethenyloxy)-	86	C5H10O	000926-65-8	33
5	2,3-Butanedione	86	C4H6O2	000431-03-8	9





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Instrument :
MSVOA_X
ClientSampleId :
CLI-109

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

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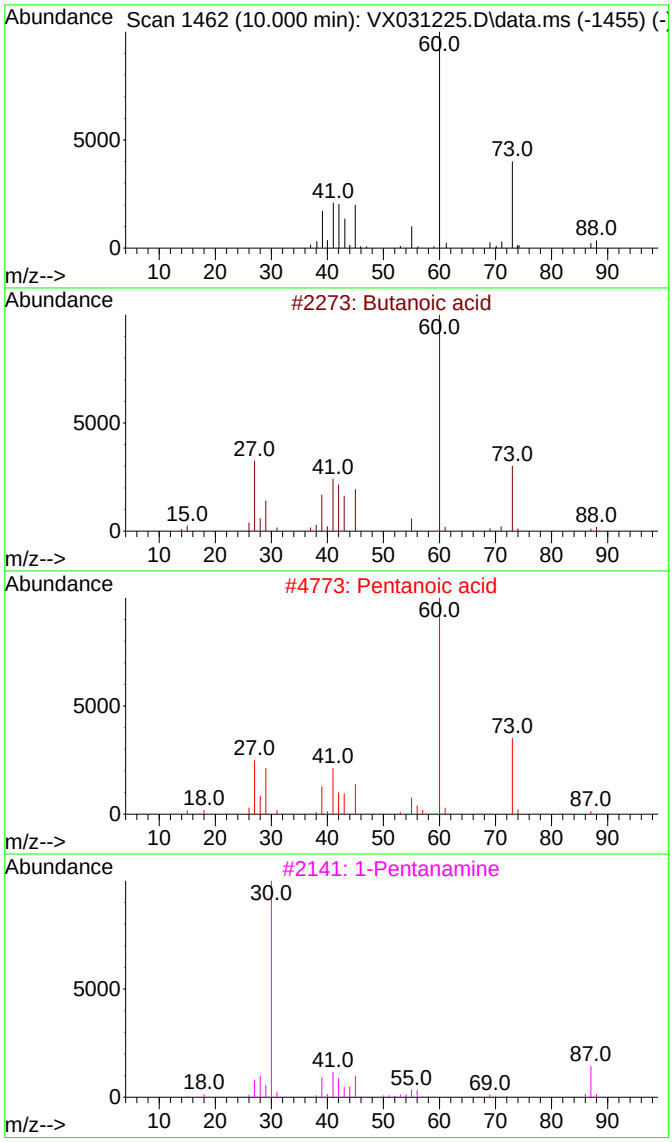
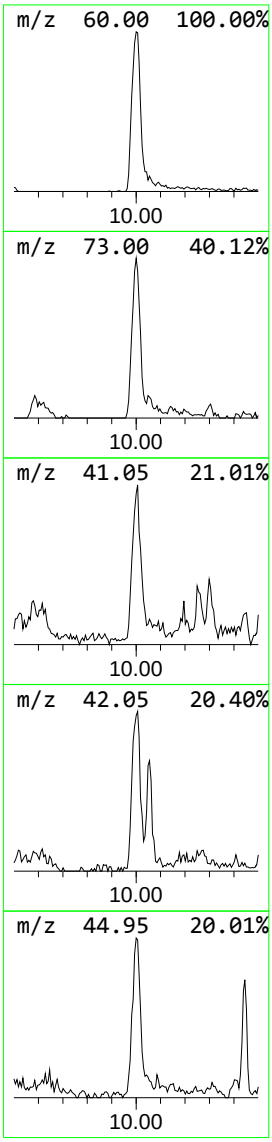
****

Peak Number 3 Butanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.000	15.25 ug/l	101299	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	91
2	Pentanoic acid	102	C5H10O2	000109-52-4	64
3	1-Pentanamine	87	C5H13N	000110-58-7	9
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	9
5	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	9





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-109

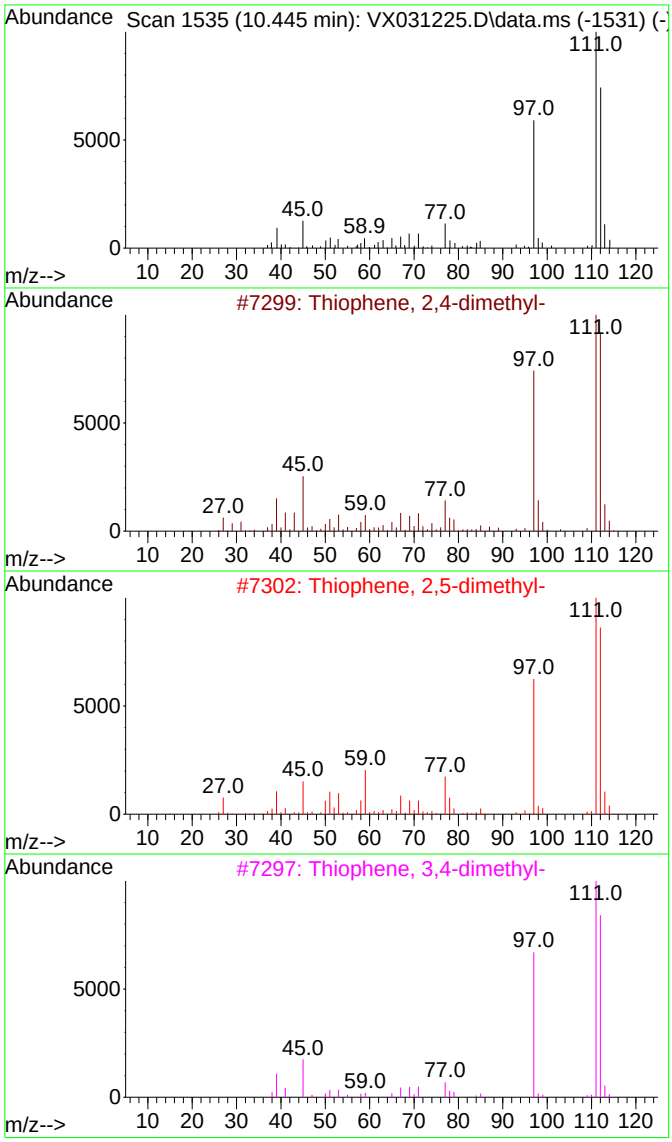
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

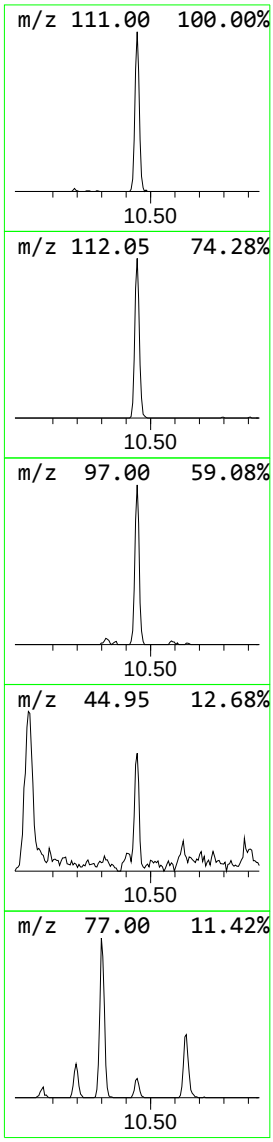
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Thiophene, 2,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.445	12.87 ug/l	85539	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 2,4-dimethyl-	112	C6H8S	000638-00-6	93
2	Thiophene, 2,5-dimethyl-	112	C6H8S	000638-02-8	90
3	Thiophene, 3,4-dimethyl-	112	C6H8S	000632-15-5	87
4	Thiophene, 2,3-dimethyl-	112	C6H8S	000632-16-6	86
5	3-Thiophenecarboxaldehyde	112	C5H4OS	000498-62-4	59





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-109

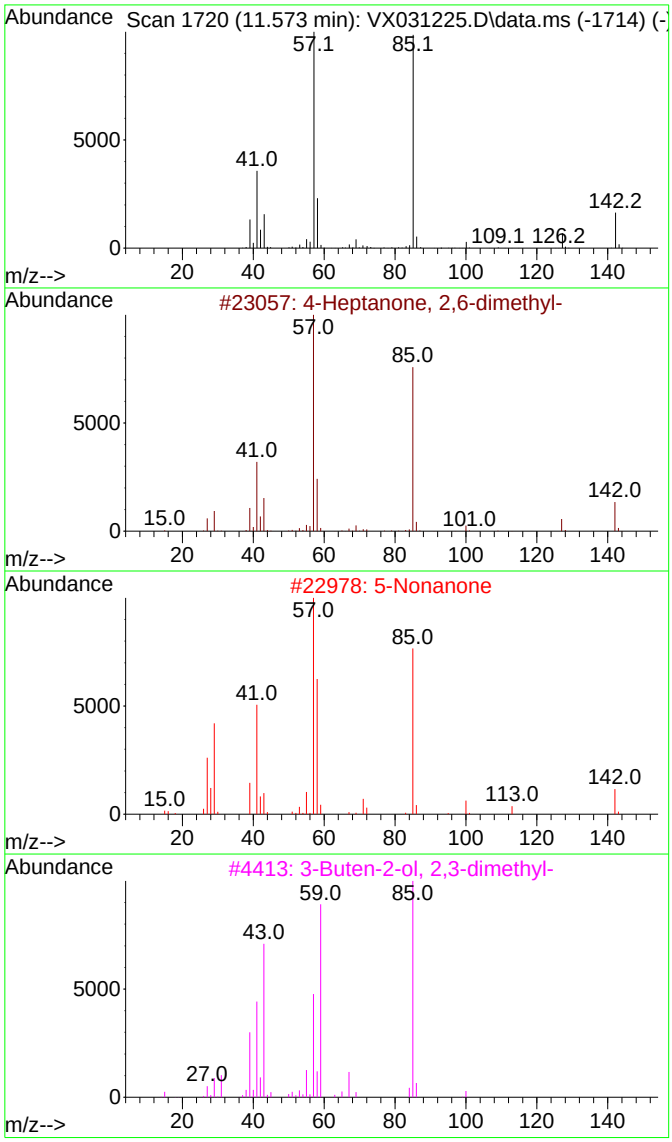
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

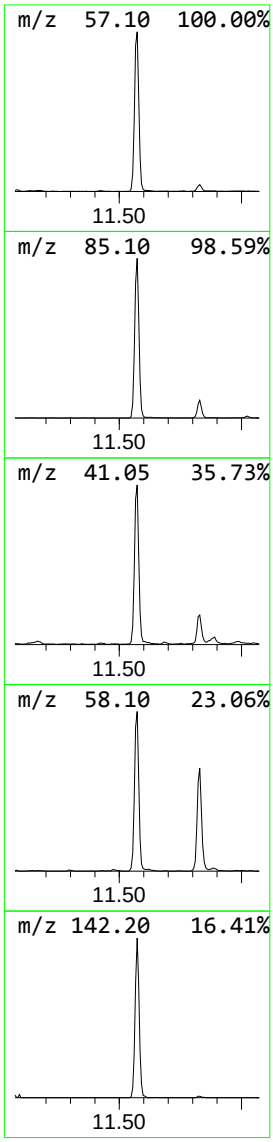
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.573	132.58 ug/l	830578	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	5-Nonanone	142	C9H18O	000502-56-7	59
3	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	53
4	2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	47
5	Acetaldehyde, bis(1-methylethyl)...	142	C8H18N2	067660-50-8	45





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
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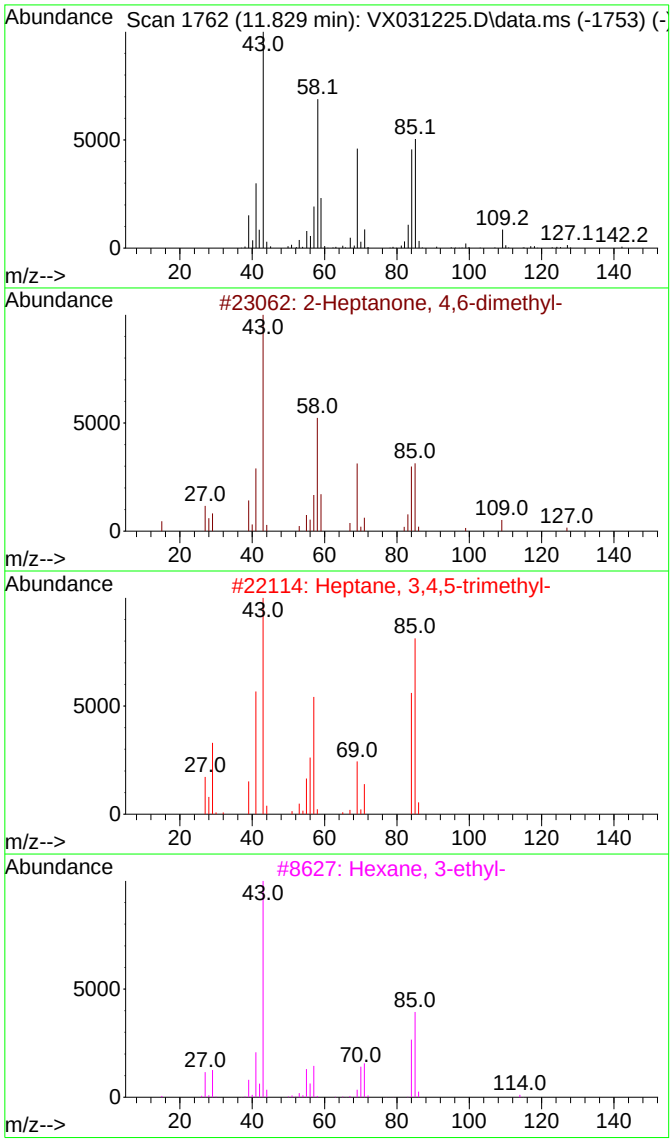
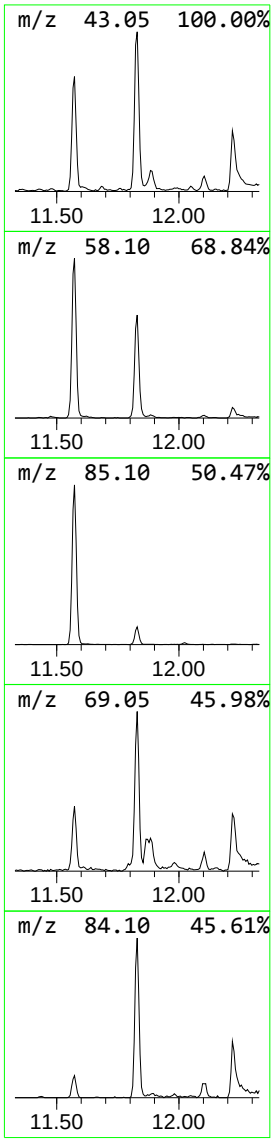
****
Peak Number 6 2-Heptanone, 4,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.829	45.31 ug/l	283867	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	72
2	Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	47
3	Hexane, 3-ethyl-	114	C8H18	000619-99-8	43
4	Butanoic acid, 3-oxo-, 2-propeny...	142	C7H10O3	001118-84-9	40
5	Oxalic acid, diisohexyl ester	258	C14H26O4	1010309-32-9	35





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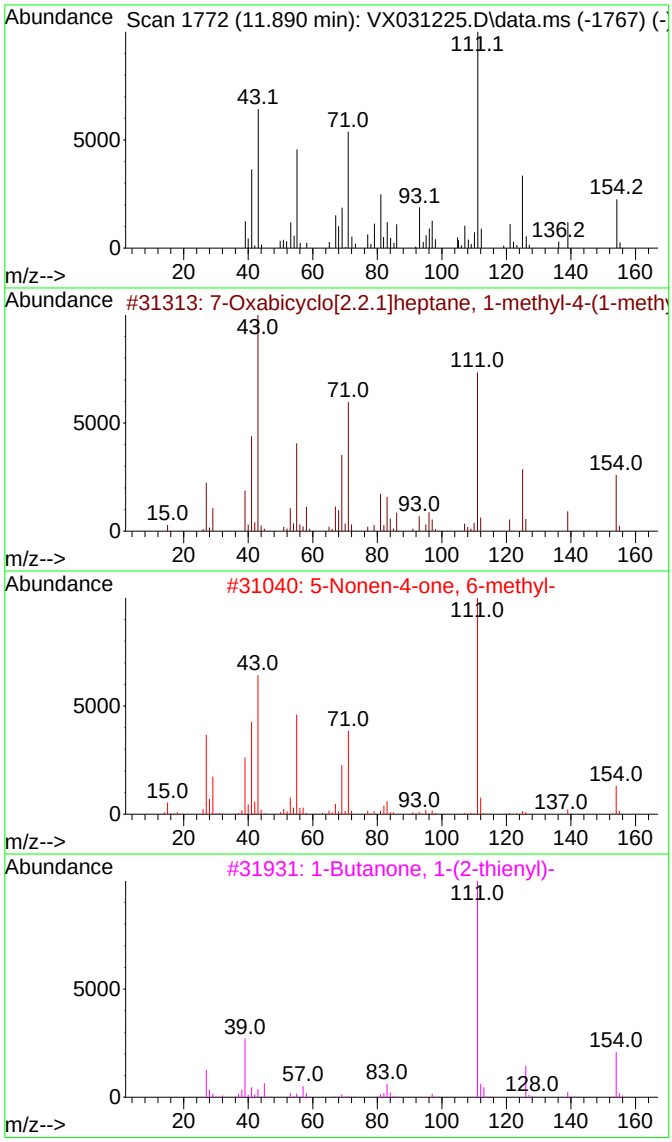
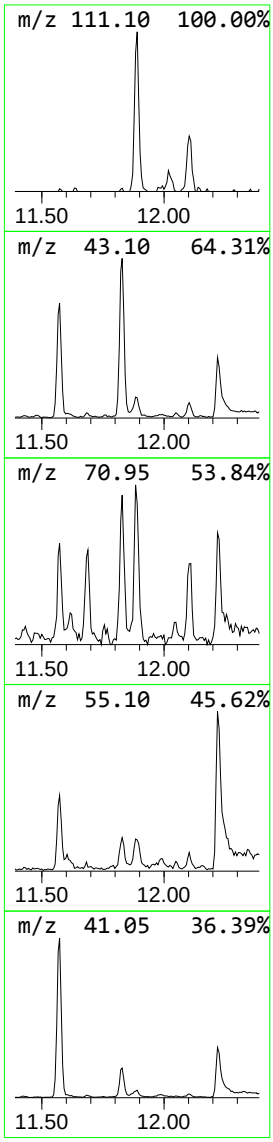
****
Peak Number 7 7-Oxabicyclo[2.2.1]heptane,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.890	13.39 ug/l	83897	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	91
2	5-Nonen-4-one, 6-methyl-	154	C10H18O	007036-98-8	47
3	1-Butanone, 1-(2-thienyl)-	154	C8H10OS	005333-83-5	35
4	5-Amino-1-methyl-2-piperidinone,...	198	C10H18N2O2	1341836-32-5	27
5	4a(2H)-Naphthalenol, octahydro-,...	154	C10H18O	001654-87-1	25





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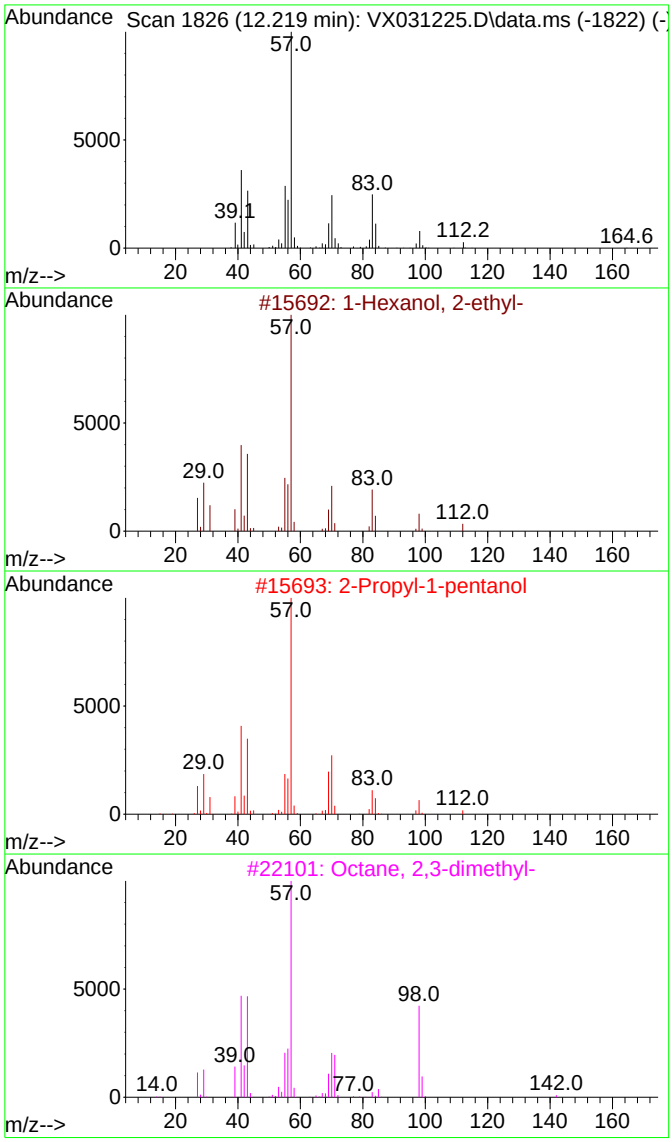
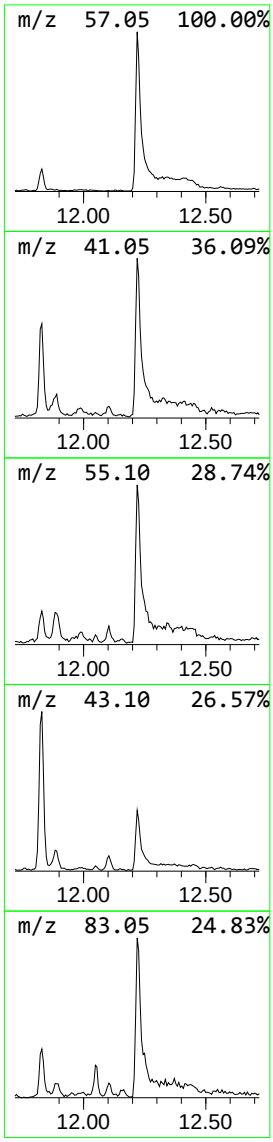
****
Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	62.69 ug/l	392716	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	90
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
3	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5	2-Decene, 5-methyl-, (Z)-	154	C11H22	074645-86-6	47





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-109

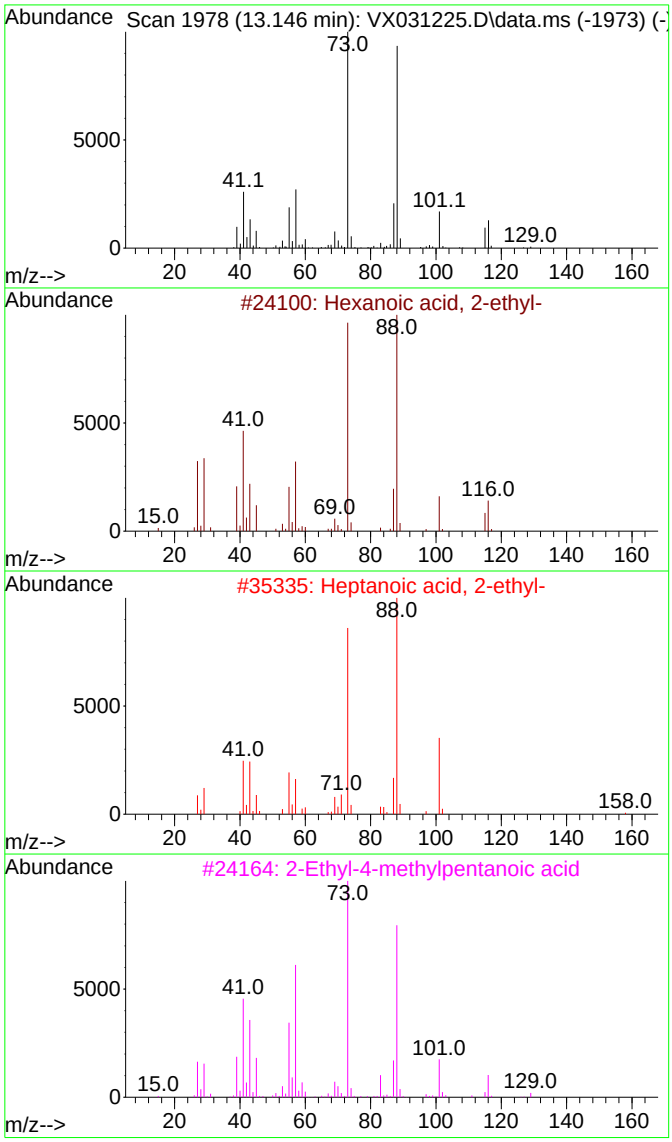
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

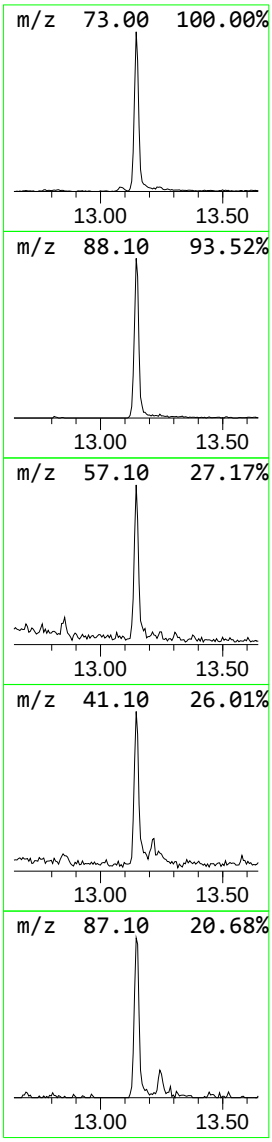
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Hexanoic acid, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.146	29.86 ug/l	187067	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	83
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
3	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	50
4	Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	38
5	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	38





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Data File : VX031225.D
Acq On : 08 Sep 2022 20:35
Operator : JC/MD
Sample : N4505-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-109

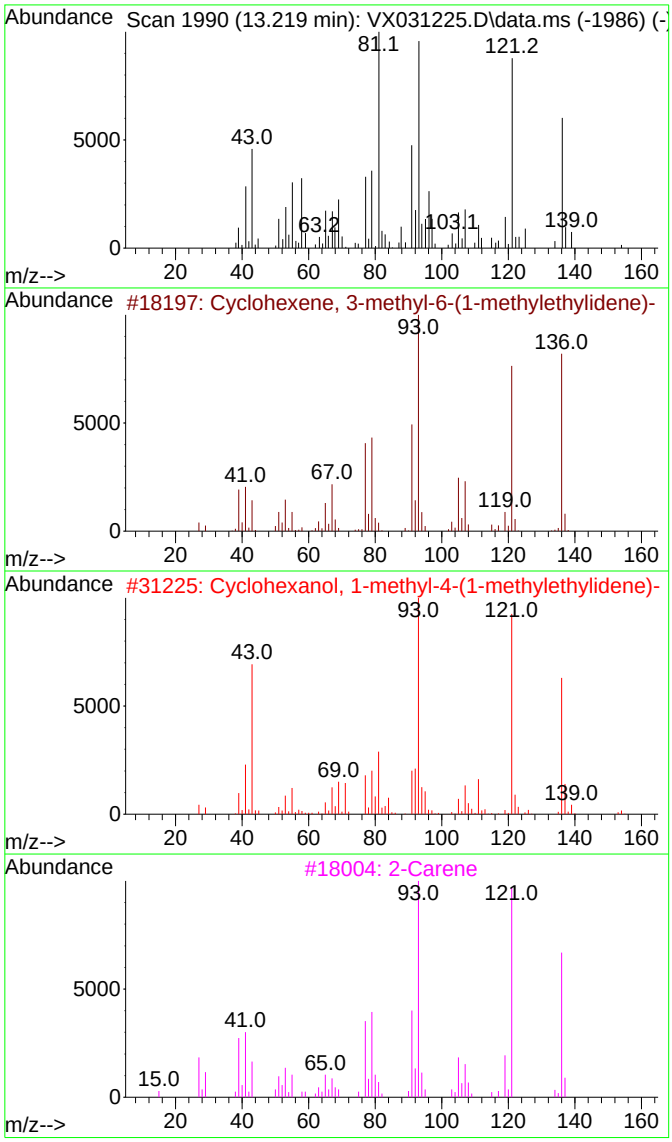
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

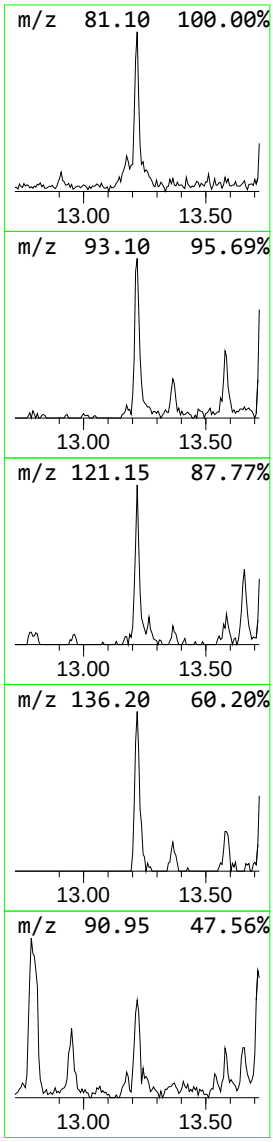
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Cyclohexene, 3-methyl-6-(1-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.219	13.00 ug/l	81422	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	000586-63-0	86
2	Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	000586-81-2	83
3	2-Carene	136	C10H16	000554-61-0	78
4	1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	64
5	(+)-4-Carene	136	C10H16	029050-33-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090822\
Data File : VX031225.D
Acq On : 08 Sep 2022 20:35
Operator : JC/MD
Sample : N4505-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CLI-109

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.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
Butanal	4.233	23.1	ug/l	103715	1	5.556	224605	50.0
2-Pentanone	7.458	13.0	ug/l	87086	2	6.769	333888	50.0
Butanoic acid	10.000	15.3	ug/l	101299	3	10.055	332233	50.0
Thiophene, 2,4-...	10.445	12.9	ug/l	85539	3	10.055	332233	50.0
4-Heptanone, 2,...	11.573	132.6	ug/l	830578	4	12.024	313226	50.0
2-Heptanone, 4,...	11.829	45.3	ug/l	283867	4	12.024	313226	50.0
7-Oxabicyclo[2....	11.890	13.4	ug/l	83897	4	12.024	313226	50.0
1-Hexanol, 2-et...	12.219	62.7	ug/l	392716	4	12.024	313226	50.0
Hexanoic acid, ...	13.146	29.9	ug/l	187067	4	12.024	313226	50.0
Cyclohexene, 3-...	13.219	13.0	ug/l	81422	4	12.024	313226	50.0