

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
 Data File : VX030150.D
 Acq On : 20 Jul 2022 22:41
 Operator : JC/MD
 Sample : N3781-01 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ORA-0037

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\82X071222W.M

Title : SW846 8260

Signal : TIC: VX030150.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.300	192	199	223	rVB	12528953	22365643	100.00%	51.892%
2	3.873	443	457	480	rBV	738378	1929208	8.63%	4.476%
3	5.391	695	706	720	rBV	116105	329313	1.47%	0.764%
4	5.556	722	733	749	rVB	198421	565049	2.53%	1.311%
5	5.964	790	800	813	rBV2	129984	348048	1.56%	0.808%
6	6.769	922	932	944	rBV2	328677	798373	3.57%	1.852%
7	8.653	1234	1241	1256	rBV	660818	1066943	4.77%	2.475%
8	8.866	1269	1276	1286	rBV	245423	364416	1.63%	0.845%
9	9.000	1291	1298	1314	rBV	4076266	5726361	25.60%	13.286%
10	9.165	1318	1325	1337	rVV	2553838	3567612	15.95%	8.277%
11	10.079	1465	1475	1484	rBV2	1859641	3201757	14.32%	7.429%
12	10.713	1572	1579	1588	rBV	159430	259911	1.16%	0.603%
13	11.085	1634	1640	1646	rBV	490982	636824	2.85%	1.478%
14	11.664	1722	1735	1741	rBV	393361	619357	2.77%	1.437%
15	11.957	1775	1783	1789	rBV	416130	518862	2.32%	1.204%
16	12.024	1789	1794	1805	rVB	639638	803061	3.59%	1.863%

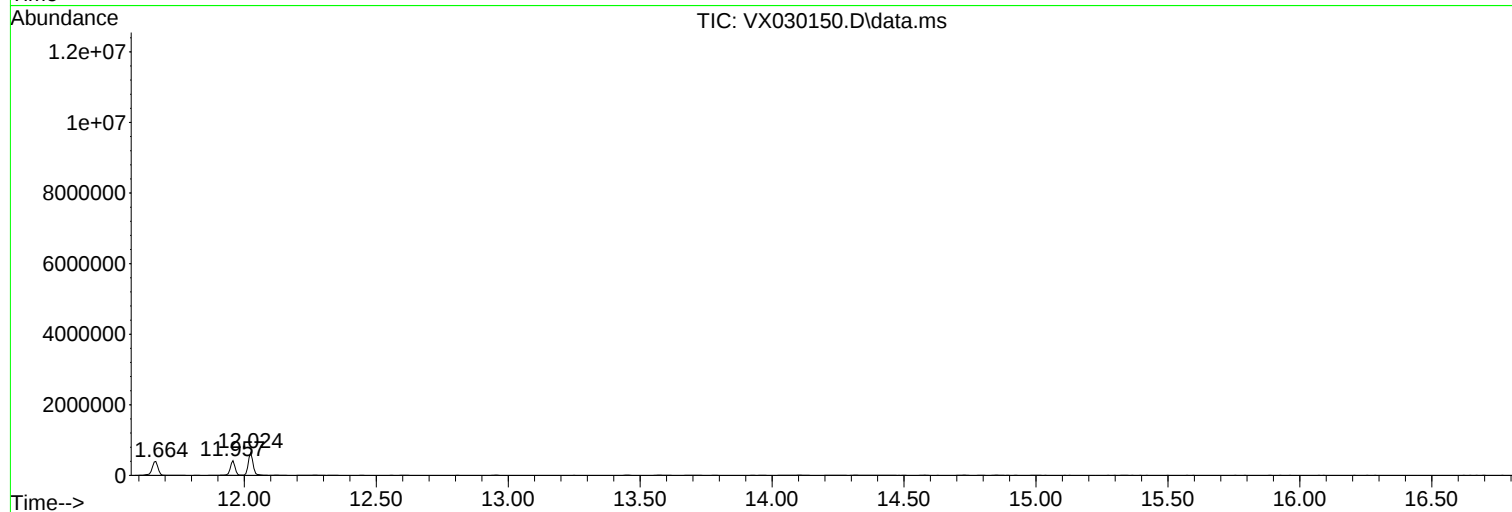
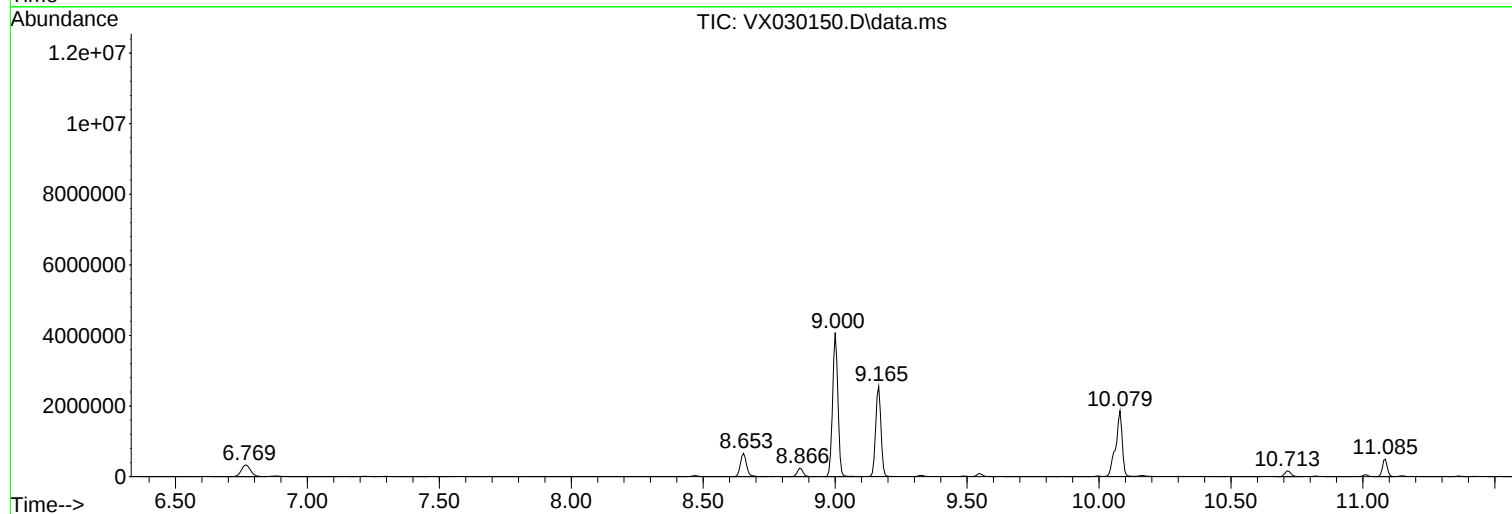
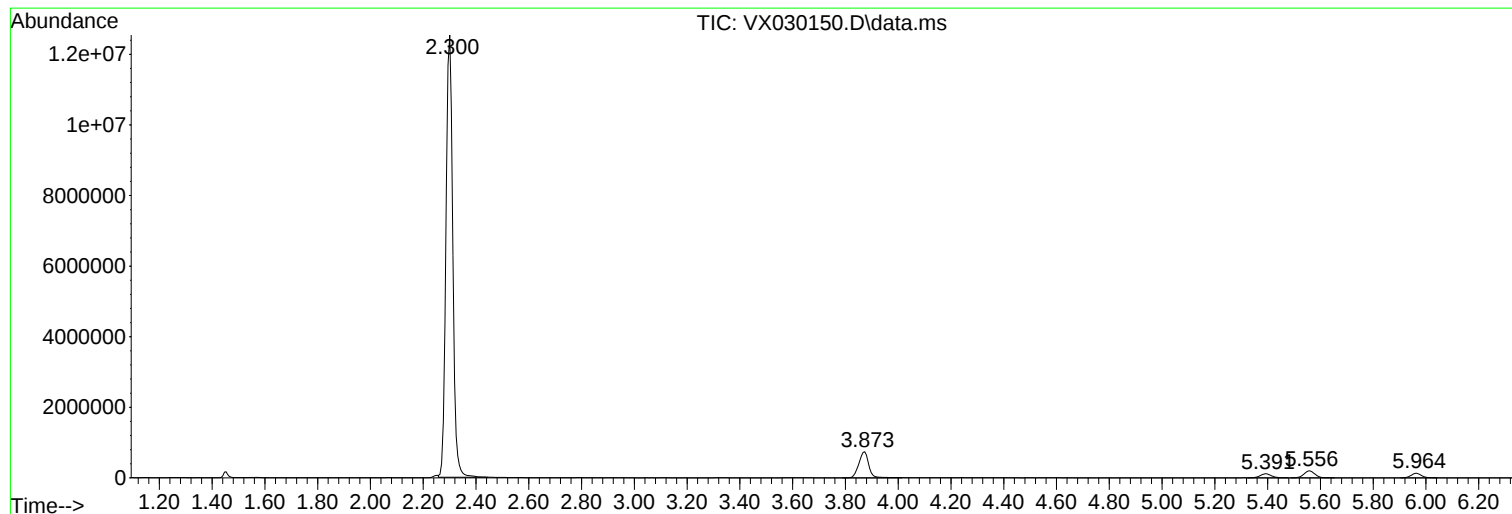
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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



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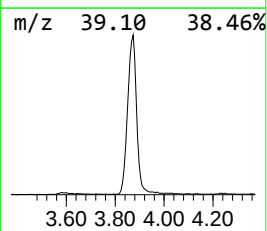
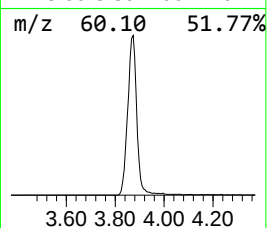
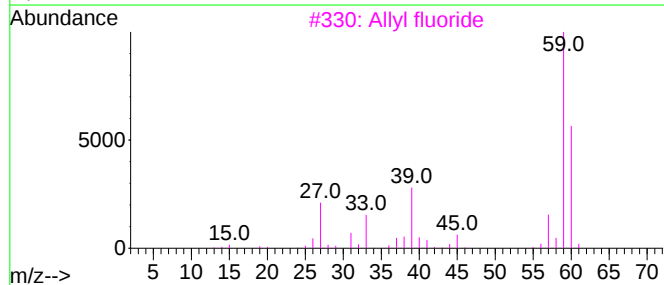
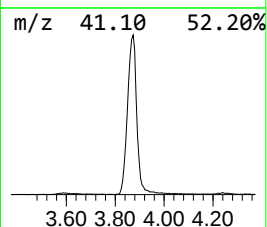
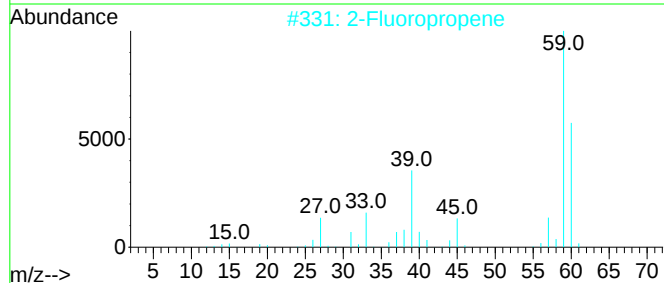
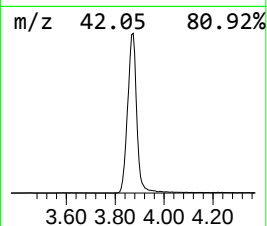
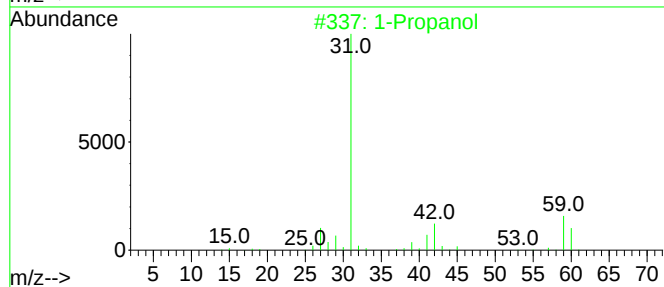
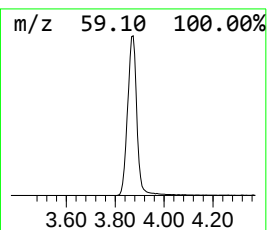
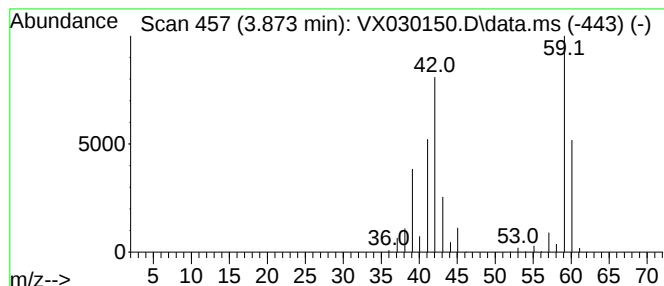
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Quant Title : SW846 8260

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

Peak Number 1 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.873	170.71 ug/l	1929210	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	59
2	2-Fluoropropene			60	C3H5F	001184-60-7	52
3	Allyl fluoride			60	C3H5F	000818-92-8	38
4	Cyclopropane			42	C3H6	000075-19-4	25
5	Formamidoxime			60	CH4N2O	000624-82-8	7



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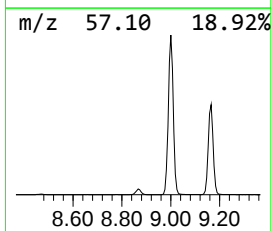
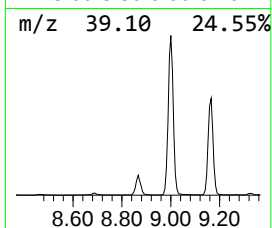
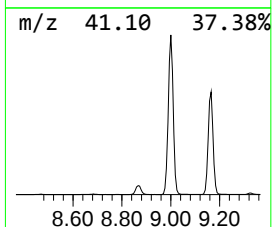
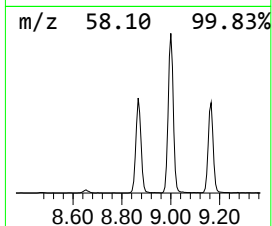
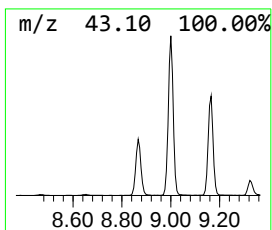
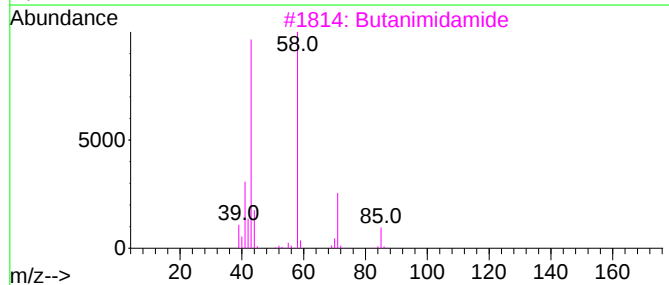
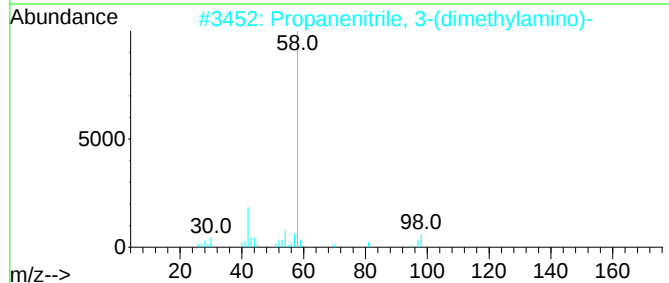
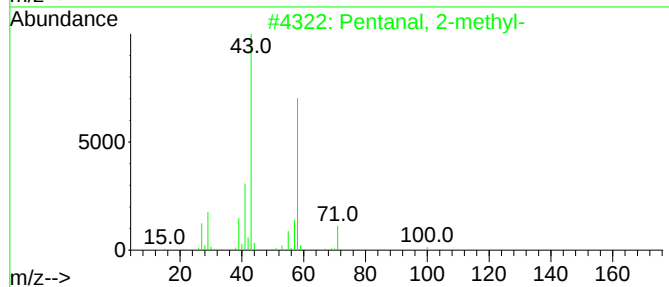
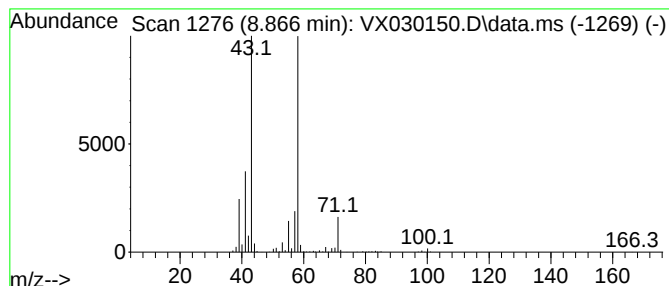
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentanal, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.866	5.69 ug/l	364416	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal, 2-methyl-	100	C6H12O	000123-15-9	91
2			Propanenitrile, 3-(dimethylamino)-	98	C5H10N2	001738-25-6	53
3			Butanimidamide	86	C4H10N2	000107-90-4	50
4			Pentanal, 2,4-dimethyl-	114	C7H14O	027944-79-2	39
5			Carbonic acid, 2-dimethylaminoet...	175	C8H17NO3	1000331-38-5	38



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

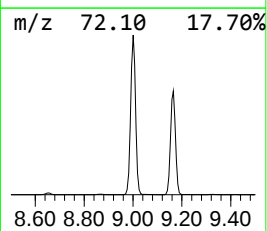
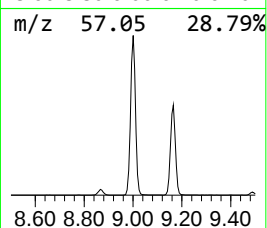
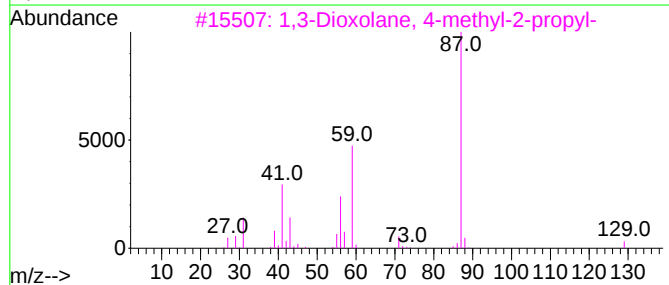
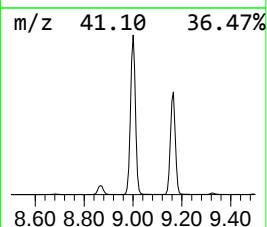
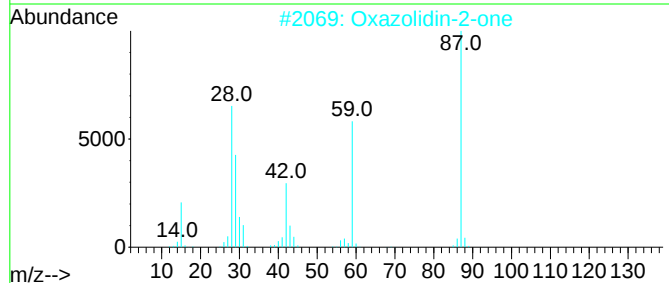
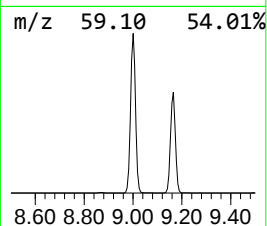
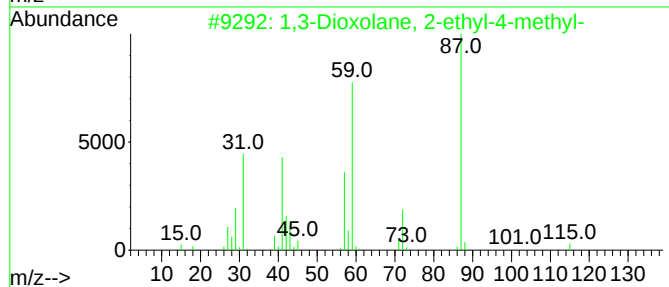
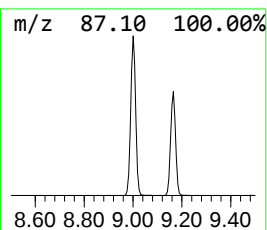
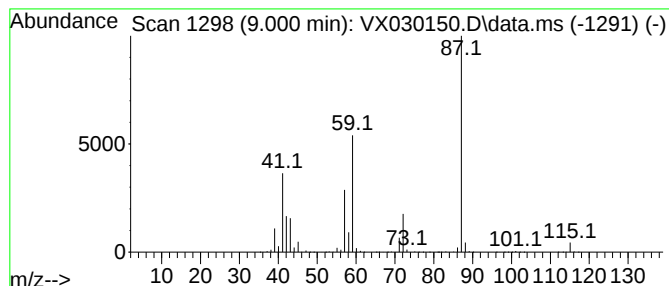
Instrument :
MSVOA_X
ClientSampleId :
ORA-0037

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Quant Title : SW846 8260

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

Peak Number 3 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.000	89.43 ug/l	5726360	Chlorobenzene-d5	10.055	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	90
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	72
3	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	64
4	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	47



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0037

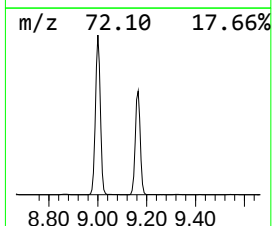
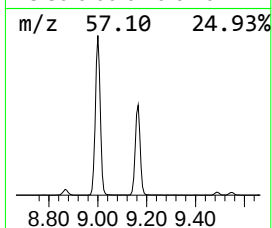
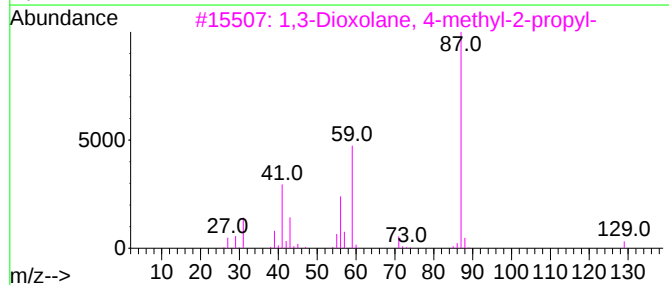
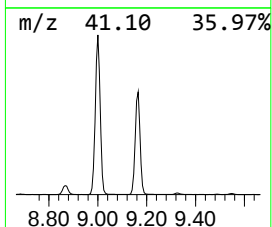
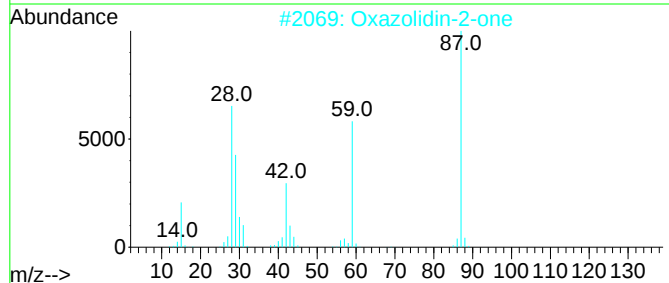
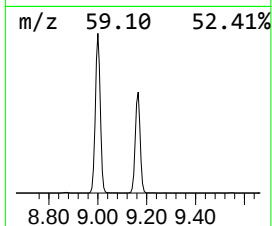
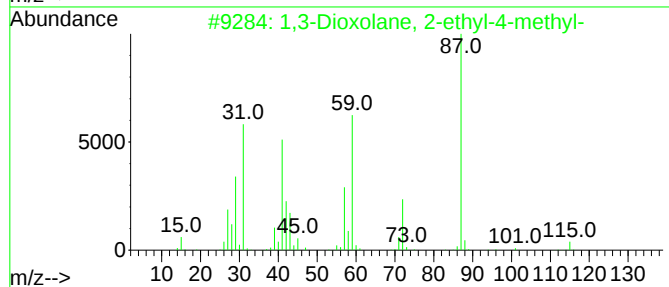
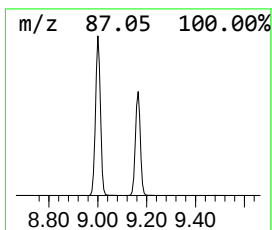
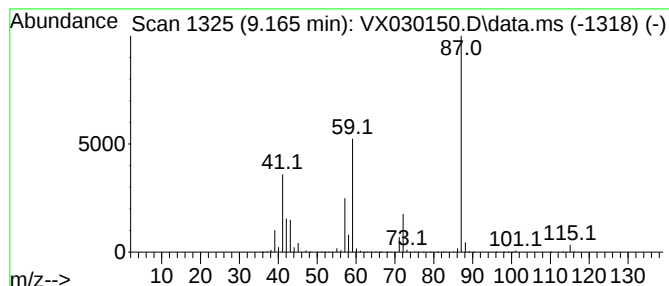
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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

Peak Number 4 Oxazolidin-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.165	55.71 ug/l	3567610	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	94
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	80
3			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	72
4			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	64
5			2-Propanone, 0-methyloxime	87	C4H9NO	003376-35-0	52



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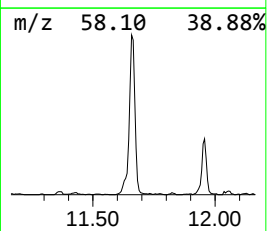
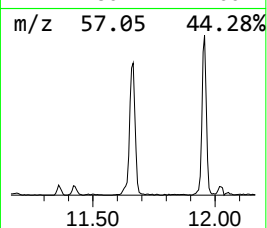
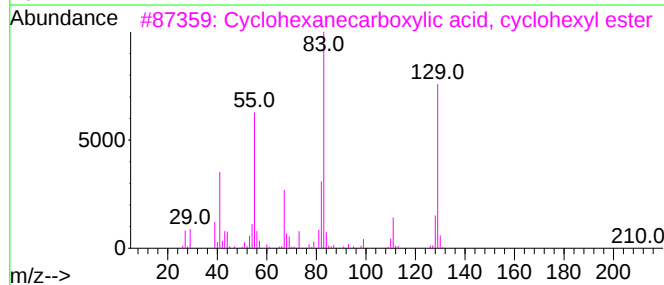
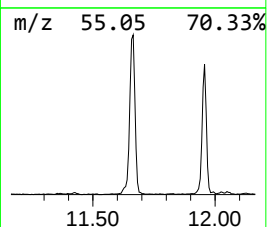
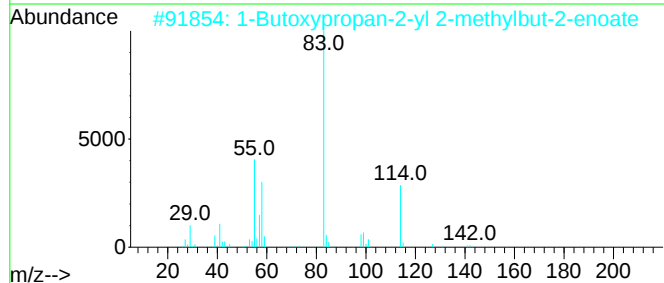
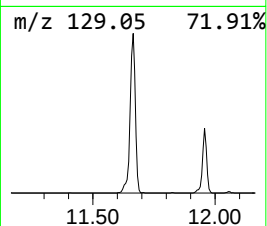
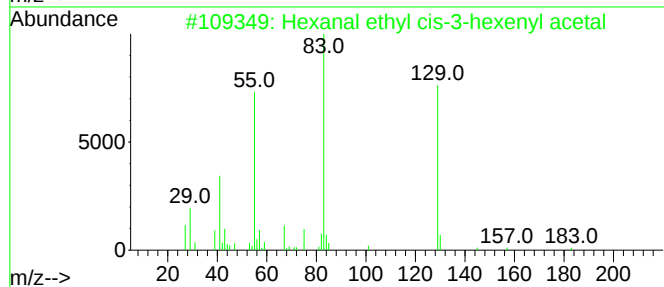
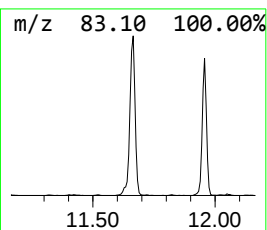
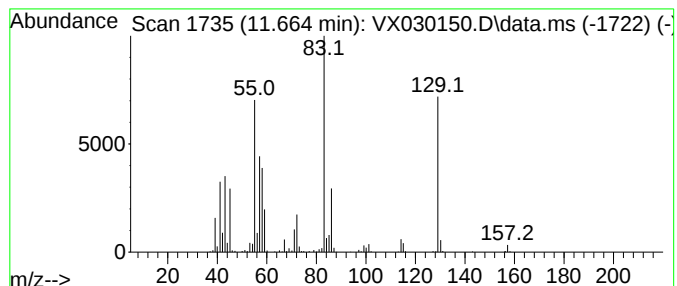
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown11.665 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.665	38.56 ug/l	619357	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal ethyl cis-3-hexenyl acetal	228	C14H28O2	1000431-42-9	43
2			1-Butoxypropan-2-yl 2-methylbut-...	214	C12H22O3	1000367-09-3	43
3			Cyclohexanecarboxylic acid, cycl...	210	C13H22O2	015840-96-7	38
4			1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	18
5			2-(2-(2-Methoxyethoxy)ethoxy)eth...	248	C12H24O5	1000367-05-6	16



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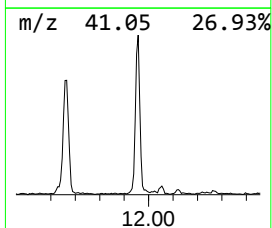
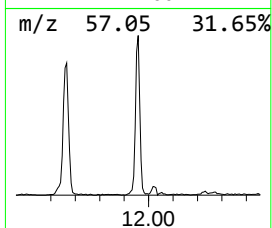
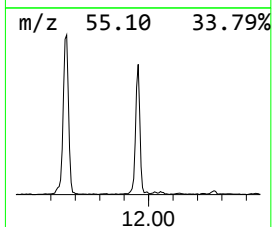
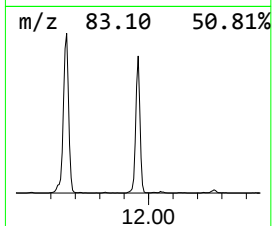
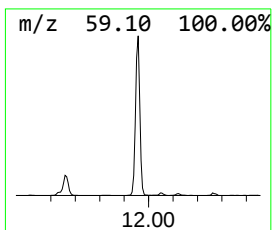
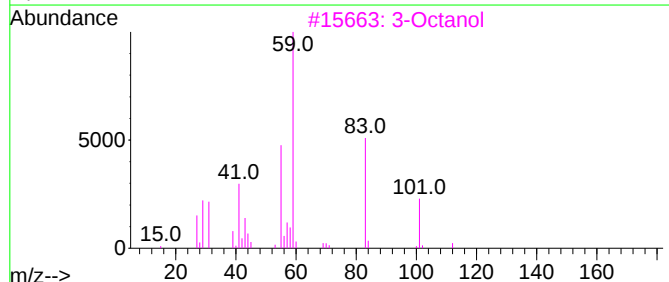
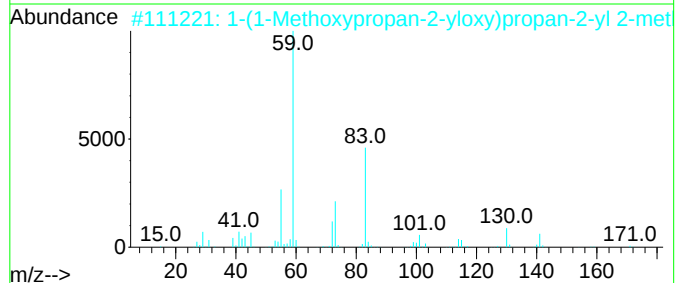
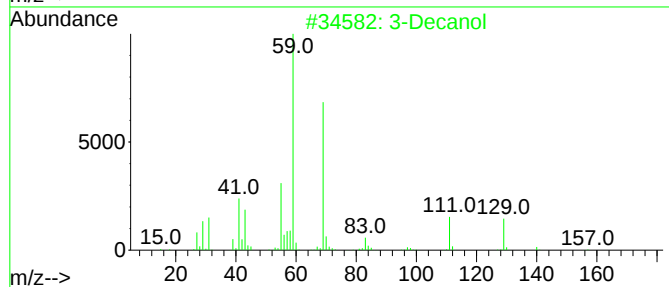
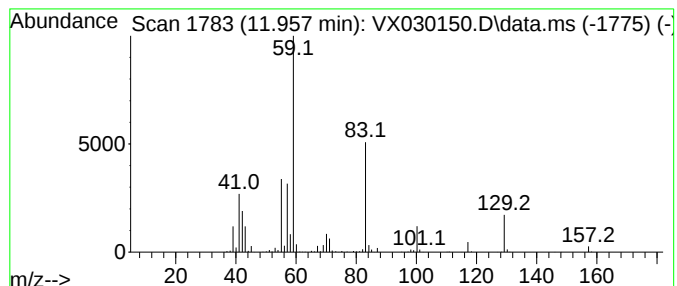
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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

Peak Number 6 unknown11.957 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	32.31 ug/l	518862	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Decanol	158	C10H22O	001565-81-7	47
2			1-(1-Methoxypropan-2-yloxy)propa...	230	C12H22O4	1000367-11-3	39
3			3-Octanol	130	C8H18O	000589-98-0	38
4			1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1000367-11-4	37
5			Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030150.D
Acq On : 20 Jul 2022 22:41
Operator : JC/MD
Sample : N3781-01 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0037

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propanol	3.873	170.7	ug/l	1929210	1	5.562	565049	50.0
Pentanal, 2-met...	8.866	5.7	ug/l	364416	3	10.055	3201760	50.0
1,3-Dioxolane, ...	9.000	89.4	ug/l	5726360	3	10.055	3201760	50.0
Oxazolidin-2-one	9.165	55.7	ug/l	3567610	3	10.055	3201760	50.0
unknown11.665	11.665	38.6	ug/l	619357	4	12.024	803061	50.0
unknown11.957	11.957	32.3	ug/l	518862	4	12.024	803061	50.0