

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060625\
 Data File : VN086880.D
 Acq On : 06 Jun 2025 20:36
 Operator : JC\MD
 Sample : Q2216-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 3851

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_N\methods\82N060625W.M
 Title : SW846 8260

Signal : TIC: VN086880.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.112	21	27	42	rVB	99855	164391	7.94%	1.307%
2	2.524	91	97	109	rBV2	71634	152210	7.35%	1.211%
3	2.706	123	128	134	rVB	17408	32607	1.58%	0.259%
4	4.448	414	424	433	rBV	18047	56894	2.75%	0.452%
5	4.548	433	441	452	rVB2	15464	47088	2.28%	0.374%
6	5.536	595	609	630	rBV2	96162	355547	17.18%	2.828%
7	7.236	891	898	906	rBV4	9411	29194	1.41%	0.232%
8	8.177	1048	1058	1062	rBV	249671	597184	28.86%	4.749%
9	8.236	1062	1068	1079	rVB	489545	1129238	54.57%	8.981%
10	8.588	1118	1128	1137	rBV	277908	633119	30.59%	5.035%
11	8.824	1163	1168	1179	rVB9	7925	21822	1.05%	0.174%
12	8.971	1187	1193	1202	rBV3	11396	26377	1.27%	0.210%
13	9.106	1206	1216	1225	rBV	733597	1498139	72.39%	11.915%
14	9.471	1269	1278	1284	rVB6	7555	20726	1.00%	0.165%
15	9.541	1284	1290	1296	rVB2	11888	23377	1.13%	0.186%
16	9.659	1304	1310	1320	rVB4	9798	23264	1.12%	0.185%
17	9.912	1345	1353	1365	rBV	273667	558945	27.01%	4.445%
18	10.453	1438	1445	1453	rBV2	16444	41255	1.99%	0.328%
19	10.571	1457	1465	1472	rVV	1088521	2069515	100.00%	16.459%
20	10.635	1472	1476	1487	rVV2	52611	116623	5.64%	0.928%
21	11.065	1543	1549	1558	rBV2	23639	67081	3.24%	0.534%
22	11.865	1677	1685	1695	rBV	913331	1685410	81.44%	13.404%
23	11.965	1697	1702	1710	rBV2	24997	55763	2.69%	0.443%
24	12.071	1714	1720	1727	rVV2	37076	77256	3.73%	0.614%
25	12.400	1772	1776	1783	rBV2	15439	31225	1.51%	0.248%
26	12.847	1846	1852	1862	rVB	733691	1240287	59.93%	9.864%
27	13.176	1904	1908	1918	rVB3	34100	80610	3.90%	0.641%
28	13.794	2006	2013	2021	rVB	939926	1629487	78.74%	12.959%
29	14.118	2063	2068	2077	rBV8	42899	109092	5.27%	0.868%

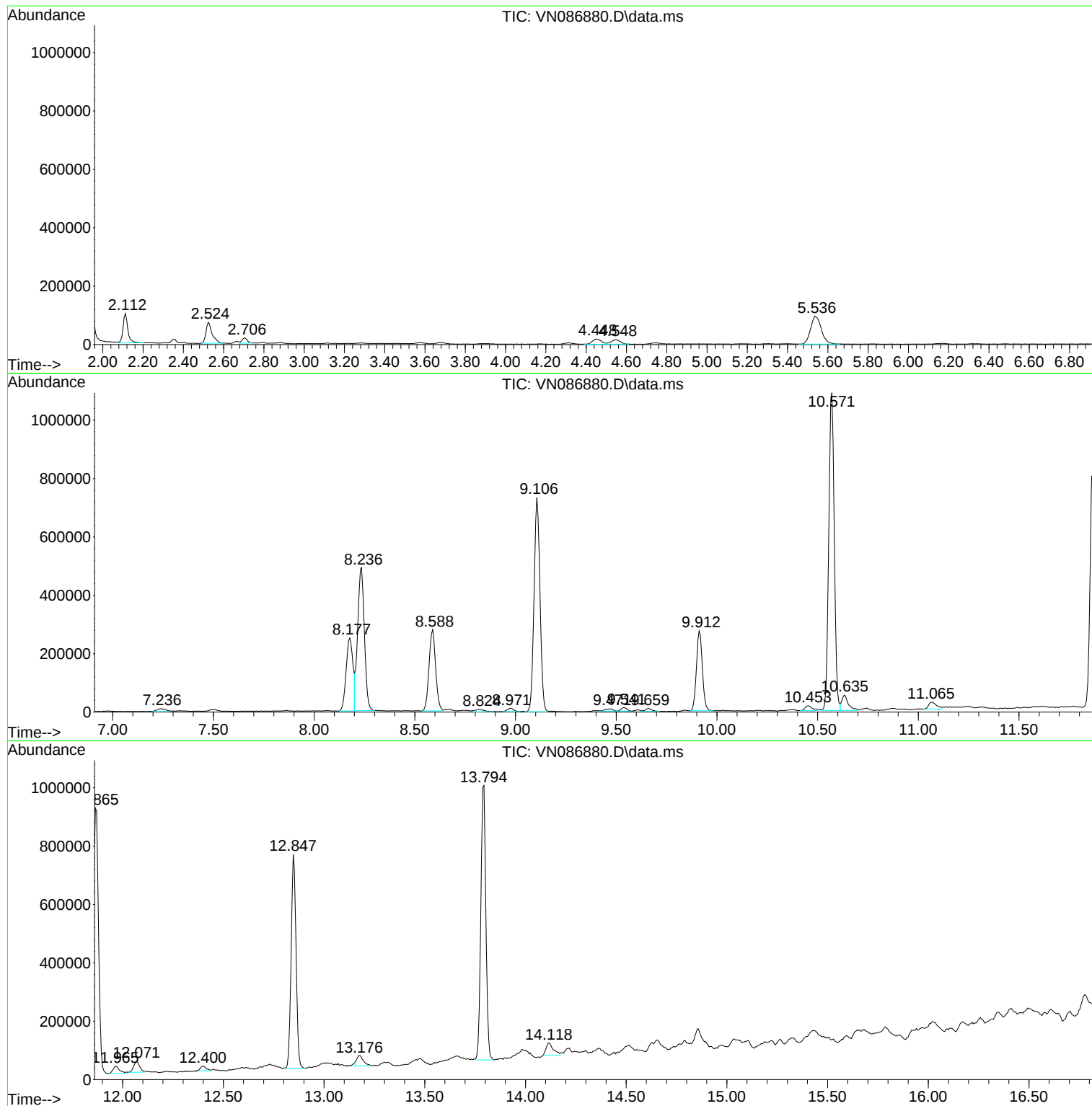
Sum of corrected areas: 12573726

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060625\
Data File : VN086880.D
Acq On : 06 Jun 2025 20:36
Operator : JC\MD
Sample : Q2216-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3851

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060625\
Data File : VN086880.D
Acq On : 06 Jun 2025 20:36
Operator : JC\MD
Sample : Q2216-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3851

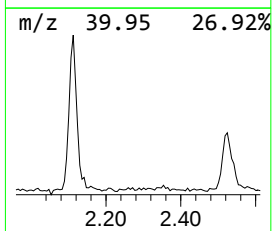
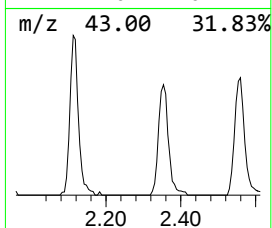
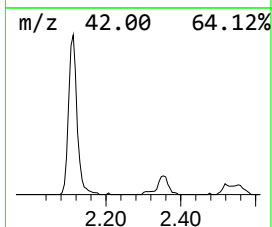
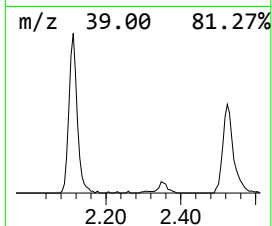
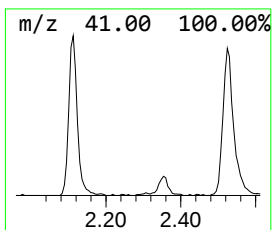
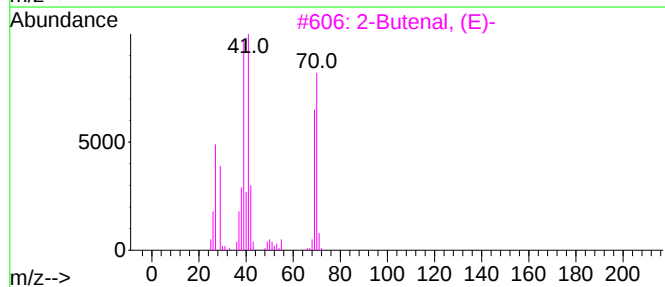
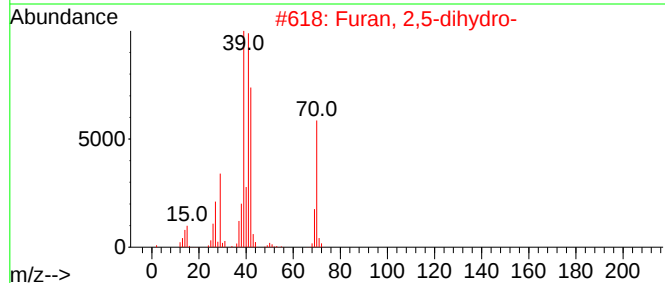
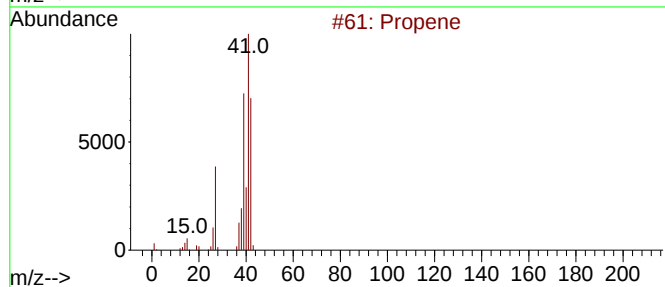
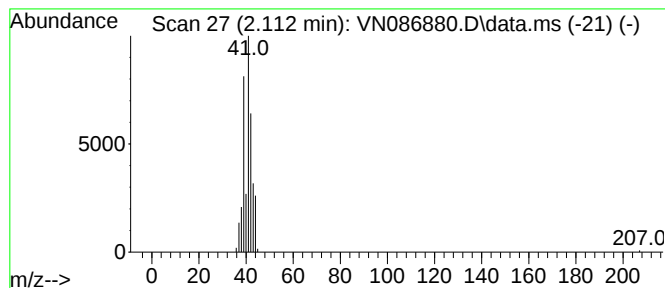
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 1 Propene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.112	7.28 ug/l	164391	Pentafluorobenzene	8.236

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	83
3			2-Butenal, (E)-	70	C4H6O	000123-73-9	78
4			3-Butenoic acid	86	C4H6O2	000625-38-7	78
5			Pyrimidin-4(3H)-one, 3-amino-2,6...	139	C6H9N3O	093098-74-9	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060625\
Data File : VN086880.D
Acq On : 06 Jun 2025 20:36
Operator : JC\MD
Sample : Q2216-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3851

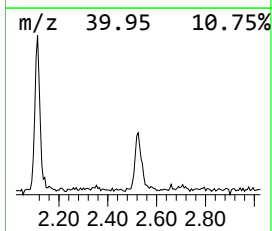
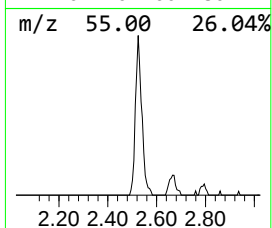
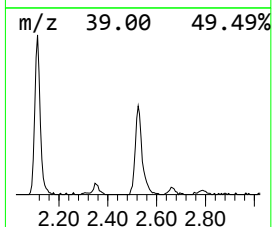
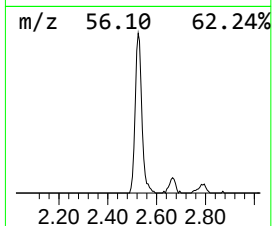
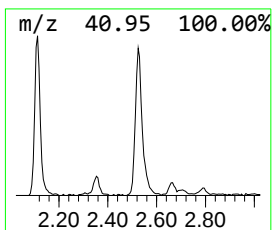
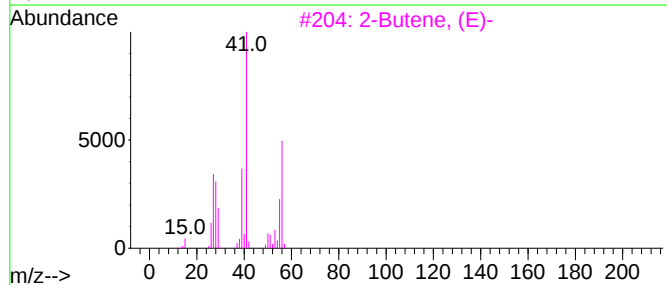
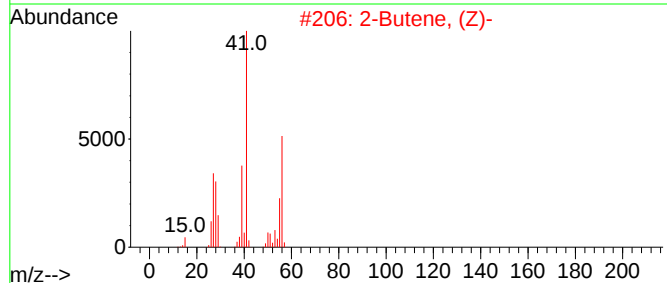
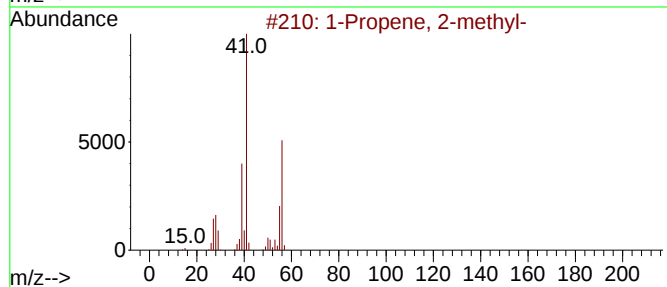
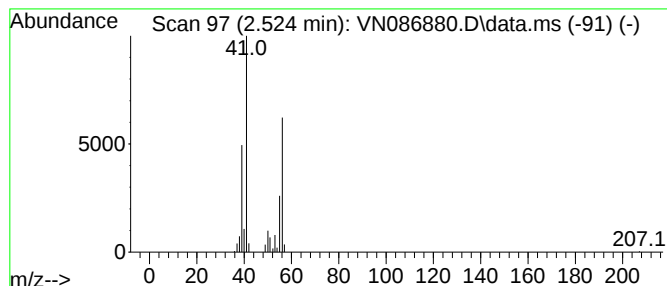
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.524	6.74 ug/l	152210	Pentafluorobenzene	8.236

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-			56	C4H8	000115-11-7	90
2	2-Butene, (Z)-			56	C4H8	000590-18-1	80
3	2-Butene, (E)-			56	C4H8	000624-64-6	80
4	2-Butene			56	C4H8	000107-01-7	72
5	Cyclobutane			56	C4H8	000287-23-0	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060625\
Data File : VN086880.D
Acq On : 06 Jun 2025 20:36
Operator : JC\MD
Sample : Q2216-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3851

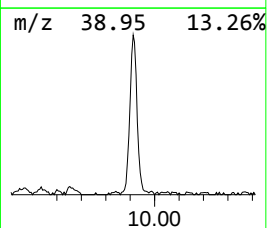
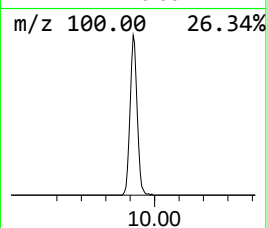
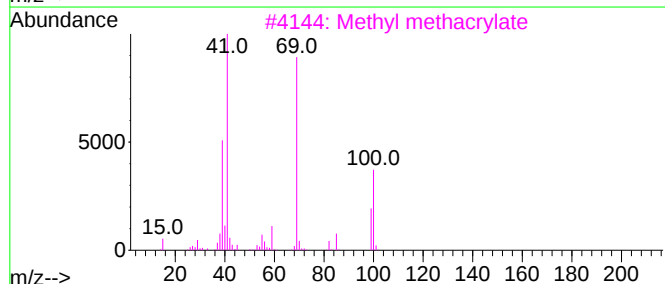
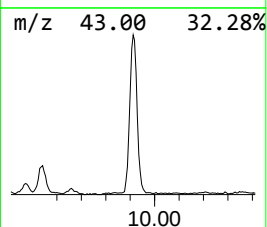
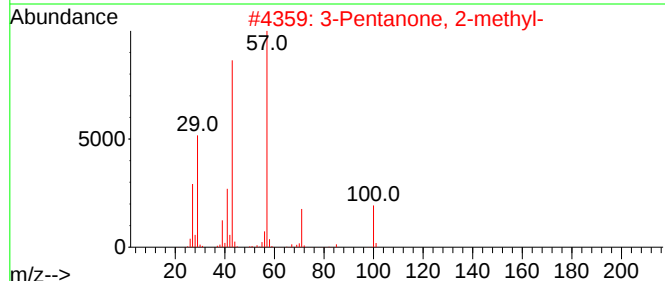
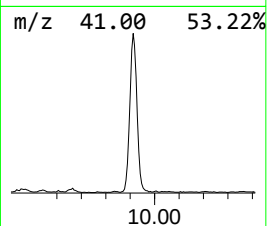
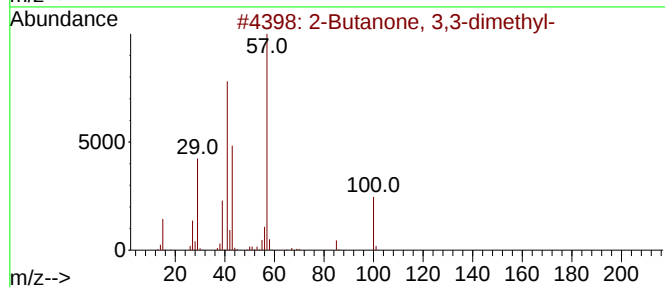
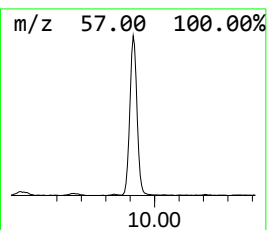
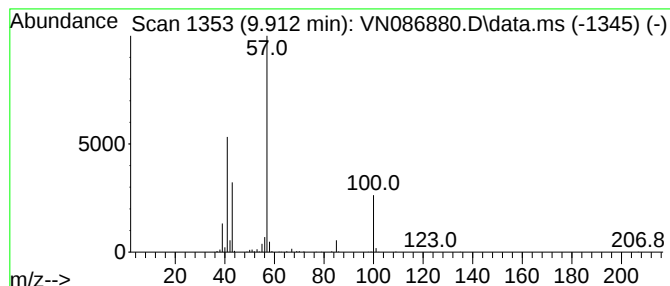
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 3 2-Butanone, 3,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.912	18.65 ug/l	558945	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	78
2			3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	59
3			Methyl methacrylate	100	C5H8O2	000080-62-6	47
4			Neopentane	72	C5H12	000463-82-1	38
5			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060625\
Data File : VN086880.D
Acq On : 06 Jun 2025 20:36
Operator : JC\MD
Sample : Q2216-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3851

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propene	2.112	7.3	ug/l	164391	1	8.236	1129240	50.0
1-Propene, 2-me...	2.524	6.7	ug/l	152210	1	8.236	1129240	50.0
2-Butanone, 3,3...	9.912	18.6	ug/l	558945	2	9.106	1498140	50.0