

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081525\
 Data File : VN087586.D
 Acq On : 15 Aug 2025 16:46
 Operator : JC\MD
 Sample : Q2840-02
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 0804-D

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\82N071625W.M

Title : SW846 8260

Signal : TIC: VN087586.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.312	54	61	66	rBV2	26986	45925	2.69%	0.492%
2	2.853	136	153	155	rBV8	61044	216431	12.69%	2.316%
3	4.547	437	441	452	rVB5	8362	24719	1.45%	0.265%
4	6.271	722	734	747	rBV5	25681	87236	5.11%	0.934%
5	8.147	1043	1053	1057	rBV	231421	539625	31.64%	5.776%
6	8.206	1057	1063	1073	rVB	351164	835315	48.97%	8.940%
7	8.559	1113	1123	1134	rBV	264941	614131	36.00%	6.573%
8	9.082	1198	1212	1223	rBV	632651	1343964	78.79%	14.385%
9	10.547	1451	1461	1470	rBV	913464	1705698	100.00%	18.256%
10	11.847	1673	1682	1694	rBV	801924	1515341	88.84%	16.219%
11	12.829	1842	1849	1863	rBV	512264	988135	57.93%	10.576%
12	13.770	2002	2009	2021	rVV	777423	1366926	80.14%	14.630%
13	14.288	2088	2097	2098	rBV4	30765	59692	3.50%	0.639%

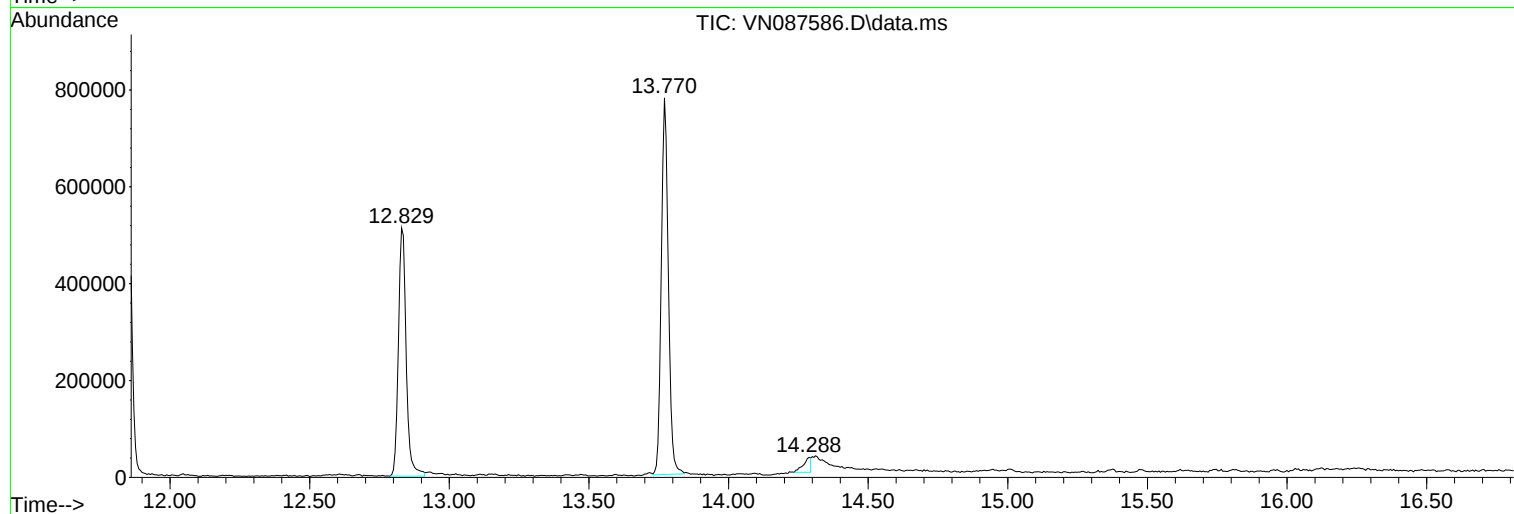
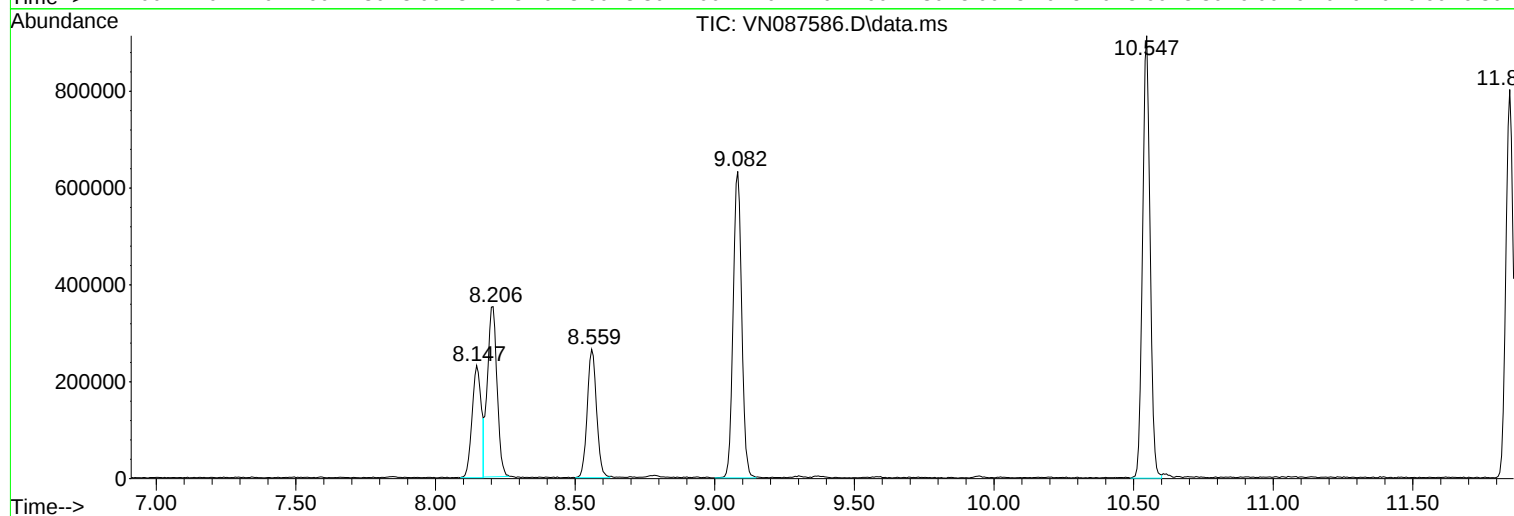
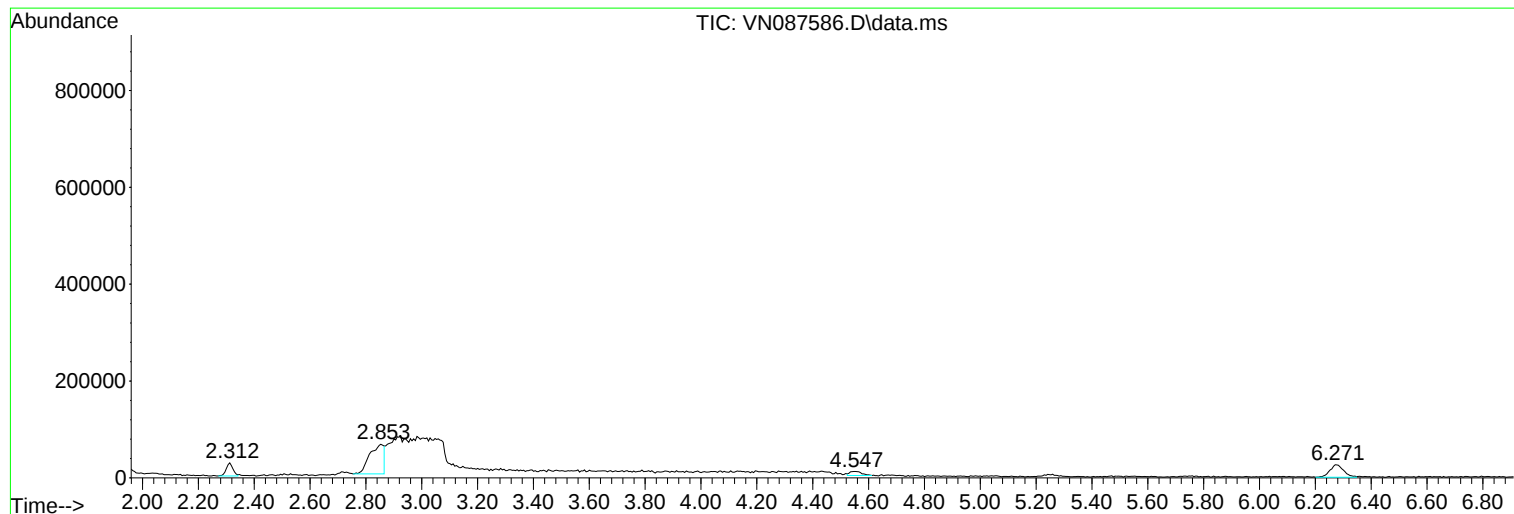
Sum of corrected areas: 9343138

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081525\
Data File : VN087586.D
Acq On : 15 Aug 2025 16:46
Operator : JC\MD
Sample : Q2840-02
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
0804-D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081525\
Data File : VN087586.D
Acq On : 15 Aug 2025 16:46
Operator : JC\MD
Sample : Q2840-02
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

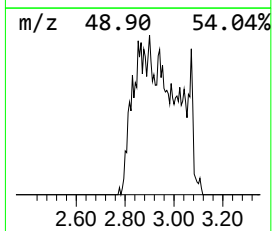
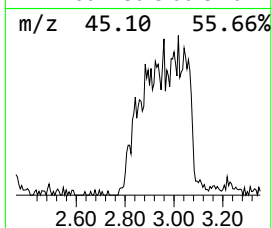
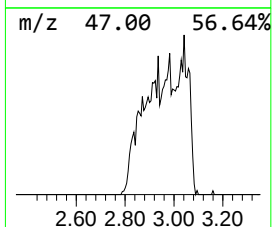
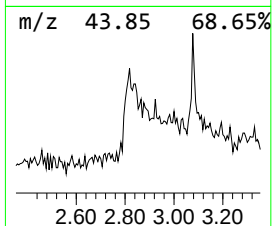
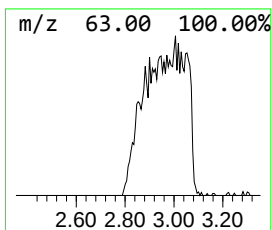
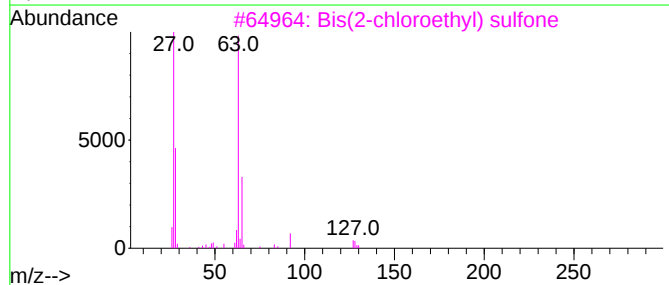
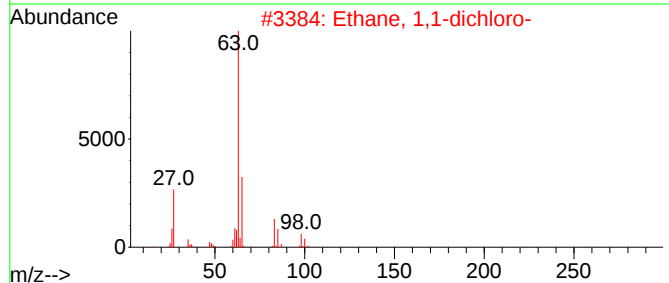
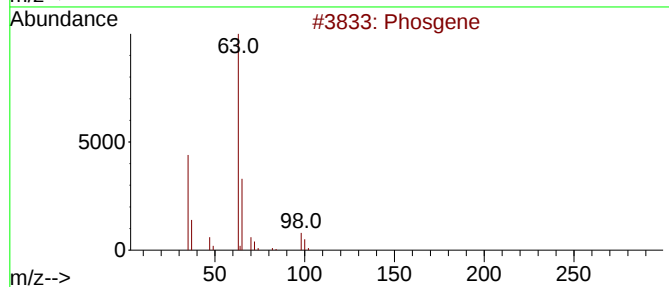
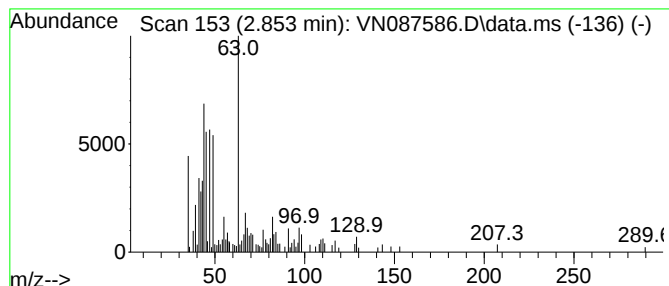
Instrument :
MSVOA_N
ClientSampleId :
0804-D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.853 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.853	12.96 ug/l	216431	Pentafluorobenzene	8.206	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosgene	98	CCl2O	000075-44-5	38
2	Ethane, 1,1-dichloro-	98	C2H4Cl2	000075-34-3	12
3	Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	12
4	2-Propanol, 1-chloro-3-fluoro-	112	C3H6ClFO	189937-18-6	12
5	Propanoic acid, 2-chloro-, methy...	122	C4H7ClO2	017639-93-9	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081525\
Data File : VN087586.D
Acq On : 15 Aug 2025 16:46
Operator : JC\MD
Sample : Q2840-02
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
0804-D

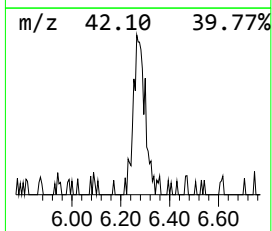
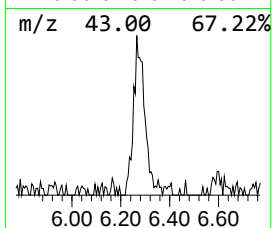
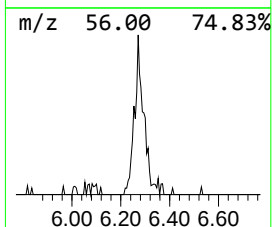
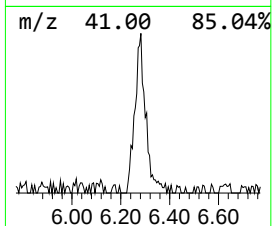
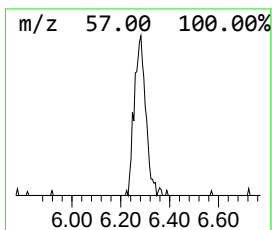
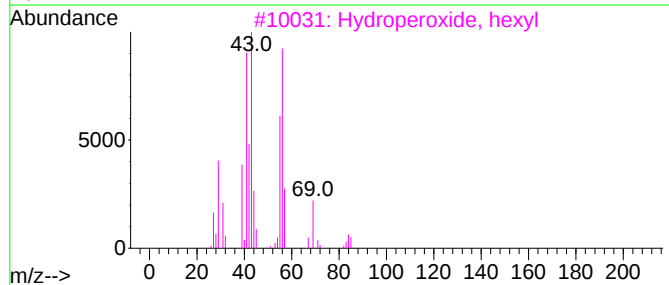
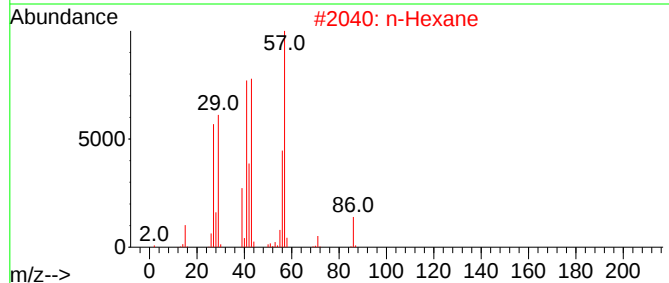
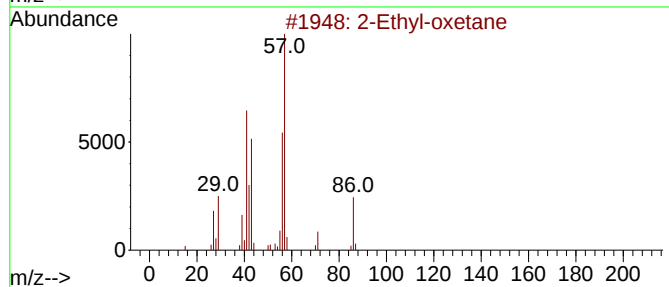
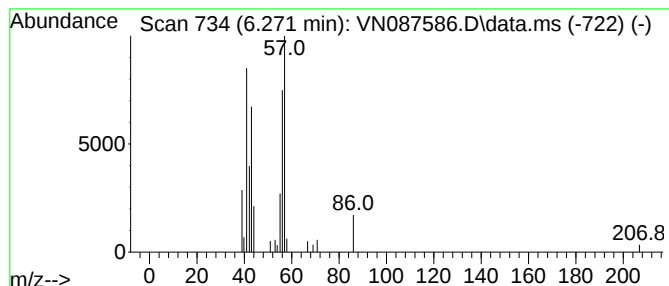
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Ethyl-oxetane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.271	5.22 ug/l	87236	Pentafluorobenzene	8.206

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	72
2			n-Hexane	86	C6H14	000110-54-3	52
3			Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	45
4			1-Butanol	74	C4H10O	000071-36-3	42
5			1-Hexene, 4-methyl-	98	C7H14	003769-23-1	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081525\
Data File : VN087586.D
Acq On : 15 Aug 2025 16:46
Operator : JC\MD
Sample : Q2840-02
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
0804-D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.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
unknown2.853	2.853	13.0	ug/l	216431	1	8.206	835315	50.0
2-Ethyl-oxetane	6.271	5.2	ug/l	87236	1	8.206	835315	50.0