

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120925\
Data File : VN088476.D
Acq On : 09 Dec 2025 13:45
Operator : JC\MD
Sample : Q3770-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
4207

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\82N112425W.M

Title : SW846 8260

Signal : TIC: VN088476.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.194	1041	1061	1071	rBV2	2489001	6670758	3.63%	2.935%
2	8.300	1071	1079	1089	rVV2	770732	1888084	1.03%	0.831%
3	8.418	1089	1099	1115	rVV	4365064	10086974	5.49%	4.438%
4	8.941	1177	1188	1203	rBV	8841535	17694256	9.64%	7.784%
5	9.565	1281	1294	1299	rBV3	1149251	3094364	1.69%	1.361%
6	10.606	1463	1471	1486	rVB3	79236700	183595550	100.00%	80.772%
7	13.135	1894	1901	1909	rVB2	1143398	2078836	1.13%	0.915%
8	14.076	2056	2061	2068	rBV	1392121	2193257	1.19%	0.965%

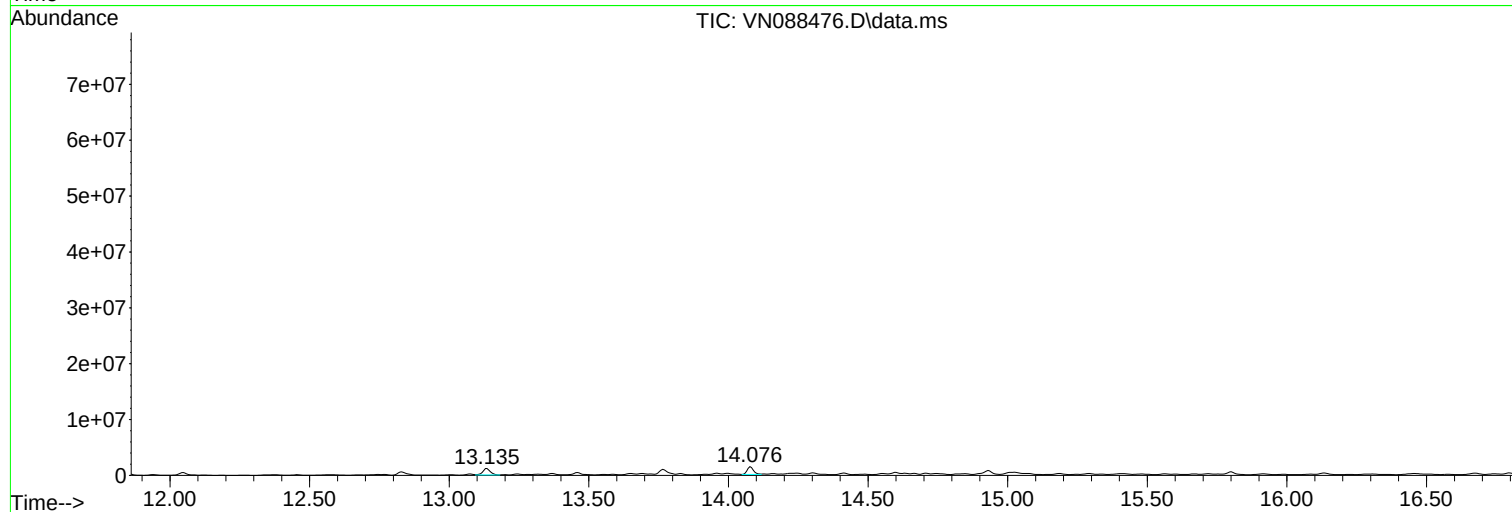
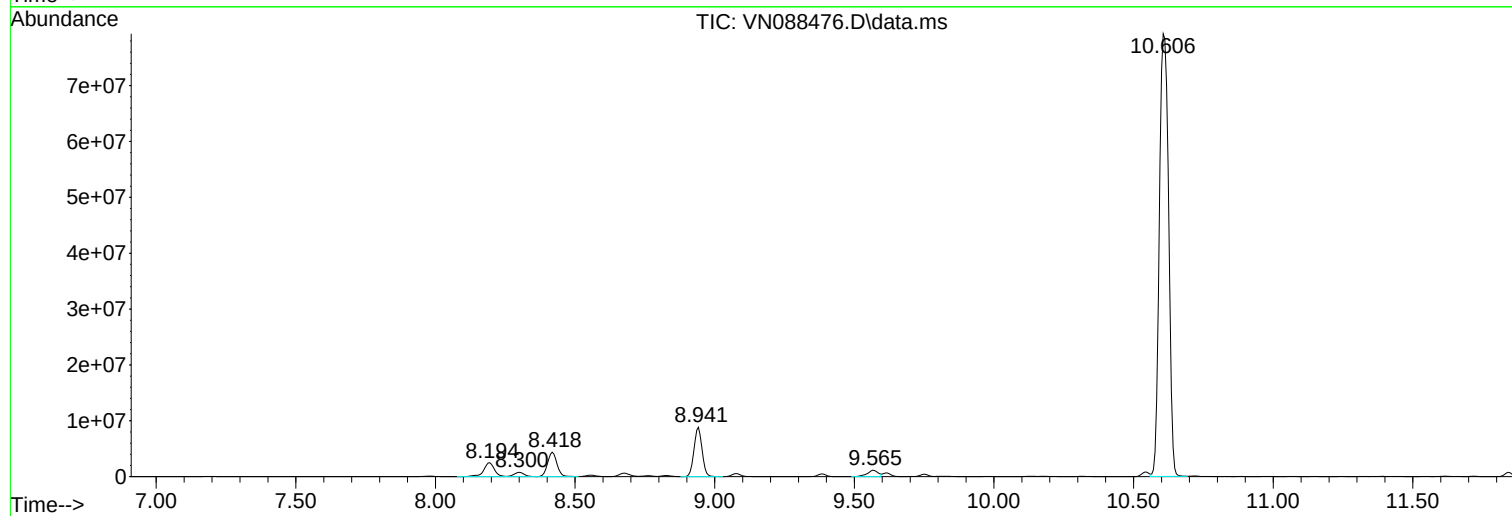
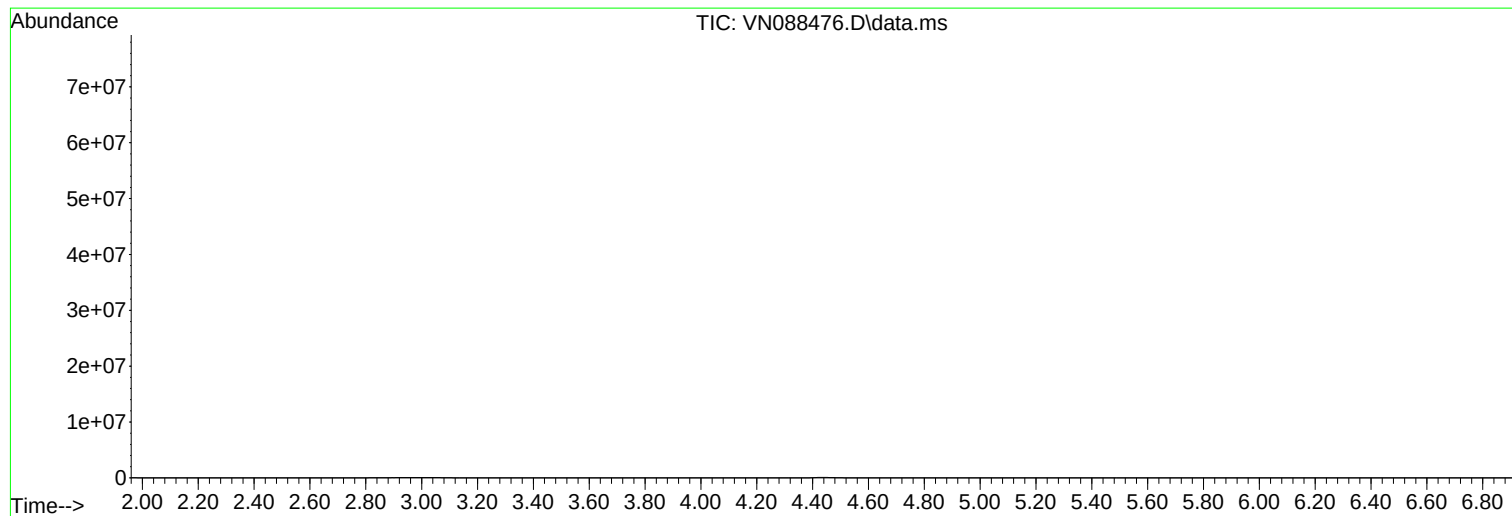
Sum of corrected areas: 227302079

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Quant Title : SW846 8260

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



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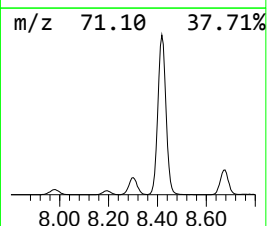
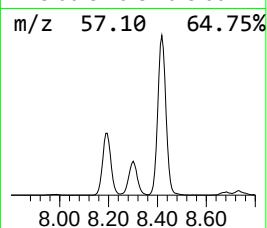
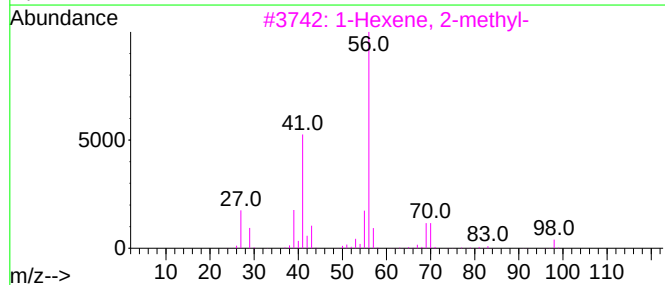
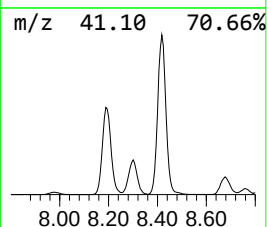
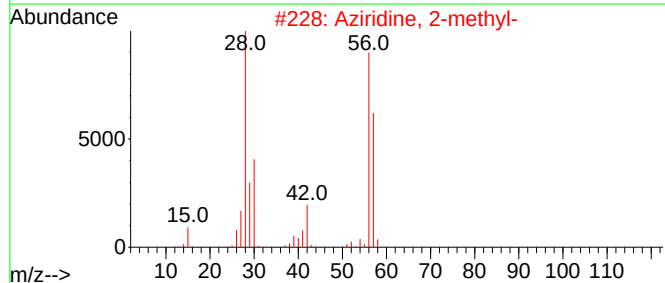
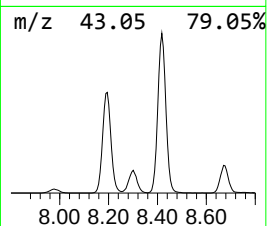
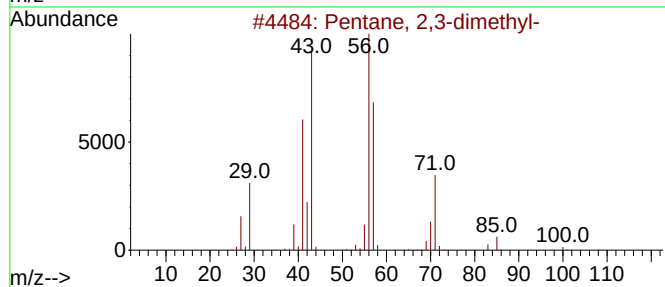
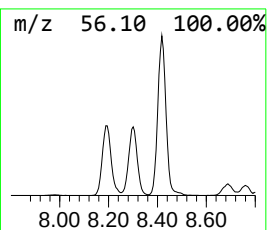
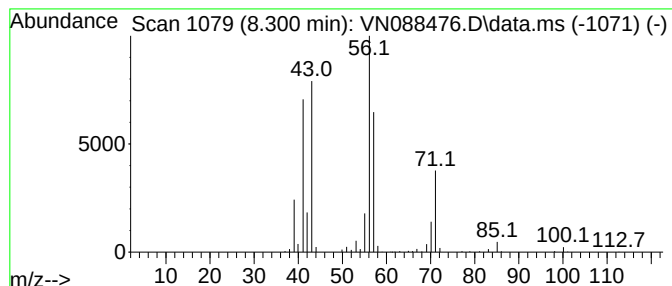
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112425W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.300	14.15 ug/l	1888080	Pentafluorobenzene	8.200

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	47
3			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	47
4			Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	42
5			Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	40



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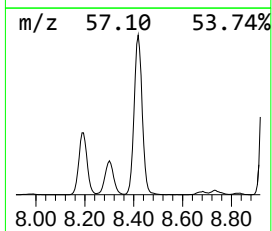
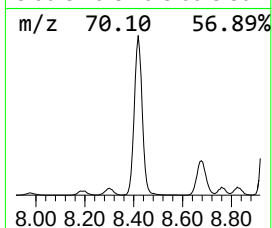
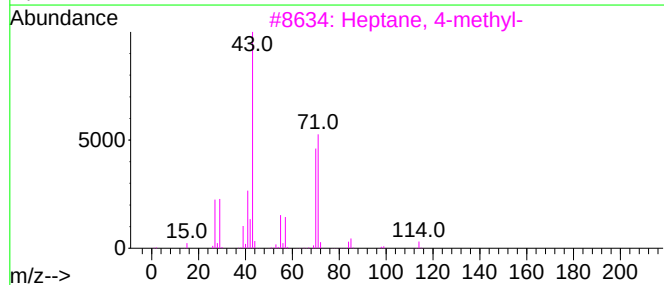
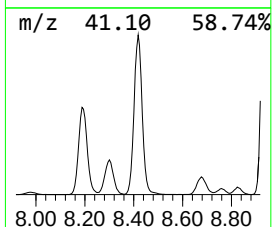
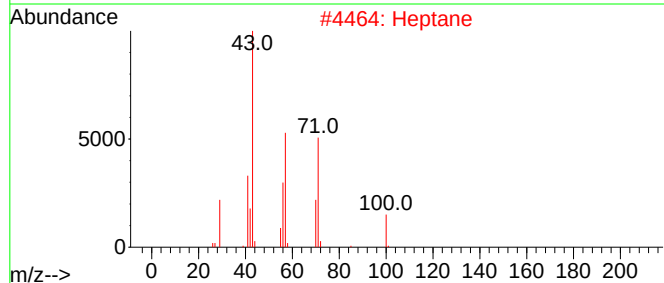
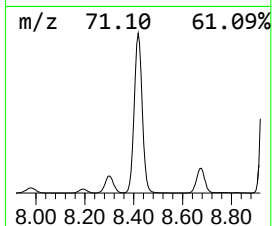
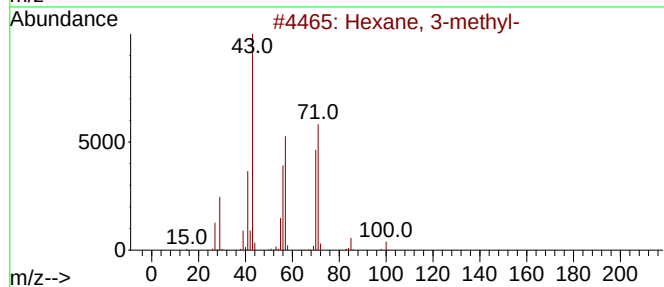
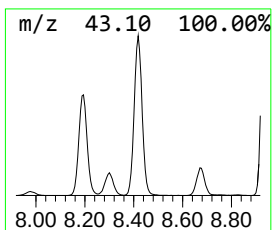
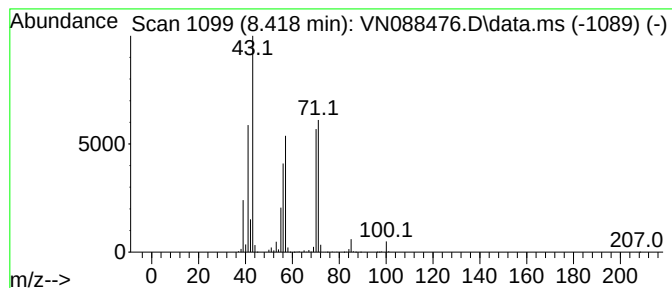
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Peak Number 2 Hexane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.418	75.61 ug/l	10087000	Pentafluorobenzene	8.200

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2			Heptane	100	C7H16	000142-82-5	80
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	53
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53



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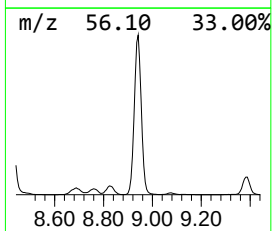
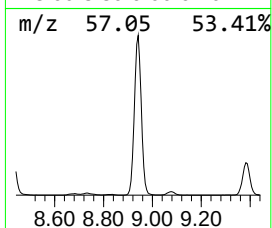
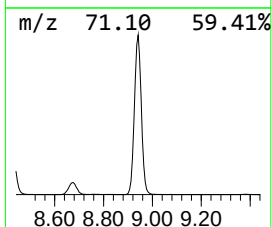
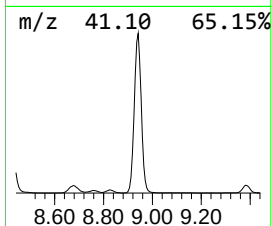
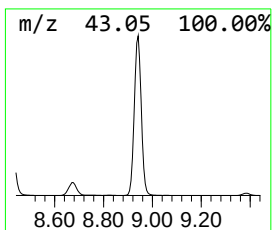
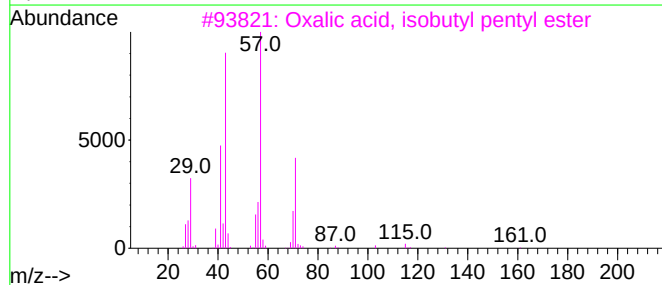
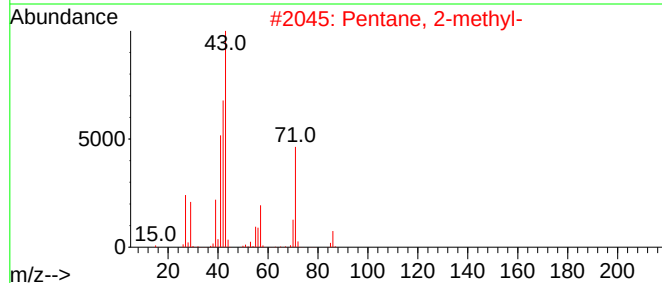
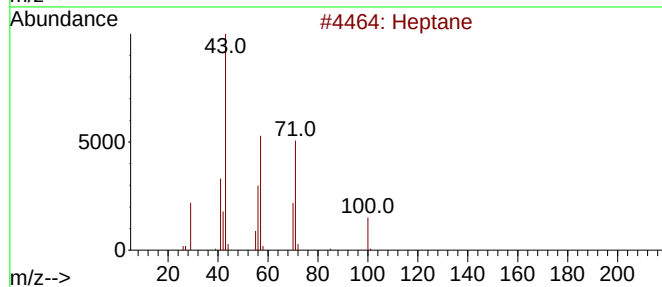
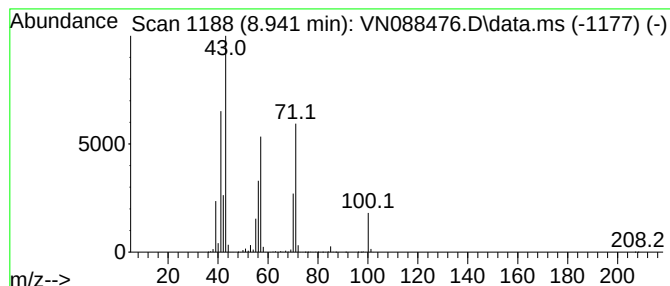
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Peak Number 3 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.941	50.00 ug/l	17694300	1,4-Difluorobenzene	9.077

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	47
3			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	42
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	38
5			3-Hexanone	100	C6H12O	000589-38-8	37



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,3-di...	8.300	14.2	ug/l	1888080	1	8.200	6670760	50.0
Hexane, 3-methyl-	8.418	75.6	ug/l	10087000	1	8.200	6670760	50.0
Heptane	8.941	50.0	ug/l	17694300	2	9.077	17694300	50.0