

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091521\
 Data File : VN068495.D
 Acq On : 15 Sep 2021 19:56
 Operator : JC/MD
 Sample : M3759-17 50X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31185

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\82N090721W.M

Title : SW846 8260

Signal : TIC: VN068495.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.242	78	94	110	rVB4	18874	37943	1.26%	0.213%
2	2.588	210	223	247	rBV	190798	339878	11.32%	1.912%
3	4.149	782	805	835	rBV	181816	522218	17.40%	2.938%
4	4.299	849	861	882	rVB2	11897	32524	1.08%	0.183%
5	6.586	1694	1714	1736	rBV4	20049	69205	2.31%	0.389%
6	7.158	1910	1927	1950	rVB	14588	40276	1.34%	0.227%
7	7.313	1964	1985	2011	rBV	24697	75126	2.50%	0.423%
8	8.024	2227	2250	2261	rBV	412694	981522	32.70%	5.522%
9	8.088	2262	2274	2303	rVB	827837	1891237	63.01%	10.641%
10	8.440	2380	2405	2430	rBV2	362146	846933	28.22%	4.765%
11	8.973	2583	2604	2650	rBV3	1383052	3001658	100.00%	16.888%
12	9.215	2677	2694	2715	rBV2	231801	464164	15.46%	2.612%
13	10.443	3132	3152	3169	rBV	1407180	2733215	91.06%	15.378%
14	10.693	3231	3245	3269	rBV3	63248	132672	4.42%	0.746%
15	11.143	3382	3413	3424	rBV	23783	70079	2.33%	0.394%
16	11.747	3613	3638	3667	rVB	1295526	2519586	83.94%	14.176%
17	12.733	3988	4006	4026	rBV	1079234	1899890	63.29%	10.689%
18	13.678	4342	4358	4380	rBV	1178768	2052721	68.39%	11.549%
19	13.771	4382	4393	4412	rVB3	33076	62724	2.09%	0.353%

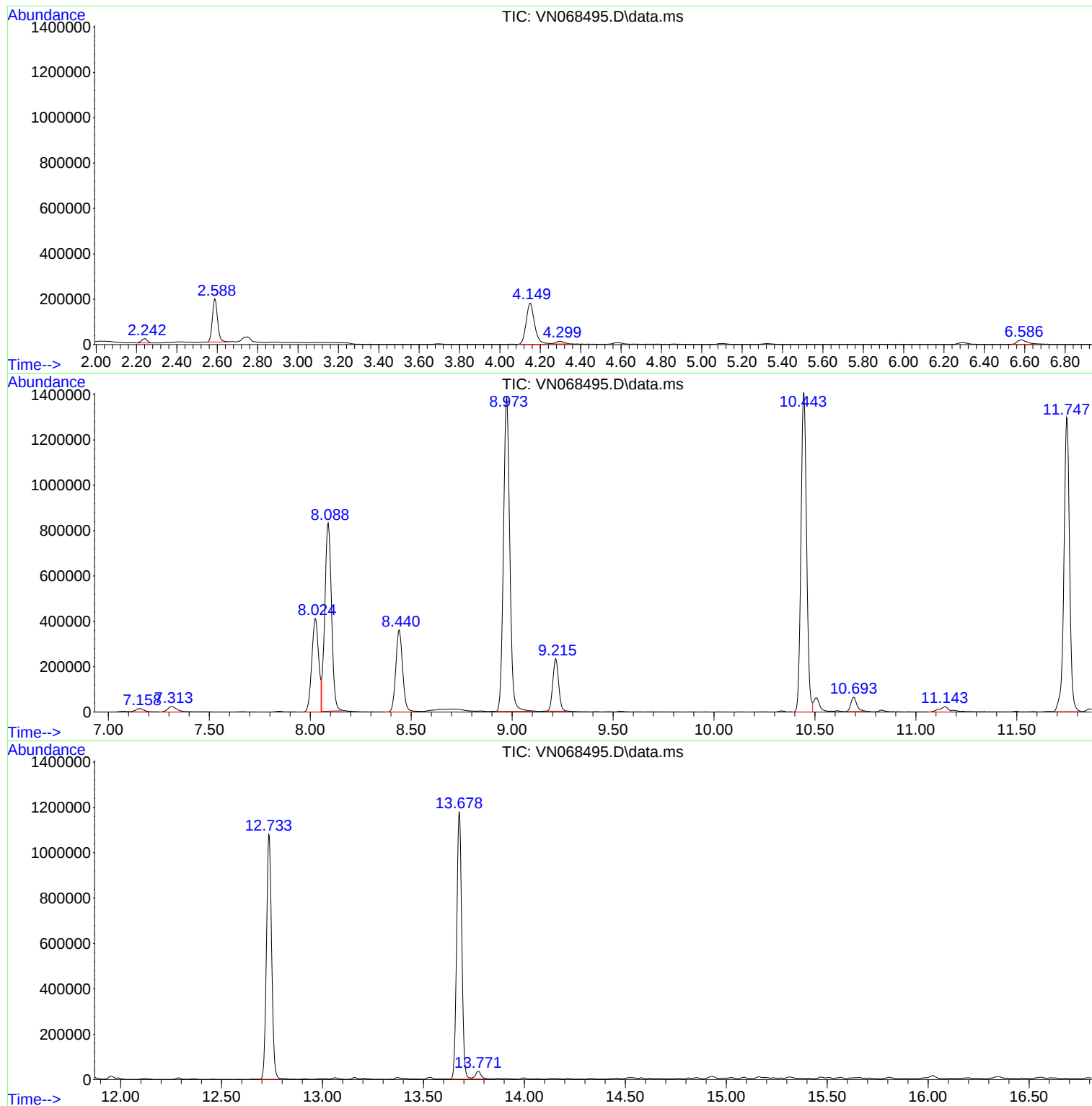
Sum of corrected areas: 17773571

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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



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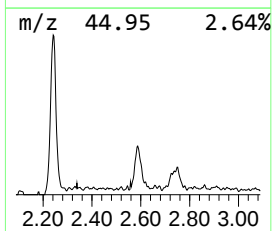
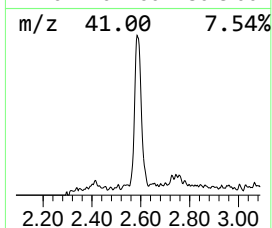
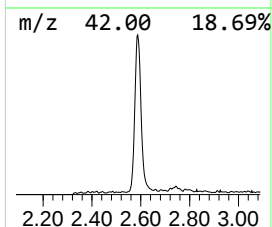
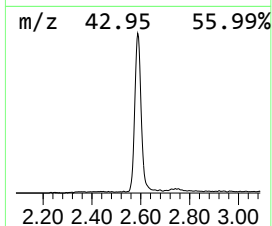
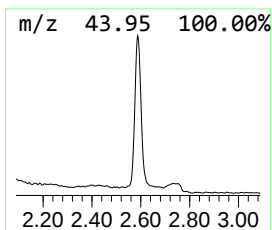
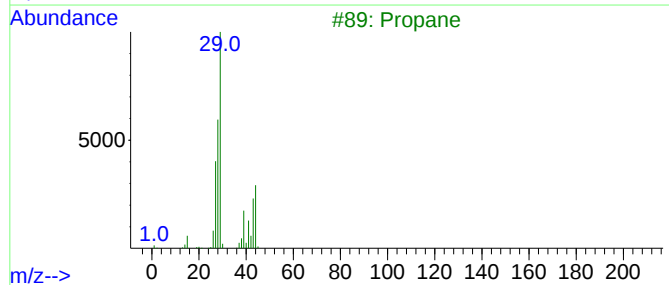
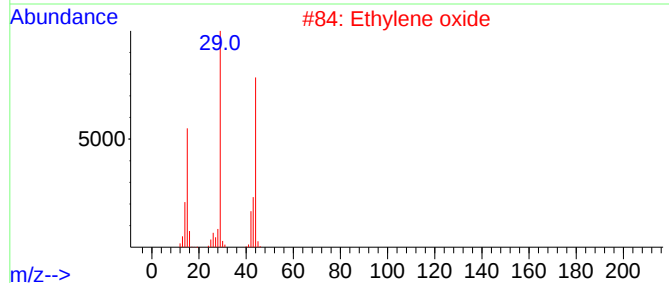
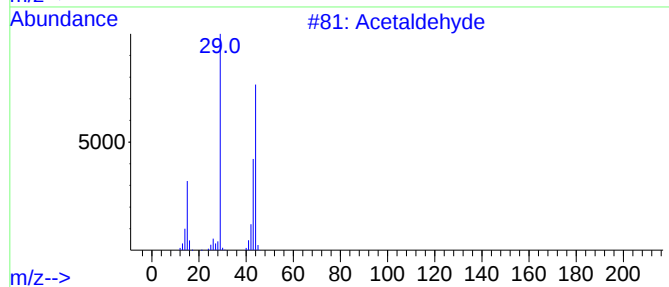
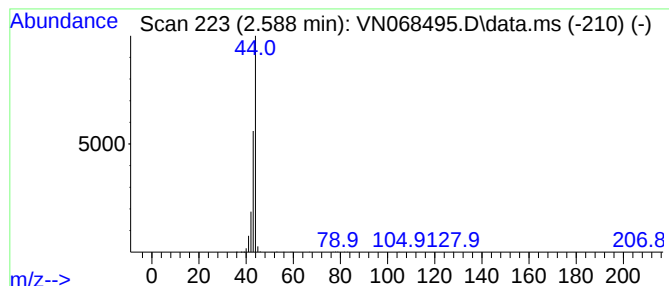
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.588	8.99 ug/l	339878	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			Acetic acid, [(aminocarbonyl)ami...	132	C3H4N2O4	000585-05-7	4
5			Acetic acid, 2-(methylaminoethyl...	117	C5H11NO2	026921-43-7	4



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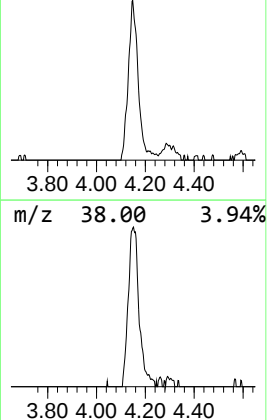
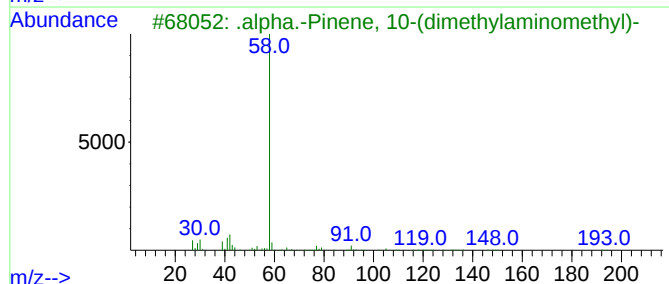
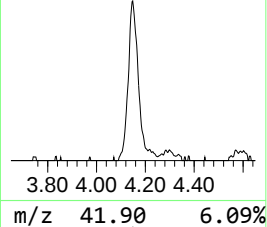
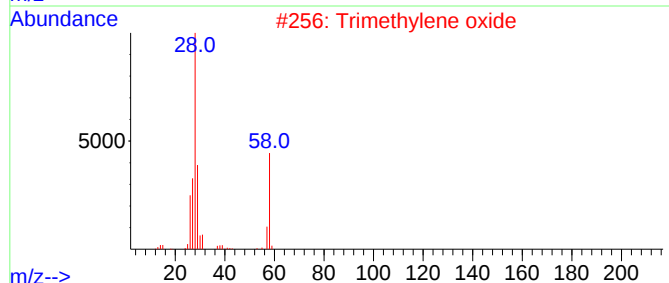
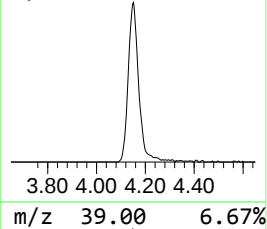
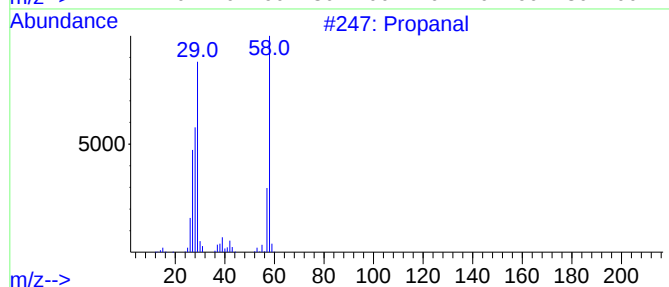
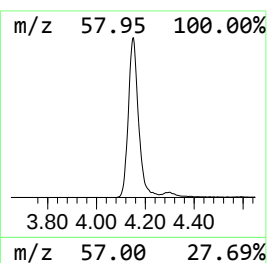
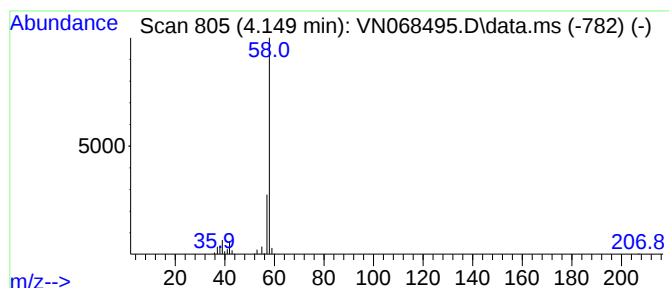
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Peak Number 2 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.149	13.81 ug/l	522218	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Trimethylene oxide	58	C3H6O	000503-30-0	9
3			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
4			2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	9
5			Propylene oxide	58	C3H6O	000075-56-9	7



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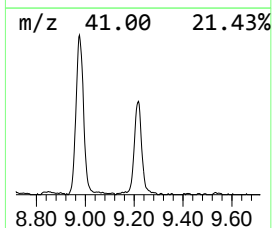
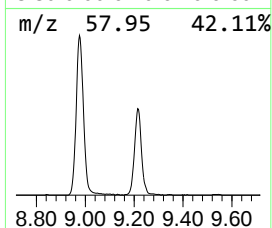
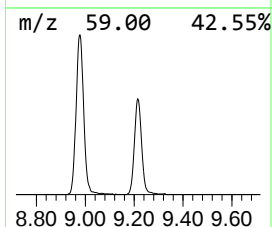
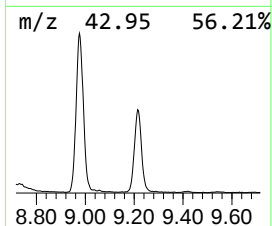
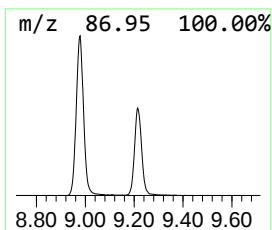
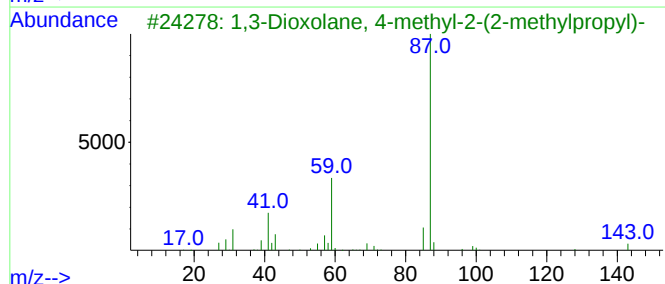
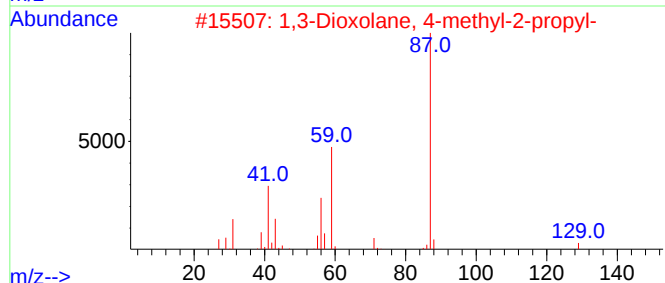
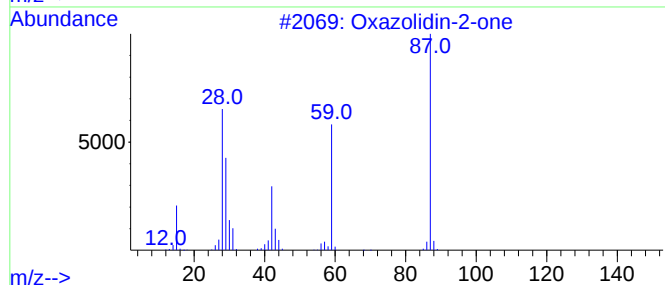
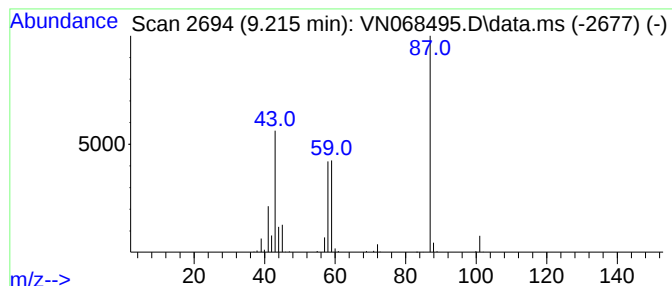
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Peak Number 3 unknown9.215 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.215	7.73 ug/l	464164	1,4-Difluorobenzene	8.971

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40
2			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	40
3			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	40
4			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	27
5			Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	23



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.588	9.0	ug/l	339878	1	8.088	1891240	50.0
Propanal	4.149	13.8	ug/l	522218	1	8.088	1891240	50.0
unknown9.215	9.215	7.7	ug/l	464164	2	8.971	3001660	50.0