Supporting Information for Publication

Raman spectroscopy applied to monitor furfural liquid-phase oxidation catalyzed by supported gold nanoparticles

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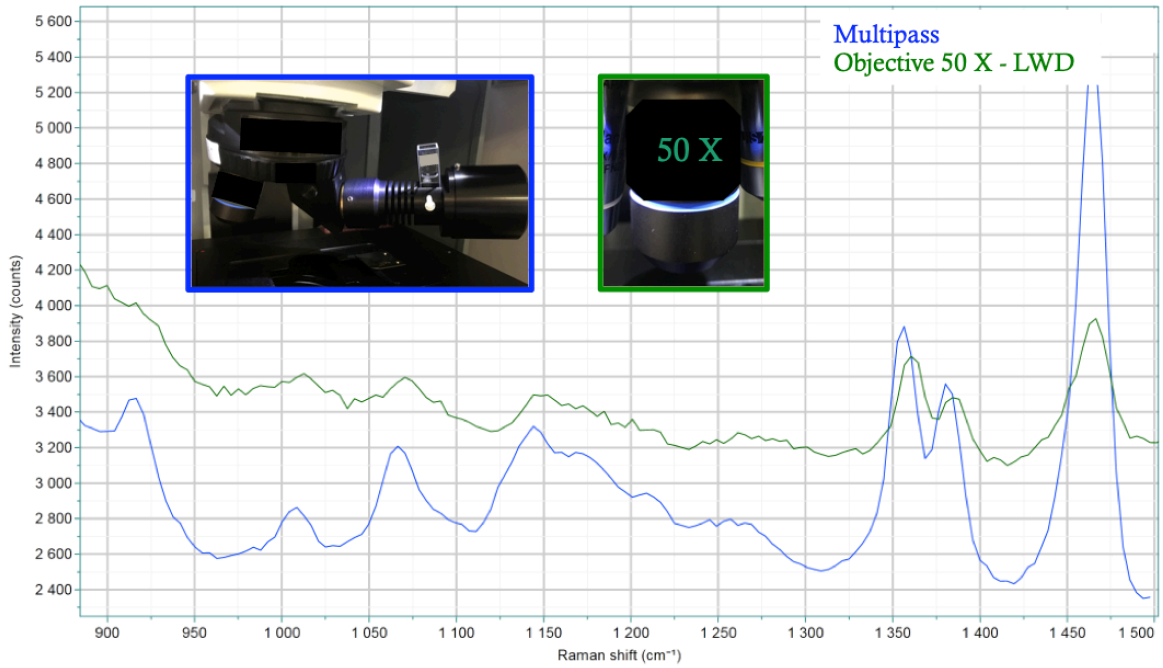

Figure S1: Comparison of the analysis of [furfural]= 64 mmol.L^{-1} by the multipass holder and conventional Raman objective (Long working distance). The multipass holder cell enables sensitivity to be increased by up to five times over the use of an objective (×50 LWD)

Calculation of conversion, selectivity, yield and carbon balance:

-The conversion (X%) represents the real amount of reagent that is converted into the products. It is expressed as follow:

$X = 100 * [n(t_0) - n(t_f)] / n(t_0)$

Where $n(t_0)$ is the mole number of furfural at t_0 and $n(t_f)$ is the number of moles of furfural after the reaction.

-The yield (Y%) is calculated using the number of the product moles obtained during the reaction. It is expressed as follow:

$Y = 100 * n\ prod(t_f) / n\ reag(t_0)$

-The selectivity (S%) is calculated comparing the yield to the conversion of the reagent, as follow:

$S = 100 * Y / X$

-The carbon balance is a very useful and necessary parameter to check the possible degradation of the furfural and it is calculated as follow:

$C\% = Cprod(t_f) / [Creag(t_f) - Creag(t_0)]$

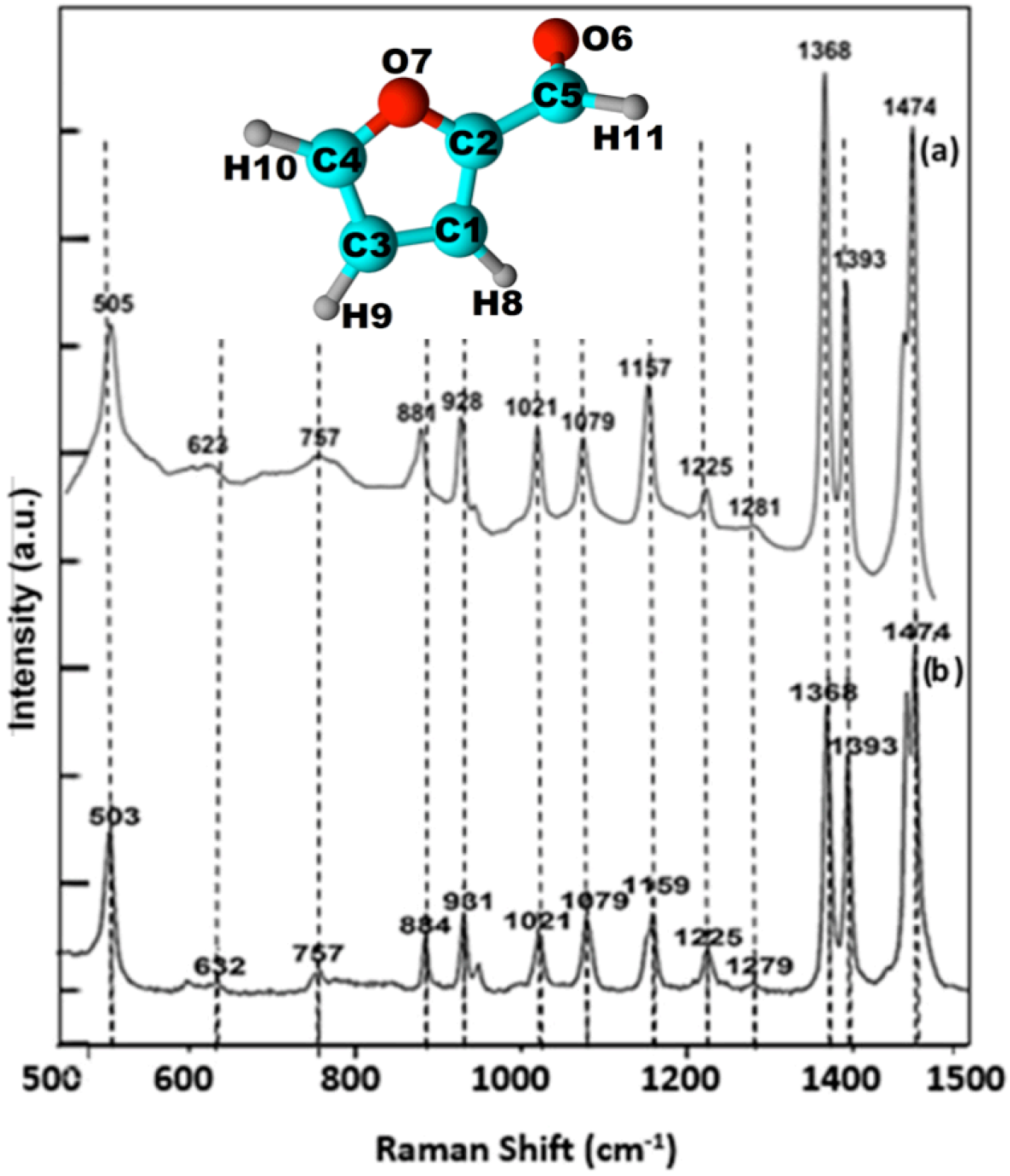

Figure S2: Full Furfural Raman spectra a) this work b) obtained by Wan *et al.* 2017
(Adapted in part with permission from [WAN ET Al. 2017,7(8), 210, NANOMATERIALS]. Copyright [2017] [MDPI])

Table S1: All Raman vibration mode assignments of furfural molecules & comparison with literature (Wan *et al.* 2017).

Raman Shift (cm^{-1})			
This work	Wan *et al.* 2017	Vibrational plane	Vibrational mode
505	503	In plane	C3-C1-H8, H8-C1-C3-H9 symmetric bend
623	632	Out plane	C3-C1-H8, H8-C1-C2-O7-C4 symmetric wag
757	757	In plane	H9-C3-C1-C2-C5-O6-H11 sway; H8-C1-C3-H9 stretch
881	884	Out plane	C1-C2-C5-H11, C3-C4-H10-O7 synchronous sway; C2-C5-O6-H11 asynchronous sway
928	931	In plane	C3-C1-H8, H8-C1-C2-O7-C4 symmetric bend
1021	1021	In plane	C2-C5-O6-H11, C3-C4-H10-O7 symmetric bend; C2-C1-C3 stretch
1079	1079	In plane	C1-C2-C5-H11, C2-C5-O6-H11 symmetric bend; C1-C2-O7-C4 stretch
1157	1159	In plane	C1-C2-C5-H11 sway; H8-C1-C2-O7-C4 stretch
1225	1225	In plane	C3-C4-H10-O7, C1-C2-C5-H11 asynchronous sway; C2-C1-C3 stretch
1281	1279	In plane	H8-C1-C3-H9, H8-C1-C2-O7-C4 asynchronous stretch; C2-C1-C3 stretch
1368	1368	In plane	H9-C3-C4-H10, C1-C2-C5-H11 synchronous sway
1393	1393	In plane	H8-C1-C3-H9, H8-C1-C2-O7-C4 asymmetric stretch; C2-C1-C3 stretch; H9-C3-C4-H10 sway; C2-C5-O6-H11 sway
1474	1474	In plane	C1-C2-O7-C4, H8-C1-C2-O7-C4 symmetric bend; C1-C2; C3-C1-H8 synchronous stretch; H9-C3-C4-H10, C1-C2-C5-H11 asynchronous sway

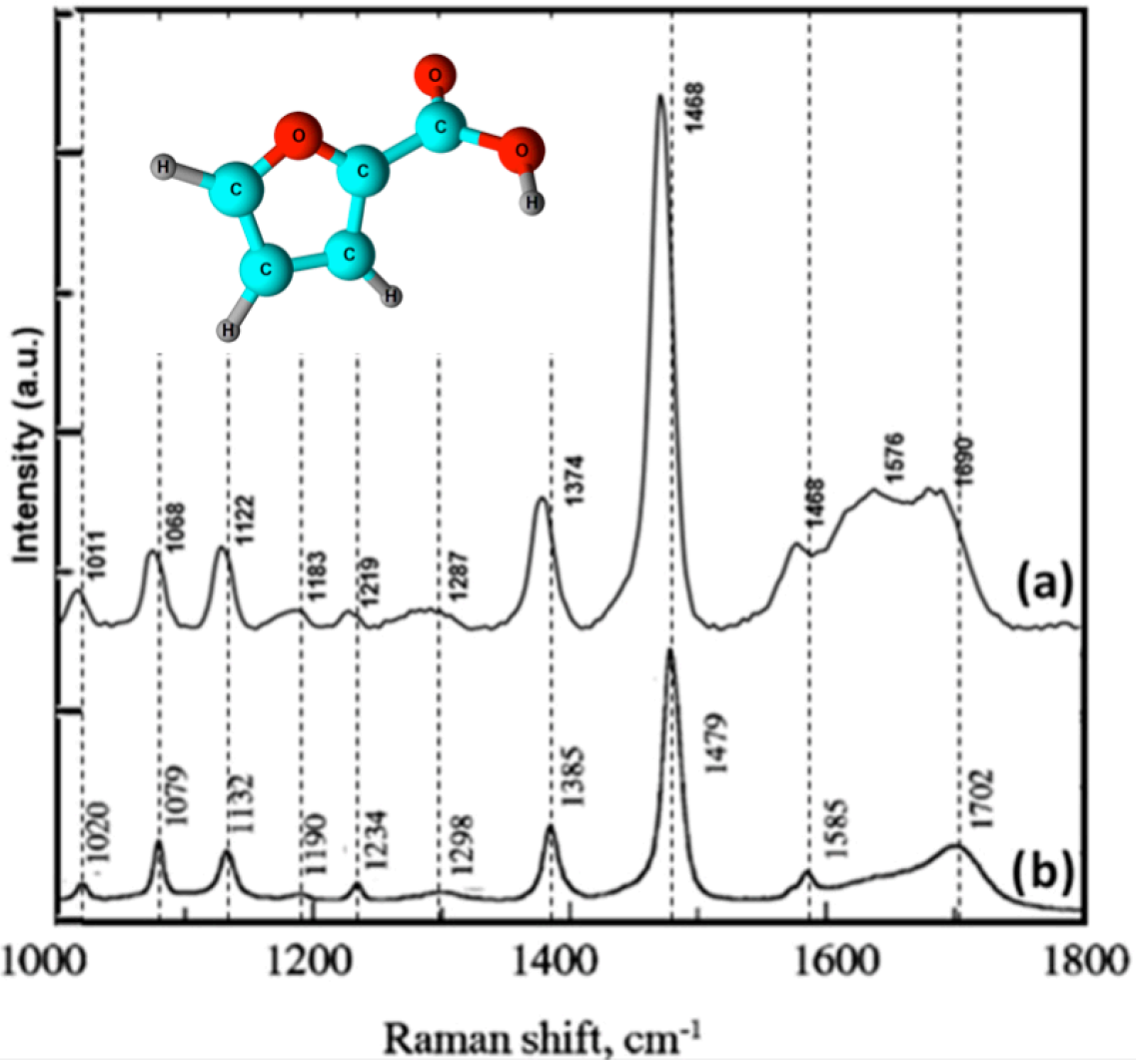

Figure S3: Furoic acid Raman spectra a) this work b) obtained by Bismondo *et al.* 2003 (Adapted in part with permission from [BISMONDO ET AL. 2003, 469-474, DALTON TRANSACTIONS]. Copyright [2003] [ROYAL SOCIETY OF CHEMISTRY])

Table S2: Comparison of all Raman Furoic acid bands obtained by our experimentation and by Bismondo *et al.* 2003

Raman Shift (cm^{-1})		
This work	Bismondo *et al.* 2017	Difference
1006	1020	14
1068	1079	11
1122	1132	10
1183	1190	7
1219	1234	15
1287	1298	11
1374	1385	11
1468	1479	10
1576	1585	11
1637 (water)	*	*
1690	1702	12

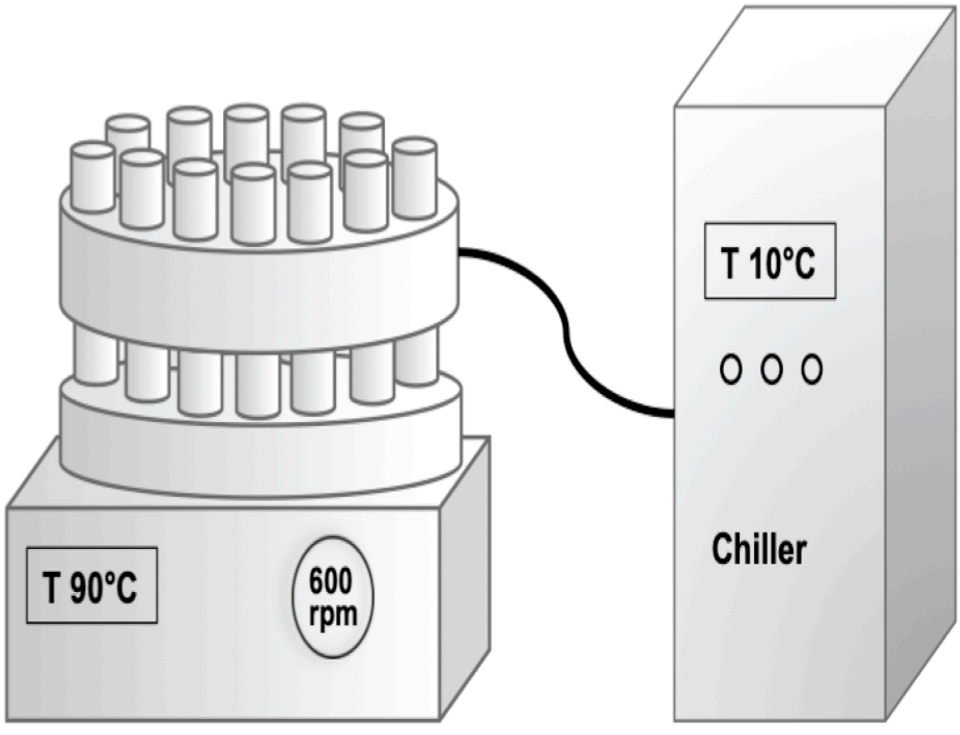

Figure S4: Schematic view of the multi-reactor system (MR)