Supporting information

Conversion of HMF to Methyl Cyclopentenolone by the Pd/Nb_2O_5 and Ca-Al Catalysts via Two-steps Procedure

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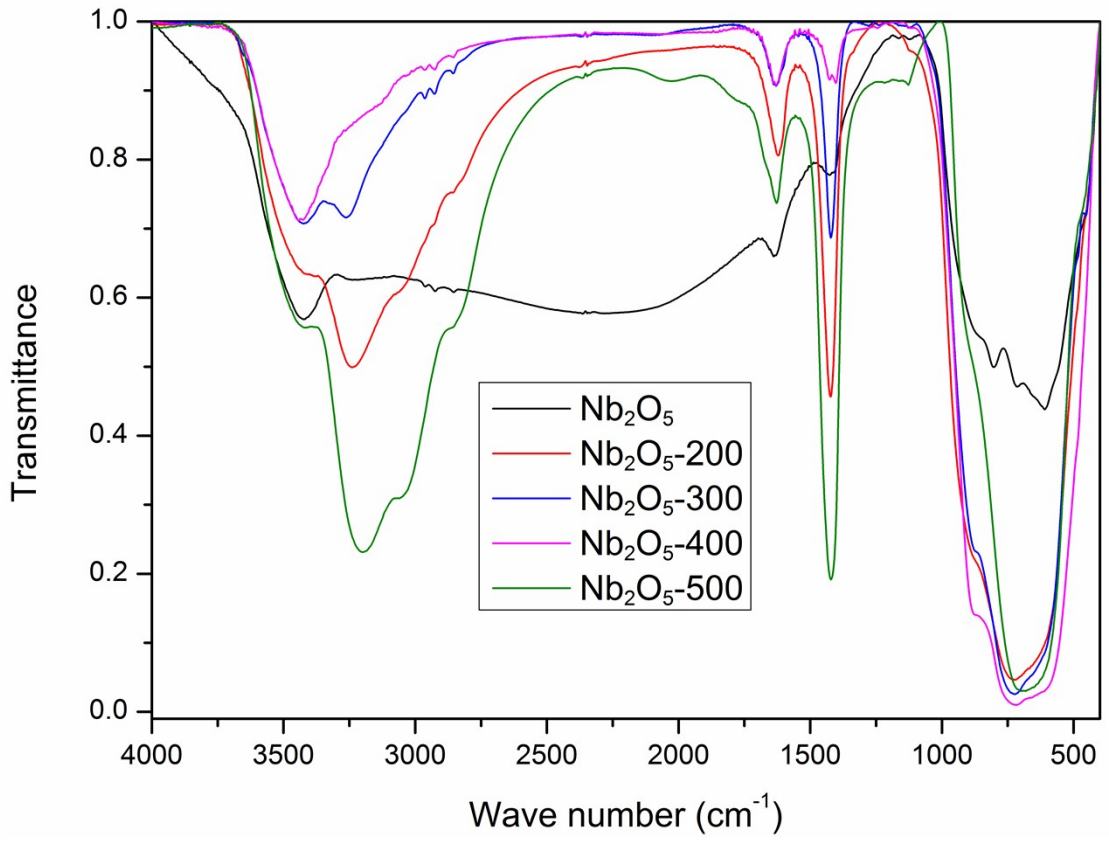

Fig. S1 FT-IR spectrum of Nb_2O_5 and Nb_2O_5-x.

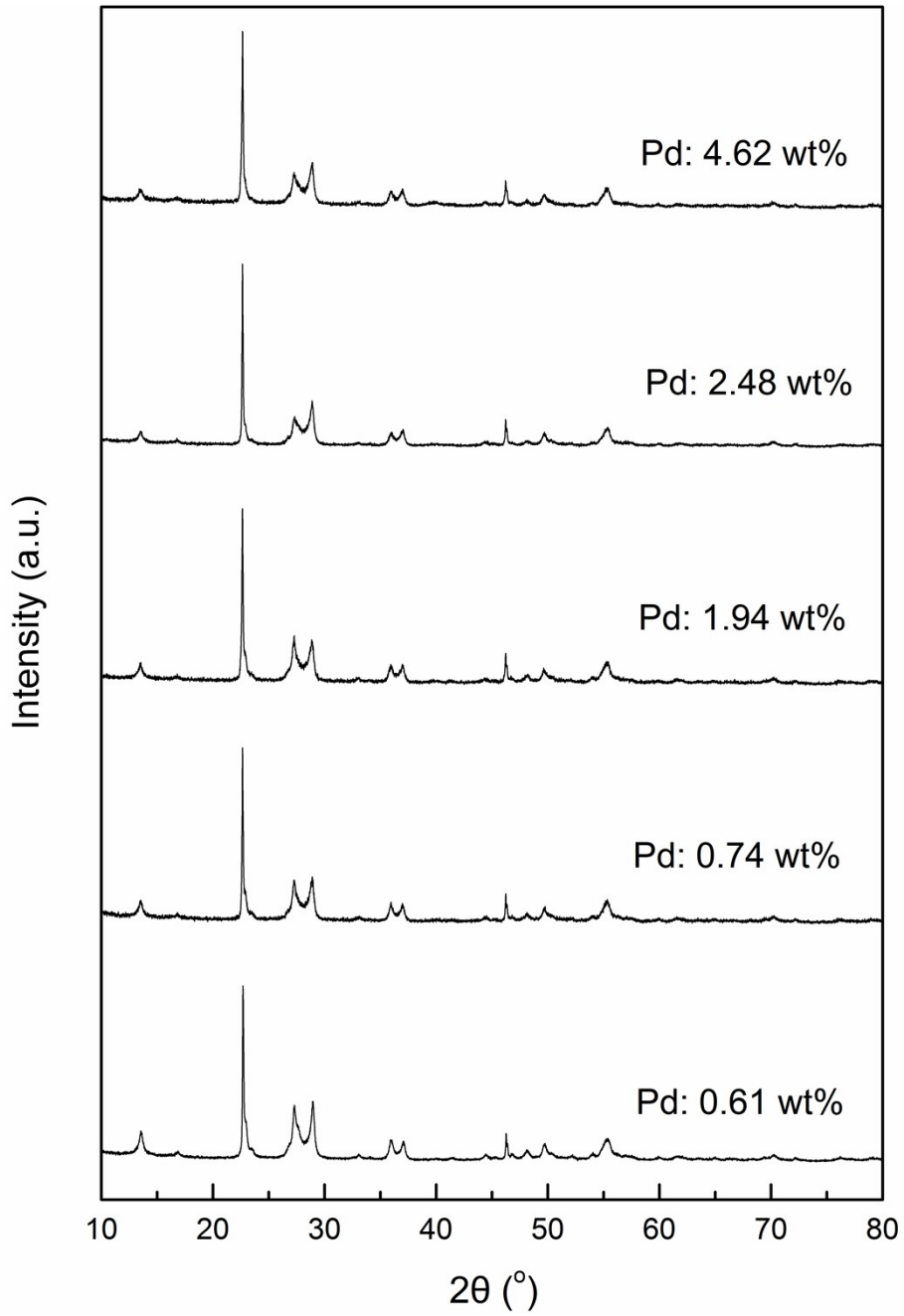

Fig. S2 The XRD patterns of Pd catalysts with different Pd contents.

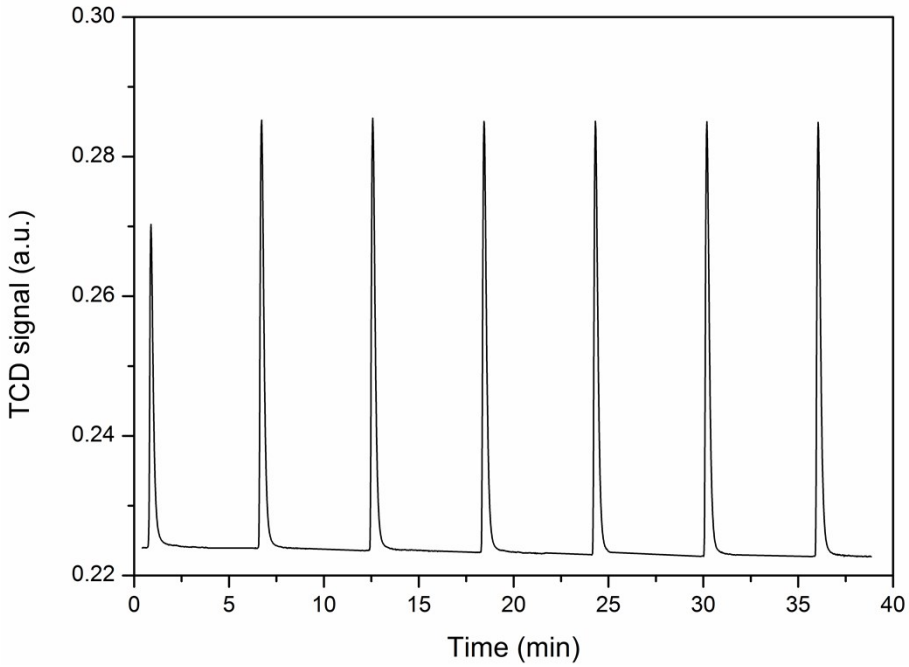

Fig. S3 The CO pulse chemisorption profiles of Pd/Nb_2O_5-400.

Table S1 The binding energy for different Pd catalylsts.

Entry	Catalysts	B.E. (eV)			
		Pd $3d_{5/2}$		Pd $3d_{3/2}$	
1	Pd-Nb_2O_5-400	334.7	336.7	339.9	341.8
2	Pd-Nb_2O_5-400-IP	334.8	336.4	340.1	341.9
3	Pd-Nb_2O_5-400-B	335.3	336.9	340.7	342.5

Table S2 Pd contents in the different catalysts.

Entry	Catalysts	Pd contents (wt.%)[a]
1	Pd-Nb_2O_5-400	0.61
2	Pd-Nb_2O_5-400-IP	0.63
3	Pd-Nb_2O_5-400-B	0.70

[a] Determined by ICP-AES.

Table S3 The Conversion of HMF to methyl cyclopentenolone. [a]

Entry	Conv. /%	HHD Select. /%[b]	NaOH /mol L^{-1}	MCP Isolated yield /%[c]
1	93	67	0.01	28
2	94	69	0.04	43
3	90	63	0.06	41
4	90	71	0.08	47
5	94	66	0.10	52
6	91	70	0.15	57
7	92	67	0.20	54
8	94	73	1.00	31

[a] Reaction conditions: Pd/Nb_2O_5-400 (20 mg), 2.00 g HMF aqueous solution (1 mmol) 413 K, 4 MPa H_2, 6 h for HMF hydrogenation and 10.0 g aqueous solution of NaOH, 4 h, room temperature for the conversion of HHD to MCP; [b] The selectivity of HHD from HMF; [c] The isolated yield of MCP based on the amount of HMF.

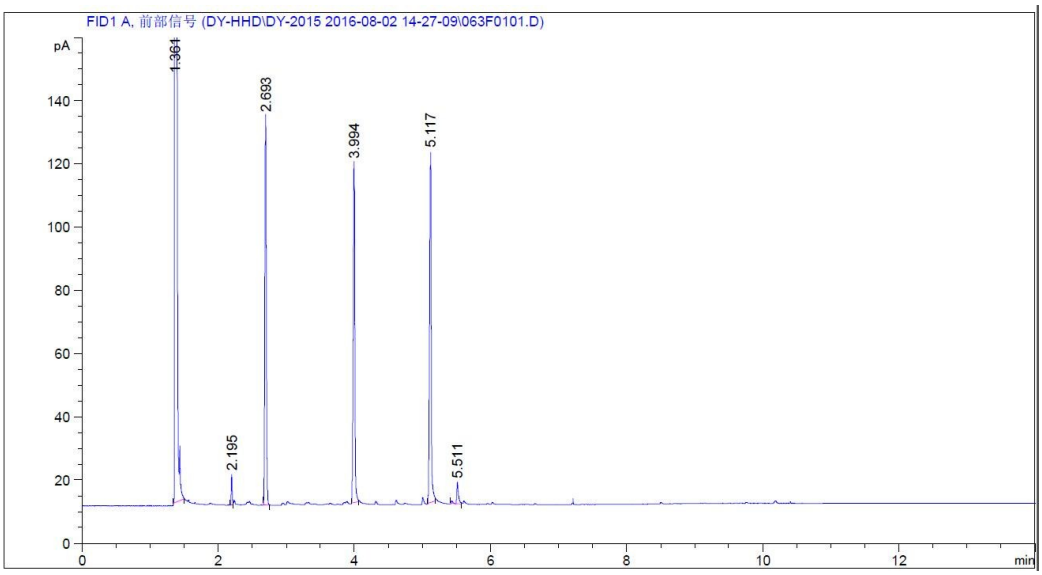

Fig. S4 Typical GC traces for the hydrogenation of HMF to HHD (Table1, Entry 4). The compounds correspond to retention time: 2.195 min (2,5-hexanedione), 2.693 min (internal standard), 3.994 min (HHD), 4.661 min (DHMF), 4.998 min (THFDM) 5.117 min (HMF).

Fig. S5 ^{1}H and ^{13}C NMR spectra of MCP.

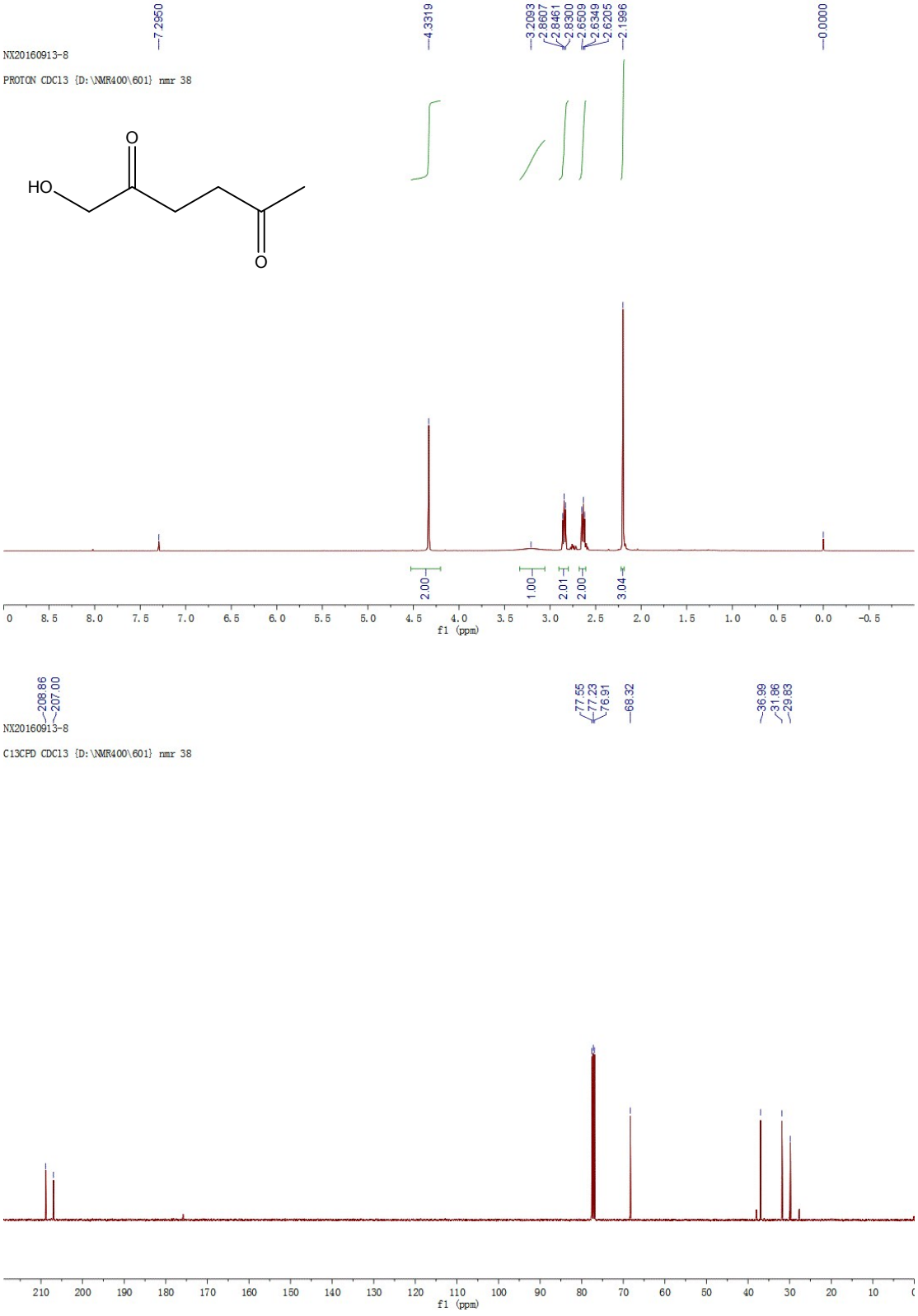

Fig. S6 ^{1}H and ^{13}C NMR spectra of HHD.