

Supplementary Information

Alcohol amines catalyzed CO₂ conversion for the synthesis of quinazoline-2, 4-(1H, 3H)-dione in water

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NMR Data

The quinazoline-2, 4-(1H, 3H)-diones were identified by matching the NMR data with those reported literature.^[1]

Quinazoline-2, 4(1H, 3H)-dione (2a).

¹H NMR (DMSO-d₆, 500 MHz) δ : 11.21 (s, 2H), 7.89 (d, J = 7.3 Hz, 1H), 7.64 (t, J = 6.9 Hz, 1H), 7.17 (d, J = 7.7 Hz, 2H); ¹³C NMR (DMSO-d₆, 126 MHz) δ : 163.29, 150.76, 141.34, 135.41, 127.41, 122.77, 115.78, 114.79.

6-Fluoroquinazoline-2, 4(1H, 3H)-dione (2b).

¹H NMR (DMSO-d₆, 500 MHz) δ : 11.30 (s, 2H), 7.63 – 7.43 (m, 2H), 7.19 (dd, J = 9.0, 4.4 Hz, 1H); ¹³C NMR (DMSO-d₆, 126 MHz) δ : 162.55, 158.67, 150.49, 137.99, 123.42, 118.03, 115.86, 112.30.

6-Chloroquinazoline-2, 4(1H, 3H)-dione (2c).

¹H NMR (DMSO-d₆, 500 MHz) δ : 11.35 (d, J = 77.6 Hz, 2H), 7.80 (d, J = 2.5 Hz, 1H), 7.67 (dd, J = 8.7, 2.5 Hz, 1H), 7.18 (d, J = 8.7 Hz, 1H); ¹³C NMR (DMSO-d₆, 126 MHz) δ : 162.26, 150.49, 140.17, 135.24, 126.73, 126.36, 117.96, 116.23.

6-Bromoquinazoline-2, 4(1H, 3H)-dione (2d).

¹H NMR (DMSO-d₆, 500 MHz) δ : 11.35 (s, 2H), 7.93 (d, J = 2.3 Hz, 1H), 7.77 (dd, J = 8.7, 2.4 Hz, 1H), 7.11 (d, J = 8.7 Hz, 1H); ¹³C NMR (DMSO-d₆, 126 MHz) δ : 162.16, 150.49, 140.51, 137.92, 129.36, 118.21, 116.65, 114.27.

7-Chloroquinazoline-2, 4(1H, 3H)-dione (2e).

¹H NMR (DMSO-d₆, 500 MHz) δ : 11.31 (s, 2H), 7.87 (d, J = 8.4 Hz, 1H), 7.19 (d, J = 10.4 Hz, 1H), 7.16 (s, 1H); ¹³C NMR (DMSO-d₆, 126 MHz) δ : 162.52, 150.62, 142.39, 139.73, 129.45, 122.90, 115.12, 113.77.

7-methylquinazoline-2, 4(1H, 3H)-dione (2f).

¹H NMR (DMSO-d₆, 500 MHz) δ : 11.12 (s, 2H), 7.76 (d, J = 8.0 Hz, 1H), 6.99 (d, J = 8.1 Hz, 1H), 6.94 (s, 1H), 2.35 (s, 3H); ¹³C NMR (DMSO-d₆, 126 MHz) δ : 163.15,

150.91, 146.02, 141.38, 127.35, 124.09, 115.50, 112.50, 21.42.

6, 7-Dimethoxyquinazoline-2, 4(1H, 3H)-dione (2g).

¹H NMR (DMSO-d₆, 500 MHz) δ : 11.10 (s, 1H), 10.92 (s, 1H), 7.26 (s, 1H), 6.68 (s, 1H), 3.83 (s, 3H), 3.79 (s, 3H); ¹³C NMR (DMSO-d₆, 126 MHz) δ : 162.86, 155.34, 150.84, 145.47, 136.99, 107.60, 106.65, 98.21, 56.26, 56.16.

FT-IR Spectra

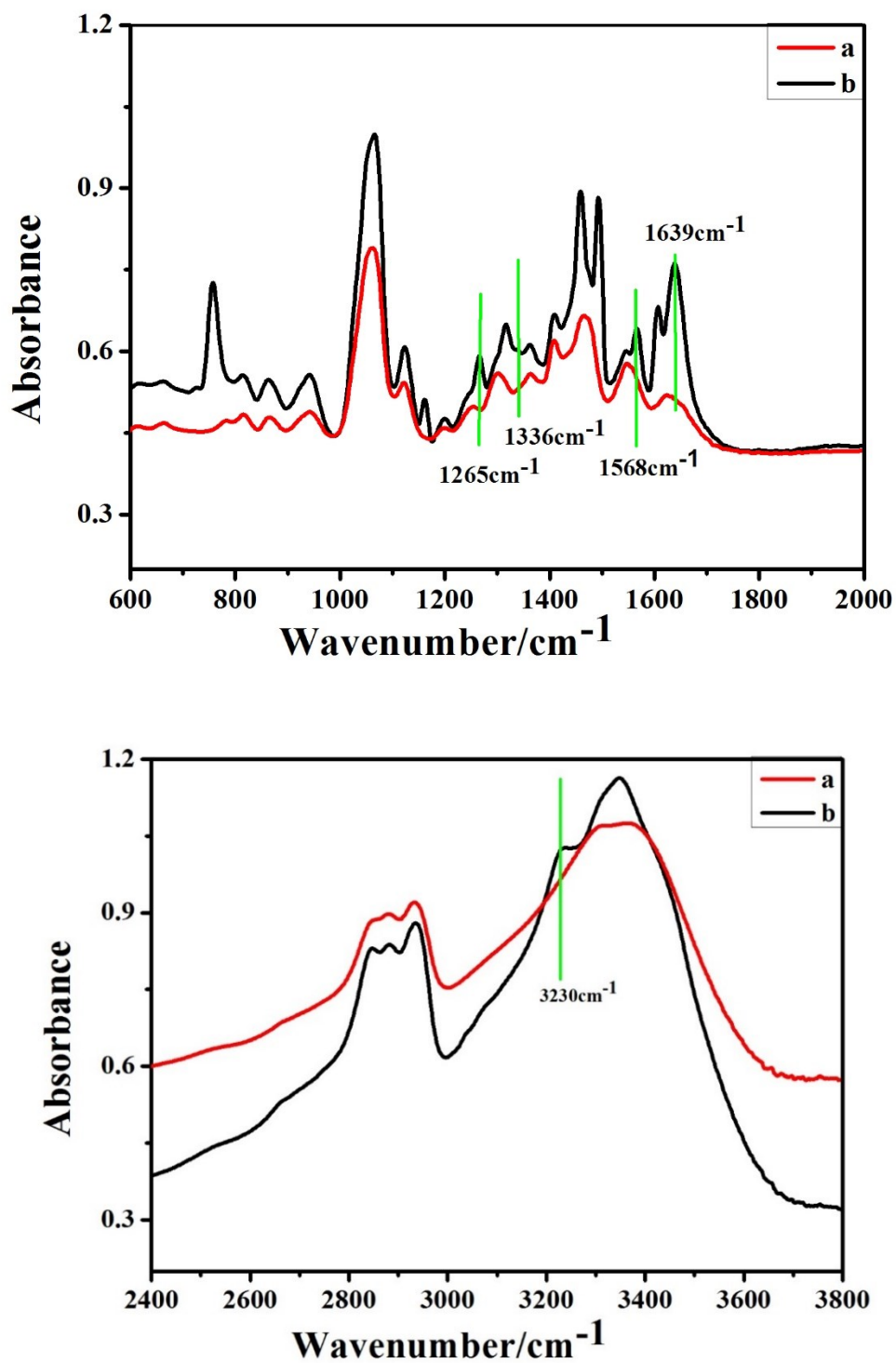
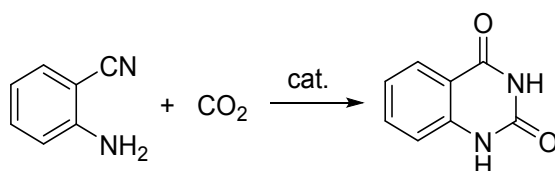


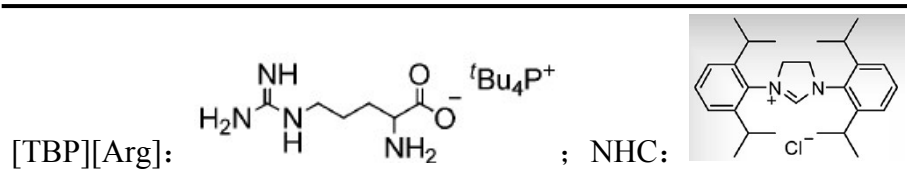
Fig S1 FT-IR spectra of reaction mixture (a) before adding CO₂ and (b) after adding CO₂.

Supplementary Table

Table S1 Several homogeneous catalysts used for synthesis of quinazoline-2,4(1H,3H)-diones.



Entry	Catalyst	Solvent	Reaction Condition	Isolated Yield (%)	Reference
1	DBU	DMF	20 °C 1 bar 24 h	97	[2]
2	TMG	Solvent free	120 °C 10 MPa 4 h	89	[3]
3	Choline	water	90 °C 2 MPa 24 h	92	[4]
4	[TBP][Arg]	DMF	100 °C 8.5 MPa 12 h	91	[5]
5	NHC, K ₂ CO ₃	DMSO	120 °C 0.1 MPa 15 h	95	[6]
6	DEA	water	100 °C 1 MPa 12 h	94	Current work



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