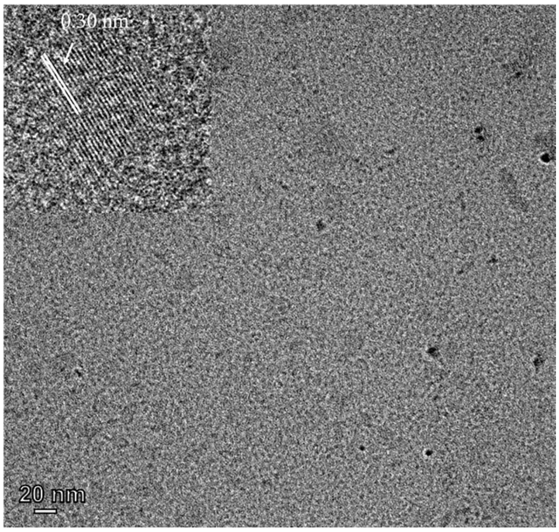
Electronic Supplementary Material (ESI) for New Journal of Chemistry.

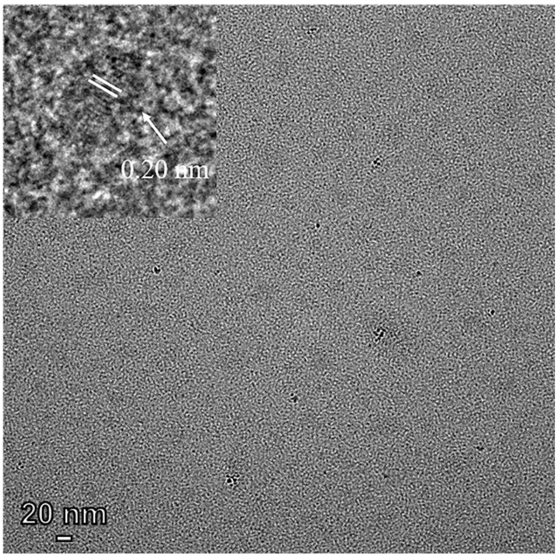
Supporting Information

Nitrogen-doped carbon dots as acid-base bifunctional and efficient catalysts for the Cycloaddition of CO_2 to Epoxides

(a)



(b)



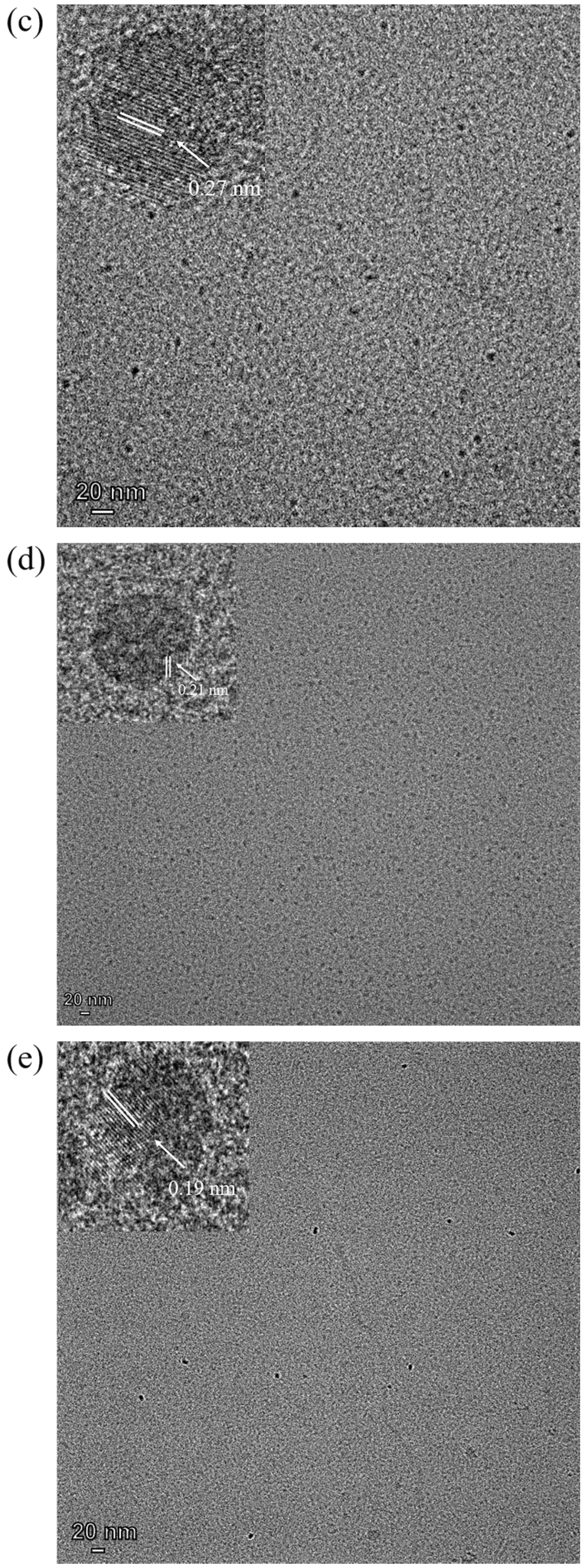


Figure S1 TEM images of (a) G-CDs, (b) GS-CDs, (c) NCDs-1, (d) NCDs-2 and (e) NCDs-3.

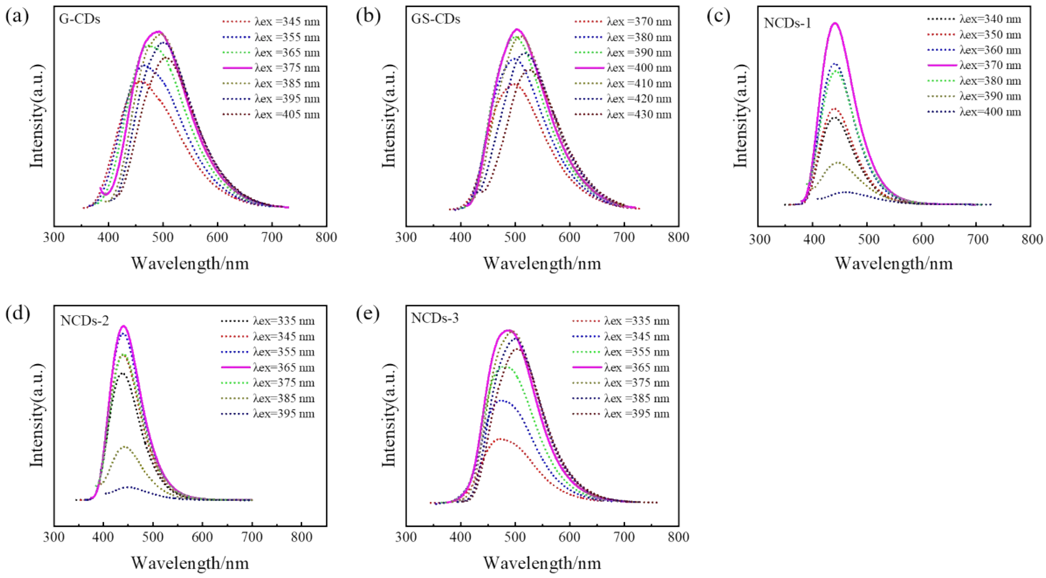


Figure S2 The fluorescence spectra of (a) G-CDs, (b) GS-CDs, (c) NCDs-1, (d) NCDs-2, and (e) NCDs-3 under different excitation wavelengths.

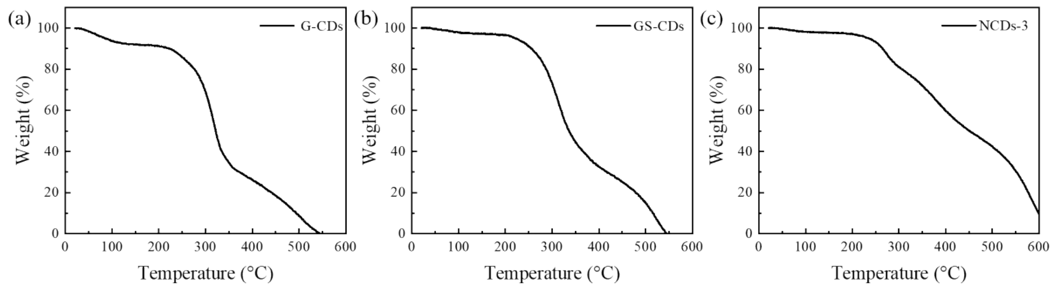


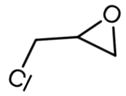
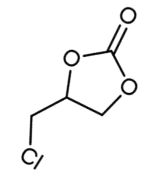
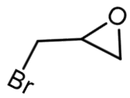
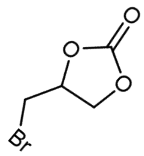
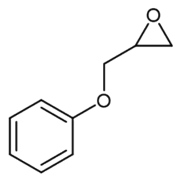
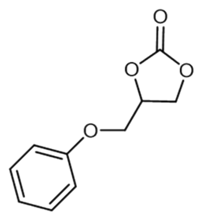
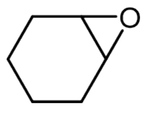
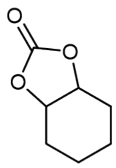
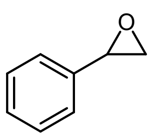
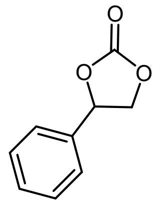
Figure S3 Thermogravimetric analysis (TGA) for (a) G-CD, (b) GS-CDs, (c) NCDs-3.

Table S1 Percentage of N atoms in NCDs-1, NCDs-2 and NCDs-3 as determined by XPS measurements

Sample	NCDs-1	NCDs-2	NCDs-3
N%	4.5% (4.42% [a])	5.2% (5.31% [a])	8.6% (9.01% [a])

[a] N content calculated by elemental analysis

Table S2 Cycloaddition reactions with various epoxides [a]

Entry	Epoxide	Product	Time (h)	Yield (%) [b]	Selectivity (%) [b]	TOF ($mmol_{yield}$/g_{cat}/h)
1			3	42	>99	17.5
2			3	75	>99	31.2
3			3	85	>99	35.4
4			3	5	>99	2.0
5			3	99	>99	41.2

[a] Conditions: 5 mmol epoxide, 40 mg NCDs-3, 2.4 mol% KI, 1 atm of CO_2, 100 °C.

[b] Yield and selectivity were calculated by ^1H NMR

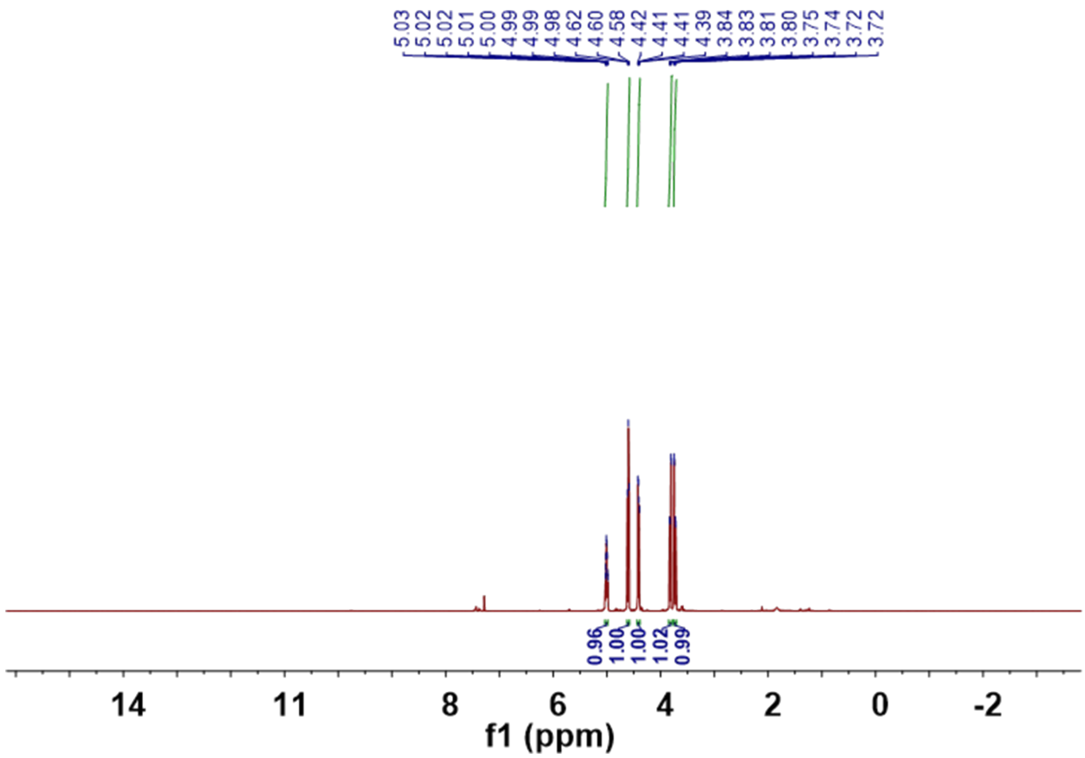


Figure S4 ^{1}H NMR spectra of 4-(chloromethyl)-1,3-dioxolan-2-one.

^{1}H NMR (500 MHz, $CDCl_3$) δ 5.01 (ddd, *J* = 14.2, 5.4, 3.6 Hz, 1H), 4.60 (t, *J* = 8.6 Hz, 1H), 4.41 (dd, *J* = 8.9, 5.7 Hz, 1H), 3.82 (dd, *J* = 12.2, 5.1 Hz, 1H), 3.73 (dd, *J* = 12.2, 3.6 Hz, 1H).

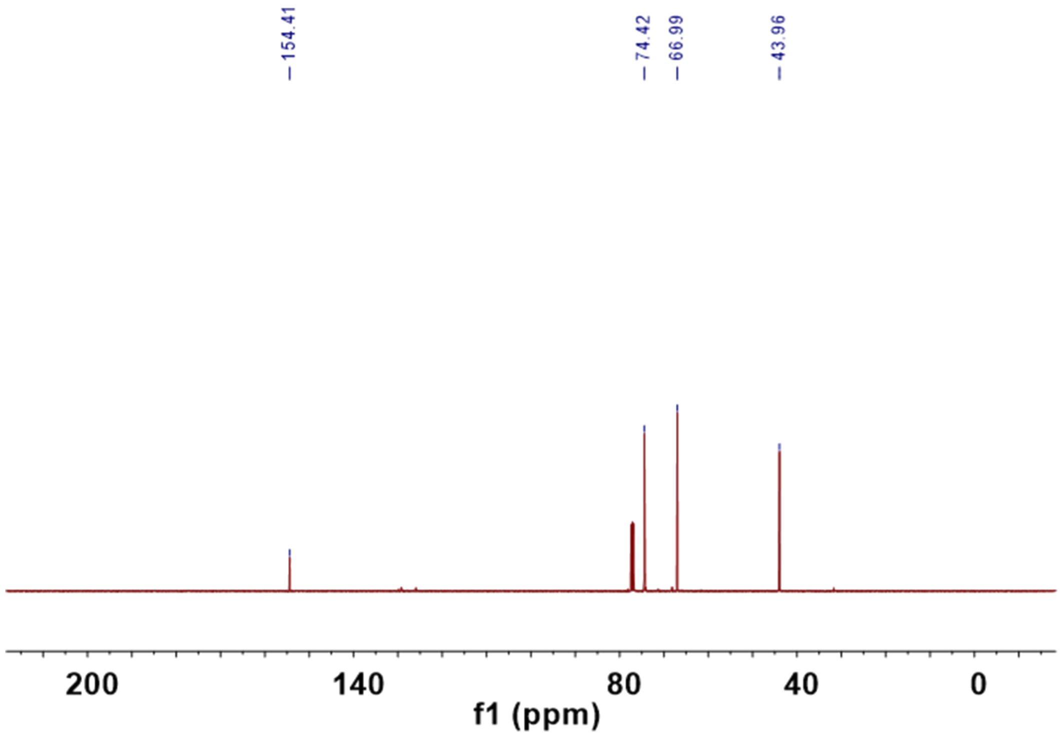


Figure S5 ^{13}C NMR spectra of 4-(chloromethyl)-1,3-dioxolan-2-one.

^{13}C NMR (126 MHz, $CDCl_3$) δ 154.41 (s), 74.42 (s), 66.99 (s), 43.96 (s).

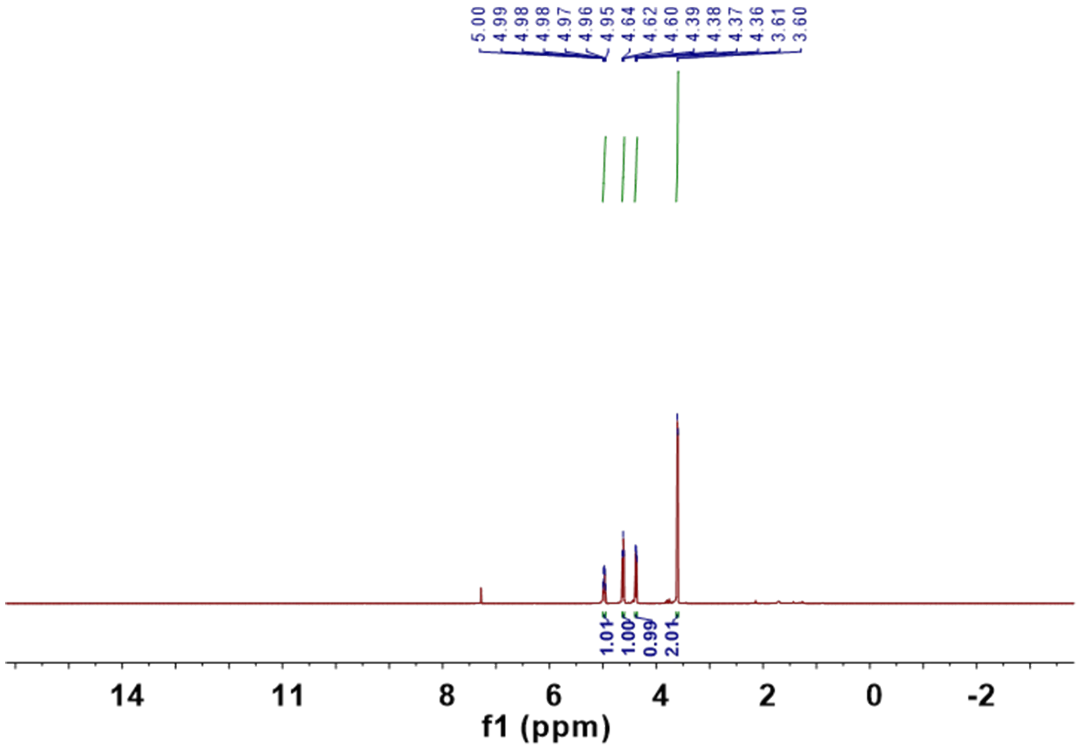


Figure S6 ^{1}H NMR spectrum of 4-(bromomethyl)-1,3-dioxolan-2-one.

^{1}H NMR (500 MHz, $CDCl_3$) δ 5.00 – 4.95 (m, 1H), 4.64 – 4.60 (m, 1H), 4.38 (dd, *J* = 8.9, 5.9 Hz, 1H), 3.60 (d, *J* = 5.2 Hz, 2H).

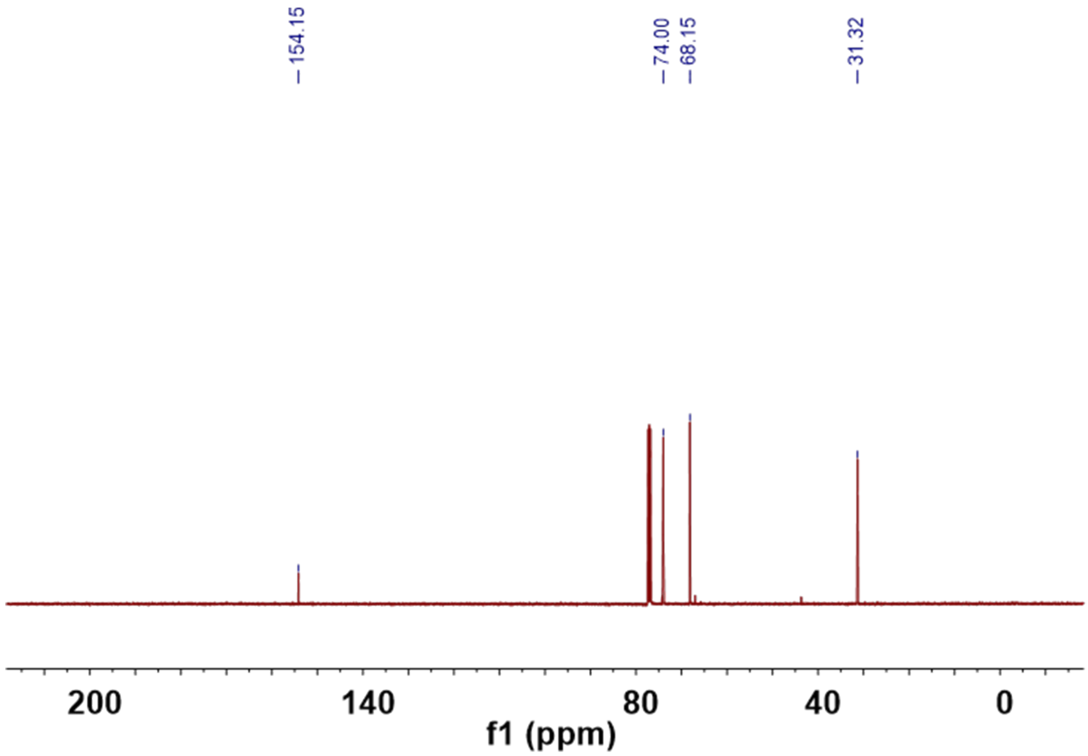


Figure S7 ^{13}C NMR spectrum of 4-(bromomethyl)-1,3-dioxolan-2-one.

^{13}C NMR (126 MHz, $CDCl_3$) δ 154.15 (s), 74.00 (s), 68.15 (s), 31.32 (s).

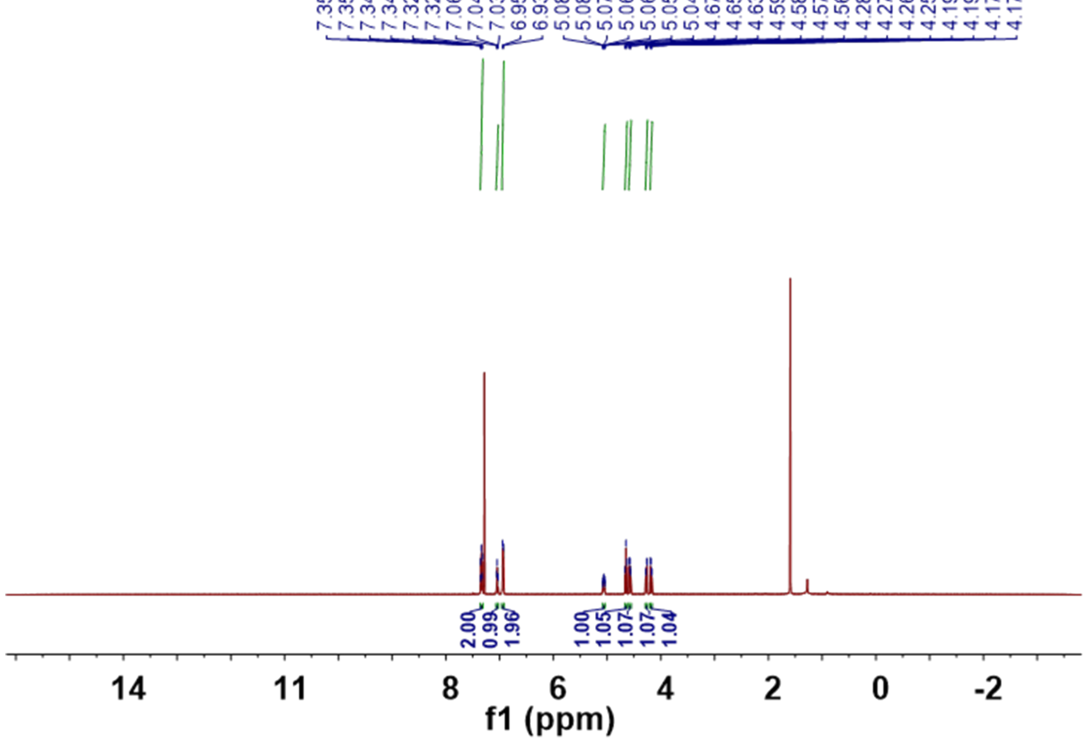


Figure S8 ^1H NMR spectra of 4-(phenoxymethyl)-1,3-dioxolan-2-one.

^1H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.31 (m, 2H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.94 (d, *J* = 7.9 Hz, 2H), 5.08 – 5.04 (m, 1H), 4.65 (t, *J* = 8.4 Hz, 1H), 4.57 (dd, *J* = 8.5, 5.9 Hz, 1H), 4.27 (dd, *J* = 10.5, 4.3 Hz, 1H), 4.18 (dd, *J* = 10.5, 3.6 Hz, 1H).

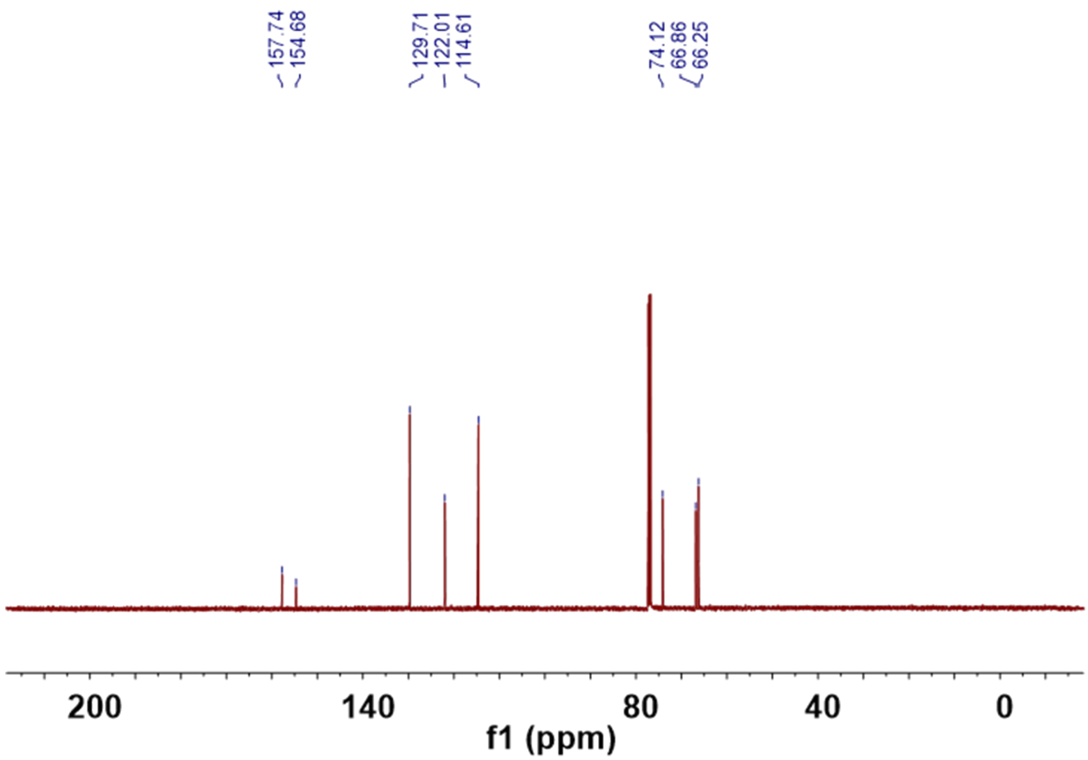


Figure S9 ^{13}C NMR spectra of 4-(phenoxymethyl)-1,3-dioxolan-2-one.
^{13}C NMR (126 MHz, $CDCl_3$) δ 157.74 (s), 154.68 (s), 129.71 (s), 122.01 (s), 114.61 (s), 74.12 (s), 66.86 (s), 66.25 (s).

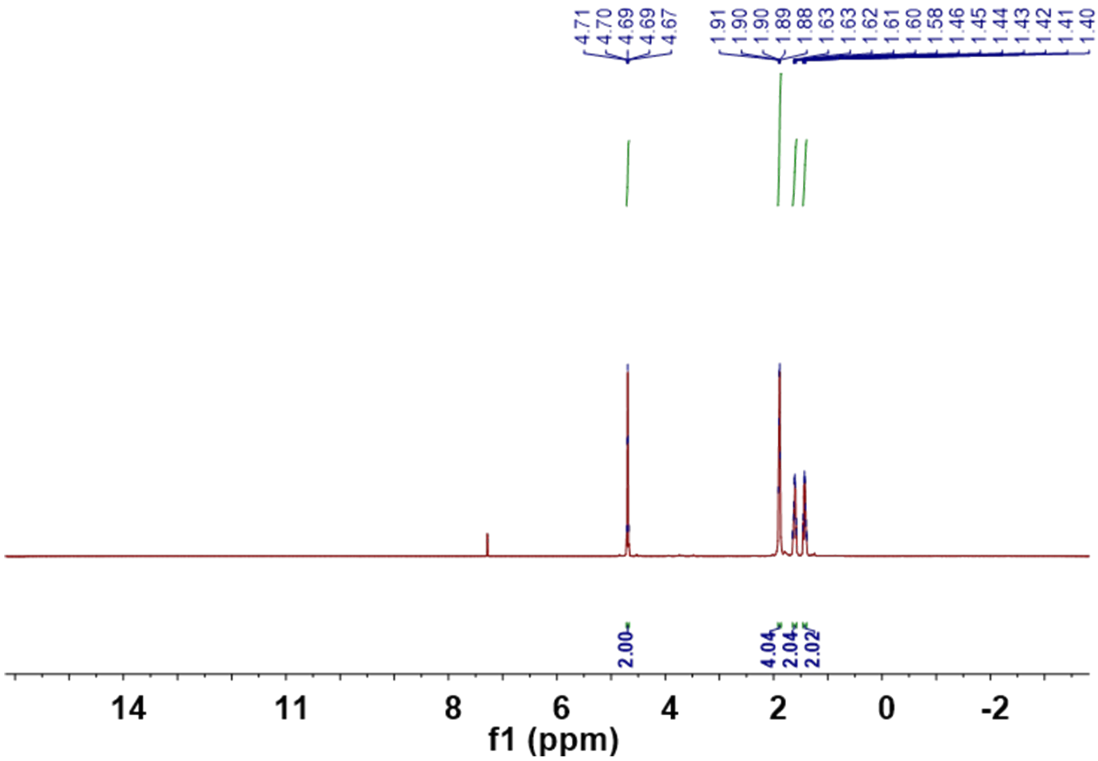


Figure S10 ^{1}H NMR spectrum of cyclohexene carbonate.

^{1}H NMR (500 MHz, $CDCl_3$) δ 4.72 – 4.67 (m, 1H), 1.92 – 1.86 (m, 2H), 1.62 (tt, J = 13.5, 6.9 Hz, 1H), 1.46 – 1.39 (m, 1H).

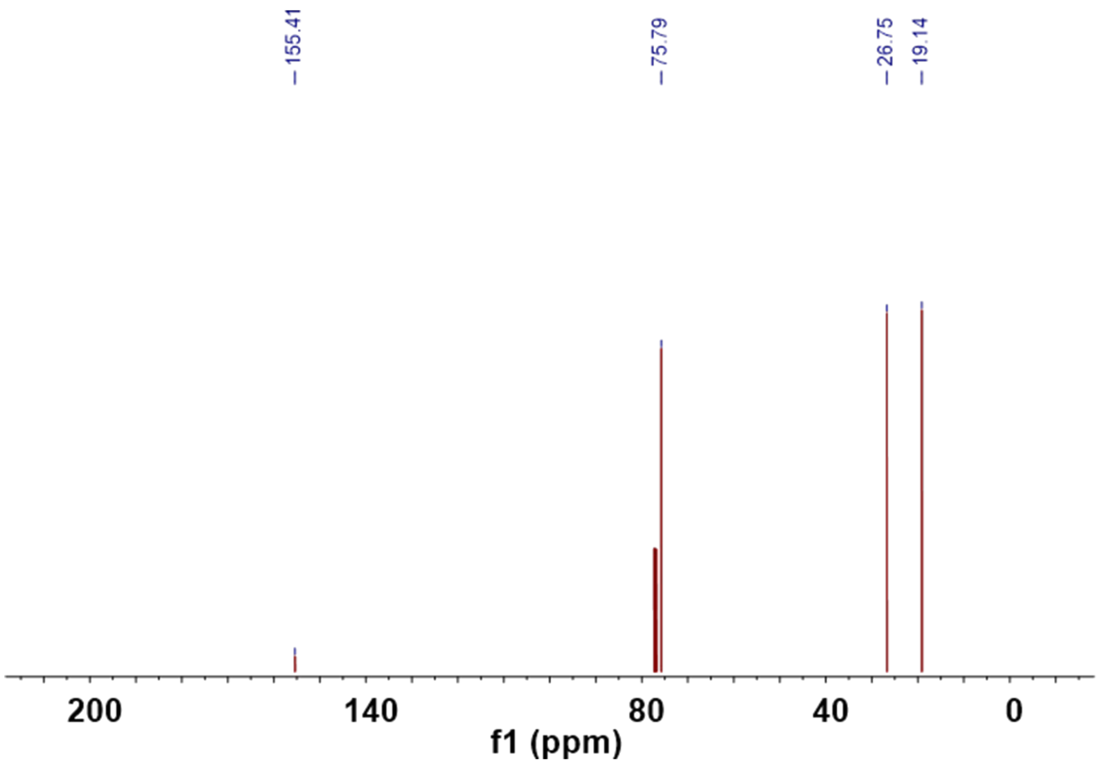


Figure S11 ^{13}C NMR spectrum of cyclohexene carbonate.

^{13}C NMR (126 MHz, $CDCl_3$) δ 155.41 (s), 75.79 (s), 26.75 (s), 19.14 (s).

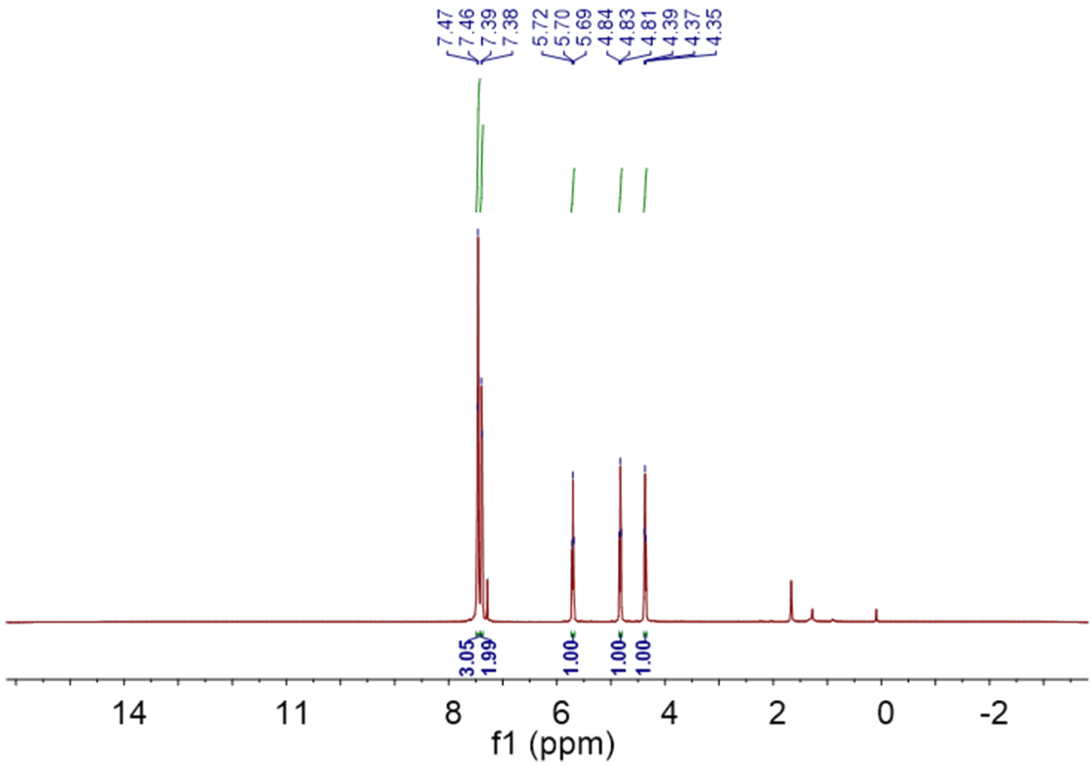


Figure S12 ¹H NMR spectrum of 4-phenyl-1, 3-dioxolan-2-one

¹H NMR (500 MHz, $CDCl_3$) δ 7.46 (d, J = 6.8 Hz, 1H), 7.39 (d, J = 7.1 Hz, 1H), 4.83 (t, J = 8.4 Hz, 1H), 4.37 (t, J = 8.2 Hz, 1H).

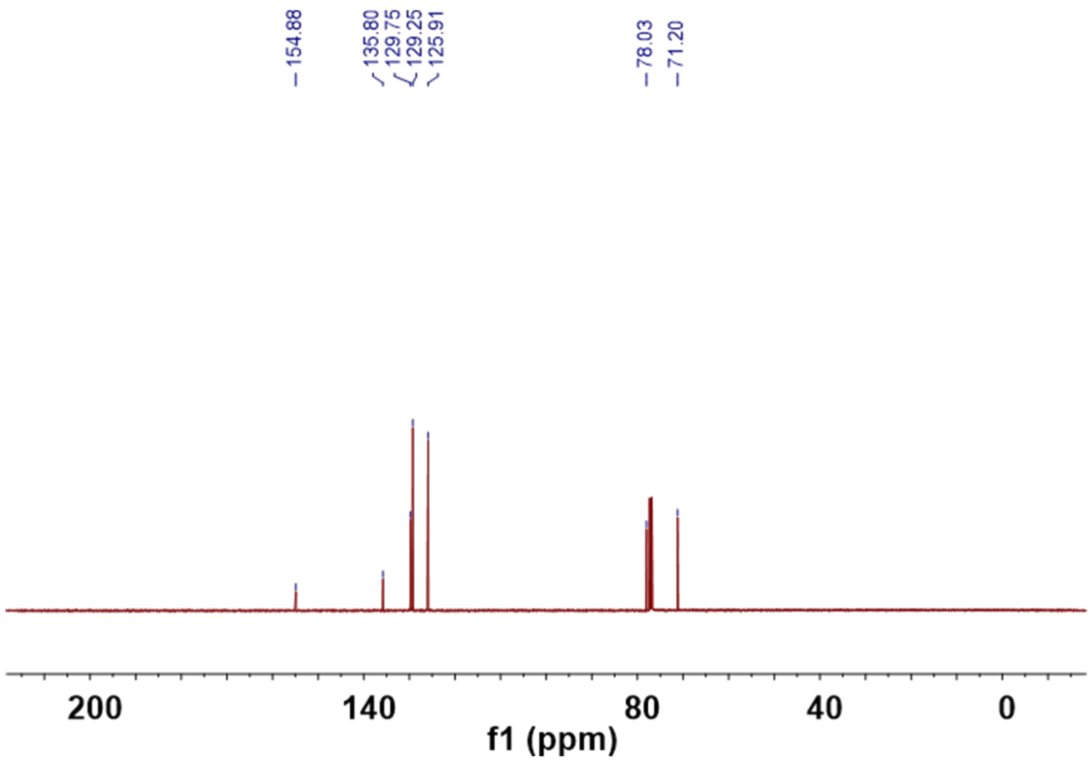


Figure S13 ^{13}C NMR spectrum of 4-phenyl-1, 3-dioxolan-2-one.
^{13}C NMR (126 MHz, $CDCl_3$) δ 154.88 (s), 135.80 (s), 129.75 (s), 129.25 (s), 125.91 (s), 78.03 (s), 71.20 (s).

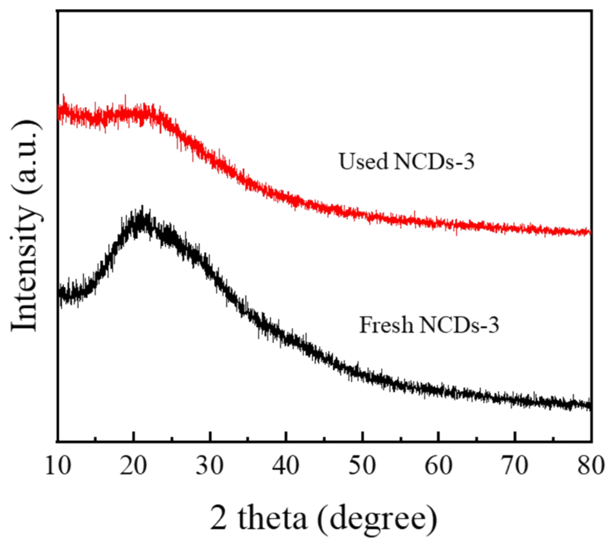


Figure S14 XRD spectra of fresh and used NCDs-3

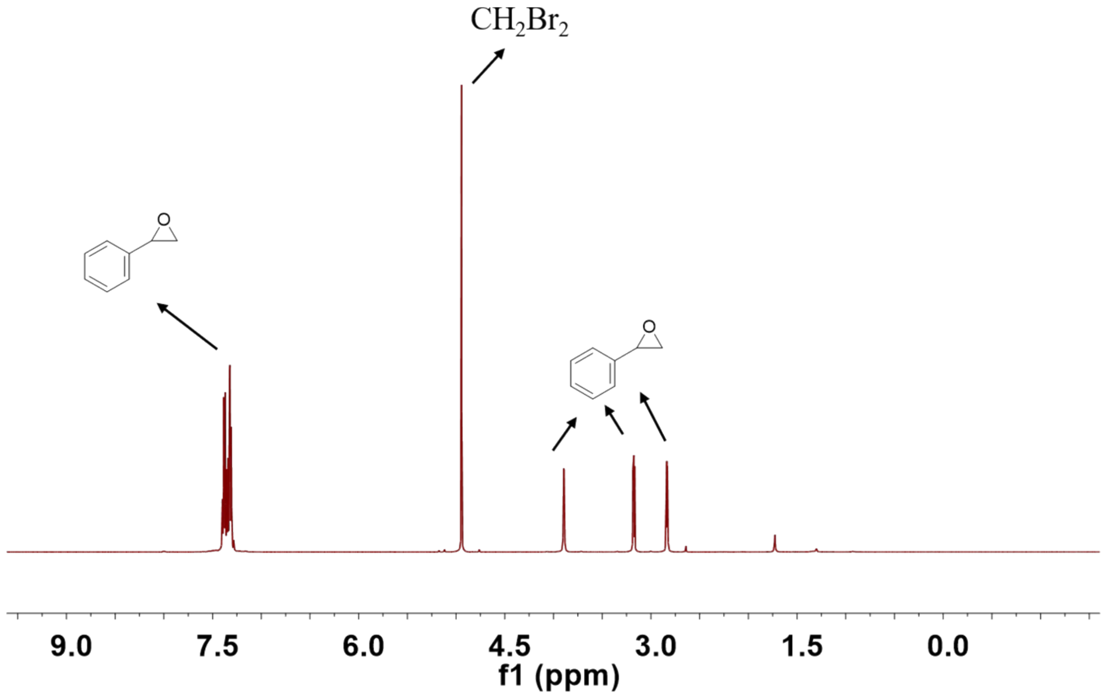


Figure S 15 the selectivity of the reaction (catalyst: 40 mg G-CDs, cocatalyst: 2.4 mol% KI as shown in Table 1)

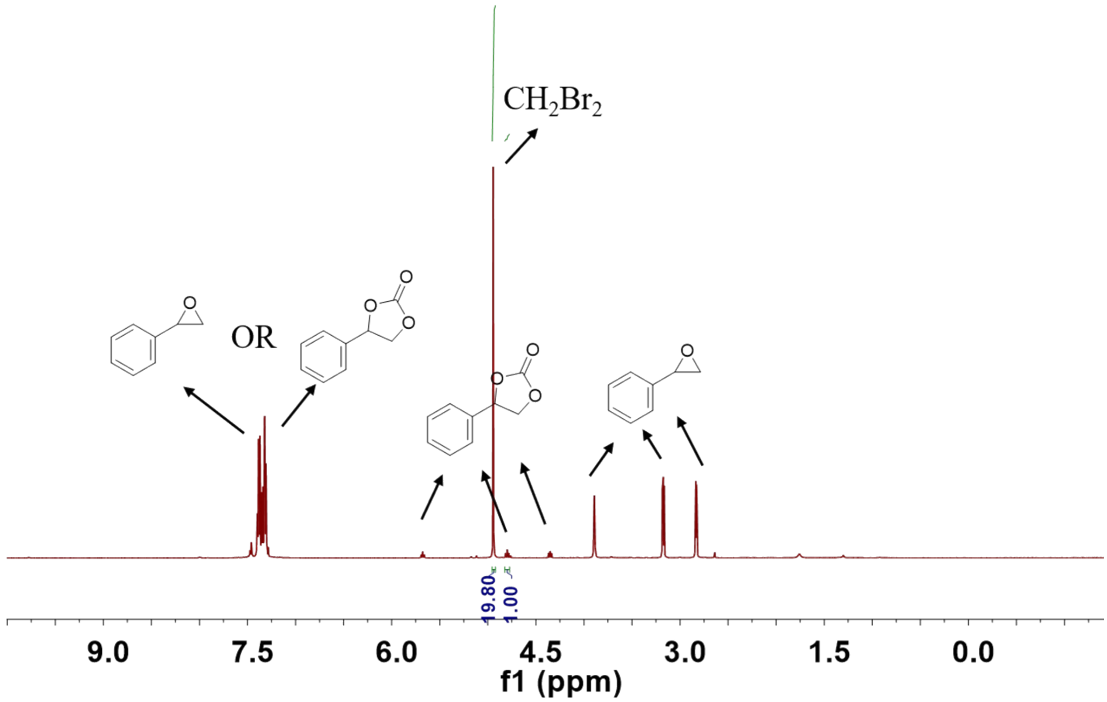


Figure S16 the selectivity of the reaction (catalyst: 40 mg GS-CDs, cocatalyst: 2.4 mol% KI as shown in Table 1)

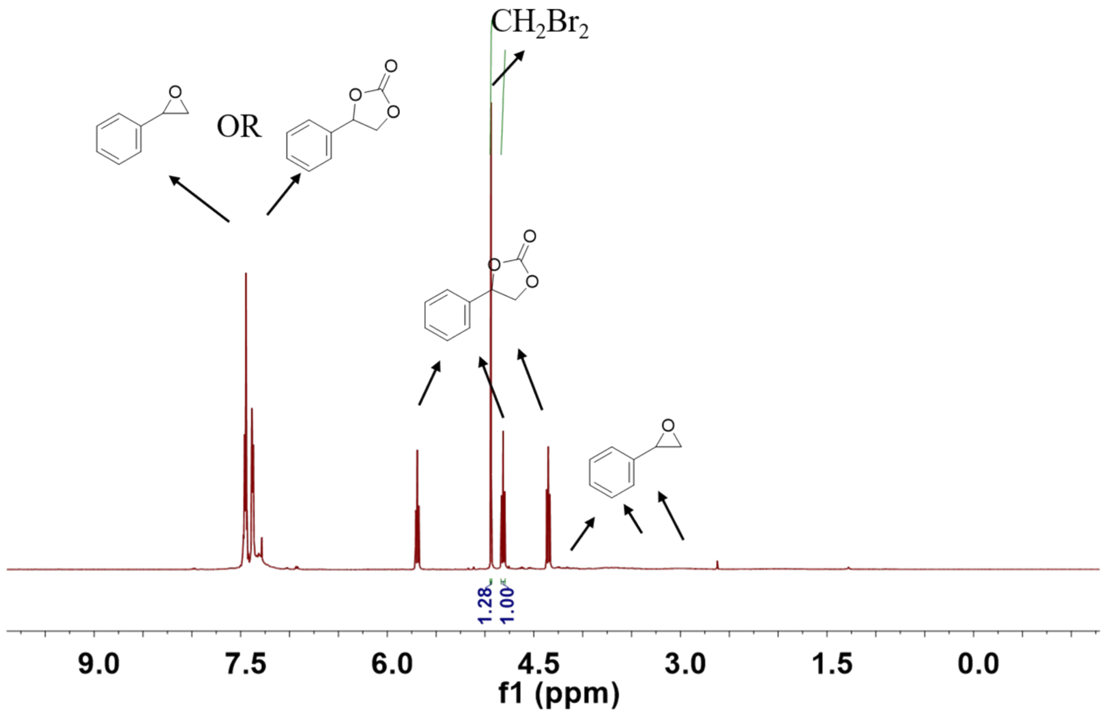


Figure S 17 the selectivity of the reaction (catalyst: 40 mg NCDs-1, cocatalyst: 2.4 mol% KI as shown in Table 1)

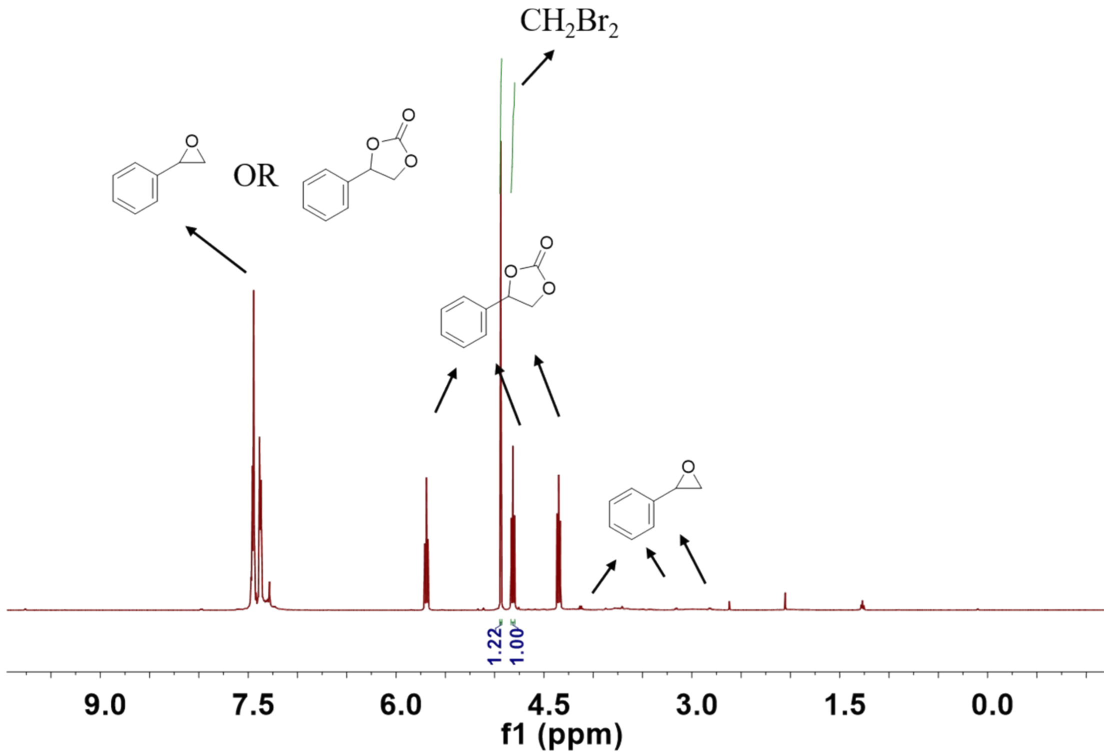


Figure S 18 the selectivity of the reaction (catalyst: 40 mg NCDs-2, cocatalyst: 2.4 mol% KI as shown in Table 1)

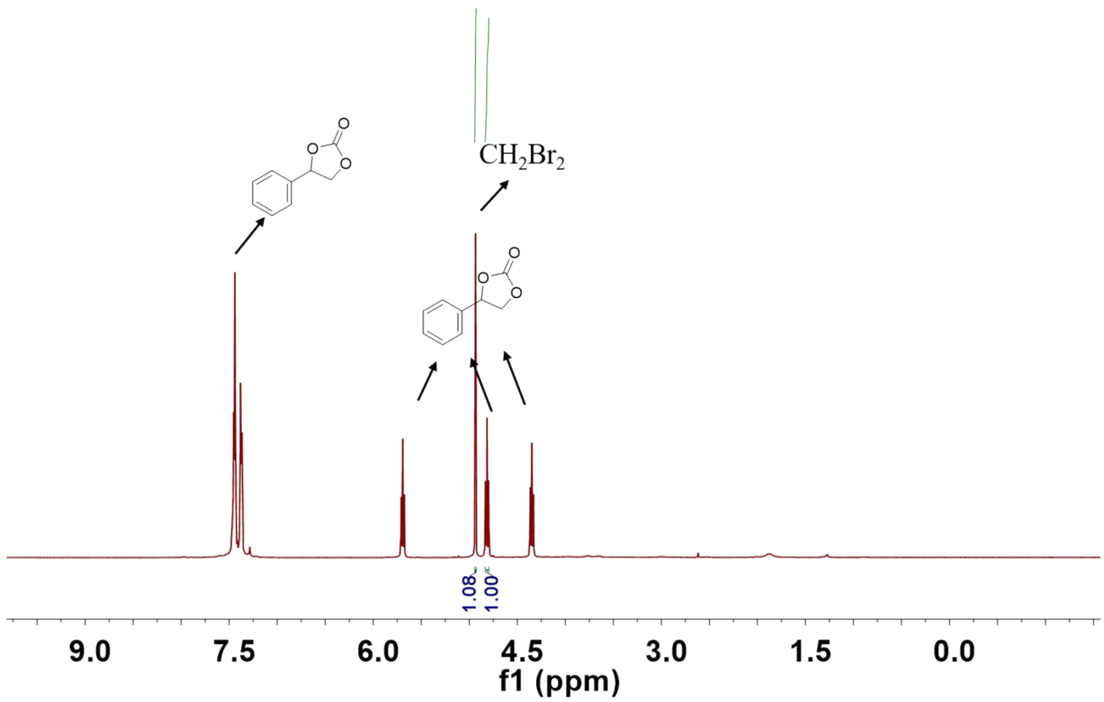


Figure S 19 the selectivity of the reaction (catalyst: 40 mg NCDs-3, cocatalyst: 2.4 mol% KI as shown in Table 1)