Supporting Information

Experimental sections

Product glutaric acid purification: Boiling the reaction mixture to decompose the remaining H_20_2 until it is checked with starch potassium iodide test paper until there is no blue color. Concentrate and remove water by vacuum distillation. When it becomes more concentrated, stop the distillation and fully cool and crystallize. Colorless crystals are obtained by suction filtration, and purified product glutaric acid can be obtained after drying.

Supporting Figures

Figure S1. MS spectra of intermediate 8.

Figure S2. IR spectra of solution after reaction.

Figure S3. IR spectra of Glutaric acid aqueous solution.

Figure S4. ^{1}H NMR spectra of product Glutaric acid.

Figure S5. ^{13}C NMR spectra of product Glutaric acid.

Figure S6. MS spectra of product Glutaric acid.

Theoretical calculation part

Table S1. Absolute calculation energies and thermodynamic corrections for the optimized geometries and transition states.

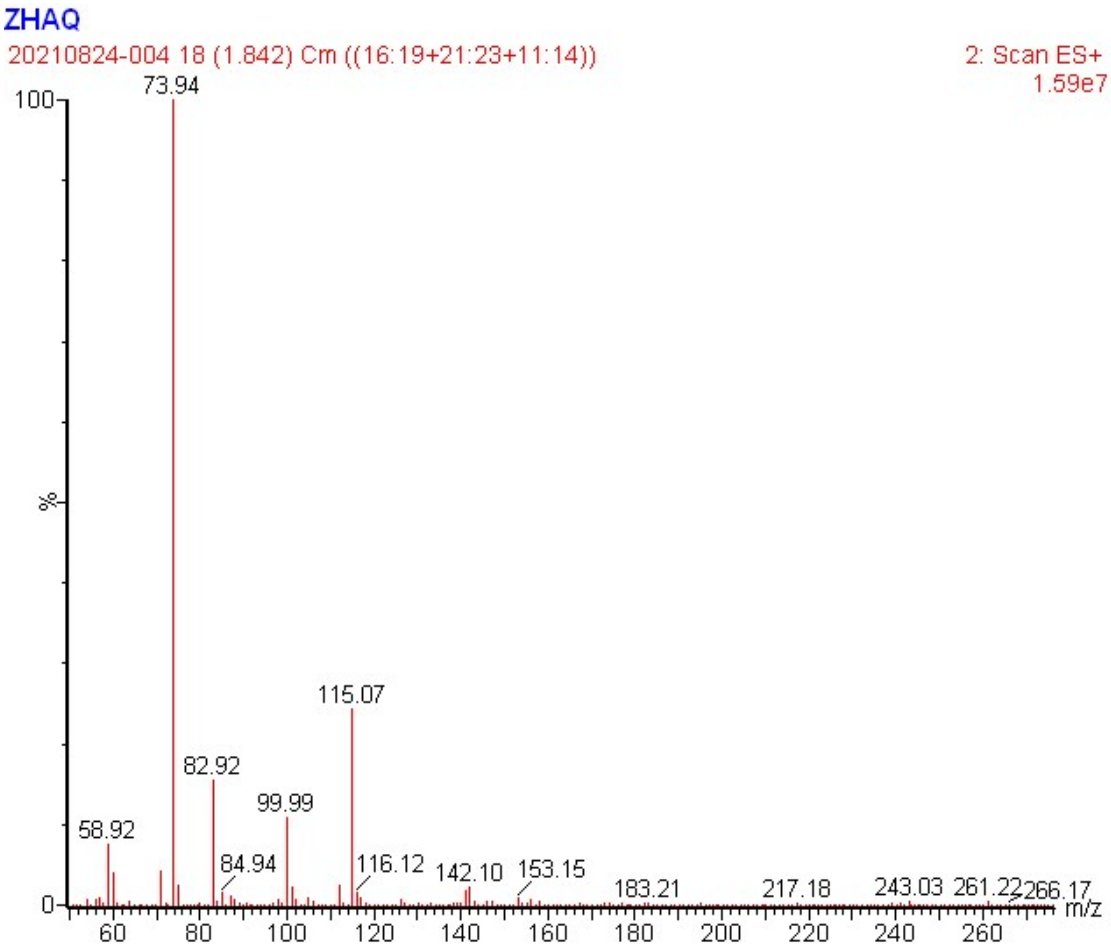

Figure S1. Mass spectra of intermediate 8.

MS, m/z: 115.07 $[M\text{-}CH_2CHOH+C_2H_3N]^+$, 99.99 $[M\text{-}H_2O]^+$, 84.94 $[M\text{-}OOH]^+$, 82.92 $[M\text{-}OH\text{-}H_2O]^+$, 73.94 $[M\text{-}CH_2CHOH]^+$.

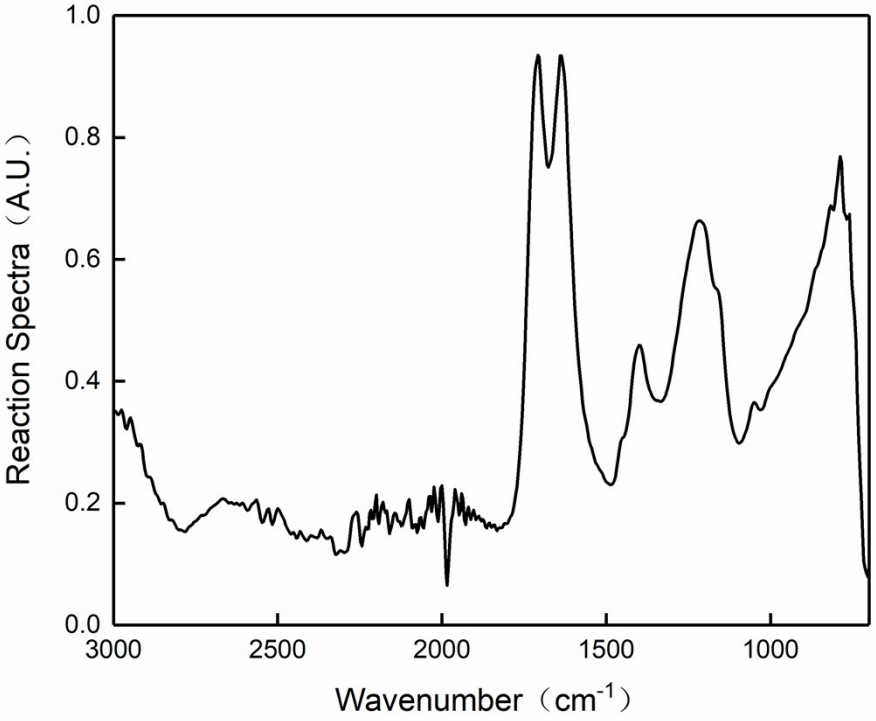

Figure S2. IR spectra of solution after reaction.

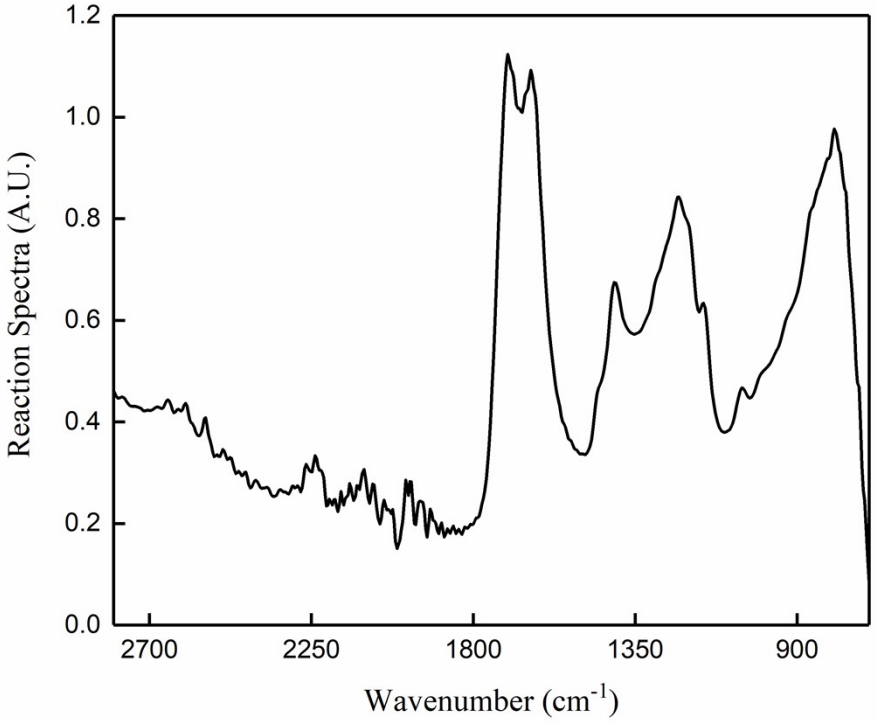

Figure S3. IR spectra of Glutaric acid aqueous solution.

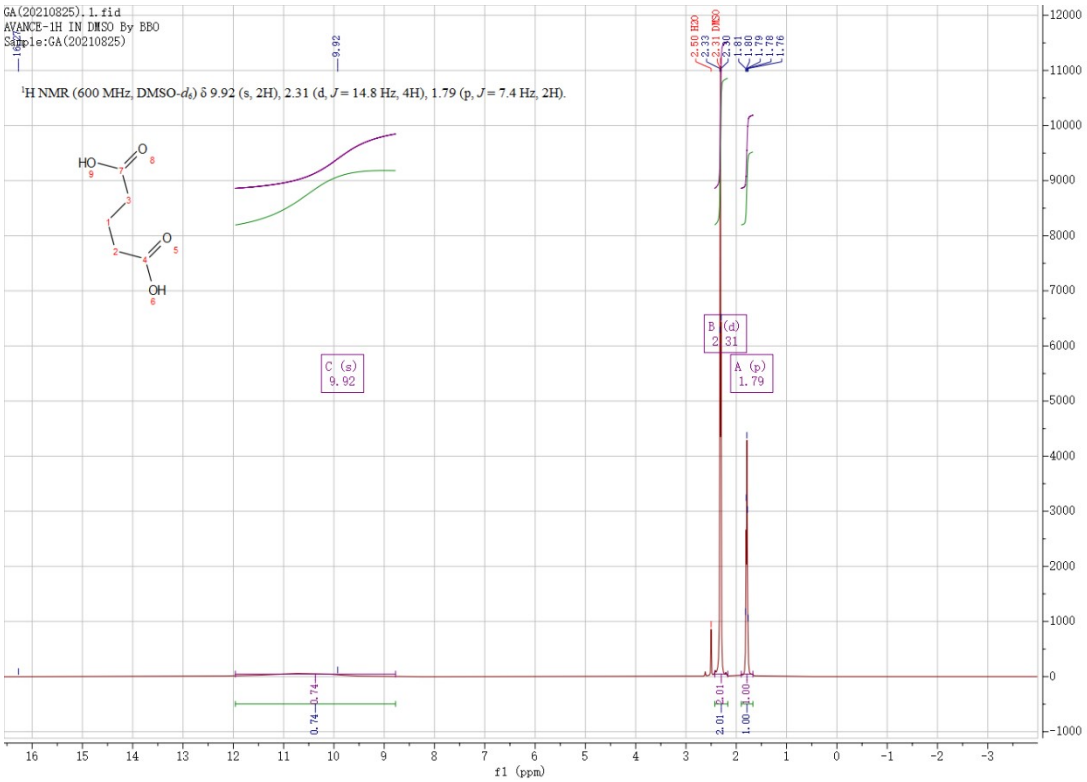

Figure S4. ^{1}H NMR spectra of product Glutaric acid.

^{1}H NMR (600 MHz, DMSO-d_6) δ 9.92 (s, 2H), 2.31 (d, J = 14.8 Hz, 4H), 1.79 (p, J = 7.4 Hz, 2H).

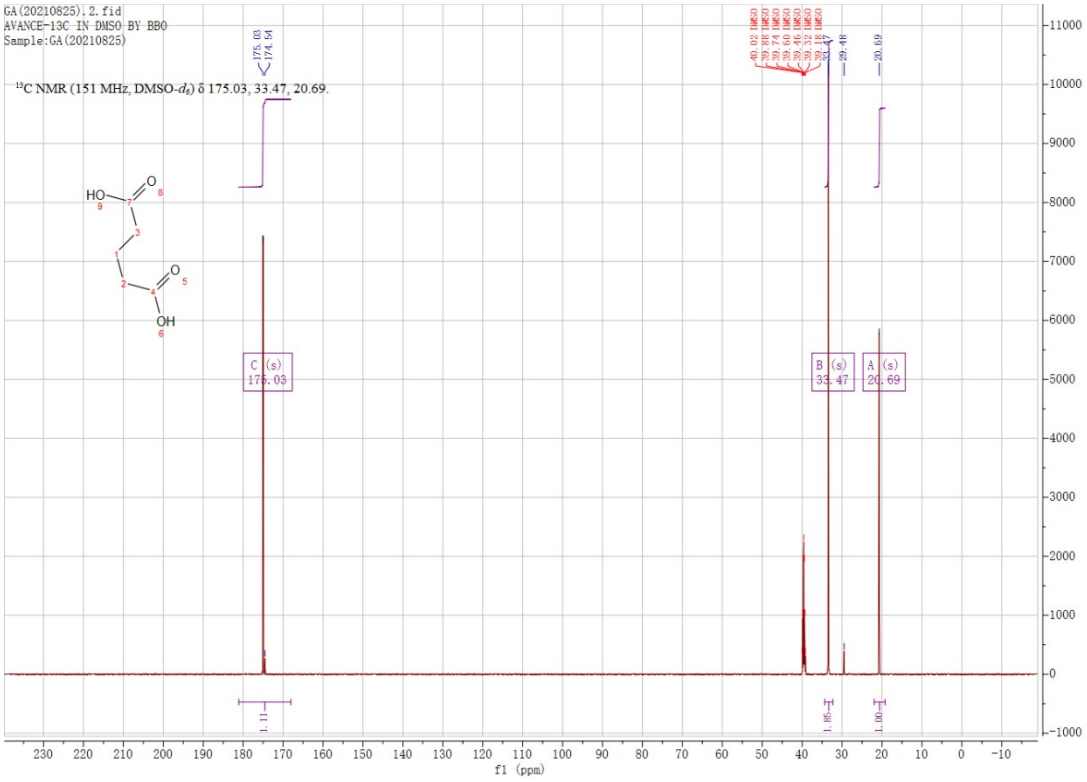

Figure S5. ^{13}C NMR spectra of product Glutaric acid.

^{13}C NMR (151 MHz, DMSO-d_6) δ 175.03, 33.47, 20.69.

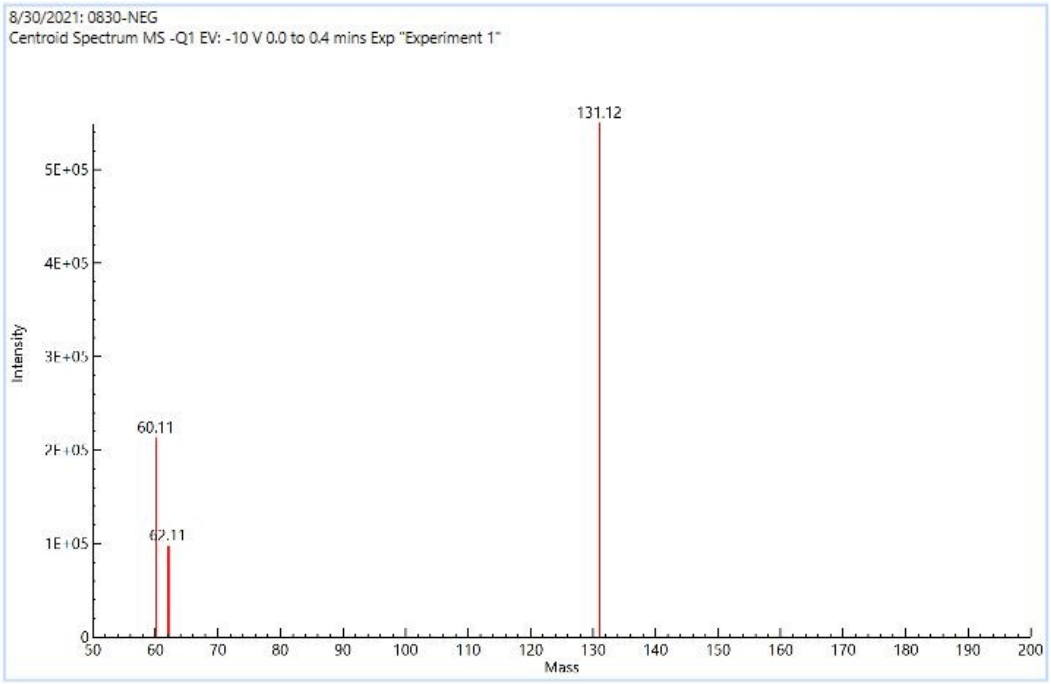

Figure S6. MS spectra of product Glutaric acid.

Table S1. Absolute calculation energies and thermodynamic corrections for the optimized geometries and transition states.

	E	Corr. (ZPE)	Corr. (H)	Corr. (G)
Initiators	-347.148752	0.161083	0.170170	0.128331
TS	-347.146885	0.159966	0.168794	0.127480
Int-1	-347.148750	0.161101	0.170177	0.128400
Int-1	-422.239326	0.166214	0.176189	0.131736
TS2	-347.134753	0.163633	0.171312	0.133379
TS2	-422.224914	0.167599	0.176400	0.135399
Int-23	-347.135571	0.163651	0.172368	0.131324
Int-28	-422.225388	0.167677	0.177387	0.133688