

Supporting Information

Tables

Table S1 Imaginary frequencies of the transition states, bonds corresponding to relative normal vibrations.

Transition States	Imaginary frequency (cm ⁻¹)	Bonds corresponding to relative normal vibrations
TS1a	-636.84	C-H, N-H
TS2b	-1035.19	C-H, N-H
TS3c	-1326.52	C-O, O-H
TS4d	-825.46	C-O, O-H

Table S2 Relative energy of Intermediate and transition states.

Transition States	Relative energy (kJ/mol)
IM1a	-163.85
TS1a	-121.46
Product-a	-184.49
IM1b	-204.89
TS1b	-139.53
Product-b	-239.04
IM1c	-129.29
TS1c	-28.28
Product-c	-152.81
IM1d	-95.11
TS1d	-8.82
Product-d	-136.44