Supplementary Materials

Analyzing the pyrolysis mechanism of avermectin via experiments and density functional theory

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Table A Associated Mulliken layout numbers(e).

Bond	Layout number	Bond	Layout number
C3”-O	0.56	C1”-O	0.55
C4’-O	0.53	C3’-O	0.54
C1’-O	0.61	C13-O	0.56
C1-O	0.64	C19-O	0.47
C8a-O	0.51	C6-O	0.55
C21-O	0.62	C25-O	0.51
C15-C16	0.76	C16-C17	0.70
C8-C9	1.33	C9-C10	0.91

Table (a) A Transition state energy results

TS	Barrier from reactant （kcal·mol^{-1}）	Energy of reaction （kcal·mol^{-1}）
TS-A1	6.58	5.85
TS-A2	0.98	0.74
TS-A3	1.31	0.95
TS-A4	42.7	12.51

Table (b) B Transition state energy results

TS	Barrier from reactant (kcal·mol^{-1})	Energy of reaction (kcal·mol^{-1})
TS-B1	6.58	5.85
TS-B2	1.02	0.74
TS-B3	69.32	41.36
TS-B4	35.70	12.51

Table (c) C Transition state energy results

TS	Barrier from reactant (kcal·mol^{-1})	Energy of reaction (kcal·mol^{-1})
TS-C1	11.09	6.70
TS-C2	50.52	25.26
TS-C3	1.31	0.95
TS-C4	35.70	12.51

Table (d) D Transition state energy results

TS	Barrier from reactant (kcal·mol^{-1})	Energy of reaction (kcal·mol^{-1})
TS-D1	9.02	8.43
TS-D2	7.12	0.14
TS-D3	5.57	0.36
TS-D4	42.70	12.51
TS-D5	64.67	40.32
TS-D6	50.52	25.26