

Identification and Mechanistic Analysis of Toxic Degradation Products in the Advanced Oxidation Pathways of Fluoroquinolone Antibiotics

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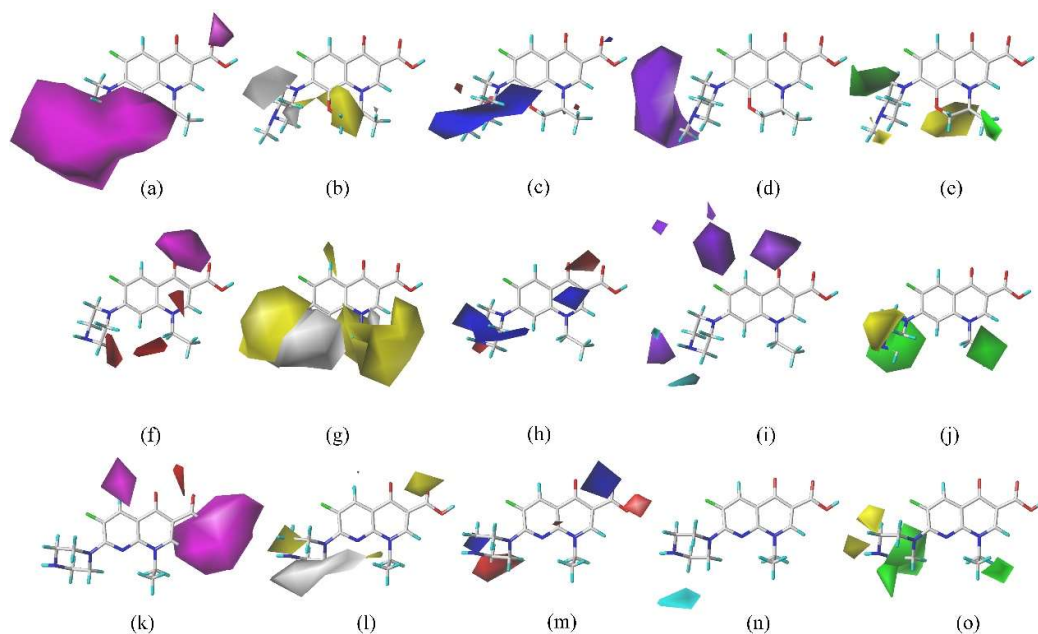


Figure S1 Equipotential diagram of FQs molecule CoMSIA model ((a) hydrogen bond receptor field of defluorinated CoMSIA model; (b) Hydrophobic field of defluorinated CoMSIA model; (c) Defluorinated CoMSIA model electrostatic field; (d) Defluorinated CoMSIA model hydrogen bond donor field; (e) Defluorinated CoMSIA model three-dimensional field; (f) Hydroxylated CoMSIA model hydrogen bond receptor field; (g) Hydrophobic field of hydroxylated CoMSIA model; (h) Hydroxylated CoMSIA model electrostatic field; (i) Hydroxylated CoMSIA model

hydrogen bond donor field; (j) Hydroxylated CoMSIA model stereo field; (k) CoMSIA model hydrogen bond receptor field for hydroxylation of piperazine ring; (l) Hydrophobic field of CoMSIA model for hydroxylation of piperazine ring; (m) CoMSIA model electrostatic field for hydroxylation of piperazine ring; (n) CoMSIA model hydrogen bond donor field for hydroxylation of piperazine ring; (o) CoMSIA model for hydroxylation of piperazine ring in three-dimensional field.

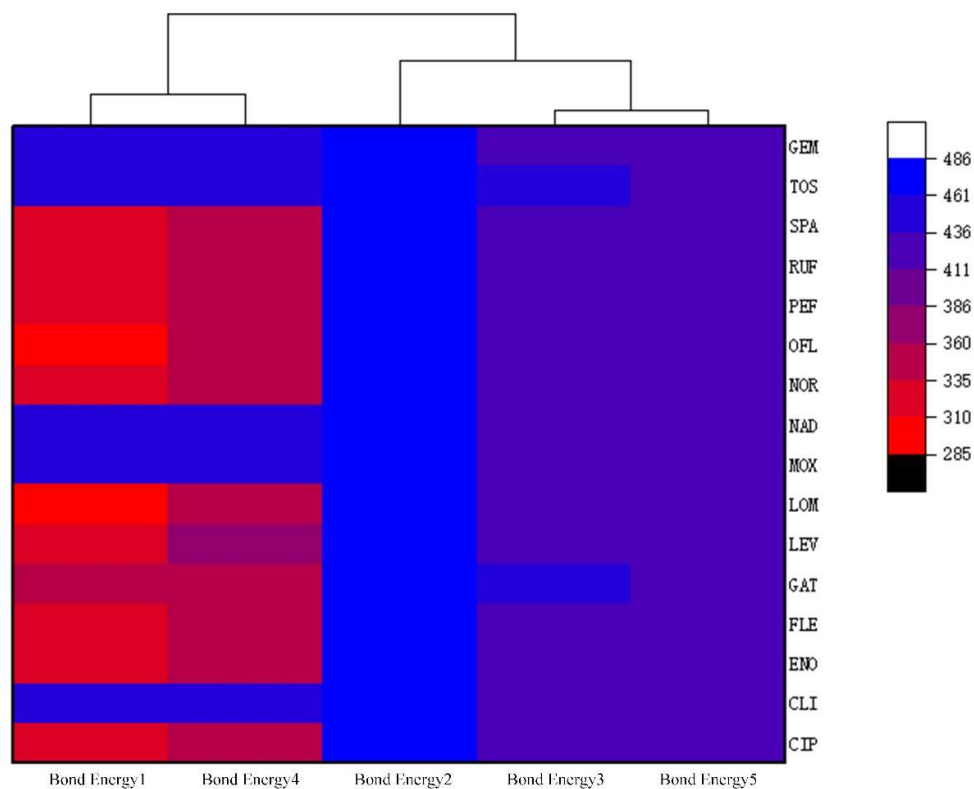


Figure S2 FQs Molecular column clustering analysis chart.