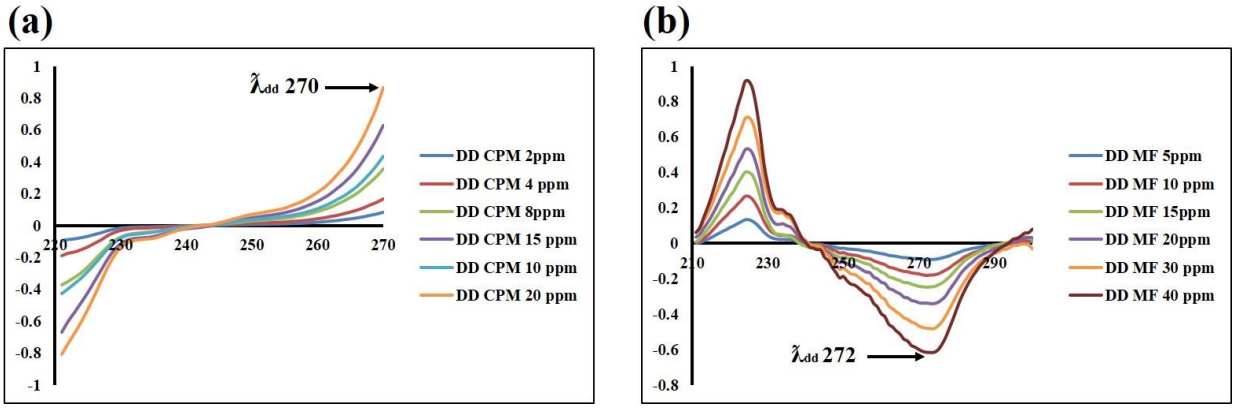

Figure S1 (a) First derivative of the ratio spectra of CP (2-20 µg/ml) in mixture using the spectrum of MF normalized as a divisor and (b) the first derivative of the ratio spectra of MF (5-40µg/ml) in mixture using the spectrum of CP normalized as a divisor

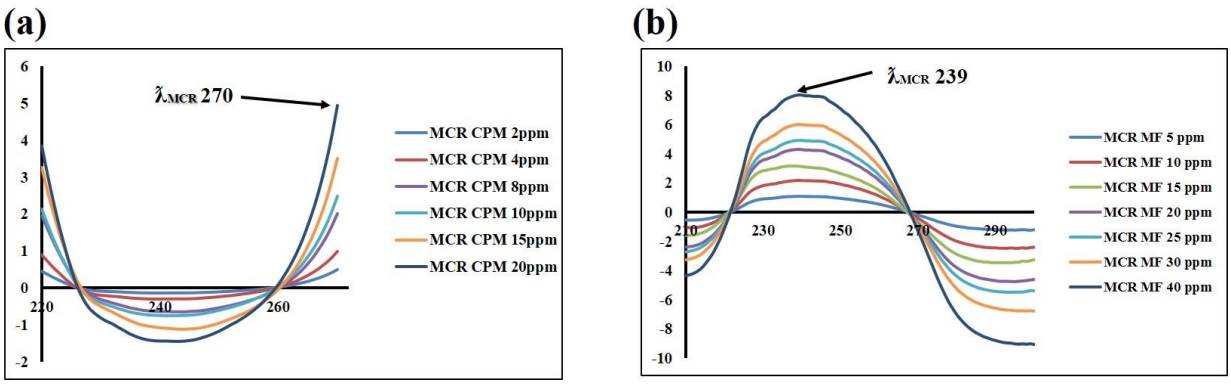

Figure S2 (a) Mean-centered ratio spectra of CP in mixture using the spectrum of MF normalized as a divisor and (b) mean-centered ratio spectra MF (5-40 µg/ml) in mixture using the spectrum of CP normalized as a divisor

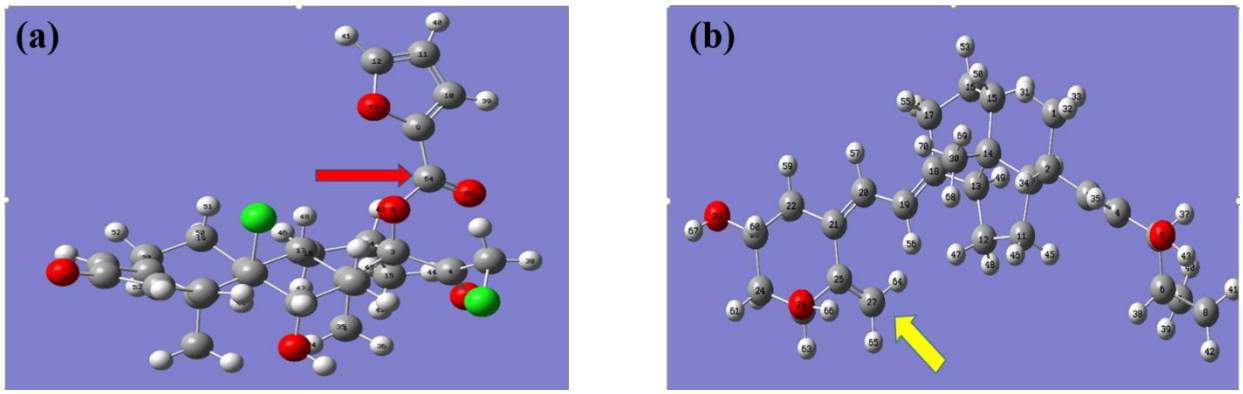

Figure S3 Gaussian output for (a) MF and (b) CP; atom numbers were represented, and C-54 and C-27 with the highest Fukui (f+), respectively, are indicated by arrows

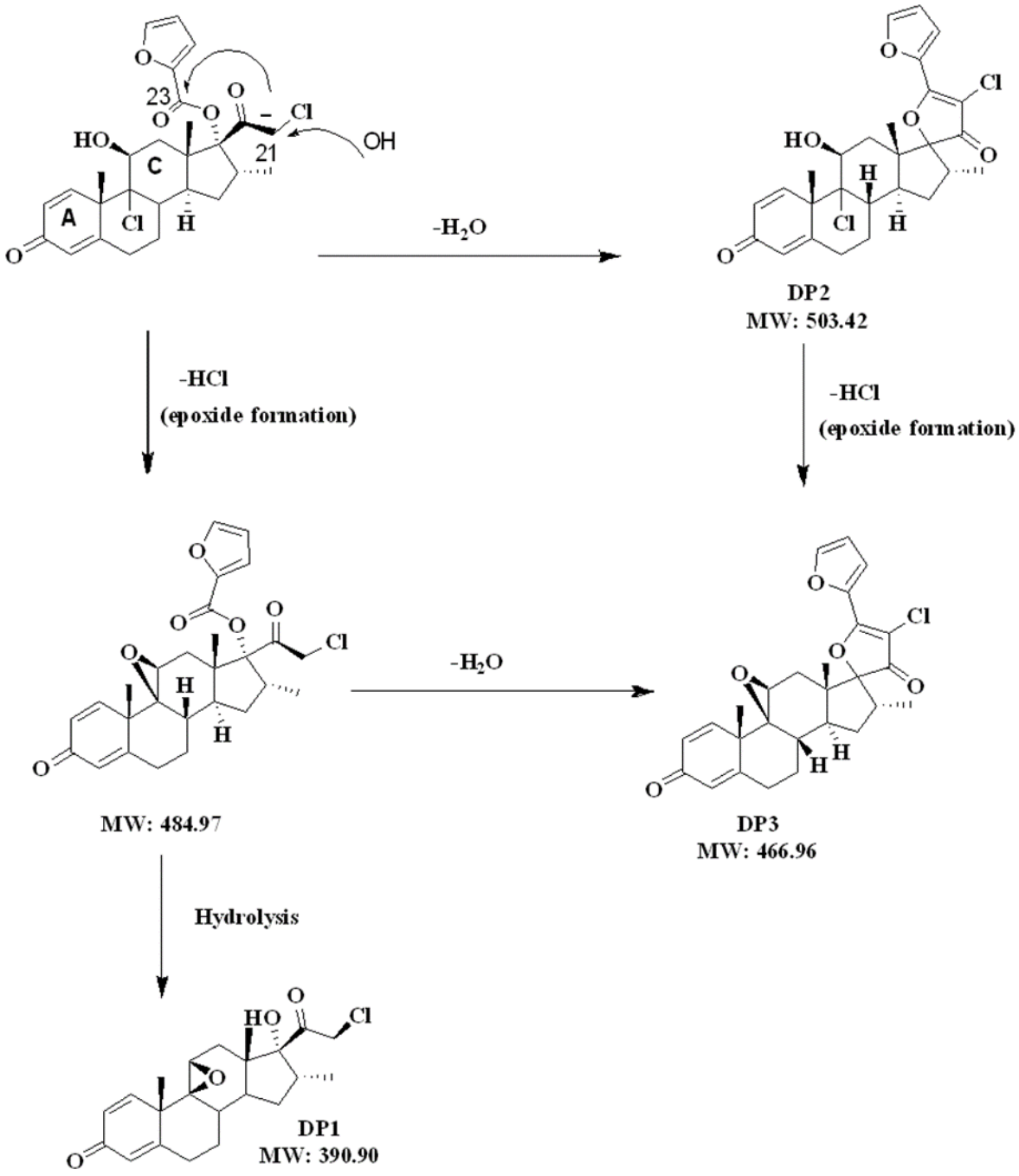

Figure S4. Plausible degradation mechanism of mometasone furoate

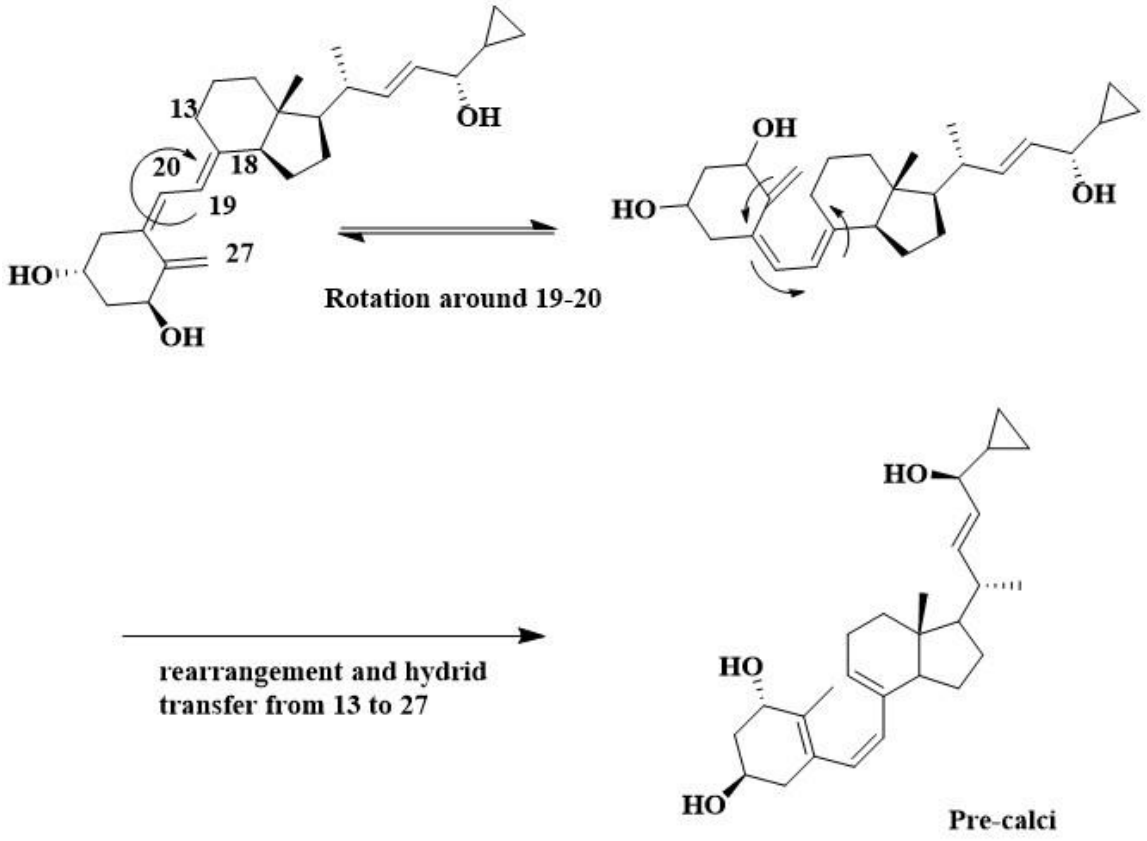

Figure S5. Plausible degradation mechanism of calcipotriol based on Fukui data

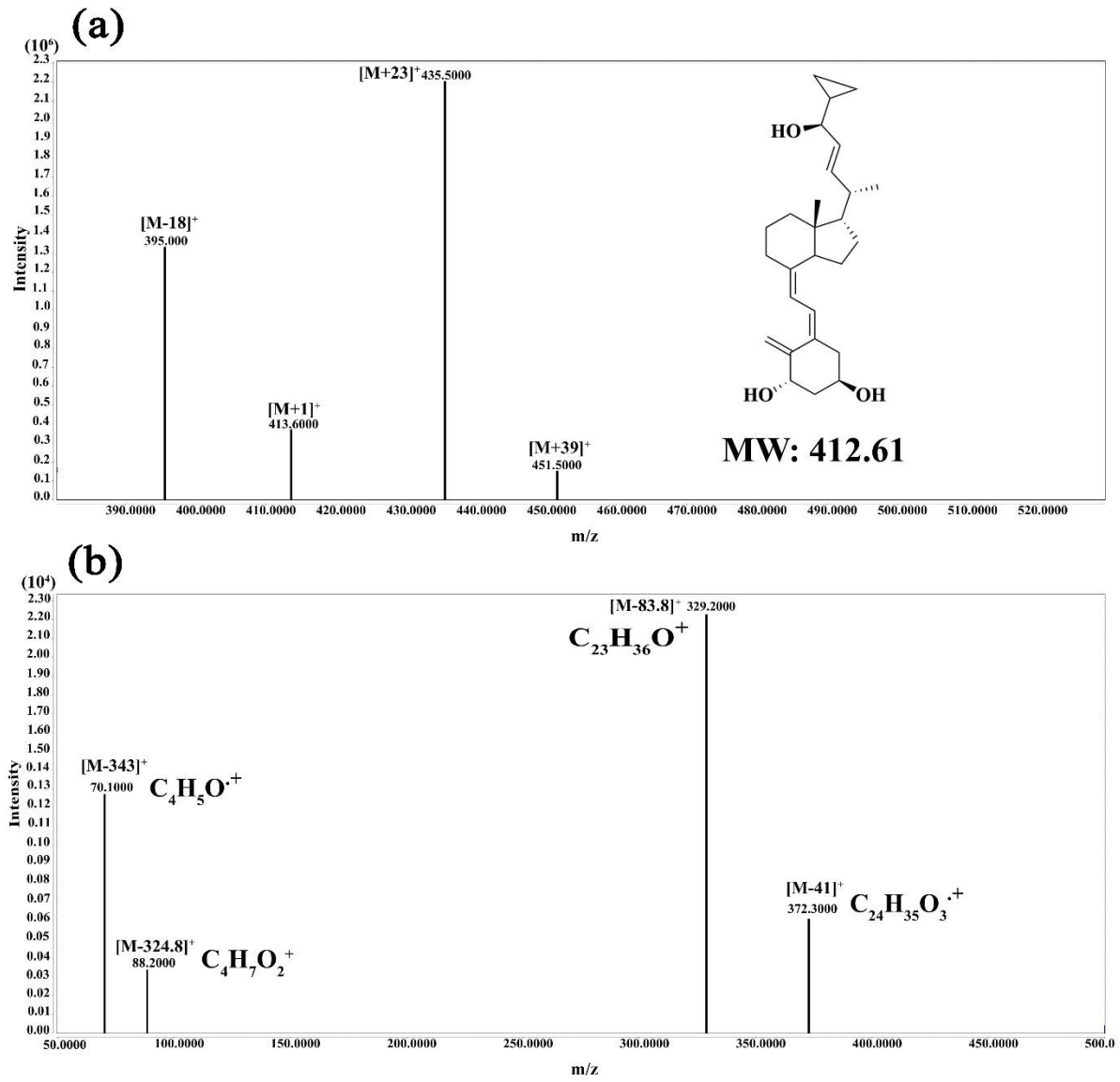

Figure S6 (a) MS spectra, (b) MS-MS spectra, and the structures of standard CP and DP4 (pre-calcipotriol)

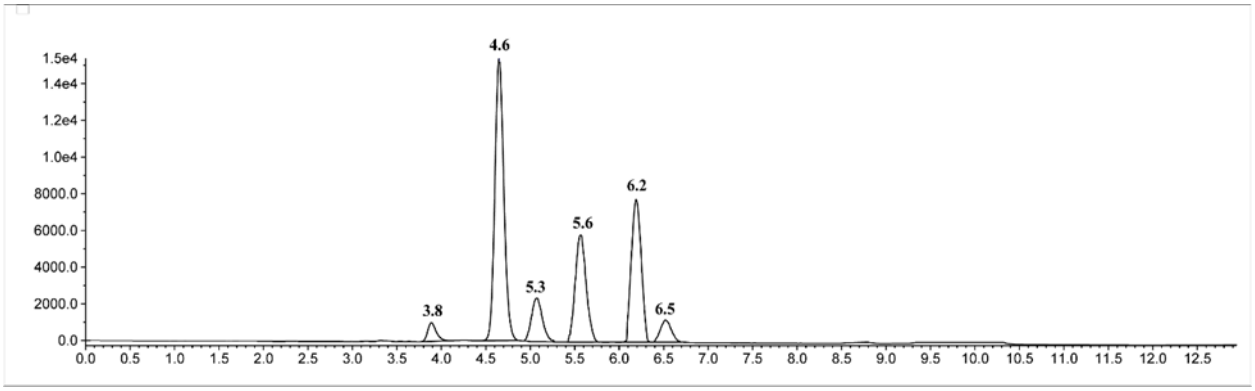

Figure S7. LC-MS Chromatogram of MF (4.6 min), degradation products of MF (3.8, 5.3 and 5.6 min) and CP (6.2 min) and degradation product of CP (6.5 min)

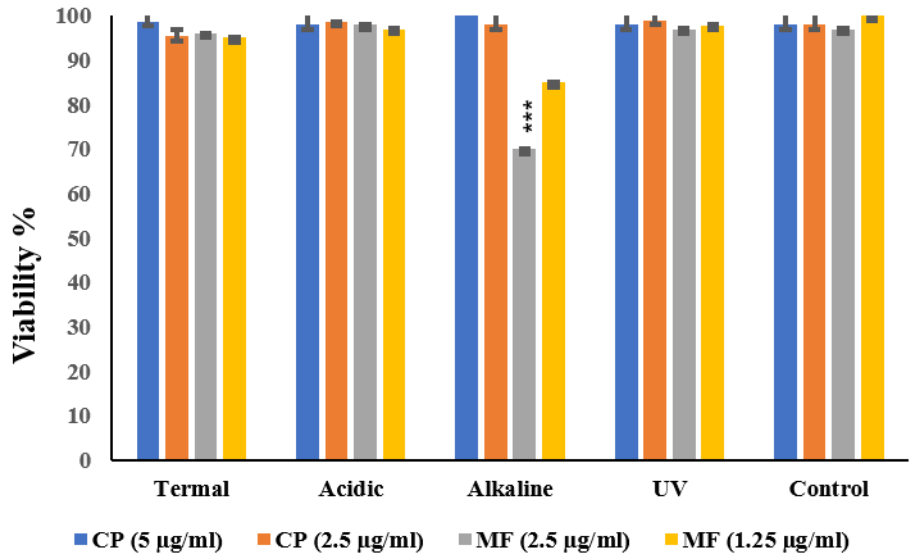

Figure S8. Cell viability of CP and MF after forced degradation on NIH/3T3 cell (***: $p < 0.001$)

R1 (t_R MF) =49.69–0.46 (% MeOH) +0.011(λ̄) – 25.34 (flow rate) -0.0001(MeOH*λ̄) +0.24(MeOH*flow) – 0.002 (λ̄* flow); (R^2=0.991) (3)
R2 (t_R CP) =112.86 -1.17(% MeOH) +0.05(λ̄) – 58.70 (flow rate) -0.0004(MeOH*λ̄) +0.62 (MeOH*flow) – 0.01 (λ̄* flow); (R^2=0.9741) (4)
R3 (AUC MF) =2.07× 10^7- 1.85 (% MeOH) – 86564 (λ̄) +1.5× 10^6 (flow rate) + 909.2(MeOH*λ̄) -32051.7 (MeOH*flow) – 648.23 (λ̄* flow); (R^2=0.9131) (5)
R4 (AUC CP) = -1.303× 10^4- 13489(% MeOH) – 5349.6 (λ̄) – 1.02× 10^5 (flow rate) - 56.15(MeOH*λ̄) +985.6 (MeOH*flow) – 169.96 (λ̄* flow); (R^2=0.8991) (6)
R5 (R) = 109.94 - 1.14(% MeOH) – 0.100 (λ̄) – 18.28 (flow rate) + 0.0009(MeOH*λ̄) +0.16 (MeOH*flow) + 0.012 (λ̄* flow); (R^2=0.9847) (7)