

A high performance thin layer chromatographic method for the simultaneous determination of curcumin I, curcumin II and curcumin III in *Curcuma longa* and herbal formulation

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Characterization of Curcumins

Curcumin I: Yellow powder, m.p. 183 0C; UV λ_{max} (MeOH) 263, 431 nm; ^1H NMR (δ , CDCl_3)(Figure S1): 5.98 (s, H-1), 6.48 (d, J = 16 Hz, H-3, 3'), 7.58 (d, J = 16 Hz, H-4, 4'), 7.05 (bs, H-6, 6'), 6.92 (d, J = 8.2Hz, H-9, 9'), 7.11 (bd, J = 8.2Hz, H-10, 10'), 3.98 (s, 2 X OCH_3). ^{13}C NMR (δ , CDCl_3)(Figure S2): 100.81 (C-1), 183.52 (C-2,2'), 121.76 (C-3,3'), 140.60 (C-4,4'), 127.69 (C-5,5'), 109.65 (C-6,6'), 147.87 (C-7,7'), 146.81 (C-8,8'), 114.85 (C-9,9'), 122.90 (C-10,10'), 55.84 (OCH_3) and Table 2. HRESI-MS: m/z 367.1188 (Calc. 367.1182) [M^+-1], 369.1328 (Calc. 369.1338) [M^++1], 391.1147 (Calc. 391.1158) [M^++Na] (Figure S1).

Curcumin II: Yellow powder, m.p. 169 0C; UV λ_{max} (MeOH) 251, 423 nm; ^1H NMR (δ , CD_3OD)(Figure S1): 5.98 (s, H-1), 6.57 (d, J = 16 Hz, H-3, 3'), 7.55 (d, J = 16 Hz, H-4, 4'), 7.19 (bs, H-6), 7.46 (d, J = 7.5 Hz. H-6', H10'), 6.80 (bd, J = 7.5 Hz H-7', H9', H-9), 7.08 (d, J =7.0 Hz, H-10), 3.83 (s, OCH_3) and Table 1. ^{13}C NMR (δ , CD_3OD)(Figure S2): 102.41 (C-1), 185.05 (C-2), 184.85 (C-2'), 122.43 (C-3), 122.16 C-3'), 142.28 (C-4), 142.05 (C-4'), 128.75 (C-5), 128.16 (C-5'), 111.88 (C-6), 131.35 (C-6', 10'), 149.57(C-7), 115.50 (C-7', C-9'), 150.63 (C-8), 161.27 (C-8'), 116.74 (C-9), 124.29 (C-10), 56.04 (OCH_3). HRESI-MS: m/z 337.1084 (Calc. 337.1076) [M^+-1], 339.1226 (Calc. 339.1232) [M^++1], 361.1043 (Calc. 361.1052) [M^++Na] (Figure S2).

Curcumin III: Yellow powder, m.p. 173 0C; UV λ_{max} (MeOH) 248, 418 nm; ^1H NMR (δ , CD_3OD)(Figure S1): 5.98 (s, H-1), 6.58 (d, J = 16 Hz, H-3, 3'), 7.56 (d, J = 16 Hz, H-4, 4'), 7.47 (d, J = 8.2 Hz, H-6, 6', 10, 10'), 6.80 (d, J = 8.2Hz, H-7, 7', 9, 9'). ^{13}C NMR (δ , CD_3OD)(Figure S2): 102.23 (C-1), 185.00 (C-2,2'), 122.15 (C-3,3'), 142.04 (C-4,4'), 128.17 (C-5,5'), 131.34 (C-6,6',10,10'), 117.07 (C-7,7',9,9'), 161.26 (C-8,8'). HRESI-MS: m/z 307.0977 (Calc. 307.0970) [M^+-1], 309.1120 (Calc. 309.1127) [M^++1], 331.0938 (Calc. 331.0946) [M^++Na] (Figure S3).

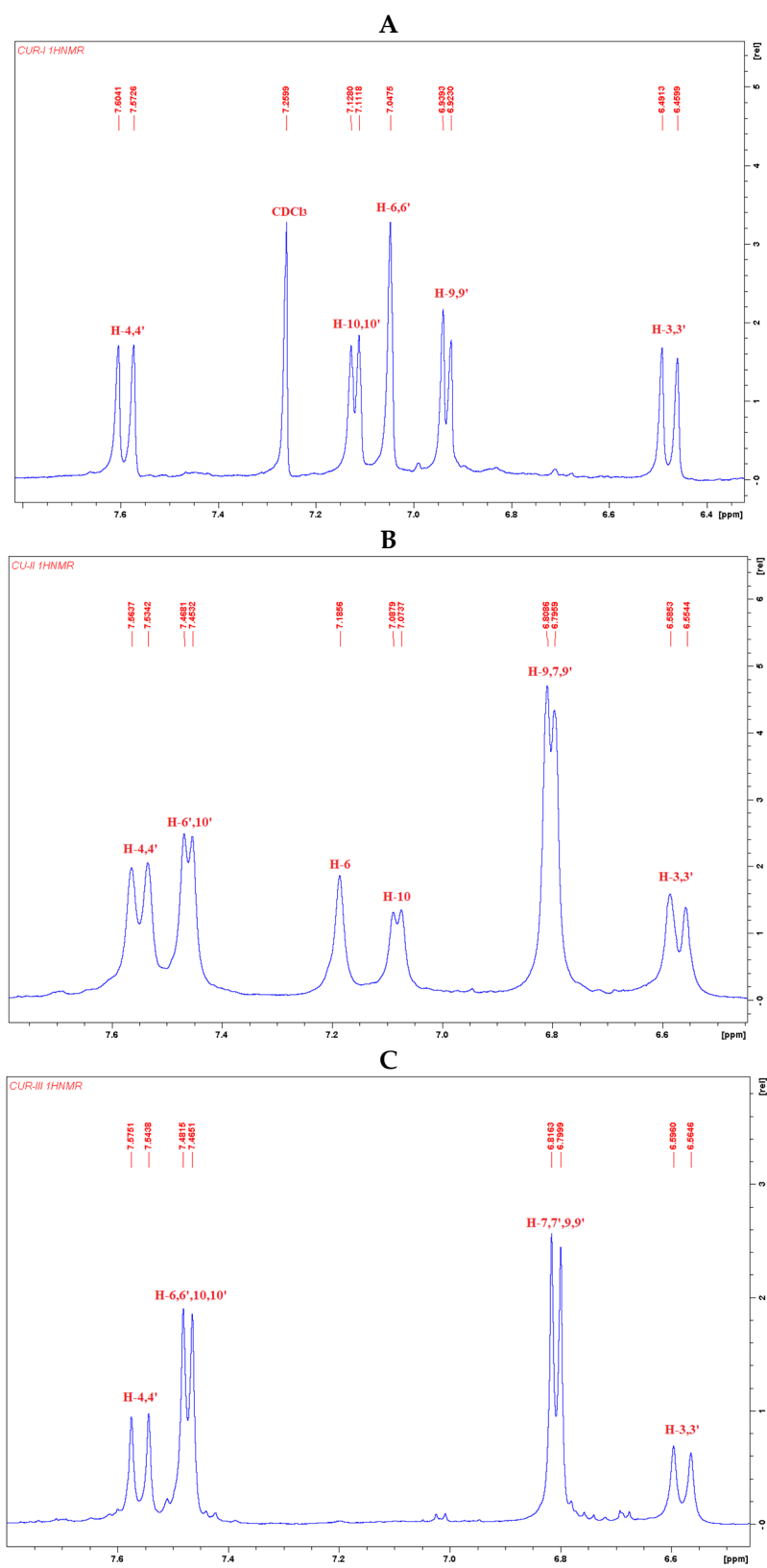


Figure S1. ¹H NMR of the aromatic protons of Curcumins I-III (A-C).

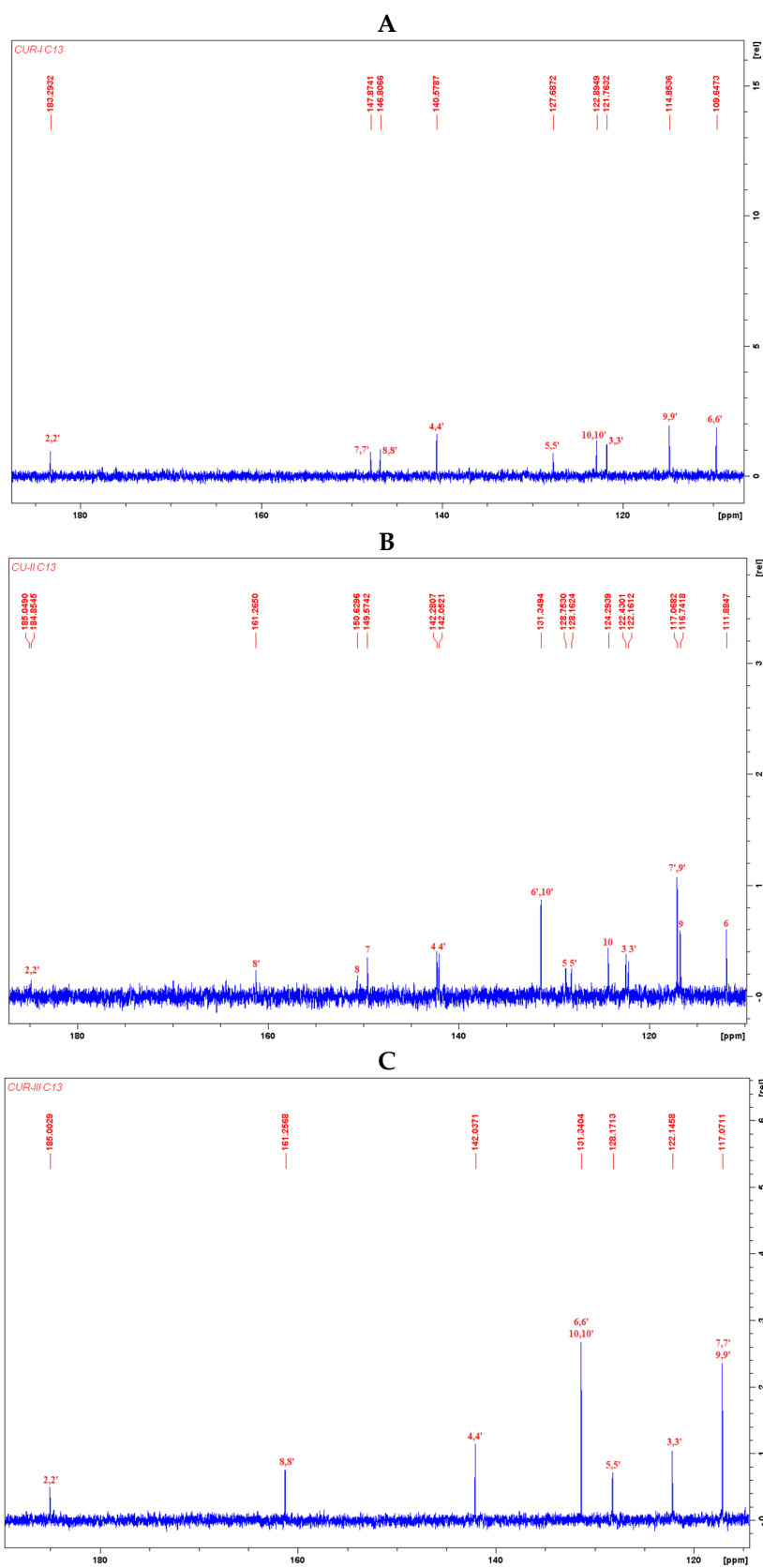
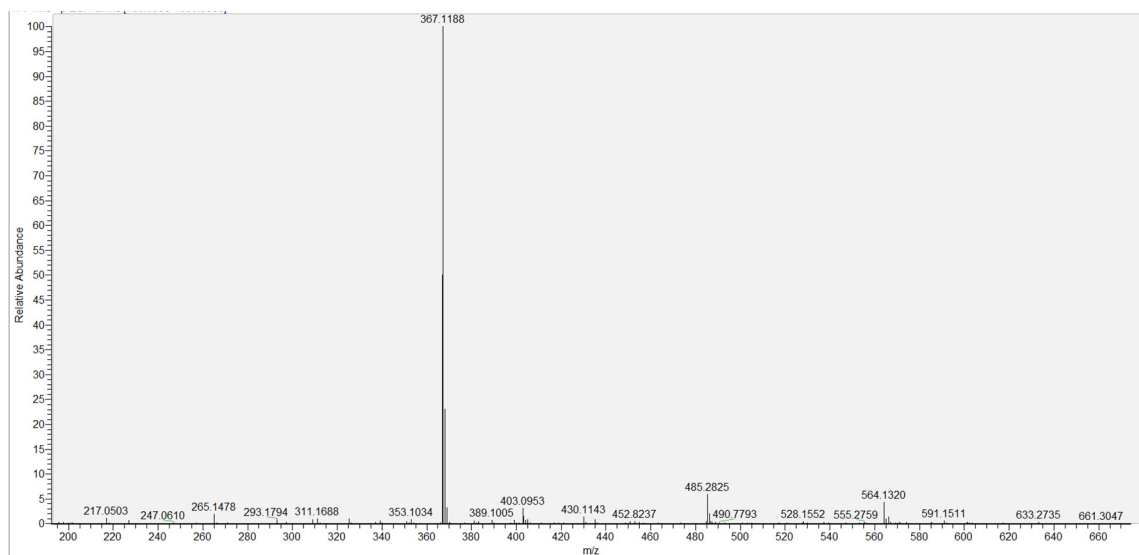
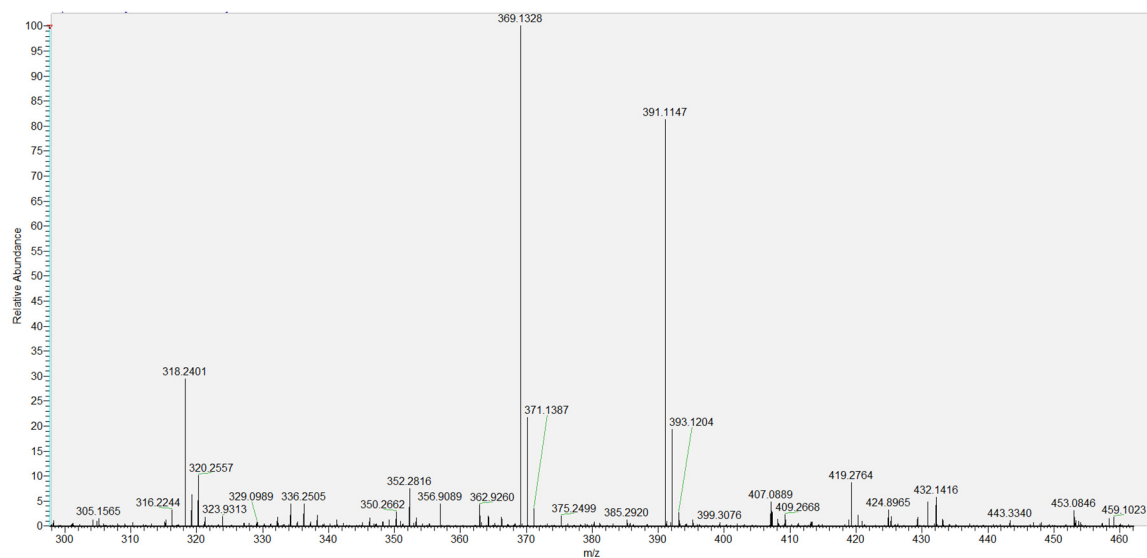


Figure S2. ^{13}C NMR of the aromatic carbons of Curcumins I-III (A-C).

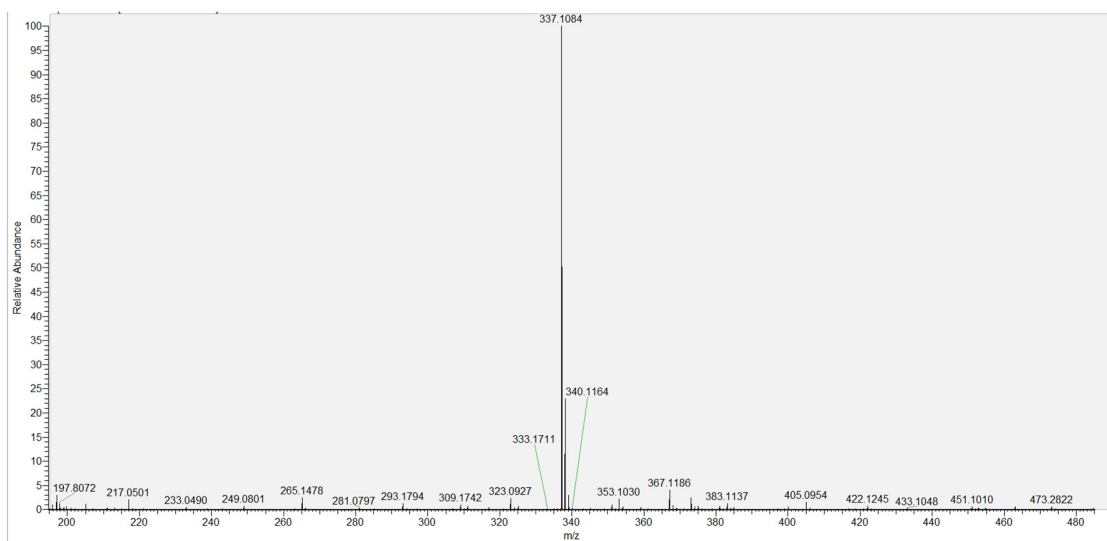


A

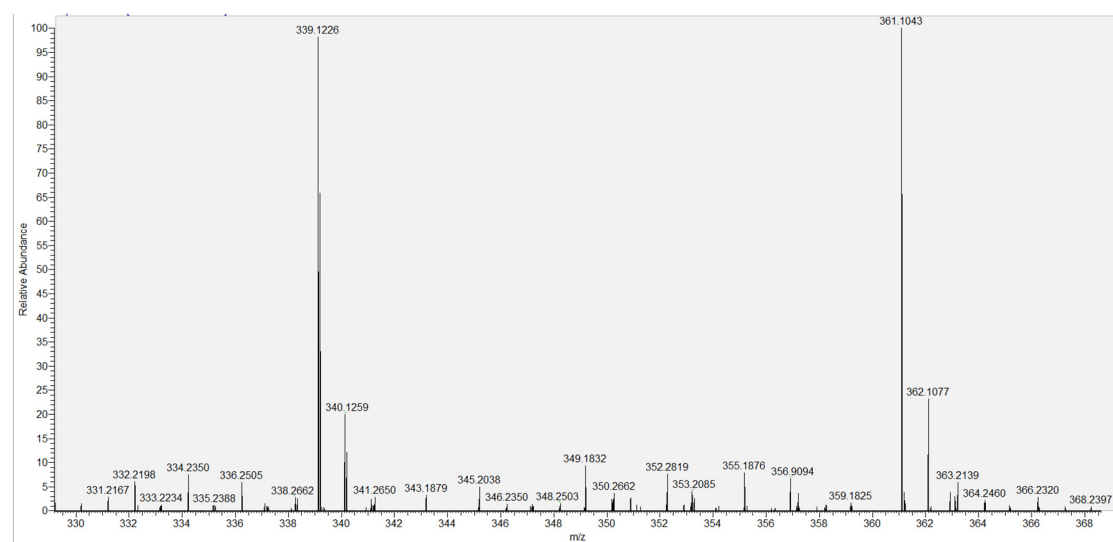


B

Figure S3. Mass spectra of Curcumin I (A: Negative Mode B: Positive Mode).

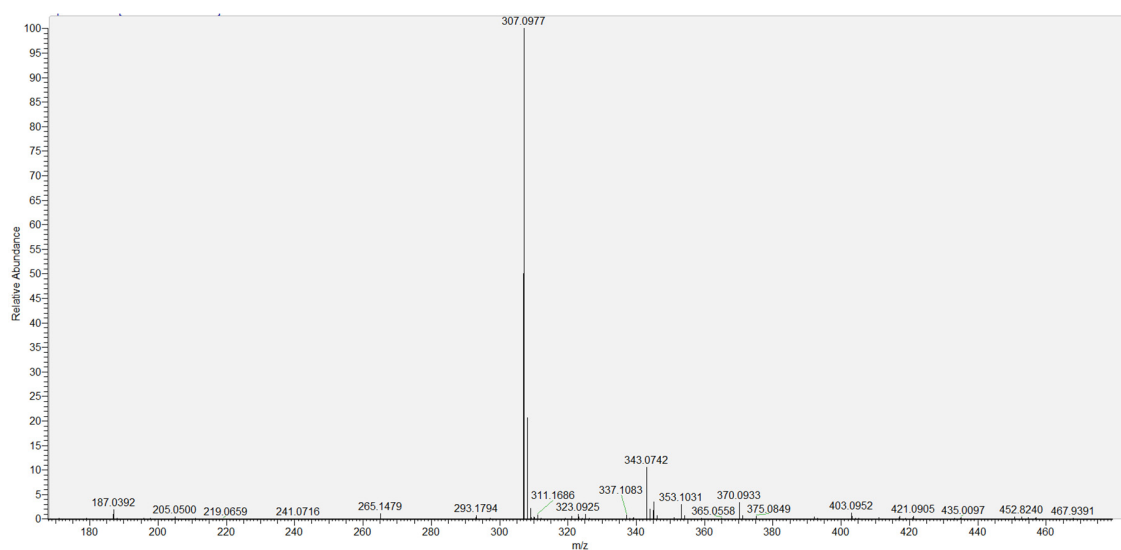


A

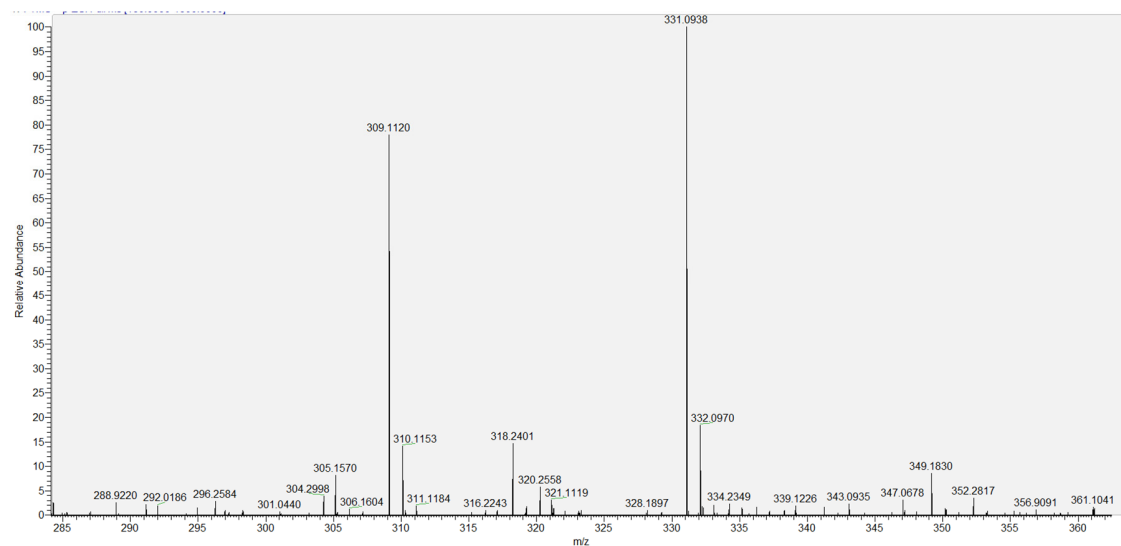


B

Figure S4. Mass spectra of Curcumin II (A: Negative Mode B: Positive Mode).



A



B

Figure S5. Mass spectra of Curcumin III (A: Negative Mode B: Positive Mode).

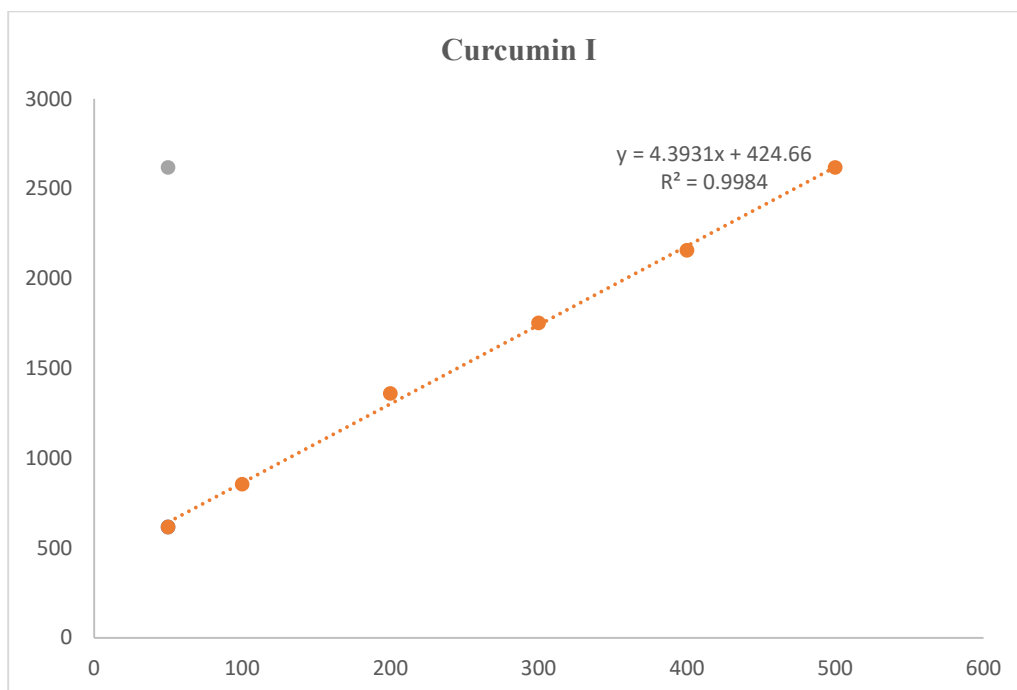


Figure S6. Calibration curve of curcumin I.

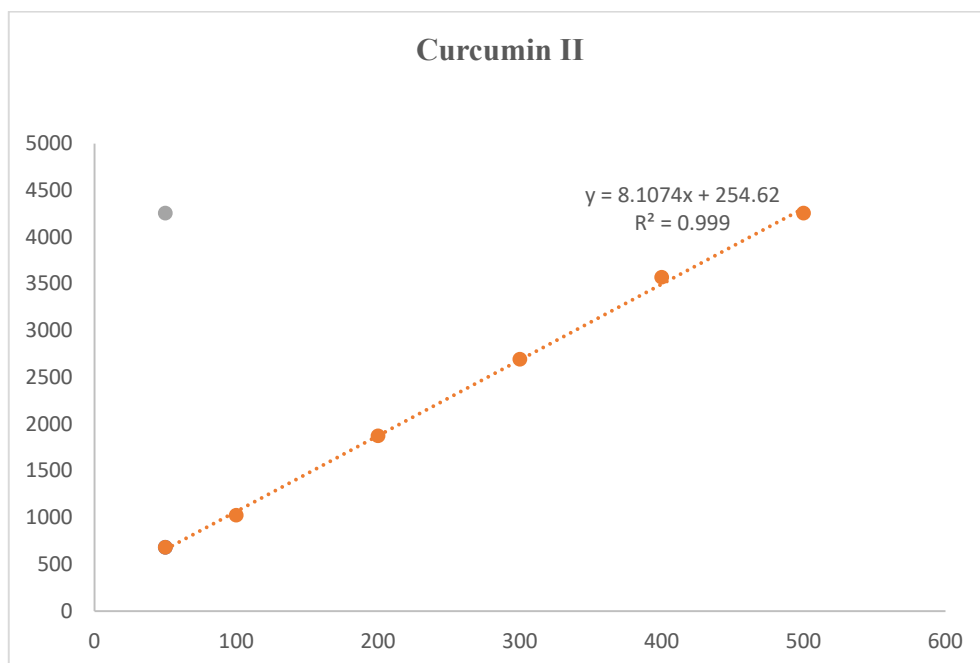


Figure S7. Calibration curve of curcumin II.

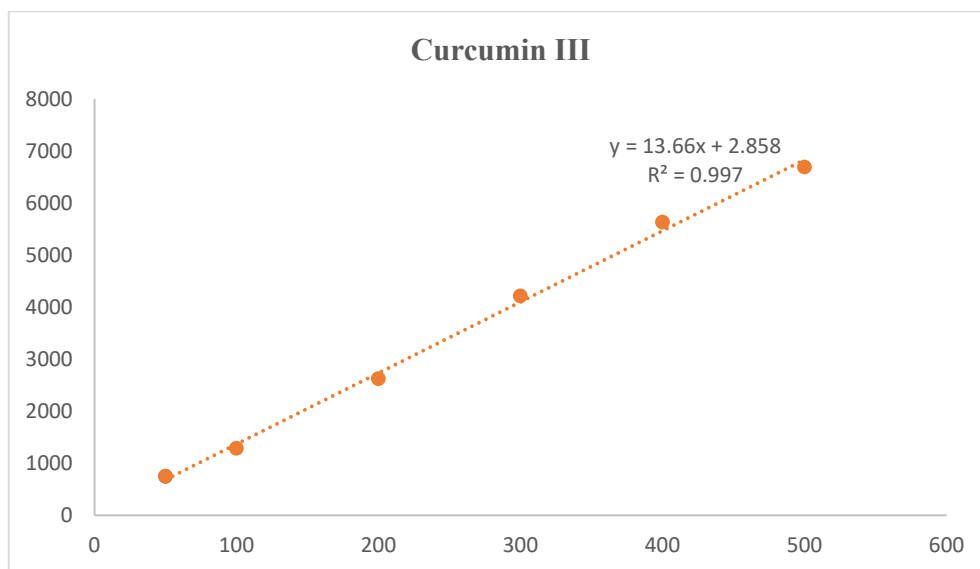


Figure S8. Calibration curve of curcumin III.

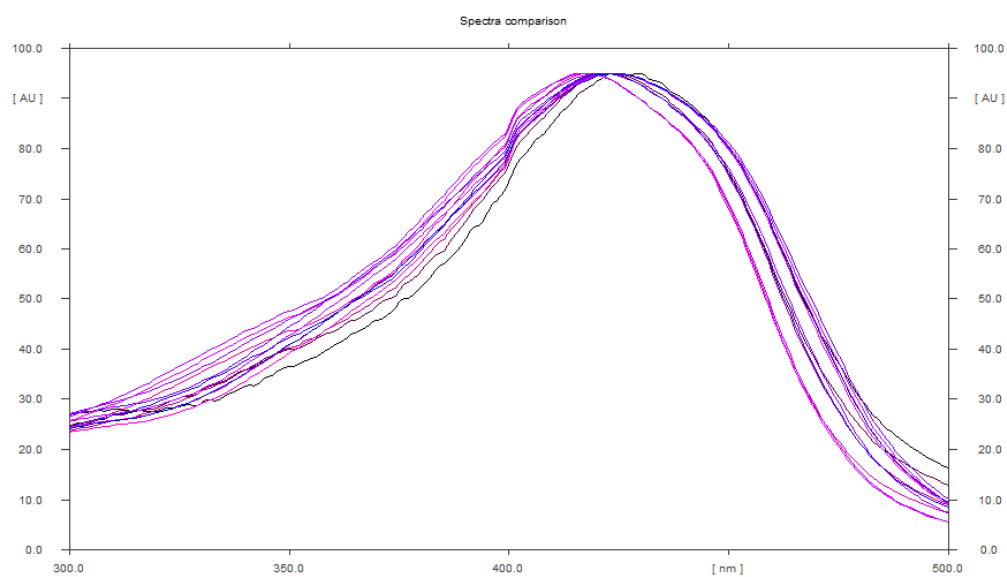


Figure S9: Overlay UV absorption spectra of curcumins I-III and corresponding spots in *C. longa* extracts and formulations.