

Supporting information

Table S1 d-Spacings(Å), 2θ Values(°) and relative intensities (%) of the ten most intense peaks in XPRD patterns of methoxyflavone polymorphs

| No | Form A | | | Form B | | |
|----|--------|-------|------------------|--------|-------|------------------|
| | d | 2θ | I/I ₀ | d | 2θ | I/I ₀ |
| 1 | 7.54 | 11.72 | 100.0 | 12.55 | 7.04 | 100.0 |
| 2 | 4.06 | 21.90 | 67.3 | 8.34 | 10.60 | 44.8 |
| 3 | 3.51 | 25.36 | 66.2 | 6.98 | 12.68 | 15.9 |
| 4 | 5.12 | 17.32 | 62.8 | 3.55 | 20.06 | 15.9 |
| 5 | 3.17 | 28.16 | 38.8 | 10.75 | 8.22 | 13.9 |
| 6 | 3.30 | 27.02 | 37.5 | 4.33 | 20.50 | 11.3 |
| 7 | 5.80 | 15.26 | 29.2 | 3.67 | 24.26 | 10.4 |
| 8 | 8.20 | 10.78 | 22.2 | 4.23 | 20.96 | 10.2 |
| 9 | 4.81 | 18.44 | 20.8 | 6.20 | 14.28 | 6.5 |
| 10 | 4.97 | 17.82 | 19.4 | 5.71 | 15.50 | 6.1 |

Table S2 Main vibrational data (cm⁻¹) with tentative assignments for polymorphs of methoxyflavone

| Vibrational data | | Vibrational assignment |
|-------------------------|------------------------|------------------------------------|
| form A | form B | |
| 3074 | 3081 | Ar-H stretch vibration |
| 1634 | 1632, 1622 | C=O stretch vibration |
| 1600, 1563, 1453 | 1600, 1566, 1451 | C=C stretch vibration |
| 1258, 1216, 1139, 1071 | 1253, 1217, 1136, 1072 | C-O stretch vibration |
| 856, 826, 758, 701, 693 | 858, 828, 754, 696 | C-H out-of-plane bending vibration |

Fig S1 TGA diagram of polymorphs of methoxyflavone

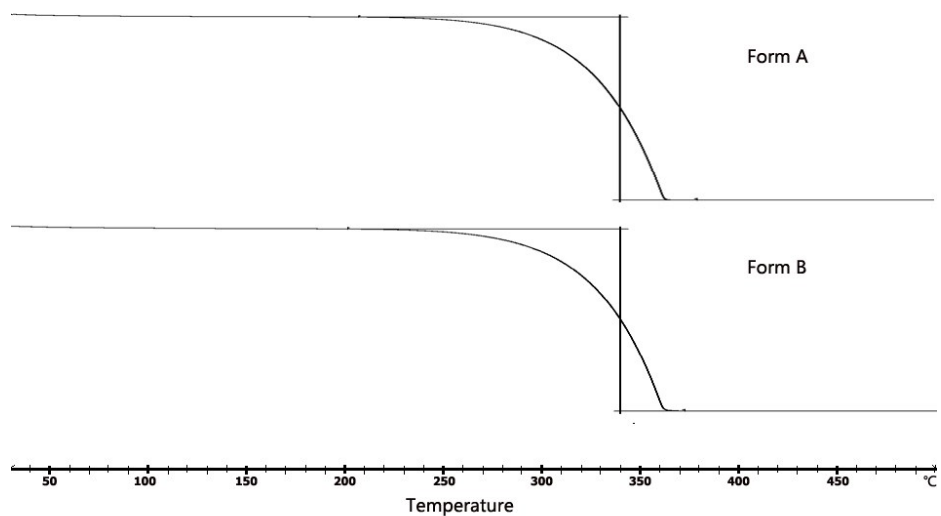


Fig S2 Polymorph transformation of methoxyflavone amorphous phase

