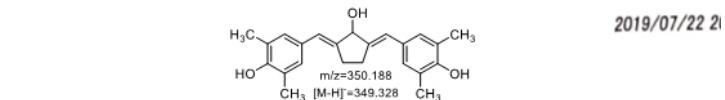


## Supplementary file 1

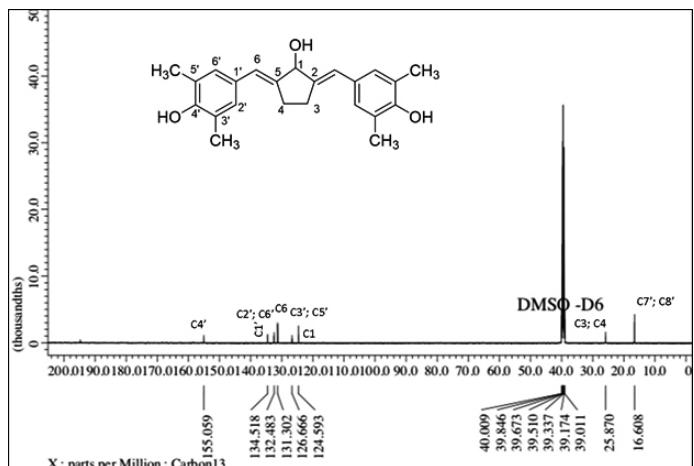


===== Shimadzu LCMSsolution 分析レポート =====

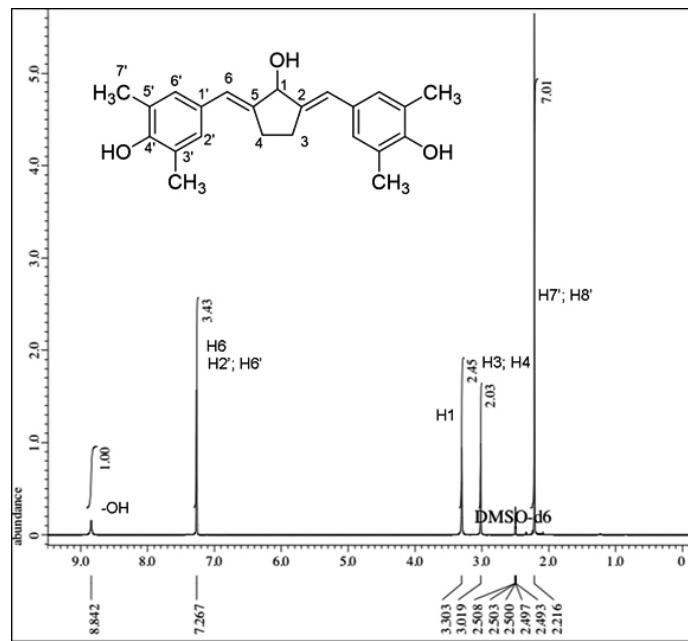
〈クロマトグラム〉

クロマトグラム  
CRL-52-350 @F:\LCMS\DATA\nakamura\_Lab\Yudi\CRL-52-350.lcd

**Figure S1.** Mass spectrometric profile of CCA-1.1



**Figure S2.** <sup>13</sup>C-NMR Spectrum of CCA-1.1



**Figure S3.** <sup>1</sup>H-NMR Spectrum of CCA-1.1

**Table S1.** RMSD value of the molecular docking study

| Ligand  | RMSD (Å) |       |       |             |            |       |       |        |        |       |
|---------|----------|-------|-------|-------------|------------|-------|-------|--------|--------|-------|
|         | HER2     | EGFR  | IKK   | ER $\alpha$ | ER $\beta$ | NQO1  | NQO2  | AKR1C1 | GST-P1 | GLO1  |
| PGV-1   | 0.721    | 1.288 | 1.539 | 1.241       | 1.539      | 1.728 | 1.003 | 1.641  | 1.156  | 1.964 |
| CCA-1.1 | 1.862    | 1.189 | 1.854 | 1.778       | 1.165      | 1.727 | 1.261 | 1.288  | 1.089  | 0.821 |