Supplementary Information

for

Rational Design and Optimization of Selenophenes with Basic Side Chains as Novel Potent Selective Estrogen Receptor Modulators (SERMs) for Breast Cancer Therapy

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PART I. Analytical techniques

$^1$H NMR and $^{13}$C NMR spectra were recorded on a Bruker AVANCE III 400 spectrometer (400 MHz, $^1$H NMR; 101 MHz, $^{13}$C NMR) at room temperature. NMR spectra were calibrated to the solvent signals of CDCl$_3$ ($\delta$ 7.26 and 77.00), Acetone-$d_6$ ($\delta$ 2.05 and 29.84, 206.26), CD$_3$OD ($\delta$ 3.31 and 49.00) or DMSO-$d_6$ ($\delta$ 2.50 and 39.43). The chemical shifts are provided in ppm and the coupling constants in Hz. The following abbreviations for multiplicities are used: s, singlet; d, doublet; t, triplet; m, multiplet. Glassware was oven-dried, assembled while hot, and cooled under an inert atmosphere. Unless otherwise noted, all reactions were conducted in an atmosphere. Reaction progress was monitored using analytical thin-layer chromatography (TLC). Visualization was achieved by UV light (254 nm). Chromatography was performed with silica gel (0.040-0.063 mm) packing. High resolution mass spectra (HRMS) were measured on IonSpec 4.7 Tesla FTMS using MALDI/DHB. Melting points were obtained on X-4 melting point apparatus (Beijing TECH Instruments, Co., Ltd.) and are uncorrected.
PART II. $^1$H NMR and $^{13}$C NMR Spectra of final compounds

9a

![Chemical Structure Image]
12b
12f

![Chemical Structure](image)

![NMR Spectrum](image)

![Another NMR Spectrum](image)
16b

\[
\text{HO} \quad \text{Se} \quad \text{HO} \\
\text{O} \quad \text{N}
\]