

## Structure and purity confirmation data of compounds KSK-60 and KSK-74

### KSK60:

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz)  $\delta$  ppm: 8.2-8.3 (m, 2H, *J*=7.6 Hz, 4Pyr-2,6H), 7.9-7.9 (m, 2H, *J*=8.8 Hz, Ph-3,5H), 7.1-7.2 (m, 2H, *J*=7.0 Hz, Ph-2,6H), 7.0-7.0 (m, 2H, *J*=8.8 Hz, 4Pyr-3,5H), 4.04 (br t, 2H, *J*=6.2 Hz, CH<sub>2</sub>-O), 3.68 (br s, 4H, Pip-3,5H), 2.95 (q, 2H, *J*=7.2 Hz, CO-CH<sub>2</sub>-CH<sub>3</sub>), 2.71 (br s, 4H, Pip-2,6H), 2.49 (m, 3H, CO-CH<sub>2</sub>-CH<sub>3</sub>), 1.7-1.8 (m, 2H, NCH<sub>2</sub>), 1.3-1.6 (m, 6H, CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>), 1.04 (m, 2H, *J*=7.0 Hz, CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>). <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>): 199.24, 162.83, 130.54, 129.85, 114.68, 108.19, 68.18, 56.99, 51.71, 45.03, 33.02, 31.22, 28.85, 26.70, 25.66, 8.77. LC-MS: purity 100.00% *t*<sub>R</sub> = 3.43, (ESI) *m/z* [M+H]<sup>+</sup> 396.22.

### KSK74:

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz)  $\delta$  ppm: 8.24 (br d, 2H, *J*=6.9 Hz, 4Pyr-2,6H), 7.88 (br d, 2H, *J*=8.6 Hz, Ph-3,5H), 7.15 (br d, 2H, *J*=6.9 Hz, Ph-2,6H), 6.97 (br d, 2H, *J*=8.6 Hz, 4Pyr-3,5H), 4.01 (br t, 2H, *J*=6.3 Hz, CH<sub>2</sub>-O), 3.71 (br s, 4H, Pip-3,5H), 2.93 (q, 2H, *J*=7.4 Hz, CO-CH<sub>2</sub>-CH<sub>3</sub>), 2.80 (br s, 4H, Pip-2,6H), 2.60 (br t, 2H, *J*=7.4 Hz, NCH<sub>2</sub>), 1.7-1.7 (m, 2H, CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>), 1.51 (br s, 2H, CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>), 1.38 (br s, 2H, CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>), 1.27 (br s, 6H, CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>), 1.02 (br t, 3H, *J*=7.2 Hz, CO-CH<sub>2</sub>-CH<sub>3</sub>). <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>): 199.34, 162.93, 162.72, 157.10, 141.08, 130.63, 129.93, 114.77, 108.51, 68.32, 56.28, 50.82, 50.81, 31.30, 29.01, 26.67, 25.89, 24.10, 14.42, 8.48. LC-MS: purity 100.00% *t*<sub>R</sub> = 4.03, (ESI) *m/z* [M+H]<sup>+</sup> 424.34.