## Synthesis, docking studies and biological activity of new benzimidazole- triazolothiadiazine derivatives as aromatase inhibitor

Ulviye ACAR ÇEVİK<sup>1,2</sup>, Betül KAYA ÇAVUŞOĞLU<sup>3</sup>, Begüm Nurpelin SAĞLIK<sup>1,2</sup>, Derya OSMANİYE<sup>1,2</sup>, Serkan LEVENT<sup>1,2</sup>, Sinem ILGIN<sup>4</sup>, Yusuf ÖZKAY<sup>\*1,2</sup>, Zafer Asım KAPLANCIKLI<sup>1</sup>

<sup>1</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Anadolu Universty, Eskişehir, Turkey

<sup>2</sup>Doping and Narcotic Compounds Analysis Laboratory, Faculty of Pharmacy, Anadolu Universty, Eskişehir, Turkey

<sup>3</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Bülent Ecevit University, Zonguldak, Turkey

<sup>4</sup> Department of Pharmaceutical Toxicology, Faculty of Pharmacy, Anadolu Universty, Eskişehir, Turkey

\* Correspondence: yozkay@anadolu.edu.tr; Tel.: +90-222-335-0580/3603



Figure S1. <sup>1</sup>H NMR spectrum of compound 5a



Figure S2. <sup>13</sup>C NMR spectrum of compound 5a



Figure S3. Mass spectrum of compound 5a



Figure S4. <sup>1</sup>H NMR spectrum of compound 5b



Figure S5. <sup>13</sup>C NMR spectrum of compound 5b



Figure S6. Mass spectrum of compound 5b



Figure S7. <sup>1</sup>H NMR spectrum of compound 5c



S8. <sup>13</sup>C NMR spectrum of compound 5c

Figure







Figure S10.  $^1\!\mathrm{H}$  NMR spectrum of compound 5d



Figure S11.  $^{\rm 13}\!C$  NMR spectrum of compound 5d



Figure S12. Mass spectrum of compound 5d



Figure S13. <sup>1</sup>H NMR spectrum of compound 5e



Figure S14. <sup>13</sup>C NMR spectrum of compound 5e



Figure S15. Mass spectrum of compound 5e



Figure S16. <sup>1</sup>H NMR spectrum of compound 5f



Figure S17. <sup>13</sup>C NMR spectrum of compound 5f



Figure S18. Mass spectrum of compound 5f



Figure S19. <sup>1</sup>H NMR spectrum of compound 5g



Figure S20. <sup>13</sup>C NMR spectrum of compound 5g







Figure S21. Mass spectrum of compound 5g



Figure S22.  $^1\!\mathrm{H}$  NMR spectrum of compound 5h



Figure S23. <sup>13</sup>C NMR spectrum of compound 5h









C23 H14 N6 S Cl2 [M+H]+ : Predicted region for 477.0450 m/z



Figure S24. Mass spectrum of compound 5h



Figure S25. <sup>1</sup>H NMR spectrum of compound 51



Figure S26. <sup>13</sup>C NMR spectrum of compound 51







Figure S28. <sup>1</sup>H NMR spectrum of compound 5j



Figure S29. <sup>13</sup>C NMR spectrum of compound 5j



Figure S30. Mass spectrum of compound 5j



Figure S31. <sup>1</sup>H NMR spectrum of compound 5k



Figure S32. <sup>13</sup>C NMR spectrum of compound 5k



Figure S33. Mass spectrum of compound 5k



Figure S34. <sup>1</sup>H NMR spectrum of compound 51



Figure S35. <sup>13</sup>C NMR spectrum of compound 51







Figure S37. <sup>1</sup>H NMR spectrum of compound 5m



Figure S38. <sup>13</sup>C NMR spectrum of compound 5m



Figure S39. Mass spectrum of compound 5m



Figure S40. <sup>1</sup>H NMR spectrum of compound 5n



Figure S41. <sup>13</sup>C NMR spectrum of compound 5n



Figure S42. Mass spectrum of compound 5n

521.0

520.5

521.5

522.0

522.5

523.5

524.0

524.5

525.0

523.0



Figure S43. <sup>1</sup>H NMR spectrum of compound 50



Figure S44. <sup>13</sup>C NMR spectrum of compound 50



Figure S45. Mass spectrum of compound 50



Figure S46. <sup>1</sup>H NMR spectrum of compound 5p



Figure S47. <sup>13</sup>C NMR spectrum of compound 5p



Figure S48. Mass spectrum of compound 5p