# Supporting Information

**Identification of Thiazoyl Guanidine Derivatives As Novel Antifungal Agents Inhibiting Ergosterol Biosynthesis for Treatment of Invasive Fungal Infections**

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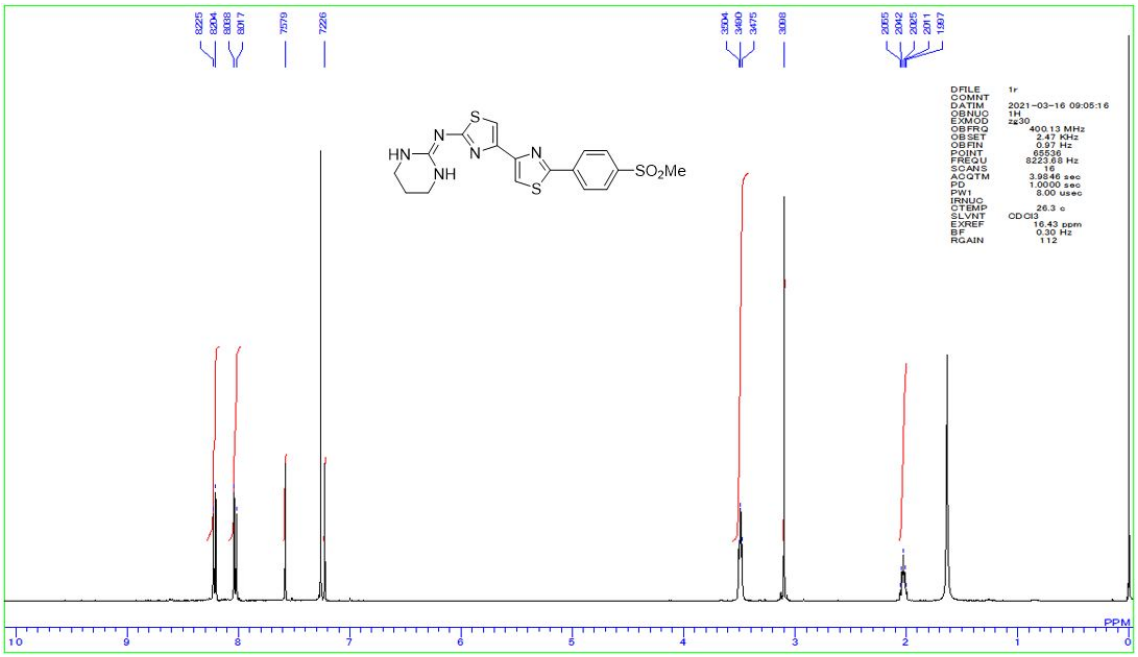
**$^1$HNMR SPECTRA OF COMPOUND 6h**

***N*-(2'-(4-(methylsulfonyl)phenyl)-[4,4'-bithiazol]-2-yl)tetrahydropyrimidin-2(1H)-imine (6h).**




**Compound purity information**

The purity of all tested compounds were determined by UPLC-MS (Table S1). The condition was described in the manuscript.

Table S1. Compound purity information

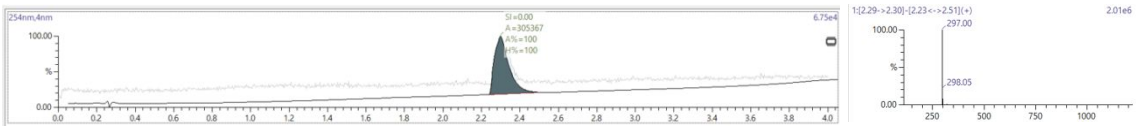
| Compound | Purity (UPLC) | Found Mass |
|---|---|---|
| **3a** | > 99.5 % | 297.0 |

| | | |
|---|---|---|
| **3b** | > 99.5 % | 325.0 |
| **3c** | > 99.5 % | 374.1 |
| **3d** | > 99.5 % | 375.0 |
| **3e** | > 99.5 % | 367.1 |
| **3f** | 97 % | 365.1 |
| **3g** | 97 % | 393.1 |
| **3h** | > 99.5 % | 393.1 |
| **4a** | > 99.5 % | 379.1 |
| **4b** | > 99.5 % | 380.1 |
| **4c** | > 99.5 % | 373.2 |
| **5a** | > 99.5 % | 335.1 |
| **5b** | > 99.5 % | 341.1 |
| **5c** | > 99.5 % | 342.0 |
| **5d** | > 99.5 % | 325.1 |
| **5e** | > 99.5 % | 326.1 |
| **6a** | > 99.5 % | 386.0 |
| **6b** | > 99.5 % | 358.0 |
| **6c** | > 99.5 % | 358.0 |

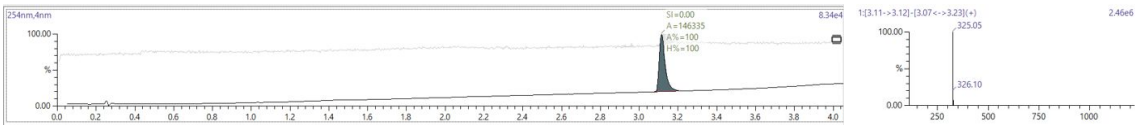
| | | |
|---|---|---|
| **6d** | > 99.5 % | 358.0 |
| **6e** | > 99.5 % | 343.0 |
| **6f** | > 99.5 % | 343.0 |
| **6g** | > 99.5 % | 343.0 |
| **6h** | > 99.5 % | 420.0 |
| **6i** | > 99.5 % | 420.0 |

**[1]LCMS SPECTRA OF COMPOUND 3a-h, 4a-c, 5a-e, 6a-i**

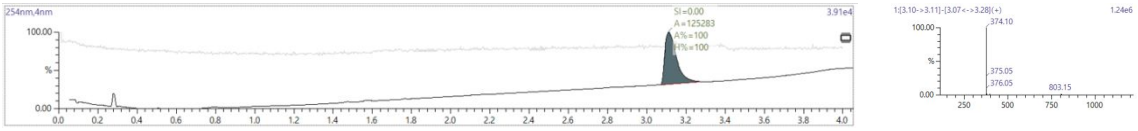
4-(2-(2,4-dimethylphenoxy)phenyl)thiazol-2-amine (3a).



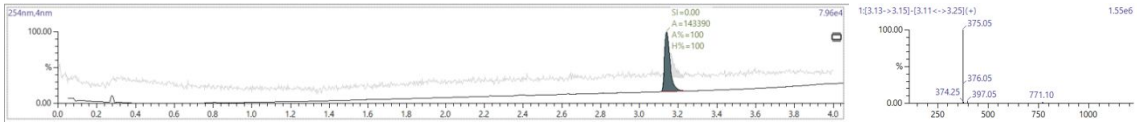
4-(2-(2,4-dimethylphenoxy)phenyl)-*N*,*N*-dimethylthiazol-2-amine (3b).



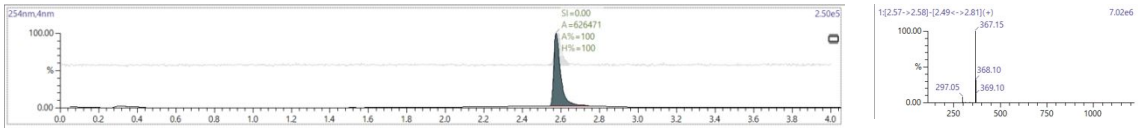
4-(2-(2,4-dimethylphenoxy)phenyl)-*N*-(pyridin-2-yl)thiazol-2-amine (3c).



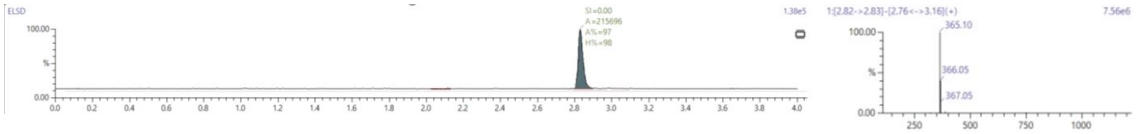
4-(2-(2,4-dimethylphenoxy)phenyl)-N-(pyrimidin-2-yl)thiazol-2-amine (3d).



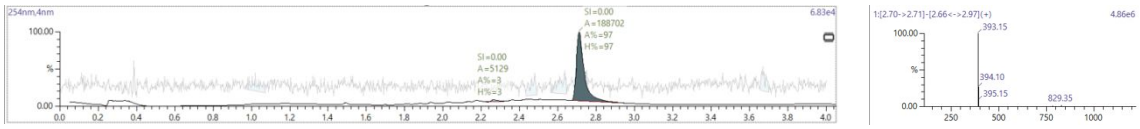
2-(4-(2-(2,4-dimethylphenoxy)phenyl)thiazol-2-yl)-1,3-dimethylguanidine (3e).



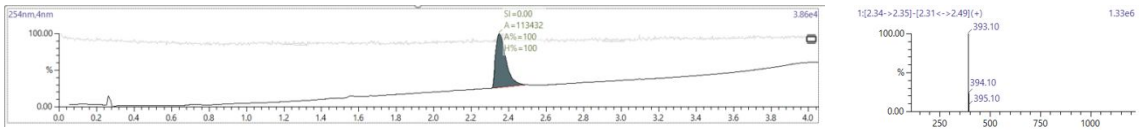
*N*-(4-(2-(2,4-dimethylphenoxy)phenyl)thiazol-2-yl)imidazolidin-2-imine (3f).



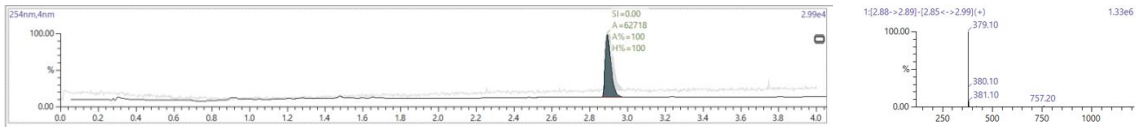
*N*-(4-(2-(2,4-dimethylphenoxy)phenyl)thiazol-2-yl)-1,3-diazepan-2-imine (3g).



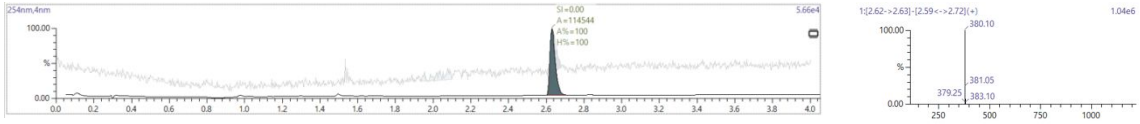
(*E*)-N-(4-(2-(2,4-dimethylphenoxy)phenyl)thiazol-2-yl)-1-methyltetrahydropyrimidin-2(1H)-imine (3h)



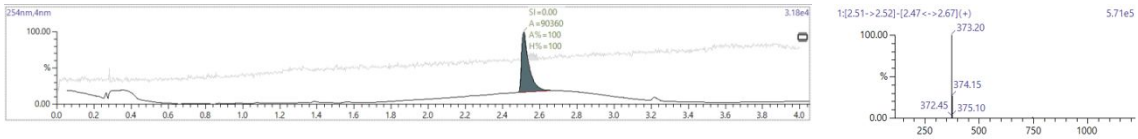
N-(5-(2-(2,4-dimethylphenoxy)phenyl)thiazol-2-yl)tetrahydropyrimidin-2(1H)-imine (4a)



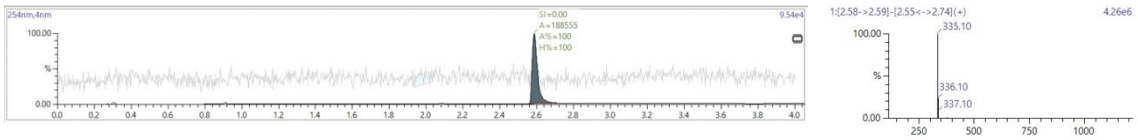

*N*-(3-(2-(2,4-dimethylphenoxy)phenyl)-1,2,4-thiadiazol-5-yl)tetrahydropyrimidin-2(1H)-imine (4b).



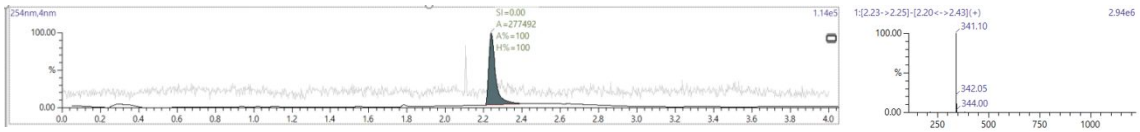

*N*-(6-(2-(2,4-dimethylphenoxy)phenyl)pyridin-2-yl)tetrahydropyrimidin-2(1H)-imine (4c).



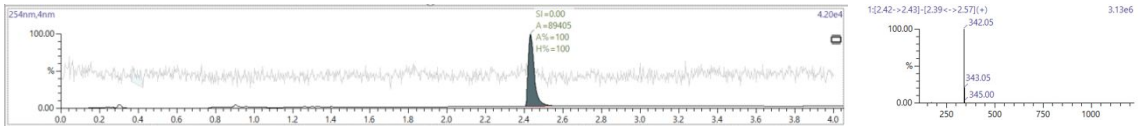

*N*-(4-([1,1'-biphenyl]-3-yl)thiazol-2-yl)tetrahydropyrimidin-2(1H)-imine (5a)



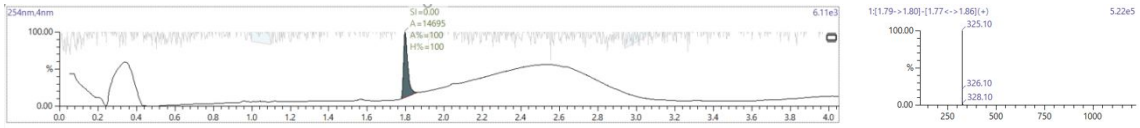

*N*-(4-(5-phenylthiophen-3-yl)thiazol-2-yl)tetrahydropyrimidin-2(1H)-imine (5b)



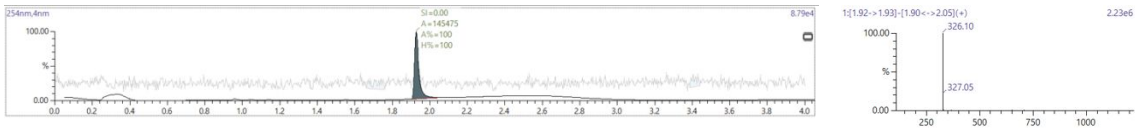

*N*-(2'-bromo-[4,4'-bithiazol]-2-yl)tetrahydropyrimidin-2(1H)-imine (5c)




*N*-(4-(1-phenyl-1H-pyrazol-3-yl)thiazol-2-yl)tetrahydropyrimidin-2(1H)-imine (5d)

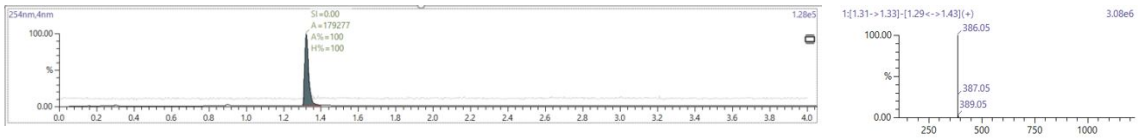



N-(4-(2-phenyloxazol-4-yl)thiazol-2-yl)tetrahydropyrimidin-2(1H)-imine (5e)

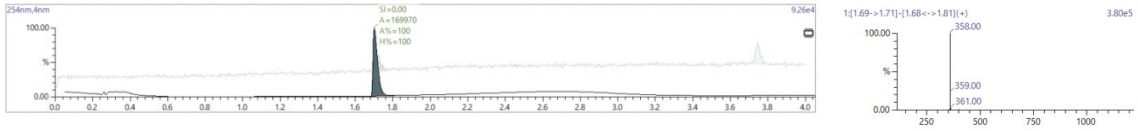



4-(2'-((tetrahydropyrimidin-2(1H)-ylidene)amino)-[4,4'-bithiazol]-2-yl)benzoic acid

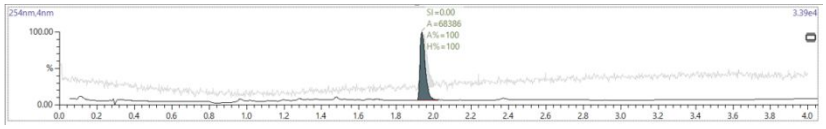
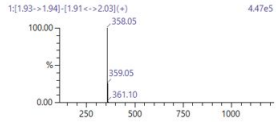
(6a)



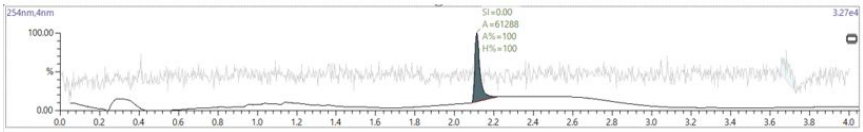
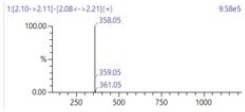

4-(2'-((tetrahydropyrimidin-2(1H)-ylidene)amino)-[4,4'-bithiazol]-2-yl)phenol (6b)



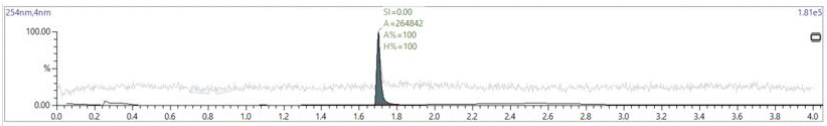
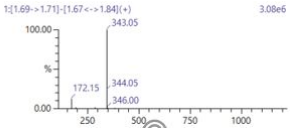

3-(2'-((tetrahydropyrimidin-2(1H)-ylidene)amino)-[4,4'-bithiazol]-2-yl)phenol (6c)

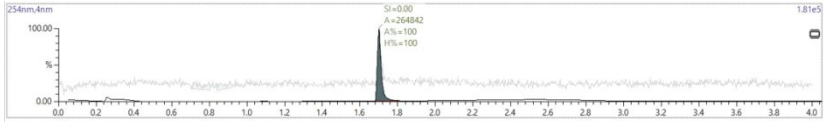
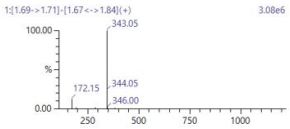
2-(2'-((tetrahydropyrimidin-2(1H)-ylidene)amino)-[4,4'-bithiazol]-2-yl)phenol (6d)

*N*-(2'-(pyridin-4-yl)-[4,4'-bithiazol]-2-yl)tetrahydropyrimidin-2(1H)-imine (6e)

*N*-(2'-(pyridin-3-yl)-[4,4'-bithiazol]-2-yl)tetrahydropyrimidin-2(1H)-imine (6f)

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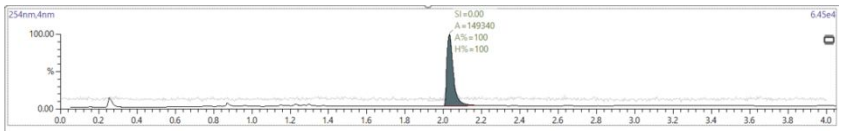
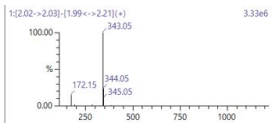
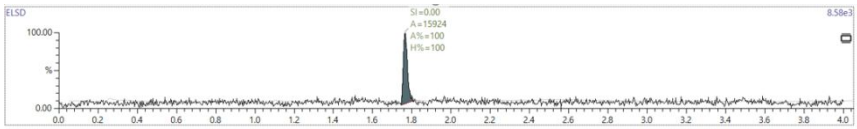
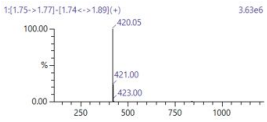



*N*-(2'-(4-(methylsulfonyl)phenyl)-[4,4'-bithiazol]-2-yl)tetrahydropyrimidin-2(1H)-imine (6h)

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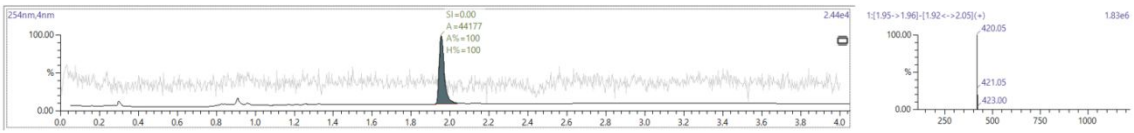
(6i)