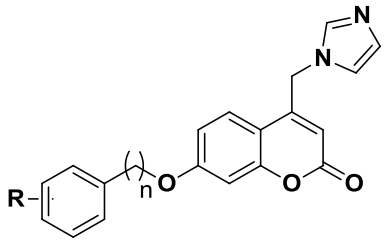
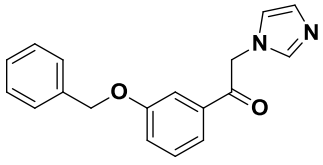
**Table 2.** CYP Inhibition and Selectivity Data of Compounds **2-27**



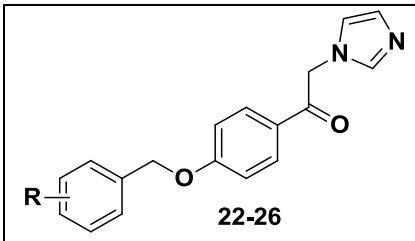
**2-20**

| Comps | R | n | CYP11B1 $IC_{50}$ nM [a,b] | CYP11B2 $IC_{50,}$ nM [a,b] | SIB[c] | CYP17 % inhibition [a,d] | CYP19 $IC_{50}$, nM [a,e] | SIC[f] |
|---|---|---|---|---|---|---|---|---|
| 2 | H | 1 | 72 | 289 | 4.1 | 3% | 150 | 2.1 |
| 3 | 3-$CH_3$ | 1 | 45 | 250 | 5.6 | 0% | 114 | 2.5 |
| 4 | 3-F | 1 | 40 | 200 | 5.0 | 0% | 113 | 2.8 |
| 5 | 3-Cl | 1 | 31 | 101 | 3.3 | 3% | 130 | 4.2 |
| 6 | 3-$CF_3$ | 1 | 20 | 150 | 7.5 | 0% | 235 | 12 |
| 7 | 3-$OCF_3$ | 1 | 5 | 125 | 25 | 3% | 207 | 41 |
| 8 | 3-$NO_2$ | 1 | 20 | 100 | 5.0 | 3% | 141 | 7.1 |
| 9 | 3-$OCH_3$ | 1 | 48 | 127 | 2.6 | 2% | 549 | 11 |
| 10 | 4-Cl | 1 | 100 | 200 | 2.0 | 1% | 178 | 1.8 |
| 11 | 4-$OCF_3$ | 1 | 25 | 250 | 10 | 1% | 481 | 19 |
| 12 | 4- $NO_2$ | 1 | 111 | 86 | 1.3 | 1% | 387 | 3.5 |
| 13 | 4-$OCH_3$ | 1 | 80 | 124 | 1.5 | 1% | 127 | 1.6 |
| 14 | 4-$OCH_2CH_2CH_3$ | 1 | 63 | 77 | 1.2 | 2% | 477 | 7.6 |
| 15 | 4-$OCH(CH_3)_2$ | 1 | 48 | 82 | 1.7 | 2% | 584 | 12 |
| 16 | H | 2 | 258 | 899 | 3.5 | 2% | 639 | 2.5 |
| 17 | 3,5-$F_2$ | 1 | 45 | 200 | 4.4 | 2% | 169 | 3.8 |
| 18 | 3,4-$F_2$ | 1 | 50 | 100 | 2.0 | 1% | 165 | 3.3 |
| 19 | 3,4-$(OCH_3)_2$ | 1 | 57 | 82 | 1.4 | 0% | 445 | 7.8 |
| 20 | 3,4,5-$(OCH_3)_3$ | 1 | 50 | 147 | 2.9 | 2% | 349 | 7.0 |



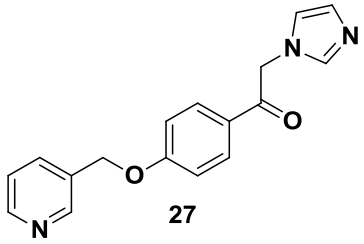
**21**

| Comps | R | CYP11B1 $IC_{50}$ nM [a,b] | CYP11B2 $IC_{50,}$ nM [a,b] | SIB[c] | CYP17 % inhibition [a,d] | CYP19 $IC_{50}$, nM [a,e] | SIC[f] |
|---|---|---|---|---|---|---|---|
| 21 | - | >500 | >500 | - | 1% | 17464 | -nd |




22-26

| Comps | R | CYP11B1 $IC_{50}$ nM [a,b] | CYP11B2 $IC_{50,}$ nM [a,b] | SIB[c] | CYP17 % inhibition [a,d] | CYP19 $IC_{50}$, nM [a,e] | SIC[f] |
|---|---|---|---|---|---|---|---|
| 22 | H | 149 | 588 | 3.9 | 1% | 4490 | 30 |
| 23 | 3-$OCF_3$ | 15 | 497 | 33 | 5% | 5855 | 390 |
| 24 | 3-$NO_2$ | 24 | 192 | 8.0 | 5% | 3708 | 155 |
| 25 | 3-CN | 30 | 222 | 7.4 | 3% | 4566 | 152 |
| 26 | 4-$OCF_3$ | 109 | 669 | 6.1 | 0% | 8299 | 76 |




27

| Comps | - | CYP11B1 $IC_{50}$ nM [a,b] | CYP11B2 $IC_{50,}$ nM [a,b] | SIB[c] | CYP17 % inhibition [a,d] | CYP19 $IC_{50}$, nM [a,e] | SIC[f] |
|---|---|---|---|---|---|---|---|
| 27 | - | 518 | 1397 | 2.7 | 6% | 31813 | 61 |
| Metyrapone | | 15 | 72 | 4.8 | 3% | 0 | nd |
| Ref A [8] | | 107 | 1423 | 13.3 | 2% | 0 | nd |
| Ref B [14] | | 2 | 33 | 16.5 | 5% | 1% | nd |

[a] Mean value of two or three experiments with a standard error always <15%. [b] Hamster fibroblasts expressing human CYP11B1 or CYP11B2;substrate 11-deoxycorticosterone, 100 nM. [c] SIB: $IC_{50}$CYP11B2/$IC_{50}$ CYP11B1. [d] *E. coli* expressing human CYP17; substrate progesterone, 2.5 μM except for ref. A and B (2.0 μM). [e] Human placental CYP19; substrate androstenedione, 500 nM. [f] SIC: $IC_{50}$ CYP19/$IC_{50}$ CYP11B1; nd , not determinable. Reference compounds, ketoconazole $IC_{50}$, 4.5 μM for CYP17 and **2** $IC_{50}$, 0.15 μM for CYP19.