In Silico Design of Bioisosteric Modifications of a Drug for the Treatment of Diabetes

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**Figure S1: TAK-875 bioisosteres structures**



1

2

3, 4

5

6

7

8

9

10

11, 12

13, 14

15

**Figure S1 (continued)**

**Figure S2: GW9508 bioisosteres structures**

|  |
| --- |
| **GW9508** |
| 20 |  | 21 |  |
| 22,23 |  | 24 |  |
| 25 |  | 26 |  |
| 27 |  | 28 |  |
| 29 |  | 30,31 |  |
| 32,33 |  | 34 |  |
| 35 |  | 36,37,38 |  |

**Table S1: TAK-875 bioisosteres corresponding numbers and pKa values**



**References**:

[1] Ballatore C, Huryn DM, Smith AB. Carboxylic acid (bio)isosteres in drug design. *ChemMedChem*. 8(3), 385–395 (2013)

[2]Hans Reich's Collection. Bordwell pKa Table.

[3] *Bioisosteric motifs cited in* - Lassalas P, Gay B, Lasfargeas C, *et al.* Structure Property Relationships of Carboxylic Acid Isosteres. *J. Med. Chem.* 59(7), 3183–3203 (2016).