**Prospects for inhibitors of PTP1B
(Protein Tyrosine Phosphatase–1B)
as anti–diabetic drugs**

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Supporting Information

A table showing the molecular structure, Lipinski parameters², PSA values³, and literature references for 64 anti-diabetic compounds used in Figure 3.

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1. Corresponding author; e-mail address: rob.hooft@serono.com.
 2. calculated using clogP (BioByte Corp., Claremont) and Tsar (Accelrys Inc., San Diego), respectively.
 3. calculated by an in-house script using Corina (Molecular Networks GmbH, Erlangen), catConf (part of the Catalyst package, Accelrys Inc., San Diego) and Cerius² (Accelrys Inc., San Diego).

Figure 3: plot of polar surface area (PSA) vs. molecular weight (MW) for 64 anti-diabetic compounds (3 triangles are non-PTP1B compounds, see text), color-coded by the number of violations against Lipinski's "Rules of 5" ($MW \leq 500$; $clogP \leq 5.0$; number of H-bond acceptors ≤ 10 ; number of H-bond donors ≤ 5).³¹ Color code: green – no violation; blue – one violation; red – two violations; black – three (or more) violations. Compounds that violate no more than one of these rules and have a $PSA < 160 \text{ \AA}^2$ (white area) are more likely to be orally bioavailable. Compound numbering is as in Fig. 2.