



Supplemental Digital Content 6. Chemical structures of PDE10A inhibitors PF-2545920 and TAK-063.

From a chemical point of view, PF-2545920 and TAK-063 are structurally distinct. While PF-2545920 has a pyrazole core, TAK-063 exhibits a pyridazine-4-one scaffold. The substituents of these compounds are also different. From a cheminformatics perspective, the structures exhibit a Tanimoto similarity of only 35% (based on RDKFingerprint), indicating significant dissimilarity. Hence, PF-2545920 can be described as structurally unrelated to TAK-063. The formulae were drawn using ACD/ChemSketch 2017.1.2 (Advanced Chemistry Development, Toronto, Canada).