

Figure 1 is a scatter plot showing the relationship between the number of atoms (X-axis, 0.0 to 0.6) and the number of rings (Y-axis, 0.0 to 0.6) for various drugs. The plot includes a solid blue line representing the linear regression and two dashed grey lines representing the confidence interval. Drugs are labeled with their names and colored dots (blue for one ring, green for two rings, red for three rings).

Drugs plotted include: Fesoterodine, Voriconazole, Cefixime, Pravastatin, Enprofylline, Mirabegron, Remoxipride, Risperidone, Lansoprazole, Rivaroxaban, Imatinib, Eprosartan, Nifedipine, Lansoprazole, Eprosartan, Febuxostat, Cerivastatin, Rosiglitazone, Meloxicam, Abiraterone, Tamsulosin, Aripiprazole, Bupropion, and Tenoxicam.

----- **Fold 2**  
----- **Fold 5**

- Mild
- Moderate
- Severe