**Data Mapping within this Dataset**

The ESI file is split into multiple sections for easier navigation. Please note the figure/table numbers run across all of the ESI files. The full file with no splitting is also available File: ESI\_Full

ESI\_1\_Synthesis and Characterization.docx

ESI\_2a\_Anion Transport Studies.docx

ESI\_2b\_Kini Determination.docx

ESI\_2c\_EC50 Determination Hill plot analyses.docx

ESI\_2d\_Anion Transport summary.docx

ESI\_3a\_QSAR Model fits.docx

ESI\_3b\_QSAR R Code CI.docx

ESI\_3c\_QSAR R Code lmer fits.docx



Figure 1 – Data mapping for this dataset showing where data were obtained or derived from

**Data Mapping for Figures and Tables in the Paper**

Figure 1: Compound Structures – obtained from file: ‘Compound\_structures\_2D.zip’, justified by Experimental Characterization file: ‘ESI\_1\_Synthesis and Characterization’

Figure 2: Log(1/EC50) vs ALOGPs Plots – plots in JMP, using EC50, ALOGPs, RT - file: ‘Tambjamine\_dataset\_cleaned.jmp’

Figure 3: Backbone structure of Tambjamines – obtained from compound structures - file: ‘Compound\_structures\_2D.zip’

Figure 4: Plots split by substituents – plots in JMP – using file: ‘Tambjamine\_dataset\_cleaned.jmp’

Figure 5: lmer fits – both ring substituents – analysis in R using file: ‘Tambjamine\_dataset\_cleaned.csv’ using R code see file: ‘ESI\_3c\_QSAR R Code lmer fits’

Figure 6: lmer fits – OMe ring substituent only - analysis in R using file: ‘Tambjamine\_dataset\_cleaned.csv’ using R code see file: ‘ESI\_3c\_QSAR R Code lmer fits’

Figure 7: Fits using compound classifications – plots in JMP – using file: ‘Tambjamine\_dataset\_cleaned.jmp’ and compound classifications

Table 1: Summary of raw data + ALOGPs – from raw data see file: ‘ESI\_2d\_ANION TRANSPORT SUMMARY’ and calculated descriptors – file: ‘Tambjamine\_dataset\_cleaned.jmp’

Table 2: Fitted Models – analysis in JMP - using file: ‘Tambjamine\_dataset\_cleaned.jmp’ see file: ‘ESI\_3a\_QSAR Model Fits’

Table 3: Confidence Intervals and Coefficients – analysis in JMP - using file: ‘Tambjamine\_dataset\_cleaned.jmp’ see file: ‘ESI\_3b\_QSAR R Code CI’

Table 4: Fits using compound classifications – analysis in JMP - using file: ‘Tambjamine\_dataset\_cleaned.jmp’ see file: ‘ESI\_3c\_QSAR R Code lmer fits’