**Supplementary File 2.** Criteria Used to Construct Classes of Deep Learning Models

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| **Cardiotoxicity Score** | **Description** | **Number of Imagesd** | **4-Class Modela** | **3-Class Modelb** | **2-Class Modelc** | |
| Class 3 | Highly toxic | 432 | Class 3 | Class 2 | Class 1 | |
| Class 2 | Toxic | 504 | Class 2 |
| Class 1 | Mildly toxic | 252 | Class 1 | Class 1 |  |  |
| Class 0 | Non-toxic | 504 | Class 0 | Class 0 | Class 0 | |

aDistinguishes highly toxic, toxic, and mildly toxic compounds from the non-toxic DMSO-treated condition (0.1%).

bBins highly toxic and toxic compounds into a single category separate from mildly toxic compounds.

cBins highly toxic and toxic compounds separate from the non-toxic DMSO-treated condition.

dThe total number of images used per class (80% of images were used to construct the neural network; the remaining 20% were used to validate the deep learning model).