

## Description of Additional Supplementary Files

**File Name: Supplementary Data 1**

**Description:** Structure of 71 nucleoside derivatives.

**File Name: Supplementary Data 2**

**Description:** Structure of 71 nucleoside derivatives.

**File Name: Supplementary Data 3**

**Description:** The details of 5566 molecular descriptors.

**File Name: Supplementary Data 4**

**Description:** The optimal combination of descriptors of each algorithm.

**File Name: Supplementary Data 5**

**Description:** Information and feature importance of the optimal model features (LR with 24 descriptors).

**File Name: Supplementary Data 6**

**Description:** The feature importance of 70 molecular descriptors based on LASSO regression.

**File Name: Supplementary Data 7**

**Description:** The predictions of optimal model for nucleoside derivatives from PubChem database.

**File Name: Supplementary Data 8**

**Description:** The validation for the hydrogel-forming ability of the 24 nucleoside derivatives.

**File Name: Supplementary Data 9**

**Description:** Search terms and search strategy of system-wide search.

**File Name: Supplementary Data 10**

**Description:** The atomic coordinates of the optimized computational models.