Development of QSRR model for hydroxamic acids using PCA-GA-BP algorithm incorporated with molecular interaction-based features

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CONTENTS

Table S1. The retention time of each analyte.........................................................1

Table S2. The docking scores of each analyte.......................................................6

Table S3. The principle components of matrix 1. ..................................................7

Table S4. The principle components of matrix 2. .................................................8

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Table S1. The retention time of each analyte.

| Compound NO. | Structure | retention time / min |
|--------------|-----------|----------------------|
| 1            | ![Structure 1](image1.png) | 3.6                  |
| 2            | ![Structure 2](image2.png) | 8.77                 |
| 3            | ![Structure 3](image3.png) | 2.71                 |
| 4            | ![Structure 4](image4.png) | 2.86                 |
| 5            | ![Structure 5](image5.png) | 4.23                 |
Table S2. The docking scores of each analyte.

| Compound NO. | Total_Score | Crash | D_SCORE | PMF_SCORE | G_SCORE | CHEMSCORE |
|--------------|-------------|-------|---------|-----------|---------|------------|
| 1            | 3.04        | -1.29 | -72.625 | -36.356   | -126.806| -16.212    |
| 2            | 1.5         | -0.94 | -83.299 | -54.325   | -137.703| -19.715    |
| 3            | 2.45        | -1.38 | -91.347 | -42.177   | -167.772| -17.575    |
| 4            | 3.51        | -1.18 | -87.542 | -44.06    | -169.457| -20.404    |
| 5            | 2.8         | -2.1  | -101.124| -46.507   | -209.161| -21.027    |
| 6            | 3.26        | -2.44 | -120.022| -58.321   | -251.997| -18.985    |
| 7            | 2.63        | -0.67 | -79.73  | -42.222   | -161.64 | -16.998    |
| 8            | 1.66        | -1.07 | -79.731 | -36.845   | -111.582| -20.181    |
| 9            | 3.21        | -1.26 | -86.354 | -33.603   | -161.909| -16.822    |
| 10           | 3.11        | -1.62 | -97.64  | -37.904   | -210.336| -20.227    |
| 11           | 4.16        | -1.38 | -96.107 | -51.894   | -194.589| -15.782    |
| 12           | 3.69        | -2.08 | -103.423| -62.16    | -222.057| -16.242    |
| 13           | 4.35        | -1.95 | -103.306| -58.944   | -211.189| -14.623    |
| 14           | 3.94        | -1.41 | -96.857 | -43.467   | -198.025| -12.939    |
| 15           | 3.04        | -1.26 | -81.698 | -40.866   | -178.101| -11.344    |
| 16           | 3.96        | -1.12 | -92.128 | -49.257   | -202.407| -14.046    |
| 17           | 2.77        | -0.88 | -77.205 | -43.882   | -160.972| -16.714    |
| 18           | 2.99        | -1.18 | -83.386 | -32.969   | -150.993| -14.744    |
| 19           | 3.45        | -1.5  | -100.604| -49.717   | -179.573| -20.229    |
| 20           | 2.33        | -1.35 | -90.196 | -45.506   | -174.371| -16.632    |
| 21           | 1.63        | -0.76 | -73.083 | -41.787   | -144.782| -16.502    |
| 22           | 2.6         | -1.1  | -90.244 | -35.359   | -175.682| -21.791    |
| 23           | 2.97        | -0.92 | -87.896 | -62.003   | -162.12 | -28.166    |
| 24           | 3.1         | -1.02 | -89.107 | -59.208   | -153.547| -14.248    |
| 25           | 2.72        | -1.25 | -83.762 | -43.364   | -171.507| -5.438     |
| 26           | 2.86        | -0.88 | -84.902 | -48.705   | -176.279| -8.387     |
| 27           | 3.9         | -2.02 | -101.804| -53.741   | -200.029| -10.295    |
Table S3. The principle components of matrix 1.

| Compound NO. | PC1  | PC2  | PC3  | PC4  | PC5  | PC6  | PC7  | PC8  |
|--------------|------|------|------|------|------|------|------|------|
| 1            | -24.64 | -6.07 | 7.96 | -0.17 | -9.43 | -3.20 | -0.85 | 0.56 |
| 2            | 25.20 | -4.65 | -2.59 | -3.17 | -2.96 | 0.36 | -0.42 | 2.00 |
| 3            | 1.71 | 3.97 | 2.22 | 2.55 | 1.45 | -2.59 | 2.52 | 0.74 |
| 4            | -1.73 | 6.54 | 0.54 | 0.96 | 0.32 | 0.00 | 1.40 | -0.28 |
| 5            | 1.95 | 4.19 | 2.54 | 1.89 | 1.72 | -2.99 | 2.08 | 0.84 |
| 6            | 14.85 | -7.31 | 7.50 | -0.91 | -5.66 | 3.22 | -0.25 | -0.54 |
| 7            | -7.95 | 7.12 | -0.84 | -5.48 | 0.14 | 0.67 | -0.86 | 0.96 |
| 8            | 7.06 | 6.50 | -3.23 | -2.59 | -2.15 | 0.27 | -0.16 | 0.34 |
| 9            | -0.07 | 5.58 | 1.72 | 0.95 | 1.15 | -1.62 | 1.13 | -0.80 |
| 10           | 8.90 | 4.96 | -2.25 | -1.28 | -1.27 | -1.52 | 0.05 | 0.28 |
| 11           | 4.87 | -9.09 | -6.15 | -2.97 | -0.68 | -3.94 | -0.97 | -1.19 |
| 12           | -0.15 | -10.08 | 0.29 | -2.49 | 2.93 | -2.96 | 0.08 | -2.05 |
| 13           | -0.05 | -8.88 | 0.53 | -2.10 | 2.77 | -0.80 | -0.24 | -0.47 |
| 14           | 10.17 | -4.24 | 7.85 | -0.29 | 2.08 | 5.57 | 2.06 | -0.46 |
| 15           | -12.84 | -4.75 | 3.83 | -3.23 | 6.86 | 2.88 | -0.83 | 3.77 |
| 16           | -4.70 | -6.58 | -0.19 | -1.88 | 3.74 | 0.10 | 0.77 | -4.90 |
| 17           | -3.65 | 7.38 | -0.73 | 0.36 | -0.49 | 1.66 | 0.68 | -0.36 |
| 18           | -2.03 | 6.31 | 0.17 | 1.64 | 0.11 | 0.36 | 1.50 | -0.66 |
| 19           | 3.62 | 2.69 | 2.95 | 3.24 | 1.80 | -4.04 | 2.57 | 0.86 |
| 20           | 7.36 | 5.28 | 4.70 | 6.75 | 3.04 | -1.03 | -8.38 | -0.75 |
| 21           | -11.36 | 9.87 | -2.70 | -5.61 | -1.45 | 3.26 | -1.42 | -2.07 |
| 22           | 9.13 | 5.20 | -2.28 | -1.96 | -1.79 | -1.10 | -0.69 | 0.66 |
| 23           | -3.43 | 7.62 | -0.54 | 0.55 | -0.47 | 1.47 | 0.58 | -0.58 |
| 24           | -7.31 | -5.35 | -4.01 | -2.90 | 1.99 | -0.89 | -1.37 | 3.33 |
| 25           | -6.73 | -4.02 | -6.52 | 4.68 | -1.53 | 2.17 | -0.79 | -0.50 |
| 26           | -4.91 | -5.41 | -5.71 | 6.47 | -1.25 | 2.86 | 0.82 | 0.25 |
| 27           | -3.25 | -6.77 | -5.05 | 6.99 | -0.95 | 1.86 | 0.99 | 1.01 |
Table S4. The principle components of matrix 2.

| Compo und NO. | PC1  | PC2  | PC3  | PC4  | PC5  | PC6  | PC7  | PC8  | PC9  |
|---------------|------|------|------|------|------|------|------|------|------|
| 1             | -24.75 | -5.42 | -6.61 | 3.92 | -9.83 | -2.62 | -1.35 | 1.75 | -1.13 |
| 2             | 24.77  | -4.01 | 3.97  | 2.55 | -2.91 | 1.61  | -1.35 | 4.93 | -1.93 |
| 3             | 1.62   | 3.65  | -3.50 | -2.46 | 1.02  | -2.37 | 1.96  | 1.71 | -0.20 |
| 4             | -1.81  | 6.35  | -1.60 | -1.35 | 0.43  | -0.26 | 1.63  | -0.36 | 0.08  |
| 5             | 2.02   | 3.56  | -3.92 | -1.75 | 1.55  | -3.27 | 1.93  | 0.71 | 0.70  |
| 6             | 14.93  | -8.11 | -6.44 | 3.83  | -5.38 | 2.51  | 0.78  | -3.55 | 3.06  |
| 7             | -8.12  | 7.63  | 1.46  | 3.98  | 1.04  | 1.40  | -0.47 | 1.36 | -0.29 |
| 8             | 6.76   | 7.20  | 3.34  | 1.10  | -1.86 | 0.78  | 0.00  | 0.92 | 0.43  |
| 9             | -0.23  | 5.42  | -2.75 | -1.21 | 1.04  | -1.41 | 1.03  | 0.51 | -1.25 |
| 10            | 8.79   | 4.91  | 1.80  | 0.22  | -0.77 | -1.71 | 0.62  | -0.85 | 1.28  |
| 11            | 4.58   | -8.65 | 7.05  | 1.59  | -0.11 | -3.87 | -0.89 | -0.28 | -0.68 |
| 12            | -0.18  | -10.17 | 0.68  | 2.77  | 3.20  | -3.35 | -0.03 | -1.80 | -0.49 |
| 13            | -0.14  | -9.13 | 0.19  | 2.19  | 3.09  | -1.12 | 0.02  | -1.25 | 0.74  |
| 14            | 10.02  | -4.88 | -7.34 | 2.00  | 1.91  | 5.64  | 2.08  | 0.27 | -2.09 |
| 15            | -12.98 | -4.63 | -3.07 | 3.17  | 6.86  | 3.43  | -1.16 | 2.55 | 2.78  |
| 16            | -4.90  | -6.53 | 0.74  | 1.58  | 3.89  | -0.13 | 0.75  | -2.30 | -4.57 |
| 17            | -3.81  | 7.36  | -0.14 | -1.25 | -0.28 | 1.65  | 0.94  | -0.32 | 0.31  |
| 18            | -2.24  | 6.25  | -1.37 | -2.24 | -0.01 | 0.49  | 1.60  | -0.04 | -0.70 |
| 19            | 3.60   | 2.08  | -4.30 | -2.65 | 1.37  | -4.22 | 2.02  | 1.00 | 0.52  |
| 20            | 7.25   | 4.52  | -6.66 | -5.70 | 1.69  | -0.47 | -8.71 | -1.57 | -0.54 |
| 21            | -11.55 | 10.66 | 3.29  | 3.76  | -0.47 | 3.62  | -0.52 | -1.97 | -0.56 |
| 22            | 8.93   | 5.55  | 2.19  | 0.85  | -1.41 | -0.82 | -0.33 | 0.25 | 0.90  |
| 23            | 0.68   | 8.15  | 6.09  | 5.33  | -0.70 | -1.17 | -0.51 | -2.98 | 0.31  |
| 24            | -7.52  | -4.94 | 4.70  | 1.46  | 2.32  | -0.48 | -1.66 | 2.55 | 2.67  |
| 25            | -7.06  | -4.01 | 5.08  | -6.40 | -2.05 | 2.34  | -0.55 | -0.15 | -0.88 |
| 26            | -5.24  | -5.45 | 4.05  | -7.55 | -2.01 | 2.77  | 0.81  | 0.03 | -0.18 |
| 27            | -3.40  | -7.36 | 3.07  | -7.74 | -1.60 | 1.03  | 1.38  | -1.10 | 1.71  |