Electronic Supplementary Information

Molecular basis of rutin inhibition of protein disulfide isomerase (PDI)
by combined \textit{in silico} and experimental methods

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Supplementary Methods

1. The purity of small-molecule chemicals was analysed by HPLC (Fig. S1). We used Welch Xtrimade C18 chromatographic column (size: 150 mm X 4.6 mm) for analysis.

|               | Concentration (µM) | Mobile phase      | Detection wavelength (nm) | Injection volume (µL) | Flow rate (ml/min) | Column pressure (MPa) |
|---------------|--------------------|-------------------|---------------------------|-----------------------|--------------------|-----------------------|
| Rutin         | 200                | CH₃OH :H₂O(1% HOAc) = 32:68 | 257                       | 20                    | 1                  | 13                    |
| Kaempferitrin | 500                | CH₃CN :H₂O(0.3%H₃PO₄) = 30:70 | 345                       | 20                    | 1                  | 10                    |
| Tiliroside    | 700                | CH₃CN :H₂O(0.04%H₃PO₄) = 15:85 | 254                       | 20                    | 1                  | 13                    |
| 2'-O-galloylhyperin | 330 | CH₃CN :H₂O(0.2%H₃PO₄) = 19:81 | 258                       | 20                    | 1                  | 12                    |

2. Binding affinity (IC₅₀) of rutin to human or murine MBP-fused PDI proteins

The MBP-fused PDI proteins (18 µM) were incubated with a gradient of 10 rutin’s concentrations differed by 2- or 3-fold and 3 repetitions in 384-well black plate at room temperature for 30 min before measurements. The total assay volume was filled to 100 µL using the assay buffer (pH 7.4) contains 150 mM NaCl, 20 mM Tris, 1 mM EDTA, 1 mM β-ME and 5% glycerin. The fluorescence emission spectrum of the mixture were measured with the excitation at 430 nm and the emission at 530 nm at room temperature on a BioTek Synergy microplate reader with a sensitivity of 100. The data were analyzed by GraphPad Prism (Fig. S3).
Supplementary Figures

Fig. S1 Purity analysis by HPLC of small-molecule chemicals used in the experimental assays. The purity of rutin, kaempferitrin, tiliroside and 2’-O-galloylhyperin were 98.75%, 94.84%, 86.02% and 96.23%, respectively.

A. Rutin (98.75%)

| Number | Retention time (Min) | Height (mV) | Area (mv. sec) | Percentage (%) |
|--------|----------------------|-------------|----------------|----------------|
| 1      | 2.07                 | 7.54        | 51.81          | 1.2464         |
| 2      | 12.28                | 120.59      | 4104.57        | 98.7536        |
B. Kaempferitrin (94.84%)  

| Number | Retention time (Min) | Height (mV) | Area (mv. sec) | Percentage (%) |
|--------|-----------------------|-------------|----------------|----------------|
| 1      | 1.93                  | 27.25       | 165.60         | 2.1367         |
| 2      | 2.01                  | 27.60       | 112.03         | 1.4455         |
| 3      | 2.39                  | 17.50       | 122.28         | 1.5778         |
| 4      | 2.89                  | 587.15      | 7350.46        | 94.8400        |
C. Tiliroside (86.02%)

| Number | Retention time (Min) | Height (mV) | Area (mv. sec) | Percentage (%) |
|--------|----------------------|-------------|----------------|----------------|
| 1      | 1.94                 | 54.35       | 417.73         | 3.3970         |
| 2      | 2.04                 | 80.41       | 493.16         | 4.0103         |
| 3      | 2.12                 | 67.40       | 299.97         | 2.4393         |
| 4      | 2.20                 | 51.89       | 508.59         | 4.1359         |
| 5      | 3.40                 | 839.19      | 10577.70       | 86.0175        |
D. 2’-O-galloylhyperin (96.23%)

| Number | Retention time (Min) | Height (mV) | Area (mv. sec) | Percentage (%) |
|--------|----------------------|-------------|----------------|----------------|
| 1      | 2.06                 | 29.02       | 107.94         | 1.8549         |
| 2      | 2.12                 | 19.04       | 92.25          | 1.5853         |
| 3      | 2.34                 | 11.22       | 19.22          | 0.3303         |
| 4      | 7.78                 | 289.38      | 5599.72        | 96.2295        |

![Graph showing retention time and peak area for 2’-O-galloylhyperin]
Fig. S2. Root-mean-square deviation (RMSD) of backbone atoms of PDI (red) and heavy atoms of rutin relative to the initial structures as a function of MD simulation time.
Fig. S3. Fluorescence assay on the interactions between rutin and human or murine MBP-fused PDI proteins. All these proteins have similar binding affinity to rutin. A-E: IC$_{50}$ values for the full-length human PDI and MBP-fused PDI proteins binding to rutin were: (A) full-length human PDI, 31.1 μM; (B) human MBP-PDI-b’x, 18.7 μM; (C) human MBP-PDI-b’xa’, 28.8 μM; (D) murine MBP-mPDI-b’x, 15.7 μM; (E) murine MBP-mPDI-b’xa’, 26.3 μM. Error bars indicate ±S.E, n=3. Standard Error: (A) the full-length human PDI, 0.18 μM; (B) human MBP-PDI-b’x, 0.16 μM; (C) the human MBP-PDI-b’xa’, 0.14 μM; (D) the murine MBP-mPDI-b’x, 0.15 μM; (E) the murine MBP-mPDI-b’xa’, 0.15 μM.
Fig. S4. Rutin does not bind to MBP as shown by fluorescence measurements of rutin in the presence of three different MBP-fusion proteins. The MBP-fusion proteins (MBP-PNGase protein (gray dash-dot line), MBP-SpoIVB protein (gray dash line) and MBP-MOC1 protein (gray dot line) at 18 μM did not have fluorescence compared to the assay buffer with excitation at 430 nm. Addition of rutin (55 μM) to these proteins (MBP-PNGase in black solid line, MBP-SpoIVB in black dash line and MBP-MOC1 in black dot line) gave the signals almost identical to rutin itself (gray solid), which has a maximum fluorescence at 550 nm.
**Fig. S5. The reduced SDS-PAGE analysis of the purified MBP-PDI-b’xa’ mutants.** The molecular weight of K328E, H354A, L355R, E359A and E359K are 71.8 kDa, 71.7 kDa, 71.9 kDa, 71.8 kDa and 71.8 kDa, respectively.
Fig. S6. Isothermal titration calorimetry (ITC) measurements of the binding affinity between the mutants of wt MBP-PDI-b’xa’ and rutin. The interactions of the mutants of wt MBP-PDI-b’xa’ to rutin was measured by ITC method. (A) K328E; (B) H354A; (C) L355R; (D) E359A; (E) E359K.
Fig. S7. Insulin reductase assay has good reproducibility as shown by three independent experiments of rutin (100 μM) inhibition on the insulin reduction catalyzed by MBP-PDI-b’xa’-H354A mutant.
Fig. S8. Small molecular inhibitors did not perturb insulin reduction assay. 100 μM of rutin (A), kaempferitrin (B), tiliroside (C) and 2'-O-galloylhyperin (D) were added into the assay solution in the absence of any PDI or its fragments.
Fig. S9. Rutin binding to PDI (MBP-PDI-b’xa’) is sensitive to GSSH/DTT ratio, but not to the mutation of H354A as shown by fluorescence-based binding assay at reducing (1 mM DTT) or oxidative (5 mM GSSG) condition.
Fig. S10. The center-of-mass (COM) distance between a and a’ domains as a function of MD simulation time. The corresponding distances in the crystal structures of PDI in the oxidized (PDB ID: 4EL1) and reduced states (PDB ID: 4EKZ)\textsuperscript{1} were displayed by red and blue dashed lines.

References
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Supplementary Tables

Table S1. Hydrogen bond interactions between rutin and PDI.

| Rutin      | PDI           | Distance (Å)\(^a\) | Occupancy (%)\(^b\) |
|------------|---------------|---------------------|---------------------|
| O@7-OH     | O@E303        | 3.2 ± 0.5           | 89.6                |
| O@4’-OH    | O@E359        | 3.4 ± 0.7           | 74.0                |
| O@5’-OH    | O@E359        | 3.4 ± 0.5           | 77.2                |
| O@4-ketone | N@H354        | 2.9 ± 0.3           | 98.8                |
| O@2-OH     | O@L355        | 2.7 ± 0.1           | 99.8                |
| O@1-ether  | N@K328        | 4.1 ± 1.1           | 40.0                |
| O@3-OH     | O@K352        | 3.8 ± 0.8           | 44.8                |
| O@4-OH     | O@E330        | 7.2 ± 2.8           | 1.6                 |
| O@5-OH     | O@E330        | 6.8 ± 1.4           | 2.8                 |

\(^a\) Average atomic distances between hydrogen bond donor and acceptor calculated on the equilibrium trajectory of MD simulations.

\(^b\) Occupancy of the formation of hydrogen bonds across the equilibrium trajectory of MD simulations.
Table S2. Chemical properties of rutin and isoquercetin.

Terms listed in the table (from left to right): partition coefficient (logP) predicted by Molinspiration (http://www.molinspiration.com/) (logPm) and ALOGPS2.1 (logPa), \(^a\) aqueous solubility (AS) in g/L predicted by ALOGPS2.1, \(^b\) drug-like score (Score) predicted by OSIRIS \(^2\) and molecular weight (MW) in Da.

|           | logPm\(^a\) | logPa\(^a\) | AS\(^b\) | Score\(^c\) | MW       |
|-----------|-------------|-------------|----------|------------|----------|
| Rutin     | -1.06       | -0.14       | 0.16     | 1.93       | 610.52   |
| Isoquercetin | -0.36       | 0.02        | 0.14     | 1.66       | 464.38   |

\(^a\) The value of logP is defined as the logarithm of the ratio of the concentrations of compound between octanol and water. It is a measurement of the lipophilicity of compounds and is used for drug absorption prediction. From the magnitude of the logP of a compound, one can infer its ease of transport through the cell membrane. According to the rule of 5 by Lipinski, \(^3\) compounds with logP greater than 5 are more likely a poor absorption or permeation.

\(^b\) AS governs both the rate of dissolution of the compound and the maximum concentration of compound reached in the gastrointestinal fluid. \(^4\)

\(^c\) The drug-like score predicted by OSIRIS\(^2\) is calculated with the summation of score values of substructure fragments that are present in the compound under investigation. The distributions of drug-like score values calculated from 15000 commercially available chemicals and 3300 traded drugs show that about 80% of the drugs have a positive drug-like score values while the big majority of chemicals accounts for the negative values. \(^2\)

References
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2. T. Sander, J. Freyss, M. von Korff, J. R. Reich and C. Rufener, *J. Chem. Inf. Model.*, 2009, 49, 232-246.
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## Supplementary Data

1. Raw experimental data of Fig. 2

1) Fig. 2A:

| Wavelength | buffer | PDI  | rutin | PDI+rutin |
|------------|--------|------|-------|-----------|
| 460        | 105    | 139  | 91    | 134       |
| 462        | 113    | 154  | 99    | 144       |
| 464        | 108    | 158  | 99    | 171       |
| 466        | 119    | 171  | 111   | 189       |
| 468        | 123    | 163  | 126   | 183       |
| 470        | 121    | 178  | 136   | 212       |
| 472        | 137    | 182  | 132   | 251       |
| 474        | 151    | 187  | 152   | 264       |
| 476        | 149    | 201  | 166   | 285       |
| 478        | 164    | 204  | 158   | 324       |
| 480        | 160    | 190  | 176   | 342       |
| 482        | 163    | 202  | 186   | 400       |
| 484        | 189    | 229  | 221   | 411       |
| 486        | 180    | 245  | 225   | 454       |
| 488        | 182    | 230  | 251   | 509       |
| 490        | 207    | 239  | 253   | 534       |
| 492        | 225    | 240  | 278   | 596       |
| 494        | 226    | 258  | 305   | 610       |
| 496        | 237    | 272  | 338   | 679       |
| 498        | 238    | 271  | 345   | 716       |
| 500        | 260    | 283  | 351   | 751       |
| 502        | 268    | 294  | 370   | 789       |
| 504        | 243    | 309  | 411   | 867       |
| 506        | 249    | 306  | 435   | 875       |
| 508        | 262    | 297  | 425   | 915       |
| 510        | 256    | 298  | 417   | 952       |
| 512        | 237    | 295  | 467   | 988       |
| 514        | 237    | 289  | 460   | 996       |
| 516        | 230    | 294  | 470   | 1001      |
| 518        | 224    | 291  | 484   | 1014      |
| 520        | 206    | 280  | 492   | 1041      |
| 522        | 227    | 276  | 513   | 1086      |
| 524        | 237    | 289  | 517   | 1071      |
| 526        | 208    | 276  | 507   | 1084      |
| 528        | 196    | 268  | 553   | 1050      |
|   |   |   |   |   |
|---|---|---|---|---|
| 530 | 193 | 268 | 545 | 1075 |
| 532 | 194 | 272 | 550 | 1079 |
| 534 | 213 | 251 | 555 | 1043 |
| 536 | 196 | 246 | 550 | 1092 |
| 538 | 182 | 258 | 564 | 1107 |
| 540 | 201 | 261 | 570 | 1059 |
| 542 | 198 | 243 | 583 | 1060 |
| 544 | 182 | 253 | 580 | 1049 |
| 546 | 200 | 240 | 596 | 994  |
| 548 | 188 | 256 | 563 | 988  |
| 550 | 164 | 245 | 562 | 946  |
| 552 | 167 | 240 | 561 | 922  |
| 554 | 179 | 228 | 549 | 905  |
| 556 | 155 | 224 | 535 | 908  |
| 558 | 168 | 231 | 548 | 877  |
| 560 | 161 | 228 | 558 | 849  |
| 562 | 175 | 225 | 529 | 853  |
| 564 | 158 | 214 | 525 | 835  |
| 566 | 165 | 204 | 516 | 828  |
| 568 | 149 | 213 | 507 | 783  |
| 570 | 158 | 203 | 493 | 725  |
| 572 | 140 | 197 | 492 | 703  |
| 574 | 138 | 184 | 476 | 715  |
| 576 | 154 | 176 | 448 | 682  |
| 578 | 130 | 174 | 468 | 666  |
| 580 | 135 | 157 | 457 | 637  |
| 582 | 133 | 180 | 428 | 618  |
| 584 | 124 | 172 | 405 | 552  |
| 586 | 117 | 175 | 413 | 561  |
| 588 | 115 | 174 | 406 | 535  |
| 590 | 117 | 163 | 382 | 529  |
| 592 | 110 | 156 | 360 | 497  |
| 594 | 117 | 152 | 372 | 493  |
| 596 | 123 | 145 | 356 | 462  |
| 598 | 112 | 116 | 360 | 488  |
| 600 | 97  | 124 | 351 | 458  |
| 602 | 89  | 131 | 340 | 420  |
| 604 | 101 | 139 | 327 | 410  |
| 606 | 105 | 122 | 319 | 398  |
| 608 | 111 | 100 | 309 | 399  |
| 610 | 87  | 121 | 330 | 402  |
| Wavelength | MBP-PDI-b'x+ rutin | MBP-PDI-b'xa'+ rutin | rutin | buffer | MBP-PDI-b'xa' | MBP-PDI-b'x |
|------------|---------------------|----------------------|-------|--------|----------------|---------------|
| 460        | 256                 | 226                  | 91    | 108    | 158            | 171           |
| 470        | 345                 | 323                  | 136   | 151    | 187            | 201           |
| 480        | 487                 | 474                  | 176   | 189    | 229            | 245           |
| 490        | 684                 | 710                  | 253   | 226    | 258            | 272           |
| 500        | 946                 | 983                  | 351   | 243    | 309            | 306           |
| 510        | 1103                | 1194                 | 417   | 230    | 294            | 294           |
| 520        | 1196                | 1288                 | 492   | 237    | 289            | 276           |
| 530        | 1233                | 1350                 | 545   | 213    | 251            | 246           |
| 540        | 1201                | 1325                 | 570   | 182    | 253            | 240           |
| 550        | 1122                | 1213                 | 562   | 179    | 228            | 224           |
| 560        | 1008                | 1093                 | 558   | 158    | 214            | 214           |
| 570        | 889                 | 947                  | 493   | 138    | 184            | 176           |
| 580        | 776                 | 824                  | 457   | 124    | 172            | 175           |
| 590        | 666                 | 679                  | 382   | 117    | 152            | 145           |
| 600        | 549                 | 570                  | 351   | 101    | 139            | 122           |
### 3) Fig. 2C

| Wavelength | MBP-mPDI-b'xa +rutin | MBP-mPDI-b'x +rutin | rutin buffer | MBP-mPDI-b'xa' | MBP-mPDI-b'x |
|------------|----------------------|----------------------|-------------|----------------|----------------|
| 460        | 207                  | 218                  | 91          | 113            | 154            | 119            |
| 470        | 266                  | 294                  | 136         | 137            | 182            | 149            |
| 480        | 346                  | 368                  | 176         | 163            | 202            | 180            |
| 490        | 464                  | 471                  | 253         | 225            | 240            | 237            |
| 500        | 646                  | 631                  | 351         | 268            | 294            | 249            |
| 510        | 763                  | 744                  | 417         | 237            | 295            | 230            |
| 520        | 824                  | 785                  | 492         | 227            | 276            | 208            |
| 530        | 851                  | 818                  | 545         | 194            | 272            | 196            |
| 540        | 865                  | 811                  | 570         | 198            | 243            | 200            |
| 550        | 810                  | 773                  | 562         | 167            | 240            | 155            |
| 560        | 731                  | 708                  | 558         | 175            | 225            | 165            |
| 570        | 670                  | 638                  | 493         | 140            | 197            | 154            |
| 580        | 573                  | 556                  | 457         | 133            | 180            | 117            |
| 590        | 494                  | 471                  | 382         | 110            | 156            | 123            |
| 600        | 409                  | 401                  | 351         | 89             | 131            | 105            |
| 610        | 361                  | 370                  | 330         | 102            | 124            | 93             |
| 620        | 304                  | 302                  | 267         | 65             | 99             | 72             |
| 630        | 254                  | 257                  | 218         | 64             | 76             | 51             |
| 640        | 221                  | 219                  | 191         | 76             | 85             | 58             |
| 650        | 184                  | 212                  | 167         | 68             | 83             | 56             |
| 660        | 180                  | 155                  | 160         | 65             | 80             | 53             |
| 670        | 133                  | 142                  | 154         | 50             | 76             | 52             |
| 680        | 134                  | 144                  | 148         | 48             | 72             | 48             |
| 690        | 124                  | 95                   | 142         | 50             | 70             | 44             |
| 700        | 89                   | 86                   | 136         | 45             | 66             | 40             |
4) Fig. 2D

| Wavelength | rutin | MBP-PDI-b'xa'+rutin | K328E | H354A |
|------------|-------|----------------------|-------|-------|
| 460        | 91    | 226                  | 219   | 220   |
| 470        | 136   | 323                  | 359   | 366   |
| 480        | 176   | 474                  | 449   | 461   |
| 490        | 253   | 710                  | 705   | 717   |
| 500        | 351   | 983                  | 900   | 926   |
| 510        | 417   | 1194                 | 1038  | 1064  |
| 520        | 492   | 1288                 | 1126  | 1137  |
| 530        | 545   | 1350                 | 1139  | 1173  |
| 540        | 570   | 1325                 | 1151  | 1184  |
| 550        | 562   | 1213                 | 1065  | 1098  |
| 560        | 558   | 1093                 | 996   | 1041  |
| 570        | 493   | 947                  | 890   | 924   |
| 580        | 457   | 824                  | 815   | 841   |
| 590        | 382   | 679                  | 624   | 653   |
| 600        | 351   | 570                  | 548   | 584   |
| 610        | 330   | 489                  | 409   | 434   |
| 620        | 267   | 402                  | 390   | 391   |
| 630        | 218   | 347                  | 347   | 324   |
| 640        | 191   | 294                  | 275   | 293   |
| 650        | 167   | 250                  | 243   | 268   |
| 660        | 160   | 207                  | 186   | 190   |
| 670        | 154   | 196                  | 175   | 170   |
| 680        | 148   | 187                  | 168   | 152   |
| 690        | 142   | 120                  | 105   | 95    |
| 700        | 136   | 153                  | 90    | 96    |

2. Raw data of Fig. 3

| Kinetic read | MBP-P DI | MBP-m PDI | MBP-P DI | MBP-m PDI | MBP-P DI | MBP-m PDI | MBP-P DI | MBP-m PDI |
|--------------|----------|-----------|----------|-----------|----------|-----------|----------|-----------|
|              | -b'x     | -b'x      | -b'xa'   | -b'xa'    | +rutin   | +rutin    | +rutin   | +rutin    |
| 0:00:32      | 0.041    | 0.043     | 0.042    | 0.042     | 0.042    | 0.041     | 0.047    | 0.042     |
| 0:01:32      | 0.042    | 0.044     | 0.042    | 0.043     | 0.043    | 0.043     | 0.047    | 0.042     |
| Time  | Pollen Count 1 | Pollen Count 2 | Pollen Count 3 | Pollen Count 4 | Pollen Count 5 | Pollen Count 6 | Pollen Count 7 | Pollen Count 8 |
|-------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| 0:02:32 | 0.042          | 0.044          | 0.042          | 0.043          | 0.042          | 0.043          | 0.048          | 0.042          |
| 0:03:32 | 0.043          | 0.046          | 0.042          | 0.043          | 0.043          | 0.046          | 0.048          | 0.043          |
| 0:04:32 | 0.042          | 0.045          | 0.042          | 0.044          | 0.043          | 0.045          | 0.048          | 0.043          |
| 0:05:32 | 0.042          | 0.045          | 0.043          | 0.044          | 0.044          | 0.044          | 0.048          | 0.043          |
| 0:06:32 | 0.042          | 0.046          | 0.043          | 0.044          | 0.044          | 0.044          | 0.049          | 0.044          |
| 0:07:32 | 0.042          | 0.046          | 0.043          | 0.048          | 0.043          | 0.044          | 0.048          | 0.044          |
| 0:08:32 | 0.042          | 0.046          | 0.043          | 0.044          | 0.043          | 0.044          | 0.048          | 0.044          |
| 0:09:32 | 0.042          | 0.046          | 0.046          | 0.045          | 0.043          | 0.044          | 0.048          | 0.043          |
| 0:10:32 | 0.042          | 0.045          | 0.053          | 0.048          | 0.043          | 0.045          | 0.049          | 0.043          |
| 0:11:32 | 0.043          | 0.046          | 0.062          | 0.056          | 0.043          | 0.045          | 0.048          | 0.043          |
| 0:12:32 | 0.042          | 0.045          | 0.073          | 0.067          | 0.043          | 0.045          | 0.048          | 0.043          |
| 0:13:32 | 0.042          | 0.046          | 0.085          | 0.08           | 0.043          | 0.045          | 0.048          | 0.043          |
| 0:14:32 | 0.042          | 0.045          | 0.098          | 0.095          | 0.043          | 0.045          | 0.049          | 0.043          |
| 0:15:32 | 0.042          | 0.046          | 0.112          | 0.11           | 0.043          | 0.045          | 0.049          | 0.043          |
| 0:16:32 | 0.042          | 0.045          | 0.125          | 0.125          | 0.042          | 0.045          | 0.049          | 0.043          |
| 0:17:32 | 0.042          | 0.047          | 0.138          | 0.14           | 0.042          | 0.045          | 0.048          | 0.043          |
| 0:18:32 | 0.042          | 0.046          | 0.153          | 0.156          | 0.042          | 0.045          | 0.049          | 0.043          |
| 0:19:32 | 0.042          | 0.045          | 0.167          | 0.17           | 0.042          | 0.044          | 0.049          | 0.044          |
| 0:20:32 | 0.042          | 0.045          | 0.182          | 0.186          | 0.042          | 0.045          | 0.049          | 0.044          |
| 0:21:32 | 0.042          | 0.045          | 0.197          | 0.2            | 0.042          | 0.044          | 0.051          | 0.046          |
| 0:22:32 | 0.042          | 0.045          | 0.21           | 0.216          | 0.042          | 0.044          | 0.055          | 0.05           |
| Time   | X1   | Y1   | X2   | Y2   | X3   | Y3   | X4   | Y4   |
|--------|------|------|------|------|------|------|------|------|
| 0:43:32| 0.104| 0.114| 0.462| 0.479| 0.117| 0.115| 0.242| 0.244|
| 0:44:32| 0.112| 0.121| 0.472| 0.486| 0.126| 0.122| 0.252| 0.254|
| 0:45:32| 0.12 | 0.13 | 0.479| 0.492| 0.135| 0.132| 0.262| 0.263|
| 0:46:32| 0.128| 0.138| 0.491| 0.502| 0.144| 0.139| 0.272| 0.274|
| 0:47:32| 0.136| 0.147| 0.497| 0.512| 0.153| 0.148| 0.281| 0.282|
| 0:48:32| 0.144| 0.155| 0.516| 0.524| 0.161| 0.157| 0.288| 0.288|
| 0:49:32| 0.152| 0.163| 0.525| 0.532| 0.171| 0.165| 0.299| 0.297|
| 0:50:32| 0.161| 0.173| 0.535| 0.54  | 0.179| 0.173| 0.307| 0.305|
| 0:51:32| 0.17 | 0.182| 0.537| 0.548| 0.187| 0.182| 0.319| 0.316|
| 0:52:32| 0.179| 0.19 | 0.546| 0.556| 0.196| 0.191| 0.324| 0.319|
| 0:53:32| 0.187| 0.2  | 0.562| 0.566| 0.206| 0.2  | 0.33 | 0.328|
| 0:54:32| 0.196| 0.208| 0.57 | 0.565| 0.216| 0.208| 0.336| 0.337|
| 0:55:32| 0.205| 0.217| 0.579| 0.582| 0.226| 0.219| 0.345| 0.343|
| 0:56:32| 0.215| 0.228| 0.58 | 0.599| 0.234| 0.226| 0.355| 0.35 |
| 0:57:32| 0.223| 0.237| 0.6  | 0.606| 0.243| 0.235| 0.361| 0.357|
| 0:58:32| 0.233| 0.245| 0.602| 0.606| 0.252| 0.244| 0.371| 0.365|
| 0:59:32| 0.241| 0.254| 0.609| 0.614| 0.261| 0.252| 0.378| 0.373|
| 1:00:32| 0.25 | 0.262| 0.619| 0.623| 0.271| 0.261| 0.387| 0.376|
| 1:01:32| 0.256| 0.271| 0.619| 0.634| 0.279| 0.269| 0.396| 0.384|
| 1:02:32| 0.264| 0.28 | 0.629| 0.634| 0.288| 0.277| 0.403| 0.387|
| 1:03:32| 0.274| 0.288| 0.632| 0.639| 0.296| 0.285| 0.409| 0.396|
| Time  | Day  | 1:04:32 | 1:05:32 | 1:06:32 | 1:07:32 | 1:08:32 | 1:09:32 | 1:10:32 | 1:11:32 | 1:12:32 | 1:13:32 | 1:14:32 | 1:15:32 | 1:16:32 | 1:17:32 | 1:18:32 | 1:19:32 | 1:20:32 | 1:21:32 | 1:22:32 | 1:23:32 |
|-------|------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
|       | 32   | 0.286   | 0.297   | 0.645   | 0.649   | 0.306   | 0.293   | 0.413   | 0.402   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.297   | 0.304   | 0.643   | 0.656   | 0.312   | 0.301   | 0.424   | 0.411   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.304   | 0.313   | 0.654   | 0.663   | 0.321   | 0.309   | 0.43    | 0.418   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.312   | 0.32    | 0.662   | 0.672   | 0.329   | 0.316   | 0.433   | 0.422   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.322   | 0.329   | 0.666   | 0.677   | 0.34    | 0.325   | 0.44    | 0.426   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.331   | 0.336   | 0.669   | 0.684   | 0.349   | 0.333   | 0.446   | 0.438   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.337   | 0.344   | 0.683   | 0.692   | 0.358   | 0.344   | 0.457   | 0.44    |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.344   | 0.354   | 0.675   | 0.693   | 0.368   | 0.346   | 0.463   | 0.45    |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.35    | 0.36    | 0.691   | 0.707   | 0.377   | 0.353   | 0.466   | 0.451   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.36    | 0.368   | 0.698   | 0.707   | 0.383   | 0.359   | 0.469   | 0.456   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.364   | 0.373   | 0.7     | 0.716   | 0.39    | 0.365   | 0.475   | 0.462   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.373   | 0.382   | 0.71    | 0.716   | 0.398   | 0.373   | 0.48    | 0.466   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.38    | 0.389   | 0.715   | 0.722   | 0.407   | 0.38    | 0.484   | 0.474   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.388   | 0.396   | 0.72    | 0.729   | 0.411   | 0.386   | 0.495   | 0.479   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.391   | 0.402   | 0.722   | 0.741   | 0.421   | 0.393   | 0.495   | 0.486   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.404   | 0.409   | 0.727   | 0.746   | 0.425   | 0.399   | 0.502   | 0.491   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.406   | 0.416   | 0.746   | 0.746   | 0.433   | 0.405   | 0.502   | 0.494   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.419   | 0.421   | 0.734   | 0.745   | 0.438   | 0.413   | 0.519   | 0.496   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.423   | 0.429   | 0.741   | 0.756   | 0.445   | 0.418   | 0.513   | 0.502   |         |         |         |         |         |         |         |         |         |         |         |         |
|       | 32   | 0.43    | 0.435   | 0.739   | 0.761   | 0.454   | 0.424   | 0.516   | 0.505   |         |         |         |         |         |         |         |         |         |         |         |         |
| Kineti c read | PDI | PDI+rutil | K328 E | K328E+rutil | H354 A | H354A+rutil | L355 R | L355R+rutil |
|-------------|-----|----------|--------|------------|--------|------------|-------|-------------|
| 0:00:32     | 0.048 | 0.073    | 0.039  | 0.041      | 0.043  | 0.041      | 0.039 | 0.042       |
| 0:01:32     | 0.056 | 0.073    | 0.039  | 0.042      | 0.044  | 0.041      | 0.039 | 0.042       |
| Time  | Value 1 | Value 2 | Value 3 | Value 4 | Value 5 | Value 6 | Value 7 | Value 8 | Value 9 |
|-------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 0:02:32 | 0.08 | 0.073 | 0.04 | 0.042 | 0.043 | 0.041 | 0.04 | 0.042 |
| 0:03:32 | 0.13 | 0.073 | 0.04 | 0.043 | 0.043 | 0.041 | 0.04 | 0.042 |
| 0:04:32 | 0.18 | 0.074 | 0.04 | 0.043 | 0.043 | 0.041 | 0.041 | 0.042 |
| 0:05:32 | 0.23 | 0.073 | 0.04 | 0.042 | 0.043 | 0.041 | 0.041 | 0.042 |
| 0:06:32 | 0.28 | 0.073 | 0.041 | 0.042 | 0.043 | 0.042 | 0.041 | 0.042 |
| 0:07:32 | 0.33 | 0.073 | 0.041 | 0.043 | 0.043 | 0.042 | 0.04 | 0.042 |
| 0:08:32 | 0.37 | 0.073 | 0.041 | 0.043 | 0.043 | 0.042 | 0.041 | 0.042 |
| 0:09:32 | 0.42 | 0.079 | 0.043 | 0.043 | 0.044 | 0.042 | 0.043 | 0.042 |
| 0:10:32 | 0.46 | 0.087 | 0.047 | 0.043 | 0.043 | 0.042 | 0.048 | 0.042 |
| 0:11:32 | 0.50 | 0.101 | 0.054 | 0.043 | 0.043 | 0.042 | 0.055 | 0.042 |
| 0:12:32 | 0.54 | 0.116 | 0.063 | 0.043 | 0.043 | 0.042 | 0.065 | 0.042 |
| 0:13:32 | 0.57 | 0.134 | 0.072 | 0.043 | 0.043 | 0.042 | 0.075 | 0.042 |
| 0:14:32 | 0.61 | 0.15 | 0.083 | 0.043 | 0.043 | 0.042 | 0.087 | 0.042 |
| 0:15:32 | 0.65 | 0.168 | 0.095 | 0.043 | 0.044 | 0.042 | 0.099 | 0.042 |
| 0:16:32 | 0.68 | 0.185 | 0.106 | 0.043 | 0.043 | 0.042 | 0.112 | 0.042 |
| 0:17:32 | 0.70 | 0.202 | 0.118 | 0.043 | 0.044 | 0.042 | 0.125 | 0.042 |
| 0:18:32 | 0.73 | 0.221 | 0.13 | 0.043 | 0.047 | 0.042 | 0.138 | 0.042 |
| 0:19:32 | 0.76 | 0.238 | 0.143 | 0.043 | 0.051 | 0.042 | 0.152 | 0.042 |
| 0:20:32 | 0.78 | 0.255 | 0.157 | 0.043 | 0.055 | 0.042 | 0.166 | 0.042 |
| 0:21:32 | 0.80 | 0.276 | 0.168 | 0.043 | 0.06 | 0.042 | 0.18 | 0.042 |
| 0:22:32 | 0.81 | 0.29 | 0.182 | 0.043 | 0.067 | 0.042 | 0.195 | 0.043 |
| Time  | Value 1 | Value 2 | Value 3 | Value 4 | Value 5 | Value 6 | Value 7 | Value 8 |
|-------|---------|---------|---------|---------|---------|---------|---------|---------|
| 0:23:3 | 0.83  | 0.31    | 0.195   | 0.043   | 0.072   | 0.042   | 0.208   | 0.042   |
| 0:24:3 | 0.85  | 0.325   | 0.207   | 0.043   | 0.079   | 0.042   | 0.221   | 0.042   |
| 0:25:3 | 0.87  | 0.342   | 0.221   | 0.043   | 0.087   | 0.042   | 0.235   | 0.042   |
| 0:26:3 | 0.88  | 0.361   | 0.233   | 0.043   | 0.094   | 0.042   | 0.248   | 0.042   |
| 0:27:3 | 0.90  | 0.377   | 0.245   | 0.043   | 0.102   | 0.042   | 0.263   | 0.043   |
| 0:28:3 | 0.91  | 0.394   | 0.259   | 0.043   | 0.11    | 0.042   | 0.275   | 0.043   |
| 0:29:3 | 0.93  | 0.407   | 0.27    | 0.043   | 0.118   | 0.042   | 0.288   | 0.043   |
| 0:30:3 | 0.94  | 0.424   | 0.284   | 0.043   | 0.126   | 0.042   | 0.304   | 0.045   |
| 0:31:3 | 0.96  | 0.438   | 0.295   | 0.044   | 0.134   | 0.042   | 0.312   | 0.047   |
| 0:32:3 | 0.97  | 0.45    | 0.305   | 0.046   | 0.143   | 0.041   | 0.326   | 0.05    |
| 0:33:3 | 0.98  | 0.468   | 0.316   | 0.049   | 0.151   | 0.042   | 0.34    | 0.054   |
| 0:34:3 | 0.99  | 0.478   | 0.326   | 0.052   | 0.16    | 0.042   | 0.352   | 0.058   |
| 0:35:3 | 1.00  | 0.491   | 0.339   | 0.055   | 0.168   | 0.042   | 0.363   | 0.062   |
| 0:36:3 | 1.01  | 0.508   | 0.353   | 0.059   | 0.176   | 0.042   | 0.373   | 0.066   |
| 0:37:3 | 1.02  | 0.518   | 0.36    | 0.063   | 0.185   | 0.042   | 0.384   | 0.07    |
| 0:38:3 | 1.03  | 0.534   | 0.372   | 0.067   | 0.194   | 0.042   | 0.394   | 0.075   |
| 0:39:3 | 1.03  | 0.545   | 0.386   | 0.071   | 0.202   | 0.043   | 0.401   | 0.081   |
| 0:40:3 | 1.04  | 0.556   | 0.394   | 0.076   | 0.21    | 0.044   | 0.416   | 0.085   |
| 0:41:3 | 1.04  | 0.569   | 0.4     | 0.081   | 0.221   | 0.046   | 0.429   | 0.09    |
| 0:42:3 | 1.04  | 0.58    | 0.409   | 0.086   | 0.225   | 0.049   | 0.438   | 0.096   |
| Time  | Value | Value | Value | Value | Value | Value | Value | Value | Value |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 0:43:3| 1.05  | 0.586 | 0.421 | 0.09  | 0.232 | 0.052 | 0.446 | 0.101 |
| 0:44:3| 1.06  | 0.597 | 0.43  | 0.097 | 0.241 | 0.056 | 0.448 | 0.107 |
| 0:45:3| 1.06  | 0.603 | 0.437 | 0.102 | 0.249 | 0.06  | 0.462 | 0.112 |
| 0:46:3| 1.07  | 0.605 | 0.449 | 0.107 | 0.257 | 0.064 | 0.47  | 0.118 |
| 0:47:3| 1.07  | 0.61  | 0.459 | 0.113 | 0.264 | 0.068 | 0.483 | 0.124 |
| 0:48:3| 1.07  | 0.619 | 0.468 | 0.118 | 0.274 | 0.072 | 0.49  | 0.13  |
| 0:49:3| 1.07  | 0.633 | 0.475 | 0.124 | 0.282 | 0.077 | 0.5   | 0.136 |
| 0:50:3| 1.08  | 0.659 | 0.481 | 0.131 | 0.289 | 0.081 | 0.508 | 0.143 |
| 0:51:3| 1.08  | 0.662 | 0.492 | 0.136 | 0.297 | 0.086 | 0.518 | 0.148 |
| 0:52:3| 1.08  | 0.671 | 0.501 | 0.143 | 0.305 | 0.09  | 0.521 | 0.154 |
| 0:53:3| 1.08  | 0.686 | 0.508 | 0.148 | 0.31  | 0.096 | 0.538 | 0.16  |
| 0:54:3| 1.09  | 0.691 | 0.518 | 0.155 | 0.32  | 0.101 | 0.548 | 0.167 |
| 0:55:3| 1.09  | 0.691 | 0.526 | 0.161 | 0.327 | 0.106 | 0.552 | 0.173 |
| 0:56:3| 1.08  | 0.7   | 0.535 | 0.166 | 0.335 | 0.112 | 0.567 | 0.18  |
| 0:57:3| 1.09  | 0.707 | 0.545 | 0.173 | 0.34  | 0.117 | 0.571 | 0.186 |
| 0:58:3| 1.09  | 0.717 | 0.549 | 0.177 | 0.348 | 0.123 | 0.581 | 0.192 |
| 0:59:3| 1.09  | 0.728 | 0.558 | 0.184 | 0.354 | 0.128 | 0.587 | 0.198 |
| 1:00:3| 1.09  | 0.731 | 0.565 | 0.19  | 0.361 | 0.134 | 0.6   | 0.205 |
| 1:01:3| 1.09  | 0.742 | 0.575 | 0.197 | 0.371 | 0.14  | 0.606 | 0.211 |
| 1:02:3| 1.10  | 0.752 | 0.584 | 0.203 | 0.377 | 0.146 | 0.608 | 0.217 |
| 1:03:3| 1.10  | 0.762 | 0.589 | 0.208 | 0.385 | 0.152 | 0.621 | 0.224 |
| 1:04:3 | 1 | 1.10 3 | 0.759 | 0.6 | 0.215 | 0.389 | 0.157 | 0.626 | 0.229 |
| 1:05:3 | 1 | 1.10 5 | 0.768 | 0.606 | 0.221 | 0.398 | 0.163 | 0.634 | 0.235 |
| 1:06:3 | 1 | 1.10 7 | 0.784 | 0.614 | 0.227 | 0.406 | 0.17 | 0.641 | 0.241 |
| 1:07:3 | 1 | 1.10 5 | 0.785 | 0.618 | 0.233 | 0.41 | 0.175 | 0.644 | 0.247 |
| 1:08:3 | 1 | 1.10 8 | 0.787 | 0.628 | 0.238 | 0.415 | 0.182 | 0.654 | 0.254 |
| 1:09:3 | 1 | 1.10 5 | 0.794 | 0.632 | 0.245 | 0.423 | 0.186 | 0.656 | 0.26 |
| 1:10:3 | 1 | 1.10 6 | 0.804 | 0.639 | 0.249 | 0.427 | 0.193 | 0.67 | 0.266 |
| 1:11:3 | 1 | 1.10 9 | 0.814 | 0.648 | 0.254 | 0.435 | 0.199 | 0.676 | 0.271 |
| 1:12:3 | 1 | 1.11 1 | 0.812 | 0.652 | 0.259 | 0.442 | 0.205 | 0.679 | 0.279 |
| 1:13:3 | 1 | 1.11 1 | 0.823 | 0.657 | 0.266 | 0.447 | 0.211 | 0.683 | 0.284 |
| 1:14:3 | 1 | 1.11 1 | 0.829 | 0.66 | 0.271 | 0.454 | 0.217 | 0.693 | 0.289 |
| 1:15:3 | 1 | 1.11 1 | 0.831 | 0.662 | 0.277 | 0.46 | 0.223 | 0.698 | 0.294 |
| 1:16:3 | 1 | 1.10 8 | 0.845 | 0.672 | 0.285 | 0.466 | 0.229 | 0.701 | 0.3 |
| 1:17:3 | 1 | 1.11 2 | 0.834 | 0.675 | 0.29 | 0.475 | 0.234 | 0.704 | 0.304 |
| 1:18:3 | 1 | 1.11 6 | 0.842 | 0.677 | 0.295 | 0.481 | 0.24 | 0.71 | 0.312 |
| 1:19:3 | 1 | 1.11 4 | 0.85 | 0.688 | 0.299 | 0.479 | 0.245 | 0.709 | 0.317 |
| 1:20:3 | 1 | 1.11 6 | 0.863 | 0.684 | 0.305 | 0.487 | 0.25 | 0.722 | 0.324 |
| 1:21:3 | 1 | 1.11 5 | 0.873 | 0.693 | 0.31 | 0.495 | 0.257 | 0.727 | 0.331 |
| 1:22:3 | 1 | 1.11 5 | 0.863 | 0.695 | 0.315 | 0.502 | 0.261 | 0.732 | 0.335 |
| 1:23:3 | 1 | 1.11 3 | 0.871 | 0.707 | 0.321 | 0.509 | 0.266 | 0.736 | 0.341 |
| Time   | E359A | E359A+rutin | E359K | E359K+rutin | Rutin |
|--------|-------|-------------|-------|-------------|-------|
| 0:00:32| 0.043 | 0.046       | 0.04  | 0.045       | 0.034 |
| 0:01:32| 0.045 | 0.046       | 0.041 | 0.045       | 0.034 |
| 0:02:32| 0.044 | 0.052       | 0.041 | 0.045       | 0.034 |
| 0:03:32| 0.045 | 0.047       | 0.041 | 0.044       | 0.034 |
| Time     | Value1 | Value2 | Value3 | Value4 | Value5 |
|----------|--------|--------|--------|--------|--------|
| 0:04:32  | 0.046  | 0.048  | 0.041  | 0.044  | 0.034  |
| 0:05:32  | 0.046  | 0.046  | 0.041  | 0.044  | 0.034  |
| 0:06:32  | 0.046  | 0.046  | 0.041  | 0.044  | 0.034  |
| 0:07:32  | 0.046  | 0.046  | 0.041  | 0.044  | 0.034  |
| 0:08:32  | 0.046  | 0.046  | 0.041  | 0.044  | 0.034  |
| 0:09:32  | 0.045  | 0.046  | 0.043  | 0.043  | 0.034  |
| 0:10:32  | 0.045  | 0.046  | 0.047  | 0.043  | 0.034  |
| 0:11:32  | 0.045  | 0.046  | 0.051  | 0.043  | 0.034  |
| 0:12:32  | 0.045  | 0.046  | 0.058  | 0.043  | 0.034  |
| 0:13:32  | 0.046  | 0.046  | 0.066  | 0.043  | 0.034  |
| 0:14:32  | 0.05   | 0.045  | 0.074  | 0.043  | 0.034  |
| 0:15:32  | 0.055  | 0.046  | 0.084  | 0.044  | 0.034  |
| 0:16:32  | 0.062  | 0.045  | 0.093  | 0.043  | 0.034  |
| 0:17:32  | 0.069  | 0.045  | 0.103  | 0.043  | 0.034  |
| 0:18:32  | 0.078  | 0.048  | 0.114  | 0.043  | 0.034  |
| 0:19:32  | 0.086  | 0.045  | 0.124  | 0.043  | 0.034  |
| 0:20:32  | 0.096  | 0.046  | 0.135  | 0.043  | 0.034  |
| 0:21:32  | 0.106  | 0.046  | 0.145  | 0.043  | 0.034  |
| 0:22:32  | 0.117  | 0.046  | 0.157  | 0.043  | 0.034  |
| 0:23:32  | 0.128  | 0.045  | 0.167  | 0.043  | 0.034  |
| 0:24:32  | 0.137  | 0.045  | 0.178  | 0.043  | 0.034  |
| 0:25:32  | 0.149  | 0.046  | 0.192  | 0.044  | 0.034  |
| 0:26:32  | 0.162  | 0.046  | 0.2   | 0.043  | 0.034  |
| 0:27:32  | 0.171  | 0.045  | 0.21   | 0.044  | 0.034  |
| 0:28:32  | 0.182  | 0.046  | 0.221  | 0.044  | 0.034  |
| 0:29:32  | 0.192  | 0.046  | 0.231  | 0.044  | 0.034  |
| 0:30:32  | 0.204  | 0.046  | 0.242  | 0.045  | 0.034  |
| 0:31:32  | 0.216  | 0.046  | 0.253  | 0.047  | 0.034  |
| 0:32:32  | 0.226  | 0.047  | 0.264  | 0.05   | 0.034  |
| 0:33:32  | 0.237  | 0.048  | 0.272  | 0.053  | 0.034  |
| 0:34:32  | 0.248  | 0.051  | 0.284  | 0.056  | 0.034  |
| 0:35:32  | 0.258  | 0.054  | 0.294  | 0.06   | 0.034  |
| 0:36:32  | 0.269  | 0.058  | 0.302  | 0.064  | 0.034  |
| 0:37:32  | 0.279  | 0.061  | 0.311  | 0.068  | 0.034  |
| 0:38:32  | 0.29   | 0.066  | 0.321  | 0.072  | 0.034  |
| 0:39:32  | 0.3    | 0.07   | 0.331  | 0.077  | 0.034  |
| 0:40:32  | 0.309  | 0.075  | 0.341  | 0.082  | 0.034  |
| 0:41:32  | 0.318  | 0.08   | 0.349  | 0.087  | 0.034  |
| 0:42:32  | 0.329  | 0.085  | 0.36   | 0.092  | 0.034  |
| 0:43:32  | 0.34   | 0.09   | 0.368  | 0.097  | 0.034  |
| 0:44:32  | 0.35   | 0.096  | 0.376  | 0.103  | 0.034  |
| Time    | Value1 | Value2 | Value3 | Value4 | Value5 |
|---------|--------|--------|--------|--------|--------|
| 0:45:32 | 0.362  | 0.102  | 0.388  | 0.108  | 0.033  |
| 0:46:32 | 0.368  | 0.107  | 0.396  | 0.114  | 0.034  |
| 0:47:32 | 0.379  | 0.113  | 0.405  | 0.12   | 0.034  |
| 0:48:32 | 0.385  | 0.119  | 0.415  | 0.125  | 0.034  |
| 0:49:32 | 0.399  | 0.125  | 0.423  | 0.131  | 0.034  |
| 0:50:32 | 0.404  | 0.131  | 0.43   | 0.137  | 0.034  |
| 0:51:32 | 0.415  | 0.137  | 0.436  | 0.143  | 0.034  |
| 0:52:32 | 0.424  | 0.144  | 0.446  | 0.149  | 0.034  |
| 0:53:32 | 0.431  | 0.15   | 0.453  | 0.155  | 0.034  |
| 0:54:32 | 0.437  | 0.157  | 0.46   | 0.162  | 0.034  |
| 0:55:32 | 0.448  | 0.164  | 0.472  | 0.167  | 0.034  |
| 0:56:32 | 0.453  | 0.169  | 0.477  | 0.172  | 0.034  |
| 0:57:32 | 0.46   | 0.175  | 0.488  | 0.177  | 0.034  |
| 0:58:32 | 0.469  | 0.181  | 0.494  | 0.184  | 0.034  |
| 0:59:32 | 0.478  | 0.188  | 0.493  | 0.19   | 0.034  |
| 1:00:32 | 0.484  | 0.195  | 0.505  | 0.197  | 0.034  |
| 1:01:32 | 0.489  | 0.201  | 0.516  | 0.205  | 0.034  |
| 1:02:32 | 0.493  | 0.207  | 0.522  | 0.21   | 0.034  |
| 1:03:32 | 0.5     | 0.214  | 0.529  | 0.215  | 0.034  |
| 1:04:32 | 0.511  | 0.22   | 0.533  | 0.223  | 0.034  |
| 1:05:32 | 0.518  | 0.226  | 0.539  | 0.228  | 0.034  |
| 1:06:32 | 0.525  | 0.232  | 0.543  | 0.234  | 0.034  |
| 1:07:32 | 0.533  | 0.239  | 0.54   | 0.239  | 0.034  |
| 1:08:32 | 0.537  | 0.245  | 0.557  | 0.246  | 0.034  |
| 1:09:32 | 0.542  | 0.25   | 0.552  | 0.249  | 0.034  |
| 1:10:32 | 0.549  | 0.257  | 0.558  | 0.257  | 0.034  |
| 1:11:32 | 0.557  | 0.262  | 0.568  | 0.261  | 0.034  |
| 1:12:32 | 0.564  | 0.268  | 0.573  | 0.268  | 0.034  |
| 1:13:32 | 0.571  | 0.275  | 0.581  | 0.273  | 0.034  |
| 1:14:32 | 0.577  | 0.28   | 0.587  | 0.276  | 0.034  |
| 1:15:32 | 0.585  | 0.285  | 0.587  | 0.28   | 0.034  |
| 1:16:32 | 0.585  | 0.292  | 0.594  | 0.288  | 0.034  |
| 1:17:32 | 0.595  | 0.298  | 0.6     | 0.297  | 0.034  |
| 1:18:32 | 0.598  | 0.303  | 0.604  | 0.302  | 0.034  |
| 1:19:32 | 0.604  | 0.311  | 0.604  | 0.308  | 0.034  |
| 1:20:32 | 0.615  | 0.318  | 0.612  | 0.313  | 0.034  |
| 1:21:32 | 0.617  | 0.322  | 0.618  | 0.317  | 0.034  |
| 1:22:32 | 0.626  | 0.33   | 0.624  | 0.323  | 0.034  |
| 1:23:32 | 0.63   | 0.334  | 0.627  | 0.324  | 0.034  |
| 1:24:32 | 0.634  | 0.339  | 0.633  | 0.331  | 0.034  |
| 1:25:32 | 0.639  | 0.343  | 0.642  | 0.336  | 0.034  |
3. Raw data of Fig. 6

1) Fig. 6A

| Kinetic read | PDI   | PDI+rutin | PDI+kaempferitin | PDI+tiliroside | PDI+2’-O-galloylhyperinin |
|--------------|-------|-----------|------------------|----------------|----------------------------|
| 0:00:32      | 0.048 | 0.073     | 0.048            | 0.044          | 0.057                      |
| 0:01:32      | 0.056 | 0.073     | 0.049            | 0.045          | 0.057                      |
| 0:02:32      | 0.085 | 0.073     | 0.051            | 0.047          | 0.058                      |
| 0:03:32      | 0.131 | 0.073     | 0.054            | 0.047          | 0.058                      |
| 0:04:32      | 0.181 | 0.074     | 0.063            | 0.047          | 0.058                      |
| 0:05:32      | 0.233 | 0.073     | 0.079            | 0.047          | 0.058                      |
| 0:06:32      | 0.283 | 0.073     | 0.099            | 0.047          | 0.057                      |
| 0:07:32      | 0.331 | 0.073     | 0.122            | 0.047          | 0.057                      |
| 0:08:32      | 0.379 | 0.073     | 0.146            | 0.048          | 0.058                      |
| 0:09:32      | 0.42  | 0.079     | 0.173            | 0.052          | 0.058                      |
|                | 1  | 6  | 0.087 | 0.198 | 0.059 | 0.058  |
|---------------|----|----|-------|-------|-------|-------|
| 0:10:32       | 0.46|    |       |       |       |       |
| 0:11:32       | 0.50|    |       |       | 0.068 | 0.059  |
| 0:12:32       | 0.54|    |       | 0.251 | 0.08  | 0.063  |
| 0:13:32       | 0.57|    |       | 0.275 | 0.094 | 0.068  |
| 0:14:32       | 0.61|    | 0.15  | 0.306 | 0.11  | 0.074  |
| 0:15:32       | 0.65|    | 0.168 | 0.33  | 0.128 | 0.082  |
| 0:16:32       | 0.68|    | 0.185 | 0.354 | 0.144 | 0.09   |
| 0:17:32       | 0.70|    | 0.202 | 0.377 | 0.161 | 0.101  |
| 0:18:32       | 0.73|    | 0.221 | 0.406 | 0.178 | 0.11   |
| 0:19:32       | 0.76|    | 0.238 | 0.427 | 0.198 | 0.122  |
| 0:20:32       | 0.78|    | 0.255 | 0.45  | 0.214 | 0.135  |
| 0:21:32       | 0.80|    | 0.276 | 0.473 | 0.23  | 0.146  |
| 0:22:32       | 0.81|    | 0.29  | 0.499 | 0.25  | 0.157  |
| 0:23:32       | 0.83|    | 0.31  | 0.521 | 0.271 | 0.173  |
| 0:24:32       | 0.85|    | 0.325 | 0.539 | 0.289 | 0.186  |
| 0:25:32       | 0.87|    | 0.342 | 0.557 | 0.304 | 0.2    |
| 0:26:32       | 0.88|    | 0.361 | 0.571 | 0.323 | 0.212  |
| 0:27:32       | 0.90|    | 0.377 | 0.58  | 0.338 | 0.225  |
| 0:28:32       | 0.91|    | 0.394 | 0.598 | 0.353 | 0.242  |
| 0:29:32       | 0.93|    | 0.407 | 0.628 | 0.363 | 0.25   |
| 0:30:32       | 0.94|    | 0.424 | 0.651 | 0.382 | 0.255  |
| Time       | Value 1 | Value 2 | Value 3 | Value 4 | Value 5 |
|-----------|---------|---------|---------|---------|---------|
| 0:31:32   | 0.96    | 0.438   | 0.672   | 0.397   | 0.265   |
| 0:32:32   | 0.97    | 0.45    | 0.691   | 0.412   | 0.282   |
| 0:33:32   | 0.98    | 0.468   | 0.71    | 0.426   | 0.294   |
| 0:34:32   | 0.99    | 0.478   | 0.726   | 0.441   | 0.307   |
| 0:35:32   | 1.00    | 0.491   | 0.738   | 0.457   | 0.314   |
| 0:36:32   | 1.01    | 0.508   | 0.75    | 0.467   | 0.326   |
| 0:37:32   | 1.02    | 0.518   | 0.759   | 0.486   | 0.336   |
| 0:38:32   | 1.03    | 0.534   | 0.767   | 0.496   | 0.348   |
| 0:39:32   | 1.03    | 0.545   | 0.782   | 0.512   | 0.358   |
| 0:40:32   | 1.04    | 0.556   | 0.8     | 0.52    | 0.37    |
| 0:41:32   | 1.04    | 0.569   | 0.814   | 0.534   | 0.382   |
| 0:42:32   | 1.04    | 0.58    | 0.828   | 0.547   | 0.399   |
| 0:43:32   | 1.05    | 0.586   | 0.833   | 0.558   | 0.414   |
| 0:44:32   | 1.06    | 0.597   | 0.843   | 0.569   | 0.42    |
| 0:45:32   | 1.06    | 0.603   | 0.856   | 0.578   | 0.435   |
| 0:46:32   | 1.07    | 0.605   | 0.874   | 0.593   | 0.442   |
| 0:47:32   | 1.07    | 0.61    | 0.875   | 0.6     | 0.452   |
| 0:48:32   | 1.07    | 0.619   | 0.882   | 0.616   | 0.46    |
| 0:49:32   | 1.07    | 0.633   | 0.896   | 0.621   | 0.471   |
| 0:50:32   | 1.08    | 0.659   | 0.905   | 0.64    | 0.478   |
| 0:51:32   | 1.08    | 0.662   | 0.906   | 0.641   | 0.488   |
| 0:52:32   | 1.08    | 0.671   | 0.919   | 0.647   | 0.493   |
| Time   | 1.09 | 0.686 | 0.923 | 0.657 | 0.509 |
|--------|------|-------|-------|-------|-------|
| 0:53:32| 1.08 | 0.691 | 0.928 | 0.67  | 0.52  |
| 0:54:32| 1.09 | 0.691 | 0.929 | 0.677 | 0.528 |
| 0:56:32| 0.7  | 0.937 | 0.692 | 0.53  |
| 0:57:32| 1.09 | 0.707 | 0.945 | 0.694 | 0.543 |
| 0:58:32| 1.09 | 0.717 | 0.954 | 0.697 | 0.553 |
| 0:59:32| 1.09 | 0.728 | 0.949 | 0.706 | 0.564 |
| 1:00:32| 1.09 | 0.731 | 0.967 | 0.707 | 0.576 |
| 1:01:32| 1.09 | 0.742 | 0.961 | 0.716 | 0.581 |
| 1:02:32| 1.10 | 0.752 | 0.956 | 0.725 | 0.584 |
| 1:03:32| 1.10 | 0.762 | 0.97  | 0.726 | 0.592 |
| 1:04:32| 1.10 | 0.759 | 0.967 | 0.737 | 0.6  |
| 1:12:32| 1.11 | 0.812 | 0.98  | 0.802 | 0.66  |
| 1:13:32| 1.11 | 0.823 | 0.98  | 0.808 | 0.672 |
| Time   | Column 1 | Column 2 | Column 3 | Column 4 | Column 5 |
|--------|----------|----------|----------|----------|----------|
| 1:14:32| 1.111    | 0.829    | 0.98     | 0.812    | 0.676    |
| 1:15:32| 1.111    | 0.831    | 0.98     | 0.806    | 0.681    |
| 1:16:32| 1.108    | 0.845    | 0.986    | 0.817    | 0.687    |
| 1:17:32| 1.112    | 0.834    | 0.991    | 0.826    | 0.695    |
| 1:18:32| 1.116    | 0.842    | 0.993    | 0.83     | 0.706    |
| 1:19:32| 1.114    | 0.85     | 0.983    | 0.839    | 0.712    |
| 1:20:32| 1.116    | 0.863    | 0.992    | 0.835    | 0.723    |
| 1:21:32| 1.115    | 0.873    | 0.979    | 0.844    | 0.726    |
| 1:22:32| 1.115    | 0.863    | 0.994    | 0.855    | 0.729    |
| 1:23:32| 1.113    | 0.871    | 0.995    | 0.852    | 0.737    |
| 1:24:32| 1.107    | 0.878    | 0.992    | 0.859    | 0.743    |
| 1:25:32| 1.107    | 0.88     | 0.995    | 0.873    | 0.746    |
| 1:26:32| 1.112    | 0.885    | 0.991    | 0.866    | 0.761    |
| 1:27:32| 1.113    | 0.882    | 0.99     | 0.874    | 0.764    |
| 1:28:32| 1.117    | 0.883    | 1.003    | 0.878    | 0.761    |
| 1:29:32| 1.12     | 0.889    | 0.989    | 0.883    | 0.771    |
| 1:30:32| 1.12     | 0.902    | 0.991    | 0.884    | 0.771    |
| 1:31:32| 1.124    | 0.907    | 0.992    | 0.889    | 0.782    |
| 1:32:32| 1.119    | 0.908    | 0.996    | 0.901    | 0.787    |
| 1:33:32| 1.127    | 0.91     | 0.993    | 0.894    | 0.792    |
| 1:34:32| 1.122    | 0.916    | 0.986    | 0.899    | 0.798    |
| 1:35:32| 1.13     | 0.909    | 0.992    | 0.907    | 0.805    |
| 1:36:32| 1.129    | 0.914    | 0.991    | 0.913    | 0.805    |
| 1:37:32| 1.127    | 0.917    | 0.993    | 0.91     | 0.815    |
| 1:38:32| 1.128    | 0.917    | 0.999    | 0.914    | 0.813    |
| 1:39:32| 1.127    | 0.923    | 1.001    | 0.917    | 0.826    |
| 1:40:32| 1.125    | 0.924    | 0.998    | 0.925    | 0.825    |

2) Fig. 6B
| Kinetic read | MBP-PDI-b'xa' (WT) | WT+rutin | WT+kaempferin | WT+tiliroside | WT+2'-O-galloylhypin |
|--------------|-------------------|---------|--------------|---------------|---------------------|
| 0:00:32      | 0.042             | 0.047   | 0.06         | 0.049         | 0.065               |
| 0:01:32      | 0.042             | 0.047   | 0.055        | 0.049         | 0.065               |
| 0:02:32      | 0.042             | 0.048   | 0.055        | 0.05          | 0.066               |
| 0:03:32      | 0.042             | 0.048   | 0.054        | 0.049         | 0.065               |
| 0:04:32      | 0.042             | 0.048   | 0.054        | 0.05          | 0.064               |
| 0:05:32      | 0.043             | 0.048   | 0.054        | 0.049         | 0.065               |
| 0:06:32      | 0.043             | 0.049   | 0.054        | 0.049         | 0.064               |
| 0:07:32      | 0.043             | 0.048   | 0.054        | 0.049         | 0.064               |
| 0:08:32      | 0.043             | 0.048   | 0.054        | 0.049         | 0.064               |
| 0:09:32      | 0.046             | 0.048   | 0.054        | 0.049         | 0.064               |
| 0:10:32      | 0.053             | 0.049   | 0.055        | 0.049         | 0.064               |
| 0:11:32      | 0.062             | 0.048   | 0.054        | 0.048         | 0.063               |
| 0:12:32      | 0.073             | 0.048   | 0.054        | 0.048         | 0.064               |
| 0:13:32      | 0.085             | 0.048   | 0.055        | 0.048         | 0.063               |
| 0:14:32      | 0.098             | 0.049   | 0.055        | 0.048         | 0.065               |
| 0:15:32      | 0.112             | 0.049   | 0.057        | 0.048         | 0.063               |
| 0:16:32      | 0.125             | 0.049   | 0.059        | 0.048         | 0.062               |
| 0:17:32      | 0.138             | 0.048   | 0.062        | 0.048         | 0.062               |
| 0:18:32      | 0.153             | 0.049   | 0.065        | 0.05          | 0.062               |
| Time (hh:mm:ss) | Column 1 | Column 2 | Column 3 | Column 4 | Column 5 |
|----------------|----------|----------|----------|----------|----------|
| 0:19:30:2 | 0.167    | 0.049    | 0.069    | 0.048    | 0.062    |
| 0:20:30:2 | 0.182    | 0.049    | 0.074    | 0.048    | 0.062    |
| 0:21:30:2 | 0.197    | 0.051    | 0.079    | 0.049    | 0.062    |
| 0:22:30:2 | 0.21     | 0.055    | 0.085    | 0.048    | 0.062    |
| 0:23:30:2 | 0.225    | 0.06     | 0.091    | 0.049    | 0.063    |
| 0:24:30:2 | 0.239    | 0.067    | 0.099    | 0.05     | 0.063    |
| 0:25:30:2 | 0.254    | 0.073    | 0.106    | 0.051    | 0.063    |
| 0:26:30:2 | 0.268    | 0.081    | 0.113    | 0.053    | 0.064    |
| 0:27:30:2 | 0.282    | 0.088    | 0.121    | 0.056    | 0.067    |
| 0:28:30:2 | 0.297    | 0.096    | 0.128    | 0.058    | 0.068    |
| 0:29:30:2 | 0.307    | 0.105    | 0.136    | 0.062    | 0.07     |
| 0:30:30:2 | 0.323    | 0.114    | 0.141    | 0.066    | 0.073    |
| 0:31:30:2 | 0.337    | 0.123    | 0.15     | 0.07     | 0.076    |
| 0:32:30:2 | 0.348    | 0.133    | 0.155    | 0.075    | 0.08     |
| 0:33:30:2 | 0.36     | 0.141    | 0.162    | 0.081    | 0.083    |
| 0:34:30:2 | 0.369    | 0.151    | 0.171    | 0.087    | 0.086    |
| 0:35:30:2 | 0.377    | 0.162    | 0.179    | 0.092    | 0.09     |
| 0:36:30:2 | 0.39     | 0.172    | 0.187    | 0.098    | 0.095    |
| 0:37:30:2 | 0.402    | 0.181    | 0.193    | 0.105    | 0.099    |
| 0:38:30:2 | 0.404    | 0.192    | 0.201    | 0.112    | 0.105    |
| 0:39:30:2 | 0.417    | 0.202    | 0.208    | 0.119    | 0.11     |
|   |     |     |     |     |     |
|---|-----|-----|-----|-----|-----|
| 2 | 0:40:3 | 0.426 | 0.212 | 0.218 | 0.127 | 0.117 |
| 2 | 0:41:3 | 0.442 | 0.222 | 0.223 | 0.134 | 0.122 |
| 2 | 0:42:3 | 0.442 | 0.232 | 0.235 | 0.141 | 0.128 |
| 2 | 0:43:3 | 0.462 | 0.242 | 0.237 | 0.149 | 0.133 |
| 2 | 0:44:3 | 0.472 | 0.252 | 0.246 | 0.157 | 0.138 |
| 2 | 0:45:3 | 0.479 | 0.262 | 0.258 | 0.165 | 0.144 |
| 2 | 0:46:3 | 0.491 | 0.272 | 0.263 | 0.172 | 0.151 |
| 2 | 0:47:3 | 0.497 | 0.281 | 0.271 | 0.181 | 0.158 |
| 2 | 0:48:3 | 0.516 | 0.288 | 0.278 | 0.189 | 0.165 |
| 2 | 0:49:3 | 0.525 | 0.299 | 0.282 | 0.196 | 0.171 |
| 2 | 0:50:3 | 0.535 | 0.307 | 0.297 | 0.204 | 0.177 |
| 2 | 0:51:3 | 0.537 | 0.319 | 0.297 | 0.214 | 0.187 |
| 2 | 0:52:3 | 0.546 | 0.324 | 0.31 | 0.221 | 0.191 |
| 2 | 0:53:3 | 0.562 | 0.33 | 0.314 | 0.23 | 0.198 |
| 2 | 0:54:3 | 0.57 | 0.336 | 0.32 | 0.238 | 0.204 |
| 2 | 0:55:3 | 0.579 | 0.345 | 0.323 | 0.242 | 0.21 |
| 2 | 0:56:3 | 0.58 | 0.355 | 0.333 | 0.25 | 0.219 |
| 2 | 0:57:3 | 0.6 | 0.361 | 0.338 | 0.258 | 0.227 |
| 2 | 0:58:3 | 0.602 | 0.371 | 0.345 | 0.268 | 0.233 |
| 2 | 0:59:3 | 0.609 | 0.378 | 0.351 | 0.275 | 0.24 |
| Time (1:00) | Value 1 | Value 2 | Value 3 | Value 4 | Value 5 |
|------------|---------|---------|---------|---------|---------|
| 0.619      | 0.387   | 0.357   | 0.281   | 0.248   |
| 0.619      | 0.396   | 0.366   | 0.287   | 0.254   |
| 0.629      | 0.403   | 0.372   | 0.298   | 0.263   |
| 0.632      | 0.409   | 0.374   | 0.303   | 0.266   |
| 0.645      | 0.413   | 0.382   | 0.308   | 0.27    |
| 0.643      | 0.424   | 0.39    | 0.313   | 0.278   |
| 0.654      | 0.43    | 0.395   | 0.323   | 0.285   |
| 0.662      | 0.433   | 0.395   | 0.332   | 0.29    |
| 0.666      | 0.44    | 0.409   | 0.335   | 0.296   |
| 0.669      | 0.446   | 0.413   | 0.344   | 0.303   |
| 0.683      | 0.457   | 0.418   | 0.348   | 0.307   |
| 0.675      | 0.463   | 0.422   | 0.353   | 0.314   |
| 0.691      | 0.466   | 0.431   | 0.358   | 0.322   |
| 0.698      | 0.469   | 0.434   | 0.365   | 0.325   |
| 0.7        | 0.475   | 0.438   | 0.377   | 0.331   |
| 0.71       | 0.48    | 0.445   | 0.381   | 0.34    |
| 0.715      | 0.484   | 0.448   | 0.389   | 0.344   |
| 0.72       | 0.495   | 0.455   | 0.39    | 0.351   |
| 0.722      | 0.495   | 0.461   | 0.4     | 0.355   |
| 0.727      | 0.502   | 0.466   | 0.403   | 0.359   |
| 0.746      | 0.502   | 0.472   | 0.406   | 0.364   |
| Time       | Value 1 | Value 2 | Value 3 | Value 4 | Value 5 |
|------------|---------|---------|---------|---------|---------|
| 1:21:3     | 0.734   | 0.519   | 0.476   | 0.412   | 0.369   |
| 1:22:3     | 0.741   | 0.513   | 0.481   | 0.416   | 0.375   |
| 1:23:3     | 0.739   | 0.516   | 0.486   | 0.423   | 0.382   |
| 1:24:3     | 0.756   | 0.528   | 0.489   | 0.43    | 0.386   |
| 1:25:3     | 0.759   | 0.536   | 0.495   | 0.432   | 0.389   |
| 1:26:3     | 0.758   | 0.538   | 0.501   | 0.441   | 0.394   |
| 1:27:3     | 0.759   | 0.538   | 0.502   | 0.447   | 0.401   |
| 1:28:3     | 0.783   | 0.544   | 0.511   | 0.449   | 0.405   |
| 1:29:3     | 0.781   | 0.548   | 0.514   | 0.454   | 0.41    |
| 1:30:3     | 0.779   | 0.549   | 0.516   | 0.457   | 0.413   |
| 1:31:3     | 0.796   | 0.553   | 0.52    | 0.462   | 0.414   |
| 1:32:3     | 0.787   | 0.554   | 0.522   | 0.466   | 0.424   |
| 1:33:3     | 0.804   | 0.558   | 0.523   | 0.471   | 0.428   |
| 1:34:3     | 0.805   | 0.564   | 0.533   | 0.475   | 0.434   |
| 1:35:3     | 0.803   | 0.574   | 0.537   | 0.482   | 0.434   |
| 1:36:3     | 0.801   | 0.57    | 0.55    | 0.482   | 0.443   |
| 1:37:3     | 0.811   | 0.577   | 0.546   | 0.484   | 0.445   |
| 1:38:3     | 0.808   | 0.579   | 0.55    | 0.493   | 0.453   |
| 1:39:3     | 0.831   | 0.58    | 0.555   | 0.499   | 0.453   |
| 1:40:3     | 0.829   | 0.585   | 0.56    | 0.5     | 0.462   |
4. Raw data of Fig. S3

1) PDI

| Concentration (μM) | 2.27E-07 | 6.8E-07 | 2.04E-06 | 6.11E-06 | 0.0000183 | 0.00005 | 0.000165 | 0.004455 |
|--------------------|----------|---------|----------|----------|-----------|----------|-----------|----------|
| Fluorescence       | 223      | 290.3   | 272      | 449      | 443.3     | 1370     | 1737.3    | 1812     |
|                    | 238      | 259.3   | 263      | 278      | 1164.3    | 1432     | 1267.3    | 1800     |
|                    | 175      | 183.3   | 236      | 397      | 777.3     | 663      | 772.3     | 1471     |

2) MBP-PDI-b’x

| Concentration (μM) | 2.27E-07 | 6.8E-07 | 2.04E-06 | 6.11E-06 | 0.0000183 | 0.00005 | 0.000165 | 0.004455 |
|--------------------|----------|---------|----------|----------|-----------|----------|-----------|----------|
| Fluorescence       | 266      | 186.3   | 215      | 356      | 872.3     | 2501     | 3723.3    | 2613     |
|                    | 171      | 100.3   | 256      | 397      | 991.3     | 2228     | 2463.3    | 2857     |
|                    | 203      | 163.3   | 179      | 628      | 1110.3    | 3385     | 2718.3    | 2389     |

3) MBP-PDI-b’xa’

| Concentration (μM) | 2.27E-07 | 6.8E-07 | 2.04E-06 | 6.11E-06 | 0.0000183 | 0.00005 | 0.000165 | 0.004455 |
|--------------------|----------|---------|----------|----------|-----------|----------|-----------|----------|
| Fluorescence       | 107      | 212.3   | 250      | 444      | 770.3     | 1073     | 1140.3    | 1373     |
|                    | 249      | 214.3   | 200      | 135      | 911.3     | 1060     | 756.3     | 1277     |
|                    | 149      | 181.3   | 244      | 388      | 322.3     | 774      | 1238.3    | 1331     |

4) MBP-mPDI-b’x

| Concentration (μM) | 2.27E-07 | 6.8E-07 | 2.04E-06 | 6.11E-06 | 0.0000183 | 0.00005 | 0.000165 | 0.004455 |
|--------------------|----------|---------|----------|----------|-----------|----------|-----------|----------|
| Fluorescence       | 110      | 236.3   | 251      | 407      | 1137.3    | 1850     | 1718.7    | 2011     |
|                    | 233      | 147.3   | 186      | 589      | 953.3     | 1071     | 1883.7    | 1949     |
|                    | 224      | 207.3   | 261      | 534      | 1030.3    | 2610     | 1720.7    | 2214     |
5) MBP-mPDI-b’xa’

| Concentration (μM) | 2.27E-07 | 6.8E-07 | 2.04E-06 | 6.11E-06 | 0.0000183 | 0.000055 | 0.000165 | 0.000495 | 0.004455 |
|-------------------|----------|----------|----------|----------|------------|----------|----------|----------|----------|
| Fluorescence      | 101      | 227.3    | 140      | 425      | 938.3      | 1005     | 1183.3   | 1760     | 1672     |
| Fluorescence      | 223      | 224.3    | 235      | 429      | 864.3      | 633      | 1573.3   | 1383     | 1527     |
| Fluorescence      | 277      | 369.3    | 265      | 501      | 758.3      | 1332     | 1424.3   | 916      | 1670     |

5. Raw data of Fig. S4

| Wavelength | rutin | MBP-PNGase+rutin | MBP-SpoIVB+rutin | MBP-MOC1+rutin | MBP-PNGase | MBP-SpoIVB | MBP-MOC | Buffer |
|------------|-------|------------------|------------------|----------------|------------|------------|---------|--------|
| 460        | 13    | 145              | 155              | 99             | 147        | 131        | 111     | 109    |
| 470        | 15    | 144              | 150              | 111            | 147        | 120        | 106     | 93     |
| 480        | 15    | 188              | 180              | 139            | 141        | 149        | 115     | 122    |
| 490        | 22    | 219              | 230              | 187            | 169        | 185        | 175     | 132    |
| 500        | 26    | 234              | 276              | 227            | 227        | 211        | 182     | 168    |
| 510        | 29    | 290              | 319              | 247            | 193        | 209        | 169     | 144    |
| 520        | 31    | 296              | 262              | 227            | 169        | 171        | 143     | 112    |
| 530        | 32    | 282              | 262              | 235            | 132        | 128        | 111     | 104    |
| 540        | 30    | 299              | 288              | 285            | 109        | 134        | 104     | 78     |
| 550        | 30    | 270              | 269              | 238            | 94         | 89         | 93      | 71     |
| 560        | 29    | 268              | 264              | 223            | 99         | 90         | 78      | 54     |
| 570        | 25    | 240              | 229              | 197            | 81         | 87         | 70      | 43     |
6. Raw data of Fig. S7

| Kinetic read | H354A+rutin | H354A+rutin | H354A+rutin |
|--------------|-------------|-------------|-------------|
| 0:00:32      | 0.035       | 0.036       | 0.039       |
| 0:01:32      | 0.035       | 0.035       | 0.045       |
| 0:02:32      | 0.035       | 0.035       | 0.041       |
| 0:03:32      | 0.035       | 0.035       | 0.041       |
| 0:04:32      | 0.035       | 0.036       | 0.041       |
| 0:05:32      | 0.036       | 0.036       | 0.042       |
| 0:06:32      | 0.036       | 0.036       | 0.043       |
| 0:07:32      | 0.038       | 0.036       | 0.041       |
| 0:08:32      | 0.036       | 0.036       | 0.042       |
| 0:09:32      | 0.036       | 0.036       | 0.062       |
| 0:10:32      | 0.036       | 0.037       | 0.053       |
| 0:11:32      | 0.036       | 0.036       | 0.06        |
| 0:12:32      | 0.036       | 0.036       | 0.041       |
| 0:13:32      | 0.039       | 0.036       | 0.041       |
| 0:14:32      | 0.036       | 0.037       | 0.042       |
| 0:15:32      | 0.036       | 0.037       | 0.041       |
| Time   | Value1 | Value2 | Value3 |
|--------|--------|--------|--------|
| 0:16:32| 0.039  | 0.038  | 0.048  |
| 0:17:32| 0.036  | 0.037  | 0.04   |
| 0:18:32| 0.037  | 0.037  | 0.04   |
| 0:19:32| 0.036  | 0.037  | 0.042  |
| 0:20:32| 0.037  | 0.038  | 0.041  |
| 0:21:32| 0.037  | 0.037  | 0.04   |
| 0:22:32| 0.036  | 0.037  | 0.06   |
| 0:23:32| 0.036  | 0.037  | 0.04   |
| 0:24:32| 0.036  | 0.037  | 0.04   |
| 0:25:32| 0.036  | 0.037  | 0.04   |
| 0:26:32| 0.039  | 0.037  | 0.041  |
| 0:27:32| 0.04   | 0.037  | 0.04   |
| 0:28:32| 0.038  | 0.038  | 0.04   |
| 0:29:32| 0.039  | 0.037  | 0.04   |
| 0:30:32| 0.037  | 0.038  | 0.041  |
| 0:31:32| 0.039  | 0.038  | 0.04   |
| 0:32:32| 0.041  | 0.039  | 0.046  |
| 0:33:32| 0.043  | 0.04   | 0.043  |
| 0:34:32| 0.047  | 0.042  | 0.044  |
| 0:35:32| 0.05   | 0.045  | 0.046  |
| 0:36:32| 0.053  | 0.048  | 0.05   |
| 0:37:32| 0.057  | 0.052  | 0.053  |
| 0:38:32| 0.062  | 0.056  | 0.057  |
| 0:39:32| 0.065  | 0.06   | 0.06   |
| 0:40:32| 0.07   | 0.064  | 0.065  |
| 0:41:32| 0.075  | 0.068  | 0.074  |
| 0:42:32| 0.08   | 0.072  | 0.085  |
| 0:43:32| 0.084  | 0.077  | 0.081  |
| 0:44:32| 0.089  | 0.082  | 0.083  |
| 0:45:32| 0.095  | 0.088  | 0.087  |
| 0:46:32| 0.1    | 0.092  | 0.104  |
| 0:47:32| 0.108  | 0.098  | 0.099  |
| 0:48:32| 0.111  | 0.104  | 0.103  |
| 0:49:32| 0.118  | 0.109  | 0.108  |
| 0:50:32| 0.122  | 0.114  | 0.114  |
| 0:51:32| 0.128  | 0.12   | 0.119  |
| 0:52:32| 0.134  | 0.126  | 0.13   |
| 0:53:32| 0.139  | 0.132  | 0.13   |
| 0:54:32| 0.146  | 0.137  | 0.136  |
| 0:55:32| 0.154  | 0.143  | 0.142  |
| 0:56:32| 0.158  | 0.15   | 0.147  |
| Time   | Value1 | Value2 | Value3 |
|--------|--------|--------|--------|
| 0:57:32| 0.165  | 0.154  | 0.163  |
| 0:58:32| 0.169  | 0.16   | 0.159  |
| 0:59:32| 0.174  | 0.167  | 0.164  |
| 1:00:32| 0.18   | 0.172  | 0.175  |
| 1:01:32| 0.191  | 0.177  | 0.176  |
| 1:02:32| 0.193  | 0.183  | 0.181  |
| 1:03:32| 0.199  | 0.189  | 0.188  |
| 1:04:32| 0.205  | 0.195  | 0.193  |
| 1:05:32| 0.21   | 0.201  | 0.198  |
| 1:06:32| 0.215  | 0.206  | 0.203  |
| 1:07:32| 0.221  | 0.212  | 0.208  |
| 1:08:32| 0.227  | 0.217  | 0.214  |
| 1:09:32| 0.237  | 0.222  | 0.222  |
| 1:10:32| 0.238  | 0.227  | 0.229  |
| 1:11:32| 0.244  | 0.234  | 0.234  |
| 1:12:32| 0.249  | 0.239  | 0.234  |
| 1:13:32| 0.255  | 0.245  | 0.241  |
| 1:14:32| 0.26   | 0.252  | 0.247  |
| 1:15:32| 0.265  | 0.255  | 0.251  |
| 1:16:32| 0.274  | 0.261  | 0.257  |
| 1:17:32| 0.276  | 0.267  | 0.265  |
| 1:18:32| 0.281  | 0.271  | 0.27   |
| 1:19:32| 0.288  | 0.276  | 0.273  |
| 1:20:32| 0.291  | 0.282  | 0.274  |
| 1:21:32| 0.296  | 0.286  | 0.281  |
| 1:22:32| 0.305  | 0.293  | 0.291  |
| 1:23:32| 0.309  | 0.297  | 0.294  |
| 1:24:32| 0.311  | 0.304  | 0.296  |
| 1:25:32| 0.316  | 0.307  | 0.304  |
| 1:26:32| 0.322  | 0.311  | 0.314  |
| 1:27:32| 0.326  | 0.318  | 0.312  |
| 1:28:32| 0.333  | 0.323  | 0.319  |
| 1:29:32| 0.337  | 0.327  | 0.323  |
| 1:30:32| 0.343  | 0.331  | 0.328  |
| 1:31:32| 0.346  | 0.334  | 0.331  |
| 1:32:32| 0.352  | 0.341  | 0.337  |
| 1:33:32| 0.357  | 0.344  | 0.341  |
| 1:34:32| 0.363  | 0.348  | 0.345  |
| 1:35:32| 0.365  | 0.353  | 0.353  |
| 1:36:32| 0.368  | 0.358  | 0.356  |
| 1:37:32| 0.373  | 0.362  | 0.358  |
7. Raw data of Fig. S8

| Kinetic read | Rutin+insulin | Kaempferitin+insulin | Tiliroside+insulin | 2'-O-galloylhyperin+insulin |
|--------------|---------------|----------------------|--------------------|-----------------------------|
| 0:00:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:01:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:02:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:03:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:04:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:05:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:06:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:07:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:08:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:09:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:10:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:11:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:12:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:13:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:14:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| 0:15:32      | 0.034         | 0.039                | 0.043              | 0.045                       |
| Time   | Value1 | Value2 | Value3 | Value4 |
|--------|--------|--------|--------|--------|
| 0:16:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:17:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:18:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:19:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:20:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:21:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:22:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:23:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:24:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:25:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:26:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:27:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:28:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:29:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:30:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:31:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:32:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:33:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:34:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:35:32| 0.034  | 0.039  | 0.043  | 0.045  |
| 0:36:32| 0.034  | 0.039  | 0.043  | 0.045  |
| Time | Value 1 | Value 2 | Value 3 | Value 4 |
|------|---------|---------|---------|---------|
| 0:37:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:38:3 | 0.034   | 0.039   | 0.043   | 0.044   |
| 0:39:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:40:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:41:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:42:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:43:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:44:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:45:3 | 0.033   | 0.039   | 0.043   | 0.045   |
| 0:46:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:47:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:48:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:49:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:50:3 | 0.034   | 0.039   | 0.043   | 0.044   |
| 0:51:3 | 0.034   | 0.039   | 0.043   | 0.044   |
| 0:52:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:53:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:54:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:55:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:56:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| Time  | Value 1 | Value 2 | Value 3 | Value 4 |
|-------|---------|---------|---------|---------|
| 0:57:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:58:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 0:59:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:00:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:01:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:02:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:03:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:04:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:05:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:06:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:07:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:08:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:09:3 | 0.034   | 0.039   | 0.043   | 0.044   |
| 1:10:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:11:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:12:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:13:3 | 0.034   | 0.04    | 0.043   | 0.045   |
| 1:14:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:15:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:16:3 | 0.034   | 0.039   | 0.043   | 0.045   |
| 1:17:3 | 0.034   | 0.039   | 0.043   | 0.045   |
8. Raw data of Fig. S9

| Wavelength (nm) | Ruti n | WT+GSSG+R utin | H354A+GSSG+R utin | WT+DTT+R utin | H354A+DTT+R utin |
|-----------------|--------|----------------|-------------------|---------------|------------------|
| 460             | 91     | 522            | 463               | 226           | 220              |
| 470             | 136    | 645            | 643               | 323           | 366              |
| 480             | 176    | 840            | 868               | 474           | 461              |
| 490             | 253    | 1110           | 1077              | 710           | 717              |
| 500             | 351    | 1483           | 1314              | 983           | 926              |
| 510             | 417    | 1702           | 1409              | 1194          | 1064             |
| 520             | 492    | 1714           | 1571              | 1288          | 1137             |
| 530             | 545    | 1683           | 1575              | 1350          | 1173             |
| 540             | 570    | 1546           | 1539              | 1325          | 1184             |
| 550             | 562    | 1419           | 1320              | 1213          | 1098             |
| 560             | 558    | 1288           | 1242              | 1093          | 1041             |
| 570             | 493    | 1137           | 1021              | 947           | 924              |
| 580             | 457    | 948            | 943               | 824           | 841              |
| 590             | 382    | 753            | 770               | 679           | 653              |
| 600             | 351    | 701            | 676               | 570           | 584              |
| 610             | 330    | 522            | 539               | 489           | 434              |
| 620             | 267    | 501            | 484               | 402           | 391              |
| 630             | 218    | 330            | 309               | 347           | 324              |
| 640             | 191    | 352            | 336               | 294           | 293              |
| 650             | 167    | 305            | 242               | 250           | 268              |
| 660             | 160    | 228            | 248               | 207           | 190              |
| 670             | 154    | 189            | 104               | 196           | 170              |
| 680             | 148    | 222            | 176               | 187           | 152              |
| 690             | 142    | 58             | 92                | 120           | 95               |
| 700             | 136    | 228            | 68                | 153           | 96               |