

|                                 | Chemistry(C) |                    | Clin. phenotype(CP) |                   | C+CP      |            |
|---------------------------------|--------------|--------------------|---------------------|-------------------|-----------|------------|
| T/P                             | Training     | Prediction         | Training            | Prediction        | Training  | Prediction |
| A.                              | .757±.043    | .729±.022          | .956±.019           | .824±.022         | .973±.016 | .855±.023  |
| AUC                             | .756±.043    | .733±.022          | .955±.020           | .823±.023         | .972±.017 | .854±.024  |
| F <sub>1</sub> <sup>&amp;</sup> | .754±.044    | .725±.024          | .956±.019           | .824±.023         | .973±.016 | .854±.024  |
| F <sub>1(+)</sub> <sup>+</sup>  | .743±.057    | .715±.036          | .959±.018           | .836±.022         | .975±.015 | .863±.022  |
| F <sub>1(-)</sub> <sup>#</sup>  | .761±.058    | .737±.034          | .952±.022           | .810±.027         | .971±.018 | .844±.028  |
| P *                             |              | < e <sup>-90</sup> |                     | < e <sup>-5</sup> |           |            |

Each data field shows average ± std from 1000 random split of Doniger *et al.*

<sup>&</sup>: total samples macro weighted F<sub>1</sub>;

<sup>+</sup>: positive sample F<sub>1</sub>;

<sup>#</sup>: negative samples F<sub>1</sub>.

\*P-value for all of A., AUC and F<sub>1</sub><sup>&</sup> of this column to last column (C + CP), T-test.