Supplementary Table 3. Data description for testing H-RACS on unexplored drug combinations and cell lines.

| Category                        | Data usage | Combinational scenarios | Drug combinations | Cell lines |
|---------------------------------|------------|-------------------------|-------------------|------------|
| A&O dataset                     |            | 33,574                  | 1,380             | 116        |
| unexplored drug combinations    | Training   | 22,320                  | 920               | 116        |
|                                 | External test | 11,254                | 460               | 116        |
| unexplored cell lines           | Training   | 22,680                  | 1380              | 77         |
|                                 | External test | 10,894                | 1378              | 39         |