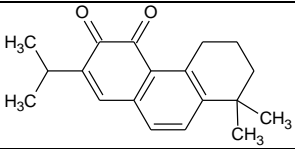
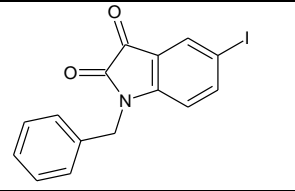
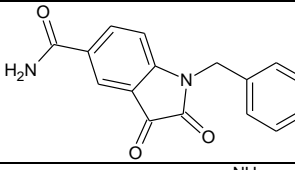
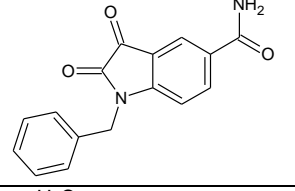
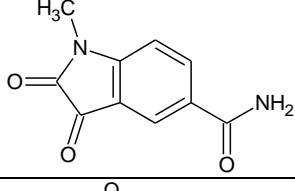
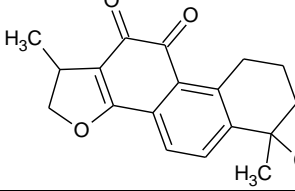
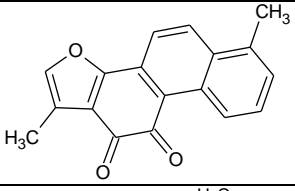
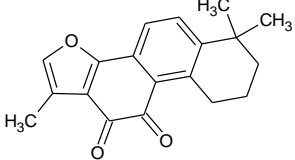
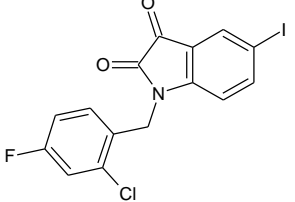
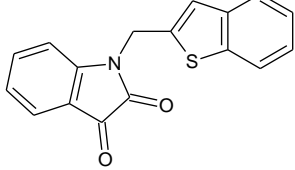
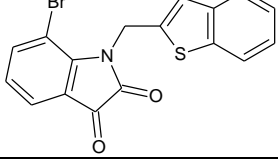
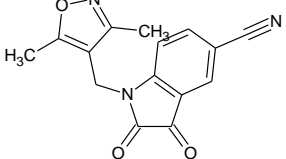
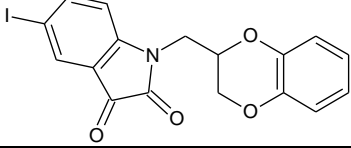
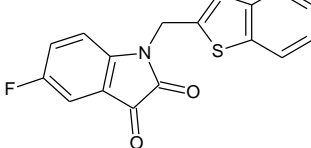
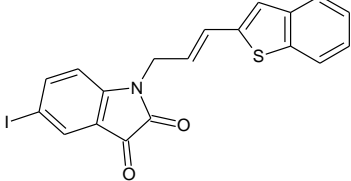
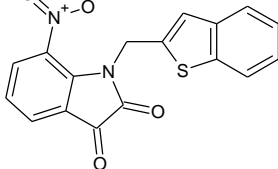
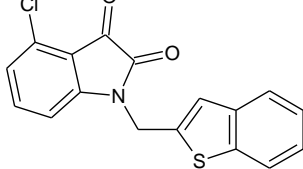
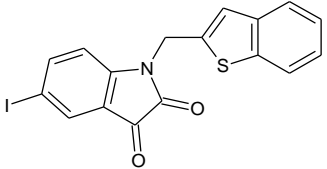
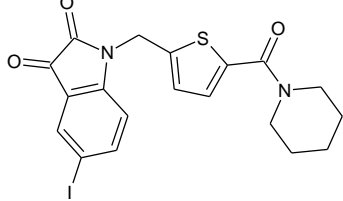
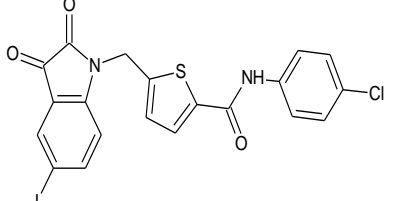
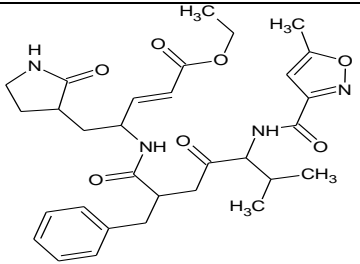
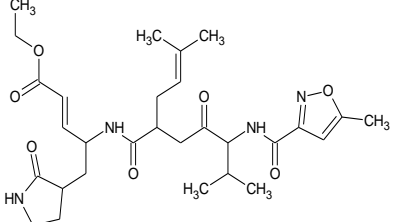
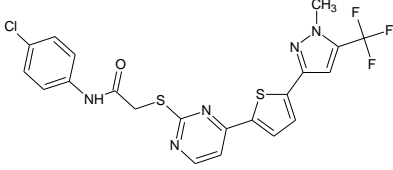
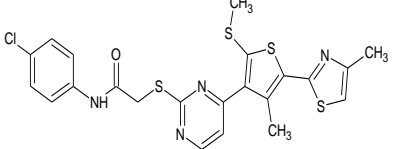
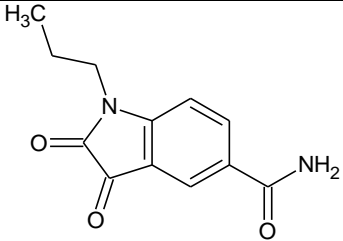


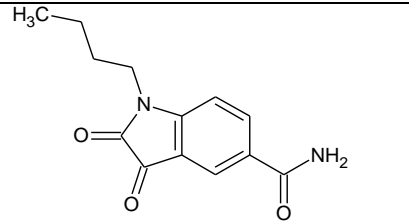
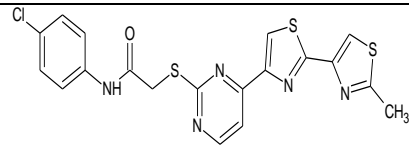
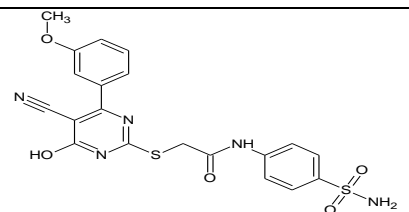
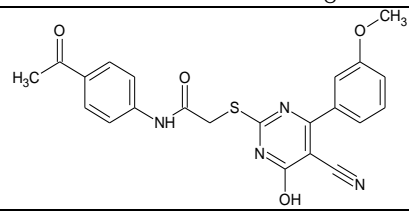
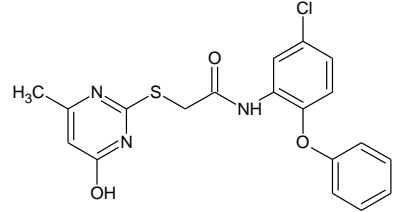
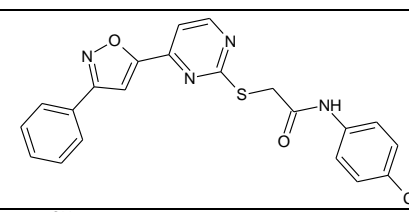
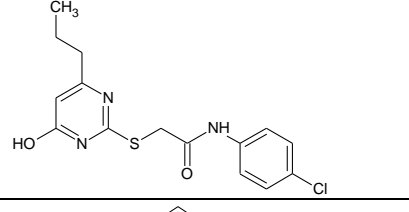
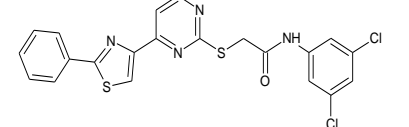
## SUPPLEMENTARY MATERIAL

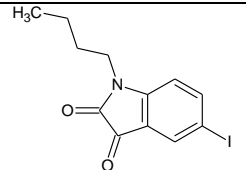
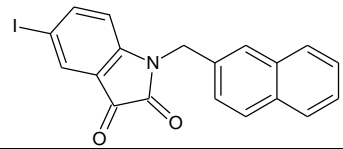
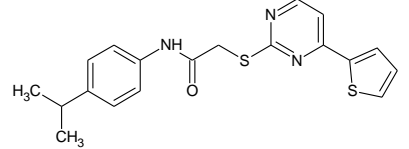
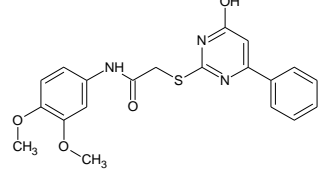
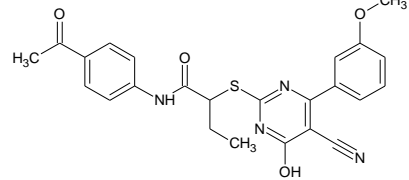
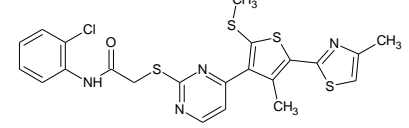
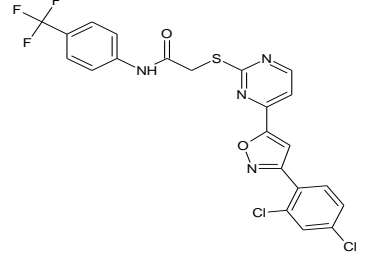
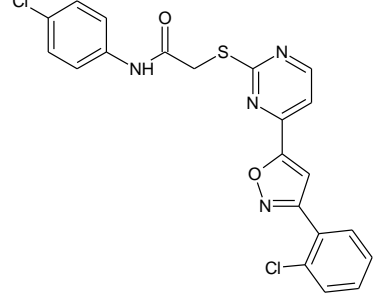
Supplementary Table 1: Structure, and Molecular Descriptors of 3C-like protease inhibitors

| Comp No | Molecular structure   | AATS8v | AATS3i | MATS6c | GATS8e | BCUT p-1h | ZMIC 2 | VE1_D |
|---------|---|--------|--------|--------|--------|-----------|--------|-------|
| 1       |    | 0.202  | 0.294  | 0.632  | 0.593  | 0.454     | 0.085  | 0.243 |
| 2       |    | 0.525  | 0.294  | 0.63   | 0.349  | 0.655     | 0.293  | 0.614 |
| 3       |    | 0.686  | 0.278  | 0.795  | 0.474  | 0.327     | 0.226  | 0.29  |
| 4       |   | 0.389  | 0.397  | 0.82   | 0.506  | 0.3       | 0.139  | 0.313 |
| 5       |  | 0      | 0.4    | 0.95   | 1      | 0.172     | 0.006  | 0.541 |
| 6       |  | 0.265  | 0.295  | 0.581  | 0.822  | 0.479     | 0.063  | 0.106 |
| 7       |  | 0.37   | 0      | 0.536  | 0.605  | 0.436     | 0.153  | 0.205 |
| 8       |  | 0.322  | 0.188  | 0.584  | 0.921  | 0.459     | 0.07   | 0.106 |

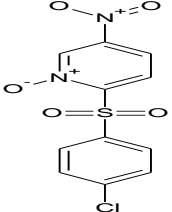
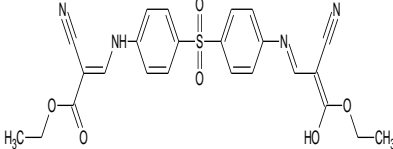
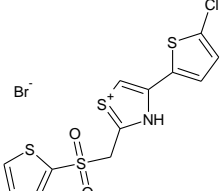
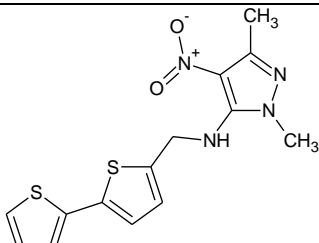
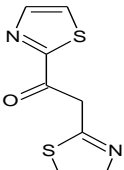
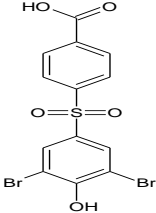
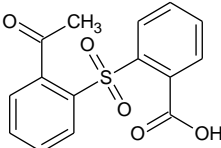
|    |   |       |       |       |       |       |       |       |
|----|---|-------|-------|-------|-------|-------|-------|-------|
| 9  |    | 0.747 | 0.415 | 0.745 | 0.44  | 0.657 | 0.271 | 0.475 |
| 10 |    | 0.788 | 0.23  | 0.581 | 0.394 | 0.55  | 0.188 | 0.447 |
| 11 |    | 0.918 | 0.168 | 0.649 | 0.391 | 0.582 | 0.237 | 0.589 |
| 12 |    | 0.284 | 0.455 | 0.583 | 0.518 | 0.309 | 0.053 | 0.064 |
| 13 |   | 0.857 | 0.539 | 0.709 | 0.32  | 0.654 | 0.268 | 0.424 |
| 14 |  | 0.84  | 0.361 | 0.747 | 0.324 | 0.55  | 0.138 | 0.417 |
| 15 |  | 0.87  | 0.197 | 0.396 | 0.328 | 0.655 | 0.254 | 0.542 |
| 16 |  | 0.846 | 0.274 | 0.777 | 0.418 | 0.562 | 0.176 | 0.7   |
| 17 |  | 0.907 | 0.21  | 0.478 | 0.427 | 0.56  | 0.183 | 0.544 |

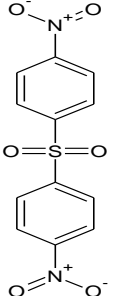
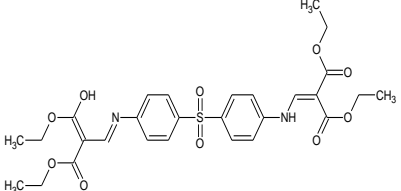
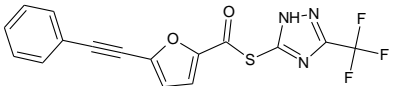
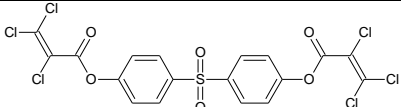
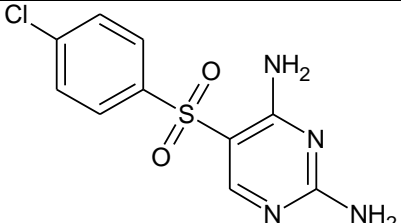
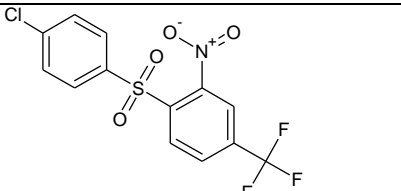
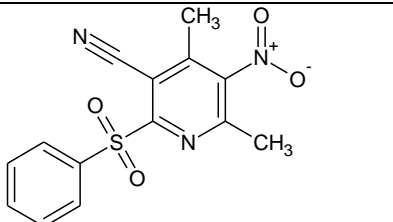
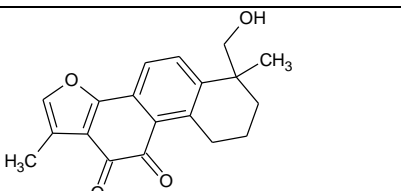
|    |   |       |       |       |       |       |       |       |
|----|---|-------|-------|-------|-------|-------|-------|-------|
| 18 |    | 0.971 | 0.123 | 0.663 | 0.392 | 0.661 | 0.269 | 0.417 |
| 19 |    | 0.549 | 0.544 | 0.846 | 0.238 | 0.661 | 0.253 | 0.534 |
| 20 |    | 0.829 | 0.306 | 0.736 | 0.214 | 0.661 | 0.375 | 0.722 |
| 21 |   | 0.426 | 0.839 | 0.315 | 0.402 | 0.467 | 0.202 | 0.076 |
| 22 |  | 0.375 | 0.859 | 0.352 | 0.418 | 0.428 | 0.175 | 0.083 |
| 23 |  | 0.79  | 0.738 | 0.45  | 0.322 | 0.601 | 0.35  | 0.607 |
| 24 |  | 0.66  | 0.333 | 0.499 | 0.394 | 1     | 0.21  | 1     |
| 25 |  | 0.15  | 0.698 | 0.793 | 0.476 | 0.234 | 0     | 0.179 |

|    |   |       |       |       |       |       |       |       |
|----|---|-------|-------|-------|-------|-------|-------|-------|
| 26 |    | 0.17  | 0.737 | 0.818 | 0.519 | 0.247 | 0.008 | 0.246 |
| 27 |    | 0.825 | 0.605 | 0.234 | 0.362 | 0.555 | 0.208 | 0.435 |
| 28 |    | 0.673 | 0.497 | 0.306 | 0.35  | 0.423 | 0.199 | 0.863 |
| 29 |    | 0.648 | 0.466 | 0.177 | 0.408 | 0.422 | 0.171 | 0.962 |
| 30 |   | 0.633 | 0.683 | 0.27  | 0.524 | 0.322 | 0.257 | 0.417 |
| 31 |  | 0.791 | 0.585 | 0.166 | 0.327 | 0.355 | 0.305 | 0.431 |
| 32 |  | 0.55  | 0.842 | 0     | 0.58  | 0.345 | 0.094 | 0.28  |
| 33 |  | 0.81  | 0.513 | 0.484 | 0.302 | 0.505 | 0.403 | 0.232 |

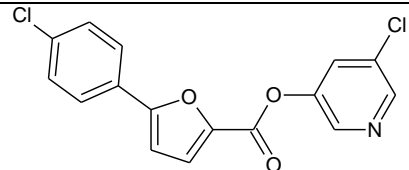
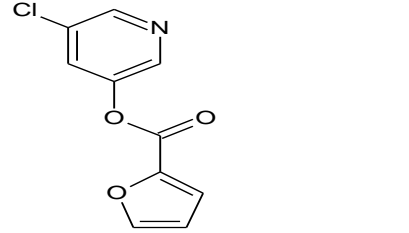
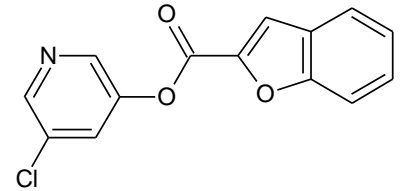
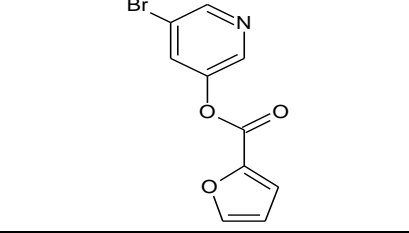
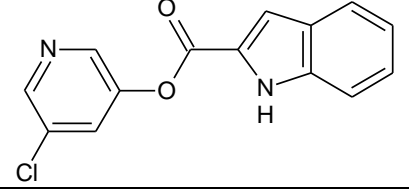
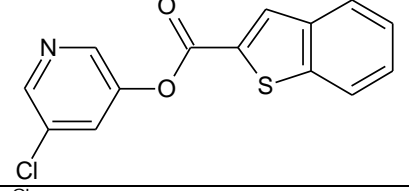
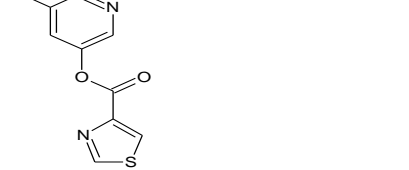
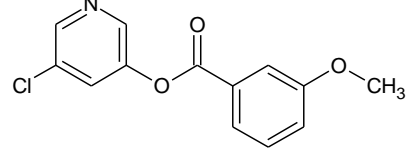
|    |   |       |       |       |       |       |       |       |
|----|---|-------|-------|-------|-------|-------|-------|-------|
| 34 |    | 0.222 | 0.675 | 0.627 | 0.329 | 0.65  | 0.114 | 0.781 |
| 35 |    | 0.836 | 0.185 | 0.615 | 0.369 | 0.657 | 0.315 | 0.424 |
| 36 |    | 0.639 | 0.531 | 0.335 | 0.58  | 0.473 | 0.153 | 0.306 |
| 37 |    | 0.566 | 0.536 | 0.212 | 0.527 | 0.386 | 0.23  | 0.253 |
| 38 |   | 0.546 | 0.497 | 0.219 | 0.345 | 0.578 | 0.162 | 0.835 |
| 39 |  | 0.655 | 0.333 | 0.65  | 0.307 | 1     | 0.21  | 0.833 |
| 40 |  | 0.885 | 0.635 | 0.652 | 0.201 | 0.358 | 0.397 | 0.478 |
| 41 |  | 0.863 | 0.569 | 0.129 | 0.35  | 0.358 | 0.375 | 0.552 |

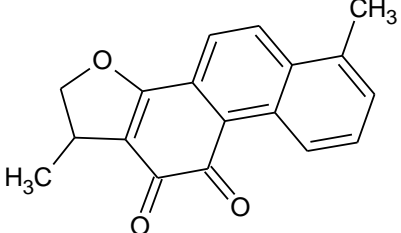
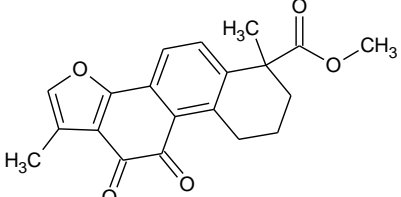
|    |  |       |       |       |       |       |       |       |
|----|--|-------|-------|-------|-------|-------|-------|-------|
| 42 |  | 0.741 | 0.36  | 0.65  | 0.383 | 0.825 | 0.522 | 0.239 |
| 43 |  | 0.664 | 1     | 0.876 | 0.459 | 0.548 | 0.241 | 0.04  |
| 44 |  | 0.433 | 0.514 | 0.725 | 0.364 | 0.751 | 0.16  | 0.151 |
| 45 |  | 0.371 | 0.327 | 0.528 | 0.169 | 0.714 | 0.184 | 0.427 |
| 46 |  | 0.562 | 0.362 | 0.521 | 0.454 | 0.988 | 0.224 | 0.536 |
| 47 |  | 0.514 | 0.358 | 0.56  | 0.491 | 0.607 | 0.048 | 0.984 |
| 48 |  | 0.282 | 0.673 | 0.42  | 0.397 | 0.741 | 0.088 | 0.003 |

|    |   |       |       |       |       |       |       |       |
|----|---|-------|-------|-------|-------|-------|-------|-------|
| 49 |    | 0.708 | 0.518 | 0.33  | 0.314 | 0.562 | 0.186 | 0.052 |
| 50 |    | 0.641 | 0.608 | 0.799 | 0.457 | 0.58  | 0.344 | 0     |
| 51 |    | 0.901 | 0.297 | 0.27  | 0.519 | 0.807 | 0.226 | 0.16  |
| 52 |   | 0.564 | 0.642 | 0.6   | 0.384 | 0.66  | 0.103 | 0.456 |
| 53 |  | 0.146 | 0.633 | 0.219 | 0     | 0.334 | 0.164 | 0.113 |
| 54 |  | 0.808 | 0.09  | 0.59  | 0.549 | 0.791 | 0.538 | 0.489 |
| 55 |  | 0.233 | 0.217 | 0.325 | 0.296 | 0.719 | 0.261 | 0     |

|    |   |       |       |       |       |       |       |       |
|----|---|-------|-------|-------|-------|-------|-------|-------|
| 56 |    | 0.663 | 0.373 | 0.046 | 0.374 | 0.546 | 0.475 | 0     |
| 57 |    | 0.506 | 0.719 | 0.691 | 0.305 | 0.583 | 0.596 | 0     |
| 58 |    | 0.819 | 0.842 | 0.193 | 0.178 | 0.262 | 0.288 | 0.325 |
| 59 |    | 1     | 0.312 | 0.824 | 0.47  | 0.572 | 1     | 0     |
| 60 |   | 0.44  | 0.55  | 1     | 0.139 | 0.583 | 0.152 | 0.201 |
| 61 |  | 0.701 | 0.422 | 0.518 | 0.445 | 0.648 | 0.362 | 0.219 |
| 62 |  | 0.294 | 0.4   | 0.455 | 0.146 | 0.708 | 0.211 | 0.243 |
| 63 |  | 0.359 | 0.225 | 0.466 | 0.671 | 0.465 | 0.043 | 0.151 |



|    |   |       |       |       |       |       |       |       |
|----|---|-------|-------|-------|-------|-------|-------|-------|
| 64 |    | 0.895 | 0.483 | 0.91  | 0.52  | 0.15  | 0.167 | 0.023 |
| 65 |    | 0.477 | 0.737 | 0.698 | 0.263 | 0     | 0.008 | 0.026 |
| 66 |    | 0.952 | 0.506 | 0.688 | 0.172 | 0.043 | 0.069 | 0.265 |
| 67 |   | 0.547 | 0.653 | 0.716 | 0.198 | 0.192 | 0.08  | 0.026 |
| 68 |  | 0.898 | 0.564 | 0.718 | 0.208 | 0.106 | 0.056 | 0.265 |
| 69 |  | 0.964 | 0.272 | 0.724 | 0.154 | 0.453 | 0.096 | 0.265 |
| 70 |  | 0.767 | 0.666 | 0.687 | 0.268 | 0.105 | 0.052 | 0.026 |
| 71 |  | 0.656 | 0.466 | 0.583 | 0.327 | 0.088 | 0.022 | 0.08  |

|    |   |       |       |       |       |       |       |       |
|----|---|-------|-------|-------|-------|-------|-------|-------|
| 72 |  | 0.31  | 0.17  | 0.52  | 0.531 | 0.458 | 0.084 | 0.205 |
| 73 |  | 0.374 | 0.182 | 0.377 | 0.347 | 0.494 | 0.065 | 0.209 |