

**Table S1.** List of Cyp protein entries with incomplete cytochrome P450 domain

| Trichoderma spp.        | Incomplete entries | Incomplete terminus | Cytochrome P-450 domain (amino acid residues) |      |
|-------------------------|--------------------|---------------------|-----------------------------------------------|------|
|                         |                    |                     | Start                                         | End  |
| <i>T. asperellum</i>    | Trias1 74589       | C                   | 8                                             | 268  |
|                         | Trias1 68713       | N                   | 109                                           | 419  |
|                         | Trias1 51693       | N                   | 242                                           | 503  |
|                         | Trias1 63192       | N                   | 185                                           | 479  |
|                         | Trias1 148485      | N                   | 235                                           | 435  |
|                         | Trias1 149507      | N                   | 158                                           | 461  |
|                         | Trias1 57351       | N                   | 207                                           | 354  |
|                         | Trias1 74377       | N                   | 106                                           | 457  |
|                         | Trias1 58239       | N                   | 160                                           | 480  |
|                         | Trias1 334617      | N                   | 206                                           | 468  |
|                         | Trias1 65994       | N                   | 164                                           | 526  |
|                         | Trias1 378536      | Pseudogene          |                                               |      |
|                         | Trias1 53084       | Pseudogene          |                                               |      |
|                         | Trias1 154835      | Pseudogene          |                                               |      |
| <i>T. atroviride</i>    | Triat2 313069      | N                   | 188                                           | 432  |
|                         | Triat2 156885      | N                   | 242                                           | 503  |
|                         | Triat2 174966      | N                   | 52                                            | 349  |
|                         | Triat2 293815      | N                   | 227                                           | 483  |
|                         | Triat2 296774      | N                   | 141                                           | 456  |
|                         | Triat2 303744      | N                   | 135                                           | 518  |
|                         | Triat2 38322       | N                   | 319                                           | 488  |
|                         | Triat2 293435      | N                   | 183                                           | 564  |
|                         | Triat2 216002      | N                   | 169                                           | 509  |
|                         | Triat2 79360       | N                   | 208                                           | 328  |
|                         | Triat2 293464      | N                   | 938                                           | 994  |
|                         | Triat2 88322       | N                   | 959                                           | 1041 |
|                         | Triat2 301918      | Pseudogene          | 101                                           | 139  |
| <i>T. citrinoviride</i> | Trici1 9295        | C                   | 104                                           | 390  |
|                         | Trici1 7681        | N                   | 219                                           | 414  |
|                         | Trici1 2997        | N                   | 5                                             | 85   |
|                         | Trici1 54417       | N                   | 198                                           | 461  |
|                         | Trici1 59297       | N                   | 166                                           | 454  |
|                         | Trici1 58984       | N                   | 241                                           | 495  |
|                         | Trici1 66123       | N                   | 174                                           | 506  |
|                         | Trici1 66522       | N                   | 226                                           | 538  |
|                         | Trici1 148916      | N                   | 216                                           | 528  |
|                         | Trici1 149423      | N                   | 139                                           | 248  |
|                         | Trici1 61028       | N                   | 331                                           | 517  |
|                         | Trici1 59740       | N                   | 36                                            | 381  |
|                         | Trici1 168800      | N                   | 1                                             | 375  |
|                         | Trici1 170026      | N                   | 322                                           | 466  |
|                         | Trici1 54905       | N                   | 318                                           | 537  |
|                         | Trici1 64273       | N                   | 113                                           | 418  |
|                         | Trici1 2998        | NC                  | 122                                           | 192  |

|                           |               |   |     |      |
|---------------------------|---------------|---|-----|------|
|                           | Trici1 169764 | N | 24  | 318  |
| <i>T. harzianum</i>       | Triha1 47771  | N | 2   | 169  |
|                           | Triha1 525301 | N | 210 | 518  |
|                           | Triha1 554415 | N | 245 | 435  |
|                           | Triha1 94359  | N | 141 | 493  |
|                           | Triha1 100004 | N | 100 | 453  |
|                           | Triha1 498331 | N | 208 | 493  |
|                           | Triha1 5267   | N | 234 | 429  |
|                           | Triha1 481072 | N | 246 | 519  |
|                           | Triha1 21965  | N | 53  | 486  |
|                           | Triha1 86064  | N | 104 | 419  |
|                           | Triha1 93338  | N | 49  | 483  |
|                           | Triha1 114691 | N | 234 | 505  |
|                           | Triha1 552903 | N | 143 | 495  |
|                           | Triha1 7362   | N | 55  | 524  |
|                           | Triha1 549187 | N | 21  | 311  |
|                           | Triha1 99484  | C | 44  | 236  |
|                           | Triha1 145743 | N | 653 | 1014 |
| <i>T. longibrachiatum</i> | Trilo1 56127  | N | 191 | 368  |
|                           | Trilo1 60327  | N | 191 | 479  |
|                           | Trilo1 356685 | N | 193 | 504  |
|                           | Trilo1 367454 | N | 75  | 183  |
|                           | Trilo1 361148 | N | 246 | 519  |
|                           | Trilo1 3525   | N | 322 | 525  |
|                           | Trilo1 361541 | N | 145 | 562  |
|                           | Trilo1 58830  | N | 279 | 456  |
|                           | Trilo1 363943 | N | 173 | 487  |
|                           | Trilo1 45702  | N | 351 | 545  |
|                           | Trilo1 51748  | N | 559 | 340  |
|                           | Trilo1 60572  | N | 221 | 511  |
|                           | Trilo1 205473 | N | 315 | 534  |
|                           | Trilo1 4413   | N | 2   | 75   |
|                           | Trilo1 69955  | C | 100 | 257  |
| <i>T. reesei</i>          | Trire2 54166  | N | 216 | 393  |
|                           | Trire2 4999   | N | 165 | 445  |
|                           | Trire2 65360  | N | 159 | 478  |
|                           | Trire2 73344  | N | 322 | 517  |
|                           | Trire2 66453  | N | 234 | 493  |
|                           | Trire2 82133  | N | 229 | 520  |
|                           | Trire2 69648  | N | 113 | 456  |
|                           | Trire2 64377  | N | 142 | 415  |
|                           | Trire2 37827  | N | 298 | 446  |
|                           | Trire2 69883  | N | 58  | 390  |
|                           | Trire2 10312  | N | 714 | 1026 |
|                           | Trire2 120889 | N | 328 | 524  |
| <i>T. virens</i>          | Trivi2 53375  | N | 164 | 554  |

|               |   |     |     |
|---------------|---|-----|-----|
| Trivi2 147960 | N | 185 | 517 |
| Trivi2 191659 | N | 1   | 184 |
| Trivi2 53058  | N | 153 | 568 |
| Trivi2 52099  | N | 216 | 393 |
| Trivi2 13758  | N | 302 | 444 |
| Trivi2 49153  | N | 207 | 527 |
| Trivi2 53278  | N | 233 | 520 |
| Trivi2 53366  | N | 226 | 507 |
| Trivi2 60000  | N | 290 | 486 |
| Trivi2 91346  | N | 165 | 490 |
| Trivi2 126116 | N | 146 | 466 |
| Trivi2 147207 | N | 158 | 431 |
| Trivi2 193168 | N | 59  | 343 |
| Trivi2 214982 | N | 208 | 493 |
| Trivi2 216144 | N | 202 | 455 |
| Trivi2 38198  | N | 180 | 503 |
| Trivi2 29262  | N | 5   | 85  |
| Trivi2 32911  | N | 92  | 419 |
| Trivi2 34391  | N | 233 | 487 |
| Trivi2 192422 | N | 191 | 453 |
| Trivi2 59906  | N | 177 | 284 |
| Trivi2 223842 | N | 79  | 163 |
| Trivi2 60068  | N | 29  | 421 |
| Trivi2 37402  | N | 340 | 561 |
| Trivi2 59079  | N | 85  | 415 |
| Trivi2 70946  | N | 383 | 494 |
| Trivi2 134374 | N | 278 | 465 |
| Trivi2 155466 | N | 223 | 459 |
| Trivi2 196674 | N | 158 | 491 |
| Trivi2 205975 | C | 46  | 222 |
| Trivi2 200187 | N | 329 | 483 |

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**Table S2.** Cytochrome P450s associated with secondary metabolism–related gene clusters

| Species              | Gene Cluster                                              | No. of CYPs per cluster | Protein ID of Cyps                                                            |
|----------------------|-----------------------------------------------------------|-------------------------|-------------------------------------------------------------------------------|
| <i>T. virens</i>     | NRPS/ Trivi2:70629                                        | 1                       | Trivi2:186579 B/Cyp55                                                         |
|                      | NRPS/ Trivi2:62540                                        | 1                       | Trivi2:212112 E//Cyp65                                                        |
|                      | NRPS/ Trivi2:70770                                        | 1                       | Trivi2:191958 E//Cyp584                                                       |
|                      | NRPS/Trivi2:70742                                         | 1                       | Trivi2:191958 E//Cyp584                                                       |
|                      | NRPS/Trivi2:78708                                         | 1                       | Trivi2:216161 E//Cyp613                                                       |
|                      | NRPS/Trivi2: 48850                                        | 1                       | Trivi2:49165 E/Cyp655                                                         |
|                      | NRPS/Trivi2: 53833 & 28610                                | 1                       | Trivi2:60180 E//Cyp627                                                        |
|                      | PKS/Trivi2:47407                                          | 1                       | Trivi2:47601 E//Cyp530                                                        |
|                      | PKS/Trivi2:51044                                          | 2                       | Trivi2:50878 E//Cyp584                                                        |
|                      | NRPS-PKS/Trivi2:48850                                     | 1                       | Trivi2:49165 E/Cyp655                                                         |
|                      | NRPS-PKS/Trivi2:53833, 28610                              | 1                       | Trivi2:60180 E//Cyp627                                                        |
|                      | NRPS-PKS/Trivi2:28610                                     | 1                       | Trivi2-60180 E//Cyp627                                                        |
|                      | NRPS-PKS/Trivi2:78708                                     | 1                       | Trivi2-216161 E//Cyp613                                                       |
|                      | NRPS-Like/Trivi2:60181                                    | 1                       | Trivi2:60180 E//Cyp627                                                        |
|                      | TC/Trivi2:224958                                          | 2                       | Trivi2:193582 E//Cyp65<br>Trivi2:181847 E//IV/Cyp551                          |
|                      | TC/Trivi2:53145                                           | 1                       | Trivi2:53201 E//Cyp5094                                                       |
|                      | TC/Trivi2:56195                                           | 3                       | Trivi2:74291 E//Cyp5094<br>Trivi2:74289 E//Cyp5117<br>Trivi2:39153 Cyp5104    |
| <i>T. atroviride</i> | NRPS/Triat2:39904 or 40716<br>NRPS/Triat2:10385 or 181616 | 1                       | Triat2:152285 E//Cyp620                                                       |
|                      | PKS/Triat2:51726 or 188840                                | 1                       | Triat2:304119 E//Cyp65                                                        |
|                      | PKS/Triat2:45854 or 217234                                | 1                       | Triat2:45536-E//Cyp584                                                        |
|                      | PKS/Triat2:45973                                          | 1                       | Triat2:263459 E//Cyp530                                                       |
|                      | PKS/Triat2:32458<br>PKS/Triat:245485/267549               | 3                       | Triat2:295844 E//Cyp548<br>Triat2:84128 E//Cyp5082<br>Triat2-295125 E-I/Cyp65 |
|                      | NRPS-PKS/<br>Triat2:51715(212102)                         | 2                       | Triat2:304119 E//Cyp65,<br>Triat2:51470 E-I/Cyp5043                           |
|                      | NRPS-Like/Triat2:224197                                   | 1                       | Triat2:319887 E//Cyp530                                                       |
| <i>T. reesei</i>     | NRPS/Trire2:24586<br>NRPS/Trire2: 60751                   | 1<br>1                  | Trire2:53168 E//Cyp613,<br>Trire2-27722 E//Cyp5046                            |
|                      | NRPS/Trire2: 271005                                       | 2                       | Trire2: 38749 E//Cyp587,<br>Trire2: 70984 E//Cyp531                           |
|                      | PKS/Trire2:65172                                          | 1                       | Trire2:65036 E//Cyp584                                                        |
|                      | PKS/Trire2:65116                                          | 1                       | Trire2:65040 E//Cyp530                                                        |
|                      | PKS/Trire2:82208<br>PKS/Trire2:73618                      | 3                       | Trire2:70161 E//Cyp584<br>Trire2:37950 E//Cyp617,<br>Trire2-102487 E//Cyp620  |
|                      | NRPS-PKS/Trire2:58285                                     | 1                       | Trire2:58953 E//Cyp655                                                        |
|                      | NRPS-PKS/Trire2:59315<br>NRPS-PKS/Trire2:4117             | 2                       | Trire2:59377 E//Cyp627<br>Trire2-78387 E//Cyp58                               |
|                      | NRPS/Trilo1: 1392769                                      | 1                       | Trilo1: 5795 E//Cyp613                                                        |

|                      |                            |   |                                                                              |
|----------------------|----------------------------|---|------------------------------------------------------------------------------|
|                      | NRPS/Trilo1: 165613        | 1 | Trilo1: 366608 E//Cyp531                                                     |
|                      | PKS/Trilo1:1470852         | 1 | Trilo1:363456 E//Cyp584                                                      |
|                      | PKS/Trilo1:1431707         | 1 | Trilo1:66680 E//Cyp530                                                       |
|                      | PKS/Trilo1:1434581         | 1 | Trilo1:62496 E//Cyp584                                                       |
|                      | PKS/Trilo1:1431707         | 2 | Trilo1:62513 E//Cyp547,<br>Trilo1:241300 E//Cyp620                           |
|                      | NRPS-PKS/Trilo1:1459985    | 1 | Trilo1:16230 E/Cyp655                                                        |
|                      | NRPS-PKS/Trilo1:1471953    | 1 | Trilo1:21463 E//Cyp58                                                        |
|                      | TC/Trilo1:1406488 or 36731 | 2 | Trilo1:23205 E//Cyp65<br>Trilo1:62189 E/IV/Cyp551                            |
|                      | TC/Trilo1:1442452 or 61665 | 1 | Trilo1:68704 E/IV/Cyp570                                                     |
|                      | NRPS/Trici1:1122832        | 1 | Trici1:21500 E/IV/Cyp548                                                     |
|                      | NRPS/Trici1:1129911        | 1 | Trici1:61488 E//Cyp5046                                                      |
|                      | NRPS/Trici1:1129911        | 1 | Trici1:68598 E//Cyp613                                                       |
|                      | PKS/Trici1:65461           | 1 | Trici1:52618 E/IV/Cyp5039                                                    |
|                      | PKS/Trici1:7685            | 1 | Trici1:59853 E//Cyp584                                                       |
|                      | PKS/Trici1:1186452         | 2 | Trici1:61780 E//Cyp617<br>Trici1:61695 E//Cyp584                             |
|                      | NRPS-PKS/Trici1:1107986    | 1 | Trici1:62893 E//Cyp627                                                       |
|                      | NRPS-PKS/Trici1:1131145    | 1 | Trici1:153235 E/Cyp655                                                       |
|                      | TC/Trici1:5384             | 2 | Trici1:5385 E/IV/Cyp551<br>Trici1:164732 E/Cyp65                             |
|                      | TC/Trici1:52419            | 2 | Trici1:4125 E//Cyp503<br>Trici1:19588 E//Cyp5181                             |
|                      | NRPS/Triha1:15930          | 1 | Triha1:507225 E//Cyp587                                                      |
|                      | NRPS/Triha1:551513         | 1 | Triha1:81578 B/Cyp55                                                         |
|                      | NRPS/Triha1:80219          | 1 | Triha1:493712 E//Cyp5246                                                     |
|                      | NRPS/Triha1:496332         | 2 | Triha1:521249 E//Cyp613<br>Triha1:483190 E//Cyp5046                          |
|                      | NRPS/Triha1:501208         | 1 | Triha1:501206 E//Cyp561                                                      |
|                      | NRPS/Triha1:7629           | 1 | Triha1-532775 E/IV/Cyp680                                                    |
|                      | PKS/Triha1:536358          | 3 | Triha1:40927 E/IV/Cyp5129<br>Triha1:488675 E/IV/Cyp631<br>Triha1:5 E//Cyp552 |
|                      | PKS/Triha1:85730           | 2 | Triha1:495469 E//Cyp540<br>Triha1:520506 E/IV/Cyp570                         |
|                      | PKS/Triha1:120155          | 1 | Triha1:521979 E//Cyp65, 7362                                                 |
|                      | PKS/Triha1:509408          | 1 | Triha1:145803 E/IV/Cyp52                                                     |
|                      | PKS/Triha1: 526013         | 1 | Triha1:501866 E//Cyp65                                                       |
|                      | NRPS-PKS/Triha1:488711     | 1 | Triha1:514484 E//Cyp65                                                       |
|                      | NRPS-PKS/Triha1:87171      | 1 | Triha1:87842 E//Cyp5068                                                      |
|                      | NRPS-PKS/Triha1:96798      | 2 | Triha1:9617 Cyp685,<br>Triha1:96879 E/II/Cyp655                              |
|                      | TC/Triha1:113113           | 1 | Triha1:507006 E//Cyp65                                                       |
|                      | TC/Triha1:523651           | 1 | Triha1:507008 E/IV/Cyp551                                                    |
| <i>T. asperellum</i> | NRPS/ Trias1:75656         | 1 | Trias1:454396 E/IV/Cyp559                                                    |
|                      | NRPS/Trias1:74656          | 1 | Trias1:166901 E/IV/Cyp548                                                    |
|                      | NRPS/Trias1:79628          | 1 | Trias1:139185 E//Cyp620                                                      |
|                      | NRPS/Trias1:89466          | 1 | Trias1:147445 E//Cyp5134                                                     |

|  |                   |   |                          |
|--|-------------------|---|--------------------------|
|  | NRPS/Trias1:71435 | 1 | Trias1:71439 E//Cyp548   |
|  | PKS/Trias1:456732 | 1 | Trias1:137162 E//Cyp5082 |