Supplementary Material for

**Crystal structure of palbociclib form A, C24H29N7O2**

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**Figure S1.** Theoretical XRD pattern for palbociclib form A for CuKα-radiation.

**Table S1.** Characteristic peak positions and intensities for palbociclib (λ = 0.7500 Å)

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| H | K | L | *d*obs (Å) | *d*calc (Å) | *∆d* | *2θ*obs (°) | *2θ*calc (°) | *∆2θ* | *I/I*o |
| 0 | 0 | 2 | 17.61274 | 17.56806 | -0.0447 | 2.445 | 2.446 | 0.001 | 0.36 |
| 1 | 0 | 0 | 11.07733 | 11.06238 | -0.015 | 3.885 | 3.885 | 0.000 | 0.23 |
| 0 | 0 | 4 | 8.7904 | 8.7840 | -0.0064 | 4.890 | 4.894 | 0.004 | 0.39 |
| 1 | 0 | 2 | 8.6134 | 8.6177 | 0.0043 | 4.980 | 4.998 | 0.018 | 0.53 |
| 1 | 0 | -4 | 7.6629 | 7.6641 | 0.0012 | 5.605 | 5.609 | 0.004 | 0.34 |
| 2 | 0 | 0 | 5.5347 | 5.5312 | -0.0035 | 7.755 | 7.775 | 0.020 | 0.15 |
| 2 | 0 | -4 | 5.1756 | 5.1687 | -0.0069 | 8.310 | 8.321 | 0.011 | 0.42 |
| 0 | 1 | 3 | 5.0661 | 5.0630 | -0.0031 | 8.485 | 8.495 | 0.010 | 0.13 |
| 0 | 1 | 4 | 4.7357 | 4.7309 | -0.0048 | 9.080 | 9.093 | 0.013 | 0.38 |
| 2 | 0 | -6 | 4.5002 | 4.4935 | -0.0067 | 9.565 | 9.574 | 0.009 | 0.38 |
| 1 | 1 | 4 | 4.1939 | 4.1900 | -0.0039 | 10.265 | 10.270 | 0.005 | 0.16 |
| 0 | 1 | 6 | 4.0559 | 4.0528 | -0.0031 | 10.605 | 10.618 | 0.013 | 0.11 |
| 2 | -1 | -1 | 3.9848 | 3.9790 | -0.0058 | 10.805 | 10.819 | 0.014 | 0.32 |
| 2 | 1 | 0 | 3.9447 | 3.9404 | -0.0043 | 10.910 | 10.922 | 0.012 | 1.00 |
| 2 | 1 | 1 | 3.8601 | 3.8556 | -0.0045 | 11.150 | 11.163 | 0.013 | 0.33 |
| 3 | 0 | -2 | 3.7462 | 3.7629 | 0.0167 | 11.490 | 11.439 | -0.051 | 0.09 |
| 3 | -1 | -2 | 3.1192 | 3.1259 | 0.0067 | 13.805 | 13.780 | -0.025 | 0.15 |
| 3 | 1 | 0 | 3.0858 | 3.0822 | -0.0036 | 13.960 | 13.977 | 0.017 | 0.11 |
| 3 | -1 | -5 | 3.01703 | 3.0136 | -0.0034 | 14.275 | 14.297 | 0.021 | 0.06 |
| 3 | 1 | 2 | 2.9573 | 2.9531 | -0.0042 | 14.570 | 14.591 | 0.021 | 0.09 |
| 3 | 0 | 6 | 2.8692 | 2.8726 | 0.0034 | 15.020 | 15.002 | -0.018 | 0.07 |

Atomic coordinates of the optimized model

CELL 0.71073 11.3249 5.6315 35.9681 90 101.51 90

LATT 1

SYMM 0.5-X,0.5+Y,0.5-Z

O1 0.6457 0.40195 0.13914

O5 0.57219 -0.10485 0.06614

N1 1.28085 1.68049 0.16829

N5 1.44953 1.91006 0.22889

H113 1.47685 2.06175 0.24456

N9 1.15084 1.40188 0.07563

N13 0.92427 0.8083 0.08677

N17 0.92404 0.78132 0.01969

N21 0.80337 0.559 0.11527

N25 1.0352 1.07024 0.05588

H85 1.04935 1.12257 0.02921

C1 1.4497 1.96414 0.1883

H1 1.54201 2.00692 0.18536

H5 1.39157 2.118 0.17793

C5 1.40493 1.74737 0.16367

H9 1.40331 1.78939 0.13385

H13 1.46762 1.59675 0.17162

C9 1.27615 1.63904 0.20859

H17 1.18183 1.60966 0.21067

H21 1.32855 1.47962 0.21998

C13 1.32402 1.85688 0.23269

H25 1.26257 2.00837 0.22363

H29 1.32334 1.81972 0.26265

C17 1.09126 1.21386 0.08634

C21 1.09032 1.16927 0.12475

H33 1.0423 1.01657 0.13259

C25 1.15429 1.32062 0.1522

H37 1.15635 1.2805 0.18193

C29 1.21778 1.51753 0.14185

C33 1.21028 1.54665 0.10222

H41 1.25493 1.69728 0.09168

C37 0.84497 0.62899 0.08332

C41 0.80167 0.51142 0.04812

C45 0.84849 0.59958 0.01722

H45 0.82279 0.52265 -0.01117

C49 0.95931 0.8807 0.0551

C53 0.69772 0.41562 0.11217

C57 0.66252 0.28112 0.07646

C61 0.71411 0.32389 0.04546

C65 0.85865 0.66719 0.15259

H49 0.94597 0.73208 0.14815

C69 0.88317 0.49808 0.18721

H53 0.80259 0.39427 0.18875

H57 0.95825 0.37673 0.18629

C73 0.90894 0.67823 0.22025

H61 0.90678 0.59742 0.24788

H65 0.99905 0.75682 0.22222

C77 0.81028 0.87116 0.20861

H69 0.72794 0.81859 0.21831

H73 0.83847 1.04409 0.22141

C81 0.7861 0.87938 0.16437

H77 0.81652 1.04573 0.15362

H81 0.69008 0.85954 0.15207

C85 0.56042 0.10313 0.07452

C89 0.44197 0.20053 0.08196

H89 0.45463 0.25616 0.11175

H93 0.41615 0.36099 0.06489

H97 0.37093 0.06626 0.07532

C93 0.67619 0.19551 0.00792

H101 0.6237 0.31392 -0.01354

H105 0.75567 0.13752 -0.00284

H109 0.62153 0.03916 0.01061