Supplementary data for the article:

Bjelogrlić, S. K.; Todorović, T. R.; Kojić, M.; Senćanski, M.; Nikolić, M.; Višnjevac, A.; Araškov, J.; Miljković, M.; Muller, C. D.; Filipović, N. R. Pd(II) Complexes with N-Heteroaromatic Hydrazone Ligands: Anticancer Activity, in Silico and Experimental Target Identification. *Journal of Inorganic Biochemistry* **2019**, *199*.
https://doi.org/10.1016/j.jinorgbio.2019.110758

```
#\#CIF_1.1

#  CIF produced by WinGX routine CIF_UPDATE
#  Created on 2018-06-05 at 11:19:12
#  Using CIFtbx version 3.0.4  1 Sep 2006

#  Dictionary name : cif_core.dic
#  Dictionary vers : 2.4.3
#  Request file    : c:\wingx\files\archive.reqdat
#  CIF files read  : exp_645 instrumental

#------------------ SECTION 1. GLOBAL INFORMATION -----------------------
----#

data_global

#------------------ AUDIT DETAILS -------------------------------------
----#

_audit_creation_date              2018-06-05
_audit_creation_method            'WinGX routine CIF_UPDATE'
_audit_conform_dict_name          cif_core.dic
_audit_conform_dict_version       2.4
_audit_conform_dict_location      ftp://ftp.iucr.org/pub/cif_core.dic
_audit_update_record              ?

#=====================================================================
======
#
# SUBMISSION DETAILS
# Name and address of author for correspondence

_publ_contact_author_name         'Višnjevac, Aleksandar'
_publ_contact_author_address
;
Physical Chemistry Division
Ruđer Boškoviæ Institute
Bijenièka 54
HR-10000 Zagreb
Croatia
;
_publ_contact_author_email         'aleksandar.visnjevac@irb.hr'
_publ_contact_author_fax           '+385 1 4680245'
_publ_contact_author_phone         '+385 1 4571203'


_publ_contact_letter
;
 Submission dated :2018-06-05

Please consider this CIF for submission to the Cambridge Crystallographic
Data Centre. I certify that all authors have seen and approved of this
submission, that all have made significant scientific contributions to
the
```

```
work reported, and that all share responsibility and accountability for
the results.

This CIF  is submitted as a personal communication

This CIF is submitted as part of a journal submission
<Insert Journal details here>

<Insert NAME here>
;


#=============================================================================
======
#
# TITLE AND AUTHOR LIST

_publ_section_title
; ?
;
_publ_section_title_footnote
; ?
;

# The loop structure below should contain the names and addresses of all
# authors, in the required order of publication. Repeat as necessary.

loop_
 _publ_author_name
 _publ_author_footnote
 _publ_author_address
?
?
;?
;

#------------------  SECTION 2. COMPOUND(S) DETAILS ----------------------
----#

data_exp_645

_audit_creation_date                    2018-06-05T11:19:12-00:00
_audit_creation_method                  'WinGX routine CIF_UPDATE'

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----#
#                   CHEMICAL INFORMATION
#
#-----------------------------------------------------------------------------
----#

_chemical_formula_sum                   'C16 H17 Cl2 N3 O2 Pd'
_chemical_formula_weight                460.62
```

```
#------------------------------------------------------------------------
----#
#                   UNIT CELL INFORMATION
#
#------------------------------------------------------------------------
----#

_symmetry_cell_setting                 monoclinic
_symmetry_space_group_name_H-M         'P 21/n'
_symmetry_space_group_name_Hall        '-P 2yn'
_symmetry_Int_Tables_number            14
loop_
    _symmetry_equiv_pos_as_xyz
'x, y, z'
'-x+1/2, y+1/2, -z+1/2'
'-x, -y, -z'
'x-1/2, -y-1/2, z-1/2'

_cell_length_a                         14.4227(3)
_cell_length_b                         7.2284(2)
_cell_length_c                         17.7189(4)
_cell_angle_alpha                      90
_cell_angle_beta                       101.744(2)
_cell_angle_gamma                      90
_cell_volume                           1808.58(8)
_cell_formula_units_Z                  4
_cell_measurement_temperature          295(2)
_cell_measurement_reflns_used          2373
_cell_measurement_theta_min            4.422
_cell_measurement_theta_max            61.899

#------------------------------------------------------------------------
----#
#                   CRYSTAL INFORMATION
#
#------------------------------------------------------------------------
----#

_exptl_crystal_description             needle
_exptl_crystal_colour                  'clear light yellow'
_exptl_crystal_size_max                0.17
_exptl_crystal_size_mid                0.03
_exptl_crystal_size_min                0.02
_exptl_crystal_density_diffrn          1.692
_exptl_crystal_F_000                   920

#------------------------------------------------------------------------
----#
#                   ABSORPTION CORRECTION
#
#------------------------------------------------------------------------
----#

_exptl_absorpt_coefficient_mu          11.115
```

```
_exptl_absorpt_correction_type          multi-scan
_exptl_absorpt_process_details
;
        CrysAlisPro 1.171.38.46 (Rigaku Oxford Diffraction, 2015)
        Empirical absorption correction using spherical harmonics,
 implemented in SCALE3 ABSPACK scaling algorithm.
;
_exptl_absorpt_correction_T_min         0.66273
_exptl_absorpt_correction_T_max         1

#------------------------------------------------------------------------
----#
#                    DATA COLLECTION
#
#------------------------------------------------------------------------
----#

_diffrn_source                          'micro-focus sealed X-ray tube'
_diffrn_source_type                     'Nova (Cu) X-ray Source'
_diffrn_ambient_temperature             295(2)
_diffrn_radiation_wavelength            1.54180
_diffrn_radiation_type                  CuK\a
_diffrn_radiation_monochromator         mirror
_diffrn_radiation_probe                 x-ray
_diffrn_detector                        'CCD plate'
_diffrn_detector_type                   Ruby
_diffrn_detector_area_resol_mean        10.4323
_diffrn_orient_matrix_type
                                'CrysAlisPro convention (1999,Acta
A55,543-557)'
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_diffrn_measurement_device_type         'Xcalibur, Ruby, Nova'
_diffrn_measurement_method              '\w scans'
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_diffrn_reflns_av_unetI/netI            0.0566
_diffrn_reflns_number                   5039
_diffrn_reflns_limit_h_min              -16
_diffrn_reflns_limit_h_max              15
_diffrn_reflns_limit_k_min              -4
_diffrn_reflns_limit_k_max              8
_diffrn_reflns_limit_l_min              -20
_diffrn_reflns_limit_l_max              17
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_diffrn_measured_fraction_theta_full
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_diffrn_reflns_Laue_measured_fraction_max
                                        0.975
_diffrn_reflns_point_group_measured_fraction_full
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_diffrn_reflns_point_group_measured_fraction_max
                                        0.975
_reflns_Friedel_coverage                0
_reflns_number_total                    2799
_reflns_number_gt                       2420
_reflns_threshold_expression            'I > 2\s(I)'

#------------------------------------------------------------------------
----#
#                   COMPUTER PROGRAMS USED
#
#------------------------------------------------------------------------
----#

_computing_data_collection
                                      'CrysAlisPro 1.171.38.46 (Rigaku OD,
2015)'
_computing_cell_refinement
                                      'CrysAlisPro 1.171.38.46 (Rigaku OD,
2015)'
_computing_data_reduction
                                      'CrysAlisPro 1.171.38.46 (Rigaku OD,
2015)'
_computing_structure_refinement         'SHELXL-2016/4 (Sheldrick, 2016)'

#------------------------------------------------------------------------
----#
#                   STRUCTURE SOLUTION
#
#------------------------------------------------------------------------
----#

_atom_sites_solution_hydrogens          mixed

#------------------------------------------------------------------------
----#
#                   REFINEMENT INFORMATION
#
#------------------------------------------------------------------------
----#

_refine_ls_structure_factor_coef        Fsqd
_refine_ls_matrix_type                  full
_refine_ls_weighting_scheme             calc
```

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_refine_ls_weighting_details
                      'w=1/[\s^2^(Fo^2^)+(0.0565P)^2^] where
P=(Fo^2^+2Fc^2^)/3'
_refine_ls_hydrogen_treatment           mixed
_refine_ls_extinction_method            none
_refine_ls_number_reflns                2799
_refine_ls_number_parameters            222
_refine_ls_number_restraints            0
_refine_ls_R_factor_all                 0.0454
_refine_ls_R_factor_gt                  0.0389
_refine_ls_wR_factor_ref                0.1019
_refine_ls_wR_factor_gt                 0.0948
_refine_ls_goodness_of_fit_ref          1.002
_refine_ls_restrained_S_all             1.002
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_refine_ls_shift/su_mean                0
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_refine_diff_density_rms                0.107

#-------------------------------------------------------------------------
----#
#                   CONSTRAINTS AND RESTRAINTS
#
#-------------------------------------------------------------------------
----#


#-------------------------------------------------------------------------
----#
#                   ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS
#
#-------------------------------------------------------------------------
----#

loop_
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    _atom_type_scat_source
C C 0.0181 0.0091 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0 0 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N N 0.0311 0.018 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0492 0.0322 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cl Cl 0.3639 0.7018 'International Tables Vol C Tables 4.2.6.8 and
6.1.1.4'
Pd Pd 0.1215 3.9337 'International Tables Vol C Tables 4.2.6.8 and
6.1.1.4'

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    _atom_site_type_symbol
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```
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    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_adp_type
    _atom_site_occupancy
    _atom_site_site_symmetry_order
    _atom_site_calc_flag
    _atom_site_refinement_flags_posn
    _atom_site_refinement_flags_adp
    _atom_site_refinement_flags_occupancy
    _atom_site_disorder_assembly
    _atom_site_disorder_group
C2 C 0.5247(3) 0.2446(8) 0.8852(3) 0.0578(12) Uani 1 1 d . . . . .
H2 H 0.557326 0.252226 0.845143 0.069 Uiso 1 1 calc R U . . .
C3 C 0.5737(4) 0.2669(9) 0.9592(3) 0.0648(14) Uani 1 1 d . . . . .
H3 H 0.63866 0.287567 0.96924 0.078 Uiso 1 1 calc R U . . .
C4 C 0.5256(4) 0.2585(9) 1.0186(3) 0.0620(13) Uani 1 1 d . . . . .
H4 H 0.557665 0.273504 1.069352 0.074 Uiso 1 1 calc R U . . .
C5 C 0.4291(3) 0.2274(7) 1.0020(3) 0.0540(12) Uani 1 1 d . . . . .
H5 H 0.395563 0.222138 1.041534 0.065 Uiso 1 1 calc R U . . .
C6 C 0.3823(3) 0.2040(6) 0.9260(2) 0.0418(10) Uani 1 1 d . . . . .
C7 C 0.2805(3) 0.1726(6) 0.9037(3) 0.0437(11) Uani 1 1 d . . . . .
C8 C 0.2224(3) 0.1545(7) 0.9630(2) 0.0443(11) Uani 1 1 d . . . . .
C9 C 0.1983(4) 0.3058(7) 1.0034(3) 0.0572(13) Uani 1 1 d . . . . .
H9 H 0.220676 0.422753 0.994381 0.069 Uiso 1 1 calc R U . . .
C10 C 0.1418(4) 0.2839(9) 1.0565(3) 0.0689(16) Uani 1 1 d . . . . .
H10 H 0.124547 0.386077 1.082415 0.083 Uiso 1 1 calc R U . . .
C11 C 0.1109(4) 0.1099(10) 1.0710(3) 0.0701(16) Uani 1 1 d . . . . .
H11 H 0.073549 0.094708 1.107661 0.084 Uiso 1 1 calc R U . . .
C12 C 0.1341(4) -0.0387(9) 1.0328(3) 0.0651(15) Uani 1 1 d . . . . .
H12 H 0.112681 -0.155327 1.04334 0.078 Uiso 1 1 calc R U . . .
C13 C 0.1894(3) -0.0196(7) 0.9780(3) 0.0535(12) Uani 1 1 d . . . . .
H13 H 0.204379 -0.122544 0.951383 0.064 Uiso 1 1 calc R U . . .
C16 C 0.0793(3) 0.1958(7) 0.8249(3) 0.0470(11) Uani 1 1 d . . . . .
H16A H 0.094267 0.312866 0.851276 0.056 Uiso 1 1 calc R U . . .
H16B H 0.065004 0.106398 0.861727 0.056 Uiso 1 1 calc R U . . .
C17 C -0.0048(3) 0.2186(7) 0.7601(3) 0.0503(12) Uani 1 1 d . . . . .
C18 C -0.1682(4) 0.2920(9) 0.7346(4) 0.0691(16) Uani 1 1 d . . . . .
H18A H -0.182663 0.195912 0.695729 0.083 Uiso 1 1 calc R U . . .
H18B H -0.161184 0.408443 0.709123 0.083 Uiso 1 1 calc R U . . .
C19 C -0.2449(4) 0.3056(9) 0.7792(4) 0.0785(19) Uani 1 1 d . . . . .
H19A H -0.247743 0.192852 0.807295 0.118 Uiso 1 1 calc R U . . .
H19B H -0.304449 0.325562 0.744472 0.118 Uiso 1 1 calc R U . . .
H19C H -0.232088 0.407237 0.814703 0.118 Uiso 1 1 calc R U . . .
N1 N 0.4312(2) 0.2120(5) 0.8685(2) 0.0458(9) Uani 1 1 d . . . . .
N14 N 0.2507(3) 0.1587(5) 0.8295(2) 0.0398(8) Uani 1 1 d . . . . .
N15 N 0.1584(3) 0.1336(6) 0.7945(2) 0.0507(10) Uani 1 1 d . . . . .
O1 O -0.0043(3) 0.2135(6) 0.6937(2) 0.0762(12) Uani 1 1 d . . . . .
O2 O -0.0816(2) 0.2472(5) 0.78978(19) 0.0586(9) Uani 1 1 d . . . . .
CL1 Cl 0.47150(9) 0.19481(19) 0.69888(8) 0.0631(4) Uani 1 1 d . . . . .
CL2 Cl 0.24375(9) 0.13054(19) 0.64895(6) 0.0561(3) Uani 1 1 d . . . . .
PD1 Pd 0.34935(2) 0.17554(5) 0.76314(2) 0.04106(16) Uani 1 1 d . . . . .
H15 H 0.157(4) 0.155(8) 0.743(3) 0.07(2) Uiso 1 1 d . . . . .
```

```
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    _atom_site_aniso_U_33
    _atom_site_aniso_U_23
    _atom_site_aniso_U_13
    _atom_site_aniso_U_12
C2 0.043(3) 0.077(3) 0.053(3) 0.004(3) 0.010(2) 0.002(3)
C3 0.036(3) 0.091(4) 0.061(3) -0.002(3) -0.004(2) -0.005(3)
C4 0.047(3) 0.082(4) 0.050(3) -0.003(3) -0.008(2) -0.001(3)
C5 0.047(3) 0.070(3) 0.042(3) -0.004(2) 0.004(2) 0.002(2)
C6 0.038(2) 0.050(3) 0.036(2) 0.0004(19) 0.0047(18) 0.0034(19)
C7 0.037(2) 0.057(3) 0.037(2) -0.004(2) 0.0073(19) -0.0003(19)
C8 0.034(2) 0.065(3) 0.032(2) -0.001(2) 0.0013(18) -0.001(2)
C9 0.053(3) 0.069(4) 0.051(3) -0.017(2) 0.013(2) -0.009(2)
C10 0.057(3) 0.099(5) 0.053(3) -0.027(3) 0.016(3) -0.002(3)
C11 0.054(3) 0.115(5) 0.044(3) -0.008(3) 0.018(2) -0.007(3)
C12 0.055(3) 0.091(4) 0.050(3) 0.014(3) 0.013(2) -0.010(3)
C13 0.045(2) 0.068(3) 0.047(3) 0.007(2) 0.007(2) 0.006(2)
C16 0.035(2) 0.069(3) 0.038(2) 0.003(2) 0.0076(19) 0.002(2)
C17 0.039(3) 0.063(3) 0.048(3) 0.003(2) 0.008(2) -0.004(2)
C18 0.041(3) 0.085(4) 0.073(4) 0.009(3) -0.010(3) 0.003(3)
C19 0.042(3) 0.096(5) 0.093(5) 0.002(3) 0.003(3) 0.005(3)
N1 0.0321(19) 0.061(2) 0.044(2) -0.0019(18) 0.0065(16) 0.0000(17)
N14 0.040(2) 0.046(2) 0.0336(19) -0.0033(15) 0.0089(16) -0.0013(15)
N15 0.036(2) 0.077(3) 0.038(2) -0.003(2) 0.0074(16) -0.0011(19)
O1 0.057(2) 0.126(4) 0.041(2) 0.005(2) -0.0014(17) 0.009(2)
O2 0.0364(17) 0.078(2) 0.057(2) 0.0057(19) 0.0003(15) -0.0007(17)
CL1 0.0571(8) 0.0812(9) 0.0591(8) 0.0060(6) 0.0306(6) 0.0021(6)
CL2 0.0565(7) 0.0744(8) 0.0367(6) -0.0017(6) 0.0078(5) -0.0057(6)
PD1 0.0383(2) 0.0493(3) 0.0366(2) 0.00148(13) 0.01021(15) 0.00074(13)


#------------------------------------------------------------------------
----#
#                   MOLECULAR GEOMETRY
#
#------------------------------------------------------------------------
----#

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
;
loop_
```

```
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    _geom_bond_atom_site_label_2
    _geom_bond_distance
    _geom_bond_site_symmetry_2
    _geom_bond_publ_flag
C2 N1 1.342(6) . ?
C2 C3 1.366(7) . ?
C3 C4 1.374(8) . ?
C4 C5 1.382(7) . ?
C5 C6 1.387(6) . ?
C6 N1 1.354(6) . ?
C6 C7 1.458(6) . ?
C7 N14 1.301(5) . ?
C7 C8 1.478(6) . ?
C8 C9 1.388(7) . ?
C8 C13 1.390(7) . ?
C9 C10 1.374(8) . ?
C10 C11 1.376(9) . ?
C11 C12 1.349(8) . ?
C12 C13 1.382(7) . ?
C16 N15 1.429(6) . ?
C16 C17 1.500(6) . ?
C17 O1 1.178(6) . ?
C17 O2 1.336(6) . ?
C18 O2 1.457(6) . ?
C18 C19 1.489(8) . ?
N1 PD1 2.013(4) . ?
N14 N15 1.361(5) . ?
N14 PD1 2.025(4) . ?
CL1 PD1 2.2884(12) . ?
CL2 PD1 2.2946(12) . ?

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    _geom_angle_atom_site_label_2
    _geom_angle_atom_site_label_3
    _geom_angle
    _geom_angle_site_symmetry_1
    _geom_angle_site_symmetry_3
    _geom_angle_publ_flag
N1 C2 C3 122.2(5) . . ?
C2 C3 C4 119.1(5) . . ?
C3 C4 C5 119.1(5) . . ?
C4 C5 C6 119.8(5) . . ?
N1 C6 C5 120.0(4) . . ?
N1 C6 C7 116.9(4) . . ?
C5 C6 C7 123.1(4) . . ?
N14 C7 C6 113.2(4) . . ?
N14 C7 C8 126.4(4) . . ?
C6 C7 C8 120.4(4) . . ?
C9 C8 C13 118.9(4) . . ?
C9 C8 C7 122.3(4) . . ?
C13 C8 C7 118.8(4) . . ?
C10 C9 C8 120.5(5) . . ?
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```
C9 C10 C11 119.6(5) . . ?
C12 C11 C10 120.7(5) . . ?
C11 C12 C13 120.7(6) . . ?
C12 C13 C8 119.6(5) . . ?
N15 C16 C17 109.2(4) . . ?
O1 C17 O2 124.9(4) . . ?
O1 C17 C16 126.3(4) . . ?
O2 C17 C16 108.8(4) . . ?
O2 C18 C19 106.6(5) . . ?
C2 N1 C6 119.7(4) . . ?
C2 N1 PD1 127.0(3) . . ?
C6 N1 PD1 113.3(3) . . ?
C7 N14 N15 124.1(4) . . ?
C7 N14 PD1 117.1(3) . . ?
N15 N14 PD1 118.8(3) . . ?
N14 N15 C16 124.7(4) . . ?
C17 O2 C18 115.9(4) . . ?
N1 PD1 N14 79.53(14) . . ?
N1 PD1 CL1 95.04(11) . . ?
N14 PD1 CL1 174.53(10) . . ?
N1 PD1 CL2 174.38(11) . . ?
N14 PD1 CL2 94.85(10) . . ?
CL1 PD1 CL2 90.57(5) . . ?

# The following lines are used to test the character set of files sent by
# network email or other means. They are not part of the CIF data set
# abcdefghijklmnopqrstuvwxyzABCDEFGHIJKLMNOPQRSTUVWXYZ0123456789
# !@#$%^&*()_+{}:"~<>?|\-=[];'`,./

# END of CIF
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