

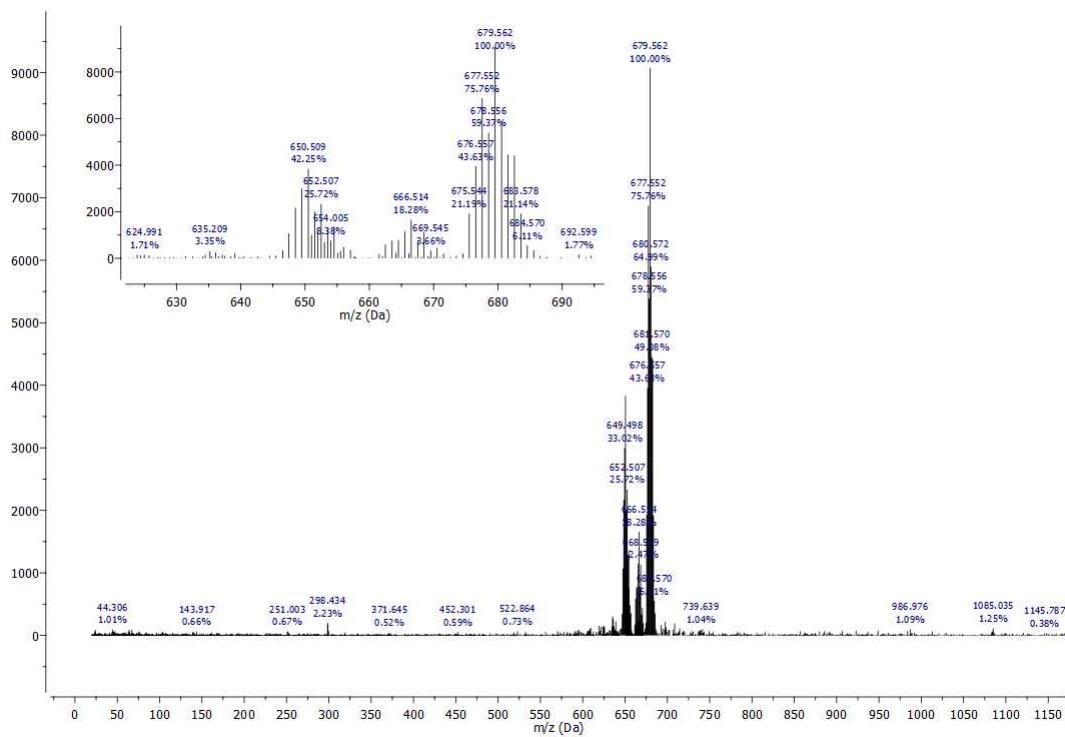
SUPPORTING INFORMATION

To the *Acta C* paper

Structural explanation of spectral features of non-symmetrical complex 2,3,7,8,12,13,17,18-octaethyl-5-((methylimino)methyl) porphyrin-palladium(II)

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Figure S1. Mass spectrum of (3).

Mass spectrum was obtained on Ultraflex II Bruker Daltonics by MALDI TOF-method following the standard procedure of the Bruker company. MS (MALDI-TOF), m/z: 680.3 (M^+), calc. for M^+ 680.2. UV-vis (CH_2Cl_2), λ_{max} ($\log \epsilon$): 397 (5.03), 515 (3.94), 550 (4.30) nm.

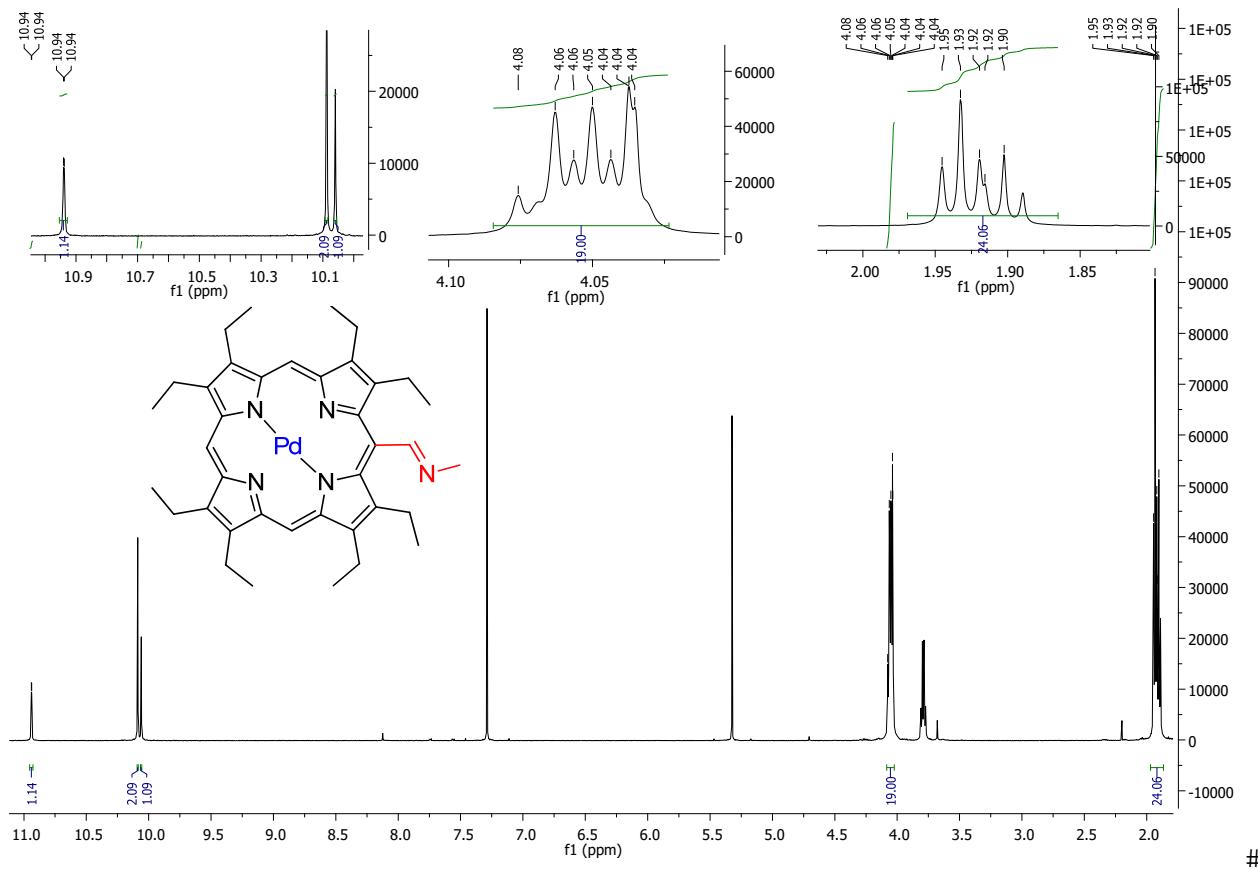


Figure S2. ^1H NMR spectrum of (3), recorded in CDCl_3 on a spectrometer Bruker Avance III 600 at 25 °C.

NMR spectrum was recorded in CDCl_3 on a spectrometer Bruker Avance III 600 at 25 °C following the standard procedure of the Bruker company. ^1H NMR (600 MHz, CDCl_3) δ : 1.90-1.95 (24H, m, -CH₂-CH₃), 4.04-4.08 (19H, m, -CH₂-CH₃ and -CH=N-CH₃), 10.06 (1H, s, meso CH), 10.09 (2H, s, meso CH) 10.94 (1H, d, CH=N-CH₃).

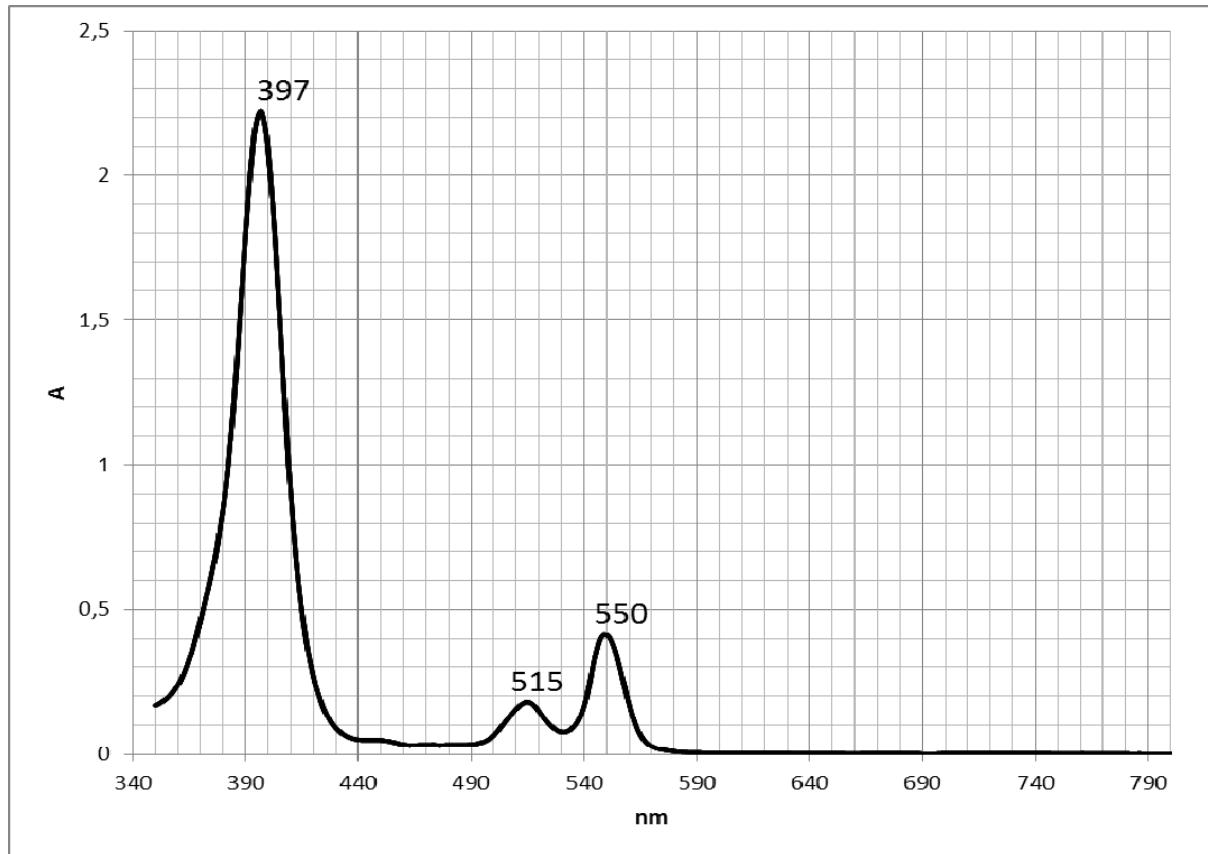


Figure S3. Absorption electronic spectrum of the title compound in CH_2Cl_2 ($c = 2.07 \cdot 10^{-5}$ mol/l). (obtained on a spectrophotometer HITACHI U-2900).

Table S1. Quantitative characteristics of the porphyrin core planarity in 38 crystal structures of porphyrin complexes with Pd from CSD. Positions of the substituents (R)–meso (m) or/and beta (b) are denoted as (m) or/and (b), respectively.

Refcode	R-position	max +/- deviation (Å)	
ATIRAW	b,m	0.24/-0.016	
ATIREA	b,m	0.21/-0.24	
BEMQEAE	b,m	0.62/-0.54	
DOWJEE	b,m	0.89/-0.79	
E BARAB	m	0.06/-0.06	
EBARIJ	-	- (CIF does not contain x,y,z)	
FOSTEM	m	0.01/-0.01	
FOSTEM10	m	0.01/-0.01	
HONKOF	m,b	0.40/-0.40	
HONKUL	m,b	0.80/-0.80	
IBAPUY	-	m	0.02/-0.02
KILPUS	b	0.03/-0.03	
KILQON	b	0.02/-0.02	
KIWPOV	m	0.03/-0.03	
MISKAB	m	0.42/-0.26	
NAYJOO	m	0.33/-0.29	
NEMYAG	m	0.065/-0.066	
OLEKIZ	m	0.52/-0.45	
OLEKUL	disorder		
OQEROS	m	0.05/-0.05	
PAPFAO	b,m	0.87/-0.79	
PDTPOR	m	0.43/-0.43	
PUJLAS	m	0.32/-0.33	
QARPUU	b,m	0.24/-0.22	
QIHYAJ	m	0.40/-0.40	

QOQBOO	m	0.02/-0.02
RIDKAR	m	0.07/-0.07
RIVLIT	m	0.24/-0.24
RIVLOZ	m	0.16/-0.17
RIVLUF	m	0.4/-0.4
ROKKAF	m	0.08/-0.08
SOBTUY	m	0.18/-0.18
VARPEL	m	0.05/-0.05
WUTREJ	m,b	0.61/-0.74
XENQOY	m	0.38/-0.26
XUBXUP	m	0.03/-0.03
YUKFEP	m,b	0.44/-0.34
ZOXQUA	m	0.31/-0.27

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