Supplementary Material for New Journal of Chemistry

Supplementary data

Table S1 Crystal data and structure refinement parameter for the quinol derivatives **2a**, **3a**, **6**, and **7**.

Compound	**2a**	**3a**	**6**	**7**
Molecular formula	$C_{26}H_{25}N_3O_2$	$C_{26}H_{25}N_3O_2$	$C_{30}H_{33}N_3O_2$	$C_{30}H_{33}N_3O_2$
Formula weight	411.50	411.50	467.61	467.61
Number of reflection used for unit cell determination (2θ range/°)	25 (23.8-29.9)	25 (22.7-23.8)	25 (28.9-29.9)	25 (23.0-24.5)
Crystal System	monoclinic	orthorhombic	monoclinic	monoclinic
Space group	$P2_1/c$	$Pna2_1$	$P2_1/c$	$P2_1/n$
a/Å	11.111(2)	13.405(6)	16.130(3)	12.007(3)
b/Å	16.954(2)	10.911(2)	8.793(3)	13.152(4)
c/Å	12.318(2)	14.405(3)	18.260(3)	16.196(5)
α/°				
β/°	113.97(1)		96.12(1)	102.99(2)
γ/°				
V/Å^3	2120.3(3)	2106(1)	2575.1(9)	2492(9)
Z	4	4	4	4
D_c/g cm^{-3}	1.289 g/ cm^{-3}	1.297 g/ cm^{-3}	1.206 g/ cm^{-3}	1.246 g/ cm^{-3}
F(000)	872.00	872.00	1000.0	1000.0
M(Mokα)/cm^{-1}	0.83	0.83	0.76	0.79
Crystal dimensions/nm	0.45×0.45×0.25	0.30×0.45×0.25	0.60×0.40×0.20	0.20×0.10×0.20
Scan mode	ω-2θ	ω-2θ	ω-2θ	ω-2θ
Scan rate in ω/°min^{-1}	4.0(up to 5 scans)	8.0(up to 5 scans)	4.0(up to 5 scans)	4.0(up to 5 scans)
Scan width/°	1.21 + 0.30 tanθ	1.58 + 0.30 tanθ	0.89 + 0.30 tanθ	0.73 + 0.30 tanθ
2θ max/°	50.0	55.0	50.0	50.0
Range of induces *h*; *k*; *l*	0, 13; 0, 20;-14,13	0, 17; 0, 14; -18, 0	±19; 9, 10; -12, -0	-13, 14; 0, 15; 15, -19
Reflections collected (unique)	3735	2516	4696	4390
Reflection observed with $I_0>2\sigma I_0$	1866	1465	3272	1453
Number of parameters	357	330	449	449
R	0.062	0.042	0.056	0.076
R_w	0.146	0.099	0.109	0.149

w	$(\sigma^2F)^{-1}$	$(\sigma^2F)^{-1}$	$(\sigma^2F)^{-1}$	$(\sigma^2F)^{-1}$
S	1.44	1.08	1.31	1.07
Max. Shift/Error in final cycle	0.00	0.00	0.00	0.00
Max. peak in final diff. map/e $Å^{-3}$	0.49	0.21	0.15	0.43
Min. peak in final diff. map/e $Å^{-3}$	-0.62	-0.18	-0.14	-0.42