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Supplementary information

Solvent-free, $[Et_3NH]$ $[HSO_4]$ catalyzed facile synthesis of hydrazone derivatives

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Table S1. Comparison of selected geometrical parameters of compound (**2f**) as determined by X-Ray diffraction and from DFT calculation (Å,°)

	Experimental [1]	**Experimental (This study)**	**DFT study**
O1-C4	1.365(2)	1.3585(14)	1.361
O2-C5	1.374(2)	1.3709(12)	1.365
O3-C6	1.370(2)	1.3607(14)	1.361
N1-N1^{i}	1.419(2)	1.4102(18)	1.389
N1-C1-C2	123.00(19)	123.03(12)	122.58
C1-N1-N1	112.25(17)	112.03(13)	112.66
N1^{i}-N1-C1-C2	179.37(18)	179.01(13)	180.00
C3-C4-O1-C8	-0.7(3)	-0.68(18)	2.29
C4-C5-O2-C9	-105.8(2)	-105.69(13)	-81.04
C7-C6-O3-C10	2.8(3)	3.0(2)	-2.13

Symmetry code: (*i*) -*x*,1-*y*, 1-*z*.

Table S2. Crystallographic data and structure refinement of compound (**2f**).

Empirical formula	$C_{20}\ H_{24}\ N_2O_6$
Formula weight	388.41
Temperature (K)	293(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	*C* 2/c
a (Å)	29.7753(9)
b (Å)	4.8973(2)
c (Å)	13.9889(4)
α (deg.)	90
β (deg.)	103.7400(10)
γ (deg.)	90
Volume ($Å^3$)	1981.47(12)
Z	4
Calculated density (g/cm^3)	1.302
Absorption coefficient (mm^{-1})	0.097
F(000)	824
Crystal size (mm)	0.55 × 0.33 × 0.31
θ range for data collection (deg.)	3.00 –27.58
Index ranges	–38<h<38, –6<k<6, –18<l<18
Reflections collected/unique	17606 /2300 [*R(int)* = 0.0421]
Completeness to θ = 25.00º	99.8 %
Refinement method	Full–matrix least–squares on F^2
Data/restraints/parameters	2300/0/130
Goodness–of–fit on F^2	1.064
Final R indices [I> 2σ(I)]	*R1* =0.0396 *wR2* = 0.1091
R indices (all data)	*R1* = 0.0489 *wR2* = 0.1214
Largest diff. peak and hole (e $Å^{-3}$)	0.170 and –0.209

References

[1]. B. Zhao, Y. Q. Feng, J. W. Guo, J. Wang, *Acta Cryst*., 2006, E62, o2413-o2414.