Electronic Supplementary Information

A highly efficient solution and solid state ESIPT fluorophore and its OLEDs application

Virgile Trannoy,[ad] Anne Léaustic,[a] Sophie Gadan,[a] Régis Guillot,[a] Clémence Allain,[b] Gilles Clavier,[b] Sandra Mazerat,[a] Bernard Geffroy*[ce] and Pei Yu*[a]

[a] Université Paris-Saclay, CNRS, Institut de Chimie Moléculaire et des Matériaux d'Orsay, 91405, Orsay, France.
[b] Université Paris-Saclay, ENS Paris-Saclay, CNRS, PPSM, 91190 Gif-sur-Yvette, France.
[c] Université Paris-Saclay, CEA, CNRS, NIMBE, LICSEN, 91191, Gif-sur-Yvette, France.
[d] Present address : Instituto de Ciencia Molecular (ICMol), Universidad de Valencia, c/ Catedratico José Beltran 2, 46980 Paterna, Spain.
[e] LPICM, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, route de Saclay, 91128 Palaiseau, France.

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X-Ray single crystal structure

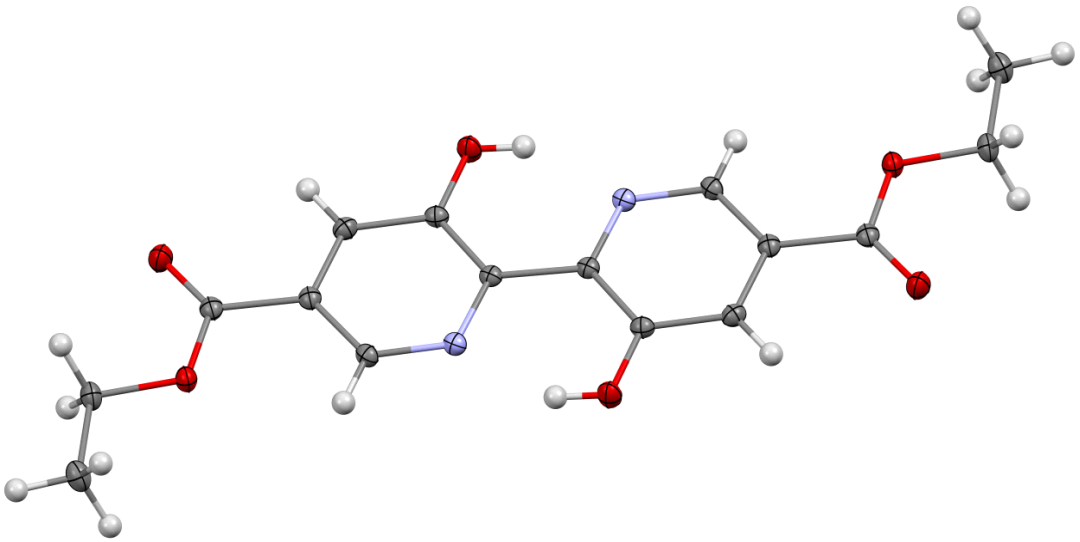


Fig. S01. An ORTEP drawing of compound **BP(OH)$_2$DCEt$_2$**. Thermal ellipsoids are shown at the 30% level.

X-ray diffraction data for compound **BP(OH)$_2$DCEt$_2$** were collected on a Kappa X8 APPEX II Bruker diffractometer equipped with a graphite-monochromated MoK$_\alpha$ radiation (λ = 0.71073 Å). Crystal was mounted on a CryoLoop (Hampton Research) with Paratone-N (Hampton Research) as cryoprotectant and then flashfrozen in a nitrogen-gas stream at 100 K. The temperature of the crystal was maintained at the selected value by means of a 700 series Cryostream cooling device to within an accuracy of ±1 K. The data were corrected for Lorentz polarization and absorption effects. The structures were solved by direct methods using SHELXS-97[SRX1] and refined against F^2 by full-matrix least-squares techniques using SHELXL-2018[SRX2] with anisotropic displacement parameters for all non-hydrogen atoms. Hydrogen atoms were located on a difference Fourier map and introduced into the calculations as a riding model with isotropic thermal parameters. All calculations were performed by using the Crystal Structure crystallographic software package WINGX.[SRX3]

The crystal data collection and refinement parameters are given in Table SX1.

The asymmetric unit of the crystal contains one-half-molecule.

CCDC 2004784 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/Community/Requestastructure.

Table SX1. Crystallographic data and structure refinement details.

Compound	**$BP(OH)_2DCEt_2$**
CCDC	2004784
Empirical Formula	$C_{16}\ H_{16}\ N_2\ O_6$
M_r	332.31
Crystal size, mm^3	0.21 x 0.09 x 0.08
Crystal system	monoclinic
Space group	*C* 2/*c*
a, Å	16.3814(6)
b, Å	11.6206(5)
c, Å	8.1169(3)
α, °	90
β, °	102.453(2)
γ, °	90
Cell volume, $Å^3$	1508.79(10)
Z ; Z’	4 ; 1/2
T, K	100(1)
Radiation type; wavelength Å	MoKα; 0.71073
F_{000}	696

μ, mm^{-1}	0.114
range, °	2.166 - 30.642
Reflections collected	15 738
Reflections unique	2 310
R_{int}	0.0341
GOF	1.060
Refl. obs. $I > 2(I)$	1 743
Parameters	111
wR_2 (all data)	0.1249
R value $I > 2(I)$	0.0415
Largest diff. peak and hole ($e^-.Å^{-3}$)	0.511 ; -0.251

[SRX1] Sheldrick, G. M. SHELXS-97, Program for Crystal Structure Solution, University of Göttingen, Göttingen, Germany, **1997**.

[SRX2] Sheldrick, G. M. *Acta Crystallogr. A* **2008**, *64*, 112-122.

[SRX3] Farrugia, L. J. *J. Appl. Cryst*. **1999**, *32*, 837-838.

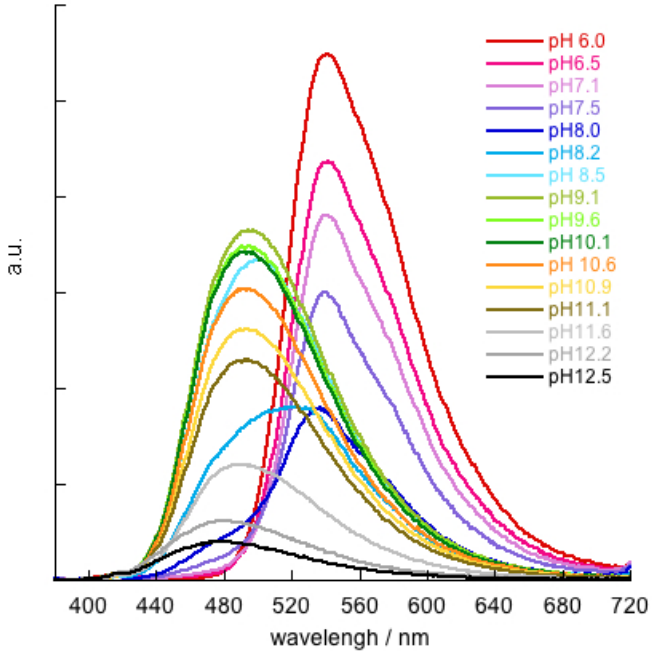


Figure S1. Fluorescence changes of $BP(OH)_2DCEt_2$ vs pH in H_2O-DMSO (3%) at RT

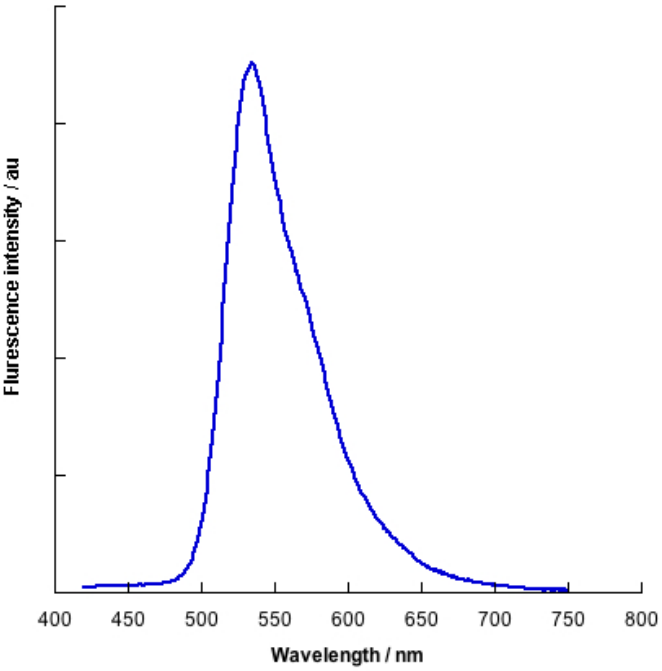


Figure S2. Fluorescence of microcrystals of $BP(OH)_2DCEt_2$ at RT

AFM images:

Tapping mode topography and phase imaging was accomplished using an Innova AFM Bruker with NanoDrive v8.02 software.
Tapping mode images were acquired using silicon tips from Nanosensors (PPP NCSTR) with a resonance frequency ranging beetween 76 and 263 kHz. Images were processed using WsXM software, freely available on internet.

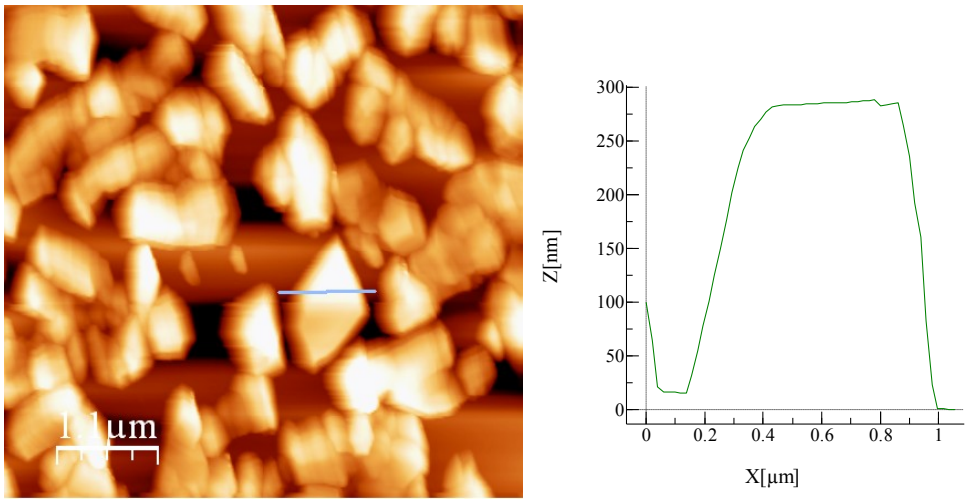


Figure S3. AFM image of a 70 nm thick neat film of $BP(OH)_2DCEt_2$ at RT where brigts spots

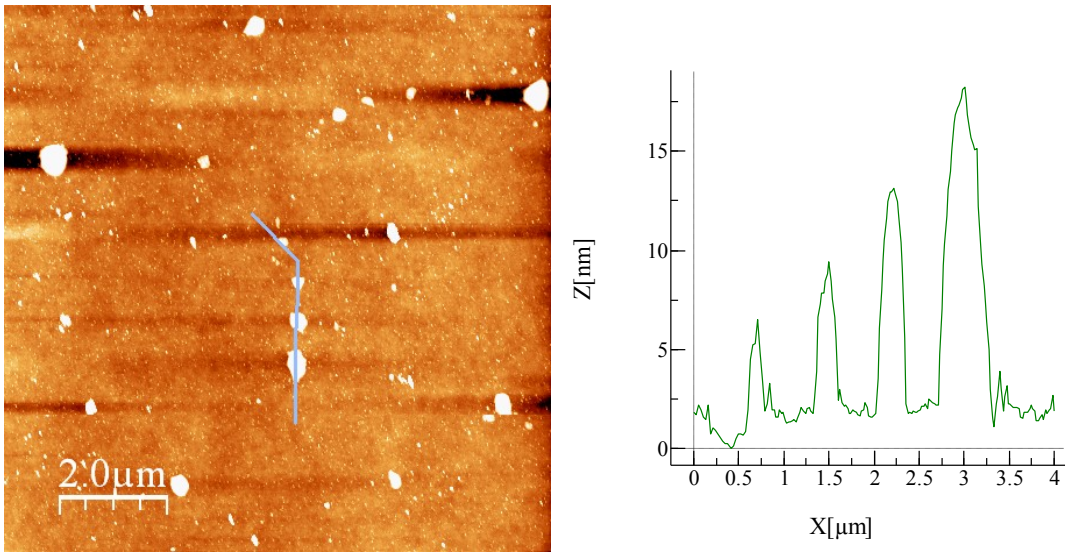
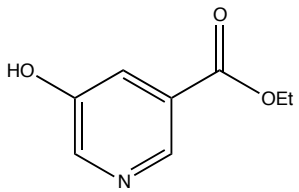
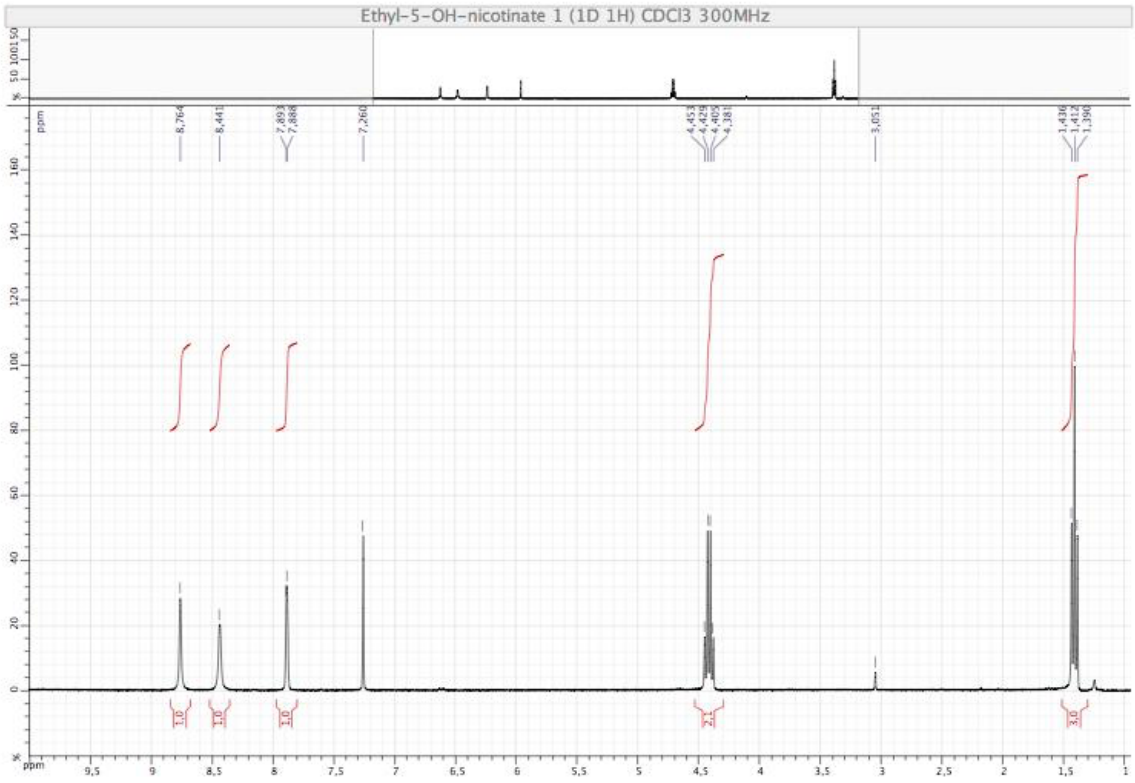
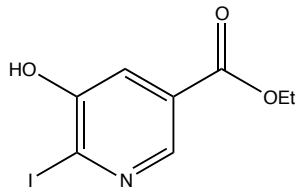
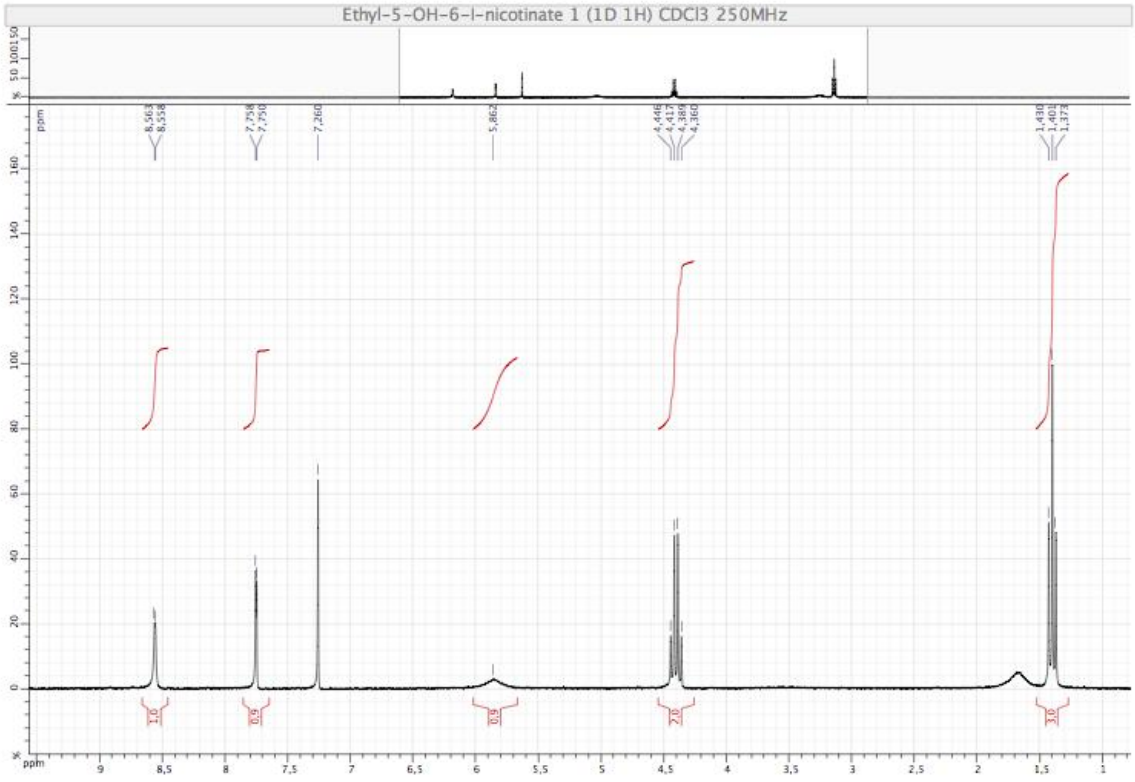


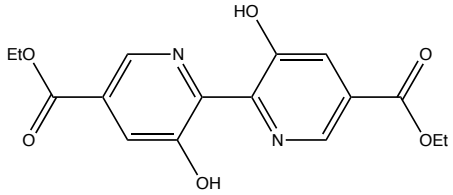
Figure S4. AFM image of DPVBi film doped with 10% of $BP(OH)_2DCEt_2$ at RT

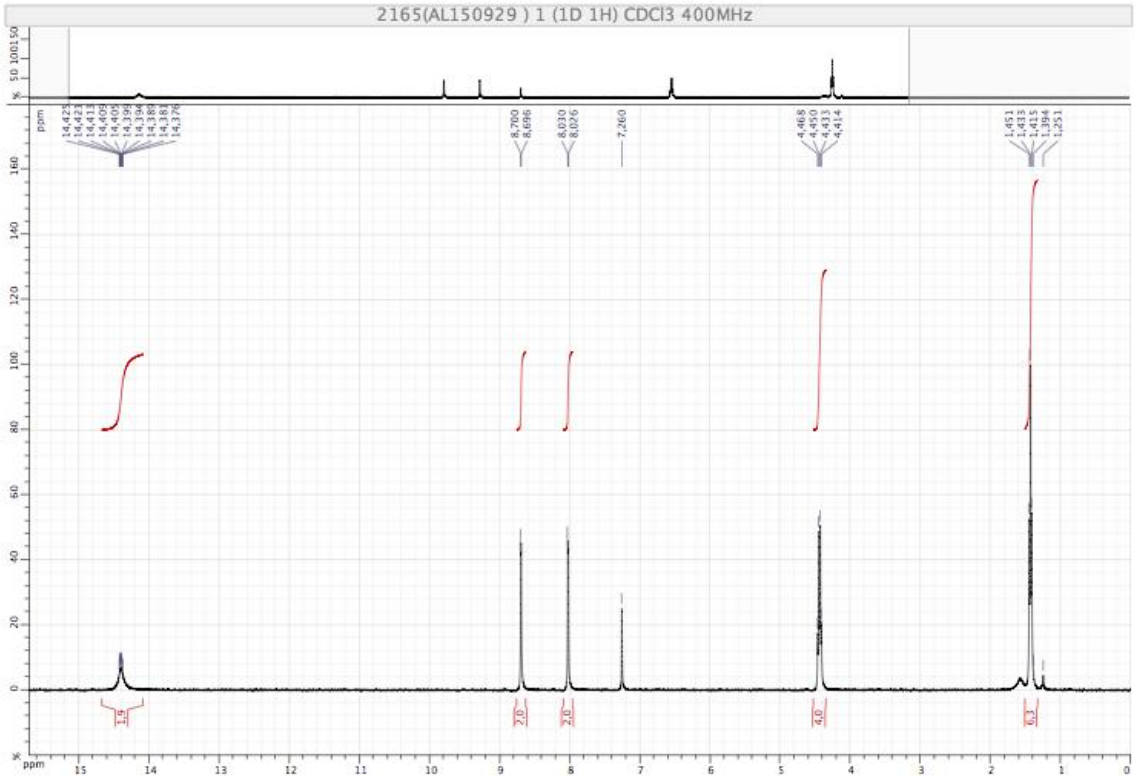

O
HO
OEt
N


Ethyl-5-OH-nicotinate 1 (1D 1H) CDCl3 300MHz
ppm
8,764
8,441
7,893
7,884
7,266
4,453
4,428
4,405
4,381
3,051
1,436
1,412
1,390
1,0
1,0
1,0
2,1
3,0


O
HO
OEt
I
N


Ethyl-5-OH-6-I-nicotinate 1 (1D 1H) CDCl3 250MHz
ppm
8,563
8,558
7,758
7,750
7,260
5,862
4,446
4,417
4,389
4,360
1,430
1,401
1,373
1,0
0,9
0,9
2,0
3,0


HO
EtO
N
O
O
N
OEt
OH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8.696
8.030
8.026
7.260
4.468
4.450
4.433
4.414
1.451
1.433
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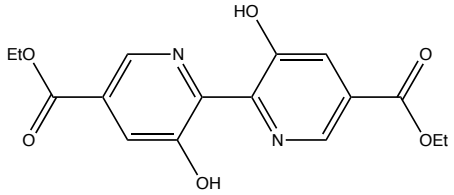
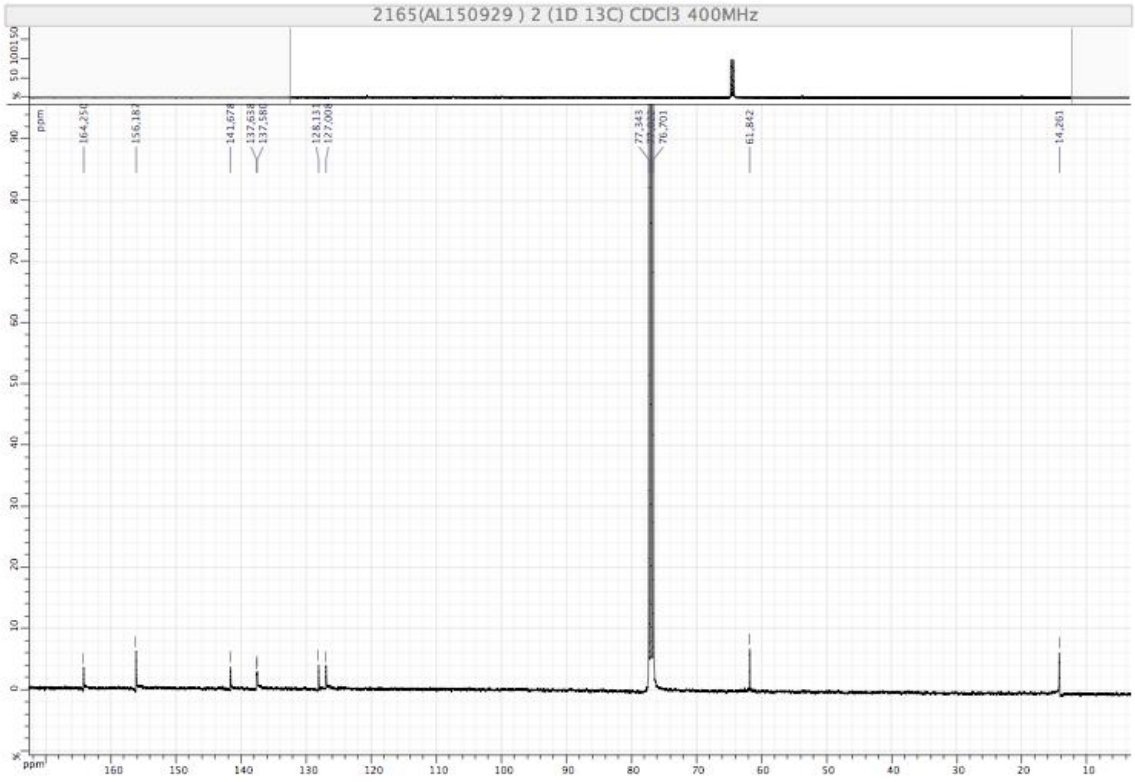
1.394
1.251
1.9
2.0
2.0
4.0
6.3


HO
EtO
N
O
O
N
OEt
OH


2165(AL150929) 2 (1D 13C) CDCl3 400MHz
ppm
164.254
156.183
141.678
137.634
137.586
128.131
127.008
77.343
76.701
61.842
14.261