

Supplemental Information

The Design of Boronic Acid Spectroscopic Reporter Compounds by Taking Advantage of the pKa-Lowering Effect of Diol-binding: Nitrophenol-based Color Reporters for Diols

Weijuan Ni,[‡] Hao Fang,[□] Greg Springsteen,[‡] and Binghe Wang^{□}*

[‡]Department of Chemistry, North Carolina State University, Raleigh, NC 27695 and [□]
Department of Chemistry, Georgia State University, 33 Gilmer St. S.E., Atlanta, GA
30303 USA

To whom correspondence should be address at

Professor Binghe Wang
Department of Chemistry
Georgia State University
33 Gilmer St. S.E.
Atlanta, GA 30303
Phone: (404) 651-0289
E-mail: wang@gsu.edu

HPLC of compound **1** (4-Nitrophenol-2-boronic acid)

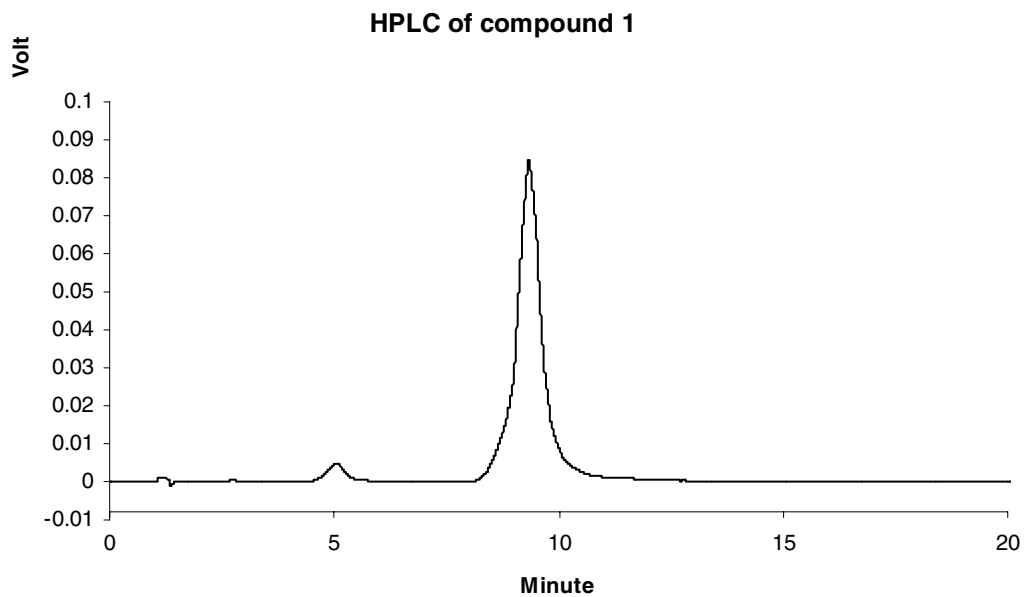
Shimidazul SPD-10AVvp UV detector

Column: ES Industries Chromegabond ODS Test Column 100×4.6mm 5 micron

Mobile Phase: 19/81 Acetonitrile/Water (containing 0.1% trifluoroacetic acid)

Flow Rate: 1.0 ml/min

Detection: UV 323 nm



Peak	Retention time (min)	Area (%)
1	5.067	3.8
2	9.342	96.2



GE NMR OMEGA

--juan/nitro/d6-ph74-021403

Date: Thu Feb 13 09:44:53 2003

OPERATOR: *****

ACQ TIME = 0.29 sec

DATA SIZE = 8192

NUM OF BLKS = 1

NUM OF SCANS = 24576

PULSE SEQUENCE:

SEQUENCE NAME = 1puls.s

OBSERVE:

NUC1 = ¹³C 101326.0 MHzSOLVENT = DMSO-d₆

SOLVENT = 400.146011 Hz

SOLVENT = 400.146011 Hz

GAIN = 10000.0

POWER LEVEL = 61

HIGH POWER = ON

DECOUPLER:

Z1 FREQUENCY = 300.515026 MHz

Z1 POWER = 63.00

Z1 MODULATION = waltz16

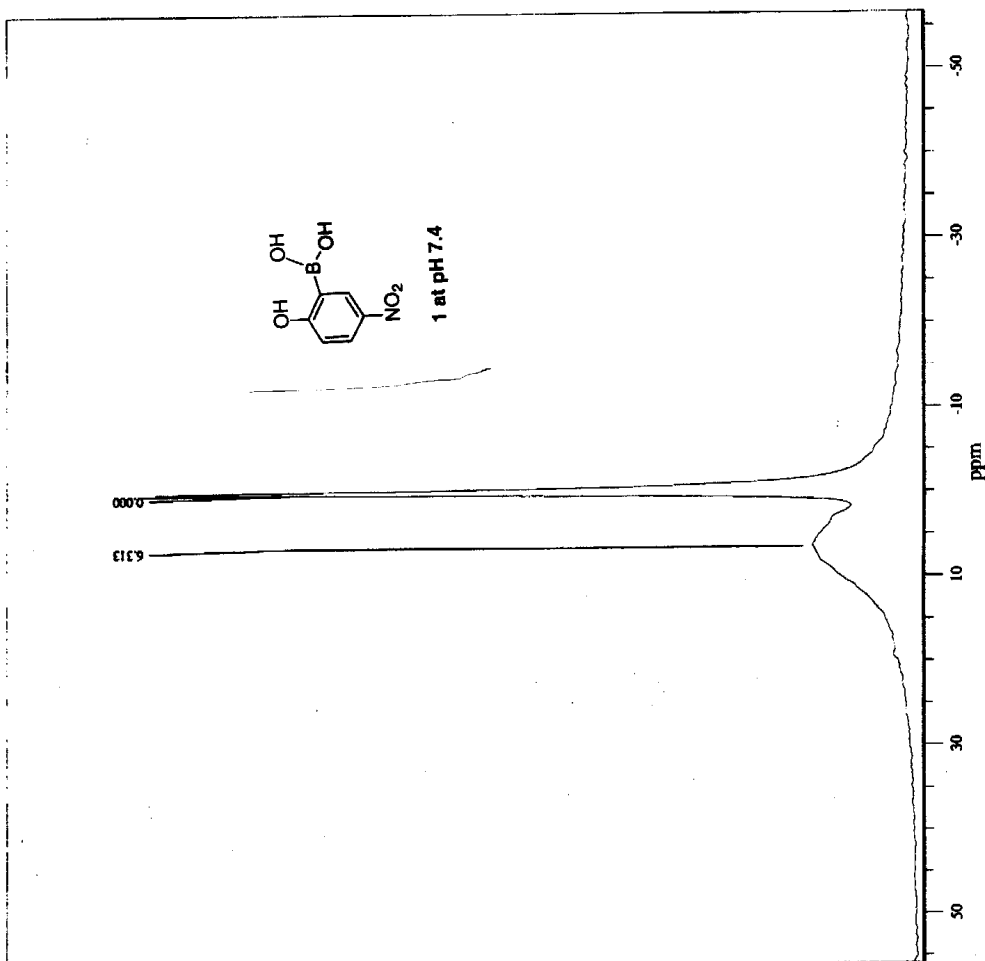
PROCESSING:

PHASE A = -9.84

PHASE B = 0.00

PLOT RANGE:

X From 55.82 TO -56.60 ppm





GE NMR OMEGA

...nitro/d6-ph74-diol-021203

Date: Tue Feb 11 21:49:34 2003

OPERATOR: *****

ACQ TIME = 8.29 sec
 DATA SIZE = 8192
 NUM OF BLKS = 1
 NUM OF SCANS = 2576

PULSE SEQUENCE:

SEQUENCE NAME = 1puls3

OBSERVE:

F1 FREQ = 96.4192840 MHz
 SPEC WIDTH = 28169.01 Hz
 SPEC OFFSET = 424.72 Hz
 GAIN = 10000.0
 POWER LEVEL = 61
 HIGH POWER = ON

DECOUPLER:

F2 FREQUENCY = 300.5215026 MHz
 F2 POWER = 63 db
 F2 MODULATION = waltz16

PROCESSING:

PHASE A = -5.33
 PHASE B = 0.00

PLOT RANGE:

X From 130.48 TO -141.67 ppm

