Supporting Information

Supramolecular Hydrogel Derived from A C_3-symmetric Boronic acid Derivative for Stimuli Responsive Release of Insulin and Doxorubicin

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Experimental Section:

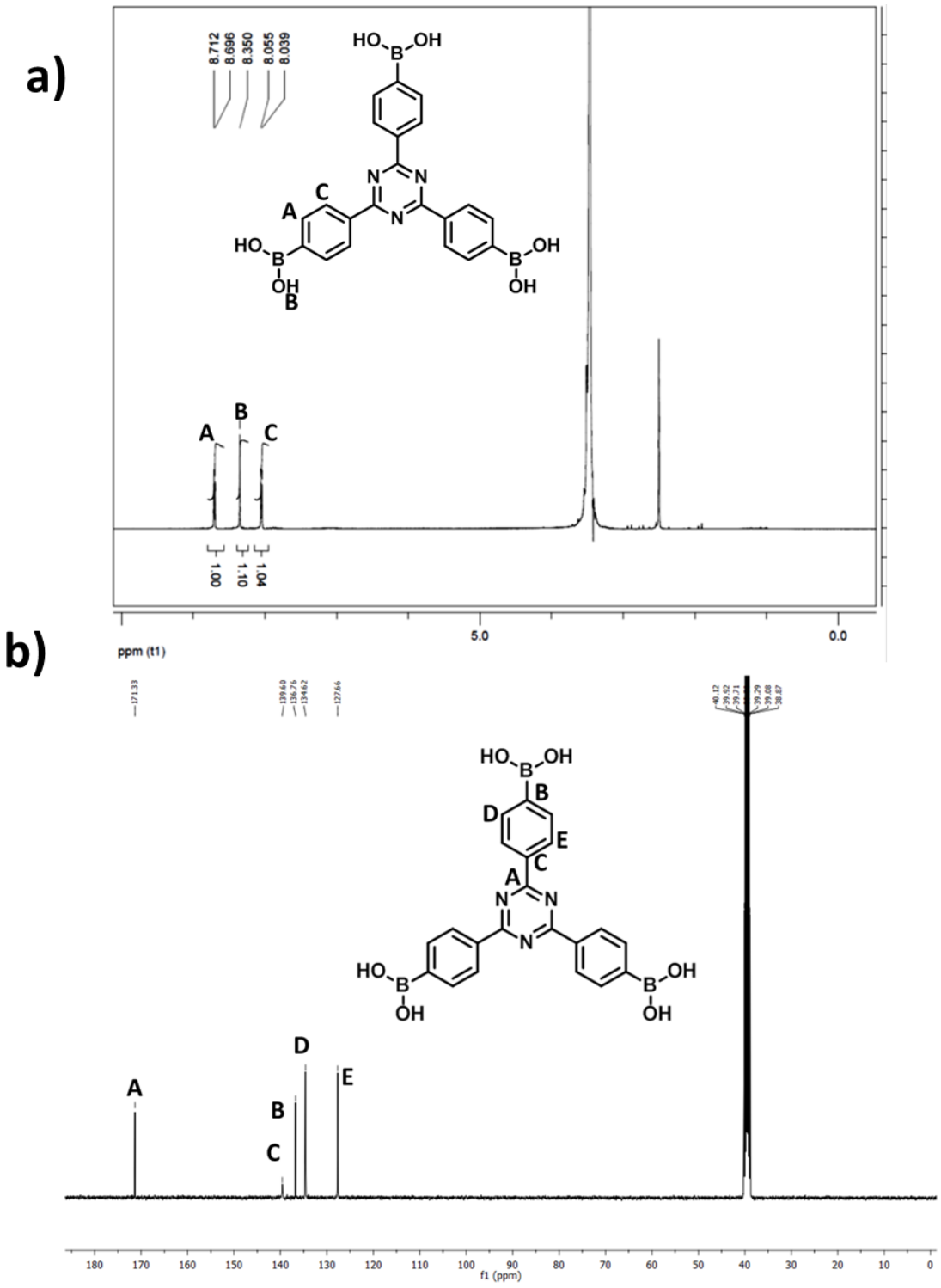

Figure S1: a) ^{1}H, b) ^{13}C NMR spectra of **HG1**.

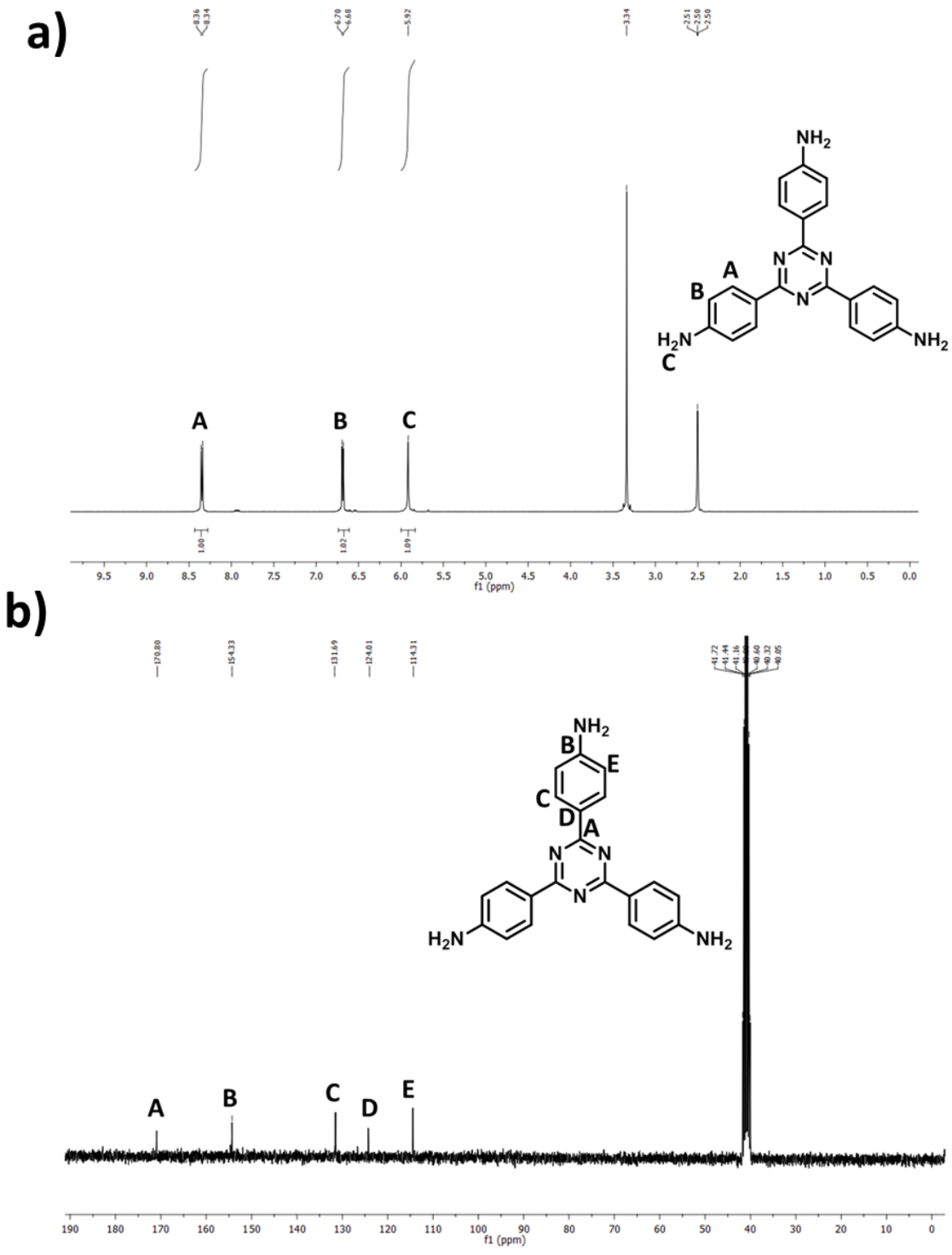

Figure S2: a) ^{1}H, b) ^{13}C NMR spectra of **NG1**.

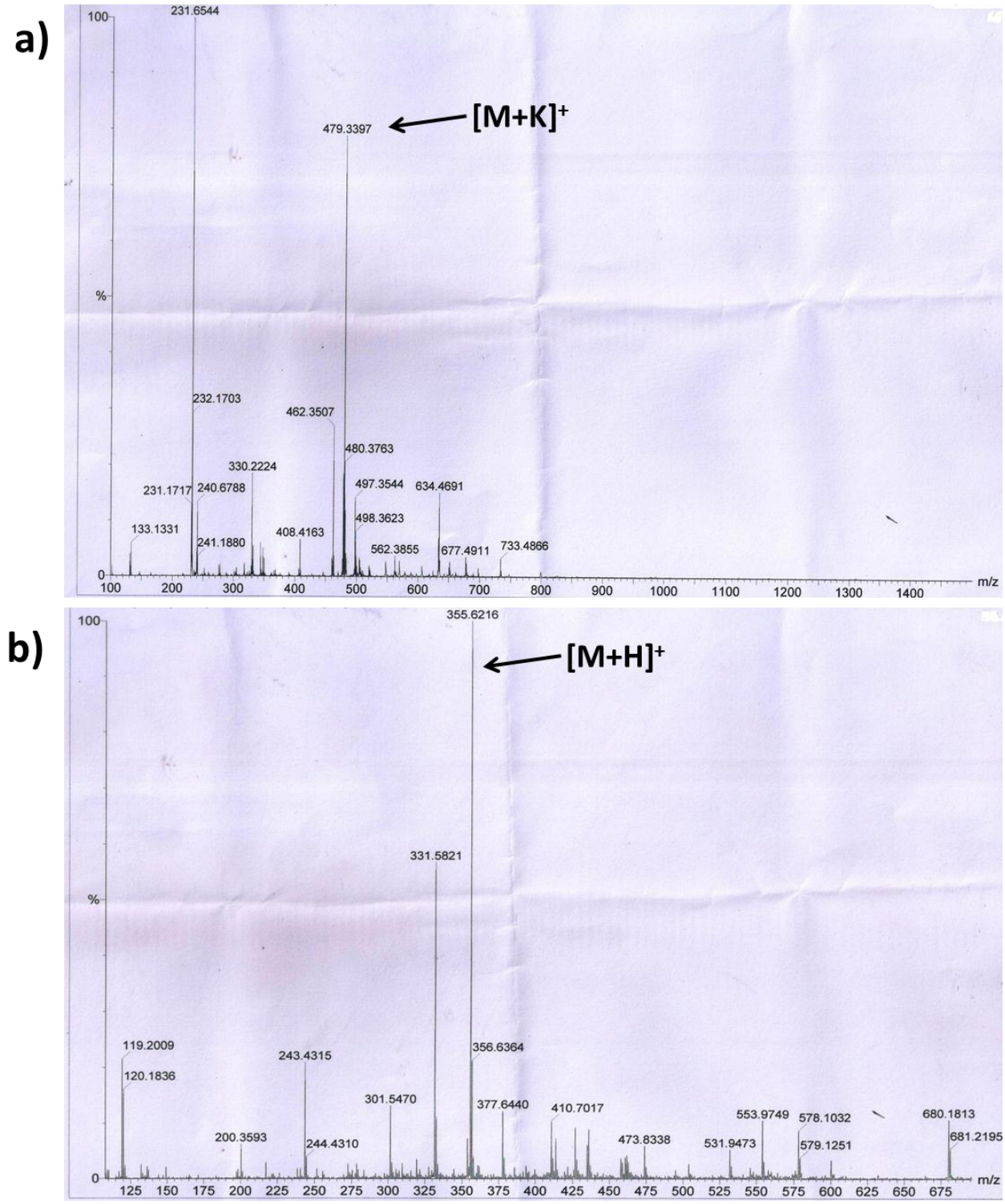

Figure S3: HRMS spectra of a) **HG1** and b) **NG1**.

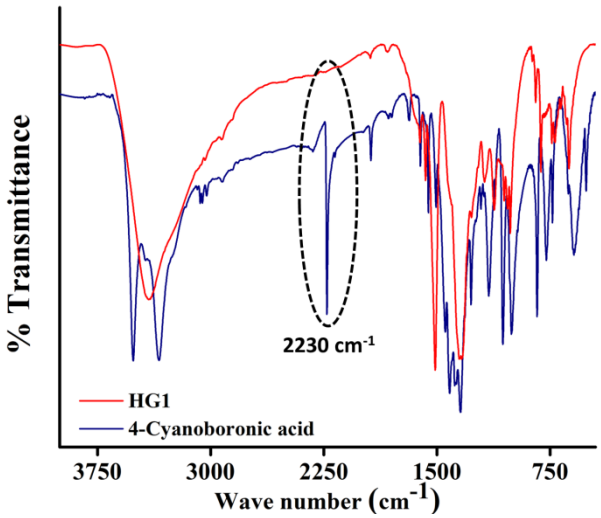

Figure S4: Comparative IR data of 4-cyanophenylboronic acid and **HG1**.

Optical, TEM and SEM images:

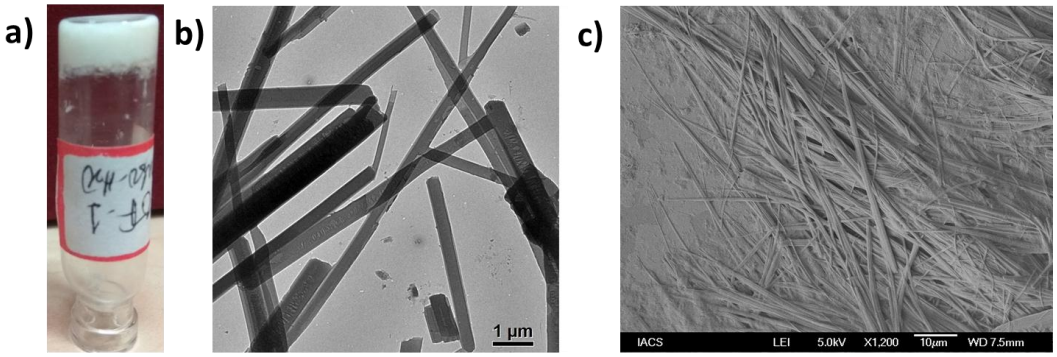

Figure S5: a) Optical, b) TEM and c) SEM images of the hydrogel.

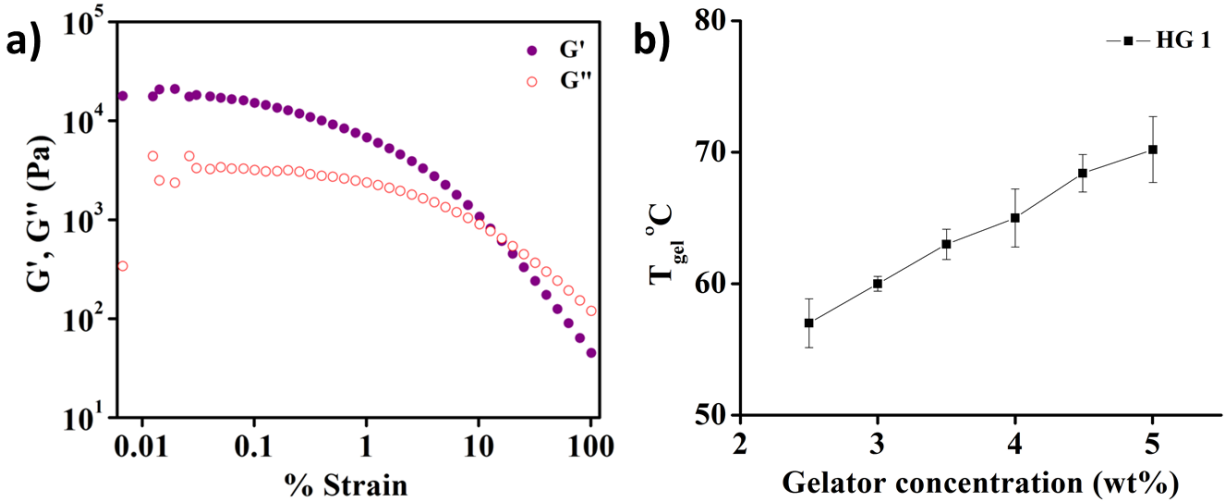

Figure S6: a) Amplitude sweep experiment, b) T_{gel} *vs.* [MGC] plot of the hydrogel **HG1**; in all the cases, 1 mL of a 2.5 wt % (w/v) gel was used.

Table S1: Gelation Table.

Gelation Solvents	Bromobenzene	Chlorobenzene	1,2-Dichlorobenzene	Toluene	o-Xylene	m-Xylene	p-Xylene	Mesitylene	Nitrobenzene	1,4-Dioxan	Methyl salicylate	DMF-water	DMSO-water	Water
HG1	INS	INS	INS	CS	INS	INS	INS	INS	CS	CS	INS	GP	GEL MGC = 2.5 wt% T_{gel} = 57 °C	INS
NG1	CS	S	S	CS	CS	CS	CS	S	S	S	GP	S	S	INS

[a]The minimum gelator concentration, (MGC) in wt % (w/v). [b]T_{gel} –Gel dissociation temperature at the respective MGC (0.4 mL). GP= Gelatinous precipitate. INS= Insoluble. CS= Colloidal solution.

pH dependent gelation:

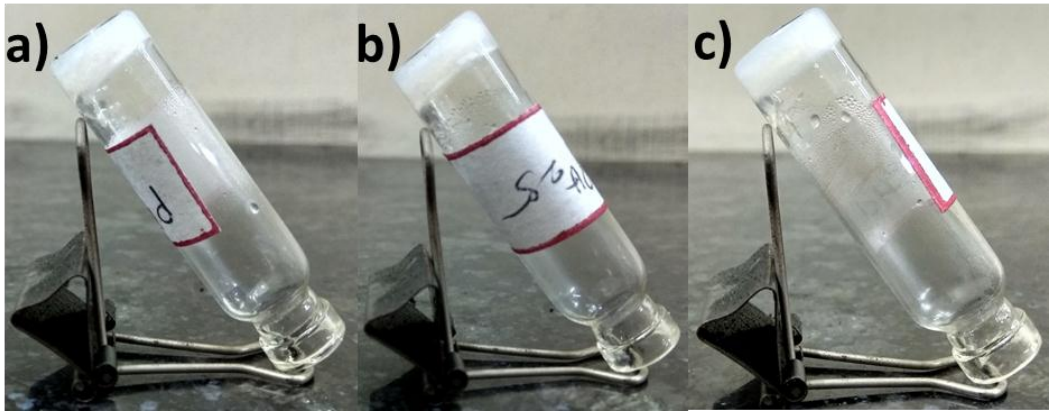

Figure S7: Picture of gel at various pH; a) at pH 3, b) at pH 5, c) at pH 7.4.

ORTEP plots and Hydrogen Bonding parameters HG1:

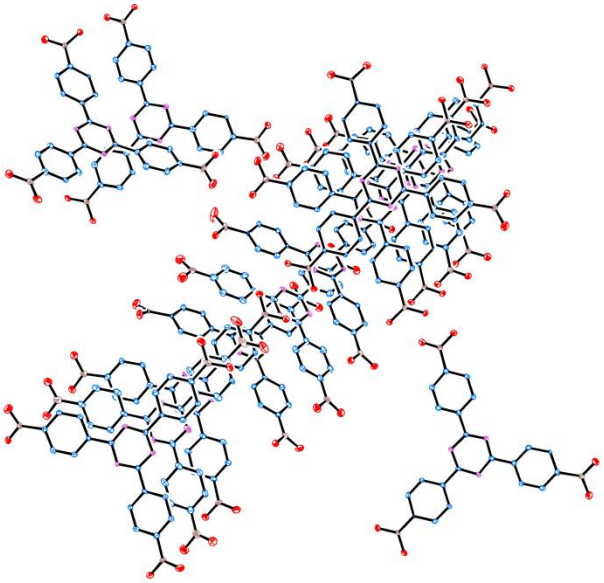

Figure S8. ORTEP plot of **HG1** (30% ellipsoid probability). Atoms are not marked to maintain the clarity.

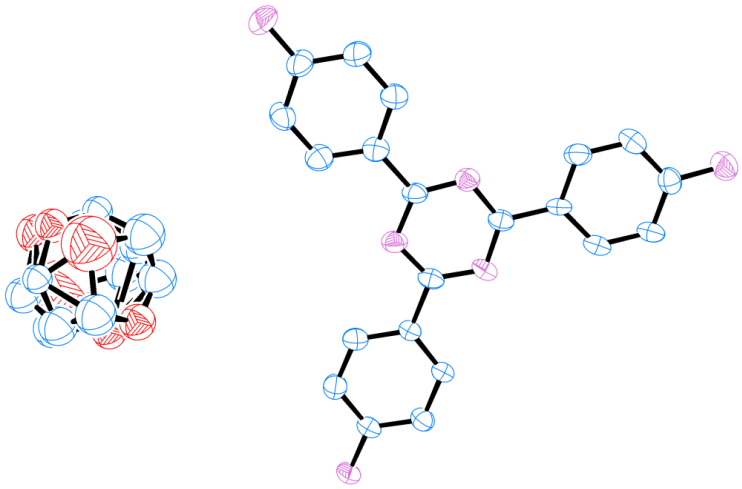

Figure S9. ORTEP plot of **NG1** (30% ellipsoid probability). Atoms are not marked to maintain the clarity.

Crystal data:

Table S2: Crystallographic parameter table.

Crystal parameters	**HG1**	**NG1**
CCDC No	1541749	1541748
empirical formula	$C_{21}H_{12}B_3N_3O_6$	$C_{25}H_{18}N_6O_2$
formula weight	434.77	434.45
crystal size/mm	0.36 × 0.3 × 0.22	0.28 × 0.18 × 0.12
crystal system	orthorhombic	Monoclinic
space group	*P*na2_1	*P*2_1/c
a /Å	31.2369(2)	19.795(7)
b/Å	44.0844(4)	5.3123(19)
c /Å	29.4269(2)	22.606(8)
$\alpha/^0$	90	90
$\beta/^0$	90	106.332(8)
$\gamma/^0$	90	90
volume/Å^3	40522.5(5)	2281.3(14)
Z	56	4
F(000)	12432.0	904.0
μ /mm^{-1}	0.603	0.084
temperature/K	100	120
R_{int}	0.0318	0.1121
range of h, k, l	$-37 \le h \le 33$, $-49 \le k \le 52$, $-34 \le l \le 31$	$-18 \le h \le 18$, $-4 \le k \le 4$, $-20 \le l \le 20$
θmin/max/°	3.357/ 67.079	1.072/ 19.097
Reflections collected/unique	212294/ 67567	10335/ 1847
data/restraints/parameters	67567/1/2840	1847/1/320
goodness of fit on F^2	1.019	1.024
final R indices [I>2σ(I)]	R_1 = 0.0888, wR_2 = 0.2409	R_1 = 0.0802, wR_2 = 0.1777
R indices (all data)	R_1 = 0.0945, wR_2 = 0.2459	R_1 = 0.1610, wR_2 = 0.2362

SXRD analysis:

Crystal structure of HG1: SXRD data revealed that **HG1** belongs to the noncentrosymmetric orthorhombic space group *P*na2_1. The asymmetric unit contained fourteen ((1,3,5-triazine-2,4,6-triyl)tris(benzene-4,1-diyl))triboronic acid (**HG1**) molecules and smeared electron densities that were SQUEEZED out as it could not be modeled. TWINROTMAT analysis from PLATON revealed that there was non-merohedral twining (59:41) present in the crystal. In the crystal structure of HG1, the boronic acid unit recognizes each other via hydrogen bonding and propagated into 2D network architecture. These 2D hydrogen bonded network having a large pore of ~ 3.0 nm, further interpenetrated for the sake of stabilization. By careful investigation of the crystal structure it was found that the eight fold interpenetration present in the crystal structure. Each of the **HG1** unit was further stacked by intermolecular π…π stacking (3.8-3.9 Å)

involving the triazine core. Loosely bound lattice occluded disordered solvent molecules were SQUEEZEd out. SQUEEZE calculations revealed that there were 85.4 electrons per asymmetric unit which might be attributed to ~1 DMSO molecule and 4 water molecules. Elemental analysis further supports the analysis.

Crystal structure of NG1: SXRD data revealed that **NG1** belongs to the centrosymmetric monoclinic space group $P2_1/c$. The asymmetric unit contained one 4,4',4''-(1,3,5-triazine-2,4,6-triyl)trianiline (**NG1**) molecule and one 1,4-dioxane molecule disordered over three positions (Refined SOF- 0.35414, 0.30393 and 0.34195). In the crystal structure of **NG1**, the solvent 1,4-dioxane remains H-bonded to one of the $-NH_2$ group of the triamine analogue. Each of the **NG1** unit was further stacked by intermolecular π…π stacking (3.5-3.6 Å).

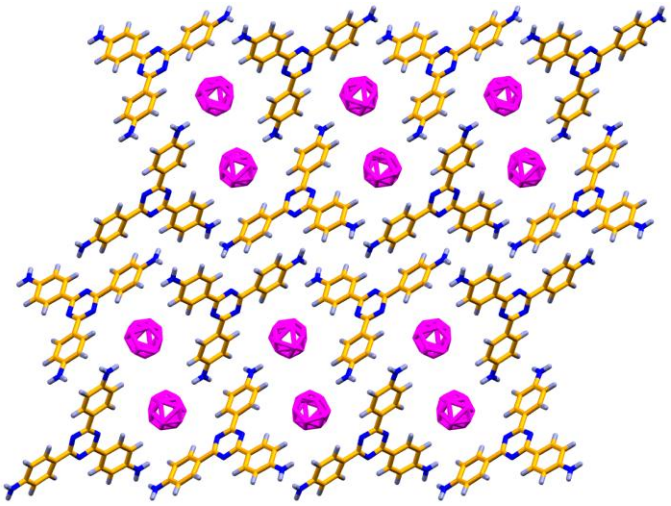

Figure S10. Packing diagram of **NG1** displaying solvent occlusion in the interstitial cavity formed by **NG1**.

TGA of HG1:

Unit cell contents = 56 molecules of **HG1** + 4782 electrons squeezed from unit cell contributed by the solvent molecules.

Monoclinic *C*2/c space group, Z = 56

Therefore FW = Unitcell contents/Z

= 1 **HG1** molecule + 85.4 electrons

(~ 1 DMSO molecule and 4 water molecules)

= 440.8 + 78.1 + 72

= 590.9

Weight loss for 1 DMSO and 4 water molecules

= 150.1/590.9 X 100%

= 25.4 % Experimental Value (25.77 %)

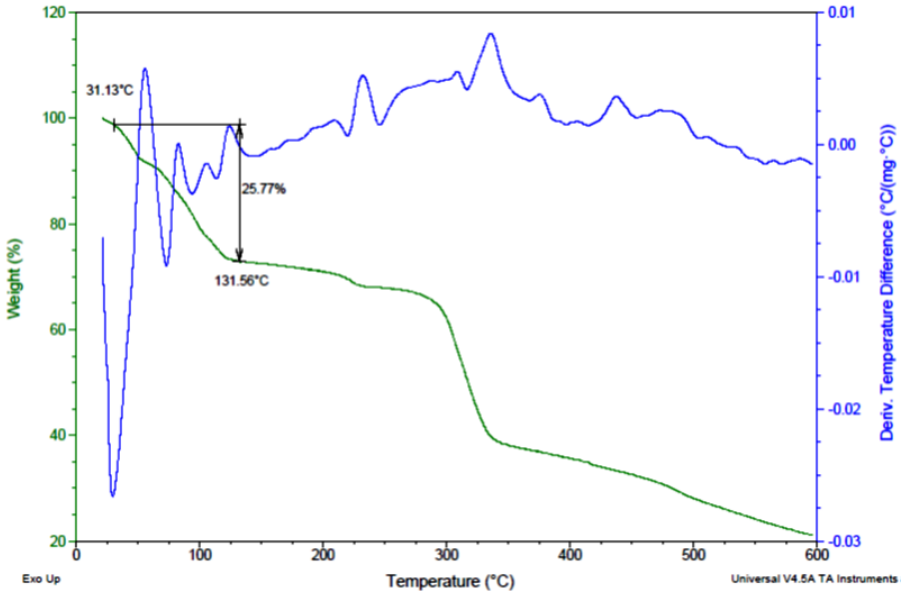

Figure S11: TGA profile of **HG1**.

NMR study for solvent detection:

50 mg crystals of **HG1** were soaked in 0.5 ml Methanol-d^4 and slightly warmed for few minutes. After that the insoluble coumpond was filtered off. The filtrate was characterised by ^{1}H NMR spectroscopy.

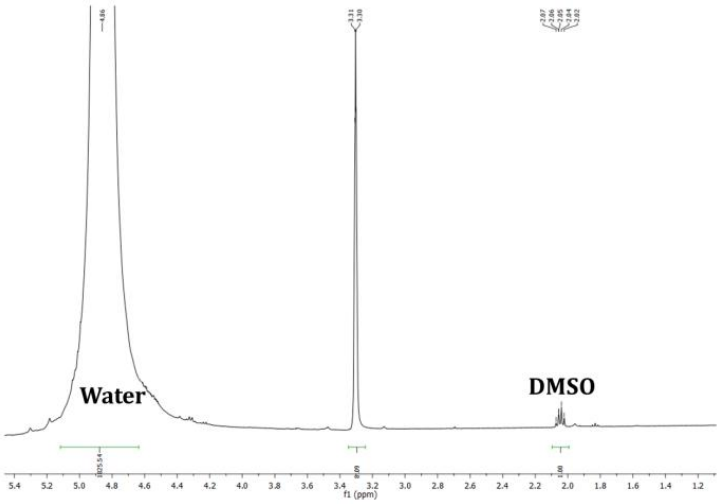

Figure S12: ^{1}H NMR spectra of the occluded water and DMSO in the crystals of **HG1**.

Powder X-ray diffraction:

HG1

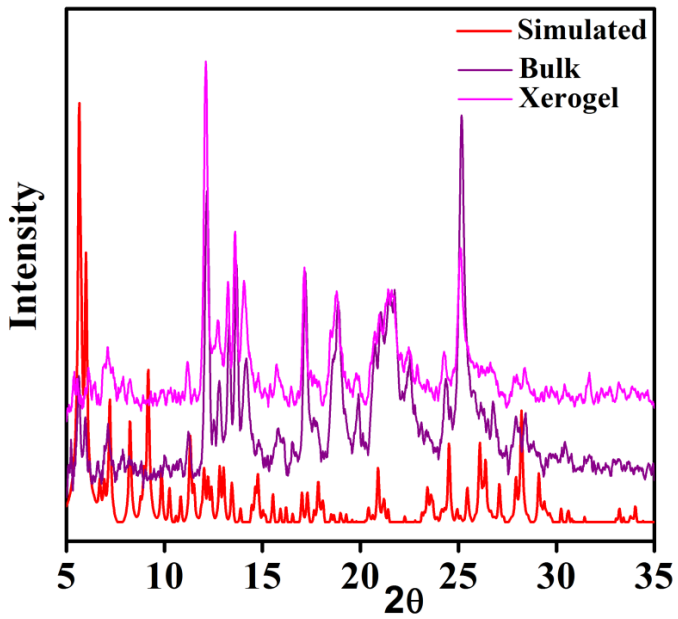

Figure S13: PXRD plot of simulated, bulk and xerogel of **HG1**.

NG1

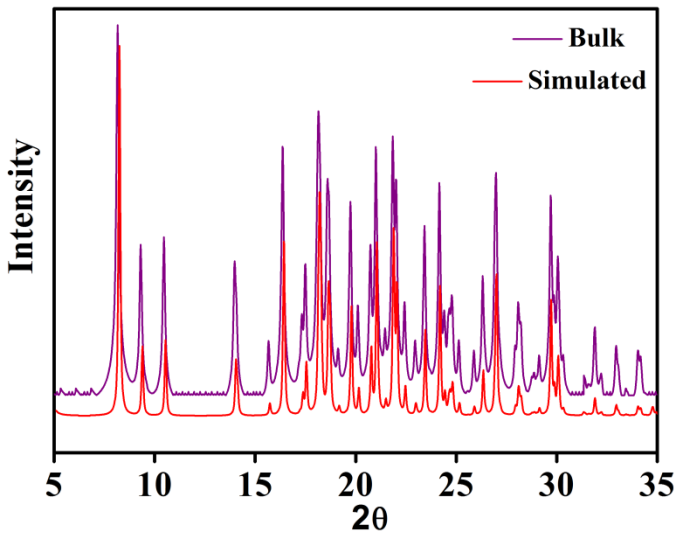

Figure S14: PXRD plot of simulated and bulk for **NG1**.

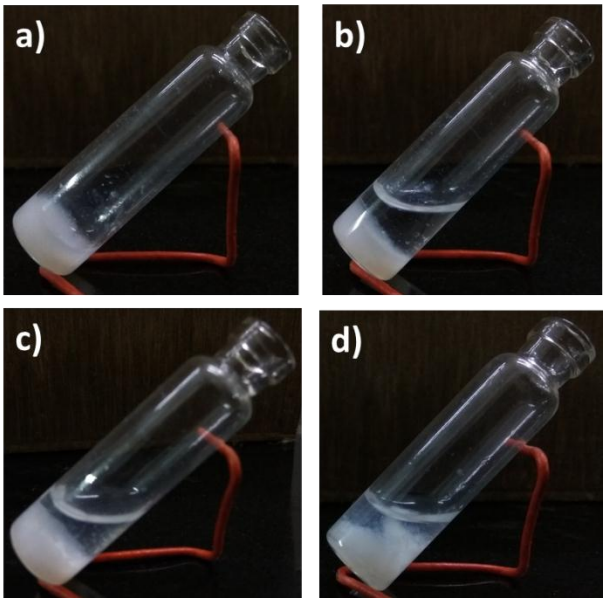

Figure S15: a) Hydrogel, b) 1.0 mM glucose solution added on the top of the hydrogel, c) After 48 hours and d) After one week of the addition of glucose solution.

Photoluminescence study for sensing glucose in solution state:

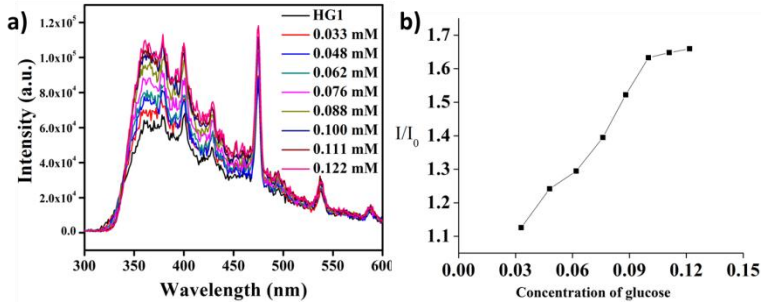

Figure S16: a) Fluorescence spectra of **HG1** with increasing glucose concentration, b) Incremental change in photoluminescence at λ = 360 nm with increasing glucose concentration.

Biological Studies

Insulin release study:

Table S3: Ratio of the two bands observed (ϕ_{209}/ϕ_{223}) from CD spectra for excreted insulin at different experimental conditions.

Insulin Solutions at various conditions	ϕ_{209}/ϕ_{223}
Standard insulin	1.14
Insulin excreted in presence of PBS	1.22
Insulin excreted in presence of 5% glucose in PBS	1.254
Insulin excreted in presence of 10% glucose in PBS	1.220
Insulin excreted in presence of 20% glucose in PBS	1.213

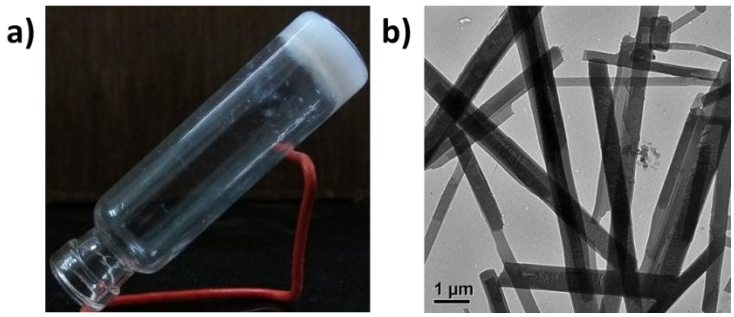

Figure S17: a) Picture of **HG1**-insulin hydrogel, b) TEM image of the **HG1**-insulin hydrogel.

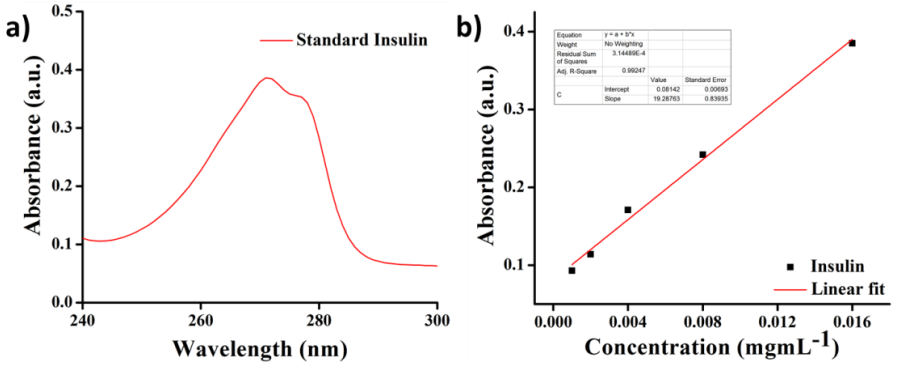

Figure S18: a) UV-Vis spectra of standard insulin, b) Calibration curve for standard insulin.

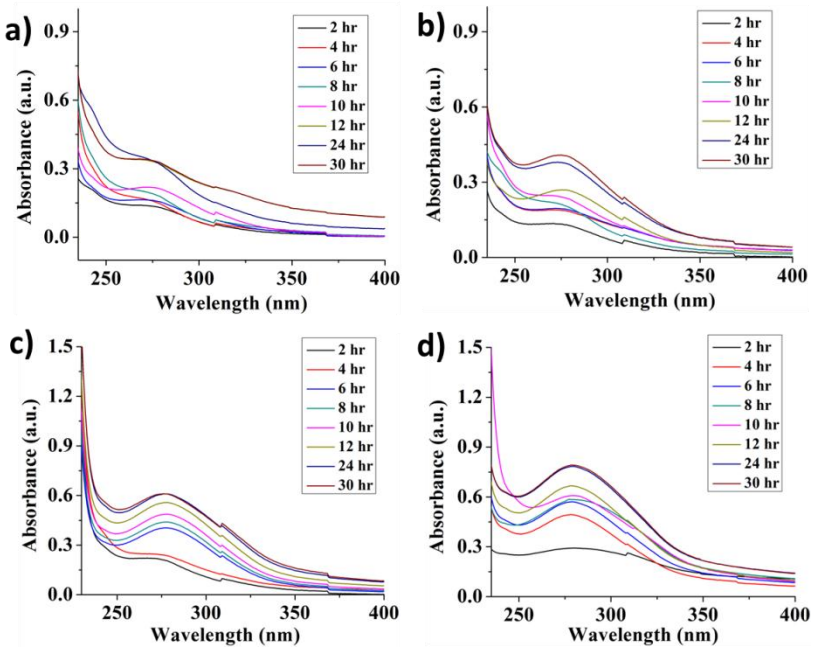

Figure S19: Release of insulin with time at different experimental conditions, a) In PBS, b) In 5% glucose in PBS, c) In 10% glucose in PBS, d) In 20% glucose in PBS.

Doxorubicin adsorption within gel matrix:

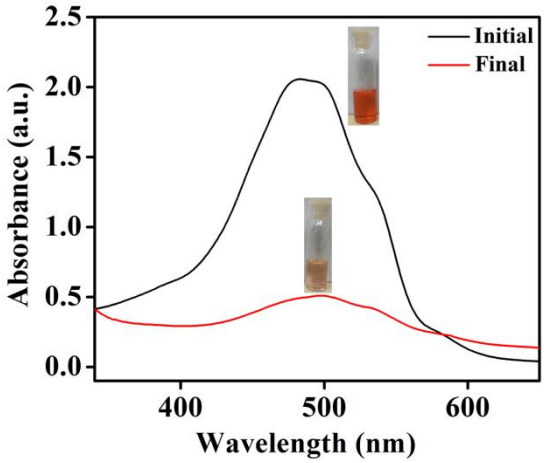

Figure S20: UV-Vis spectroscopy before (black) and after (red) DOX adsorption.

MTT assay:

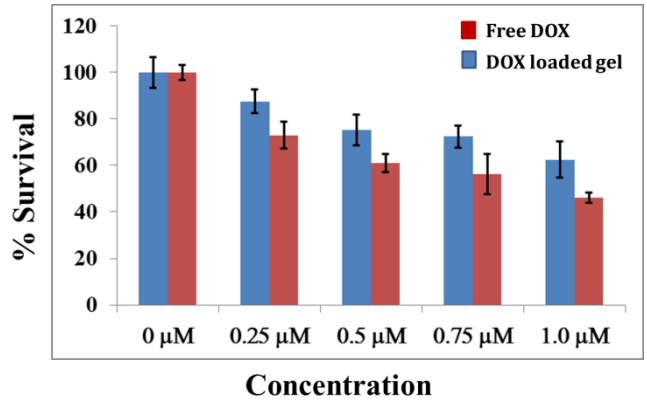

Figure S21: MTT assay of DOX solution (maroon) and DOX loaded hydrogel (sky).

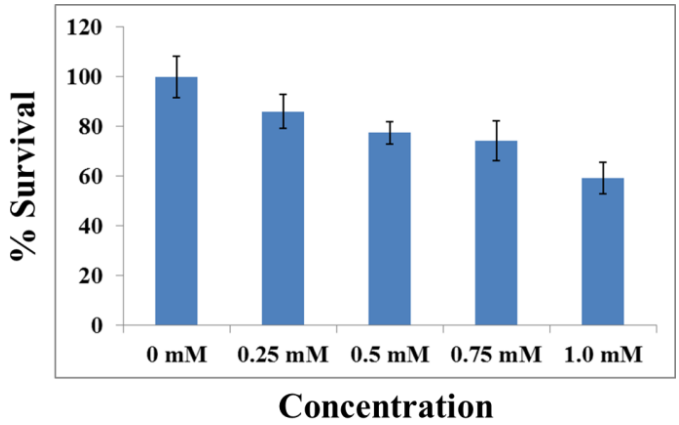

Figure S22: MTT assay of **HG1**.

Cell imaging:

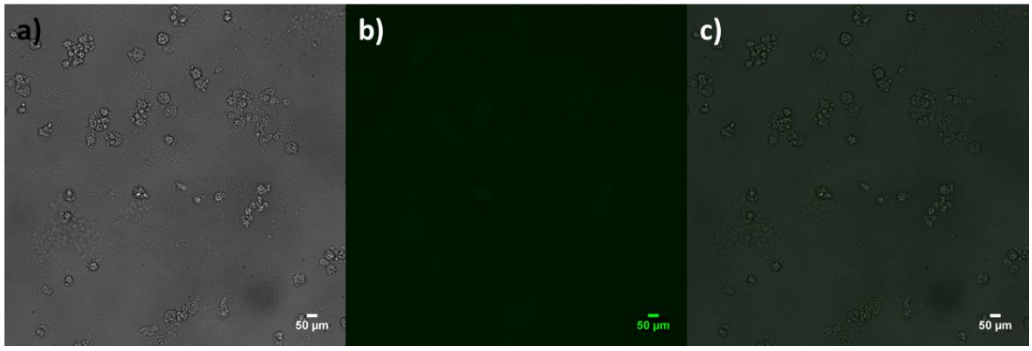

Figure S23. Fluorescent microscopic images of the RAW 264.7 cells displaying (a) bright field, (b) fluorescence, and (c) overlay of the images when incubated with the **HG1** for 4 h.

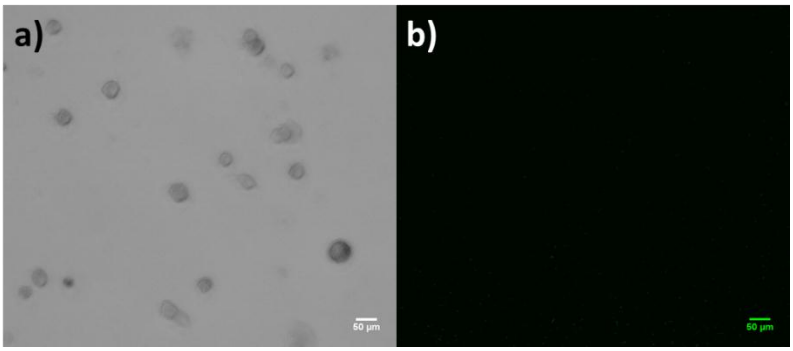

Figure S24: RAW 264.7 cells incubated without **HG1** displaying no auto-fluorescence. Fluorescence microscopic images of a) bright field, b) fluorescence.

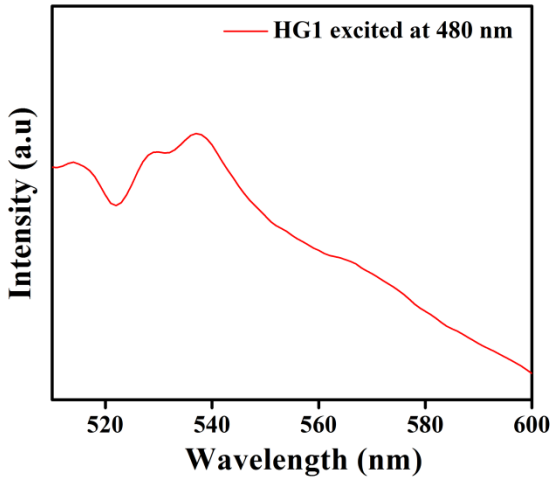

Figure S25: Fluorescence image of **HG1** when excited at 480 nm.

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: HG1

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Bond precision:  C-C = 0.0081 A          Wavelength=1.54184

Cell:            a=31.2369(2)     b=44.0844(4)     c=29.4269(2)
                 alpha=90         beta=90          gamma=90
Temperature:     100 K
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Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C21 H12 B3 N3 O6 [+ solvent]	C21 H18 B3 N3 O6
Sum formula	C21 H12 B3 N3 O6 [+ solvent]	C21 H18 B3 N3 O6
Mr	434.77	441.25
Dx,g cm-3	0.998	0.998
Z	56	56
Mu (mm-1)	0.603	0.603
F000	12432.0	12432.0
F000’	12474.26	
h,k,lmax	37,52,35	37,52,34
Nref	72406[36975]	67567
Tmin,Tmax	0.805,0.876	0.367,0.725
Tmin’	0.805	

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Correction method= # Reported T Limits: Tmin=0.367 Tmax=0.725
AbsCorr = GAUSSIAN

Data completeness= 1.83/0.93      Theta(max)= 67.079

R(reflections)= 0.0789( 61407)    wR2(reflections)= 0.2210( 67567)

S = 1.029                 Npar= 4160
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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT213_ALERT_2_B Atom C0AA has ADP max/min Ratio ..... 4.6 prolat

Author Response: This alert is due to disorder associated with the corresponding atom. We didn't model the disorder as we didn't get sufficient electron density for the other atoms associated with the disorder atom which is mandatory for maintaining proper chemical sense.

PLAT430_ALERT_2_B Short Inter D...A Contact O005 .. O00C .. 2.77 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O009 .. O00O .. 2.71 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O00A .. O00X .. 2.78 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O00E .. O00J .. 2.75 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O00F .. O01M .. 2.73 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O00G .. O00K .. 2.74 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O00L .. O00S .. 2.84 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O00M .. O06W .. 2.80 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O00N .. O01F .. 2.73 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

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Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O00R   .. O00W   ..   2.69 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O00T   .. O019   ..   2.74 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O00V   .. O02A   ..   2.75 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O00Y   .. O016   ..   2.76 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O00Z   .. O01Z   ..   2.76 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O011   .. O012   ..   2.70 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O013   .. O04H   ..   2.71 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O014   .. O02Y   ..   2.79 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O017   .. O02K   ..   2.76 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O018   .. O01R   ..   2.78 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O01B   .. O0B8   ..   2.79 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O01C   .. O045   ..   2.76 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O01D   .. O03B   ..   2.77 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O01H   .. O03N   ..   2.69 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O01P   .. O035   ..   2.77 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O01W   .. O04J   ..   2.77 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O01X   .. O05L   ..   2.76 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O022   .. O02H   ..   2.78 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O023   .. O03J   ..   2.76 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O024   .. O03K   ..   2.72 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O026   .. O02P   ..   2.70 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O027   .. O02I   ..   2.75 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O028   .. O02Q   ..   2.72 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O02C   .. O038   ..   2.75 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O02J   .. O03U   ..   2.70 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O02L   .. O03I   ..   2.84 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O02M   .. O033   ..   2.73 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O02R   .. O02V   ..   2.77 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O03X   .. O0B3   ..   2.69 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

PLAT430_ALERT_2_B Short Inter D...A Contact O04G   .. O074   ..   2.76 Ang.

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O05U   ..  O063    ..       2.73 Ang.
```

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O082   ..  O0B6    ..       2.80 Ang.
```

Author Response: There are fourteen independent molecules in the asymmetric unit. For this reason some atom(s) are in closer proximity of the other atom(s). This alert is due to the presense higher number of molecules which might lead to shorter intermolecular distances between the molecules which is responsible for extended H-bonding and pi-pi stacking.

Alert level C

```
CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
            calculated from the _atom_site* data lies outside
            the range 0.99 <> 1.01
           From the CIF: _cell_formula_units_Z                  56
           From the CIF: _chemical_formula_weight           441.25
           TEST: Calculate formula weight from _atom_site_*
           atom     mass    num     sum
           C        12.01   21.00  252.23
           H         1.01   12.00   12.10
           B        10.81    3.00   32.43
           N        14.01    3.00   42.02
           O        16.00    6.00   95.99
           Calculated formula weight              434.77
DENSD01_ALERT_1_C  The ratio of the submitted crystal density and that
            calculated from the formula is outside the range 0.99 <> 1.01
            Crystal density given    =      0.998
            Calculated crystal density =      1.012
STRVA01_ALERT_4_C           Flack test results are ambiguous.
           From the CIF: _refine_ls_abs_structure_Flack    0.590
           From the CIF: _refine_ls_abs_structure_Flack_su    0.120
PLAT046_ALERT_1_C Reported Z, MW and D(calc) are Inconsistent ....      1.013 Check
PLAT213_ALERT_2_C Atom C0BJ            has ADP max/min Ratio .....        3.1 prolat
```

Author Response: This alert is due to disorder associated with the corresponding atom. We didn't model the disorder as we didn't get sufficient electron density for the other atoms associated with the disorder atom which is mandatory for maintaining proper chemical sense.

```
PLAT220_ALERT_2_C Non-Solvent Resd 5   O   Ueq(max)/Ueq(min) Range        3.2 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd12   C   Ueq(max)/Ueq(min) Range        3.4 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C0DQ Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C0DX Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C0E9 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       B0DB Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       B0DK Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       B0DJ Check
```

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C0E3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C0E5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C0EK Check
PLAT334_ALERT_2_C Small Average Benzene  C-C Dist. C03C   -C05H         1.37 Ang.
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00813 Ang.
PLAT907_ALERT_2_C Flack x > 0.5, Structure needs to be Inverted? .       0.59 Check
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C21 H18 B3 N3 O6
           Atom count from the _atom_site data:  C21 H12 B3 N3 O6
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z   56
          From the CIF: _chemical_formula_sum  C21 H18 B3 N3 O6
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C       1176.00   1176.00    0.00
          H       1008.00    672.00  336.00
          B        168.00    168.00    0.00
          N        168.00    168.00    0.00
          O        336.00    336.00    0.00
PLAT014_ALERT_1_G N.O.K. _shelx_fab_checksum found in CIF ........     Please Check
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.11 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      73.08 Why ?
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..............    0.00040 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............    0.00020 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure       ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       629 Note
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON         16 Info
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed          ! Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
  43 ALERT level B = A potentially serious problem, consider carefully
  19 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  61 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

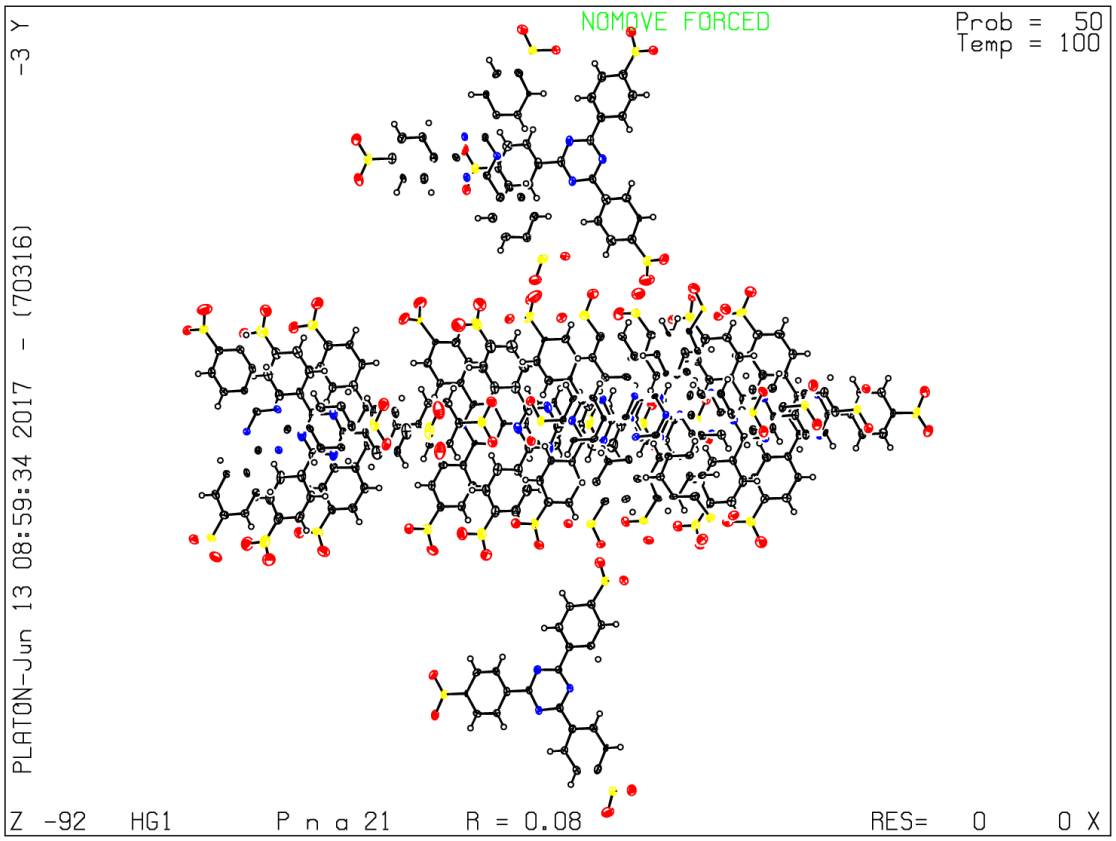
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 27/03/2017; check.def file version of 24/03/2017

Datablock HG1 - ellipsoid plot



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: NG1

```
Bond precision:  C-C = 0.0142 A          Wavelength=0.71073

Cell:            a=19.795(7)    b=5.3123(19)         c=22.606(8)
                 alpha=90       beta=106.332(8)      gamma=90
Temperature:     120 K

                Calculated                Reported
Volume          2281.3(14)                2281.3(14)
Space group     P 21/c                    P 1 21/c 1
Hall group      -P 2ybc                   -P 2ybc
                C21 H18 N6, 0.342(C4 O2),
Moiety formula  0.304(C3 O), 0.708(C2 O), C21 H18 N6, 2(C2 O)
                0.304(C O)
Sum formula     C25 H18 N6 O2             C25 H18 N6 O2
Mr              434.45                    434.45
Dx,g cm-3       1.265                     1.265
Z               4                         4
Mu (mm-1)       0.084                     0.084
F000            904.0                     904.0
F000'           904.34
h,k,lmax        18,4,20                   18,4,20
Nref            1856                      1847
Tmin,Tmax       0.982,0.990               0.604,0.744
Tmin'           0.977

Correction method= # Reported T Limits: Tmin=0.604 Tmax=0.744
AbsCorr = MULTI-SCAN

Data completeness= 0.995          Theta(max)= 19.097

R(reflections)= 0.0802( 886)      wR2(reflections)= 0.2362( 1847)

S = 1.024                 Npar= 320
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

REFNR01_ALERT_3_A Ratio of reflections to parameters is < 6 for a centrosymmetric structure

sine(theta)/lambda	0.4603
Proportion of unique data used	1.0000
Ratio reflections to parameters	5.7719

Author Response: The crystal was difracting poor and data quality was also poor. Multiple collection of data with more X-ray exposure doesn't improve data quality.

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4603

Author Response: The crystal is poorly diffracting. Multiple collection of data with more X-ray exposure doesn't improve data quality.

PLAT088_ALERT_3_A Poor Data / Parameter Ratio ..... 5.80 Note

Author Response: This alert is due to poor data quality.

Alert level B

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01419 Ang.

Author Response: This alert is due to poor data quality.

Alert level C

PLAT018_ALERT_1_C	_diffrn_measured_fraction_theta_max .NE. *_full				!	Check
PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..				48	%
PLAT234_ALERT_4_C	Large Hirshfeld Difference C12	--	C13	..	0.16	Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of				C19	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)				O3	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)				O5	Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N4	--	H4A ...	Please	Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N4	--	H4B ...	Please	Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N5	--	H5A ...	Please	Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N6	--	H6A ...	Please	Check

---

Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.13	Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)..	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)..	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)..	100%	Note

```
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5)..       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6)..       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   2.05) in Resd. #          2 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   1.22) in Resd. #          3 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   1.06) in Resd. #          4 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   1.06) in Resd. #          5 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.61) in Resd. #          6 Check
PLAT398_ALERT_2_G Deviating  C-O-C  Angle from 120 Deg for O6          140.3 Degree
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C31    --  C30     .       1.98 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C25    --  C24     .       1.99 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         79 Check
              C26  -O3   -C27     1.555   1.555   1.555             43.00 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          1 Note
```

```
   3 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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```

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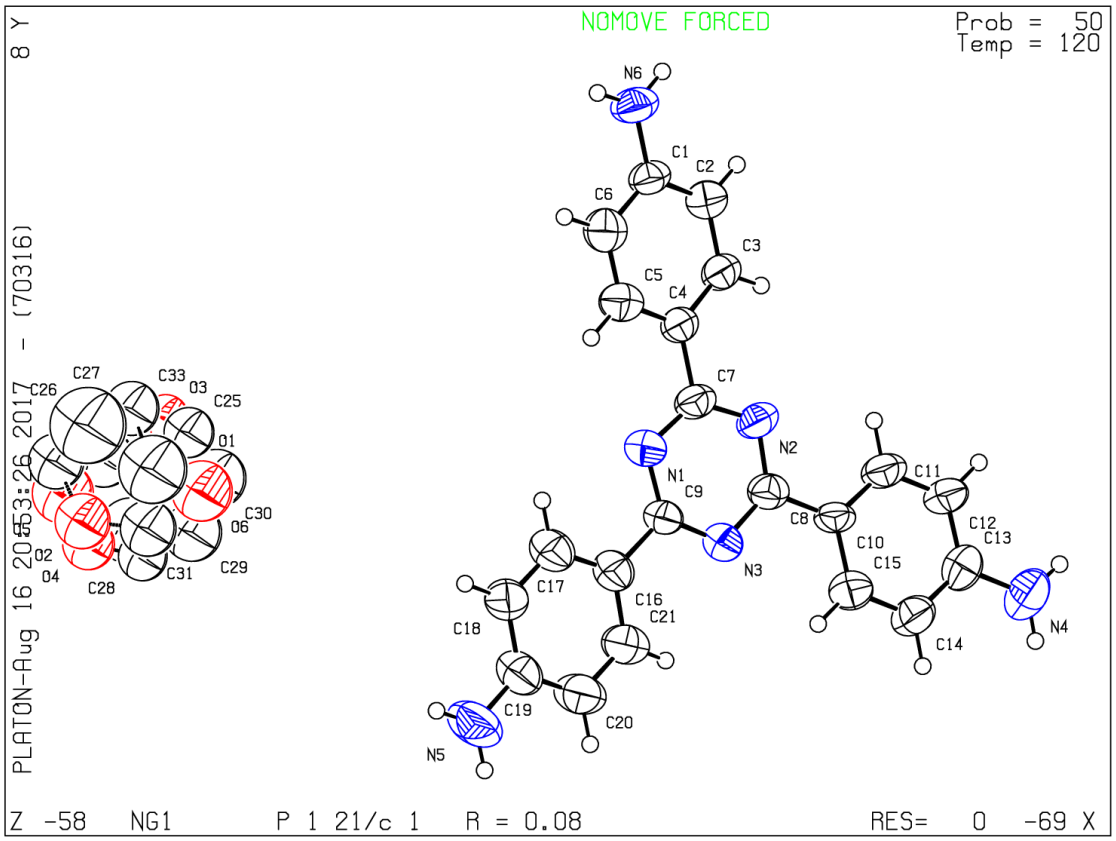
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/08/2017; check.def file version of 27/07/2017

Datablock NG1 - ellipsoid plot



Search Overview

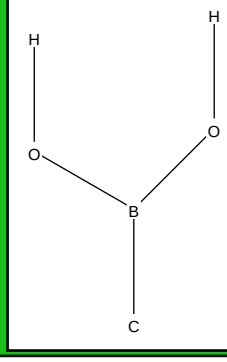
Search:	search4
Date/Time done:	Mon May 01 12:48:32 2017
Database(s):	CSD version 5.38 updates (Nov 2016) CSD version 5.38 (November 2016) CSD version 5.38 (November 2016)
Restriction Info:	No refcode restrictions applied
Filters:	3D coordinates determined No powder structures Only Organics
Percentage Completed:	100%
Number of Hits:	323

Single query used. Search found structures that:

match

Query 1

Query 1



Search: search4 (Mon May 01 12:48:32 2017): Hits 1-4

ASILIZ

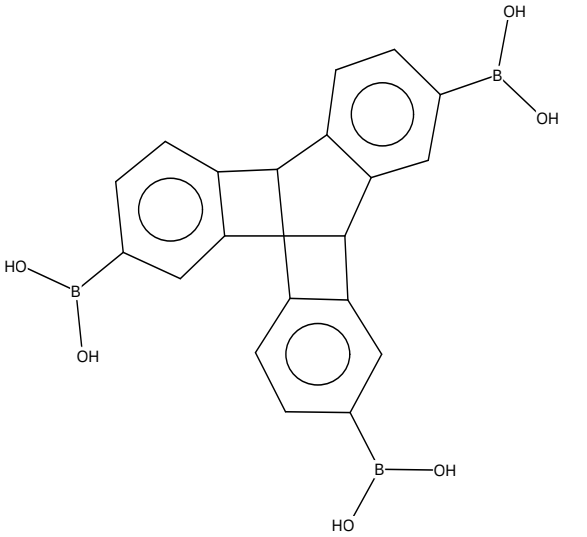
Reference: Gang Zhang, F.Rominger, M.Mastalerz (2016) *Cryst.Growth Des.* ,

Formula: $C_{20}\,H_{17}\,B_3\,O_6,7(H_2\,O_1)$

Compound Name: pentacyclo[6.6.6.0^{2,7}.0^{9,14}.0^{15,20}]icosa-2,4,6,9,11,13,15,17,19-nonaene-4,12,17-triyltriboronic acid heptahydrate

Space Group:	C2/c	***Cell:***	***a***	23.412(2)	***b***	11.249(1)	***c***	22.232(3)
Space Group No.:	15	***(Å,°)***	α	90.00	β	120.77(0)	γ	90.00

R-Factor (%): 7.62 ***Temperature(K):*** 200 ***Density(g/cm^3):*** 1.352



H_2O

EVIROS

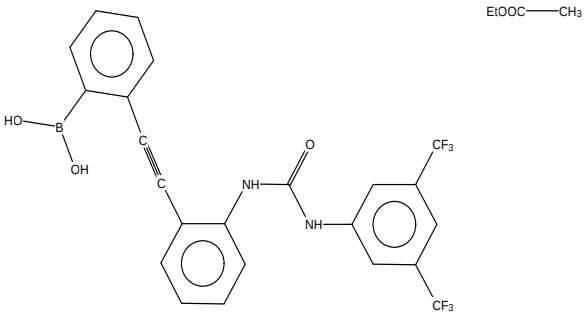
Reference: K.W.Bentley, D.Proano, C.Wolf (2016) *Nat.Commun.* ,***7***, 12539

Formula: $C_{23}\,H_{15}\,B_1\,F_6\,N_2\,O_3,C_4\,H_8\,O_2$

Compound Name: (2-((2-(((3,5-bis(trifluoromethyl)phenyl)carbamoyl)amino)phenyl)ethynyl)phenyl)boronic acid ethyl acetate solvate

Space Group:	P212121	***Cell:***	***a***	7.202(0)	***b***	14.548(0)	***c***	25.193(1)
Space Group No.:	19	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 4.18 ***Temperature(K):*** 173 ***Density(g/cm^3):*** 1.460



ISANOH

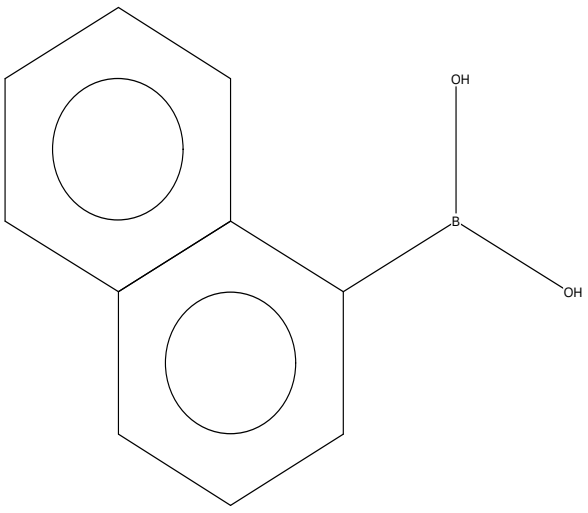
Reference: K.Bemisderfer, A.Y.Nazarenko (2016) *Acta Crystallogr.,Sect.E:Cryst.Commun.* ,***72***,1285

Formula: $C_{10}\,H_9\,B_1\,O_2$

Compound Name: 1-naphthylboronic acid

Space Group:	Pna21	***Cell:***	***a***	9.665(0)	***b***	6.229(0)	***c***	29.178(1)
Space Group No.:	33	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.46 ***Temperature(K):*** 173 ***Density(g/cm^3):*** 1.301



ISANOH01

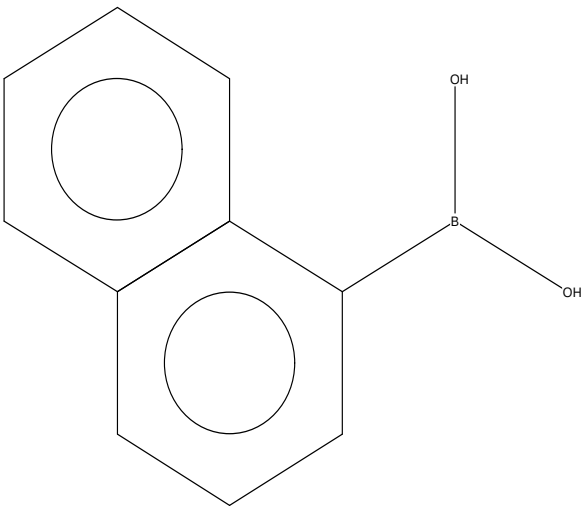
Reference: K.Bemisderfer, A.Y.Nazarenko (2016) *Acta Crystallogr.,Sect.E:Cryst.Commun.* ,***72***,1285

Formula: $C_{10}\,H_9\,B_1\,O_2$

Compound Name: 1-naphthylboronic acid

Space Group:	P21/c	***Cell:***	***a***	14.847(1)	***b***	6.102(0)	***c***	9.680(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	93.98(0)	γ	90.00

R-Factor (%): 3.45 ***Temperature(K):*** 173 ***Density(g/cm^3):*** 1.306



Search: search4 (Mon May 01 12:48:32 2017): Hits 5-8

ACEPAA

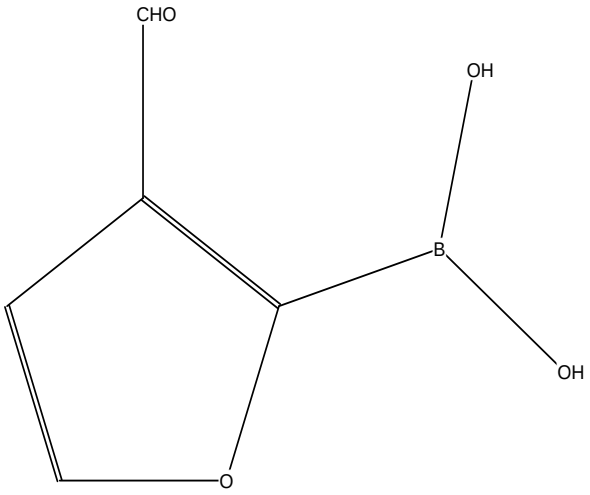
Reference: B.Zarychta, K.Ejsmont, M.Bujak, J.Zaleski, A.Sporzynski, A.Miskiewicz, A.Strutynska, J.Serwatowski (2004) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**60,**o1925

Formula: $C_5 H_5 B_1 O_4$

Compound Name: 3-Formyl-2-furanboronic acid

Space Group:	P21/c	***Cell:***	***a***	3.660(1)	***b***	14.252(2)	***c***	11.447(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	98.09(1)	γ	90.00

R-Factor (%): 4.29 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.572



AFOLUC

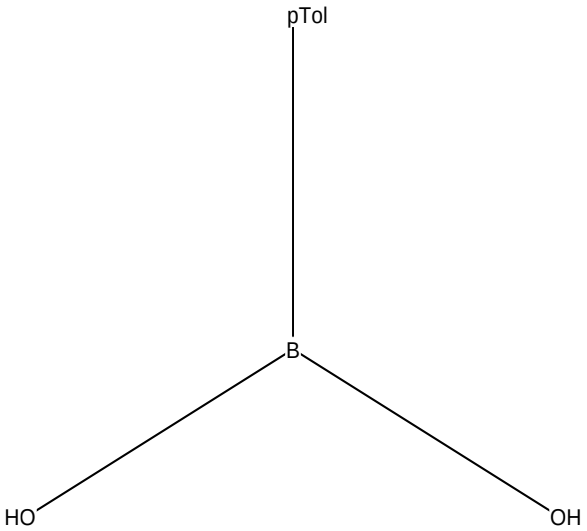
Reference: C.Zheng, B.F.Spielvogel, R.Y.Smith, N.S.Hosmane (2001) *Z.Kristallogr.-New Cryst.Struct.* ,**216,**341

Formula: $C_7 H_9 B_1 O_2$

Compound Name: 4-Methylphenylboronic acid

Space Group:	Iba2	***Cell:***	***a***	17.016(5)	***b***	19.164(5)	***c***	9.722(5)
Space Group No.:	45	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 6.42 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.139



APOROO

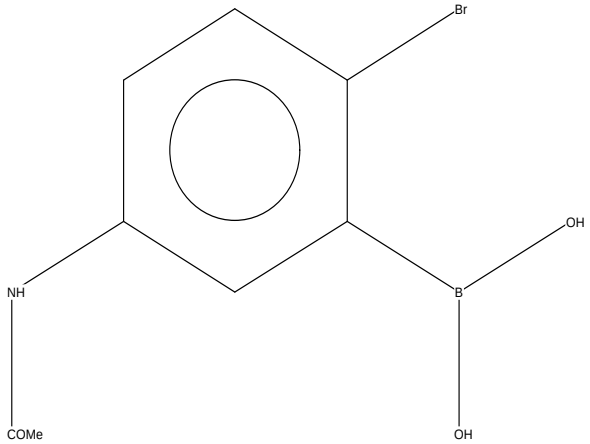
Reference: A.J.Close, P.Kemmitt, S.Mark Roe, J.Spencer (2016) *Org.Biomol.Chem.* ,**14,**6751

Formula: $C_8 H_9 B_1 Br_1 N_1 O_3$

Compound Name: (5-acetamido-2-bromophenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	7.245(0)	***b***	10.625(0)	***c***	12.411(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	90.96(0)	γ	90.00

R-Factor (%): 4.32 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.793



AVOTIO

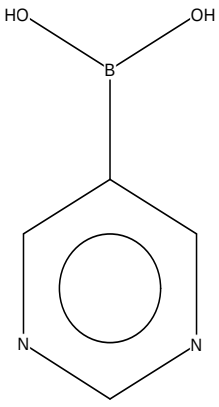
Reference: N.Saygili, A.S.Batsanov, M.R.Bryce (2004) *Org.Biomol.Chem.* ,**2,**852

Formula: $C_4 H_5 B_1 N_2 O_2,0.5(H_2 O_1)$

Compound Name: 5-Pyrimidylboronic acid hemihydrate

Space Group:	P21212	***Cell:***	***a***	7.647(0)	***b***	21.062(5)	***c***	3.635(0)
Space Group No.:	18	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.18 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.508



H_2O

Search: search4 (Mon May 01 12:48:32 2017): Hits 9-12

BAGFAS

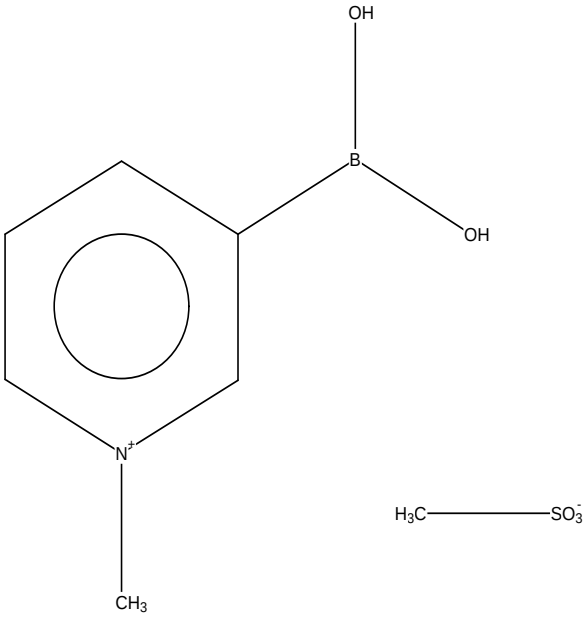
Reference: S.Iwatsuki, Y.Kanamitsu, H.Danjo, K.Ishihara (2011) *X-ray.Str.Anal.Online.* ,**27,**61

Formula: $C_6 H_9 B_1 N_1 O_2\ ^{1+}, C_1 H_3 O_3 S_1\ ^{1-}$

Compound Name: 3-(Dihydroxyboryl)-1-methylpyridinium methanesulfonate

Space Group:	P21/c	***Cell:***	***a***	8.946(1)	***b***	8.838(1)	***c***	13.850(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	105.28(3)	γ	90.00

R-Factor (%): 4.03 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.465



BAGYOZ

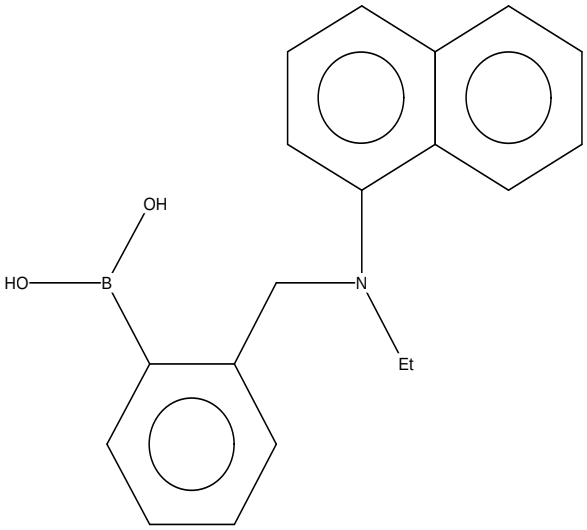
Reference: A.Adamczyk-Wozniak, R.M.Fratila, I.D.Madura, A.Pawelko, A.Sporzynski, M.Tumanowicz, A.H.Velders, J.Zyla (2011) *Tetrahedron Lett.* ,**52,**6639

Formula: $C_{19} H_{20} B_1 N_1 O_2$

Compound Name: (2-((Ethyl(1-naphthyl)amino)methyl)phenyl)boronic acid

Space Group:	P-1	***Cell:***	***a***	8.161(0)	***b***	8.387(0)	***c***	12.243(1)
Space Group No.:	2	***(Å,°)***	α	102.17(1)	β	93.18(0)	γ	105.12(0)

R-Factor (%): 3.25 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.291



BAJTEM

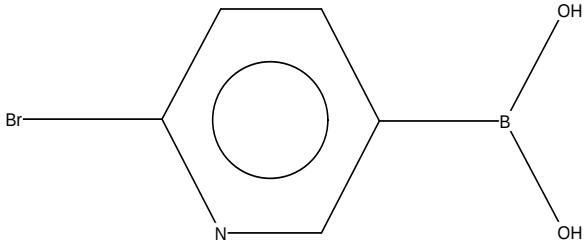
Reference: P.R.Parry, Changsheng Wang, A.S.Batsanov, M.R.Bryce, B.Tarbit (2002) *J.Org.Chem.* ,**67,**7541

Formula: $C_5 H_5 B_1 Br_1 N_1 O_2$

Compound Name: 2-bromo-5-pyridylboronic acid

Space Group:	P21/c	***Cell:***	***a***	7.535(2)	***b***	6.941(1)	***c***	13.877(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	96.81(4)	γ	90.00

R-Factor (%): 3.59 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.860



BAJTEM01

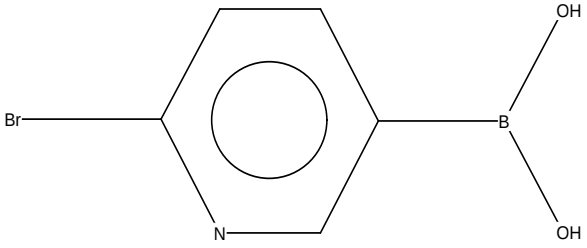
Reference: P.R.Parry, Changsheng Wang, A.S.Batsanov, M.R.Bryce, B.Tarbit (2002) *J.Org.Chem.* ,**67,**7541

Formula: $C_5 H_5 B_1 Br_1 N_1 O_2$

Compound Name: 2-bromo-5-pyridylboronic acid

Space Group:	P21/c	***Cell:***	***a***	7.346(1)	***b***	6.938(1)	***c***	13.727(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	96.62(1)	γ	90.00

R-Factor (%): 1.89 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.929



Search: search4 (Mon May 01 12:48:32 2017): Hits 13-16

BAJTEM02

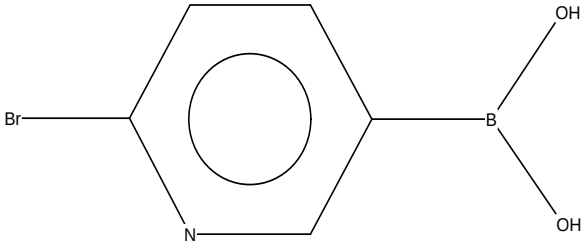
Reference: J.Sopkova-de Oliveira Santos, J.-C.Lancelot, A.Bouillon, S.Rault (2003) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**59,**o111

Formula: $C_5 H_5 B_1 Br_1 N_1 O_2$

Compound Name: (6-Bromopyridin-3-yl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	7.499(0)	***b***	6.918(0)	***c***	13.825(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	96.57(1)	γ	90.00

R-Factor (%): 4.90 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.881



BAJTIQ

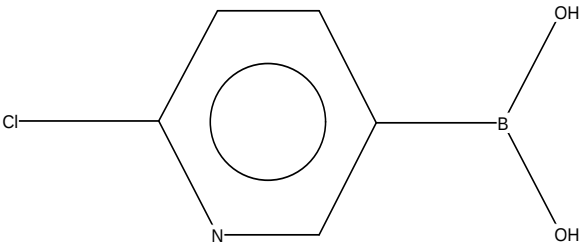
Reference: P.R.Parry, Changsheng Wang, A.S.Batsanov, M.R.Bryce, B.Tarbit (2002) *J.Org.Chem.* ,**67,**7541

Formula: $C_5 H_5 B_1 Cl_1 N_1 O_2$

Compound Name: 2-chloro-5-pyridylboronic acid

Space Group:	P21/n	***Cell:***	***a***	8.906(1)	***b***	7.277(1)	***c***	10.389(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	96.55(1)	γ	90.00

R-Factor (%): 2.94 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.563



BASQET

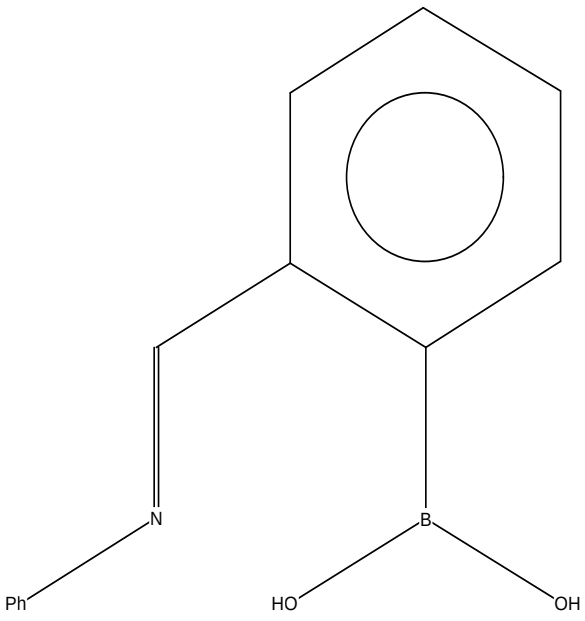
Reference: A.Adamczyk-Wozniak, M.K.Cyranski, B.T.Fraczak, A.Lewandowska, I.D.Madura, A.Sporzynski (2012) *Tetrahedron* ,**68,** 3761

Formula: $C_{13} H_{12} B_1 N_1 O_2$

Compound Name: (2-((Phenylimino)methyl)phenyl)boronic acid

Space Group:	C2/c	***Cell:***	***a***	21.472(4)	***b***	7.842(1)	***c***	16.178(3)
Space Group No.:	15	***(Å,°)***	α	90.00	β	123.98(3)	γ	90.00

R-Factor (%): 3.13 ***Temperature(K):*** 150 ***Density(g/cm³):*** 1.324



BASQIX

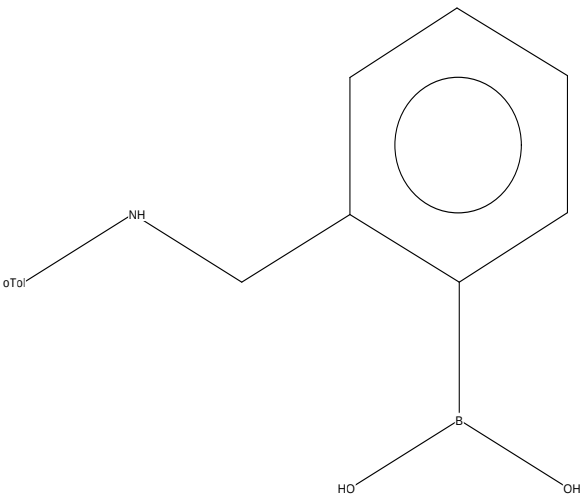
Reference: A.Adamczyk-Wozniak, M.K.Cyranski, B.T.Fraczak, A.Lewandowska, I.D.Madura, A.Sporzynski (2012) *Tetrahedron* ,**68,** 3761

Formula: $C_{14} H_{16} B_1 N_1 O_2$

Compound Name: (2-(((2-Methylphenyl)amino)methyl)phenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	10.678(2)	***b***	9.437(1)	***c***	12.986(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	105.80(3)	γ	90.00

R-Factor (%): 3.52 ***Temperature(K):*** 150 ***Density(g/cm³):*** 1.272



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BASQOD

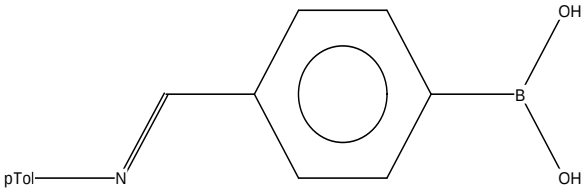
Reference: A.Adamczyk-Wozniak, M.K.Cyranski, B.T.Fraczak, A.Lewandowska, I.D.Madura, A.Sporzynski (2012) *Tetrahedron* ,**68,** 3761

Formula: $C_{14}\,H_{14}\,B_1\,N_1\,O_2$

Compound Name: (4-(((4-Methylphenyl)imino)methyl)phenyl)boronic acid

Space Group:	P-1	***Cell:***	***a***	6.958(1)	***b***	9.887(2)	***c*** 18.691(4)
Space Group No.:	2	***(Å,°)***	α	94.00(3)	β	91.62(3)	γ 104.18(3)

R-Factor (%): 3.39 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.278



BAVJIS

Reference: T.Beringhelli, G.D'Alfonso, D.Donghi, D.Maggioni, P.Mercandelli, A.Sironi (2003) *Organometallics* ,**22,**1588

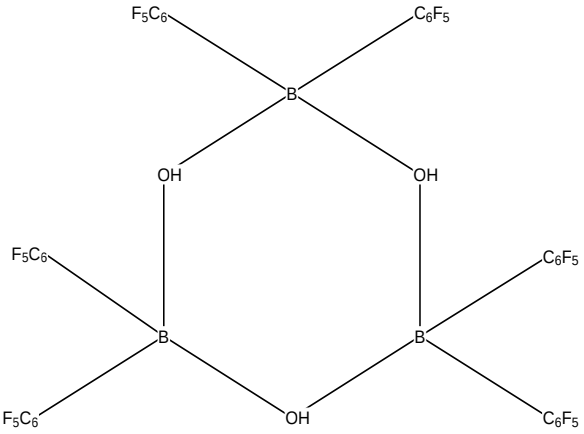
Formula: $C_{36}\,H_3\,B_3\,F_{30}\,O_3$

Compound Name: tris((μ_2-Hydroxo)-bis(pentafluorophenyl)-boron)

Synonym: Cyclo-tris(bis(pentafluorophenyl)borinic acid)

Space Group:	P21/c	***Cell:***	***a***	19.575(3)	***b***	13.127(2)	***c*** 14.823(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	98.14(1)	γ 90.00

R-Factor (%): 3.32 ***Temperature(K):*** 295 ***Density(g/cm^3):*** 1.913



BEQMER

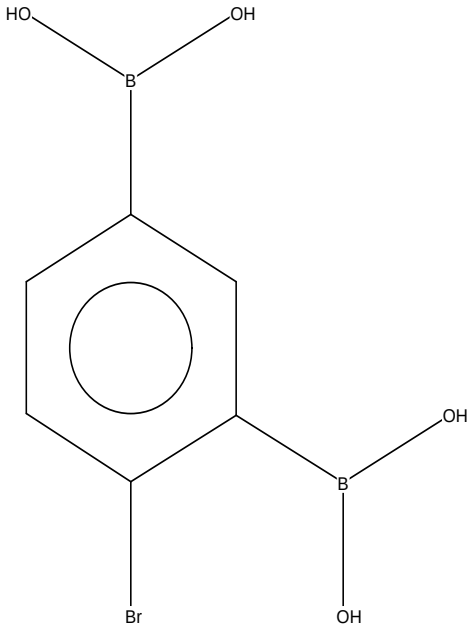
Reference: K.Durka, S.Lulinski, J.Smetek, M.Dabrowski, J.Serwatowski, K.Wozniak (2013) *Eur.J.Org.Chem.* ,3023

Formula: $C_6\,H_7\,B_2\,Br_1\,O_4$

Compound Name: (4-Bromo-1,3-phenylene)diboronic acid

Space Group:	Cc	***Cell:***	***a***	28.918(3)	***b***	3.770(0)	***c*** 16.676(1)
Space Group No.:	9	***(Å,°)***	α	90.00	β	109.88(1)	γ 90.00

R-Factor (%): 4.10 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.901



BEWYAE

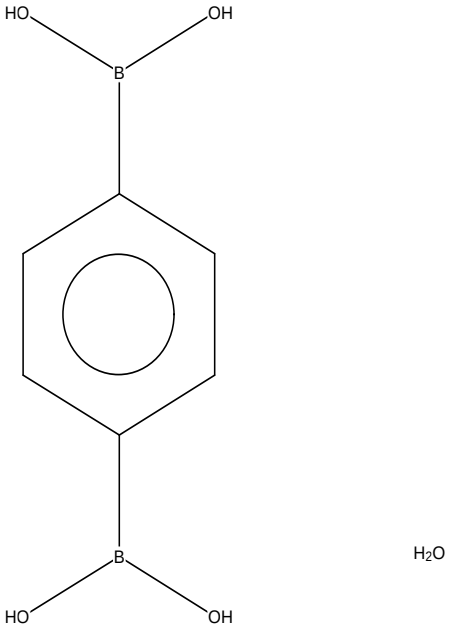
Reference: P.Rodriguez-Cuamatzi, G.Vargas-Daz, H.Hopfl (2004) *Angew.Chem.,Int.Ed.* ,**43,**3041

Formula: $C_6\,H_8\,B_2\,O_4{,}4(H_2\,O_1)$

Compound Name: 1,4-Phenylenediboronic acid tetrahydrate

Space Group:	P-1	***Cell:***	***a***	4.940(2)	***b***	8.727(4)	***c*** 14.216(6)
Space Group No.:	2	***(Å,°)***	α	95.03(0)	β	91.79(0)	γ 101.48(0)

R-Factor (%): 4.40 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.322



Search: search4 (Mon May 01 12:48:32 2017): Hits 21-24

BEWYAE01

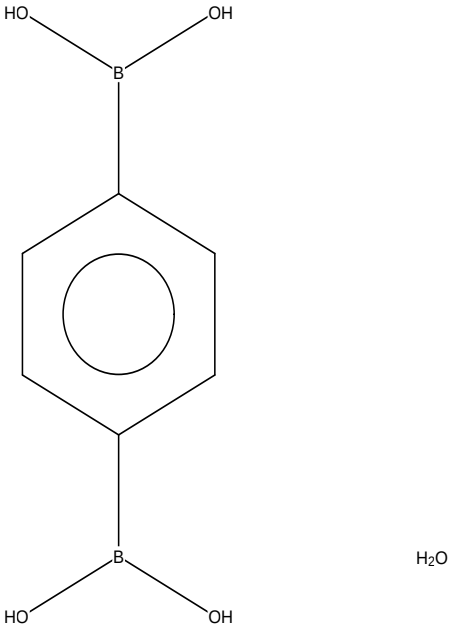
Reference: T.Morawitz, H.-W.Lerner, M.Bolte (2006)
CSD Communication(Private Communication) ,

Formula: $C_6 H_8 B_2 O_4,4(H_2 O_1)$

Compound Name: 1,4-Phenylenediboronic acid tetrahydrate

Space Group:	P-1	***Cell:***	***a*** 4.942(0)	***b*** 8.744(1)	***c*** 14.259(2)
Space Group No.:	2	***(Å,°)***	α 95.38(1)	β 91.14(1)	γ 101.26(1)

R-Factor (%): 4.79 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.314



BPHBAC

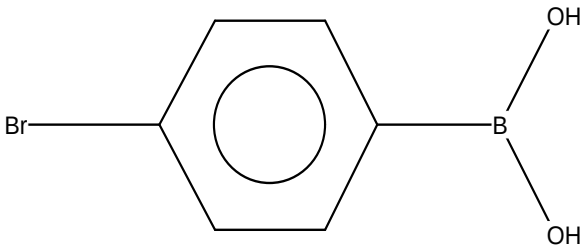
Reference: Z.V.Zvonkova, V.P.Gluskova (1958)
Kristallografiya(Russ.)(Crystallogr.Rep.) ,**3,**559

Formula: $C_6 H_6 B_1 Br_1 O_2$

Compound Name: p-Bromophenylboronic acid

Space Group:	P6/mcc	***Cell:***	***a*** 28.730	***b*** 28.730	***c*** 9.740
Space Group No.:	192	***(Å,°)***	α 90.00	β 90.00	γ 120.00

R-Factor (%): 24.00 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.724



BPHBAC01

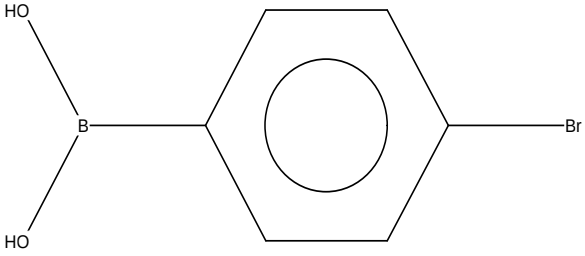
Reference: M.R.Shimpi, N.SeethaLekshmi, V.R.Pedireddi (2007)
Cryst.Growth Des. ,**7,**1958

Formula: $C_6 H_6 B_1 Br_1 O_2$

Compound Name: 4-Bromophenylboronic acid

Space Group:	P-1	***Cell:***	***a*** 5.010(3)	***b*** 7.241(4)	***c*** 10.989(6)
Space Group No.:	2	***(Å,°)***	α 103.30(8)	β 97.06(9)	γ 100.52(9)

R-Factor (%): 6.22 ***Temperature(K):*** 133 ***Density(g/cm³):*** 1.775



BUDREY

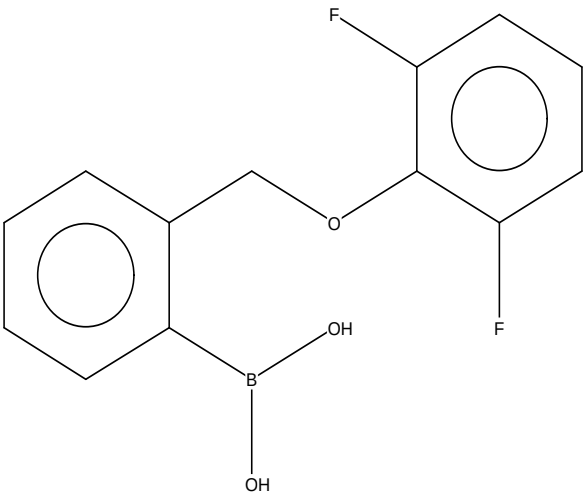
Reference: T.Klis, J.Serwatowski (2009)
Acta Crystallogr.,Sect.E:Struct.Rep.Online ,**65,**o2348

Formula: $C_{13} H_{11} B_1 F_2 O_3$

Compound Name: (2-((2,6-Difluorophenoxy)methyl)phenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a*** 7.666(0)	***b*** 14.230(1)	***c*** 11.360(1)
Space Group No.:	14	***(Å,°)***	α 90.00	β 101.15(0)	γ 90.00

R-Factor (%): 3.00 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.442



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CAKYUK

Reference: S.Varughese, Y.Azim, G.R.Desiraju (2010) *J.Pharm.Sci.* , **99,**3743

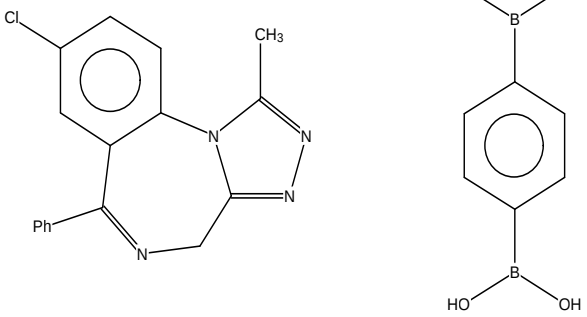
Formula: $C_{17}\,H_{13}\,Cl_1\,N_4{,}0.5(C_6\,H_8\,B_2\,O_4)$

Compound Name: 8-Chloro-1-methyl-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine hemikis(1,4-phenylenediboronic acid)

Synonym: Alprazolam hemikis(1,4-benzenediboronic acid)

Space Group:	P-1	***Cell:***	***a***	11.881(9)	***b***	13.279(9)	***c***	14.544(8)
Space Group No.:	2	***(Å,°)***	α	63.89(0)	β	71.17(0)	γ	88.44(0)

R-Factor (%): 5.25 ***Temperature(K):*** 298 ***Density(g/cm^3):*** 1.346



CAKZAR

Reference: S.Varughese, Y.Azim, G.R.Desiraju (2010) *J.Pharm.Sci.* , **99,**3743

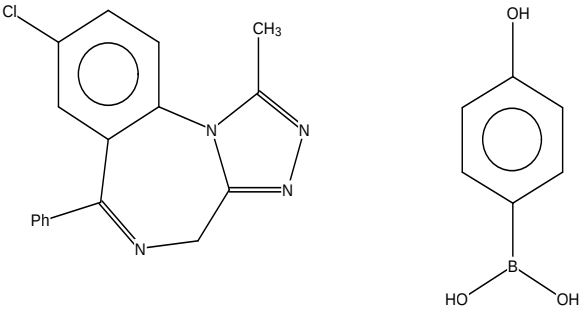
Formula: $C_{17}\,H_{13}\,Cl_1\,N_4{,}C_6\,H_7\,B_1\,O_3$

Compound Name: 8-Chloro-1-methyl-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine (4-hydroxyphenyl)boronic acid

Synonym: Alprazolam 4-hydroxyphenylboronic acid

Space Group:	P-1	***Cell:***	***a***	7.687(2)	***b***	10.986(2)	***c***	13.731(3)
Space Group No.:	2	***(Å,°)***	α	71.76(0)	β	83.14(0)	γ	83.76(0)

R-Factor (%): 4.58 ***Temperature(K):*** 298 ***Density(g/cm^3):*** 1.361



CAQZAW

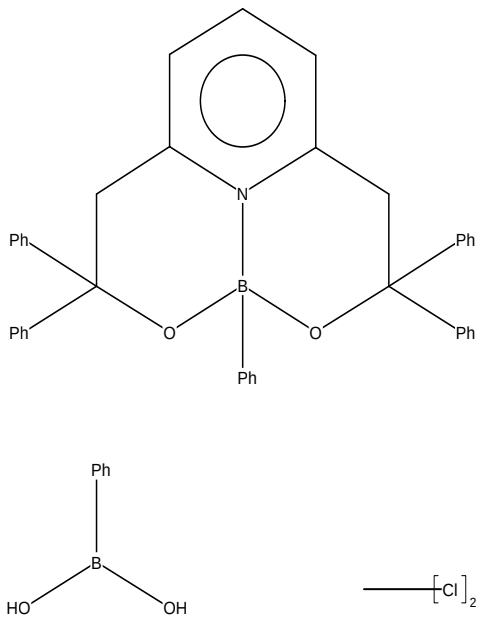
Reference: G.Vargas, N.Farfan, R.Santillan, A.Gutierrez, E.Gomez, V.Barba (2005) *Inorg.Chim.Acta* , **358,**2996

Formula: $C_{39}\,H_{32}\,B_1\,N_1\,O_2{,}C_6\,H_7\,B_1\,O_2{,}0.5(C_1\,H_2\,Cl_2)$

Compound Name: (2,6-bis(2,2-Diphenyl-2-oxyethyl)pyridyl)phenylboron phenylboronic acid dichloromethane solvate

Space Group:	P1	***Cell:***	***a***	10.403(2)	***b***	12.451(2)	***c***	16.425(3)
Space Group No.:	1	***(Å,°)***	α	102.74(3)	β	95.43(3)	γ	110.12(3)

R-Factor (%): 4.23 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.252



CEZHUK

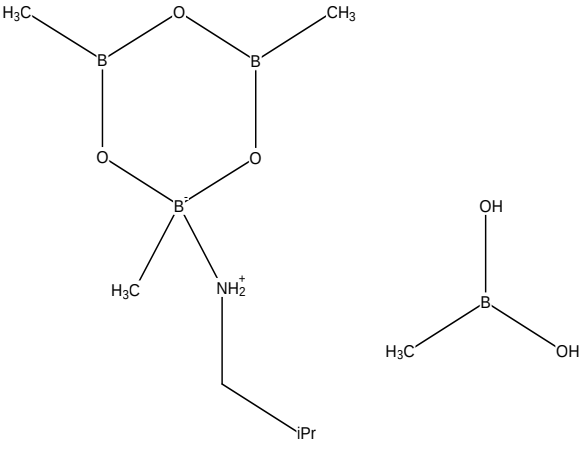
Reference: M.A.Beckett, D.S.Brassington, P.Owen, M.B.Hursthouse, M.E.Light, K.M.A.Malik, K.S.Varma (1999) *J.Organomet.Chem.* , **585,**7

Formula: $C_7\,H_{20}\,B_3\,N_1\,O_3{,}C_1\,H_5\,B_1\,O_2$

Compound Name: Isobutylamine trimethylboroxine dihydroxy(methyl)borane

Space Group:	P21/c	***Cell:***	***a***	9.342(2)	***b***	22.300(4)	***c***	15.935(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	106.49(3)	γ	90.00

R-Factor (%): 6.16 ***Temperature(K):*** 150 ***Density(g/cm^3):*** 1.079



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CIQHAN

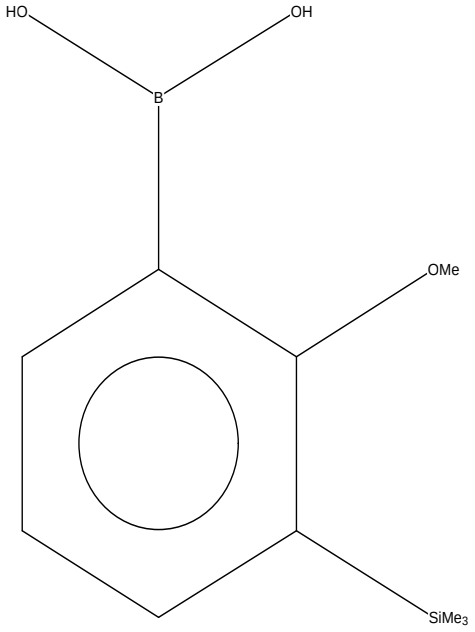
Reference: K.Durka, S.Lulinski, J.Serwatowski (2013) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**69,**o1818

Formula: $C_{10}\,H_{17}\,B_1\,O_3\,Si_1$

Compound Name: (2-Methoxy-3-(trimethylsilyl)phenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	9.183(1)	***b***	9.708(1)	***c***	14.142(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	104.26(1)	γ	90.00

R-Factor (%): 3.39 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.218



CITNOJ

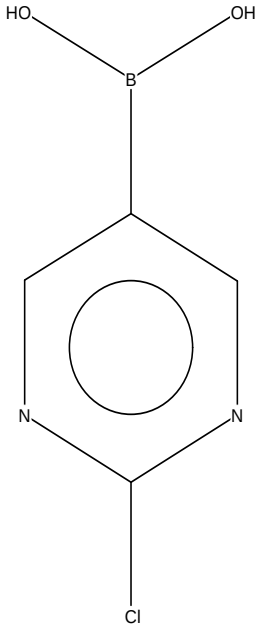
Reference: K.M.Clapham, A.E.Smith, A.S.Batsanov, L.McIntyre, A.Pountney, M.R.Bryce, B.Tarbit (2007) *Eur.J.Org.Chem.* ,5712

Formula: $C_4\,H_4\,B_1\,Cl_1\,N_2\,O_2$

Compound Name: 2-Chloro-5-pyrimidylboronic acid

Space Group:	P21/n	***Cell:***	***a***	6.644(2)	***b***	14.578(4)	***c***	7.155(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	116.60(1)	γ	90.00

R-Factor (%): 5.14 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.697



DAVPAT

Reference: A.Lemmerer (2012) *J.Chem.Cryst.* ,**42,**498

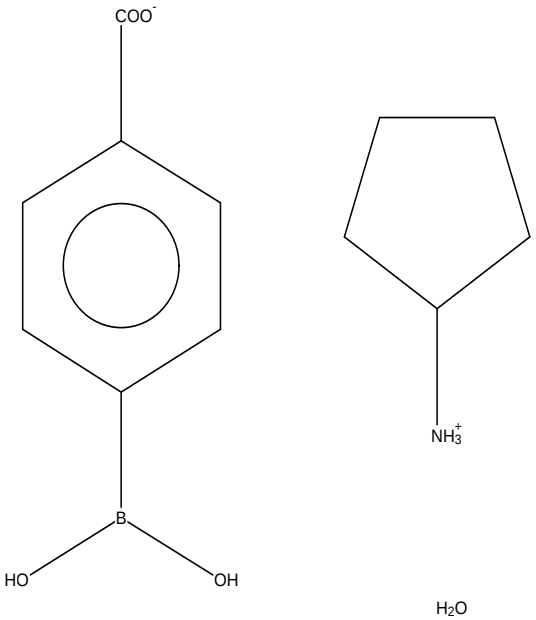
Formula: $C_5\,H_{12}\,N_1\,^{1+}$,$C_7\,H_6\,B_1\,O_4\,^{1-}$,3($H_2\,O_1$)

Compound Name: Cyclopentanaminium 4-(dihydroxyboryl)benzoate trihydrate

Synonym: cyclopentylammnonium 4-carboxyboronate trihydrate

Space Group:	Cc	***Cell:***	***a***	16.927(0)	***b***	10.339(0)	***c***	9.748(0)
Space Group No.:	9	***(Å,°)***	α	90.00	β	107.01(0)	γ	90.00

R-Factor (%): 4.40 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.242



DECROT

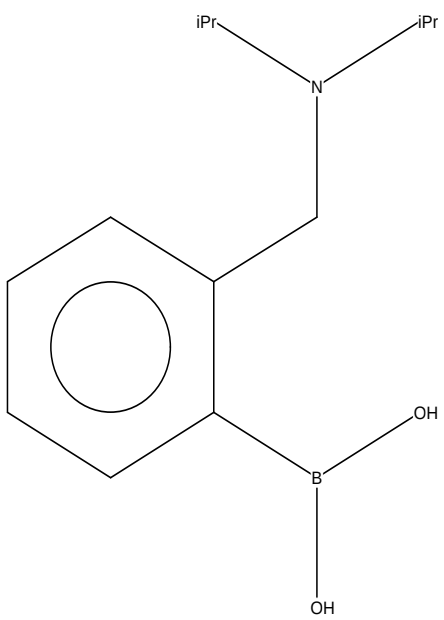
Reference: S.W.Coghlan, R.L.Giles, J.A.K.Howard, L.G.F.Patrick, M.R.Probert, G.E.Smith, A.Whiting (2005) *J.Organomet.Chem.* ,**690,** 4784

Formula: $C_{13}\,H_{22}\,B_1\,N_1\,O_2$

Compound Name: (2-(Diisopropylaminomethyl)phenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	13.620(0)	***b***	7.658(0)	***c***	13.486(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	109.61(0)	γ	90.00

R-Factor (%): 4.09 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.179



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DEWYAG

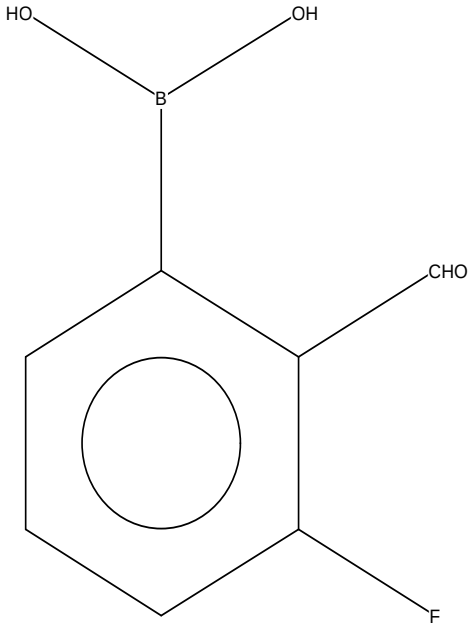
Reference: S.Lulinski, I.Madura, J.Serwatowski, H.Szatylowicz, J.Zachara (2007) *New J.Chem.* ,**31,**144

Formula: $C_7 H_6 B_1 F_1 O_3$

Compound Name: 3-Fluoro-2-formylphenylboronic acid

Space Group:	P-1	***Cell:***	***a***	7.214(0)	***b***	7.619(0)	***c*** 8.101(1)
Space Group No.:	2	***(Å,°)***	α	102.96(1)	β	106.80(1)	γ 111.39(0)

R-Factor (%): 3.27 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.512



DEWYEK

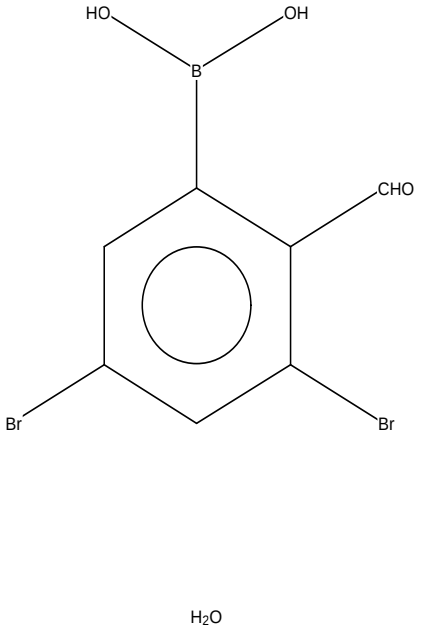
Reference: S.Lulinski, I.Madura, J.Serwatowski, H.Szatylowicz, J.Zachara (2007) *New J.Chem.* ,**31,**144

Formula: $C_7 H_5 B_1 Br_2 O_3,H_2 O_1$

Compound Name: 3,5-Dibromo-2-formylphenylboronic acid monohydrate

Space Group:	P-1	***Cell:***	***a***	7.056(1)	***b***	8.375(1)	***c*** 9.656(2)
Space Group No.:	2	***(Å,°)***	α	89.99(1)	β	99.61(1)	γ 108.33(1)

R-Factor (%): 2.53 ***Temperature(K):*** 293 ***Density(g/cm³):*** 2.029



DISSAA

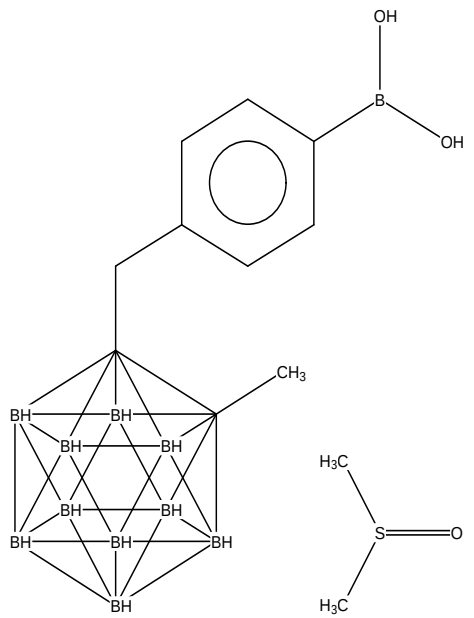
Reference: Erhong Hao, B.Fabre, F.R.Fronczek, M.G.H.Vicente (2007) *Chem.Mater.* ,**19,**6195

Formula: $C_{10} H_{21} B_{11} O_2,C_2 H_6 O_1 S_1$

Compound Name: (4-((2-Methyl-1,2-dicarba-closo-dodecaboran-1-yl)methyl)phenyl)boronic acid dimethylsulfoxide solvate

Space Group:	P21/c	***Cell:***	***a***	19.767(2)	***b***	7.661(1)	***c*** 14.602(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	111.66(0)	γ 90.00

R-Factor (%): 4.40 ***Temperature(K):*** 90 ***Density(g/cm³):*** 1.197



DIXTIO

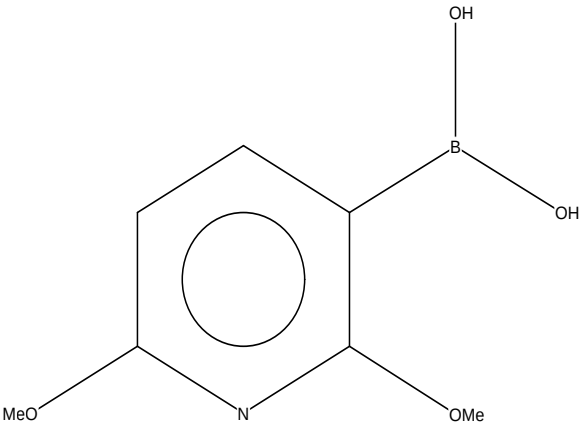
Reference: A.E.Smith, K.M.Clapham, A.S.Batsanov, M.R.Bryce, B.Tarbit (2008) *Eur.J.Org.Chem.* ,1458

Formula: $C_7 H_{10} B_1 N_1 O_4$

Compound Name: (2,6-Dimethoxy-3-pyridyl)boronic acid

Space Group:	Pbca	***Cell:***	***a***	6.862(0)	***b***	15.825(1)	***c*** 32.167(3)
Space Group No.:	61	***(Å,°)***	α	90.00	β	90.00	γ 90.00

R-Factor (%): 9.07 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.392



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DIXTOU

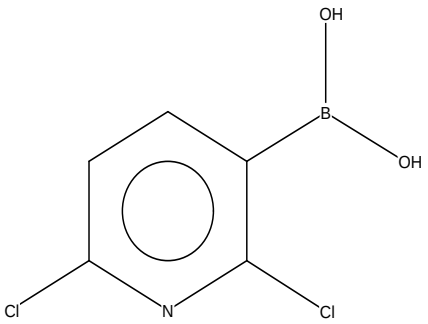
Reference: A.E.Smith, K.M.Clapham, A.S.Batsanov, M.R.Bryce, B.Tarbit (2008) *Eur.J.Org.Chem.* ,1458

Formula: $C_5 H_4 B_1 Cl_2 N_1 O_2$,0.5($H_2 O_1$)

Compound Name: 2,6-Dichloro-3-pyridyl boronic acid hemihydrate

Space Group:	P21/n	***Cell:***	***a***	6.828(1)	***b***	31.106(4)	***c***	7.797(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	95.25(3)	γ	90.00

R-Factor (%): 3.65 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.618



H_2O

DIXTUA

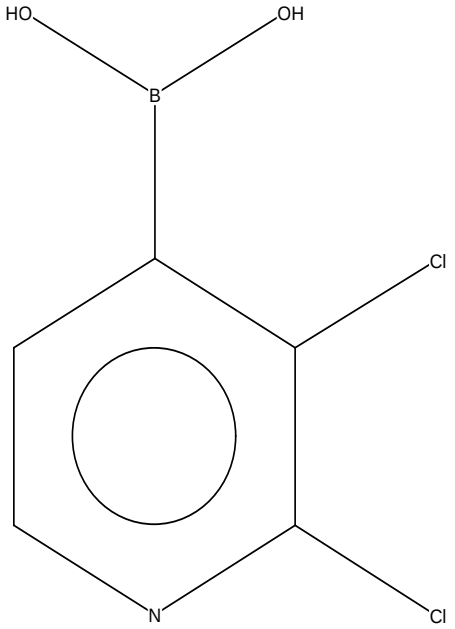
Reference: A.E.Smith, K.M.Clapham, A.S.Batsanov, M.R.Bryce, B.Tarbit (2008) *Eur.J.Org.Chem.* ,1458

Formula: $C_5 H_4 B_1 Cl_2 N_1 O_2$

Compound Name: (2,3-Dichloro-4-pyridyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	8.970(2)	***b***	8.666(2)	***c***	10.216(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	106.22(1)	γ	90.00

R-Factor (%): 3.45 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.671



DIXVAI

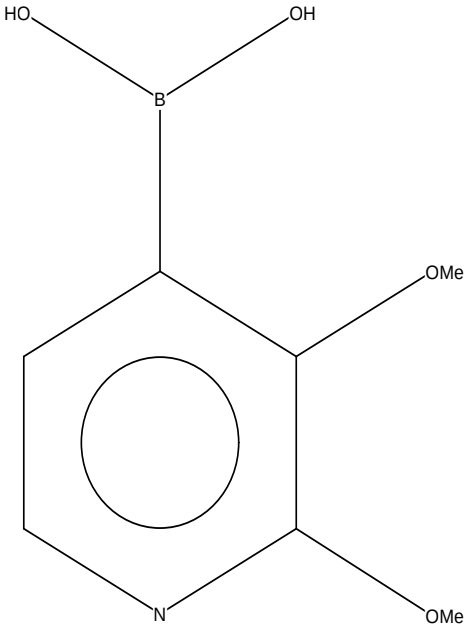
Reference: A.E.Smith, K.M.Clapham, A.S.Batsanov, M.R.Bryce, B.Tarbit (2008) *Eur.J.Org.Chem.* ,1458

Formula: $C_7 H_{10} B_1 N_1 O_4$

Compound Name: 2,3-Dimethoxy-4-pyridylboronic acid

Space Group:	Pna21	***Cell:***	***a***	14.759(0)	***b***	3.874(0)	***c***	14.744(0)
Space Group No.:	33	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 2.55 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.442



DOBKUA

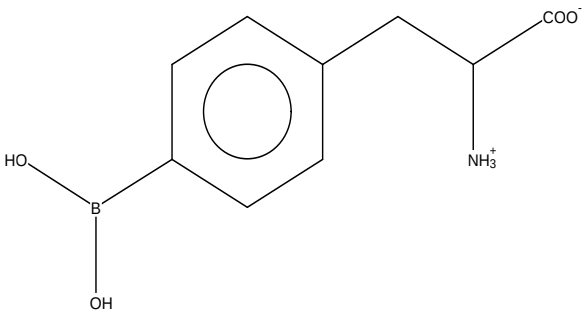
Reference: B.K.Shull, D.E.Spielvogel, R.Gopalaswamy, S.Sankar, P.D.Boyle, G.Head, K.Devito (2000) *J.Chem.Soc.,Perkin Trans.2* ,557

Formula: $C_9 H_{12} B_1 N_1 O_4$

Compound Name: L-p-Boronophenylalanine

Space Group:	P21	***Cell:***	***a***	5.347(0)	***b***	7.323(0)	***c***	12.171(0)
Space Group No.:	4	***(Å,°)***	α	90.00	β	102.38(0)	γ	90.00

R-Factor (%): 3.10 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.491



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DOVHON

Reference: I.D.Madura, K.Czerwinska, D.Soldanska (2014)
Cryst.Growth Des. ,**14,**5912

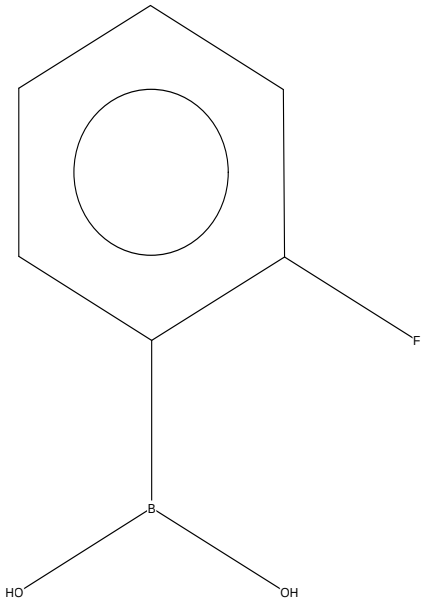
Formula: $C_6 H_6 B_1 F_1 O_2$

Compound Name: (2-fluorophenyl)boronic acid

Synonym: (o-fluorophenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	5.102(0)	***b***	5.557(0)	***c***	22.059(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	94.73(0)	γ	90.00

R-Factor (%): 3.43 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.491



DOVHUT

Reference: I.D.Madura, K.Czerwinska, D.Soldanska (2014)
Cryst.Growth Des. ,**14,**5912

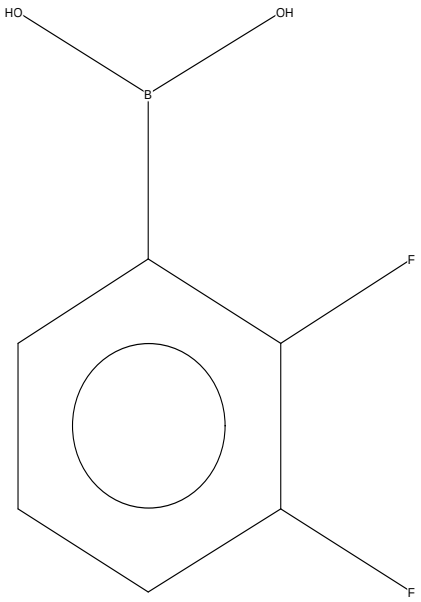
Formula: $C_6 H_5 B_1 F_2 O_2$

Compound Name: (2,3-difluorophenyl)boronic acid

Synonym: (o,m-difluorophenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	8.966(0)	***b***	4.957(0)	***c***	29.717(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	97.59(0)	γ	90.00

R-Factor (%): 3.04 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.602



DOVJEF

Reference: I.D.Madura, K.Czerwinska, D.Soldanska (2014)
Cryst.Growth Des. ,**14,**5912

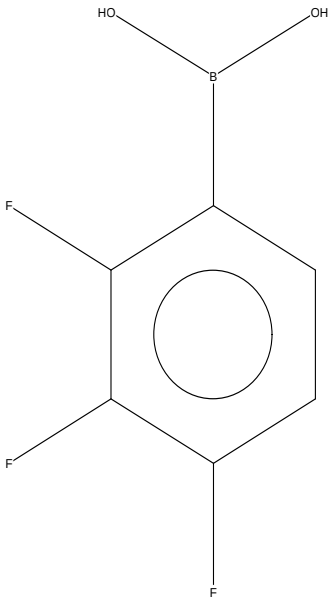
Formula: $C_6 H_4 B_1 F_3 O_2$

Compound Name: (2,3,4-trifluorophenyl)boronic acid

Synonym: (o,m,p-trifluorophenyl)boronic acid

Space Group:	P-1	***Cell:***	***a***	4.376(0)	***b***	5.024(0)	***c***	15.640(1)
Space Group No.:	2	***(Å,°)***	α	96.48(0)	β	94.14(0)	γ	92.84(0)

R-Factor (%): 3.09 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.717



DOVJIJ

Reference: I.D.Madura, K.Czerwinska, D.Soldanska (2014)
Cryst.Growth Des. ,**14,**5912

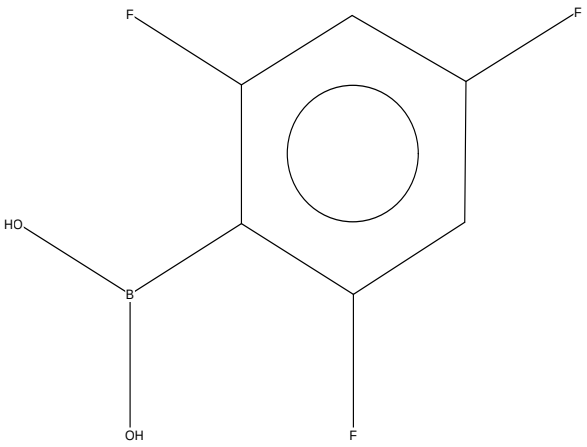
Formula: $C_6 H_4 B_1 F_3 O_2$

Compound Name: (2,4,6-trifluorophenyl)boronic acid

Synonym: (o,o,p-trifluorophenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	5.003(0)	***b***	5.334(0)	***c***	24.218(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	90.26(0)	γ	90.00

R-Factor (%): 2.82 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.808



Search: search4 (Mon May 01 12:48:32 2017): Hits 45-48

DOVJOP

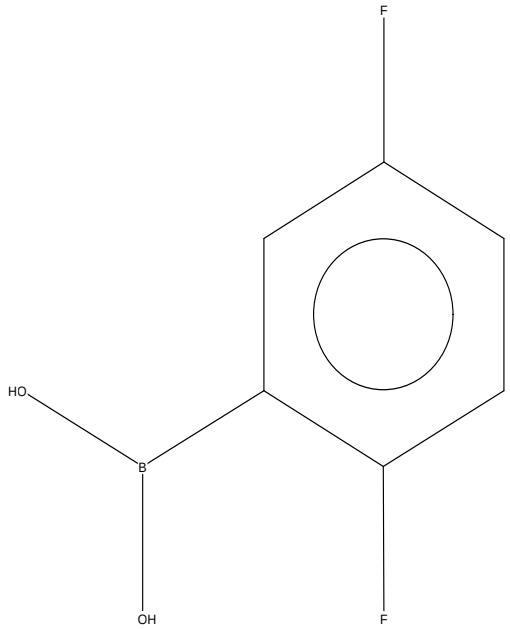
Reference: I.D.Madura, K.Czerwinska, D.Soldanska (2014) *Cryst.Growth Des.* ,**14,**5912

Formula: $C_6 H_5 B_1 F_2 O_2$

Compound Name: (2,5-difluorophenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	4.153(0)	***b***	5.114(0)	***c***	30.732(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	90.07(0)	γ	90.00

R-Factor (%): 3.09 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.607



DOVJOP01

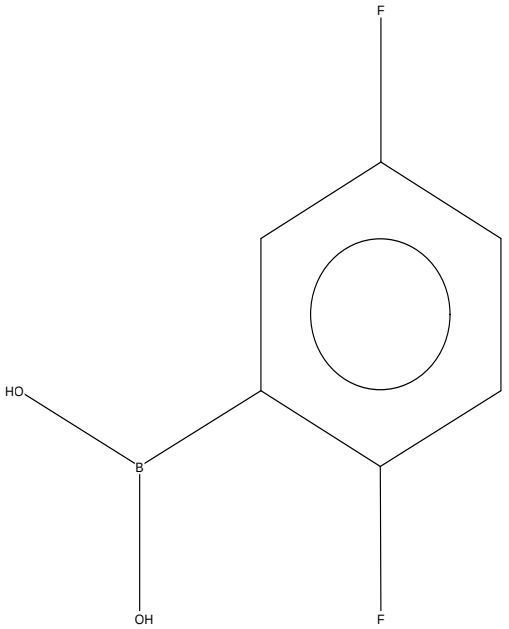
Reference: I.D.Madura, K.Czerwinska, D.Soldanska (2014) *Cryst.Growth Des.* ,**14,**5912

Formula: $C_6 H_5 B_1 F_2 O_2$

Compound Name: (2,5-difluorophenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	4.958(0)	***b***	5.526(0)	***c***	23.484(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	93.97(0)	γ	90.00

R-Factor (%): 4.66 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.634



EFIDIH

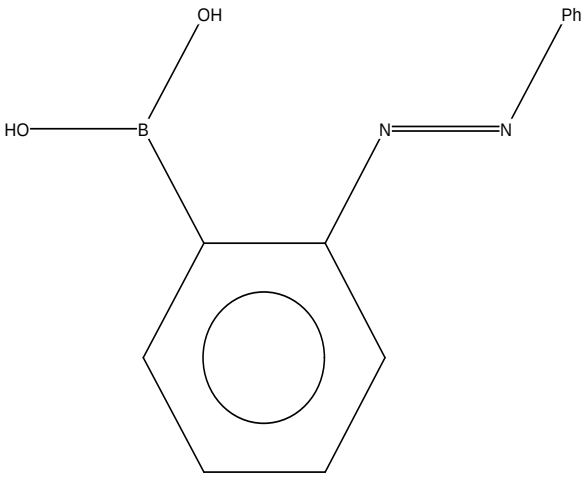
Reference: J.Yoshino, N.Kano, T.Kawashima (2008) *Tetrahedron* ,**64,** 7774

Formula: $C_{12} H_{11} B_1 N_2 O_2$

Compound Name: (E)-(2-(Phenylazo)phenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	14.436(7)	***b***	5.080(2)	***c***	16.529(8)
Space Group No.:	14	***(Å,°)***	α	90.00	β	112.49(0)	γ	90.00

R-Factor (%): 3.32 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.341



EFIDON

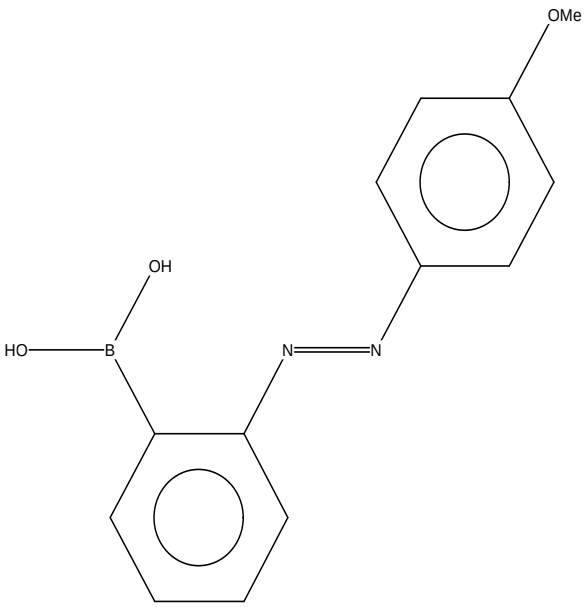
Reference: J.Yoshino, N.Kano, T.Kawashima (2008) *Tetrahedron* ,**64,** 7774

Formula: $C_{13} H_{13} B_1 N_2 O_3$

Compound Name: (E)-(2-(4-Methoxyphenylazo)phenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	11.469(6)	***b***	5.253(2)	***c***	21.151(11)
Space Group No.:	14	***(Å,°)***	α	90.00	β	103.18(0)	γ	90.00

R-Factor (%): 3.62 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.371



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EHIZOM

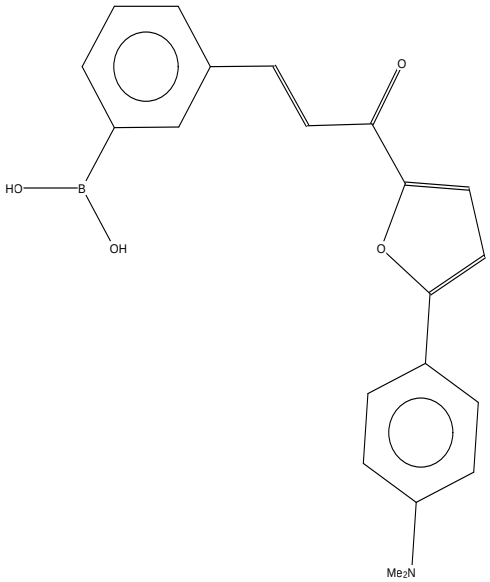
Reference: Seung-Jin Jung, Jun Young Lee, Tae Ho Kim, Dong-Eun Lee, Jongho Jeon, Seung Dae Yang, Min Goo Hur, Jung-Joon Min, Yong Dae Park (2016) *Bioorg.Med.Chem.Lett.* ,**26,** 1784

Formula: $C_{21}\,H_{20}\,B_1\,N_1\,O_4$

Compound Name: (3-(3-(5-(4-(Dimethylamino)phenyl)-2-furyl)-3-oxoprop-1-en-1-yl)phenyl) boronic acid

Space Group:	C2/c	***Cell:***	***a***	18.551(0)	***b***	14.327(0)	***c***	14.463(0)
Space Group No.:	15	***(Å,°)***	α	90.00	β	105.96(0)	γ	90.00

R-Factor (%): 6.70 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.298



EJAGAZ

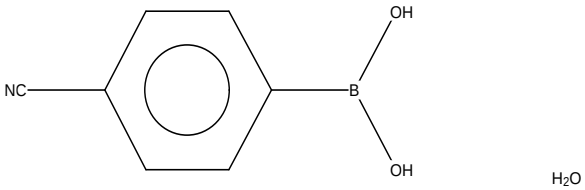
Reference: A.M.Mfuh, J.D.Doyle, Bhuwan Chhetri, H.D.Arman, O.V.Larionov (2016) *J.Am.Chem.Soc.* ,**138,**2985

Formula: $C_7\,H_6\,B_1\,N_1\,O_2{,}2(H_2\,O_1)$

Compound Name: (4-cyanophenyl)boronic acid dihydrate

Space Group:	P-1	***Cell:***	***a***	3.769(0)	***b***	8.510(1)	***c***	14.058(1)
Space Group No.:	2	***(Å,°)***	α	93.31(0)	β	91.47(0)	γ	94.63(0)

R-Factor (%): 6.63 ***Temperature(K):*** 98 ***Density(g/cm³):*** 1.355



EJUXAK

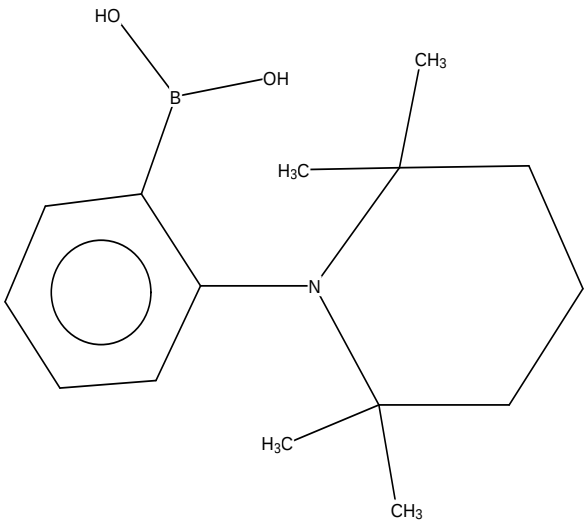
Reference: M.-A.Legare, E.Rochette, J.L.Lavergne, N.Bouchard, F.-G.Fontaine (2016) *Chem.Commun.* ,**52,**5387

Formula: $C_{15}\,H_{24}\,B_1\,N_1\,O_2$

Compound Name: (2-(2,2,6,6-Tetramethylpiperidin-1-yl)phenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	13.854(0)	***b***	7.816(0)	***c***	15.243(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	115.86(0)	γ	90.00

R-Factor (%): 4.27 ***Temperature(K):*** 150 ***Density(g/cm³):*** 1.168



ETOLAA

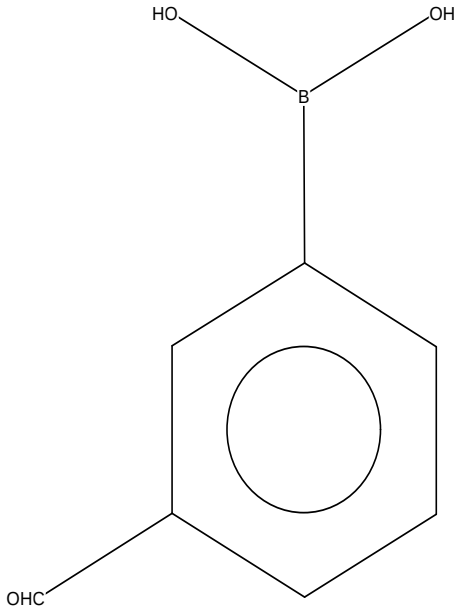
Reference: B.Zarychta, J.Zaleski, A.Sporzynski, M.Dabrowski, J.Serwatowski (2004) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* , **60,**o344

Formula: $C_7\,H_7\,B_1\,O_3$

Compound Name: (3-Formylphenyl)boronic acid

Space Group:	C2/c	***Cell:***	***a***	22.635(2)	***b***	3.733(0)	***c***	17.126(2)
Space Group No.:	15	***(Å,°)***	α	90.00	β	102.05(0)	γ	90.00

R-Factor (%): 3.63 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.407



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FAKTER

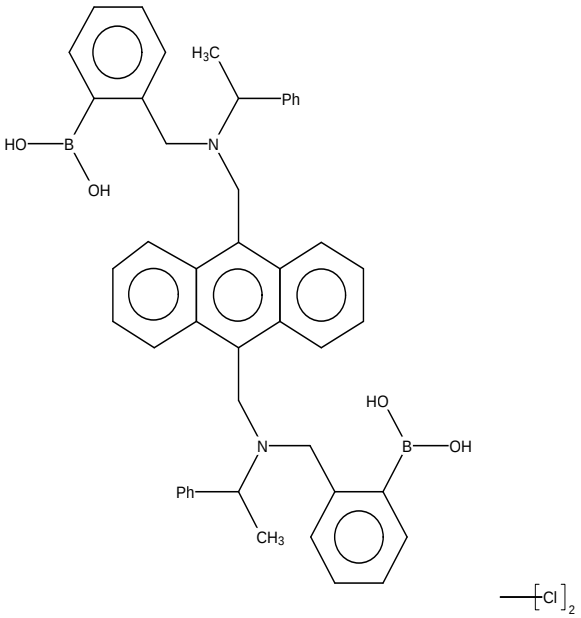
Reference: Jianzhang Zhao, M.G.Davidson, M.F.Mahon, G.Kociok-Kohn, T.D.James (2004) *J.Am.Chem.Soc.* ,**126,**16179

Formula: $C_{46}H_{46}B_2N_2O_4,0.25(C_1H_2Cl_2)$

Compound Name: (R,R)-(-)-9,10-bis(N-((2-(Dihydroxyboryl)phenyl)methyl)-N-(1-phenylethyl)aminomethyl)anthracene dichloromethane solvate

Space Group:	P21	***Cell:***	***a***	12.425(0)	***b***	25.943(0)	***c***	14.708(0)
Space Group No.:	4	***(Å,°)***	α	90.00	β	114.26(0)	γ	90.00

R-Factor (%): 6.27 ***Temperature(K):*** 150 ***Density(g/cm³):*** 1.128



FECSEM

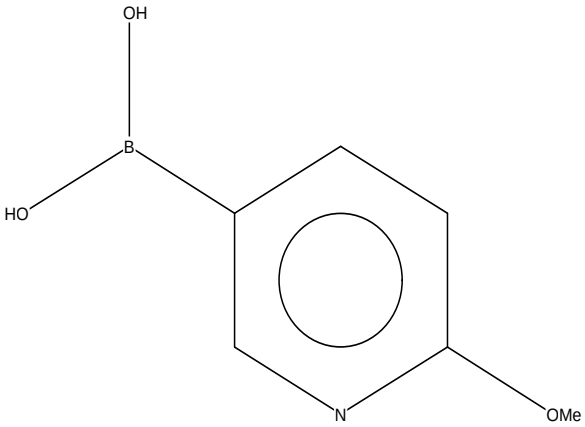
Reference: A.E.Thompson, G.Hughes, A.S.Batsanov, M.R.Bryce, P.R.Parry, B.Tarbit (2005) *J.Org.Chem.* ,**70,**388

Formula: $C_6H_8B_1N_1O_3$

Compound Name: 2-Methoxy-5-pyridylboronic acid

Space Group:	P-1	***Cell:***	***a***	7.071(1)	***b***	9.898(2)	***c***	10.636(2)
Space Group No.:	2	***(Å,°)***	α	85.74(1)	β	89.27(1)	γ	74.64(1)

R-Factor (%): 4.29 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.419



FEJGIL

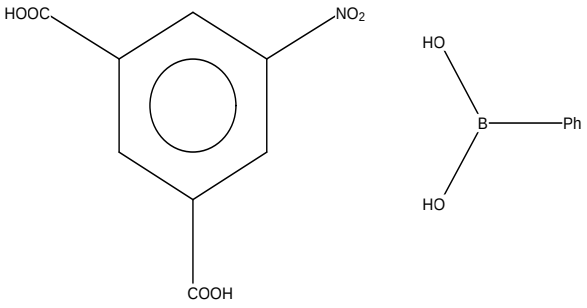
Reference: P.Rodriguez-Cuamatzi, O.I.Arillo-Flores, M.I.Bernal-Uruchurtu, H.Hopfl (2005) *Cryst.Growth Des.* ,**5,**167

Formula: $C_8H_5N_1O_6,C_6H_7B_1O_2,2(H_2O_1)$

Compound Name: 5-nitroisophthalic acid phenyl boronic acid dihydrate

Space Group:	P-1	***Cell:***	***a***	8.498(1)	***b***	9.810(1)	***c***	11.594(1)
Space Group No.:	2	***(Å,°)***	α	68.79(0)	β	69.65(0)	γ	83.61(0)

R-Factor (%): 7.04 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.451



H_2O

FEJGOR

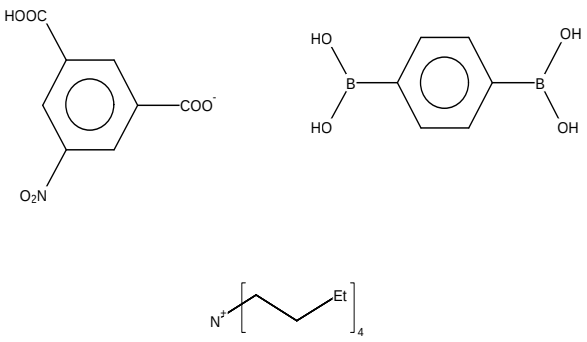
Reference: P.Rodriguez-Cuamatzi, O.I.Arillo-Flores, M.I.Bernal-Uruchurtu, H.Hopfl (2005) *Cryst.Growth Des.* ,**5,**167

Formula: $C_{16}H_{36}N_1{}^{1+},C_8H_4N_1O_6{}^{1-},0.5(C_6H_8B_2O_4)$

Compound Name: tetrabutylammonium 5-nitrohydrogenisophthalate 1,4-phenylenediboronic acid

Space Group:	P21/c	***Cell:***	***a***	9.634(1)	***b***	15.200(1)	***c***	19.600(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	97.71(0)	γ	90.00

R-Factor (%): 6.07 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.251



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FEJGUX

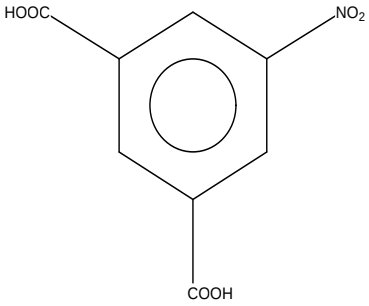
Reference: P.Rodriguez-Cuamatzi, O.I.Arillo-Flores, M.I.Bernal-Uruchurtu, H.Hopfl (2005) *Cryst.Growth Des.* ,**5,**167

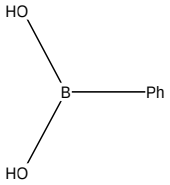
Formula: $C_8 H_5 N_1 O_6$,$C_6 H_7 B_1 O_2$,$H_2 O_1$

Compound Name: 5-nitrohydrogenisophthalate phenyl boronic acid monohydrate

Space Group:	P21/n	***Cell:***	***a*** 8.640(1)	***b*** 21.251(3)	***c*** 9.681(1)
Space Group No.:	14	***(Å,°)***	α 90.00	β 112.11(0)	γ 90.00

R-Factor (%): 6.66 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.416





H_2O

FEJHAE

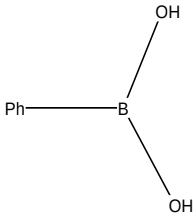
Reference: P.Rodriguez-Cuamatzi, O.I.Arillo-Flores, M.I.Bernal-Uruchurtu, H.Hopfl (2005) *Cryst.Growth Des.* ,**5,**167

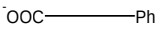
Formula: $C_7 H_5 O_2^{1-}$,$C_6 H_7 B_1 O_2$,$C_{16} H_{36} N_1^{1+}$

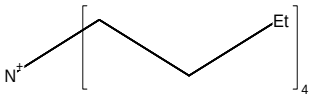
Compound Name: phenylboronic acid tetra-n-butylammonium benzoate

Space Group:	P21/c	***Cell:***	***a*** 10.559(1)	***b*** 17.448(1)	***c*** 16.253(1)
Space Group No.:	14	***(Å,°)***	α 90.00	β 91.31(0)	γ 90.00

R-Factor (%): 9.13 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.077







FETDAK

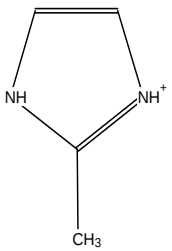
Reference: C.B.Aakeroy, J.Desper, B.Levin (2005) *CrystEngComm* ,**7,** 102

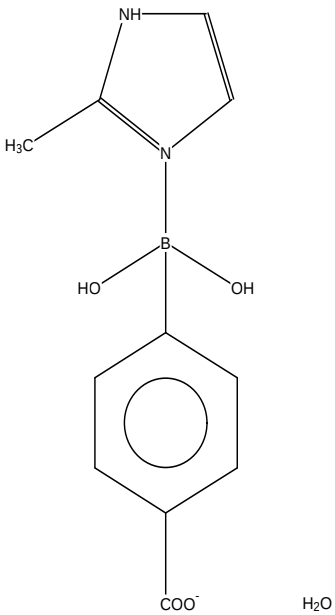
Formula: $C_4 H_7 N_2^{1+}$,$C_{11} H_{12} B_1 N_2 O_4^{1-}$,$H_2 O_1$

Compound Name: 2-Methylimidazolium (4-carboxybenzene)(2-methylimidazolyl)boronate monohydrate

Space Group:	P-1	***Cell:***	***a*** 7.300(0)	***b*** 7.695(0)	***c*** 15.668(1)
Space Group No.:	2	***(Å,°)***	α 86.51(0)	β 76.78(0)	γ 80.87(0)

R-Factor (%): 4.45 ***Temperature(K):*** 203 ***Density(g/cm³):*** 1.367





H_2O

FETDEO

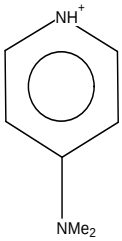
Reference: C.B.Aakeroy, J.Desper, B.Levin (2005) *CrystEngComm* ,**7,** 102

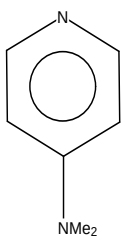
Formula: $3(C_7 H_{11} N_2^{1+})$,$2(C_7 H_{10} N_2)$,$3(C_7 H_6 B_1 O_4^{1-})$,$3(H_2 O_1)$

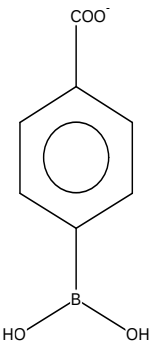
Compound Name: tris(4-(Dimethylamino)pyridinium) bis(4-(dimethylamino)pyridine) tris(4-carboxybenzeneboronate) trihydrate

Space Group:	P21/c	***Cell:***	***a*** 17.866(3)	***b*** 17.879(3)	***c*** 19.370(3)
Space Group No.:	14	***(Å,°)***	α 90.00	β 107.96(0)	γ 90.00

R-Factor (%): 6.41 ***Temperature(K):*** 203 ***Density(g/cm³):*** 1.312







H_2O

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FETDIS

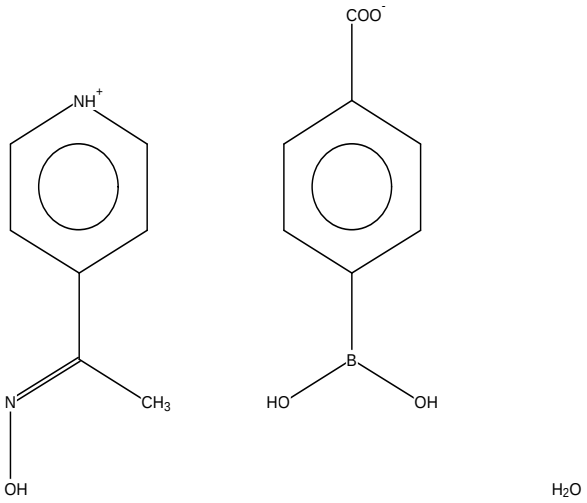
Reference: C.B.Aakeroy, J.Desper, B.Levin (2005) *CrystEngComm* ,**7,** 102

Formula: $C_7 H_9 N_2 O_1$ $^{1+}$,$C_7 H_6 B_1 O_4$ $^{1-}$,2($H_2 O_1$)

Compound Name: 4-Acetylpyridine oxime 4-carboxybenzeneboronate dihydrate

Space Group:	P1	***Cell:***	***a***	5.855(0)	***b***	8.572(0)	***c***	8.688(0)
Space Group No.:	1	***(Å,°)***	α	69.04(0)	β	89.41(0)	γ	77.33(0)

R-Factor (%): 4.55 ***Temperature(K):*** 203 ***Density(g/cm^3):*** 1.417



H_2O

FETZUA

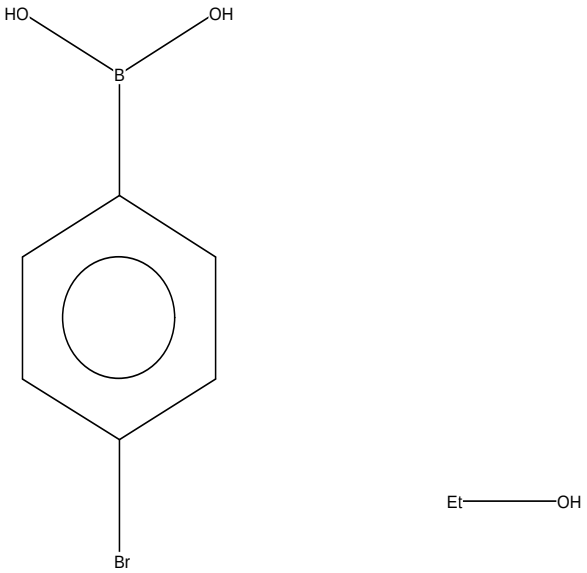
Reference: N.S.P.Bhuvanesh, J.H.Reibenspies (2005) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**61,**o362

Formula: $C_6 H_6 B_1 Br_1 O_2$,0.04($C_2 H_6 O_1$)

Compound Name: 4-Bromophenylboronic acid ethanol solvate

Space Group:	C2/m	***Cell:***	***a***	29.186(1)	***b***	9.825(0)	***c***	12.029(0)
Space Group No.:	12	***(Å,°)***	α	90.00	β	101.90(0)	γ	90.00

R-Factor (%): 4.95 ***Temperature(K):*** 110 ***Density(g/cm^3):*** 1.595



FOVMOT

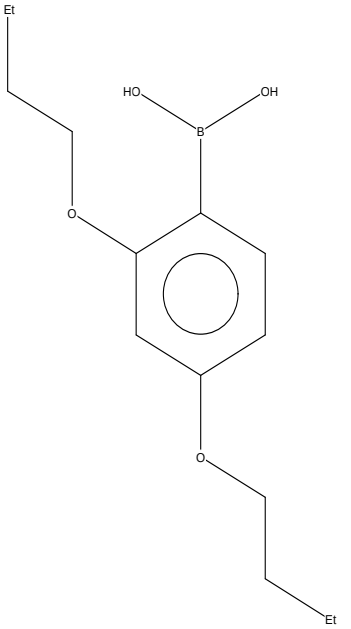
Reference: M.Dabrowski, S.Lulinski, J.Serwatowski, A.Wilmowicz (2009) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**65,**o1669

Formula: $C_{14} H_{23} B_1 O_4$

Compound Name: (2,4-Di-n-butoxyphenyl)boronic acid

Space Group:	P-1	***Cell:***	***a***	5.313(0)	***b***	11.361(1)	***c***	13.736(1)
Space Group No.:	2	***(Å,°)***	α	112.75(1)	β	94.31(1)	γ	100.39(1)

R-Factor (%): 3.40 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.190



FUBKOD

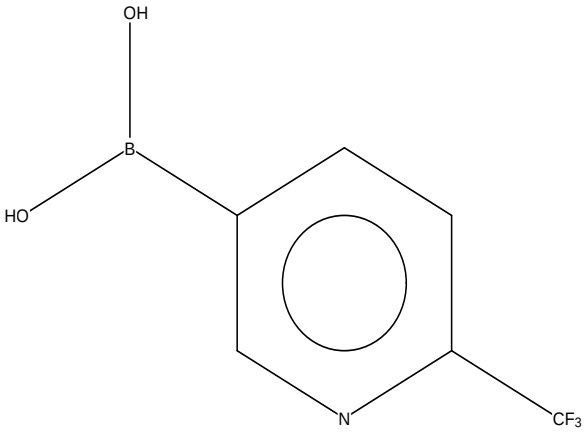
Reference: K.M.Clapham, A.S.Batsanov, M.R.Bryce, B.Tarbit (2009) *Org.Biomol.Chem.* ,**7,**2155

Formula: $C_6 H_5 B_1 F_3 N_1 O_2$

Compound Name: 6-(Trifluoromethyl)-3-pyridylboronic acid

Space Group:	P21/c	***Cell:***	***a***	7.737(0)	***b***	7.042(0)	***c***	13.874(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	95.18(1)	γ	90.00

R-Factor (%): 3.84 ***Temperature(K):*** 120 ***Density(g/cm^3):*** 1.684



Search: search4 (Mon May 01 12:48:32 2017): Hits 65-68

FUBLIY

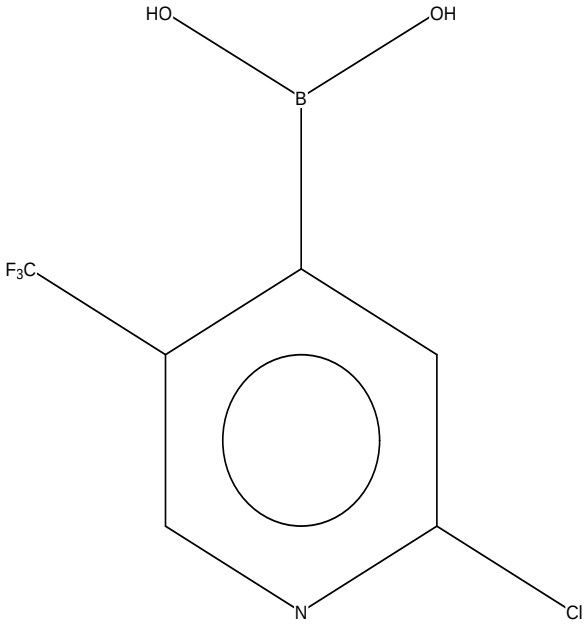
Reference: K.M.Clapham, A.S.Batsanov, M.R.Bryce, B.Tarbit (2009) *Org.Biomol.Chem.* ,**7,**2155

Formula: $C_6 H_4 B_1 Cl_1 F_3 N_1 O_2$

Compound Name: 2-Chloro-5-(trifluoromethyl)-4-pyridylboronic acid

Space Group:	C2/c	***Cell:***	***a***	24.080(4)	***b***	7.804(1)	***c***	9.385(1)
Space Group No.:	15	***(Å,°)***	α	90.00	β	96.42(3)	γ	90.00

R-Factor (%): 2.61 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.708



FUQBOK

Reference: D.Pla, O.Sadek, S.Cadet, B.Mestre-Voegtle, E.Gras (2015) *Dalton Trans.* ,**44,**18340

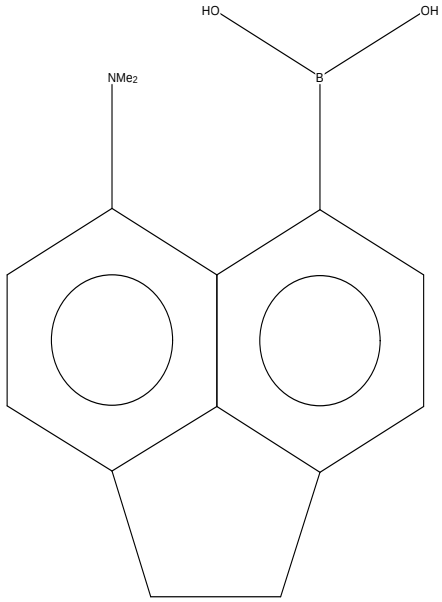
Formula: $C_{14} H_{16} B_1 N_1 O_2$

Compound Name: 6-(Dihydroxyboryl)-N,N-dimethyl-1,2-dihydroacenaphthylen-5-amine

Synonym: (6-(dimethylamino)-1,2-dihydroacenaphthylen-5-yl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	11.566(1)	***b***	10.175(1)	***c***	12.084(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	117.25(0)	γ	90.00

R-Factor (%): 5.10 ***Temperature(K):*** 193 ***Density(g/cm³):*** 1.267



FUWHIP

Reference: M.Regueiro-Figueroa, K.Djanashvili, D.Esteban-Gomez, A.de Blas, C.Platas-Iglesias, T.Rodriguez-Blas (2010) *Eur.J.Org.Chem.* ,3237

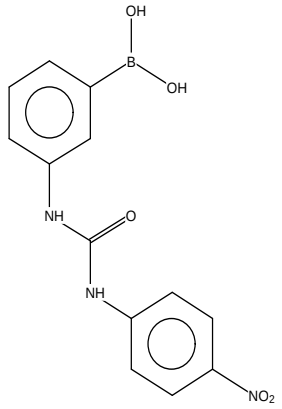
Formula: $C_{13} H_{12} B_1 N_3 O_5, C_2 H_6 O_1 S_1$

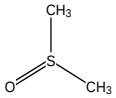
Compound Name: (3-(((4-Nitrophenyl)carbamoyl)amino)phenyl)boronic acid dimethylsulfoxide solvate

Synonym: 3-(3-(4-Nitrophenyl)ureido)phenylboronic acid dimethylsulfoxide solvate

Space Group:	P21/c	***Cell:***	***a***	13.653(0)	***b***	12.884(0)	***c***	19.965(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	105.75(0)	γ	90.00

R-Factor (%): 4.07 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.490





FUZLES

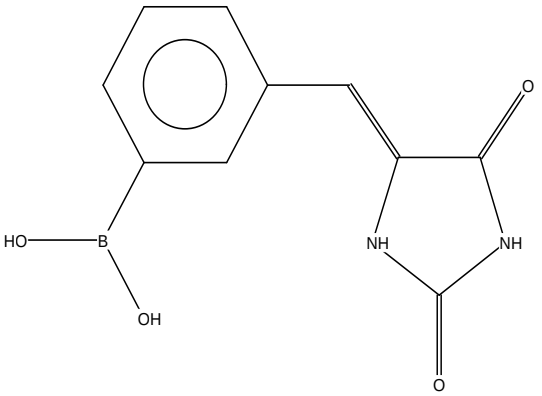
Reference: E.A.Gwynne, J.C.Holt, J.R.Dwan, F.E.Appoh, C.M.Vogels, A.Decken, S.A.Westcott (2010) *Helv.Chim.Acta* ,**93,**1093

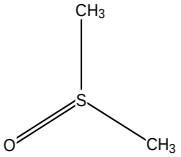
Formula: $C_{10} H_9 B_1 N_2 O_4, C_2 H_6 O_1 S_1$

Compound Name: (3-((Z)-(2,5-Dioxoimidazolidin-4-ylidene)methyl)phenyl)boronic acid dimethylsulfoxide solvate

Space Group:	P-1	***Cell:***	***a***	8.739(1)	***b***	8.931(1)	***c***	9.351(1)
Space Group No.:	2	***(Å,°)***	α	83.92(0)	β	79.18(0)	γ	83.42(0)

R-Factor (%): 3.26 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.452





Search: search4 (Mon May 01 12:48:32 2017): Hits 69-72

GANBUU

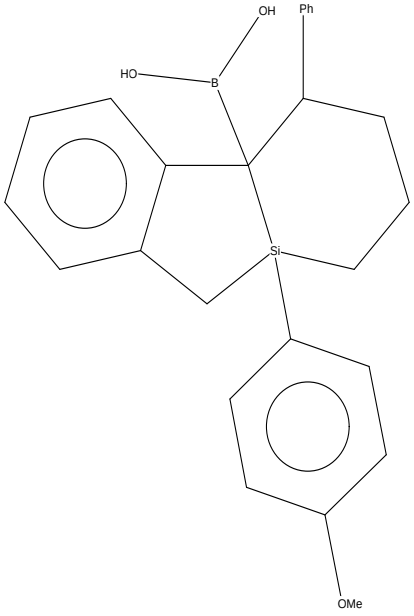
Reference: R.Shintani, K.Moriya, T.Hayashi (2011) *J.Am.Chem.Soc.* , **133,**16440

Formula: $C_{25}\,H_{27}\,B_1\,O_3\,Si_1$

Compound Name: (5-(4-Methoxyphenyl)-1-phenyl-1,2,3,4,5,6-hexahydro-10bH-silino[2,1-a][2]benzosilol-10b-yl)boronic acid

Space Group:	P-1	***Cell:***	***a*** 8.601(0)	***b*** 9.324(0)	***c*** 14.184(0)
Space Group No.:	2	***(Å,°)***	α 81.49(0)	β 72.95(0)	γ 77.97(0)

R-Factor (%): 6.56 ***Temperature(K):*** 93 ***Density(g/cm^3):*** 1.299



GENTOJ

Reference: B.Shivachev, R.Petrova, E.Naydenova (2006) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* , **62,**o3887

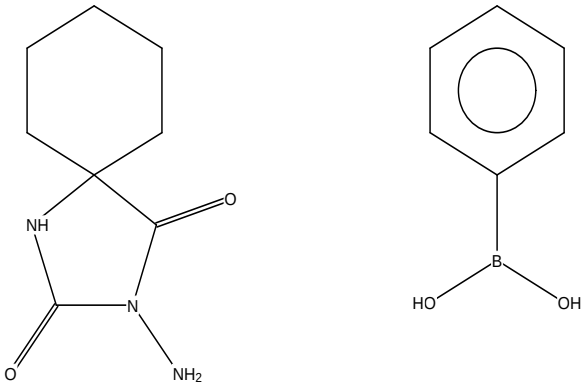
Formula: $C_8\,H_{13}\,N_3\,O_2,C_6\,H_7\,B_1\,O_2$

Compound Name: 3-Amino-1,3-diazaspiro(4.5)decane-2,4-dione phenylboronic acid

Synonym: 3'-Aminocyclohexanespiro-5'-hydantoin phenylboronic acid

Space Group:	P-1	***Cell:***	***a*** 6.043(1)	***b*** 12.094(1)	***c*** 12.301(1)
Space Group No.:	2	***(Å,°)***	α 62.51(0)	β 89.29(0)	γ 80.18(0)

R-Factor (%): 6.15 ***Temperature(K):*** 290 ***Density(g/cm^3):*** 1.293



GESJIZ

Reference: S.Varughese, S.B.Sinha, G.R.Desiraju (2011) *Sci.China.Chem.* , **54,**1909

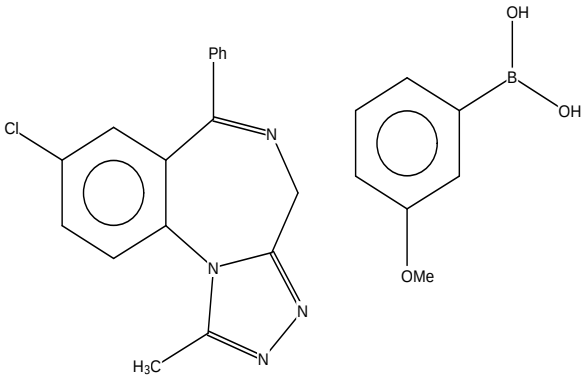
Formula: $2(C_{17}\,H_{13}\,Cl_1\,N_4),C_7\,H_9\,B_1\,O_3$

Compound Name: bis(8-chloro-1-methyl-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine) (3-methoxyphenyl)boronic acid

Synonym: bis(Alprazolam) (3-methoxyphenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a*** 14.390(3)	***b*** 20.776(4)	***c*** 13.075(3)
Space Group No.:	14	***(Å,°)***	α 90.00	β 111.85(0)	γ 90.00

R-Factor (%): 7.97 ***Temperature(K):*** 150 ***Density(g/cm^3):*** 1.409



GESJOF

Reference: S.Varughese, S.B.Sinha, G.R.Desiraju (2011) *Sci.China.Chem.* , **54,**1909

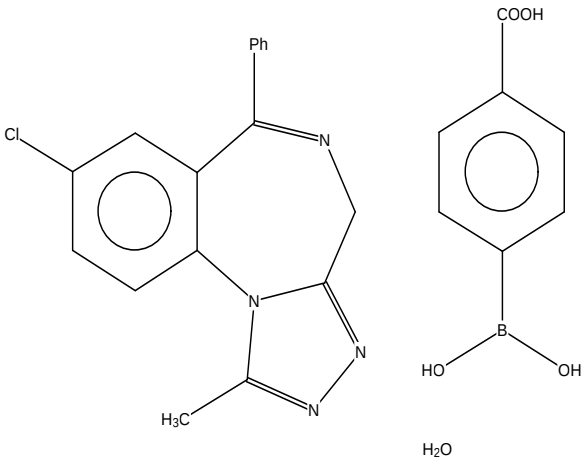
Formula: $2(C_{17}\,H_{13}\,Cl_1\,N_4),C_7\,H_7\,B_1\,O_4,H_2\,O_1$

Compound Name: bis(8-chloro-1-methyl-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine) 4-(dihydroxyboryl)benzoic acid monohydrate

Synonym: bis(Alprazolam) 4-(dihydroxyboryl)benzoic acid monohydrate

Space Group:	P-1	***Cell:***	***a*** 11.883(1)	***b*** 13.186(3)	***c*** 14.236(3)
Space Group No.:	2	***(Å,°)***	α 116.42(0)	β 107.89(0)	γ 90.64

R-Factor (%): 6.75 ***Temperature(K):*** 150 ***Density(g/cm^3):*** 1.422



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GESJUL

Reference: S.Varughese, S.B.Sinha, G.R.Desiraju (2011)
Sci.China.Chem. ,**54,**1909

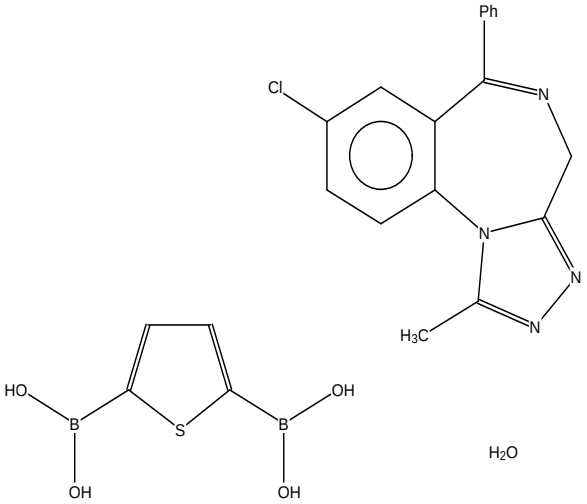
Formula: $2(C_{17}\,H_{13}\,Cl_1\,N_4),C_4\,H_6\,B_2\,O_4\,S_1,0.5(H_2\,O_1)$

Compound Name: bis(8-chloro-1-methyl-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine) 2,5-bis(dihydroxyboryl)thiophene hemihydrate

Synonym: bis(Alprazolam) 2,5-bis(dihydroxyboryl)thiophene hemihydrate

Space Group:	P-1	***Cell:***	***a***	11.915(0)	***b***	13.154(0)	***c***	14.525(0)
Space Group No.:	2	***(Å,°)***	α	63.82(0)	β	69.60(0)	γ	88.71(0)

R-Factor (%): 8.39 ***Temperature(K):*** 150 ***Density(g/cm^3):*** 1.402



GESKAS

Reference: S.Varughese, S.B.Sinha, G.R.Desiraju (2011)
Sci.China.Chem. ,**54,**1909

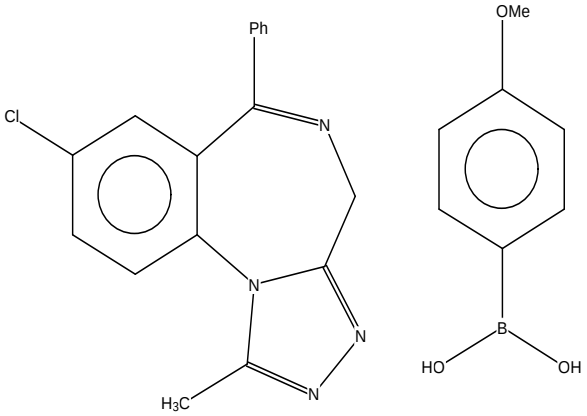
Formula: $C_{17}\,H_{13}\,Cl_1\,N_4,C_7\,H_9\,B_1\,O_3$

Compound Name: 8-chloro-1-methyl-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine (4-methoxyphenyl)boronic acid

Synonym: Alprazolam (4-methoxyphenyl)boronic acid

Space Group:	Pccn	***Cell:***	***a***	19.413(1)	***b***	25.444(2)	***c***	9.162(7)
Space Group No.:	56	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 8.22 ***Temperature(K):*** 150 ***Density(g/cm^3):*** 1.352



GESKEW

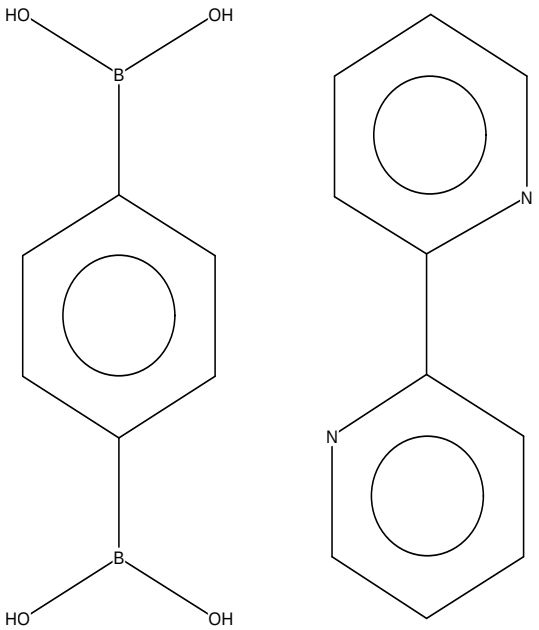
Reference: S.Varughese, S.B.Sinha, G.R.Desiraju (2011)
Sci.China.Chem. ,**54,**1909

Formula: $C_6\,H_8\,B_2\,O_4,C_{10}\,H_8\,N_2$

Compound Name: 1,4-Phenylenediboronic acid 2,2'-bipyridine

Space Group:	P-1	***Cell:***	***a***	5.432(2)	***b***	7.525(1)	***c***	10.745(1)
Space Group No.:	2	***(Å,°)***	α	102.10(0)	β	104.37(0)	γ	101.47(0)

R-Factor (%): 6.57 ***Temperature(K):*** 150 ***Density(g/cm^3):*** 1.333



GESKIA

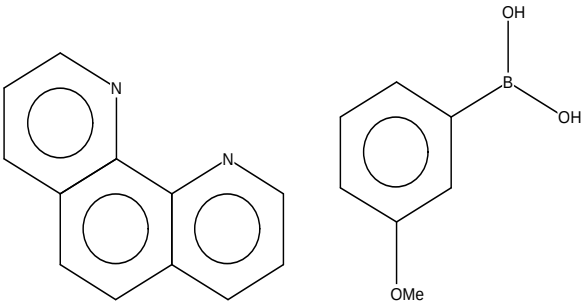
Reference: S.Varughese, S.B.Sinha, G.R.Desiraju (2011)
Sci.China.Chem. ,**54,**1909

Formula: $C_{12}\,H_8\,N_2,C_7\,H_9\,B_1\,O_3$

Compound Name: (3-Methoxyphenyl)boronic acid 1,10-phenanthroline

Space Group:	Pbca	***Cell:***	***a***	11.763(1)	***b***	11.426(1)	***c***	24.684(1)
Space Group No.:	61	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 4.24 ***Temperature(K):*** 295 ***Density(g/cm^3):*** 1.330



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GESKOG

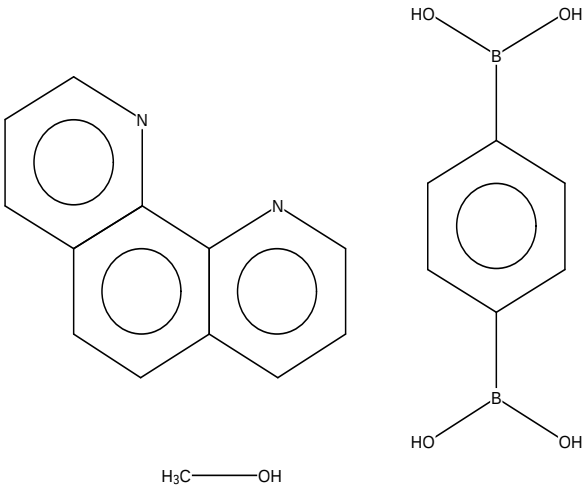
Reference: S.Varughese, S.B.Sinha, G.R.Desiraju (2011)
Sci.China.Chem. ,**54,**1909

Formula: $2(C_{12}H_8N_2),C_6H_8B_2O_4,C_1H_4O_1$

Compound Name: 1,4-Phenylenediboronic acid bis(1,10-phenanthroline) methanol solvate

Space Group:	P21/c	***Cell:***	***a***	3.961(1)	***b***	17.194(3)	***c***	22.861(4)
Space Group No.:	14	***(Å,°)***	α	90.00	β	90.92(1)	γ	90.00

R-Factor (%): 8.40 ***Temperature(K):*** 150 ***Density(g/cm³):*** 1.191



GESKUM

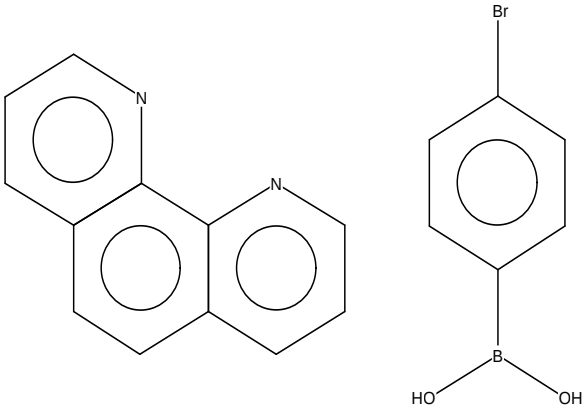
Reference: S.Varughese, S.B.Sinha, G.R.Desiraju (2011)
Sci.China.Chem. ,**54,**1909

Formula: $C_{12}H_8N_2,C_6H_6B_1Br_1O_2$

Compound Name: (4-Bromophenyl)boronic acid 1,10-phenanthroline

Space Group:	Pca21	***Cell:***	***a***	18.522(3)	***b***	6.466(1)	***c***	14.384(2)
Space Group No.:	29	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 5.87 ***Temperature(K):*** 150 ***Density(g/cm³):*** 1.469



GESLAT

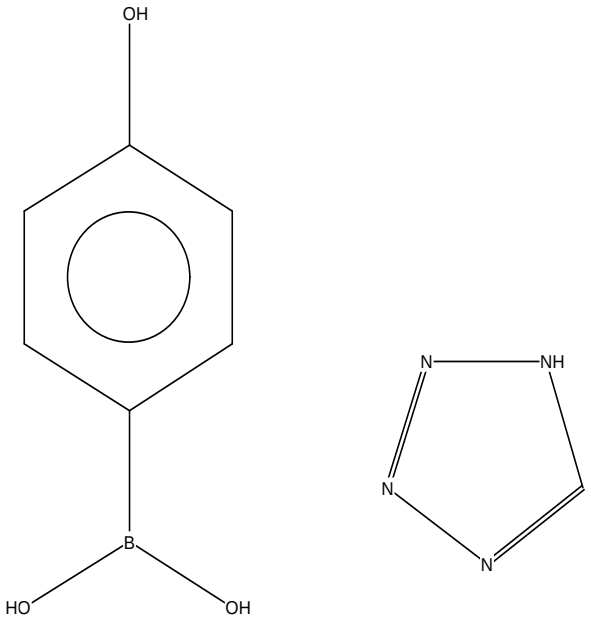
Reference: S.Varughese, S.B.Sinha, G.R.Desiraju (2011)
Sci.China.Chem. ,**54,**1909

Formula: $2(C_6H_7B_1O_3),C_1H_2N_4$

Compound Name: bis((4-Hydroxyphenyl)boronic acid) 1H-tetrazole

Space Group:	P21/c	***Cell:***	***a***	10.201(3)	***b***	13.900(3)	***c***	12.749(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	118.83(1)	γ	90.00

R-Factor (%): 7.91 ***Temperature(K):*** 150 ***Density(g/cm³):*** 1.451



GISVIO

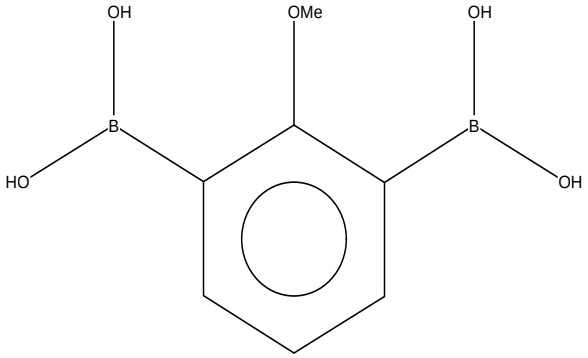
Reference: M.Dabrowski, S.Lulinski, J.Serwatowski (2008)
Acta Crystallogr.,Sect.E:Struct.Rep.Online ,**64,**o414

Formula: $C_7H_{10}B_2O_5$

Compound Name: (2-Methoxy-1,3-phenylene)diboronic acid

Space Group:	P-1	***Cell:***	***a***	5.026(0)	***b***	7.647(1)	***c***	12.454(1)
Space Group No.:	2	***(Å,°)***	α	79.01(1)	β	81.90(1)	γ	77.25(1)

R-Factor (%): 3.06 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.426



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GITLAX

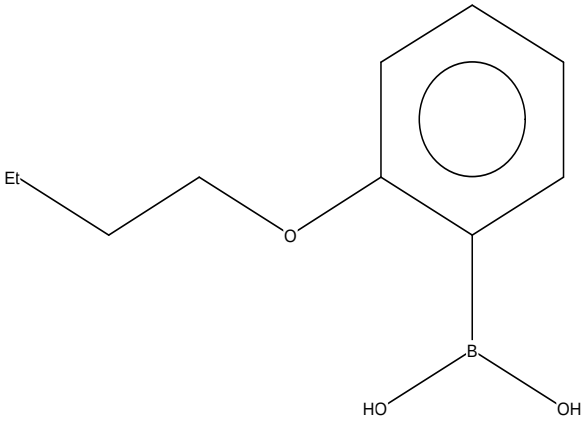
Reference: M.Dabrowski, S.Lulinski, J.Serwatowski (2008) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**64,**o437

Formula: $C_{10}\,H_{15}\,B_1\,O_3$

Compound Name: (2-Butoxyphenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	7.481(0)	***b***	15.351(0)	***c***	9.282(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	94.30(0)	γ	90.00

R-Factor (%): 3.20 ***Temperature(K):*** 102 ***Density(g/cm³):*** 1.212



GODGUC

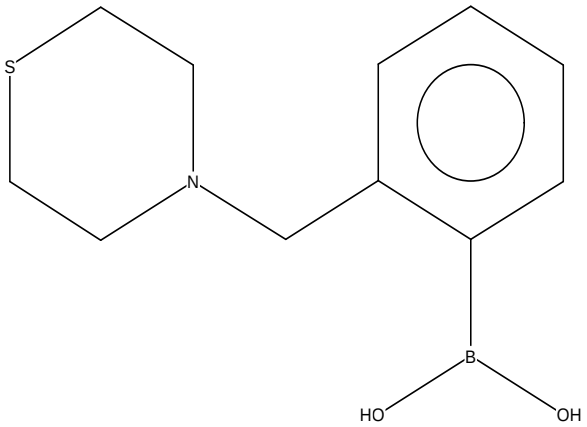
Reference: A.Adamczyk-Wozniak, Z.Brzozka, M.K.Cyranski, A.Filipowicz-Szymanska, P.Klimentowska, A.Zubrowska, K.Zukowski, A.Sporzynski (2008) *Appl.Organomet.Chem.* ,**22,**427

Formula: $C_{11}\,H_{16}\,B_1\,N_1\,O_2\,S_1$

Compound Name: o-(Thiomorpholinomethyl)phenylboronic acid

Space Group:	Pbca	***Cell:***	***a***	10.665(0)	***b***	12.388(0)	***c***	18.421(0)
Space Group No.:	61	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 2.87 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.294



GODHAJ

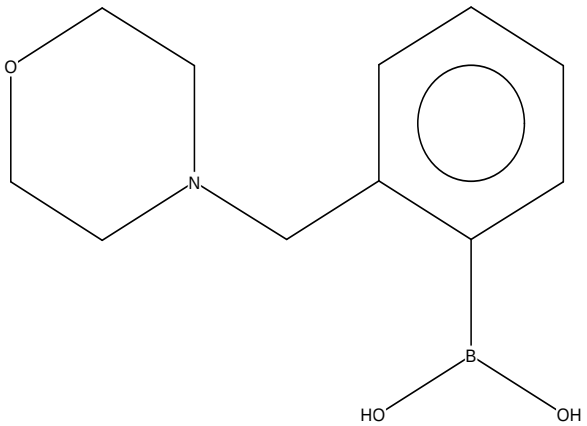
Reference: A.Adamczyk-Wozniak, Z.Brzozka, M.K.Cyranski, A.Filipowicz-Szymanska, P.Klimentowska, A.Zubrowska, K.Zukowski, A.Sporzynski (2008) *Appl.Organomet.Chem.* ,**22,**427

Formula: $C_{11}\,H_{16}\,B_1\,N_1\,O_3$

Compound Name: o-(Morpholinomethyl)phenylboronic acid

Space Group:	C2/c	***Cell:***	***a***	42.454(1)	***b***	9.504(0)	***c***	18.920(0)
Space Group No.:	15	***(Å,°)***	α	90.00	β	112.14(0)	γ	90.00

R-Factor (%): 3.33 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.246



GUCSAA

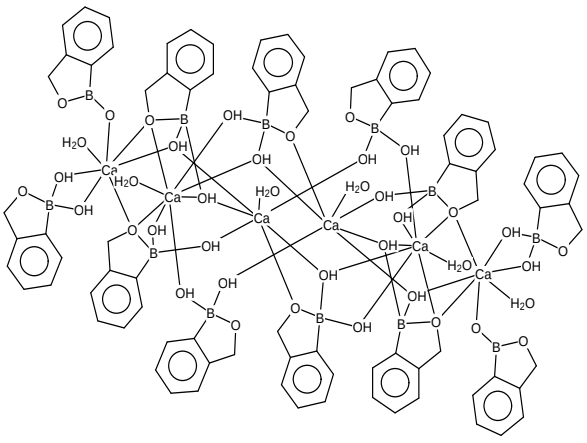
Reference: Saad Sene, S.Begu, C.Gervais, G.Renaudin, A.Mesbah, M.E.Smith, P.Hubert Mutin, A.van der Lee, J.-M.Nedelec, C.Bonhomme, D.Laurencin (2015) *Chem.Mater.* ,**27,**1242

Formula: $C_{84}\,H_{104}\,B_{12}\,Ca_6\,O_{40}$

Compound Name: bis(μ_3-Benzoxaborole-O,O,O',O'')-bis(μ_3-benzoxaborole-O,O,O',O',O'', O'')-bis(μ_2-benzoxaborole-O,O')-bis(μ_2-benzoxaborole-O,O,O',O'')-bis(benzoxaborole)-bis(benzoxaborolate)-hexa-aqua-hexa-calcium

Space Group:	P-1	***Cell:***	***a***	10.431(0)	***b***	14.533(0)	***c***	16.115(0)
Space Group No.:	2	***(Å,°)***	α	98.11(0)	β	98.05(0)	γ	101.48(0)

R-Factor (%): 5.13 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.511



Search: search4 (Mon May 01 12:48:32 2017): Hits 85-88

GUCSUU

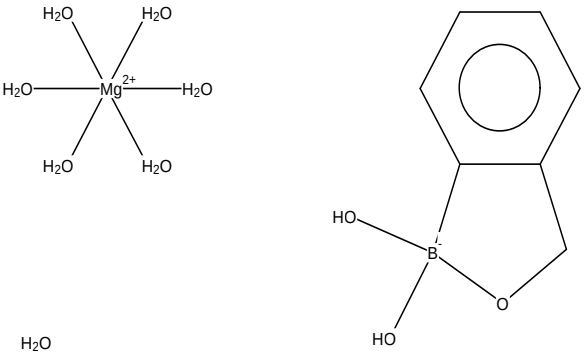
Reference: Saad Sene, S.Begu, C.Gervais, G.Renaudin, A.Mesbah, M.E.Smith, P.Hubert Mutin, A.van der Lee, J.-M.Nedelec, C.Bonhomme, D.Laurencin (2015) *Chem.Mater.* ,**27,**1242

Formula: $H_{12}\ Mg_1\ O_6\ ^{2+}$,2($C_7\ H_8\ B_1\ O_3\ ^{1-}$),4($H_2\ O_1$)

Compound Name: Hexa-aqua-magnesium bis(hydrogen benzoxaborole) tetrahydrate

Space Group:	Pbca	***Cell:***	***a***	8.237(0)	***b***	12.147(0)	***c***	24.792(1)
Space Group No.:	61	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.62 ***Temperature(K):*** 175 ***Density(g/cm³):*** 1.356



HEVZIS

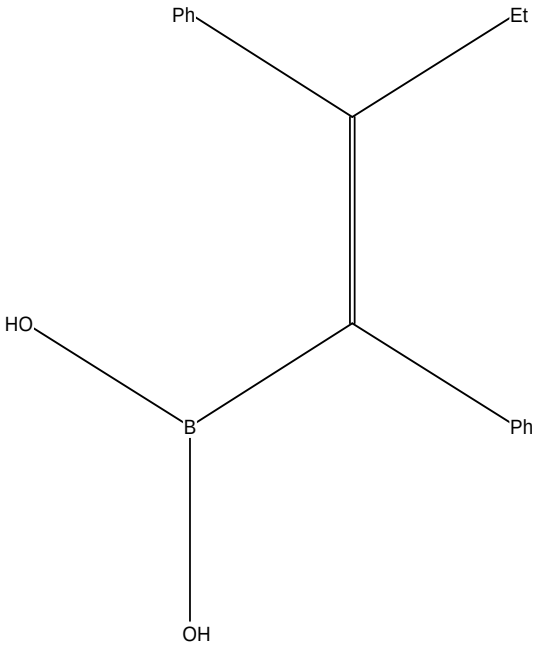
Reference: N.F.McKinley, D.F.O'Shea (2006) *J.Org.Chem.* ,**71,**9552

Formula: $C_{16}\ H_{17}\ B_1\ O_2$

Compound Name: (E)-1,2-Diphenyl-1-butene boronic acid

Space Group:	C2/c	***Cell:***	***a***	17.871(4)	***b***	5.213(1)	***c***	30.632(6)
Space Group No.:	15	***(Å,°)***	α	90.00	β	101.33(0)	γ	90.00

R-Factor (%): 8.33 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.197



HIRGEV

Reference: D.Zhang, L.E.Harrington, H.Tanaka, R.Pelton (2007) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**63,**o4628

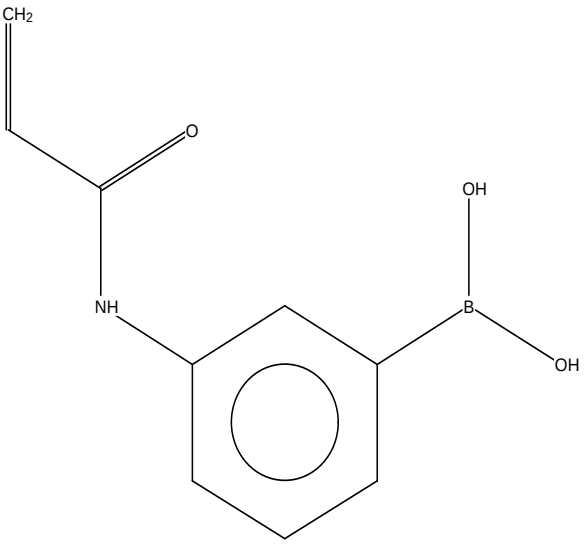
Formula: $C_9\ H_{10}\ B_1\ N_1\ O_3$

Compound Name: (3-(acryloylamino)phenyl)boronic acid

Synonym: (3-(Propen-3-amido)phenyl)boronic acid

Space Group:	Fdd2	***Cell:***	***a***	18.626(4)	***b***	42.112(8)	***c***	5.054(1)
Space Group No.:	43	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.85 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.280



HOXPIU

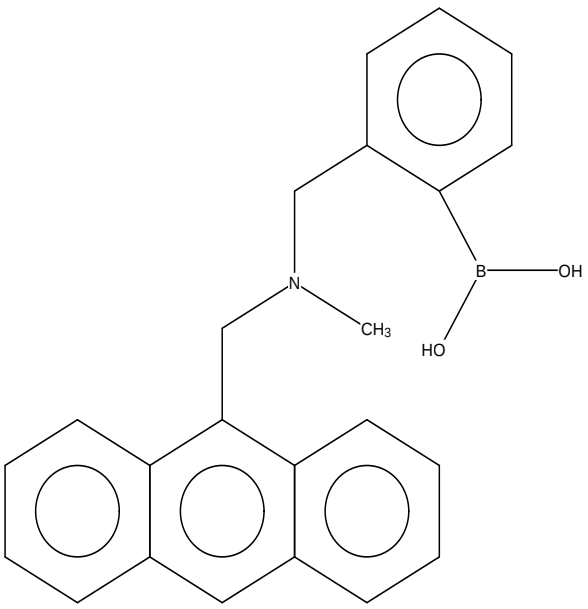
Reference: Lu Zhang, J.A.Kerszulis, R.J.Clark, Tao Ye, Lei Zhu (2009) *Chem.Commun.* ,2151

Formula: $C_{23}\ H_{22}\ B_1\ N_1\ O_2$

Compound Name: (2-(((9-Anthrylmethyl)(methyl)amino)methyl)phenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	9.864(1)	***b***	12.478(1)	***c***	15.734(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	98.54(0)	γ	90.00

R-Factor (%): 3.91 ***Temperature(K):*** 153 ***Density(g/cm³):*** 1.232



Search: search4 (Mon May 01 12:48:32 2017): Hits 89-92

HUXXII

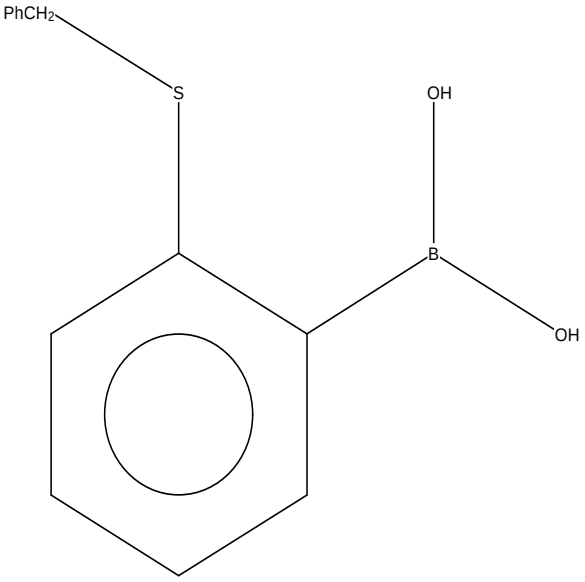
Reference: T.Klis, J.Serwatowski, G.Wesela-Bauman, M.Zadrozna (2010) *Tetrahedron Lett.* ,**51,**1685

Formula: $C_{13}H_{13}B_1O_2S_1$

Compound Name: (2-(Benzylsulfanyl)phenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	8.595(1)	***b***	5.037(1)	***c***	27.961(6)
Space Group No.:	14	***(Å,°)***	α	90.00	β	94.61(3)	γ	90.00

R-Factor (%): 3.52 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.344



HUYRAU

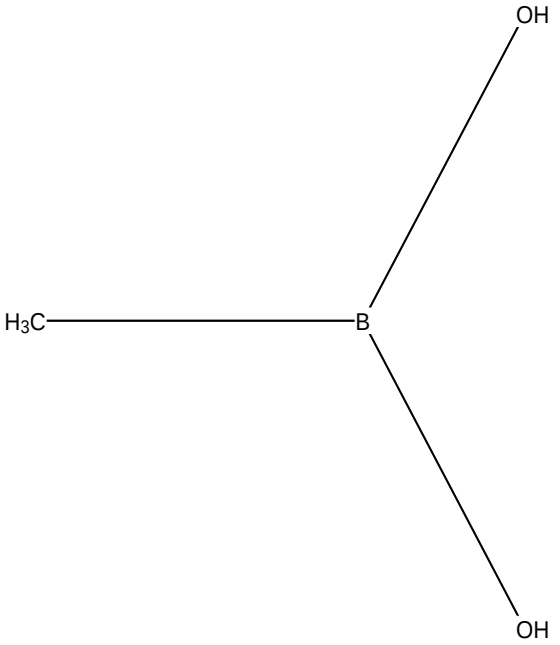
Reference: J.M.Stoddard, K.J.Shea (2003) *Organometallics* ,**22,**1124

Formula: $C_1H_5B_1O_2$

Compound Name: Methylboronic acid

Space Group:	P-1	***Cell:***	***a***	6.225(4)	***b***	8.680(6)	***c***	10.845(7)
Space Group No.:	2	***(Å,°)***	α	112.60(1)	β	94.16(1)	γ	94.31(1)

R-Factor (%): 8.88 ***Temperature(K):*** 158 ***Density(g/cm³):*** 1.112



IGERAO

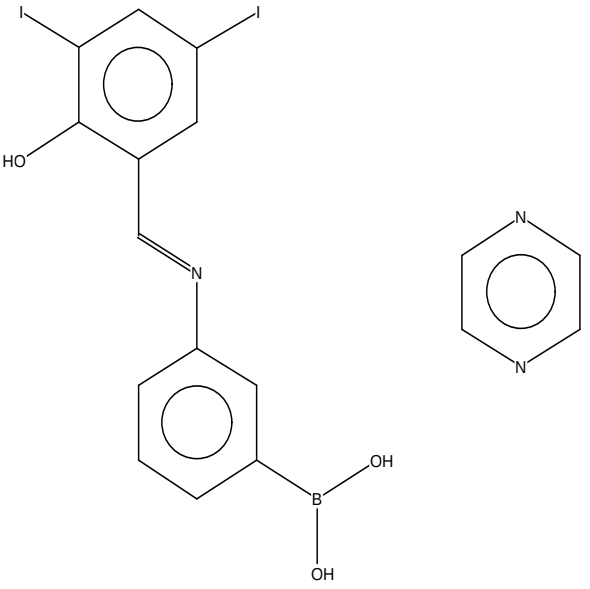
Reference: V.Barba, R.Hernandez, H.Hopfl, R.Santillan, N.Farfan (2009) *J.Organomet.Chem.* ,**694,**2127

Formula: $C_{13}H_{10}B_1I_2N_1O_3,C_4H_4N_2$

Compound Name: (3-((2-Hydroxy-3,5-diiodobenzylidene)amino)phenyl)boronic acid pyrazine solvate

Space Group:	P21/n	***Cell:***	***a***	4.280(0)	***b***	21.944(3)	***c***	20.376(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	94.93(0)	γ	90.00

R-Factor (%): 4.80 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.996



IHOREE

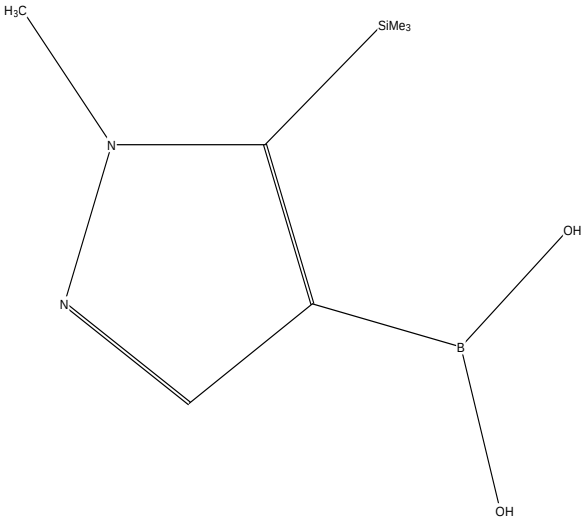
Reference: K.Durka, A.Gorska, T.Klis, M.Kublicki, J.Serwatowski, K.Wozniak (2015) *Tetrahedron Lett.* ,**56,**1855

Formula: $C_7H_{15}B_1N_2O_2Si_1$

Compound Name: (1-methyl-5-(trimethylsilyl)-1H-pyrazol-4-yl)boronic acid

Space Group:	P-1	***Cell:***	***a***	7.627(0)	***b***	12.349(0)	***c***	12.708(0)
Space Group No.:	2	***(Å,°)***	α	108.31(0)	β	94.15(0)	γ	107.90(0)

R-Factor (%): 3.62 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.239



Search: search4 (Mon May 01 12:48:32 2017): Hits 93-96

IHORII

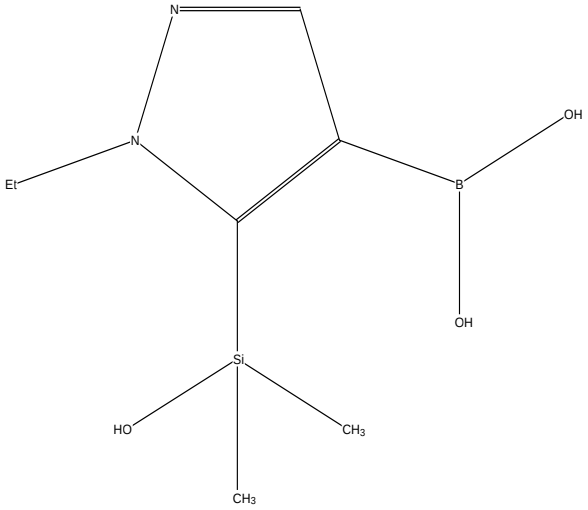
Reference: K.Durka, A.Gorska, T.Klis, M.Kublicki, J.Serwatowski, K.Wozniak (2015) *Tetrahedron Lett.* ,**56,**1855

Formula: $C_7 H_{15} B_1 N_2 O_3 Si_1$

Compound Name: (1-ethyl-5-(hydroxy(dimethyl)silyl)-1H-pyrazol-4-yl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	7.599(0)	***b***	13.118(0)	***c***	11.702(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	105.84(1)	γ	90.00

R-Factor (%): 5.79 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.267



IHORUU

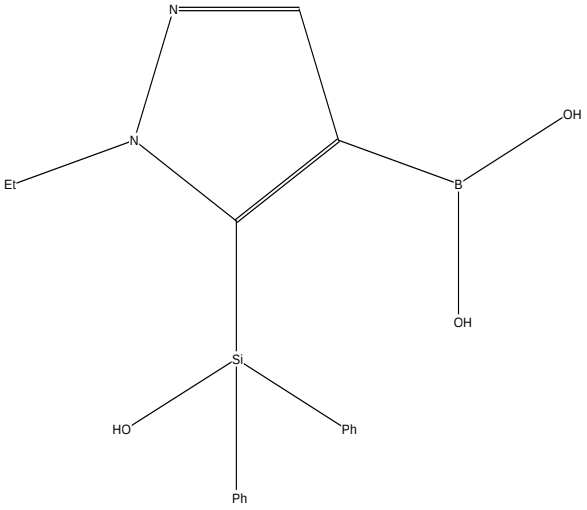
Reference: K.Durka, A.Gorska, T.Klis, M.Kublicki, J.Serwatowski, K.Wozniak (2015) *Tetrahedron Lett.* ,**56,**1855

Formula: $C_{17} H_{19} B_1 N_2 O_3 Si_1$

Compound Name: (1-ethyl-5-(hydroxy(diphenyl)silyl)-1H-pyrazol-4-yl)boronic acid

Space Group:	P-1	***Cell:***	***a***	7.435(0)	***b***	13.785(1)	***c***	17.618(1)
Space Group No.:	2	***(Å,°)***	α	88.34(0)	β	78.70(0)	γ	85.29(0)

R-Factor (%): 5.96 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.273



IHOSAB

Reference: K.Durka, A.Gorska, T.Klis, M.Kublicki, J.Serwatowski, K.Wozniak (2015) *Tetrahedron Lett.* ,**56,**1855

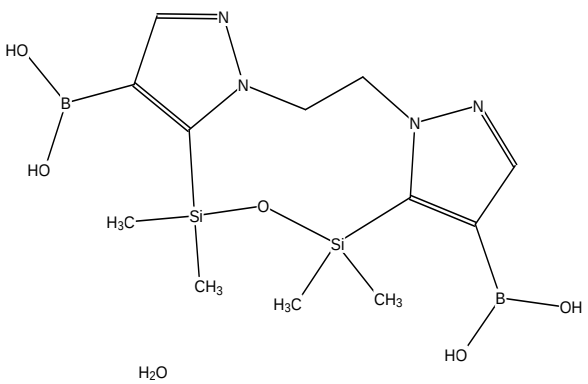
Formula: $C_{12} H_{22} B_2 N_4 O_5 Si_2, H_2 O_1$

Compound Name: (4,4,6,6-tetramethyl-11,12-dihydro-4H,6H-dipyrazolo[5,1-c:1',5'-g][1,4,7,2,9]oxadiazadisilonine-3,7-diyl)diboronic acid monohydrate

Synonym: 1-oxo-2,9-bis-(dimethylsila)-3,4-(5,1-(pirazole-4-dihydroxyboryl)-yl)-7,8-(1,5-(pirazole-4-dihydroxyboryl)-yl)-cyclononane monohydrate

Space Group:	C2/c	***Cell:***	***a***	19.308(0)	***b***	17.119(0)	***c***	12.755(0)
Space Group No.:	15	***(Å,°)***	α	90.00	β	104.98(0)	γ	90.00

R-Factor (%): 4.44 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.299



IKIFAJ

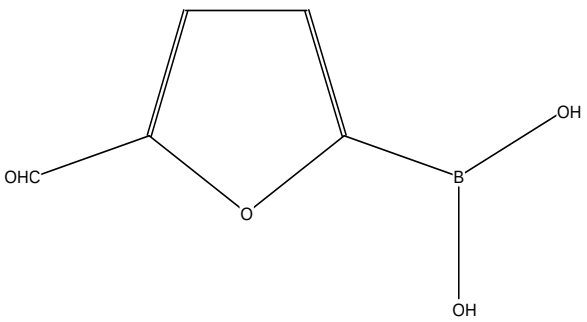
Reference: K.Ejsmont, J.Zaleski, A.Sporzynski, M.Lewandowski (2003) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**59,**o1324

Formula: $C_5 H_5 B_1 O_4$

Compound Name: 5-Formyl-2-furanboronic acid

Space Group:	P21/n	***Cell:***	***a***	3.755(0)	***b***	7.758(2)	***c***	20.694(4)
Space Group No.:	14	***(Å,°)***	α	90.00	β	91.31(3)	γ	90.00

R-Factor (%): 4.74 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.542



Search: search4 (Mon May 01 12:48:32 2017): Hits 97-100

IRASIF

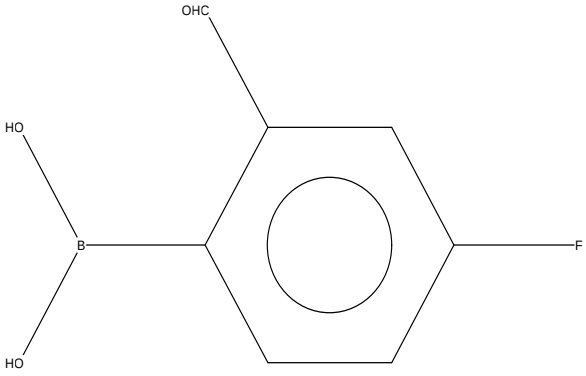
Reference: K.Kowalska, A.Adamczyk-Wozniak, P.Gajowiec, B.Gierczyk, E.Kaczorowska, L.Popenda, G.Schroeder, A.Sikorski, A.Sporzynski (2016) *J.Fluorine Chem.* ,**187,**1

Formula: $C_7 H_6 B_1 F_1 O_3$

Compound Name: (4-fluoro-2-formylphenyl)boronic acid

Space Group:	C2/c	***Cell:***	***a*** 30.045(1)	***b*** 3.754(0)	***c*** 13.516(0)
Space Group No.:	15	***(Å,°)***	α 90.00	β 90.39(0)	γ 90.00

R-Factor (%): 4.63 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.464



IRASOL

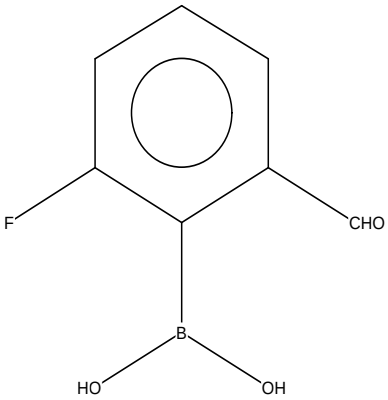
Reference: K.Kowalska, A.Adamczyk-Wozniak, P.Gajowiec, B.Gierczyk, E.Kaczorowska, L.Popenda, G.Schroeder, A.Sikorski, A.Sporzynski (2016) *J.Fluorine Chem.* ,**187,**1

Formula: $C_7 H_6 B_1 F_1 O_3,H_2 O_1$

Compound Name: (2-fluoro-6-formylphenyl)boronic acid monohydrate

Space Group:	P21/c	***Cell:***	***a*** 7.540(0)	***b*** 8.180(0)	***c*** 14.096(0)
Space Group No.:	14	***(Å,°)***	α 90.00	β 99.16(0)	γ 90.00

R-Factor (%): 8.42 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.439



H_2O

ITIGEY

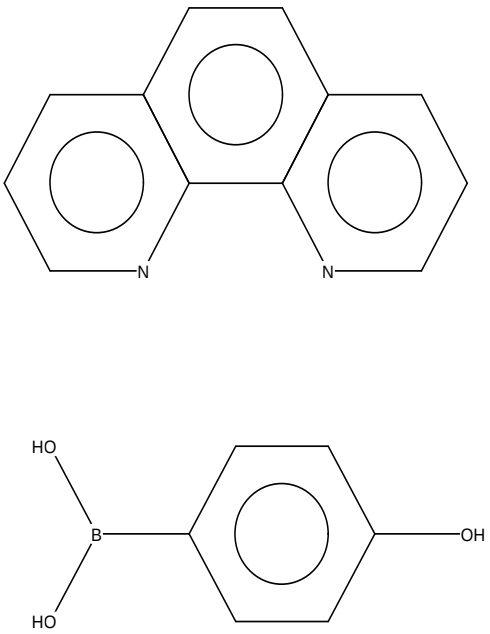
Reference: M.Talwelkar, V.R.Pedireddi (2010) *Tetrahedron Lett.* ,**51,** 6901

Formula: $C_{12} H_8 N_2,C_6 H_7 B_1 O_3$

Compound Name: (4-Hydroxyphenyl)boronic acid 1,10-phenanthroline

Space Group:	P21/c	***Cell:***	***a*** 12.435(3)	***b*** 10.941(3)	***c*** 12.177(3)
Space Group No.:	14	***(Å,°)***	α 90.00	β 108.18(1)	γ 90.00

R-Factor (%): 5.25 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.343



ITIQIL

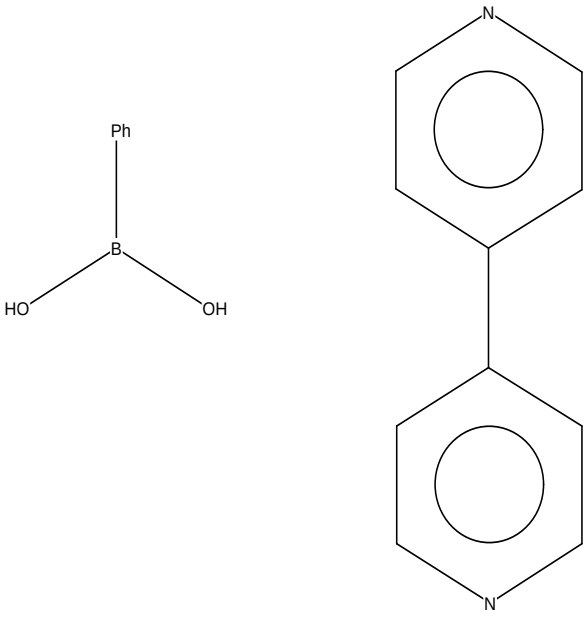
Reference: V.R.Pedireddi, N.S.Lekshmi (2004) *Tetrahedron Lett.* ,**45,** 1903

Formula: $C_6 H_7 B_1 O_2,2(C_{10} H_8 N_2)$

Compound Name: Phenylboronic acid bis(4,4'-bipyridine)

Space Group:	Fdd2	***Cell:***	***a*** 26.519(23)	***b*** 9.245(8)	***c*** 17.612(15)
Space Group No.:	43	***(Å,°)***	α 90.00	β 90.00	γ 90.00

R-Factor (%): 5.22 ***Temperature(K):*** 140 ***Density(g/cm³):*** 1.336



Search: search4 (Mon May 01 12:48:32 2017): Hits 101-104

ITIQOR

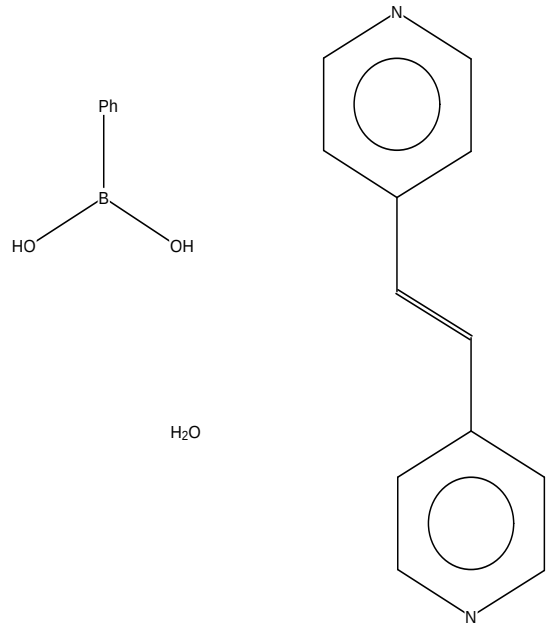
Reference: V.R.Pedireddi, N.S.Lekshmi (2004) *Tetrahedron Lett.* ,**45,** 1903

Formula: $C_6 H_7 B_1 O_2$,$C_{12} H_{10} N_2$,$H_2 O_1$

Compound Name: Phenylboronic acid 1,2-bis(4-pyridyl)ethene monohydrate

Space Group:	P21/c	***Cell:***	***a***	6.860(2)	***b***	19.092(5)	***c***	12.829(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	96.47(1)	γ	90.00

R-Factor (%): 3.97 ***Temperature(K):*** 140 ***Density(g/cm³):*** 1.282



ITIQUX

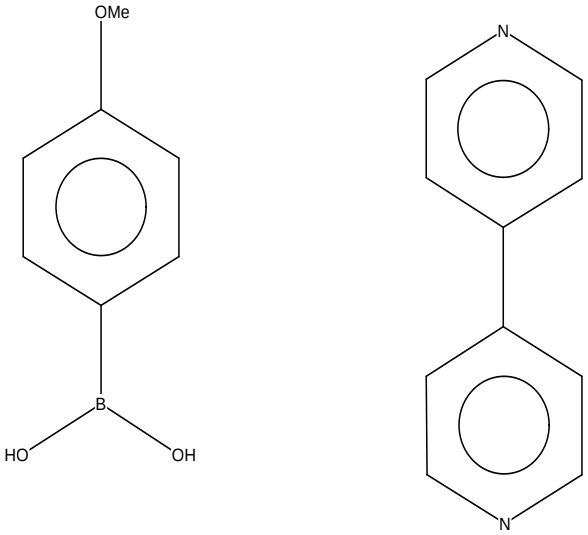
Reference: V.R.Pedireddi, N.S.Lekshmi (2004) *Tetrahedron Lett.* ,**45,** 1903

Formula: $2(C_7 H_9 B_1 O_3)$,$C_{10} H_8 N_2$

Compound Name: bis(4-Methoxyphenylboronic acid) 4,4-bipyridine

Space Group:	C2/c	***Cell:***	***a***	23.736(6)	***b***	5.216(1)	***c***	18.544(5)
Space Group No.:	15	***(Å,°)***	α	90.00	β	96.11(1)	γ	90.00

R-Factor (%): 4.63 ***Temperature(K):*** 140 ***Density(g/cm³):*** 1.339



ITIRAE

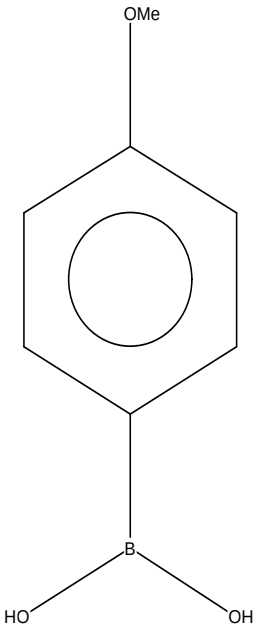
Reference: V.R.Pedireddi, N.S.Lekshmi (2004) *Tetrahedron Lett.* ,**45,** 1903

Formula: $C_7 H_9 B_1 O_3$

Compound Name: 4-Methoxyphenylboronic acid

Space Group:	P21/n	***Cell:***	***a***	11.259(3)	***b***	5.064(1)	***c***	13.878(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	111.04(1)	γ	90.00

R-Factor (%): 3.41 ***Temperature(K):*** 140 ***Density(g/cm³):*** 1.367



IYAXAH

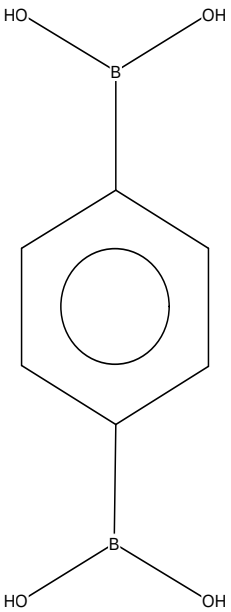
Reference: P.Rodriguez-Cuamatzi, G.Vargas-Diaz, T.Maris, J.D.Wuest, H.Hopfl (2004) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* , **60,**o1316

Formula: $C_6 H_8 B_2 O_4$

Compound Name: 1,4-Phenylenediboronic acid

Space Group:	P-1	***Cell:***	***a***	4.989(3)	***b***	5.305(3)	***c***	7.368(4)
Space Group No.:	2	***(Å,°)***	α	104.43(1)	β	97.89(0)	γ	93.80(1)

R-Factor (%): 5.00 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.479



Search: search4 (Mon May 01 12:48:32 2017): Hits 105-108

KAJPIU

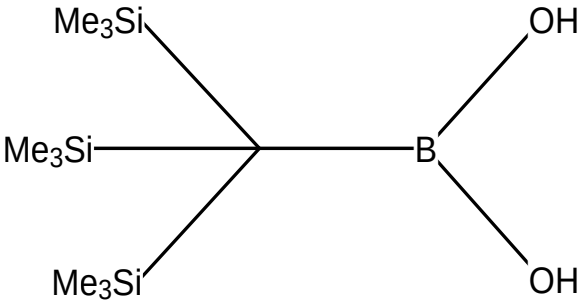
Reference: S.S.Al-Juaid, C.Eaborn, M.N.A.El-Kheli, P.B.Hitchcock, P.D.Lickiss, M.E.Molla, J.D.Smith, J.A.Zora (1989) *J.Chem.Soc.,Dalton Trans.* ,447

Formula: $C_{10}\,H_{29}\,B_1\,O_2\,Si_3$

Compound Name: Dihydroxy-(tris(trimethylsilyl)methyl)borane

Space Group:	Pna21	***Cell:***	***a***	15.675(2)	***b***	16.121(2)	***c***	14.662(2)
Space Group No.:	33	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 16.30 ***Temperature(K):*** 295 ***Density(g/cm³):*** 0.991



KECJIM

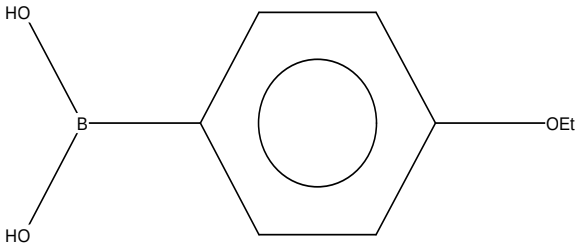
Reference: P.Rogowska, M.K.Cyranski, A.Sporzynski, A.Ciesielski (2006) *Tetrahedron Lett.* ,**47,**1389

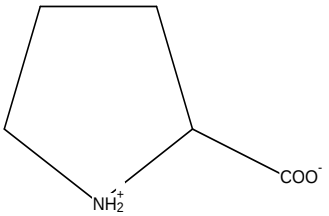
Formula: $C_8\,H_{11}\,B_1\,O_3,C_5\,H_9\,N_1\,O_2$

Compound Name: L-Proline 4-ethoxyphenylboronic acid

Space Group:	P1	***Cell:***	***a***	7.376(0)	***b***	7.830(0)	***c***	12.959(1)
Space Group No.:	1	***(Å,°)***	α	84.11(0)	β	78.72(0)	γ	73.91(0)

R-Factor (%): 5.25 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.326





KECJOS

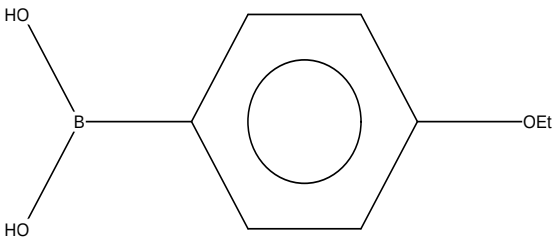
Reference: P.Rogowska, M.K.Cyranski, A.Sporzynski, A.Ciesielski (2006) *Tetrahedron Lett.* ,**47,**1389

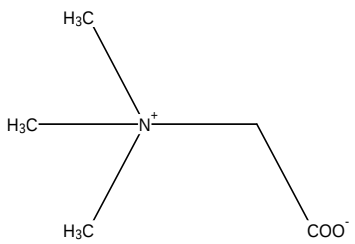
Formula: $C_8\,H_{11}\,B_1\,O_3,C_5\,H_{11}\,N_1\,O_2$

Compound Name: Betaine 4-ethoxyphenylboronic acid

Space Group:	P21/n	***Cell:***	***a***	19.222(2)	***b***	9.179(1)	***c***	19.337(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	118.75(1)	γ	90.00

R-Factor (%): 3.86 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.258





KEGNAM

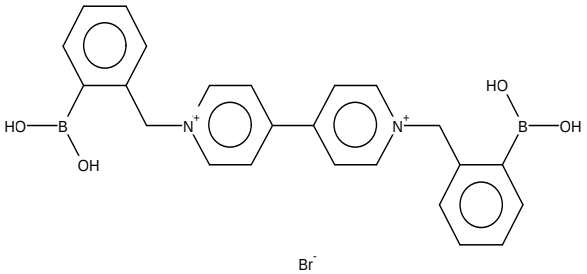
Reference: S.Gamsey, N.A.Baxter, Z.Sharrett, D.B.Cordes, M.M.Olmstead, R.A.Wessling, B.Singaram (2006) *Tetrahedron* ,**62,** 6321

Formula: $C_{24}\,H_{24}\,B_2\,N_2\,O_4\,^{2+},2(Br_1\,^{1-})$

Compound Name: 1,1'-bis(2-(Dihydroxyboryl)benzyl)-4,4'-bipyridinium dibromide

Space Group:	P21/c	***Cell:***	***a***	9.054(0)	***b***	9.682(0)	***c***	14.391(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	107.57(0)	γ	90.00

R-Factor (%): 3.06 ***Temperature(K):*** 166 ***Density(g/cm³):*** 1.618



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KEGNEQ

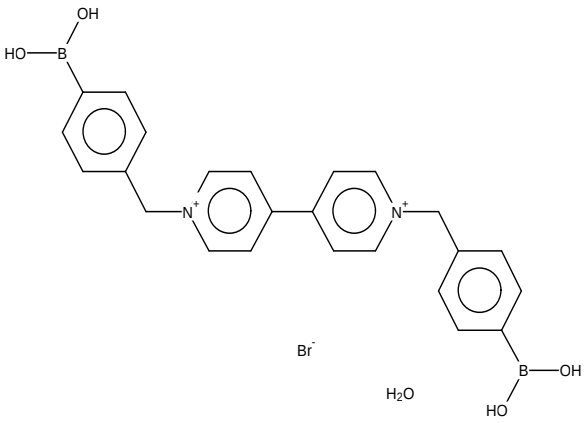
Reference: S.Gamsey, N.A.Baxter, Z.Sharrett, D.B.Cordes, M.M.Olmstead, R.A.Wessling, B.Singaram (2006) *Tetrahedron* ,**62,** 6321

Formula: $C_{24}H_{24}B_2N_2O_4^{2+},2(Br_1^{1-}),5(H_2O_1)$

Compound Name: 1,1'-bis(4-(Dihydroxyboryl)benzyl)-4,4'-bipyridinium dibromide pentahydrate

Space Group:	P21/c	***Cell:***	***a***	16.932(5)	***b***	28.674(8)	***c***	12.118(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	103.96(0)	γ	90.00

R-Factor (%): 8.27 ***Temperature(K):*** 90 ***Density(g/cm^3):*** 1.573



KEGNIU

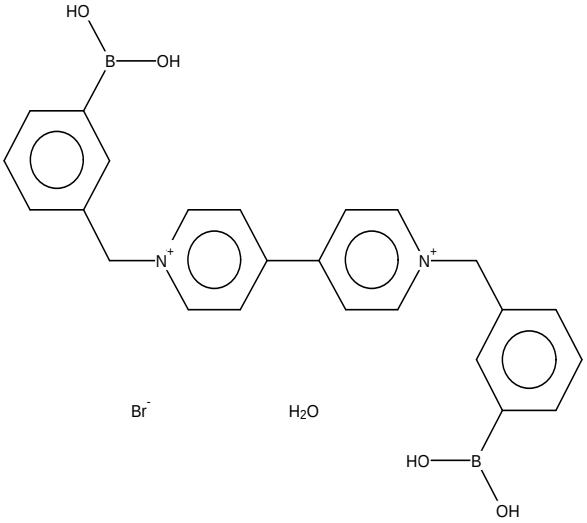
Reference: S.Gamsey, N.A.Baxter, Z.Sharrett, D.B.Cordes, M.M.Olmstead, R.A.Wessling, B.Singaram (2006) *Tetrahedron* ,**62,** 6321

Formula: $C_{24}H_{24}B_2N_2O_4^{2+},2(Br_1^{1-}),H_2O_1$

Compound Name: 1,1'-bis(3-(Dihydroxyboryl)benzyl)-4,4'-bipyridinium dibromide monohydrate

Space Group:	P21/c	***Cell:***	***a***	14.395(1)	***b***	14.037(0)	***c***	12.759(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	104.30(0)	γ	90.00

R-Factor (%): 2.93 ***Temperature(K):*** 90 ***Density(g/cm^3):*** 1.606



KERQOP

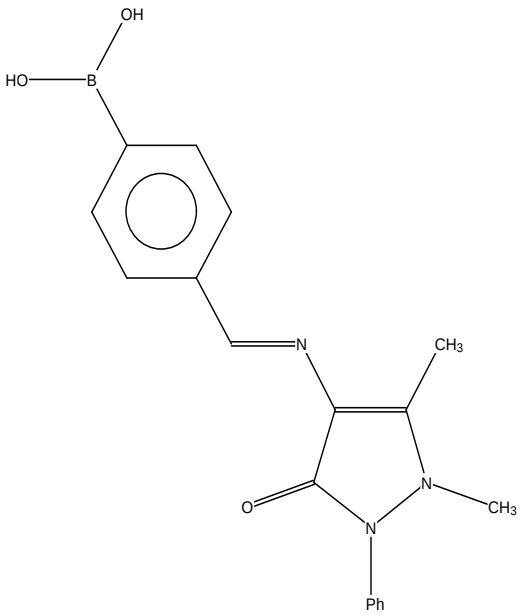
Reference: Yi-Feng Sun, He-Ping Wang, Yong Chen, Zhi-Yong Chen, Ji-Kun Li (2012) *Spectrochim.Acta,Part A* ,**97,**568

Formula: $C_{18}H_{18}B_1N_3O_3$

Compound Name: (4-(((1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)imino) methyl)phenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	13.990(6)	***b***	6.624(3)	***c***	18.751(9)
Space Group No.:	14	***(Å,°)***	α	90.00	β	102.44(0)	γ	90.00

R-Factor (%): 3.93 ***Temperature(K):*** 298 ***Density(g/cm^3):*** 1.312



KEZDOK

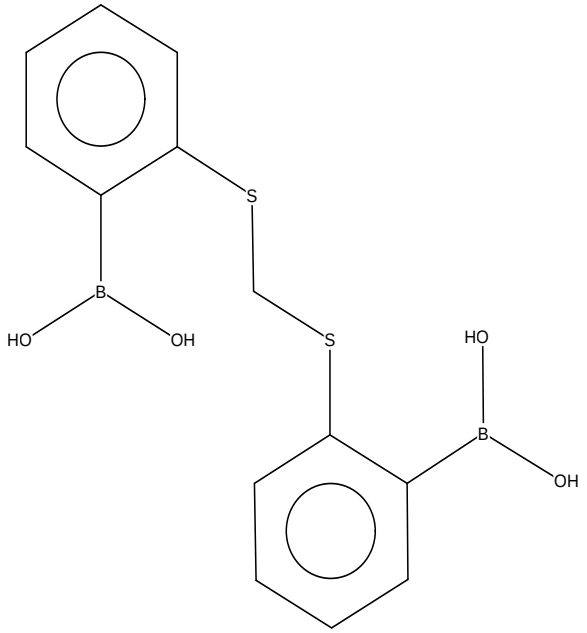
Reference: M.Dabrowski, K.Durka, T.Klis, J.Serwatowski, K.Wozniak (2013) *Tetrahedron* ,**69,**3159

Formula: $C_{13}H_{14}B_2O_4S_2$

Compound Name: (Methylenebis(sulfanediyl-2,1-phenylene))diboronic acid

Space Group:	P21/c	***Cell:***	***a***	24.450(1)	***b***	5.074(0)	***c***	24.739(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	106.85(0)	γ	90.00

R-Factor (%): 5.71 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.447



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KOJQAC

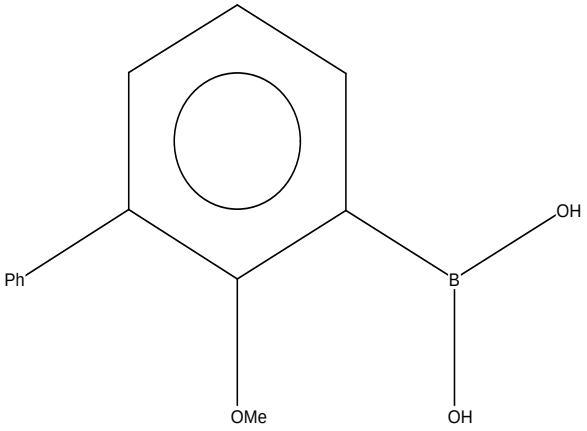
Reference: C.J.Davies, A.Gregory, P.Griffith, T.Perkins, K.Singh, G.A.Solan (2008) *Tetrahedron* ,**64,**9857

Formula: $C_{13}H_{13}B_1O_3$

Compound Name: (2-Methoxy-3-biphenyl)boronic acid

Space Group:	P-1	***Cell:***	***a***	7.714(0)	***b***	8.287(0)	***c***	9.785(0)
Space Group No.:	2	***(Å,°)***	α	67.47(0)	β	85.43(0)	γ	88.71(0)

R-Factor (%): 4.21 ***Temperature(K):*** 150 ***Density(g/cm³):*** 1.315



KUGBOE

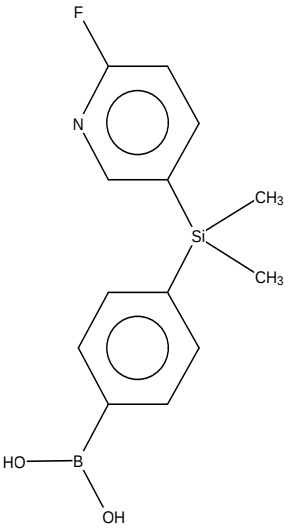
Reference: D.Troegel, F.Moller, C.Burschka, R.Tacke (2009) *Organometallics* ,**28,**3218

Formula: $C_{13}H_{15}B_1F_1N_1O_2Si_1,0.5(C_3H_6O_1)$

Compound Name: 4-((2-Fluoro-5-pyridyl)dimethylsilyl)phenylboronic acid acetone solvate

Space Group:	P21/n	***Cell:***	***a***	6.696(1)	***b***	22.190(3)	***c***	11.153(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	97.82(1)	γ	90.00

R-Factor (%): 4.41 ***Temperature(K):*** 193 ***Density(g/cm³):*** 1.231



KUGBUK

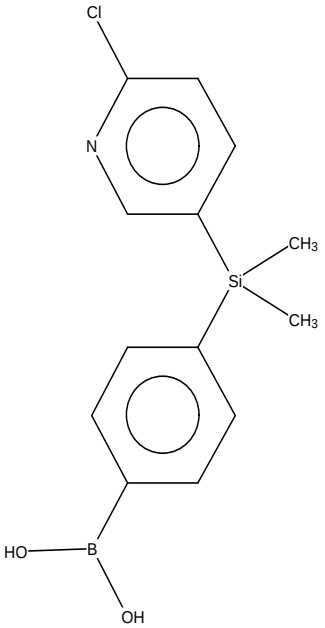
Reference: D.Troegel, F.Moller, C.Burschka, R.Tacke (2009) *Organometallics* ,**28,**3218

Formula: $C_{13}H_{15}B_1Cl_1N_1O_2Si_1$

Compound Name: 4-((2-Chloro-5-pyridyl)dimethylsilyl)phenylboronic acid

Space Group:	C2/c	***Cell:***	***a***	20.509(0)	***b***	15.689(0)	***c***	9.798(0)
Space Group No.:	15	***(Å,°)***	α	90.00	β	105.42(0)	γ	90.00

R-Factor (%): 3.79 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.275



KUQYEB

Reference: A.Vega, M.Zarate, H.Tlahuext, H.Hopfl (2010) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**66,**o219

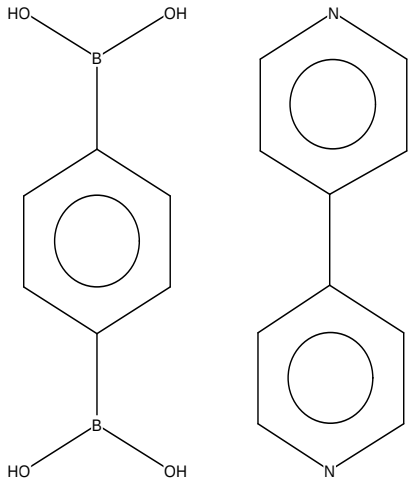
Formula: $2(C_{10}H_8N_2),C_6H_8B_2O_4,2(H_2O_1)$

Compound Name: bis(1,4-Phenylenediboronic acid) 4,4'-bipyridine dihydrate

Synonym: Benzene-1,4-diboronic acid bis(4,4'-bipyridine) dihydrate

Space Group:	P-1	***Cell:***	***a***	6.826(0)	***b***	10.191(1)	***c***	18.834(2)
Space Group No.:	2	***(Å,°)***	α	98.83(0)	β	90.80(0)	γ	98.00(0)

R-Factor (%): 4.77 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.333



H_2O

Search: search4 (Mon May 01 12:48:32 2017): Hits 117-120

LABCUM

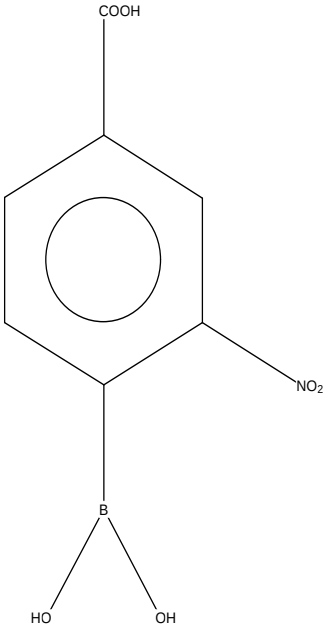
Reference: S.Soundararajan, E.N.Duesler, J.H.Hageman (1993) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**49,**690

Formula: $C_7 H_6 B_1 N_1 O_6$

Compound Name: 4-Carboxy-2-nitrobenzeneboronic acid

Space Group:	P21/n	***Cell:***	***a***	10.542(2)	***b***	6.411(1)	***c***	13.105(4)
Space Group No.:	14	***(Å,°)***	α	90.00	β	106.47(2)	γ	90.00

R-Factor (%): 5.30 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.650



LABMIN

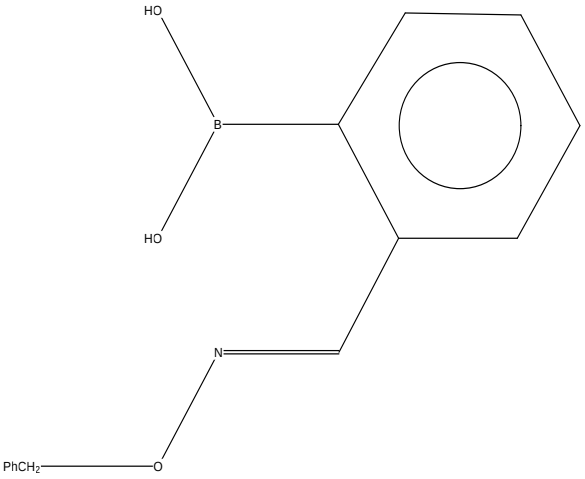
Reference: C.J.Stress, P.J.Schmidt, D.G.Gillingham (2016) *Org.Biomol.Chem.* ,**14,**5529

Formula: $C_{14} H_{14} B_1 N_1 O_3$

Compound Name: (2-(((Benzyloxy)imino)methyl)phenyl)boronic acid

Space Group:	C2/c	***Cell:***	***a***	18.525(1)	***b***	15.228(1)	***c***	18.962(1)
Space Group No.:	15	***(Å,°)***	α	90.00	β	94.10(0)	γ	90.00

R-Factor (%): 3.86 ***Temperature(K):*** 123 ***Density(g/cm³):*** 1.270



LEDVOH

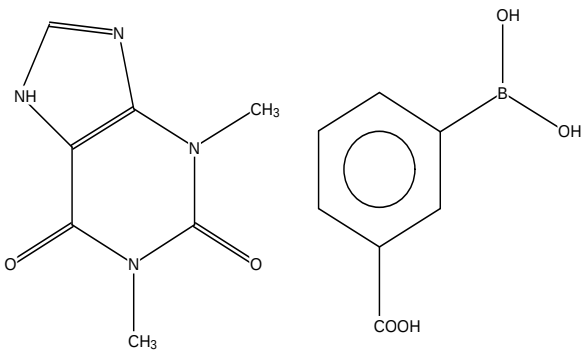
Reference: V.Dyulgerov, R.P.Nikolova, L.T.Dimova, B.L.Shivachev (2012) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**68,**o2320

Formula: $C_7 H_8 N_4 O_2$,$C_7 H_7 B_1 O_4$

Compound Name: 3-(Dihydroxyboryl)benzoic acid 1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione

Space Group:	P21/c	***Cell:***	***a***	13.185(4)	***b***	9.189(3)	***c***	13.287(4)
Space Group No.:	14	***(Å,°)***	α	90.00	β	109.04(3)	γ	90.00

R-Factor (%): 4.96 ***Temperature(K):*** 290 ***Density(g/cm³):*** 1.511



LEGMUH

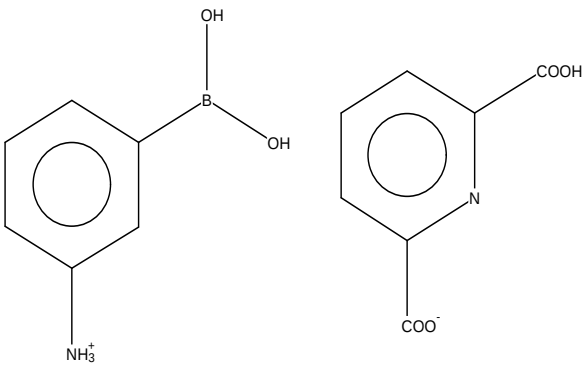
Reference: Chunhua Ge, Xiangdong Zhang, Rui Zhang, Chenglong Zhang (2012) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* , **68,**o2559

Formula: $C_6 H_9 B_1 N_1 O_2^{1+}$,$C_7 H_4 N_1 O_4^{1-}$

Compound Name: 3-(Dihydroxyboryl)anilinium 6-carboxypyridine-2-carboxylate

Space Group:	P21/n	***Cell:***	***a***	7.707(0)	***b***	14.047(1)	***c***	13.085(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	106.96(0)	γ	90.00

R-Factor (%): 3.71 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.491



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LEYNAF

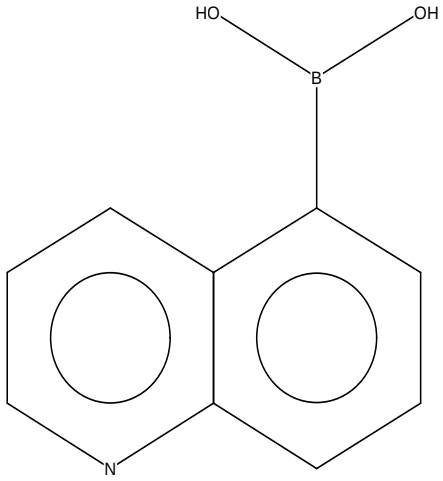
Reference: Yangling Zhang, Minyong Li, S.Chandrasekaran, Xingming Gao, Xikui Fang, Hsiau-Wei Lee, K.Hardcastle, J.Yang, Binghe Wang (2007) *Tetrahedron* ,**63,**3287

Formula: $C_9 H_8 B_1 N_1 O_2,H_2 O_1$

Compound Name: 5-Quinolineboronic acid monohydrate

Space Group:	C2/c	***Cell:***	***a***	17.536(1)	***b***	7.131(0)	***c***	15.271(0)
Space Group No.:	15	***(Å,°)***	α	90.00	β	93.58(0)	γ	90.00

R-Factor (%): 4.67 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.331



H_2O

LIXLAG

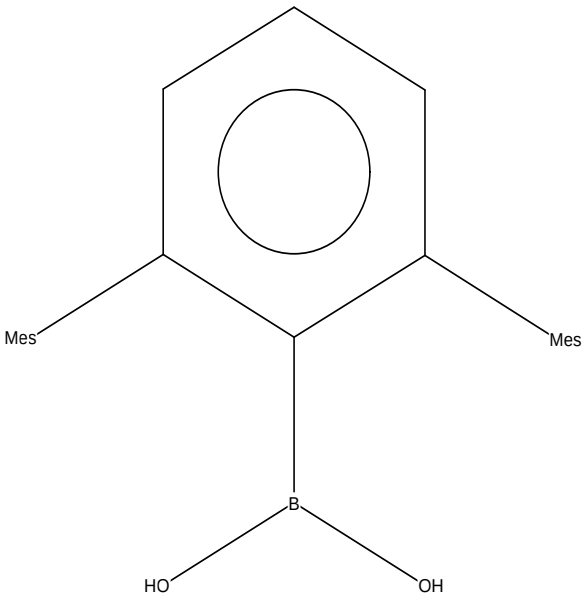
Reference: D.A.Dickie, I.S.MacIntosh, D.D.Ino, Qi He, O.A.Labeodan, M.C.Jennings, G.Schatte, C.J.Walsby, J.A.C.Clyburne (2008) *Can.J.Chem.* ,**86,**20

Formula: $C_{24} H_{27} B_1 O_2$

Compound Name: 2,6-bis(2,4,6-Trimethylphenyl)phenol boronic acid

Space Group:	Cmc21	***Cell:***	***a***	23.178(6)	***b***	12.981(0)	***c***	6.747(0)
Space Group No.:	36	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 7.05 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.172



LIYHOR

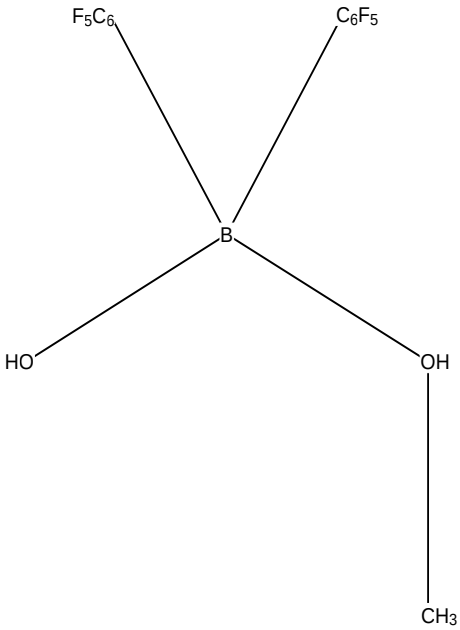
Reference: D.Donghi, D.Maggioni, T.Beringhelli, G.D'Alfonso, P.Mercandelli, A.Sironi (2008) *Eur.J.Inorg.Chem.* ,1645

Formula: $C_{13} H_5 B_1 F_{10} O_2$

Compound Name: Hydroxy-(methanol)-bis(pentafluorophenyl)-boron

Space Group:	P-1	***Cell:***	***a***	6.014(2)	***b***	10.101(2)	***c***	12.425(2)
Space Group No.:	2	***(Å,°)***	α	73.02(1)	β	77.49(1)	γ	73.48(1)

R-Factor (%): 3.49 ***Temperature(K):*** 110 ***Density(g/cm³):*** 1.911



LOXCOS

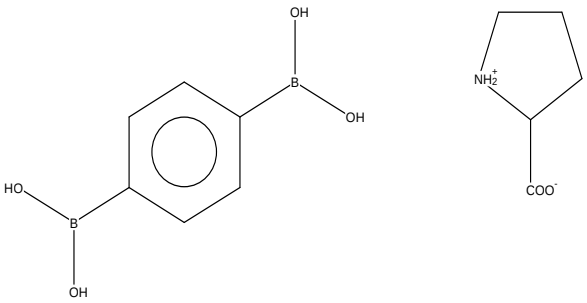
Reference: J.Hernandez-Paredes, A.L.Olvera-Tapia, J.I.Arenas-Garcia, H.Hopfl, H.Morales-Rojas, D.Herrera-Ruiz, A.I.Gonzaga-Morales, L.Rodriguez-Fragoso (2015) *CrystEngComm* , **17,**5166

Formula: $C_6 H_8 B_2 O_4,2(C_5 H_9 N_1 O_2)$

Compound Name: bis(pyrrolidinium-2-carboxylate) 1,4-phenylenediboronic acid

Space Group:	P1	***Cell:***	***a***	6.894(1)	***b***	7.632(1)	***c***	9.917(1)
Space Group No.:	1	***(Å,°)***	α	79.29(0)	β	71.22(0)	γ	81.68(0)

R-Factor (%): 4.84 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.360



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LOXCUY

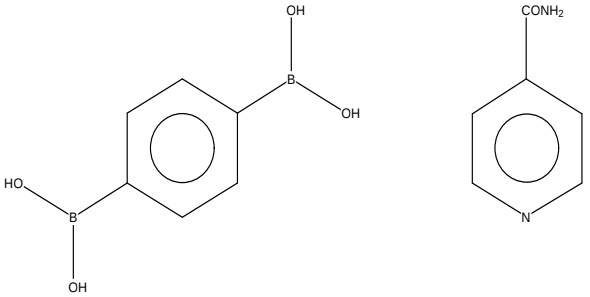
Reference: J.Hernandez-Paredes, A.L.Olvera-Tapia, J.I.Arenas-Garcia, H.Hopfl, H.Morales-Rojas, D.Herrera-Ruiz, A.I.Gonzaga-Morales, L.Rodriguez-Fragoso (2015) *CrystEngComm* , **17,**5166

Formula: $C_6 H_8 B_2 O_4$,2($C_6 H_6 N_2 O_1$)

Compound Name: 1,4-phenylenediboronic acid bis(isonicotinamide)

Space Group:	P21/c	***Cell:***	***a***	7.869(1)	***b***	5.103(0)	***c***	23.951(4)
Space Group No.:	14	***(Å,°)***	α	90.00	β	90.47(0)	γ	90.00

R-Factor (%): 3.73 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.416



LOXDAF

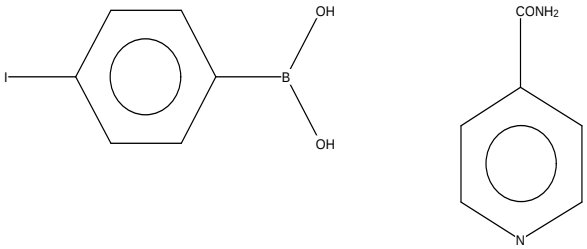
Reference: J.Hernandez-Paredes, A.L.Olvera-Tapia, J.I.Arenas-Garcia, H.Hopfl, H.Morales-Rojas, D.Herrera-Ruiz, A.I.Gonzaga-Morales, L.Rodriguez-Fragoso (2015) *CrystEngComm* , **17,**5166

Formula: $C_6 H_6 B_1 I_1 O_2$,$C_6 H_6 N_2 O_1$

Compound Name: (4-iodophenyl)boronic acid isonicotinamide

Space Group:	P-1	***Cell:***	***a***	5.111(0)	***b***	11.294(1)	***c***	12.093(1)
Space Group No.:	2	***(Å,°)***	α	76.59(0)	β	84.83(0)	γ	78.49(0)

R-Factor (%): 3.27 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.848



LOXDEJ

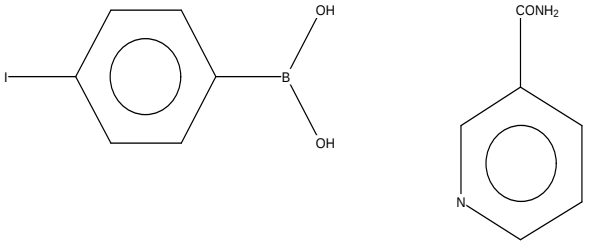
Reference: J.Hernandez-Paredes, A.L.Olvera-Tapia, J.I.Arenas-Garcia, H.Hopfl, H.Morales-Rojas, D.Herrera-Ruiz, A.I.Gonzaga-Morales, L.Rodriguez-Fragoso (2015) *CrystEngComm* , **17,**5166

Formula: $C_6 H_6 B_1 I_1 O_2$,$C_6 H_6 N_2 O_1$

Compound Name: (4-iodophenyl)boronic acid nicotinamide

Space Group:	Pca21	***Cell:***	***a***	34.686(8)	***b***	4.009(0)	***c***	10.092(2)
Space Group No.:	29	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 5.31 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.751



LOXDIN

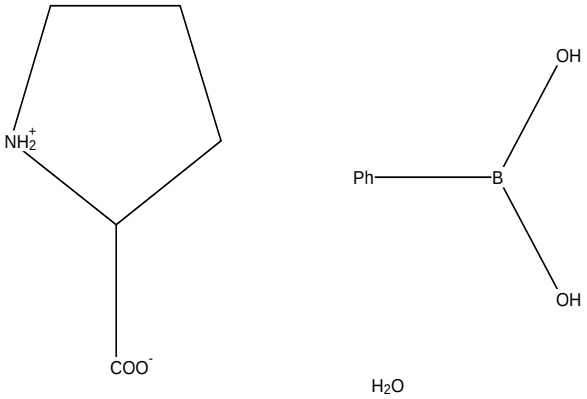
Reference: J.Hernandez-Paredes, A.L.Olvera-Tapia, J.I.Arenas-Garcia, H.Hopfl, H.Morales-Rojas, D.Herrera-Ruiz, A.I.Gonzaga-Morales, L.Rodriguez-Fragoso (2015) *CrystEngComm* , **17,**5166

Formula: $C_5 H_9 N_1 O_2$,$C_6 H_7 B_1 O_2$,$H_2 O_1$

Compound Name: pyrrolidinium-2-carboxylate phenylboronic acid monohydrate

Space Group:	P21	***Cell:***	***a***	7.686(1)	***b***	5.846(1)	***c***	14.933(3)
Space Group No.:	4	***(Å,°)***	α	90.00	β	103.95(0)	γ	90.00

R-Factor (%): 4.34 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.301



Search: search4 (Mon May 01 12:48:32 2017): Hits 129-132

MAPZIO

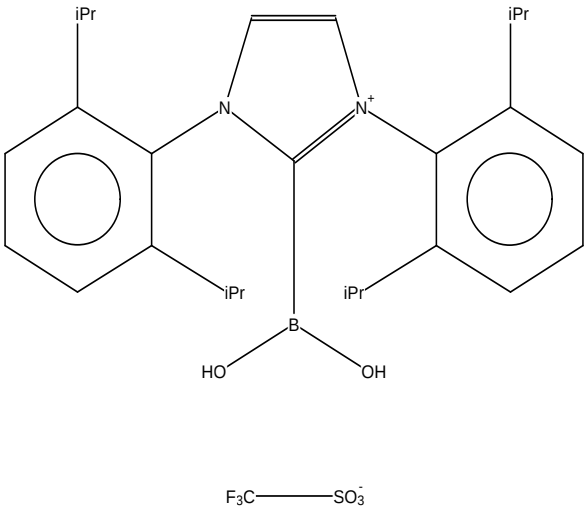
Reference: A.Solovyev, S.J.Geib, E.Lacte, D.P.Curran (2012)
Organometallics ,**31,**54

Formula: $C_{27}\,H_{38}\,B_1\,N_2\,O_2\,^{1+},C_1\,F_3\,O_3\,S_1\,^{1-}$

Compound Name: 2-(Dihydroxyboryl)-1,3-bis(2,6-diisopropylphenyl)-1H-imidazol-3-ium trifluoromethanesulfonate

Space Group:	P-1	***Cell:***	***a***	11.596(6)	***b***	15.429(8)	***c***	19.414(10)
Space Group No.:	2	***(Å,°)***	α	69.98(1)	β	77.44(1)	γ	86.11(1)

R-Factor (%): 7.22 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.215



MIDYOO

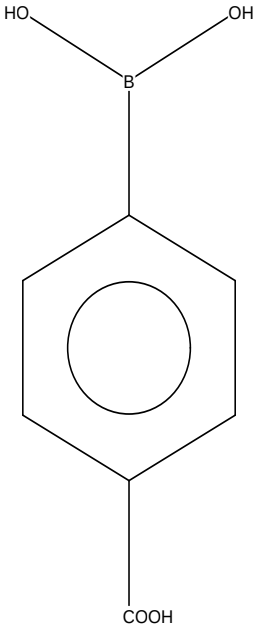
Reference: N.SeethaLekshmi, V.R.Pedireddi (2007)
Cryst.Growth Des. ,**7,**944

Formula: $C_7\,H_7\,B_1\,O_4$

Compound Name: 4-Carboxyphenylboronic acid

Space Group:	C2/c	***Cell:***	***a***	11.378(5)	***b***	9.825(5)	***c***	7.245(3)
Space Group No.:	15	***(Å,°)***	α	90.00	β	120.08(2)	γ	90.00

R-Factor (%): 7.58 ***Temperature(K):*** 133 ***Density(g/cm³):*** 1.573



MIDYUU

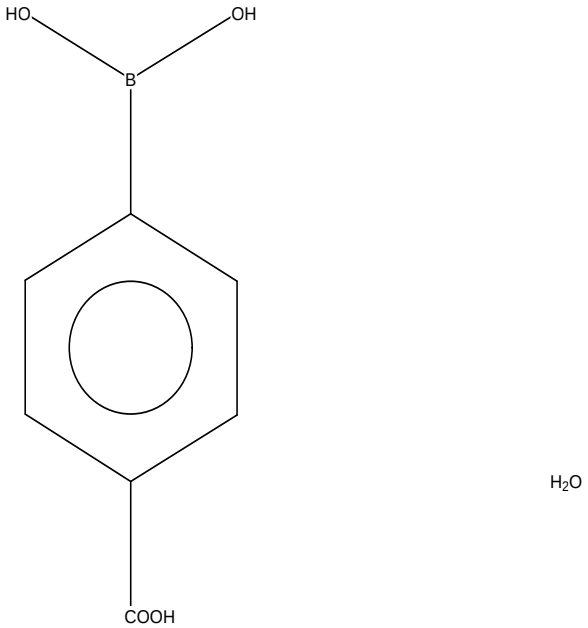
Reference: N.SeethaLekshmi, V.R.Pedireddi (2007)
Cryst.Growth Des. ,**7,**944

Formula: $C_7\,H_7\,B_1\,O_4,H_2\,O_1$

Compound Name: 4-Carboxyphenylboronic acid monohydrate

Space Group:	Ccc2	***Cell:***	***a***	7.566(5)	***b***	11.929(7)	***c***	9.769(6)
Space Group No.:	37	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 7.13 ***Temperature(K):*** 298 ***Density(g/cm³):*** 1.386



MIDZAB

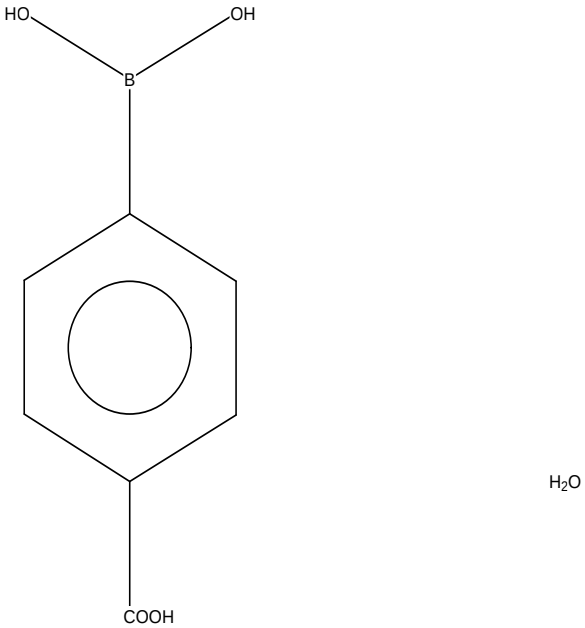
Reference: N.SeethaLekshmi, V.R.Pedireddi (2007)
Cryst.Growth Des. ,**7,**944

Formula: $C_7\,H_7\,B_1\,O_4,0.25(H_2\,O_1)$

Compound Name: 4-Carboxyphenylboronic acid hydrate

Space Group:	Fddd	***Cell:***	***a***	13.140(3)	***b***	18.138(5)	***c***	25.328(7)
Space Group No.:	70	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 5.14 ***Temperature(K):*** 133 ***Density(g/cm³):*** 1.500



Search: search4 (Mon May 01 12:48:32 2017): Hits 133-136

MOKKON

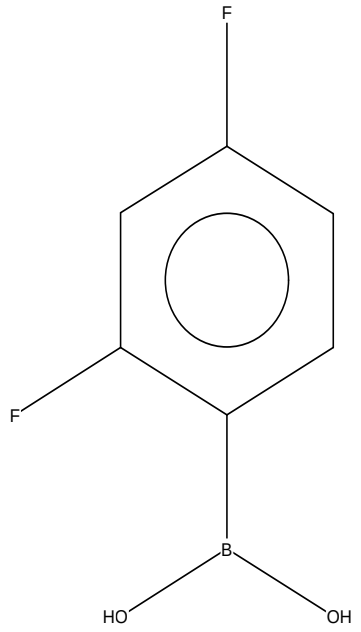
Reference: P.Rodriguez-Cuamatzi, H.Tlahuext, H.Hopfl (2009) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**65,**o44

Formula: $C_6 H_5 B_1 F_2 O_2$

Compound Name: 2,4-Difluorophenylboronic acid

Space Group:	P21/n	***Cell:***	***a***	3.762(1)	***b***	12.347(4)	***c***	14.620(4)
Space Group No.:	14	***(Å,°)***	α	90.00	β	95.45(0)	γ	90.00

R-Factor (%): 5.57 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.552



MOKKON01

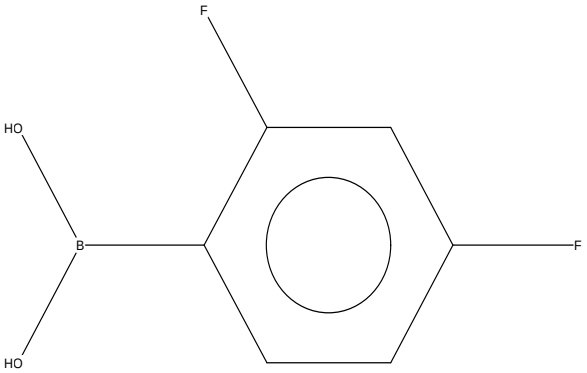
Reference: I.D.Madura, K.Czerwinska, D.Soldanska (2014) *Cryst.Growth Des.* ,**14,**5912

Formula: $C_6 H_5 B_1 F_2 O_2$

Compound Name: (2,4-difluorophenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	3.679(0)	***b***	12.287(0)	***c***	14.318(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	93.06(0)	γ	90.00

R-Factor (%): 3.57 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.623



MOPFON

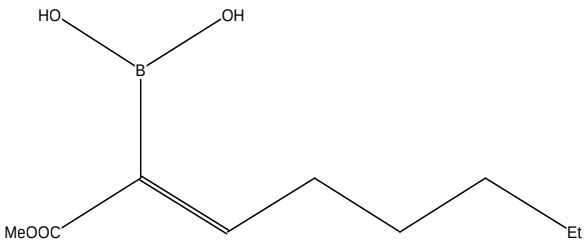
Reference: B.H.Lipshutz, Z.V.Boskovic, D.H.Aue (2008) *Angew.Chem.,Int.Ed.* ,**47,**10183

Formula: $C_9 H_{17} B_1 O_4$

Compound Name: (1-Methoxy-1-oxo-2-octen-2-yl)boronic acid

Space Group:	P-1	***Cell:***	***a***	8.766(5)	***b***	11.011(6)	***c***	11.640(7)
Space Group No.:	2	***(Å,°)***	α	100.48(0)	β	94.29(0)	γ	91.90(1)

R-Factor (%): 7.49 ***Temperature(K):*** 230 ***Density(g/cm³):*** 1.207



MORTET

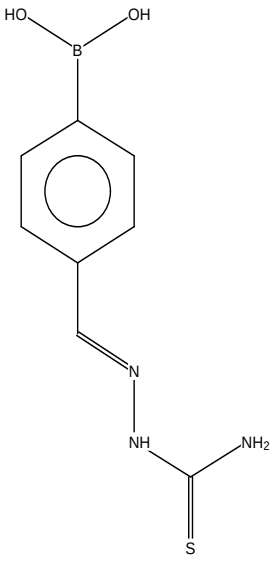
Reference: J.W.Hicks, C.B.Kyle, C.M.Vogels, S.L.Wheaton, F.J.Baerlocher, A.Decken, S.A.Westcott (2008) *Chem.Biodiversity* ,**5,** 2415

Formula: $C_8 H_{10} B_1 N_3 O_2 S_1, H_2 O_1$

Compound Name: 4-((E)-(Thiosemicarbazono)methyl)phenylboronic acid monohydrate

Space Group:	C2/c	***Cell:***	***a***	28.928(6)	***b***	4.817(0)	***c***	20.418(4)
Space Group No.:	15	***(Å,°)***	α	90.00	β	127.66(0)	γ	90.00

R-Factor (%): 4.02 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.422



H_2O

Search: search4 (Mon May 01 12:48:32 2017): Hits 137-140

MOYLES

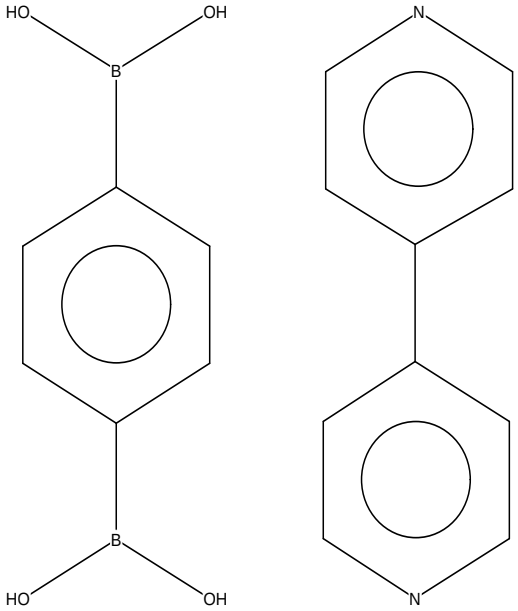
Reference: P.Rodriquez-Cuamatzi, R.Luna-Garcia, A.Torres-Huerta, M.I.Bernal-Uruchurtu, V.Barba, H.Hopfl (2009) *Cryst.Growth Des.* ,**9,** 1575

Formula: $C_6 H_8 B_2 O_4$,2($C_{10} H_8 N_2$)

Compound Name: 1,4-Phenylenediboronic acid bis(4,4'-bipyridine)

Space Group:	P21/c	***Cell:***	***a*** 14.891(2)	***b*** 9.377(1)	***c*** 17.420(3)
Space Group No.:	14	***(Å,°)***	α 90.00	β 107.81(0)	γ 90.00

R-Factor (%): 7.96 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.371



MOYLIW

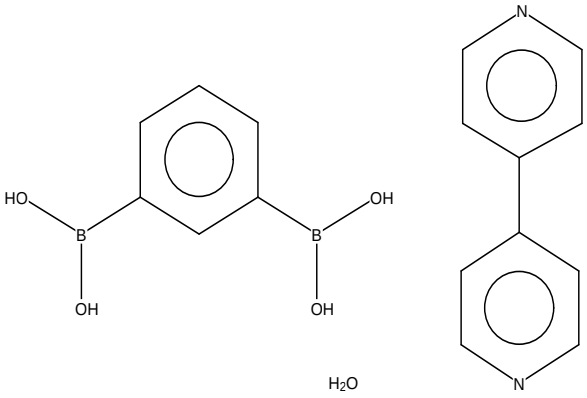
Reference: P.Rodriquez-Cuamatzi, R.Luna-Garcia, A.Torres-Huerta, M.I.Bernal-Uruchurtu, V.Barba, H.Hopfl (2009) *Cryst.Growth Des.* ,**9,** 1575

Formula: $C_6 H_8 B_2 O_4$,2($C_{10} H_8 N_2$),2($H_2 O_1$)

Compound Name: 1,3-Phenylenediboronic acid bis(4,4'-bipyridine) dihydrate

Space Group:	C2/c	***Cell:***	***a*** 18.820(3)	***b*** 6.828(1)	***c*** 20.112(3)
Space Group No.:	15	***(Å,°)***	α 90.00	β 99.17(0)	γ 90.00

R-Factor (%): 7.29 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.339



MOYLOC

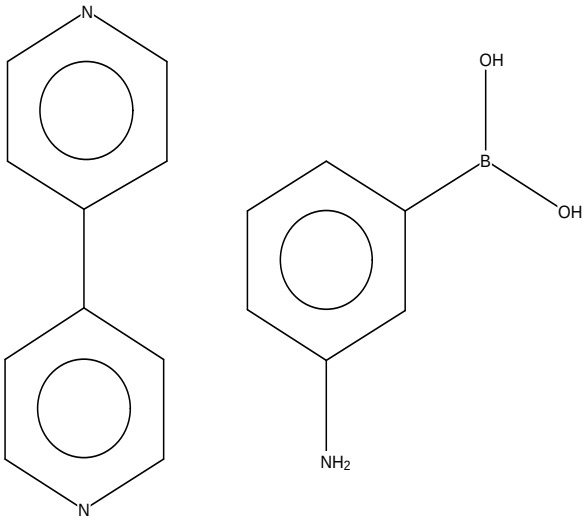
Reference: P.Rodriquez-Cuamatzi, R.Luna-Garcia, A.Torres-Huerta, M.I.Bernal-Uruchurtu, V.Barba, H.Hopfl (2009) *Cryst.Growth Des.* ,**9,** 1575

Formula: 2($C_{10} H_8 N_2$),$C_6 H_8 B_1 N_1 O_2$

Compound Name: (3-Aminophenyl)boronic acid bis(4,4'-bipyridine)

Space Group:	Cc	***Cell:***	***a*** 16.778(1)	***b*** 9.062(0)	***c*** 15.838(1)
Space Group No.:	9	***(Å,°)***	α 90.00	β 114.39(0)	γ 90.00

R-Factor (%): 3.99 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.361



MOYMAP

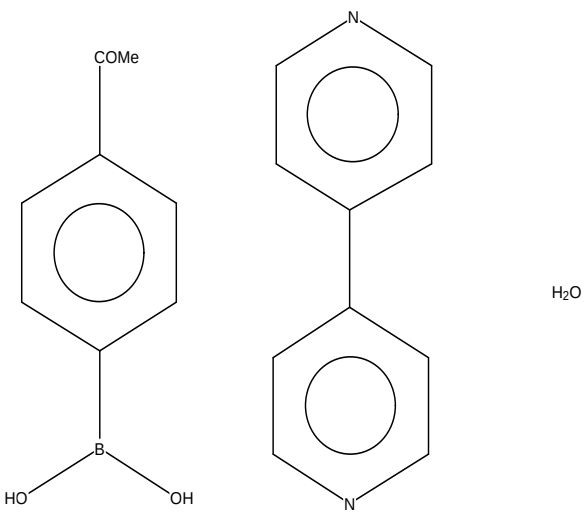
Reference: P.Rodriquez-Cuamatzi, R.Luna-Garcia, A.Torres-Huerta, M.I.Bernal-Uruchurtu, V.Barba, H.Hopfl (2009) *Cryst.Growth Des.* ,**9,** 1575

Formula: $C_8 H_9 B_1 O_3$,2($C_{10} H_8 N_2$),2($H_2 O_1$)

Compound Name: (4-Acetylphenyl)boronic acid bis(4,4'-bipyridine) dihydrate

Space Group:	Cc	***Cell:***	***a*** 24.159(4)	***b*** 7.649(1)	***c*** 18.434(3)
Space Group No.:	9	***(Å,°)***	α 90.00	β 130.43(0)	γ 90.00

R-Factor (%): 6.16 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.312



Search: search4 (Mon May 01 12:48:32 2017): Hits 141-144

MUCJUQ

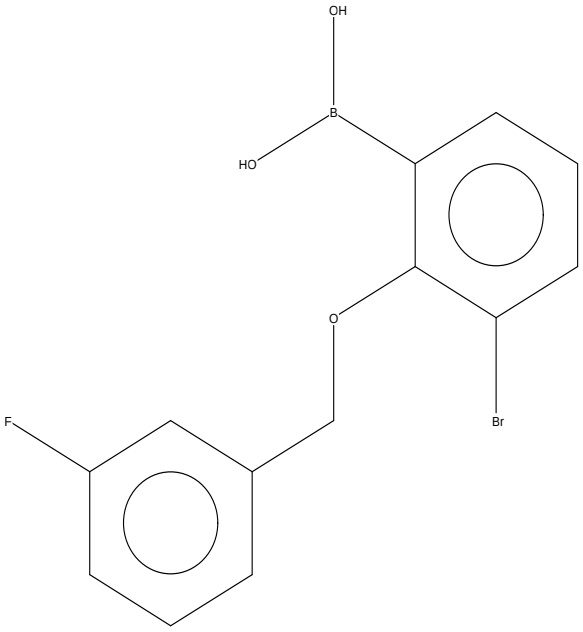
Reference: K.Kacprzak, T.Klis, J.Serwatowski (2009)
Acta Crystallogr.,Sect.E:Struct.Rep.Online ,**65,**o2250

Formula: $C_{13}H_{11}B_1Br_1F_1O_3$

Compound Name: (3-Bromo-2-((3-fluorobenzyl)oxy)phenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	14.913(2)	***b***	4.021(0)	***c***	21.945(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	101.57(1)	γ	90.00

R-Factor (%): 3.86 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.674



MULQER

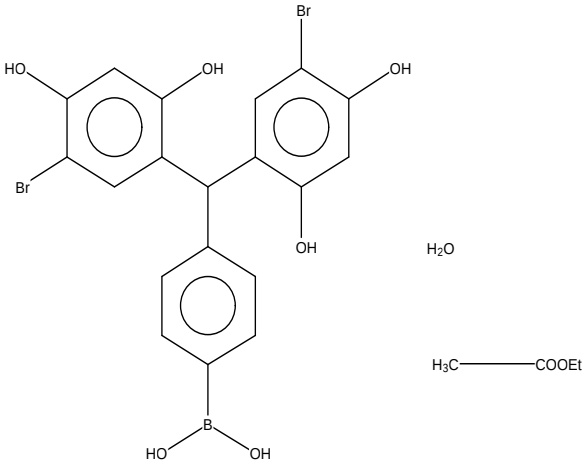
Reference: Youjun Yang, R.M.Strongin, F.R.Fronczek (2015)
CSD Communication(Private Communication) ,

Formula: $C_{19}H_{15}B_1Br_2O_6.2(C_4H_8O_2).H_2O_1$

Compound Name: (4-(bis(5-bromo-2,4-dihydroxyphenyl)methyl)phenyl)boronic acid ethyl acetate solvate monohydrate

Space Group:	P-1	***Cell:***	***a***	10.695(7)	***b***	11.568(6)	***c***	13.286(9)
Space Group No.:	2	***(Å,°)***	α	74.04(2)	β	78.53(2)	γ	86.53(3)

R-Factor (%): 7.40 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.510



MUWYOT

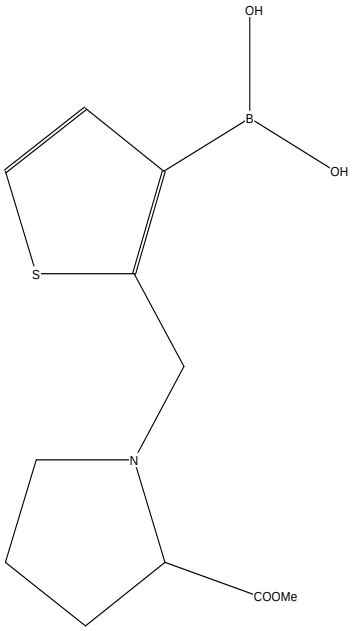
Reference: Lei Zhu, S.H.Shabbir, M.Gray, V.M.Lynch, S.Sorey, E.V.Anslyn (2006) *J.Am.Chem.Soc.* ,**128,**1222

Formula: $C_{11}H_{16}B_1N_1O_4S_1$

Compound Name: Methyl 1-((3-(dihydroxyboryl)-2-thienyl)methyl)prolinate

Space Group:	P21/n	***Cell:***	***a***	10.115(0)	***b***	8.948(0)	***c***	14.699(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	99.35(0)	γ	90.00

R-Factor (%): 4.18 ***Temperature(K):*** 153 ***Density(g/cm³):*** 1.362



MUWYUZ

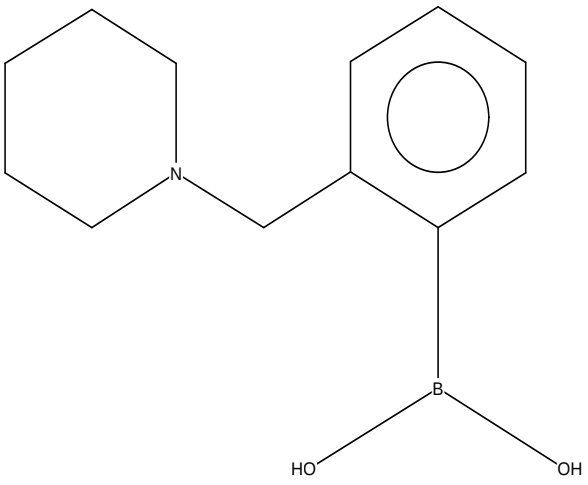
Reference: Lei Zhu, S.H.Shabbir, M.Gray, V.M.Lynch, S.Sorey, E.V.Anslyn (2006) *J.Am.Chem.Soc.* ,**128,**1222

Formula: $C_{12}H_{18}B_1N_1O_2$

Compound Name: (2-(Piperidin-1-ylmethyl)phenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	10.557(0)	***b***	10.873(0)	***c***	11.507(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	114.30(0)	γ	90.00

R-Factor (%): 3.87 ***Temperature(K):*** 153 ***Density(g/cm³):*** 1.209



Search: search4 (Mon May 01 12:48:32 2017): Hits 145-148

MUWYUZ01

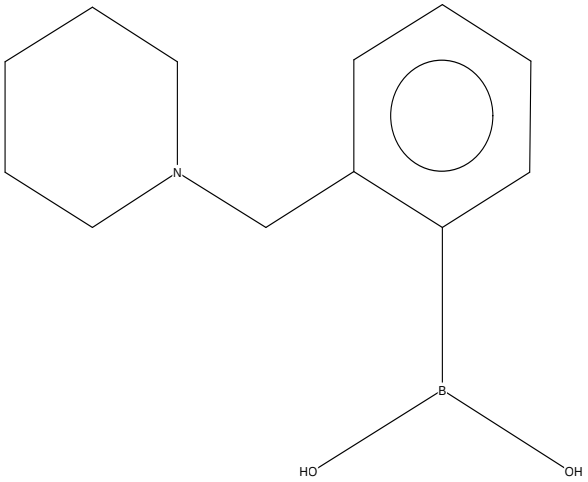
Reference: A.Adamczyk-Wozniak, I.Madura, A.Pawelko, A.Sporzynski, A.Zubrowska, J.Zyla (2011) *Central Eur.J.Chem.* ,**9,**199

Formula: $C_{12}H_{18}B_1N_1O_2$

Compound Name: (2-(Piperidin-1-ylmethyl)phenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	10.510(0)	***b***	10.827(0)	***c***	11.508(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	114.66(0)	γ	90.00

R-Factor (%): 3.34 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.223



NEBSOE

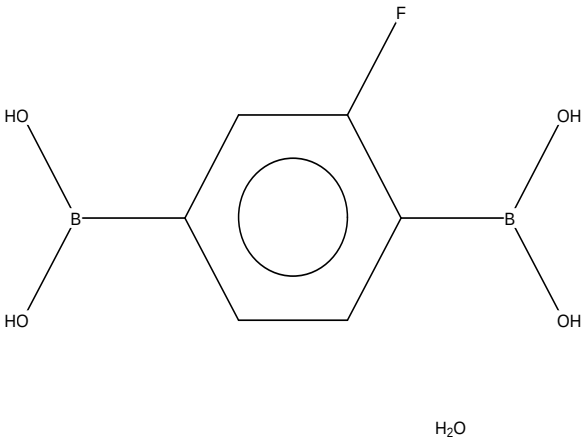
Reference: K.Durka, K.N.Jarzembska, R.Kaminski, S.Lulinski, J.Serwatowski, K.Wozniak (2012) *Cryst.Growth Des.* ,**12,**3720

Formula: $C_6H_7B_2F_1O_4,H_2O_1$

Compound Name: (2-fluoro-1,4-phenylene)diboronic acid monohydrate

Space Group:	Cccm	***Cell:***	***a***	12.049(0)	***b***	7.277(0)	***c***	10.055(0)
Space Group No.:	66	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 4.02 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.520



NEBSUK

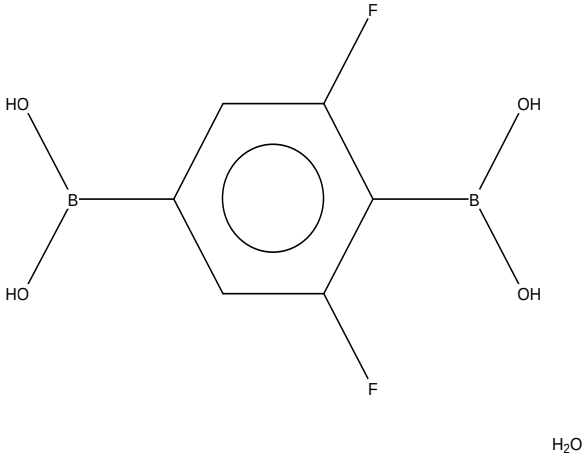
Reference: K.Durka, K.N.Jarzembska, R.Kaminski, S.Lulinski, J.Serwatowski, K.Wozniak (2012) *Cryst.Growth Des.* ,**12,**3720

Formula: $C_6H_6B_2F_2O_4,H_2O_1$

Compound Name: (2,6-difluoro-1,4-phenylene)diboronic acid monohydrate

Space Group:	Cccm	***Cell:***	***a***	12.207(2)	***b***	7.329(1)	***c***	10.081(1)
Space Group No.:	66	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.02 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.618



NEBTAR

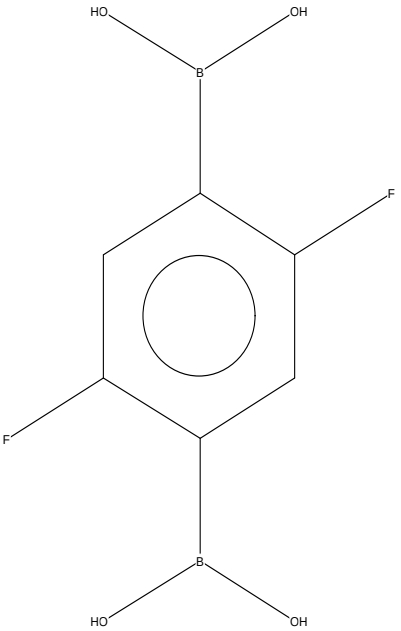
Reference: K.Durka, K.N.Jarzembska, R.Kaminski, S.Lulinski, J.Serwatowski, K.Wozniak (2012) *Cryst.Growth Des.* ,**12,**3720

Formula: $C_6H_6B_2F_2O_4$

Compound Name: (2,5-Difluoro-1,4-phenylene)diboronic acid

Space Group:	P-1	***Cell:***	***a***	4.984(1)	***b***	5.257(1)	***c***	7.423(3)
Space Group No.:	2	***(Å,°)***	α	74.67(1)	β	84.64(1)	γ	89.00(1)

R-Factor (%): 6.45 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.794



Search: search4 (Mon May 01 12:48:32 2017): Hits 149-152

NEBTEV

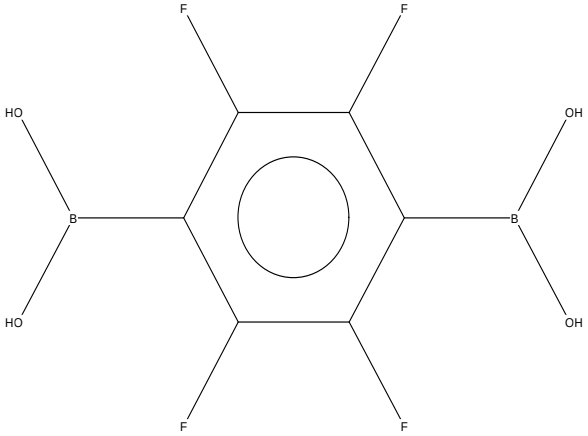
Reference: K.Durka, K.N.Jarzembska, R.Kaminski, S.Lulinski, J.Serwatowski, K.Wozniak (2012) *Cryst.Growth Des.* ,**12,**3720

Formula: $C_6 H_4 B_2 F_4 O_4$

Compound Name: (2,3,5,6-Tetrafluoro-1,4-phenylene)diboronic acid

Space Group:	P21/n	***Cell:***	***a***	8.426(1)	***b***	5.024(0)	***c***	10.166(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	106.25(0)	γ	90.00

R-Factor (%): 5.54 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.911



NEBTIZ

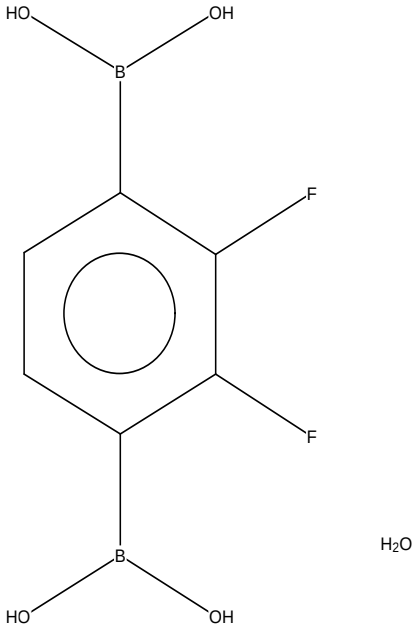
Reference: K.Durka, K.N.Jarzembska, R.Kaminski, S.Lulinski, J.Serwatowski, K.Wozniak (2012) *Cryst.Growth Des.* ,**12,**3720

Formula: $C_6 H_6 B_2 F_2 O_4,2(H_2 O_1)$

Compound Name: (2,3-Difluoro-1,4-phenylene)diboronic acid dihydrate

Space Group:	P21/c	***Cell:***	***a***	9.551(0)	***b***	28.212(1)	***c***	7.652(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	109.57(0)	γ	90.00

R-Factor (%): 3.52 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.626



NEYVIX

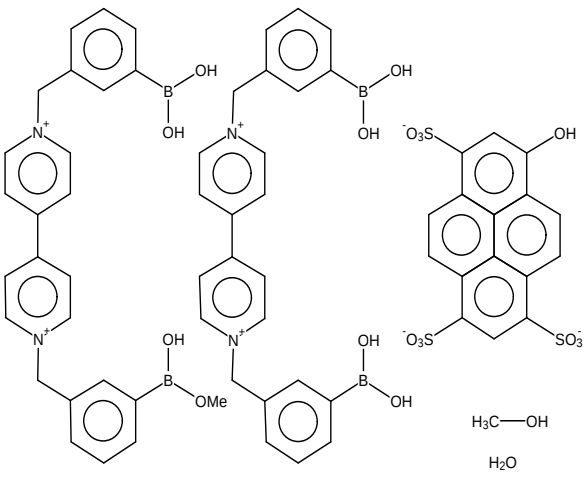
Reference: S.Gamsey, A.Miller, M.M.Olmstead, C.M.Beavers, L.C.Hirayama, S.Pradhan, R.A.Wessling, B.Singaram (2007) *J.Am.Chem.Soc.* ,**129,**1278

Formula: $2(C_{25} H_{26} B_2 N_2 O_4 {}^{2+}),C_{24} H_{24} B_2 N_2 O_4 {}^{2+},2(C_{16} H_7 O_{10} S_3 {}^{3-}),2(C_1 H_4 O_1),2(H_2 O_1)$

Compound Name: (4,4'-bis(3-(dihydroxyboryl)benzyl)-4,4'-bipyridinium) (4-(3-(dihydroxyboryl)benzyl)-4'-(3-(hydroxy(methoxy)boryl)benzyl)-4,4'-bipyridinium) bis(8-hydroxypyrene-1,3,6-trisulfonate) methanol solvate dihydrate

Space Group:	P-1	***Cell:***	***a***	9.593(1)	***b***	13.911(1)	***c***	20.342(2)
Space Group No.:	2	***(Å,°)***	α	102.13(0)	β	90.32(0)	γ	105.61(0)

R-Factor (%): 6.29 ***Temperature(K):*** 93 ***Density(g/cm³):*** 1.509



NIQCUM

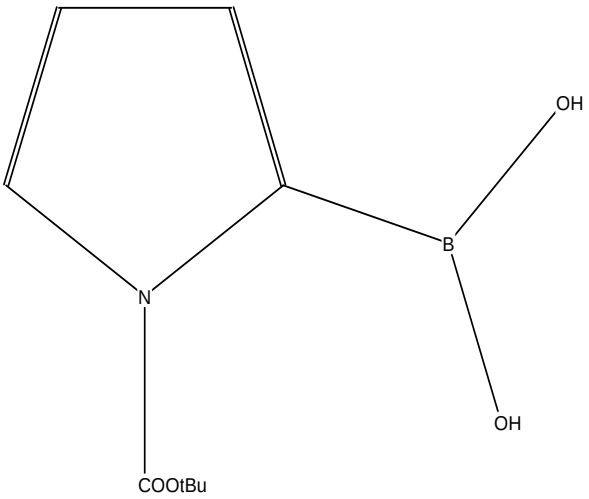
Reference: M.E.Light, I.E.D.Vega, P.A.Gale (2007) *CSD Communication(Private Communication)* ,

Formula: $C_9 H_{14} B_1 N_1 O_4$

Compound Name: (1-(t-Butoxycarbonyl)-1H-pyrrol-2-yl)boronic acid

Space Group:	Pbca	***Cell:***	***a***	12.925(1)	***b***	9.596(1)	***c***	17.570(1)
Space Group No.:	61	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 4.12 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.286



Search: search4 (Mon May 01 12:48:32 2017): Hits 153-156

NIQCUM01

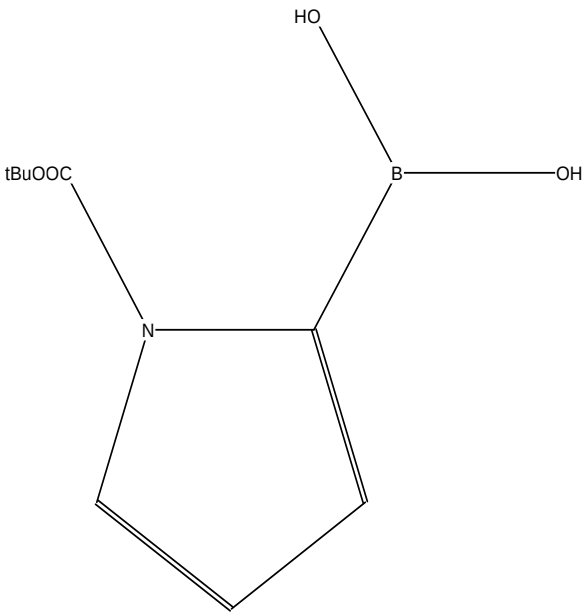
Reference: T.Klis, J.Serwatowski (2008)
Acta Crystallogr.,Sect.E:Struct.Rep.Online ,**64,**o1054

Formula: $C_9 H_{14} B_1 N_1 O_4$

Compound Name: t-Butyl 2-(dihydroxyboryl)pyrrole-1-carboxylate

Space Group:	Pbca	***Cell:***	***a***	12.918(1)	***b***	9.588(0)	***c***	17.581(1)
Space Group No.:	61	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.06 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.287



NIQCUM02

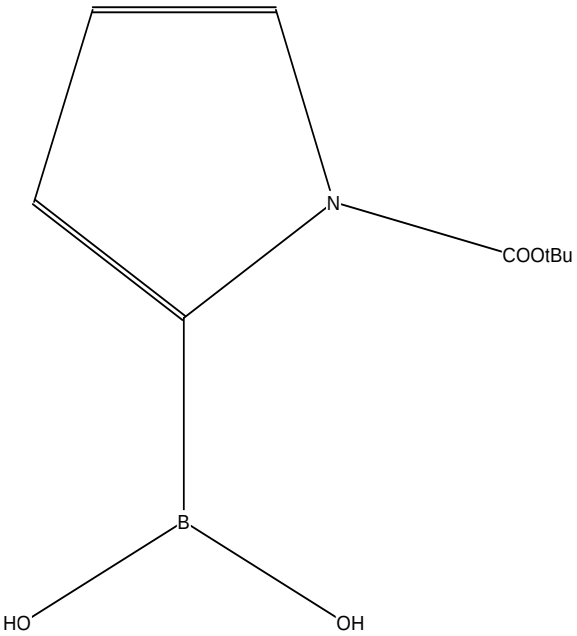
Reference: Zheng Zhong, Guo-Qiang Lin, Zhi-Hua Sun, Bing Wang (2009) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**65,**o687

Formula: $C_9 H_{14} B_1 N_1 O_4$

Compound Name: t-Butyl 2-(dihydroxyboryl)pyrrole-1-carboxylate

Space Group:	Pbca	***Cell:***	***a***	13.014(3)	***b***	9.940(2)	***c***	17.417(4)
Space Group No.:	61	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 4.16 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.244



NIQCUM03

Reference: S.Enthaler, M.Weidauer, E.Irran (2014)
CSD Communication(Private Communication) ,

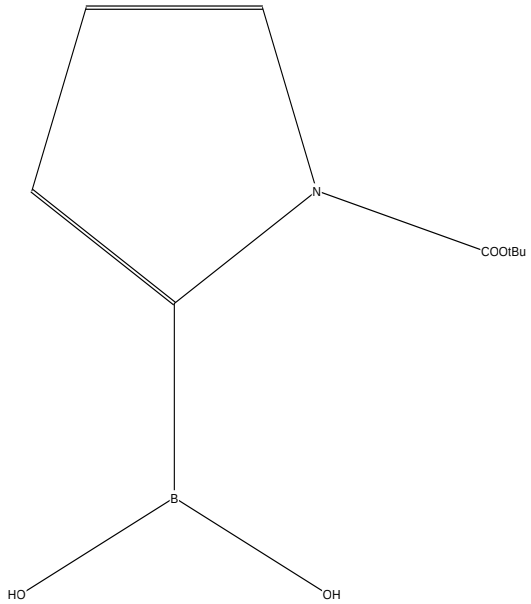
Formula: $C_9 H_{14} B_1 N_1 O_4$

Compound Name: t-Butyl 2-(dihydroxyboryl)pyrrole-1-carboxylate

Synonym: (1-(t-butoxycarbonyl)-1H-pyrrol-2-yl)boronic acid

Space Group:	Pbca	***Cell:***	***a***	12.958(0)	***b***	9.645(0)	***c***	17.592(0)
Space Group No.:	61	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.06 ***Temperature(K):*** 150 ***Density(g/cm³):*** 1.275



NIQYUI

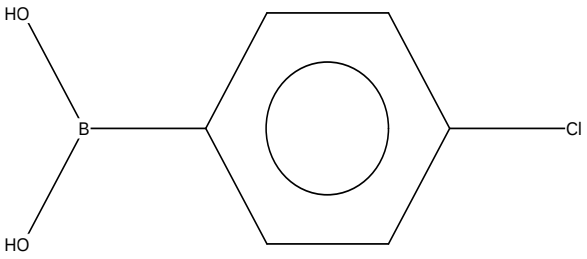
Reference: M.R.Shimpi, N.SeethaLekshmi, V.R.Pedireddi (2007)
Cryst.Growth Des. ,**7,**1958

Formula: $C_6 H_6 B_1 Cl_1 O_2$

Compound Name: 4-Chlorophenylboronic acid

Space Group:	P21/c	***Cell:***	***a***	14.678(4)	***b***	5.951(2)	***c***	9.030(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	105.72(4)	γ	90.00

R-Factor (%): 3.85 ***Temperature(K):*** 133 ***Density(g/cm³):*** 1.368



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NIQZAP

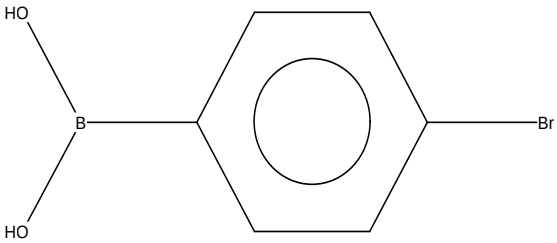
Reference: M.R.Shimpi, N.SeethaLekshmi, V.R.Pedireddi (2007) *Cryst.Growth Des.* ,**7,**1958

Formula: $C_6 H_6 B_1 Br_1 O_2$,0.75($H_2 O_1$)

Compound Name: 4-Bromophenylboronic acid hydrate

Space Group:	Ibam	***Cell:***	***a***	14.427(9)	***b***	24.973(1)	***c***	9.901(6)
Space Group No.:	72	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 7.28 ***Temperature(K):*** 133 ***Density(g/cm³):*** 1.596



H_2O

NIQZET

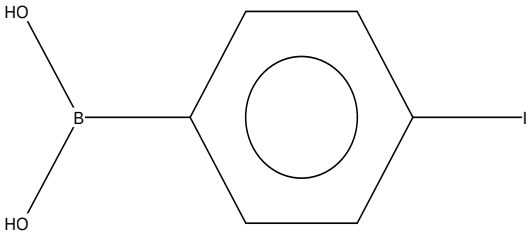
Reference: M.R.Shimpi, N.SeethaLekshmi, V.R.Pedireddi (2007) *Cryst.Growth Des.* ,**7,**1958

Formula: $C_6 H_6 B_1 I_1 O_2$,0.5($H_2 O_1$)

Compound Name: 4-Iodophenylboronic acid hemihydrate

Space Group:	Ibam	***Cell:***	***a***	15.157(8)	***b***	24.837(1)	***c***	9.872(5)
Space Group No.:	72	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 5.63 ***Temperature(K):*** 133 ***Density(g/cm³):*** 1.836



H_2O

NIQZET01

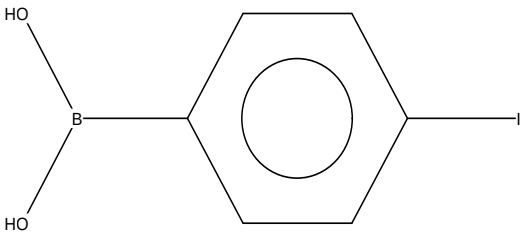
Reference: M.R.Shimpi, N.SeethaLekshmi, V.R.Pedireddi (2007) *Cryst.Growth Des.* ,**7,**1958

Formula: $C_6 H_6 B_1 I_1 O_2$,0.5($H_2 O_1$)

Compound Name: 4-Iodophenylboronic acid hemihydrate

Space Group:	Ibam	***Cell:***	***a***	19.280(6)	***b***	18.881(6)	***c***	9.854(3)
Space Group No.:	72	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 5.25 ***Temperature(K):*** 133 ***Density(g/cm³):*** 1.902



H_2O

NITFOL

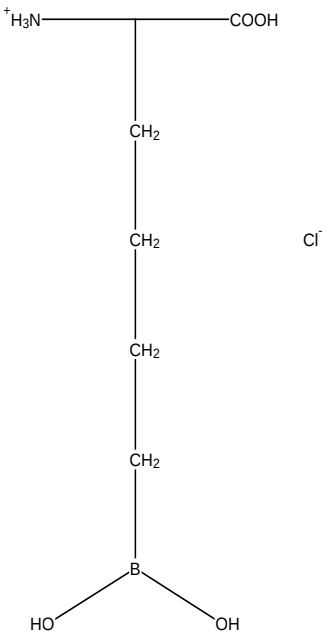
Reference: R.Baggio, D.Elbaum, Z.F.Kanyo, P.J.Carroll, R.C.Cavalli, D.E.Ash, D.W.Christianson (1997) *J.Am.Chem.Soc.* ,**119,**8107

Formula: $C_6 H_{15} B_1 N_1 O_4$ $^{1+}$,Cl_1 $^{1-}$

Compound Name: 2(S)-Amino-6-boronohexanoic acid hydrochloride

Space Group:	P212121	***Cell:***	***a***	9.914(2)	***b***	20.213(2)	***c***	5.180(0)
Space Group No.:	19	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 7.68 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.353



Search: search4 (Mon May 01 12:48:32 2017): Hits 161-164

NUGRUE

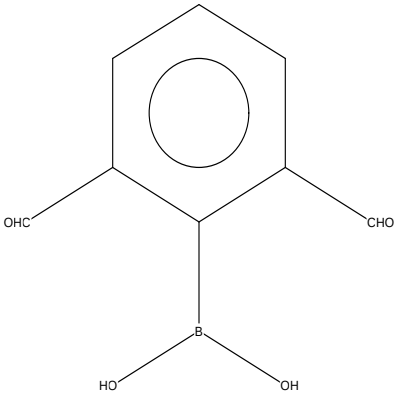
Reference: A.Adamczyk-Wozniak, K.Ejsmont, B.Gierczyk, E.Kaczorowska, A.Matuszewska, G.Schroeder, A.Sporzynski, B.Zarychta (2015) *J.Organomet.Chem.* ,**788,**36

Formula: $C_8 H_7 B_1 O_4,H_2 O_1$

Compound Name: (2,6-Diformylphenyl)boronic acid monohydrate

Space Group:	P21/n	***Cell:***	***a***	6.911(0)	***b***	11.554(0)	***c***	11.415(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	93.02(0)	γ	90.00

R-Factor (%): 2.98 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.430



H_2O

NUPQIZ

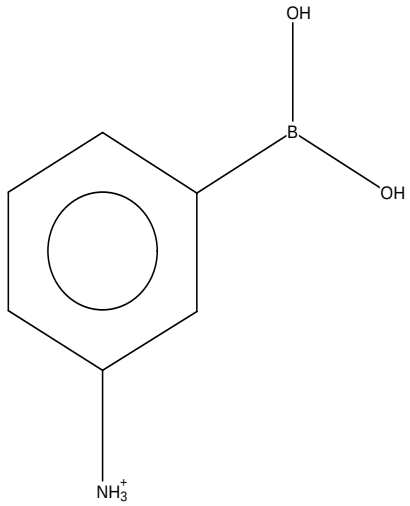
Reference: A.Vega, R.Luna, H.Tlahuext, H.Hopfl (2010) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**66,**o1035

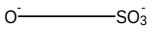
Formula: $C_6 H_9 B_1 N_1 O_2\ ^{1+},0.5(O_4 S_1\ ^{2-})$

Compound Name: 3-(Dihydroxyboryl)anilinium hemisulfate

Space Group:	P21/c	***Cell:***	***a***	5.359(0)	***b***	15.695(3)	***c***	20.489(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	101.42(0)	γ	90.00

R-Factor (%): 7.77 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.463





NUPZAB

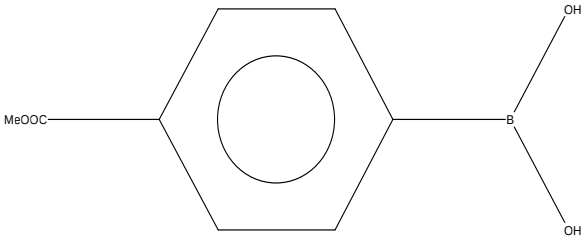
Reference: K.J.Flanagan, M.O.Senge (2015) *Acta Crystallogr.,Sect.E:Cryst.Commun.* ,**71,**1151

Formula: $C_8 H_9 B_1 O_4$

Compound Name: (4-(methoxycarbonyl)phenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	11.245(0)	***b***	12.067(0)	***c***	6.860(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	105.12(0)	γ	90.00

R-Factor (%): 3.23 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.330



NUSPIB

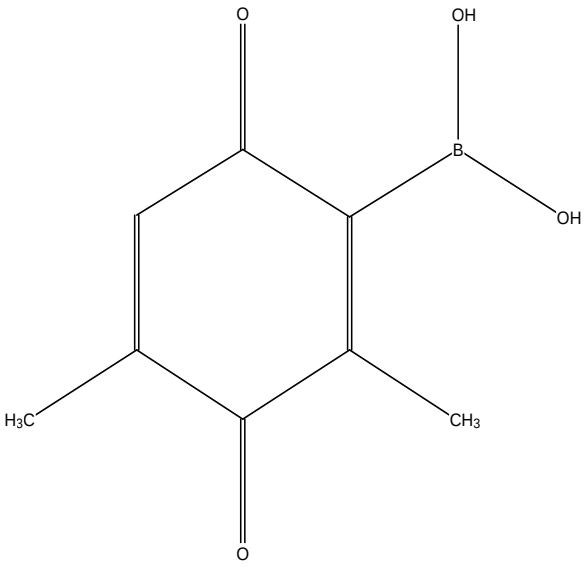
Reference: M.Veguillas, M.C.Redondo, I.Garcia, M.Ribagorda, M.C.Carreno (2010) *Chem.-Eur.J.* ,**16,**3707

Formula: $C_8 H_9 B_1 O_4$

Compound Name: (2,4-Dimethyl-3,6-dioxocyclohexa-1,4-dien-1-yl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	8.197(0)	***b***	17.978(1)	***c***	5.597(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	95.24(0)	γ	90.00

R-Factor (%): 3.78 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.455



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OCAJUY

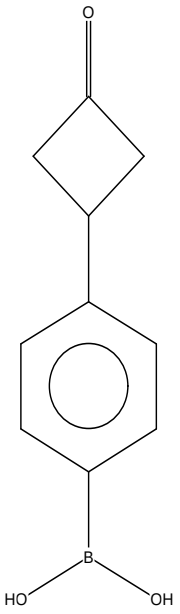
Reference: Jem-Mau Lo, Shyh-Ming Chen, Mei-Hsun Chen, Yu-Jen Chen, Fen-Ling Liao, Tian-Huey Lu (2004) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**60,**o1851

Formula: $C_{10}\,H_{11}\,B_1\,O_3$

Compound Name: 3-(4-Dihyroxyborylphenyl)cyclobutanone

Space Group:	P21/c	***Cell:***	***a***	11.465(1)	***b***	9.832(0)	***c***	8.367(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	98.55(0)	γ	90.00

R-Factor (%): 3.41 ***Temperature(K):*** 294 ***Density(g/cm^3):*** 1.353



OCEFAF

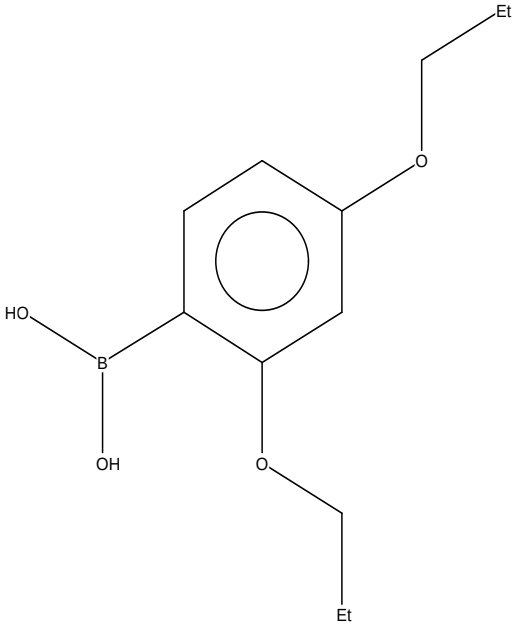
Reference: M.Dabrowski, K.Durka, S.Lulinski, J.Serwatowski (2011) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**67,**o3455

Formula: $C_{12}\,H_{19}\,B_1\,O_4$

Compound Name: (2,4-Dipropoxyphenyl)boronic acid

Space Group:	P-1	***Cell:***	***a***	7.963(0)	***b***	8.801(1)	***c***	9.318(1)
Space Group No.:	2	***(Å,°)***	α	101.59(1)	β	91.92(1)	γ	90.83(1)

R-Factor (%): 3.26 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.237



OGAYUR

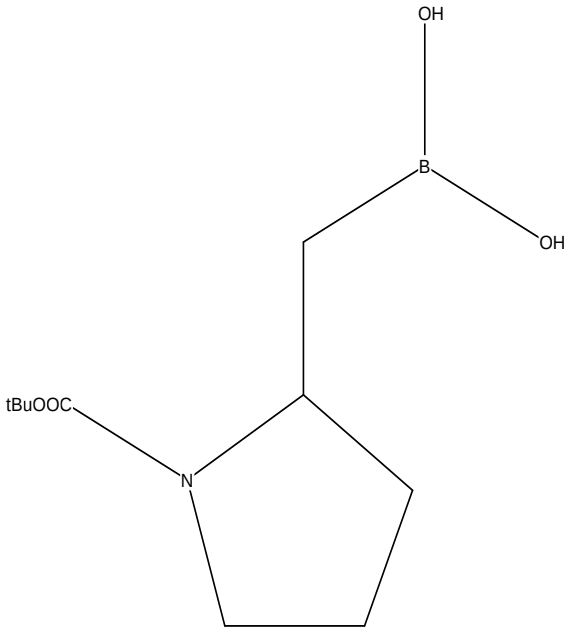
Reference: K.Arnold, A.S.Batsanov, B.Davies, C.Grosjean, T.Schutz, A.Whiting, K.Zawatzky (2008) *Chem.Commun.* ,3879

Formula: $C_{10}\,H_{20}\,B_1\,N_1\,O_4$

Compound Name: (S)-N-(1,1-Dimethylethoxycarbonyl)-(pyrrolidin-2-yl)methylboronic acid

Space Group:	P212121	***Cell:***	***a***	9.338(0)	***b***	11.500(1)	***c***	12.064(1)
Space Group No.:	19	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.06 ***Temperature(K):*** 120 ***Density(g/cm^3):*** 1.174



OHAZOO

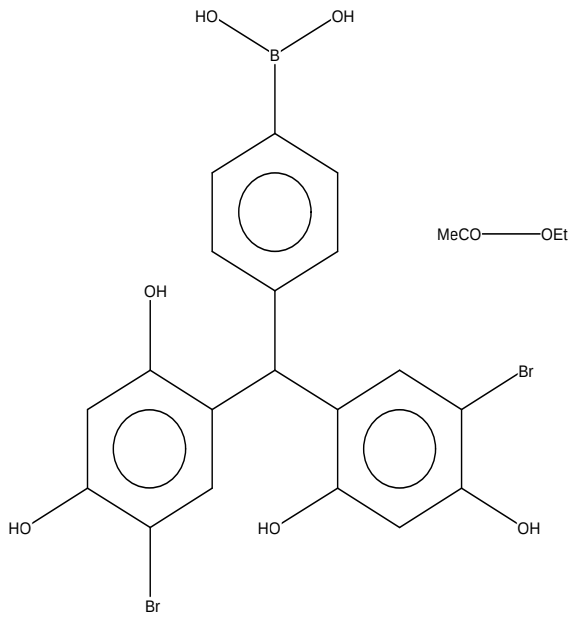
Reference: D.R.Billodeaux, P.T.Lewis, R.M.Strongin, F.R.Fronczek (2015) *CSD Communication(Private Communication)* ,

Formula: $C_{19}\,H_{15}\,B_1\,Br_2\,O_6{.}2.5(C_4\,H_8\,O_2)$

Compound Name: (4-(bis(5-bromo-2,4-dihydroxyphenyl)methyl)phenyl)boronic acid ethyl acetate solvate

Space Group:	C2/c	***Cell:***	***a***	13.781(3)	***b***	18.780(4)	***c***	25.035(5)
Space Group No.:	15	***(Å,°)***	α	90.00	β	95.91(3)	γ	90.00

R-Factor (%): 10.20 ***Temperature(K):*** 180 ***Density(g/cm^3):*** 1.505



Search: search4 (Mon May 01 12:48:32 2017): Hits 169-172

OLEXAF

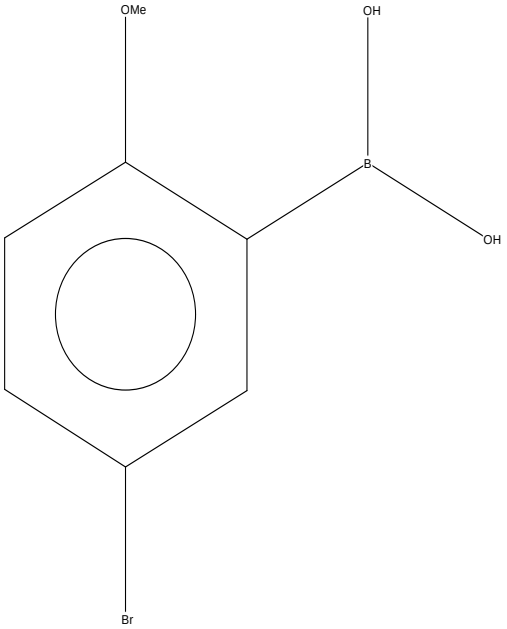
Reference: Di Qiu, Fanyang Mo, Zhitong Zheng, Yan Zhang, Jianbo Wang (2010) *Org.Lett.* ,**12,**5474

Formula: $C_7 H_8 B_1 Br_1 O_3$

Compound Name: (5-Bromo-2-methoxyphenyl)boronic acid

Space Group:	P-1	***Cell:***	***a***	7.606(1)	***b***	8.082(1)	***c***	8.250(1)
Space Group No.:	2	***(Å,°)***	α	68.67(3)	β	69.49(3)	γ	85.84(3)

R-Factor (%): 8.65 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.736



OLEXOT

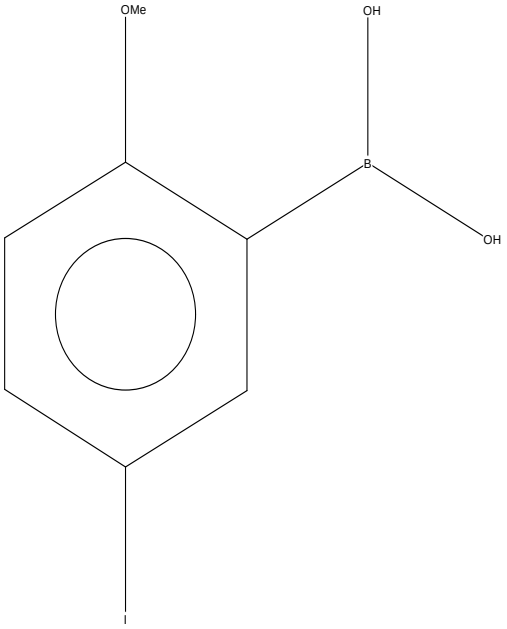
Reference: Di Qiu, Fanyang Mo, Zhitong Zheng, Yan Zhang, Jianbo Wang (2010) *Org.Lett.* ,**12,**5474

Formula: $C_7 H_8 B_1 I_1 O_3$

Compound Name: (5-Iodo-2-methoxyphenyl)boronic acid

Space Group:	P-1	***Cell:***	***a***	7.741(1)	***b***	8.062(1)	***c***	8.440(1)
Space Group No.:	2	***(Å,°)***	α	69.97(3)	β	72.46(3)	γ	86.33(3)

R-Factor (%): 5.45 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.958



OLIDOC

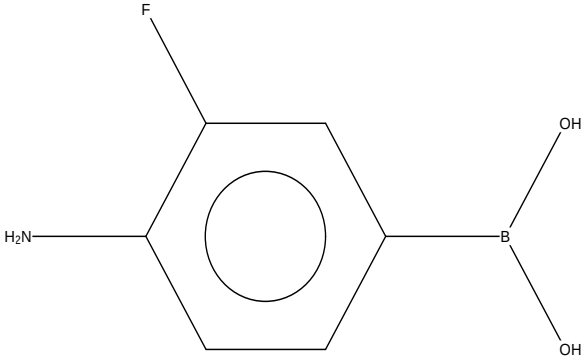
Reference: S.Das, V.L.Alexeev, A.C.Sharma, S.J.Geib, S.A.Asher (2003) *Tetrahedron Lett.* ,**44,**7719

Formula: $C_6 H_7 B_1 F_1 N_1 O_2$

Compound Name: 4-Amino-3-fluorophenylboronic acid

Space Group:	P21/c	***Cell:***	***a***	15.370(6)	***b***	5.247(1)	***c***	9.370(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	105.83(0)	γ	90.00

R-Factor (%): 4.94 ***Temperature(K):*** 150 ***Density(g/cm³):*** 1.416



OQUJUG

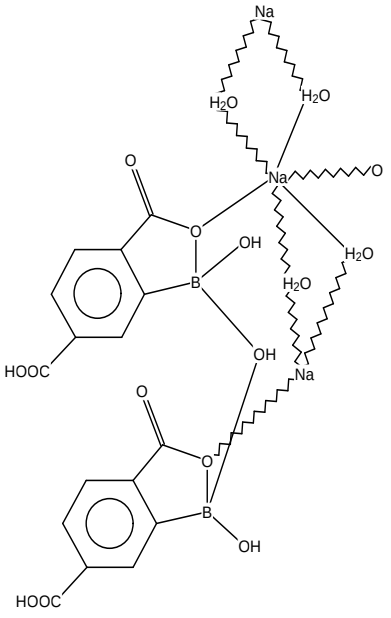
Reference: S.Simmons, A.Fratini, V.Benin (2011) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**67,**m123

Formula: $(C_{16} H_{15} B_2 Na_1 O_{13})n$

Compound Name: catena-(bis(μ$_2$-Aqua)-(μ$_2$-bis(6-carboxy-1-hydroxy-3-oxo-1,3-dihydro-2,1-benzoxaborol-1-yl)oxidanium)-sodium)

Space Group:	P-1	***Cell:***	***a***	6.720(0)	***b***	7.112(0)	***c***	19.280(1)
Space Group No.:	2	***(Å,°)***	α	80.06(0)	β	81.80(0)	γ	83.04(0)

R-Factor (%): 4.56 ***Temperature(K):*** 140 ***Density(g/cm³):*** 1.709



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PAQMAX

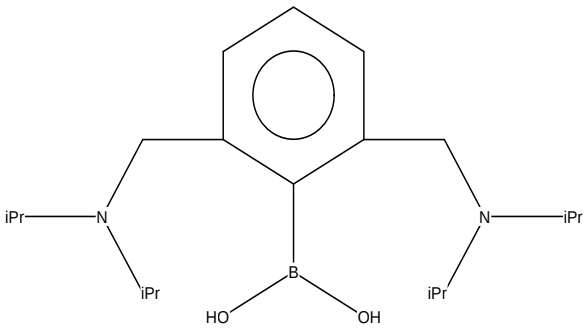
Reference: A.Sakakura, R.Yamashita, T.Ohkubo, M.Akakura, K.Ishihara (2011) *Aust.J.Chem.* ,**64,**1458

Formula: $C_{20}\,H_{37}\,B_1\,N_2\,O_2$

Compound Name: (2,6-bis((diisopropylamino)methyl)phenyl)boronic acid

Space Group:	Pnn2	***Cell:***	***a***	11.198(3)	***b***	11.845(3)	***c***	8.277(2)
Space Group No.:	34	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.87 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.054



PAXSUD

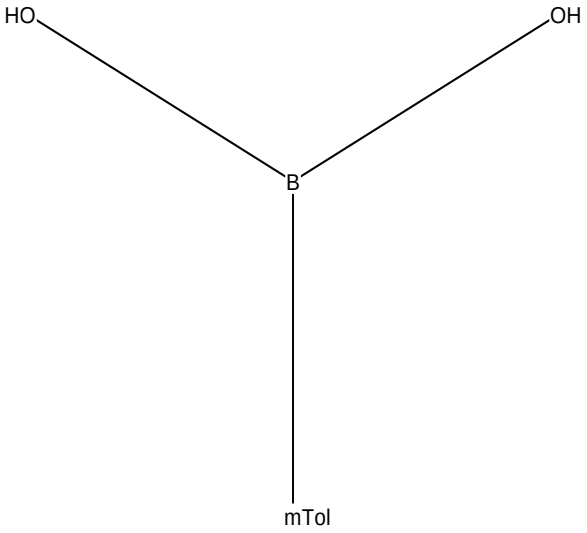
Reference: C.B.Aakeroy, J.Desper, B.Levin, D.J.Salmon (2004) *Trans.Am.Crystallogr.Assoc.* ,**39,**123

Formula: $C_7\,H_9\,B_1\,O_2$

Compound Name: 3-Methylbenzeneboronic acid

Space Group:	P21/c	***Cell:***	***a***	15.063(4)	***b***	5.671(1)	***c***	9.101(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	94.85(0)	γ	90.00

R-Factor (%): 3.87 ***Temperature(K):*** 203 ***Density(g/cm³):*** 1.166



PAXTAK

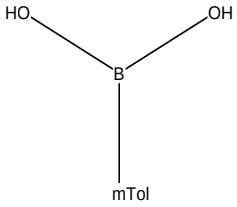
Reference: C.B.Aakeroy, J.Desper, B.Levin, D.J.Salmon (2004) *Trans.Am.Crystallogr.Assoc.* ,**39,**123

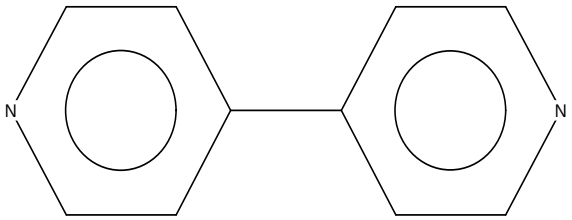
Formula: $C_7\,H_9\,B_1\,O_2,1.5(C_{10}\,H_8\,N_2)$

Compound Name: 3-Methylbenzeneboronic acid sesquikis(4,4'-bipyridine)

Space Group:	C2/c	***Cell:***	***a***	20.266(1)	***b***	9.271(0)	***c***	22.304(1)
Space Group No.:	15	***(Å,°)***	α	90.00	β	113.79(0)	γ	90.00

R-Factor (%): 5.14 ***Temperature(K):*** 163 ***Density(g/cm³):*** 1.283





PAXTEO

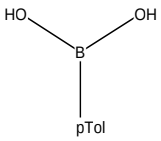
Reference: C.B.Aakeroy, J.Desper, B.Levin, D.J.Salmon (2004) *Trans.Am.Crystallogr.Assoc.* ,**39,**123

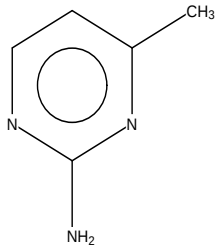
Formula: $C_7\,H_9\,B_1\,O_2,C_5\,H_7\,N_3$

Compound Name: 2-Amino-4-methylpyrimidine 4-methylbenzeneboronic acid

Space Group:	P21/c	***Cell:***	***a***	9.508(1)	***b***	11.939(1)	***c***	11.266(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	102.72(0)	γ	90.00

R-Factor (%): 4.74 ***Temperature(K):*** 203 ***Density(g/cm³):*** 1.305





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PAXTIS

Reference: C.B.Aakeroy, J.Desper, B.Levin, D.J.Salmon (2004) *Trans.Am.Crystallogr.Assoc.* ,**39,**123

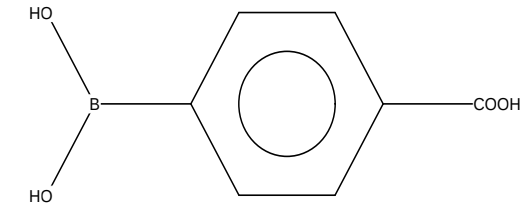
Formula: $C_7 H_7 B_1 O_4$,$C_{10} H_8 N_2$

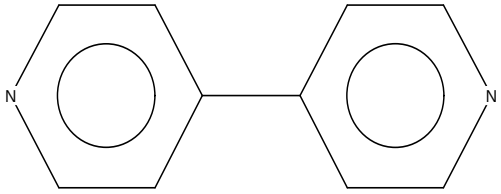
Compound Name: 4-Carboxybenzeneboronic acid 4,4'-bipyridine

Synonym: PDB Chemical Component code: 4CB

Space Group:	P1	***Cell:***	***a*** 3.955(0)	***b*** 8.361(1)	***c*** 11.670(2)
Space Group No.:	1	***(Å,°)***	α 101.61(0)	β 98.91(0)	γ 98.04(0)

R-Factor (%): 4.46 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.455





PAYYAP

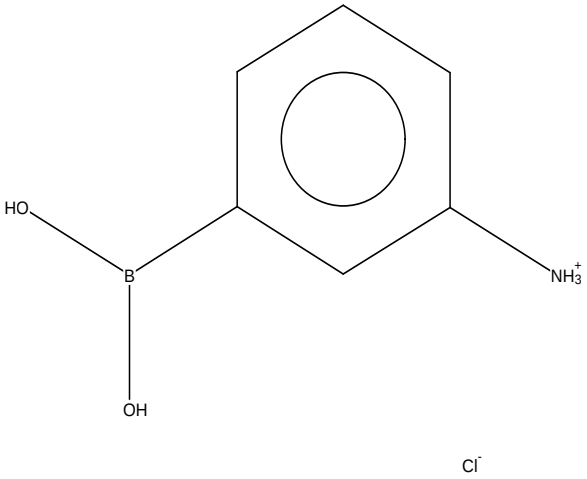
Reference: Hong-Feng Li, Xiang-Yun Wang, Qing-Chuan Yang, Yuan-Fang Liu (1995) *Gaodeng Xuexiao Huaxue Xuebao(Chin.)(Chem.J.Chin.Univ.(Chinese Edition))* , **16,**1841

Formula: $C_6 H_9 B_1 N_1 O_2$ $^{1+}$,Cl_1 $^{1-}$

Compound Name: 3-(Dihydroxyboryl)phenylammonium chloride

Space Group:	P21/c	***Cell:***	***a*** 5.193(3)	***b*** 15.802(14)	***c*** 10.307(8)
Space Group No.:	14	***(Å,°)***	α 90.00	β 102.43(6)	γ 90.00

R-Factor (%): 3.33 ***Temperature(K):*** 295 ***Density(g/cm^3):*** 1.394



PEPNUU

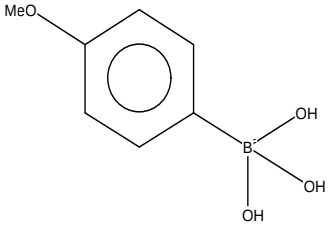
Reference: A.N.Cammidge, V.H.M.Goddard, H.Gopee, N.L.Harrison, D.L.Hughes, C.J.Schubert, B.M.Sutton, G.L.Watts, A.J.Whitehead (2006) *Org.Lett.* ,**8,**4071

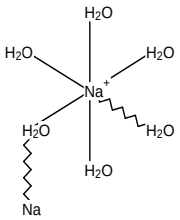
Formula: $(H_{10} Na_1 O_5$ $^{1+})n$,$n(C_7 H_{10} B_1 O_4$ $^{1-})$

Compound Name: catena-($(\mu_2$-aqua)-tetraaqua-sodium (4-methoxyphenyl)boronate)

Space Group:	P212121	***Cell:***	***a*** 6.126(2)	***b*** 7.352(1)	***c*** 29.508(5)
Space Group No.:	19	***(Å,°)***	α 90.00	β 90.00	γ 90.00

R-Factor (%): 3.51 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.409





PEYLOV

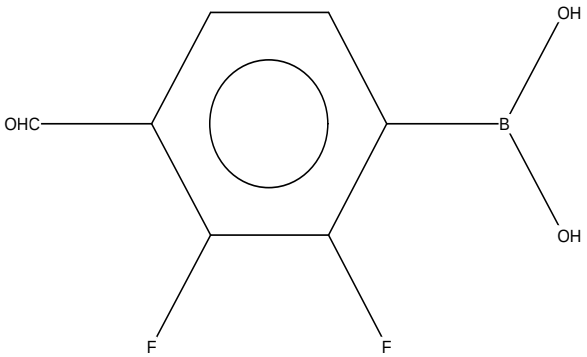
Reference: T.Klis, S.Lulinski, J.Serwatowski (2007) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**63,**o145

Formula: $C_7 H_5 B_1 F_2 O_3$

Compound Name: 2,3-Difluoro-4-formylphenylboronic acid

Space Group:	P21/c	***Cell:***	***a*** 7.915(1)	***b*** 9.853(1)	***c*** 9.814(1)
Space Group No.:	14	***(Å,°)***	α 90.00	β 94.20(1)	γ 90.00

R-Factor (%): 3.87 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.618



Search: search4 (Mon May 01 12:48:32 2017): Hits 181-184

PHBORA

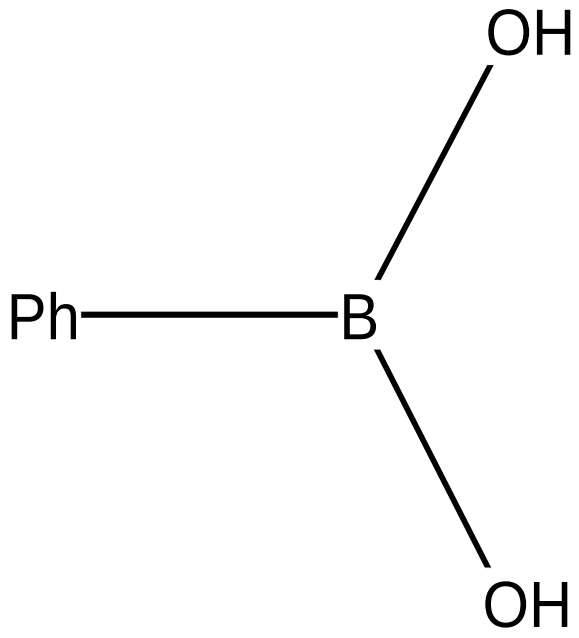
Reference: S.J.Rettig, J.Trotter (1977) *Can.J.Chem.* ,**55,**3071

Formula: $C_6 H_7 B_1 O_2$

Compound Name: Phenylboronic acid

Space Group:	Iba2	***Cell:***	***a***	17.905(0)	***b***	15.326(0)	***c***	9.811(0)
Space Group No.:	45	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.10 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.203



PHBORA01

Reference: M.K.Cyranski, A.Jezierska, P.Klimentowska, J.J.Panek, A.Sporzynski (2008) *J.Phys.Org.Chem.* ,**21,**472

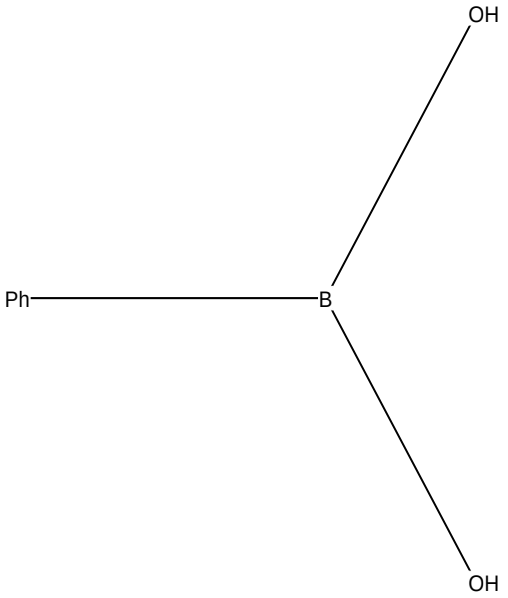
Formula: $C_6 H_7 B_1 O_2$

Compound Name: phenylboronic acid

Synonym: PDB Chemical Component code: PBC

Space Group:	Iba2	***Cell:***	***a***	15.095(3)	***b***	17.867(4)	***c***	9.729(1)
Space Group No.:	45	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 2.86 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.235



PICJOB

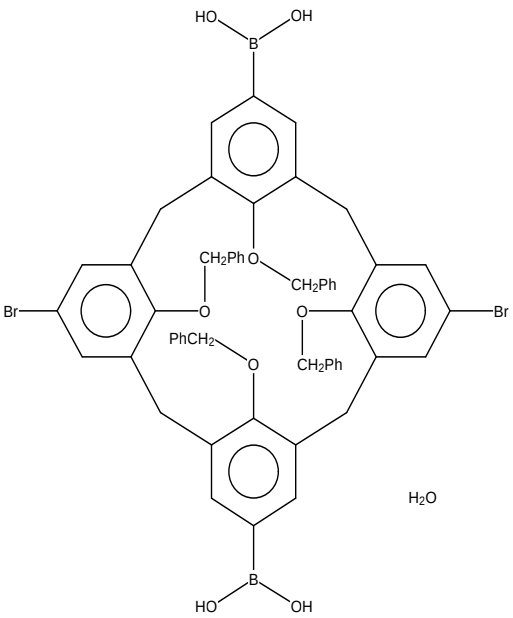
Reference: R.M.McKinlay, J.L.Atwood (2007) *Angew.Chem.,Int.Ed.* , **46,**2394

Formula: $C_{56} H_{48} B_2 Br_2 O_8$,0.83($H_2 O_1$)

Compound Name: (5,17-Dibromo-25,26,27,28-tetrakis(benzyloxy)calix(4)arene-11,23-diyl) diboronic acid hydrate

Space Group:	R-3	***Cell:***	***a***	27.437(2)	***b***	27.437(2)	***c***	34.726(4)
Space Group No.:	148	***(Å,°)***	α	90.00	β	90.00	γ	120.00

R-Factor (%): 9.38 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.380



PUBLEE

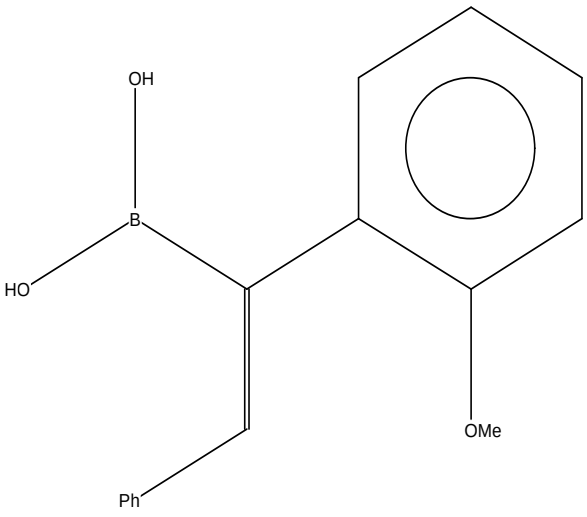
Reference: T.Tricotet, P.Fleming, J.Cotter, A.-M.L.Hogan, C.Strohmann, V.H.Gessner, D.F.O'Shea (2009) *J.Am.Chem.Soc.* ,**131,** 3142

Formula: $C_{15} H_{15} B_1 O_3$

Compound Name: (E)-(1-(2-Methoxyphenyl)-2-phenylvinyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	16.132(4)	***b***	20.076(5)	***c***	8.573(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	99.49(0)	γ	90.00

R-Factor (%): 4.21 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.233



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QACYEA

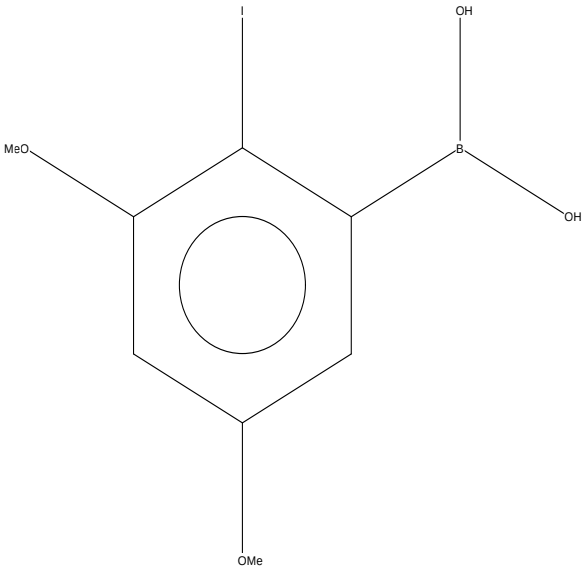
Reference: R.M.Al-Zoubi, D.G.Hall (2010) *Org.Lett.* ,**12,**2480

Formula: $C_8 H_{10} B_1 I_1 O_4$

Compound Name: (2-Iodo-3,5-dimethoxyphenyl)boronic acid

Space Group:	Pbca	***Cell:***	***a*** 9.172(0)	***b*** 14.092(0)	***c*** 16.179(0)
Space Group No.:	61	***(Å,°)***	α 90.00	β 90.00	γ 90.00

R-Factor (%): 1.79 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.956



QACYIE

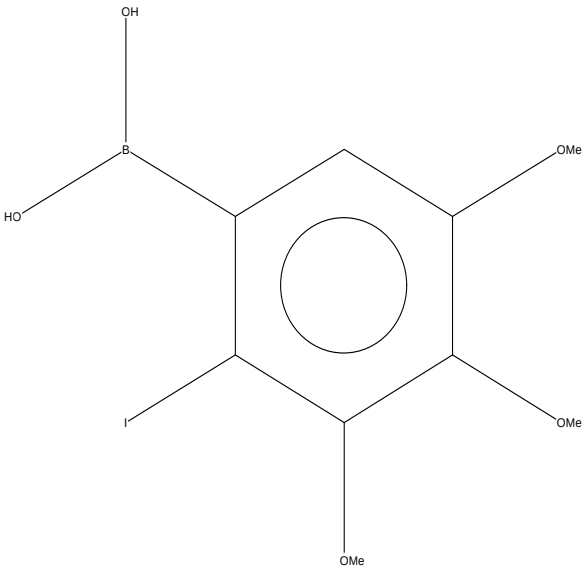
Reference: R.M.Al-Zoubi, D.G.Hall (2010) *Org.Lett.* ,**12,**2480

Formula: $C_9 H_{12} B_1 I_1 O_5$

Compound Name: (2-Iodo-3,4,5-trimethoxyphenyl)boronic acid

Space Group:	P-1	***Cell:***	***a*** 7.318(0)	***b*** 9.705(1)	***c*** 9.749(1)
Space Group No.:	2	***(Å,°)***	α 60.44(0)	β 77.03(0)	γ 86.28(0)

R-Factor (%): 1.62 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.915



QAQCIW

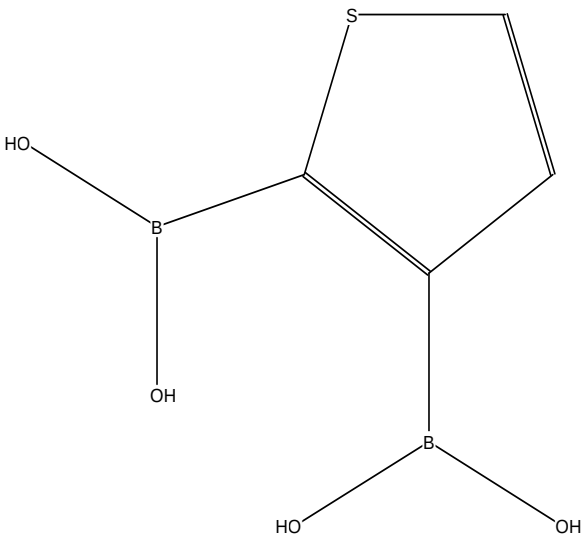
Reference: E.Borowska, K.Durka, S.Lulinski, J.Serwatowski, K.Wozniak (2012) *Eur.J.Org.Chem.* ,2208

Formula: $C_4 H_6 B_2 O_4 S_1.1.5(H_2 O_1)$

Compound Name: Thiene-2,3-diyldiboronic acid sesquihydrate

Space Group:	C2/c	***Cell:***	***a*** 11.088(0)	***b*** 11.845(0)	***c*** 13.283(0)
Space Group No.:	15	***(Å,°)***	α 90.00	β 104.72(0)	γ 90.00

R-Factor (%): 3.00 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.565



H_2O

QIWRIZ

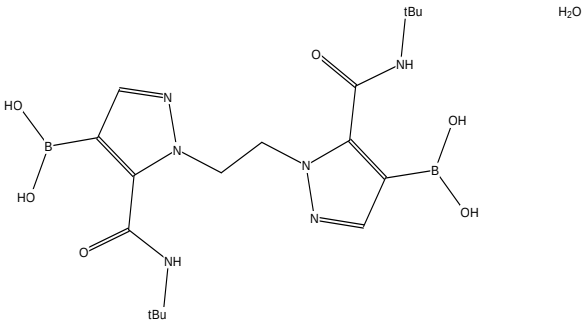
Reference: K.Durka, A.Gorska, T.Klis, J.Serwatowski, K.Wozniak (2014) *Tetrahedron Lett.* ,**55,**1234

Formula: $C_{18} H_{30} B_2 N_6 O_6.H_2 O_1$

Compound Name: (ethane-1,2-diylbis(5-(t-butylcarbamoyl)-1H-pyrazole-1,4-diyl))diboronic acid monohydrate

Space Group:	P-1	***Cell:***	***a*** 9.968(0)	***b*** 10.600(0)	***c*** 13.071(0)
Space Group No.:	2	***(Å,°)***	α 94.61(0)	β 106.91(0)	γ 110.02(0)

R-Factor (%): 4.42 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.273



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QIXCEH

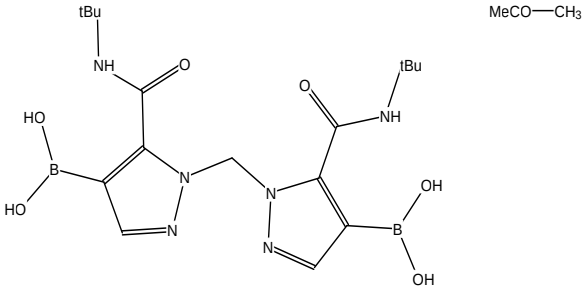
Reference: K.Durka, A.Gorska, T.Klis, J.Serwatowski, K.Wozniak (2014) *Tetrahedron Lett.* ,**55,**1234

Formula: $C_{17}H_{28}B_2N_6O_6,C_3H_6O_1$

Compound Name: (methylenebis(5-(t-butylcarbamoyl)-1H-pyrazole-1,4-diyl))diboronic acid acetone solvate

Space Group:	P21/c	***Cell:***	***a***	9.980(0)	***b***	17.865(0)	***c***	15.370(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	92.33(0)	γ	90.00

R-Factor (%): 5.09 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.194



QUSPAW

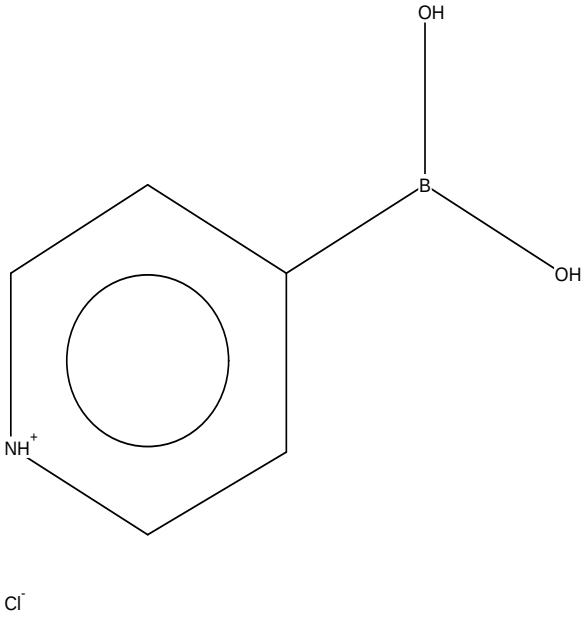
Reference: J.J.Campos-Gaxiola, A.Vega-Paz, P.Roman-Bravo, H.Hopfl, M.Sanchez-Vazquez (2010) *Cryst.Growth Des.* ,**10,**3182

Formula: $C_5H_7B_1N_1O_2\ ^{1+},Cl_1\ ^{1-}$

Compound Name: 4-Pyridineboronic acid hydrochloride

Space Group:	Pc	***Cell:***	***a***	6.196(0)	***b***	5.328(0)	***c***	11.357(1)
Space Group No.:	7	***(Å,°)***	α	90.00	β	105.13(0)	γ	90.00

R-Factor (%): 3.27 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.463



RAPZUF

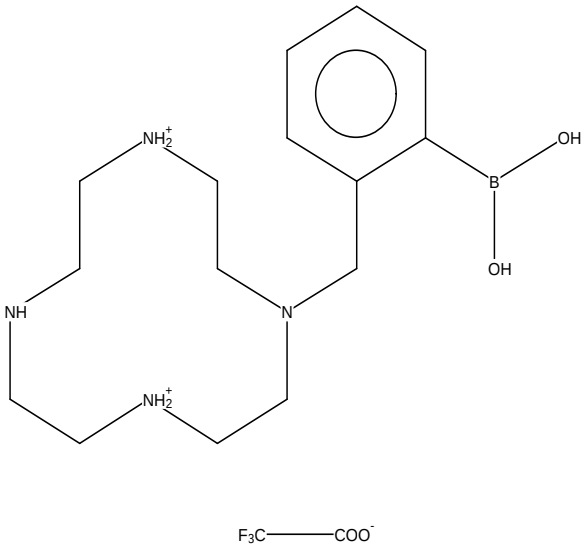
Reference: M.Kitamura, T.Suzuki, R.Abe, T.Ueno, S.Aoki (2011) *Inorg.Chem.* ,**50,**11568

Formula: $C_{15}H_{29}B_1N_4O_2\ ^{2+},2(C_2F_3O_2\ ^{1-})$

Compound Name: 4-(2-(Dihydroxyboryl)benzyl)-4,10-diaza-1,7-diazoniacyclododecane bis(trifluoroacetate)

Space Group:	P21/c	***Cell:***	***a***	9.392(5)	***b***	12.179(7)	***c***	21.872(12)
Space Group No.:	14	***(Å,°)***	α	90.00	β	94.89(0)	γ	90.00

R-Factor (%): 7.24 ***Temperature(K):*** 123 ***Density(g/cm³):*** 1.424



REHDOY

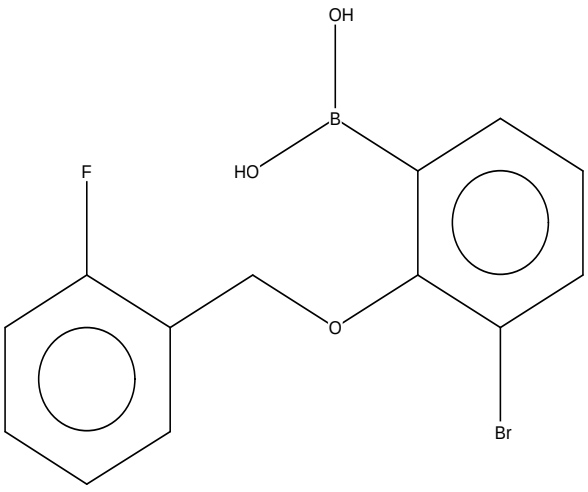
Reference: J.Serwatowski, T.Klis, K.Kacprzak (2006) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**62,**o1308

Formula: $C_{13}H_{11}B_1Br_1F_1O_3$

Compound Name: 3-Bromo-2-(2-fluorobenzyloxy)phenylboronic acid

Space Group:	P-1	***Cell:***	***a***	4.023(0)	***b***	15.278(2)	***c***	21.685(3)
Space Group No.:	2	***(Å,°)***	α	105.08(1)	β	90.03(1)	γ	92.09(1)

R-Factor (%): 4.86 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.678



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ROBJAV

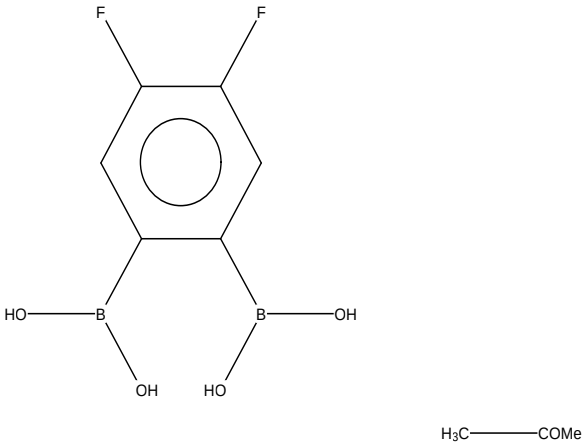
Reference: K.Durka, S.Lulinski, J.Serwatowski, K.Wozniak (2014) *Organometallics* ,**33,**1608

Formula: $2(C_6 H_6 B_2 F_2 O_4),C_3 H_6 O_1$

Compound Name: (4,5-Difluoro-1,2-phenylene)diboronic acid acetone solvate

Space Group:	P21/n	***Cell:***	***a***	12.704(0)	***b***	11.756(0)	***c***	13.153(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	94.28(0)	γ	90.00

R-Factor (%): 4.73 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.565



ROBJEZ

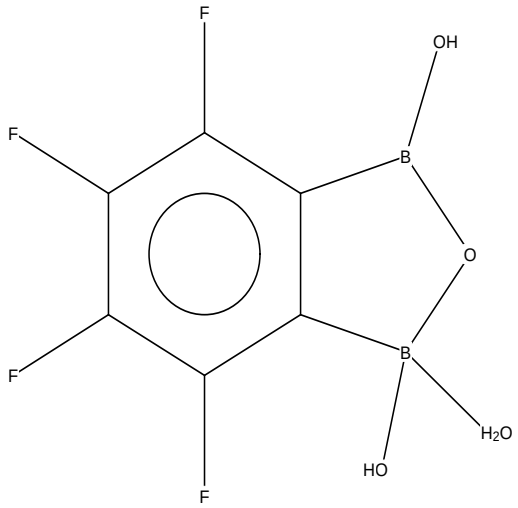
Reference: K.Durka, S.Lulinski, J.Serwatowski, K.Wozniak (2014) *Organometallics* ,**33,**1608

Formula: $C_6 H_4 B_2 F_4 O_4,3(H_2 O_1)$

Compound Name: 3-Aqua-4,5,6,7-tetrafluoro-2,1,3-benzoxadiborole-1,3-diol trihydrate

Space Group:	P-1	***Cell:***	***a***	4.406(0)	***b***	10.555(0)	***c***	14.046(0)
Space Group No.:	2	***(Å,°)***	α	108.89(0)	β	93.46(0)	γ	99.73(0)

R-Factor (%): 3.50 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.603



H_2O

ROBJID

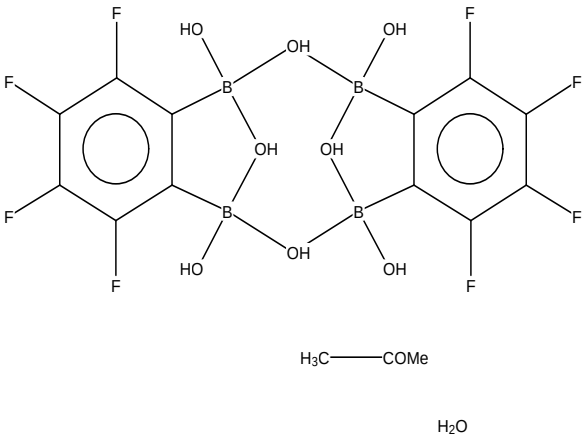
Reference: K.Durka, S.Lulinski, J.Serwatowski, K.Wozniak (2014) *Organometallics* ,**33,**1608

Formula: $C_{12} H_8 B_4 F_8 O_8,C_3 H_6 O_1,2(H_2 O_1)$

Compound Name: 1,2,3,4,8,9,10,11-Octafluoro-5,14:7,12-diepoxydibenzo[c,h][1,6,2,5,7,10]dioxatetraborecine acetone solvate dihydrate

Space Group:	P21/c	***Cell:***	***a***	7.026(1)	***b***	10.811(2)	***c***	28.360(6)
Space Group No.:	14	***(Å,°)***	α	90.00	β	92.29(1)	γ	90.00

R-Factor (%): 9.64 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.757



H_2O

ROGKUU

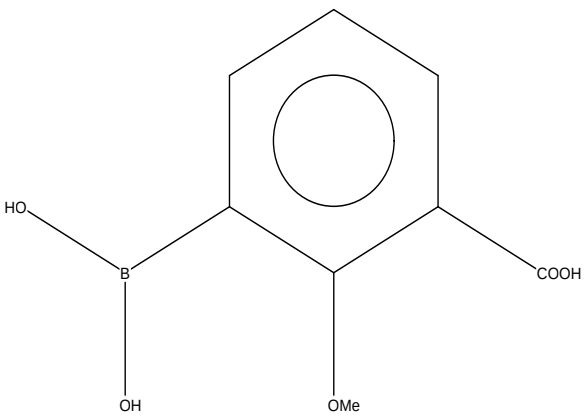
Reference: S.Lulinski (2008) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**64,**o1963

Formula: $C_8 H_9 B_1 O_5$

Compound Name: 3-carboxy-2-methoxyphenylboronic acid

Space Group:	P-1	***Cell:***	***a***	4.845(0)	***b***	7.756(0)	***c***	12.106(0)
Space Group No.:	2	***(Å,°)***	α	79.48(0)	β	79.58(0)	γ	76.12(0)

R-Factor (%): 3.50 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.514



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ROGMEF

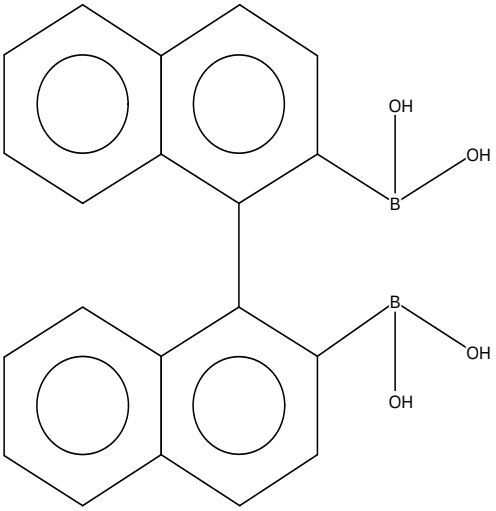
Reference: B.Schilling, V.Kaiser, D.E.Kaufmann (1997) *Chem.Ber.* , **130,**923

Formula: $C_{20}\,H_{16}\,B_2\,O_4$,2($C_4\,H_{10}\,O_1$)

Compound Name: 1,1'-Binaphthyl-2,2'-diboronic acid diethyl ether solvate

Space Group:	P21/c	***Cell:***	***a***	16.395(2)	***b***	9.200(3)	***c***	19.300(4)
Space Group No.:	14	***(Å,°)***	α	90.00	β	100.25(3)	γ	90.00

R-Factor (%): 8.07 ***Temperature(K):*** 210 ***Density(g/cm³):*** 1.137



ROKCAX

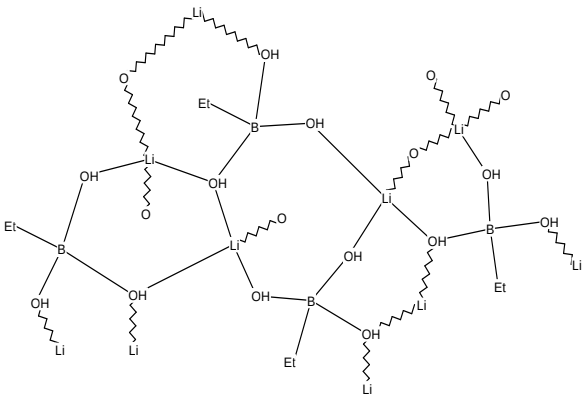
Reference: D.A.Aubry, G.G.Stanley, F.R.Fronczek (2014) *CSD Communication(Private Communication)* ,

Formula: $(C_8\,H_{32}\,B_4\,Li_4\,O_{12})n$

Compound Name: catena-[tetrakis(μ$_4$-ethyl(trihydroxy)borate)-tetra-lithium]

Space Group:	P212121	***Cell:***	***a***	5.105(0)	***b***	17.464(1)	***c***	21.706(2)
Space Group No.:	19	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.79 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.343



ROKJUX

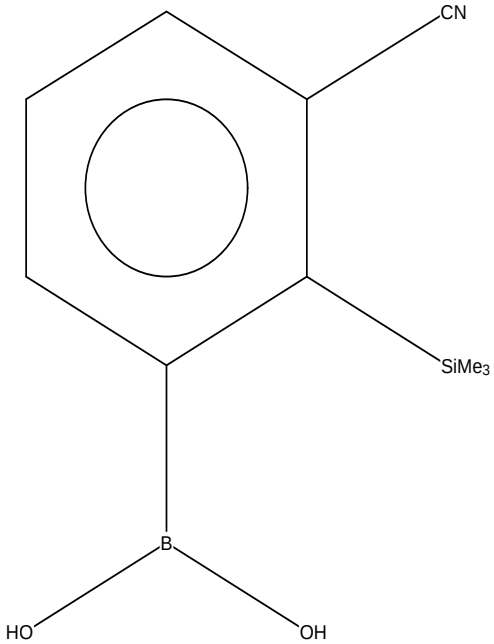
Reference: S.Lulinski, K.Zajac (2008) *J.Org.Chem.* , **73,**7785

Formula: $C_{10}\,H_{14}\,B_1\,N_1\,O_2\,Si_1$

Compound Name: 3-Cyano-2-trimethylsilylphenylboronic acid

Space Group:	I2/a	***Cell:***	***a***	23.951(5)	***b***	8.511(1)	***c***	23.986(13)
Space Group No.:	15	***(Å,°)***	α	90.00	β	91.92(3)	γ	90.00

R-Factor (%): 6.78 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.191



RONLIP

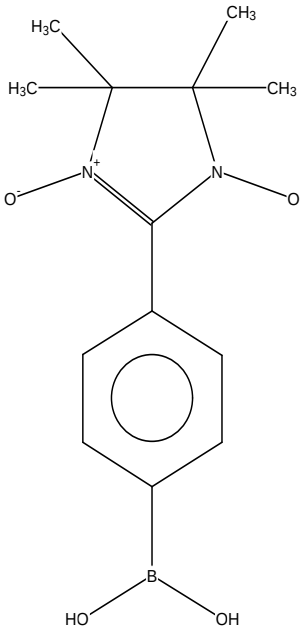
Reference: T.Akita, K.Kobayashi (1997) *Adv.Mater.* , **9,**346

Formula: $C_{13}\,H_{18}\,B_1\,N_2\,O_4$

Compound Name: 2-(4'-Dihydroxyborylphenyl)-4,4,5,5-tetramethylimidazoline-3-oxide 1-oxyl radical

Space Group:	P21/n	***Cell:***	***a***	10.503(3)	***b***	20.882(4)	***c***	6.434(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	90.31(2)	γ	90.00

R-Factor (%): 4.80 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.304



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RORLUH

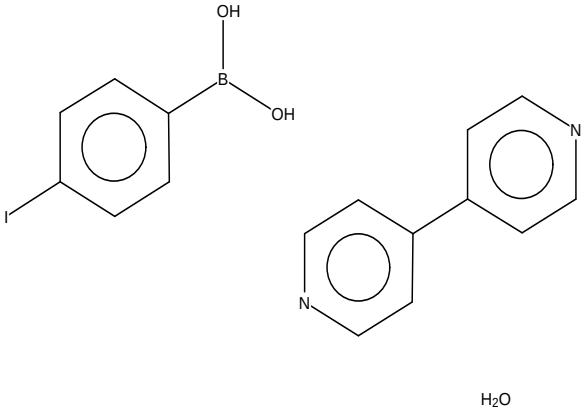
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 I_1 O_2$,$C_{10} H_8 N_2$,$H_2 O_1$

Compound Name: (4-Iodophenyl)boronic acid 4,4'-bipyridine monohydrate

Space Group:	P21/n	***Cell:***	***a***	13.251(5)	***b***	6.858(3)	***c***	18.594(8)
Space Group No.:	14	***(Å,°)***	α	90.00	β	103.50(7)	γ	90.00

R-Factor (%): 3.95 ***Temperature(K):*** 133 ***Density(g/cm³):*** 1.706



H_2O

RORMAO

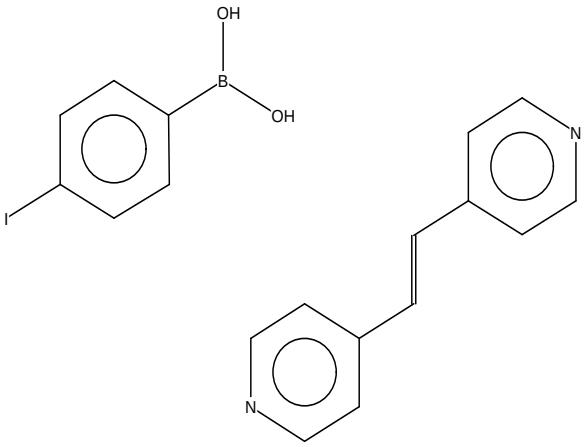
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 I_1 O_2$,$1.5(C_{12} H_{10} N_2)$

Compound Name: (4-Iodophenyl)boronic acid sesquikis(trans-1,2-bis(4-pyridyl)ethene)

Space Group:	P-1	***Cell:***	***a***	10.129(4)	***b***	10.900(4)	***c***	12.521(4)
Space Group No.:	2	***(Å,°)***	α	69.96(0)	β	66.85(0)	γ	70.21(0)

R-Factor (%): 5.49 ***Temperature(K):*** 298 ***Density(g/cm³):*** 1.492



RORMES

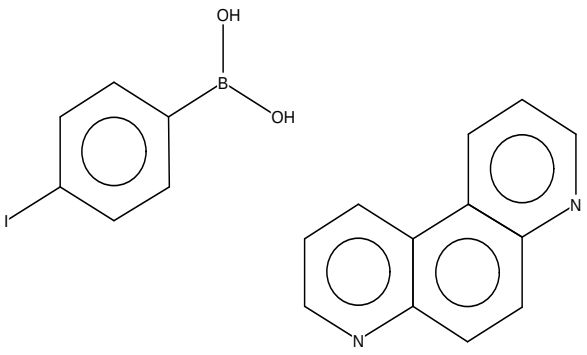
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 I_1 O_2$,$0.5(C_{12} H_8 N_2)$

Compound Name: (4-Iodophenyl)boronic acid hemikis(4,7-phenanthroline)

Space Group:	P21/c	***Cell:***	***a***	7.202(2)	***b***	34.347(8)	***c***	21.339(5)
Space Group No.:	14	***(Å,°)***	α	90.00	β	105.66(0)	γ	90.00

R-Factor (%): 4.20 ***Temperature(K):*** 298 ***Density(g/cm³):*** 1.766



RORMIW

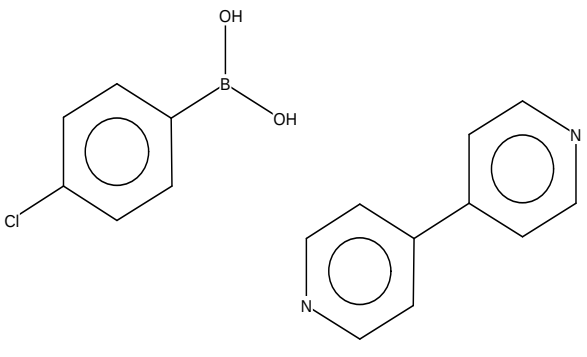
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 Cl_1 O_2$,$C_{10} H_8 N_2$,$H_2 O_1$

Compound Name: (4-Chlorophenyl)boronic acid 4,4'-bipyridine monohydrate

Space Group:	P21/n	***Cell:***	***a***	12.606(5)	***b***	6.878(3)	***c***	18.873(8)
Space Group No.:	14	***(Å,°)***	α	90.00	β	102.79(0)	γ	90.00

R-Factor (%): 5.66 ***Temperature(K):*** 133 ***Density(g/cm³):*** 1.376



H_2O

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RORMOC

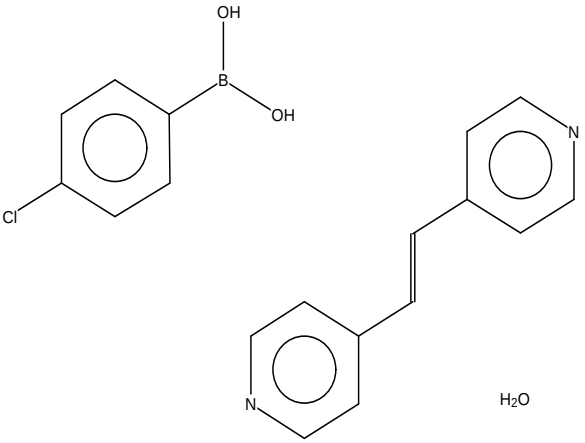
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 Cl_1 O_2,C_{12} H_{10} N_2,H_2 O_1$

Compound Name: (4-Chlorophenyl)boronic acid (trans-1,2-bis(4-pyridyl)ethene) monohydrate

Space Group:	P-1	***Cell:***	***a***	12.259(5)	***b***	12.938(2)	***c***	13.211(3)
Space Group No.:	2	***(Å,°)***	α	96.91(1)	β	116.79(2)	γ	99.83(2)

R-Factor (%): 4.65 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.319



RORMUI

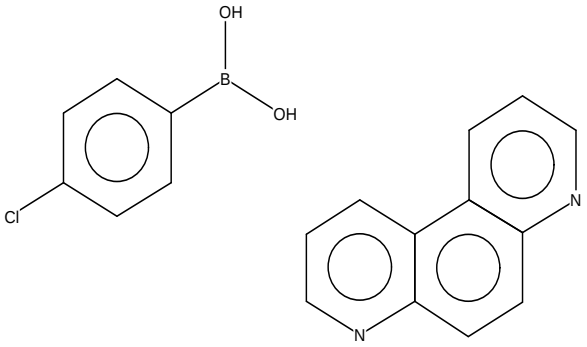
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 Cl_1 O_2,C_{12} H_8 N_2$

Compound Name: (4-Chlorophenyl)boronic acid 4,7-phenanthroline

Space Group:	P-1	***Cell:***	***a***	7.506(2)	***b***	9.118(2)	***c***	11.635(4)
Space Group No.:	2	***(Å,°)***	α	79.24(3)	β	88.39(2)	γ	84.33(2)

R-Factor (%): 2.75 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.436



RORNAP

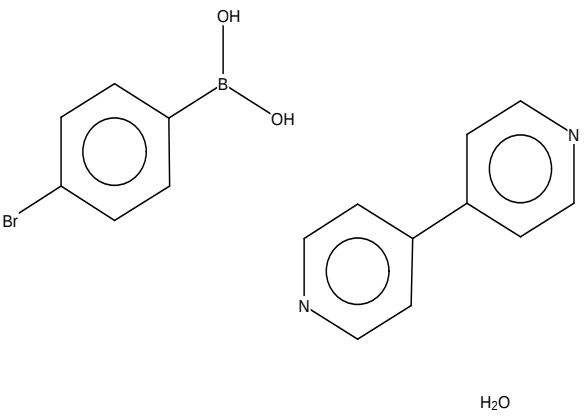
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 Br_1 O_2,C_{10} H_8 N_2,H_2 O_1$

Compound Name: (4-Bromophenyl)boronic acid 4,4'-bipyridine monohydrate

Space Group:	P21/n	***Cell:***	***a***	12.805(3)	***b***	6.834(1)	***c***	18.647(4)
Space Group No.:	14	***(Å,°)***	α	90.00	β	102.74(3)	γ	90.00

R-Factor (%): 3.32 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.565



RORNET

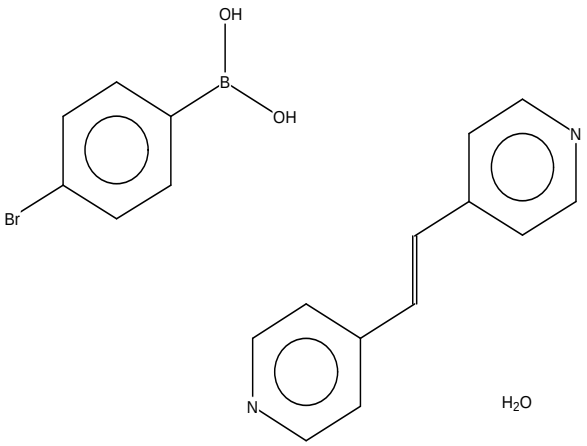
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 Br_1 O_2,C_{12} H_{10} N_2,H_2 O_1$

Compound Name: (4-Bromophenyl)boronic acid (trans-1,2-bis(4-pyridyl)ethene) monohydrate

Space Group:	P-1	***Cell:***	***a***	12.301	***b***	12.969	***c***	13.309
Space Group No.:	2	***(Å,°)***	α	96.25(1)	β	116.94(1)	γ	100.13(1)

R-Factor (%): 3.85 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.464



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RORNIX

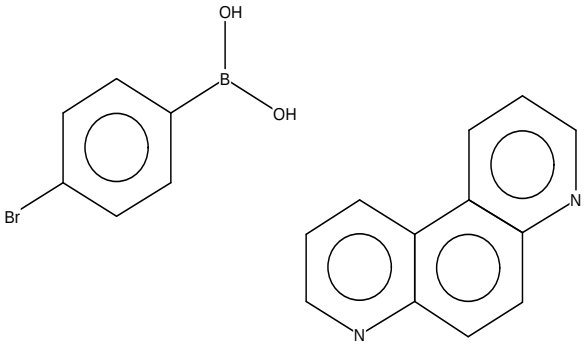
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 Br_1 O_2,C_{12} H_8 N_2$

Compound Name: (4-Bromophenyl)boronic acid 4,7-phenanthroline

Space Group:	P-1	***Cell:***	***a***	7.621(4)	***b***	9.054(5)	***c***	11.668(6)
Space Group No.:	2	***(Å,°)***	α	80.58(2)	β	88.21(2)	γ	84.07(2)

R-Factor (%): 2.89 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.602



RORNOD

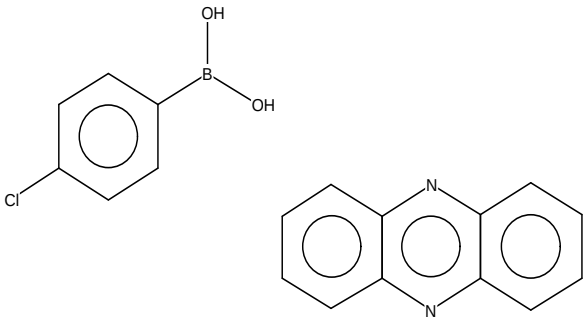
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 Cl_1 O_2,C_{12} H_8 N_2$

Compound Name: (4-Chlorophenyl)boronic acid phenazine

Space Group:	P-1	***Cell:***	***a***	6.939(4)	***b***	9.959(5)	***c***	12.125(7)
Space Group No.:	2	***(Å,°)***	α	80.17(1)	β	87.69(1)	γ	83.07(1)

R-Factor (%): 4.05 ***Temperature(K):*** 301 ***Density(g/cm³):*** 1.364



RORNUJ

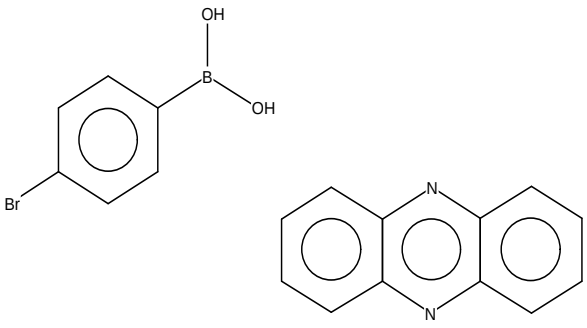
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 Br_1 O_2,2(C_{12} H_8 N_2),H_2 O_1$

Compound Name: (4-Bromophenyl)boronic acid bis(phenazine) monohydrate

Space Group:	P-1	***Cell:***	***a***	8.982(6)	***b***	12.482(8)	***c***	13.945(8)
Space Group No.:	2	***(Å,°)***	α	109.23(0)	β	95.72(0)	γ	110.22(0)

R-Factor (%): 5.19 ***Temperature(K):*** 301 ***Density(g/cm³):*** 1.431



H_2O

RORPAR

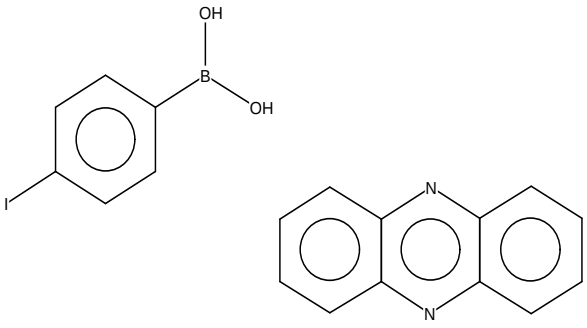
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 I_1 O_2,2(C_{12} H_8 N_2),H_2 O_1$

Compound Name: (4-Iodophenyl)boronic acid bis(phenazine) monohydrate

Space Group:	P-1	***Cell:***	***a***	8.996(5)	***b***	12.502(6)	***c***	14.051(7)
Space Group No.:	2	***(Å,°)***	α	109.40(0)	β	94.07(0)	γ	110.19(0)

R-Factor (%): 3.76 ***Temperature(K):*** 300 ***Density(g/cm³):*** 1.520



H_2O

Search: search4 (Mon May 01 12:48:32 2017): Hits 213-216

RORPEV

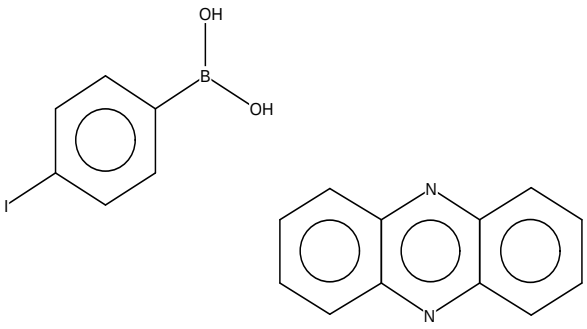
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 I_1 O_2,C_{12} H_8 N_2$

Compound Name: (4-Iodophenyl)boronic acid phenazine

Space Group:	P21/c	***Cell:***	***a***	19.700(8)	***b***	7.072(3)	***c***	25.731(10)
Space Group No.:	14	***(Å,°)***	α	90.00	β	107.70(0)	γ	90.00

R-Factor (%): 5.40 ***Temperature(K):*** 300 ***Density(g/cm³):*** 1.665



RORPIZ

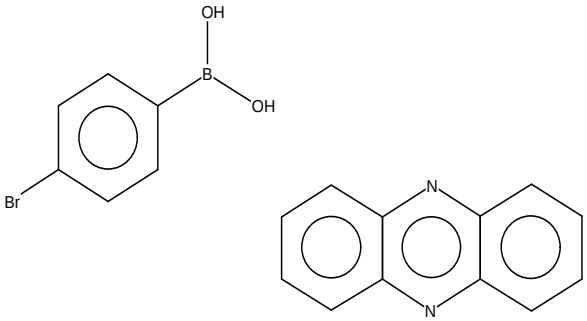
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 Br_1 O_2,C_{12} H_8 N_2,H_2 O_1$

Compound Name: (4-Bromophenyl)boronic acid phenazine monohydrate

Space Group:	P-1	***Cell:***	***a***	7.095(4)	***b***	10.015(6)	***c***	13.341(8)
Space Group No.:	2	***(Å,°)***	α	90.95(1)	β	95.04(1)	γ	93.99(1)

R-Factor (%): 7.32 ***Temperature(K):*** 301 ***Density(g/cm³):*** 1.407



H_2O

RORPOF

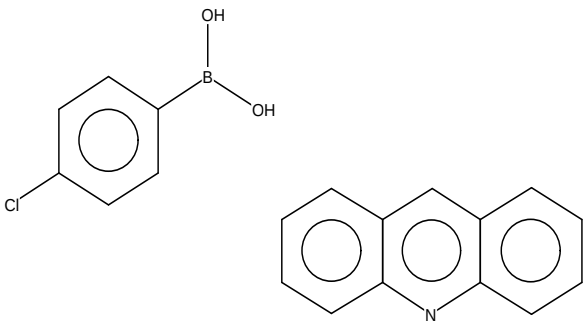
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 Cl_1 O_2,C_{13} H_9 N_1$

Compound Name: (4-Chlorophenyl)boronic acid acridine

Space Group:	P21/n	***Cell:***	***a***	11.092(6)	***b***	7.246(4)	***c***	21.061(13)
Space Group No.:	14	***(Å,°)***	α	90.00	β	99.21(1)	γ	90.00

R-Factor (%): 6.65 ***Temperature(K):*** 301 ***Density(g/cm³):*** 1.334



RORPUL

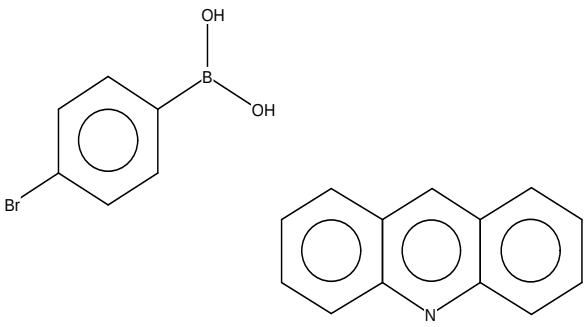
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 Br_1 O_2,C_{13} H_9 N_1$

Compound Name: (4-Bromophenyl)boronic acid acridine

Space Group:	P-1	***Cell:***	***a***	7.218(4)	***b***	11.132(6)	***c***	11.861(7)
Space Group No.:	2	***(Å,°)***	α	109.40(1)	β	104.45(0)	γ	94.52(0)

R-Factor (%): 4.81 ***Temperature(K):*** 301 ***Density(g/cm³):*** 1.473



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RORQAS

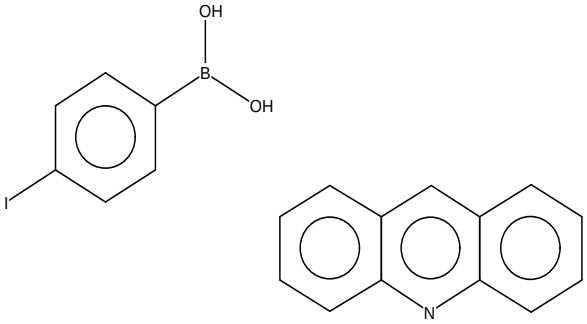
Reference: S.SeethaLekshmi, S.Varughese, L.Giri, V.R.Pedireddi (2014) *Cryst.Growth Des.* ,**14,**4143

Formula: $C_6 H_6 B_1 I_1 O_2$,$C_{13} H_9 N_1$

Compound Name: (4-Iodophenyl)boronic acid acridine

Space Group:	P-1	***Cell:***	***a*** 7.384(8)	***b*** 11.183(9)	***c*** 12.070(2)
Space Group No.:	2	***(Å,°)***	α 110.30(0)	β 103.06(0)	γ 94.72(0)

R-Factor (%): 9.20 ***Temperature(K):*** 301 ***Density(g/cm³):*** 1.582



RUTJOH

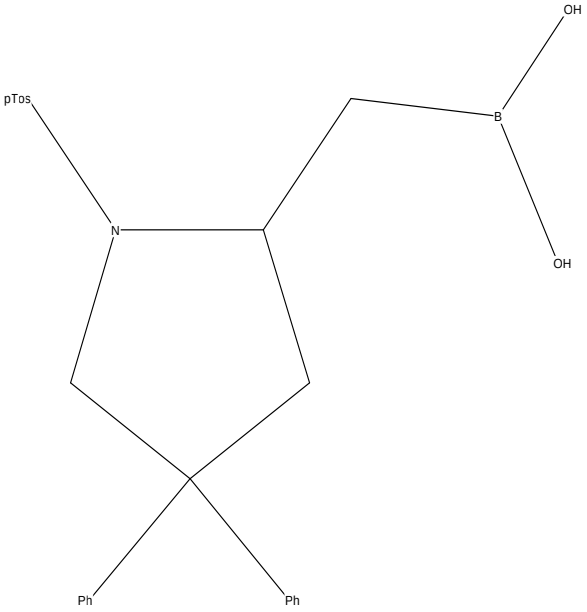
Reference: Chun-Hua Yang, Yu-Shi Zhang, Wen-Wen Fan, Dr G.-Q.Liu, P.Dr Y.-M.Li (2015) *Angew.Chem.,Int.Ed.* ,**54,**12636

Formula: $C_{24} H_{26} B_1 N_1 O_4 S_1$

Compound Name: ((1-((4-methylphenyl)sulfonyl)-4,4-diphenylpyrrolidin-2-yl)methyl)boronic acid

Space Group:	P21/c	***Cell:***	***a*** 8.828(1)	***b*** 11.463(2)	***c*** 22.233(4)
Space Group No.:	14	***(Å,°)***	α 90.00	β 100.89(3)	γ 90.00

R-Factor (%): 6.33 ***Temperature(K):*** 113 ***Density(g/cm³):*** 1.309



SAFSID

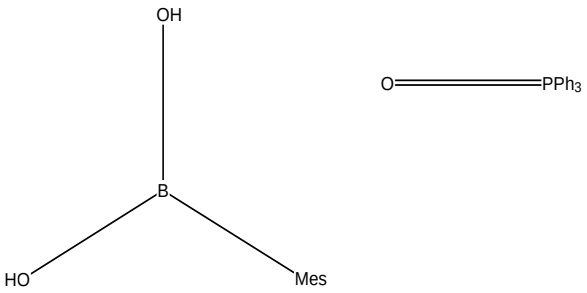
Reference: S.Rosca, M.Olaru, C.I.Rat (2012) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**68,**o31

Formula: $C_{18} H_{15} O_1 P_1$,$C_9 H_{13} B_1 O_2$

Compound Name: (2,4,6-Trimethylphenyl)boronic acid triphenylphosphine oxide

Space Group:	P21/c	***Cell:***	***a*** 12.218(4)	***b*** 12.339(4)	***c*** 16.983(5)
Space Group No.:	14	***(Å,°)***	α 90.00	β 95.65(0)	γ 90.00

R-Factor (%): 8.30 ***Temperature(K):*** 297 ***Density(g/cm³):*** 1.153



SIKCIZ

Reference: A.S.Batsanov, C.Grosjean, T.Schutz, A.Whiting (2007) *J.Org.Chem.* ,**72,**6276

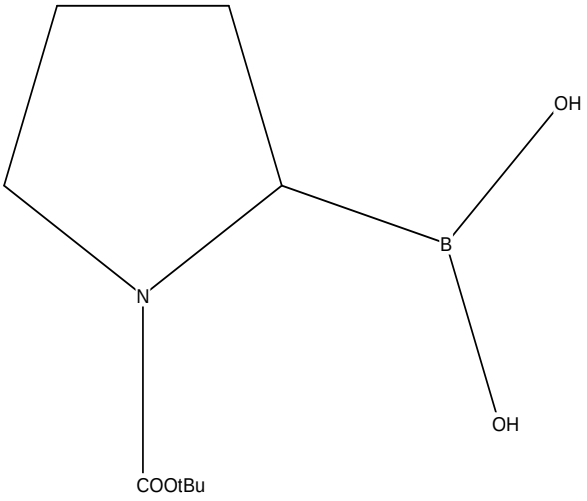
Formula: $C_9 H_{18} B_1 N_1 O_4$

Compound Name: (S)-N-(1,1-Dimethylethoxycarbonyl)-(pyrrolidin-2-yl)boronic acid

Synonym: (S)-(1-(t-Butoxycarbonyl)pyrrolidin-2-yl)boronic acid

Space Group:	P212121	***Cell:***	***a*** 6.541(0)	***b*** 9.216(0)	***c*** 20.015(2)
Space Group No.:	19	***(Å,°)***	α 90.00	β 90.00	γ 90.00

R-Factor (%): 2.95 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.184



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SOWHUI

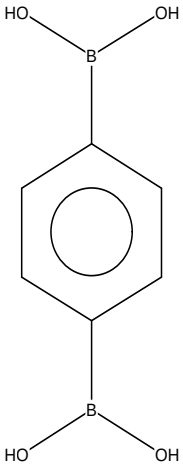
Reference: R.Sarma, J.B.Baruah (2009) *J.Mol.Struct.* ,**920,**350

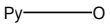
Formula: $C_6 H_8 B_2 O_4$,2($C_5 H_5 N_1 O_1$)

Compound Name: p-Phenylenediboronic acid bis(pyridine N-oxide)

Space Group: P21/c ***Cell:*** ***a*** 10.685(13) ***b*** 7.111(9) ***c*** 12.140(14)
Space Group No.: 14 ***(Å,°)*** α 90.00 β 115.05(3) γ 90.00

R-Factor (%): 10.93 ***Temperature(K):*** 296 ***Density(g/cm³):*** 1.415





SOWJAQ

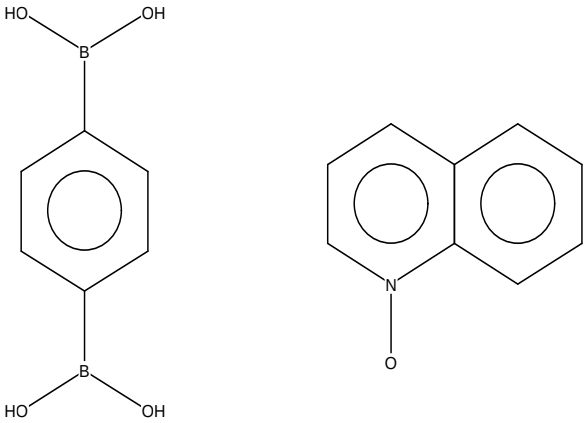
Reference: R.Sarma, J.B.Baruah (2009) *J.Mol.Struct.* ,**920,**350

Formula: $C_6 H_8 B_2 O_4$,2($C_9 H_7 N_1 O_1$)

Compound Name: 1,4-Phenylenediboronic acid bis(quinoline N-oxide)

Space Group: P-1 ***Cell:*** ***a*** 6.807(1) ***b*** 7.777(2) ***c*** 11.578(4)
Space Group No.: 2 ***(Å,°)*** α 106.45(1) β 99.51(1) γ 101.72(0)

R-Factor (%): 4.58 ***Temperature(K):*** 296 ***Density(g/cm³):*** 1.354



SOWJEU

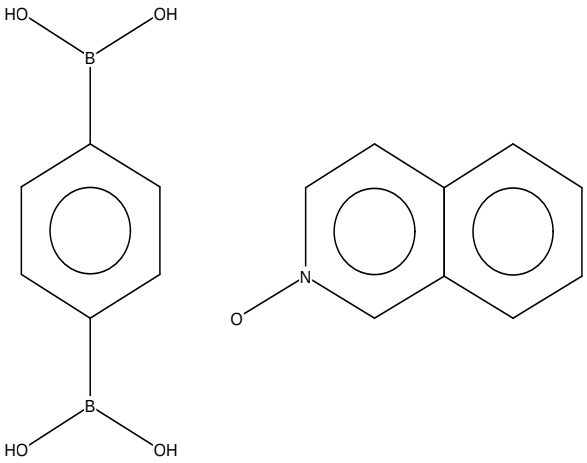
Reference: R.Sarma, J.B.Baruah (2009) *J.Mol.Struct.* ,**920,**350

Formula: $C_6 H_8 B_2 O_4$,4($C_9 H_7 N_1 O_1$)

Compound Name: 1,4-Phenylenediboronic acid tetrakis(isoquinoline-N-oxide)

Space Group: P-1 ***Cell:*** ***a*** 8.104(0) ***b*** 10.057(0) ***c*** 12.627(0)
Space Group No.: 2 ***(Å,°)*** α 84.15(0) β 78.47(0) γ 67.19(0)

R-Factor (%): 7.10 ***Temperature(K):*** 296 ***Density(g/cm³):*** 1.334



SOWJIY

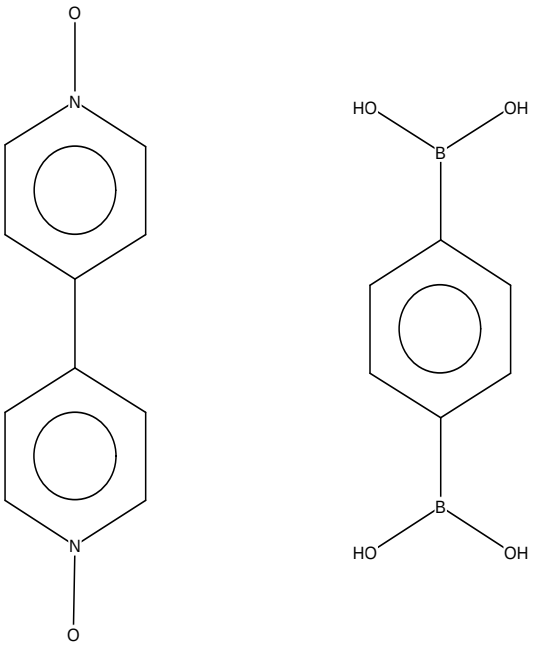
Reference: R.Sarma, J.B.Baruah (2009) *J.Mol.Struct.* ,**920,**350

Formula: $C_{10} H_8 N_2 O_2$,$C_6 H_8 B_2 O_4$

Compound Name: 1,4-Phenylenediboronic acid 4,4'-bipyridine-N,N'-dioxide

Space Group: P-1 ***Cell:*** ***a*** 6.669(0) ***b*** 7.598(1) ***c*** 8.285(1)
Space Group No.: 2 ***(Å,°)*** α 100.16(1) β 106.99(0) γ 92.94(0)

R-Factor (%): 4.54 ***Temperature(K):*** 296 ***Density(g/cm³):*** 1.496



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SUHPIU

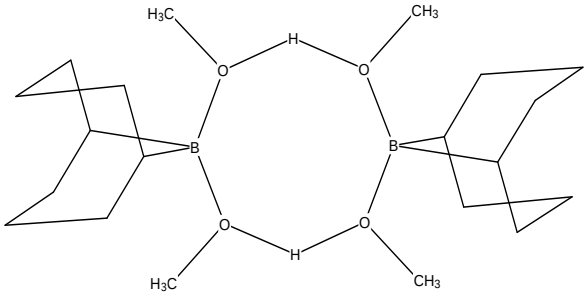
Reference: R.Koster, R.Kucznierz, W.Schussler, D.Blaser, R.Boese (1993) *Liebigs Ann.* ,189

Formula: $C_{20}H_{42}B_2O_4$

Compound Name: 1,5-Cyclo-octanediyl(dimethoxy)boric acid dimer

Space Group:	P-1	***Cell:***	***a***	6.839(2)	***b***	8.146(4)	***c***	9.821(4)
Space Group No.:	2	***(Å,°)***	α	87.13(4)	β	72.75(3)	γ	76.36(3)

R-Factor (%): 4.73 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.204



TASCEW

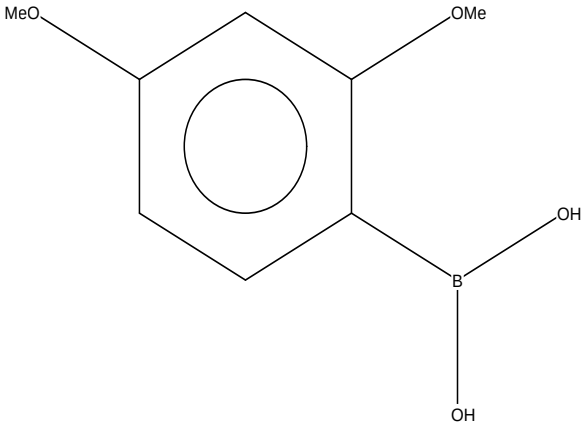
Reference: Youjun Yang, J.O.Escobedo, A.Wong, C.M.Schowalter, M.C.Touchy, Lijuan Jiao, W.E.Crowe, F.R.Fronczek, R.M.Strongin (2005) *J.Org.Chem.* ,**70,**6907

Formula: $C_8H_{11}B_1O_4$

Compound Name: 2,4-Dimethoxyphenylboronic acid

Space Group:	P-1	***Cell:***	***a***	6.992(2)	***b***	7.916(2)	***c***	7.998(2)
Space Group No.:	2	***(Å,°)***	α	94.75(1)	β	94.53(1)	γ	96.54(1)

R-Factor (%): 3.60 ***Temperature(K):*** 105 ***Density(g/cm³):*** 1.384



TECCEL

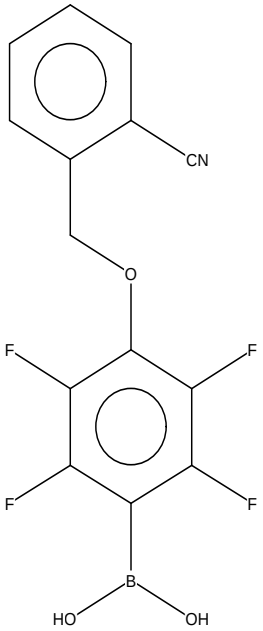
Reference: K.Durka, K.Gontarczyk, T.Klis, J.Serwatowski, K.Wozniak (2012) *Appl.Organomet.Chem.* ,**26,**287

Formula: $C_{14}H_8B_1F_4N_1O_3$

Compound Name: (4-((2-Cyanobenzyl)oxy)-2,3,5,6-tetrafluorophenyl)boronic acid

Space Group:	P-1	***Cell:***	***a***	4.976(0)	***b***	5.938(0)	***c***	21.801(1)
Space Group No.:	2	***(Å,°)***	α	95.55(0)	β	92.23(0)	γ	95.31(0)

R-Factor (%): 4.83 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.693



TENROV

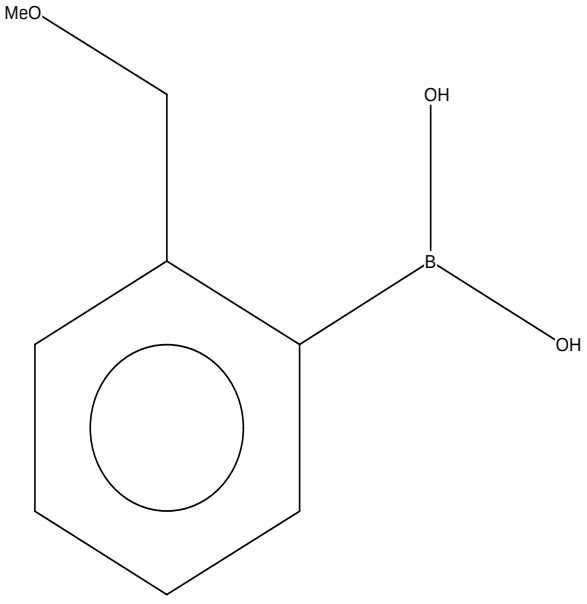
Reference: A.Adamczyk-Wozniak, Z.Brzozka, M.Dabrowski, I.D.Madura, R.Scheidsbach, E.Tomecka, K.Zukowski, A.Sporzynski (2013) *J.Mol.Struct.* ,**1035,**190

Formula: $C_8H_{11}B_1O_3$

Compound Name: (2-(Methoxymethyl)phenyl)boronic acid

Space Group:	Pca21	***Cell:***	***a***	20.092(0)	***b***	6.467(0)	***c***	13.240(0)
Space Group No.:	29	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.61 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.282



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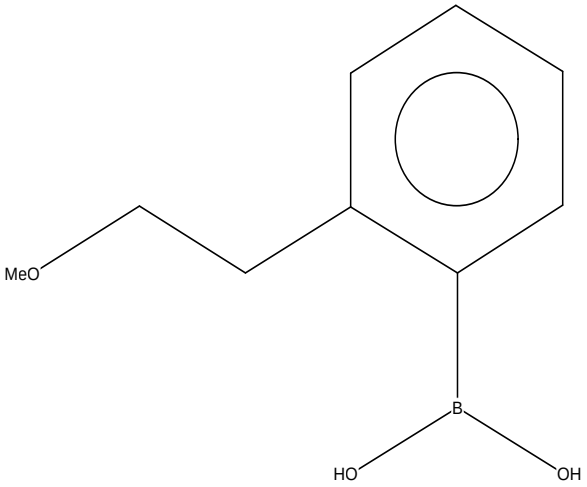
TENRUB

Reference: A.Adamczyk-Wozniak, Z.Brzozka, M.Dabrowski, I.D.Madura, R.Scheidsbach, E.Tomecka, K.Zukowski, A.Sporzynski (2013) *J.Mol.Struct.* ,**1035,**190

Formula: $C_9 H_{13} B_1 O_3$

Compound Name: (2-(2-Methoxyethyl)phenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	8.085(0)	***b***	12.220(0)	***c*** 10.593(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	104.10(0)	γ 90.00
R-Factor (%):	3.20	***Temperature(K):***	100		***Density(g/cm³):***	1.178	



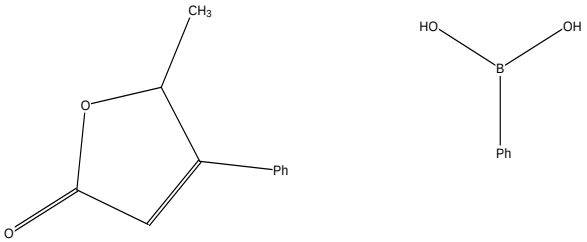
TILLUX

Reference: Rui Zhang, Qin Xu, Kai Chen, Peng Gu, Min Shi (2013) *Eur.J.Org.Chem.* ,7366

Formula: $C_{11} H_{10} O_2$,$C_6 H_7 B_1 O_2$

Compound Name: 5-methyl-4-phenylfuran-2(5H)-one phenylboronic acid

Space Group:	P-1	***Cell:***	***a***	9.203(1)	***b***	9.774(1)	***c*** 9.955(1)
Space Group No.:	2	***(Å,°)***	α	92.80(0)	β	109.36(0)	γ 108.17(0)
R-Factor (%):	4.79	***Temperature(K):***	293		***Density(g/cm³):***	1.243	



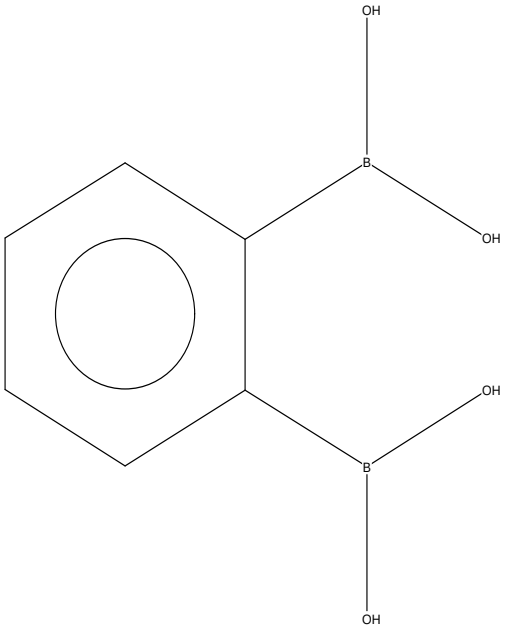
TIRXUP

Reference: K.Durka, K.N.Jarzembska, R.Kaminski, S.Lulinski, J.Serwatowski, K.Wozniak (2013) *Cryst.Growth Des.* ,**13,**4181

Formula: $C_6 H_8 B_2 O_4$

Compound Name: 1,2-phenylenediboronic acid

Space Group:	P21/n	***Cell:***	***a***	5.802(0)	***b***	11.974(0)	***c*** 11.544(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	95.39(0)	γ 90.00
R-Factor (%):	2.49	***Temperature(K):***	100		***Density(g/cm³):***	1.379	



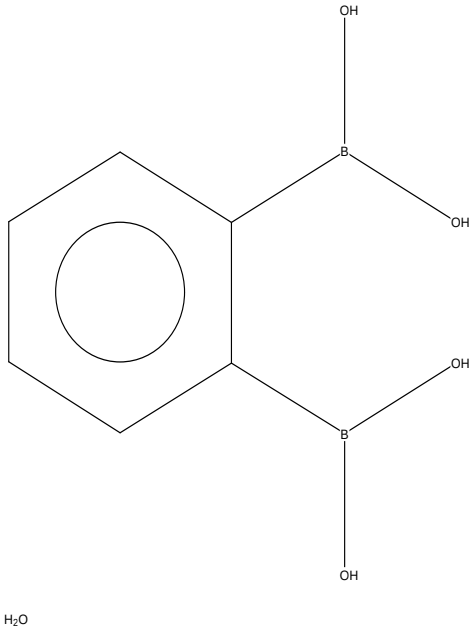
TIRYAW

Reference: K.Durka, K.N.Jarzembska, R.Kaminski, S.Lulinski, J.Serwatowski, K.Wozniak (2013) *Cryst.Growth Des.* ,**13,**4181

Formula: $C_6 H_8 B_2 O_4$,$2(H_2 O_1)$

Compound Name: 1,2-Phenylenediboronic acid dihydrate

Space Group:	P21/n	***Cell:***	***a***	11.258(0)	***b***	5.145(0)	***c*** 16.821(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	92.44(0)	γ 90.00
R-Factor (%):	3.28	***Temperature(K):***	100		***Density(g/cm³):***	1.376	



H_2O

Search: search4 (Mon May 01 12:48:32 2017): Hits 233-236

TIRYEA

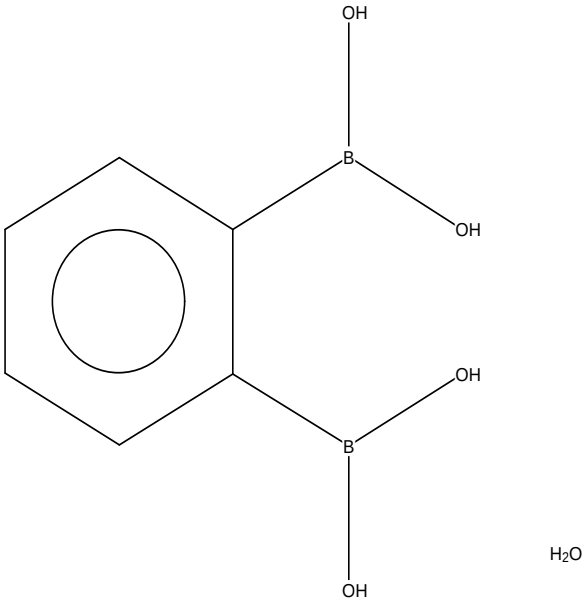
Reference: K.Durka, K.N.Jarzembska, R.Kaminski, S.Lulinski, J.Serwatowski, K.Wozniak (2013) *Cryst.Growth Des.* ,**13,**4181

Formula: $C_6 H_8 B_2 O_4,H_2 O_1$

Compound Name: 1,2-Phenylenediboronic acid monohydrate

Space Group:	R-3	***Cell:***	***a*** 29.475(0)	***b*** 29.475(0)	***c*** 6.169(0)
Space Group No.:	148	***(Å,°)***	α 90.00	β 90.00	γ 120.00

R-Factor (%): 5.06 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.183



TITDEG

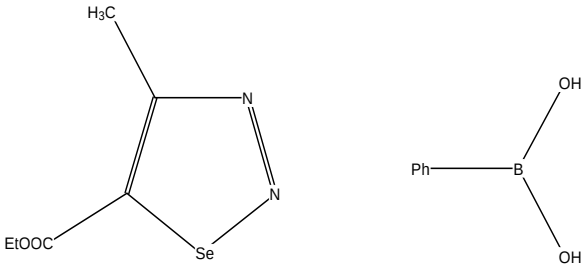
Reference: P.Arsenyan, K.Oberte, S.Belyakov (2007) *Khim.Get.Soedin.,SSSR(Russ.)(Chem.Heterocycl.Compd.)* ,289

Formula: $C_6 H_8 N_2 O_2 Se_1,C_6 H_7 B_1 O_2$

Compound Name: 4-Methyl-5-ethoxycarbonyl-1,2,3-selenadiazole phenylboronic acid

Space Group:	P-1	***Cell:***	***a*** 7.467(0)	***b*** 10.098(0)	***c*** 11.169(0)
Space Group No.:	2	***(Å,°)***	α 107.75(0)	β 98.40(0)	γ 107.91(0)

R-Factor (%): 4.41 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.539



TIWWIG

Reference: M.K.Cyranski, A.Jezierska, P.Klimentowska, J.J.Panek, G.Z.Zukowska, A.Sporzynski (2008) *J.Chem.Phys.* ,**128,**124512

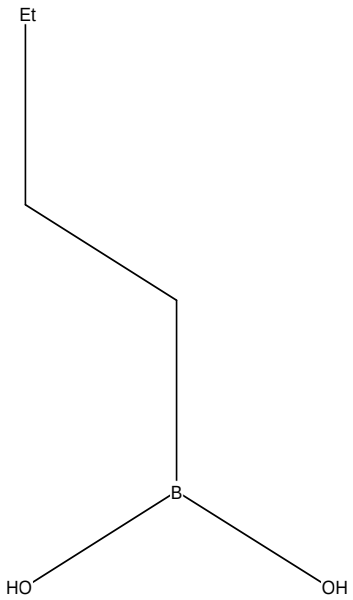
Formula: $C_4 H_{11} B_1 O_2$

Compound Name: n-Butylboronic acid

Synonym: PDB Chemical Component code: BUB

Space Group:	P21/c	***Cell:***	***a*** 11.264(1)	***b*** 5.757(0)	***c*** 9.609(0)
Space Group No.:	14	***(Å,°)***	α 90.00	β 101.72(0)	γ 90.00

R-Factor (%): 4.09 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.110



TUNGAK

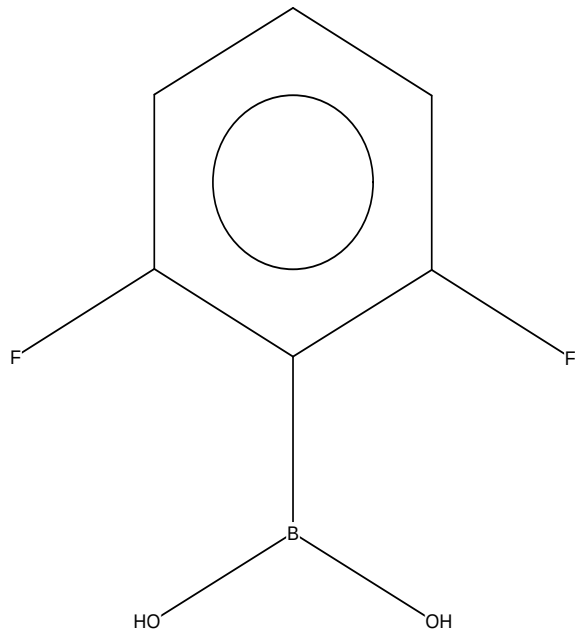
Reference: D.C.Bradley, I.S.Harding, A.D.Keefe, M.Motevalli, Dao Hong Zheng (1996) *J.Chem.Soc.,Dalton Trans.* ,3931

Formula: $C_6 H_5 B_1 F_2 O_2$

Compound Name: (2,6-Difluorophenyl)dihydroxyborane

Space Group:	P21/n	***Cell:***	***a*** 23.631(3)	***b*** 5.498(10)	***c*** 5.033(10)
Space Group No.:	14	***(Å,°)***	α 90.00	β 91.61(1)	γ 90.00

R-Factor (%): 4.28 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.605



Search: search4 (Mon May 01 12:48:32 2017): Hits 237-240

TUNGAK01

Reference: I.D.Madura, K.Czerwinska, D.Soldanska (2014)
Cryst.Growth Des. ,**14,**5912

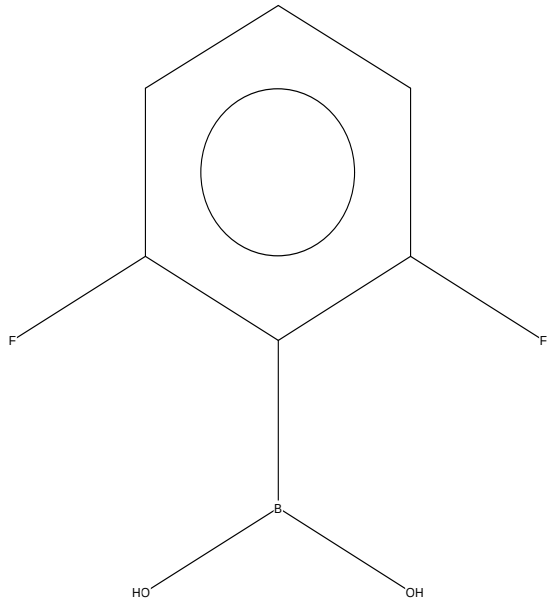
Formula: $C_6 H_5 B_1 F_2 O_2$

Compound Name: (2,6-difluorophenyl)boronic acid

Synonym: (diorthofluorophenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	5.027(0)	***b***	5.394(0)	***c***	23.233(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	91.90(0)	γ	90.00

R-Factor (%): 3.24 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.666



TUNNEW

Reference: A.Vega, M.Zarate, H.Tlahuext, H.Hopfl (2010)
Acta Crystallogr.,Sect.E:Struct.Rep.Online ,**66,**o1260

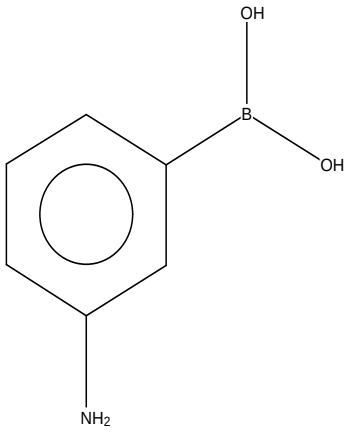
Formula: $C_6 H_8 B_1 N_1 O_2,H_2 O_1$

Compound Name: 3-Aminophenylboronic acid monohydrate

Synonym: PDB Chemical Component code: APB

Space Group:	P21/c	***Cell:***	***a***	7.121(0)	***b***	13.855(1)	***c***	7.848(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	100.66(0)	γ	90.00

R-Factor (%): 3.20 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.353



H_2O

TUNQID

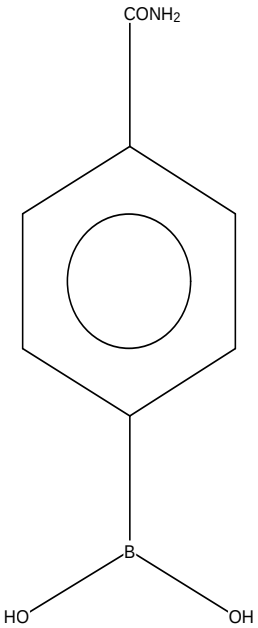
Reference: M.D.Apostolova, R.P.Nikolova, B.L.Shivachev (2010)
Acta Crystallogr.,Sect.E:Struct.Rep.Online ,**66,**o1273

Formula: $C_7 H_8 B_1 N_1 O_3$

Compound Name: (4-Carbamoylphenyl)boronic acid

Space Group:	P-1	***Cell:***	***a***	4.997(2)	***b***	5.351(2)	***c***	7.297(1)
Space Group No.:	2	***(Å,°)***	α	103.91(1)	β	98.69(2)	γ	93.14(1)

R-Factor (%): 5.30 ***Temperature(K):*** 290 ***Density(g/cm^3):*** 1.470



UCETUS

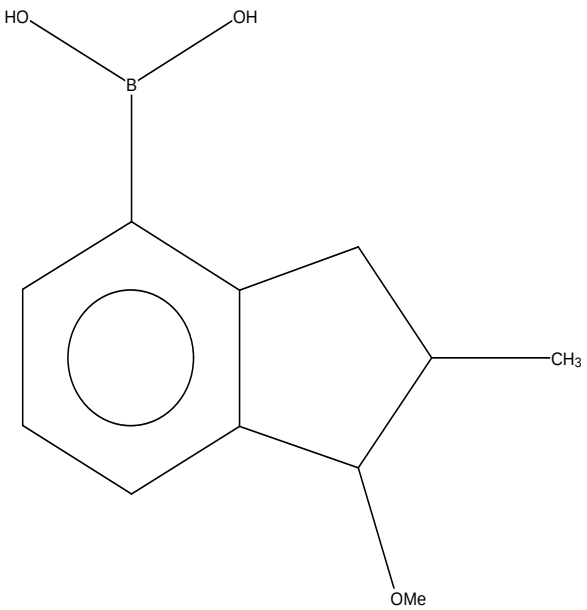
Reference: V.V.Izmer, A.Y.Lebedev, M.V.Nikulin, A.N.Ryabov, A.F.Asachenko, A.V.Lygin, D.A.Sorokin, A.Z.Voskoboynikov (2006)
Organometallics ,**25,**1217

Formula: $C_{11} H_{15} B_1 O_3$

Compound Name: trans-1-Methoxy-2-methyl-2,3-dihydroinden-4-yl boronic acid

Space Group:	P-1	***Cell:***	***a***	7.777(1)	***b***	8.536(1)	***c***	8.748(1)
Space Group No.:	2	***(Å,°)***	α	80.84(3)	β	72.12(3)	γ	78.97(3)

R-Factor (%): 4.31 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.269



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UJABUE

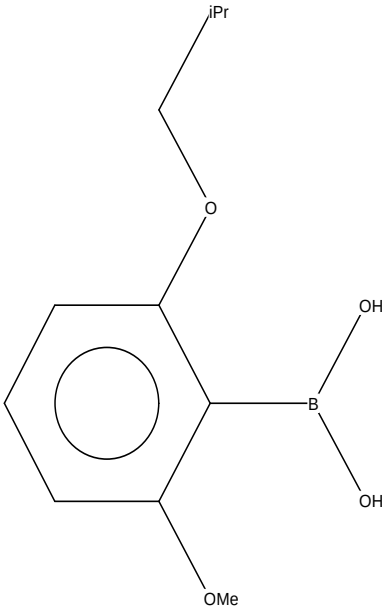
Reference: M.K.Cyranski, P.Klimentowska, A.Rydzewska, J.Serwatowski, A.Sporzynski, D.K.Stepien (2012) *CrystEngComm* ,**14,** 6282

Formula: $C_{11}\,H_{17}\,B_1\,O_4$

Compound Name: (2-Isobutoxy-6-methoxyphenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	7.571(1)	***b***	14.670(2)	***c***	10.660(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	91.73(1)	γ	90.00

R-Factor (%): 4.15 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.257



UJACAL

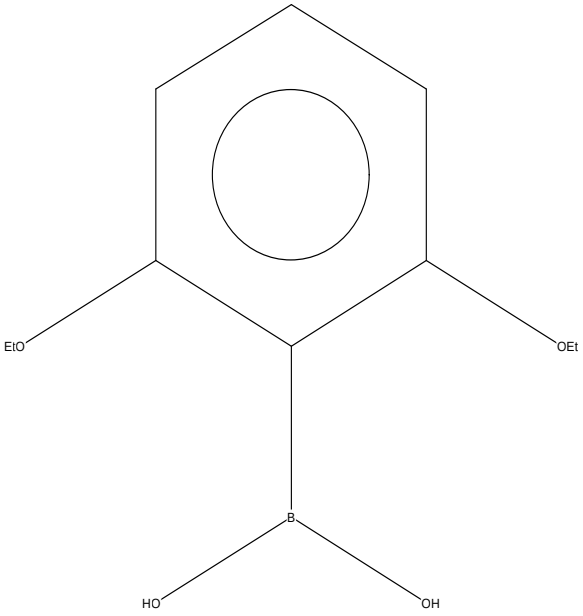
Reference: M.K.Cyranski, P.Klimentowska, A.Rydzewska, J.Serwatowski, A.Sporzynski, D.K.Stepien (2012) *CrystEngComm* ,**14,** 6282

Formula: $C_{10}\,H_{15}\,B_1\,O_4$

Compound Name: 2,6-Diethoxyphenylboronic acid

Space Group:	P21/c	***Cell:***	***a***	20.081(0)	***b***	15.533(0)	***c***	15.096(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	109.72(0)	γ	90.00

R-Factor (%): 4.52 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.259



UJACAL01

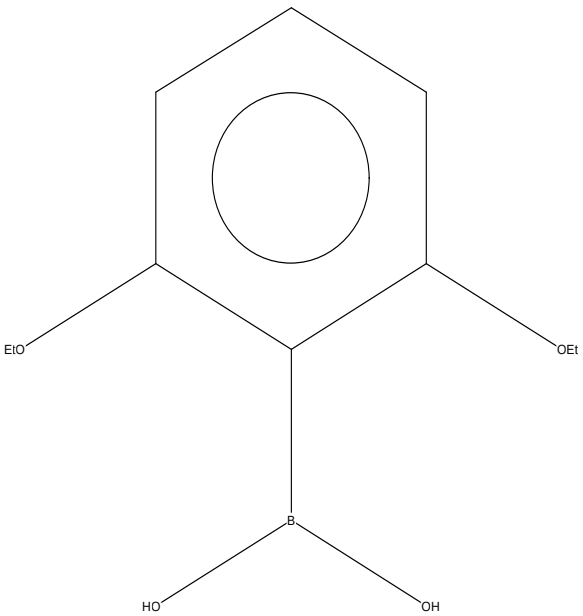
Reference: M.K.Cyranski, P.Klimentowska, A.Rydzewska, J.Serwatowski, A.Sporzynski, D.K.Stepien (2012) *CrystEngComm* ,**14,** 6282

Formula: $C_{10}\,H_{15}\,B_1\,O_4$

Compound Name: 2,6-Diethoxyphenylboronic acid

Space Group:	P21/n	***Cell:***	***a***	15.188(2)	***b***	5.017(0)	***c***	15.737(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	117.18(2)	γ	90.00

R-Factor (%): 4.26 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.308



UJACIT

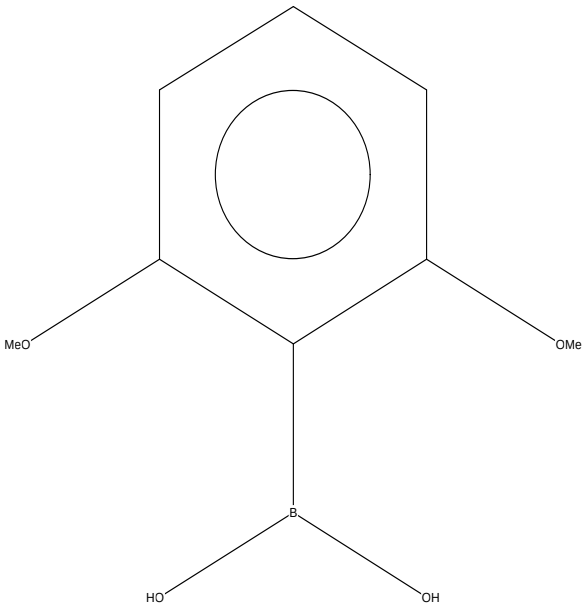
Reference: M.K.Cyranski, P.Klimentowska, A.Rydzewska, J.Serwatowski, A.Sporzynski, D.K.Stepien (2012) *CrystEngComm* ,**14,** 6282

Formula: $C_8\,H_{11}\,B_1\,O_4$

Compound Name: 2,6-Dimethoxyphenylboronic acid

Space Group:	C2/c	***Cell:***	***a***	14.405(1)	***b***	8.471(0)	***c***	22.271(1)
Space Group No.:	15	***(Å,°)***	α	90.00	β	98.17(0)	γ	90.00

R-Factor (%): 4.30 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.348



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UJACIT01

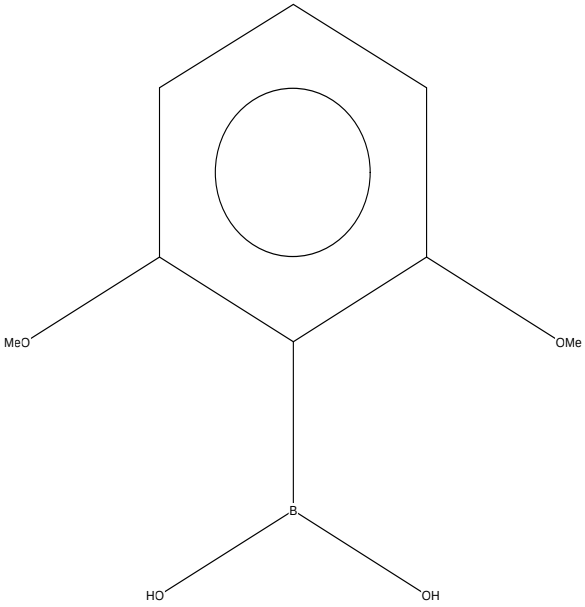
Reference: M.K.Cyranski, P.Klimentowska, A.Rydzewska, J.Serwatowski, A.Sporzynski, D.K.Stepien (2012) *CrystEngComm* ,**14,** 6282

Formula: $C_8 H_{11} B_1 O_4$

Compound Name: 2,6-Dimethoxyphenylboronic acid

Space Group:	P-4n2	***Cell:***	***a***	13.376(0)	***b***	13.376(0)	***c***	5.033(0)
Space Group No.:	118	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 2.32 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.342



UJACUF

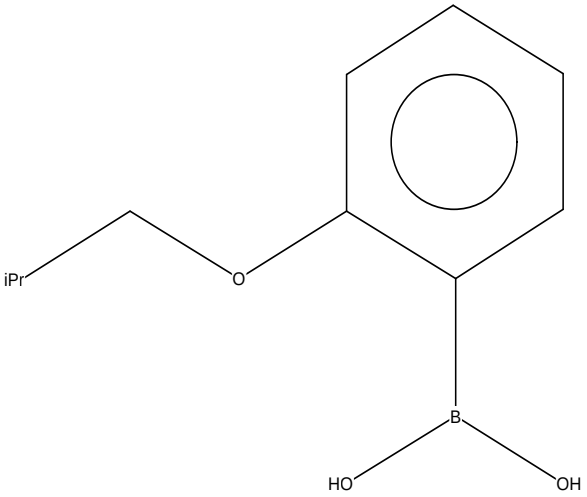
Reference: M.K.Cyranski, P.Klimentowska, A.Rydzewska, J.Serwatowski, A.Sporzynski, D.K.Stepien (2012) *CrystEngComm* ,**14,** 6282

Formula: $C_{10} H_{15} B_1 O_3$

Compound Name: (2-Isobutoxyphenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	12.909(2)	***b***	12.984(1)	***c***	18.437(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	134.64(3)	γ	90.00

R-Factor (%): 3.99 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.172



UJADAM

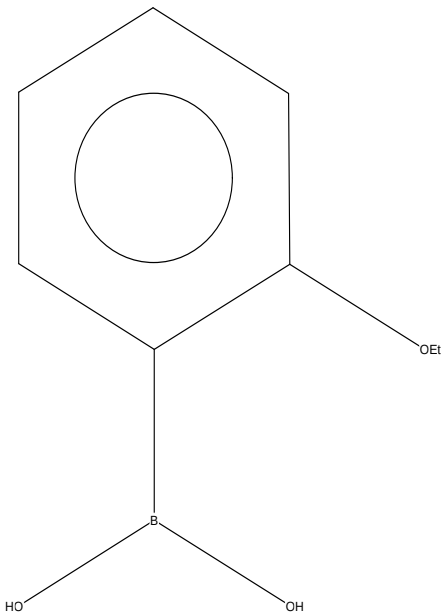
Reference: M.K.Cyranski, P.Klimentowska, A.Rydzewska, J.Serwatowski, A.Sporzynski, D.K.Stepien (2012) *CrystEngComm* ,**14,** 6282

Formula: $C_8 H_{11} B_1 O_3$

Compound Name: (2-Ethoxyphenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	5.418(1)	***b***	14.812(3)	***c***	10.728(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	103.29(3)	γ	90.00

R-Factor (%): 3.41 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.316



UJADEQ

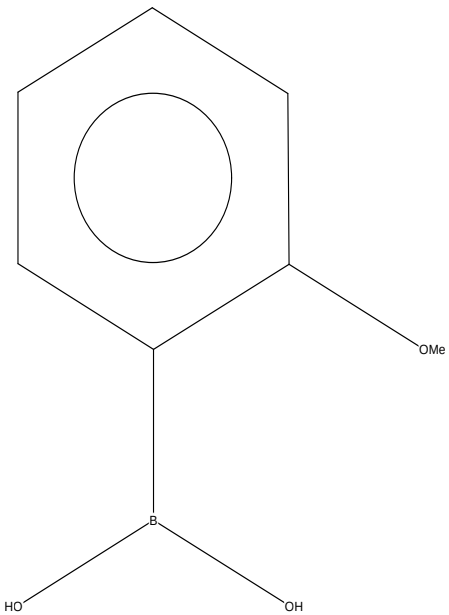
Reference: M.K.Cyranski, P.Klimentowska, A.Rydzewska, J.Serwatowski, A.Sporzynski, D.K.Stepien (2012) *CrystEngComm* ,**14,** 6282

Formula: $C_7 H_9 B_1 O_3$

Compound Name: (2-Methoxyphenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	7.718(0)	***b***	14.454(0)	***c***	7.284(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	113.43(0)	γ	90.00

R-Factor (%): 3.81 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.354



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ULUQUP

Reference: M.TalwelkarShimpi, S.Oberg, L.Giri, V.R.Pedireddi (2016)
RSC Advances ,**6,**43060

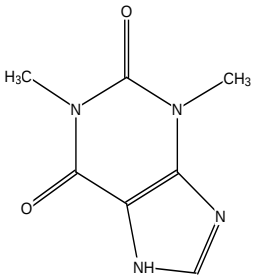
Formula: $C_7 H_8 N_4 O_2$,$C_6 H_6 B_1 Cl_1 O_2$

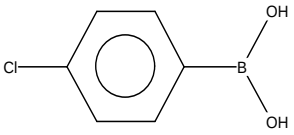
Compound Name: (4-chlorophenyl)boronic acid 1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione

Synonym: theophylline (4-chlorophenyl)boronic acid

Space Group:	P-1	***Cell:***	***a***	7.510(1)	***b***	9.471(2)	***c***	11.878(2)
Space Group No.:	2	***(Å,°)***	α	85.63(3)	β	79.47(4)	γ	68.96(3)

R-Factor (%): 7.53 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.442





ULURAW

Reference: M.TalwelkarShimpi, S.Oberg, L.Giri, V.R.Pedireddi (2016)
RSC Advances ,**6,**43060

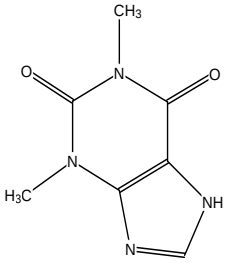
Formula: $C_7 H_8 N_4 O_2$,$C_6 H_6 B_1 I_1 O_2$

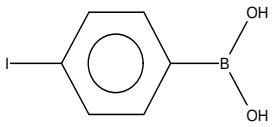
Compound Name: (4-iodophenyl)boronic acid 1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione

Synonym: (4-iodophenyl)boronic acid theophylline

Space Group:	P-1	***Cell:***	***a***	7.475(0)	***b***	9.623(2)	***c***	11.957(3)
Space Group No.:	2	***(Å,°)***	α	87.25(1)	β	80.94(1)	γ	71.63(1)

R-Factor (%): 5.97 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.763





ULUREA

Reference: M.TalwelkarShimpi, S.Oberg, L.Giri, V.R.Pedireddi (2016)
RSC Advances ,**6,**43060

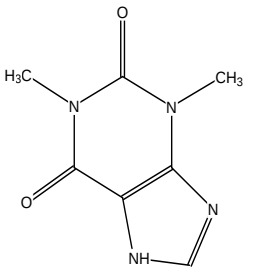
Formula: $C_7 H_8 N_4 O_2$,$C_6 H_7 B_1 O_3$

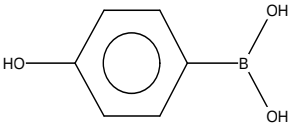
Compound Name: (4-hydroxyphenyl)boronic acid 1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione

Synonym: (4-hydroxyphenyl)boronic acid theophylline

Space Group:	P21/c	***Cell:***	***a***	12.858(3)	***b***	8.215(1)	***c***	14.199(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	98.03(0)	γ	90.00

R-Factor (%): 4.56 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.423





ULURIE

Reference: M.TalwelkarShimpi, S.Oberg, L.Giri, V.R.Pedireddi (2016)
RSC Advances ,**6,**43060

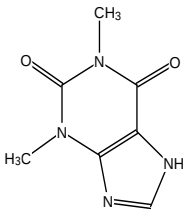
Formula: $2(C_7 H_8 N_4 O_2)$,$C_6 H_8 B_2 O_4$,$0.5(H_2 O_1)$

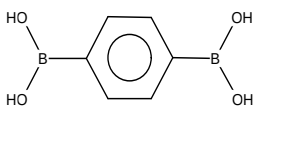
Compound Name: 1,4-phenylenediboronic acid bis(1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione) hemihydrate

Synonym: 1,4-phenylenediboronic acid bis(theophylline) hemihydrate

Space Group:	P-1	***Cell:***	***a***	8.528(2)	***b***	8.711(2)	***c***	9.661(3)
Space Group No.:	2	***(Å,°)***	α	109.74(1)	β	94.47(1)	γ	104.78

R-Factor (%): 7.73 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.383





H_2O

Search: search4 (Mon May 01 12:48:32 2017): Hits 253-256

UMUHOZ

Reference: S.M.Cornet, K.B.Dillon, C.D.Entwistle, M.A.Fox, A.E.Goeta, H.P.Goodwin, T.B.Marder, A.L.Thompson (2003) *Dalton Trans.* ,4395

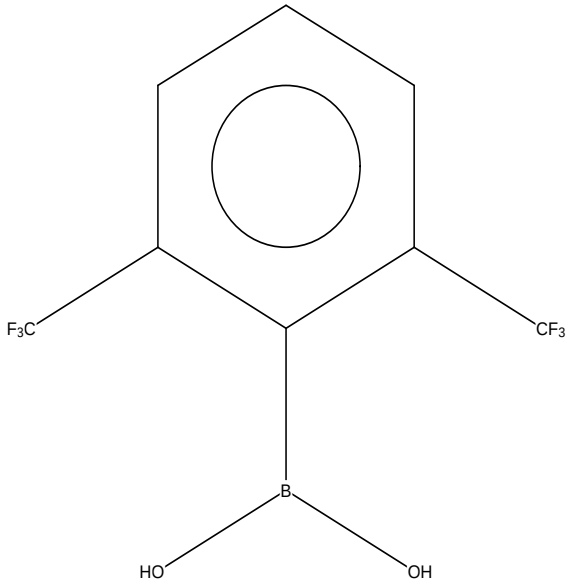
Formula: $C_8 H_5 B_1 F_6 O_2$

Compound Name: (2,6-bis(Trifluoromethyl)phenyl)-dihydroxy-borane

Synonym: (2,6-bis(Trifluoromethyl)phenyl)boronic acid

Space Group:	P21212	***Cell:***	***a***	14.086(1)	***b***	14.462(1)	***c***	5.003(0)
Space Group No.:	18	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.05 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.681



UPUNUQ

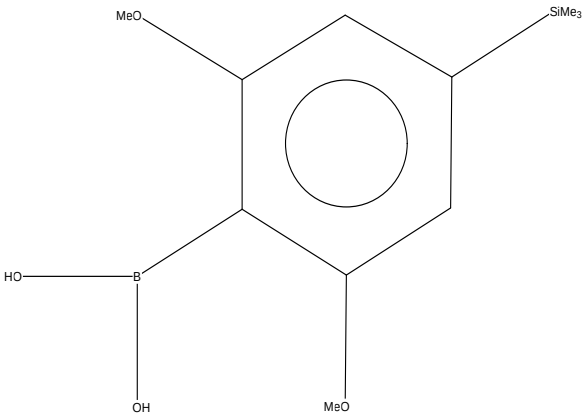
Reference: J.E.Barnsley, G.E.Shillito, C.B.Larsen, H.van der Salm, L.E.Wang, N.T.Lucas, K.C.Gordon (2016) *J.Phys.Chem.A* ,**120,**1853

Formula: $C_{11} H_{19} B_1 O_4 Si_1$

Compound Name: (2,6-dimethoxy-4-(trimethylsilyl)phenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	7.769(1)	***b***	12.973(2)	***c***	13.791(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	103.16(0)	γ	90.00

R-Factor (%): 3.84 ***Temperature(K):*** 91 ***Density(g/cm³):*** 1.247



USAKEF

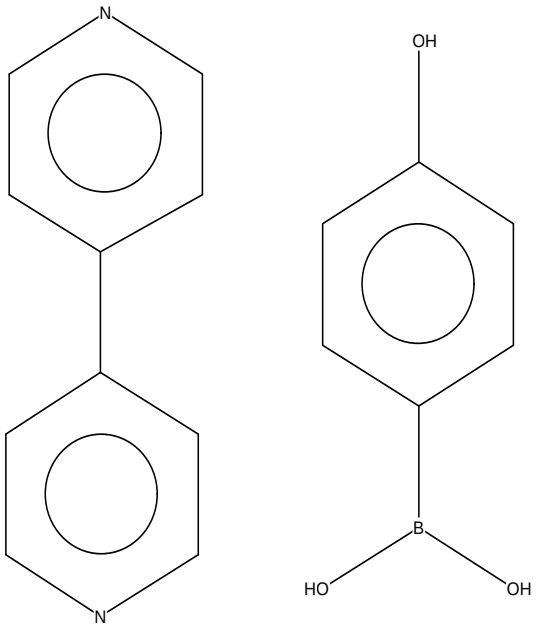
Reference: M.Talwelkar, V.R.Pedireddi (2010) *Tetrahedron Lett.* ,**51,** 6901

Formula: $1.5(C_{10} H_8 N_2),C_6 H_7 B_1 O_3$

Compound Name: (4-Hydroxyphenyl)boronic acid 4,4'-bipyridine

Space Group:	P-1	***Cell:***	***a***	13.960(9)	***b***	17.186(1)	***c***	25.222(5)
Space Group No.:	2	***(Å,°)***	α	92.64(1)	β	100.65(1)	γ	111.18(1)

R-Factor (%): 9.09 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.348



USAKIJ

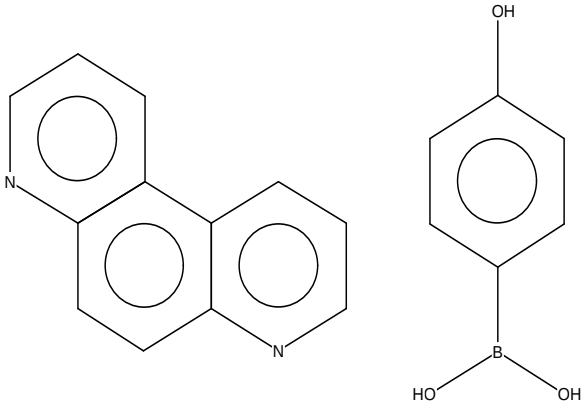
Reference: M.Talwelkar, V.R.Pedireddi (2010) *Tetrahedron Lett.* ,**51,** 6901

Formula: $C_{12} H_8 N_2,C_6 H_7 B_1 O_3$

Compound Name: (4-Hydroxyphenyl)boronic acid 4,7-phenanthroline

Space Group:	P21/n	***Cell:***	***a***	7.229(1)	***b***	20.718(4)	***c***	11.036(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	107.58(1)	γ	90.00

R-Factor (%): 6.60 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.341



Search: search4 (Mon May 01 12:48:32 2017): Hits 257-260

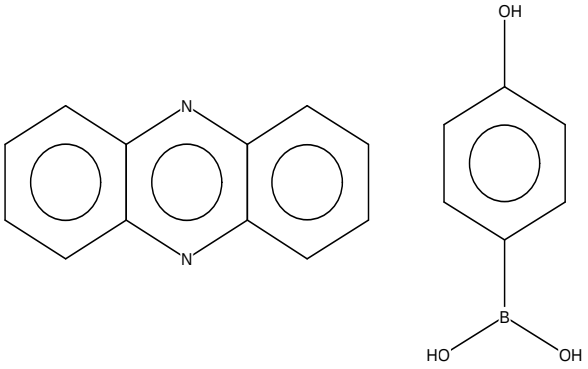
USAKOP

Reference: M.Talwelkar, V.R.Pedireddi (2010) *Tetrahedron Lett.* ,**51,** 6901

Formula: $C_{12}H_8N_2,C_6H_7B_1O_3$

Compound Name: (4-Hydroxyphenyl)boronic acid phenazine

Space Group:	P21/n	***Cell:***	***a***	8.405(5)	***b***	23.225(12)	***c*** 9.102(5)
Space Group No.:	14	***(Å,°)***	α	90.00	β	115.18(0)	γ 90.00
R-Factor (%):	6.13	***Temperature(K):***	273		***Density(g/cm³):***		1.314



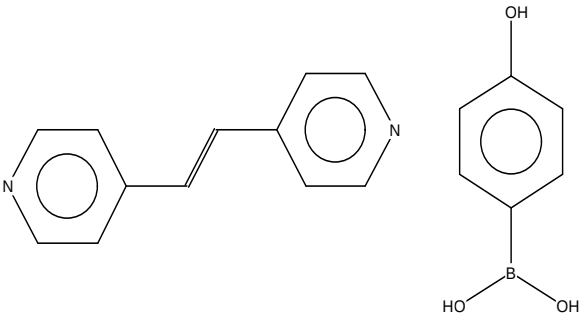
USAKUV

Reference: M.Talwelkar, V.R.Pedireddi (2010) *Tetrahedron Lett.* ,**51,** 6901

Formula: $2(C_{12}H_{10}N_2),C_6H_7B_1O_3,2(H_2O_1)$

Compound Name: (4-Hydroxyphenyl)boronic acid bis(4,4'-ethene-1,2-diyldipyridine) dihydrate

Space Group:	Pbca	***Cell:***	***a***	14.153(5)	***b***	18.022(6)	***c*** 22.548(6)
Space Group No.:	61	***(Å,°)***	α	90.00	β	90.00	γ 90.00
R-Factor (%):	16.31	***Temperature(K):***	293		***Density(g/cm³):***		1.244



H_2O

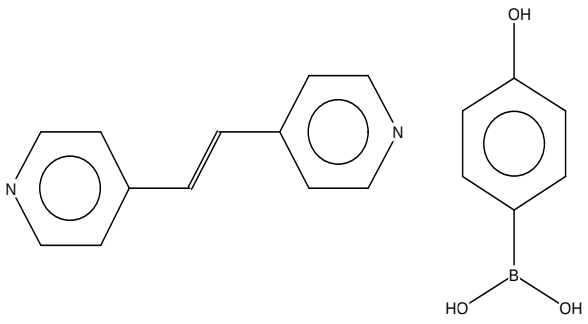
USALAC

Reference: M.Talwelkar, V.R.Pedireddi (2010) *Tetrahedron Lett.* ,**51,** 6901

Formula: $C_{12}H_{10}N_2,C_6H_7B_1O_3,H_2O_1$

Compound Name: (4-Hydroxyphenyl)boronic acid 4,4'-ethene-1,2-diyldipyridine monohydrate

Space Group:	P-1	***Cell:***	***a***	9.269(6)	***b***	9.322(7)	***c*** 11.591(8)
Space Group No.:	2	***(Å,°)***	α	90.80(2)	β	104.90(2)	γ 112.48(2)
R-Factor (%):	16.42	***Temperature(K):***	293		***Density(g/cm³):***		1.266



H_2O

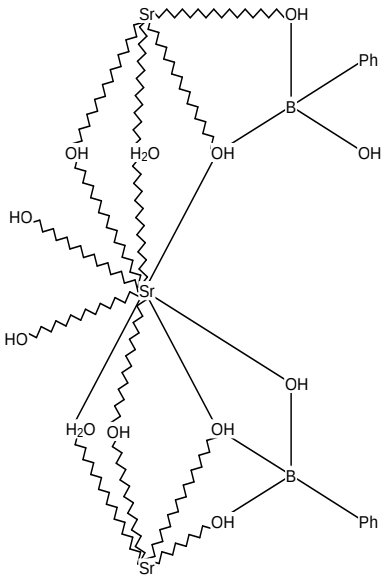
UZUMIM

Reference: M.Reinholdt, J.Croissant, L.Di Carlo, D.Granier, P.Gaveau, S.Begu, J.-M.Devoisselle, P.H.Mutin, M.E.Smith, C.Bonhomme, C.Gervais, A.van der Lee, D.Laurencin (2011) *Inorg.Chem.* ,**50,**7802

Formula: $(C_{12}H_{18}B_2O_7Sr_1)n$

Compound Name: catena-[(μ_2-Phenylboronato-O,O',O'')-(μ_2-phenylboronato-O,O')-(μ_2-aqua)-strontium]

Space Group:	P21/c	***Cell:***	***a***	6.219(0)	***b***	7.957(0)	***c*** 30.764(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	92.78(0)	γ 90.00
R-Factor (%):	6.40	***Temperature(K):***	175		***Density(g/cm³):***		1.675



Search: search4 (Mon May 01 12:48:32 2017): Hits 261-264

VEFCIT

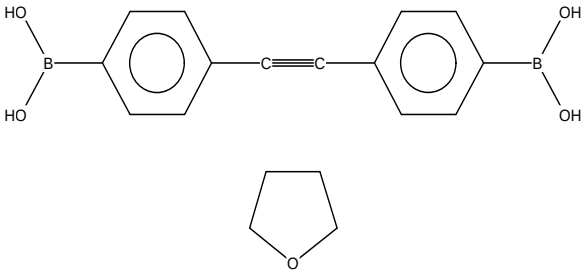
Reference: K.E.Maly, T.Maris, J.D.Wuest (2006) *CrystEngComm* ,**8,**33

Formula: $C_{14}H_{12}B_2O_4,3(C_4H_8O_1)$

Compound Name: 1,2-Ethynediylbis(4,1-phenylene)diboronic acid tetrahydrofuran solvate

Space Group:	P-1	***Cell:***	***a***	6.541(0)	***b***	9.420(0)	***c***	10.812(1)
Space Group No.:	2	***(Å,°)***	α	92.16(0)	β	104.38(0)	γ	96.51(0)

R-Factor (%): 7.19 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.252



VEFCOZ

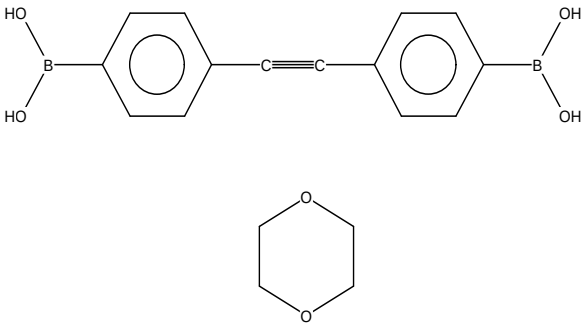
Reference: K.E.Maly, T.Maris, J.D.Wuest (2006) *CrystEngComm* ,**8,**33

Formula: $C_{14}H_{12}B_2O_4,3(C_4H_8O_2)$

Compound Name: 1,2-Ethynediylbis(4,1-phenylene)diboronic acid 1,4-dioxane solvate

Space Group:	P-1	***Cell:***	***a***	6.710(0)	***b***	7.445(0)	***c***	14.138(0)
Space Group No.:	2	***(Å,°)***	α	94.67(0)	β	102.78(0)	γ	98.33(0)

R-Factor (%): 7.25 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.301



VEFCUF

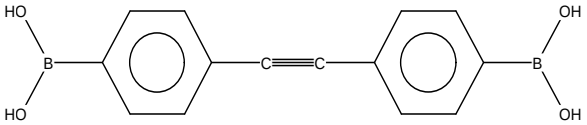
Reference: K.E.Maly, T.Maris, J.D.Wuest (2006) *CrystEngComm* ,**8,**33

Formula: $C_{14}H_{12}B_2O_4$

Compound Name: 1,2-Ethynediylbis(4,1-phenylene)diboronic acid

Space Group:	P21/n	***Cell:***	***a***	11.343(0)	***b***	5.069(0)	***c***	11.581(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	103.74(0)	γ	90.00

R-Factor (%): 3.53 ***Temperature(K):*** 200 ***Density(g/cm³):*** 1.365



VEXFUZ

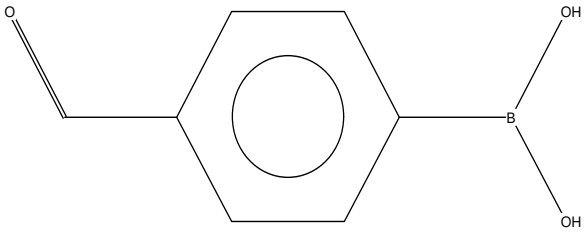
Reference: H.Feulner, G.Linti, H.Noth (1990) *Chem.Ber.* ,**123,**1841

Formula: $C_7H_7B_1O_3$

Compound Name: p-Formylbenzeneboronic acid

Space Group:	P-1	***Cell:***	***a***	7.323(2)	***b***	7.459(2)	***c***	7.464(2)
Space Group No.:	2	***(Å,°)***	α	82.89	β	68.68	γ	68.55

R-Factor (%): 9.72 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.409



Search: search4 (Mon May 01 12:48:32 2017): Hits 265-268

VEXFUZ01

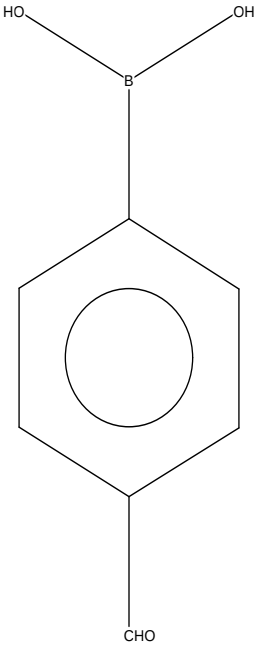
Reference: H.Feulner, G.Linti, H.Noth (1990) *Chem.Ber.* ,**123,**1841

Formula: $C_7 H_7 B_1 O_3$

Compound Name: p-Formylbenzeneboronic acid

Space Group:	C2/c	***Cell:***	***a***	11.177(5)	***b***	9.891(4)	***c***	7.330(4)
Space Group No.:	15	***(Å,°)***	α	90.00	β	119.37(3)	γ	90.00

R-Factor (%): 14.52 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.410



VEXFUZ02

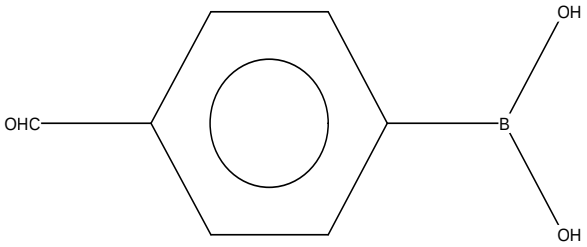
Reference: F.R.Fronczek, N.N.St.Luce, R.M.Strongin (2001) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**57,**1423

Formula: $C_7 H_7 B_1 O_3$

Compound Name: 4-Formylphenylboronic acid

Space Group:	Cc	***Cell:***	***a***	11.124(0)	***b***	9.872(0)	***c***	7.199(0)
Space Group No.:	9	***(Å,°)***	α	90.00	β	119.07(0)	γ	90.00

R-Factor (%): 3.80 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.441



VIVPUM

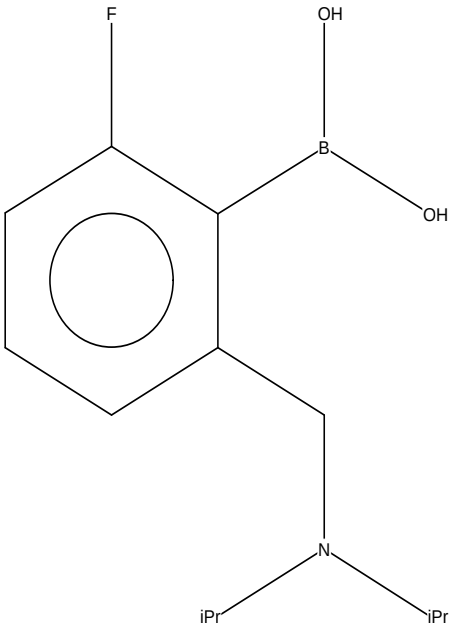
Reference: K.Arnold, A.S.Batsanov, B.Davies, A.Whiting (2008) *Green Chemistry* ,**10,**124

Formula: $C_{13} H_{21} B_1 F_1 N_1 O_2$

Compound Name: N,N-Diisopropyl-3-fluorobenzylamine-2-boronic acid

Space Group:	P21/c	***Cell:***	***a***	13.748(2)	***b***	7.701(1)	***c***	13.781(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	110.97(1)	γ	90.00

R-Factor (%): 3.74 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.234



VIVQAT

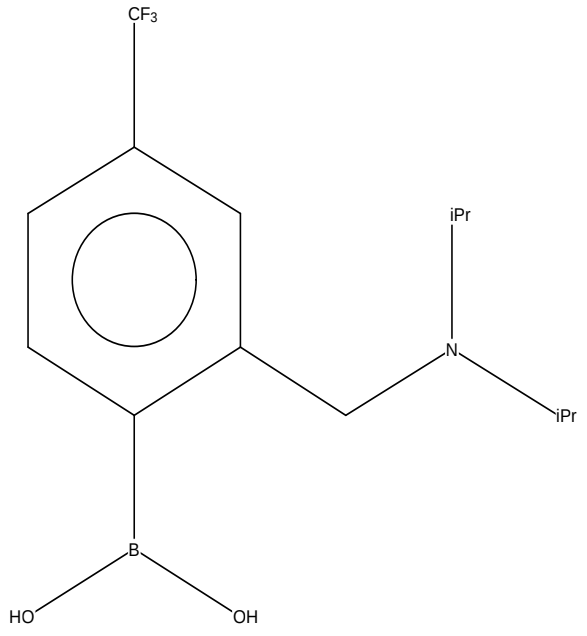
Reference: K.Arnold, A.S.Batsanov, B.Davies, A.Whiting (2008) *Green Chemistry* ,**10,**124

Formula: $C_{14} H_{21} B_1 F_3 N_1 O_2$

Compound Name: N,N-Diisopropyl-5-trifluoromethylbenzylamine-2-boronic acid

Space Group:	P21/c	***Cell:***	***a***	15.465(1)	***b***	7.785(0)	***c***	13.255(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	105.71(1)	γ	90.00

R-Factor (%): 4.20 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.311



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VOSZOU

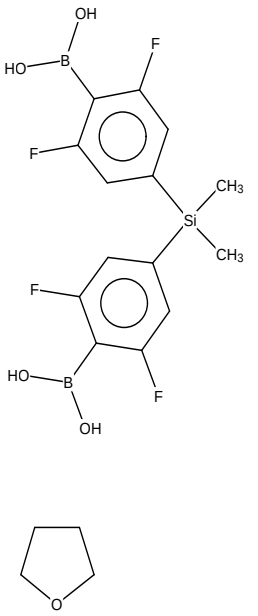
Reference: K.Gontarczyk, K.Durka, P.Klimkowski, S.Lulinski, J.Serwatowski, K.Wozniak (2015) *J.Organomet.Chem.* ,**783,**1

Formula: $C_{14}H_{14}B_2F_4O_4Si_1,0.5(C_4H_8O_1)$

Compound Name: bis(4-Dihydroxyboryl-3,5-difluorophenyl)dimethylsilane tetrahydrofuran solvate

Space Group:	P-1	***Cell:***	***a***	11.372(1)	***b***	14.212(0)	***c***	14.377(1)
Space Group No.:	2	***(Å,°)***	α	67.67(0)	β	70.99(0)	γ	67.21(0)

R-Factor (%): 9.25 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.399



VOSZUA

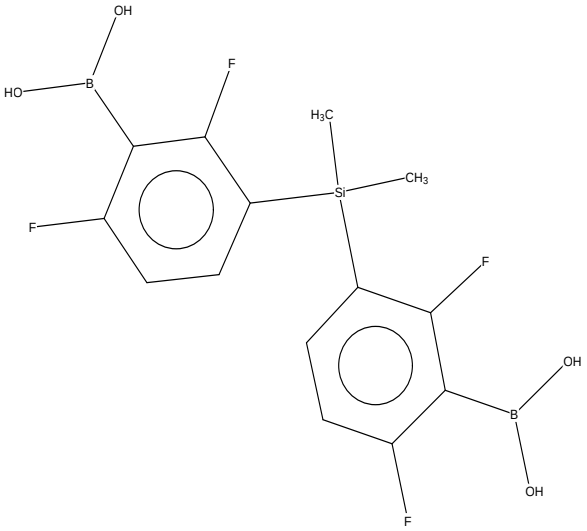
Reference: K.Gontarczyk, K.Durka, P.Klimkowski, S.Lulinski, J.Serwatowski, K.Wozniak (2015) *J.Organomet.Chem.* ,**783,**1

Formula: $C_{14}H_{14}B_2F_4O_4Si_1$

Compound Name: bis(3-Dihydroxyboryl-2,4-difluorophenyl)dimethylsilane

Space Group:	Pnna	***Cell:***	***a***	12.286(0)	***b***	18.087(0)	***c***	7.335(0)
Space Group No.:	52	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 4.52 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.516



VUWHAY

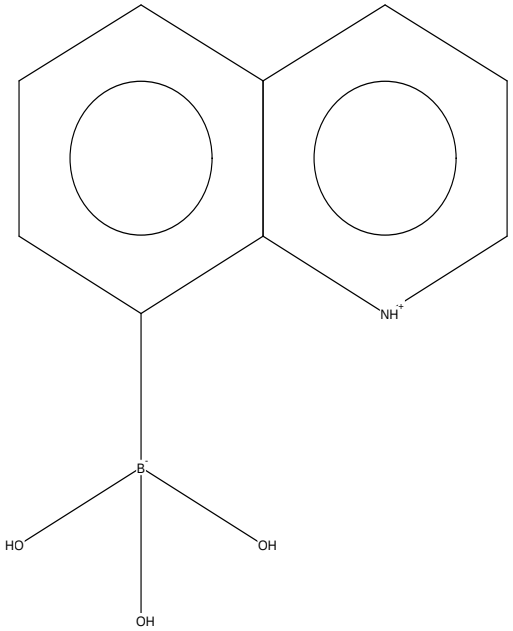
Reference: Jung-Ho Son, Sem Raj Tamang, J.C.Yarbrough, J.D.Hoefelmeyer (2015) *Z.Naturforsch.,B:Chem.Sci.* ,**70,**775

Formula: $C_9H_{10}B_1N_1O_3$

Compound Name: trihydroxy(quinolinium-8-yl)borate

Space Group:	P21/c	***Cell:***	***a***	7.154(0)	***b***	15.845(1)	***c***	7.932(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	114.86(0)	γ	90.00

R-Factor (%): 5.48 ***Temperature(K):*** 101 ***Density(g/cm³):*** 1.555



WADQIC

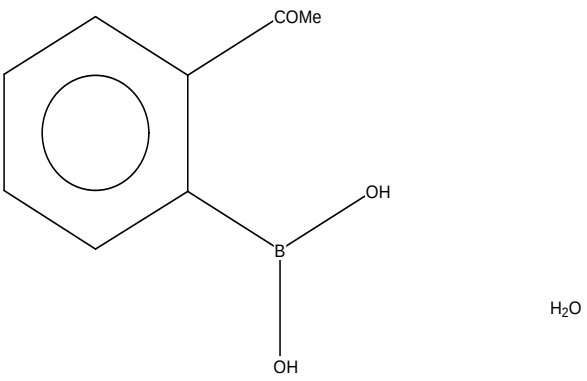
Reference: A.Ganguly, C.Y.Meyers, P.D.Robinson (2003) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**59,**o759

Formula: $C_8H_9B_1O_3,H_2O_1$

Compound Name: 2-Acetylphenylboronic acid monohydrate

Space Group:	P21/c	***Cell:***	***a***	7.884(4)	***b***	8.128(1)	***c***	14.500(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	100.47(2)	γ	90.00

R-Factor (%): 3.40 ***Temperature(K):*** 296 ***Density(g/cm³):*** 1.323



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WAJXEL

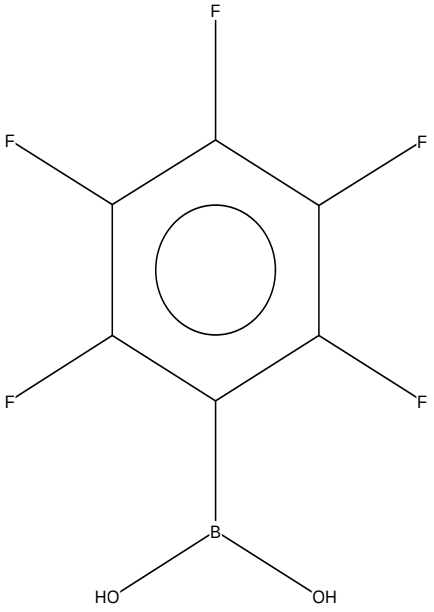
Reference: P.N.Horton, M.B.Hursthouse, M.A.Beckett, M.P.Rugen-Hankey (2004) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* , **60,**o2204

Formula: $C_6 H_2 B_1 F_5 O_2$

Compound Name: Pentafluorophenylboronic acid

Space Group:	P21/c	***Cell:***	***a***	12.621(0)	***b***	6.295(0)	***c***	9.397(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	98.25(0)	γ	90.00

R-Factor (%): 4.40 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.905



WAJXEL01

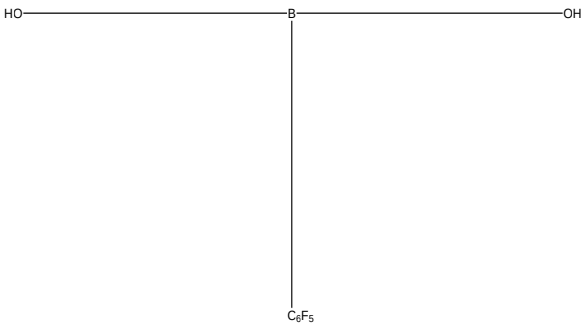
Reference: T.D.Grayfer, A.Yu.Makarov, I.Yu.Bagryanskaya, I.G.Irtegova, Y.V.Gatilov, A.V.Zibarev (2015) *Heteroat.Chem.* ,**26,**42

Formula: $C_6 H_2 B_1 F_5 O_2$

Compound Name: (pentafluorophenyl)boronic acid

Space Group:	P21	***Cell:***	***a***	7.455(1)	***b***	5.007(0)	***c***	10.055(1)
Space Group No.:	4	***(Å,°)***	α	90.00	β	96.78(0)	γ	90.00

R-Factor (%): 3.96 ***Temperature(K):*** 240 ***Density(g/cm³):*** 1.888



WAPDIB

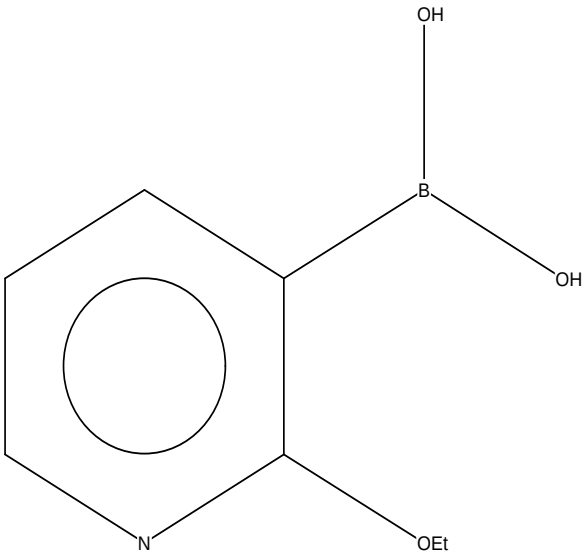
Reference: A.E.Thompson, A.S.Batsanov, M.R.Bryce, N.Saygili, P.R.Parry, B.Tarbit (2005) *Tetrahedron* ,**61,**5131

Formula: $C_7 H_{10} B_1 N_1 O_3$

Compound Name: 2-Ethoxy-3-pyridylboronic acid

Space Group:	P21/n	***Cell:***	***a***	3.940(1)	***b***	14.335(2)	***c***	14.226(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	94.60(1)	γ	90.00

R-Factor (%): 3.99 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.385



WAYVEZ

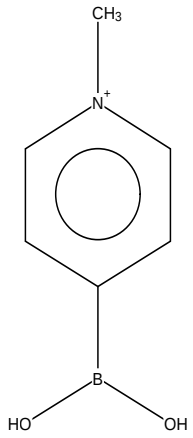
Reference: S.Iwatsuki, Y.Kanamitsu, H.Ohara, M.Kawahata, H.Danjo, K.Ishihara (2012) *X-ray.Str.Anal.Online.* ,**28,**63

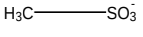
Formula: $C_6 H_9 B_1 N_1 O_2\ ^{1+}, C_1 H_3 O_3 S_1\ ^{1-}, H_2 O_1$

Compound Name: 4-(Dihydroxyboryl)-1-methylpyridinium methanesulfonate monohydrate

Space Group:	P-1	***Cell:***	***a***	5.694(1)	***b***	7.805(2)	***c***	13.522(3)
Space Group No.:	2	***(Å,°)***	α	99.46(3)	β	91.45(3)	γ	108.01(1)

R-Factor (%): 4.32 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.484





H_2O

Search: search4 (Mon May 01 12:48:32 2017): Hits 277-280

WEJCIY

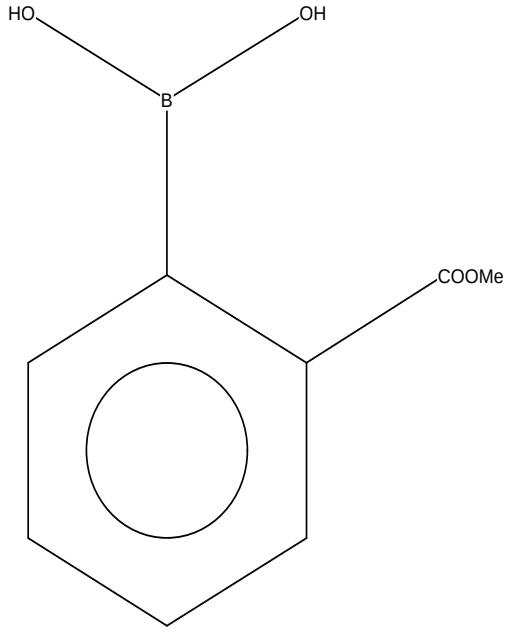
Reference: S.Lulinski, J.Serwatowski (2006)
Acta Crystallogr.,Sect.C:Cryst.Struct.Commun. ,**62,**o301

Formula: $C_8 H_9 B_1 O_4$

Compound Name: 2-(Methoxycarbonyl)phenylboronic acid

Space Group:	P21/m	***Cell:***	***a***	8.276(0)	***b***	19.712(0)	***c***	8.732(0)
Space Group No.:	11	***(Å,°)***	α	90.00	β	115.01(0)	γ	90.00

R-Factor (%): 3.25 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.389



WENZUL

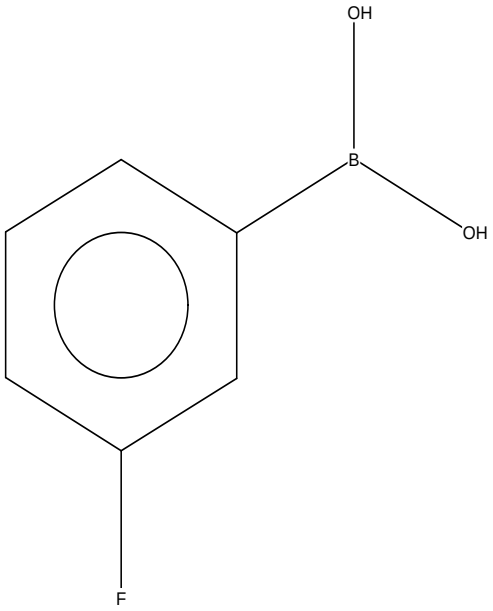
Reference: Ya-Ming Wu, Chang-Chuan Dong, Shan Liu, Hong-Jun Zhu, Yi-Zu Wu (2006)
Acta Crystallogr.,Sect.E:Struct.Rep.Online ,**62,**o4236

Formula: $C_6 H_6 B_1 F_1 O_2$

Compound Name: 3-Fluorophenylboronic acid

Space Group:	P21/c	***Cell:***	***a***	5.756(1)	***b***	5.027(1)	***c***	22.402(5)
Space Group No.:	14	***(Å,°)***	α	90.00	β	91.19(3)	γ	90.00

R-Factor (%): 8.43 ***Temperature(K):*** 294 ***Density(g/cm³):*** 1.434



WIYMEX

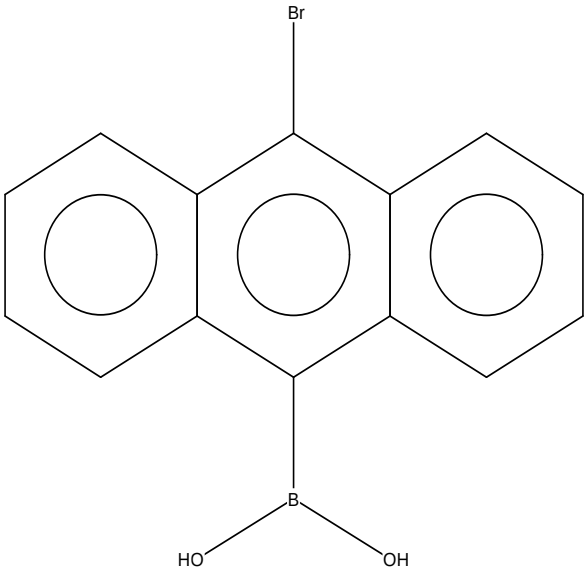
Reference: M.Filthaus, I.M.Oppel, H.F.Bettinger (2008)
Org.Biomol.Chem. ,**6,**1201

Formula: $C_{14} H_{10} B_1 Br_1 O_2$

Compound Name: (10-bromo-9-anthracenyl)boronic acid

Space Group:	P21212	***Cell:***	***a***	14.468(0)	***b***	17.094(1)	***c***	4.920(0)
Space Group No.:	18	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 2.40 ***Temperature(K):*** 108 ***Density(g/cm³):*** 1.643



WIYMOH

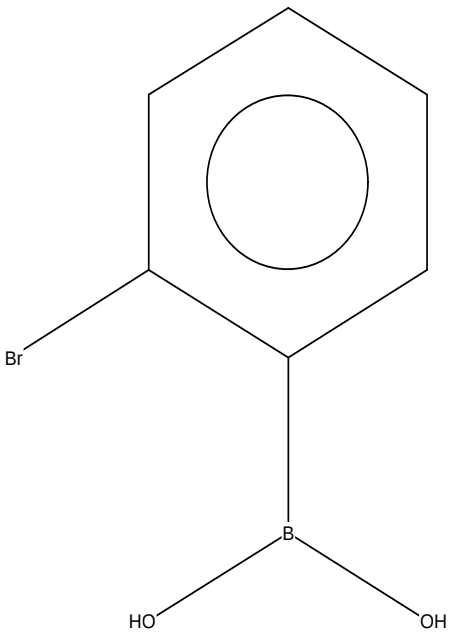
Reference: M.Filthaus, I.M.Oppel, H.F.Bettinger (2008)
Org.Biomol.Chem. ,**6,**1201

Formula: $C_6 H_6 B_1 Br_1 O_2$

Compound Name: 2-bromophenylboronic acid

Space Group:	P-1	***Cell:***	***a***	4.957(0)	***b***	7.056(1)	***c***	10.757(1)
Space Group No.:	2	***(Å,°)***	α	95.77(1)	β	92.22(1)	γ	96.61(1)

R-Factor (%): 2.41 ***Temperature(K):*** 108 ***Density(g/cm³):*** 1.796



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WIYMOH01

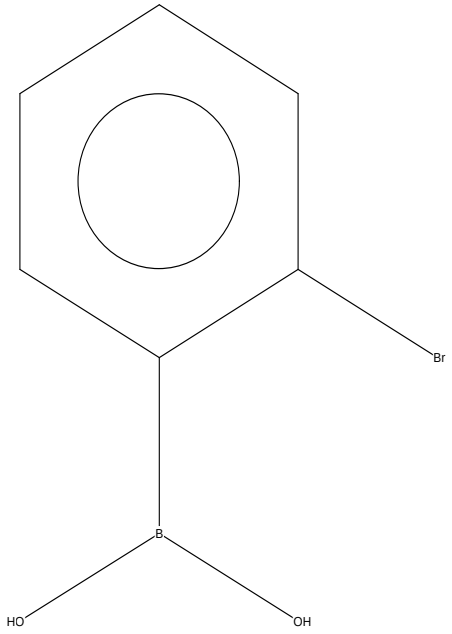
Reference: A.Schnurr, M.Bolte (2010)
CSD Communication(Private Communication) ,

Formula: $C_6 H_6 B_1 Br_1 O_2$

Compound Name: (2-Bromophenyl)boronic acid

Space Group: P-1 ***Cell:*** ***a*** 4.945(0) ***b*** 7.073(0) ***c*** 10.756(1)
Space Group No.: 2 ***(Å,°)*** α 95.09(0) β 92.76(0) γ 96.84(0)

R-Factor (%): 4.18 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.796



WIYMUN

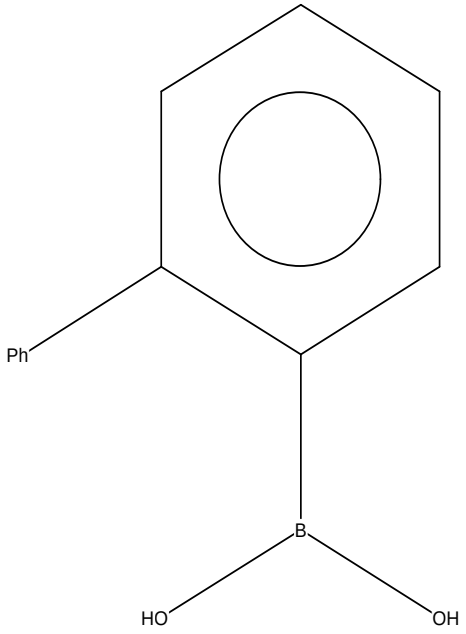
Reference: M.Filthaus, I.M.Oppel, H.F.Bettinger (2008)
Org.Biomol.Chem. ,**6,**1201

Formula: $C_{12} H_{11} B_1 O_2$

Compound Name: (1,1'-biphenyl-2-yl)boronic acid

Space Group: P-1 ***Cell:*** ***a*** 8.264(0) ***b*** 9.289(0) ***c*** 14.548(1)
Space Group No.: 2 ***(Å,°)*** α 98.51(0) β 105.00(1) γ 99.90(0)

R-Factor (%): 6.15 ***Temperature(K):*** 108 ***Density(g/cm³):*** 1.264



WIYMUN01

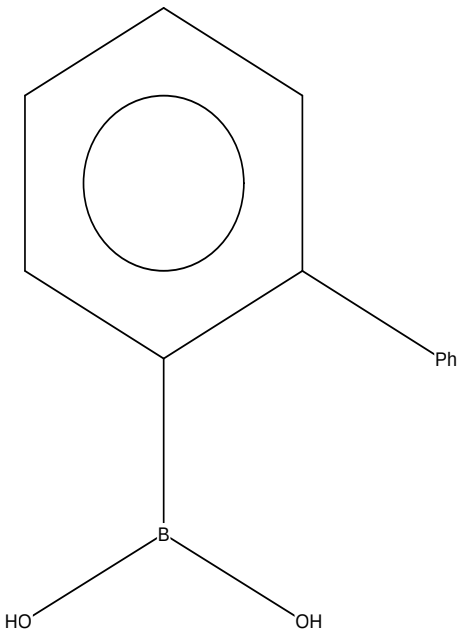
Reference: Su-Zhen Bai, Xin-Hua Lou, Hong-Mei Li, Wei-Chun Yang, Hui Shi (2010) *Z.Kristallogr.-New Cryst.Struct.* ,**225,**295

Formula: $C_{12} H_{11} B_1 O_2$

Compound Name: 2-Biphenylboronic acid

Space Group: P-1 ***Cell:*** ***a*** 8.313(1) ***b*** 9.420(1) ***c*** 14.687(3)
Space Group No.: 2 ***(Å,°)*** α 99.25(0) β 104.53(0) γ 100.31(0)

R-Factor (%): 4.34 ***Temperature(K):*** 296 ***Density(g/cm³):*** 1.230



WIYNAU

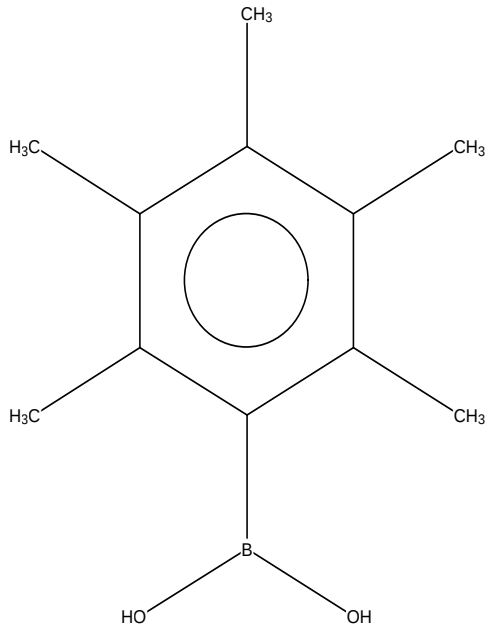
Reference: M.Filthaus, I.M.Oppel, H.F.Bettinger (2008)
Org.Biomol.Chem. ,**6,**1201

Formula: $C_{11} H_{17} B_1 O_2$

Compound Name: (2,3,4,5,6-pentamethylphenyl)boronic acid

Space Group: Aba2 ***Cell:*** ***a*** 31.624(4) ***b*** 15.161(1) ***c*** 9.156(1)
Space Group No.: 41 ***(Å,°)*** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.06 ***Temperature(K):*** 108 ***Density(g/cm³):*** 1.162



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WIYPEA

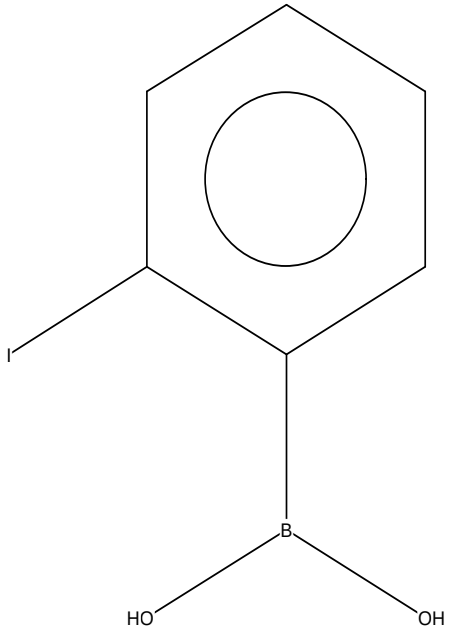
Reference: R.M.Al-Zoubi, O.Marion, D.G.Hall (2008) *Angew.Chem.,Int.Ed.* ,**47,**2876

Formula: $C_6 H_6 B_1 I_1 O_2$

Compound Name: 2-iodophenylboronic acid

Space Group:	P-1	***Cell:***	***a***	4.913(0)	***b***	7.259(0)	***c***	11.190(1)
Space Group No.:	2	***(Å,°)***	α	93.44(0)	β	92.23(0)	γ	95.73(0)

R-Factor (%): 2.57 ***Temperature(K):*** 193 ***Density(g/cm³):*** 2.078



WUMKAS

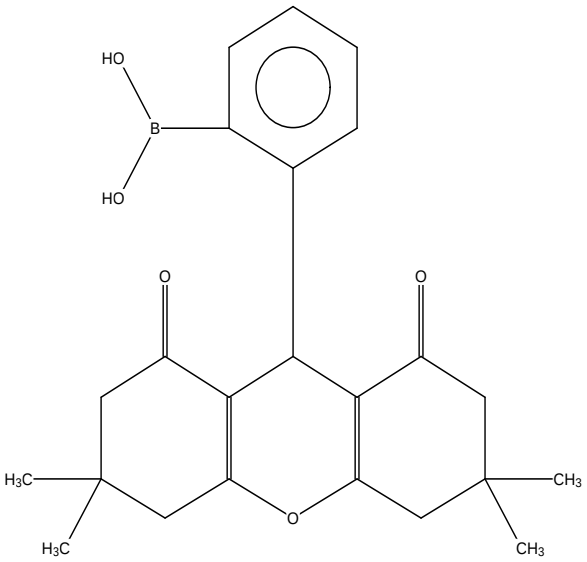
Reference: O.Rusin, R.M.Strongin, F.R.Fronczek (2015) *CSD Communication(Private Communication)* ,

Formula: $C_{23} H_{27} B_1 O_5$

Compound Name: (2-(3,3,6,6-tetramethyl-1,8-dioxo-2,3,4,5,6,7,8,9-octahydro-1H-xanthen-9-yl)phenyl)boronic acid

Space Group:	P-1	***Cell:***	***a***	10.018(2)	***b***	10.634(2)	***c***	21.644(6)
Space Group No.:	2	***(Å,°)***	α	77.47(0)	β	77.66(0)	γ	67.46(1)

R-Factor (%): 5.20 ***Temperature(K):*** 110 ***Density(g/cm³):*** 1.273



XAJNUU

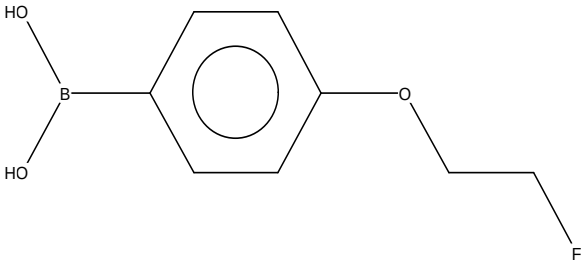
Reference: B.Beutel, C.G.Daniliuc, B.Riemann, M.Schafers, G.Haufe (2016) *Bioorg.Med.Chem.* ,**24,**902

Formula: $C_8 H_{10} B_1 F_1 O_3$

Compound Name: (4-(2-Fluoroethoxy)phenyl)boronic acid

Space Group:	C2/c	***Cell:***	***a***	18.893(0)	***b***	5.032(0)	***c***	19.247(0)
Space Group No.:	15	***(Å,°)***	α	90.00	β	107.63(0)	γ	90.00

R-Factor (%): 4.67 ***Temperature(K):*** 223 ***Density(g/cm³):*** 1.402



XAVHUZ

Reference: M.Ikeda, T.Tanida, T.Yoshii, I.Hamachi (2011) *Adv.Mater.* , **23,**2819

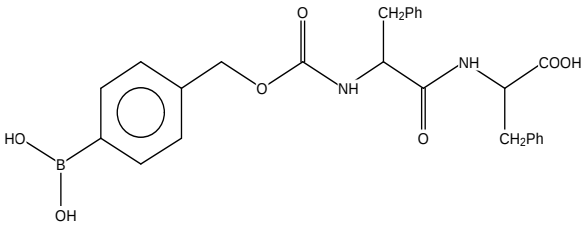
Formula: $C_{26} H_{27} B_1 N_2 O_7$

Compound Name: N-(((4-(Dihydroxyboryl)benzyl)oxy)carbonyl)phenylalanylphenylalanine

Synonym: Acyclic peptide (2 residues): PHE*-PHE

Space Group:	P21212	***Cell:***	***a***	20.532(0)	***b***	24.694(1)	***c***	9.831(0)
Space Group No.:	18	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 7.49 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.307



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XECHOD

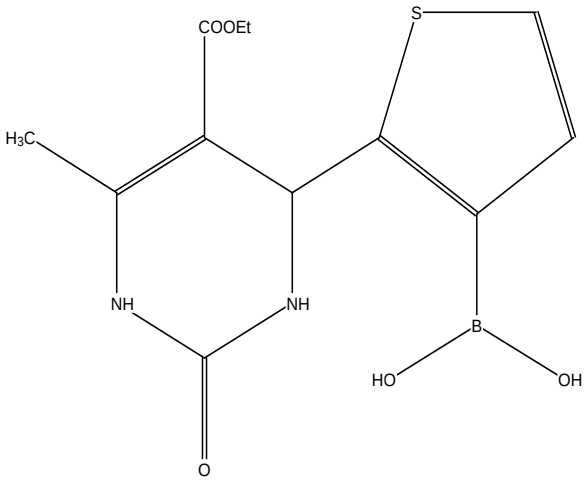
Reference: J.M.Blacquiere, O.Sicora, C.M.Vogels, M.Cuperlovic-Culf, A.Decken, R.J.Quellette, S.A.Westcott (2005) *Can.J.Chem.* ,**83,**2052

Formula: $C_{12}\,H_{15}\,B_1\,N_2\,O_5\,S_1$

Compound Name: 2-(5-Ethoxycarbonyl-4-methyl-2-oxo-3,6-dihydro-1H-pyrimidin-6-yl)thiene 3-boronic acid

Space Group:	P21/n	***Cell:***	***a***	10.991(0)	***b***	12.027(0)	***c***	11.696(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	108.79(0)	γ	90.00

R-Factor (%): 3.75 ***Temperature(K):*** 198 ***Density(g/cm³):*** 1.407



XECHUJ

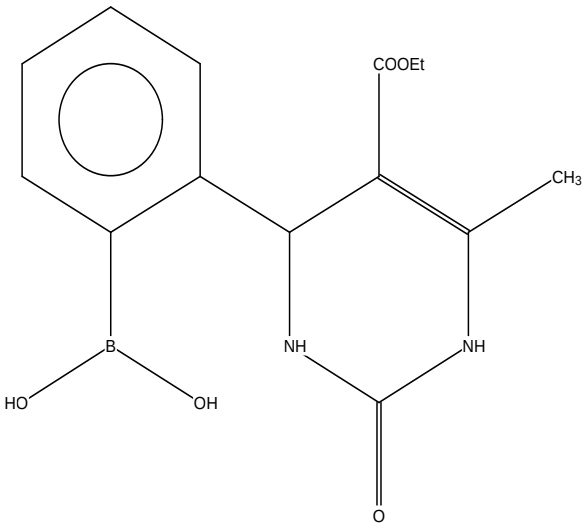
Reference: J.M.Blacquiere, O.Sicora, C.M.Vogels, M.Cuperlovic-Culf, A.Decken, R.J.Quellette, S.A.Westcott (2005) *Can.J.Chem.* ,**83,**2052

Formula: $C_{14}\,H_{17}\,B_1\,N_2\,O_5$

Compound Name: 2-(5-Ethoxycarbonyl-4-methyl-2-oxo-3,6-dihydro-1H-pyrimidin-6-yl) phenylboronic acid

Space Group:	P21/n	***Cell:***	***a***	11.528(0)	***b***	11.969(0)	***c***	11.618(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	109.43(0)	γ	90.00

R-Factor (%): 4.37 ***Temperature(K):*** 198 ***Density(g/cm³):*** 1.336



XETLOY

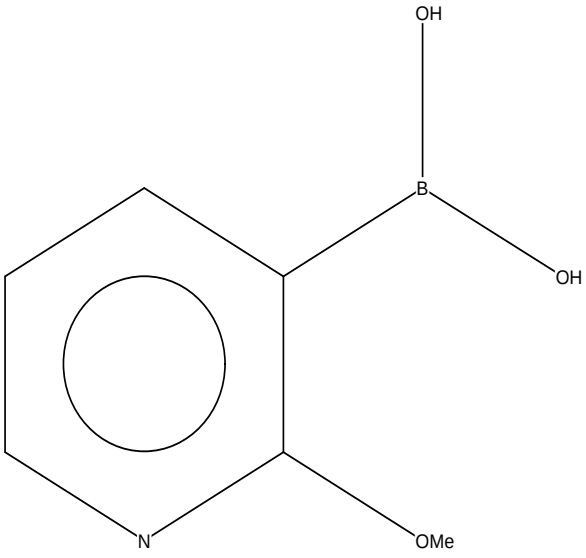
Reference: M.Dabrowski, S.Lulinski, J.Serwatowski, M.Szczerbinska (2006) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**62,**o702

Formula: $C_6\,H_8\,B_1\,N_1\,O_3$

Compound Name: (2-Methoxy-3-pyridyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	7.634(0)	***b***	25.740(1)	***c***	7.244(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	100.86(0)	γ	90.00

R-Factor (%): 3.00 ***Temperature(K):*** 102 ***Density(g/cm³):*** 1.453



XOQVIJ

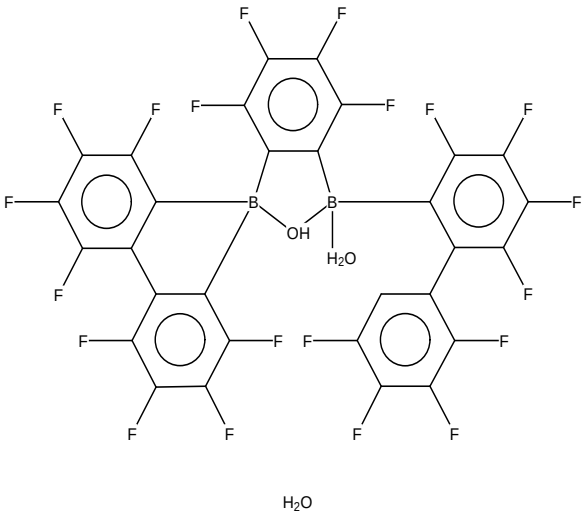
Reference: S.P.Lewis, Jianfang Chai, S.Collins, T.J.J.Sciarone, L.D.Henderson, Cheng Fan, M.Parvez, W.E.Piers (2009) *Organometallics* ,**28,**249

Formula: $C_{30}\,H_4\,B_2\,F_{20}\,O_2,6(H_2\,O_1)$

Compound Name: (μ_2-Hydroxo)-(μ_2-3,4,5,6-tetrafluoro-o-phenylene)-(2-(2,3,4,5-tetrafluorophenyl)-3,4,5,6-tetrafluorophenyl)-(3,3',4,4',5,5',6,6'-octafluorobiphenyl-2,2'-diyl)-aqua-di-boron hexahydrate

Space Group:	Pbca	***Cell:***	***a***	10.163(2)	***b***	19.094(2)	***c***	35.176(5)
Space Group No.:	61	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 4.62 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.763



H_2O

Search: search4 (Mon May 01 12:48:32 2017): Hits 293-296

XOSDOZ

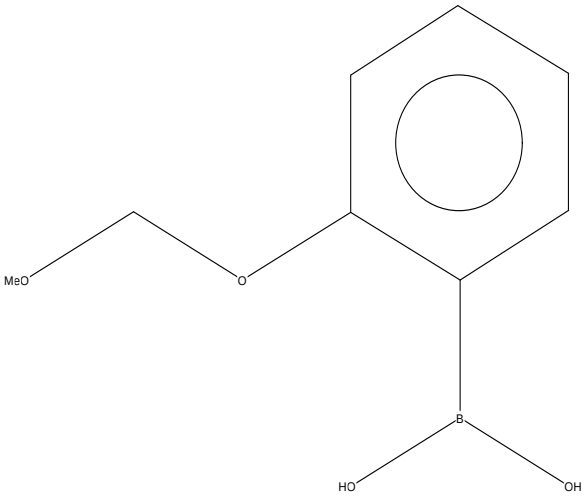
Reference: A.Adamczyk-Wozniak, M.K.Cyranski, A.Dabrowska, B.Gierczyk, P.Klimentowska, G.Schroeder, A.Zubrowska, A.Sporzynski (2009) *J.Mol.Struct.* ,**920,**430

Formula: $C_8 H_{11} B_1 O_4$

Compound Name: (2-(Methoxymethoxy)phenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	5.278(0)	***b***	12.555(1)	***c***	13.737(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	94.16(1)	γ	90.00

R-Factor (%): 3.60 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.331



XOSDUF

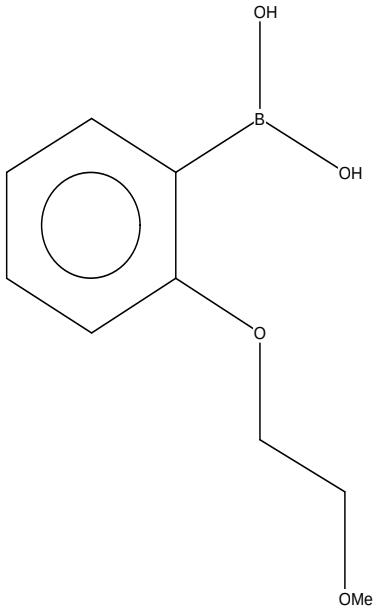
Reference: A.Adamczyk-Wozniak, M.K.Cyranski, A.Dabrowska, B.Gierczyk, P.Klimentowska, G.Schroeder, A.Zubrowska, A.Sporzynski (2009) *J.Mol.Struct.* ,**920,**430

Formula: $C_9 H_{13} B_1 O_4$

Compound Name: (2-(2-Methoxyethoxy)phenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	10.847(1)	***b***	12.203(1)	***c***	23.256(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	99.00(1)	γ	90.00

R-Factor (%): 2.85 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.285



XOSFAN

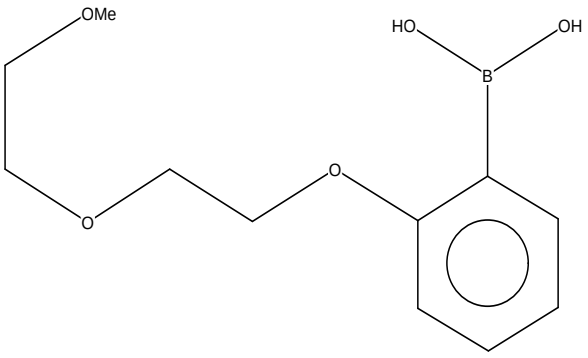
Reference: A.Adamczyk-Wozniak, M.K.Cyranski, A.Dabrowska, B.Gierczyk, P.Klimentowska, G.Schroeder, A.Zubrowska, A.Sporzynski (2009) *J.Mol.Struct.* ,**920,**430

Formula: $C_{11} H_{17} B_1 O_5$

Compound Name: (2-(2-(2-Methoxyethoxy)ethoxy)phenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	11.181(0)	***b***	7.345(0)	***c***	15.420(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	95.64(0)	γ	90.00

R-Factor (%): 3.55 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.265



XUVBAR

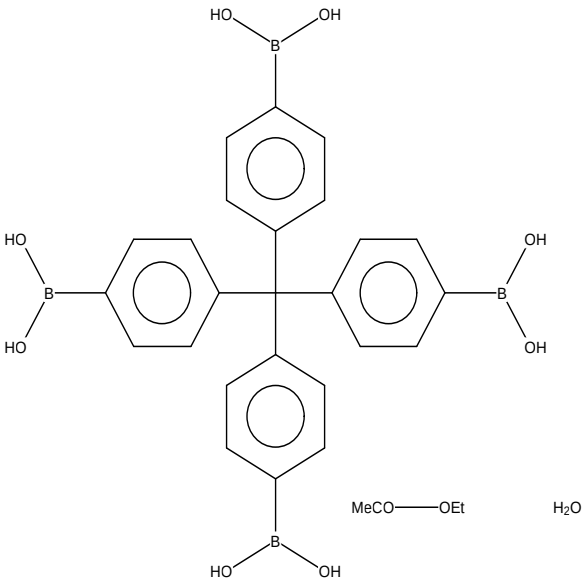
Reference: J.-H.Fournier, T.Maris, J.D.Wuest, Wenzhuo Guo, E.Galoppini (2003) *J.Am.Chem.Soc.* ,**125,**1002

Formula: $C_{25} H_{24} B_4 O_8$,5($C_4 H_8 O_2$),$H_2 O_1$

Compound Name: (Methanetetrayltetra-4,1-phenylene)tetrakis(boronic acid) pentakis(ethyl acetate) hydrate clathrate

Space Group:	I41/a	***Cell:***	***a***	10.627(11)	***b***	10.627(11)	***c***	41.608(6)
Space Group No.:	88	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 9.78 ***Temperature(K):*** 226 ***Density(g/cm³):*** 1.349



Search: search4 (Mon May 01 12:48:32 2017): Hits 297-300

XUVBEV

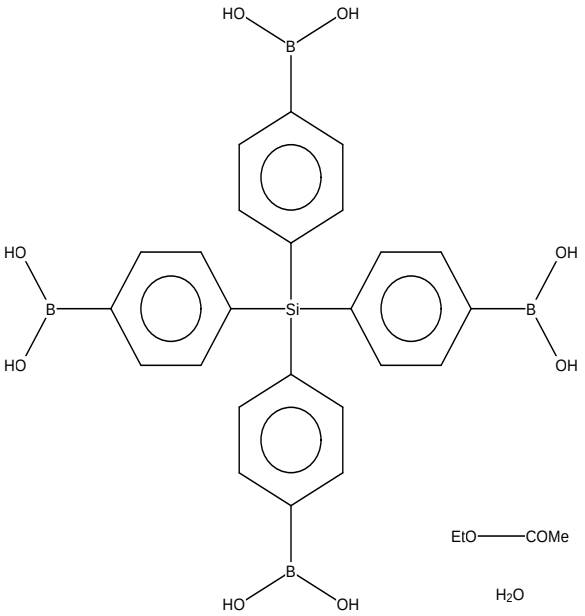
Reference: J.-H.Fournier, T.Maris, J.D.Wuest, Wenzhuo Guo, E.Galoppini (2003) *J.Am.Chem.Soc.* ,**125,**1002

Formula: $C_{24}\,H_{24}\,B_4\,O_8\,Si_1,5(C_4\,H_8\,O_2),H_2\,O_1$

Compound Name: (Silanetetrayltetra-4,1-phenylene)tetrakis(boronic acid) pentakis(ethyl acetate) hydrate clathrate

Space Group:	I41/a	***Cell:***	***a***	10.837(1)	***b***	10.837(1)	***c***	45.603(9)
Space Group No.:	88	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 7.58 ***Temperature(K):*** 210 ***Density(g/cm³):*** 1.203



XUVTUF

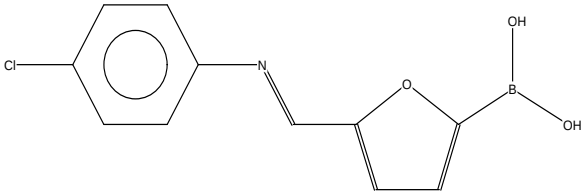
Reference: V.E.Gonzalez, P.Lacroix, V.Barba (2015) *Inorg.Chim.Acta* , **438,**23

Formula: $C_{11}\,H_9\,B_1\,Cl_1\,N_1\,O_3$

Compound Name: (5-((4-chlorophenyl)carbonoimidoyl)-2-furyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	7.523(3)	***b***	10.036(4)	***c***	15.503(6)
Space Group No.:	14	***(Å,°)***	α	90.00	β	102.03(0)	γ	90.00

R-Factor (%): 3.32 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.447



YEJLIK

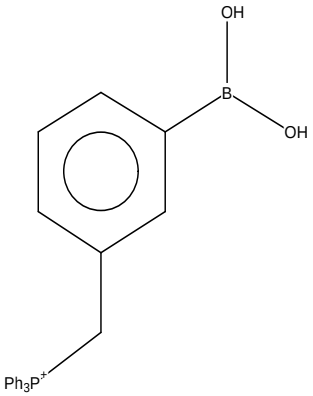
Reference: L.J.Farrugia, R.C.Hartley, S.J.McQuaker, M.P.Murphy (2012) *CSD Communication(Private Communication)* ,

Formula: $C_{25}\,H_{23}\,B_1\,O_2\,P_1\,^{1+},Br_1\,^{1-}$

Compound Name: (3-(Dihydroxyboryl)benzyl)(triphenyl)phosphonium bromide

Space Group:	Pn	***Cell:***	***a***	9.808(0)	***b***	9.476(0)	***c***	12.025(0)
Space Group No.:	7	***(Å,°)***	α	90.00	β	94.75(0)	γ	90.00

R-Factor (%): 1.99 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.423



Br-

YEJLIK01

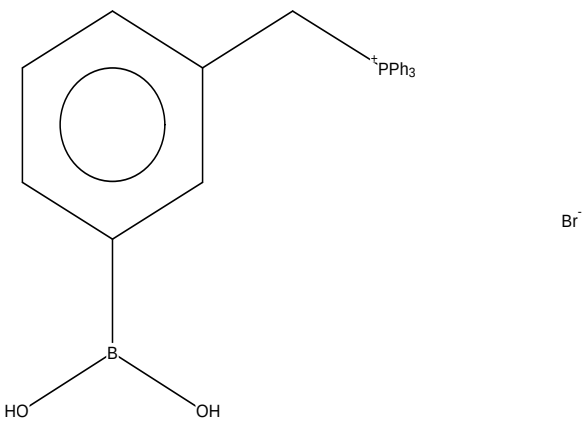
Reference: G.J.Tizzard, M.B.Hursthouse, J.Spencer (2009) *University of Southampton, Crystal Structure Report Archive* ,1047

Formula: $C_{25}\,H_{23}\,B_1\,O_2\,P_1\,^{1+},Br_1\,^{1-}$

Compound Name: (3-(dihydroxyboryl)benzyl)(triphenyl)phosphonium bromide

Space Group:	Pn	***Cell:***	***a***	9.828(0)	***b***	9.488(0)	***c***	12.039(0)
Space Group No.:	7	***(Å,°)***	α	90.00	β	94.74(0)	γ	90.00

R-Factor (%): 4.28 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.416



Search: search4 (Mon May 01 12:48:32 2017): Hits 301-304

YESZAY

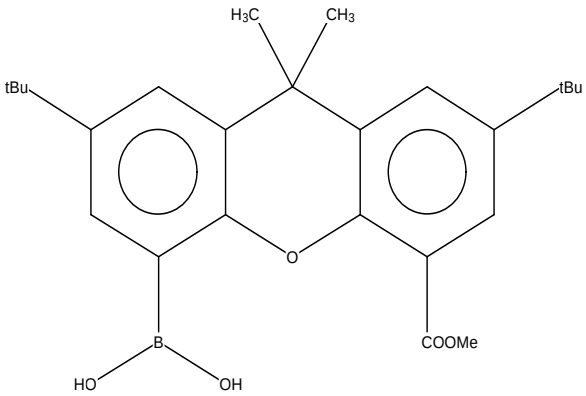
Reference: J.Y.Yang, J.Bachmann, D.G.Nocera (2006) *J.Org.Chem.* , **71,**8706

Formula: $C_{25}H_{33}B_1O_5$

Compound Name: Methyl 5-(boronic acid)-2,7-di-t-butyl-9,9-dimethyl-9H-xanthene-4-carboxylate

Space Group:	P-1	***Cell:***	***a***	9.157(7)	***b***	11.143(10)	***c***	12.500(11)
Space Group No.:	2	***(Å,°)***	α	77.03(1)	β	83.05(1)	γ	79.42(1)

R-Factor (%): 9.70 ***Temperature(K):*** 467 ***Density(g/cm³):*** 1.157



YICHIB

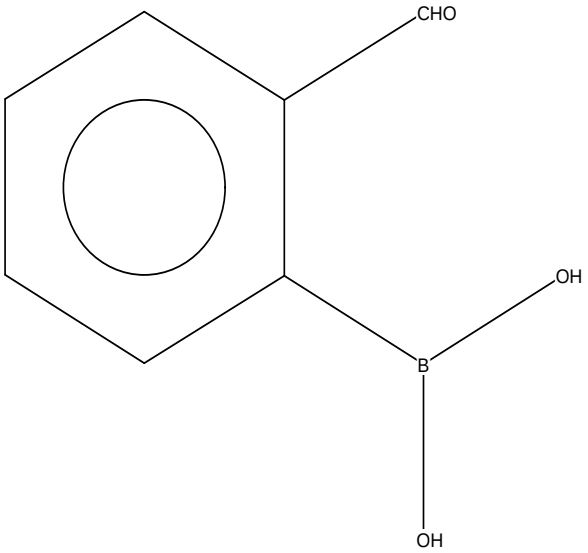
Reference: W.H.Scouten, X.-C.Liu, N.Khangin, D.F.Mullica, E.L.Sappenfield (1994) *J.Chem.Cryst.* ,**24,**621

Formula: $C_7H_7B_1O_3$

Compound Name: o-Formylbenzeneboronic acid

Space Group:	P21/n	***Cell:***	***a***	3.883	***b***	13.225	***c***	14.029
Space Group No.:	14	***(Å,°)***	α	90.00	β	92.16	γ	90.00

R-Factor (%): 3.70 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.383



YICHIB01

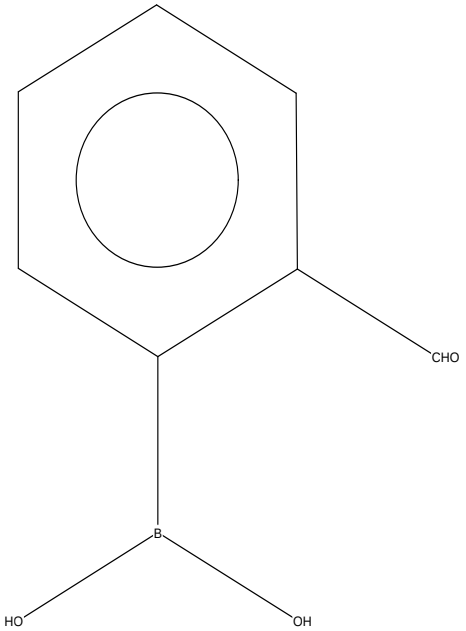
Reference: I.D.Madura, A.Adamczyk-Wozniak, A.Sporzynski (2015) *J.Mol.Struct.* ,**1083,**204

Formula: $C_7H_7B_1O_3$

Compound Name: 2-Formylphenyl boronic acid

Space Group:	P21/c	***Cell:***	***a***	3.781(0)	***b***	13.099(0)	***c***	13.984(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	91.11(0)	γ	90.00

R-Factor (%): 3.72 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.438



YICHOH

Reference: W.H.Scouten, X.-C.Liu, N.Khangin, D.F.Mullica, E.L.Sappenfield (1994) *J.Chem.Cryst.* ,**24,**621

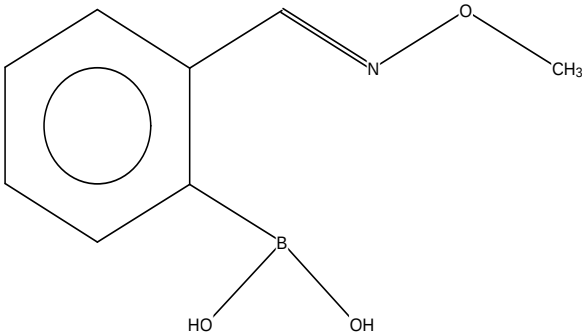
Formula: $C_8H_{10}B_1N_1O_3$

Compound Name: o-Methoxyiminomethylbenzeneboronic acid

Synonym: o-Boronobenzalmethoxyamine

Space Group:	Pccn	***Cell:***	***a***	14.158	***b***	17.156	***c***	7.734
Space Group No.:	56	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 5.80 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.266



Search: search4 (Mon May 01 12:48:32 2017): Hits 305-308

YIPJIS

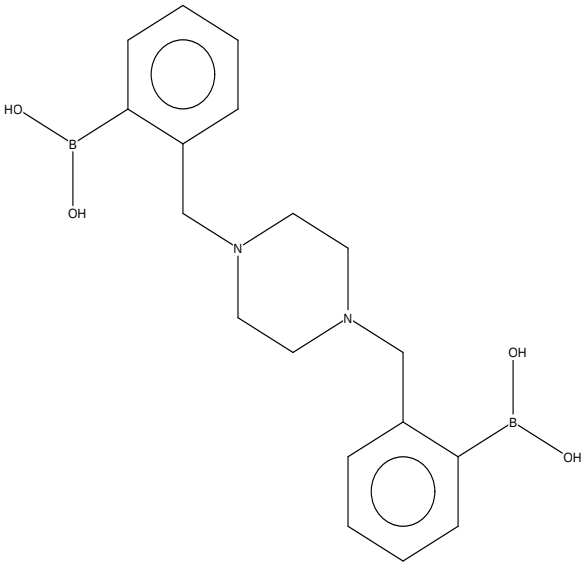
Reference: A.Adamczyk-Wozniak, K.M.Borys, I.D.M.S.Michalek, A.Pawelko (2013) *Tetrahedron* ,**69,**8936

Formula: $C_{18}H_{24}B_2N_2O_4$

Compound Name: (Piperazine-1,4-diylbis(methylene-2,1-phenylene))diboronic acid

Space Group:	P21/c	***Cell:***	***a***	6.037(0)	***b***	7.749(0)	***c*** 19.983(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	92.89(0)	γ 90.00

R-Factor (%): 3.56 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.259



YIPJOY

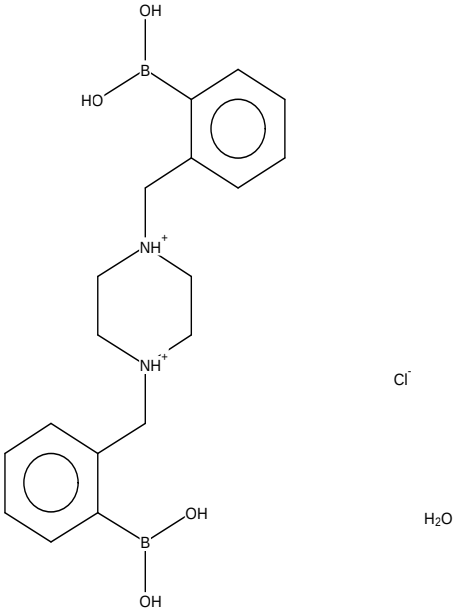
Reference: A.Adamczyk-Wozniak, K.M.Borys, I.D.M.S.Michalek, A.Pawelko (2013) *Tetrahedron* ,**69,**8936

Formula: $C_{18}H_{26}B_2N_2O_4^{2+},6(H_2O_1),2(Cl_1^{1-})$

Compound Name: 1,4-bis(2-(dihydroxyboryl)benzyl)piperazinediium dichloride hexahydrate

Space Group:	P21/c	***Cell:***	***a***	11.571(0)	***b***	16.199(0)	***c*** 7.147(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	107.98(0)	γ 90.00

R-Factor (%): 2.71 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.395



YIWKOE

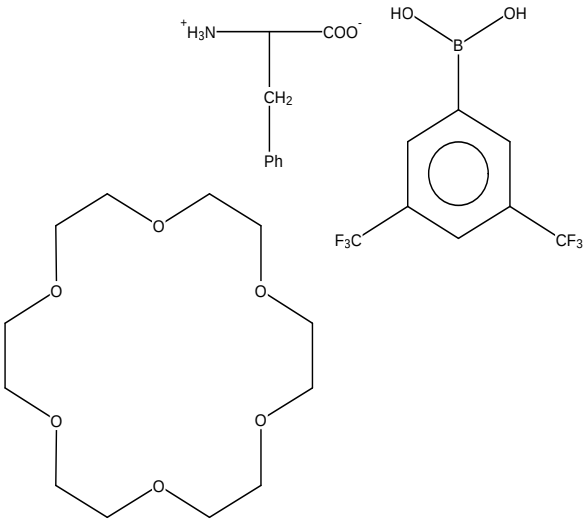
Reference: M.T.Reetz, J.Huff, J.Rudolph, K.Tollner, A.Deege, R.Goddard (1994) *J.Am.Chem.Soc.* ,**116,**11588

Formula: $C_9H_{11}N_1O_2,C_8H_5B_1F_6O_2,C_{12}H_{24}O_6$

Compound Name: Phenylalanine 3,5-bis(trifluoromethyl)phenylboronic acid 18-crown-6

Space Group:	P1	***Cell:***	***a***	8.853	***b***	9.261	***c*** 12.141
Space Group No.:	1	***(Å,°)***	α	85.39	β	89.00	γ 61.38

R-Factor (%): 9.30 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.311



YOQZIO

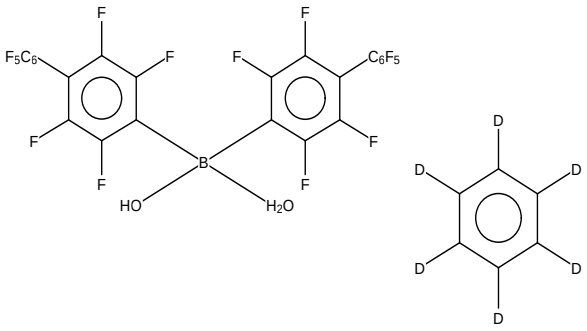
Reference: E.Martin, D.L.Hughes, M.B.Hursthouse, L.Male, S.J.Lancaster (2009) *Dalton Trans.* ,1593

Formula: $C_{24}H_3B_1F_{18}O_2,3(C_6D_6)$

Compound Name: bis(2,2',3,3',4',5,5',6,6'-nonafluorobiphenyl-4-yl)(aqua)(hydroxy)boron perdeuterobenzene solvate

Space Group:	P-1	***Cell:***	***a***	7.081(0)	***b***	14.562(0)	***c*** 18.471(0)
Space Group No.:	2	***(Å,°)***	α	92.21(0)	β	95.50(0)	γ 99.80(0)

R-Factor (%): 5.20 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.653



Search: search4 (Mon May 01 12:48:32 2017): Hits 309-312

YUTQEL

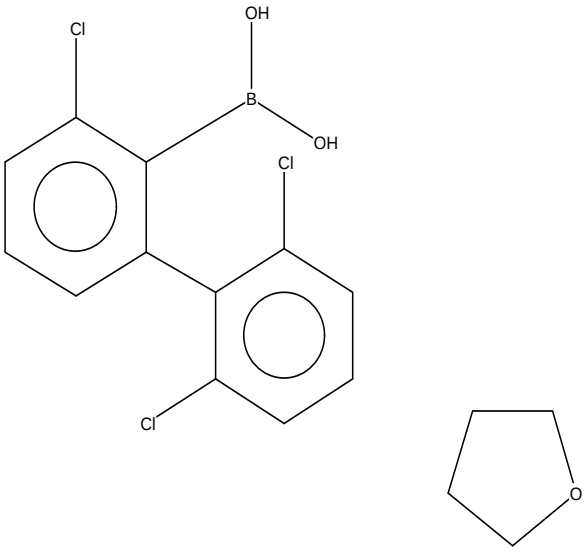
Reference: K.Durka, T.Klis, J.Serwatowski (2015) *Acta Crystallogr.,Sect.E:Cryst.Commun.* ,**71,**1471

Formula: $C_{12}H_8B_1Cl_3O_2{,}C_4H_8O_1$

Compound Name: (2',3,6'-trichlorobiphenyl-2-yl)boronic acid tetrahydrofuran solvate

Space Group:	P-1	***Cell:***	***a***	8.331(0)	***b***	8.712(0)	***c***	12.431(0)
Space Group No.:	2	***(Å,°)***	α	98.68(0)	β	97.74(0)	γ	99.40(0)

R-Factor (%): 3.35 ***Temperature(K):*** 130 ***Density(g/cm³):*** 1.429



YUTTUE

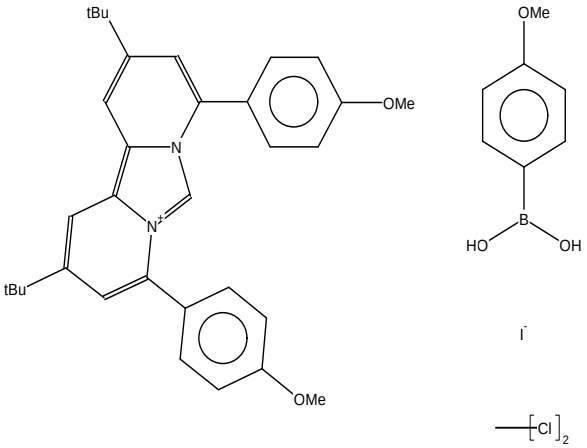
Reference: N.Maeta, J.Yamamoto, Shin-ichi Fuku-en, Rong Shang, Y.Yamamoto (2015) *Z.Anorg.Allg.Chem.* ,**641,**2199

Formula: $C_{33}H_{37}N_2O_2{}^{1+}{,}C_7H_9B_1O_3{,}I_1{}^{1-}{,}2(C_1H_2Cl_2)$

Compound Name: 2,10-di-t-butyl-4,8-bis(4-methoxyphenyl)pyrido[1',2':3,4]imidazo[1,5-a]pyridin-5-ium ((4-methoxyphenyl)boronic acid) iodide dichloromethane solvate

Space Group:	P21/n	***Cell:***	***a***	10.166(0)	***b***	18.027(1)	***c***	25.044(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	91.93(0)	γ	90.00

R-Factor (%): 4.51 ***Temperature(K):*** 173 ***Density(g/cm³):*** 1.365



ZAPDAV

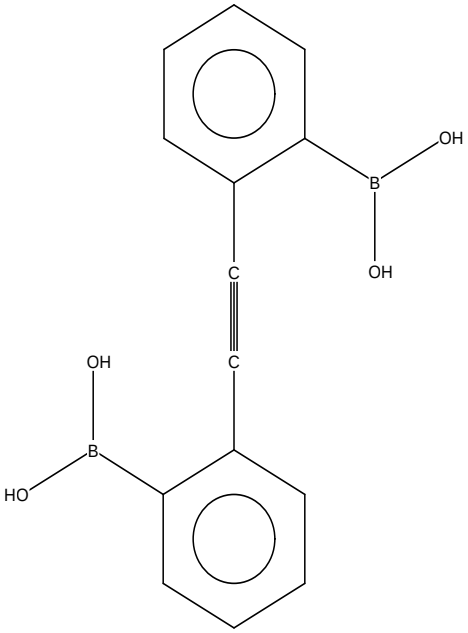
Reference: M.Pilkington, J.D.Wallis, S.Larsen (1995) *Chem.Commun.* ,1499

Formula: $C_{14}H_{12}B_2O_4$

Compound Name: 2,2'-Ethynylenedibenzeneboronic acid

Space Group:	P21/n	***Cell:***	***a***	7.794(2)	***b***	5.079(1)	***c***	16.458(4)
Space Group No.:	14	***(Å,°)***	α	90.00	β	103.39(2)	γ	90.00

R-Factor (%): 4.13 ***Temperature(K):*** 122 ***Density(g/cm³):*** 1.393



ZIGPAG

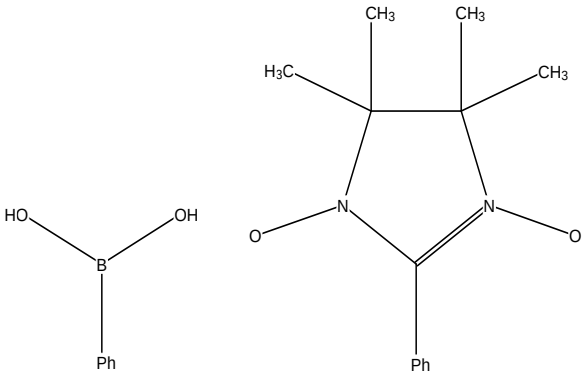
Reference: T.Akita, Y.Mazaki, K.Kobayashi (1995) *Chem.Commun.* , 1861

Formula: $C_6H_7B_1O_2{,}C_{13}H_{17}N_2O_2$

Compound Name: Phenyl nitronyl nitroxide radical phenylboronic acid

Space Group:	P21/n	***Cell:***	***a***	14.764(3)	***b***	9.482(3)	***c***	13.686(2)
Space Group No.:	14	***(Å,°)***	α	90.00	β	90.20(3)	γ	90.00

R-Factor (%): 3.89 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.231



Search: search4 (Mon May 01 12:48:32 2017): Hits 313-316

ZIGPAG01

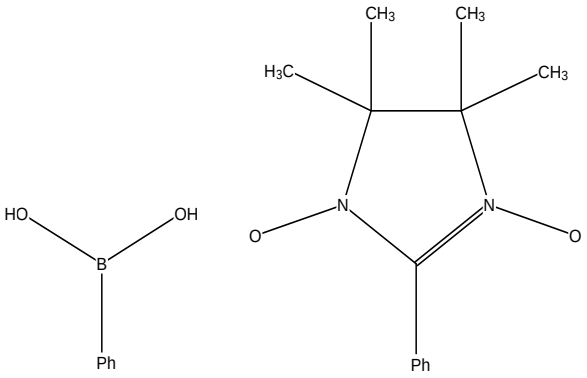
Reference: Y.Pontillon, T.Akita, A.Grand, K.Kobayashi, E.Lelievre-Berna, J.Pecaut, E.Ressouche, J.Schweizer (1999) *J.Am.Chem.Soc.* ,**121,**10126

Formula: $C_6 H_7 B_1 O_2$,$C_{13} H_{17} N_2 O_2$

Compound Name: Phenyl nitronyl nitroxide radical phenylboronic acid

Space Group:	P-1	***Cell:***	***a***	9.360(0)	***b***	13.640(0)	***c***	14.532(0)
Space Group No.:	2	***(Å,°)***	α	92.08	β	90.23(0)	γ	91.26(0)

R-Factor (%): 7.11 ***Temperature(K):*** 143 ***Density(g/cm³):*** 1.273



ZIGPAG02

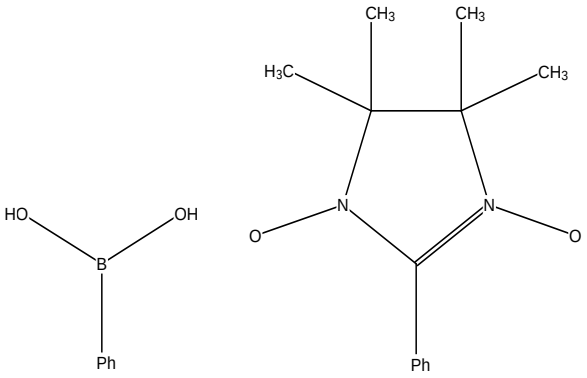
Reference: Y.Pontillon, T.Akita, A.Grand, K.Kobayashi, E.Lelievre-Berna, J.Pecaut, E.Ressouche, J.Schweizer (1999) *J.Am.Chem.Soc.* ,**121,**10126

Formula: $C_6 H_7 B_1 O_2$,$C_{13} H_{17} N_2 O_2$

Compound Name: Phenyl nitronyl nitroxide radical phenylboronic acid

Space Group:	P-1	***Cell:***	***a***	14.500(10)	***b***	9.360	***c***	13.660(20)
Space Group No.:	2	***(Å,°)***	α	92.08	β	89.75	γ	91.26

R-Factor (%): 4.90 ***Temperature(K):*** 5 ***Density(g/cm³):*** 1.274



ZILBEB

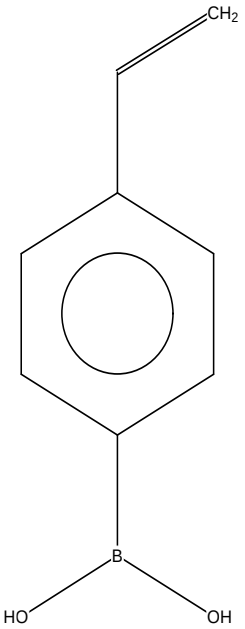
Reference: G.J.Gainsford, R.H.Meinhold, A.D.Woolhouse (1995) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**51,**2694

Formula: $C_8 H_9 B_1 O_2$

Compound Name: Styrylboronic acid

Space Group:	P21/c	***Cell:***	***a***	19.362(16)	***b***	5.128(6)	***c***	8.159(6)
Space Group No.:	14	***(Å,°)***	α	90.00	β	100.11(6)	γ	90.00

R-Factor (%): 5.50 ***Temperature(K):*** 193 ***Density(g/cm³):*** 1.232



ZOHDUX

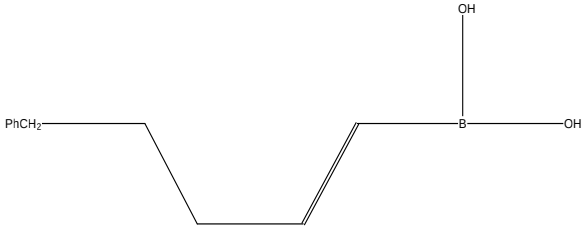
Reference: T.Gelbrich, D.Sampson, M.B.Hursthouse (2000) *University of Southampton, Crystal Structure Report Archive* ,528

Formula: $C_{11} H_{15} B_1 O_2$

Compound Name: (5-phenylpent-1-en-1-yl)boronic acid

Space Group:	Pbca	***Cell:***	***a***	7.515(0)	***b***	9.392(0)	***c***	30.737(0)
Space Group No.:	61	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 5.47 ***Temperature(K):*** 150 ***Density(g/cm³):*** 1.164



Search: search4 (Mon May 01 12:48:32 2017): Hits 317-320

ZOQVEI

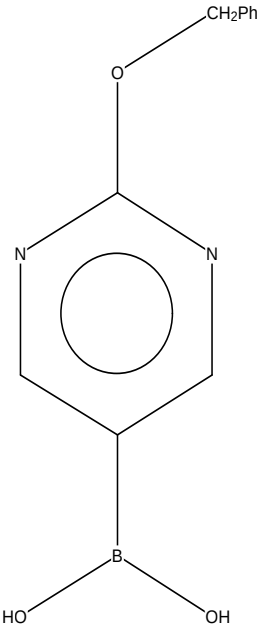
Reference: K.Durka, T.Klis, J.Serwatowski (2014)
Acta Crystallogr.,Sect.E:Struct.Rep.Online ,**70,**o1259

Formula: $C_{11}H_{11}B_1N_2O_3$

Compound Name: (2-(Benzyloxy)pyrimidin-5-yl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	5.498(1)	***b***	30.432(1)	***c***	6.709(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	113.54(4)	γ	90.00

R-Factor (%): 5.33 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.485



ZUCREW

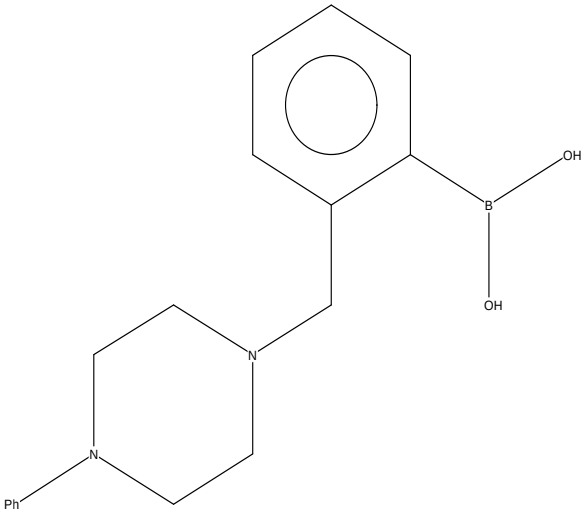
Reference: A.Adamczyk-Wozniak, K.Czerwinska, I.D.Madura, A.Matuszewska, A.Sporzynski, A.Zubrowska-Zembrzuska (2015)
New J.Chem. ,**39,**4308

Formula: $C_{17}H_{21}B_1N_2O_2$

Compound Name: (2-((4-phenylpiperazin-1-yl)methyl)phenyl)boronic acid

Space Group:	P21/c	***Cell:***	***a***	13.309(0)	***b***	6.012(0)	***c***	19.833(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	108.65(0)	γ	90.00

R-Factor (%): 3.45 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.308



ZUCRIA

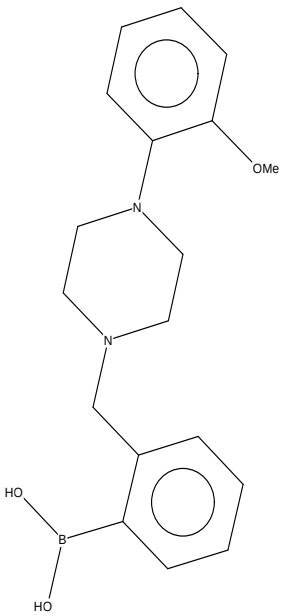
Reference: A.Adamczyk-Wozniak, K.Czerwinska, I.D.Madura, A.Matuszewska, A.Sporzynski, A.Zubrowska-Zembrzuska (2015)
New J.Chem. ,**39,**4308

Formula: $C_{18}H_{23}B_1N_2O_3$

Compound Name: (2-((4-(2-methoxyphenyl)piperazin-1-yl)methyl)phenyl)boronic acid

Space Group:	I2/a	***Cell:***	***a***	12.198(0)	***b***	19.205(0)	***c***	15.542(0)
Space Group No.:	15	***(Å,°)***	α	90.00	β	96.00(0)	γ	90.00

R-Factor (%): 3.92 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.197



ZUCROG

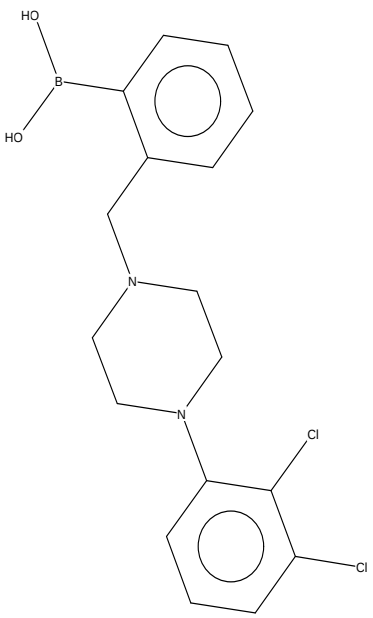
Reference: A.Adamczyk-Wozniak, K.Czerwinska, I.D.Madura, A.Matuszewska, A.Sporzynski, A.Zubrowska-Zembrzuska (2015)
New J.Chem. ,**39,**4308

Formula: $C_{17}H_{19}B_1Cl_2N_2O_2$

Compound Name: (2-((4-(2,3-dichlorophenyl)piperazin-1-yl)methyl)phenyl)boronic acid

Space Group:	P-1	***Cell:***	***a***	7.916(0)	***b***	10.313(0)	***c***	11.833(0)
Space Group No.:	2	***(Å,°)***	α	88.46(0)	β	72.90(0)	γ	69.37(0)

R-Factor (%): 4.88 ***Temperature(K):*** 120 ***Density(g/cm³):*** 1.408



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ZUCRUM

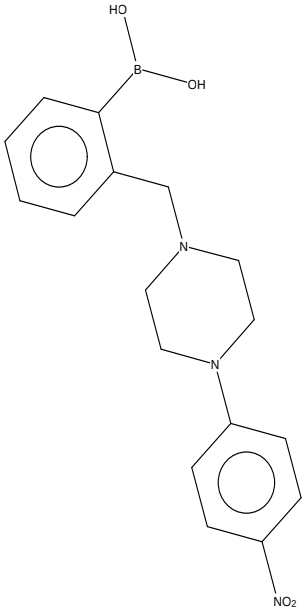
Reference: A.Adamczyk-Wozniak, K.Czerwinska, I.D.Madura, A.Matuszewska, A.Sporzynski, A.Zubrowska-Zembrzuska (2015) *New J.Chem.* ,**39,**4308

Formula: $C_{17}\,H_{20}\,B_1\,N_3\,O_4$

Compound Name: (2-((4-(4-nitrophenyl)piperazin-1-yl)methyl)phenyl)boronic acid

Space Group:	P21/n	***Cell:***	***a***	10.326(0)	***b***	9.107(0)	***c***	18.038(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	90.71(0)	γ	90.00

R-Factor (%): 3.64 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.336



ZUCSAT

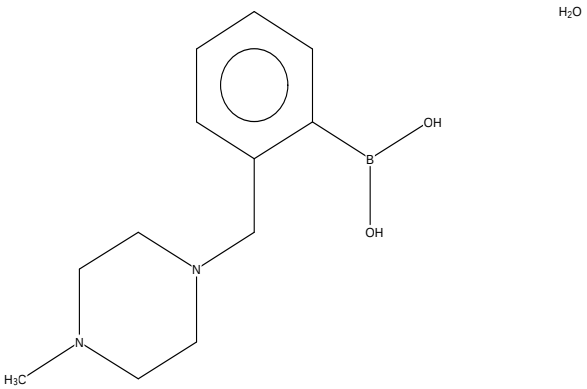
Reference: A.Adamczyk-Wozniak, K.Czerwinska, I.D.Madura, A.Matuszewska, A.Sporzynski, A.Zubrowska-Zembrzuska (2015) *New J.Chem.* ,**39,**4308

Formula: $C_{12}\,H_{19}\,B_1\,N_2\,O_2,H_2\,O_1$

Compound Name: (2-((4-methylpiperazin-1-yl)methyl)phenyl)boronic acid monohydrate

Space Group:	Pna21	***Cell:***	***a***	12.878(0)	***b***	10.186(0)	***c***	10.365(0)
Space Group No.:	33	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.73 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.232



ZUCSIB

Reference: A.Adamczyk-Wozniak, K.Czerwinska, I.D.Madura, A.Matuszewska, A.Sporzynski, A.Zubrowska-Zembrzuska (2015) *New J.Chem.* ,**39,**4308

Formula: $C_{24}\,H_{27}\,B_1\,N_2\,O_2,C_3\,H_6\,O_1$

Compound Name: (2-((4-(diphenylmethyl)piperazin-1-yl)methyl)phenyl)boronic acid acetone solvate

Space Group:	P21/c	***Cell:***	***a***	24.604(0)	***b***	11.768(0)	***c***	17.522(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	93.83(0)	γ	90.00

R-Factor (%): 3.58 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.166