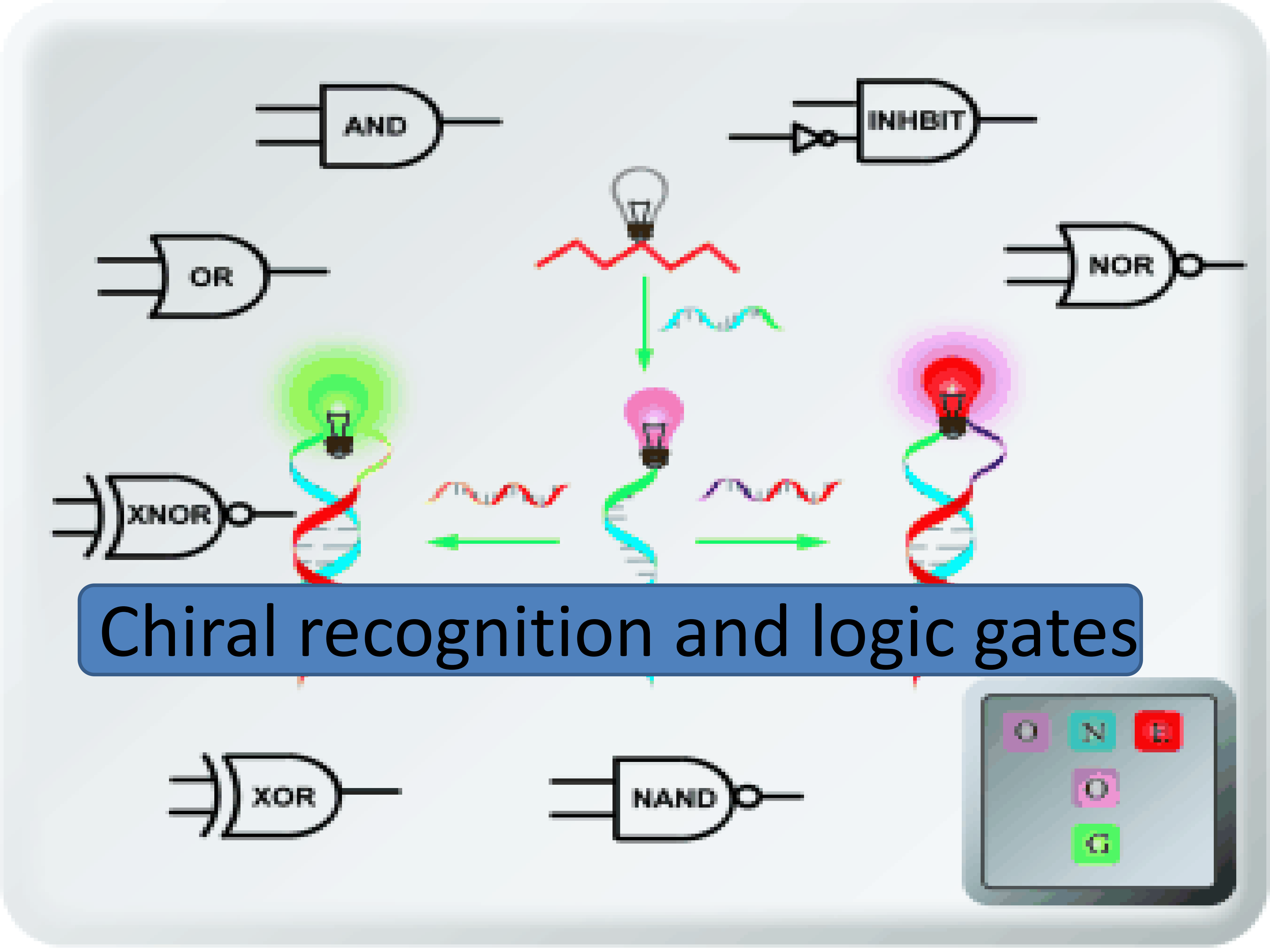
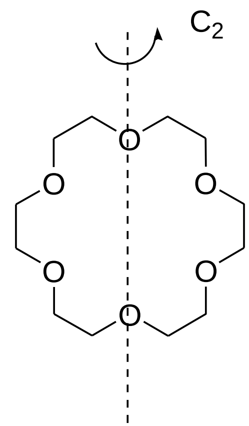

AND
INHBIT
OR
NOR
XNOR
XOR
NAND
Chiral recognition and logic gates
O
N
E
O
G

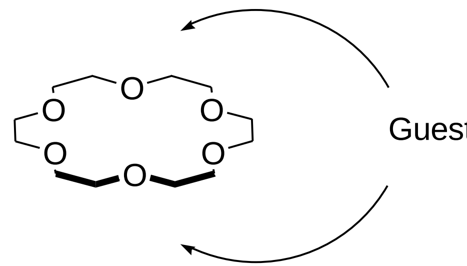
Recognition of chiral guests

- Discrimination between enantiomeric species
- Enantiomers cannot be separated by physical properties
- To separate them they should be converted into diastereomers
- Only chiral hosts can be used
- The thermodynamically more stable HOST.GUEST pair will be formed (matched, mismatched)
- Preference of one enantiomer over the other
- Host preferably belongs to C_2 or D_2 symmetry group

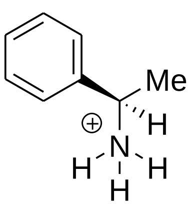
Achiral host – chiral guest

Achiral Host - Chiral Guest

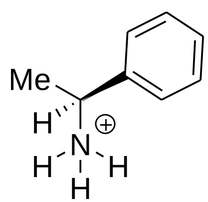




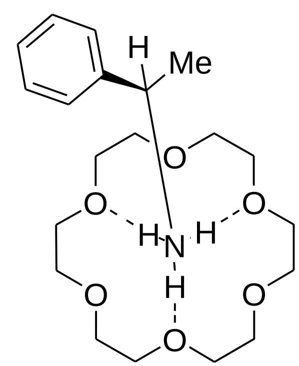
no preference of either side



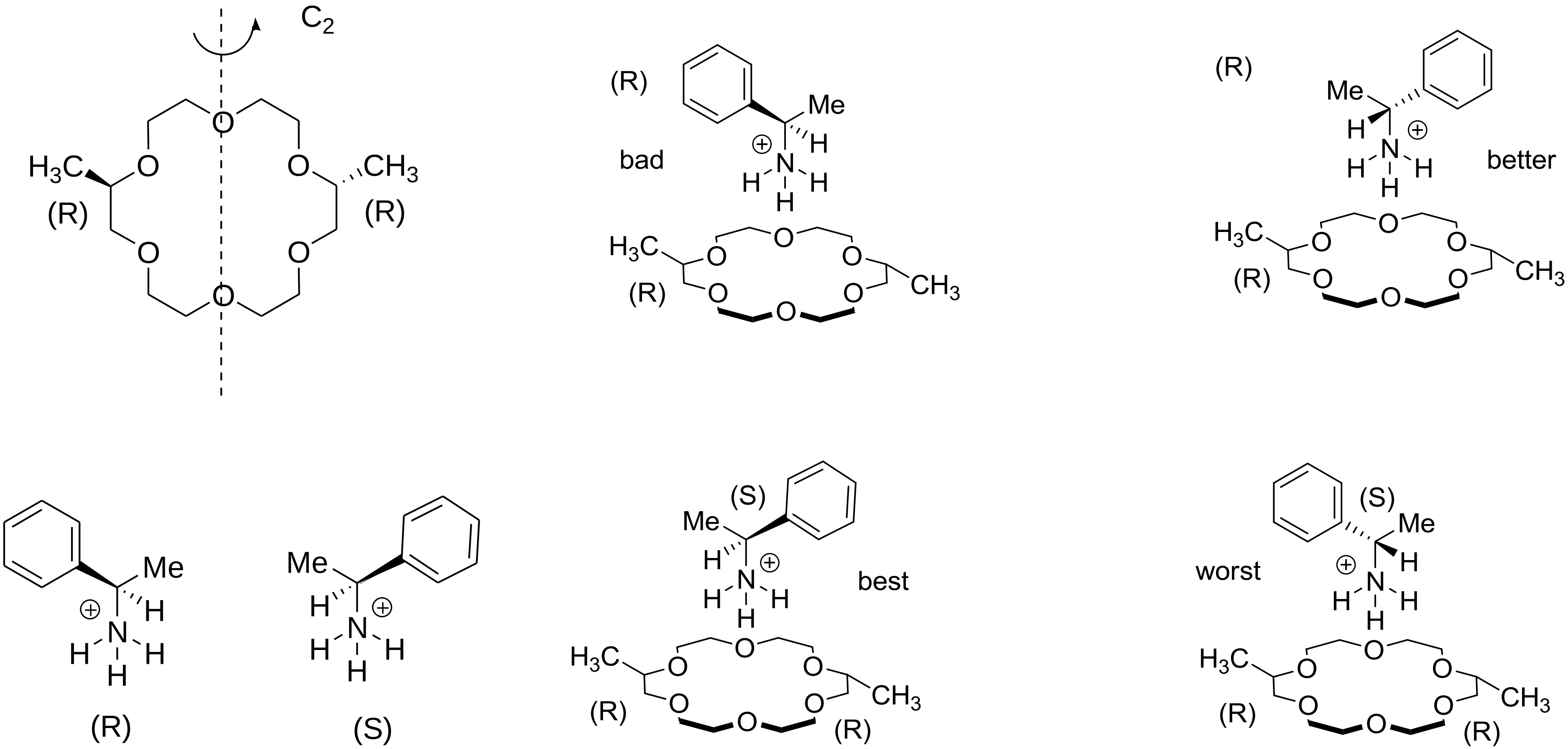
(R)



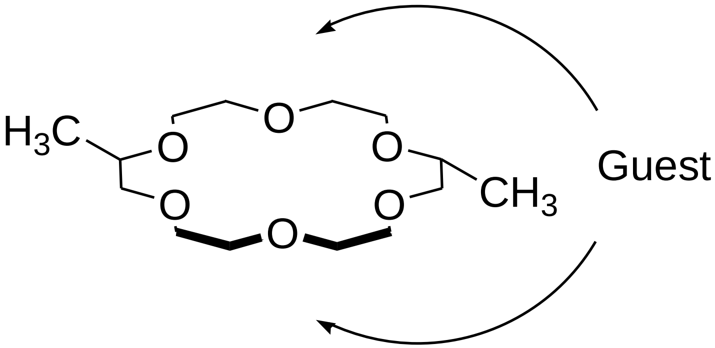
(S)



Chiral host – chiral guest

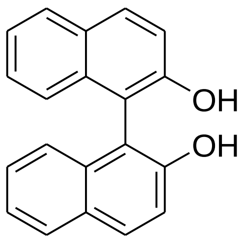


Symmetry of host

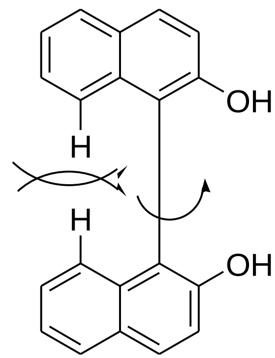


- C2 symmetric hosts have the same faces
- In general host and guest have heterochiral preference (R-S, S-R)

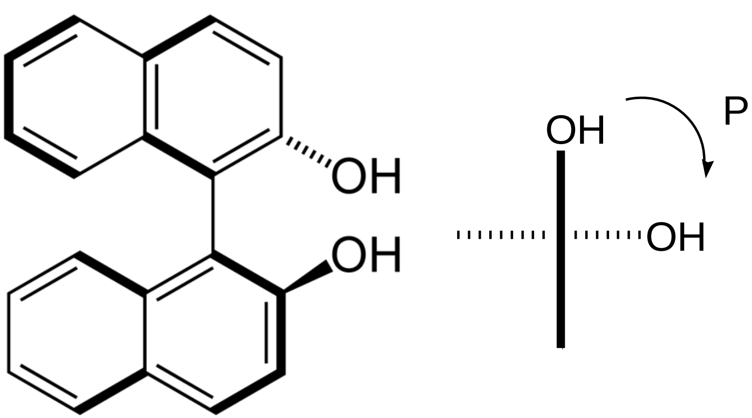
Binol the ultimate chiral element, axial chirality



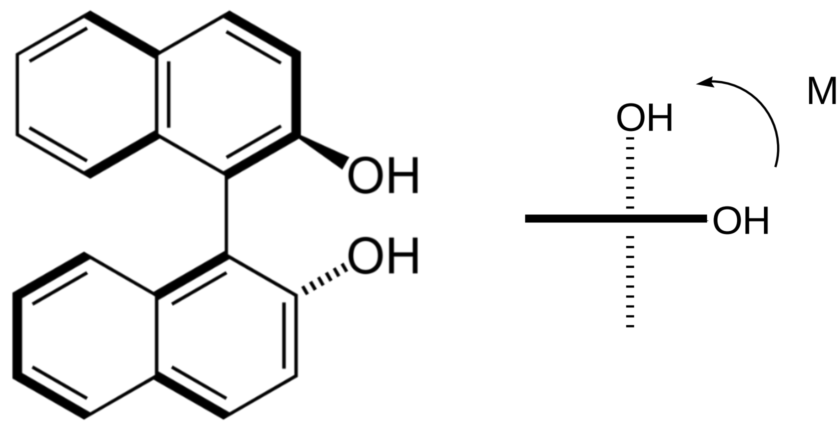
1,1'-bi-2,2'-naphtol
BINOL



Restricted rotation due to H-H banging

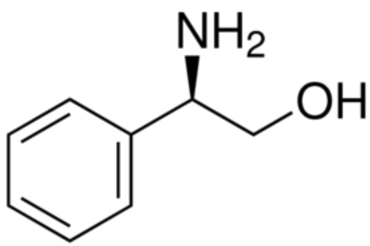


(R)-BINOL

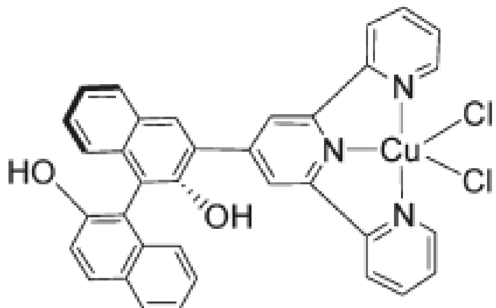


(S)-BINOL

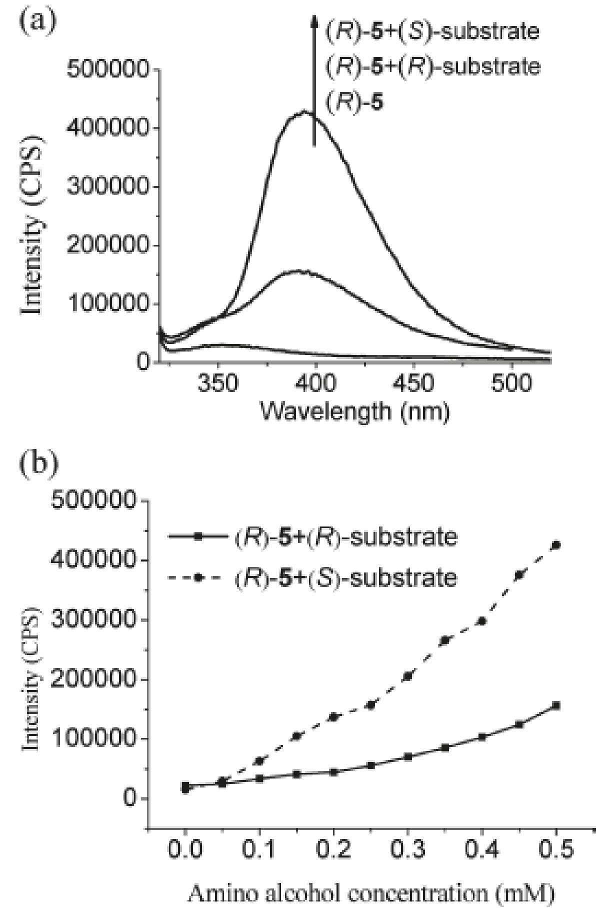
Recognition of aminoalcohols



phenylglycinol

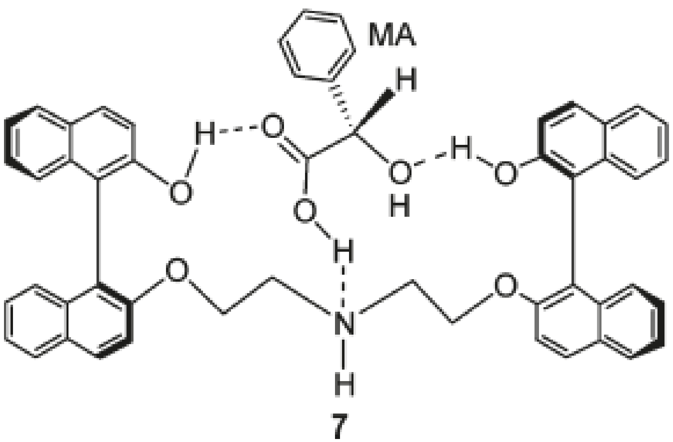


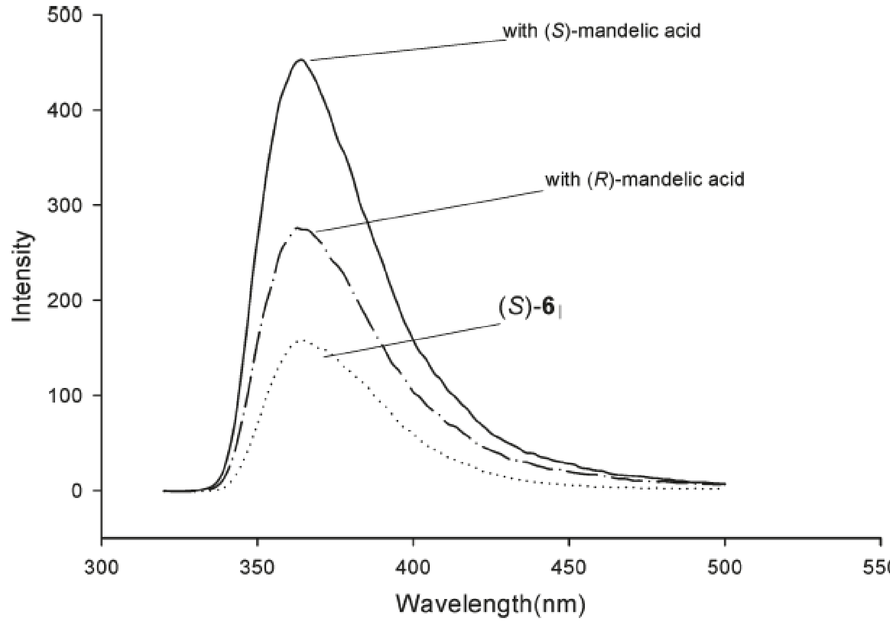
(*R*)-**5**



- fluorescence of 5 is completely quenched (LMCT)
- replacement by aminoalcohol restores fluorescence

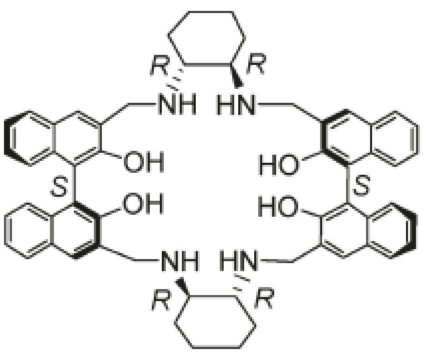
Recognition of α-hydroxy carboxylic acid





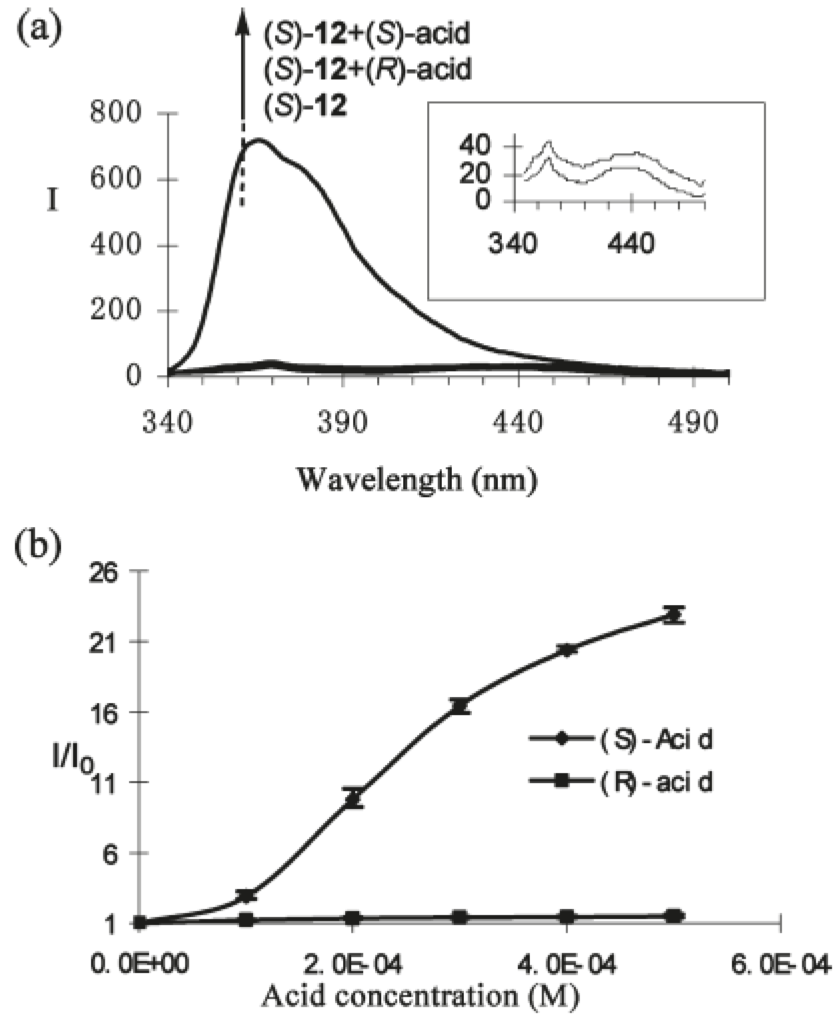
- PET from N is turned off → fluorescence enhancement
- $I_S/I_0 = 2.87$
- ef $[=(I_S - I_0)/(I_R - I_0)] = 2.49$

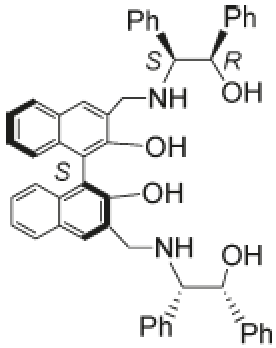
Recognition of α-hydroxy carboxylic acids



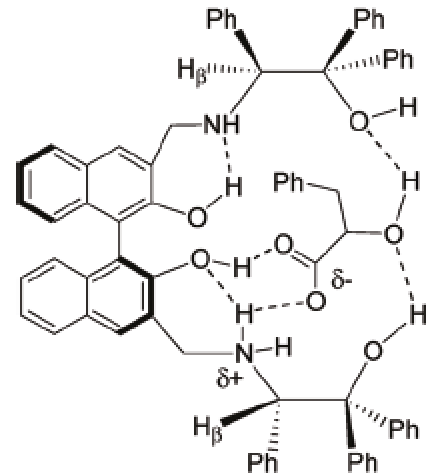
(*S*)-**12**

ef = 46

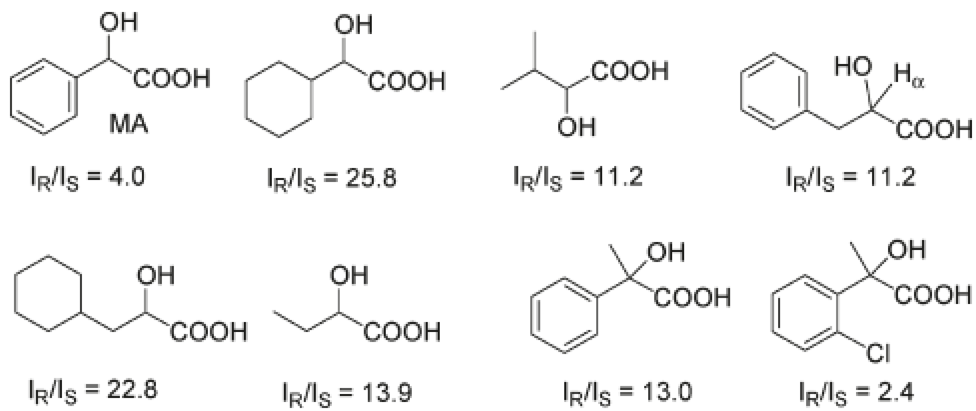




(*S*)-**14**

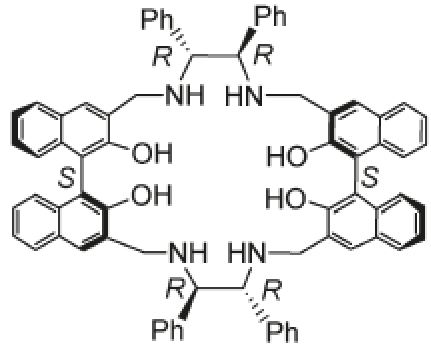


proposed 1:1 complex of (*S*)-**15**+(*R*)-phenyllactic acid.

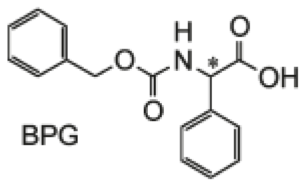


Fluorescent enantioselectivity of (S)-15 toward various chiral R-hydroxycarboxylic acids

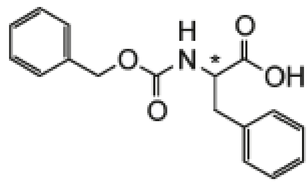
Recognition of amino acids



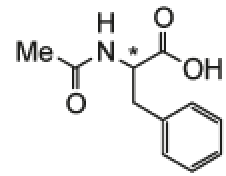
(*S*)-**11**



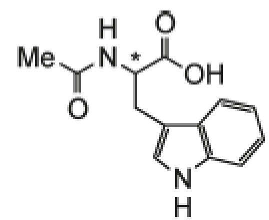
ef = 5.7



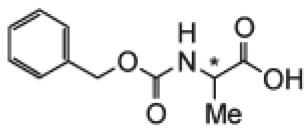
ef = 1.9



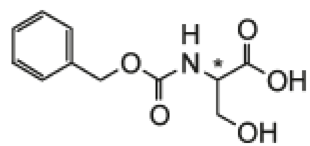
ef = 1.7



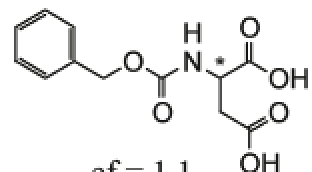
ef = 2.2



ef = 1.7



ef = 1.2



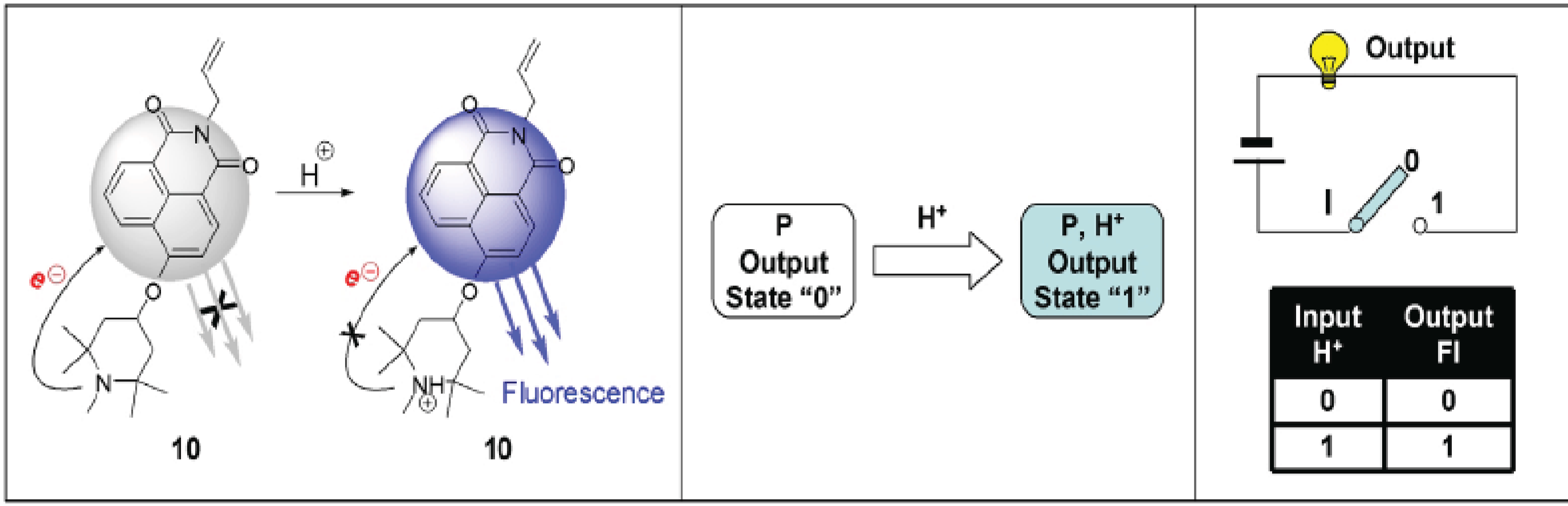
ef = 1.1

Enantioselectivity of (R)-11 in the fluorescent recognition of various amino acid derivatives

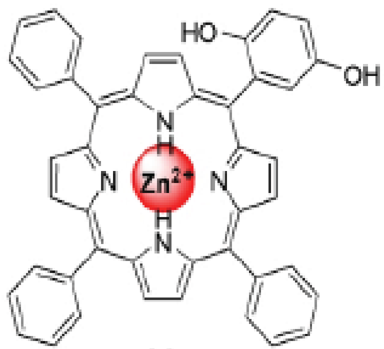
Logic gates

- Logic operations at molecular level
- Miniaturization
- Molecular wires
- Binary units (0, 1)
- Integrated logic (e.g. not+and = NAND) in one gate
- Further miniaturization
- Single (yes, not) and multiple input (and, or etc.) gates

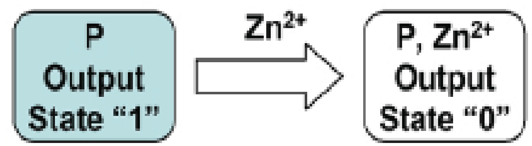
YES operation

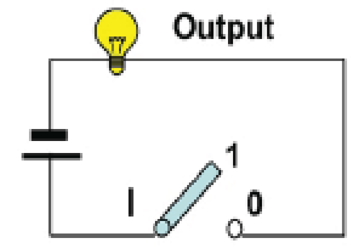


NOT operation



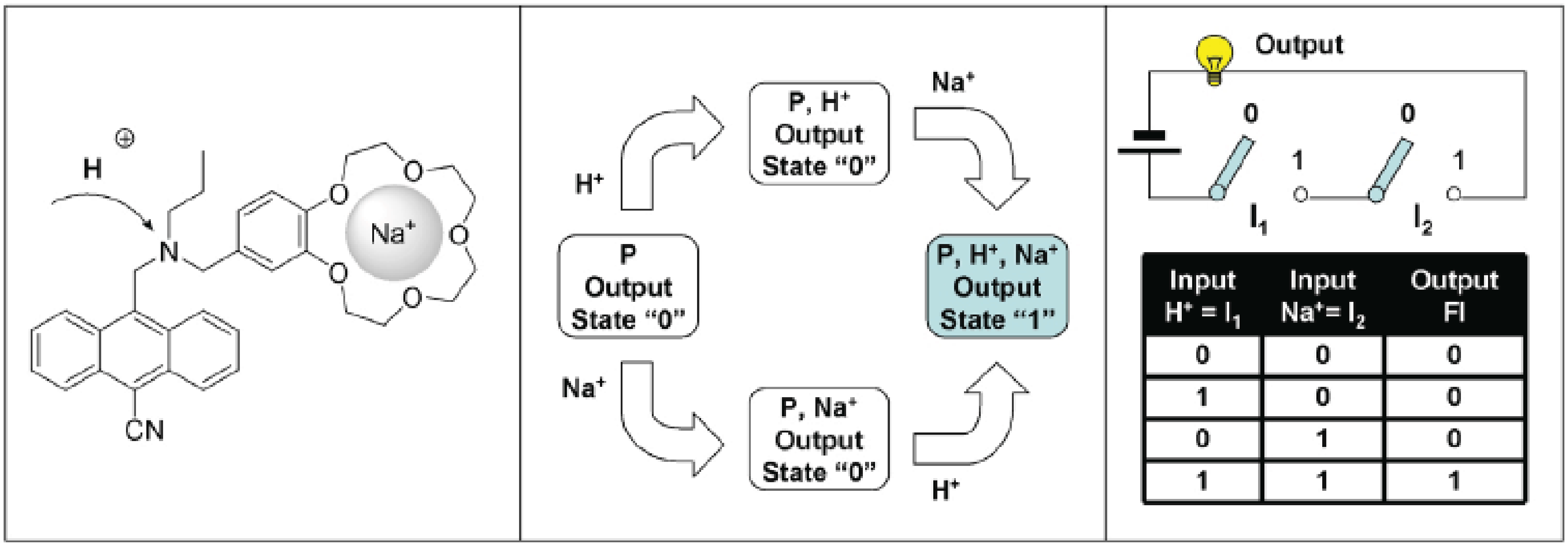
39



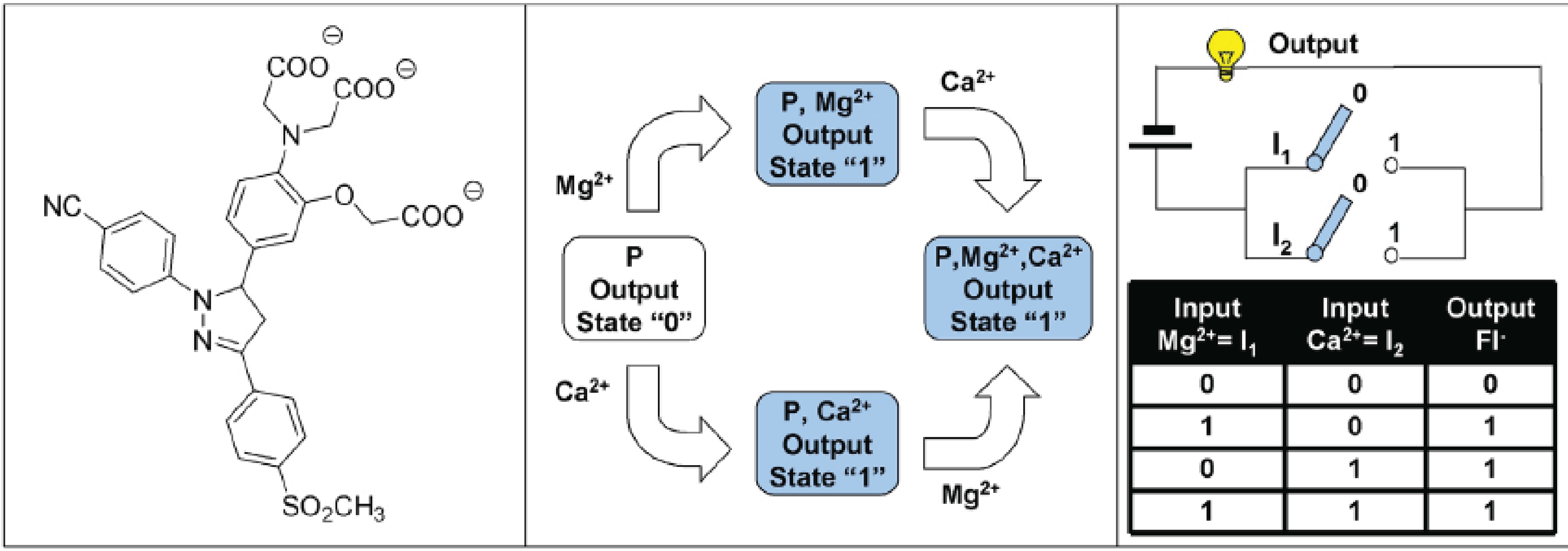


Input Zn^{2+}	Output Fl
0	1
1	0

AND logic

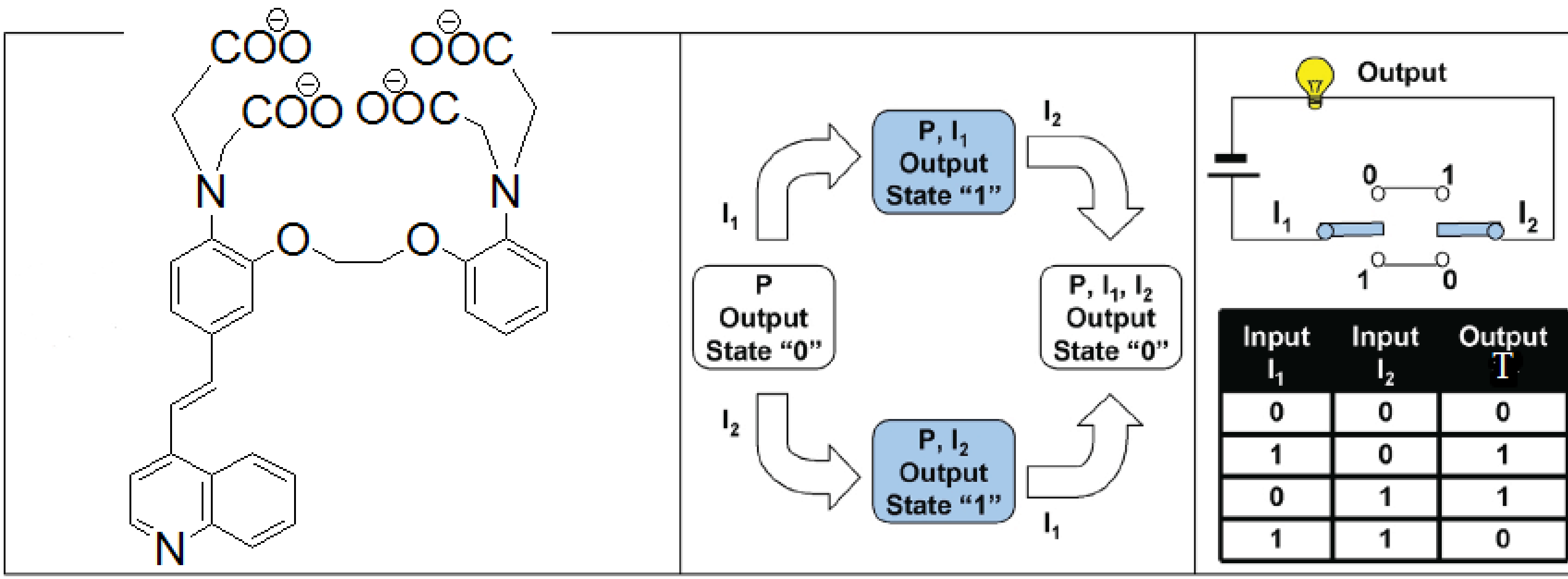

H ⊕
N
Na+
O
CN
H+
Na+
P
Output
State "0"
P, H+
Output
State "0"
P, Na+
Output
State "0"
P, H+, Na+
Output
State "1"
Output
0
1
I1
I2
Input H+ = I1
Input Na+ = I2
Output Fl
0 0 0
1 0 0
0 1 0
1 1 1

OR logic



Input $Mg^{2+} = I_1$	Input $Ca^{2+} = I_2$	Output Fl·
0	0	0
1	0	1
0	1	1
1	1	1

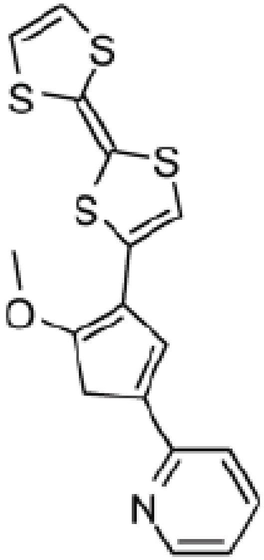
XOR logic (exclusive Or –either/or)



Input I_1	Input I_2	Output T
0	0	0
1	0	1
0	1	1
1	1	0

- Output is true if either but not both is present
- no input λabs = 394 nm
- protonation λabs = 478 nm
- calcium λabs = 347 nm
- both λabs = 396 nm

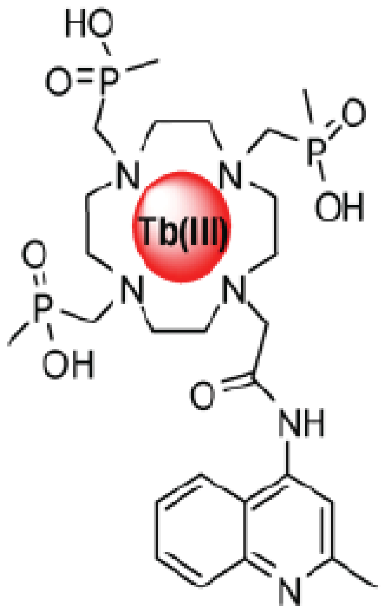
NAND logic (NOT+AND)



Input Fe^{2+}	Input $NOBF_4$	Output FI
0	0	1
1	0	1
0	1	1
1	1	0

- Output is false if both input present
- AND followed by negation
- Fe^{3+} quenches fluorescence

INHIBIT logic (AND + NOT)

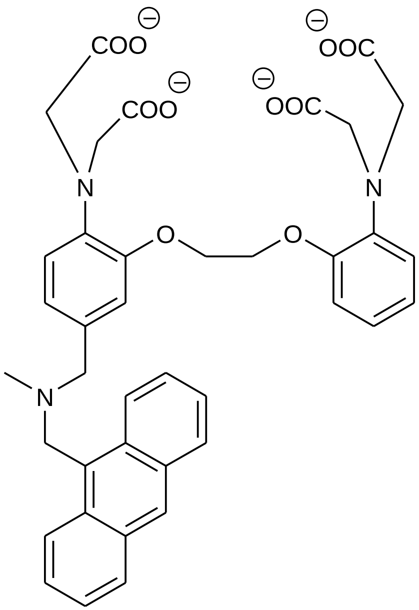


Input H^+	Input O_2	Output Fl
0	0	0
1	0	1
0	1	0
1	1	0

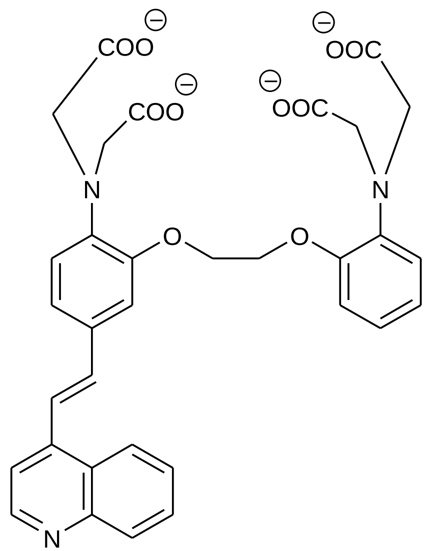
- Tb complex is luminescent in oxygen free media
- protonation of the sensitizer allows for excitation of the quinoline and FRET

Half-adder (AND + XOR)

AND



XOR



Input A	Input B	Output F (Carry)	Output T (Sum)	A+B
		AND	XOR	
0	0	0	0	00
1	0	0	1	01
0	1	0	1	01
1	1	1	0	10

- The two gates are compatible
- There are examples where the two gates are in one molecule