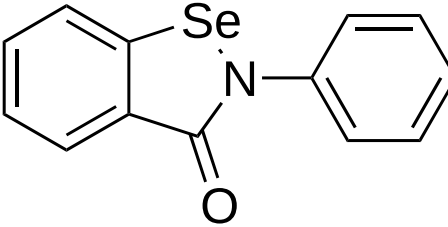
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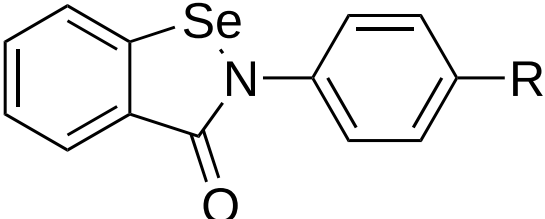
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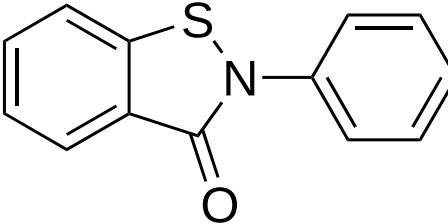
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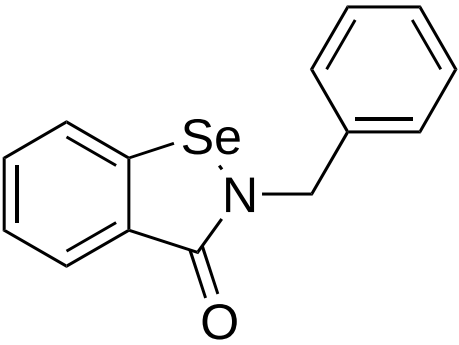
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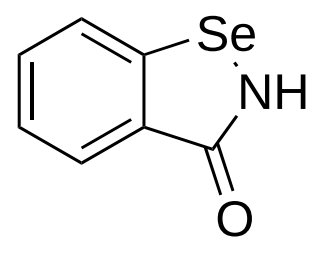
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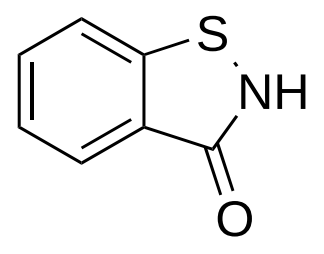
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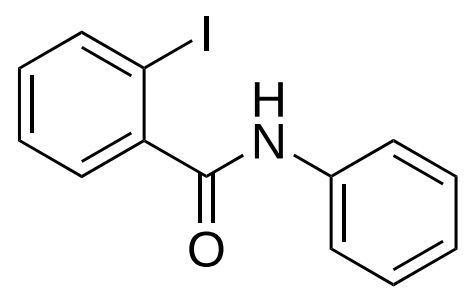
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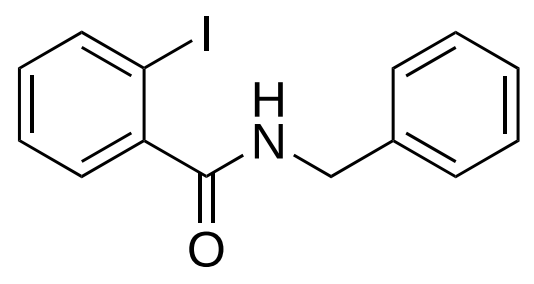
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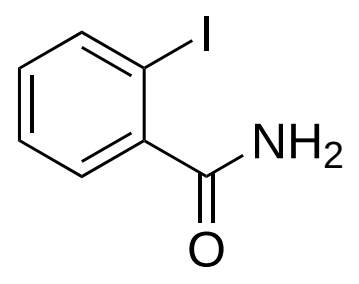
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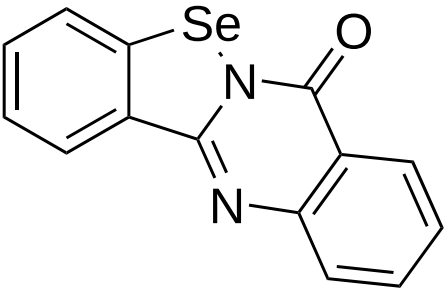
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O
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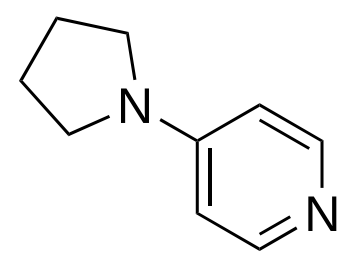
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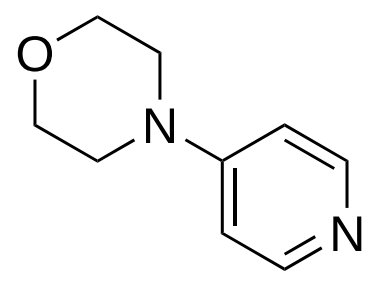
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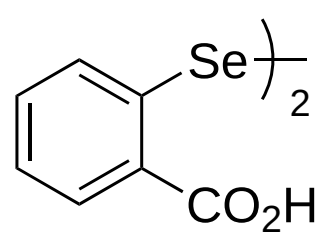
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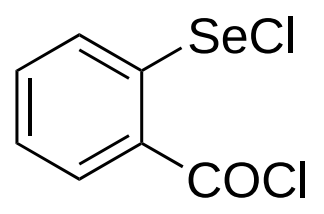
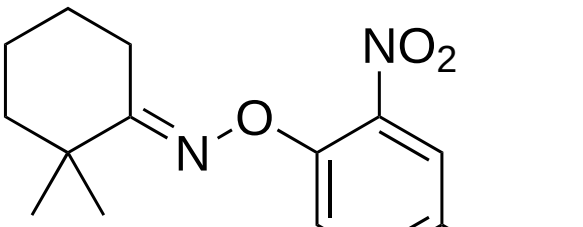
CO2H


SeCl
COCl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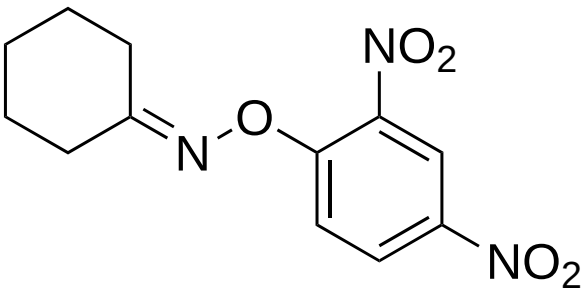
NO2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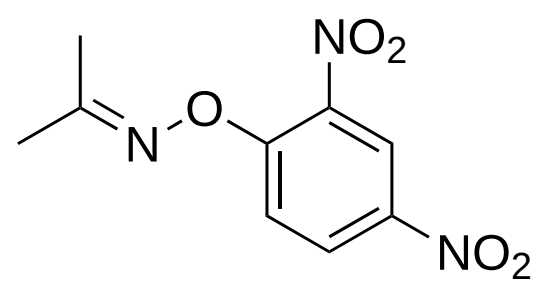
NO2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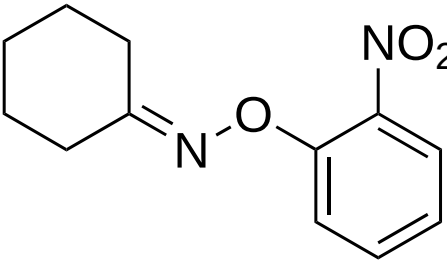
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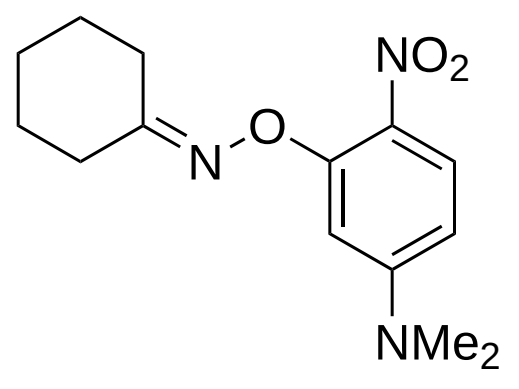
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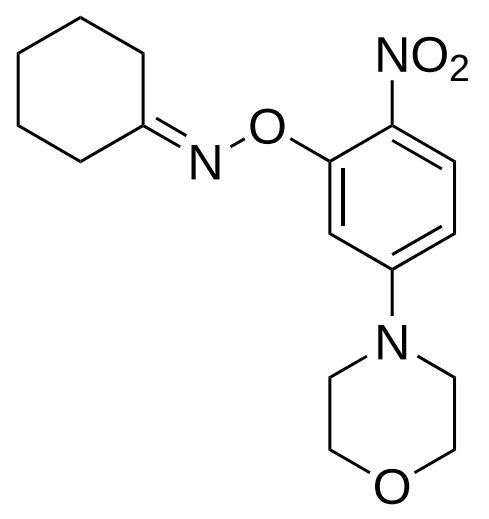
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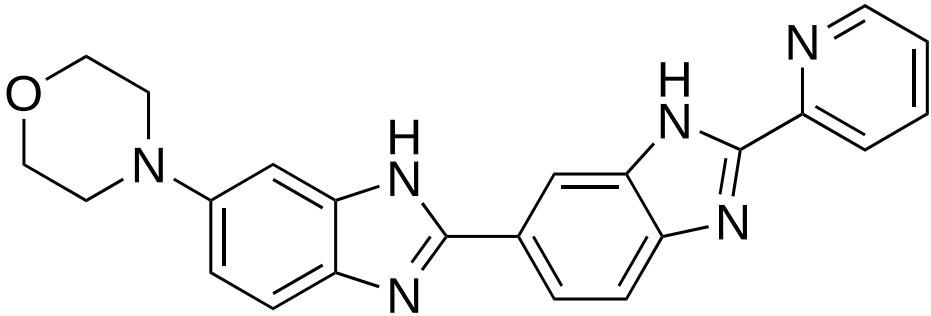
O
N
O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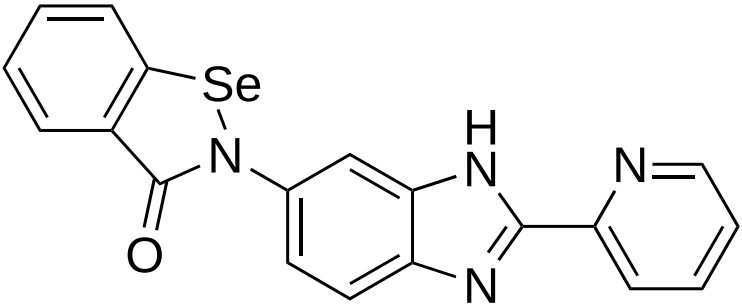
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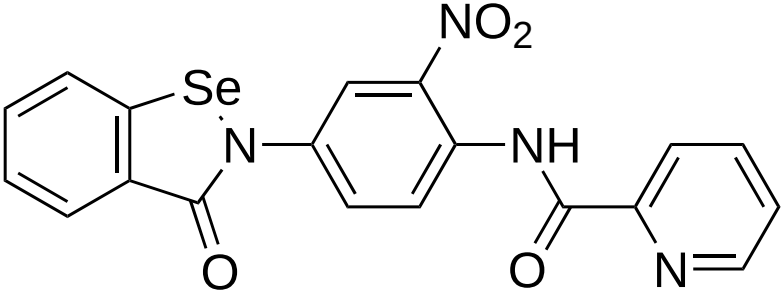
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NH
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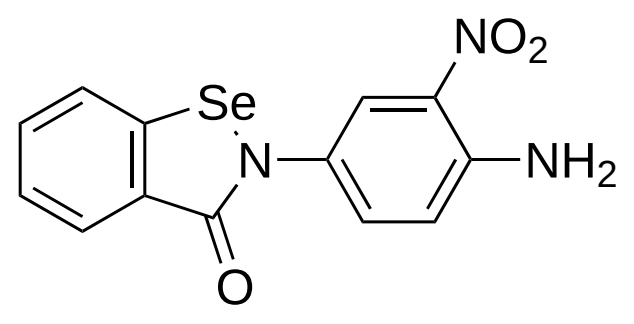
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NH2
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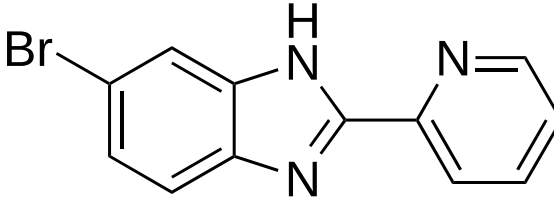
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N
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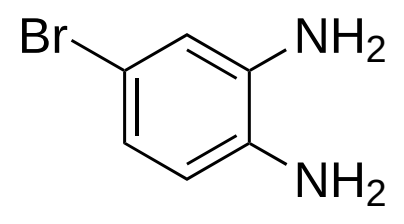
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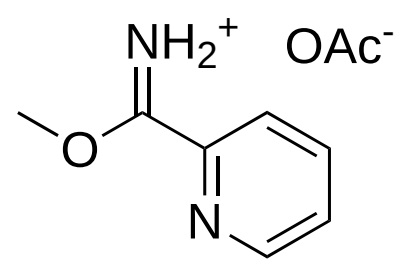
NH2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OAc-
O
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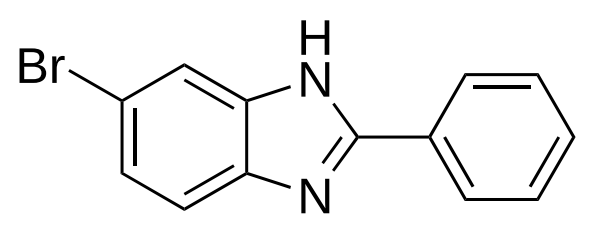
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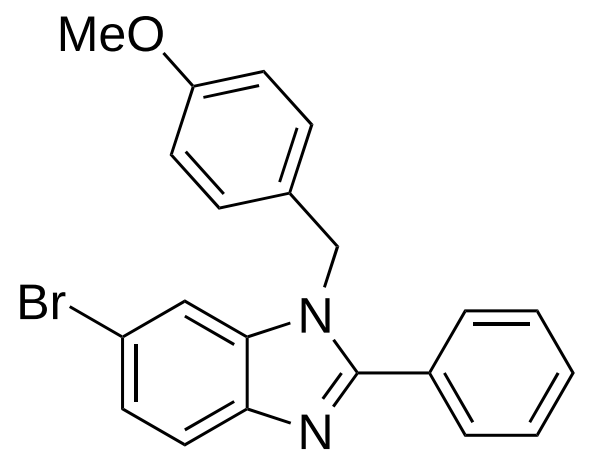
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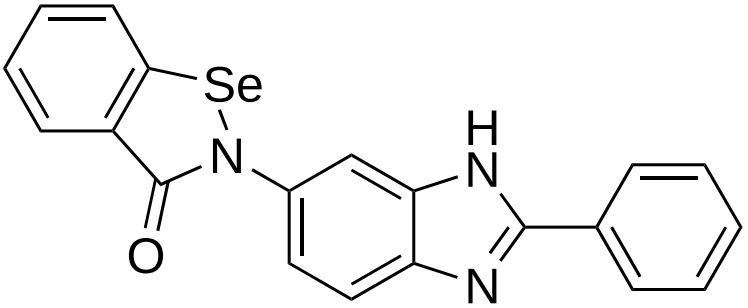
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H
N
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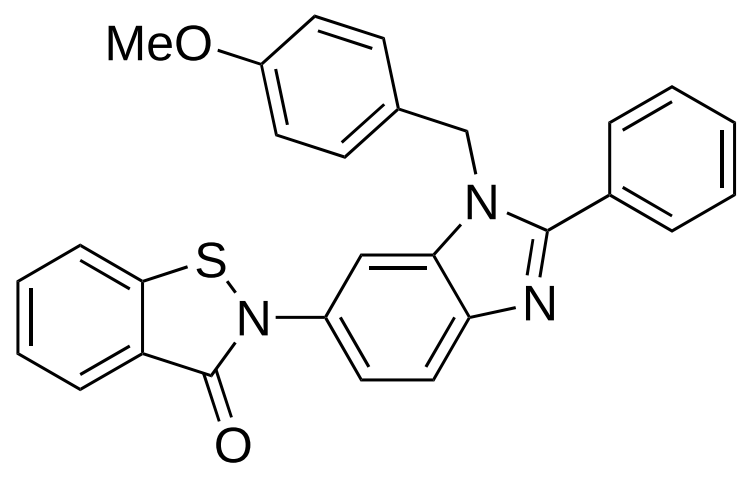
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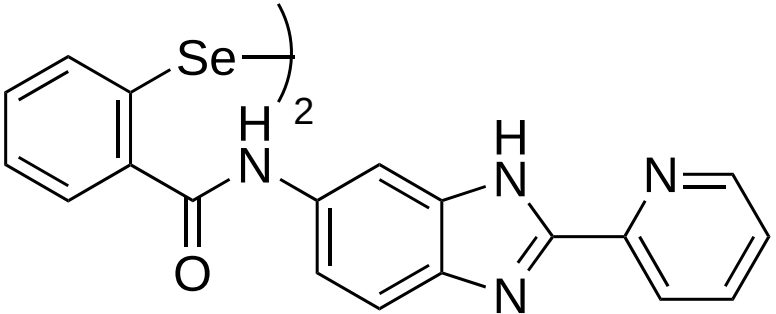
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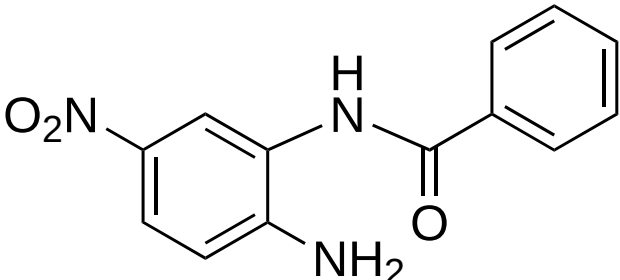
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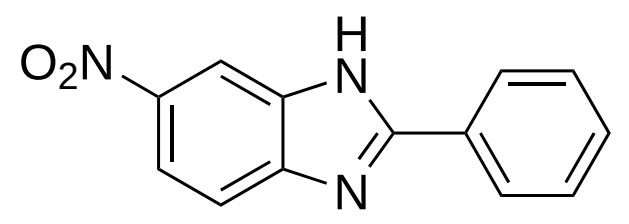
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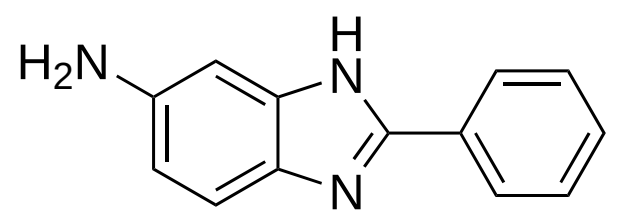
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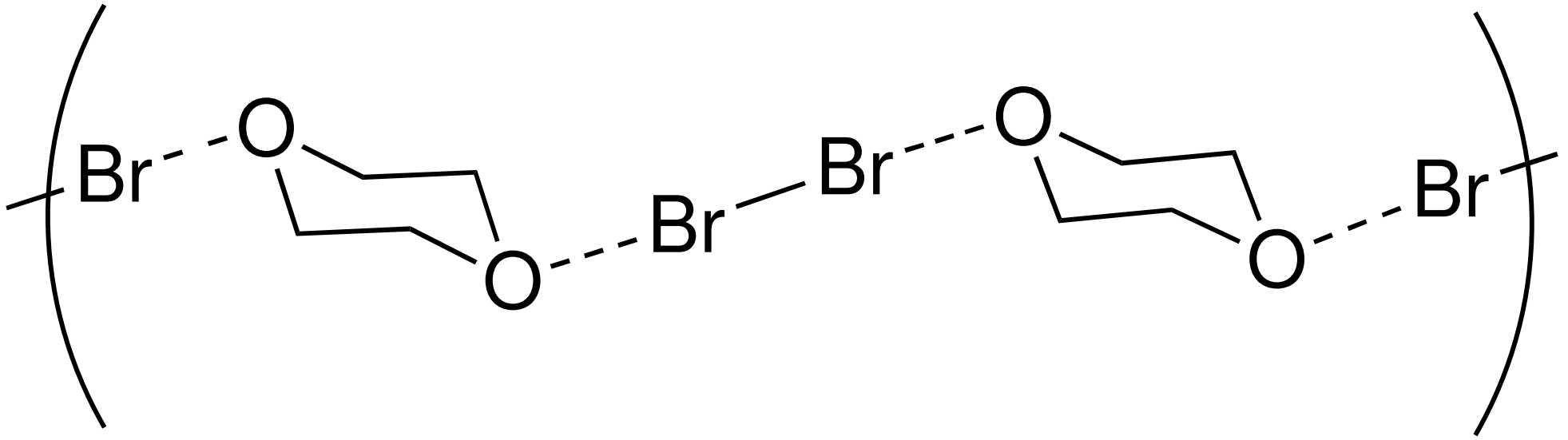
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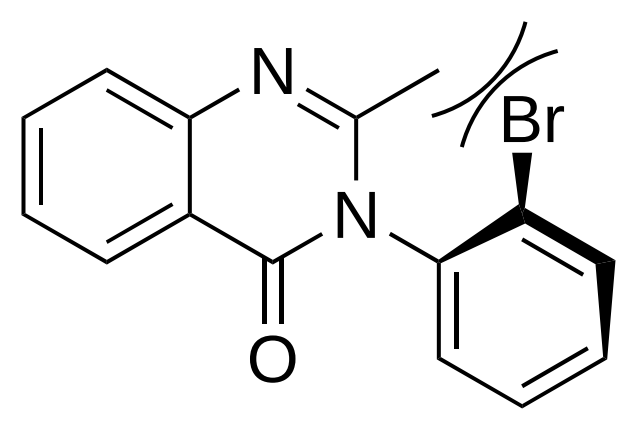
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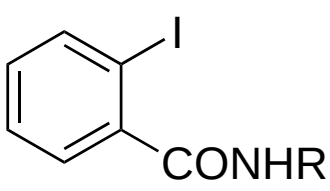
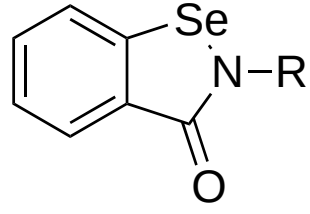


CuI, 1,10-phenanthroline,
Se, K_2CO_3

DMF, 110°C, 5h

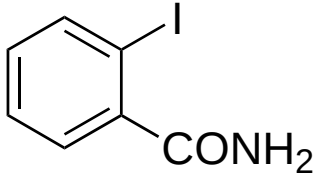


1 R = Ph, 69%

1a R = Bn, 53%

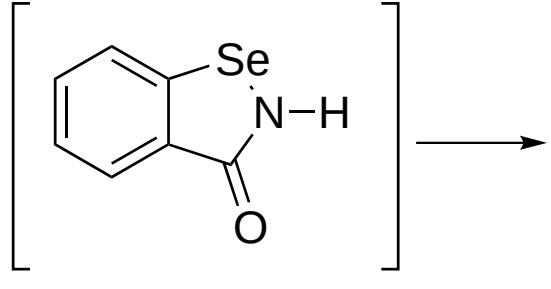
2 and **2a**

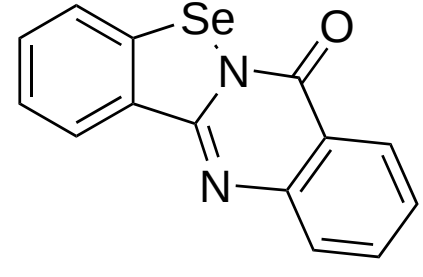
1 and **1a**



CuI, 1,10-phenanthroline,
Se, K_2CO_3

DMF, 110°C, 5h, 15%

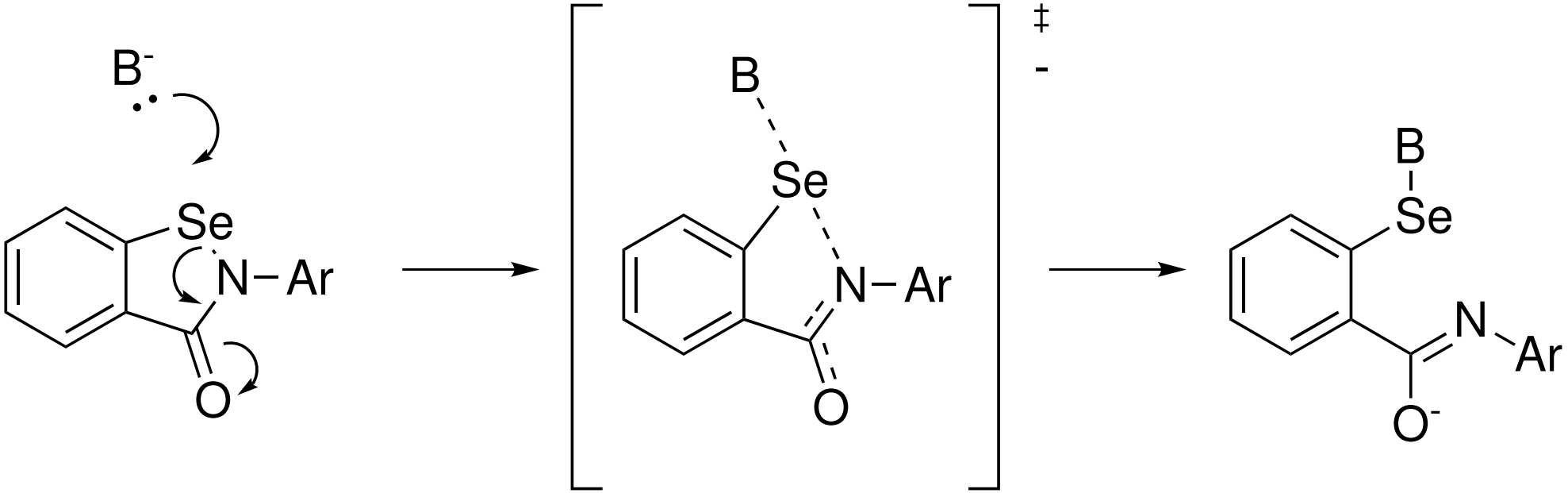


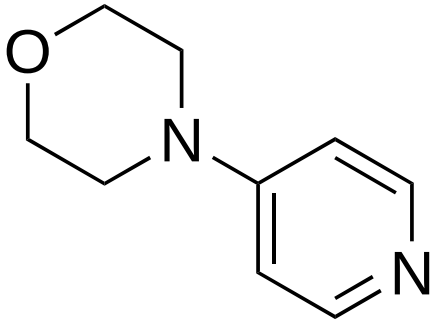


2b

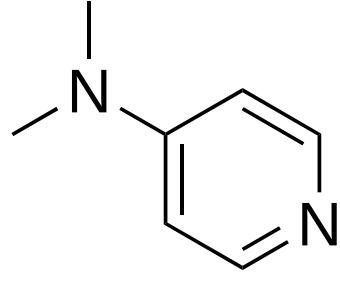
1b

3

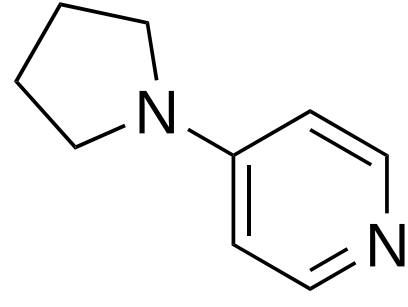

B-
Se
N
Ar
O
B
Se
N
Ar
O
‡
-
B
Se
N
Ar
O-



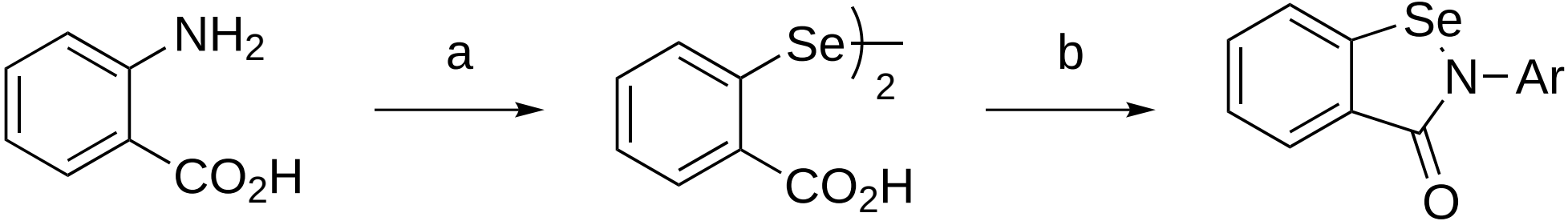
4a



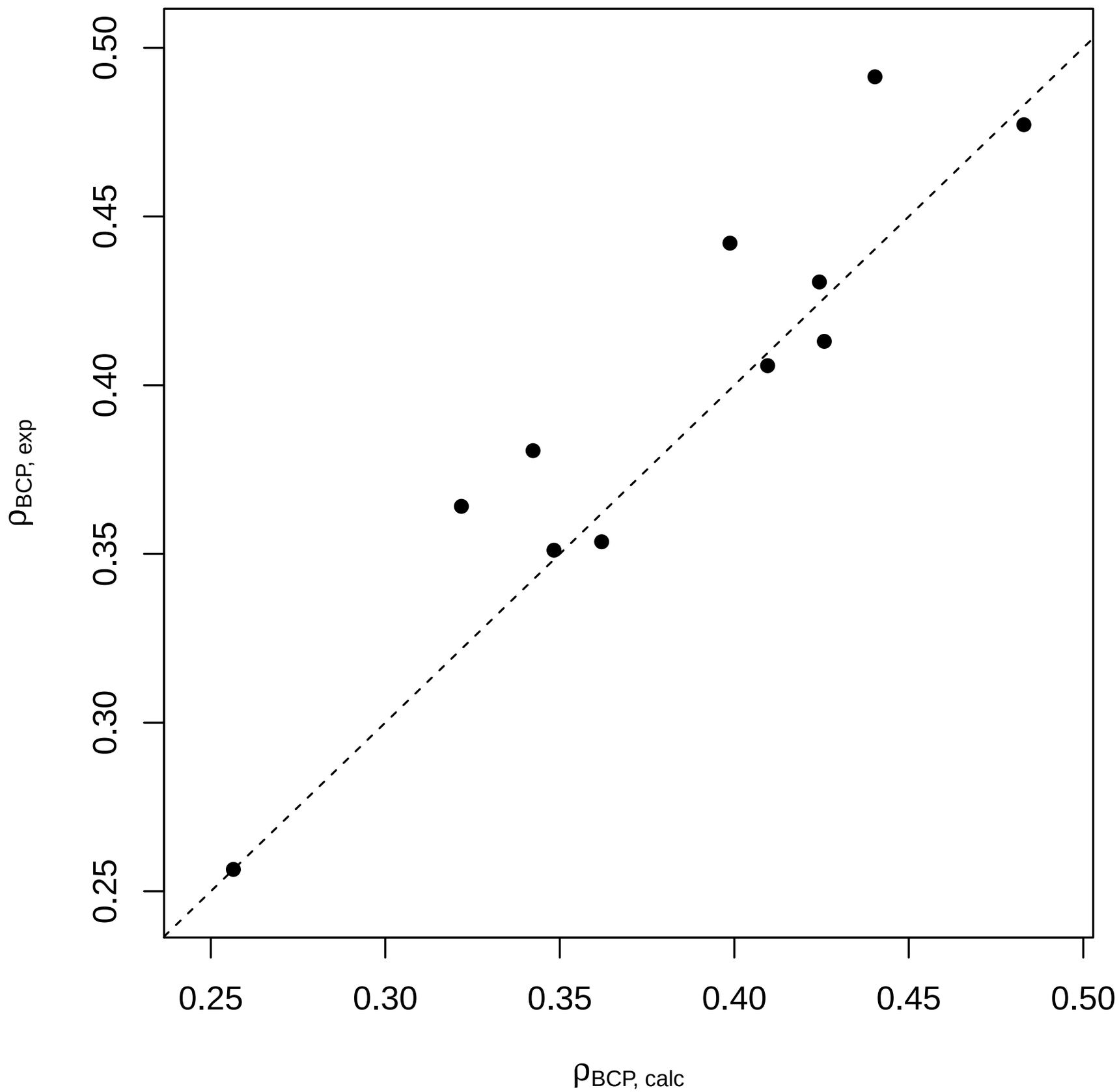
DMAP

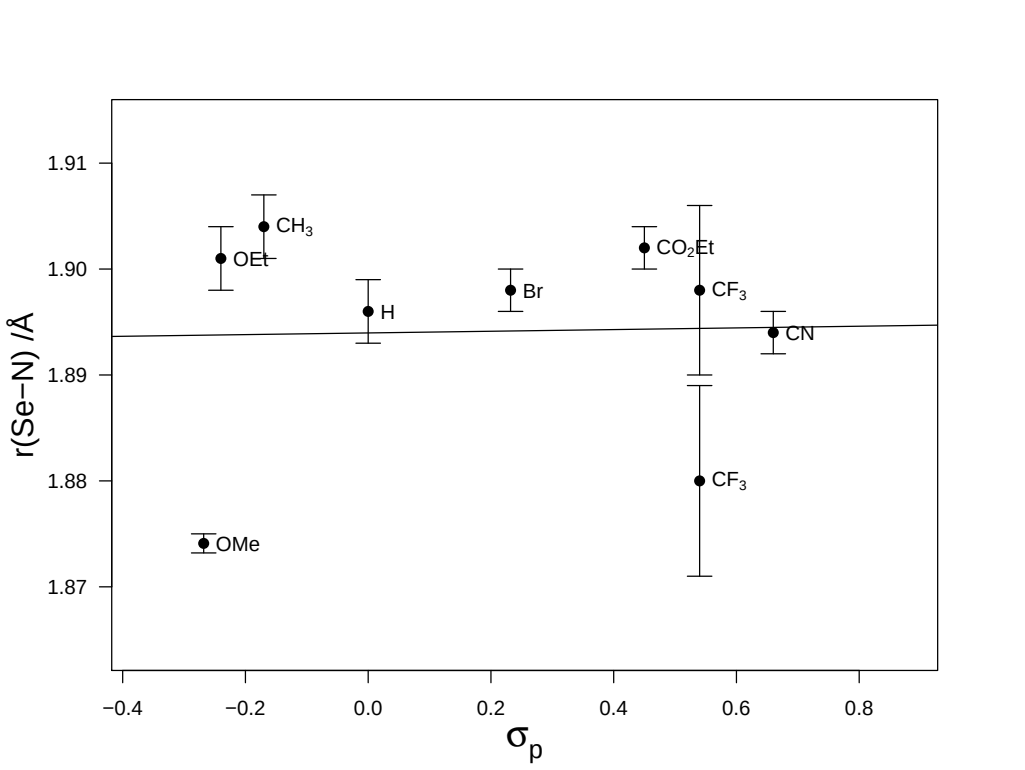


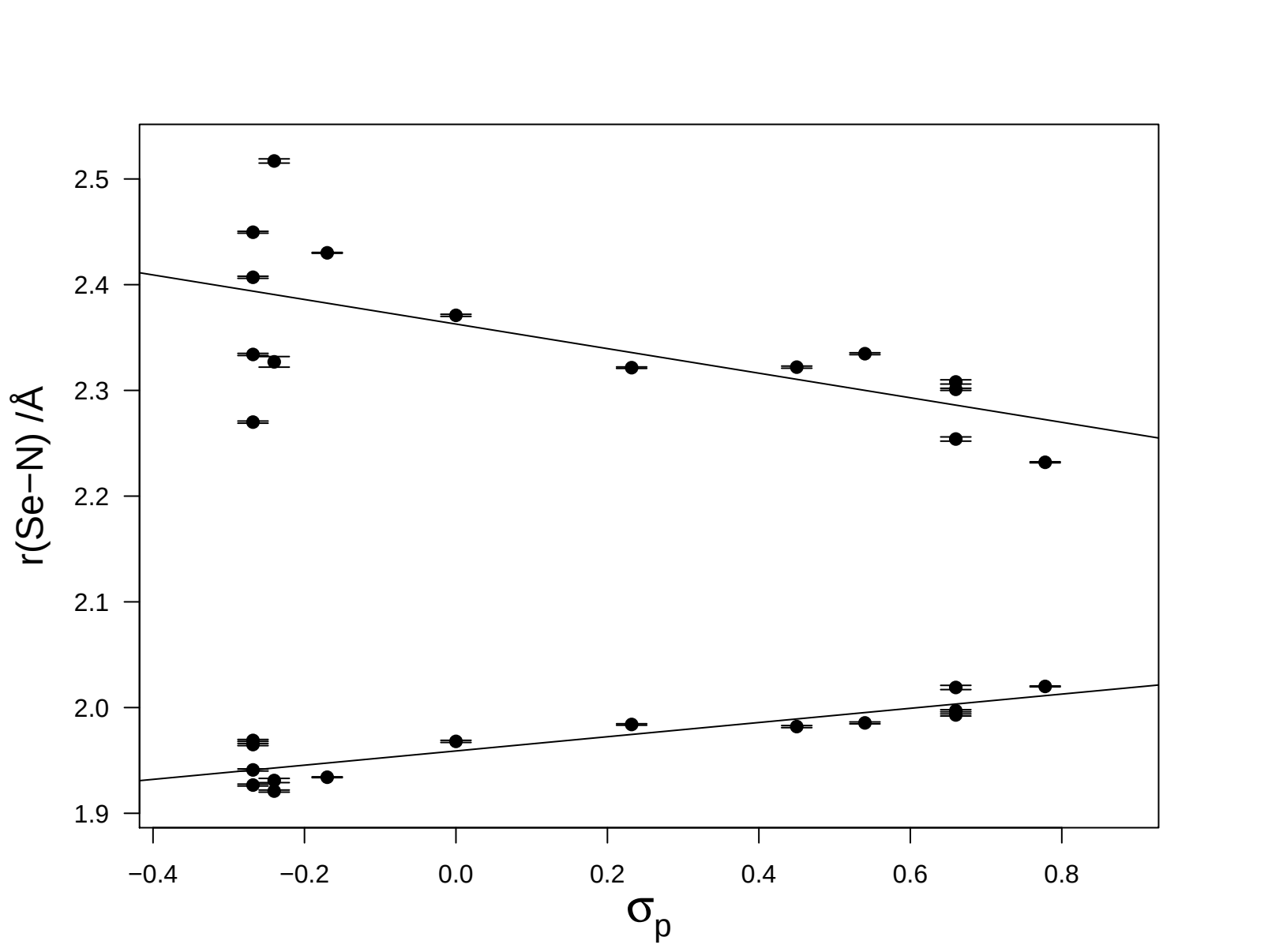
4b

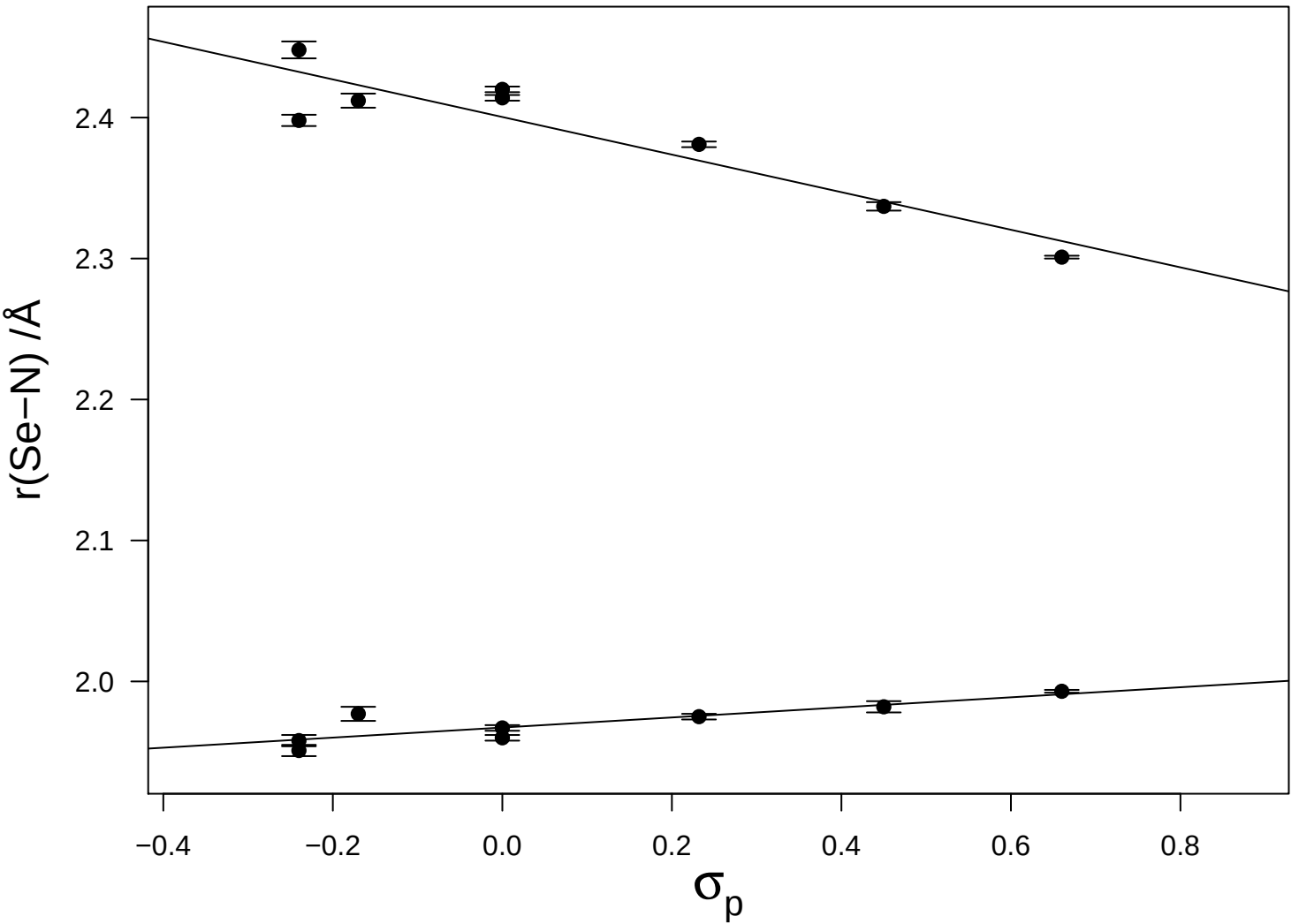


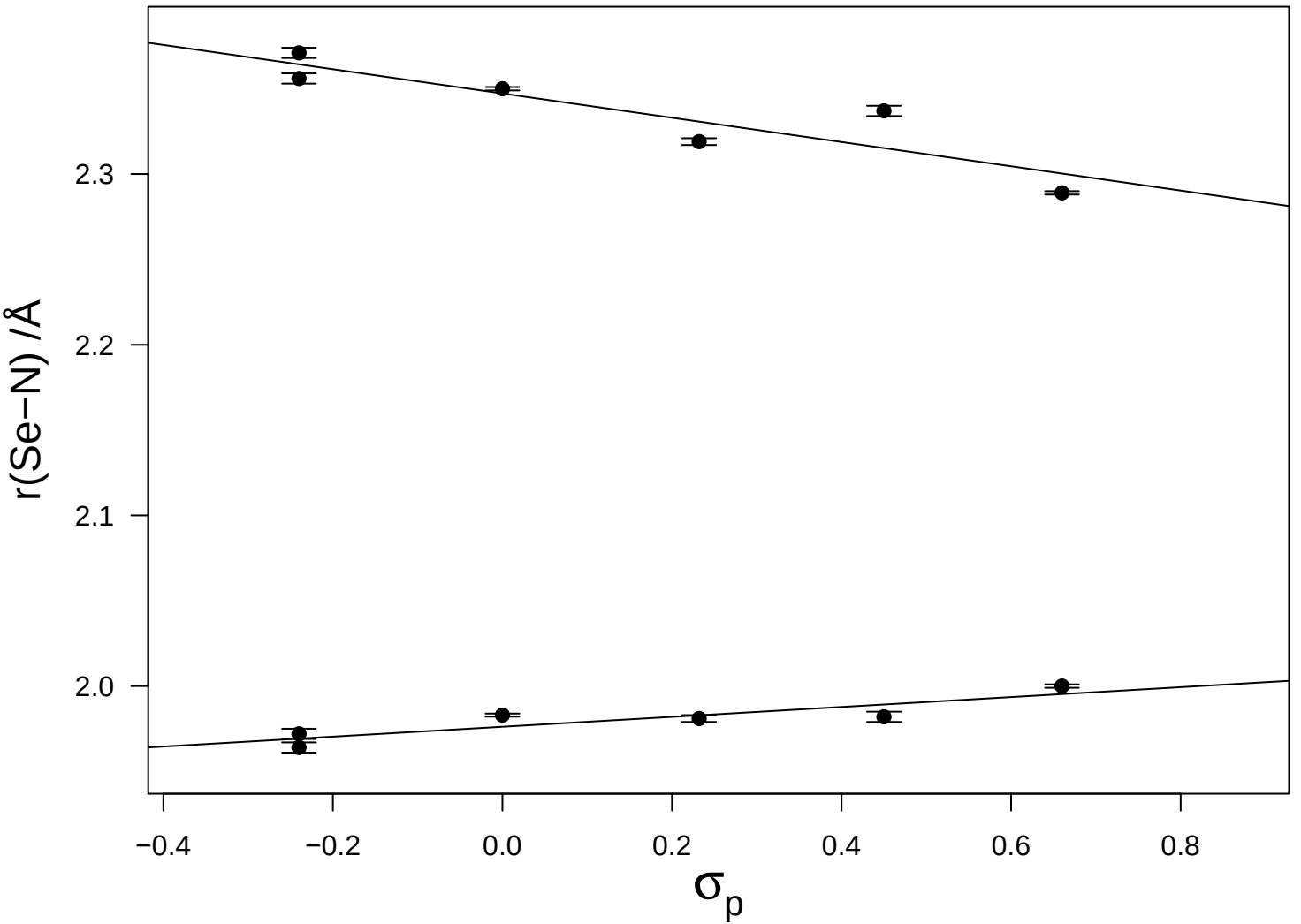
5 **1**

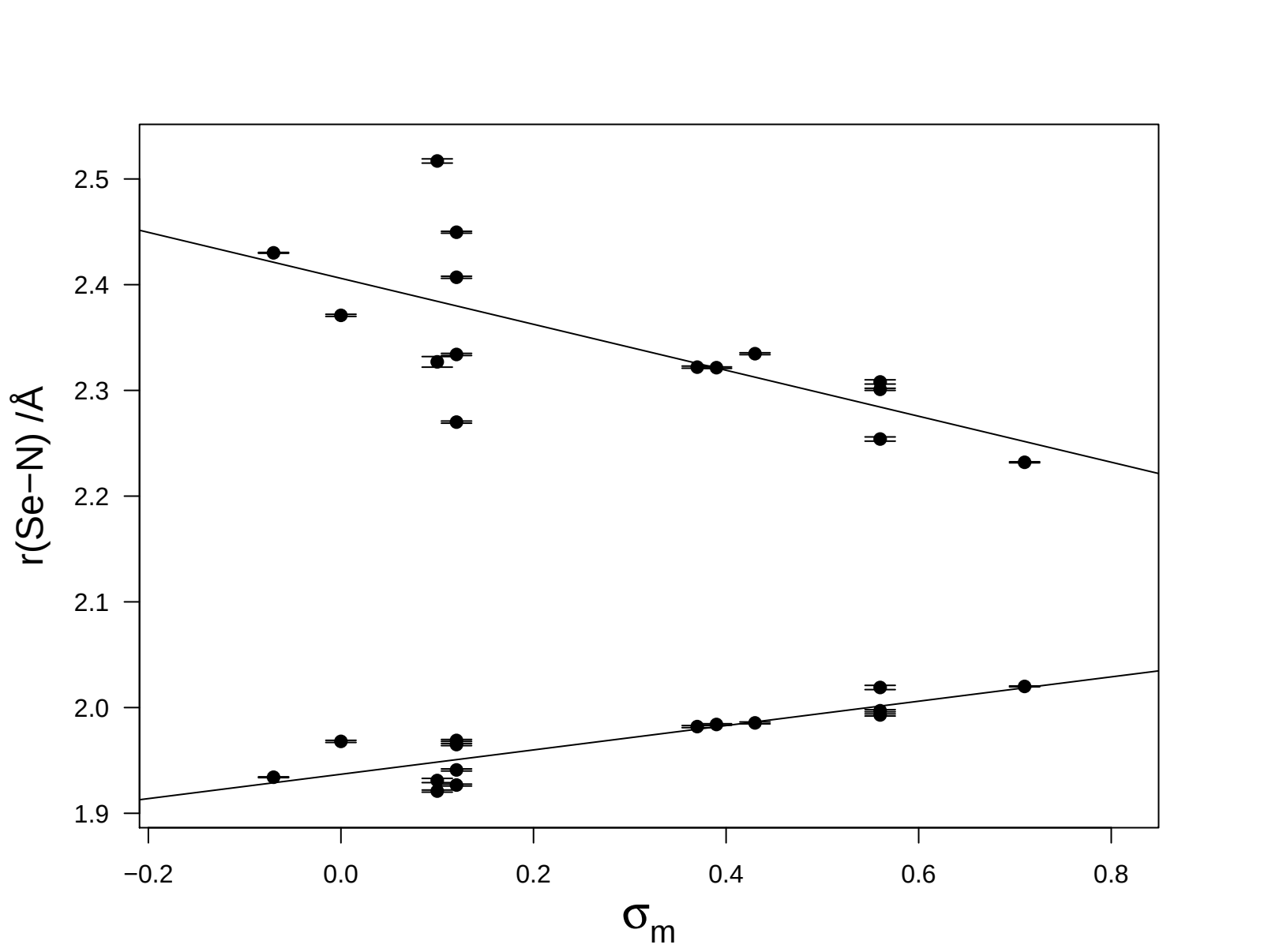

0.25
0.30
0.35
0.40
0.45
0.50
ρBCP, exp
ρBCP, calc

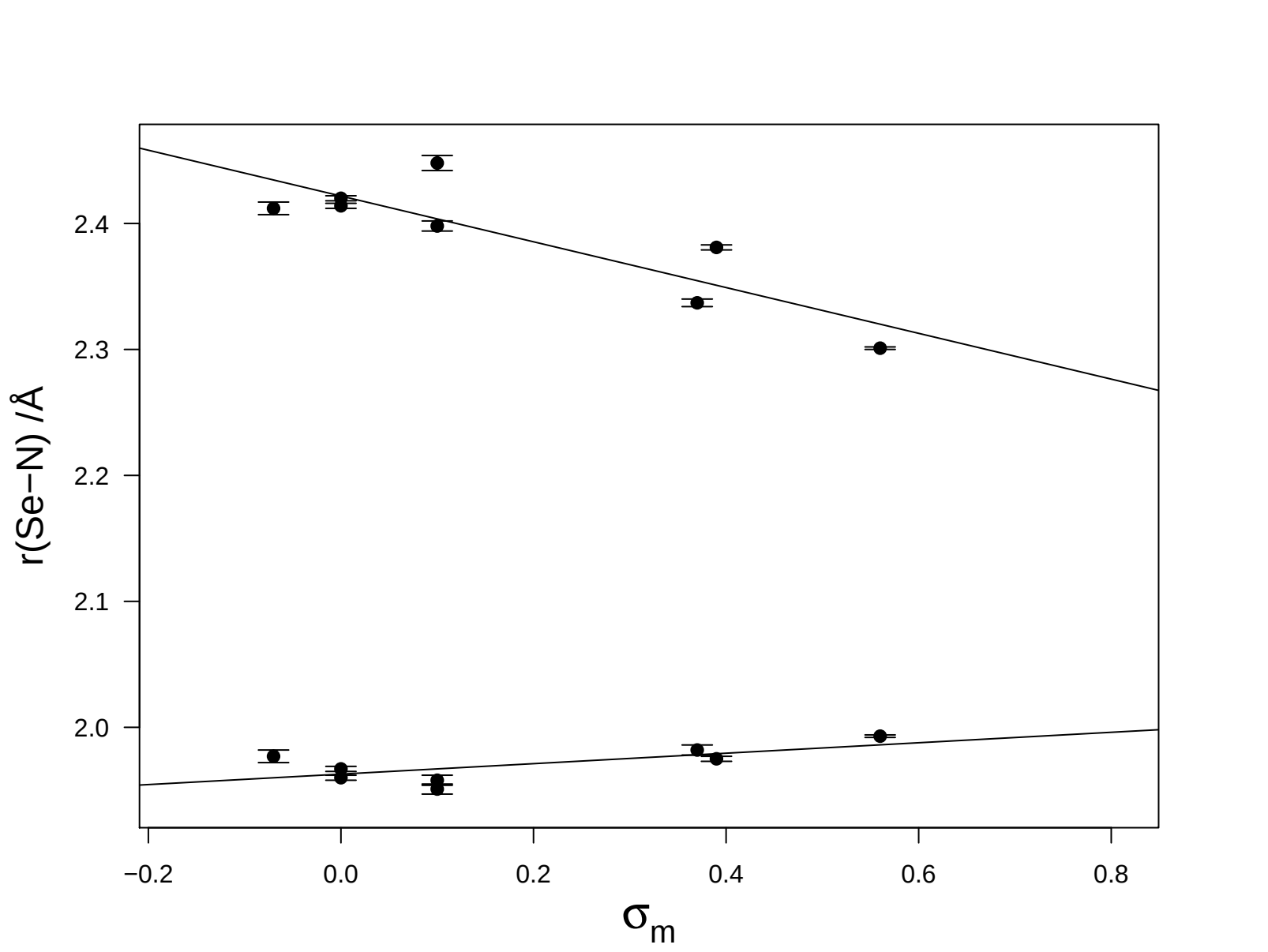

1.91
1.90
1.89
1.88
1.87
r(Se−N) /Å
CH3
OEt
H
Br
CO2Et
CF3
CN
CF3
OMe
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
σp

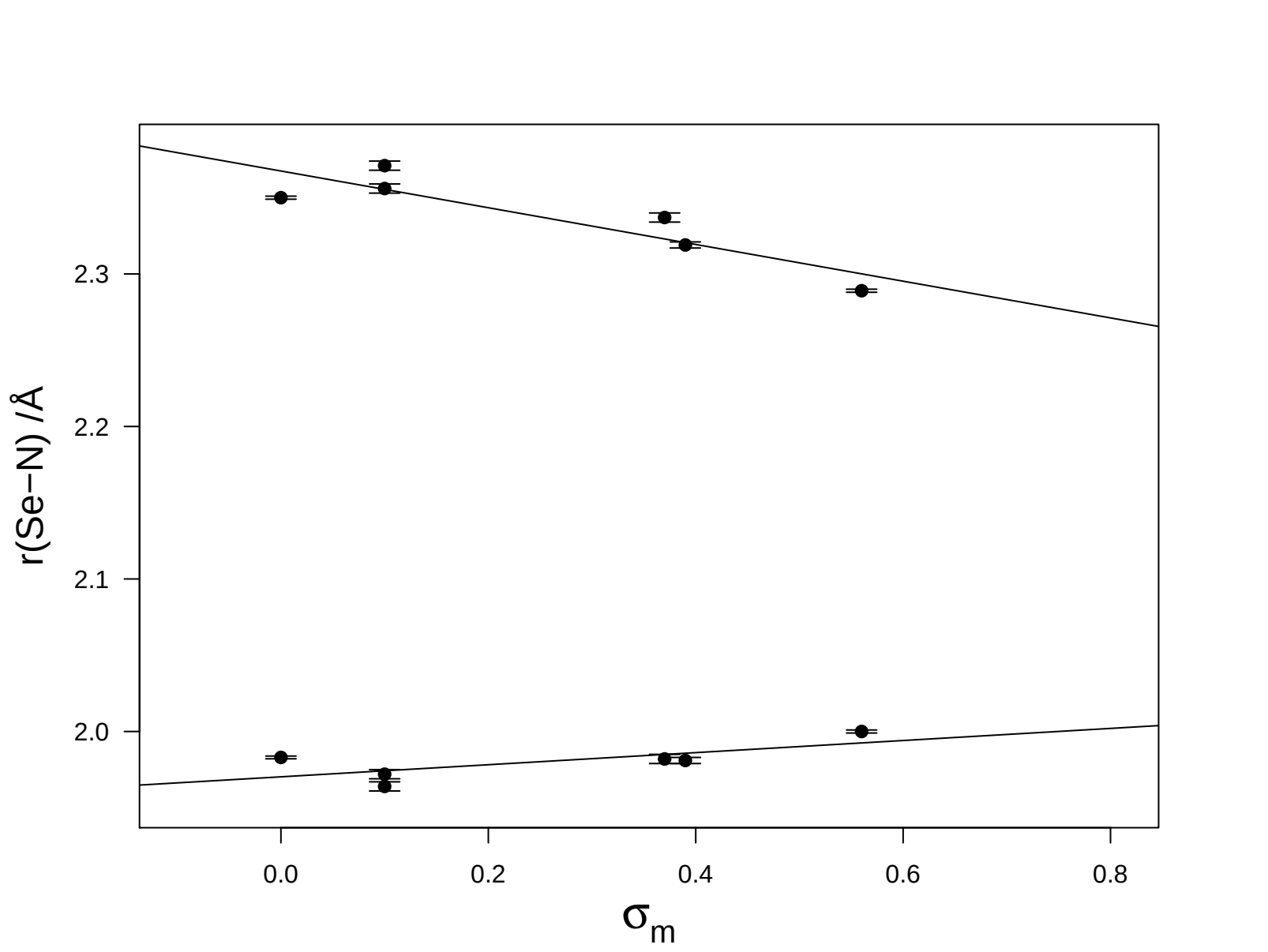

r(Se–N) /Å
2.5
2.4
2.3
2.2
2.1
2.0
1.9
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
σp

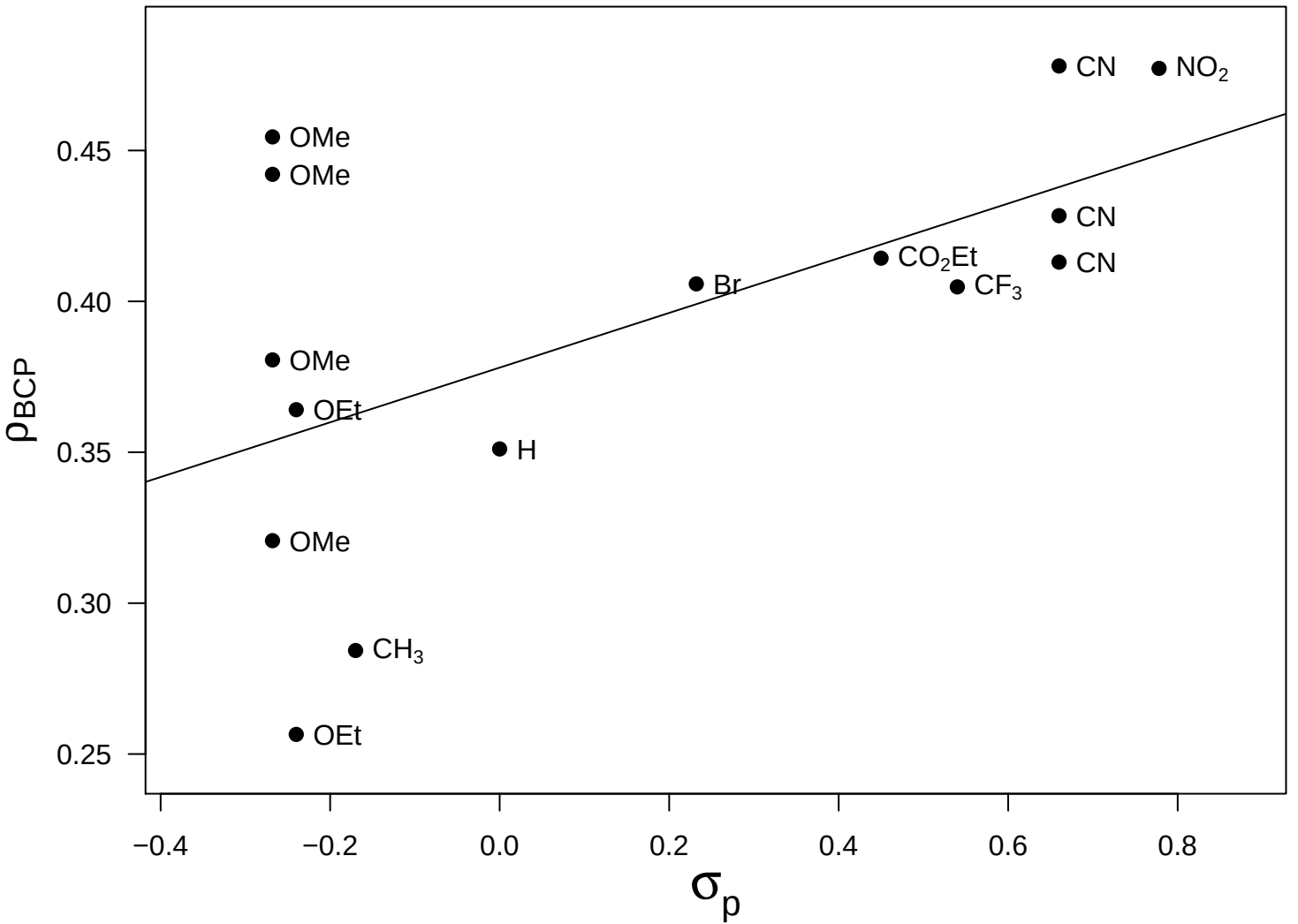

r(Se–N) /Å
2.4
2.3
2.2
2.1
2.0
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
σp

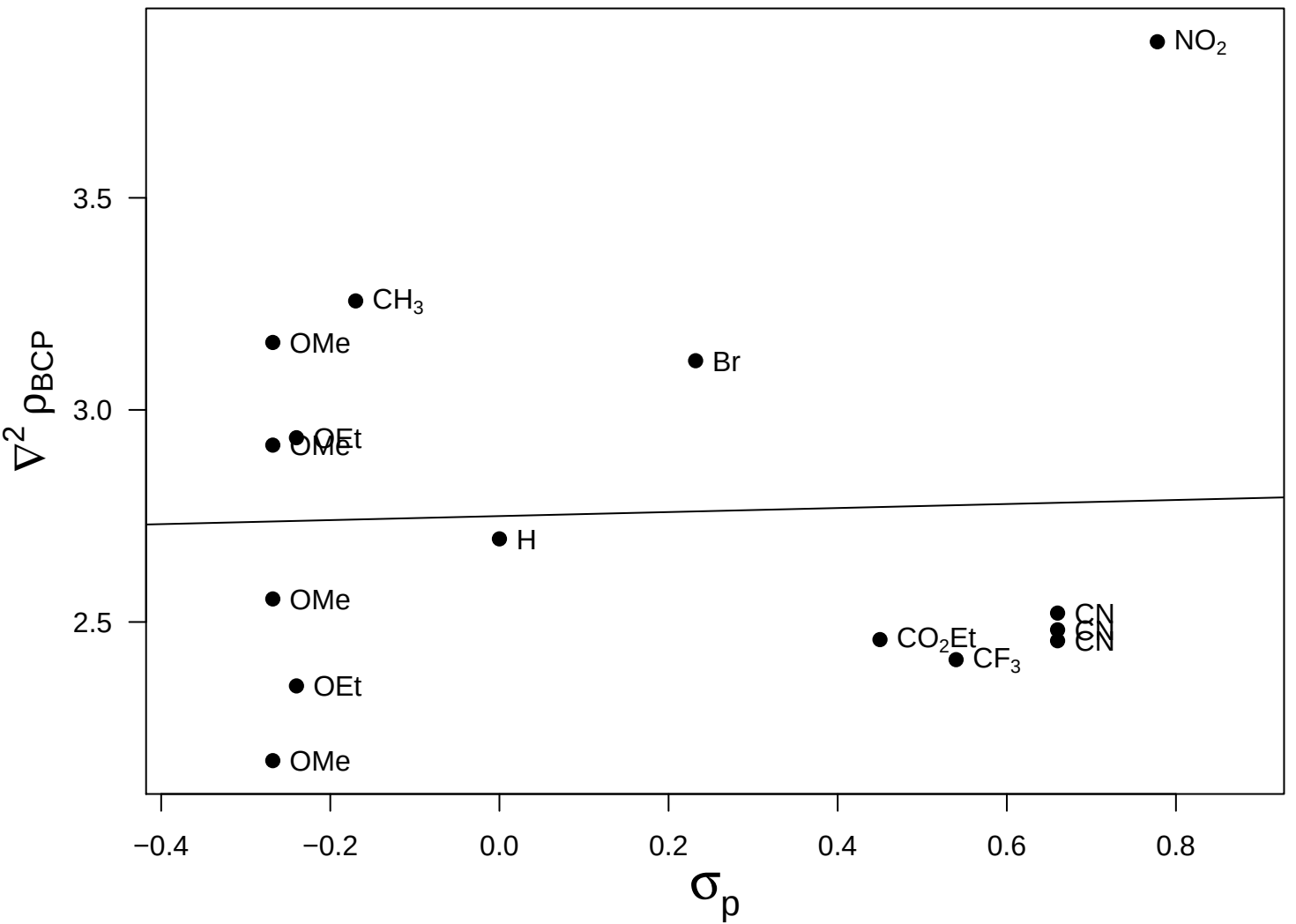

r(Se–N) /Å
2.0
2.1
2.2
2.3
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
σp

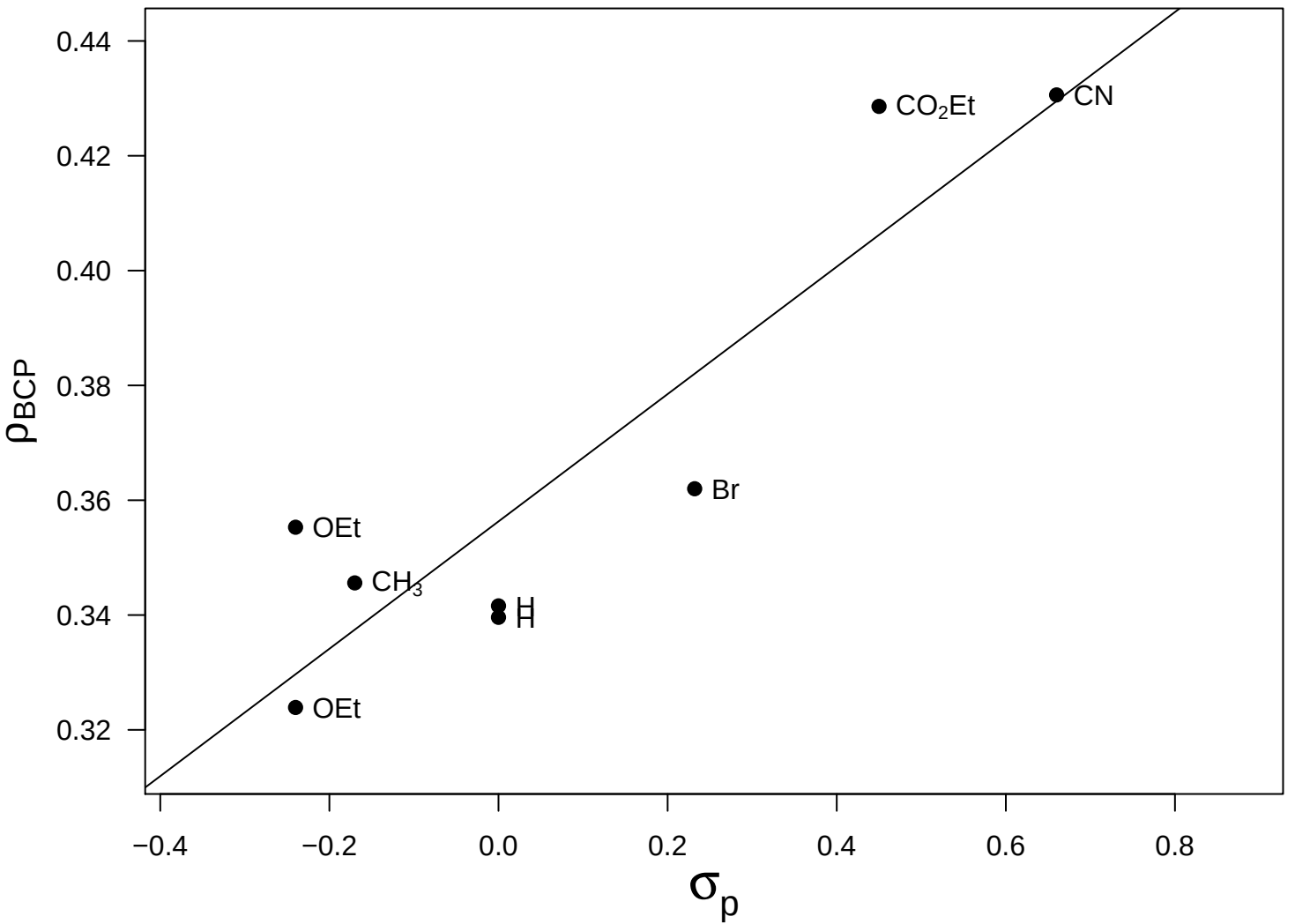

r(Se–N) /Å
2.5
2.4
2.3
2.2
2.1
2.0
1.9
−0.2
0.0
0.2
0.4
0.6
0.8
σm

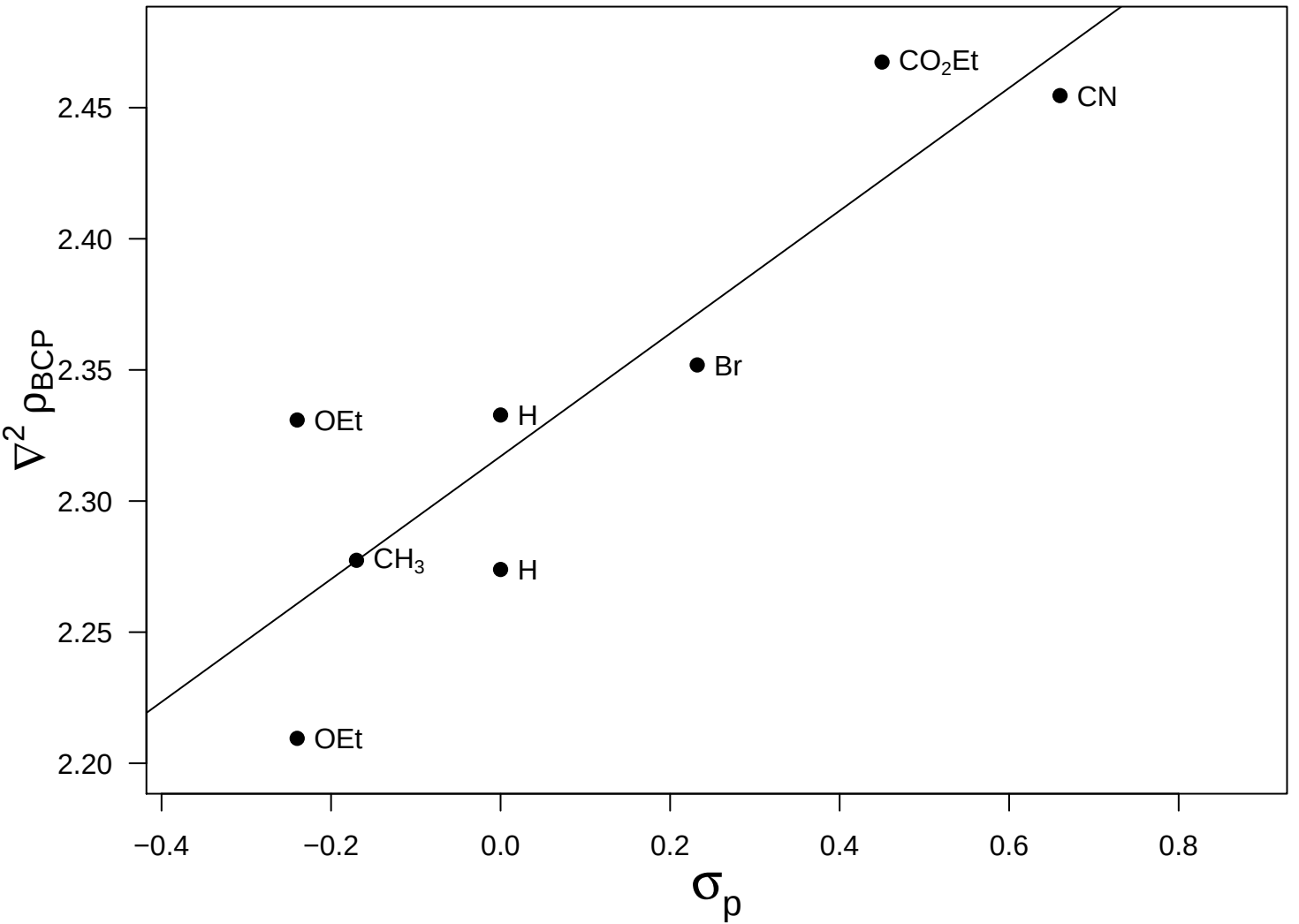

r(Se–N) /Å
2.4
2.3
2.2
2.1
2.0
−0.2
0.0
0.2
0.4
0.6
0.8
σm

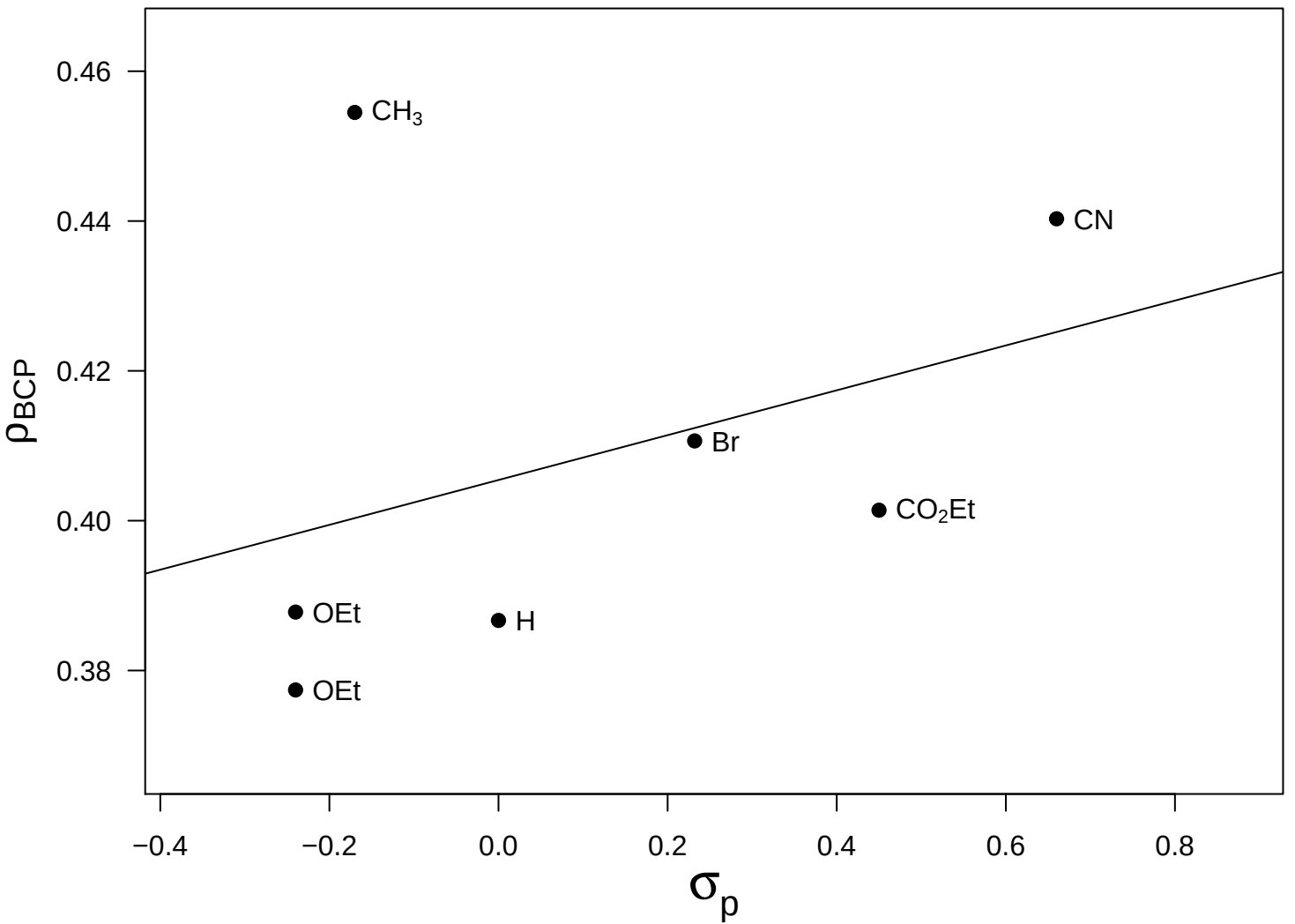

r(Se–N) /Å
2.3
2.2
2.1
2.0
0.0
0.2
0.4
0.6
0.8
σm

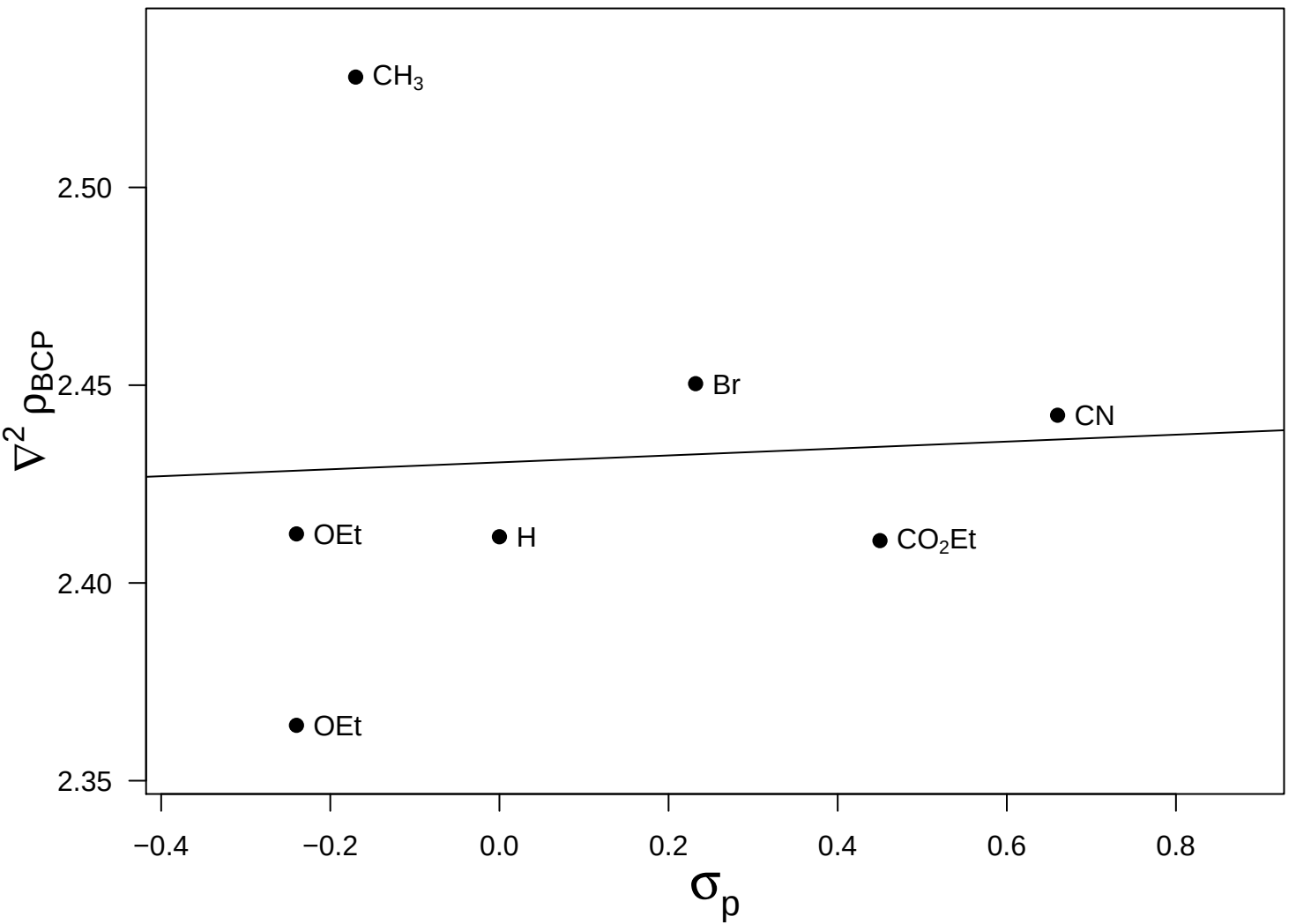

CN
NO2
OMe
OMe
CN
CO2Et
CN
Br
CF3
OMe
OEt
H
OMe
CH3
OEt
0.45
0.40
0.35
0.30
0.25
ρBCP
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
σp

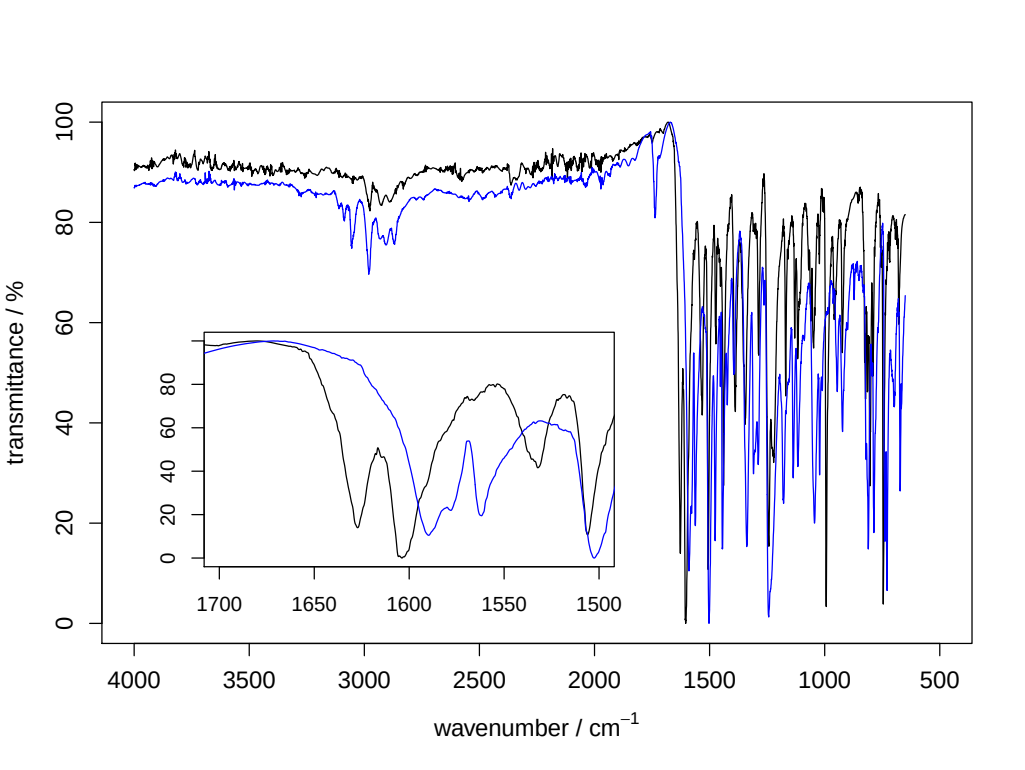

NO2
CH3
OMe
Br
OMe
OEt
H
OMe
CO2Et
CF3
CN
CN
CN
OEt
OMe
3.5
3.0
2.5
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
∇2 ρBCP
σp

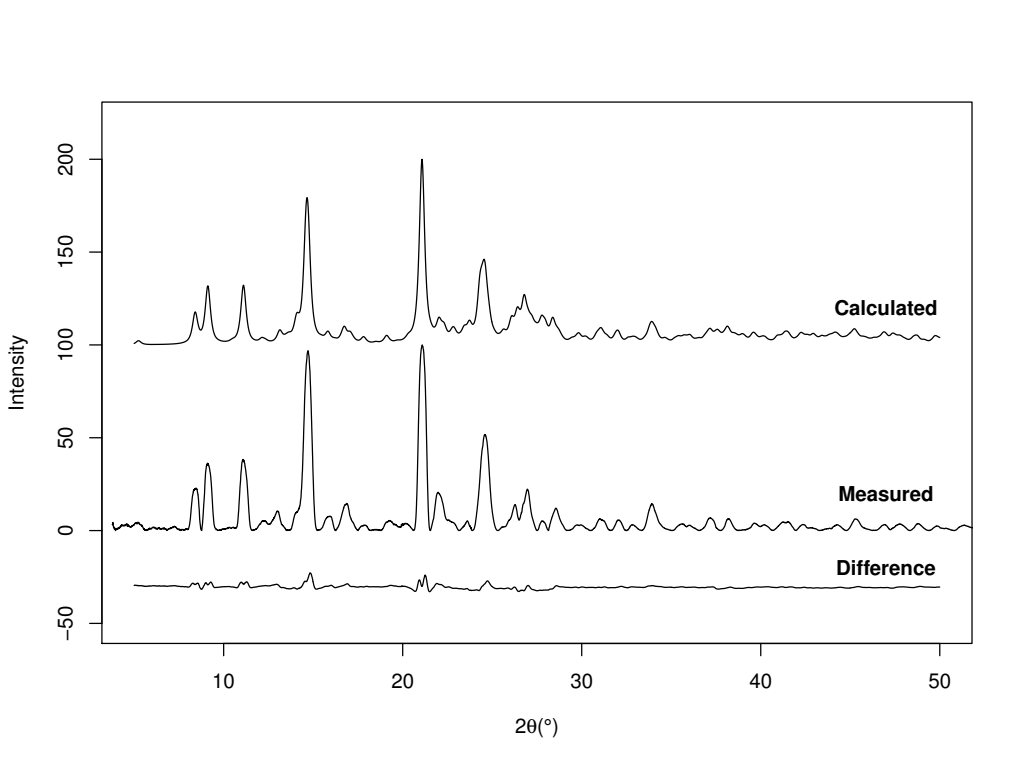

0.44
0.42
0.40
0.38
0.36
0.34
0.32
ρBCP
CO2Et
CN
Br
OEt
CH3
H
OEt
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
σp

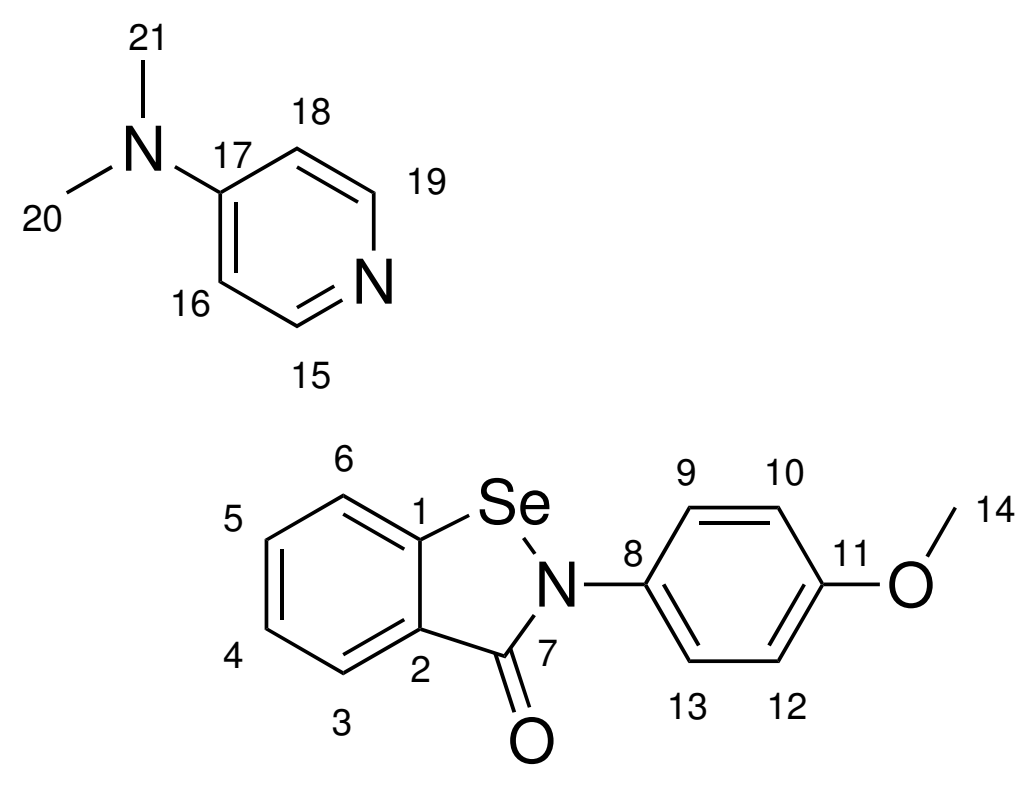

CO_2Et
CN
Br
OEt
H
CH_3
H
OEt
2.45
2.40
2.35
2.30
2.25
2.20
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
$\nabla^2 \rho_{BCP}$
σ_p

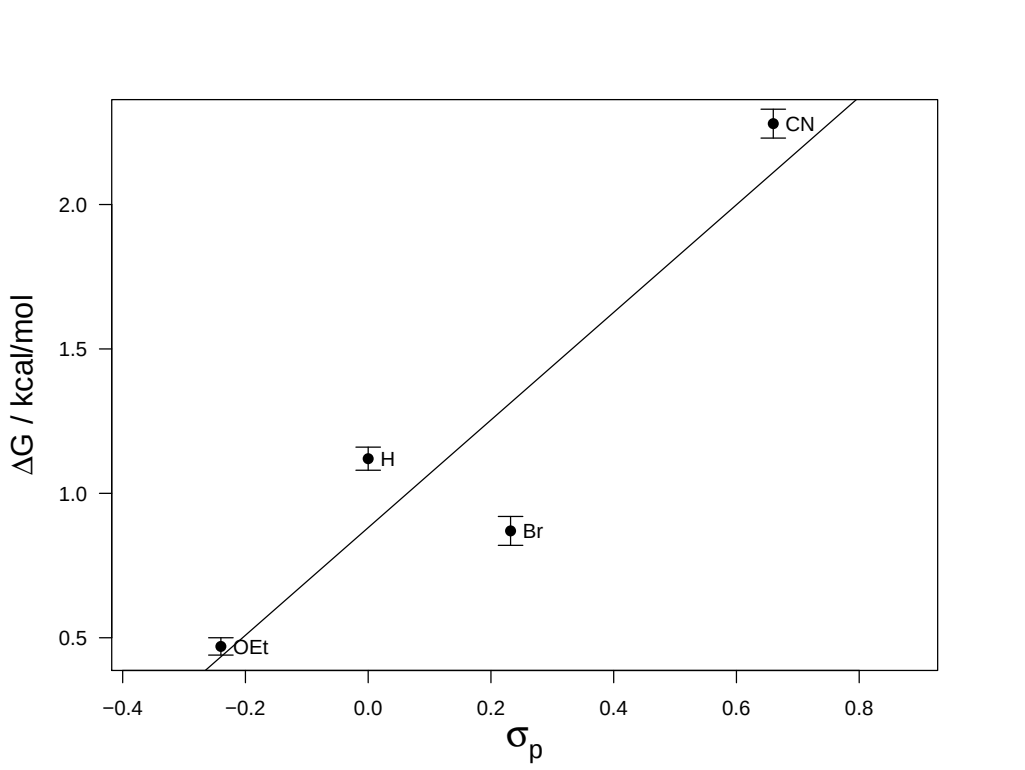

0.46
0.44
0.42
0.40
0.38
ρ_{BCP}
CH_3
CN
Br
CO_2Et
OEt
H
OEt
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
σ_p

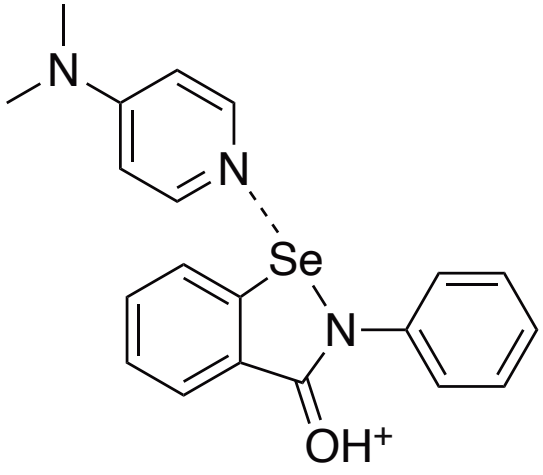

CH3
Br
CN
OEt
H
CO2Et
OEt
2.50
2.45
2.40
2.35
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
∇2 ρBCP
σp


transmittance / %
0
20
40
60
80
100
4000
3500
3000
2500
2000
1500
1000
500
wavenumber / cm^{-1}
0
20
40
60
80
1700
1650
1600
1550
1500


Intensity
200
150
100
50
0
−50
Calculated
Measured
Difference
10
20
30
40
50
2θ(°)

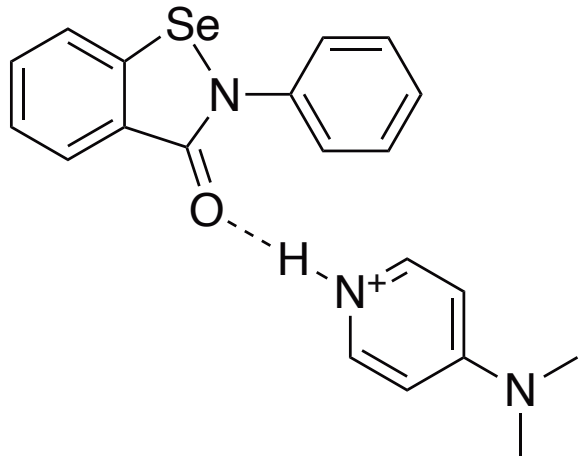

21
18
N
17
19
20
N
16
15
6
9
10
5
1
Se
8
11
14
N
O
4
2
7
3
13
12
O


CN
H
Br
OEt
2.0
1.5
1.0
0.5
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
ΔG / kcal/mol
σp



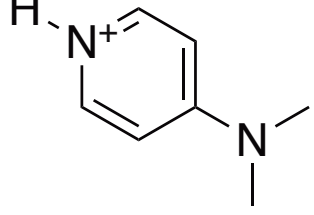
m/z: 398.08

or

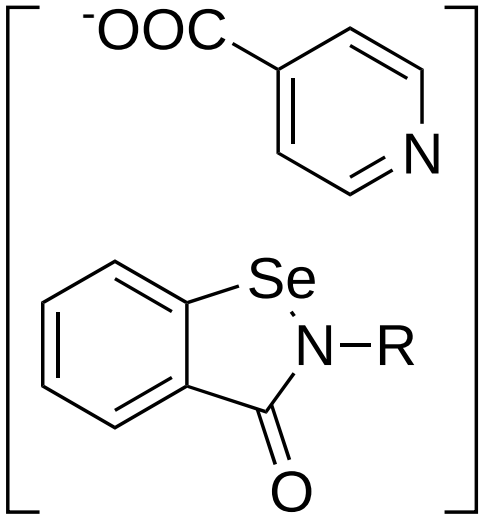


m/z: 398.08

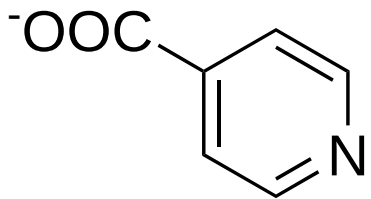
CID



m/z: 123.09



CID

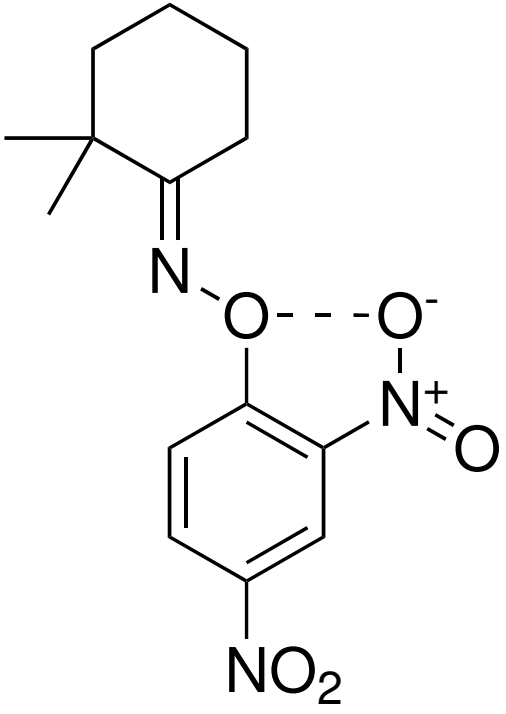


1 R = Ph

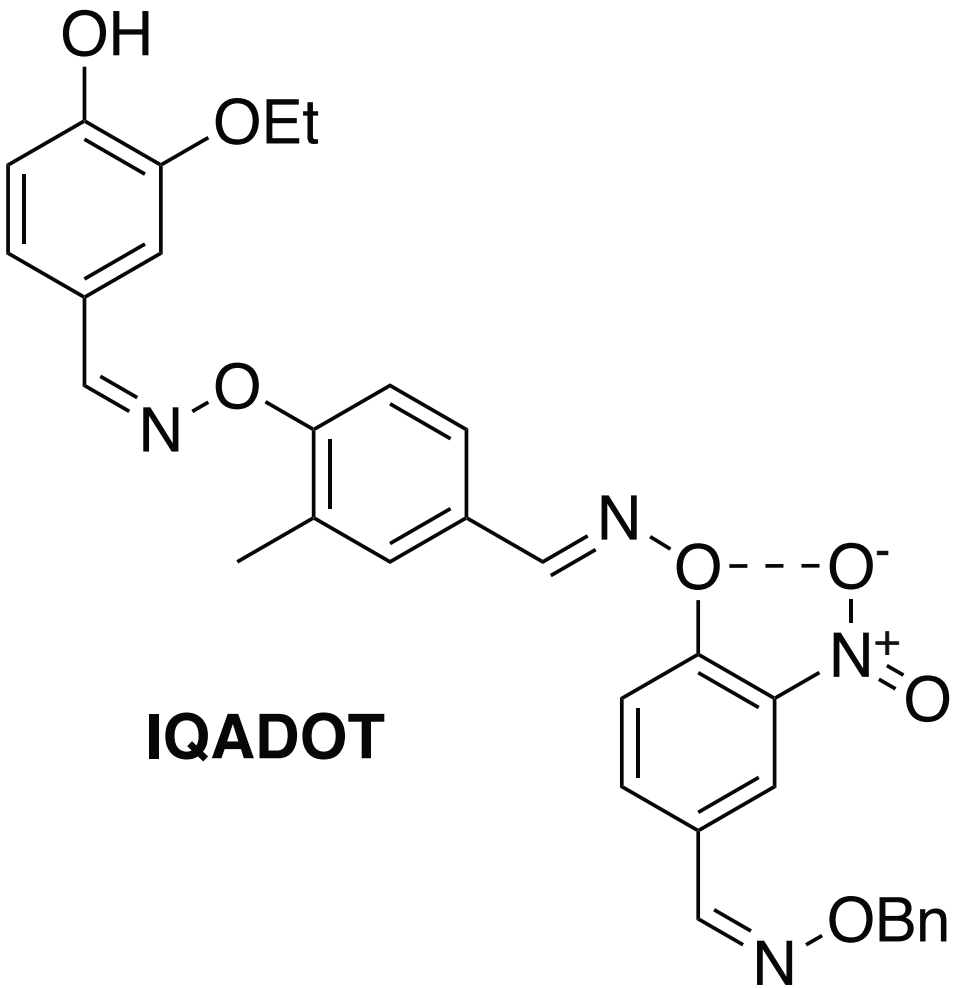
1a R = Bn

m/z: 397.01

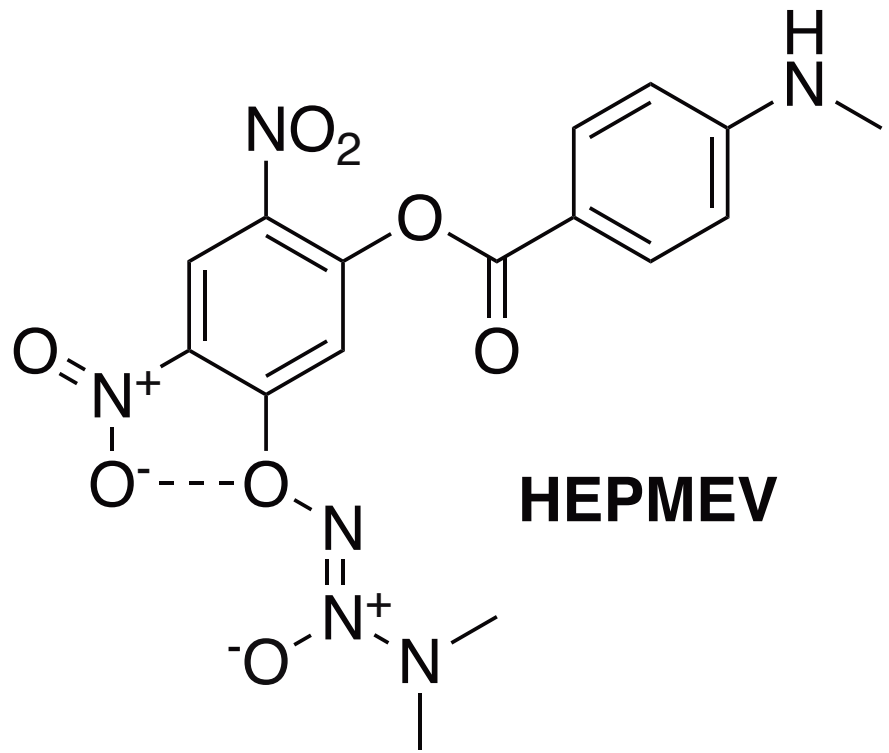
m/z: 122.02



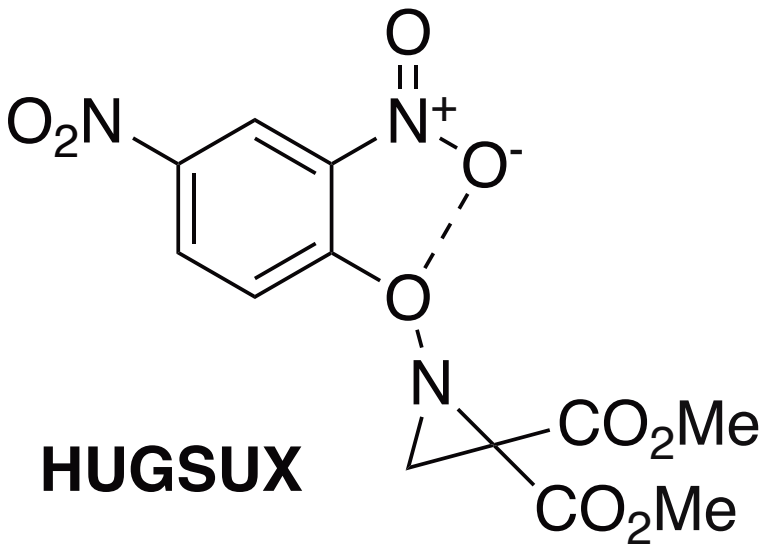
7



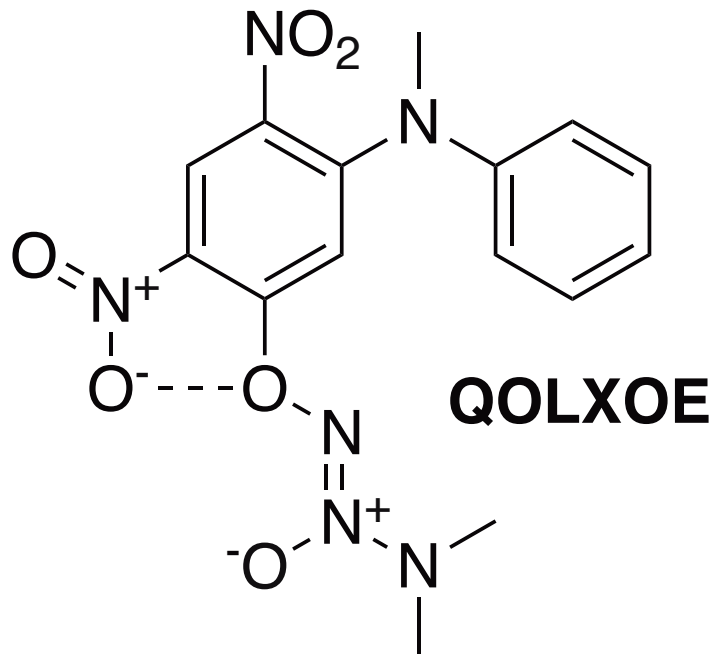
IQADOT



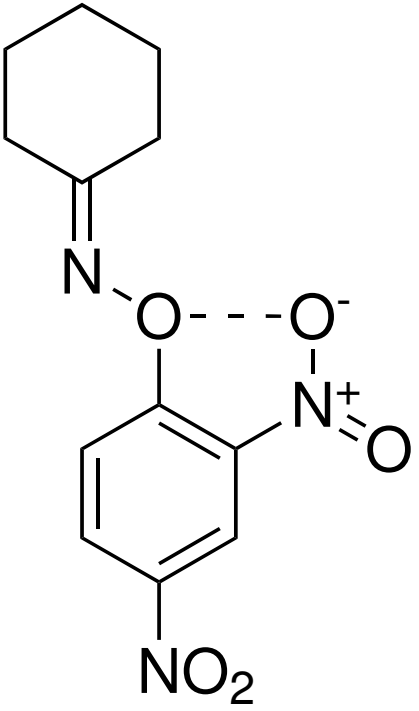
HEPMEV



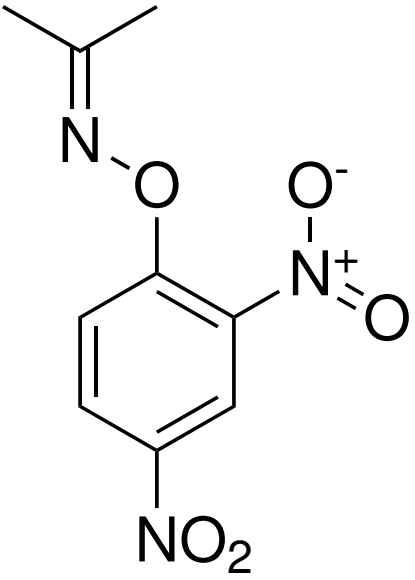
HUGSUX



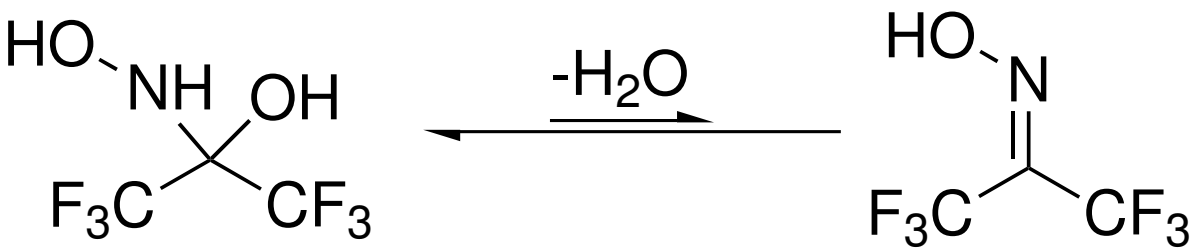
QOLXOE

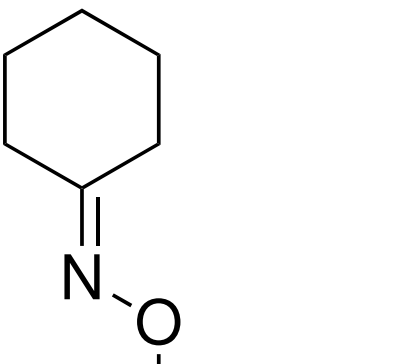


8

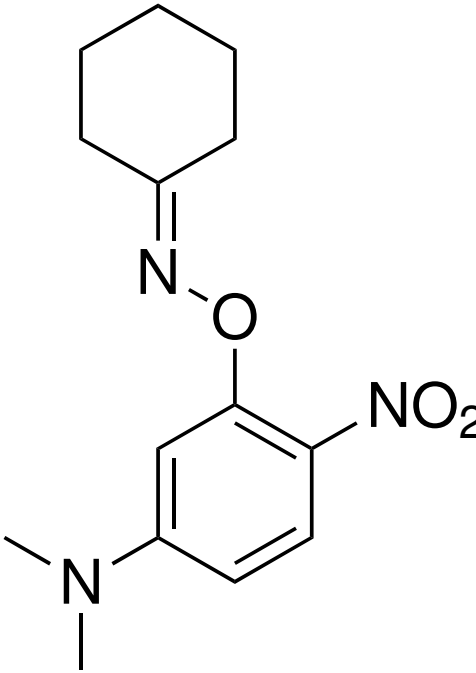


9

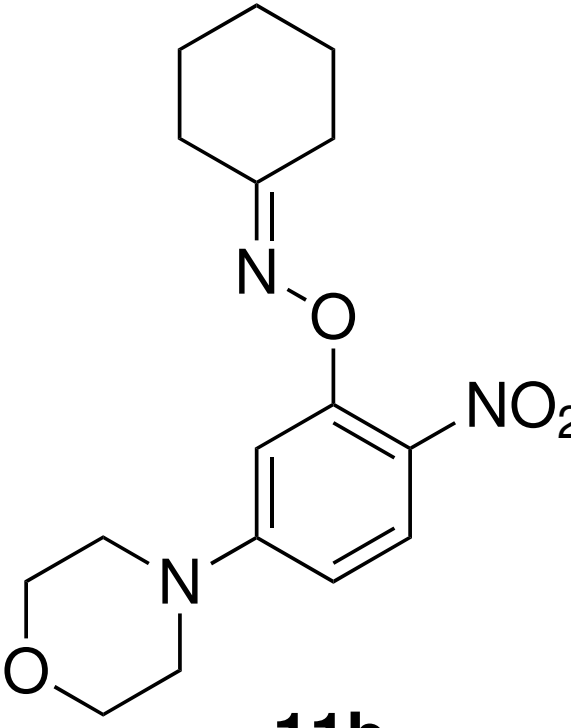

HO
NH
OH
F3C
CF3
-H2O
HO
N
F3C
CF3



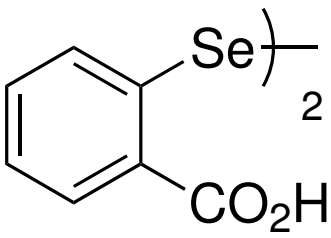
10



11a

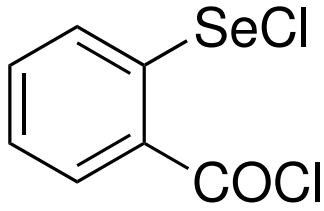


11b



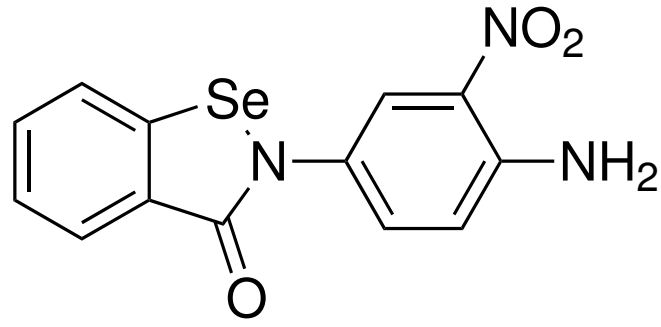
5

a



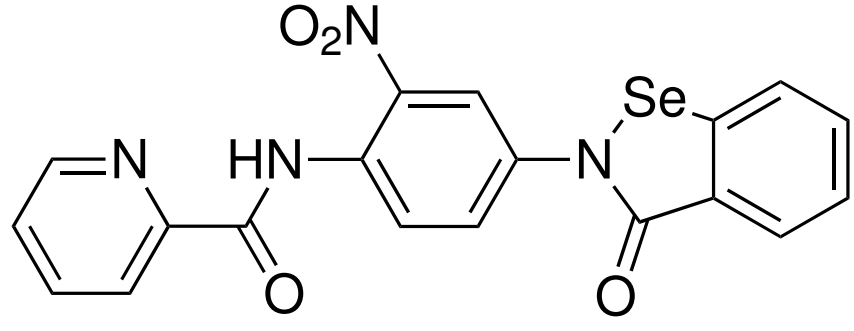
6

b



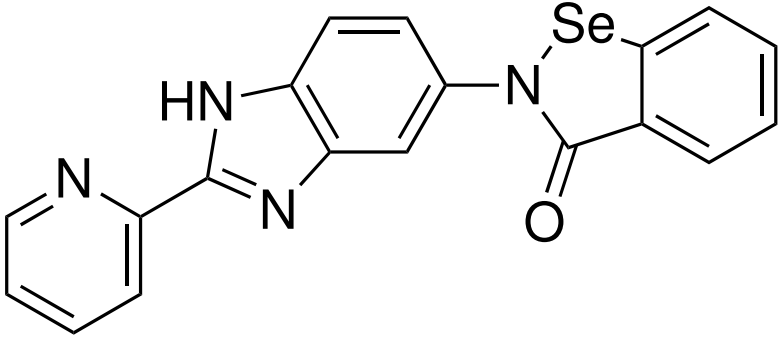
15

c

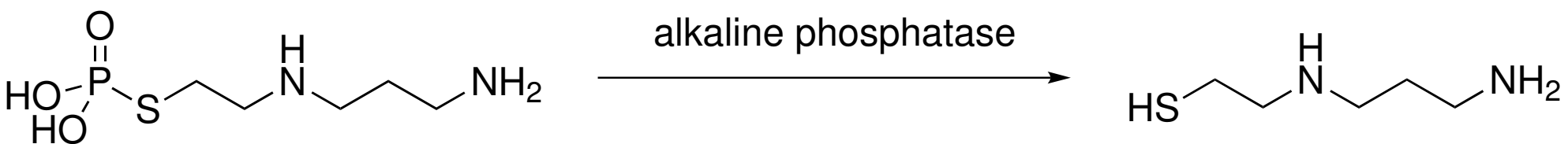


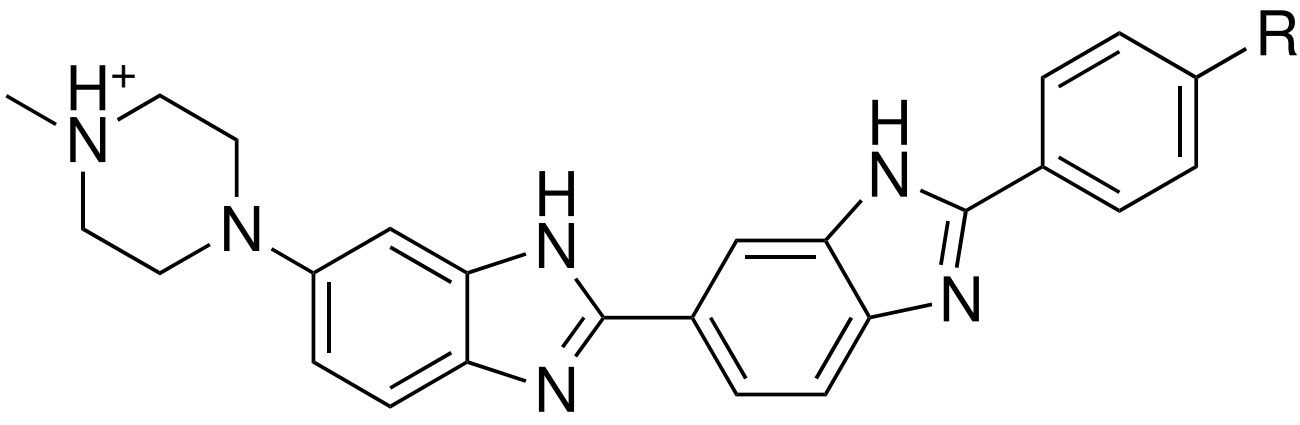
14

d

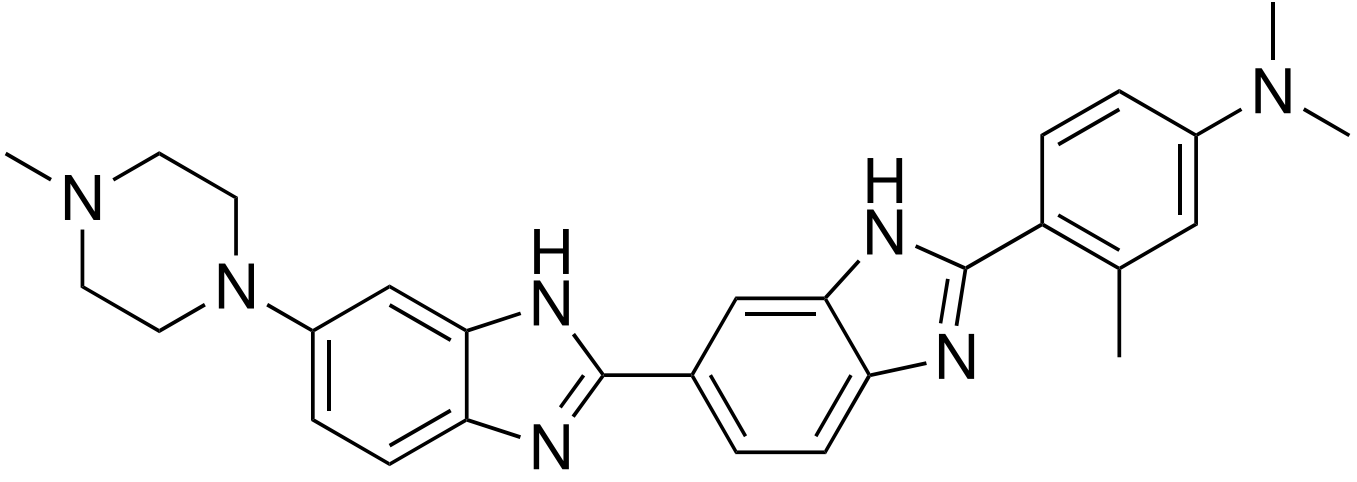


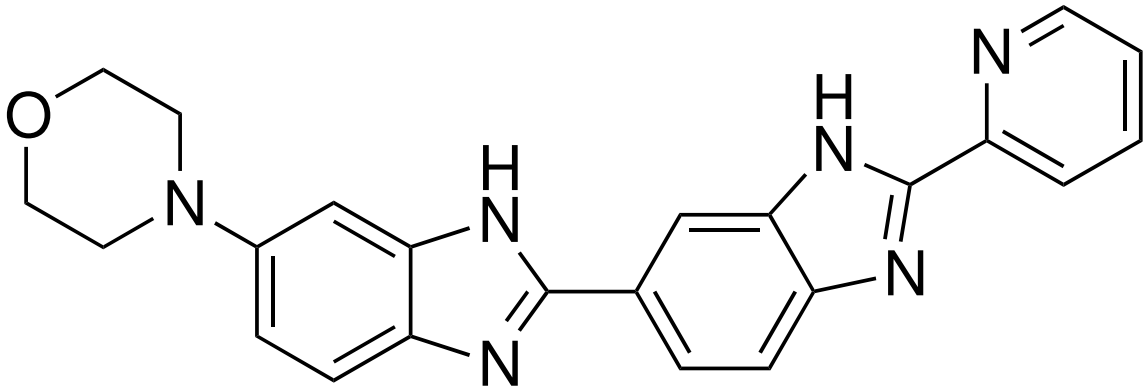
13


O
HO
P
HO
S
H
N
NH2
alkaline phosphatase
HS
H
N
NH2

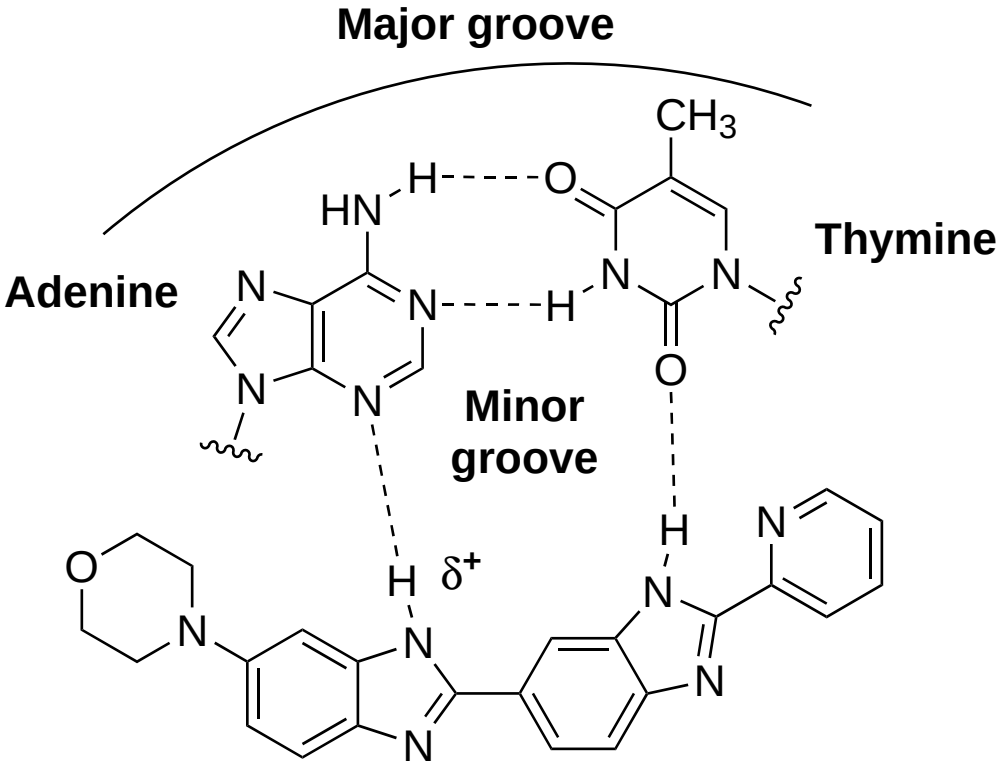


Hoechst 33258 R: OH
Hoechst 33342 R: OCH_2CH_3
Hoechst 34580 R: $N(CH_3)_2$

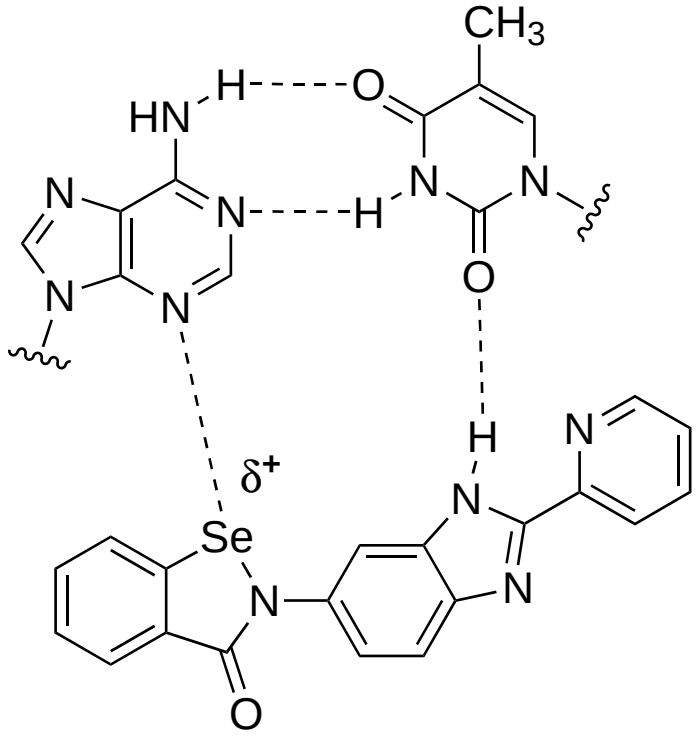




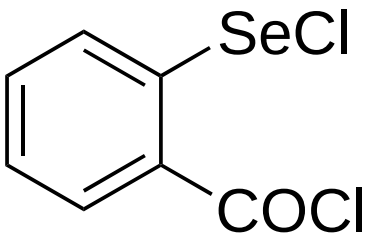
12



12

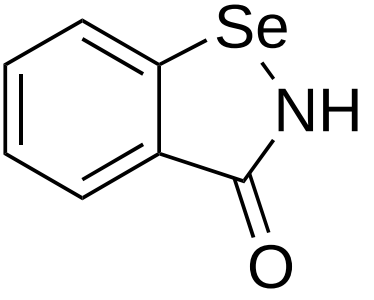


13



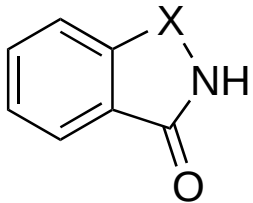
NH_3 (aq)

MeCN, rt, 10 min, 87%



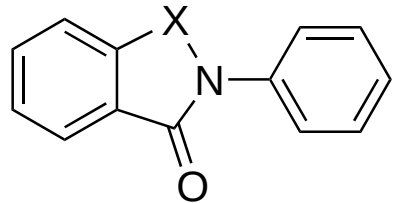
6

1b



PhBr, CuI, DMEDA, K_2CO_3

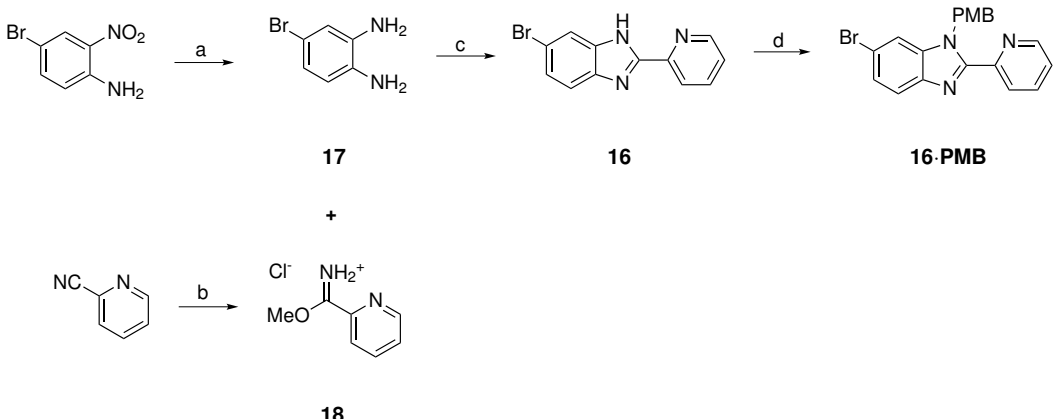
4Å sieves, 1,4-dioxane , 120ºC, 18 h, 45%

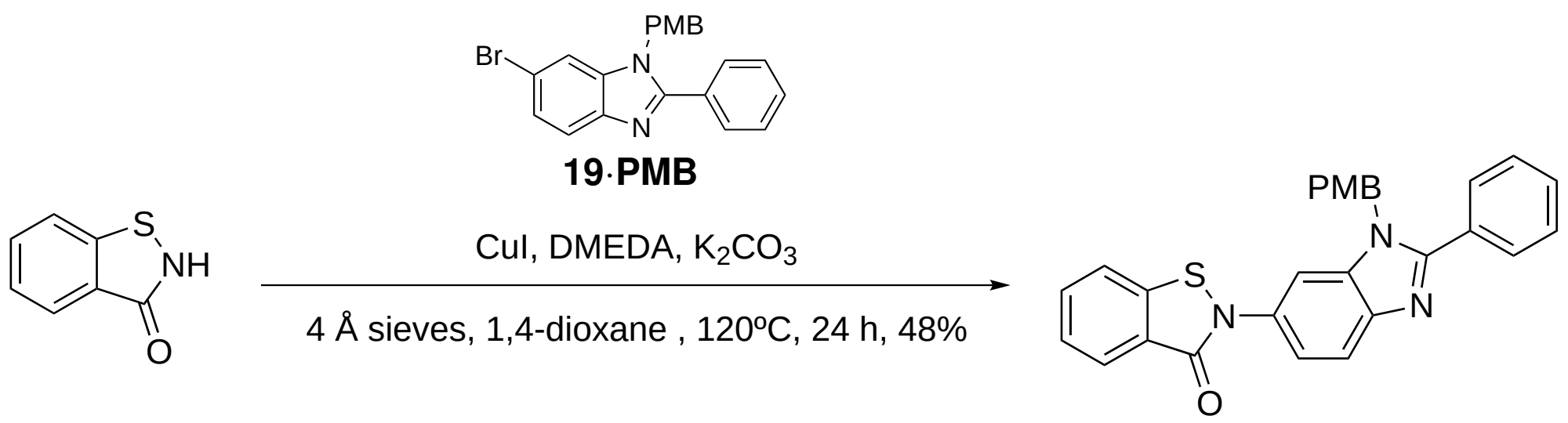


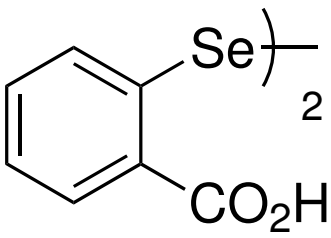
X = S, Se

1b and **1b·S**

1 and **1·S**

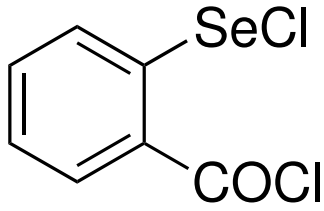

Br
NO2
NH2
a
Br
NH2
NH2
c
Br
H
N
N
d
Br
PMB
N
N
17
16
16·PMB
+
NC
N
b
Cl-
NH2+
MeO
N
18


PMB
Br
N
N
19·PMB
S
NH
O
CuI, DMEDA, K2CO3
4 Å sieves, 1,4-dioxane , 120ºC, 24 h, 48%
PMB
N
S
N
N
O
1b·S
20·S·PMB



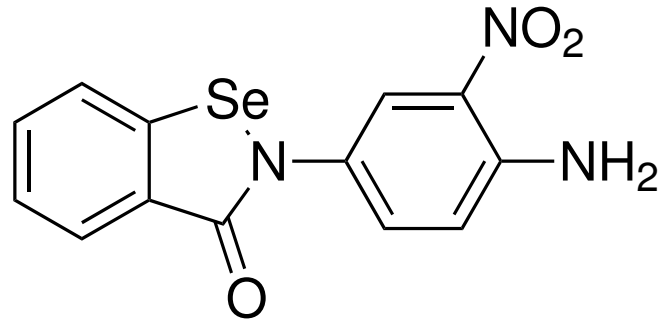
5

a



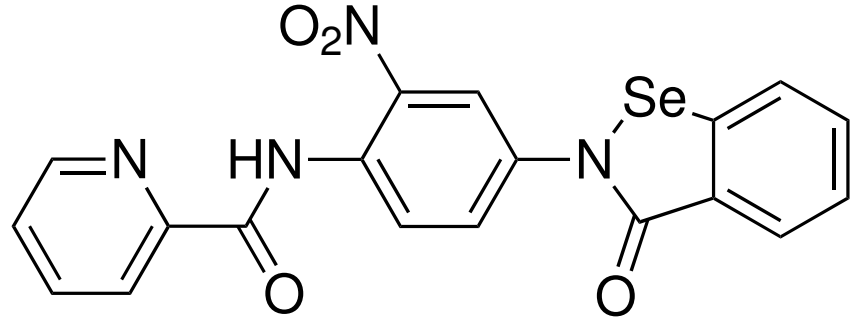
6

b



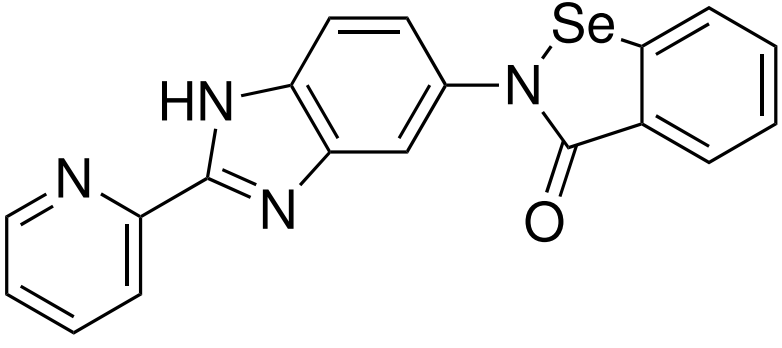
15

c

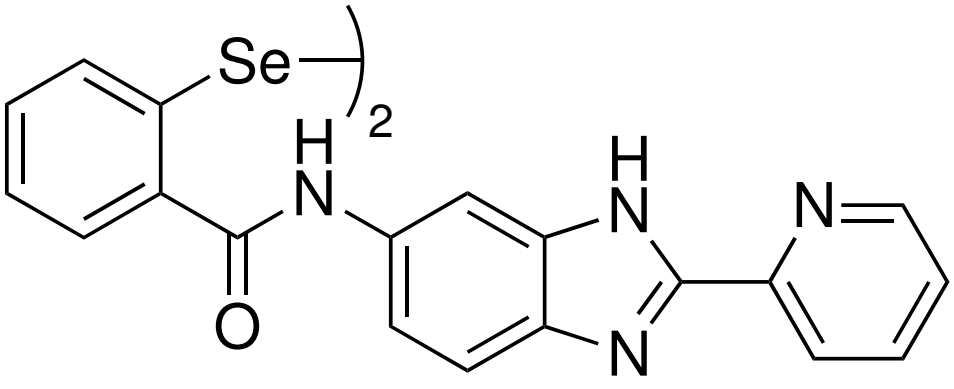


14

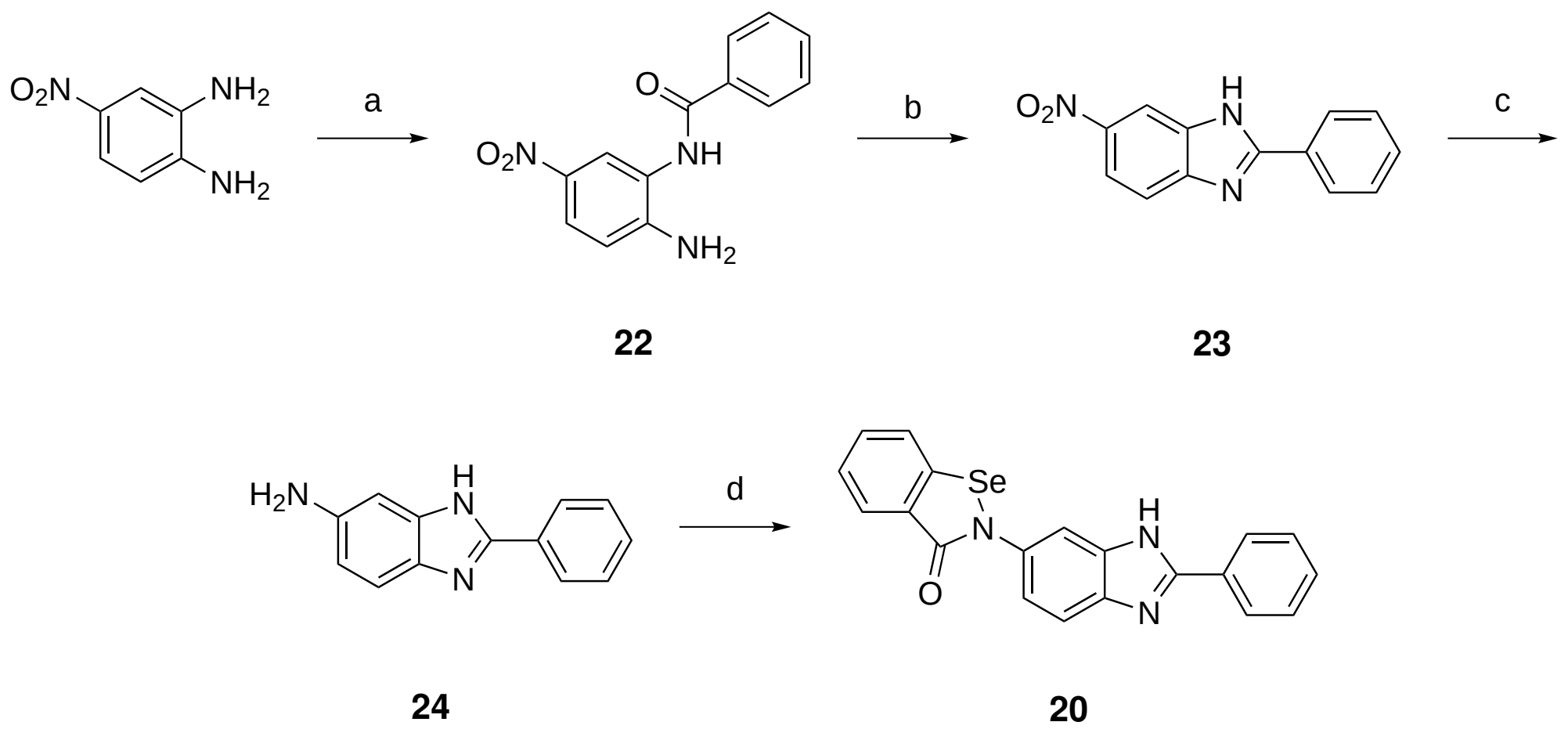
d

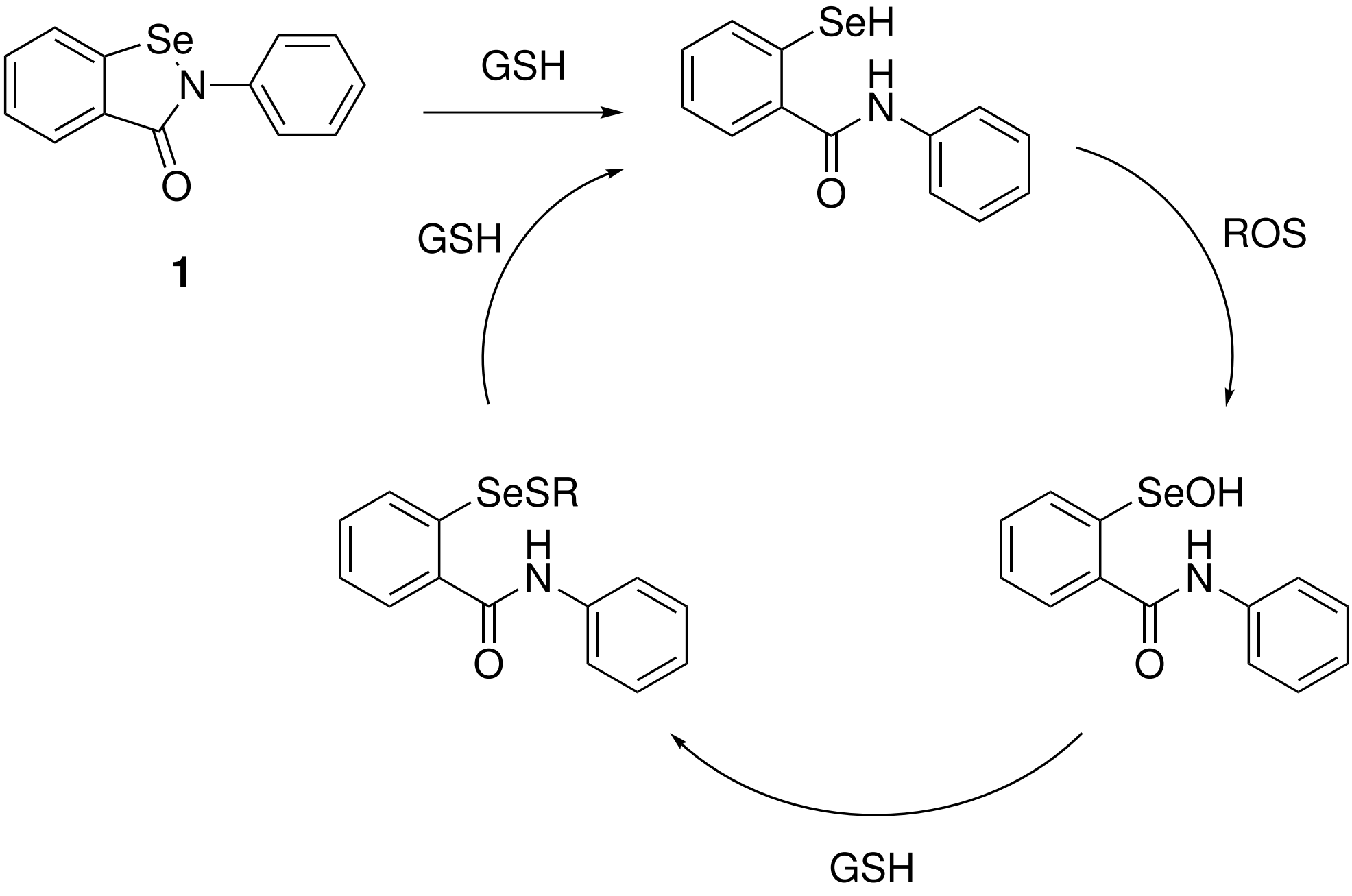


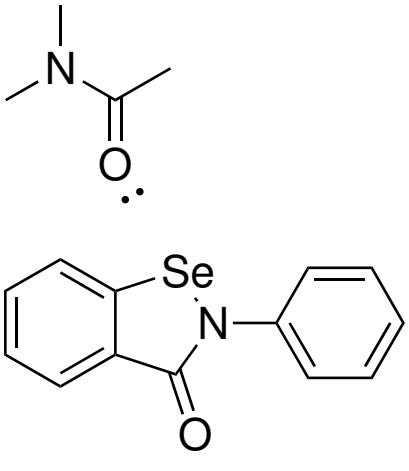
13



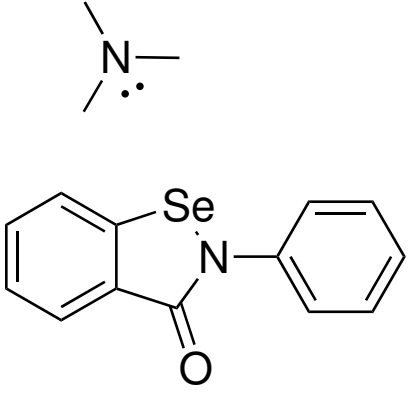
21


O2N
NH2
NH2
a
O
NH
O2N
NH2
22
b
H
N
O2N
N
23
c
H2N
H
N
N
24
d
Se
N
O
H
N
N
20

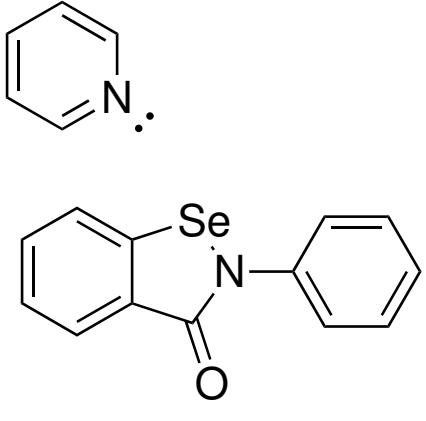

Se
N
O
1
GSH
SeH
H
N
O
ROS
SeOH
H
N
O
GSH
SeSR
H
N
O
GSH



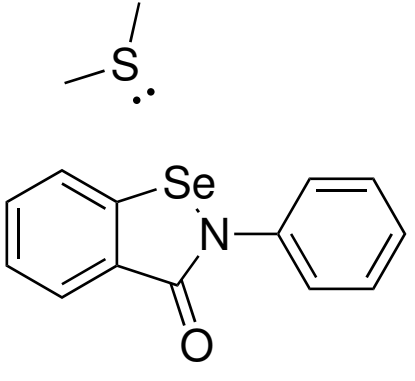
1•DMAc



1•TMA



1•py



1•DMS