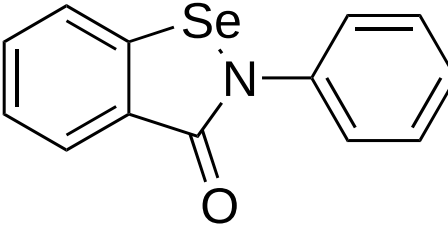
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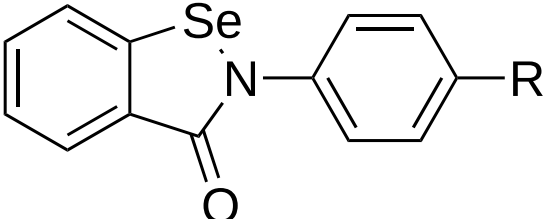
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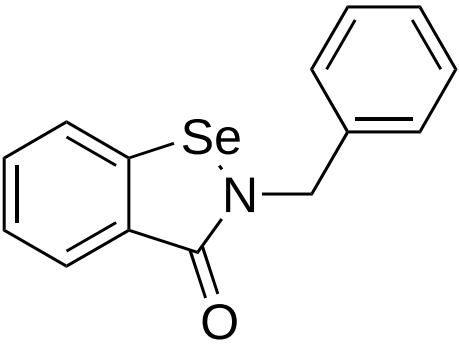
O
R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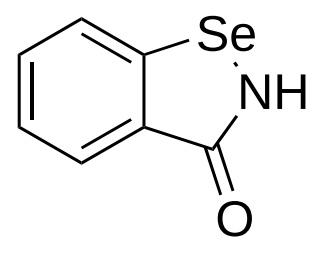
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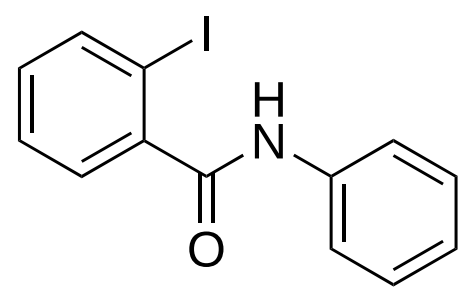
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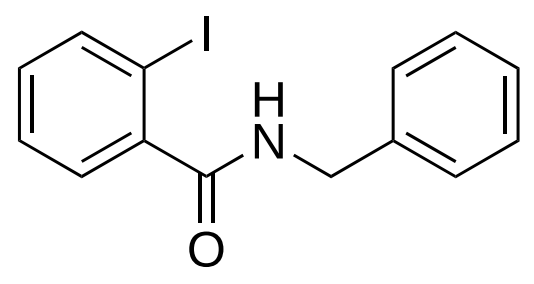
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N
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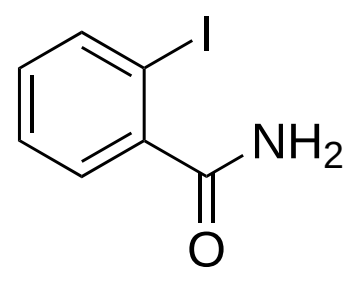
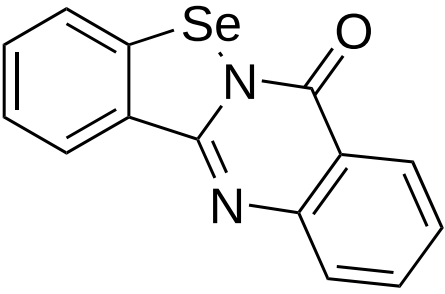

I
NH2
O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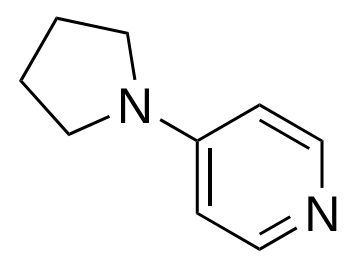
O
N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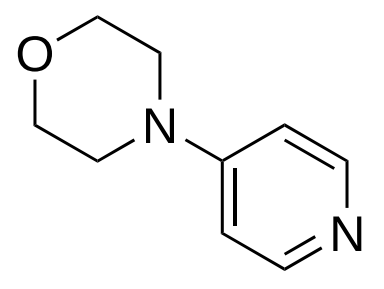
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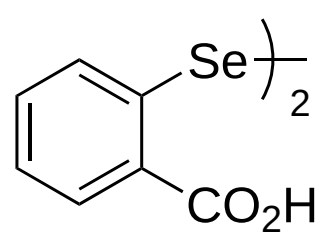
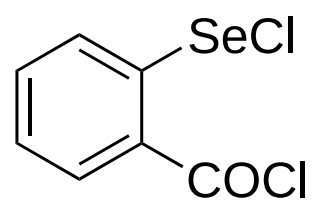
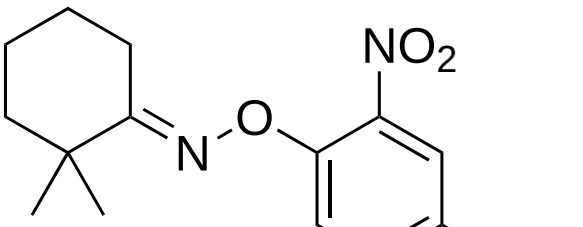
N
N


Se
2
CO2H


SeCl
COCl


NO2
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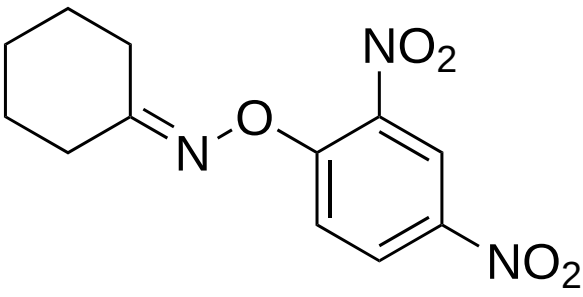
NO2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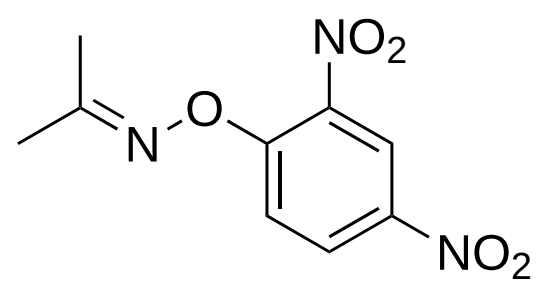
O
NO2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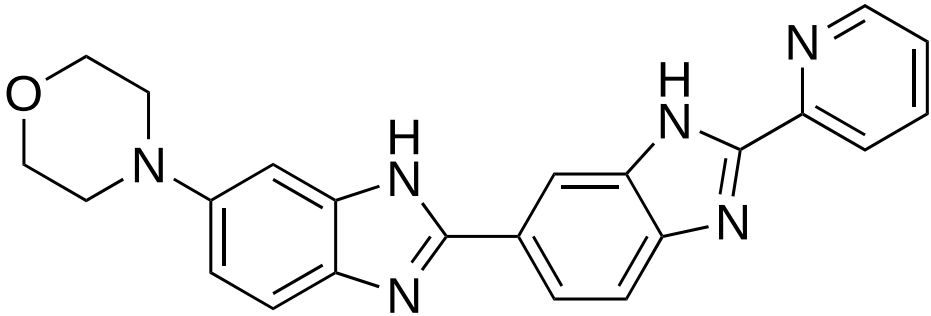
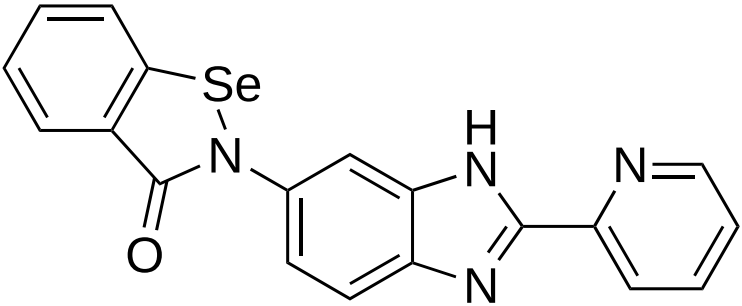
NO2


O
N
H
N
N
H
N
N
N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O
H
N
N
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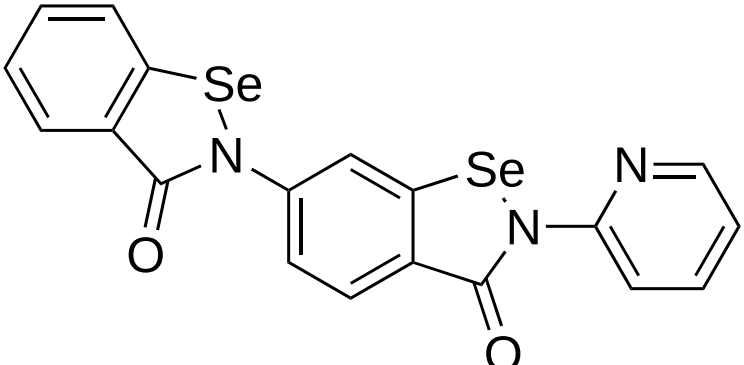
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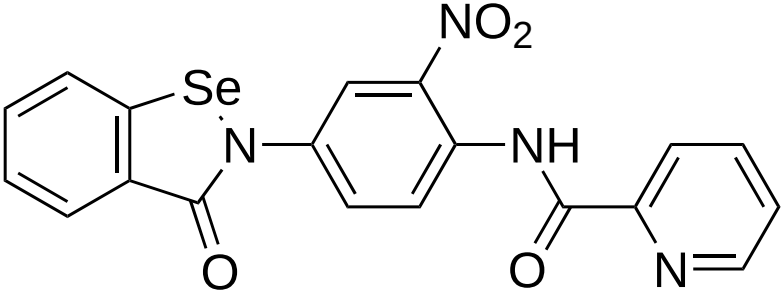
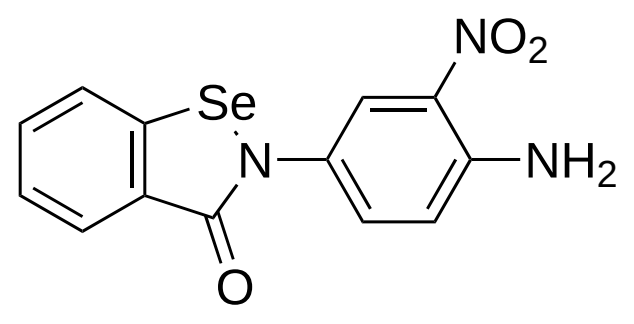
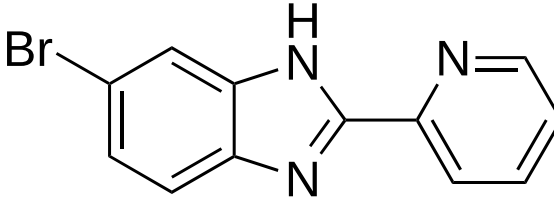
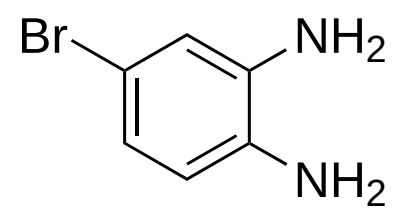
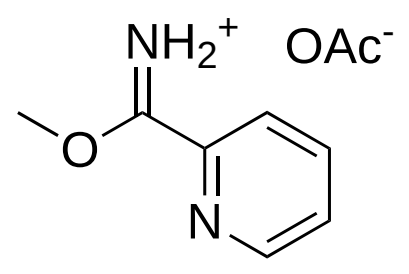
O
Se
N
N
O

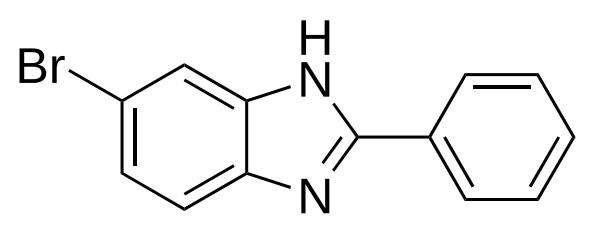

NO2
Se
N
NH
O
O
N

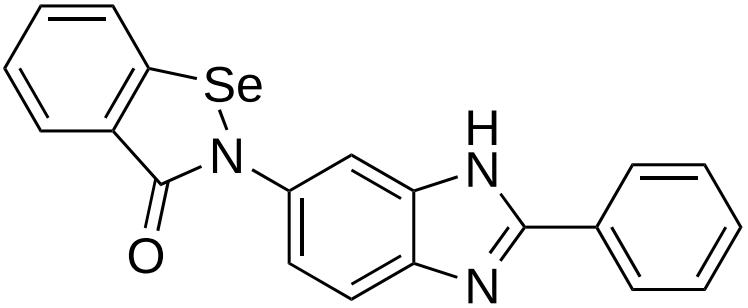

NO2
Se
N
NH2
O

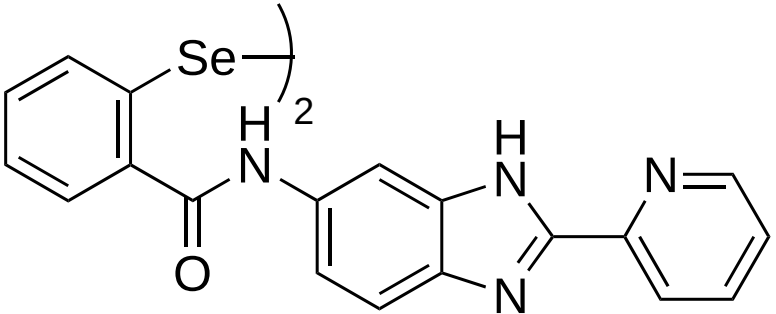

Br
H
N
N
N

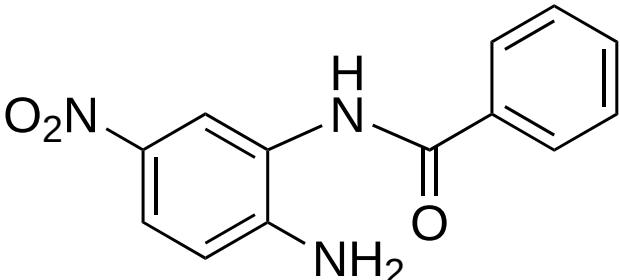

Br
NH2
NH2

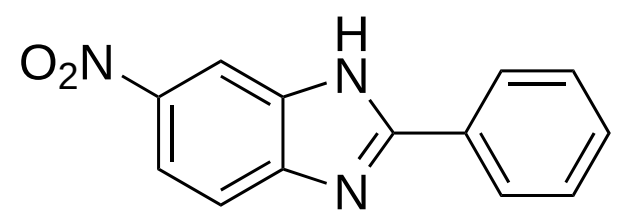

NH2+
OAc-
O
N

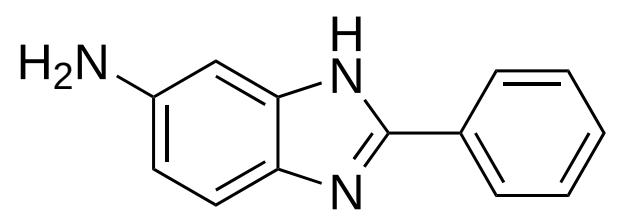

Br
H
N
N

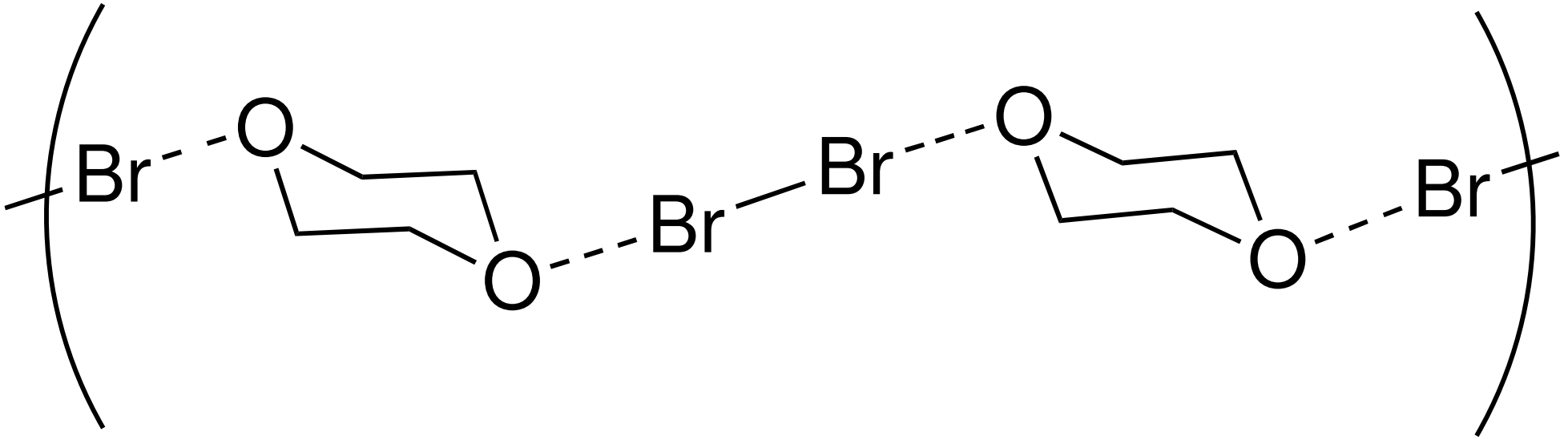

Se
N
O
H
N
N

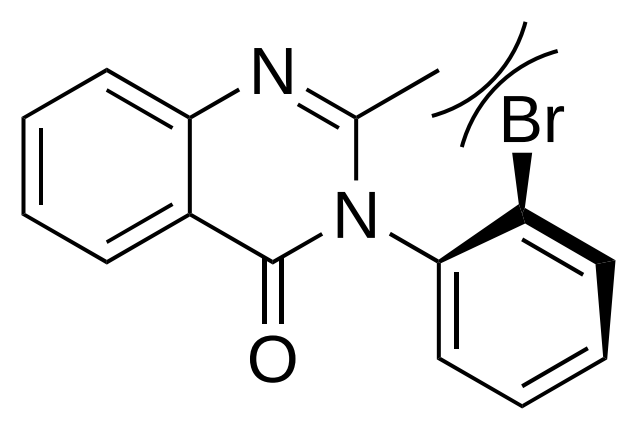

Se
H
2
N
H
N
N
O
N


O2N
H
N
O
NH2


O2N
H
N
N


H2N
H
N
N


Br
O
O
Br
Br
O
O
Br


N
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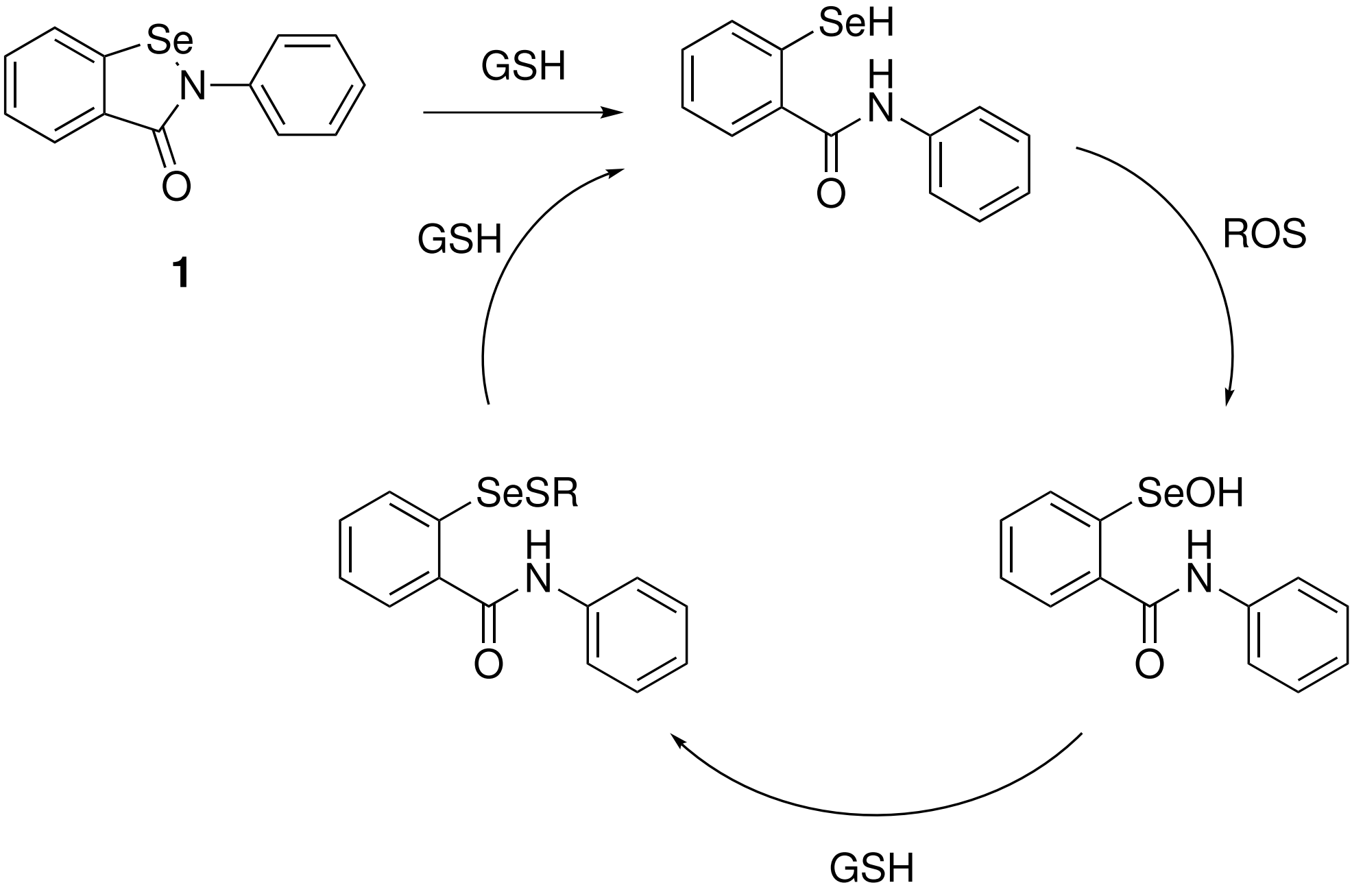
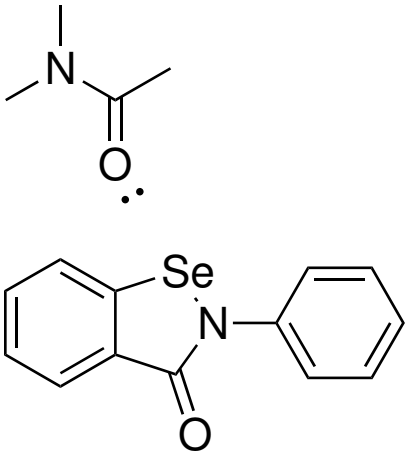
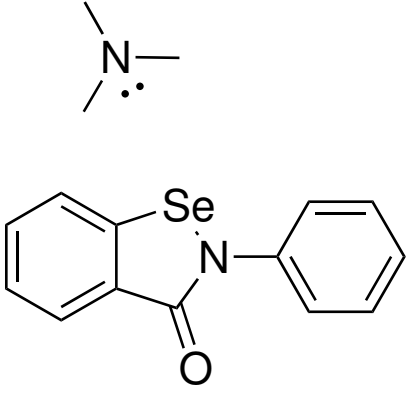
Br
O

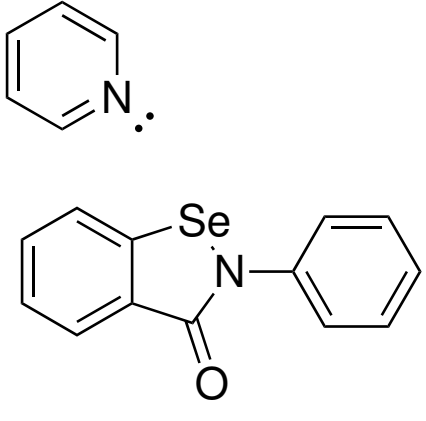

Se
N
O
1
GSH
SeH
H
N
O
ROS
SeOH
H
N
O
GSH
SeSR
H
N
O
GSH



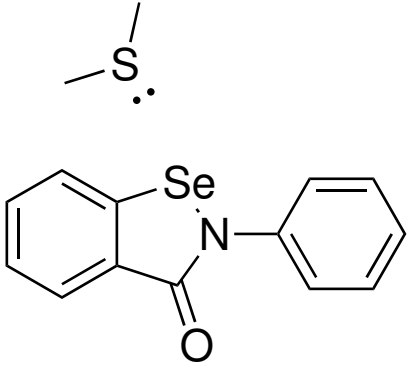
1•DMAc



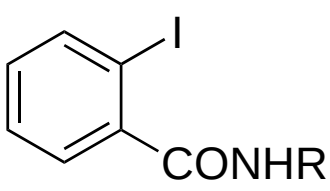
1•TMA



1•py

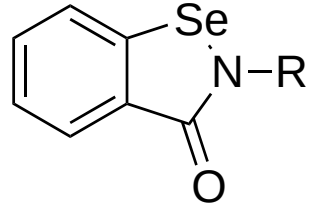


1•DMS



CuI, 1,10-phenanthroline,
Se, K_2CO_3

DMF, 110°C, 5h

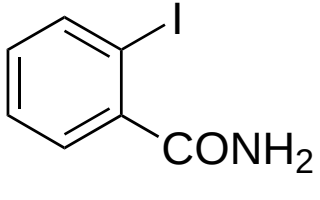


1 R = Ph, 69%

1a R = Bn, 53%

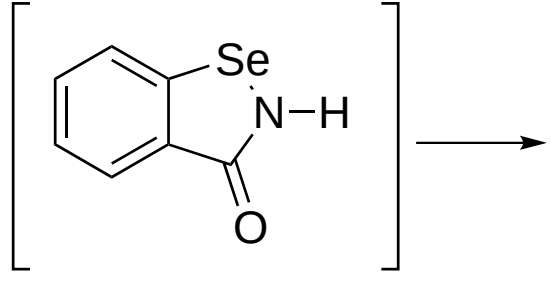
2 and **2a**

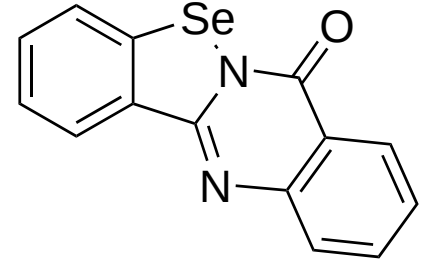
1 and **1a**



CuI, 1,10-phenanthroline,
Se, K_2CO_3

DMF, 110°C, 5h, 15%

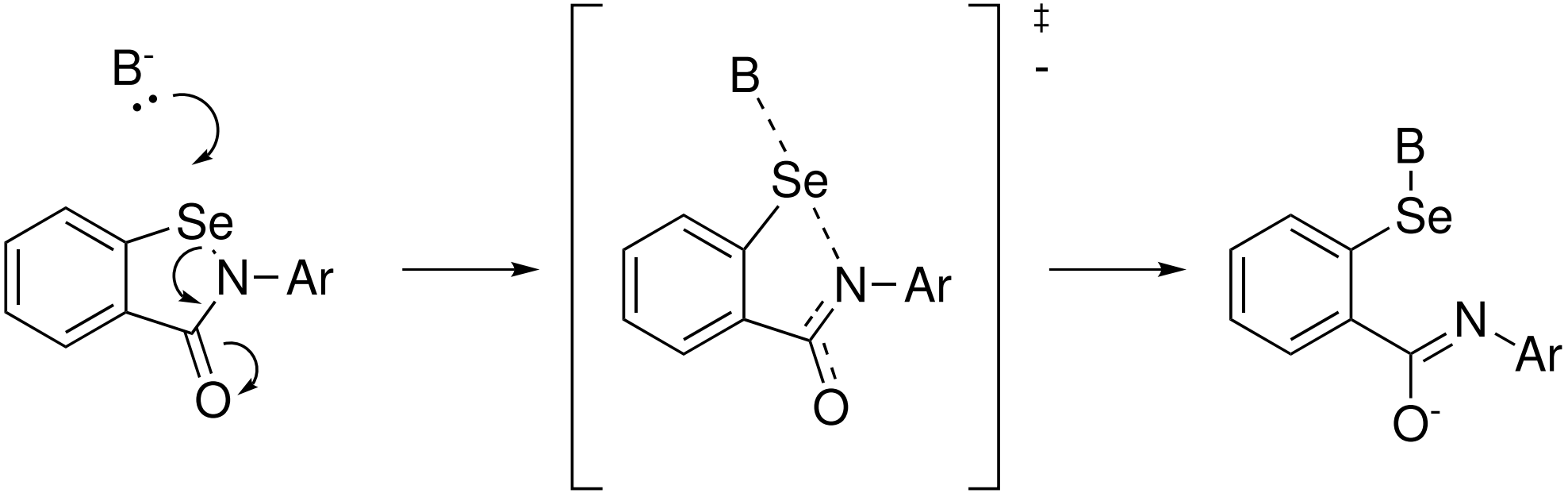


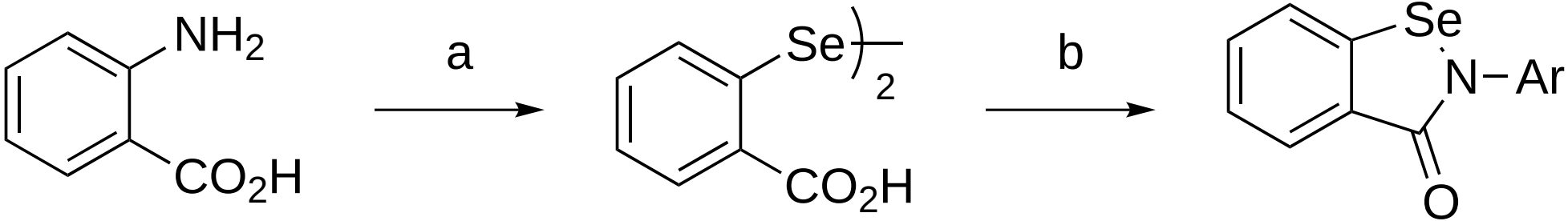


2b

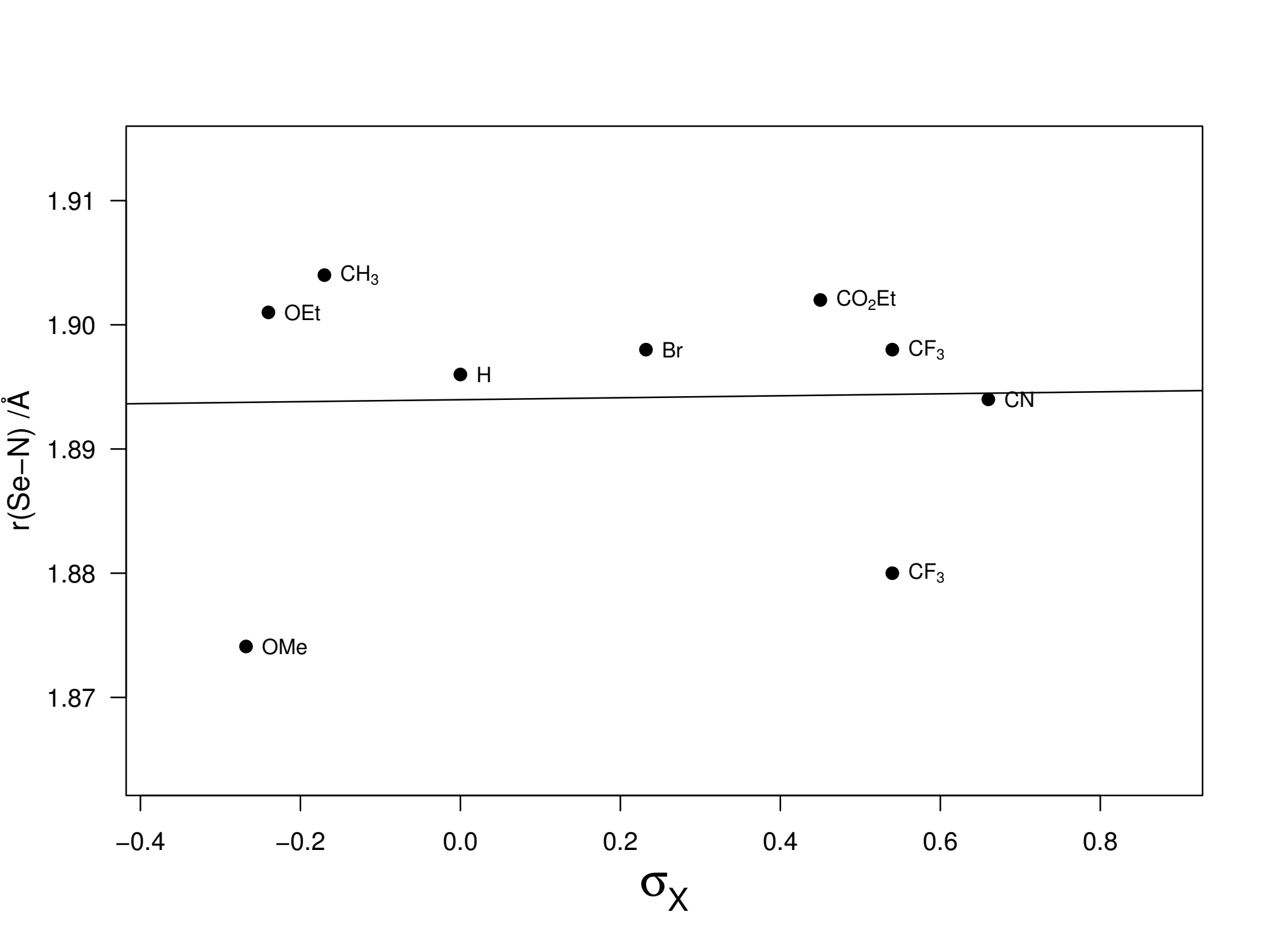
1b

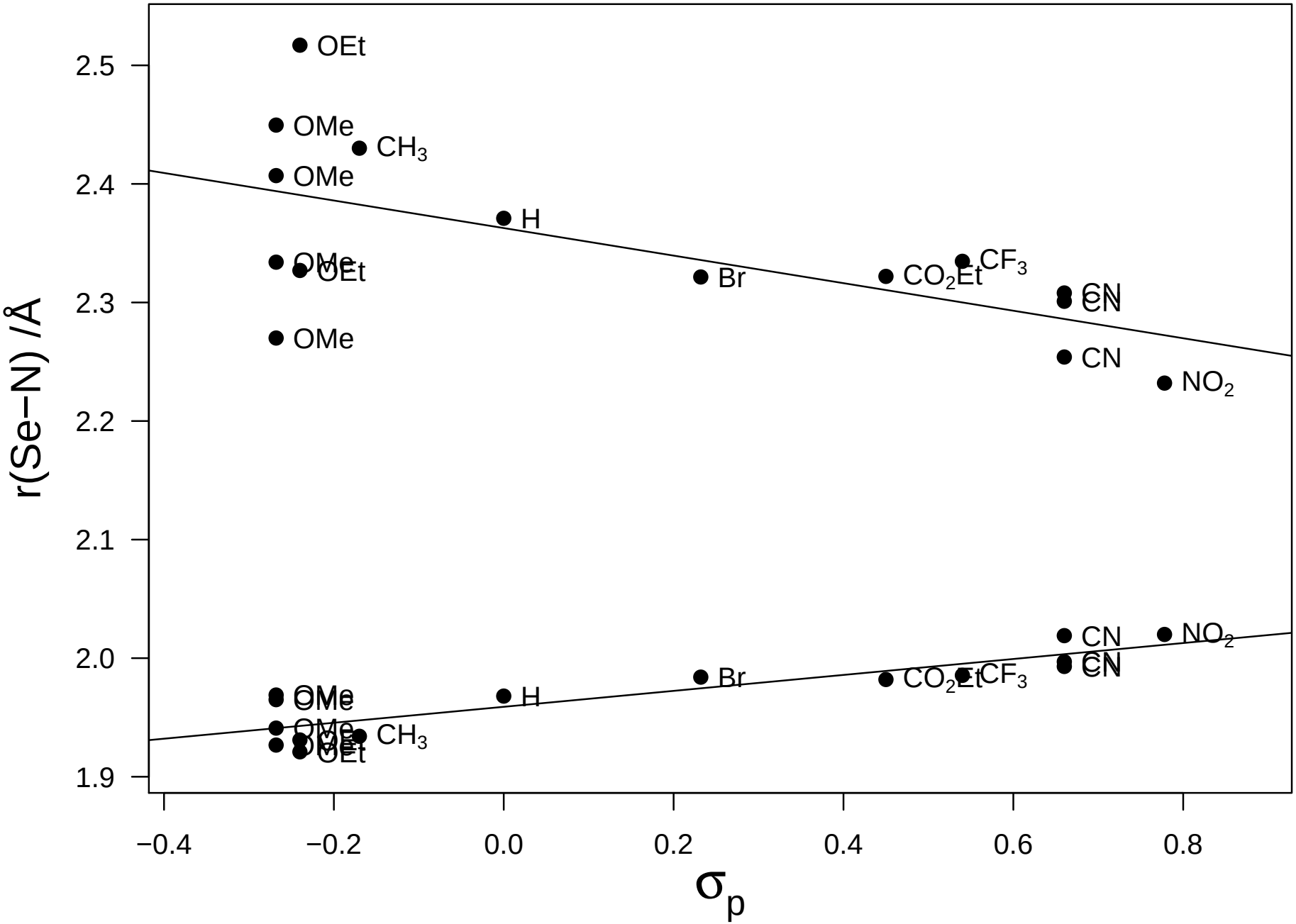
3

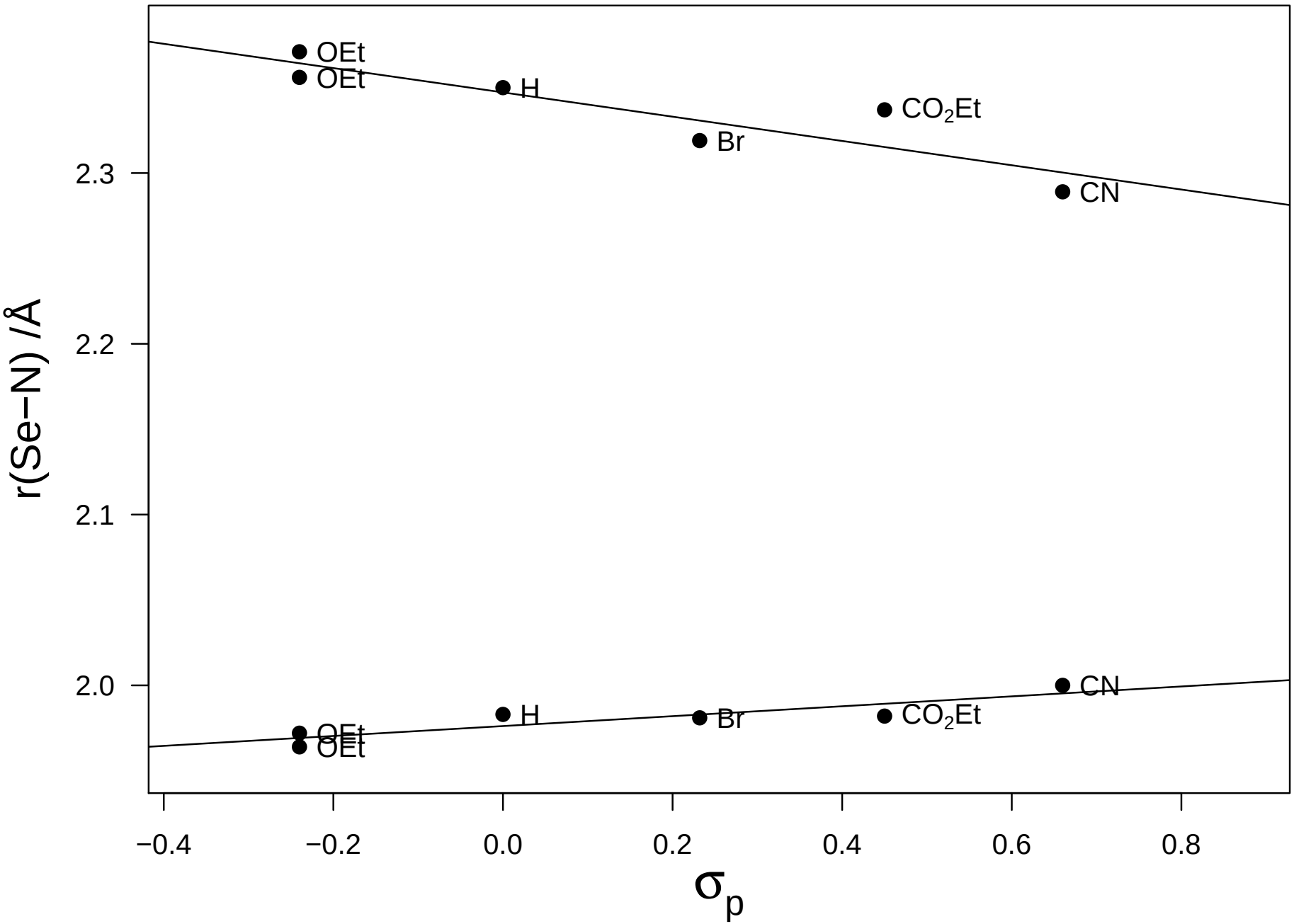

B-
Se
N
Ar
O
B
Se
N
Ar
O
‡
-
B
Se
N
Ar
O-

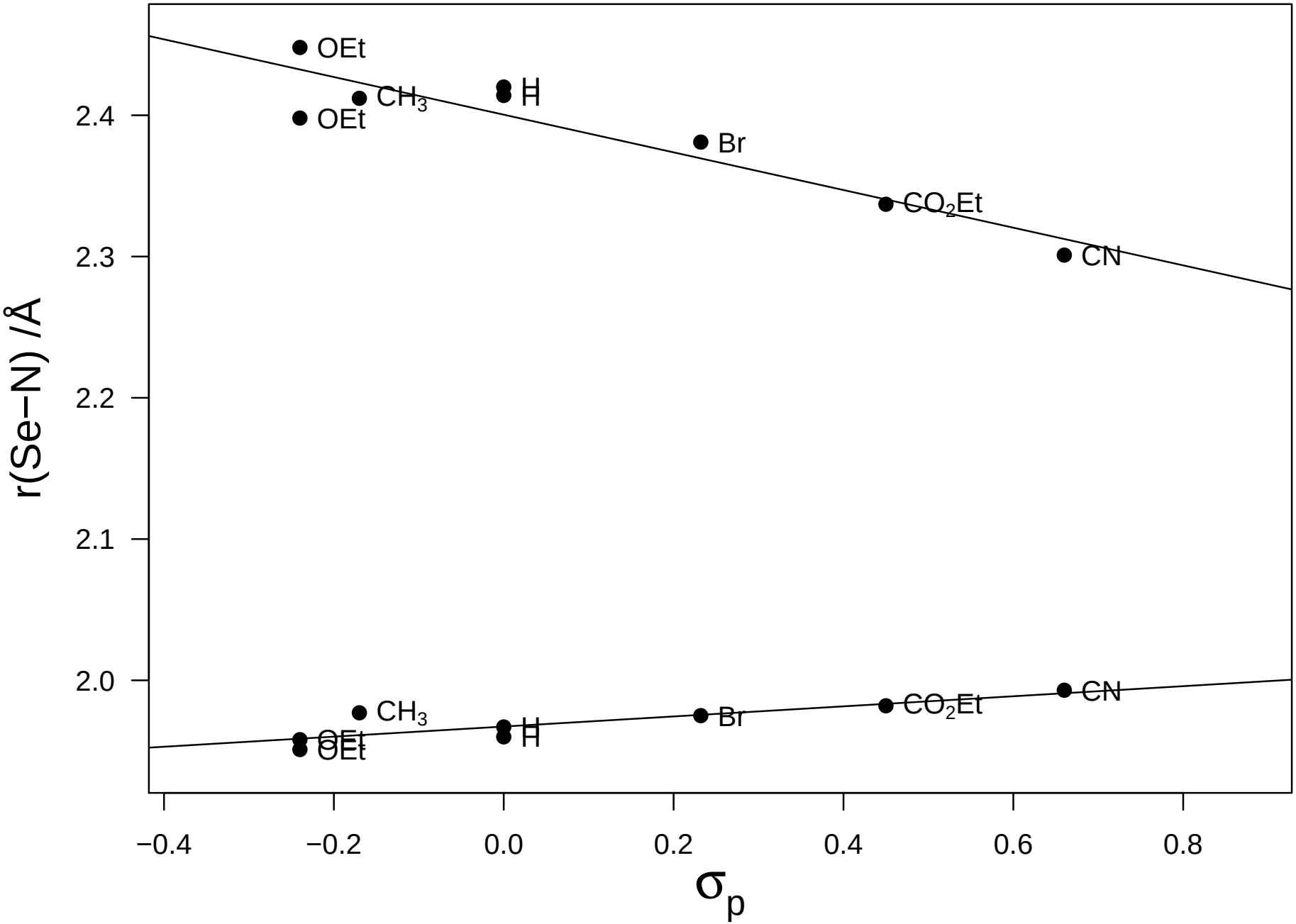


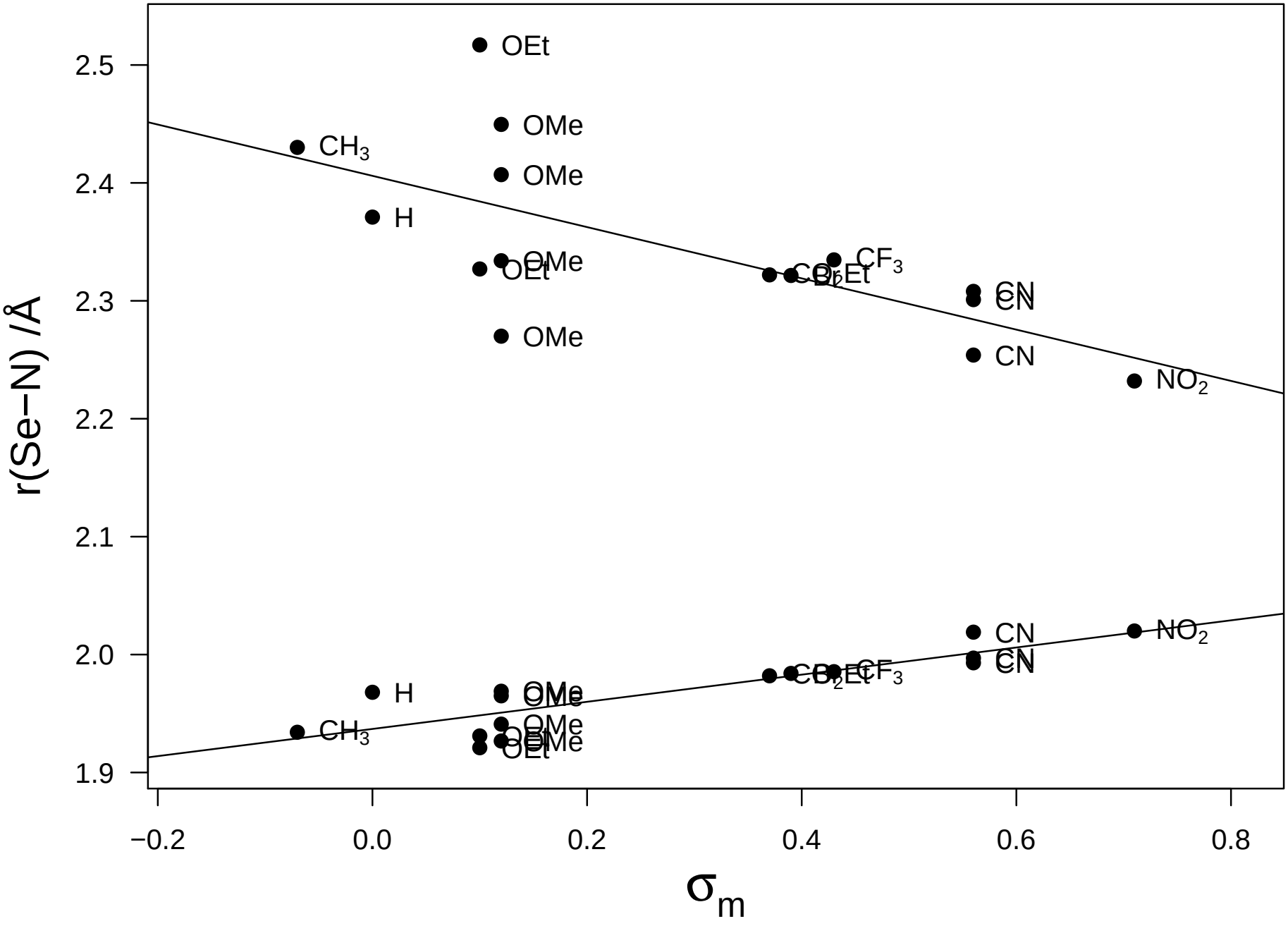
5 **1**

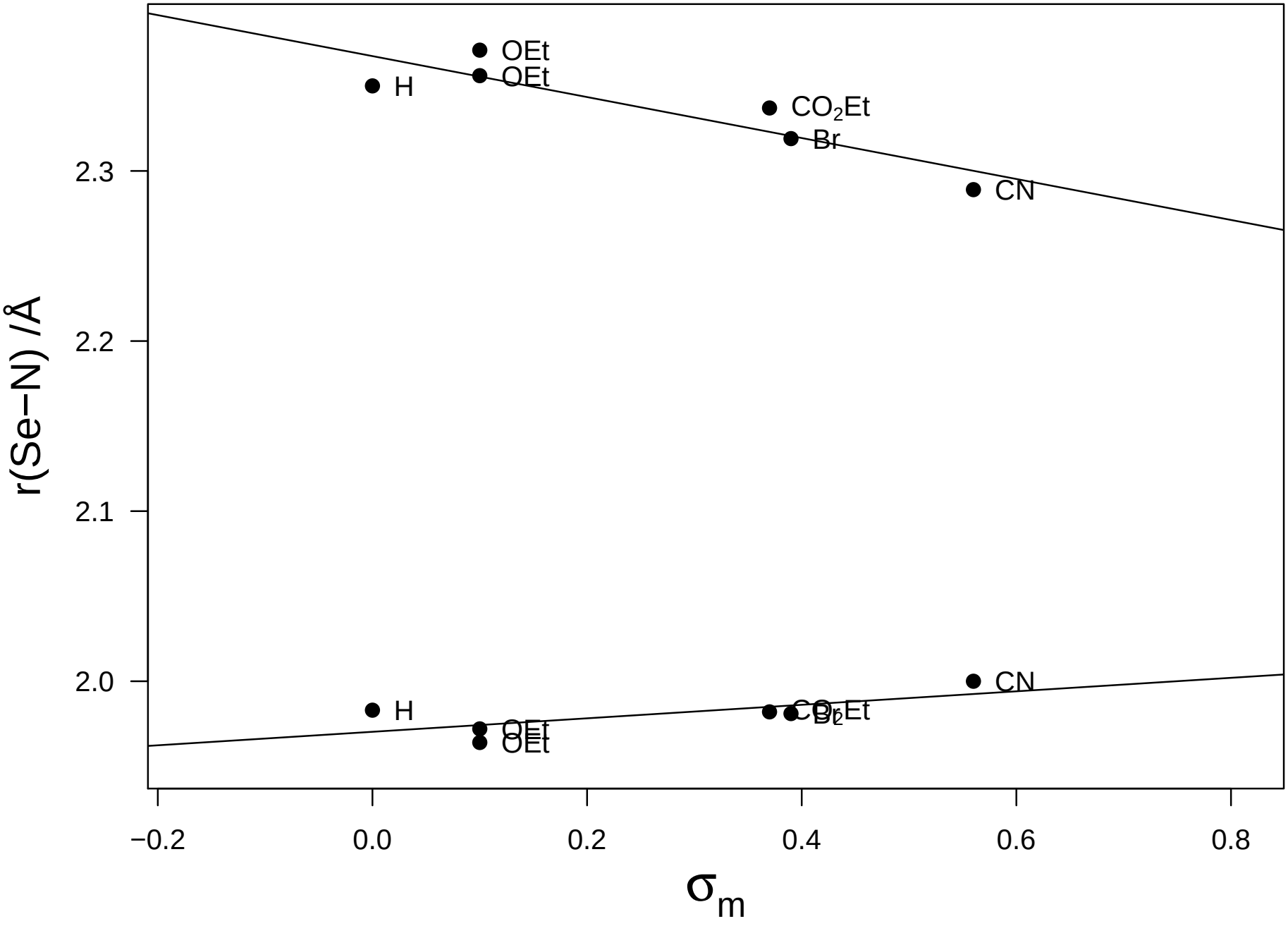

1.91
1.90
1.89
1.88
1.87
r(Se–N) /Å
CH3
OEt
CO2Et
Br
CF3
H
CN
CF3
OMe
–0.4
–0.2
0.0
0.2
0.4
0.6
0.8
σX

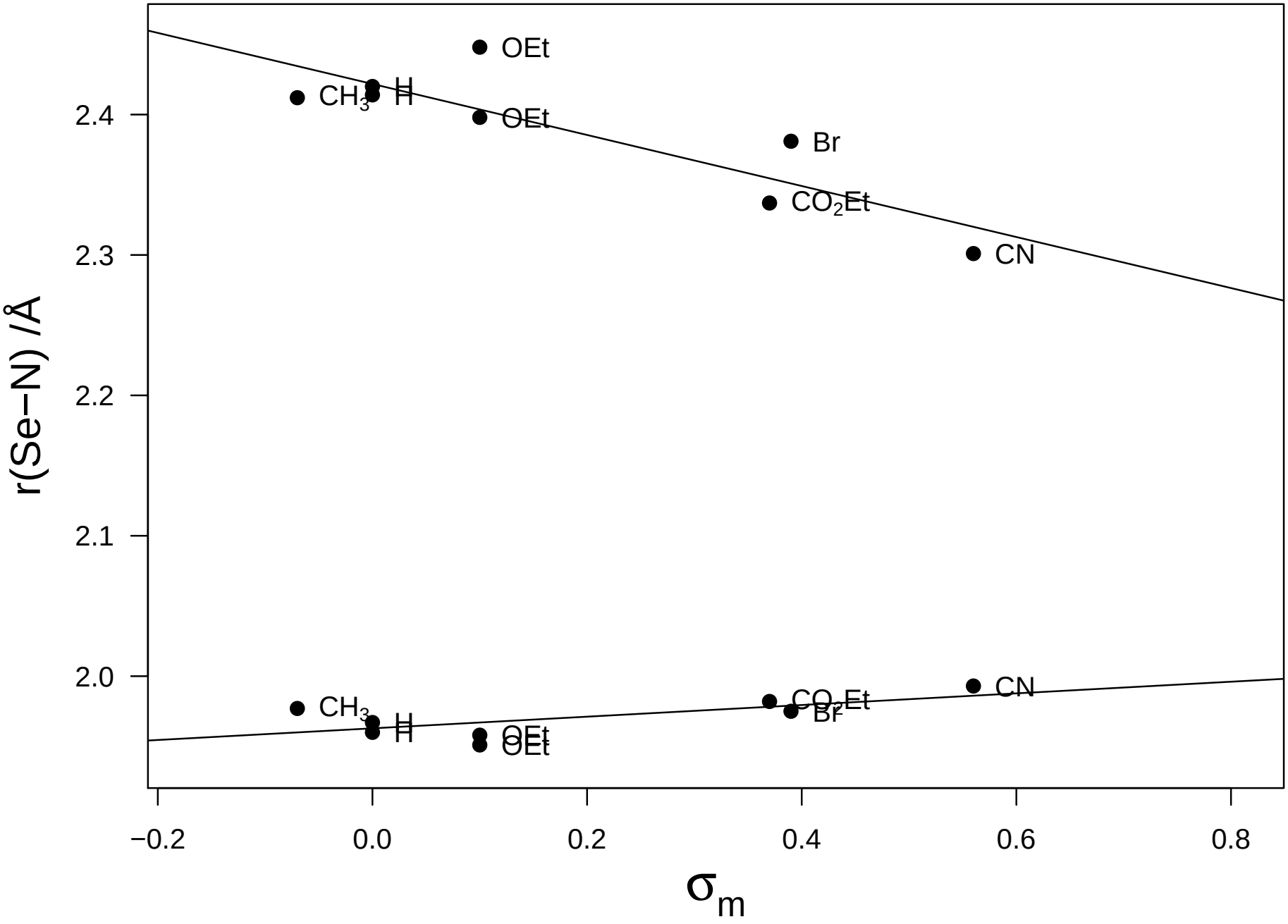

OEt
OMe
CH3
OMe
H
OMe
OEt
Br
CO2Et
CF3
CN
CN
OMe
CN
NO2
CN
NO2
CN
Br
H
CO2Et
CF3
CH3
OEt
2.5
2.4
2.3
2.2
2.1
2.0
1.9
r(Se−N) /Å
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
σp

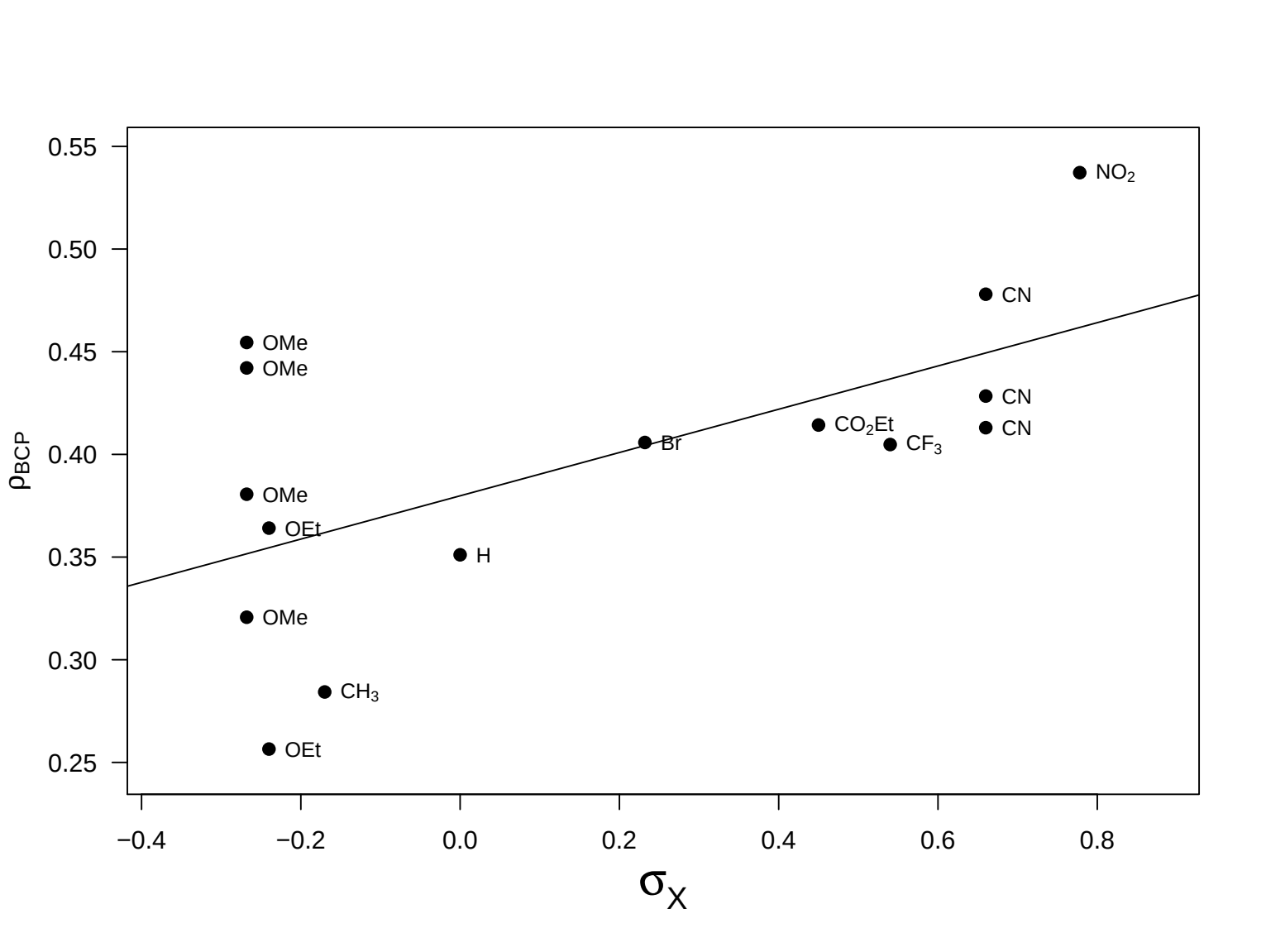

OEt
OEt
H
CO2Et
Br
CN
CN
H
Br
CO2Et
OEt
OEt
2.3
2.2
2.1
2.0
r(Se−N) /Å
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
σp

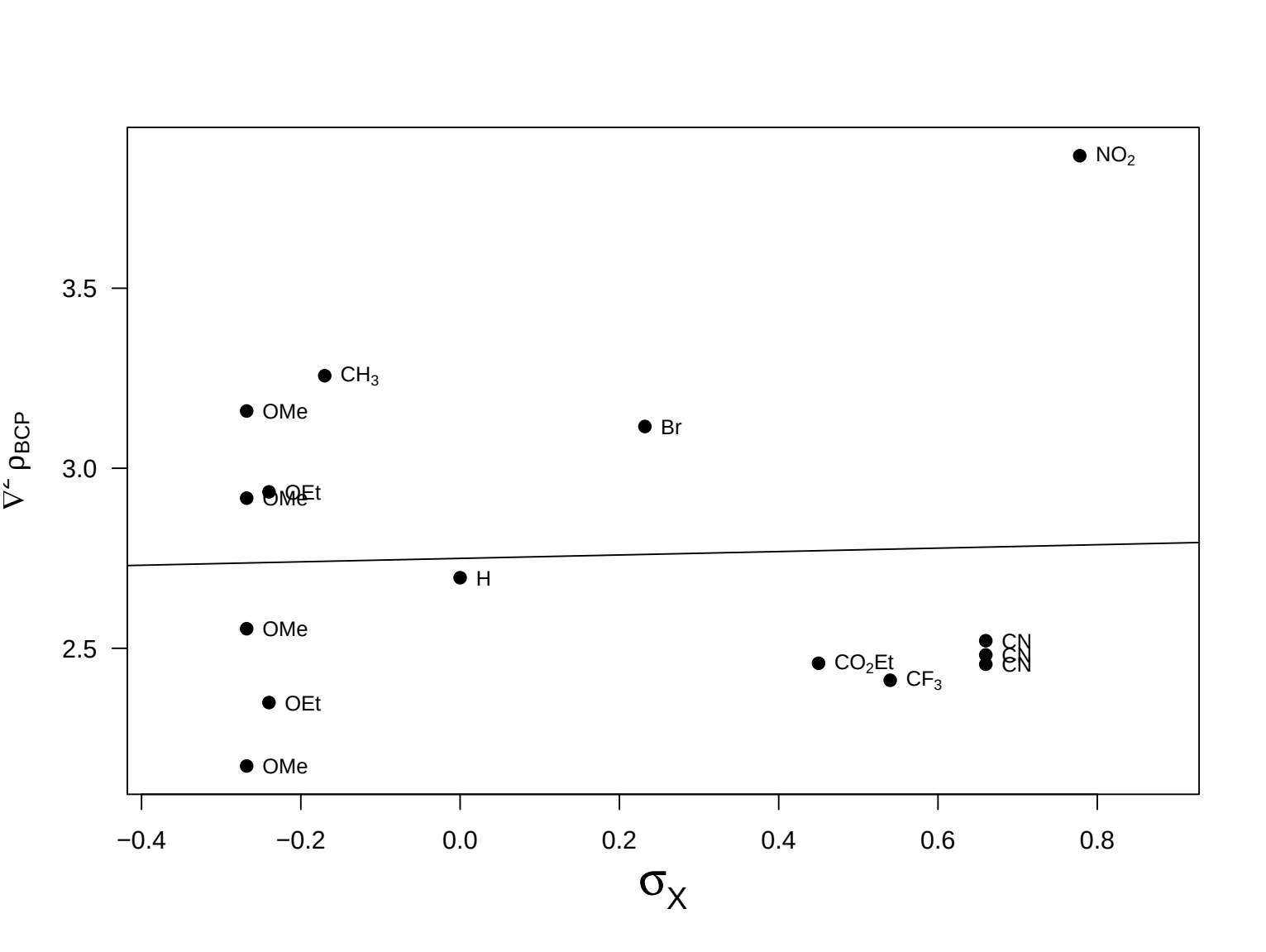

OEt
CH3
OEt
H
H
Br
CO2Et
CN
CH3
OEt
OEt
H
H
Br
CO2Et
CN
2.4
2.3
2.2
2.1
2.0
r(Se−N) /Å
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
σp

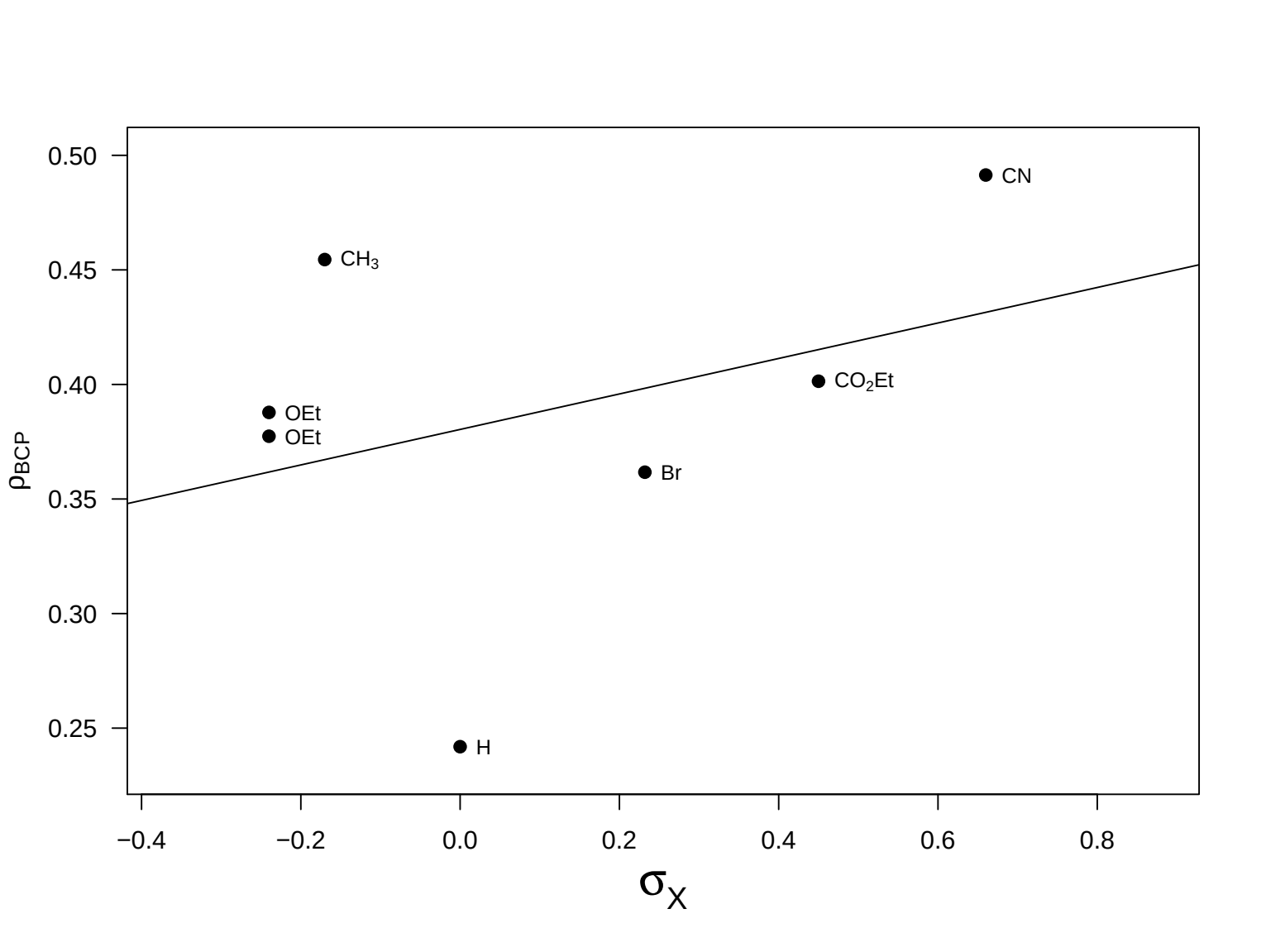

r(Se–N) /Å
2.5
2.4
2.3
2.2
2.1
2.0
1.9
OEt
OMe
OMe
CH3
H
OMe
OEt
OMe
CF3
CO2Et
CN
CN
CN
NO2
CN
NO2
CN
CO2Et
CF3
H
CH3
OMe
OMe
OEt
−0.2
0.0
0.2
0.4
0.6
0.8
σm

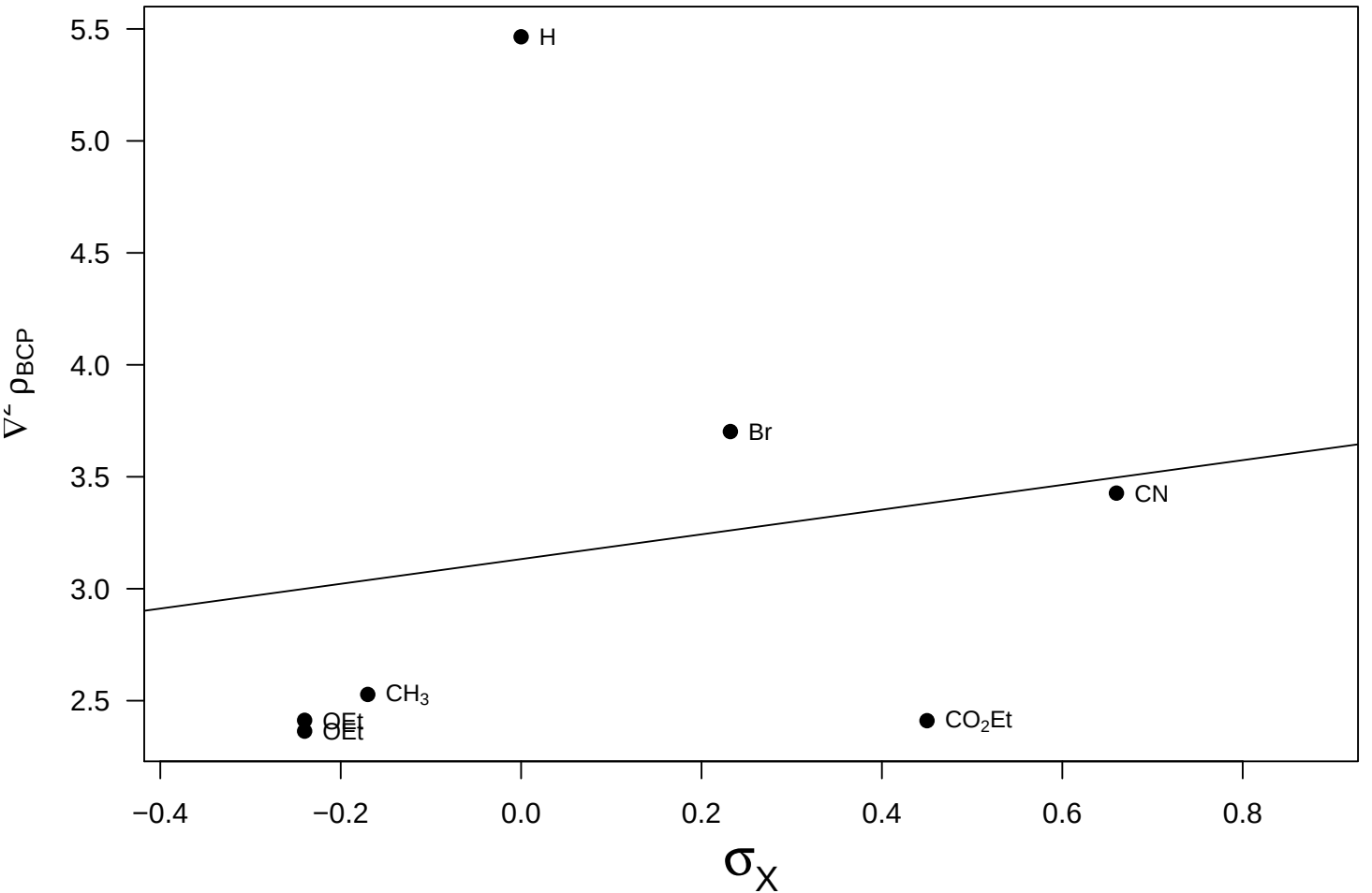

OEt
OEt
H
CO2Et
Br
CN
H
CN
2.3
2.2
2.1
2.0
r(Se–N) /Å
−0.2
0.0
0.2
0.4
0.6
0.8
σm

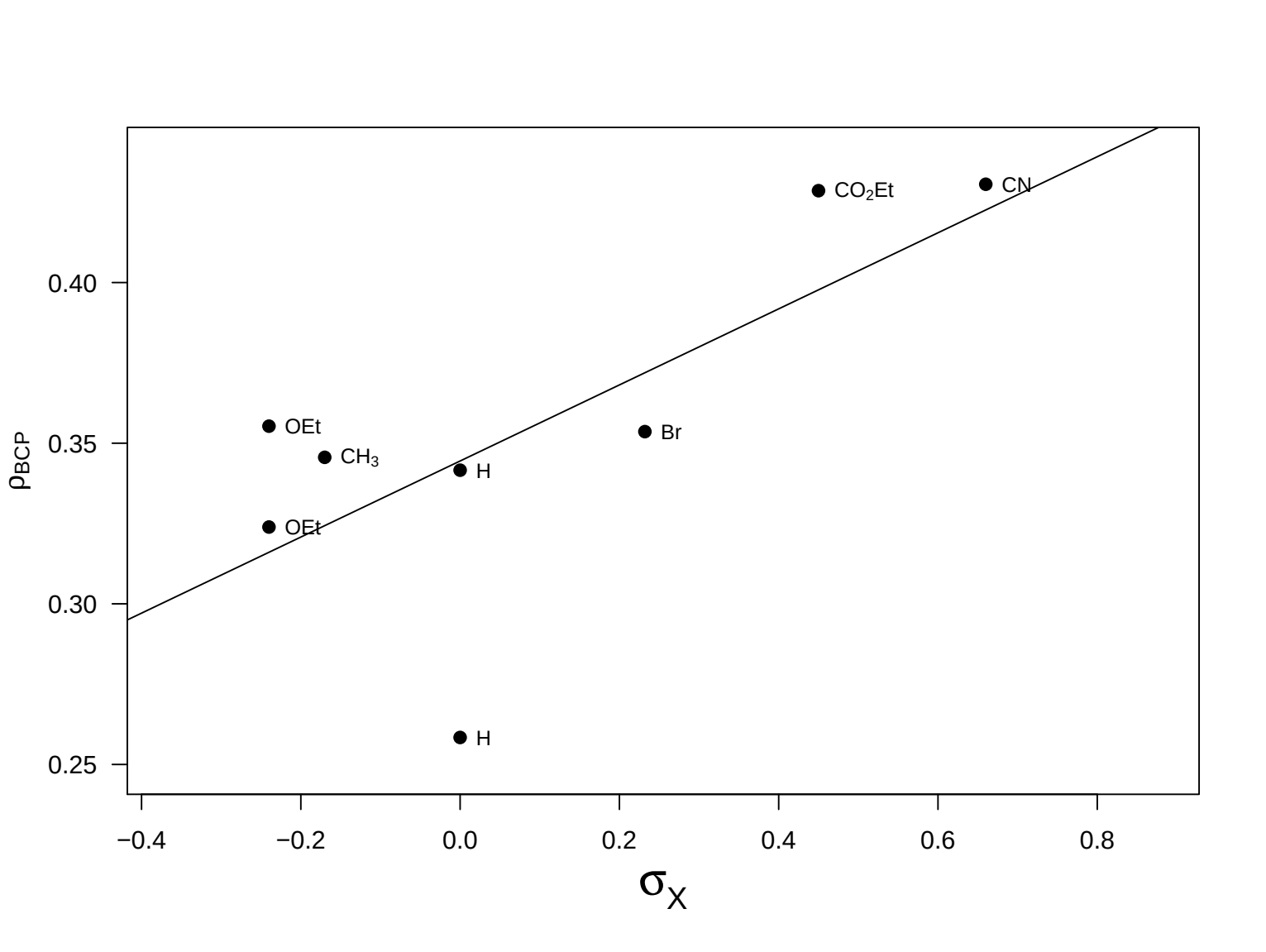

OEt
CH3
H
OEt
Br
CO2Et
CN
CH3
H
OEt
OEt
Br
CO2Et
CN
2.4
2.3
2.2
2.1
2.0
r(Se−N) /Å
−0.2
0.0
0.2
0.4
0.6
0.8
σm

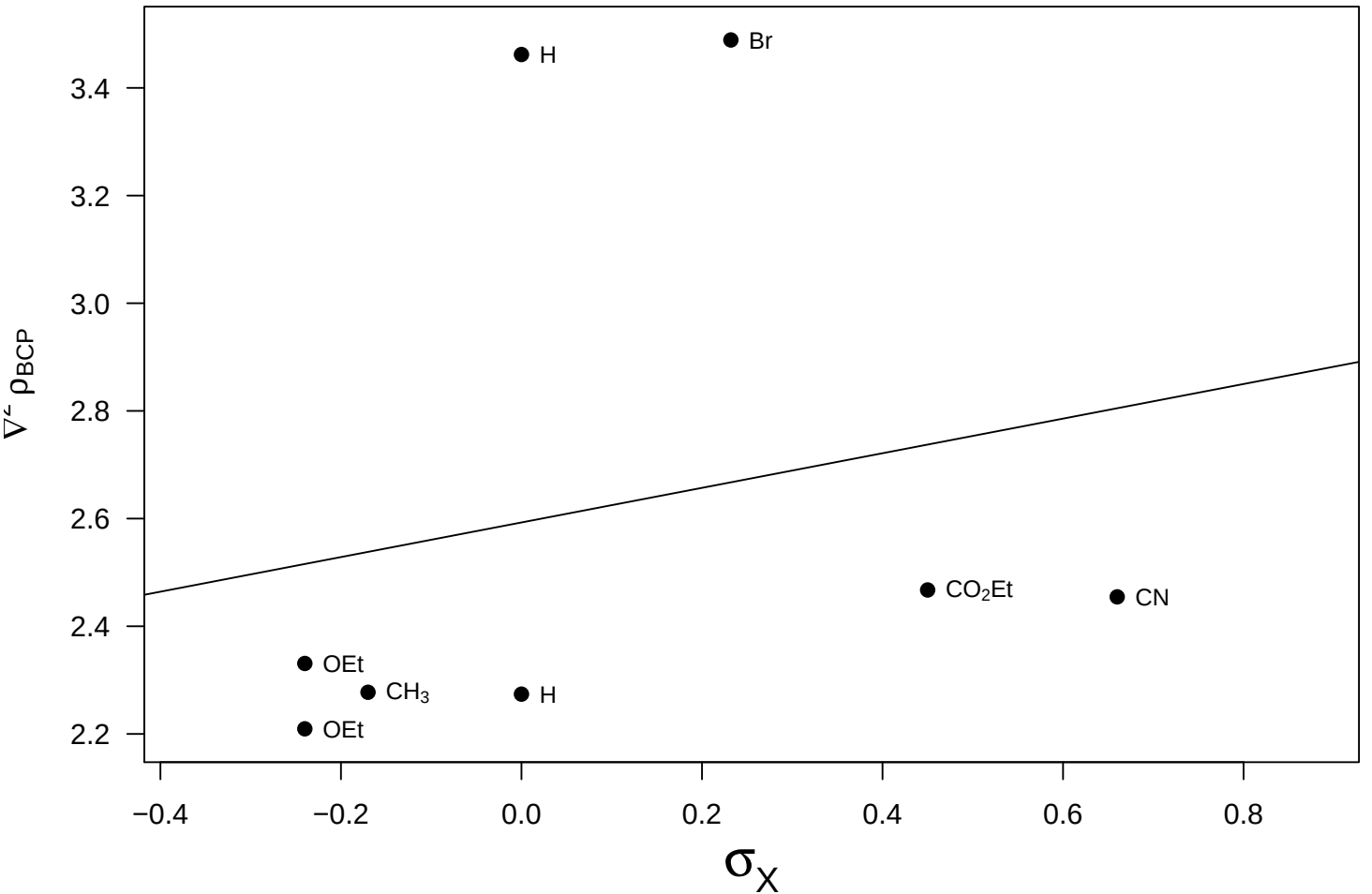

0.55
0.50
0.45
0.40
0.35
0.30
0.25
ρ_{BCP}
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
σ_X
NO_2
CN
OMe
OMe
CN
CO_2Et
CN
Br
CF_3
OMe
OEt
H
OMe
CH_3
OEt

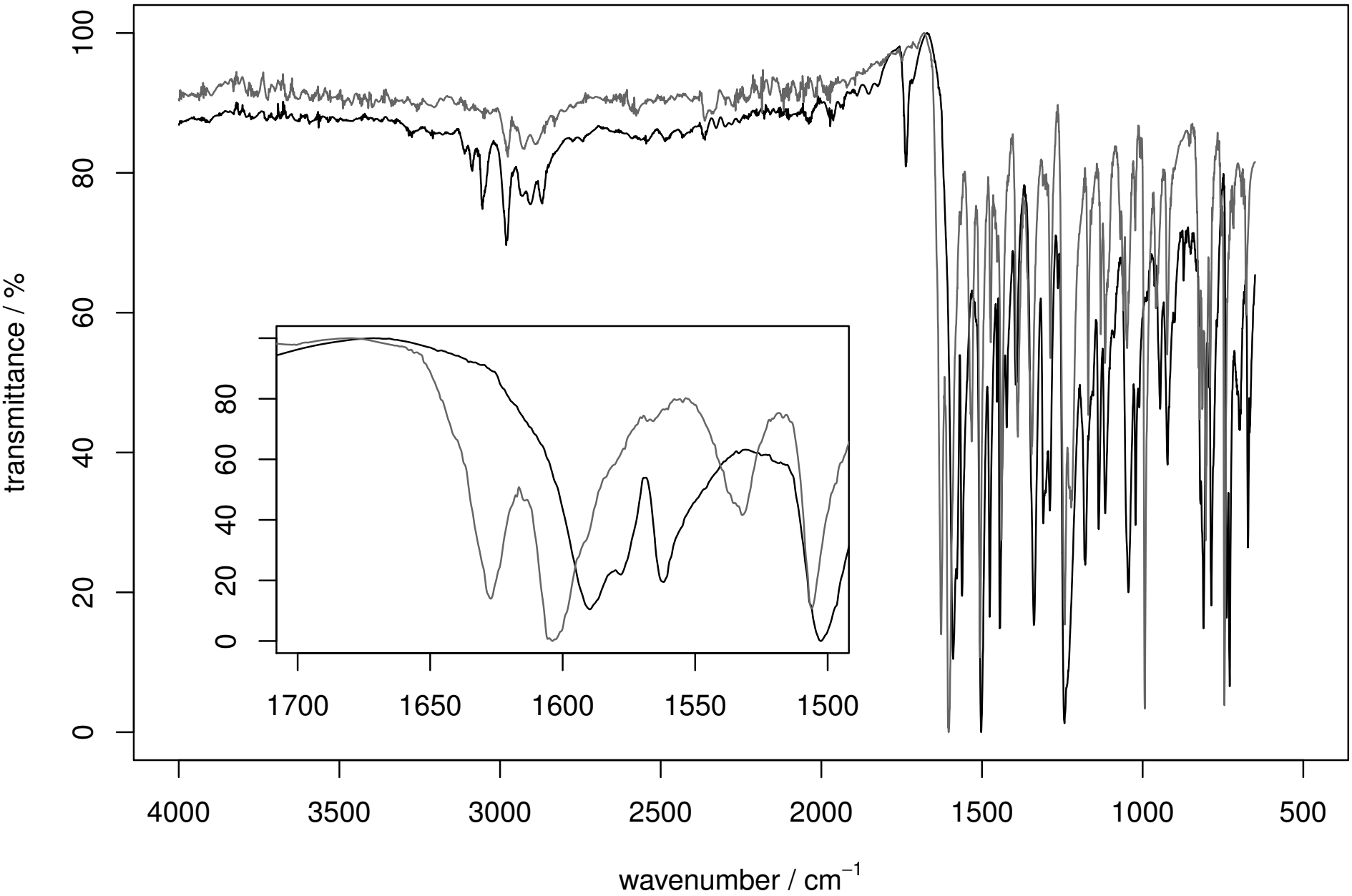

NO2
CH3
OMe
Br
OEt
OMe
H
OMe
CO2Et
CF3
CN
CN
CN
OEt
OMe
3.5
3.0
2.5
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
∇² ρBCP
σX

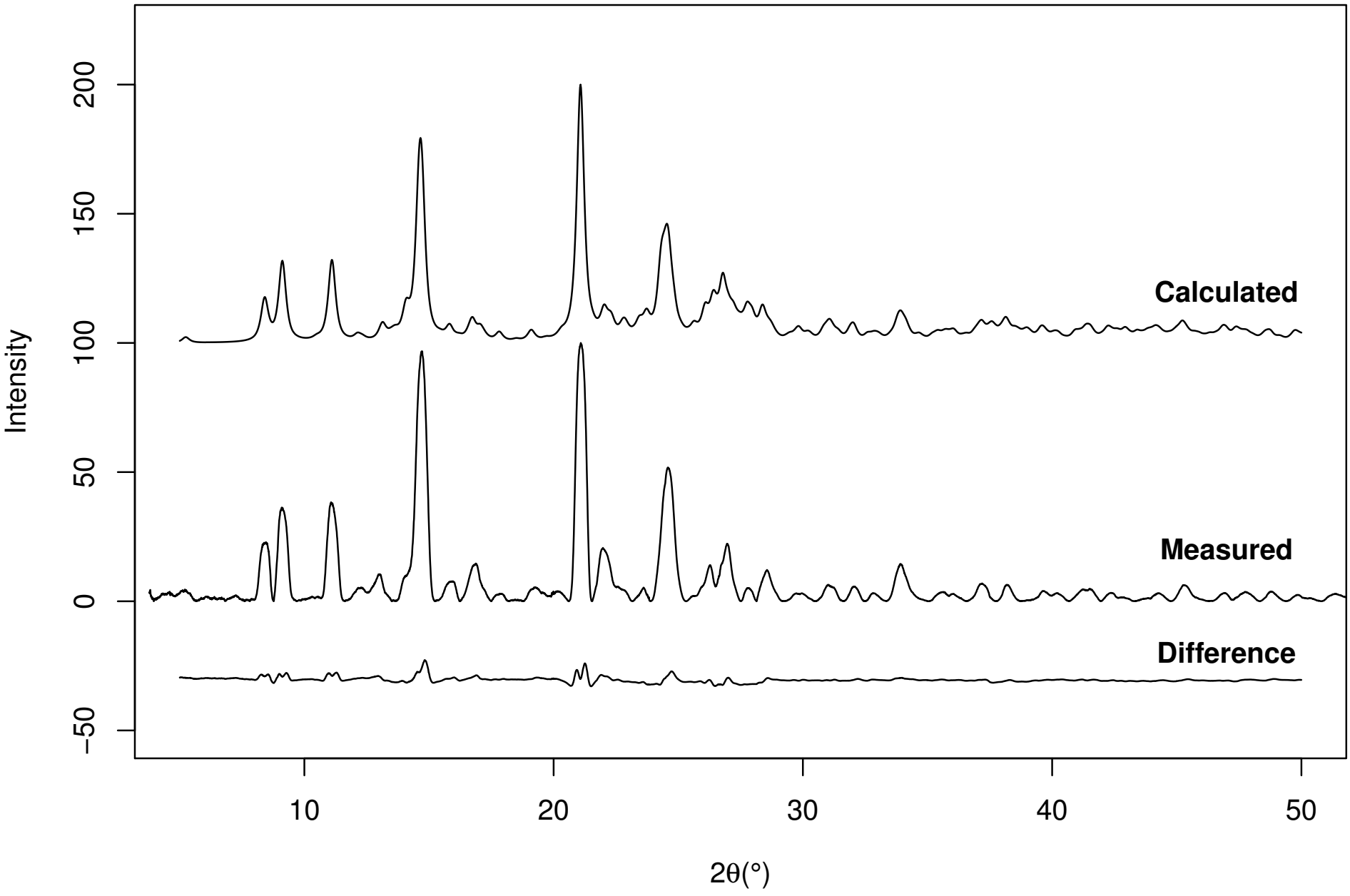

0.50
0.45
0.40
0.35
0.30
0.25
ρ_{BCP}
CN
CH_3
CO_2Et
OEt
OEt
Br
H
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
σ_X

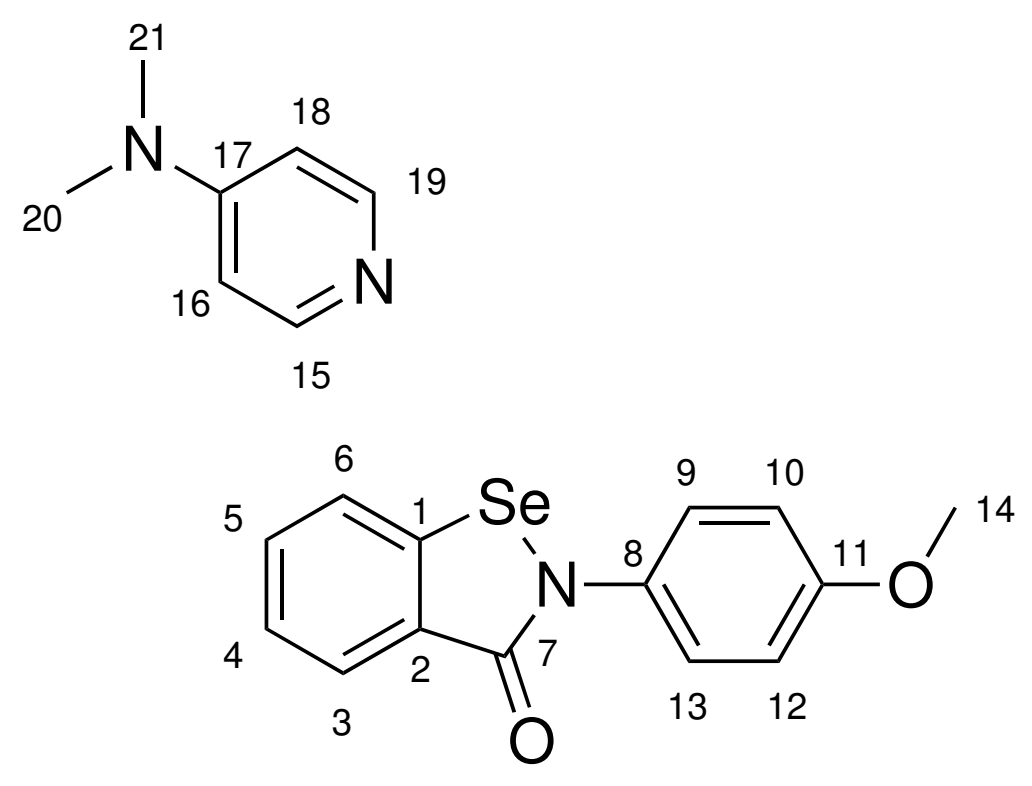

5.5
5.0
4.5
4.0
3.5
3.0
2.5
$\nabla^2 \rho_{BCP}$
H
Br
CN
CH_3
OEt
OEt
CO_2Et
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
σ_X

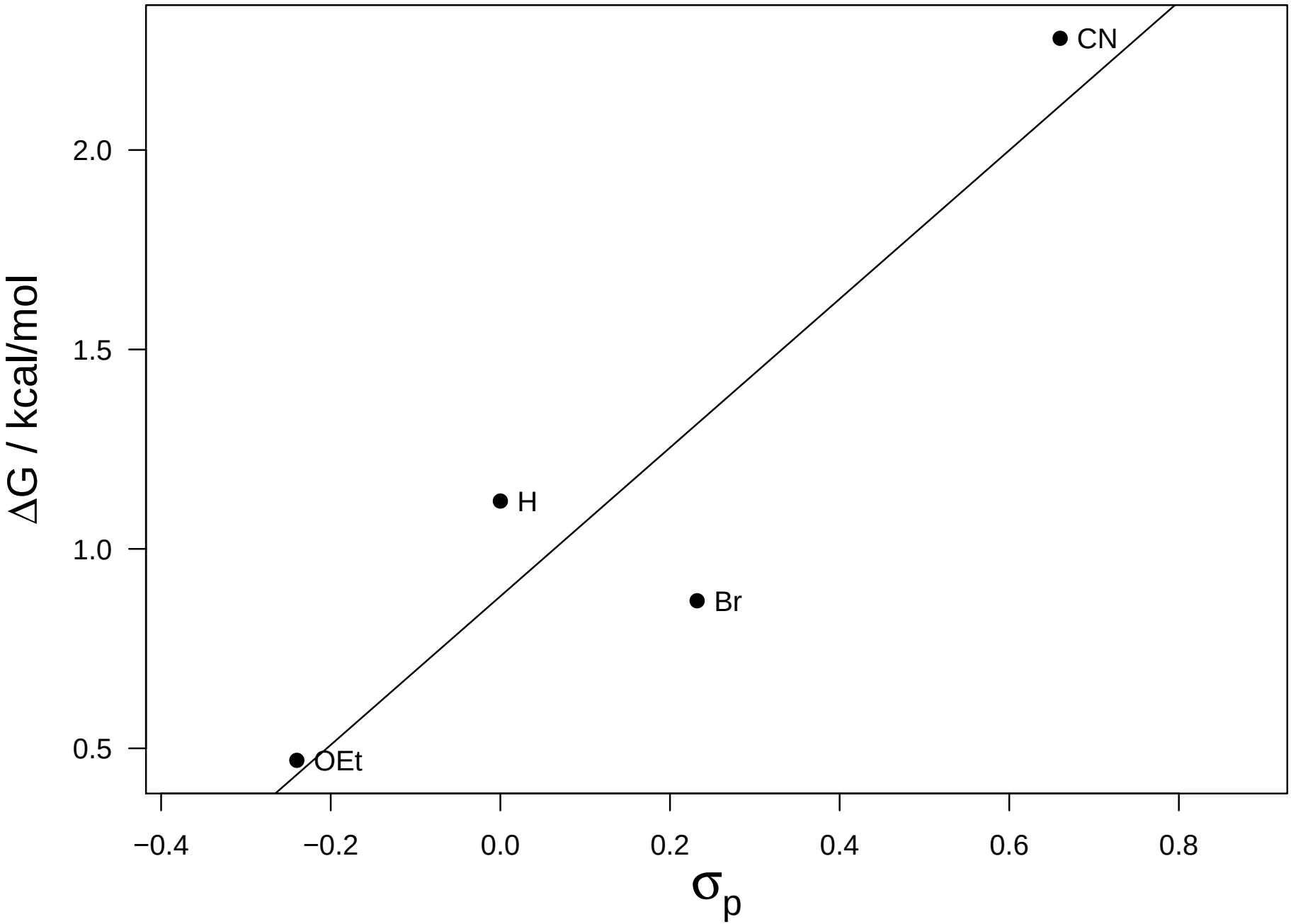

CO_2Et
CN
OEt
CH_3
H
Br
OEt
H
0.40
0.35
0.30
0.25
ρ_{BCP}
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
σ_X

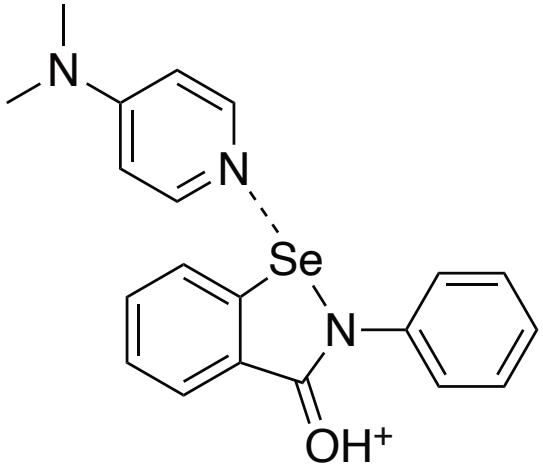

H
Br
CO2Et
CN
OEt
CH3
H
OEt
3.4
3.2
3.0
2.8
2.6
2.4
2.2
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
∇² ρBCP
σX


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(°)

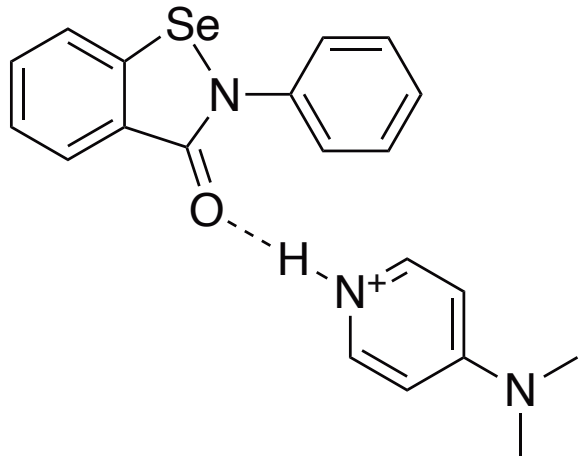

21
18
N
17
19
20
N
16
15
6
9
10
5
1
Se
8
11
14
N
O
4
2
7
3
13
12
O


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



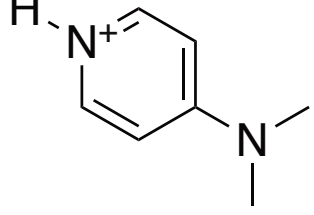
m/z: 398.08

or

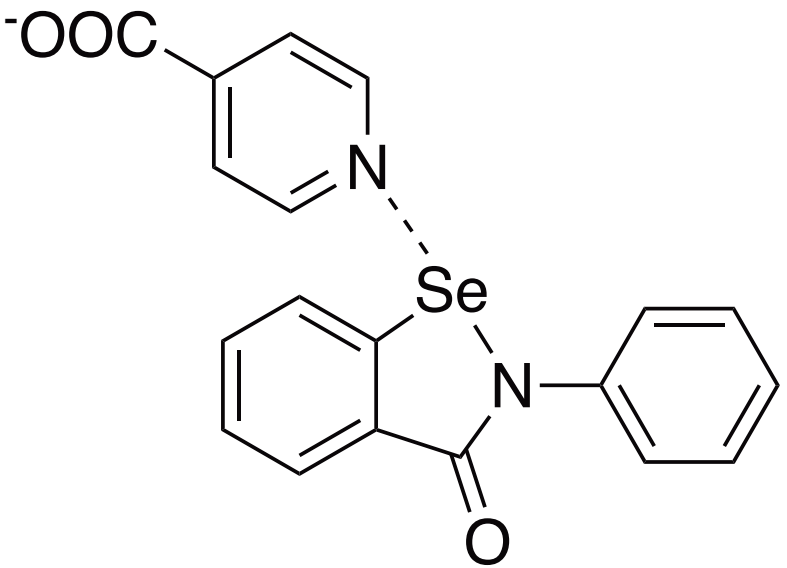


m/z: 398.08

CID

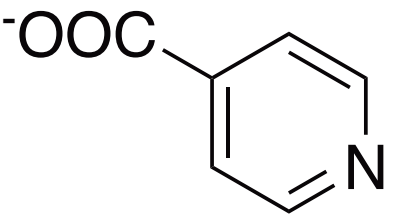


m/z: 123.09

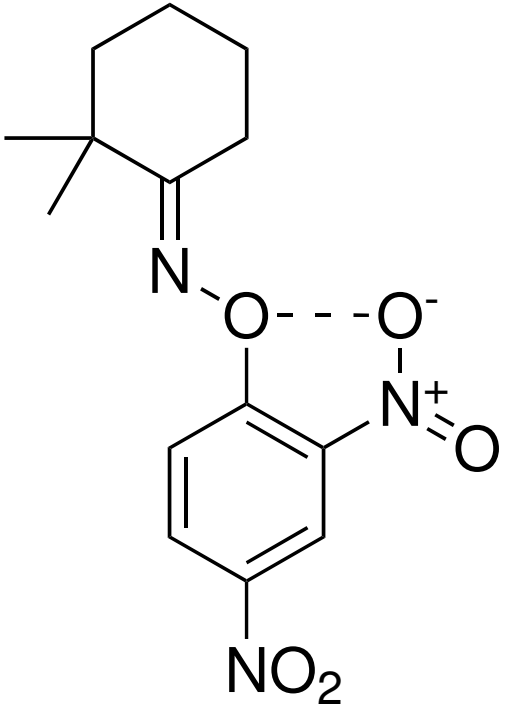


m/z: 397.01

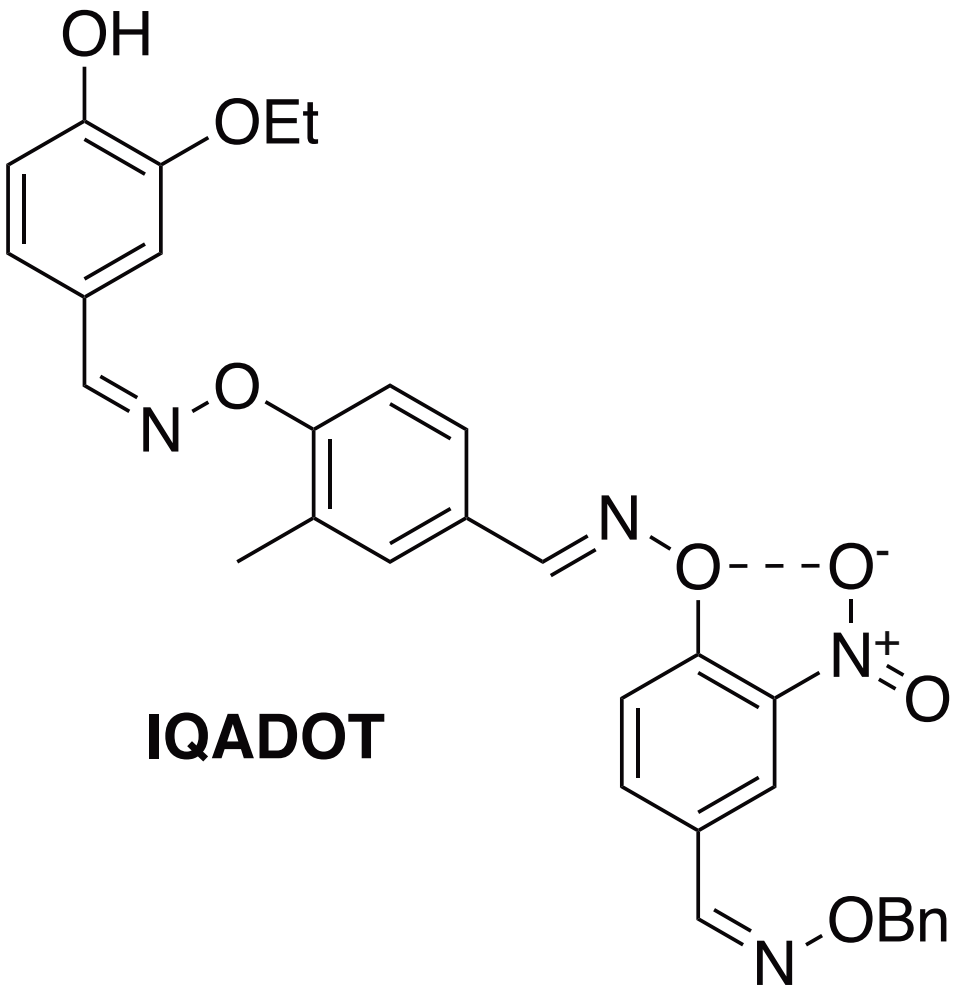
CID



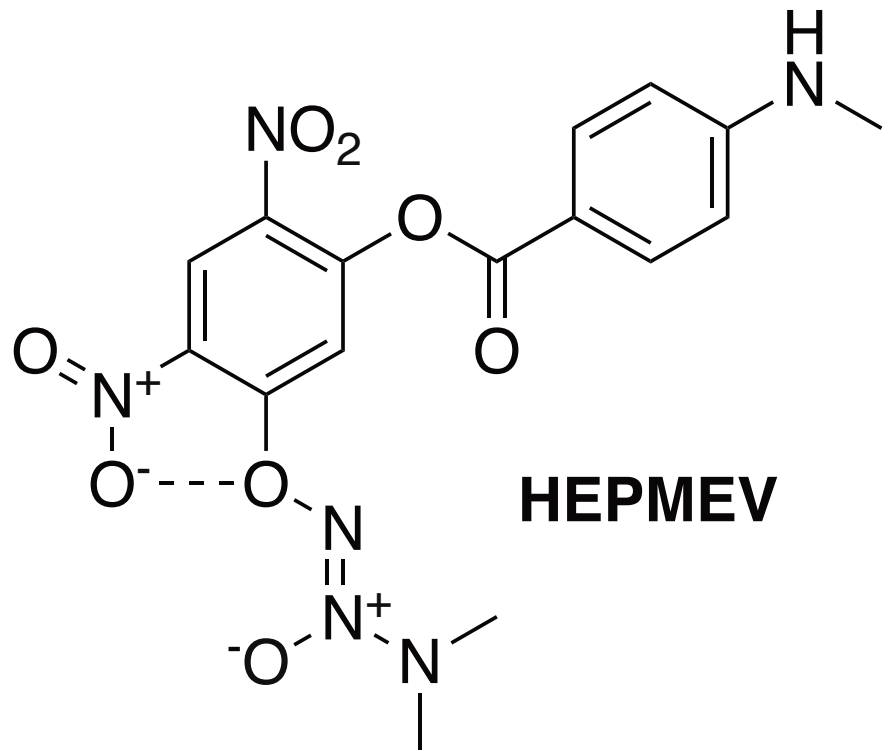
m/z: 122.02



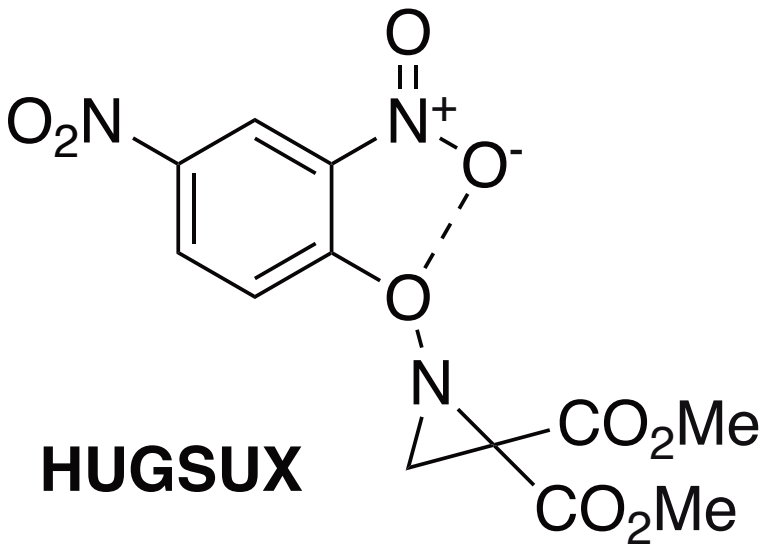
7



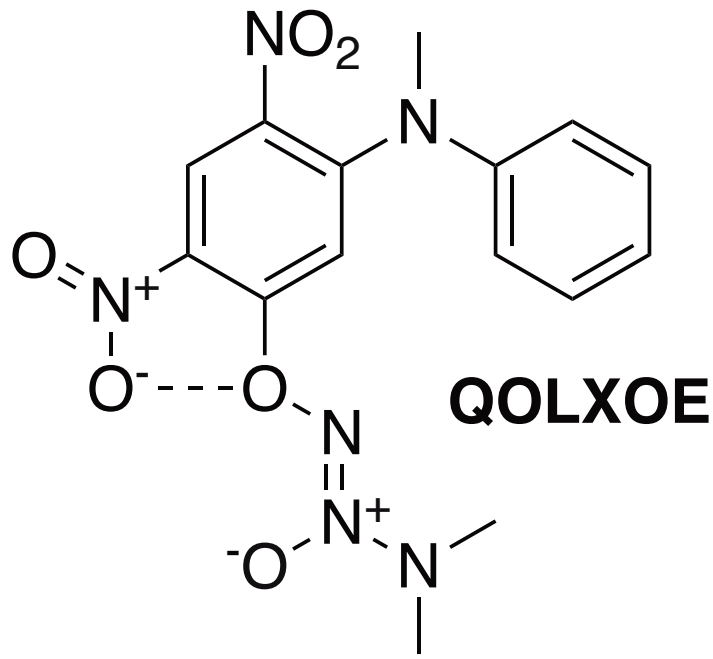
IQADOT



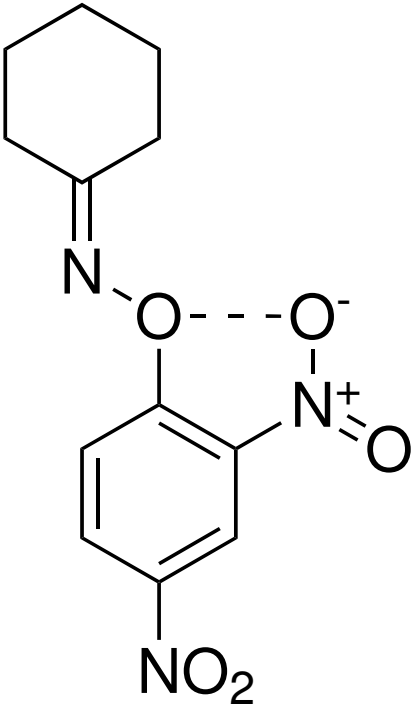
HEPMEV



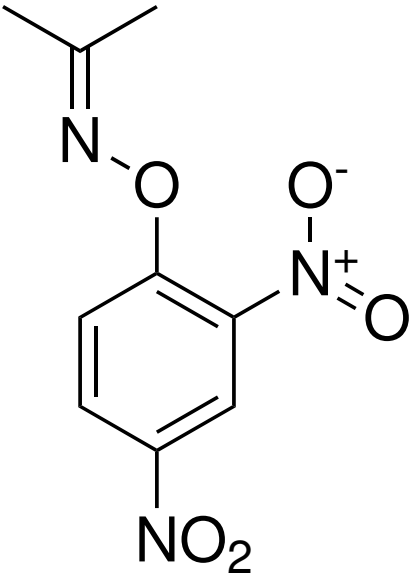
HUGSUX



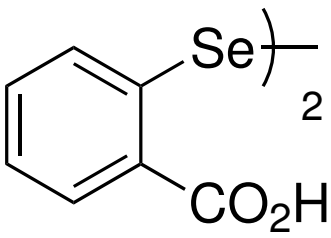
QOLXOE



8

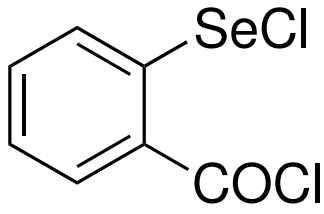


9



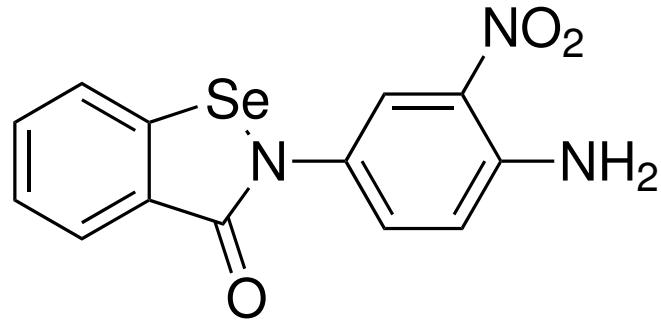
5

a



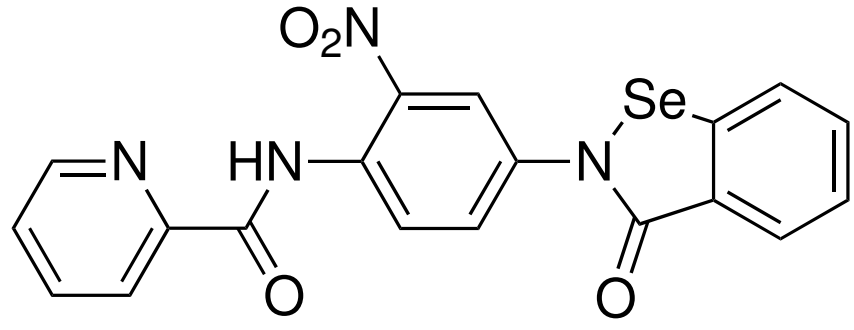
6

b



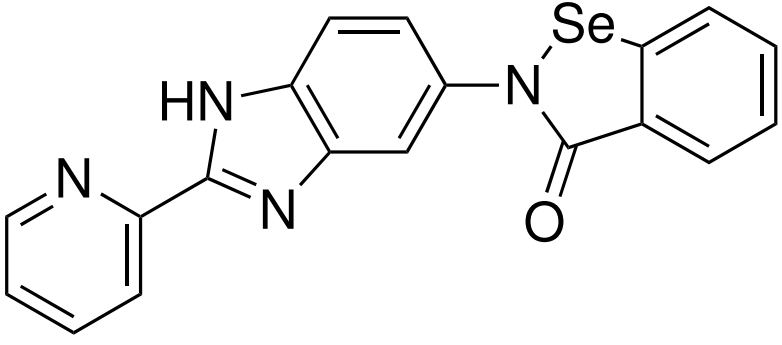
14

c

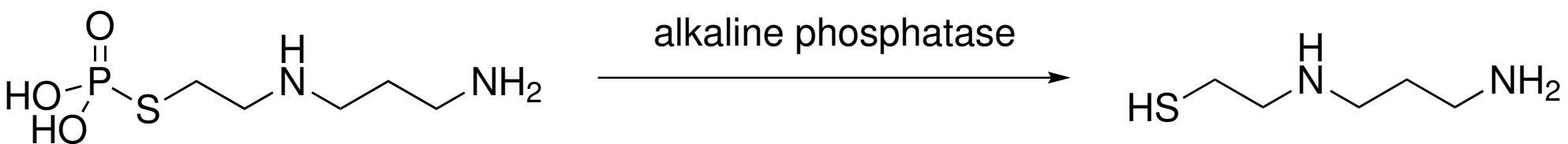


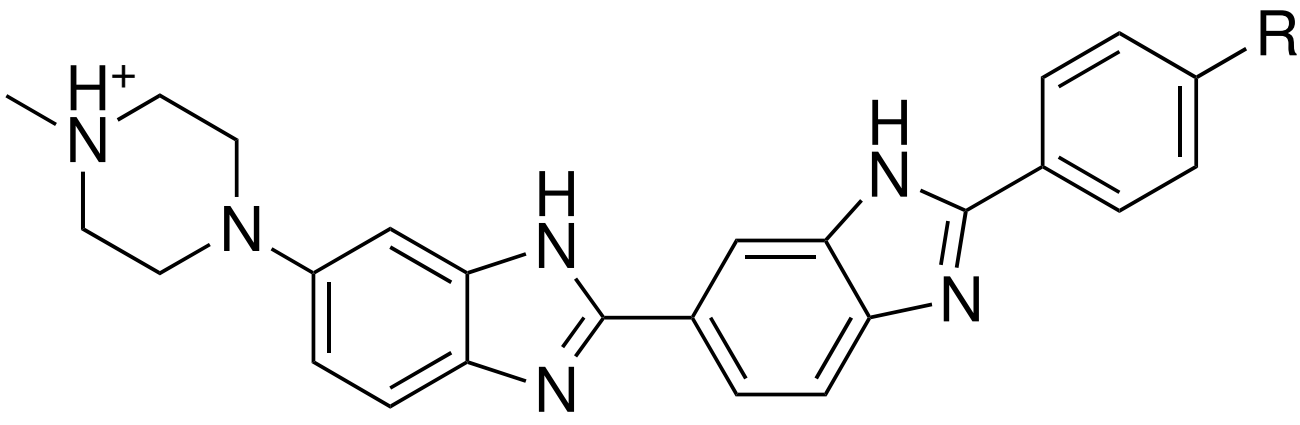
13

d

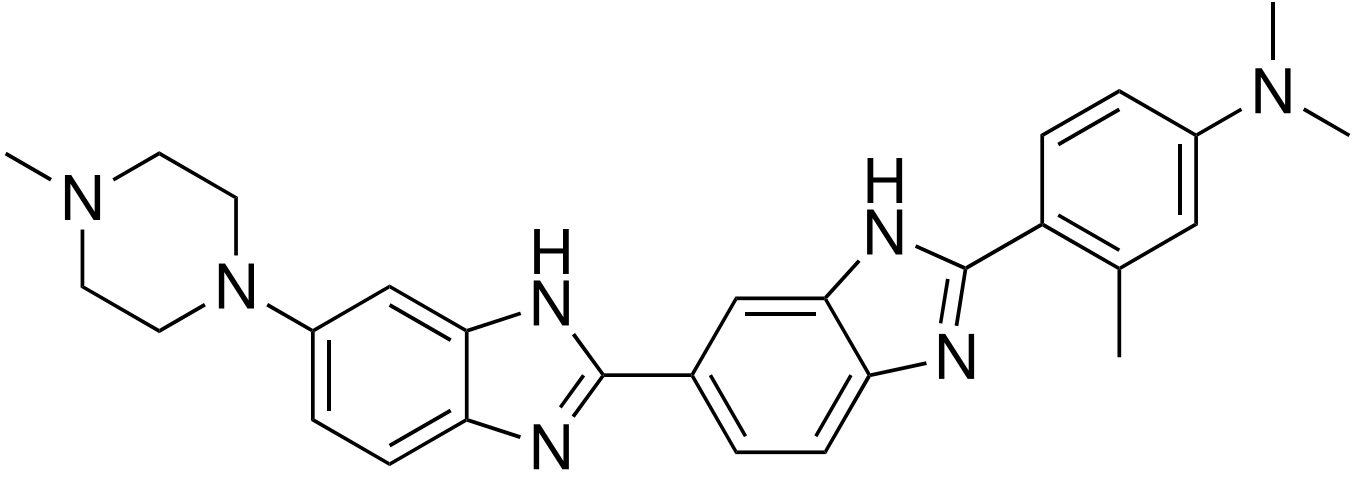


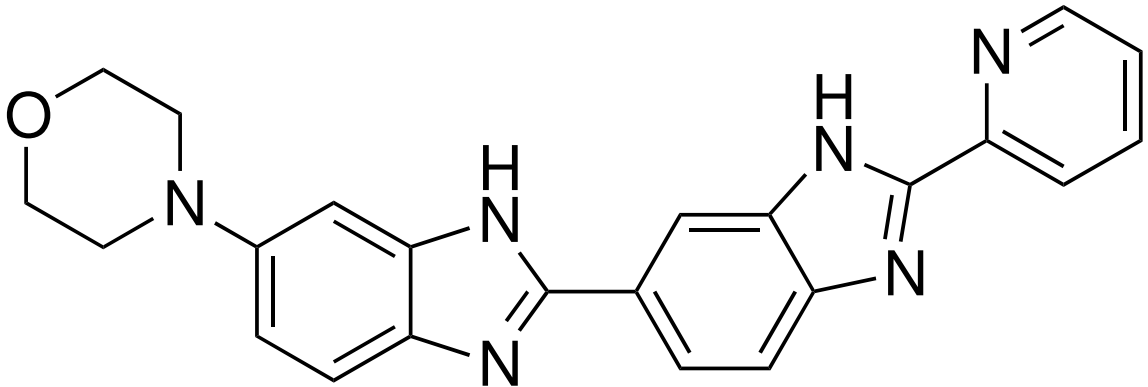
11


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

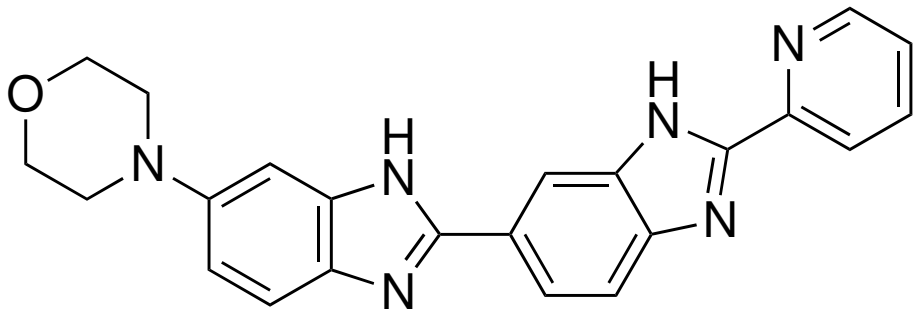


Hoechst 33258 R: OH
Hoechst 33342 R: OCH_2CH_3
Hoechst 34580 R: $N(CH_3)_2$

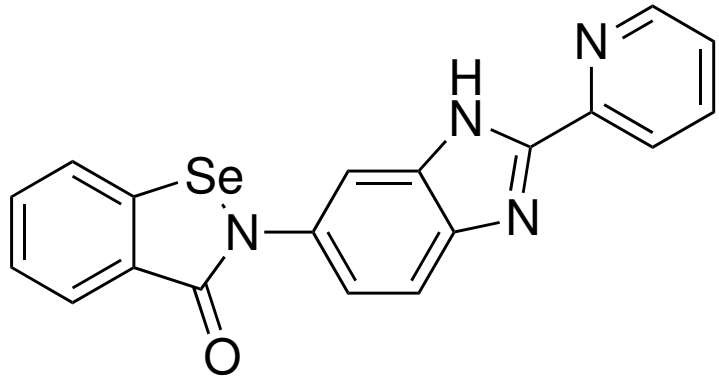




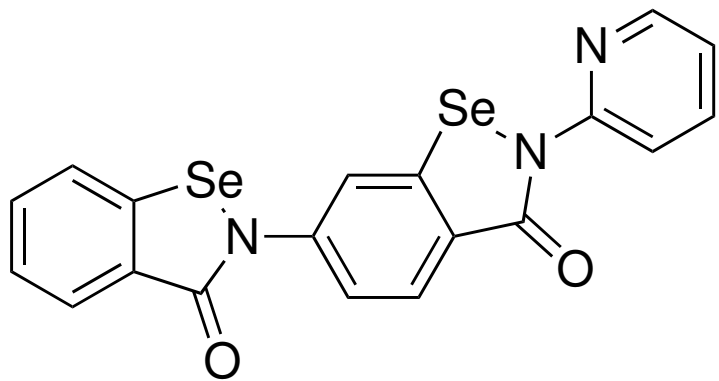
10



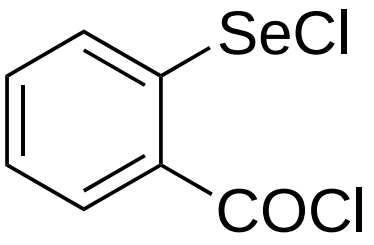
10



11

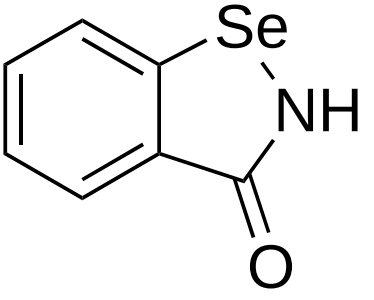


12



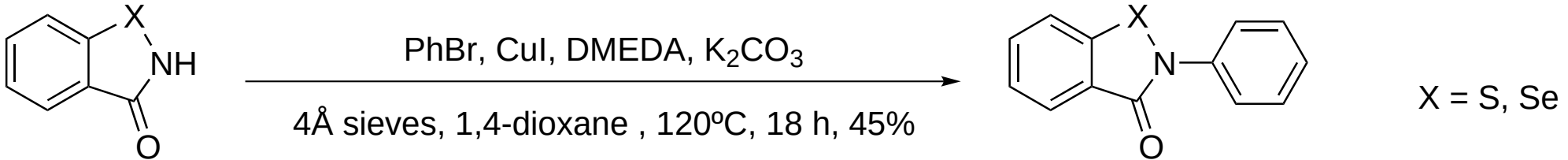
NH_3 (aq)

MeCN, rt, 10 min, 87%

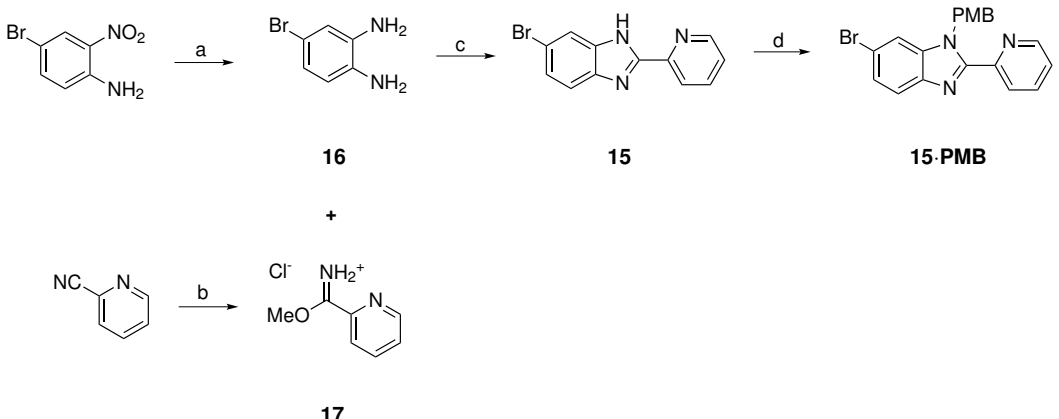


6

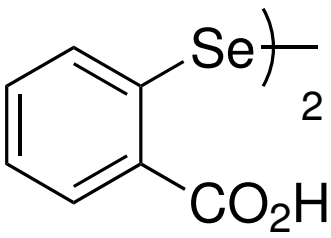
1b


X
NH
O
PhBr, CuI, DMEDA, K2CO3
4Å sieves, 1,4-dioxane , 120ºC, 18 h, 45%
X
N
O
X = S, Se

1b **1**

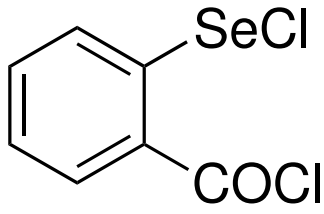

Br
NO2
NH2
a
Br
NH2
NH2
c
Br
H
N
N
d
Br
PMB
N
N
16
15
15·PMB
+
NC
N
b
Cl-
NH2+
MeO
N
17

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



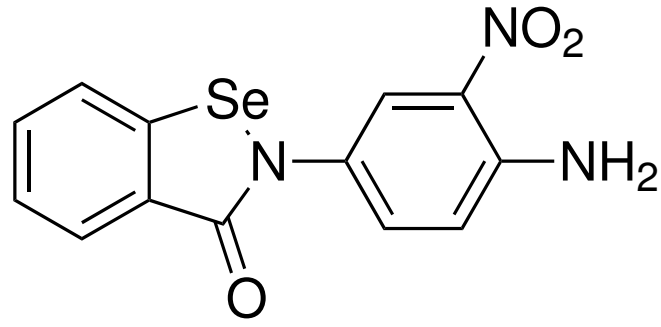
5

a



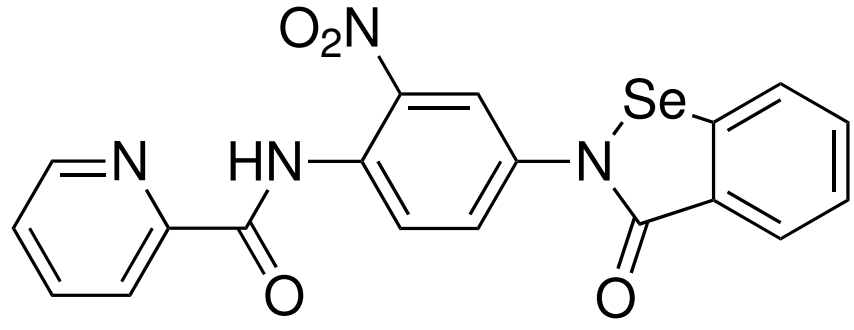
6

b



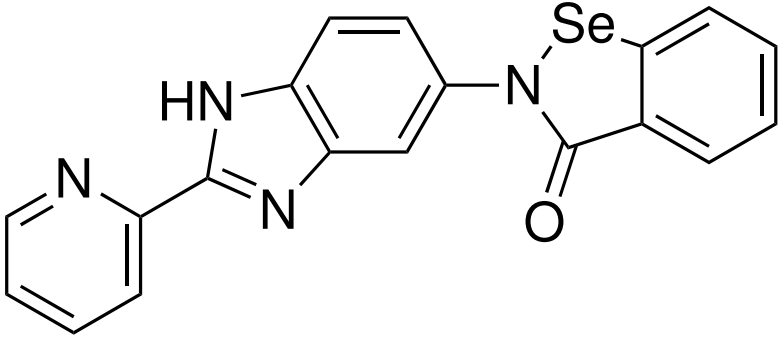
14

c

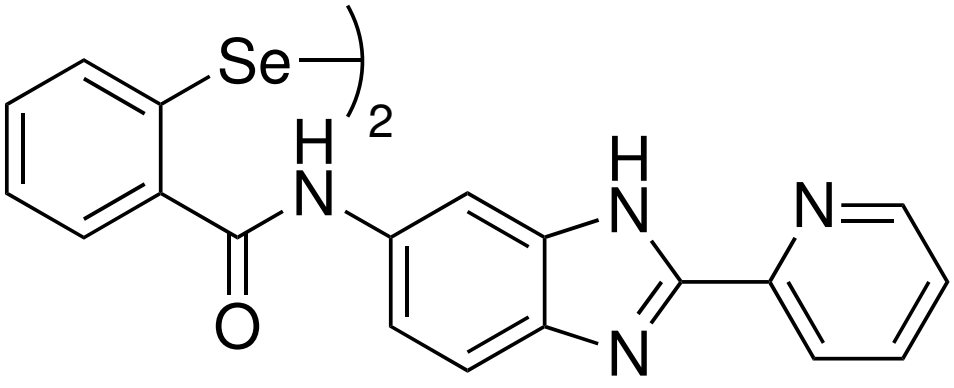


13

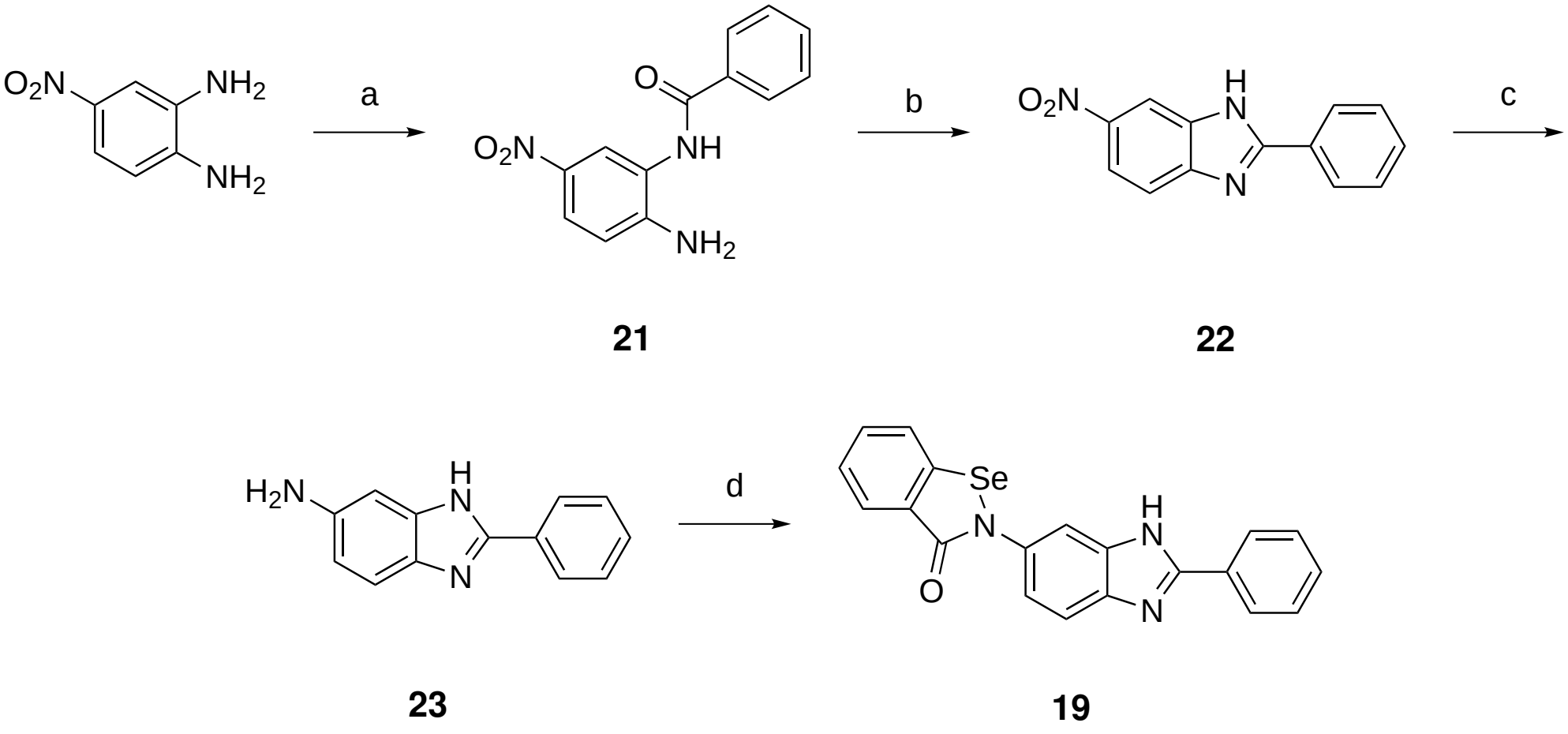
d



11



20


O2N
NH2
NH2
a
O
NH
O2N
NH2
21
b
H
N
O2N
N
22
c
H2N
H
N
N
23
d
Se
N
O
H
N
N
19