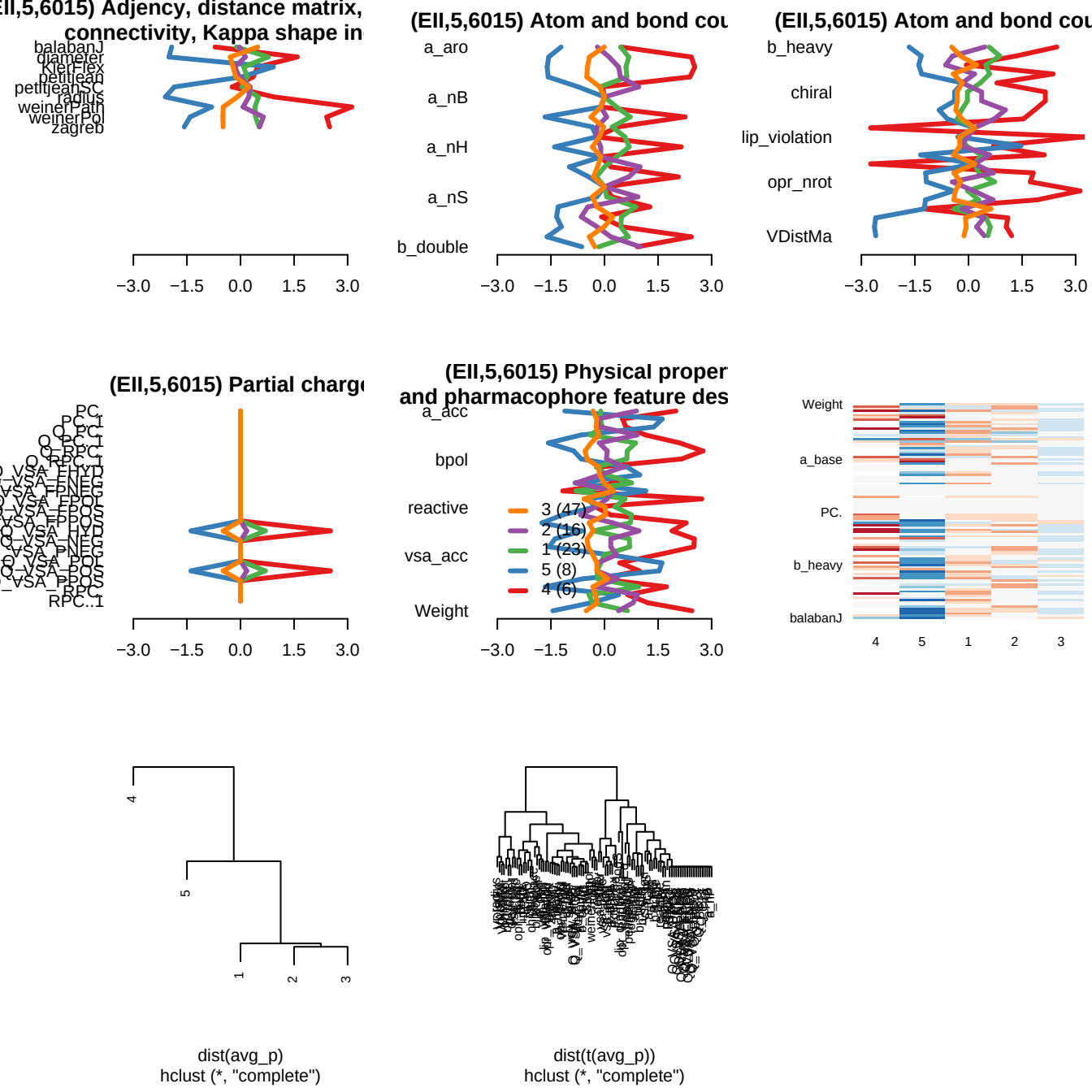
(EII,5,6015) Adjency, distance matrix, connectivity, Kappa shape in
balabanJ
diameter
KlerFlex
petitjean
petitjeanSC
radius
weinerPath
weinerPol
zagreb
−3.0 −1.5 0.0 1.5 3.0
(EII,5,6015) Atom and bond cou
a_aro
a_nB
a_nH
a_nS
b_double
−3.0 −1.5 0.0 1.5 3.0
(EII,5,6015) Atom and bond cou
b_heavy
chiral
lip_violation
opr_nrot
VDistMa
−3.0 −1.5 0.0 1.5 3.0
(EII,5,6015) Partial charge
PC.
PC.1
Q.PC.1
Q.RPC.
Q.RPC.1
RPC..1
−3.0 −1.5 0.0 1.5 3.0
(EII,5,6015) Physical proper
and pharmacophore feature des
a_acc
bpol
reactive
vsa_acc
Weight
3 (47)
2 (16)
1 (23)
5 (8)
4 (6)
−3.0 −1.5 0.0 1.5 3.0
Weight
a_base
PC.
b_heavy
balabanJ
4 5 1 2 3
4
5
1 2 3
dist(avg_p)
hclust (*, "complete")
dist(t(avg_p))
hclust (*, "complete")