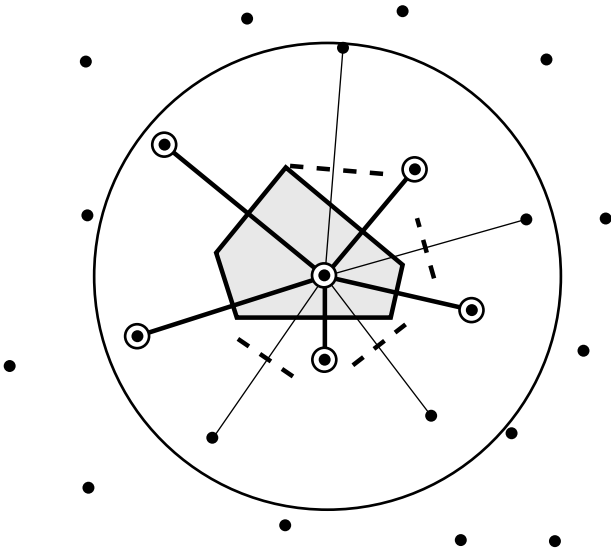


Figure 1 - Voronoi Construct



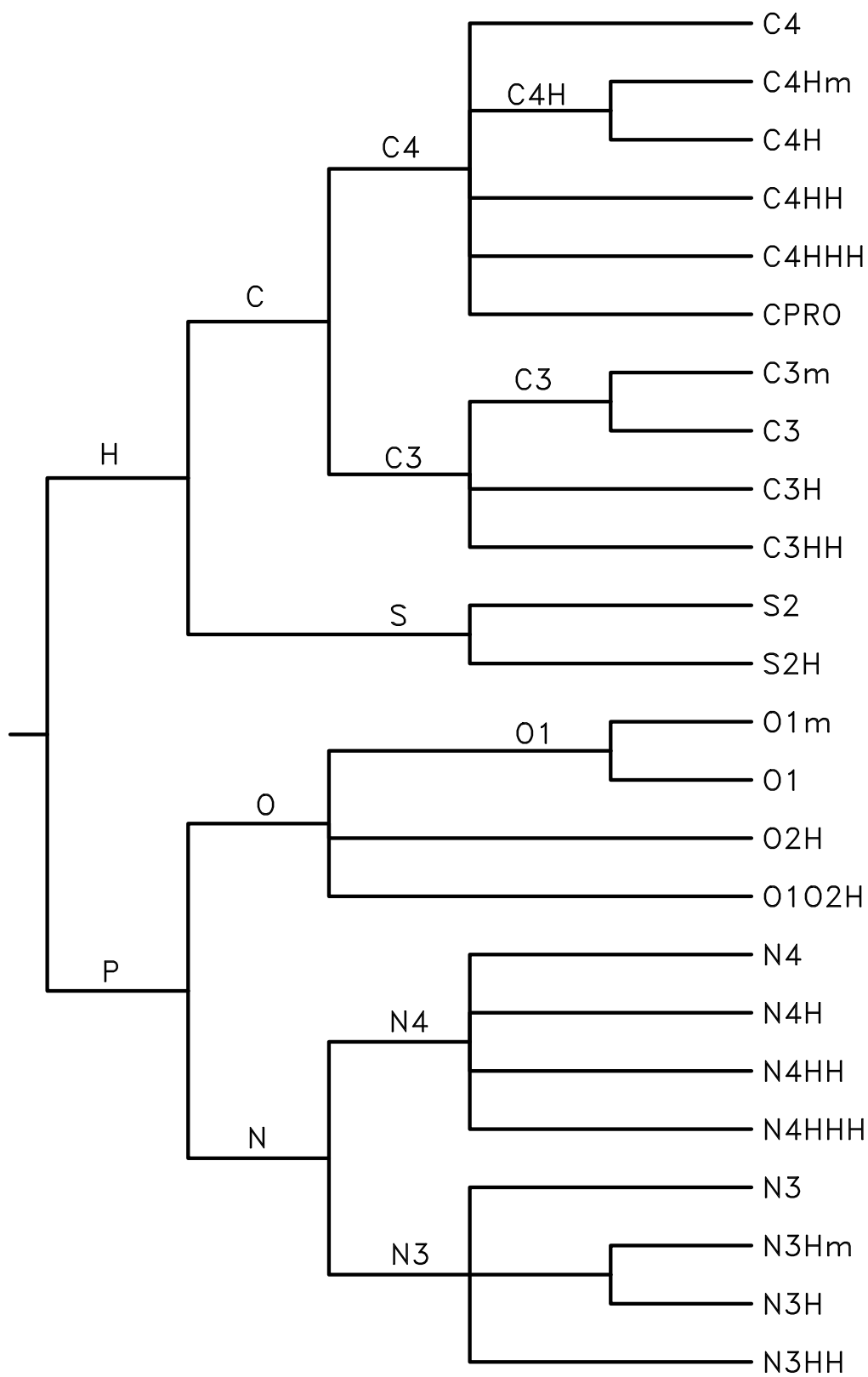


Fig. 2A - Chemical Tree

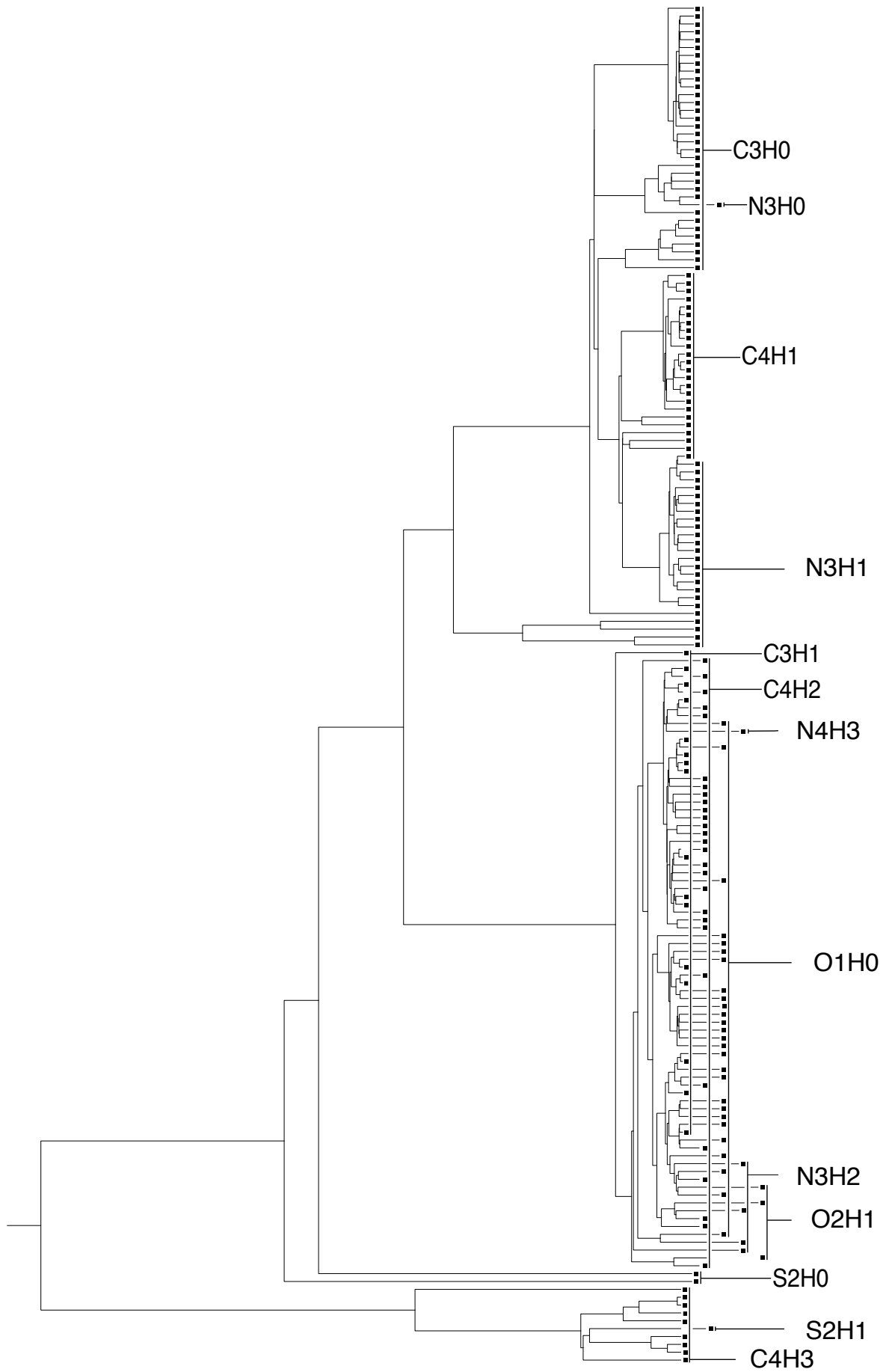


Fig. 2B-Single Linkage Tree

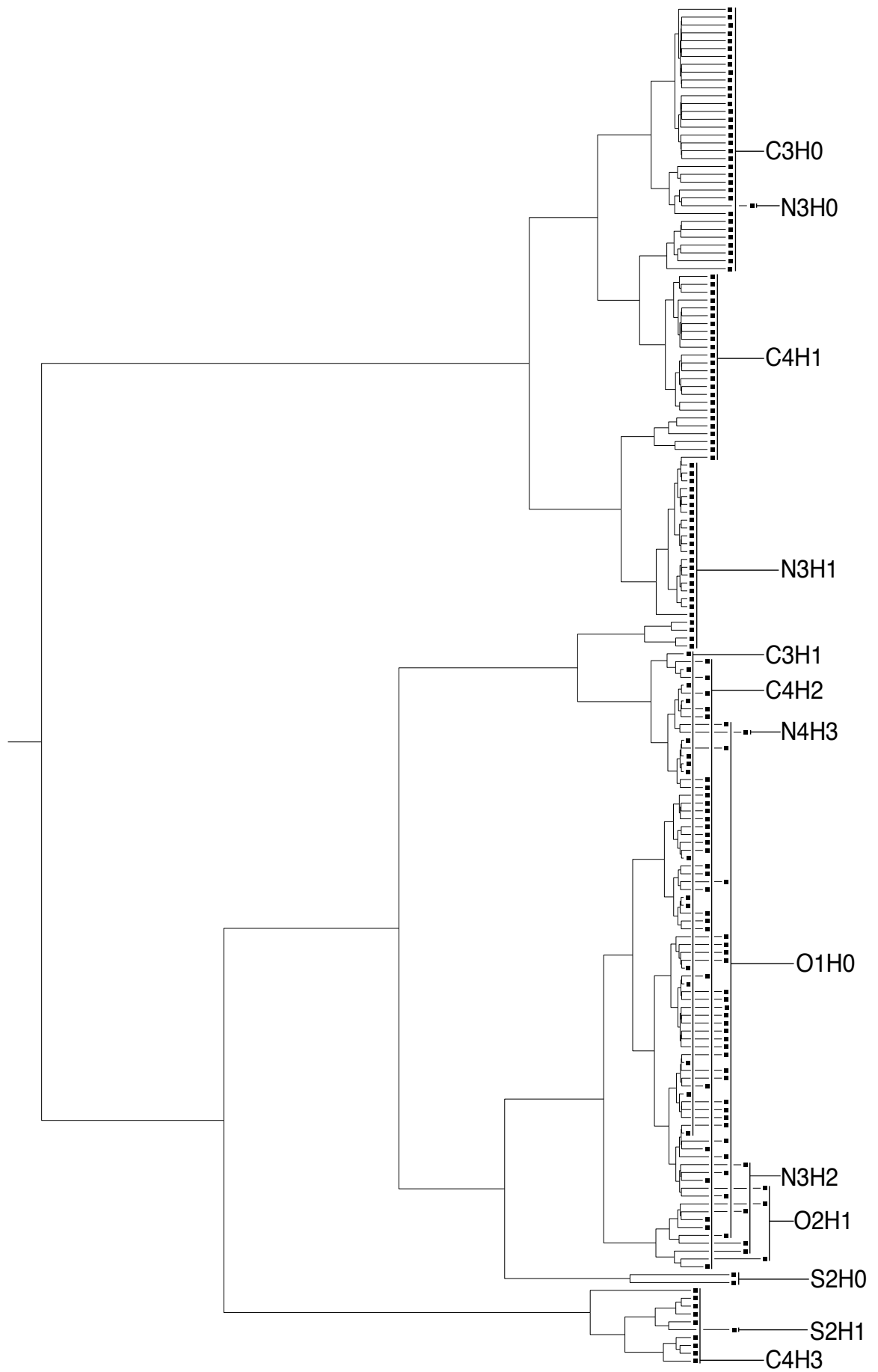


Fig. 2C - Multi-Linkage Tree

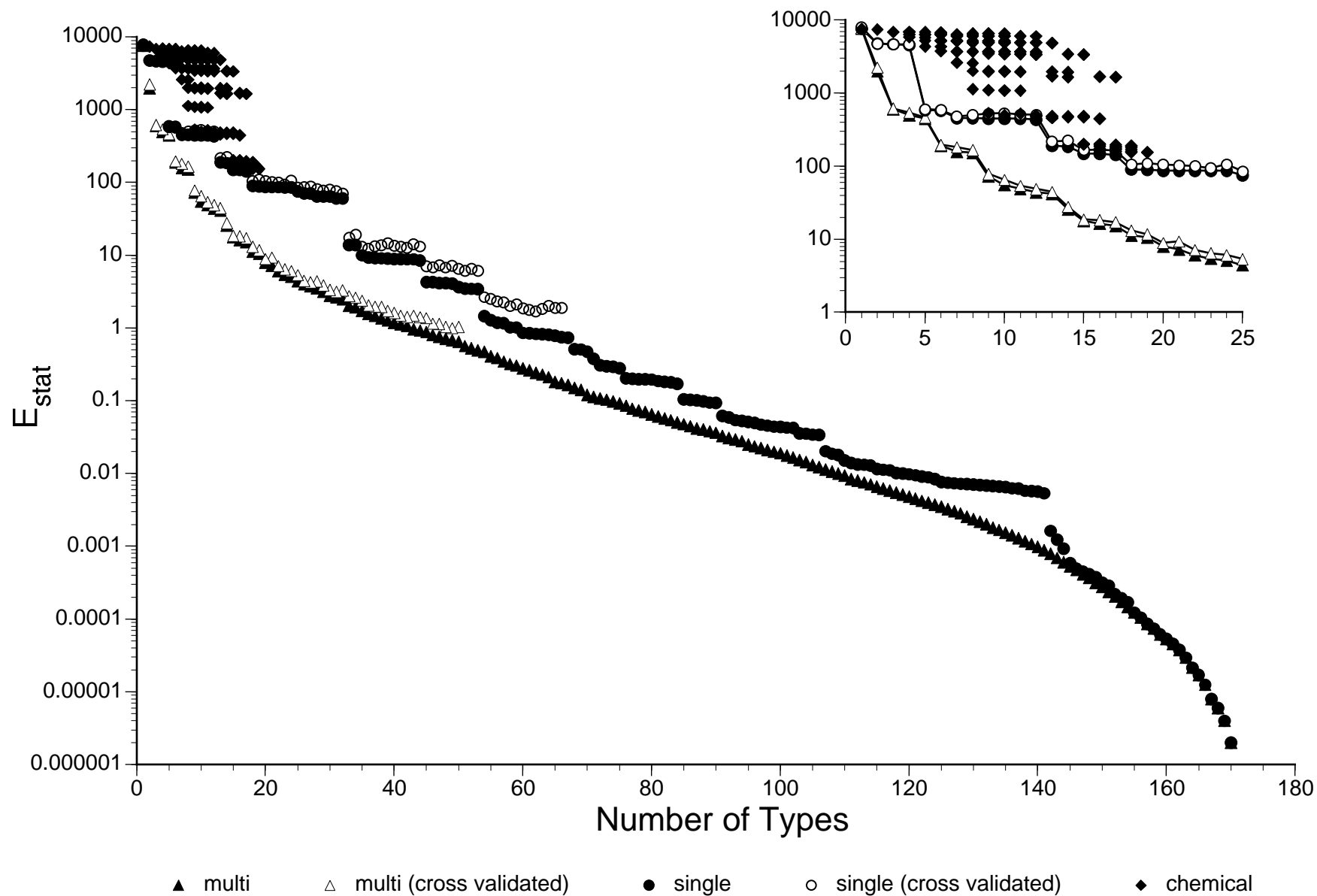


Fig. 3

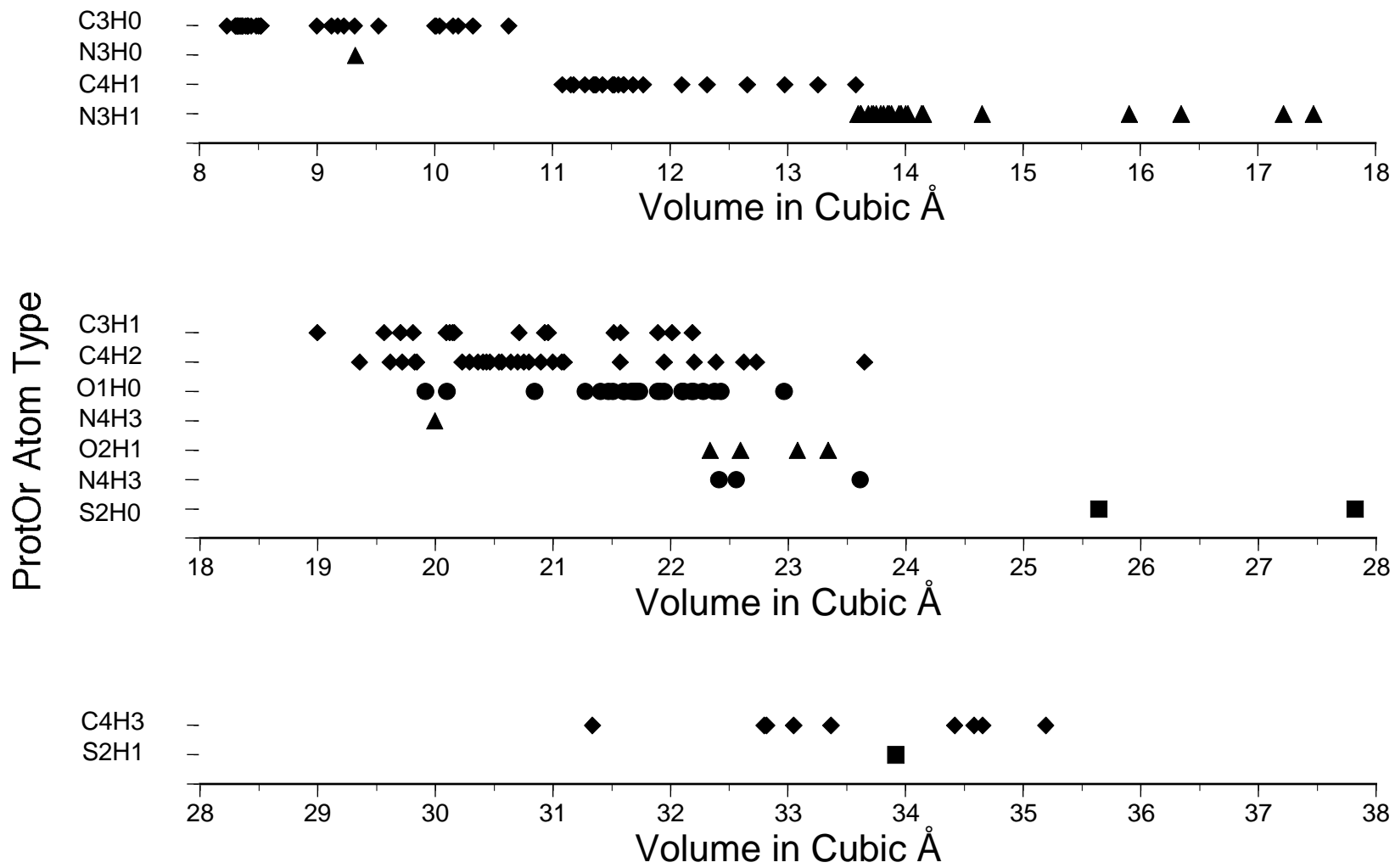


Fig. 4

Table 1
ProtOr Volumes

ProtOr radii set	
atom	radii
C3H0	1.61
C3H1	1.76
C4H1	1.88
C4H2	1.88
C4H3	1.88
N3H0	1.64
N3H1	1.64
N3H2	1.64
N4H3	1.64
O1H0	1.42
O2H1	1.46
S2H0	1.77
S2H1	1.77

Atom Type	num (173)	Comments	Protein Atoms
C3H0s	20	carbonyl carbons with branching (mainchain carbonyls from residues with a C , so no gly carbon)	ALA_C,ARG_C,ASN_C,ASP_C,CSS_C,CYS_C,GLN_C,GLU_C,HIS_C,ILE_C,LEU_C,LYS_C,MET_C,PHE_C,PRO_C,SER_C,THR_C,TRP_C,TYR_C,VAL_C
C3H0b	13	carboxyl and carbonyl carbons w/o branching (side chain and glycine's) and aromatic carbons w/o hydrogen	ARG_CZ,ASN_CG,ASP_CG,GLN_CD,GLU_CD,GLY_C,HIS_CG,PHE_CG,TRP_CD2,TRP_CE2,TRP_CG,TYR_CG,TYR_CZ
C4H1s	18	aliphatic carbons with one hydrogen and branching from all three heavy atom bonds	ARG_CA,ASN_CA,ASP_CA,CSS_CA,CYS_CA,GLN_CA,GLU_CA,HIS_CA,ILE_CA,LEU_CA,LYS_CA,MET_CA,PHE_CA,SER_CA,THR_CA,TRP_CA,TYR_CA,VAL_CA
C4H1b	6	aliphatic carbons with one hydrogen and no branching through at least one heavy atom bond	ALA_CA,ILE_CB,LEU_CG,PRO_CA,THR_CB,VAL_CB
C3H1s	8	small aromatic carbons with one hydrogen	HIS_CD2,HIS_CE1,PHE_CD1,TRP_CD1,TYR_CD1,TYR_CD2,TYR_CE1,TYR_CE2
C3H1b	8	big aromatic carbons with one hydrogen	PHE_CD2,PHE_CE1,PHE_CE2,PHE_CZ,TRP_CE3,TRP_CH2,TRP_CZ2,TRP_CZ3
C4H2s	21	aliphatic carbons with two hydrogens, small	ARG_CB,ARG_CD,ARG_CG,ASN_CB,ASP_CB,GLN_CB,GLN_CG,GLU_CB,GLU_CG,GLY_CA,HIS_CB,LEU_CB,LYS_CB,LYS_CD,LYS_CG,MET_CB,PHE_CB,PRO_CD,SER_CB,TRP_CB,TYR_CB
C4H2b	7	aliphatic carbons with two hydrogens, big	CSS_CB,CYS_CB,ILE_CG1,LYS_CE,MET_CG,PRO_CB,PRO_CG
C4H3u	9	aliphatic carbons with three hydrogens, i.e. methyl groups	ALA_CB,ILE_CD1,ILE_CG2,LEU_CD1,LEU_CD2,MET_CE,THR_CG2,VAL_CG1,VAL_CG2
N3H0u	1	imide nitrogens (only member is Pro N)	PRO_N
N3H1s	20	amide nitrogens with one hydrogen (all other mainchain N's)	ALA_N,ARG_N,ASN_N,ASP_N,CSS_N,CYS_N,GLN_N,GLU_N,GLY_N,HIS_N,ILE_N,LEU_N,LYS_N,MET_N,PHE_N,SER_N,THR_N,TRP_N,TYR_N,VAL_N
N3H1b	4	amide nitrogens with one hydrogen (on sidechains)	ARG_NE,HIS_ND1,HIS_NE2,TRP_NE1
N3H2u	4	all amide nitrogens with 2 hydrogens (only on sidechains)	ARG_NH1,ARG_NH2,ASN_ND2,GLN_NE2
N4H3u	1	amide nitrogen charged, with 3 hydrogens	LYS_NZ
O1H0u	27	all oxygens in carboxyl or carbonyl groups (no distinction made between oxygens in carboxyl group)	ALA_O,ARG_O,ASN_O,ASN_OD1,ASP_O,ASP_OD1,ASP_OD2,CSS_O,CYS_O, GLN_O, GLN_OE1, GLU_O, GLU_OE1, GLU_OE2, GLY_O, HIS_O, ILE_O, LEU_O, LYS_O, MET_O, PHE_O, PRO_O, SER_O, THR_O, TRP_O, TYR_O, VAL_O
O2H1u	3	all hydroxyl atoms	SER_OG,THR_OG1,TYR_OH
S2H0u	2	sulfurs with no hydrogens	CSS_SG,MET_SD
S2H1u	1	sulfurs with one hydrogen	CYS_SG

Table 2. Summary of ProtOr Type Set