Table 1: Small molecule building blocks. CG particle type, corresponding chemical building block, and examples of molecules in which such a block appears. The atoms the CG block is taken to represent are also shown in the 2D chemical structures, with T-beads, S-beads, and R-beads depicted in blue, green, and red, respectively.
† Indicates that the (group of) atom(s) is shared with neighboring beads.
* Indicates molecules considered in this work (DOI: 10.33774/chemrxiv-2021-1qmq9); others are from the Martini 3 main paper (DOI: 10.1038/s41592-021-01098-3).

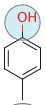
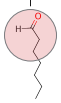
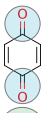
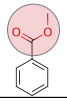
type	chemical building block	examples	
		2D	name (mapping)
P2	CH_3CH_2-COOH		propanoic acid (P2)
SP2	CH_3-COOH		acetic acid (SP2)
P1	$(CH_3)_2CH-OH$		isopropanol (P1)
TP1d	$-CH_2OH$ (bonded to $-CF_3$)		2,2,2-trifluoroethanol (SX4e-TP1d)
SN6	$-CH^{\dagger}=C(-OH)-CH^{\dagger}=$		*phenol ($(TC5)_2$-SN6)
	$-CH_2{}^{\dagger}-CH(-OH)-CH_2{}^{\dagger}-$		*cyclopentanol (SN6-SC3)
SN6d	$-CH^{\dagger}=C(-NH_2)-CH^{\dagger}=$		*aniline ($(TC5)_2$-SN6d)
TN6d	$=CH^{\dagger}-NH-CH^{\dagger}=$		*pyrrole ($(TC5)_2$-TN6d)
TN6	$=C(-OH)-$		*p-cresol ($(TC5)_2$-TC5-TN6)
N6a	$-(CH_2)_2-CH(=O)$		heptanal (C1-N6a)
TN6a	$-CH=N-$		*pyridine ($(TC5)_2$-TN6a)
	$=C=O$		*benzoquinone (TN6a-$(TC5)_2$-TN6a)
SN5a	$-O-CH_2-O-$		*1,3-dioxolane (SN5a-TC3)
N4a	$-C(=O)-O-CH_3$		*methyl-benzoate (N4a-$(TC5)_3$)

Table 1: (continued)

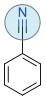
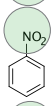
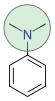
	$CH_3-C(=O)-O-CH_3$		methyl-acetate (N4a)
SN4a	$-CH_2-O-CH_2-$		*tetrahydropyran (SC3-SN4a)
	$-C(=O)-CH_3$		*acetophenone (SN4a-$(TC5)_3$)
TN4a	$-CH_2^{\dagger}-O-CH_2^{\dagger}-$		*tetrahydrofuran (SC3-TN4a)
	$-C\equiv N$		*benzonitrile ($(TC5)_3$-TN4a)
	$-CH(=O)$		*benzaldehyde ($(TC5)_3$-TN4a)
SN3r	CH_3-O-CH_3		*dimethyl ether (SN3r)
SN3a	$-CH_2-O-CH_2-$		*1,4-dioxane (SN3a-SN3a)
SN3a	$-NO_2$		*nitrobenzene ($(TC5)_3$-SN3a)
SN2a	$=C(-O-CH_3)-$		*o-methylanisole (SN2a-TC4-$(TC5)_2$)
TN2a	$=CH^{\dagger}-O-CH^{\dagger}=$		*furan ($(TC5)_2$-TN2a)
	$-O-CH_3$		*methoxybenzene ($(TC5)_3$-TN2a)
SN1	$-N(-CH_3)_2$		*N,N-dimethylaniline ($(TC5)_3$-SN1)
TN1	$-N(-CH_3)-$		*1-methylimidazole (TC5-TN1-TN6a)
SC6	$-CH^{\dagger}=C(-SH)-CH^{\dagger}=$		*thiophenol ($(TC5)_2$-SC6)
	$-CH_2-S-CH_2-$		*tetrahydrothiophene (SC6-TC3)
TC6	$=CH^{\dagger}-S-CH^{\dagger}=$		*thiophene ($(TC5)_2$-TC6)
TC5	$-CH=CH-$		*benzene ($(TC5)_3$)

Table 1: (continued)

	$-CH=CH_2$		*styrene ($(TC5)_4$)
TC5e	$(-)_2C=C(-)_2$		*naphthalene ($(TC5)_2$-TC5e-$(TC5)_2$)
C4	$CH_3-CH=CH-CH_3$		1-butene (C4)
SC4	$-CH^{\dagger}=C(-CH_3)-CH^{\dagger}=$		*toluene ($(TC5)_2$-SC4)
TC4	$=C(-CH_3)-$		*o-methylanisole (SN2a-TC4-$(TC5)_2$)
SX4e	$-CF_3$		*benzotrifluoride ($(TC5)_3$-SX4e)
	$-CF_3$		2,2,2-trifluoroethanol (SX4e-TP1d)
SC3	$-(CH_2)_3-$		*cyclohexane (SC3-SC3)
	$-CH_2{}^{\dagger}-CH(-CH_3)-CH_2{}^{\dagger}-$		*methylcyclopentane (SC3-SC3)
TC3	$-CH_2-CH_3$		*ethylbenzene ($(TC5)_3$-TC3)
	$-CH_2-CH_2-$		*tetrahydrothiophene (SC6-TC3)
SX3	$-CH^{\dagger}=C(-Cl)-CH^{\dagger}=$		*chlorobenzene ($(TC5)_2$-SX3)
SC2	$-(CH_2)_2-(CH_3)$		*3-propyl-thiophene (TC6-$(TC5)_2$-SC2)
X2	$CHCl_3$		*trichloromethane (X2)
SX2	$-CH^{\dagger}=C(-Br)-CH^{\dagger}=$		*bromobenzene ($(TC5)_2$-SX2)
C1	$CH_3-(CH_2)_2-CH_3$		butane (C1)
X1	$-CH^{\dagger}=C(-I)-CH^{\dagger}=$		*iodobenzene ($(TC5)_2$-X1)

Bead (charge)	Cation	Bead (charge)	Anion
TQ5 (+1)	sodium	TQ5 (-1)	chloride
SQ4 (+1)	potassium	SQ4 (-1)	bromide
TQ5p (+1)	ammonium	SQ2(-1)	iodine
Q4p/SQ4p (+1)	alkyl ammonium	Q2(-1)	tetrafluoroborate
Q3p/SQ3p (+1)	alkyl methyl ammonium	Q1 (-1)	hexafluorophosphate
Q2p/SQ2p (+1)	alkyl dimethyl ammonium	SQ1 (-1)	thiocyanate
Q2 (+1)	tetramethyl ammonium	SQ3 (-1)	nitrate
Q1 (+1)	choline (lipid head))	Q2 (-1)	perchlorate
Q1 (+1)	tetramethyl phosphonium	Q5n/SQ5n (-1)	carboxylate
SQ3p (+1)	guanidinium	Q4n/SQ4n (-1)	sulfonate
TD (+2)	magnesium	Q5 (-1)	phosphate (lipid head)
SD/TD* (+2)	calcium	D (-2)	phosphate

* Depending of the application, TD could be useful.