

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	$\text{CH}_3\text{CH}_2\text{COOH}$		propanoic acid (P2)
SP2	CH_3COOH		acetic acid (SP2)
P1	$(\text{CH}_3)_2\text{CHOH}$		isopropanol (P1)
TP1d	$-\text{CH}_2\text{OH}$ (bonded to $-\text{CF}_3$)		2,2,2-trifluoroethanol (SX4e-TP1d)
SN6	$-\text{CH}^\dagger=\text{C}(-\text{OH})-\text{CH}^\dagger=$		*phenol ((TC5) ₂ -SN6)
	$-\text{CH}_2^\dagger-\text{CH}(-\text{OH})-\text{CH}_2^\dagger-$		*cyclopentanol (SN6-SC3)
SN6d	$-\text{CH}^\dagger=\text{C}(-\text{NH}_2)-\text{CH}^\dagger=$		*aniline ((TC5) ₂ -SN6d)
TN6d	$=\text{CH}^\dagger-\text{NH}-\text{CH}^\dagger=$		*pyrrole ((TC5) ₂ -TN6d)
TN6	$=\text{C}(-\text{OH})-$		*p-cresol ((TC5) ₂ -TC5-TN6)
N6a	$-(\text{CH}_2)_2-\text{CH}(=\text{O})$		heptanal (C1-N6a)
TN6a	$-\text{CH}=\text{N}-$		*pyridine ((TC5) ₂ -TN6a)
	$=\text{C}=\text{O}$		*benzoquinone (TN6a-(TC5) ₂ -TN6a)
SN5a	$-\text{O}-\text{CH}_2-\text{O}-$		*1,3-dioxolane (SN5a-TC3)
N4a	$-\text{C}(=\text{O})-\text{O}-\text{CH}_3$		*methyl-benzoate (N4a-(TC5) ₃)

Table 1: (continued)




































	$\text{CH}_3-\text{C}(=\text{O})-\text{O}-\text{CH}_3$		methyl-acetate (N4a)
SN4a	$-\text{CH}_2-\text{O}-\text{CH}_2-$		*tetrahydropyran (SC3-SN4a)
	$-\text{C}(=\text{O})-\text{CH}_3$		*acetophenone (SN4a-(TC5) ₃)
TN4a	$-\text{CH}_2^\dagger-\text{O}-\text{CH}_2^\dagger-$		*tetrahydrofuran (SC3-TN4a)
	$-\text{C}\equiv\text{N}$		*benzonitrile ((TC5) ₃ -TN4a)
	$-\text{CH}(=\text{O})$		*benzaldehyde ((TC5) ₃ -TN4a)
SN3r	$\text{CH}_3-\text{O}-\text{CH}_3$		*dimethyl ether (SN3r)
SN3a	$-\text{CH}_2-\text{O}-\text{CH}_2-$		*1,4-dioxane (SN3a-SN3a)
SN3a	$-\text{NO}_2$		*nitrobenzene ((TC5) ₃ -SN3a)
SN2a	$=\text{C}(-\text{O}-\text{CH}_3)-$		*o-methylanisole (SN2a-TC4-(TC5) ₂)
TN2a	$=\text{CH}^\dagger-\text{O}-\text{CH}^\dagger=$		*furan ((TC5) ₂ -TN2a)
	$-\text{O}-\text{CH}_3$		*methoxybenzene ((TC5) ₃ -TN2a)
SN1	$-\text{N}(-\text{CH}_3)_2$		*N,N-dimethylaniline ((TC5) ₃ -SN1)
TN1	$-\text{N}(-\text{CH}_3)-$		*1-methylimidazole (TC5-TN1-TN6a)
SC6	$-\text{CH}^\dagger=\text{C}(-\text{SH})-\text{CH}^\dagger=$		*thiophenol ((TC5) ₂ -SC6)
	$-\text{CH}_2-\text{S}-\text{CH}_2-$		*tetrahydrothiophene (SC6-TC3)
TC6	$=\text{CH}^\dagger-\text{S}-\text{CH}^\dagger=$		*thiophene ((TC5) ₂ -TC6)
TC5	$-\text{CH}=\text{CH}-$		*benzene ((TC5) ₃)

Table 1: (continued)

	$-\text{CH}=\text{CH}_2$		*styrene ((TC5) ₄)
TC5e	$(-)_2\text{C}=\text{C}(-)_2$		*naphthalene ((TC5) ₂ -TC5e-(TC5) ₂)
C4	$\text{CH}_3-\text{CH}=\text{CH}-\text{CH}_3$		1-butene (C4)
SC4	$-\text{CH}^\dagger=\text{C}(-\text{CH}_3)-\text{CH}^\dagger=$		*toluene ((TC5) ₂ -SC4)
TC4	$=\text{C}(-\text{CH}_3)-$		*o-methylanisole (SN2a-TC4-(TC5) ₂)
SX4e	$-\text{CF}_3$		*benzotrifluoride ((TC5) ₃ -SX4e)
	$-\text{CF}_3$		2,2,2-trifluoroethanol (SX4e-TP1d)
SC3	$-(\text{CH}_2)_3-$		*cyclohexane (SC3-SC3)
	$-\text{CH}_2^\dagger-\text{CH}(-\text{CH}_3)-\text{CH}_2^\dagger-$		*methylcyclopentane (SC3-SC3)
TC3	$-\text{CH}_2-\text{CH}_3$		*ethylbenzene ((TC5) ₃ -TC3)
	$-\text{CH}_2-\text{CH}_2-$		*tetrahydrothiophene (SC6-TC3)
SX3	$-\text{CH}^\dagger=\text{C}(-\text{Cl})-\text{CH}^\dagger=$		*chlorobenzene ((TC5) ₂ -SX3)
SC2	$-(\text{CH}_2)_2-(\text{CH}_3)$		*3-propyl-thiophene (TC6-(TC5) ₂ -SC2)
X2	CHCl_3		*trichloromethane (X2)
SX2	$-\text{CH}^\dagger=\text{C}(-\text{Br})-\text{CH}^\dagger=$		*bromobenzene ((TC5) ₂ -SX2)
C1	$\text{CH}_3-(\text{CH}_2)_2-\text{CH}_3$		butane (C1)
X1	$-\text{CH}^\dagger=\text{C}(-\text{I})-\text{CH}^\dagger=$		*iodobenzene ((TC5) ₂ -X1)