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 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 ₃ CH ₂ -COOH	O	propanoic acid (P2)
SP2	$\mathrm{CH_{3}}\mathrm{-COOH}$	HO	acetic acid (SP2)
P1	$(\mathrm{CH_3})_2\mathrm{CH-OH}$	OH	isopropanol (P1)
TP1d	$-\mathrm{CH_2OH}$ (bonded to $-\mathrm{CF_3}$)	OH F F	2,2,2-trifluoroethanol (SX4e-TP1d)
SN6	$-\mathrm{CH}^\dagger{=}\mathrm{C}(-\mathrm{OH}){-}\mathrm{CH}^\dagger{=}$	OH	*phenol ((TC5) ₂ -SN6)
	$-\mathrm{CH_2}^\dagger - \mathrm{CH}(-\mathrm{OH}) - \mathrm{CH_2}^\dagger -$	OH	*cyclopentanol (SN6-SC3)
SN6d	$-\mathrm{CH}^{\dagger}\mathrm{=}\mathrm{C}(-\mathrm{NH}_{2})\mathrm{-}\mathrm{CH}^{\dagger}\mathrm{=}$	NH ₂	*aniline ((TC5) ₂ -SN6d)
TN6d	$=\!\!\mathrm{C}\mathrm{H}^{\dagger}\!-\!\mathrm{N}\mathrm{H}\!-\!\mathrm{C}\mathrm{H}^{\dagger}\!=$	H	*pyrrole ((TC5) ₂ -TN6d)
TN6	=C(-OH)-	OH OH	* p -cresol ((TC5) ₂ -TC5-TN6)
N6a	$-(\mathrm{CH}_2)_2 - \mathrm{CH}(=\mathrm{O})$	H	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	$-C(=O)-O-CH_3$	000	*methyl-benzoate (N4a-(TC5) ₃)

[†] Indicates that the (group of) atom(s) is shared with neighboring beads.

$$CH_3-C(=O)-O-CH_3 \qquad \qquad \text{methyl-acetate (N4a)}$$

$$SN4a \quad -CH_2-O-CH_2- \qquad \qquad \text{*tetrahydropyran (SC3-SN4a)}$$

$$-C(=O)-CH_3 \qquad \qquad \text{*acetophenone (SN4a-(TC5)_3)}$$

$$TN4a \quad -CH_2^{\dagger}-O-CH_2^{\dagger}- \qquad \qquad \text{*tetrahydrofuran (SC3-TN4a)}$$

$$-C\equiv N \qquad \qquad \text{*benzonitrile ((TC5)_3-TN4a)}$$

$$-CH(=O) \qquad \qquad \text{*benzaldehyde ((TC5)_3-TN4a)}$$

$$SN3a \quad -CH_2-O-CH_2- \qquad \qquad \text{*introbenzene ((TC5)_3-SN3a)}$$

$$SN3a \quad -NO_2 \qquad \qquad \text{*nitrobenzene ((TC5)_3-SN3a)}$$

$$SN2a \quad =C(-O-CH_3)- \qquad \qquad \text{*o-methylanisole (SN2a-TC4-(TC5)_2)}$$

$$TN2a \quad =CH^{\dagger}-O-CH^{\dagger}= \qquad \text{*furan ((TC5)_2-TN2a)}$$

$$-O-CH_3 \qquad \qquad \text{*methoxybenzene ((TC5)_3-SN1)}$$

$$SN1 \quad -N(-CH_3)_2 \qquad \qquad \text{*N,N-dimethylaniline ((TC5)_3-SN1)}$$

$$TN1 \quad -N(-CH_3)- \qquad \qquad \text{*introbenzene ((TC5)_3-SN1)}$$

$$SC6 \quad -CH^{\dagger}=C(-SH)-CH^{\dagger}= \qquad \text{*thiophenol ((TC5)_2-SC6)}$$

$$-CH_2-S-CH_2- \qquad \qquad \text{*tetrahydrothiophene (SC6-TC3)}$$

$$TC6 \quad =CH^{\dagger}-S-CH^{\dagger}= \qquad \text{*thiophene ((TC5)_2-TC6)}$$

$$TC5 \quad -CH=CH- \qquad \text{*benzene ((TC5)_4)}$$

$$TC5e (-)_2C=C(-)_2$$

*naphthalene
$$((TC5)_2$$
- $TC5e$ - $(TC5)_2)$

$$C4$$
 $CH_3-CH=CH-CH_3$



$$SC4$$
 $-CH^{\dagger}=C(-CH_3)-CH^{\dagger}=$



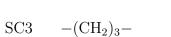
$$TC4 = C(-CH_3)-$$



*
$$o$$
-methylanisole (SN2a-TC4-(TC5)₂)

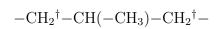
$$SX4e - CF_3$$
 $-CF_3$



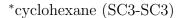




$$2,2,2$$
-trifluoroethanol (SX4e-TP1d)







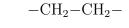


*methylcyclopentane (SC3-SC3)

TC3



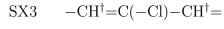
*ethylbenzene ((TC5)₃-TC3)



 $-CH_2-CH_3$



*tetrahydrothiophene (SC6-TC3)





*chlorobenzene ((TC5)₂-SX3)



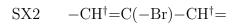


*3-propyl-thiophene (TC6-(TC5)₂-SC2)

X2 $CHCl_3$



*trichloromethane (X2)





*bromobenzene ((TC5)₂-SX2)

C1 $CH_3-(CH_2)_2-CH_3$



butane (C1)

 $-\mathrm{CH}^{\dagger} = \mathrm{C}(-\mathrm{I}) - \mathrm{CH}^{\dagger} =$ X1

*iodobenzene ((TC5)₂-X1)