

Supplementary material

Retention Time Prediction with Message-Passing Neural Networks

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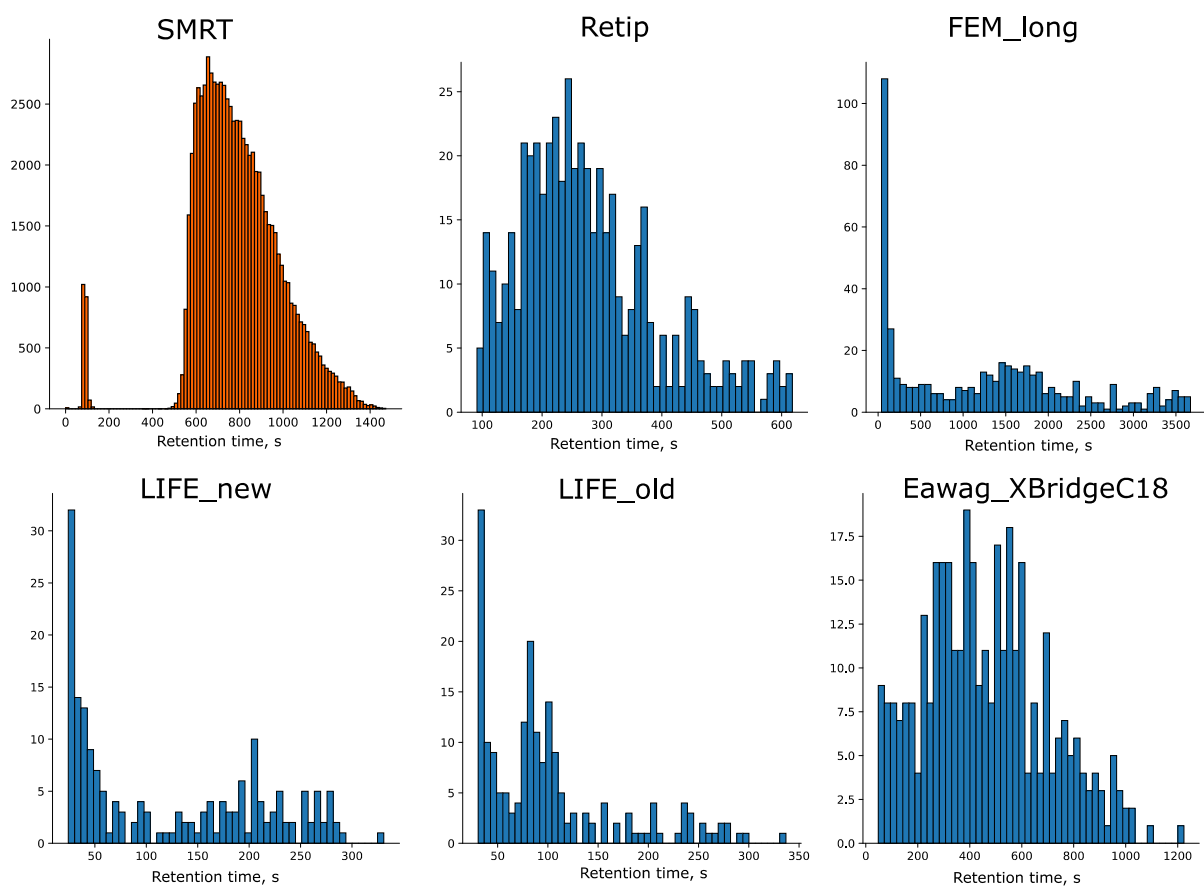


Figure S1. Retention time distribution across the investigated datasets.

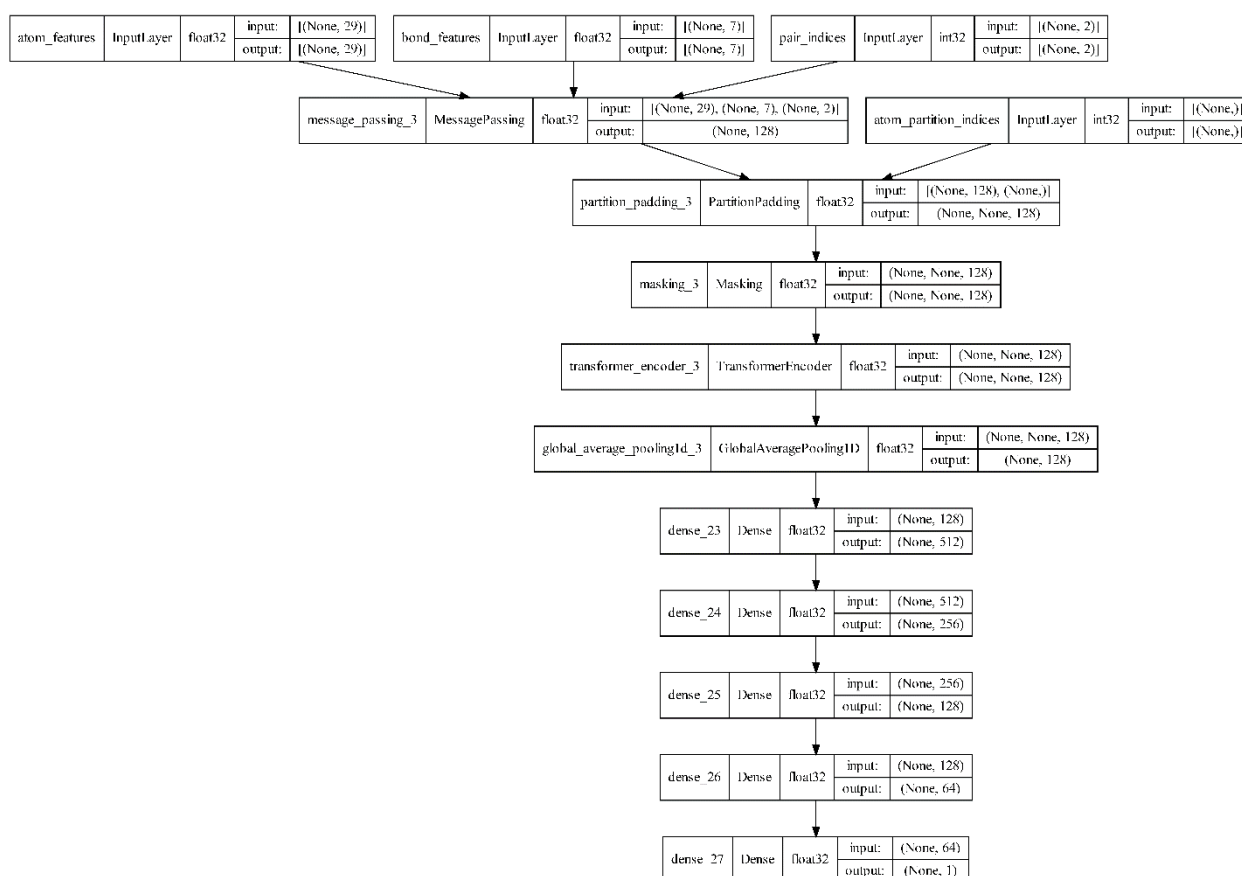


Figure S2. The detailed architecture of the proposed message-passing neural network.

Table S1. Atom and bond features.

Atom features	
Symbol	'Br', 'C', 'Cl', 'F', 'H', 'I', 'N', 'O', 'P', 'S', 'Si'
N hydrogens	0, 1, 2, 3, 4
Valence	0, 1, 2, 3, 4, 5, 6
Hybridization	"s", "sp", "sp2", "sp3"
Aromatic	True, False
Bond features	
Bond type	"single", "double", "triple", "aromatic"
Conjugated	True, False