Generating flavor molecules using Scientific Machine Learning

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Supporting Information

Table S1 - Pytorch default parameters' values for Adam optimizer.

Parameters	Learning rate	Betas	Eps	Weight decay	AMSGrad	Maximize
Default values	1.00×10^{-3}	(0.90, 0.99)	1.00×10^{-8}	0.00	False	False

The defined hyperparameters are presented in the following table, Table S2.

Table S2 - Deep generative model hyperparameters.

Parameters	Deep Generative Model's Value
α	-
Batch size	20
Block size	1000
Epochs	1000
Generation epoch	790
GGNN activation function	SELU
GGNN depth	4
GGNN dropout probability	0
GGNN hidden dimension	250
GGNN width	100
Initial learning rate	1.00×10^{-4}
Learning rate decay factor	0.99
Learning rate decay interval	10
Loss function	Kullback-Leibler divergence
Maximum relative learning rate	1.00
Message passing layers	3

Message size – input size of GRU	100
Minimum relative learning rate	1.00×10^{-4}
MLP activation function	SoftMax
MLP depth (Layers 1 and 2)	4
MLP dropout probability (Layers 1 and 2)	0
MLP hidden dimension (Layers 1 and 2)	500
Number of samples	200
Optimizer	Adam
σ	-
Weight decay	0
Weight initialization	Uniform