Time/Space Consumption

Table info: The training time, inference time, and GPU memory consumption of random batches of 32 molecules (16 molecules for GemNet and 3-E-DisGNN) from the original MD17 dataset. The format is training time in ms, inference time in ms, and inference GPU memory consumption in MB.

	2-F-DisGNN	**DimeNet**	**DimeNet_dense**	**3-E-DisGNN**	**GemNet**	**TorchMD**	**GNN-LF**
Aspirin	232/56/3644	727/133/5790	378/101/3886	OOM/OOM/OOM	2823/612/15980	188/32/2065	65/10/2791
Benzene	125/26/2134	669/94/1831	370/98/1876	383/90/6124	2242/393/3761	478/33/918	29/8/95
Ethanol	114/18/1852	672/95/784	373/104/1568	192/41/3438	2256/344/1565	417/32/532	59/8/54
Malonaldehyde	88/16/1852	657/88/784	369/96/1568	194/41/3438	2237/355/1565	753/32/532	57/7/68
Naphthalene	185/42/3140	614/112/4470	388/105/3032	OOM/312/17248	2613/498/11661	265/32/1694	61/9/175
Salicylic Acid	147/33/2640	619/92/3489	381/109/2384	OOM/197/12488	2577/430/8182	239/34/1418	59/9/176
Toluene	134/30/2640	595/113/3148	372/99/2358	OOM/164/10528	2495/423/7153	896/45/1322	62/8/176
Uracil	108/22/2134	595/107/1782	376/104/1876	383/90/6124	2165/354/3735	118/32/907	66/8/99
Average	142/30/2505	643/104/2760	376/102/2319	-	2426/426/670	419/34/1174	57/ 9/140