Correction to
Graph neural networks for the prediction of infinite dilution activity coefficients

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This is a correction notice to our original work published by Digital Discovery, RSC titled "Graph neural networks for the prediction of infinite dilution activity coefficients" with DOI: 10.1039/D1DD00037C. Our original work makes use of a dataset originally retrieved and published by [2]. On April 2023, a correction was published on this same dataset noticing that out of the 5194 data points in the original dataset 24 entries contained errors. In 18 of them iodomethane was incorrectly used instead of diiodomethane. The other 6 contained a typo of incorrect placement of the decimal point in the experimental value of the infinite dilution activity coefficient.[1].

We have re-run our computational experiments and analysis to observe the impact of this correction in our original work. Overall, the correction have led to minor implications on the models accuracy and coverage percentage. The accuracy of the GNN-based models was in general slightly improved. Moreover, the original analysis, general conclusions and findings remain the same.

A summary of the impacts of the dataset correction can be found below:

- After the cleaning process described in Section 2.2 of the original manuscript the number of solvents in the dataset changed from 262 to 261 since iodomethane is no longer present as a solvent.

- The accuracy of all mechanistic models slightly increased (cf. Table C1). The most prominent example is MOSCED which remains as the mechanistic model with the highest accuracy as originally explained in the manuscript. However, the trend of models' performance remain the same.

- The coverage percentage of UNIFAC (Ly) and MOSCED slightly decreased (cf. Table C1) given that di-iodomethane cannot be predicted using such models.

- Overall, for *GNN single* the accuracy remained within the original error margins. However, in general, the error margins themselves were slightly decreased after the correction.

- The accuracy of *GNN ensemble* slightly increased.

- The trends of the GNN-based models' performance remain the same compared to all mechanistic models (cf. Figure C1).

- The trends of the GNN and hybrid models' performance remain the same compared to all mechanistic models (cf. Figure C3). A slight improvement of the GNN model (according to the error density metric) could be now observed compared to the MOSCED model (cf. Figure C4).

Table C1: Comparison of the <mark>original</mark> and <mark>corrected</mark> values of the models accuracy and coverage percentage corresponding to Table 3 in the original manuscript. The percentage change is also specified for each model and metric. For the GNN-based models the coverage percentage remains 100%.

| Model	Sys. covered	MAE	SDEP	MSE	RMSE	R^2	MAPE
Hildebrand	54.66%	2.55×10^5	9.89×10^6	9.79×10^{13}	9.90×10^6	-7.92×10^9	4.26×10^5
Hildebrand	54.66%	2.55×10^5	9.89×10^6	9.79×10^{13}	9.90×10^6	-7.92×10^9	4.26×10^5
change	0%	0%	0%	0%	0%	0%	0%
HSP	56.23%	15.86	122.23	15190.81	123.25	-0.27	66.90
HSP	56.23%	16.03	122.37	15232.31	123.42	-0.27	66.95
change	0%	-1.06%	-0.11%	-0.27%	-0.14%	0%	-0.07%
UNIFAC (Ly)	93.91%	10.32	59.17	3607.61	60.06	0.56	32.65
UNIFAC (Ly)	94.52%	10.61	59.28	3626.24	60.22	0.56	32.99
change	-0.65%	-2.73%	-0.19%	-0.51%	-0.27%	0%	-1.03%
UNIFAC	94.52%	10.44	60.39	3755.53	61.28	0.54	32.06
UNIFAC	94.52%	10.68	60.66	3794.03	61.60	0.54	32.37
change	0%	-2.25%	-0.45%	-1.01%	-0.52%	0%	-0.96%
COSMO-RS	97.22%	10.64	66.98	4599.82	67.82	0.43	28.37
COSMO-RS	97.22%	10.78	67.18	4628.81	68.04	0.43	28.43
change	0%	-1.30%	-0.30%	-0.63%	-0.32%	0%	-0.21%
UNIFAC (Do)	94.91%	8.23	56.50	3260.48	57.10	0.60	25.88
UNIFAC (Do)	94.91%	8.54	56.82	3301.85	57.46	0.59	26.28
change	0%	-3.63%	-0.56%	-1.25%	-0.63%	1.69%	-1.52%
Abraham	44.27%	4.16	33.58	1144.72	33.84	0.90	21.93
Abraham	44.27%	4.18	33.58	1144.97	33.84	0.90	22.05
change	0%	-0.48%	0%	-0.02%	0%	0%	-0.54%
MOSCED	45.69%	2.78	12.58	165.94	12.88	0.48	19.88
MOSCED	46.12%	3.15	13.49	191.80	13.85	0.44	20.58
change	-0.93%	-11.75%	-6.75%	-13.48%	-7.00%	9.09%	-3.40%
GNN single (train)		3.97±0.46	30.78±7.01	1012.48±505.61	31.04±7.01	0.88±0.06	13.58±0.65
GNN single (train)		4.07±0.57	31.06±9.83	1077.93±757.29	31.33±9.82	0.88±0.08	13.80±0.52
change mean		-2.46%	-0.90%	-6.07%	-0.93%	0%	-1.59%
change std		(-19.30%)	(-28.69%)	(-33.23%)	(-28.62%)	(-25.00%)	(25.00%)
GNN single (valid)		4.87±2.14	30.65±18.13	1296.35±1331.09	31.06±18.21	0.80±0.27	18.24±2.77
GNN single (valid)		3.83±1.59	20.31±11.90	571.35±573.56	20.70±11.96	0.89±0.09	18.65±2.69
change mean		27.15%	50.91%	126.89%	50.05%	-10.11%	-2.20%
change std		(34.59%)	(52.35%)	(132.08%)	(52.26%)	(200%)	(2.97%)
GNN single (test)		4.36±0.33	30.49±2.79	956.33±177.64	30.80±2.81	0.77±0.04	24.94±2.07
GNN single (test)		4.26±0.60	29.60±6.22	933.44±419.07	29.91±6.24	0.78±0.1	25.27±1.14
change mean		2.35%	3.01%	2.45%	2.98%	-1.28%	-1.31%
change std		(-45.00%)	(-55.14%)	(-57.61%)	(-54.97%)	(-60%)	(81.58%)
GNN single (complete)		4.12±0.36	31.26±5.44	1023.98±382.36	31.53±5.44	0.87±0.05	16.22±0.90
GNN single (complete)		4.09±0.49	30.37±8.32	1008.47±610.84	30.65±88.31	0.87±0.08	16.48±0.61
change mean		0.73%	2.93%	1.54%	2.87%	0%	-1.58%
change std		(-26.53%)	(-34.62%)	(-37.40%)	(-93.84%)	(-37.50%)	(47.54%)
GNN ensemble (train/valid)		3.22	23.49	562.21	23.71	0.93	11.96
GNN ensemble (train/valid)		3.48	25.79	677.18	26.02	0.92	12.19
change		-7.47%	-8.92%	-16.98%	-8.88%	1.09%	-1.89%
GNN ensemble (test)		3.61	26.49	715.03	26.74	0.83	22.41
GNN ensemble (test)		3.91	26.73	729.69	27.01	0.82	22.66
change		-7.67%	-0.90%	-2.01%	-1.00%	1.22%	-1.10%
GNN ensemble (complete)		3.30	24.12	592.78	24.35	0.92	14.05
GNN ensemble (complete)		3.57	25.98	687.68	26.22	0.91	14.29
change		-7.56%	-7.16%	-13.80%	-7.13%	1.10%	-1.68%
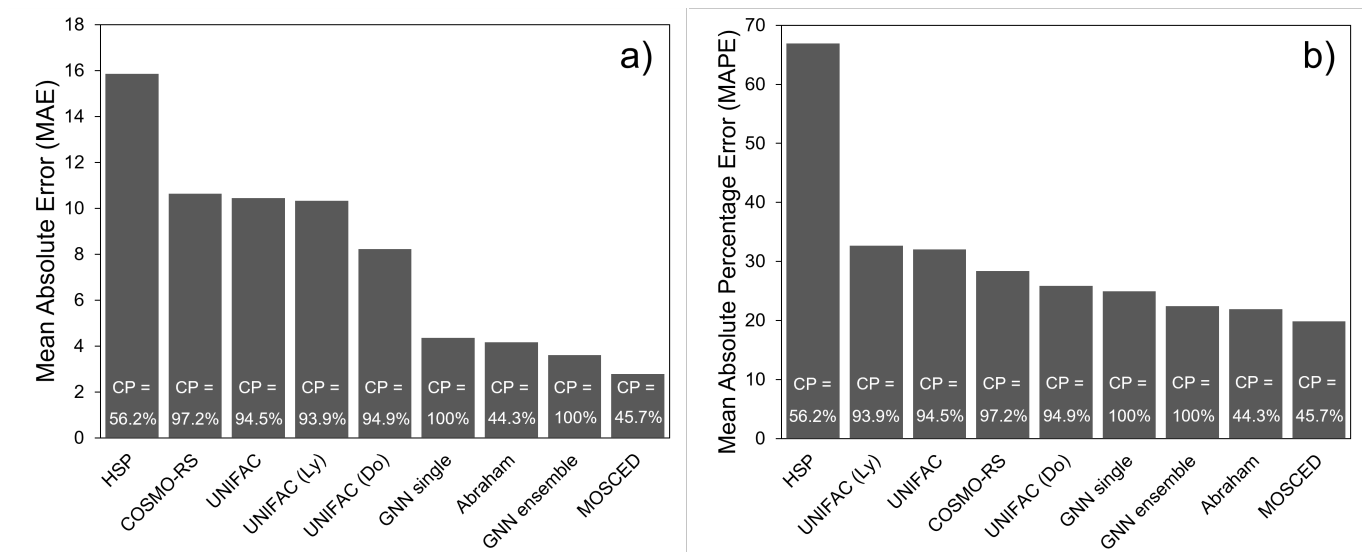
Figure C1: Corrected figure showing the performance of all models. Corresponding to Figure 4 of the original manuscript.
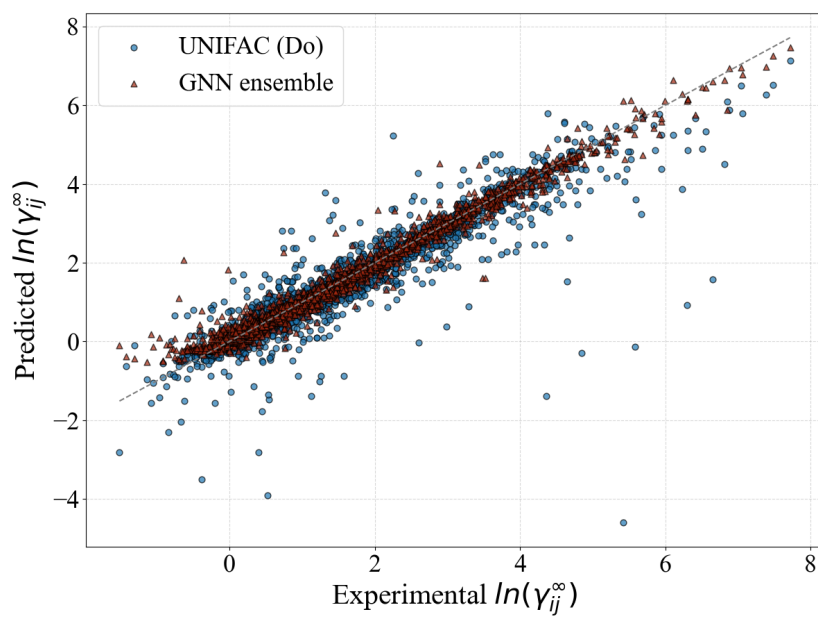

Figure C2: Corrected figure comparing the performance of GNN ensemble and UNIFAC (Do) models. Corresponding to Figure 5 of the original manuscript.
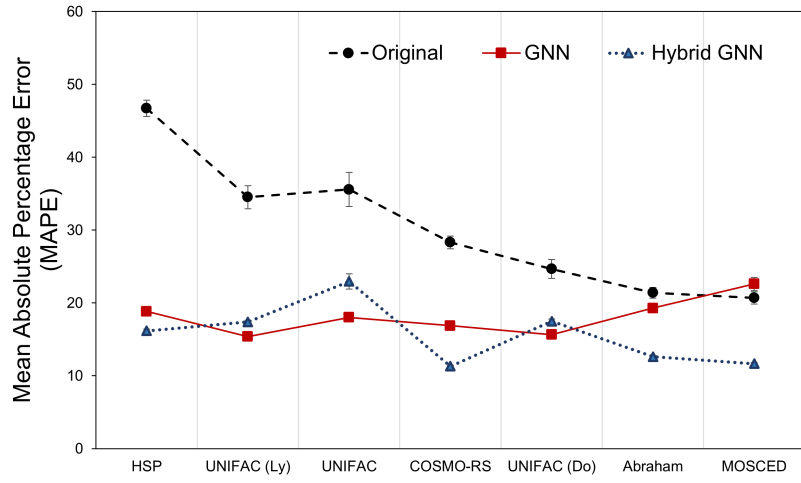
Figure C3: Corrected figure comparing the performance of GNN-based models and original models. Corresponding to Figure 6 of the original manuscript.
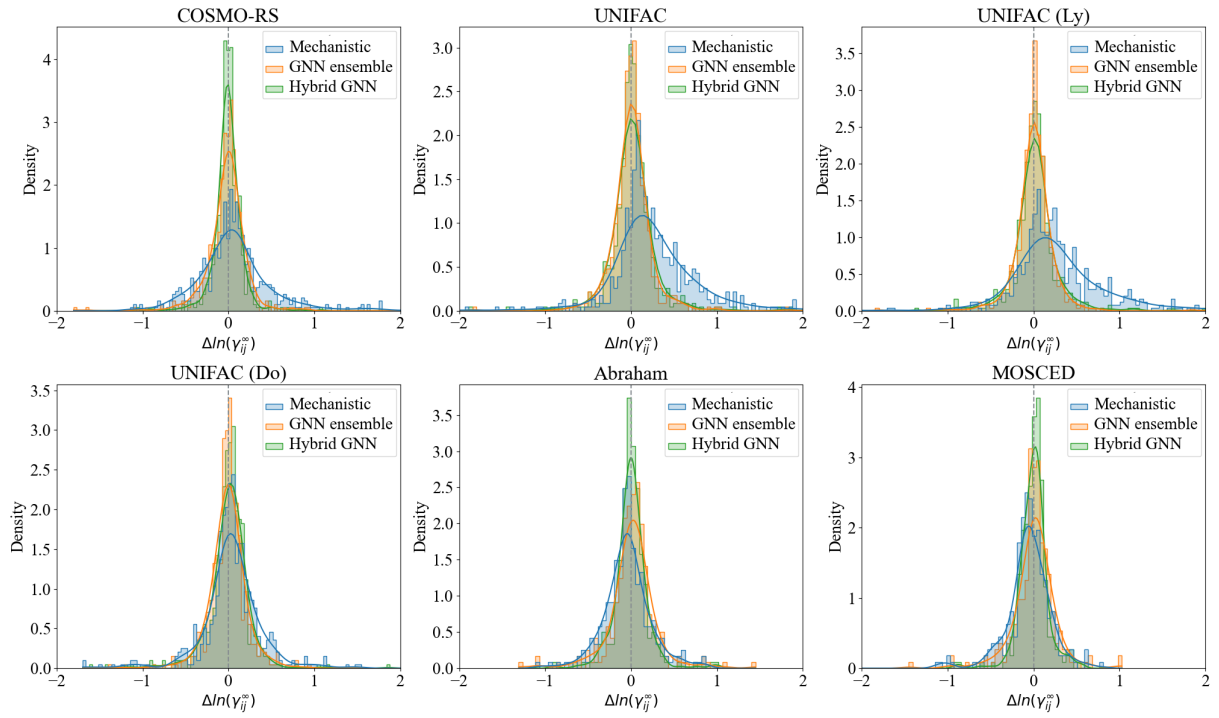

Figure C4: Corrected figure comparing the error density of GNN-based models and original models. Corresponding to Figure 7 of the original manuscript.
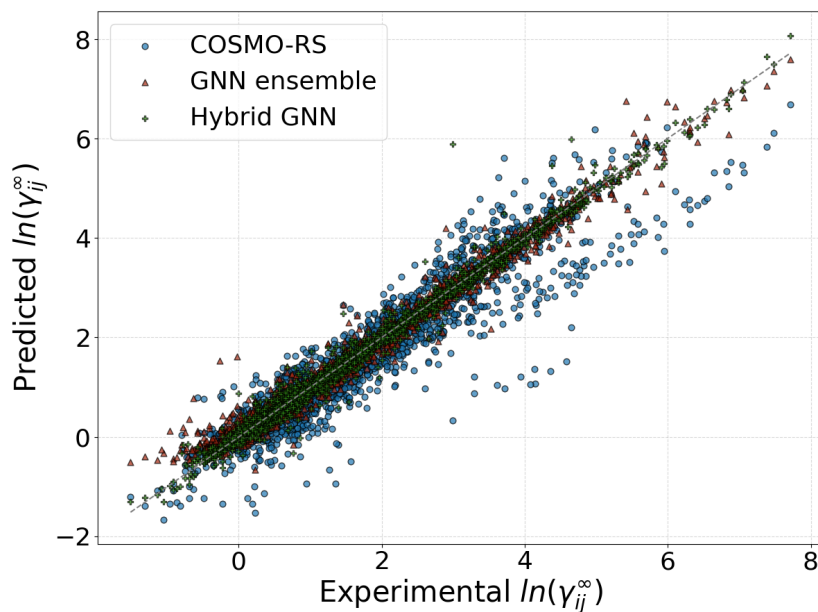
Figure C5: Corrected figure comparing the performance of GNN and hybrid models and COSMO-RS. Corresponding to Figure 8 of the original manuscript.

References

[1] Thomas Brouwer and Boelo Schuur. "Erratum for "Model performances evaluated for infinite dilution activity coefficients prediction at 298.15 K"". In: *Industrial & Engineering Chemistry Research* 62.14 (2023), pp. 6016–6017.

[2] Thomas Brouwer and Boelo Schuur. "Model performances evaluated for infinite dilution activity coefficients prediction at 298.15 K". In: *Industrial & Engineering Chemistry Research* 58.20 (2019), pp. 8903–8914.