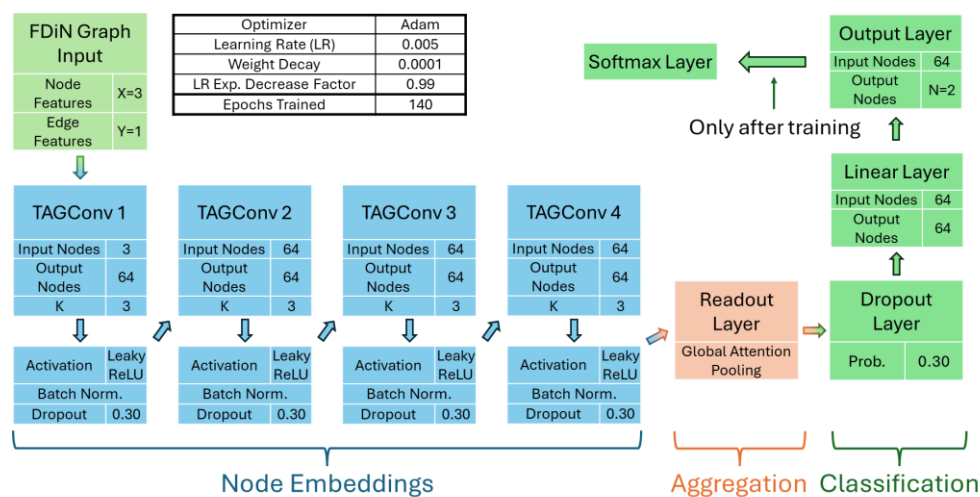
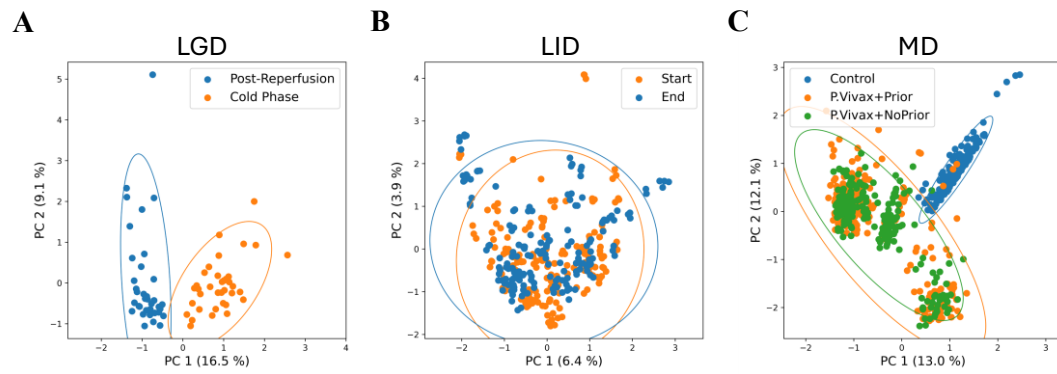


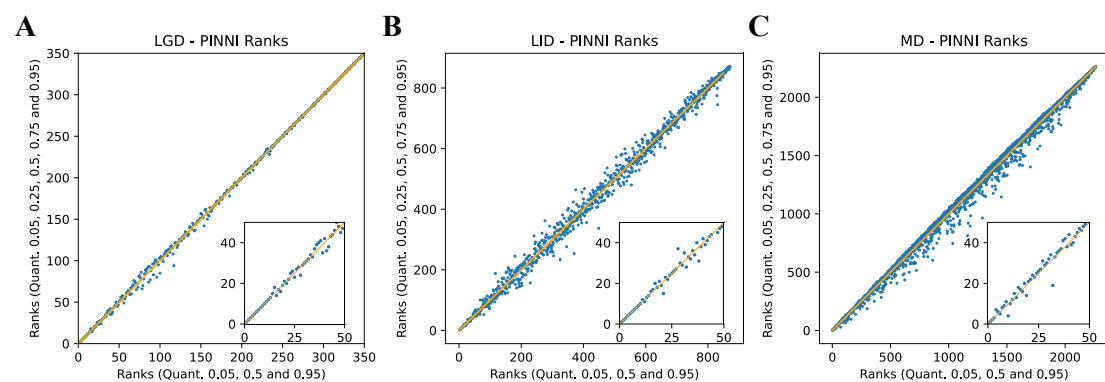
Supplementary Figures



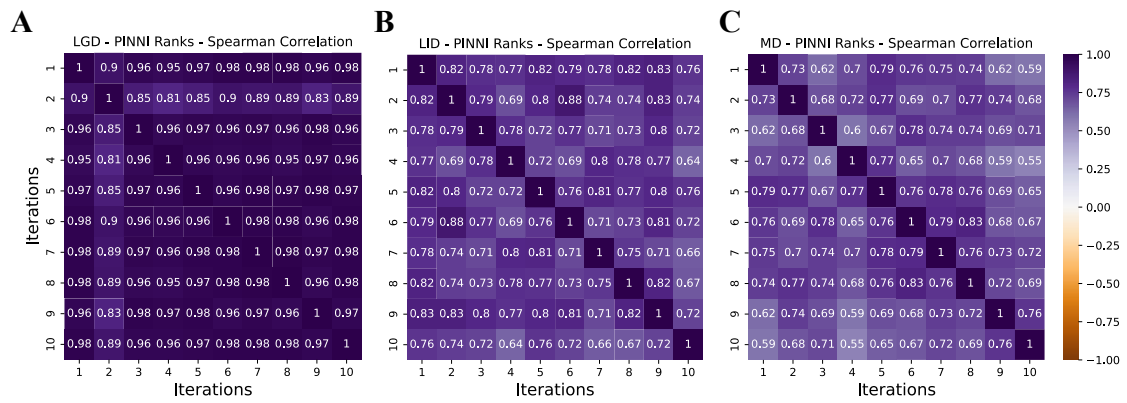
Supplementary Figure 1: Diagram of the FDiGNN architecture used for LGD. X and Y represent the number of node and edge features of the input while N is the number of dataset classes. Abbreviations: ReLU: Rectified Linear Unit; Exp.: Exponential.



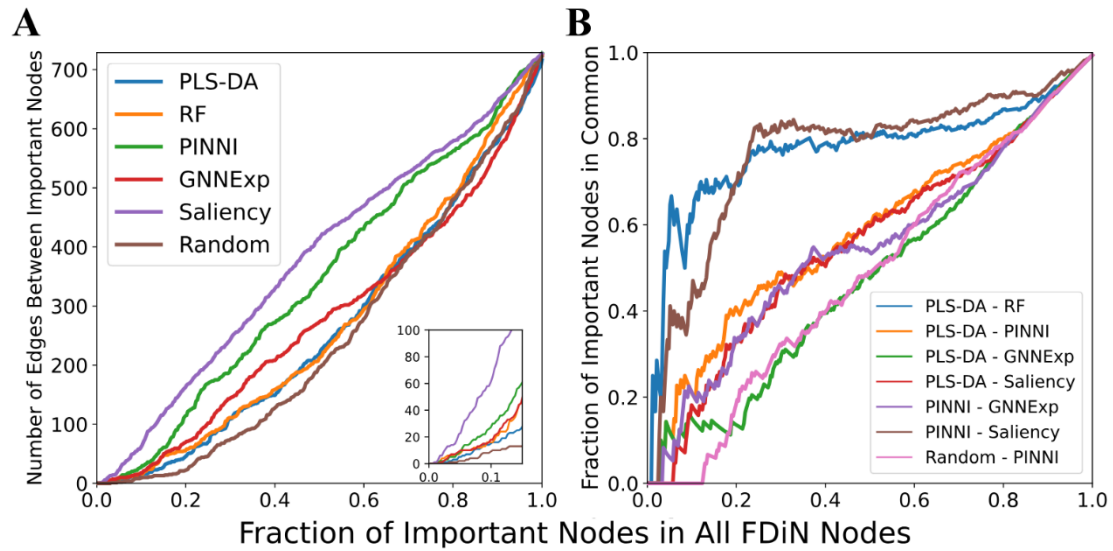
Supplementary Figure 2: Sample projection of the first two components of Principal Component Analysis. PCA of **A)** LGD, **B)** LID and **C)** MD. Ellipses drawn for each class in each PCA correspond to the confidence interval at 95%. Number in parenthesis in the axis titles represent the percentage of variance explained by the corresponding component. PC – Principal Components.



Supplementary Figure 3: Comparison between PINNI ranks obtained from allowing choices over 5 quantiles (0.05, 0.25, 0.50, 0.75 and 0.95) and over 3 quantiles (0.05, 0.50 and 0.95). Orange line shows case where equal ranks are obtained in both cases. Insets on the lower right are a zoom on the first section of the plot.

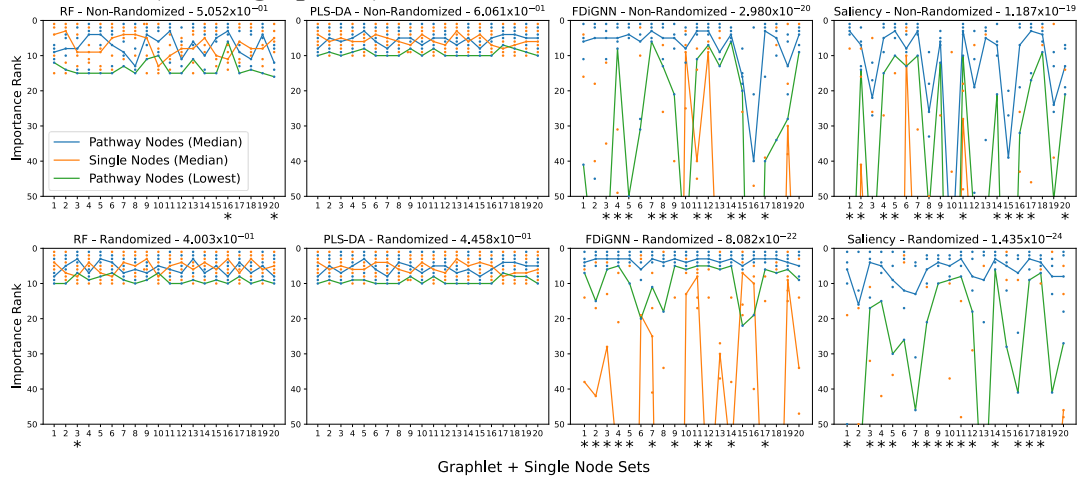


Supplementary Figure 4: Spearman Correlation between PINNI rankings over 10 FDiGNN model fitting iterations.

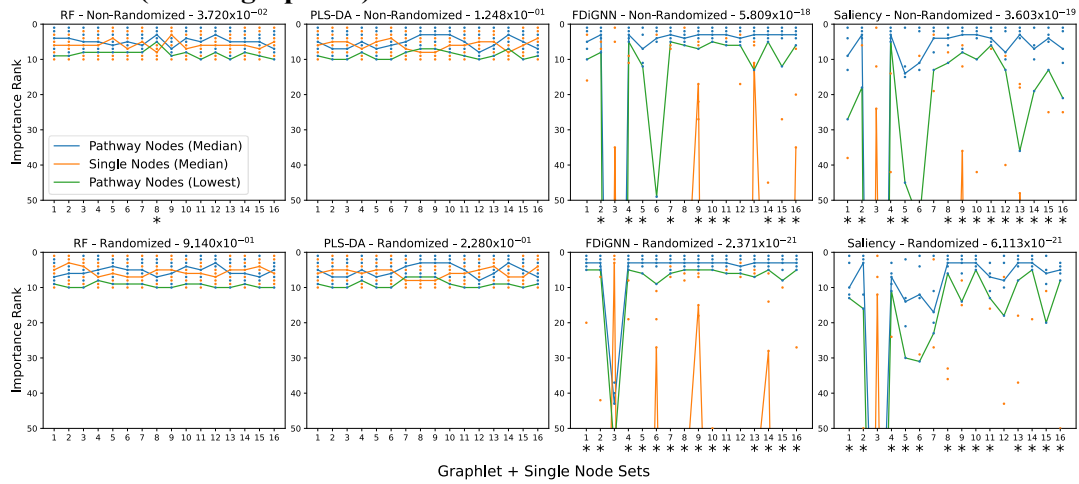


Supplementary Figure 5: Comparing important nodes through Gini importance for RF, VIP scores for PLS-DA, and PINNI, GNNExplainer and Saliency for FDiGNN models, on the LGD dataset, with FDiN constructed without pathway knowledge. A) Number of FDiN edges established between topmost important nodes. Insets are a zoom on the first section of the plot. **B)** Fraction of important nodes in common between models. *Random* is a randomly ordered list of nodes and represents the background of the comparison.

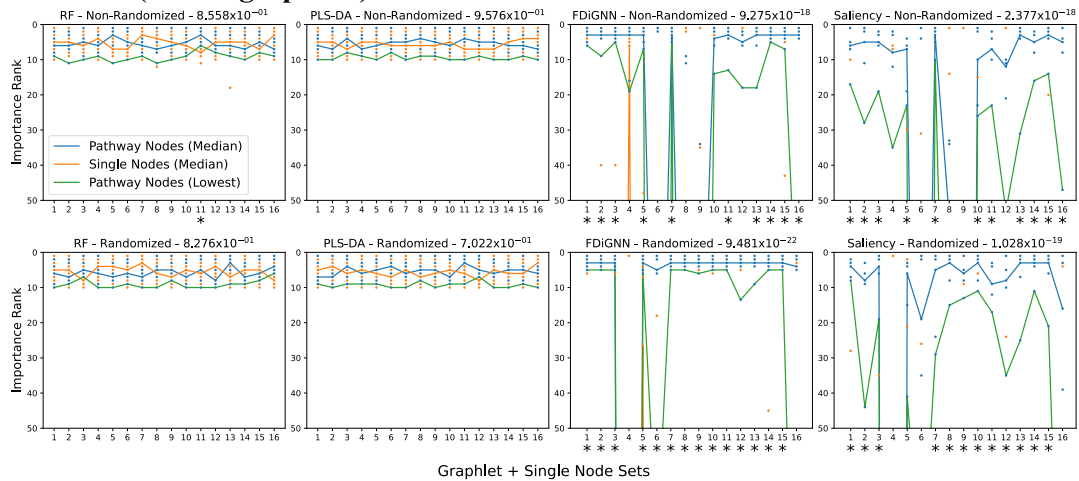
A – LGD (5 node graphlets)



B – LID (5 node graphlets)

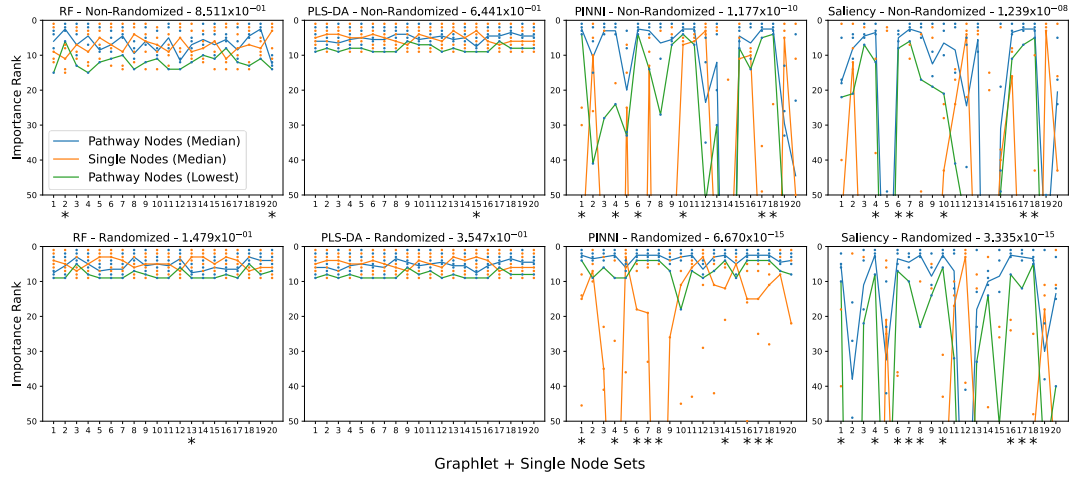


C – MD (5 node graphlets)



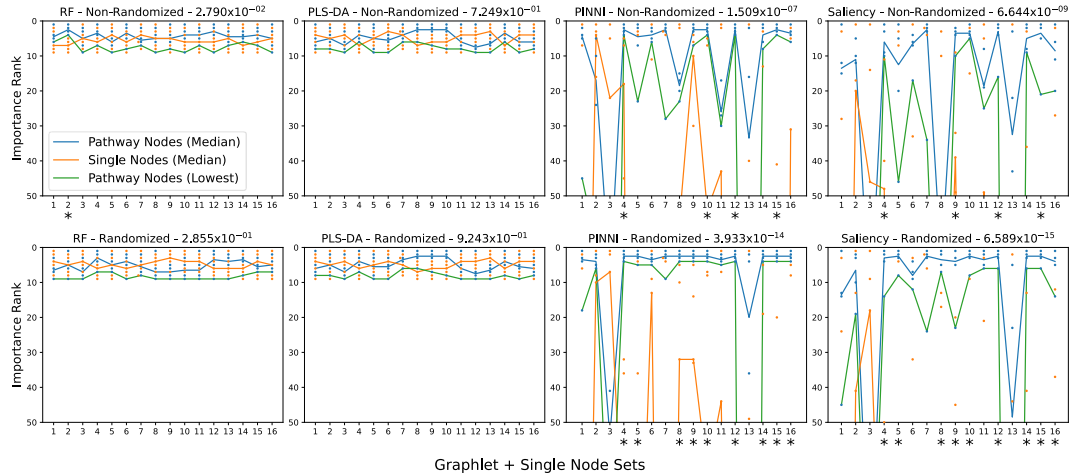
Supplementary Figure 6: Node Importance ranks of pathway and single nodes from Gini importance of RF, VIP scores of PLS-DA and PINNI score and Saliency from FDIINN models in 5-node graphlet simulations. Results are shown for the A) LGD, B) LID and C) MD benchmarks. In each 5-node graphlet simulation, a random 5-length graphlet is randomly selected, representing pathway nodes, and 5 nodes with no connection to each other or the graphlet are also selected as single nodes. Chart titles include the Mann-Whitney test p -value considering all ranks of the pathway nodes and of the single nodes across all simulations in that chart. Dots show the individual ranks of the selected nodes in each simulation with the blue line connecting the medians of the pathway node ranks in each simulation, the orange line the medians of the single nodes and the green line the worst-case ranked pathway node. Simulations have a * symbol below them if there is a significant difference (p -value below 0.05) between the ranks of pathway and single nodes (Mann-Whitney test). Only the top 50 ranks in each case are shown.

A – LGD (4 node graphlets)



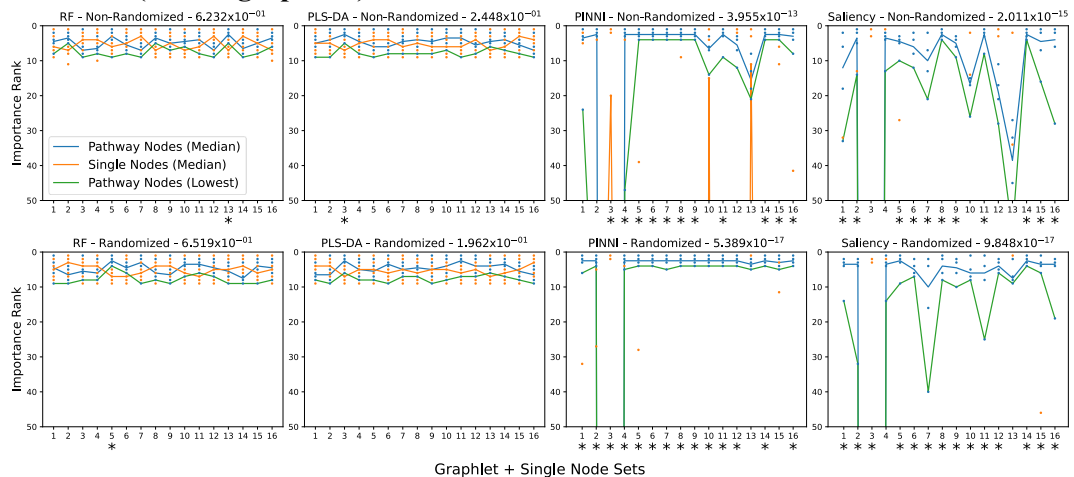
Graphlet + Single Node Sets

B – LID (4 node graphlets)



Graphlet + Single Node Sets

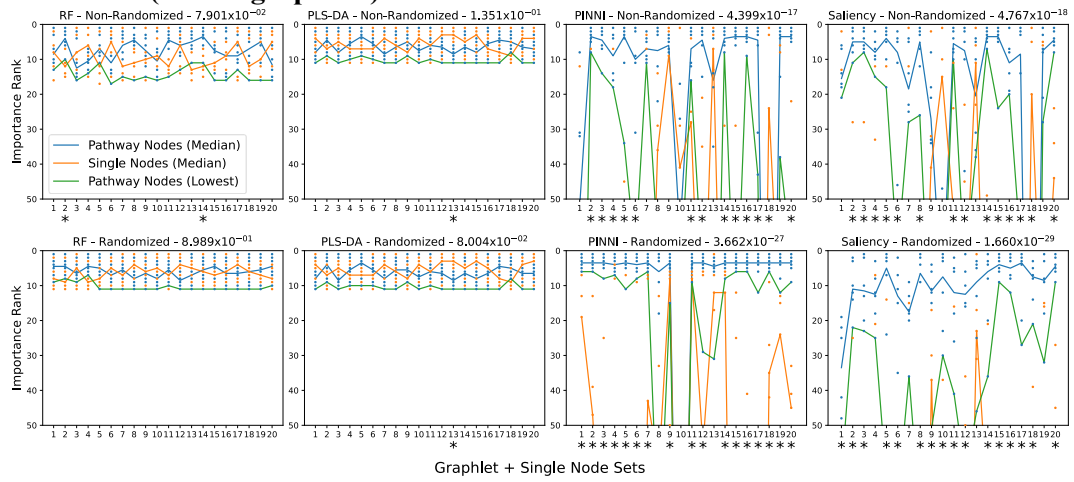
C – MD (4 node graphlets)



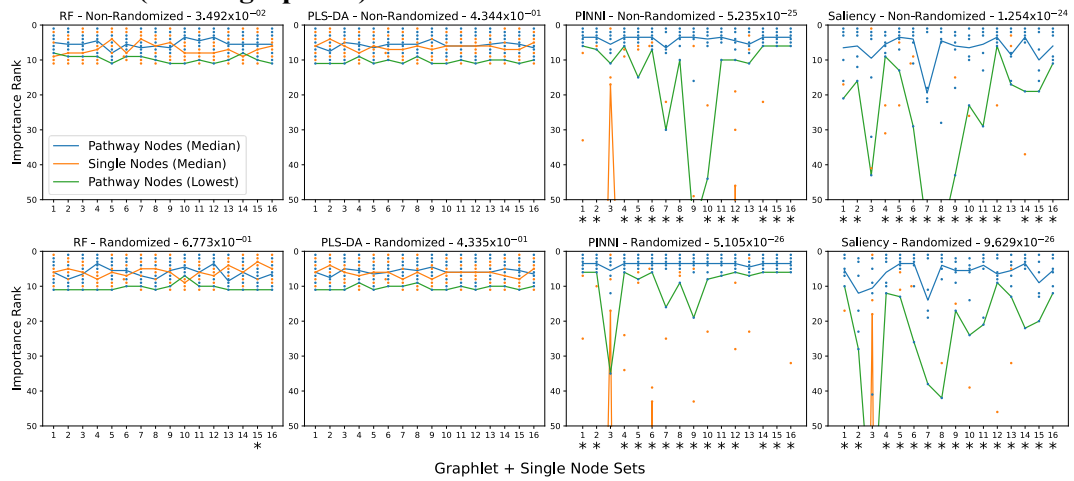
Graphlet + Single Node Sets

Supplementary Figure 7: Node Importance ranks of pathway and single nodes from Gini importance of RF, VIP scores of PLS-DA and PINNI score and Saliency from FDiGNN models in 4-node graphlet simulations. Results are shown for the A) LGD, B) LID and C) MD benchmarks. In each 4-node graphlet simulation, a random 4-length graphlet is randomly selected, representing pathway nodes, and 5 nodes with no connection to each other or the graphlet are also selected as single nodes. Chart titles include the Mann-Whitney test p -value considering all ranks of the pathway nodes and of the single nodes across all simulations in that chart. Dots show the individual ranks of the selected nodes in each simulation with the blue line connecting the medians of the pathway node ranks in each simulation, the orange line the medians of the single nodes and the green line the worst-case ranked pathway node. Simulations have a * symbol below them if there is a significant difference (p -value below 0.05) between the ranks of pathway and single nodes (Mann-Whitney test). Only the top 50 ranks in each case are shown.

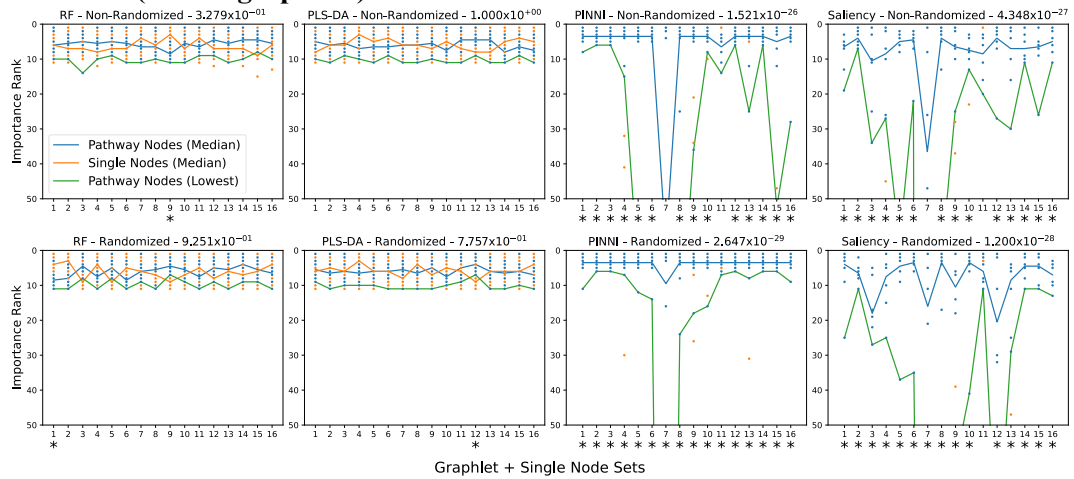
A – LGD (6 node graphlets)



B – LID (6 node graphlets)

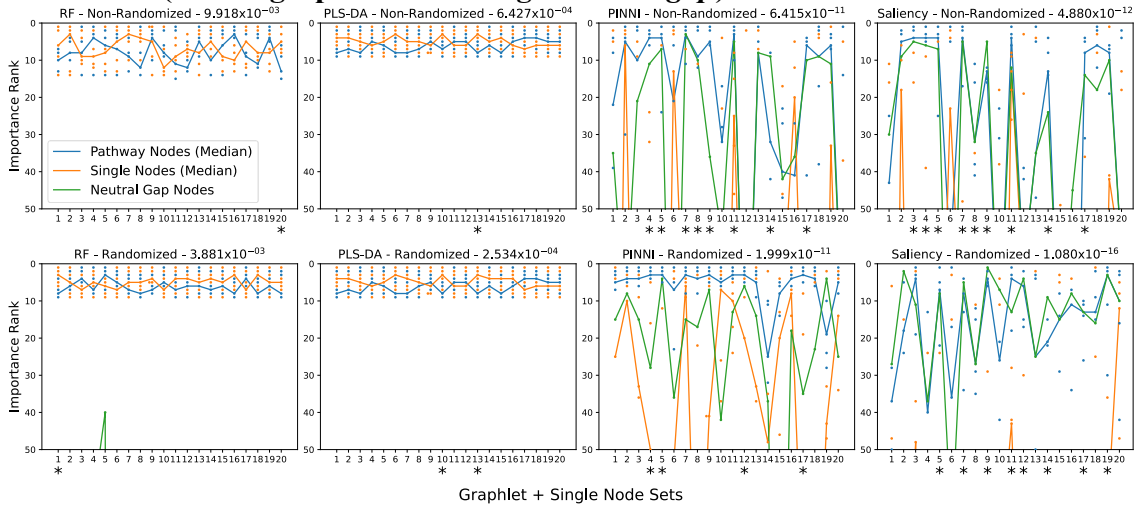


C – MD (6 node graphlets)

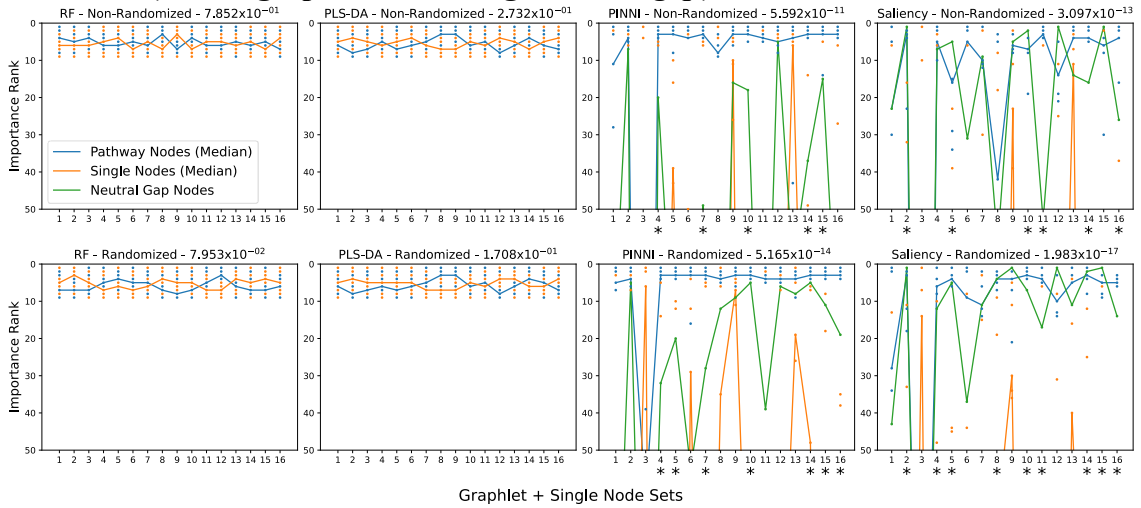


Supplementary Figure 8: Node Importance ranks of pathway and single nodes from Gini importance of RF, VIP scores of PLS-DA and PINNI score and Saliency from FdGNN models in 6-node graphlet simulations. Results are shown for the A) LGD, B) LID and C) MD benchmarks. In each 6-node graphlet simulation, a random 6-length graphlet is randomly selected, representing pathway nodes, and 5 nodes with no connection to each other or the graphlet are also selected as single nodes. Chart titles include the Mann-Whitney test p -value considering all ranks of the pathway nodes and of the single nodes across all simulations in that chart. Dots show the individual ranks of the selected nodes in each simulation with the blue line connecting the medians of the pathway node ranks in each simulation, the orange line the medians of the single nodes and the green line the worst-case ranked pathway node. Simulations have a * symbol below them if there is a significant difference (p -value below 0.05) between the ranks of pathway and single nodes (Mann-Whitney test). Only the top 50 ranks in each case are shown.

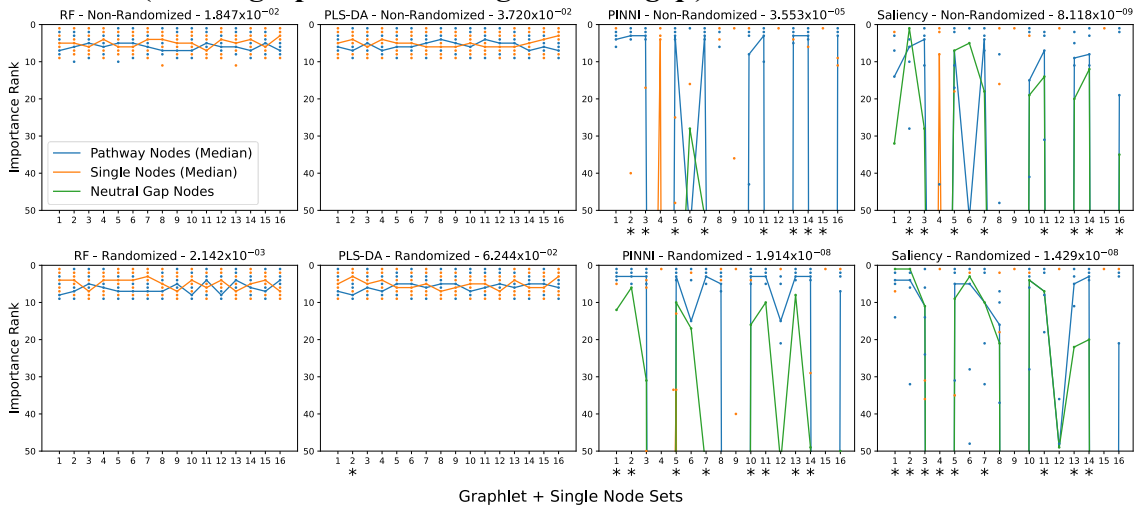
A – LGD (5 node graphlets including a *neutral gap*)



B – LID (5 node graphlets including a *neutral gap*)



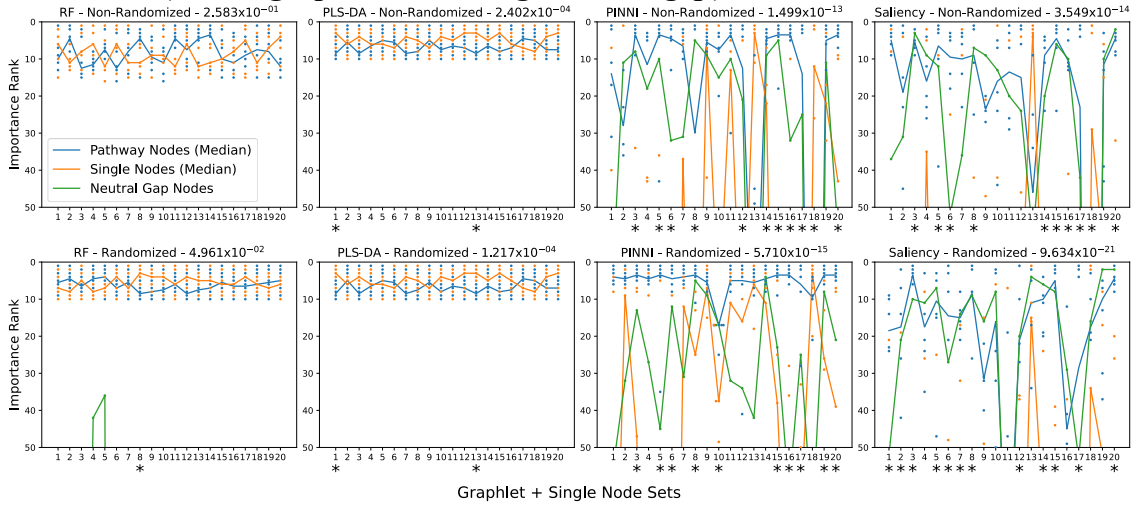
C – MD (5 node graphlets including a *neutral gap*)



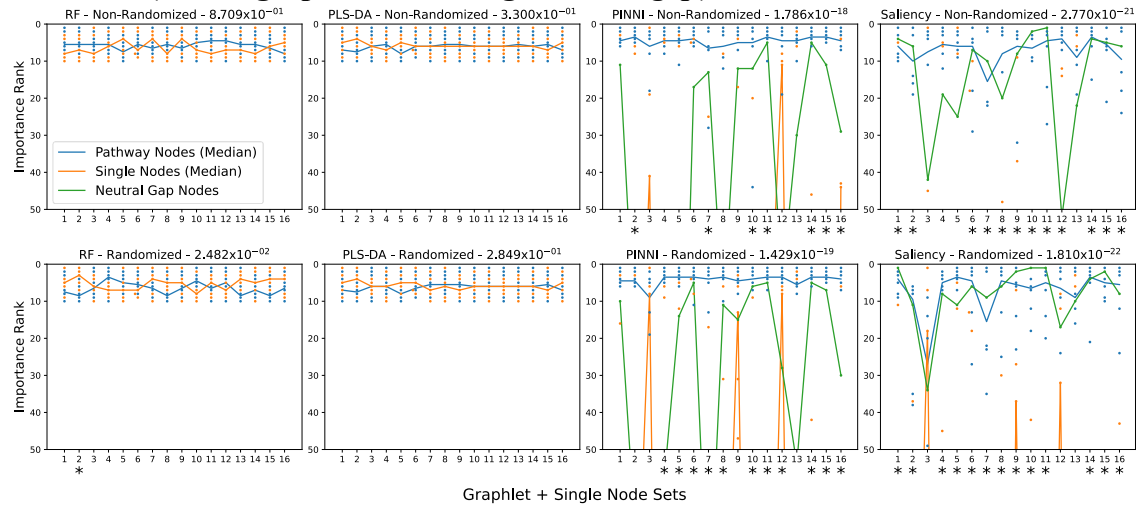
Supplementary Figure 9: Node Importance ranks of pathway, single, and *neutral gap* nodes from Gini importance of RF, VIP scores of PLS-DA and PINNI score and Saliency from FDIGNN models in 5-node graphlet including a *neutral gap* simulations. Results are shown for the **A) LGD, B) LID and C) MD** benchmarks. In each 5-node graphlet including a *neutral gap* simulation, a random 5-length graphlet is randomly selected, representing pathway nodes, and 5 nodes with no connection to each other or the graphlet are also selected as single nodes. The *neutral gap* is a graphlet node with the highest degree assigned with intensities with intermediate random values between

all samples. Chart titles include the Mann-Whitney test p -value considering all ranks of the pathway nodes (including the *neutral gap*) and of the single nodes across all simulations in that chart. Dots show the individual ranks of the selected nodes in each simulation performed with the blue line connecting each simulation medians of the pathway node ranks, the orange line the medians of the single nodes and the green line the ranks of the *neutral gaps*. Simulations have a * symbol below them if there is a significant difference (p -value below 0.05) between the ranks of pathway (including the *neutral gap*) and single nodes (Mann-Whitney test). Only the top 50 ranks in each case are shown.

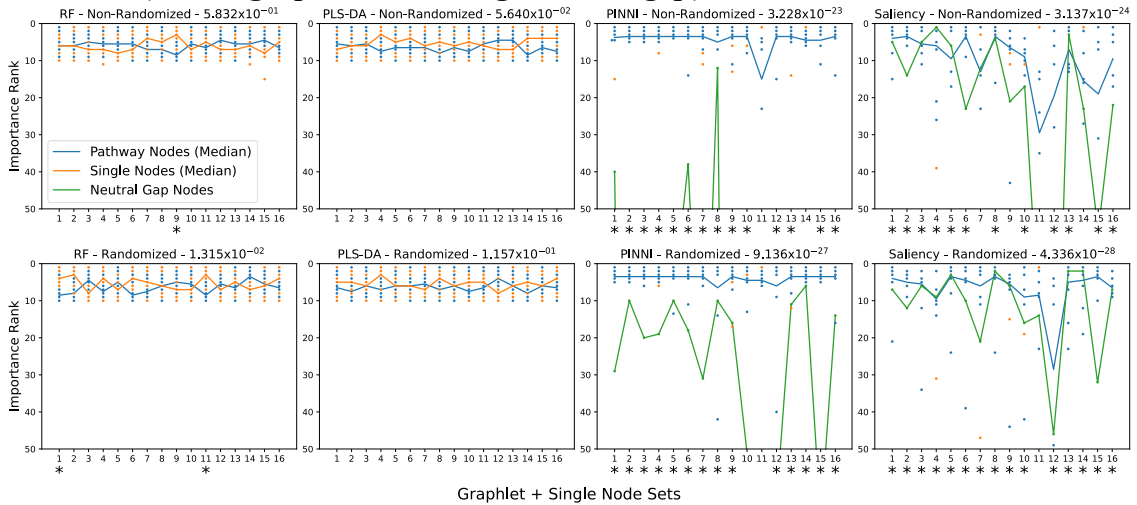
A – LGD (6 node graphlets including a *neutral gap*)



B – LID (6 node graphlets including a *pinball* gap)



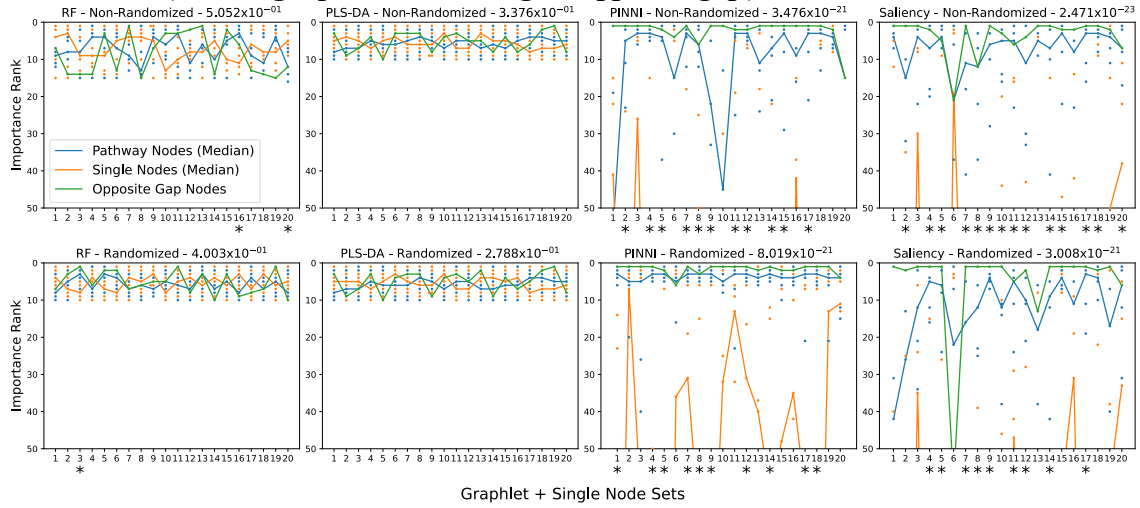
C – MD (6 node graphlets including a *neutral gap*)



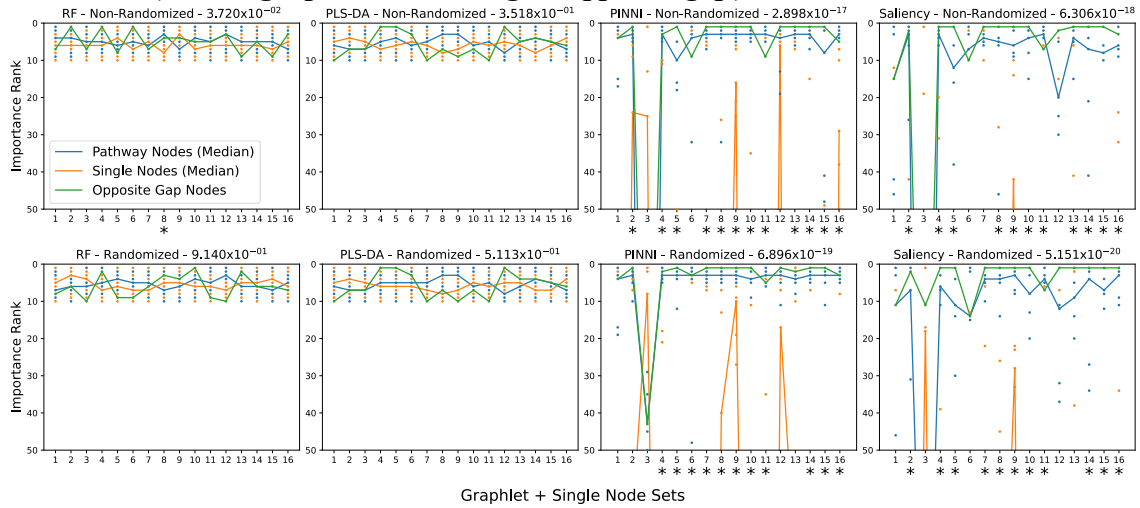
Supplementary Figure 10: Node Importance ranks of pathway, and single, and *neutral gap* nodes from Gini importance of RF, VIP scores of PLS-DA and PINNI score and Saliency from FDiGNN models in 6-node graphlet including a *neutral gap* simulations. Results are shown for the A) LGD, B) LID and C) MD benchmarks. In each 6-node graphlet including a *neutral gap* simulation, a random 6-length graphlet is randomly selected, representing pathway nodes, and 5 nodes with no connection to each other or the graphlet are also selected as single nodes. The *neutral gap* is a graphlet node with the highest degree assigned with intensities with intermediate random values between

all samples. Chart titles include the Mann-Whitney test p -value considering all ranks of the pathway nodes (including the *neutral gap*) and of the single nodes across all simulations in that chart. Dots show the individual ranks of the selected nodes in each simulation performed with the blue line connecting each simulation medians of the pathway node ranks, the orange line the medians of the single nodes and the green line the ranks of the *neutral gaps*. Simulations have a * symbol below them if there is a significant difference (p -value below 0.05) between the ranks of pathway (including the *neutral gap*) and single nodes (Mann-Whitney test). Only the top 50 ranks in each case are shown.

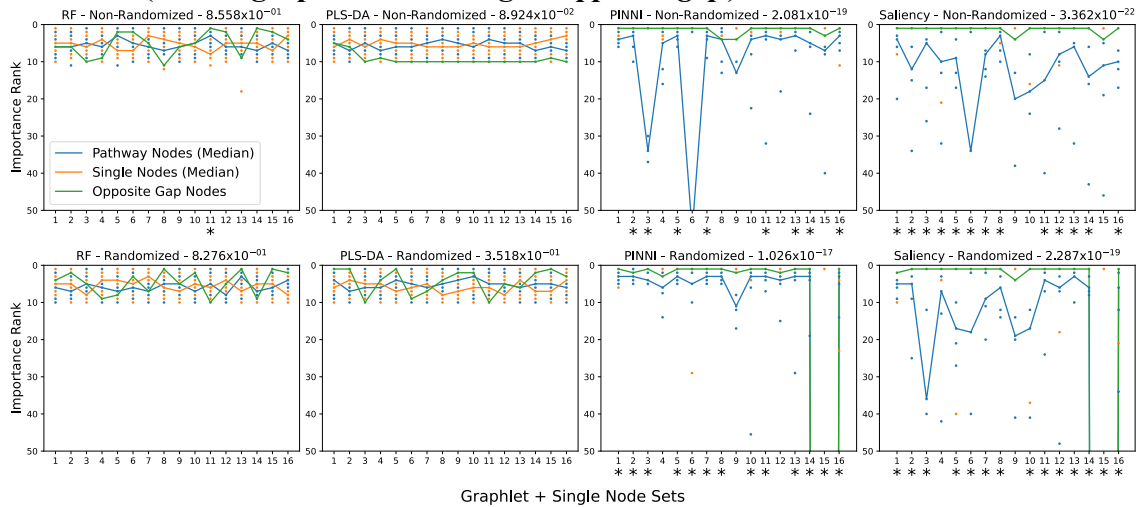
A – LGD (5 node graphlets including an *opposite gap*)



B – LID (5 node graphlets including an *opposite gap*)



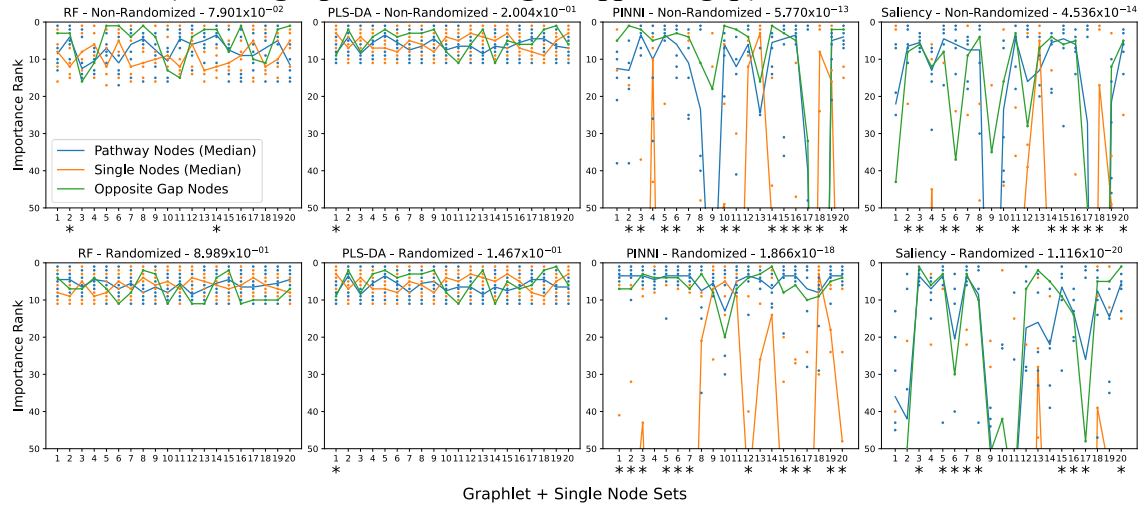
C – MD (5 node graphlets including an *opposite gap*)



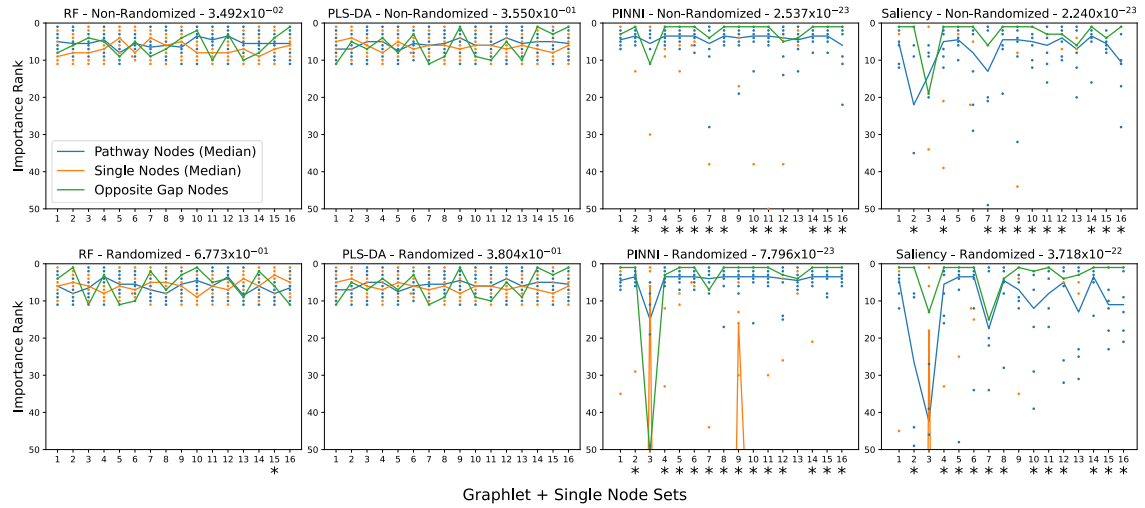
Supplementary Figure 11: Node Importance ranks of pathway, and single, and *opposite gap* nodes from Gini importance of RF, VIP scores of PLS-DA and PINNI score and Saliency from FDIGNN models in 5-node graphlet including an *opposite gap* simulations. Results are shown for the **A) LGD, B) LID and C) MD** benchmarks. In each 5-node graphlet including an *opposite gap* simulation, a random 5-length graphlet is randomly selected, representing pathway nodes, and 5 nodes with no connection to each other or the graphlet are also selected as single nodes. The *opposite gap* is a graphlet node with the highest degree assigned with either high or low intensities across the samples

to have an opposite relationship of intensities to the remaining pathway nodes. Chart titles include the Mann-Whitney test p -value considering all ranks of the pathway nodes (including the *opposite gap*) and of the single nodes across all simulations in that chart. Dots show the individual ranks of the selected nodes in each simulation performed with the blue line connecting each simulation medians of the pathway node ranks, the orange line the medians of the single nodes and the green line the ranks of the *opposite gaps*. Simulations have a * symbol below them if there is a significant difference (p -value below 0.05) between the ranks of pathway (including the *opposite gap*) and single nodes (Mann-Whitney test). Only the top 50 ranks in each case are shown.

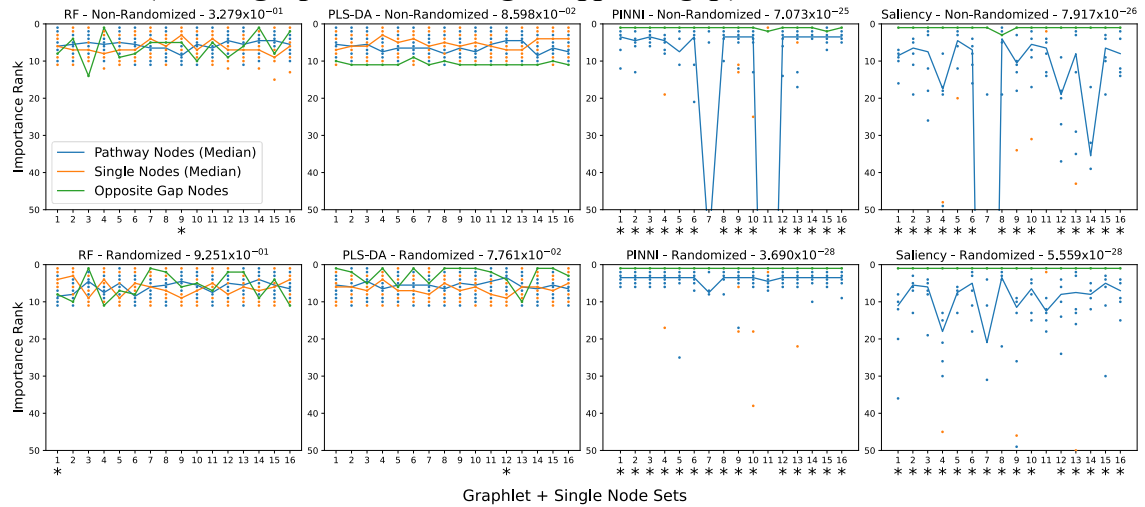
A – LGD (6 node graphlets including an *opposite gap*)



B – LID (6 node graphlets including an *opposite gap*)

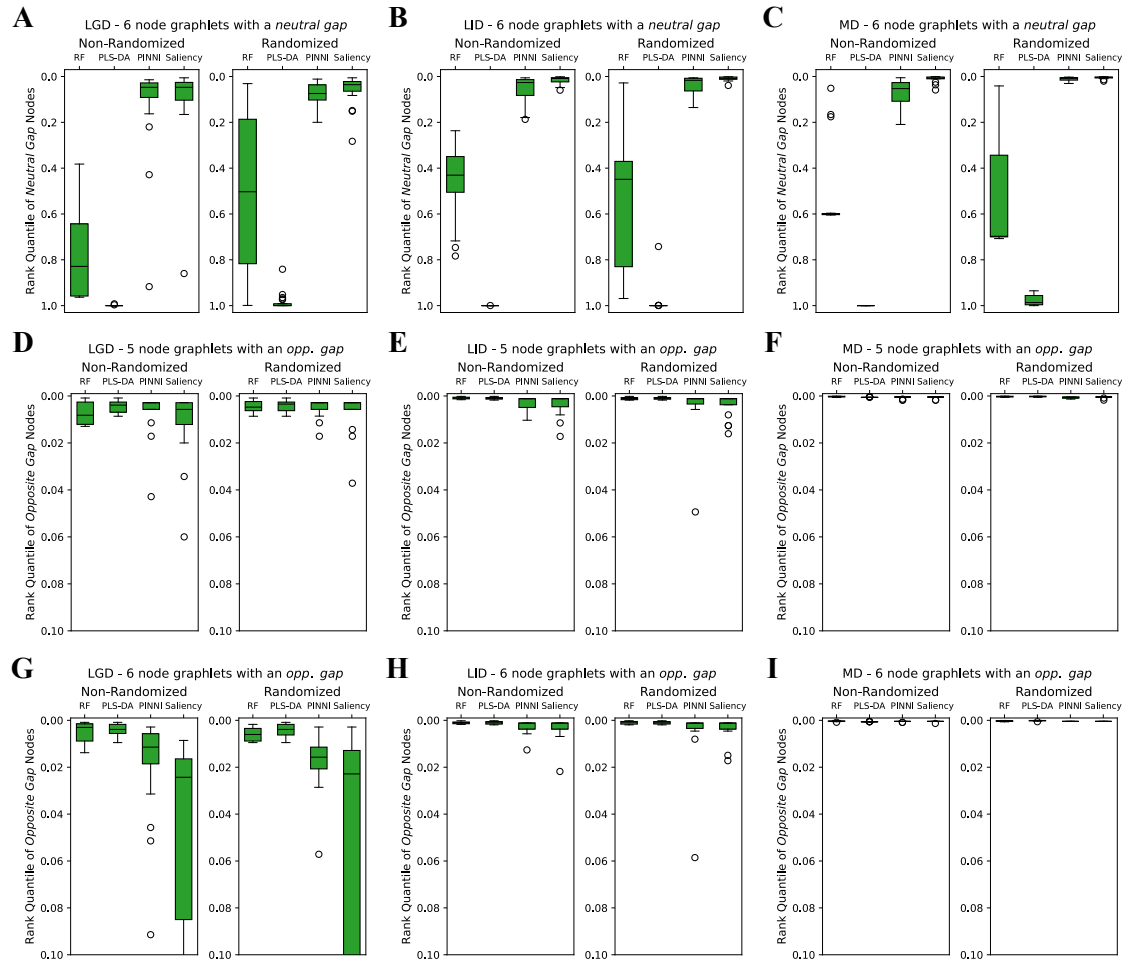


C – MD (6 node graphlets including an *opposite gap*)



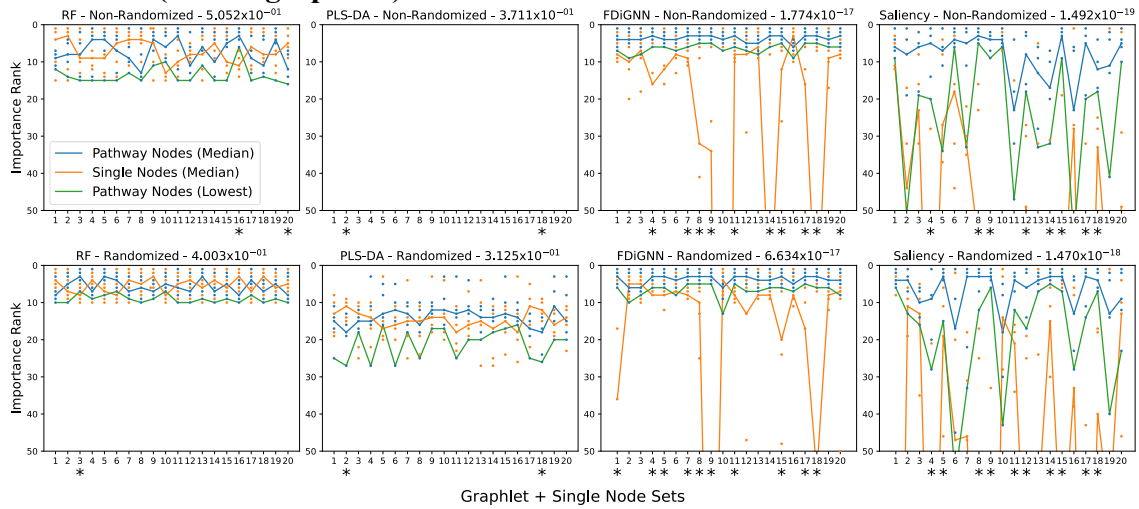
Supplementary Figure 12: Node Importance ranks of pathway, and single, and *opposite gap* nodes from Gini importance of RF, VIP scores of PLS-DA and PINNI score and Saliency from FDIGNN models in 6-node graphlet including an *opposite gap* simulations. Results are shown for the **A) LGD, B) LID and C) MD** benchmarks. In each 6-node graphlet including an *opposite gap* simulation, a random 6-length graphlet is randomly selected, representing pathway nodes, and 5 nodes with no connection to each other or the graphlet are also selected as single nodes. The *opposite gap* is a graphlet node with the highest degree assigned with either high or low intensities across the samples

to have an opposite relationship of intensities to the remaining pathway nodes. Chart titles include the Mann-Whitney test p -value considering all ranks of the pathway nodes (including the *opposite gap*) and of the single nodes across all simulations in that chart. Dots show the individual ranks of the selected nodes in each simulation performed with the blue line connecting each simulation medians of the pathway node ranks, the orange line the medians of the single nodes and the green line the ranks of the *opposite gaps*. Simulations have a * symbol below them if there is a significant difference (p -value below 0.05) between the ranks of pathway (including the *opposite gap*) and single nodes (Mann-Whitney test). Only the top 50 ranks in each case are shown.

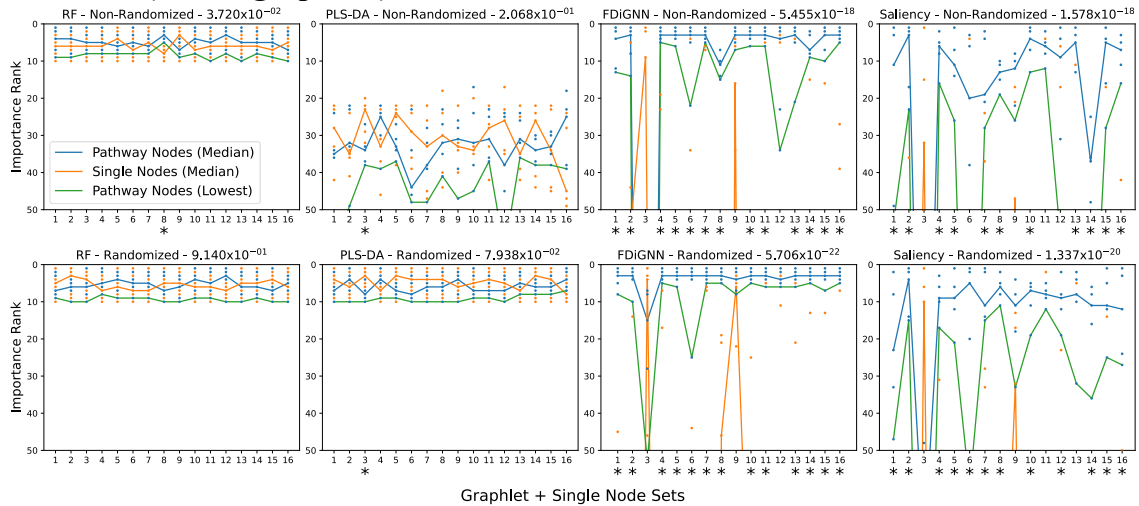


Supplementary Figure 13: Distribution of the rank quantiles of the *neutral* or *opposite gap* nodes in each simulation, according to the four importance rankings. 6-node graphlets with a *neutral gap* results are shown for **A)** LGD, **B)** LID and **C)** MD benchmarks. 5-node graphlets with an *opposite gap* results are shown for **D)** LGD, **E)** LID and **F)** MD benchmarks. 6-node graphlets with an *opposite gap* results are shown for **G)** LGD, **H)** LID and **I)** MD benchmarks. The *neutral gap* or *opposite gap* (Opp. Gap) select one of the highest degree nodes in the selected 5- or 6-node graphlets to have intermediate values between all samples – the *neutral gap* – or to have the opposite relationship of intensities to the remaining pathway nodes – the *opposite gap*.

A – LGD (5 node graphlets) – Lower Effect Sizes



B – LID (5 node graphlets) – Lower Effect Sizes



Supplementary Figure 14: Node Importance ranks of pathway and single nodes from Gini importance of RF, VIP scores of PLS-DA and PINNI score and Saliency from FDiGNN models in 5-node graphlet simulations with mild effect sizes for pathway and single nodes. Results are shown for the **A)** LGD and **B)** LID benchmarks. In each 5-node graphlet simulation, a random 5-length graphlet is randomly selected, representing pathway nodes, and 5 nodes with no connection to each other or the graphlet are also selected as single nodes. Chart titles include the Mann-Whitney test p-value considering all ranks of the pathway nodes and of the single nodes across all simulations in that chart. Dots show the individual ranks of the selected nodes in each simulation with the blue line connecting the medians of the pathway node ranks in each simulation, the orange line the medians of the single nodes and the green line the worst-case ranked pathway node. Simulations have a * symbol below them if there is a significant difference (p-value below 0.05) between the ranks of pathway and single nodes (Mann-Whitney test). Only the top 50 ranks in each case are shown.

Supplementary Tables

Supplementary Table 1: General characteristics of the benchmark datasets after pre-processing and treatment.
Abbreviations: P.vivax+Prior – Patients infected with *P. vivax* that had been infected in the past, P.vivax+NoPrior – Patients infected with *P. vivax* that had not been infected in the past (Control are not infected samples). * – The MD dataset illustrates what to expect when formulas are assigned in a much less accurate way and is here deployed to show what our approach can still do with mainstream, less performing mass spectrometers when benchmarking for molecular formula assignment from spectral data alone.

Dataset	Samples	Features	Features/ Sample (Range)	Classes	Samples/Class	FDiN nodes	FDiN edges
LGD	72	1159	1066 (530 – 1141)	2	36	350	799
LID	354	5700	2117 (1782 – 2720)	2	177	871	1676
MD*	627	17087	5168 (2334 – 6649)	3	237 'P.vivax+Prior', 213 'P.vivax+NoPrior', 177 'Control'	2264	5404

Supplementary Table 2: List of chemical elemental transformations used to build the FDiNs.

Elemental Transformations	Reaction Type Examples
O (-NH)	Deamination
NH₃ (-O)	Transamination
H₂	Hydrogenation / Dehydrogenation
CH₂	Methylation
O	Oxygenation / Hydroxylation
H₂O	Condensation / Dehydration / Cyclization
NCH	Transfer of a formidoyl group
CO	Formylation
CHOH	Hydroxymethylation
S	Transfer of a -SH group
C₂H₂O	Acetylation
CONH	Transfer of a carbamoyl group
CO₂	Carboxylation / Decarboxylation
SO₃	Sulphation
PO₃H	Phosphorylation

Supplementary Table 3: Characteristics of the FDiGNN models for the different datasets. Other details not shown are identical among all datasets and shown in **Sup. Figure 2**.

Datasets	LGD	LID	MD
Number of Parameters in FDiGNN	55 043	30 083	55 108
TAG layers			
Number	4	4	4
Hidden Channels	64	64	64
K	3	1	3
Other layers			
Dropout Probability	0.30	0.15	0.30
Leaky ReLU Activation between classifier layers	No	No	Yes
Training Parameters			
Optimizer	Adam	Adam	Adam
Learning Rate (LR)	0.005	0.005	0.001
Weight Decay	0.0001	0.0001	0.0001
LR Exp. Decrease Factor	0.99	0.99	0.99
Epochs Trained	140	160	500

Supplementary Table 4: Distribution of quantile choices for PINNI maximum effect perturbations. Comparison is made between a five-quantile set and a three-quantile set.

Dataset	Quantiles	5-quantile set		3-quantile set	
		Number	Percentage	Number	Percentage
LGD	0.05	14577	57.85	15151	60.12
	0.25	909	3.61		
	0.50	413	1.64	1537	6.10
	0.75	1552	6.16		
	0.95	7749	30.75	8512	33.78
LID	0.05	164264	53.27	173187	56.17
	0.25	12785	4.15	-	-
	0.50	10245	3.32	19693	6.39
	0.75	16762	5.44		
	0.95	104278	33.82	115454	37.44
MD	0.05	110291	25.78	124978	29.21
	0.25	18613	4.35		
	0.50	17952	4.20	34678	8.10
	0.75	40170	9.39		
	0.95	240870	56.29	268240	62.69

Supplementary Table 5: Spearman Correlation between PINNI rankings of the 16 or 20 simulations to the closeness centrality of the corresponding nodes in the dataset's FDiN considering all nodes, only the pathway nodes or the single nodes for each set within each simulation. Original is the original model with no modification. E.g. for the 5-Graphlet Simulation on the LGD, 20 sets of graphlets were used. Therefore, all 20 sets of ranks were used to calculate the correlation. Lowest correlation (closer to 0) is in bold for each case.

Dataset	Simulation	Changes	All Nodes	Pathway Nodes	Single Nodes
LGD	Original		-0.807	-	-
	5-Graphlet	Non-Randomized	-0.637	-0.192	-0.538
		Randomized	-0.464	-0.224	-0.524
	6-Graphlet	Non-Randomized	-0.617	-0.287	-0.498
		Randomized	-0.463	-0.306	-0.509
	4-Graphlet	Non-Randomized	-0.634	-0.250	-0.327
		Randomized	-0.435	-0.206	-0.168
	5-Graphlet with a <i>neutral gap</i>	Non-Randomized	-0.705	-0.334	-0.679
		Randomized	-0.426	-0.010	-0.420
	6-Graphlet with a <i>neutral gap</i>	Non-Randomized	-0.624	-0.125	-0.500
		Randomized	-0.452	-0.255	-0.471
	5-Graphlet with an <i>opposite gap</i>	Non-Randomized	-0.653	-0.145	-0.489
		Randomized	-0.494	-0.195	-0.485
LID	5-Graphlet	Non-Randomized	-0.356	-0.095	-0.426
		Randomized	-0.390	-0.111	-0.408
	6-Graphlet	Non-Randomized	-0.360	-0.107	-0.414
		Randomized	-0.371	-0.109	-0.347
	4-Graphlet	Non-Randomized	-0.327	-0.310	-0.323
		Randomized	-0.265	-0.064	-0.251
	5-Graphlet with a <i>neutral gap</i>	Non-Randomized	-0.403	-0.058	-0.383
		Randomized	-0.325	0.030	-0.334
	6-Graphlet with a <i>neutral gap</i>	Non-Randomized	-0.321	-0.034	-0.400
		Randomized	-0.383	-0.013	-0.413
	5-Graphlet with an <i>opposite gap</i>	Non-Randomized	-0.372	-0.112	-0.303
		Randomized	-0.345	-0.007	-0.373
MD	5-Graphlet	Non-Randomized	-0.148	0.213	-0.047
		Randomized	-0.208	-0.053	-0.201
	6-Graphlet	Non-Randomized	-0.165	-0.090	-0.142
		Randomized	-0.165	-0.073	-0.226
	4-Graphlet	Non-Randomized	-0.163	0.128	-0.133
		Randomized	-0.172	0.024	-0.163
	5-Graphlet with a <i>neutral gap</i>	Non-Randomized	-0.194	-0.009	-0.157
		Randomized	-0.211	-0.096	-0.159
	6-Graphlet with a <i>neutral gap</i>	Non-Randomized	-0.188	-0.126	-0.033
		Randomized	-0.186	-0.126	-0.111
	5-Graphlet with an <i>opposite gap</i>	Non-Randomized	-0.173	-0.164	-0.132
		Randomized	-0.230	-0.172	-0.256
	6-Graphlet with an <i>opposite gap</i>	Non-Randomized	-0.154	-0.034	-0.227
		Randomized	-0.151	0.027	-0.056

Supplementary Table 6: Top 11 most significant pathways from Pathway Enrichment Analysis on LID considering the top 5% of FDiGNN ranked nodes as significant. Methodology explained in the Methods. Pathway database used was SMPDB. Abbreviations: Met. – Metabolites, BH – Benjamini-Hochberg multiple test correction.

Rank	Pathway	Nr. Metabolites Ranks	Nr. Metabolites Dataset	Probability	Adjusted (BH) Probability
1	Arginine and Proline Metabolism	8	8	0.000011	0.000339
2	Purine Metabolism	7	7	0.000052	0.000786
3	Histidine Metabolism	6	6	0.000235	0.002346
4	Tryptophan Metabolism	4	4	0.004269	0.013435
5	Urea Cycle	4	4	0.004269	0.013435
6	Nicotinate and Nicotinamide Metabolism	4	4	0.004269	0.013435
7	Aspartate Metabolism	4	4	0.004269	0.013435
8	Glutathione Metabolism	4	4	0.004269	0.013435
9	Ammonia Recycling	4	4	0.004269	0.013435
10	Glycine and Serine Metabolism	5	6	0.004926	0.013435
11	Glutamate Metabolism	5	6	0.004926	0.013435

Supplementary Table 7: Top 5 most significant pathways from Pathway Enrichment Analysis on MD considering the top 25% of FDiGNN ranked nodes as significant. Methodology explained in the Methods. Pathway database used was SMPDB. Abbreviations: Met. – Metabolites, BH – Benjamini-Hochberg multiple test correction.

Rank	Pathway	Nr. Metabolites Ranks	Nr. Metabolites Dataset	Probability	Adjusted (BH) Probability
1	Histidine Metabolism	4	5	0.0031	0.0769
2	Fructose and Mannose Degradation	3	3	0.0045	0.0769
3	Tyrosine Metabolism	4	6	0.0083	0.0937
4	Estrone Metabolism	3	4	0.0159	0.1354
5	Alpha Linolenic Acid and Linoleic Acid Metabolism	4	10	0.0684	0.2536

Supplementary Table 8: Top 20 most over-represented pathways using sets of most important metabolites ranked by PINNI or VIP scores or Gini importance. Fractions of important metabolites were 10% for LGD and 5% for LID and 25% for MD.

Pathway	# dataset / # pathway	p-value	Adjusted (BH)	Impact
<i>LGD PINNI</i>				
Pyruvate Metabolism	4 / 5	0.01244	0.23168	0.88725
Citric Acid Cycle	4 / 5	0.01244	0.23168	0.99543
Glutamate Metabolism	6 / 11	0.02376	0.23168	0.61878
Arginine and Proline Metabolism	6 / 11	0.02376	0.23168	0.67943
D-Arginine and D-Ornithine Metabolism	3 / 4	0.04525	0.34223	0.83717
Propanoate Metabolism	4 / 7	0.06006	0.34223	0.65308
Spermidine and Spermine Biosynthesis	3 / 5	0.09447	0.34223	0.38010
Tryptophan Metabolism	3 / 5	0.09447	0.34223	0.40313
Glycine and Serine Metabolism	5 / 11	0.09572	0.34223	0.67549
Methionine Metabolism	5 / 11	0.09572	0.34223	0.61015
Warburg Effect	4 / 8	0.09975	0.34223	0.50142
Valine, Leucine, and Isoleucine Degradation	4 / 9	0.14915	0.34223	0.54303
Cysteine Metabolism	2 / 3	0.14985	0.34223	0.71874
Folate Metabolism	2 / 3	0.14985	0.34223	0.65483
Phenylacetate Metabolism	2 / 3	0.14985	0.34223	0.50704
Threonine and 2-Oxobutanoate Degradation	2 / 3	0.14985	0.34223	0.89689
Pantothenate and CoA Biosynthesis	2 / 3	0.14985	0.34223	0.70980
Urea Cycle	3 / 6	0.15795	0.34223	0.61155
Pyrimidine Metabolism	3 / 7	0.23137	0.43143	0.77033
Aspartate Metabolism	3 / 7	0.23137	0.43143	0.32597
<i>LGD VIP</i>				
Arginine and Proline Metabolism	4 / 11	0.03827	0.56052	0.46157
Threonine and 2-Oxobutanoate Degradation	2 / 3	0.04669	0.56052	0.91553
Ammonia Recycling	3 / 8	0.07189	0.56052	0.48824
Galactose Metabolism	2 / 4	0.08623	0.56052	0.55252
Transfer of Acetyl Groups into Mitochondria	2 / 4	0.08623	0.56052	0.69049
Fructose and Mannose Degradation	2 / 4	0.08623	0.56052	0.66630
Pyruvate Metabolism	2 / 5	0.13276	0.57529	0.65390
Citric Acid Cycle	2 / 5	0.13276	0.57529	0.74783
Glutathione Metabolism	2 / 5	0.13276	0.57529	0.54444
Glutamate Metabolism	3 / 11	0.16503	0.59798	0.38289
Urea Cycle	2 / 6	0.18399	0.59798	0.45917
Phenylalanine and Tyrosine Metabolism	2 / 6	0.18399	0.59798	0.16893

Propanoate Metabolism	2 / 7	0.23807	0.66090	0.47272
Tyrosine Metabolism	2 / 7	0.23807	0.66090	0.31746
Warburg Effect	2 / 8	0.29346	0.66090	0.37670
Histidine Metabolism	2 / 8	0.29346	0.66090	0.51400
Valine, Leucine, and Isoleucine Degradation	2 / 9	0.34895	0.66090	0.46594
Folate Metabolism	1 / 3	0.35587	0.66090	0.64894
Starch and Sucrose Metabolism	1 / 3	0.35587	0.66090	0.55239
Cysteine Metabolism	1 / 3	0.35587	0.66090	0.52878
<i>LGD Gini</i>				
Ammonia Recycling	4 / 8	0.01926	0.56070	0.60715
Nicotinate and Nicotinamide Metabolism	3 / 6	0.04734	0.56070	0.59890
Pyrimidine Metabolism	3 / 7	0.07486	0.56070	0.76479
Warburg Effect	3 / 8	0.10822	0.56070	0.50739
Galactose Metabolism	2 / 4	0.11502	0.56070	0.55252
Lysine Degradation	2 / 4	0.11502	0.56070	0.24699
Transfer of Acetyl Groups into Mitochondria	2 / 4	0.11502	0.56070	0.69049
Fructose and Mannose Degradation	2 / 4	0.11502	0.56070	0.66630
Pyruvate Metabolism	2 / 5	0.17423	0.61773	0.65390
Glutathione Metabolism	2 / 5	0.17423	0.61773	0.54444
Citric Acid Cycle	2 / 5	0.17423	0.61773	0.74783
Arginine and Proline Metabolism	3 / 11	0.23514	0.66210	0.47005
Urea Cycle	2 / 6	0.23768	0.66210	0.57230
Amino Sugar Metabolism	2 / 6	0.23768	0.66210	0.55628
Histidine Metabolism	2 / 8	0.36767	0.75289	0.51400
Threonine and 2-Oxobutanoate Degradation	1 / 3	0.40540	0.75289	0.81242
Phenylacetate Metabolism	1 / 3	0.40540	0.75289	0.49296
Folate Metabolism	1 / 3	0.40540	0.75289	0.64894
Starch and Sucrose Metabolism	1 / 3	0.40540	0.75289	0.55239
Cysteine Metabolism	1 / 3	0.40540	0.75289	0.52878
<i>LID PINNI</i>				
Arginine and Proline Metabolism	8 / 8	0.00001	0.00034	1.00000
Purine Metabolism	7 / 7	0.00005	0.00079	1.00000
Histidine Metabolism	6 / 6	0.00023	0.00235	1.00000
Tryptophan Metabolism	4 / 4	0.00427	0.01343	1.00000
Urea Cycle	4 / 4	0.00427	0.01343	1.00000
Nicotinate and Nicotinamide Metabolism	4 / 4	0.00427	0.01343	1.00000
Ammonia Recycling	4 / 4	0.00427	0.01343	1.00000
Aspartate Metabolism	4 / 4	0.00427	0.01343	1.00000
Glutathione Metabolism	4 / 4	0.00427	0.01343	1.00000
Glycine and Serine Metabolism	5 / 6	0.00493	0.01343	0.99999
Glutamate Metabolism	5 / 6	0.00493	0.01343	0.99999

Methionine Metabolism	3 / 4	0.05681	0.10653	0.99999
Bile Acid Biosynthesis	3 / 4	0.05681	0.10653	0.98911
Propanoate Metabolism	3 / 4	0.05681	0.10653	0.99999
Phenylalanine and Tyrosine Metabolism	3 / 4	0.05681	0.10653	0.99999
Valine, Leucine, and Isoleucine Degradation	3 / 4	0.05681	0.10653	0.99994
Tyrosine Metabolism	3 / 5	0.11611	0.20491	0.99982
Carnitine Synthesis	2 / 4	0.28743	0.47905	0.89508
Fatty Acid Biosynthesis	2 / 7	0.60092	0.86948	0.91936
Arachidonic Acid Metabolism	3 / 11	0.60288	0.86948	0.06145
<i>LID VIP</i>				
Carnitine Synthesis	2 / 4	0.03356	0.50346	0.89508
Tryptophan Metabolism	2 / 4	0.03356	0.50346	0.38745
Glycine and Serine Metabolism	2 / 6	0.07673	0.57549	0.38745
Histidine Metabolism	2 / 6	0.07673	0.57549	0.33776
Arginine and Proline Metabolism	2 / 8	0.13096	0.68113	0.32816
Starch and Sucrose Metabolism	1 / 3	0.22976	0.68113	0.21137
Valine, Leucine, and Isoleucine Degradation	1 / 4	0.29516	0.68113	0.53964
Urea Cycle	1 / 4	0.29516	0.68113	0.00000
Aspartate Metabolism	1 / 4	0.29516	0.68113	0.00000
Methionine Metabolism	1 / 4	0.29516	0.68113	0.34590
Phenylalanine and Tyrosine Metabolism	1 / 4	0.29516	0.68113	0.03012
Nicotinate and Nicotinamide Metabolism	1 / 4	0.29516	0.68113	0.38745
Galactose Metabolism	1 / 4	0.29516	0.68113	0.21137
Tyrosine Metabolism	1 / 5	0.35557	0.76194	0.86080
Purine Metabolism	1 / 7	0.46278	0.92555	0.00000
Phosphatidylcholine Biosynthesis	1 / 30	0.95173	1.00000	0.31882
Androgen and Estrogen Metabolism	0 / 5	1.00000	1.00000	0.00000
Glutamate Metabolism	0 / 6	1.00000	1.00000	0.00000
Fatty Acid Biosynthesis	0 / 7	1.00000	1.00000	0.00000
Retinol Metabolism	0 / 8	1.00000	1.00000	0.00000
<i>LID Gini</i>				
Fructose and Mannose Degradation	2 / 3	0.04918	0.73773	1.00000
Starch and Sucrose Metabolism	2 / 3	0.04918	0.73773	0.94695
Galactose Metabolism	2 / 4	0.09043	0.90431	0.94695
Histidine Metabolism	2 / 6	0.19133	1.00000	0.13656
Arginine and Proline Metabolism	2 / 8	0.30285	1.00000	0.13061
Pentose Phosphate Pathway	1 / 3	0.36149	1.00000	0.00632
Valine, Leucine, and Isoleucine Degradation	1 / 4	0.45185	1.00000	0.53964
Ammonia Recycling	1 / 4	0.45185	1.00000	0.19463

Urea Cycle	1 / 4	0.45185	1.00000	0.00000
Aspartate Metabolism	1 / 4	0.45185	1.00000	0.00000
Tryptophan Metabolism	1 / 4	0.45185	1.00000	0.00000
Phenylalanine and Tyrosine Metabolism	1 / 4	0.45185	1.00000	0.03012
Carnitine Synthesis	1 / 4	0.45185	1.00000	0.00000
Glycine and Serine Metabolism	1 / 6	0.59792	1.00000	0.00000
Purine Metabolism	1 / 7	0.65648	1.00000	0.00000
Retinol Metabolism	1 / 8	0.70700	1.00000	0.00000
Nicotinate and Nicotinamide Metabolism	0 / 4	1.00000	1.00000	0.00000
Phosphatidylethanolamine Biosynthesis	0 / 29	1.00000	1.00000	0.00000
Arachidonic Acid Metabolism	0 / 11	1.00000	1.00000	0.00000
Steroidogenesis	0 / 9	1.00000	1.00000	0.00000
<i>MD PINNI</i>				
Histidine Metabolism	4 / 5	0.00315	0.07686	0.04873
Fructose and Mannose Degradation	3 / 3	0.00452	0.07686	0.00000
Tyrosine Metabolism	4 / 6	0.00826	0.09366	0.04839
Estrone Metabolism	3 / 4	0.01593	0.13540	0.01255
Alpha Linolenic Acid and Linoleic Acid Metabolism	4 / 10	0.06840	0.25364	0.38911
Lysine Degradation	2 / 3	0.07460	0.25364	0.04596
Valine, Leucine, and Isoleucine Degradation	2 / 3	0.07460	0.25364	0.72065
Glutathione Metabolism	2 / 3	0.07460	0.25364	0.05132
Arginine and Proline Metabolism	2 / 3	0.07460	0.25364	0.05142
Ubiquinone Biosynthesis	2 / 3	0.07460	0.25364	0.04358
Vitamin K Metabolism	3 / 7	0.09574	0.29592	0.04836
Glutamate Metabolism	2 / 4	0.13327	0.34856	0.05132
Folate Metabolism	2 / 4	0.13327	0.34856	0.04880
Bile Acid Biosynthesis	4 / 14	0.19458	0.42227	0.02694
Androstenedione Metabolism	2 / 5	0.19871	0.42227	0.01131
Starch and Sucrose Metabolism	2 / 5	0.19871	0.42227	0.20197
Tryptophan Metabolism	2 / 6	0.26710	0.53420	0.27908
Arachidonic Acid Metabolism	3 / 12	0.32832	0.60062	0.02829
Androgen and Estrogen Metabolism	2 / 7	0.33564	0.60062	0.01069
Porphyrin Metabolism	1 / 3	0.42663	0.69073	0.53284
<i>MD VIP</i>				
Phosphatidylethanolamine Biosynthesis	27 / 92	0.01002	0.20418	0.65239
Phosphatidylcholine Biosynthesis	27 / 93	0.01201	0.20418	0.65239
Glutamate Metabolism	2 / 4	0.19137	1.00000	0.05132
Starch and Sucrose Metabolism	2 / 5	0.27757	1.00000	0.20197
Tryptophan Metabolism	2 / 6	0.36335	1.00000	0.27908
Lysine Degradation	1 / 3	0.50384	1.00000	0.04596

Porphyryn Metabolism	1 / 3	0.50384	1.00000	0.53284
Arginine and Proline Metabolism	1 / 3	0.50384	1.00000	0.05142
Galactose Metabolism	1 / 3	0.50384	1.00000	0.21247
Ubiquinone Biosynthesis	1 / 3	0.50384	1.00000	0.04358
Glutathione Metabolism	1 / 3	0.50384	1.00000	0.05132
Valine, Leucine, and Isoleucine Degradation	1 / 3	0.50384	1.00000	0.72065
Fructose and Mannose Degradation	1 / 3	0.50384	1.00000	0.00000
Sphingolipid Metabolism	2 / 9	0.58998	1.00000	0.03259
Oxidation of Branched-Chain Fatty Acids	1 / 4	0.60799	1.00000	0.03285
Folate Metabolism	1 / 4	0.60799	1.00000	0.04880
Estrone Metabolism	1 / 4	0.60799	1.00000	0.01255
Alpha Linolenic Acid and Linoleic Acid Metabolism	2 / 10	0.65140	1.00000	0.38911
Cardiolipin Biosynthesis	2 / 10	0.65140	1.00000	0.21030
Androstenedione Metabolism	1 / 5	0.69060	1.00000	0.01131
<i>MD Gini</i>				
Alpha Linolenic Acid and Linoleic Acid Metabolism	6 / 10	0.00880	0.29929	0.77281
Sphingolipid Metabolism	4 / 9	0.10892	0.68931	0.07517
Tryptophan Metabolism	3 / 6	0.12103	0.68931	0.28746
Tyrosine Metabolism	3 / 6	0.12103	0.68931	0.09713
Valine, Leucine, and Isoleucine Degradation	2 / 3	0.12164	0.68931	0.95515
Galactose Metabolism	2 / 3	0.12164	0.68931	1.00000
Steroidogenesis	3 / 7	0.17948	0.79097	0.09270
Folate Metabolism	2 / 4	0.20937	0.79097	0.09603
Glutamate Metabolism	2 / 4	0.20937	0.79097	0.05132
Histidine Metabolism	2 / 5	0.30125	0.89260	0.09590
Starch and Sucrose Metabolism	2 / 5	0.30125	0.89260	0.81949
Steroid Biosynthesis	2 / 6	0.39136	0.89260	0.11488
Androgen and Estrogen Metabolism	2 / 7	0.47611	0.89260	0.01775
Vitamin K Metabolism	2 / 7	0.47611	0.89260	0.05394
Fructose and Mannose Degradation	1 / 3	0.52490	0.89260	0.04617
Arginine and Proline Metabolism	1 / 3	0.52490	0.89260	0.05142
Porphyryn Metabolism	1 / 3	0.52490	0.89260	0.53284
Lysine Degradation	1 / 3	0.52490	0.89260	0.04596
Glutathione Metabolism	1 / 3	0.52490	0.89260	0.05132
Fatty Acid Biosynthesis	4 / 17	0.53273	0.89260	0.09914