

Cluster #75 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 75, from importance channel 1 (*aggregator*), represents a motif consisting of 8.3 (± 1.7) nodes. The concept is generally associated with an impact of 1.1 (± 0.6) on the prediction outcome.

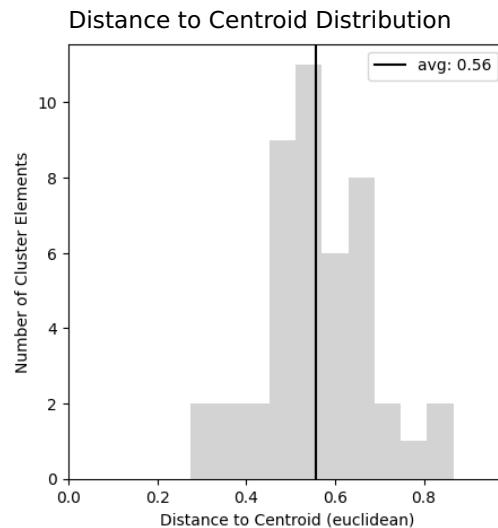
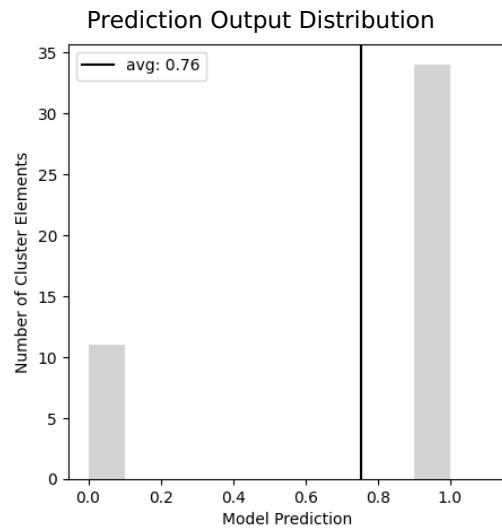
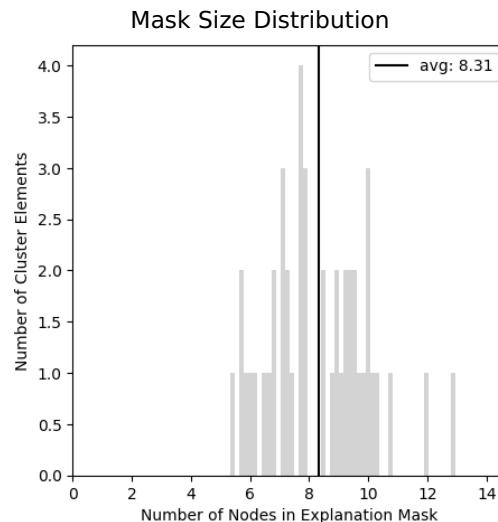
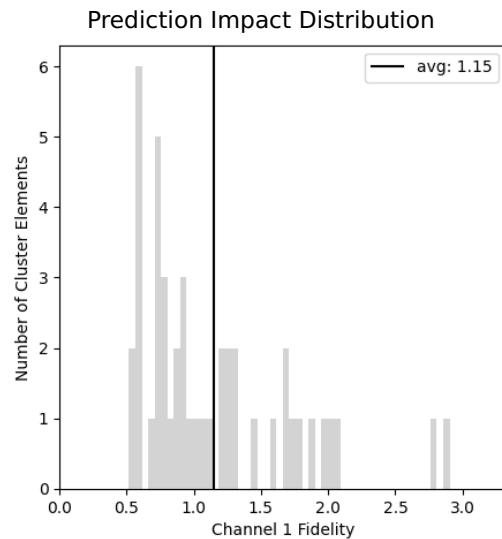
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	45
Channel Index	1.0 (0.0)

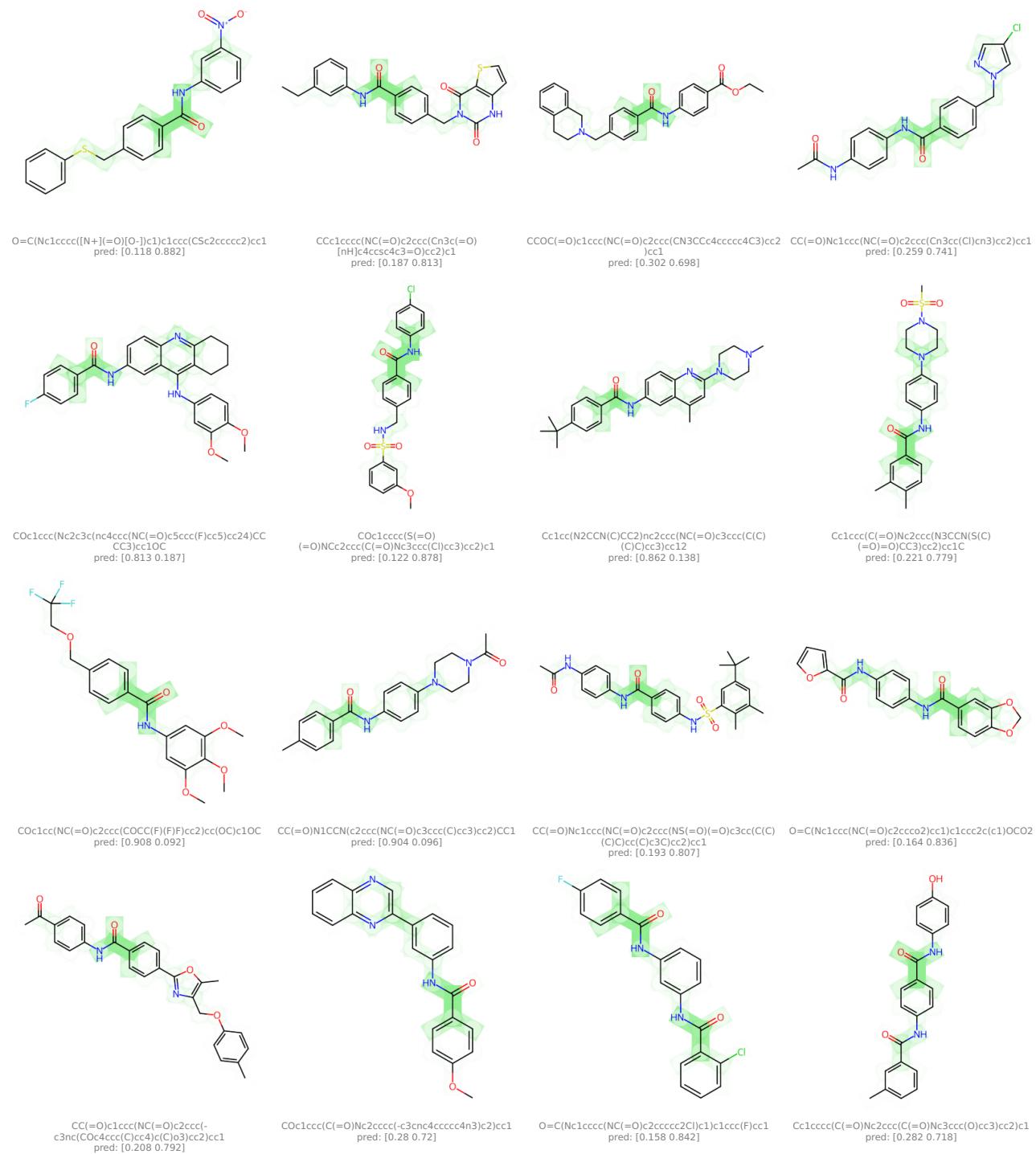
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #76 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 76, from importance channel 1 (*aggregator*), represents a motif consisting of 8.4 (± 2.2) nodes. The concept is generally associated with an impact of 1.5 (± 0.7) on the prediction outcome.

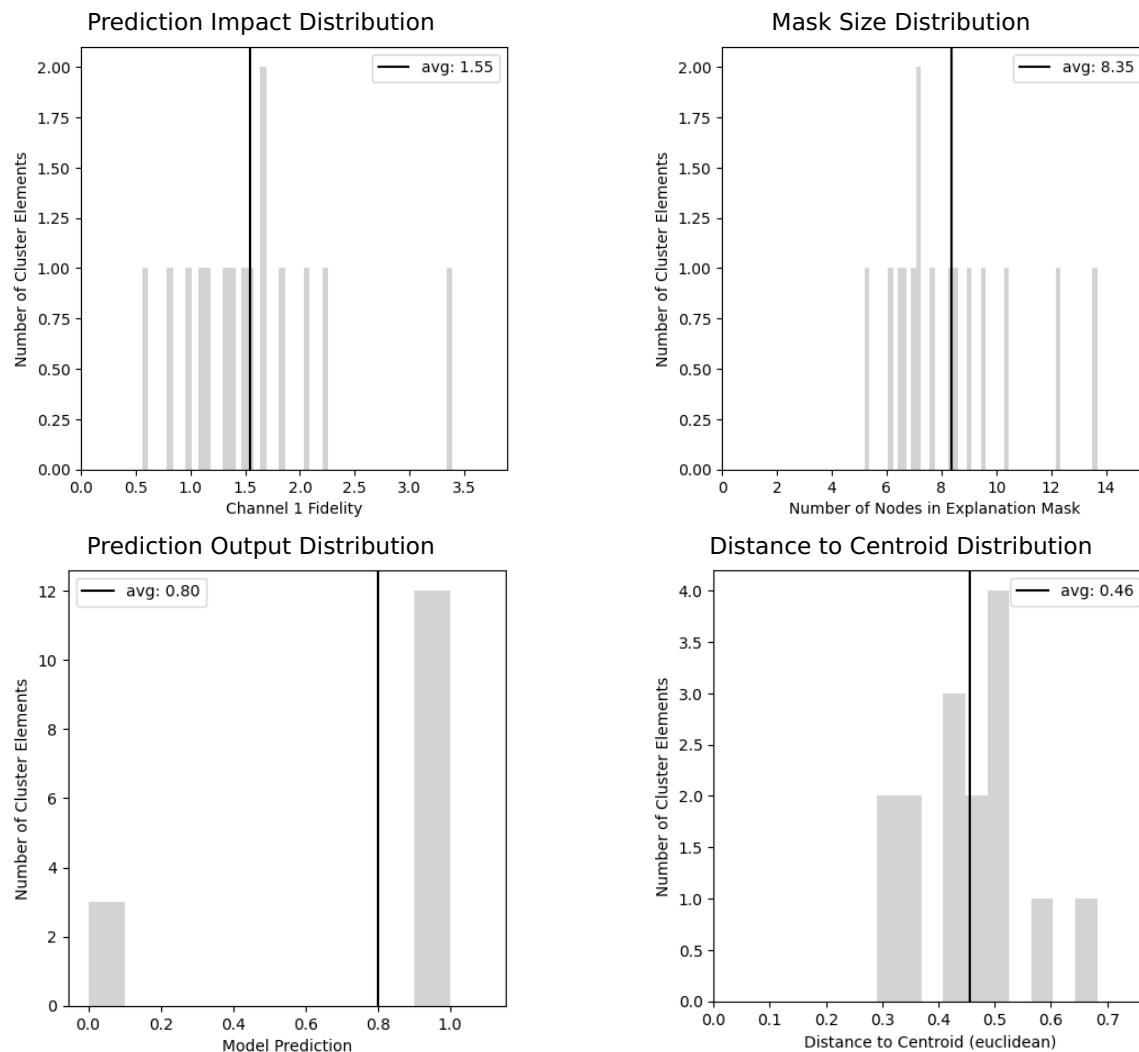
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	15
Channel Index	1.0 (0.0)

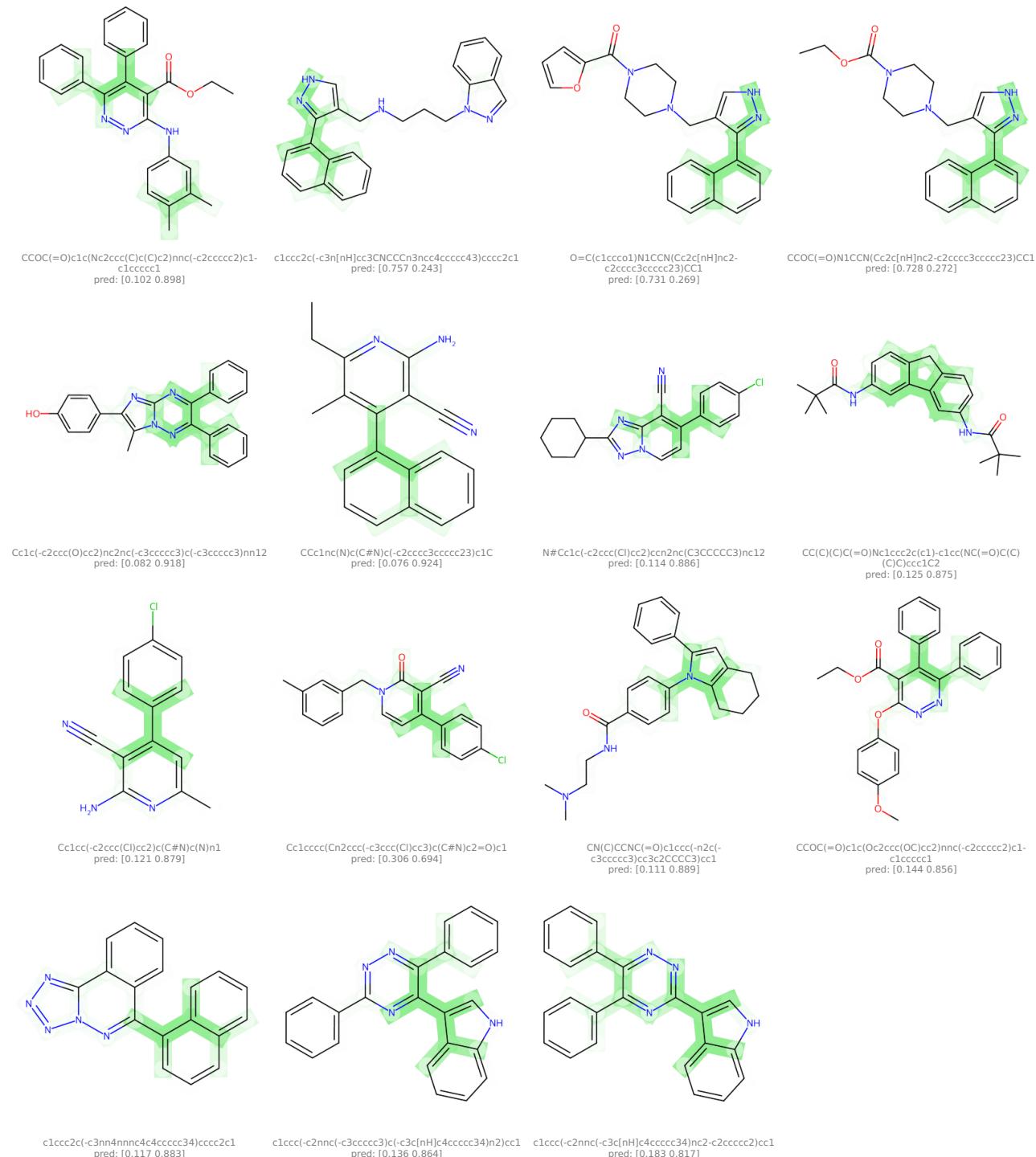
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #77 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 77, from importance channel 1 (*aggregator*), represents a motif consisting of 8.5 (± 1.4) nodes. The concept is generally associated with an impact of 1.0 (± 0.0) on the prediction outcome.

Properties

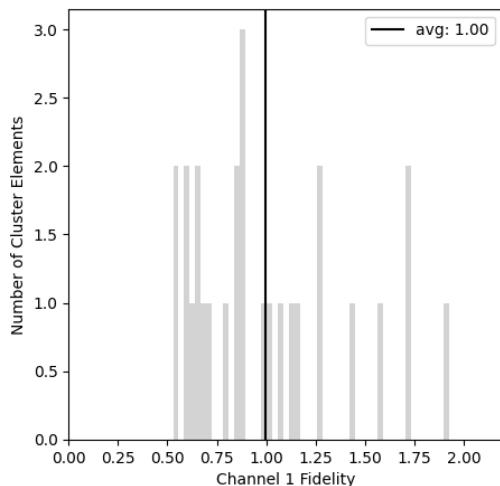
ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	27
Channel Index	1.0 (0.0)

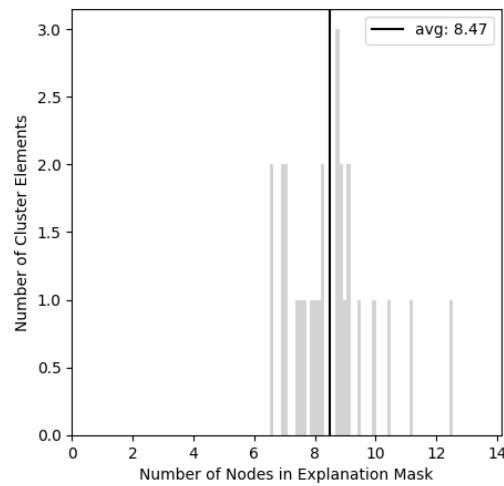
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.

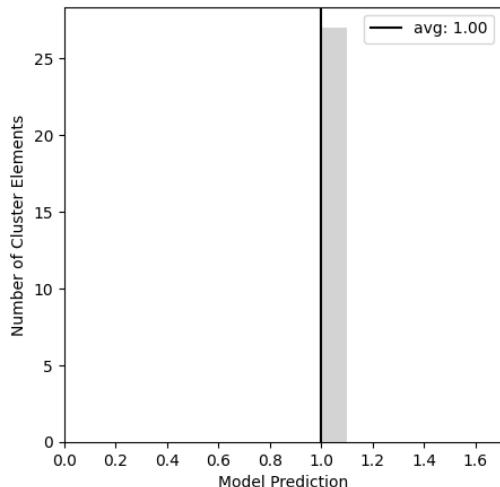
Prediction Impact Distribution



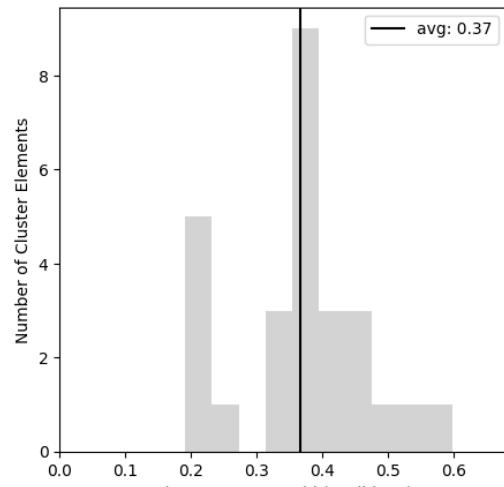
Mask Size Distribution



Prediction Output Distribution

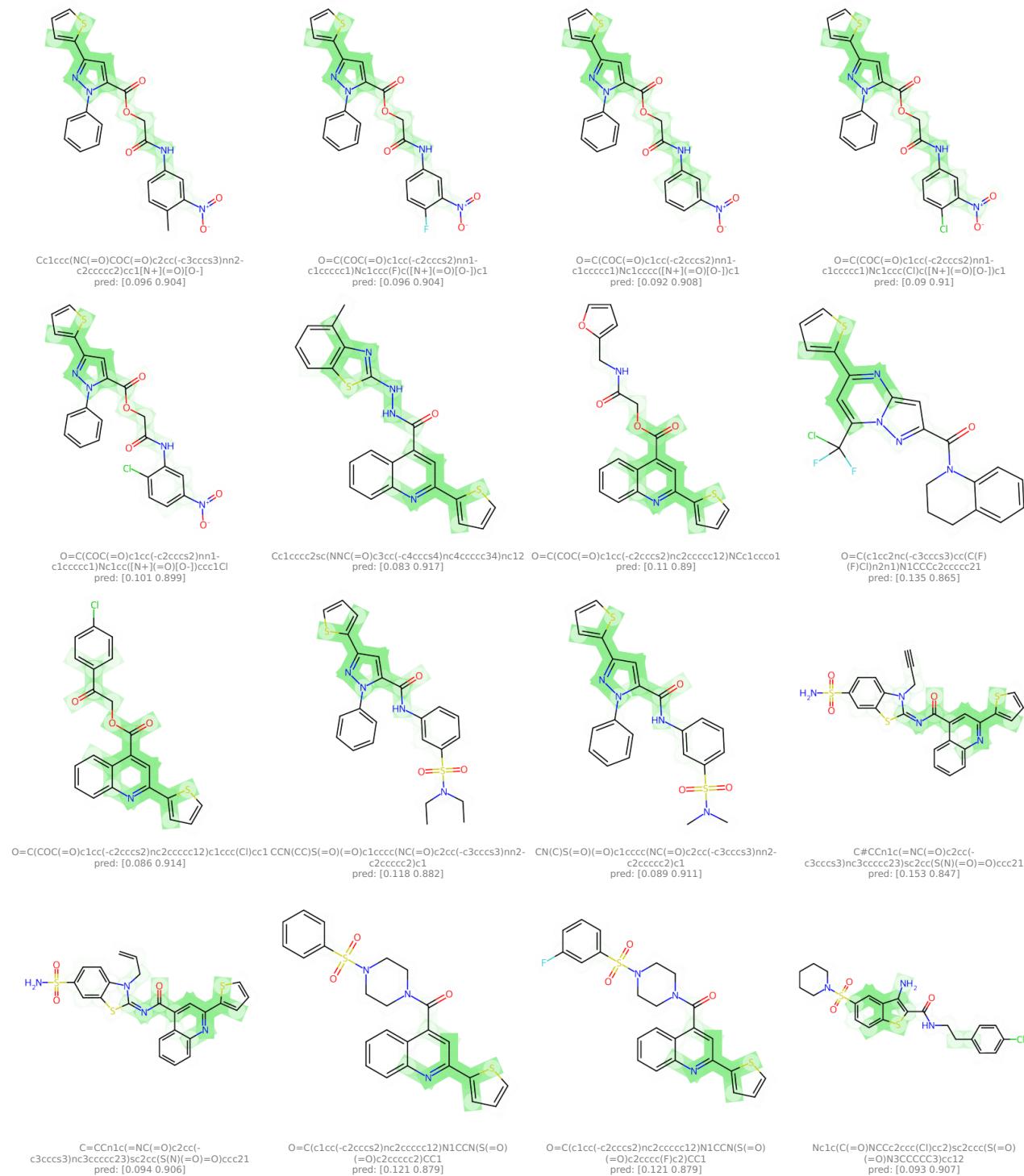


Distance to Centroid Distribution



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #78 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 78, from importance channel 1 (*aggregator*), represents a motif consisting of 8.8 (± 0.4) nodes. The concept is generally associated with an impact of 1.0 (± 0.1) on the prediction outcome.

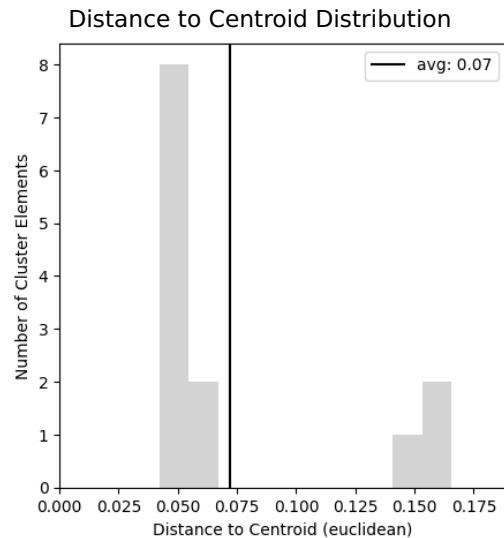
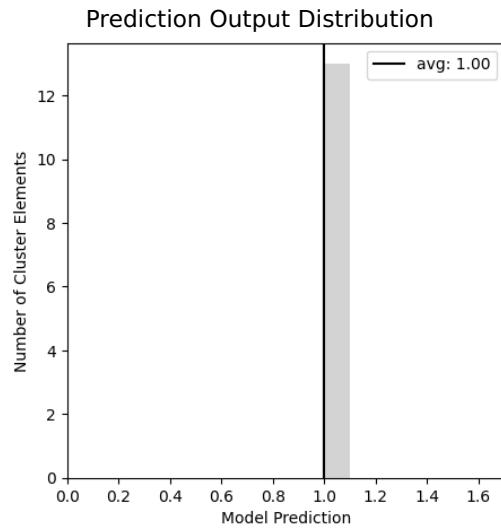
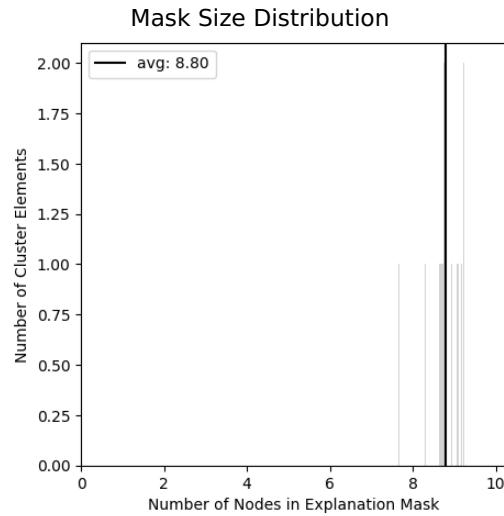
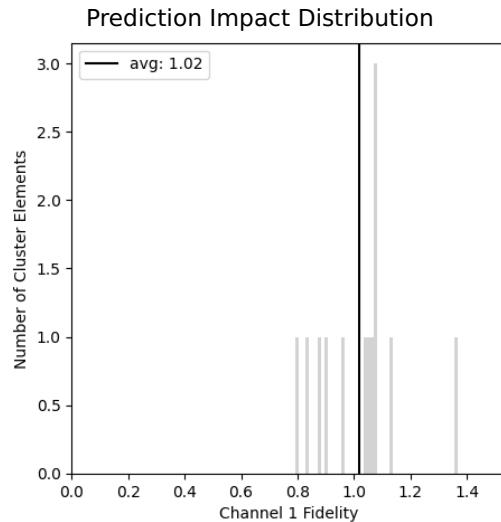
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	13
Channel Index	1.0 (0.0)

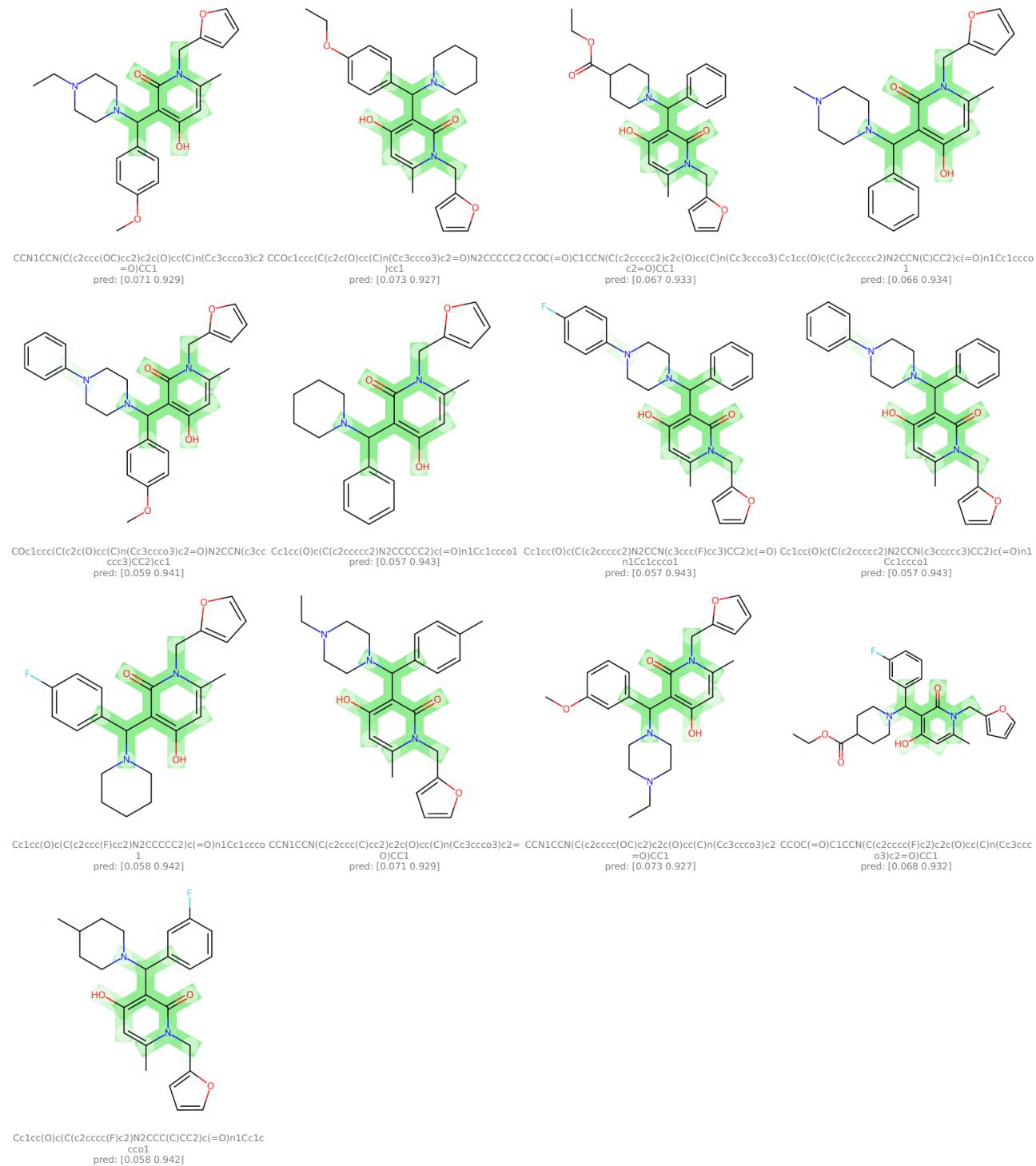
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #79 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 79, from importance channel 1 (*aggregator*), represents a motif consisting of 7.9 (± 2.7) nodes. The concept is generally associated with an impact of 1.0 (± 0.3) on the prediction outcome.

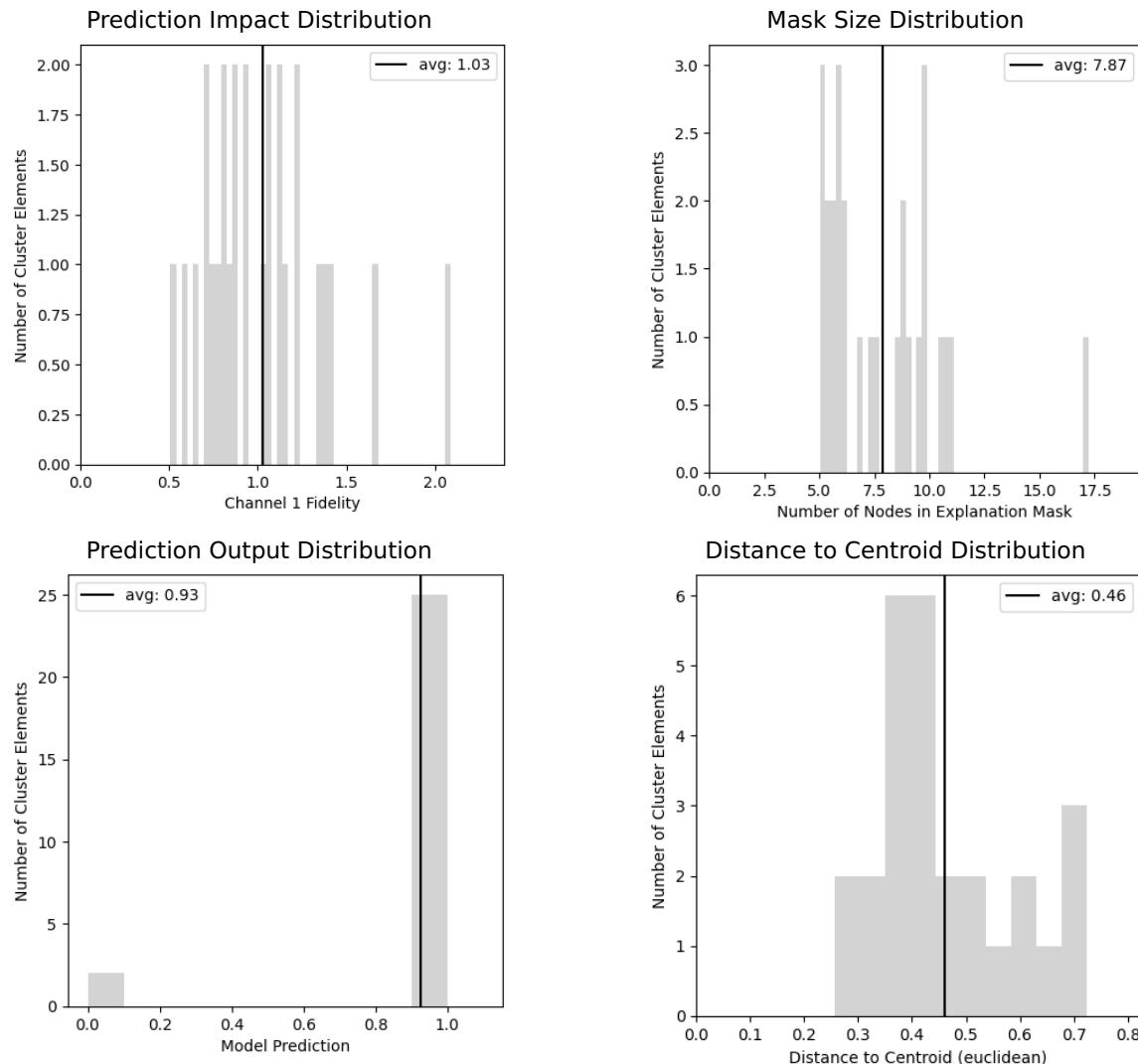
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	27
Channel Index	1.0 (0.0)

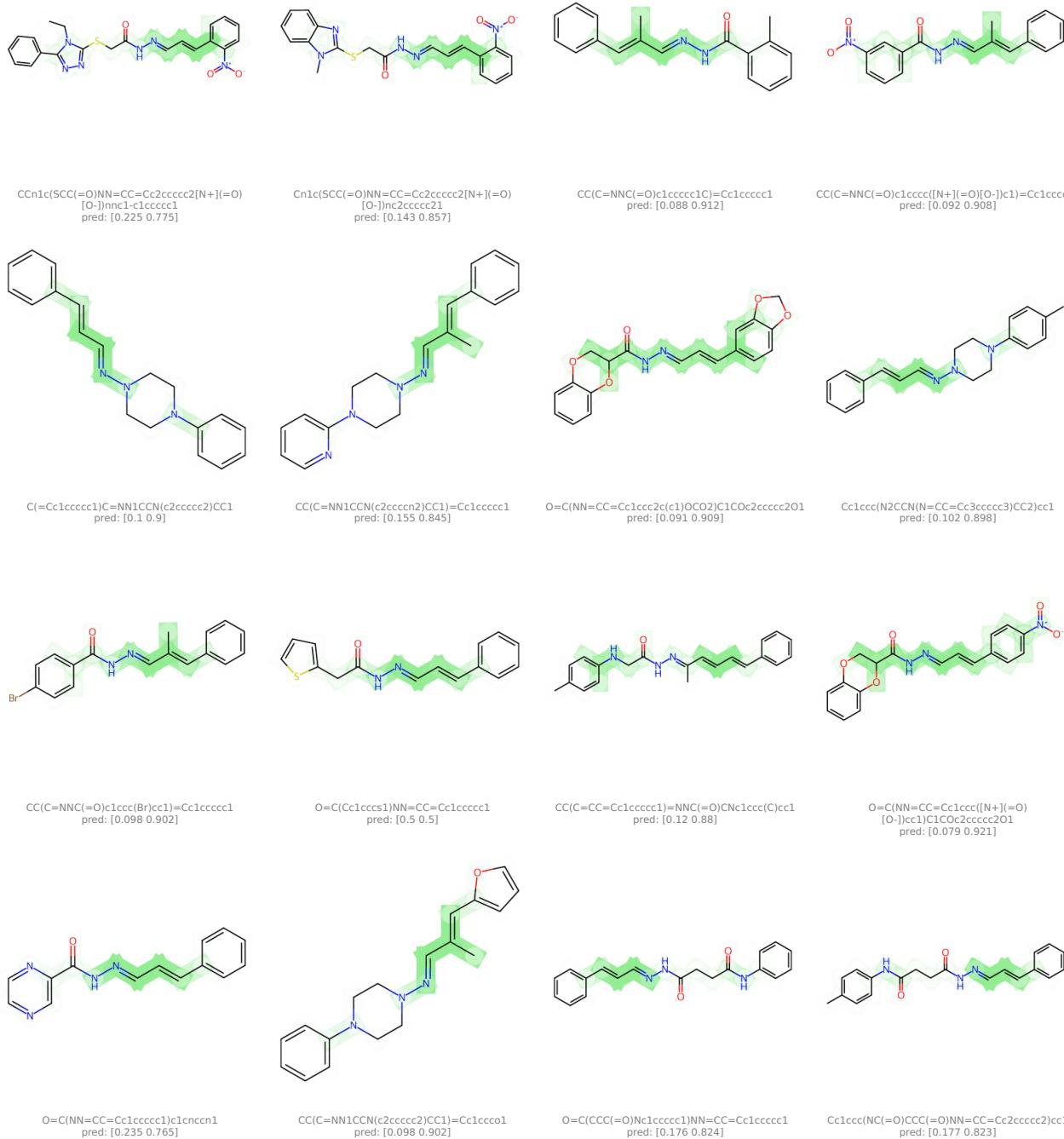
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #80 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 80, from importance channel 1 (*aggregator*), represents a motif consisting of 7.1 (± 1.0) nodes. The concept is generally associated with an impact of 0.9 (± 0.4) on the prediction outcome.

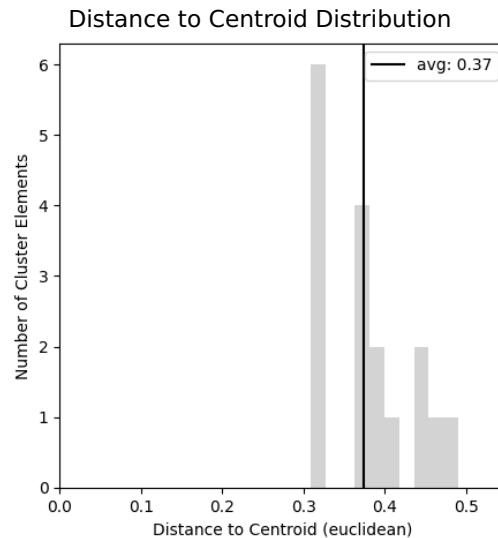
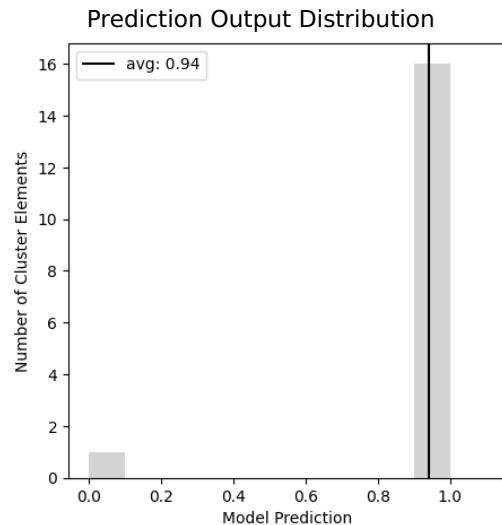
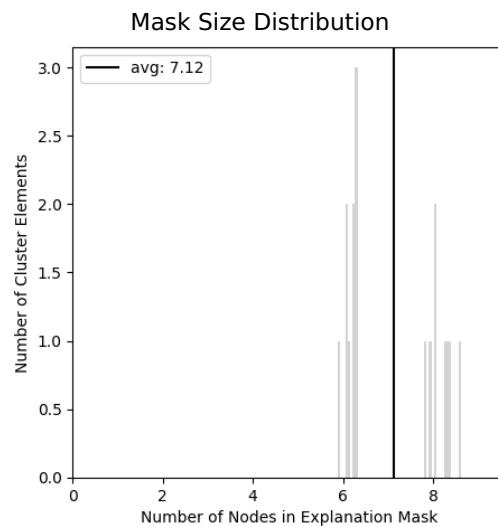
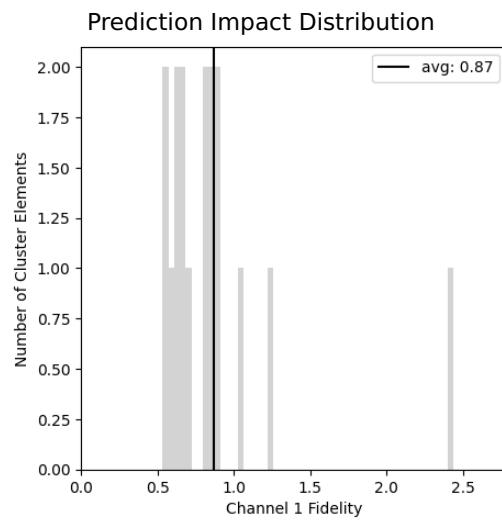
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	17
Channel Index	1.0 (0.0)

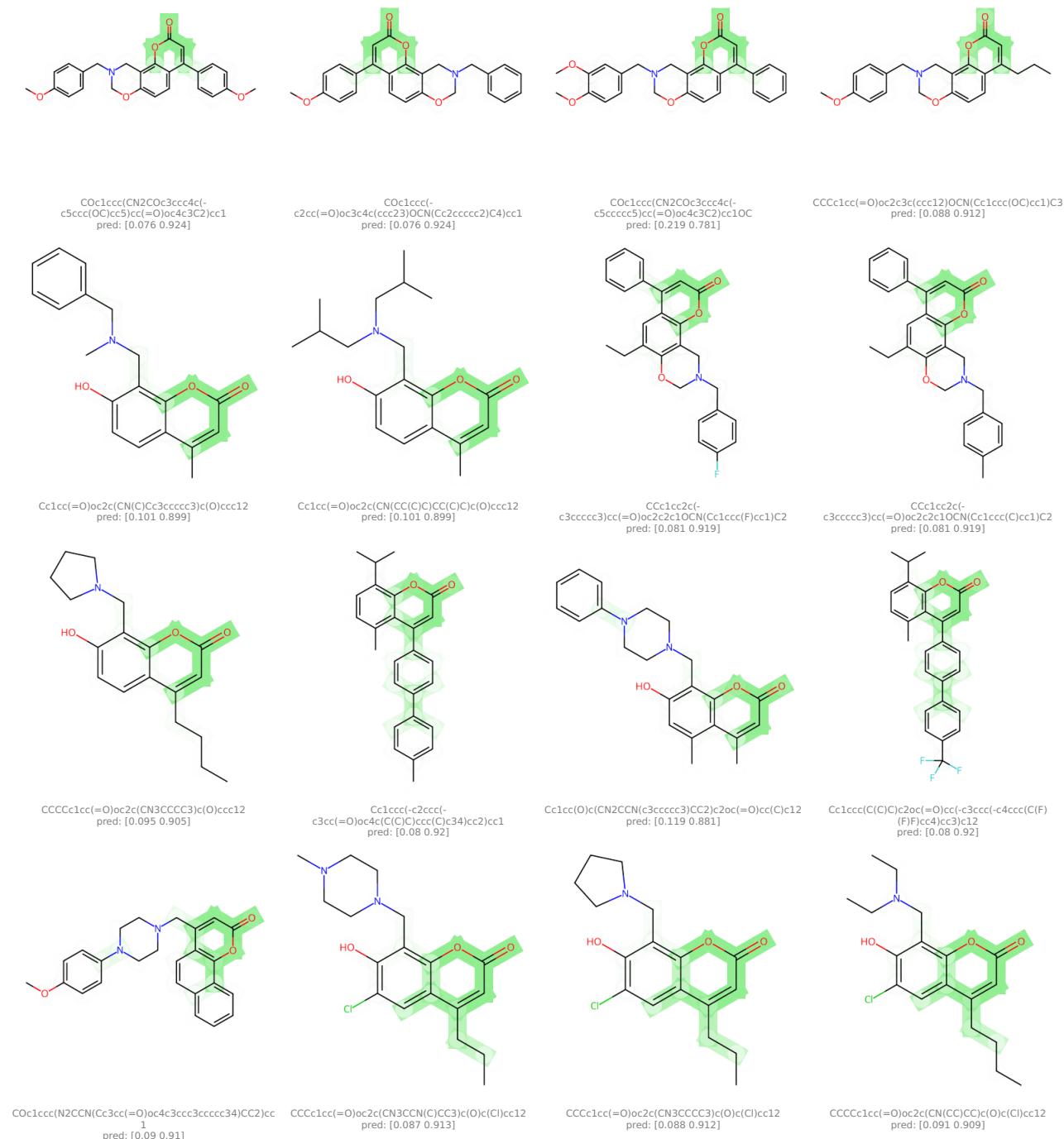
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #81 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 81, from importance channel 1 (*aggregator*), represents a motif consisting of 8.1 (± 1.1) nodes. The concept is generally associated with an impact of 0.8 (± 0.2) on the prediction outcome.

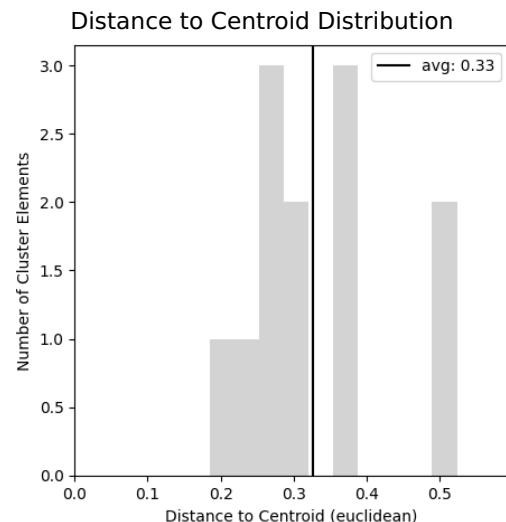
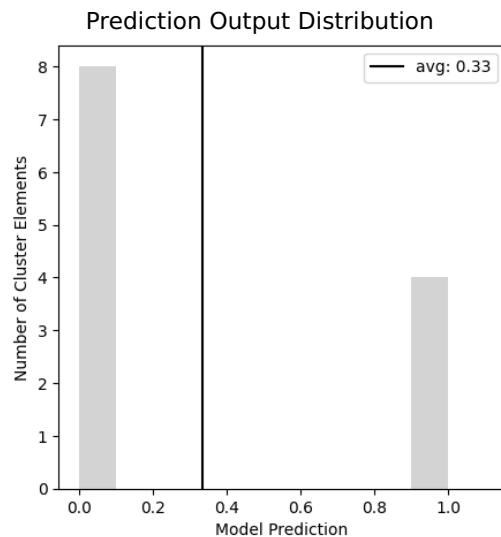
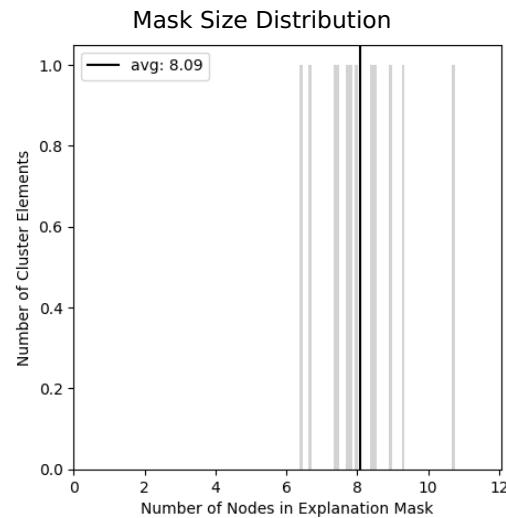
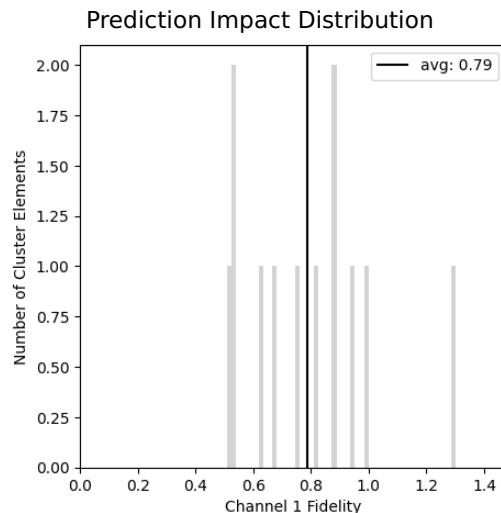
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	12
Channel Index	1.0 (0.0)

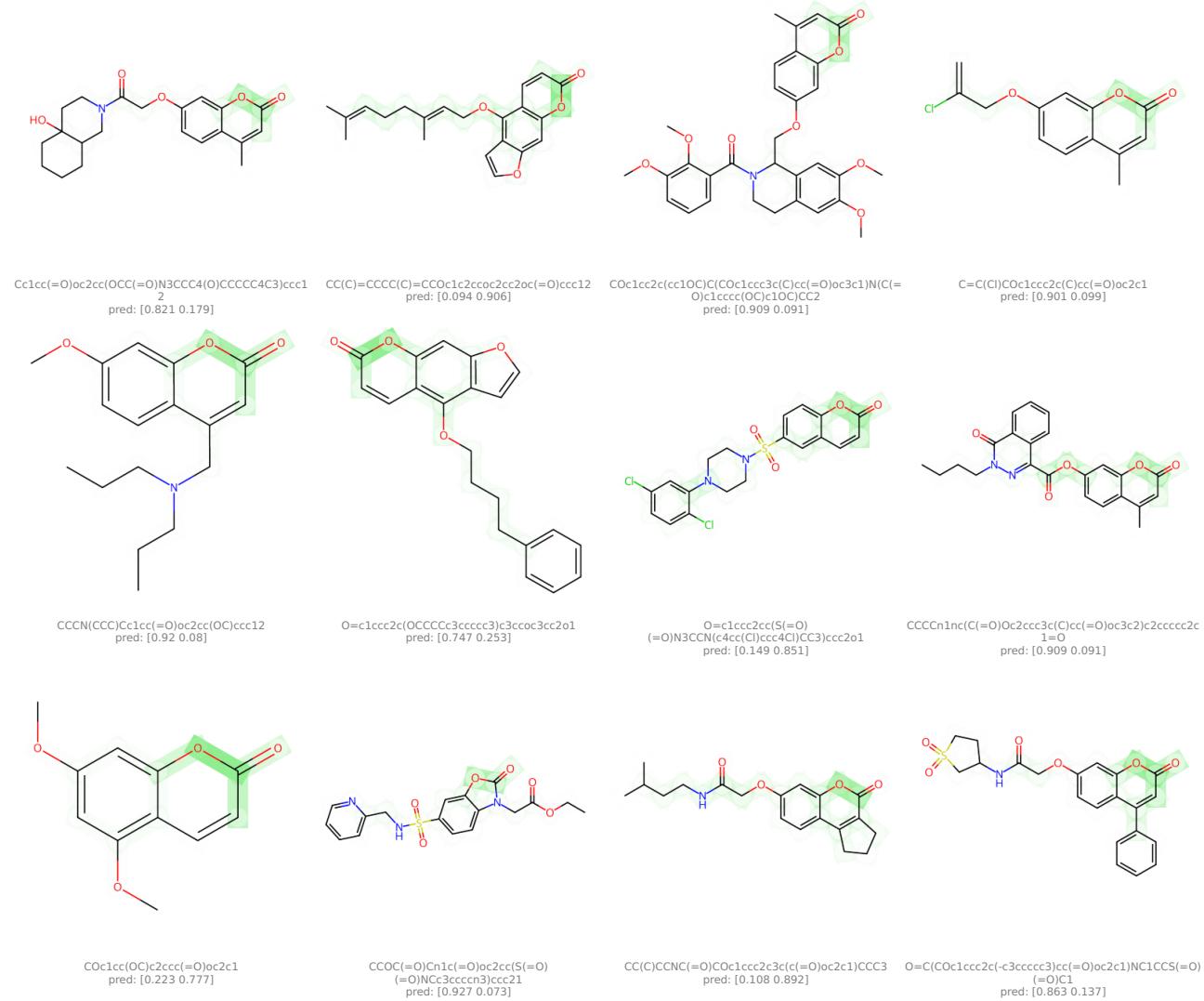
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #82 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 82, from importance channel 1 (*aggregator*), represents a motif consisting of 9.0 (± 1.6) nodes. The concept is generally associated with an impact of 1.5 (± 0.5) on the prediction outcome.

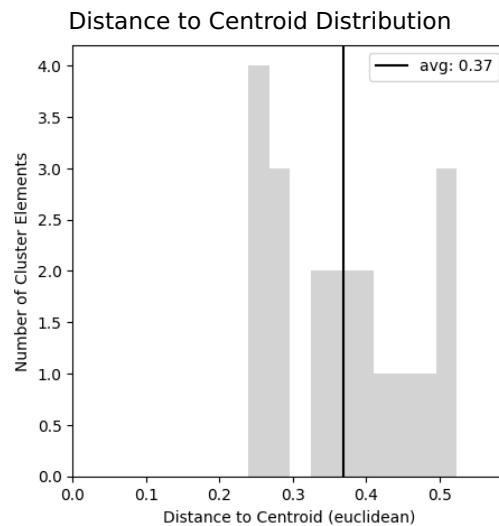
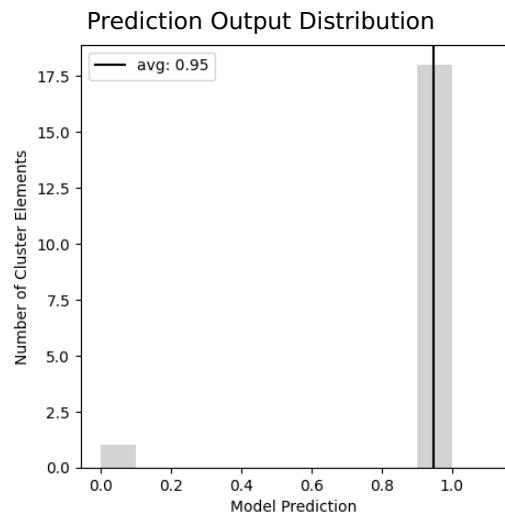
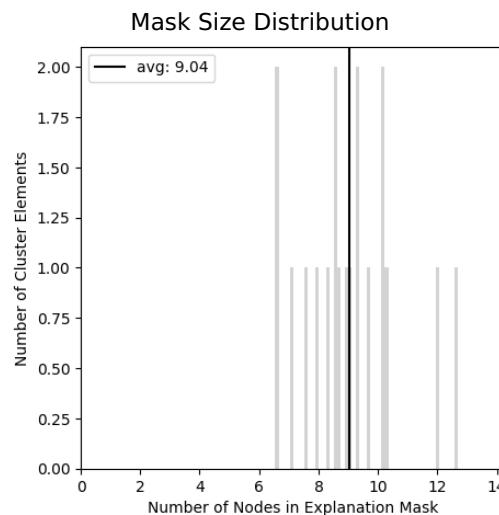
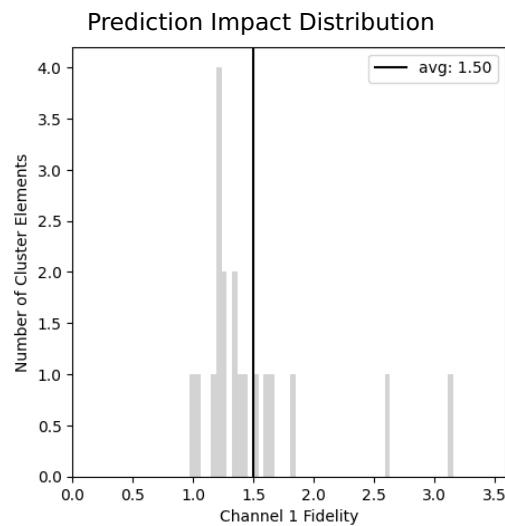
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	19
Channel Index	1.0 (0.0)

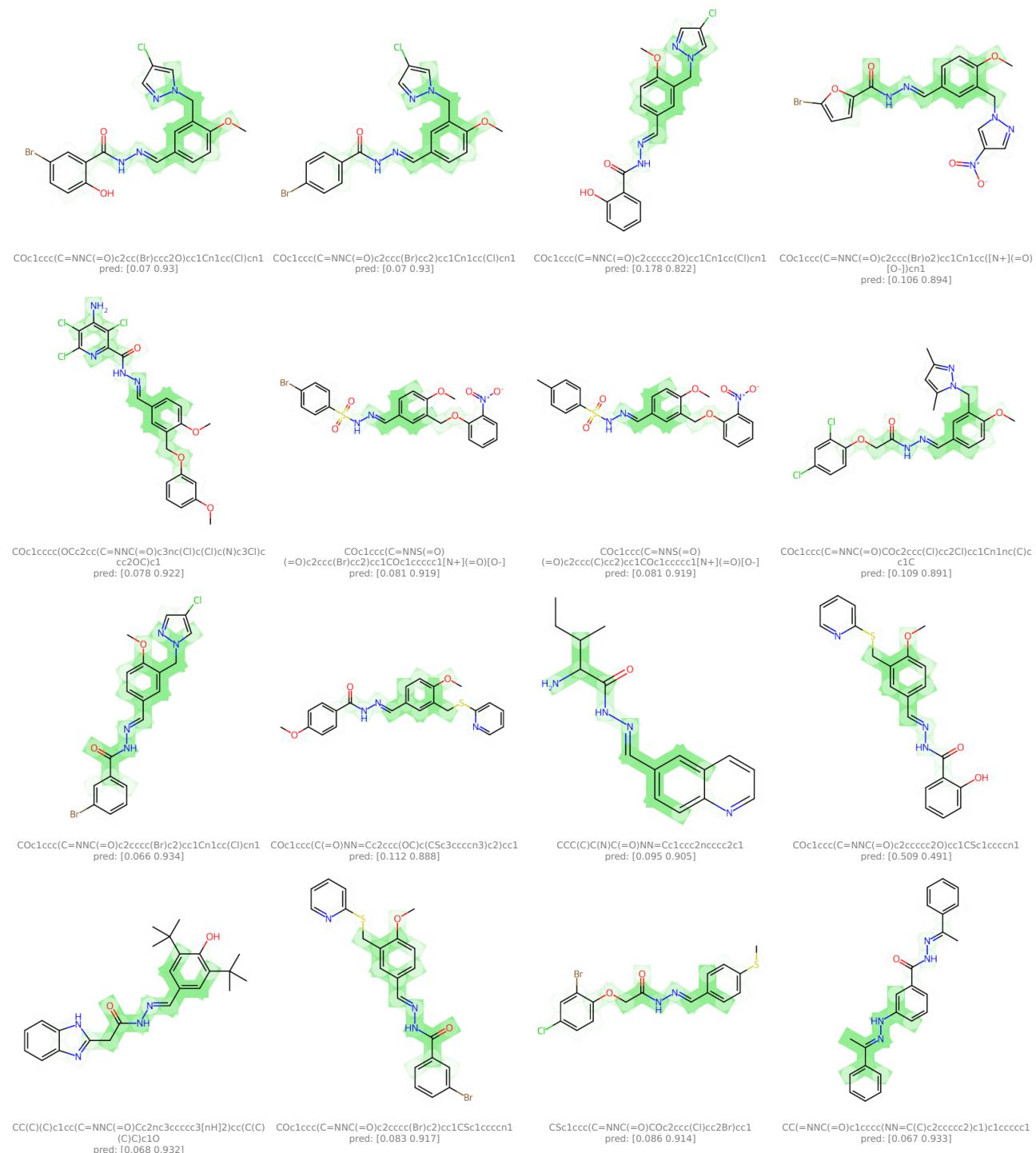
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #83 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 83, from importance channel 1 (*aggregator*), represents a motif consisting of 7.5 (± 1.7) nodes. The concept is generally associated with an impact of 1.6 (± 0.7) on the prediction outcome.

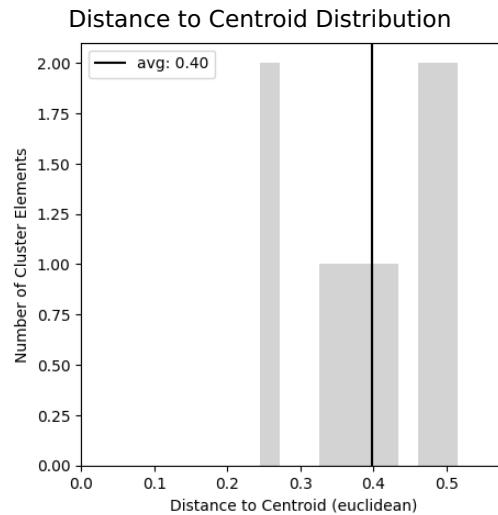
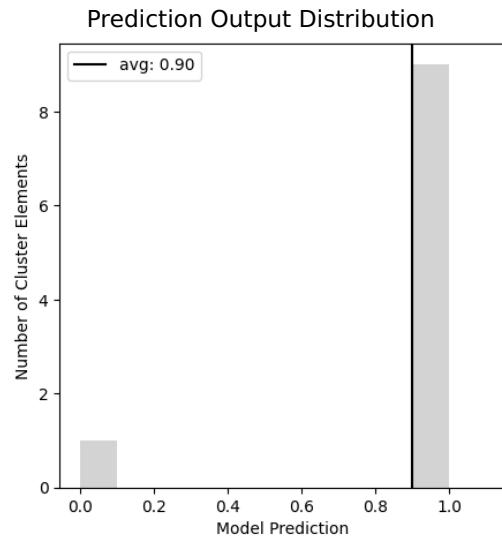
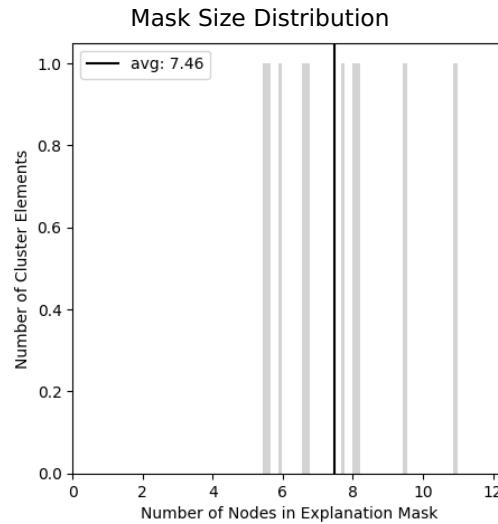
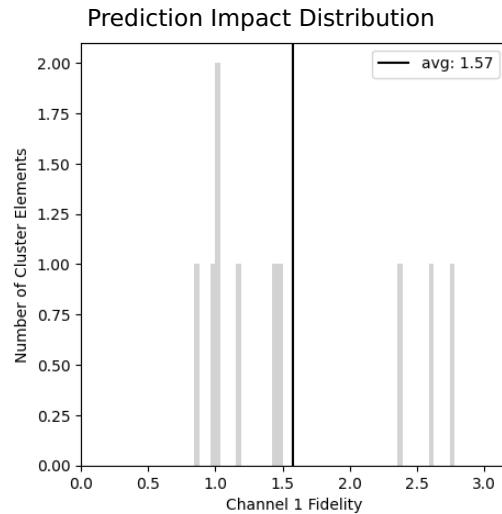
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	10
Channel Index	1.0 (0.0)

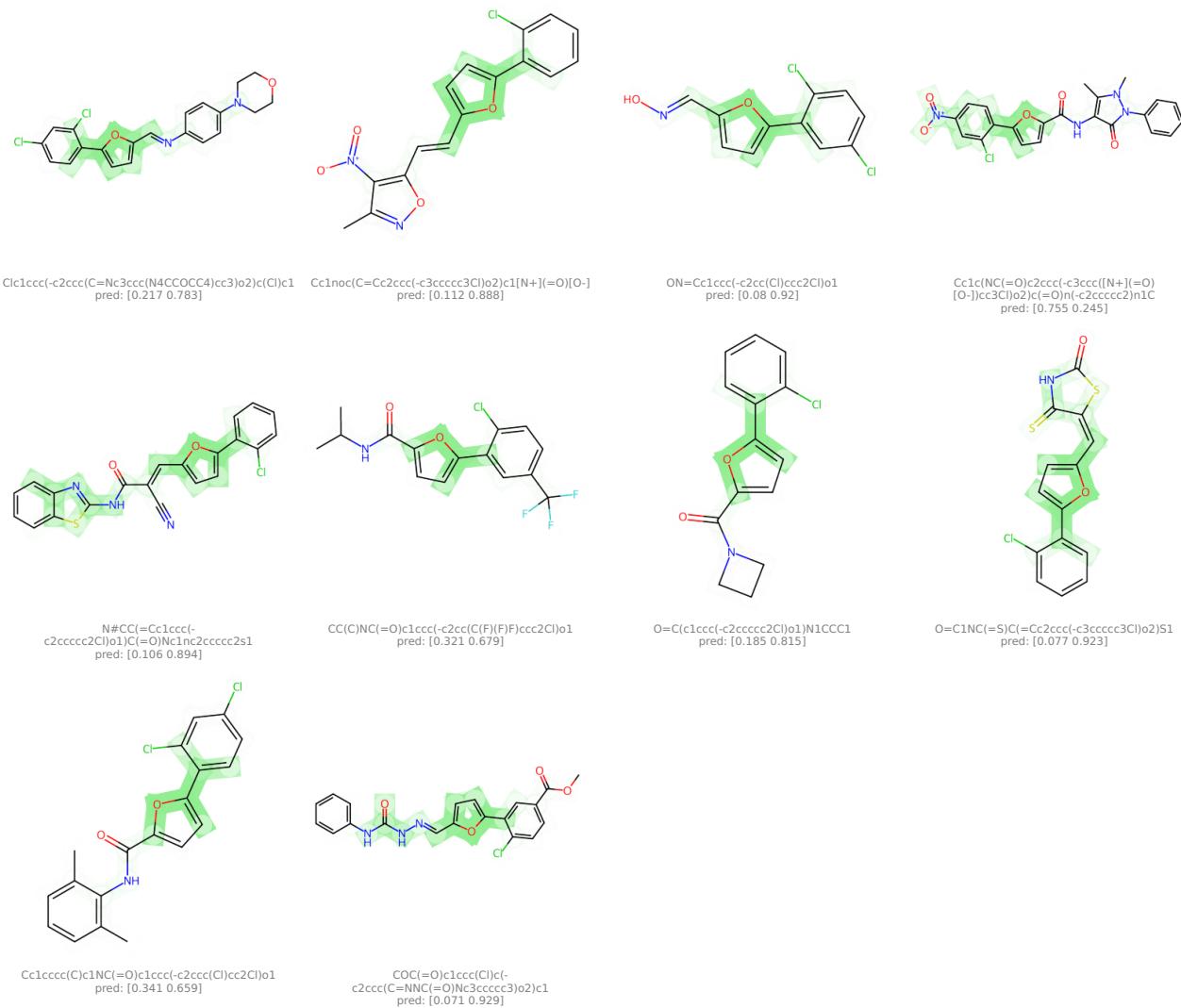
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #84 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 84, from importance channel 1 (*aggregator*), represents a motif consisting of 8.0 (± 0.5) nodes. The concept is generally associated with an impact of 0.9 (± 0.5) on the prediction outcome.

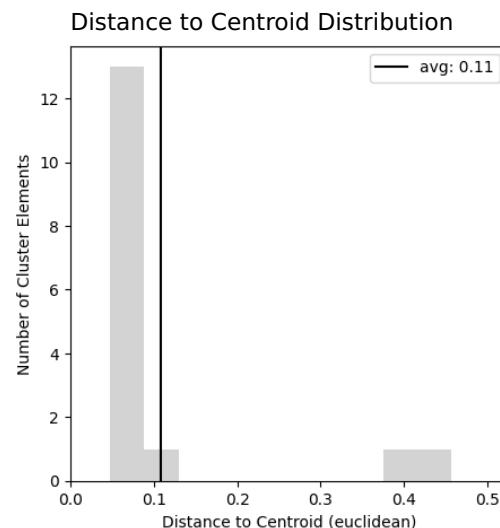
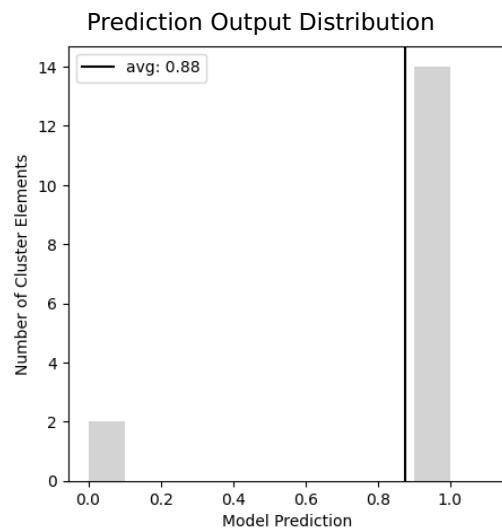
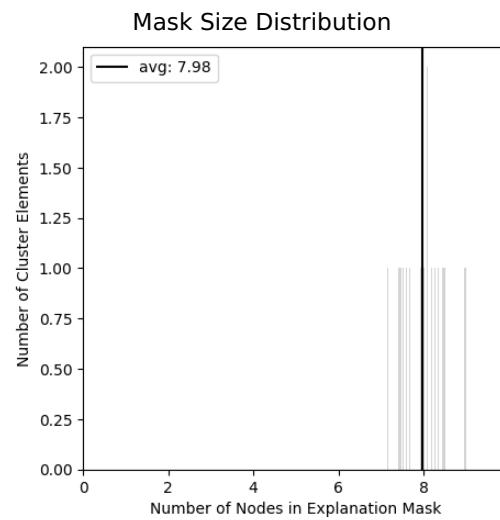
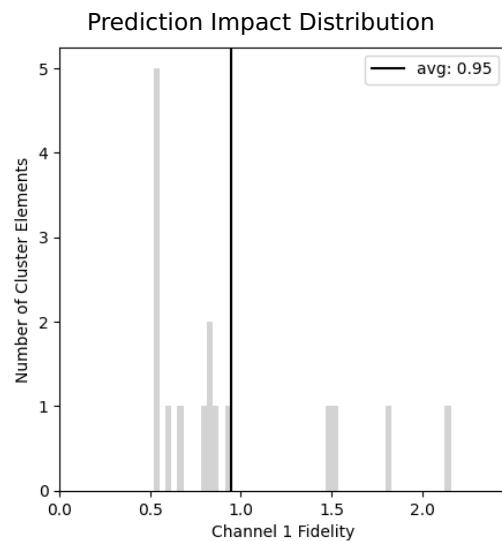
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	16
Channel Index	1.0 (0.0)

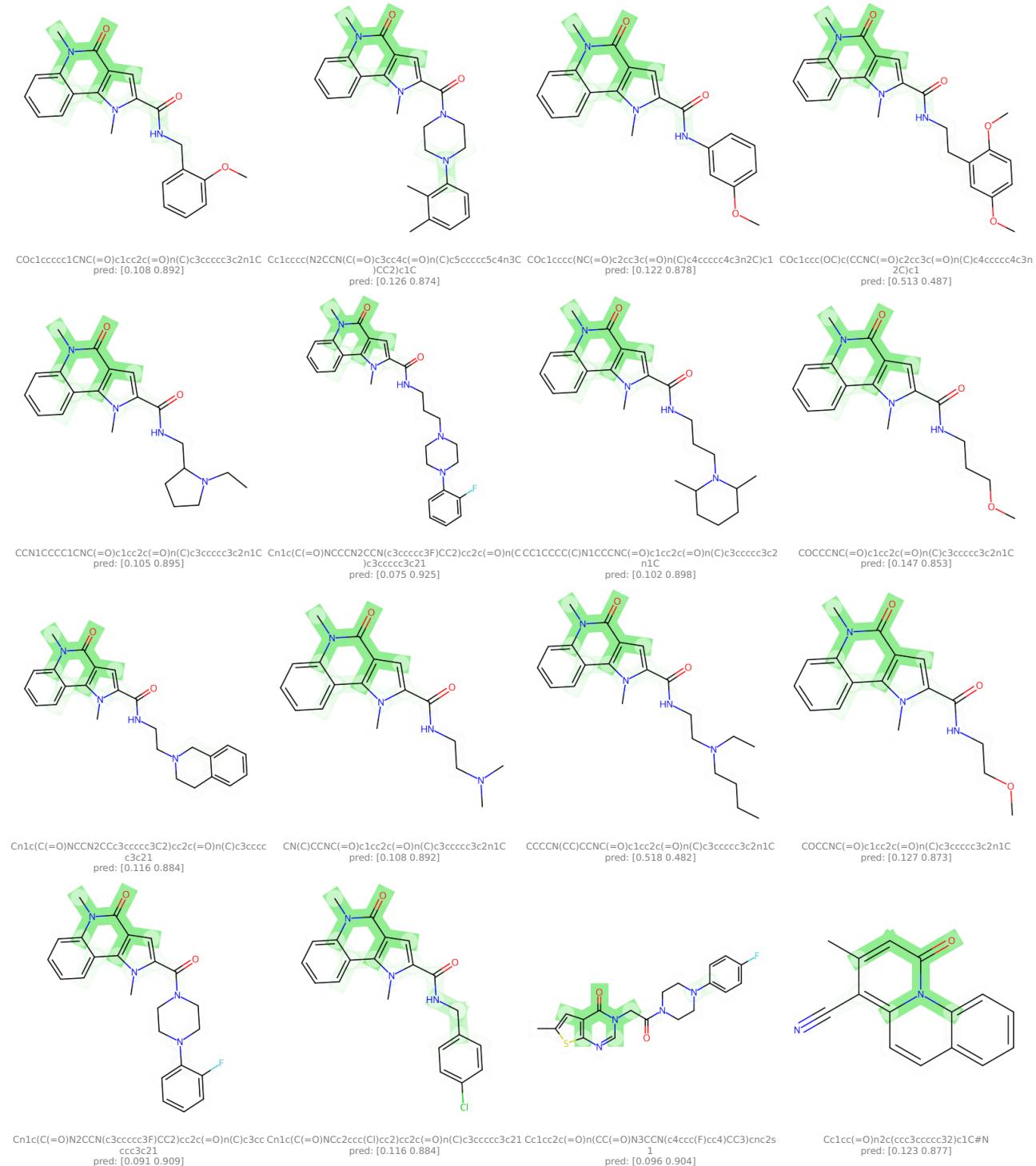
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #85 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 85, from importance channel 1 (*aggregator*), represents a motif consisting of 7.2 (± 1.6) nodes. The concept is generally associated with an impact of 0.8 (± 0.1) on the prediction outcome.

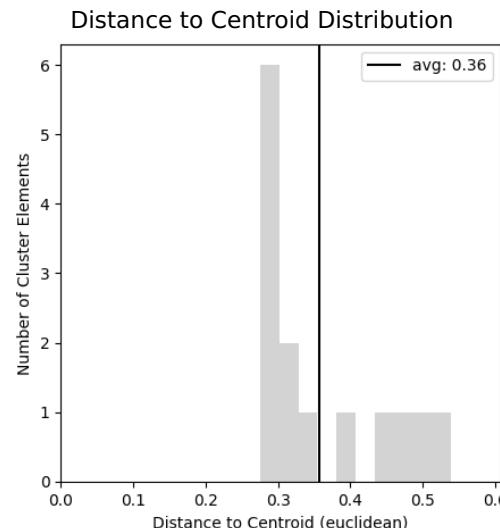
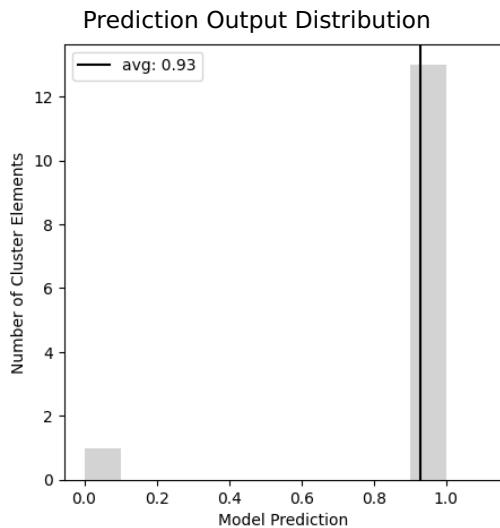
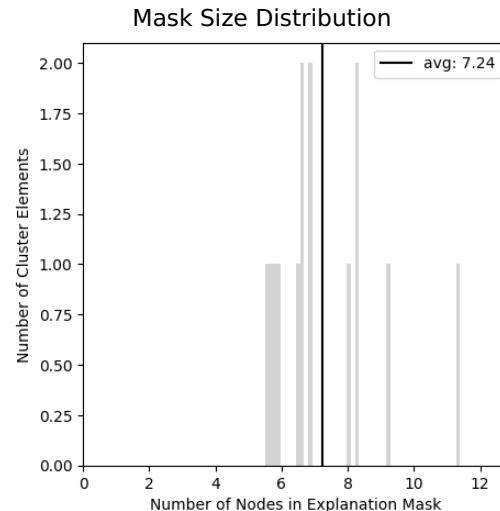
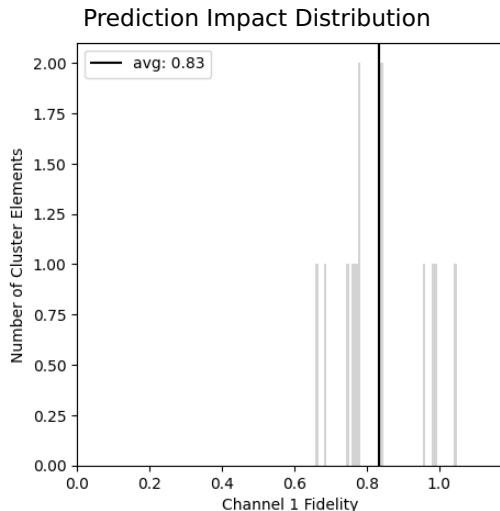
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	14
Channel Index	1.0 (0.0)

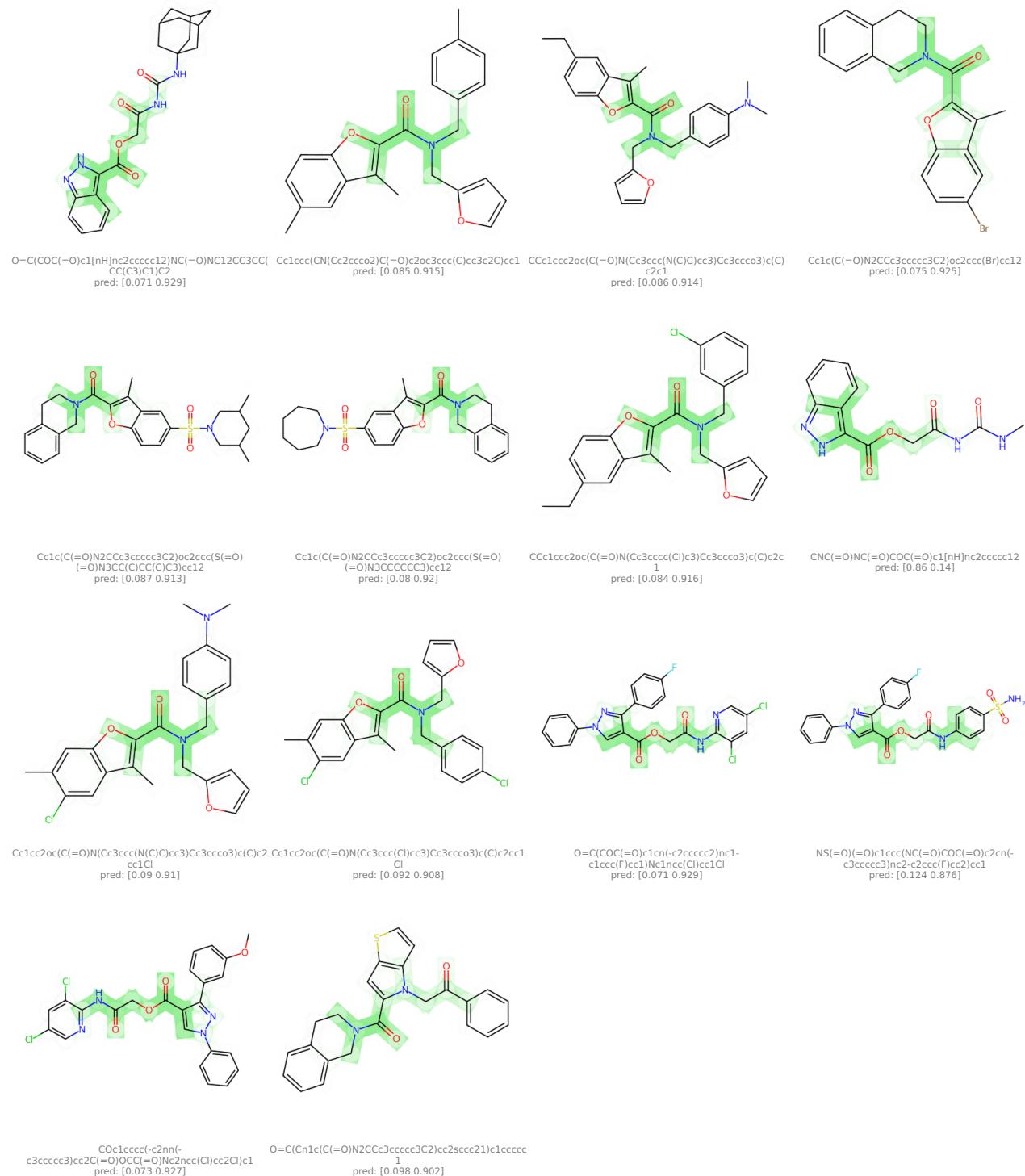
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #86 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 86, from importance channel 1 (*aggregator*), represents a motif consisting of 8.6 (± 1.6) nodes. The concept is generally associated with an impact of 1.2 (± 0.7) on the prediction outcome.

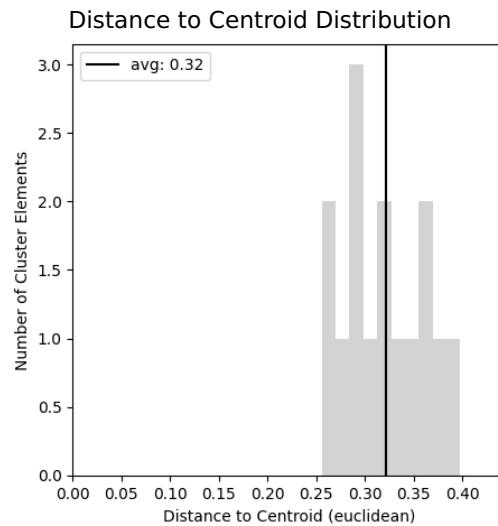
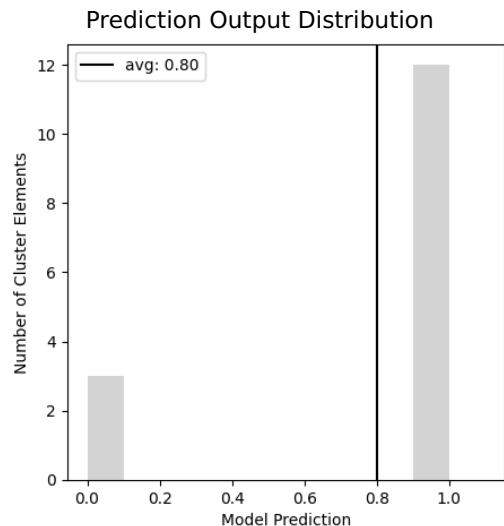
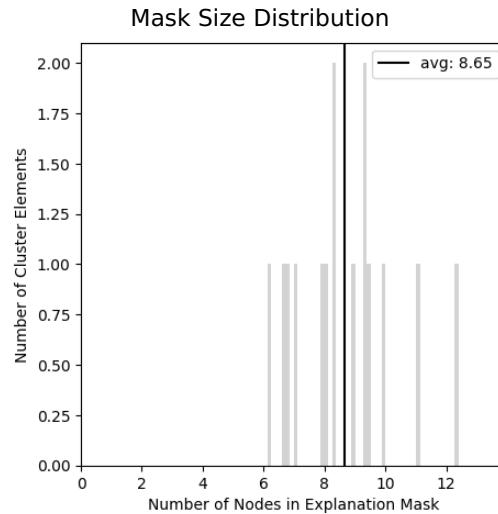
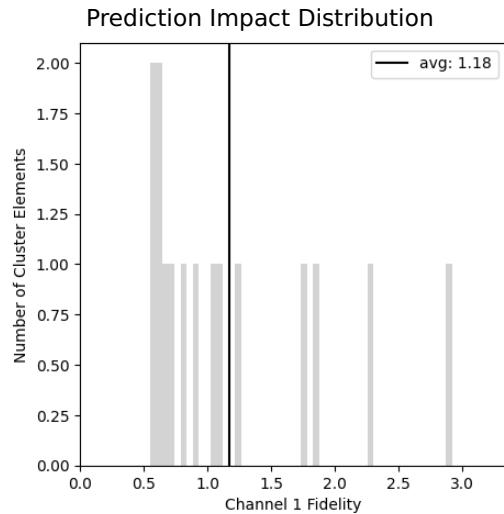
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	15
Channel Index	1.0 (0.0)

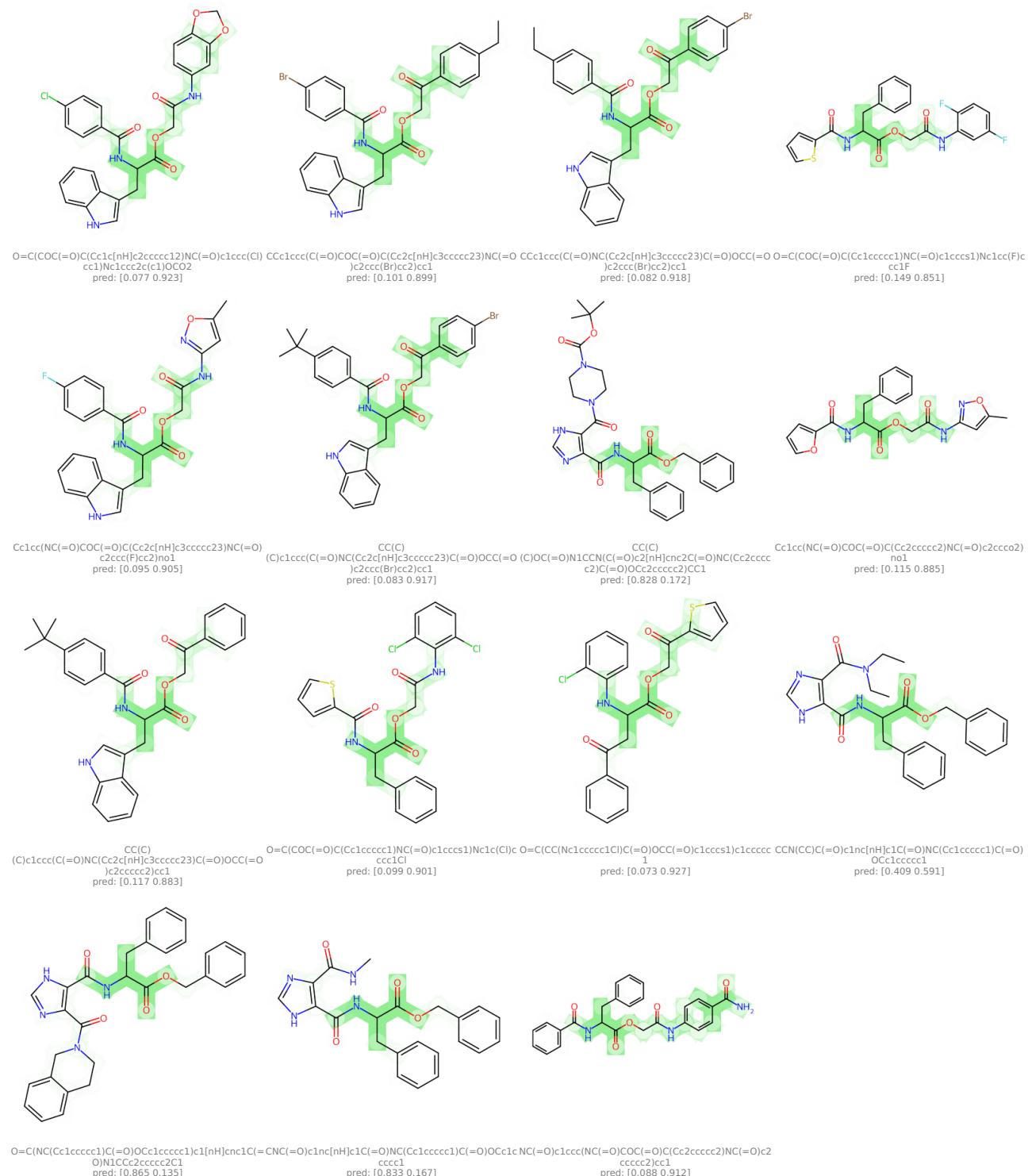
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #87 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 87, from importance channel 1 (*aggregator*), represents a motif consisting of 9.5 (± 1.1) nodes. The concept is generally associated with an impact of 1.4 (± 0.5) on the prediction outcome.

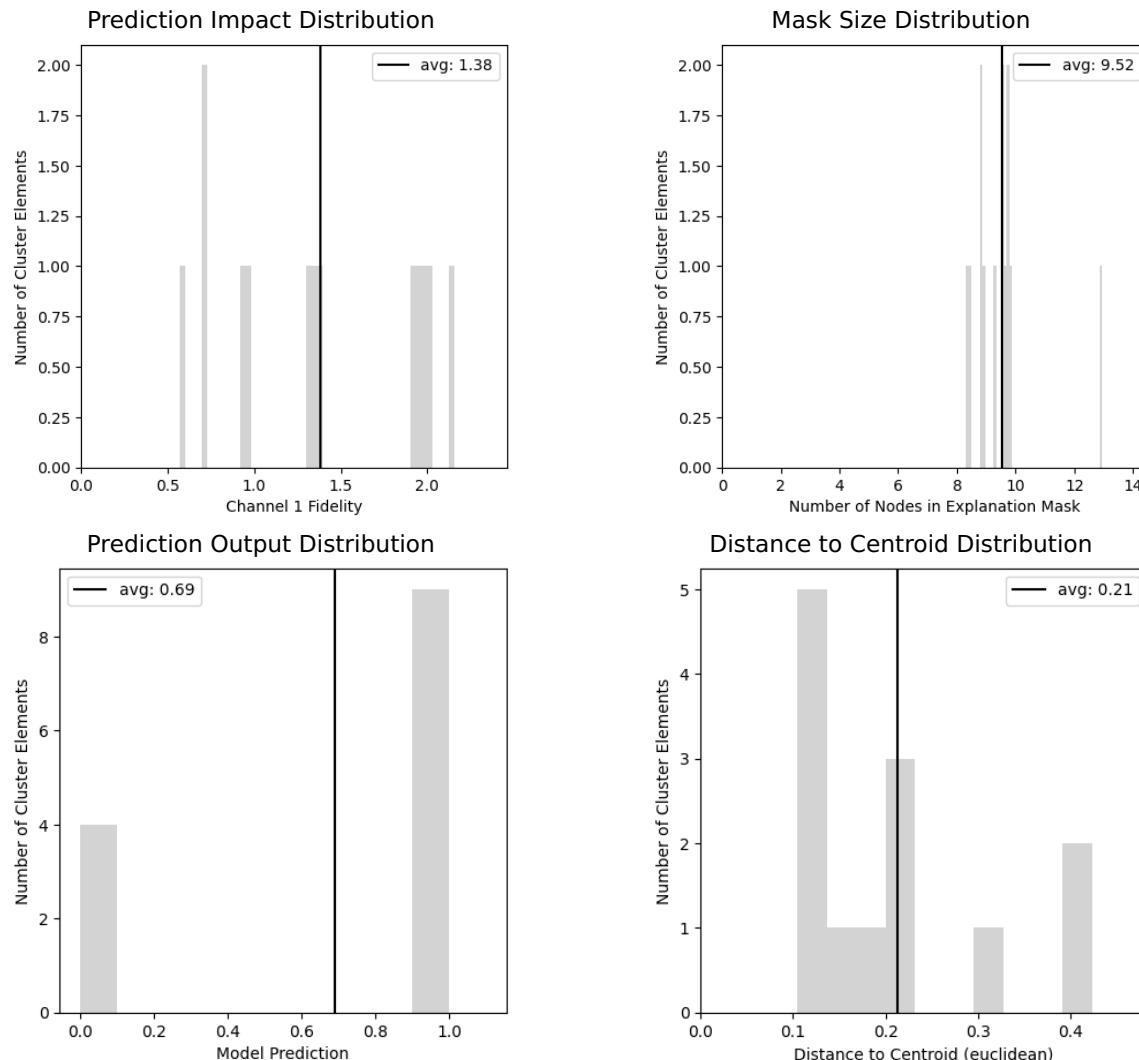
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	13
Channel Index	1.0 (0.0)

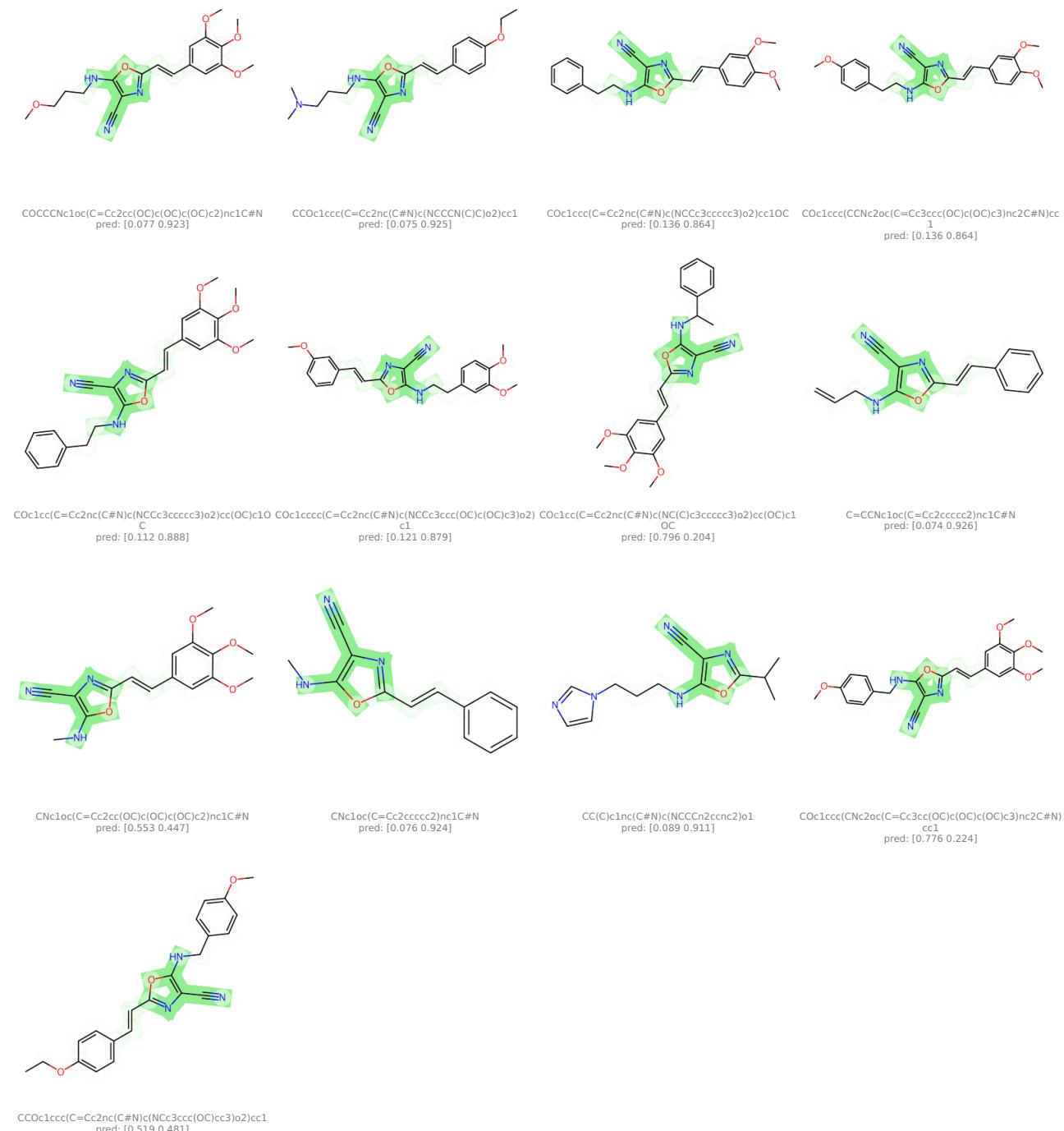
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #88 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 88, from importance channel 1 (*aggregator*), represents a motif consisting of 7.9 (± 2.0) nodes. The concept is generally associated with an impact of 1.1 (± 0.5) on the prediction outcome.

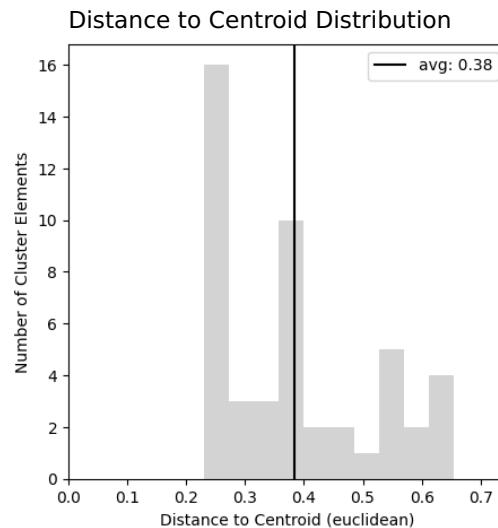
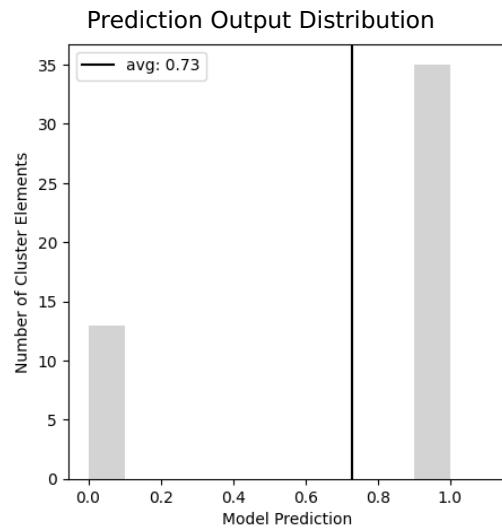
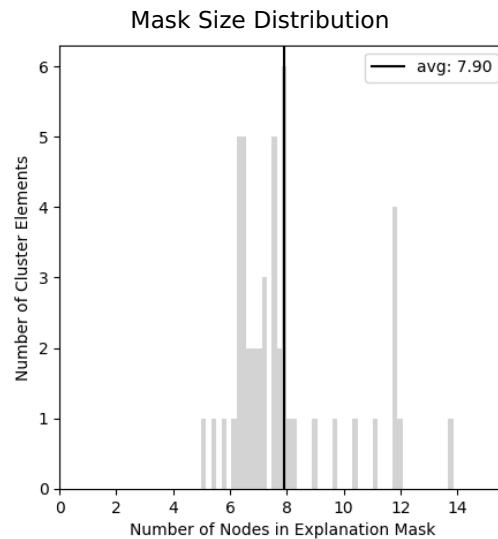
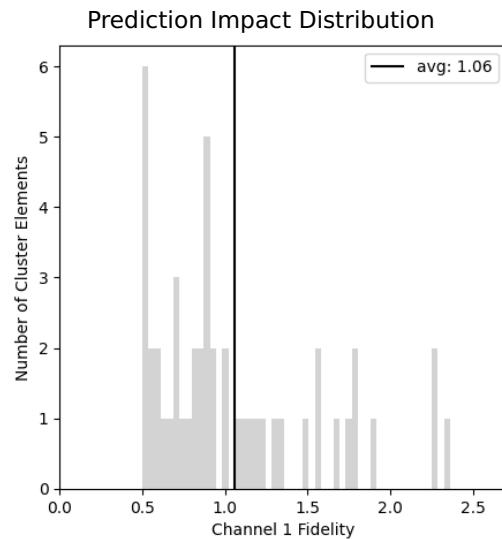
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	48
Channel Index	1.0 (0.0)

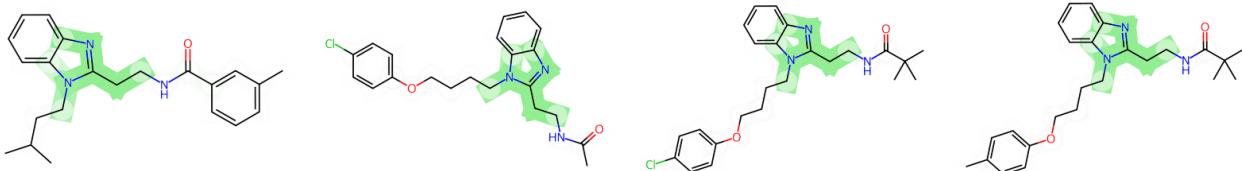
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.

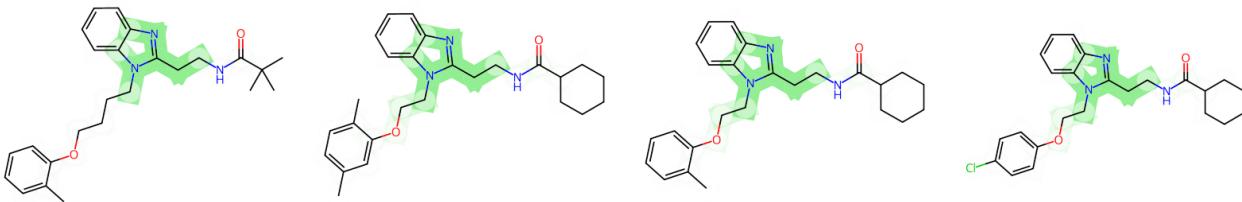


Cc1cccc(C(=O)NCc2nc3cccc3n2CCC(C)c1
pred: [0.084 0.916]

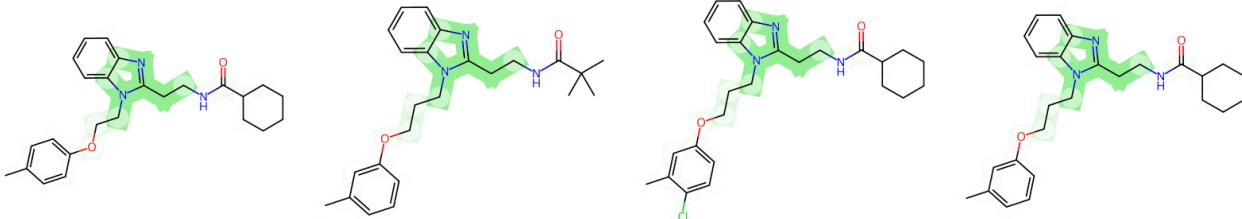
CC(=O)NCCc1nc2cccc2n1CCCCo1ccc(Cl)cc1
pred: [0.498 0.502]

CC(C)(C)C(=O)NCCc1nc2cccc2n1CCCCo1ccc(Cl)cc1
pred: [0.906 0.094]

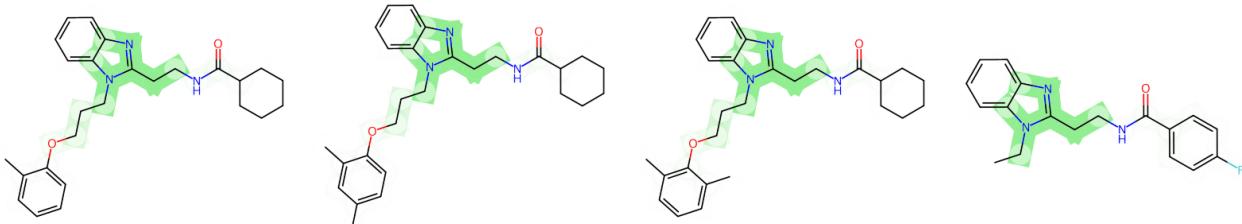
Cc1ccc(OCCCCn2c(CCNC(=O)C(C)C)c3cccc32 Cc1cccc1OCCn1c(CCNC(=O)C2CCCCC2)nc2cccc21 O=C(NCCc1nc2cccc2n1CCo1ccc(Cl)cc1)C1CCCCC1
pred: [0.906 0.094]



Cc1cccc1OCCCCn1c(CCNC(=O)C(C)C)c3cccc21 Cc1ccc(C)c(OCCn2c(CCNC(=O)C3CCCCC3)nc3cccc32 Cc1cccc1OCCn1c(CCNC(=O)C2CCCCC2)nc2cccc21 O=C(NCCc1nc2cccc2n1CCo1ccc(Cl)cc1)C1CCCCC1
pred: [0.908 0.092] pred: [0.084 0.916]



Cc1ccc(OCCn2c(CCNC(=O)C3CCCCC3)nc3cccc32)cc1 Cc1cccc(OCCn2c(CCNC(=O)C(C)C)c3cccc32)c1 Cc1cc(OCCn2c(CCNC(=O)C3CCCCC3)nc3cccc32)cc1 Cc1cccc(OCCn2c(CCNC(=O)C3CCCCC3)nc3cccc32)
pred: [0.077 0.923] pred: [0.899 0.101] pred: [0.073 0.927] pred: [0.074 0.926]



Cc1cccc1OCCn1c(CCNC(=O)C2CCCCC2)nc2cccc21 Cc1ccc(OCCn2c(CCNC(=O)C3CCCCC3)nc3cccc32)c1 Cc1cccc(C)c1OCCn1c(CCNC(=O)C2CCCCC2)nc2cccc21 Cc1cccc(C)c1OCCn1c(CCNC(=O)C2CCCCC2)nc2cccc21
pred: [0.081 0.919] pred: [0.246 0.754] pred: [0.084 0.916] pred: [0.159 0.841]

Cluster #89 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 89, from importance channel 1 (*aggregator*), represents a motif consisting of 7.8 (± 1.2) nodes. The concept is generally associated with an impact of 1.3 (± 0.6) on the prediction outcome.

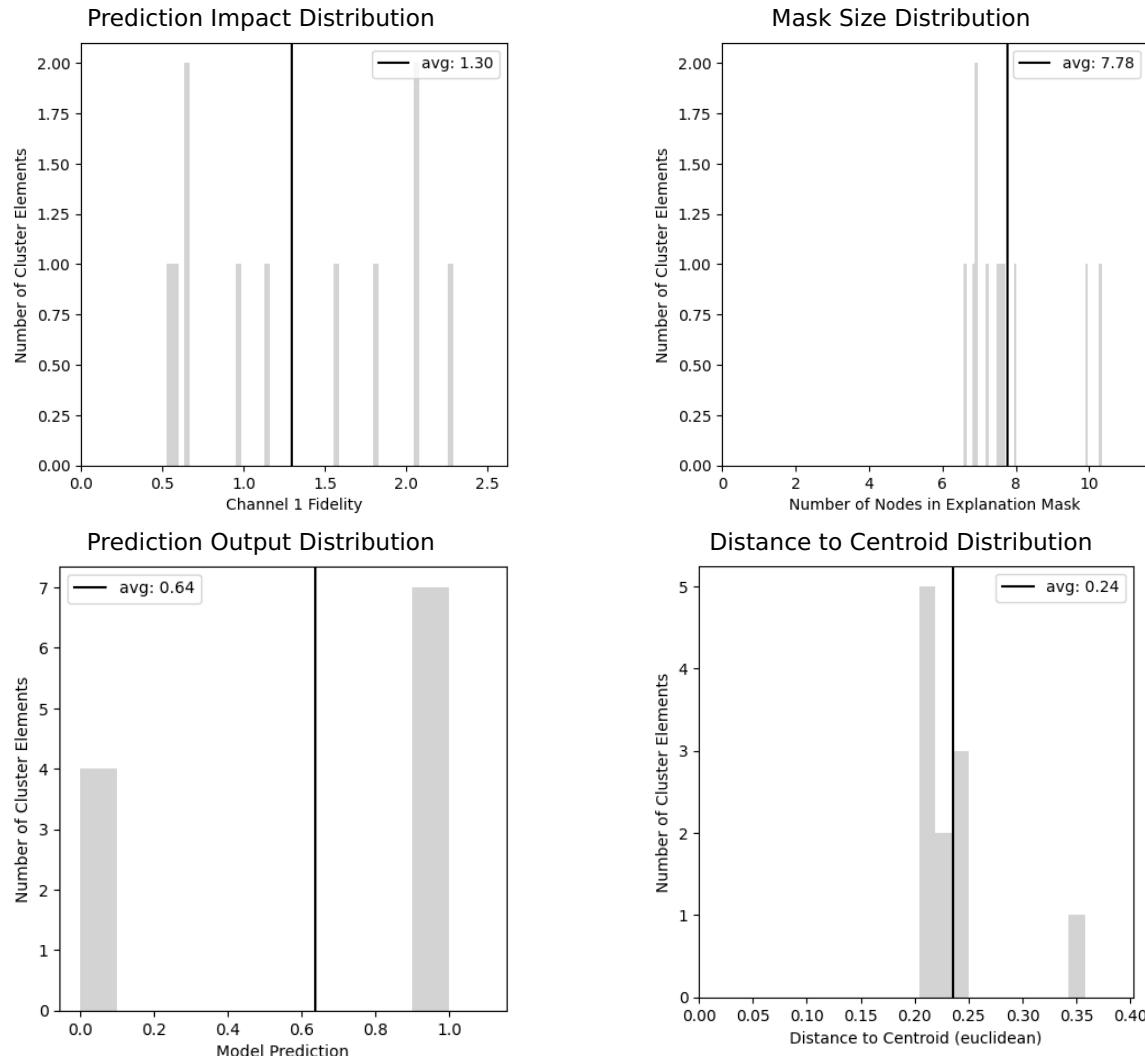
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	11
Channel Index	1.0 (0.0)

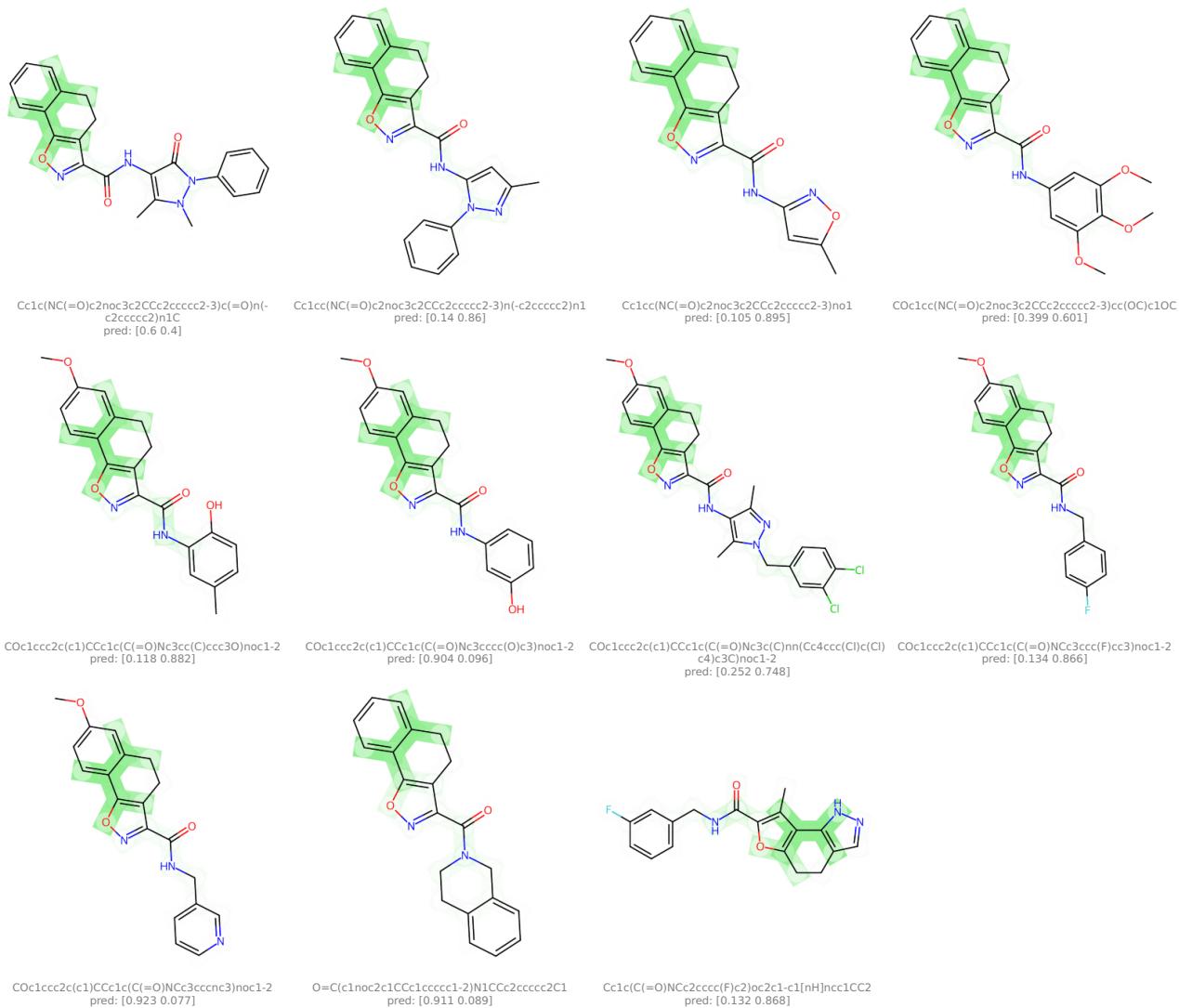
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #90 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 90, from importance channel 1 (*aggregator*), represents a motif consisting of 8.7 (± 0.9) nodes. The concept is generally associated with an impact of 1.5 (± 0.7) on the prediction outcome.

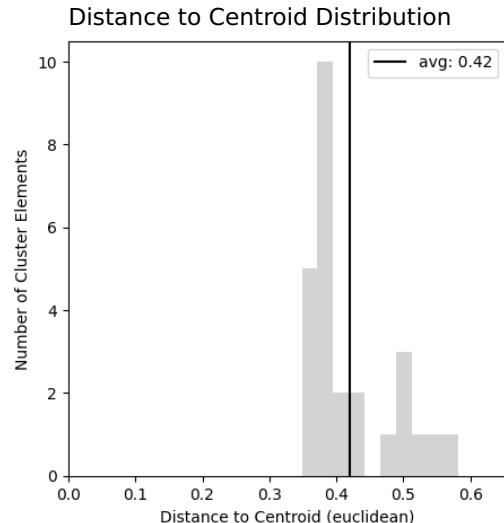
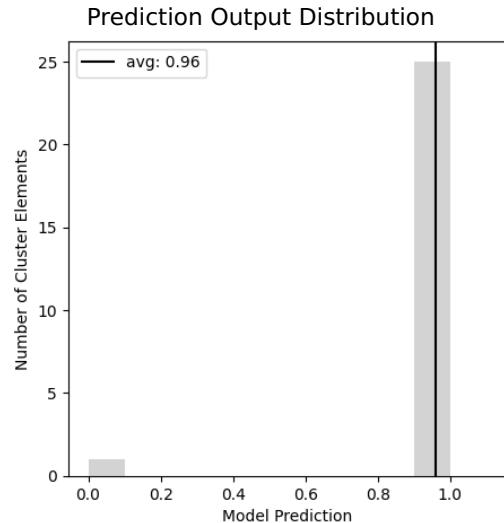
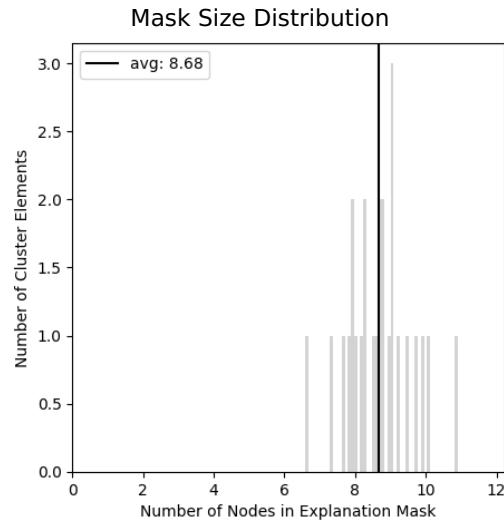
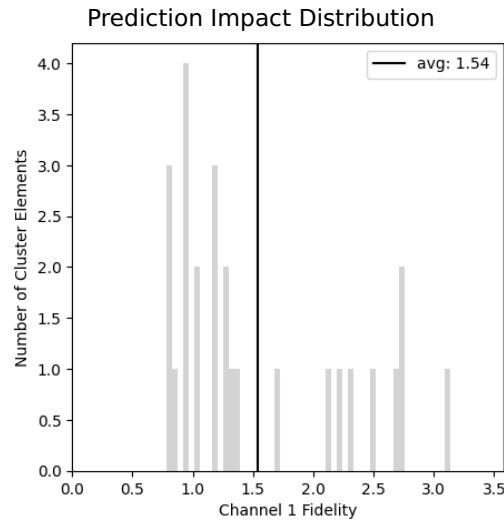
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	26
Channel Index	1.0 (0.0)

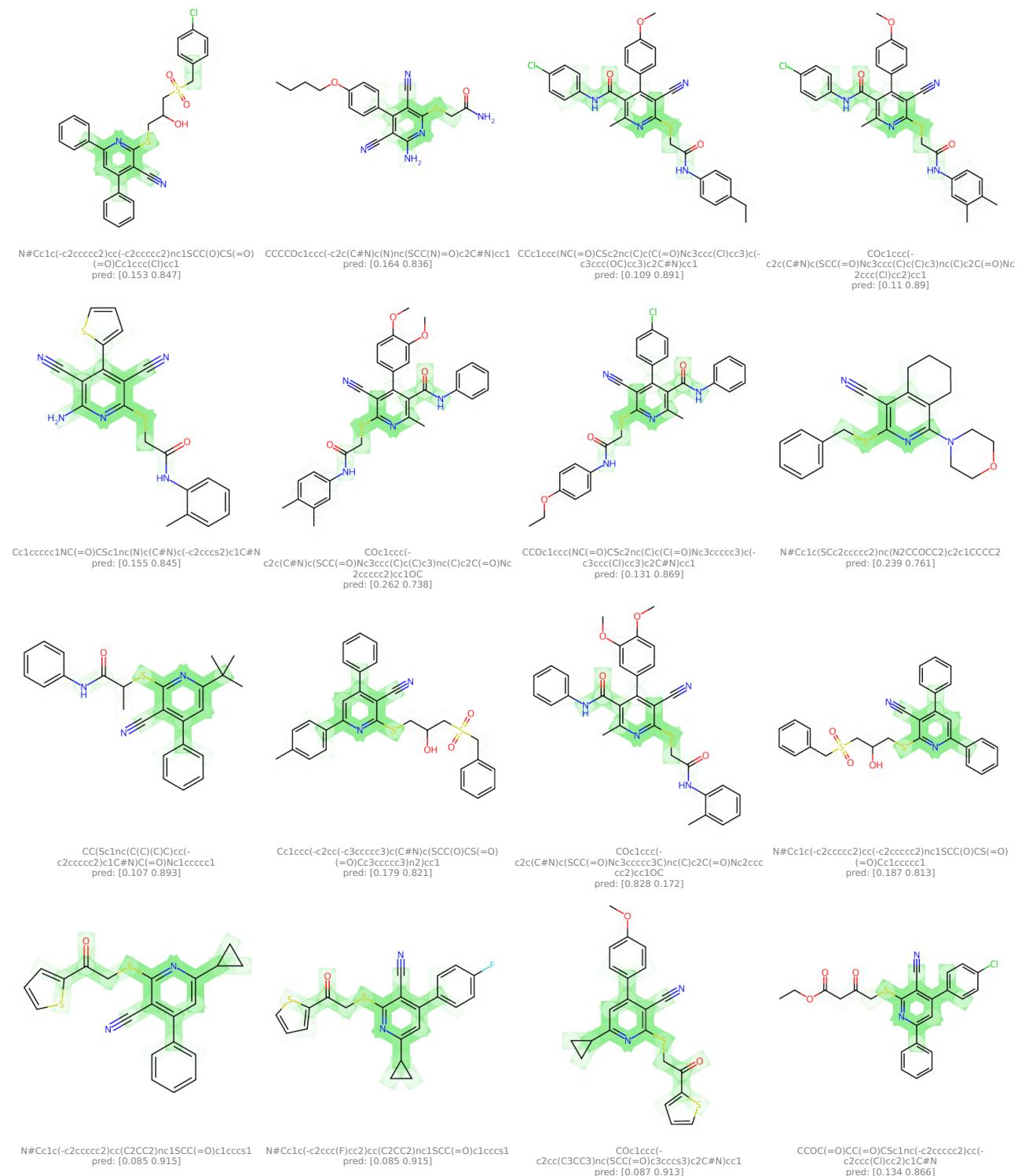
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #91 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 91, from importance channel 1 (*aggregator*), represents a motif consisting of 7.7 (± 1.6) nodes. The concept is generally associated with an impact of 1.5 (± 0.6) on the prediction outcome.

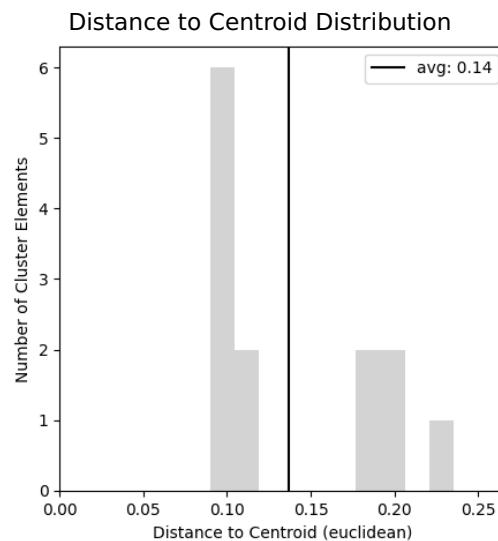
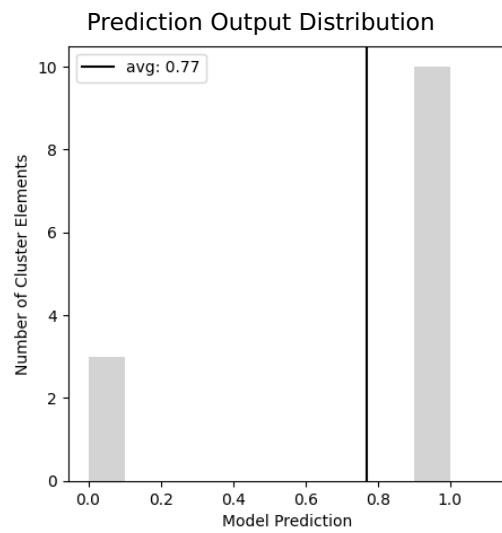
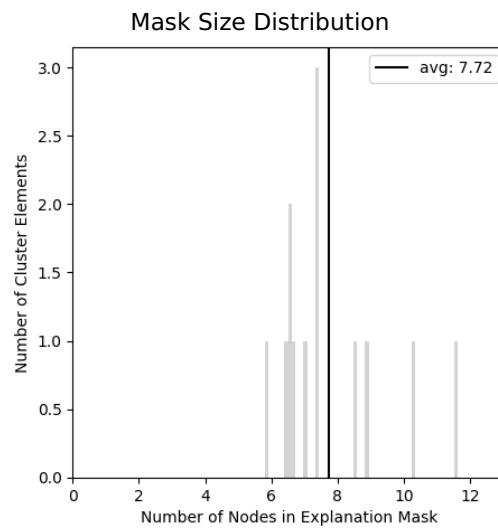
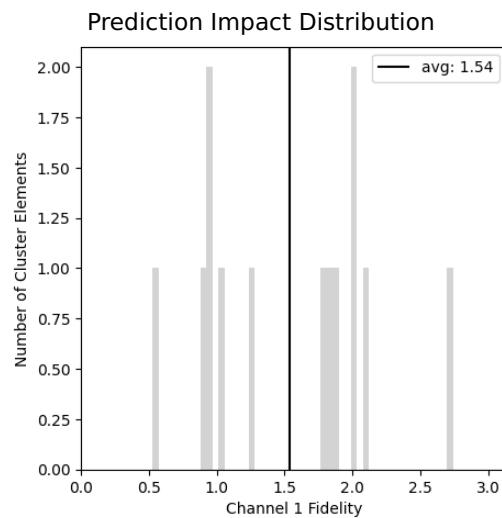
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	13
Channel Index	1.0 (0.0)

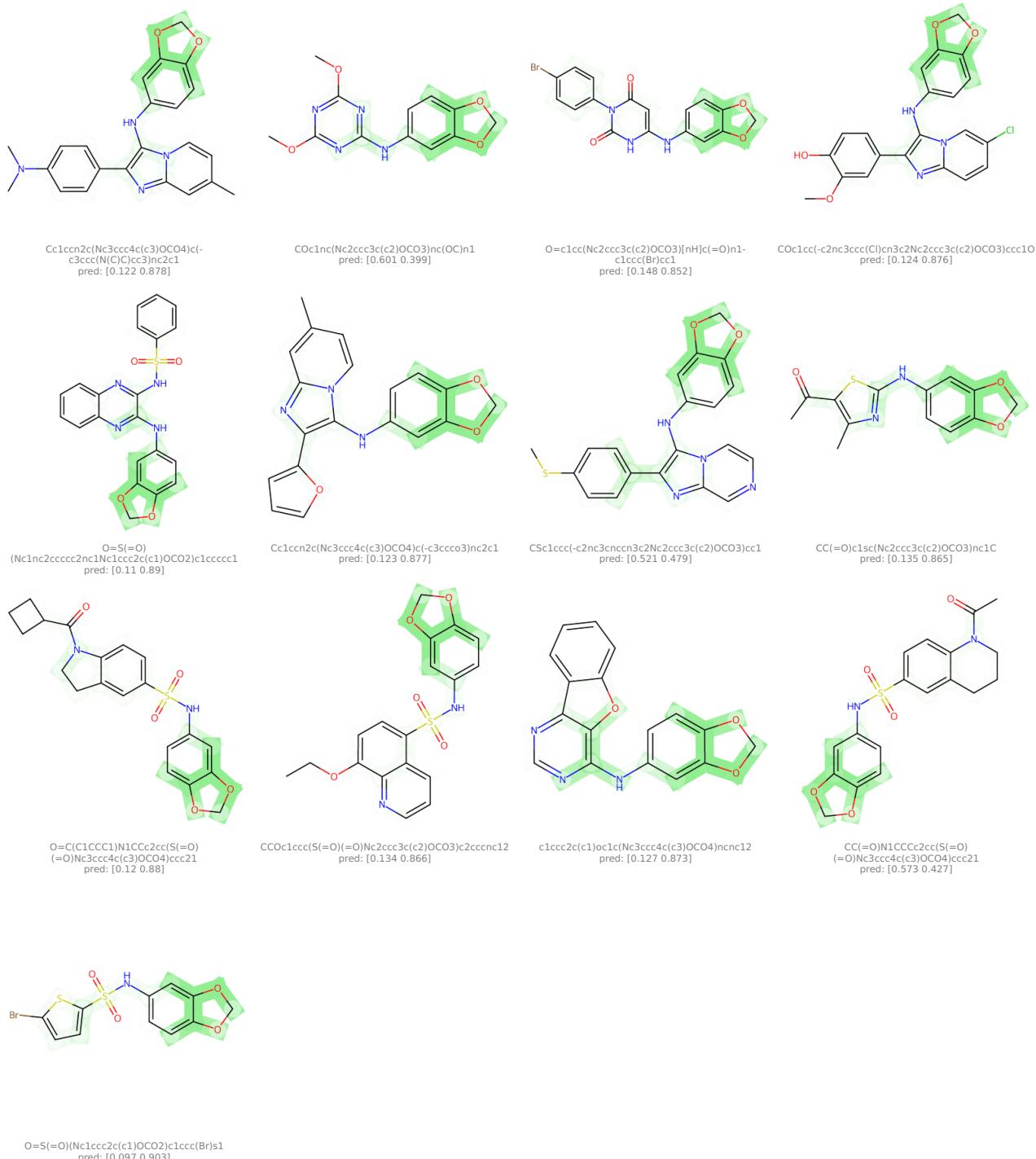
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #92 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 92, from importance channel 1 (*aggregator*), represents a motif consisting of 8.6 (± 0.6) nodes. The concept is generally associated with an impact of 1.7 (± 0.9) on the prediction outcome.

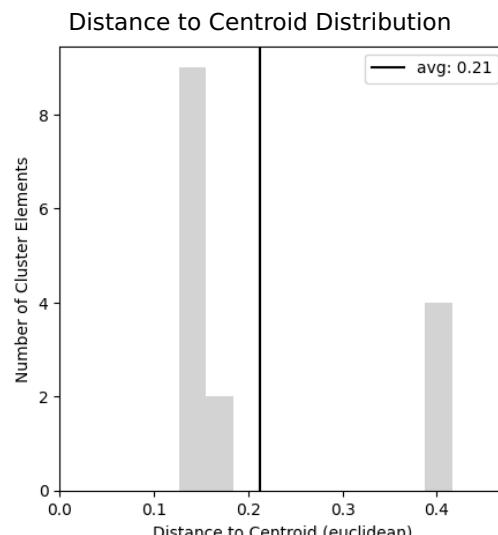
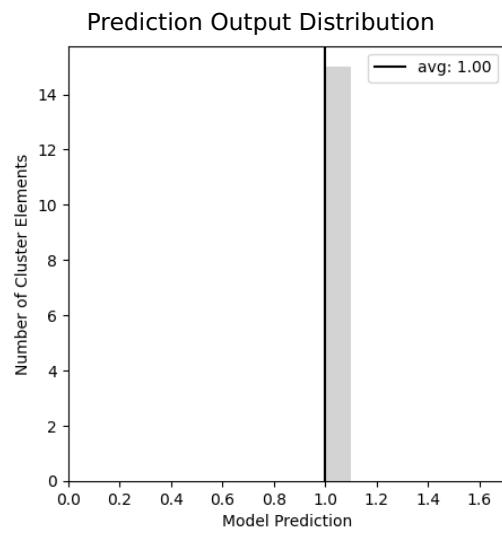
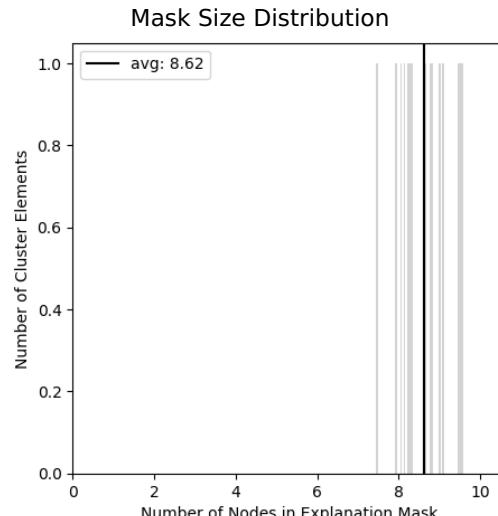
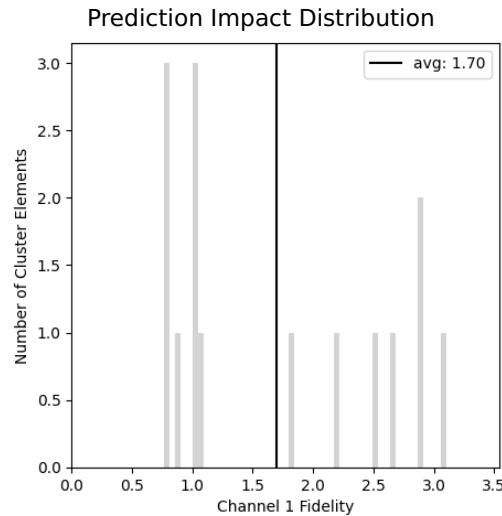
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	15
Channel Index	1.0 (0.0)

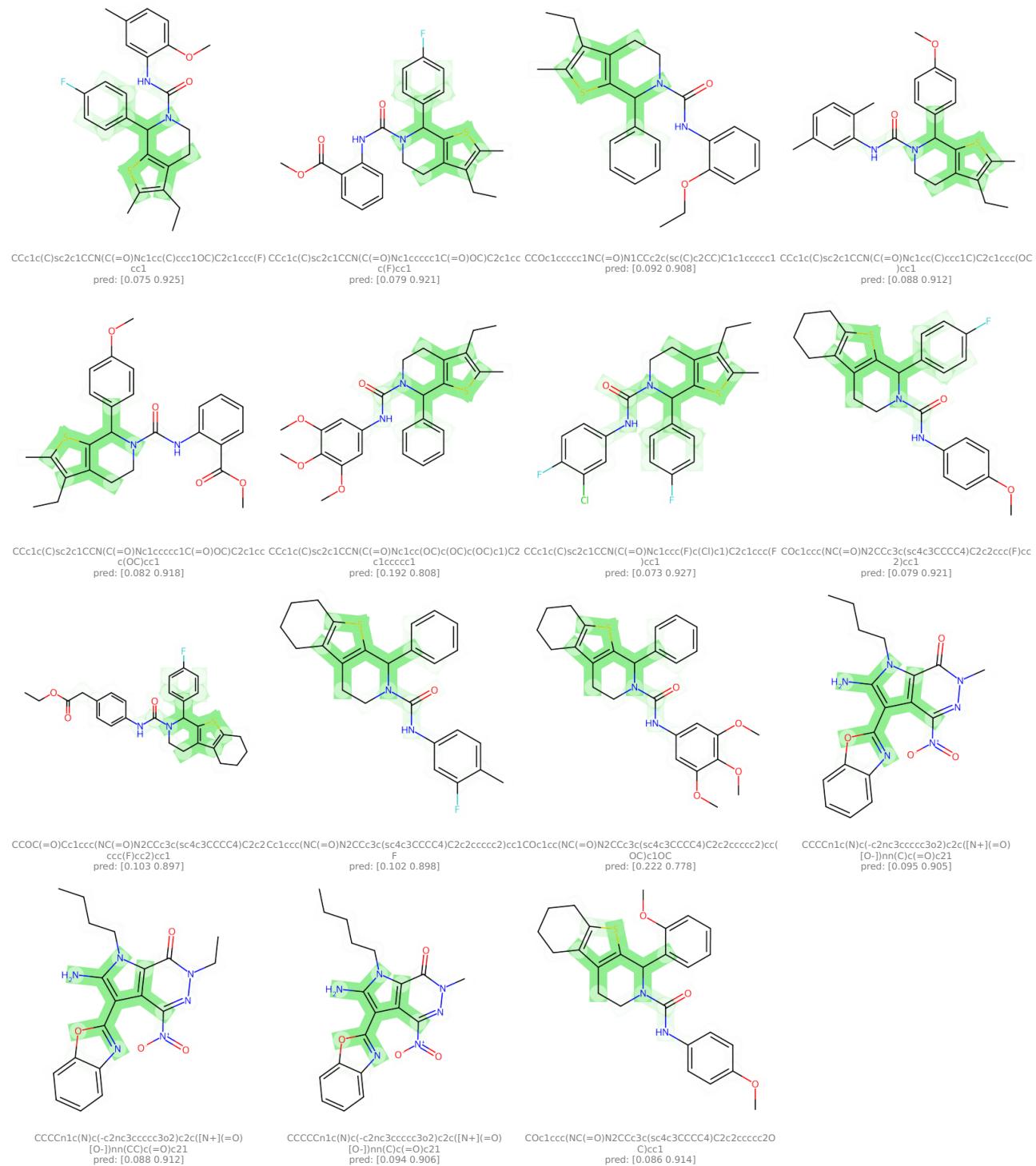
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #93 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 93, from importance channel 1 (*aggregator*), represents a motif consisting of 8.2 (± 1.6) nodes. The concept is generally associated with an impact of 1.2 (± 0.6) on the prediction outcome.

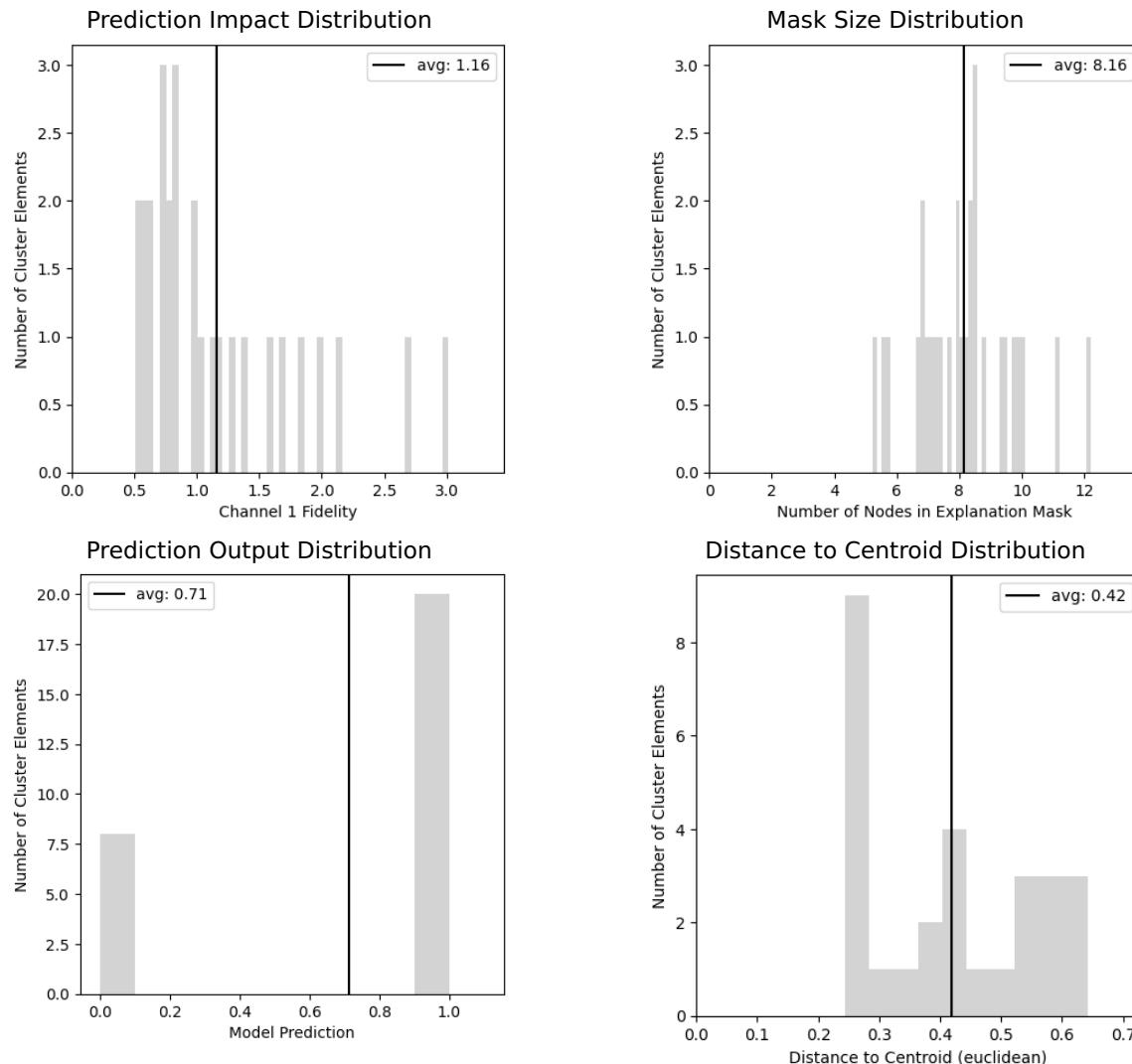
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	28
Channel Index	1.0 (0.0)

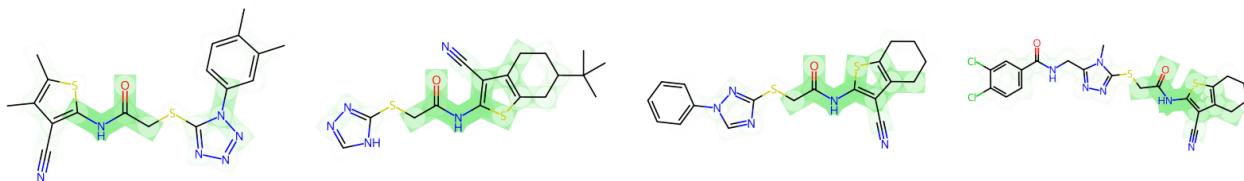
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.

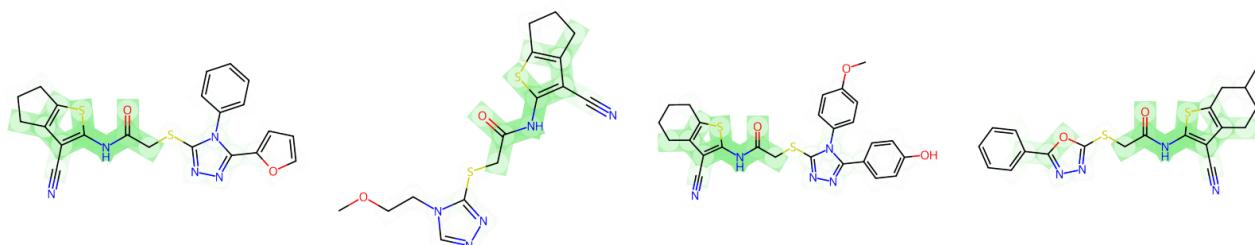


Cc1ccc(-n2nnnc2SCC(=O)Nc2sc(C)c(C)c2#N)cc1C CC(C)(C)C1Cc2c(sc(NC(=O)CSc3nn[nH]3)c2C#N)C1 N#Cc1c(NC(=O)CSc2ncn(-c3cccc3)n2)sc2c1CCCC2 Cn1c(CNC(=O)c2cc(Cl)c(Cl)c2)nn1SCC(=O)Nc1sc2c c1C#N)CCCC2
pred: [0.098 0.902]

CC(C)(C)C1Cc2c(sc(NC(=O)CSc3nn[nH]3)c2C#N)C1 N#Cc1c(NC(=O)CSc2ncn(-c3cccc3)n2)sc2c1CCCC2 Cn1c(CNC(=O)c2cc(Cl)c(Cl)c2)nn1SCC(=O)Nc1sc2c c1C#N)CCCC2
pred: [0.501 0.499]

Cn1c(CNC(=O)c2cc(Cl)c(Cl)c2)nn1SCC(=O)Nc1sc2c c1C#N)CCCC2
pred: [0.144 0.856]

Cn1c(CNC(=O)c2cc(Cl)c(Cl)c2)nn1SCC(=O)Nc1sc2c c1C#N)CCCC2
pred: [0.137 0.863]

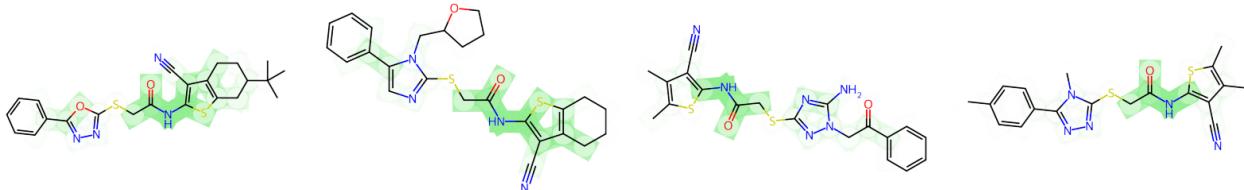


N#Cc1c(NC(=O)CSc2nn(-c3ccco3)n2- c2cccc2)sc2c1CCCC2
pred: [0.146 0.854]

COCc1cnnn1SCC(=O)Nc1sc2(c1C#N)CCCC2
pred: [0.881 0.119]

COc1ccc(-n2c(SCC(=O)Nc3sc4(c3C#N)CCCC4)nn2- c2ccc(O)cc2)cc1
pred: [0.085 0.915]

CC1Cc2c(sc(NC(=O)CSc3nn(-c4cccc4)o3)c2C#N)C1
pred: [0.089 0.911]



CC(C)(C)C1Cc2c(sc(NC(=O)CSc3nn(-c4cccc4)o3)c2C#N)C1
pred: [0.083 0.917]

N#Cc1c(NC(=O)CSc2ncc(-c3cccc3)n2)sc2c1CCCC2
pred: [0.128 0.872]

Cc1sc(NC(=O)CSc2nc(N)n(CC(=O)c3cccc3)n2)c(C#N)Cc1ccc(-c2nnc(SCC(=O)Nc3sc(C)c(C)c3C#N)n2)cc1
pred: [0.152 0.848]

CCOC(=O)c1sc(NC(=O)CSc2n[nH]c(-c3ccc(Cl)cc3)n2)c(C#N)c1C
pred: [0.806 0.194]

Cc1ccc(C(=O)OCC(=O)Nc2sc3c(c2C#N)CCCC3)cc1NC Cc1ccc(C(=O)OCC(=O)Nc2sc3c(c2C#N)CCCC3)cc1N
pred: [0.11 0.89]

Cc1ccc(C(=O)OCC(=O)Nc2sc3c(c2C#N)CCCC3)cc1N C(=O)c1ccco1
pred: [0.11 0.89]

Cc1ccc(C(=O)OCC(=O)Nc2sc3c(c2C#N)CCCC3)cc1N C(=O)c1ccco1
pred: [0.087 0.913]

Cluster #94 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 94, from importance channel 1 (*aggregator*), represents a motif consisting of 8.1 (± 0.8) nodes. The concept is generally associated with an impact of 1.2 (± 0.8) on the prediction outcome.

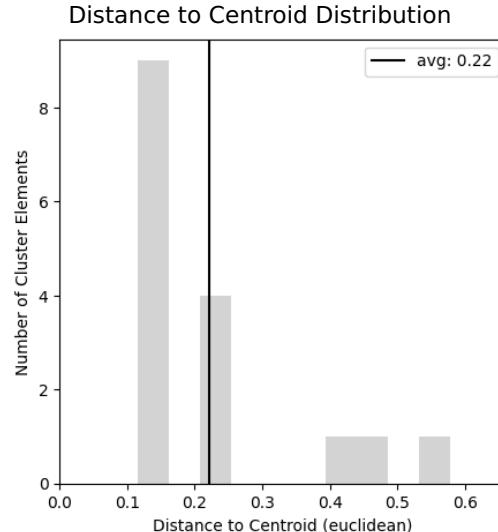
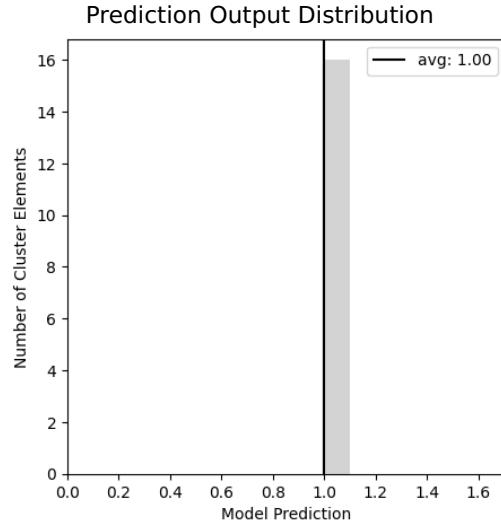
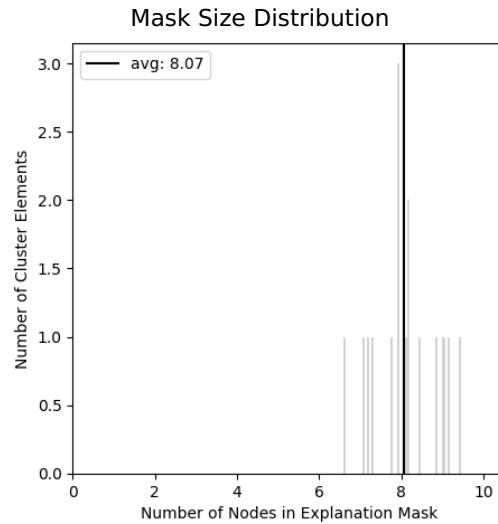
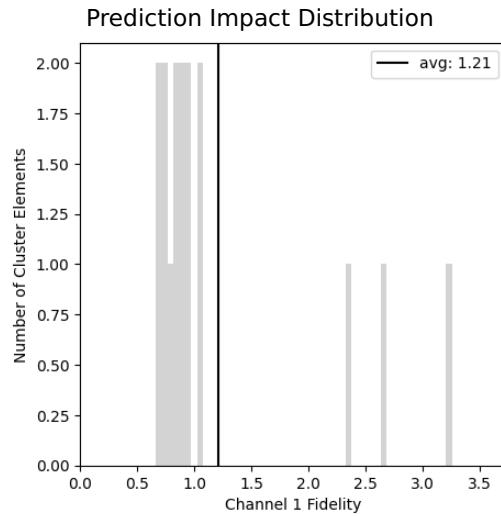
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	16
Channel Index	1.0 (0.0)

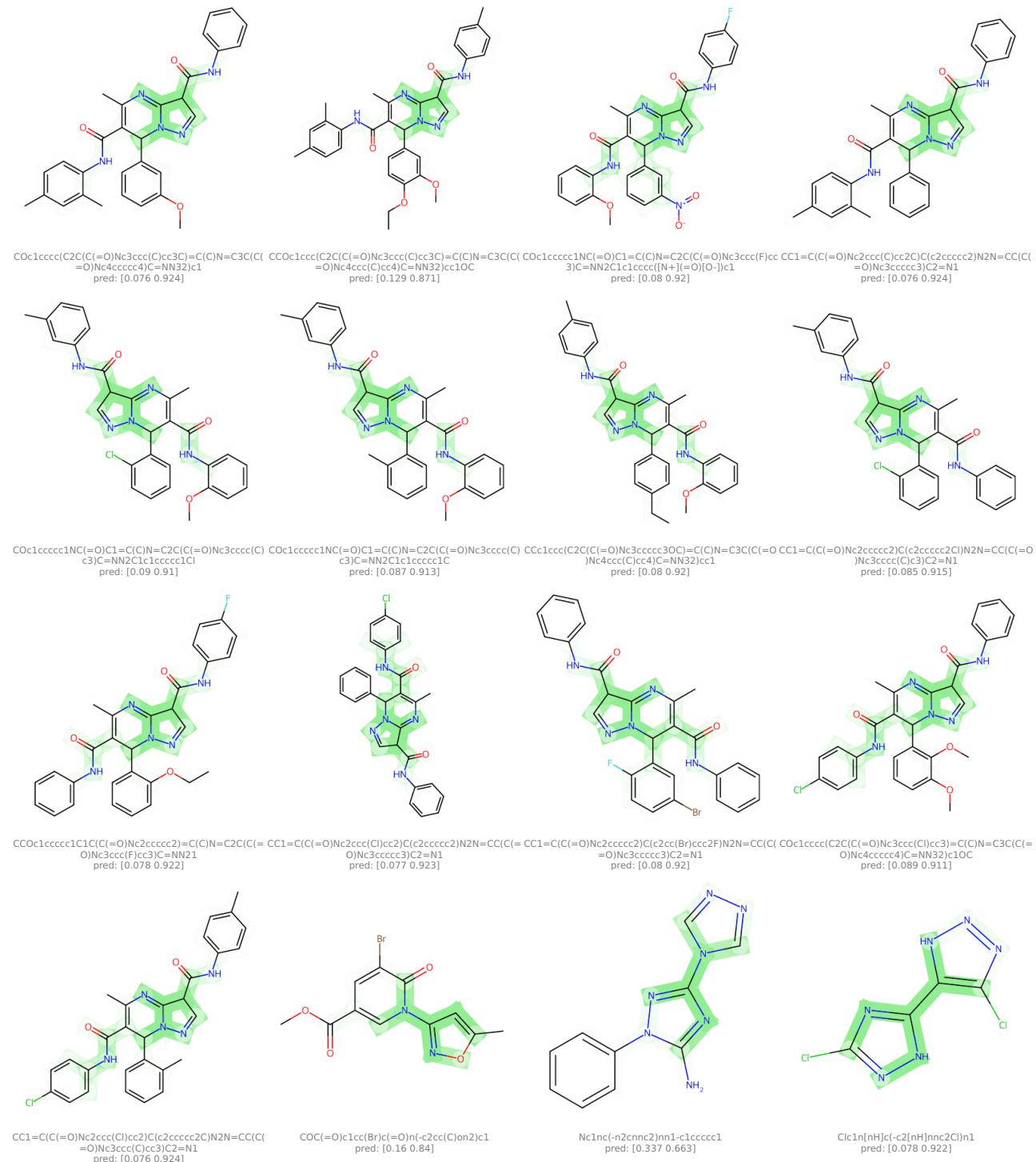
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

① This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #95 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 95, from importance channel 1 (*aggregator*), represents a motif consisting of 7.7 (± 0.6) nodes. The concept is generally associated with an impact of 1.0 (± 0.6) on the prediction outcome.

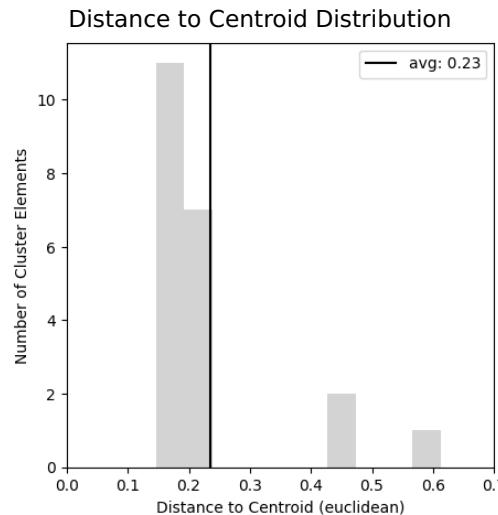
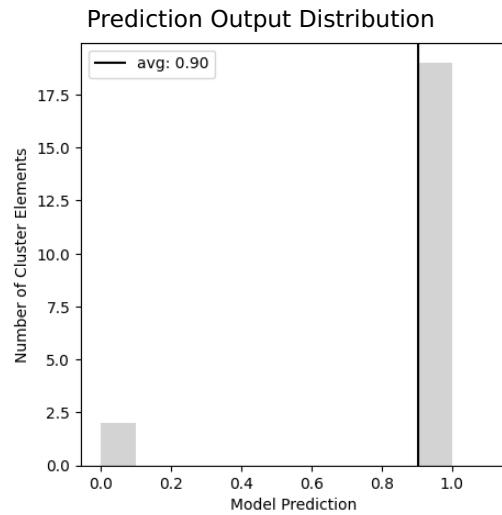
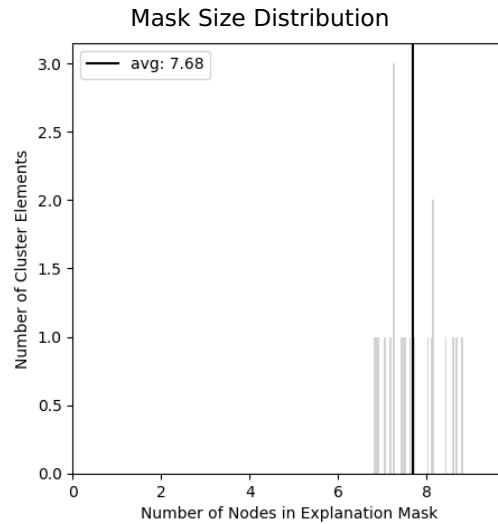
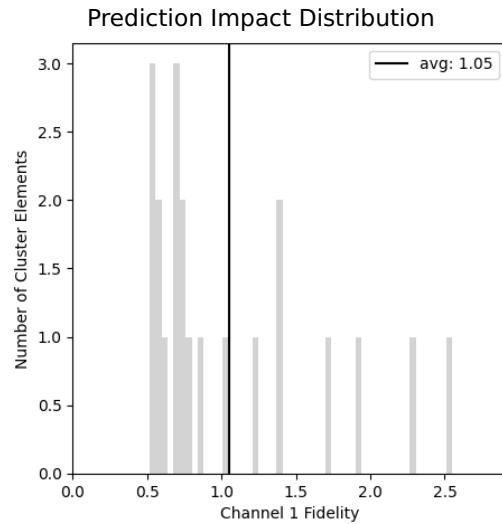
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	21
Channel Index	1.0 (0.0)

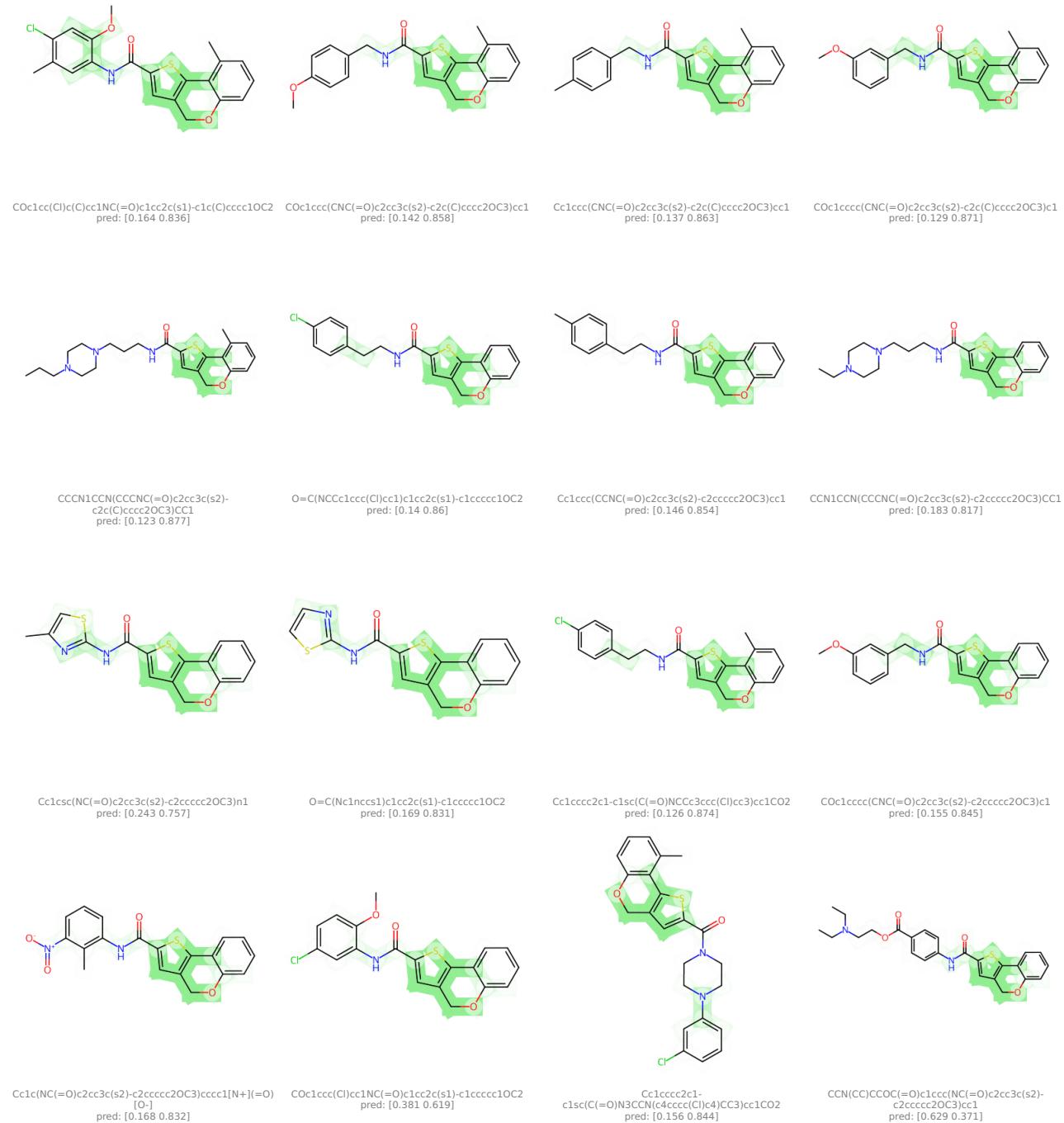
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #96 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 96, from importance channel 1 (*aggregator*), represents a motif consisting of 7.9 (± 1.1) nodes. The concept is generally associated with an impact of 1.3 (± 0.6) on the prediction outcome.

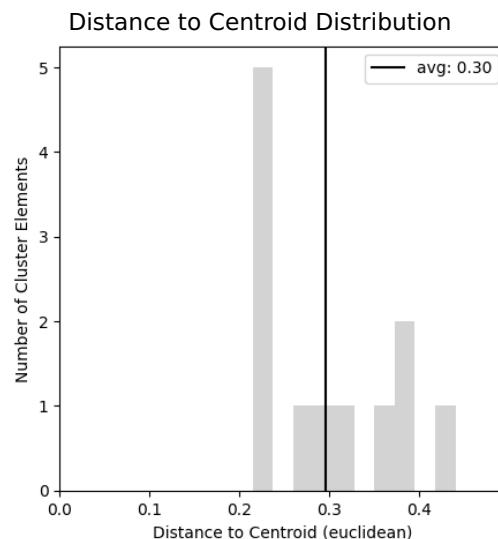
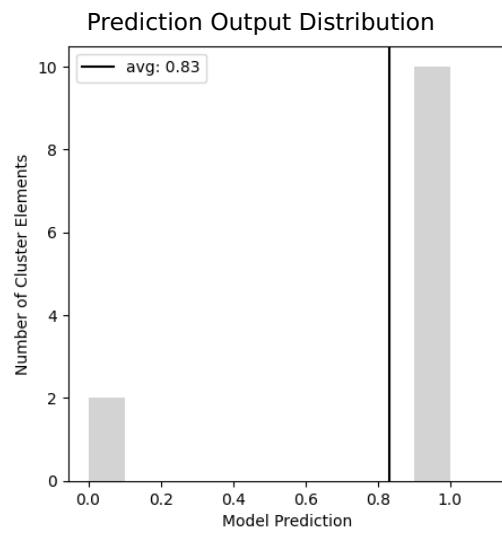
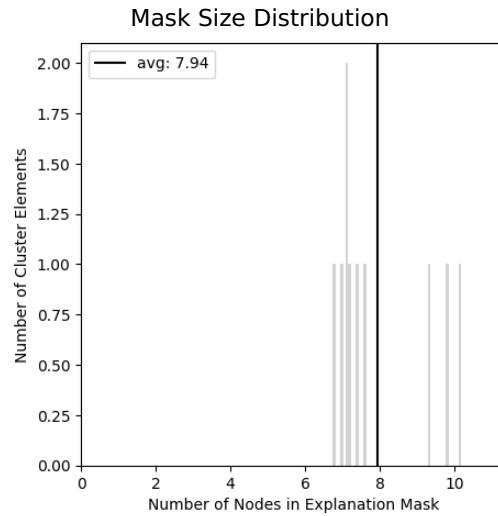
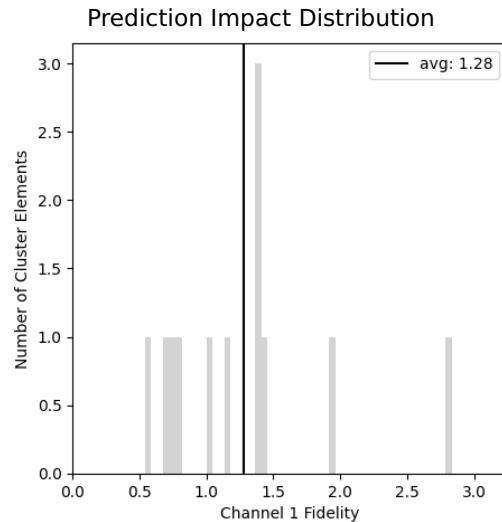
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	12
Channel Index	1.0 (0.0)

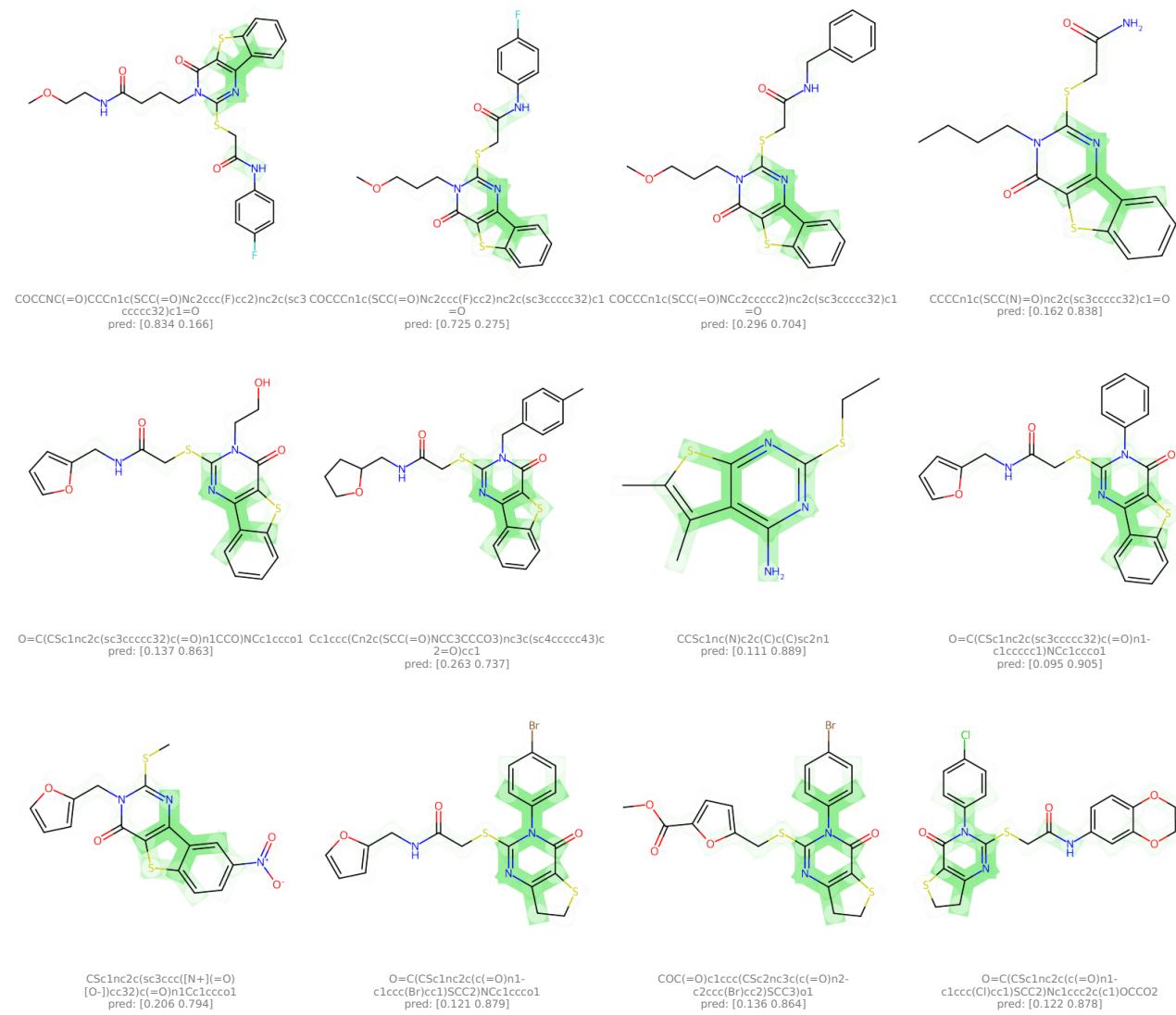
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #97 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 97, from importance channel 1 (*aggregator*), represents a motif consisting of 7.8 (± 1.0) nodes. The concept is generally associated with an impact of 1.2 (± 0.5) on the prediction outcome.

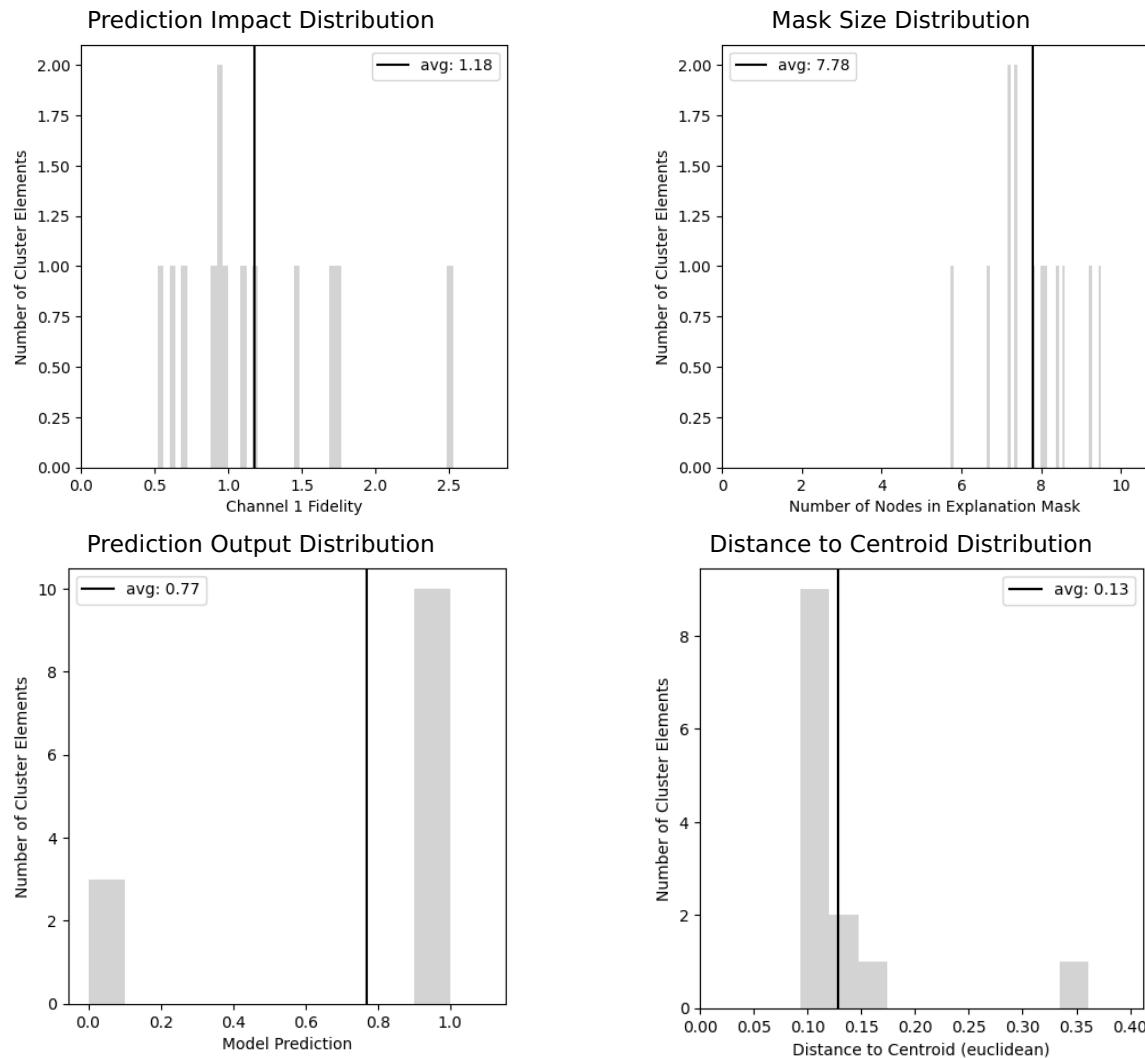
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	13
Channel Index	1.0 (0.0)

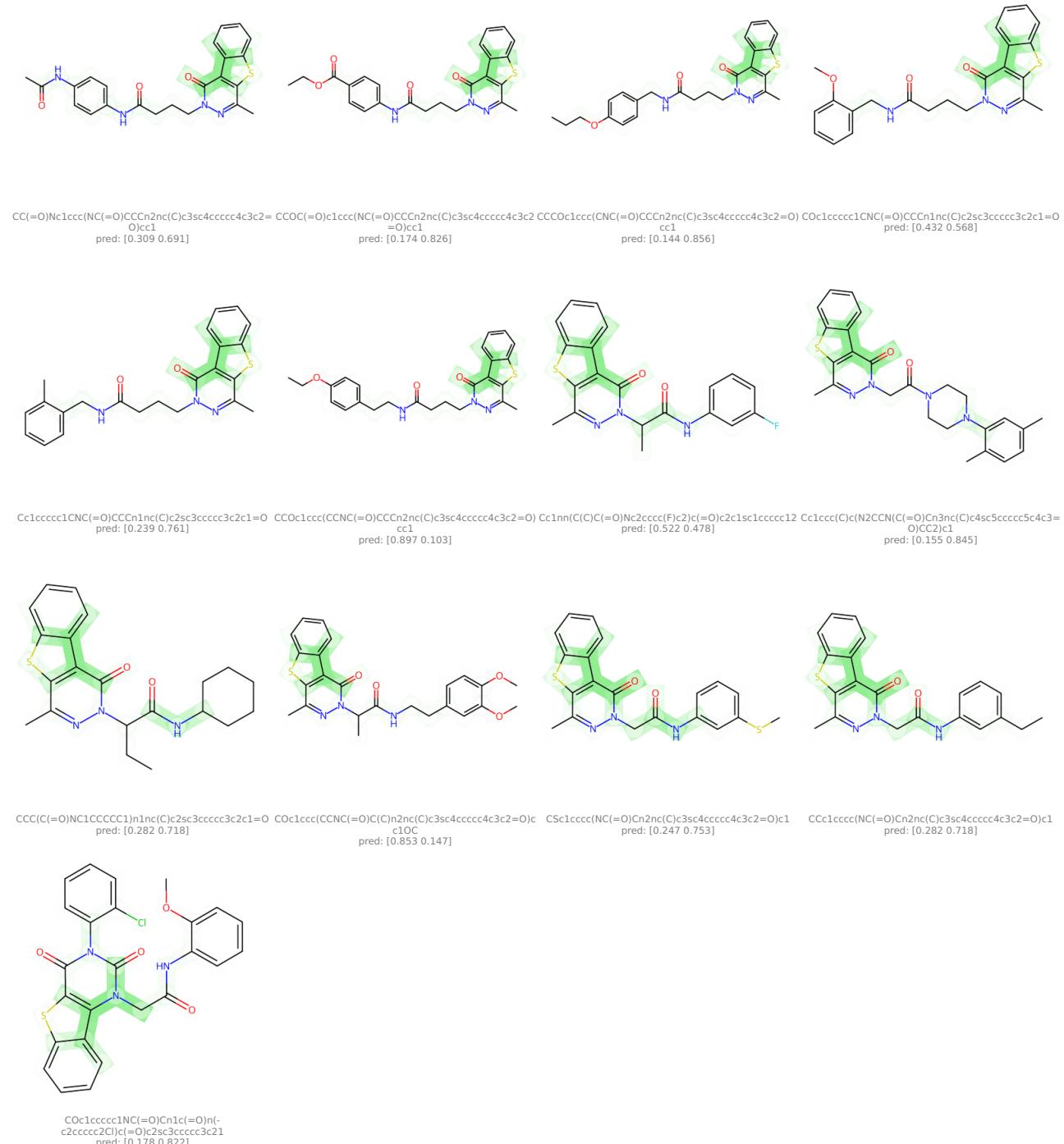
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #98 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 98, from importance channel 1 (*aggregator*), represents a motif consisting of 8.5 (± 1.3) nodes. The concept is generally associated with an impact of 1.1 (± 0.5) on the prediction outcome.

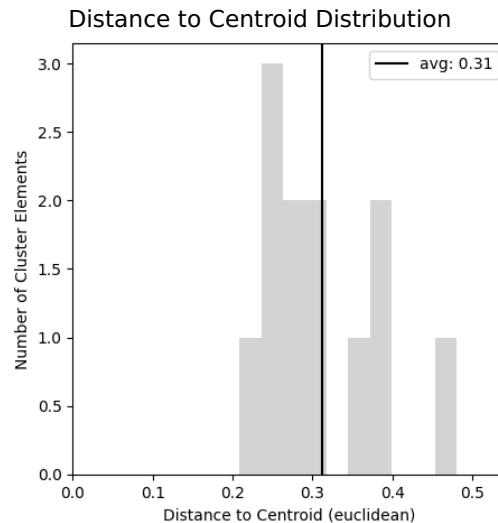
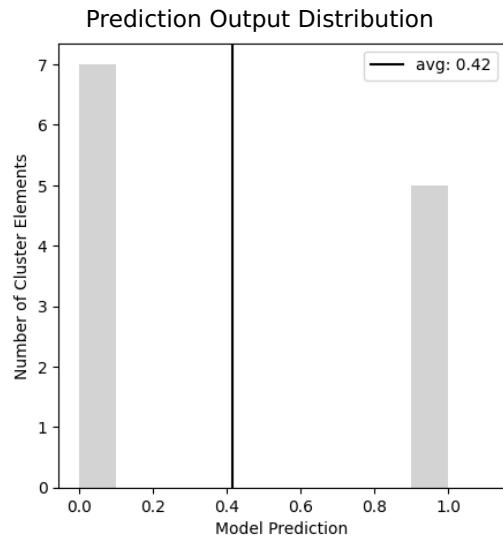
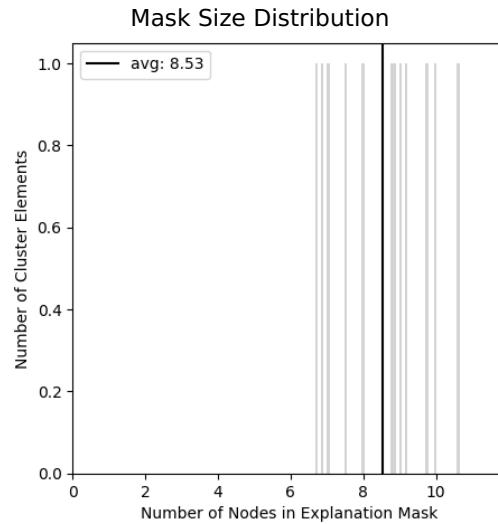
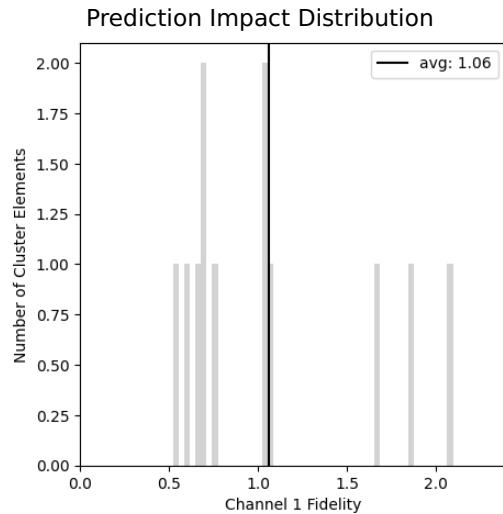
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	12
Channel Index	1.0 (0.0)

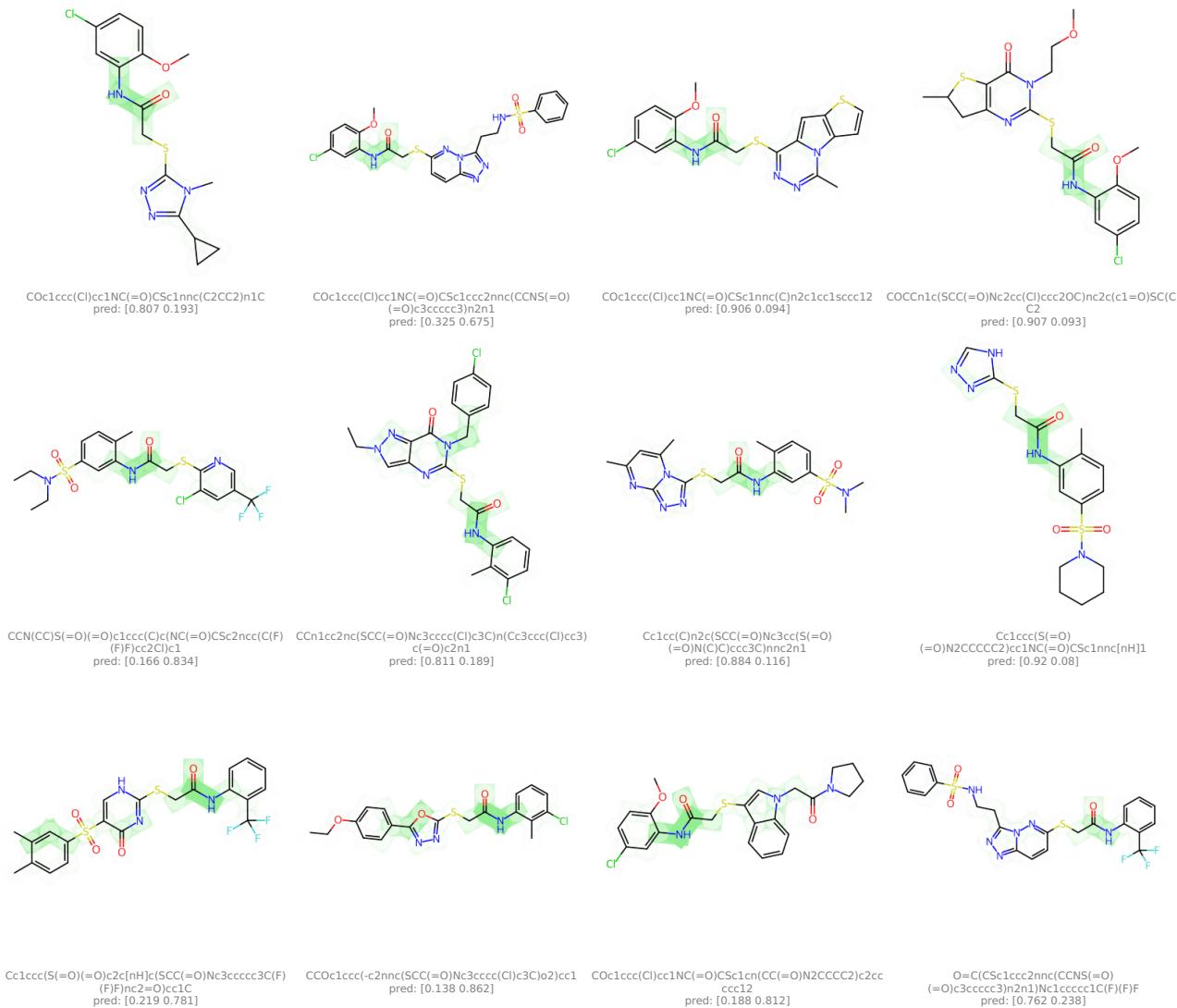
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #99 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 99, from importance channel 1 (*aggregator*), represents a motif consisting of 8.1 (± 1.4) nodes. The concept is generally associated with an impact of 0.9 (± 0.3) on the prediction outcome.

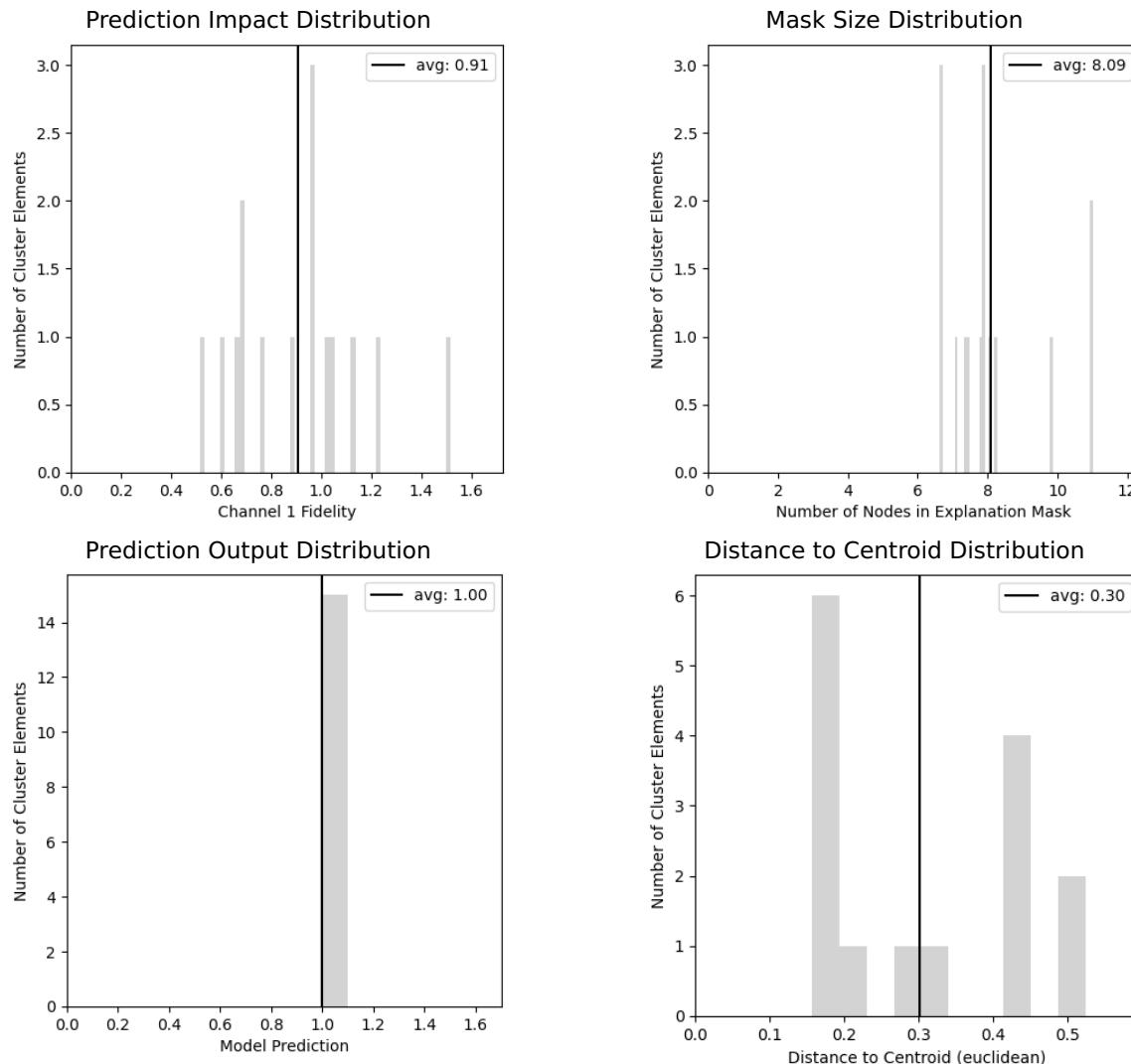
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	15
Channel Index	1.0 (0.0)

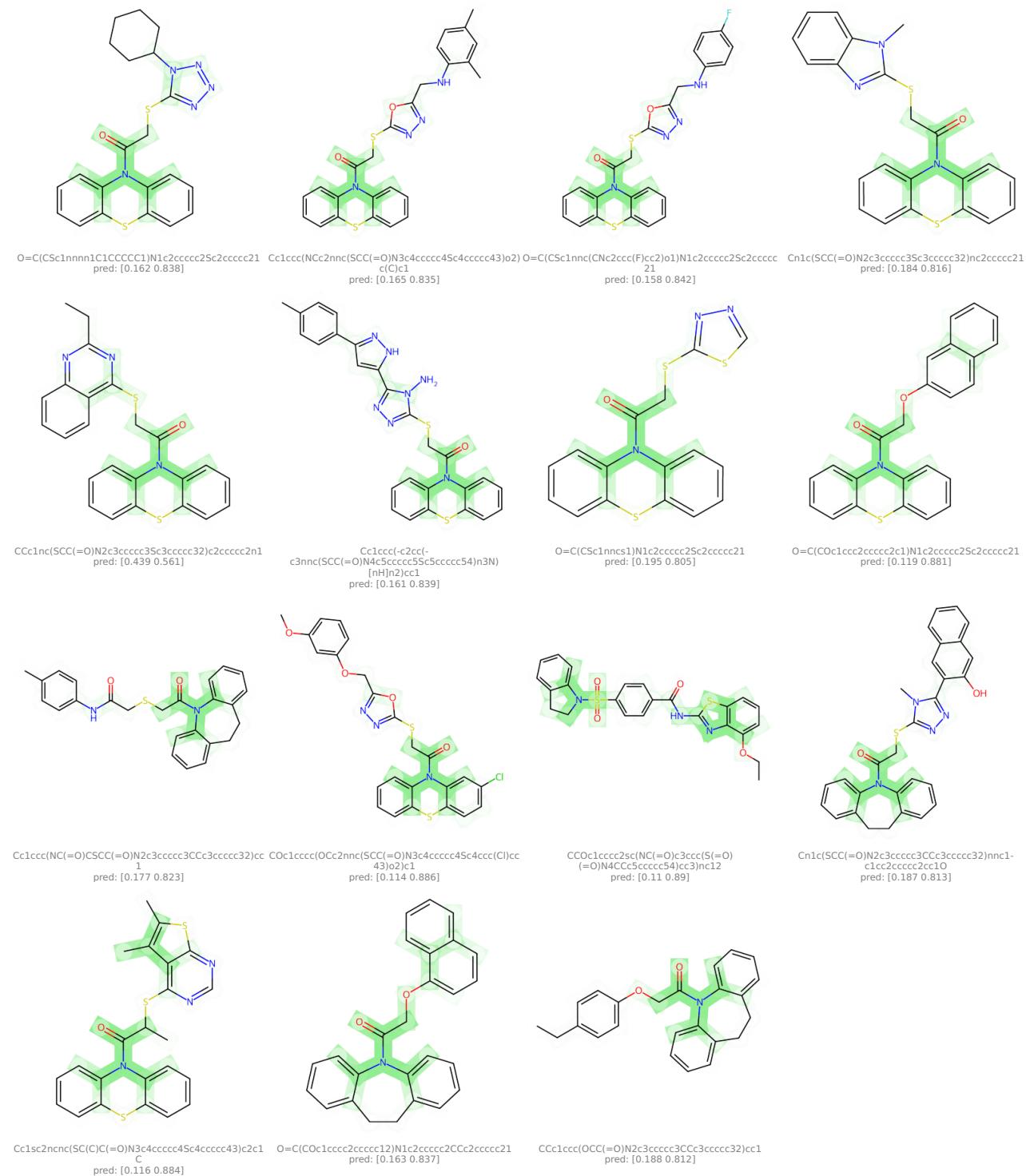
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #100 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 100, from importance channel 1 (*aggregator*), represents a motif consisting of 8.2 (± 1.8) nodes. The concept is generally associated with an impact of 0.9 (± 0.3) on the prediction outcome.

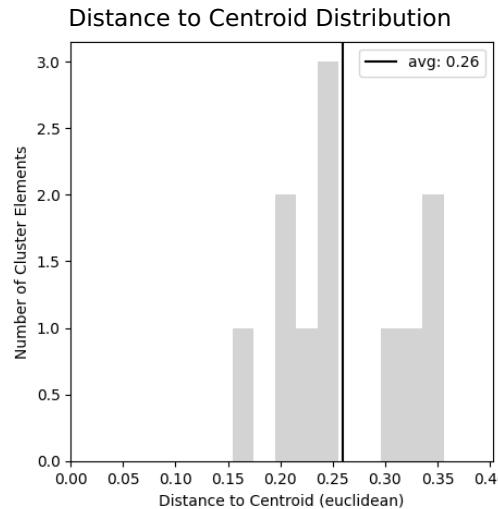
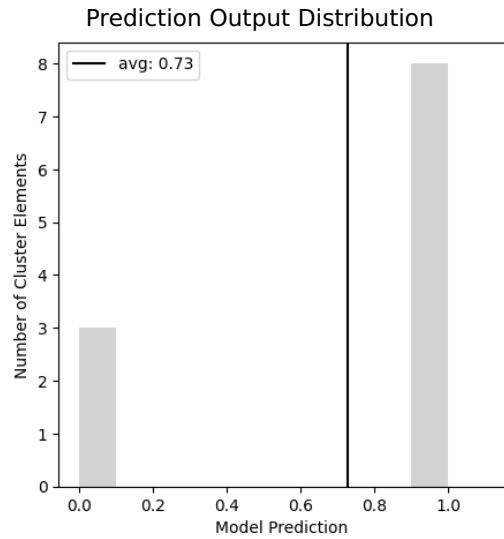
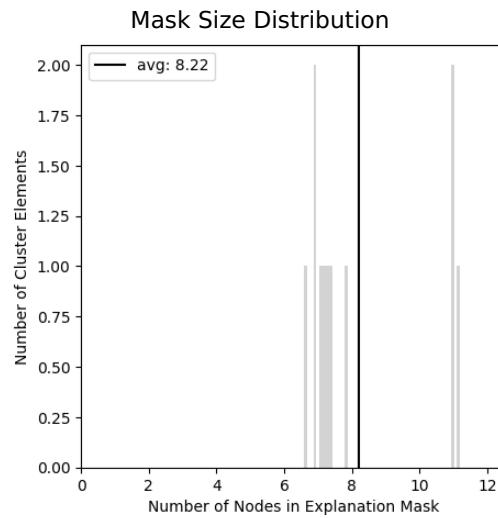
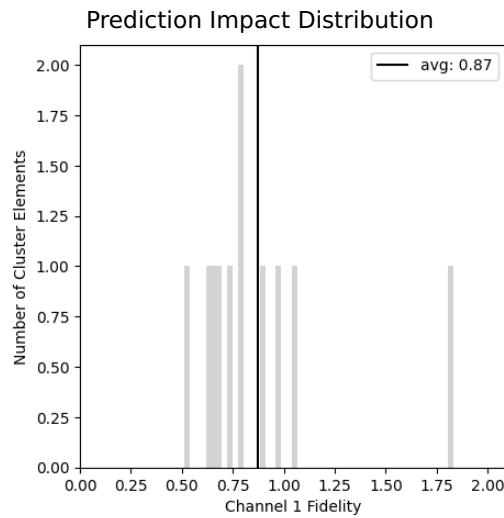
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	11
Channel Index	1.0 (0.0)

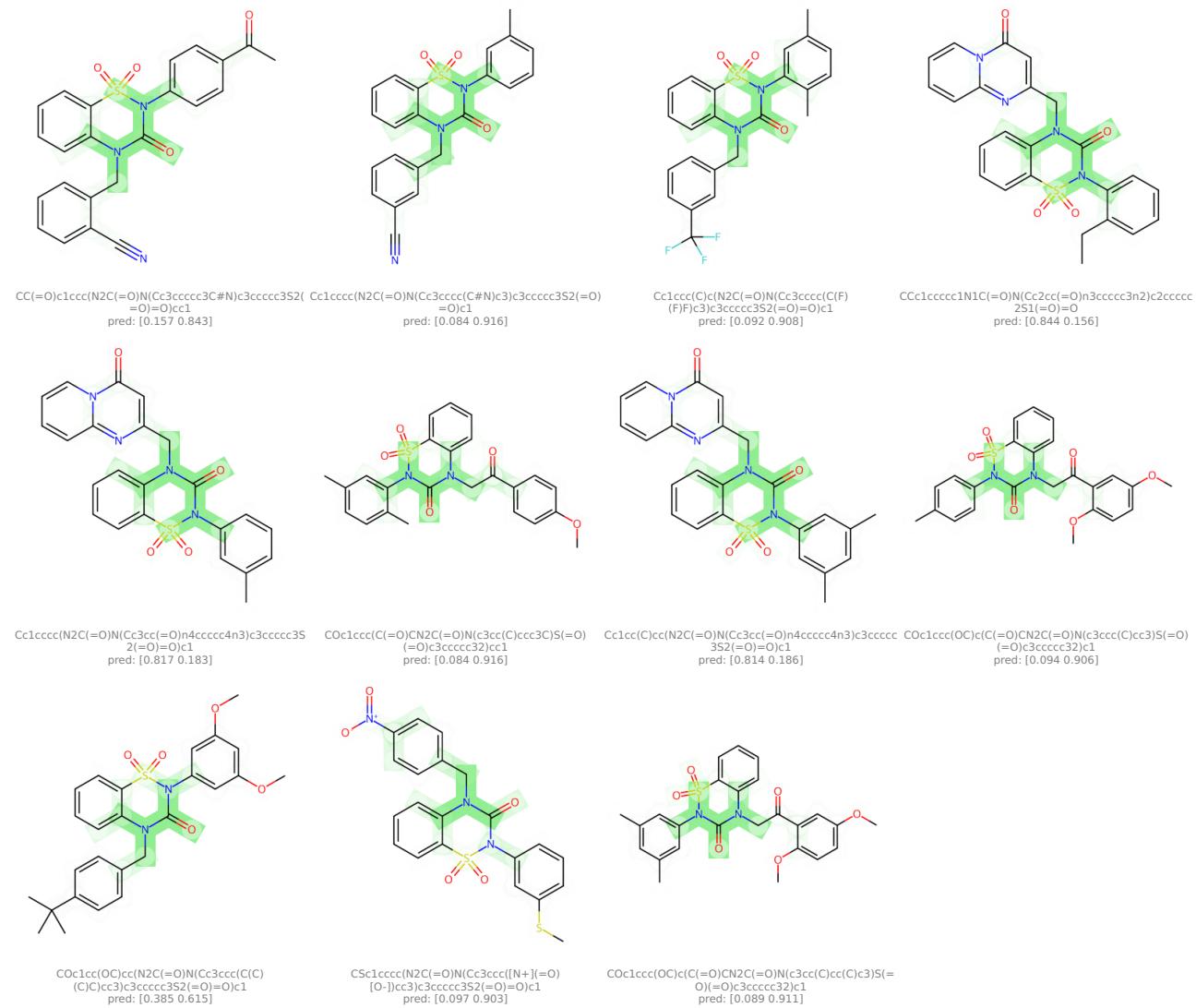
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #101 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 101, from importance channel 1 (*aggregator*), represents a motif consisting of 7.9 (± 1.2) nodes. The concept is generally associated with an impact of 1.0 (± 0.5) on the prediction outcome.

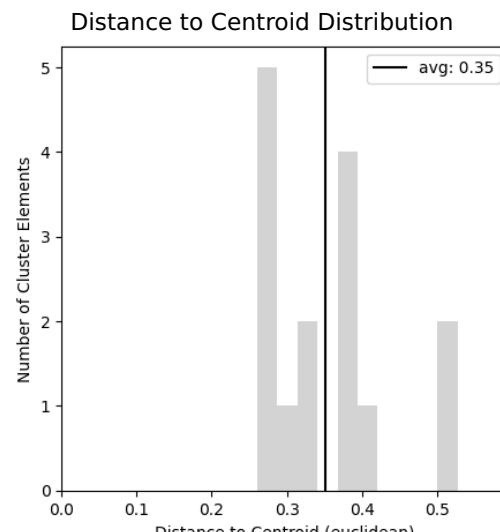
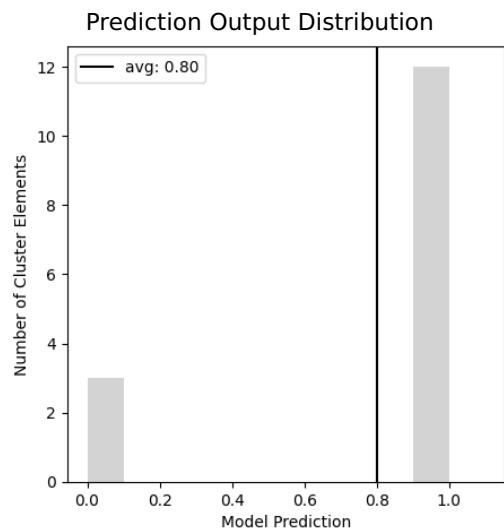
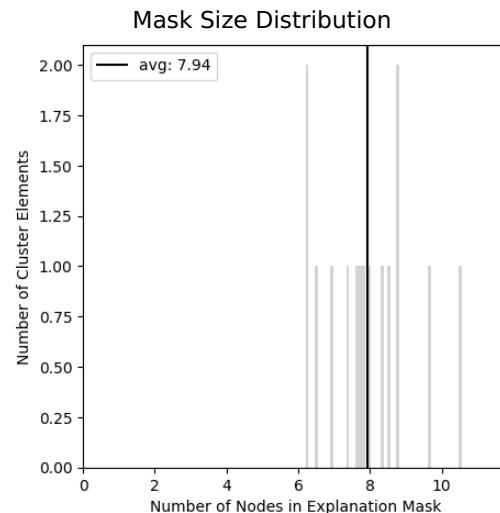
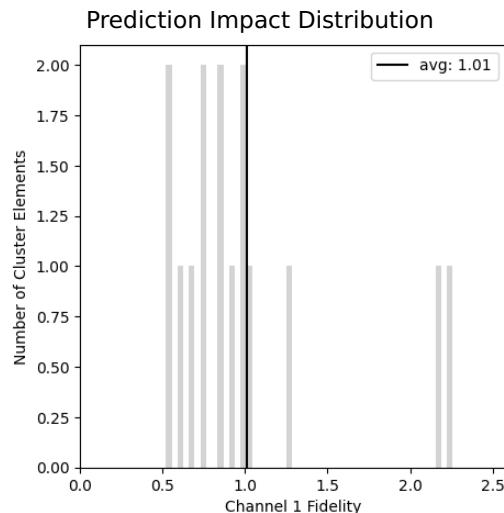
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	15
Channel Index	1.0 (0.0)

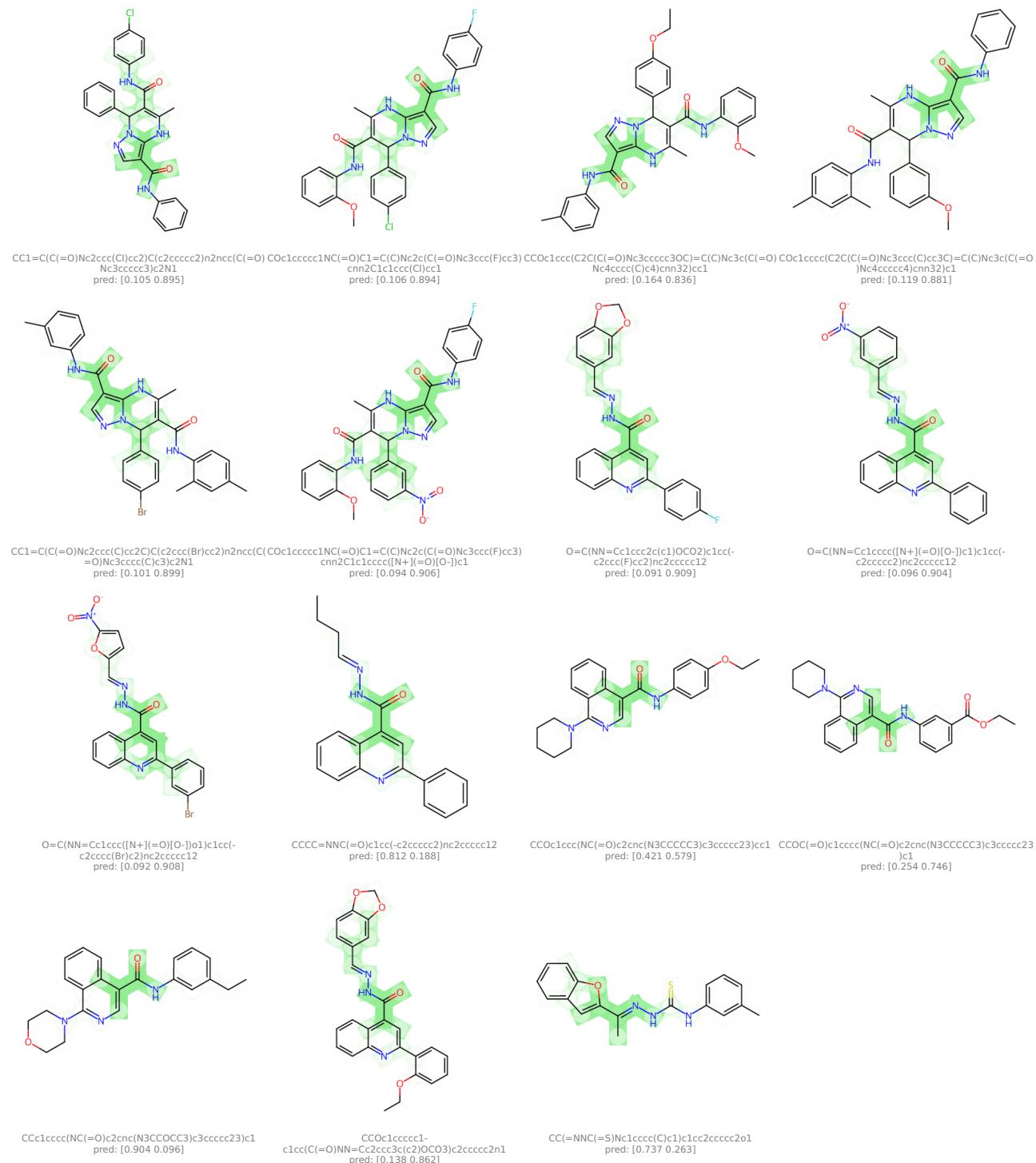
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #102 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 102, from importance channel 1 (*aggregator*), represents a motif consisting of 8.2 (± 0.9) nodes. The concept is generally associated with an impact of 1.0 (± 0.3) on the prediction outcome.

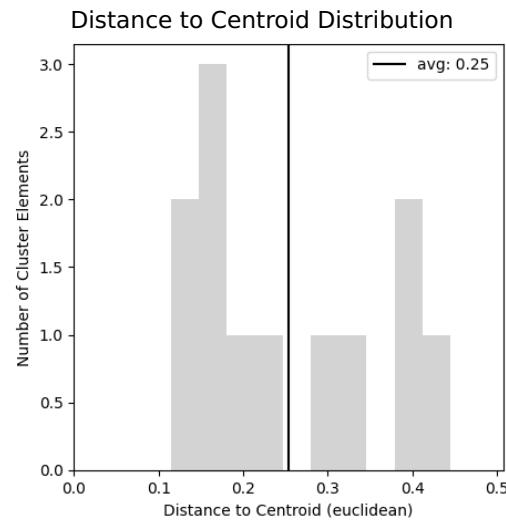
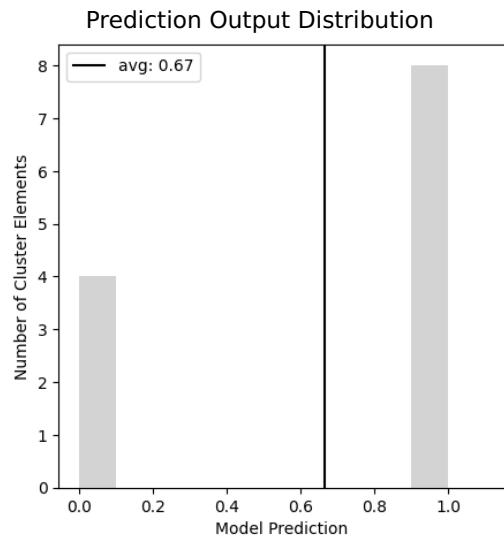
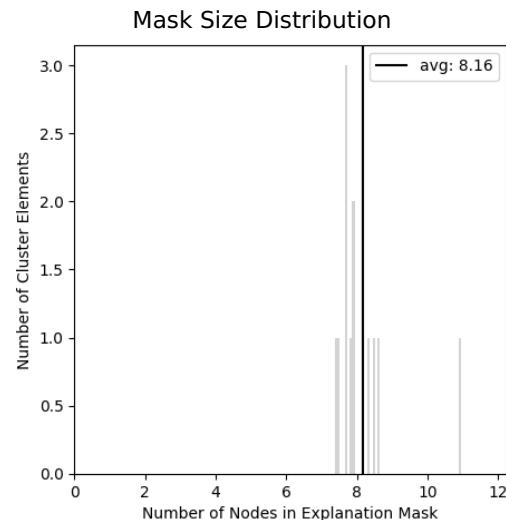
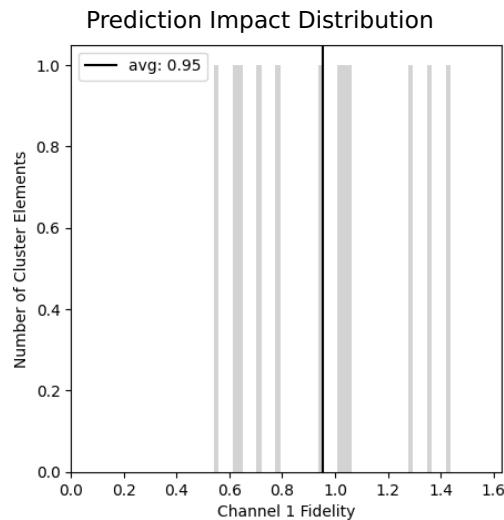
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	12
Channel Index	1.0 (0.0)

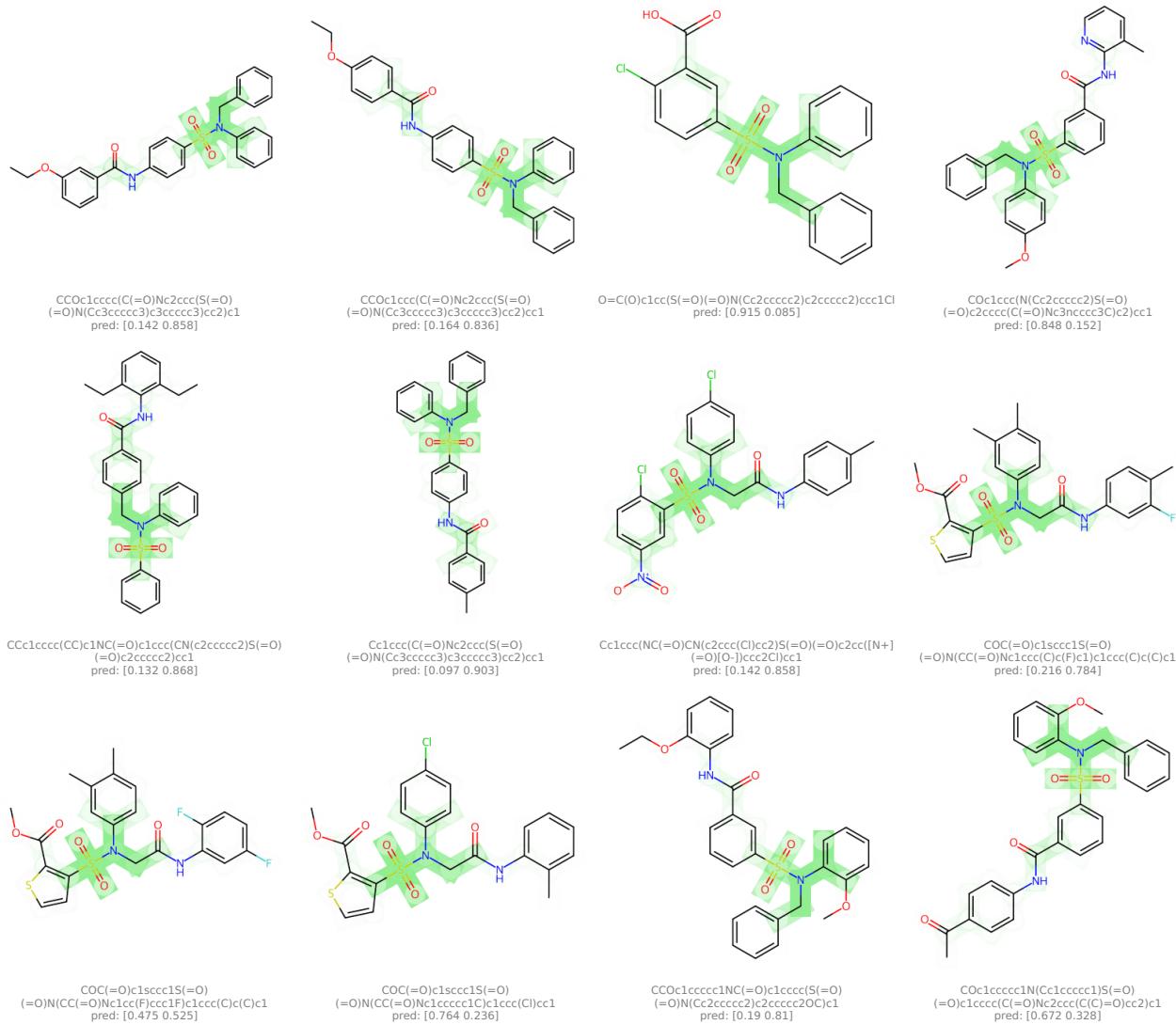
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #103 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 103, from importance channel 1 (*aggregator*), represents a motif consisting of $7.4 (\pm 0.7)$ nodes. The concept is generally associated with an impact of $1.0 (\pm 0.4)$ on the prediction outcome.

Properties

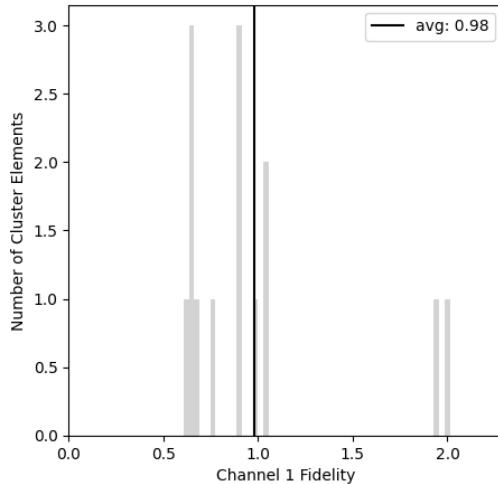
ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	14
Channel Index	1.0 (0.0)

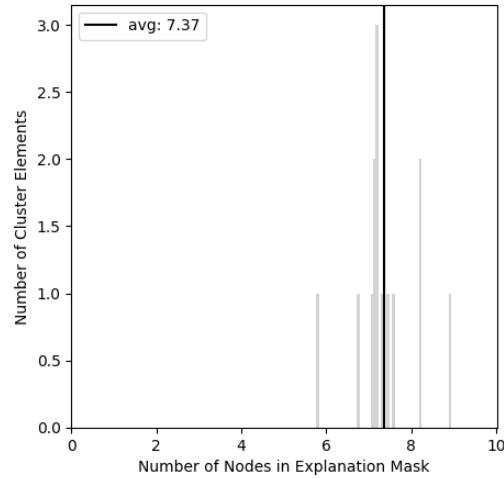
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.

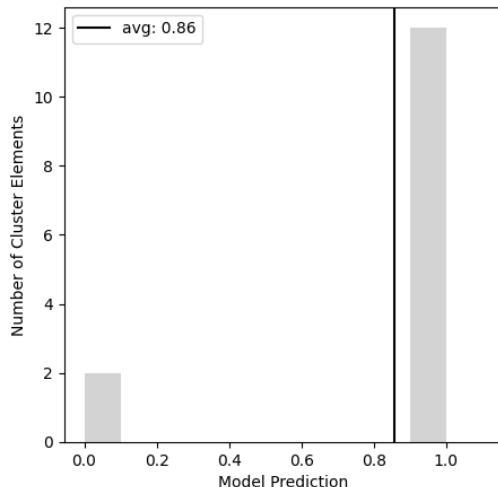
Prediction Impact Distribution



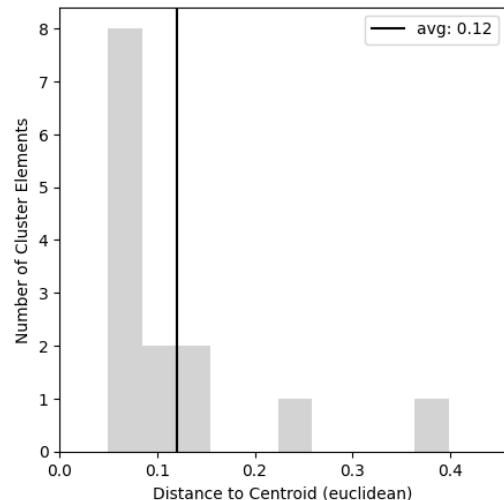
Mask Size Distribution



Prediction Output Distribution

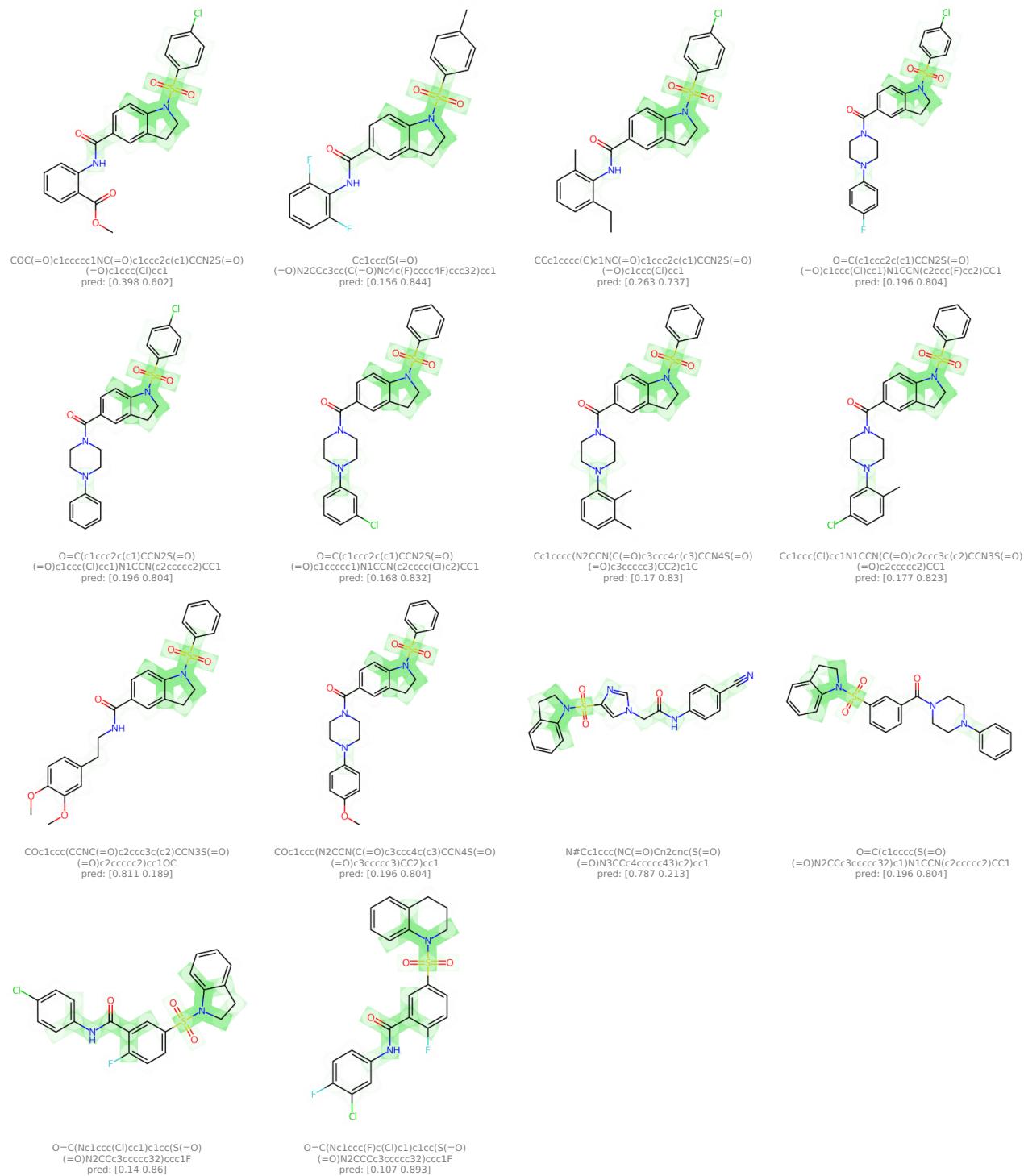


Distance to Centroid Distribution



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #104 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 104, from importance channel 1 (*aggregator*), represents a motif consisting of $7.6 (\pm 0.4)$ nodes. The concept is generally associated with an impact of $1.2 (\pm 0.6)$ on the prediction outcome.

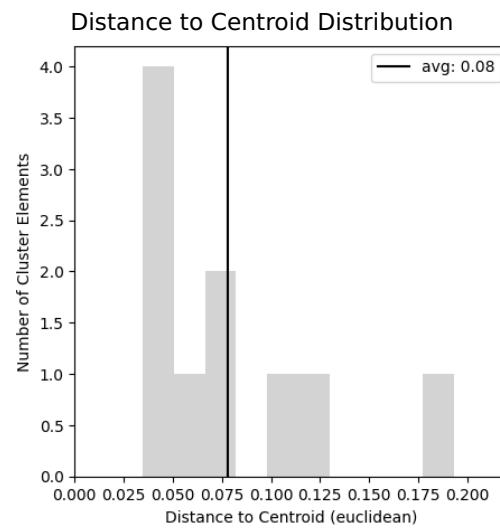
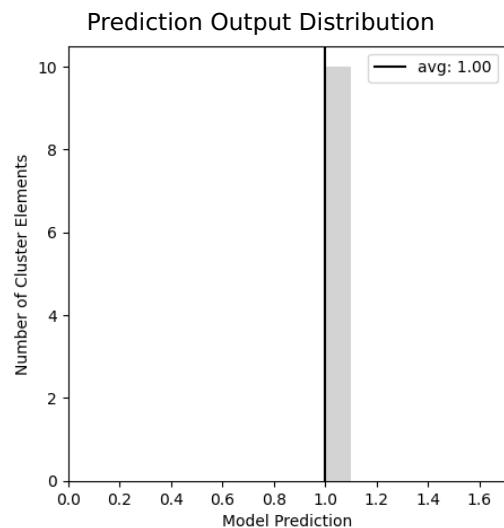
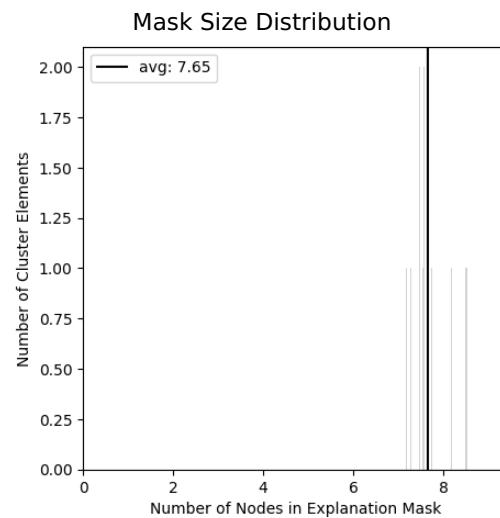
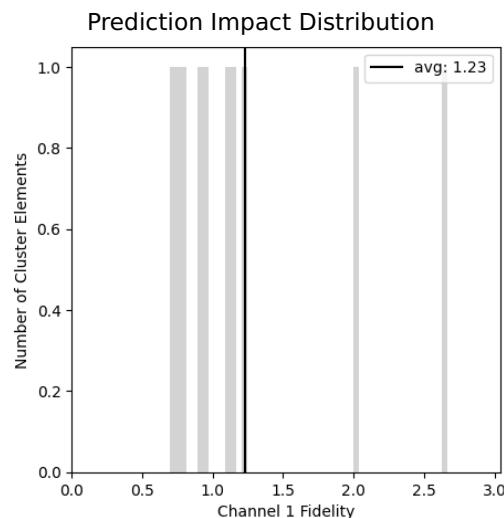
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	10
Channel Index	1.0 (0.0)

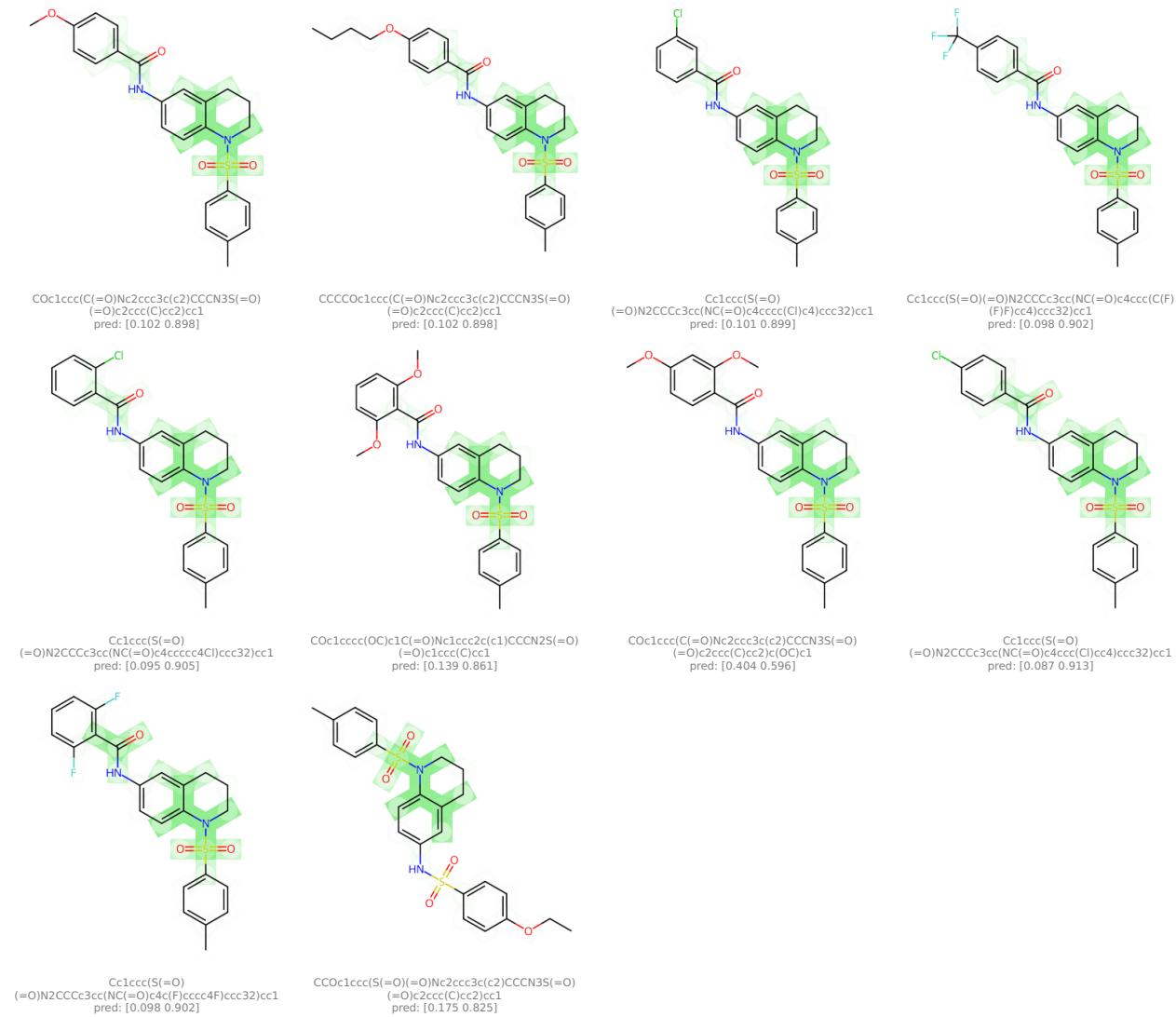
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #105 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 105, from importance channel 1 (*aggregator*), represents a motif consisting of 7.5 (± 1.6) nodes. The concept is generally associated with an impact of 1.4 (± 0.6) on the prediction outcome.

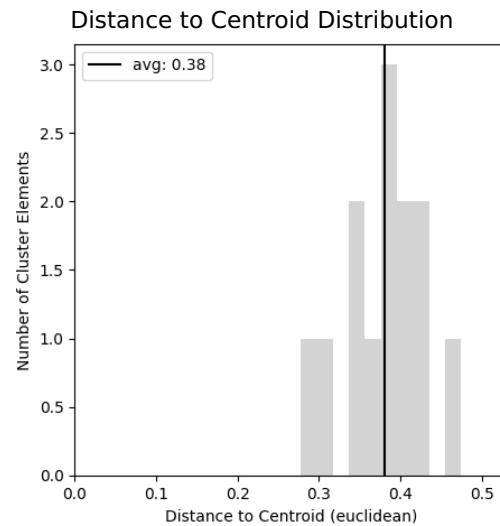
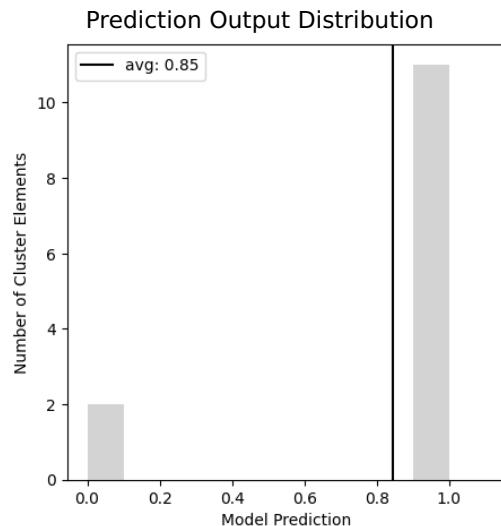
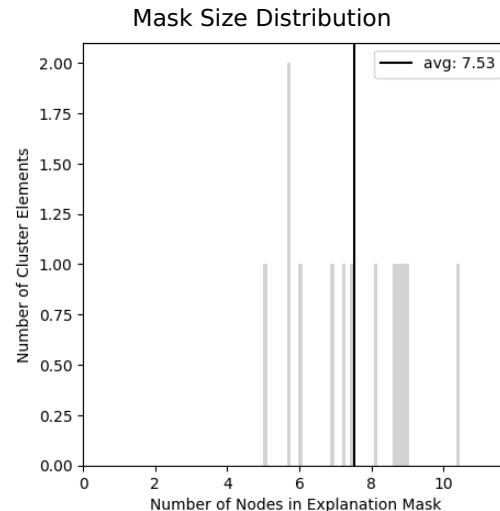
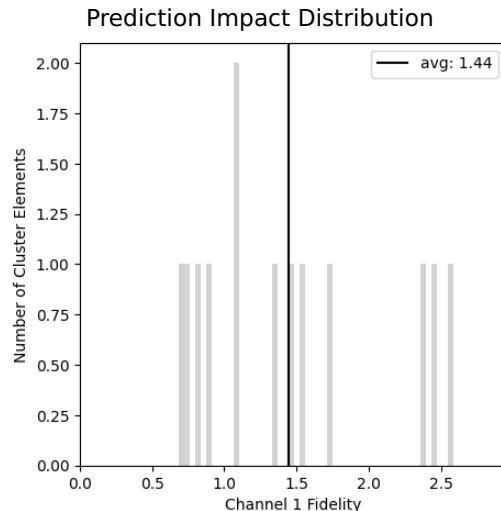
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	13
Channel Index	1.0 (0.0)

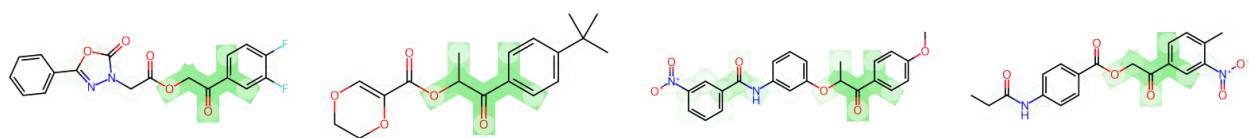
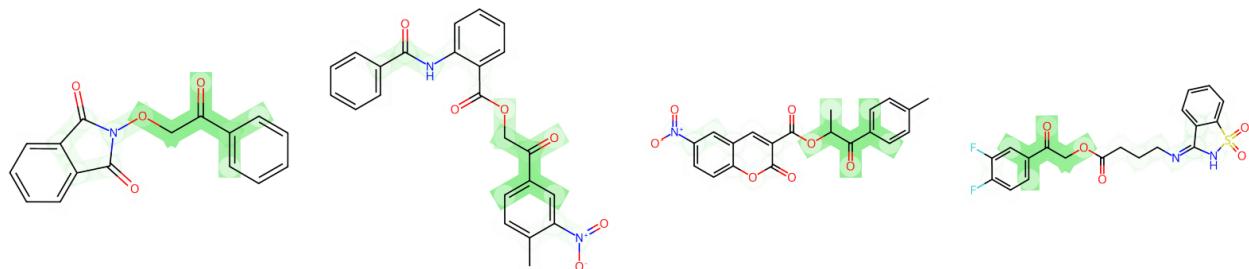
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.

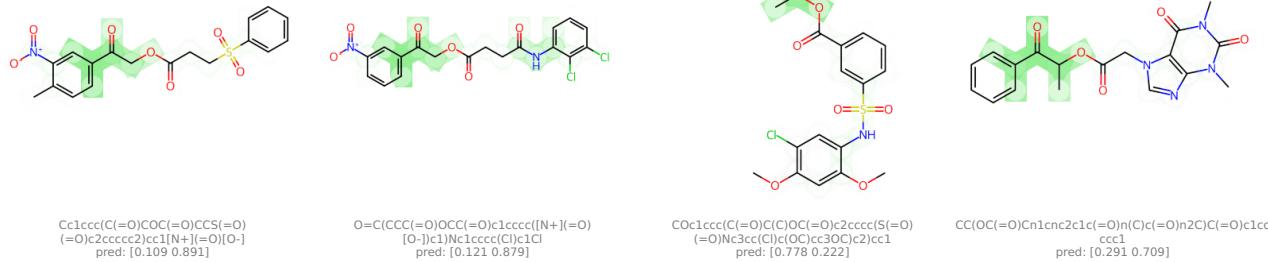


O=C(Cn1nc(-c2ccccc2)oc1=O)OCC(=O)c1ccc(F)c(F)c1
pred: [0.096 0.904]

CC(OC(=O)C1=COCCO1)C(=O)c1ccc(C(C)(C)C)cc1
pred: [0.862 0.138]

COc1ccc(C(=O)C(Oc2cccc(NC(=O)c3cccc([N+](=O)[O-])c3)cc2)cc1
pred: [0.106 0.894]

CCC(=O)Nc1ccc(C(=O)OCC(=O)c2ccc(C([N+](=O)[O-])c2)cc1
pred: [0.138 0.862]



Cluster #106 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 106, from importance channel 1 (*aggregator*), represents a motif consisting of 8.5 (± 1.8) nodes. The concept is generally associated with an impact of 1.1 (± 0.5) on the prediction outcome.

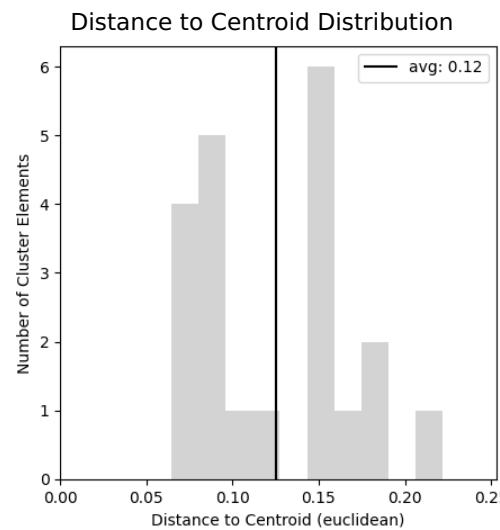
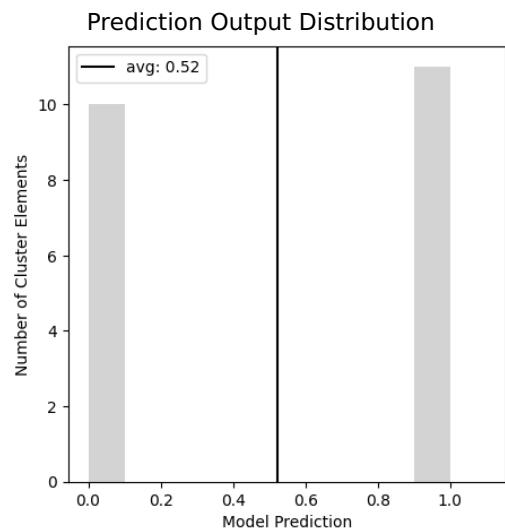
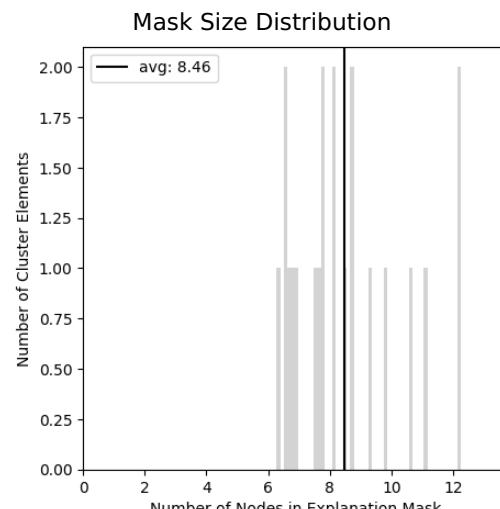
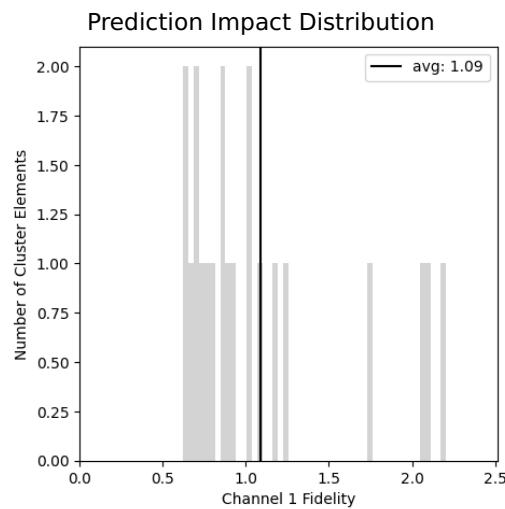
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	21
Channel Index	1.0 (0.0)

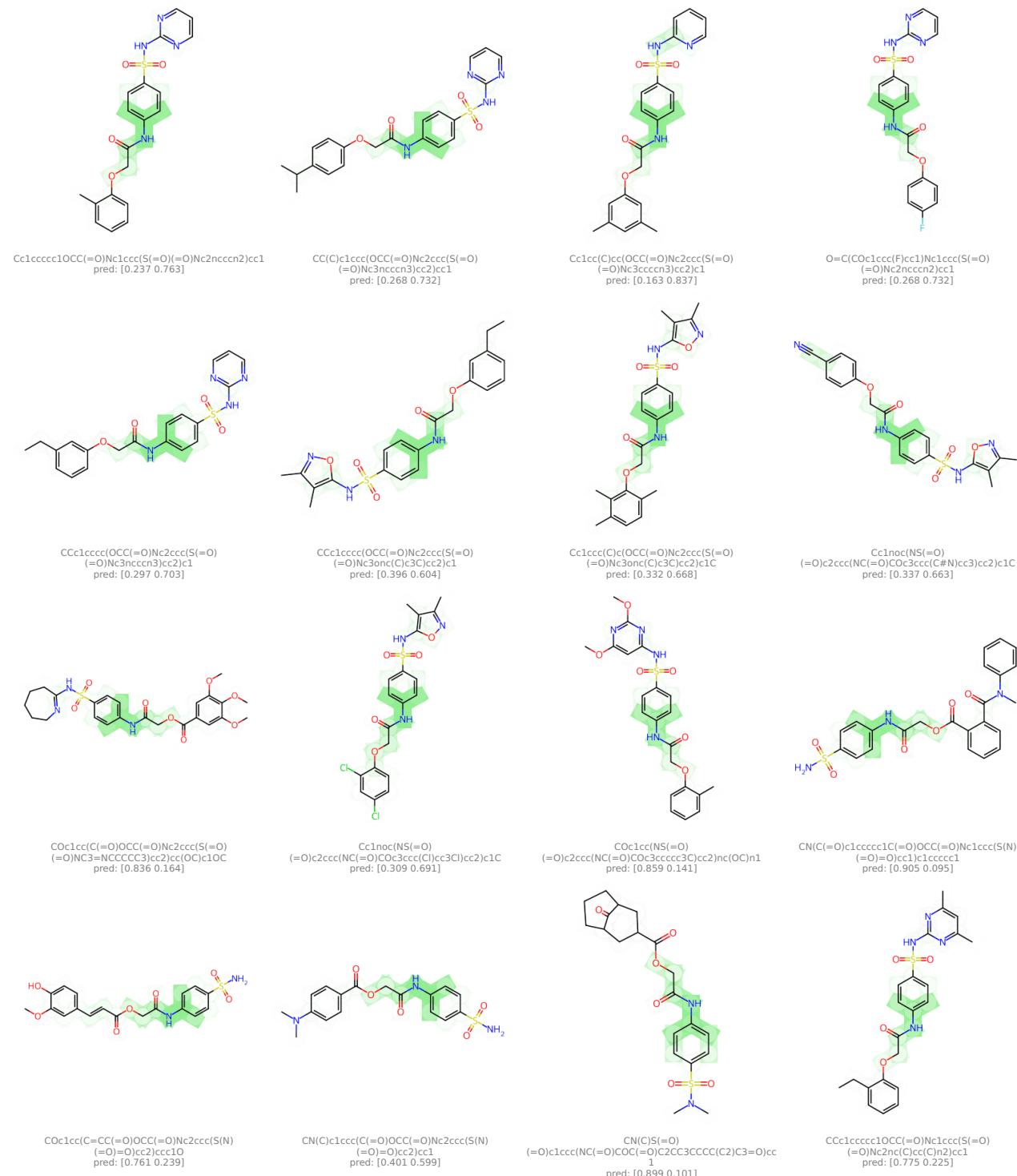
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #107 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 107, from importance channel 1 (*aggregator*), represents a motif consisting of $8.6 (\pm 2.0)$ nodes. The concept is generally associated with an impact of $2.0 (\pm 0.8)$ on the prediction outcome.

Properties

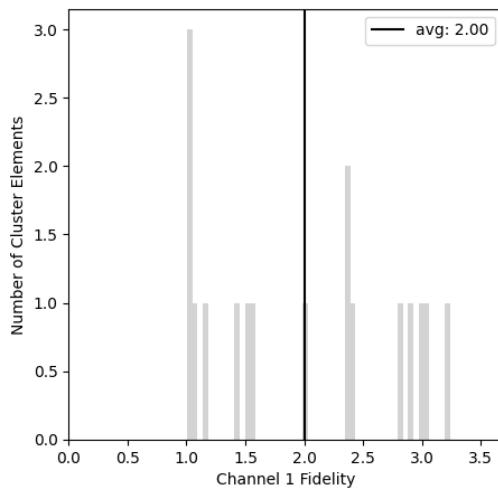
ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	17
Channel Index	1.0 (0.0)

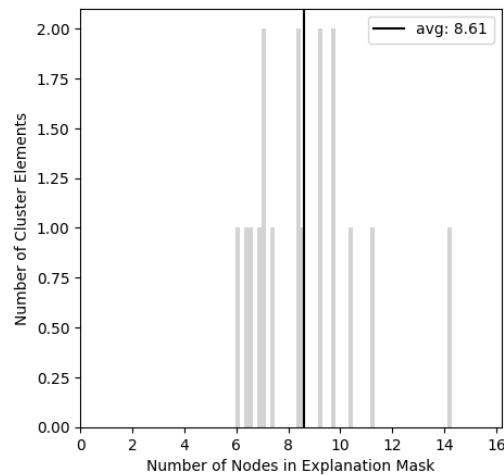
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.

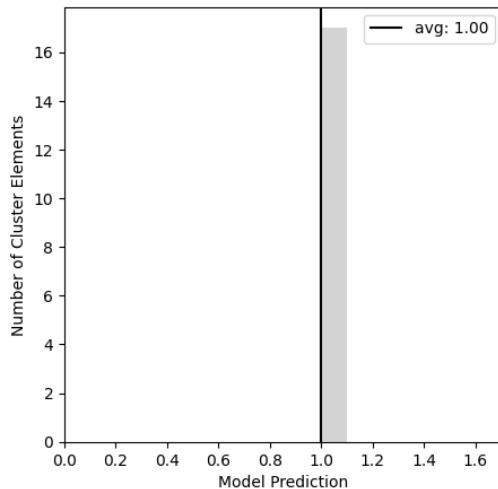
Prediction Impact Distribution



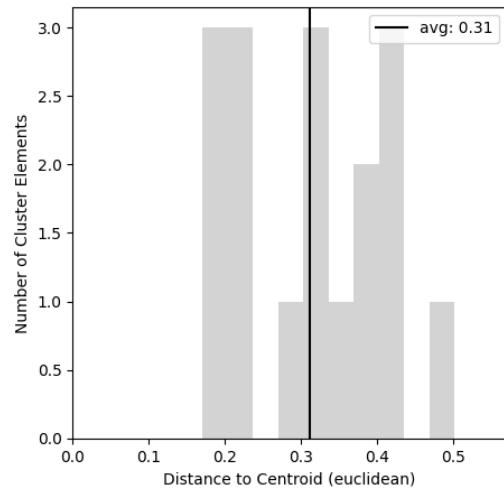
Mask Size Distribution



Prediction Output Distribution

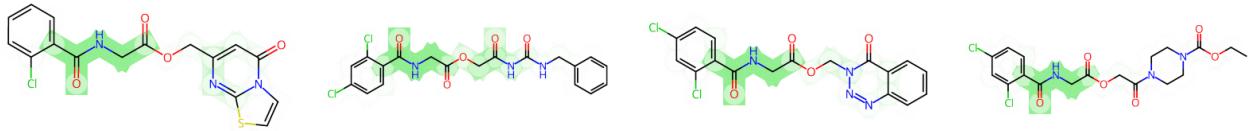


Distance to Centroid Distribution

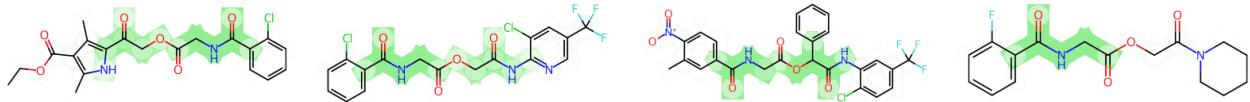


Example Elements

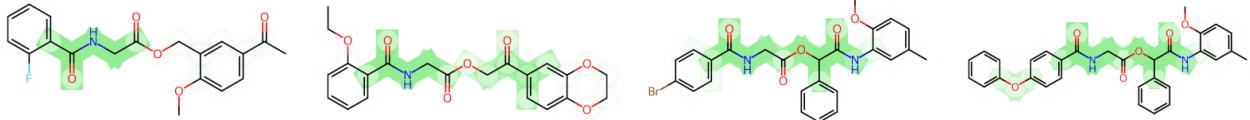
ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



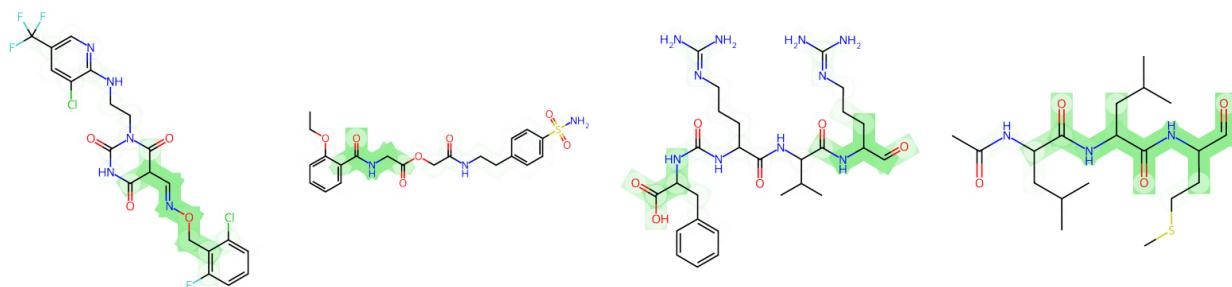
<chem>O=C(CNC(=O)c1ccccc1Cl)OCc1cc(=O)n2ccsc2n1</chem>	<chem>O=C(COC(=O)CNC(=O)c1ccc(Cl)cc1Cl)NC(=O)NCC1CC</chem>	<chem>O=C(CNC(=O)c1ccc(Cl)cc1Cl)OCn1nncc2cccc2c1=O</chem>	<chem>CCOC(=O)N1CCN(C(=O)COc(=O)CNC(=O)c2ccc(Cl)cc2)CC1</chem>
pred: [0.159 0.841]	<chem>ccc1</chem> pred: [0.07 0.93]	pred: [0.093 0.907]	pred: [0.246 0.754]



<chem>CCOC(=O)c1cc(C)[nH]c(C(=O)COc(=O)CNC(=O)c2cccc2Cl)c1C</chem>	<chem>O=C(COC(=O)CNC(=O)c1ccccc1Cl)Nc1ncc(C(F)(F)F)cc1Cl</chem>	<chem>Cc1cc(C(=O)NCC(=O)OC(C(=O)Nc2cc(C(F)(F)F)cc2Cl)c2cccc2c1)N+[+](=O)[O-]</chem>	<chem>O=C(CNC(=O)c1ccccc1F)OCC(=O)N1CCCCC1</chem>
[nH]c(C(=O)COc(=O)CNC(=O)c2cccc2Cl)c1C pred: [0.063 0.937]	pred: [0.082 0.918]	pred: [0.064 0.936]	pred: [0.079 0.921]



<chem>CCOc1ccc(C(=O)c1cccOC(=O)CNC(=O)c1ccccc1F)</chem>	<chem>CCOc1ccccc1C(=O)NCC(=O)OCC(=O)c1cc2c(c1)OCC Oo1ccc(C)cc1NC(=O)C(OC(=O)CNC(=O)c1ccc(Br)cc1COc1ccc(C)cc1NC(=O)C(OC(=O)CNC(=O)c1ccc(Oc2ccc2Cl)c1)cc1c1</chem>
pred: [0.357 0.643]	<chem>O2</chem> pred: [0.077 0.923]
pred: [0.067 0.933]	



<chem>O=C1NC(=O)N(CCNC2ncc(C(F)(F)Cc2Cl)c1)C(=O)C1=NOCC1c(F)cccc1Cl</chem>	<chem>CCOc1ccccc1C(=O)NCC(=O)OCC(=O)NCCc1ccc(S(N)CC(C)C(NC(=O)O)C(CCN=C(N)N)NC(=O)NC(Cc1cccc1)CSCCC(C=O)NC(=O)C(CC(C)C)NC(=O)C(CC(C)C)NC(C(=O)O)C(=O)NC(C(=O)O)C(CCN=C(N)N)pred: [0.11 0.89]</chem>	<chem>=O</chem>
pred: [0.177 0.823]	pred: [0.073 0.927]	pred: [0.34 0.66]

Cluster #108 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 108, from importance channel 1 (*aggregator*), represents a motif consisting of 8.0 (± 0.9) nodes. The concept is generally associated with an impact of 1.1 (± 0.4) on the prediction outcome.

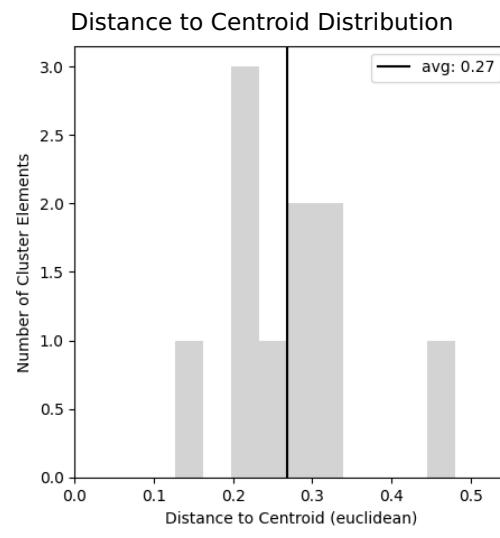
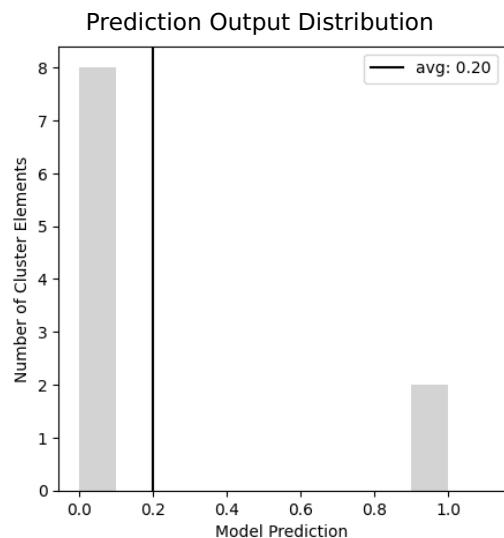
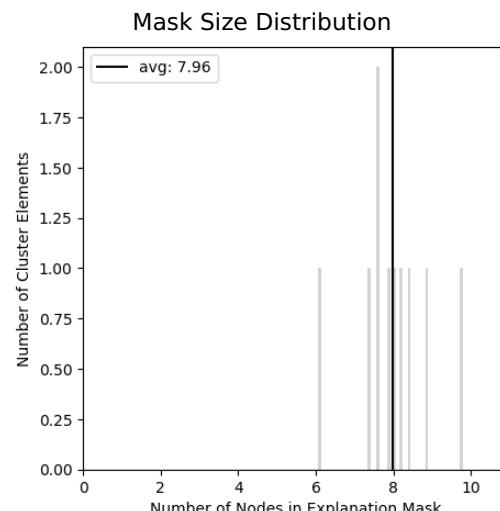
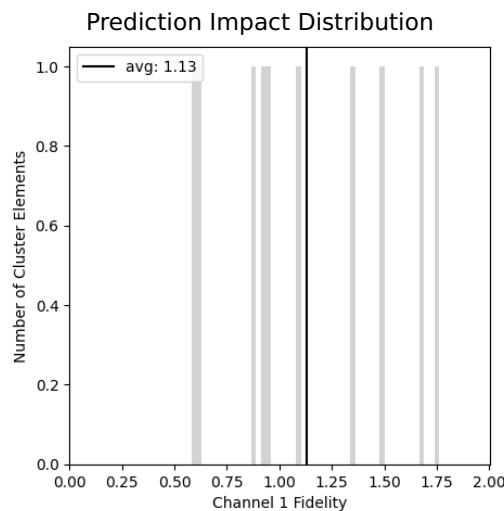
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	10
Channel Index	1.0 (0.0)

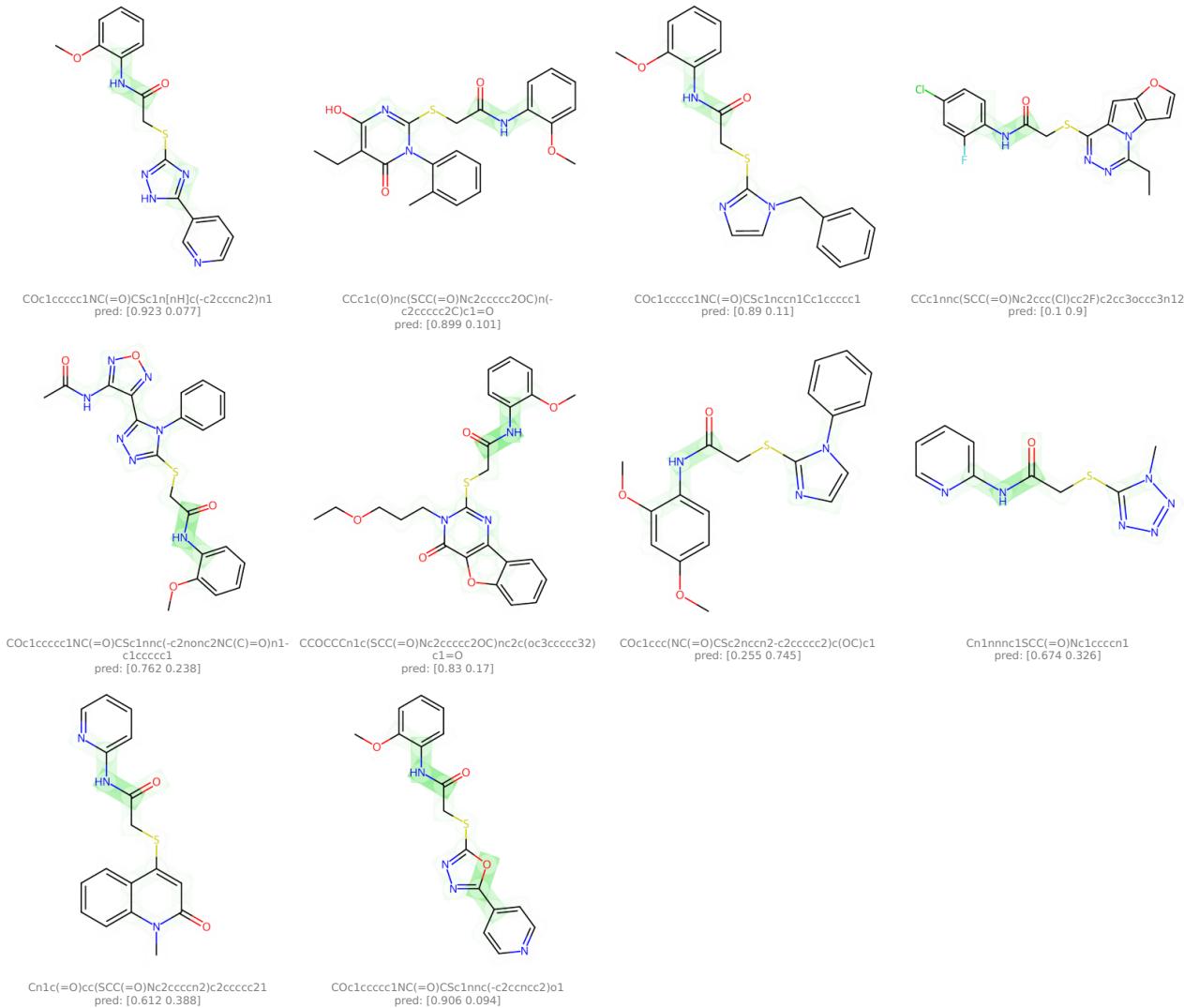
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #109 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 109, from importance channel 1 (*aggregator*), represents a motif consisting of 8.0 (± 1.4) nodes. The concept is generally associated with an impact of 0.9 (± 0.3) on the prediction outcome.

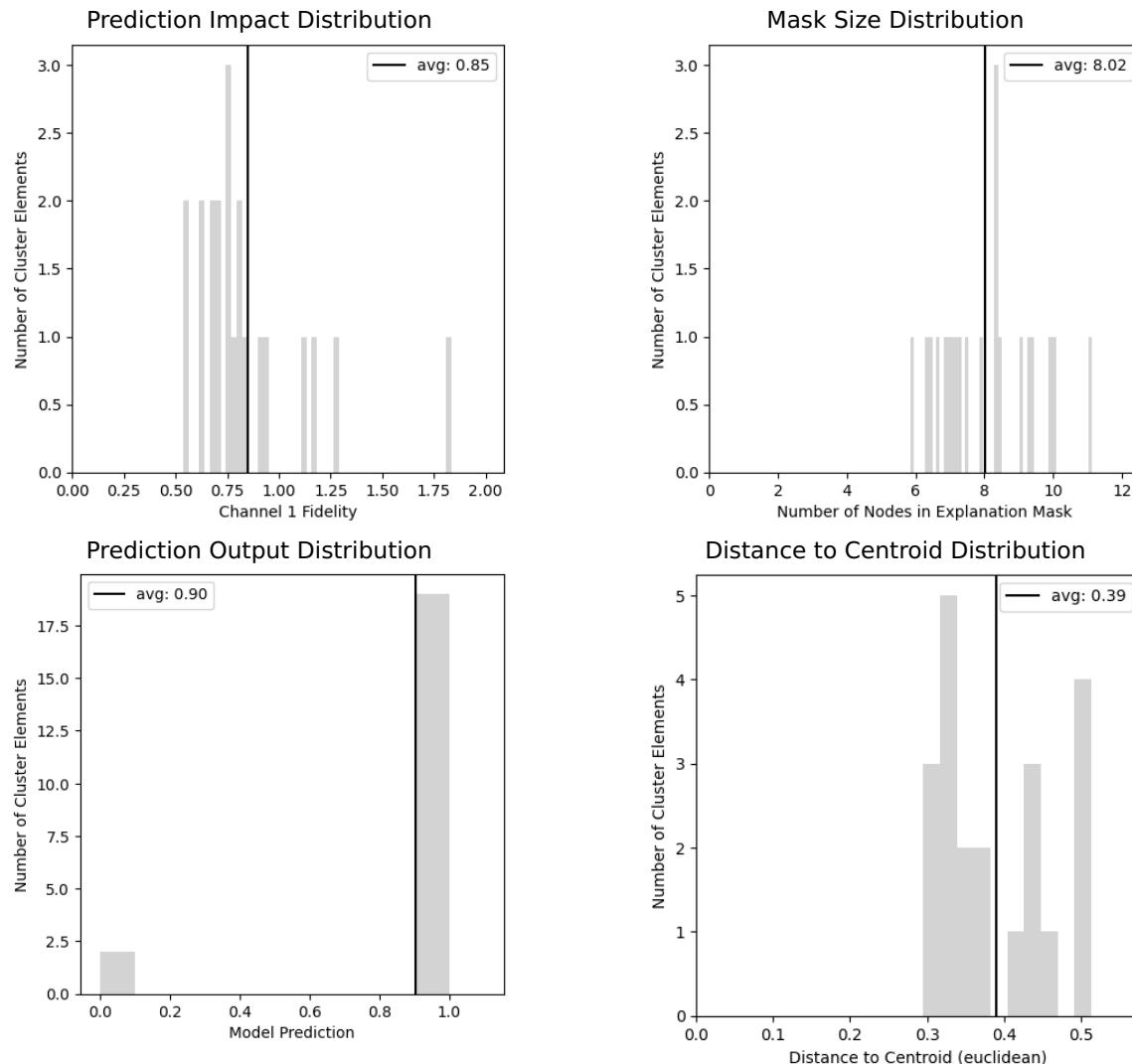
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	21
Channel Index	1.0 (0.0)

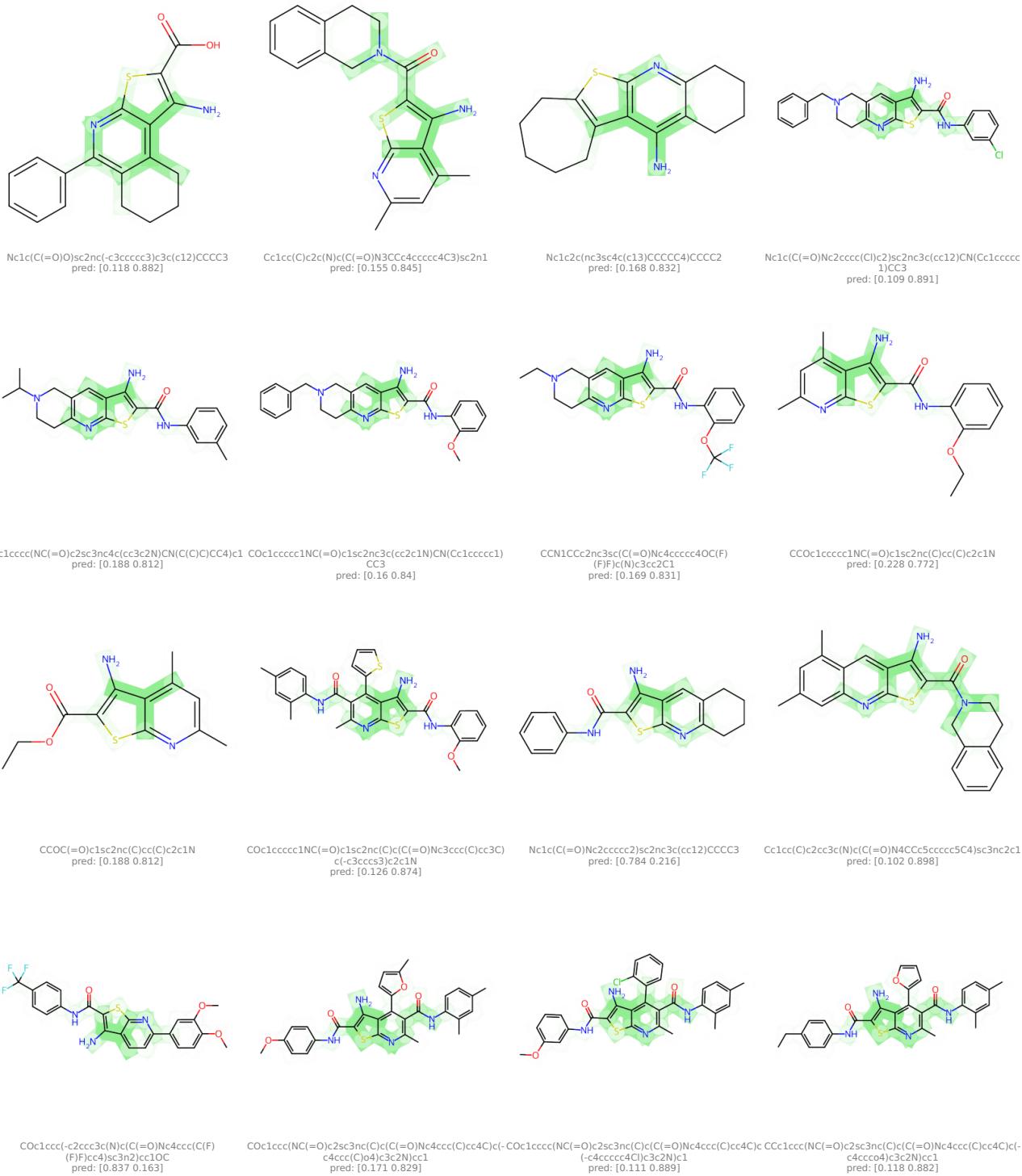
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

① This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #110 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 110, from importance channel 1 (*aggregator*), represents a motif consisting of 9.3 (± 1.1) nodes. The concept is generally associated with an impact of 0.9 (± 0.4) on the prediction outcome.

Properties

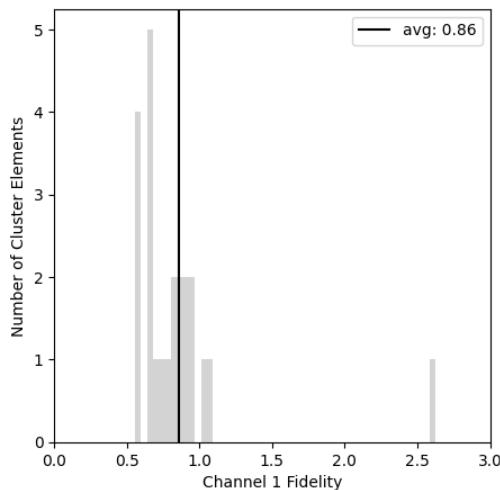
ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	23
Channel Index	1.0 (0.0)

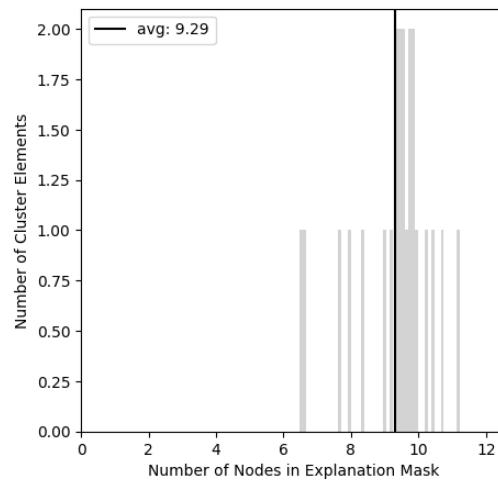
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.

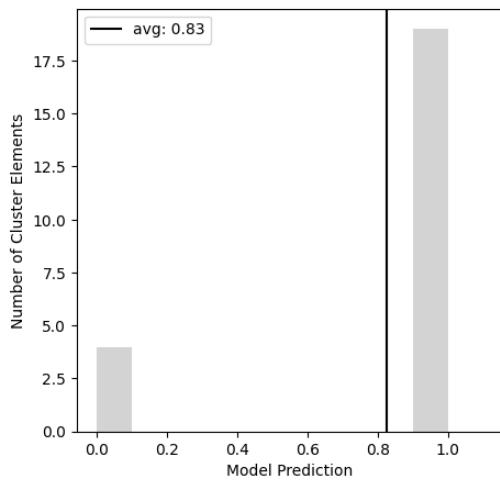
Prediction Impact Distribution



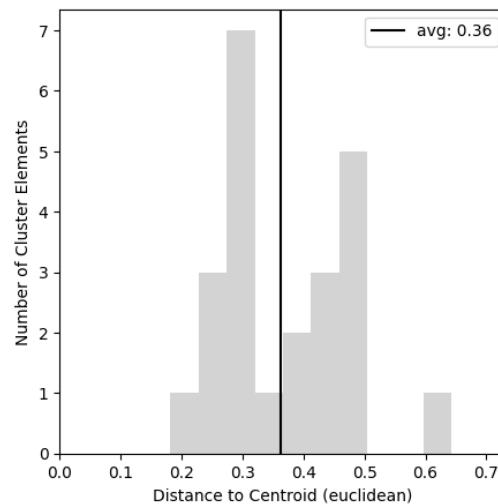
Mask Size Distribution



Prediction Output Distribution

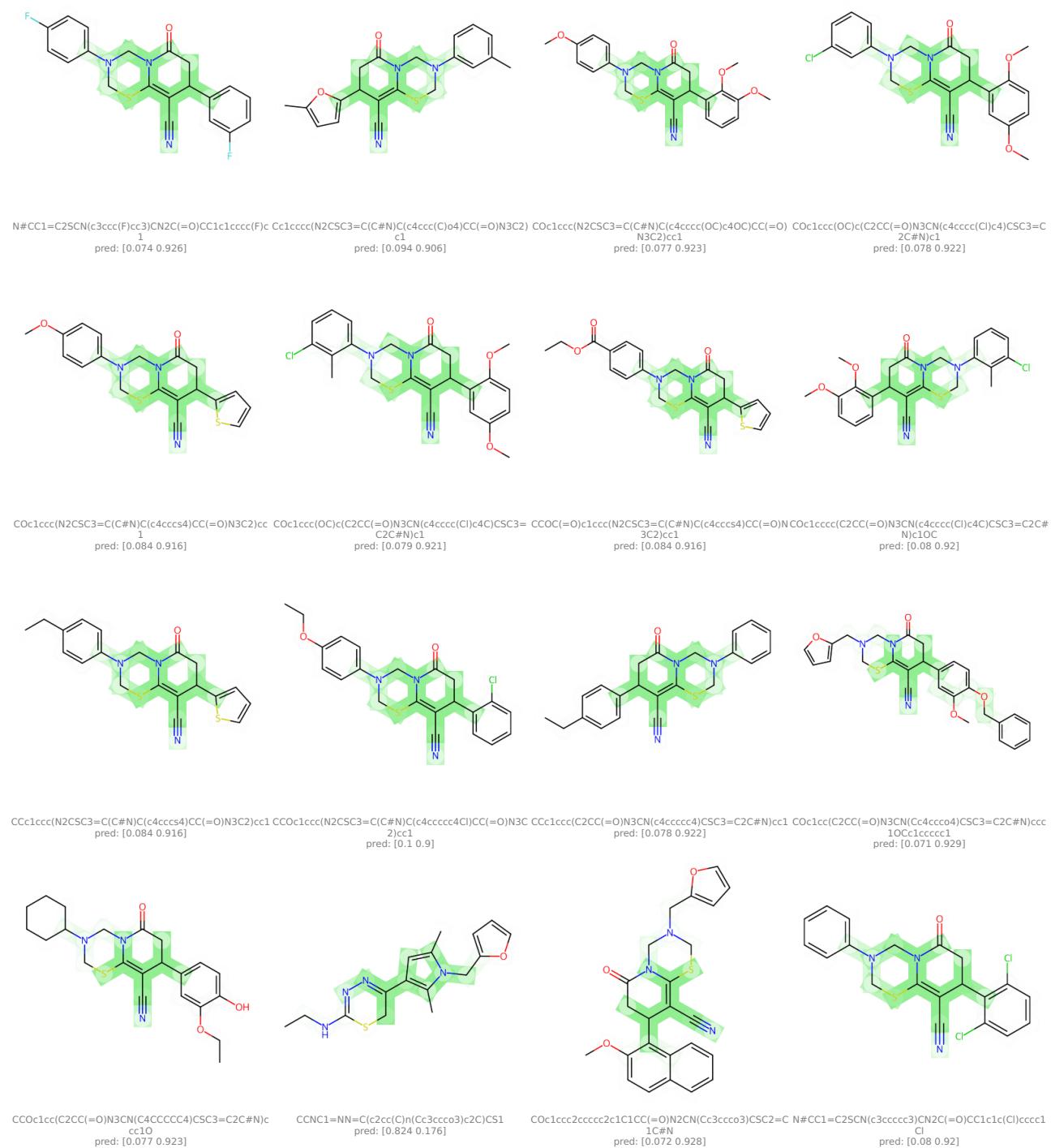


Distance to Centroid Distribution



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #111 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 111, from importance channel 1 (*aggregator*), represents a motif consisting of 7.2 (± 1.3) nodes. The concept is generally associated with an impact of 1.4 (± 0.7) on the prediction outcome.

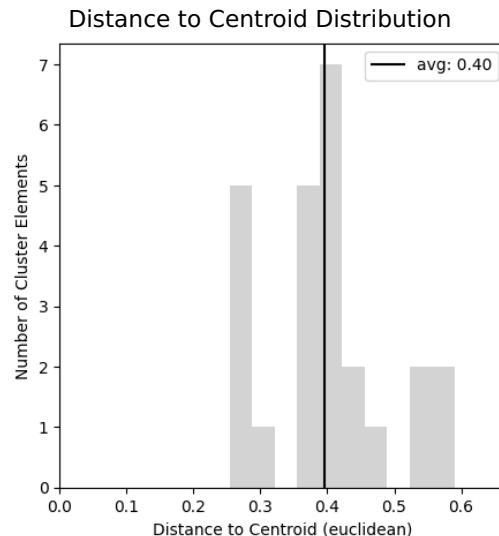
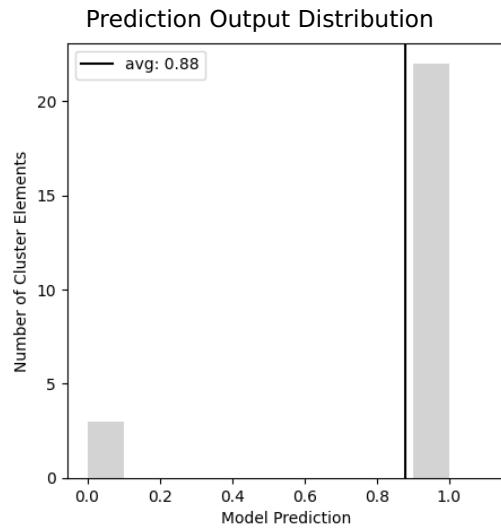
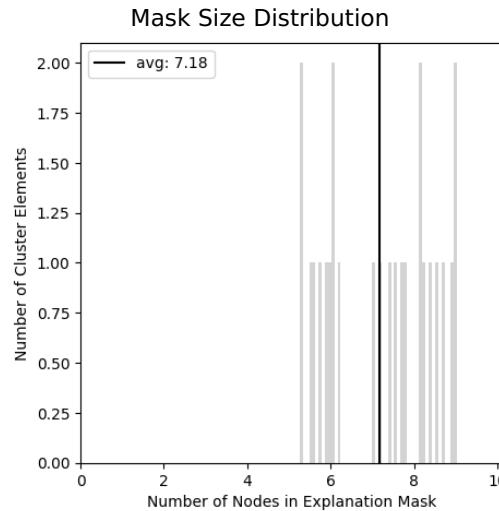
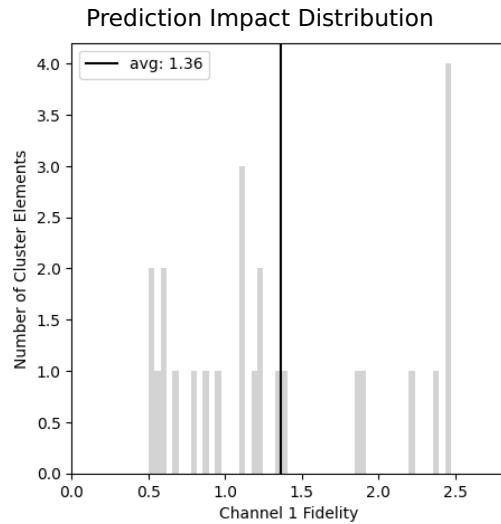
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	25
Channel Index	1.0 (0.0)

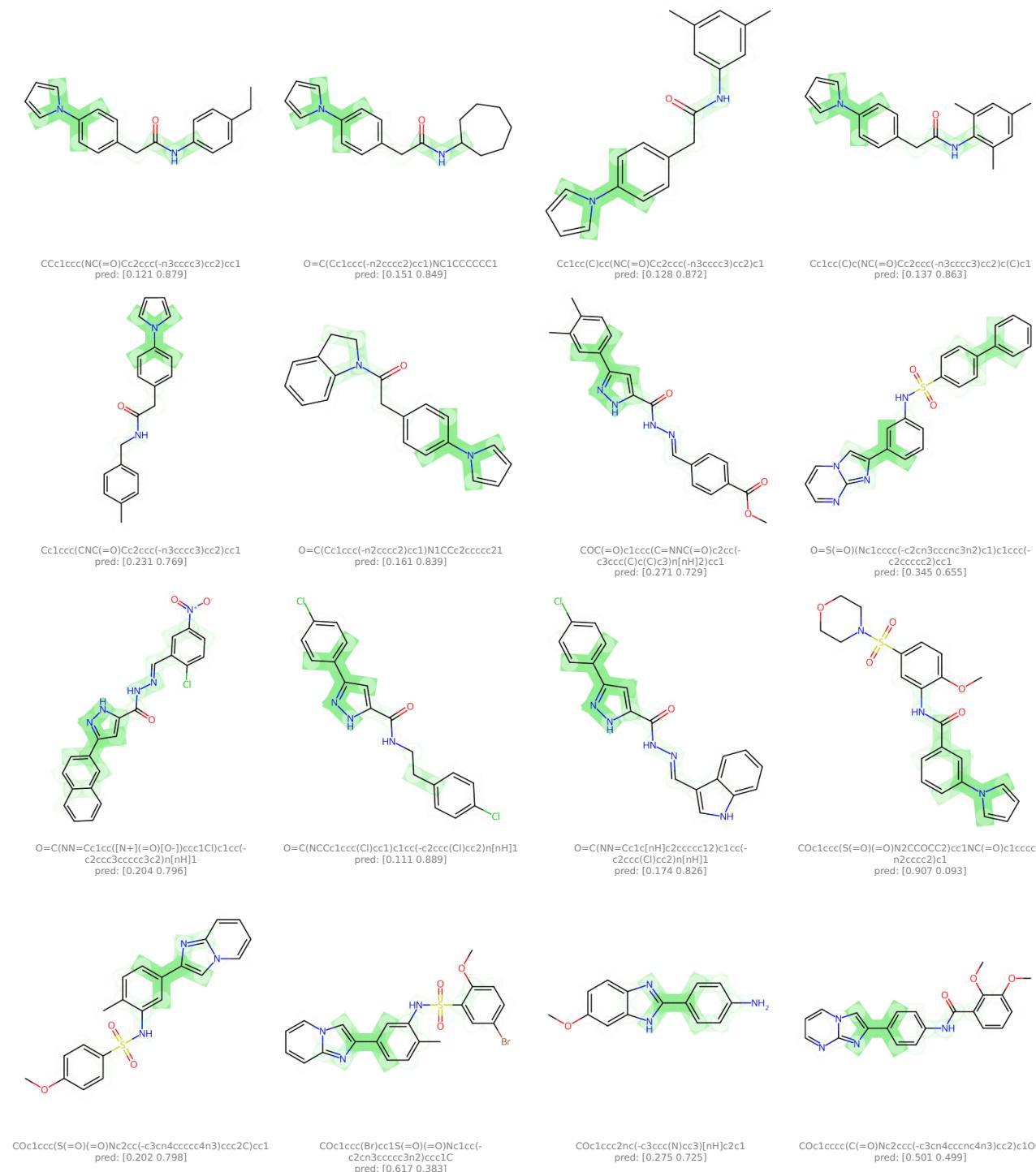
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.



Cluster #112 - aggregator

Summary

ⓘ This is a summary about the most important properties of the cluster. It lists which explanation channel the cluster is from, what the average size of the explanation is as well as the average impact of this clusters members to the prediction outcome of the model.

Cluster 112, from importance channel 1 (*aggregator*), represents a motif consisting of 8.3 (± 1.7) nodes. The concept is generally associated with an impact of 1.4 (± 0.7) on the prediction outcome.

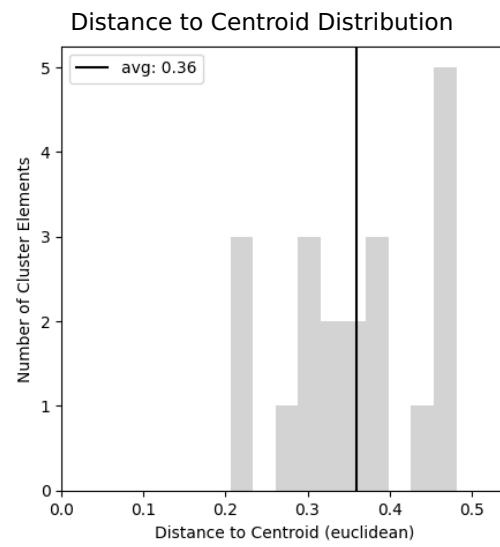
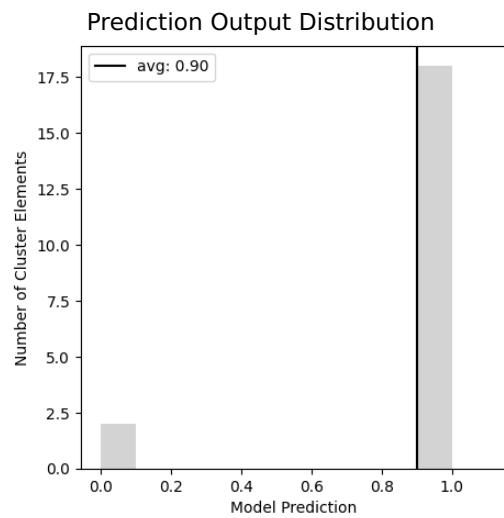
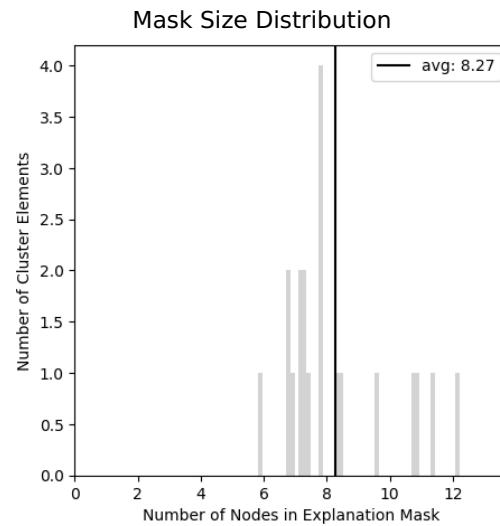
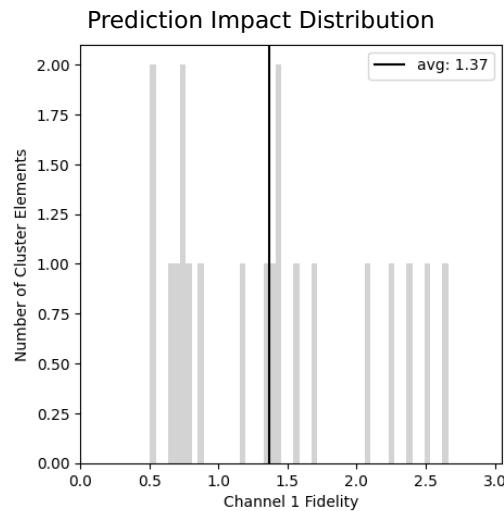
Properties

ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	20
Channel Index	1.0 (0.0)

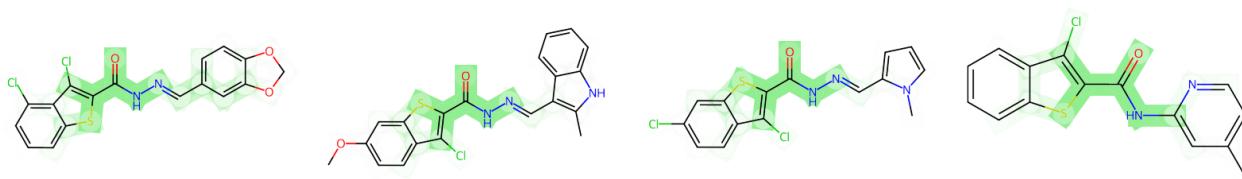
Member Statistics

ⓘ This section shows various statistical distributions about some aspects of the various cluster members. As distributions over the cluster members, the vertical axis always shows the number of elements associated with a certain properties and the horizontal axis shows the different values that the properties can take.



Example Elements

① This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some sort of common pattern even though the base graphs may differ.

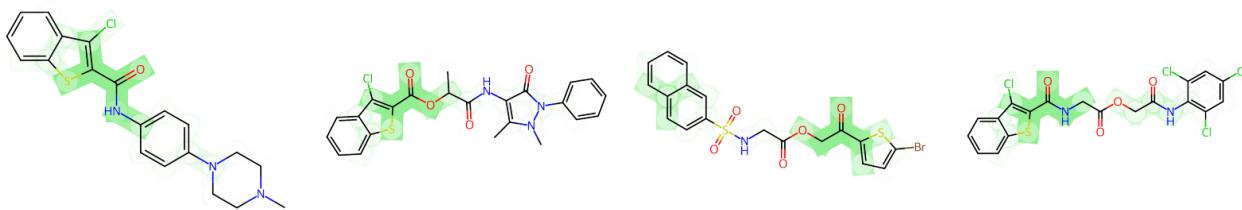


O=C(NN=Cc1ccc2c(c1)OCO2)c1sc2cccc(Cl)c2c1Cl
pred: [0.1 0.9]

COc1ccc2c(C)c(C(=O)NN=Cc3c(C)[nH]c4cccc34)sc2c1
pred: [0.109 0.891]

Cn1cccc1C=NNC(=O)c1sc2cc(Cl)ccc2c1Cl
pred: [0.116 0.884]

Cc1ccnc(NC(=O)c2sc3cccc3c2Cl)c1
pred: [0.129 0.871]

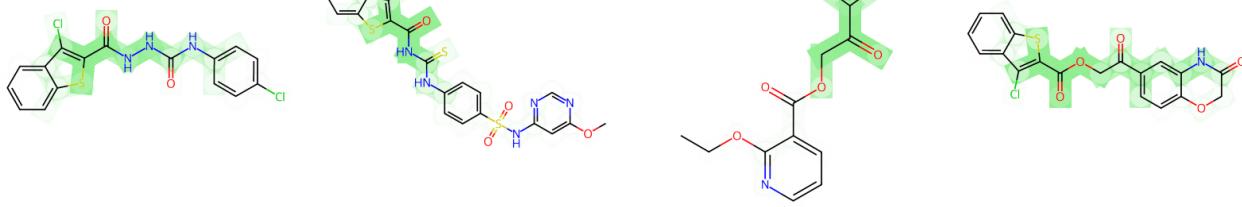


CN1CCN(c2ccc(NC(=O)c3sc4cccc4c3Cl)cc2)CC1
pred: [0.362 0.638]

Cc1c(NC(=O)C(C)OC(=O)c2sc3cccc3c2Cl)c(=O)n(-c2cccc2c1)Nc1
pred: [0.384 0.616]

O=C(CNS(=O)(=O)c1ccc2cccc2c1)OCC(=O)c1ccc(Br)s1
pred: [0.109 0.891]

O=C(COC(=O)NC(=O)c1sc2cccc2c1Cl)Nc1c(Cl)cc(Cl)c1
pred: [0.085 0.915]

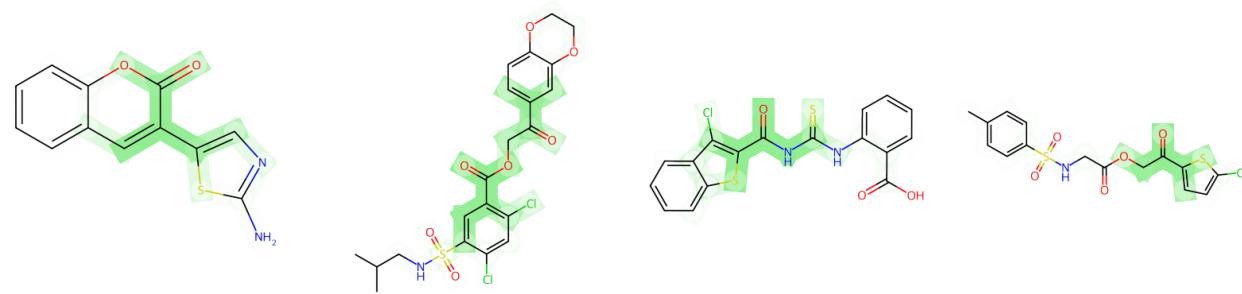


O=C(NNC(=O)c1sc2cccc2c1Cl)Nc1ccc(Cl)cc1
pred: [0.1 0.9]

COc1cc(NS(=O)(=O)c2ccc(NC(=S)NC(=O)c3sc4cccc4c3Cl)cc2)ncn1
pred: [0.158 0.842]

CCOc1cccc1C(=O)OCC(=O)c1ccc(Br)s1
pred: [0.436 0.564]

O=C1COc2ccc(C(=O)COC(=O)c3sc4cccc4c3Cl)cc2N1
pred: [0.098 0.902]



Nc1ncc(-c2cc3cccc3o2=O)s1
pred: [0.098 0.902]

CCC(C)CNS(=O)(=O)c1cc(C(=O)OCC(=O)c2ccc3c(c2)OC(=O)O)Nc1Cl
pred: [0.154 0.846]

O=c1cccc1NC(=S)NC(=O)c1sc2cccc2c1Cl
pred: [0.114 0.886]

Cc1ccc(S(=O)(=O)NCC(=O)OCC(=O)c2ccc(Cl)s2)cc1
pred: [0.156 0.844]