

# Cluster #113 - 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 113, from importance channel 1 (*aggregator*), represents a motif consisting of  $7.6 (\pm 1.5)$  nodes. The concept is generally associated with an impact of  $1.4 (\pm 0.7)$  on the prediction outcome.

## Properties

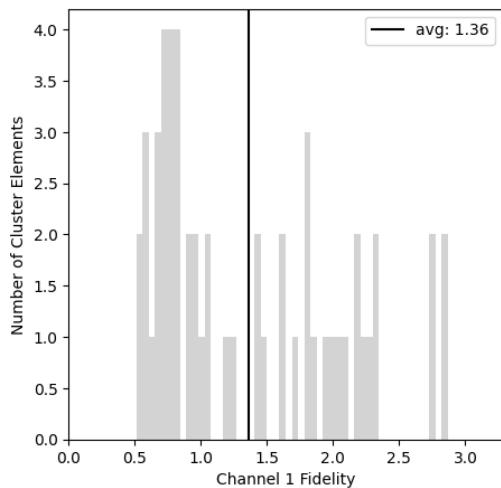
ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	54
Channel Index	1.0 (0.0)

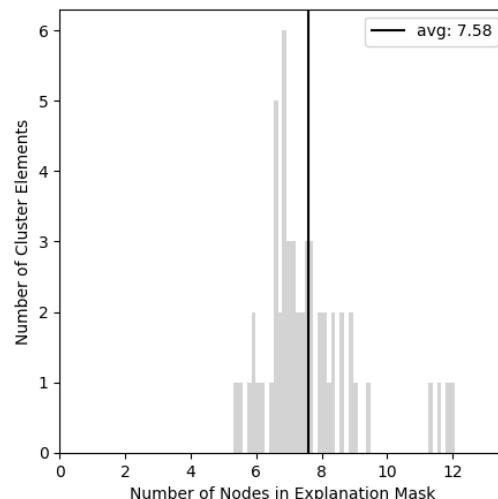
## Member Statistics

ⓘ 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.

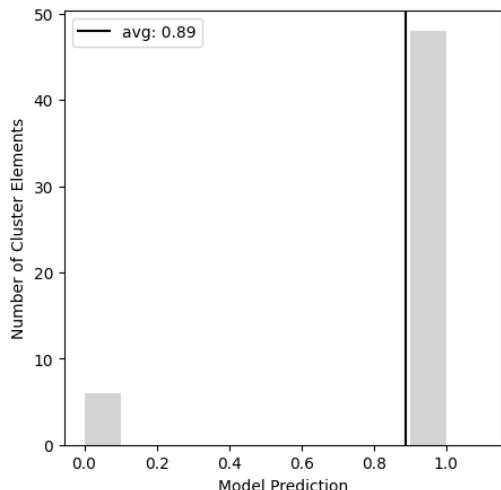
Prediction Impact Distribution



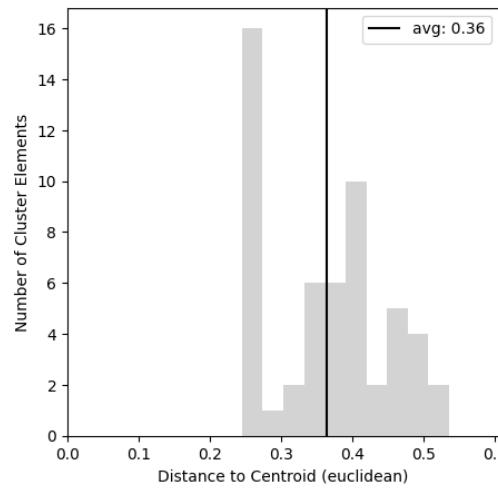
Mask Size Distribution



Prediction Output Distribution

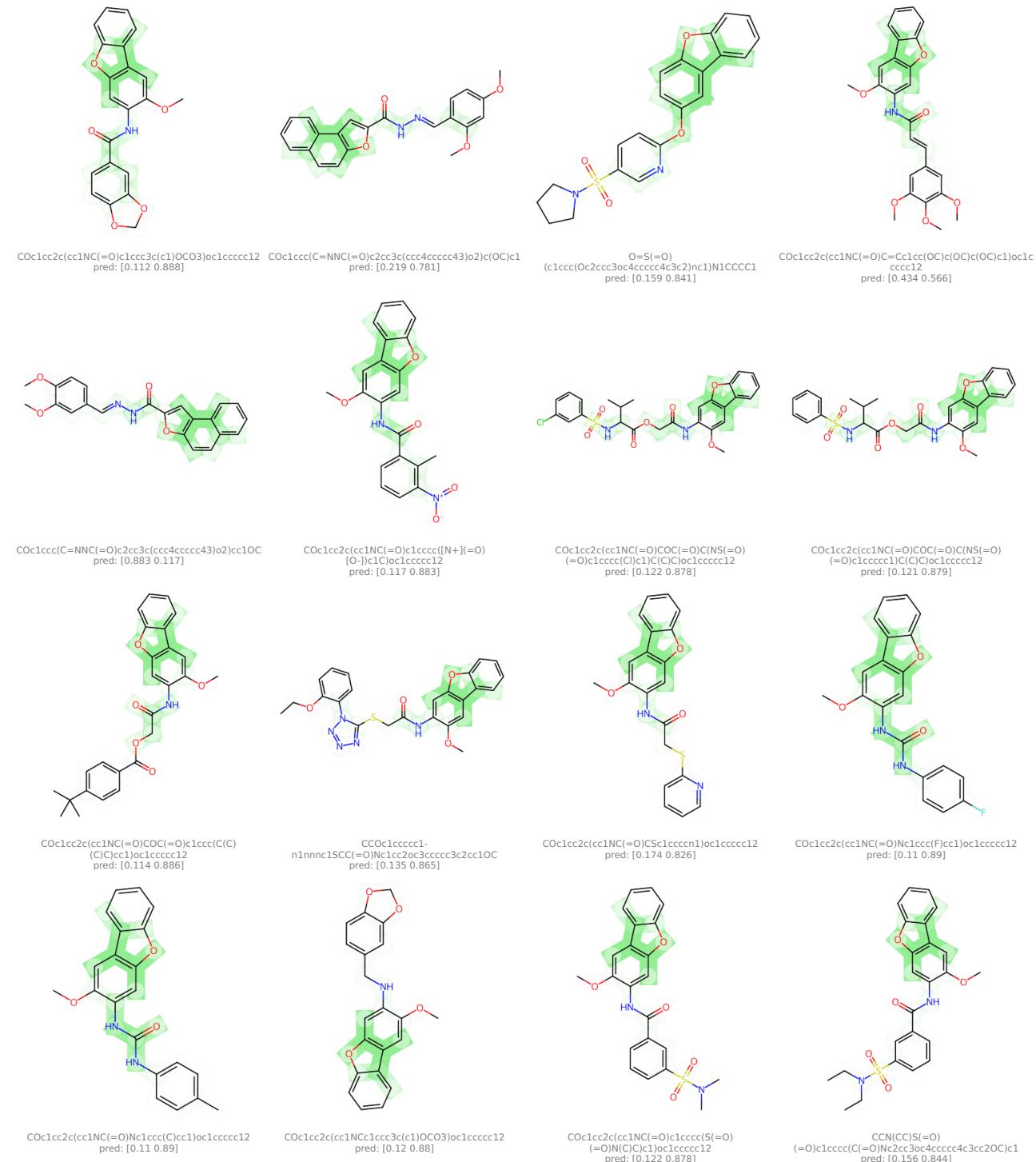


Distance to Centroid Distribution



## 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 #114 - 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 114, from importance channel 1 (*aggregator*), represents a motif consisting of 7.7 ( $\pm 0.9$ ) nodes. The concept is generally associated with an impact of 1.1 ( $\pm 0.6$ ) on the prediction outcome.

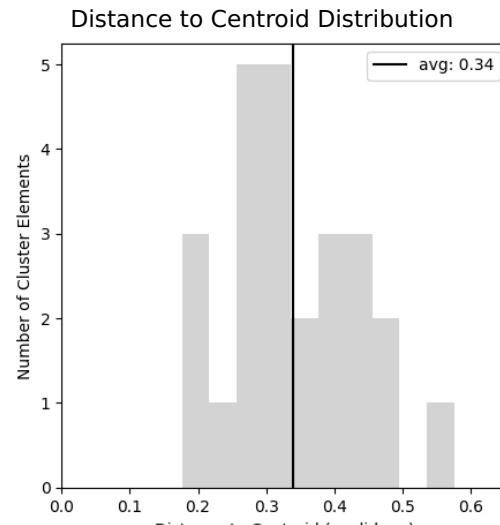
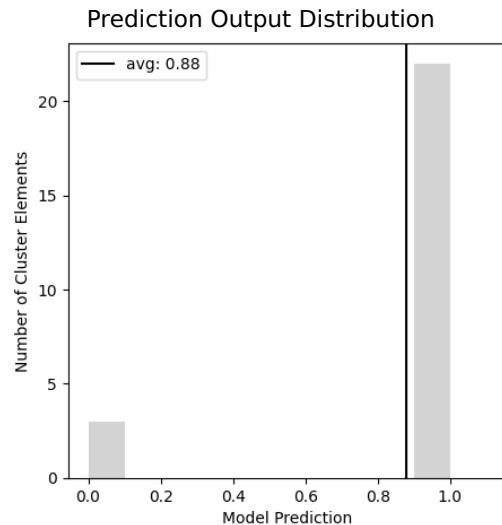
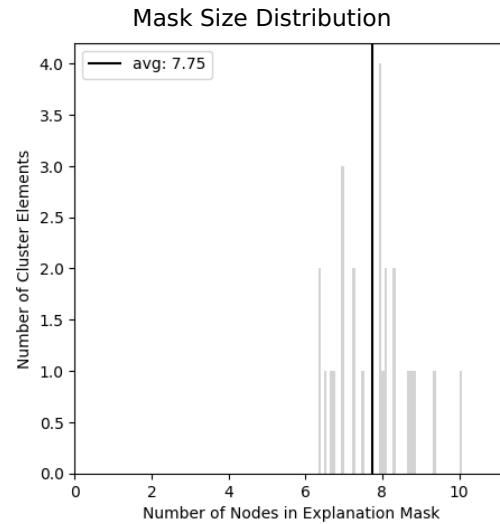
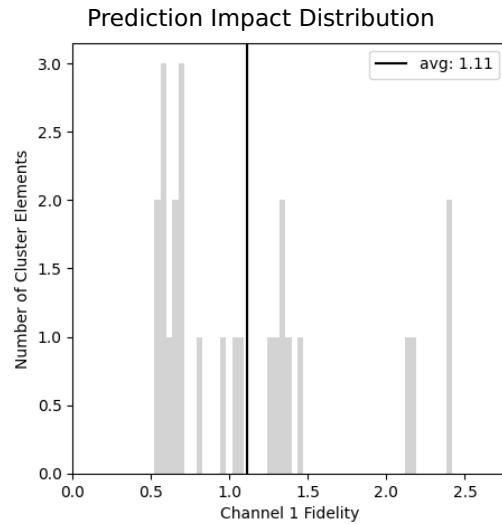
## Properties

ⓘ 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:	25
Channel Index	1.0 (0.0)

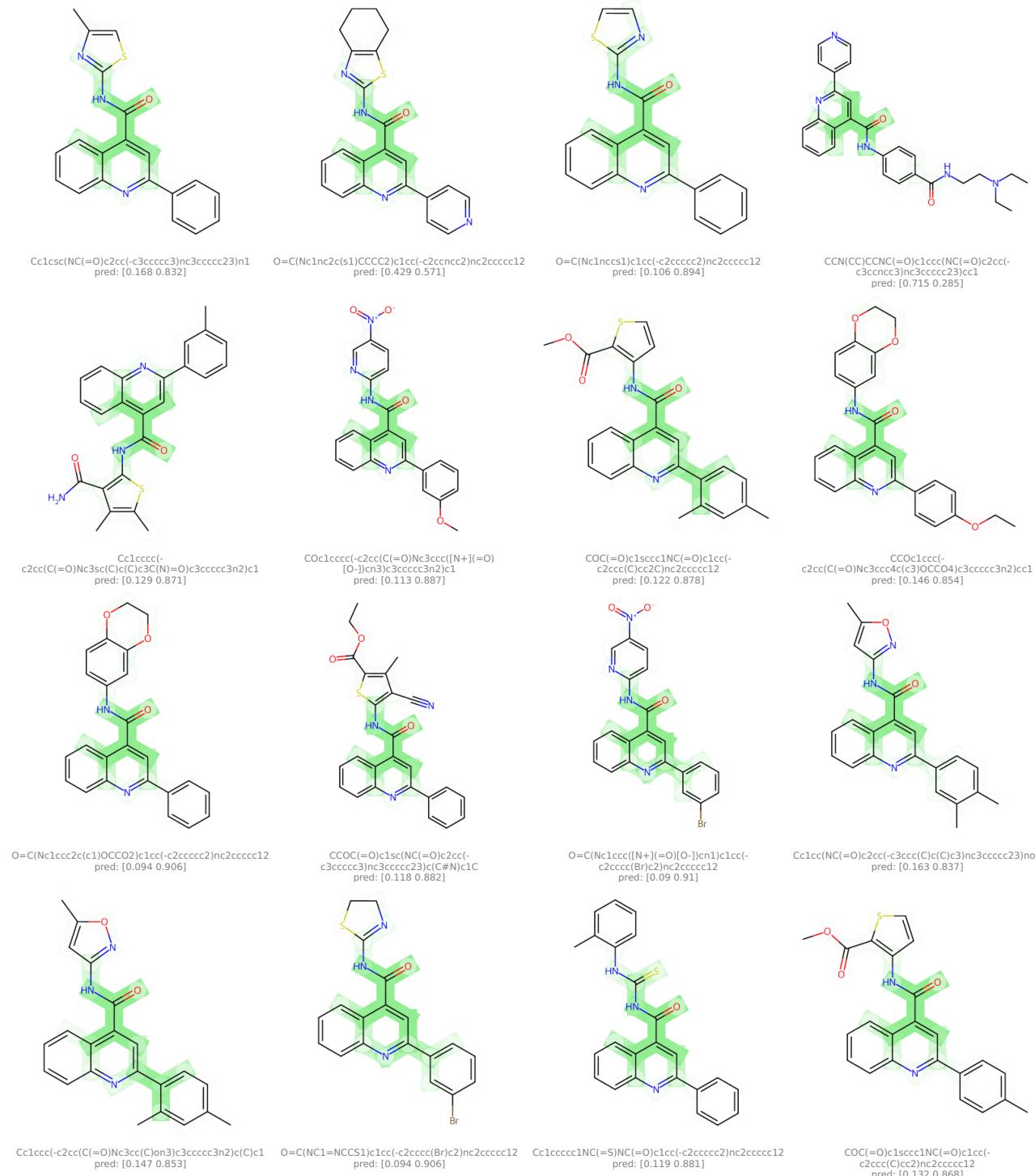
## Member Statistics

ⓘ 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 #115 - 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 115, from importance channel 1 (*aggregator*), represents a motif consisting of 7.4 ( $\pm 1.3$ ) nodes. The concept is generally associated with an impact of 1.2 ( $\pm 0.4$ ) on the prediction outcome.

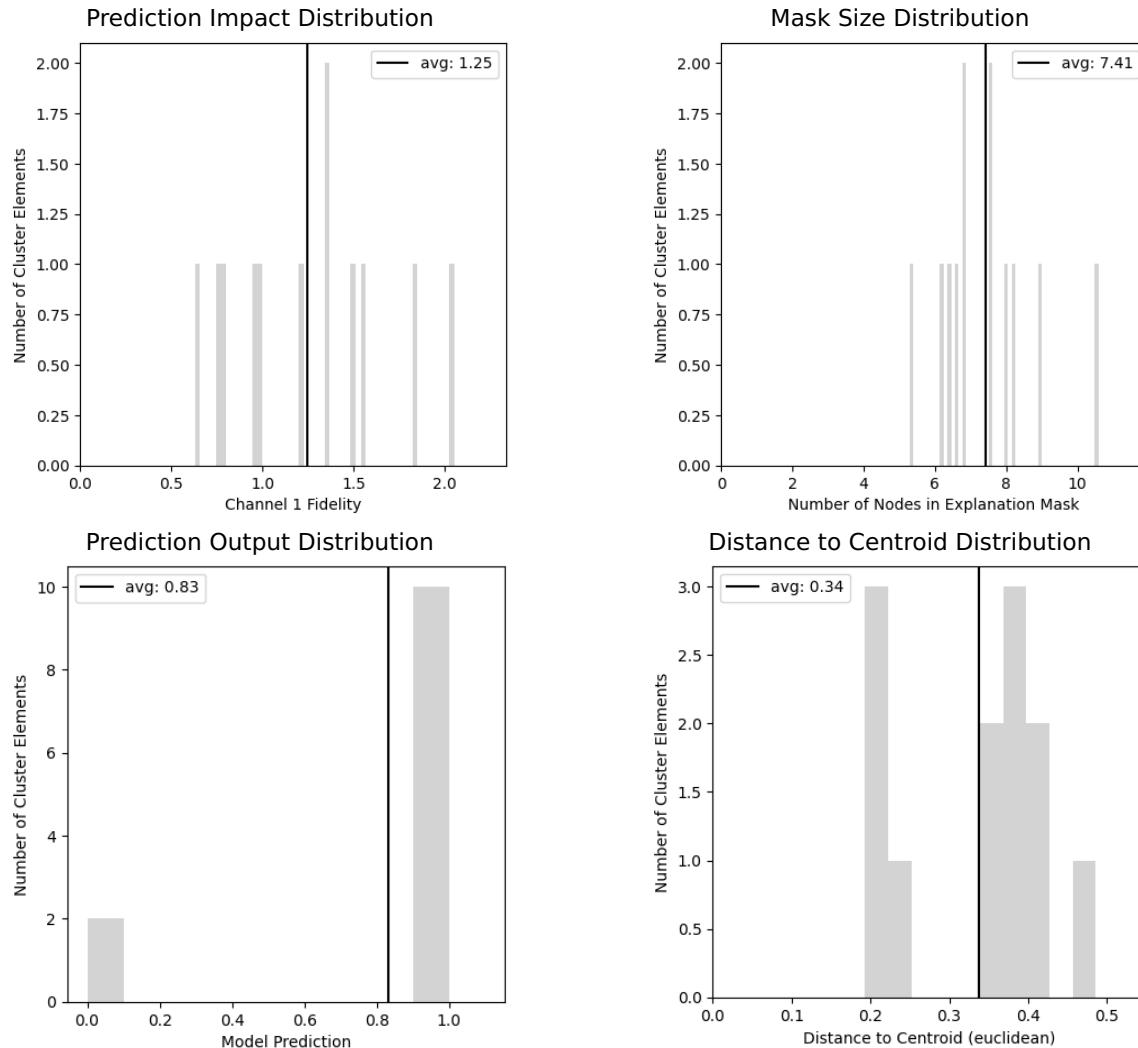
## Properties

ⓘ 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:	12
Channel Index	1.0 (0.0)

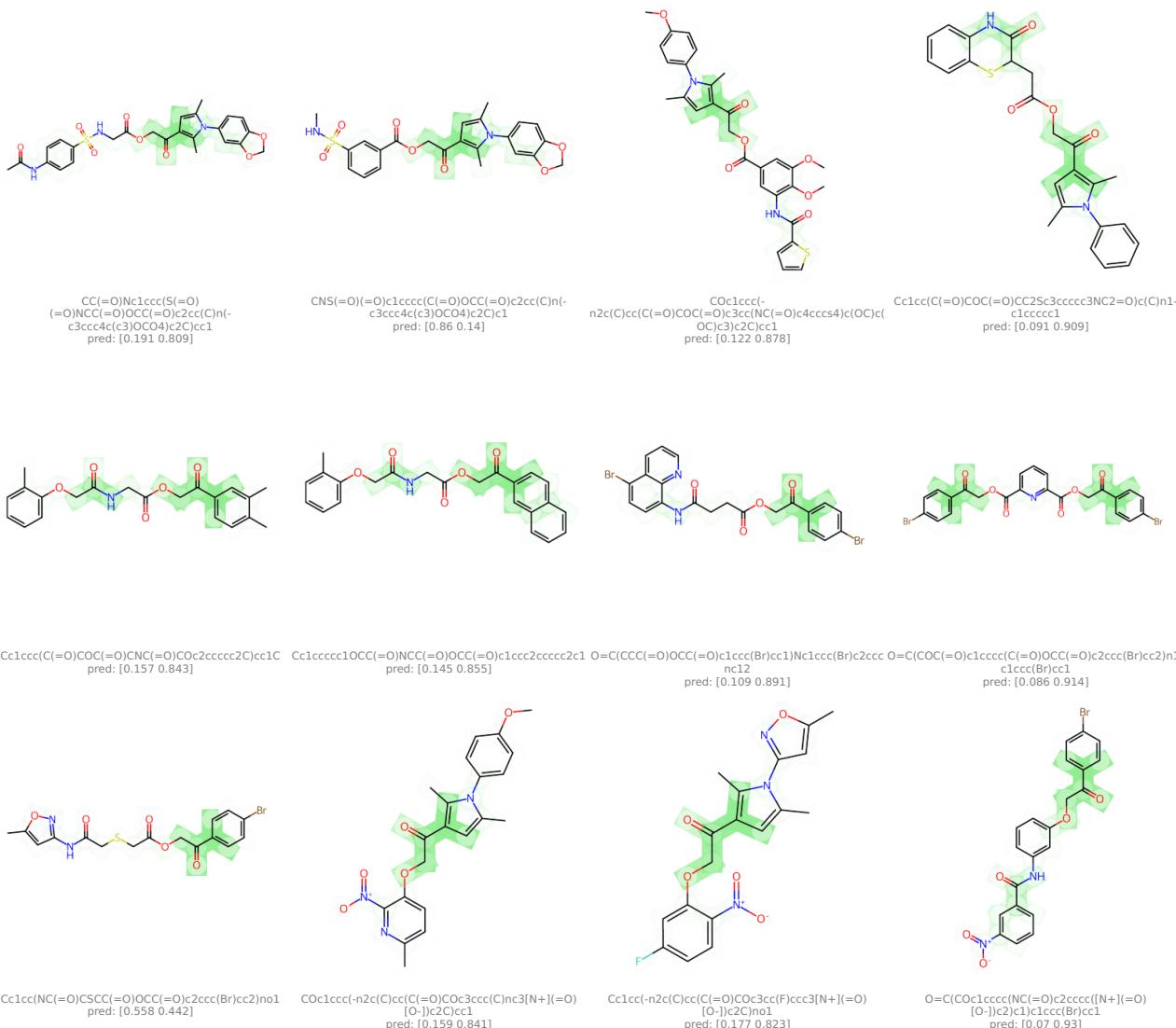
## Member Statistics

ⓘ 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

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 #116 - 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 116, from importance channel 1 (*aggregator*), represents a motif consisting of 8.3 ( $\pm 1.7$ ) nodes. The concept is generally associated with an impact of 1.1 ( $\pm 0.5$ ) on the prediction outcome.

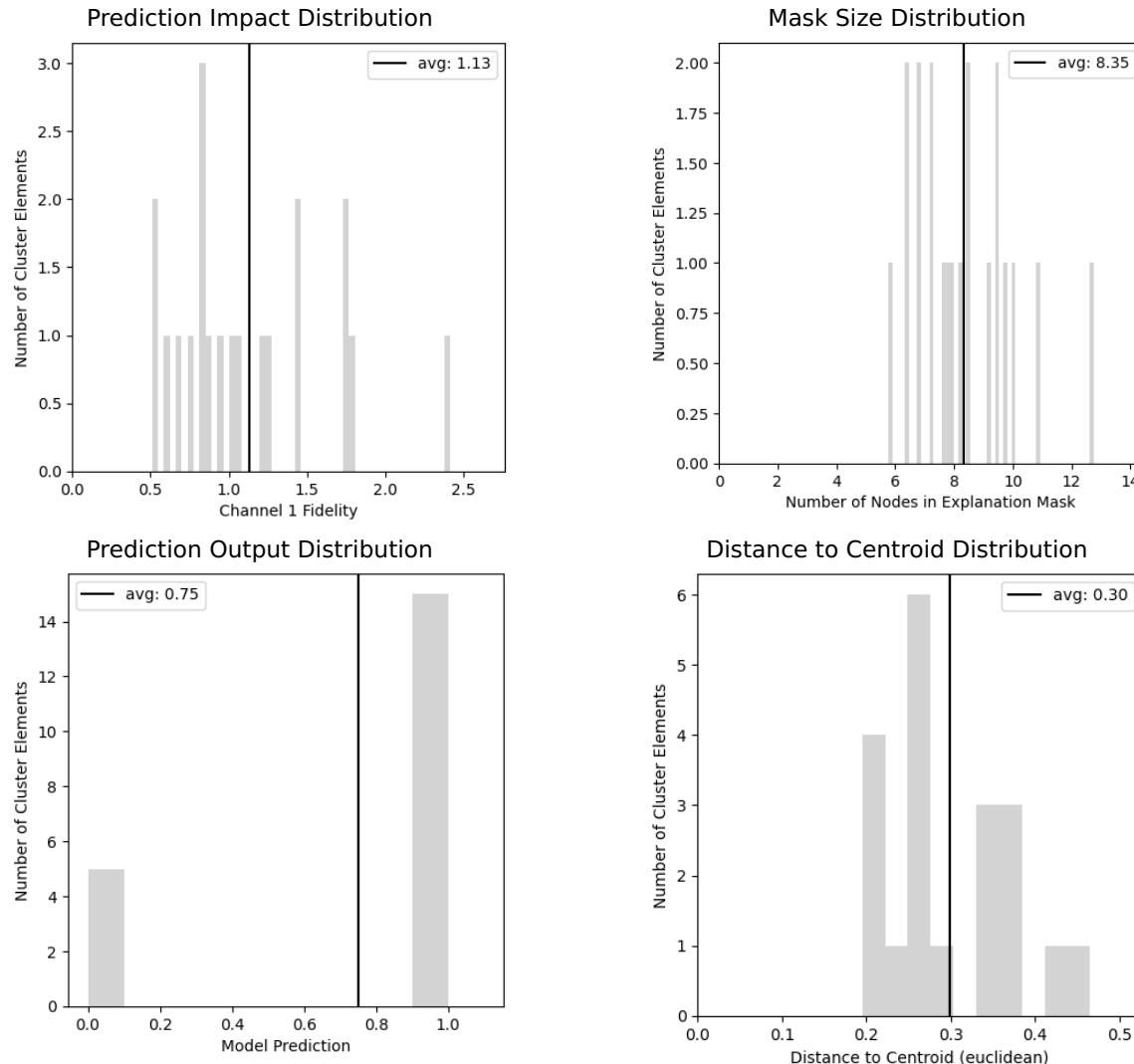
## Properties

ⓘ 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:	20
Channel Index	1.0 (0.0)

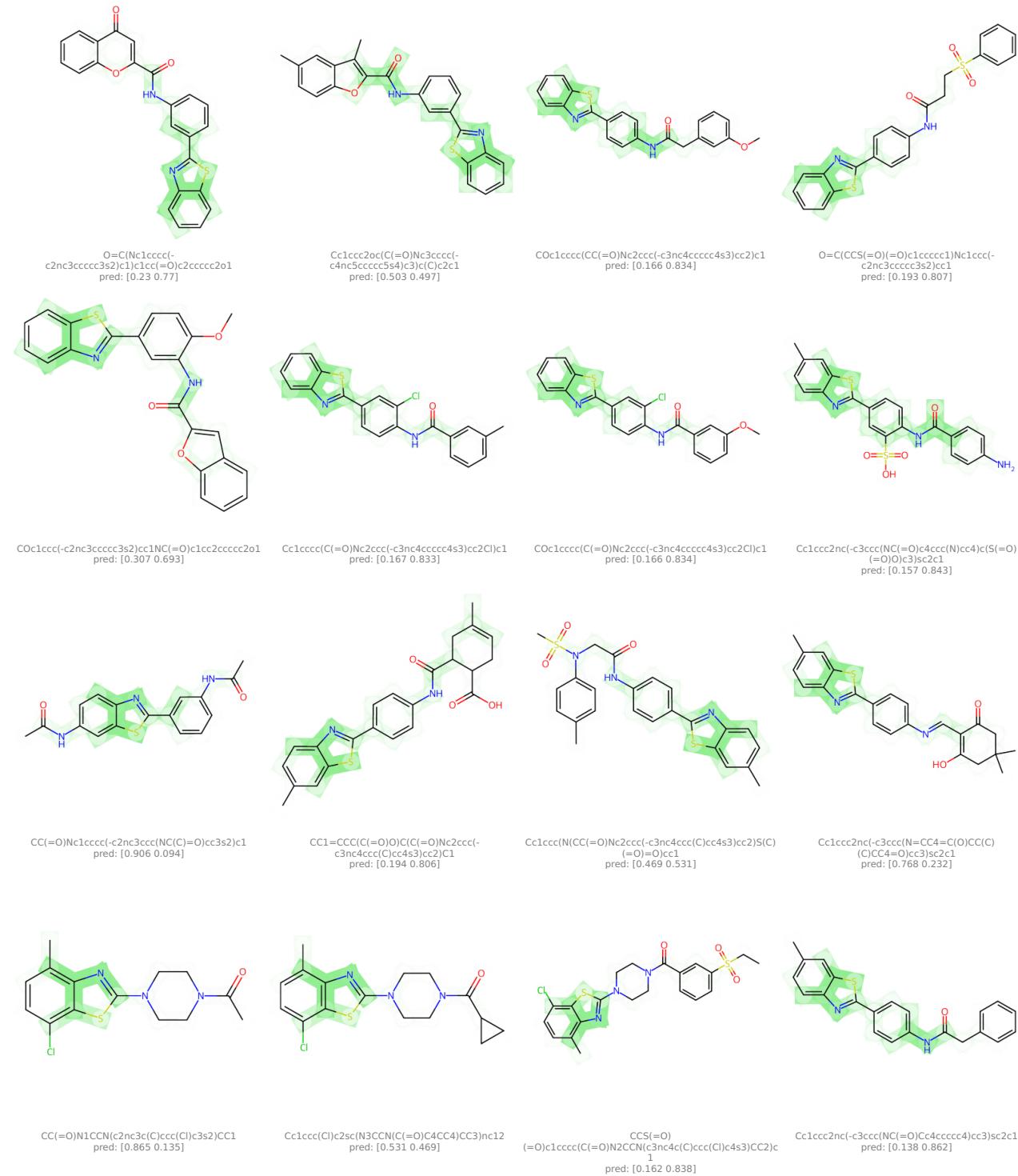
## Member Statistics

ⓘ 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

ⓘ 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 #117 - 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 117, from importance channel 1 (*aggregator*), represents a motif consisting of 9.0 ( $\pm 2.1$ ) nodes. The concept is generally associated with an impact of 1.1 ( $\pm 0.6$ ) on the prediction outcome.

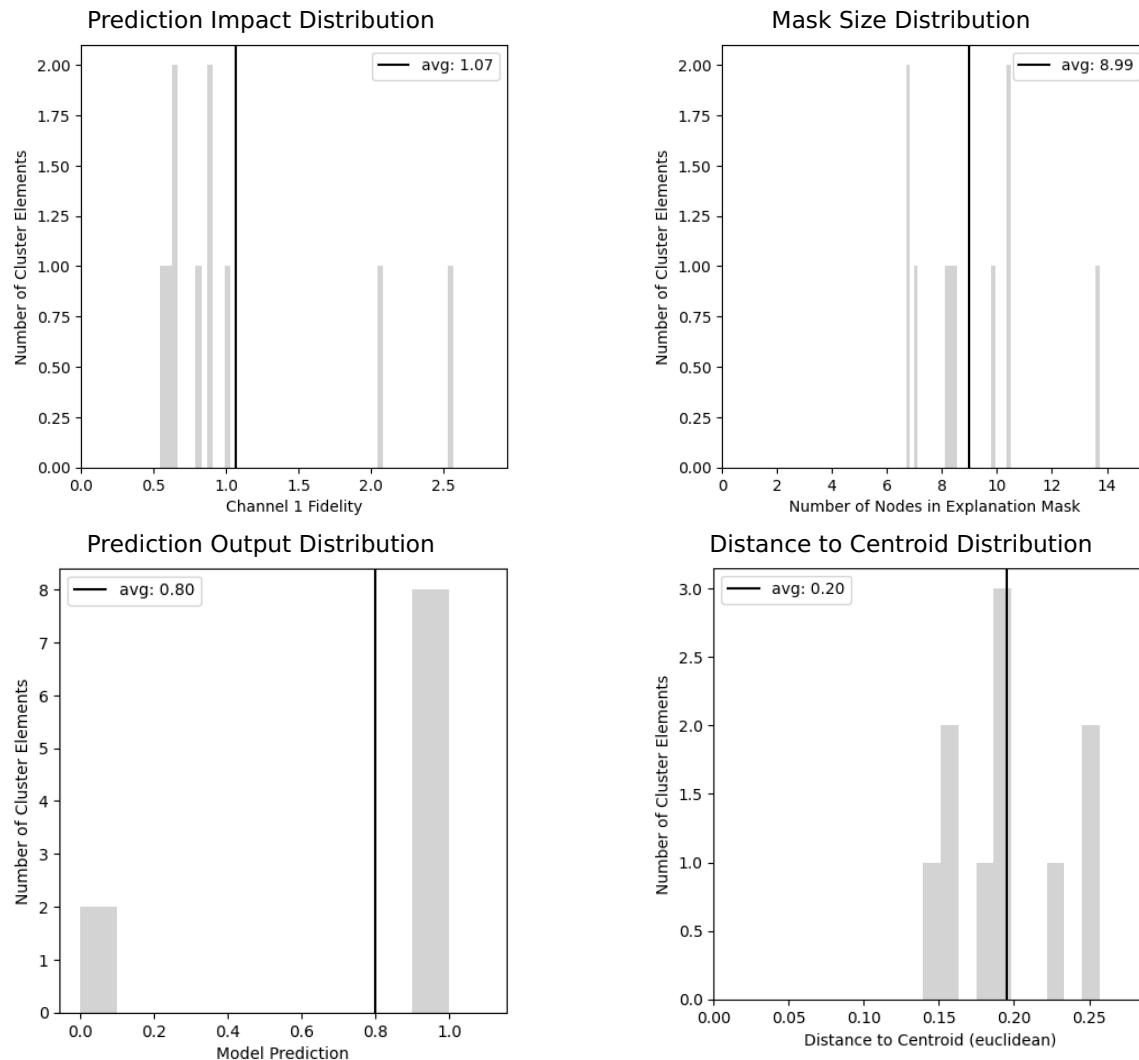
## Properties

ⓘ 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)

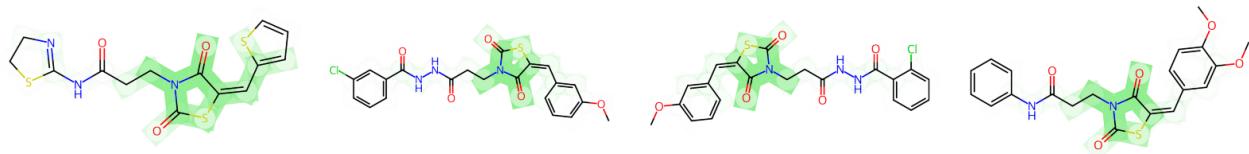
## Member Statistics

ⓘ 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.

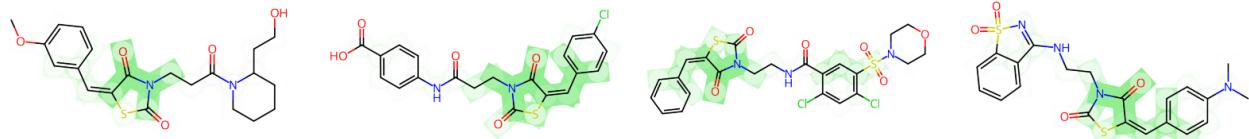


## Example Elements

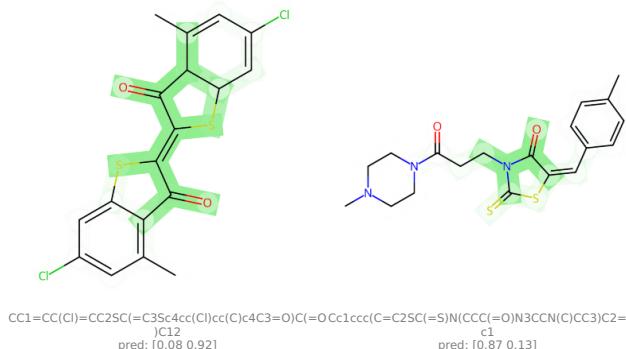
ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some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



O=C(CCN1C(=O)SC(=Cc2cccs2)C1=O)NC1=NCCS1 pred: [0.098 0.902]    COc1cccc(C=C2SC(=O)N(CCC(=O)NNC(=O)c3cccc(Cl)COc1cccc(C=C2SC(=O)N(CCC(=O)NNC(=O)c3cccc3C)COc1ccc(C=C2SC(=O)N(CCC(=O)Ne3cccc3)C2=O)cc1)c3)C2=O)c1 pred: [0.105 0.895]    Oc1ccc(cc1)C(=O)N(Cc2ccccc2)C(=O)c1cc(Cl)c(Cl)c1 pred: [0.105 0.895]    CC(=O)N(c1ccccc1)Cc2ccccc2 pred: [0.181 0.819]



COc1cccc(C=C2SC(=O)N(CCC(=O)N3CCCCC3CCO)C2 pred: [0.873 0.127]    O=C(CCN1C(=O)SC(=Cc2ccc(Cl)cc2)C1=O)Nc1ccc(C(=O)NCCN1C(=O)SC(=Cc2cccc2)C1=O)c1cc(S(=O)(=O)N2CCOCC2)c1(Cl)c1Cl pred: [0.106 0.894]    O=c1ccc(cc1)C(=O)N(Cc2ccccc2)C(=O)c1cc(Cl)c(Cl)c1 pred: [0.157 0.843]    CN(C)c1ccc(C=C2SC(=O)N(CCNC3=NS(=O)(=O)c4cccc43)C2=O)cc1 pred: [0.155 0.845]



# Cluster #118 - 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 118, from importance channel 1 (*aggregator*), represents a motif consisting of 8.5 ( $\pm 0.9$ ) nodes. The concept is generally associated with an impact of 1.3 ( $\pm 0.6$ ) on the prediction outcome.

## Properties

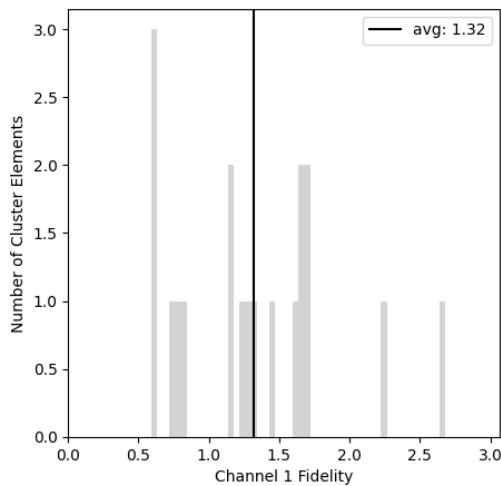
ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

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

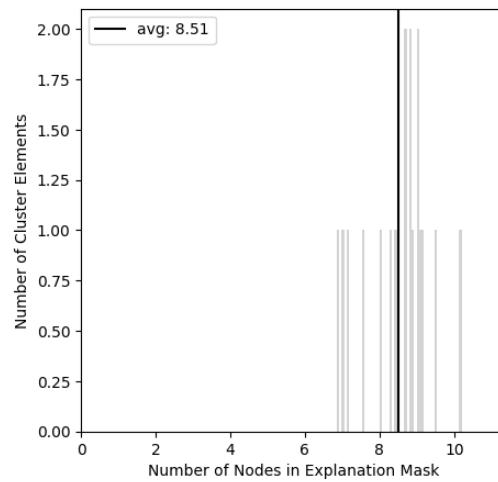
## Member Statistics

ⓘ 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.

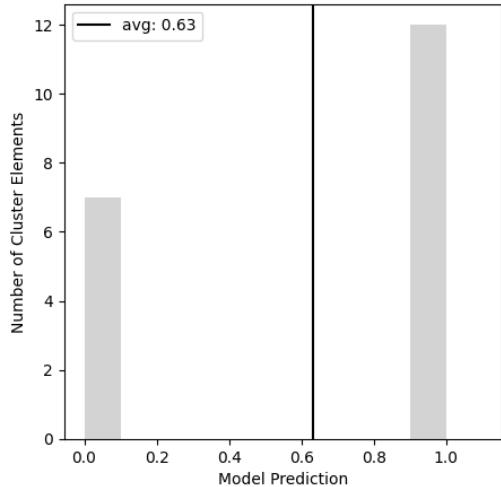
Prediction Impact Distribution



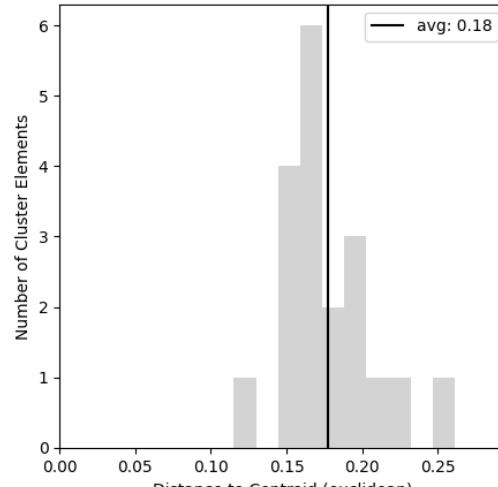
Mask Size Distribution



Prediction Output Distribution

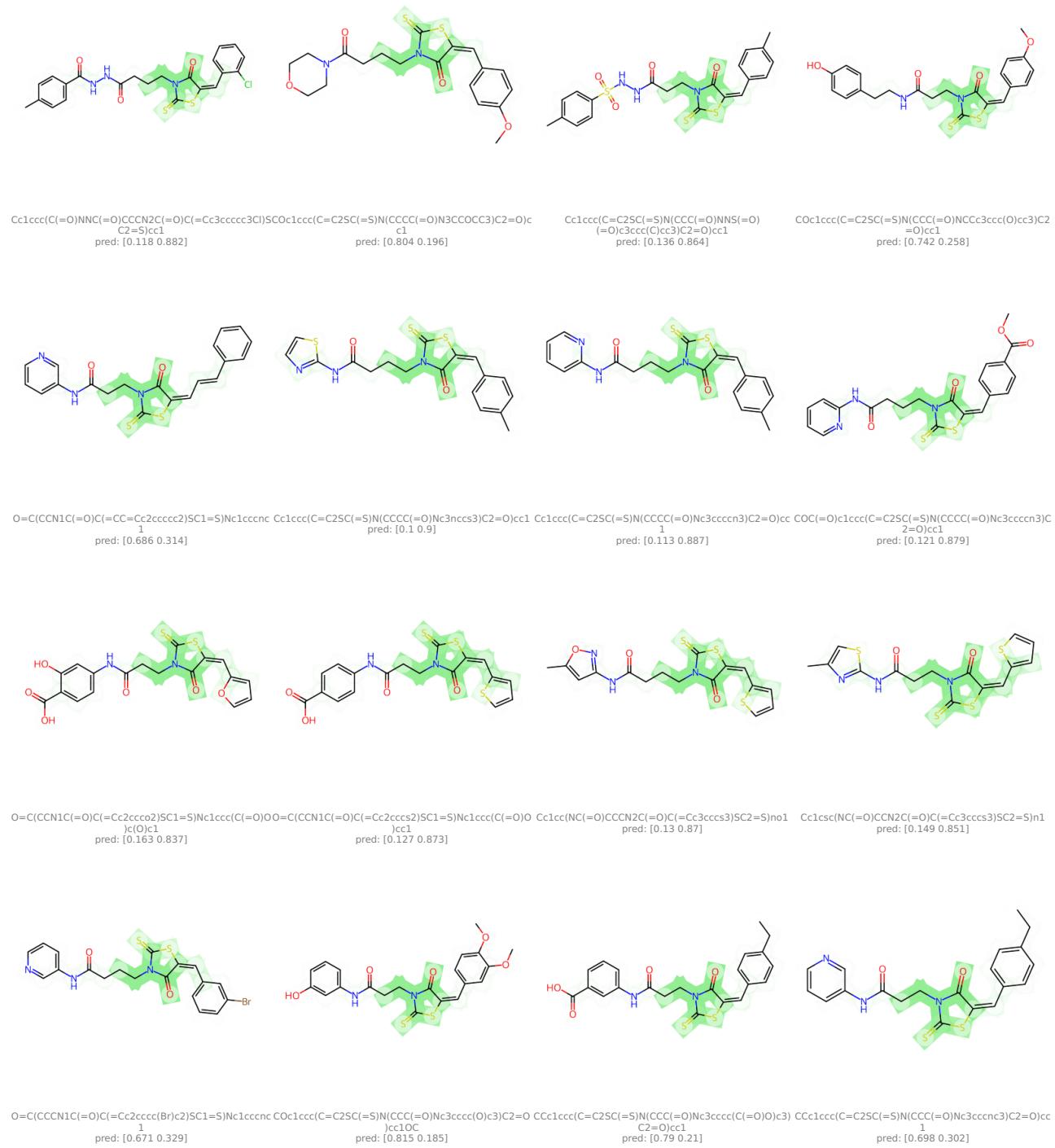


Distance to Centroid Distribution



## 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 #119 - 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 119, from importance channel 1 (*aggregator*), represents a motif consisting of  $8.1 (\pm 0.9)$  nodes. The concept is generally associated with an impact of  $1.0 (\pm 0.4)$  on the prediction outcome.

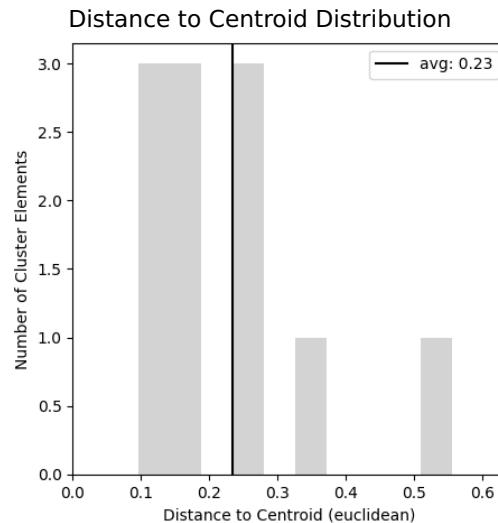
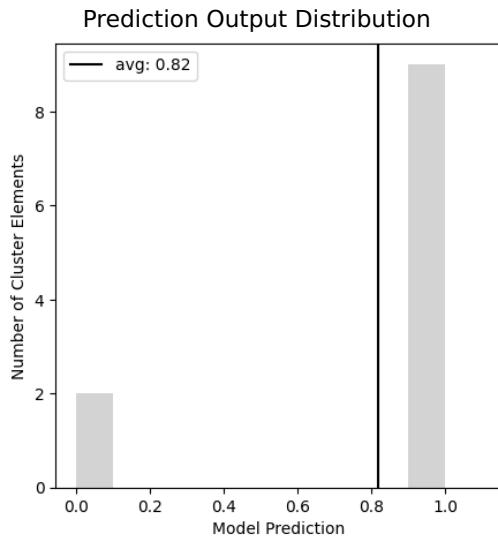
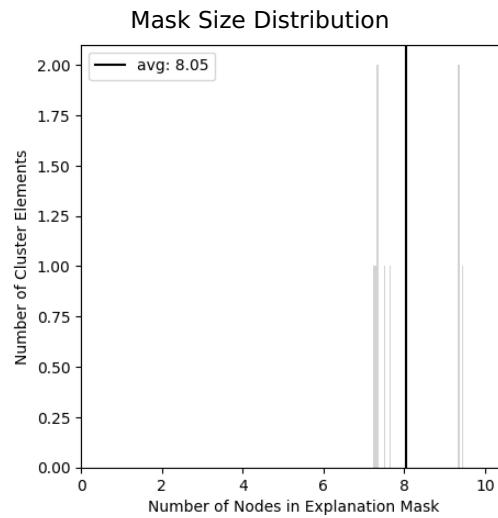
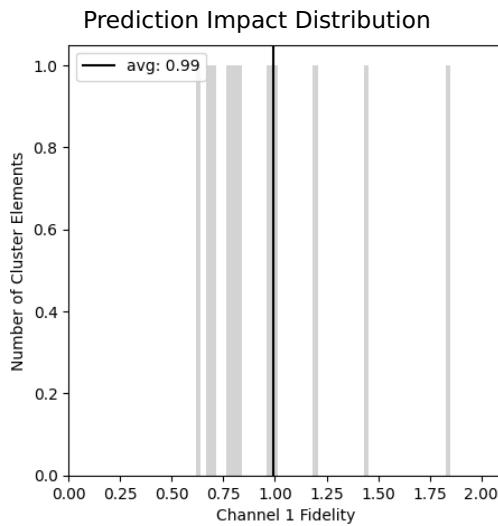
## Properties

ⓘ 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:	11
Channel Index	1.0 (0.0)

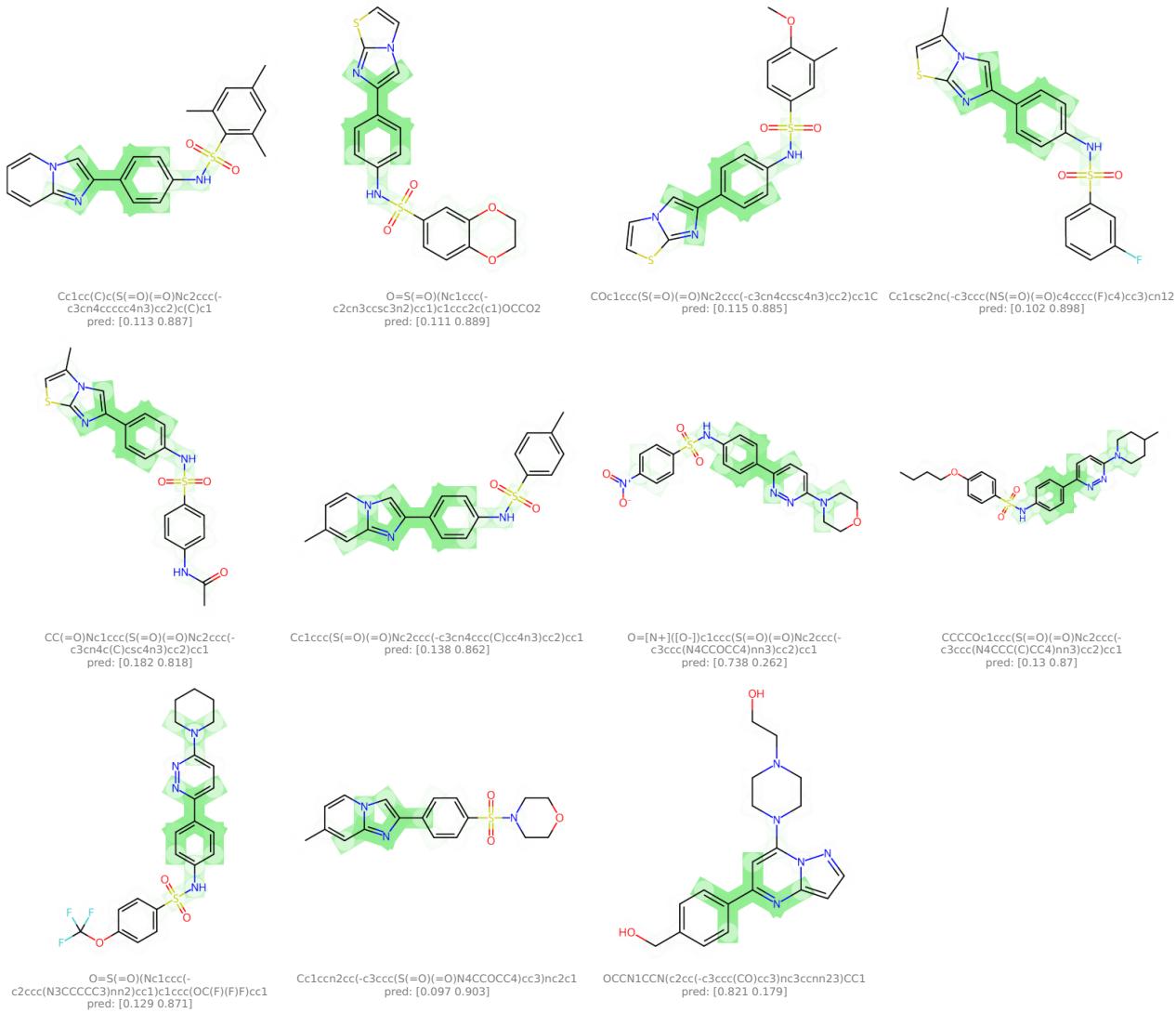
## Member Statistics

ⓘ 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 #120 - 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 120, from importance channel 1 (*aggregator*), represents a motif consisting of 8.2 ( $\pm 1.5$ ) nodes. The concept is generally associated with an impact of 1.0 ( $\pm 0.5$ ) on the prediction outcome.

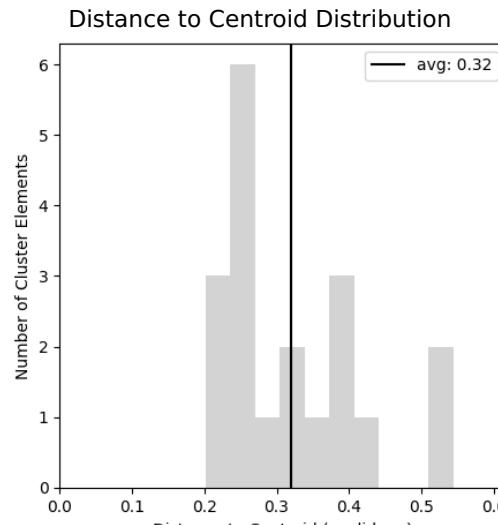
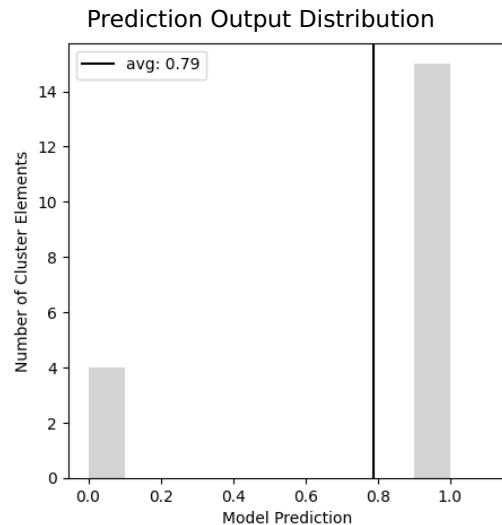
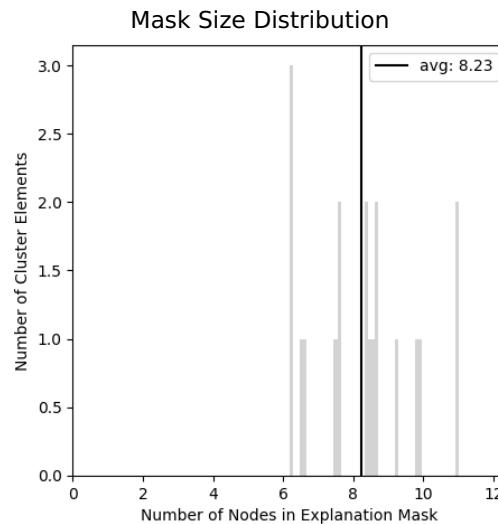
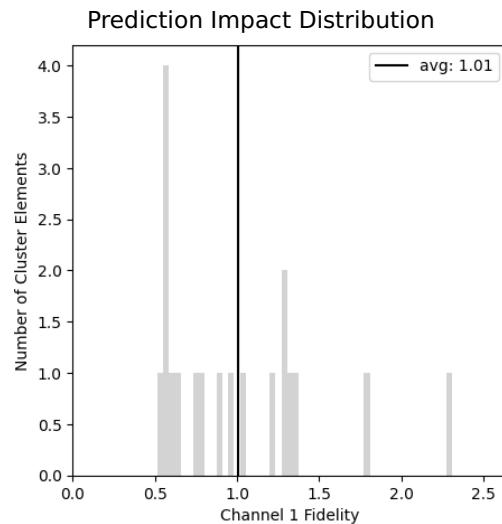
## Properties

ⓘ 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)

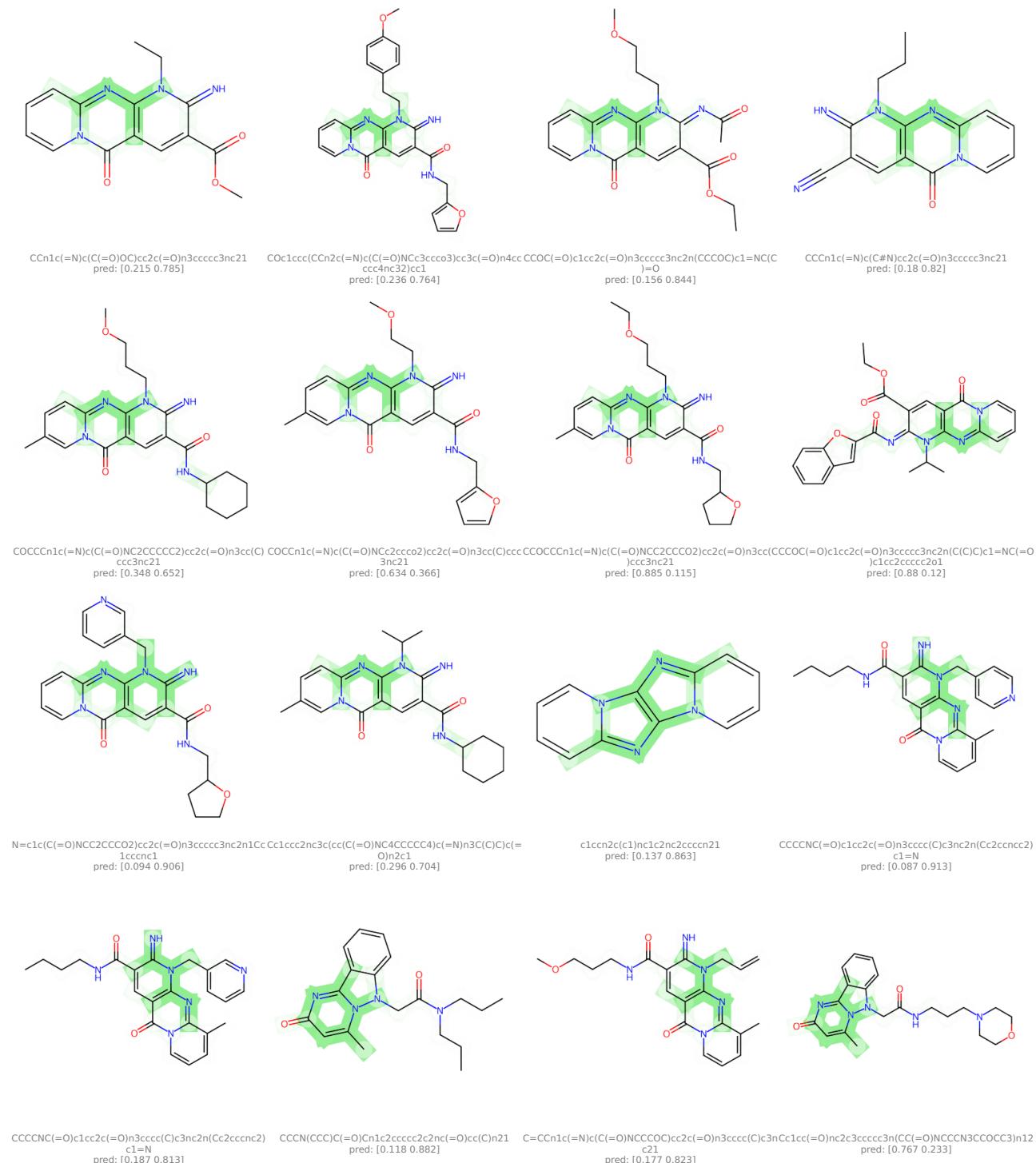
## Member Statistics

ⓘ 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 #121 - 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 121, from importance channel 1 (*aggregator*), represents a motif consisting of 7.4 ( $\pm 1.3$ ) nodes. The concept is generally associated with an impact of 0.7 ( $\pm 0.1$ ) on the prediction outcome.

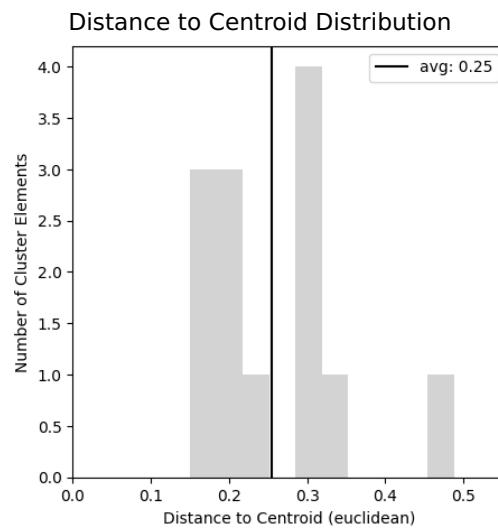
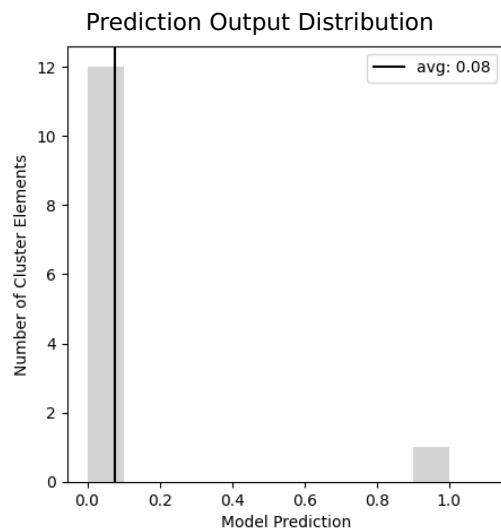
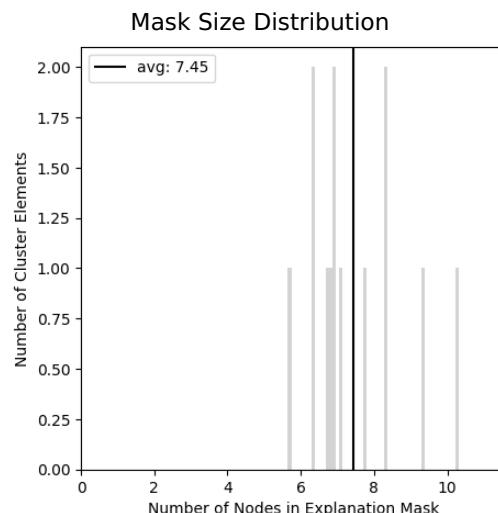
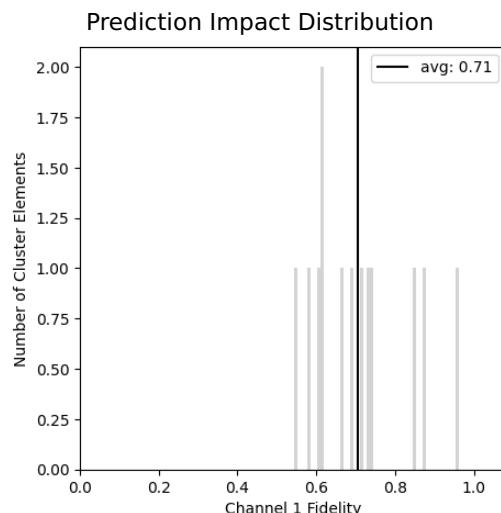
## Properties

ⓘ 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)

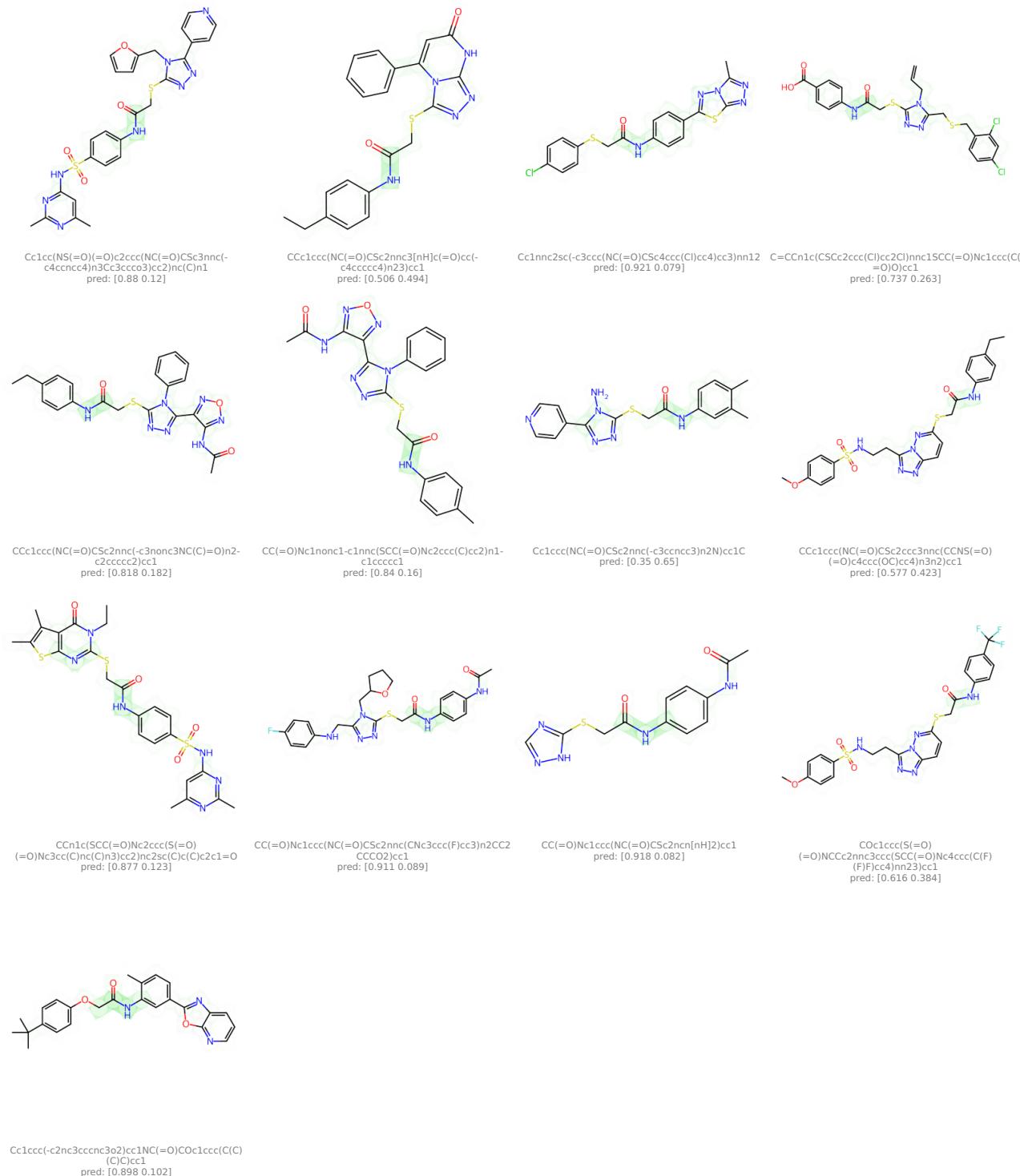
## Member Statistics

ⓘ 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 #122 - 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 122, from importance channel 1 (*aggregator*), represents a motif consisting of 8.0 ( $\pm 1.5$ ) nodes. The concept is generally associated with an impact of 1.2 ( $\pm 0.2$ ) on the prediction outcome.

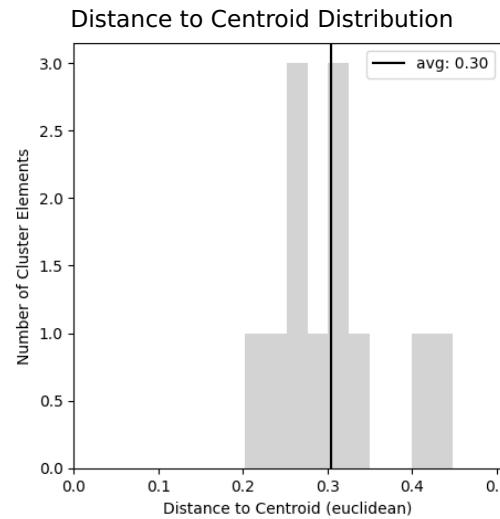
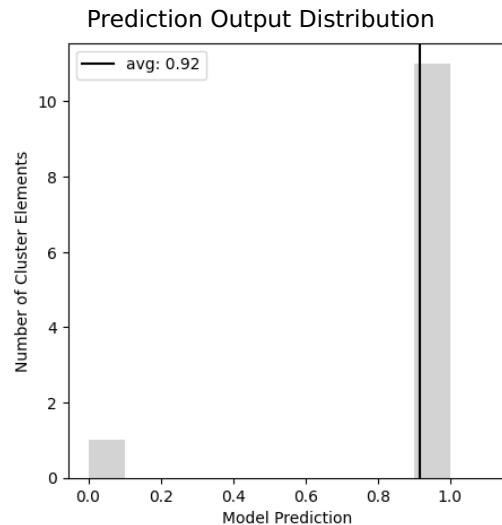
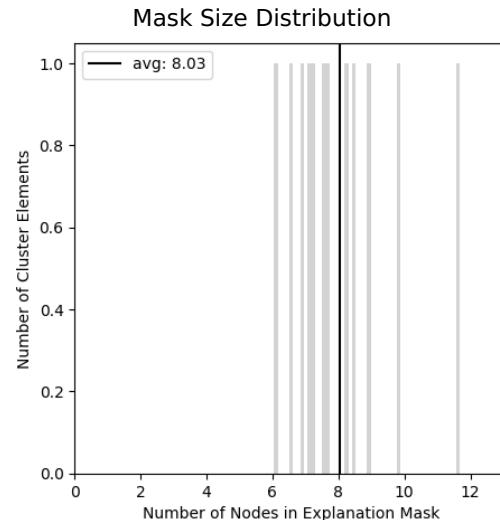
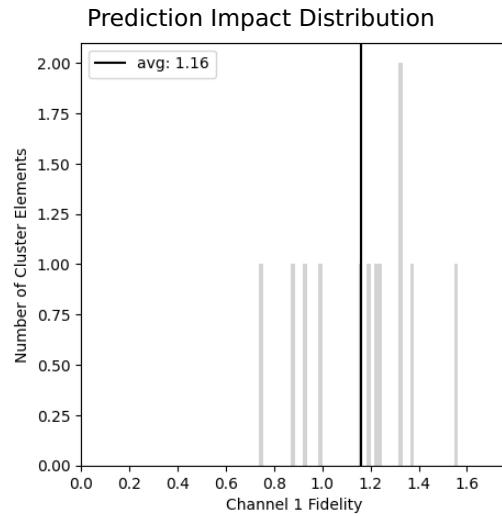
## Properties

ⓘ 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)

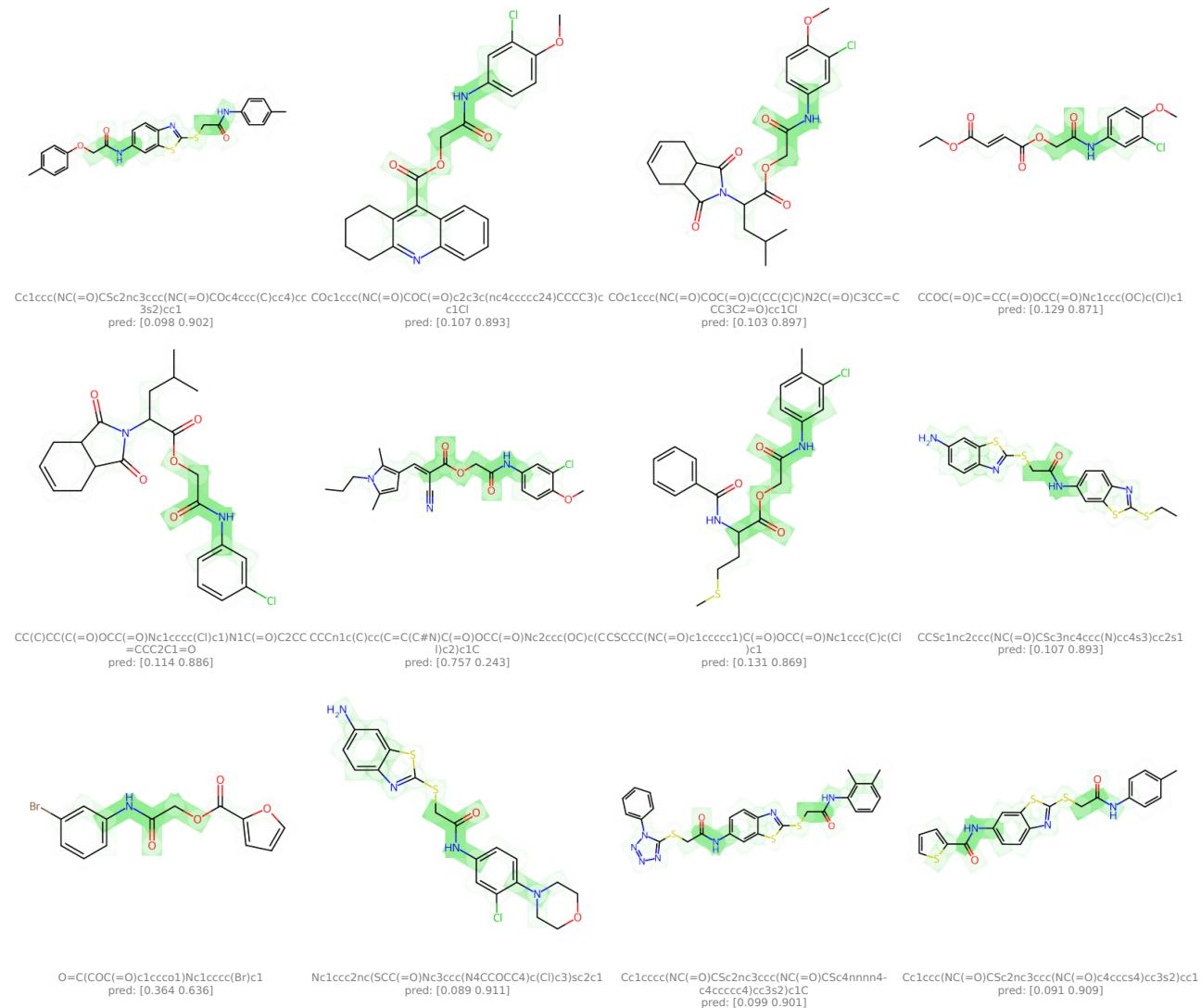
## Member Statistics

ⓘ 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 #123 - 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 123, from importance channel 1 (*aggregator*), represents a motif consisting of 7.4 ( $\pm 1.1$ ) nodes. The concept is generally associated with an impact of 1.3 ( $\pm 0.7$ ) on the prediction outcome.

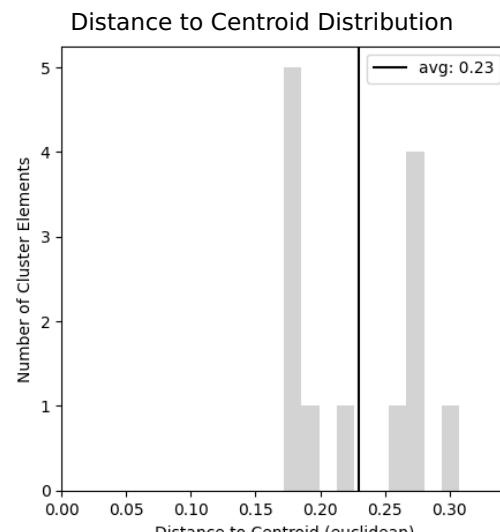
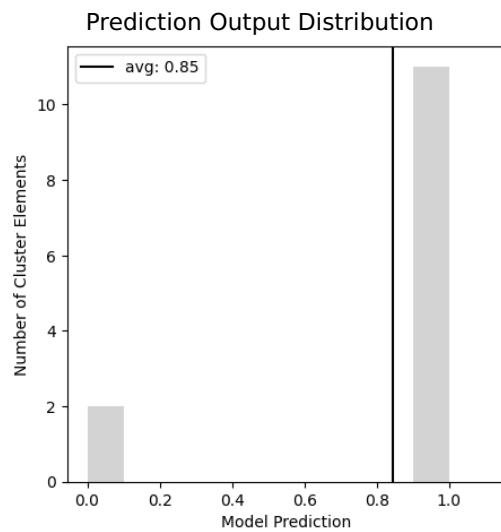
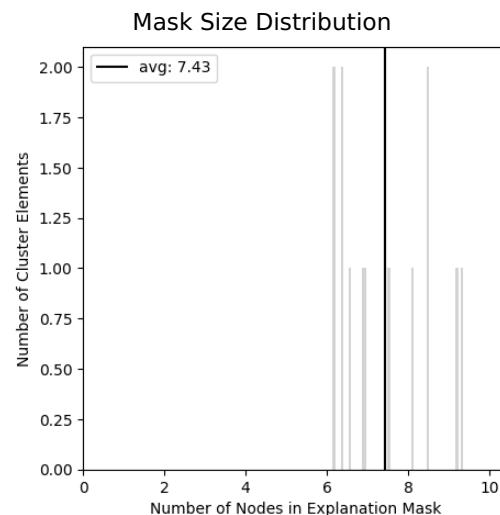
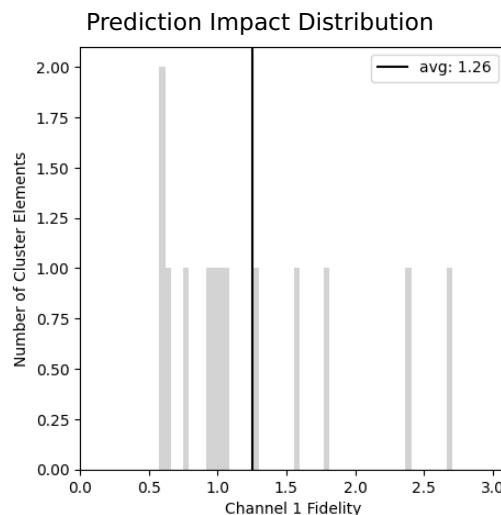
## Properties

ⓘ 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:	13
Channel Index	1.0 (0.0)

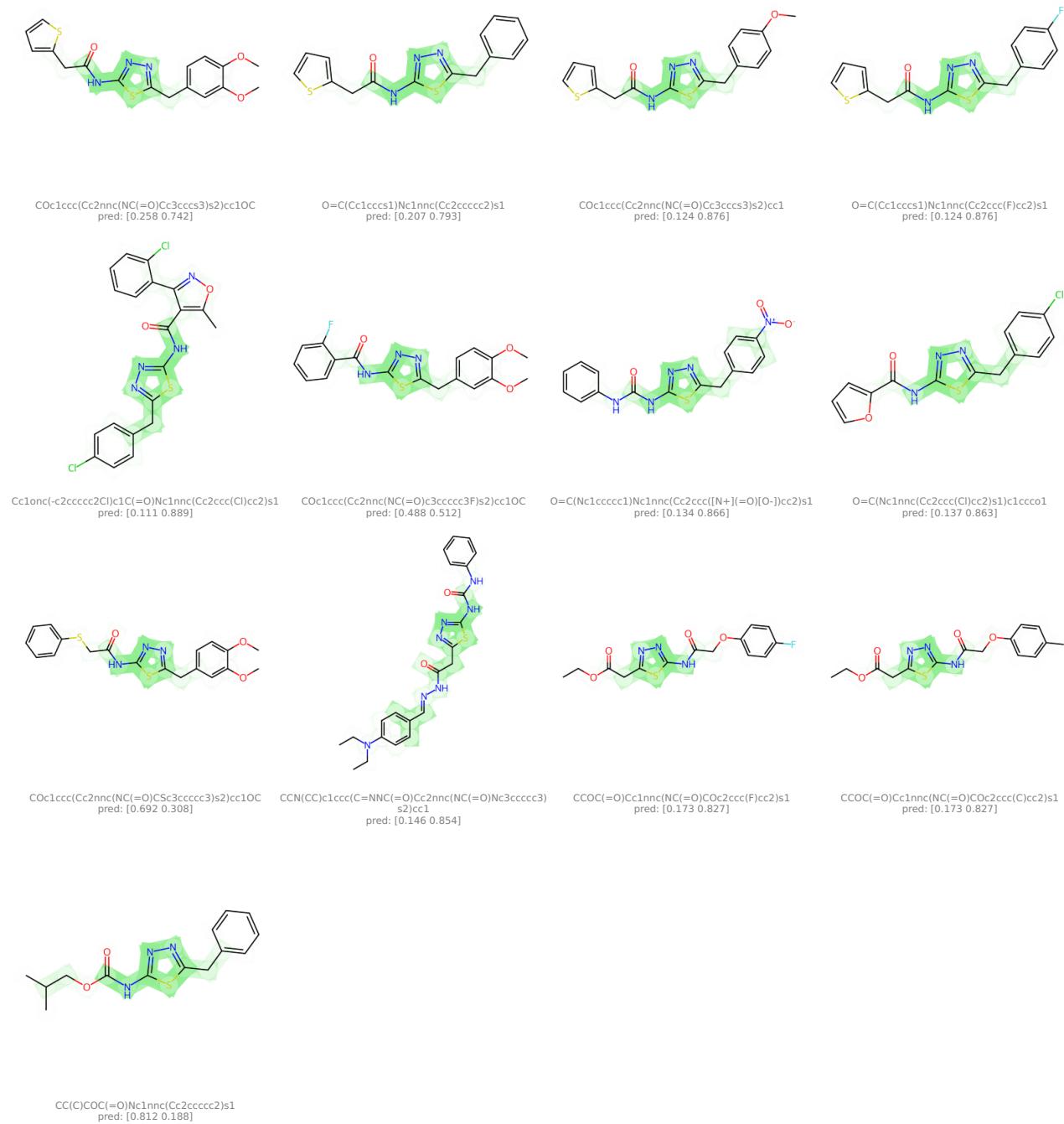
## Member Statistics

ⓘ 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 #124 - 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 124, from importance channel 1 (*aggregator*), represents a motif consisting of 8.5 ( $\pm 1.7$ ) nodes. The concept is generally associated with an impact of 1.1 ( $\pm 0.5$ ) on the prediction outcome.

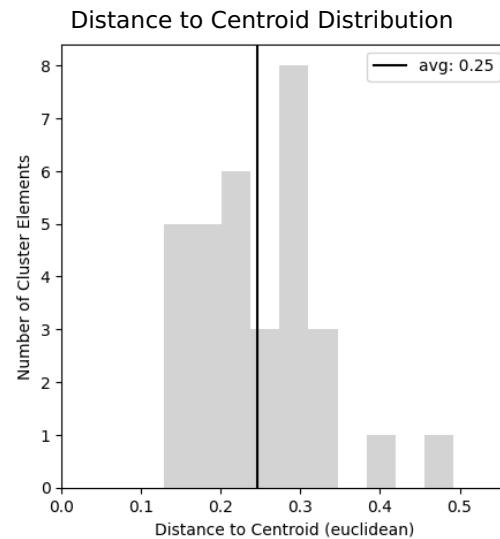
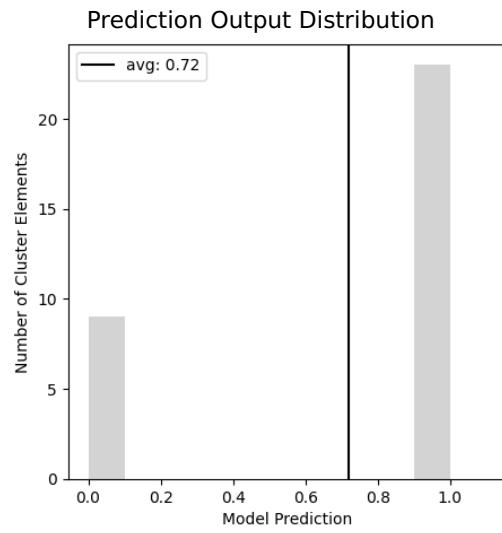
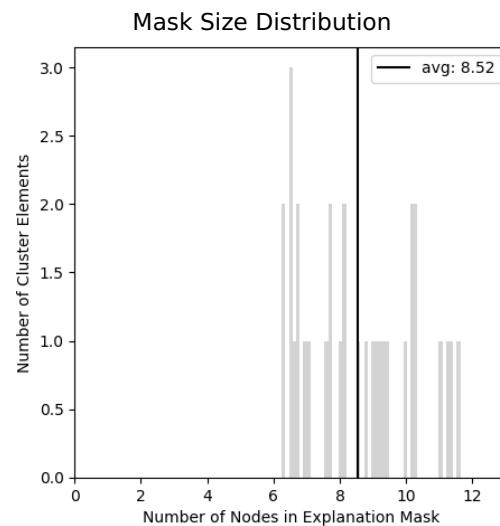
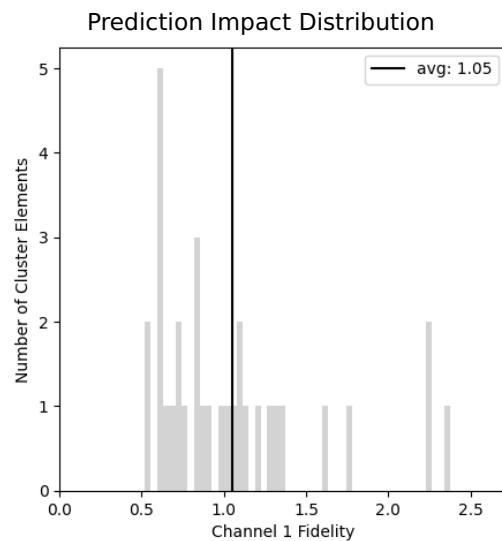
## Properties

ⓘ 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:	32
Channel Index	1.0 (0.0)

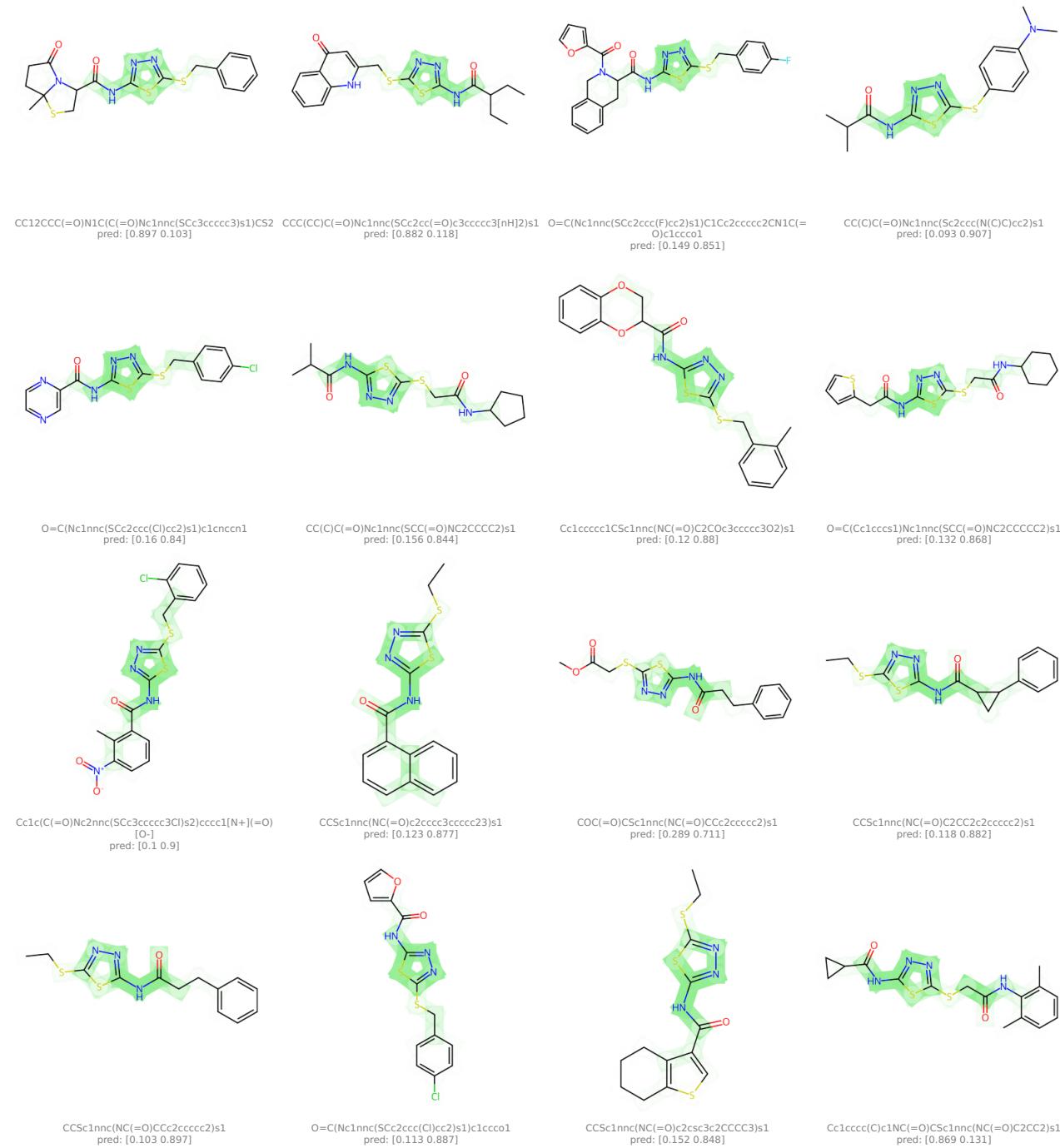
## Member Statistics

ⓘ 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 #125 - 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 125, from importance channel 1 (*aggregator*), represents a motif consisting of **8.1** ( $\pm 1.2$ ) nodes. The concept is generally associated with an impact of **1.3** ( $\pm 0.5$ ) on the prediction outcome.

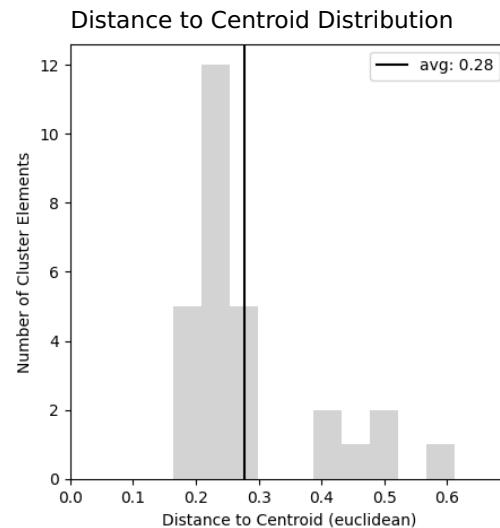
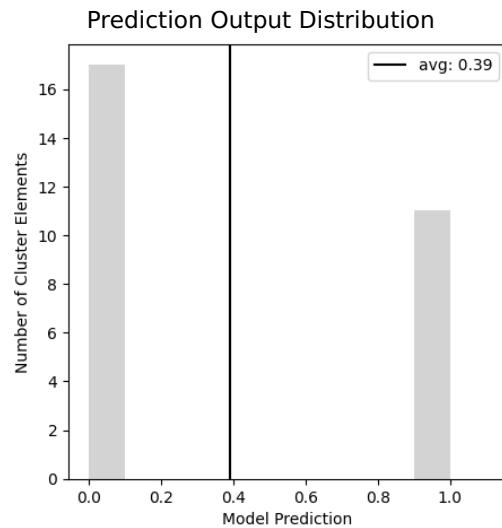
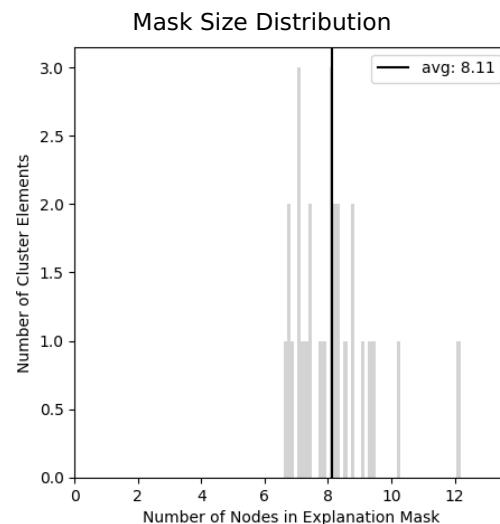
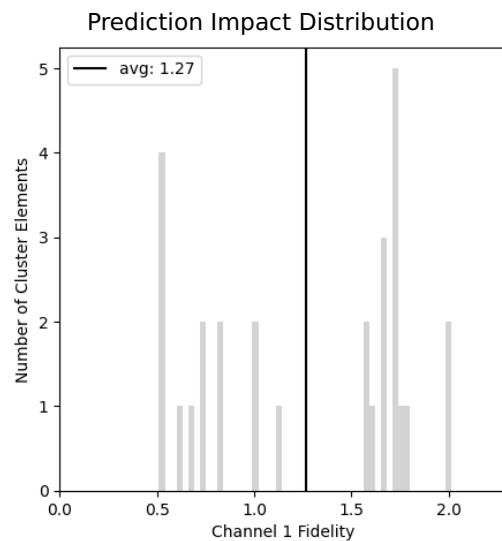
## Properties

ⓘ 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:	28
Channel Index	1.0 (0.0)

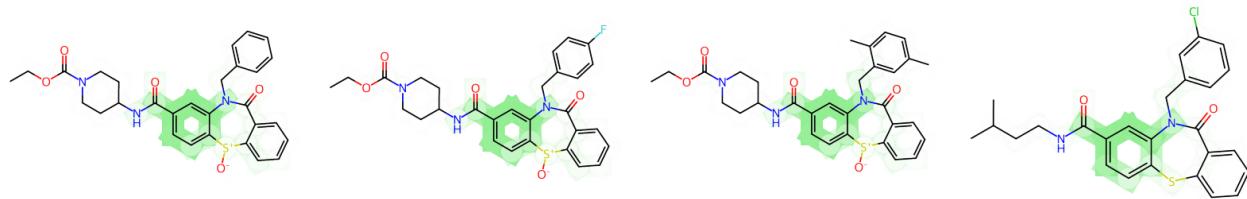
## Member Statistics

ⓘ 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.

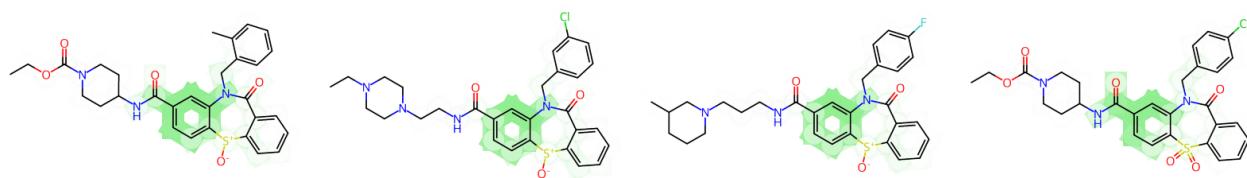


## Example Elements

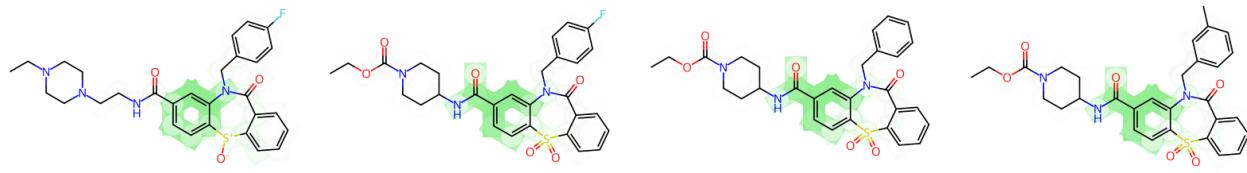
ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some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



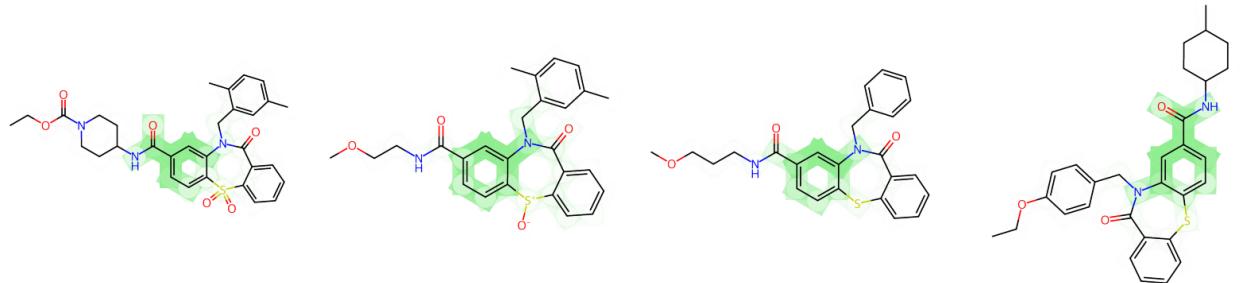
CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2cccc2)C( CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2ccc(F)cc2) CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2cc(C)ccc2 CC(C)CCNC(=O)c1ccc2c(c1)N(Cc1cccc(Cl)c1)C(=O)c1 =O)c2cccc2[S+][O-])CC1 C(=O)c2cccc2[S+][O-])CC1 pred: [0.609 0.391]  
C(=O)c2cccc2[S+][O-])CC1 pred: [0.61 0.39]  
CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2cc(C)ccc2 CC(C)CCNC(=O)c1ccc2c(c1)N(Cc1cccc(Cl)c1)C(=O)c1 ccccc1S2 pred: [0.627 0.373]  
pred: [0.892 0.108]



CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2cccc2)C CCN1CCN(CCNC(=O)c2ccc3c(c2)N(Cc2ccc(Cl)c2)C( CC1CCCN(CCCNC(=O)c2ccc3c(c2)N(Cc2ccc(F)cc2)C(= CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2ccc(Cl)c2)C(=O)c2cccc2[S+][O-])CC1 O)c2cccc2[S+][O-])CC1 pred: [0.625 0.375]  
O)c2cccc2[S+][O-])CC1 pred: [0.481 0.519]  
CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2cccc2)C( CC1CCCN(CCCNC(=O)c2ccc3c(c2)N(Cc2ccc(Cl)c2)C(= CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2ccc(Cl)c2)C(=O)c2cccc2[S+][O-])CC1 O)c2cccc2[S+][O-])CC1 pred: [0.821 0.179]  
)C(=O)c2cccc2S3(=O)=O)CC1 pred: [0.595 0.405]



CCN1CCN(CCNC(=O)c2ccc3c(c2)N(Cc2ccc(F)cc2)C(=O)CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2ccc(Cl)c2) C(=O)c2cccc2[S+][O-])CC1 C(=O)c2cccc2S3(=O)=O)CC1 pred: [0.473 0.527]  
CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2ccc(Cl)c2)C( CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2ccc(Cl)c2)C(=O)c2cccc2[S+][O-])CC1 C(=O)c2cccc2S3(=O)=O)CC1 pred: [0.595 0.405]  
CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2ccc(Cl)c2)C( CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2ccc(Cl)c2)C(=O)c2cccc2[S+][O-])CC1 C(=O)c2cccc2S3(=O)=O)CC1 pred: [0.594 0.406]  
CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2ccc(Cl)c2)C( CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2ccc(Cl)c2)C(=O)c2cccc2[S+][O-])CC1 C(=O)c2cccc2S3(=O)=O)CC1 pred: [0.592 0.408]



CCOC(=O)N1CCC(NC(=O)c2ccc3c(c2)N(Cc2cc(Cl)ccc2 COCCNC(=O)c1ccc2c(c1)N(Cc1cc(C)ccc1C)(=O)c1cc COCCNC(=O)c1ccc2c(c1)N(Cc1cccc1)C(=O)c1ccccCCOc1ccc(CN2C(=O)c3cccc3Sc3ccc(C(=O)NC4CCCCC)C(=O)c2cccc2S3(=O)=O)CC1 C(=O)c2cccc2[S+][O-])CC1 pred: [0.606 0.394]  
CC1S2 pred: [0.523 0.477]  
CC1S2 pred: [0.615 0.385]  
CC1S2 pred: [0.707 0.293]

# Cluster #126 - 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 126, from importance channel 1 (*aggregator*), represents a motif consisting of 7.9 ( $\pm 1.2$ ) nodes. The concept is generally associated with an impact of 1.2 ( $\pm 0.6$ ) on the prediction outcome.

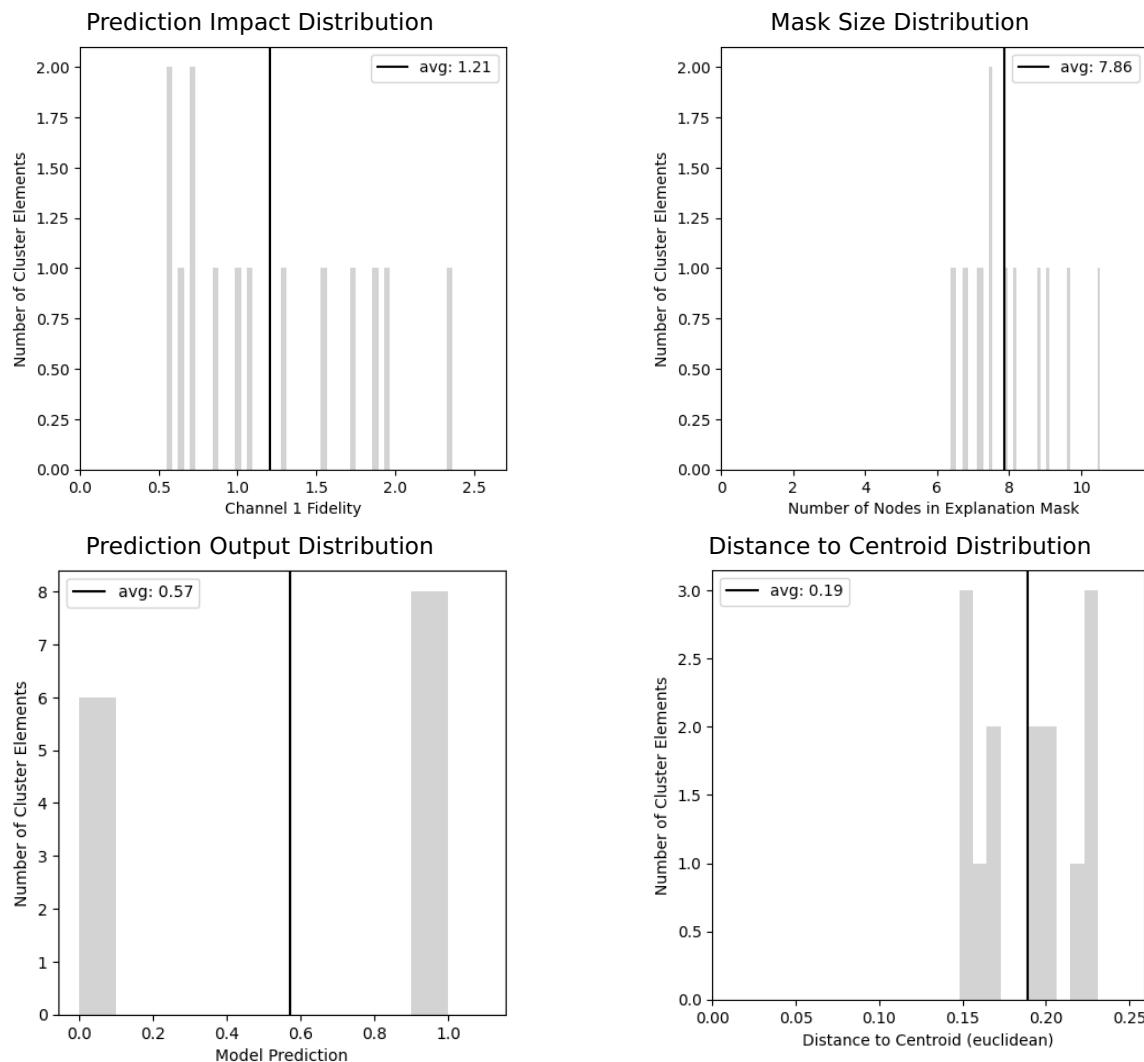
## Properties

ⓘ 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:	14
Channel Index	1.0 (0.0)

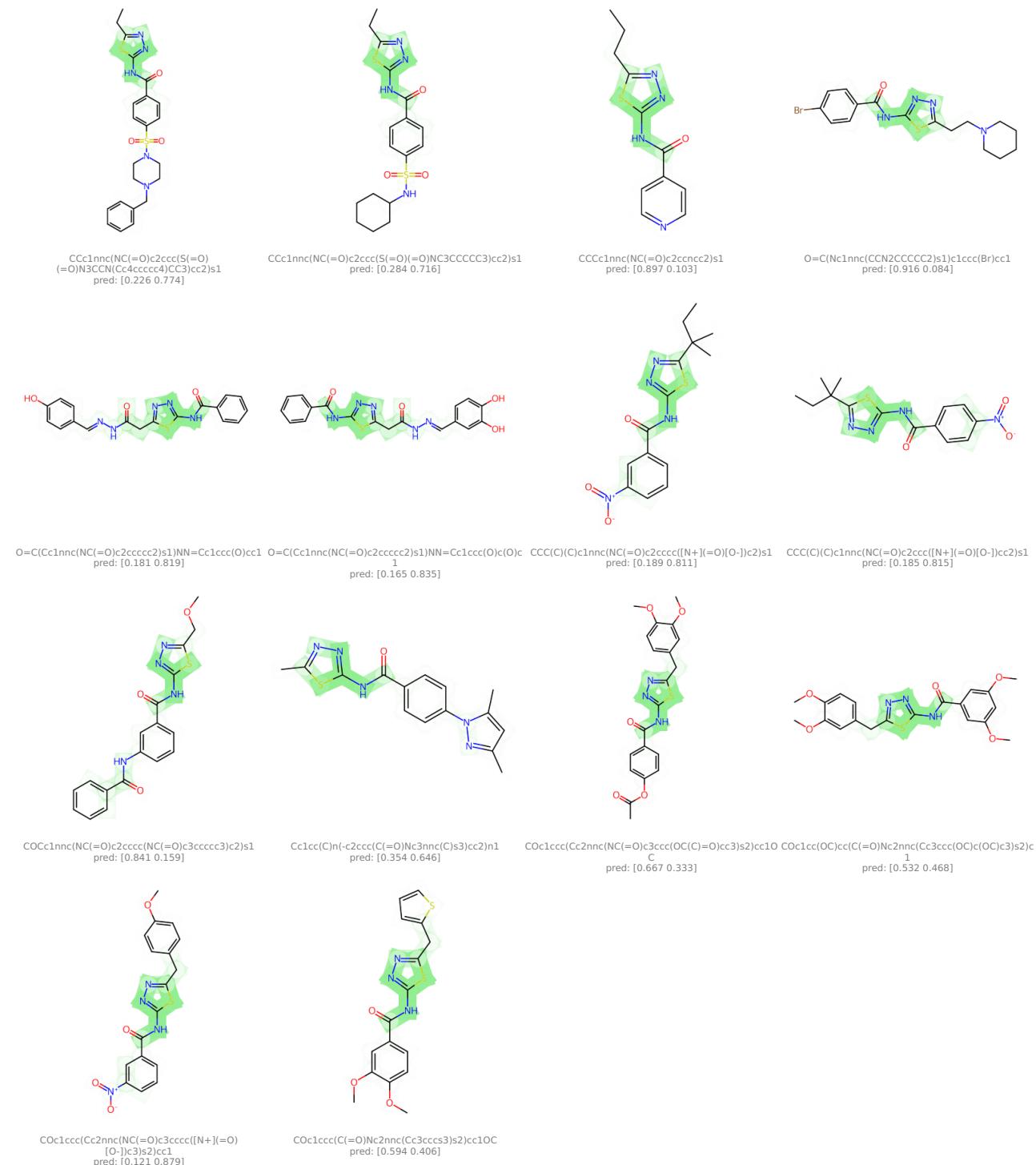
## Member Statistics

ⓘ 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 #127 - 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 127, from importance channel 1 (*aggregator*), represents a motif consisting of 7.3 ( $\pm 1.2$ ) nodes. The concept is generally associated with an impact of 1.2 ( $\pm 0.6$ ) on the prediction outcome.

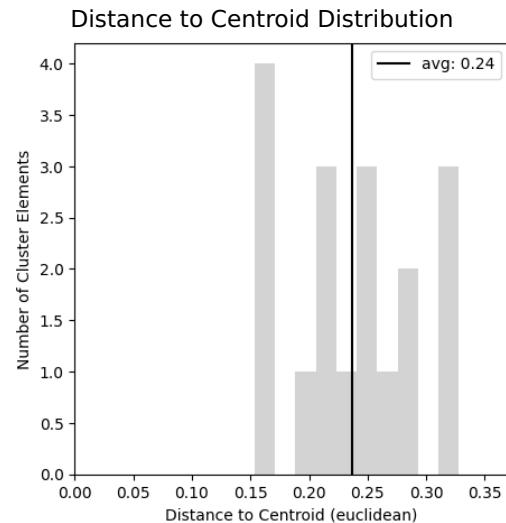
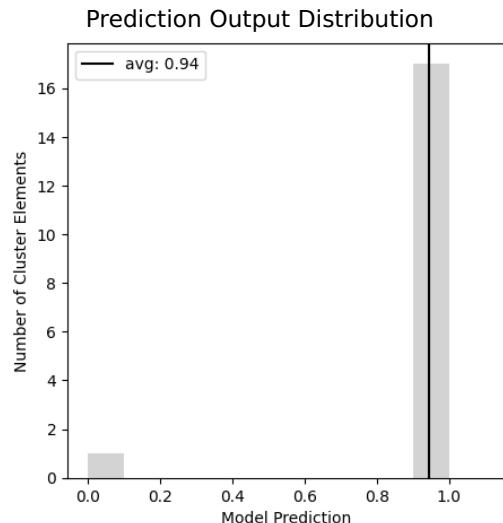
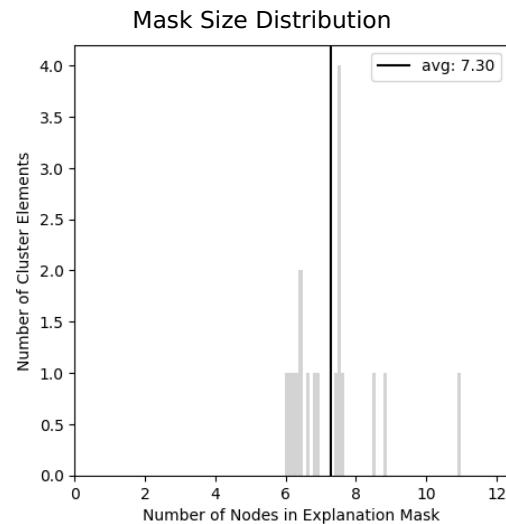
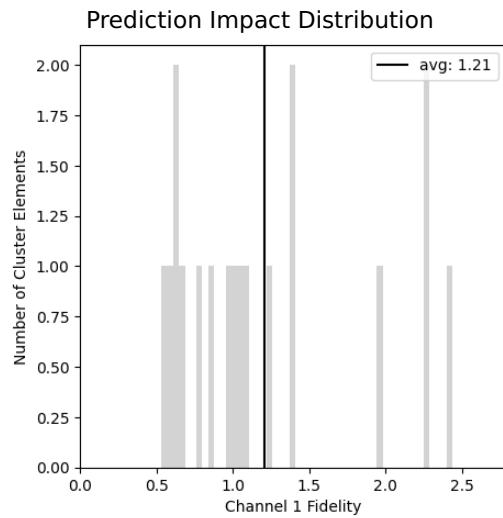
## Properties

ⓘ 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:	18
Channel Index	1.0 (0.0)

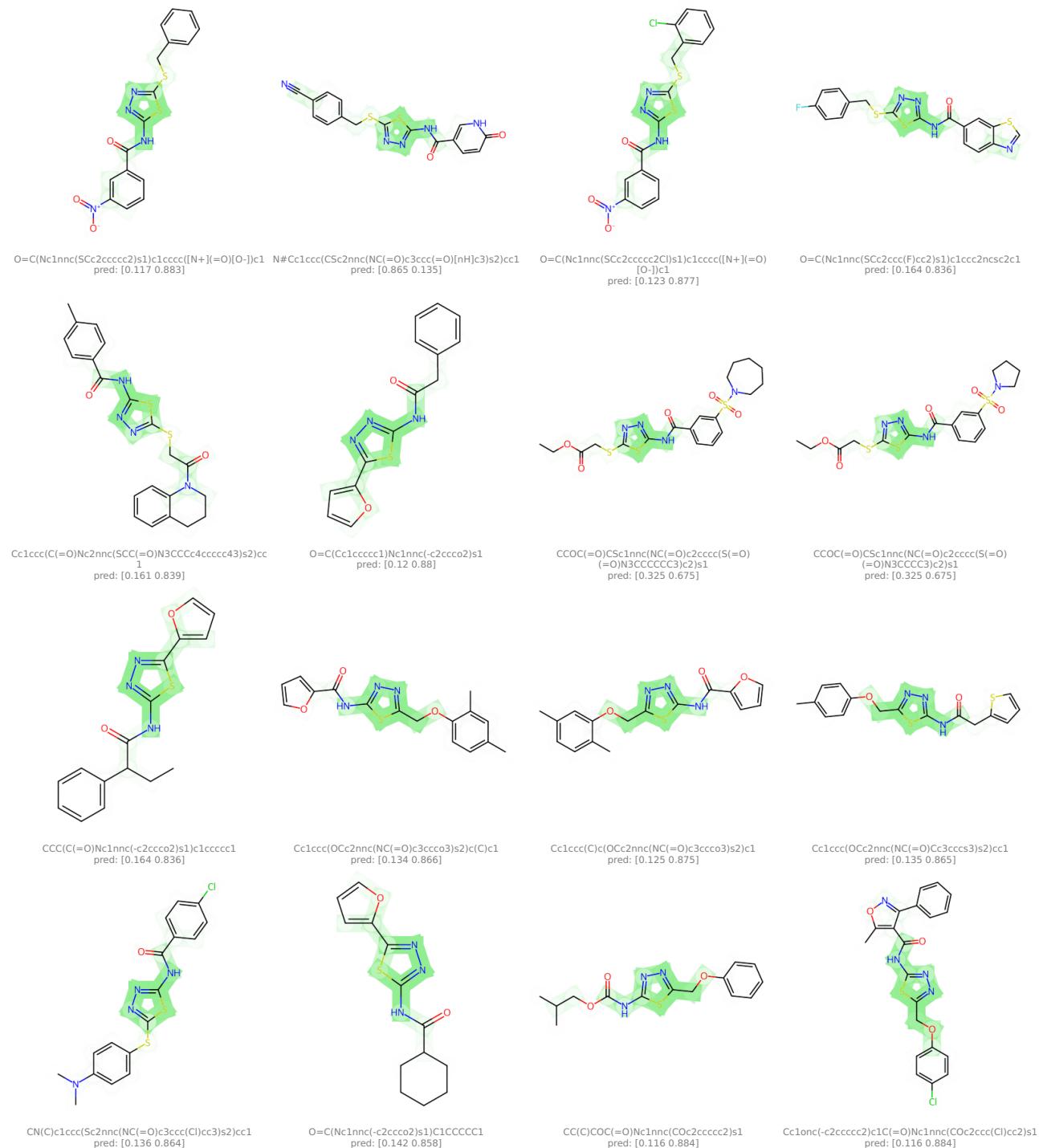
## Member Statistics

ⓘ 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 #128 - 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 128, from importance channel 1 (*aggregator*), represents a motif consisting of 7.5 ( $\pm 1.3$ ) nodes. The concept is generally associated with an impact of 1.4 ( $\pm 0.6$ ) on the prediction outcome.

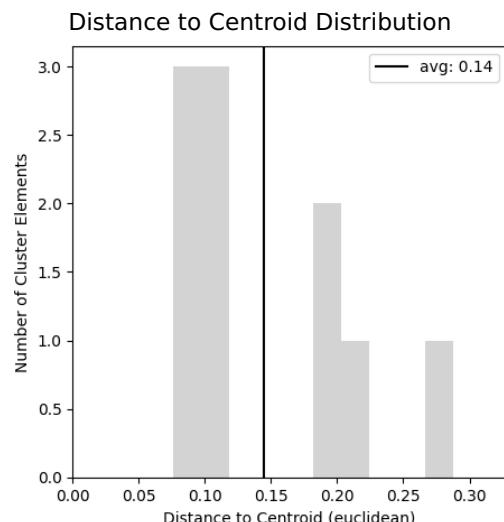
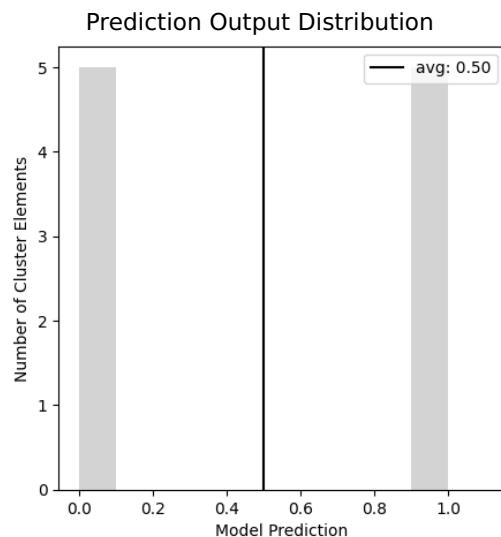
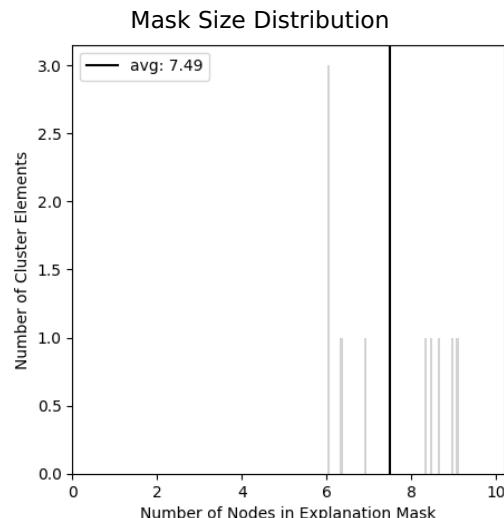
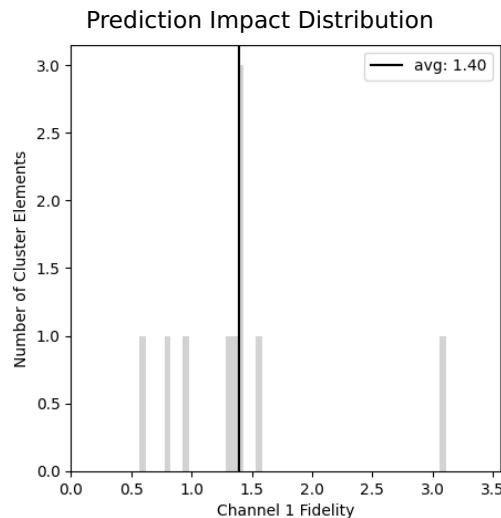
## Properties

ⓘ 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)

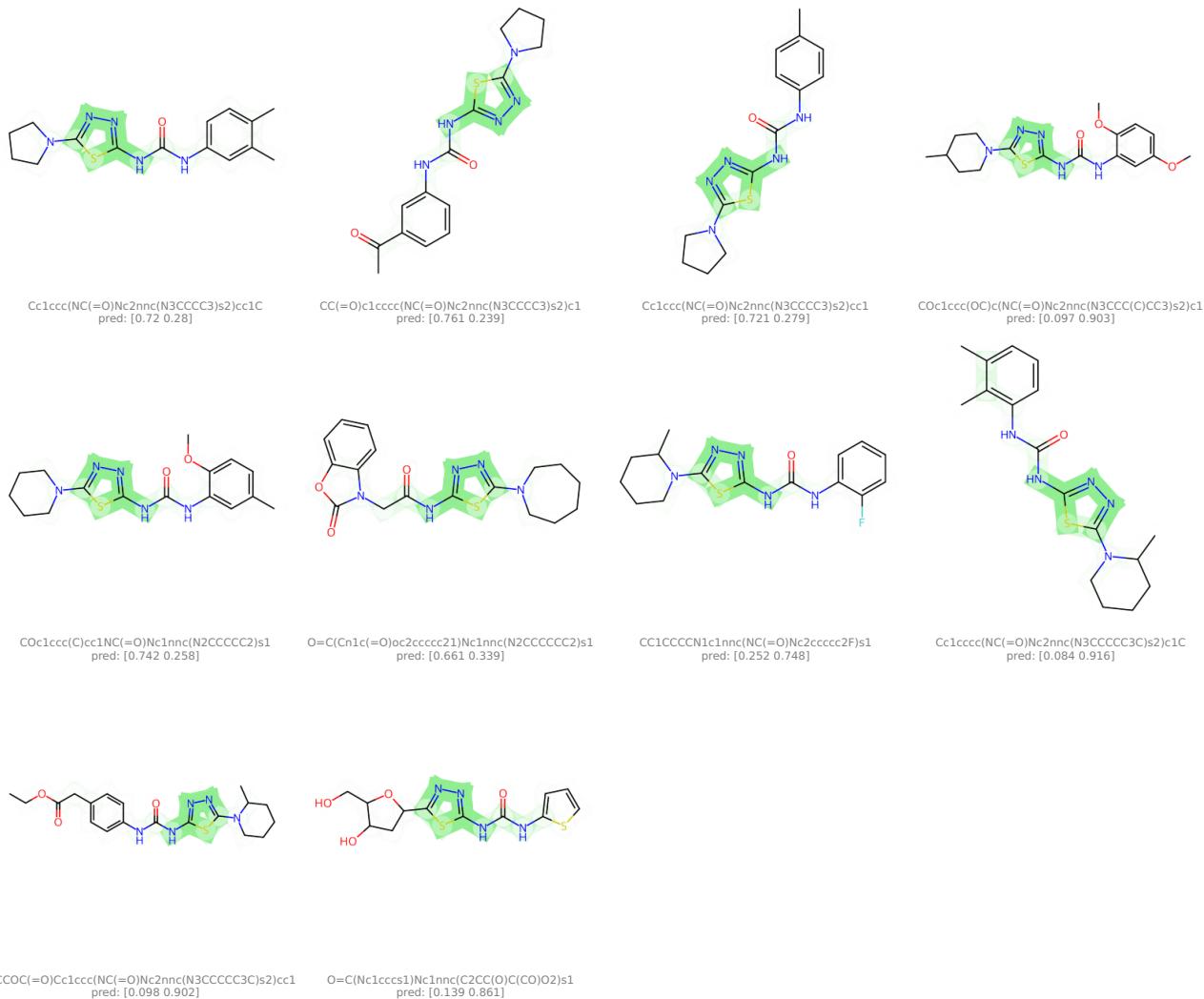
## Member Statistics

ⓘ 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 #129 - 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 129, from importance channel 1 (*aggregator*), represents a motif consisting of  $7.3 (\pm 0.8)$  nodes. The concept is generally associated with an impact of  $1.4 (\pm 0.7)$  on the prediction outcome.

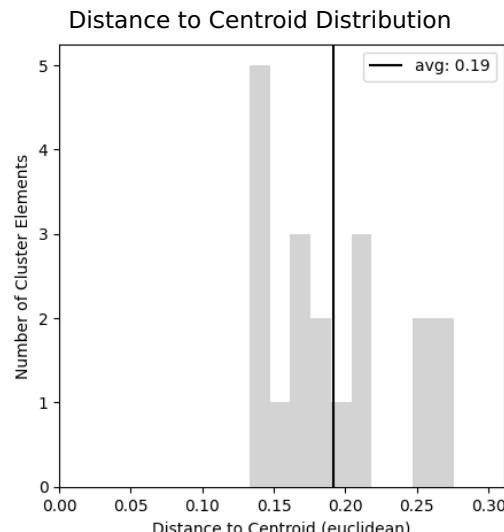
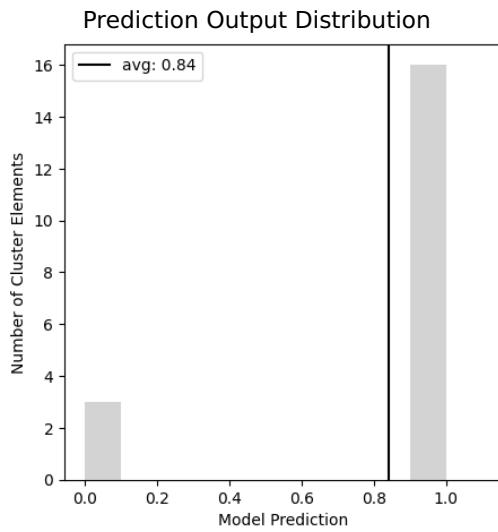
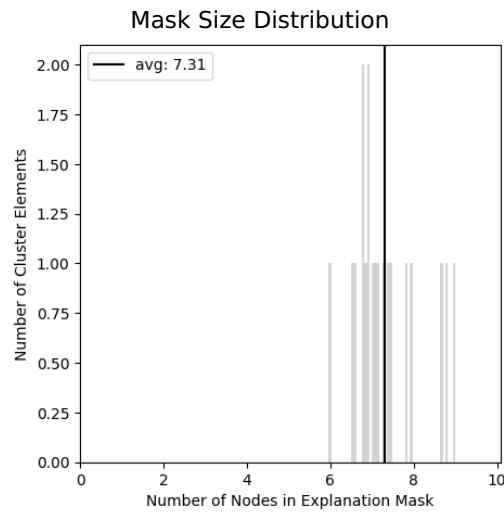
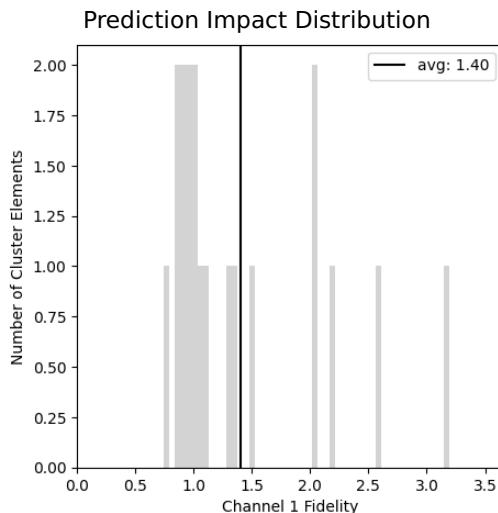
## Properties

ⓘ 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:	19
Channel Index	1.0 (0.0)

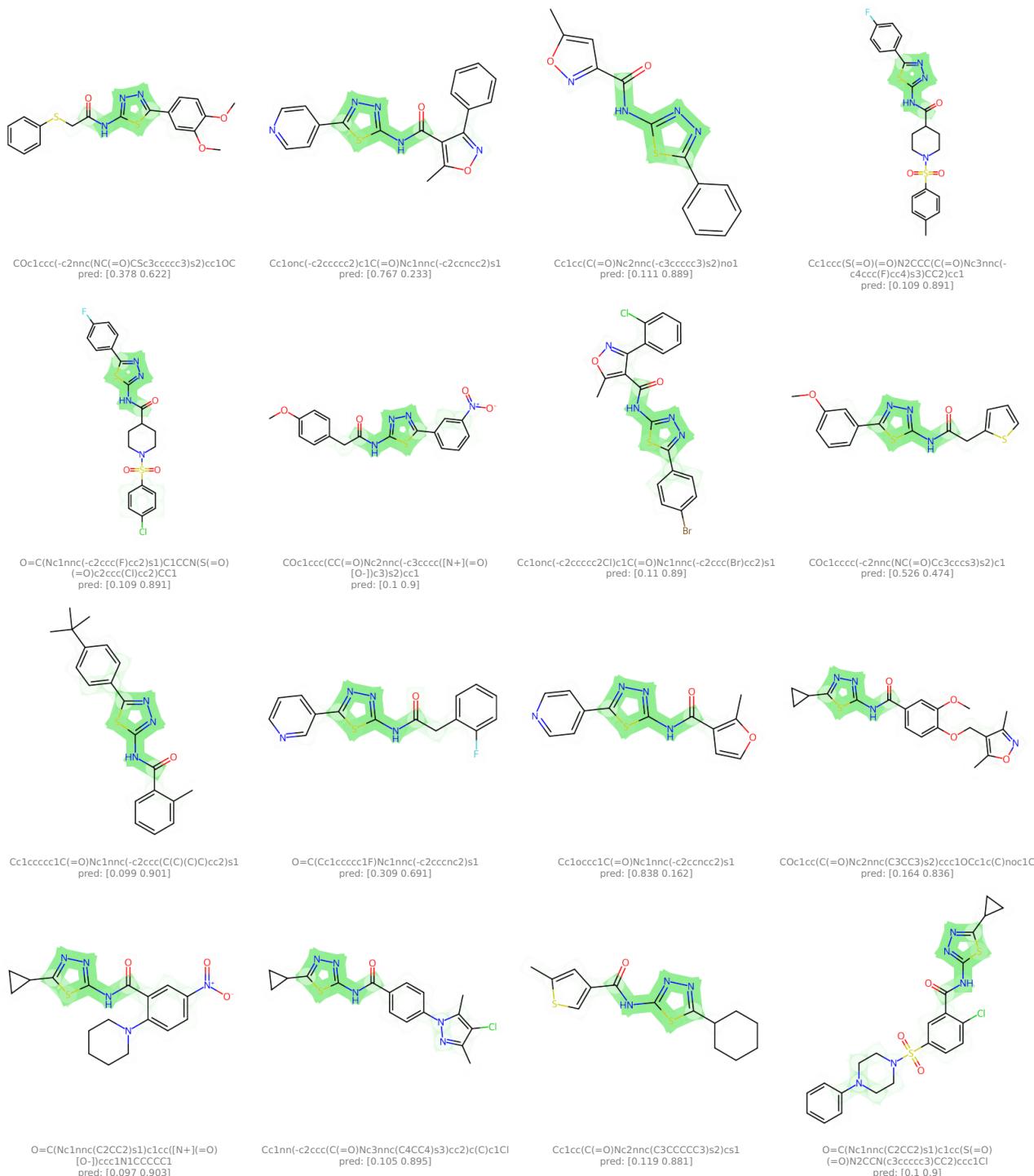
## Member Statistics

ⓘ 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 #130 - 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 130, from importance channel 1 (*aggregator*), represents a motif consisting of 7.2 ( $\pm 0.9$ ) nodes. The concept is generally associated with an impact of 0.7 ( $\pm 0.2$ ) on the prediction outcome.

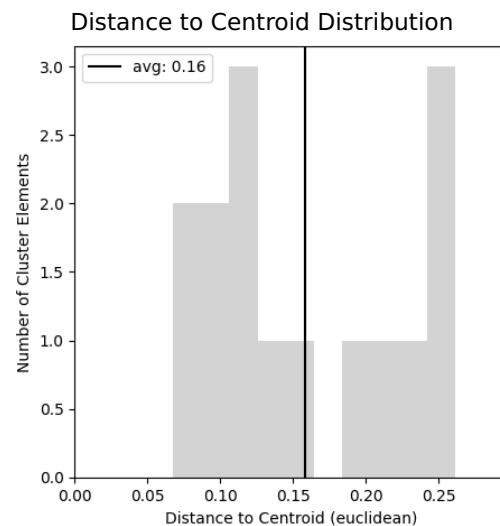
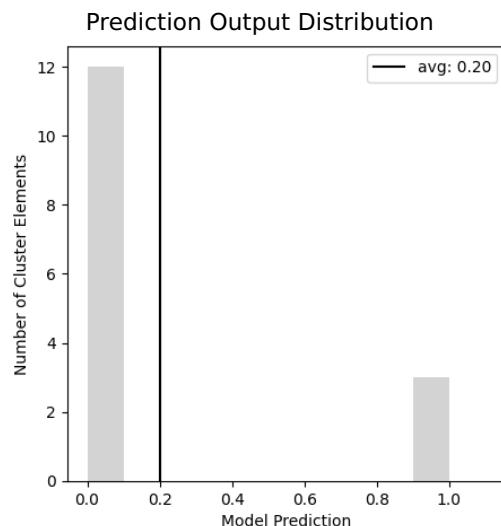
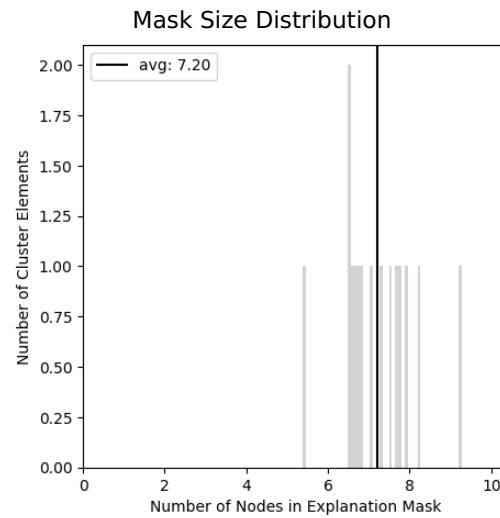
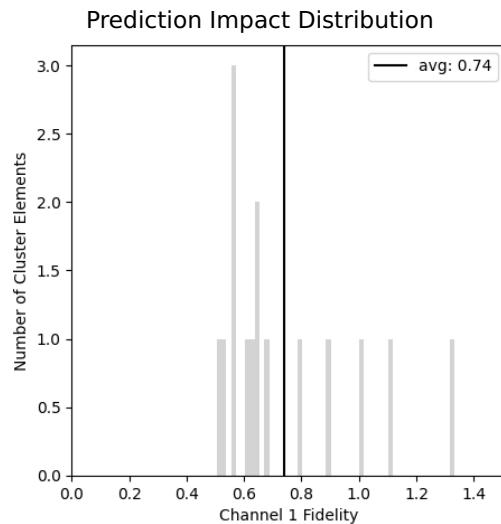
## Properties

ⓘ 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:	15
Channel Index	1.0 (0.0)

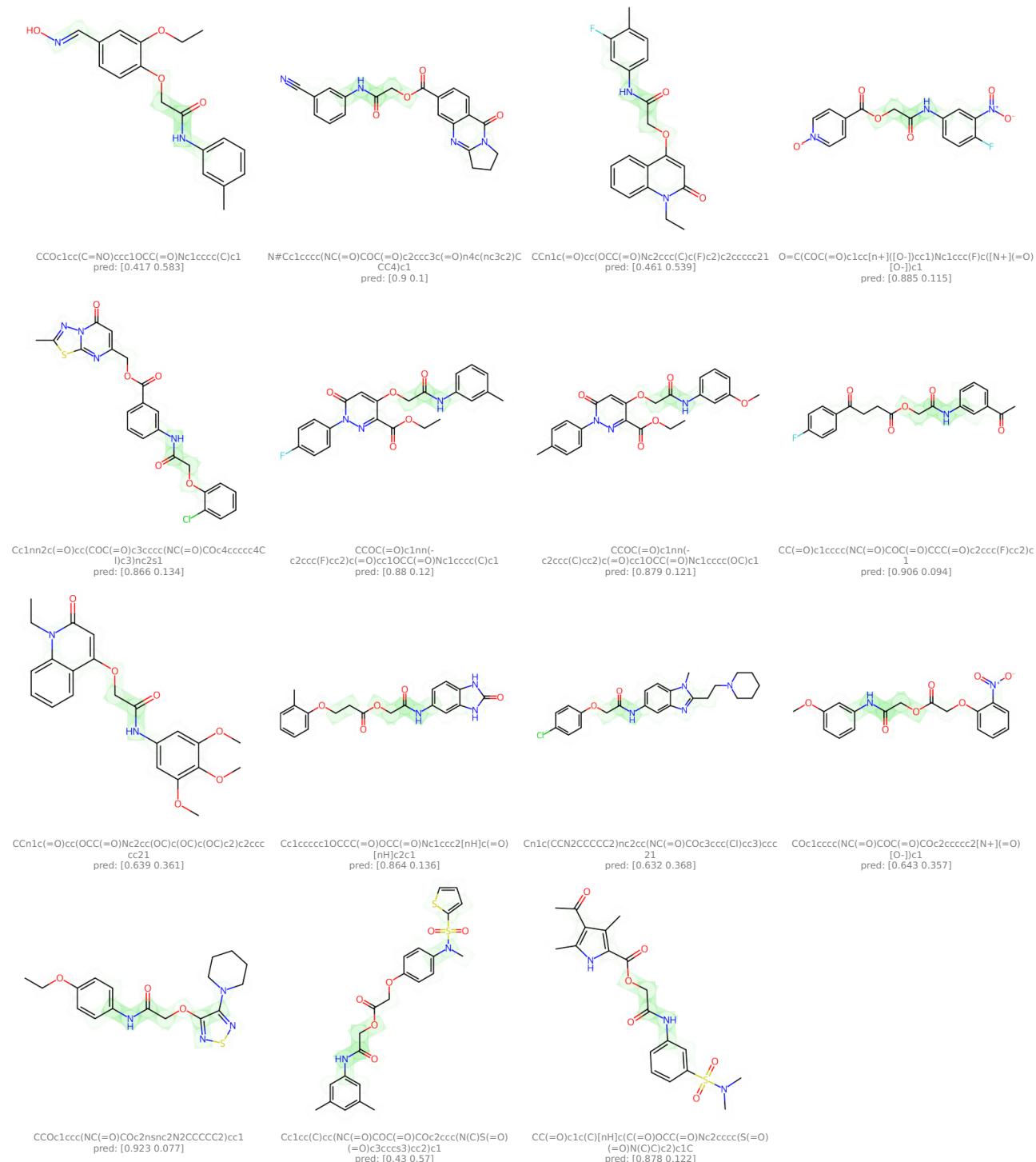
## Member Statistics

ⓘ 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 #131 - 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 131, from importance channel 1 (*aggregator*), represents a motif consisting of 7.8 ( $\pm 1.2$ ) nodes. The concept is generally associated with an impact of 0.8 ( $\pm 0.4$ ) on the prediction outcome.

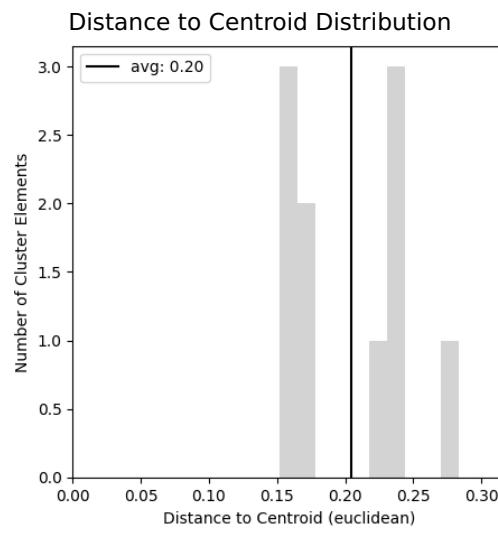
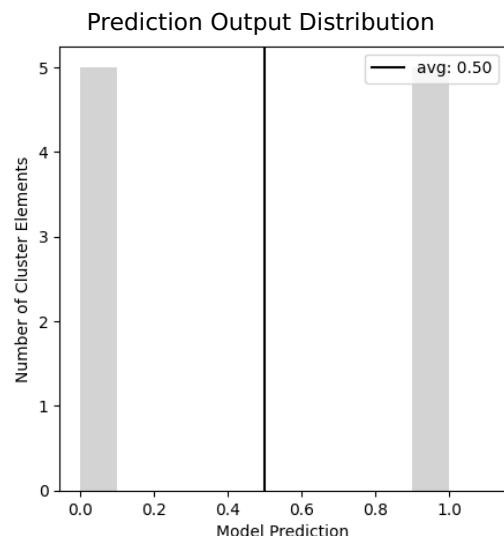
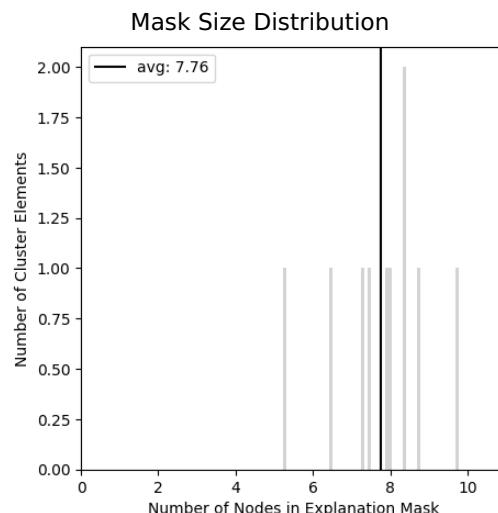
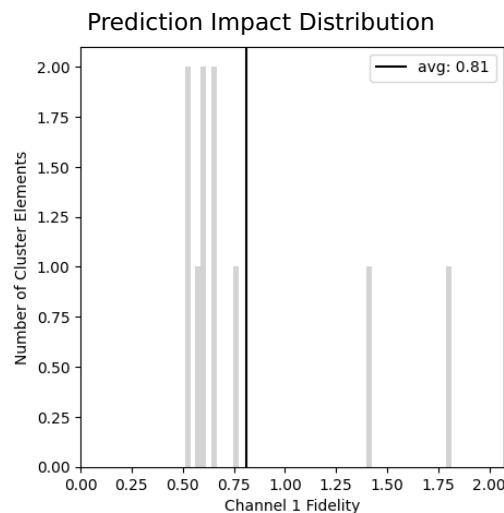
## Properties

ⓘ 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:	10
Channel Index	1.0 (0.0)

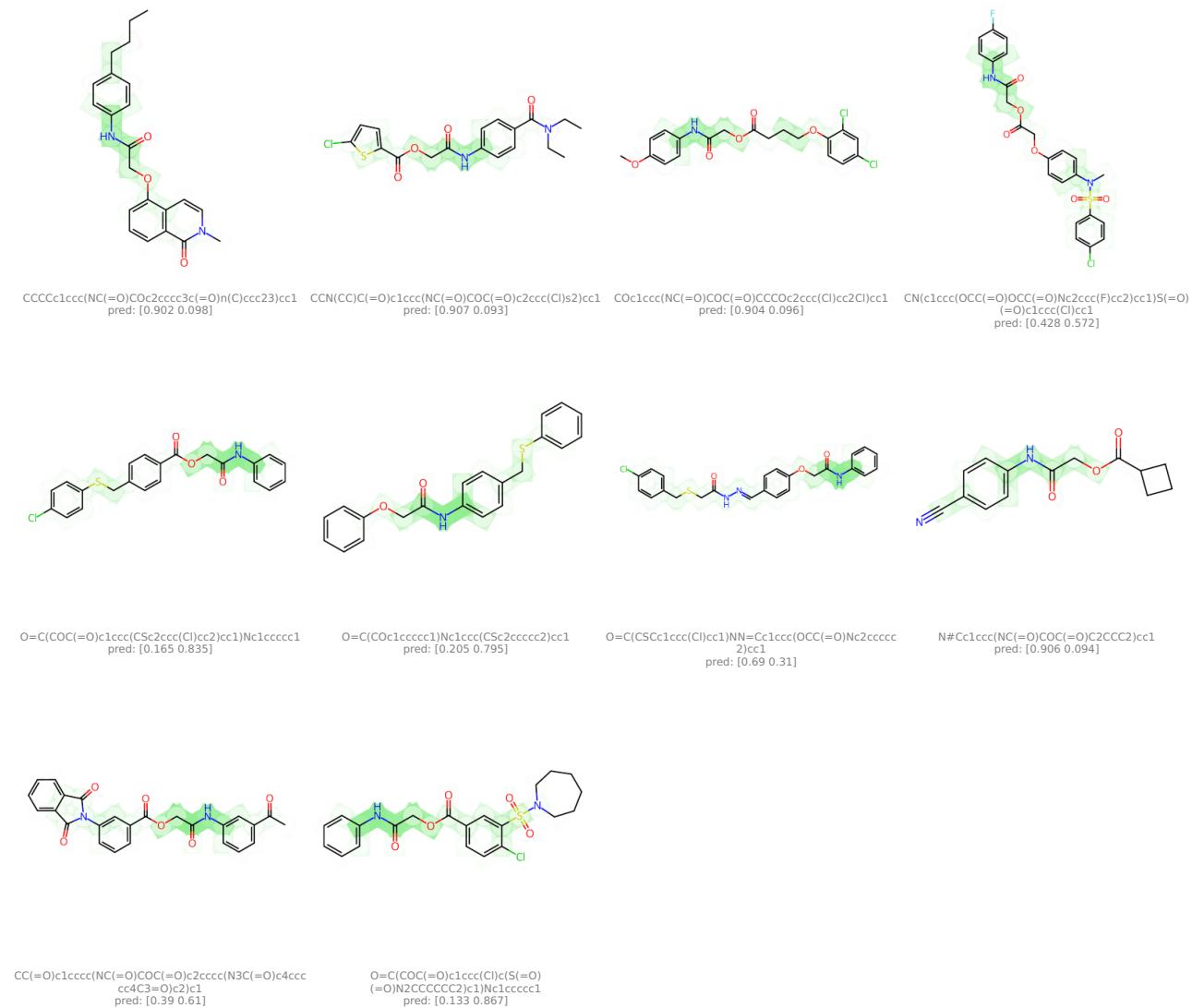
## Member Statistics

ⓘ 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 #132 - 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 132, from importance channel 1 (*aggregator*), represents a motif consisting of 8.7 ( $\pm 1.9$ ) nodes. The concept is generally associated with an impact of 1.1 ( $\pm 0.6$ ) on the prediction outcome.

## Properties

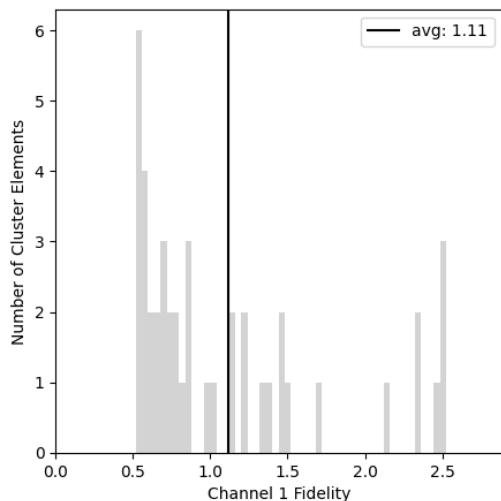
ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	44
Channel Index	1.0 (0.0)

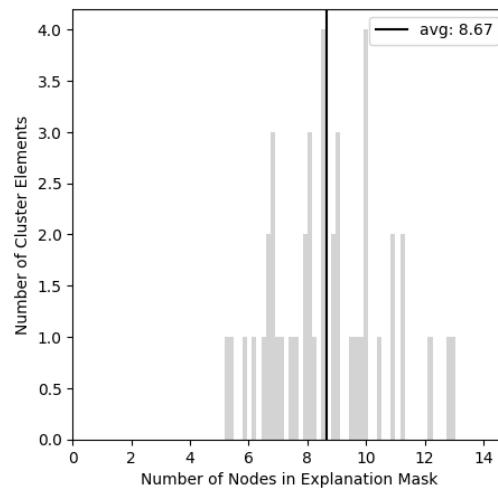
## Member Statistics

ⓘ 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.

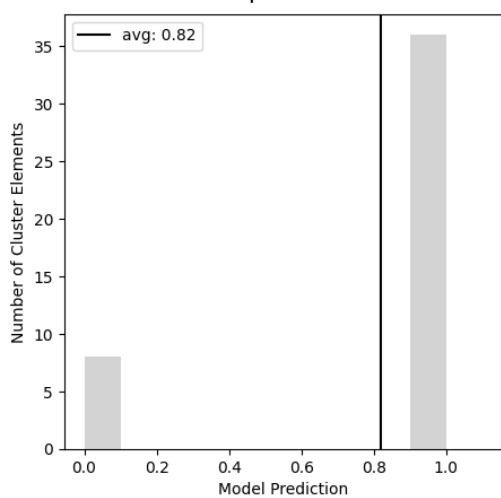
Prediction Impact Distribution



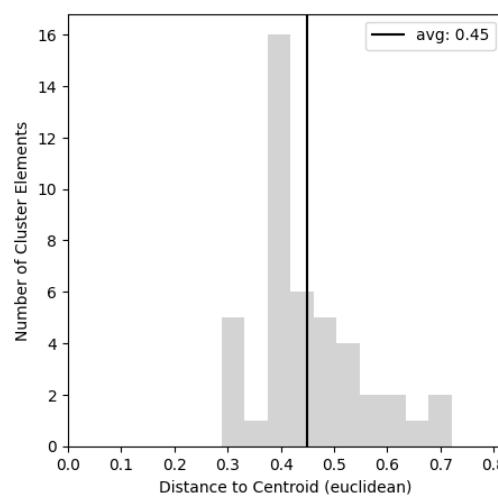
Mask Size Distribution



Prediction Output Distribution

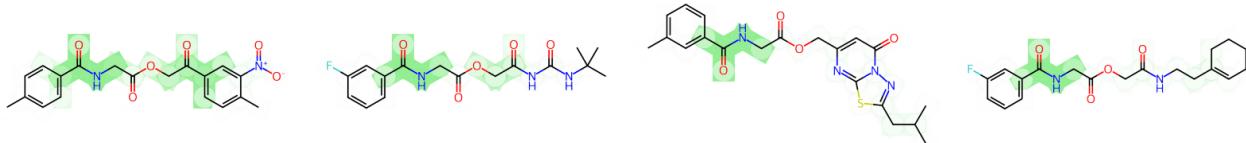


Distance to Centroid Distribution



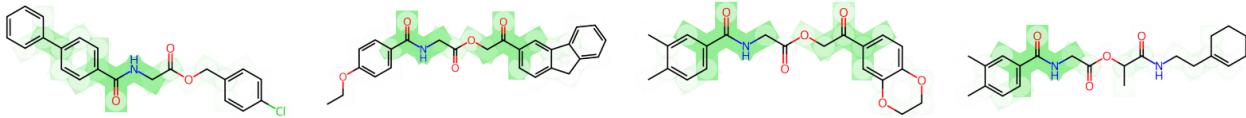
## Example Elements

ⓘ 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.



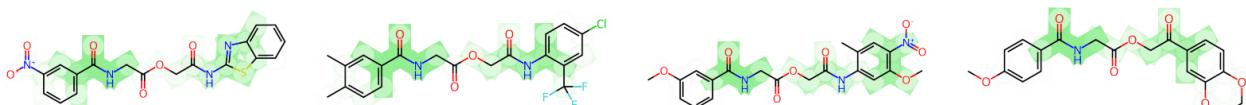
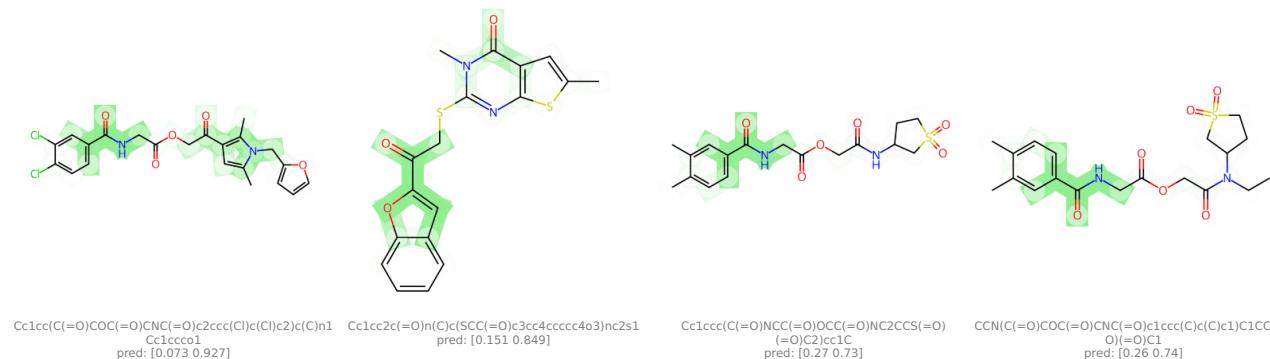
Cc1ccc(C(=O)NCC(=O)OCC(=O)c2ccc(C)c([N+](=O)[O-])c2cc1 pred: [0.178 0.822]  
CC(C)(C)NC(=O)NC(=O)COC(=O)CNC(=O)c1cccc(F)c1

Cc1cccc(C(=O)NCC(=O)OCC(=O)c2cc2n3nc(CC(C)C)sc3 pred: [0.795 0.205]  
O=C(COC(=O)CNC(=O)c1cccc(F)c1)NCCCC1=CCCCC1 pred: [0.125 0.875]



O=C(CNC(=O)c1ccc(c2ccccc2)cc1)Oc1ccc(Cl)cc1 pred: [0.085 0.915]  
CCOc1ccc(C(=O)NCC(=O)OCC(=O)c2ccc3c(c2)c2ccccc2C3)cc1 pred: [0.163 0.837]

Cc1ccc(C(=O)NCC(=O)OCC(=O)c2ccc3c(c2)OCCO3)cc1 pred: [0.081 0.919]  
Cc1ccc(C(=O)NCC(=O)OCC(=O)c1ccc(C)c1)C1CC=CCCCC2 pred: [0.142 0.858]



O=C(COC(=O)CNC(=O)c1cccc([N+](=O)[O-])c1)Nc1nc2ccccc2s1 pred: [0.081 0.919]  
Cc1ccc(C(=O)NCC(=O)OCC(=O)Nc2ccc(Cl)cc2C(F)(F)F)cc1 pred: [0.077 0.923]

Cc1cccc(C(=O)NCC(=O)OCC(=O)Nc2cc(OC)c([N+](=O)[O-])c2)cc1 pred: [0.098 0.902]  
Cc1ccc(C(=O)NCC(=O)OCC(=O)c2ccc3c(c2)OCCO3)cc1 pred: [0.124 0.876]

# Cluster #133 - 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 133, from importance channel 1 (*aggregator*), represents a motif consisting of  $7.5 (\pm 0.6)$  nodes. The concept is generally associated with an impact of  $1.1 (\pm 0.5)$  on the prediction outcome.

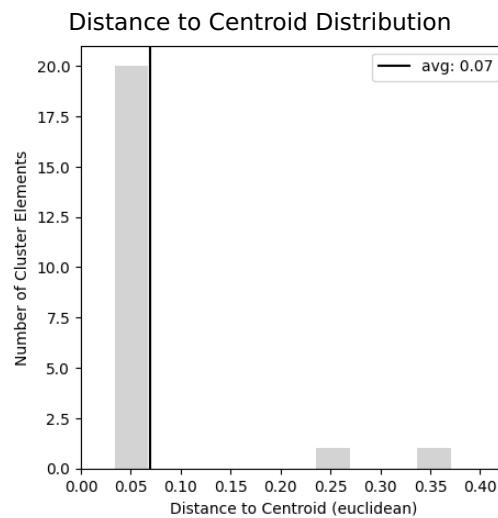
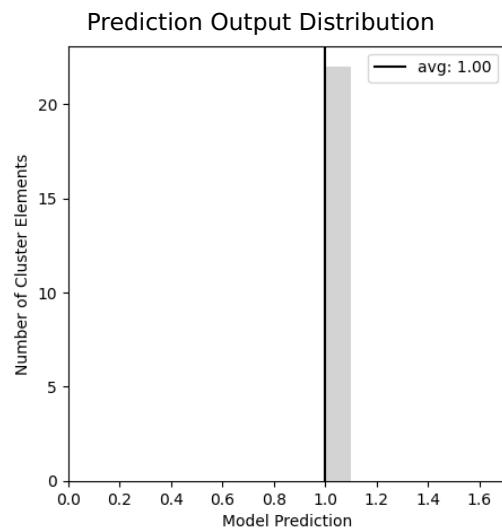
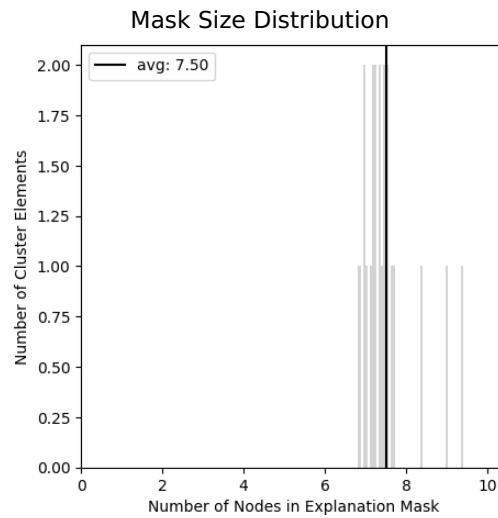
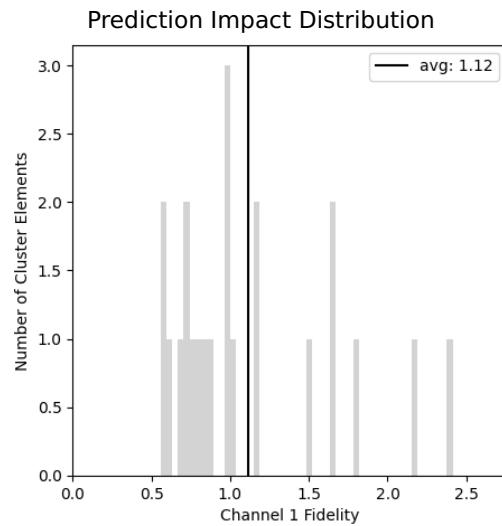
## Properties

ⓘ 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:	22
Channel Index	1.0 (0.0)

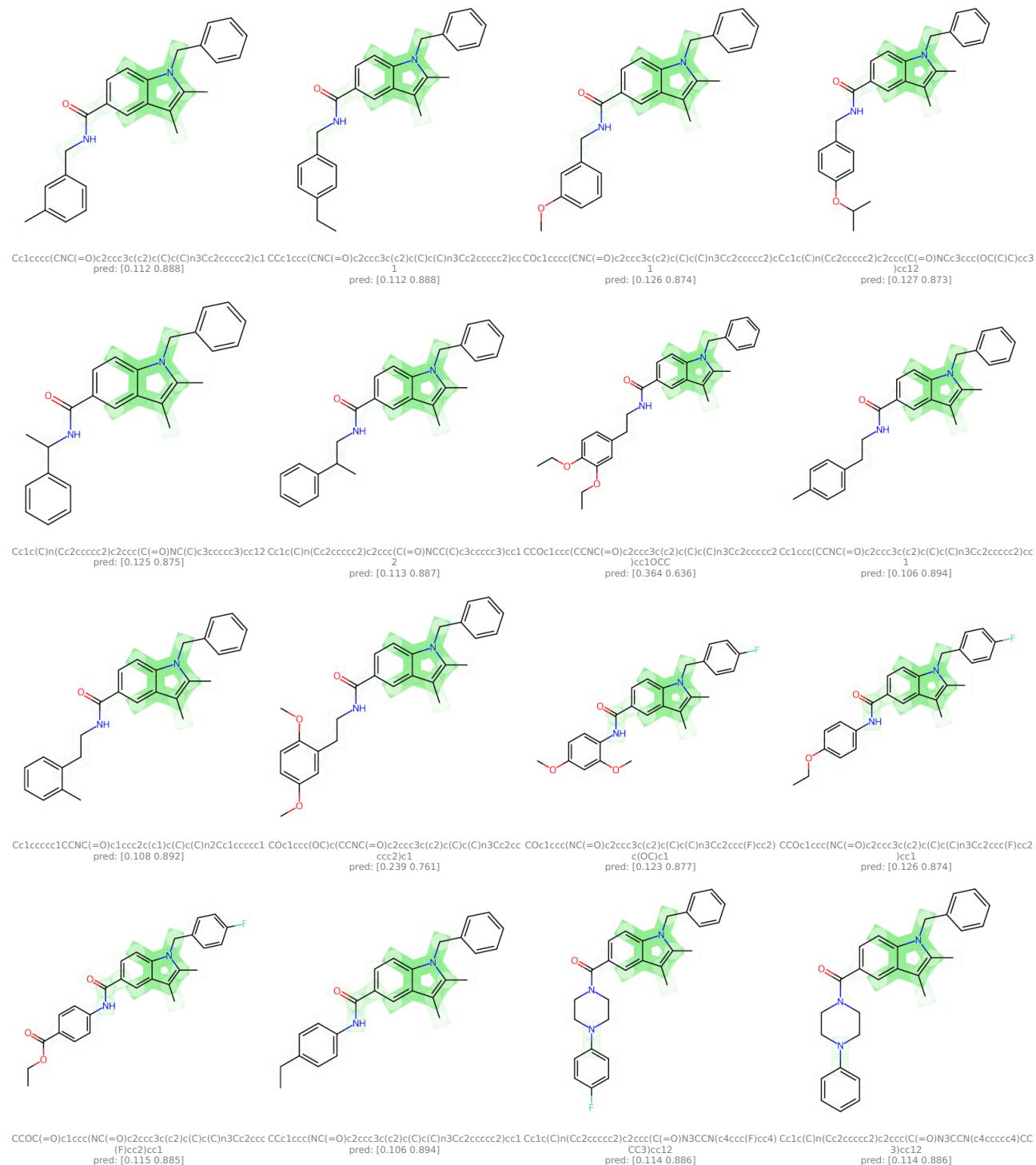
## Member Statistics

ⓘ 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 #134 - 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 134, from importance channel 1 (*aggregator*), represents a motif consisting of 8.7 ( $\pm 1.1$ ) nodes. The concept is generally associated with an impact of 1.9 ( $\pm 0.6$ ) on the prediction outcome.

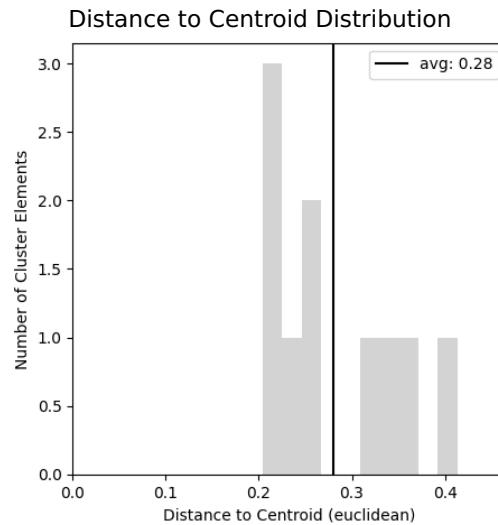
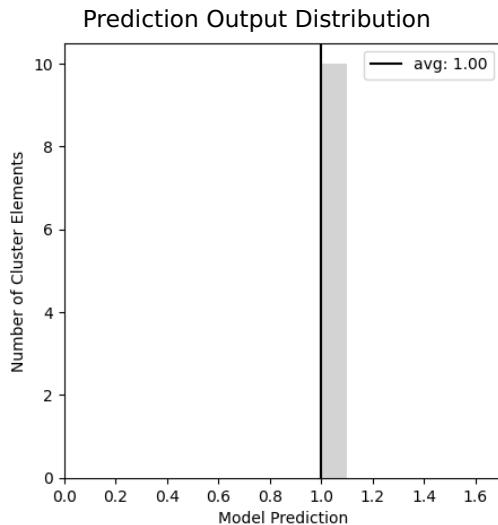
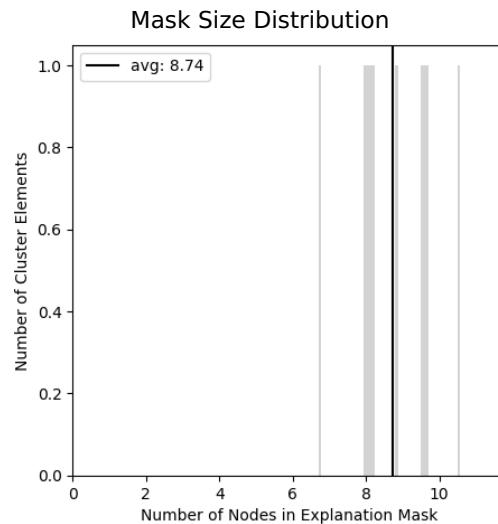
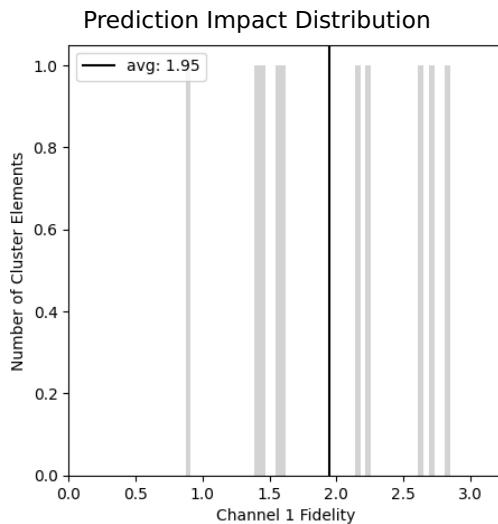
## Properties

ⓘ 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)

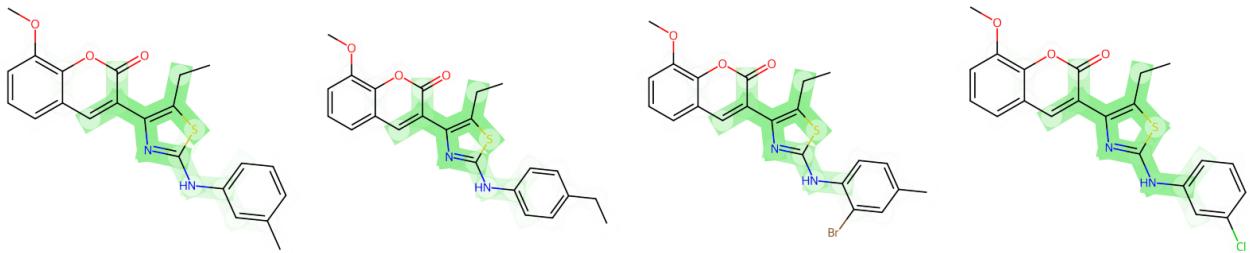
## Member Statistics

ⓘ 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.

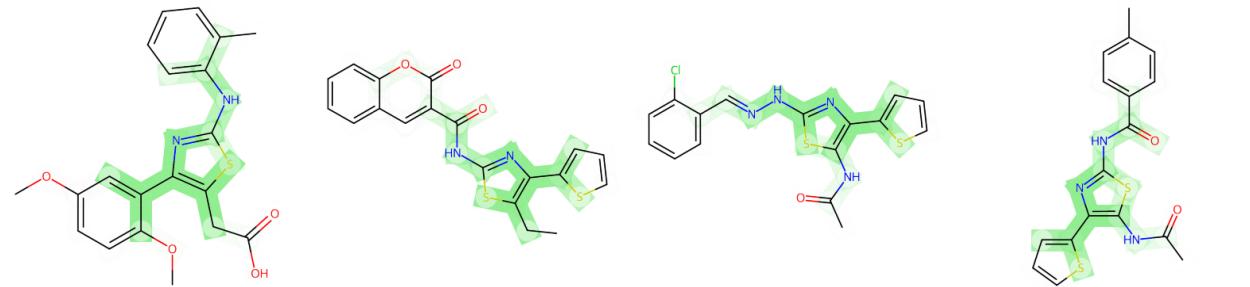


## Example Elements

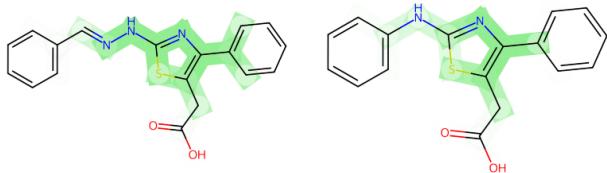
ⓘ This section shows the visualization of some example members of the cluster. A cluster member is a combination of a base graph and an explanation mask, whereby the masks indicates what kind of motif the cluster represents. In the best case, the explanation masks (highlighted nodes and edges) show some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



CCc1sc(Nc2cccc(C)c2)nc1-c1cc2cccc(OC)c2oc1=O pred: [0.086 0.914]    CCc1ccc(Nc2nc(-c3cc4ccccc(OC)c4o3=O)c(CC)s2)cc1 pred: [0.086 0.914]    CCc1sc(Nc2ccc(C)cc2Br)nc1-c1cc2cccc(OC)c2oc1=O pred: [0.089 0.911]    CCc1sc(Nc2cccc(Cl)c2)nc1-c1cc2cccc(OC)c2oc1=O pred: [0.085 0.915]



COc1ccc(OC)c(-c2nc(Nc3cccc3C)sc2CC(=O)O)c1 pred: [0.295 0.705]    CCc1sc(NC(=O)c2cc3cccc3oc2=O)nc1-c1cccs1 pred: [0.091 0.909]    CC(=O)Nc1sc(NN=Cc2cccc2Cl)nc1-c1cccs1 pred: [0.144 0.856]    CC(=O)Nc1sc(NC(=O)c2ccc(C)cc2)nc1-c1cccs1 pred: [0.112 0.888]



O=C(O)Cc1sc(NN=Cc2cccc2)nc1-c1ccccc1 pred: [0.151 0.849]    O=C(O)Cc1sc(Nc2cccc2)nc1-c1ccccc1 pred: [0.209 0.791]

# Cluster #135 - 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 135, from importance channel 1 (*aggregator*), represents a motif consisting of 7.8 ( $\pm 1.4$ ) nodes. The concept is generally associated with an impact of 1.5 ( $\pm 0.6$ ) on the prediction outcome.

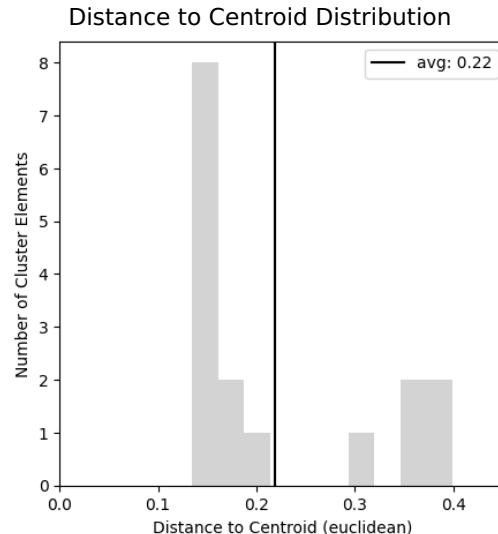
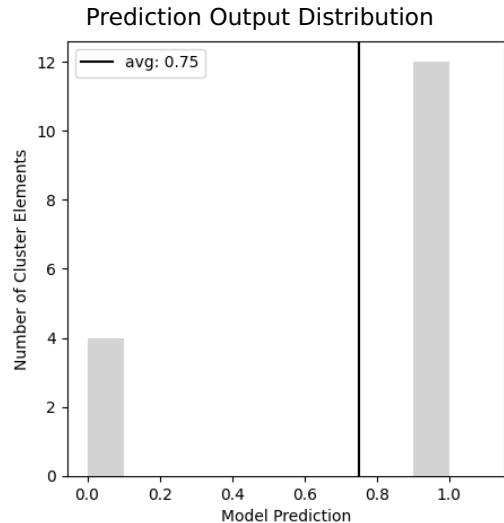
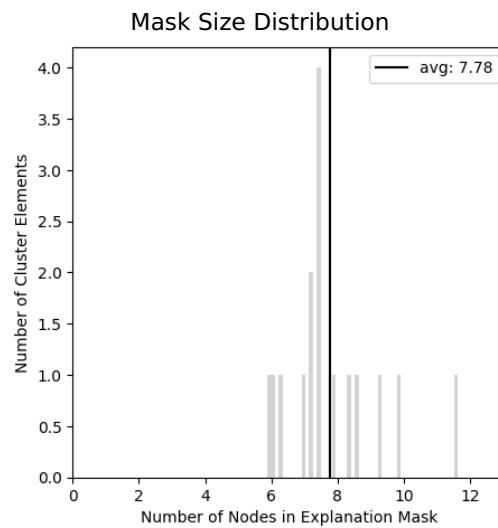
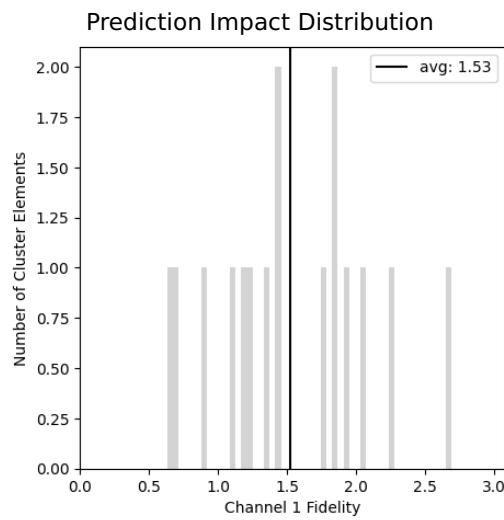
## Properties

ⓘ 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:	16
Channel Index	1.0 (0.0)

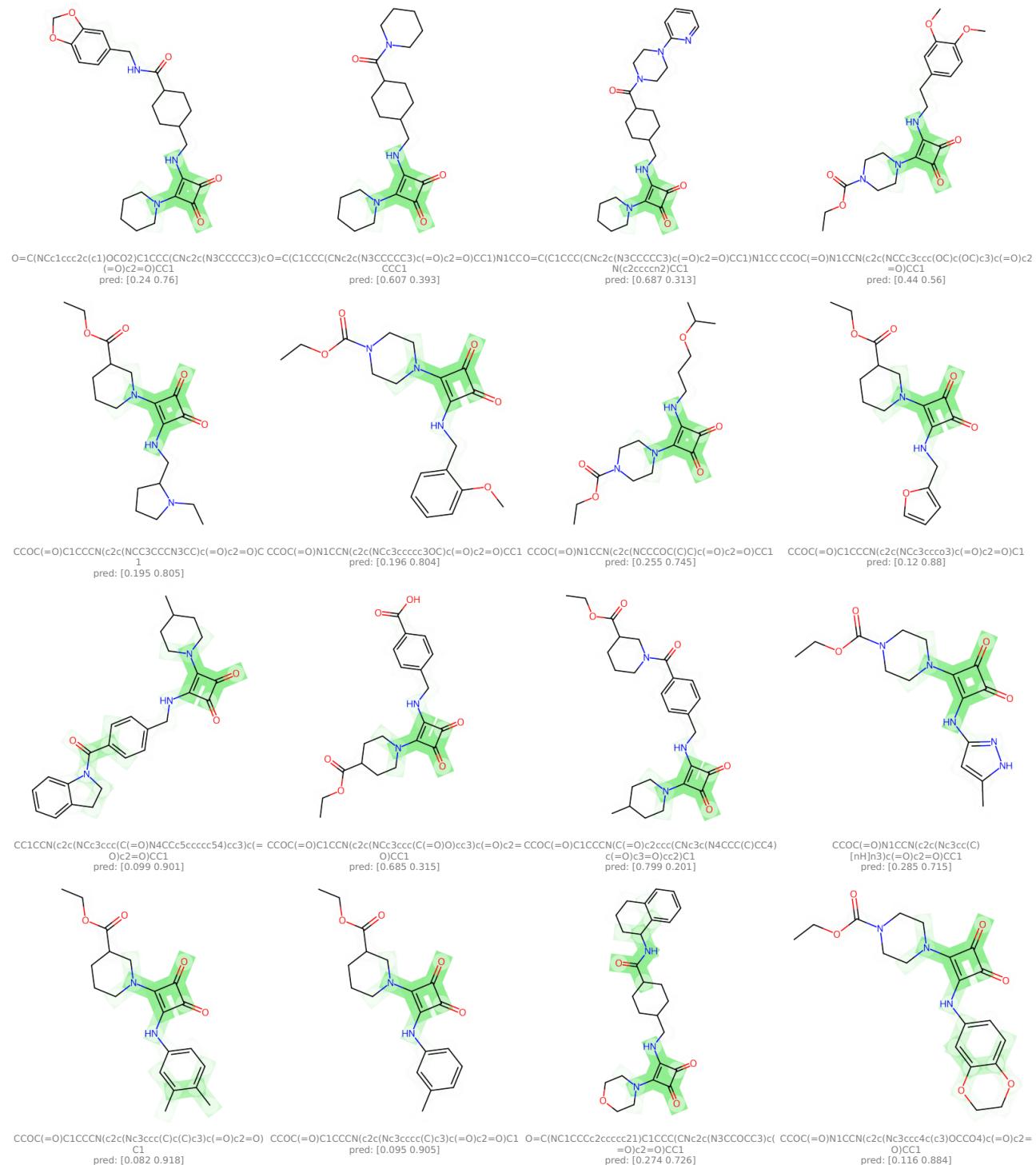
## Member Statistics

ⓘ 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 #136 - 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 136, from importance channel 1 (*aggregator*), represents a motif consisting of 7.9 ( $\pm 0.4$ ) nodes. The concept is generally associated with an impact of 0.8 ( $\pm 0.4$ ) on the prediction outcome.

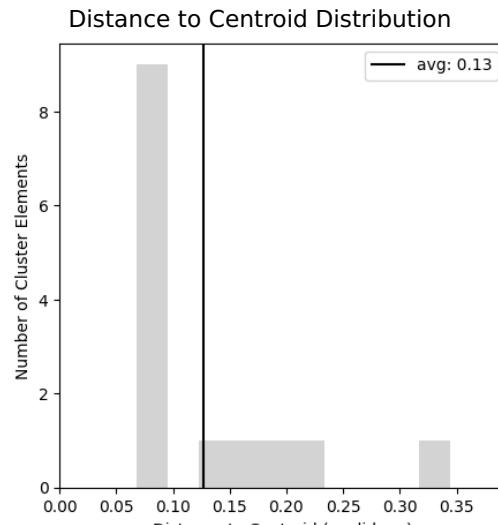
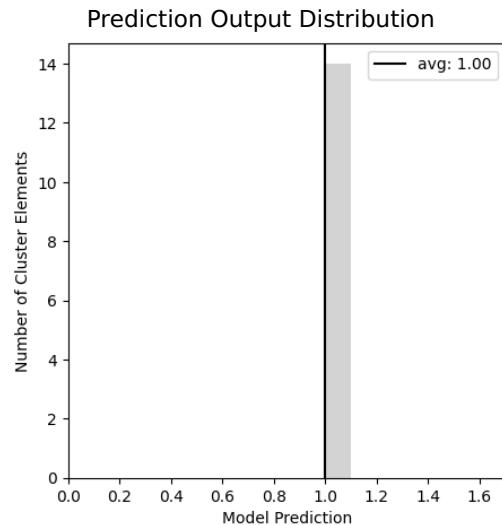
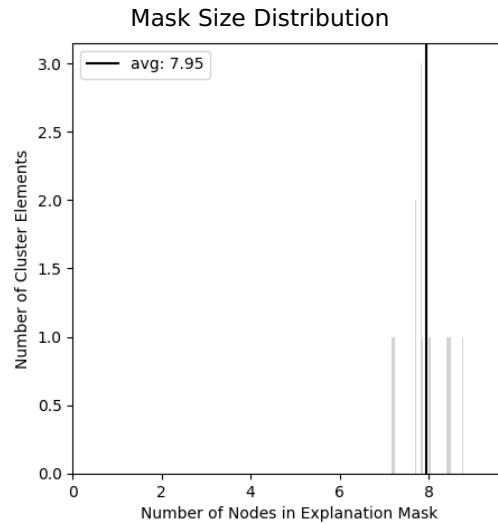
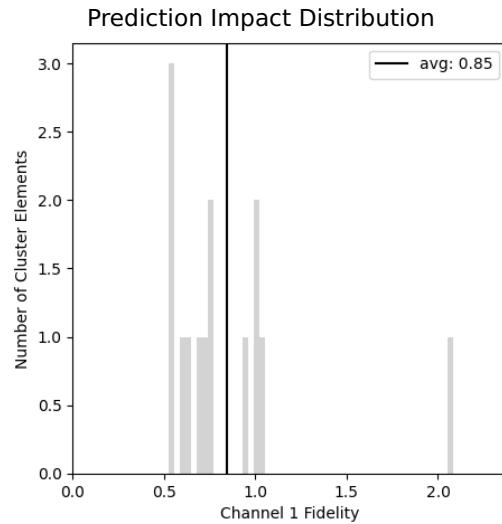
## Properties

ⓘ 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)

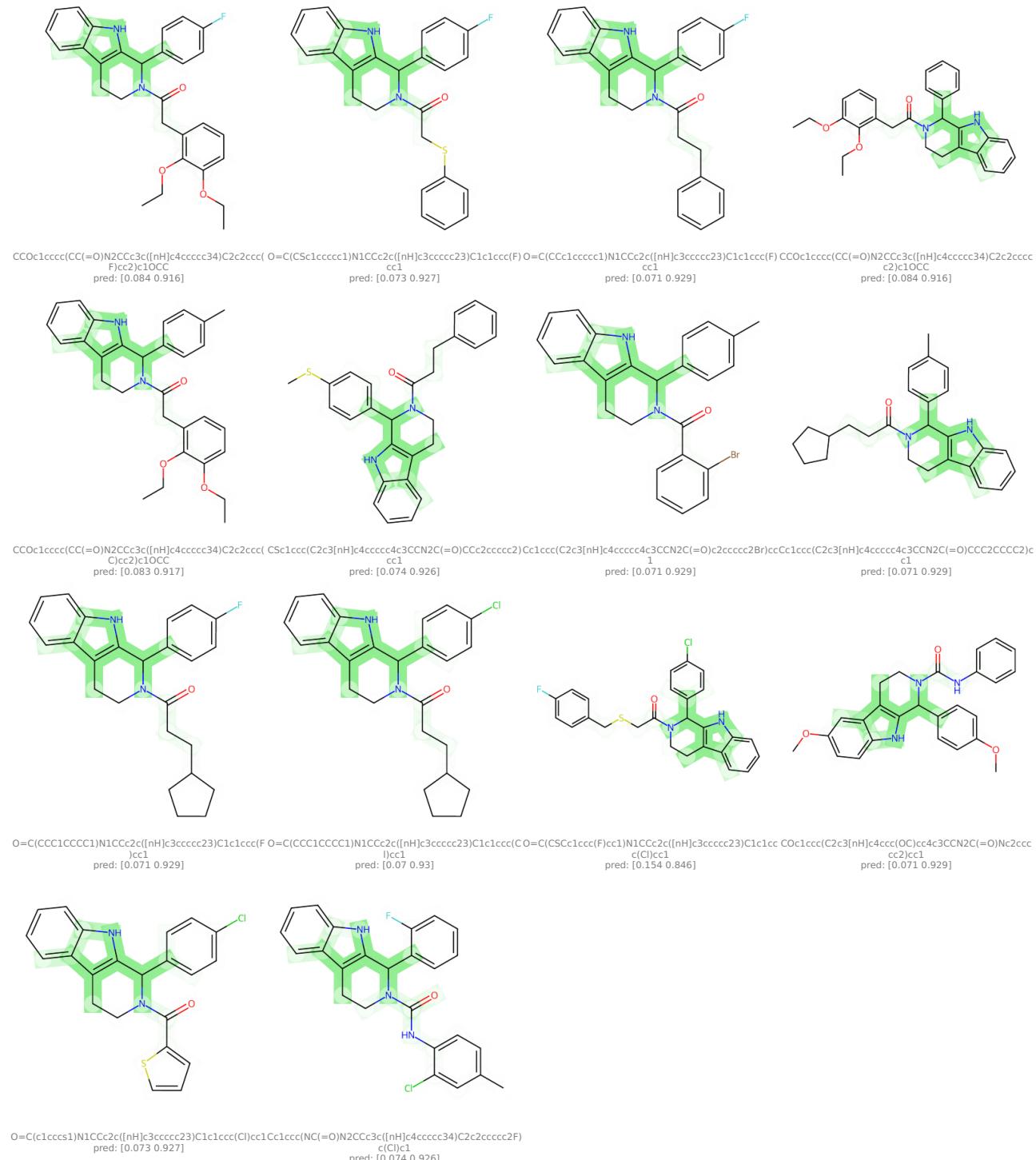
## Member Statistics

ⓘ 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.



## 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 #137 - 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 137, from importance channel 1 (*aggregator*), represents a motif consisting of 10.8 ( $\pm 2.4$ ) nodes. The concept is generally associated with an impact of 1.5 ( $\pm 0.7$ ) on the prediction outcome.

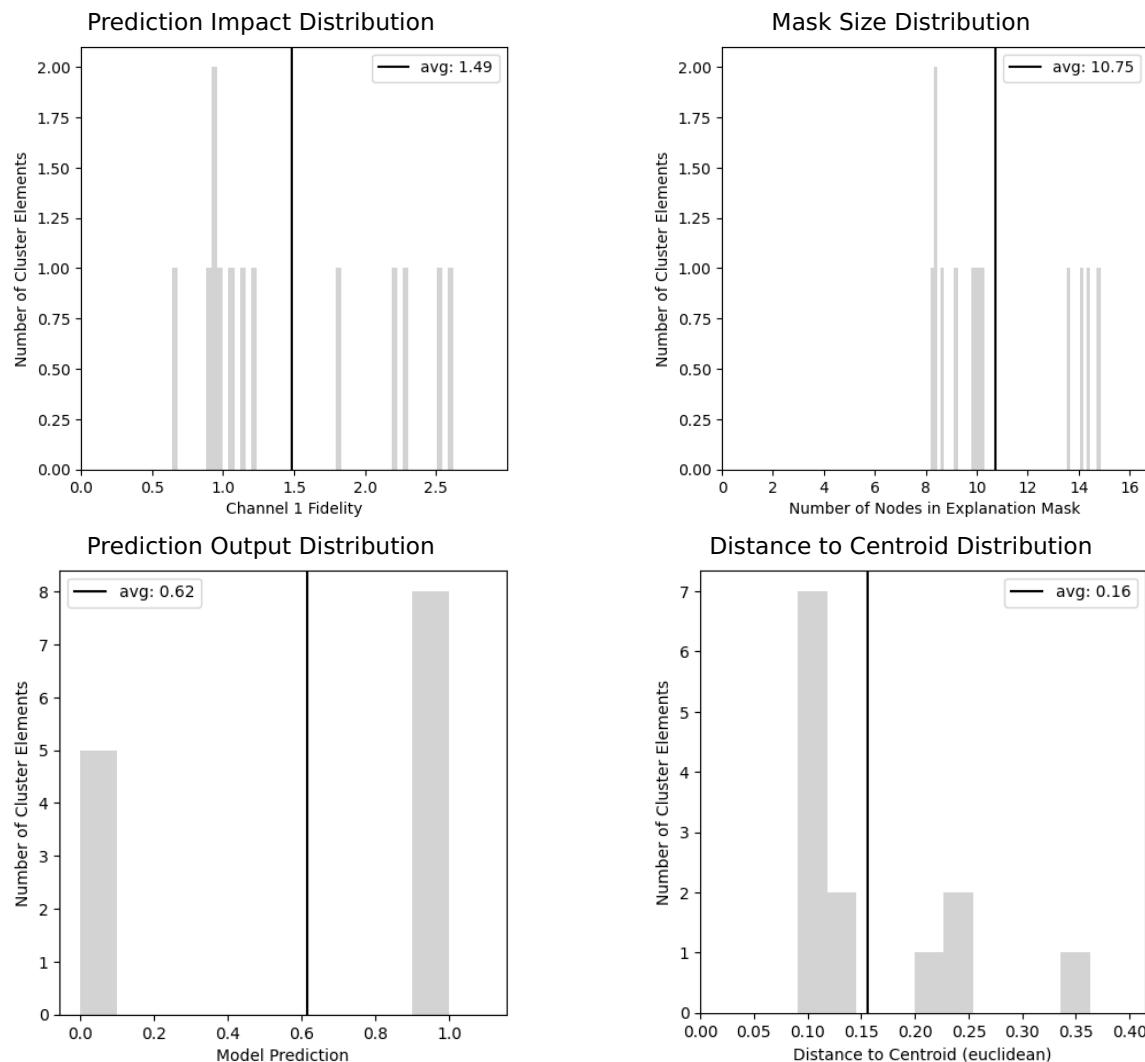
## Properties

ⓘ 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:	13
Channel Index	1.0 (0.0)

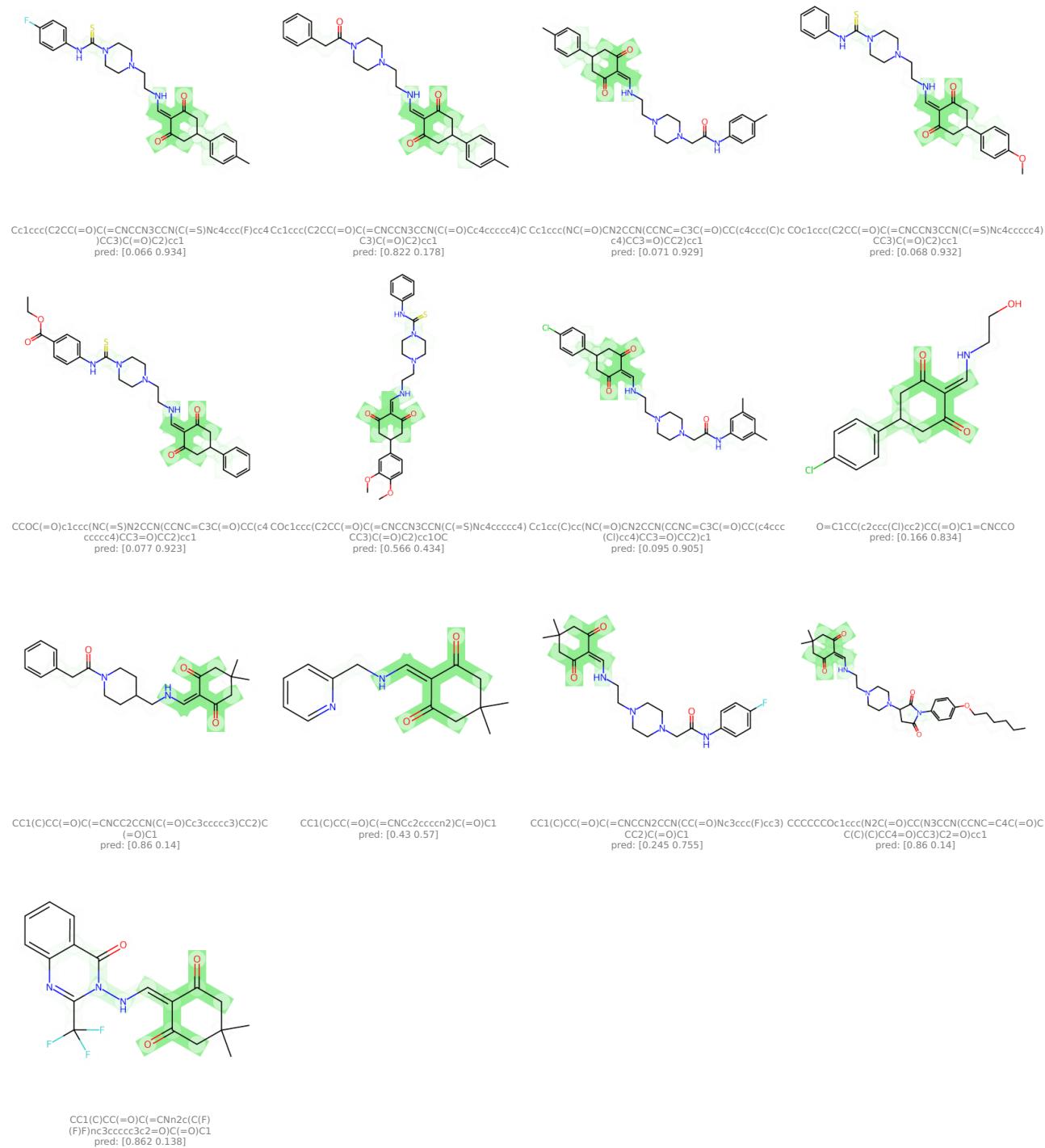
## Member Statistics

ⓘ 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 #138 - 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 138, from importance channel 1 (*aggregator*), represents a motif consisting of **8.1** ( $\pm 0.7$ ) nodes. The concept is generally associated with an impact of **1.1** ( $\pm 0.4$ ) on the prediction outcome.

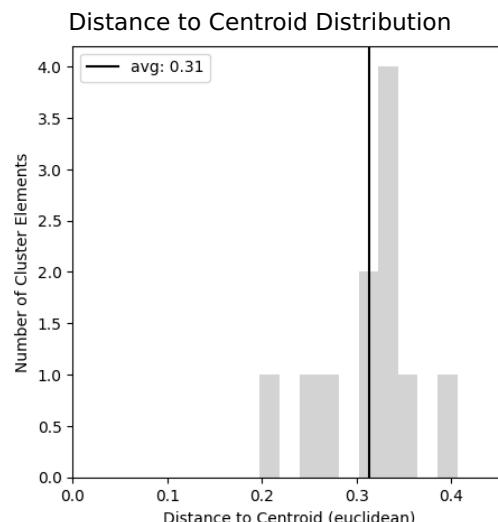
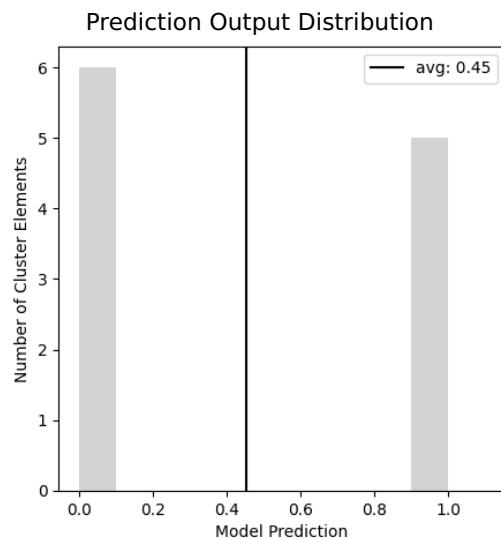
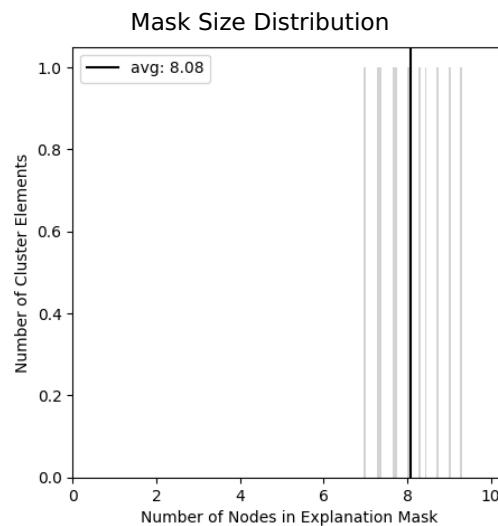
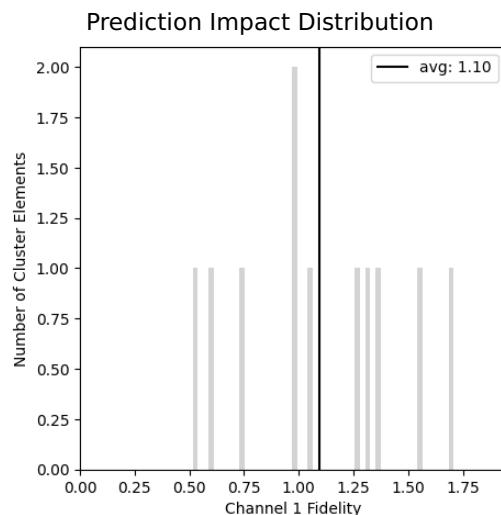
## Properties

ⓘ 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:	11
Channel Index	1.0 (0.0)

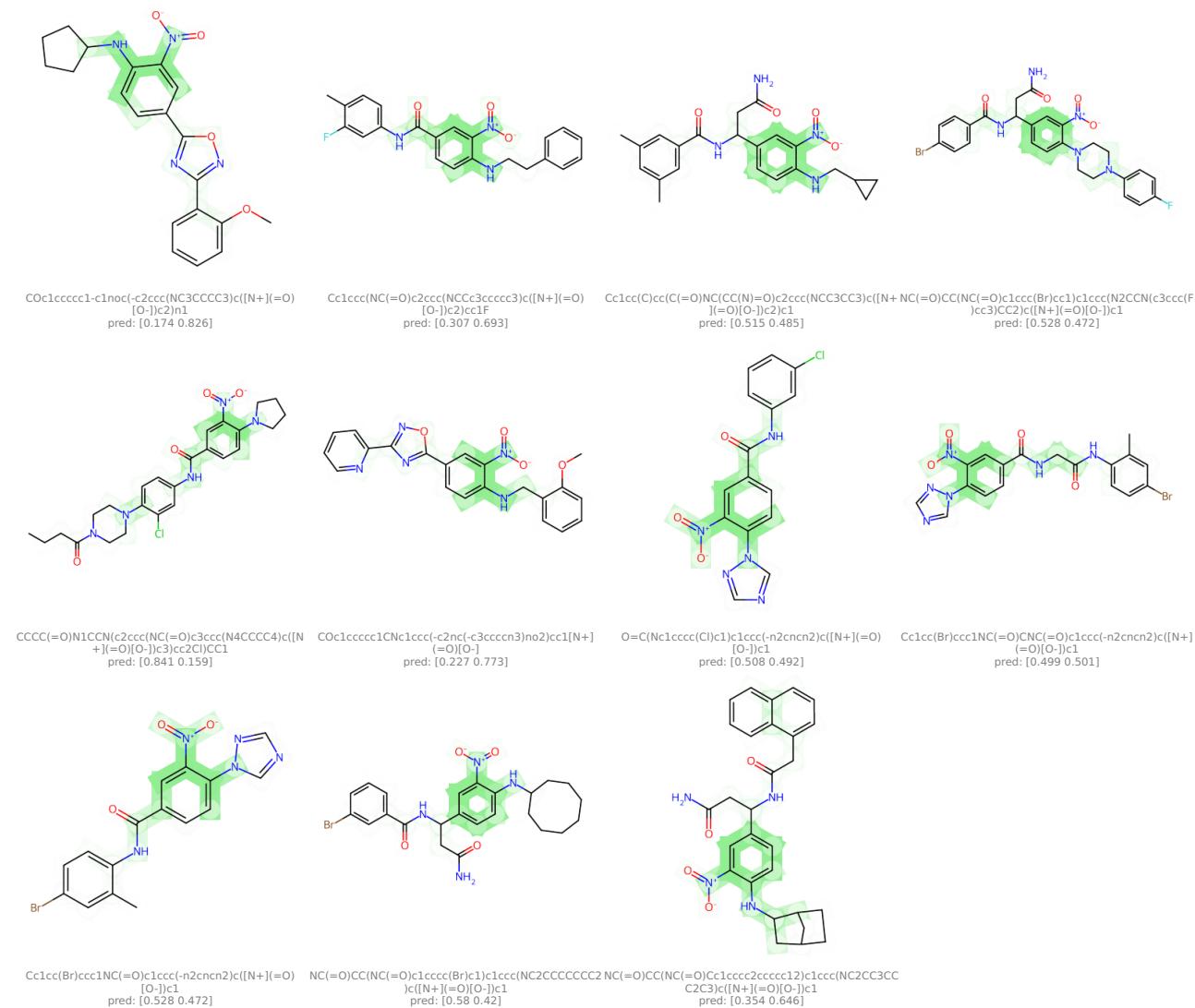
## Member Statistics

ⓘ 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 #139 - 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 139, from importance channel 1 (*aggregator*), represents a motif consisting of **9.1** ( $\pm 1.5$ ) nodes. The concept is generally associated with an impact of **0.9** ( $\pm 0.4$ ) on the prediction outcome.

## Properties

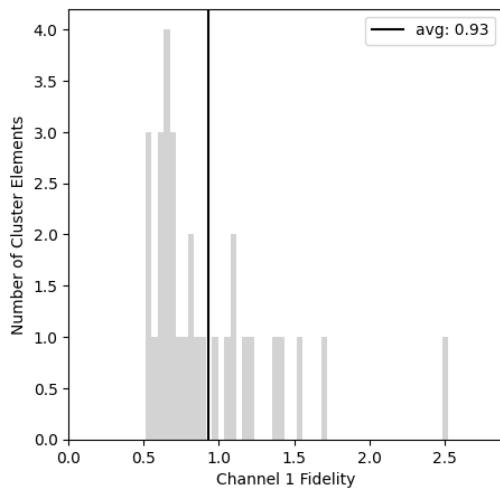
ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	31
Channel Index	1.0 (0.0)

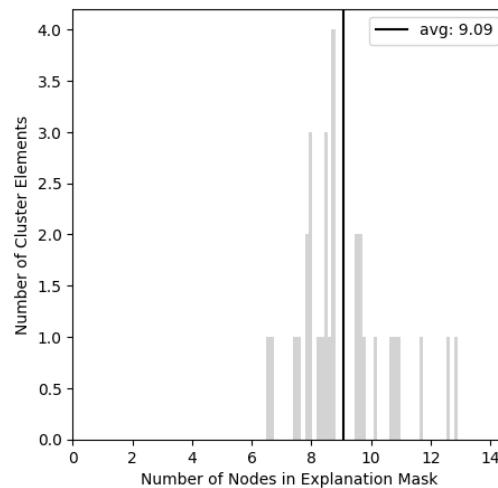
## Member Statistics

ⓘ 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.

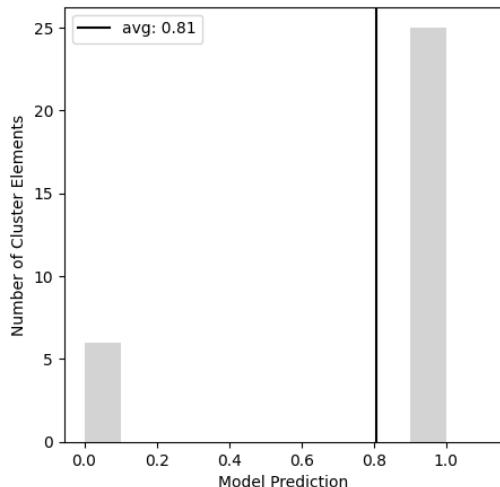
Prediction Impact Distribution



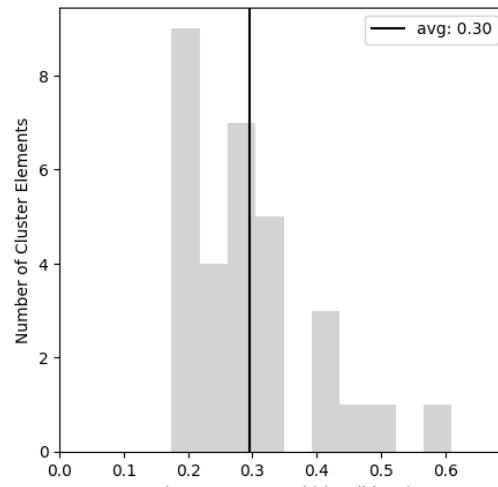
Mask Size Distribution



Prediction Output Distribution

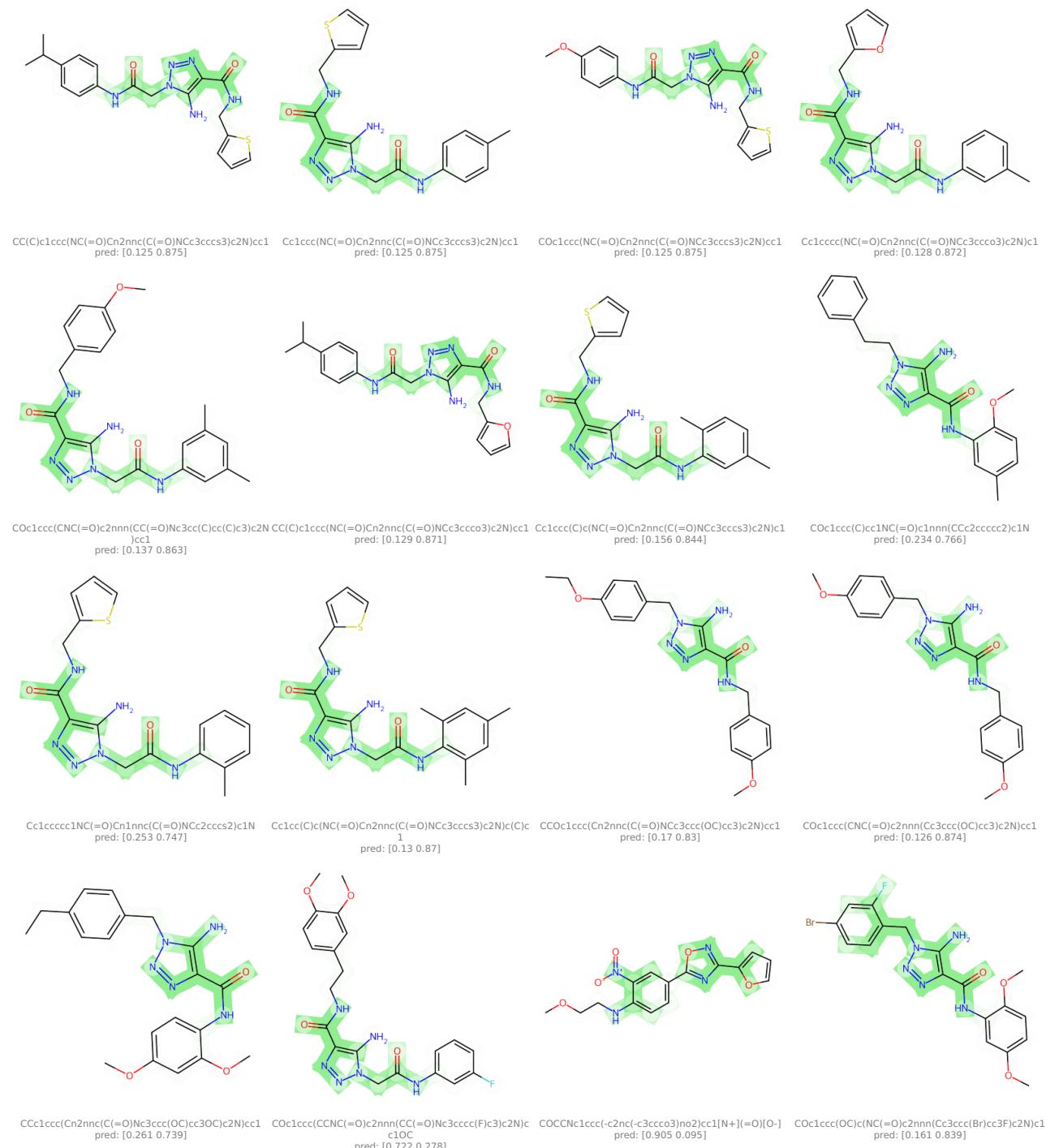


Distance to Centroid Distribution



## 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 #140 - 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 140, from importance channel 1 (*aggregator*), represents a motif consisting of  $9.9 (\pm 1.8)$  nodes. The concept is generally associated with an impact of  $1.2 (\pm 0.7)$  on the prediction outcome.

## Properties

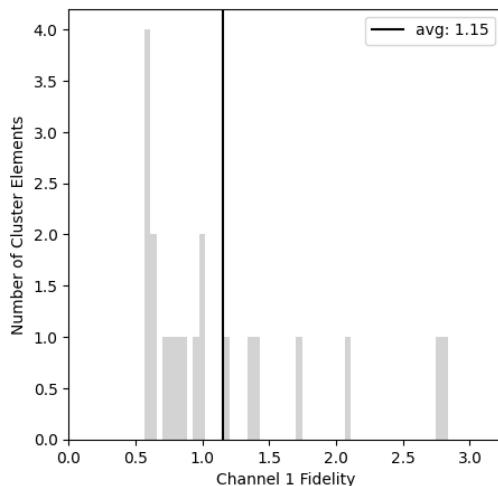
ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

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

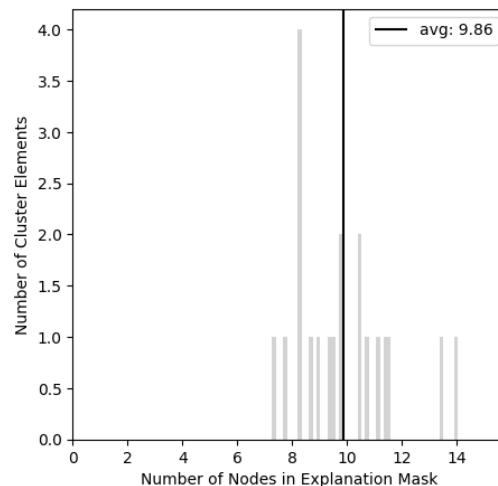
## Member Statistics

ⓘ 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.

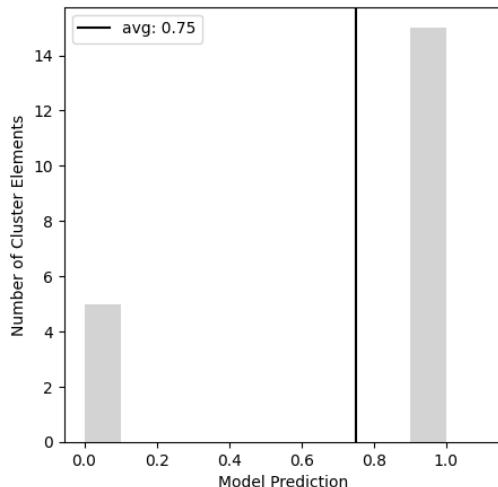
Prediction Impact Distribution



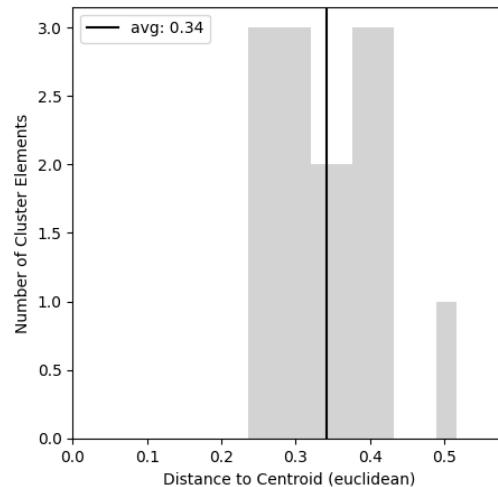
Mask Size Distribution



Prediction Output Distribution

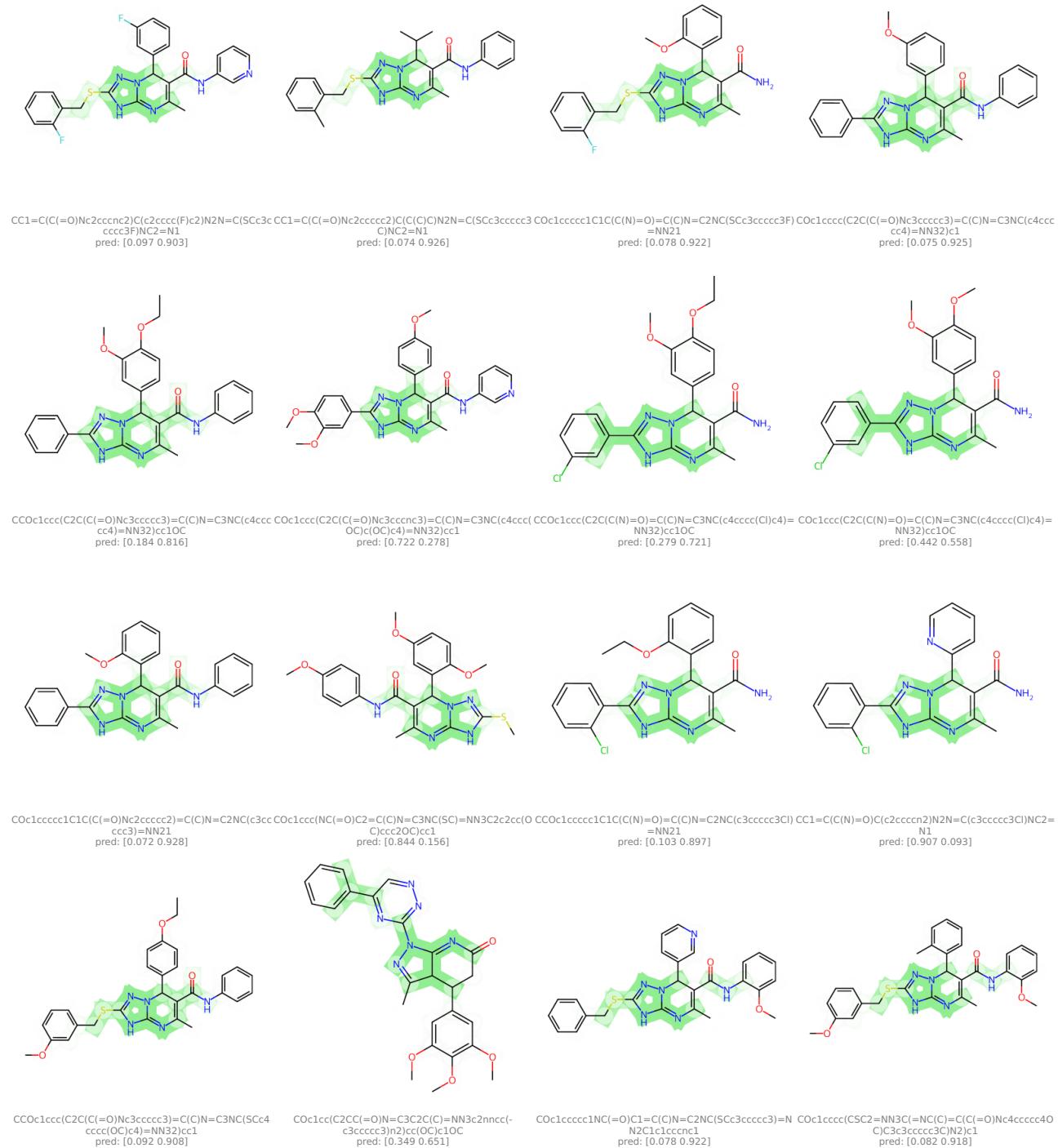


Distance to Centroid Distribution



## 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 #141 - 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 141, from importance channel 1 (*aggregator*), represents a motif consisting of 6.7 ( $\pm 0.8$ ) nodes. The concept is generally associated with an impact of 1.0 ( $\pm 0.5$ ) on the prediction outcome.

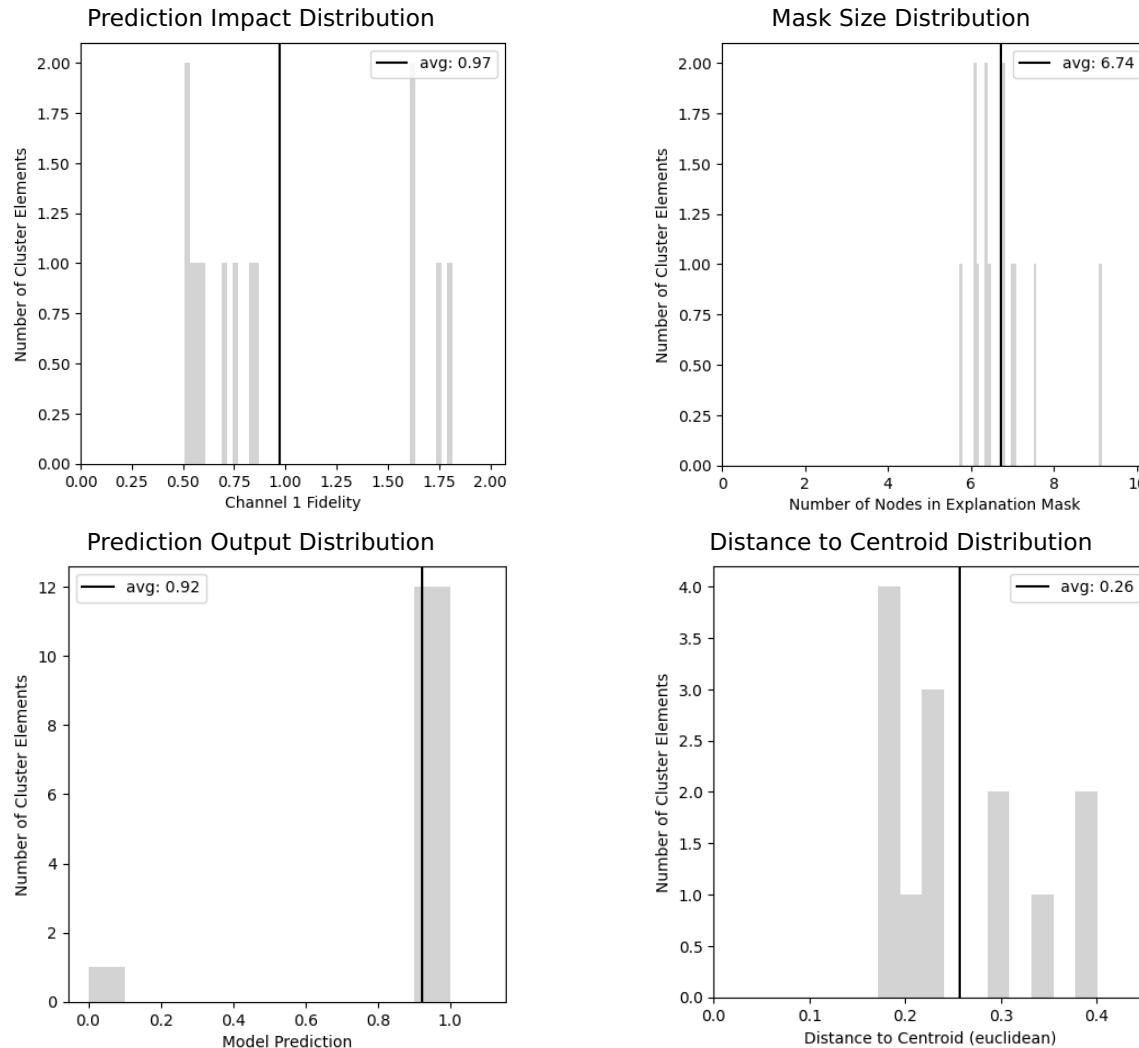
## Properties

ⓘ 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)

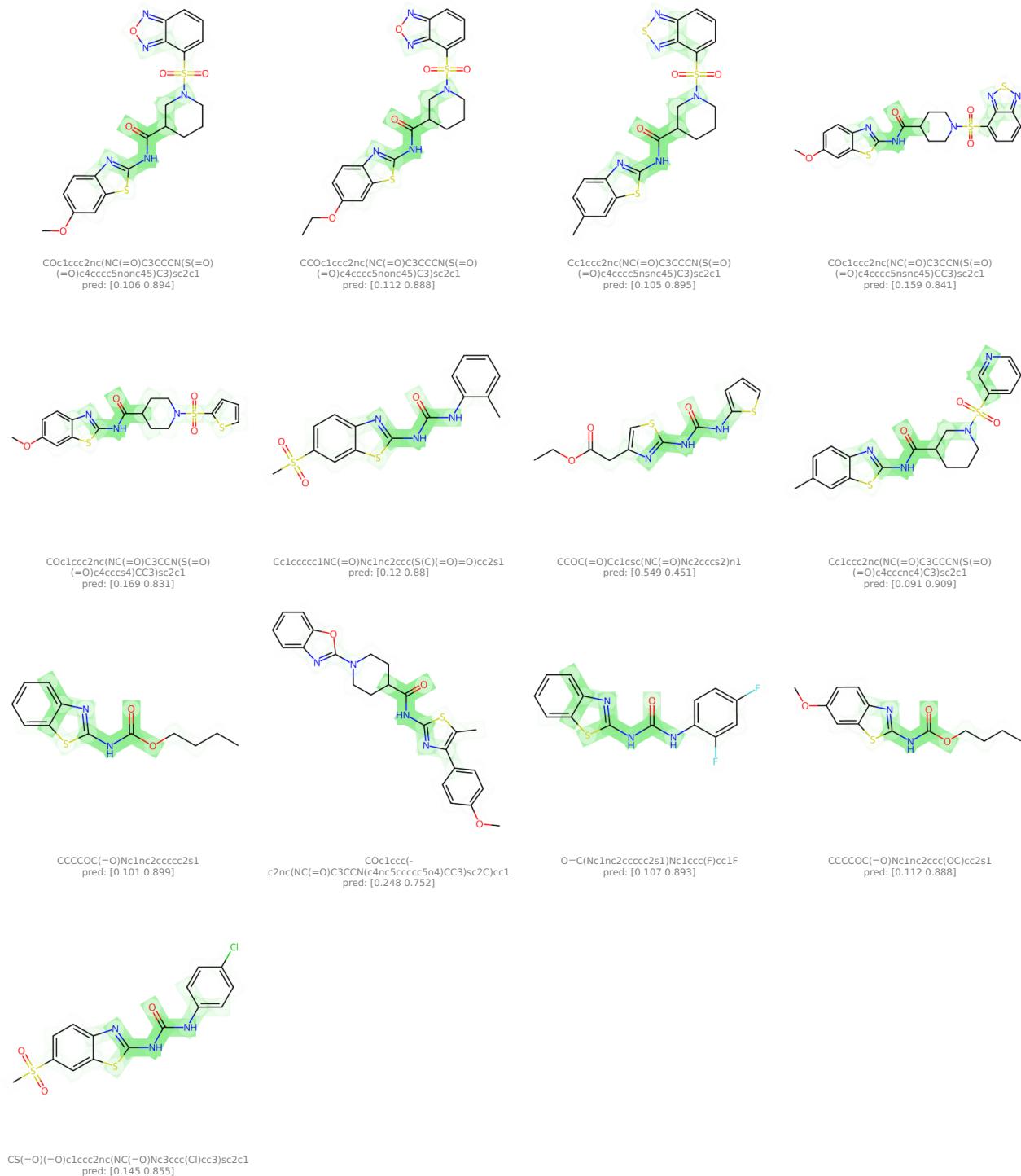
## Member Statistics

ⓘ 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 #142 - 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 142, from importance channel 1 (*aggregator*), represents a motif consisting of 12.4 ( $\pm 2.3$ ) nodes. The concept is generally associated with an impact of 1.6 ( $\pm 0.8$ ) on the prediction outcome.

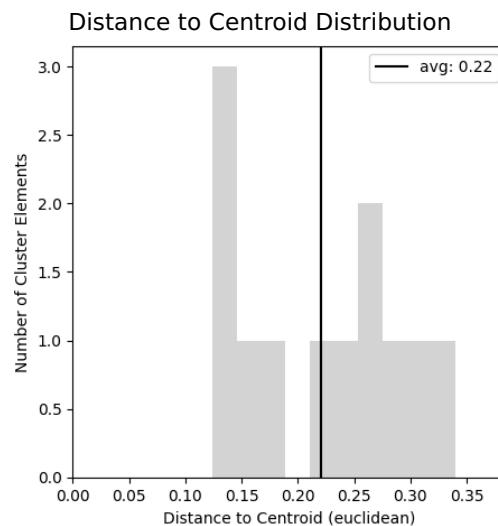
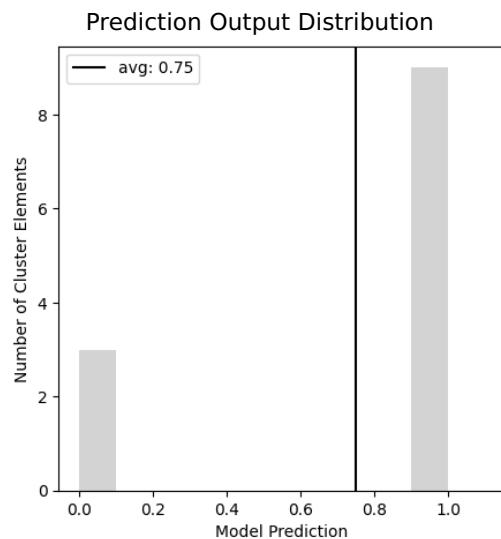
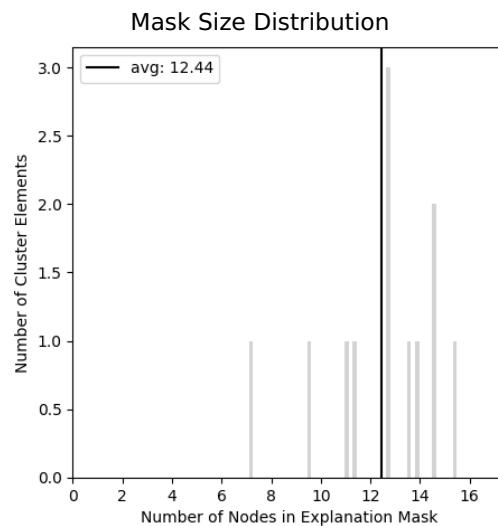
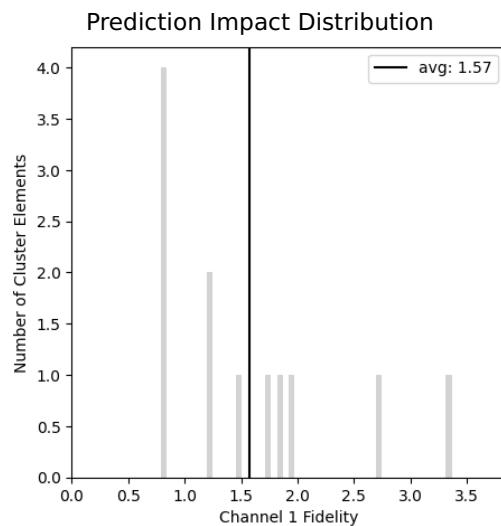
## Properties

ⓘ 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:	12
Channel Index	1.0 (0.0)

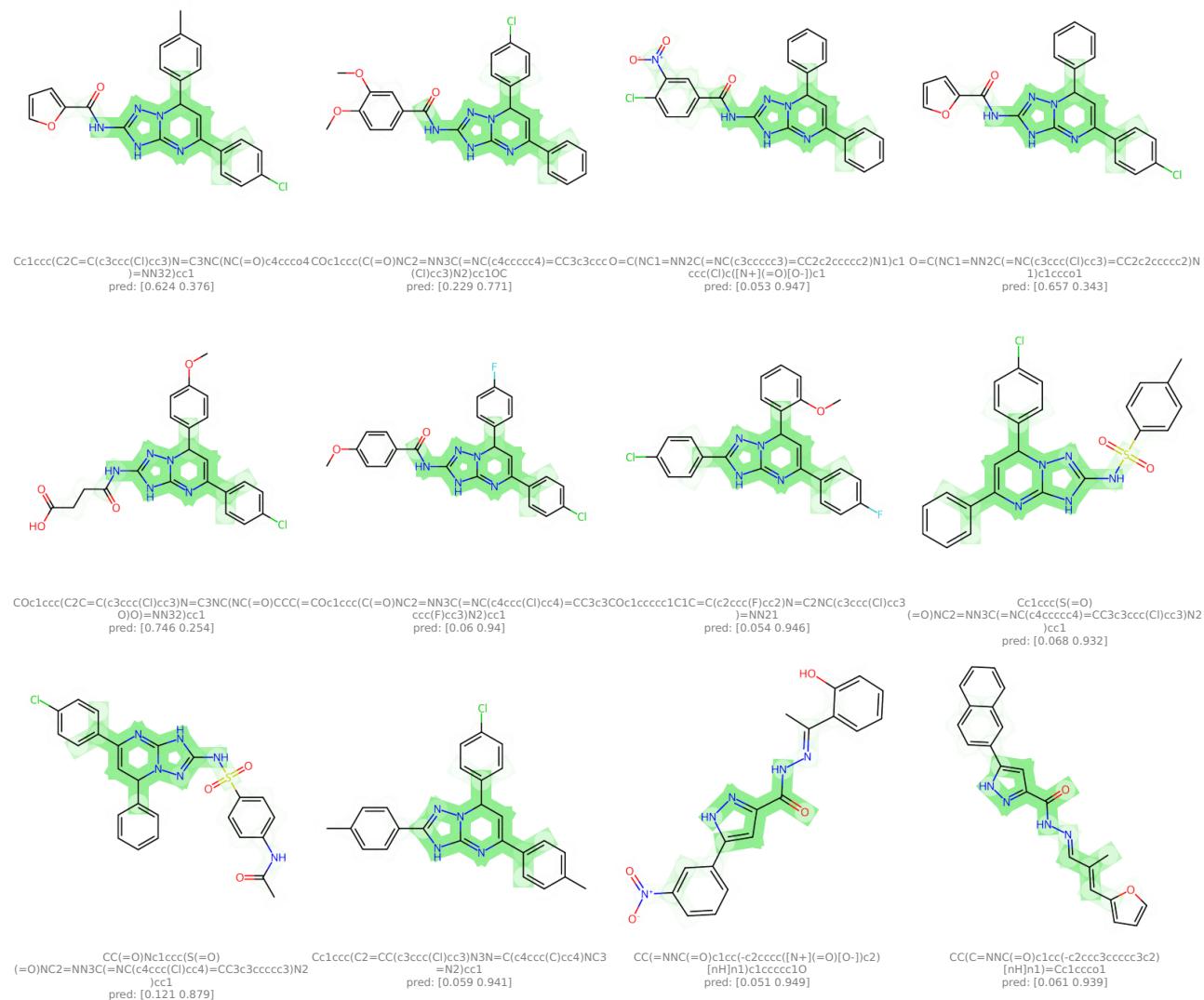
## Member Statistics

ⓘ 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 #143 - 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 143, from importance channel 1 (*aggregator*), represents a motif consisting of  $8.4 (\pm 0.5)$  nodes. The concept is generally associated with an impact of  $0.6 (\pm 0.0)$  on the prediction outcome.

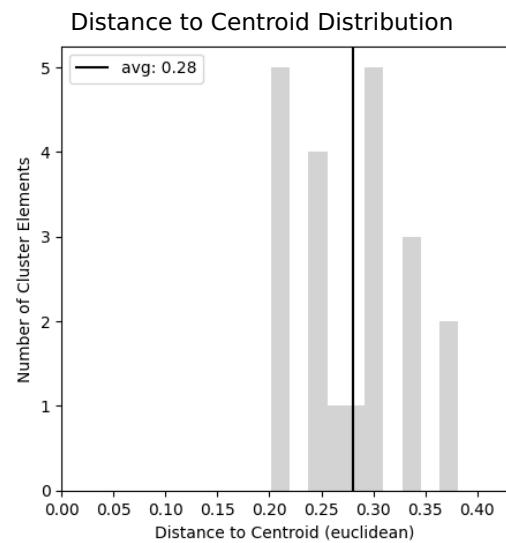
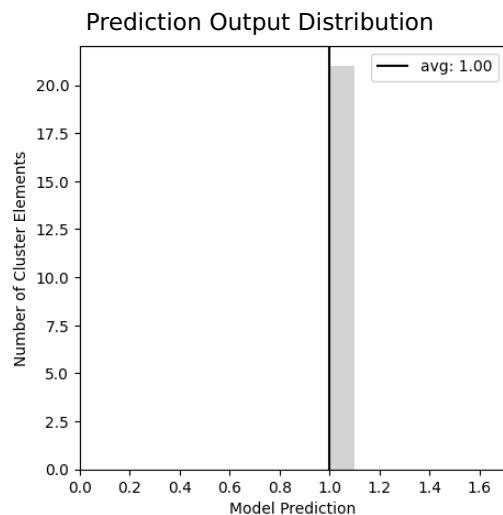
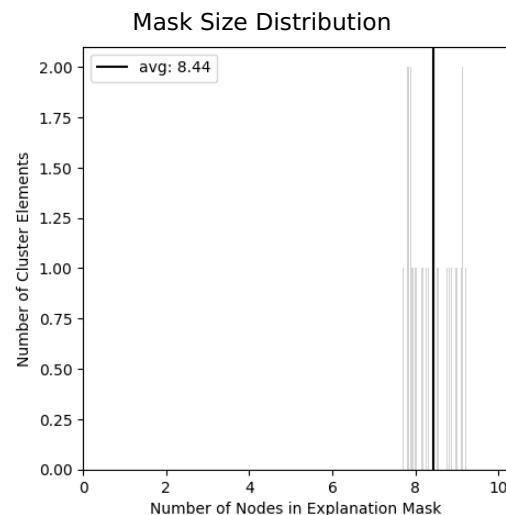
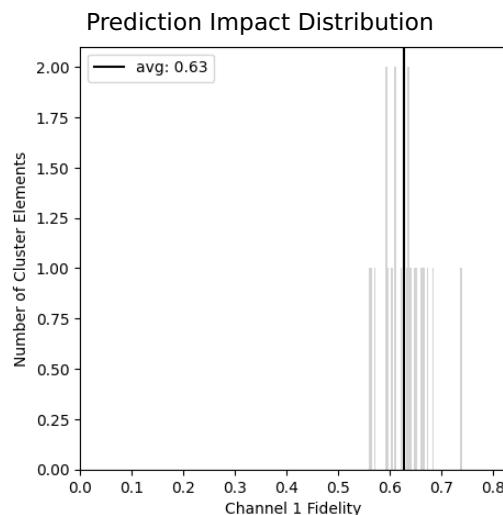
## Properties

ⓘ 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:	21
Channel Index	1.0 (0.0)

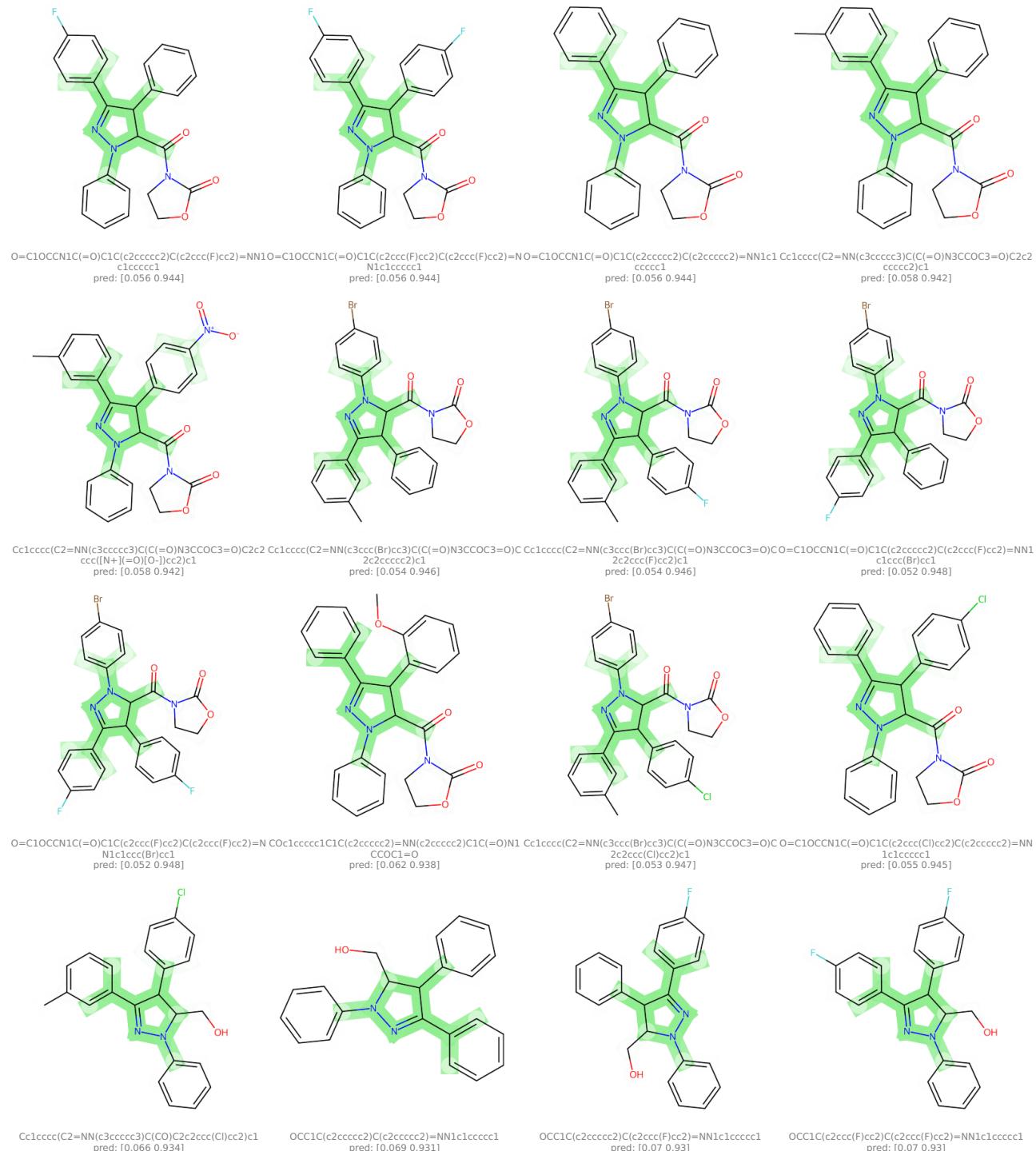
## Member Statistics

ⓘ 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 #144 - 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 144, from importance channel 1 (*aggregator*), represents a motif consisting of 8.5 ( $\pm 1.9$ ) nodes. The concept is generally associated with an impact of 1.2 ( $\pm 0.5$ ) on the prediction outcome.

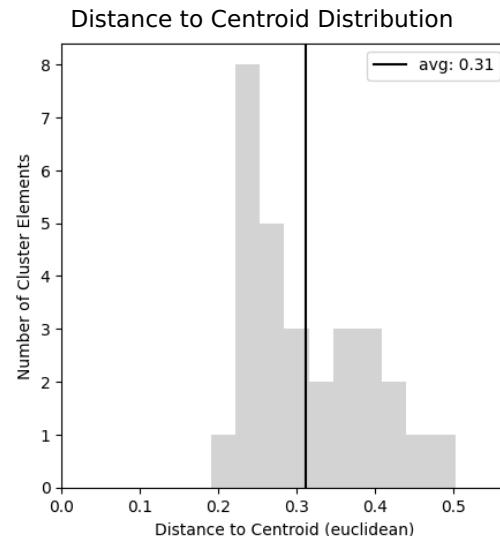
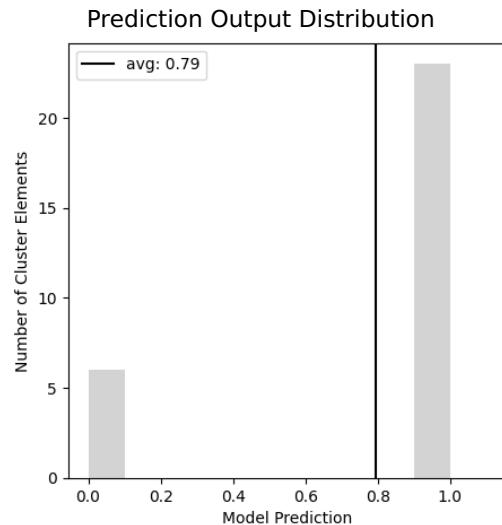
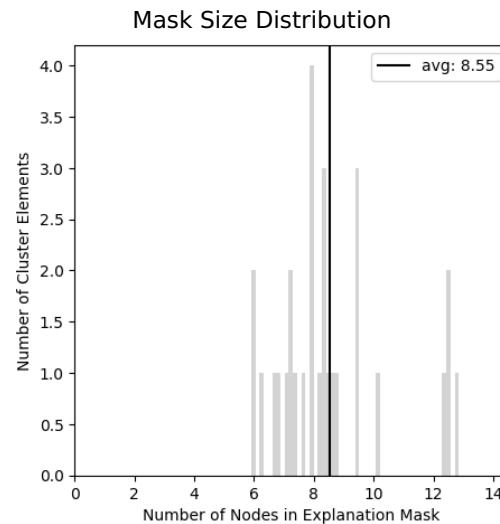
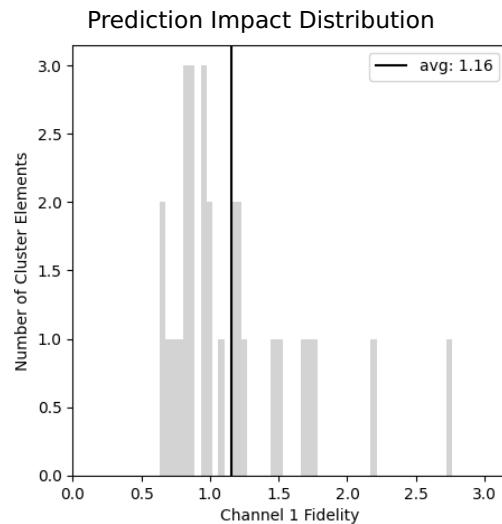
## Properties

ⓘ 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:	29
Channel Index	1.0 (0.0)

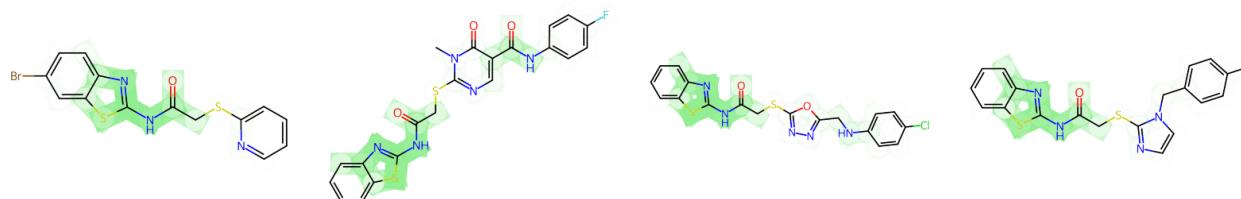
## Member Statistics

ⓘ 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.

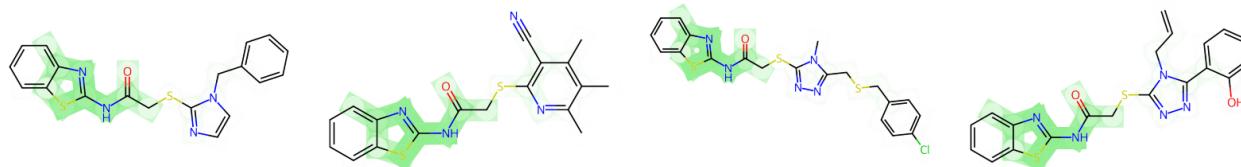


O=C(CSc1ccccc1)Nc1nc2ccc(Br)cc2s1  
pred: [0.151 0.849]

Cn1c(SCC(=O)Nc2nc3cccc3s2)nc(C(=O)Nc2ccc(F)cc2)c1=O  
pred: [0.817 0.183]

O=C(CS1nnc(Nc2ccc(Cl)cc2)o1)Nc1nc2cccc2s1  
pred: [0.116 0.884]

Cc1ccc(Cn2ccnc2SCC(=O)Nc2nc3cccc3s2)cc1  
pred: [0.87 0.13]

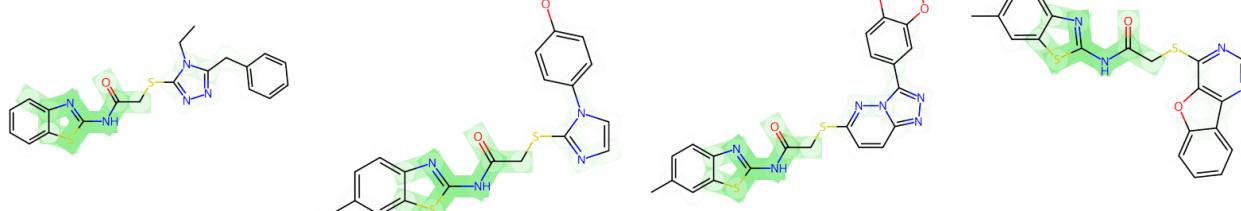


O=C(CSc1nccn1Cc1cccc1)Nc1nc2cccc2s1  
pred: [0.871 0.129]

Cc1nc(SCC(=O)Nc2nc3cccc3s2)c(C#N)c(C)c1  
pred: [0.133 0.867]

Cn1c(CSCc2ccc(Cl)cc2)nnc1SCC(=O)Nc1nc2cccc2s1  
pred: [0.139 0.861]

C=CCn1c(SCC(=O)Nc2nc3cccc3s2)nnc1-c1cccc1O  
pred: [0.103 0.897]

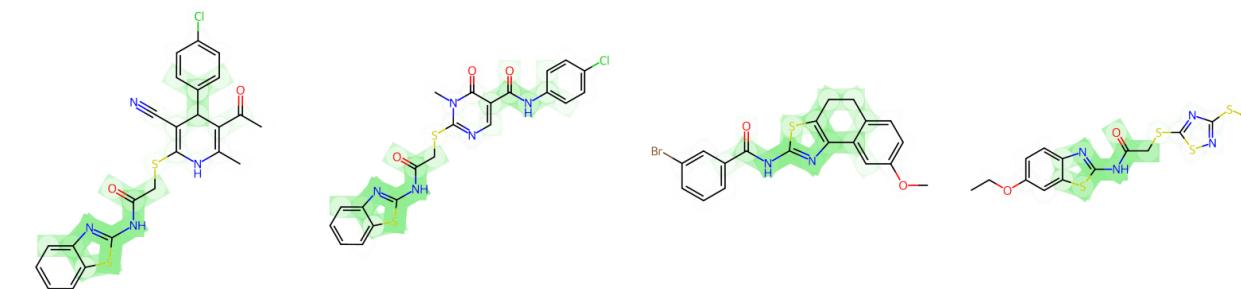


CCn1c(Cc2cccc2)nnc1SCC(=O)Nc1nc2cccc2s1  
pred: [0.121 0.879]

CCOc1ccc(-n2ccnc2SCC(=O)Nc2nc3ccc(C)c3s2)cc1  
pred: [0.451 0.549]

COc1ccc(-c2nncc(CSC(=O)Nc4nc5ccc(C)cc5s4)nn23)cc1OC  
pred: [0.867 0.133]

Cc1ccc2nc(NC(=O)CSc3ncnc4c3ccc34)sc2c1  
pred: [0.119 0.881]



CC(=O)C1=C(C)NC(SCC(=O)Nc2nc3cccc3s2)=C(C#N Cn1c(SCC(=O)Nc2nc3cccc3s2)nc(C(=O)Nc2ccc(Cl)c2)c1=O  
pred: [0.105 0.895]

pred: [0.803 0.197]

COc1ccc2c(c1)-c1nc(NC(=O)c3cccc(Br)c3)sc1CC2  
pred: [0.113 0.887]

CCOc1ccc2nc(NC(=O)CSc3ncnc4c3ccc34)sc2c1  
pred: [0.159 0.841]

# Cluster #145 - 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 145, from importance channel 1 (*aggregator*), represents a motif consisting of **9.4 ( $\pm 0.8$ )** nodes. The concept is generally associated with an impact of **0.9 ( $\pm 0.2$ )** on the prediction outcome.

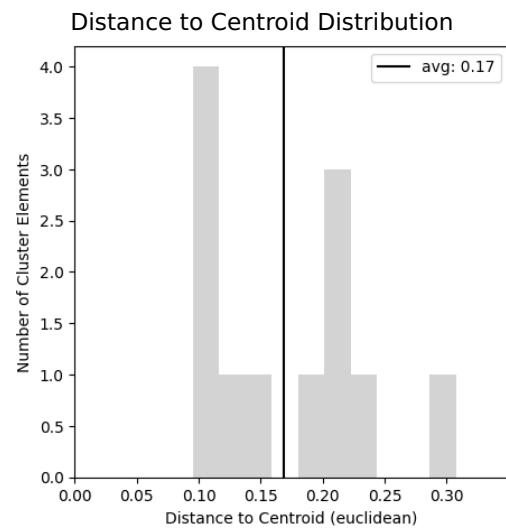
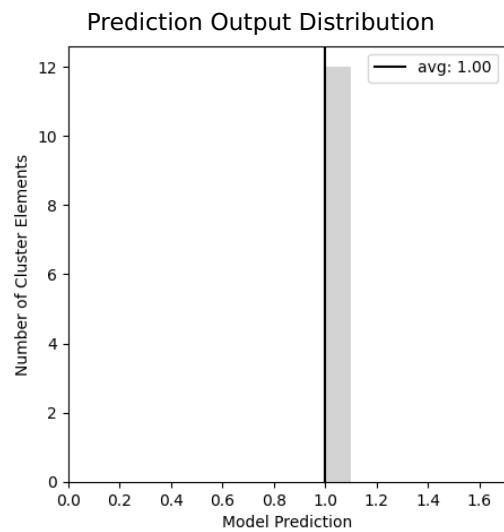
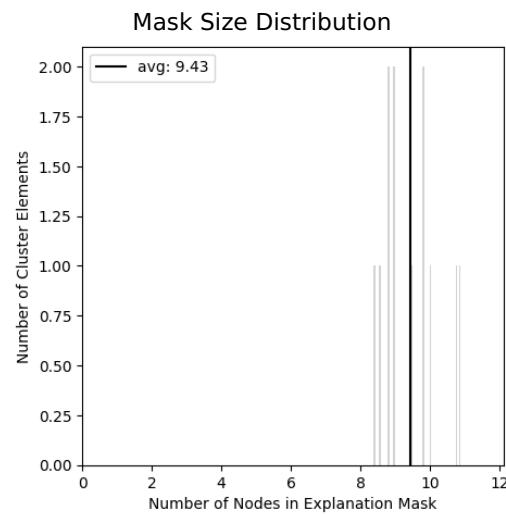
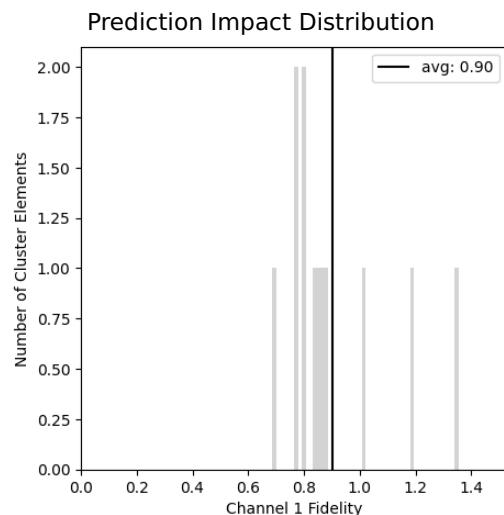
## Properties

ⓘ 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)

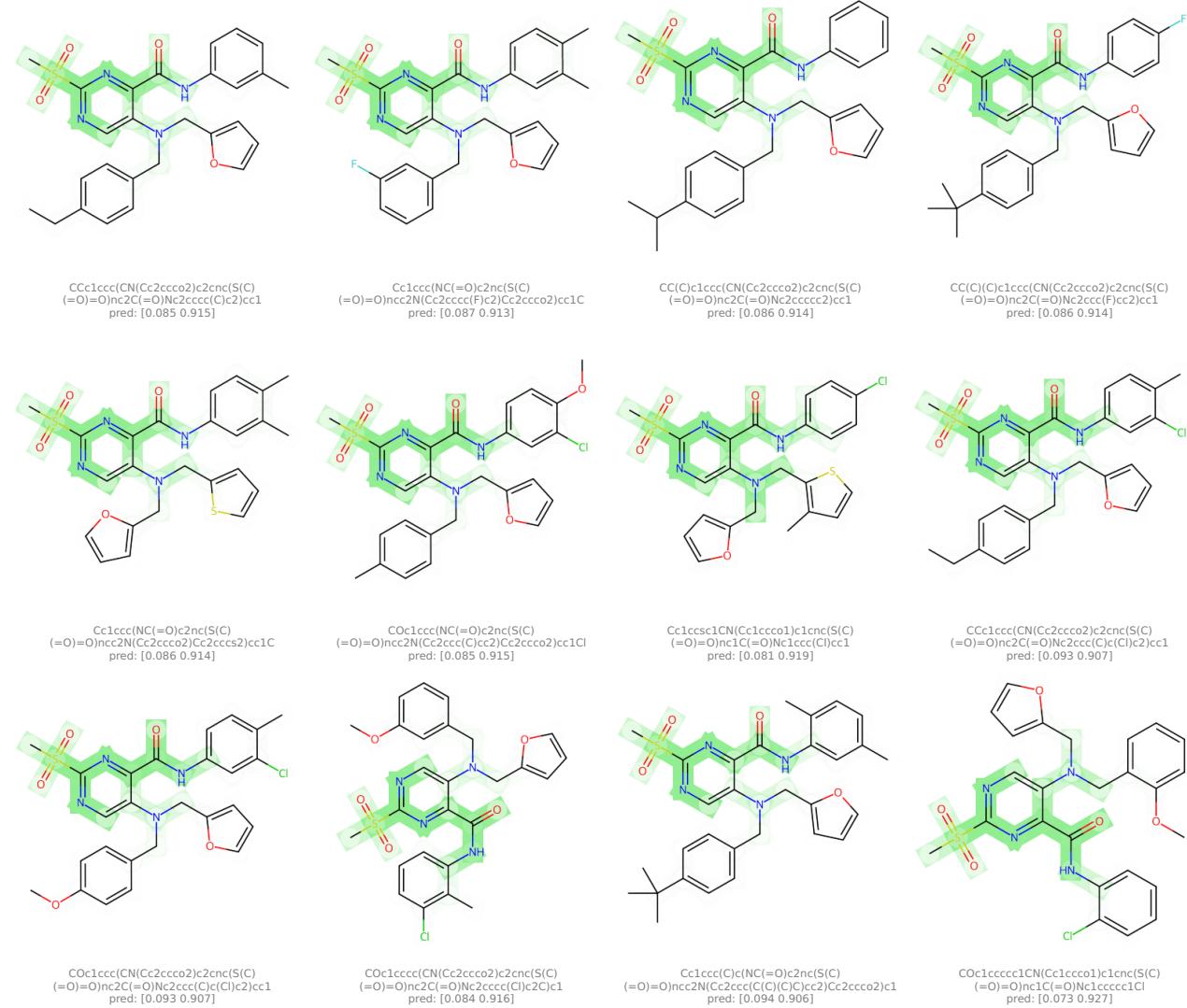
## Member Statistics

ⓘ 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 #146 - 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 146, from importance channel 1 (*aggregator*), represents a motif consisting of 8.4 ( $\pm 1.3$ ) nodes. The concept is generally associated with an impact of 1.4 ( $\pm 0.5$ ) on the prediction outcome.

## Properties

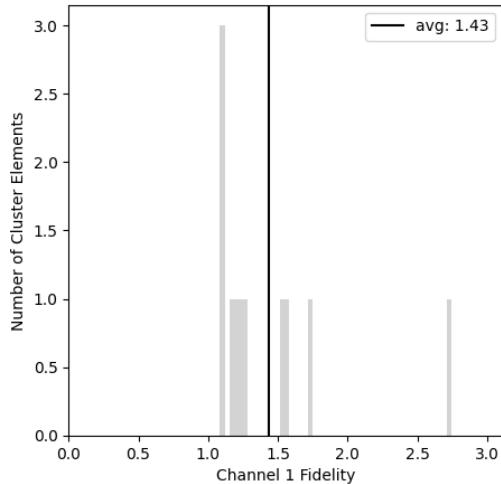
ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

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

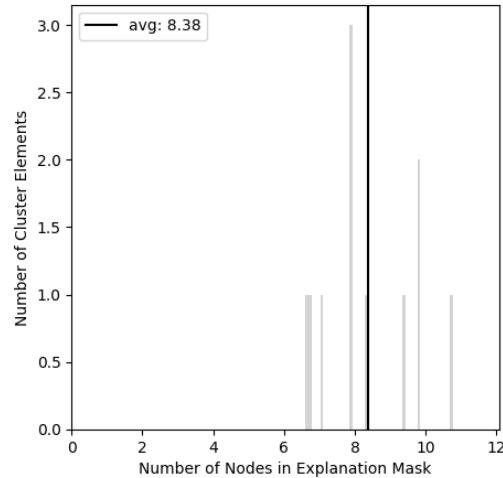
## Member Statistics

ⓘ 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.

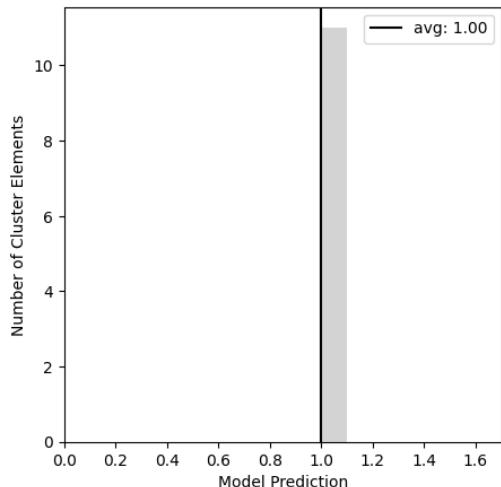
Prediction Impact Distribution



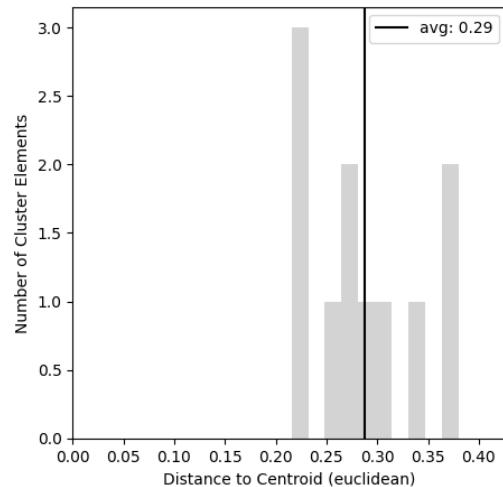
Mask Size Distribution



Prediction Output Distribution

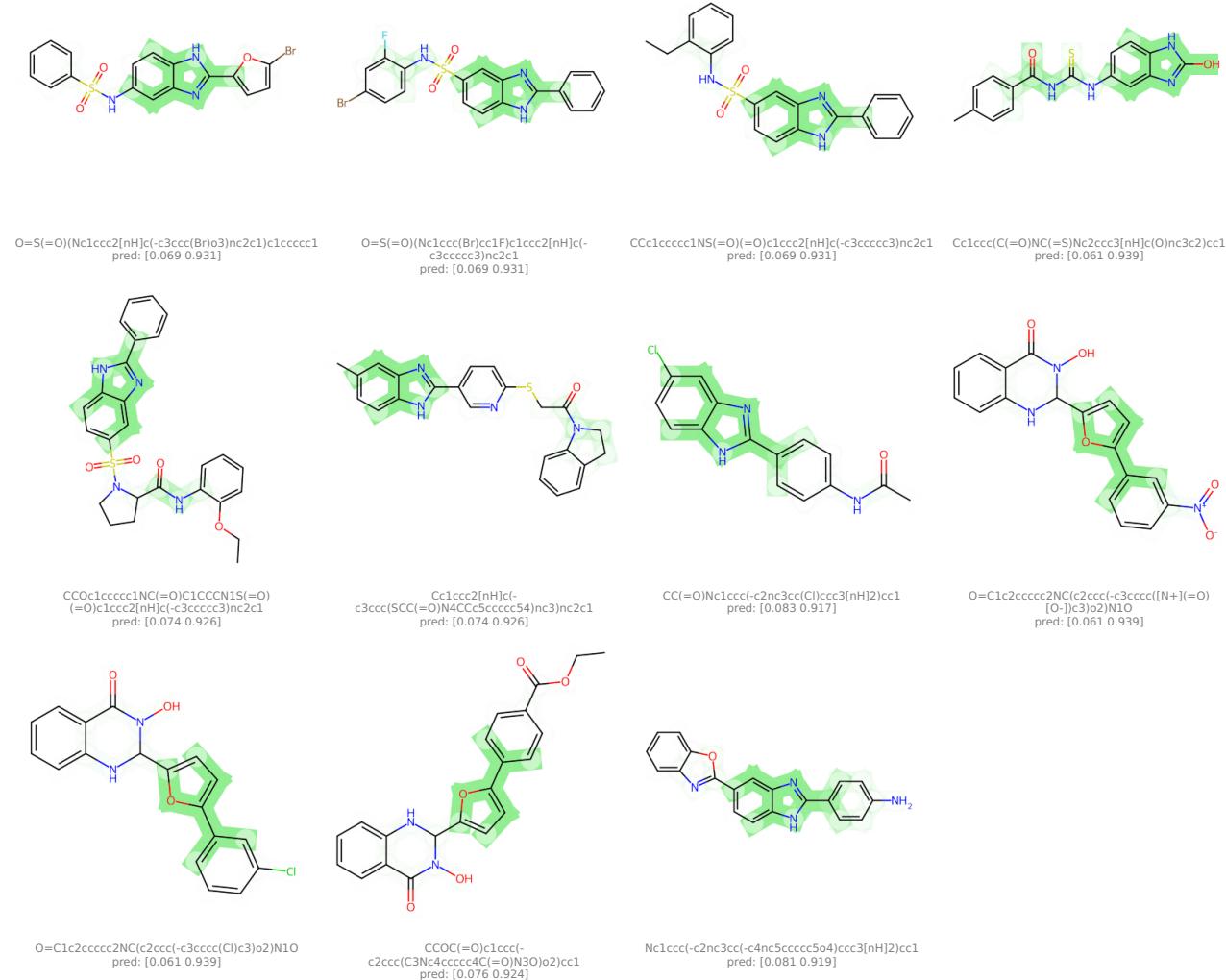


Distance to Centroid Distribution



## 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 #147 - 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 147, from importance channel 1 (*aggregator*), represents a motif consisting of 8.9 ( $\pm 1.5$ ) nodes. The concept is generally associated with an impact of 1.0 ( $\pm 0.6$ ) on the prediction outcome.

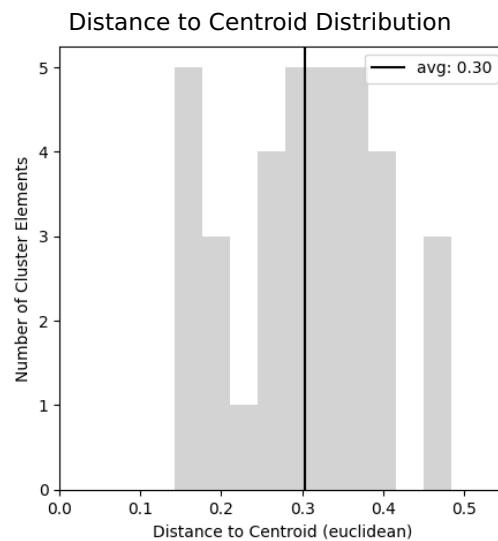
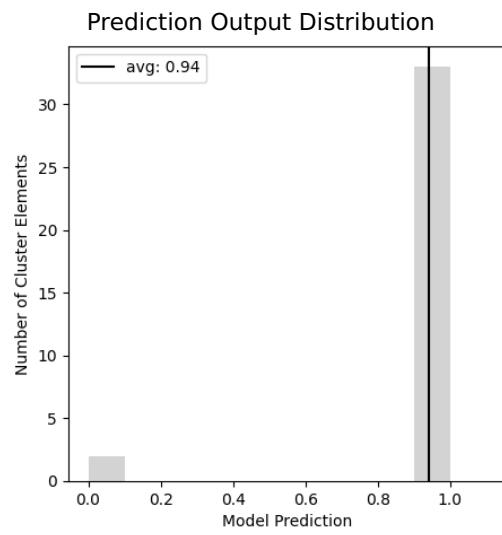
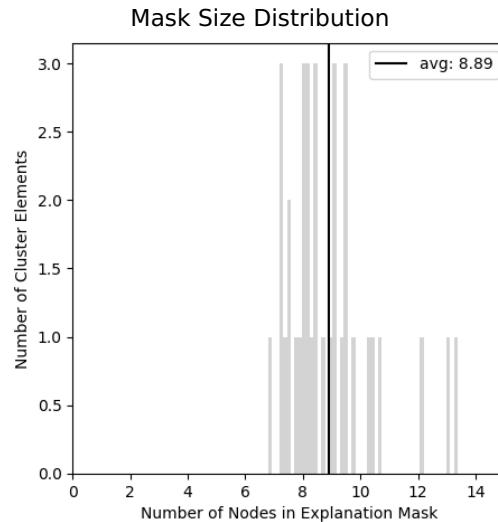
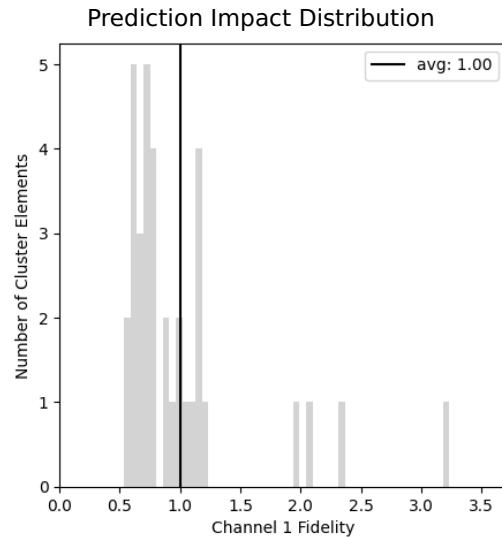
## Properties

ⓘ 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:	35
Channel Index	1.0 (0.0)

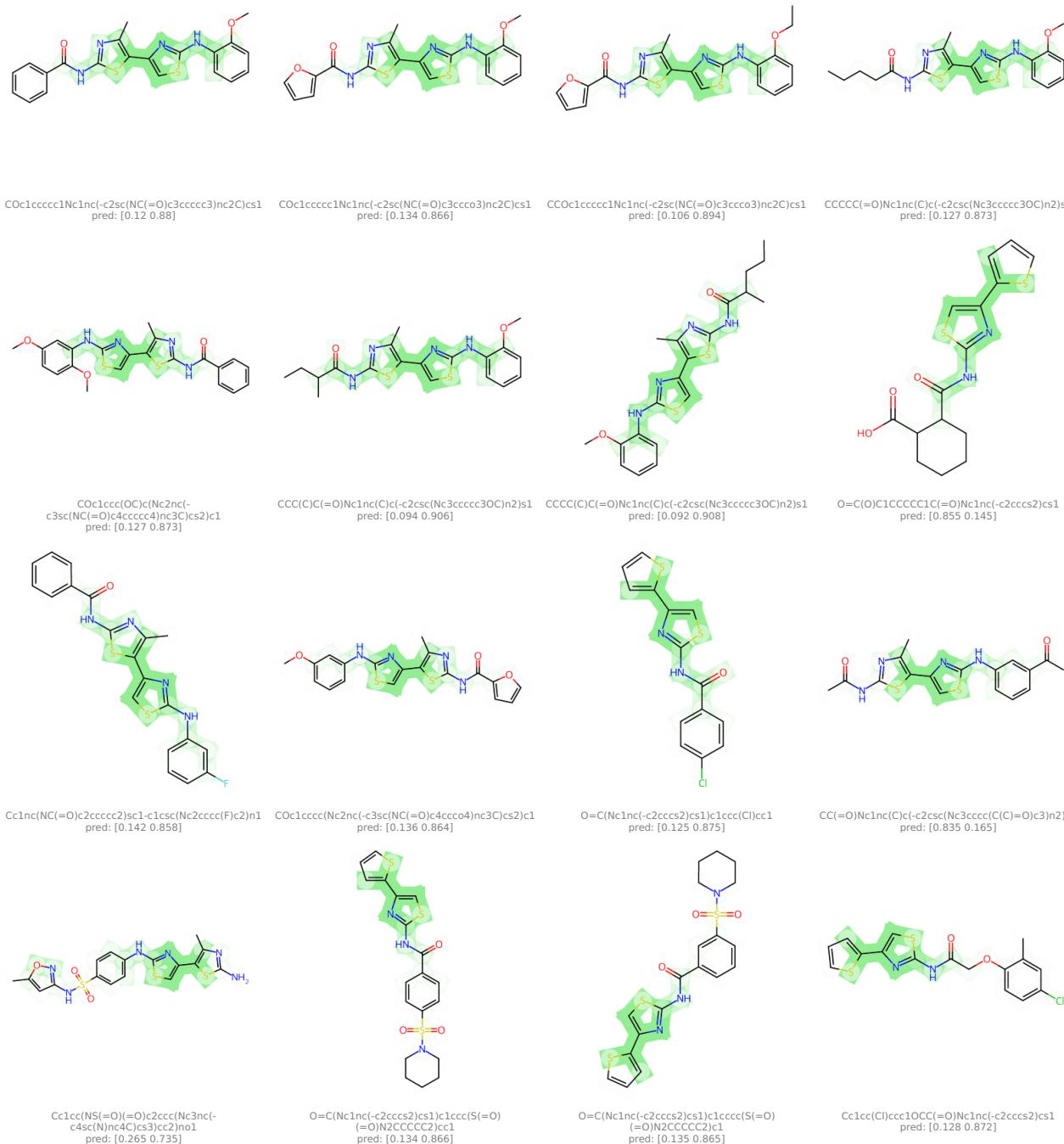
## Member Statistics

ⓘ 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 #148 - 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 148, from importance channel 1 (*aggregator*), represents a motif consisting of **8.4 ( $\pm 1.9$ )** nodes. The concept is generally associated with an impact of **1.1 ( $\pm 0.4$ )** on the prediction outcome.

## Properties

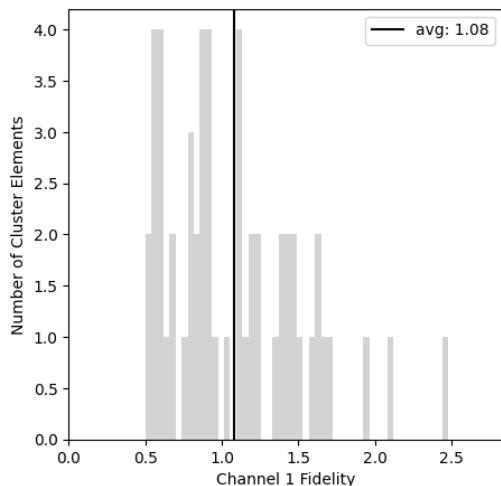
ⓘ This section shows some numeric information about the cluster in a tabular format. The left column is a description of the property and the right column shows the value of that property.

No. Cluster Members:	54
Channel Index	1.0 (0.0)

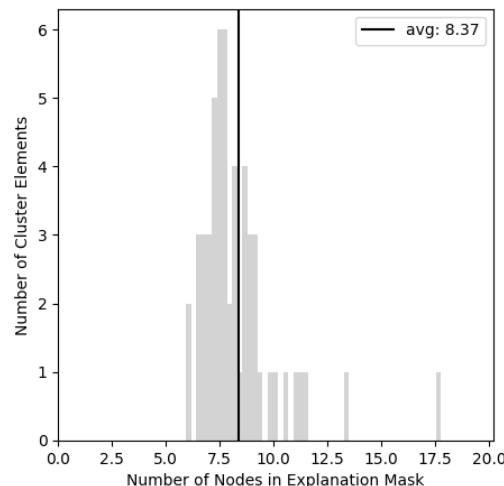
## Member Statistics

ⓘ 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.

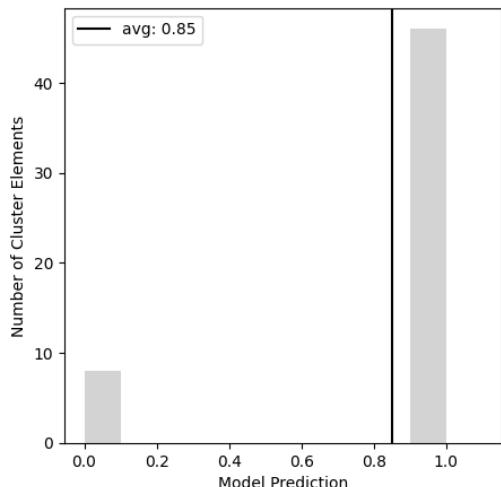
Prediction Impact Distribution



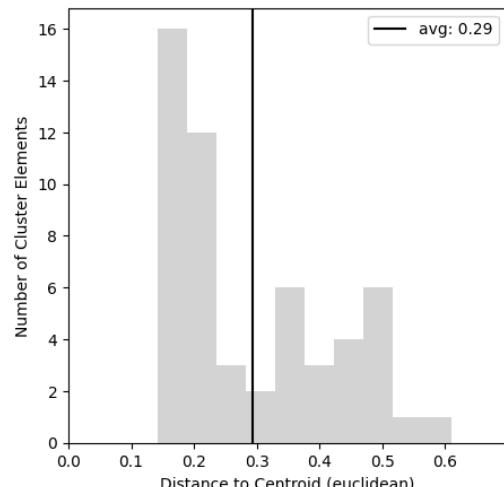
Mask Size Distribution



Prediction Output Distribution

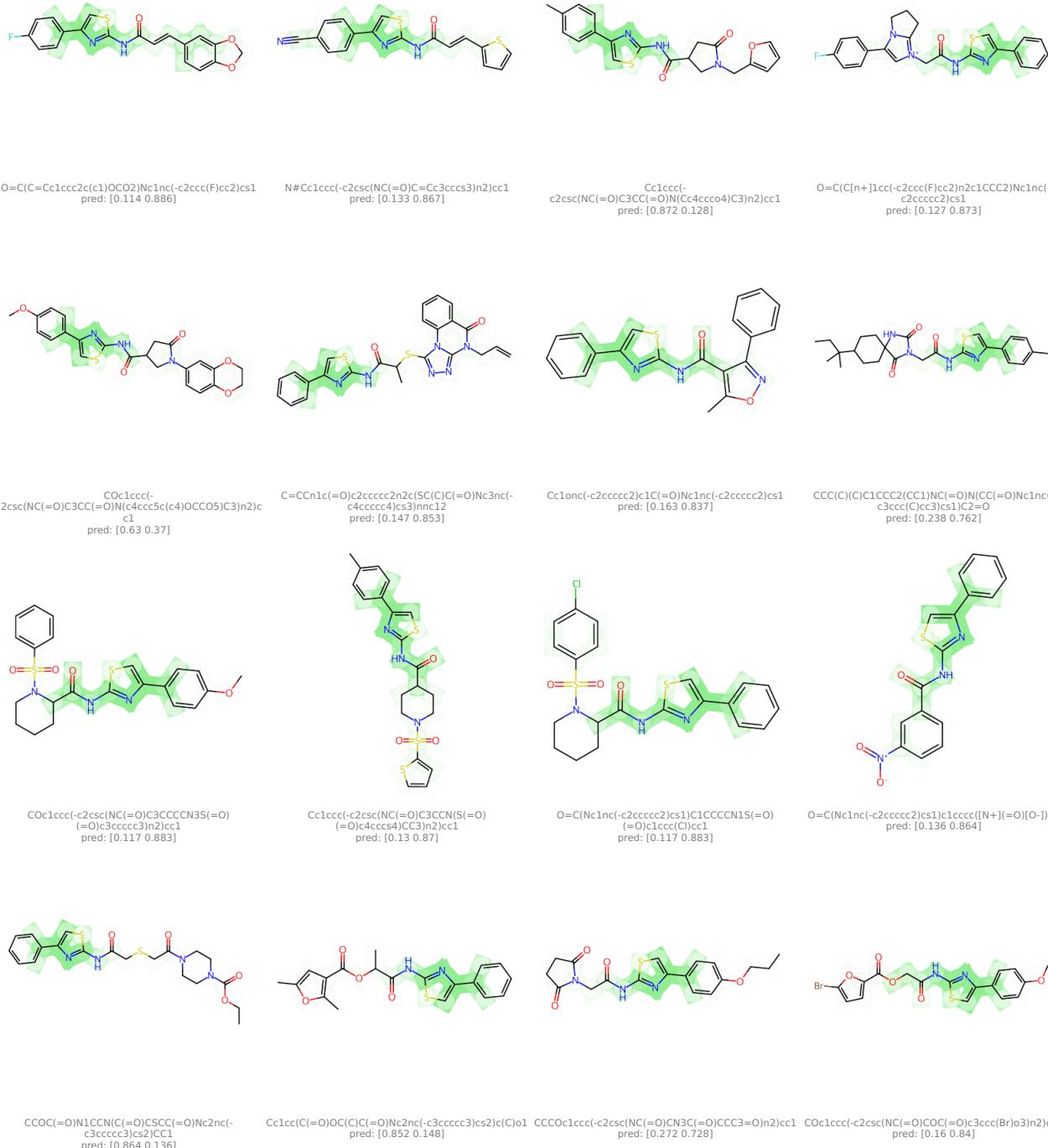


Distance to Centroid Distribution



## 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 #149 - 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 149, from importance channel 1 (*aggregator*), represents a motif consisting of 9.1 ( $\pm 1.4$ ) nodes. The concept is generally associated with an impact of 1.6 ( $\pm 0.7$ ) on the prediction outcome.

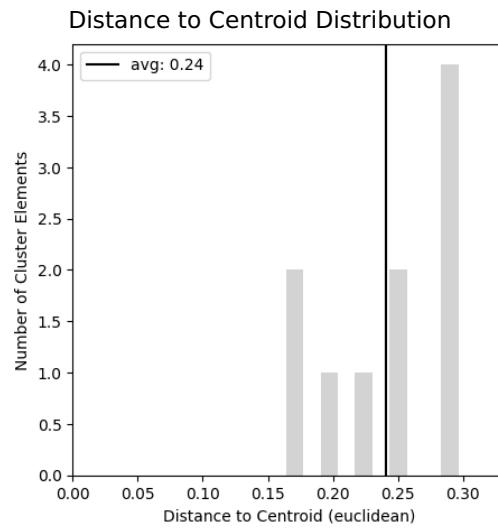
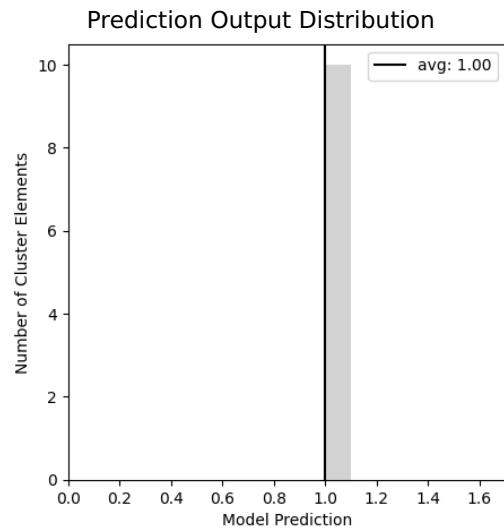
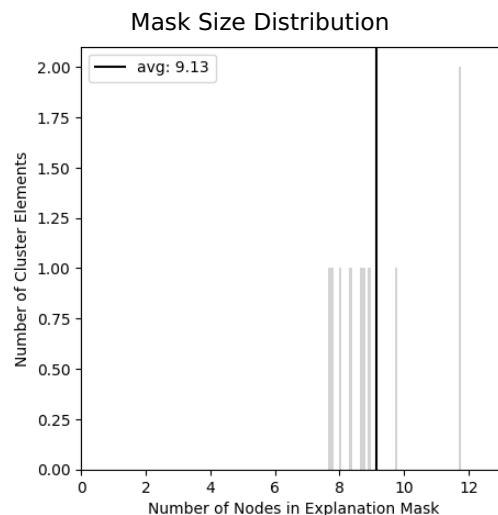
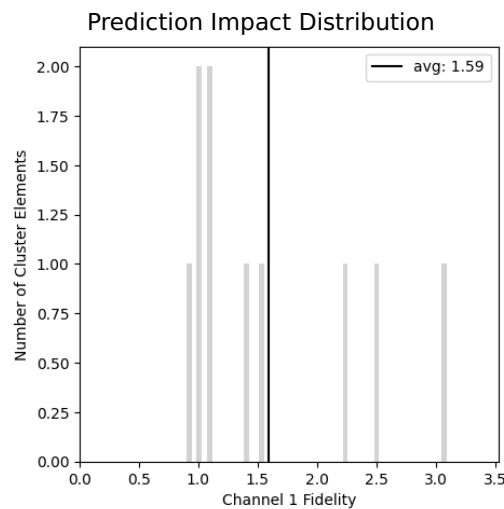
## Properties

ⓘ 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)

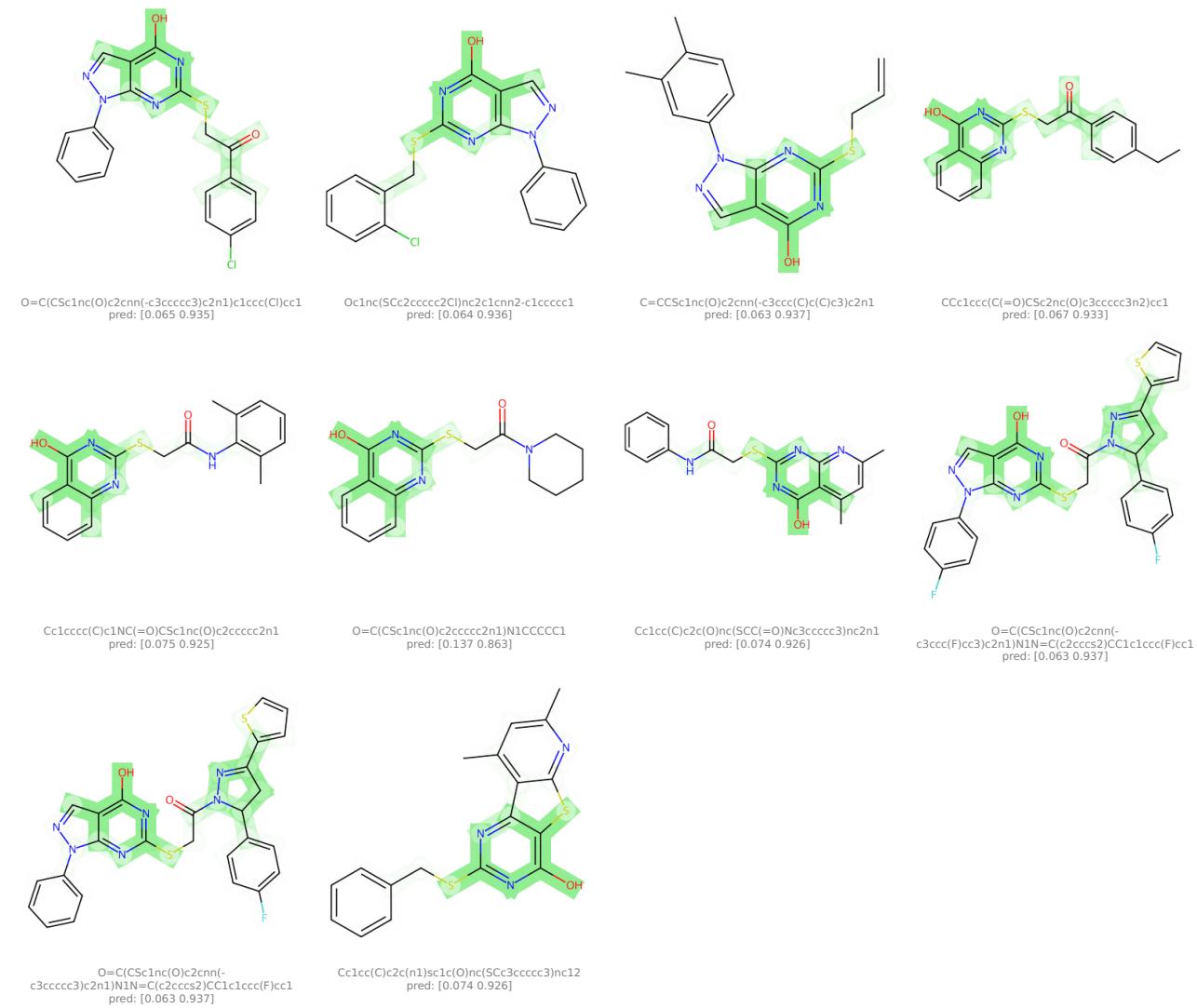
## Member Statistics

ⓘ 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 #150 - 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 150, from importance channel 1 (*aggregator*), represents a motif consisting of 8.3 ( $\pm 2.0$ ) nodes. The concept is generally associated with an impact of 1.6 ( $\pm 0.6$ ) on the prediction outcome.

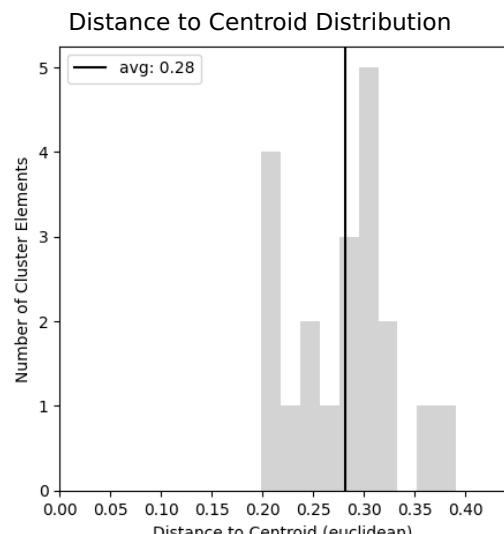
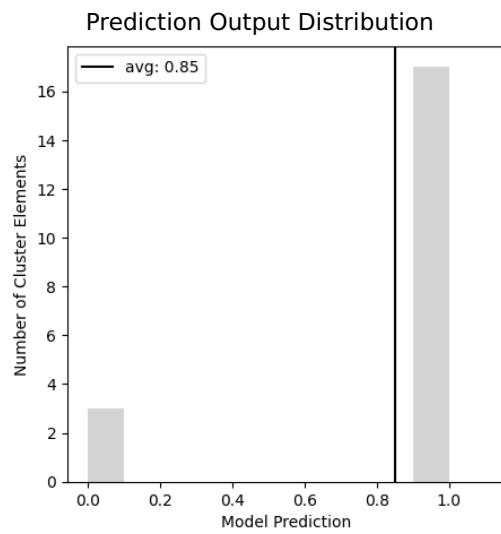
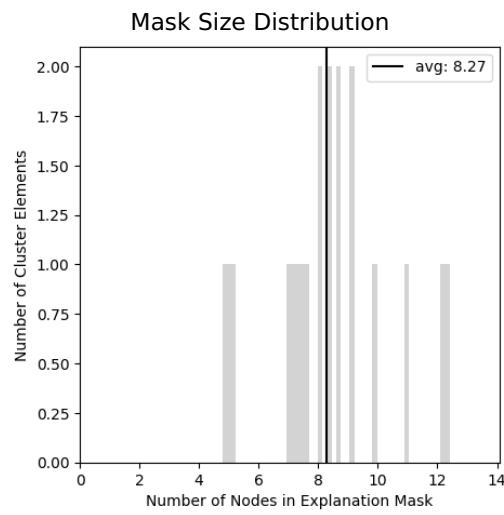
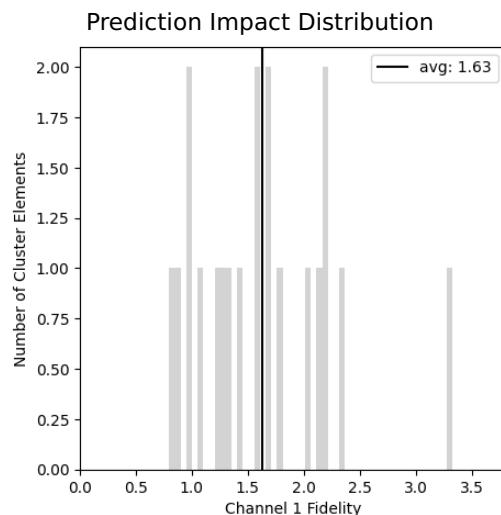
## Properties

ⓘ 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:	20
Channel Index	1.0 (0.0)

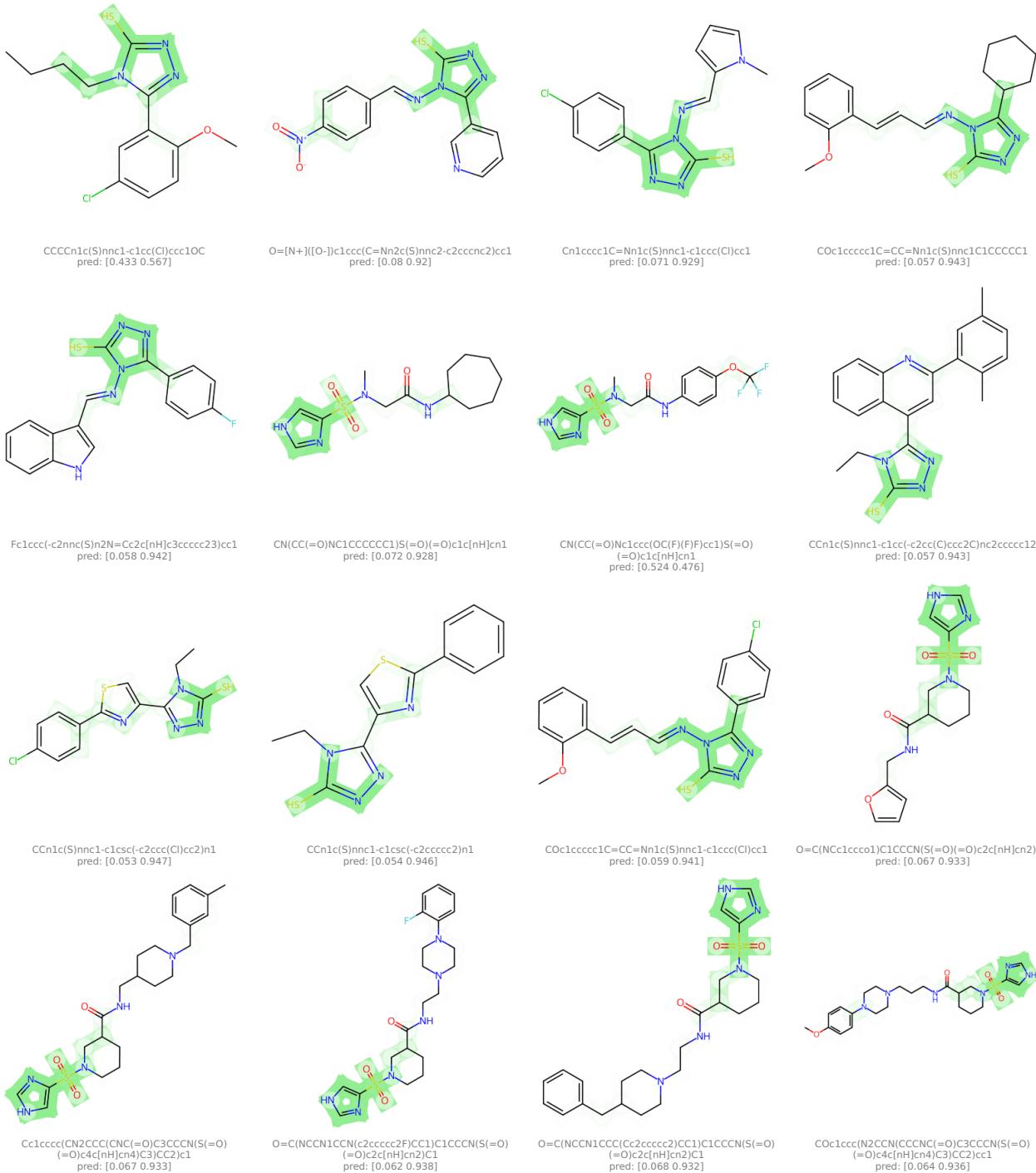
## Member Statistics

ⓘ 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

ⓘ 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 #151 - 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 151, from importance channel 1 (*aggregator*), represents a motif consisting of 8.3 ( $\pm 2.0$ ) nodes. The concept is generally associated with an impact of 2.4 ( $\pm 0.7$ ) on the prediction outcome.

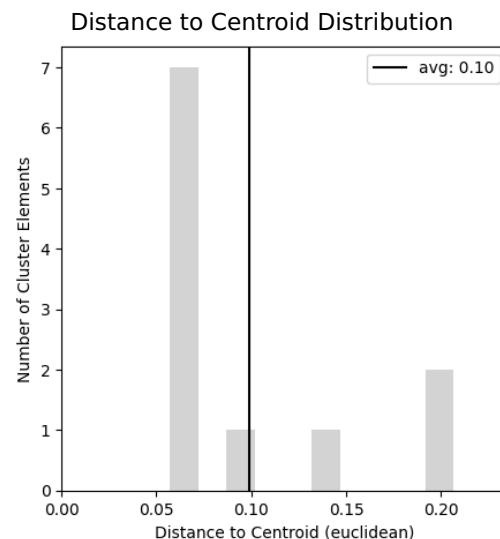
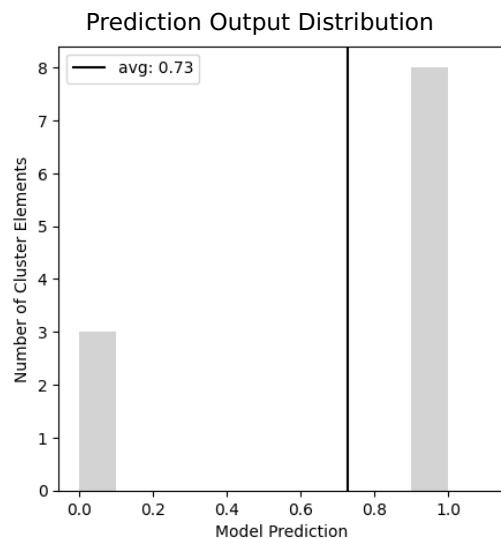
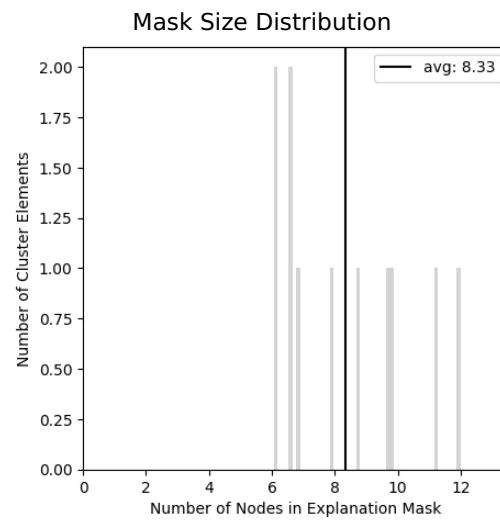
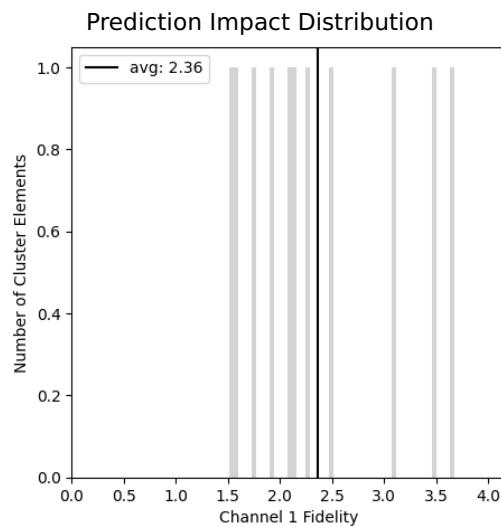
## Properties

ⓘ 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:	11
Channel Index	1.0 (0.0)

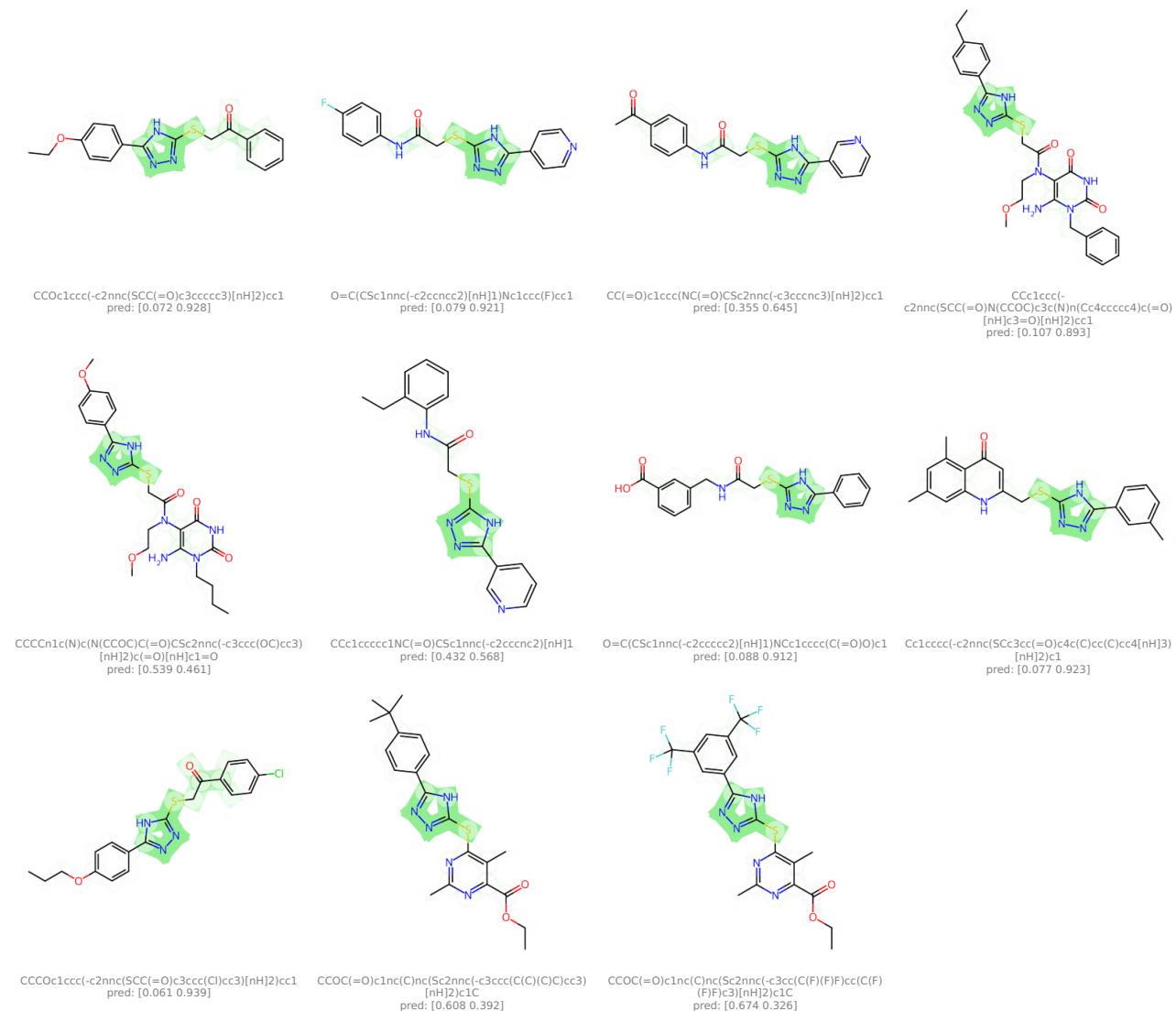
## Member Statistics

ⓘ 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 #152 - 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 152, from importance channel 1 (*aggregator*), represents a motif consisting of  $9.6 (\pm 1.8)$  nodes. The concept is generally associated with an impact of  $1.5 (\pm 0.7)$  on the prediction outcome.

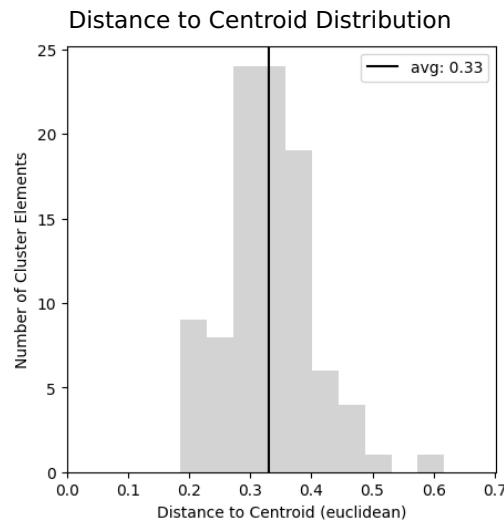
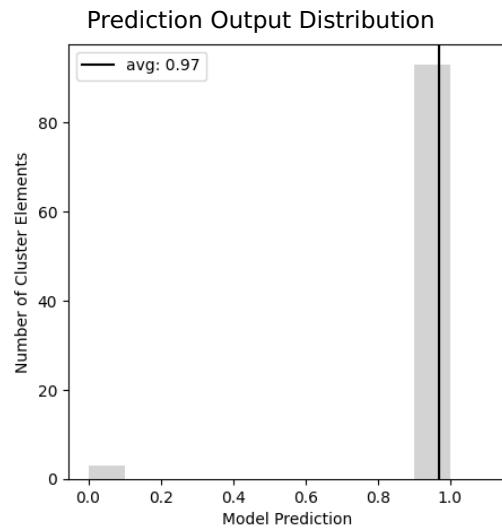
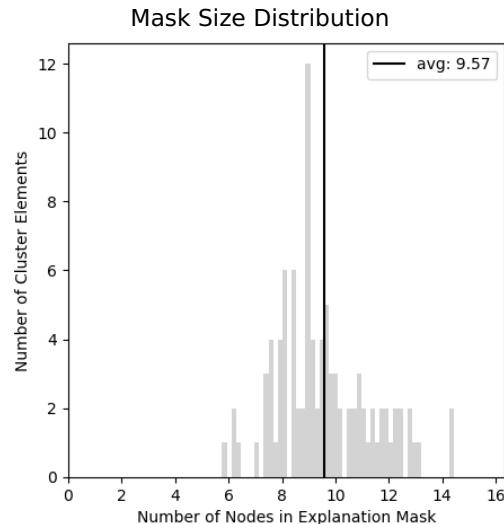
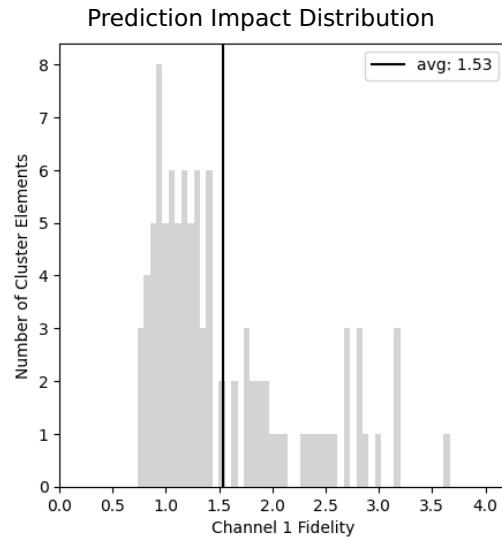
## Properties

ⓘ 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:	96
Channel Index	1.0 (0.0)

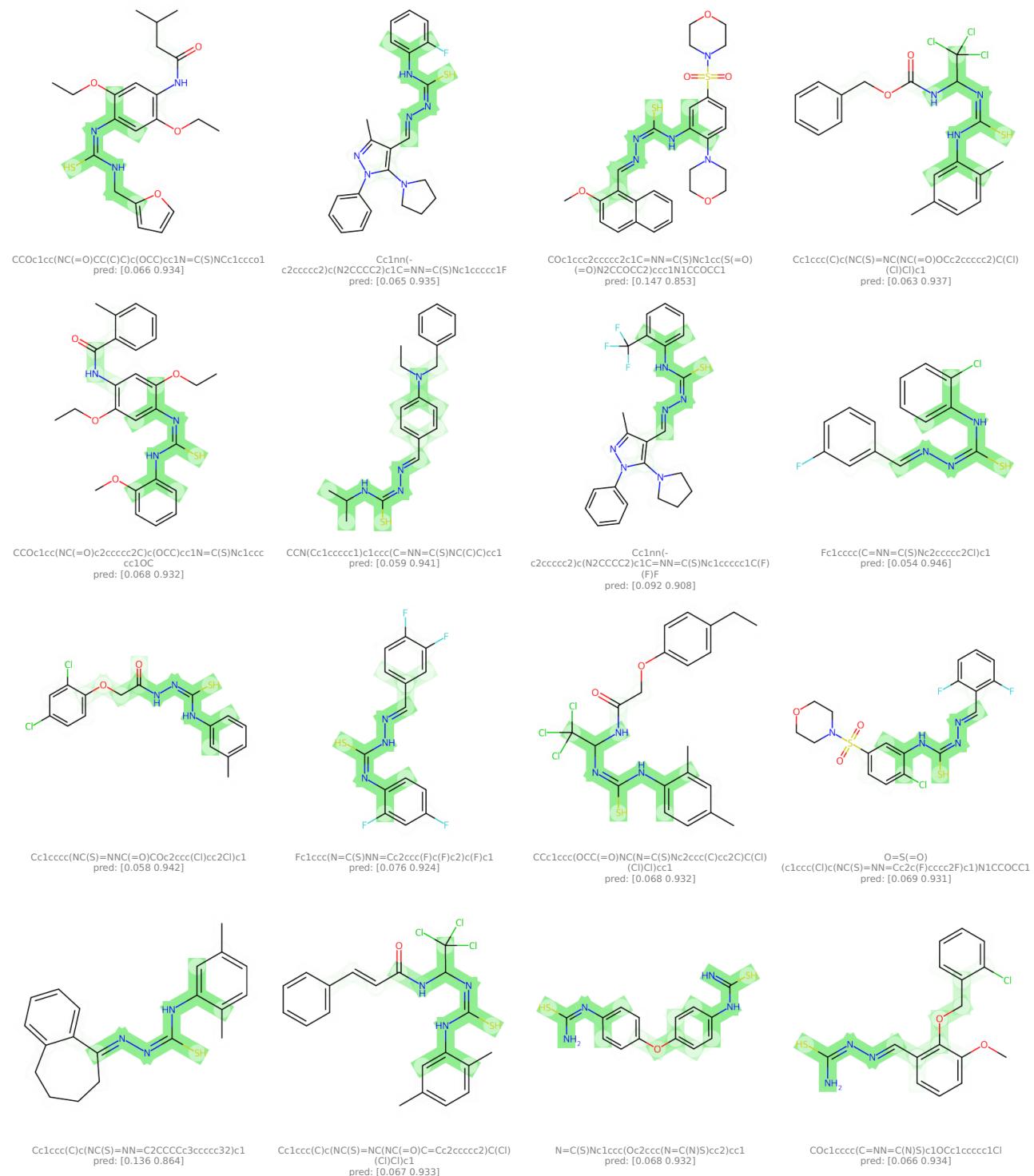
## Member Statistics

ⓘ 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 #153 - 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 153, from importance channel 1 (*aggregator*), represents a motif consisting of 9.0 ( $\pm 1.2$ ) nodes. The concept is generally associated with an impact of 1.7 ( $\pm 0.9$ ) on the prediction outcome.

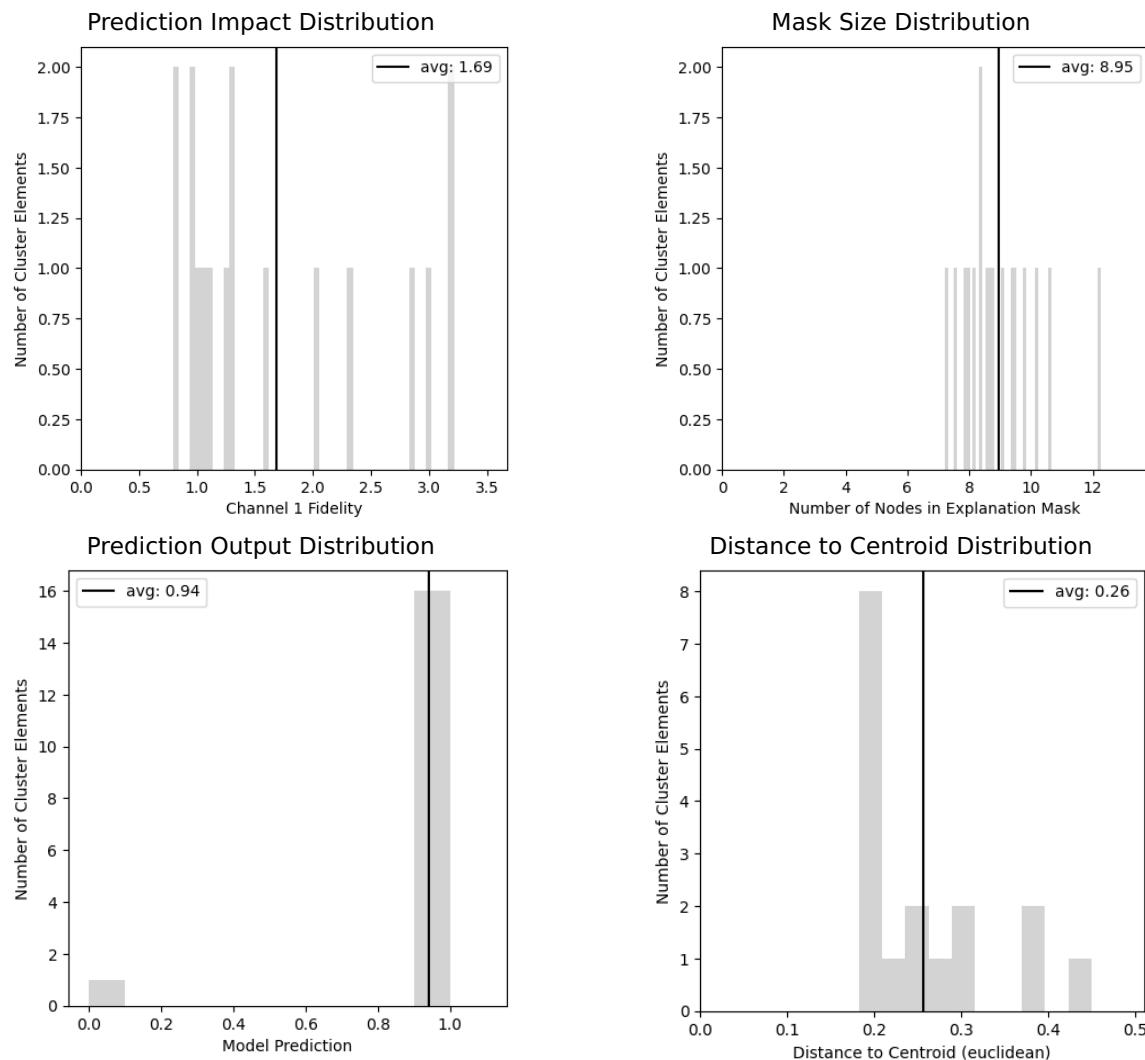
## Properties

ⓘ 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:	17
Channel Index	1.0 (0.0)

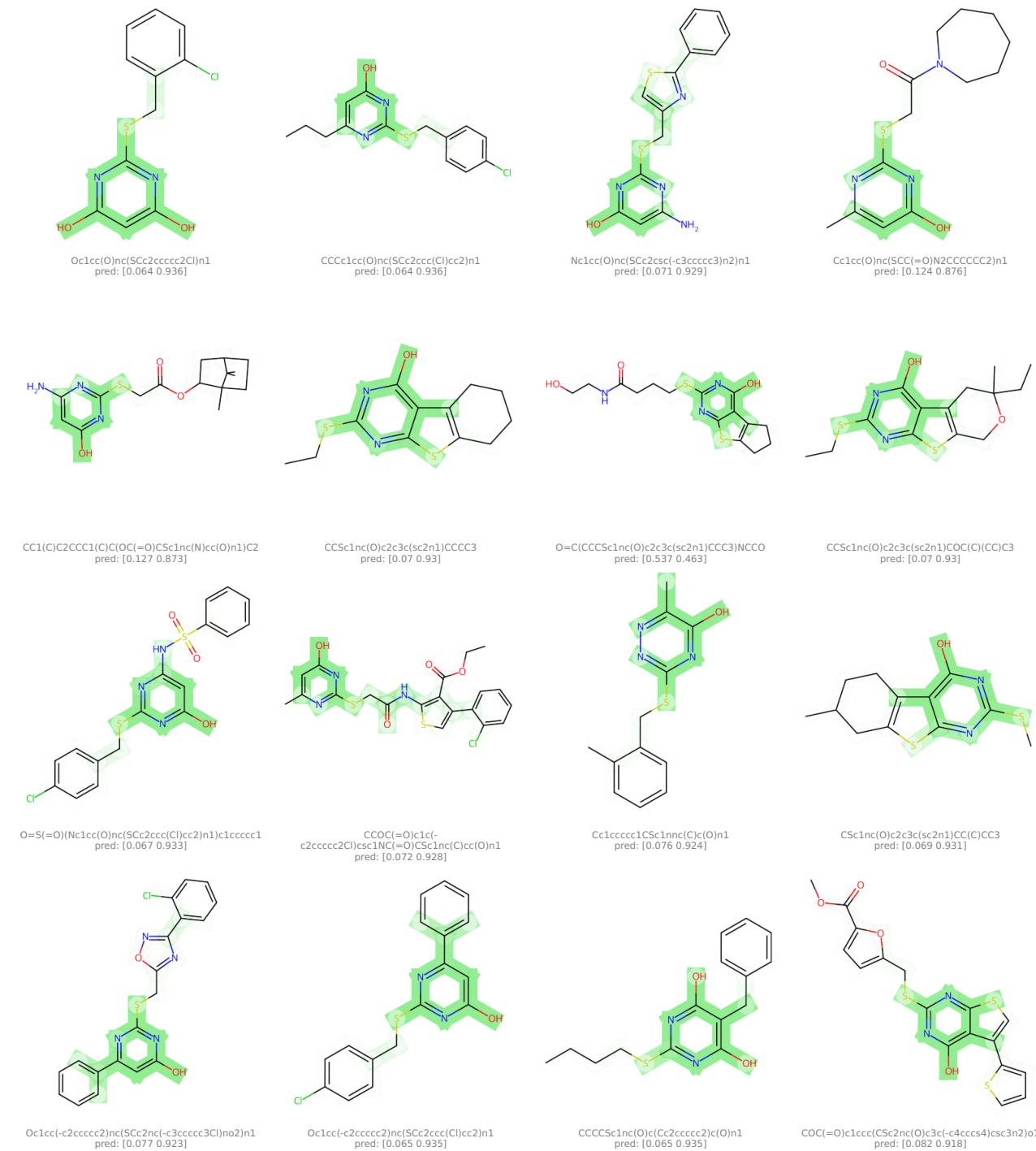
## Member Statistics

ⓘ 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 #154 - 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 154, from importance channel 1 (*aggregator*), represents a motif consisting of **9.1** ( $\pm 0.5$ ) nodes. The concept is generally associated with an impact of **1.6** ( $\pm 1.0$ ) on the prediction outcome.

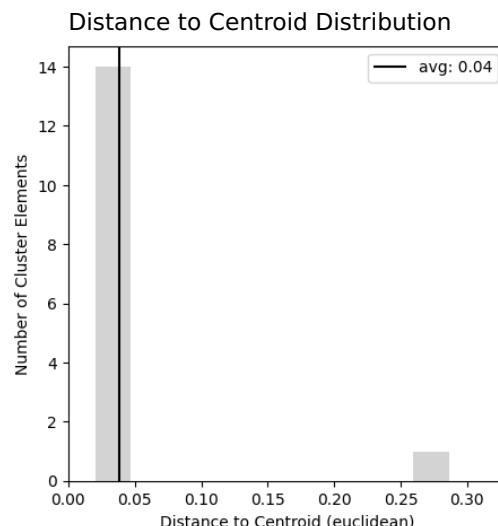
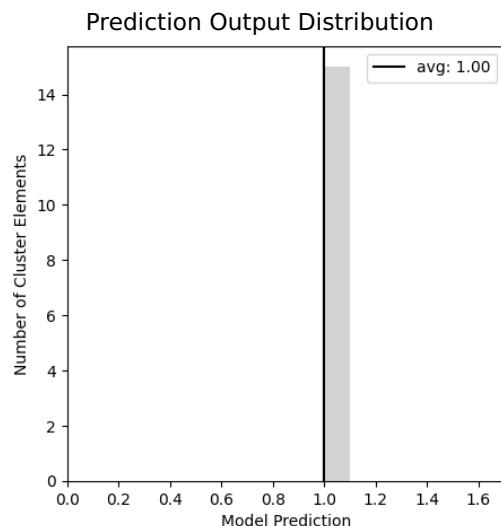
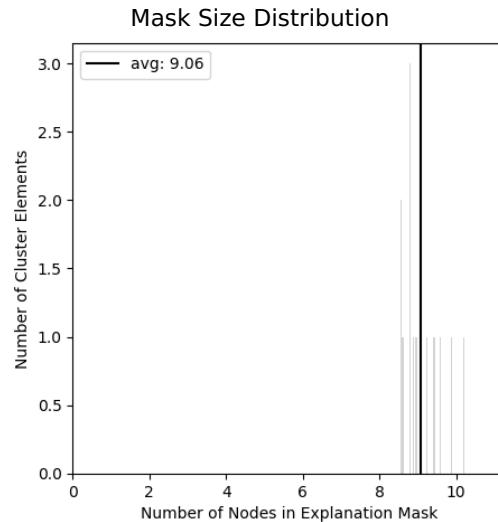
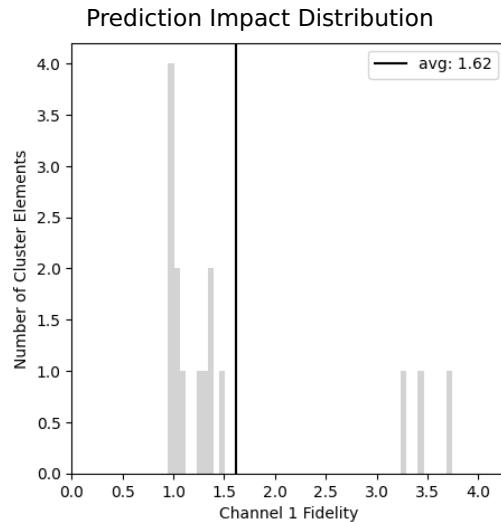
## Properties

ⓘ 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:	15
Channel Index	1.0 (0.0)

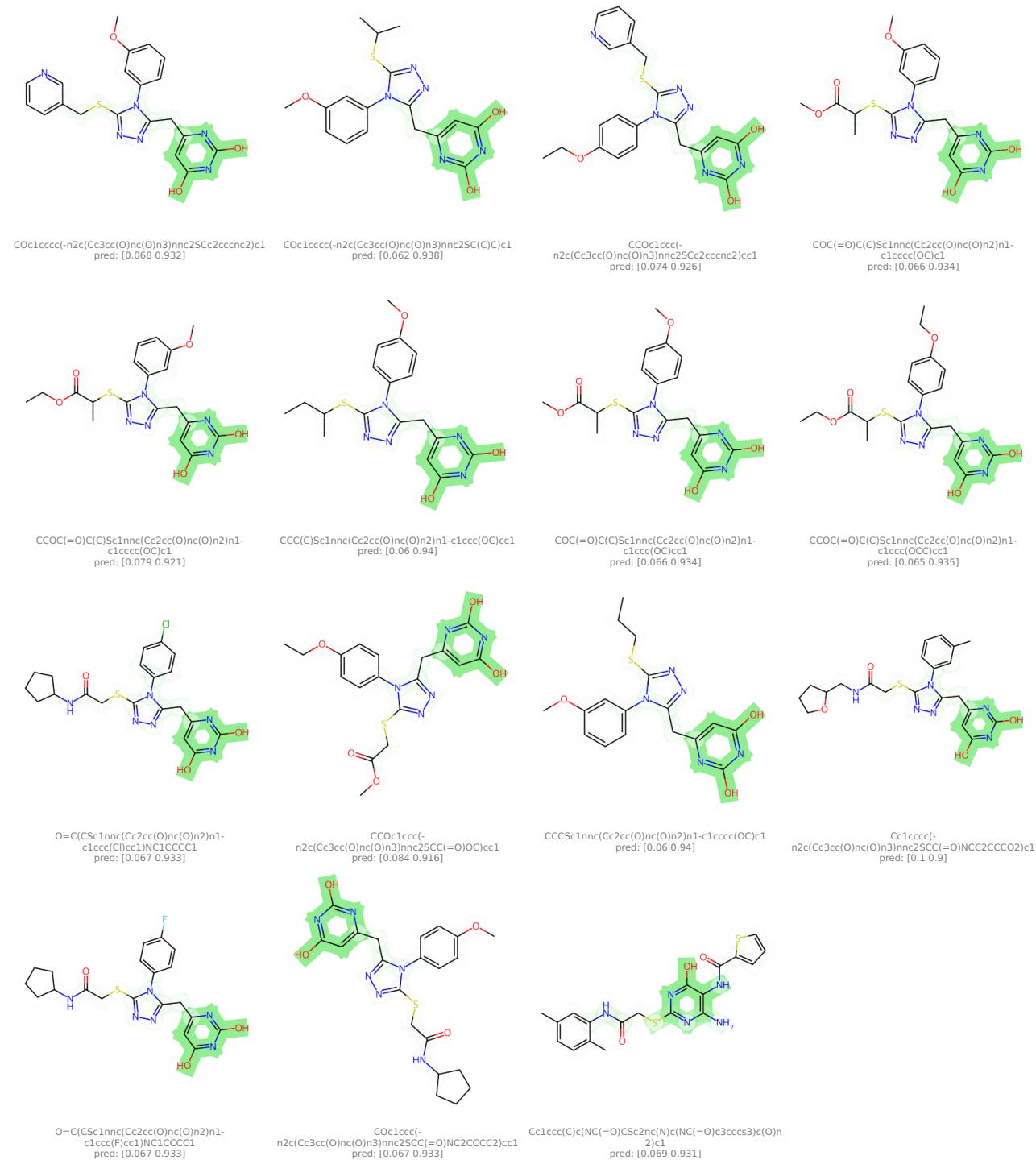
## Member Statistics

ⓘ 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 #155 - 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 155, from importance channel 1 (*aggregator*), represents a motif consisting of 9.3 ( $\pm 1.7$ ) nodes. The concept is generally associated with an impact of 1.9 ( $\pm 0.8$ ) on the prediction outcome.

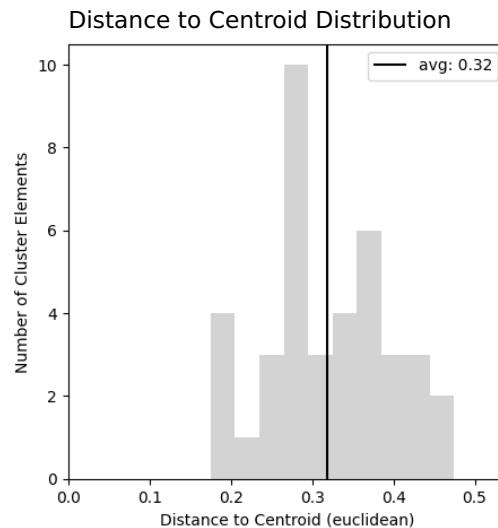
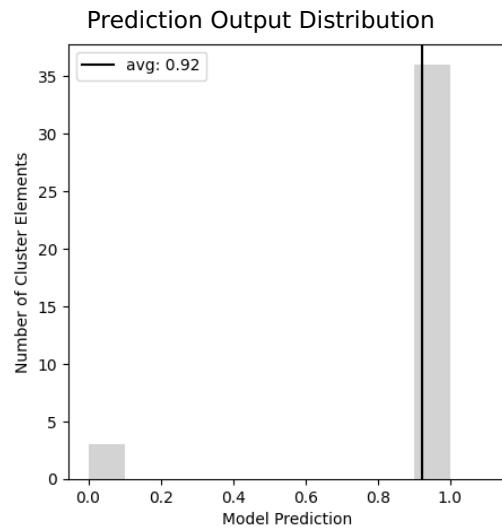
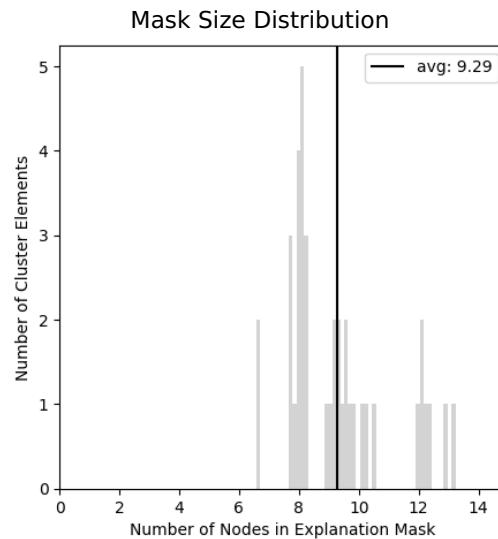
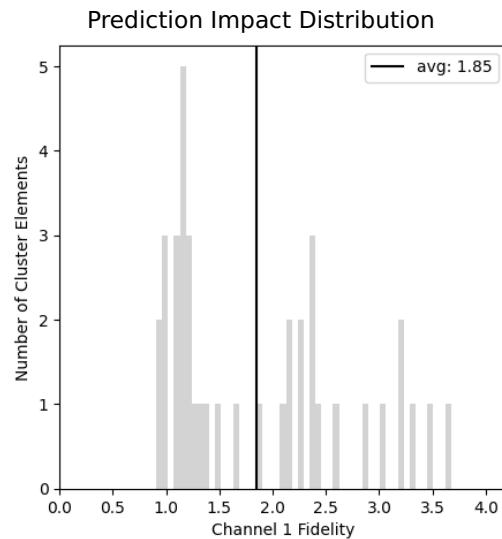
## Properties

ⓘ 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:	39
Channel Index	1.0 (0.0)

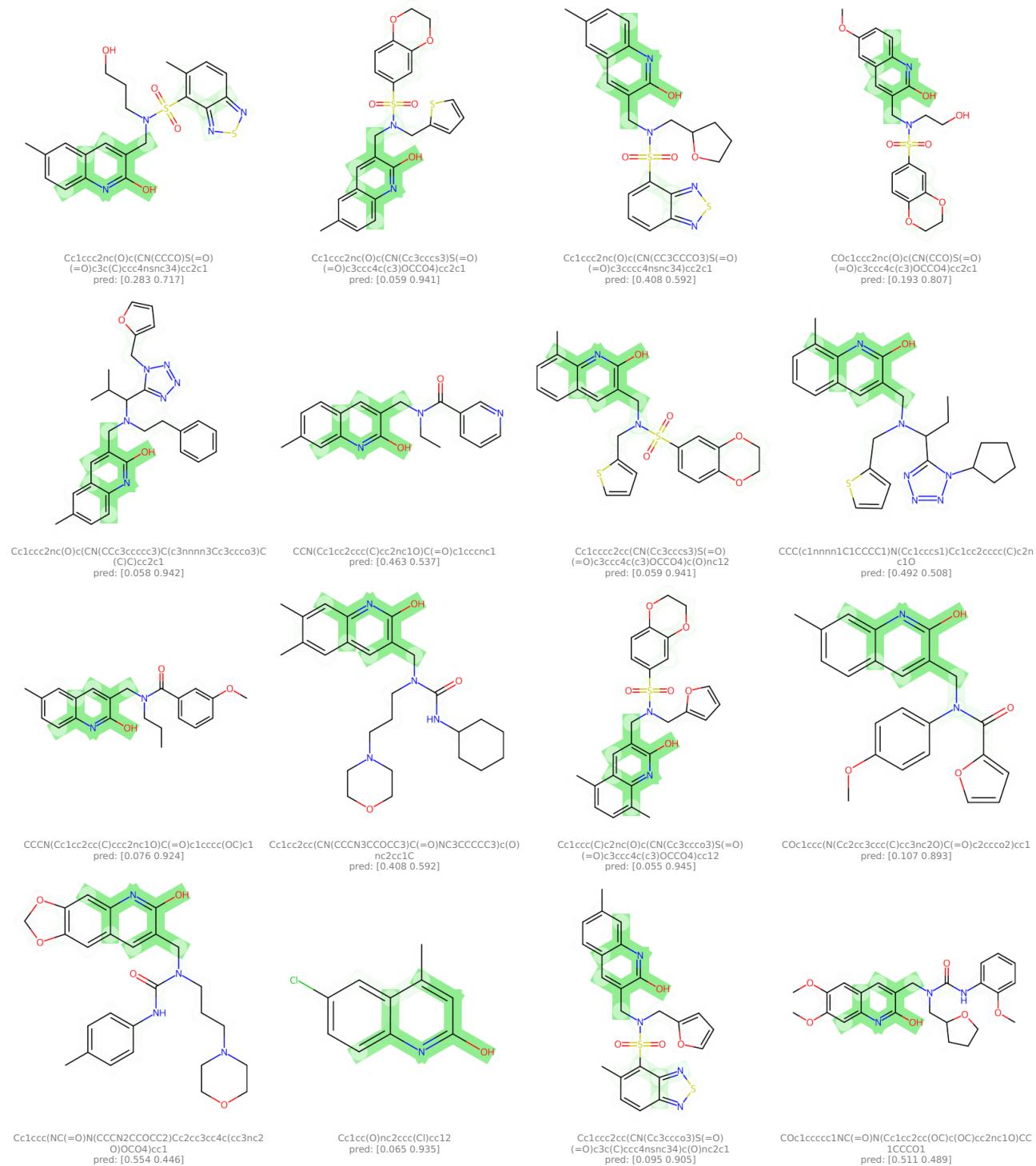
## Member Statistics

ⓘ 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 #156 - 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 156, from importance channel 1 (*aggregator*), represents a motif consisting of 8.4 ( $\pm 2.4$ ) nodes. The concept is generally associated with an impact of 2.4 ( $\pm 1.0$ ) on the prediction outcome.

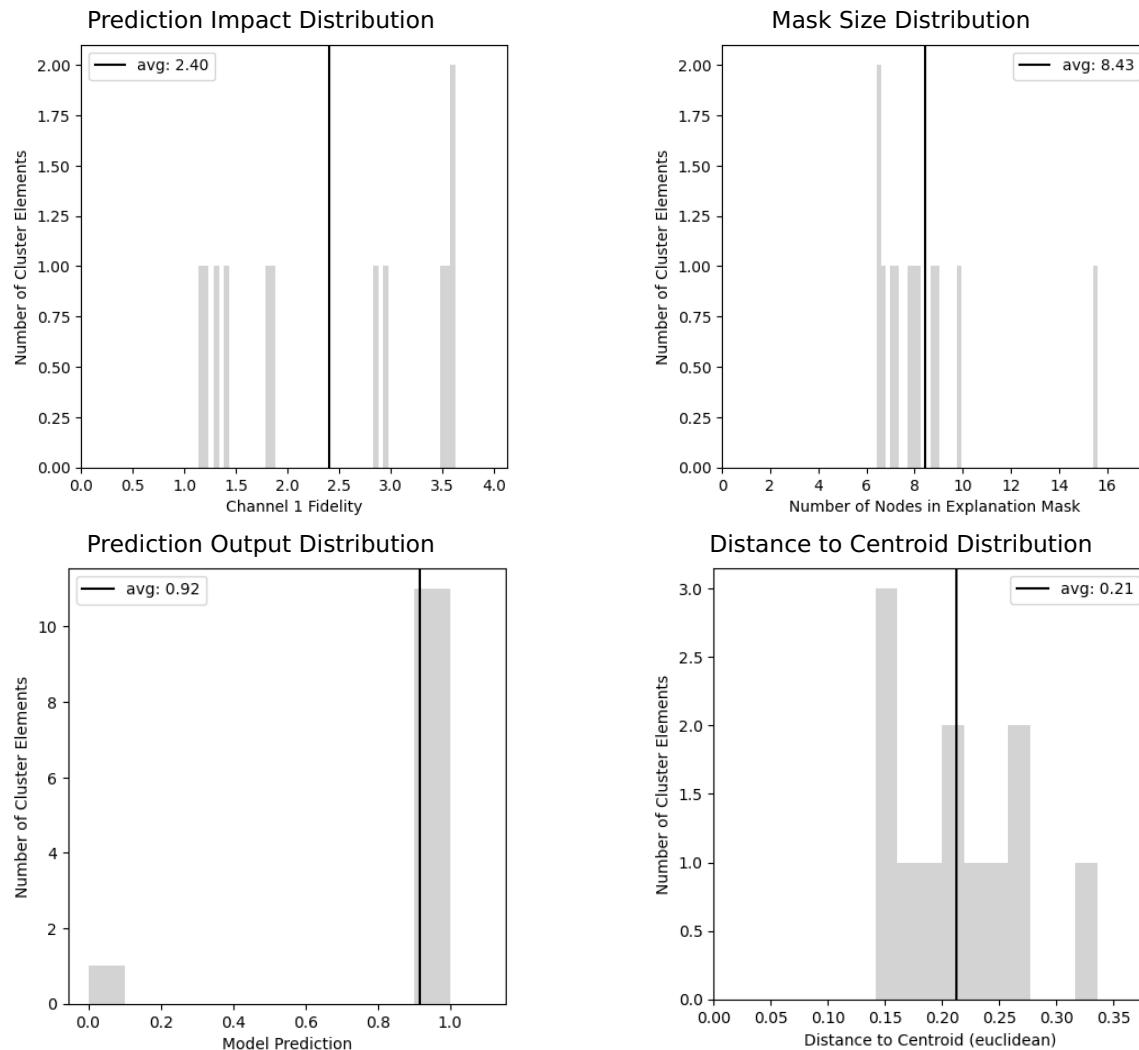
## Properties

ⓘ 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:	12
Channel Index	1.0 (0.0)

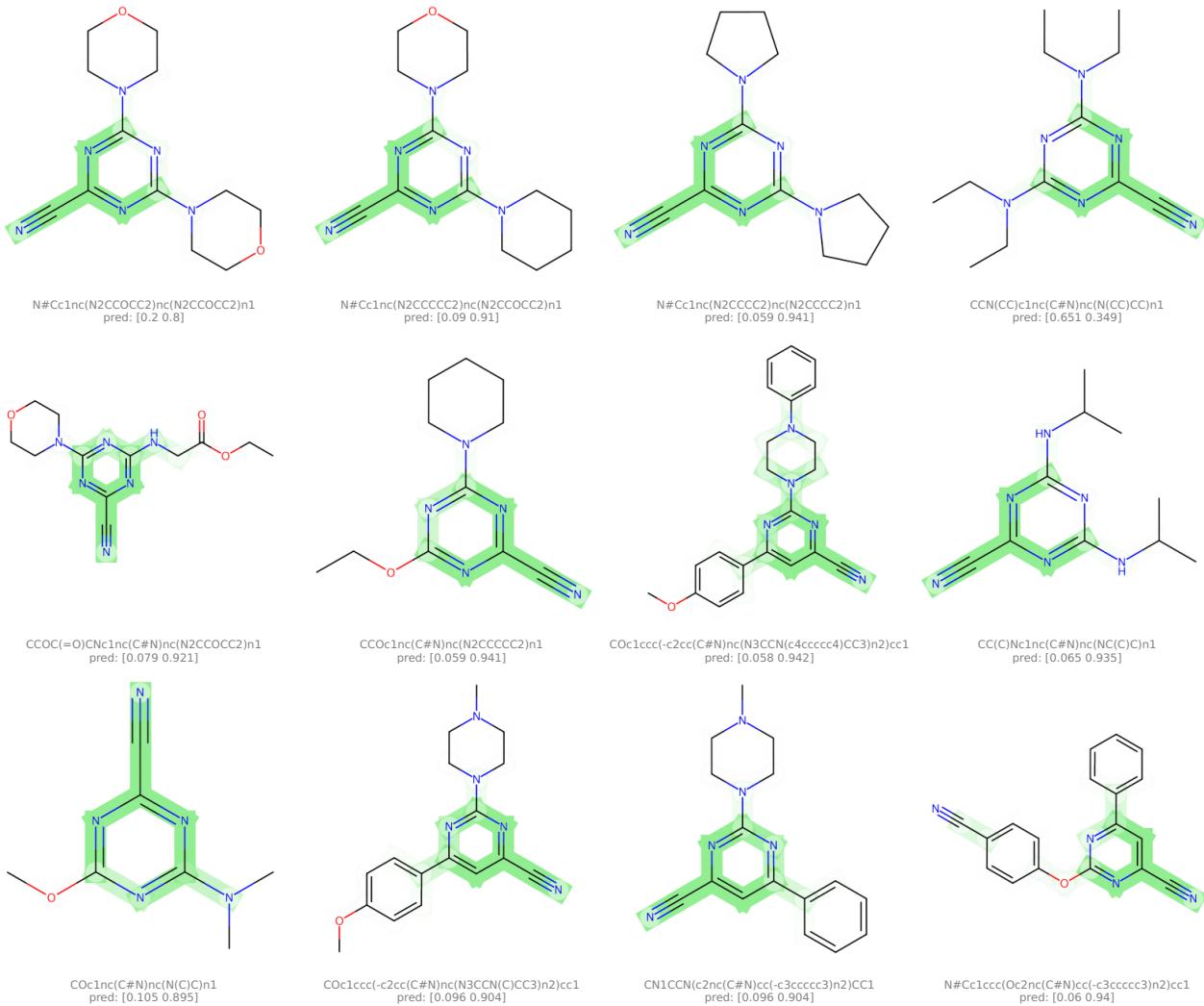
## Member Statistics

ⓘ 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 #157 - 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 157, from importance channel 1 (*aggregator*), represents a motif consisting of 9.1 ( $\pm 1.9$ ) nodes. The concept is generally associated with an impact of 1.7 ( $\pm 0.9$ ) on the prediction outcome.

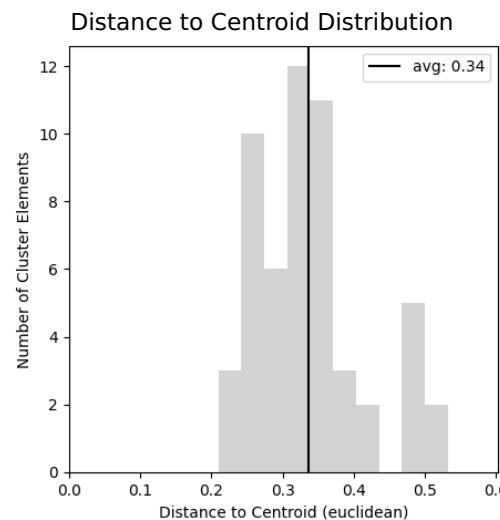
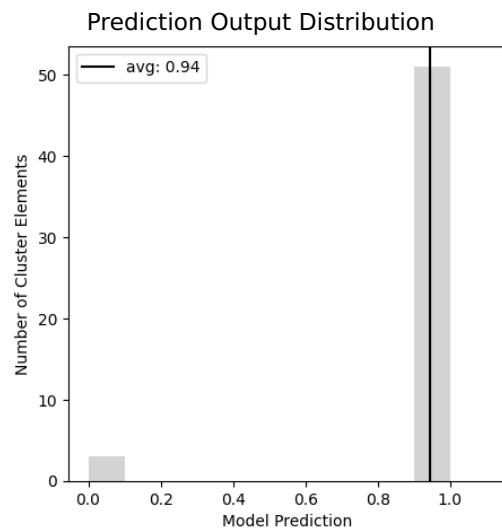
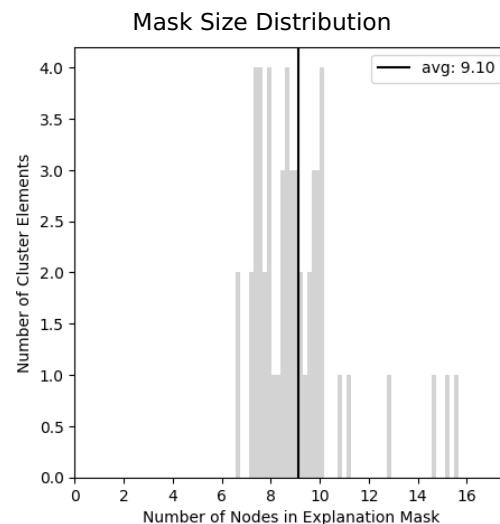
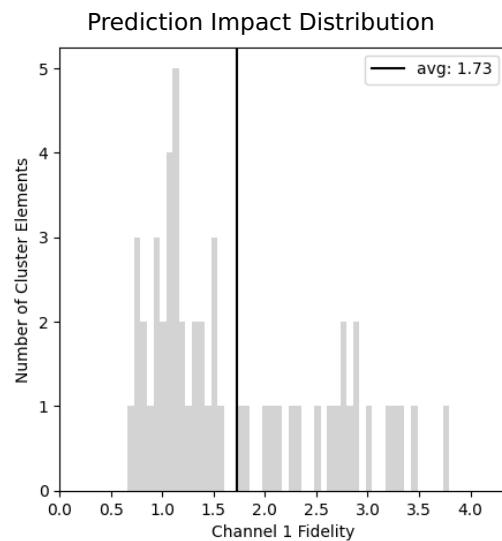
## Properties

ⓘ 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:	54
Channel Index	1.0 (0.0)

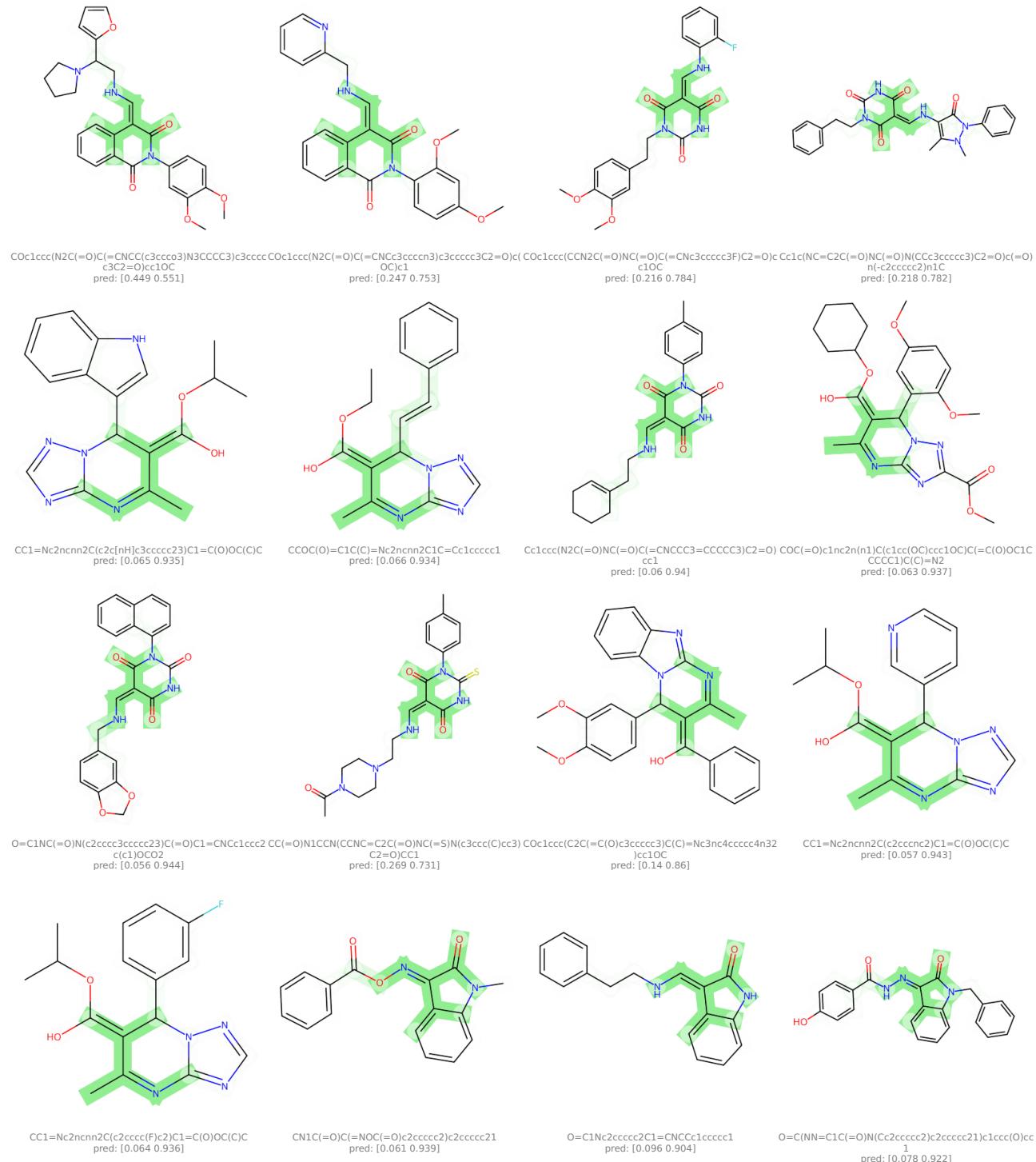
## Member Statistics

ⓘ 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 #158 - 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 158, from importance channel 1 (*aggregator*), represents a motif consisting of  $9.6 (\pm 1.2)$  nodes. The concept is generally associated with an impact of  $2.5 (\pm 0.8)$  on the prediction outcome.

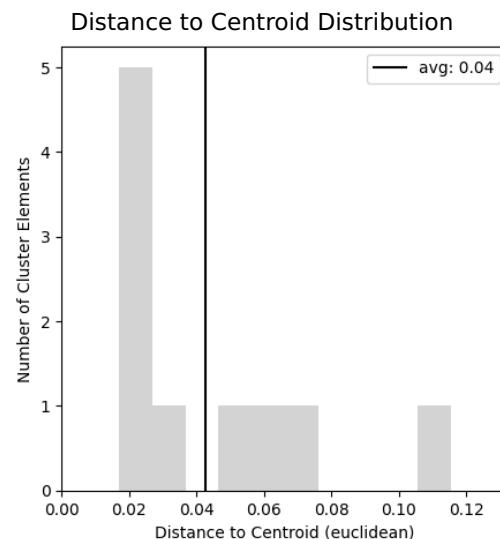
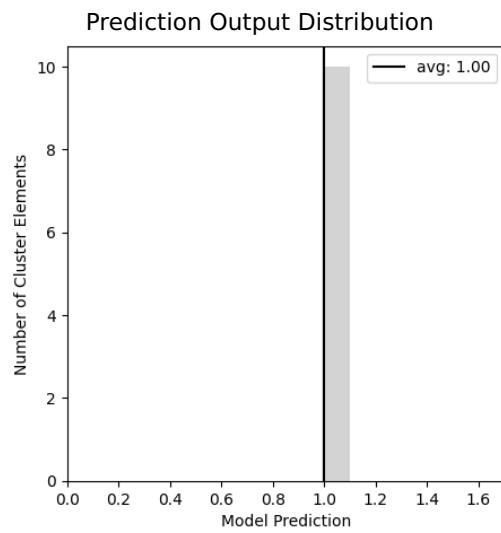
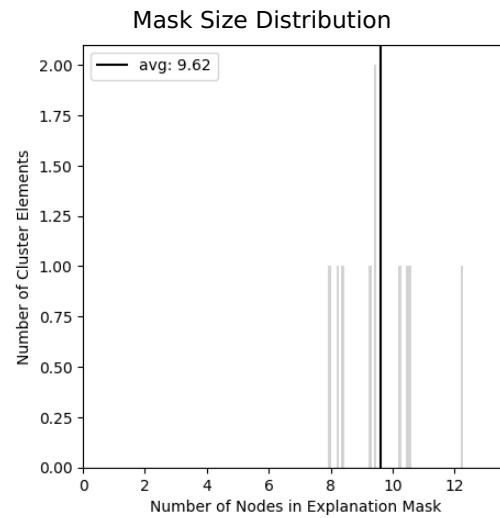
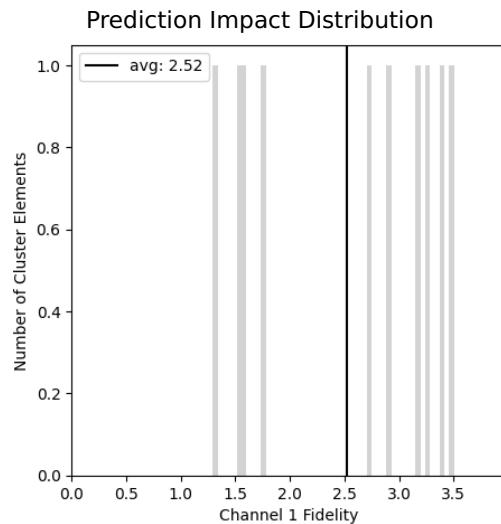
## Properties

ⓘ 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:	10
Channel Index	1.0 (0.0)

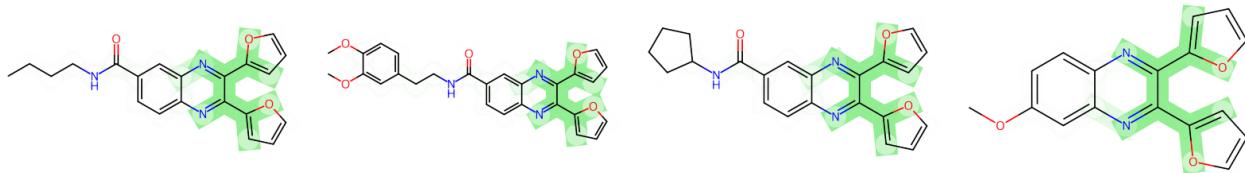
## Member Statistics

ⓘ 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.

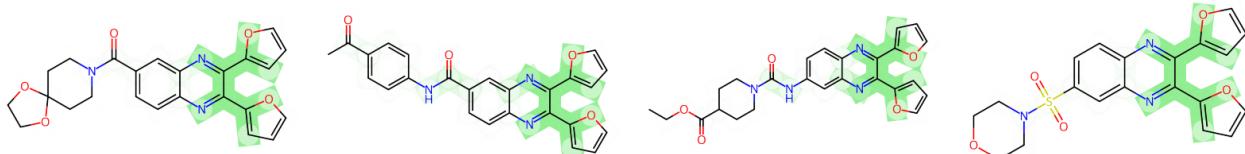


CCCCNC(=O)c1ccc2nc(-c3ccco3)c(-c3ccco3)nc2c1  
pred: [0.125 0.875]

COc1ccc(CCNC(=O)c2ccc3nc(-c4ccco4)c(-c4ccco4)nc3c2)cc1OC  
pred: [0.091 0.909]

O=C(NC1CCCC1)c1ccc2nc(-c3ccco3)c(-c3ccco3)nc2c1  
pred: [0.076 0.924]

COc1ccc2nc(-c3ccco3)c(-c3ccco3)nc2c1  
pred: [0.078 0.922]

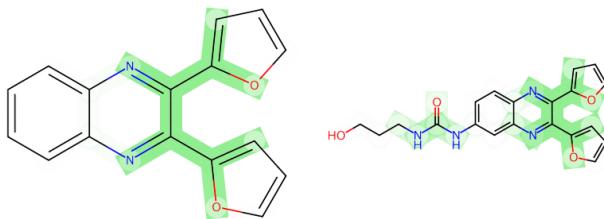


O=C(c1ccc2nc(-c3ccco3)c(-c3ccco3)nc2c1)N1CCC2(CC1)OCCO2  
pred: [0.177 0.823]

CC(=O)c1ccc(CCNC(=O)c2ccc3nc(-c4ccco4)c(-c4ccco4)nc3c2)cc1  
pred: [0.109 0.891]

CCOC(=O)C1CCN(C(=O)Nc2ccc3nc(-c4ccco4)c(-c4ccco4)nc3c2)CC1  
pred: [0.09 0.91]

O=S(=O)(c1ccc2nc(-c3ccco3)c(-c3ccco3)nc2c1)N1CCOCC1  
pred: [0.055 0.945]



c1coc(-c2nc3cccc3nc2-c2ccco2)c1  
pred: [0.074 0.926]

O=C(NCCCO)Nc1ccc2nc(-c3ccco3)c(-c3ccco3)nc2c1  
pred: [0.143 0.857]