# QSAR model for Glucocorticoid Receptor (GR) antagonism (v1.0)

ProtoED by ProtoQSAR

## ProtoED

ProtoED is a computational tool designed to predict whether a compound will act as an agonist or antagonist on various hormonal receptors, facilitating the assessment of the compound's potential to disrupt the endocrine system.

By employing QSAR models, ProtoED offers an efficient alternative to experimental assays by enabling rapid and accurate predictions of compound-receptor interactions, serving as a valuable tool in chemical and pharmacological research.

This module promotes the use of alternative methods, helping to reduce the need for *in vivo* testing and supporting decision-making processes regarding potential risks to human health and the environment.

## Endpoint

**Human health effects: Glucocorticoid receptor antagonism.**

The glucocorticoid receptor (GR) is an evolutionarily conserved nuclear receptor superfamily protein that mediates the diverse actions of glucocorticoids as a ligand-dependent transcription factor. This receptor is a protein that shuttles from the cytoplasm to the nucleus upon binding to its ligand glucocorticoid hormone, where it modulates the transcription rates of glucocorticoid-responsive genes positively or negatively. Glucocorticoid receptor antagonism occurs when compounds bind to the GR but do not activate it, thereby preventing the effects of endogenous glucocorticoids. This antagonism can be used therapeutically but may also disrupt homeostatic regulation of inflammation and metabolism.

## Metrics

### Training set

| Experimental values | QSAR predictions | |
|---|---|---|
| | **inactive** | **antagonist** |
| **inactive** | 1331 | 114 |
| **antagonist** | 159 | 1277 |

### Validation set

| Experimental values | QSAR predictions | |
|---|---|---|
| | **inactive** | **antagonist** |
| **inactive** | 436 | 46 |
| **antagonist** | 74 | 405 |

| Parameters | Training | Validation |
|---|---|---|
| Accuracy | 0.91 | 0.88 |
| Sensitivity / recall | 0.89 | 0.85 |
| Specificity | 0.92 | 0.90 |
| Precision | 0.92 | 0.90 |
| Negative predictive value | 0.89 | 0.85 |
| F-score | 0.90 | 0.87 |
| Matthews Correlation Coefficient | 0.81 | 0.75 |
| Critical Success Index | 0.82 | 0.77 |
| Area under the ROC | 0.91 | 0.88 |