Generating structural alerts from toxicology datasets using the local interpretable model-agnostic explanations method

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Supplementary Material

Sampling process

The data points are created around the instance of interest using a Gaussian distribution. This sampling process is designed to generate perturbed samples, which are then used to approximate the behavior of the underlying model locally. The locality-awareness in LIME refers to the fact that the explanation generated by LIME focuses on the local behavior of the model around a specific instance. By sampling data points in the vicinity of the instance of interest, LIME captures the local decision boundaries and feature importance. Regarding the distances between samples and perturbed samples, LIME does not directly utilize the Gaussian distance between their features. Instead, it perturbs the features of the original instance by sampling from the Gaussian distribution and creates synthetic samples. These synthetic samples are then used to approximate the behavior of the model in the local neighborhood of the instance. The distances between the perturbed samples and the original instance are typically measured using a similarity metric, such as the Euclidean distance or cosine similarity, depending on the nature of the features. The choice of distance metric depends on the specific implementation and the type of data being analyzed.

In LIME, the perturbation process involves generating 5000 synthetic samples by perturbing a maximum of 10 input features of a target instance. These perturbations are done by randomly sampling binary values (0 and 1) for each feature according to the training distribution using Gaussian sampling. The goal is to observe how these perturbations affect the model predictions and use them to explain the model behavior locally. To measure the closeness between the target instance and the perturbed samples, a distance metric is used as explained in the previous paragraph. The choice of distance metric depends on the nature of the data. It was chosen here a standard Euclidean distance.

The LimeTabularExplainer class was run in the classification mode. The kernel width for the exponential kernel was set to 0.75 times the squared root of the number of features, which was well stablished by the LIME developers.[1] The kernel width parameter determines the locality of the perturbations applied to the input data. Changing the kernel width can have an impact on the results of LIME in the following ways: 1) local interpretability: a smaller kernel width results in more

local interpretability. When the kernel width is small, LIME focuses on a smaller region around each instance to generate perturbed samples. This can lead to more precise and fine-grained explanations specific to the local behavior of the model; 2) sensitivity to noise: decreasing the kernel width makes LIME more sensitive to noise in the data. As the perturbations become more localized, any noise present in the dataset may have a greater influence on the explanation. This can lead to less stable or reliable explanations if the data contains noisy or irrelevant features; 3) coverage of global patterns: increasing the kernel width allows LIME to capture larger-scale patterns in the data. A wider kernel considers a larger neighborhood around each instance, which can help identify global trends and dependencies in the model behavior. This may be useful when the model relies on broader contextual information that is not the situation presented in this study; 4) computational efficiency: The choice of kernel width can affect the computational efficiency of LIME. A smaller kernel width requires generating a larger number of perturbed samples to adequately cover the local neighborhood, increasing the computational cost. Conversely, a wider kernel may require fewer samples, resulting in faster computation. The selection of the kernel width in LIME depends on the specific characteristics of the data, the complexity of the model, and the desired level of interpretability. It is often a hyperparameter that needs to be tuned through experimentation to achieve the most meaningful and reliable explanations for the given scenario.[2] For sake of checking consistency and reliability, the explanation was tested with the kernel width of 3, 10, 16, and 22.

For the categorical features found in this study, the procedure perturbs by sampling according to the training distribution, and making a binary feature that is 1 when the value is the same as the instance being explained. The categorical features are discretized into quartiles. For classifiers, the prediction function outputs prediction probabilities that produce explanations for the label with the highest prediction probability. In the explain_instance class, it generates explanations for a prediction. It was generated neighborhood data by randomly perturbing features from the instance as mentioned previously. Then, locally weighted linear models are learnt on this neighborhood data to explain each of the samples in an interpretable way.

The loss function used in LIME can vary depending on the application and the surrogate model being used. LIME finds a local linear model that approximates the behavior of the underlying complex model. The loss function typically tries to minimize the difference between the predictions of the linear model and the predictions of the complex model for the perturbed samples. In LIME, the choice of loss function depends on the specific application and the surrogate model being used. The loss function is designed to approximate the behavior of the complex model being explained and to find a local linear model that mimics its predictions. In this study, the binary cross-entropy loss is typically used when the predictions of the complex model involve probability distributions, such as in binary classification tasks. It calculates the distance between the predicted probabilities of the surrogate model and the true probabilities obtained from the complex model. The surrogate model in LIME is chosen to be a decision tree because it is interpretable and should be able to approximate the behavior of the original model. This model is relatively simple and allows easy interpretation of the relationship between the input features and the predictions.

The overall process of LIME can be summarized as follows:

1. Select a target instance for which you want to explain the model prediction.

2. Perturb the features of the target instance by sampling binary values according to the training distribution, generating synthetic samples.

3. Calculate the distances between the target instance and the perturbed samples using a chosen distance metric.

4. Assign weights to the perturbed samples based on their distances, with closer samples receiving higher weights.

5. Train a surrogate model using the perturbed samples and their corresponding predictions from the original complex model.

6. Interpret the surrogate model to understand the importance and contribution of different features towards the model prediction for the target instance.

For a given task, LIME performs a data perturbation creating a new dataset around the observation by sampling the distribution generated from the training. In this dataset, features are selected based on this distribution and categorical

values based on its frequency of appearance. Then, the distance is calculated between perturbation and original data. The model predicts the probability on new data and select the m features that best describes the model output from the perturbed data. Finally, a linear model is fit on data with m dimensions weighted by similarity and the weights of this linear model are used as explanation.

After generating a model, LIME explains the training data with categorical values and feature names using the LimeTabularExplainer function in the classification mode. The categorical names are input as a dictionary that maps the categorical features to their values using a list of indexes of categorical features. The usage, input, and output of these function is shown below:

```python
from lime import lime_tabular
feature_names = ["fp_%s"  % x for x in range(1024)]
explainer = lime_tabular.LimeTabularExplainer(train_dataset.X,
                                              feature_names=feature_names,
                                              categorical_features=feature_names,
                                              class_names=['not toxic', 'toxic'],
                                              discretize_continuous=True)
```

In this way, the explainer object is created for LIME that takes the training dataset and names for the features as circular fingerprints using the fp_mol function as follows:

```python
def fp_mol(mol, fp_length=1024):
    d = {}
    feat = dc.feat.CircularFingerprint(sparse=True, smiles=True, size=1024)
    retval = feat._featurize(mol)
    for k, v in retval.items():
        index = k % fp_length
        if index not in d:
            d[index] = set()
        d[index].add(v['smiles'])
    return d
```

This fp_mol function returns a dictionary mapping the fingerprint index to the list of SMILES strings that activated that fingerprint. As there are not natural names for our features, they are just numbered in the feature_names object. The class names of the Tox21 dataset are toxicity assays, so they are called 0 as "not toxic" and 1 as "toxic".

The evaluation function eval_model(model, i) is used for each molecule to attempt to explain why the model predicts a molecule to be toxic for each task i. This function takes a 2d numpy array (samples, features) and returns predictions (samples) as follows:

```python
def eval_model(my_model,i):
    def eval_closure(x):
        ds = dc.data.NumpyDataset(x, n_tasks=12)
        predictions = my_model.predict(ds)[:,i]
        return predictions
    return eval_closure
```

The output is stored in the model_fn object and the list of toxic molecules in the test set that is correctly predicted to be toxic is obtained with a threshold of 0.8 as in the following:

```python
for i in range(12):
    model_fn = eval_model(model,i)
    lista_active_id = np.where((test_dataset.y[:,i] == 1) * (model.predict(test_dataset)[:,0,1] > 0.8))[0]
```

Then, the 12 tasks are looped evaluating the model over the list of toxic molecules in the test set and storing the model in the model_fn object. Then, this list was input with the model_fn object into the explain_instance class to figure out why the molecule was predicted to be toxic. The explainer predicts the most sensitive features to the prediction, i. e., the elements in the fingerprint that correspond to one or more fragments. The output is stored in the exp object that has the information of which fragments contributed to the prediction. The lime.explanation module in the LIME library has visualization and mapping functions that returns the explainers. The as_map() class generates the map of explanations with labels and a list of tuples with the feature id and its weights. This class is used to get this information in a more suitable format for processing. The keys in this map are the labels and the value for each key is a list of tuples with the fingerprint_index and its respective weight that is converted to a dictionary mapping indices to weights as follows:

```
for active_id in lista_active_id:
    exp = explainer.explain_instance(test_dataset.X[active_id],
                                     model_fn, num_features=1024, top_labels=1)

    # What fragments activated what fingerprints in our active molecule?
    my_fragments = fp_mol(Chem.MolFromSmiles(test_dataset.ids[active_id]))
    q = [key for key in exp.as_map().keys()][0]
    map = exp.as_map()[q]
    dic = dict(map)
```

In the my_fragments object, the fragments are present for each molecule of interest, and the fragment_weights object (fragment_weight = dict(exp.as_map()[1])) contains which fragments contributed to the prediction. All this information is printed as follows:

```
for index in my_fragments:
    if index in fragment_weight:
        print(index, my_fragments[index], fragment_weight[index])
```

The weights are assigned by LIME and represent the contribution of a fragment in a molecule to the prediction in a value from 0 up to (-1) or (+1). However, the sum of these weights for each molecule is not necessarily equal to 1. The weights are still the contribution of a fragment to the prediction. Each molecule has many fragments and each of its fragments contributes positively (positive weight) or negatively (negative weight) to the toxicity prediction. It may be possible that a single molecule has some fragments with a positive contribution to the prediction and others that do not. So, a molecule is classified as "toxic" or "non-toxic" by the model by separately summing all the positive and negative contributions to find out if the sum of the positive weights is greater than the sum of the negative weights, or not. If the final balance of the sum resulted in negative numbers, when considering all the toxicity weight contributions of their respective fragments, it means that the negative contributions of some fragments are larger than the positive contributions. Therefore, based on this fact, the molecule in question is considered "non-toxic" because the absolute value of the sum of negative weights is larger than the absolute value of the sum of positive weights.

References

1. M. T. Ribeiro, S. Singh and C. Guestrin, arXiv, 2016, preprint, arXiv:1602.04938, DOI: 10.48550/arXiv.1602.04938.

2. V. Giorgio, B. Enrico, C. Frederico, arXiv, 2020, preprint, arXiv: 2006.05714, DOI: 10.48550/arXiv.2006.05714

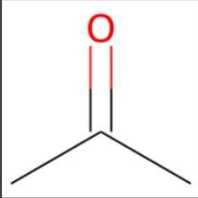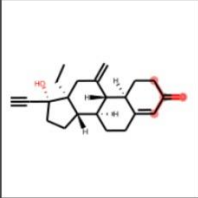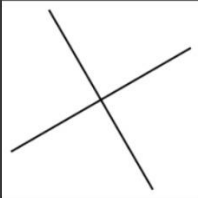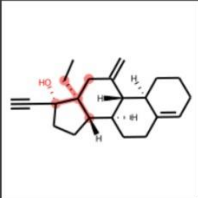**Table S1.** Number of molecules classified as toxic or non-toxic for each task.

Task	Clintox		Sider	
	Toxic	Non-toxic	Toxic	Non-toxic
NR-AR	74	0	62	0
NR-AR-LBD	56	5	46	1
NR-AhR	5	1	3	2
NR-Aromatase	2	3	2	1
NR-ER	35	4	28	7
NR-ER-LBD	25	2	21	3
NR-PPAR-γ	0	0	0	0
SR-ARE	10	7	9	5
SR-ATAD5	3	2	1	0
SR-HSE	3	0	1	0
SR-MMP	15	4	10	2
SR-p53	7	2	4	1

Table S2. Classification of Clintox molecules for task 11 (SR-p53).

SR-p53

Task	Molecule Index	Molecule Id	Result	Toxicity	Non-Toxicity
11	101	Nc1ccc(N=Nc2ccccc2)c(N)n1	YES	0,37141	-0,183608804
11	190	C[C@]12CC[C@@H]3c4ccc(O)	YES	0,488552	-0,488239442
11	191	C[C@]12CC[C@@H]3c4ccc(O)	YES	0,494497	-0,459122147
11	192	C[C@]12CC[C@@H]3c4ccc(O(	YES	0,885043	-0,615036074
11	193	C#C[C@]1(O)CC[C@H]2[C@@	NO	0,540393	-0,610418354
11	199	C[C@]12CC[C@H]3[C@@H](C	YES	0,810673	-0,635185453
11	216	C[C@]1(O)CC[C@H]2[C@@H]:	NO	0,74109	-0,74994214
11	252	CC#C[C@]1(O)CC[C@H]2[C@(	YES	1,072263	-1,001839159
11	569	COC(=O)Nc1nc2cc(C(=O)c3ccc	YES	0,664281	-0,304463491

YES	7	78%
NO	2	22%

Table S3. Contribution of toxicity of two fragments against the NR-AR task using the Sider dataset. The quantity is the counting frequency of appearance after running the LIME method.

Task	Fragment SMILES		Quantity	ROMol	Total Weight		Active Molecules	Highlight First Active Molecule
0	CC(C)=O		54		3.266208	[3, 14, 15, 110, 116, 118, 153, 189, 190, 213,...		
	CC(C)(C)C		87		3.158524	[2, 3, 14, 14, 15, 15, 39, 40, 110, 110, 116, ...		
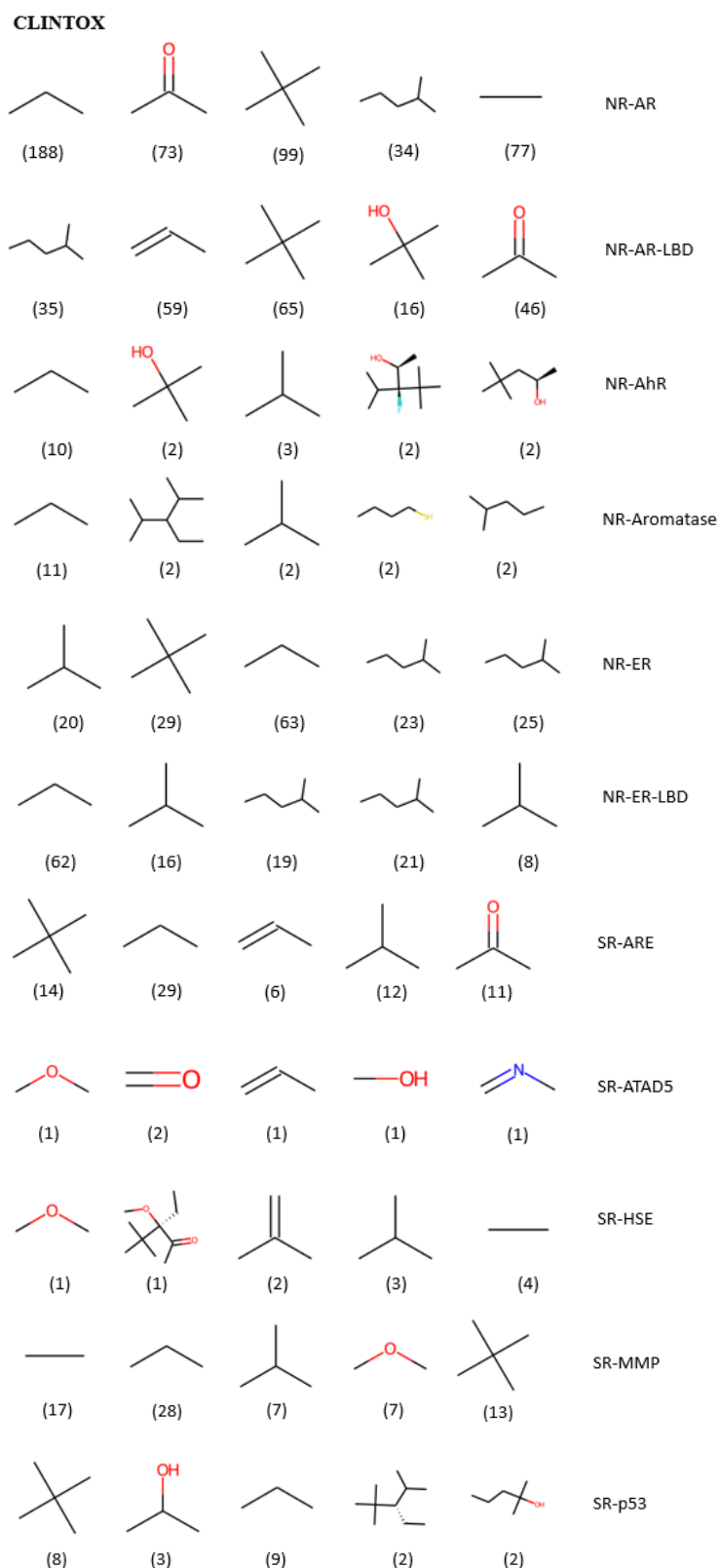
Figure S1. Five small fragments that most influenced the increase in toxicity for each of the 12 tasks in the Clintox dataset. Descending order of toxic influence from left to right. The number in parentheses is the number of fragment hits in each task.
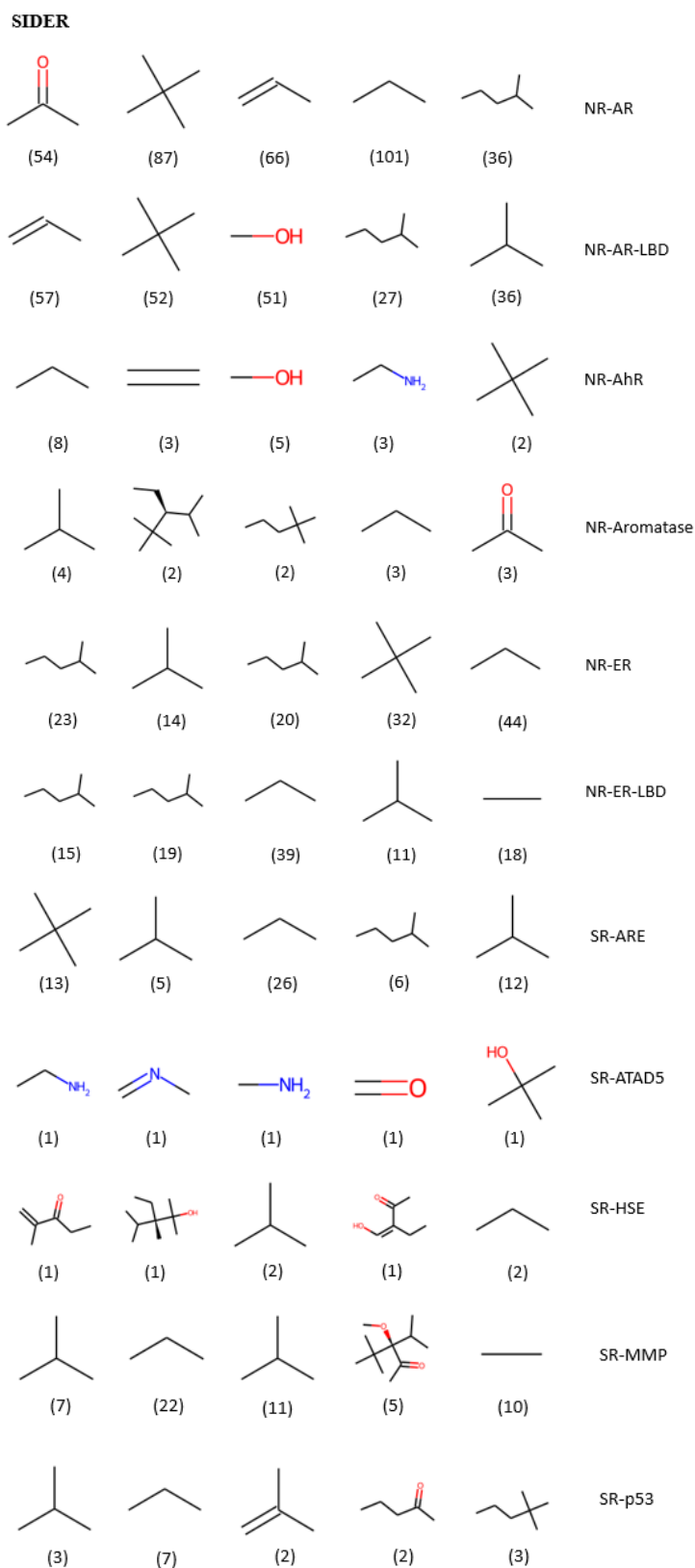
Figure S2. Five small fragments that most influenced the increase in toxicity for each of the 12 tasks in the Sider dataset. Descending order of toxic influence from left to right. The number in parentheses is the number of fragment hits in each task.
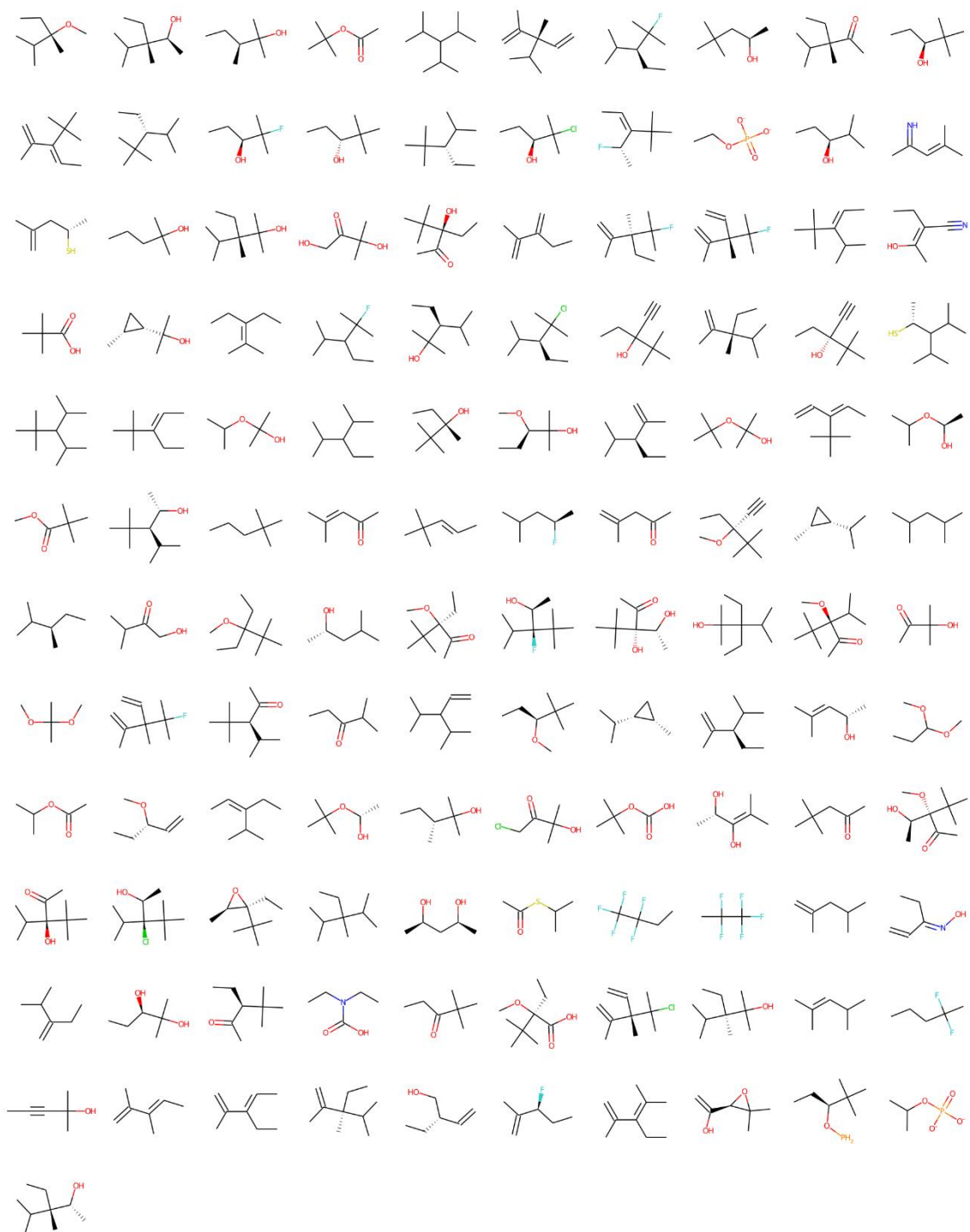
Figure S3. Structural alerts that most influenced the increase in toxicity for all of the 12 tasks in the Clintox dataset (Run #2). The order does not represent the toxic influence of each fragment.
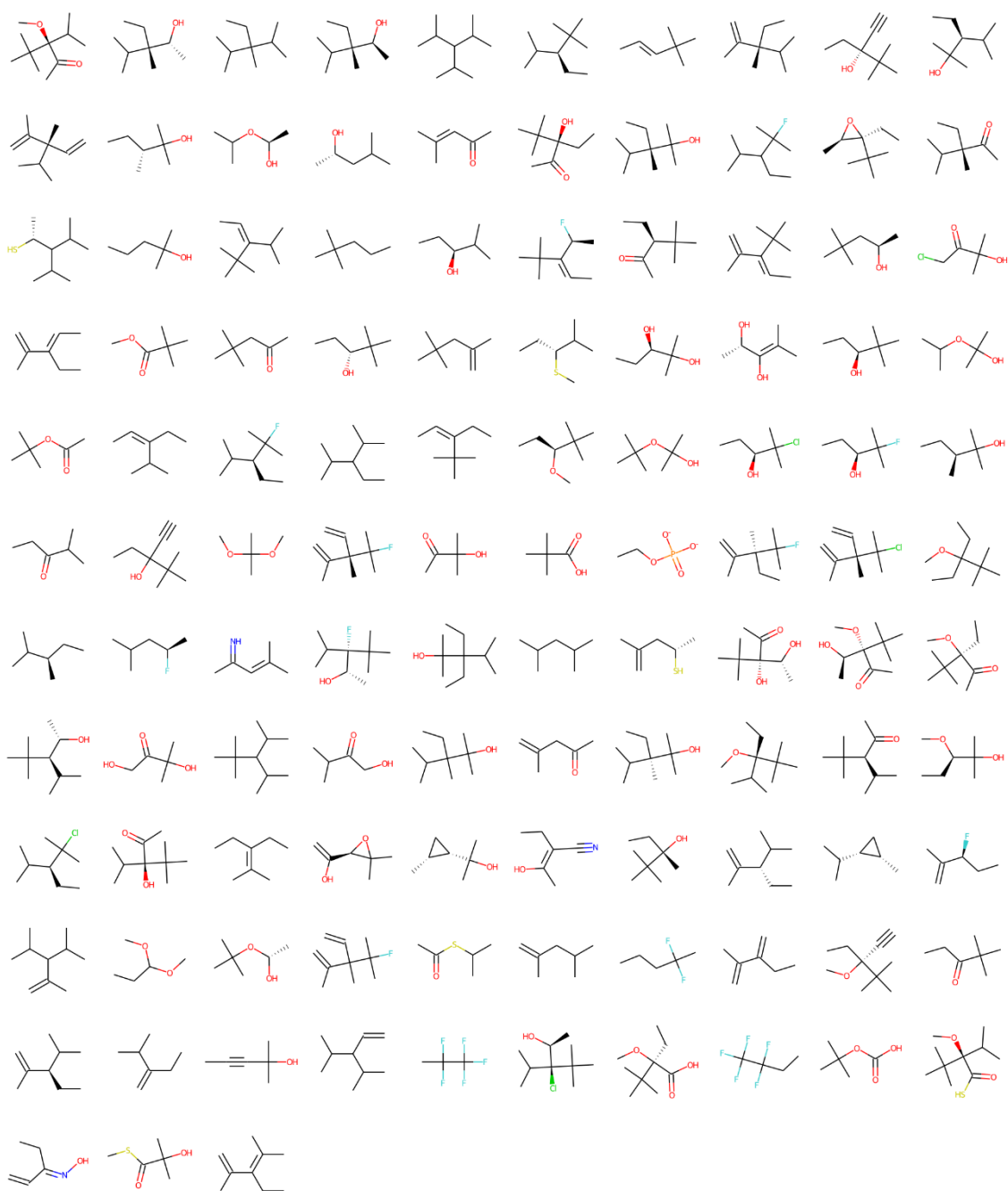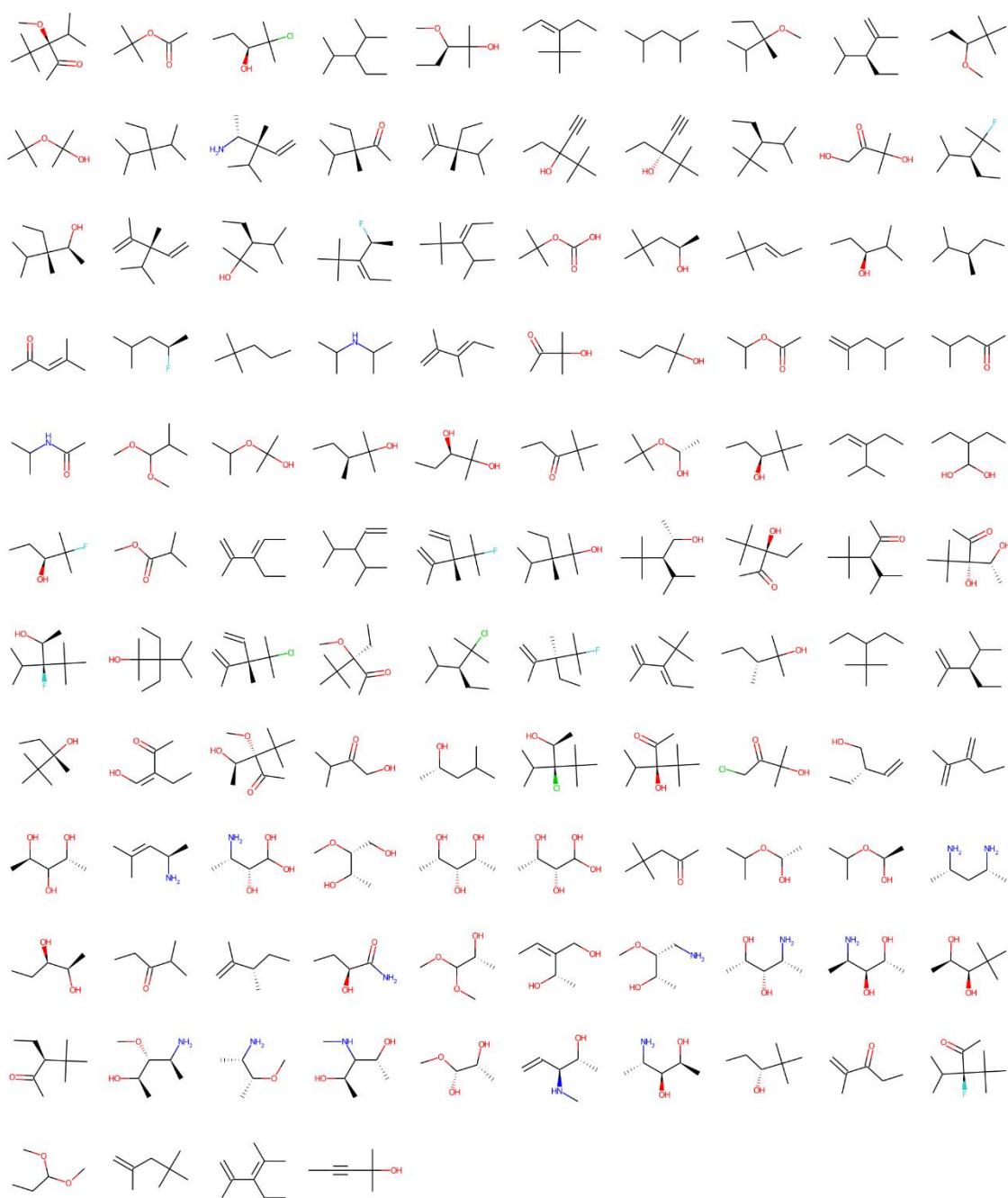
Figure S4. Structural alerts that most influenced the increase in toxicity for all of the 12 tasks in the Clintox dataset (Run #3). The order does not represent the toxic influence of each fragment.
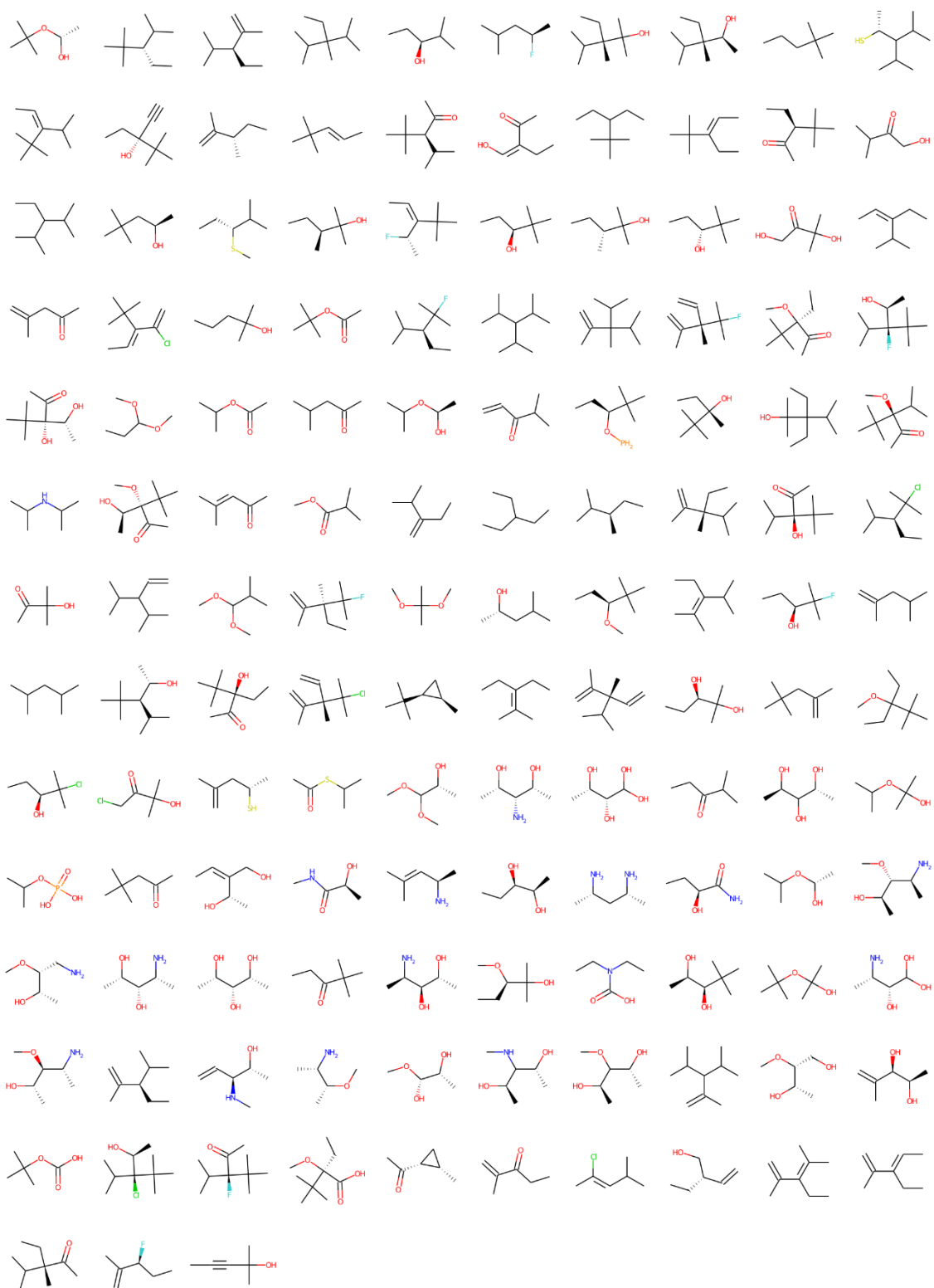
Figure S5. Structural alerts that most influenced the increase in toxicity for all the 12 tasks in the Sider dataset (Run #2). The order does not represent the toxic influence of each fragment.
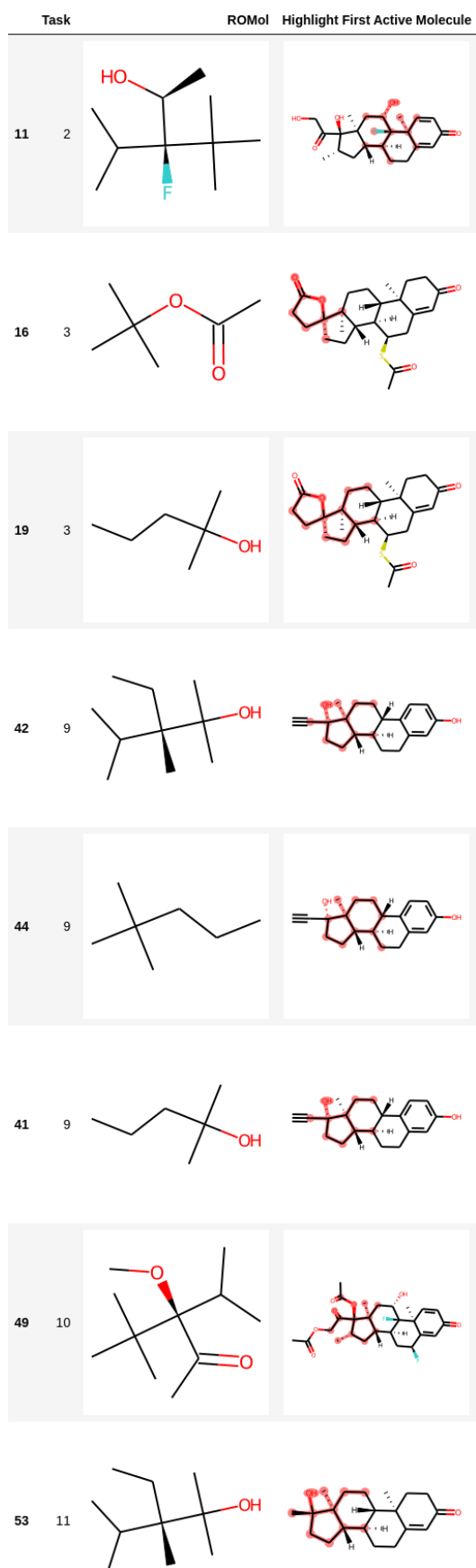
Figure S6. Structural alerts that most influenced the increase in toxicity for all the 12 tasks in the Sider dataset (Run #3). The order does not represent the toxic influence of each fragment.

Task		ROMol	Highlight First Active Molecule
11	2		
16	3		
19	3		
42	9		
44	9		
41	9		
49	10		
53	11		

Figure S7. Representation of the several fragments highlighted in the first active molecule of some tasks for the Clintox dataset (Run #2).
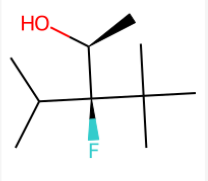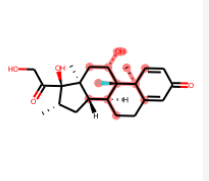
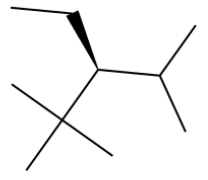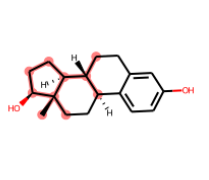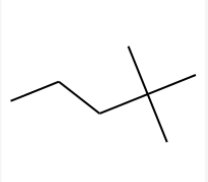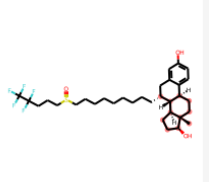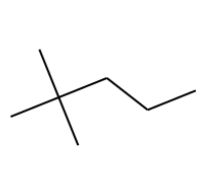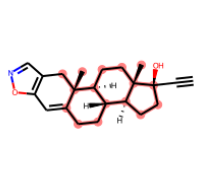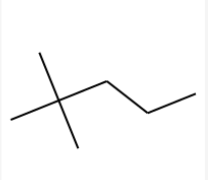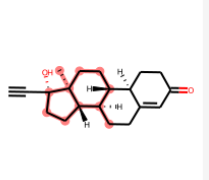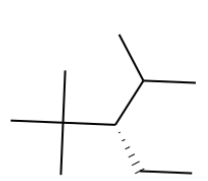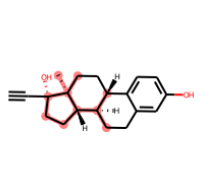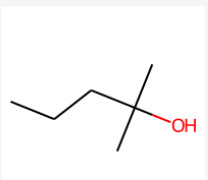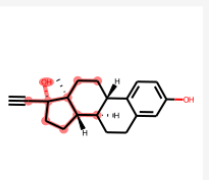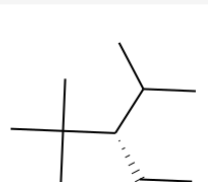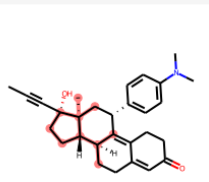| Task		ROMol	Highlight First Active Molecule
14	2		
18	3		
17	3		
19	3		
32	7		
39	9		
40	9		
52	11		

Figure S8. Representation of the several fragments highlighted in the first active molecule of some tasks for the Clintox dataset (Run #3).
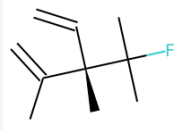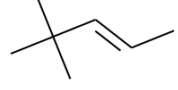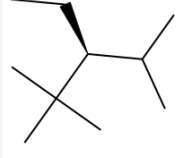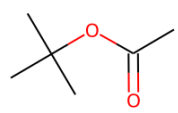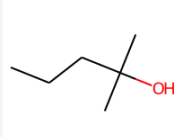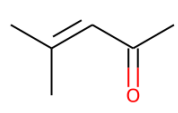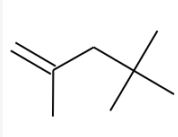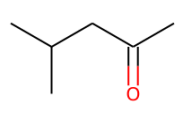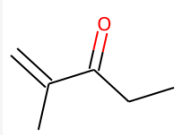
Task		ROMol	Highlight First Active Molecule
14	2		
13	2		
15	3		
16	3		
17	3		
19	3		
43	9		
42	9		
41	9		

Figure S9. Representation of the several fragments highlighted in the first active molecule of some tasks for the Sider dataset (Run #2).
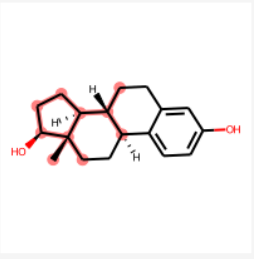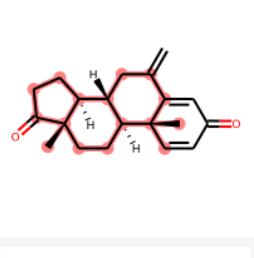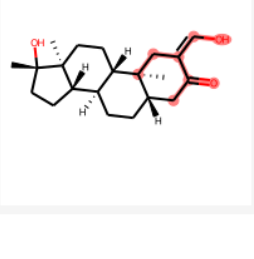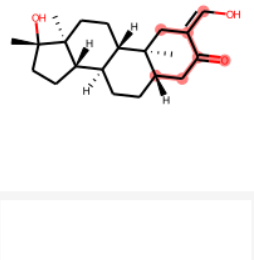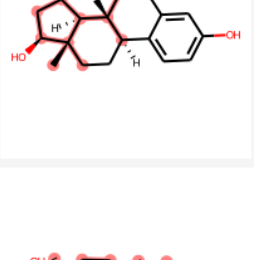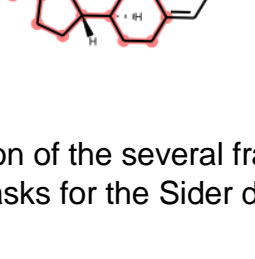
Task		ROMol	Highlight First Active Molecule
15	3		
18	3		
43	9		
44	9		
51	11		
52	11		

Figure S10. Representation of the several fragments highlighted in the first active molecule of some tasks for the Sider dataset (Run #3).
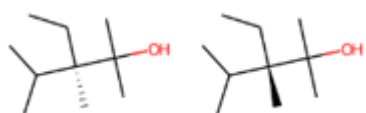
Figure S11. Representation of repeated structures in Clintox/ECFP (Run #2).
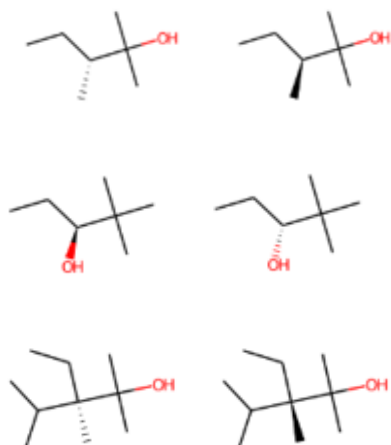
Figure S12. Representation of repeated structures in Clintox/ECFP (Run #3).
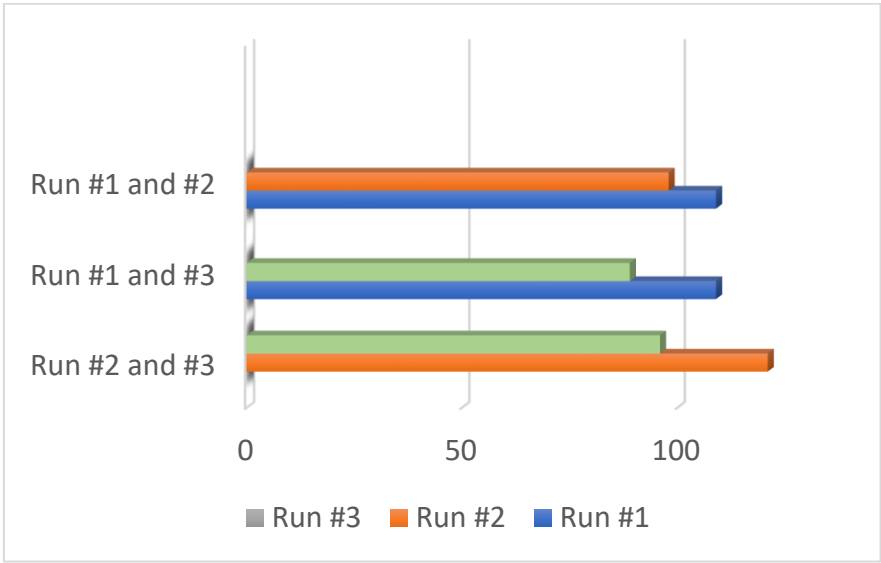
Figure S13. Similarity between each pair of runs using the Clintox dataset (Runs #1, #2 and #3). The x-axis is the number of alerts in each run.
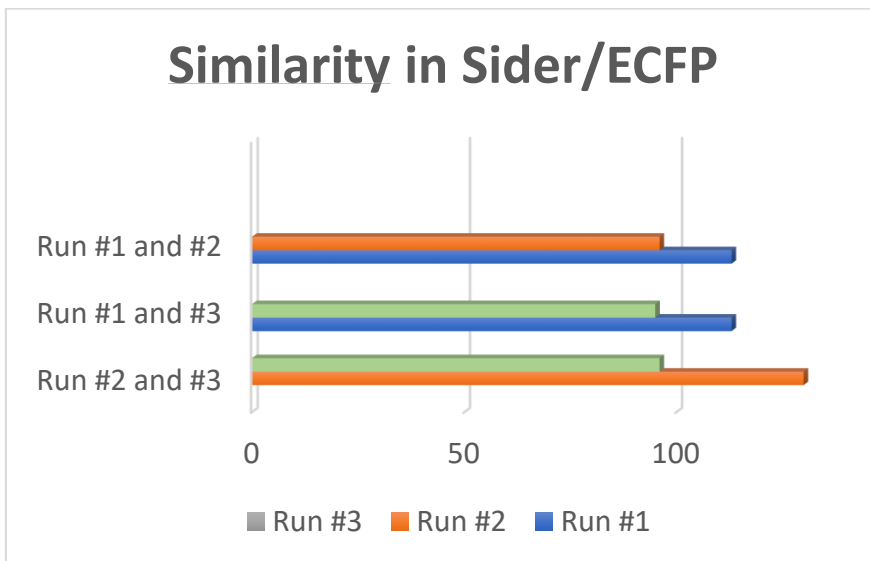
Figure S14. Similarity between each pair of runs using the Sider dataset (Runs #1, #2 and #3). The x-axis is the number of alerts in each run.
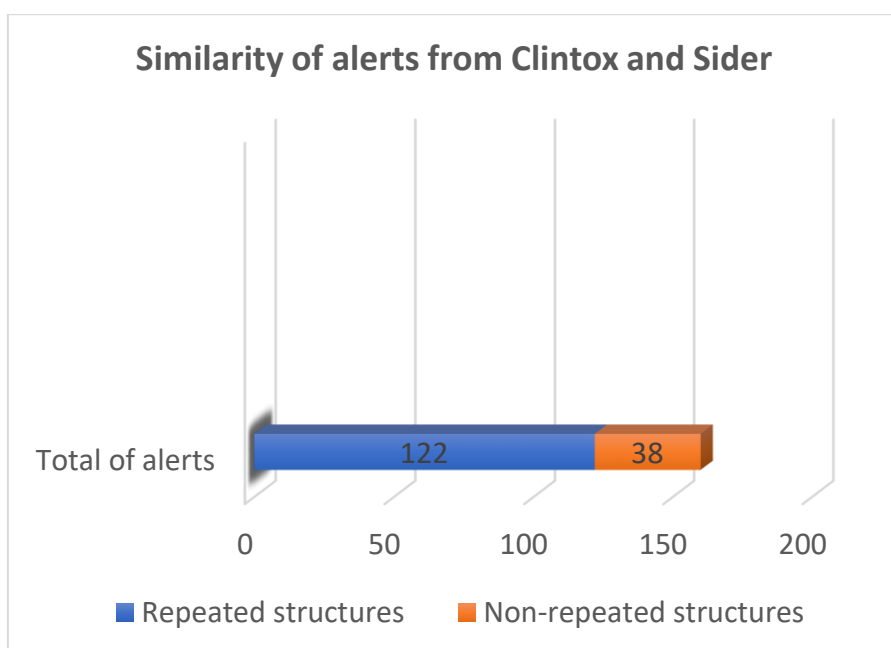
Figure S15. Number of repeated (orange) and non-repeated (blue) structural alerts in both Clintox and Sider datasets. The x-axis is the number of structural alerts generated in the Clintox and Sider dataset.

Attachments

Structural alert lists (SMARTS pattern)

Structural alert list (SMARTS pattern) from Clintox dataset Run #1

[#6]-[#6](-[#6])-[#6](-[#6]-[#6])-[#6](-[#6])-[#6]

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[#6]-[#6]-[#6@H](-[#8]-[#6])-[#6](-[#6])(-[#6])-[#6]

[#6]-[#6](-[#6])-[#6](-[#6]=[#6])-[#6](-[#6])-[#6]

[#6]-[#6](-[#6])-[#6](-[#6](-[#6])-[#6])-[#6](-[#6])-[#6]

[#6]-[#6](-[#6])-[#6@H](-[#6]-[#6])-[#6](=[#6])-[#6]

[#6]-[#6](-[#6])(-[#6])-[#6](=[#6]-[#6])-[#6]-[#6]

[#6]-[#6]-[#6@H](-[#8])-[#6](-[#6])(-[#6])-[#9]

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[#6]-[#6]=[#6](-[#6@H](-[#6])-[#9])-[#6](-[#6])(-[#6])-[#6]

[#6]=[#6](-[#6])-[#6@](-[#6])(-[#6]-[#6])-[#6](-[#6])-[#6]

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[#6]-[#6](-[#6])-[#6@H](-[#6]-[#6])-[#6](-[#6])(-[#6])-[#9]

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[#6]#[#6]-[#6@](-[#8])(-[#6]-[#6])-[#6](-[#6])(-[#6])-[#6]

[#6]-[#6]-[#6@@](-[#6])(-[#6](-[#6])-[#6])-[#6@@H](-[#6])-[#8]

[#6]-[#6]=[#6](-[#6](-[#6])-[#6])-[#6](-[#6])(-[#6])-[#6]

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[#6]-[#6](-[#6])-[#6@H](-[#6]-[#6])-[#6](-[#6])(-[#6])-[#17]

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[#6]-[#6](-[#6])(-[#8])-[#6](=[#8])-[#6]-[#17]

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Structural alert list (SMARTS pattern) from Clintox dataset Run #2

[#6]-[#6]-[#6@](-[#6])(-[#8]-[#6])-[#6](-[#6])-[#6]

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[#6]-[#6](-[#6])(-[#8])-[#6@@H](-[#6])-[#6]-[#6]

[#6]-[#6](-[#6])(-[#6])-[#8]-[#6](-[#6])=[#8]

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[#6]-[#6@@H](-[#8])-[#6]-[#6](-[#6])(-[#6])-[#6]

[#6]-[#6]-[#6@](-[#6])(-[#6](-[#6])=[#8])-[#6](-[#6])-[#6]

[#6]-[#6]-[#6@H](-[#8])-[#6](-[#6])(-[#6])-[#6]

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[#6]-[#6]-[#6@H](-[#8])-[#6](-[#6])(-[#6])-[#9]

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[#6]=[#6](-[#6])-[#6@](-[#6])(-[#6]-[#6])-[#6](-[#6])(-[#6])-[#9]

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Structural alert list (SMARTS pattern) from Clintox dataset Run #3

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Structural alert list (SMARTS pattern) from Sider dataset Run #1

[#6]-[#6]-[#6@H](-[#8])-[#6](-[#6])(-[#6])-[#6]

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[#6]-[#6](-[#6])(-[#8])-[#6](-[#6])=[#8]

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[#6]-[#6]-[#6@H](-[#8])-[#6](-[#6])(-[#6])-[#9]

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[#6]-[#8]-[#6@@H](-[#8])-[#6@@H](-[#6])-[#8]

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[#6]-[#6@H](-[#8])-[#6@@H](-[#8])-[#6](-[#8])-[#8]

[#6]-[#8]-[#6@H](-[#6]-[#8])-[#6@H](-[#6])-[#8]

[#6]=[#6](-[#6])-[#6@@H](-[#8])-[#6@@H](-[#6])-[#8]

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[#6]-[#6](=[#8])-[#6@@](-[#9])(-[#6](-[#6])-[#6])-[#6](-[#6])(-[#6])-[#6]

[#6]-[#6](-[#17])=[#6]-[#6](-[#6])-[#6]

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Structural alert list (SMARTS pattern) from Sider dataset Run #2

[#6]-[#6](-[#6])(-[#6])-[#8]-[#6@H](-[#6])-[#8]

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[#6]-[#6]-[#6@H](-[#8])-[#6](-[#6])-[#6]

[#6]-[#6](-[#6])-[#6]-[#6@@H](-[#6])-[#9]

[#6]-[#6]-[#6@@](-[#6])(-[#6](-[#6])-[#6])-[#6](-[#6])(-[#6])-[#8]

[#6]-[#6]-[#6@](-[#6])(-[#6@H](-[#6])-[#8])-[#6](-[#6])-[#6]

[#6]-[#6]-[#6]-[#6](-[#6])(-[#6])-[#6]

[#6]-[#6](-[#6])-[#6](-[#6](-[#6])-[#6])-[#6@@H](-[#6])-[#16]

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[#6]-[#6](-[#6])(-[#6])-[#6](=[#6]-[#6])-[#6]-[#6]

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[#6]-[#6](-[#6])-[#6](=[#8])-[#6]-[#8]

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[#6]-[#8]-[#6](-[#6]-[#6])-[#8]-[#6]

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[#6]-[#6]-[#6@H](-[#8])-[#6](-[#6])(-[#6])-[#9]

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[#6]-[#6@@H](-[#8])-[#6@H](-[#8])-[#6]-[#6]

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[#6]-[#6]-[#6@H](-[#8])-[#6](-[#7])=[#8]

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[#6]-[#8]-[#6@H](-[#6]-[#7])-[#6@H](-[#6])-[#8]

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[#6]-[#6]-[#7](-[#6]-[#6])-[#6](=[#8])-[#8]

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[#6]-[#6](-[#6])(-[#6])-[#8]-[#6](-[#6])(-[#6])-[#8]

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[#6]-[#8]-[#6@@H](-[#8])-[#6@@H](-[#6])-[#8]

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[#6]-[#6](-[#6])(-[#6])-[#8]-[#6](=[#8])-[#8]

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[#6]-[#6](=[#8])-[#6@@](-[#9])(-[#6](-[#6])-[#6])-[#6](-[#6])(-[#6])-[#6]

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[#6]-[#6@H]1-[#6]-[#6@H]-1-[#6](-[#6])=[#8]

[#6]=[#6](-[#6])-[#6](=[#8])-[#6]-[#6]

[#6]-[#6](-[#17])=[#6]-[#6](-[#6])-[#6]

[#6]=[#6]-[#6@H](-[#6]-[#6])-[#6]-[#8]

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[#6]-[#6](=[#6])-[#6@@H](-[#9])-[#6]-[#6]

[#6]-[#6](-[#6])(-[#8])-[#6]#[#6]-[#6]

Structural alert list (SMARTS pattern) from Sider dataset Run #3

[#6]-[#8]-[#6@](-[#6](-[#6])=[#8])(-[#6](-[#6])-[#6])-[#6](-[#6])(-[#6])-[#6]

[#6]-[#6](-[#6])(-[#6])-[#8]-[#6](-[#6])=[#8]

[#6]-[#6]-[#6@H](-[#8])-[#6](-[#6])(-[#6])-[#17]

[#6]-[#6](-[#6])-[#6](-[#6]-[#6])-[#6](-[#6])-[#6]

[#6]-[#6](-[#6])(-[#8])-[#6@@H](-[#6]-[#6])-[#8]-[#6]

[#6]-[#6]=[#6](-[#6]-[#6])-[#6](-[#6])(-[#6])-[#6]

[#6]-[#6](-[#6])-[#6]-[#6](-[#6])-[#6]

[#6]-[#6]-[#6@](-[#6])(-[#8]-[#6])-[#6](-[#6])-[#6]

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