Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supporting Information for:

Beyond the static picture: a machine learning and molecular dynamics insight on singlet fission

Natalia Szczepkowsk[1], Iga Pregowska[1], Diana Radovanovici[1], and Luis Enrique Aguilar Suarez[1]

[1]Amsterdam University College, Science Park 113, 1098 XG Amsterdam

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1. GitLab repository

Link for dowload and consultion here: https://uva-hva.gitlab.host/l.e.aguilarsuarez/singletfission

2. Supplementary Tables

Table 1: The structure of the neural network consisted of 1 hidden layers with 64 nodes. Mean absolute (MAE) and coefficient of determination (R^2) for diffent runs where the activation function, the loss function and the train/test split were varied.

		MSE		MAE		Huber	
Activation Function	Train/test	MAE	R^2	MAE	R^2	MAE	R^2
ReLU	90/10	0.2390	0.8448	0.2066	0..8374	0.2001	0.8247
	80/20	0.2556	0.7659	0.2734	0.7430	0.2799	0.7421
	70/30	0.2821	0.8132	0.2882	0.7539	0.2619	0.7527
LeakyReLU	90/10	0.2090	0.7746	0.2525	0.8642	0.2314	0.8648
	80/20	0.2551	0.8159	0.3016	0.7700	0.2951	0.7690
	70/30	0.2804	0.8585	0.3506	0.7909	0.2755	0.8214
ELU	90/10	0.3007	0.8213	0.2063	0.7950	0.2480	0.8220
	80/20	0.2935	0.7995	0.2930	0.7509	0.3004	0.7470
	70/30	0.3181	0.8488	0.2791	0.7506	0.2849	0.7877

Table 2: The structure of the neural network consisted of 2 hidden layers with (64,32) nodes in the first and second layer, respectively. Mean absolute (MAE) and coefficient of determination (R^2) for diffent runs where the activation function, the loss function and the train/test split were varied.

		MSE		MAE		Huber	
Activation Function	Train/test	MAE	R^2	MAE	R^2	MAE	R^2
ReLU	90/10	0.1842	0.8924	0.1878	0.8925	0.2059	0.8397
	80/20	0.2370	0.8587	0.2324	0.8565	0.2199	0.8796
	70/30	0.2249	0.8762	0.2137	0.8825	0.2212	0.8877
LeakyReLU	90/10	0.1873	0.8995	0.1905	0.8809	0.1989	0.8846
	80/20	0.2462	0.8589	0.2293	0.8809	0.2425	0.8675
	70/30	0.2167	0.8846	0.2181	0.8605	0.2180	0.8855
ELU	90/10	0.1892	0.8770	0.2378	0.8230	0.2665	0.8726
	80/20	0.2562	0.8108	0.2032	0.8134	0.2537	0.8162
	70/30	0.2654	0.7988	0.2139	0.8018	0.1948	0.7990

Table 3: The structure of the neural network consisted of 2 hidden layers with (64,32) nodes in the first and second layer, respectively. The first layer is followed by dropout regularization. Mean absolute (MAE) and coefficient of determination (R^2) for differnt runs where the activation function, the loss function and the train/test split were varied.

		MSE		MAE		Huber	
Activation Function	Train/test	MAE	R^2	MAE	R^2	MAE	R^2
ReLU	90/10	0.1820	0.9078	0.1649	0.9262	0.1796	0.9118
	80/20	0.2757	0.7739	0.2625	0.7852	0.2774	0.7742
	70/30	0.2528	0.8310	0.2219	0.8624	0.2518	0.8340
LeakyReLU	90/10	0.1776	0.9155	0.1607	0.9274	0.1884	0.9044
	80/20	0.2722	0.7846	0.2795	0.7603	0.2641	0.7987
	70/30	0.2583	0.8164	0.2085	0.8702	0.2484	0.8271
ELU	90/10	0.1936	0.8790	0.1952	0.8719	0.1954	0.8797
	80/20	0.2746	0.7383	0.2708	0.7571	0.2726	0.7406
	70/30	0.2578	0.8116	0.2381	0.8398	0.2521	0.8148

3. Supplementary Figures

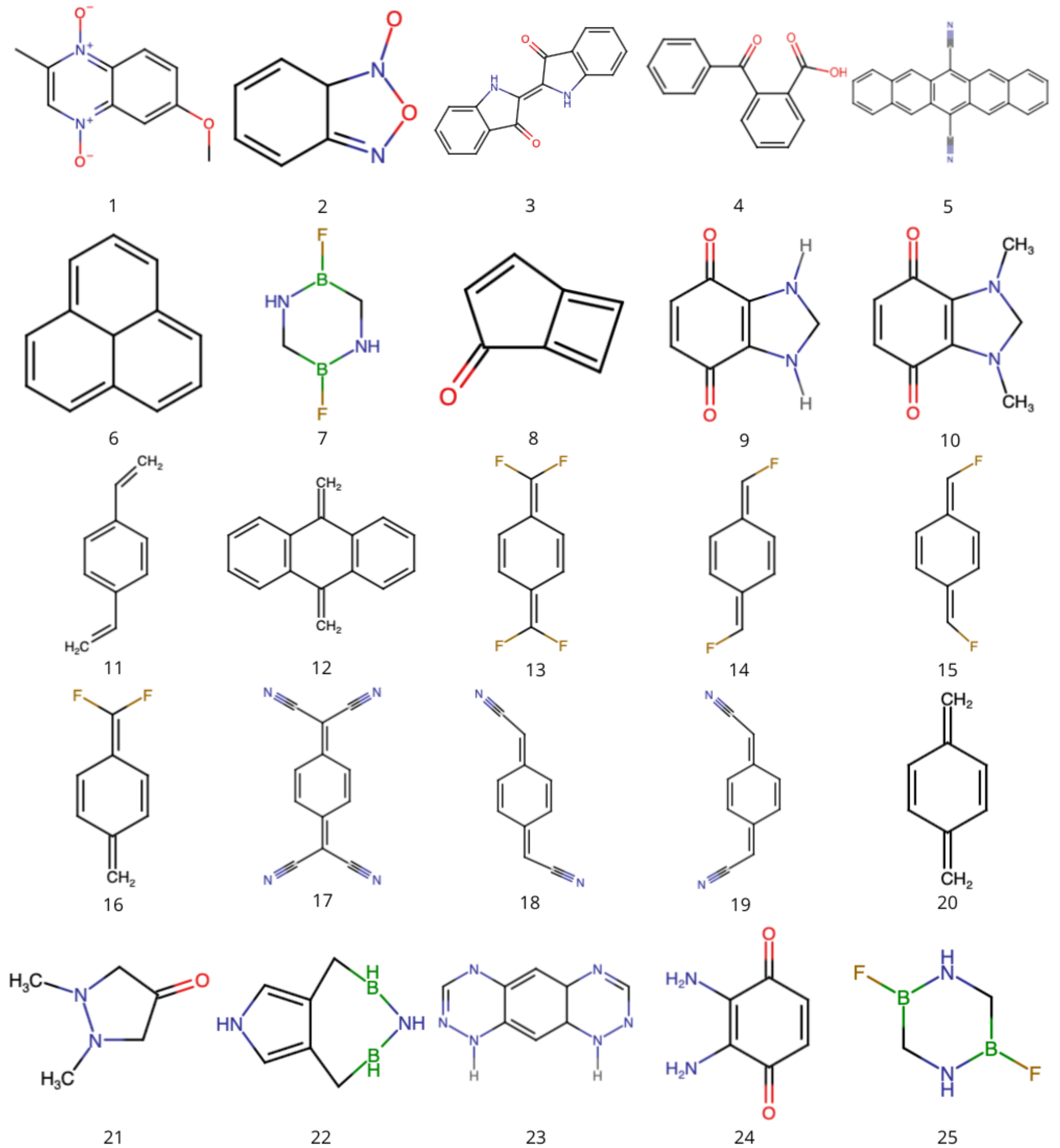


Figure 1: Structures 1-25 of the moelcules studies in the machine learnign algorithm

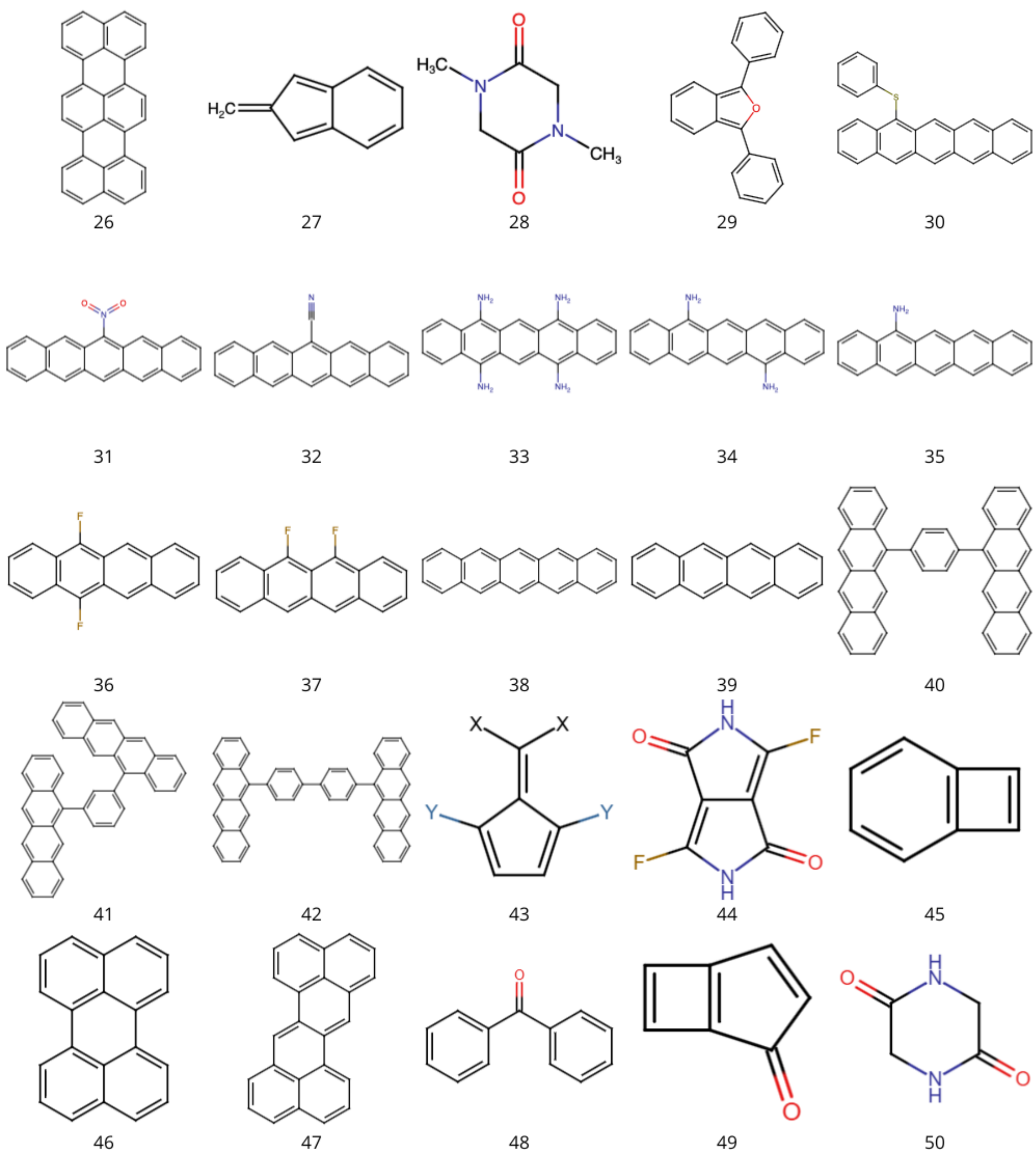
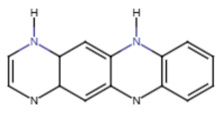


Figure 2: Structures 26-50 of the moelcules studies in the machine learnign algorithm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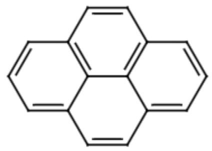
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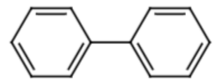
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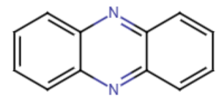
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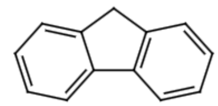
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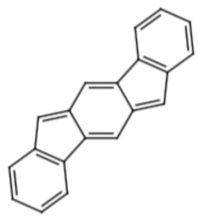
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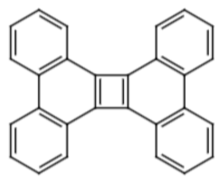
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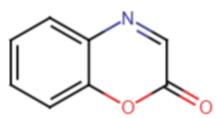
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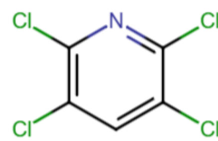
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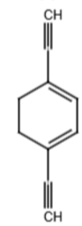
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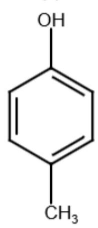
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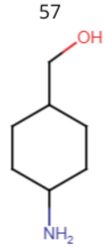
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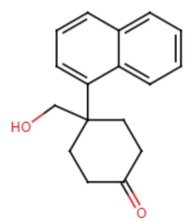
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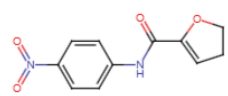
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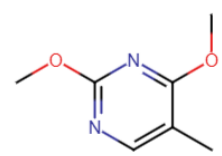
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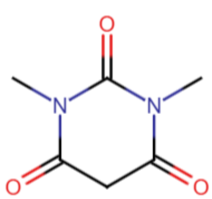
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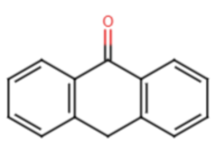
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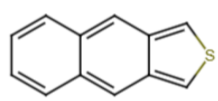
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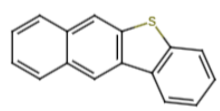
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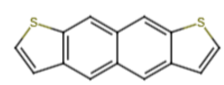
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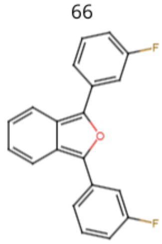
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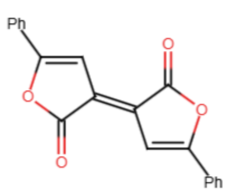
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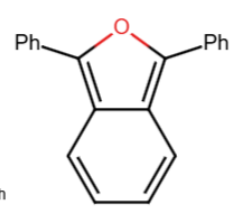
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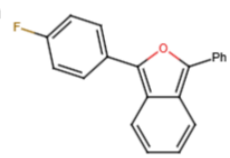
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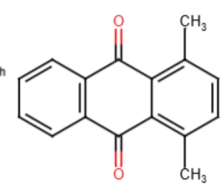
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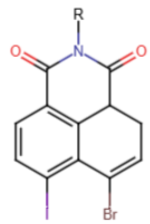
Figure 3: Structures 51-75 of the moelcules studies in the machine learnign algorithm



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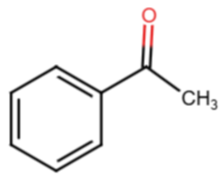

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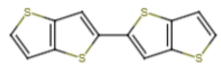

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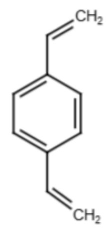

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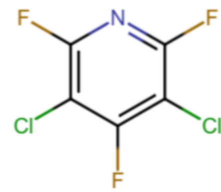

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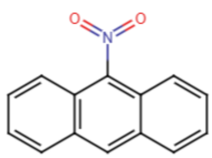

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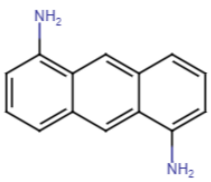

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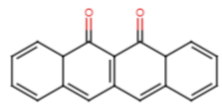

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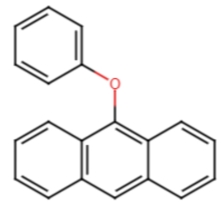

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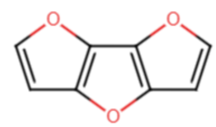

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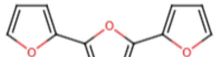

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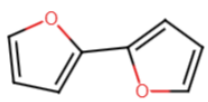

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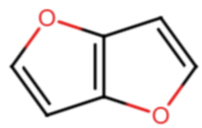

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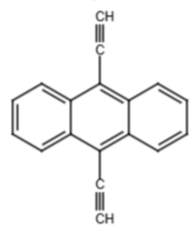

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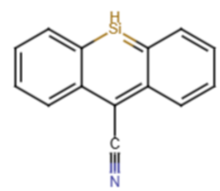

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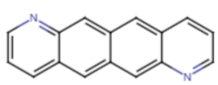

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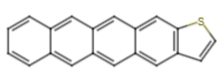

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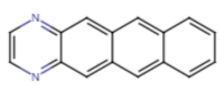

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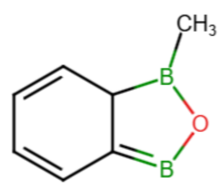

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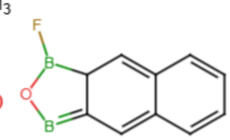

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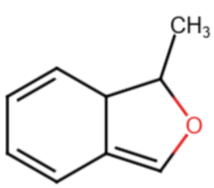

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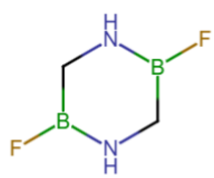

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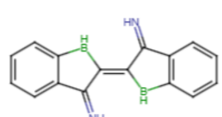

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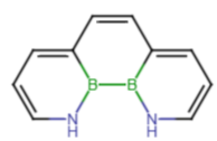

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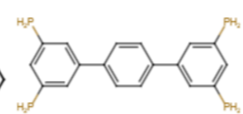

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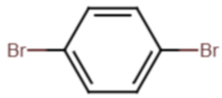
Figure 4: Structures 76-100 of the moelcules studies in the machine learnign algorithm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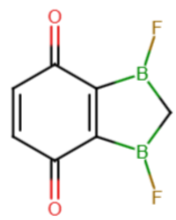
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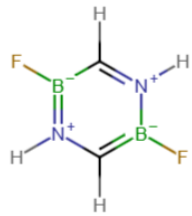
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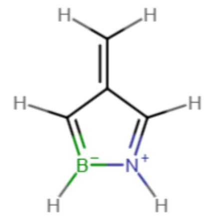
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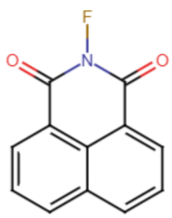
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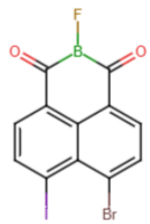
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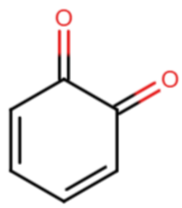
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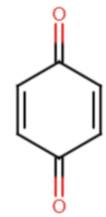
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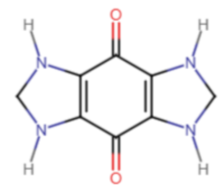
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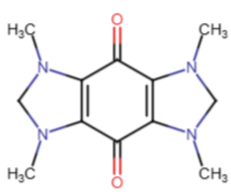
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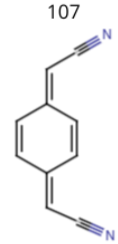
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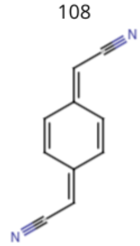
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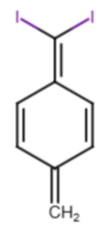
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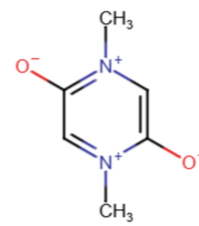
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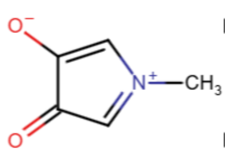
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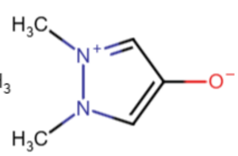
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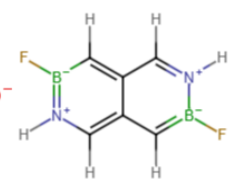
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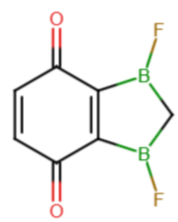
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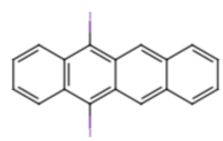
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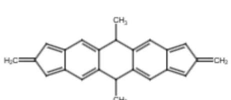
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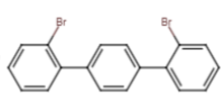
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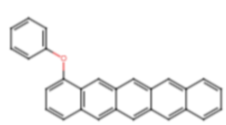
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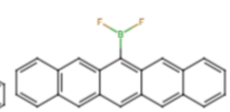
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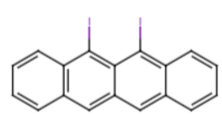
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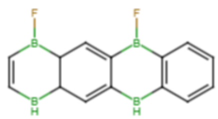
Figure 5: Structures 101-125 of the moelcules studies in the machine learnign algorithm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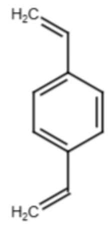
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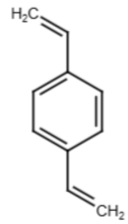
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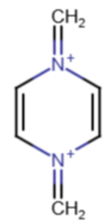
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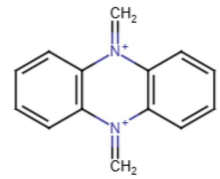
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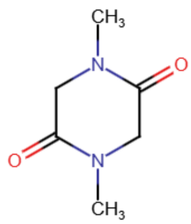
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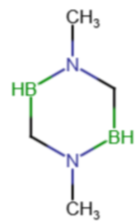
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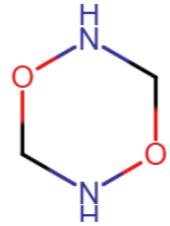
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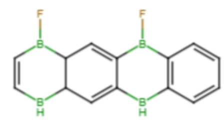
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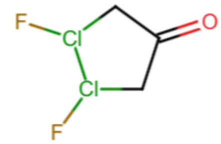
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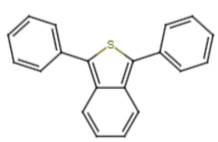
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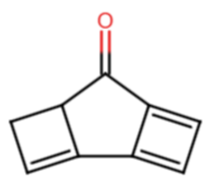
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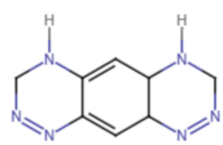
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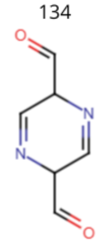
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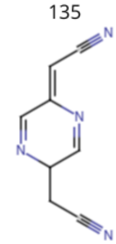
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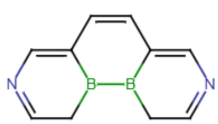
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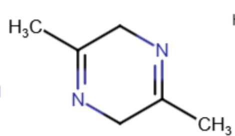
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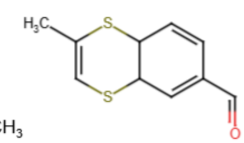
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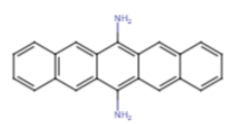
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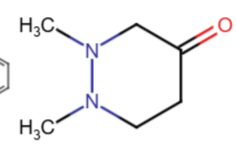
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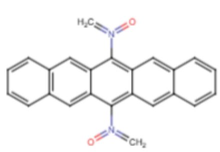
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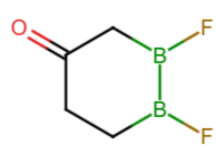
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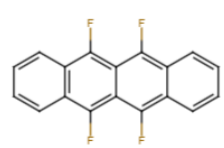
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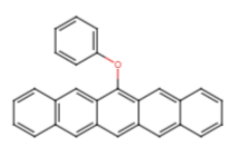
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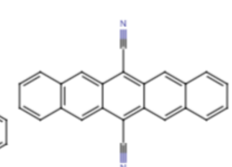
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Figure 6: Structures 126-150 of the moelcules studies in the machine learnign algorithm

(1) Architecture: One hidden layer
Hidden layer size: 64
Activation function: ReLU
Loss function: MSE

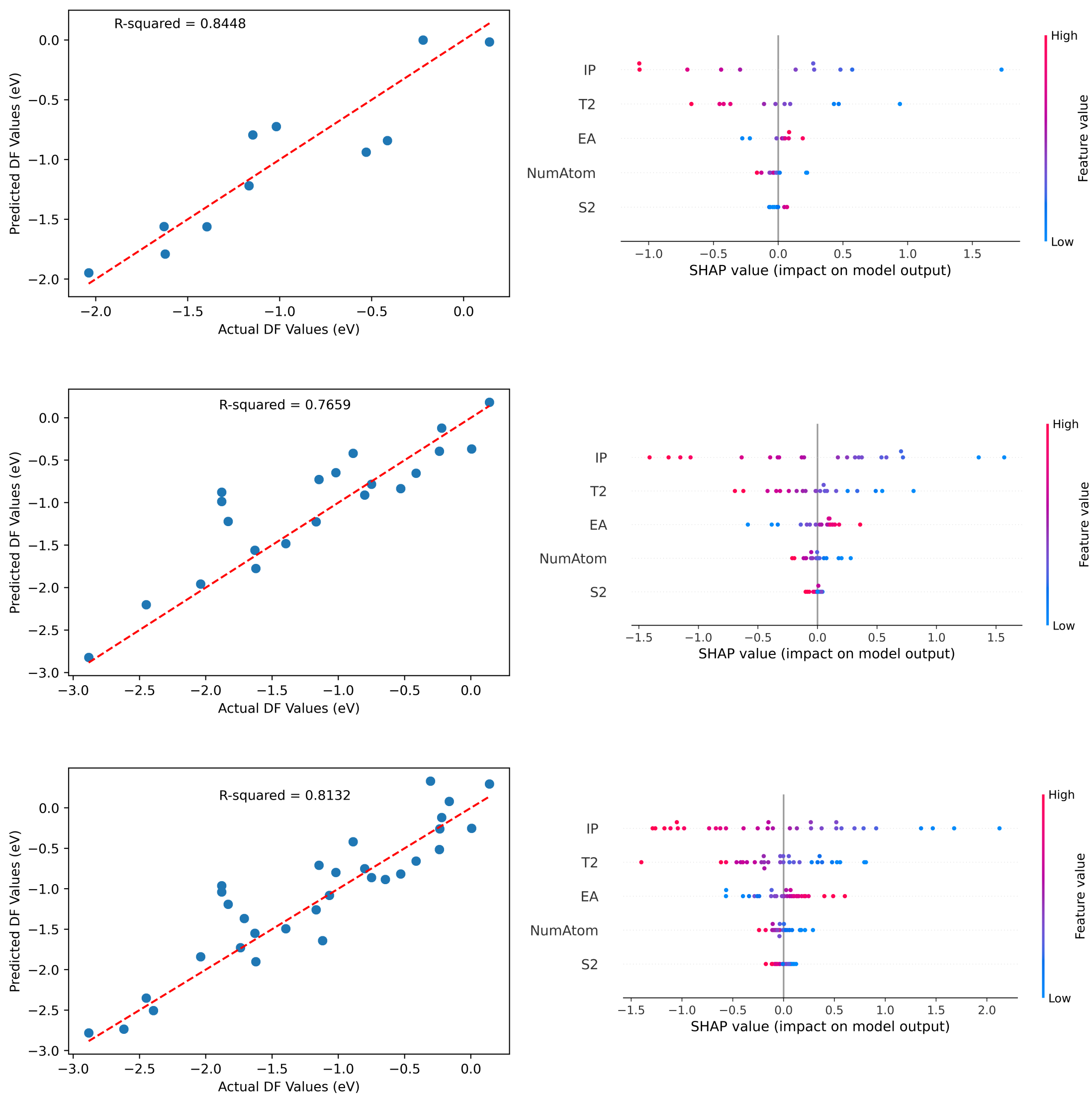


Figure 7: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(2) Architecture: One hidden layer
Hidden layer size: 64
Activation function: ReLU
Loss function: MAE

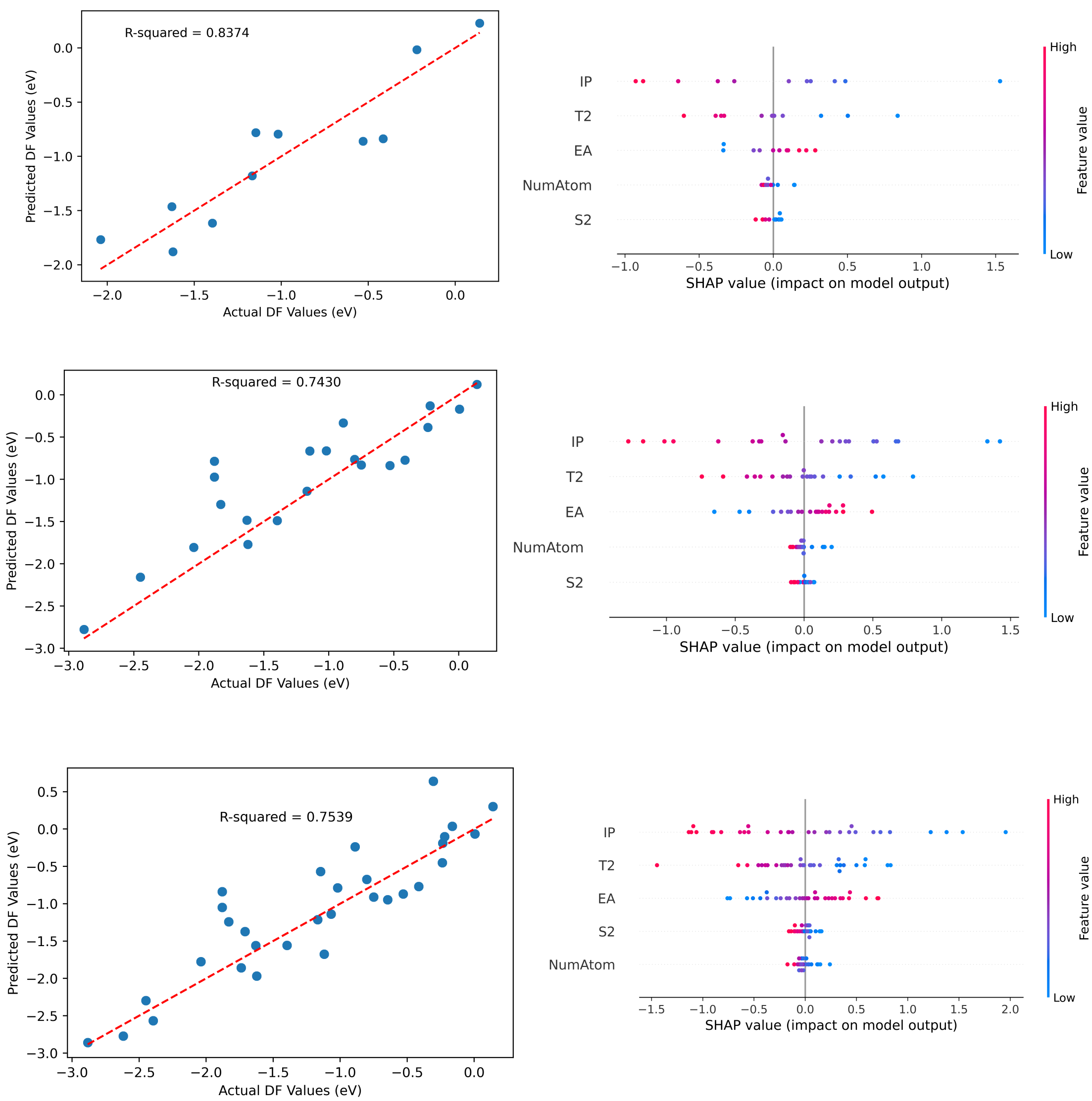


Figure 8: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

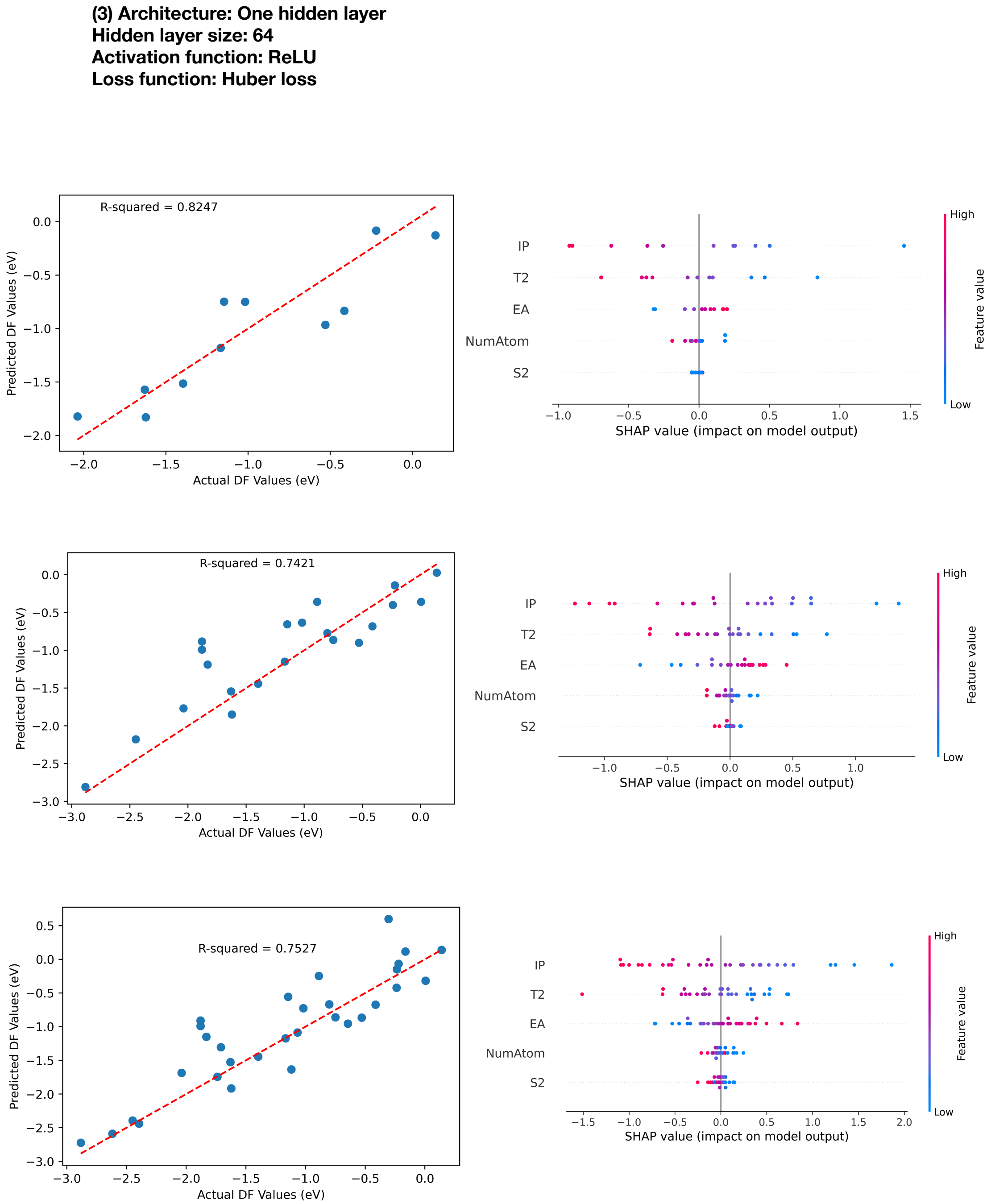


Figure 9: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

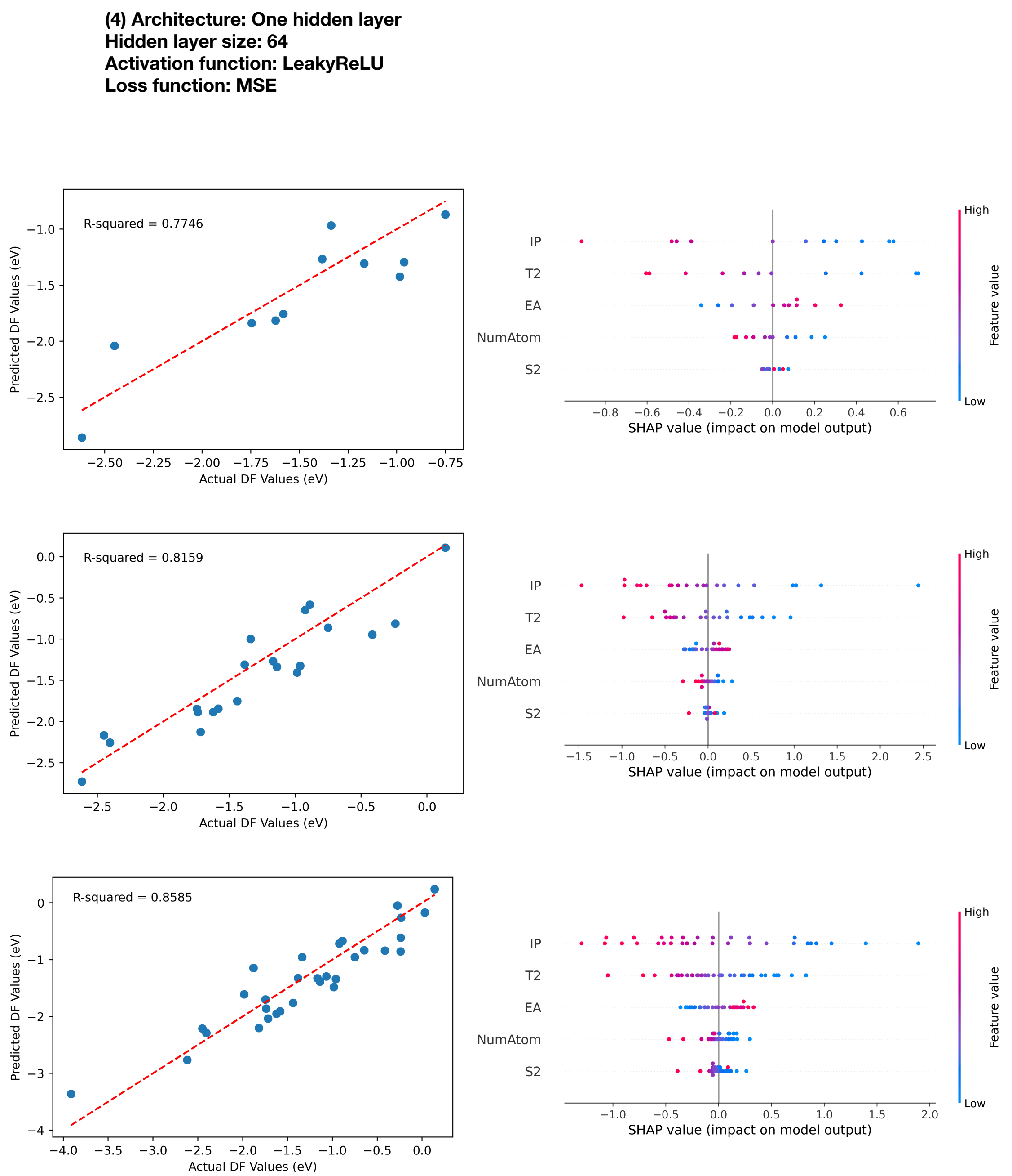


Figure 10: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(5) Architecture: One hidden layer
Hidden layer size: 64
Activation function: LeakyReLU
Loss function: MAE

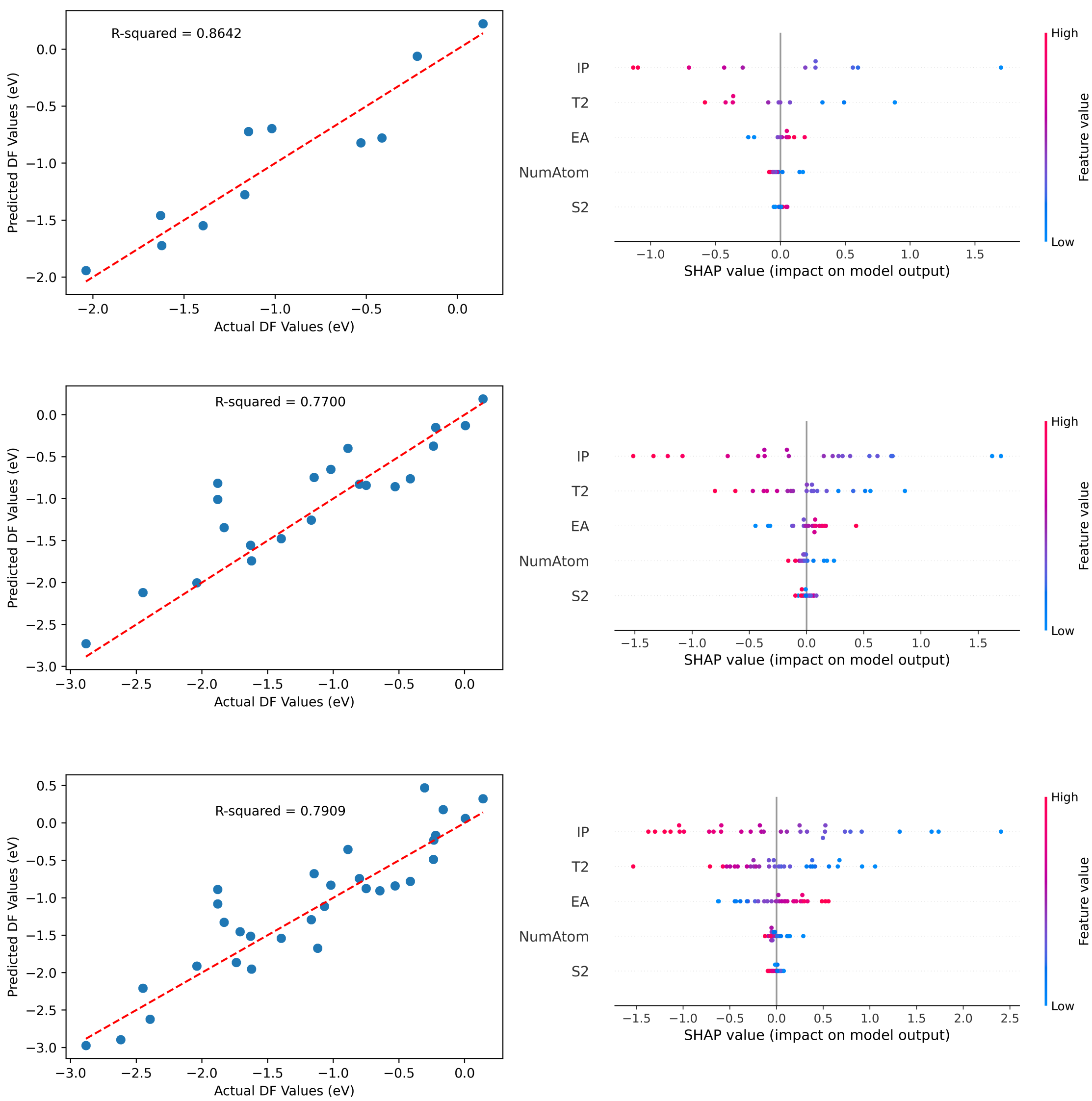


Figure 11: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

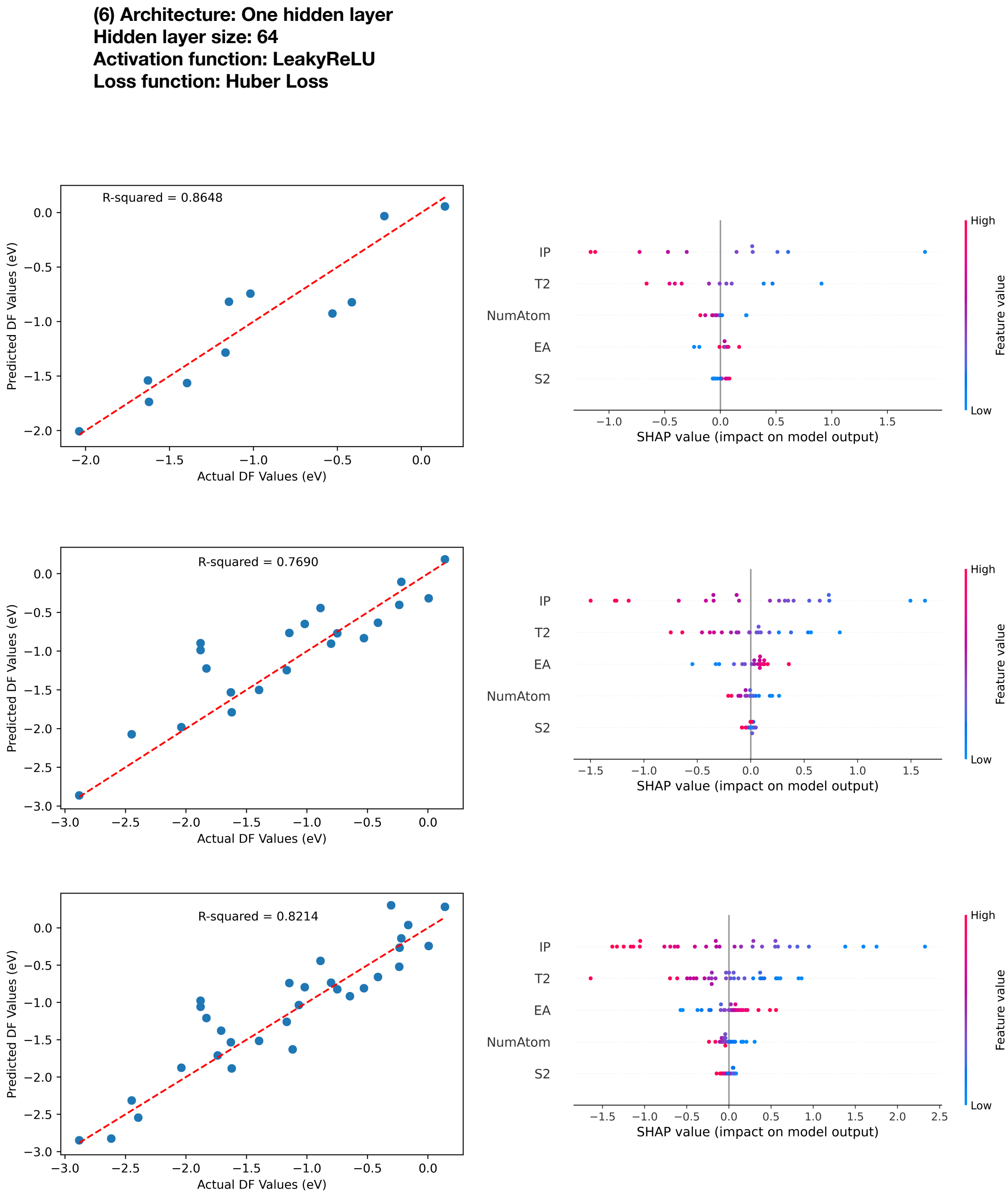


Figure 12: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(7) Architecture: One hidden layer
Hidden layer size: 64
Activation function: ELU
Loss function: MSE

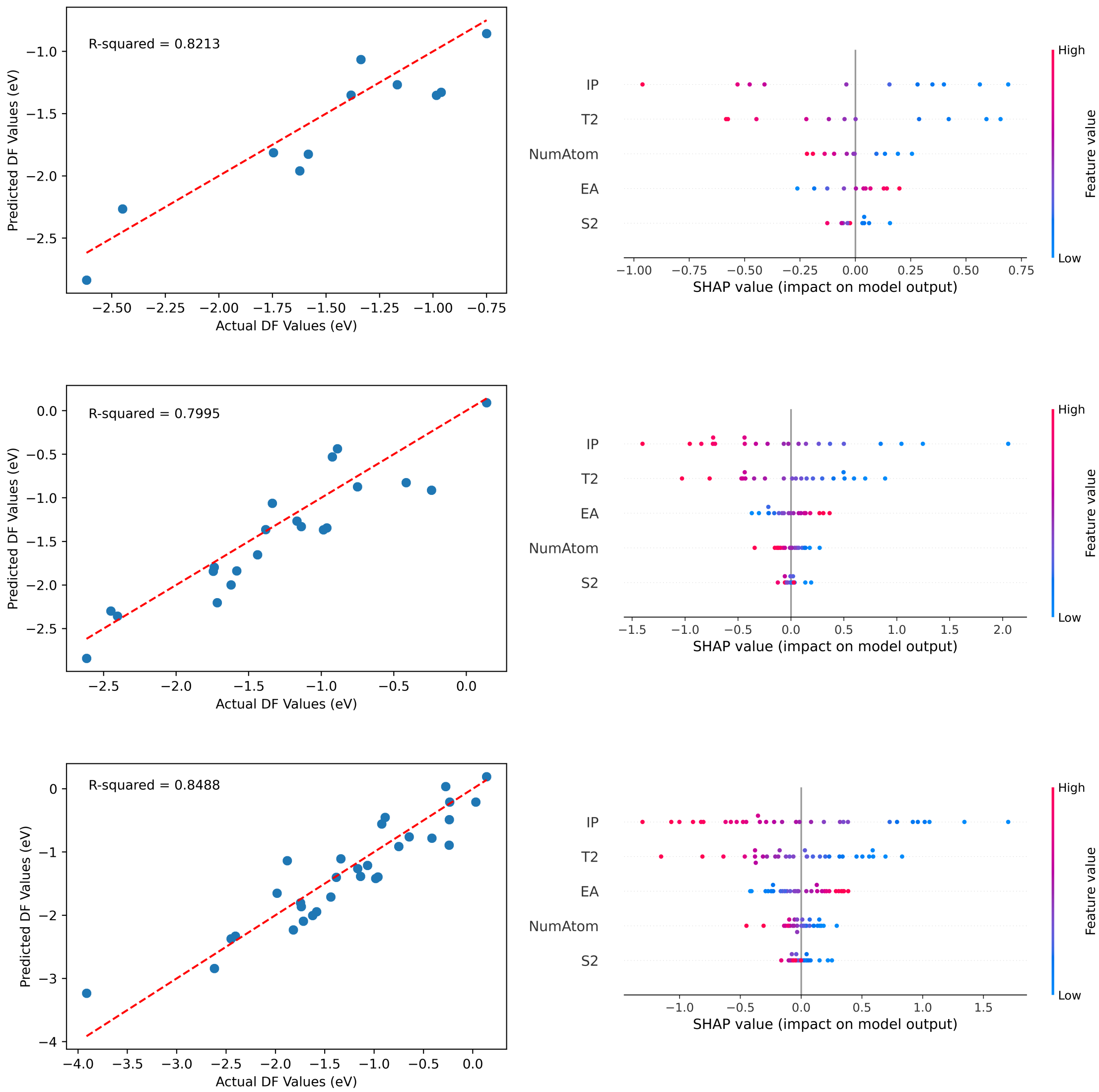


Figure 13: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

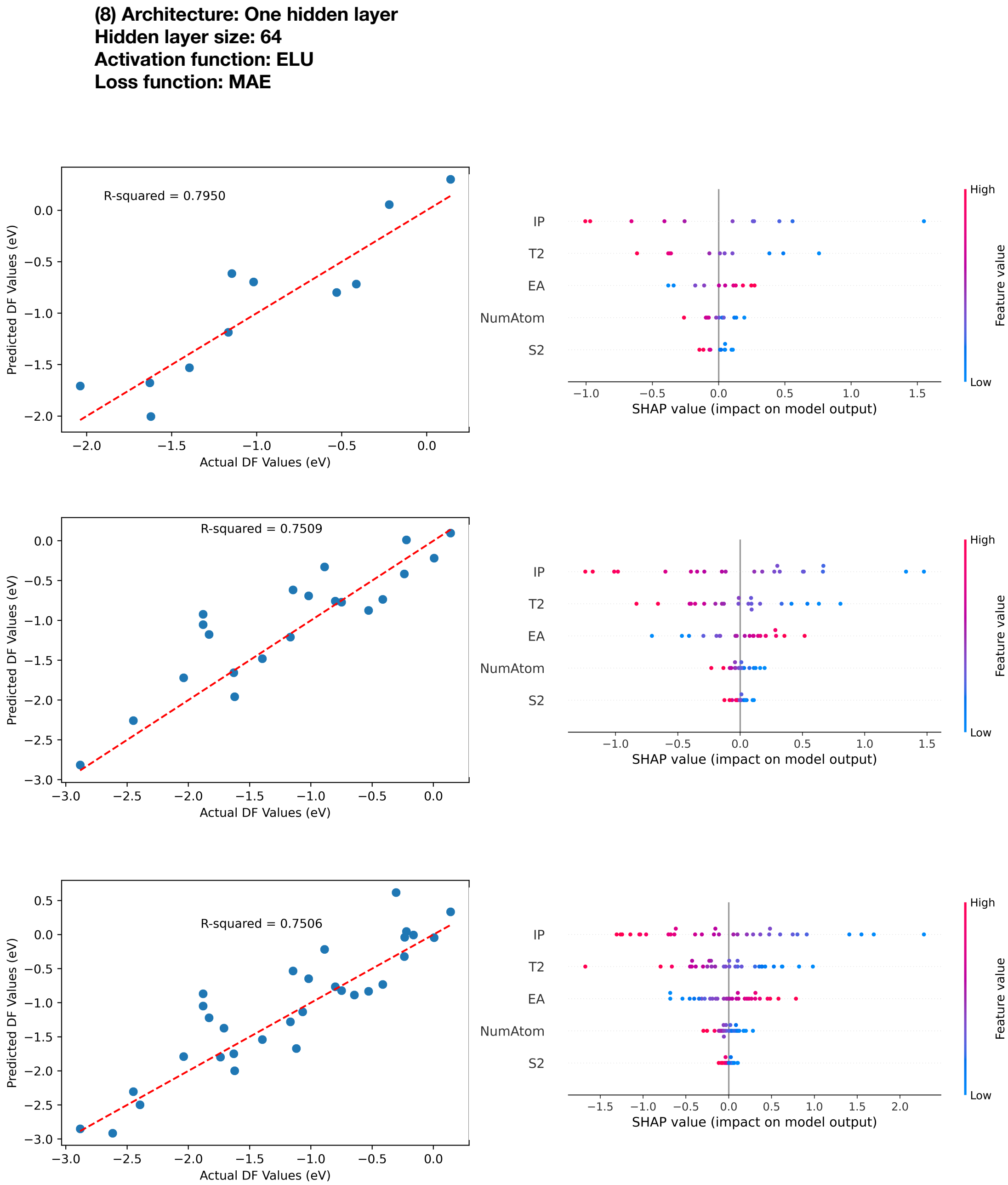


Figure 14: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(9) Architecture: One hidden layer
Hidden layer size: 64
Activation function: ELU
Loss function: Smooth

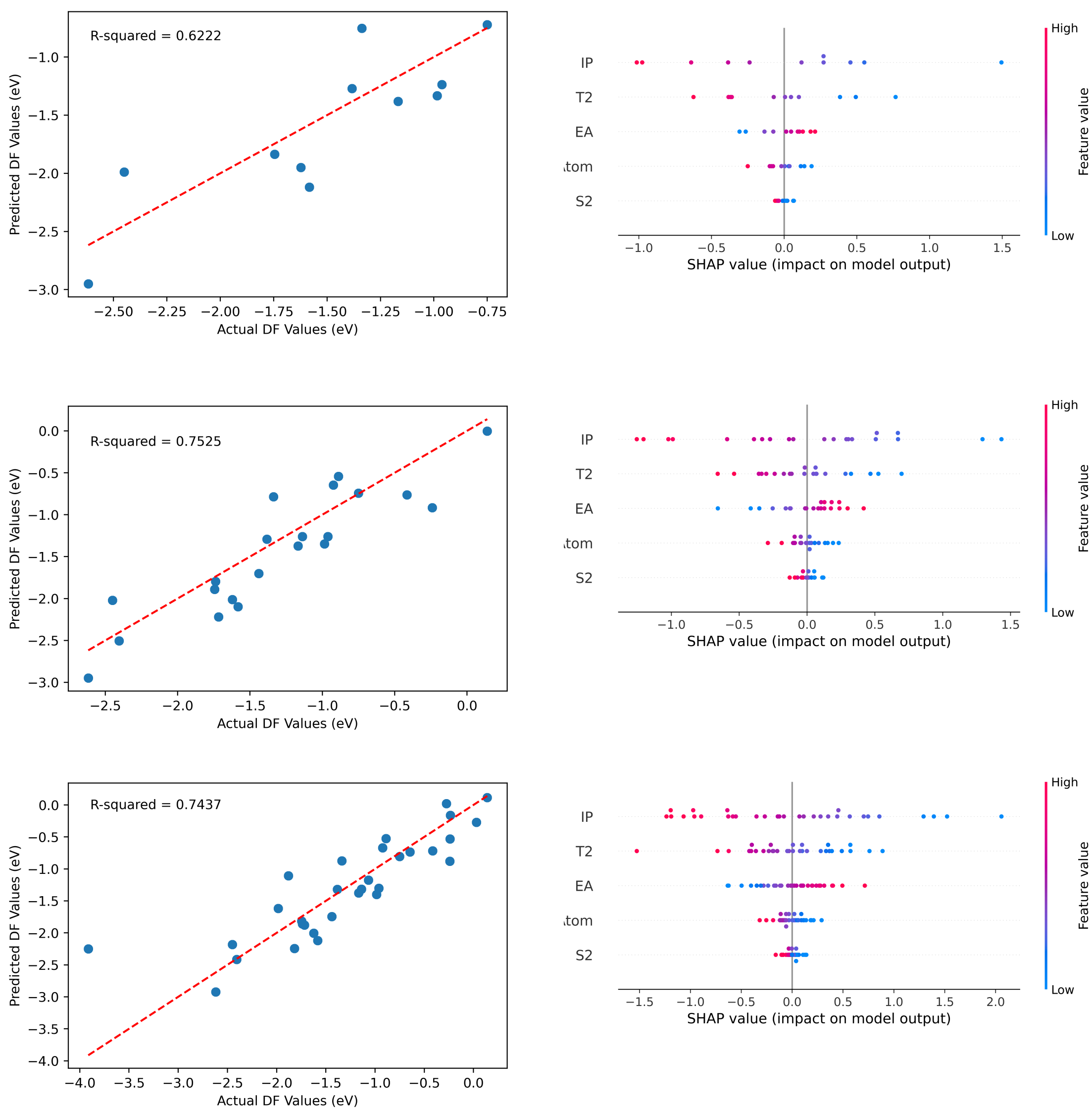
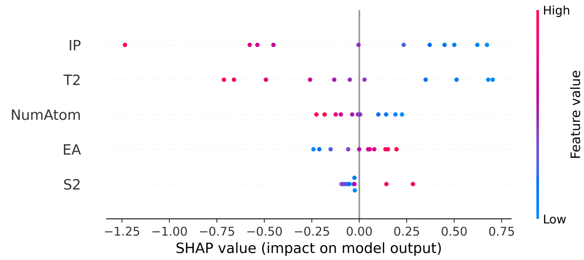
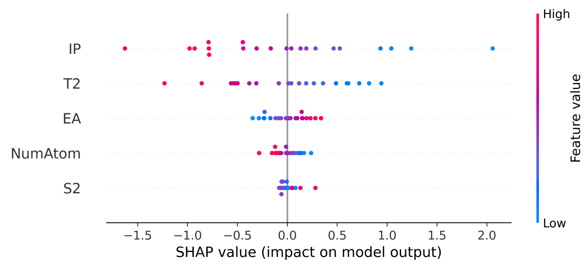


Figure 15: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(10) Architecture: One hidden layer
Hidden layer size: 64
Activation function: Tanh
Loss function: MSE





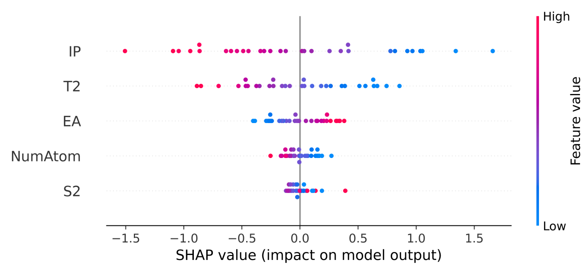


Figure 16: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(11) Architecture: One hidden layer
Hidden layer size: 64
Activation function: Tanh
Loss function: MAE

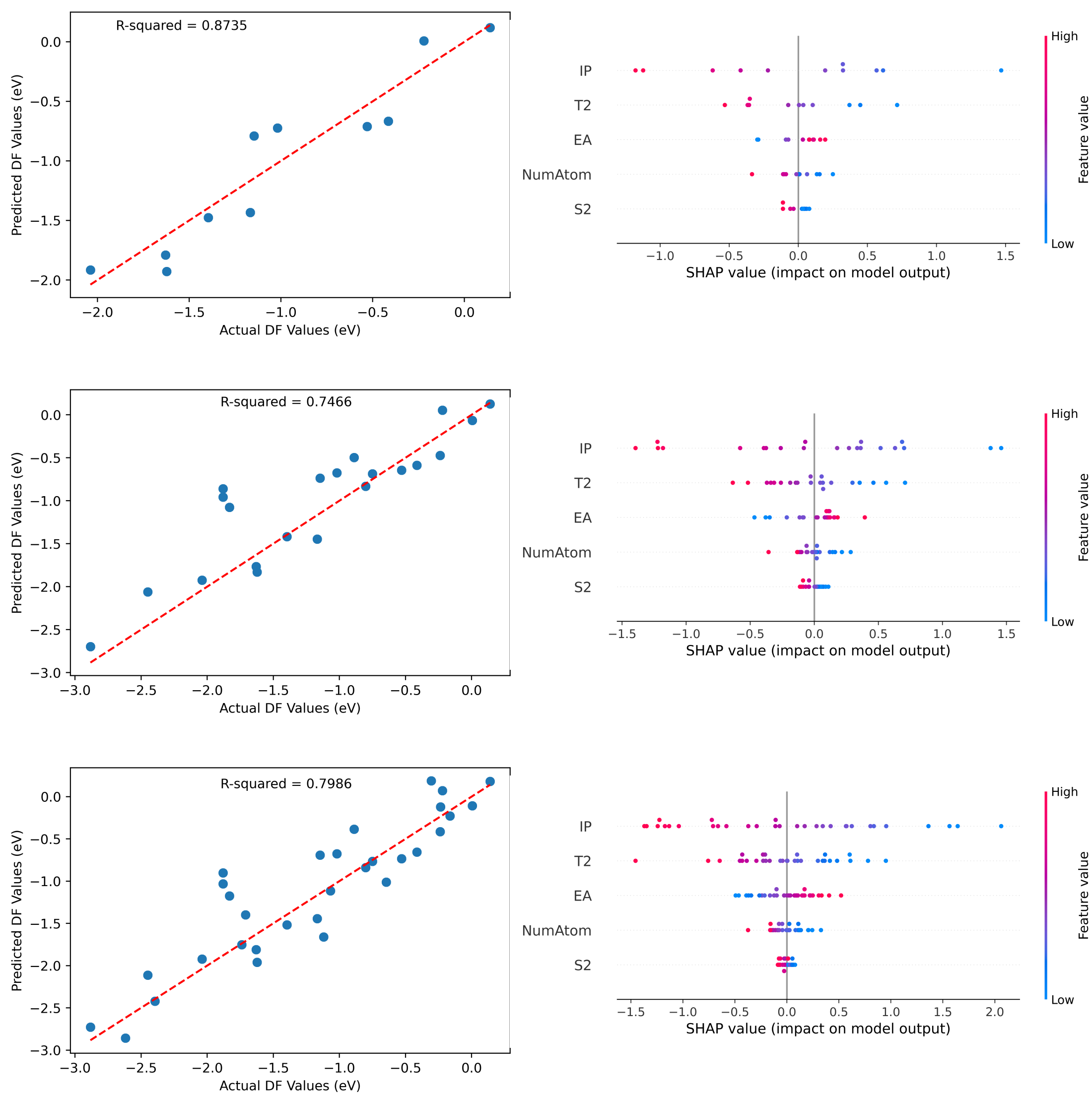


Figure 17: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

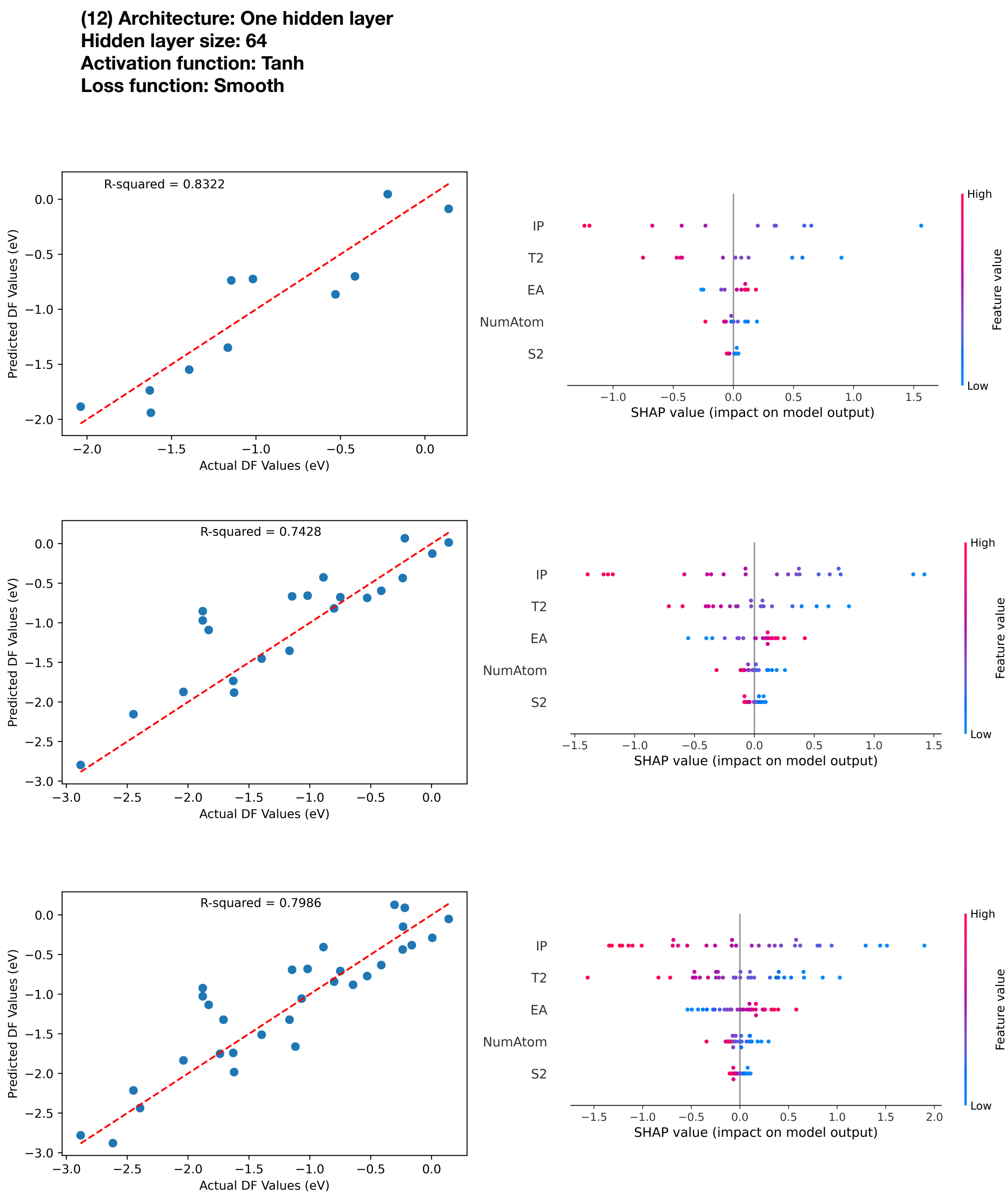


Figure 18: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(13) Architecture: Two hidden layers
Hidden layer size: 64, 32
Activation function: ReLU
Loss function: MSE

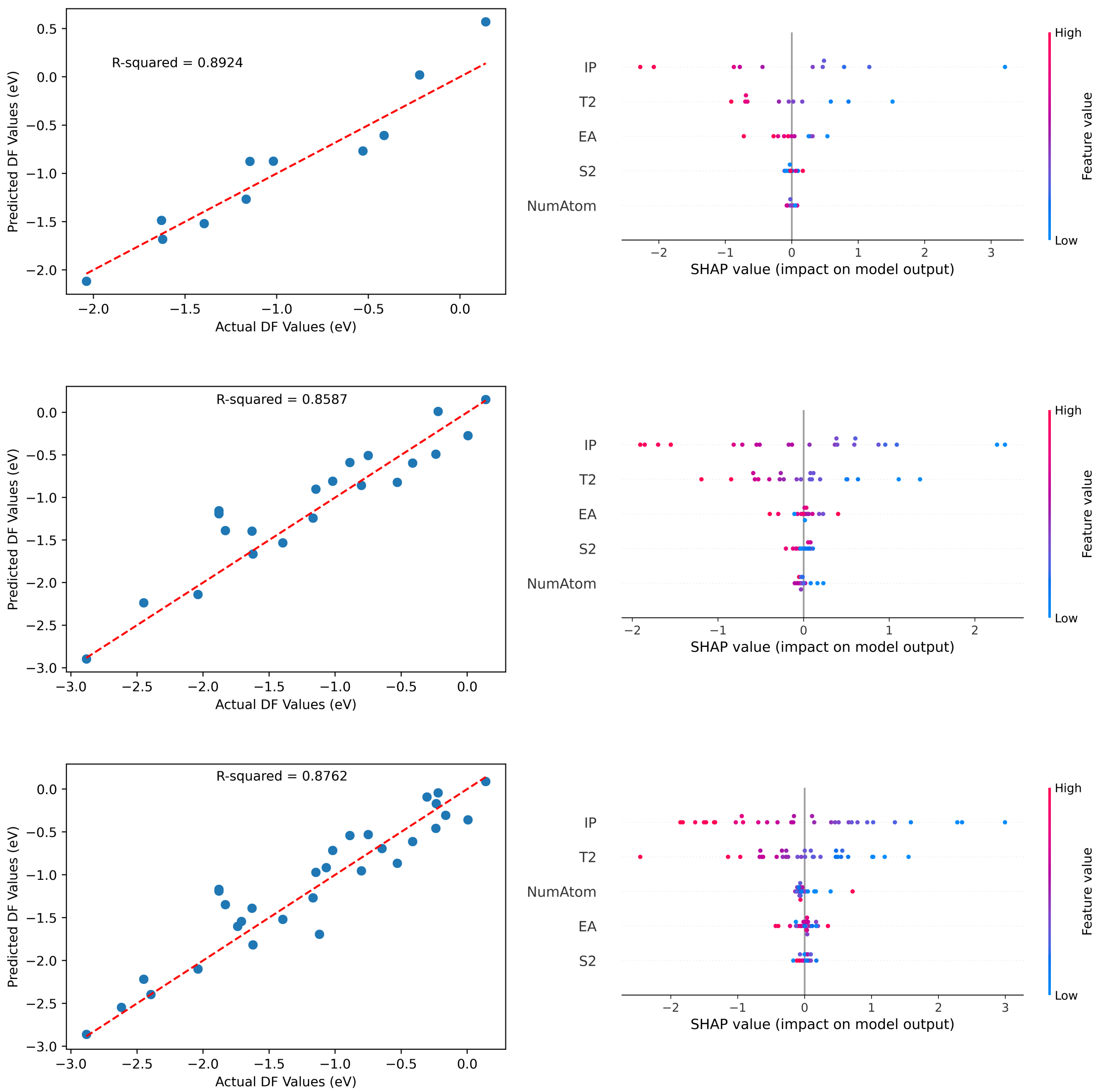


Figure 19: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(14) Architecture: Two hidden layers
Hidden layer size: 64, 32
Activation function: ReLU
Loss function: MAE

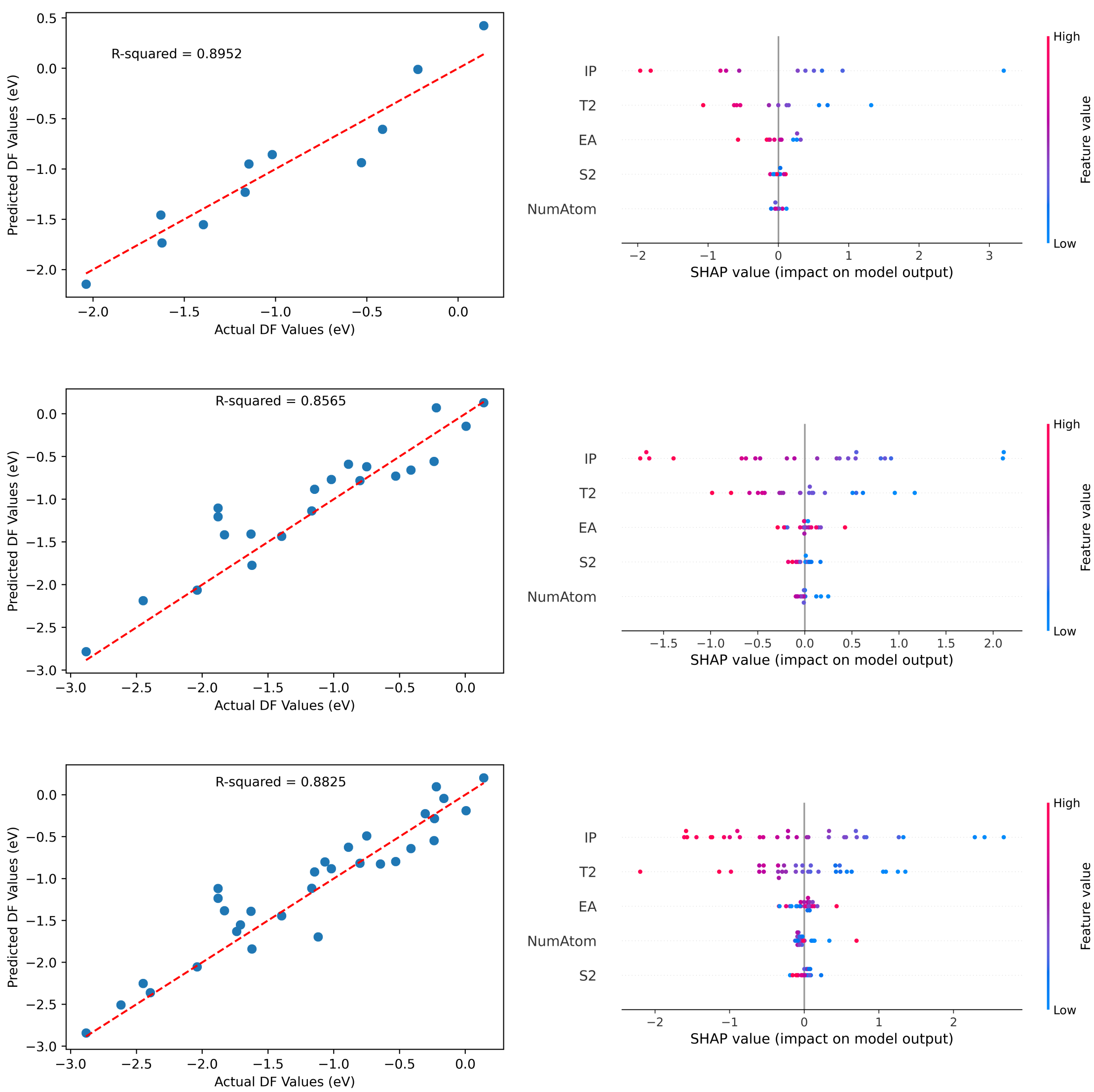


Figure 20: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(15) Architecture: Two hidden layers
Hidden layer size: 64,32
Activation function: ReLU
Loss function: Smooth

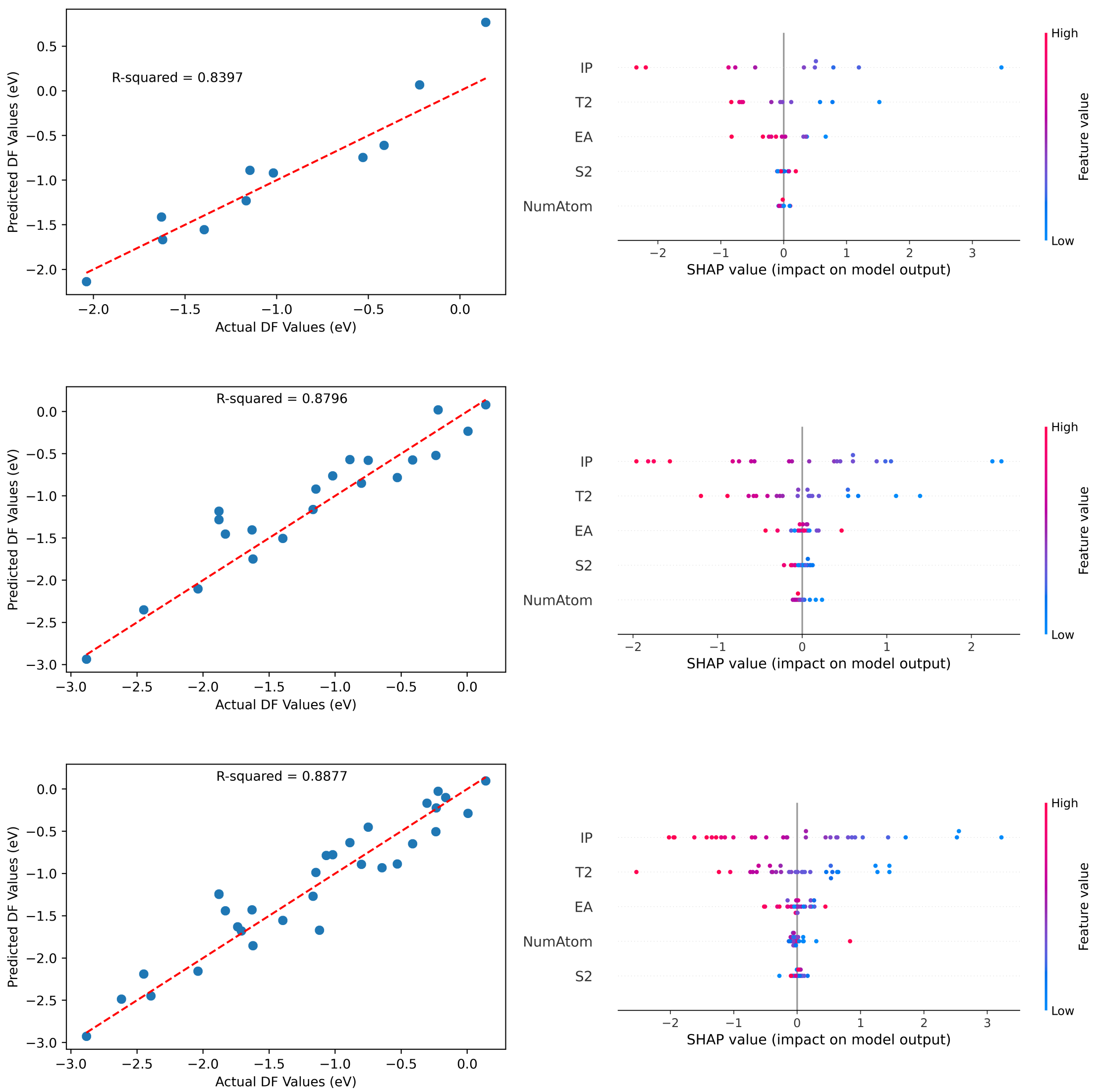


Figure 21: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

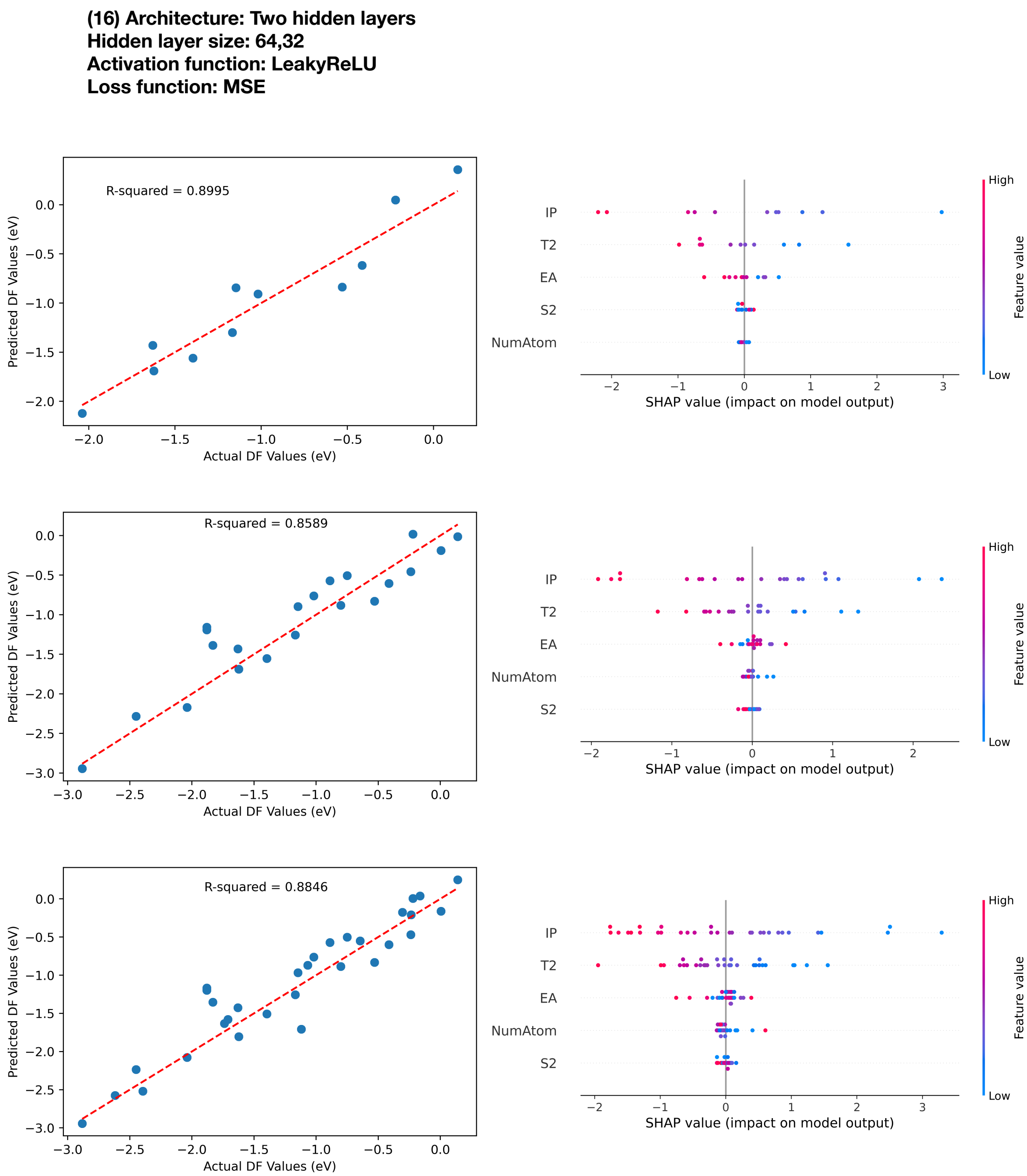


Figure 22: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(17) Architecture: Two hidden layers
Hidden layer size: 64,32
Activation function: LeakyReLU
Loss function: MAE

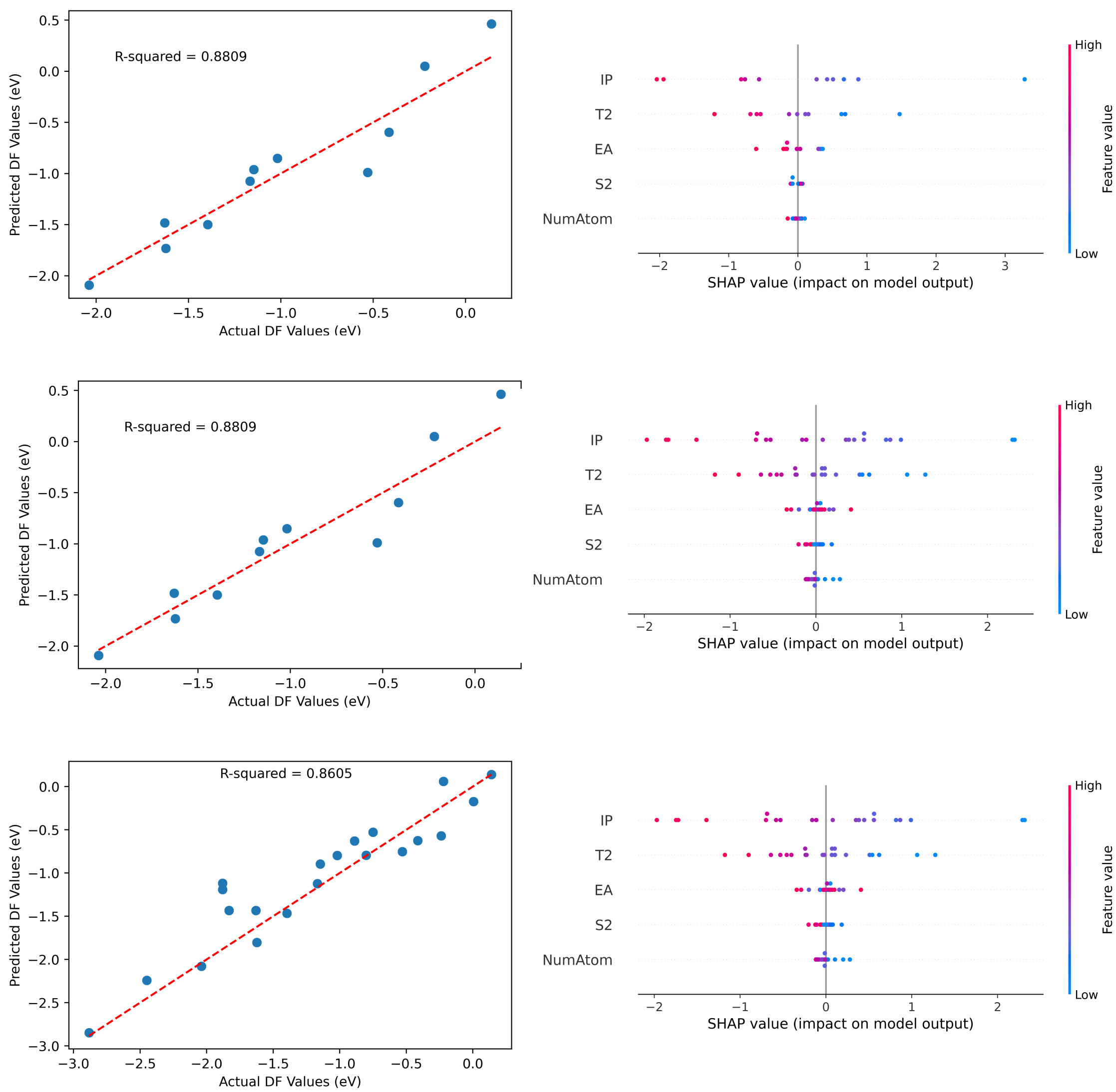


Figure 23: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(18) Architecture: Two hidden layers
Hidden layer size: 64,32
Activation function: LeakyReLU
Loss function: Smooth

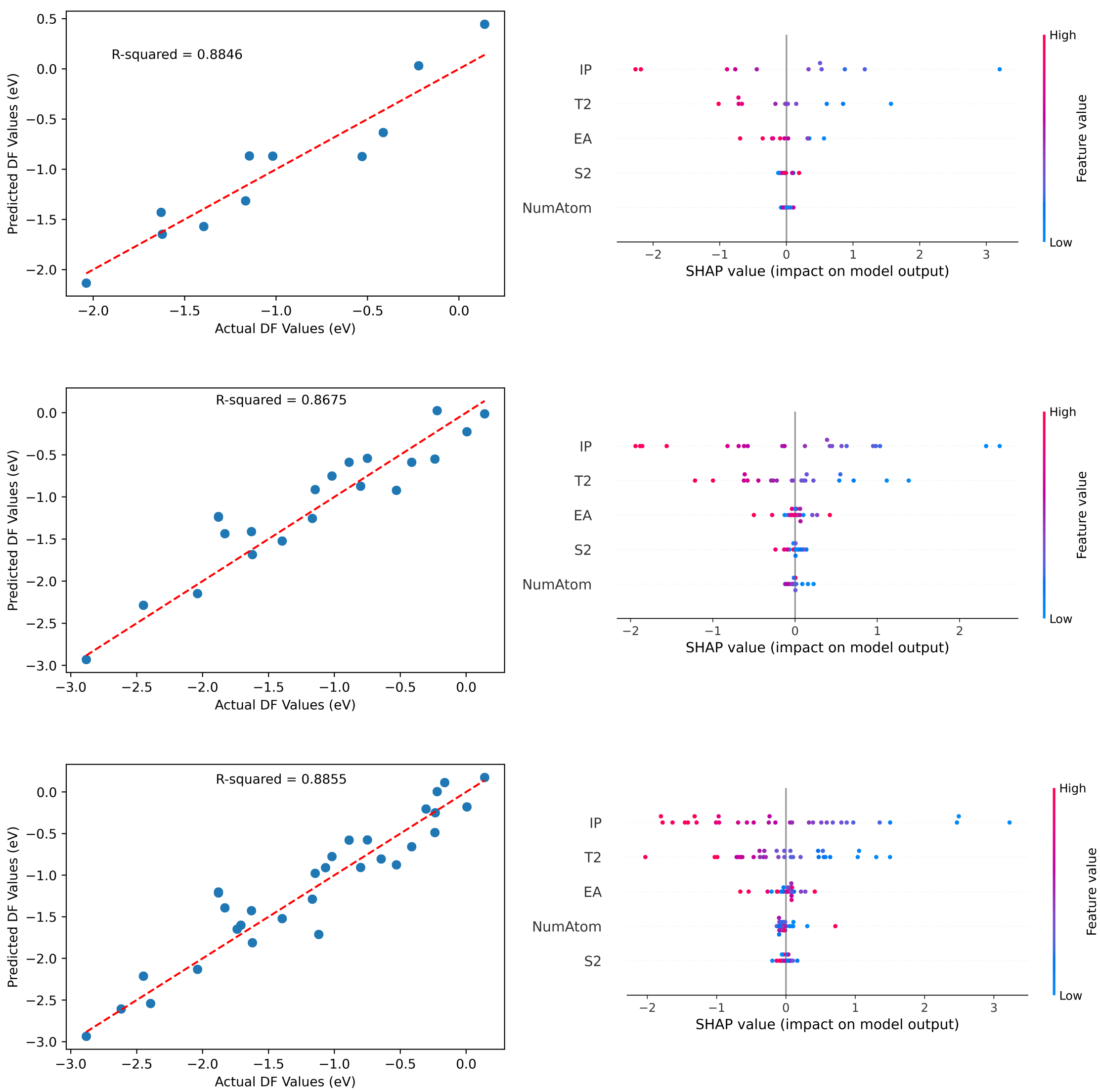


Figure 24: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

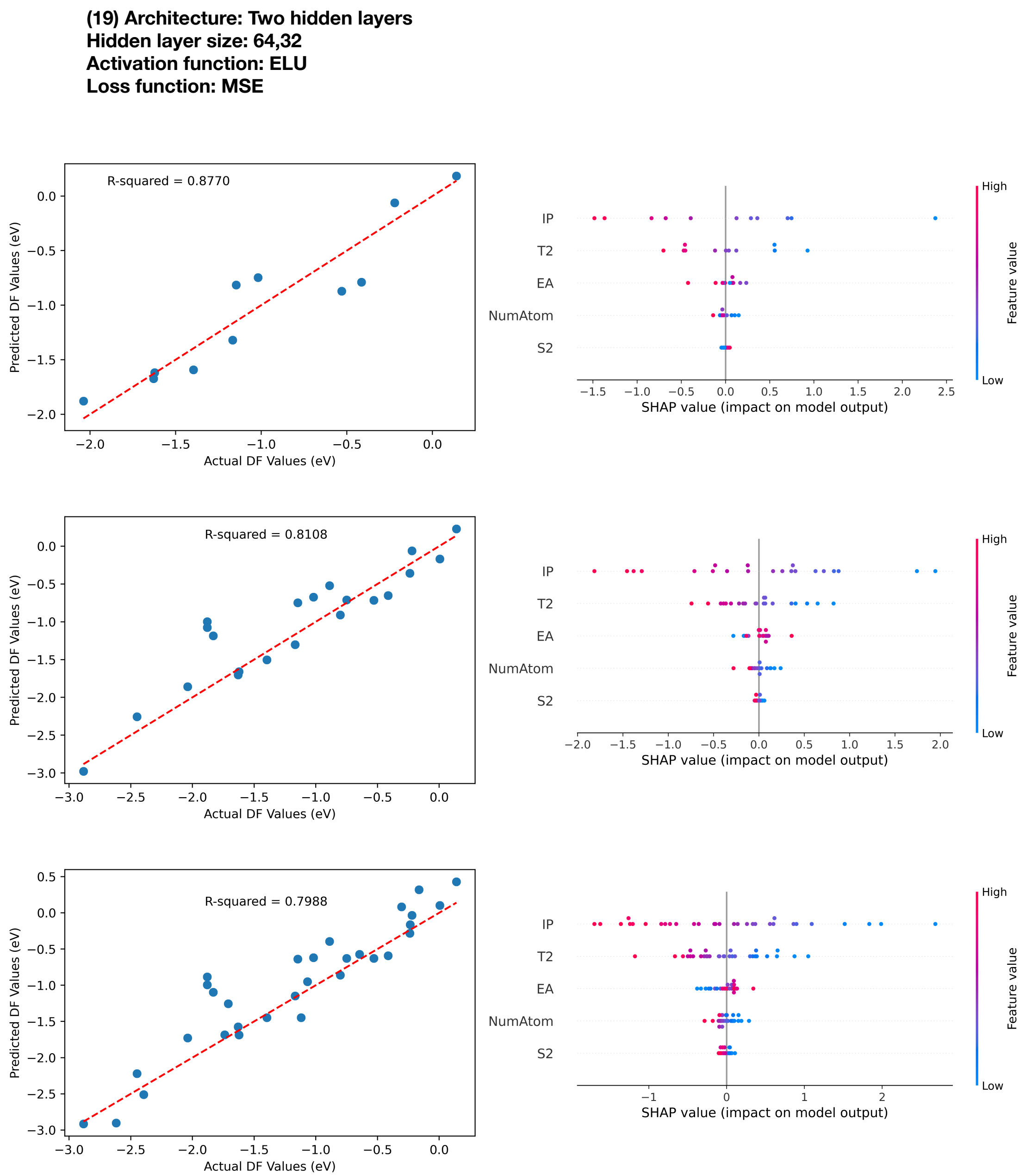


Figure 25: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

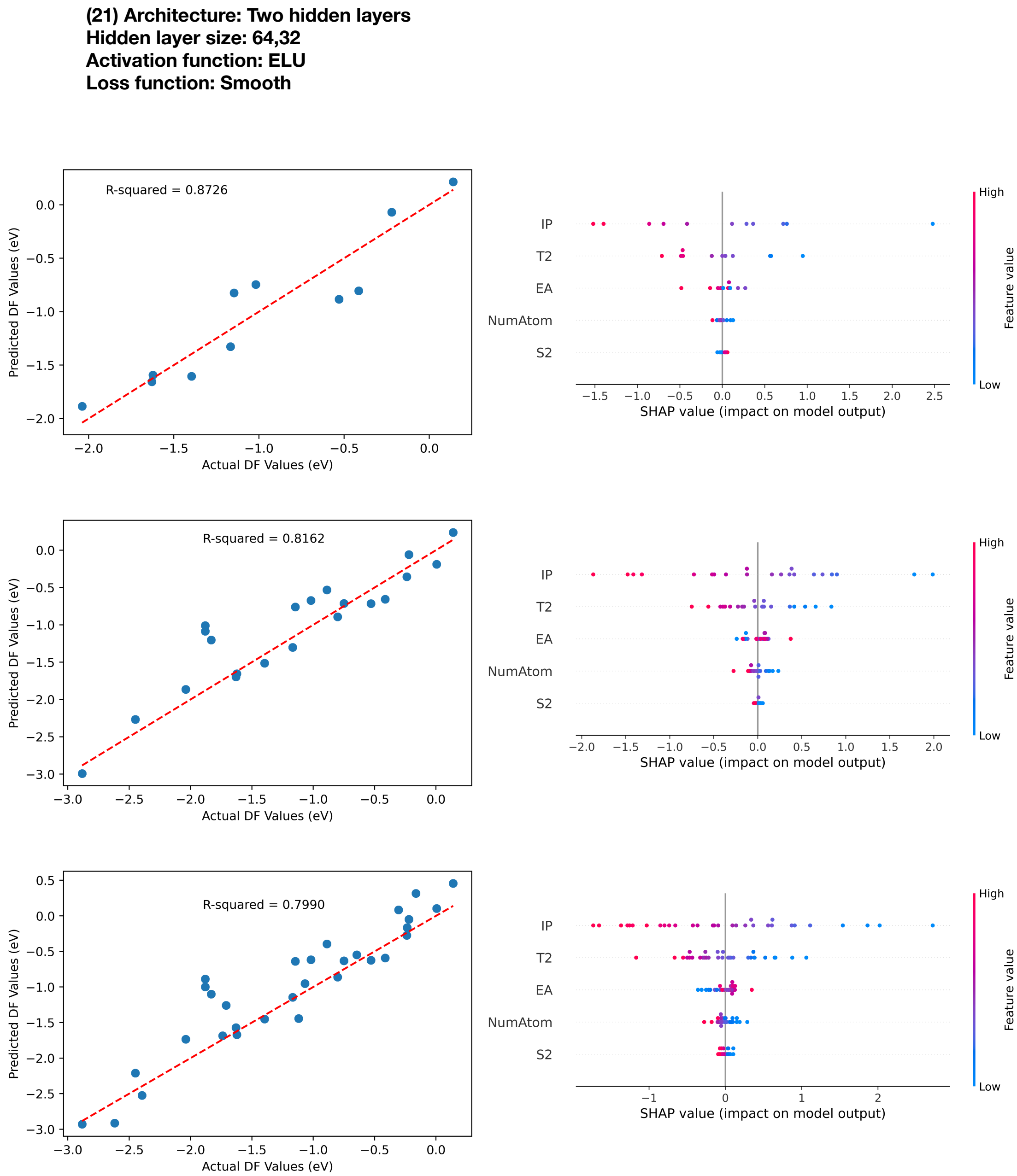


Figure 26: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

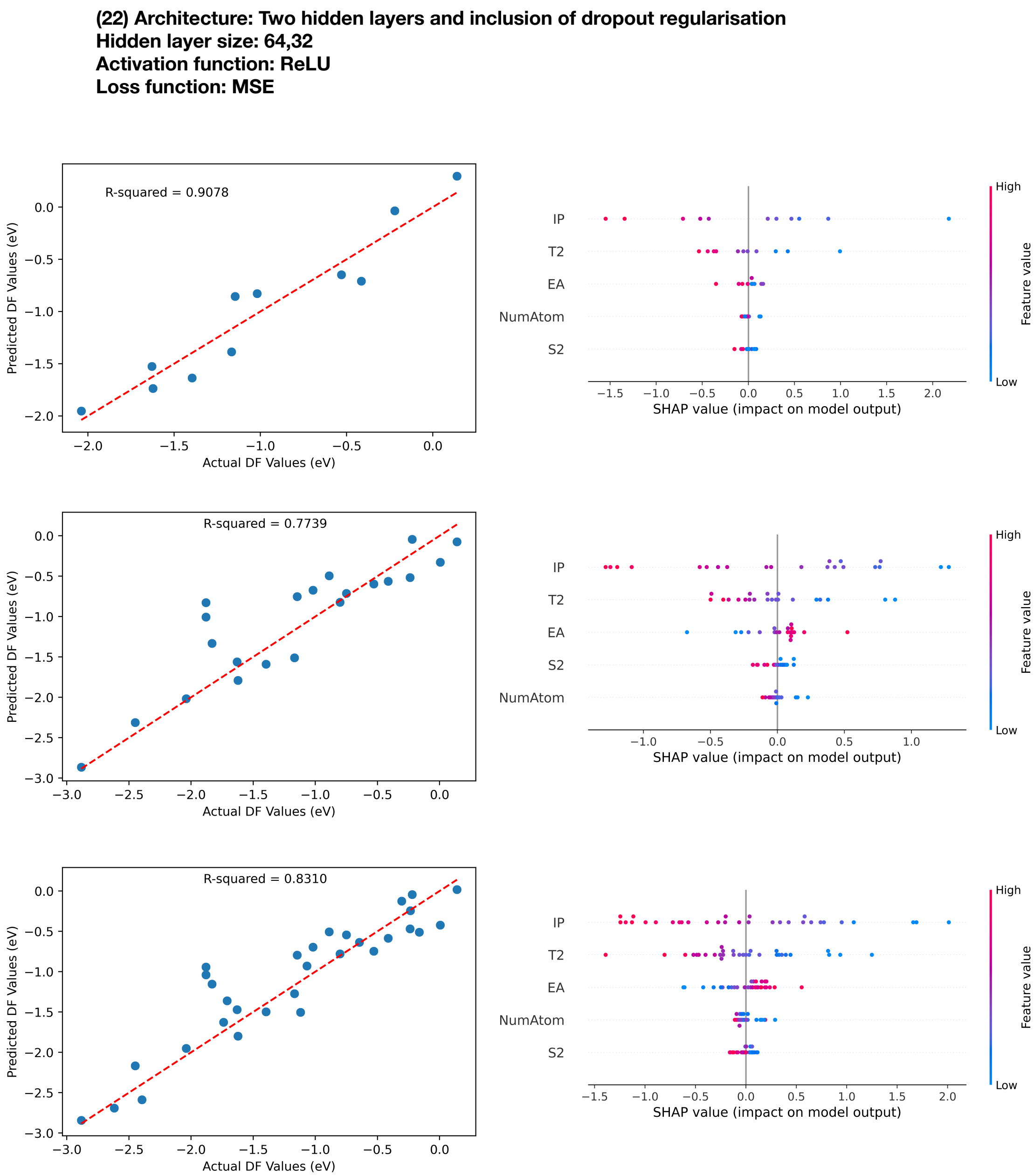


Figure 27: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

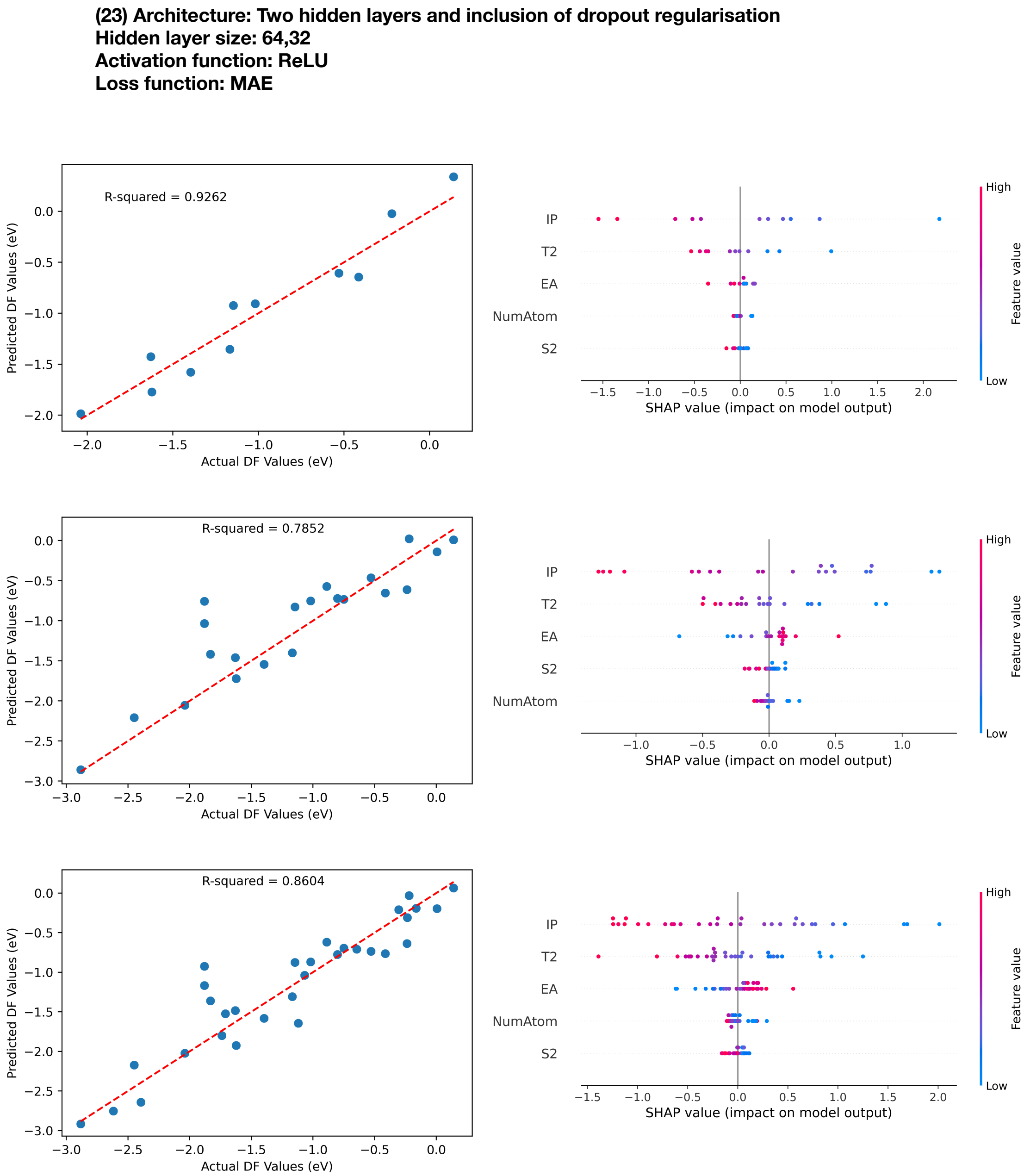


Figure 28: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

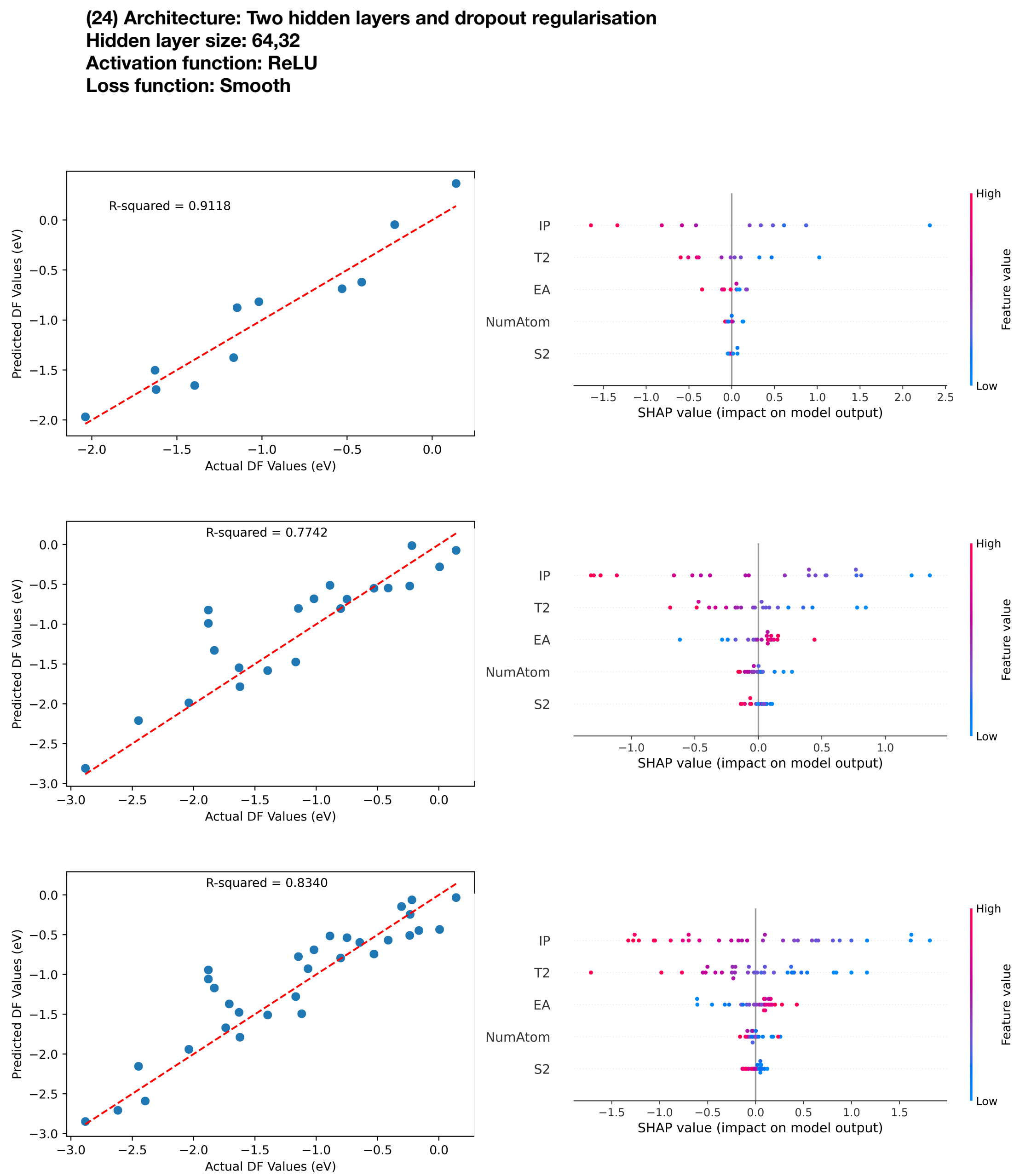


Figure 29: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(25) Architecture: Two hidden layers and dropout regularisation
Hidden layer size: 64,32
Activation function: LeakyReLU
Loss function: MSE

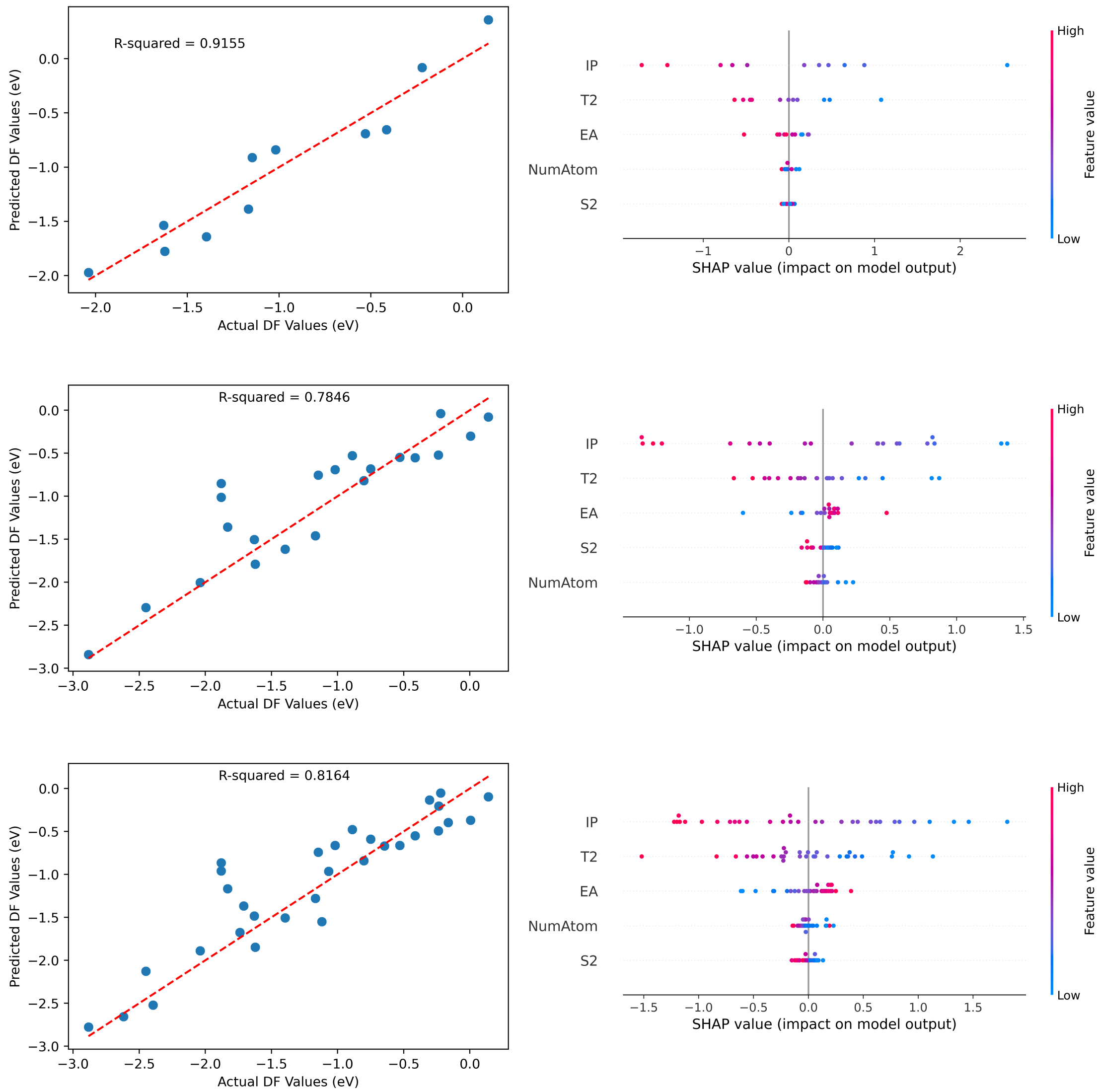


Figure 30: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(26) Architecture: Two hidden layers and dropout regularisation
Hidden layer size: 64,32
Activation function: LeakyReLU
Loss function: MAE

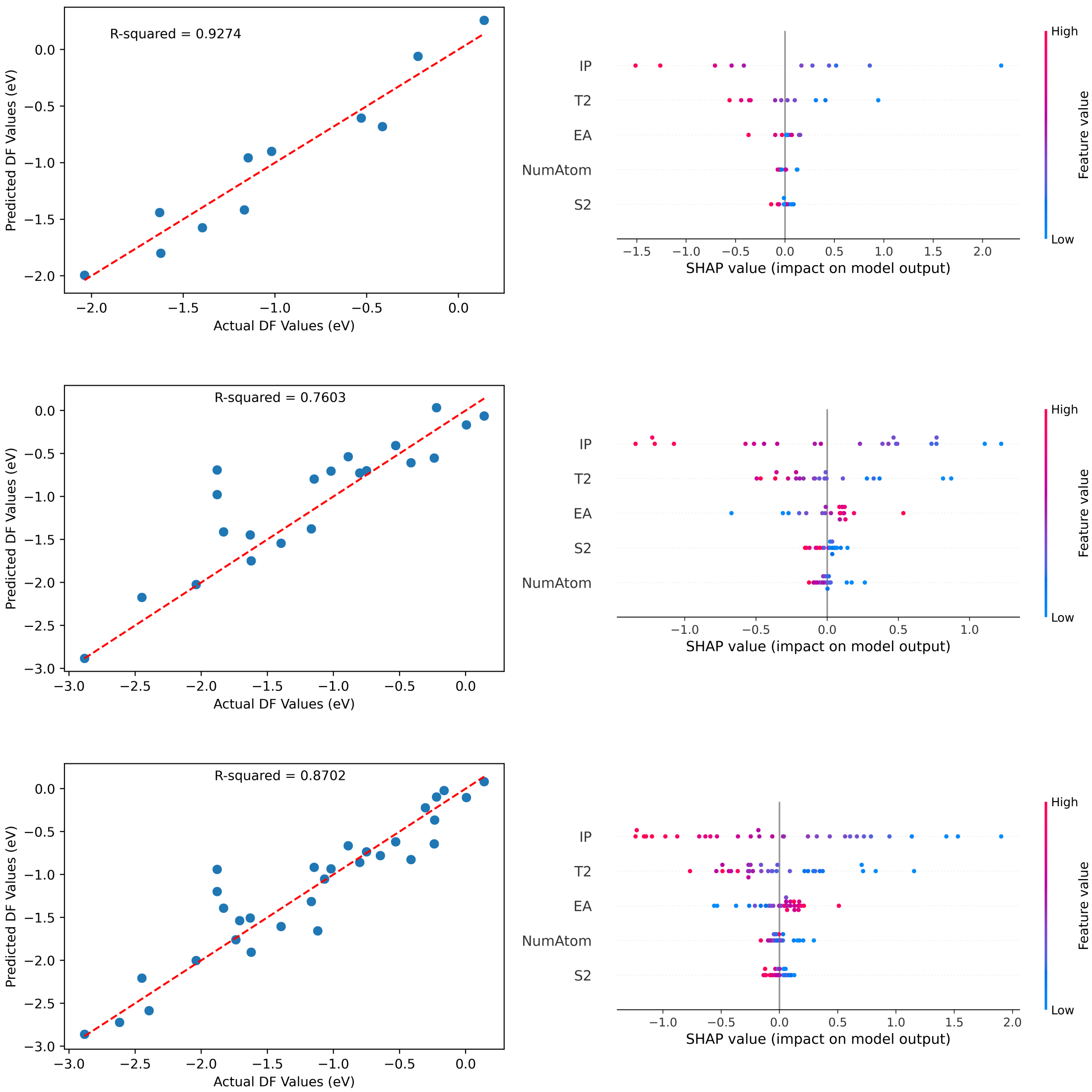


Figure 31: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

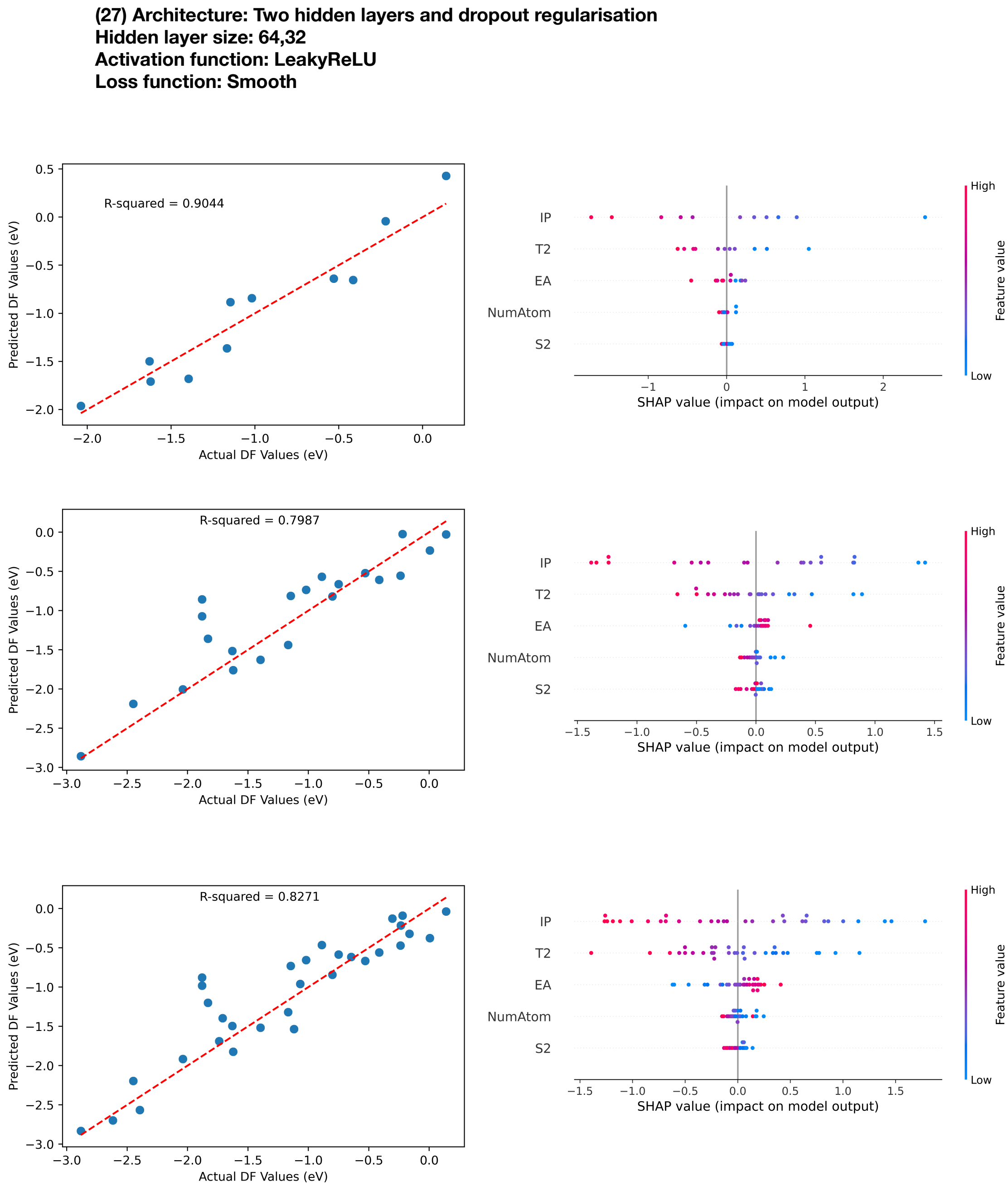


Figure 32: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

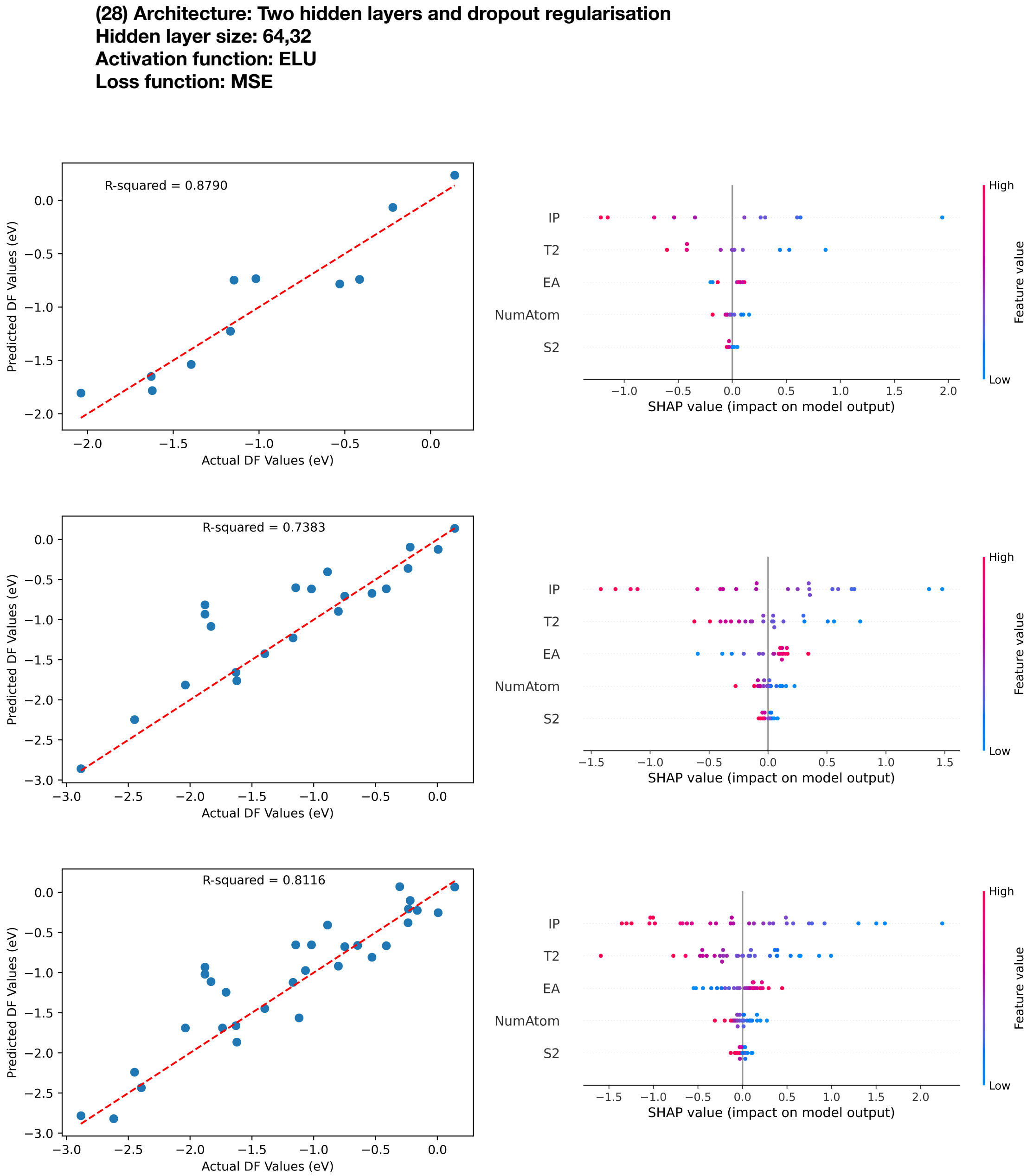


Figure 33: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(29) Architecture: Two hidden layers and dropout regularisation
Hidden layer size: 64,32
Activation function: ELU
Loss function: MAE

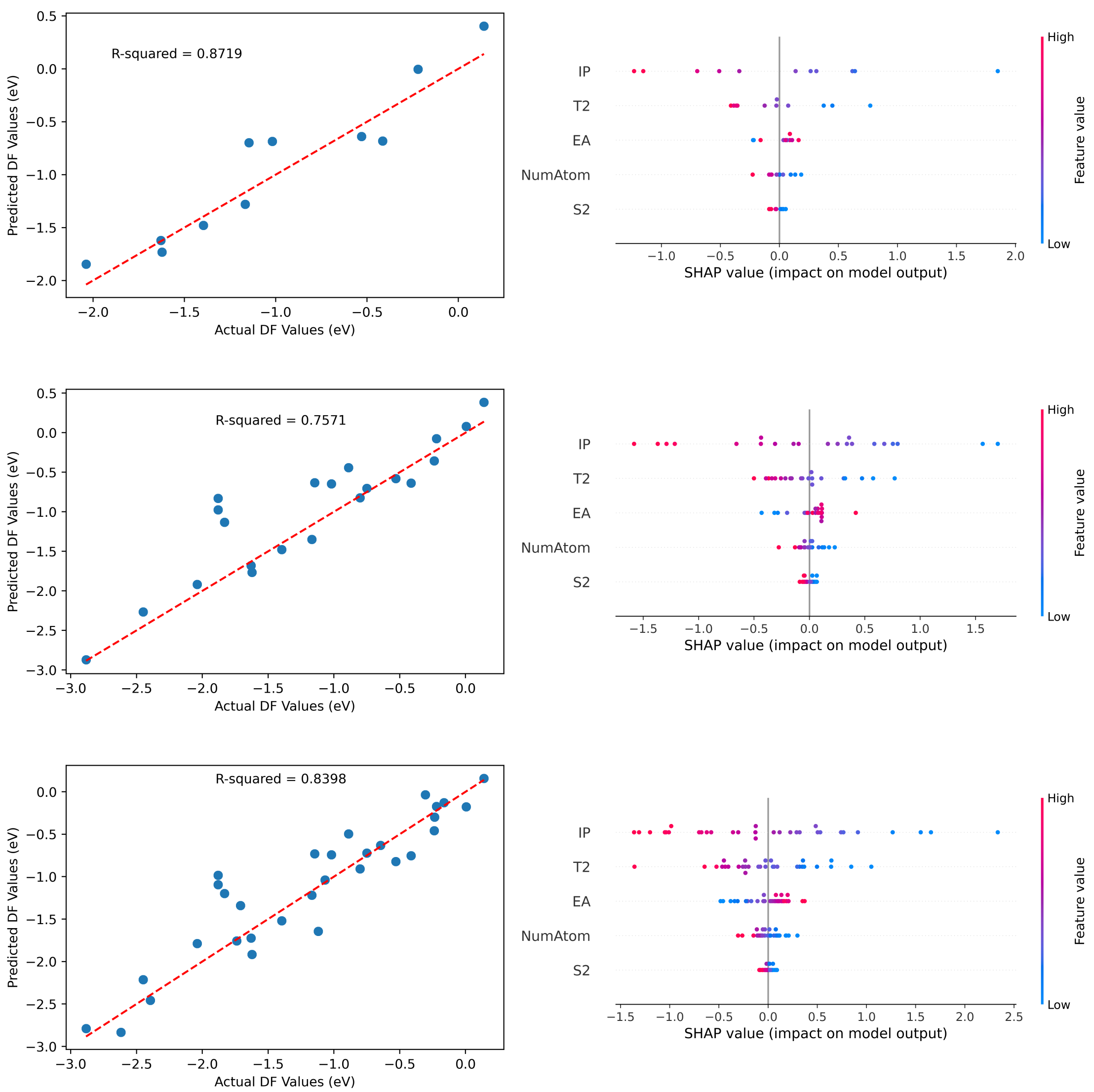


Figure 34: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

(30) Architecture: Two hidden layers and dropout regularisation
Hidden layer size: 64,32
Activation function: ELU
Loss function: Smooth

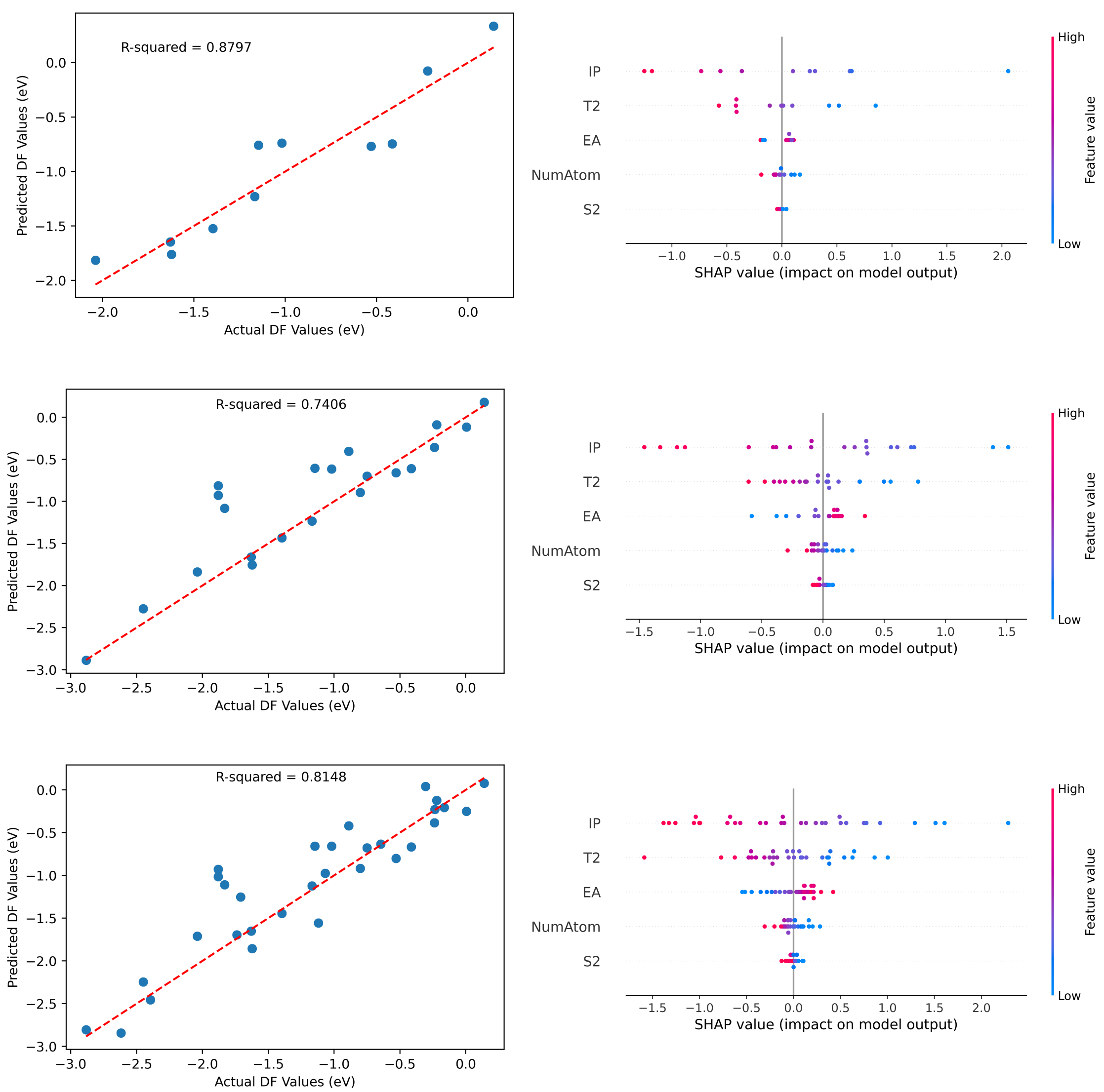


Figure 35: Actual vs predicted driving forces (in eV) for a neural netowrk whose configuration is explained at the begginign of the figure. The plots in the top correspond to a train/test split of 90/10, the plots in the middle to a train/test split of 80/20 and the plots at the bottom to a train/test spolit of 70/30.

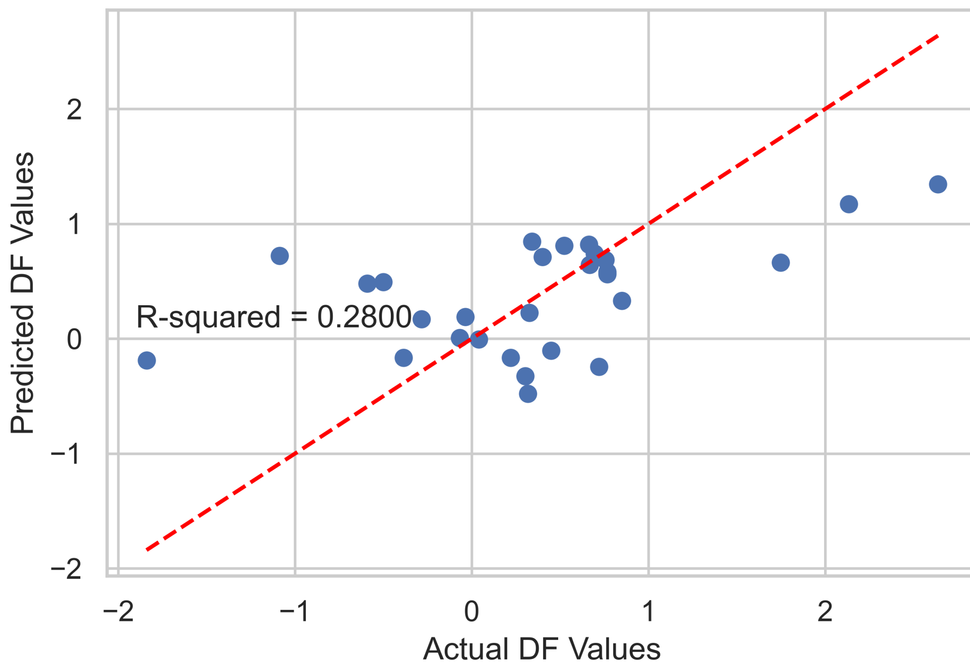


Figure 36: Actual vs predicted driving force (DF, in eV) obtained from a multiple linear regression. The red dashed line indicates the perfect linear agreement.

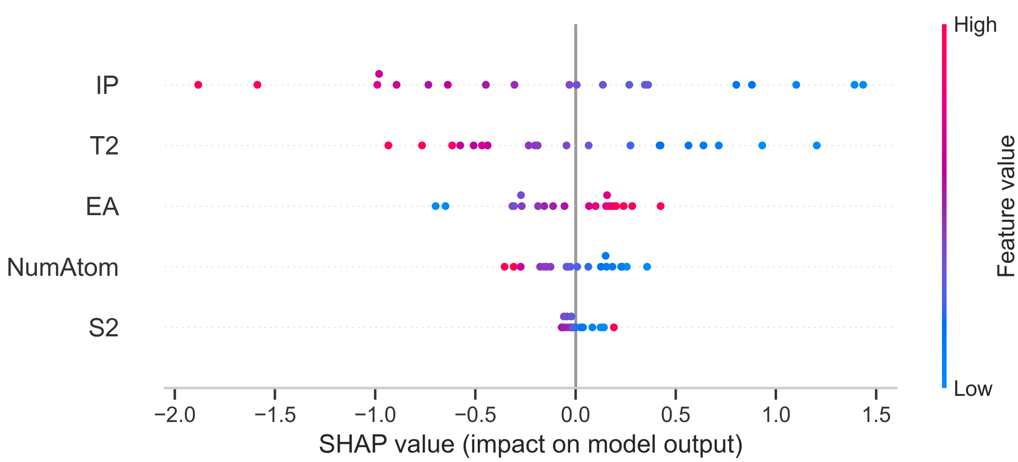


Figure 37: Beeswarm plot in which the descriptors have been ranked based on their mean absolute SHAP value. The following electronic states are represented: first and second triplets (T_1, T_2), first and second singlets (S_1, S_2), electron affinity (EA), ionization potential (IP) and total number of atoms (NumAtom). The feature value color scale represents the range of each feature. The presented plot is for fold 5 of cross-validation.

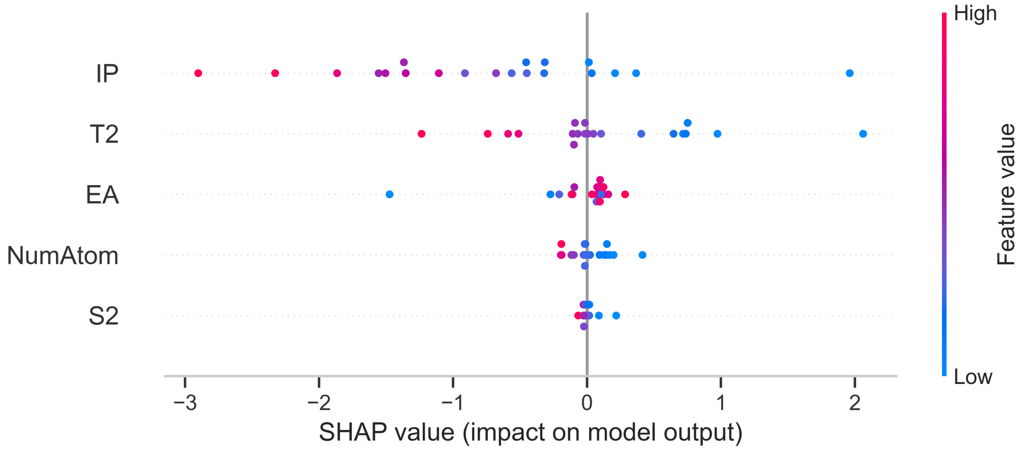


Figure 38: Beeswarm plot in which the descriptors have been ranked based on their mean absolute SHAP value. The following electronic states are represented: first and second triplets (T_1, T_2), first and second singlets (S_1, S_2), electron affinity (EA), ionization potential (IP) and total number of atoms (NumAtom). The feature value color scale represents the range of each feature. The presented plot is for fold 4 of cross-validation.

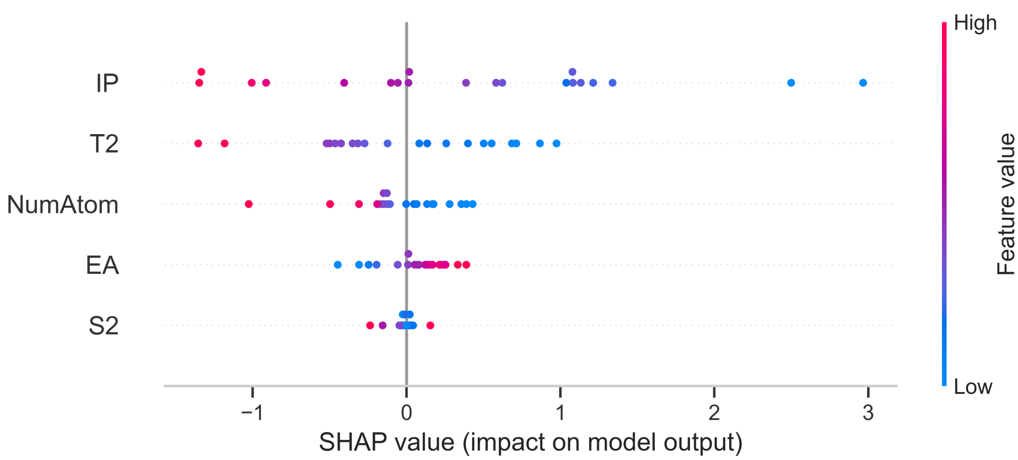


Figure 39: Beeswarm plot in which the descriptors have been ranked based on their mean absolute SHAP value. The following electronic states are represented: first and second triplets (T_1, T_2), first and second singlets (S_1, S_2), electron affinity (EA), ionization potential (IP) and total number of atoms (NumAtom). The feature value color scale represents the range of each feature. The presented plot is for fold 3 of cross-validation.

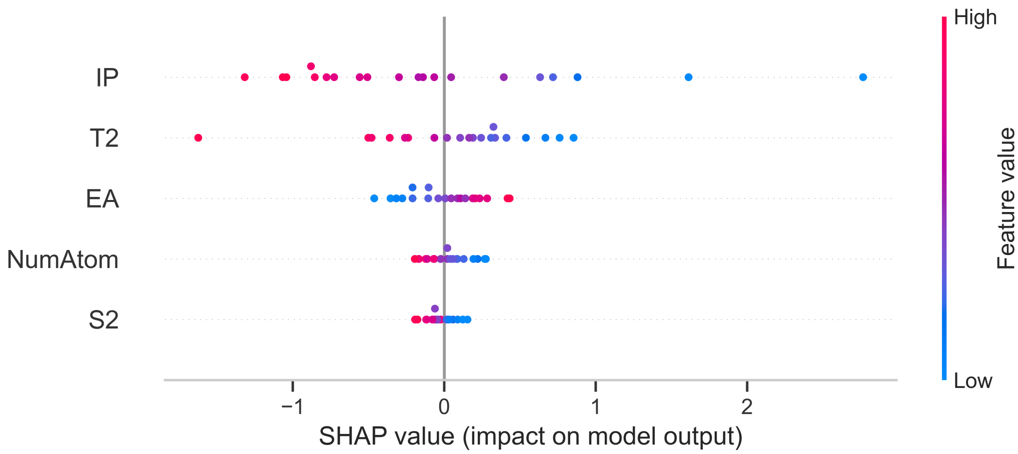


Figure 40: Beeswarm plot in which the descriptors have been ranked based on their mean absolute SHAP value. The following electronic states are represented: first and second triplets (T_1, T_2), first and second singlets (S_1, S_2), electron affinity (EA), ionization potential (IP) and total number of atoms (NumAtom). The feature value color scale represents the range of each feature. The presented plot is for fold 2 of cross-validation.