Additivity part 1 - Data

- Substituent,Benzene,,Pyridine,
- Combination,ΔVC(pred),ΔVC(cal),ΔVC(pred),ΔVC(cal)
- "NO2,NO2,NO2",63.6,65.7,59.7,63.7
- "NC,NC,NC",54.0,59.5,50.6,57.5
- "CHO,CHO,CHO",41.4,39.6,35.5,35.8
- "Cl,Cl,Cl",21.0,26.7,19.6,25.1
- "OH,OH,OH",-6.0,-1.9,-10.3,-4.6
- "Me,Me,Me",-9.9,-10.6,-11.2,-12.3
- "OMe,OMe,OMe",-15.0,-10.0,-18.3,-13.4
- "NH2,NH2,NH2",-27.0,-19.9,-33.4,-25.5
- "NO2,NC,CHO",53.0,51.3,48.6,53.9
- "NO2,CHO,OMe",30.0,28.3,25.6,28.4
- "NC,OMe,NH2",4.0,8.4,-0.4,7.0
- "NC,Cl,OH",23.0,28.6,20.0,28.3
- "OH,Me,NH2",-14.3,-11.1,-18.3,-9.5

- %%%%%%%%%%%%%% benzene_mean_val %%%%%%%%%%%%%%

	R^2	MAE	MSE	MAPE	MedAE
Linear Regression	0.030789	23.508366	775.411750	1.026871	19.125395
Ridge	0.875168	7.109008	102.667214	0.186575	2.663963
Random Forest	0.739952	12.685167	212.997317	0.379778	11.364500
Multi-layer Perceptron	0.640093	14.881345	290.578446	0.450464	15.053874

- %%%%%%%%%%%%%% benzene_sum_val %%%%%%%%%%%%%%

	R^2	MAE	MSE	MAPE	MedAE
Linear Regression	0.991508	1.230847	3.729706	0.060466	1.424942
Ridge	0.991322	1.331812	3.852332	0.060712	1.428169
Random Forest	0.481229	12.531000	268.474970	0.634259	8.262000
Multi-layer Perceptron	0.794099	9.581244	109.852056	0.421857	10.836345

- %%%%%%%%%%%%%% pyridine_mean_val %%%%%%%%%%%%%%

	R^2	MAE	MSE	MAPE	MedAE
Linear Regression	-0.071576	12.954087	227.277350	0.402694	16.521082
Ridge	-0.166467	14.048085	247.171187	0.447433	17.786699
Random Forest	-1.032685	17.924000	430.458035	0.506462	13.056500
Multi-layer Perceptron	-2.102150	25.431644	657.136919	0.891334	25.539679

- %%%%%%%%%%%%%% pyridine_sum_val %%%%%%%%%%%%%%

	R^2	MAE	MSE	MAPE	MedAE
Linear Regression	0.975874	1.905188	15.527231	0.354354	0.626821
Ridge	0.974969	2.106037	16.106140	0.372908	0.705771
Random Forest	0.868838	8.188333	83.266695	0.443761	6.107000
Multi-layer Perceptron	0.811018	9.757333	120.723271	0.655735	8.940324

Advanced metrics result

pyridine_sum_val
Linear Regression
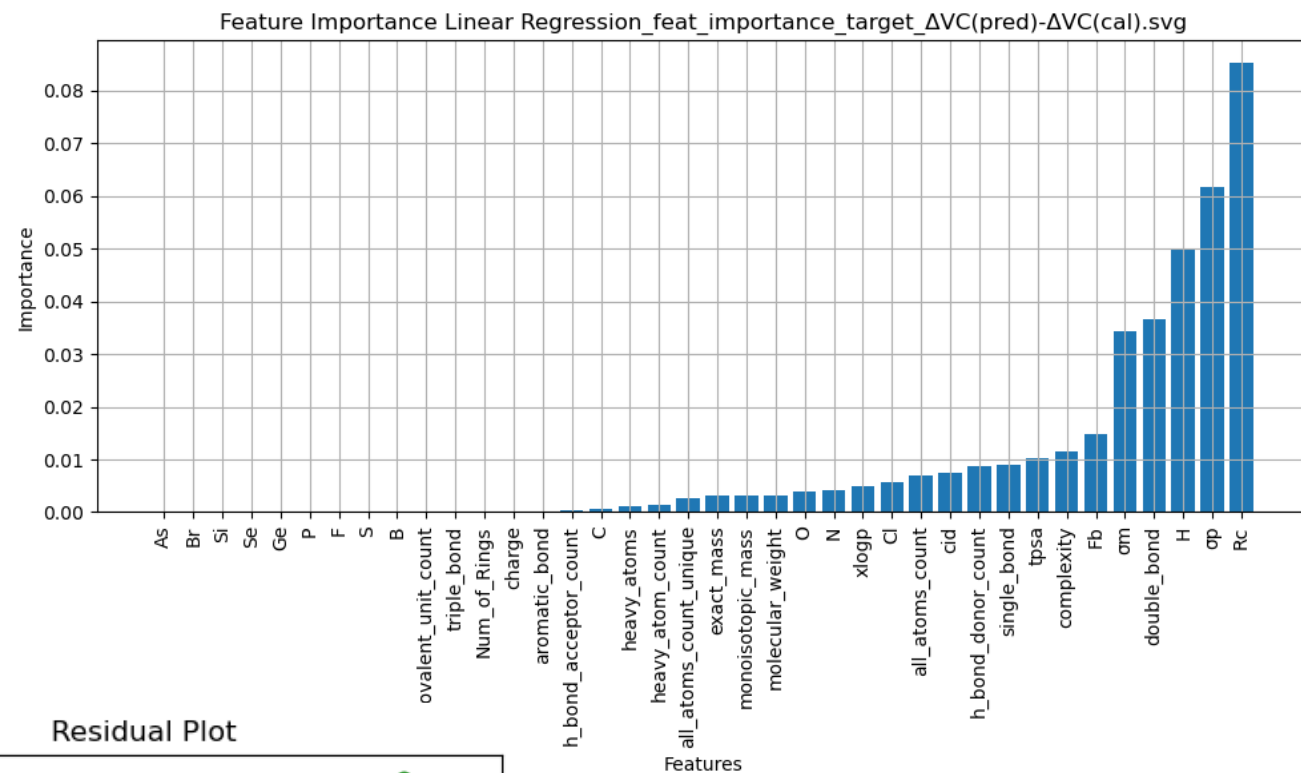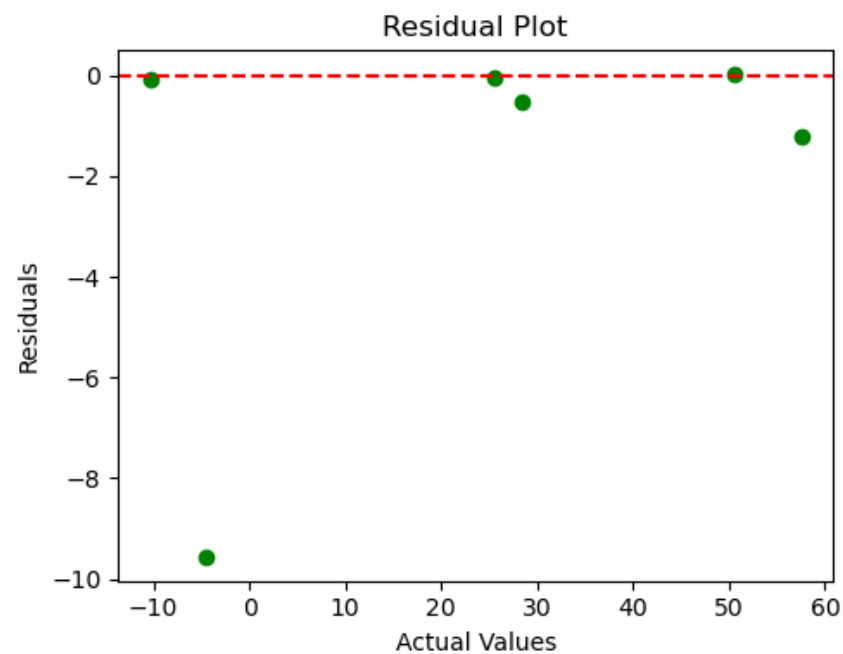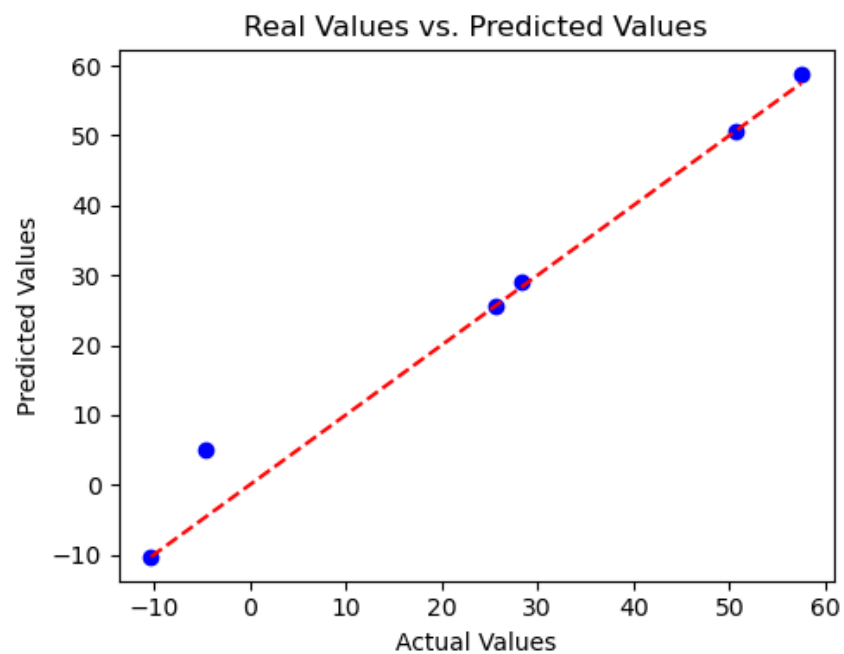
benzene_sum_val
Linear Regression
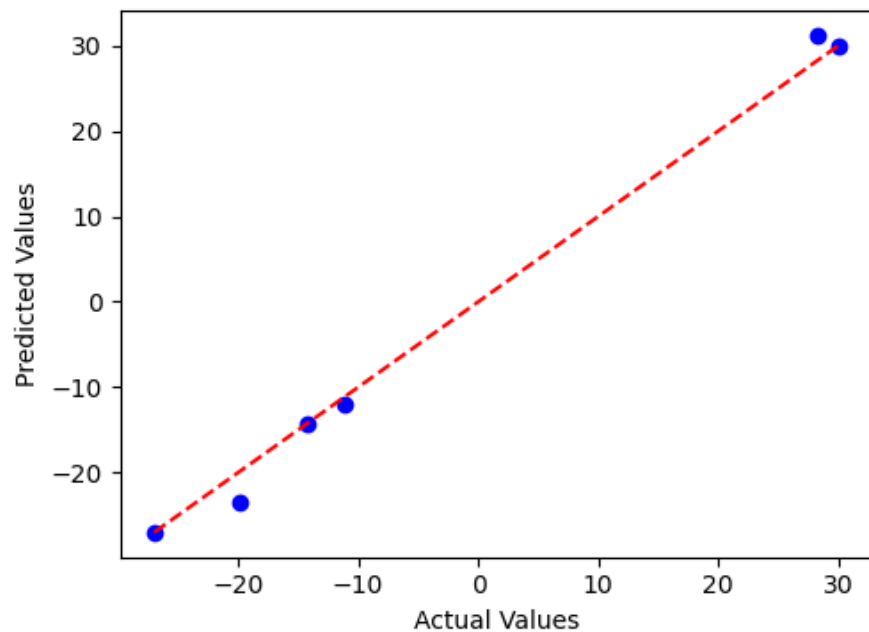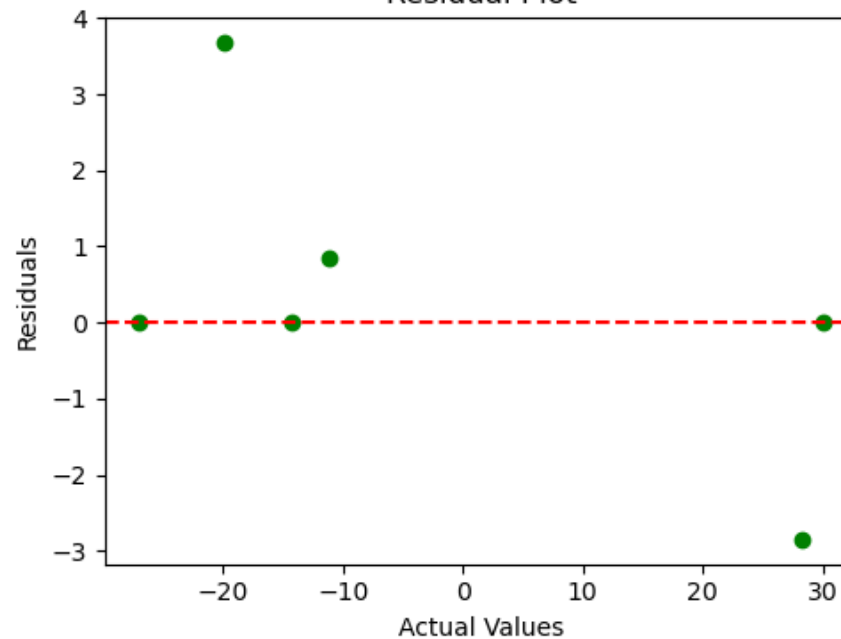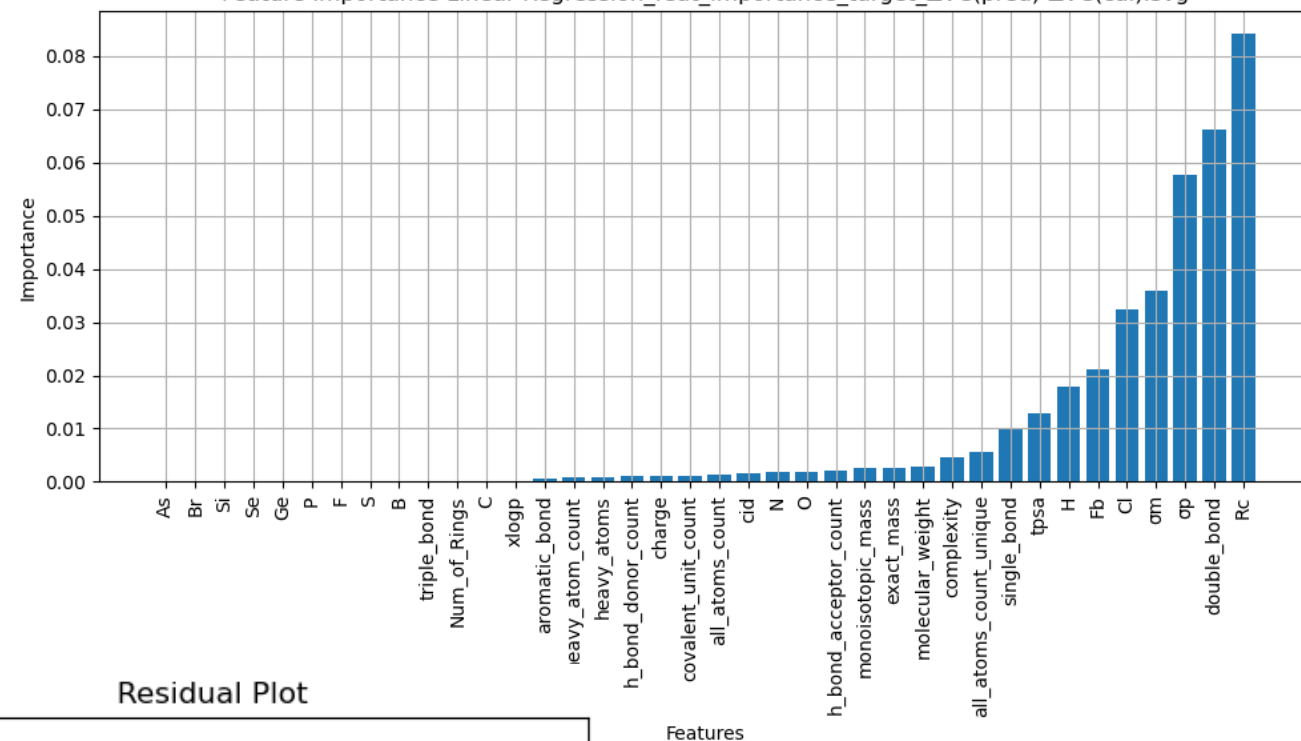
Additivity part 2 - Data

- Substituent,Pyrene,Pyrene,Butadiene,Butadiene,Butadiyne,Butadiyne
- Combination,ΔVC(pred),ΔVC(cal),ΔVC(pred),ΔVC(cal),ΔVC(pred),ΔVC(cal)
- "NO2,NO2",50.8,51.7,58.6,62.4,61.7,65.2
- "NC,NC",41.4,41.8,44.2,46.1,47.9,49.7
- "CHO,CHO",16.2,16.7,20.2,18.0,18.1,19.5
- "Cl,Cl",44.0,44.1,40.2,40.7,27.6,27.5
- "OH,OH",40.6,40.6,25.6,25.6,20.7,20.3
- "Me,Me",3.9,3.9,-5.2,-5.6,-16.4,-17.2
- "OMe,OMe",37.0,37.0,28.6,27.6,13.5,11.9
- "NH2,NH2",23.0,22.9,9.2,7.8,-5.5,-6.0
- "NO2,NC",49.5,50.2,54.3,63.5,58.6,62.6
- "Cl,OH",45.2,45.1,26.8,33.4,18.1,17.6
- "Me,NH2",25.3,25.2,13.9,21.2,-22.5,-23.9
- "NC,Me",14.4,14.5,14.8,21.2,16.5,17.0
- "CHO,OMe",45.8,45.6,51.0,52.1,-7.9,-8.0

Advanced metrics result
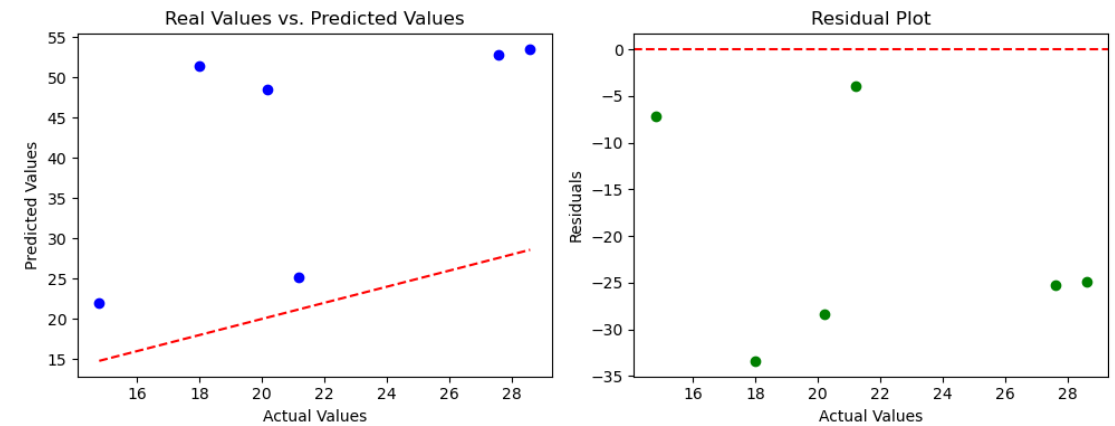
- %%%%%%%%%%%%%% Pyrene_sum_val %%%%%%%%%%%%%%

	R^2	MAE	MSE	MAPE	MedAE
Linear Regression	-5.277286	22.940000	713.304167	1.185936	25.995000
Ridge	-1.756561	16.613795	313.240087	0.802664	17.463418
Random Forest	-2.232027	16.849167	367.271589	0.788154	16.568000
Multi-layer Perceptron	0.183778	7.797503	92.788831	0.249821	7.732875

- %%%%%%%%%%%%%% Butadiene_sum_val %%%%%%%%%%%%%%

	R^2	MAE	MSE	MAPE	MedAE
Linear Regression	-25.086817	20.484722	539.689759	0.951703	25.051489
Ridge	-14.423126	15.400684	313.053474	0.770000	10.761975
Random Forest	-24.652795	21.437833	540.111914	1.126243	25.429500
Multi-layer Perceptron	-4.708690	8.194730	124.318141	0.340405	4.910471

- %%%%%%%%%%%%%% Butadiyne_sum_val %%%%%%%%%%%%%%

	R^2	MAE	MSE	MAPE	MedAE
Linear Regression	0.780495	6.520833	61.990104	0.247723	5.475000
Ridge	0.780443	6.746804	62.030717	0.249387	5.740049
Random Forest	-0.546711	20.259833	436.320651	0.615886	23.063000
Multi-layer Perceptron	0.890712	4.590308	31.134301	0.116155	2.854944

- Pyrene_sum_val
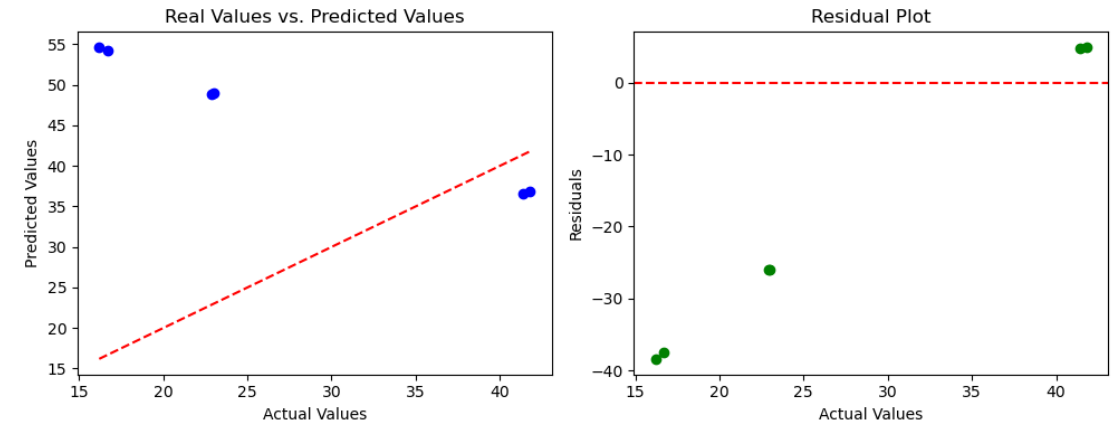
- Butadiene_sum_val

- Butadiyne_sum_val