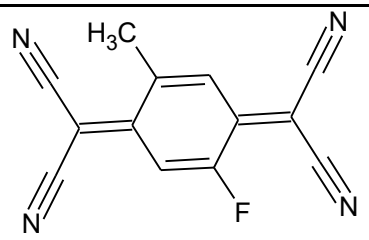
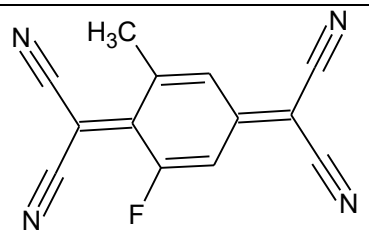
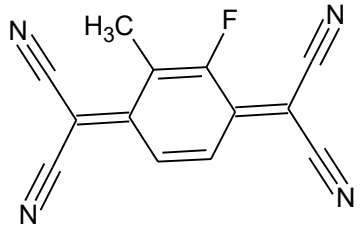
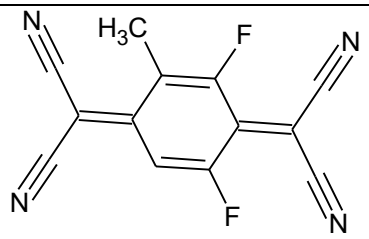
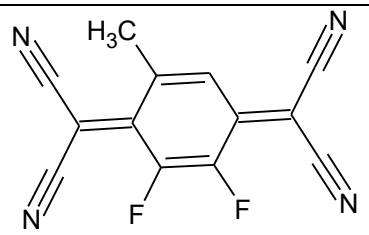
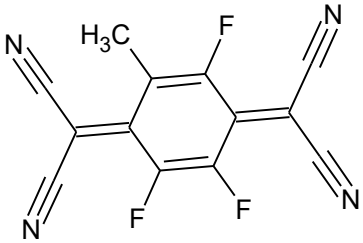
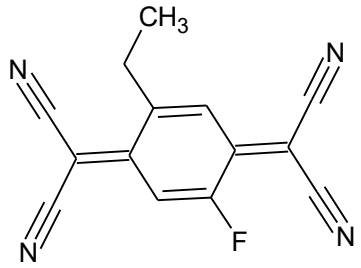
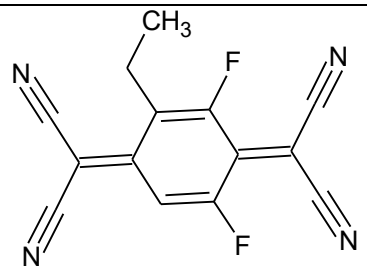
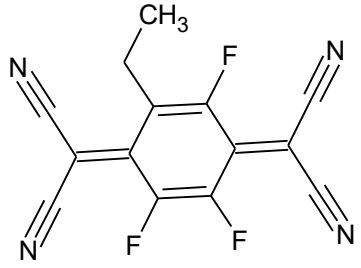
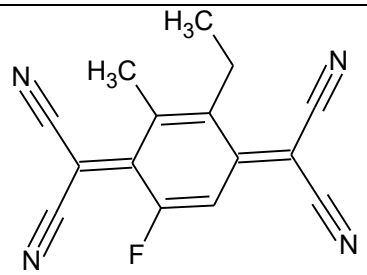
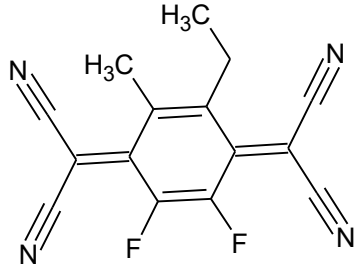
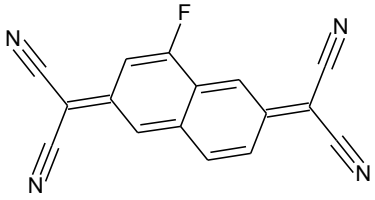
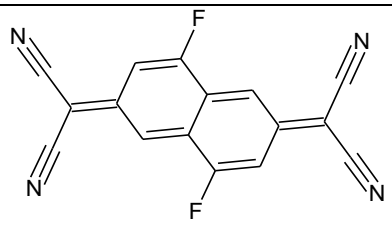
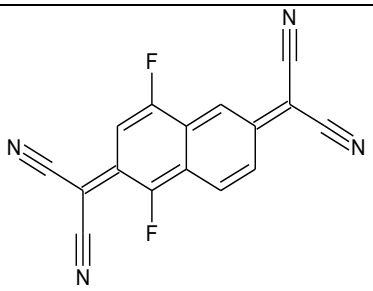
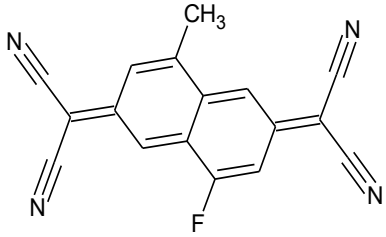
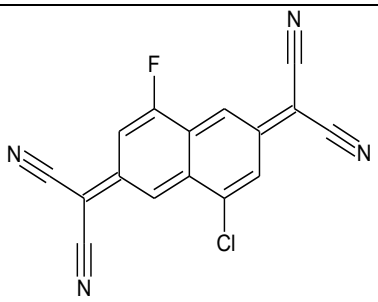
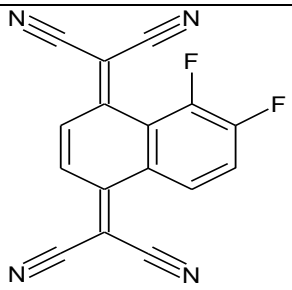
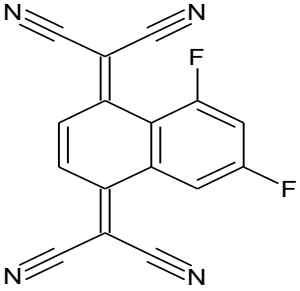
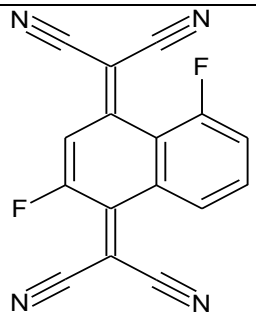
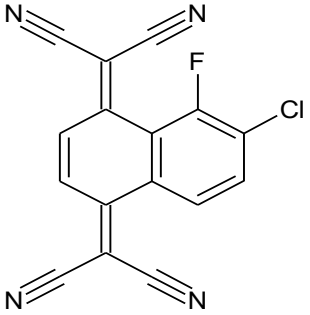
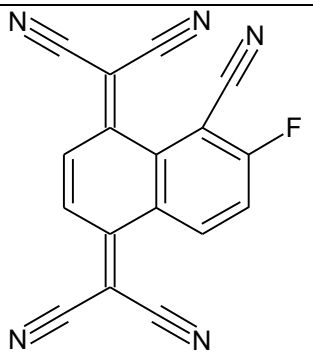
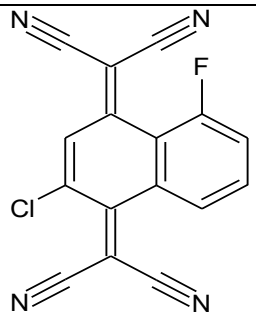
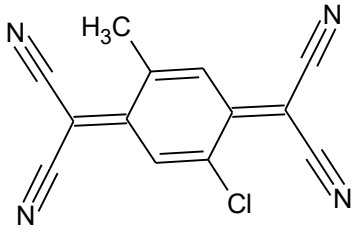
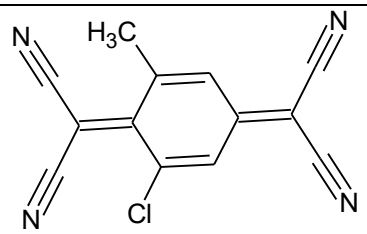
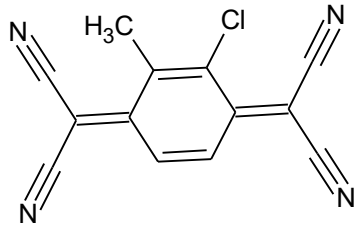
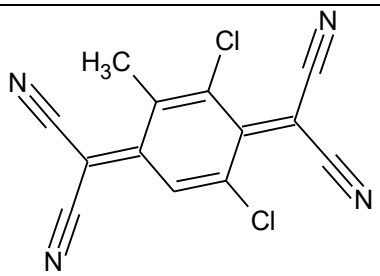
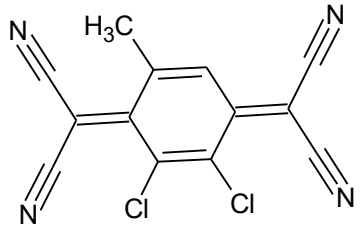
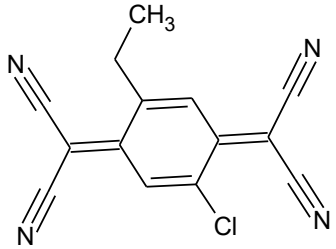
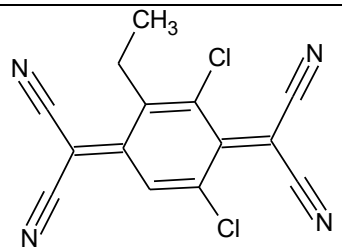
Table 2. Structures of the molecules with electronic affinities, enthalpy and free enthalpy of formation (in kcal/mol), entropy of formation (in cal/mol.K) and predicted values of the first reduction potentials by the model

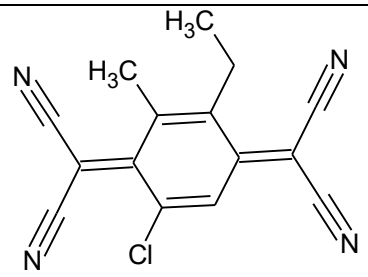
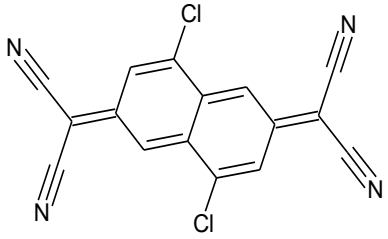
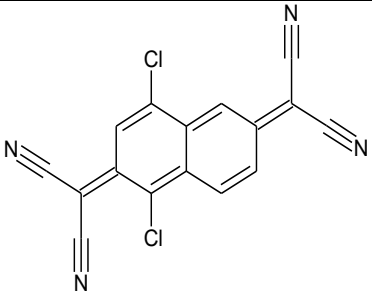
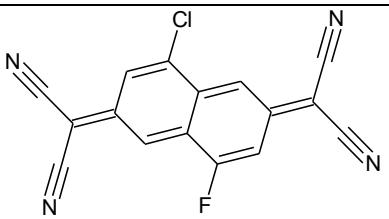
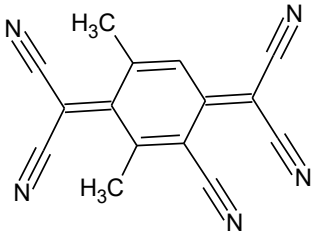
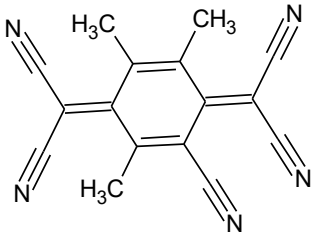
CODE	STRUCTURE	EA(eV)	$\Delta_f H^0_{298}$	$\Delta_f S^0_{298}$	$\Delta_f G^0_{298}$	E^1_{theo}(eV)
HA_1		4.8296	-679.3970	-683.7894	**-475.5252**	**+0.225**
HA_2		4.8301	-678.4663	-683.4527	**-474.6949**	**+0.226**
HA_3		4.8232	-679.5116	-683.5790	**-475.7025**	**+0.222**
HA_4		4.9333	-722.1295	-689.8052	**-516.4641**	**+0.285**
HA_5		4.9428	-717.2853	-689.5758	**-511.6883**	**+0.290**
HA_6		5.0361	-759.4023	-695.2990	**-552.0989**	**+0.343**

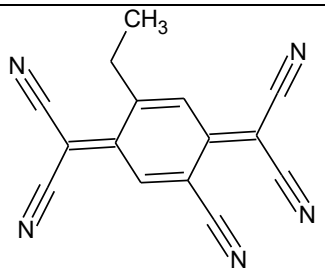
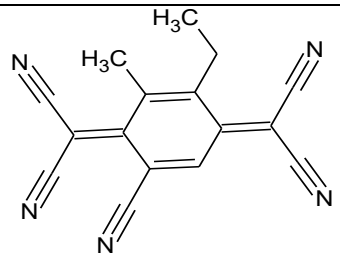
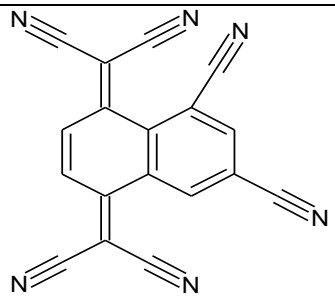
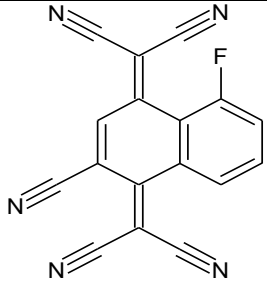
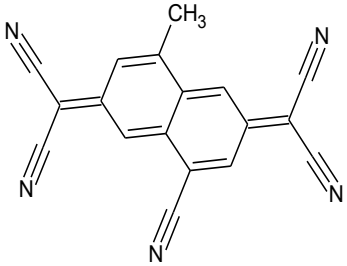
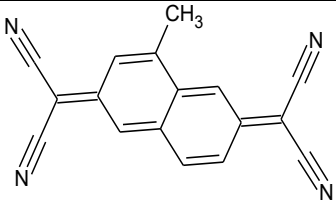
HA_7		4.7811	-727.1942	-769.7532	**-497.6922**	**+0.198**
HA_8		4.9224	-769.9580	-775.3523	**-538.7867**	**+0.278**
HA_9		5.0242	-807.1517	-780.9998	**-574.2966**	**+0.336**
HA_10		4.7150	-769.1650	-856.1801	**-513.8949**	**+0.160**
HA_11		4.8222	-806.5883	-861.7518	**-549.6571**	**+0.221**
HA_12		4.8911	-786.3961	-790.4428	**-550.7255**	**+0.260**

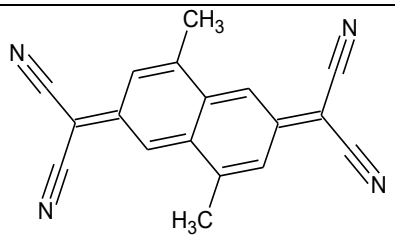
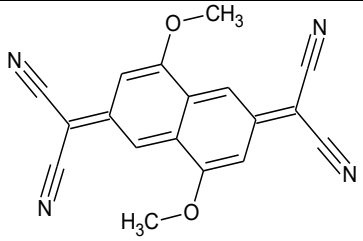
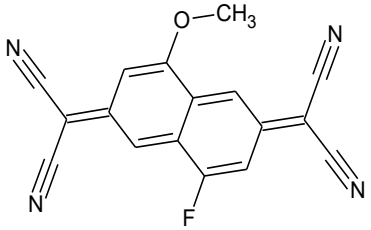
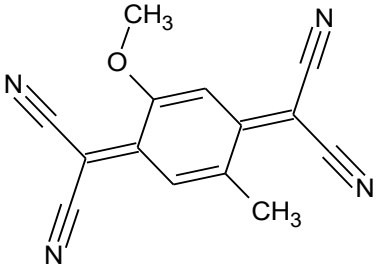
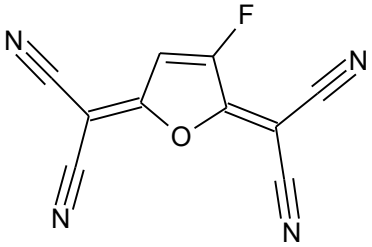
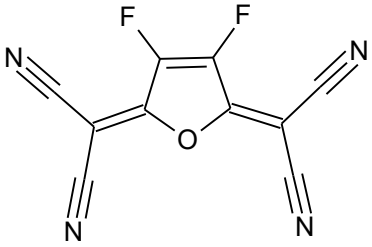
HA_13		4.9809	-833.1055	-796.6859	**-595.5736**	**+0.312**
HA_14		4.9624	-829.9836	-796.7301	**-592.4385**	**+0.301**
HA_15		4.8132	-839.3523	-876.1204	**-578.1370**	**+0.216**
HA_16		4.9169	-738.4343	-789.3573	**-503.0874**	**+0.275**
HA_17		4.4845	-825.9193	-798.0371	**-587.9845**	**+0.028**
HA_18		4.5033	-829.7167	-798.1297	**-591.7543**	**+0.039**

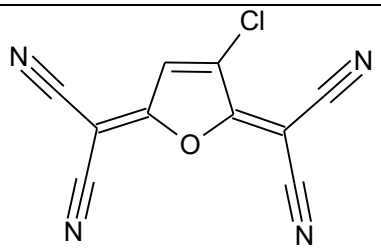
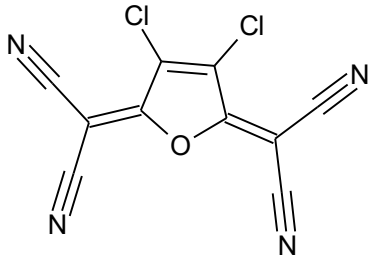
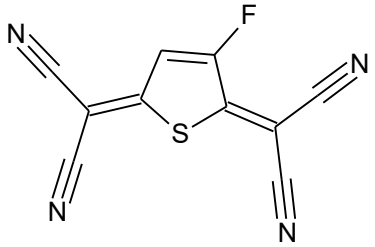
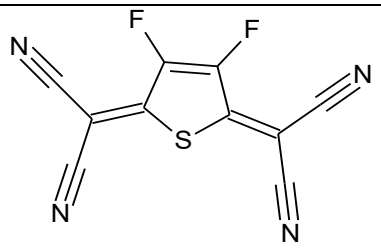
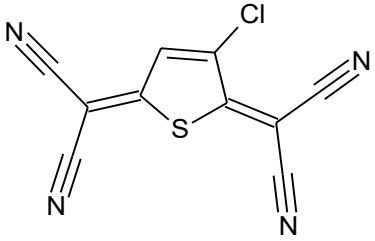
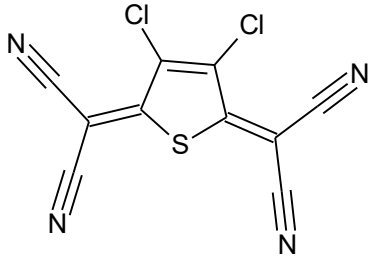
HA_19		4.4924	-825.9167	-798.4139	**-587.8696**	**+0.033**
HA_20		4.5177	-781.1794	-797.1347	**-543.5137**	**+0.047**
HA_21		4.4965	-809.6874	-835.6944	**-560.5252**	**+0.035**
HA_22		4.4088	-775.5356	-797.4883	**-537.7644**	**-0.015**
HA_23		4.8546	-629.0663	-682.3882	**-425.6123**	**+0.240**

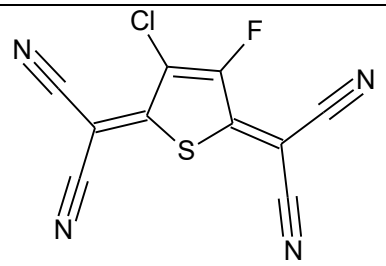
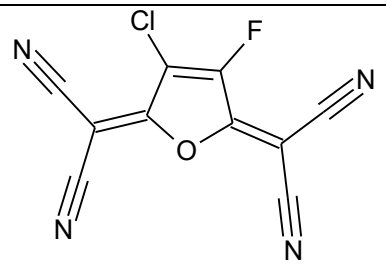
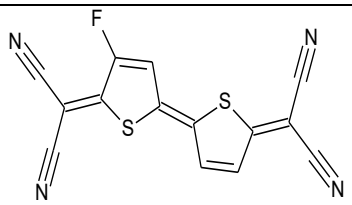
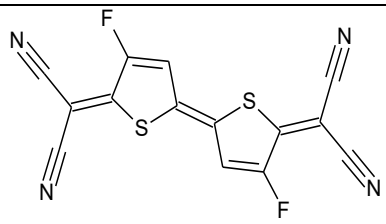
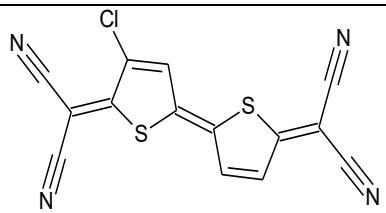
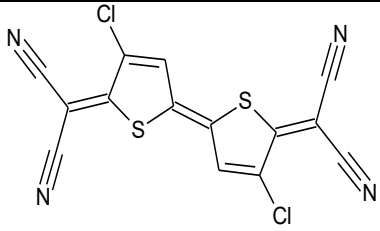
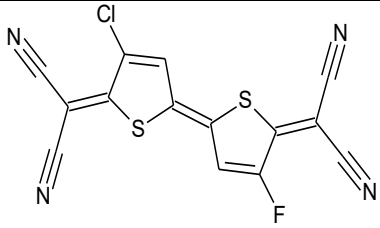
HA_24		4.8516	-625.6382	-678.3199	**-423.3971**	**+0.238**
HA_25		4.8440	-625.8938	-679.7700	**-423.2204**	**+0.234**
HA_26		4.8424	-615.6768	-686.7523	**-410.9216**	**+0.233**
HA_27		4.8728	-615.7542	-687.4889	**-410.7794**	**+0.250**
HA_28		4.8078	-676.8576	-768.4930	**-447.7314**	**+0.213**
HA_29		4.8511	-663.2647	-772.8213	**-432.8480**	**+0.238**

HA_30		4.6328	-717.7242	-854.8841	**-462.8405**	**+0.113**
HA_31		5.0250	-736.9996	-794.5106	**-500.1163**	**+0.337**
HA_32		5.0353	-730.0270	-794.2812	**-493.2121**	**+0.343**
HA_33		5.0029	-785.1724	-795.6193	**-547.9585**	**+0.324**
HA_34		4.9120	-744.3658	-800.9765	**-505.5547**	**+0.272**
HA_35		4.5996	-789.4068	-887.0351	**-524.9373**	**+0.094**

HA_36		5.0555	-746.7061	-800.5914	**-508.0098**	**+0.354**
HA_37		4.9020	-788.2483	-887.1550	**-523.7430**	**+0.267**
HA_38		4.7722	-827.9232	-866.5326	**-569.5665**	**+0.193**
HA_39		4.6976	-845.8148	-829.8876	**-598.3838**	**+0.150**
HA_40		5.0410	-860.9337	-907.4405	**-590.3803**	**+0.346**
HA_41		4.7259	-792.2955	-869.8878	**-532.9384**	**+0.166**

HA_42		4.6510	-844.9316	-955.6538	**-560.0034**	**+0.123**
HA_43		4.4246	-1037.6904	-1022.2047	**-732.9200**	**-0.006**
HA_44		4.7019	-935.5956	-90.4790	**-664.4344**	**+0,152**
HA_45		4.4823	-781.7151	-796.4268	**-544.2605**	**+0.027**
HA_46		4.6508	-642.4129	-508.8625	**-490.6955**	**+0.123**
HA_47		4.7406	-678.6842	-514.5394	**-525.2742**	**+0.175**

HA_48		4.6949	-596.8113	-507.9685	**-445.3605**	**+0.148**
HA_49		4.7659	-591.2228	-513.4081	**-438.1502**	**+0.189**
HA_50		4.6810	-569.5601	-507.5234	**-418.2420**	**+0.141**
HA_51		4.7877	-607.3958	-513.3708	**-454.3342**	**+0.201**
HA_52		4.7264	-522.1114	-506.6273	**-371.0604**	**+0.166**
HA_53		4.8103	-515.8053	-512.2921	**-363.0654**	**+0.214**

HA_54		4.7953	-562.9540	-512,8115	**-410.0593**	**+0.206**
HA_55		4.7487	-635.8761	-513.8769	**-482.6637**	**+0.179**
HA_56		4.5245	-740.3662	-729.7692	**-522.7855**	**+0.051**
HA_57		4.5746	-782.0717	-735.9302	**-562.6541**	**+0.080**
HA_58		4.5762	-693.2846	-728.8605	**-475.9748**	**+0.081**
HA_59		4.6742	-687.9550	-734.0517	**-469.0975**	**+0.137**
HA_60		4.6249	-735.0176	-734.9773	**-515.8841**	**+0.108**