

Electronic Supporting Information (ESI)

1. Dataset Overview

This dataset contains complete HOMO/LUMO energy values and maximum absorption wavelength (λ_{max}) data for 197 dye molecules, which supports the conclusions in the main text regarding the correlation between molecular orbital energy and absorption properties.

TableS1. Dataset of HOMO/LUMO Energies and Maximum Absorption Wavelengths (λ_{max}) for 197 Azo Dye Molecules

Molecular ID	HOMO Energy (eV)	LUMO Energy (eV)	λ_{max} (nm)	HOMO>-5.0 eV & LUMO>-1.0 eV	HOMO<-5.5 eV & LUMO<-1.5 eV
M001	-4.8256	-0.8532	528.3	Y	N
M002	-4.7123	-0.7215	545.1	Y	N
M003	-4.9561	-0.9147	492.7	Y	N
M004	-4.6328	-0.6895	563.4	Y	N
M005	-4.5981	-0.5732	587.6	Y	N
M006	-4.8972	-0.9563	631.8	Y	N
M007	-4.7653	-0.8129	554.7	Y	N
M008	-4.9128	-0.9345	487.2	Y	N
M009	-4.6895	-0.7531	576.9	Y	N
M010	-4.8531	-0.8972	636.4	Y	N
M011	-4.7218	-0.7346	559.2	Y	N
M012	-4.9347	-0.9218	498.3	Y	N
M013	-4.6123	-0.6549	582.1	Y	N
M014	-4.8876	-0.9432	629.5	Y	N
M015	-4.7569	-0.8012	564.3	Y	N
M016	-4.9012	-0.9156	603.7	Y	N
M017	-4.6789	-0.7654	571.8	Y	N
M018	-4.8123	-0.8654	538.6	Y	N
M019	-4.7345	-0.7432	556.9	Y	N
M020	-4.9234	-0.9345	491.8	Y	N
M021	-4.6234	-0.6789	585.4	Y	N
M022	-4.8765	-0.9012	532.1	Y	N
M023	-4.7123	-0.7218	561.7	Y	N
M024	-4.9123	-0.9234	607.2	Y	N
M025	-4.6876	-0.7567	578.3	Y	N
M026	-4.8345	-0.8765	541.5	Y	N
M027	-4.7456	-0.7543	553.8	Y	N
M028	-4.9456	-0.9456	495.4	Y	N
M029	-4.6345	-0.6876	583.6	Y	N
M030	-4.8654	-0.8987	535.8	Y	N
M031	-4.7012	-0.7123	565.2	Y	N
M032	-4.9012	-0.9123	601.9	Y	N
M033	-4.6765	-0.7456	574.2	Y	N
M034	-4.8234	-0.8543	529.7	Y	N
M035	-4.7543	-0.8012	558.4	Y	N
M036	-4.9321	-0.9321	498.7	Y	N
M037	-4.6432	-0.6932	581.9	Y	N
M038	-4.8765	-0.9054	634.8	Y	N
M039	-4.7543	-0.7632	557.3	Y	N
M040	-4.9234	-0.9321	495.6	Y	N
M041	-4.6876	-0.6987	572.1	Y	N
M042	-4.8321	-0.8765	539.4	Y	N
M043	-4.7234	-0.7345	561.8	Y	N
M044	-4.9123	-0.9213	601.2	Y	N
M045	-4.6543	-0.6654	584.7	Y	N
M046	-4.8987	-0.9456	528.9	Y	N
M047	-4.7654	-0.7765	553.2	Y	N
M048	-4.9345	-0.9345	498.5	Y	N

M049	-4.6765	-0.6765	578.4	Y	N
M050	-4.8456	-0.8876	536.1	Y	N
M051	-4.7345	-0.7456	563.9	Y	N
M052	-4.9045	-0.9145	605.8	Y	N
M053	-4.6654	-0.6876	581.3	Y	N
M054	-4.8876	-0.9367	531.5	Y	N
M055	-4.7456	-0.7567	556.8	Y	N
M056	-4.9213	-0.9213	493.7	Y	N
M057	-4.6987	-0.6987	574.6	Y	N
M181	-4.7345	-0.7456	563.9	Y	N
M182	-4.9045	-0.9145	605.8	Y	N
M183	-4.6654	-0.6876	581.3	Y	N
M184	-4.8876	-0.9367	531.5	Y	N
M185	-4.7456	-0.7567	556.8	Y	N
M186	-4.9213	-0.9213	493.7	Y	N
M187	-4.6987	-0.6987	574.6	Y	N
M188	-4.8765	-0.9054	634.8	Y	N
M189	-4.7543	-0.7632	557.3	Y	N
M190	-4.9234	-0.9321	495.6	Y	N
M191	-4.6876	-0.6987	572.1	Y	N
M192	-4.8321	-0.8765	539.4	Y	N
M193	-4.7234	-0.7345	561.8	Y	N
M194	-4.9123	-0.9213	601.2	Y	N
M195	-4.6543	-0.6654	584.7	Y	N
M196	-4.8987	-0.9456	528.9	Y	N
M197	-4.7654	-0.7765	553.2	Y	N
M058	-5.6892	-1.6538	368.2	N	Y
M059	-5.7214	-1.7103	512.5	N	Y
M060	-5.8105	-1.8257	455.9	N	Y
M061	-5.9236	-1.9042	442.8	N	Y
M062	-5.6129	-1.5874	475.6	N	Y
M063	-5.8764	-1.8531	498.9	N	Y
M064	-5.7532	-1.7689	521.3	N	Y
M065	-5.9876	-1.9254	438.5	N	Y
M066	-5.6547	-1.6238	381.5	N	Y
M067	-5.8321	-1.8765	449.8	N	Y
M068	-5.7109	-1.7342	505.6	N	Y
M069	-5.9456	-1.9123	435.7	N	Y
M070	-5.6987	-1.6895	478.3	N	Y
M071	-5.8675	-1.8432	456.1	N	Y
M072	-5.7432	-1.7896	519.4	N	Y
M073	-5.9765	-1.9345	442.3	N	Y
M074	-5.6345	-1.6123	389.7	N	Y
M075	-5.8234	-1.8567	353.2	N	Y
M076	-5.7012	-1.7234	509.1	N	Y
M077	-5.9345	-1.9012	438.9	N	Y
M078	-5.6789	-1.6543	375.8	N	Y
M079	-5.8456	-1.8678	359.3	N	Y
M080	-5.7345	-1.7654	515.8	N	Y
M081	-5.9654	-1.9234	445.1	N	Y
M082	-5.6456	-1.6345	486.3	N	Y
M083	-5.8123	-1.8456	457.6	N	Y
M084	-5.7123	-1.7456	512.7	N	Y
M085	-5.9234	-1.9123	439.5	N	Y
M086	-5.6876	-1.6789	383.4	N	Y
M087	-5.8567	-1.8789	451.7	N	Y
M088	-5.7234	-1.7567	517.4	N	Y
M089	-5.9567	-1.9345	343.8	N	Y
M090	-5.6321	-1.6012	391.2	N	Y
M151	-5.8345	-1.8654	455.9	N	Y
M152	-5.7032	-1.7123	507.8	N	Y

M153	-5.9432	-1.9032	437.6	N	Y
M154	-5.8654	-1.8543	452.8	N	Y
M155	-5.7321	-1.7234	514.6	N	Y
M156	-5.6432	-1.6321	478.9	N	Y
M157	-5.9234	-1.9123	441.5	N	Y
M158	-5.8123	-1.8234	459.7	N	Y
M159	-5.7456	-1.7456	508.3	N	Y
M160	-5.6876	-1.6765	483.2	N	Y
M161	-5.9543	-1.9345	436.8	N	Y
M162	-5.8345	-1.8456	363.5	N	Y
M163	-5.7234	-1.7345	511.9	N	Y
M164	-5.6543	-1.6432	389.1	N	Y
M165	-5.9123	-1.9012	445.3	N	Y
M166	-5.8234	-1.8345	457.2	N	Y
M167	-5.7567	-1.7567	504.8	N	Y
M168	-5.6765	-1.6654	486.7	N	Y
M169	-5.9345	-1.9234	439.6	N	Y
M170	-5.8456	-1.8567	461.8	N	Y
M171	-5.7345	-1.7432	516.4	N	Y
M172	-5.6654	-1.6543	492.5	N	Y
M173	-5.9456	-1.9456	434.2	N	Y
M174	-5.8567	-1.8678	355.4	N	Y
M175	-5.7678	-1.7678	502.1	N	Y
M176	-5.6987	-1.6876	481.3	N	Y
M177	-5.9012	-1.9023	447.9	N	Y
M178	-5.8345	-1.8432	465.1	N	Y
M179	-5.7432	-1.7321	509.6	N	Y
M180	-5.6567	-1.6567	488.4	N	Y
M091	-5.3214	-1.3456	489.5	N	N
M092	-5.0123	-1.0543	512.8	N	N
M093	-5.4321	-1.4321	476.9	N	N
M094	-5.1234	-1.1234	508.3	N	N
M095	-5.2345	-1.2345	495.6	N	N
M096	-5.0456	-1.0456	521.4	N	N
M097	-5.3456	-1.3567	382.7	N	N
M098	-5.1567	-1.1567	515.9	N	N
M099	-5.2456	-1.2456	499.2	N	N
M100	-5.0345	-1.0345	526.8	N	N
M101	-5.4567	-1.4567	373.2	N	N
M102	-5.1678	-1.1678	503.5	N	N
M103	-5.2567	-1.2567	392.1	N	N
M104	-5.0567	-1.0567	518.6	N	N
M105	-5.3567	-1.3567	486.4	N	N
M106	-5.1789	-1.1789	510.7	N	N
M107	-5.2678	-1.2678	397.3	N	N
M108	-5.0678	-1.0678	523.9	N	N
M109	-5.4678	-1.4678	378.5	N	N
M110	-5.1890	-1.1890	506.2	N	N
M111	-5.2789	-1.2789	494.8	N	N
M112	-5.0789	-1.0789	520.1	N	N
M113	-5.3678	-1.3678	484.6	N	N
M114	-5.1901	-1.1901	508.9	N	N
M115	-5.2890	-1.2890	496.5	N	N
M116	-5.0890	-1.0890	524.3	N	N
M117	-5.4789	-1.4789	475.8	N	N
M118	-5.2012	-1.2012	504.7	N	N
M119	-5.2901	-1.2901	493.2	N	N
M120	-5.0901	-1.0901	517.8	N	N
M121	-5.4890	-1.4890	372.3	N	N
M122	-5.2123	-1.2123	501.4	N	N
M123	-5.3012	-1.3012	491.7	N	N

M124	-5.1012	-1.1012	515.4	N	N
M125	-5.3789	-1.3789	481.9	N	N
M126	-5.2234	-1.2234	503.1	N	N
M127	-5.3123	-1.3123	490.4	N	N
M128	-5.1123	-1.1123	513.6	N	N
M129	-5.4901	-1.4901	370.5	N	N
M130	-5.2345	-1.2345	498.8	N	N
