Supporting Information File

Δ-Machine Learning of Triplet Excitation Energies in Organic Chromophores

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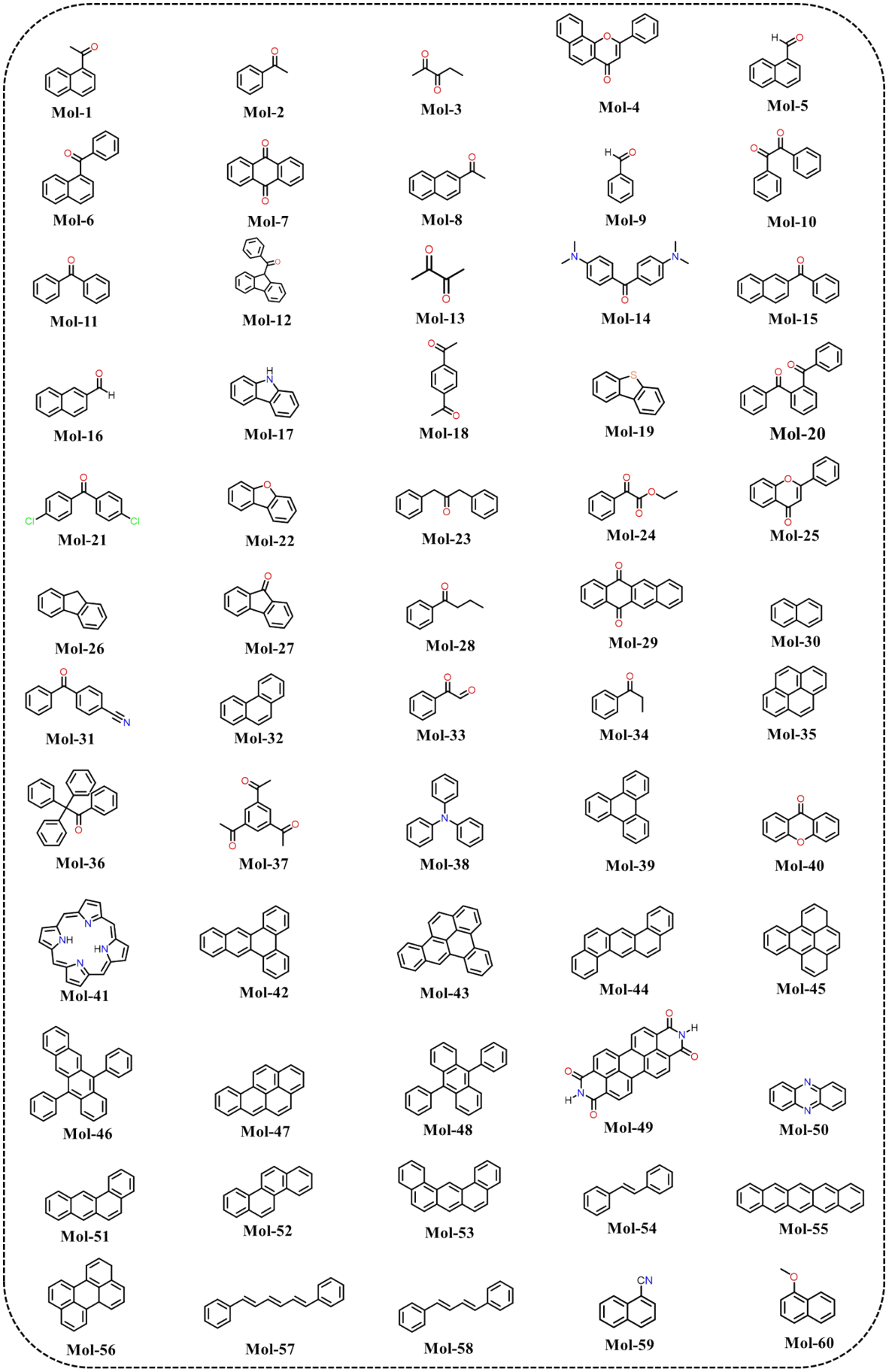
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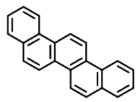

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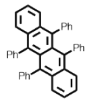

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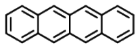

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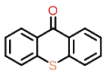

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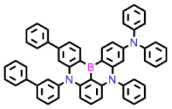

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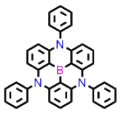

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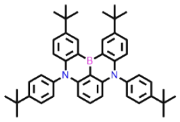

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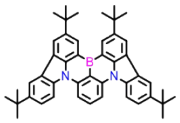

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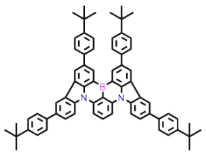

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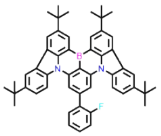

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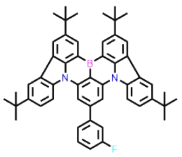

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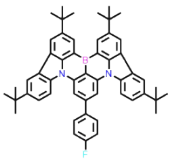

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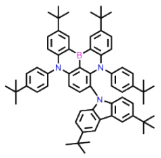

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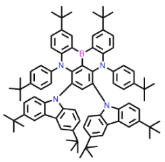

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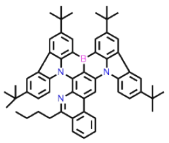

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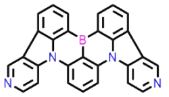

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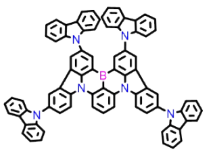

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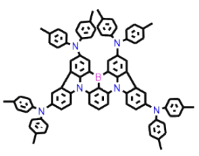

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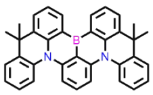

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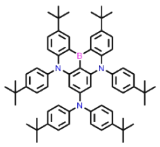

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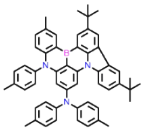

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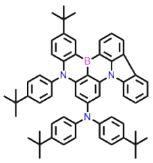

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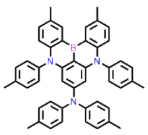

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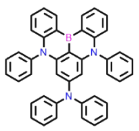

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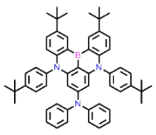

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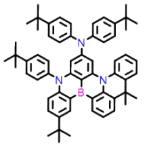

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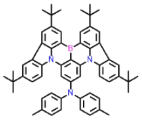

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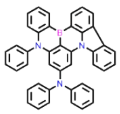

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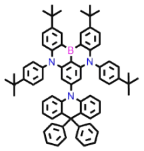

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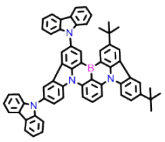

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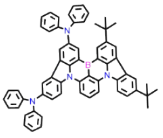

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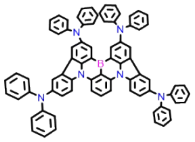

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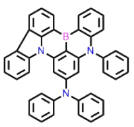

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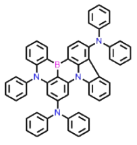

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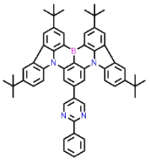

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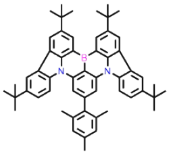

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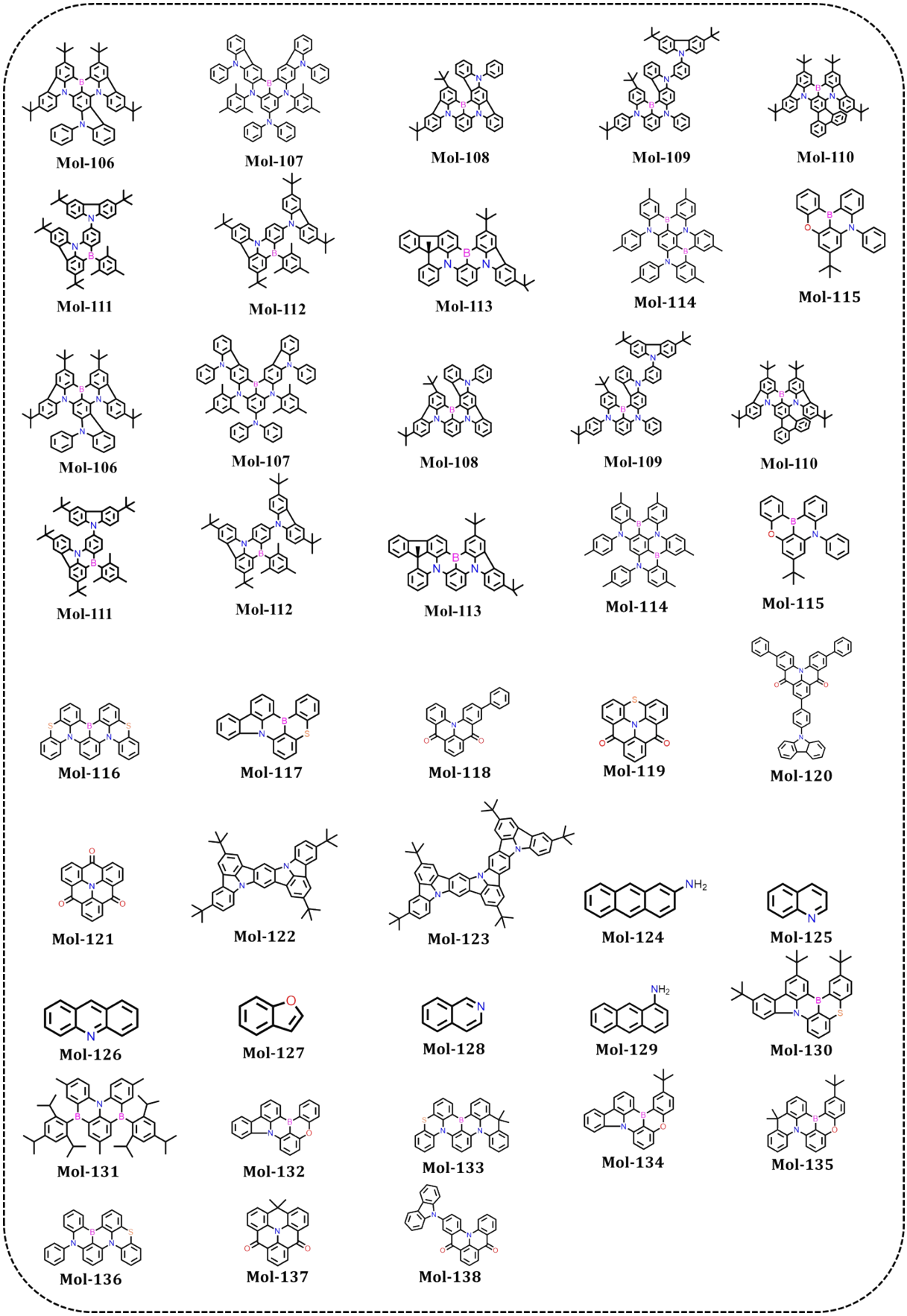


Figure S1: The molecular structure of all the molecules used in this study.

Table S1: The experimental T_1 energies (eV) of all the molecules that are used in this study.

Id	SMILES	Experimental T_1 Energy
Mol-1	c1cc2c(cc1)cccc2C(=O)C	2.45
Mol-2	c1c(cccc1)C(=O)C	3.19
Mol-3	C(=O)(C(=O)CC)C	2.37
Mol-4	c1(=O)cc(oc2c1ccc1c2cccc1)c1ccccc1	2.70
Mol-5	c1cc2c(cc1)cccc2C=O	2.44
Mol-6	c1cc2c(cc1)cccc2C(=O)c1ccccc1	2.49
Mol-7	c1cc2c(cc1)C(=O)c1c(cccc1)C2=O	2.71
Mol-8	c1cc2c(cc1)ccc(c2)C(=O)C	2.57
Mol-9	c1c(cccc1)C=O	3.12
Mol-10	c1c(cccc1)C(=O)C(=O)c1ccccc1	2.33
Mol-11	c1ccc(cc1)C(=O)c1ccccc1	2.68
Mol-12	c1ccc2c(-c3c(C2C(=O)c2ccccc2)cccc3)c1	2.90
Mol-13	C(=O)(C(=O)C)C	2.38
Mol-14	c1cc(ccc1N(C)C)C(=O)c1ccc(cc1)N(C)C	2.65
Mol-15	c1cc2c(cc1)ccc(c2)C(=O)c1ccccc1	2.58
Mol-16	c1cc2c(cc1)ccc(c2)C=O	2.58
Mol-17	c1ccc2c(c1)c1c(cccc1)[nH]2	3.04
Mol-18	c1(ccc(cc1)C(=O)C)C(=O)C	2.94
Mol-19	c1ccc2c(c1)c1c(cccc1)s2	3.02
Mol-20	c1(c(cccc1)C(=O)c1ccccc1)C(=O)c1ccccc1	3.02
Mol-21	c1(ccc(cc1)C(=O)c1ccc(cc1)Cl)Cl	2.95
Mol-22	c1ccc2c(c1)c1c(cccc1)o2	3.04
Mol-23	c1c(cccc1)CC(=O)Cc1ccccc1	3.13
Mol-24	CCOC(=O)C(=O)c1ccccc1	2.68
Mol-25	c1c2c(ccc1)oc(cc2=O)c1ccccc1	2.69
Mol-26	c1ccc2c(-c3c(C2)cccc3)c1	2.93
Mol-27	c1cc2-c3c(cccc3)C(=O)c2cc1	2.31
Mol-28	c1cc(ccc1)C(=O)CCC	3.17
Mol-29	c12cc3c(cc1C(=O)c1ccccc1C2=O)cccc3	2.42
Mol-30	c1cc2c(cc1)cccc2	2.64
Mol-31	c1ccc(cc1)C(=O)c1ccc(cc1)C#N	2.88
Mol-32	c1cc2c(cc1)c1c(cc2)cccc1	2.70
Mol-33	c1c(cccc1)C(=O)C=O	2.71
Mol-34	c1cc(ccc1)C(=O)CC	3.24
Mol-35	c1cc2c3c(c1)ccc1c3c(cc2)ccc1	2.11
Mol-36	C(=O)(C(c1ccccc1)(c1ccccc1)c1ccccc1)c1ccccc1	3.18
Mol-37	c1c(cc(cc1C(=O)C)C(=O)C)C(=O)C	3.04
Mol-38	N(c1ccccc1)(c1ccccc1)c1ccccc1	2.89
Mol-39	c1cc2c(cc1)c1c(c3c2cccc3)cccc1	3.07
Mol-40	c1cc2c(cc1)c(=O)c1c(cccc1)o2	3.22
Mol-41	c\1/2=C\C3=N/C(=C\c4ccc(/C=C\5/N=C(/C=c(/cc1)\[nH]2)C=C5)[nH]4)/C=C3	1.57

Mol-42	c1cc2c(cc1)cc1c(c2)c2c(c3c1cccc3)cccc2	2.20
Mol-43	c12cc3c4c(c1cccc2)ccc1c4c(c2c3cccc2)ccc1	2.03
Mol-44	c12c(cc3c(c1)c1c(cc3)cccc1)c1c(cccc1)cc2	2.26
Mol-45	c1cc2c3c(c1)ccc1c3c(c3c2cccc3)ccc1	2.29
Mol-46	c12cc3c(cc1cccc2)c(c1c(c3c2ccccc2)cccc1)c1ccccc1	1.20
Mol-47	c12cc3c4c(c1cccc2)ccc1c4c(cc3)ccc1	1.82
Mol-48	c1cc2c(cc1)c(c1c(c2c2ccccc2)cccc1)c1ccccc1	1.77
Mol-49	c1c2c3c4c(c1)c1ccc5c6c1c(c4ccc3C(=O)NC2=O)ccc6C(=O)NC5=O	1.20
Mol-50	c1cc2c(cc1)nc1c(cccc1)n2	1.93
Mol-51	c1cc2c(cc1)cc1c(c2)ccc2c1cccc2	2.05
Mol-52	c12c(ccc3c1cccc3)c1c(cccc1)cc2	2.49
Mol-53	c1cc2c(c3c1cccc3)cc1c(c2)ccc2c1cccc2	2.29
Mol-54	c1ccc(cc1)/C=C/c1ccccc1	2.14
Mol-55	c12cc3c(cc1cccc2)cc1c(c3)cc2c(c1)cccc2	0.86
Mol-56	c1cc2c3c(c1)c1cccc4c1c(c3ccc2)ccc4	1.53
Mol-57	c1ccc(cc1)/C=C/C=C/C=C/c1ccccc1	1.54
Mol-58	c1ccc(cc1)/C=C/C=C/c1ccccc1	1.83
Mol-59	c1cc2c(cc1)cccc2C#N	2.49
Mol-60	c1cc2c(cc1)cccc2OC	2.59
Mol-61	c12c(ccc3c1ccc1c3cccc1)c1c(cccc1)cc2	2.49
Mol-62	c12c(c3c(c(c1cccc2)c1ccccc1)c(c1c(c3c2ccccc2)cccc1)c1ccccc1)c1ccccc1	1.14
Mol-63	c1cc2c(cc1)nccn2	2.64
Mol-64	c12cc3c(cc1cccc2)cc1c(c3)cccc1	1.27
Mol-65	c1c2c3c4c(c1)ccc1c4c4c5c3c(cc2)ccc5ccc4cc1	2.40
Mol-66	c1cc2c(cc1)c(=O)c1c(cccc1)s2	2.84
Mol-67	b12c3ccccc3n(c3c2c(ccc3)n(c2c1cccc2)c1ccccc1)c1ccccc1	2.49
Mol-68	b12c3ccc(cc3n(c3c2c(ccc3)n(c2c1ccc(c2)N(c1ccccc1)c1ccccc1)c1ccccc1)c1cc(ccc1)c1ccccc1)c1ccccc1	2.47
Mol-69	b12c3c4cccc3n(c3c2c(ccc3)n(c2c1c(ccc2)n4c1ccccc1)c1ccccc1)c1ccccc1	2.97
Mol-70	b12c3cc(ccc3n(c3c2c(ccc3)n(c2c1cc(cc2)C(C)(C)C)c1ccc(cc1)C(C)(C)C)c1ccc(cc1)C(C)(C)C)C(C)(C)C	2.63
Mol-71	b12c3cc(cc4c3n(c3c2c(ccc3)n2c3c1cc(cc3c1c2ccc(c1)C(C)(C)C)C(C)(C)C)c1c4cc(cc1)C(C)(C)C)C(C)(C)C	2.53
Mol-72	b12c3cc(cc4c3n(c3c2c(ccc3)n2c3c1cc(cc3c1c2ccc(c1)c1ccc(cc1)C(C)(C)C)c1ccc(cc1)C(C)(C)C)c1c4cc(cc1)c1ccc(cc1)C(C)(C)C)c1ccc(cc1)C(C)(C)C	2.50
Mol-73	b12c3cc(cc4c3n(c3c2c(cc(c3)c2c(cccc2)F)n2c3c1cc(cc3c1c2ccc(c1)C(C)(C)C)C(C)(C)C)c1c4cc(cc1)C(C)(C)C)C(C)(C)C	2.35
Mol-74	b12c3cc(cc4c3n(c3c2c(cc(c3)c2cccc(c2)F)n2c3c1cc(cc3c1c2ccc(c1)C(C)(C)C)C(C)(C)C)c1c4cc(cc1)C(C)(C)C)C(C)(C)C	2.40
Mol-75	b12c3cc(cc4c3n(c3c2c(cc(c3)c2ccc(cc2)F)n2c3c1cc(cc3c1c2ccc(c1)C(C)(C)C)C(C)(C)C)c1c4cc(cc1)C(C)(C)C)C(C)(C)C	2.39
Mol-76	c12c3c(ccc1n1c4c(c5c1ccc(c5)C(C)(C)C)cc(cc4)C(C)(C)C)n1c4ccc(cc4c4c1c(b3c1c3n2c2c(c3cc(c1)C(C)(C)C)cc(cc2)C(C)(C)C)cc(c4)C(C)(C)C)C(C)(C)C	2.42
Mol-77	c12c3c(c(cc1n1c4c(c5c1ccc(c5)C(C)(C)C)cc(cc4)C(C)(C)C)n1c4ccc(cc4c4c1ccc(c4)C(C)(C)C)C(C)(C)C)n1c4ccc(cc4c4c1c(b3c1c3n2c2c(c3cc(c1)C(C)(C)C)cc(cc2)C(C)(C)C)cc(c4)C(C)(C)C)C(C)(C)C	2.27
Mol-78	c12c3c(c4c(c1)c1c(c(n4)CCCC)cccc1)n1c4ccc(cc4c4c1c(b3c1c3n2c2c(c3c	2.19

	c(c1)C(C)(C)C)cc(cc2)C(C)(C)C)cc(c4)C(C)(C)C)C(C)(C)C	
Mol-79	b12c3cccc4c3n(c3c2c(ccc3)n2c3c1cccc3c1c2cccc1)c1c4cccc1	2.47
Mol-80	b12c3cccc4c3n(c3c2c(ccc3)n2c3c1cccc3c1c2ccnc1)c1c4cncc1	2.58
Mol-81	b12c3cc(cc4c3n(c3c2c(ccc3)n2c3c1cc(cc3c1c2ccc(c1)n1c2ccccc2c2c1cccc2)n1c2c(cccc2)c2c1cccc2)c1c4cc(cc1)n1c2ccccc2c2c1cccc2)n1c2c(cccc2)c2c1cccc2	2.33
Mol-82	b12c3cc(cc4c3n(c3c2c(ccc3)n2c3c1cc(cc3c1c2ccc(c1)N(c1ccc(cc1)C)c1ccc(cc1)C)N(c1ccc(cc1)C)c1ccc(cc1)C)c1c4cc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)N(c1ccc(cc1)C)c1ccc(cc1)C	2.03
Mol-83	b12c3c(cccc3n3-c4ccccc4C(c4c3c2ccc4)(C)C)n2-c3ccccc3C(c3c2c1ccc3)(C)C	2.40
Mol-84	b12c3cc(ccc3n(c3c2c(cc(c3)N(c2ccc(cc2)C(C)(C)C)c2ccc(cc2)C(C)(C)C)n(c2c1cc(cc2)C(C)(C)C)c1ccc(cc1)C(C)(C)C)c1ccc(cc1)C(C)(C)C)C(C)(C)C	2.57
Mol-85	b12c3cc(ccc3n(c3c2c(cc(c3)N(c2ccc(cc2)C)c2ccc(cc2)C)n2c3c1cc(cc3c1c2ccc(c1)C(C)(C)C)C(C)(C)C)c1ccc(cc1)C)C	2.47
Mol-86	b12c3cc(cc4c3n(c3c2c(cc(c3)N(c2ccc(cc2)C)c2ccc(cc2)C)n2c3c1cc(cc3c1c2ccc(c1)C(C)(C)C)C(C)(C)C)c1c4cc(cc1)C(C)(C)C)C(C)(C)C	2.45
Mol-87	b12c3ccccc3n(c3c2c(cc(c3)N(c2ccccc2)c2ccccc2)n2c3c1cccc3c1c2cccc1)c1ccccc1	2.51
Mol-88	b12c3cc(ccc3n(c3c2c(cc(c3)N(c2ccc(cc2)C(C)(C)C)c2ccc(cc2)C(C)(C)C)n2c3c1cccc3c1c2cccc1)c1ccc(cc1)C(C)(C)C)C(C)(C)C	2.49
Mol-89	b12c3cc(ccc3n(c3c2c(cc(c3)N(c2ccc(cc2)C)c2ccc(cc2)C)n(c2c1cc(cc2)C)c1ccc(cc1)C)c1ccc(cc1)C)C	2.53
Mol-90	b12c3ccccc3n(c3c2c(cc(c3)N(c2ccccc2)c2ccccc2)n(c2c1cccc2)c1ccccc1)c1ccccc1	2.71
Mol-91	b12c3cc(ccc3n(c3c2c(cc(c3)N(c2ccccc2)c2ccccc2)n(c2c1cc(cc2)C(C)(C)C)c1ccc(cc1)C(C)(C)C)c1ccc(cc1)C(C)(C)C)C(C)(C)C	2.68
Mol-92	b12c3c(cccc3)n(c3c1c(ccc3N(c1ccc(cc1)C(C)(C)C)c1ccc(cc1)C(C)(C)C)n1-c3c(cccc3)C(c3c1c2ccc3)(C)C)c1ccc(cc1)C(C)(C)C	2.53
Mol-93	b12c3cc(ccc3n(c3c2c(cc(c3)N2c3ccccc3C(c3c2cccc3)(c2ccccc2)c2ccccc2)n(c2c1cc(cc2)C(C)(C)C)c1ccc(cc1)C(C)(C)C)c1ccc(cc1)C(C)(C)C)C(C)(C)C	2.56
Mol-94	b12c3cc(cc4c3n(c3c2c(ccc3)n2c3c1cc(cc3c1c2ccc(c1)n1c2ccccc2c2c1cccc2)n1c2ccccc2c2c1cccc2)c1c4cc(cc1)C(C)(C)C)C(C)(C)C	2.39
Mol-95	b12c3cc(cc4c3n(c3c2c(ccc3)n2c3c1cc(cc3c1c2ccc(c1)N(c1ccccc1)c1ccccc1)N(c1ccccc1)c1ccccc1)c1c4cc(cc1)C(C)(C)C)C(C)(C)C	2.19
Mol-96	b12c3cc(cc4c3n(c3c2c(ccc3)n2c3c1cc(cc3c1c2ccc(c1)N(c1ccccc1)c1ccccc1)N(c1ccccc1)c1ccccc1)c1c4cc(cc1)N(c1ccccc1)c1ccccc1)N(c1ccccc1)c1ccccc1	2.14
Mol-97	c1ccc(cc1)N(c1cc2n(c3ccccc3)c3ccccc3b3c2c(c1)n1c2ccccc2c2c1c3ccc2)c1ccccc1	2.59
Mol-98	c1ccc(cc1)N(c1cc2n(c3ccccc3)c3ccccc3b3c2c(c1)n1c2ccccc2c2c1c3ccc2N(c1ccccc1)c1ccccc1)c1ccccc1	2.54
Mol-99	CC(c1ccc2c(c1)c1cc(cc3c1n2c1cc(cc2c1b3c1cc(cc3c1n2c1ccc(cc31)C(C)(C)C)C(C)(C)C)c1cnc(nc1)c1ccccc1)C(C)(C)C)(C)C	2.32
Mol-100	Cc1cc(C)c(c(c1)C)c1cc2c3c(c1)n1c4ccc(cc4c4c1c(b3c1c3n2c2ccc(cc2c3cc(c1)C(C)(C)C)C(C)(C)C)cc(c4)C(C)(C)C)C(C)(C)C	2.50
Mol-101	CC(c1ccc2c(c1)c1cc(cc3c1n2c1cc(cc2c1b3c1cc(cc3c1n2c1ccc(cc31)C(C)(C)C)C(C)(C)C)c1cc(cc(c1)c1ccccc1)c1ccccc1)C(C)(C)C)(C)C	2.50
Mol-102	CC(c1ccc2c(c1)c1cc(cc3c1n2c1cc(cc2c1b3c1cc(cc3c1n2c1ccc(cc31)C(C)(C)C)C(C)(C)C)c1ccc(cc1)n1c2ccccc2c2c1cccc2)C(C)(C)C)(C)C	2.47
Mol-103	CC(c1ccc2c(c1)c1cc(cc3c1n2c1cc(cc2c1b3c1cc(cc3c1n2c1ccc(cc31)C(C)(	2.42

	C)C)C(C)(C)C)c1cccc(c1)n1c2ccccc2c2c1cccc2)C(C)(C)C)(C)C	
Mol-104	b12c3cc(ccc3n(c3c2c(cc(c3)c2cc(cc(c2)C(C)(C)C)C(C)(C)C)n(c2c1cc(cc2)C(C)(C)C)c1ccc(cc1)C(C)(C)C)c1ccc(cc1)C(C)(C)C)C(C)(C)C	2.58
Mol-105	Cc1ccccc1N(c1cc2c3c(c1)n(c1c(C)cccc1C)c1c(b3c3c(n2c2c(C)cccc2C)cc(cc3)c2ccccc2)ccc(c1)c1ccccc1)c1cccc(c1)c1ccccc1	2.56
Mol-106	CC(c1ccc2c(c1)c1cc(cc3c1n2c1cc2c(c4c1b3c1cc(cc3c1n4c1ccc(cc31)C(C)(C)C)C(C)(C)C)c1c(n2c2ccccc2)cccc1)C(C)(C)C)(C)C	2.39
Mol-107	Cc1cc(C)c(c(c1)C)n1c2cc3n(c4ccccc4)c4c(c3cc2b2c3c1cc(cc3n(c1c2cc2c3ccccc3n(c2c1)c1ccccc1)c1c(C)cc(cc1C)C)N(c1ccccc1)c1ccccc1)cccc4	2.59
Mol-108	CC(c1cc2b3c4c5c(cc6c4n(c4c3c(n3c2c(c1)c1cc(ccc31)C(C)(C)C)ccc4)c1c6cccc1)n(c1c5cccc1)c1ccccc1)(C)C	2.16
Mol-109	CC(c1cc2b3c4c5c(cc6c4n(c4c3c(n3c2c(c1)c1cc(ccc31)C(C)(C)C)ccc4)c1c6cccc1)n(c1c5cccc1)c1cccc(c1)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C)(C)C	2.20
Mol-110	CC(c1cc2c3cc(ccc3n3c2c(c1)b1c2c3cc3c(c2n2c4c1cc(cc4c1c2ccc(c1)C(C)(C)C)C(C)(C)C)c1ccccc1c1c3cccc1)C(C)(C)C)(C)C	2.33
Mol-111	Cc1cc(C)c(c(c1)C)b1c2ccc(cc2n2c3c1cc(cc3c1c2ccc(c1)C(C)(C)C)C(C)(C)C)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C	2.60
Mol-112	Cc1cc(C)c(c(c1)C)b1c2cc(ccc2n2c3c1cc(cc3c1c2ccc(c1)C(C)(C)C)C(C)(C)C)n1c2ccc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C	2.52
Mol-113	CC(c1cc2b3c4c(cccc4n4c2c(c1)c1cc(ccc41)C(C)(C)C)n1-c2ccccc2[C@]2(c4c1c3ccc4-c1c2cccc1)C)(C)C	2.45
Mol-114	b12c3c(ccc(c3)C)n(c3c2c2c4c(c3)n(c3ccc(cc3)C)c3ccc(cc3b4c3c(n2c2c1cc(cc2)C)ccc(c3)C)C)c1ccc(cc1)C	2.54
Mol-115	b12c3ccccc3oc3c2c(cc(c3)C(C)(C)C)n(c2c1cccc2)c1ccccc1	2.77
Mol-116	b12c3cccc4c3n(-c3ccccc3S4)c3c2c(ccc3)n2-c3c(cccc3)Sc3c2c1ccc3	2.44
Mol-117	b12c3cccc4c3n(c3c1c(ccc3)sc1c2cccc1)c1c4cccc1	2.52
Mol-118	n12c3c(cccc3)c(=O)c3c2c(ccc3)c(=O)c2c1ccc(c2)c1ccccc1	2.42
Mol-119	n12c3c4cccc3Sc3c1c(ccc3)c(=O)c1c2c(ccc1)c4=O	2.07
Mol-120	n12c3c(cc(cc3)c3ccccc3)c(=O)c3c2c(cc(c3)c2ccc(cc2)n2c3ccccc3c3c2cccc3)c(=O)c2c1ccc(c2)c1ccccc1	2.38
Mol-121	n12c3c4cccc3c(=O)c3c1c(ccc3)c(=O)c1c2c(ccc1)c4=O	2.68
Mol-122	c12cc3c(cc1c1cc(cc4c1n2c1c4cc(cc1)C(C)(C)C)C(C)(C)C)n1c2c3cc(cc2c2c1ccc(c2)C(C)(C)C)C(C)(C)C	2.55
Mol-123	c12cc3c(cc1c1cc(cc4c1n2c1c4cc(cc1)C(C)(C)C)C(C)(C)C)n1c2c3cc(cc2c2c1cc1c(c2)n2c3c1cc(cc3c1c2ccc(c1)C(C)(C)C)C(C)(C)C)C(C)(C)C	2.49
Mol-124	c1cc2c(cc1)cc1c(c2)cc(cc1)N	1.86
Mol-125	c1cc2c(cc1)cccn2	2.68
Mol-126	c1cc2c(cc1)cc1c(cccc1)n2	1.95
Mol-127	c12c(cccc1)occ2	3.05
Mol-128	c1cc2c(cc1)cncc2	2.63
Mol-129	c1cc2c(cc1)cc1c(c2)c(ccc1)N	1.86
Mol-130	b12c3cc(cc4c3n(c3c1c(ccc3)sc1c2cc(cc1)C(C)(C)C)c1c4cc(cc1)C(C)(C)C)C(C)(C)C	2.58
Mol-131	n12c3c(cc(cc3b(c3c1ccc(c3)C)c1c(cc(cc1C(C)C)C(C)C)C(C)C)C)b(c1c2ccc(c1)C)c1c(cc(cc1C(C)C)C(C)C)C(C)C	2.41
Mol-132	b12c3cccc4c3n(c3c1c(ccc3)oc1c2cccc1)c1c4cccc1	2.63
Mol-133	b12c3cccc4c3n(-c3c(cccc3)S4)c3c1c(ccc3)n1-c3c(cccc3)C(c3c1c2ccc3)(C)C	2.31
Mol-134	b12c3cc(ccc3oc3c2c(ccc3)n2c3c1cccc3c1c2cccc1)C(C)(C)C	2.76
Mol-135	b12c3cc(ccc3oc3c2c(ccc3)n2-c3c(cccc3)C(c3c2c1ccc3)(C)C)C(C)(C)C	2.66

Mol-136	b12c3cccc4c3n(-c3ccccc3S4)c3c2c(ccc3)n(c2c1cccc2)c1ccccc1	2.51
Mol-137	n12c3c4cccc3C(c3c1c(ccc3)c(=O)c1c2c(ccc1)c4=O)(C)C	2.47
Mol-138	n12c3c(cccc3)c(=O)c3c2c(ccc3)c(=O)c2c1ccc(c2)n1c2ccccc2c2c1cccc2	2.58

OPTIMIZED HYPERPARAMETERS

Table S2: Optimized hyperparameters of the Chemprop model for TDDFT method.

Hyperparameter	Value
depth	6
message-hidden-dim	700
ffn-hidden-dim	1200
ffn-num-layers	2
dropout	0.1
epochs	100

Table S3: Optimized hyperparameters of the Chemprop model for ΔSCF method.

Hyperparameter	Value
depth	4
message-hidden-dim	1200
ffn-hidden-dim	1500
ffn-num-layers	2
dropout	0.0
epochs	100

Table S4: Optimized hyperparameters of the Chemprop model for xTB/sTDA method.

Hyperparameter	Value
depth	5
message-hidden-dim	1900
ffn-hidden-dim	1600
ffn-num-layers	1
dropout	0.0
epochs	100

CROSS-VALIDATION

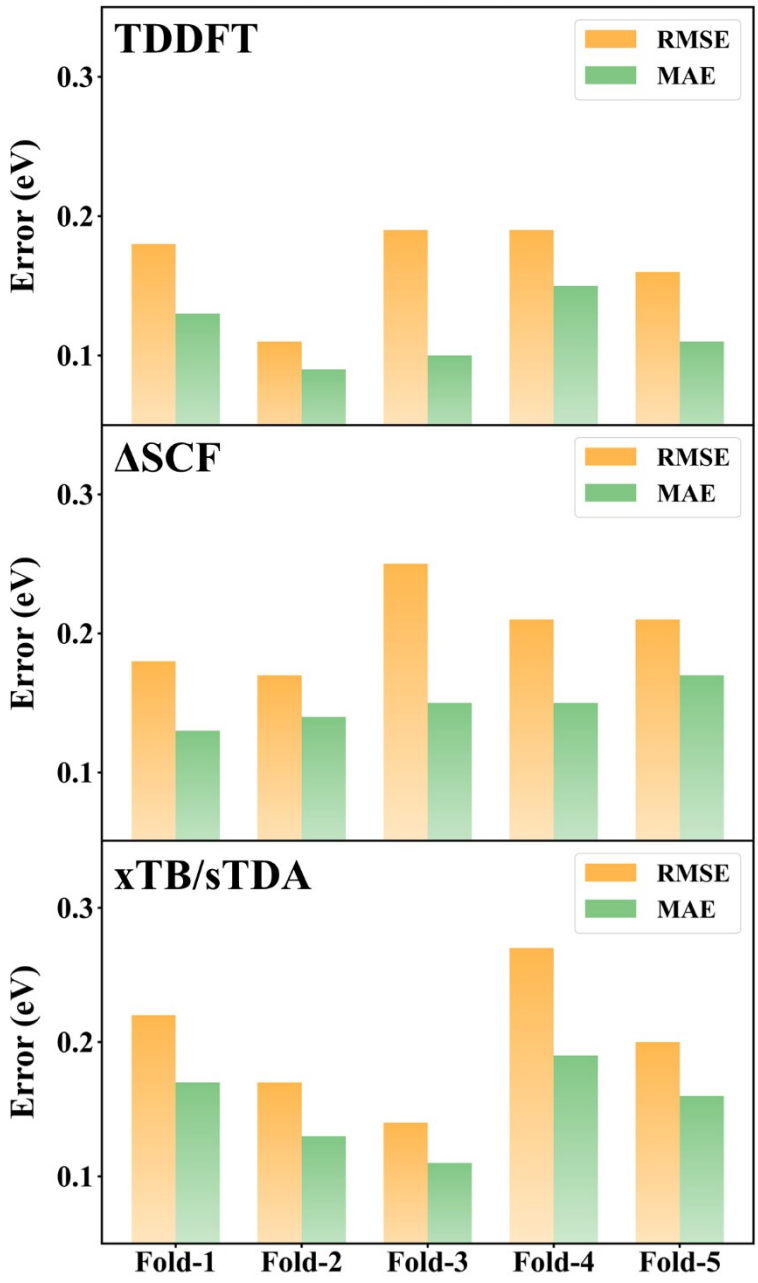


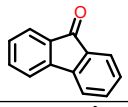
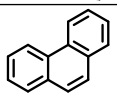
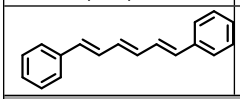
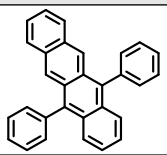
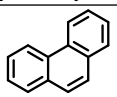
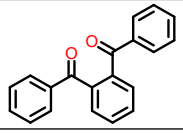
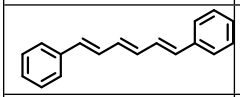
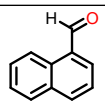
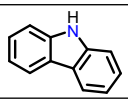
Figure S2: Computed five-fold cross-validation for the training dataset.

LIST OF MOLECULES

Table S5: List of molecules in the test dataset that satisfied the stringent criteria of a pre-correction error $|\Delta E| \geq 0.38$ eV, a post-correction error $|\Delta E| \leq 0.10$ eV, and a minimum improvement of 50% across all three QM methods. The T_1 excitation energies of all molecules are reported in eV.

DATA AND CODE AVAILABILITY

All the training and test datasets, pre-trained models, and automated python scripts used in this study have been deposited in a GitHub repository to ensure reproducibility of the reported results.

TDDFT						
Molecule	**Experiment**	**TDDFT**	**TDDFT + Δ-MPNN**	**Uncorrected |ΔE|**	**Corrected |ΔE|**	**Improvement (%)**
	2.38	1.96	2.34	0.42	0.04	90.48
ΔSCF						
Molecule	**Experiment**	**ΔSCF**	**ΔSCF + Δ-MPNN**	**Uncorrected |ΔE|**	**Corrected |ΔE|**	**Improvement (%)**
	2.31	2.73	2.27	0.42	0.04	90.48
	2.70	3.22	2.73	0.52	0.03	94.23
	1.54	1.91	1.49	0.37	0.05	86.49
xTB/sTDA						
Molecule	**Experiment**	**xTB/sTDA**	**xTB/sTDA + Δ-MPNN**	**Uncorrected |ΔE|**	**Corrected |ΔE|**	**Improvement (%)**
	1.20	1.71	1.18	0.51	0.02	96.08
	2.70	3.69	2.64	0.99	0.06	93.94
	3.02	3.63	3.08	0.61	0.06	90.16
	1.54	2.21	1.56	0.67	0.02	97.01
	2.44	3.14	2.48	0.70	0.04	94.28
	3.04	3.78	3.10	0.74	0.06	91.89

GitHub link: https://github.com/PyGhosh/Delta-MPNN

Table S6: R^2, RMSE and MAE values of the 5 representative test molecules between experimental T_1 values and TDDFT T_1 values using different exchange-correlation functionals.

B3LYP		
TDDFT		
R^2	**RMSE (eV)**	**MAE (eV)**
0.86	0.20	0.13
CAM-B3LYP		
TDDFT		
R^2	**RMSE (eV)**	**MAE (eV)**
0.77	0.25	0.22
ω-B97X-D		
TDDFT		
R^2	**RMSE (eV)**	**MAE (eV)**
0.78	0.25	0.21