Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary material for

TD-DFT based fine-tuning of molecular excitation energies using evolutionary algorithms

Sailesh Abburu, Vishwesh Venkatraman, and Bjørn K. Alsberg

Table S1: Table summarises the experimentally observed λ_{max} and predictions using CAM-B3LYP, B3LYP and PBE0 DFT functionals of the molecules in the test set. The figures are rounded to the nearest integer. The errors in prediction $\Delta\lambda_{max}$ is given by $\lambda_{max}^{Exp} - \lambda_{max}^{pred}$.

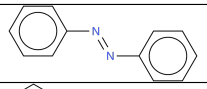
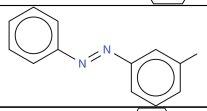
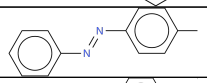
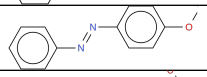
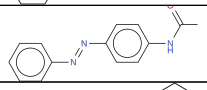
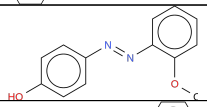
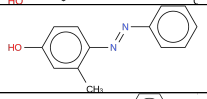
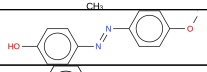
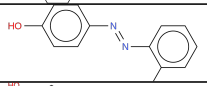
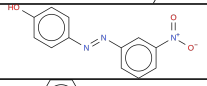
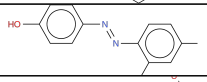
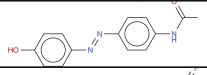
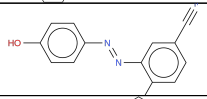
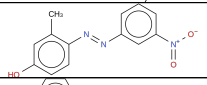
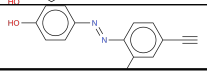
Molecule	**Structure**	λ_{max}^{Exp}	$\lambda_{max}^{CAM-B3LYP}$	$\Delta\lambda_{max}$	λ_{max}^{B3LYP}	$\Delta\lambda_{max}$	λ_{max}^{PBE0}	$\Delta\lambda_{max}$
M01		318	324	-6	352	-34	343	-25
M02		322	325	-3	356	-34	345	-23
M03		333	331	2	361	-28	351	-18
M04		345	346	-1	381	-36	370	-25
M05		348	351	-3	389	-41	378	-30
M06		351	350	1	385	-34	374	-23
M07		354	352	2	384	-30	374	-20
M08		357	354	3	390	-33	379	-22
M09		360	352	8	386	-26	375	-15
M10		362	345	17	378	-16	367	-5
M11		366	358	8	394	-28	383	-17
M12		368	361	7	400	-32	388	-20
M13		372	355	17	390	-18	379	-7
M14		375	356	19	388	-13	377	-2
M15		378	369	9	409	-31	398	-20

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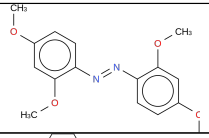
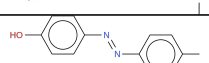
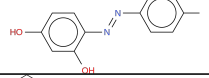
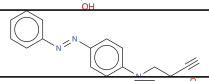
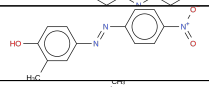
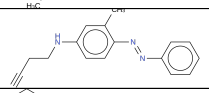
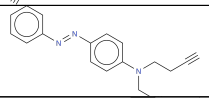
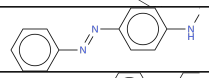
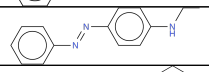
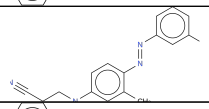
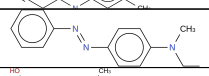
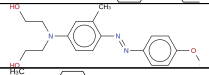
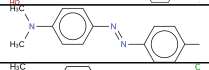
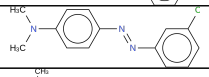
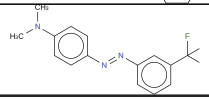
Table S1: Table summarises the experimentally observed λ_{max} and predictions using CAM-B3LYP, B3LYP and PBE0 DFT functionals of the molecules in the test set. The figures are rounded to the nearest integer. The errors in prediction $\Delta\lambda_{max}$ is given by $\lambda_{max}^{Exp} - \lambda_{max}^{pred}$.

Molecule	**Structure**	λ_{max}^{Exp}	$\lambda_{max}^{CAM-B3LYP}$	$\Delta\lambda_{max}$	λ_{max}^{B3LYP}	$\Delta\lambda_{max}$	λ_{max}^{PBE0}	$\Delta\lambda_{max}$
M16		381	370	11	406	-25	395	-14
M17		385	370	15	409	-24	397	-12
M18		387	362	25	396	-9	385	2
M19		390	364	26	406	-16	394	-4
M20		393	374	19	444	-51	422	-29
M21		396	377	19	418	-22	406	-10
M22		399	379	20	428	-29	415	-16
M23		402	378	24	421	-19	408	-6
M24		405	378	27	421	-16	409	-4
M25		408	382	26	423	-15	411	-3
M26		411	385	26	433	-22	420	-9
M27		414	392	22	442	-28	428	-14
M28		417	393	24	442	-25	428	-11
M29		420	390	30	438	-18	426	-6
M30		423	391	32	439	-16	426	-3

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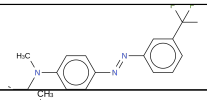
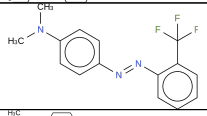
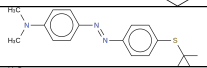
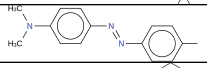
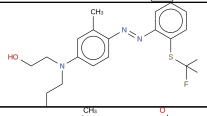
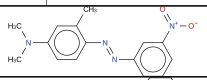
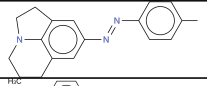
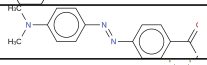
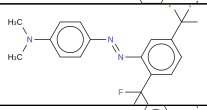
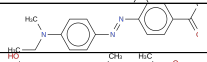
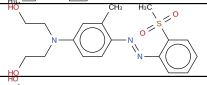
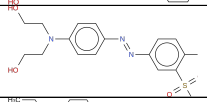
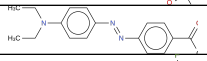
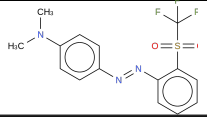
Molecule	**Structure**	λ_{max}^{Exp}	$\lambda_{max}^{CAM-B3LYP}$	$\Delta\lambda_{max}$	λ_{max}^{B3LYP}	$\Delta\lambda_{max}$	λ_{max}^{PBE0}	$\Delta\lambda_{max}$
M31		426	392	34	440	-14	427	-1
M32		429	399	30	445	-16	433	-4
M33		432	400	32	451	-19	438	-6
M34		435	388	47	436	-1	422	13
M35		438	410	28	460	-22	447	-9
M36		441	405	36	449	-8	436	5
M37		444	408	36	461	-17	448	-4
M38		447	410	37	472	-25	456	-9
M39		450	407	43	453	-3	441	9
M40		454	411	43	473	-19	457	-3
M41		456	404	52	454	2	441	15
M42		460	401	59	466	-6	449	11
M43		462	414	48	475	-13	459	3
M44		466	412	54	455	11	444	22

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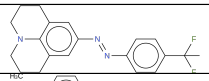
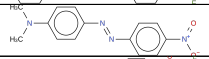
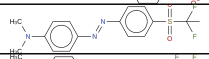
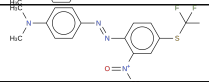
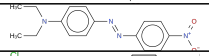
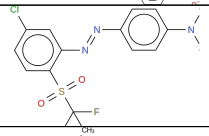
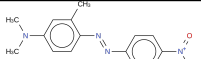
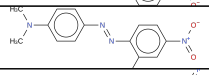
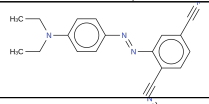
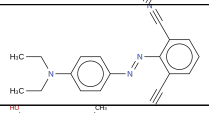
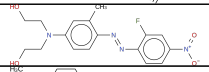
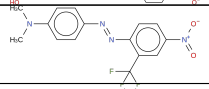
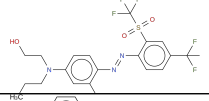
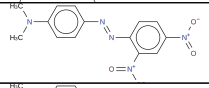
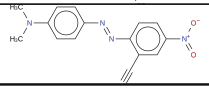
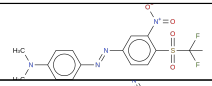
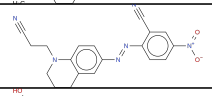
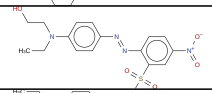
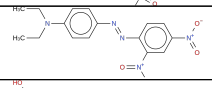
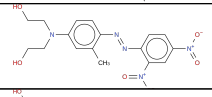
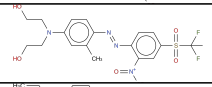
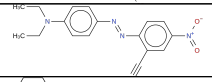
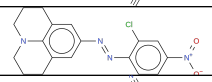
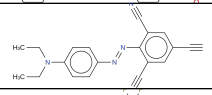
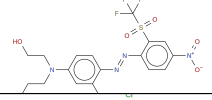
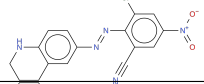
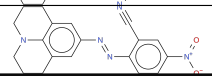
Table S1: Table summarises the experimentally observed λ_{max} and predictions using CAM-B3LYP, B3LYP and PBE0 DFT functionals of the molecules in the test set. The figures are rounded to the nearest integer. The errors in prediction $\Delta\lambda_{max}$ is given by $\lambda_{max}^{Exp} - \lambda_{max}^{pred}$.

Molecule	**Structure**	λ_{max}^{Exp}	$\lambda_{max}^{CAM-B3LYP}$	$\Delta\lambda_{max}$	λ_{max}^{B3LYP}	$\Delta\lambda_{max}$	λ_{max}^{PBE0}	$\Delta\lambda_{max}$
M45		471	419	52	468	3	455	16
M46		475	432	43	537	-62	506	-31
M47		476	416	60	470	6	456	20
M48		481	421	60	539	-58	498	-17
M49		483	436	47	542	-59	510	-27
M50		486	419	67	461	25	450	36
M51		489	443	46	543	-54	512	-23
M52		492	444	48	550	-58	519	-27
M53		495	425	70	480	15	464	31
M54		503	441	62	486	17	474	29
M55		508	451	57	554	-46	523	-15
M56		510	449	61	546	-36	517	-7
M57		513	420	93	468	45	455	58
M58		515	448	67	562	-47	528	-13
M59		520	457	63	547	-27	520	0

Continued on next page

Table S1: Table summarises the experimentally observed λ_{max} and predictions using CAM-B3LYP, B3LYP and PBE0 DFT functionals of the molecules in the test set. The figures are rounded to the nearest integer. The errors in prediction $\Delta\lambda_{max}$ is given by $\lambda_{max}^{Exp} - \lambda_{max}^{pred}$.

Molecule	**Structure**	λ_{max}^{Exp}	$\lambda_{max}^{CAM-B3LYP}$	$\Delta\lambda_{max}$	λ_{max}^{B3LYP}	$\Delta\lambda_{max}$	λ_{max}^{PBE0}	$\Delta\lambda_{max}$
M60		522	430	92	469	53	537	-15
M61		526	458	68	550	-24	522	4
M62		528	460	68	550	-22	518	10
M63		530	464	66	568	-38	534	-4
M64		533	451	82	564	-31	530	3
M65		538	441	97	548	-10	508	30
M66		540	464	76	553	-13	526	14
M67		545	478	67	583	-38	552	-7
M68		562	471	91	513	49	501	61
M69		564	463	101	554	10	530	34
M70		565	486	79	556	9	534	31
M71		575	486	89	579	-4	550	25