Supplementary Material for:

Benchmark assessment of collinear, mixed-reference, and spin-adapted variants of spin-flip time-dependent density functional theory, for closed- and open-shell molecules

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March 18, 2026

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Table S1: Vertical transition energies for the QUEST 1 data set.

Molecule	State[a]	Excitation Energy (eV)[b]				Error (eV)[c]		
		TD-	spin-flip[d]		TBE	TD-	spin-flip[d]	
		B3LYP	SF	SA-SF		B3LYP	SF	SA-SF
acetaldehyde	^{1}A$''$(V; $n \rightarrow \pi^*$)	4.29	4.43	4.60	4.31	−0.02	0.12	0.29
	^{3}A$''$(V; $n \rightarrow \pi^*$)	3.67	3.09	3.80	3.97	−0.30	−0.88	−0.18
acetylene	$^1\Sigma_u^-$(V; $\pi \rightarrow \pi^*$)	6.60	6.21	6.94	7.10	−0.50	−0.89	−0.16
	$^1\Delta_u$(V; $\pi \rightarrow \pi^*$)	6.76	6.88	7.08	7.44	−0.68	−0.56	−0.36
ammonia	^{1}A$_2$(R; $n \rightarrow$ 3s)	5.96	6.00	7.18	6.59	−0.63	−0.59	0.59
	^{1}E(R; $n \rightarrow$ 3p)	7.21	7.36	7.60	8.16	−0.95	−0.80	−0.56
	^{3}A$_2$(R; $n \rightarrow$ 3s)	5.69	5.99	6.55	6.31	−0.63	−0.32	0.24
carbon monoxide	$^1\Pi$(V; $n \rightarrow \pi^*$)	8.55	7.09	8.24	8.49	0.06	−1.40	−0.25
	$^1\Sigma^-$(V; $\pi \rightarrow \pi^*$)	9.64	8.35	9.44	9.92	−0.28	−1.57	−0.48
	$^3\Pi$(V; $n \rightarrow \pi^*$)	6.01	6.75	6.14	6.28	−0.27	0.47	−0.14
cyclopropene	^{1}B$_1$(V; $\sigma \rightarrow \pi^*$)	6.15	6.09	6.40	6.68	−0.53	−0.59	−0.28
	^{1}B$_2$(V; $\pi \rightarrow \pi^*$)	6.38	6.37	6.50	6.79	−0.41	−0.42	−0.29
	^{3}B$_2$(V; $\pi \rightarrow \pi^*$)	4.08	4.56	4.06	4.38	−0.30	0.18	−0.32
diazomethane	^{1}A$_2$(V; $\pi \rightarrow \pi^*$)	3.02	2.95	3.11	3.14	−0.12	−0.19	−0.03
	^{1}B$_1$(R; $\pi \rightarrow$ 3s)	5.16	4.66	5.58	5.54	−0.38	−0.88	0.04
	^{1}A$_1$(V; $\pi \rightarrow \pi^*$)	5.93	4.99	5.86	5.90	0.03	−0.91	−0.04
	^{3}A$_2$(V; $\pi \rightarrow \pi^*$)	2.58	1.85	2.63	2.79	−0.21	−0.94	−0.16
dinitrogen	$^1\Pi_g$(V; $n \rightarrow \pi^*$)	9.29	8.40	9.13	9.34	−0.05	−0.94	−0.21
	$^1\Sigma_u^-$(V; $\pi \rightarrow \pi^*$)	9.34	8.50	9.37	9.88	−0.54	−1.38	−0.51
	$^3\Sigma_u^+$(V; $\pi \rightarrow \pi^*$)	7.51	7.44	7.85	7.70	−0.19	−0.26	0.15
ethylene	^{1}B$_{3u}$(R; $\pi \rightarrow$ 3s)	6.63	6.59	6.72	7.39	−0.76	−0.80	−0.67
	^{1}B$_{1u}$(V; $\pi \rightarrow \pi^*$)	7.18	7.23	7.31	7.93	−0.75	−0.70	−0.62
	^{3}B$_{1u}$(V; $\pi \rightarrow \pi^*$)	4.42	4.81	4.29	4.54	−0.12	0.27	−0.25
formaldehyde	^{1}A$_2$(V; $n \rightarrow \pi^*$)	3.94	4.09	4.22	3.98	−0.04	0.11	0.24
	^{1}B$_2$(R; $n \rightarrow$ 3s)	6.38	6.40	6.88	7.23	−0.85	−0.83	−0.35
	^{3}A$_2$(V; $n \rightarrow \pi^*$)	3.27	2.69	3.39	3.58	−0.31	−0.89	−0.19
formamide	^{1}A$''$(V; $n \rightarrow \pi^*$)	5.57	5.16	5.38	5.65	−0.08	−0.49	−0.27
	^{1}A$'$(R; $n \rightarrow$ 3s)	6.11	6.56	6.87	6.81	−0.70	−0.25	0.06
	^{3}A$''$(V; $n \rightarrow \pi^*$)	5.05	4.99	5.51	5.38	−0.33	−0.39	0.13
hydrogen chloride	$^1\Pi$(CT)	7.35	7.54	7.81	7.84	−0.49	−0.30	−0.03
hydrogen sulfide	^{1}A$_2$(R; $n \rightarrow$ 4p)	5.75	5.75	5.90	6.18	−0.43	−0.43	−0.28
	^{1}B$_1$(R; $n \rightarrow$ 4s)	5.97	5.85	6.45	6.24	−0.27	−0.39	0.21
	^{3}A$_2$(R; $n \rightarrow$ 4p)	5.42	5.72	6.05	5.81	−0.39	−0.09	0.23
ketene	^{1}A$_2$(V; $\pi \rightarrow \pi^*$)	3.89	3.94	4.13	3.85	0.04	0.09	0.28
	^{1}B$_1$(R; $n \rightarrow$ 3s)	5.63	5.54	5.93	6.01	−0.38	−0.47	0.08
	^{3}A$_2$(V; $n \rightarrow \pi^*$)	3.53	3.07	3.65	3.77	−0.25	−0.70	0.12
methanamine	^{1}A$''$(V; $n \rightarrow \pi^*$)	5.12	5.27	5.42	5.23	−0.11	0.04	0.19
	^{3}A$''$(V; $n \rightarrow \pi^*$)	4.20	3.90	4.50	4.65	−0.45	−0.75	−0.15
nitrosomethane	^{1}A$''$(V; $n \rightarrow \pi^*$)	1.92	1.94	1.99	1.96	−0.05	−0.02	0.03
	^{1}A$'$(V; $n, n \rightarrow \pi^*, \pi^*$)	5.60	4.74	4.75	4.76	0.84	−0.03	−0.01
	^{3}A$''$(V; $n \rightarrow \pi^*$)	0.86	1.37	0.89	1.16	−0.30	0.21	−0.27
streptocyanine-C1	^{1}B$_2$(V; $\pi \rightarrow \pi^*$)	7.90	7.43	7.13	7.13	0.77	0.30	0.00
	^{3}B$_2$(V; $\pi \rightarrow \pi^*$)	5.11	5.74	5.28	5.52	−0.41	0.22	−0.24
thioformaldehyde	^{1}B$_1$(R; $n \rightarrow$ 3s)	2.23	2.24	2.46	2.22	0.01	0.02	0.24
	^{1}B$_2$(R; $n \rightarrow$ 4s)	5.40	4.80	5.86	5.96	−0.56	−1.16	−0.10
	^{3}A$_2$(V; $n \rightarrow \pi^*$)	1.67	2.06	1.93	1.95	−0.28	0.11	−0.02
water	^{1}B$_1$(R; $n \rightarrow$ 3s)	6.93	6.81	8.14	7.62	−0.69	−0.81	0.51
	^{1}A$_2$(R; $n \rightarrow$ 3p)	8.34	8.38	8.53	9.41	−1.07	−1.03	−0.88
	^{3}B$_1$(R; $n \rightarrow$ 3s)	6.58	6.68	7.33	7.25	−0.67	−0.57	0.08
MAE						0.40	0.55	0.25
RMSE						0.48	0.67	0.31
Mean						−0.33	−0.46	−0.10

[a] Characterized as valence (V), Rydberg (R), or charge transfer (CT), according to Ref. 1.
[b] TDDFT calculations use the aug-cc-pVTZ basis set and TBE values are from Ref. 1.
[c] Relative to TBE values [Eq. (16)].
[d] Using the BH&HLYP functional.

Table S2: Vertical transition energies for the QUEST 3 data set.

Molecule	State	Excitation Energy (eV)[a]					Error (eV)[b]			
		TD-	spin-flip[c]			TBE	TD-	spin-flip[c]		
		B3LYP	SF	MRSF	SA-SF		B3LYP	SF	MRSF	SA-SF
acetone	$^1A_2(n \rightarrow \pi^*)$	4.43	4.58	4.35	4.78	4.47	−0.04	0.11	−0.12	0.31
	$^1B_2(n \rightarrow 3s)$	5.76	5.96	6.02	6.45	6.46	−0.70	−0.50	−0.44	−0.01
	$^3A_2(n \rightarrow \pi^*)$	3.84	3.27	3.44	3.99	4.13	−0.29	−0.86	−0.69	−0.14
acrolein	$^1A''(n \rightarrow \pi^*)$	3.59	3.86	3.58	3.99	3.78	−0.19	0.08	−0.20	0.21
	$^1A'(\pi \rightarrow \pi^*)$	6.20	5.60	6.24	6.42	6.69	−0.49	−1.09	−0.45	−0.27
	$^3A''(n \rightarrow \pi^*)$	3.06	2.53	2.83	3.40	3.51	−0.45	−0.98	−0.68	−0.11
benzene	$^1B_{2u}(\pi \rightarrow \pi^*)$	5.42	4.40	5.41	5.54	5.06	0.36	−0.66	0.35	0.48
	$^1B_{1u}(\pi \rightarrow \pi^*)$	6.03	5.87	6.29	6.30	6.45	−0.42	−0.58	−0.16	−0.15
	$^3B_{1u}(\pi \rightarrow \pi^*)$	4.19	3.81	4.57	4.66	4.16	0.03	−0.35	0.41	0.50
butadiene	$^1B_u(\pi \rightarrow \pi^*)$	5.70	5.70	5.77	5.59	6.22	−0.52	−0.52	−0.45	−0.63
	$^1B_g(\pi \rightarrow 3s)$	5.96	5.80	5.93	5.98	6.33	−0.37	−0.53	−0.40	−0.35
	$^3B_u(\pi \rightarrow \pi^*)$	3.17	3.62	3.12	3.47	3.36	−0.19	0.26	−0.24	0.11
cyanoacetylene	$^1\Sigma^-(\pi \rightarrow \pi^*)$	5.15	4.96	5.44	5.46	5.80	−0.65	−0.84	−0.36	−0.34
	$^1\Delta(\pi \rightarrow \pi^*)$	5.31	5.54	5.51	5.75	6.07	−0.76	−0.53	−0.56	−0.32
	$^3\Sigma^+(\pi \rightarrow \pi^*)$	4.15	4.66	5.09	5.22	4.44	−0.29	0.22	0.65	0.78
cyanoformaldehyde	$^1A''(n \rightarrow \pi^*)$	3.72	3.90	3.58	4.03	3.81	−0.09	0.09	−0.23	0.22
	$^1A''(\pi \rightarrow \pi^*)$	5.48	6.33	6.45	6.72	6.46	−0.98	−0.13	−0.01	0.26
	$^3A''(n \rightarrow \pi^*)$	3.07	2.46	2.65	3.25	3.44	−0.37	−0.98	−0.79	−0.19
cyanogen	$^1\Sigma_u^-(\pi \rightarrow \pi^*)$	5.65	5.41	5.99	6.08	6.39	−0.74	−0.98	−0.40	−0.31
	$^1\Delta_u(\pi \rightarrow \pi^*)$	5.86	6.10	6.06	6.36	6.66	−0.80	−0.56	−0.60	−0.30
cyclopentadiene	$^1B_2(\pi \rightarrow \pi^*)$	5.13	5.15	5.24	5.19	5.54	−0.41	−0.39	−0.30	−0.35
	$^1A_2(\pi \rightarrow 3s)$	5.34	5.38	5.42	5.38	5.78	−0.44	−0.40	−0.36	−0.40
	$^3B_2(\pi \rightarrow \pi^*)$	3.11	3.54	3.07	3.35	3.31	−0.20	0.23	−0.24	0.04
cyclopropenone	$^1B_1(n \rightarrow \pi^*)$	4.00	4.06	4.02	4.24	4.26	−0.26	−0.20	−0.24	−0.02
	$^1A_2(n \rightarrow \pi^*)$	5.50	4.76	5.31	5.37	5.55	−0.05	−0.79	−0.24	−0.18
	$^3B_1(n \rightarrow \pi^*)$	3.60	2.98	3.43	3.76	3.93	−0.33	−0.95	−0.50	−0.17
cyclopropenethione	$^1A_2(n \rightarrow \pi^*)$	3.04	2.70	3.41	3.14	3.41	−0.37	−0.71	0.00	−0.27
	$^1B_1(n \rightarrow \pi^*)$	3.40	3.18	3.50	3.39	3.45	−0.05	−0.27	0.05	−0.06
	$^3A_2(n \rightarrow \pi^*)$	2.87	2.40	3.02	3.07	3.28	−0.41	−0.88	−0.26	−0.21
diacetylene	$^1\Sigma_u^-(\pi \rightarrow \pi^*)$	4.72	4.56	4.68	5.09	5.33	−0.61	−0.77	−0.65	−0.24
	$^1\Delta_u(\pi \rightarrow \pi^*)$	4.84	5.09	4.80	5.29	5.60	−0.76	−0.51	−0.80	−0.31
furan	$^1A_2(\pi \rightarrow 3s)$	5.53	5.47	5.56	5.68	6.09	−0.56	−0.62	−0.53	−0.41
	$^1B_2(\pi \rightarrow \pi^*)$	5.98	5.84	6.07	6.03	6.37	−0.39	−0.53	−0.30	−0.34
	$^3B_2(\pi \rightarrow \pi^*)$	4.05	4.36	3.85	4.14	4.20	−0.15	0.16	−0.35	−0.06
glyoxal	$^1A_u(n \rightarrow \pi^*)$	2.57	3.14	3.12	3.10	2.88	−0.31	0.26	0.24	0.22
	$^3A_u(n \rightarrow \pi^*)$	1.97	2.09	2.52	2.60	2.49	−0.52	−0.40	0.03	0.11
imidazole	$^1A''(\pi \rightarrow 3s)$	5.16	5.13	5.74	5.39	5.71	−0.55	−0.58	0.03	−0.32
	$^1A'(\pi \rightarrow \pi^*)$	5.93	5.85	6.27	6.13	6.41	−0.48	−0.56	−0.14	−0.28
	$^3A'(\pi \rightarrow \pi^*)$	4.54	4.90	5.66	4.67	4.73	−0.19	0.17	0.93	−0.06
isobutene	$^1B_1(\pi \rightarrow 3s)$	5.71	5.90	6.16	6.02	6.46	−0.75	−0.56	−0.30	−0.44
	$^1A_1(\pi \rightarrow 3p)$	6.38	6.63	6.40	6.50	7.01	−0.63	−0.38	−0.61	−0.51
	$^3A_1(\pi \rightarrow \pi^*)$	4.35	4.78	5.99	4.29	4.53	−0.18	0.25	1.46	−0.24
methylenecyclopropene	$^1B_2(\pi \rightarrow \pi^*)$	4.08	4.37	4.38	5.25	4.28	−0.20	0.09	0.10	0.97
	$^1B_1(\pi \rightarrow 3s)$	4.90	4.94	5.09	5.71	5.44	−0.54	−0.50	−0.35	0.27
	$^3B_2(\pi \rightarrow \pi^*)$	3.11	3.57	3.15	3.44	3.49	−0.38	0.08	−0.34	−0.05

[a] TDDFT calculations use the aug-cc-pVTZ basis set and TBE values are from Ref. 2.
[b] Relative to TBE values [Eq. (16)].
[c] Using the BH&HLYP functional.

Table S3: Continuation of Table S2.

Molecule	State	Excitation Energy (eV)[a]					Error (eV)[b]			
		TD-	spin-flip[c]			TBE	TD-	spin-flip[c]		
		B3LYP	SF	MRSF	SA-SF		B3LYP	SF	MRSF	SA-SF
propynal	$^1A''(n \rightarrow \pi^*)$	3.72	3.91	3.58	4.04	3.80	−0.08	0.11	−0.22	0.24
	$^1A''(\pi \rightarrow \pi^*)$	4.70	5.49	5.58	5.87	5.54	−0.84	−0.05	0.04	0.33
	$^3A''(n \rightarrow \pi^*)$	3.12	2.49	2.70	3.31	3.47	−0.35	−0.98	−0.77	−0.16
pyrazine	$^1B_{3u}(n \rightarrow \pi^*)$	3.99	4.50	4.51	4.46	4.15	−0.16	0.35	0.36	0.31
	$^1A_u(n \rightarrow \pi^*)$	4.70	4.65	5.46	5.29	4.98	−0.28	−0.33	0.48	0.31
	$^3B_{3u}(n \rightarrow \pi^*)$	3.28	4.11	3.89	3.96	3.59	−0.31	0.52	0.30	0.37
pyridazine	$^1B_1(n \rightarrow \pi^*)$	3.64	4.02	4.00	3.98	3.83	−0.19	0.19	0.17	0.15
	$^1A_2(n \rightarrow \pi^*)$	4.16	4.08	4.49	4.88	4.37	−0.21	−0.29	0.12	0.51
	$^3B_1(n \rightarrow \pi^*)$	2.83	3.49	3.16	3.30	3.19	−0.36	0.30	−0.03	0.11
pyridine	$^1B_1(n \rightarrow \pi^*)$	4.82	4.97	4.95	5.29	4.95	−0.13	0.02	0.00	0.34
	$^1B_2(\pi \rightarrow \pi^*)$	5.11	5.58	5.20	5.77	5.14	−0.03	0.44	0.06	0.63
	$^3A_1(\pi \rightarrow \pi^*)$	4.12	4.82	4.11	4.61	4.30	−0.18	0.52	−0.19	0.31
pyrimidine	$^1B_1(n \rightarrow \pi^*)$	4.31	4.68	4.78	4.86	4.44	−0.13	0.24	0.34	0.42
	$^1A_2(n \rightarrow \pi^*)$	4.63	4.78	5.15	5.20	4.85	−0.22	−0.07	0.30	0.35
	$^3B_1(n \rightarrow \pi^*)$	3.79	4.57	4.34	4.54	4.09	−0.30	0.48	0.25	0.45
pyrrole	$^1A_2(\pi \rightarrow 3s)$	4.73	4.73	5.25	4.91	5.24	−0.51	−0.51	0.01	−0.33
	$^1B_1(\pi \rightarrow 3p)$	5.44	5.45	5.79	5.64	6.00	−0.56	−0.55	−0.21	−0.36
	$^3B_2(\pi \rightarrow \pi^*)$	4.36	4.66	5.19	4.45	4.51	−0.15	0.15	0.68	−0.06
tetrazine	$^1B_{3u}(n \rightarrow \pi^*)$	2.31	2.81	2.82	2.75	2.47	−0.16	0.34	0.35	0.28
	$^1A_u(n \rightarrow \pi^*)$	3.46	3.70	4.28	4.03	3.69	−0.23	0.01	0.59	0.34
	$^3B_{3u}(n \rightarrow \pi^*)$	1.56	2.35	2.23	2.28	1.85	−0.29	0.50	0.38	0.43
thioacetone	$^1A_2(n \rightarrow \pi^*)$	2.56	2.59	2.43	2.84	2.53	0.03	0.06	−0.10	0.31
	$^1B_2(n \rightarrow 4s)$	4.90	4.49	5.14	5.64	5.56	−0.66	−1.07	−0.42	0.08
	$^3A_2(n \rightarrow \pi^*)$	2.10	2.44	1.84	2.34	2.33	−0.23	0.11	−0.49	0.01
thiophene	$^1A_1(\pi \rightarrow \pi^*)$	5.67	5.67	5.48	5.66	5.64	0.03	0.03	−0.17	0.02
	$^1A_2(\pi \rightarrow 3s)$	5.79	5.79	5.68	5.82	5.98	−0.19	−0.19	−0.30	−0.16
	$^3B_2(\pi \rightarrow \pi^*)$	3.79	4.11	3.62	3.92	3.97	−0.18	0.14	−0.35	−0.05
thiopropynal	$^1A''(n \rightarrow \pi^*)$	2.01	2.00	1.88	2.21	2.03	−0.02	−0.03	−0.15	0.18
	$^3A''(n \rightarrow \pi^*)$	1.50	1.91	1.35	1.80	1.80	−0.30	0.11	−0.46	0.00
triazine	$^1A''_1(n \rightarrow \pi^*)$	4.48	4.48	5.04	4.67	4.72	−0.24	−0.24	0.32	−0.05
	$^1A''_2(n \rightarrow \pi^*)$	4.59	4.97	5.17	4.87	4.75	−0.16	0.22	0.42	0.12
	$^3A''_2(n \rightarrow \pi^*)$	3.99	4.36	4.74	4.89	4.33	−0.34	0.03	0.41	0.56
MAE							0.34	0.42	0.35	0.27
RMSE							0.41	0.50	0.43	0.33
Mean							−0.33	−0.23	-0.10	0.03

[a] TDDFT calculations use the aug-cc-pVTZ basis set and TBE values are from Ref. 2.
[b] Relative to TBE values [Eq. (16)].
[c] Using the BH&HLYP functional.

Table S4: Vertical transition energies for exotic molecules in the QUEST 4 data set.

Molecule	State	Excitation Energy (eV)[a]				Errors (eV)[b]		
		TD-B3LYP	spin-flip[c]		TBE	TD-B3LYP	spin-flip[c]	
			SF	SA-SF			SF	SA-SF
CF_2O	$^1A_2$	7.09	6.97	7.74	7.31	−0.22	−0.34	0.43
	$^3A_2$	6.56	5.91	6.77	7.06	−0.50	−1.15	−0.29
CCl_2	$^1B_1$	2.62	2.64	2.49	2.59	0.03	0.05	-0.10
	$^1A_2$	4.16	3.42	4.26	4.40	−0.24	−1.02	−0.14
	$^3B_1$	1.12	1.66	1.15	1.22	−0.10	0.44	−0.07
CClF	$^1A''$	3.59	3.58	3.38	3.55	0.04	0.03	−0.17
CF_2	$^1B_1$	5.11	4.97	4.78	5.09	0.02	−0.12	−0.31
	$^3B_1$	2.52	3.36	2.62	2.77	−0.25	0.59	−0.15
CF_2N_2	$^1B_1$	3.49	3.69	3.63	3.74	−0.25	−0.05	−0.11
	$^3B_1$	2.59	3.14	2.75	3.03	−0.44	0.11	−0.28
CHFO	$^1A''$	5.91	5.53	6.31	5.96	−0.05	−0.43	0.35
	$^3A''$	5.27	4.61	5.40	5.73	−0.46	−1.12	−0.33
HCCl	$^1A''$	1.95	2.10	1.96	1.98	−0.03	0.12	−0.02
HCF	$^1A''$	2.47	2.62	2.47	2.49	−0.02	0.13	−0.02
HCP	$^1\Sigma^-$	4.67	3.99	4.73	4.84	−0.17	−0.85	−0.11
	$^1\Delta$	4.67	4.68	4.84	5.15	−0.48	−0.47	−0.31
HPO	$^1A''$	2.44	2.57	2.47	2.47	−0.03	0.10	0.00
HPS	$^1A''$	1.57	1.60	1.70	1.59	−0.02	0.01	0.11
HSiF	$^1A''$	3.08	3.30	3.01	3.05	0.03	0.25	−0.04
$SiCl_2$	$^1B_1$	3.97	4.03	3.74	3.91	0.06	0.12	−0.17
	$^3B_1$	2.41	2.86	2.60	2.48	−0.07	0.38	0.12
CH_2Si	$^1A_2$	2.18	2.14	1.94	2.11	0.07	0.03	−0.17
	$^1B_2$	3.93	3.64	3.75	3.78	0.15	−0.14	−0.03
MAE						0.16	0.35	0.17
RMSE						0.23	0.50	0.21
Mean						−0.13	−0.15	−0.08

[a] TDDFT calculations use the aug-cc-pVTZ basis set and TBE values are from Ref. 3.
[b] Relative to TBE values [Eq. (16)].
[c] Using the BH&HLYP functional.

Table S5: Vertical transition energies for radicals in the QUEST 4 data set.

Molecule	State	Excitation Energy (eV)[a]						Error (eV)[b]				
		LR-TDDFT			spin-flip[c]		TBE	LR-TDDFT			spin-flip[c]	
		B3LYP	BH&HLYP	ωB97M-V	SA-SF	SF		B3LYP	BH&HLYP	ωB97M-V	SA-SF	SF
allyl	$^2B_1$	3.94	4.34	3.88	3.54	3.53	3.43	0.51	0.91	0.45	0.11	0.10
	$^4A_2$	–	–	–	5.73	5.47	6.01	–	–	–	−0.28	−0.54
BeF	$^2\Pi$	4.16	4.20	4.01	3.54	3.63	4.15	0.01	0.05	−0.14	−0.61	−0.52
BeH	$^2\Pi$	2.58	2.61	2.19	2.29	2.23	2.49	0.09	0.12	−0.30	−0.20	−0.26
	$^2\Pi$	4.86	5.17	4.64	6.25	6.08	6.45	−1.59	−1.28	−1.81	−0.20	−0.37
	$^4\Pi$	–	–	–	5.90	5.61	5.88	–	–	–	0.02	−0.26
BH_2	$^2B_1$	1.34	1.34	0.94	1.08	1.18	1.18	0.16	0.16	−0.24	−0.10	0.00
	$^4A_2$				5.78	5.63	5.36				0.43	0.28
CH	$^2\Delta$	3.23	3.23	3.08	3.01	1.73	2.94	0.29	0.29	0.14	0.07	−1.21
	$^2\Sigma^-$	3.54	3.23	3.22	3.30	3.05	3.31	0.23	−0.08	−0.09	−0.01	−0.26
	$^4\Sigma^-$	–	–	–	1.03	0.95	0.72	–	–	–	0.31	0.23
CH_3	$^2A_1'$	5.21	5.74	5.08	6.13	6.14	5.86	−0.65	−0.12	−0.78	0.27	0.28
	$^2E'$	6.22	6.85	6.16	7.05	7.15	6.96	−0.74	−0.11	−0.80	0.09	0.19
CN	$^2\Pi$	1.21	1.21	0.92	0.56	0.81	1.38	−0.17	−0.17	−0.46	−0.82	−0.57
	$^4\Sigma^+$	–	–	–	6.89	6.62	6.04	–	–	–	0.85	0.58
CO^+	$^2\Pi$	3.38	3.86	3.26	2.46	2.66	3.26	0.12	0.60	0.00	−0.80	−0.60
	$^4\Sigma^+$	–	–	–	6.73	7.61	7.28	–	–	–	−0.55	0.33
F_2BO	$^2B_1$	1.01	0.91	0.91	0.71	0.66	0.71	0.30	0.20	0.20	0.00	−0.05
F_2BS	$^2B_1$	0.64	0.61	0.34	0.48	0.48	0.48	0.16	0.13	−0.14	0.00	0.00
H_2BO	$^2B_1$	2.42	2.16	2.25	0.97	1.02	2.17	0.25	−0.01	0.08	−1.20	−1.15
HCO	$^2A''$	2.26	2.40	2.09	2.39	2.29	2.09	0.17	0.31	0.00	0.30	0.19
	$^2A'$	5.03	5.82	4.90	6.20	6.06	5.45	0.42	0.37	−0.55	0.75	0.61
	$^4A''$	–	–	–	6.11	5.70	6.39	–	–	–	−0.26	−0.67
HOC	$^2A''$	1.11	1.06	0.81	0.85	0.82	0.93	0.18	0.13	−0.12	−0.08	−0.11
	$^4A''$				3.93	3.76	3.84				0.09	−0.09
H_2PO	$^2A''$	2.71	2.89	2.67	2.14	1.92	2.81	−0.10	0.08	−0.14	−0.67	−0.89
	$^2A'$	4.36	4.24	4.28	4.63	4.84	4.21	0.15	0.03	0.07	0.42	0.63
	$^4A''$	–	–	–	5.83	5.43	6.32	–	–	–	−0.49	−0.89
H_2PS	$^2A''$	1.23	1.25	1.15	0.84	0.83	1.15	0.08	0.10	0.00	−0.31	−0.34
	$^4A''$	–	–	–	4.93	4.71	5.12	–	–	–	−0.19	−0.41
NH_2	$^2A_1$	2.36	2.34	2.33	2.10	2.18	2.12	0.24	0.22	0.21	−0.02	0.06
	$^4B_1$	–	–	–	7.59	7.29	7.29	–	–	–	0.30	0.00
CH_3NO_2	$^2B_2$	1.95	2.58	2.33	2.04	1.76	2.05	−0.10	0.53	0.28	−0.01	−0.29
	$^4A_2$	–	–	–	4.13	3.48	4.34	–	–	–	−0.21	−0.86
PH_2	$^2A_1$	2.93	2.98	2.63	2.71	2.85	2.77	0.16	0.21	−0.14	−0.06	0.08
	$^4A_2$	–	–	–	6.26	7.10	6.16	–	–	–	0.10	0.93
vinyl	$^2A''$	3.30	3.44	3.14	2.96	2.96	3.31	−0.01	0.13	−0.17	−0.35	−0.35
	$^2A'$	4.51	4.83	4.32	4.25	4.31	4.69	−0.18	0.14	−0.37	−0.44	−0.38
	$^4A'$	–	–	–	4.28	4.06	4.56	–	–	–	−0.28	−0.50
MAE								0.28	0.27	0.31	0.31	0.37
RMSE								0.43	0.39	0.48	0.44	0.50
Mean								−0.03	0.13	−0.20	−0.16	−0.20

[a]TDDFT calculations use the aug-cc-pVTZ basis set and TBE values are from Ref. 3. Five of the QUEST 4 species have been removed and are considered separately in Table 4.
[b]Relative to TBE values [Eq. (16)].
[c]Using the BH&HLYP functional.

Table S6: Vertical transition energies for the QUEST 5 data set.

Molecule	State[a]	Excitation Energy (eV)[b]				Error (eV)[c]		
		TD-	spin-flip[d]		TBE	TD-	spin-flip[d]	
		B3LYP	SA-SF	SF		B3LYP	SA-SF	SF
aza-napthalene	$^1B_{3g}(V; n \rightarrow \pi^*)$	2.80	3.57	3.60	3.14	−0.34	0.43	0.46
	$^1B_{2u}(V; \pi \rightarrow \pi^*)$	4.15	4.31	3.91	4.28	−0.13	0.03	−0.37
benzoquinone	$^1B_{1g}(V; n \rightarrow \pi^*)$	2.51	3.24	3.26	2.82	−0.31	0.42	0.44
	$^3B_{1g}(V; n \rightarrow \pi^*)$	2.04	2.95	2.42	2.58	−0.54	0.37	−0.16
cyclopentadienethione	$^1A_2(V; n \rightarrow \pi^*)$	1.58	1.81	1.70	1.70	−0.12	0.11	0.00
	$^1B_2(V; \pi \rightarrow \pi^*)$	2.25	2.98	2.49	2.63	−0.38	0.35	−0.14
	$^1A_1(V; \pi \rightarrow \pi^*)$	5.03	4.84	3.69	4.96	0.07	−0.12	−1.27
	$^3A_2(V; n \rightarrow \pi^*)$	1.08	1.44	0.92	1.47	−0.39	−0.03	−0.55
cyclopentadienone	$^1A_2(V; n \rightarrow \pi^*)$	2.73	3.18	3.29	2.94	−0.21	0.24	0.35
	$^1B_2(V; \pi \rightarrow \pi^*)$	3.08	3.84	3.59	3.58	−0.41	0.26	0.01
	$^3B_2(V; \pi \rightarrow \pi^*)$	1.88	2.21	2.34	2.29	−0.14	−0.08	0.05
diazirine	$^1B_1(V; n \rightarrow \pi^*)$	3.95	3.92	3.89	4.09	−0.47	−0.17	−0.20
	$^1A_2(V; \sigma \rightarrow \pi^*)$	6.80	5.72	6.34	7.27	−0.07	−1.55	−0.93
	$^1B_2(R; n \rightarrow 3s)$	7.37	7.34	7.21	7.44	−0.47	−0.10	−0.23
	$^1A_1(R; n \rightarrow 3p)$	7.56	8.01	7.51	8.03	−0.40	−0.02	−0.52
	$^3B_1(V; n \rightarrow \pi^*)$	3.09	3.10	3.44	3.49	−0.32	−0.39	−0.05
hexatriene	$^1B_u(V; \pi \rightarrow \pi^*)$	5.05	4.51	4.94	5.37	−0.56	−0.86	−0.43
	$^1A_u(R; \pi \rightarrow 3s)$	5.23	5.59	4.98	5.79	−0.49	−0.20	−0.81
	$^1B_g(R; \pi \rightarrow 3p)$	5.45	5.72	5.27	5.94	−0.22	−0.22	−0.67
	$^3B_u(V; \pi \rightarrow \pi^*)$	2.51	2.92	2.99	2.73	−0.38	0.19	0.26
maleimide	$^1B_1(V; n \rightarrow \pi^*)$	3.42	4.59	4.41	3.80	−0.36	0.79	0.61
	$^1A_2(V; n \rightarrow \pi^*)$	4.16	4.89	5.09	4.52	−0.26	0.37	0.57
	$^1B_2(V; \pi \rightarrow \pi^*)$	4.63	5.25	5.15	4.89	−0.19	0.36	0.26
	$^1B_2(V; \pi \rightarrow \pi^*)$	6.02	6.13	6.28	6.21	−0.55	−0.08	0.07
	$^3B_1(V; n \rightarrow \pi^*)$	3.02	3.54	3.89	3.57	0.21	−0.03	0.32
naphthalene	$^1B_{3u}(V; \pi \rightarrow \pi^*)$	4.48	4.56	3.95	4.27	−0.36	0.29	−0.32
	$^1B_{2u}(V; \pi \rightarrow \pi^*)$	4.54	4.81	4.88	4.90	−0.45	−0.09	−0.02
	$^1A_u(R; \pi \rightarrow 3s)$	5.20	5.53	5.13	5.65	−0.37	−0.12	−0.52
	$^1B_{1g}(V; \pi \rightarrow \pi^*)$	5.47	5.89	5.23	5.84	−0.08	0.05	−0.61
nitroxyl	$^1A''(V; n \rightarrow \pi^*)$	1.66	1.76	1.72	1.74	−0.62	0.02	−0.02
	$^1A'(R)$	5.65	6.25	4.32	6.27	−0.62	−0.02	−1.95
	$^3A''(V; n \rightarrow \pi^*)$	0.55	0.61	1.12	0.88	−0.33	−0.27	0.24
octatetraene	$^1B_u(V; \pi \rightarrow \pi^*)$	4.40	3.89	4.24	4.78	−0.38	−0.89	−0.54
	$^1A_g(V; \pi \rightarrow \pi^*)$	4.86	4.91	4.38	4.90	−0.04	0.01	−0.52
	$^3B_u(V; \pi \rightarrow \pi^*)$	2.12	2.59	2.60	2.36	−0.25	0.23	0.24
streptocyanine-C3	$^1B_2(V; \pi \rightarrow \pi^*)$	5.79	4.77	5.15	4.82	0.97	−0.05	0.33
	$^3B_2(V; \pi \rightarrow \pi^*)$	3.13	3.26	3.53	3.44	−0.31	−0.18	0.09
streptocyanine-C5	$^1B_2(V; \pi \rightarrow \pi^*)$	4.70	3.55	4.01	3.64	1.06	−0.09	0.37
	$^3B_2(V; \pi \rightarrow \pi^*)$	2.23	2.40	2.54	2.47	−0.24	−0.07	0.07
thioacrolein	$^1A''(V; n \rightarrow \pi^*)$	2.08	2.34	2.21	2.11	−0.03	0.23	0.10
	$^3A''(V; n \rightarrow \pi^*)$	1.62	1.98	1.35	1.91	−0.29	0.07	−0.56
MAE						0.35	0.26	0.40
RMSE						0.41	0.39	0.51
Mean						−0.24	−0.02	−0.16

[a] Characterized as valence (V) or Rydberg (R), according to Ref. 4.
[b] TDDFT calculations use the aug-cc-pVTZ basis set and TBE values are from Ref. 4.
[c] Relative to TBE values [Eq. (16)].
[d] Using the BH&HLYP functional.

Table S7: Tuned range separation parameters for the QUEST 6 molecules, used in TD-LRC-ω_{GDD}PBE calculations.

Molecule	ω (bohr^{-1})^a
aminobenzonitrile	0.312
aniline	0.317
azulene	0.300
β-dipeptide	0.307
benzonitrile	0.319
benzothiadiazole	0.310
DMABN	0.302
dimethylaniline	0.305
dipeptide	0.315
hydrogen chloride	0.439
nitroaniline	0.317
nitrobenzene	0.325
nitrodimethylaniline	0.306
nitropyridine N-oxide	0.330
N-phenylpyrrole	0.297
phthalazine	0.312
quinoxaline	0.310
twisted DMABN	0.302
twisted PP	0.297

^{a}LRC-ωPBE/aug-cc-pVTZ

Table S8: Vertical transition energies for the QUEST 6 data set of intramolecular ^{1}CT excitations.

Molecules	State	Excitation Energy (eV)[a]				Error (eV)[b]		
		SA-SF[c]	LR-TDDFT		TBE	SA-SF[c]	LR-TDDFT	
			B3LYP	LRC-ωPBE[d]			B3LYP	LRC-ωPBE[d]
aminobenzonitrile	$A_1(\pi \rightarrow \pi^*)$	5.09	5.10	5.17	5.09	0.00	0.01	0.08
aniline	$A_1(\pi \rightarrow \pi^*)$	5.30	5.44	5.65	5.50	−0.20	−0.06	0.15
azulene	$A_1(\pi \rightarrow \pi^*)$	3.48	3.74	3.78	3.85	−0.37	−0.11	−0.08
azulene	$B_2(\pi \rightarrow \pi^*)$	4.73	4.76	4.75	4.50	0.23	0.25	0.25
β-dipeptide	$A''(n_1 \rightarrow \pi_2^*)$	8.39	7.27	8.67	8.90	−0.43	−1.70	−0.23
benzonitrile	$A_2(\pi_{CN} \rightarrow \pi^*)$	7.07	6.21	6.73	7.05	0.02	−0.84	−0.32
benzothiadiazole	$B_2(\pi \rightarrow \pi^*)$	3.86	3.99	4.29	4.29	−0.43	−0.30	0.00
DMABN	$A_1(\pi \rightarrow \pi^*)$	4.88	4.88	4.95	4.86	0.02	0.02	0.09
dimethylaniline	$B_2(\pi \rightarrow \pi^*)$	4.71	4.51	4.66	4.39	0.32	0.12	0.27
	$A_1(\pi \rightarrow \pi^*)$	5.48	5.06	5.47	5.40	0.08	−0.34	0.07
dipeptide	$A''(n_1 \rightarrow \pi^*)$	7.90	6.34	7.87	8.15	−0.25	−1.81	−0.28
hydrogen chloride	$\Pi(n \rightarrow \sigma^*)$	7.81	7.35	8.08	7.84	−0.03	−0.49	0.24
nitroaniline	$A_1(\pi \rightarrow \pi^*)$	4.16	4.12	4.69	4.40	−0.24	−0.28	0.29
nitrobenzene	$A_1(\pi \rightarrow \pi^*)$	4.98	4.89	5.33	5.41	−0.43	−0.52	−0.08
nitrodimethylaniline	$A_1(\pi \rightarrow \pi^*)$	3.95	3.86	4.30	4.14	−0.19	−0.28	0.16
nitropyridine *N*-oxide	$A_1(\pi \rightarrow \pi^*)$	3.63	4.13	4.30	4.10	−0.47	0.03	0.20
N-phenylpyrrole	$B_2(\pi \rightarrow \pi^*)$	5.12	4.79	5.28	5.32	−0.20	−0.53	−0.04
	$A_1(\pi \rightarrow \pi^*)$	5.74	5.04	5.62	5.85	−0.10	−0.81	−0.23
phthalazine	$A_2(n \rightarrow \pi^*)$	4.23	3.54	3.95	3.91	0.32	−0.37	0.04
quinoxaline	$B_2(n \rightarrow \pi^*)$	4.71	4.21	4.69	4.64	0.07	−0.42	0.05
	$A_1(\pi \rightarrow \pi^*)$	5.11	5.93	5.95	5.66	−0.55	0.27	0.29
twisted DMABN	$A_2(n \rightarrow \pi^*)$	4.41	3.20	3.93	4.11	0.30	−0.91	−0.18
	$B_1(n \rightarrow \pi^*)$	4.70	3.87	4.75	4.74	−0.04	−0.87	0.01
twisted PP	$B_2(\pi \rightarrow \pi^*)$	5.54	4.34	5.41	5.58	−0.04	−1.24	−0.17
	$A_1(\pi \rightarrow \pi^*)$	5.57	4.44	5.96	5.64	−0.07	−1.20	0.32
MAE						0.22	0.55	0.16
RMSE						0.28	0.74	0.19
Mean						−0.11	−0.50	−0.03

[a] TDDFT calculations use the aug-cc-pVTZ basis set except where noted, and TBE values are from Ref. 5.
[b] Relative to TBE values [Eq. (16)].
[c] Using the BH&HLYP functional.
[d] Using GDD tuning for ω.[6]

Table S9: Vertical transition energies for bicyclic systems (QUEST 7 data set).

Molecule	State[a]	Excitation Energy (eV)[b]				Error (eV)[c]		
		TD-	spin-flip[d]		TBE	TD-	spin-flip[d]	
		B3LYP	SA-SF	SF		B3LYP	SA-SF	SF
azulene	$^1B_2(V;\pi\rightarrow\pi^*)$	2.46	2.37	2.45	2.17	0.29	0.20	0.28
	$^1A_1(CT;\pi\rightarrow\pi^*)$	3.74	3.48	3.11	3.84	−0.10	−0.36	−0.73
	$^1B_2(CT;\pi\rightarrow\pi^*)$	4.55	4.73	3.88	4.49	0.06	0.24	−0.61
	$^1A_2(R)$	4.76	4.81	4.59	4.86	−0.10	−0.05	−0.27
	$^1A_1(V;\pi\rightarrow\pi^*)$	4.91	4.93	4.98	4.91	0.00	0.02	0.07
	$^3B_2(V;\pi\rightarrow\pi^*)$	2.00	2.15	2.11	2.19	−0.19	−0.04	−0.08
BOD	$^1B_2(V;\pi\rightarrow\pi^*)$	4.29	3.92	4.14	4.52	−0.23	−0.60	−0.38
	$^1A_1(V;\pi\rightarrow\pi^*)$	4.98	4.99	4.37	4.91	0.07	0.08	−0.54
	$^1A_2(V;n\rightarrow\pi^*)$	5.13	5.09	4.75	5.28	−0.15	−0.19	−0.53
	$^1B_1(V;n/\sigma\rightarrow\pi^*)$	5.50	5.57	5.10	5.83	−0.33	−0.26	−0.73
	$^3B_2(V;\pi\rightarrow\pi^*)$	2.50	2.77	2.80	2.74	−0.24	0.03	0.06
BTD	$^1B_2(CT;\pi\rightarrow\pi^*)$	3.99	3.86	3.36	4.23	−0.24	−0.37	−0.87
	$^1A_1(V,\pi\rightarrow\pi^*)$	4.59	4.45	4.67	4.36	0.23	0.09	0.31
	$^1A_2(V;n\rightarrow\pi^*)$	4.66	5.04	4.77	4.80	−0.14	0.24	−0.03
	$^1B_1(V;n/\sigma\rightarrow\pi^*)$	5.18	5.63	5.37	5.42	−0.25	0.21	−0.05
	$^3A_1(V;\pi\rightarrow\pi^*)$	3.22	3.24	3.36	3.49	−0.27	−0.25	−0.13
DPP	$^1B_u(V;\pi\rightarrow\pi^*)$	3.60	3.64	3.80	3.54	0.06	0.10	0.26
	$^1A_u(V;n\rightarrow\pi^*)$	3.75	3.75	3.82	3.86	−0.11	−0.11	−0.04
	$^1A_g(V;\pi\rightarrow\pi^*)$	3.91	4.26	4.08	3.91	0.00	0.35	0.17
	$^1B_g(V;n\rightarrow\pi^*)$	4.05	4.71	4.55	4.31	−0.26	0.40	0.24
	$^3B_u(V;\pi\rightarrow\pi^*)$	1.73	2.06	2.11	1.93	−0.20	0.13	0.18
FF	$^1A_u(R)$	5.04	5.17	4.91	5.43	−0.40	−0.26	−0.52
	$^1B_u(V;\pi\rightarrow\pi^*)$	5.26	5.23	5.23	5.46	−0.20	−0.23	−0.23
	$^1B_g(R)$	5.52	5.58	5.26	5.86	−0.34	−0.28	−0.60
	$^3B_u(V;\pi\rightarrow\pi^*)$	5.77	5.60	4.19	5.99	−0.22	−0.39	−1.80
	$^3B_u(V;\pi\rightarrow\pi^*)$	3.35	3.60	3.68	3.58	−0.23	0.02	0.10
phthalazine	$^1A_2(CT;n\rightarrow\pi^*)$	3.54	3.43	3.69	3.87	−0.33	−0.44	−0.18
	$^1B_1(CT;n\rightarrow\pi^*)$	4.00	4.23	3.86	4.28	−0.28	−0.05	−0.42
	$^1B_2(V;\pi\rightarrow\pi^*)$	4.79	5.30	4.52	5.15	−0.36	0.15	−0.63
	$^1B_1(CT;n\rightarrow\pi^*)$	5.15	5.72	5.49	5.74	−0.59	−0.02	−0.25
	$^3A_2(CT;n\rightarrow\pi^*)$	3.28	3.93	3.35	3.63	−0.35	0.30	−0.28
PP	$^1A_u(R)$	4.11	4.36	4.08	4.55	−0.44	−0.19	−0.47
	$^1B_g(R)$	4.23	4.55	4.26	4.75	−0.52	−0.20	−0.49
	$^1A_u(R)$	4.61	4.89	4.62	5.13	−0.52	−0.24	−0.51
	$^1B_g(R)$	4.78	5.27	4.98	5.15	−0.37	0.12	−0.17
	$^3B_u(V;\pi\rightarrow\pi^*)$	3.62	3.87	3.94	3.84	−0.22	0.03	0.10
quinoxaline	$^1B_1(V;n\rightarrow\pi^*)$	3.57	4.12	4.10	3.79	−0.22	0.33	0.31
	$^1A_1(V;\pi\rightarrow\pi^*)$	4.21	4.71	4.16	4.26	−0.05	0.45	−0.10
	$^1B_2(CT;\pi\rightarrow\pi^*)$	4.51	5.11	4.22	4.59	−0.08	0.52	−0.37
	$^1A_2(V;n\rightarrow\pi^*)$	4.84	5.56	5.33	5.09	−0.25	0.48	0.25
	$^3B_1(V;n\rightarrow\pi^*)$	3.06	3.70	3.83	3.35	−0.29	0.35	0.48
TTF	$^1B_{3u}(V;\pi\rightarrow\sigma^*)$	2.51	3.01	3.08	2.79	−0.28	0.22	0.29
	$^1B_{2u}(V;\pi\rightarrow\pi^*)$	3.30	3.47	3.64	3.74	−0.44	−0.27	−0.10
	$^1B_{1g}(V;\pi\rightarrow\sigma^*)$	3.64	3.88	4.05	3.98	−0.34	−0.10	0.07
	$^1B_{2g}$(mixed)	3.74	4.12	4.07	4.05	−0.31	0.07	0.02
	$^3B_{1u}(V;\pi\rightarrow\pi^*)$	2.74	2.91	2.72	2.99	−0.25	−0.08	−0.27
TT	$^1B_u(V;\pi\rightarrow\pi^*)$	4.91	5.00	4.46	4.96	−0.05	−0.04	−0.50
	$^1B_u(V;\pi\rightarrow\pi^*)$	5.01	5.22	5.00	5.22	−0.21	0.00	−0.22
	$^1B_g(R)$	5.16	5.43	5.07	5.41	−0.25	−0.02	−0.34
	$^1A_u(R)$	5.16	5.50	5.18	5.52	−0.36	0.02	−0.30
	$^3B_u(V;\pi\rightarrow\pi^*)$	3.28	3.59	3.64	3.47	−0.19	0.12	0.17
MAE						0.24	0.20	0.34
RMSE						0.28	0.25	0.45
Mean						−0.22	0.01	−0.20

[a] Characterized as valence (V), Rydberg (R), or charge transfer (CT), according to Ref. 7.
[b] TDDFT calculations use the aug-cc-pVTZ basis set and TBE values are from Ref. 7.
[c] Relative to TBE values [Eq. (16)].
[d] Using the BH&HLYP functional.

Table S10: Error statistics for vertical transition energies (from the singlet ground state) in cyclazine derivatives.

Molecule[a]	State	TBE[b] (eV)	Error (eV)[c]		
			spin-flip[d]		TD-
			SF	SA-SF	B3LYP
1	S_1	2.72	0.20	0.28	0.23
	T_1	2.94	−0.02	0.27	−0.21
2	S_1	0.98	0.03	0.08	0.29
	T_1	1.11	−0.18	0.09	−0.04
3	S_1	1.56	0.06	0.09	0.27
	T_1	1.66	−0.24	0.12	−0.10
4	S_1	2.18	0.19	0.09	0.23
	T_1	2.30	−0.17	0.13	−0.17
5	S_1	2.13	0.12	0.13	0.25
	T_1	2.23	−0.24	0.14	−0.15
6	S_1	0.83	−0.06	0.01	0.30
	T_1	0.90	−0.33	0.05	−0.03
7	S_1	0.69	−0.11	−0.03	0.30
	T_1	0.74	−0.36	0.01	−0.02
8	S_1	0.55	−0.18	−0.05	0.30
	T_1	0.58	−0.39	−0.03	−0.01
9	S_1	1.26	0.07	0.14	0.31
	T_1	1.46	−0.25	0.15	−0.10
10	S_1	1.52	−0.34	0.72	0.30
	T_1	1.83	−0.24	0.68	−0.11
MAE			0.19	0.16	0.19
RMSE			0.25	0.22	0.21
Mean			0.15	−0.12	0.09

[a] Numbering corresponds to Fig. 20.
[b] From Ref. 8.
[c] Relative to TBE values [Eq. (16)]. All calculations use the aug-cc-pVTZ basis set.
[d] Using the BH&HLYP functional.