

Supplementary information for:

Resilience of Hund's rule in the Chemical Space of Small Organic Molecules

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Assessment of methods for data-generation

For calculating the energies of the S_1 and T_1 excited states of all molecules in the bigQM7 ω dataset, we have evaluated the cost-accuracy trade-off in various approximations stemming from the choice of the basis set, accuracy of geometries, approximation of molecular integrals with resolution-of-identity, and the Tamm-Dancoff approximation (TDA) to time-dependent density functional theory (TDDFT). To this end, we have selected ten triangular molecules from a previous study¹ with the theoretical best estimates (TBEs) for the energies of S_1 and T_1 determined using frozen-core CCSD(T)/cc-pVTZ geometries. From the same study, we collected energies from ADC(2) and the TDDFT-SCS-PBE-QIDH methods using the aug-cc-pVTZ basis set. With these values as references, we evaluated the accuracy of ADC(2) and TDA using the smaller basis set def2-TZVP.

For all benchmark systems, S_1 and T_1 energies, along with the S_1 - T_1 gaps determined with various theoretical methods, are collected in Table S1, Table S2, and Table S3. The accuracies of different methods are quantified via the error metrics, mean signed error (MSE), mean absolute error (MAE), standard deviation of the error (SDE), minimum error (minE),

and maximum error (maxE) in Table S4. We evaluate these metrics using the aforesaid TBEs¹ as the reference. To understand the impact of the choice of geometries, we have performed geometry optimization of these ten molecules at the ω B97X-D3/def2-TZVP level.

From Table S1, we find that when using frozen-core CCSD(T)/cc-pVTZ geometries, ADC(2)/def2-TZVP predicts similar energies as ADC(2)/aug-cc-pVTZ. However, the error metrics in Table S4 suggest that for all S_1 - T_1 gaps, the SDE drops from 0.034 eV to 0.011 eV, indicating the smaller basis set def2-TZVP to perform better in the ADC(2) calculations. We also note similar improvement for S_1 and T_1 energies. This trend is in line with the observation made in an earlier study² that ADC2/aug-cc-pVDZ yields a more accurate S_1 - T_1 gap for triangular molecules than ADC(2)/aug-cc-pVTZ due to a favorable error cancellation. ADC(2)/def2-TZVP values determined using ω B97X-D3/def2-TZVP geometries (see Table S3) very closely resemble ADC(2)/def2-TZVP values determined using CCSD(T)/cc-pVTZ geometries (see Table S1). Further, while the change in geometry has a small influence on the error metrics for S_1 and T_1 energies, due to the cancellation of effects, the metrics for the S_1 - T_1 gap are less influenced.

We also compare the TDDFT/SCS-PBE-QIDH/aug-cc-pVTZ (determined using CCSD(T)/cc-pVTZ geometries) results from Ref. 1, to TDA analog in Table S2. In this Table, we have also reported TDDFT values calculated by us using geometries from Ref. 1 and find our results to agree with previously reported values precisely, assuring that our computational settings are consistent with the previous study. Moving from TDDFT to TDA, the largest effect is seen for molecule 6. At the TDDFT level, this system’s S_1 - T_1 gap is -0.32 eV, which increases to -0.03 eV at the TDA level. However, we find the TDA value better to approximate the TBE value of -0.07 eV from Table S1. For the S_1 - T_1 gap, TDDFT values of MSE, MAE, and SDE are -0.033 , 0.055 , and 0.081 eV, respectively, which drop to 0.034 , 0.034 , and 0.012 eV when using TDA. The SDE of TDA is 8-fold smaller than that of TDDFT, indicating smaller non-systematic errors in the predictions.

The TDA calculations when performed using def2-TZVP basis set, in combinaton with

ω B97X-D3/def2-TZVP geometries (Table S3), result in increasing MSE and MAE for S_1 and T_1 energies. However, due to the cancellation of effects, the MAE and SDE for the S_1 - T_1 gap are smaller than TDDFT/aug-cc-pVTZ and TDA/aug-cc-pVTZ (see Table S4); the latter two using CCSD(T)/cc-pVTZ geometries from Ref. 1.

Hence, combining the favorable effects of TDA and a smaller basis set, we have used TDA-TDDFT/def2-TZVP in combination with various DFT approximations to generate the excited state energetics of the bigQM7 ω dataset.

Table S1: Energies of the S_1 and T_1 states with respect to the S_0 ground state along with the singlet-triplet gap, S_1 - T_1 , of 10 triangular benchmark systems reported in Ref. 1. ADC(2)/def2-TZVP results are compared with theoretical best estimate (TBE) and ADC(2)/aug-cc-pVTZ values from Ref. 1. All values are in eV and # indicates compound number. In all calculations, we used geometries determined with the CCSD(T)/cc-pVTZ method reported in Ref. 1.

#	TBE ^a			ADC(2)/aug-cc-pVTZ ^a			ADC(2)/def2-TZVP ^b		
	S_1	T_1	S_1 - T_1	S_1	T_1	S_1 - T_1	S_1	T_1	S_1 - T_1
1	2.717	2.936	-0.219	2.675	2.921	-0.246	2.665	2.915	-0.250
2	0.979	1.111	-0.131	1.001	1.138	-0.137	1.001	1.139	-0.138
3	1.562	1.663	-0.101	1.551	1.664	-0.113	1.548	1.665	-0.117
4	2.177	2.296	-0.119	2.159	2.298	-0.139	2.153	2.295	-0.142
5	2.127	2.230	-0.103	2.098	2.225	-0.127	2.093	2.225	-0.132
6	0.833	0.904	-0.071	0.851	0.945	-0.094	0.854	0.950	-0.096
7	0.693	0.735	-0.042	0.708	0.782	-0.074	0.714	0.791	-0.078
8	0.554	0.583	-0.029	0.565	0.635	-0.070	0.575	0.646	-0.071
9	1.264	1.463	-0.199	1.274	1.488	-0.214	1.271	1.487	-0.216
10	1.522	1.827	-0.305	1.639	2.074	-0.435	1.526	1.840	-0.314

^a From Ref. 1.

^b This work.

Table S2: Energies of the S_1 and T_1 states with respect to the S_0 ground state along with the singlet-triplet gap, S_1-T_1 , of 10 triangular benchmark systems reported in Ref. 1. All energies were determined using TDDFT or its Tamm–Dancoff approximation (TDA) employing the SCS-PBE-QIDH double-hybrid DFT method and the aug-cc-pVTZ basis set. All values are in eV and # indicates compound number. In all calculations, we used geometries determined with the CCSD(T)/cc-pVTZ method reported in Ref. 1.

#	TDDFT/aug-cc-pVTZ ^a			TDDFT/aug-cc-pVTZ ^b			TDA/aug-cc-pVTZ ^b		
	S_1	T_1	S_1-T_1	S_1	T_1	S_1-T_1	S_1	T_1	S_1-T_1
1	2.770	2.987	-0.217	2.770	2.986	-0.216	2.845	3.055	-0.210
2	1.039	1.163	-0.124	1.037	1.161	-0.124	1.112	1.196	-0.084
3	1.621	1.685	-0.064	1.620	1.685	-0.065	1.696	1.749	-0.053
4	2.239	2.340	-0.101	2.238	2.339	-0.101	2.317	2.405	-0.088
5	2.188	2.245	-0.057	2.186	2.243	-0.057	2.264	2.331	-0.067
6	0.881	1.201	-0.320	0.879	1.202	-0.323	0.959	0.986	-0.027
7	0.728	0.825	-0.097	0.726	0.824	-0.098	0.809	0.808	0.001
8	0.574	0.673	-0.099	0.573	0.672	-0.099	0.658	0.647	0.011
9	1.305	1.538	-0.233	1.305	1.538	-0.233	1.398	1.567	-0.169
10	1.566	1.906	-0.340	1.566	1.906	-0.340	1.659	1.947	-0.288

^a From Ref. 1.

^b This work.

Table S3: ADC(2) and TDA-SCS-PBE-QIDH energies of the S_1 and T_1 states with respect to the S_0 ground state along with the singlet-triplet gap, S_1-T_1 , of 10 triangular benchmark systems reported in Ref. 1. All values are in eV and # indicates compound number. All calculations were performed using the def2-TZVP basis set, and geometries calculated with the ω B97X-D3/def2-TZVP method.

#	ADC(2)/def2-TZVP			TDA/def2-TZVP		
	S_1	T_1	S_1-T_1	S_1	T_1	S_1-T_1
1	2.691	2.935	-0.244	2.865	3.070	-0.205
2	1.021	1.158	-0.137	1.135	1.219	-0.084
3	1.569	1.684	-0.115	1.716	1.770	-0.054
4	2.175	2.313	-0.139	2.336	2.420	-0.084
5	2.115	2.243	-0.128	2.283	2.350	-0.067
6	0.884	0.982	-0.098	0.995	1.027	-0.032
7	0.752	0.830	-0.078	0.857	0.860	-0.003
8	0.620	0.689	-0.069	0.715	0.706	0.009
9	1.265	1.480	-0.215	1.390	1.558	-0.168
10	1.518	1.828	-0.310	1.648	1.931	-0.283

Table S4: Error metrics for predicting the S_1 & T_1 energetics of 10 triangular benchmark systems reported in Ref. 1. Values are reported for various theoretical methods in comparison with the theoretical best estimates from Ref. 1. MSE: mean signed error, MAE: mean absolute error, SDE: standard deviation of the error, minE: minimal error, maxE: maximal error are in eV.

Method	Energy	MSE	MAE	SDE	minE	maxE
ADC(2)/aug-cc-pVTZ ^a	S_1	0.009	0.029	0.041	-0.042	0.117
	T_1	0.042	0.046	0.072	-0.015	0.247
	S_1-T_1	-0.033	0.033	0.034	-0.130	-0.006
	mean	0.006	0.036	0.049	-0.062	0.119
ADC(2)/def2-TZVP ^b	S_1	-0.003	0.022	0.025	-0.052	0.022
	T_1	0.021	0.026	0.027	-0.021	0.063
	S_1-T_1	-0.024	0.024	0.011	-0.042	-0.007
	mean	-0.002	0.024	0.021	-0.038	0.026
ADC(2)/def2-TZVP ^c	S_1	0.018	0.027	0.031	-0.026	0.066
	T_1	0.040	0.040	0.038	-0.001	0.106
	S_1-T_1	-0.021	0.021	0.011	-0.040	-0.005
	mean	0.012	0.029	0.027	-0.022	0.056
TDDFT-SCS-PBE-QIDH/aug-cc-pVTZ ^a	S_1	0.048	0.048	0.013	0.020	0.062
	T_1	0.082	0.082	0.076	0.015	0.297
	S_1-T_1	-0.033	0.055	0.081	-0.249	0.046
	mean	0.032	0.062	0.057	-0.071	0.135
TDA-SCS-PBE-QIDH/aug-cc-pVTZ ^b	S_1	0.129	0.129	0.011	0.104	0.140
	T_1	0.094	0.094	0.018	0.064	0.120
	S_1-T_1	0.034	0.034	0.012	0.009	0.048
	mean	0.086	0.086	0.014	0.059	0.103
TDA-SCS-PBE-QIDH/def2-TZVP ^c	S_1	0.151	0.151	0.013	0.126	0.164
	T_1	0.116	0.116	0.011	0.095	0.134
	S_1-T_1	0.035	0.035	0.010	0.014	0.047
	mean	0.101	0.101	0.011	0.078	0.115

^a Using CCSD(T)/cc-pVTZ geometries from Ref. 1.

^b This work, using CCSD(T)/cc-pVTZ geometries from Ref. 1.

^c Using ω B97X-D3/def2-TZVP geometries, this work.

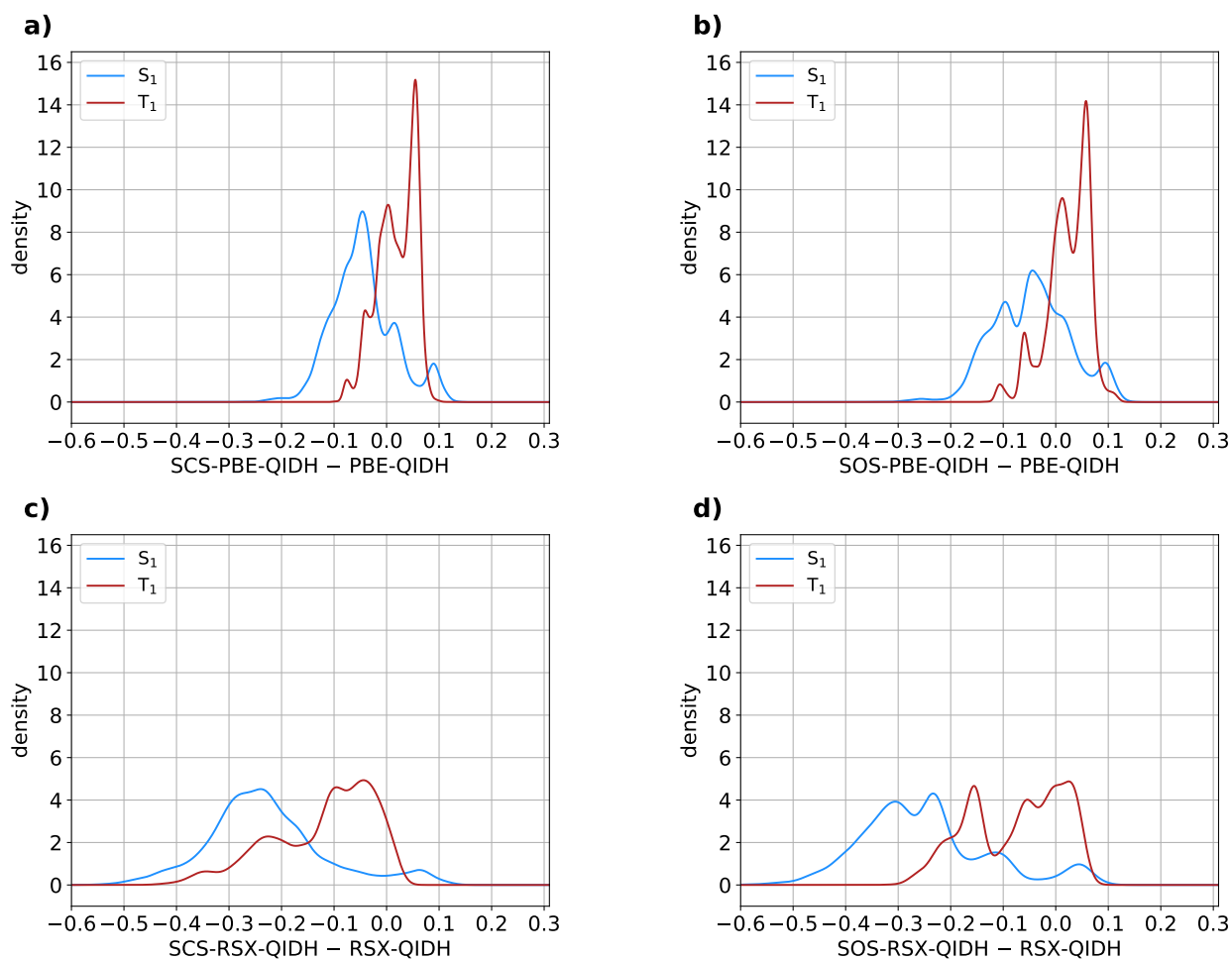


Figure S1: Probability density of the shift in S_1 and T_1 energies (in eV) of 12,880 molecules with the introduction of spin-component-scaling (SCS) and opposite-spin-component-scaling (SOS) in PBE-QIDH and RSX-QIDH methods.

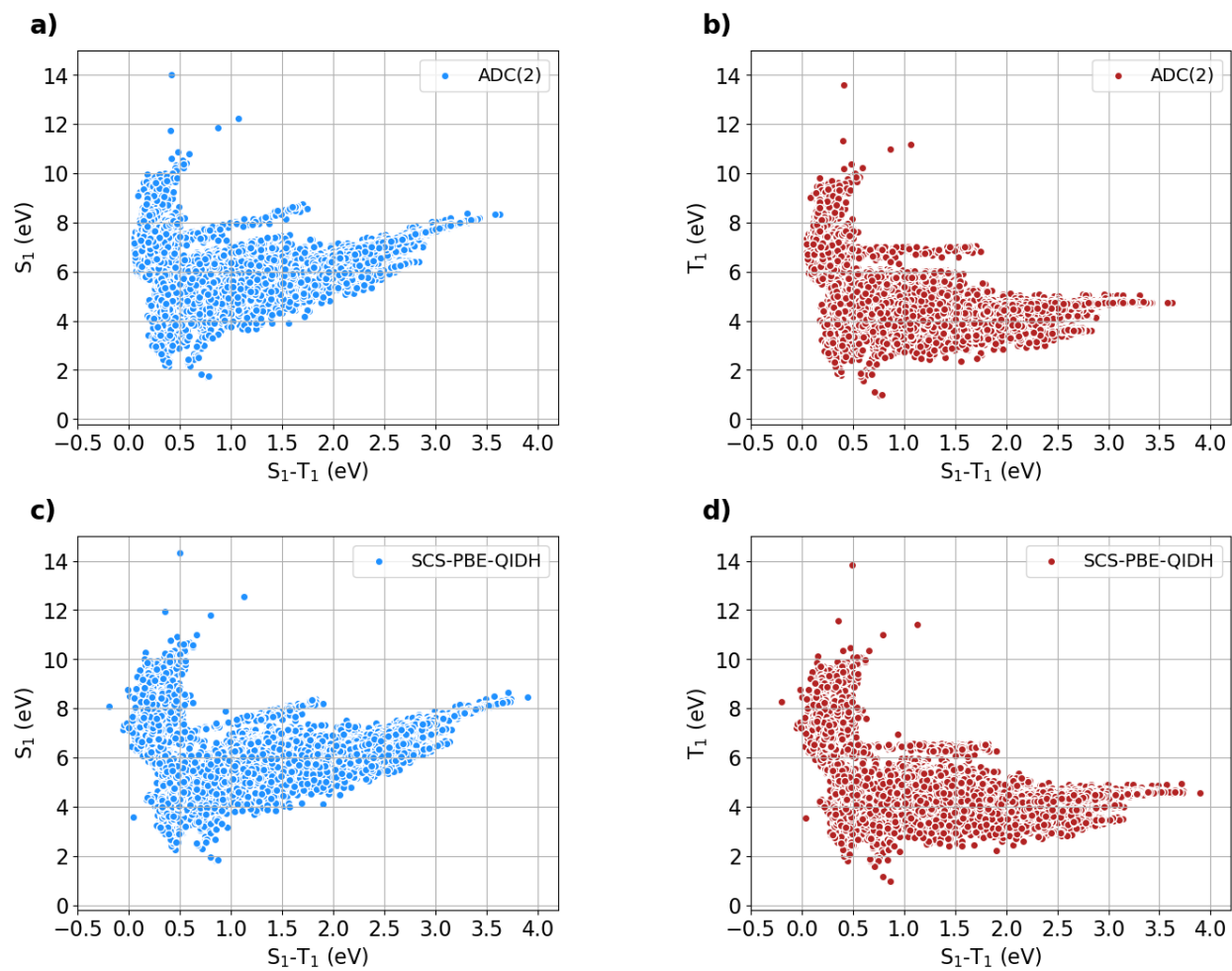


Figure S2: Distribution of S_1 and T_1 energies of 12,880 molecules calculated with ADC(2) and SCS-PBE-QIDH methods shown jointly with the $S_1 - T_1$ gap.

```
[1]: import pymoldis

df=pymoldis.get_data('bigqm7w_S1T1')
df.describe()
```

	Natoms	S1_SCSPEQIDH(eV)	T1_SCSPEQIDH(eV)	f01_SCSPEQIDH(au)	S1_ADC2(eV)	T1_ADC2(eV)	f01_ADC2(au)
count	12879.000000	12879.000000	12879.000000	12879.000000	12879.000000	12879.000000	12879.000000
mean	14.412144	6.287543	4.989370	0.099150	6.080681	5.009070	0.085172
std	2.907145	1.220643	1.372904	0.218265	1.196321	1.277183	0.169825
min	2.000000	1.809000	0.957000	0.000000	1.708240	0.945684	0.000000
25%	12.000000	5.657500	4.038000	0.001136	5.465241	4.093702	0.001144
50%	14.000000	6.393000	4.568000	0.007151	6.189377	4.732365	0.010504
75%	16.000000	7.011000	5.616000	0.050613	6.818060	5.924219	0.073313
max	23.000000	14.339000	13.844000	1.785412	14.010585	13.599737	1.362576

```
[2]: df.columns

[2]: Index(['SMI', 'Natoms', 'atoms', 'coords(Ang)', 'S1_SCSPEQIDH(eV)',
          'T1_SCSPEQIDH(eV)', 'f01_SCSPEQIDH(au)', 'S1_ADC2(eV)', 'T1_ADC2(eV)',
          'f01_ADC2(au)'],
          dtype='object')
```

Figure S3: Example query 1: Import the module `pymoldis` in Python code, load the `bigQM7 ω` dataset and perform a simple query to get an overall summary of the dataset using `.describe()` and the names of all the columns using the `columns` functionalities of `Pandas` module. Screenshot of a Jupyter notebook available at <https://github.com/mol-dis-group/pymoldis>. Note that, in `pymoldis`, we have removed the entries for the O_2 molecule as it is stable as a triplet in its ground state.


```
[1]: import pymoldis
import pandas as pd

df=pymoldis.get_data('bigqm7w_S1T1')
```

```
[2]: diff_S1=df['S1_SCSPEQIDH(eV)']-df['S1_ADC2(eV)']
diff_T1=df['T1_SCSPEQIDH(eV)']-df['T1_ADC2(eV)']
diff_S1T1=(df['S1_SCSPEQIDH(eV)']-df['T1_SCSPEQIDH(eV)'])-(df['S1_ADC2(eV)'] -df['T1_ADC2(eV)'] )
```

```
[3]: diff=pd.concat([diff_S1, diff_T1, diff_S1T1],axis=1)
diff.columns=['Delta S1 (DFT-ADC2) (eV)','Delta T1(DFT-ADC2) (eV)','Deta S1T1 (DFT-ADC2) (eV)']
diff.describe()
```

[3]:	Delta S1 (DFT-ADC2) (eV)	Delta T1(DFT-ADC2) (eV)	Deta S1T1 (DFT-ADC2) (eV)
count	12879.000000	12879.000000	12879.000000
mean	0.206861	-0.019700	0.226561
std	0.170101	0.199748	0.196457
min	-0.383320	-0.746130	-0.249989
25%	0.109476	-0.158107	0.069795
50%	0.200098	-0.053379	0.211206
75%	0.302947	0.087925	0.354126
max	1.039420	0.931055	1.295653

Figure S4: Example query 2: Import `pymoldis`, calculate the deviations of SCS-PBE-QIDH predictions from ADC(2) values of S_1 , T_1 , and S_1-T_1 energies, and get a summary of all three deviations.

```
[1]: import pymoldis
import matplotlib.pyplot as plt

df=pymoldis.get_data('bigqm7w_S1T1')
```

```
[2]: s1=df['S1_ADC2(eV)']
t1=df['T1_ADC2(eV)']
stg_adc2=s1-t1
```

```
[3]: s1=df['S1_SCSPEQIDH(eV)']
t1=df['T1_SCSPEQIDH(eV)']
stg_dft=s1-t1
```

```
[4]: plt.scatter(stg_adc2, stg_dft)
plt.xlabel('$S_1-T_1$ from ADC(2) (eV)')
plt.ylabel('$S_1-T_1$ from SCS-PBE-QIDH (eV)')
plt.title('Scatter plot')
plt.show()
```

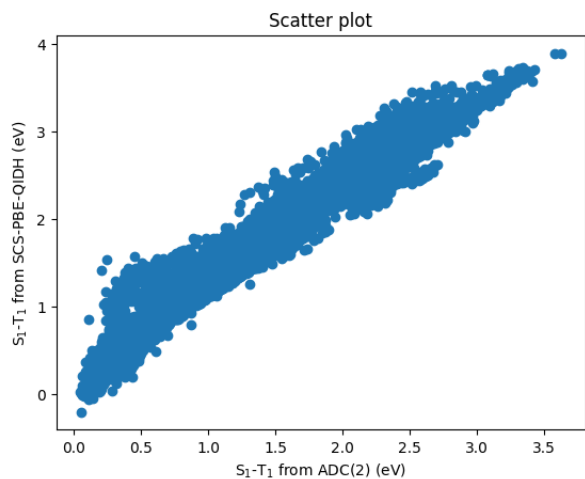


Figure S5: Example query 3: Import `pymoldis`, load S_1-T_1 energies from the SCS-PBE-QIDH and ADC(2) methods, and make a scatterplot.

```
[1]: import pymoldis
import pandas as pd

df=pymoldis.get_data('bigqm7w_S1T1')

S1T1_DFT=df['S1_SCSQBQIDH(eV)'] - df['T1_SCSQBQIDH(eV)']

NEntries=15

SmallGap_DFT_vals=S1T1_DFT.nsmallest(NEntries)

SMIs=df.iloc[SmallGap_DFT_vals.index]['SMI']

result = pd.concat([SMIs, SmallGap_DFT_vals], axis=1)
result.columns = ['SMI','S1-T1(eV)']
print(result)
```

	SMI	S1-T1(eV)
2674	'CC1(C)OC1(C)C'	-0.199
6449	'CCC1(C)CN1C'	-0.054
9153	'OC1CC2CN2C1'	-0.046
900	'CN1CC1(C)C'	-0.024
12679	'CC1CCC2CN12'	-0.019
9675	'CCC1(CF)CC1'	-0.012
12783	'CC1C2CCN1C2'	-0.008
12675	'CC1CCN2CC12'	-0.003
899	'CC1OC1(C)C'	0.007
6451	'CN1CC1(C)CO'	0.011
2232	'C1CN2CC1C2'	0.012
9204	'CC1CC2CN1C2'	0.017
3692	'CCN1CC1(C)C'	0.023
2154	'CCC1CN1C'	0.028
9122	'C1CC2CN(C1)C2'	0.028

Figure S6: Example query 4: Find 15 molecules in the bigQM7 ω dataset with the smallest S_1 - T_1 energy gaps according to the SCS-PBE-QIDH/def2-TZVP method.

```
[1]: import pymoldis
import pandas as pd

df=pymoldis.get_data('bigqm7w_S1T1')
```

Find molecules with the least S1-T1 gap in DFT and ADC2

```
[2]: diff_dft=df['S1_SCSPEQIDH(eV)'] - df['T1_SCSPEQIDH(eV)']
diff_adc2=df['S1_ADC2(eV)'] - df['T1_ADC2(eV)']

N_smallest=5
entries_dft=df.iloc[diff_dft.abs().nsmallest(N_smallest).index]
entries_adc2=df.iloc[diff_adc2.abs().nsmallest(N_smallest).index]
```

Union of both sets

```
[3]: union_df=pd.concat([entries_dft, entries_adc2]).drop_duplicates()
print(union_df[['SMI']])

SMI
12675 'CC1CCN2CC12'
899 'CC10C1(C)C'
12783 'CC1C2CCN1C2'
6451 'CN1CC1(C)CO'
2232 'C1CN2CC1C2'
12810 'C1C2C3C1N3C2'
2674 'CC1(C)OC1(C)C'
9204 'CC1CC2CN1C2'
9151 'CC1CC2CN2C1'
```

Intersection of both sets

```
[4]: intersection_df=pd.merge(entries_dft, entries_adc2, how='inner')
print(intersection_df[['SMI']])

SMI
0 'C1CN2CC1C2'
```

Figure S7: Example query 5: Find 5 molecules in the bigQM7 ω dataset with the smallest S₁-T₁ energy gaps according to the SCS-PBE-QIDH/def2-TZVP and the ADC(2) methods. Then, find the union and intersection of both sets.

```
[1]: import pymoldis

df=pymoldis.get_data('bigqm7w_S1T1')
```

```
[2]: index=2232
xyzfile='Mol_002232.xyz' # The XYZ will also be stored in this file
pymoldis.makexyz(index,df,xyzfile)
```

```
15
Mol_002232.xyz
C 1.16551200 0.75720200 -0.00000400
C 1.07023400 -0.80010900 0.00000300
N -0.39240300 -1.04289800 0.00000500
C -0.82255300 -0.01894200 1.01610000
C -0.33864800 1.03267300 -0.00000400
C -0.82255400 -0.01895100 -1.01609900
H 1.66444500 1.15390500 -0.88491300
H 1.66444600 1.15391200 0.88490200
H 1.51620400 -1.25541900 0.88379500
H 1.51620300 -1.25542600 -0.88378600
H -0.32334700 -0.08922200 1.98477500
H -1.90392100 -0.04919600 1.14389800
H -0.67188200 2.06893800 -0.00000900
H -0.32334800 -0.08923900 -1.98477400
H -1.90392200 -0.04920600 -1.14389600
```

Figure S8: Example query 6: Get the Cartesian coordinates of the equilibrium geometry of a molecule in the bigQM7 ω dataset (determined at the ω B97-XD/def2-TZVP level) using an index (perhaps one of them from the queries shown in Figure S6 or Figure S7.).


```
[1]: import pymoldis
df=pymoldis.get_data('bigqm7w_S1T1')
```

```
[2]: pymoldis.print_MolFormula(df) # to print all molecular formulas in the dataset
```

```
Item: C5_H9_N1_01, Frequency: 319
Item: C4_H8_N2_01, Frequency: 295
Item: C6_H10_01, Frequency: 293
Item: C5_H11_N1_01, Frequency: 287
Item: C4_H6_N2_01, Frequency: 262
Item: C5_H8_02, Frequency: 255
Item: C5_H7_N1_01, Frequency: 239
Item: C6_H11_N1, Frequency: 236
Item: C6_H8_01, Frequency: 236
Item: C5_H8_N2, Frequency: 222
Item: C5_H10_N2, Frequency: 222
Item: C4_H7_N1_02, Frequency: 207
Item: C6_H13_N1, Frequency: 197
Item: C6_H12_01, Frequency: 193
Item: C5_F1_H9_01, Frequency: 189
Item: C5_H10_02, Frequency: 188
Item: C6_H9_N1, Frequency: 177
Item: C4_H10_N2_01, Frequency: 176
```

```
[3]: Formula='C3_H4_O4' # pick a molecular formula
indices=pymoldis.get_ConstitutionalIsomers(df,Formula) # get the indices of the constitutional isomers for the formula
indices
```

```
[3]: [2561, 3104, 5980, 6029, 7426, 9915]
```

```
[4]: print(df[['SMI', 'S1_SCSPEQIDH(eV)', 'S1_ADC2(eV)']].iloc[indices]) # get the properties of interest
```

	SMI	S1_SCSPEQIDH(eV)	S1_ADC2(eV)
2561	'OC(=O)CC(O)=O'	5.956	5.845653
3104	'OC(=O)COC=O'	6.013	5.933349
5980	'OCC(=O)C(O)=O'	3.768	3.651278
6029	'COC(=O)C(O)=O'	4.498	4.358432
7426	'O=C1OCOC1'	7.023	6.928801
9915	'O=COCOC=O'	5.926	5.845559

Figure S11: Example query 9: Get a list of all molecular formula (atomic compositions) spanned by the bigQM7w molecules. Pick a molecular formula, and for the corresponding constitutional isomers, get indices, SMILES, and energetics.

```
[1]: import pymoldis
df=pymoldis.get_data('bigqm7w_S1T1')
```

```
[2]: def svg_from_smiles(SMI):
    from rdkit import Chem
    from rdkit.Chem import Draw
    from rdkit.Chem.Draw import rdMolDraw2D
    from io import StringIO

    mol=Chem.MolFromSmiles(SMI)
    drawer=rdMolDraw2D.MolDraw2DSVG(300, 300)
    drawer.DrawMolecule(mol)
    drawer.FinishDrawing()
    svg=drawer.GetDrawingText()

    return svg
```

```
[3]: from IPython.display import SVG

index=2232
smiles=(df.iloc[index]['SMI']).strip("")
print(smiles)
image=svg_from_smiles(smiles)
SVG(image)
C1CN2CC1C2
```

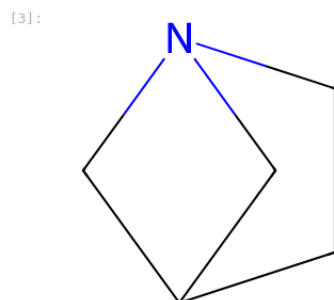


Figure S12: Example query 10: For an index in the bigQM7 ω dataset, get the corresponding SMILES, and visualize the cartoon representation using the rdkit module

MINIMUM ENERGY COORDINATES (ANGSTROM) OF STRUCTURE 1 IN FIGURE 6
Calculated with wB97X-D3/def2-TZVP

N	0.390872	1.428585	1.624955
C	0.708861	1.815707	0.253755
C	0.575682	3.347565	0.045517
C	0.089341	3.961412	1.361490
H	-0.131796	3.573618	-0.756278
H	1.533710	3.788806	-0.241382
C	1.283999	2.122298	2.548251
C	1.118564	3.662217	2.456078
H	0.778668	4.076750	3.408734
H	2.070037	4.145241	2.219926
H	1.071210	1.764467	3.558078
C	-0.992622	1.786176	1.923318
C	-1.241399	3.307219	1.744630
H	-0.039013	5.039944	1.249580
H	-1.985937	3.494278	0.966417
H	-1.626810	3.750993	2.666145
H	1.723467	1.477122	0.032424
H	-1.642047	1.200697	1.268645
H	-1.207181	1.472821	2.947557
H	2.307905	1.823158	2.312964
H	0.038048	1.268226	-0.412274

MINIMUM ENERGY COORDINATES (ANGSTROEM) OF STRUCTURE 2 IN FIGURE 6
Calculated with wB97X-D3/def2-TZVP

N	0.059194	1.259689	-0.034749
C	0.181223	1.369404	-1.395803
C	-0.296127	2.902657	-1.396472
C	0.054220	3.314306	0.129364
H	-1.363092	3.048798	-1.581413
H	0.243182	3.522982	-2.117687
C	1.181099	1.199343	0.750894
C	1.520318	2.753136	0.525266
H	1.915932	3.242972	1.419373
H	2.223629	2.952868	-0.286825
C	1.528474	-0.295853	0.278838
H	0.899558	1.113411	1.801396
C	-1.183797	1.210035	0.541175
C	-1.055725	2.697881	1.134222
H	0.050930	4.414046	0.217821
H	-1.993011	3.260095	1.099742
H	-0.688225	2.748816	2.162011
C	-0.289605	-0.146435	-1.640642
H	1.235079	1.394086	-1.677194
C	0.064753	-0.795176	-0.200259
H	0.247777	-0.642054	-2.453944
H	-1.356951	-0.264126	-1.843230
H	1.929624	-0.922619	1.080084
H	2.228482	-0.357077	-0.558021
C	-1.048484	-0.352316	0.888450
H	0.066962	-1.894859	-0.288843
H	-1.956302	1.270798	-0.226817
H	-0.683096	-0.565357	1.895970
H	-1.983093	-0.906070	0.762965

MINIMUM ENERGY COORDINATES (ANGSTROM) OF STRUCTURE 3 IN FIGURE 6
Calculated with wB97X-D3/def2-TZVP

N	0.379208	1.545025	1.615145
C	0.522414	1.919464	0.194214
C	0.040684	3.378560	-0.020385
C	0.070623	4.079408	1.341912
H	-0.971796	3.397890	-0.435621
H	0.687101	3.882379	-0.742271
C	1.397206	2.264418	2.406877
C	1.412052	3.764525	2.012063
H	1.569465	4.382515	2.898662
H	2.237474	3.978652	1.325930
H	1.089246	2.185002	3.450570
C	-0.962585	1.942004	2.086010
C	-1.045306	3.486323	2.208089
H	-0.060595	5.156597	1.225223
H	-2.028676	3.834363	1.884747
H	-0.923759	3.801422	3.249156
H	1.589067	1.872414	-0.031392
H	-1.668148	1.617693	1.319548
C	-1.351177	1.237061	3.350943
C	-2.472023	0.550734	3.501386
H	-0.672436	1.330637	4.194999
H	-3.177772	0.431281	2.685513
H	-2.727656	0.079541	4.442427
C	2.748725	1.623174	2.311812
C	3.451742	1.226245	3.359832
H	3.172792	1.510693	1.317038
H	4.436513	0.788344	3.252706
H	3.063378	1.320067	4.368993
C	-0.151387	0.943751	-0.723295
C	0.442594	0.367902	-1.755661
H	-1.200067	0.730826	-0.531445
H	-0.090516	-0.308915	-2.411831
H	1.487653	0.552956	-1.982883

MINIMUM ENERGY COORDINATES (ANGSTROEM) OF STRUCTURE 4 IN FIGURE 6
Calculated with wB97X-D3/def2-TZVP

N	0.355841	1.689193	1.598935
C	0.654217	1.567608	0.241850
C	0.916390	3.184956	0.110907
C	0.117101	3.739458	1.383964
H	0.492086	3.569881	-0.818793
H	1.953136	3.517290	0.137921
C	1.382307	1.891585	2.521578
C	0.949315	3.463932	2.724722
H	0.351171	3.699694	3.603907
H	1.834938	4.101303	2.773002
C	1.206907	0.380433	3.106052
C	-0.962678	1.564839	2.037086
C	-1.333716	3.064287	1.474371
H	-0.010959	4.829075	1.268782
H	-1.838994	3.113681	0.510825
H	-1.969501	3.596206	2.185549
C	1.368005	0.121696	0.488440
C	0.595592	-0.357605	1.814591
H	2.440757	0.147130	0.671914
H	1.195988	-0.565099	-0.340160
H	0.525997	0.275976	3.949162
H	2.159615	-0.058002	3.402458
C	-0.972163	-0.025668	1.682064
H	0.723680	-1.446292	1.930783
H	-1.563157	-0.604598	2.391255
H	-1.320345	-0.286401	0.684087
C	-1.319803	1.664616	3.508357
C	-2.446498	1.175892	4.005664
H	-0.689579	2.244579	4.167756
H	-3.139819	0.593203	3.409219
H	-2.718670	1.354144	5.037962
C	2.830237	1.995063	2.078788
C	3.843275	1.830891	2.916769
H	3.056792	2.300071	1.066856
H	4.862687	2.000213	2.594920
H	3.698317	1.535684	3.950444
C	-0.433615	1.319396	-0.787093
C	-0.169445	0.856936	-2.000303
H	-1.452131	1.607214	-0.567215
H	-0.950220	0.771167	-2.744907
H	0.828234	0.554823	-2.300199

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