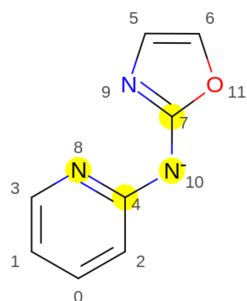


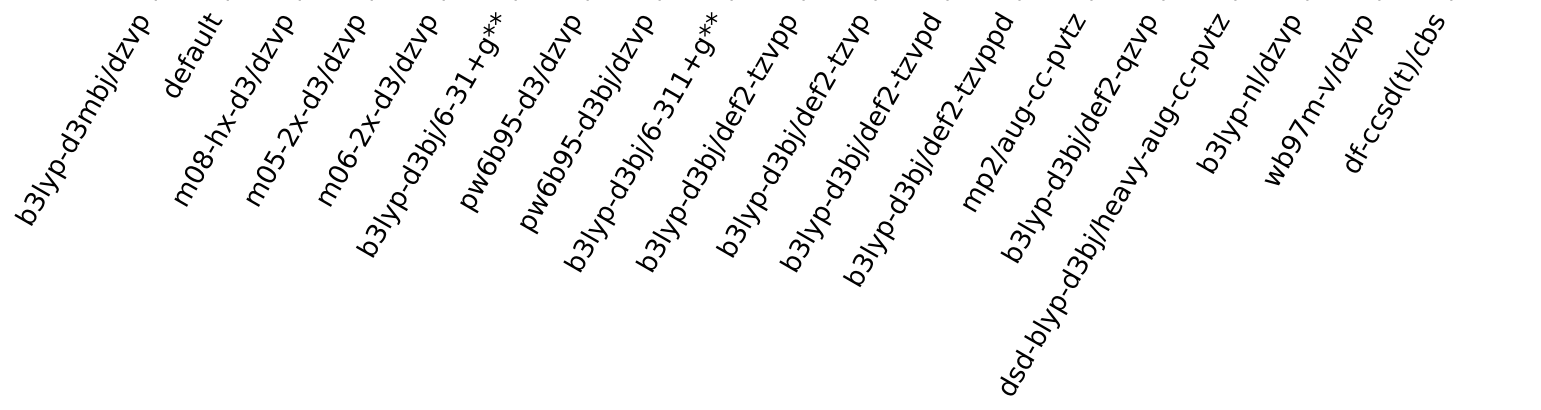
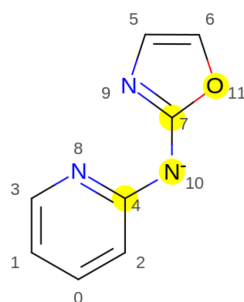
Wall time in seconds (in log scale)



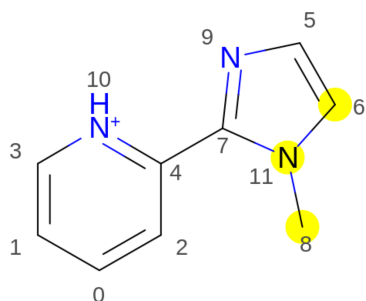
Bar chart showing Wall time in seconds (in log scale) for various computational methods. The y-axis ranges from 10^1 to 10^4 seconds. The x-axis lists the methods. The wall time increases significantly for the methods listed on the right side of the chart.

| Method | Wall time (seconds) |
|------------------------|---------------------|
| b3lyp-d3mbj/dzvp | ~15 |
| default | ~15 |
| m05-2x-d3/dzvp | ~25 |
| m08-hx-d3/dzvp | ~25 |
| m06-2x-d3/dzvp | ~30 |
| pw6b95-d3/dzvp | ~30 |
| b3lyp-d3bj/dzvp | ~30 |
| pw6b95-d3bj/dzvp | ~35 |
| b3lyp-d3bj/6-31+g** | ~35 |
| b3lyp-d3bj/6-311+g** | ~38 |
| b3lyp-d3bj/def2-tzvp | ~50 |
| b3lyp-d3bj/def2-tzvpp | ~52 |
| b3lyp-d3bj/def2-tzvppd | ~80 |
| mp2/aug-cc-pvtz | ~100 |
| b3lyp-d3bj/def2-qzvp | ~110 |
| b3lyp-nl/dzvp | ~130 |
| wb97m-v/dzvp | ~140 |
| df-ccsd(t)/cbs | ~150 |

Wall time in seconds (in log scale)

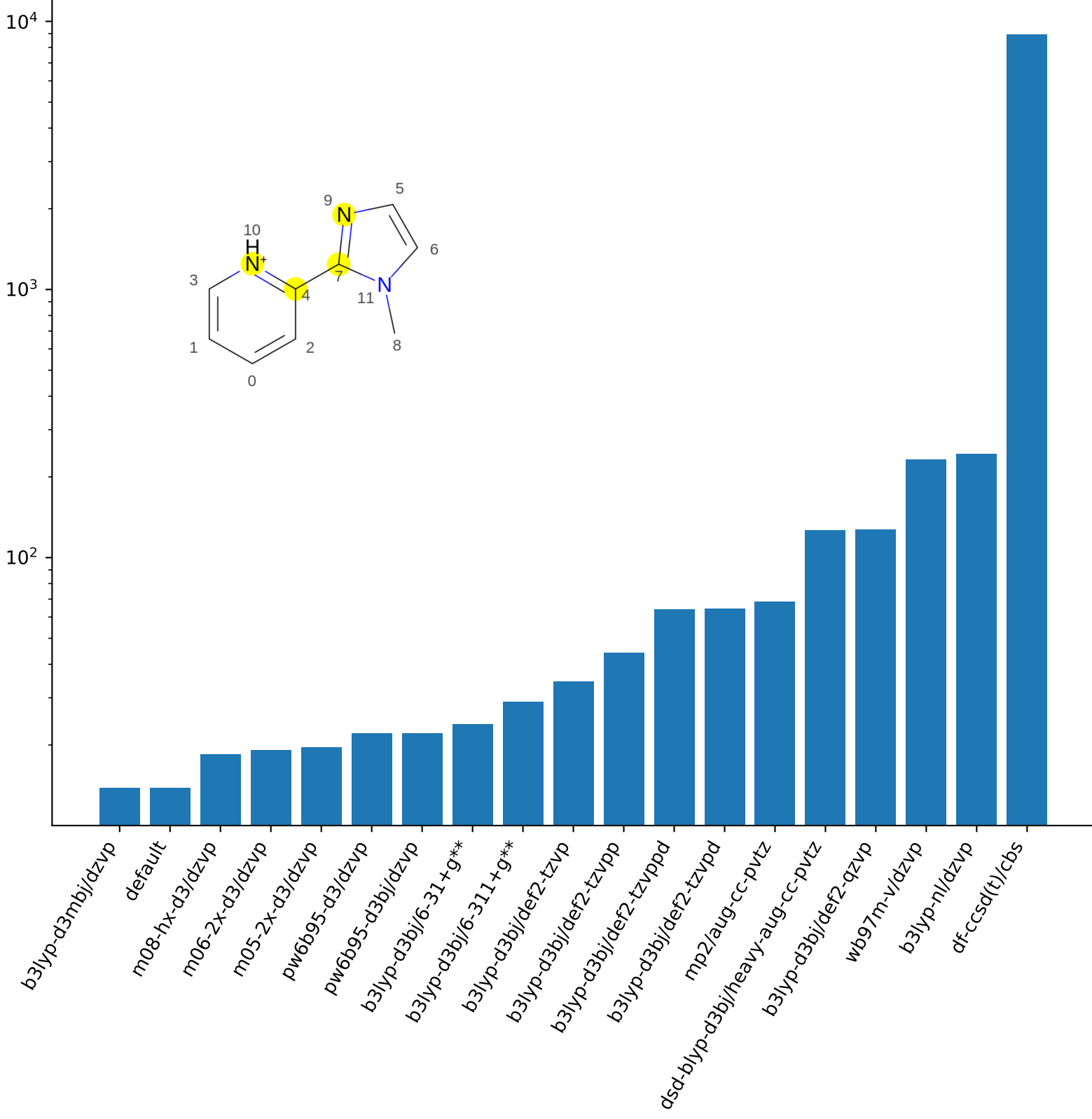


Wall time in seconds (in log scale)

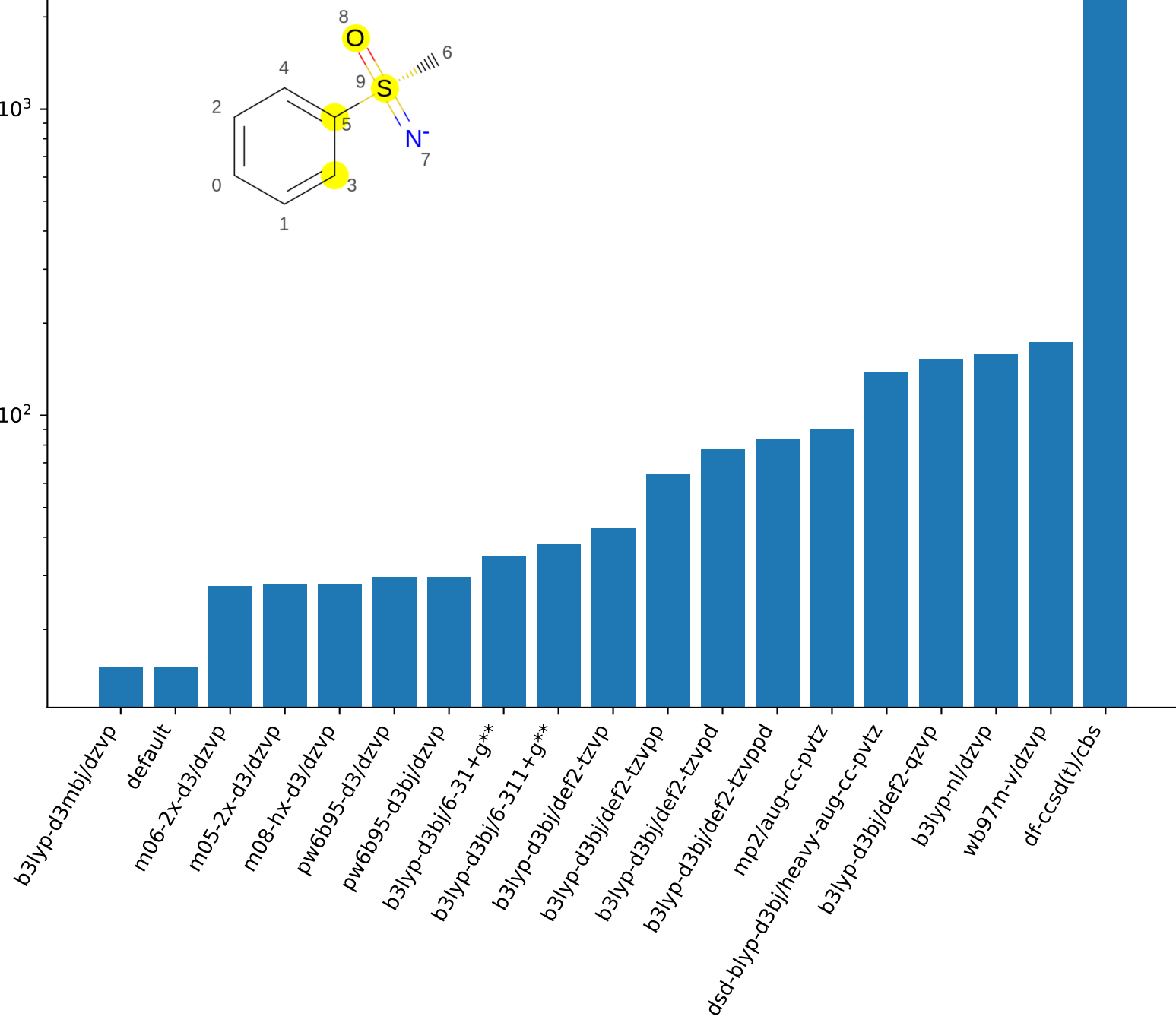


m08-hx-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3mbj/dzvp
default
m06-2x-d3/dzvp
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

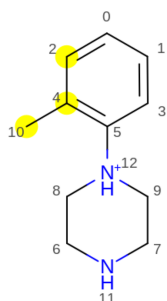
Wall time in seconds (in log scale)



Wall time in seconds (in log scale)



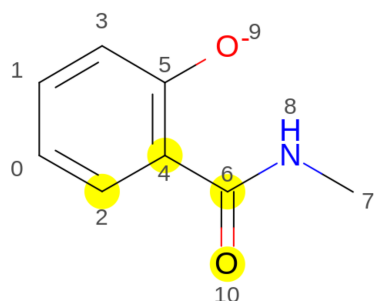
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The y-axis ranges from 10^2 to 10^4 seconds. The x-axis lists the methods. The wall time increases significantly for the methods listed from left to right, with the final method (df-ccsd(t)/cbs) showing the highest wall time, exceeding 10^4 seconds.

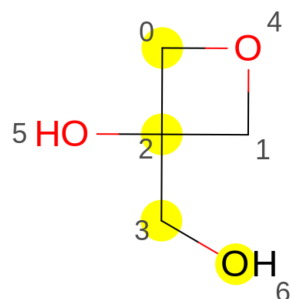
| Method | Wall time (seconds) |
|------------------------|---------------------|
| b3lyp-d3mbj/dzvp | ~200 |
| default | ~200 |
| m05-2x-d3/dzvp | ~300 |
| pw6b95-d3/dzvp | ~300 |
| pw6b95-d3bj/dzvp | ~300 |
| m08-hx-d3/dzvp | ~300 |
| m06-2x-d3/dzvp | ~300 |
| b3lyp-d3bj/6-31+g** | ~300 |
| b3lyp-d3bj/6-311+g** | ~400 |
| b3lyp-d3bj/def2-tzvp | ~500 |
| b3lyp-d3bj/def2-tzvpp | ~700 |
| b3lyp-d3bj/def2-tzvppd | ~1100 |
| b3lyp-d3bj/def2-tzvppd | ~1400 |
| mp2/aug-cc-pvtz | ~2000 |
| b3lyp-d3bj/def2-qzvp | ~2200 |
| b3lyp-nl/dzvp | ~3000 |
| wb97m-v/dzvp | ~4000 |
| df-ccsd(t)/cbs | > 10000 |

Wall time in seconds (in log scale)



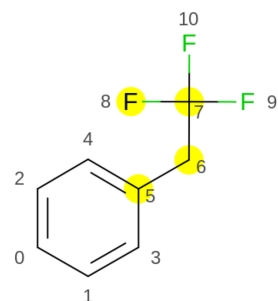
m05-2x-d3/dzvp
m08-hx-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3mbj/dzvp
default
m06-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

Wall time in seconds (in log scale)



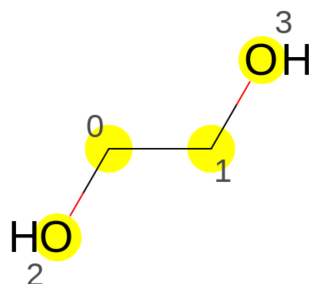
b3lyp-d3mbj/dzvp
default
b3lyp-d3bj/6-31+g**
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m08-hx-d3/dzvp
m06-2x-d3/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

Wall time in seconds (in log scale)

 10^3 10^2 10^1

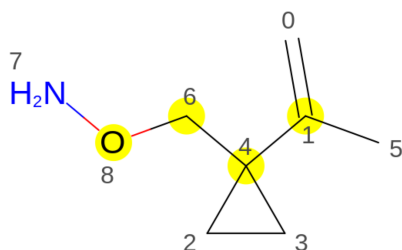
b3lyp-d3mbj/dzvp
default
m06-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m08-hx-d3/dzvp
m05-2x-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

Wall time in seconds (in log scale)



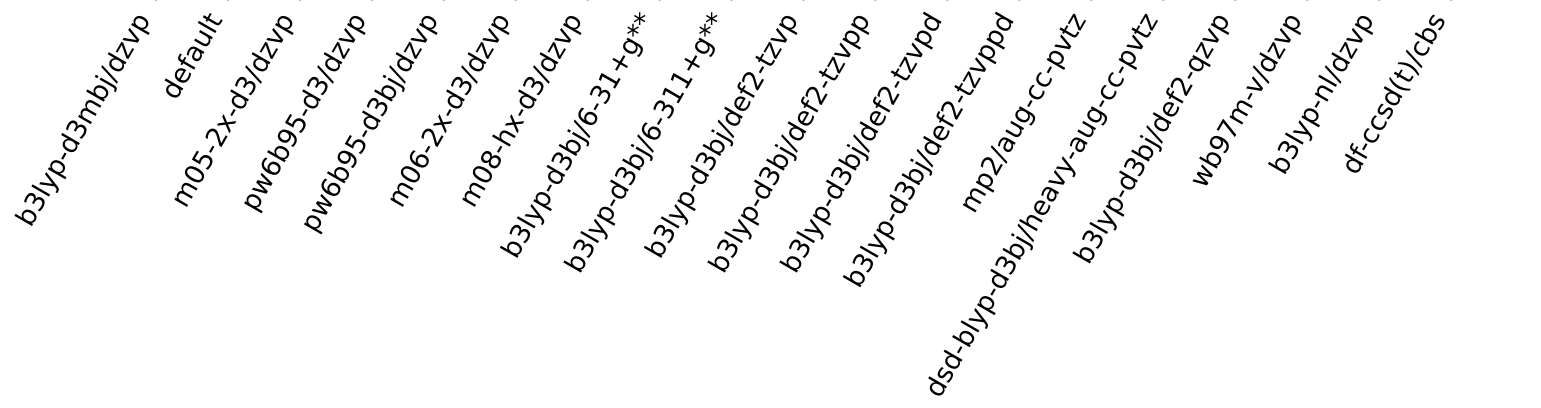
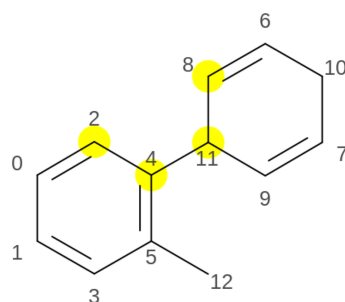
b3lyp-d3mbj/dzvp
default
b3lyp-d3bj/6-31+g**
m06-2x-d3/dzvp
b3lyp-d3bj/6-311+g**
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m08-hx-d3/dzvp
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

Wall time in seconds (in log scale)

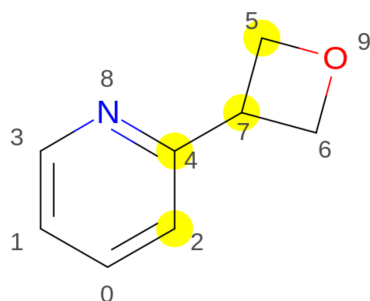


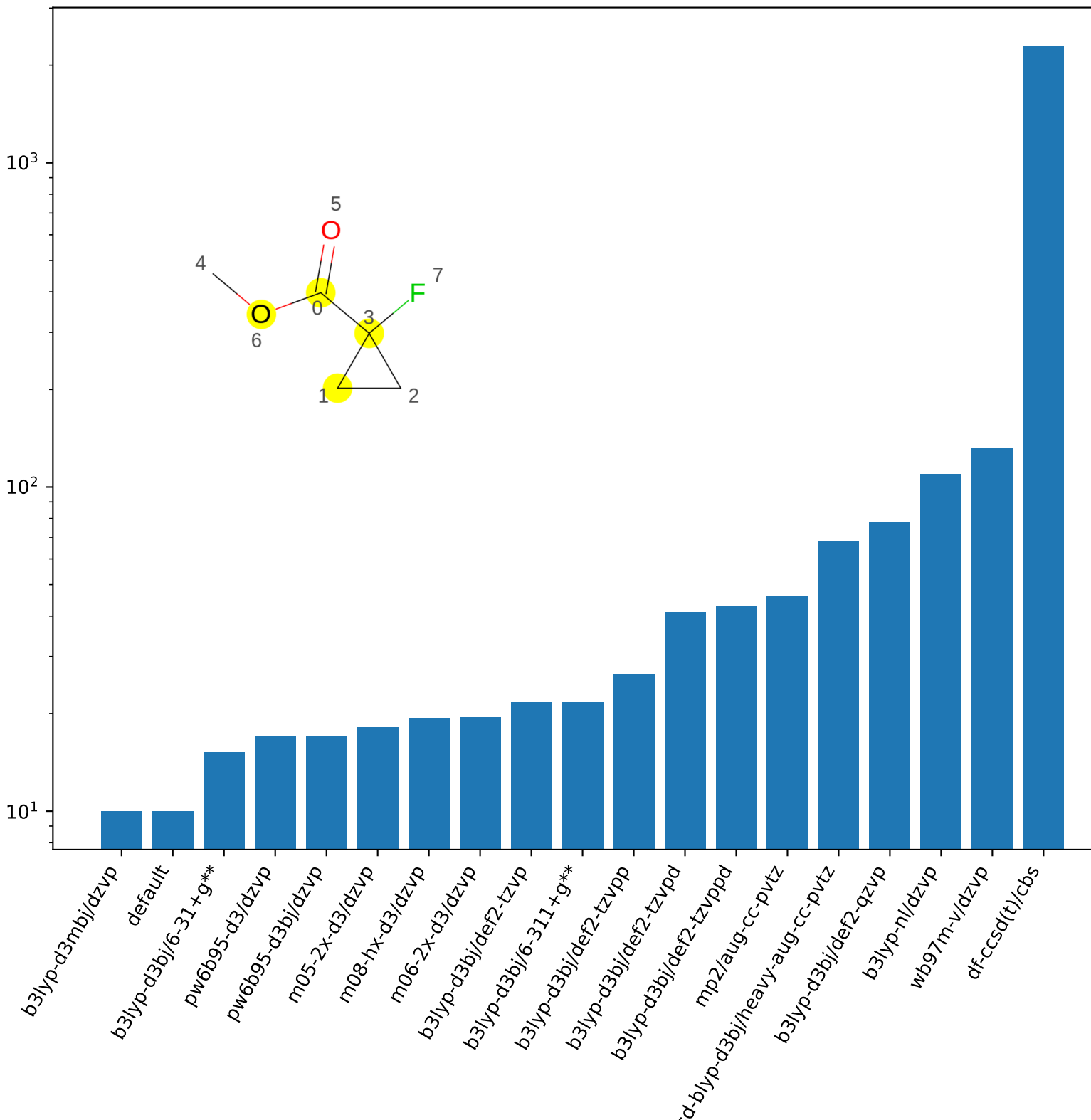
b3lyp-d3mbj/dzvp
default
m05-2x-d3/6-31+g**
m08-hx-d3/dzvp
m06-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

Wall time in seconds (in log scale)

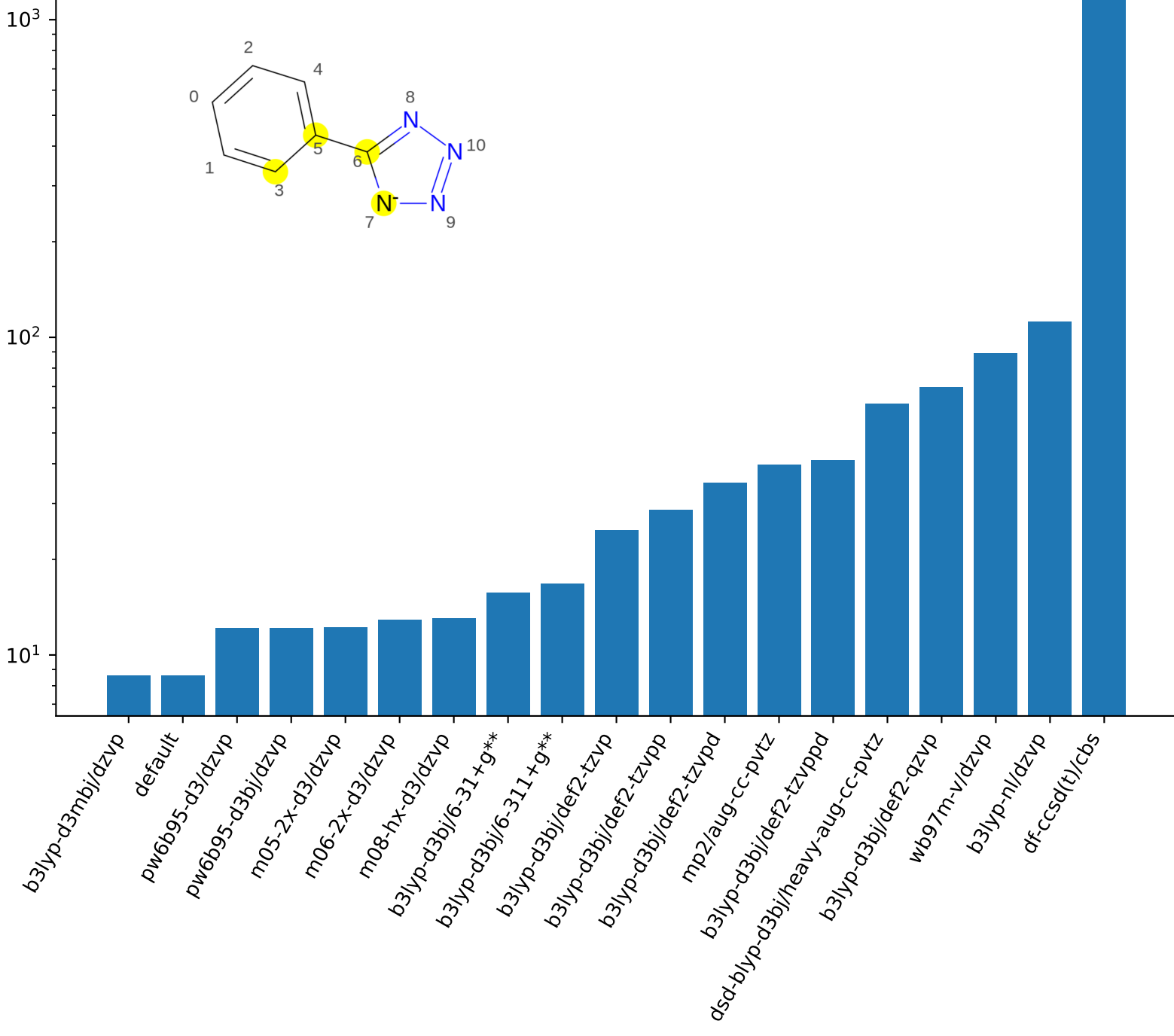


Wall time in seconds (in log scale)

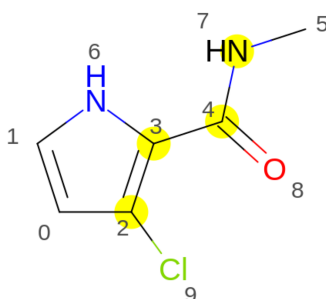
 10^3 10^2 10^1 *b3lyp-d3mbj/dzvp**default**pw6b95-d3/dzvp**pw6b95-d3bj/dzvp**b3lyp-d3bj/6-31+g****m05-2x-d3/dzvp**m06-2x-d3/dzvp**m08-hx-d3/dzvp**b3lyp-d3bj/6-311+g****b3lyp-d3bj/def2-tzvp**mp2/aug-cc-pvtz**b3lyp-d3bj/def2-tzvpd**b3lyp-d3bj/def2-tzvppd**dsd-blyp-d3bj/heavy-aug-cc-pvtz**b3lyp-d3bj/def2-qzvp**wb97m-v/dzvp**b3lyp-nl/dzvp**df-ccsd(t)/cbs*



Wall time in seconds (in log scale)



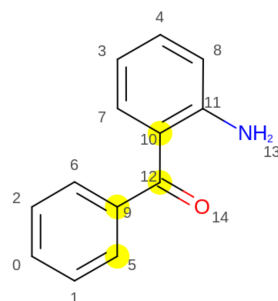
Wall time in seconds (in log scale)



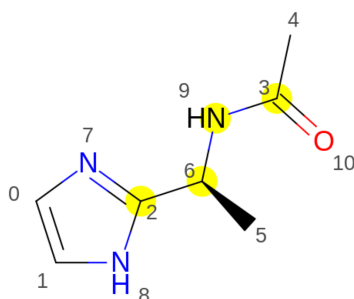
Bar chart showing Wall time in seconds (in log scale) for various computational methods. The y-axis ranges from 10¹ to 10³ seconds. The x-axis lists the methods. The wall time increases significantly for the methods listed on the right side of the chart.

| Method | Wall time (seconds) |
|---------------------------------|---------------------|
| b3lyp-d3mbj/dzvp | ~9 |
| default | ~9 |
| m05-2x-d3/dzvp | ~13 |
| pw6b95-d3/dzvp | ~13 |
| pw6b95-d3bj/dzvp | ~13 |
| m06-2x-d3/dzvp | ~14 |
| m08-hx-d3/dzvp | ~15 |
| b3lyp-d3bj/6-31+g** | ~15 |
| b3lyp-d3bj/6-311+g** | ~16 |
| b3lyp-d3bj/def2-tzvp | ~22 |
| b3lyp-d3bj/def2-tzvpp | ~32 |
| b3lyp-d3bj/def2-tzvppd | ~38 |
| mp2/aug-cc-pvtz | ~40 |
| b3lyp-d3bj/def2-tzvppd | ~45 |
| b3lyp-d3bj/def2-qzvp | ~60 |
| dsd-blyp-d3bj/heavy-aug-cc-pvtz | ~65 |
| b3lyp-nl/dzvp | ~115 |
| wb97m-v/dzvp | ~125 |
| df-ccsd(t)/cbs | ~3500 |

Wall time in seconds (in log scale)

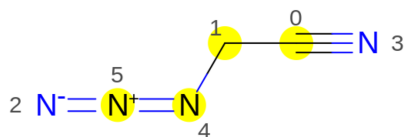


b3lyp-d3mbj/dzvp
default
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
mp2/aug-cc-pvtz
d3d-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs



b3lyp-d3mbj/dzvp
default
m08-hx-d3/dzvp
b3lyp-d3bj/6-31+g**
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m06-2x-d3/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvppd
d3sd.b3lyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

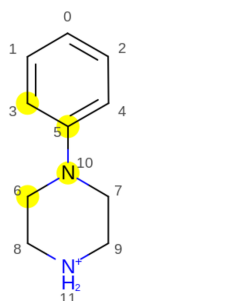
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The Y-axis ranges from 10^1 to 10^2 . The X-axis lists the methods. The wall time increases significantly for the methods listed on the right side of the chart.

| Method | Wall time (seconds) |
|---------------------------------|---------------------|
| b3lyp-d3mbj/dzvp | ~2.5 |
| default | ~2.5 |
| m08-hx-d3-31+g** | ~3.5 |
| m05-2x-d3/dzvp | ~4.5 |
| m06-2x-d3/dzvp | ~4.5 |
| pw6b95-d3/dzvp | ~4.5 |
| pw6b95-d3bj/dzvp | ~4.5 |
| b3lyp-d3bj/6-311+g** | ~4.5 |
| b3lyp-d3bj/def2-tzvp | ~5.5 |
| mp2/aug-cc-pvtz | ~6.5 |
| b3lyp-d3bj/def2-tzvpp | ~7.5 |
| b3lyp-d3bj/def2-tzvpd | ~7.5 |
| dsd-blyp-d3bj/heavy-aug-cc-pvtz | ~9.5 |
| b3lyp-d3bj/def2-qzvp | ~18.5 |
| b3lyp-nl/dzvp | ~20.5 |
| wb97m-v/dzvp | ~28.5 |
| df-ccsd(t)/cbs | ~145 |

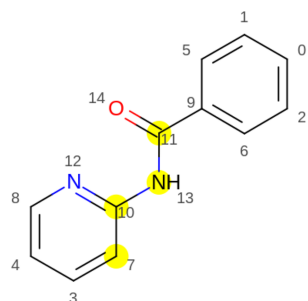
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The y-axis ranges from 10¹ to 10⁴ seconds. The x-axis lists the methods. The wall time increases significantly for the methods listed on the right side of the chart.

| Method | Wall time (seconds) |
|---------------------------------|---------------------|
| b3lyp-d3mbj/dzvp | ~20 |
| default | ~20 |
| m05-2x-d3/dzvp | ~22 |
| m08-hx-d3/dzvp | ~23 |
| m06-2x-d3/dzvp | ~25 |
| pw6b95-d3/dzvp | ~28 |
| pw6b95-d3bj/dzvp | ~28 |
| b3lyp-d3bj/6-31+g** | ~32 |
| b3lyp-d3bj/6-311+g** | ~40 |
| b3lyp-d3bj/def2-tzvp | ~48 |
| b3lyp-d3bj/def2-tzvpp | ~70 |
| b3lyp-d3bj/def2-tzvppd | ~80 |
| mp2/aug-cc-pvtz | ~95 |
| b3lyp-d3bj/def2-tzvppd | ~100 |
| d3d-blyp-d3bj/heavy-aug-cc-pvtz | ~150 |
| b3lyp-d3bj/def2-qzvp | ~200 |
| wb97m-v/dzvp | ~400 |
| b3lyp-nl/dzvp | ~420 |
| df-ccsd(t)/cbs | ~18000 |

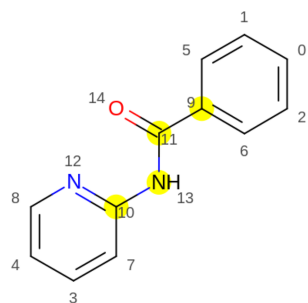
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The y-axis ranges from 10^2 to 10^4 seconds. The x-axis lists the computational methods. The wall time increases significantly for the methods listed on the right side of the chart, reaching over 10^4 seconds for the final method.

| Computational Method | Wall time in seconds (approx.) |
|---------------------------------|--------------------------------|
| b3lyp-d3mbj/dzvp | 200 |
| default | 200 |
| m06-2x-d3/dzvp | 300 |
| m08-hx-d3/dzvp | 300 |
| m05-2x-d3/dzvp | 350 |
| pw6b95-d3/dzvp | 350 |
| pw6b95-d3bj/dzvp | 350 |
| b3lyp-d3bj/6-31+g** | 350 |
| b3lyp-d3bj/6-311+g** | 400 |
| b3lyp-d3bj/def2-tzvp | 500 |
| b3lyp-d3bj/def2-tzvpp | 600 |
| b3lyp-d3bj/def2-tzvppd | 800 |
| mp2/aug-cc-pvtz | 1000 |
| b3lyp-d3bj/def2-qzvp | 1500 |
| dsd-blyp-d3bj/heavy-aug-cc-pvtz | 1800 |
| wb97m-v/dzvp | 3500 |
| b3lyp-nl/dzvp | 4000 |
| df-ccsd(t)/cbs | 35000 |

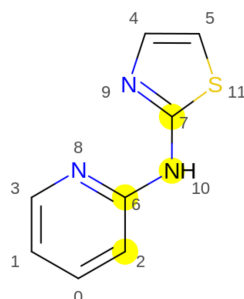
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is plotted on the y-axis (log scale).

| Method | Wall time (seconds) |
|---------------------------------|---------------------|
| b3lyp-d3mbj/dzvp | ~20 |
| default | ~20 |
| m08-hx-d3/dzvp | ~22 |
| m05-2x-d3/dzvp | ~25 |
| m06-2x-d3/dzvp | ~26 |
| pw6b95-d3/dzvp | ~27 |
| pw6b95-d3bj/dzvp | ~28 |
| b3lyp-d3bj/6-31+g** | ~30 |
| b3lyp-d3bj/6-311+g** | ~35 |
| b3lyp-d3bj/def2-tzvp | ~45 |
| b3lyp-d3bj/def2-tzvpp | ~55 |
| b3lyp-d3bj/def2-tzvppd | ~75 |
| mp2/aug-cc-pvtz | ~90 |
| b3lyp-d3bj/def2-qzvp | ~120 |
| dsd-blyp-d3bj/heavy-aug-cc-pvtz | ~180 |
| wb97m-v/dzvp | ~220 |
| b3lyp-nl/dzvp | ~350 |
| df-ccsd(t)/cbs | ~3500 |

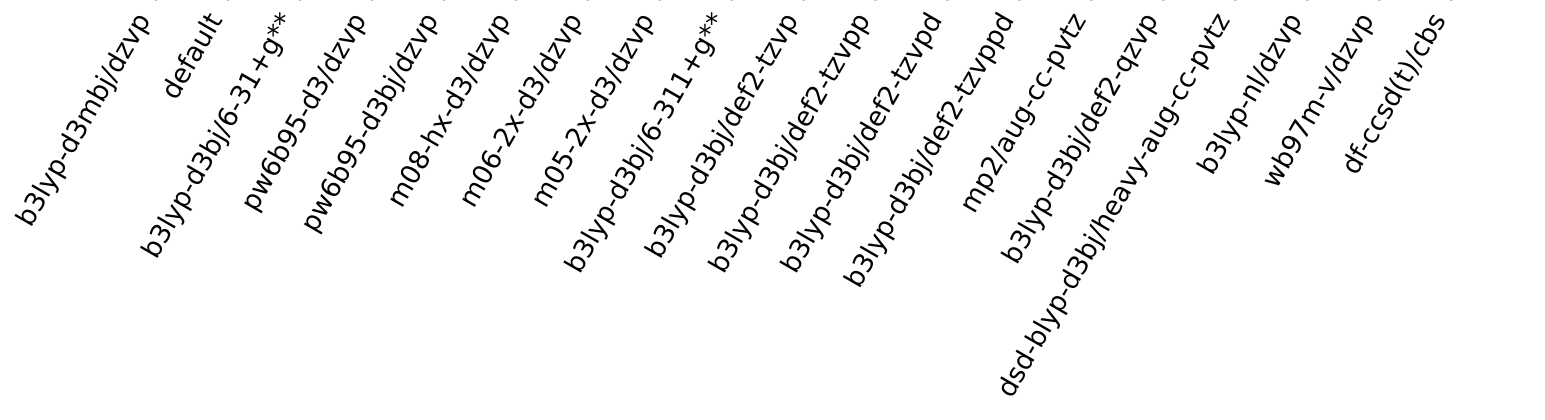
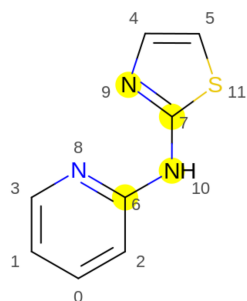
Wall time in seconds (in log scale)

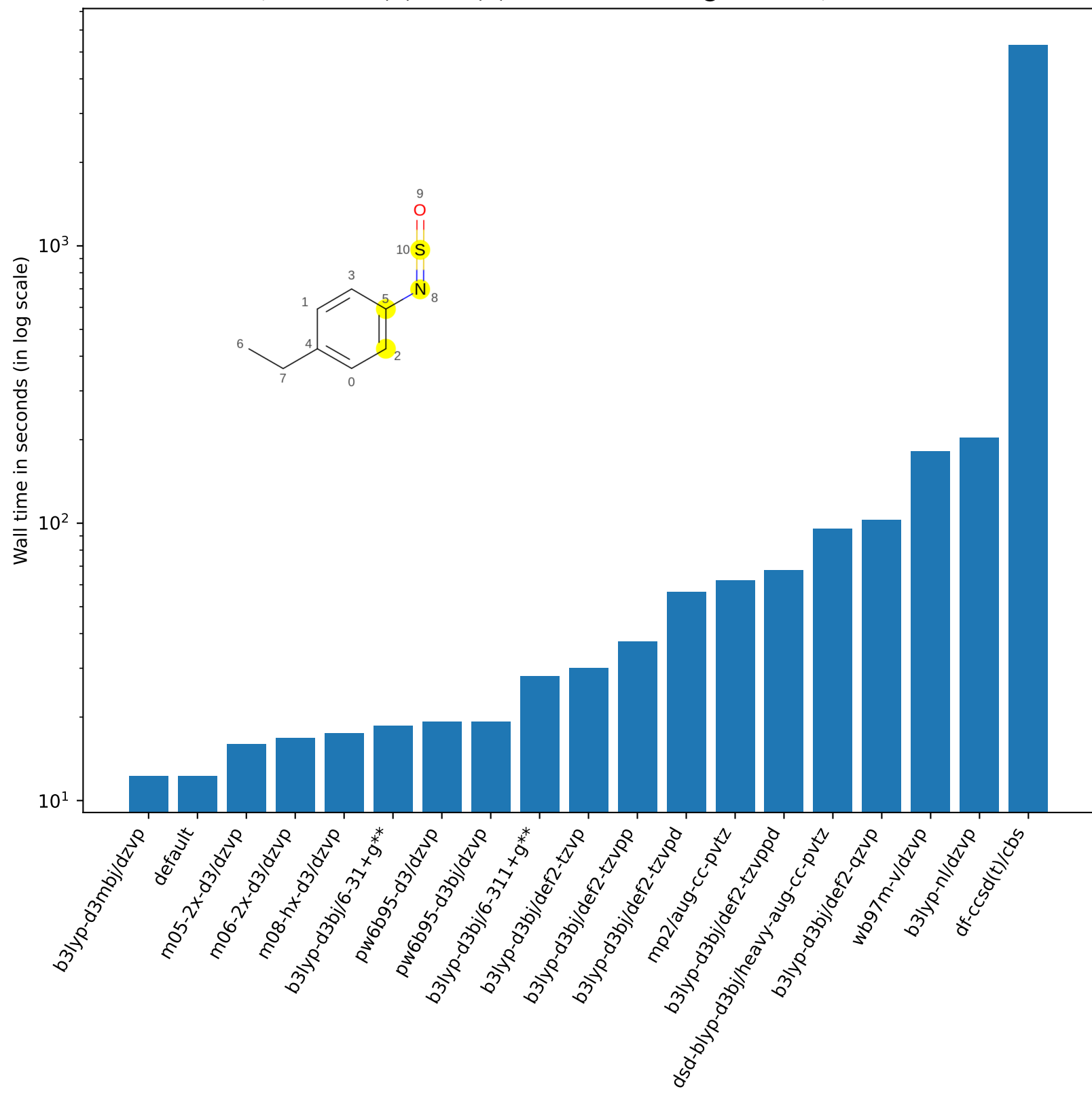


Bar chart showing Wall time in seconds (in log scale) for various computational methods. The y-axis ranges from 10¹ to 10³ seconds. The x-axis lists the methods. The wall time increases significantly for the methods listed on the right side of the chart.

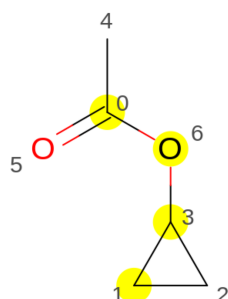
| Method | Wall time (seconds) |
|------------------------|---------------------|
| b3lyp-d3mbj/dzvp | ~11 |
| default | ~11 |
| m08-hx-d3/dzvp | ~17 |
| m05-2x-d3/dzvp | ~18 |
| pw6b95-d3/dzvp | ~18 |
| pw6b95-d3bj/dzvp | ~18 |
| m06-2x-d3/dzvp | ~18 |
| b3lyp-d3bj/6-31+g** | ~20 |
| b3lyp-d3bj/6-311+g** | ~23 |
| b3lyp-d3bj/def2-tzvp | ~26 |
| b3lyp-d3bj/def2-tzvpp | ~35 |
| mp2/aug-cc-pvtz | ~50 |
| b3lyp-d3bj/def2-tzvppd | ~55 |
| b3lyp-d3bj/def2-tzvppd | ~55 |
| b3lyp-d3bj/def2-tzvppd | ~55 |
| b3lyp-d3bj/def2-tzvppd | ~95 |
| wb97m-v/dzvp | ~100 |
| b3lyp-nl/dzvp | ~160 |
| df-ccsd(t)/cbs | ~170 |
| b3lyp-d3bj/def2-tzvppd | ~500 |

Wall time in seconds (in log scale)



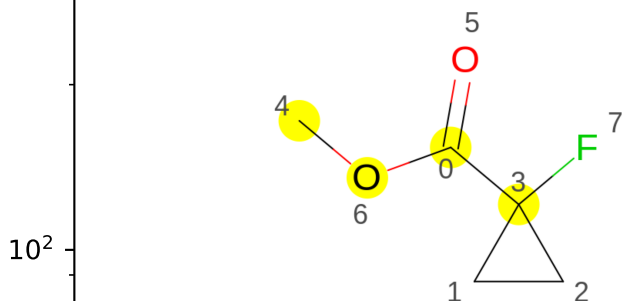


Wall time in seconds (in log scale)



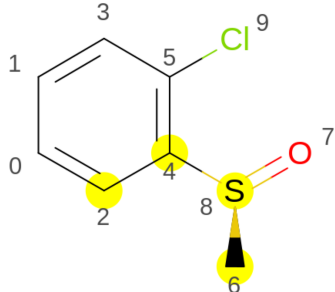
b3lyp-d3mbj/dzvp
default
m06-2x-d3/dzvp
b3lyp-d3bj/6-31+g**
m08-hx-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
m05-2x-d3/dzvp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvppd
d3lyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvpp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

Wall time in seconds (in log scale)

10¹10²

b3lyp-d3mbj/dzvp
default
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
b3lyp-d3bj/6-31+g**
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
d3d-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

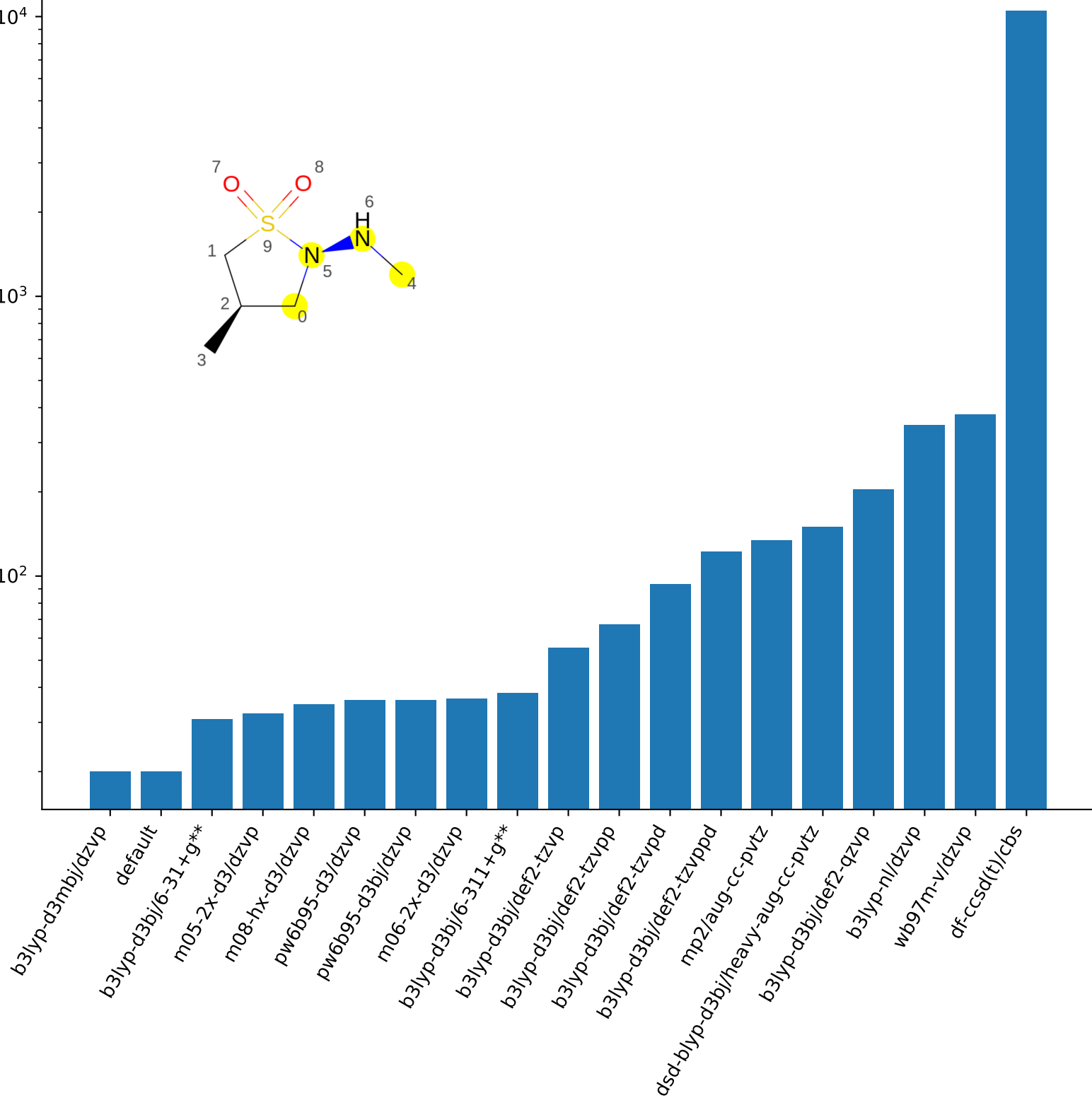
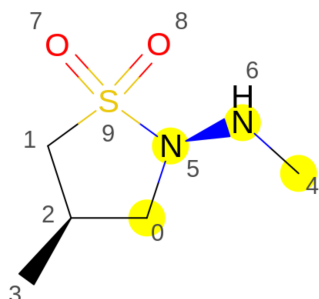
Wall time in seconds (in log scale)



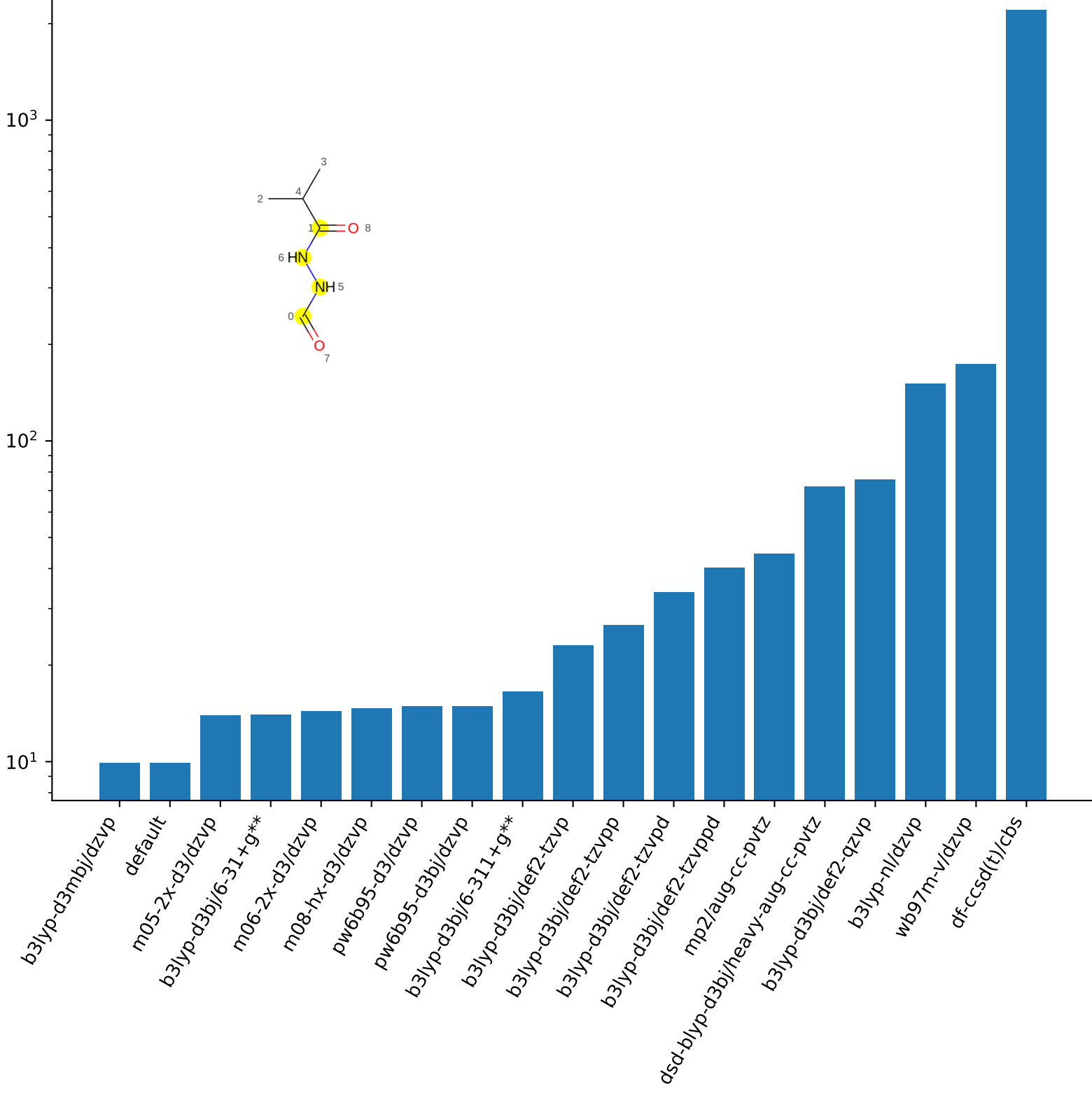
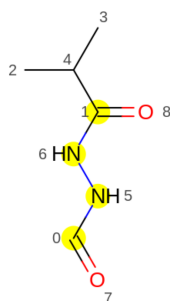
Bar chart showing Wall time in seconds (in log scale) for various computational methods. The methods are listed on the x-axis, and the wall time is shown on the y-axis (log scale).

| Method | Wall time (seconds) |
|---------------------------------|---------------------|
| b3lyp-d3mbj/dzvp | ~8.5 |
| default | ~8.5 |
| m06-2x-d3/dzvp | ~13.5 |
| b3lyp-d3bj/6-31+g** | ~14.5 |
| pw6b95-d3/dzvp | ~14.5 |
| pw6b95-d3bj/dzvp | ~14.5 |
| m08-hx-d3/dzvp | ~14.5 |
| m05-2x-d3/dzvp | ~15.5 |
| b3lyp-d3bj/6-311+g** | ~20.5 |
| b3lyp-d3bj/def2-tzvp | ~22.5 |
| b3lyp-d3bj/def2-tzvpp | ~26.5 |
| b3lyp-d3bj/def2-tzvppd | ~38.5 |
| mp2/aug-cc-pvtz | ~45.5 |
| b3lyp-d3bj/def2-tzvppd | ~48.5 |
| dsd-blyp-d3bj/heavy-aug-cc-pvtz | ~65.5 |
| b3lyp-d3bj/def2-qzvvp | ~75.5 |
| wb97m-v/dzvp | ~115.5 |
| b3lyp-nl/dzvp | ~125.5 |
| df-ccsd(t)/cbs | ~3500.5 |

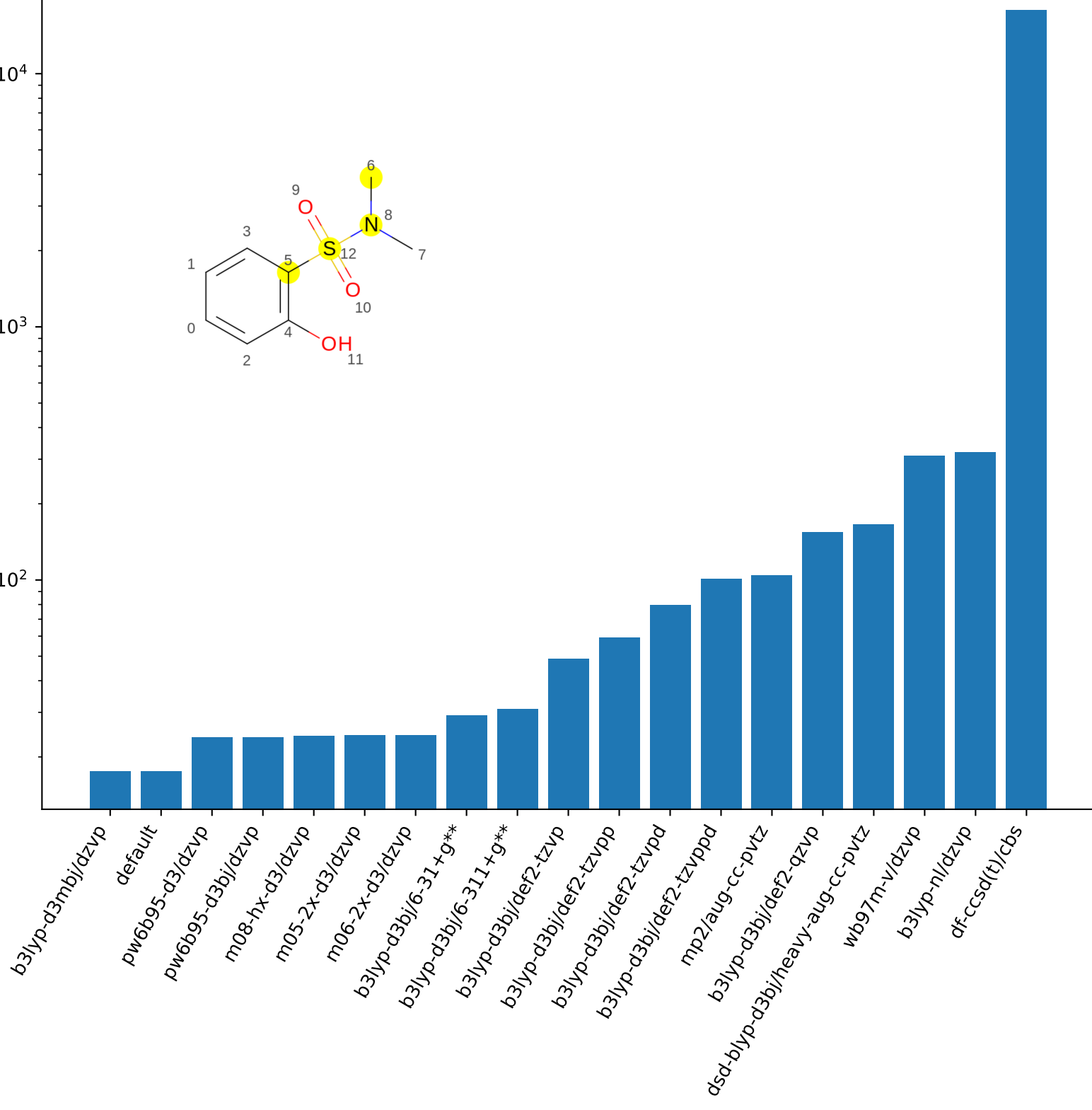
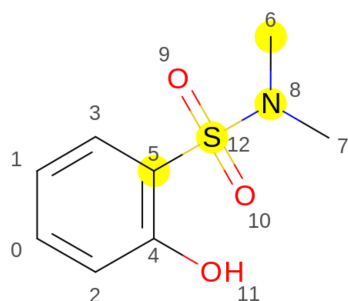
Wall time in seconds (in log scale)



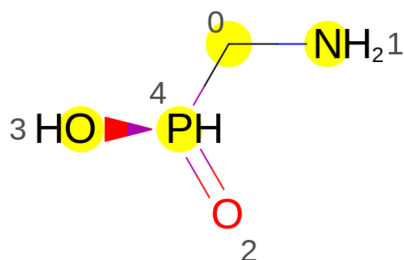
Wall time in seconds (in log scale)



Wall time in seconds (in log scale)



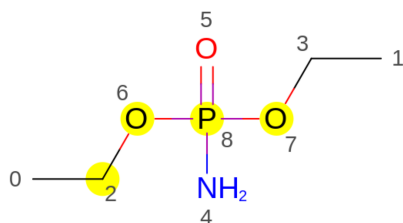
Wall time in seconds (in log scale)



Bar chart showing Wall time in seconds (in log scale) for various computational methods. The y-axis is logarithmic, ranging from 10¹ to 10². The x-axis lists 20 different computational methods. The wall time increases significantly for the last few methods, with 'df-ccsd(t)/cbs' being the most computationally expensive.

| Method | Wall time (seconds) |
|------------------------|---------------------|
| b3lyp-d3mbj/dzvp | ~5.5 |
| default | ~5.5 |
| m08-hx-d3/dzvp | ~9.0 |
| m06-2x-d3/dzvp | ~9.2 |
| m05-2x-d3/dzvp | ~9.8 |
| b3lyp-d3bj/6-311+g** | ~10.0 |
| b3lyp-d3bj/6-31+g** | ~10.1 |
| pw6b95-d3/dzvp | ~10.5 |
| pw6b95-d3bj/dzvp | ~10.6 |
| b3lyp-d3bj/def2-tzvp | ~16.5 |
| b3lyp-d3bj/def2-tzvpp | ~17.5 |
| mp2/aug-cc-pvtz | ~18.5 |
| b3lyp-d3bj/def2-tzvppd | ~19.5 |
| b3lyp-d3bj/def2-pvtz | ~28.5 |
| wb97m-v/dzvp | ~42.5 |
| b3lyp-nl/dzvp | ~58.5 |
| df-ccsd(t)/cbs | ~100.0 |

Wall time in seconds (in log scale)



b3lyp-d3mbj/dzvp
default
b3lyp-d3bj/6-31+g**
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
d3-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvvp
wb97m-v/dzvp
b3lyp-n/dzvp
df-ccsd(t)/cbs

mol: 58, CPU: AMD EPYC 7601 32-Core Processor, # of threads: 4

