

Supplementary material

for

**Comparative Analysis of Phosphodiesterase Type 5 Inhibitors and
Usnic Acid: Exploring Therapeutic Potential in Pulmonary Arterial
Hypertension**

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Cartesian coordinates of optimized geometries of investigated compounds

Sildenafil (SIL) ($G=-1883.476868$ a.u)

0 1

C	-1.14991400	-5.02437400	1.21901300
C	-1.91743000	-3.70311500	1.14030700
C	-2.69937200	-3.56287200	-0.18368900
C	-3.39942300	-2.24990600	-0.30191800
N	-4.74628700	-2.13260700	-0.41052400
N	-5.12481700	-0.82837600	-0.49979100
C	-6.50767100	-0.39741200	-0.64324900
C	-3.99896700	-0.08140900	-0.44306600
C	-3.82889900	1.37535700	-0.50373100
O	-4.79974800	2.14239400	-0.61075900
N	-2.51877000	1.75279100	-0.43889600
C	-1.53206300	0.85104300	-0.30226200
N	-1.61031400	-0.49136600	-0.23135300
C	-2.88648500	-0.93386100	-0.31675200
C	-0.13508000	1.38996500	-0.28802400
C	0.85293000	0.67566800	-0.96654100
C	2.16411700	1.14857000	-1.04459600
C	2.50973600	2.36262500	-0.45274100
C	1.54581200	3.08037000	0.24960700
C	0.23037000	2.59895100	0.35971200
O	-0.71827600	3.21588300	1.09479100
C	-0.48521400	4.52816100	1.60863900
C	-1.78815800	4.99829100	2.22984200
S	3.41595000	0.17237400	-1.87597600
O	4.51715300	1.08494500	-2.20185600
O	2.73471100	-0.62961800	-2.89722900
N	4.06098400	-0.93995600	-0.79173300
C	5.00031200	-0.50502600	0.24741000
C	4.34617000	-0.46787200	1.63142200
N	3.73028600	-1.76056900	1.93873700
C	3.19541000	-1.79284300	3.29145800
C	2.70866600	-2.09829000	0.94464700
C	3.32871400	-2.16527200	-0.45405100
H	-0.60222000	-5.10128700	2.16291200
H	-0.42263600	-5.10970000	0.40416000
H	-1.82329900	-5.88690500	1.15512300
H	-1.22997700	-2.85501900	1.21962600
H	-2.61743100	-3.62355200	1.98106800
H	-3.41714800	-4.38647300	-0.29183600
H	-1.99471300	-3.64721900	-1.02066200
H	-5.43621500	-2.86865200	-0.45005500

H	-6.93943500	-0.79101500	-1.56841900
H	-7.10152000	-0.71756900	0.21816300
H	-6.45298300	0.69454600	-0.68397300
H	0.57469100	-0.24702200	-1.46039000
H	3.51892500	2.74609000	-0.55342200
H	1.82378500	4.01567000	0.71895400
H	-0.17517500	5.19449200	0.79260700
H	0.32316500	4.50483500	2.35376600
H	-1.67527200	6.01580600	2.61679500
H	-2.58655100	4.98600200	1.48400100
H	-2.07977900	4.34257800	3.05490000
H	5.41043500	0.46684200	-0.03030700
H	5.82787400	-1.22603400	0.26216500
H	3.61016700	0.35820400	1.67456000
H	5.11582500	-0.26126300	2.38473300
H	2.79510300	-2.78925500	3.50637400
H	3.99563700	-1.58780500	4.01014600
H	2.38664000	-1.05650000	3.46168800
H	1.87171500	-1.37411700	0.95020200
H	2.29225400	-3.08158800	1.19588300
H	4.04902100	-2.99317400	-0.48619400
H	2.57427400	-2.34764100	-1.22023400

Tadalafil (**TAD**) ($G=-1314.510959$ a.u)

0 1

C	-5.40647400	2.16755700	-0.27910100
C	-5.30318100	1.56653600	0.99420900
C	-4.16699300	0.85370600	1.35829400
C	-3.11129800	0.73750900	0.43423600
C	-1.83353700	0.11306500	0.41633400
C	-1.30422000	0.40157300	-0.86002100
N	-2.09897000	1.13305500	-1.65030100
C	-3.21824500	1.35335000	-0.86882000
C	-4.37608800	2.06687600	-1.20965800
C	0.05340400	-0.09193900	-1.25758400
N	0.20396600	-1.50123000	-0.69585100
C	0.70109500	-2.46707300	-1.51065000
O	1.19936200	-2.30418000	-2.61749700
C	0.62338600	-3.89652800	-0.94672900
N	1.09370900	-3.93668800	0.47547900
C	0.37754500	-2.78617700	1.37134600
O	0.55445300	-2.88838600	2.54809400
C	-0.51671500	-1.90780700	0.53633500
C	-1.06235000	-0.73491700	1.36557500

C	0.99510800	-5.28040000	1.12785400
C	1.24577000	0.76693300	-0.82474100
C	2.50095700	0.53077600	-1.40151600
C	3.63479300	1.28256000	-1.04861700
C	3.45492100	2.27672000	-0.10679100
O	4.38824300	3.13719800	0.42478400
C	3.63215500	4.08001000	1.19653000
O	2.31712300	3.54882700	1.37679400
C	2.20887700	2.52366100	0.46251600
C	1.08596200	1.79466700	0.12772700
H	1.25922300	-4.53808500	-1.55640000
H	-0.40175100	-4.27896300	-0.96510700
H	2.07884600	-3.65344400	0.48487800
H	-6.30779600	2.71947700	-0.53349000
H	-6.12441600	1.66718100	1.69935400
H	-4.09895400	0.40046900	2.34600400
H	-4.45435600	2.52910800	-2.18989600
H	0.09359900	-0.21891600	-2.34091400
H	-1.39564100	-2.51409000	0.24225600
H	-1.67755000	-1.15643400	2.16673400
H	-0.21721000	-0.22182300	1.85225100
H	1.30249400	-5.17540900	2.16742900
H	1.63886600	-5.98507700	0.59962500
H	-0.04270100	-5.61204300	1.07962200
H	2.59364000	-0.24571100	-2.15428000
H	4.60302200	1.10398300	-1.50298300
H	3.57390900	5.03435500	0.65238800
H	4.10813400	4.21586600	2.17175300
H	0.11502400	2.01199100	0.55771900

Avanafil (**AVA**) ($G=-1960.891028$ a.u)

0 1

C	0.41926100	0.14327000	0.79183200
C	-5.03895100	-4.59418800	-1.95215400
C	-4.25003200	-2.85506800	-0.52246000
C	-4.46237300	-1.60267400	0.07859700
C	-3.51469300	-1.02833500	0.91831400
C	-2.31100100	-1.69059400	1.18464600
C	-2.09341900	-2.93446900	0.58757800
C	-3.04290000	-3.51342000	-0.25305500
C	-1.27776100	-1.07663900	2.11943800
C	-0.07753300	2.19709100	-0.10879800
C	1.97615400	1.35475300	-0.54813200
C	1.73728700	0.21150200	0.21746300
C	2.72725300	-0.86740600	0.41687100

C	5.03753200	-1.62828900	0.20239000
C	6.40309200	-1.06502000	-0.11693400
C	7.71161700	0.69653300	-0.73782400
C	8.84581700	-0.10274200	-0.66152600
C	8.64031500	-1.43143800	-0.28728400
C	-0.63112600	4.47797300	-0.91206500
C	-1.93946100	5.27851300	-0.83016200
C	-2.60961800	4.74730300	0.44962800
C	-2.26203600	3.24828000	0.44749500
C	-3.30817900	2.38284700	-0.26410700
N	0.04553800	-0.91890700	1.53811400
N	-0.46486100	1.13622300	0.62093300
N	1.11891600	2.35446600	-0.73118300
N	4.00466800	-0.63803100	-0.00083900
N	6.48726600	0.22449300	-0.46735400
N	7.42962000	-1.92272100	-0.01460000
N	-0.97028900	3.21025900	-0.25322100
O	-5.23410000	-3.33415200	-1.32670500
O	2.43848400	-1.96106500	0.94038000
O	-4.42531000	2.27484800	0.61394800
Cl	-5.96164100	-0.73925400	-0.25944800
H	-5.93804500	-4.77471800	-2.54223600
H	-4.16564800	-4.58453700	-2.61606200
H	-4.92285200	-5.39775000	-1.21431000
H	-3.71416900	-0.05080400	1.34662600
H	-1.16235000	-3.46446600	0.76945400
H	-2.84078600	-4.47951600	-0.69960700
H	-1.16090200	-1.71383800	3.00370700
H	-1.62914700	-0.10029900	2.45891600
H	2.92492600	1.46946200	-1.07230200
H	4.86855200	-2.51506000	-0.42162400
H	5.03337400	-1.99477100	1.23747300
H	7.77485200	1.74476100	-1.02272600
H	9.83437400	0.28388500	-0.88122000
H	9.47430300	-2.12605700	-0.20386300
H	-0.28650600	4.30510300	-1.93474600
H	0.18714400	4.97721900	-0.37645100
H	-2.56537500	5.06677900	-1.70405700
H	-1.76194500	6.35701800	-0.80736400
H	-3.69014700	4.90645800	0.48115000
H	-2.17319700	5.22933600	1.33154900
H	-2.14696900	2.84630000	1.45808700
H	-2.86778900	1.40220500	-0.47673600
H	-3.59393500	2.84681500	-1.22186900
H	0.73875700	-1.66532200	1.57441100
H	4.33301500	0.28440700	-0.25124800

H	-5.06570300	1.67050800	0.21322100
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Usnic Acid (UA) ($G=-1221.914487$ a.u)

0 1

C	-0.73956500	0.06620600	0.62209300
C	-0.88042700	0.24999800	2.17898500
C	0.64291500	0.50178800	0.18320800
H	-0.05891800	-0.25949500	2.68719200
H	-1.83130800	-0.15271300	2.53683000
H	-0.83071100	1.31694500	2.40784600
C	-0.65329000	-1.39747600	0.31124300
C	-1.98825800	0.73444700	0.03784500
C	1.42000200	-0.63327100	0.08005900
C	1.24824200	1.77191600	0.09054100
C	-1.72388700	-2.18647500	0.09711200
O	0.63942700	-1.79572300	0.21404200
C	-3.14925200	-0.11013900	-0.13724000
O	-1.97093500	1.96453800	-0.13291400
C	2.80723000	-0.63771800	-0.12131600
C	2.63480200	1.86161500	-0.11542000
O	0.52697300	2.89952500	0.19406800
C	-2.99793300	-1.53053100	-0.06315400
H	-1.65921300	-3.25187600	-0.08386500
C	-4.47454600	0.41269000	-0.44798100
C	3.65564400	-1.82355500	-0.24822800
C	3.39023000	0.67711700	-0.20720800
C	3.32393800	3.19462400	-0.24559300
H	-0.43597700	2.67801200	0.10700700
O	-4.02535500	-2.31712800	-0.23709000
C	-4.73952600	1.88507700	-0.61084200
O	-5.44306100	-0.37649000	-0.57996700
C	3.07668900	-3.21880400	-0.17188700
O	4.88238300	-1.70342500	-0.42395000
O	4.70472200	0.81435700	-0.40176600
H	-4.83200000	-1.67609200	-0.40534400
H	-4.40645900	2.44425200	0.26733500
H	-4.16928800	2.28753300	-1.45250300
H	-5.80884300	2.02317000	-0.77489600
H	5.07904900	-0.11127200	-0.45656200
H	2.58451700	-3.38787000	0.79024800
H	2.31864900	-3.37253400	-0.94520000
H	3.89131700	-3.93153100	-0.30223200
H	3.93957300	3.40996000	0.63543200
H	3.99665500	3.19855700	-1.10793100
H	2.59168500	3.99467300	-0.35605900