Supporting Information for

Non-covalent interactions in glutathione peroxidase active center and their influence on the enzyme activity

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Table of Content

Coordinates of atoms of GPx-1 active center cut out from the enzyme X-Ray and used for initial guess for calculations

C	-2.98501100	2.80132700	1.08645500
O	-3.69889300	3.79415500	1.11237300
Se	-0.05569500	0.53274300	0.38240900
O	-1.48771100	-0.20025500	-0.16278900
C	-4.79959100	0.03844800	-0.61066400
O	-4.95850400	-0.28473900	-1.79068500
C	4.10549000	2.73953400	-0.56532500
O	4.23958700	3.03330700	-1.74996300
C	2.28451800	-2.35788800	-1.71300500
C	1.82184500	-1.09769100	-2.21046200
C	0.60540200	-2.30775700	2.29828900
O	0.02889900	-1.21099200	2.30754500
C	2.73250700	-0.07440700	2.26651500
O	2.46103000	1.11325900	2.47864400
O	-2.02481700	2.61071900	-1.92214600
H	-1.93170300	3.28064100	-2.61382200
H	-2.21093300	1.74904500	-2.38647500
O	-2.30646800	0.07891700	-2.67857300
H	-2.02035600	-0.11607300	-1.75039100
H	-3.26403800	-0.12344200	-2.67254700
C	3.66369100	-2.53277300	-1.47881500
H	4.04491700	-3.49138000	-1.11660500
C	4.53222000	-1.47179900	-1.72581300
H	5.60355800	-1.59679000	-1.55112000
C	4.05059500	-0.22782800	-2.19301600
H	4.73994300	0.60082600	-2.36152100
C	2.69319500	-0.02404200	-2.43736100
H	2.32967200	0.94553700	-2.77976100

C	1.12587100	-3.19994800	-1.57908400
H	1.09957300	-4.22679200	-1.22231900
C	0.04337600	-2.45845200	-1.99329400
H	-1.00813100	-2.72532000	-2.04488700
N	0.45698600	-1.20026900	-2.37180200
H	-0.16770700	-0.49933600	-2.75771700
N	2.89748200	2.58675400	0.02525400
H	2.05331100	2.63645500	-0.54217400
H	2.79837000	2.27198200	0.99464600
C	5.30137300	2.46024600	0.32985500
H	5.61562600	1.41518700	0.17094100
H	6.13583000	3.10950400	0.03411200
H	5.07733600	2.59168500	1.39801900
N	3.19961700	-0.49786000	1.07728300
H	3.39236500	-1.46782500	0.86515900
H	3.26074000	0.15118000	0.29745800
C	2.58315100	-1.12296100	3.35773100
H	3.57955400	-1.29359000	3.79835400
H	1.95351600	-0.66995700	4.13290400
C	1.99710400	-2.45865400	2.90336200
H	1.92856300	-3.14333500	3.76485900
H	2.64880600	-2.97320100	2.17695700
N	0.05116800	-3.40664700	1.77359500
H	0.55636400	-4.28310500	1.74395100
H	-0.86782100	-3.32787500	1.31460000
O	-2.39134800	-2.59009100	0.62606100
H	-2.01937800	-1.69259600	0.44894300
C	-3.41454600	-2.84406300	-0.31084500
H	-3.17079300	-2.40578300	-1.29518900
H	-3.50251800	-3.93463600	-0.44875300

C	-4.76894300	-2.30111400	0.15188000
H	-5.06379200	-2.79216400	1.09069000
H	-5.53091200	-2.52328300	-0.61032600
N	-4.75001900	-0.86583300	0.38927800
H	-4.52013300	-0.53062200	1.31859300
C	-4.60263700	1.49158200	-0.18894300
H	-5.48371600	1.85342800	0.36603000
H	-4.51106700	2.09429300	-1.10532800
N	-3.40995100	1.59300600	0.63102000
H	-2.69394200	0.88756300	0.41381700
C	-1.52813300	2.88044300	1.54823300
H	-1.52533300	3.53588500	2.43289600
H	-0.99028600	3.44474900	0.76831600
C	-0.76889100	1.60607100	1.89488400
H	-1.35220000	0.87105000	2.46372200
H	0.14735700	1.82437300	2.46102100
O	0.17584300	1.84723100	-0.80316200
H	-0.69045500	2.21466400	-1.19326900

Optimized coordinates of atoms of GPx-1 active center in –SeH form

C 2.72713700 -2.76604300 0.71216500

O 2.66483900 -3.09408700 -0.46500600

Se 0.17380500 -0.63993000 0.62009600

O 2.06905400 -0.08307300 -2.07471400

C 4.62834700 -0.18759500 -0.20221600

O 5.08362700 0.13869800 -1.29480600

C -4.28803800 -2.62641000 -1.01906100

O -4.69594700 -2.46904600 -2.15726300

C -1.70884200 3.03127600 -1.69982200

C -0.89500900 1.93752200 -2.10753000

C -1.22264000 2.18150500 2.56763800

O -0.26149400 1.76657300 3.20891400

C -2.80422500 -0.50145800 2.07038100

O -2.43667000 -1.66835100 2.19578200

O 1.08568900 -2.63189700 -2.59591300

H 1.63154700 -3.09272900 -1.92301100

H 1.88311000 -0.92411700 -2.54552700

O 2.93543000 0.65454400 -2.96919500

H 1.47831500 -0.32791200 0.01895600

H 3.79987600 0.54625300 -2.51215800

C -3.09556400 2.84116600 -1.59675400

H -3.74286900 3.66156700 -1.30871000

C -3.62882700 1.60427700 -1.92110700

H -4.69979700 1.45138300 -1.87631300

C -2.80782500 0.54221100 -2.34306000

H -3.26419300 -0.40294000 -2.61030400

C -1.43395300 0.69288900 -2.43265600

H -0.80615900 -0.12266300 -2.76355500

C -0.83016500 4.14583700 -1.49470400

H -1.10365700 5.14581900 -1.20072200

C 0.43806200 3.70768700 -1.77322900

H 1.37206000 4.24446300 -1.75542400

N 0.40584400 2.38218300 -2.13071700

H 1.21019800 1.83283100 -2.39733500

N -2.96297900 -2.73410100 -0.72925600

H -2.30659300 -2.83773100 -1.49027100

H -2.64271900 -2.86556900 0.21844800

C -5.22799500 -2.69303100 0.16777800

H -5.89043700 -1.82805600 0.13638800

H -5.84690100 -3.58500100 0.06190600

H -4.70991500 -2.72336700 1.12523400

N -3.18609500 0.00363700 0.88326600

H -3.39040800 0.97492000 0.73354600

H -3.05721000 -0.55939100 0.05424900

C -2.87702200 0.41402000 3.28167400

H -3.86193200 0.26889700 3.73353600

H -2.14133800 0.04318100 3.99245100

C -2.64240500 1.90560400 3.03295600

H -2.76987000 2.43957900 3.97709500

H -3.37535100 2.32468000 2.34043500

N -1.10095600 2.91809900 1.44821700

H -1.87991800 3.07840100 0.83271500

H -0.19277300 3.05757700 1.03590500

O 2.38549600 1.96321100 2.32761700

H 1.45817600 1.89371500 2.63588100

C 2.40326400 2.44091400 0.99313000

H 1.59103400 1.99668200 0.41073000

H 2.30011600 3.53249700 0.95675400

C 3.73276300 2.05262300 0.36866600

H 4.54040900 2.64616700 0.80718500

H 3.72494100 2.23256100 -0.70465900

N 3.97255900 0.64267300 0.61636700

H 3.61188400 0.31278000 1.49802100

C 4.85063700 -1.61071900 0.32177800

H 5.81019100 -1.63128200 0.84128200

H 4.91782400 -2.26145200 -0.54537500

N 3.81010600 -2.10698700 1.20064600

H 3.86297300 -1.92952100 2.18960700

C 1.59389400 -3.00722400 1.68779600

H 1.97493900 -3.50982500 2.58354700

H 0.89153800 -3.67831000 1.19823200

C 0.89068400 -1.71540300 2.11086200

H 1.53494300 -1.05846000 2.69237200

H 0.00661900 -1.94076200 2.70311200

O -0.21792700 -2.66055400 -1.97380200

H -0.10781000 -2.05178400 -1.20817800

Optimized coordinates of atoms of GPx-1 active center in –SeOH form

C 2.58302300 -2.67212000 0.92154400

O 2.50803300 -3.37850000 -0.07930200

Se 0.14492600 -0.28073900 0.72198100

O 1.75578700 0.11752300 -0.03090700

C 4.78353700 -0.63920800 -0.63325600

O 4.41012800 -0.70518100 -1.79904600

C -4.74191600 -2.37182100 -0.06014800

O -5.29014700 -2.67874500 -1.10673300

C -2.17311200 2.43310100 -1.97490800

C -1.59484900 1.16926400 -2.27372000

C -0.13125800 2.65940300 2.40487700

O 0.52993400 2.09690300 3.26367300

C -2.54754200 0.40288100 2.06589400

O -2.21452200 -0.76403500 2.30730000

O 0.49532800 -3.28776400 -1.86076700

H 1.15184800 -3.58208700 -1.18666600

H 1.31465300 -1.78880800 -2.43175900

O 1.72800100 -0.89927300 -2.49081200

H 1.76848100 -0.29333900 -0.93343000

H 2.69334200 -1.02432100 -2.53938100

C -3.56806000 2.52922500 -1.87345200

H -4.03951300 3.48344400 -1.67054100

C -4.33474600 1.39022500 -2.05623800

H -5.41298300 1.45203700 -1.98626100

C -3.74140500 0.14542700 -2.33463300

H -4.36627800 -0.73022600 -2.45070700

C -2.36579900 0.02089100 -2.44556900

H -1.91032300 -0.93752700 -2.65813800

C -1.08785800 3.36560900 -1.86449100

H -1.15770300 4.42555900 -1.68150600

C 0.06604300 2.66358500 -2.09814700

H 1.08812600 3.00178300 -2.10778300

N -0.23198700 1.34555100 -2.33980800

H 0.44425500 0.62744700 -2.57040600

N -3.40360100 -2.47659400 0.12684100

H -2.83881400 -2.87723600 -0.60756500

H -2.95853000 -2.17611700 0.98411500

C -5.52572100 -1.81805800 1.11424900

H -5.99412700 -0.88188700 0.80852800

H -6.32298200 -2.52012000 1.35689200

H -4.91254600 -1.64217800 1.99678600

N -3.15832700 0.73322300 0.91990800

H -3.34699900 1.68427200 0.65819600

H -3.26347300 0.04195200 0.19089000

C -2.31788100 1.51555300 3.07097100

H -3.29411200 1.77225700 3.49160100

H -1.70664200 1.10763900 3.87251900

C -1.65040900 2.78076200 2.52347000

H -1.82365800 3.59781500 3.22855300

H -2.08524700 3.09980800 1.57464300

N 0.40908800 3.28999000 1.33785100

H -0.16152700 3.49083000 0.53128400

H 1.40335600 3.20223600 1.16675700

O 3.09075300 2.44524300 0.20223900

H 2.58410000 1.60784200 0.25269100

C 3.84148600 2.37969800 -0.99423100

H 3.31709100 1.78708300 -1.74812100

H 3.96173300 3.39314000 -1.38534300

C 5.23275400 1.78972500 -0.76600600

H 5.82241700 2.46957000 -0.15188200

H 5.73596900 1.66699100 -1.72727400

N 5.21553000 0.50670100 -0.07409700

H 5.46098300 0.50298000 0.90056700

C 4.81842100 -1.87097200 0.28190700

H 5.74740300 -1.88234600 0.85594800

H 4.78572500 -2.74847700 -0.35700500

N 3.69640300 -1.95267200 1.19865100

H 3.64935900 -1.29814200 1.96145700

C 1.46677700 -2.60865600 1.94978000

H 1.84806200 -3.04543500 2.87972200

H 0.67449400 -3.25999600 1.58669700

C 0.90685800 -1.22291800 2.25675000

H 1.63227500 -0.53253000 2.68696700

H 0.07019200 -1.29380700 2.94875500

O -0.66789900 -3.01769600 -1.04757700

H -0.44886800 -2.15576100 -0.62497500

Optimized coordinates of atoms of GPx-1 active center in –SeOOH form

C -3.19433900 2.63985100 1.14482800

O -3.98739800 3.55055600 1.35029700

Se -0.15382300 0.55408800 0.18717900

O -1.54299800 -0.15698400 -0.43800300

C -5.02349900 -0.17872700 -0.43747500

O -5.35701000 -0.43996500 -1.59460500

C 4.16782700 2.83935900 -0.42127200

O 4.39698800 3.16992700 -1.58154600

C 2.56116700 -2.29425000 -1.69116000

C 2.39271300 -0.95956800 -2.15309000

C 0.52580300 -2.31214900 2.25494700

O -0.10798300 -1.25443000 2.21136800

C 2.62982200 -0.06052100 2.36788300

O 2.38805100 1.14187700 2.50779700

O -2.10408200 2.86760500 -1.93661700

H -2.02817600 3.57157000 -2.58976100

H -2.50441700 2.08631200 -2.39123300

O -2.87063600 0.43299200 -2.80794700

H -2.35245500 0.08633200 -2.05383500

H -3.78876100 0.16182400 -2.63061500

C 3.83438300 -2.70796400 -1.27527000

H 3.99598800 -3.72149200 -0.92873700

C 4.88513700 -1.80649100 -1.32585000

H 5.87327700 -2.11663800 -1.01153300

C 4.69212100 -0.49065800 -1.78290600

H 5.52876400 0.19404600 -1.81467200

C 3.44585100 -0.04918200 -2.20039200

H 3.30857700 0.96764100 -2.54234500

C 1.27805000 -2.92752600 -1.77890800

H 1.03346200 -3.94021400 -1.50712700

C 0.40489800 -2.00025200 -2.27490500

H -0.64848400 -2.07923100 -2.47607400

N 1.06958000 -0.81509200 -2.49929700

H 0.64833300 0.03146200 -2.84186600

N 2.92262700 2.61821100 0.04371800

H 2.13585200 2.68462500 -0.58604500

H 2.75508800 2.28130800 0.98762300

C 5.28607800 2.63140200 0.57783300

H 5.88865200 1.78224000 0.25197500

H 5.92888100 3.51098400 0.57734800

H 4.92454800 2.44336600 1.58761300

N 3.18451600 -0.54817700 1.24836900

H 3.35559400 -1.52704300 1.10212000

H 3.36509200 0.05778000 0.46245400

C 2.34420300 -1.04858000 3.48212800

H 3.27052800 -1.18173000 4.04726100

H 1.62792300 -0.56564400 4.14185700

C 1.82313200 -2.41372700 3.04323300

H 1.62984400 -3.02338400 3.92959500

H 2.56290000 -2.97083500 2.46262700

N 0.11106900 -3.42258800 1.63638100

H 0.65855100 -4.26507300 1.65764600

H -0.75094300 -3.39544200 1.09405000

O -2.27798200 -2.72030000 0.20296200

H -1.97735400 -1.80080900 0.04098200

C -3.44365700 -2.97353700 -0.56597100

H -3.38355700 -2.46873200 -1.53354200

H -3.49351900 -4.04816000 -0.75215100

C -4.71712900 -2.54721300 0.15858100

H -4.80437900 -3.09047700 1.09891000

H -5.58188300 -2.78607500 -0.46122900

N -4.74310400 -1.12593400 0.47165000

H -4.40224400 -0.82849500 1.37167500

C -4.87528400 1.25969100 0.03973100

H -5.65288300 1.49462000 0.76928500

H -5.02146800 1.91136200 -0.82254700

N -3.56431200 1.44570700 0.63323400

H -2.83280200 0.82455700 0.28550500

C -1.71335900 2.82115600 1.44979800

H -1.66579700 3.46215400 2.33132400

H -1.29663900 3.41488100 0.63310900

C -0.86027000 1.59123800 1.72394600

H -1.36121900 0.83321800 2.32108200

H 0.06252700 1.86208100 2.23639200

O 0.13932100 1.89179500 -0.94788700

H -0.71208800 2.30453600 -1.29040700

Figure S1. Electron density (blue) and electrostatic potential (red) distribution along bond paths for non-covalent interactions in GPx-1 active center in –SeH form. Positions of minima are shown by dashed lines.

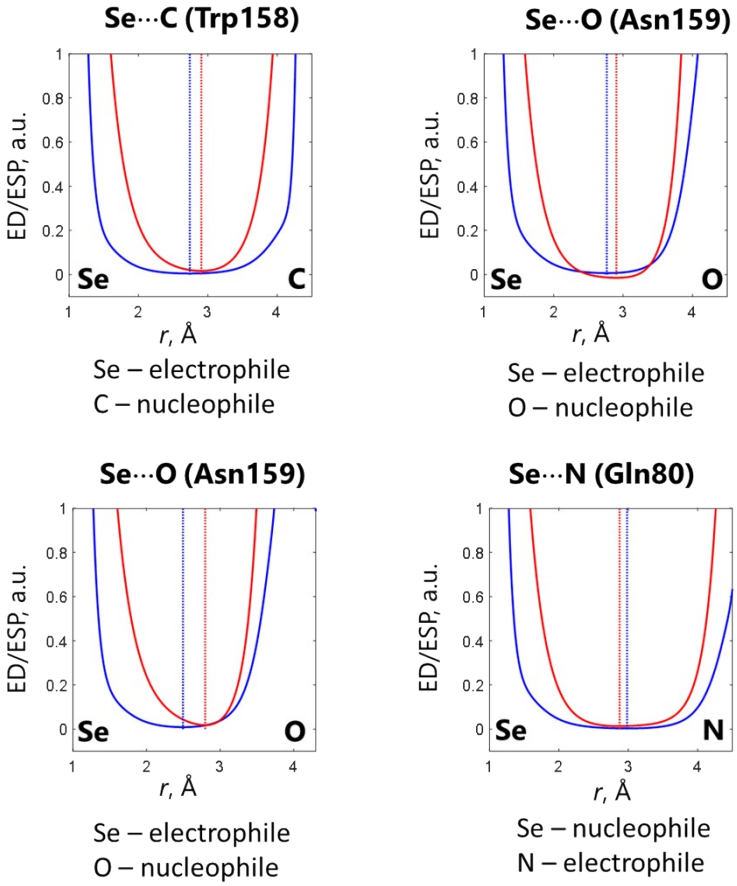
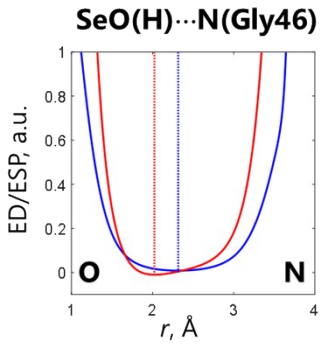
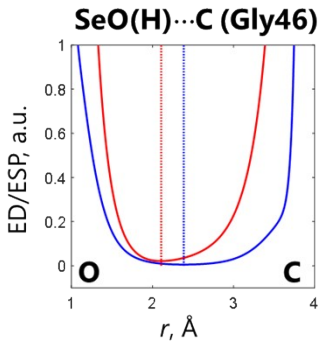


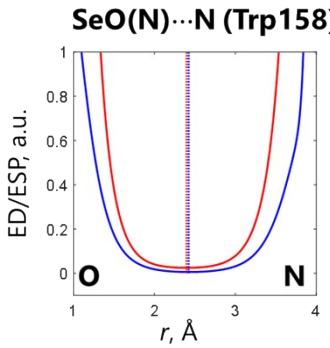
Figure S2. Electron density (blue) and electrostatic potential (red) distribution along bond paths for non-covalent interactions in GPx-1 active center in –SeOH form. Positions of minima are shown by dashed lines.



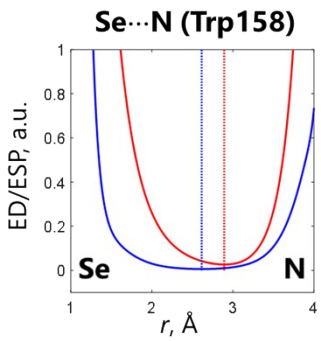
N – electrophile
O – nucleophile



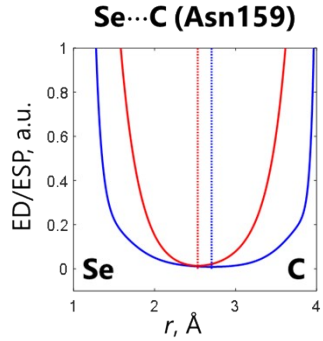
C – electrophile
O – nucleophile



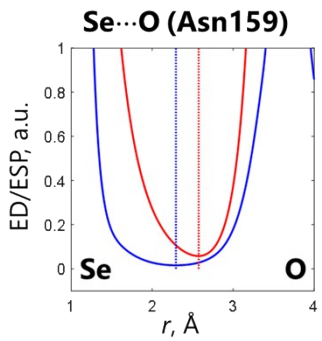
N – electrophile
O – nucleophile



Se – electrophile
O – nucleophile



C – electrophile
Se – nucleophile



Se – electrophile
O – nucleophile

Figure S3. Electron density (blue) and electrostatic potential (red) distribution along bond paths for non-covalent interactions in GPx-1 active center in –SeOOH form. Positions of minima are shown by dashed lines.