

## SUPPLEMENTARY INFORMATION

# Mechanistic Insight into SARS-CoV-2 M<sup>pro</sup> Inhibition by Organoselenides: The Ebselen Case Study

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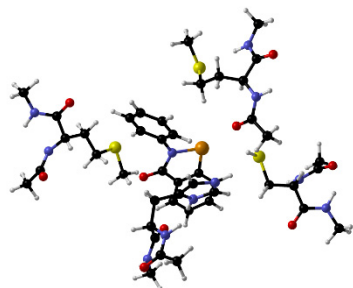
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**Table S1.** Coordinates (Å) energies (E, Hartree) and number of imaginary frequencies (Nimag) of stationary points as computed at B3LYP-D3(BJ)/6-311G(d,p),cc-pVTZ level of theory.

## EbSe

### RC



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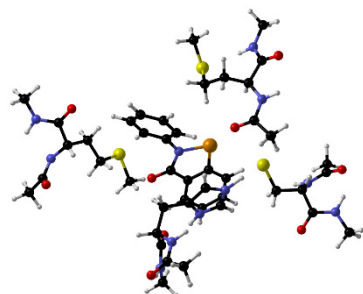
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H	-0.125236000	-6.913808000	4.917952000
H	-1.135948000	-5.948278000	5.988225000
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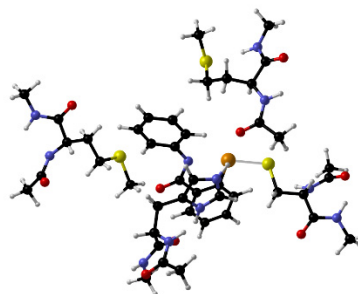
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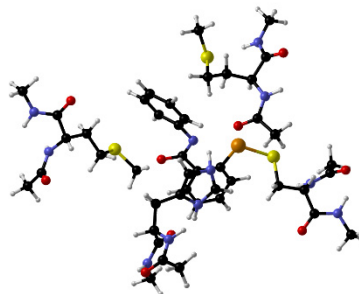
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O	-8.708949000	-1.073520000	0.454110000
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H	-10.747937000	-1.915403000	-0.978936000

H	-9.345523000	-2.410223000	-1.923742000
N	-8.560464000	0.461205000	-1.218856000
C	-7.496796000	1.246630000	-0.600070000
C	-7.955770000	2.593006000	-0.052309000
O	-7.136554000	3.384824000	0.390237000
C	-6.338217000	1.446377000	-1.590990000
C	-5.643268000	0.139409000	-1.962868000
S	-4.519862000	0.426695000	-3.373213000
C	-3.879884000	-1.262402000	-3.592328000
H	-7.157745000	0.667993000	0.263385000
H	-6.733292000	1.926773000	-2.495376000
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H	-5.069549000	-0.248088000	-1.116866000
H	-6.372816000	-0.621930000	-2.253002000
H	-3.159829000	-1.219832000	-4.410449000
H	-4.686164000	-1.948765000	-3.861990000
H	-3.367098000	-1.585792000	-2.685602000
H	-8.718948000	0.608728000	-2.204805000
N	-9.291256000	2.823535000	-0.085560000
C	-9.888013000	4.022390000	0.472417000
H	-9.877333000	2.074601000	-0.417958000
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H	-10.520176000	4.522701000	-0.265864000
C	8.123855000	-0.268157000	-3.620752000
C	7.978112000	-0.842781000	-2.228686000
O	8.864256000	-0.728961000	-1.385155000
H	7.440892000	-0.720039000	-4.341878000
H	9.152844000	-0.401874000	-3.952555000
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N	6.802969000	-1.473223000	-1.973290000
C	6.366417000	-1.798097000	-0.623338000
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O	6.189746000	-4.111821000	-0.000802000
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S	4.331655000	-0.021053000	-1.200105000
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C	8.993882000	-4.378227000	0.268896000
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H	9.613854000	-4.697642000	-0.574804000
C	4.747749000	1.512541000	3.022529000
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O	2.594998000	1.798603000	2.019936000
H	5.547529000	2.118390000	3.449623000
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N	3.980405000	3.617206000	2.119628000
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C	0.718582000	4.747145000	0.762845000
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C	0.221842000	7.472967000	0.365243000

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C	-0.298278000	-2.850626000	-2.693861000
C	0.594789000	-3.528976000	-3.511183000
C	1.904573000	-3.062871000	-3.628297000
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H	9.194860000	-0.780012000	-4.023627000	C	-2.583518000	3.468917000	2.346259000
H	8.051440000	0.531539000	-3.728821000	C	-1.437579000	2.896921000	2.891280000
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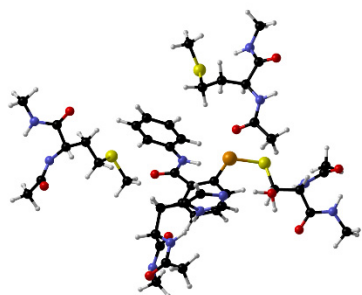
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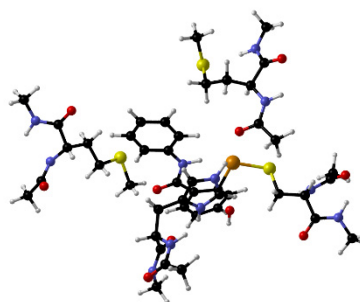
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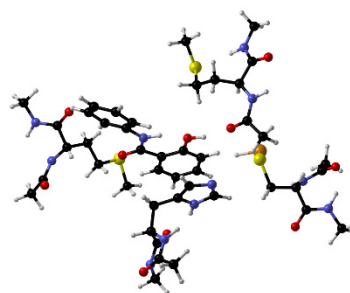
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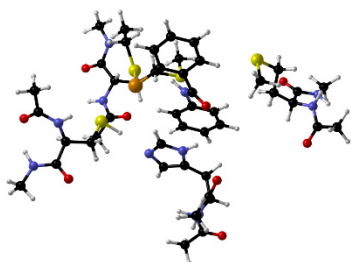
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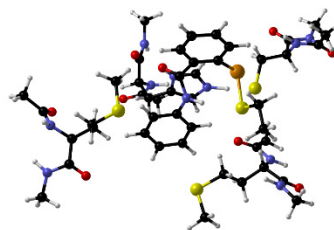
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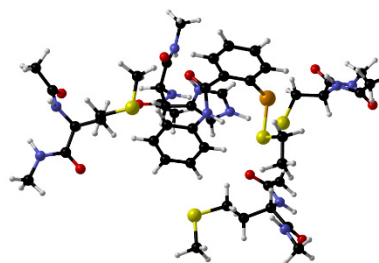
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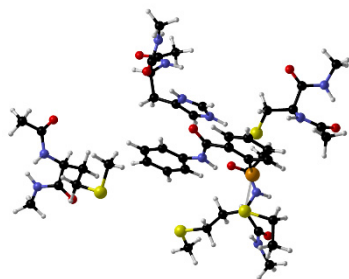
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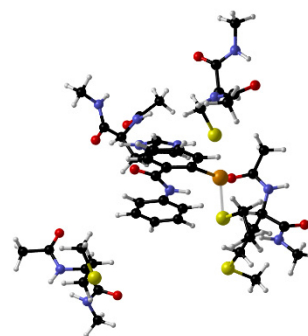
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Pinhb(-)



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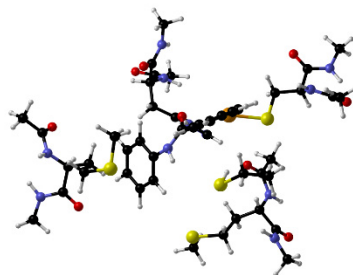
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H	-0.136215000	-4.767601000	1.844451000
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H	-4.898641000	-0.712138000	-2.418908000				
H	-3.773526000	-2.822536000	-1.750219000				
H	-2.238231000	-2.849783000	0.178058000				
H	-1.454473000	-1.732953000	2.122116000				
S	1.015900000	-3.190052000	0.935536000				

**Table S2.** Electronic ( $\Delta E$ ) and Gibbs ( $\Delta G_{\text{solv}}$ ) free energies (kcal mol<sup>-1</sup>) relative to the RC for Ebselen (EbSe) mechanism.

	$\Delta E$	$\Delta G_{\text{solv}}$
RC	0.00	0.00
TS1	14.90	15.16
TCI	3.42	3.41
TS2	31.16	29.93
Pinhb	-8.83	-6.86

**Table S3.** Electronic ( $\Delta E$ ) and Gibbs ( $\Delta G_{\text{solv}}$ ) free energies (kcal mol<sup>-1</sup>) relative to the RC for Ebselen ethanethiolate (EbSeS) mechanism.

	$\Delta E$	$\Delta G_{\text{solv}}$
RC	0.00	0.00
TS1	9.15	8.83
IP	8.58*	9.62*
TCI	-3.33	1.25
Pinhb(-)	4.02	5.20
Pinhb	-2.44	-1.78

\* $\Delta G_{\text{solv}}$  of the IP is higher in energy than the TS1 required to reach such minimum, this is likely an effect of the thermodynamic corrections, strongly dependent on frequency calculations, due to the fact that the two stationary points are very close in energy. The correct behaviour (i.e. with the minimum (IP) at lower energy than the TS (TS1) required to reach it is correctly present in the electronic energies. In both cases, the two structures are almost isoenergetic.