# Supplementary material

## Supplementary Figure Legends

**Figure S1**: ACE inhibition assay by (A) Captopril and (B) Lisinopril.

**Figure S2:** HPLC-DAD profiles of compounds **1, 2** and **3** purified from fraction (F1) using preparative recycling HPLC.

**Figure S3:** Total ion chromatogram (TIC) of the most active fraction with annotated peaks related to purified compounds (**A**) and LC-ESI-MS/MS based characterization of compounds **1-3** shown in (**B, C** and **D**), respectively.

**Figure S4** : FTIR spectrum of Compound **1**,**2** and **3.**

**Figure S5:** Proton NMR spectrum of compound **1**.

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**Figure S7:** Proton NMR spectrum of compound **2**.

**Figure S8:** C-13 NMR spectrum of compound **2.**

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**Figure S10:** C-13 NMR spectrum of compound **3**.

**Figure S11:** (A) 2D Structure of lisinopril, (B) 3D structure of lisinopril, (C) 3D interaction of lisinopril with ACE generated through Chimera, and (D) 2D interactions of lisinopril with ACE generated through PoseView.

**Figure S12:** (A) 2D Structure of captopril, (B) 3D structure of captopril (C) 3D interaction of captopril with ACE generated through Chimera, and (D) 2D interactions of captopril with ACE generated through PoseView.

## Supplementary Table Legends

**Table S1**: Reaction initial velocity of ACE in enzymatic assay.

**Table S1**: ACE inhibitory activity of plant extracts.

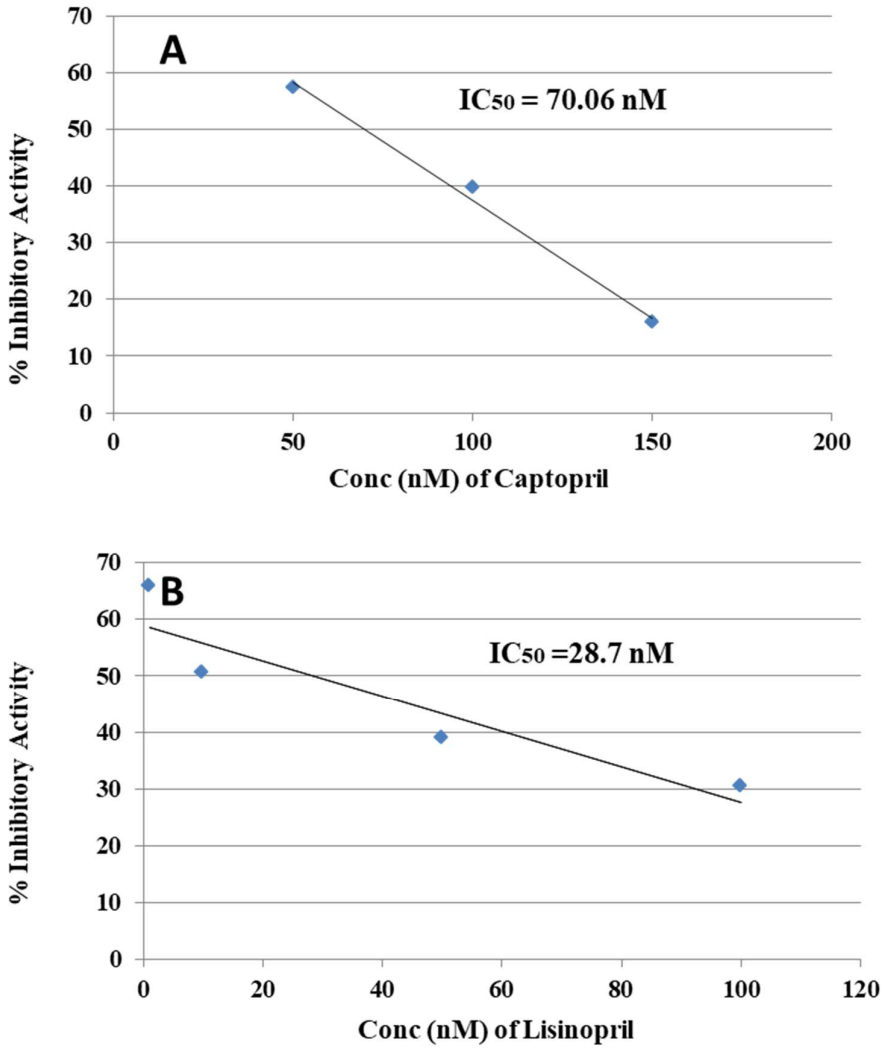


**Figure S1**: ACE inhibition assay by (A) Captopril and (B) Lisinopril.

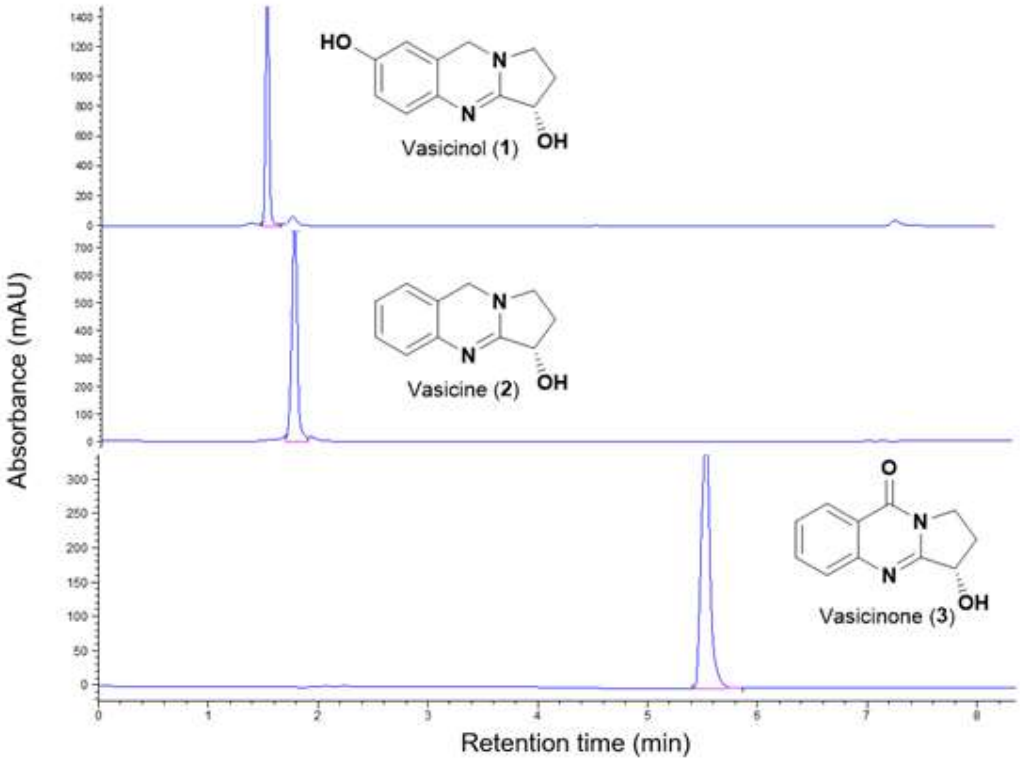


**Figure S2:** HPLC-DAD profiles of compounds **1, 2** and **3** purified from fraction (F1) using preparative recycling HPLC.

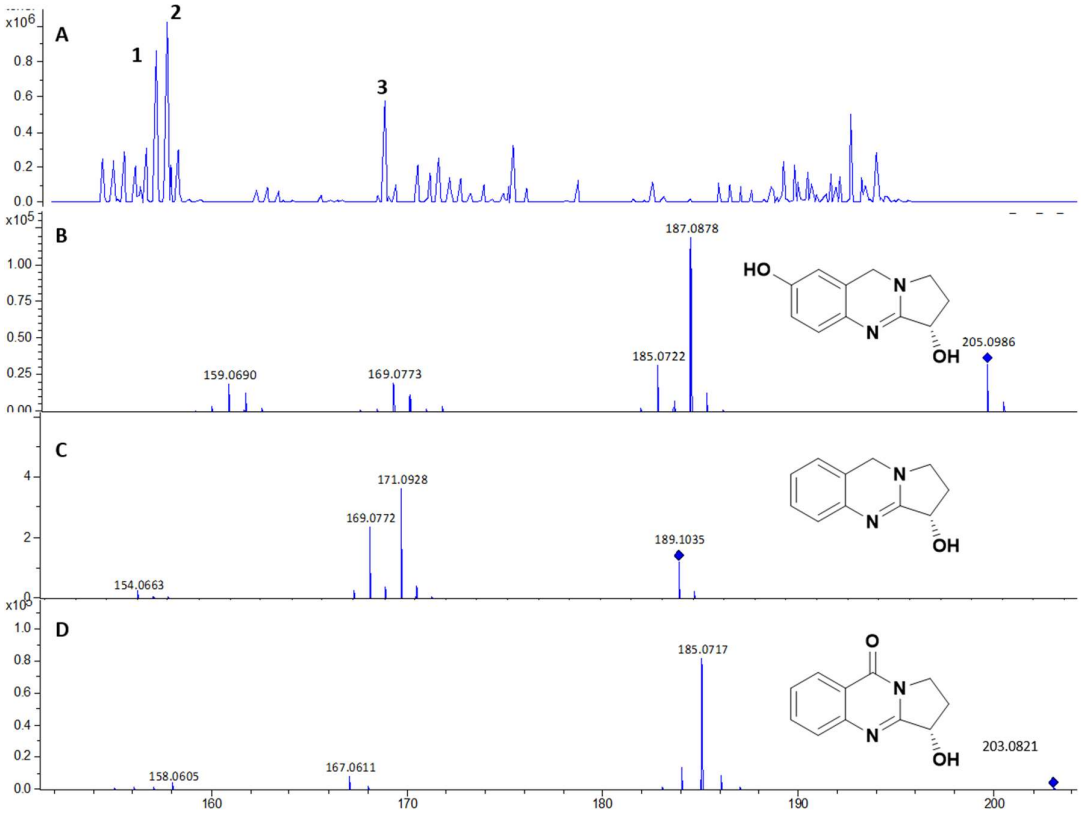


**Figure S3:** Total ion chromatogram (TIC) of the most active fraction with annotated peaks related to purified compounds (**A**) and LC-ESI-MS/MS based characterization of compounds **1-3** shown in (**B, C** and **D**), respectively.

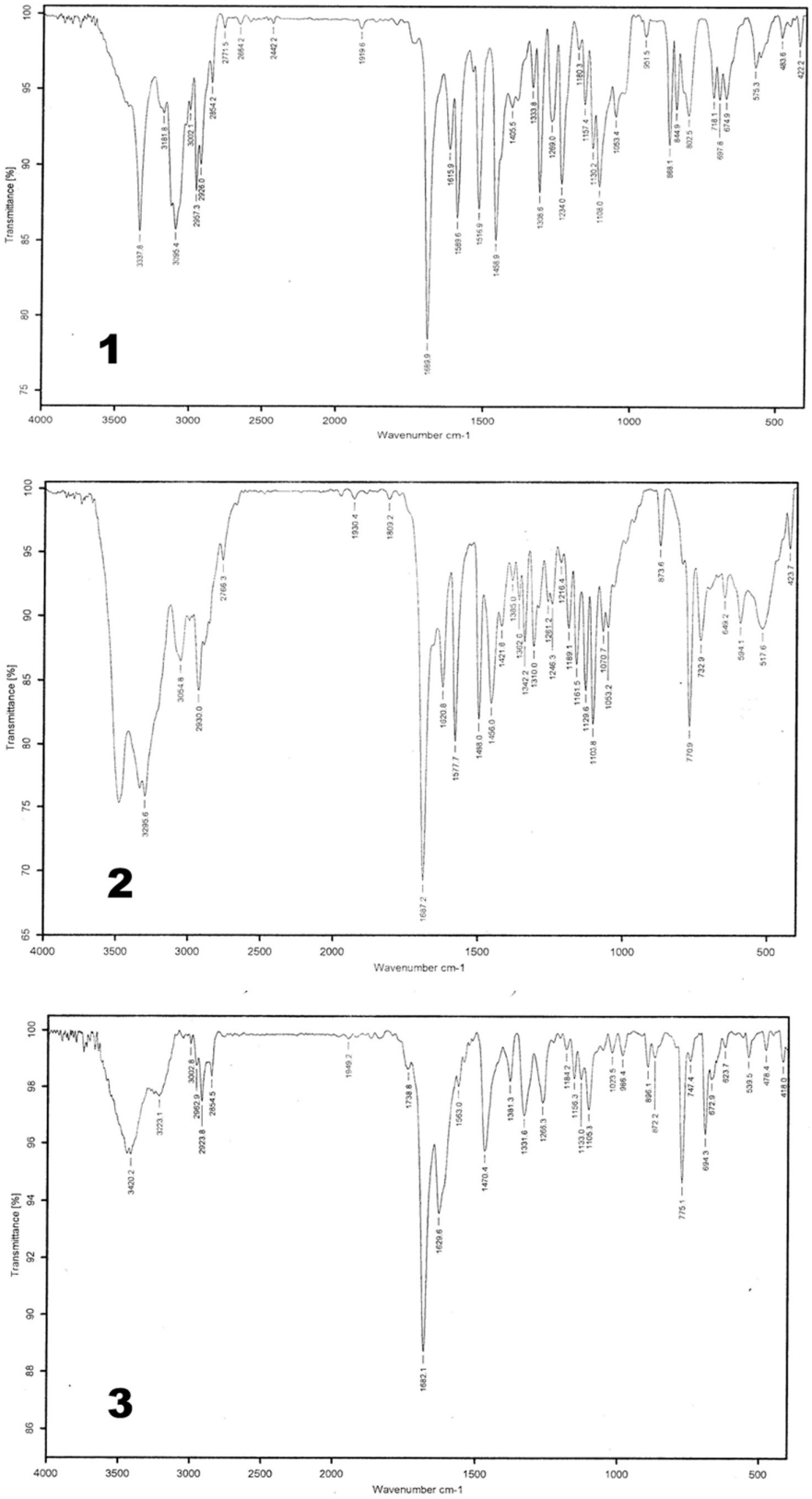


**Figure S4** : FT-IR spectrum of Compound **1**,**2** and **3.**

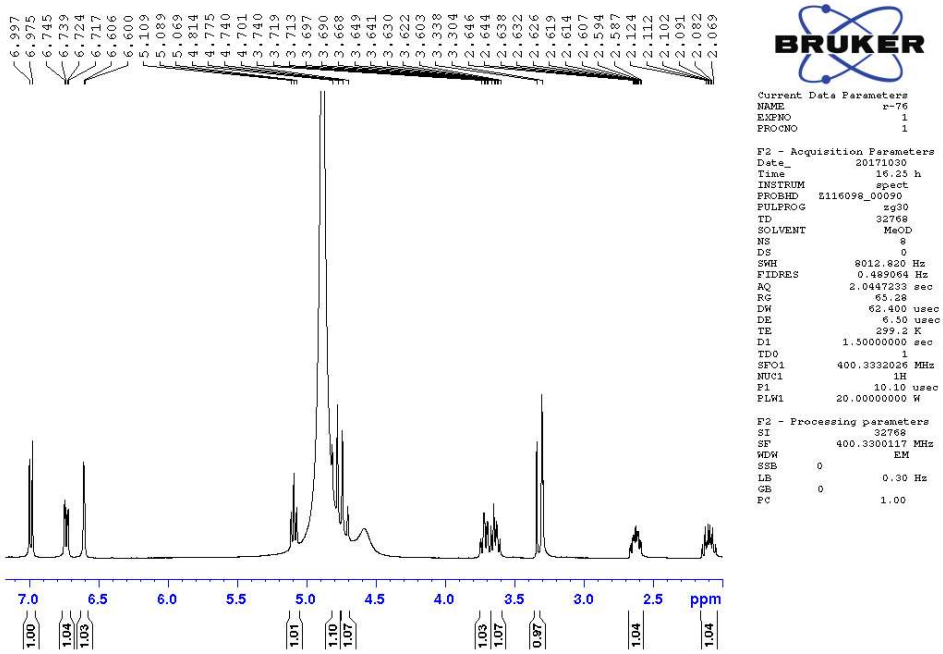


**Figure S5:** Proton NMR spectrum of compound **1**.

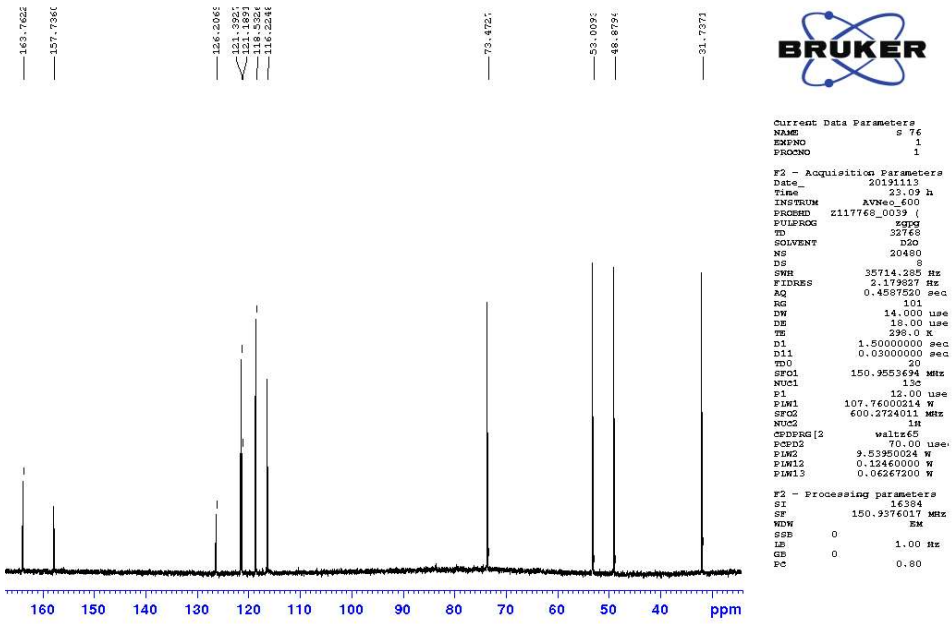


**Figure S6:** C-13 NMR spectrum of compound **1.**

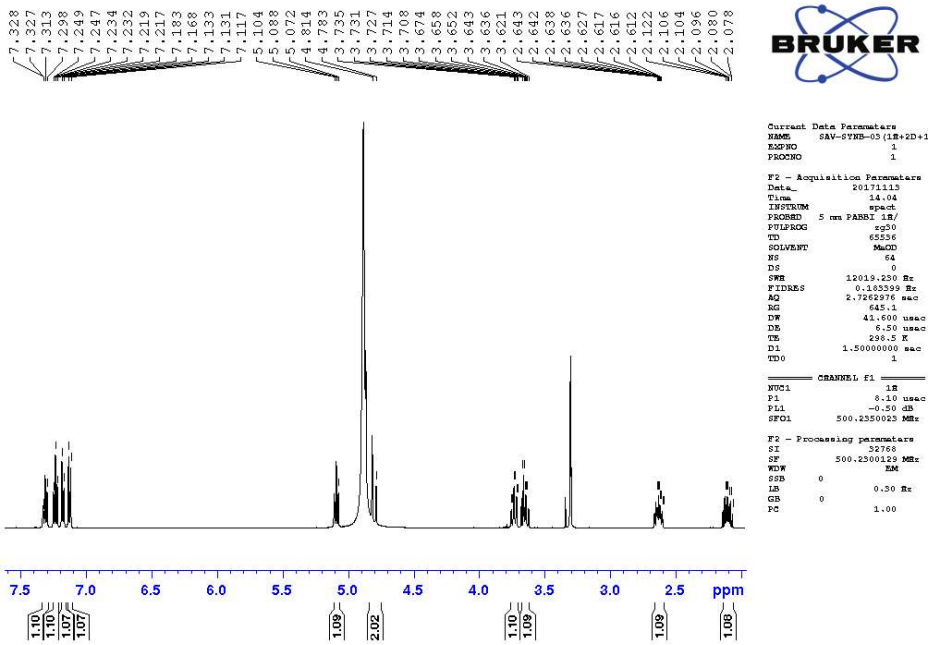


**Figure S7:** Proton NMR spectrum of compound **2**.

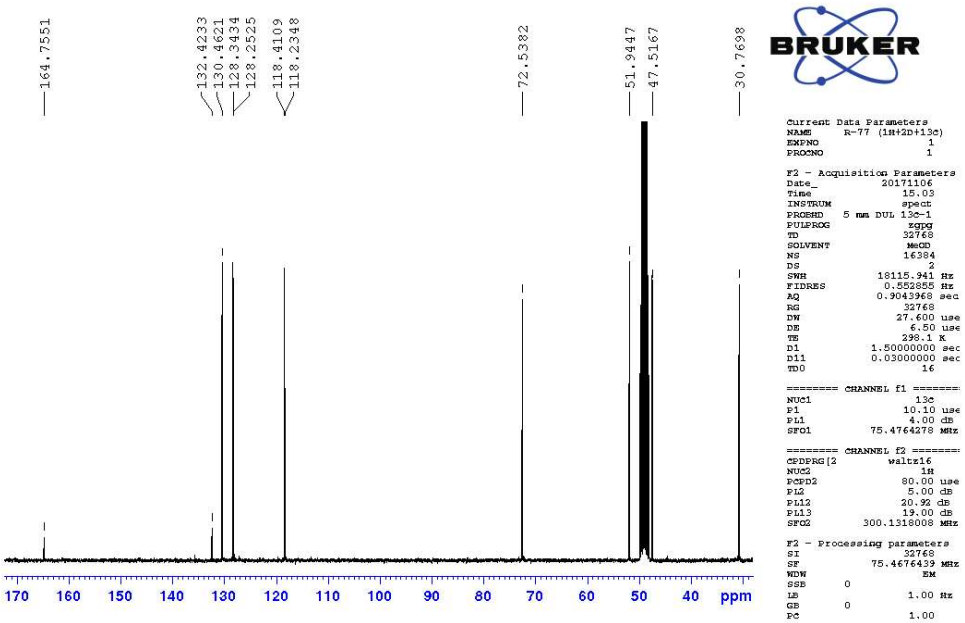


**Figure S8:** C-13 NMR spectrum of compound **2.**

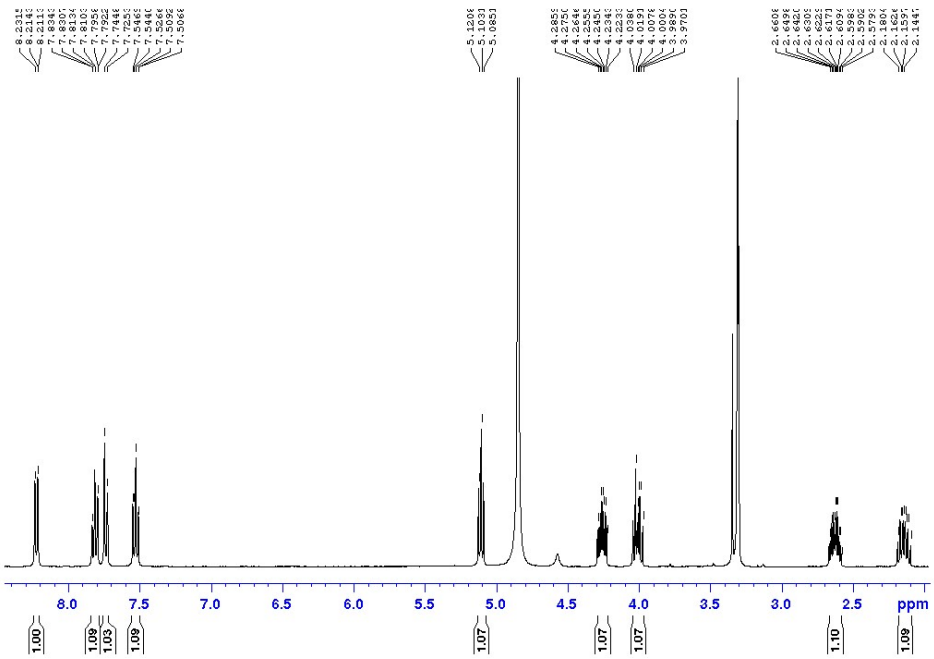


**Figure S9:** Proton NMR spectrum of compound **3**.

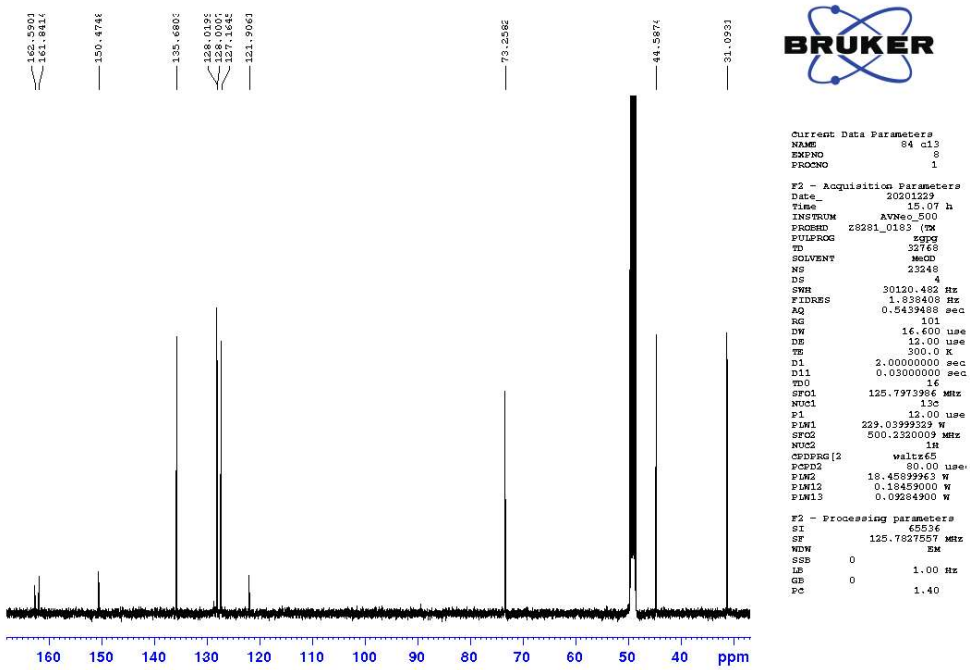


**Figure S10:** C-13 NMR spectrum of compound **3**.

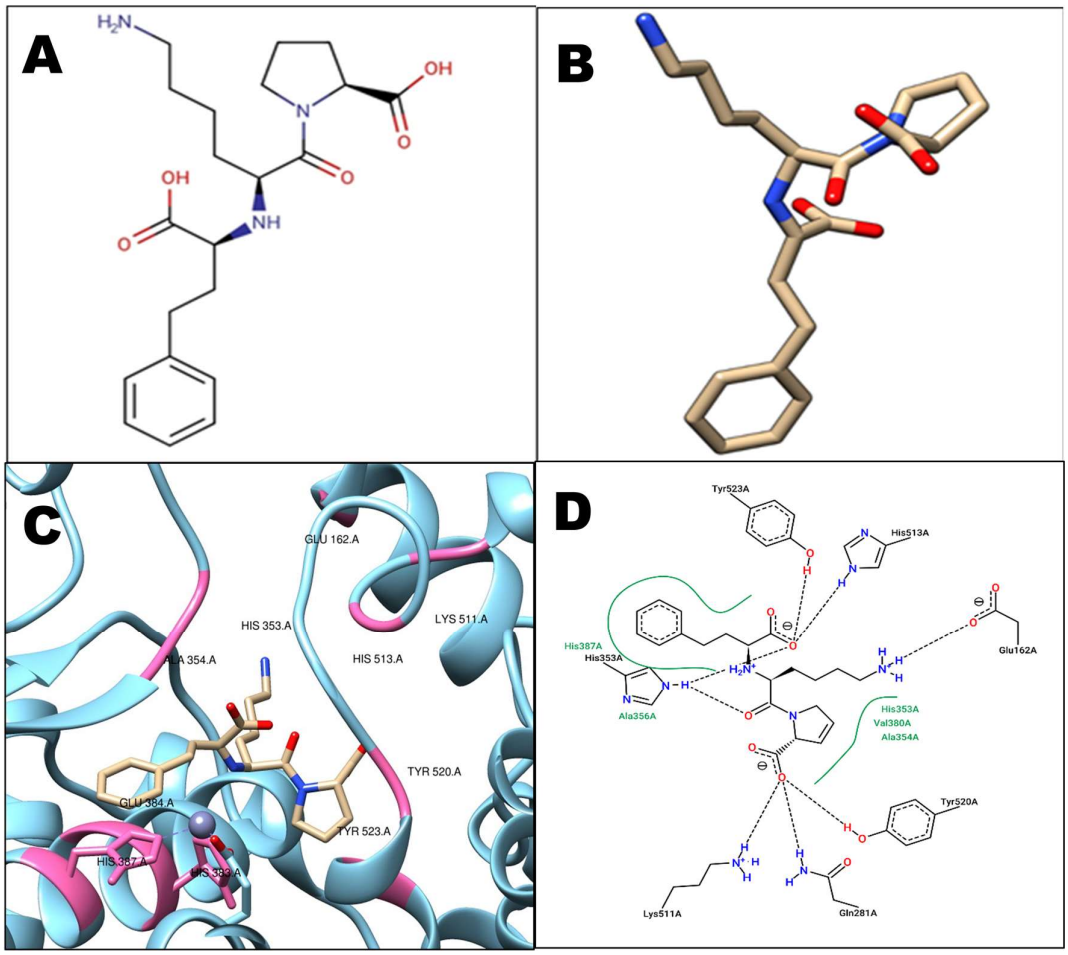


**Figure S11:** (A) 2D Structure of lisinopril, (B) 3D structure of lisinopril, (C) 3D interaction of lisinopril with ACE generated through Chimera, and (D) 2D interactions of lisinopril with ACE generated through PoseView.

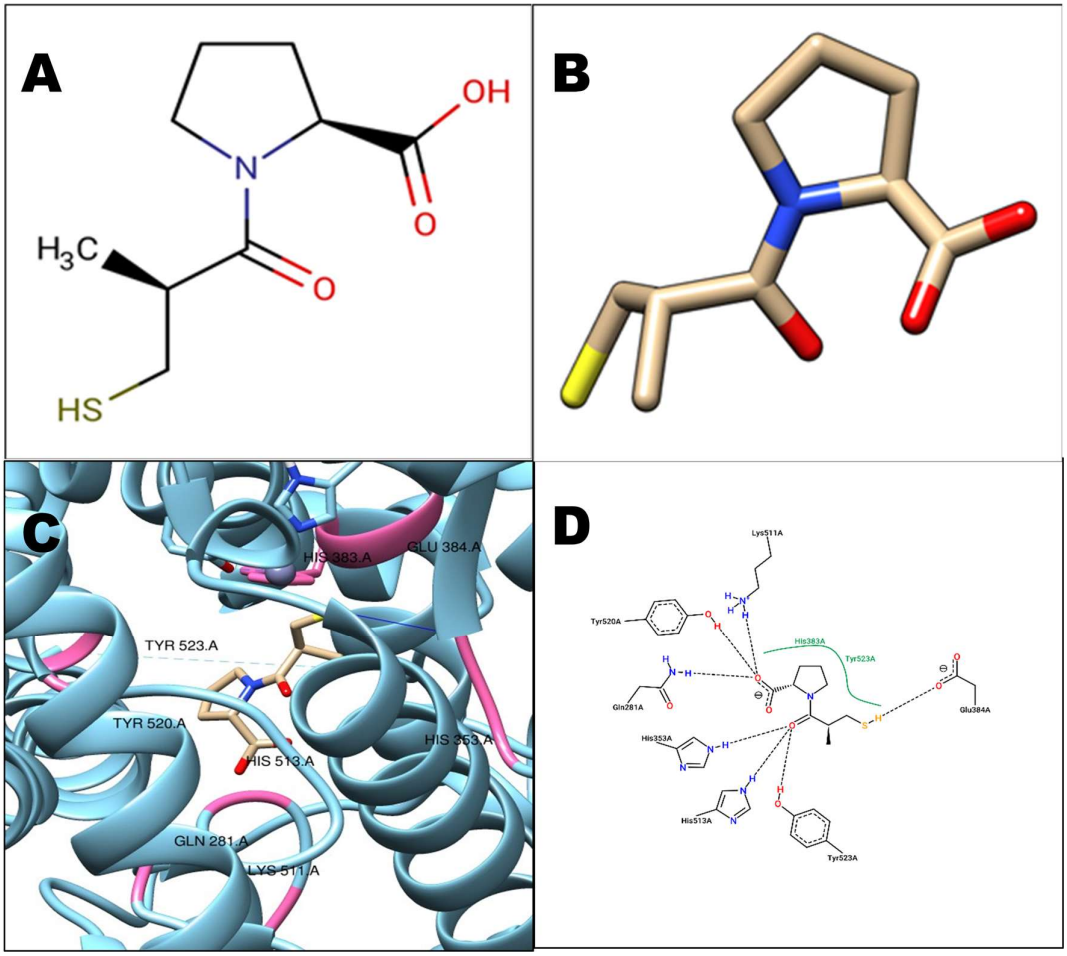


**Figure S12:** (A) 2D Structure of captopril, (B) 3D structure of captopril (C) 3D interaction of captopril with ACE generated through Chimera, and (D) 2D interactions of captopril with ACE generated through PoseView.

**Table S1:** Reaction initial velocity of ACE in enzymatic assay.

| Points | Cf-Ci (mM) | tf-ti (min) | $v^0$ (mM/min) |
|---|---|---|---|
| 1 | 0.750 | 10 | 0.0750 |
| 2 | 0.371 | 10 | 0.0371 |
| Average reaction velocity for initial 20 minutes | | | 0.056 |

**Table S2**: ACE inhibitory activity of plant extracts.

| S. No. | Code | Name of plant | %Inhibitory activity | Activity |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | AG | *Alpinia galangal* | 6.15 | Active |
| 2 | ZV | *Ziziphus vulgaris* | 25.92 | Active |
| 3 | BO | *Borago officinalis* | 10.08 | Active |
| 4 | AO | *Althaea officinalis* | 6.69 | Active |
| 5 | CL | *Cordia latifolia* | 8.60 | Active |
| 6 | VO | *Viola odorata* | > 5% | In active |
| 7 | GG | *Glycyrrhiza glabra* | > 5% | In active |
| 8 | PL | *Piper longum* | > 5% | In active |
| 9 | AV | *Adhatoda vasica* | 10.15 | Active |
| 10 | HO | *Hyssopus officinalis* | > 5% | In active |
| 11 | AT | *Anemone tetrasepala* | 10.52 | Active |
| 12 | AN | *Anemone obtusiloba* | > 5% | In active |
| 13 | AF | *Aquliegia fragrans* | 12.82 | Active |
| 14 | CQ | *Cissus quadrangularis* | 9.78 | Active |
| 15 | FI | *Fagonia indica* | 11.45 | Active |
| 16 | EO | *Emblica officinalis* | > 5% | In active |
| 17 | CA | *Centella asciatica* | > 5% | In active |
| 18 | AS | *Amomum subulatum* | > 5% | In active |
| 19 | DD | *Delphinium denudatum* | > 5% | In active |
| 20 | LA | *Lavandula angustifolia* | > 5% | In active |
| 21 | CD | *Canscora decussate* | > 5% | In active |
| 22 | GB | *Ginko biloba* | > 5% | In active |
| 23 | HM | *Herpestis monniera* | > 5% | In active |