**SUPPLEMENTARY MATERIAL**

*Communication*

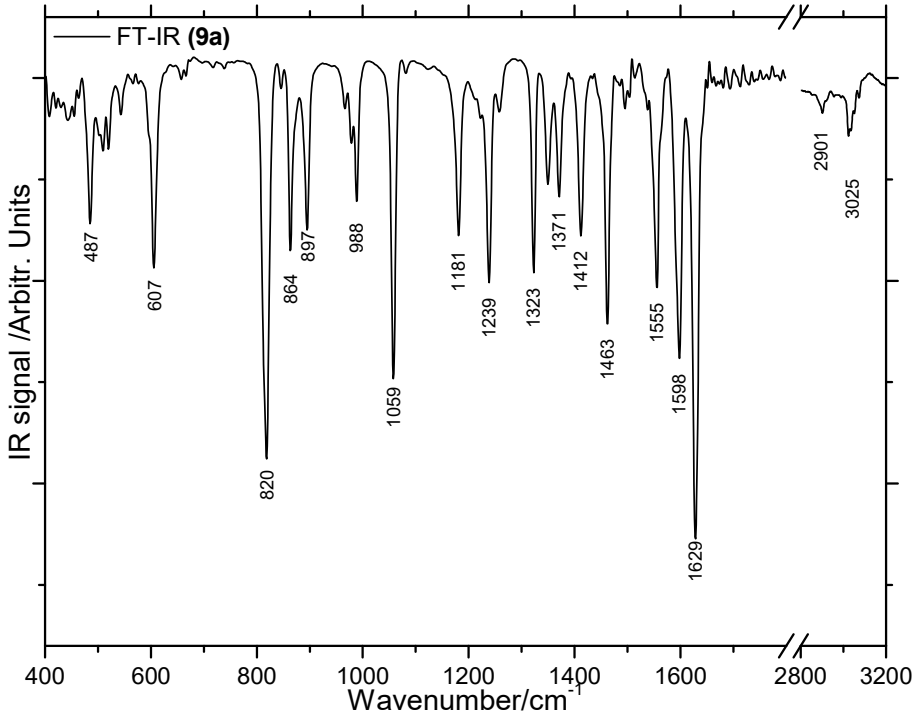
# Resveratrol-Schiff base hybrid compounds with selective antibacterial activity: Synthesis, biological activity, and computational study

**Rodrigo Sánchez-González [1], Patricio Leyton [1], Luis F. Aguilar [1], Mauricio Reyna-Jeldes [2-4], Claudio Coddou [2-4], Katy Díaz [5,*], Marco Mellado [6,*]**

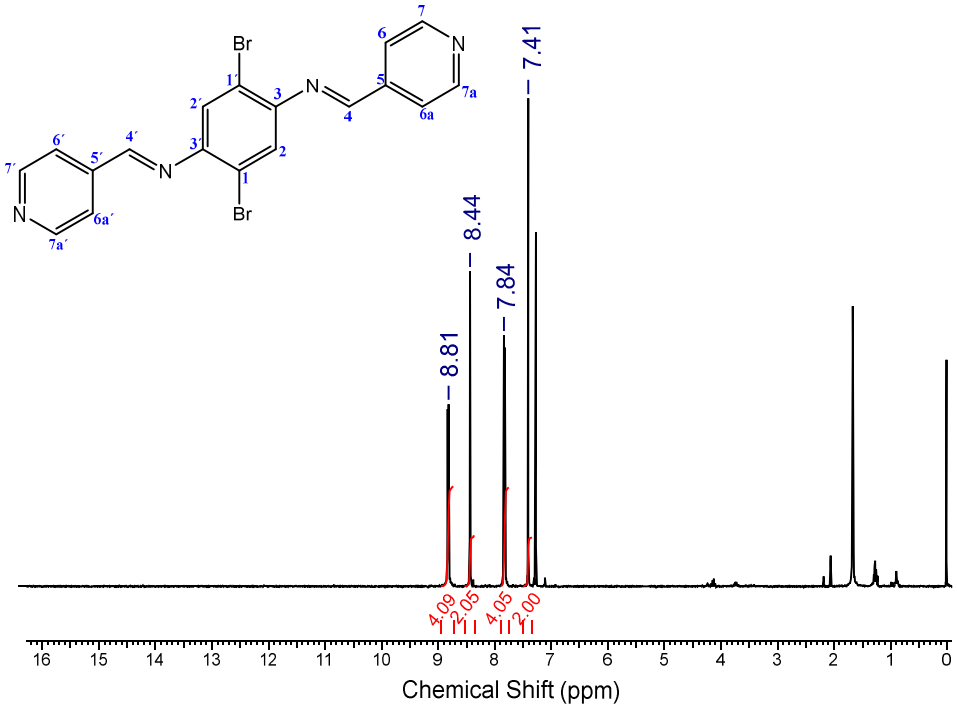
[1] Instituto de Química, Facultad de Ciencias, Pontificia Universidad Católica de Valparaíso, Valparaíso 2373223, Chile; rodrigo.sanchez.g@pucv.cl (R.S-G.); patricio.leyton@pucv.cl (P.L.)
[2] Departamento de Ciencias Biomédicas, Facultad de Medicina, Universidad Católica Del Norte, Coquimbo 1781421, Chile; mauricio.reyna@ucn.cl (M.R-J.); ccoddou@ucn.cl (C.C.)
[3] Millennium Nucleus for the Study of Pain (MiNuSPain), Santiago 8330025, Chile; mauricio.reyna@ucn.cl (M.R-J.); ccoddou@ucn.cl (C.C.)
[4] Núcleo para el Estudio del Cáncer a Nivel Básico, Aplicado y Clínico, Universidad Católica del Norte, Antofagasta 1270709, Chile; mauricio.reyna@ucn.cl (M.R-J.); ccoddou@ucn.cl (C.C.)
[5] Departamento de Química, Universidad Técnica Federico Santa María, Valparaíso 2390123, Chile; katy.diaz@usm.cl (K.D.)
[6] Instituto de Investigación y Postgrado, Facultad de Ciencias de la Salud, Universidad Central de Chile, Santiago 8330507, Chile; marco.mellado@ucentral.cl (M.M.)
* Correspondence: katy.diaz@usm.cl (K.D.); marco.mellado@ucentral.cl (M.M.)

## Table of Content

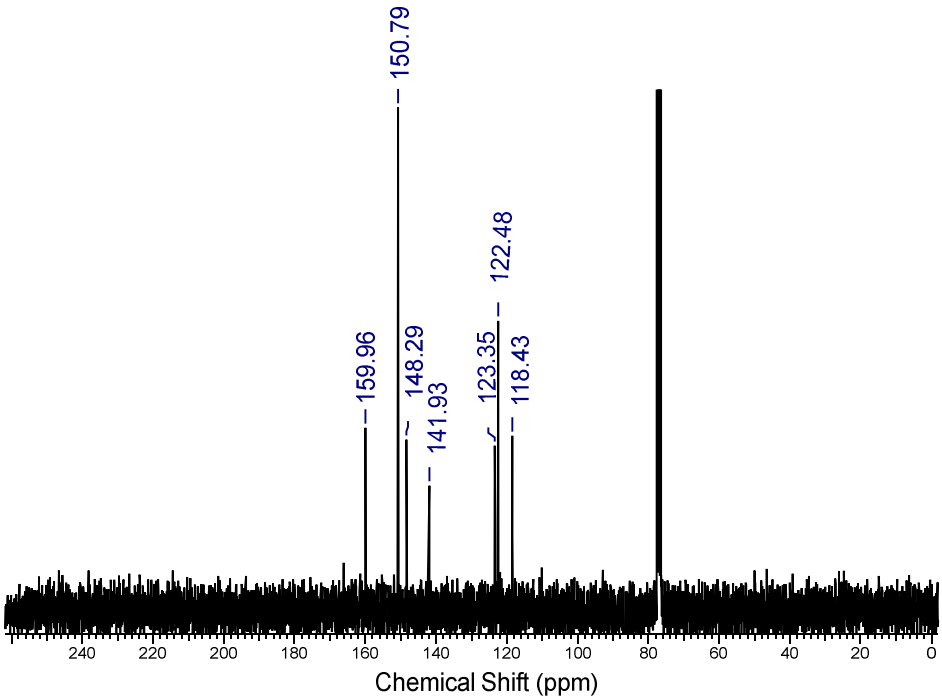
# Spectra S1-S18: FT-IR, $^{1}$H-NMR and $^{13}$C-NMR spectra for symmetric (9a-9e) and asymmetric (10a) imines



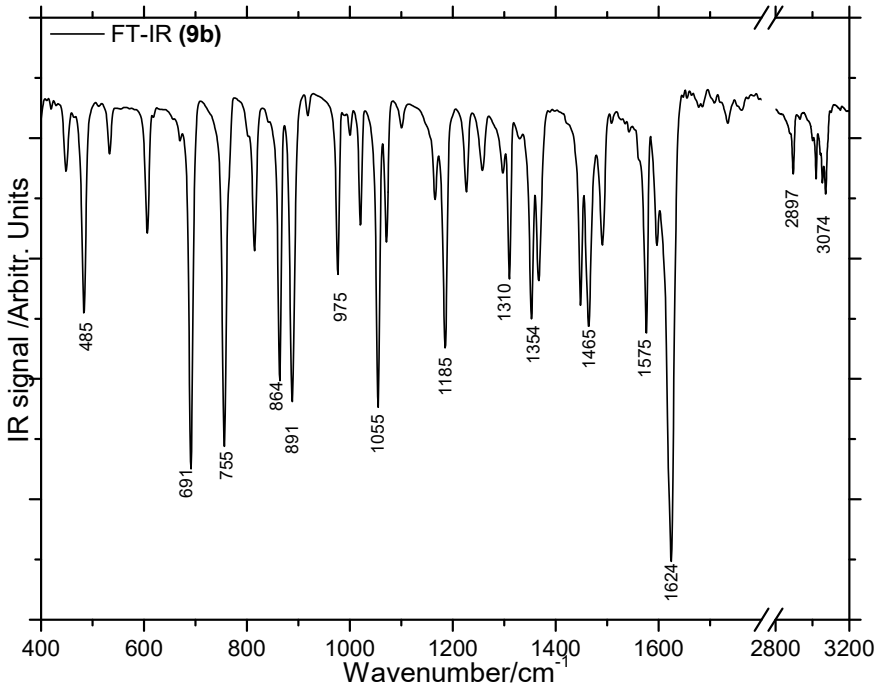

**Spectra S1:** FT-IR of compound **9a**



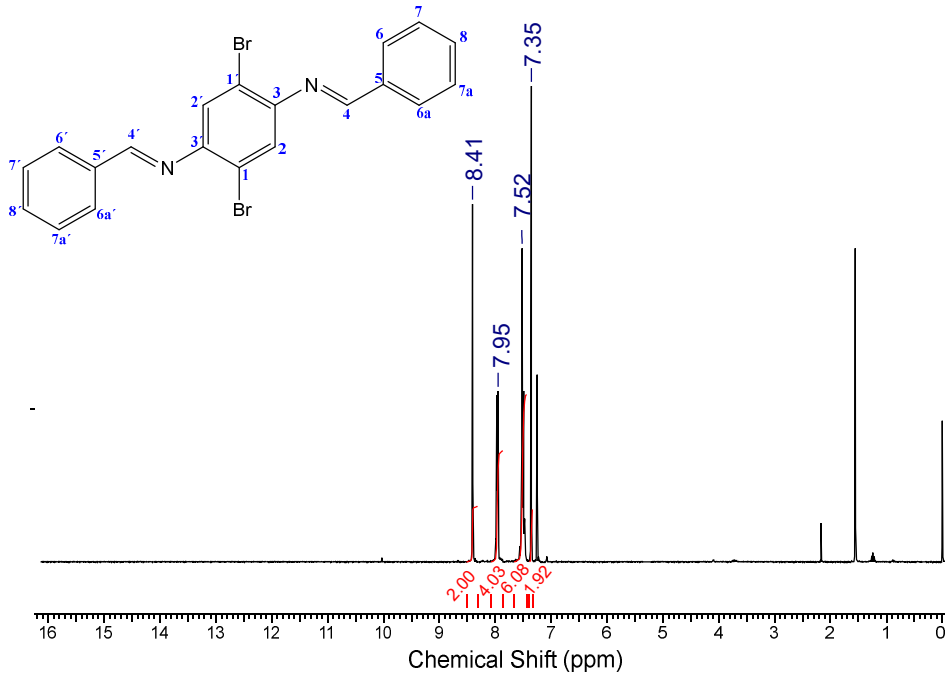

**Spectra S2:** $^{1}$H-NMR of compound **9a**



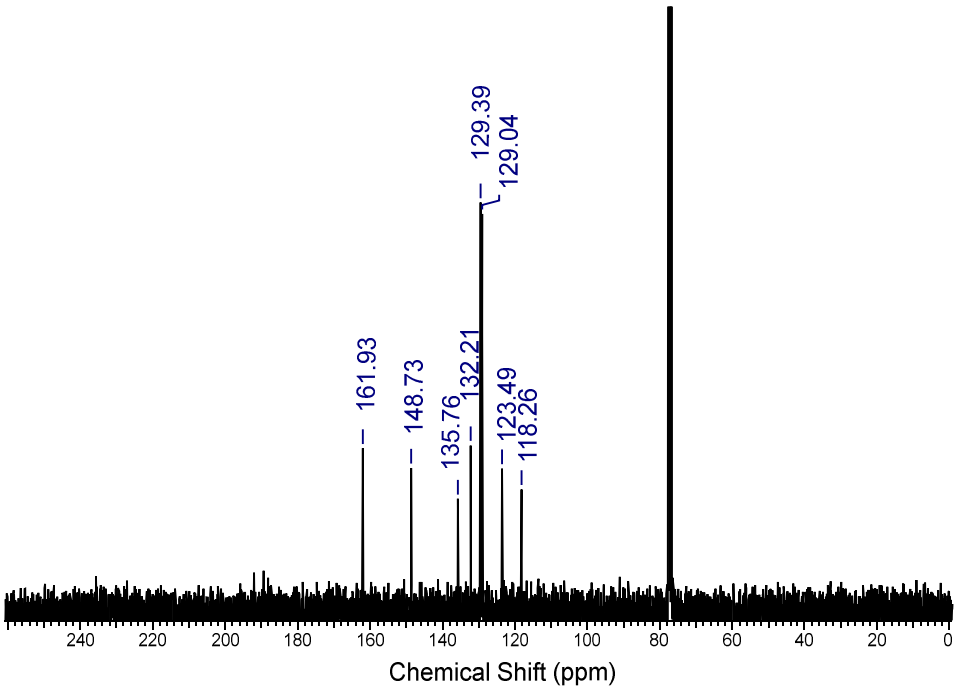

**Spectra S3:** $^{13}$C-NMR of compound **9a**



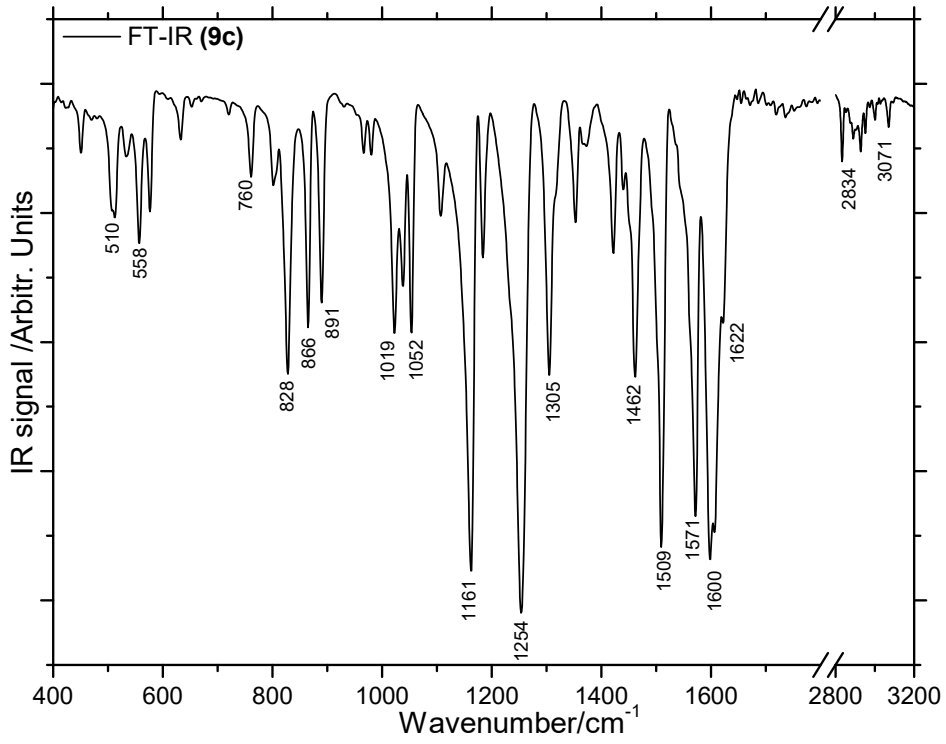

**Spectra S4:** FT-IR of compound **9b**



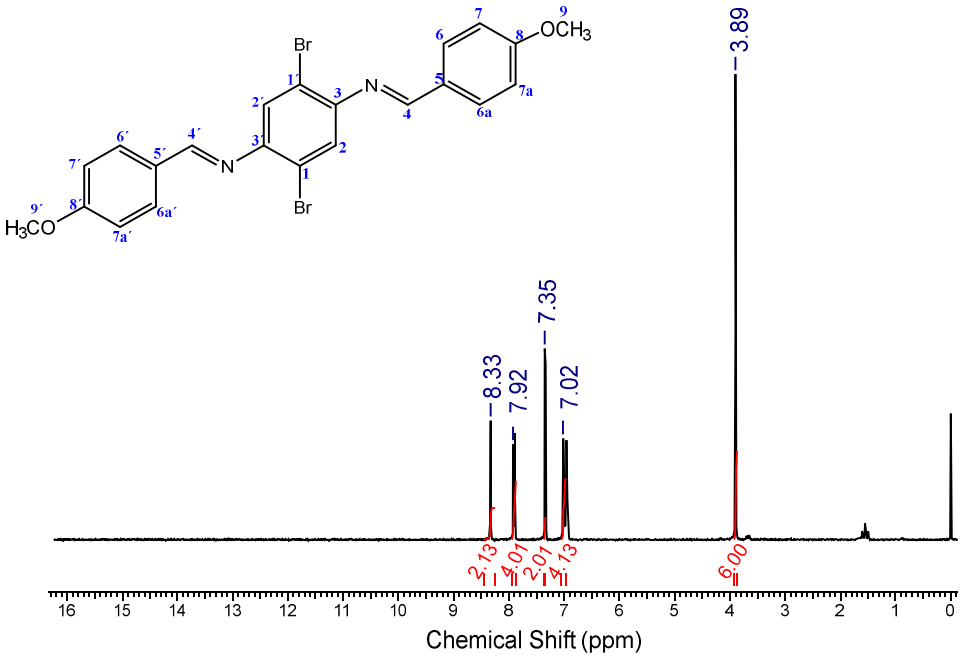

**Spectra S5:** $^{1}$H-NMR of compound **9b**



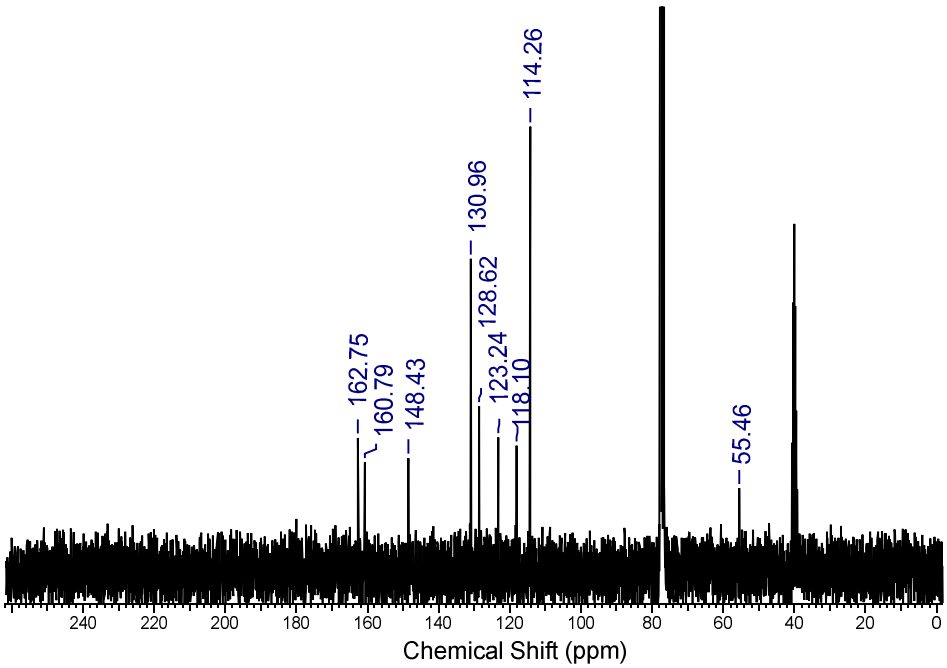

**Spectra S6:** $^{13}$C-NMR of compound **9b**



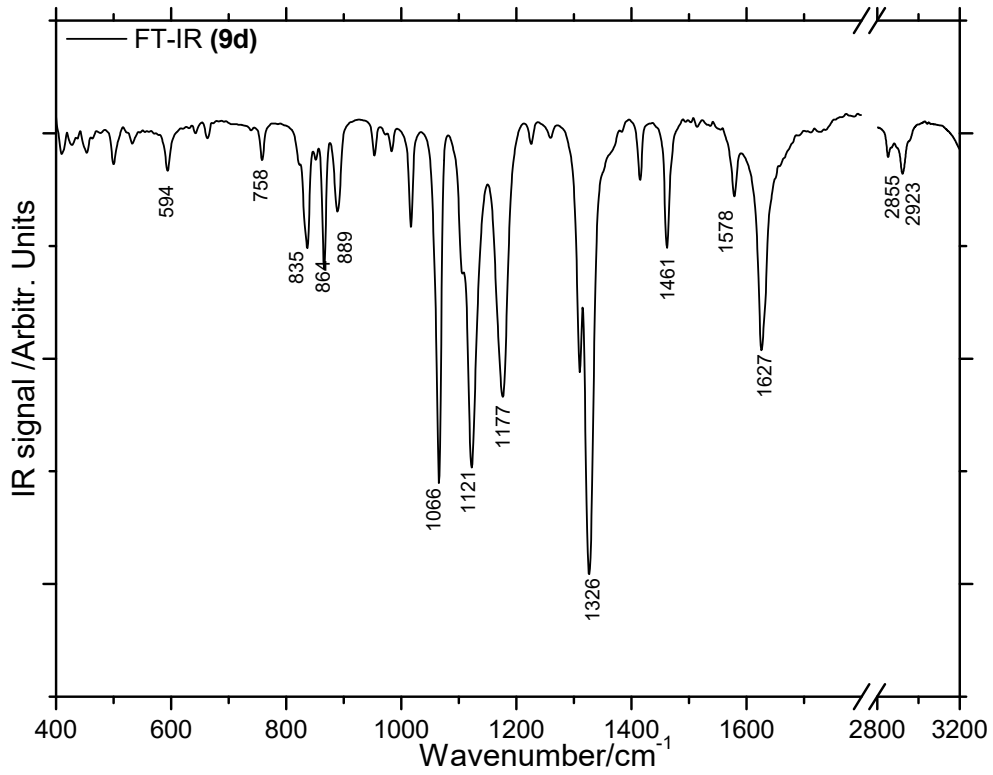

**Spectra S7:** FT-IR of compound **9c**



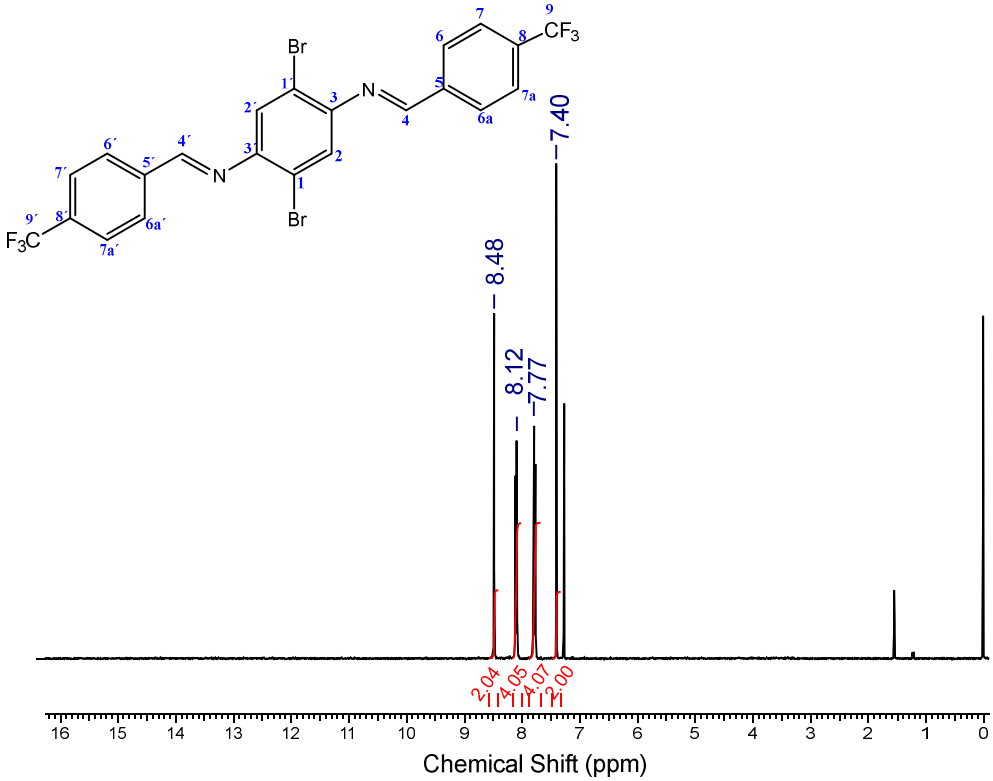

**Spectra S8:** [1]H-NMR of compound **9c**



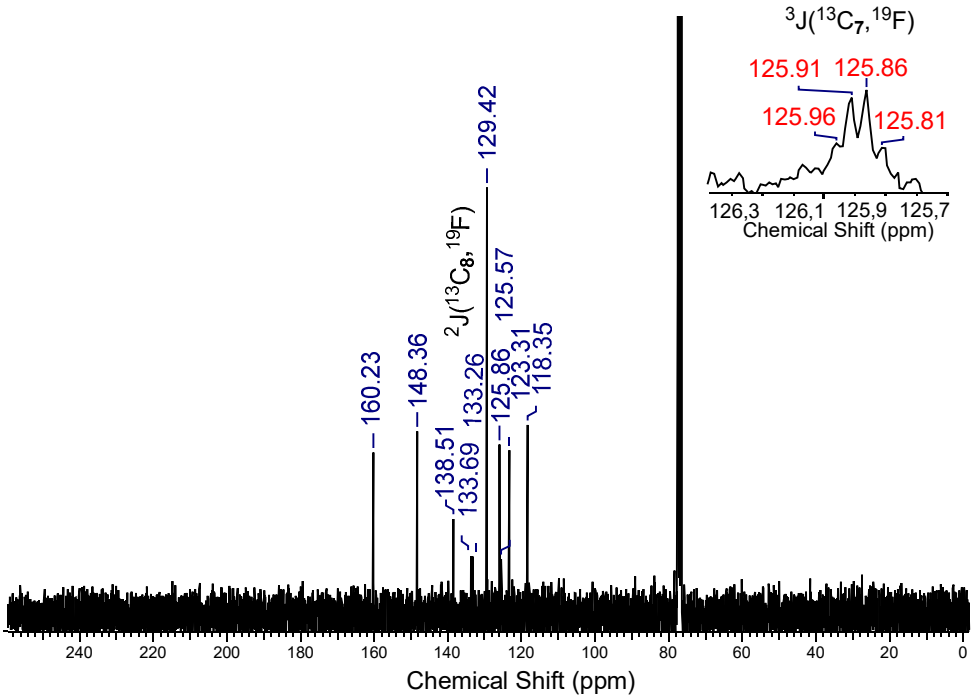

**Spectra S9:** $^{13}$C-NMR of compound **9c**



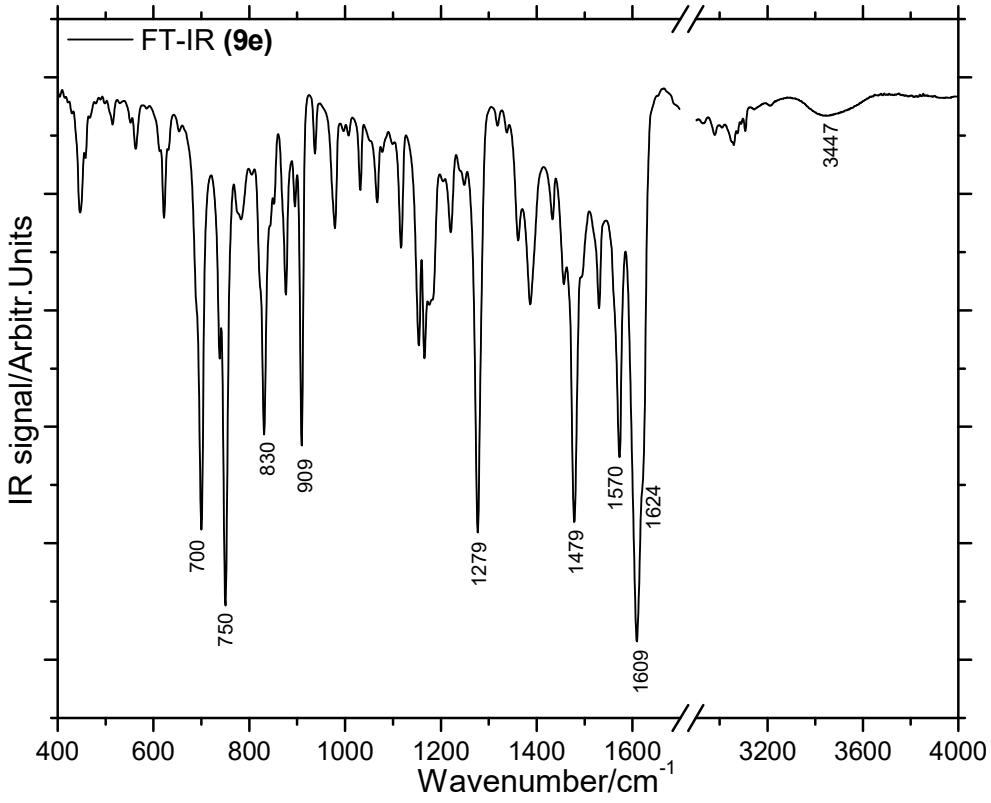

**Spectra S10:** FT-IR of compound **9d**



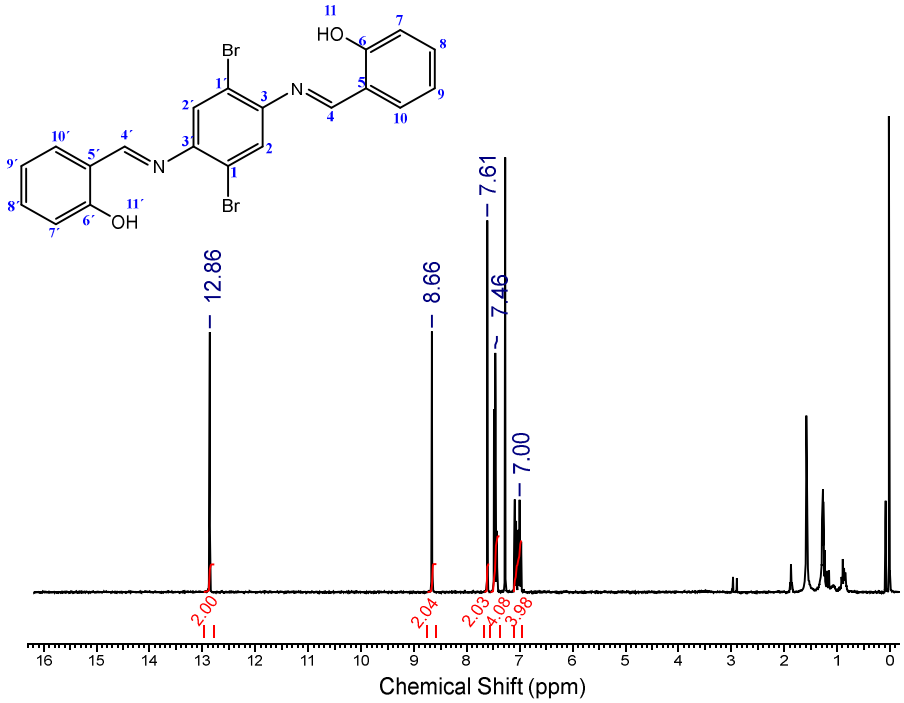

**Spectra S11:** [1]H-NMR of compound **9d**



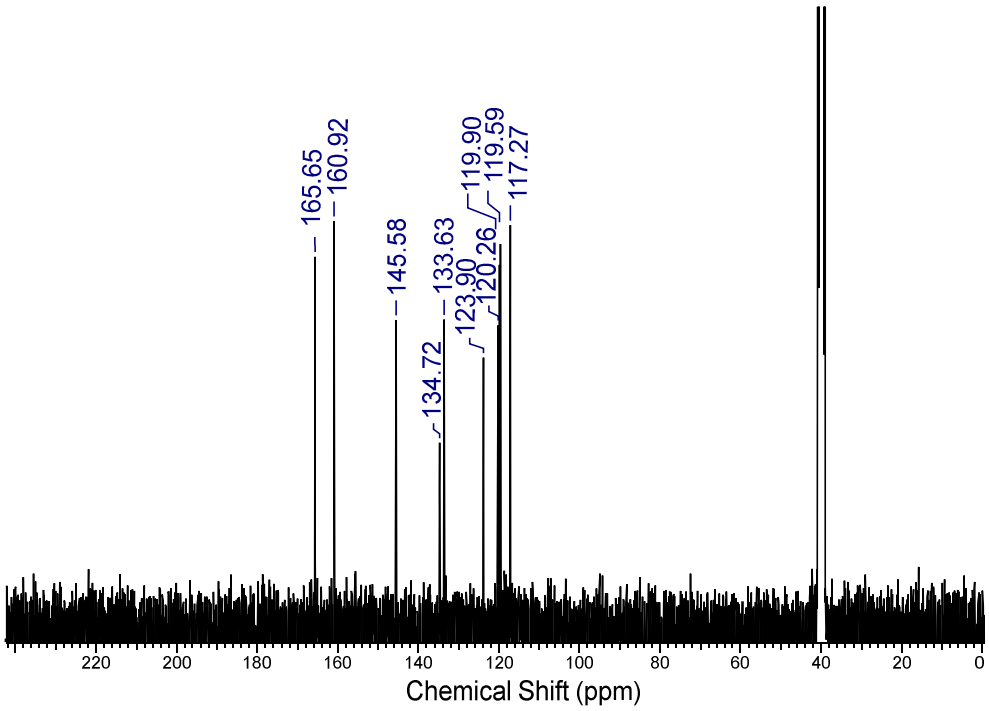

**Spectra S12:** $^{13}$C-NMR of compound **9d**



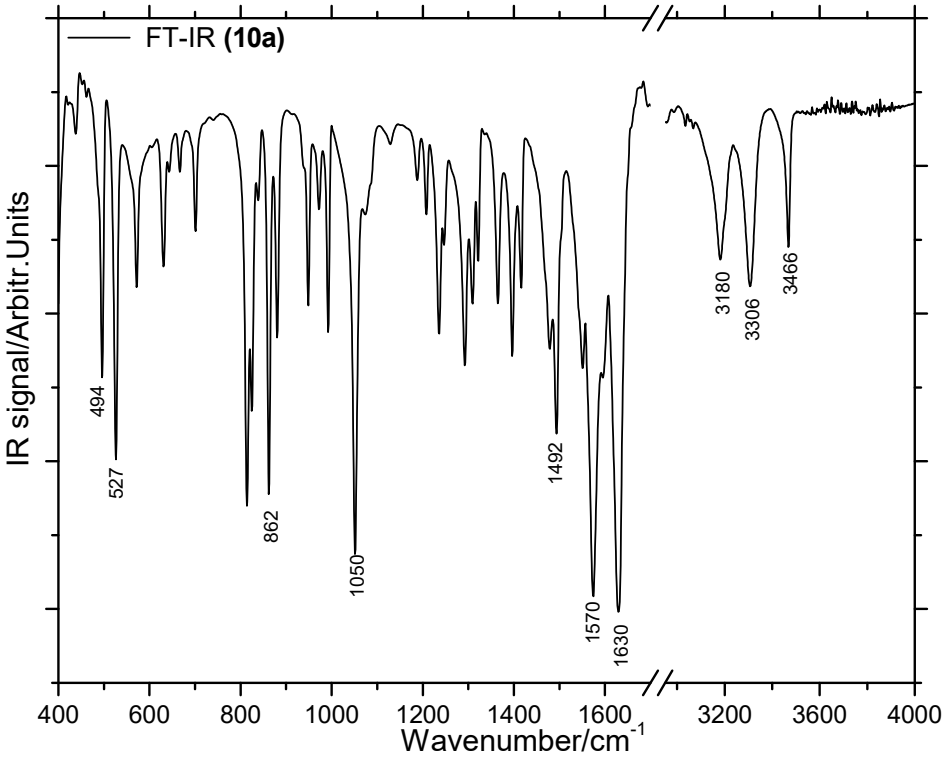

**Spectra S13:** FT-IR of compound **9e**



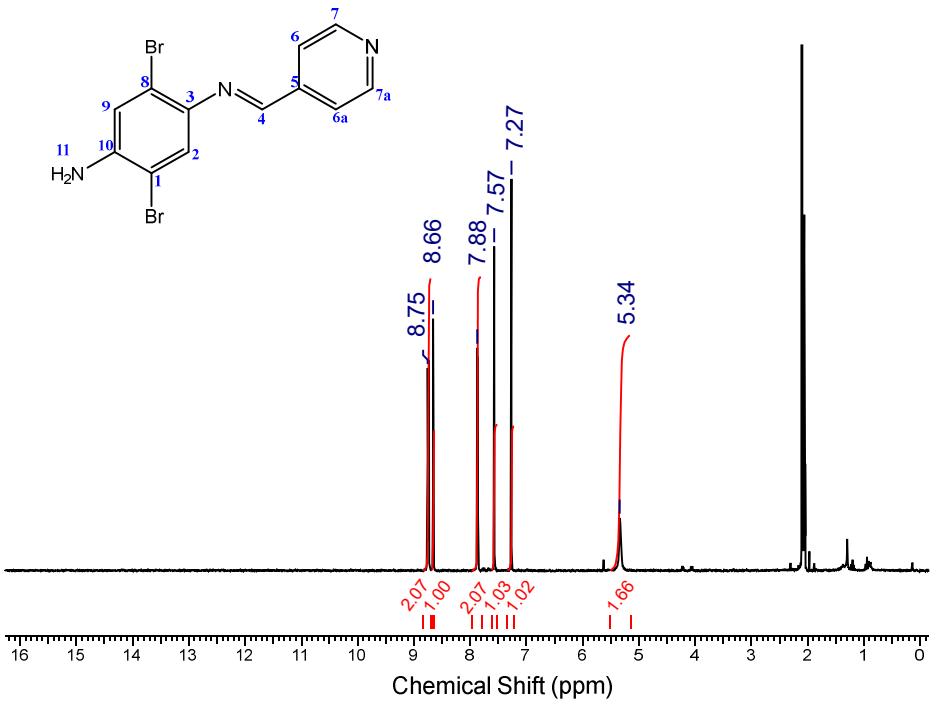

**Spectra S14:** [1]H-NMR of compound **9e**



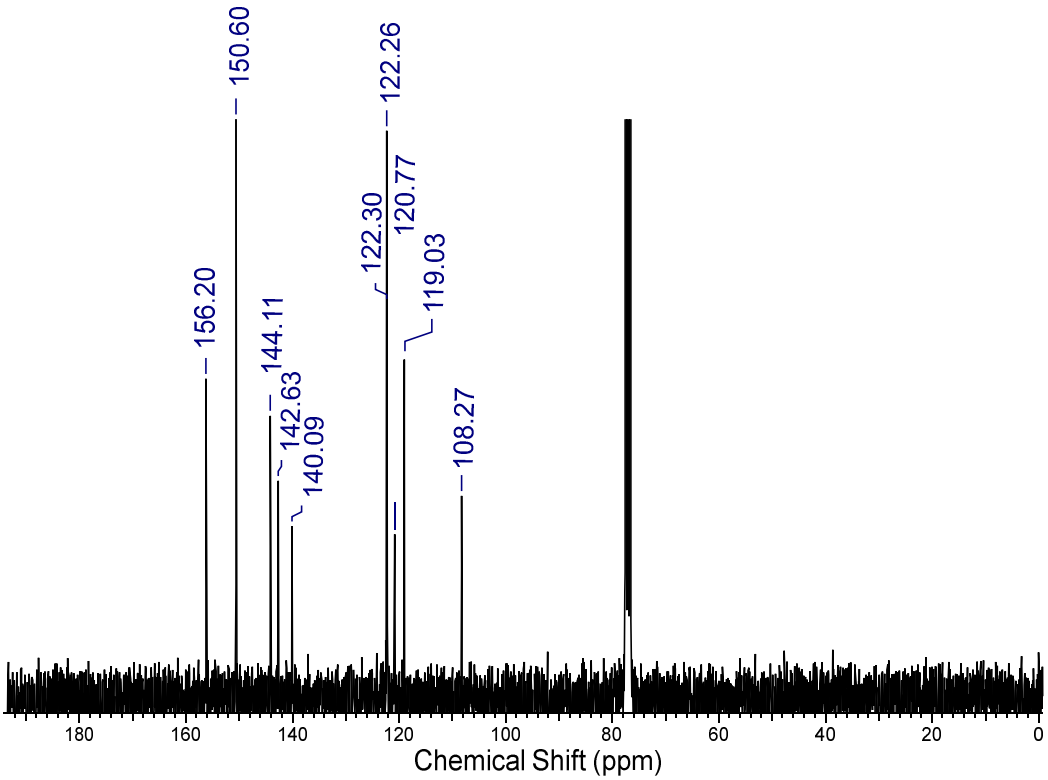

**Spectra S15:** $^{13}$C-NMR of compound **9e**




**Spectra S16:** FT-IR of compound **10a**




**Spectra S17:** $^{1}$H-NMR of compound **10a**




**Spectra S18:** $^{13}$C-NMR of compound **10a**

# Figures S1-S6: Molecular docking results

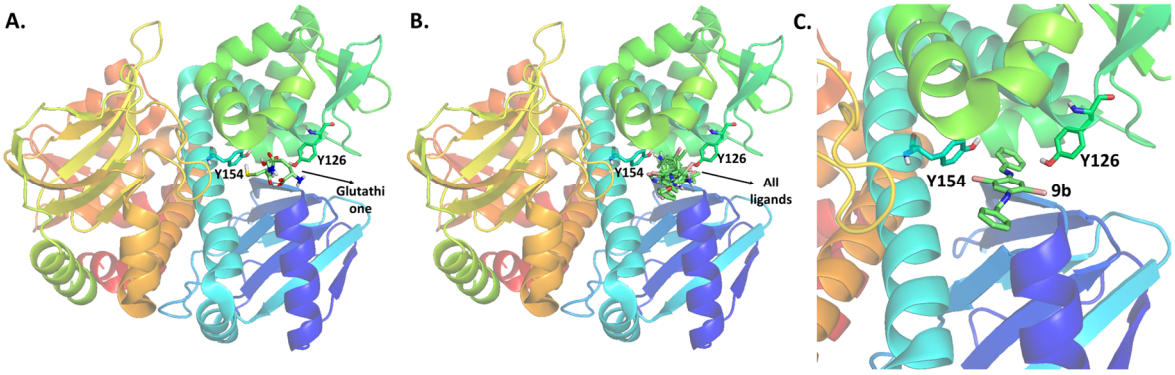



**Figure S1:** Molecular docking results for active compounds on positive regulatory factor A (PrfA, PDB ID: ILRR). **A.** 3D-overview for native ligand on the active site of PrfA. **B.** 3D-overview for active compounds on the active site of PrfA. **C.** Detailed interaction between key residues and the most active compound (**9b**).

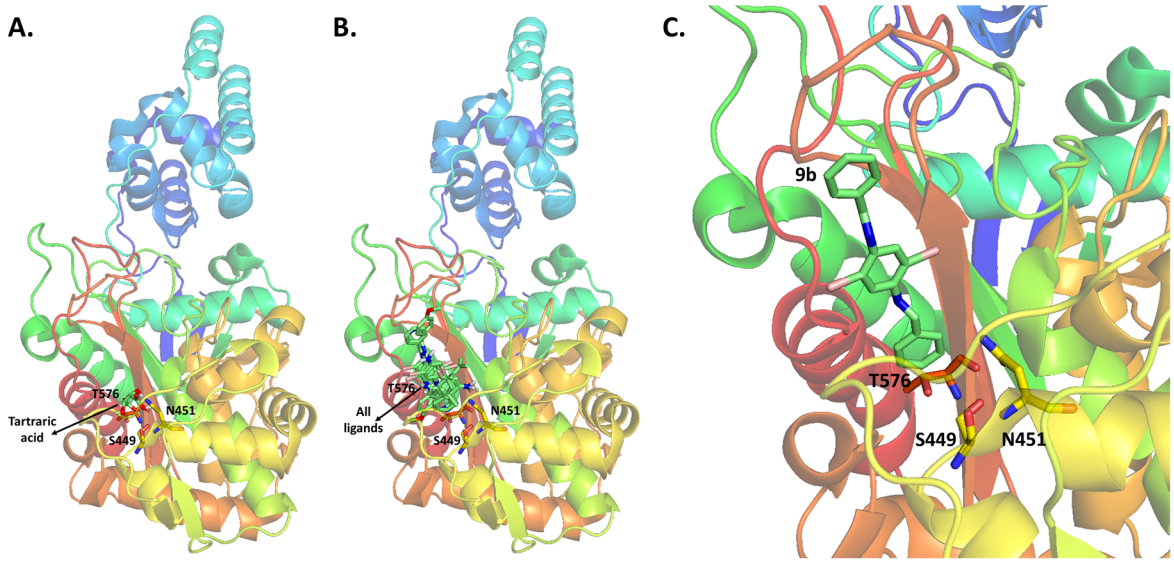



**Figure S2:** Molecular docking results for active compounds on penicillin-binding protein 4 (PBPs4, PDB ID: 3ZG8). **A.** 3D-overview for native ligand the on active site of PBPs4. **B.** 3D-overview for active compounds the on active site of PBPs4. **C.** Detailed interaction between key residues and the most active compound (**9b**).

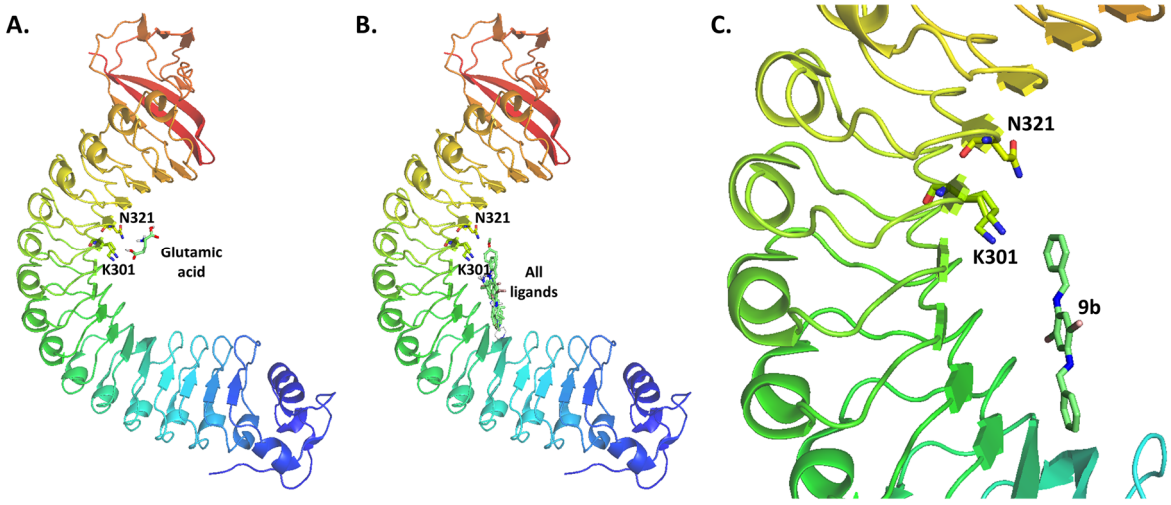



**Figure S3:** Molecular docking results for active compounds on internalin A (PDB ID: 1O6V). **A.** 3D-overview for native ligand on the active site of internalin A. **B.** 3D-overview for active compounds on the active site of internalin A. **C.** Detailed interactions between key residues and the most active compound (**9b**).

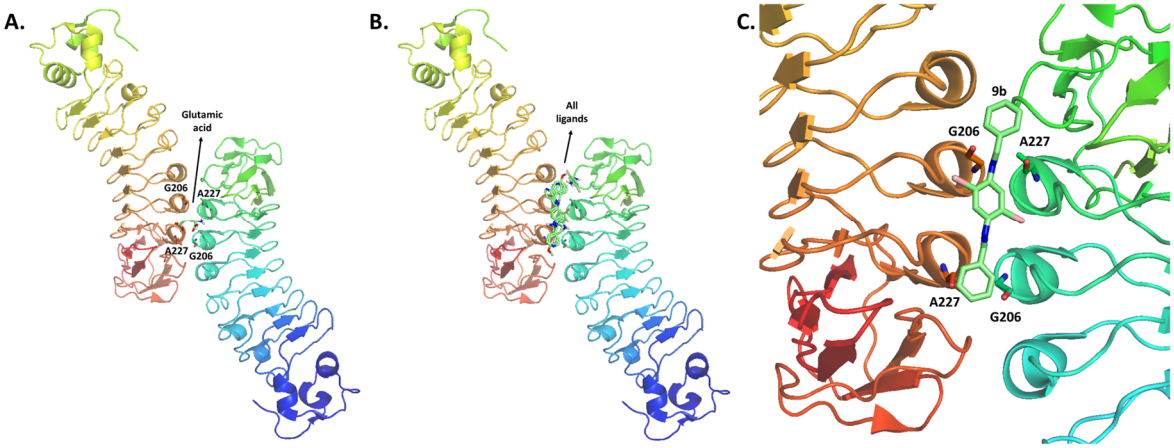



**Figure S4:** Molecular docking results for the active compounds against internalin B (PDB ID: 2WQU). **A.** 3D-overview for native ligand on the active site of internalin B. **B.** 3D-overview for active compounds on the active site of internalin B. **C.** Detailed interaction between key residues and the most active compound (**9b**).

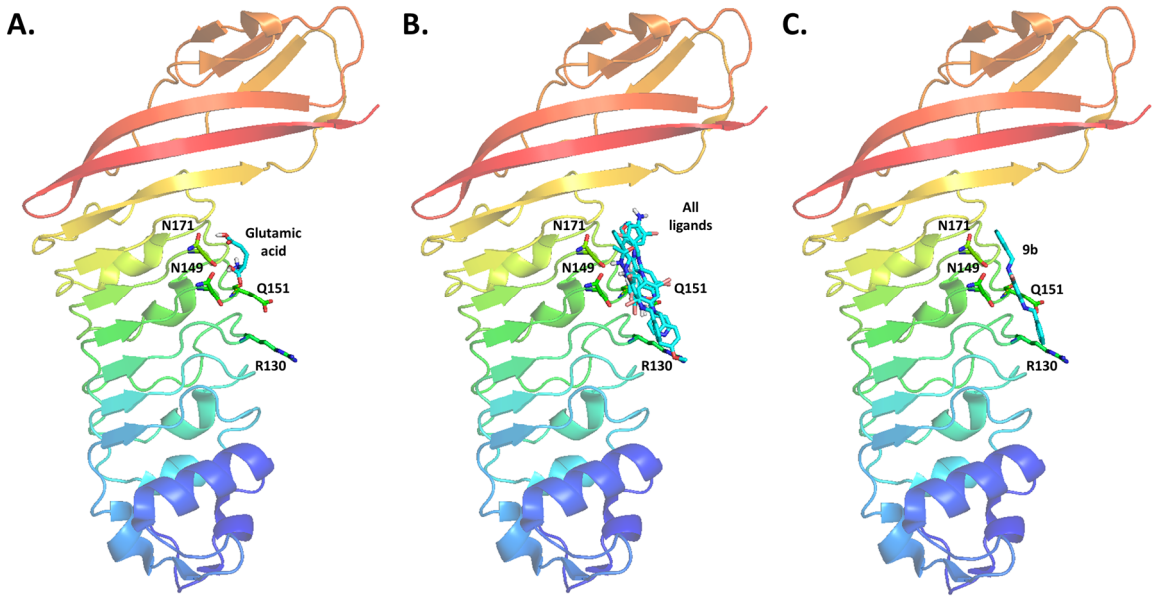



**Figure S5:** Molecular docking result for active compounds against internalin C (PDB ID: 1XEU). **A.** 3D-Overview for native ligand on the active site of internalin C. **B.** 3D-overview for active compounds on the active site of internalin C. **C.** Detailed interaction between key residues and the most active compound (**9b**).

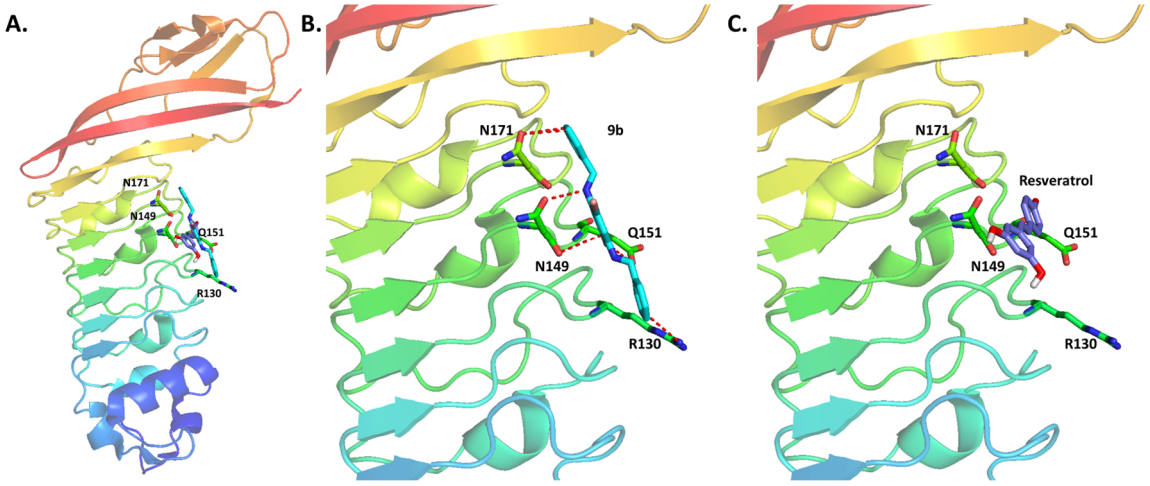



**Figure S6**: Molecular docking results for compound **9b** and **resveratrol** against internalin C (PDB ID: 1XEU). **A.** 3D-overview for compound **9b** and **resveratrol** on the active site of internalin C. **B.** Detailed interaction between key residues and compound **9b. C.** Detailed interaction between key residues and **resveratrol**.