Supporting information

Novel 3-Arylethynyl-subsititued Thieno[3,4-b]pyrazine Derivatives as a Human Transglutaminase 2 Inhibitors.

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3 compounds GK-414-430
3D Structure presented Docking results of **GK-13**

3D Structure presented Docking results of **GK-428**
3D Structure presented Docking results of **GK-419**

3D Structure presented Docking results of **GK-421**
3D Structure presented Docking results of **GK-423**

3D Structure presented Docking results of **GK-425**
The viewing 3D-molecular volume and IC50 of chosen thieno[3,4-b]pyrazine derivatives from 1st screening using the SRB test

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<th>Code</th>
<th>3D-molecular volume</th>
<th>IC50</th>
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<td>GK-13</td>
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<td>GK-414</td>
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*3D-molecular volume calculated by using the software Discovery studio 4.0
GK-428: $^1$H NMR Spectrum

GK-428: $^{13}$C NMR Spectrum
GK-428: LC/MS Spectrum

GK-428: Mass Spectrum
GK-428 : High Resolution Mass Spectrum
2 - $^{13}$C NMR Spectrum
2 - LC/MS Spectrum

2 - Mass Spectrum
3 - $^1$H NMR Spectrum

3 - $^{13}$C NMR Spectrum
4 - $^1$H NMR Spectrum

4 - $^{13}$C NMR Spectrum
4 – LC/MS Spectrum

4 – Mass Spectrum
GK-414: $^1$H NMR Spectrum

GK-414: $^{13}$C NMR Spectrum
GK-414: LC/MS Spectrum

GK-414: Mass Spectrum
GK-414: High Resolution Mass Spectrum
GK-416: $^1$H NMR Spectrum

GK-416: $^{13}$C NMR Spectrum
GK-416: LC/MS Spectrum

GK-416: Mass Spectrum
GK-416 : High Resolution Mass Spectrum
GK-417: $^1$H NMR Spectrum

GK-416: $^{13}$C NMR Spectrum
GK-417: LC/MS Spectrum

GK-417: Mass Spectrum
GK-417: High Resolution Mass Spectrum
GK-418: $^1$H NMR Spectrum

GK-418: $^{13}$C NMR Spectrum
GK-418: LC/MS Spectrum

GK-418: Mass Spectrum
GK-418: High Resolution Mass Spectrum
GK-419: $^1$H NMR Spectrum

419 - $^{13}$C NMR Spectrum
GK-419: LC/MS Spectrum

GK-419: Mass Spectrum
GK-419 : High Resolution Mass Spectrum
GK-421: $^1$H NMR Spectrum

GK-421: $^{13}$C NMR Spectrum
GK-421: LC/MS Spectrum

GK-421: Mass Spectrum
GK-421 : High Resolution Mass Spectrum
GK-422: $^1$H NMR Spectrum

GK-422: $^{13}$C NMR Spectrum
GK-422 : LC/MS Spectrum

GK-422 : Mass Spectrum
GK-422: High Resolution Mass Spectrum
GK-423: $^1$H NMR Spectrum

GK-423: $^{13}$C NMR Spectrum
GK-423 : High Resolution Mass Spectrum
GK-424: $^1$H NMR Spectrum

GK-424: $^{13}$C NMR Spectrum
GK-424: LC/MS Spectrum

GK-424: Mass Spectrum
GK-424 : High Resolution Mass Spectrum
GK-425: $^1$H NMR Spectrum

GK-425: $^{13}$C NMR Spectrum
GK-425: LC/MS Spectrum

GK-425: Mass Spectrum
GK-425: High Resolution Mass Spectrum
GK-426: $^1$H NMR Spectrum

GK-426: $^{13}$C NMR Spectrum
GK-426: LC/MS Spectrum

GK-426: Mass Spectrum
GK-426 : High Resolution Mass Spectrum
GK-427: $^1$H NMR Spectrum

GK-427: $^{13}$C NMR Spectrum
GK-427 : LC/MS Spectrum

GK-427 : Mass Spectrum
GK-427 : High Resolution Mass Spectrum
GK-430 : $^1$H NMR Spectrum

GK-430 : $^{13}$C NMR Spectrum
GK-430 : LC/MS Spectrum

GK-430 : ass Spectrum
GK-430: High Resolution Mass Spectrum