

Supporting Informations.

Life-Threatening Cardiogenic Shock Related to Venlafaxine Poisoning—A Case Report with Metabolomic Approach

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Figure S1. Total ion chromatogram of QC 1/1 in (A) positive and (B) negative ion mode.

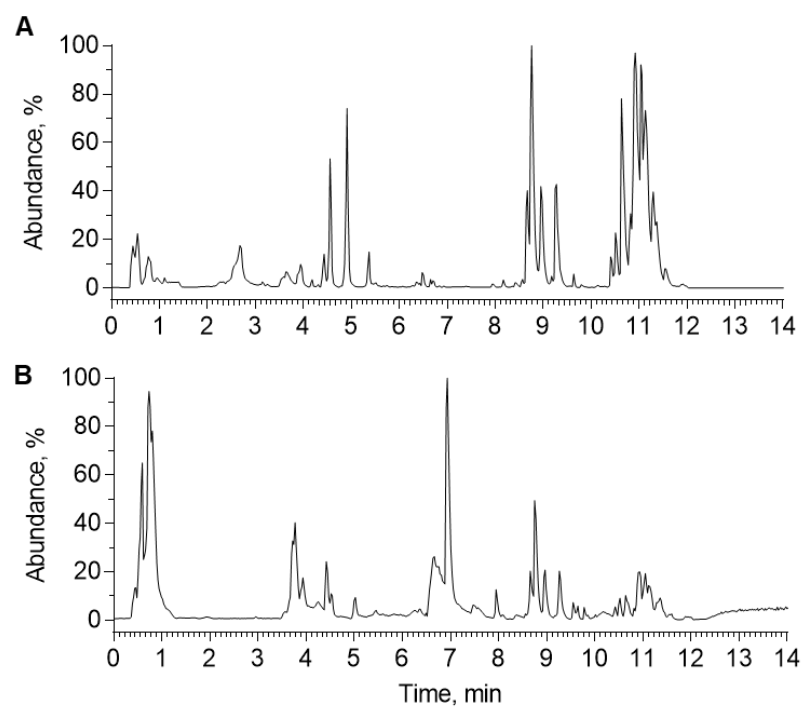


Figure S2. Proposed fragmentation patterns of venlafaxine based on the inspection of the MS/MS spectra obtained through the analysis of the commercial standard.

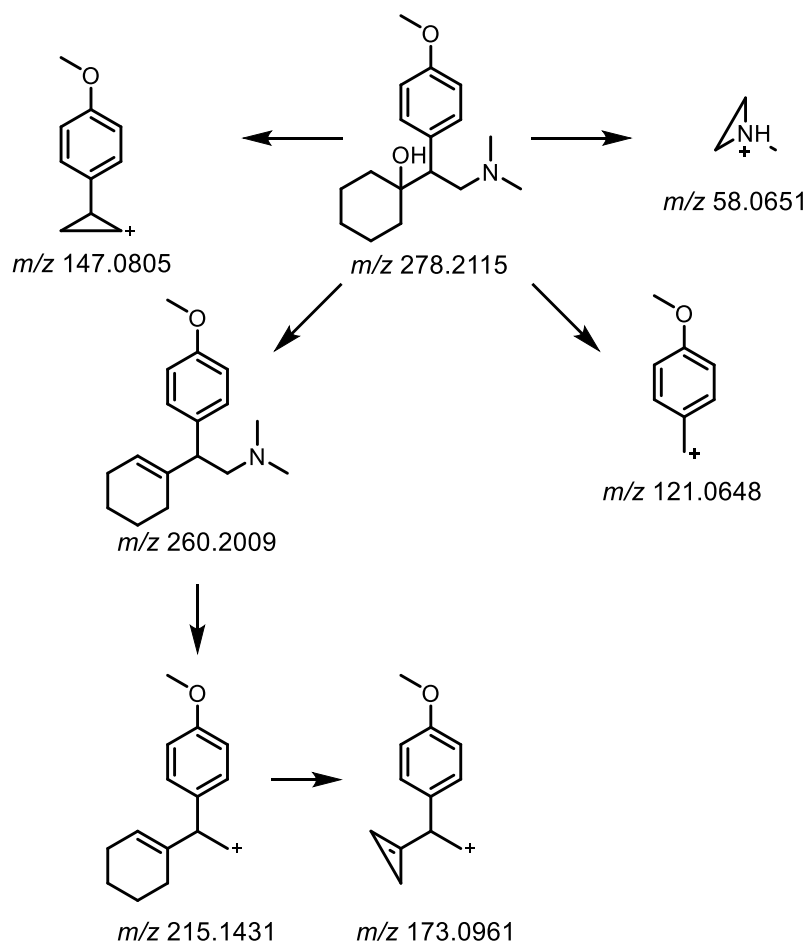


Figure S3. Isomers of hydroxylated venlafaxine metabolites. Extracted ion chromatogram at m/z 294.2064 corresponding to the [M+H]⁺ ion of hydroxyl venlafaxine.

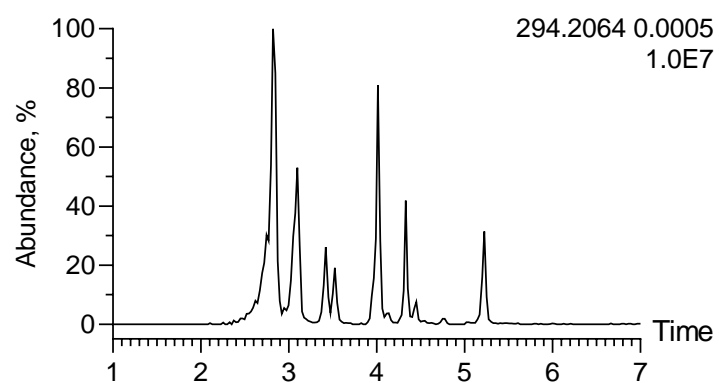


Figure S4. Metabolic network of venlafaxine and its phase I and II metabolites.

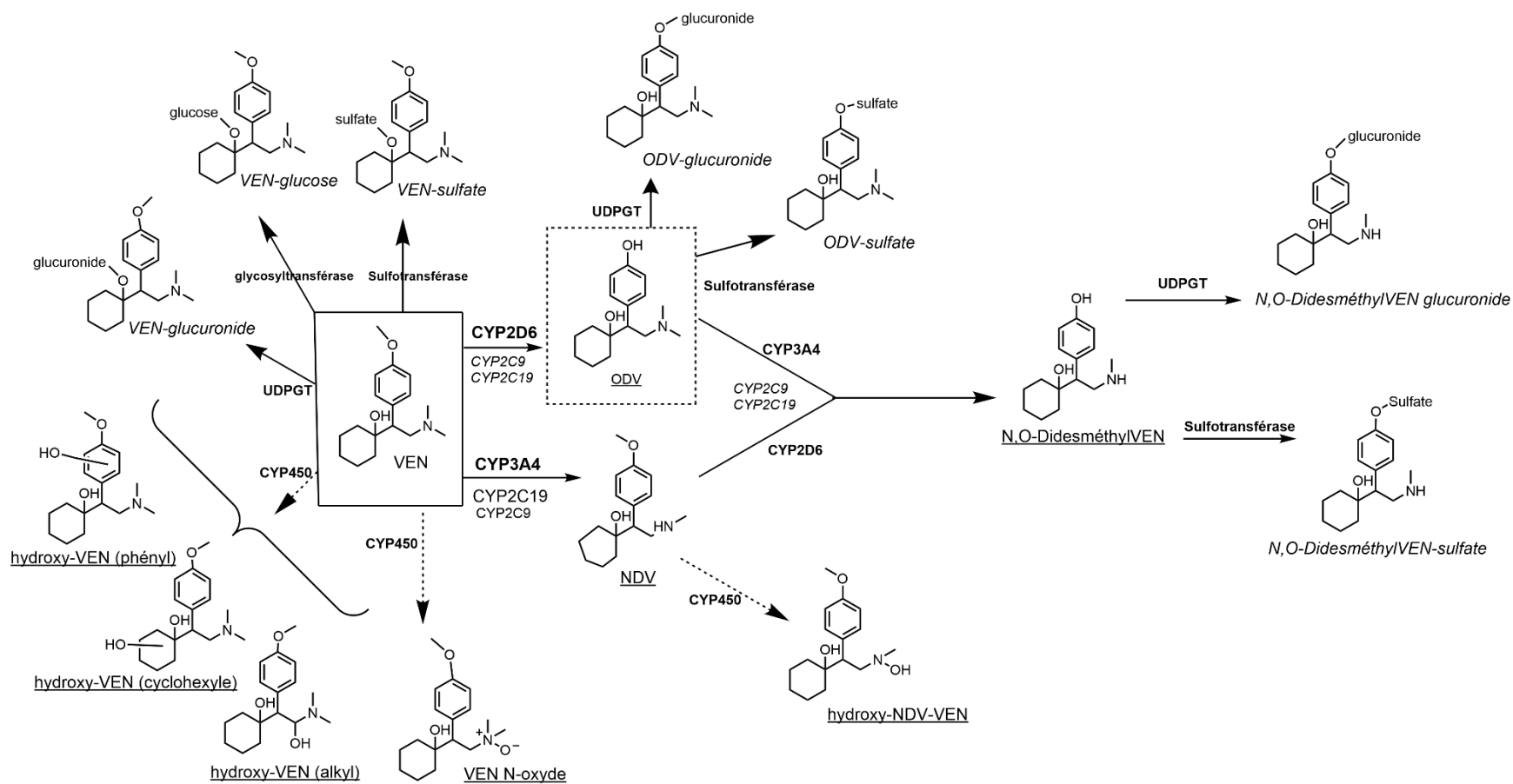


Table S1. Analytical features of venlafaxine and its annotated metabolites.

| Name | t _R | Precursor ion <i>m/z</i> | Formula | Product ions <i>m/z</i> |
|---|----------------|-----------------------------|---|---|
| Venlafaxine | 4.90 | 278.2115 | C ₁₇ H ₂₇ NO ₂ | 58.0660, 121.0649, 173.0962, 215.1431, 260.2009 |
| O-desmethyl-venlafaxine | 3.96 | 264.1958 | C ₁₆ H ₂₅ NO ₂ | 58.0661, 84.0452, 107.0496, 133.0651, 159.0805, 201.1277, 246.1850 |
| N-desmethyl-venlafaxine | 4.87 | 264.1958 | C ₁₆ H ₂₅ NO ₂ | 121.0651, 147.0806, 173.0963, 215.1432, 246.1854 |
| N,O-Didesmethyl-Venlafaxine | 3.9 | 250.1801 | C ₁₅ H ₂₃ NO ₂ | 107.0496, 133.0649, 159.0804, 201.1267, 232.1690 |
| N,N,O-tridesmethyl-Venlafaxine | 3.8 | 236.1645 | C ₁₄ H ₂₁ NO ₂ | 107.0497, 133.0651, 159.0808, 201.1271, 232.1694 |
| Venlafaxine N-Oxide | 5.22 | 294.2062 | C ₁₇ H ₂₇ NO ₃ | 58.0660, 121.0651, 215.1440 |
| OH-Venlafaxine - Alkyl | 4.01 | 294.2064 | C ₁₇ H ₂₇ NO ₃ | 58.0661, 121.0652, 171.0806, 213.1271, 276.1962 |
| OH-Venlafaxine -Cyclohexyl | 2.84 | 294.2062 | C ₁₇ H ₂₇ NO ₃ | 58.0661, 121.0650, 171.0805, 213.1278, 276.1962 |
| OH-Venlafaxine - Phenyl | 4.33 | 294.2063 | C ₁₇ H ₂₇ NO ₃ | 58.0661, 107.0862, 137.0599, 199.1118, 278.1953 |
| O-Desmethyl-Venlafaxine-N-Oxide | 4.25 | 280.1906 | C ₁₆ H ₂₅ NO ₃ | 107.0496 |
| N-Desmethyl-Hydroxy-Venlafaxine | 2.92 | 280.1906 | C ₁₆ H ₂₅ NO ₃ | 84.0451, 121.0651, 171.0799, 262.1804 |
| Venlafaxine Hexose | 4.91 | 440.2639 | C ₂₃ H ₃₇ NO ₇ | 58.0661, 121.0651, 147.0805, 173.0957, 260.2007, 278.2114 |
| Venlafaxine Glucuronide | 5.02 | 454.2431 | C ₂₃ H ₃₅ NO ₈ | 58.0661, 121.0651, 135.0805, 147.0806, 173.0957, 215.1432, 260.2006, 278.2112 |
| O-desmethyl-Venlafaxine-Glucuronide | 3.25 | 440.2275 | C ₂₂ H ₃₃ NO ₈ | 58.0660, 107.0496, 133.0649, 173.0966, 201.1273, 246.1847, 264.1951 |
| O-desmethyl Venlafaxine-sulfate | 4.23 | 344.1536 | C ₁₆ H ₂₅ NO ₅ S | 58.0661, 107.0496, 133.0651, 159.0805, 192.1019, 206.1179, 246.1851 |
| N,O-Didesmethyl-Venlafaxine-Glucuronide | 3.17 | 426.2118 | C ₂₁ H ₃₁ NO ₈ | 137.0598, 151.0755, 178.0863, 192.1020 |
| N,O-Didesmethyl-Venlafaxine-Sulfate | 4.2 | 328.1228 | C ₁₅ H ₂₃ NO ₅ S | 137.0597, 151.0757, 178.0865, 192.1025 |