

# Salt or/and Cocrystal? The Case of the Antidepressant Drug

## Venlafaxine

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Table S1 The salt-bond and hydrogen-bond geometry (in Å and deg)

|             | D—H...A                                               | d(D...A)(Å) | ∠(DHA)(deg) | symmetry code        |
|-------------|-------------------------------------------------------|-------------|-------------|----------------------|
| VLF–DA(1:1) | N <sub>1</sub> –H <sub>1</sub> ...O <sub>2</sub>      | 3.101       | 122.02      |                      |
|             | N <sub>1</sub> –H <sub>1</sub> ...O <sub>3</sub>      | 3.376       | 141.23      | [ -x, -y+1, -z+1 ]   |
|             | N <sub>1</sub> –H <sub>1</sub> ...O <sub>4</sub>      | 2.794       | 142.78      | [ -x, -y+1, -z+1 ]   |
|             | O <sub>2</sub> –H <sub>2A</sub> ...O <sub>3</sub>     | 2.774       | 163.60      | [ -x, -y+1, -z+1 ]   |
| VLF–DA(1:2) | N <sub>1b</sub> –H <sub>1b</sub> ...O <sub>9b</sub>   | 2.668       | 155.39      | [ -x+1, -y+1, -z+1 ] |
|             | O <sub>2b</sub> –H <sub>2Ab</sub> ...O <sub>10b</sub> | 2.932       | 159.18      |                      |
|             | O <sub>4b</sub> –H <sub>4Ab</sub> ...O <sub>10b</sub> | 2.527       | 154.17      | [ -x+1, -y+1, -z ]   |

Table S2 The main powder XRD peaks of VLF–DA (1:1) salt, VLF–DA (1:2) salt cocrystal and the raw materials.

| No. | samples                    | PXRD peaks                                                                                           |
|-----|----------------------------|------------------------------------------------------------------------------------------------------|
| 1   | VLF                        | 8.18°, 11.18°, 16.98°, 23.85°, 26.22°                                                                |
| 2   | DA                         | 19.42°, 21.24°, 22.92°, 23.44°, 24.78°, 29.56°, 32.44°                                               |
| 3   | VLF–DA(1:1) salt           | 7.18°, 7.42°, 12.36°, 13.58°, 14.42°, 15.46°, 17.42°, 17.98°, 19.72°, 22.00°, 26.72°, 27.54°, 30.32° |
| 4   | VLF–DA(1:2) salt cocrystal | 13.66°, 14.66°, 15.10°, 17.20°, 17.94°, 20.16°, 21.58°, 22.74°, 26.50°, 27.30°                       |

Figure S1 TG patterns of VLF–DA (1:1) salt and VLF–DA (1:2) salt cocrystal

