**"Eco-friendly Multivariate Curve Resolution-Alternating Least Squares and Chromatographic Quantifications of Some Veterinary Drug Residues in Pharmaceutical Industrial Wastewater"**

# Electronic Supporting Information (ESI)

## List of tables

**Table. S1: The concentration matrix used for preparation of the calibration model and validation set of IVM, RFX and SDD.**

| Mixture no. | Calibration model (µg/mL) | | | Validation set (µg/mL) | | |
|---|---|---|---|---|---|---|
| | IVM | RFX | SDD | IVM | RFX | SDD |
| **1** | 5 | 5 | 5 | 4 | 2 | 2 |
| **2** | 1 | 9 | 1 | 8 | 4 | 6 |
| **3** | 9 | 1 | 1 | 6 | 6 | 8 |
| **4** | 3 | 9 | 9 | 2 | 8 | 2 |
| **5** | 9 | 5 | 3 | 4 | 2 | 4 |
| **6** | 5 | 3 | 9 | 6 | 6 | 4 |
| **7** | 3 | 1 | 5 | 4 | 4 | 6 |
| **8** | 3 | 7 | 3 | 2 | 8 | 6 |
| **9** | 7 | 5 | 3 | 8 | 6 | 8 |
| **10** | 9 | 9 | 7 | 6 | 2 | 2 |
| **11** | 7 | 3 | 9 | 2 | 2 | 2 |
| **12** | 5 | 3 | 7 | 4 | 4 | 4 |
| **13** | 3 | 7 | 5 | 6 | 6 | 6 |
| **14** | 5 | 7 | 9 | 8 | 8 | 8 |
| **15** | 9 | 3 | 7 | 8.5 | 8.5 | 8.5 |
| **16** | 3 | 3 | 1 | | | |
| **17** | 1 | 1 | 3 | | | |
| **18** | 5 | 7 | 9 | | | |
| **19** | 3 | 1 | 1 | | | |
| **20** | 1 | 5 | 9 | | | |

**Table. S2: System suitability parameters for the proposed TLC-densitometry and HPLC methods.**

| Parameters | TLC-densitometry | | | Reference value [52] | HPLC | | |
|---|---|---|---|---|---|---|---|
| | IVM | RFX | SDD | | IVM | RFX | SDD |
| $t_R$ (min) | ----- | ----- | ----- | ----- | 6.7 ± 0.3 | 2.6 ± 0.2 | 3.7 ± 0.1 |
| $R_f$ value | 0.73 ±0.03 | 0.28 ±0.02 | 0.58 ±0.04 | ----- | ----- | ----- | ----- |
| Resolution ($R_s$) [a] | 6 | ----- | 3.73 | $R_s > 1.5$ | 43.04 | ----- | 15.19 |
| Tailing factor (T) | 1 | 1.09 | 1 | $T < 2$ | 1.09 | 1 | 1 |
| Capacity factor (K) | ----- | ----- | ----- | 1-10 acceptable | 5.17 | 1.37 | 2.40 |
| Selectivity factor (α) [a] | 2.5 | ----- | 2 | $\alpha > 1$ | 3.76 | ----- | 1.75 |
| No. of theoretical plates (N) | ----- | ----- | ----- | $N \geq 2000$ | 54492.56 | 18048.43 | 43743.40 |
| HETP (mm) | ----- | ----- | ----- | The smaller the value, the higher the column efficiency | $4 \times 10^{-3}$ | $13 \times 10^{-3}$ | $4 \times 10^{-3}$ |

[a] The parameters were calculated using RFX as reference

**Table. S3: Analysis of real spiked wastewater samples (spiked with 5 µg/mL of studied drugs standards) by using the proposed methods.**

| Samples [a] | MCR-ALS | | | | | | TLC-densitometry | | | | | | HPLC | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | IVM | | RFX | | SDD | | IVM | | RFX | | SDD | | IVM | | RFX | | SDD | |
| | T.C [b] | D.R [c] | T.C [b] | D.R [c] | T.C [b] | D.R [c] | T.C [b] | D.R [c] | T.C [b] | D.R [c] | T.C [b] | D.R [c] | T.C [b] | D.R [c] | T.C [b] | D.R [c] | T.C [b] | D.R [c] |
| W.W 1 | 11.07 | 6.07 | 4.99 | ----- | 10.88 | 5.88 | 11.00 | 6.00 | 4.99 | ---- | 11.11 | 6.11 | 11.08 | 6.08 | 4.99 | ---- | 11.06 | 6.06 |
| W.W 2 | 10.05 | 5.05 | 4.96 | ----- | 10.16 | 5.16 | 10.00 | 5.00 | 5.04 | ---- | 10.28 | 5.28 | 10.01 | 5.01 | 4.92 | ---- | 10.27 | 5.27 |
| W.W 3 | 12.39 | 7.39 | 10.11 | 5.11 | 10.72 | 5.72 | 12.45 | 7.45 | 10.10 | 5.10 | 10.57 | 5.57 | 12.42 | 7.42 | 10.13 | 5.13 | 10.51 | 5.51 |
| W.W 4 | 9.13 | 4.13 | 11.19 | 6.19 | 4.99 | ----- | 9.07 | 4.07 | 11.10 | 6.10 | 4.998 | ---- | 9.14 | 4.14 | 11.13 | 6.13 | 5.00 | ---- |
| W.W 5 | 10.60 | 5.60 | 4.95 | ----- | 11.30 | 6.30 | 10.67 | 5.67 | 5.00 | ---- | 11.25 | 6.25 | 10.71 | 5.71 | 5.00 | ---- | 11.28 | 6.28 |

[a] Samples are calculated in µg/mL.

[b] Total drug concentration of the spiked sample in µg/mL.

[c] Drug residue in µg/mL after the subtraction of the added standard.

# List of figures

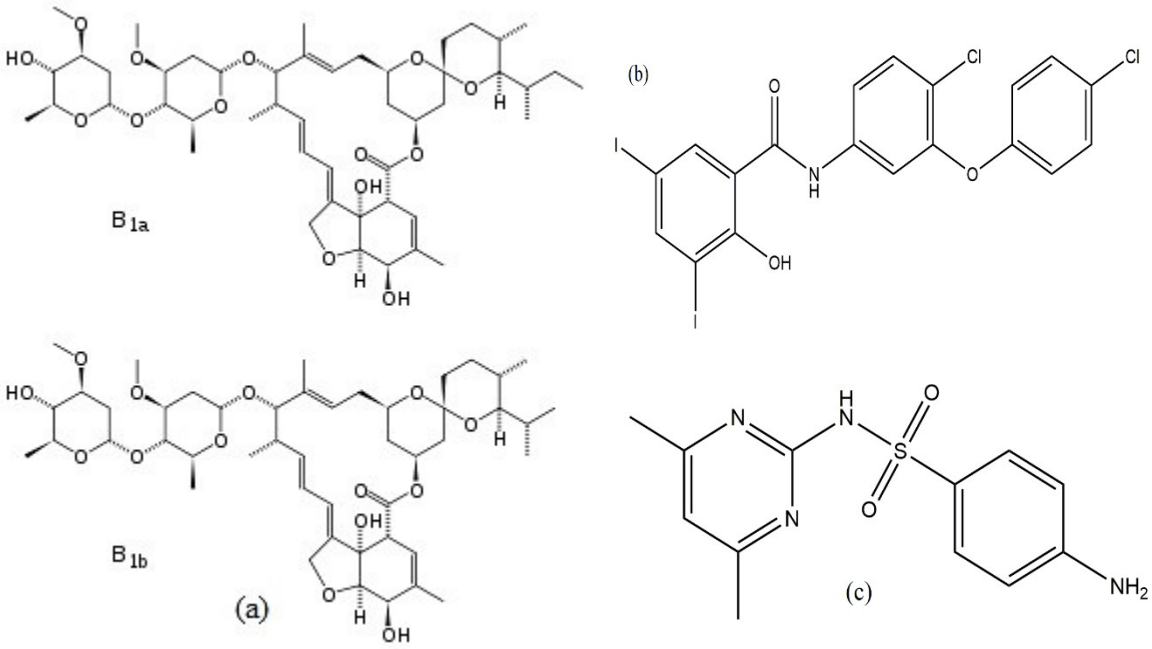


**Figure S1: Chemical structures of (a) IVM, (b) RFX, and (c) SDD**

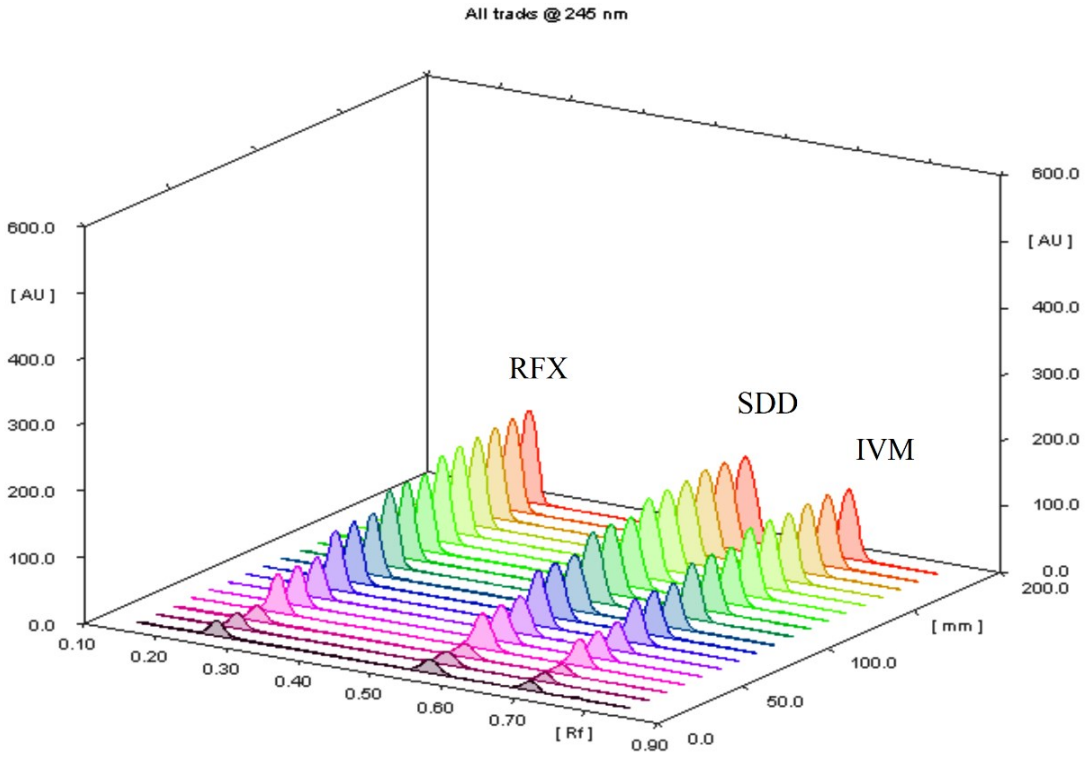


**Figure S2: 3D-TLC densitogram showing linearity range (0.1-1 µg/band) of IVM, RFX and SDD.**

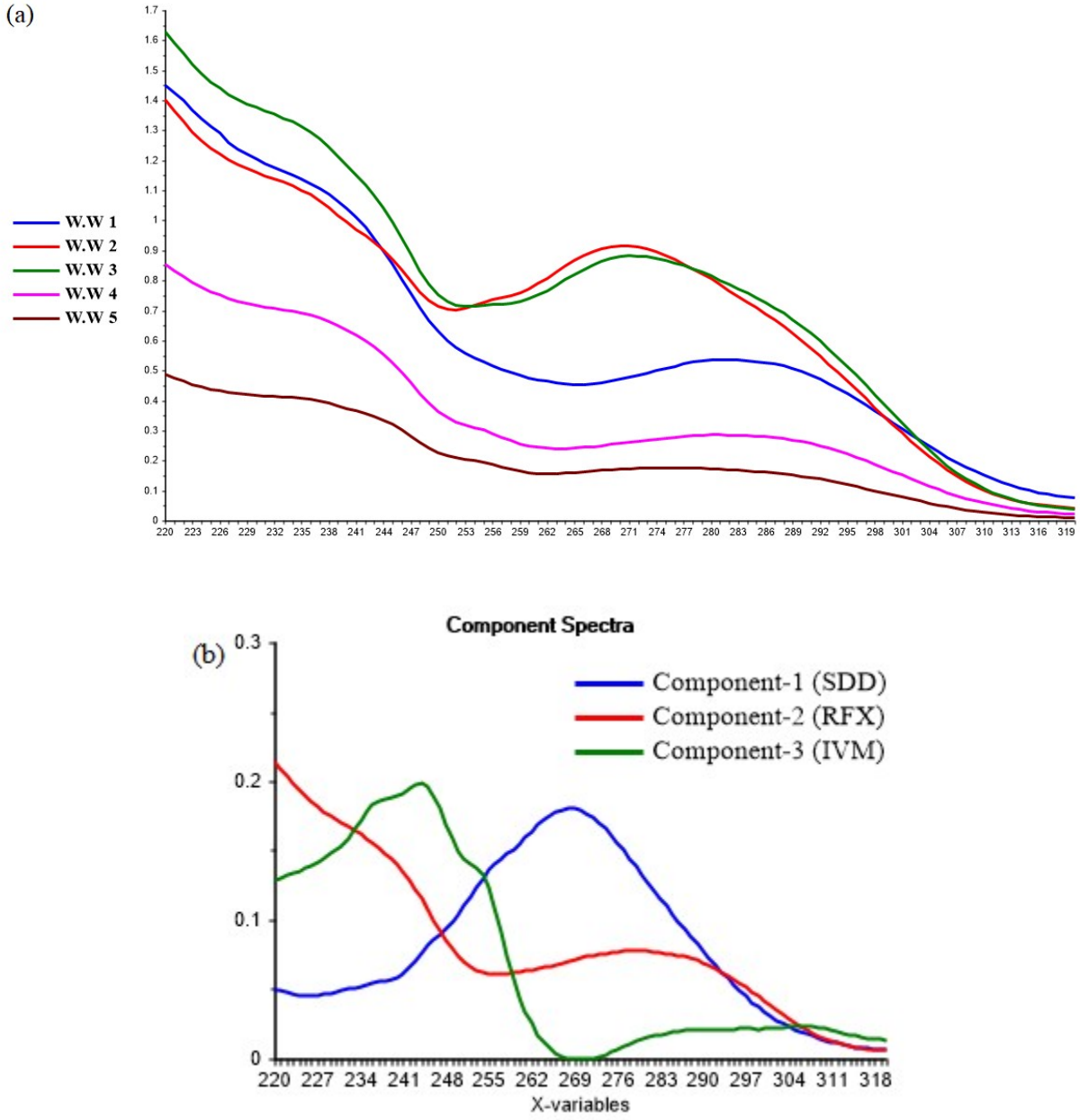


**Figure S3:**

**(a) UV spectra of real industrial wastewater samples after SPE.**

**(b) Resolved MCR-ALS pure spectra profiles of the target pharmaceuticals in wastewater samples.**