Predicting environmental concentrations of carbamazepine and oxcarbazepine and their main metabolites in a coastal system


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Predicted environmental concentrations of carbamazepine, oxcarbazepine and their main metabolites in a coastal system


Introduction
Pharmaceuticals are widely released in aquatic environment through treated wastewaters. They reach coastal zone indirectly via streams or directly through marine outfalls however data concerning this contamination in coastal waters are scarce.

Environmental Risk Assessment (ERA) of pharmaceuticals have been conducted mostly in surface waters and has not been performed in coastal zone. The first step of ERA is to evaluate the exposure through predictive environmental concentration (PEC) values.

The aim of this study was to predict the occurrence of some pharmaceuticals in a coastal area subjected to treated wastewater (TWW) reject through a marine outfall (Fig 2.). Among pharmaceuticals, Carbamazepine, Oxcarbazepine and their main metabolites (Fig 1.) were chosen. CBZ has been proposed as an indicator of wastewater contamination and has been already detected in Mediterranean (Munaron et al., 2011).

Prediction was performed based on local pharmaceuticals consumption recording and a review of pharmacokinetics data. PECs values were estimated in TWW and at the marine outfall and compared with MECs obtained by direct quantification and with POCS implementation.

Materials and methods

PEC
Medical care consumption data (g of CBZ and OxCBZ sales per month)
Pharmacokinetics data (% of excreted forms: parents compounds and metabolites)
% elimination in STEP, flux effluent

PEC effluent: Sales (g) * % excreted/ % elimination* flux effluent

PEC coastal zone: PEC/100 (TGD, 2003)

MEC
MEC effluents: 24h homogenate effluents sampling (n=8)
Filtration, SPE OASIS HLB, analysis LC-MS (Ledlercq et al., 2009)

MEC coastal zone: POCS implementation for one month near the submarine outfall (n=6)
Analysis as described by Munaron et al. (2011)

Results - Discussion

Table 1: Consumption data of CBZ and OxCBZ from January to June 2011

<table>
<thead>
<tr>
<th></th>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>CBZ</td>
<td>10427</td>
<td>9554</td>
<td>11914</td>
<td>9659</td>
<td>10047</td>
<td>10222</td>
</tr>
<tr>
<td>OxCBZ</td>
<td>2517.5</td>
<td>2240</td>
<td>2070</td>
<td>2242.5</td>
<td>3217.5</td>
<td>2572.5</td>
</tr>
</tbody>
</table>

Table 2: PEC in coastal zone (ng/L)

<table>
<thead>
<tr>
<th>Molecule</th>
<th>CBZ</th>
<th>OxCBZ</th>
<th>10-OHCbz</th>
<th>10427.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>CBZ</td>
<td>2.7.7</td>
<td>0.9.2</td>
<td>3.3.4</td>
<td>10.5.17</td>
</tr>
<tr>
<td>OxCBZ</td>
<td>0.6.4</td>
<td>0.1.6</td>
<td>nd</td>
<td>0.2.2</td>
</tr>
<tr>
<td>10-OHCbz</td>
<td>0.2.2</td>
<td>0.2.2</td>
<td>nd</td>
<td>0.2.2</td>
</tr>
</tbody>
</table>

Table 3: concentrations in POCS in ng/g of sorbent

<table>
<thead>
<tr>
<th>Molecule</th>
<th>POCS Sorbent</th>
<th>CBZ</th>
<th>OxCBZ</th>
<th>10-OHCbz</th>
</tr>
</thead>
<tbody>
<tr>
<td>CBZ</td>
<td>0.6.4</td>
<td>1.6</td>
<td>nd</td>
<td>0.2.2</td>
</tr>
<tr>
<td>OxCBZ</td>
<td>0.2.2</td>
<td>2.2</td>
<td>nd</td>
<td>0.2.2</td>
</tr>
</tbody>
</table>

Cbez and OxCBz are excreted as parent compounds or metabolites, free or conjugated as glucuronides (Fig 4)

Cbez and OxCBz are stable from January to June (Fig 3)

Conclusion

Further studies have to be performed for PEC estimation in coastal area including a hydrodynamic numeric model, which take into account diffusion, advection in seawater.

References


Acknowledgments

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