Table TS1. Properties or variables of the homologous series of chloromethyl-ketone derivatives with an acetyl group at R₁ and a chloromethyl group at R₃ taken from ChEMBL database.

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<th>Cmpn.</th>
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<th>Qed weighted</th>
<th>acd logp</th>
<th>Lipinski Ro5 vltns.</th>
<th>rtb</th>
<th>Heavy atoms</th>
<th>Density [g/cm³]</th>
<th>Boiling point [°C] at 760mmHg</th>
<th>Enthalpy of vaporization [kJ/mol]</th>
<th>ACD/LogD (pH 7.4)</th>
<th>ACD/LogP (pH 7.4)</th>
<th>ACD/KOC (pH 7.4)</th>
<th>Polarizabilit[10⁻²² cm³]</th>
<th>Surface tension [dyne/cm]</th>
<th>Molar volume [cm³]</th>
<th>No. of C in R₂</th>
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Cmpn.: compound (boldface) and Chemical Abstract Service (CAS) number.

hba Lipinski = 3 in all cases.

hbd Lipinski = 1 in all cases.

Polar surface area = 71.00Å² in all cases.

psa = 46.17Å² in all cases.