The third filter (**MCF-3**) evaluates physico-chemical parameters of compounds and classifies them in accordance with Lipinski's "rule of 5" (LR5) of drug-likeness and Veber's "rule of 2" (VR2). However, this filter is not universal as the rules tend to reflect a compound's likely bioavailability rather than efficacy. For example, it should be noted that the majority of anti-infective or oncolytic drugs do not conform to either LR5 or VR2. We recommend using human medicinal chemistry expertise to further analyze the compounds flagged with the MCF-3. Some examples:

Parameters/Criteria	Comments
H-bond donors: HBD ≤ 5	(LR5) HBD ≤ 5
H-bond acceptors: HBA ≤ 10	(LR5) HBA ≤ 10
Rotatable bonds: RB ≤ 10	(VR2) RB ≤ 10
ElogD ≤ 5, ElogD ≥-2	Special HPLC estimation of logD for new compounds
ClogP ≤ 5	(LR5) ClogP ≤ 5
Molecular weight: MW ≤ 600	(LR5) MW ≤ 500
HBD + HBA ≤ 12 or Polar surface area: PSA ≤ 140 Å^2	HBD + HBA ≤ 12 or (VR2) PSA ≤ 140 Å^2
Water solubility: SW ≥ - 4.5	Calculated with ChemoSoft software
Possibility of structural variation without MW increase	Structural lead-likeness
Possibility of water solubility optimization without HBD + HBA increase	Structural lead-likeness
Number of condensed rings ≤ 3	Structural lead-likeness
Two or more points of structural variation	Structural lead-likeness