



Variations of radius of gyration for the D130V-Eg5 backbone atoms upon binding to DHPMT derivatives, **b)** Variation of number of intramolecular H-bonds for D130V-Eg5 structure upon binding to DHPMT derivatives, **c)** variation of D130V-Eg5 SASA upon binding to DHPMT derivatives and **d)** variation of DHPMT SASA upon their binding to D130V-Eg5 structure; (R)-2/D130V-Eg5 (orange), (R)-4/D130V-Eg5 (black), (R)-5/D130V-Eg5 (yellow), (R)-5/L214I-Eg5 (violet) and (R)-5/R119L-Eg5 (green), monastrol/D130V (blue), monastrol/L214I (brown) and monastrol/R119L (red)