

Electronic Supplementary Information

Functionalization of protein hexahistidine tags by functional nanoreactors

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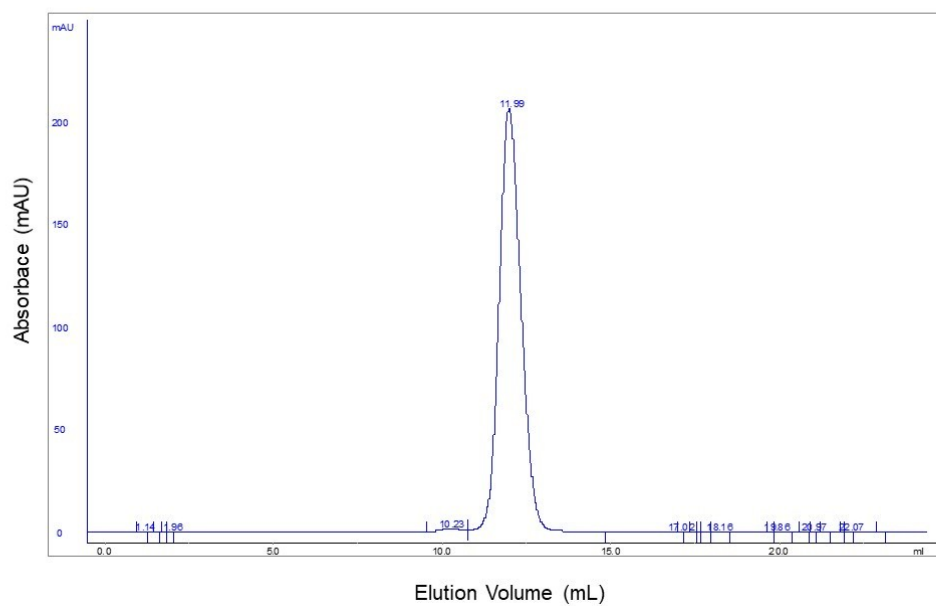
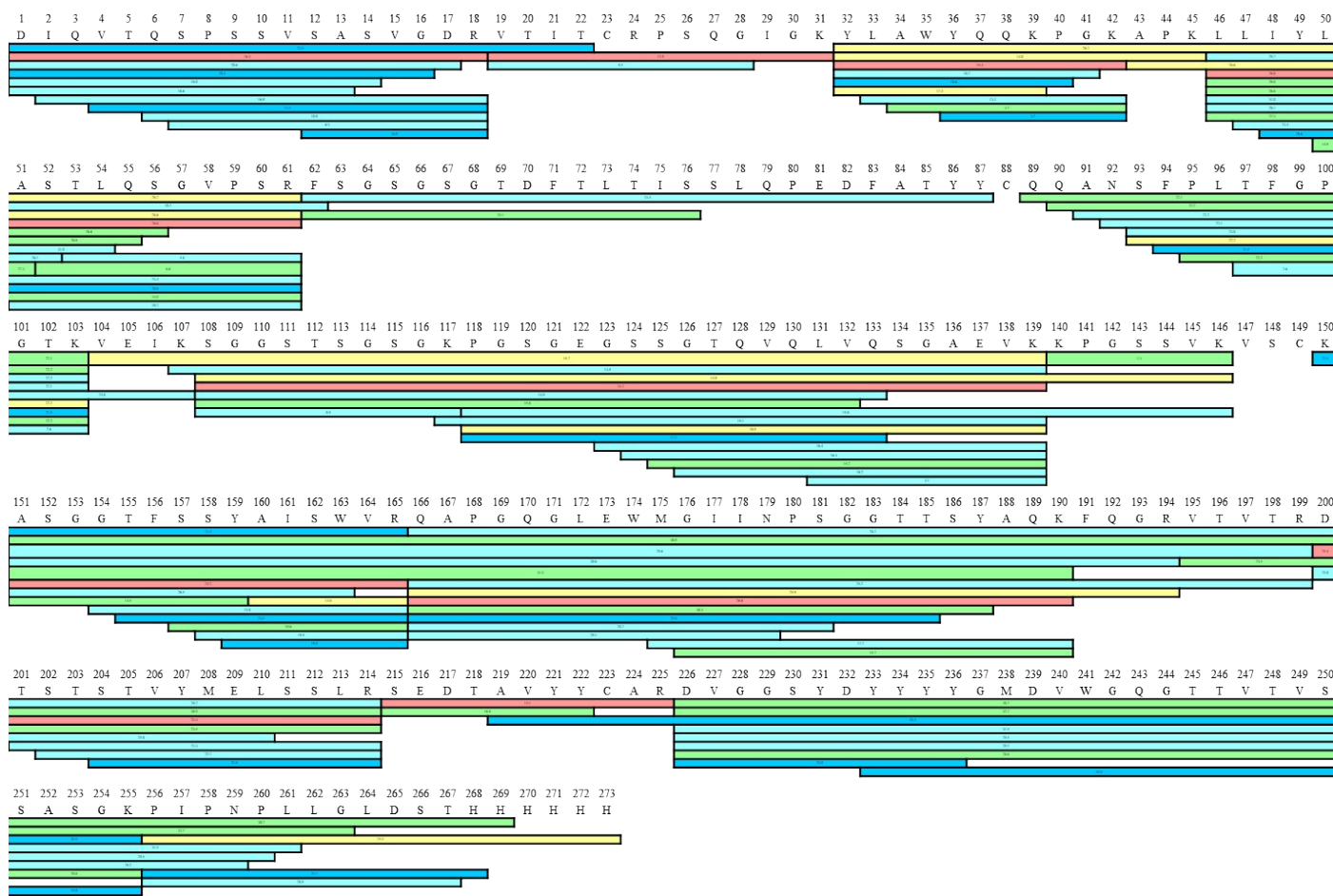


Figure ESI1. SEC profile (milli Absorbance Units, mAU at 280 nm plotted against Elution Volume, mL) of CRB0137. The scFv was diluted in PBS to a concentration of 1.25 mg/mL and loaded onto a Superdex 75 10/300 column (GE Healthcare) at a flow rate of 0.5 mL/min. CRB0137 Elution Volume is 11.99 mL. The monomer pool contained a residual aggregate level of 0.6%.



Color code for signal intensity

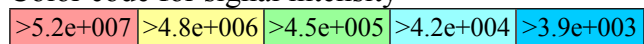
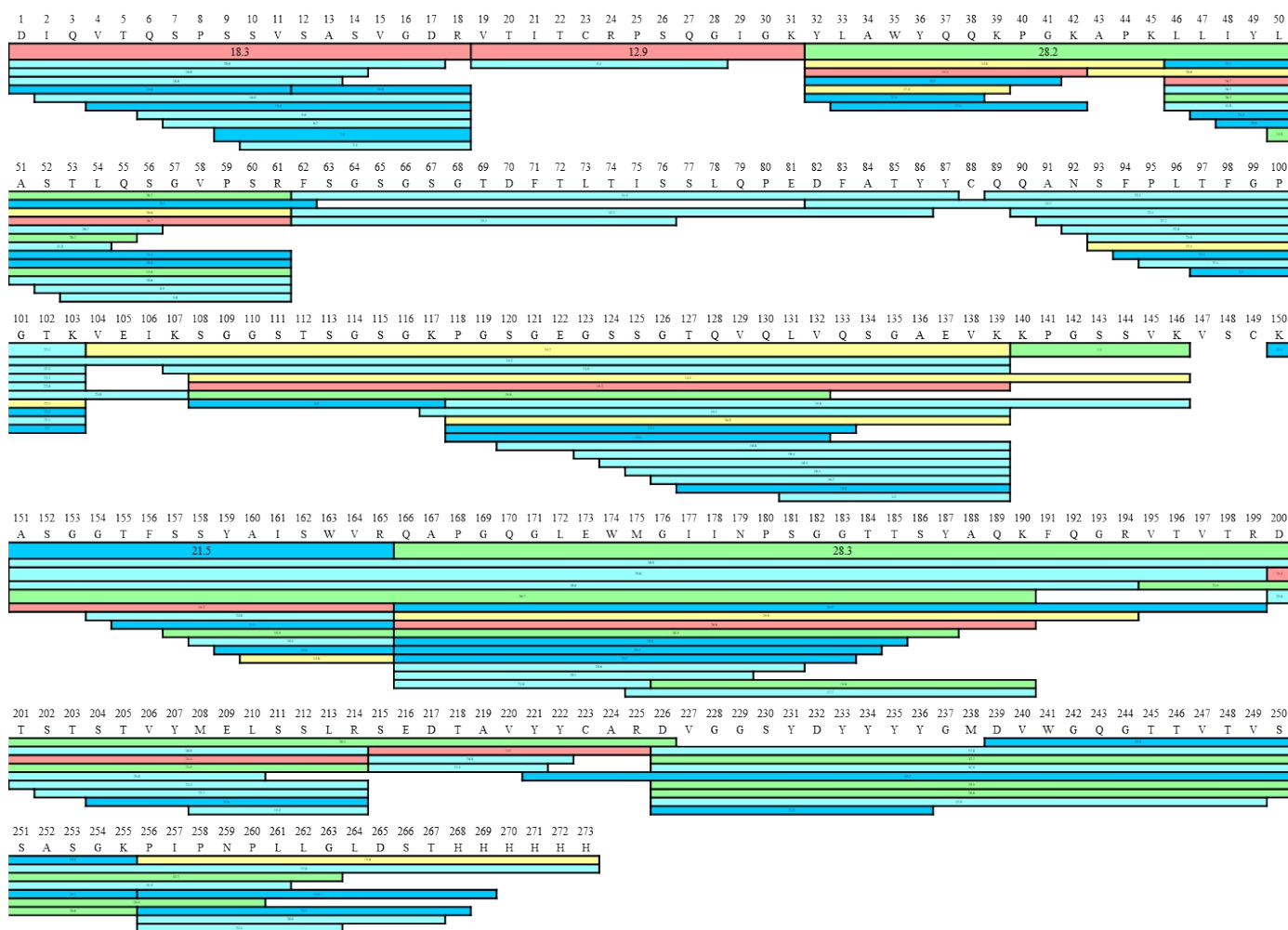


Figure ESI2. Sequence coverage map of CRB0137 digested with trypsin (98.5%), first experiment.



Color code for signal intensity

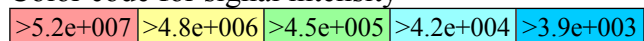


Figure ESI3. Sequence coverage map of CRB0137 digested with trypsin (98.9%), second experiment.

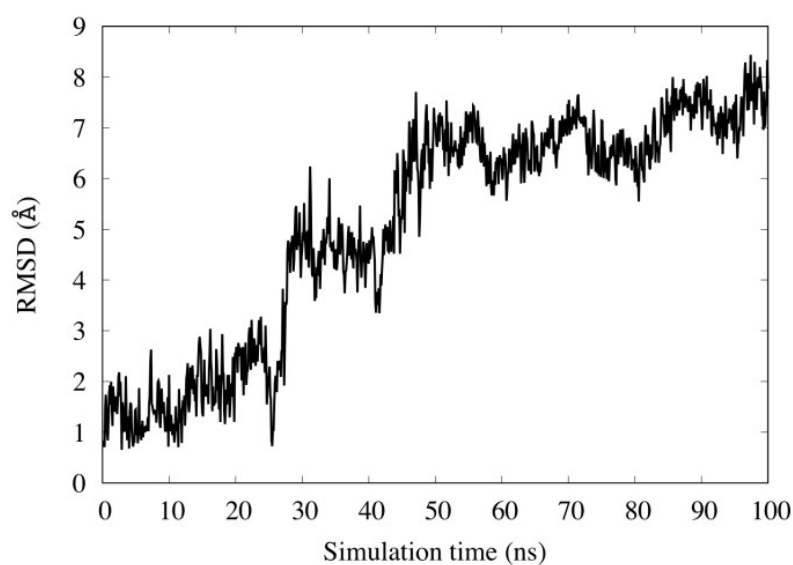


Figure ESI4. Root mean square deviations (rmsd) of the α -carbon positions of the terminal stretch of amino acids $^{259}\text{NPLLGLDSTHHHHH}^{273}$ during the dynamic run with respect to the initial positions.

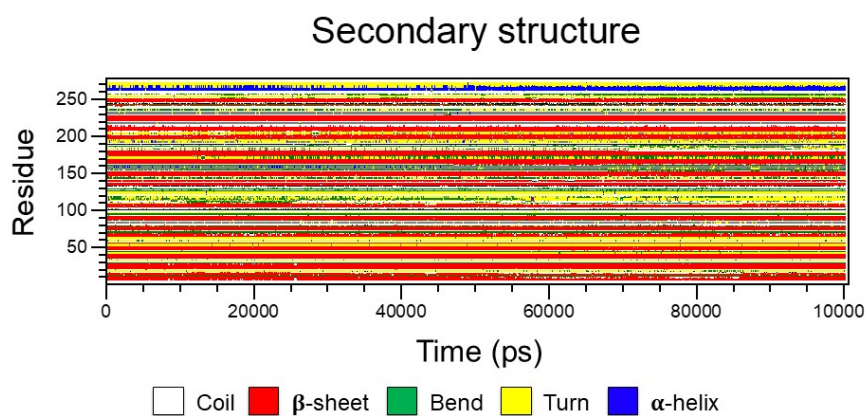


Figure ESI5. Evolution of the single-chain Fv antibody CRB0137 secondary structure during the 100 ns dynamics run.

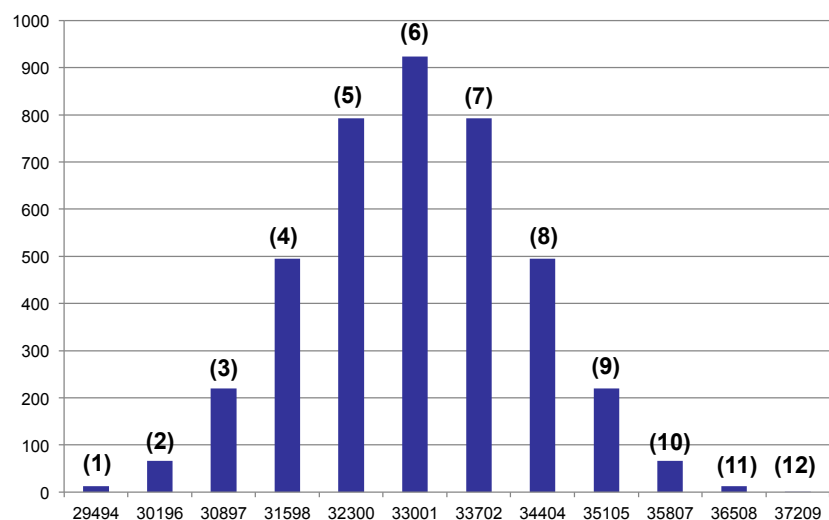


Figure ESI6. Simulated theoretical mass spectrum of the product of reaction between CRB0137 and MBHA derivative **3**. The value in parentheses is the number of naphthalene substituents (i. e. the grafting degree) for each CRB0137 molecule.

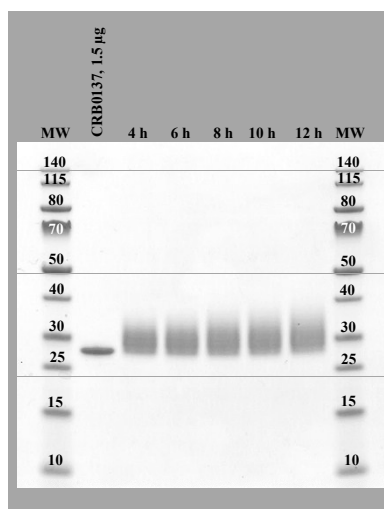
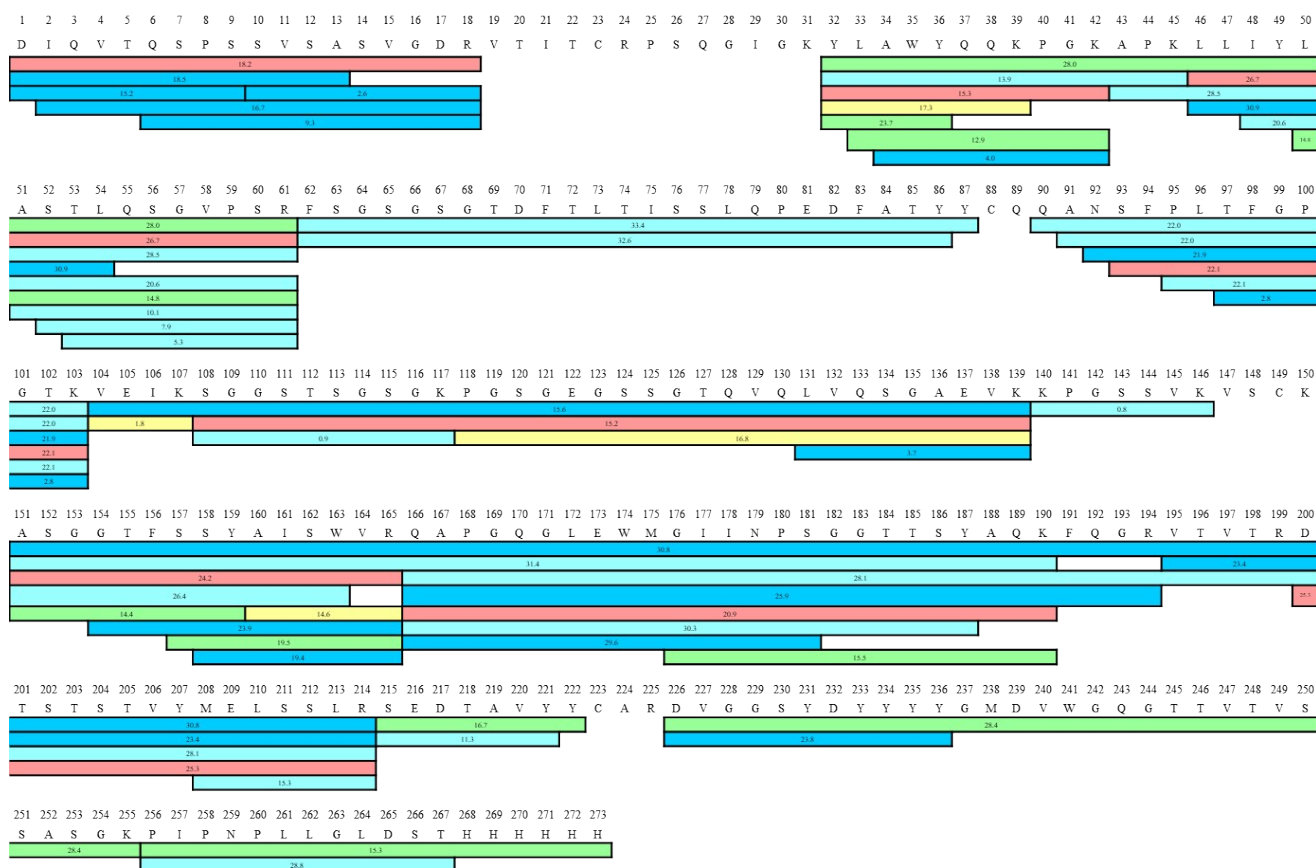


Figure ESI7. SDS-PAGE analysis of a kinetics experiment (reaction mixture after 4, 6, 8, 10, and 12 hours of reaction at 25 °C) compared with native CRB0137 molecule.



Color code for signal intensity

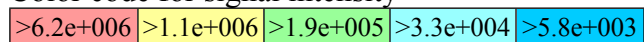
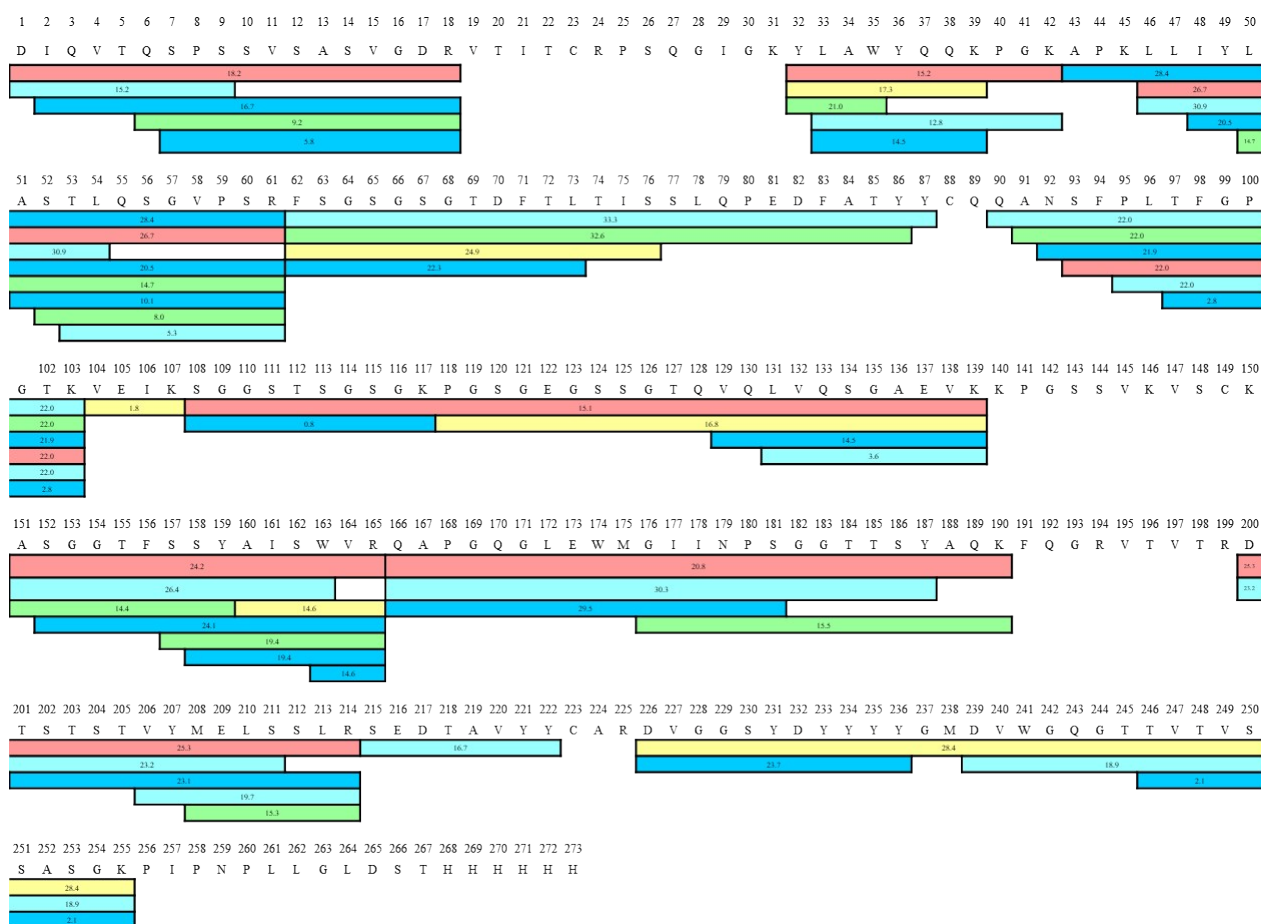


Figure ESI8. Sequence coverage map of the sample obtained after 8 h of reaction time digested with trypsin (91.9%).



Color code for signal intensity

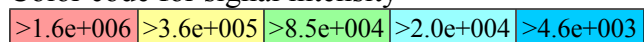


Figure ESI9. Sequence coverage map of the sample obtained after 12 h of reaction time digested with trypsin (79.5%).