

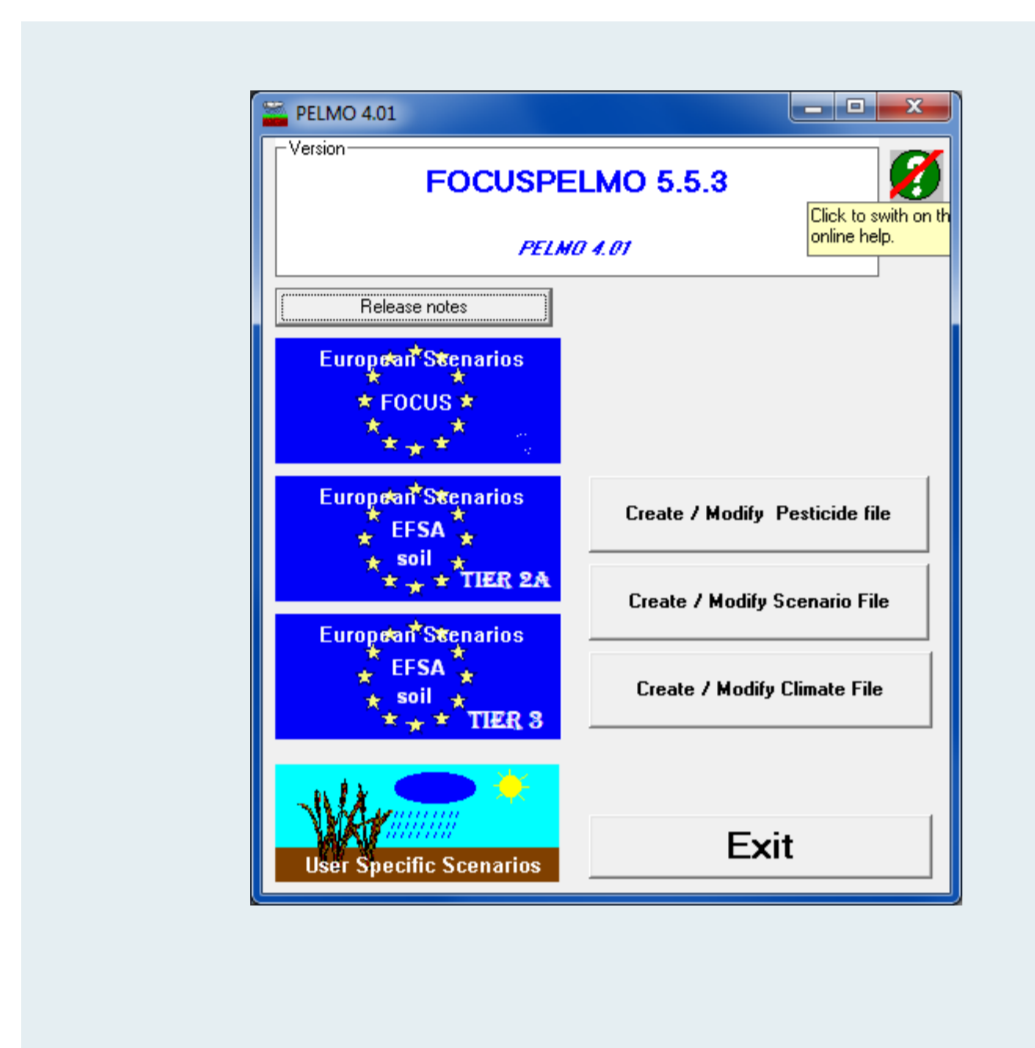
SorpKinAnalysis – Implementation of a two-site aged sorption model in accordance with EFSA PPR Panel (2018)

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The aim is to get input parameters for risk assessment

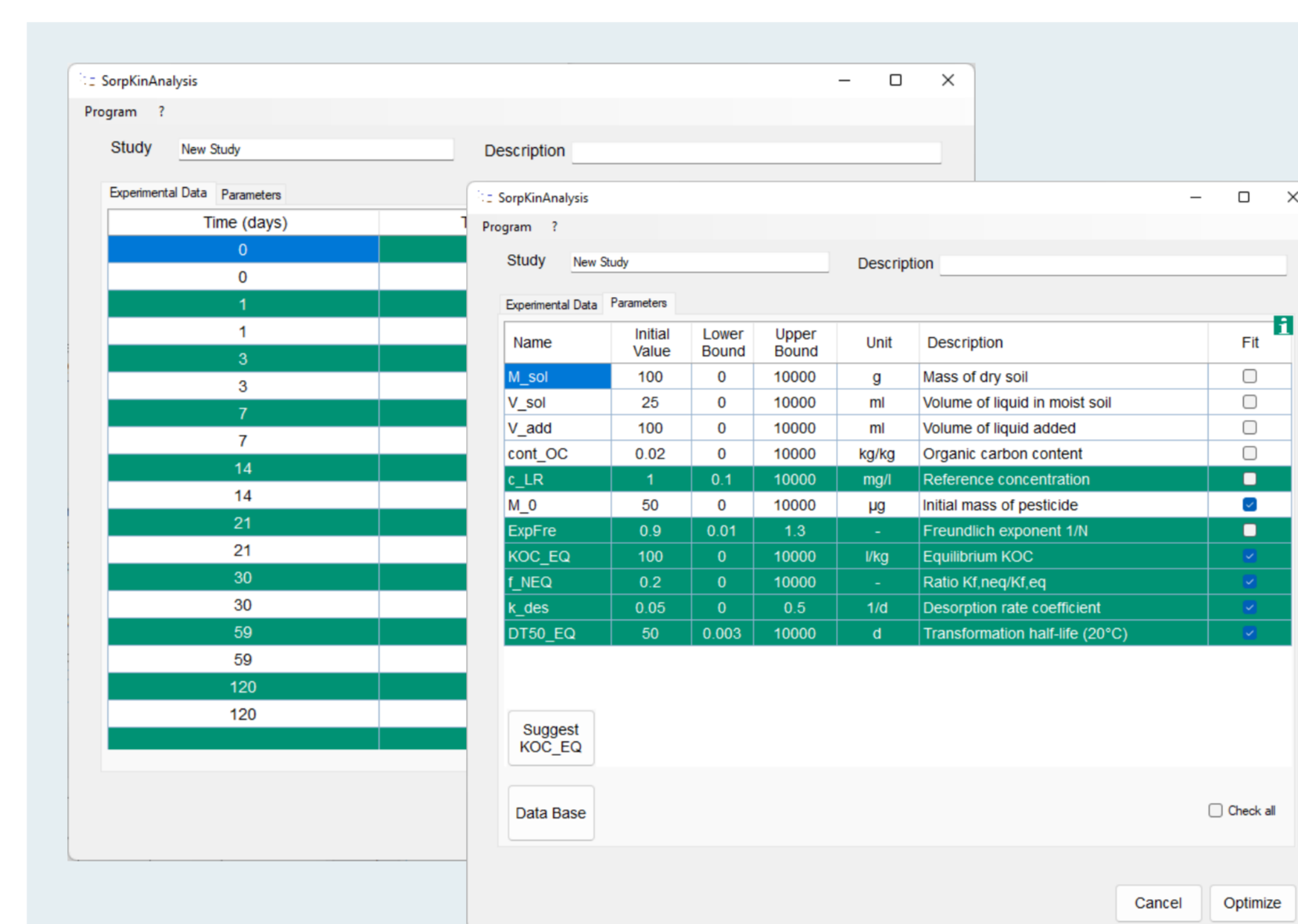
- Leaching assessments are sensitive to changes in aged sorption parameters
- Parameters can be used for higher tier calculations to get more realistic PEC_{GW} and PEC_{SW}



Form of the higher tier model PELMO

The input is experimental aged sorption study data

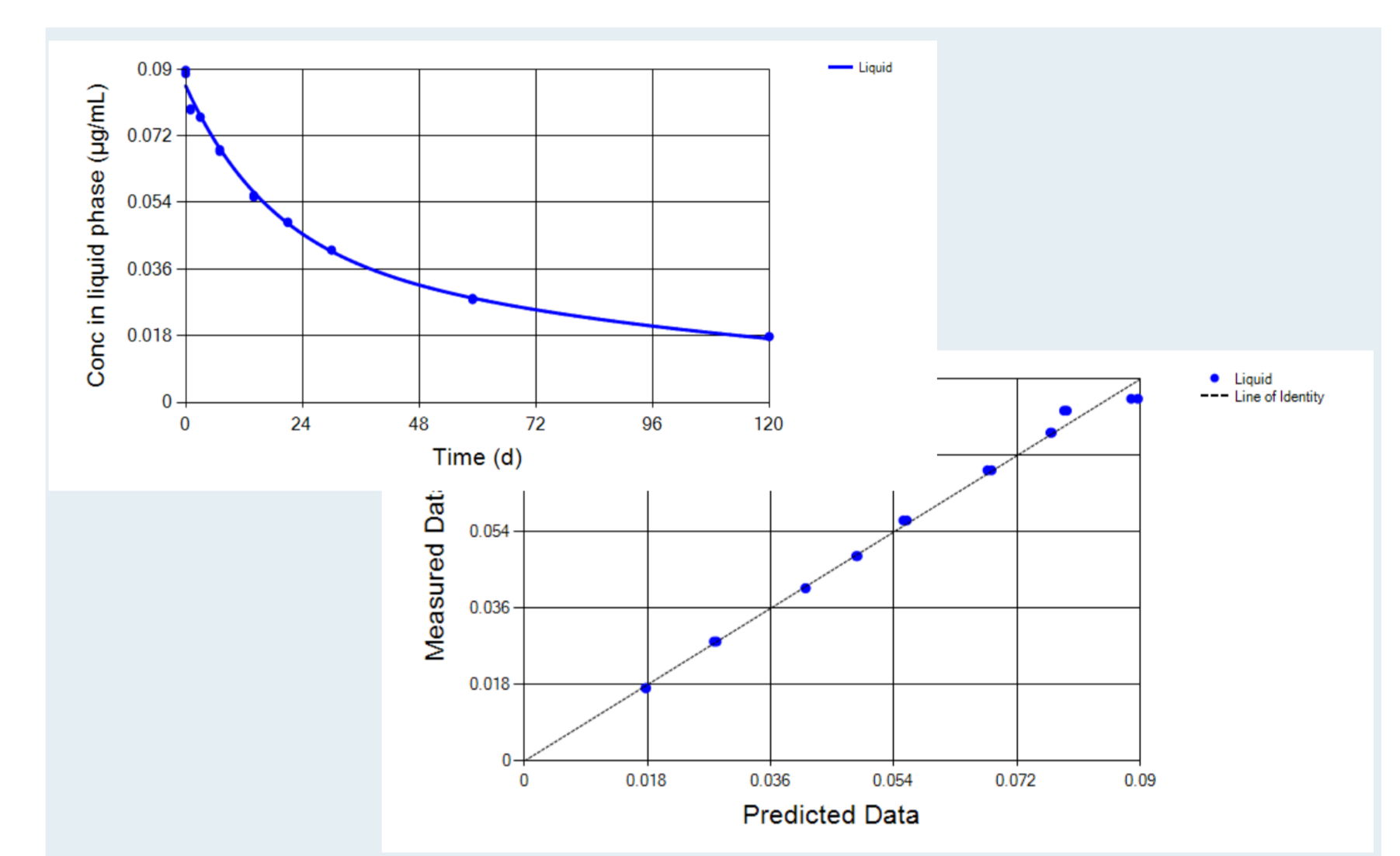
- Mass in soil (μg)
- Concentration in liquid phase ($\mu\text{g/mL}$)



Input forms of SorpKinAnalysis

The output is sorption parameter values with goodness of fit

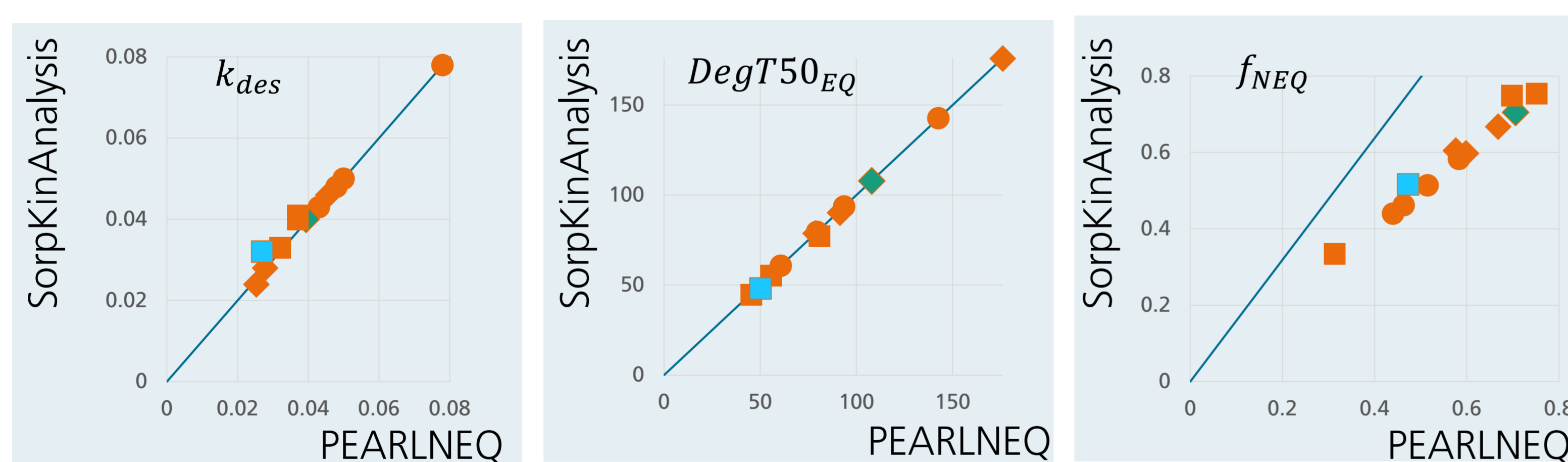
- Parameter values for
 - k_{des} Desorption rate
 - f_{NEQ} Ration non-equilibrium/ equilibrium
 - $DegT50_{EQ}$ Transformation half-life (20°C)
- Charts presenting the visual result



Visual result plots of SorpKinAnalysis

SorpKinAnalysis delivers similar results as PEARLNEQ

- Case study: Parameter values were compared using a ECPA data set with 3 substances, 4 soils each (EFSA PPR Panel 2018)
- χ^2 values of SorpKinAnalysis were similar to the values of PEARLNEQ
- Both models use different solver: Nelder-Mead-Simplex (SorpKinAnalysis) versus Gauss-Marquardt-Levenberg (PEARLNEQ)
- Different initial values may lead to slightly different results



● ECPA-01: rather stable, low sorption ; ◆ ECPA-06: rather stable, moderate sorption; ■ ECPA-07: high persistency, moderate sorption

Visual comparison of parameter values obtained by PEARLNEQ and SorpKinAnalysis

SorpKinAnalysis is a user-friendly alternative for sorption analysis

- SorpKinAnalysis is a user-friendly stand-alone software in accordance with EFSA PPR Panel (2018)
- SorpKinAnalysis gives comparable results as PEARLNEQ
- SorpKinAnalysis is able to obtain the additional input parameters needed for EU leaching simulations including aged sorption
- SorpKinAnalysis is freely available at software.ime.fraunhofer.de

A more detailed analysis of SorpKinAnalysis can be found in Fuchs (2019).

Statistical comparison of two specific data sets of PEARLNEQ and SorpKinAnalysis

	Most similar: ECPA-06 soil A		Least similar: ECPA-07 soil D	
	PEARLNEQ	SorpKinAnalysis	PEARLNEQ	SorpKinAnalysis
Model Error (χ^2)	2.93	2.67	3.41	3.15
Weighted ME (χ^2)	2.02	1.79	4.71	4.23

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