Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering.

Supplemental Material for:

Kinetics of Furfural Electrochemical Hydrogenation and Hydrogenolysis in Acidic Media on Copper

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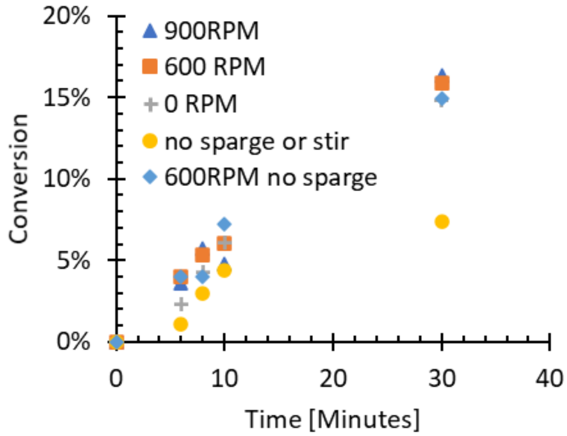

Figure S1. Impact of forced convection on the conversion of FF over 30 minutes. Conditions: 100 mM FF initial concentration, -0.560 V vs RHE, 25°C, 80:20 v:v DI water to acetonitrile with 0.5 M H_2SO_4.Unless indicated otherwise in the legend, experiments were run with 60 mL/min N_2 sparging in the catholyte.

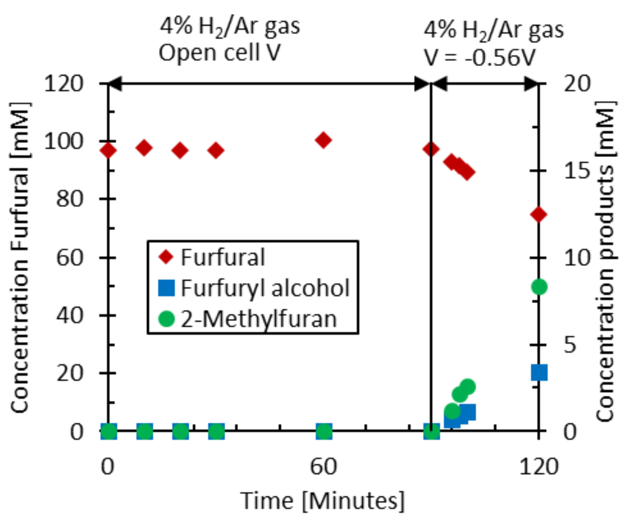

Figure S2. The concentration of FF, FA, and MF over 2 hours with sparging of 4%H_2/Ar at 60 mL/min. Applied potential of -560mV between 90 and 120 minutes. Conditions: 100 mM FF initial concentration, 25°C, 80:20 v:v DI water to acetonitrile with 0.5 M H_2SO_4.

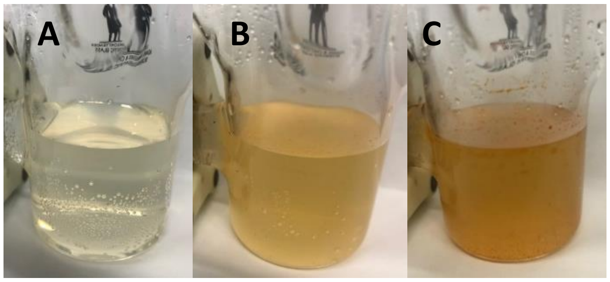

Figure S3. Electrolyte at difference temperatures (15 (A), 35 (B), 45 (C) °C) after 30 minutes electrolysis. Conditions: 100 mM FF initial concentration, -0.560 V vs RHE, 80:20 v:v DI water to acetonitrile with 0.5 M H_2SO_4.

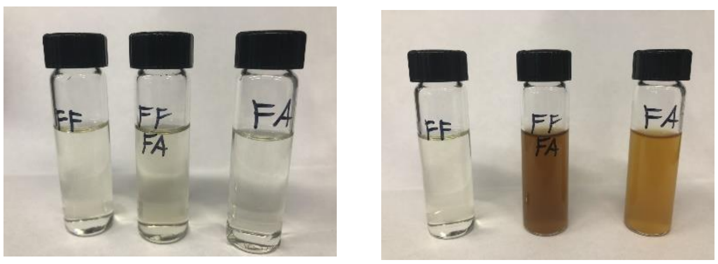

Figure S4. Impact of temperature on discoloring of catholyte solution. 100 mM FF, 100 mM FF + 25 mM FA, 25 mM FA, 30 minutes in bath at 45 °C, in 80:20 v:v DI water to acetonitrile with 0.5 M sulfuric acid.

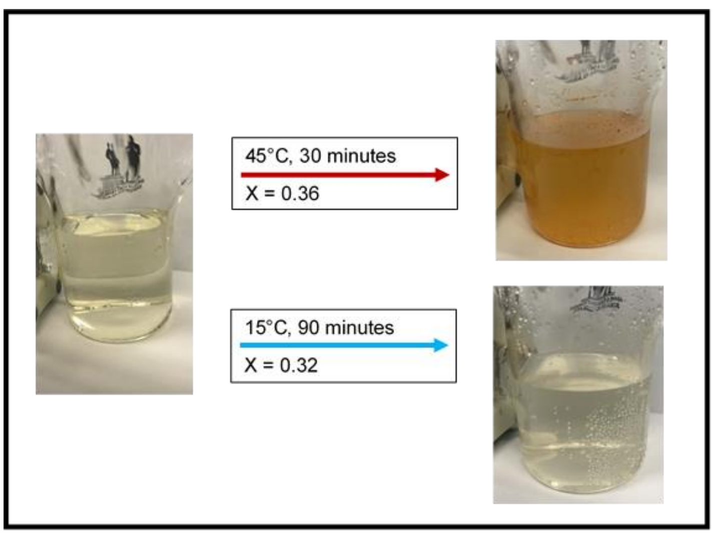

Figure S5. Effect of temperature on the color of the electrolyte after electrolysis to similar conversion. Conditions: 100 mM FF initial concentration, -0.560 V vs RHE, 80:20 v:v DI water to acetonitrile with 0.5 M H_2SO_4.

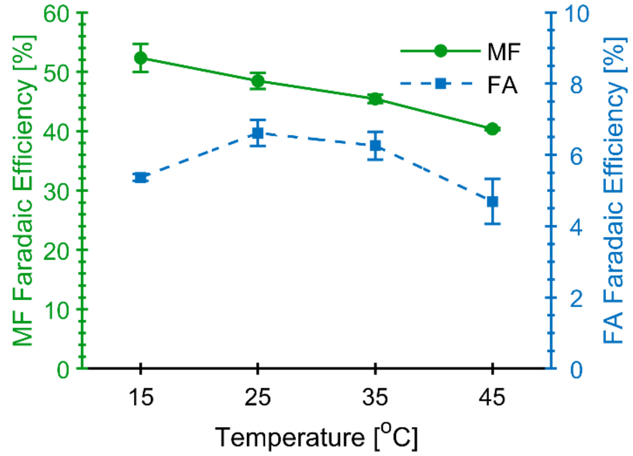

Figure S6. Faradaic efficiency of FA and MF production from FF ECH. Conditions: 30 minutes of electrolysis, 100 mM FF initial concentration, -0.560 V vs RHE, 80:20 v:v DI water to acetonitrile with 0.5 M H_2SO_4.

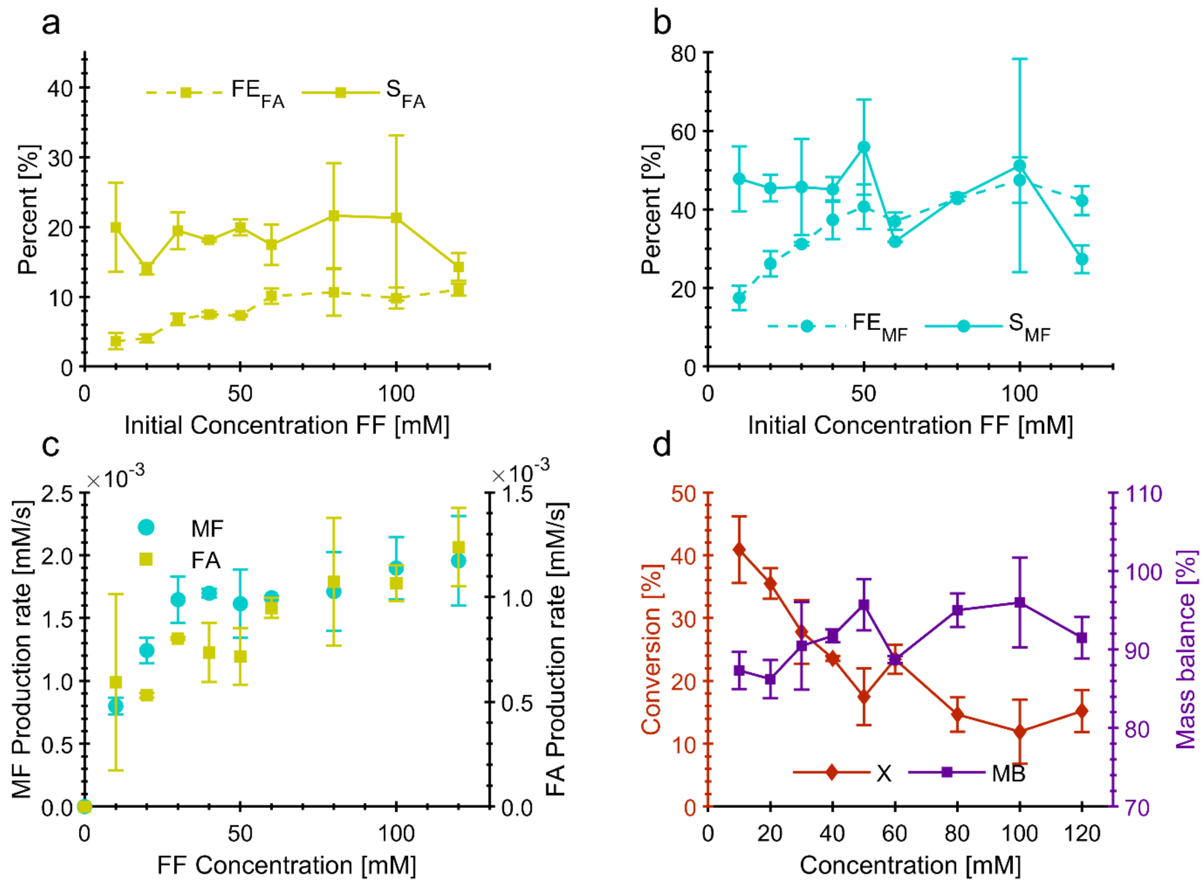

Figure S7. The Faradaic efficiency and selectivity towards (a) FA and (b) MF. (c) The production rates of FF and MF from the ECH of FF. (d) The conversion and mass balance closure from FF ECH. Conditions: 10 to 120 mM concentration of FF, 25°C, -0.560 V vs RHE, 80:20 v:v DI water to acetonitrile with 0.1 M H_2SO_4.

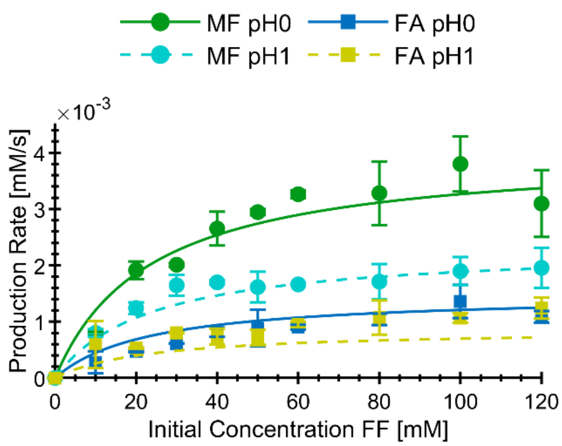

Figure S8. F2-NCLH, M7-NCLH. The model for FA at pH 1 drops from experimental data due to second order dependency on proton.

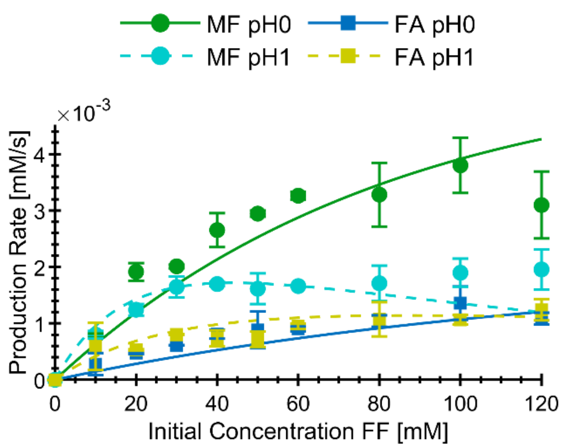

Figure S9. Competitive Langmuir-Hinshelwood fitting. M1-CLH, F1-CLH.

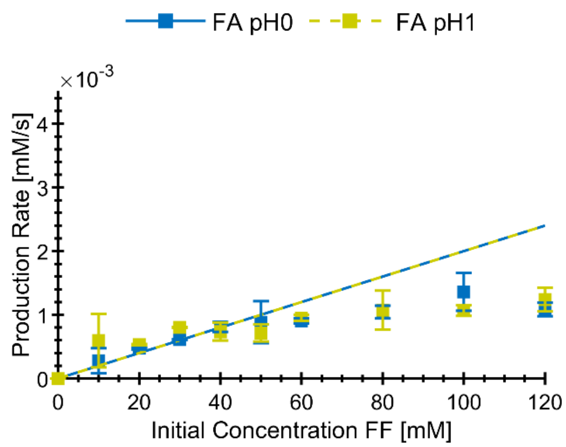

Figure S10. Adsorption limited case for FA production from FF ECH.

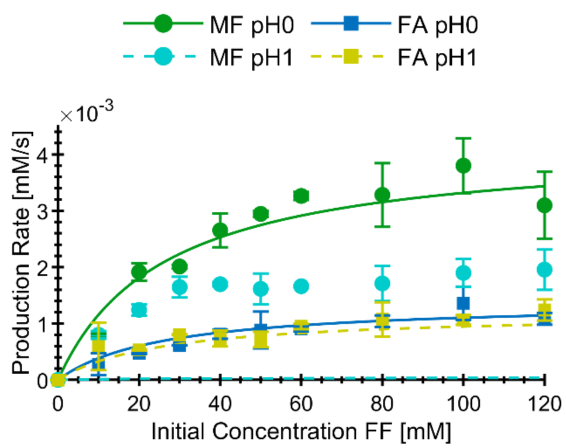

Figure S11. F1-NCLH, M7-NCER. The model for MF at pH 1 drops from experimental data due to dependency on proton.

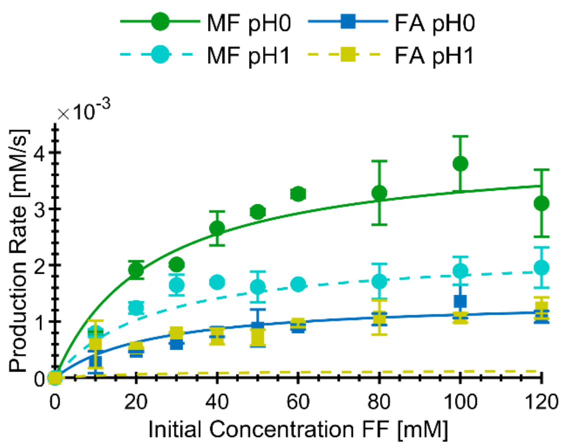

Figure S12. F1-NCER, M7-NCLH. The model for FA at pH 1 drops from experimental data due to dependency on proton.

Table S1. The standard potential of the Ag/AgCl reaction at temperatures tested in this work.

T	**E^0_{AgAgCl}**
°C	**V**
15	0.216
25	0.209
35	0.202
45	0.195

Table S2. Data for Faradaic efficiency and average current density for varied potential experiments in Figure 1.

	30 minutes	30 minutes	
V [Volts]	Faradaic Efficiency FA	Faradaic Efficiency MF	average j [mA/cm^2]
-0.485	0.0144	0.0438	-4.71
-0.517	0.0114	0.0439	-11.9
-0.552	0.0116	0.0409	-17.2
-0.572	0.00784	0.0461	-22.1
-0.597	0.00648	0.0382	-34.8
-0.645	0.00429	0.0362	-42.2

Table S3. Data for varied temperature experiments in Figure 3. Conditions: 30 minutes of electrolysis, 100 mM FF initial concentration, -0.560 V vs RHE, 80:20 v:v DI water to acetonitrile with 0.5 M H_2SO_4.

	T	Degrees C	15	25	35	45
30 minutes	**X**		0.102	0.141	0.249	0.357
30 minutes	**S_{FA}**		0.130	0.150	0.131	0.094
30 minutes	**S_{MF}**		0.635	0.548	0.475	0.404
30 minutes	**FE_{FA}**		0.054	0.066	0.063	0.047
30 minutes	**FE_{MF}**		0.523	0.485	0.454	0.404
30 minutes	Furanic mass balance		0.976	0.958	0.907	0.830
Initial	Rate FA	[mM/s *10^3]	0.856	1.359	2.070	2.547
Initial	Rate MF	[mM/s *10^3]	3.211	3.801	5.618	6.281
	Average current density	mA/cm^2	-13.4	-18.7	-29.2	-40.3

Table S4. Data for varied concentration of FF at pH 0, shown in Figures 4 and 6. Conditions: 10 to 120 mM concentration of FF, 25°C, -0.560 V vs RHE, 80:20 v:v DI water to acetonitrile with 0.5 M H_2SO_4.

Concentration of FF [mM]	**10**	**20**	**30**	**40**	**50**	**60**	**80**	**100**	**120**
Rate MF [mM/s *10^3]	0.784	1.915	2.011	2.653	2.945	3.263	3.282	3.801	3.097
Rate FA [mM/s *10^3]	0.278	0.474	0.613	0.810	0.885	0.904	1.044	1.359	1.083
X	0.348	0.338	0.292	0.252	0.279	0.252	0.177	0.153	0.115
S_{FA}	0.140	0.108	0.110	0.114	0.126	0.109	0.137	0.143	0.141
S_{MF}	0.511	0.526	0.535	0.517	0.483	0.488	0.554	0.569	0.508
Furanic mass balance	0.883	0.882	0.900	0.912	0.897	0.903	0.948	0.957	0.960
FE_{FA}	0.032	0.033	0.040	0.045	0.048	0.050	0.054	0.063	0.063
FE_{MF}	0.237	0.330	0.392	0.408	0.372	0.450	0.432	0.499	0.448
Average current density [mA/cm^2]	-8.27	-12.9	-12.7	-15.0	-19.2	-18.4	-18.1	-18.7	-16.6

Table S5. Data for varied concentration of FF at pH 1, shown in Figures 6 and S5. Conditions: 10 to 120 mM concentration of FF, 25°C, -0.560 V vs RHE, 80:20 v:v DI water to acetonitrile with 0.1 M H_2SO_4.

Concentration of FF [mM]	**10**	**20**	**30**	**40**	**50**	**60**	**80**	**100**	**120**
Rate MF [mM/s *10^3]	0.800	1.242	1.646	1.697	1.614	1.645	1.711	1.897	1.956
Rate FA [mM/s *10^3]	0.594	0.531	0.802	0.736	0.717	1.011	1.073	1.066	1.239
X	0.409	0.355	0.278	0.236	0.175	0.234	0.147	0.119	0.152
S_{FA}	0.199	0.140	0.195	0.181	0.199	0.174	0.216	0.213	0.143
S_{MF}	0.478	0.454	0.457	0.451	0.559	0.318	0.431	0.512	0.273
Furanic mass balance	0.873	0.862	0.905	0.917	0.957	0.887	0.950	0.960	0.915
FE_{FA}	0.036	0.040	0.068	0.075	0.073	0.101	0.106	0.098	0.110
FE_{MF}	0.175	0.262	0.312	0.373	0.407	0.370	0.427	0.474	0.422
Average current density [mA/cm^2]	-12.5	-12.7	-12.2	-12.1	-13.2	-14.5	-13.4	-12.2	-12.5

Derivations for equations used in Figure 6:

Derivations for rate equations:

NCLH F1 M7:

K1: $H^+ + e^- + T \rightleftharpoons H{\bullet}T$

K2: $FF + S \rightleftharpoons FF{\bullet}S$

FA production:

(RDS_{FA}): $FF{\bullet}S + H{\bullet}T \rightarrow (fur\text{-}CH_2O){\bullet}S + T$

$(fur\text{-}CH_2O){\bullet}S + H{\bullet}T \rightleftharpoons FA{\bullet}S + T$

$FA{\bullet}S \rightleftharpoons FA + S$

MF production:

(K3): $FF{\bullet}S + H{\bullet}T \rightleftharpoons (fur\text{-}CHOH){\bullet}S + T$

(RDS_{MF}): $(fur\text{-}CHOH){\bullet}S + H{\bullet}T \rightarrow (fur\text{-}CH){\bullet}S + H_2O + T$

$(fur\text{-}CH){\bullet}S + 2H{\bullet}T \rightleftharpoons MF{\bullet}S + 2T$

$MF{\bullet}S \rightleftharpoons MF + S$

$$Site_{Tot} = S_{Vac} + T_{vac} + FF \bullet S + H \bullet T$$

$$S_{Tot} = S_{Vac} + FF \bullet S$$

$$T_{Tot} = T_{vac} + H \bullet T$$

$$1 = \frac{S_{Tot}}{S_{Tot}} = \frac{S_{Vac} + FF \bullet S}{S_{Tot}} = \frac{S_{Vac}}{S_{Tot}} + \frac{FF \bullet S}{S_{Tot}} = \theta_{Vac} + \theta_{FF}$$

$$1 = \frac{T_{Tot}}{T_{Tot}} = \frac{T_{vac} + H \bullet T}{T_{Tot}} = \frac{T_{Vac}}{T_{Tot}} + \frac{(H \bullet T)}{T_{Tot}} = \theta'_{Vac} + \theta_{H}$$

Where θ'_{Vac} corresponds to unoccupied hydrogen boding sites and θ_{Vac} corresponds to unoccupied furfural bonding sites

Further assuming the surface is saturated (no vacant sites) will give:

$$1 = \theta_{FF}$$

$$1 = \theta_{H}$$

For the respective sites

So for Furfural:

$$\theta_{FF} = \frac{FF \bullet S}{S_{Tot}} = \frac{FF \bullet S}{S_{Vac} + FF \bullet S}$$

And H:

$$\theta_{H} = \frac{H \bullet T}{T_{Tot}} = \frac{H \bullet T}{T_{Vac} + H \bullet T}$$

$FF \bullet S \text{ and } H \bullet T$ are found using their adsorption reactions.

$$FF \bullet S = K_2[FF]S_{Vac}$$

Where [FF] is the concentration of FF, K2 = k2_forward / k2_backwards.

$$H \bullet T = K_1[H^+]T_{Vac} = K_1\, \alpha_H T_{Vac}$$

Where $[H^+]$ is the concentration of H^+, K1 = k1_forward / k1_backwards

The rate is determined from the RDS as

$$R_{FA} = k_{RDS}\, \theta_H * \theta_{FF}$$

$$R_{FA} = k_{RDS_{FA}} * \frac{FF \bullet S}{S_{Vac} + FF \bullet S} * \frac{H \bullet T}{T_{Vac} + H \bullet T}$$

$$R_{FA} = k_{RDS} * \frac{K_2[FF]S_{Vac}}{S_{Vac} + K_2[FF]S_{Vac}} * \frac{K_1\, \alpha_H T_{Vac}}{T_{Vac} + K_1\, \alpha_H T_{Vac}}$$

$$R_{FA} = k_{RDS} * \frac{K_2[FF]S_{Vac}}{(1 + K_2[FF]) * S_{Vac}} * \frac{K_1\, \alpha_H T_{Vac}}{(1 + K_1\, \alpha_H) * T_{Vac}}$$

$$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_1\, \alpha_H\, S_{Vac} T_{Vac}}{(1 + K_2[FF])(1 + K_1\, \alpha_H) S_{Vac} T_{Vac}}$$

$$\boldsymbol{R_{FA}} = \frac{\boldsymbol{k_{RDS_{FA}} K_2 [FF] K_1\ \alpha_H}}{\boldsymbol{(1 + K_2[FF])(1 + K_1\ \alpha_H)}}$$

$$R_{MF} = k_{RDS_{MF}} * \ (\theta_H)^2 * \theta_{FF}$$

$$R_{MF} = k_{RDS_{MF}} * \frac{FF \bullet S}{S_{Vac} + FF \bullet S} * \frac{H \bullet T}{T_{Vac} + H \bullet T} * \frac{H \bullet T}{T_{Vac} + H \bullet T}$$

$$FF \bullet S = K_2[FF]S_{Vac}$$

Where K2 = k2 forward / k2 backwards

$$H \bullet T = K_1[H^+]T_{Vac} = K_1\ \alpha_H T_{Vac}$$

Where K1 = k1 forward / k1 backwards

$$R_{MF} = K_3 k_{RDS_{MF}} * \frac{FF \bullet S}{S_{Vac} + FF \bullet S} * \left(\frac{H \bullet T}{T_{Vac} + H \bullet T}\right)^2$$

$$R_{MF} = K_3 k_{RDS_{MF}} * \frac{K_2[FF]S_{Vac}}{S_{Vac} + K_2[FF]S_{Vac}} * \left(\frac{K_1\ \alpha_H T_{Vac}}{T_{Vac} + K_1\ \alpha_H T_{Vac}}\right)^2$$

$$R_{MF} = K_3 k_{RDS_{MF}} * \frac{K_2[FF]S_{Vac}}{S_{Vac} + K_2[FF]S_{Vac}} * \left(\frac{K_1\ \alpha_H T_{Vac}}{T_{Vac} + K_1\ \alpha_H T_{Vac}}\right)^2$$

$$R_{MF} = \frac{K_3 k_{RDS_{MF}}\ K_2\ (K_1)^2 [FF]\ (\alpha_H)^2 S_{Vac} {T_{Vac}}^2}{(S_{Vac} + K_2[FF]S_{Vac}) * (T_{Vac} + K_1\ \alpha_H T_{Vac})^2}$$

$$R_{MF} = \frac{K_3 k_{RDS_{MF}}\ K_2\ (K_1)^2 [FF]\ (\alpha_H)^2 S_{Vac} {T_{Vac}}^2}{(S_{Vac} + K_2[FF]S_{Vac}) * (T_{Vac} + K_1\ \alpha_H T_{Vac})^2}$$

$$R_{MF} = \frac{K_3 k_{RDS_{MF}}\ K_2\ (K_1)^2 [FF]\ (\alpha_H)^2}{(1 + K_2[FF]) * (1 + K_1\ \alpha_H)^2}$$

$$\boldsymbol{R_{MF}} = \frac{\boldsymbol{K_3 k_{RDS_{MF}}\ K_2\ [FF](K_1)^2(\alpha_H)^2}}{\boldsymbol{(1 + K_2[FF]) * (1 + K_1\ \alpha_H)^2}}$$

NCLH F3 M4:

FA production:

FF•S + H•T → (fur-CHOH)•S + T

(fur-CHOH)•S + H•T ⇌ FA•S + T

FA•S ⇌ FA + S

MF production, mh6 then C-O cleavage (RLS), NCLH

FF•S + H•T ⇌ (fur-CH_2O)•S + T

(fur-CH_2O)•S + 2 H•T → (fur-CH_2)•S + H_2O + 2T

(fur-CH_2)•S + H•T ⇌ MF•S + T

MF•S ⇌ MF + S

$$R_{FA} = k_{RDS_{FA}} * \alpha_H * \theta_{FF}$$

$$R_{FA} = k_{RDS_{FA}} * \alpha_H * \frac{FF \bullet S}{S_{Vac} + FF \bullet S}$$

$$R_{FA} = \frac{k_{RDS_{FA}} K_2 [FF] K_1 \, \alpha_H}{(1 + K_2[FF])(1 + K_1 \, \alpha_H)}$$

$$R_{FA} = K_3 k_{RDS_{FA}} * (\alpha_H)^3 \ * \theta_{FF}$$

$$R_{FA} = K_3 k_{RDS_{FA}} * (\alpha_H)^3 * \frac{FF \bullet S}{S_{Vac} + FF \bullet S}$$

$$R_{MF} = \frac{k_{RDS_{MF}} \, K_2 \, [FF] K_3 (K_1)^3 (\alpha_H)^3}{(1 + K_2[FF]) * (1 + K_1 \, \alpha_H)^3}$$

NCER F1 M7:

FA production:

(RDS_{FA}): FF•S + H^+ + e^- → (fur-CH_2O)•S

(fur-CH_2O)•S + H^+ + e^- ⇌ FA•S

FA•S ⇌ FA + S

MF production:

K3: FF•S + H^+ + e^- ⇌ (fur-CHOH)•S

(RDS_{MF}): (fur-CHOH)•S + H^+ + e^- → (fur-CH)•S + H_2O

(fur-CH)•S + 2H^+ + 2e^- ⇌ MF•S

MF•S ⇌ MF + S

$$R_{FA} = k_{RDS_{FA}} * \alpha_H * \theta_{FF}$$

$$R_{FA} = k_{RDS_{FA}} * \alpha_H * \frac{FF \bullet S}{S_{Vac} + FF \bullet S}$$

$$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1 + K_2[FF])}$$

$$R_{MF} = K_3 k_{RDS_{MF}} * \ (\alpha_H)^2 * \theta_{FF}$$

$$R_{MF} = K_3 k_{RDS_{MF}} * \frac{FF \bullet S}{S_{Vac} + FF \bullet S} * \ (\alpha_H)^2$$

$$R_{MF} = \frac{K_3 k_{RDS_{MF}} * K_2[FF] * K_3 (\alpha_H)^2}{(1 + K_2[FF])}$$

CER F1 M7:

For the competitive adsorption case:

K1: $H^+ + e^- + S \rightleftharpoons H \bullet S$

K2: $FF + S \rightleftharpoons FF \bullet S$

FA production:

(RDS_{FA}): $FF \bullet S + H^+ + e^- \rightarrow (fur\text{-}CH_2O) \bullet S$

$(fur\text{-}CH_2O) \bullet S + H^+ + e^- \rightleftharpoons FA \bullet S$

$FA \bullet S \rightleftharpoons FA + S$

MF production:

K3: $FF \bullet S + H^+ + e^- \rightleftharpoons (fur\text{-}CHOH) \bullet S$

(RDS_{MF}): $(fur\text{-}CHOH) \bullet S + H^+ + e^- \rightarrow (fur\text{-}CH) \bullet S + H_2O$

$(fur\text{-}CH) \bullet S + 2H^+ + 2e^- \rightleftharpoons MF \bullet S$

$MF \bullet S \rightleftharpoons MF + S$

$$S_{Tot} = S_{Vac} + FF \bullet S + H \bullet S$$

$$1 = \frac{S_{Tot}}{S_{Tot}} = \frac{S_{Vac} + FF \bullet S + H \bullet S}{S_{Tot}} = \frac{S_{Vac}}{S_{Tot}} + \frac{FF \bullet S}{S_{Tot}} + \frac{(H \bullet S)}{S_{Tot}} = \theta_{Vac} + \theta_{FF} + \theta_H$$

Further assuming the surface is saturated (no vacant sites) will give:

$$1 = \theta_{FF} + \theta_H$$

So for Furfural:

$$\theta_{FF} = \frac{FF \bullet S}{S_{Tot}} = \frac{FF \bullet S}{S_{Vac} + FF \bullet S + H \bullet S}$$

And H:

$$\theta_H = \frac{H \bullet S}{S_{Tot}} = \frac{H \bullet S}{S_{Vac} + FF \bullet S + H \bullet S}$$

$FF \bullet S \text{ and } H \bullet S$ are found using their adsorption reactions.

$$FF \bullet S = K_2[FF]S_{vac}$$

Where [FF] is the concentration of FF, K2 = k2_forward / k2_backwards.

$$H \bullet S = K_1[H^+]S_{vac} = K_1\, \alpha_H S_{vac}$$

Where $[H^+]$ is the concentration of H^+, K1 = k1_forward / k1_backwards.

$$R_{FA} = k_{RDS_{FA}} * \alpha_H * \theta_{FF}$$

$$R_{FA} = k_{RDS_{FA}} * \alpha_H * \frac{FF \bullet S}{S_{Vac} + FF \bullet S + H \bullet S}$$

$$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1 + K_2[FF] + K_1\, \alpha_H)}$$

$$R_{MF} = K_3 k_{RDS_{MF}} * (\alpha_H)^2 * \theta_{FF}$$

$$R_{MF} = K_3 k_{RDS_{MF}} * \frac{FF \bullet S}{S_{Vac} + FF \bullet S + H \bullet S} * (\alpha_H)^2$$

$$R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * K_3(\alpha_H)^2}{(1 + K_2[FF] + K_1\, \alpha_H)}$$

Table S6. Elementary reactions, rate equations, rate constants, 95% confidence interval, and notes on fit for derived schemes of FF ECH. Bolded rows have figures showing fit on Figures S6, S7, S9, S10.

Model	Elementary Reactions FA	Elementary Reactions MF	Rate Equations	Rate Constants	95% Confidence Interval	Reasonableness of fit, Reduced chi-square Hypothetical Reduced chi square 14.2%
	Prior to listed elementary steps, the following occurs: 1. (K1) H^+ + e^- + T ⇌ H•T 2. (K2) FF + S ⇌ FF•S Or in the case of competitive adsorption number 1 changes to: 1. (K1) H^+ + e^- + S ⇌ H•S	Prior to listed elementary steps, the following occurs: 1. (K1) H^+ + e^- + T ⇌ H•T 2. (K2) FF + S ⇌ FF•S Or in the case of competitive adsorption number 1 changes to: 1. (K1) H^+ + e^- + S ⇌ H•S				
M1-CLH F1-CLH	**FF•S + H•S → (fur-CH_2O)•S + S (fur-CH_2O)•S + H•S ⇌ FA•S + S FA•S ⇌ FA + S**	**FF•S + 2H•S → (fur-CH)•S +H_2O + 2S (fur-CH)•S + 2H•S ⇌ MF•S + 2S MF•S ⇌ MF + S**	$\boldsymbol{R_{FA} = \frac{k_{RDS_{FA}} K_2 K_1 [FF]\, \alpha_H}{(1 + K_2[FF] + K_1\, \alpha_H)^2}}$ $\boldsymbol{R_{MF} = \frac{k_{RDS_{MF}} K_2 (K_1)^2 [FF]\, (\alpha_H)^2}{(1 + K_2[FF] + K_1\, \alpha_H)^3}}$	**K1= 12.4459 K2= 0.0276 k_{RDSFA}= 0.0083 k_{RDSMF}= 0.0383**	**8.6035 16.2884 0.0142 0.0411 0.0062 0.0105 0.0308 0.0458**	**No FA = 706.39 MF = 1537.4 $FA_{14.2}$ = 18.899 $MF_{14.2}$ = 29.26**
M1 NCLH F1(orF3) NCLH	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + 2 H•T → (fur-CH)•S + 2T + H_2O (fur-CH)•S + 2 H•T ⇌ MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2 [FF] K_1\, \alpha_H}{(1 + K_2[FF])(1 + K_1\, \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2\, [FF] (K_1)^2 (\alpha_H)^2}{(1 + K_2[FF]) * (1 + K_1\, \alpha_H)^2}$	K1= 25.8707 K2= 0.0419 k_{RDSFA}= 0.0015 k_{RDSMF}= 0.0044	20.1170 31.6243 0.0268 0.0570 0.0012 0.0017 0.0039 0.0049	Yes FA = 133.6155 MF = 17.4774 $FA_{14.2}$ = 2.9472 $MF_{14.2}$ = 1.3164
M1 NCLH F1 ncER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + 2 H•T → (fur-CH)•S + 2T + H_2O (fur-CH)•S + 2 H•T ⇌ MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2\, [FF] (K_1)^2 (\alpha_H)^2}{(1 + K_2[FF]) * (1 + K_1\, \alpha_H)^2}$	K1= 25.0275 K2= 0.0415 k_{RDSFA}= 0.0014 k_{RDSMF}= 0.0044	13.4594 36.5956 0.0100 0.0731 0.0008 0.0019 0.0033 0.0056	No (FA pH 1 underestimated) FA = 833.9357 MF = 18.8835 $FA_{14.2}$ = 21.1013 $MF_{14.2}$ = 1.3681
M1 cER F1 cER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + $2H^+$ + $2e^-$ → (fur-CH)•S + H_2O (fur-CH)•S + $2H^+$ + $2e^-$ ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1 + K_2[FF] + K_1\, \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * (\alpha_H)^2}{(1 + K_2[FF] + K_1\, \alpha_H)}$	K1= 89.9992 K2= 0.4405 k_{RDSFA}= 0.0046 k_{RDSMF}=0.0121	-6965.7 7145.7 -34.150 35.031 -0.0037 0.0129 -0.0092 0.0335	No CI span 0 FA = 424.26 MF = 1422.3 $FA_{14.2}$ = 11.833 $MF_{14.2}$ = 24.164
M1 nER F1 NCLH	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + $2H^+$ + $2e^-$ → (fur-CH)•S + H_2O (fur-CH)•S + $2H^+$ + $2e^-$ ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2 [FF] K_1\, \alpha_H}{(1 + K_2[FF])(1 + K_1\, \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * (\alpha_H)^2}{(1 + K_2[FF])}$	K1= 53.5348 K2= 0.0381 k_{RDSFA}= 0.0014 k_{RDSMF}= 0.0042	-311.0506 418.1203 -0.0201 0.0964 0.0002 0.0026 0.0021 0.0063	CI span 0 FA = 73.941 MF = 1511.8 $FA_{14.2}$ = 1.8073 $MF_{14.2}$ = 24.725

M1 nER F1 nER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + $2H^+$ + $2e^-$ → (fur-CH)•S + H_2O (fur-CH)•S + $2H^+$ + $2e^-$ ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * (\alpha_H)^2}{(1+K_2[FF])}$	No K1 k_{RDSMF}= 0.0039 K2= 0.0519 k_{RDSFA}= 0.0014	0.0020 0.0059 -0.0389 0.1426 0.0003 0.0024	pH1 underestimate CI spans 0 FA = 867.62 MF = 1522.5 $FA_{14.2}$ = 21.94 $MF_{14.2}$ = 25.517
M1 NCLH F2 NCLH	FF•S + H•T ⇌ (fur-CH_2O)•S + T (fur-CH_2O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + 2 H•T → (fur-CH)•S + 2T + H_2O (fur-CH)•S + 2 H•T ⇌ MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 (K_1)^2 (\alpha_H)^2}{(1+K_2[FF])(1+K_1\,\alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}}\, K_2\,[FF](K_1)^2(\alpha_H)^2}{(1+K_2[FF]) * (1+K_1\,\alpha_H)^2}$	K1= 25.5304 K2= 0.0416 K3*k_{RDSFA}= 0.0014 k_{RDSMF}= 0.0044	13.3617 37.6990 0.0092 0.0740 0.0008 0.0020 0.0032 0.0056	FA pH 1 underestimated FA = 257.4317 MF = 16.2129 $FA_{14.2}$ = 5.5874 $MF_{14.2}$ = 1.2443
M1 NCLH F2 nER	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S + T K3 (fur-CH_2O)•S + H^+ + e^- → FA•S + T FA•S ⇌ FA + S	FF•S + 2 H•T → (fur-CH)•S + 2T + H_2O (fur-CH)•S + 2 H•T ⇌ MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\,(\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\, K_2\,[FF](K_1)^2(\alpha_H)^2}{(1+K_2[FF]) * (1+K_1\,\alpha_H)^2}$	K1= 25.0298 K2= 0.0416 K3*k_{RDSFA}= 0.0013 k_{RDSMF}= 0.0044	12.4757 37.5840 0.0071 0.0760 0.0007 0.0019 0.0032 0.0057	FA pH 1 underestimated FA = 962.1698 MF = 18.8943 $FA_{14.2}$ = 25.0032 $MF_{14.2}$ = 1.369
M1 cER F2 cER	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S + T K3 (fur-CH_2O)•S + H^+ + e^- → FA•S + T FA•S ⇌ FA + S	FF•S + $2H^+$ + $2e^-$ → (fur-CH)•S + H_2O (fur-CH)•S + $2H^+$ + $2e^-$ ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\,(\alpha_H)^2}{(1+K_2[FF]+K_1\,\alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * (\alpha_H)^2}{(1+K_2[FF]+K_1\,\alpha_H)}$	K1= 49.9997 K2= 0.2382 K3*k_{RDSFA}= 0.0041 k_{RDSMF}= 0.0124	-7987.5 8087.5 -37.4 37.9 -0.004834 0.01293 -0.01348 0.03829	pH0 no plateau No pH1 fit CI spans 0 FA = 933.79 MF = 1424.6 $FA_{14.2}$ = 24.42 $MF_{14.2}$ = 24.243
M1 nER F2 NCLH	FF•S + H•T ⇌ (fur-CH_2O)•S + T (fur-CH_2O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + $2H^+$ + $2e^-$ → (fur-CH)•S + H_2O (fur-CH)•S + $2H^+$ + $2e^-$ ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 (K_1)^2 (\alpha_H)^2}{(1+K_2[FF])(1+K_1\,\alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * (\alpha_H)^2}{(1+K_2[FF])}$	K1= 54.4314 K2= 0.03998 K3*k_{RDSFA}= 0.001455 k_{RDSMF}= 0.004108	-147.93 256.79 -0.0223280 0.1023057 0.0002406 0.0026696 0.002027 0.006188	Both pH 1 underestimated FA = 127.45 MF = 1512.9 $FA_{14.2}$ = 2.8739 $MF_{14.2}$ = 24.79
M1 nER F2 nER	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S + T K3 (fur-CH_2O)•S + H^+ + e^- → FA•S + T FA•S ⇌ FA + S	FF•S + $2H^+$ + $2e^-$ → (fur-CH)•S + H_2O (fur-CH)•S + $2H^+$ + $2e^-$ ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\,(\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * (\alpha_H)^2}{(1+K_2[FF])}$	No K1 K2= 0.0518 K3*k_{RDSFA}= 0.0013 k_{RDSMF}= 0.0039	-0.0414 0.1451 0.0002 0.0023 0.0019 0.0060	No pH 1 fit CI spans 0 FA = 989.5 MF = 1522.5 $FA_{14.2}$ = 25.673 $MF_{14.2}$ = 25.514
M2-NCLH F1-NCLH	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + 2 H•T ⇌ (fur-CH)•S + 2T + H_2O K3m (fur-CH)•S + 2 H•T → MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_1\,\alpha_H}{(1+K_2[FF])(1+K_1\,\alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}}\, K_2\,[FF] K_3 (K_1)^4(\alpha_H)^4}{(1+K_2[FF]) * (1+K_1\,\alpha_H)^4}$	K1= 61.3608 K2= 0.0372 k_{RDSFA}= 0.0015 K3*k_{RDSMF}= 0.0046	50.3976 72.3240 0.0262 0.0481 0.0013 0.0017 0.0041 0.0051	MF pH0 is overestimated FA = 79.4092 MF = 16.7545 $FA_{14.2}$ = 1.8557 $MF_{14.2}$ = 1.125
M2-NCLH F1-ncER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + 2 H•T ⇌ (fur-CH)•S + 2T + H_2O K3m (fur-CH)•S + 2 H•T → MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\, K_2\,[FF] K_3 (K_1)^4(\alpha_H)^4}{(1+K_2[FF]) * (1+K_1\,\alpha_H)^4}$	K1= 60.5516 K2= 0.0371 k_{RDSFA}= 0.0015 K3*k_{RDSMF}= 0.0046	35.0190 86.0842 0.0106 0.0635 0.0009 0.0021 0.0035 0.0058	MF pH0 is overestimated FA pH 1 underestimated FA = 843.7316 MF = 16.3183 $FA_{14.2}$ = 21.0598 $MF_{14.2}$ = 1.1354
M2-cER F1-cER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + $2H^+$ + $2e^-$ ⇌ (fur-CH)•S + H_2O K3m (fur-CH)•S + $2H^+$ + $2e^-$ → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1+K_2[FF]+K_1\,\alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}}\, K_2\,[FF] K_3\,(\alpha_H)^4}{(1+K_2[FF]+K_1\,\alpha_H)}$	K1= 69.9994 K2= 0.3498 k_{RDSFA}= 0.004520 K3*k_{RDSMF}= 0.01175	-4697.2 4837.2 -23.5 24.2 -0.004104 0.01314 -0.00998 0.0335	pH0 no plateau pH1 underestimated CI span 0 FA = 432.14 MF = 1581.6 $FA_{14.2}$ = 12.003 $MF_{14.2}$ = 26.543
M2-ncER F1-NCLH	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + $2H^+$ + $2e^-$ ⇌ (fur-CH)•S + H_2O K3m (fur-CH)•S + $2H^+$ + $2e^-$ → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_1\,\alpha_H}{(1+K_2[FF])(1+K_1\,\alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}}\, K_2\,[FF] K_3 (\alpha_H)^4}{(1+K_2[FF])}$	K1= 53.5348 K2= 0.0380 k_{RDSFA}= 0.0014 K3*k_{RDSMF}= 0.0042	-317.1332 424.2029 -0.0213 0.0973 0.0002 0.0026 0.0020 0.0063	MF pH1 underestimated CI span 0 FA = 73.769 MF = 1564.1 $FA_{14.2}$ = 1.8016 $MF_{14.2}$ = 25.488

M2-ncER F1-ncER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + 2H^+ + 2e^- ⇌ (fur-CH)•S + H_2O K3m (fur-CH)•S + 2H^+ + 2e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2 [FF] K_3 (\alpha_H)^4}{(1+K_2[FF])}$	K2 = 0.0518 k_{RDSFA}= 0.0014 K3*k_{RDSMF}= 0.0039	-0.0404 0.1440 0.0003 0.0024 0.0019 0.0059	pH1 underestimated CI span 0 FA = 867.38 MF = 1575.7 $FA_{14.2}$ = 21.932 $MF_{14.2}$ = 26.289
M2-NCLH F2-NCLH Different K3	FF•S + H•T ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + 2 H•T ⇌ (fur-CH)•S + 2T + H_2O K3m (fur-CH)•S + 2 H•T → MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 (K_1)^2 (\alpha_H)^2}{(1+K_2[FF])(1+K_1\,\alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2 [FF] K_3 (K_1)^4 (\alpha_H)^4}{(1+K_2[FF]) * (1+K_1\,\alpha_H)^4}$	K1= 63.5271 K2= 0.0372 K3f* k_{RDSFA}= 0.0016 K3m*k_{RDSMF}= 0.0046	51.2927 75.7615 0.0255 0.0489 0.0013 0.0018 0.0041 0.0051	MF pH0 overestimated FA = 128.7596 MF = 17.8285 $FA_{14.2}$ = 2.6676 $MF_{14.2}$ = 1.0935
M2-NCLH F2-ncER Different K3	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + 2 H•T ⇌ (fur-CH)•S + 2T + H_2O K3m (fur-CH)•S + 2 H•T → MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\,(\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2 [FF] K_3 (K_1)^4 (\alpha_H)^4}{(1+K_2[FF]) * (1+K_1\,\alpha_H)^4}$	K1= 60.5522 K2= 0.0372 K3f*k_{RDSFA}= 0.0014 K3m*k_{RDSMF}= 0.0046	32.7710 88.3335 0.0081 0.0662 0.0008 0.0020 0.0033 0.0059	MF pH0 overestimated FA pH1 underestimated FA = 970.1969 MF = 16.4139 $FA_{14.2}$ = 24.978 $MF_{14.2}$ = 1.1389
M2-cER F2-cER Different K3	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + 2H^+ + 2e^- ⇌ (fur-CH)•S + H_2O K3m (fur-CH)•S + 2H^+ + 2e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\,(\alpha_H)^2}{(1+K_2[FF]+K_1\,\alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2 [FF] K_3\,(\alpha_H)^4}{(1+K_2[FF]+K_1\,\alpha_H)}$	K1= 49.9997 K2= 0.2375 K3f*k_{RDSFA}= 0.0041 K3m*k_{RDSMF}= 0.0122	-26430 26530 -123.1 123.6 -0.00533 0.0135 -0.0147 0.0392	pH0 no plat pH1 underestimate CI span 0 FA = 933.68 MF = 1582.7 $FA_{14.2}$ = 24.419 $MF_{14.2}$ = 26.609
M2-ncER F2-NCLH Different K3	FF•S + H•T ⇌ (fur-CH_2O)•S + T K3 (fur-CH_2O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + 2H^+ + 2e^- ⇌ (fur-CH)•S + H_2O K3m (fur-CH)•S + 2H^+ + 2e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 (K_1)^2 (\alpha_H)^2}{(1+K_2[FF])(1+K_1\,\alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2 [FF] K_3 (K_1)^4 (\alpha_H)^4}{(1+K_2[FF]) * (1+K_1\,\alpha_H)^4}$	K1= 54.4314 K2= 0.0398 K3f*k_{RDSFA}= 0.0015 K3m*k_{RDSMF}= 0.0041	-151.2809 260.1438 -0.0236 0.1033 0.0002 0.0027 0.0020 0.0062	MF underestimate CI span 0 FA = 127.27 MF = 1565 $FA_{14.2}$ = 2.8678 $MF_{14.2}$ = 25.551
M2-ncER F2-ncER Different K3	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + 2H^+ + 2e^- ⇌ (fur-CH)•S + H_2O K3m (fur-CH)•S + 2H^+ + 2e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\,(\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2 [FF] K_3 (K_1)^4 (\alpha_H)^4}{(1+K_2[FF]) * (1+K_1\,\alpha_H)^4}$	K2= 0.0517 K3f*k_{RDSFA}= 0.0013 K3m*k_{RDSMF}= 0.0039	-0.0430 0.1464 0.0002 0.0023 0.0019 0.0060	pH1 underestimate CI span 0 FA = 989.29 MF = 1575.7 $FA_{14.2}$ = 25.666 $MF_{14.2}$ = 26.286
M3-NCLH F3-NCLH	FF•S + H•T → (fur-CHOH)•S + T (fur-CHOH)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + 2 H•T ⇌ (fur-CH_2)•S + H_2O + 2T (fur-CH_2)•S + H•T ⇌ MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_1\,\alpha_H}{(1+K_2[FF])(1+K_1\,\alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2 [FF] K_1\,\alpha_H}{(1+K_2[FF]) * (1+K_1\,\alpha_H)}$	K1= 13.9766 K2= 0.0365 k_{RDSFA}= 0.0017 k_{RDSMF}= 0.0045	9.8607 18.0925 0.0228 0.0503 0.0014 0.0020 0.0039 0.0052	FA pH1 underestimate slightly FA = 227.3041 MF = 23.7925 $FA_{14.2}$ = 4.5861 $MF_{14.2}$ = 1.0291
M3-NCLH F3-ncER	FF•S + H^+ + e^- → (fur-CHOH)•S (fur-CHOH)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + 2 H•T ⇌ (fur-CH_2)•S + H_2O + 2T (fur-CH_2)•S + H•T ⇌ MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\,\alpha_H}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2 [FF] K_1\,\alpha_H}{(1+K_2[FF]) * (1+K_1\,\alpha_H)}$	K1= 11.3090 K2= 0.0365 k_{RDSFA}= 0.0015 k_{RDSMF}= 0.0047	5.1165 17.5015 0.0104 0.0625 0.0009 0.0021 0.0035 0.0060	FA for pH1 underestimate FA = 842.3117 MF = 15.5348 $FA_{14.2}$ = 21.0229 $MF_{14.2}$ = 1.1225
M3-cER F3-cER	FF•S + H^+ + e^- → (fur-CHOH)•S (fur-CHOH)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + 2H^+ + 2e^- ⇌ (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\,\alpha_H}{(1+K_2[FF]+K_1\,\alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * \alpha_H}{(1+K_2[FF]+K_1\,\alpha_H)}$	K1= 89.999 K2= 0.44629 k_{RDSFA}= 0.004546 k_{RDSMF}= 0.012776	-1932.6 2112.6 -9.814 10.7001 -0.000475 0.008616 -0.002263 0.02329	pH0 no plateau pH1 ~0 CI span 0 FA = 425.75 MF = 328.34 $FA_{14.2}$ = 11.878 $MF_{14.2}$ = 7.4384
M3-ncER F3-NCLH	FF•S + H•T → (fur-CHOH)•S + T (fur-CHOH)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + 2H^+ + 2e^- ⇌ (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_1\,\alpha_H}{(1+K_2[FF])(1+K_1\,\alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * \alpha_H}{(1+K_2[FF])}$	K1= 21.1527 K2= 0.0000 k_{RDSFA}= 7.5230 k_{RDSMF}= 0.0300	-0.0062 0.0104 -0.0000 0.0000 -0.0019 0.0034 -2.6538 2.6539	No CI span 0 FA = 75.497 MF = 1059.1 $FA_{14.2}$ = 1.8597 $MF_{14.2}$ = 18.111

M3-ncER F3-ncER	FF•S + H^+ + e^- → (fur-CHOH)•S (fur-CHOH)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + $2H^+$ + $2e^-$ ⇌ (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3\ \alpha_H}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * \alpha_H}{(1+K_2[FF])}$	K2= 0.0463 k_{RDSFA}= 0.0014 k_{RDSMF}= 0.0043	-0.0203 0.1129 0.0004 0.0024 0.0024 0.0061	pH1 underestimate CI span 0 FA = 869.77 MF = 1063.8 $FA_{14.2}$ = 22.014 $MF_{14.2}$ = 18.837
M3-NCLH F4-NCLH	FF•S + H•T ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + 2 H•T ⇌ (fur-CH_2)•S + H_2O + 2T (fur-CH_2)•S + H•T ⇌ MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3(K_1)^2(\alpha_H)^2}{(1+K_2[FF])(1+K_1\ \alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF]K_1\ \alpha_H}{(1+K_2[FF]) * (1+K_1\ \alpha_H)}$	K1= 19.8191 K2= 0.0442 K3* k_{RDSFA}= 0.0017 k_{RDSMF}= 0.0040	11.3401 28.2982 0.0210 0.0674 0.0013 0.0021 0.0033 0.0046	Ok fit MF pH0 underestimate slightly FA pH1 underestimate FA = 351.6171 MF = 43.4334 $FA_{14.2}$ = 7.7721 $MF_{14.2}$ = 1.2336
M3-NCLH F4-ncER	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + 2 H•T ⇌ (fur-CH_2)•S + H_2O + 2T (fur-CH_2)•S + H•T ⇌ MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3\ (\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF]K_1\ \alpha_H}{(1+K_2[FF]) * (1+K_1\ \alpha_H)}$	K1= 11.3102 K2= 0.0366 K3* k_{RDSFA}= 0.0014 k_{RDSMF}= 0.0047	4.5723 18.0481 0.0080 0.0652 0.0008 0.0020 0.0034 0.0061	FA for pH1 is ~0 FA = 968.9656 MF = 15.6373 $FA_{14.2}$ = 24.9478 $MF_{14.2}$ = 1.1258
M3-cER F4-cER	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + $2H^+$ + $2e^-$ ⇌ (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3\ (\alpha_H)^2}{(1+K_2[FF]+K_1\ \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * \alpha_H}{(1+K_2[FF]+K_1\ \alpha_H)}$	K1= 89.9990 K2= 0.45146 K3* k_{RDSFA}= 0.00388 k_{RDSMF}= 0.012672	-2310 2490 -11.84 12.75 -0.000313 0.008089 -0.000604 0.0247	no plateau CI span 0 FA = 929.81 MF = 331.92 $FA_{14.2}$ = 24.35 $MF_{14.2}$ = 7.4754
M3-ncER F4-NCLH	FF•S + H•T ⇌ (fur-CHOH)•S + T K3 (fur-CHOH)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + $2H^+$ + $2e^-$ ⇌ (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3(K_1)^2(\alpha_H)^2}{(1+K_2[FF])(1+K_1\ \alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * \alpha_H}{(1+K_2[FF])}$	K1= 54.4314 K2= 0.04123 K3* k_{RDSFA}= 0.001446 k_{RDSMF}= 0.004256	-117.2 226.1 -0.01131 0.09378 -0.004385 0.02453 -0.02520 0.05991	no plateau CI span 0 FA = 129.09 MF = 1061.9 $FA_{14.2}$ = 2.931 $MF_{14.2}$ = 18.196
M3-ncER F4-ncER	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + $2H^+$ + $2e^-$ ⇌ (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3\ (\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * \alpha_H}{(1+K_2[FF])}$	K2= 0.0463 K3* k_{RDSFA}= 0.0013 k_{RDSMF}= 0.0043	-0.0226 0.1151 0.0003 0.0023 0.0023 0.0062	pH1 too low for both CI span 0 FA = 991.31 MF = 1063.8 $FA_{14.2}$ = 25.734 $MF_{14.2}$ = 18.836
M4-NCLH F2-NCLH Same K3	FF•S + H•T ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur-CH_2O)•S + T (fur-CH_2O)•S + 2 H•T → (fur-CH_2)•S + H_2O + 2T (fur-CH_2)•S + H•T ⇌ MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3(K_1)^2(\alpha_H)^2}{(1+K_2[FF])(1+K_1\ \alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF]K_3(K_1)^3(\alpha_H)^3}{(1+K_2[FF]) * (1+K_1\ \alpha_H)^3}$	K1= 47.7835 K2= 0.0370 K3*k_{RDSFA}= 0.0016 K3*k_{RDSMF}= 0.0046	37.8010 57.7659 0.0247 0.0492 0.0014 0.0019 0.0040 0.0051	Fits ok, FA pH1 underestimate slightly FA = 164.2111 MF = 20.3403 $FA_{14.2}$ = 3.3165 $MF_{14.2}$ = 1.0854
M4-NCLH F2-ncER Same K3	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur-CH_2O)•S + T (fur-CH_2O)•S + 2 H•T → (fur-CH_2)•S + H_2O + 2T (fur-CH_2)•S + H•T ⇌ MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3\ (\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF]K_3(K_1)^3(\alpha_H)^3}{(1+K_2[FF]) * (1+K_1\ \alpha_H)^3}$	K1= 44.2368 K2= 0.0373 K3* k_{RDSFA}= 0.0014 K3*k_{RDSMF}= 0.0046	23.3021 65.1716 0.0081 0.0665 0.0008 0.0020 0.0033 0.0059	FA pH1 underestimate FA = 970.0632 MF = 16.4123 $FA_{14.2}$ = 24.9801 $MF_{14.2}$ = 1.1368
M4-cER F2-cER Same K3	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + $2H^+$ + $2e^-$ → (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3\ (\alpha_H)^2}{(1+K_2[FF]+K_1\ \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF]K_3\ (\alpha_H)^3}{(1+K_2[FF]+K_1\ \alpha_H)}$	K1= 49.999 K2= 0.2383 K3*k_{RDSFA}= 0.003951 K3*k_{RDSMF}= 0.01240	-8446.6 8546.6 -39.56 40.03 -0.004809 0.01271 -0.01369 0.03849	pH0 no plateau pH1 underestimate CI span 0 FA = 933.6 MF = 1568.1 $FA_{14.2}$ = 24.418 $MF_{14.2}$ = 26.392
M4-ncER F2-NCLH Same K3	FF•S + H•T ⇌ (fur-CH_2O)•S + T K3 (fur-CH_2O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + $2H^+$ + $2e^-$ → (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3(K_1)^2(\alpha_H)^2}{(1+K_2[FF])(1+K_1\ \alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF]K_3\ (\alpha_H)^3}{(1+K_2[FF])}$	K1= 54.4314 K2= 0.0399 K3* k_{RDSFA}= 0.0015 K3*k_{RDSMF}= 0.0041	-150.9769 259.8398 -0.0235 0.1032 0.0002 0.0027 0.0020 0.0062	MF pH1 underestimate FA = 127.29 MF = 1560.2 $FA_{14.2}$ = 2.8683 $MF_{14.2}$ = 25.481

M4-ncER F2-ncER Same K3	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + 2H^+ + 2e^- → (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 (\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2[FF] K_3 (\alpha_H)^3}{(1+K_2[FF])}$	K2= 0.0517 K3* k_{RDSFA}= 0.0013 K3*k_{RDSMF}= 0.0039	-0.0429 0.1463 0.0002 0.0023 0.0019 0.0060	pH1 underestimate FA = 989.31 MF = 1570.8 $FA_{14.2}$ = 25.667 $MF_{14.2}$ = 26.216
M4-NCLH F3-NCLH	FF•S + H•T → (fur-CHOH)•S + T (fur-CHOH)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur-CH_2O)•S + T (fur-CH_2O)•S + 2 H•T → (fur-CH_2)•S + H_2O + 2T (fur-CH_2)•S + H•T ⇌ MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_1 \alpha_H}{(1+K_2[FF])(1+K_1 \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2[FF] K_3 (K_1)^3 (\alpha_H)^3}{(1+K_2[FF]) * (1+K_1 \alpha_H)^3}$	K1= 39.7590 K2= 0.0338 k_{RDSFA}= 0.0016 K3*k_{RDSMF}= 0.0048	32.4953 47.0227 0.0233 0.0443 0.0013 0.0018 0.0043 0.0054	Fits good. FA = 96.3147 MF = 14.3861 $FA_{14.2}$ = 2.0375 $MF_{14.2}$ = 1.2107
M4-NCLH F3-ncER	FF•S + H^+ + e^- → (fur-CHOH)•S (fur-CHOH)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur-CH_2O)•S + T (fur-CH_2O)•S + 2 H•T → (fur-CH_2)•S + H_2O + 2T (fur-CH_2)•S + H•T ⇌ MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2[FF] K_3 (K_1)^3 (\alpha_H)^3}{(1+K_2[FF]) * (1+K_1 \alpha_H)^3}$	K1= 44.2348 K2= 0.0372 k_{RDSFA}= 0.0015 K3*k_{RDSMF}= 0.0046	24.9992 63.4705 0.0106 0.0638 0.0009 0.0021 0.0035 0.0058	FA pH1 underestimate FA = 843.6229 MF = 16.3433 $FA_{14.2}$ = 21.0633 $MF_{14.2}$ = 1.1337
M4-cER F3-cER	FF•S + H^+ + e^- → (fur-CHOH)•S (fur-CHOH)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + 2H^+ + 2e^- → (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1+K_2[FF]+K_1 \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2[FF] K_3 (\alpha_H)^3}{(1+K_2[FF]+K_1 \alpha_H)}$	K1= 89.9991 K2= 0.4494 k_{RDSFA}= 0.0045 K3*k_{RDSMF}= 0.0118	-7.5681 7.7481 -0.0378 0.0387 -0.0000 0.0000 -0.0000 0.0000	pH0 no plateau pH1 underestimate CI span 0 FA = 426.61 MF = 1566.6 $FA_{14.2}$ = 11.903 $MF_{14.2}$ = 26.315
M4-ncER F3-NCLH	FF•S + H•T → (fur-CHOH)•S + T (fur-CHOH)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + 2H^+ + 2e^- → (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_1 \alpha_H}{(1+K_2[FF])(1+K_1 \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2[FF] K_3 (\alpha_H)^3}{(1+K_2[FF])}$	K1= 53.5348 K2= 0.0380 k_{RDSFA}= 0.0014 K3*k_{RDSMF}= 0.0042	-316.5812 423.6509 -0.0212 0.0972 0.0002 0.0026 0.0020 0.0063	MF pH1 underestimate FA = 73.785 MF = 1559.3 $FA_{14.2}$ = 1.8021 $MF_{14.2}$ = 25.418
M4-ncER F3-ncER	FF•S + H^+ + e^- → (fur-CHOH)•S (fur-CHOH)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + 2H^+ + 2e^- → (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2[FF] K_3 (\alpha_H)^3}{(1+K_2[FF])}$	K2= 0.0518 k_{RDSFA}= 0.0014 K3*k_{RDSMF}= 0.0039	-0.0403 0.1438 0.0003 0.0024 0.0019 0.0059	pH1 underestimate FA = 867.4 MF = 1570.9 $FA_{14.2}$ = 21.932 $MF_{14.2}$ = 26.219
M4-NCLH F4-NCLH Different K3	FF•S + H•T ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur-CH_2O)•S + T (fur-CH_2O)•S + 2 H•T → (fur-CH_2)•S + H_2O + 2T (fur-CH_2)•S + H•T ⇌ MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 (K_1)^2 (\alpha_H)^2}{(1+K_2[FF])(1+K_1 \alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2[FF] K_3 (K_1)^3 (\alpha_H)^3}{(1+K_2[FF]) * (1+K_1 \alpha_H)^3}$	K1= 47.7835 K2= 0.0370 K3f* k_{RDSFA}= 0.0016 K3m*k_{RDSMF}= 0.0046	37.8010 57.7659 0.0247 0.0492 0.0014 0.0019 0.0040 0.0051	Fits ok, FA pH1 underestimate slightly FA = 164.2111 MF = 20.3403 $FA_{14.2}$ = 3.3165 $MF_{14.2}$ = 1.0854
M4-NCLH F4-ncER Different K3	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur-CH_2O)•S + T (fur-CH_2O)•S + 2 H•T → (fur-CH_2)•S + H_2O + 2T (fur-CH_2)•S + H•T ⇌ MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 (\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2[FF] K_3 (K_1)^3 (\alpha_H)^3}{(1+K_2[FF]) * (1+K_1 \alpha_H)^3}$	K1= 44.2368 K2= 0.0373 K3f* k_{RDSFA}= 0.0014 K3m*k_{RDSMF}= 0.0046	23.3021 65.1716 0.0081 0.0665 0.0008 0.0020 0.0033 0.0059	FA pH1 underestimate FA = 970.0632 MF = 16.4123 $FA_{14.2}$ = 24.9801 $MF_{14.2}$ = 1.1368
M4-cER F4-cER Different K3	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + 2H^+ + 2e^- → (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 (\alpha_H)^2}{(1+K_2[FF]+K_1 \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} K_2[FF] K_3 (\alpha_H)^3}{(1+K_2[FF]+K_1 \alpha_H)}$	K1= 49.999 K2= 0.2383 K3f*k_{RDSFA}= 0.003951 K3m*k_{RDSMF}= 0.01240	-8446.6 8546.6 -39.56 40.03 -0.004809 0.01271 -0.01369 0.03849	pH0 no plateau pH1 underestimate CI span 0 FA = 933.6 MF = 1568.1 $FA_{14.2}$ = 24.418 $MF_{14.2}$ = 26.392

M4-ncER F4-NCLH Different K3	FF•S + H•T ⇌ (fur-CHOH)•S + T K3 (fur-CHOH)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH$_2$O)•S K3 (fur-CH$_2$O)•S + 2H^+ + 2e^- → (fur-CH$_2$)•S + H_2O (fur-CH$_2$)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3(K_1)^2(\alpha_H)^2}{(1+K_2[FF])(1+K_1\,\alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}}\,K_2\,[FF]K_3\,(\alpha_H)^3}{(1+K_2[FF])}$	K1= 54.4314 K2= 0.0399 K3f* k_{RDSFA}= 0.0015 K3m*k_{RDSMF}= 0.0041	-150.9769 259.8398 -0.0235 0.1032 0.0002 0.0027 0.0020 0.0062	MF pH1 underestimate FA = 127.29 MF = 1560.2 $FA_{14.2}$ = 2.8683 $MF_{14.2}$ = 25.481
M4-ncER F4-ncER Different K3	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH$_2$O)•S K3 (fur-CH$_2$O)•S + 2H^+ + 2e^- → (fur-CH$_2$)•S + H_2O (fur-CH$_2$)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3\,(\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\,K_2\,[FF]K_3\,(\alpha_H)^3}{(1+K_2[FF])}$	K2= 0.0517 K3f* k_{RDSFA}= 0.0013 K3m*k_{RDSMF}= 0.0039	-0.0429 0.1463 0.0002 0.0023 0.0019 0.0060	pH1 underestimate FA = 989.31 MF = 1570.8 $FA_{14.2}$ = 25.667 $MF_{14.2}$ = 26.216
M5-NCLH F2-NCLH Same K3	FF•S + H•T ⇌ (fur-CH$_2$O)•S K3 (fur-CH$_2$O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur-CH$_2$O)•S + T (fur-CH$_2$O)•S + 2 H•T ⇌ (fur-CH$_2$)•S + H_2O + 2T (fur-CH$_2$)•S + H•T → MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3(K_1)^2(\alpha_H)^2}{(1+K_2[FF])(1+K_1\,\alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K1= 63.5271 K2= 0.0372 K3* k_{RDSFA}= 0.0016 K3*K4*k_{RDSMF}= 0.0046	51.2927 75.7615 0.0255 0.0489 0.0013 0.0018 0.0041 0.0051	Good fit FA = 128.7596 MF = 17.8285 $FA_{14.2}$ = 2.6676 $MF_{14.2}$ = 1.0935
M5-NCLH F2-ncER Same K3	FF•S + H^+ + e^- ⇌ (fur-CH$_2$O)•S K3 (fur-CH$_2$O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur-CH$_2$O)•S + T (fur-CH$_2$O)•S + 2 H•T ⇌ (fur-CH$_2$)•S + H_2O + 2T (fur-CH$_2$)•S + H•T → MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3\,(\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K1= 60.5522 K2= 0.0372 K3* k_{RDSFA}= 0.0014 K3*K4*k_{RDSMF}= 0.0046	32.7710 88.3335 0.0081 0.0662 0.0008 0.0020 0.0033 0.0059	FA pH1 underestimate FA = 970.1969 MF = 16.4139 $FA_{14.2}$ = 24.978 $MF_{14.2}$ = 1.1389
M5-cER F2-cER Same K3	FF•S + H^+ + e^- ⇌ (fur-CH$_2$O)•S K3 (fur-CH$_2$O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH$_2$O)•S (fur-CH$_2$O)•S + 2H^+ + 2e^- ⇌ (fur-CH$_2$)•S + H_2O (fur-CH$_2$)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3\,(\alpha_H)^2}{(1+K_2[FF]+K_1\,\alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4\,(\alpha_H)^4}{(1+K_2[FF]+K_1\,\alpha_H)}$	K1= 49.9997 K2= 0.2375 K3* k_{RDSFA}= 0.0041 K3*K4*k_{RDSMF}= 0.0122	-2643.0 2653.0 -12.3 12.4 0.000532 0.00134 -0.001474 0.00392	pH1 underestimate pH0 no plateau FA = 933.68 MF = 1582.7 $FA_{14.2}$ = 24.419 $MF_{14.2}$ = 26.609
M5-ncER F2-NCLH Same K3	FF•S + H•T ⇌ (fur-CH$_2$O)•S + T K3 (fur-CH$_2$O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH$_2$O)•S (fur-CH$_2$O)•S + 2H^+ + 2e^- ⇌ (fur-CH$_2$)•S + H_2O (fur-CH$_2$)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3(K_1)^2(\alpha_H)^2}{(1+K_2[FF])(1+K_1\,\alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K1= 54.4314 K2= 0.0398 K3* k_{RDSFA}= 0.0015 K3*K4*k_{RDSMF}= 0.0041	-151.2809 260.1438 -0.0236 0.1033 0.0002 0.0027 0.0020 0.0062	MF pH1 underestimate FA = 127.27 MF = 1565 $FA_{14.2}$ = 2.8678 $MF_{14.2}$ = 25.551
M5-ncER F2-ncER Same K3	FF•S + H^+ + e^- ⇌ (fur-CH$_2$O)•S K3 (fur-CH$_2$O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH$_2$O)•S (fur-CH$_2$O)•S + 2H^+ + 2e^- ⇌ (fur-CH$_2$)•S + H_2O (fur-CH$_2$)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3\,(\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K2= 0.0517 K3* k_{RDSFA}= 0.0013 K3*K4*k_{RDSMF}= 0.0039	-0.0430 0.1464 0.0002 0.0023 0.0019 0.0060	pH1 underestimate FA = 989.29 MF = 1575.7 $FA_{14.2}$ = 25.666 $MF_{14.2}$ = 26.286
M5-NCLH F3-NCLH	FF•S + H•T → (fur-CHOH)•S + T (fur-CHOH)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur-CH$_2$O)•S + T (fur-CH$_2$O)•S + 2 H•T ⇌ (fur-CH$_2$)•S + H_2O + 2T (fur-CH$_2$)•S + H•T → MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_1\,\alpha_H}{(1+K_2[FF])(1+K_1\,\alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K1= 61.3608 K2= 0.0372 k_{RDSFA}= 0.0015 K3*K4*k_{RDSMF}= 0.0046	50.3976 72.3240 0.0262 0.0481 0.0013 0.0017 0.0041 0.0051	Good fit FA = 79.4092 MF = 16.7545 $FA_{14.2}$ = 1.8557 $MF_{14.2}$ = 1.125
M5-NCLH F3-ncER	FF•S + H^+ + e^- → (fur-CHOH)•S (fur-CHOH)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur-CH$_2$O)•S + T (fur-CH$_2$O)•S + 2 H•T ⇌ (fur-CH$_2$)•S + H_2O + 2T (fur-CH$_2$)•S + H•T → MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K1= 60.5516 K2= 0.0371 k_{RDSFA}= 0.0015 K3*K4*k_{RDSMF}= 0.0046	35.0190 86.0842 0.0106 0.0635 0.0009 0.0021 0.0035 0.0058	FA pH1 underestimate FA = 843.7316 MF = 16.3183 $FA_{14.2}$ = 21.0598 $MF_{14.2}$ = 1.1354
M5-cER F3-cER	FF•S + H^+ + e^- → (fur-CHOH)•S (fur-CHOH)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH$_2$O)•S (fur-CH$_2$O)•S + 2H^+ + 2e^- ⇌ (fur-CH$_2$)•S + H_2O (fur-CH$_2$)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1+K_2[FF]+K_1\,\alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4\,(\alpha_H)^4}{(1+K_2[FF]+K_1\,\alpha_H)}$	K1= 69.9994 K2= 0.3498 k_{RDSFA}= 0.0045 K3*K4*k_{RDSMF}= 0.0118	-4.6972 4.8372 -0.0235 0.0242 -0.0000 0.0000 -0.0000 0.0000	pH1 underestimate pH0 no plateau FA = 432.14 MF = 1581.6 $FA_{14.2}$ = 12.003 $MF_{14.2}$ = 26.543

M5-ncER F3-NCLH	FF•S + H•T → (fur-CHOH)•S + T (fur-CHOH)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S (fur-CH_2O)•S + $2H^+$ + $2e^-$ ⇌ (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_1\ \alpha_H}{(1+K_2[FF])(1+K_1\ \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF] K_3 K_4 (\alpha_H)^4}{(1+K_2[FF])}$	K1= 53.5348 K2= 0.0380 k_{RDSFA}= 0.0014 K3*K4*k_{RDSMF}= 0.0042	-317.1332 424.2029 -0.0213 0.0973 0.0002 0.0026 0.0020 0.0063	MF pH1 underestimate FA = 73.769 MF = 1564.1 $FA_{14.2}$ = 1.8016 $MF_{14.2}$ = 25.488
M5-ncER F3-ncER	FF•S + H^+ + e^- → (fur-CHOH)•S (fur-CHOH)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S (fur-CH_2O)•S + $2H^+$ + $2e^-$ ⇌ (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF] K_3 K_4 (\alpha_H)^4}{(1+K_2[FF])}$	K2= 0.0518 k_{RDSFA}= 0.0014 K3*K4*k_{RDSMF}= 0.0039	-0.0404 0.1440 0.0003 0.0024 0.0019 0.0059	pH1 underestimate FA = 867.38 MF = 1575.7 $FA_{14.2}$ = 21.932 $MF_{14.2}$ = 26.289
M5-NCLH F4-NCLH Different K3	FF•S + H•T ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur-CH_2O)•S + T (fur-CH_2O)•S + 2 H•T ⇌ (fur-CH_2)•S + H_2O + 2T (fur-CH_2)•S + H•T → MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 (K_1)^2 (\alpha_H)^2}{(1+K_2[FF])(1+K_1\ \alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF] K_3 K_4 (K_1)^4 (\alpha_H)^4}{(1+K_2[FF]) * (1+K_1\ \alpha_H)^4}$	K1= 63.5271 K2= 0.0372 K3f* k_{RDSFA}= 0.0016 K3m*K4*k_{RDSMF}= 0.0046	51.2927 75.7615 0.0255 0.0489 0.0013 0.0018 0.0041 0.0051	Good fit FA = 128.7596 MF = 17.8285 $FA_{14.2}$ = 2.6676 $MF_{14.2}$ = 1.0935
M5-NCLH F4-ncER Different K3	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur-CH_2O)•S + T (fur-CH_2O)•S + 2 H•T ⇌ (fur-CH_2)•S + H_2O + 2T (fur-CH_2)•S + H•T → MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\ (\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF] K_3 K_4 (K_1)^4 (\alpha_H)^4}{(1+K_2[FF]) * (1+K_1\ \alpha_H)^4}$	K1= 60.5522 K2= 0.0372 K3f* k_{RDSFA}= 0.0014 K3m*K4*k_{RDSMF}= 0.0046	32.7710 88.3335 0.0081 0.0662 0.0008 0.0020 0.0033 0.0059	FA pH1 underestimate FA = 970.1969 MF = 16.4139 $FA_{14.2}$ = 24.978 $MF_{14.2}$ = 1.1389
M5-cER F4-cER Different K3	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S (fur-CH_2O)•S + $2H^+$ + $2e^-$ ⇌ (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\ (\alpha_H)^2}{(1+K_2[FF]+K_1\ \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF] K_3 K_4\ (\alpha_H)^4}{(1+K_2[FF]+K_1\ \alpha_H)}$	K1= 49.9997 K2= 0.2375 K3f* k_{RDSFA}= 0.0041 K3m*K4*k_{RDSMF}= 0.0122	-2643.0 2653.0 -12.3 12.4 0.000532 0.00134 -0.001474 0.00392	pH1 underestimate pH0 no plateau FA = 933.68 MF = 1582.7 $FA_{14.2}$ = 24.419 $MF_{14.2}$ = 26.609
M5-ncER F4-NCLH Different K3	FF•S + H•T ⇌ (fur-CHOH)•S + T K3 (fur-CHOH)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S (fur-CH_2O)•S + $2H^+$ + $2e^-$ ⇌ (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 (K_1)^2 (\alpha_H)^2}{(1+K_2[FF])(1+K_1\ \alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF] K_3 K_4 (K_1)^4 (\alpha_H)^4}{(1+K_2[FF]) * (1+K_1\ \alpha_H)^4}$	K1= 54.4314 K2= 0.0398 K3f* k_{RDSFA}= 0.0015 K3m*K4*k_{RDSMF}= 0.0041	-151.2809 260.1438 -0.0236 0.1033 0.0002 0.0027 0.0020 0.0062	MF pH1 underestimate FA = 127.27 MF = 1565 $FA_{14.2}$ = 2.8678 $MF_{14.2}$ = 25.551
M5-ncER F4-ncER Different K3	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S (fur-CH_2O)•S + $2H^+$ + $2e^-$ ⇌ (fur-CH_2)•S + H_2O (fur-CH_2)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\ (\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF] K_3 K_4 (K_1)^4 (\alpha_H)^4}{(1+K_2[FF]) * (1+K_1\ \alpha_H)^4}$	K2= 0.0517 K3f* k_{RDSFA}= 0.0013 K3m*K4*k_{RDSMF}= 0.0039	-0.0430 0.1464 0.0002 0.0023 0.0019 0.0060	pH1 underestimate FA = 989.29 MF = 1575.7 $FA_{14.2}$ = 25.666 $MF_{14.2}$ = 26.286
M6-NCLH F1-NCLH	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + H•T → (fur- CHOH)•S + T (fur-CHOH)•S + H•T ⇌ (fur-CH)•S + H_2O + T (fur-CH)•S + 2H•T ⇌ MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_1\ \alpha_H}{(1+K_2[FF])(1+K_1\ \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF] K_1\ \alpha_H}{(1+K_2[FF]) * (1+K_1\ \alpha_H)}$	K1= 13.9766 K2= 0.0365 k_{RDSFA}= 0.0017 k_{RDSMF}= 0.0045	9.8607 18.0925 0.0228 0.0503 0.0014 0.0020 0.0039 0.0052	Fits ok, FA pH1 underestimate slightly FA = 227.3041 MF = 23.7925 $FA_{14.2}$ = 4.5861 $MF_{14.2}$ = 1.0291
M6-NCLH F1-ncER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H•T → (fur- CHOH)•S + T (fur-CHOH)•S + H•T ⇌ (fur-CH)•S + H_2O + T (fur-CH)•S + 2H•T ⇌ MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1+K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF] K_1\ \alpha_H}{(1+K_2[FF]) * (1+K_1\ \alpha_H)}$	K1= 11.3090 K2= 0.0365 k_{RDSFA}= 0.0015 k_{RDSMF}= 0.0047	5.1165 17.5015 0.0104 0.0625 0.0009 0.0021 0.0035 0.0060	FA pH1 underestimate FA = 842.3117 MF = 15.5348 $FA_{14.2}$ = 21.0229 $MF_{14.2}$ = 1.1225
M6-cER F1-cER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- → (fur-CHOH)•S (fur-CHOH)•S + H^+ + e^- ⇌ (fur-CH)•S + H_2O (fur-CH)•S + $2H^+$ + $2e^-$ ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1+K_2[FF]+K_1\ \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * \alpha_H}{(1+K_2[FF]+K_1\ \alpha_H)}$	K1= 89.999 K2= 0.44629 k_{RDSFA}= 0.004546 k_{RDSMF}= 0.012776	-1932.6 2112.6 -9.814 10.7001 -0.000475 0.008616 -0.002263 0.02329	pH1 underestimate CI span 0 FA = 425.75 MF = 328.34 $FA_{14.2}$ = 11.878 $MF_{14.2}$ = 7.4384
M6-ncER F1-NCLH	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + H^+ + e^- → (fur-CHOH)•S (fur-CHOH)•S + H^+ + e^- ⇌ (fur-CH)•S + H_2O (fur-CH)•S + $2H^+$ + $2e^-$ ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_1\ \alpha_H}{(1+K_2[FF])(1+K_1\ \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * \alpha_H}{(1+K_2[FF])}$	K1= 21.1527 K2= 0.0000 k_{RDSFA}= 7.5230 k_{RDSMF}= 0.0300	-0.0062 0.0104 -0.0000 0.0000 -0.0019 0.0034 -2.6538 2.6539	No plateau CI span 0 FA = 75.497 MF = 1059.1 $FA_{14.2}$ = 1.8597 $MF_{14.2}$ = 18.111

M6-ncER F1-ncER	FF•S + H$^+$ + e$^-$ → (fur-CH$_2$O)•S (fur-CH$_2$O)•S + H$^+$ + e$^-$ ⇌ FA•S FA•S ⇌ FA + S	FF•S + H$^+$ + e$^-$ → (fur-CHOH)•S (fur-CHOH)•S + H$^+$ + e$^-$ ⇌ (fur-CH)•S + H$_2$O (fur-CH)•S + 2H$^+$ + 2e$^-$ ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * \alpha_H}{(1 + K_2[FF])}$	K2= 0.0463 k_{RDSFA}= 0.0014 k_{RDSMF}= 0.0043	-0.0203 0.1129 0.0004 0.0024 0.0024 0.0061	pH1 underestimate CI span 0 FA = 869.77 MF = 1063.8 FA$_{14.2}$ = 22.014 MF$_{14.2}$ = 18.837
M6-NCLH F2-NCLH	FF•S + H•T ⇌ (fur-CH$_2$O)•S K3 (fur-CH$_2$O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H•T → (fur- CHOH)•S + T (fur-CHOH)•S + H•T ⇌ (fur-CH)•S + H$_2$O + T (fur-CH)•S + 2H•T ⇌ MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3(K_1)^2(\alpha_H)^2}{(1 + K_2[FF])(1 + K_1\ \alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF]K_1\ \alpha_H}{(1 + K_2[FF]) * (1 + K_1\ \alpha_H)}$	K1= 19.8191 K2= 0.0442 K3*k_{RDSFA}= 0.0017 k_{RDSMF}= 0.0040	11.3401 28.2982 0.0210 0.0674 0.0013 0.0021 0.0033 0.0046	Ok fit MF pH0 underestimate slightly FA pH1 underestimate FA = 351.6171 MF = 43.4334 FA$_{14.2}$ = 7.7721 MF$_{14.2}$ = 1.2336
M6-NCLH F2-ncER	FF•S + H$^+$ + e$^-$ ⇌ (fur-CH$_2$O)•S K3 (fur-CH$_2$O)•S + H$^+$ + e$^-$ → FA•S FA•S ⇌ FA + S	FF•S + H•T → (fur- CHOH)•S + T (fur-CHOH)•S + H•T ⇌ (fur-CH)•S + H$_2$O + T (fur-CH)•S + 2H•T ⇌ MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3\ (\alpha_H)^2}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF]K_1\ \alpha_H}{(1 + K_2[FF]) * (1 + K_1\ \alpha_H)}$	K1= 11.3102 K2= 0.0366 K3*k_{RDSFA}= 0.0014 k_{RDSMF}= 0.0047	4.5723 18.0481 0.0080 0.0652 0.0008 0.0020 0.0034 0.0061	FA pH1 underestimate FA = 968.9656 MF = 15.6373 FA$_{14.2}$ = 24.9478 MF$_{14.2}$ = 1.1258
M6-cER F2-cER	FF•S + H$^+$ + e$^-$ ⇌ (fur-CH$_2$O)•S K3 (fur-CH$_2$O)•S + H$^+$ + e$^-$ → FA•S FA•S ⇌ FA + S	FF•S + H$^+$ + e$^-$ → (fur-CHOH)•S (fur-CHOH)•S + H$^+$ + e$^-$ ⇌ (fur-CH)•S + H$_2$O (fur-CH)•S + 2H$^+$ + 2e$^-$ ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3\ (\alpha_H)^2}{(1 + K_2[FF] + K_1\ \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * \alpha_H}{(1 + K_2[FF] + K_1\ \alpha_H)}$	K1= 89.9990 K2= 0.45146 K3* k_{RDSFA}= 0.00388 k_{RDSMF}= 0.012672	-2310 2490 -11.84 12.75 -0.000313 0.008089 -0.000604 0.0247	No plateau CI span 0 FA = 929.81 MF = 331.92 FA$_{14.2}$ = 24.35 MF$_{14.2}$ = 7.4754
M6-ncER F2-NCLH	FF•S + H•T ⇌ (fur-CH$_2$O)•S + T K3 (fur-CH$_2$O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H$^+$ + e$^-$ → (fur-CHOH)•S (fur-CHOH)•S + H$^+$ + e$^-$ ⇌ (fur-CH)•S + H$_2$O (fur-CH)•S + 2H$^+$ + 2e$^-$ ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3(K_1)^2(\alpha_H)^2}{(1 + K_2[FF])(1 + K_1\ \alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * \alpha_H}{(1 + K_2[FF])}$	K1= 54.4314 K2= 0.04123 K3* k_{RDSFA}= 0.001446 k_{RDSMF}= 0.004256	-117.2 226.1 -0.01131 0.09378 -0.004385 0.02453 -0.02520 0.05991	No plateau CI span 0 FA = 129.09 MF = 1061.9 FA$_{14.2}$ = 2.931 MF$_{14.2}$ = 18.196
M6-ncER F2-ncER	FF•S + H$^+$ + e$^-$ ⇌ (fur-CH$_2$O)•S K3 (fur-CH$_2$O)•S + H$^+$ + e$^-$ → FA•S FA•S ⇌ FA + S	FF•S + H$^+$ + e$^-$ → (fur-CHOH)•S (fur-CHOH)•S + H$^+$ + e$^-$ ⇌ (fur-CH)•S + H$_2$O (fur-CH)•S + 2H$^+$ + 2e$^-$ ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_3\ (\alpha_H)^2}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * \alpha_H}{(1 + K_2[FF])}$	K2= 0.0463 K3*k_{RDSFA}= 0.0013 k_{RDSMF}= 0.0043	-0.0226 0.1151 0.0003 0.0023 0.0023 0.0062	pH1 underestimate CI span 0 FA = 991.31 MF = 1063.8 FA$_{14.2}$ = 25.734 MF$_{14.2}$ = 18.836
M7-NCLH F1-NCLH	FF•S + H•T → (fur-CH$_2$O)•S + T (fur-CH$_2$O)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur- CHOH)•S + T (fur-CHOH)•S + H•T → (fur-CH)•S + H$_2$O + T (fur-CH)•S + 2H•T ⇌ MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_1\ \alpha_H}{(1 + K_2[FF])(1 + K_1\ \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF]K_3(K_1)^2\ (\alpha_H)^2}{(1 + K_2[FF]) * (1 + K_1\ \alpha_H)^2}$	K1= 25.8707 K2= 0.0419 k_{RDSFA}= 0.0015 K3*k_{RDSMF}= 0.0044	20.1170 31.6243 0.0268 0.0570 0.0012 0.0017 0.0039 0.0049	Good fit FA = 133.6155 MF = 17.4774 FA$_{14.2}$ = 2.9472 MF$_{14.2}$ = 1.3164
M7-NCLH **F1-ncER**	**FF•S + H$^+$ + e$^-$ → (fur-CH$_2$O)•S** **(fur-CH$_2$O)•S + H$^+$ + e$^-$ ⇌ FA•S** **FA•S ⇌ FA + S**	**FF•S + H•T ⇌ (fur- CHOH)•S + T** **(fur-CHOH)•S + H•T → (fur-CH)•S + H$_2$O + T** **(fur-CH)•S + 2H•T ⇌ MF•S + 2T** **MF•S ⇌ MF + S**	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\ K_2\ [FF]K_3(K_1)^2\ (\alpha_H)^2}{(1 + K_2[FF]) * (1 + K_1\ \alpha_H)^2}$	**K1= 25.0275** **K2= 0.0415** **k_{RDSFA}= 0.0014** **K3*k_{RDSMF}= 0.0044**	**13.4594 36.5956** **0.0100 0.0731** **0.0008 0.0019** **0.0033 0.0056**	**FA pH1 underestimate** **FA = 833.9357** **MF = 18.8835** **FA$_{14.2}$ = 21.1013** **MF$_{14.2}$ = 1.3681**
M7-cER F1-cER	FF•S + H$^+$ + e$^-$ → (fur-CH$_2$O)•S (fur-CH$_2$O)•S + H$^+$ + e$^-$ ⇌ FA•S FA•S ⇌ FA + S	FF•S + H$^+$ + e$^-$ ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H$^+$ + e$^-$ → (fur-CH)•S + H$_2$O (fur-CH)•S + 2H$^+$ + 2e$^-$ ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1 + K_2[FF] + K_1\ \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * K_3(\alpha_H)^2}{(1 + K_2[FF] + K_1\ \alpha_H)}$	K1= 89.9992 K2= 0.4405 k_{RDSFA}= 0.0046 K3*k_{RDSMF}=0.0121	-6965.7 7145.7 -34.150 35.031 -0.0037 0.0129 -0.0092 0.0335	pH1 underestimate pH 0 no plateau FA = 424.26 MF = 1422.3 FA$_{14.2}$ = 11.833 MF$_{14.2}$ = 24.164
M7-ncER **F1-NCLH**	**FF•S + H•T → (fur-CH$_2$O)•S + T** **(fur-CH$_2$O)•S + H•T ⇌ FA•S + T** **FA•S ⇌ FA + S**	**FF•S + H$^+$ + e$^-$ ⇌ (fur-CHOH)•S K3** **(fur-CHOH)•S + H$^+$ + e$^-$ → (fur-CH)•S + H$_2$O** **(fur-CH)•S + 2H$^+$ + 2e$^-$ ⇌ MF•S** **MF•S ⇌ MF + S**	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF]K_1\ \alpha_H}{(1 + K_2[FF])(1 + K_1\ \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * K_3(\alpha_H)^2}{(1 + K_2[FF])}$	**K1= 53.5348** **K2= 0.0381** **k_{RDSFA}= 0.0014** **K3*k_{RDSMF}= 0.0042**	**-311.0507 418.1204** **-0.0201 0.0964** **0.0002 0.0026** **0.0021 0.0063**	**MF pH1 underestimate** **FA = 73.941** **MF = 1511.8** **FA$_{14.2}$ = 1.8073** **MF$_{14.2}$ = 24.725**

M7-ncER F1-ncER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → (fur-CH)•S + H_2O (fur-CH)•S + 2H^+ + 2e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * K_3(\alpha_H)^2}{(1 + K_2[FF])}$	K2= 0.0519 k_{RDSFA}= 0.0014 K3*k_{RDSMF}= 0.0039	-0.0389 0.1426 0.0003 0.0024 0.0020 0.0059	pH1 underestimate FA = 867.62 MF = 1522.5 $FA_{14.2}$ = 21.94 $MF_{14.2}$ = 25.517
M7-NCLH **F2-NCLH**	**FF•S + H•T ⇌ (fur-CH_2O)•S K3** **(fur-CH_2O)•S + H•T → FA•S + T** **FA•S ⇌ FA + S**	**FF•S + H•T ⇌ (fur- CHOH)•S + T** **(fur-CHOH)•S + H•T → (fur-CH)•S + H_2O + T** **(fur-CH)•S + 2H•T ⇌ MF•S + 2T** **MF•S ⇌ MF + S**	$\boldsymbol{R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3(K_1)^2(\alpha_H)^2}{(1 + K_2[FF])(1 + K_1\,\alpha_H)^2}}$ $\boldsymbol{R_{MF} = \frac{k_{RDS_{MF}}\, K_2\,[FF] K_3(K_1)^2\,(\alpha_H)^2}{(1 + K_2[FF]) * (1 + K_1\,\alpha_H)^2}}$	**K1= 27.4264** **K2= 0.0425** **K3f*k_{RDSFA}= 0.0016** **K3m*k_{RDSMF}= 0.0043**	**20.3862 34.4667** **0.0245 0.0605** **0.0013 0.0019** **0.0037 0.0049**	**FA pH1 underestimate** **FA = 257.4317** **MF = 16.2129** **$FA_{14.2}$ = 5.5874** **$MF_{14.2}$ = 1.2443**
M7-NCLH F2-ncER	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur- CHOH)•S + T (fur-CHOH)•S + H•T → (fur-CH)•S + H_2O + T (fur-CH)•S + 2H•T ⇌ MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\,(\alpha_H)^2}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\, K_2\,[FF] K_3(K_1)^2\,(\alpha_H)^2}{(1 + K_2[FF]) * (1 + K_1\,\alpha_H)^2}$	K1= 25.0298 K2= 0.0416 K3f*k_{RDSFA}= 0.0013 K3m*k_{RDSMF}= 0.0044	12.4757 37.5840 0.0071 0.0760 0.0007 0.0019 0.0032 0.0057	FA pH1 underestimate FA = 962.1698 MF = 18.8943 $FA_{14.2}$ = 25.0032 $MF_{14.2}$ = 1.369
M7-cER F2-cER	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → (fur-CH)•S + H_2O (fur-CH)•S + 2H^+ + 2e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\,(\alpha_H)^2}{(1 + K_2[FF] + K_1\,\alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * K_3(\alpha_H)^2}{(1 + K_2[FF] + K_1\,\alpha_H)}$	K1= 49.9997 K2= 0.2382 K3f*k_{RDSFA}= 0.0041 K3m*k_{RDSMF}= 0.0124	-7987.5 8087.5 -37.4 37.9 -0.004834 0.01293 -0.01348 0.03829	pH1 underestimate pH 0 no plateau FA = 933.79 MF = 1424.6 $FA_{14.2}$ = 24.42 $MF_{14.2}$ = 24.243
M7-ncER F2-NCLH	FF•S + H•T ⇌ (fur-CH_2O)•S + T K3 (fur-CH_2O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → (fur-CH)•S + H_2O (fur-CH)•S + 2H^+ + 2e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3(K_1)^2(\alpha_H)^2}{(1 + K_2[FF])(1 + K_1\,\alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * K_3(\alpha_H)^2}{(1 + K_2[FF])}$	K1= 54.4314 K2= 0.0400 K3f*k_{RDSFA}= 0.0015 K3m*k_{RDSMF}= 0.0041	-147.9319 256.7948 -0.0223 0.1023 0.0002 0.0027 0.0020 0.0062	MF pH1 underestimate FA = 127.45 MF = 1512.9 $FA_{14.2}$ = 2.8739 $MF_{14.2}$ = 24.79
M7-ncER F2-ncER	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → (fur-CH)•S + H_2O (fur-CH)•S + 2H^+ + 2e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\,(\alpha_H)^2}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * K_3(\alpha_H)^2}{(1 + K_2[FF])}$	K2= 0.0518 K3f*k_{RDSFA}= 0.0013 K3m*k_{RDSMF}= 0.0039	-0.0414 0.1451 0.0002 0.0023 0.0019 0.0060	pH1 goes underestimate FA = 989.5 MF = 1522.5 $FA_{14.2}$ = 25.673 $MF_{14.2}$ = 25.514
M7-NCLH F4-NCLH	FF•S + H•T ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur- CHOH)•S + T (fur-CHOH)•S + H•T → (fur-CH)•S + H_2O + T (fur-CH)•S + 2H•T ⇌ MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3(K_1)^2(\alpha_H)^2}{(1 + K_2[FF])(1 + K_1\,\alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}}\, K_2\,[FF] K_3(K_1)^2\,(\alpha_H)^2}{(1 + K_2[FF]) * (1 + K_1\,\alpha_H)^2}$	K1= 27.4264 K2= 0.0425 K3*k_{RDSFA}= 0.0016 K3*k_{RDSMF}= 0.0043	20.3862 34.4667 0.0245 0.0605 0.0013 0.0019 0.0037 0.0049	FA pH1 underestimate FA = 257.4317 MF = 16.2129 $FA_{14.2}$ = 5.5874 $MF_{14.2}$ = 1.2443
M7-NCLH F4-ncER	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur- CHOH)•S + T (fur-CHOH)•S + H•T → (fur-CH)•S + H_2O + T (fur-CH)•S + 2H•T ⇌ MF•S + 2T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\,(\alpha_H)^2}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}}\, K_2\,[FF] K_3(K_1)^2\,(\alpha_H)^2}{(1 + K_2[FF]) * (1 + K_1\,\alpha_H)^2}$	K1= 25.0298 K2= 0.0416 K3*k_{RDSFA}= 0.0013 K3*k_{RDSMF}= 0.0044	12.4757 37.5840 0.0071 0.0760 0.0007 0.0019 0.0032 0.0057	FA pH1 underestimate FA = 962.1698 MF = 18.8943 $FA_{14.2}$ = 25.0032 $MF_{14.2}$ = 1.369
M7-cER F4-cER	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → (fur-CH)•S + H_2O (fur-CH)•S + 2H^+ + 2e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\,(\alpha_H)^2}{(1 + K_2[FF] + K_1\,\alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * K_3(\alpha_H)^2}{(1 + K_2[FF] + K_1\,\alpha_H)}$	K1= 49.9997 K2= 0.2382 K3*k_{RDSFA}= 0.0041 K3*k_{RDSMF}= 0.0124	-7987.5 8087.5 -37.4 37.9 -0.004834 0.01293 -0.01348 0.03829	pH1 underestimate pH 0 no plateau FA = 933.79 MF = 1424.6 $FA_{14.2}$ = 24.42 $MF_{14.2}$ = 24.243
M7-ncER F4-NCLH	FF•S + H•T ⇌ (fur-CHOH)•S + T K3 (fur-CHOH)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → (fur-CH)•S + H_2O (fur-CH)•S + 2H^+ + 2e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3(K_1)^2(\alpha_H)^2}{(1 + K_2[FF])(1 + K_1\,\alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * K_3(\alpha_H)^2}{(1 + K_2[FF])}$	K1= 54.4314 K2= 0.0400 K3*k_{RDSFA}= 0.0015 K3*k_{RDSMF}= 0.0041	-147.9319 256.7948 -0.0223 0.1023 0.0002 0.0027 0.0020 0.0062	MF pH1 underestimate FA = 127.45 MF = 1512.9 $FA_{14.2}$ = 2.8739 $MF_{14.2}$ = 24.79
M7-ncER F4-ncER	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → (fur-CH)•S + H_2O (fur-CH)•S + 2H^+ + 2e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3\,(\alpha_H)^2}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} * K_2[FF] * K_3(\alpha_H)^2}{(1 + K_2[FF])}$	K2= 0.0518 K3*k_{RDSFA}= 0.0013 K3*k_{RDSMF}= 0.0039	-0.0414 0.1451 0.0002 0.0023 0.0019 0.0060	pH1 underestimate FA = 989.5 MF = 1522.5 $FA_{14.2}$ = 25.673 $MF_{14.2}$ = 25.514

M8-NCLH F1-NCLH	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur- CHOH)•S + T K3 (fur-CHOH)•S + H•T ⇌ (fur-CH)•S + H_2O + T K4 (fur-CH)•S + 2H•T → MF•S + 2T MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_1\,\alpha_H}{(1+K_2[FF])(1+K_1\,\alpha_H)}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K1= 61.3608 K2= 0.0372 k_{RDSFA}= 0.0015 K3*K4*k_{RDSMF}= 0.0046	50.3976 72.3240 0.0262 0.0481 0.0013 0.0017 0.0041 0.0051	Good fit FA = 79.4092 MF = 16.7545 $FA_{14.2}$ = 1.8557 $MF_{14.2}$ = 1.125
M8-NCLH F1-ncER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur- CHOH)•S + T K3 (fur-CHOH)•S + H•T ⇌ (fur-CH)•S + H_2O + T K4 (fur-CH)•S + 2H•T → MF•S + 2T MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}*K_2[FF]*\alpha_H}{(1+K_2[FF])}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K1= 60.5516 K2= 0.0371 k_{RDSFA}= 0.0015 K3*K4*k_{RDSMF}= 0.0046	35.0190 86.0842 0.0106 0.0635 0.0009 0.0021 0.0035 0.0058	FA pH1 underestimate FA = 843.7316 MF = 16.3183 $FA_{14.2}$ = 21.0598 $MF_{14.2}$ = 1.1354
M8-cER F1-cER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- ⇌ (fur-CH)•S + H_2O K4 (fur-CH)•S + 2H^+ + 2e^- → MF•S MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}*K_2[FF]*\alpha_H}{(1+K_2[FF]+K_1\,\alpha_H)}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4\,(\alpha_H)^4}{(1+K_2[FF]+K_1\,\alpha_H)}$	K1= 69.9994 K2= 0.3498 k_{RDSFA}= 0.0045 K3*K4*k_{RDSMF}= 0.0118	-4.6972 4.8372 -0.0235 0.0242 -0.0000 0.0000 -0.0000 0.0000	pH1 underestimate pH0 no plateau FA = 432.14 MF = 1581.6 $FA_{14.2}$ = 12.003 $MF_{14.2}$ = 26.543
M8-ncER F1-NCLH	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- ⇌ (fur-CH)•S + H_2O K4 (fur-CH)•S + 2H^+ + 2e^- → MF•S MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_1\,\alpha_H}{(1+K_2[FF])(1+K_1\,\alpha_H)}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(\alpha_H)^4}{(1+K_2[FF])}$	K1= 53.5348 K2= 0.0380 k_{RDSFA}= 0.0014 K3*K4*k_{RDSMF}= 0.0042	-317.1332 424.2029 -0.0213 0.0973 0.0002 0.0026 0.0020 0.0063	MF pH1 underestimate FA = 73.769 MF = 1564.1 $FA_{14.2}$ = 1.8016 $MF_{14.2}$ = 25.488
M8-ncER F1-ncER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- ⇌ (fur-CH)•S + H_2O K4 (fur-CH)•S + 2H^+ + 2e^- → MF•S MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}*K_2[FF]*\alpha_H}{(1+K_2[FF])}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(\alpha_H)^4}{(1+K_2[FF])}$	K2= 0.0518 k_{RDSFA}= 0.0014 K3*K4*k_{RDSMF}= 0.0039	-0.0404 0.1440 0.0003 0.0024 0.0019 0.0059	pH1 underestimate FA = 867.38 MF = 1575.7 $FA_{14.2}$ = 21.932 $MF_{14.2}$ = 26.289
M8-NCLH F2-NCLH Different K3	FF•S + H•T ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur- CHOH)•S + T K3 (fur-CHOH)•S + H•T ⇌ (fur-CH)•S + H_2O + T K4 (fur-CH)•S + 2H•T → MF•S + 2T MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_3(K_1)^2(\alpha_H)^2}{(1+K_2[FF])(1+K_1\,\alpha_H)^2}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K1= 63.5271 K2= 0.0372 K3f*k_{RDSFA}= 0.0016 K3m*K4*k_{RDSMF}= 0.0046	51.2927 75.7615 0.0255 0.0489 0.0013 0.0018 0.0041 0.0051	Good fit FA = 128.7596 MF = 17.8285 $FA_{14.2}$ = 2.6676 $MF_{14.2}$ = 1.0935
M8-NCLH F2-ncER Different K3	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur- CHOH)•S + T K3 (fur-CHOH)•S + H•T ⇌ (fur-CH)•S + H_2O + T K4 (fur-CH)•S + 2H•T → MF•S + 2T MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_3\,(\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K1= 60.5522 K2= 0.0372 K3f*k_{RDSFA}= 0.0014 K3m*K4*k_{RDSMF}= 0.0046	32.7710 88.3335 0.0081 0.0662 0.0008 0.0020 0.0033 0.0059	FA pH1 underestimate FA = 970.1969 MF = 16.4139 $FA_{14.2}$ = 24.978 $MF_{14.2}$ = 1.1389
M8-cER F2-cER Different K3	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- ⇌ (fur-CH)•S + H_2O K4 (fur-CH)•S + 2H^+ + 2e^- → MF•S MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_3\,(\alpha_H)^2}{(1+K_2[FF]+K_1\,\alpha_H)}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4\,(\alpha_H)^4}{(1+K_2[FF]+K_1\,\alpha_H)}$	K1= 49.9997 K2= 0.2383 K3f*k_{RDSFA}= 0.00394 K3m*K4*k_{RDSMF}= 0.0124	-26430 26530 -123.1 123.6 -0.00533 0.0135 -0.0147 0.0392	pH1 underestimate pH0 no plateau FA = 933.68 MF = 1582.7 $FA_{14.2}$ = 24.419 $MF_{14.2}$ = 26.609
M8-ncER F2-NCLH Different K3	FF•S + H•T ⇌ (fur-CH_2O)•S + T K3 (fur-CH_2O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- ⇌ (fur-CH)•S + H_2O K4 (fur-CH)•S + 2H^+ + 2e^- → MF•S MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_3(K_1)^2(\alpha_H)^2}{(1+K_2[FF])(1+K_1\,\alpha_H)^2}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K1= 54.4314 K2= 0.0398 K3f*k_{RDSFA}= 0.0015 K3m*K4*k_{RDSMF}= 0.0041	-151.2809 260.1438 -0.0236 0.1033 0.0002 0.0027 0.0020 0.0062	MF pH1 underestimate FA = 127.27 MF = 1565 $FA_{14.2}$ = 2.8678 $MF_{14.2}$ = 25.551
M8-ncER F2-ncER Different K3	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- ⇌ (fur-CH)•S + H_2O K4 (fur-CH)•S + 2H^+ + 2e^- → MF•S MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_3\,(\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K2= 0.0517 K3f*k_{RDSFA}= 0.0013 K3m*K4*k_{RDSMF}= 0.0039	-0.0430 0.1464 0.0002 0.0023 0.0019 0.0060	pH1 underestimate FA = 127.27 MF = 1565 $FA_{14.2}$ = 2.8678 $MF_{14.2}$ = 25.551

M8-NCLH F4-NCLH Same K3	FF•S + H•T ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur- CHOH)•S + T K3 (fur-CHOH)•S + H•T ⇌ (fur-CH)•S + H_2O + T K4 (fur-CH)•S + 2H•T → MF•S + 2T MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_3(K_1)^2(\alpha_H)^2}{(1+K_2[FF])(1+K_1\,\alpha_H)^2}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K1= 63.5271 K2= 0.0372 K3*k_{RDSFA}= 0.0016 K3*K4*k_{RDSMF}= 0.0046	51.2927 75.7615 0.0255 0.0489 0.0013 0.0018 0.0041 0.0051	Good fit FA = 128.7596 MF = 17.8285 $FA_{14.2}$ = 2.6676 $MF_{14.2}$ = 1.0935
M8-NCLH F4-ncER Same K3	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H•T ⇌ (fur- CHOH)•S + T K3 (fur-CHOH)•S + H•T ⇌ (fur-CH)•S + H_2O + T K4 (fur-CH)•S + 2H•T → MF•S + 2T MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_3\,(\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K1= 60.5522 K2= 0.0372 K3*k_{RDSFA}= 0.0014 K3*K4*k_{RDSMF}= 0.0046	32.7710 88.3335 0.0081 0.0662 0.0008 0.0020 0.0033 0.0059	FA pH1 underestimate FA = 970.1969 MF = 16.4139 $FA_{14.2}$ = 24.978 $MF_{14.2}$ = 1.1389
M8-cER F4-cER Same K3	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- ⇌ (fur-CH)•S + H_2O K4 (fur-CH)•S + $2H^+$ + $2e^-$ → MF•S MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_3\,(\alpha_H)^2}{(1+K_2[FF]+K_1\,\alpha_H)}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4\,(\alpha_H)^4}{(1+K_2[FF]+K_1\,\alpha_H)}$	K1= 49.9997 K2= 0.2375 K3*k_{RDSFA}= 0.0041 K3*K4*k_{RDSMF}= 0.0122	-26430 26530 -123.1 123.6 -0.00533 0.0135 -0.0147 0.0392	No FA = 933.68 MF = 1582.7 $FA_{14.2}$ = 24.419 $MF_{14.2}$ = 26.609
M8-ncER F4-NCLH Same K3	FF•S + H•T ⇌ (fur-CHOH)•S + T K3 (fur-CHOH)•S + H•T → FA•S + T FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- ⇌ (fur-CH)•S + H_2O K4 (fur-CH)•S + $2H^+$ + $2e^-$ → MF•S MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_3(K_1)^2(\alpha_H)^2}{(1+K_2[FF])(1+K_1\,\alpha_H)^2}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K1= 54.4314 K2= 0.0398 K3*k_{RDSFA}= 0.0015 K3*K4*k_{RDSMF}= 0.0041	-151.2809 260.1438 -0.0236 0.1033 0.0002 0.0027 0.0020 0.0062	MF pH1 underestimate FA = 127.27 MF = 1565 $FA_{14.2}$ = 2.8678 $MF_{14.2}$ = 25.551
M8-ncER F4-ncER Same K3	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FF•S + H^+ + e^- ⇌ (fur-CHOH)•S K3 (fur-CHOH)•S + H^+ + e^- ⇌ (fur-CH)•S + H_2O K4 (fur-CH)•S + $2H^+$ + $2e^-$ → MF•S MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_3\,(\alpha_H)^2}{(1+K_2[FF])}$ $R_{MF}=\frac{k_{RDS_{MF}}\,K_2\,[FF]K_3K_4(K_1)^4(\alpha_H)^4}{(1+K_2[FF])*(1+K_1\,\alpha_H)^4}$	K2= 0.0517 K3*k_{RDSFA}= 0.0013 K3*K4*k_{RDSMF}= 0.0039	-0.0430 0.1464 0.0002 0.0023 0.0019 0.0060	pH1 underestimate FA = 127.27 MF = 1565 $FA_{14.2}$ = 2.8678 $MF_{14.2}$ = 25.551
M9 NCLH F1(3) NCLH	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H•T → (fur-CH_2)•S +H_2O + T (fur-CH_2)•S + H•T ⇌ MF•S + T MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_1\,\alpha_H}{(1+K_2[FF])(1+K_1\,\alpha_H)}$ $R_{MF}=\frac{k_{RDS_{MF}}k_{RDS_{FA}}K_2[FF](K_1)^3\,(\alpha_H)^3}{(1+K_2[FF])(1+K_1\,\alpha_H)^3}$	K1= 45.405 K2= 0.0373 k_{RDSFA}= 0.00152 k_{RDSMF}= 3.037	36.928 53.883 0.026187 0.048375 0.0013123 0.0017319 2.7016 3.3729	Good fit Large kMFrds FA = 97.524 MF = 18.527 $FA_{14.2}$ = 2.1401 $MF_{14.2}$ = 1.1337
M9 NCLH F1(3) ncER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H•T → (fur-CH_2)•S +H_2O + T (fur-CH_2)•S + H•T ⇌ MF•S + T MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}*K_2[FF]*\alpha_H}{(1+K_2[FF])}$ $R_{MF}=\frac{k_{RDS_{MF}}k_{RDS_{FA}}K_2[FF](K_1)^3(\alpha_H)^3}{(1+K_2[FF])(1+K_1\,\alpha_H)^3}$	K1= 44.378 K2= 0.0371 k_{RDSFA}= 0.00150 k_{RDSMF}= 3.093	25.191 63.565 0.0108 0.0634 0.000941 0.00207 2.080 4.105	pH1 FA underestimate FA = 846.14 MF = 17.659 $FA_{14.2}$ = 21.092 $MF_{14.2}$ = 1.15
M9 cER F1(3) cER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H^+ + e^- → (fur-CH_2)•S +H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}*K_2[FF]*\alpha_H}{(1+K_2[FF]+K_1\,\alpha_H)}$ $R_{MF}=\frac{k_{RDS_{MF}}k_{RDS_{FA}}*K_2[FF]*(\alpha_H)^3}{(1+K_2[FF]+K_1\,\alpha_H)}$	K1= 649.9927 K2= 3.07 k_{RDSFA}= 0.00715 k_{RDSMF}= 0.2705	-456660 457960 - 2164.3 2170.5 -0.020276 0.034575 -0.38756 0.9286	No FA = 405.77 MF = 1967.1 $FA_{14.2}$ = 17.382 $MF_{14.2}$ = 43.109
M9 ncER F1(3) NCLH	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H^+ + e^- → (fur-CH_2)•S +H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_1\,\alpha_H}{(1+K_2[FF])(1+K_1\,\alpha_H)}$ $R_{MF}=\frac{k_{RDS_{MF}}k_{RDS_{FA}}*K_2[FF]*(\alpha_H)^3}{(1+K_2[FF])}$	K1= 141.18 K2= 0.031123 k_{RDSFA}= 0.00155 k_{RDSMF}= 2.9713	-1957.9 2240.2 -0.014633 0.07688 0.00024462 0.0028494 0.86974 5.073	pH1 MF underestimate FA = 53.304 MF = 1556.4 $FA_{14.2}$ = 1.4333 $MF_{14.2}$ = 25.243
M9 ncER F1(3) ncER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H^+ + e^- → (fur-CH_2)•S +H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}*K_2[FF]*\alpha_H}{(1+K_2[FF])}$ $R_{MF}=\frac{k_{RDS_{MF}}k_{RDS_{FA}}*K_2[FF]*(\alpha_H)^3}{(1+K_2[FF])}$	K2= 0.0306 k_{RDSFA}= 0.0016 k_{RDSMF}= 2.901	-0.020187 0.081432 0.000242 0.0029619 0.96399 4.8388	pH 1 underestimate FA = 831.54 MF = 1556.3 $FA_{14.2}$ = 20.718 $MF_{14.2}$ = 25.242
M9 NCLH F2(4) NCLH	FF•S + H•T ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H•T → (fur-CH_2)•S +H_2O + T (fur-CH_2)•S + H•T ⇌ MF•S + T MF•S ⇌ MF + S	$R_{FA}=\frac{k_{RDS_{FA}}K_2[FF]K_3(K_1)^2(\alpha_H)^2}{(1+K_2[FF])(1+K_1\,\alpha_H)^2}$ $R_{MF}=\frac{k_{RDS_{MF}}k_{RDS_{FA}}K_2[FF](K_1)^3\,(\alpha_H)^3}{(1+K_2[FF])(1+K_1\,\alpha_H)^3}$	K1= 48.2854 K2= 0.0367 K3*k_{RDSFA}= 0.0016 k_{RDSMF}= 2.8087	38.1424 58.4283 0.0245 0.0489 0.0014 0.0019 2.4639 3.1536	Good fit Large kMFrds FA = 162.91 MF = 20.956 $FA_{14.2}$ = 3.2831 $MF_{14.2}$ = 1.0767

M9 NCLH F2(4) ncER	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H•T → (fur-CH_2)•S +H_2O + T (fur-CH_2)•S + H•T ⇌ MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 \, (\alpha_H)^2}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} k_{RDS_{FA}} K_2[FF](K_1)^3 \, (\alpha_H)^3}{(1 + K_2[FF])(1 + K_1 \, \alpha_H)^3}$	K1= 44.3802 K2= 0.0372 K3*k_{RDSFA}= 0.0014 k_{RDSMF}= 3.3353	23.4973 65.2632 0.0083 0.0662 0.0008 0.0020 2.0610 4.6096	pH1 FA underestimate FA = 972.06 MF = 17.74 $FA_{14.2}$ = 25.004 $MF_{14.2}$ = 1.1535
M9 cER F2(4) cER	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H^+ + e^- → (fur-CH_2)•S +H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 \, (\alpha_H)^2}{(1 + K_2[FF] + K_1 \, \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} k_{RDS_{FA}} * K_2[FF] * (\alpha_H)^3}{(1 + K_2[FF] + K_1 \, \alpha_H)}$	K1= 50 K2= 0.2431 K3*k_{RDSFA}= 0.00446 k_{RDSMF}= 0.0392	-41190 41290 -196.76 197.25 -0.041636 0.050553 -1.0806 1.1589	No FA = 904.79 MF = 2082.3 $FA_{14.2}$ = 24.277 $MF_{14.2}$ = 48.834
M9 ncER F2(4) NCLH	FF•S + H•T ⇌ (fur-CH_2O)•S + T K3 (fur-CH_2O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H^+ + e^- → (fur-CH_2)•S +H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 (K_1)^2 (\alpha_H)^2}{(1 + K_2[FF])(1 + K_1 \, \alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}} k_{RDS_{FA}} * K_2[FF] * (\alpha_H)^3}{(1 + K_2[FF])}$	K1= 174.39 K2= 0.031124 K3*k_{RDSFA}= 0.001519 k_{RDSMF}= 2.9932	-1476 1825 -0.01539 0.07764 0.0002139 0.002824 0.83026 5.1561	pH1 MF underestimate FA = 56.199 MF = 1556.1 $FA_{14.2}$ = 1.3878 $MF_{14.2}$ = 25.215
M9 ncER F2(4) ncER	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H^+ + e^- → (fur-CH_2)•S +H_2O (fur-CH_2)•S + H^+ + e^- ⇌ MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 \, (\alpha_H)^2}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} k_{RDS_{FA}} * K_2[FF] * (\alpha_H)^3}{(1 + K_2[FF])}$	K2= 0.0310 K3*k_{RDSFA}= 0.0015 k_{RDSMF}= 3.1173	-0.0220 0.0840 0.000136 0.00283 0.8350 5.3995	pH1 underestimate FA = 960.83 MF = 1556.5 $FA_{14.2}$ = 24.721 $MF_{14.2}$ = 25.246
M10 NCLH F1(3) NCLH	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H•T ⇌ (fur-CH_2)•S +H_2O + T (fur-CH_2)•S + H•T → MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_1 \, \alpha_H}{(1 + K_2[FF])(1 + K_1 \, \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} k_{RDS_{FA}} K_2[FF] K_3 (K_1)^4 (\alpha_H)^4}{(1 + K_2[FF])(1 + K_1 \, \alpha_H)^4}$	K1= 61.79 K2= 0.0371 k_{RDSFA}= 0.00149 K3*k_{RDSMF}= 3.107	50.795 72.788 0.026264 0.047877 0.0012902 0.0016922 2.769 3.445	Good fit FA = 80.986 MF = 18.183 $FA_{14.2}$ = 1.8824 $MF_{14.2}$ = 1.1368
M10 NCLH F1(3) ncER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H•T ⇌ (fur-CH_2)•S +H_2O + T (fur-CH_2)•S + H•T → MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} k_{RDS_{FA}} K_2[FF] K_3 (K_1)^4 (\alpha_H)^4}{(1 + K_2[FF])(1 + K_1 \, \alpha_H)^4}$	K1= 44.3777 K2= 0.0371 k_{RDSFA}= 0.0015 K3*k_{RDSMF}= 3.0926	25.1909 63.5645 0.0108 0.0634 0.0009 0.0021 2.0802 4.1049	pH1 FA underestimate FA = 845.5 MF = 17.52 $FA_{14.2}$ = 21.076 $MF_{14.2}$ = 1.1433
M10 cER F1(3) cER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H^+ + e^- ⇌ (fur-CH_2)•S +H_2O (fur-CH_2)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1 + K_2[FF] + K_1 \, \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} k_{RDS_{FA}} K_2[FF] K_3 \, (\alpha_H)^4}{(1 + K_2[FF] + K_1 \, \alpha_H)}$	K1= 649.9927 K2= 3.0700 k_{RDSFA}= 0.00715 K3*k_{RDSMF}= 0.2705	-456990 458290 -2166 2172 -0.0202 0.0346 -0.3848 0.9292	No FA = 405.46 MF = 1969.4 $FA_{14.2}$ = 17.363 $MF_{14.2}$ = 43.143
M10 ncER F1(3) NCLH	FF•S + H•T → (fur-CH_2O)•S + T (fur-CH_2O)•S + H•T ⇌ FA•S + T FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H^+ + e^- ⇌ (fur-CH_2)•S +H_2O (fur-CH_2)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_1 \, \alpha_H}{(1 + K_2[FF])(1 + K_1 \, \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} k_{RDS_{FA}} K_2[FF] K_3 \, (\alpha_H)^4}{(1 + K_2[FF])}$	K1= 141.18 K2= 0.03111 k_{RDSFA}= 0.00155 K3*k_{RDSMF}= 2.97	-1961 2244 -0.0147 0.0769 0.000242 0.00285 0.8661 5.074	pH1 MF underestimate FA = 53.281 MF = 1561.3 $FA_{14.2}$ = 1.4327 $MF_{14.2}$ = 25.314
M10 ncER F1(3) ncER	FF•S + H^+ + e^- → (fur-CH_2O)•S (fur-CH_2O)•S + H^+ + e^- ⇌ FA•S FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H^+ + e^- ⇌ (fur-CH_2)•S +H_2O (fur-CH_2)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} * K_2[FF] * \alpha_H}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} k_{RDS_{FA}} K_2[FF] K_3 \, (\alpha_H)^4}{(1 + K_2[FF])}$	K2= 0.0306 k_{RDSFA}= 0.0016 K3*k_{RDSMF}= 2.9014	-0.0202 0.0814 0.0002 0.0030 0.9640 4.8388	pH1 underestimate FA = 831.51 MF = 1561.3 $FA_{14.2}$ = 20.718 $MF_{14.2}$ = 25.313
M10 NCLH F2(4) NCLH	FF•S + H•T ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H•T ⇌ (fur-CH_2)•S +H_2O + T (fur-CH_2)•S + H•T → MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 (K_1)^2 (\alpha_H)^2}{(1 + K_2[FF])(1 + K_1 \, \alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}} k_{RDS_{FA}} K_2[FF] K_3 (K_1)^4 (\alpha_H)^4}{(1 + K_2[FF])(1 + K_1 \, \alpha_H)^4}$	K1= 64.0528 K2= 0.0371 K3f*k_{RDSFA}= 0.0016 K3m*k_{RDSMF}= 2.9081	51.7728 76.3328 0.0255 0.0487 0.0014 0.0018 2.5722 3.2440	Good fit FA = 131.1 MF = 19.914 $FA_{14.2}$ = 2.7014 $MF_{14.2}$ = 1.1121
M10 NCLH F2(4) ncER	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H•T ⇌ (fur-CH_2)•S +H_2O + T (fur-CH_2)•S + H•T → MF•S + T MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 \, (\alpha_H)^2}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} k_{RDS_{FA}} K_2[FF] K_3 (K_1)^4 (\alpha_H)^4}{(1 + K_2[FF])(1 + K_1 \, \alpha_H)^4}$	K1= 60.9433 K2= 0.0370 K3f*k_{RDSFA}= 0.0014 K3m*k_{RDSMF}= 3.3302	33.0553 88.8314 0.0083 0.0656 0.0008 0.0020 2.0587 4.6017	pH1 FA underestimate FA = 971.43 MF = 17.569 $FA_{14.2}$ = 24.988 $MF_{14.2}$ = 1.1456
M10 cER F2(4) cER	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H^+ + e^- ⇌ (fur-CH_2)•S +H_2O (fur-CH_2)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2[FF] K_3 \, (\alpha_H)^2}{(1 + K_2[FF] + K_1 \, \alpha_H)}$ $R_{MF} = \frac{k_{RDS_{MF}} k_{RDS_{FA}} K_2[FF] K_3 \, (\alpha_H)^4}{(1 + K_2[FF] + K_1 \, \alpha_H)}$	K1= 49.9997 K2= 0.2431 K3f*k_{RDSFA}= 0.0045 K3m*k_{RDSMF}= 0.0392	-41198 41298 -196.1 196.7 -0.0416 0.0506 -1.078 1.156	No FA = 904.82 MF = 2082.5 $FA_{14.2}$ = 24.277

						$MF_{14.2}$ = 48.837
M10 ncER F2(4) NCLH	FF•S + H•T ⇌ (fur-CH_2O)•S + T K3 (fur-CH_2O)•S + H•T → FA•S + T FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H^+ + e^- ⇌ (fur-CH_2)•S +H_2O (fur-CH_2)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2 [FF] K_3 (K_1)^2 (\alpha_H)^2}{(1 + K_2[FF])(1 + K_1\,\alpha_H)^2}$ $R_{MF} = \frac{k_{RDS_{MF}} k_{RDS_{FA}} K_2 [FF] K_3\,(\alpha_H)^4}{(1 + K_2[FF])}$	K1= 174.39 K2= 0.0311 K3f*k_{RDSFA}= 0.00151 K3m*k_{RDSMF}= 2.9916	-1451.5 1800.3 -0.01548 0.07770 0.0002118 0.00283 0.8265 5.157	pH1 MF underestimate FA = 56.189 MF = 1560.9 $FA_{14.2}$ = 1.3874 $MF_{14.2}$ = 25.285
M10 ncER F2(4) ncER	FF•S + H^+ + e^- ⇌ (fur-CH_2O)•S K3 (fur-CH_2O)•S + H^+ + e^- → FA•S FA•S ⇌ FA + S	FA•S ⇌ FA + S FA•S + H^+ + e^- ⇌ (fur-CH_2)•S +H_2O (fur-CH_2)•S + H^+ + e^- → MF•S MF•S ⇌ MF + S	$R_{FA} = \frac{k_{RDS_{FA}} K_2 [FF] K_3\,(\alpha_H)^2}{(1 + K_2[FF])}$ $R_{MF} = \frac{k_{RDS_{MF}} k_{RDS_{FA}} K_2 [FF] K_3\,(\alpha_H)^4}{(1 + K_2[FF])}$	K2= 0.0310 K3f*k_{RDSFA}= 0.0015 K3m*k_{RDSMF}= 3.1156	-0.0221 0.0841 0.000134 0.0028 0.8318 5.3995	pH1 underestimate FA = 960.81 MF = 1561.4 $FA_{14.2}$ = 24.721 $MF_{14.2}$ = 25.317