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K-368-M

SUPPLEMENTARY MATERIAL FOR THE MICROFILM EDITION

Table 1. Values of $T_1(D)$, $T_{1\rho}(D)$ and $T_1(I_zC_z)$ in ms at 500 and 600 Mz for the free PLCC SH2 domain (A) and the pY1021 complex (B). Errors are provided in parentheses.

A. Free PLCC SH2

	500 MHz			600 MHz		
Residue	$T_1(D)$	$T_{1\rho}(D)$	$T_1(I_zC_z)$	$T_1(D)$	$T_{1\rho}(D)$	$T_1(I_zC_z)$
A5	64.50 (0.69)	24.80 (0.16)	381.35 (11.9)	67.19 (1.43)	27.57 (0.37)	436.53 (8.63)
A14	43.72 (1.69)	9.32 (0.16)	288.05 (13.2)	51.34 (1.09)	9.74 (0.10)	322.37 (7.83)
L16δ1[a]	27.38 (3.64)	8.58 (1.13)	177.74 (17.2)	20.83 (5.56)	8.68 (1.20)	156.70 (8.50)
T17	51.26 (1.18)	9.15 (0.39)	259.98 (10.77)	61.84 (2.13)	9.33 (0.14)	296.55 (21.88)
A19	37.55 (1.16)	8.24 (0.13)	258.42 (8.73)	39.41 (1.06)	8.80 (0.36)	282.11 (12.14)
A21	34.58 (0.91)	8.21 (0.44)	174.28 (3.63)	36.86 (1.36)	7.64 (0.27)	178.61 (6.33)
M24	137.10 (3.88)	37.52 (0.96)	603.40 (22.89)	155.09 (7.36)	38.53 (1.25)	670.47 (32.49)
L25δ2[a]	47.32 (2.10)	11.43 (0.45)	233.09 (10.21)	51.65 (1.00)	12.67 (0.68)	257.13 (11.25)
M26	152.21 (3.36)	41.53 (1.48)	984.21 (74.74)	184.50 (6.86)	44.28 (1.27)	1094.67 (100.7)
V28γ1	46.51 (1.29)	12.69 (0.34)	321.60 (14.07)	57.21 (1.46)	13.53 (0.18)	336.25 (7.75)
V28γ2	44.94 (0.83)	15.16 (0.47)	296.61 (6.80)	48.62 (1.00)	14.64 (0.19)	331.45 (9.48)
A33	41.40 (1.59)	8.05 (0.25)	225.41 (9.80)	49.79 (1.76)	8.51 (0.14)	256.41 (12.70)
L35δ1	48.58 (6.30)	9.68 (0.50)	163.03 (19.55)	57.95 (2.36)	12.05 (0.41)	206.16 (12.33)
L35δ2	30.41 (2.36)	11.42 (0.97)	178.94 (11.60)	40.08 (3.09)	10.01 (0.84)	180.75 (9.23)
V36γ1	40.47 (2.00)	10.63 (0.35)	221.17 (10.78)	45.39 (1.88)	11.09 (0.37)	210.05 (6.11)
V36γ2	54.58 (4.13)	8.85 (0.29)	200.19 (4.47)	63.82 (3.38)	9.57 (0.24)	215.16 (7.47)
A46	55.81 (1.23)	9.31 (0.33)	267.54 (16.83)	72.21 (3.11)	10.10 (0.57)	271.20 (15.31)

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I47δ	80.38 (3.38)	12.29 (0.39)	269.64 (11.08)	94.47 (6.82)	12.70 (0.48)	330.47 (29.39)
I47γ2	55.61 (1.31)	10.60 (0.22)	250.03 (8.02)	71.04 (2.37)	11.05 (0.30)	260.77 (13.47)
A51	28.05 (0.88)	7.92 (0.29)	190.56 (5.63)	28.76 (0.80)	7.41 (0.13)	208.67 (4.54)
I55δ	59.86 (2.51)	16.96 (0.53)	319.92 (29.89)	70.91 (2.09)	18.59 (0.28)	326.15 (13.81)
I55γ2	46.19 (1.31)	9.65 (0.17)	210.43 (5.80)	55.07 (2.31)	10.21 (0.33)	253.58 (12.42)
V60γ1	34.48 (0.91)	10.42 (0.35)	192.00 (3.71)	34.10 (0.83)	10.88 (0.26)	218.07 (6.05)
V60γ2	40.84 (1.05)	12.27 (0.42)	228.97 (3.48)	46.13 (1.22)	13.18 (0.35)	258.79 (8.20)
T66	29.91 (1.04)	12.66 (0.38)	233.31 (5.66)	34.33 (0.71)	13.40 (0.38)	271.80 (5.97)
V67γ1	36.29 (0.60)	16.34 (0.23)	239.59 (5.69)	41.07 (0.83)	16.82 (0.30)	262.86 (5.27)
V67γ2	28.50 (0.79)	14.17 (0.34)	184.74 (3.80)	30.08 (0.44)	14.26 (0.07)	209.48 (2.67)
M68	159.40 (2.79)	51.44 (2.52)	728.59 (45.60)	176.01 (4.96)	54.24 (2.42)	876.70 (50.74)
L69δ1	58.32 (1.19)	25.62 (0.37)	295.40 (10.29)	65.66 (1.78)	28.16 (0.64)	299.51 (6.85)
L69δ2	60.82 (1.27)	26.97 (0.91)	305.40 (12.63)	62.89 (1.95)	25.96 (0.55)	336.72 (13.79)
L77δ1	46.26 (0.95)	19.28 (0.47)	251.34 (6.61)	50.02 (0.81)	19.99 (0.47)	264.68 (11.80)
L77δ2	46.51 (1.01)	19.97 (0.47)	249.36 (6.95)	52.25 (1.10)	21.86 (0.41)	244.36 (6.75)
V78γ1	33.81 (0.42)	12.80 (0.22)	239.81 (5.05)	36.32 (0.70)	13.70 (0.30)	270.12 (4.00)
V78γ2	43.20 (0.80)	14.27 (0.25)	246.30 (9.50)	49.89 (1.23)	14.62 (0.23)	278.91 (8.34)
L80δ1	44.06 (4.21)	14.06 (1.31)	209.51 (22.04)	48.05 (3.22)	14.75 (0.64)	221.24 (9.39)
L80δ2	48.46 (4.04)	13.76 (1.17)	195.46 (32.88)	66.11 (4.26)	15.02 (0.54)	190.80 (16.82)
I81δ	73.13 (3.05)	13.74 (0.50)	224.22 (9.71)	85.05 (3.13)	13.58 (0.32)	255.21 (12.37)
I81γ2	37.98 (1.82)	7.51 (0.16)	219.32 (7.77)	39.26 (1.89)	8.41 (0.35)	229.66 (11.14)
L89δ1	49.74 (1.04)	12.02 (0.61)	276.24 (8.44)	54.26 (2.10)	12.48 (0.72)	294.22 (21.05)
L89δ2	36.12 (2.66)	11.42 (1.21)	179.66 (9.12)	44.46 (5.99)	11.11 (0.81)	178.88 (10.71)
M93	68.11 (0.92)	24.14 (0.85)	335.50 (7.69)	78.43 (2.77)	23.77 (0.50)	365.70 (13.47)
L95δ1	16.66 (1.17)	6.20 (0.45)	129.14 (5.19)	23.02 (1.69)	7.81 (0.49)	137.92 (3.54)
L95δ2	63.03 (3.08)	9.95 (0.47)	229.68 (8.38)	84.51 (3.11)	9.78 (0.24)	249.84 (13.75)

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I99δ	73.78 (2.50)	21.10 (0.90)	324.64 (11.45)	82.55 (2.98)	21.97 (0.56)	353.71 (16.15)
I99γ2	50.85 (0.96)	11.18 (0.11)	271.06 (9.70)	57.61 (1.76)	11.42 (0.14)	298.06 (16.25)

B. PLCC SH2-pY1021 Complex

	500 MHz			600 MHz		
Residue	$T_1(D)$	$T_{1\rho}(D)$	$T_1(I_zC_z)$	$T_1(D)$	$T_{1\rho}(D)$	$T_1(I_zC_z)$
A5	62.40 (0.71)	27.30 (0.47)	383.27 (11.10)	65.32 (0.90)	27.72 (0.31)	447.50 (12.41)
A14	46.53 (1.16)	11.61 (0.29)	292.57 (7.83)	49.80 (0.51)	10.66 (0.15)	294.21 (10.80)
L16δ1[a]	19.43 (1.27)	9.87 (0.65)	154.30 (13.84)	19.71 (2.83)	7.99 (0.70)	191.76 (7.37)
T17	50.75 (1.10)	9.59 (0.25)	314.58 (17.73)	57.96 (1.14)	10.11 (0.36)	325.00 (14.05)
A19	36.40 (0.72)	9.55 (0.30)	271.76 (11.27)	41.38 (1.02)	9.40 (0.18)	285.33 (8.56)
A21	34.18 (0.81)	8.78 (0.54)	173.35 (3.33)	39.21 (1.39)	9.24 (0.38)	178.94 (3.61)
M24	131.68 (3.57)	42.25 (1.58)	659.04 (26.84)	152.31 (3.21)	41.61 (0.75)	735.65 (39.74)
L25δ2[a]	43.51 (1.44)	12.44 (0.57)	237.18 (7.32)	50.17 (3.16)	12.53 (0.85)	298.26 (18.27)
M26	150.67 (2.68)	47.76 (2.21)	933.73 (28.67)	174.72 (3.71)	45.36 (1.29)	1083.82 (88.37)
V28γ1	51.11 (1.34)	13.83 (0.34)	333.99 (26.45)	54.55 (1.42)	13.71 (0.20)	387.32 (18.16)
V28γ2	44.38 (0.82)	15.31 (0.21)	298.24 (9.87)	48.52 (0.93)	15.01 (0.40)	342.47 (14.00)
A33	44.77 (1.41)	9.03 (0.39)	233.62 (6.39)	48.63 (0.65)	9.35 (0.29)	246.03 (5.55)
L35δ1	50.77 (5.15)	10.17 (0.74)	213.28 (24.96)	62.84 (4.98)	11.16 (0.85)	185.78 (9.46)
L35δ2	33.86 (2.62)	9.80 (0.73)	191.97 (9.91)	32.96 (2.80)	9.95 (0.29)	212.45 (13.43)
V36γ1	40.63 (1.13)	10.38 (0.21)	226.22 (2.52)	39.49 (1.47)	10.89 (0.33)	251.11 (10.77)
V36γ2	53.79 (2.19)	10.03 (0.42)	219.62 (7.14)	59.33 (1.79)	9.97 (0.25)	242.27 (10.98)
A46	57.98 (2.91)	9.16 (0.28)	250.24 (11.52)	72.39 (2.97)	10.23 (0.17)	290.70 (13.29)
I47δ[b]	77.73 (3.64)	13.83 (0.50)	272.22 (7.85)	91.94 (3.72)	13.55 (0.18)	309.00 (15.14)
A51	27.92 (0.86)	7.71 (0.34)	196.00 (3.34)	29.21 (0.83)	8.23 (0.28)	198.94 (7.73)

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I55δ	60.80 (1.14)	17.04 (0.95)	314.78 (11.73)	68.40 (4.57)	17.89 (1.16)	333.48 (13.96)
I55γ2	47.98 (1.28)	10.79 (0.34)	232.56 (10.98)	55.05 (1.20)	10.78 (0.31)	258.99 (9.92)
V60γ1	33.67 (1.07)	11.72 (0.26)	207.40 (5.52)	35.72 (0.97)	11.98 (0.28)	209.08 (4.69)
V60γ2	39.14 (1.20)	11.63 (0.27)	217.19 (5.72)	46.47 (1.40)	13.40 (0.25)	253.97 (6.84)
T66	29.37 (0.51)	13.76 (0.34)	258.95 (7.99)	33.44 (0.63)	14.23 (0.46)	305.79 (10.71)
V67γ1	36.22 (0.78)	16.81 (0.49)	242.59 (4.76)	39.13 (0.58)	17.64 (0.39)	267.89 (7.06)
V67γ2	26.95 (0.70)	14.29 (0.33)	191.08 (3.63)	28.81 (0.36)	15.16 (0.51)	213.99 (5.41)
M68	176.44 (2.91)	76.45 (5.69)	851.42 (25.08)	192.59 (4.20)	78.63 (3.38)	1091.43 (75.95)
L69δ1	51.20 (1.55)	26.45 (1.25)	274.87 (11.34)	56.01 (1.73)	26.96 (1.15)	293.06 (9.60)
L69δ2	50.09 (1.90)	25.71 (0.80)	214.41 (9.60)	48.98 (0.96)	26.20 (0.84)	251.27 (8.51)
L77δ1	44.19 (1.06)	20.32 (0.74)	277.77 (10.44)	45.69 (0.87)	21.68 (0.73)	291.39 (9.04)
L77δ2	48.17 (1.41)	24.39 (0.71)	236.70 (8.38)	51.55 (1.20)	22.57 (0.84)	263.55 (7.97)
V78γ1	33.50 (0.65)	13.45 (0.33)	243.76 (7.76)	36.71 (0.45)	14.79 (0.20)	267.79 (7.72)
V78γ2	43.17 (1.07)	14.87 (0.42)	265.66 (8.38)	47.39 (0.64)	15.47 (0.32)	293.27 (8.61)
L80δ1	49.81 (4.11)	13.14 (1.05)	191.47 (18.04)	48.96 (2.60)	17.96 (1.24)	218.65 (16.25)
L80δ2	42.57 (3.94)	17.11 (2.05)	190.94 (19.50)	52.53 (4.88)	16.72 (1.03)	222.75 (15.83)
I81δ	69.23 (4.31)	14.45 (0.58)	251.44 (8.04)	82.33 (5.70)	15.61 (0.70)	265.44 (5.35)
I81γ2	34.91 (0.93)	9.35 (0.22)	213.41 (9.68)	38.46 (1.20)	9.21 (0.21)	219.14 (13.64)
L89δ1	46.04 (3.26)	14.04 (0.58)	223.74 (12.47)	46.18 (2.46)	13.64 (0.55)	237.49 (12.13)
L89δ2	33.59 (3.43)	13.88 (2.02)	152.30 (10.66)	44.92 (5.40)	12.52 (1.61)	178.71 (26.50)
M93	68.32 (1.34)	22.77 (0.60)	342.50 (15.34)	85.79 (2.38)	22.62 (0.86)	335.06 (17.18)
L95δ1	16.79 (2.08)	6.49 (0.30)	138.73 (7.60)	22.47 (2.08)	8.50 (0.40)	144.42 (3.16)
L95δ2	54.90 (2.05)	10.53 (0.30)	270.69 (18.43)	77.59 (3.25)	10.47 (0.36)	269.83 (8.64)
I99δ[b]	77.85 (2.88)	20.99 (0.61)	353.75 (17.75)	87.88 (2.41)	23.20 (0.70)	382.41 (17.73)

[a]Peaks for L16δ2 and L25δ1 overlap. [b]I47γ2 overlaps with I99γ2.

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Table 2. Values of S^2_{axis} and τ_e for the free PLCC SH2 domain and the pY1021 complex.

	Free PLCC SH2		PLCC SH2 - pY1021 Complex	
Residue	S^2_{axis}	τ_e (ns)	S^2_{axis}	τ_e (ns)
A5	0.220 (0.002)	0.033 (0.000)	0.221 (0.004)	0.033 (0.000)
A14	0.761 (0.008)	0.038 (0.001)	0.765 (0.011)	0.036 (0.001)
L16δ1[a]	0.691 (0.110)	0.088 (0.014)	0.640 (0.067)	0.118 (0.008)
T17	0.825 (0.016)	0.029 (0.001)	0.884 (0.019)	0.026 (0.001)
A19	0.844 (0.016)	0.051 (0.001)	0.864 (0.019)	0.046 (0.001)
A21	0.917 (0.036)	0.054 (0.002)	0.891 (0.044)	0.050 (0.002)
M24	0.176 (0.005)	0.013 (0.000)	0.184 (0.004)	0.013 (0.000)
L25δ2[a]	0.581 (0.028)	0.039 (0.001)	0.620 (0.034)	0.040 (0.002)
M26	0.156 (0.005)	0.012 (0.000)	0.169 (0.006)	0.011 (0.000)
V28γ1	0.511 (0.008)	0.038 (0.001)	0.580 (0.010)	0.034 (0.001)
V28γ2	0.428 (0.008)	0.045 (0.001)	0.464 (0.008)	0.043 (0.001)
A33	0.891 (0.014)	0.039 (0.002)	0.921 (0.025)	0.035 (0.001)
L35δ1	0.654 (0.026)	0.033 (0.002)	0.818 (0.053)	0.025 (0.003)
L35δ2	0.598 (0.055)	0.062 (0.004)	0.765 (0.043)	0.060 (0.006)
V36γ1	0.626 (0.020)	0.047 (0.002)	0.739 (0.017)	0.046 (0.002)
V36γ2	0.828 (0.020)	0.026 (0.002)	0.883 (0.022)	0.025 (0.001)
A46	0.807 (0.029)	0.025 (0.001)	0.918 (0.015)	0.017 (0.001)
I47δ	0.623 (0.017)	0.016 (0.001)	0.670 (0.010)	0.014 (0.001)
I47γ2	0.695 (0.014)	0.027 (0.001)	a	a
A51	0.899 (0.020)	0.075 (0.002)	0.955 (0.033)	0.070 (0.002)
I55δ	0.365 (0.009)	0.030 (0.001)	0.445 (0.026)	0.029 (0.001)

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I55γ2	0.741 (0.014)	0.036 (0.001)	0.783 (0.024)	0.031 (0.001)
V60γ1	0.582 (0.018)	0.063 (0.002)	0.591 (0.015)	0.060 (0.002)
V60γ2	0.502 (0.017)	0.048 (0.001)	0.599 (0.014)	0.045 (0.002)
T66	0.420 (0.015)	0.069 (0.001)	0.423 (0.015)	0.071 (0.001)
V67γ1	0.311 (0.007)	0.059 (0.001)	0.336 (0.012)	0.058 (0.001)
V67γ2	0.333 (0.005)	0.079 (0.001)	0.350 (0.016)	0.081 (0.001)
M68	0.118 (0.005)	0.012 (0.000)	0.080 (0.005)	0.011 (0.000)
L69δ1	0.196 (0.004)	0.036 (0.001)	0.201 (0.014)	0.041 (0.001)
L69δ2	0.201 (0.007)	0.036 (0.001)	0.191 (0.010)	0.046 (0.001)
L77δ1	0.275 (0.008)	0.046 (0.001)	0.270 (0.011)	0.049 (0.001)
L77δ2	0.248 (0.007)	0.045 (0.001)	0.237 (0.012)	0.044 (0.001)
V78γ1	0.430 (0.009)	0.064 (0.001)	0.442 (0.009)	0.061 (0.001)
V78γ2	0.431 (0.008)	0.046 (0.001)	0.468 (0.012)	0.044 (0.001)
L80δ1	0.429 (0.027)	0.046 (0.003)	0.478 (0.038)	0.041 (0.003)
L80δ2	0.462 (0.025)	0.034 (0.002)	0.416 (0.039)	0.043 (0.004)
I81δ	0.556 (0.015)	0.020 (0.001)	0.571 (0.021)	0.020 (0.002)
I81γ2	0.936 (0.025)	0.049 (0.002)	0.860 (0.022)	0.050 (0.002)
L89δ1	0.567 (0.032)	0.037 (0.001)	0.536 (0.023)	0.043 (0.003)
L89δ2	0.579 (0.055)	0.055 (0.005)	0.544 (0.103)	0.055 (0.007)
M93	0.255 (0.007)	0.030 (0.001)	0.326 (0.010)	0.025 (0.001)
L95δ1	0.830 (0.069)	0.124 (0.009)	0.936 (0.068)	0.113 (0.011)
L95δ2	0.814 (0.020)	0.018 (0.001)	0.852 (0.024)	0.019 (0.001)
I99δ	0.304 (0.009)	0.026 (0.001)	0.356 (0.012)	0.021 (0.001)
I99γ2	0.634 (0.007)	0.034 (0.001)	a	a

[a]L16δ2 and L25δ1 overlap in spectra of free SH2; L16δ2 and I47γ2 overlap with L25δ1 and I99γ2, respectively, in spectra of the PLCC SH2-pY1021 complex.