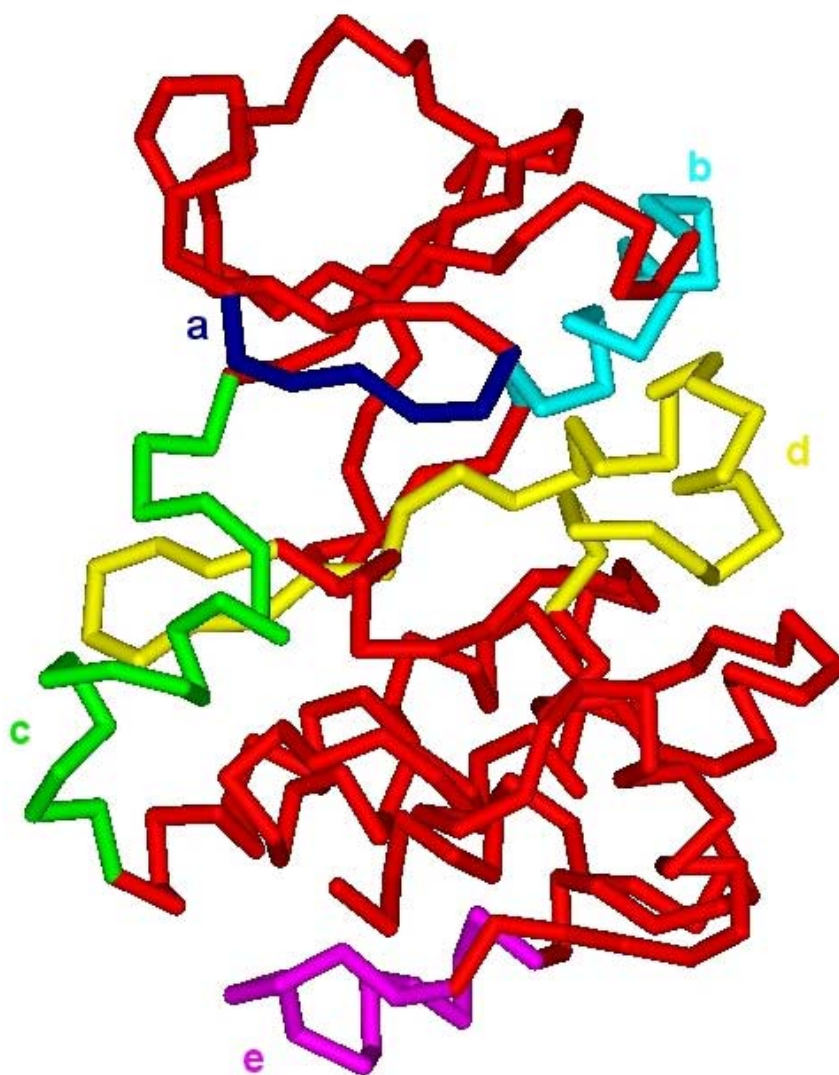


Electronic Supplementary Material

Jesús Mendieta and Federico Gago

In silico Activation of Src Tyrosine Kinase Reveals the Molecular Basis for Intramolecular Autophosphorylation

Figure 1. C α trace of Src tyrosine kinase catalytic domain highlighting in different colours the structural regions (a–e) depicted in Figure 2 of the main text.

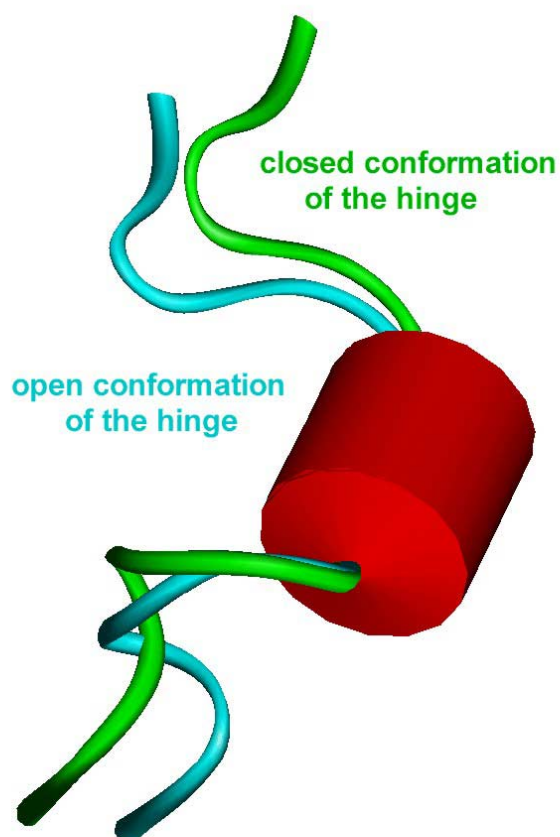


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Figure 2. Detailed view of the hinge region in both the open (cyan ribbon) and closed forms of the Src holoenzyme. Helix C (red cylinder) has been used for superimposing both structures so as to highlight strand displacements. This supplement is available in JPEG format (Mendieta_Supp.jpg).



AMBER PREP file for ADP

0 0 2

ADP3-

atf.data

ADF INT 1
CORRECT OMIT DU BEG

0.0							
	ADF	INT	DU	BEG			
1	DU	DU	M	0.000000	0.000000	0.000000	0.000000
2	DU	DU	M	1.000000	0.000000	0.000000	0.000000
3	DU	DU	M	1.000000	1.000000	0.000000	0.000000
4	O3B	OS	M	11.229000	-0.104000	-0.773000	-0.930618
5	PB	P	M	10.837000	-1.684000	-0.609000	1.279020
6	O1B	O2	E	9.367000	-1.694000	-0.593000	-0.930618
7	O2B	O2	E	11.536000	-2.345000	0.506000	-0.930618
8	O3A	OS	M	11.375000	-2.315000	-1.963000	-0.317167
9	PA	P	M	10.677000	-2.716000	-3.347000	1.073710
10	O1A	O2	E	9.984000	-4.014000	-3.162000	-0.972744
11	O2A	O2	E	9.855000	-1.611000	-3.892000	-0.972744
12	O5'	OS	M	11.901000	-2.931000	-4.268000	-0.449500
13	C5'	CT	M	12.765000	-1.786000	-4.647000	-0.022553
14	H5'1	H1	E	13.528000	-1.640000	-3.883000	0.118770
15	H5'2	H1	E	12.157000	-0.885000	-4.730000	0.118770
16	C4'	CT	M	13.390000	-2.056000	-5.899000	0.122030
17	H4'	H1	E	13.964000	-1.175000	-6.187000	0.166850
18	O4'	OS	E	14.279000	-3.162000	-5.900000	-0.386076
19	C3'	CT	M	12.338000	-2.346000	-6.976000	0.138880
19	H3'	H1	E	11.378000	-1.893000	-6.730000	0.053710
20	O3'	OH	S	12.742000	-1.826000	-8.266000	-0.628799
21	HO'3	HO	E	11.914000	-1.483000	-8.773000	0.411280
22	C2'	CT	M	12.366000	-3.864000	-7.106000	0.133400
23	H2'	H1	E	11.669000	-4.255000	-6.366000	0.097320
24	O2'	OH	S	12.010000	-4.491000	-8.327000	-0.603634
25	HO'2	HO	E	11.258000	-3.954000	-8.782000	0.389400
26	C1'	CT	M	13.876000	-4.170000	-6.859000	0.096000
27	H1'	H1	E	14.458000	-4.089000	-7.777000	0.129180
28	N9	N*	M	13.988000	-5.428000	-6.075000	-0.023033
29	C8	CK	M	13.098000	-5.951000	-5.127000	0.078510
30	H8	H5	E	12.167000	-5.497000	-4.790000	0.247240
31	N7	NB	M	13.605000	-7.098000	-4.724000	-0.583894
32	C5	CB	M	14.775000	-7.352000	-5.386000	0.098070
33	C6	CA	M	15.693000	-8.411000	-5.354000	0.674200
34	N6	N2	B	15.513000	-9.481000	-4.577000	-0.883754
35	H61	H	E	16.207000	-10.242000	-4.578000	0.398200
36	H62	H	E	14.679000	-9.546000	-3.976000	0.398200
37	N1	NC	M	16.708000	-8.205000	-6.182000	-0.771792
38	C2	CQ	M	16.932000	-7.134000	-6.975000	0.563920
39	H2	H5	E	17.833000	-7.107000	-7.588000	0.047710
40	N3	NC	M	16.079000	-6.109000	-7.029000	-0.739670
41	C4	CB	M	15.082000	-6.305000	-6.242000	0.314830

LOOP CLOSING EXPLICIT

O4' C1'
C4 C5
C4 N9

IMPROPER

C8 C4 N9 C1'
C6 H61 N6 H62
N7 N9 C8 H8
N1 N3 C2 H2
C5 N1 C6 N6

DONE
STOP

AMBER PREP file for ATP

0 0 2

ATP4-

atf.data

ATF INT 1

CORRECT OMIT DU BEG

0.0

1	DU	DU	M	0	-1	-2	0.0000	0.0000	0.0000	0.000000000
2	DU	DU	M	1	0	-1	3.7968	0.0000	0.0000	0.000000000
3	DU	DU	M	2	1	0	1.3437	119.9987	-90.0000	0.000000000
4	O3G	O2	M	3	2	1	4.6527	120.1039	179.8629	-0.972744285
5	PG	P	M	4	3	2	1.4953	179.9570	82.2725	1.486200000
6	O1G	O2	E	5	4	3	1.5039	105.9491	146.2236	-0.972744285
7	O2G	O2	E	5	4	3	1.4698	122.4896	276.0098	-0.972744285
8	O3B	OS	M	5	4	3	1.6216	112.0347	31.5857	-0.416366000
9	PB	P	M	8	5	4	1.6362	128.4996	310.8911	1.279020000
10	O1B	O2	E	9	8	5	1.4701	104.3140	45.5120	-0.972744285
11	O2B	O2	E	9	8	5	1.4725	113.3176	276.3854	-0.972744285
12	O3A	OS	M	9	8	5	1.5877	102.5009	160.4746	-0.317167000
13	PA	P	M	12	9	8	1.6014	133.5080	261.0467	1.073710000
14	O1A	O2	E	13	12	9	1.4831	108.3834	281.2405	-0.972744285
15	O2A	O2	E	13	12	9	1.4814	111.9523	50.4957	-0.972744285
16	O5'	OS	M	13	12	9	1.5473	101.8149	166.6435	-0.449500000
17	C5'	CT	M	16	13	12	1.4834	120.3385	293.0055	-0.022553000
18	H5'1	H1	E	17	16	13	1.0894	109.4558	86.4837	0.118770000
19	H5'2	H1	E	17	16	13	1.0900	109.4473	326.4974	0.118770000
20	C4'	CT	M	17	16	13	1.4249	109.4638	206.4995	0.122030000
21	H4'	H1	E	20	17	16	1.0900	108.0887	176.2119	0.166850000
22	O4'	OS	E	20	17	16	1.4192	115.0281	296.2119	-0.386076000
23	C3'	CT	M	20	17	16	1.5334	110.6560	56.7476	0.138880000
24	H3'	H1	E	23	20	17	1.0900	111.4976	24.3666	0.053710000
25	O3'	OH	S	23	20	17	1.4476	111.5103	144.3562	-0.628799000
26	HO'3	HO	E	25	23	20	1.0304	109.5136	215.7193	0.411280000
27	C2'	CT	M	23	20	17	1.5241	103.6401	258.0531	0.133400000
28	H2'	H1	E	27	23	20	1.0896	106.7138	87.6350	0.097320000
29	O2'	OH	S	27	23	20	1.4177	120.5959	207.6379	-0.603634000
30	HO'2	HO	E	29	27	23	1.0301	109.4760	324.9998	0.389400000
31	C1'	CT	M	22	20	17	1.4489	111.6203	121.1296	0.096000000
32	H1'	H1	E	31	22	20	1.0904	110.9134	99.6914	0.129180000
33	N9	N*	M	31	22	20	1.4866	102.6342	226.3744	-0.023033000
34	C8	CK	M	33	31	22	1.4015	128.6351	78.8195	0.078510000
35	H8	H5	E	34	33	31	1.0898	126.6387	358.6073	0.247240000
36	N7	NB	M	34	33	31	1.3175	106.7008	178.5901	-0.583894000
37	C5	CB	M	36	34	33	1.3681	110.0321	359.0193	0.098070000
38	C6	CA	M	37	36	34	1.4016	133.5593	180.8793	0.674200000
39	N6	N2	B	38	37	36	1.3349	122.0374	1.2666	-0.883754000
40	H61	H	E	39	38	37	1.0299	120.0073	180.0053	0.398200000
41	H62	H	E	39	38	37	1.0298	119.9564	0.0000	0.398200000
42	N1	NC	M	38	37	36	1.3259	111.6710	180.6308	-0.771792000
43	C2	CQ	M	42	38	37	1.3508	128.1143	1.2630	0.563920000
44	H2	H5	E	43	42	38	1.0899	119.1289	178.6612	0.047710000
45	N3	NC	M	43	42	38	1.3350	121.7486	358.6458	-0.739670000
46	C4	CB	M	45	43	42	1.2852	110.7044	0.3793	0.314830000

LOOP CLOSING EXPLICIT

O4' C1'
C4 C5
C4 N9

IMPROPER

C8 C4 N9 C1'
C6 H61 N6 H62
N7 N9 C8 H8
N1 N3 C2 H2
C5 N1 C6 N6

DONE
STOP