

Supporting Information

Modulators of 14-3-3 Protein-Protein Interactions

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14-3-3 crystal structures (July 2017)

PDB ID	Name	Resolution	Isoform	Organism	Ligand	Ref.
1A37	14-3-3ζ/C-RafpS259	3.60 Å	Zeta	Human	-	Liddington, RC et al. (1998) ¹
1A38	14-3-3ζ/R18	3.35 Å	Zeta	Human	-	Liddington, RC et al. (1998) ¹
1A40	14-3-3ζ	2.80 Å	Zeta	Human	-	Liddington, RC et al. (1995) ²
1QJA	14-3-3ζ/MODE2	2.00 Å	Zeta	Human	-	Yaffe, MB et al. (1999) ³
1QJB	14-3-3ζ/MODE1	2.00 Å	Zeta	Human	-	Yaffe, MB et al. (1999) ³
1IB1	14-3-3ζ/AANAT	2.60 Å	Zeta	Human	-	Dyda, F et al. (2001) ⁴
1O9C	T14-3c	2.60 Å	Isoform c	Tobacco	Citrate	Oecking, C. et al. (2003) ⁵
1O9D	T14-3c/PMA2pS955	2.30 Å	Isoform c	Tobacco	-	Oecking, C. et al. (2003) ⁵
1O9E	T14-3c/FC-A	2.60 Å	Isoform c	Tobacco	Fusicoccin A	Oecking, C. et al. (2003) ⁵
1O9F	T14-3c/PMA2pS955/FC-A	2.70 Å	Isoform c	Tobacco	Fusicoccin A	Oecking, C. et al. (2003) ⁵
1YWT	14-3-3σ/MODE1	2.40 Å	Sigma	Human	-	Yaffe, MB. et al. (2005) ⁶
1YZ5	14-3-3σ	2.80 Å	Sigma	Human	-	Hermeking, H. et al. (2005) ⁷
2BQ0	14-3-3β	2.50 Å	Beta	Human	-	Doyle, DA. et al. (2006) ⁸
2BR9	14-3-3ε/ConsPep	1.75 Å	Epsilon	Human	-	Doyle, DA. et al. (2006) ⁸
2BTP	14-3-3τ/ConsPep	2.80 Å	Tau	Human	-	Doyle, DA. et al. (2006) ⁸
2C23	14-3-3β/ExoS	2.65 Å	Beta	Human	-	Doyle, DA. et al. (2006) ⁸
2C63	14-3-3η/ConsPep	2.15 Å	Eta	Human	-	Doyle, DA. et al. (2006) ⁸
2C74	14-3-3 η/ConsPep	2.70 Å	Eta	Human	-	Doyle, DA. et al. (2006) ⁸
2B05	14-3-3γ/MODE1	2.55 Å	Gamma	Human	-	-
2C1J	14-3-3ζ/H3pS10K9Ac	2.60 Å	Zeta	Human	-	Mahadevan, LC. et al. (2005) ⁹
2C1N	14-3-3ζ/H3pS10	2.00 Å	Zeta	Human	-	Mahadevan, LC. et al. (2005) ⁹
2NPM	14-3-3/ConsPep	2.52 Å		Cryptosporidium parvum	-	Hui, R. et al. (2011) ¹⁰

2O8P	14-3-3/ConsPep	1.82 Å		Cryptosporidium parvum	-	Hui, R. et al. (2011) ¹⁰
3EFZ	14-3-3/ConsPep	2.08 Å		Cryptosporidium parvum	-	Hui, R. et al. (2011) ¹⁰
2O98	T14-3c/PMA2_CT52	2.70 Å	Isoform c	Tobacco	Fusicoccin A	Oecking, C. et al. (2007) ¹¹
2O02	14-3-3ζ/ExoS	1.50 Å	Zeta	Human/P. aeruginosa	-	Hallberg, B. et al. (2007) ¹²
2V7D	14-3-3ζ/IntegBpT758	2.50 Å	Zeta	Human	-	Fagerholm, SC. et al. (2008) ¹³
3E6Y	T14-3c/PMA2_pT955/CN-A	2.50 Å	Isoform c	Tobacco	Cotylenin A	Ottmann, C. et al. (2009) ¹⁴
3CU8	14-3-3ζ/C-RafpS259	2.40 Å	Zeta	Human	-	Ottmann, C. et al. (2010) ¹⁵
3LW1	14-3-3σ/p53pT387	1.28 Å	Sigma	Human	-	Ottmann, C. et al. (2010) ¹⁵
3M50	T14-3e/PMA2_CT30/Epibestatin	2.60 Å	Isoform e	Nicotiana	Epibestatin	Ottmann, C. et al. (2010) ¹⁵
3M51	T14-3e/PMA2_CT30/Pyrrrolidone1	3.25 Å	Isoform e	Nicotiana	Pyrrrolidone 1	Ottmann, C. et al. (2010) ¹⁵
3IQJ	14-3-3σ/C-RafpS259 (10mer)	1.15 Å	Sigma	Human	-	Ottmann, C. et al. (2010) ¹⁵
3IQU	14-3-3σ/C-RafpS259 (6mer)	1.05 Å	Sigma	Human	-	Ottmann, C. et al. (2010) ¹⁵
3IQV	14-3-3σ/C-RafpS259 (6mer)/FC-A	1.20 Å	Sigma	Human	Fusicoccin A	Ottmann, C. et al. (2010) ¹⁵
2WH0	14-3-3ζ/PKCpS346pS368	2.25 Å	Zeta	Human	-	McDonald, NQ. et al. (2009) ¹⁶
3MHR	14-3-3σ/YAPpS127	1.15 Å	Sigma	Human	-	Ottmann, C. et al. (2010) ¹⁷
3NKX	14-3-3ζ/C-RafpS259	2.40 Å	Zeta	Human	-	Ottmann, C. et al. (2010) ¹⁸
3O8I	14-3-3σ/C-RafpS259/fragment	2.00 Å	Sigma	Human	fragment	Ottmann, C. et al. (2010) ¹⁸
3AXY	GF-14c/Hd3a/OsFD1	2.40 Å	Isoform c	Rice	-	Shimamoto, K. et al. (2011) ¹⁹
3RDH	14-3-3ζ/FOBISIN101	2.40 Å	Zeta	Human	FOBISIN101	Fu, H. et al. (2011) ²⁰
3P1N	14-3-3σ/TASK3pS373	1.40 Å	Sigma	Human	-	Ottmann, C. et al. (2013) ²¹
3P1O	14-3-3σ/TASK3pS373/FC-A	1.90 Å	Sigma	Human	Fusicoccin A	Ottmann, C. et al. (2013) ²¹
3P1P	14-3-3σC38N_N166H/TASK3pS373	1.90 Å	Sigma	Human	-	Ottmann, C. et al. (2013) ²¹

3P1Q	14-3-3 σ C38N_N166H/TASK3pS373/FC-A	1.70 Å	Sigma	Human	Fusicoccin A	Ottmann, C. et al. (2013) ²¹
3P1R	14-3-3 σ C38V_N166H/TASK3pS373	1.70 Å	Sigma	Human	-	Ottmann, C. et al. (2013) ²¹
3P1S	14-3-3 σ C38V_N166H/TASK3pS373/FC-A	1.65 Å	Sigma	Human	Fusicoccin A	Ottmann, C. et al. (2013) ²¹
3UAL	14-3-3 ϵ /MLF1pS34	1.80 Å	Epsilon	Human	-	Ottmann, C. et al. (2012) ²²
3UBW	14-3-3 ϵ /MLF1pS34/fragment	1.90 Å	Epsilon	Human	fragment	Ottmann, C. et al. (2012) ²²
4DNK	14-3-3 β	2.20 Å	Beta	Human	phosphate	-
3UZD	14-3-3 γ /HDAC4pS350	1.86 Å	Gamma	Human	-	Min, J. et al. (2012) ²³
4E2E	14-3-3 γ /HDAC4pS350	2.25 Å	Gamma	Human	-	-
3U9X	14-3-3 σ /pyridoxalPD	1.80 Å	Sigma	Human	Pyridoxal-P-derivative	Ottmann, C. et al. (2012) ²⁴
4DX0	T14-3 ϵ /PMA2_CT30/pyrazole	3.40 Å	Isoform e	Tobacco	Pyrazole	Ottmann, C. et al. (2012) ²⁵
4DAT	14-3-3 σ /PADI6pS446	1.40 Å	Sigma	Human	-	Ottmann, C. et al. (2012) ²⁶
4DAU	14-3-3 σ /PADI6pS10	2.20 Å	Sigma	Human	-	Ottmann, C. et al. (2012) ²⁶
3SPR	14-3-3 σ C38V_N166H/TASK3pS373/FC-THF	1.99 Å	Sigma	Human	Fusicoccin THF	Ottmann, C. et al. (2013) ²¹
3SMK	14-3-3 σ C38V_N166H/TASK3pS373/CN-A	2.10 Å	Sigma	Human	Cotlenin A	Ottmann, C. et al. (2013) ²¹
3SML	14-3-3 σ C38N_N166H/TASK3pS373/FC-A aglycone	1.90 Å	Sigma	Human	Fusicoccin A aglycone	Ottmann, C. et al. (2013) ²¹
3SMM	14-3-3 σ C38N_N166H/TASK3pS373/FC-J aglycone	2.00 Å	Sigma	Human	Fusicoccin J aglycone	Ottmann, C. et al. (2013) ²¹
3SMN	14-3-3 σ C38N_N166H/TASK3pS373/FC THF	2.00 Å	Sigma	Human	Fusicoccin THF	Ottmann, C. et al. (2013) ²¹
3SMO	14-3-3 σ C38V_N166H/TASK3pS373/FC-J aglycone	1.80 Å	Sigma	Human	Fusicoccin J aglycone	Ottmann, C. et al. (2013) ²¹
3UX0	14-3-3 σ /TASK3pS373/FC-H	1.75 Å	Sigma	Human	Fusicoccin H	Ottmann, C. et al. (2013) ²¹
4FR3	14-3-3 σ /TASK3pS373/FC-H derivative	1.90 Å	Sigma	Human	16-O-Me-Fusicoccin H	Ottmann, C. et al. (2013) ²¹
3SP5	14-3-3 σ /TASK3pS373/Cotlenol	1.80 Å	Sigma	Human	Cotlenol	Ottmann, C. et al. (2013) ²¹

4FJ3	14-3-3 ζ /C-RafpS233pS259	1.95 Å	Zeta	Human	-	Ottmann, C. et al. (2012) ²⁷
4GNT	14-3-3 β /ChREBP	2.41 Å	Beta	Human	-	Uyeda, K. et al. (2012) ²⁸
3TOL	14-3-3 σ /inhibitor	1.60 Å	Sigma	Human	Phosphonate B5	Ottmann, C. et al. (2013) ²⁹
3TOM	14-3-3 σ /inhibitor	1.75 Å	Sigma	Human	Phosphonate B8	Ottmann, C. et al. (2013) ²⁹
4DHM	14-3-3 σ /inhibitor	1.70 Å	Sigma	Human	Phosphonate B11	Ottmann, C. et al. (2013) ²⁹
4DHN	14-3-3 σ /inhibitor	1.80 Å	Sigma	Human	Phosphonate B10	Ottmann, C. et al. (2013) ²⁹
4DHO	14-3-3 σ /inhibitor	1.70 Å	Sigma	Human	Phosphonate B9	Ottmann, C. et al. (2013) ²⁹
4DHP	14-3-3 σ /inhibitor	1.75 Å	Sigma	Human	Phosphonate B7	Ottmann, C. et al. (2013) ²⁹
4DHQ	14-3-3 σ /inhibitor	1.75 Å	Sigma	Human	Phosphonate B6	Ottmann, C. et al. (2013) ²⁹
4DHR	14-3-3 σ /inhibitor	1.40 Å	Sigma	Human	Phosphonate B4	Ottmann, C. et al. (2013) ²⁹
4DHS	14-3-3 σ /inhibitor	1.74 Å	Sigma	Human	Phosphonate B3	Ottmann, C. et al. (2013) ²⁹
4DHT	14-3-3 σ /inhibitor	1.80 Å	Sigma	Human	Phosphonate B2	Ottmann, C. et al. (2013) ²⁹
4DHU	14-3-3 σ /inhibitor	1.67 Å	Sigma	Human	Phosphonate B1	Ottmann, C. et al. (2013) ²⁹
4HQW	14-3-3 σ /molecular tweezer	2.35 Å	Sigma	Human	CLR01	Ottmann, C. et al. (2013) ³⁰
4HRU	14-3-3 σ /molecular tweezer	3.15 Å	Sigma	Human	CLR01	Ottmann, C. et al. (2013) ³⁰
4JC3	14-3-3 σ /ERapT594	2.05 Å	Sigma	Human	-	Ottmann, C. et al. (2013) ³¹
4JDD	14-3-3 σ /ERapT594/FC-A	2.10 Å	Sigma	Human	Fusicoccin A	Ottmann, C. et al. (2013) ³¹
4F7R	g14-3-3	3.20 Å	-	Giardia intestinalis	Phosphate	Lalle, M. et al. (2014) ³²
4BG6	14-3-3 ζ /Rnd3pS240	2.30 Å	Zeta	Human	-	Ridley, AJ. et al. (2013) ³³
4HKC	14-3-3 ζ /α4pS1011	2.20 Å	Zeta	Human	-	Campbell, ID. et al. (2013) ³⁴
4IEA	14-3-3 σ /C-RafpS629	1.70 Å	Sigma	Human	-	Ottmann, C. et al. (2013) ³⁵
4IHL	14-3-3 ζ /C-RafpS233pS259/CN-A	2.20 Å	Zeta	Human	-	Ottmann, C. et al. (2013) ³⁵
4J6S	14-3-3 γ /THpS19	3.08 Å	Gamma	Human	-	Martinez, A. et al. (2014) ³⁶
4FL5	14-3-3 σ /TaupS214	1.90 Å	Sigma	Human	-	Ottmann, C. et al. (2015) ³⁷
5BTV	14-3-3 σ /TaupS324	1.90 Å	Sigma	Human	-	Ottmann, C. et al. (2015) ³⁷

4N7G	14-3-3ζ/ExoS	2.25 Å	Zeta	Human	-	Ottmann, C. et al. (2014) ³⁸
4N7Y	14-3-3ζ/ExoSDerPep	2.16 Å	Zeta	Human	βRS8	Ottmann, C. et al. (2014) ³⁸
4N84	14-3-3ζ/ExoSDerPep	2.50 Å	Zeta	Human	βSS12	Ottmann, C. et al. (2014) ³⁸
4O46	14-3-3γ/NS1pS228	2.90 Å	Gamma	Human/Influenza		Min, J. et al. (2014) ³⁹
4WRQ	14-3-3ζ/ChibbypS20	2.41 Å	Zeta	Human	-	Choy et al. (2015) ⁴⁰
4QLI	14-3-3σ/SnailpT177	1.45 Å	Sigma	Human	-	-
4ZDR	14-3-3ζ/LKB1	2.90 Å	Zeta	Human	-	Zhu, Y. et al. (2015) ⁴¹
4Y32	14-3-3σ/Tau109B	1.70 Å	Sigma	Human	Tau109B	Ottmann, C. et al. (2015) ⁴²
4Y3B	14-3-3σ/Tau201D	1.80 Å	Sigma	Human	Tau201D	Ottmann, C. et al. (2015) ⁴²
4Y5I	14-3-3σ/Tau126B	1.40 Å	Sigma	Human	Tau126B	Ottmann, C. et al. (2016) ⁴²
5D2D	14-3-3ζ/CFTRpS753pS768	2.10 Å	Zeta	Human	-	Ottmann, C. et al. (2016) ⁴³
5D3E	14-3-3γ/CFTRpS768pS795	2.75 Å	Gamma	Human	-	Ottmann, C. et al. (2016) ⁴³
5D3F	14-3-3ζ/CFTRpS753pS768/FC-A	2.74 Å	Zeta	Human	Fusicoccin A	Ottmann, C. et al. (2016) ⁴³
5F74	14-3-3β/ChREBP/AMP	2.35 Å	Beta	Human	Adenosine monophosphate	Uyeda, K. et al. (2012) ⁴⁴
5IQP	14-3-3τ	2.60 Å	Tau	Human	-	Gamblin, SJ. et al. (1995) ⁴⁵
AZQ0	g14-3-3/A8Ap	3.10 Å		Giardia intestinalis	-	Lalle, M. et al. (2015) ⁴⁶
5BY9	g14-3-3 polygly	4.00 Å		Giardia intestinalis	-	Lalle, M. et al. (2015) ⁴⁶
5EWZ	14-3-3ζ/Gab2pS210pT391	1.95 Å	Zeta	Human	-	Ottmann, C. et al. (2016) ⁴⁷
5EXA	14-3-3ζ/Gab2pT391/ISIR-005	1.70 Å	Zeta	Human	ISIR-005	Ottmann, C. et al. (2016) ⁴⁷
5J31	14-3-3ζ/ExoS derivative	2.40 Å	Zeta	Human/P. aeruginosa	Peptide H	Grossmann, TN. et al. (2016) ⁴⁸
5LTW	14-3-3σ/HSPB6	4.50 Å	Sigma	Human	-	Strelkov, SV. et al. (2017) ⁴⁹
5LU1	14-3-3σ/HSPB6pS16 (8mer)	2.40 Å	Sigma	Human	-	Strelkov, SV. et al. (2017) ⁴⁹
5LU2	14-3-3σ/HSPB6pS16 (13mer)	2.50 Å	Sigma	Human	-	Strelkov, SV. et al. (2017) ⁴⁹
5MY9	14-3-3σ/LRRK2pS935	1.33 Å	Sigma	Human	-	Ottmann, C. et al. (2017) ⁵⁰
5MYC	14-3-3σ/LRRK2pS910	1.46 Å	Sigma	Human	-	Ottmann, C. et al. (2017) ⁵⁰

5NAS	14-3-3 ζ /PI4KIIIbP294	2.08 Å	Zeta	Human	-	-
5WX N	14-3-3 ζ /LKB1pT336	2.93 Å	Zeta	Human	-	Wu, J. et al. (2017) ⁵¹
5JIT	14-3-3 ζ /Cdc25pS216 (38mer)/CLR01	2.38 Å	Zeta	Human	CLR01	-
5JIV	14-3-3 ζ /Cdc25pS216 (38mer)/CLR01	2.45 Å	Zeta	Human	CLR01	-
5JM4	14-3-3 ζ /ExoS-adamantyl	2.34 Å	Zeta	Human	ExoS-adamantyl	-
5N10	14-3-3 ζ /FGG-ER β /Q8	1.60 Å	Beta	Human	Cucubit[8]Juril	Ottmann, C. et al. (2017) ⁵²
5N75	14-3-3 σ /TAZpS89	1.80 Å	Sigma	Human	-	Ottmann, C. et al. (2017) ⁵³
5N5R	14-3-3 σ /TAZpS89/NV1	1.80 Å	Sigma	Human	Fragment NV1	Ottmann, C. et al. (2017) ⁵³
5N5T	14-3-3 σ /TAZpS89/NV2	1.80 Å	Sigma	Human	Fragment NV2	Ottmann, C. et al. (2017) ⁵³
5N5 W	14-3-3 σ /TAZpS89/NV2	1.37 Å	Sigma	Human	Fragment NV3	Ottmann, C. et al. (2017) ⁵³

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