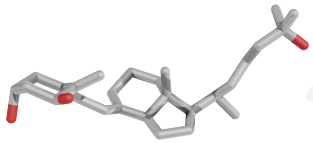
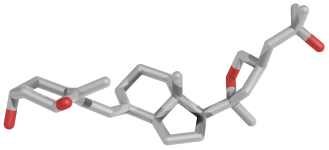
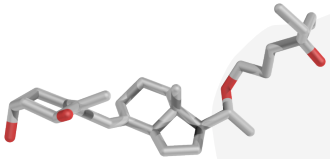
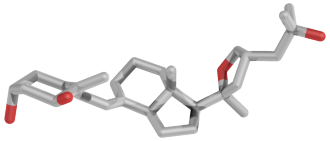
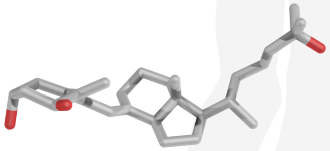
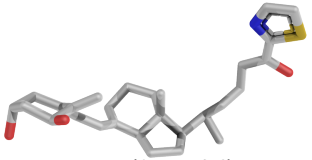
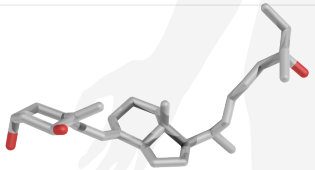
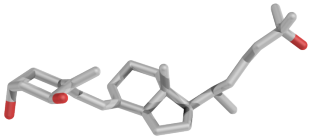
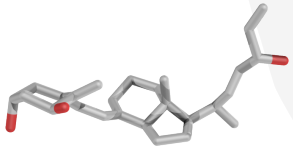
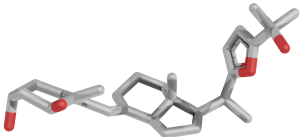
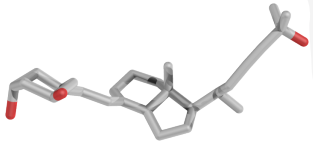
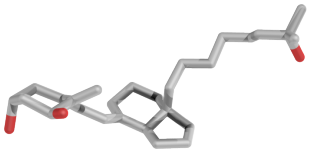
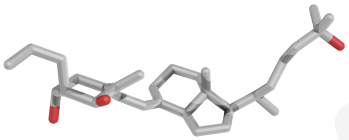
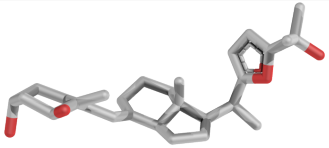
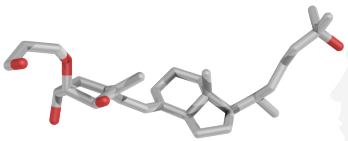
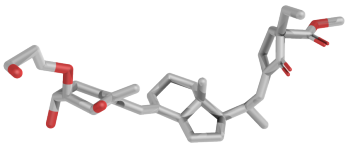
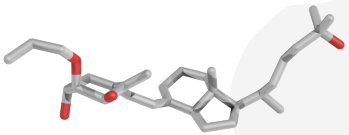
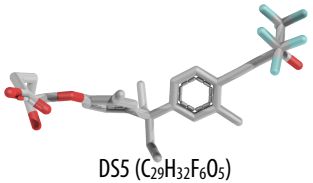
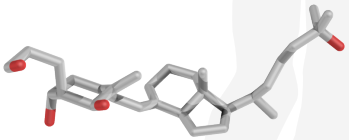
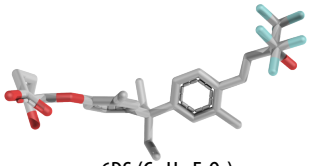
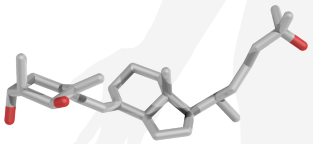
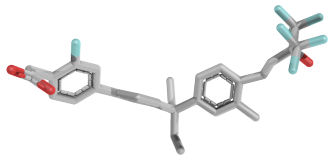
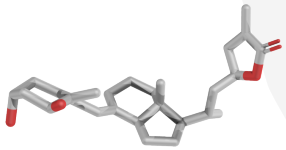
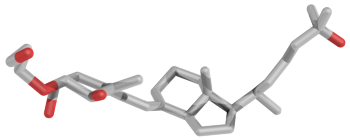
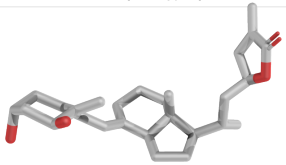
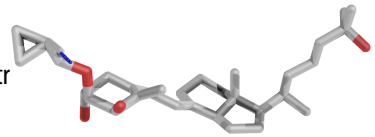
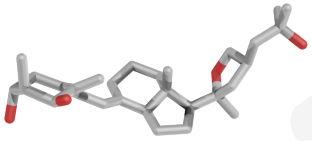
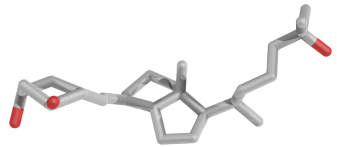
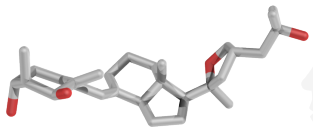
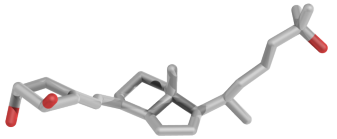
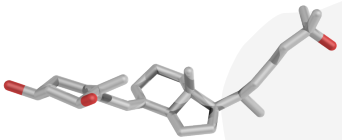
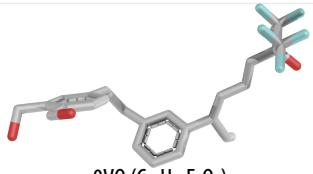
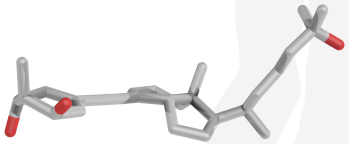
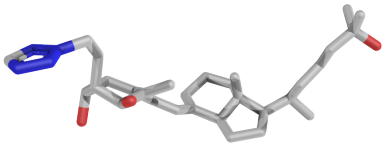
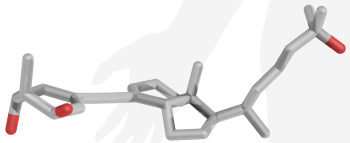
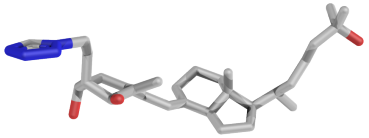
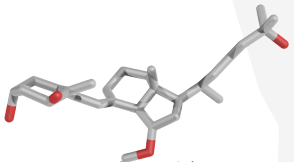
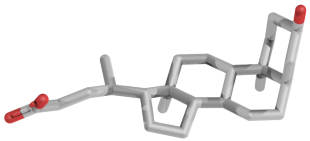
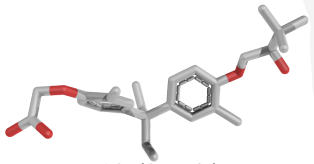
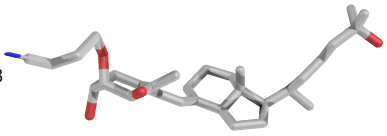
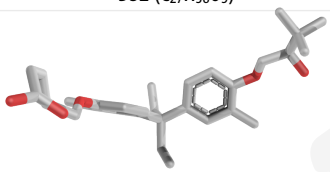
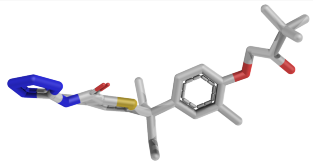
Supporting Information

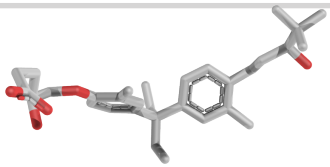
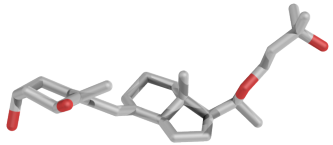
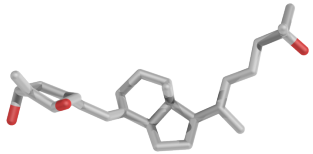
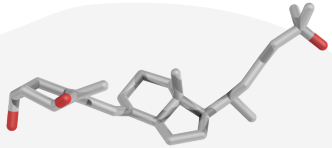
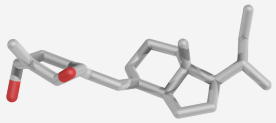
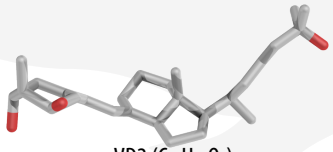
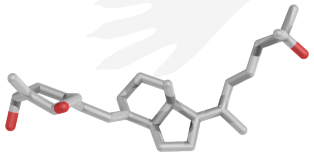
"Vitamin D and its synthetic analogs" by Miguel A. Maestro, Ferdinand Molnár and Carsten Carlberg

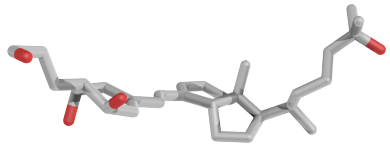
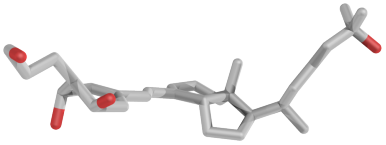
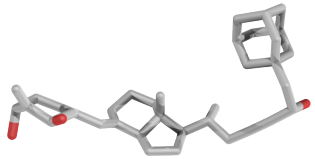
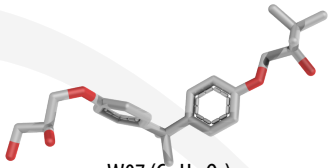
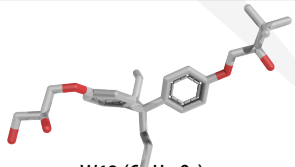
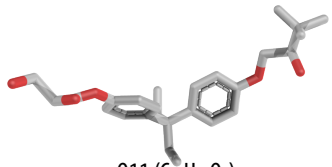
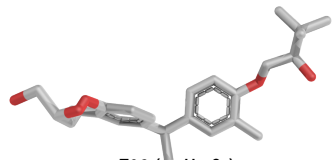
Table S1 describes all 143 publically available VDR ligand crystal structures with individual hyperlinks to the PDB and Pubmed databases.

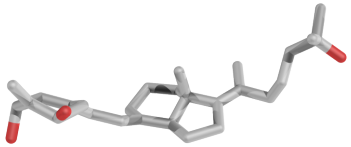
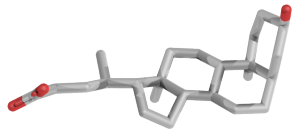
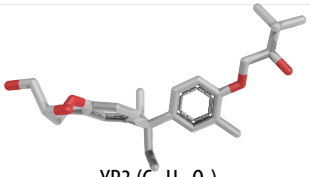
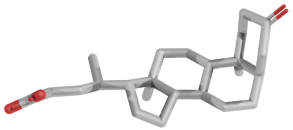
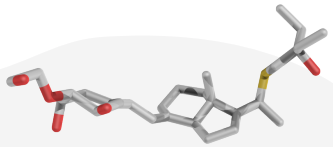
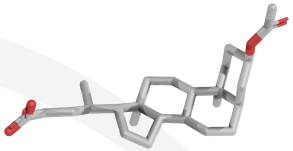
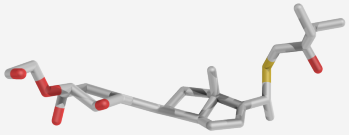
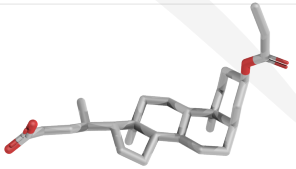
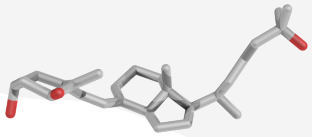
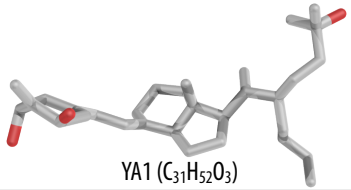
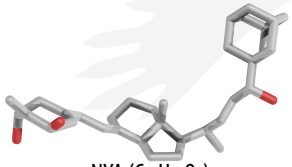
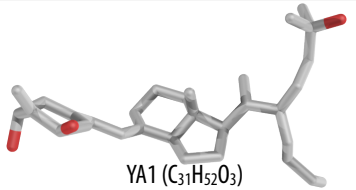
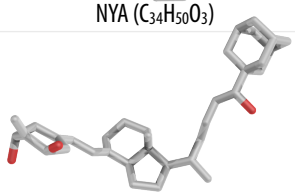
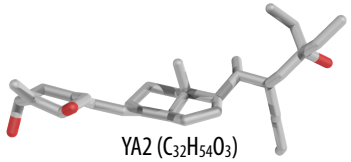
Orthologue	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]
HUMAN	1DB1	1.8 Å	[28]	Calcitriol (1,25D_3)	 VDX ($C_{27}H_{44}O_3$)	3CS4	2 Å	[99]	AMCR277A	 COV ($C_{28}H_{44}O_4$)
	1IE8	1.52 Å	[90]	Lexacalcitol (KH1060)	 KH1 ($C_{29}H_{48}O_4$)	3CS6	1.8 Å		AMCR277B	 OCO ($C_{28}H_{44}O_4$)
	1IE9	1.4 Å		20-epi calcitriol (MC1288)	 VDX ($C_{27}H_{44}O_3$)	3KPZ	1.9 Å	[100]	ZK203278	 ZNE ($C_{28}H_{41}NO_3S$)
	1S0Z	2.5 Å	[91]	Seocalcitol (EB1089)	 EB1 ($C_{30}H_{46}O_3$)	3M7R	1.8 Å	[101]	1,25D_3 **hVDR_H305Q**	 VDX ($C_{27}H_{44}O_3$)
	1S19	2.1 Å		Calcipotriol (MC903)	 MC9 ($C_{27}H_{40}O_3$)	3OGT	1.75 Å	—	Same as 3TKC	 FMV ($C_{28}H_{40}O_4$)
	1TXI	1.9 Å	[92]	Inecalcitol (TX522)	 TX5 ($C_{27}H_{40}O_3$)	3P8X	1.7 Å	[102]	20(17→18)-abeo-1α,25-dihydroxy-22-homo-21-norvitamin D_3	 ZYD ($C_{27}H_{44}O_3$)
	2HAM	1.9 Å	[93]	2α-propyl-1,25D_3	 C33 ($C_{30}H_{50}O_3$)	3TKC	1.75 Å	[103]	(20S)-[5-(2-Hydroxypropan-2-yl)furan-2yl]-22,23,24,25,26,27-hexanor-1α-hydroxyvitamin D_3	 FMV ($C_{28}H_{40}O_4$)

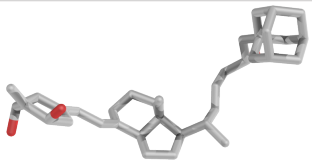
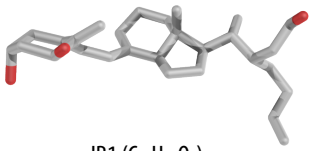
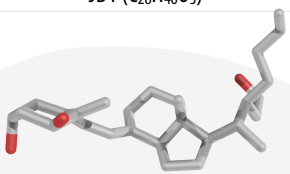
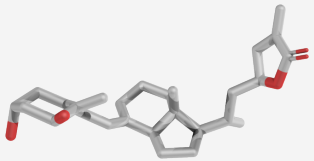
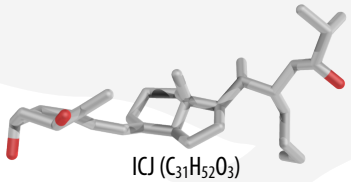
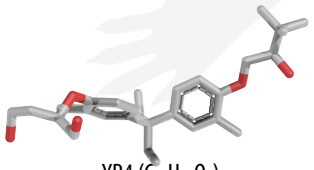
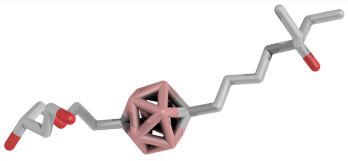
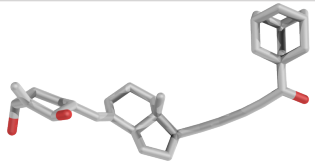
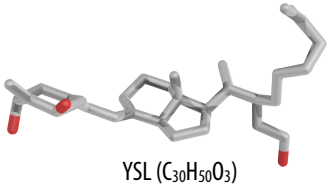
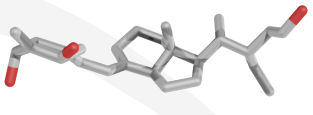
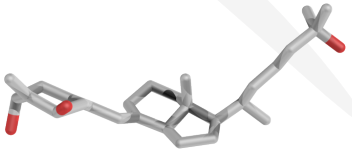
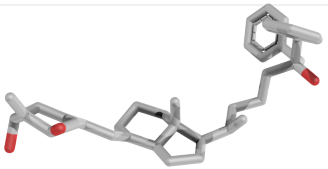
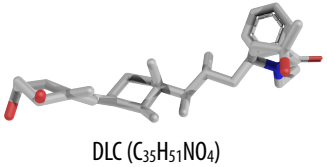
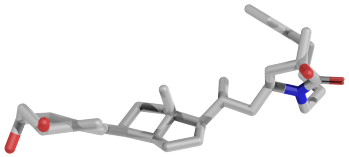
Orthologue	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]
HUMAN	2HAR	1.9 Å	[93]	2α-(3-hydroxy-1-propoxy)-1,25D_3	 OCC ($C_{30}H_{50}O_5$)	3VHW	2.43 Å	[104]	2-(3-hydroxypropoxy)-25-oxocyclopentane-carboxylate-1α-hydroxyvitamin D_3	 VHW ($C_{34}H_{50}O_7$)
	2HAS	1.96 Å		2α-(1-propoxy)-1,25D_3	 C30 ($C_{30}H_{50}O_4$)	3W0A	1.8 Å		(4S)-4-hydroxy-5-[2-methyl-4-(3-{3-methyl-4-[4,4,4-trifluoro-3-hydroxy- 3-(trifluoromethyl) but-1-yn-1-yl]phenyl}pentan-3-yl)phenoxy]pentanoic acid	 DS5 ($C_{29}H_{32}F_6O_5$)
	2HB7	1.8 Å		2α(3-hydroxy-1-propyl) -1,25D_3	 01C ($C_{30}H_{50}O_4$)	3W0C	1.9 Å	[105]	(4S)-4-hydroxy-5-[2-methyl-4-(3-{3-methyl-4-[(1E)-4,4,4-trifluoro-3-hydroxy-3 (trifluoromethyl)but-1-en-1-yl]phenyl}pentan-3yl) phenoxy]pentanoic acid	 6DS ($C_{29}H_{34}F_6O_5$)
	2HB8	2 Å		2α-methyl-1,25D_3	 MVD ($C_{28}H_{46}O_3$)	3W0Y	1.98 Å		[3-fluoro-2'-methyl-4'-(3-{3-methyl-4-[(1E)-4,4,4-trifluoro-3-hydroxy-3-(trifluoromethyl)but-1-en-1-yl]phenyl}pentan-3-yl)biphenyl-4-yl]acetic acid	 DS4 ($C_{32}H_{31}F_7O_3$)
	3A2I	3.27 Å	[94]	TEI-9647 **hVDR_H305F**	 TEJ ($C_{27}H_{38}O_4$)	3WGP	2 Å	—	2β-(3-hydroxy-1-propoxy)-1,25D_3 (see PDBID: 2HAR)	 ED9 ($C_{30}H_{50}O_5$)
	3A2J	2.7 Å		TEI-9647 **hVDR_H305F/H397F**	 TEJ ($C_{27}H_{38}O_4$)	3WWR	3.18 Å	[106]	2α-oxy-methylcyclopropanecarbonitrile-1,25D_3	 3AJ ($C_{32}H_{49}O_4$)
	3A3Z	1.72 Å	[95]	2α-methyl-AMCR277A(C23S)	 2MV ($C_{29}H_{46}O_4$)	3X31	2.11 Å	[107]	7,8-*cis*-14-*epi*-19-*nor*-1,25D_3	 41V ($C_{26}H_{44}O_3$)

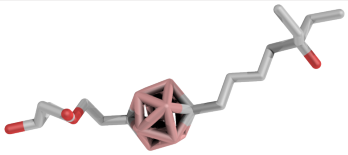
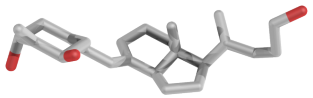
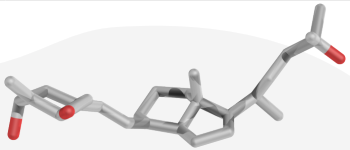
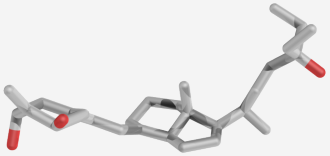
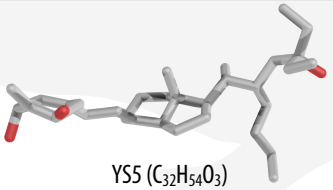
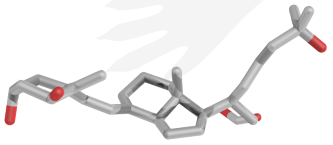
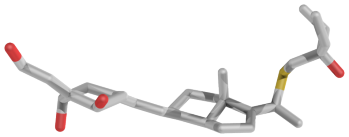
Orthologue	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]
HUMAN	3A40	1.45 Å	[95]	2α-methyl-AMCR277B(C23R)	 3EV ($C_{27}H_{44}O_3$)	3X36	1.93 Å	[107]	7,8-*cis*-19-*nor*-1,25D_3	 41W ($C_{26}H_{44}O_3$)
	3A78	1.9 Å	[96]	1,25-3-epi-D_3	 3EV ($C_{27}H_{44}O_3$)	4G2I	1.8 Å	[108]	CD4528	 0VQ ($C_{25}H_{26}F_6O_3$)
	3AUQ	2.64 Å	[76]	14-epi-2α-methyl-1α , 25(OH)$_2$-6,7-dehydro-19-norvitamin D_3	 CA9 ($C_{27}H_{42}O_3$)	4ITE	2.49 Å	[109]	2α-[2-(tetrazol-2-yl)ethyl]-1,25D_3	 TEY ($C_{30}H_{48}N_4O_3$)
	3AUR	2.21 Å		14-epi-2β-methyl-1α, 25(OH)2-6,7-dehydro-19-norvitamin D_3	 CA9 ($C_{27}H_{42}O_3$)	4ITF	2.84 Å		2α-[2-(tetrazol-1-yl)ethyl]-1,25D_3	 TFY ($C_{30}H_{48}N_4O_3$)
	3AX8	2.6 Å	[97]	15R-methoxy-1,25D_3	 EIM ($C_{28}H_{46}O_4$)	4Q0A	1.9 Å	[110]	Lithocholic acid	 4OA ($C_{24}H_{40}O_3$)
	3AZ1	1.5 Å	[98]	(4-{1-Ethyl-1-[4-(2-hydroxy-3,3-dimethyl-butoxy)-3- methyl-phenyl]-propyl}-2-methyl-phenoxy)-acetic acid	 DS2 ($C_{27}H_{38}O_5$)	5GT4 (4PA2)	1.83 Å	[106]	2α-oxy-butanenitrile-1,25D_3	 2KB ($C_{31}H_{49}NO_4$)
	3AZ2	1.69 Å		5-(4-{1-Ethyl-1-[4-(2-hydroxy-3,3-dimethyl-butoxy)-3- methyl-phenyl]-propyl}-2-methyl-phenoxy)-pentanoic acid	 DS3 ($C_{30}H_{44}O_5$)	5V39	2.2 Å	[111]	5-(3-{4-[(2S)-2-hydroxy- 3,3-dimethylbutoxy]-3-methyl phenyl}pentan-3-yl)-3-methyl-N-(1H-tetrazol -5-yl)thiophene-2-carboxamide	 8VM ($C_{25}H_{35}N_5O_3S$)

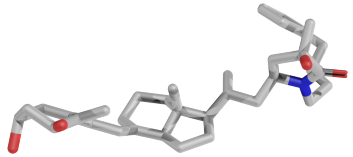
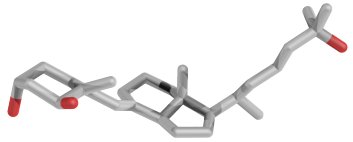
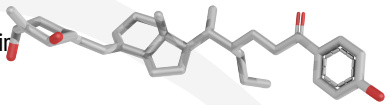
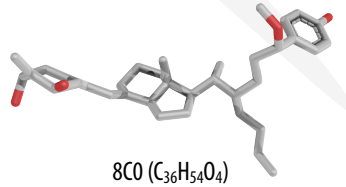
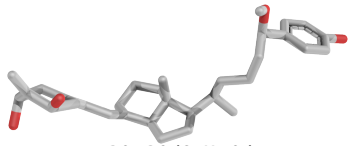
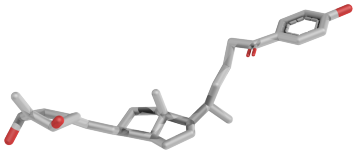
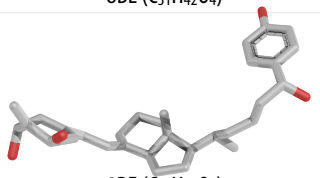
Orthologue	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]
HUMAN	3AZ3	1.36 Å	[98]	5-(4-{1-Ethyl-1-[4-(3-hydroxy-4,4-dimethyl-pentyl)-3-methyl-phenyl]-propyl}-2-methyl-pheno-xy)-4(S)-hydroxy- pentanoic acid	 DS6 ($C_{31}H_{46}O_5$)
	3B0T	1.3 Å	—	1,25-22-oxa-D_3 (Maxacalcitol)	 MCZ ($C_{26}H_{42}O_4$)
RAT	1RJK	1.99 Å	[113]	2-methylene-19-nor-(20S)-1,25D_3 + DRIP205 (NR2)[4]	 VDZ ($C_{27}H_{44}O_3$)
	1RK3	2.2 Å		1,25D_3 + DRIP 205 (NR2)[4]	 VDX ($C_{27}H_{44}O_3$)
	1RKG	1.9 Å		1α-hydroxy-2-methylene-19-nor-(20S)-bishomopregnacalciferol + DRIP 205 (NR2)[4]	 VD1 ($C_{23}H_{36}O_2$)
	1RKH	2.28 Å		2α-methylene-19-nor-1,25D_3 + DRIP205 (NR2)[4]	 VD2 ($C_{27}H_{46}O_3$)
	2O4J	1.74 Å	[114]	17Z-1,25-17(20)-dehydro-2-methylene-19-nor-D_3 + DRIP205 (NR2)[4]	 VD4 ($C_{27}H_{42}O_3$)

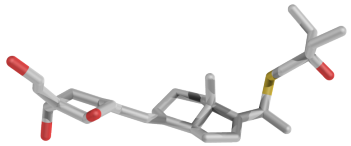
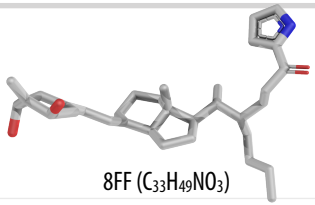
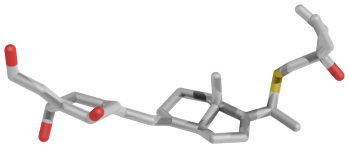
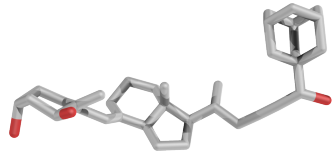
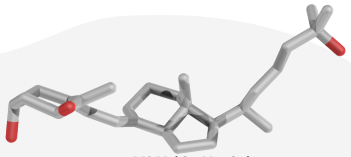
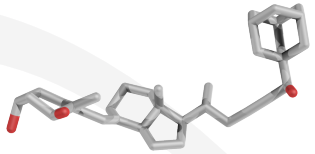
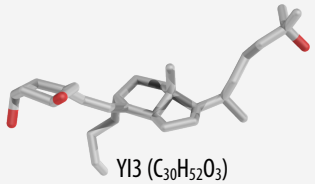
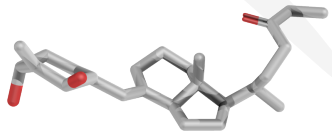
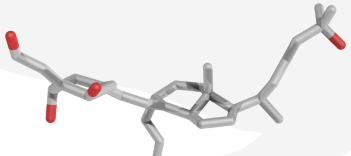
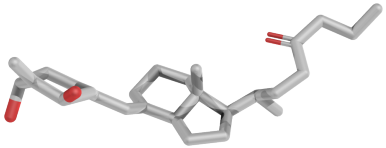
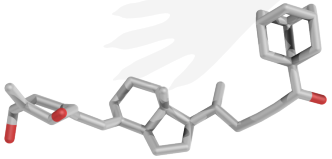
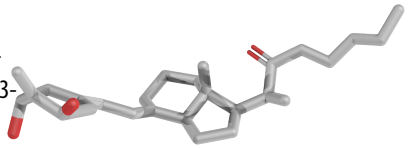
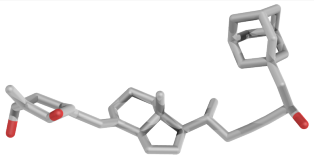
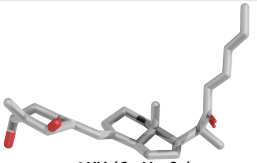
PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]
5YSY	2.0 Å	[112]	14-epi-2α-(3-hydroxypropyl)-19-nortachysterol	 90L ($C_{29}H_{48}O_4$)
5YT2	2.0 Å		14-epi-2β-(3-hydroxypropyl)-19-nortachysterol	 900 ($C_{29}H_{48}O_4$)
3VTD	2.7 Å	[122]	2-methylidene-25S-26-adamantyl-19,27-dinor vitammin-1,25D_3 (ADTK4) + DRIP205 (NR2)[4]	 TKD ($C_{36}H_{52}O_3$)
3W0G	1.94 Å	[123]	(2S)-3-{4-[2-(4-{[(2R)-2-hydroxy-3,3-dimethylbutyl] oxy} phenyl)propan-2-yl]phenoxy} propane-1,2-diol + DRIP205 (NR2)[4]	 W07 ($C_{24}H_{34}O_5$)
3W0H	1.8 Å		(2S)-3-{4-[4-(4-{[(2R)-2-hydroxy-3,3-dimethylbutyl] oxy} phenyl)heptan-4-yl]phenoxy} propane-1,2-diol + DRIP205 (NR2)[4]	 W12 ($C_{28}H_{42}O_5$)
3W0I	1.9 Å		(2S)-3-{4-[3-(4-{[(2R)-2-hydroxy-3,3-dimethylbutyl] oxy} phenyl)pentan-3-yl]phenoxy} propane-1,2-diol + DRIP205 (NR2)[4]	 011 ($C_{26}H_{38}O_5$)
3W0J	1.84 Å		(2S)-3-{4-[2-(4-{[(2R)-2-hydroxy-3,3-dimethylbutyl] oxy}-3-methylphenyl)propan- 2-yl]-2-methylphenoxy propane-1,2-diol + DRIP205 (NR2)[4]	 T08 ($C_{26}H_{38}O_5$)

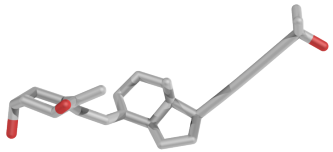
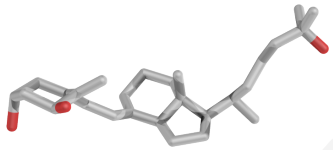
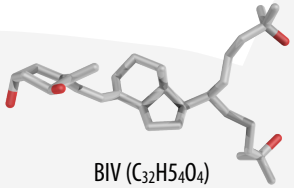
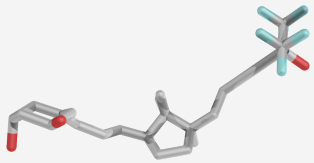
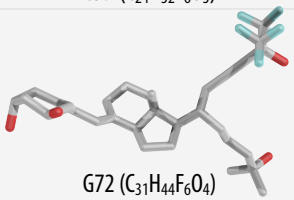
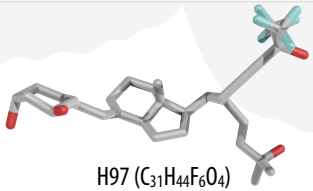
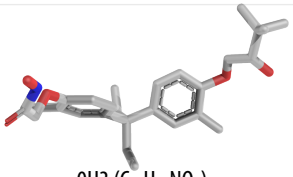
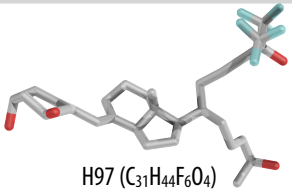
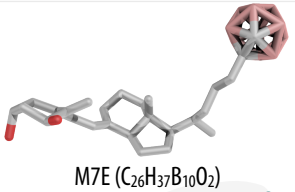
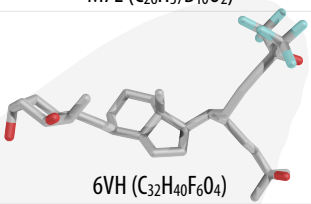
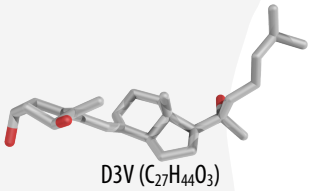
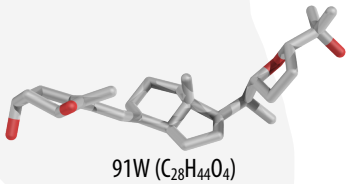
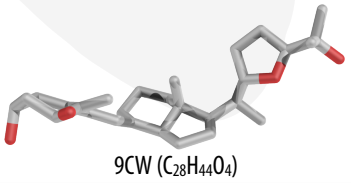
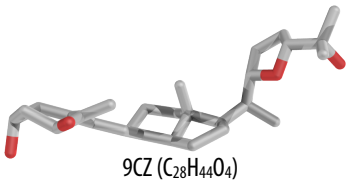
Orthologue	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]
RAT	2O4R	1.98 Å	[114]	17E-1,25-17(20)-dehydro-2-methylene-19-nor-D_3 + DRIP205 (NR2)[4]	 VD5 ($C_{27}H_{42}O_3$)	3W5P	1.9 Å	[124]	Lithocholic acid + DRIP205 (NR2)[4]	 4OA ($C_{24}H_{40}O_3$)
	2ZFX	1.99 Å	[115]	YR301 + DRIP205 (NR2)[4]	 YR3 ($C_{28}H_{42}O_5$)	3W5Q	1.9 Å		3-keto-lithocholic acid + DRIP205 (NR2)[4]	 3KL ($C_{24}H_{38}O_3$)
	2ZL9	1.9 Å		(20S)-1,25-2β-(2-hydroxy ethoxy)-16-ene-22-thia -26,27-dimethyl-19,24-dinor-D_3 + DRIP205 (NR2)[4]	 VDA ($C_{28}H_{46}O_5S$)	3W5R	2.2 Å		Lithocholic acid acetate + DRIP205 (NR2)[4]	 LOA ($C_{26}H_{42}O_4$)
	2ZLA	2 Å	[116]	(20R)-1,25-2β-(2-hydroxy ethoxy)-16-ene-22-thia -26,27-dimethyl-19,24-dinor-D_3 + DRIP205 (NR2)[4]	 VDB ($C_{28}H_{46}O_5S$)	3W5T	2.29 Å		Lithocholic acid propionate + DRIP205 (NR2)[4]	 LHP ($C_{27}H_{44}O_4$)
	2ZLC	2 Å		$1,25D_3$ + DRIP205 (NR2)[4]	 VDX ($C_{27}H_{44}O_3$)	3WT5	1.9 Å		22R-Butyl-2-methylidene-26,27-dimethyl-19,24-dinor-1α, 25-$1,25D_3$ + DRIP205 (NR2)[4]	 YA1 ($C_{31}H_{52}O_3$)
	2ZMH	2.1 Å	[117]	(25R)-25-adamantyl-1,25-2-methylene-22,23-didehydro-19,26,27-trinor-20-epi-D_3 + DRIP205 (NR2)[4]	 NYA ($C_{34}H_{50}O_3$)	3WT6	2 Å	[125]	22R-Butyl-2-methylidene-26,27-dimethyl-19,24-dinor-1α, 25-$1,25D_3$ + DRIP205 (NR2)[4]	 YA1 ($C_{31}H_{52}O_3$)
	2ZMI	1.7 Å		(24R)-24-adamantyl-1,24-2-methylene-22,23-didehydro-19,25, 26,27-tetranor-20-epi-D_3 + DRIP205 (NR2)[4]	 TT2 ($C_{35}H_{52}O_3$)	3WT7	2.4 Å		22R-Butyl-2-methylidene-26,27-dimethyl-19,24-dinor-$1,25D_3$ + DRIP205 (NR2)[4]	 YA2 ($C_{32}H_{54}O_3$)

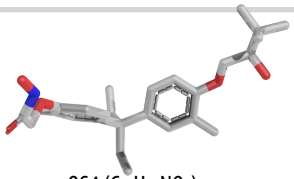
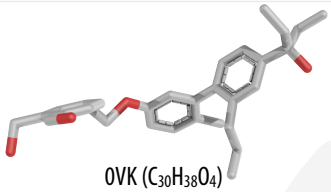
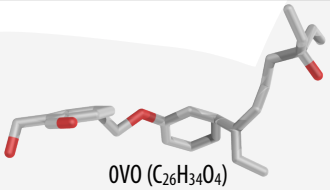
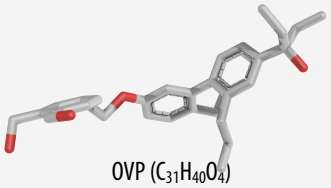
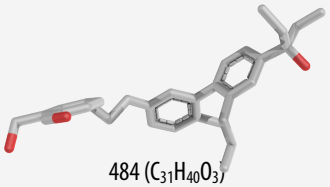
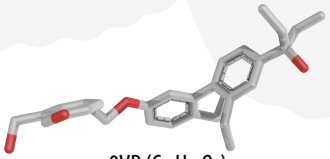
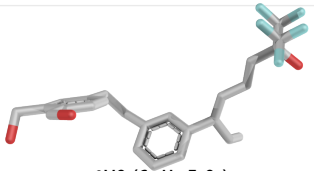
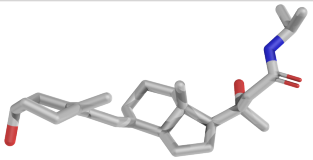
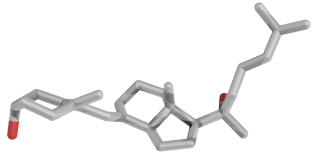
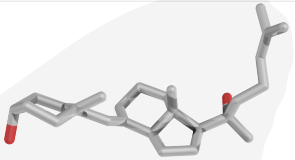
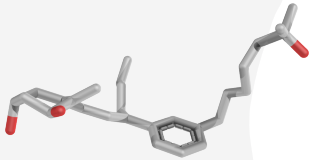
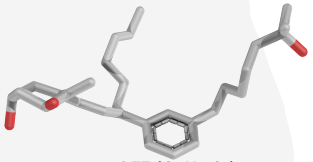
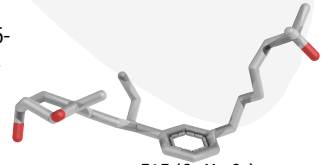
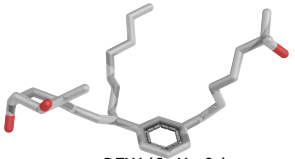
Orthologue	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]
RAT	2ZMJ	2.35 Å	[117]	26-adamantyl-1,25R-2-methylene-22,23-didehydro-19,27-dinor-20-epi-D_3 + DRIP205 (NR2)[4]	 MI4 ($C_{36}H_{54}O_3$)
	2ZXM	3.01 Å	[118]	(22S)-butyl-1,24-24,25,26-trinor-D_3 + DRIP205 (NR2)[4]	 JB1 ($C_{28}H_{46}O_3$)
	2ZXN	2.1 Å		20S(22S)-butyl-1,24-24,25,26-trinor-D_3 + DRIP205 (NR2)[4]	 JC1 ($C_{28}H_{46}O_3$)
	3A2H	2.5 Å	[94]	TEI-9647 + DRIP205 (NR2)[4]	 TEJ ($C_{27}H_{38}O_4$)
	3AFR	2 Å	[119]	22S-Butyl-1,24R-dihydroxyvitamin D_3 + DRIP205 (NR2)[4]	 ICJ ($C_{31}H_{52}O_3$)
	3AUN	1.81 Å	[120]	YR335 + DRIP205 (NR2)[4]	 YR4 ($C_{29}H_{44}O_5$)
	3VJS	1.93 Å	[78]	1-(2-[(S)-2,4-Dihydroxybutoxy]ethyl)-12-(5-ethyl-5-hydroxyheptyl)-1,12-dicarba-closo-dodecaborane + DRIP205 (NR2)[4]	 10S ($C_{17}H_{42}B_{10}O_4$)
	4YNK	2.3 Å	[126]	25-Hydroxy-25(or 26)-adamantyl-17-[20(22),23-diynyl]-19,21,26,27-tetranorvitamin-1,25D_3 + DRIP205 (NR2)[4]	 YW2 ($C_{34}H_{44}O_3$)
	5AWJ	2.2 Å	[127]	2-methylene-22S-Hexyl-19,25,26,27-tetranor-1,25D_3 + DRIP205 (NR2)[4]	 YSL ($C_{30}H_{50}O_3$)
	5AWK	2.9 Å		2-methylene-22S-ethyl-19,25,26,27-tetranor-1,25D_3 + DRIP205 (NR2)[4]	 YSE ($C_{26}H_{42}O_3$)
	5B41	1.89 Å	[128]	2-methylidene-19-nor-1,25D_3 + DRIP205 (NR2)[4]	 YSV ($C_{27}H_{44}O_3$)
	5B5B	2 Å	[129]	2-methylidene-26,27-diphenyl-19-nor-1,25D_3 + DRIP205 (NR2)[4]	 AKX ($C_{39}H_{52}O_3$)
	5GIC	2.35 Å	[130]	26,23-lactam-N-phenethyl-1,25D_3 + DRIP205 (NR2)[4]	 DLC ($C_{35}H_{51}NO_4$)
	5GID	2.15 Å		26,23-lactam-N-phenylbutyl-1,25D_3 + DRIP205 (NR2)[4]	 VDP ($C_{37}H_{53}NO_4$)

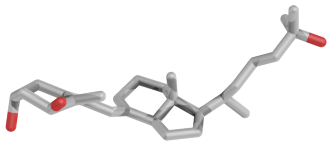
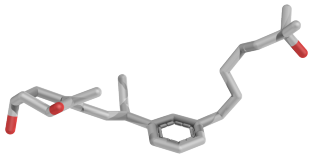
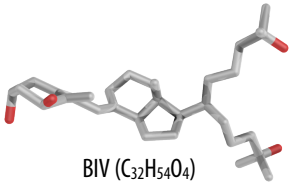
Orthologue	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]
RAT	3VJT	2 Å	[78]	1-(2-[(R)-2,4-Dihydroxybutoxy]ethyl)-12-(5-ethyl-5-hydroxyheptyl)-1,12-dicarba-closo-dodecaborane + DRIP205 (NR2)[4]	 10R ($C_{17}H_{42}B_{10}O_4$)
	3VRT	2.4 Å		2-methylidene-17-[(2R)-5-hydroxypentan-2-yl]- + DRIP205 (NR2)[4]	 YS2 ($C_{24}H_{38}O_3$)
	3VRU	2 Å		2-methylidene-17-[(2R)-5-hydroxy-5-methylhexan-2-yl]-1,25D_3 + DRIP205 (NR2)[4]	 YS3 ($C_{26}H_{42}O_3$)
	3VRV	1.9 Å	[54]	2-methylidene-17-[(2R)-5-ethyl-5-hydroxyheptan-2-yl]- + DRIP205 (NR2)[4]	 YSD ($C_{28}H_{46}O_3$)
	3VRW	2.4 Å		2-methylidene-17-[(2R,3S)-3-butyl-5-ethyl-5-hydroxyheptan-2-yl]-1,25D_3 + DRIP205 (NR2)[4]	 YS5 ($C_{32}H_{54}O_3$)
	3VT3	1.7 Å	[121]	1,25D_3 **rVDR_R270L** + DRIP 205 (NR2)[4]	 EDO FMT ($C_{27}H_{44}O_3$)
	3VT4	1.9 Å		2Z-hydroxyethylidene-16-ene-22-thia-1,25-dinorvitamin D_3 **rVDR_R270L** + DRIP 205 (NR2)[4]	 5YI ($C_{28}H_{44}O_4S$)

PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]
5GIE	2.39 Å	[130]	26,23-lactam-N-phenylbutyl-1,25D_3 + DRIP205 (NR2)[4]	 VDP ($C_{37}H_{53}NO_4$)
5H1E	2.6 Å	[131]	1,25D_3 + TIF2 (NR2)[5]	 VDX ($C_{27}H_{44}O_3$)
5XPL	2.05 Å	[132]	22S-butyl-25-hydroxyphenyl- 2-methylidene-19,26,27-trinor-25-oxo-1-hydroxyvitamin D_3 + TIF2 (NR2)[5]	 8C9 ($C_{35}H_{50}O_4$)
5XPM	2.2 Å		22S-Butyl-25RS-hydroxyphenyl-25-methoxy-2-methylidene -19 ,26,27-trinor-1-hydroxyvitamin D_3 + DRIP205 (NR2)[4]	 8C0 ($C_{36}H_{54}O_4$)
5XPN	1.96 Å		25RS-(hydroxyphenyl)-25-methoxy-2-methylidene-19,26,27-trinor-1-hydroxyvitamin D_3 + DRIP205 (NR2)[4]	 8BO 9RO ($C_{32}H_{46}O_4$)
5XPO	2.28 Å		25-(hydroxyphenyl)-2-methylidene-19,26,27-trinor-25-oxo-1-hydroxyvitamin D_3 + DRIP205 (NR2)[4]	 8BL ($C_{31}H_{42}O_4$)
5XPP	2.85 Å		25RS-(Hydroxyphenyl)-2-methylidene-19,26,27-trinor -1,25D_3 + DRIP205 (NR2)[4]	 8BF ($C_{31}H_{44}O_4$)

Orthologue	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]
RAT	3VT5	2.11 Å	[121]	2E-hydroxyethylidene-16-ene-22-thia-1,25-dinorvitamin D_3 **rVDR_R270L** + DRIP 205 (NR2)[4]	 YI2 ($C_{28}H_{44}O_4S$)	5XUQ	2.8 Å	—	2-methylidene-19,26,27-trinor-22-(S)-butyl-1-hydroxy-25-oxo-25-(1H-pyrrol-2-yl)-vitamin D_3 + DRIP205 (NR2)[4]	 8FF ($C_{33}H_{49}NO_3$)
	3VT6	2.3 Å		2Z-hydroxyethylidene-16-ene-22-thia-1,25-dinorvitamin D_3 **rVDR_WT** + DRIP 205 (NR2)[4]	 5YI ($C_{28}H_{44}O_4S$)	5XZF	2.1 Å	[133]	25S-(Adamantan-1-yl)-26,27-dinor-23-yne-1α,25D_3 (ADRO1) + DRIP205 (NR2)[4]	 8J0 ($C_{35}H_{50}O_3$)
	3VT7	1.65 Å		1,25D_3 **rVDR_W282R** + DRIP 205 (NR2)[4]	 VDX ($C_{27}H_{44}O_3$)	5XZH	2 Å		25R-(Adamantan-1-yl)-26,27-dinor-23-yne-1α,25D_3 (ADRO2) + DRIP205 (NR2)[4]	 8J3 ($C_{35}H_{50}O_3$)
	3VT8	2.1 Å		9α-butyl-1,25-norvitamin D_3 **rVDR_W282R** + DRIP 205 (NR2)[4]	 YI3 ($C_{30}H_{52}O_3$)	5ZWE	2.72 Å		1,3-Dihydroxy-2-methylidene-9,10-secoestra-5,7-dien-17-(hept-1-en-3-one) + DRIP205 (NR2)[4]	 9K0 ($C_{26}H_{38}O_3$)
	3VT9	2.35 Å		2-hydroxyethylidene-9α-(prop-2-en-1-yl)-1,25-norvitamin D_3 **rVDR_W282R** + DRIP 205 (NR2)[4]	 5Y4 ($C_{31}H_{51}O_4$)	5ZWF	2.1 Å	[134]	1,3-Dihydroxy-2-methylidene-9,10-secoestra-5,7-dien-17(-oct-2-en-4-one) + DRIP205 (NR2)[4]	 9KR ($C_{27}H_{40}O_3$)
	3VTB	2 Å	[122]	2-methylidene-25S-25-adamantyl-19,26,27-trinorvitamin-1,25D_3 (ADTK1) + DRIP 205 (NR2)[4]	 TKA ($C_{35}H_{50}O_3$)	5ZWH	2.38 Å		1,3-Dihydroxy-2-methylidene-9,10-secoestra-5,7-dien-17-(oct-6-en-4-yn-3-one) + DRIP205 (NR2)[4]	 9KX 9N9 ($C_{27}H_{36}O_3$)
	3VTC	1.5 Å		2-methylidene-25R-26-adamantyl-19,27-dinorvitammin 1,25D_3 (ADTK3) + DRIP 205 (NR2)[4]	 EDO, TK3 ($C_{36}H_{52}O_3$)	5ZWI	2.4 Å		1,3-Dihydroxy-2-methylidene-9,10-secoestra-5,7-dien-17-(octa-4,6-dien-3-one) + DRIP205 (NR2)[4]	 9KX ($C_{27}H_{38}O_3$)

Orthologue	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]
ZEBRAFISH	2HBH	2.65 Å	[135]	21-nor-20(22),23-diyne-1,25D_3 + SRC1 (NR2)[6]	 XE4 ($C_{26}H_{34}O_3$)
	2HC4	2.2 Å	[136]	1,25D_3 + SRC1 (NR2)[6]	 VDX ($C_{27}H_{44}O_3$)
	2HCD	2.6 Å		Gemini + SRC1 (NR2)[6]	 BIV ($C_{32}H_{54}O_4$)
	3DR1	2.7 Å	[137]	CD578 + SRC1 (NR2)[6]	 C5D ($C_{24}H_{32}F_6O_3$)
	3O1D	2.4 Å	[138]	Gemini-0072 + SRC1 (NR2)[6]	 G72 ($C_{31}H_{44}F_6O_4$)
	3O1E	2.5 Å		Gemini-0097 + SRC1 (NR2)[6]	 H97 ($C_{31}H_{44}F_6O_4$)
	4FHH	2.33 Å	[139]	JF-C72 + SRC1 (NR2)[6]	 0U3 ($C_{27}H_{39}NO_5$)
	4RUP	2.75 Å	[140]	Gemini-0097 **zVDR_L337H** + SRC1 (NR2)[6]	 H97 ($C_{31}H_{44}F_6O_4$)
	5E7V	2.4 Å	[44]	1α-hydroxy-27-nor-25-o-carbonyl-vitamin D_3 + SRC1 (NR2)[6]	 M7E ($C_{26}H_{37}B_{10}O_2$)
	5LGA	2.5 Å	[141]	BXL0124 + TIF2 (NR2)[5]	 6VH ($C_{32}H_{40}F_6O_4$)
	5MX7	1.98 Å	[142]	1α,20S-dihydroxyvitamin D_3 + SRC1 (NR2)[6]	 D3V ($C_{27}H_{44}O_3$)
	5NKY	2.1 Å		(22S)-[(5′S)-(2″-hydroxy-2″-propyl)-(2′R)-tetrahydrofuryl]-22,23,24,25,26,27-hexanor-1,25D_3 + SRC1 (NR2)[6]	 91W ($C_{28}H_{44}O_4$)
	5NMA	2.8 Å	[143]	(22S)-[(5′R)-(2″-hydroxy-2″-propyl)-(2′S)-tetrahydrofuryl]-22,23,24,25,26,27-hexanor-1,25D_3 + SRC1 (NR2)[6]	 9CW ($C_{28}H_{44}O_4$)
	5NMB	2.5 Å		(22S)-[(5′S)-(2″-hydroxy-2″-propyl)-(2′S)-tetrahydrofuryl]-22,23,24,25,26,27-hexanor-1,25D_3 + SRC1 (NR2)[6]	 9CZ ($C_{28}H_{44}O_4$)

Orthologue	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]
ZEBRAFISH	4FHI	2.4 Å	[139]	JF-C71 + SRC1 (NR2)[6]	 OS4 ($C_{27}H_{39}NO_5$)
	4G1D	2.9 Å		CD4720 + SRC1 (NR2)[6]	 0VK ($C_{30}H_{38}O_4$)
	4G1Y	2.85 Å		CD3938 + SRC1 (NR2)[6]	 0VO ($C_{26}H_{34}O_4$)
	4G1Z	2.5 Å	[108]	CD4802 + SRC1 (NR2)[6]	 0VP ($C_{31}H_{40}O_4$)
	4G20	2.9 Å		CD4849 + SRC1 (NR2)[6]	 484 ($C_{31}H_{40}O_3$)
	4G21	2.9 Å		CD4742 + SRC1 (NR2)[6]	 0VP ($C_{31}H_{40}O_4$)
	4G2H	2.5 Å		CD4528 + SRC1 (NR2)[6]	 0VQ ($C_{25}H_{26}F_6O_3$)
	5OW7	2.1 Å		20-*N*-isopropylacetamide-1,20S-dihydroxyvitamin D_3 + SRC1 (NR2)[6]	 AYK ($C_{26}H_{41}NO_3$)
	5OW9	2.4 Å	[144]	20S-hydroxyvitamin D_3 + SRC1 (NR2)[6]	 AYT ($C_{27}H_{44}O_2$)
	5OWD	2.15 Å		24-ene-20S-hydroxyvitamin D_3 + SRC1 (NR2)[6]	 B0B ($C_{27}H_{42}O_2$)
	6FO7	2.59 Å		(1R,3S,Z)-5-{(E)-3-[3-(6-Hydroxy-6-methylheptyl) phenyl]hept-2-en-1-ylidene}-4- methylene cyclohexane-1,3-diol + SRC1 (NR2)[6]	 LX3 ($C_{28}H_{42}O_3$)
	6FO8	2.3 Å	[83]	(1R,3S,Z)-5-{(E)-3-[3-(6-Hydroxy-6-methylheptyl) phenyl]non-2-en-1-ylidene}-4- methylene cyclohexane-1,3-diol + SRC1 (NR2)[6]	 DZT ($C_{30}H_{46}O_3$)
	6FO9	2.7 Å		(1R,3S,Z)-5-{(E)-3-[3-(6-Hydroxy-6-methylheptyl) phenyl]hex-2-en-1-ylidene} -4-methylenecyclohexane- 1,3-diol + SRC1 (NR2)[6]	 E0E ($C_{27}H_{40}O_3$)
	6FOB	2.75 Å		(1R,3S,Z)-5-{(E)-3-[3-(6-Hydroxy-6-methylheptyl) phenyl]dec-2-en-1-ylidene}-4- methylene cyclohexane-1,3-diol + SRC1 (NR2)[6]	 DZW ($C_{31}H_{48}O_3$)

Orthologue	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]	PDBID[1]	Resolution[2]	Reference	Ligand Name/Notes	Ligand Conformation[3]
ZEBRAFISH	4RUJ	2.35 Å	[140]	1,25D_3 **zVDR_L337H** + SRC1 (NR2)[6]	 VDX ($C_{27}H_{44}O_3$)	6FOD	2.5 Å	[83]	(1R,3S,Z)-5-{(E)-3-[3-(6-Hydroxy-6-methylheptyl)phenyl]pent-2-en-1-ylidene}-4- methylene cyclohexane-1,3-diol + SRC1 (NR2)[6]	 E05 ($C_{26}H_{38}O_3$)
	4RUO	2.81 Å		Gemini **zVDR_L337H** + SRC1 (NR2)[6]	 BIV ($C_{32}H_{54}O_4$)					
UNRELEASED	4XWQ	-	-	1,25D_3-26,23-lactams (DLAMS)		4XY0	-	-	1,25D_3-26,23-lactams (DLAMS)	
	4XXZ	-	-	1,25D_3-26,23-lactams (DLAMS)		4XY1	-	-	1,25D_3-26,23-lactams (DLAMS)	

[1] Protein Data Bank identifier
[2] Atomic resolution of the crystal structure in Ångström
[3] The conformation of the ligand extracted from the crystal structure
[4] Synthetic peptide corresponding to NR2 Box of DRIP205/TRAP220/MED1 625-KNHPMLMNLLKDN-637
[5] Synthetic peptide corresponding to NR2 Box of TIF2/NCOA2 740-KENALLRYLLDKD-752
[6] Synthetic peptide corresponding to NR2 Box of SRC1/NCOA1 686-RHKILHRLLQEGSPS-700
— no publication available