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X-ray structure and *in silico* molecular docking of a natural phaeosphaeride A derivative for targets associated with kinase cascades

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Table of contents:

X-ray study of AV-6

Table S1 Crystal data and structure refinement for AV-6

Identification code	AV-6
Empirical formula	$C_{19}H_{30}N_2O_4$
Formula weight	350.45
Temperature/K	100.0(5)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	11.88260(10)
b/Å	9.55000(10)
c/Å	17.21700(10)
α/°	90
β/°	107.8250(10)
γ/°	90
Volume/Å^3	1859.98(3)
Z	4
ρ_{calc}g/cm^3	1.251
μ/mm^{-1}	0.707
F(000)	760.0
Crystal size/mm^3	0.24 × 0.22 × 0.16
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.392 to 139.968
Index ranges	-14 ≤ h ≤ 14, -11 ≤ k ≤ 11, -20 ≤ l ≤ 20
Reflections collected	28159
Independent reflections	7060 [R_{int} = 0.0345, R_{sigma} = 0.0306]
Data/restraints/parameters	7060/1/459
Goodness-of-fit on F^2	1.042
Final R indexes [I>=2σ (I)]	R_1 = 0.0295, wR_2 = 0.0754
Final R indexes [all data]	R_1 = 0.0299, wR_2 = 0.0757
Largest diff. peak/hole / e Å^{-3}	0.22/-0.16
Flack parameter	0.02(5)

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for AV-6. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	4375.9(11)	8926.8(13)	8875.6(8)	17.3(3)
O2	3820.5(12)	12553.6(13)	9421.8(8)	20.2(3)
O3	481.8(12)	8252.2(16)	8984.3(9)	27.0(3)
O4	1113.5(12)	5855.0(15)	8239.3(8)	23.0(3)
N2	1917.6(14)	6758.9(17)	8776.7(9)	18.6(3)
N17	2670.4(13)	10904.7(16)	10170.4(9)	16.2(3)

C1	1478.6(17)	8062(2)	8953.8(11)	18.7(4)
C3	3028.3(16)	6940.5(19)	8644.5(10)	16.8(4)
C4	3341.4(16)	8399(2)	8886.0(10)	15.5(3)
C5	2464.7(16)	9051(2)	9085.9(11)	16.8(4)
C6	2502.0(16)	10569.8(19)	9302.0(11)	15.6(3)
C7	3500.8(16)	11249.2(19)	9013.7(11)	16.6(4)
C8	4616.9(16)	10314.6(19)	9257.1(11)	15.7(4)
C9	5657.2(16)	10892(2)	9027.3(11)	18.5(4)
C10	6725.5(16)	9915(2)	9262.8(12)	19.5(4)
C11	7846.8(17)	10574(2)	9167.2(11)	19.5(4)
C12	7750.5(17)	11064(2)	8308.6(11)	22.4(4)
C13	8897.7(19)	11733(3)	8281.1(13)	27.8(4)
C14	3635.9(18)	5995(2)	8372.2(12)	22.7(4)
C15	3059.5(17)	11528(2)	8098.4(11)	21.1(4)
C16	981.2(19)	4594(2)	8652.1(13)	25.8(4)
C18	3098.1(17)	9784(2)	10774.5(11)	21.0(4)
C19	2964.1(19)	10424(2)	11553.2(12)	26.1(4)
C20	1928.0(18)	11464(2)	11263.9(12)	23.9(4)
C21	1588.8(17)	11410(2)	10329.8(12)	22.7(4)
O1'	5367.3(11)	1041.1(14)	6177.7(8)	19.1(3)
O2'	4348.7(12)	-2555.7(14)	5530.5(9)	23.2(3)
O3'	1326.4(12)	1711.2(16)	5935.8(9)	25.4(3)
O4'	2570.0(13)	4111.7(15)	6700.7(8)	22.6(3)
N2'	2955.3(14)	3195.1(17)	6199.2(9)	19.2(3)
N17'	2528.1(13)	-905.7(17)	4795.2(9)	18.0(3)
C1'	2361.4(17)	1896(2)	6004.0(11)	18.7(4)
C3'	4187.7(17)	3018(2)	6377.7(11)	19.2(4)
C4'	4309.5(16)	1559(2)	6139.5(10)	17.5(4)
C5'	3256.9(16)	909(2)	5906.4(11)	17.2(4)
C6'	3115.1(16)	-606.6(19)	5669.6(11)	17.4(4)
C7'	4375.6(17)	-1284.9(19)	5964.4(11)	18.5(4)
C8'	5295.6(16)	-317.3(19)	5766.2(11)	17.6(4)
C9'	6546.1(17)	-890(2)	6002.1(12)	21.5(4)
C10'	7417.6(18)	116(2)	5803.7(13)	23.8(4)
C11'	8628.8(18)	-516(2)	5885.7(12)	22.3(4)
C12'	9307.3(19)	-1057(2)	6732.1(12)	26.1(4)
C13'	10532(2)	-1548(3)	6754.5(14)	32.9(5)
C14'	5024(2)	3960(2)	6675.5(14)	29.6(5)
C15'	4707.1(19)	-1624(2)	6869.0(12)	24.5(4)
C16'	2064.9(19)	5347(2)	6260.5(13)	26.2(4)
C18'	2491.0(18)	215(2)	4202.2(12)	23.7(4)
C19'	1665(2)	-390(3)	3409.9(12)	29.0(5)
C20'	802.3(18)	-1325(2)	3684.4(12)	25.5(4)
C21'	1278.7(17)	-1328(2)	4618.6(12)	22.5(4)

Table S3 Anisotropic Displacement Parameters ($Å^2×10^3$) for AV-6. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	17.9(6)	12.7(6)	22.9(6)	-2.4(5)	8.7(5)	-2.2(5)
O2	28.2(7)	11.4(6)	23.7(6)	-3.2(5)	11.9(5)	-3.3(5)
O3	20.6(7)	24.6(8)	37.4(8)	-3.0(6)	11.2(6)	-3.1(6)
O4	26.0(7)	17.3(7)	22.4(6)	-1.5(5)	2.6(5)	-7.2(6)
N2	18.4(7)	14.6(7)	22.0(7)	-3.0(6)	5.1(6)	-5.1(6)
N17	18.1(7)	14.7(7)	17.1(7)	-0.8(6)	7.2(6)	1.1(6)
C1	20.0(9)	17.0(9)	18.8(8)	1.0(7)	5.6(7)	-1.4(7)
C3	19.4(9)	13.7(9)	16.0(8)	0.2(7)	3.8(7)	-2.4(7)
C4	16.5(8)	15.4(9)	13.9(8)	1.3(6)	3.6(6)	-1.6(7)
C5	19.2(9)	15.4(9)	16.0(8)	0.0(7)	5.6(6)	-1.0(7)
C6	16.6(8)	13.5(8)	16.9(8)	0.0(7)	5.4(6)	0.2(6)
C7	20.3(9)	11.8(8)	19.0(9)	-0.5(7)	7.8(7)	-1.2(7)
C8	19.0(9)	12.4(8)	16.5(8)	-2.8(7)	6.6(7)	-4.0(7)
C9	19.4(9)	15.7(9)	21.6(8)	1.0(7)	8.1(7)	-2.7(7)
C10	18.3(9)	16.7(9)	24.7(9)	2.9(7)	8.4(7)	-0.2(7)
C11	18.8(9)	18.8(9)	21.1(9)	1.4(7)	6.1(7)	-1.6(7)
C12	21.2(9)	25.3(10)	21.4(9)	2.8(8)	7.3(7)	-1.1(8)
C13	26.9(10)	33.5(12)	26.0(9)	2.7(9)	12.6(8)	-6.1(9)
C14	26.9(9)	16.5(9)	26.0(9)	-2.0(8)	9.9(7)	-1.8(8)
C15	25.5(10)	18.7(9)	19.8(9)	2.3(7)	7.9(7)	2.7(7)
C16	28.9(10)	17.2(9)	30.3(10)	1.1(8)	7.6(8)	-7.2(8)
C18	23.2(9)	19.9(9)	19.8(9)	2.3(7)	6.4(7)	4.0(7)
C19	28.3(10)	31.3(11)	19.4(9)	1.1(8)	8.5(8)	3.6(9)
C20	26.8(10)	25.6(10)	22.6(9)	0.6(8)	12.5(8)	1.7(8)
C21	22.0(9)	24.9(10)	23.7(9)	2.4(8)	10.5(7)	6.6(8)
O1'	16.7(6)	14.8(6)	25.1(6)	-3.8(5)	5.2(5)	1.2(5)
O2'	26.9(7)	13.1(6)	27.2(7)	-4.4(5)	4.7(5)	1.3(5)
O3'	21.5(7)	23.1(7)	32.8(7)	-2.8(6)	10.3(6)	0.5(6)
O4'	31.8(7)	15.9(7)	20.7(6)	-3.3(5)	9.1(5)	7.2(5)
N2'	21.7(8)	14.8(8)	21.1(7)	-5.5(6)	6.5(6)	3.5(6)
N17'	20.2(8)	15.5(7)	19.1(7)	-1.8(6)	7.0(6)	-2.4(6)
C1'	23.5(9)	16.1(9)	16.0(8)	-0.6(7)	5.4(7)	1.4(7)
C3'	22.0(9)	16.9(9)	17.4(8)	-0.9(7)	4.2(7)	3.6(7)
C4'	20.3(9)	17.0(9)	14.8(8)	0.0(7)	4.7(7)	1.7(7)
C5'	19.9(8)	15.5(9)	16.4(8)	-0.6(7)	5.7(6)	0.8(7)
C6'	20.4(9)	13.6(9)	18.8(8)	-1.1(7)	7.0(7)	-1.6(7)
C7'	23.0(9)	12.3(9)	20.3(9)	-1.6(7)	6.9(7)	-0.4(7)
C8'	21.3(9)	12.2(8)	18.5(8)	-2.7(7)	4.8(7)	1.7(7)
C9'	21.5(9)	17.3(9)	25.3(9)	-0.9(8)	6.3(7)	2.2(7)
C10'	22.0(9)	20.3(10)	28.8(10)	4.1(8)	7.5(8)	2.9(8)
C11'	23.2(10)	21.0(10)	22.8(9)	2.6(8)	7.2(8)	2.4(8)
C12'	27.0(10)	29.7(11)	22.0(9)	2.5(8)	8.0(8)	7.8(9)
C13'	28.7(11)	42.4(13)	28.1(10)	9.6(9)	9.5(8)	13.7(10)

C14'	26.5(10)	18.9(10)	39.1(11)	-9.0(9)	3.7(8)	0.5(8)
C15'	29.0(10)	20.7(10)	22.7(9)	3.9(8)	6.1(8)	0.2(8)
C16'	30.1(10)	18.3(10)	29.0(10)	-0.9(8)	7.2(8)	6.9(8)
C18'	28.0(10)	21.5(10)	20.5(9)	-0.5(8)	5.8(8)	-7.4(8)
C19'	33.4(11)	31.5(11)	20.0(9)	-2.6(8)	5.2(8)	-10.2(9)
C20'	21.1(9)	33.9(11)	21.4(9)	-5.0(8)	6.4(7)	-2.6(8)
C21'	19.7(9)	26.8(10)	21.5(9)	-2.9(8)	7.1(7)	-4.7(8)

Table S4 Bond Lengths for AV-6.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C4	1.334(2)	O1'	C4'	1.334(2)
O1	C8	1.468(2)	O1'	C8'	1.468(2)
O2	C7	1.424(2)	O2'	C7'	1.420(2)
O3	C1	1.215(2)	O3'	C1'	1.212(2)
O4	N2	1.405(2)	O4'	N2'	1.401(2)
O4	C16	1.432(2)	O4'	C16'	1.431(2)
N2	C1	1.418(3)	N2'	C1'	1.416(3)
N2	C3	1.417(2)	N2'	C3'	1.411(2)
N17	C6	1.481(2)	N17'	C6'	1.480(2)
N17	C18	1.470(2)	N17'	C18'	1.470(2)
N17	C21	1.475(2)	N17'	C21'	1.477(2)
C1	C5	1.468(3)	C1'	C5'	1.469(3)
C3	C4	1.469(3)	C3'	C4'	1.472(3)
C3	C14	1.328(3)	C3'	C14'	1.322(3)
C4	C5	1.346(3)	C4'	C5'	1.343(3)
C5	C6	1.495(3)	C5'	C6'	1.499(3)
C6	C7	1.561(2)	C6'	C7'	1.567(3)
C7	C8	1.546(3)	C7'	C8'	1.547(3)
C7	C15	1.524(2)	C7'	C15'	1.520(3)
C8	C9	1.513(2)	C8'	C9'	1.517(3)
C9	C10	1.527(3)	C9'	C10'	1.526(3)
C10	C11	1.527(3)	C10'	C11'	1.527(3)
C11	C12	1.521(3)	C11'	C12'	1.523(3)
C12	C13	1.519(3)	C12'	C13'	1.518(3)
C18	C19	1.525(3)	C18'	C19'	1.529(3)
C19	C20	1.541(3)	C19'	C20'	1.540(3)
C20	C21	1.534(3)	C20'	C21'	1.533(3)

Table S5 Bond Angles for AV-6.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C4	O1	C8	112.92(14)	C4'	O1'	C8'	112.93(14)
N2	O4	C16	110.25(14)	N2'	O4'	C16'	110.60(14)

O4	N2	C1	117.39(15)	O4'	N2'	C1'	117.42(15)
O4	N2	C3	116.66(15)	O4'	N2'	C3'	116.97(15)
C3	N2	C1	110.43(15)	C3'	N2'	C1'	110.81(15)
C18	N17	C6	117.87(15)	C18'	N17'	C6'	118.05(15)
C18	N17	C21	103.82(14)	C18'	N17'	C21'	103.95(15)
C21	N17	C6	113.71(14)	C21'	N17'	C6'	113.13(14)
O3	C1	N2	124.62(18)	O3'	C1'	N2'	124.59(18)
O3	C1	C5	129.75(18)	O3'	C1'	C5'	130.14(18)
N2	C1	C5	105.63(15)	N2'	C1'	C5'	105.26(16)
N2	C3	C4	103.79(15)	N2'	C3'	C4'	103.69(16)
C14	C3	N2	127.40(18)	C14'	C3'	N2'	127.57(18)
C14	C3	C4	128.81(18)	C14'	C3'	C4'	128.73(19)
O1	C4	C3	120.60(16)	O1'	C4'	C3'	120.61(17)
O1	C4	C5	128.15(17)	O1'	C4'	C5'	128.37(18)
C5	C4	C3	111.24(16)	C5'	C4'	C3'	111.03(17)
C1	C5	C6	128.66(17)	C1'	C5'	C6'	128.71(17)
C4	C5	C1	107.85(16)	C4'	C5'	C1'	108.08(17)
C4	C5	C6	123.11(17)	C4'	C5'	C6'	122.98(17)
N17	C6	C5	116.44(15)	N17'	C6'	C5'	116.20(15)
N17	C6	C7	110.50(14)	N17'	C6'	C7'	110.84(14)
C5	C6	C7	106.96(15)	C5'	C6'	C7'	107.12(15)
O2	C7	C6	108.72(14)	O2'	C7'	C6'	108.51(14)
O2	C7	C8	107.11(14)	O2'	C7'	C8'	107.34(14)
O2	C7	C15	108.23(15)	O2'	C7'	C15'	108.31(15)
C8	C7	C6	110.27(15)	C8'	C7'	C6'	110.58(15)
C15	C7	C6	110.30(15)	C15'	C7'	C6'	110.01(16)
C15	C7	C8	112.09(15)	C15'	C7'	C8'	111.97(15)
O1	C8	C7	111.48(14)	O1'	C8'	C7'	111.21(14)
O1	C8	C9	105.97(14)	O1'	C8'	C9'	106.37(14)
C9	C8	C7	114.87(15)	C9'	C8'	C7'	115.21(16)
C8	C9	C10	112.80(16)	C8'	C9'	C10'	112.93(16)
C9	C10	C11	113.69(16)	C9'	C10'	C11'	114.58(16)
C12	C11	C10	115.02(16)	C12'	C11'	C10'	115.49(17)
C13	C12	C11	111.00(16)	C13'	C12'	C11'	110.58(17)
N17	C18	C19	102.92(16)	N17'	C18'	C19'	102.67(16)
C18	C19	C20	105.19(16)	C18'	C19'	C20'	104.54(16)
C21	C20	C19	104.17(16)	C21'	C20'	C19'	104.85(16)
N17	C21	C20	103.97(15)	N17'	C21'	C20'	103.92(15)

Table S6 Torsion Angles for AV-6.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C4	C5	C1	176.46(16)	O1'	C4'	C5'	C1'	177.43(17)
O1	C4	C5	C6	3.0(3)	O1'	C4'	C5'	C6'	2.5(3)
O1	C8	C9	C10	-55.12(19)	O1'	C8'	C9'	C10'	-55.5(2)

O2	C7	C8	O1	179.15(13)	O2'	C7'	C8'	O1'	178.85(13)
O2	C7	C8	C9	-60.30(19)	O2'	C7'	C8'	C9'	-60.03(19)
O3	C1	C5	C4	−172.40(19)	O3'	C1'	C5'	C4'	−172.66(19)
O3	C1	C5	C6	0.5(3)	O3'	C1'	C5'	C6'	1.9(3)
O4	N2	C1	O3	32.5(3)	O4'	N2'	C1'	O3'	31.3(3)
O4	N2	C1	C5	−147.80(15)	O4'	N2'	C1'	C5'	−149.09(14)
O4	N2	C3	C4	146.62(14)	O4'	N2'	C3'	C4'	147.98(15)
O4	N2	C3	C14	-33.9(3)	O4'	N2'	C3'	C14'	-33.1(3)
N2	C1	C5	C4	7.9(2)	N2'	C1'	C5'	C4'	7.8(2)
N2	C1	C5	C6	−179.17(17)	N2'	C1'	C5'	C6'	−177.64(17)
N2	C3	C4	O1	177.00(15)	N2'	C3'	C4'	O1'	175.91(15)
N2	C3	C4	C5	-4.08(19)	N2'	C3'	C4'	C5'	-4.6(2)
N17	C6	C7	O2	-34.33(19)	N17'	C6'	C7'	O2'	-33.3(2)
N17	C6	C7	C8	82.81(17)	N17'	C6'	C7'	C8'	84.14(18)
N17	C6	C7	C15	−152.85(15)	N17'	C6'	C7'	C15'	−151.66(15)
N17	C18	C19	C20	28.7(2)	N17'	C18'	C19'	C20'	31.0(2)
C1	N2	C3	C4	9.19(18)	C1'	N2'	C3'	C4'	9.73(19)
C1	N2	C3	C14	−171.35(18)	C1'	N2'	C3'	C14'	-171.3(2)
C1	C5	C6	N17	79.5(2)	C1'	C5'	C6'	N17'	76.1(2)
C1	C5	C6	C7	−156.45(17)	C1'	C5'	C6'	C7'	−159.41(17)
C3	N2	C1	O3	169.55(17)	C3'	N2'	C1'	O3'	169.40(17)
C3	N2	C1	C5	-10.72(19)	C3'	N2'	C1'	C5'	-11.0(2)
C3	C4	C5	C1	-2.4(2)	C3'	C4'	C5'	C1'	-2.0(2)
C3	C4	C5	C6	−175.78(16)	C3'	C4'	C5'	C6'	−176.92(16)
C4	O1	C8	C7	-41.84(19)	C4'	O1'	C8'	C7'	-43.06(19)
C4	O1	C8	C9	−167.48(14)	C4'	O1'	C8'	C9'	−169.23(15)
C4	C5	C6	N17	-108.6(2)	C4'	C5'	C6'	N17'	-110.1(2)
C4	C5	C6	C7	15.5(2)	C4'	C5'	C6'	C7'	14.4(2)
C5	C6	C7	O2	−161.99(14)	C5'	C6'	C7'	O2'	−161.04(14)
C5	C6	C7	C8	-44.85(18)	C5'	C6'	C7'	C8'	-43.56(19)
C5	C6	C7	C15	79.49(18)	C5'	C6'	C7'	C15'	80.64(19)
C6	N17	C18	C19	−170.90(15)	C6'	N17'	C18'	C19'	−171.25(16)
C6	N17	C21	C20	171.55(15)	C6'	N17'	C21'	C20'	170.30(16)
C6	C7	C8	O1	61.01(18)	C6'	C7'	C8'	O1'	60.66(18)
C6	C7	C8	C9	−178.43(14)	C6'	C7'	C8'	C9'	−178.22(15)
C7	C8	C9	C10	−178.65(15)	C7'	C8'	C9'	C10'	−179.18(16)
C8	O1	C4	C3	-	C8'	O1'	C4'	C3'	-

				170.81(15)					168.37(15)
C8	O1	C4	C5	10.5(2)	C8'	O1'	C4'	C5'	12.3(3)
C8	C9	C10	C11	−170.43(15)	C8'	C9'	C10'	C11'	−169.42(16)
C9	C10	C11	C12	-59.2(2)	C9'	C10'	C11'	C12'	-60.1(2)
C10	C11	C12	C13	178.64(17)	C10'	C11'	C12'	C13'	−175.38(19)
C14	C3	C4	O1	-2.4(3)	C14'	C3'	C4'	O1'	-3.0(3)
C14	C3	C4	C5	176.48(19)	C14'	C3'	C4'	C5'	176.5(2)
C15	C7	C8	O1	-62.29(19)	C15'	C7'	C8'	O1'	-62.41(19)
C15	C7	C8	C9	58.3(2)	C15'	C7'	C8'	C9'	58.7(2)
C16	O4	N2	C1	−116.29(18)	C16'	O4'	N2'	C1'	−113.92(18)
C16	O4	N2	C3	109.27(18)	C16'	O4'	N2'	C3'	110.59(19)
C18	N17	C6	C5	16.0(2)	C18'	N17'	C6'	C5'	19.9(2)
C18	N17	C6	C7	−106.27(17)	C18'	N17'	C6'	C7'	−102.68(18)
C18	N17	C21	C20	42.23(19)	C18'	N17'	C21'	C20'	41.02(19)
C18	C19	C20	C21	-3.4(2)	C18'	C19'	C20'	C21'	-6.4(2)
C19	C20	C21	N17	-23.1(2)	C19'	C20'	C21'	N17'	-20.5(2)
C21	N17	C6	C5	−105.84(19)	C21'	N17'	C6'	C5'	−101.76(19)
C21	N17	C6	C7	131.91(16)	C21'	N17'	C6'	C7'	135.68(16)
C21	N17	C18	C19	-44.14(18)	C21'	N17'	C18'	C19'	-45.01(19)

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for AV-6.

Atom	*x*	*y*	*z*	U(eq)
H2	3765.3	12495.79	9895.56	30
H6	1735.04	10995.39	8973.54	19
H8	4867.79	10185.98	9862.47	19
H9A	5887.51	11806.13	9300.93	22
H9B	5414.08	11054.38	8430.96	22
H10A	6533.92	9063.86	8919.46	23
H10B	6880.31	9623.07	9837.74	23
H11A	8066.92	11384.87	9541.34	23
H11B	8495.69	9881.18	9339.88	23
H12A	7561.18	10256.16	7930.73	27
H12B	7099.26	11752.04	8125.42	27
H13A	8814.94	12036.22	7722.59	42
H13B	9540.98	11049.15	8456.19	42
H13C	9077.31	12544.41	8646.81	42
H14A	3329.31	5076.6	8242.4	27
H14B	4377.26	6237.64	8307.12	27
H15A	2303.85	12027.95	7961.62	32

H15B	2950.75	10635.85	7803.21	32
H15C	3640.32	12098.98	7941.74	32
H16A	421.54	3970.44	8270.61	39
H16B	682.24	4820.65	9108.15	39
H16C	1749.25	4126.09	8860.21	39
H18A	3933.82	9550.91	10839.69	25
H18B	2611.21	8928.03	10617.45	25
H19A	3697.48	10914.58	11864.14	31
H19B	2785.23	9690.78	11904.61	31
H20A	1256.76	11172.82	11453.78	29
H20B	2176.87	12419.31	11468.11	29
H21A	921.76	10757.7	10102.04	27
H21B	1364.62	12350.34	10089.98	27
H2'	3846.91	-2491.93	5066.62	35
H6'	2630.73	-1053.45	5985.18	21
H8'	5031.28	-144.81	5164.43	21
H9'A	6544.71	-1783.85	5710.86	26
H9'B	6814.51	-1089.83	6594.69	26
H10C	7525.6	936.13	6170.95	29
H10D	7069.14	456.72	5237.68	29
H11C	8522.45	-1299.47	5493.5	27
H11D	9117.07	203.88	5727.25	27
H12C	9377.37	-301.74	7138.36	31
H12D	8868.44	-1843.57	6877.9	31
H13D	10462.8	-2261.25	6333.42	49
H13E	10936.29	-1947.22	7291.86	49
H13F	10987.47	-751.02	6652.59	49
H14C	4818.96	4879.66	6793.75	35
H14D	5830.85	3717.52	6771.24	35
H15D	4062.72	-2147.22	6978.61	37
H15E	4843.24	-751.5	7184.01	37
H15F	5429.07	-2190.72	7027.54	37
H16D	1384.11	5089.7	5795.04	39
H16E	2657.56	5819.6	6063.58	39
H16F	1807.31	5978.97	6621.57	39
H18C	3286.71	401.48	4154.46	28
H18D	2168.01	1091.78	4355.51	28
H19C	2114.15	-946.28	3119.49	35
H19D	1236.31	366.71	3045.07	35
H20C	-8.65	-936.26	3495.69	31
H20D	790.02	-2285.59	3465.91	31
H21C	841.82	-652.23	4854.7	27
H21D	1216.46	-2271.65	4839.68	27

Experimental

Single crystals of $C_{19}H_{30}N_2O_4$, **AV-6**, were collected. A suitable crystal was selected and tested on a **XtaLAB Synergy, Single source at home/near, HyPix** diffractometer. The crystal was kept at 100.0(5) K during data collection. Using Olex2 [S1], the

structure was solved with the ShelXT [S2] structure solution program using Intrinsic Phasing and refined with the ShelXL [S3] refinement package using Least Squares minimisation.

S1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339.
S2. G. M. Sheldrick, *Acta Crystallogr.*, 2015, **A71**, 3.
S3. G. M. Sheldrick, *Acta Crystallogr.*, 2015, **C71**, 3.

Crystal structure determination of AV-6

Crystal Data for $C_{19}H_{30}N_2O_4$ (M =350.45 g/mol): monoclinic, space group $P2_1$ (no. 4), a = 11.88260(10) Å, b = 9.55000(10) Å, c = 17.21700(10) Å, β = 107.8250(10)°, V = 1859.98(3) Å^3, Z = 4, T = 100.0(5) K, μ(CuKα) = 0.707 mm^{-1}, *Dcalc* = 1.251 g/cm^3, 28159 reflections measured (5.392° ≤ 2Θ ≤ 139.968°), 7060 unique (R_{int} = 0.0345, R_{sigma} = 0.0306) which were used in all calculations. The final R_1 was 0.0295 (I > 2σ(I)) and wR_2 was 0.0757 (all data).

Refinement model description

Number of restraints - 1, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups
 At 1.5 times of:
  All C(H,H,H) groups, All O(H) groups
2.a Ternary CH refined with riding coordinates:
 C6(H6), C8(H8), C6'(H6'), C8'(H8')
2.b Secondary CH2 refined with riding coordinates:
 C9(H9A,H9B), C10(H10A,H10B), C11(H11A,H11B), C12(H12A,H12B), C18(H18A,H18B),
 C19(H19A,H19B), C20(H20A,H20B), C21(H21A,H21B), C9'(H9'A,H9'B), C10'(H10C,
 H10D), C11'(H11C,H11D), C12'(H12C,H12D), C18'(H18C,H18D), C19'(H19C,H19D),
 C20'(H20C,H20D), C21'(H21C,H21D)
2.c X=CH2 refined with riding coordinates:
 C14(H14A,H14B), C14'(H14C,H14D)
2.d Idealised Me refined as rotating group:
 C13(H13A,H13B,H13C), C15(H15A,H15B,H15C), C16(H16A,H16B,H16C), C13'(H13D,H13E,
 H13F), C15'(H15D,H15E,H15F), C16'(H16D,H16E,H16F)
2.e Idealised tetrahedral OH refined as rotating group:
 O2(H2), O2'(H2')
```

***In-silico* binding of AV-6**

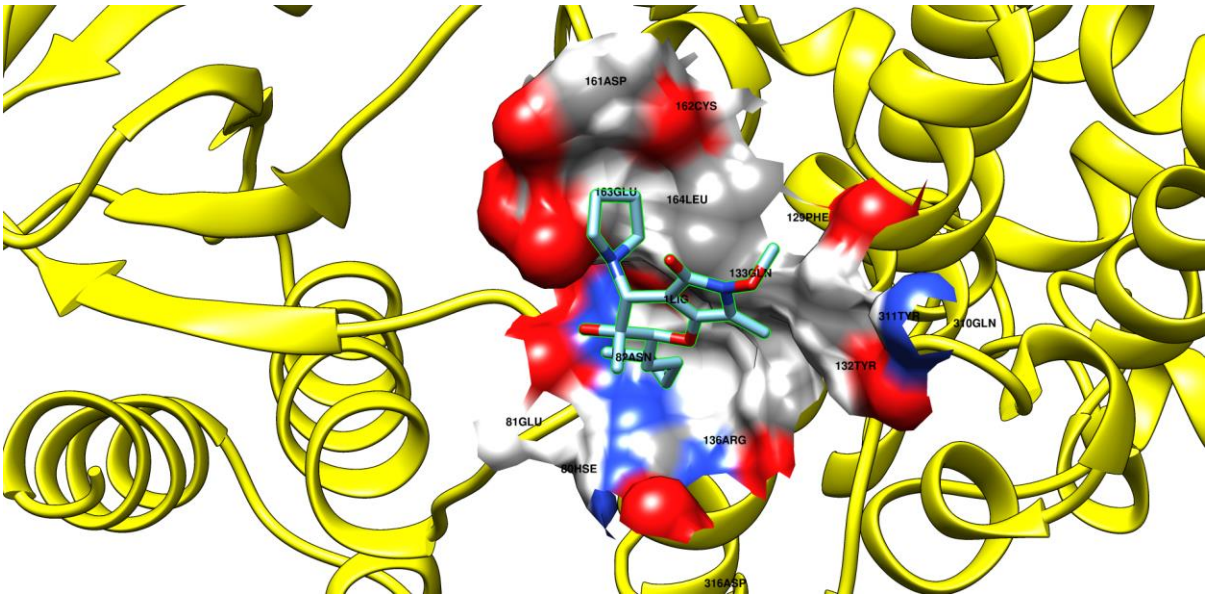

Figure S1 Binding of AV-6 to MAPK11; marked are amino acid residues, which are located at a distance of 5 or less Angstroms to the ligand.

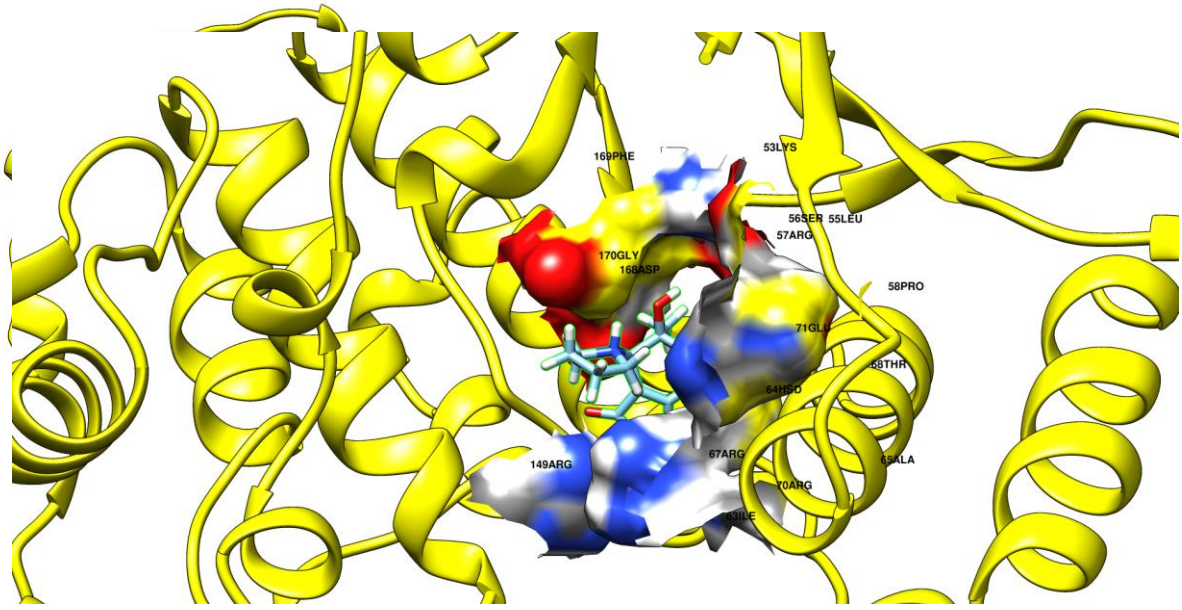

Figure S2 Binding of **AV-6** to MAPK12; marked are amino acid residues, which are located at a distance of 5 or less Angstroms to the ligand.

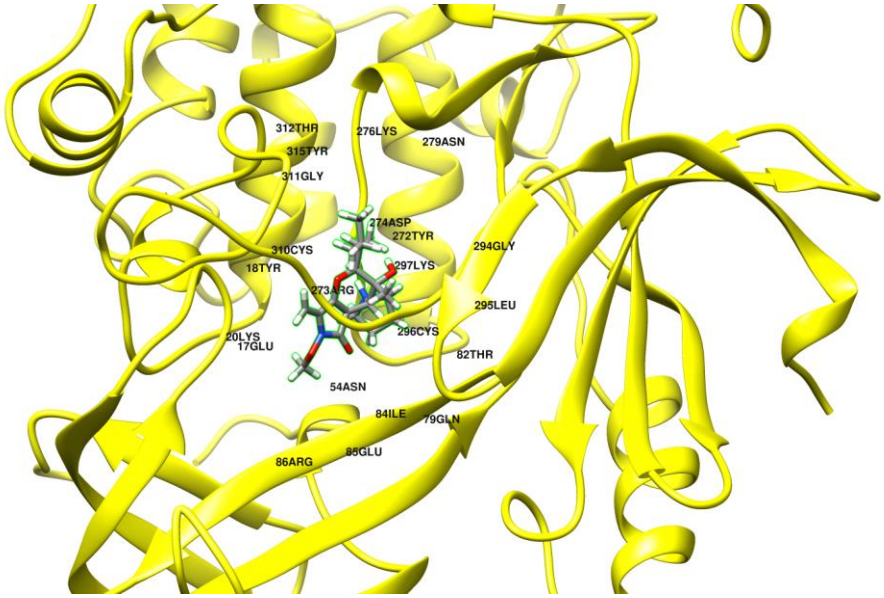

Figure S3 Binding of **AV-6** to AKT1; marked are amino acid residues, which are located at a distance of 5 or less Angstroms to the ligand.