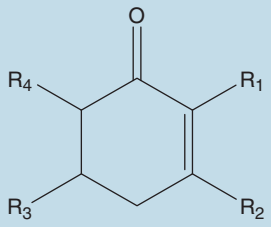
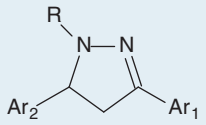
ID	R1	R2	R3	R4	
	H	C_6H_5	C_6H_5	CO_2Et	
C6	H	C_6H_5	*p*-$C_6H_4OCH_3$	CO_2Et	
C5	H	C_6H_5	*p*-C_6H_4Br	CO_2Et	
C3	H	C_6H_5	*p*-$C_6H_4NO_2$	CO_2Et	
C1	H	*p*-C_6H_4Br	*p*-$C_6H_4OCH_3$	CO_2Et	
C25	H	C_6H_5	*p*-$C_6H_4OCH_3$	H	
AAZ16-56	H	*p*-$C_6H_4OCH_3$	C_6H_5	CO_2Et	
AAZ10-50	H	*m*- $C_6H_4OCH_3$	C_6H_5	CO_2Et	
AKA57-B	H	C_6H_5	m-$C_6H_4NO_2$	CO_2Et	

ID	miLogP	TPSA	natoms	MW	nOH	nOHNH	nviolations	nrotb	Volume	CPRC ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand
C6	4.203	52.61	26	350.414	4	0	0	6	328.345	−0.26	−0.25	−0.77	−0.30
C5	4.955	43.376	25	399.284	3	0	0	5	320.684	−0.35	−0.24	−0.77	−0.52
C3	4.105	89.2	27	365.385	6	0	0	6	326.133	−0.38	−0.29	−0.87	−0.41
C1	5.012	52.61	27	429.31	4	0	1	6	346.23	−0.32	−0.28	−0.72	−0.46
C25	3.865	26.305	21	278.351	2	0	0	3	266.998	−0.19	−0.47	−0.65	−0.18
AAZ16-56	4.203	52.61	26	350.414	4	0	0	6	328.345	−0.26	−0.25	−0.77	−0.30
AAZ10-50	4.179	52.61	26	350.414	4	0	0	6	328.345	−0.25	−0.25	−0.78	−0.28
AKA57-B	4.081	89.2	27	365.385	6	0	0	6	326.133	−0.39	−0.30	−0.87	−0.41

ID	Ar1	Ar2	R	
AAZ17-A-58	C_6H_5	p-$C_6H_4OCH_3$	H	
AAZ18-59	C_6H_5	p-$C_6H_4OCH_3$	$COCH_3$	

ID	miLogP	TPSA	natoms	MW	nOH	nOHNH	nviolations	nrotb	Volume	CPRC ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand
AAZ17-A-58	3.374	33.625	19	252.317	3	1	0	3	239.448	−0.64	−0.81	−1.00	−1.15
AAZ18-59	2.98	41.907	22	294.354	4	0	0	3	275.374	−0.63	−0.83	−1.25	−1.14

Supplementary Fig. S1. C25 analog structure descriptions with calculated molecular properties and bioactivities.