Supporting Information for

Synthesis and biological evaluation of novel 2,3-pyrazole ring-substituted-4,4-dimethyl lithocholic acid derivatives as selective protein tyrosine phosphatase 1B (PTP1B) inhibitors with cellular efficacy

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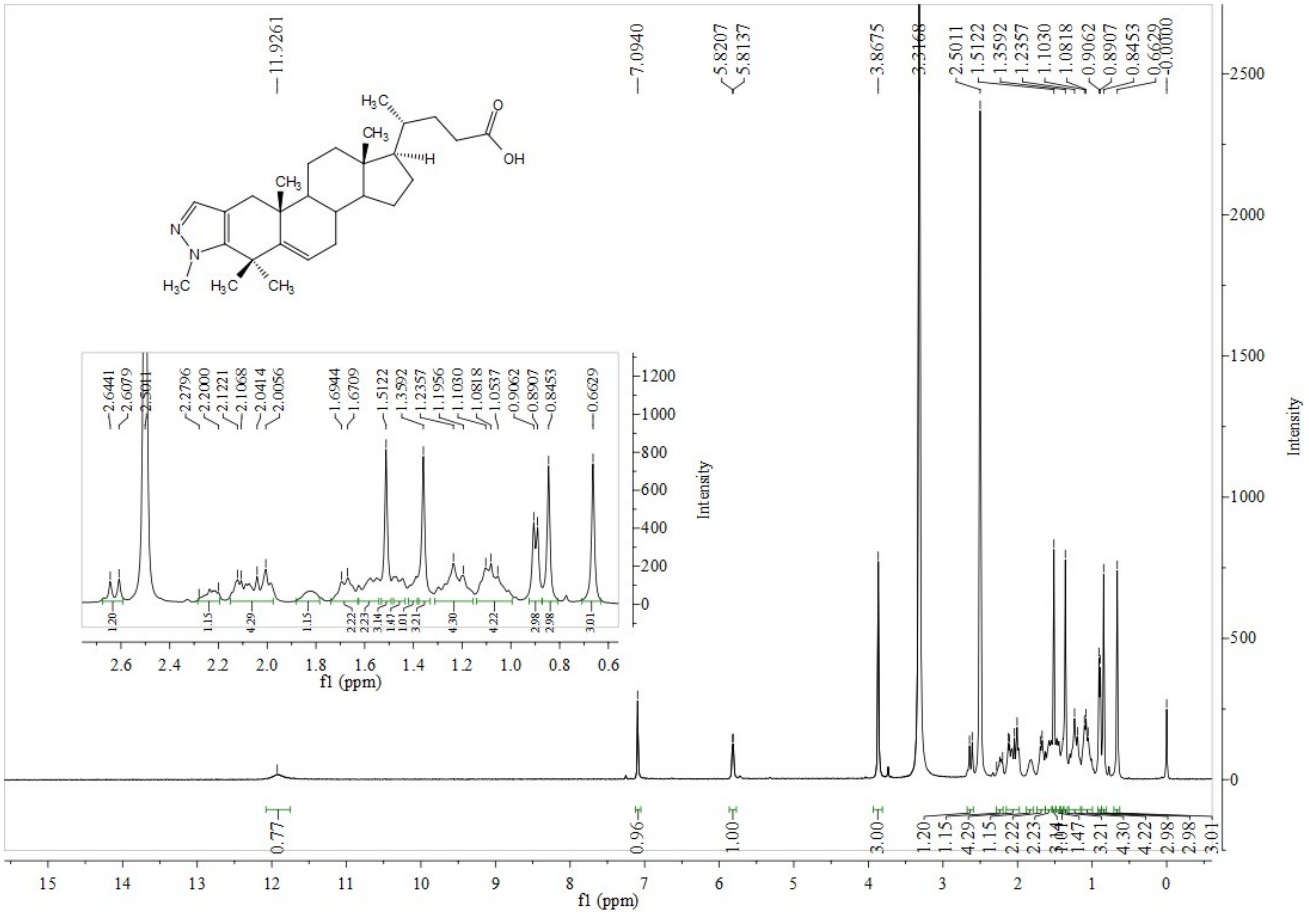

Fig S1: ^{1}H NMR of compound **25a** (in the solvent of DMSO-d6, 400MHz)

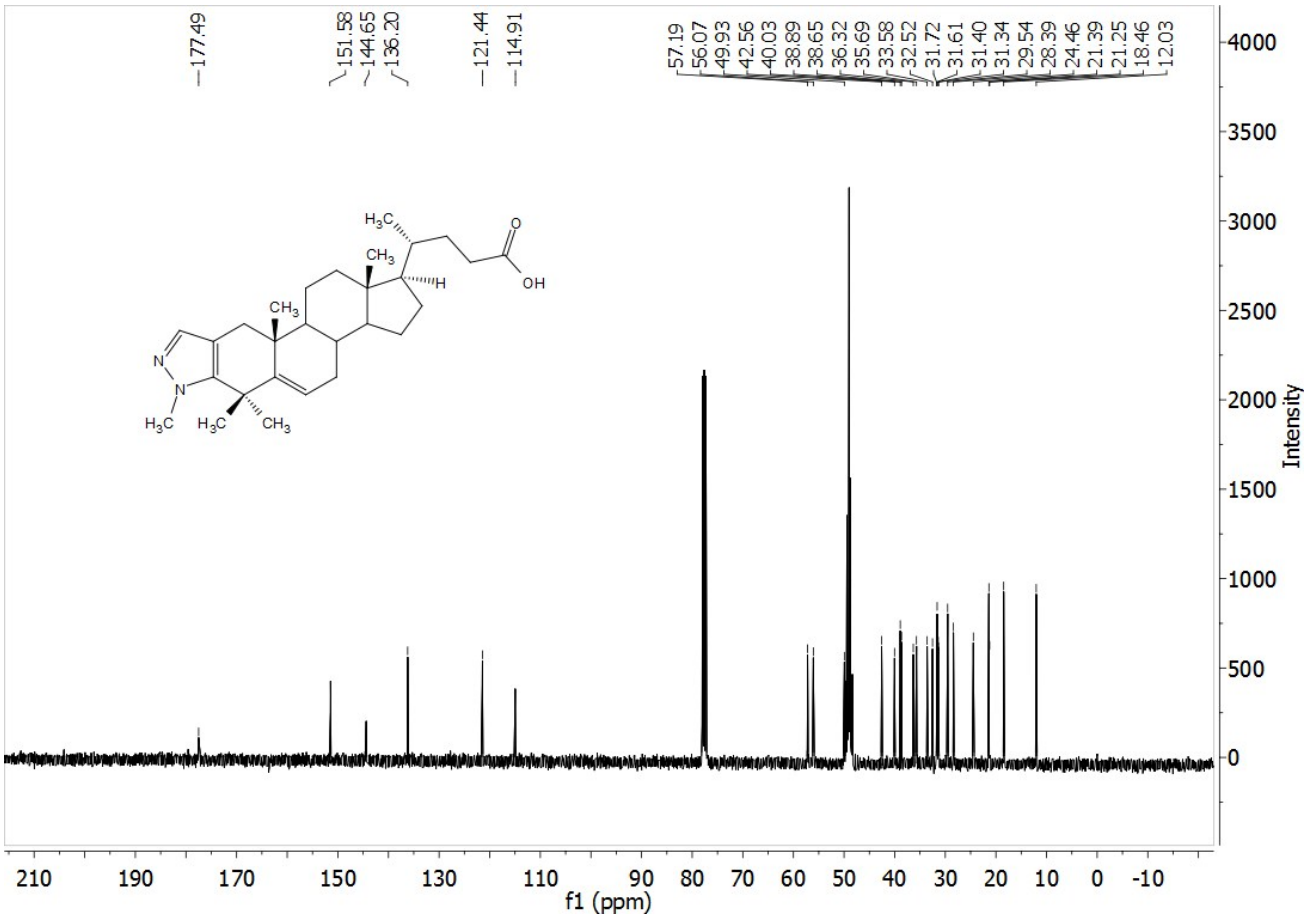

Fig S2: ^{13}C NMR of compound **25a** (in the solvent of $CDCl_3/CD_3OD$=2/1, v/v, 101MHz)

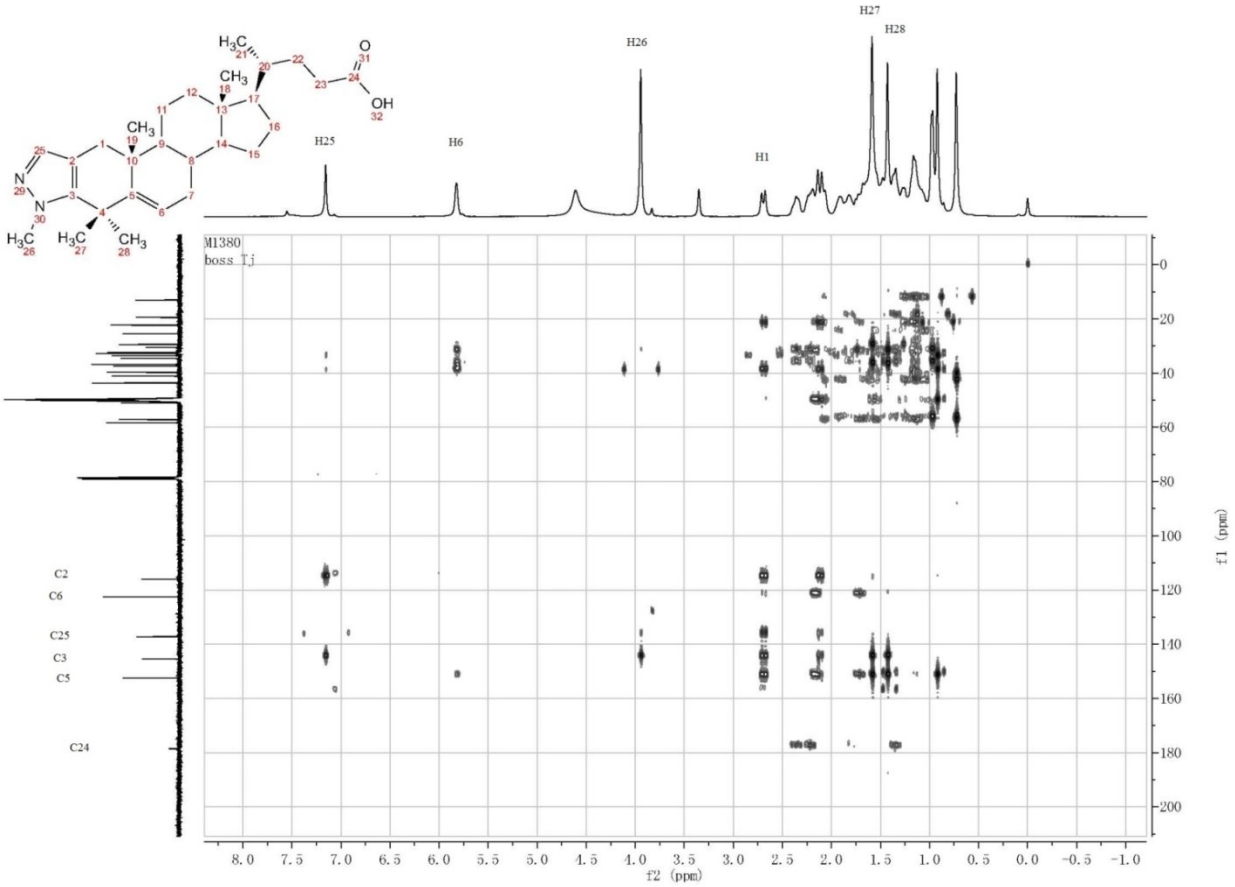

Fig S3: HMBC spectrum of compound **25a** (in the solvent of in the solvent of $CDCl_3/CD_3OD$=2/1, v/v)

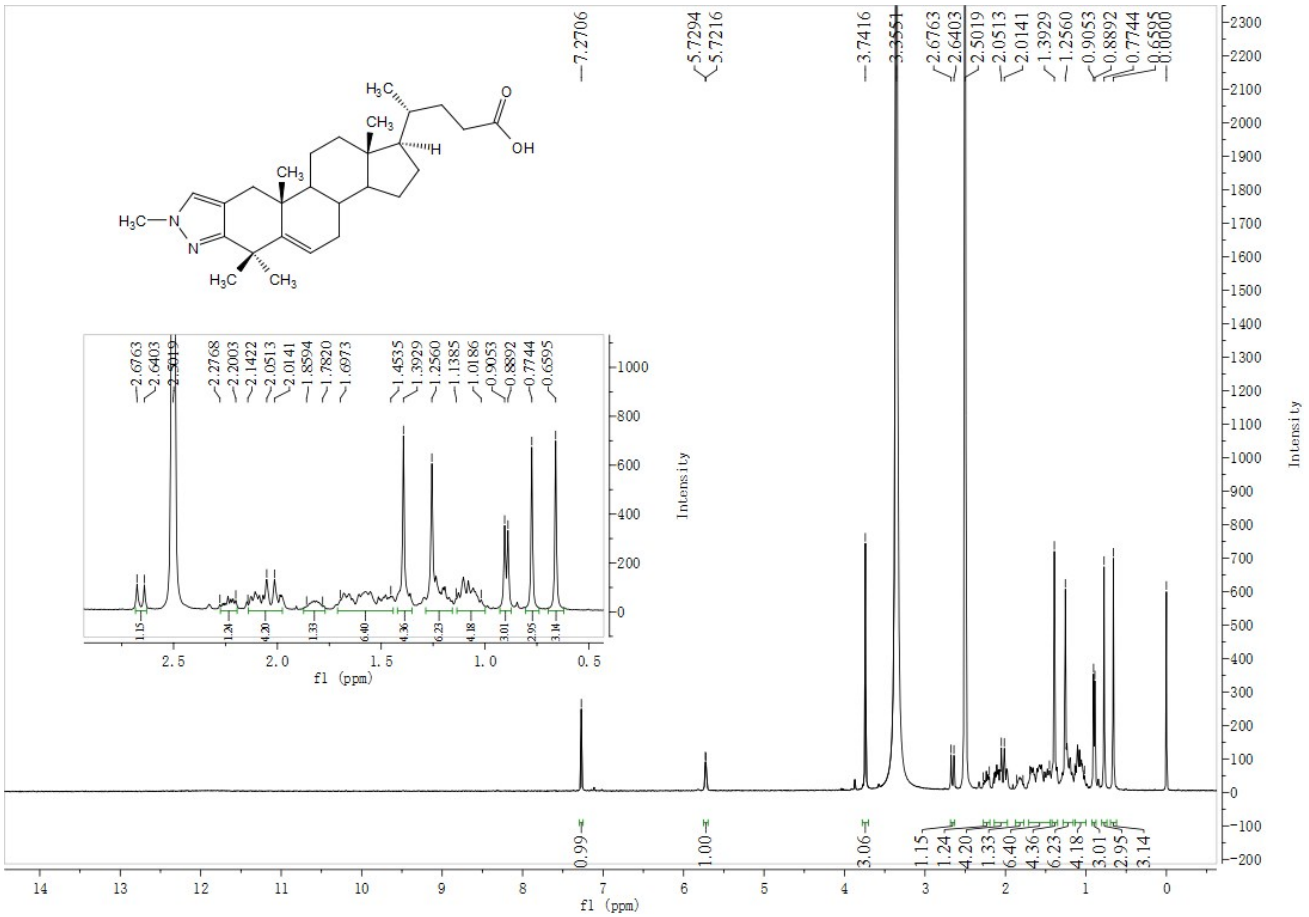

Fig S4: ^{1}H NMR of compound **25b** (in the solvent of DMSO-d6, 400MHz)

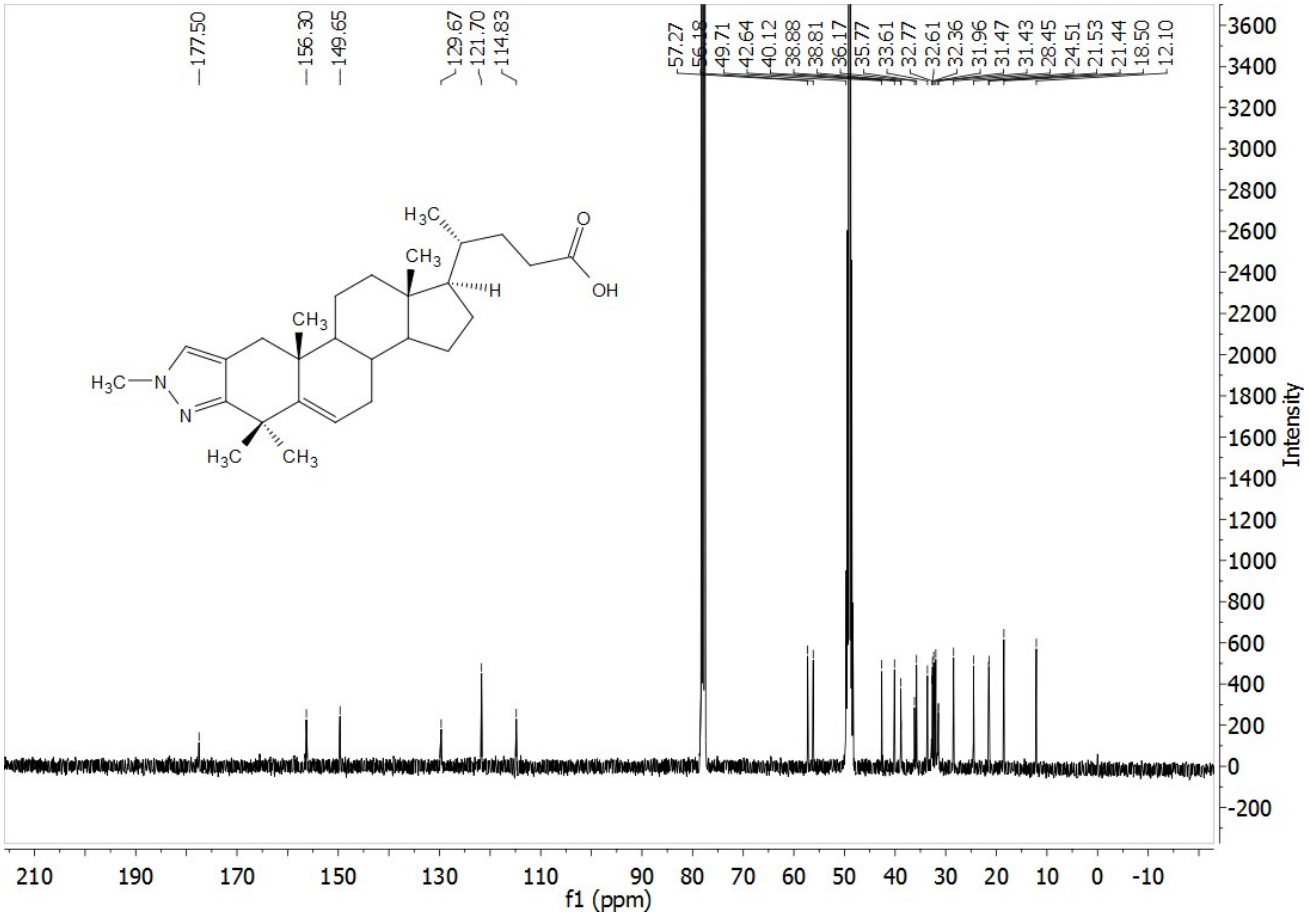

Fig S5: ^{13}C NMR of compound **25b** (in the solvent of $CDCl_3/CD_3OD$=2/1, v/v, 101MHz)

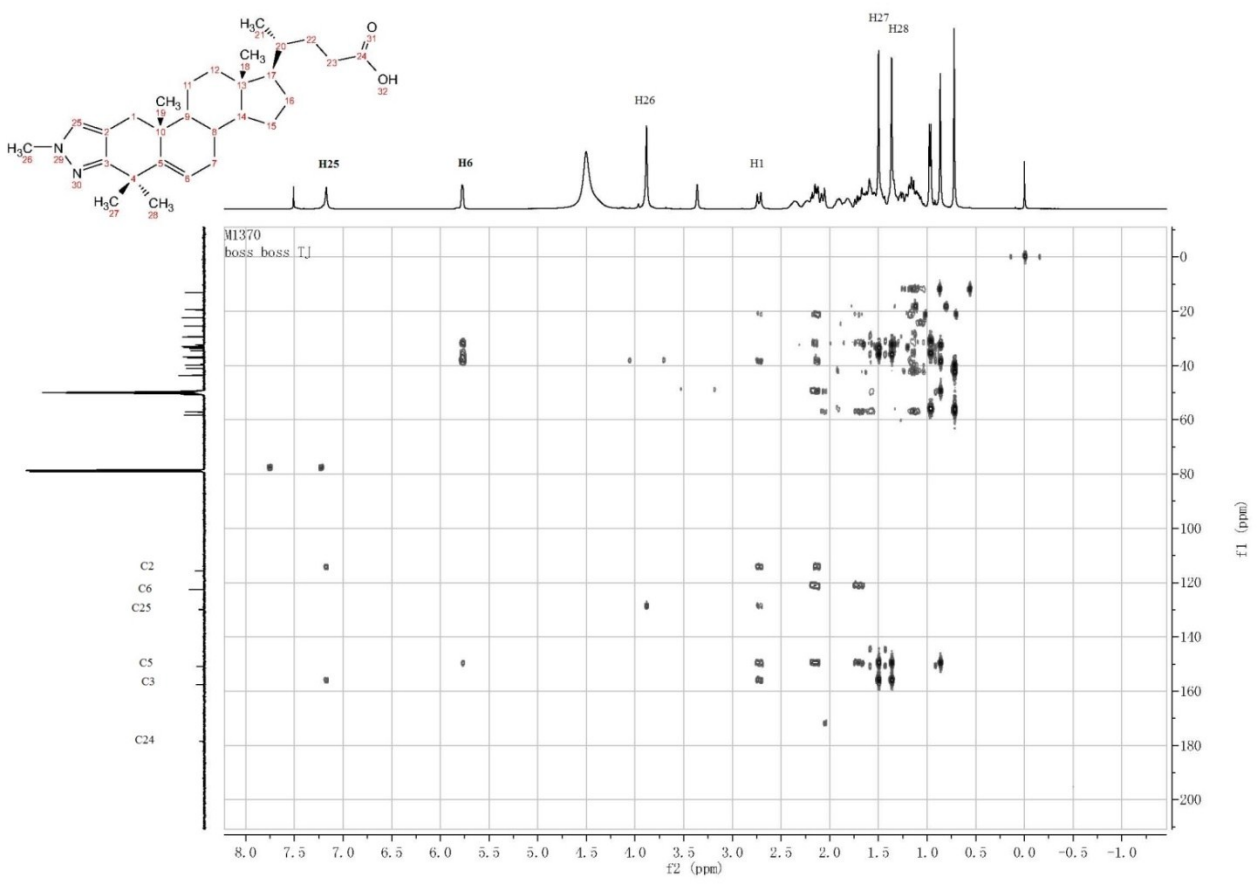

Fig S6: HMBC spectrum of compound **25b** (in the solvent of in the solvent of $CDCl_3/CD_3OD$=2/1, v/v)

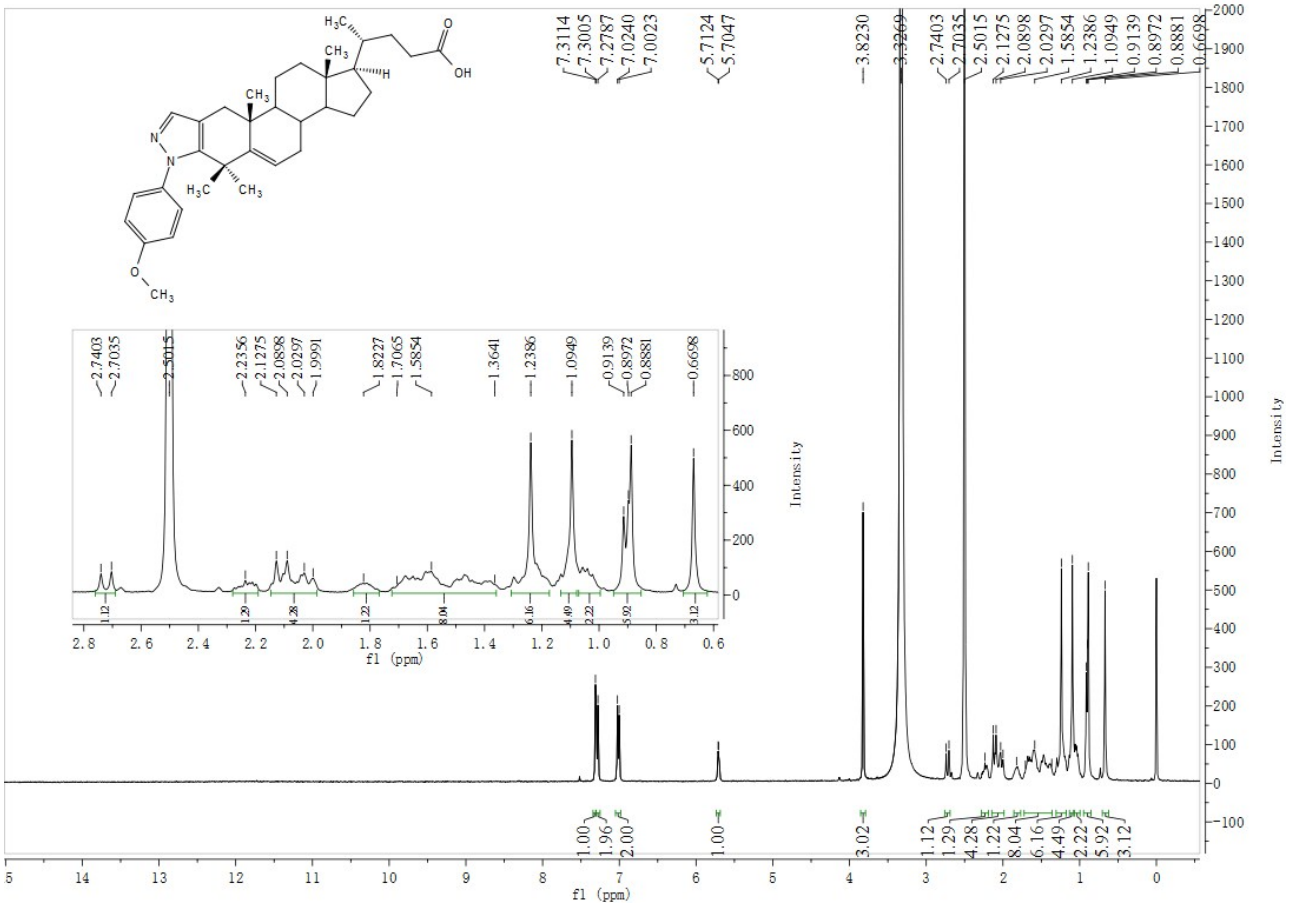

Fig S7: ^{1}H NMR of compound **26** (in the solvent of DMSO-d6, 400MHz)

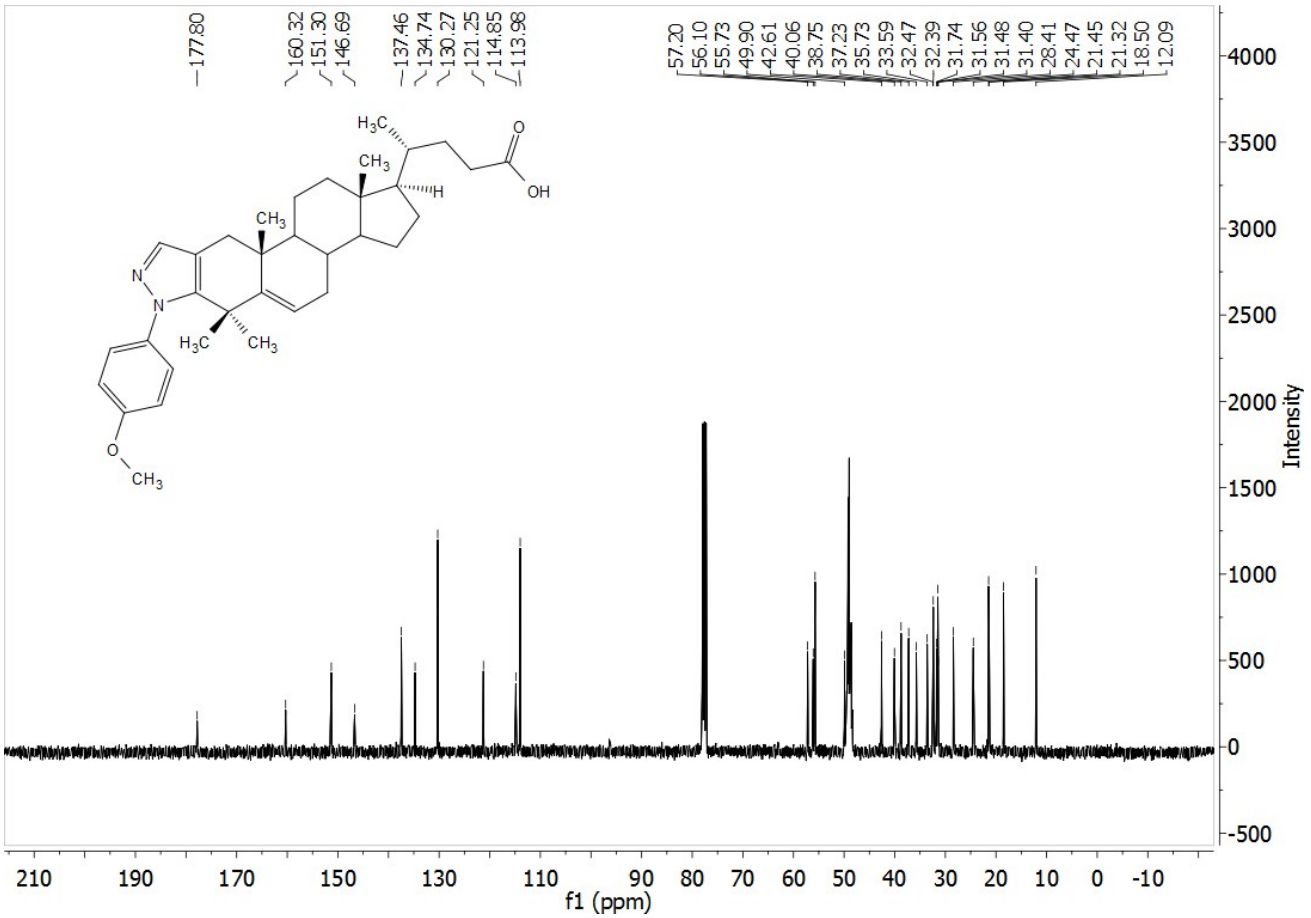

Fig S8: ^{13}C NMR of compound **26** (in the solvent of $CDCl_3/CD_3OD$=2/1, v/v, 101MHz)

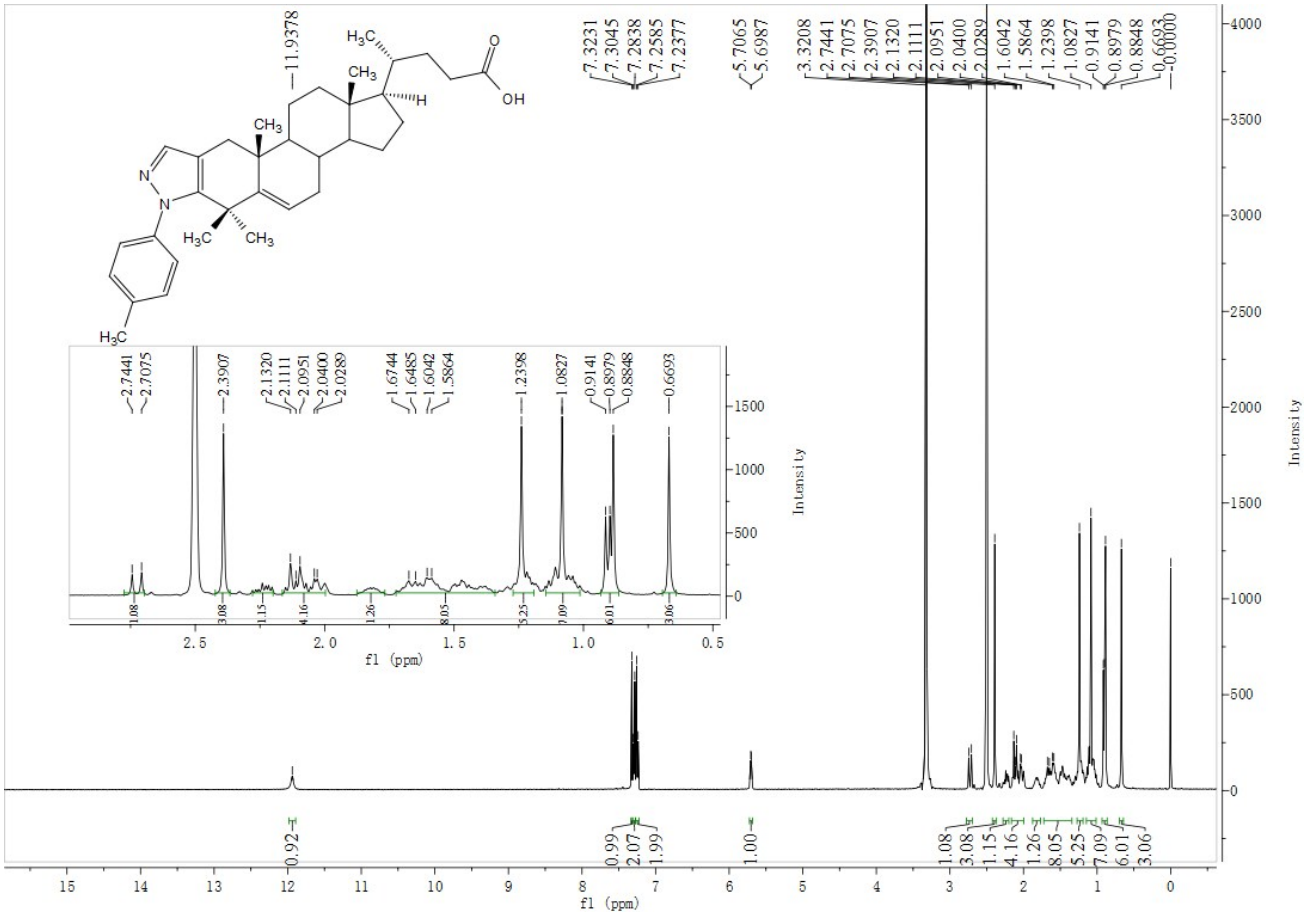

Fig S9: ^{1}H NMR of compound **27** (in the solvent of DMSO-d6, 400MHz)

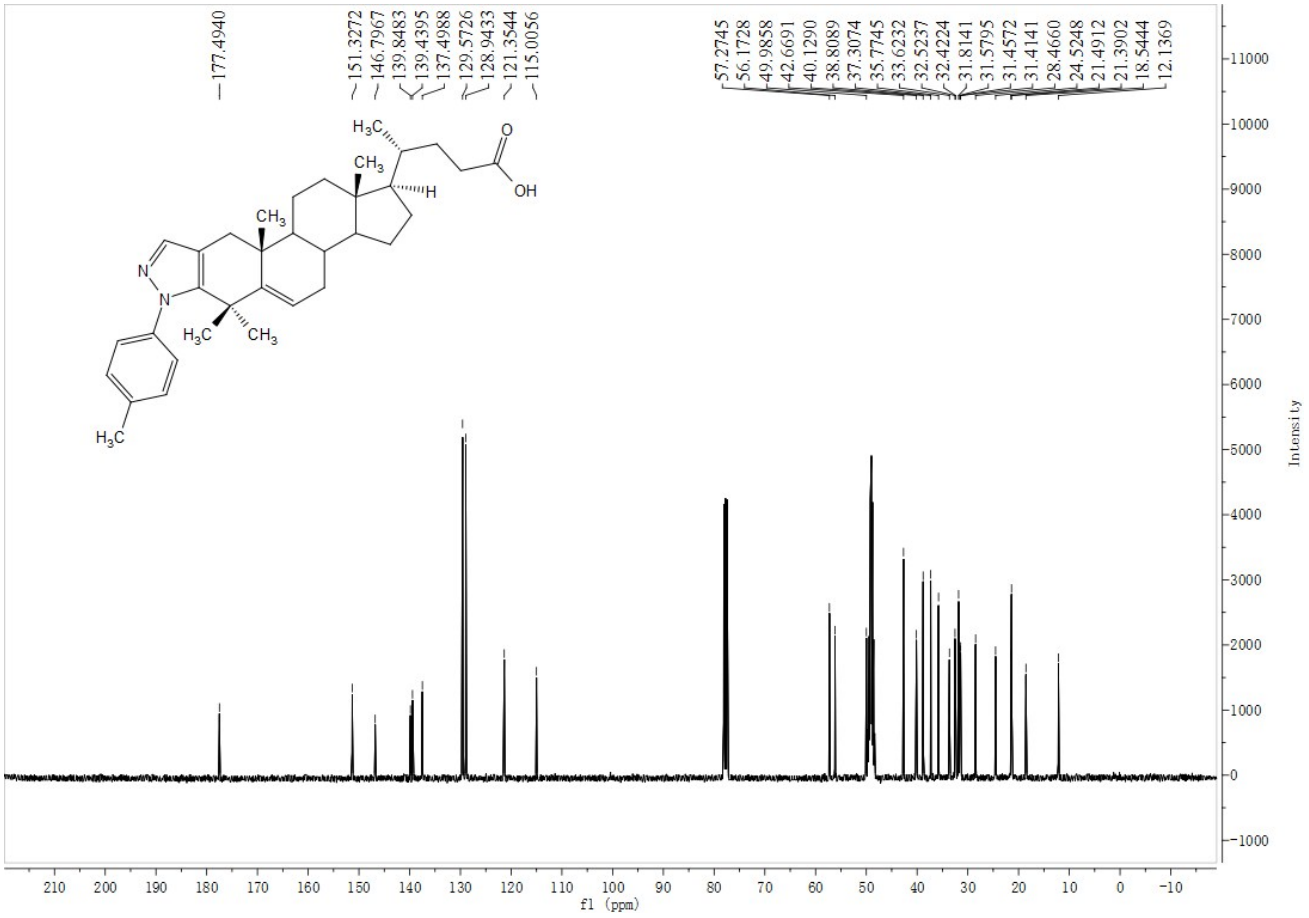

Fig S10: ^{13}C NMR of compound **27** (in the solvent of $CDCl_3/CD_3OD$=2/1, v/v, 101MHz)

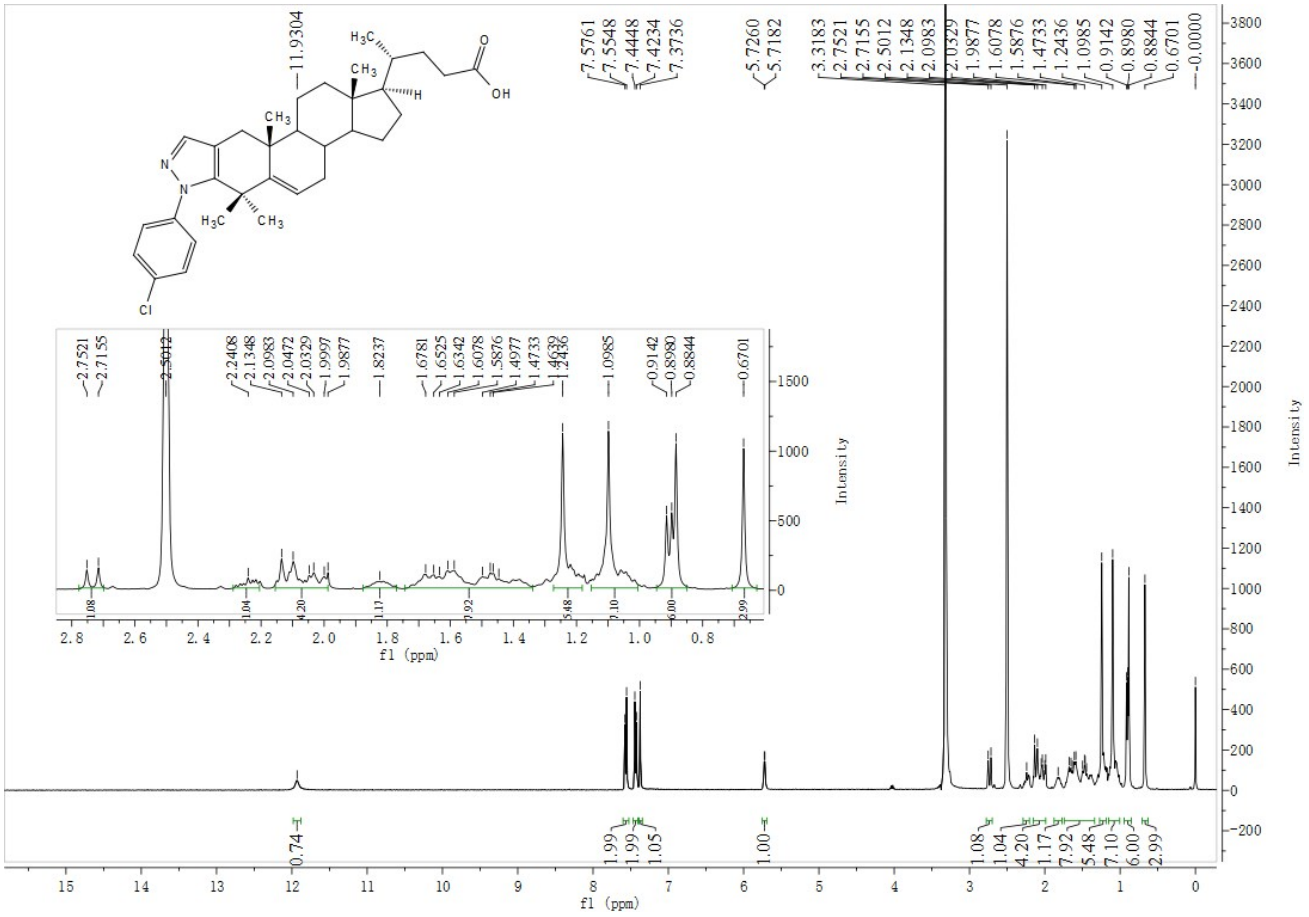

Fig S11: ^{1}H NMR of compound **28** (in the solvent of DMSO-d6, 400MHz)

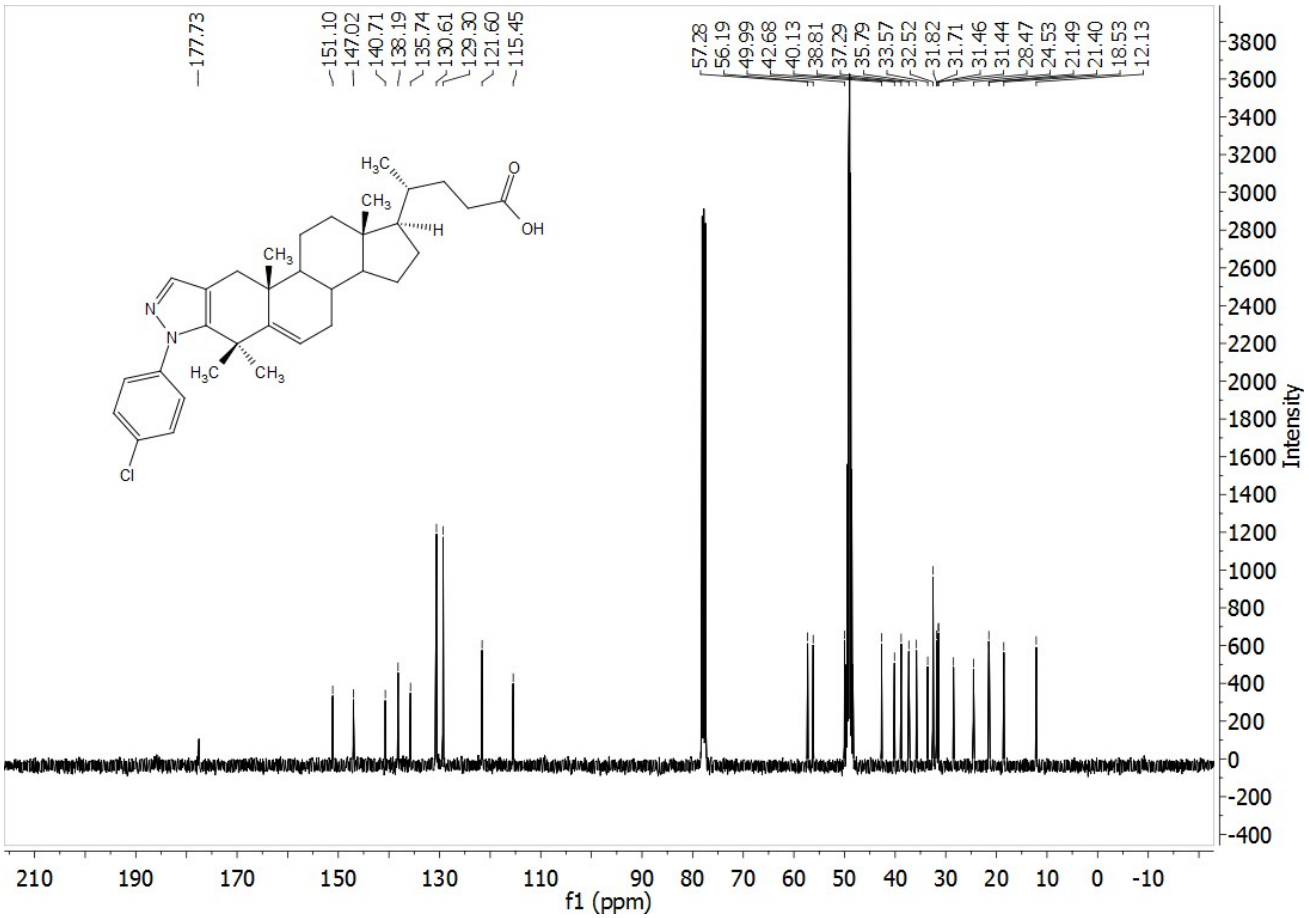

Fig S12: ^{13}C NMR of compound **28** (in the solvent of $CDCl_3/CD_3OD$=2/1, v/v, 101MHz)

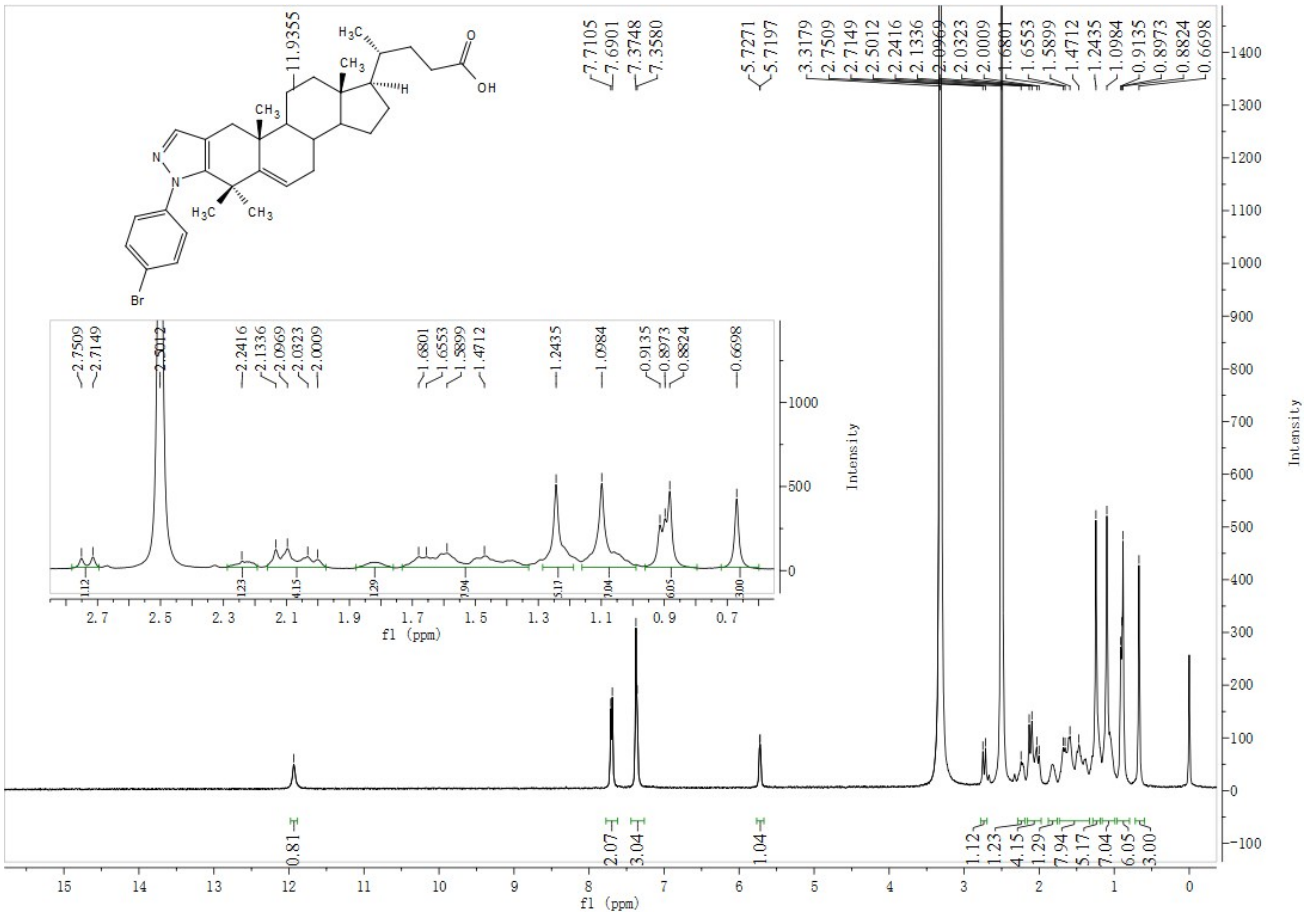

Fig S13: ^{1}H NMR of compound **29** (in the solvent of DMSO-d6, 400MHz)

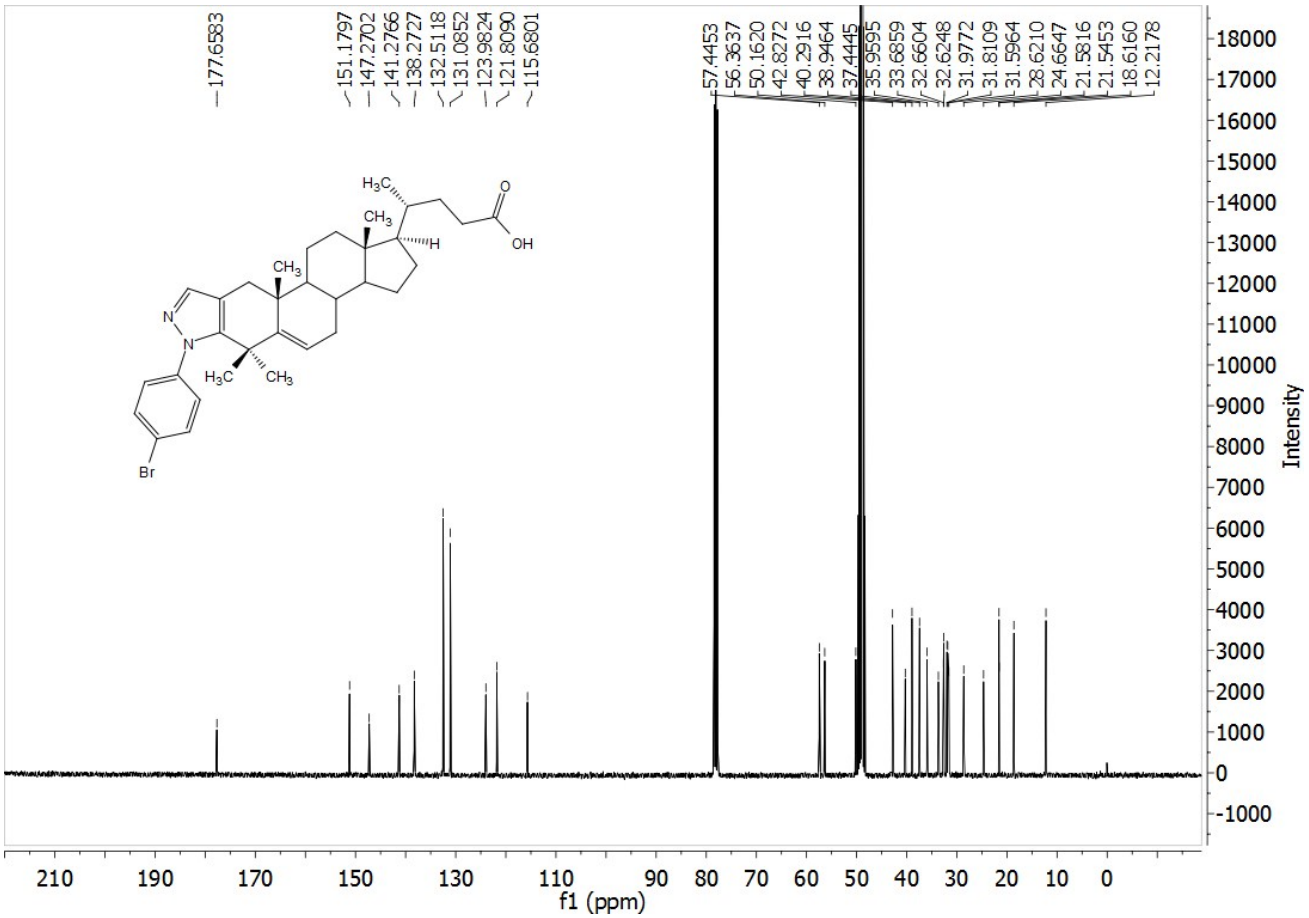

Fig S14: ^{13}C NMR of compound **29** (in the solvent of $CDCl_3/CD_3OD$=2/1, v/v, 101MHz)

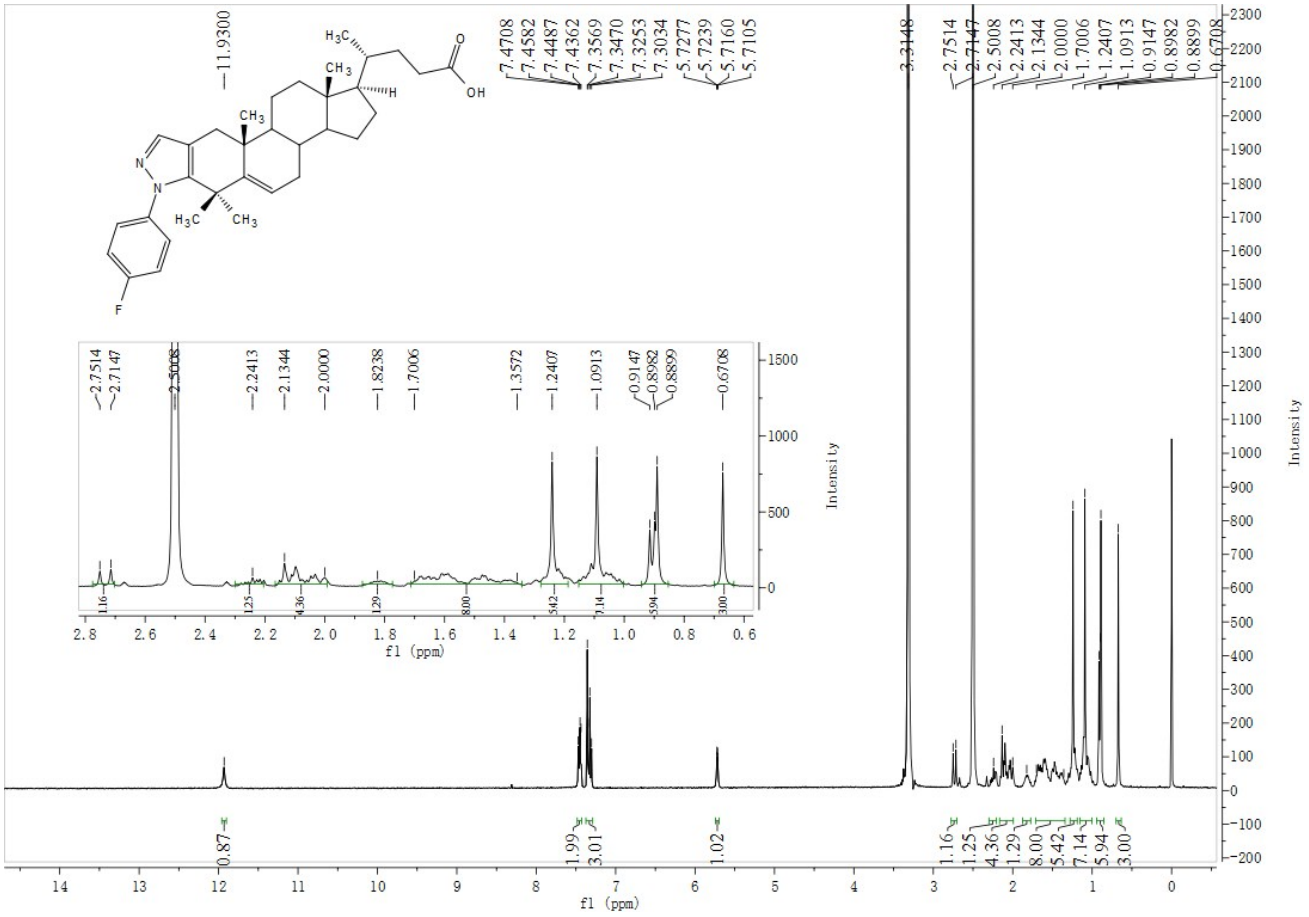

Fig S15: ^{1}H NMR of compound **30** (in the solvent of DMSO-d6, 400MHz)

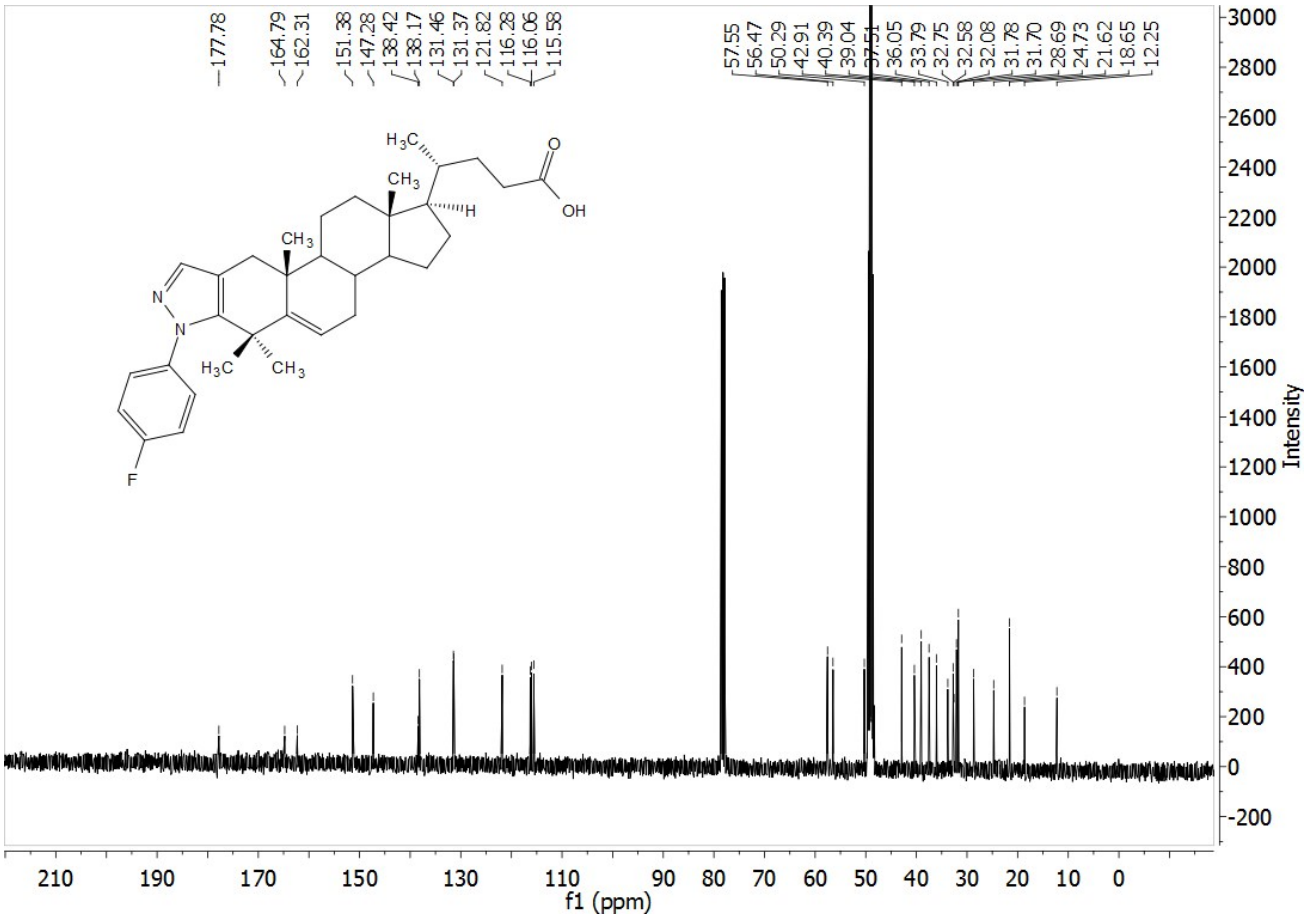

Fig S16: ^{13}C NMR of compound **30** (in the solvent of $CDCl_3/CD_3OD$=2/1, v/v, 101MHz)

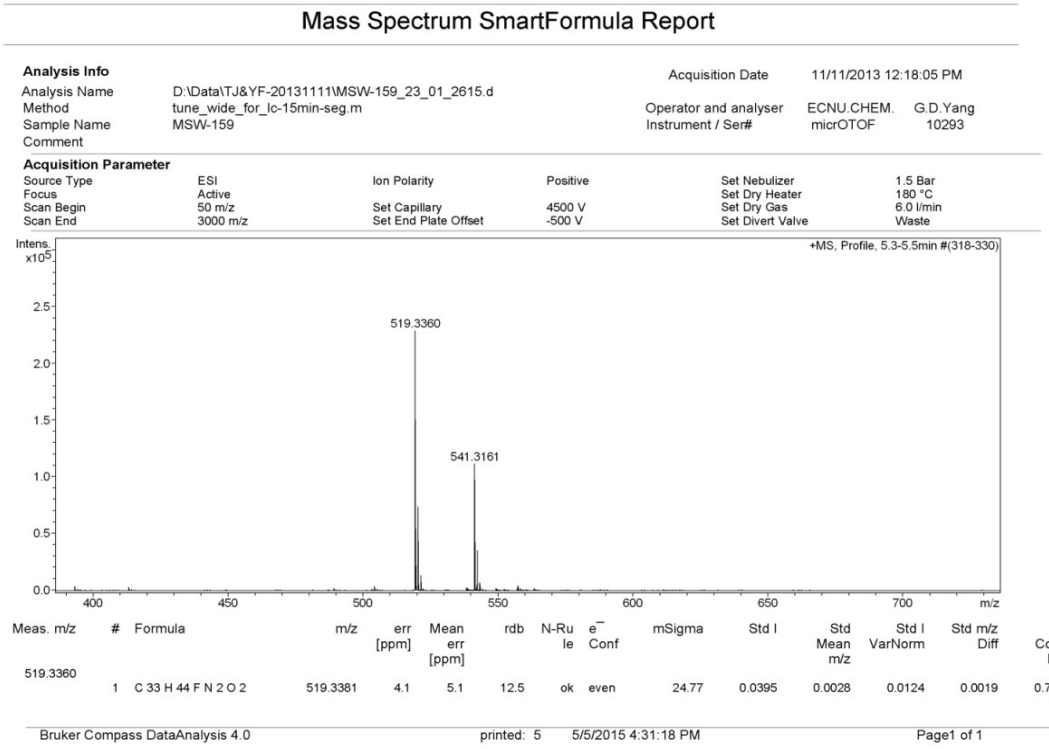

Fig S17: HRMS of compound **30**

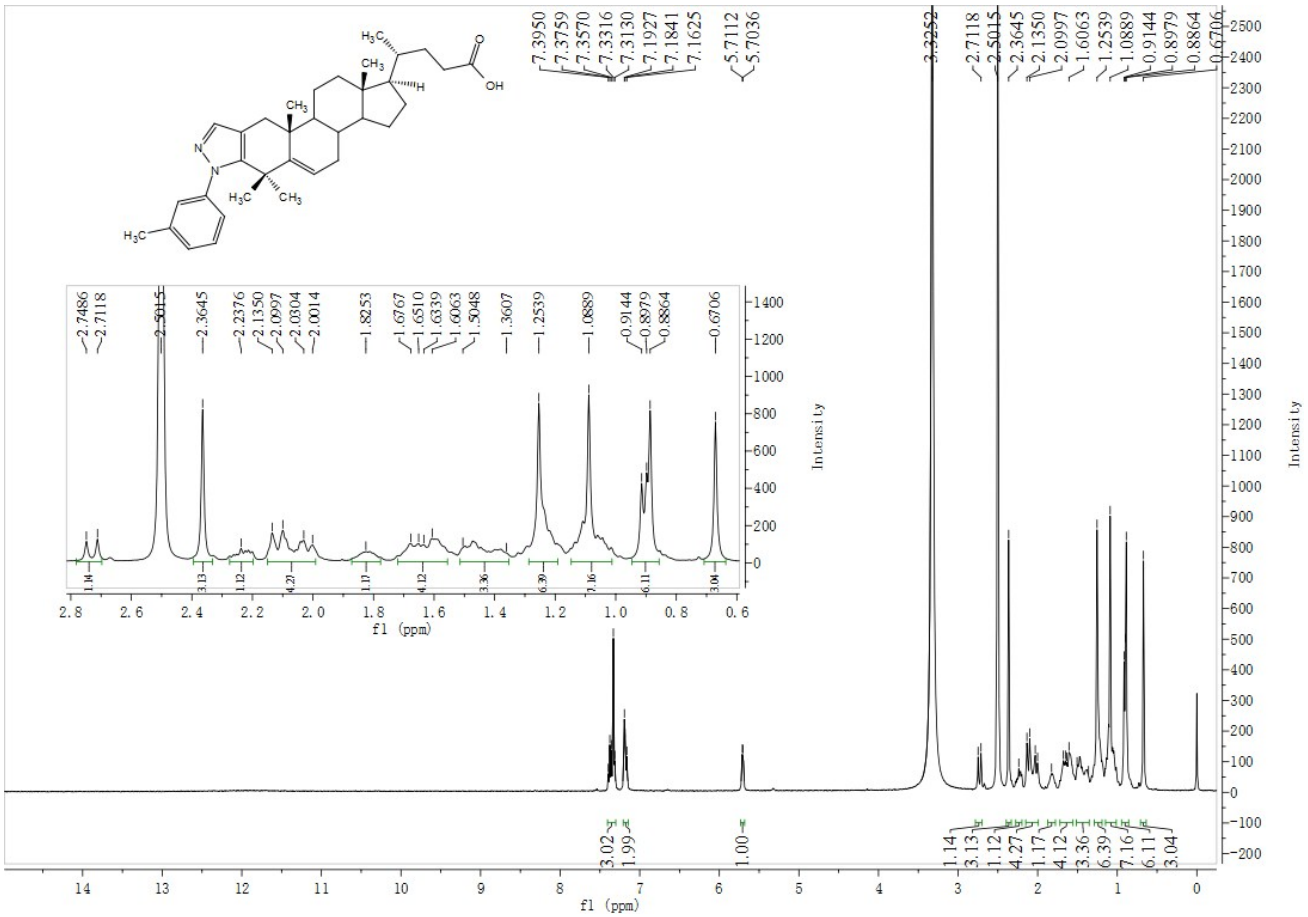

Fig S18: ^{1}H NMR of compound **31** (in the solvent of DMSO-d6, 400MHz)

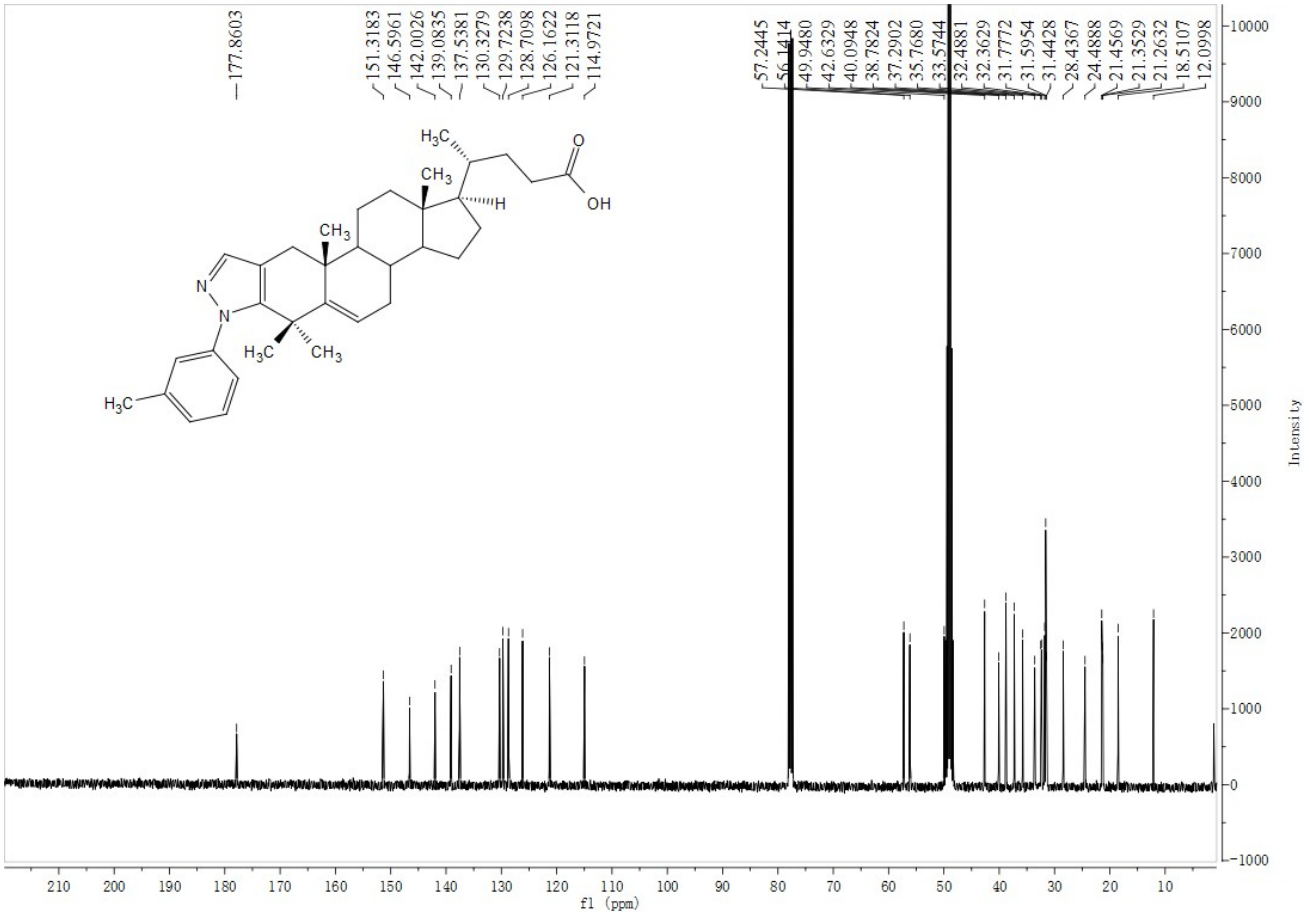

Fig S19: ^{13}C NMR of compound **31** (in the solvent of $CDCl_3/CD_3OD$=2/1, v/v, 101MHz)

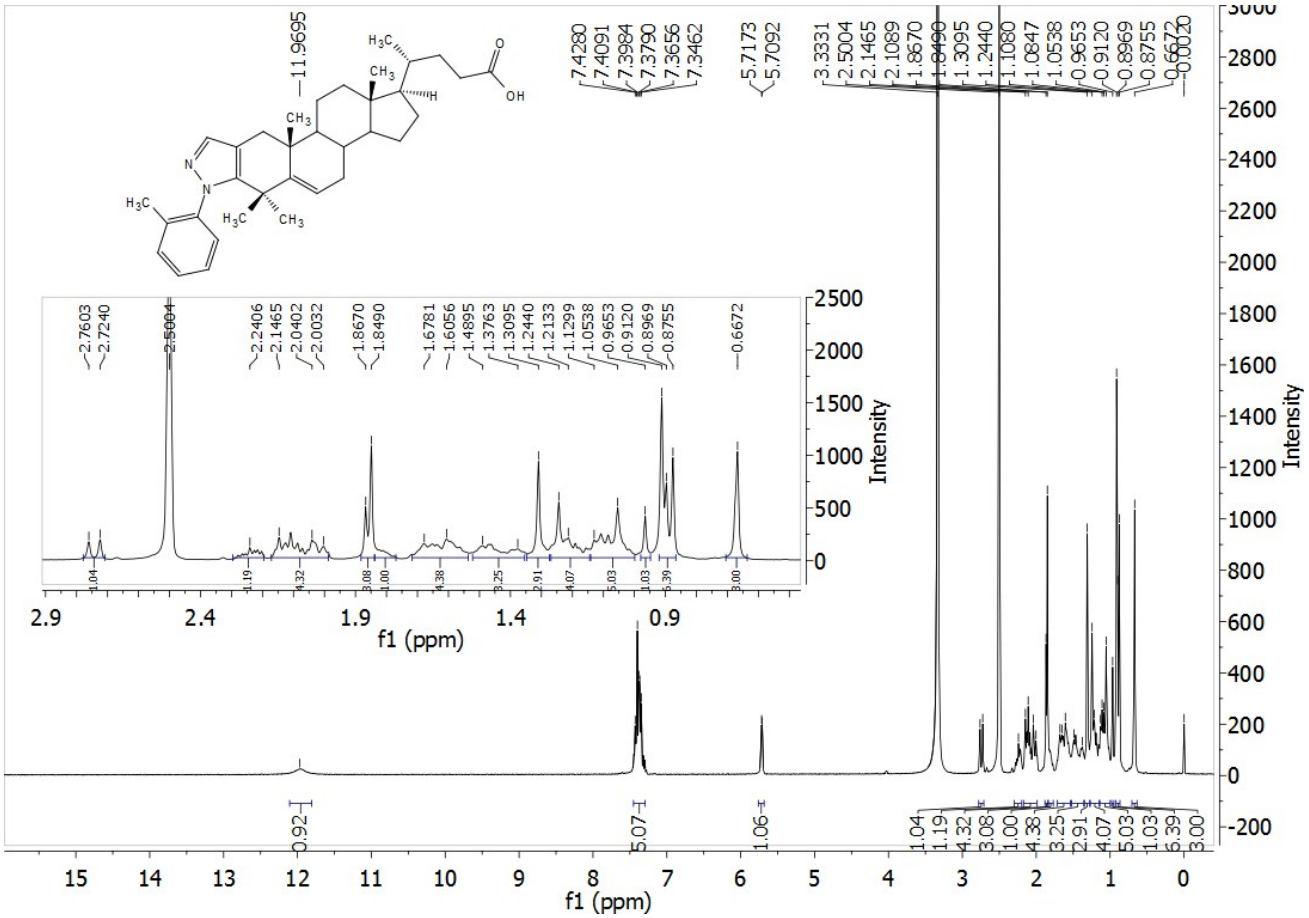

Fig S20: ^{1}H NMR of compound **32** (in the solvent of DMSO-d6, 400MHz)

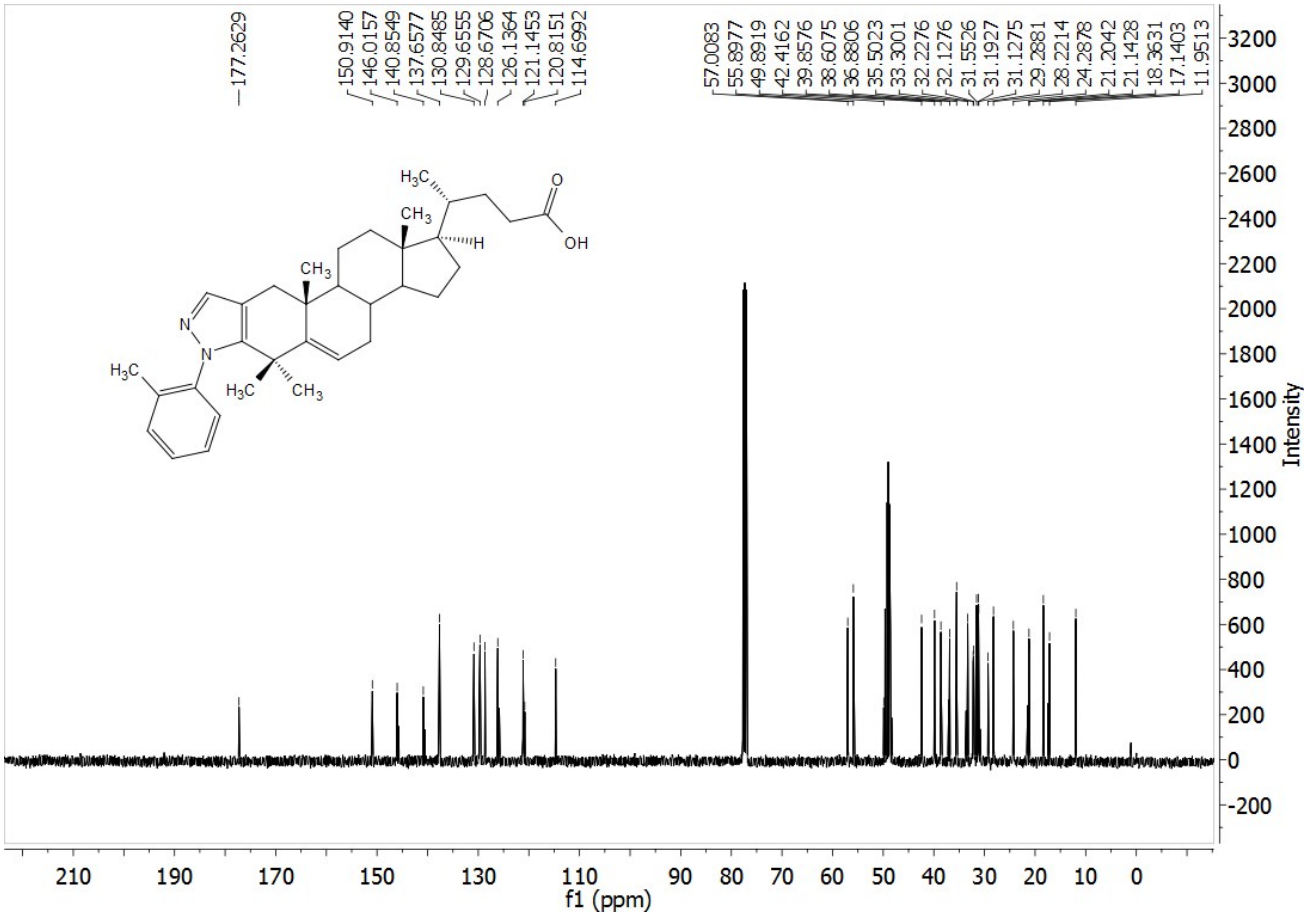

Fig S21: ^{13}C NMR of compound **32** (in the solvent of $CDCl_3/CD_3OD$=2/1, v/v, 101MHz)

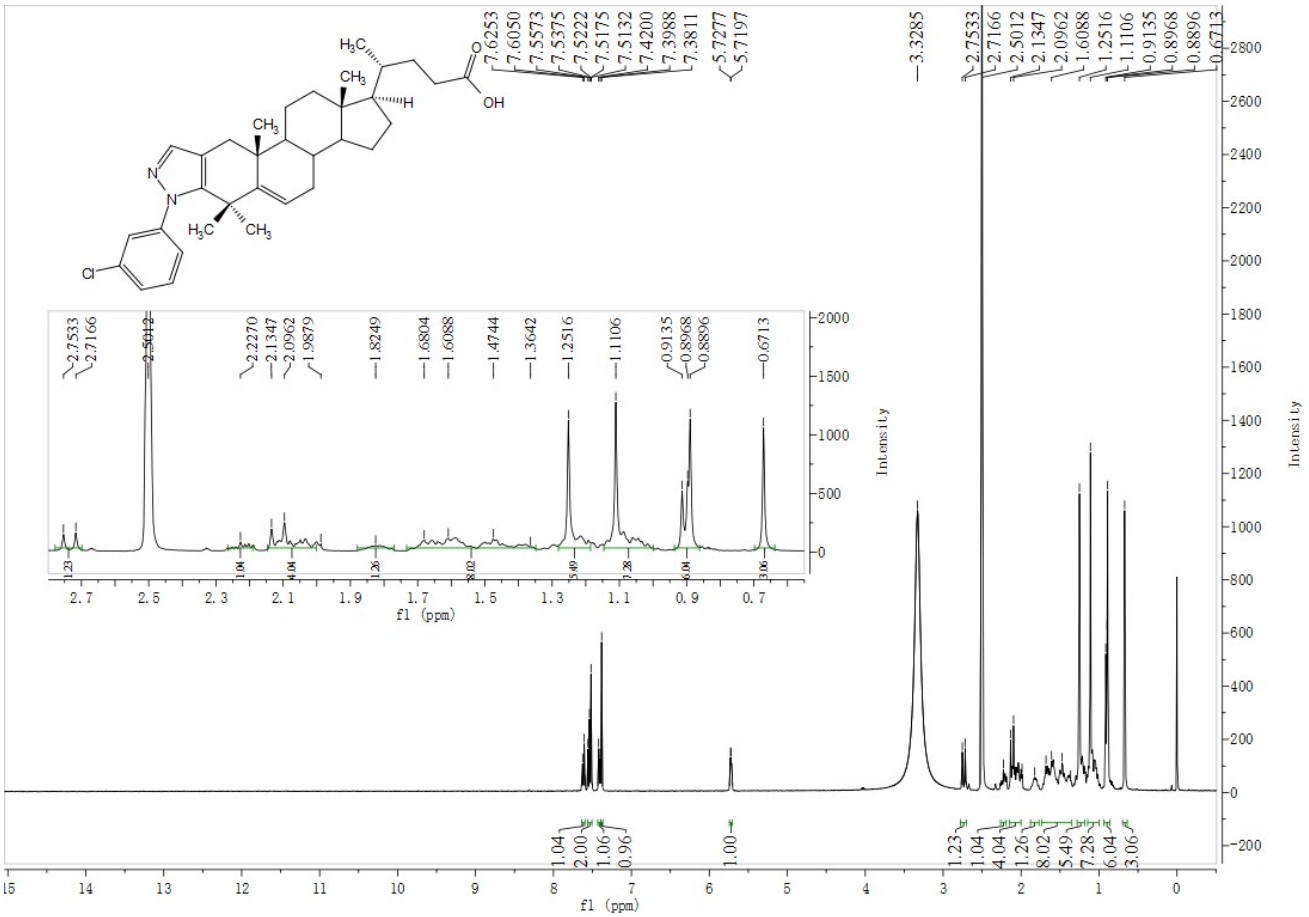

Fig S22: ^{1}H NMR of compound **33** (in the solvent of DMSO-d6, 400MHz)

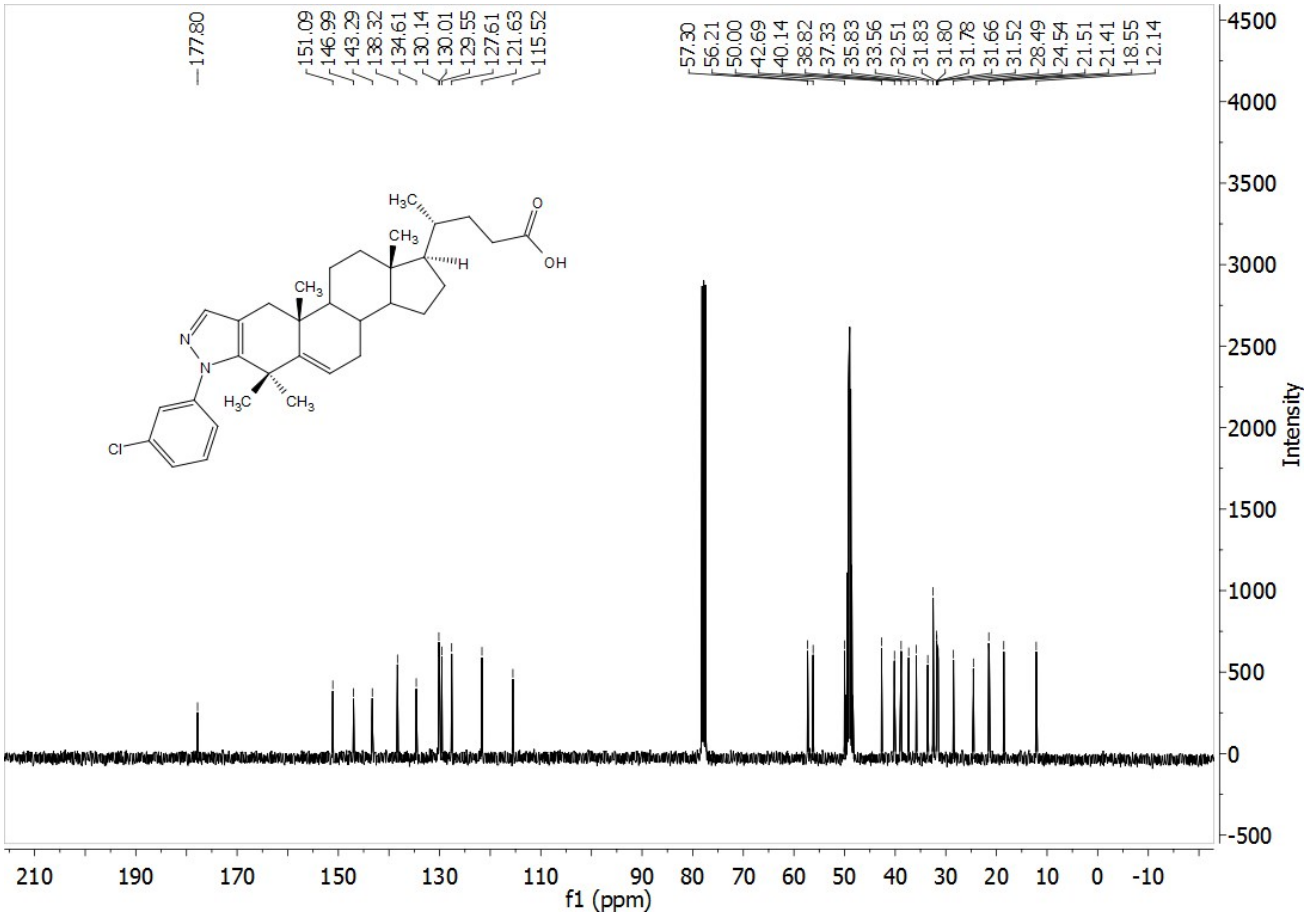

Fig S23: ^{13}C NMR of compound **33** (in the solvent of $CDCl_3/CD_3OD$=2/1, v/v, 101MHz)

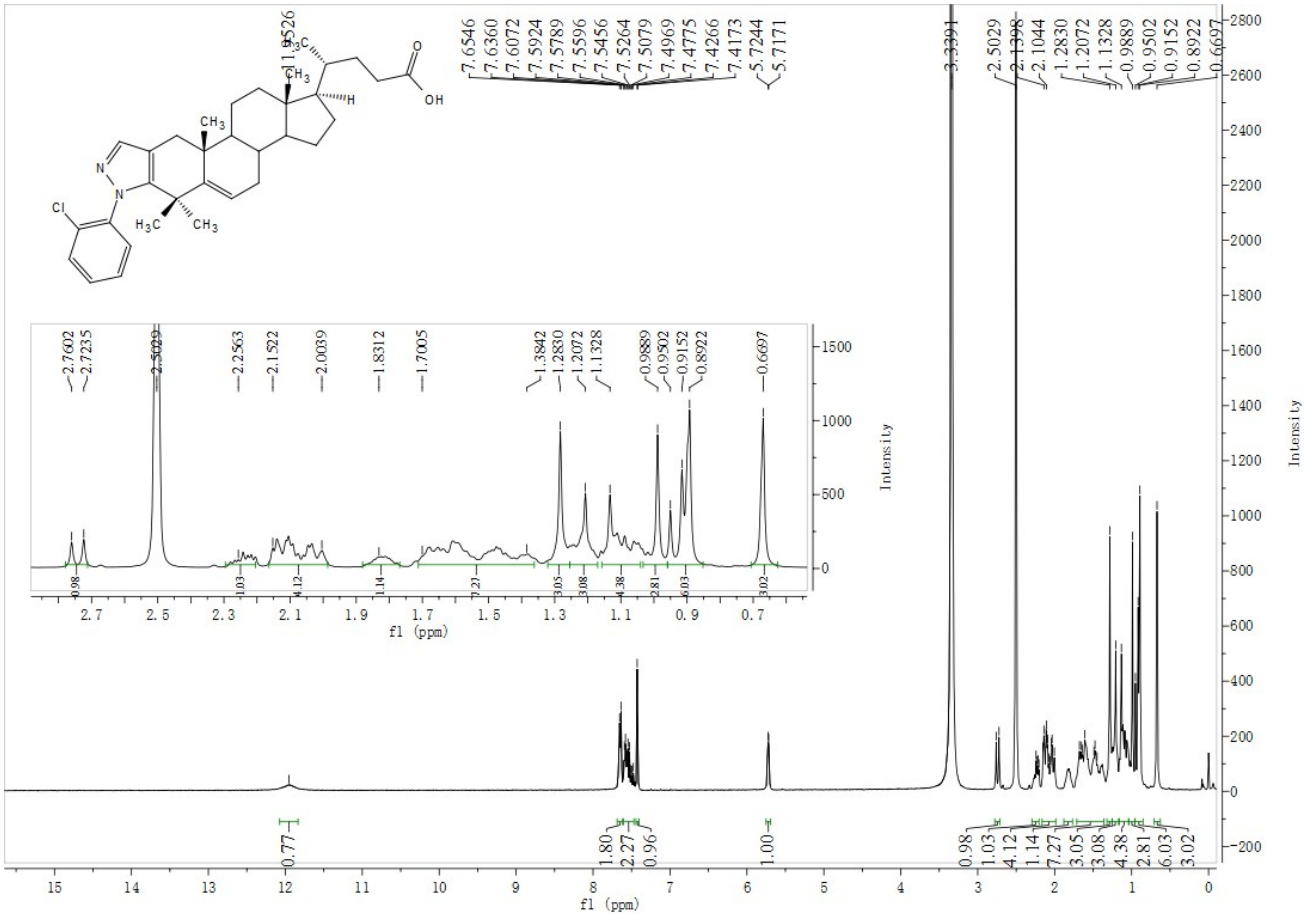

Fig S24: ^{1}H NMR of compound **34** (in the solvent of DMSO-d6, 400MHz)

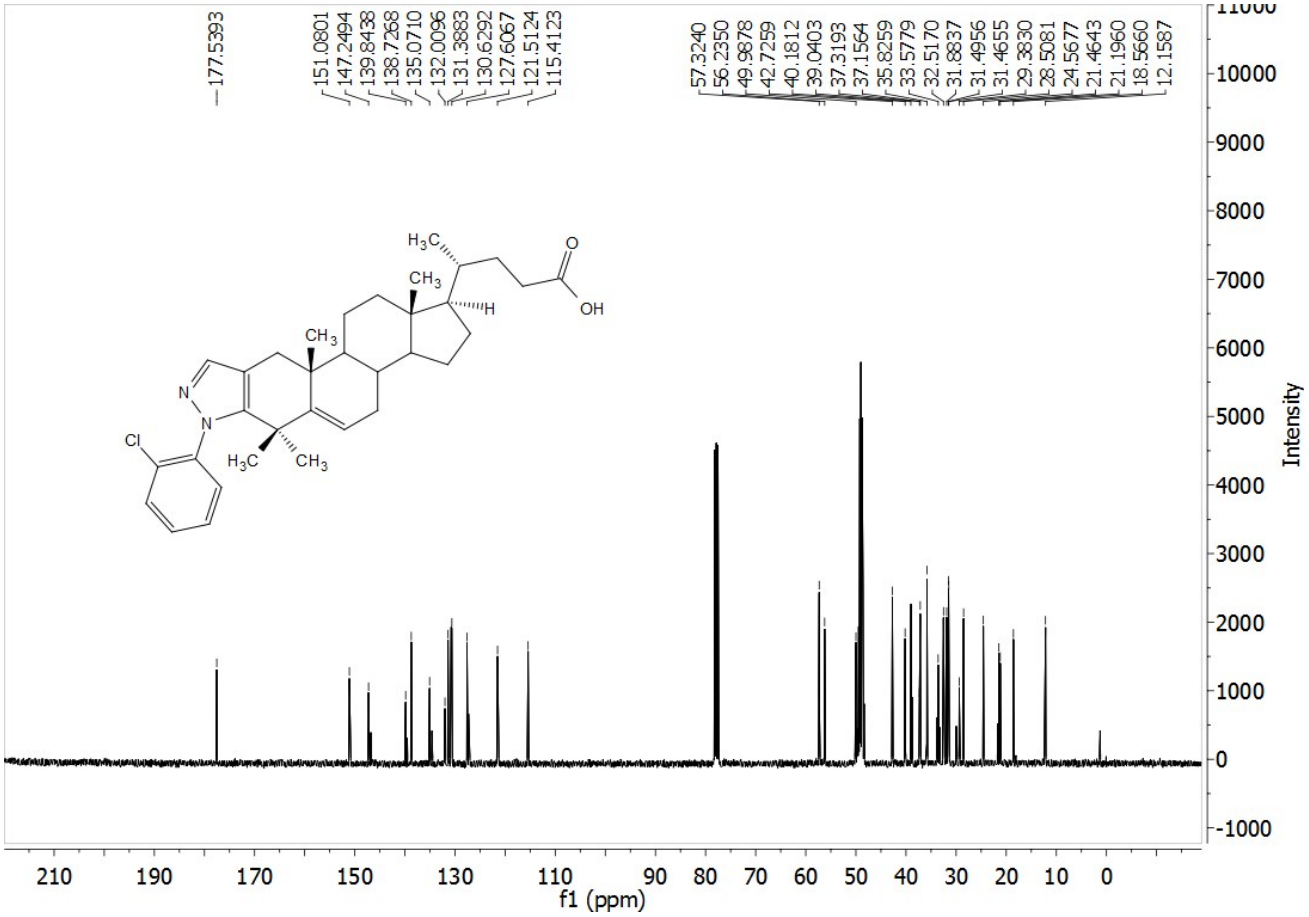

Fig S25: ^{13}C NMR of compound **34** (in the solvent of $CDCl_3/CD_3OD$=2/1, v/v, 101MHz)

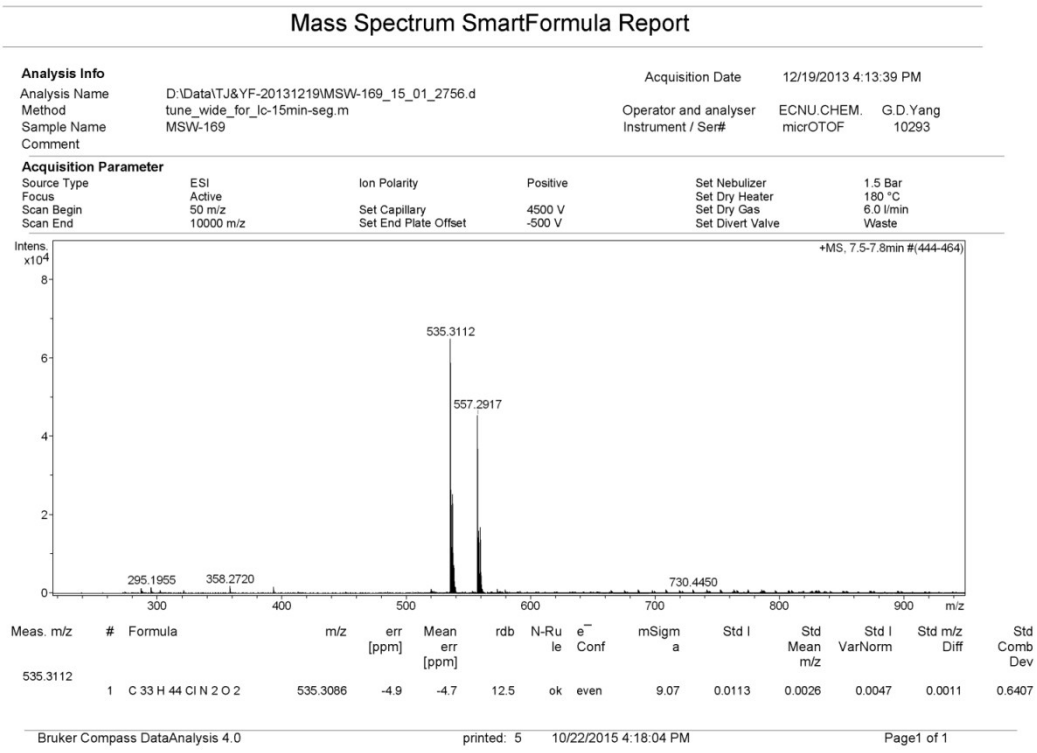

Fig S26: HRMS of compound **34**

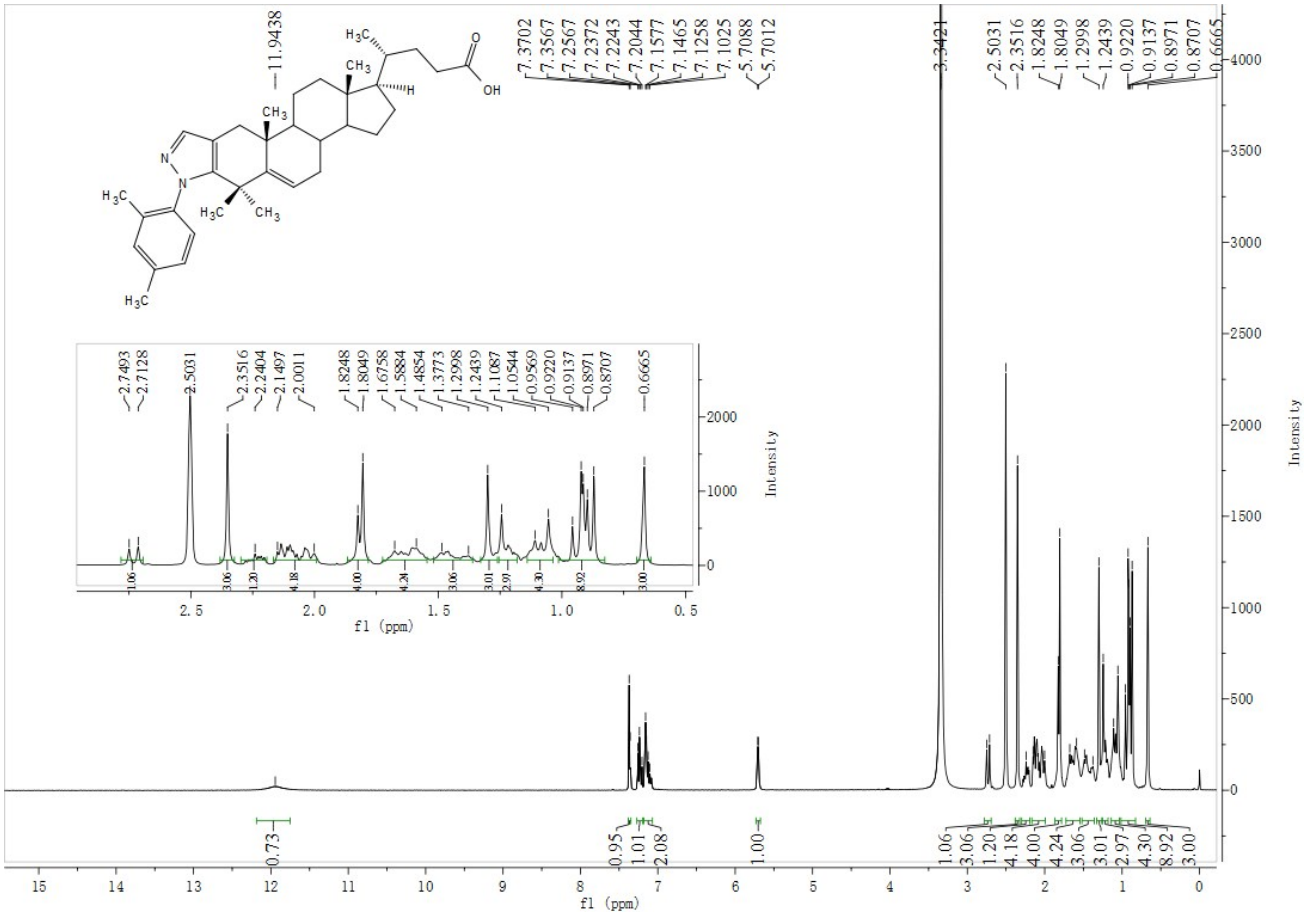

Fig S27: ^{1}H NMR of compound **35** (in the solvent of DMSO-d6, 400MHz)

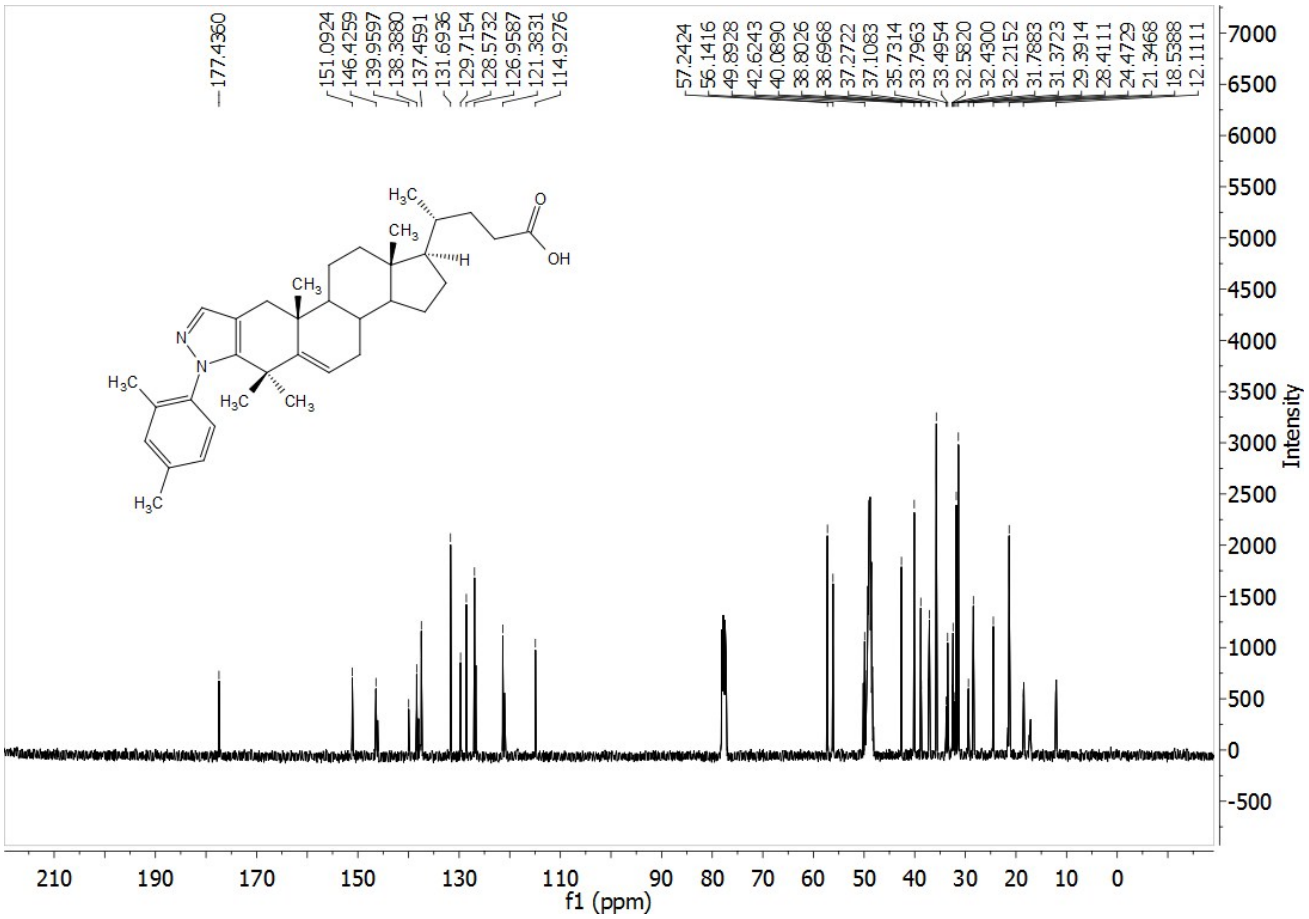

Fig S28: ^{13}C NMR of compound **35** (in the solvent of $CDCl_3/CD_3OD$=2/1, v/v, 101MHz)

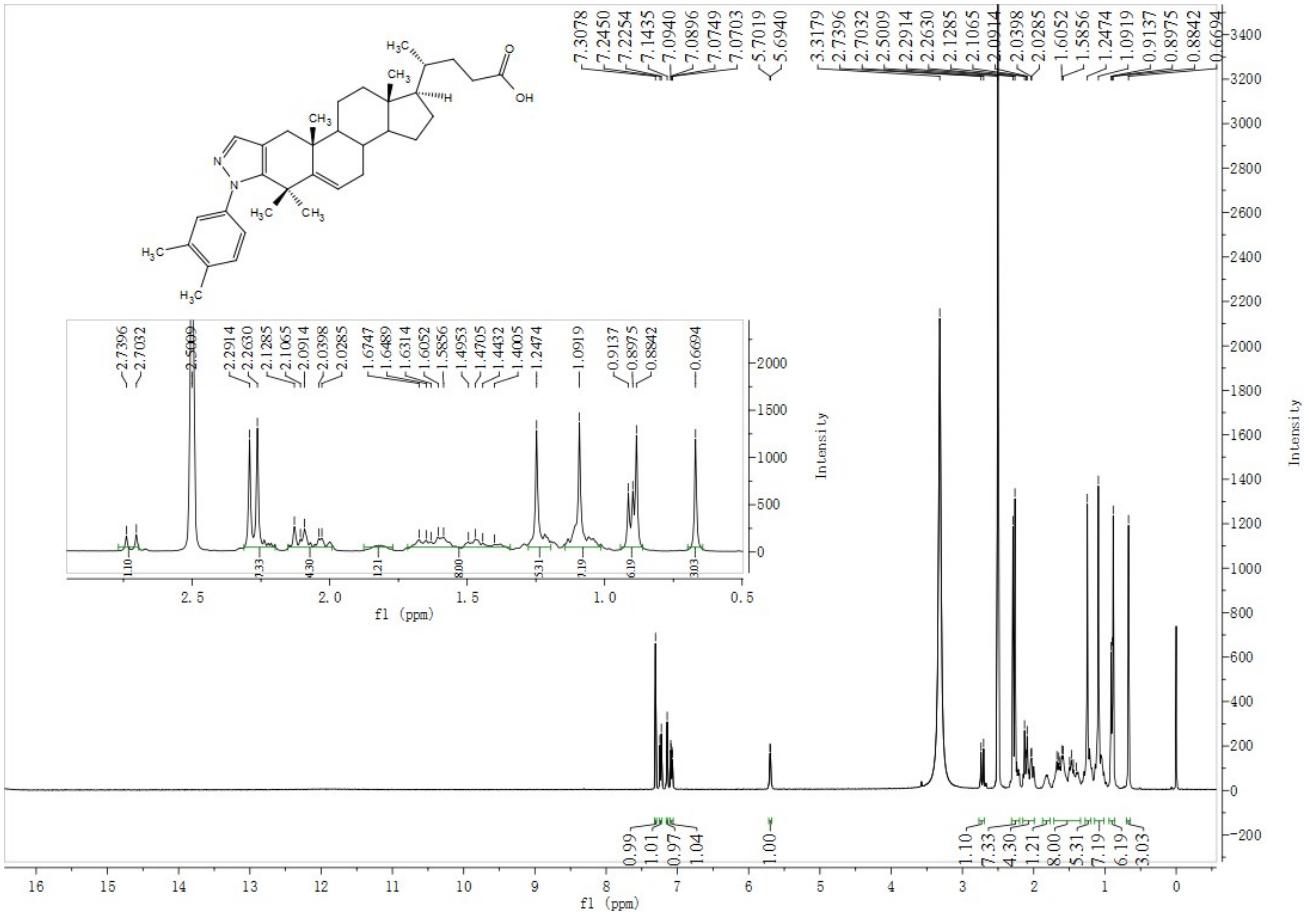

Fig S29: ^{1}H NMR of compound **36** (in the solvent of DMSO-d6, 400MHz)

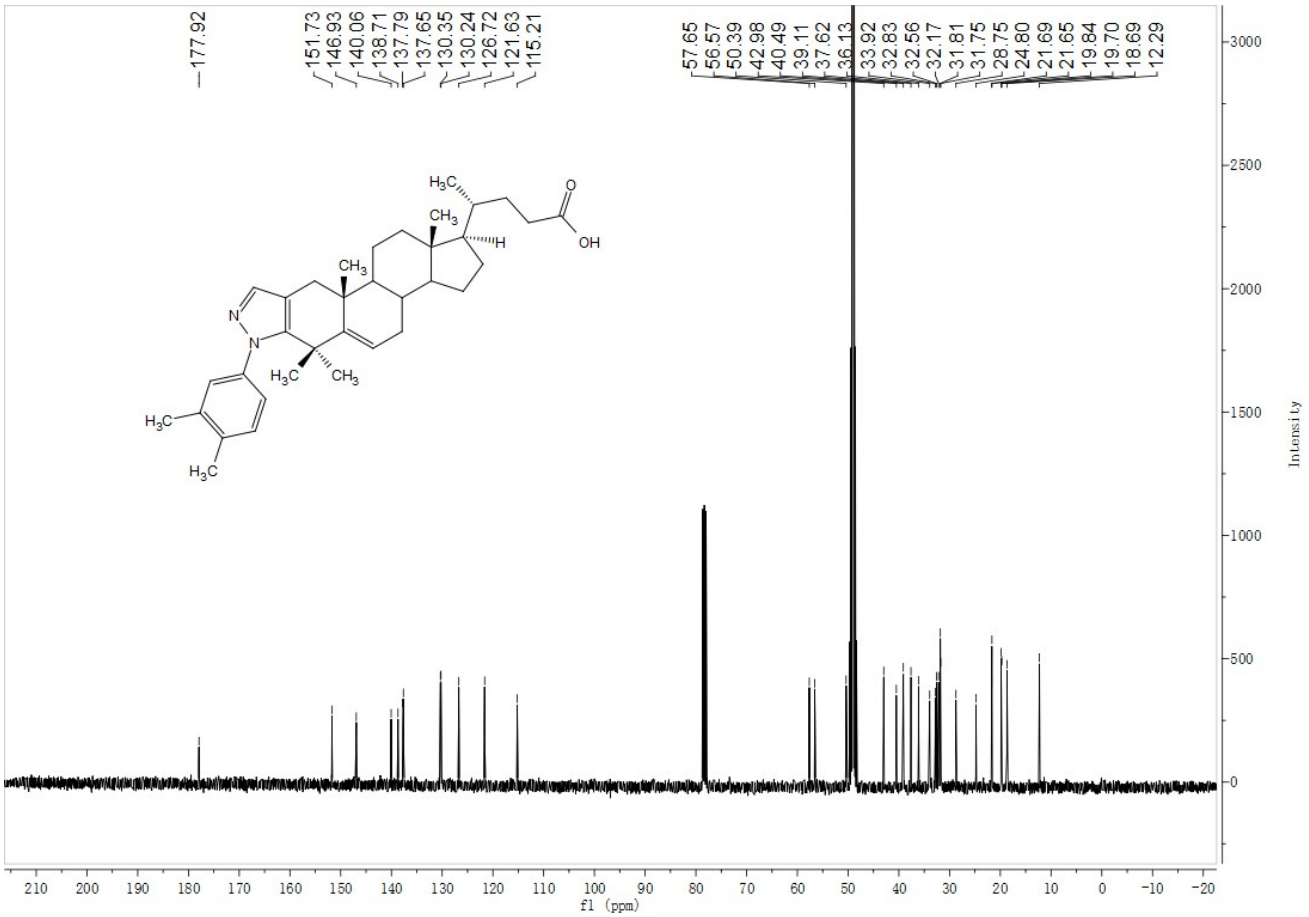

Fig S30: ^{13}C NMR of compound **36** (in the solvent of $CDCl_3/CD_3OD$=2/1, v/v, 101MHz)

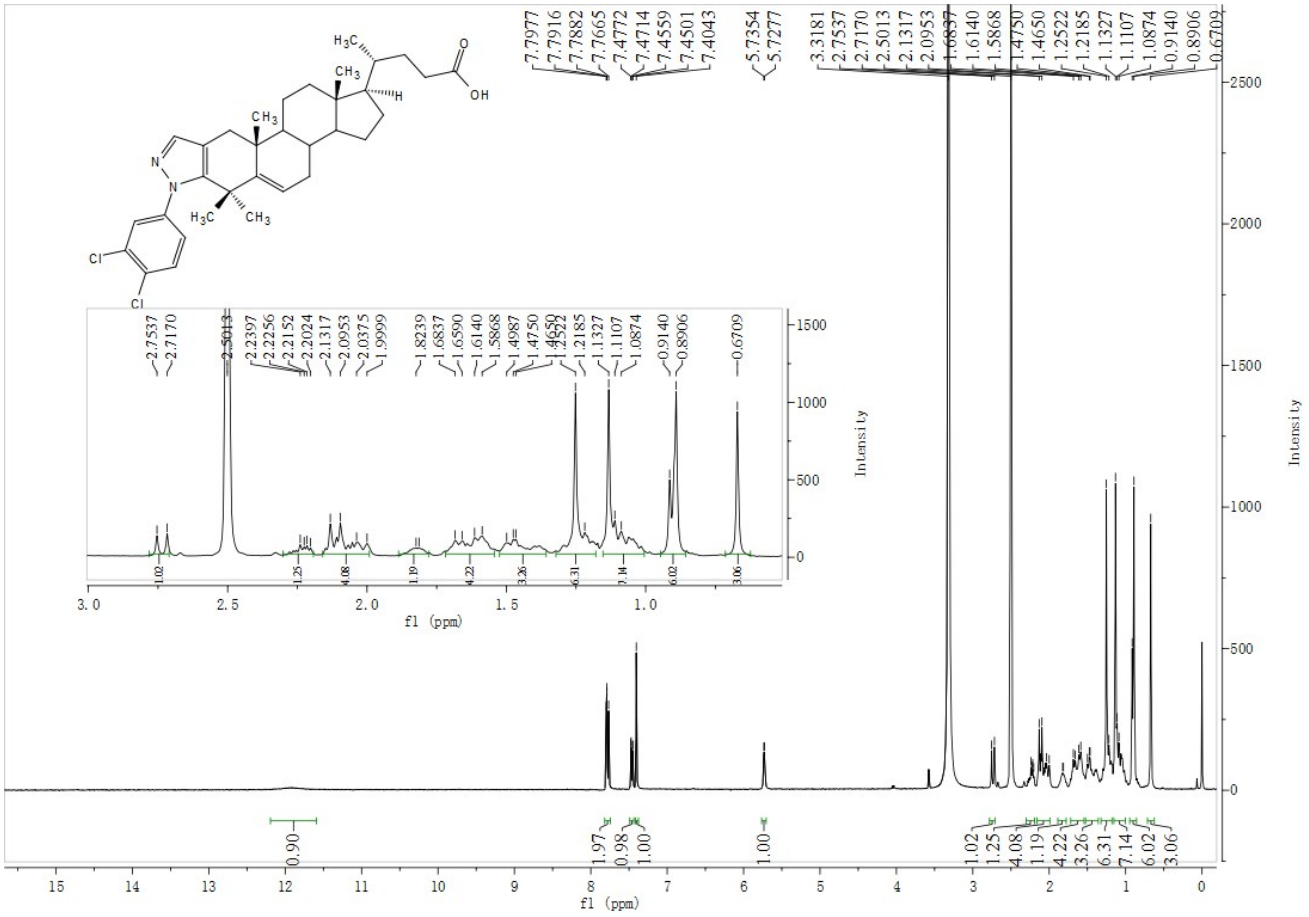

Fig S31: ^{1}H NMR of compound **37** (in the solvent of DMSO-d6, 400MHz)

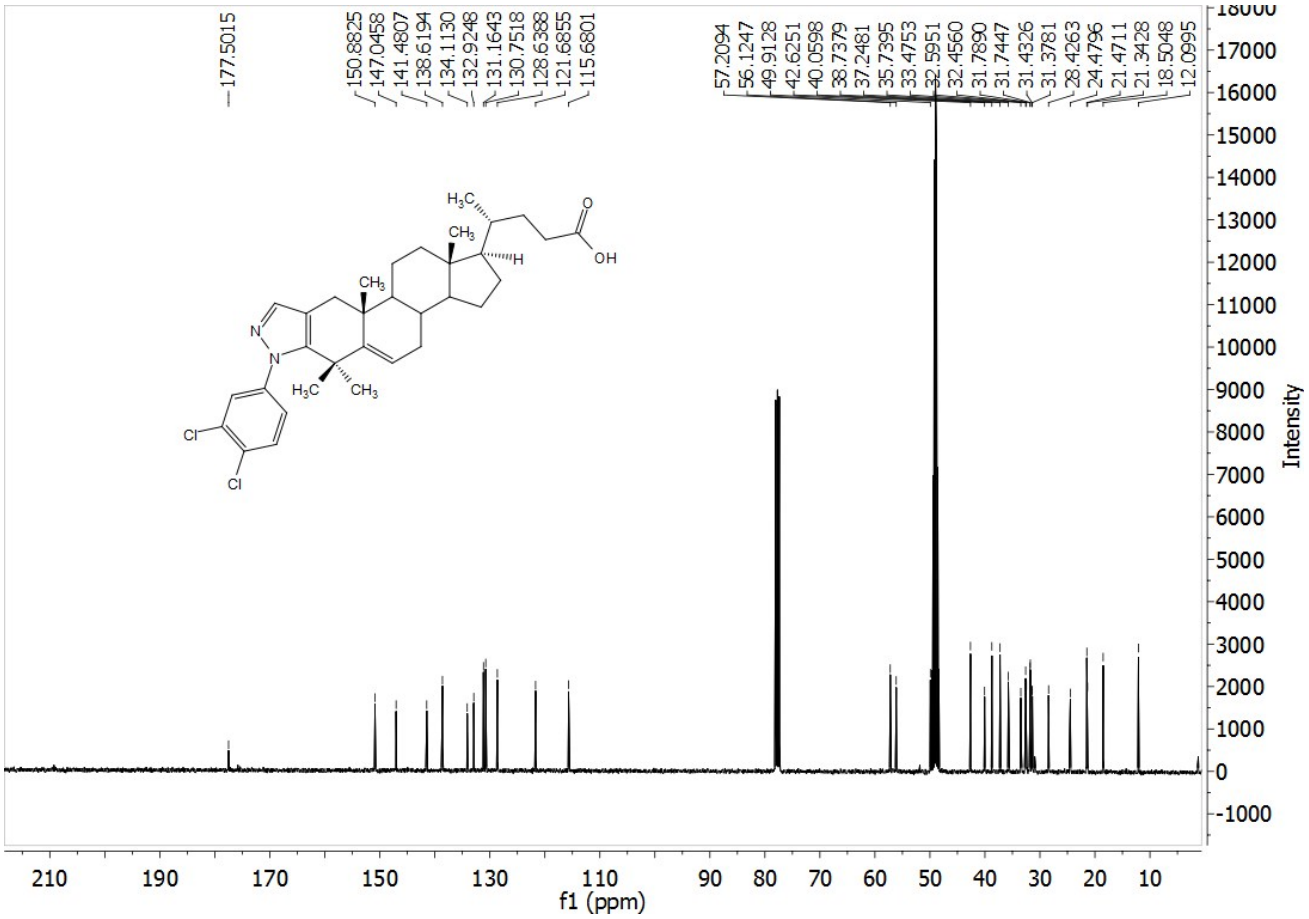

Fig S32: ^{13}C NMR of compound **37** (in the solvent of $CDCl_3/CD_3OD$=2/1, v/v, 101MHz)

Crystal data for compound **33**

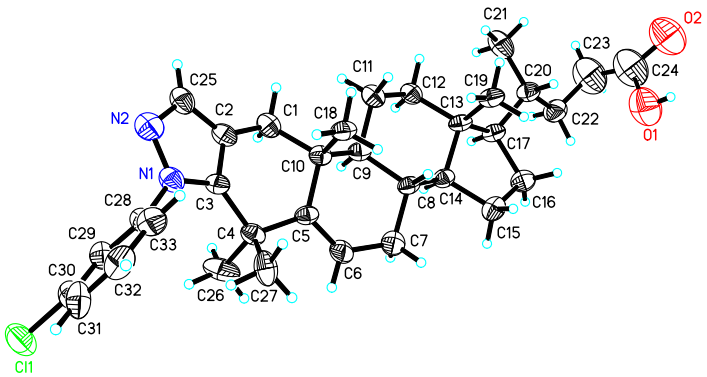

Fig S33: X-ray structure of compound **33**, the crystal data has been deposited in CCDC with number 1401731

Table S1: Crystal data and structure refinement for compound **33**

Identification code	cd214518	
Empirical formula	C_{33} H_{45} Cl N_2 O_3	
Formula weight	553.16	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 12.474(3) Å	α= 90°
	b = 6.1241(17) Å	β= 100.744(6)°
	c = 19.930(6) Å	γ = 90°
Volume	1495.8(7) $Å^3$	
Z	2	
Density (calculated)	1.228 Mg/m^3	
Absorption coefficient	0.163 mm^{-1}	
F(000)	596	
Crystal size	0.176 x 0.101 x 0.065 mm^3	
Theta range for data collection	1.788 to 25.486°	
Index ranges	-15<=h<=9, -7<=k<=7, -23<=l<=24	

Reflections collected	8648
Independent reflections	5385 [R(int) = 0.0381]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.5966
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5385 / 61 / 393
Goodness-of-fit on F^2	0.915
Final R indices [I>2sigma(I)]	R1 = 0.0591, wR2 = 0.1311
R indices (all data)	R1 = 0.1150, wR2 = 0.1582
Absolute structure parameter	0.15(8)
Extinction coefficient	n/a
Largest diff. peak and hole	0.287 and -0.140 e.$Å^{-3}$

Table S2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for compound **33**

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Cl(1)	9624(1)	9248(4)	5681(1)	108(1)
N(1)	7028(3)	8884(9)	3380(2)	62(1)
N(2)	6138(4)	7577(9)	3374(3)	73(1)
O(3)	5103(6)	2905(16)	5597(4)	209(4)
C(1)	6853(4)	6778(9)	1668(3)	59(2)
C(2)	6724(4)	7297(9)	2375(3)	56(2)
C(3)	7388(4)	8735(9)	2777(3)	52(1)
C(4)	8362(4)	9858(9)	2573(3)	54(1)
C(5)	8237(3)	9803(8)	1787(3)	48(1)
C(6)	9018(4)	10657(10)	1506(3)	63(2)
C(7)	9071(4)	10820(10)	770(3)	63(2)
C(8)	8033(3)	10045(8)	295(3)	47(1)
C(9)	7525(4)	8158(8)	634(3)	49(1)
C(10)	7227(3)	8824(9)	1320(3)	45(1)
C(11)	6592(4)	7076(9)	139(3)	56(2)
C(12)	6871(4)	6488(9)	-556(3)	55(1)
C(13)	7283(3)	8462(8)	-903(3)	49(1)
C(14)	8273(3)	9338(9)	-387(3)	48(1)

C(15)	8804(4)	10964(10)	-804(3)	62(2)
C(16)	8609(4)	9966(10)	-1526(3)	62(2)
C(17)	7838(4)	7988(9)	-1524(3)	53(1)
C(18)	6313(4)	10531(10)	1234(3)	62(2)
C(19)	6379(4)	10151(9)	-1081(3)	63(2)
C(20)	7118(4)	7614(10)	-2230(3)	57(1)
C(21)	6320(5)	5695(12)	-2241(3)	88(2)
C(22)	7850(5)	7218(12)	-2761(3)	77(2)
C(25)	5959(4)	6640(10)	2768(3)	67(2)
C(26)	9393(4)	8592(13)	2904(3)	92(2)
C(27)	8458(5)	12227(10)	2822(3)	78(2)
C(28)	7430(4)	10070(11)	3989(3)	60(2)
C(29)	8239(4)	9207(11)	4475(3)	63(2)
C(30)	8593(4)	10317(12)	5070(3)	68(2)
C(31)	8132(6)	12265(14)	5194(4)	86(2)
C(32)	7306(6)	13104(12)	4719(4)	89(2)
C(33)	6939(5)	12016(11)	4113(4)	78(2)
O(1)	7121(15)	11100(30)	-3393(7)	142(5)
O(2)	5954(11)	9470(30)	-4246(7)	169(4)
C(23)	7260(20)	6920(50)	-3490(9)	149(5)
C(24)	6680(30)	8950(50)	-3710(16)	151(5)
O(1')	6738(11)	10140(20)	-3697(8)	99(5)
O(2')	5900(20)	7400(50)	-4386(14)	184(11)
C(23')	7299(15)	6960(50)	-3480(10)	41(5)
C(24')	6440(30)	8100(70)	-3883(19)	152(5)
N(1)	7028(3)	8884(9)	3380(2)	62(1)

Table S3: Bond lengths [Å] and angles [°] for compound **33**

Cl(1)-C(30)	1.727(6)	N(1)-C(3)	1.362(6)
N(1)-N(2)	1.367(6)	N(1)-C(28)	1.423(7)
N(2)-C(25)	1.319(7)	O(3)-H(3C)	0.8287
O(3)-H(3D)	0.8233	C(1)-C(2)	1.482(8)
C(1)-C(10)	1.546(7)	C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700	C(2)-C(3)	1.363(7)
C(2)-C(25)	1.400(7)	C(3)-C(4)	1.517(7)
C(4)-C(27)	1.531(8)	C(4)-C(5)	1.544(8)

C(4)-C(26)	1.541(7)	C(5)-C(6)	1.320(7)
C(5)-C(10)	1.542(6)	C(6)-C(7)	1.485(8)
C(6)-H(6)	0.9300	C(7)-C(8)	1.530(7)
C(7)-H(7A)	0.9700	C(7)-H(7B)	0.9700
C(8)-C(14)	1.510(7)	C(8)-C(9)	1.533(7)
C(8)-H(8)	0.9800	C(9)-C(11)	1.529(7)
C(9)-C(10)	1.537(7)	C(9)-H(9)	0.9800
C(10)-C(18)	1.533(7)	C(11)-C(12)	1.532(7)
C(11)-H(11A)	0.9700	C(11)-H(11B)	0.9700
C(12)-C(13)	1.529(7)	C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700	C(13)-C(19)	1.523(7)
C(13)-C(14)	1.547(6)	C(13)-C(17)	1.554(7)
C(14)-C(15)	1.524(7)	C(14)-H(14)	0.9800
C(15)-C(16)	1.541(8)	C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700	C(16)-C(17)	1.547(7)
C(16)-H(16A)	0.9700	C(16)-H(16B)	0.9700
C(17)-C(20)	1.538(7)	C(17)-H(17)	0.9800
C(18)-H(18A)	0.9600	C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600	C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600	C(19)-H(19C)	0.9600
C(20)-C(22)	1.540(7)	C(20)-C(21)	1.538(8)
C(20)-H(20)	0.9800	C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600	C(21)-H(21C)	0.9600
C(22)-C(23')	1.477(19)	C(22)-C(23)	1.513(17)
C(22)-H(22A)	0.9602	C(22)-H(22B)	0.9603
C(22)-H(22C)	0.9601	C(22)-H(22D)	0.9315
C(25)-H(25)	0.9300	C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600	C(26)-H(26C)	0.9600
C(27)-H(27A)	0.9600	C(27)-H(27B)	0.9600

C(27)-H(27C)	0.9600	C(28)-C(29)	1.368(7)
C(28)-C(33)	1.383(8)	C(29)-C(30)	1.367(8)
C(29)-H(29)	0.9300	C(30)-C(31)	1.366(9)
C(31)-C(32)	1.364(9)	C(31)-H(31)	0.9300
C(32)-C(33)	1.381(9)	C(32)-H(32)	0.9300
C(33)-H(33)	0.9300	O(1)-C(24)	1.52(3)
O(1)-H(1)	0.8200	O(2)-C(24)	1.31(3)
C(23)-C(24)	1.46(2)	C(23)-H(23A)	0.9700
C(23)-H(23B)	0.9700	O(1')-C(24')	1.33(4)
O(1')-H(1')	0.8200	O(2')-C(24')	1.18(4)
C(23')-C(24')	1.40(2)	C(23')-H(23C)	0.9700
C(23')-H(23D)	0.9700		
C(3)-N(1)-N(2)	110.7(5)	C(3)-N(1)-C(28)	131.7(5)
N(2)-N(1)-C(28)	117.5(5)	C(25)-N(2)-N(1)	105.1(5)
H(3C)-O(3)-H(3D)	144.9	C(2)-C(1)-C(10)	110.4(5)
C(2)-C(1)-H(1A)	109.6	C(10)-C(1)-H(1A)	109.6
C(2)-C(1)-H(1B)	109.6	C(10)-C(1)-H(1B)	109.6
H(1A)-C(1)-H(1B)	108.1	C(3)-C(2)-C(25)	105.1(5)
C(3)-C(2)-C(1)	122.4(5)	C(25)-C(2)-C(1)	132.5(5)
N(1)-C(3)-C(2)	107.3(5)	N(1)-C(3)-C(4)	128.2(5)
C(2)-C(3)-C(4)	124.4(5)	C(3)-C(4)-C(27)	111.1(5)
C(3)-C(4)-C(5)	109.1(4)	C(27)-C(4)-C(5)	109.6(5)
C(3)-C(4)-C(26)	107.7(4)	C(27)-C(4)-C(26)	109.2(5)
C(5)-C(4)-C(26)	110.0(5)	C(6)-C(5)-C(10)	118.8(5)
C(6)-C(5)-C(4)	118.6(5)	C(10)-C(5)-C(4)	122.6(4)
C(5)-C(6)-C(7)	128.2(5)	C(5)-C(6)-H(6)	115.9
C(7)-C(6)-H(6)	115.9	C(6)-C(7)-C(8)	113.7(4)
C(6)-C(7)-H(7A)	108.8	C(8)-C(7)-H(7A)	108.8
C(6)-C(7)-H(7B)	108.8	C(8)-C(7)-H(7B)	108.8

H(7A)-C(7)-H(7B)	107.7	C(14)-C(8)-C(7)	111.0(4)
C(14)-C(8)-C(9)	110.4(4)	C(7)-C(8)-C(9)	109.5(4)
C(14)-C(8)-H(8)	108.7	C(7)-C(8)-H(8)	108.7
C(9)-C(8)-H(8)	108.7	C(11)-C(9)-C(8)	111.7(4)
C(11)-C(9)-C(10)	114.0(4)	C(8)-C(9)-C(10)	112.3(4)
C(11)-C(9)-H(9)	106.0	C(8)-C(9)-H(9)	106.0
C(10)-C(9)-H(9)	106.0	C(18)-C(10)-C(9)	112.3(4)
C(18)-C(10)-C(5)	108.0(4)	C(9)-C(10)-C(5)	109.6(4)
C(18)-C(10)-C(1)	108.8(4)	C(9)-C(10)-C(1)	109.1(4)
C(5)-C(10)-C(1)	108.9(4)	C(9)-C(11)-C(12)	114.3(4)
C(9)-C(11)-H(11A)	108.7	C(12)-C(11)-H(11A)	108.7
C(9)-C(11)-H(11B)	108.7	C(12)-C(11)-H(11B)	108.7
H(11A)-C(11)-H(11B)	107.6	C(13)-C(12)-C(11)	112.1(4)
C(13)-C(12)-H(12A)	109.2	C(11)-C(12)-H(12A)	109.2
C(13)-C(12)-H(12B)	109.2	C(11)-C(12)-H(12B)	109.2
H(12A)-C(12)-H(12B)	107.9	C(19)-C(13)-C(12)	110.2(4)
C(19)-C(13)-C(14)	112.6(4)	C(12)-C(13)-C(14)	105.5(4)
C(19)-C(13)-C(17)	111.2(4)	C(12)-C(13)-C(17)	116.8(4)
C(14)-C(13)-C(17)	100.1(4)	C(8)-C(14)-C(15)	118.8(4)
C(8)-C(14)-C(13)	115.4(4)	C(15)-C(14)-C(13)	103.8(4)
C(8)-C(14)-H(14)	105.9	C(15)-C(14)-H(14)	105.9
C(13)-C(14)-H(14)	105.9	C(14)-C(15)-C(16)	103.9(5)
C(14)-C(15)-H(15A)	111.0	C(16)-C(15)-H(15A)	111.0
C(14)-C(15)-H(15B)	111.0	C(16)-C(15)-H(15B)	111.0
H(15A)-C(15)-H(15B)	109.0	C(15)-C(16)-C(17)	107.4(4)
C(15)-C(16)-H(16A)	110.2	C(17)-C(16)-H(16A)	110.2
C(15)-C(16)-H(16B)	110.2	C(17)-C(16)-H(16B)	110.2
H(16A)-C(16)-H(16B)	108.5	C(20)-C(17)-C(16)	111.8(4)
C(20)-C(17)-C(13)	119.1(4)	C(16)-C(17)-C(13)	103.0(4)

C(20)-C(17)-H(17)	107.5	C(16)-C(17)-H(17)	107.5
C(13)-C(17)-H(17)	107.5	C(10)-C(18)-H(18A)	109.5
C(10)-C(18)-H(18B)	109.5	H(18A)-C(18)-H(18B)	109.5
C(10)-C(18)-H(18C)	109.5	H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5	C(13)-C(19)-H(19A)	109.5
C(13)-C(19)-H(19B)	109.5	H(19A)-C(19)-H(19B)	109.5
C(13)-C(19)-H(19C)	109.5	H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5	C(17)-C(20)-C(22)	109.4(4)
C(17)-C(20)-C(21)	113.2(5)	C(22)-C(20)-C(21)	109.5(5)
C(17)-C(20)-H(20)	108.2	C(22)-C(20)-H(20)	108.2
C(21)-C(20)-H(20)	108.2	C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5	H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5	H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5	C(23')-C(22)-C(20)	117.1(9)
C(23)-C(22)-C(20)	115.7(10)	C(23)-C(22)-H(22A)	110.8
C(20)-C(22)-H(22A)	108.2	C(23)-C(22)-H(22B)	105.1
C(20)-C(22)-H(22B)	108.0	H(22A)-C(22)-H(22B)	108.7
C(23')-C(22)-H(22C)	100.1	C(20)-C(22)-H(22C)	107.3
C(23')-C(22)-H(22D)	117.1	C(20)-C(22)-H(22D)	104.9
H(22C)-C(22)-H(22D)	109.8	N(2)-C(25)-C(2)	111.8(5)
N(2)-C(25)-H(25)	124.1	C(2)-C(25)-H(25)	124.1
C(4)-C(26)-H(26A)	109.5	C(4)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5	C(4)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5	H(26B)-C(26)-H(26C)	109.5
C(4)-C(27)-H(27A)	109.5	C(4)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5	C(4)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5	H(27B)-C(27)-H(27C)	109.5
C(29)-C(28)-C(33)	119.9(6)	C(29)-C(28)-N(1)	120.2(6)
C(33)-C(28)-N(1)	119.7(5)	C(30)-C(29)-C(28)	119.9(6)

C(30)-C(29)-H(29)	120.0	C(28)-C(29)-H(29)	120.0
C(29)-C(30)-C(31)	120.8(6)	C(29)-C(30)-Cl(1)	120.1(5)
C(31)-C(30)-Cl(1)	119.1(6)	C(32)-C(31)-C(30)	119.5(7)
C(32)-C(31)-H(31)	120.2	C(30)-C(31)-H(31)	120.2
C(31)-C(32)-C(33)	120.6(7)	C(31)-C(32)-H(32)	119.7
C(33)-C(32)-H(32)	119.7	C(32)-C(33)-C(28)	119.1(6)
C(32)-C(33)-H(33)	120.4	C(28)-C(33)-H(33)	120.4
C(24)-O(1)-H(1)	109.4	C(24)-C(23)-C(22)	108(2)
C(24)-C(23)-H(23A)	106.9	C(22)-C(23)-H(23A)	112.2
C(24)-C(23)-H(23B)	110.7	C(22)-C(23)-H(23B)	110.9
H(23A)-C(23)-H(23B)	107.9	O(2)-C(24)-C(23)	133(3)
O(2)-C(24)-O(1)	106(2)	C(23)-C(24)-O(1)	120(2)
C(24')-O(1')-H(1')	109.5	C(24')-C(23')-C(22)	132(2)
C(24')-C(23')-H(23C)	101.3	C(22)-C(23')-H(23C)	101.4
C(24')-C(23')-H(23D)	108.5	C(22)-C(23')-H(23D)	104.2
H(23C)-C(23')-H(23D)	107.2	O(2')-C(24')-O(1')	131(3)
O(2')-C(24')-C(23')	124(4)	O(1')-C(24')-C(23')	100(3)

Table S4: Torsion angles [°] for compound **33**

C(3)-N(1)-N(2)-C(25)	-0.1(6)	C(28)-N(1)-N(2)-C(25)	-178.3(5)
C(10)-C(1)-C(2)-C(3)	-35.1(7)	C(10)-C(1)-C(2)-C(25)	141.7(6)
N(2)-N(1)-C(3)-C(2)	-0.4(6)	C(28)-N(1)-C(3)-C(2)	177.6(6)
N(2)-N(1)-C(3)-C(4)	-178.4(5)	C(28)-N(1)-C(3)-C(4)	-0.4(10)
C(25)-C(2)-C(3)-N(1)	0.6(6)	C(1)-C(2)-C(3)-N(1)	178.1(5)
C(25)-C(2)-C(3)-C(4)	178.7(5)	C(1)-C(2)-C(3)-C(4)	-3.7(8)
N(1)-C(3)-C(4)-C(27)	-40.9(7)	C(2)-C(3)-C(4)-C(27)	141.4(5)
N(1)-C(3)-C(4)-C(5)	-161.9(5)	C(2)-C(3)-C(4)-C(5)	20.4(7)
N(1)-C(3)-C(4)-C(26)	78.7(7)	C(2)-C(3)-C(4)-C(26)	-99.0(6)
C(3)-C(4)-C(5)-C(6)	-178.4(5)	C(27)-C(4)-C(5)-C(6)	59.6(7)

C(26)-C(4)-C(5)-C(6)	-60.5(7)	C(3)-C(4)-C(5)-C(10)	2.6(7)
C(27)-C(4)-C(5)-C(10)	-119.4(5)	C(26)-C(4)-C(5)-C(10)	120.5(5)
C(10)-C(5)-C(6)-C(7)	-0.1(9)	C(4)-C(5)-C(6)-C(7)	-179.1(5)
C(5)-C(6)-C(7)-C(8)	5.2(9)	C(6)-C(7)-C(8)-C(14)	-155.9(5)
C(6)-C(7)-C(8)-C(9)	-33.8(6)	C(14)-C(8)-C(9)-C(11)	-48.3(5)
C(7)-C(8)-C(9)-C(11)	-170.8(4)	C(14)-C(8)-C(9)-C(10)	-178.0(3)
C(7)-C(8)-C(9)-C(10)	59.6(5)	C(11)-C(9)-C(10)-C(18)	-62.4(6)
C(8)-C(9)-C(10)-C(18)	66.0(5)	C(11)-C(9)-C(10)-C(5)	177.6(4)
C(8)-C(9)-C(10)-C(5)	-54.0(5)	C(11)-C(9)-C(10)-C(1)	58.4(5)
C(8)-C(9)-C(10)-C(1)	-173.2(4)	C(6)-C(5)-C(10)-C(18)	-98.7(6)
C(4)-C(5)-C(10)-C(18)	80.3(6)	C(6)-C(5)-C(10)-C(9)	23.9(6)
C(4)-C(5)-C(10)-C(9)	-157.1(4)	C(6)-C(5)-C(10)-C(1)	143.3(5)
C(4)-C(5)-C(10)-C(1)	-37.8(6)	C(2)-C(1)-C(10)-C(18)	-65.8(6)
C(2)-C(1)-C(10)-C(9)	171.3(4)	C(2)-C(1)-C(10)-C(5)	51.7(5)
C(8)-C(9)-C(11)-C(12)	49.1(6)	C(10)-C(9)-C(11)-C(12)	177.8(4)
C(9)-C(11)-C(12)-C(13)	-55.0(6)	C(11)-C(12)-C(13)-C(19)	-65.4(6)
C(11)-C(12)-C(13)-C(14)	56.4(5)	C(11)-C(12)-C(13)-C(17)	166.5(4)
C(7)-C(8)-C(14)-C(15)	-57.2(6)	C(9)-C(8)-C(14)-C(15)	-178.8(4)
C(7)-C(8)-C(14)-C(13)	178.5(5)	C(9)-C(8)-C(14)-C(13)	56.9(5)
C(19)-C(13)-C(14)-C(8)	60.4(6)	C(12)-C(13)-C(14)-C(8)	-59.9(5)
C(17)-C(13)-C(14)-C(8)	178.5(4)	C(19)-C(13)-C(14)-C(15)	-71.5(5)
C(12)-C(13)-C(14)-C(15)	168.2(4)	C(17)-C(13)-C(14)-C(15)	46.6(5)
C(8)-C(14)-C(15)-C(16)	-163.7(4)	C(13)-C(14)-C(15)-C(16)	-33.9(5)
C(14)-C(15)-C(16)-C(17)	7.8(5)	C(15)-C(16)-C(17)-C(20)	149.9(4)
C(15)-C(16)-C(17)-C(13)	20.8(5)	C(19)-C(13)-C(17)-C(20)	-45.8(6)
C(12)-C(13)-C(17)-C(20)	81.8(6)	C(14)-C(13)-C(17)-C(20)	-165.0(5)
C(19)-C(13)-C(17)-C(16)	78.6(5)	C(12)-C(13)-C(17)-C(16)	-153.8(4)
C(14)-C(13)-C(17)-C(16)	-40.6(5)	C(16)-C(17)-C(20)-C(22)	59.1(6)
C(13)-C(17)-C(20)-C(22)	179.0(5)	C(16)-C(17)-C(20)-C(21)	-178.5(4)

C(13)-C(17)-C(20)-C(21)	-58.5(7)	C(17)-C(20)-C(22)-C(23')	-176.4(14)
C(21)-C(20)-C(22)-C(23')	59.0(15)	C(17)-C(20)-C(22)-C(23)	-177.3(14)
C(21)-C(20)-C(22)-C(23)	58.1(14)	N(1)-N(2)-C(25)-C(2)	0.5(7)
C(3)-C(2)-C(25)-N(2)	-0.7(7)	C(1)-C(2)-C(25)-N(2)	-177.9(6)
C(3)-N(1)-C(28)-C(29)	-85.0(8)	N(2)-N(1)-C(28)-C(29)	92.9(6)
C(3)-N(1)-C(28)-C(33)	100.3(7)	N(2)-N(1)-C(28)-C(33)	-81.9(7)
C(33)-C(28)-C(29)-C(30)	-2.8(9)	N(1)-C(28)-C(29)-C(30)	-177.5(5)
C(28)-C(29)-C(30)-C(31)	1.4(9)	C(28)-C(29)-C(30)-Cl(1)	-179.3(4)
C(29)-C(30)-C(31)-C(32)	0.3(10)	Cl(1)-C(30)-C(31)-C(32)	-179.0(5)
C(30)-C(31)-C(32)-C(33)	-0.6(11)	C(31)-C(32)-C(33)-C(28)	-0.8(11)
C(29)-C(28)-C(33)-C(32)	2.5(9)	N(1)-C(28)-C(33)-C(32)	177.3(6)
C(23')-C(22)-C(23)-C(24)	-89(70)	C(20)-C(22)-C(23)-C(24)	64(3)
C(22)-C(23)-C(24)-O(2)	-169(3)	C(22)-C(23)-C(24)-O(1)	28(4)
C(23)-C(22)-C(23')-C(24')	72(68)	C(20)-C(22)-C(23')-C(24')	44(4)
C(22)-C(23')-C(24')-O(2')	-159(4)	C(22)-C(23')-C(24')-O(1')	43(4)