Figure S1. ^{1}H NMR spectra of 1, D_2O, $(CD_3)_2CO$ as standard.

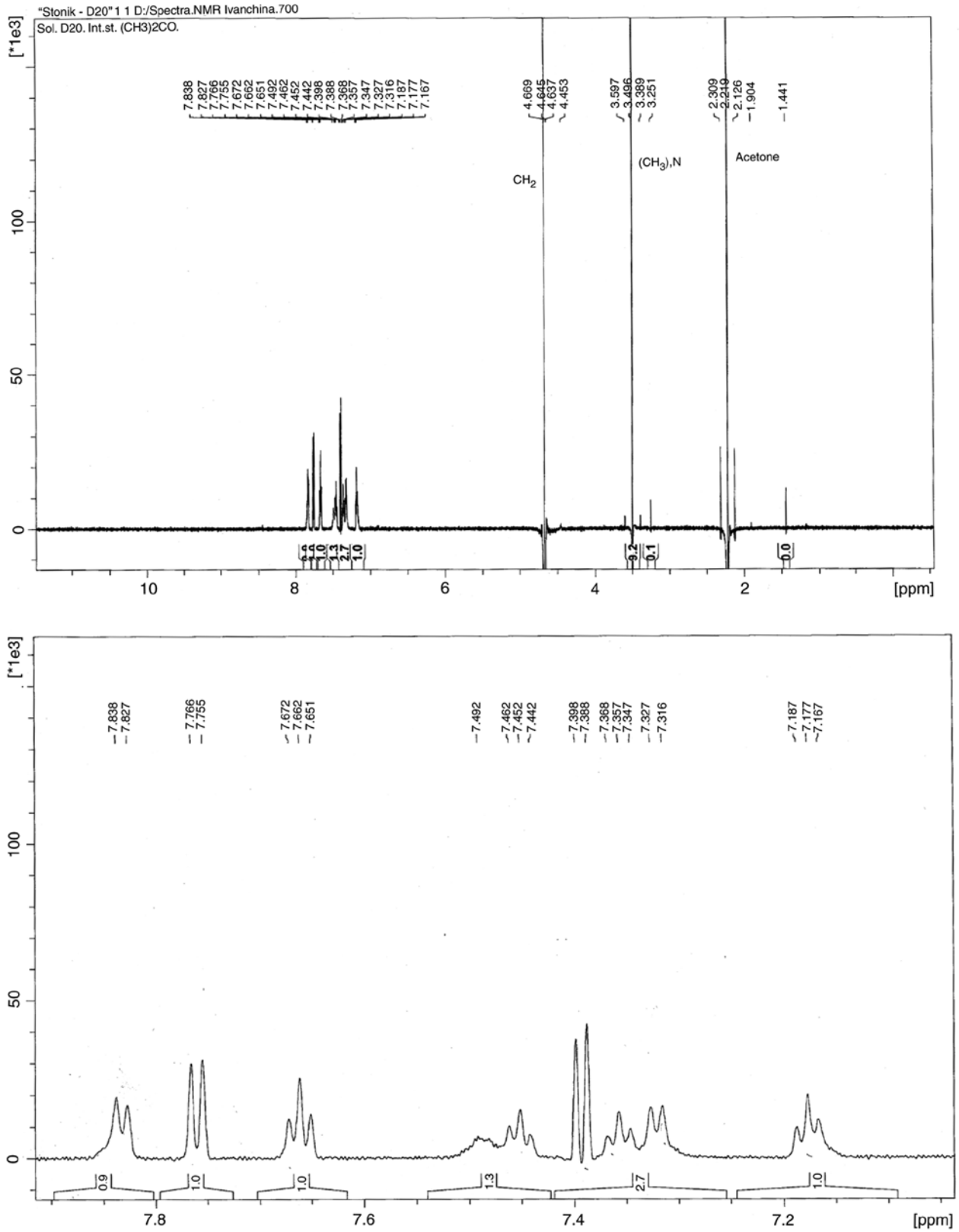

Figure S2. ^{13}C NMR spectra of 1, DEPT, $(CD_3)_2SO$.

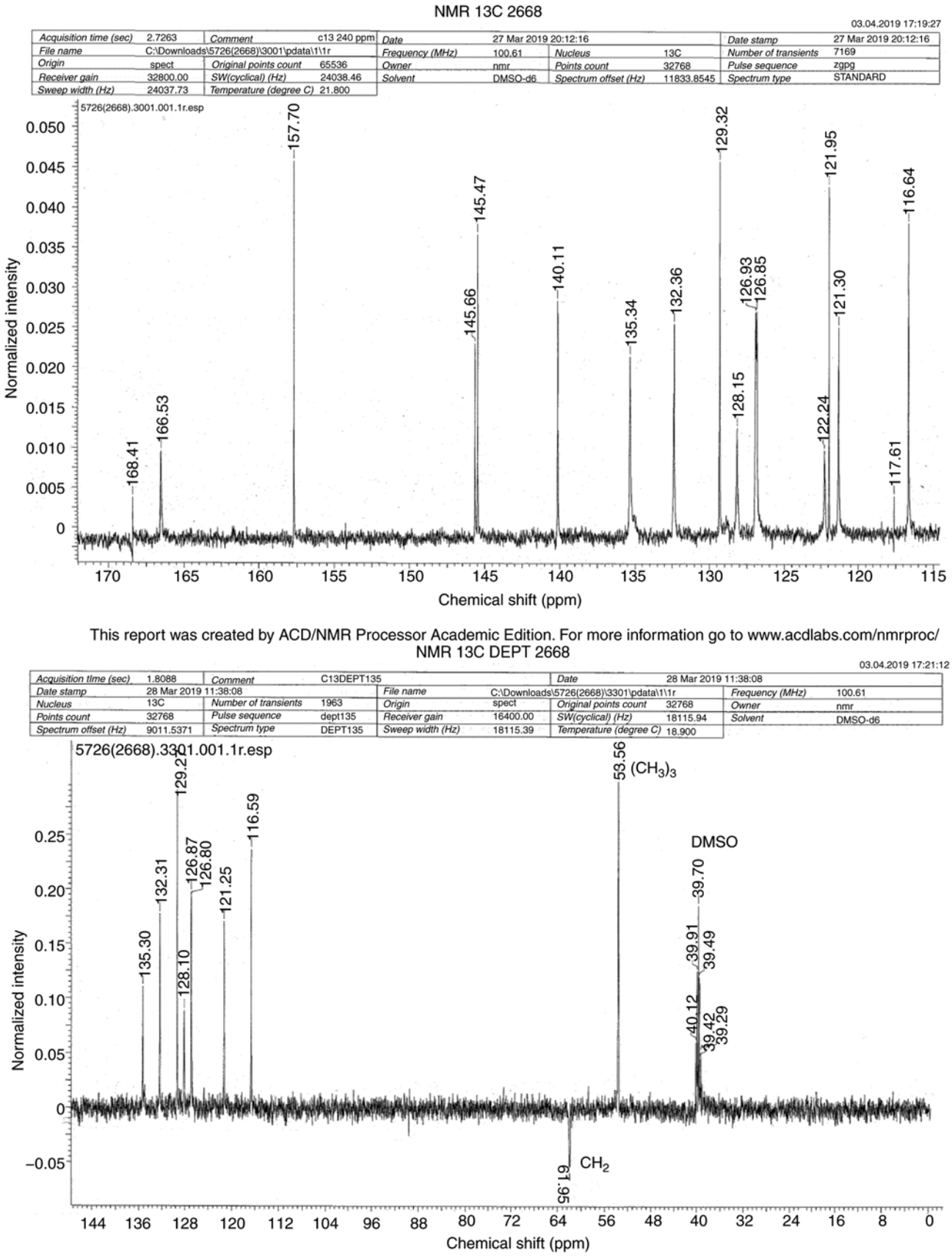

Figure S3. IR spectrum of 1, KBr.

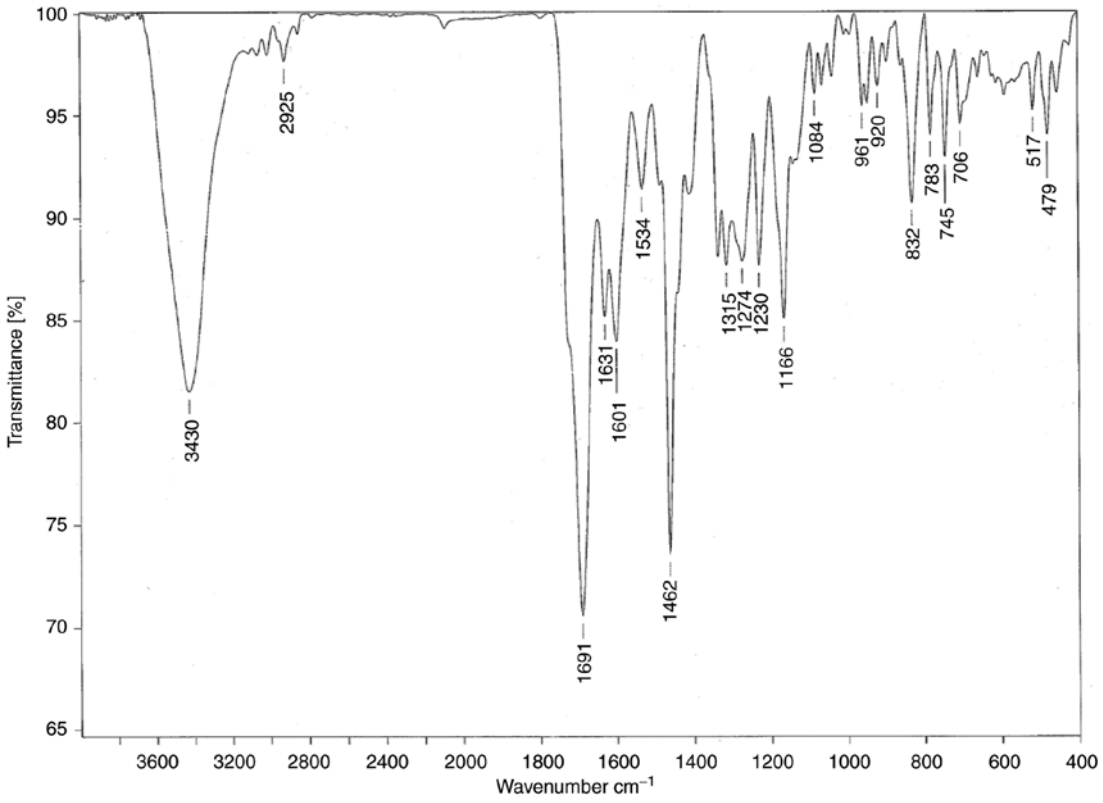

Figure S4. (+) ESI HRMS and (+) ESI HRMS/MS of 1.

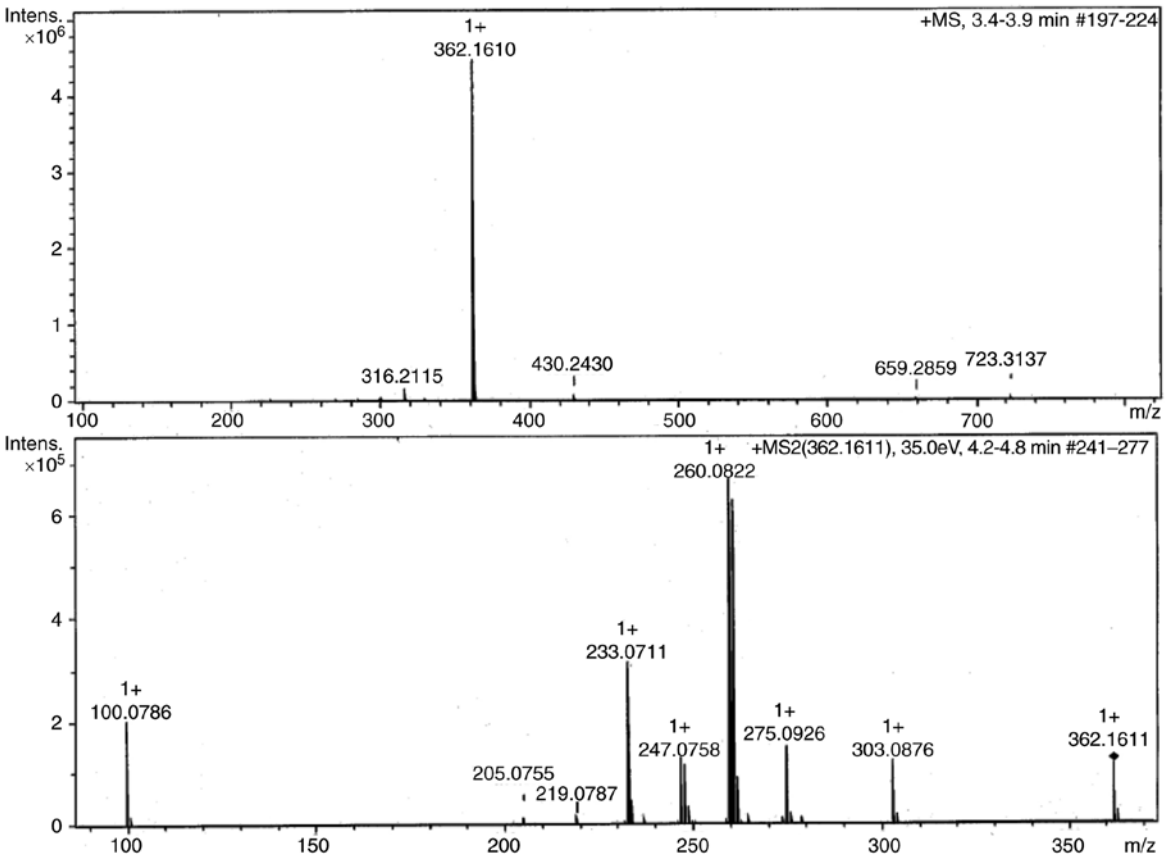

Figure S5. Elemental unit in the crystal of 1.

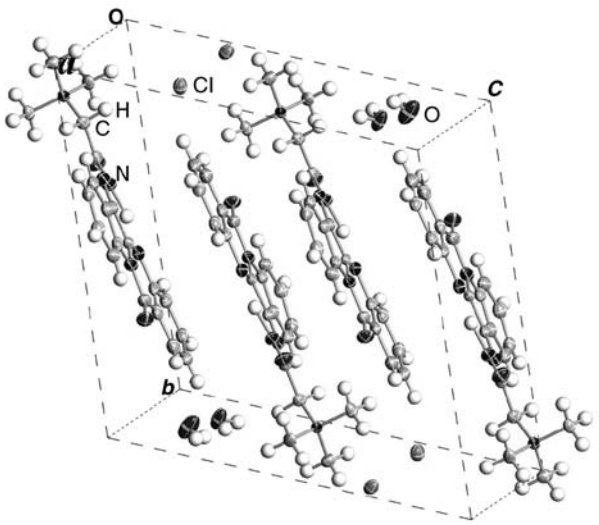

Table SI. X-ray analysis of 1 and crystal data of 1 and structure refinement for x2.

Item	Value	
Identification code	x2	
Empirical formula	$C_{20}H_{22}N_5O_3Cl$	
Molecular mass	415.87	
Temperature	173(2) K	
Wavelength	0.71073 E	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions		
	a=10.8609(4)	E α=69.714(2)°
	b=13.4641(5)	E β=75.979(2)°
	c=14.8893(5)	E γ=79.247(2)°
Volume	1968.77(13) E^3	
Z	4	
Density (calculated)	1.403 mg/m^3	
Absorption coefficient	0.227 mm^{-1}	
F(000)	872	
Crystal size	0.200x0.130x0.130 mm^3	
Theta range for data collection	1.486 to 28.535°	
Index ranges	-14<=h<=14, -18<=k<=17, -18<=l<=20	
Reflections collected	34626	
Independent reflections	9966 [R(int)=0.0213]	
Completeness to theta=25.242°	100.0%	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	9966/6/545	
Goodness-of-fit on F^2	0.989	
Final R indices [I>2sigma(I)]	R1=0.0494, wR2=0.1465	
R indices (all data)	R1=0.0626, wR2=0.1592	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.117 and -0.419 $e.E^{-3}$	
CCDC no.1964205		

Table SII. Interatomic distances in MT.[a]

Bond	d, Å	Bond	d, Å	Bond	d, Å
Molecule a					
N1-C1	1.503(2)	N2-H1	1.40	N5-C14	1.389(2)
N1-C2	1.501(2)	N4-H1	1.75[b]	C14-C15	1.467(2)
N1-C3	1.505(2)	C7-C8	1.449(2)	C15-C16	1.404(2)
N1-C4	1.496(2)	C8-C9	1.399(2)	C16-N4	1.402(2)
C4-C5	1.520(2)	C9-C10	1.383(2)	C16-C17	1.409(2)
C5-N2	1.371(2)	C10-C11	1.395(2)	C17-C18	1.383(2)
N2-N3	1.375(2)	C11-C12	1.392(2)	C18-C19	1.397(2)
N3-C7	1.311(2)	C12-C13	1.386(2)	C19-C20	1.374(2)
C7-C6	1.468(2)	C13-C8	1.382(2)	C20-C15	1.396(2)
C6-N4	1.296(2)	N5-C6	1.387(2)	C5-O1	1.206(2)
		N5-C9	1.434(2)	C14-O2	1.225(2)

[a]As indicated in Fig. 2. [b]The sum of Van-der-Waals radiuses of nitrogen and hydrogen atoms=1.55+1.09 Å.

Table SIII. Comparative evaluation of dynamics of the tumor growth renewal after treatment with DOX alone and in combination with MT.

Group	30-th day[a]		40-th day		50-th day		60-th day	
	Survived animals, %	Of them with tumor, %	Survived animals, %	Of them with tumor, %	Survived animals, %	Of them with tumor, %	Survived animals, %	Of them with tumor, %
DOX	100	20	100	40	80	50	67	70
DOX+MT 5 mg/kg	100	10	100	20	90	20	78	40
DOX+MT 10 mg/kg	100	0	100	0	100	10	100	10

DOX, doxorubicin treatment; DOX + MT, joint administration of doxorubicin and mostotrin. [a]Beginning of secondary tumor growth after treatment was detected on 30th day of the experiment, to that moment MT group had no surviving animals.

Table SIV. The evaluation of antitumor activity at application of MT, DOX and the combination of MT+DOX using the model of solid Ehrlich's adenocarcinoma.

	10 day		13 day		17 day		22 day	
Group	V, mm^3	TGI, %	V, mm^3	TGI, %	V, mm^3	TGI, %	V, mm^3	TGI, %
Contr(-)	116.3±2.3	-	177.0±3.4	-	424.9±5.7	-	633.4±7.5	-
DOX	102.1±2.8	12.2±2.8	138.7±2.1	21.6±2.1	345.2±3.4	18.7±3.4	514.1±3.2[a]	18.8±3.2
MT	115.2±2.9	0.9±2.9	176.1±3.0	0.5±3.05	414.3±4.6	2.5±4.6	614.6±5.6	2.9±5.6
MT+DOX	100.1±2.7	13.9±2.7	118.3±3.6[a]	33.1±3.6[c]	329.2±3.8[a]	22.5±3.8	497.2±3.6[b]	21.5±3.6

MT, compound 1; DOX, doxorubicin; DOX + MT, joint administration of 1 and doxorubicin. V, tumor volume; TGI, inhibition tumor growth. Results are presented as mean tumor volume ± SEM, n=7 for each group, [a]$P<0.05$, [b]$P<0.01$ vs. negative control group; [c]$P<0.05$ vs. DOX group (Tukey's test).