

Supplementary Materials

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Copies of NMR Spectra

Figure S1. Copy of ^1H NMR spectrum of the derivative **2**.

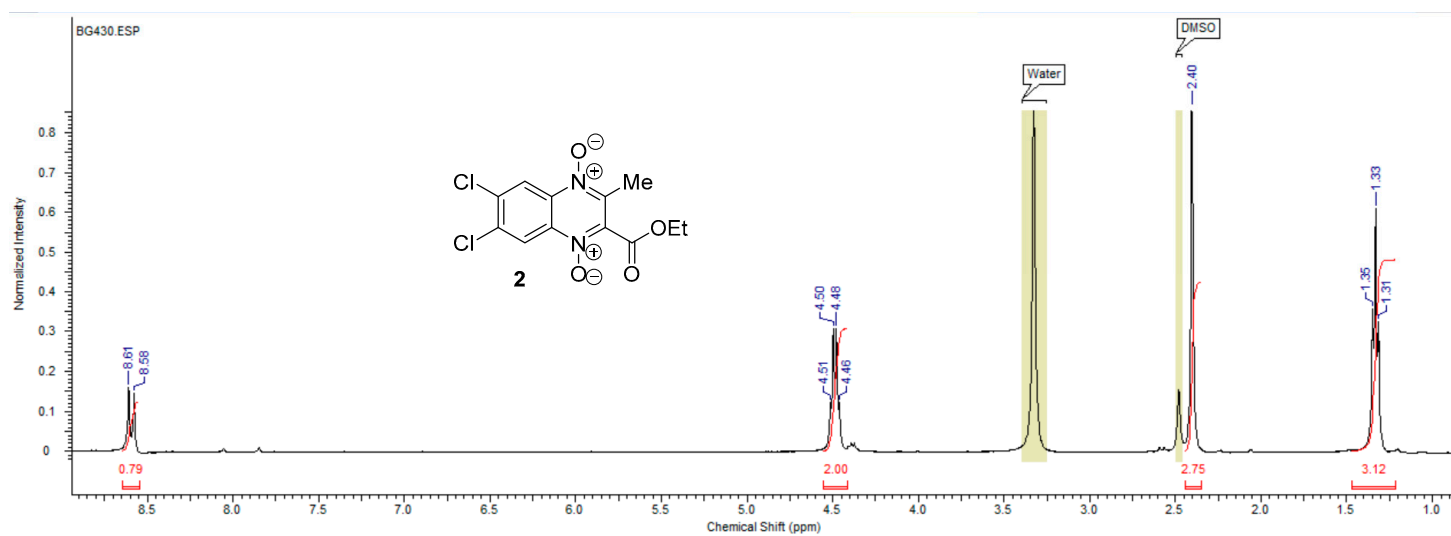


Figure S2. Copy of ^{13}C NMR spectrum of the derivative **2**.

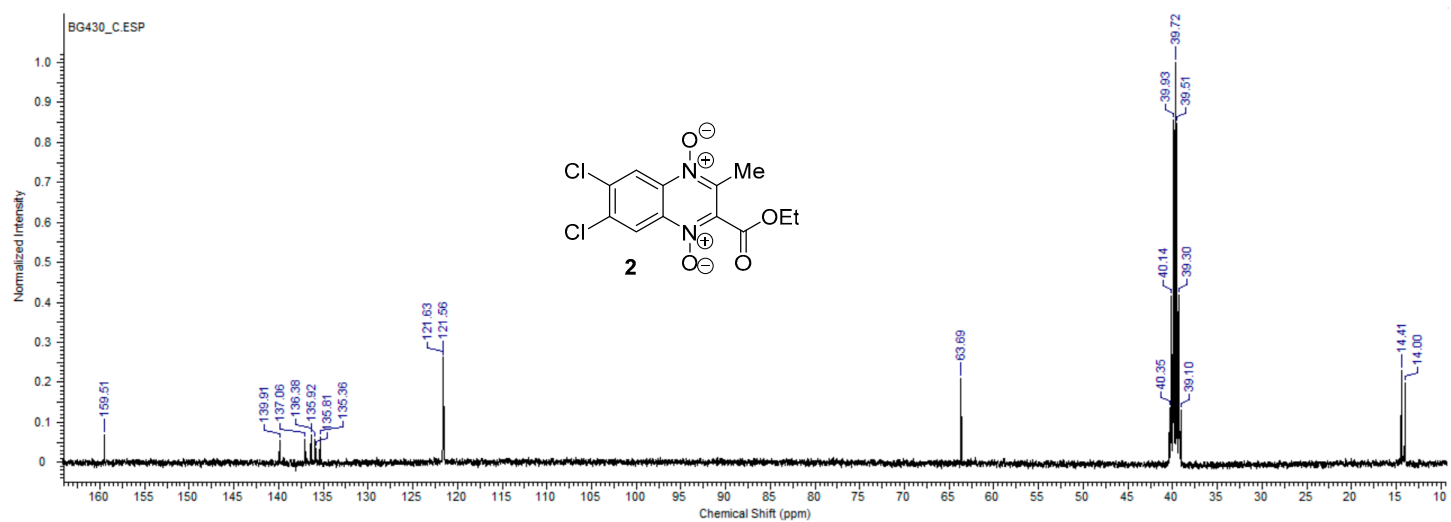


Figure S3. Copy of ^1H NMR spectrum of the derivative **3**.

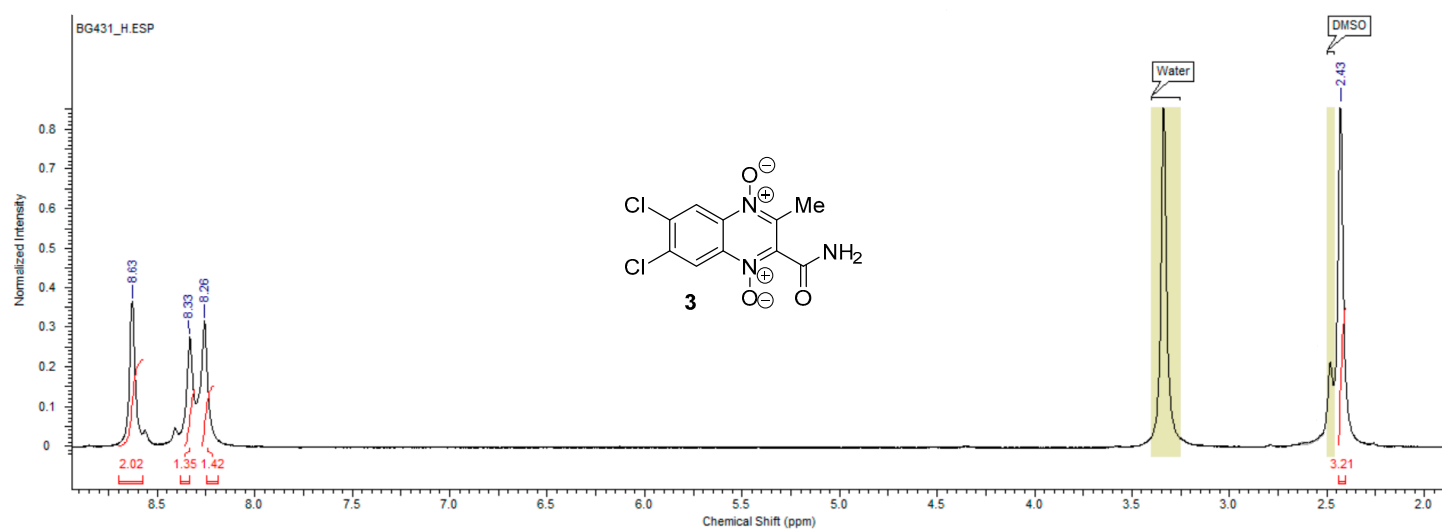


Figure S4. Copy of ^{13}C NMR spectrum of the derivative **3**.

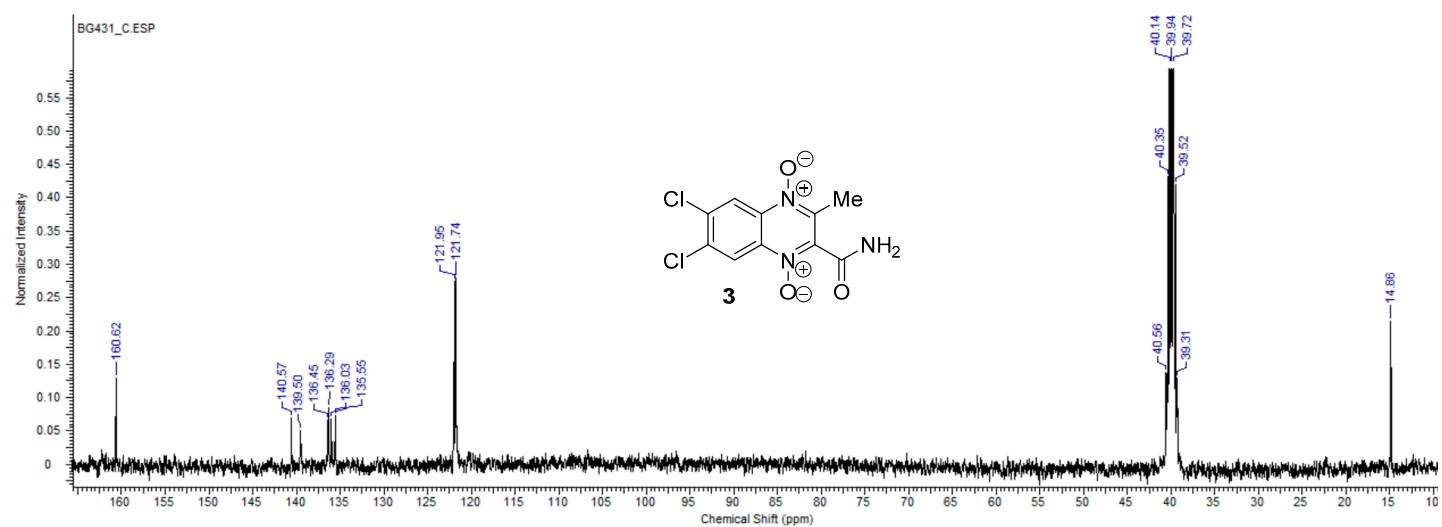


Figure S5. Copy of ^1H NMR spectrum of the derivative **4**.

BG-127 DMSO- d_6

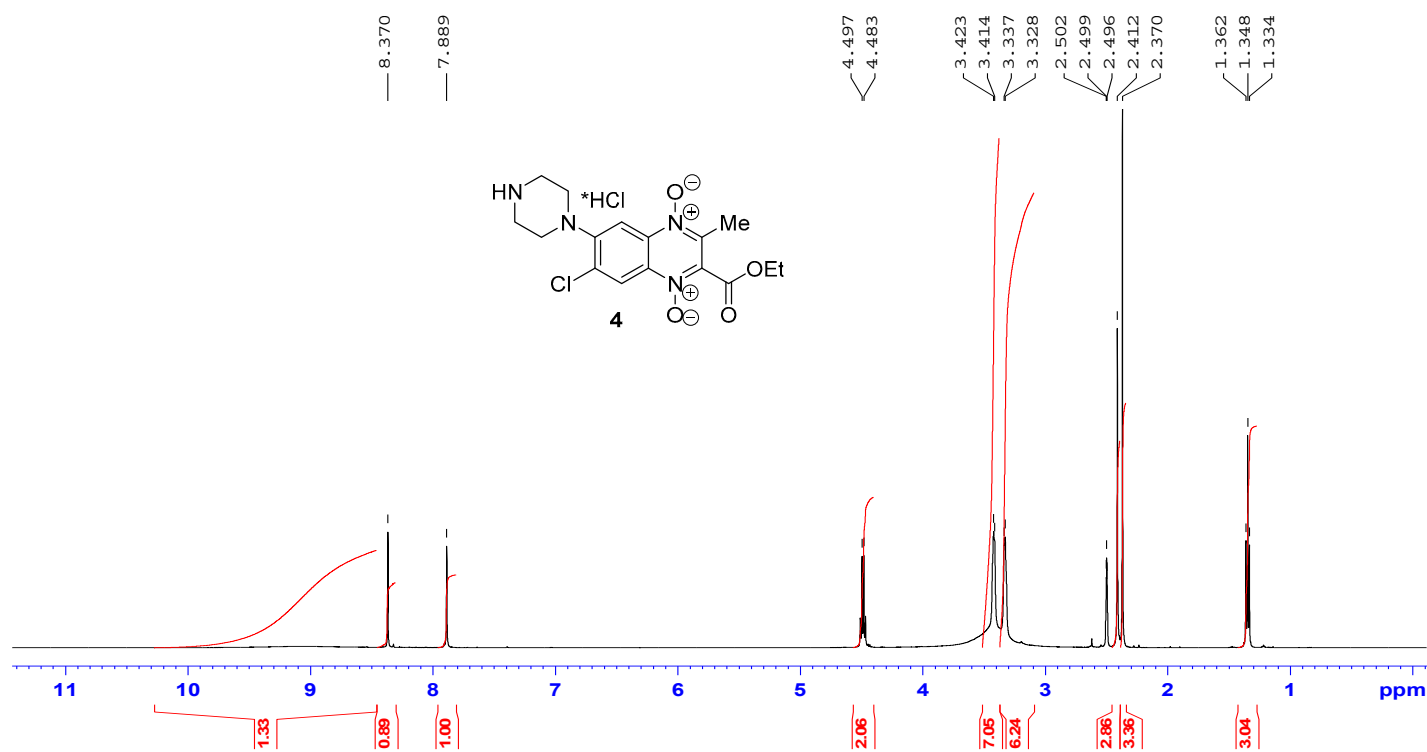


Figure S6. Copy of ^{13}C NMR spectrum of the derivative **4**.

BG-127 DMSO- d_6

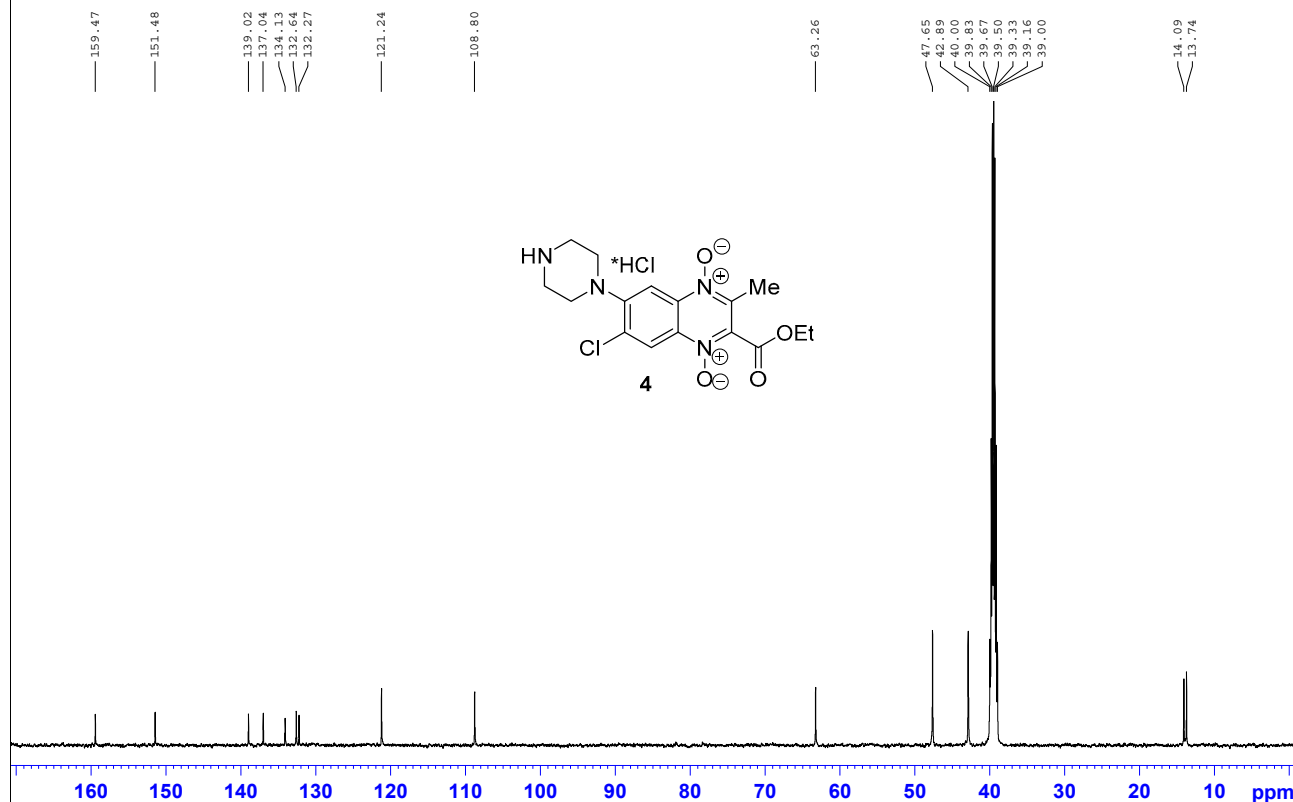


Figure S7. Copy of ^1H NMR spectrum of the derivative **5**.

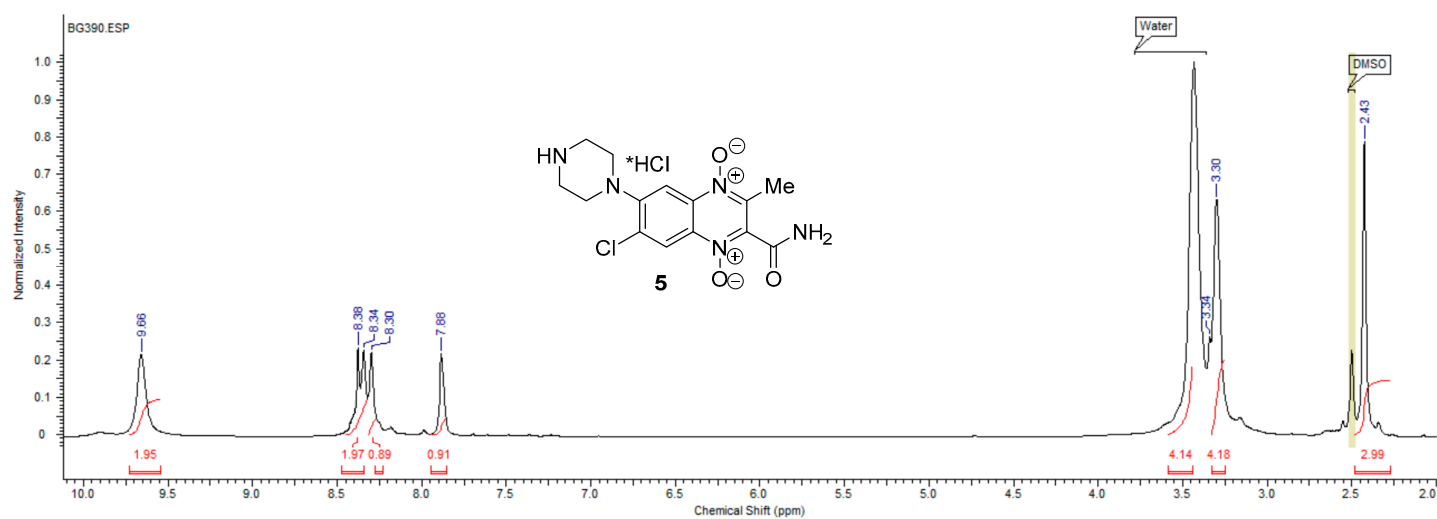


Figure S8. Copy of ^{13}C NMR spectrum of the derivative **5**.

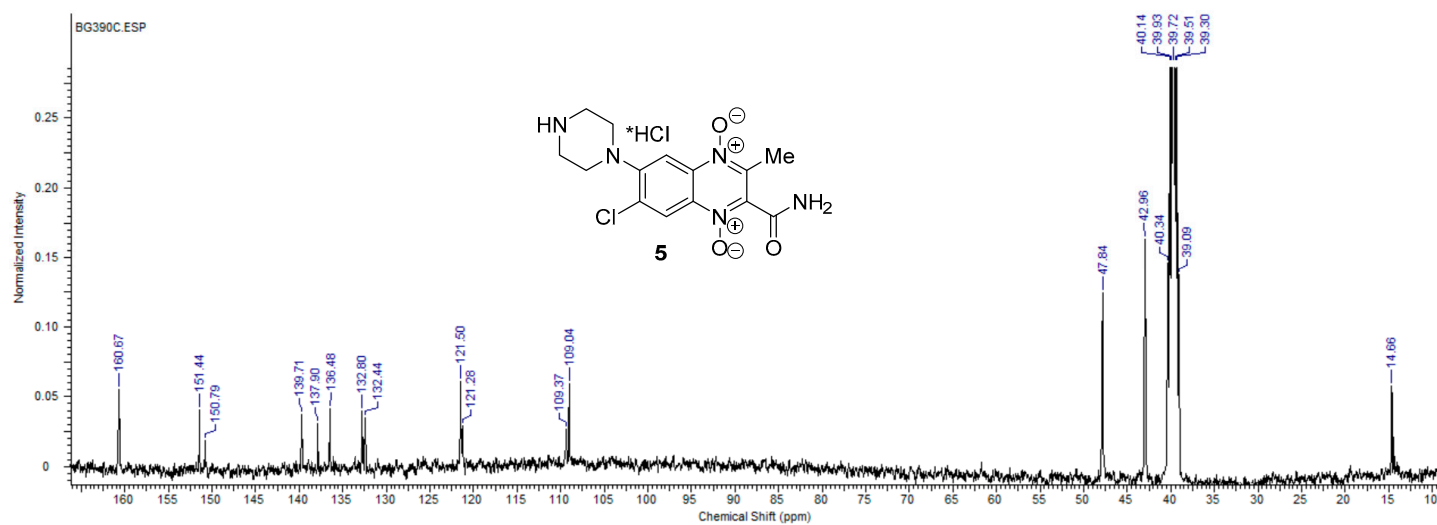


Figure S9. Copy of ^1H NMR spectrum of the derivative **6**.

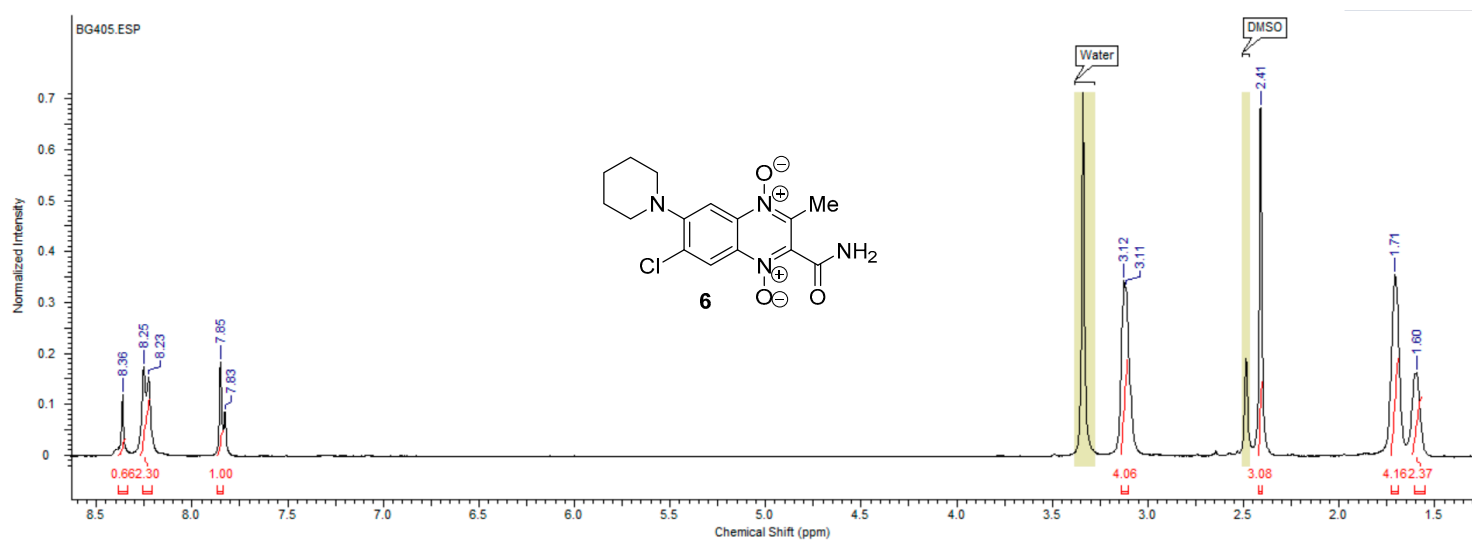


Figure S10. Copy of ^{13}C NMR spectrum of the derivative **6**.

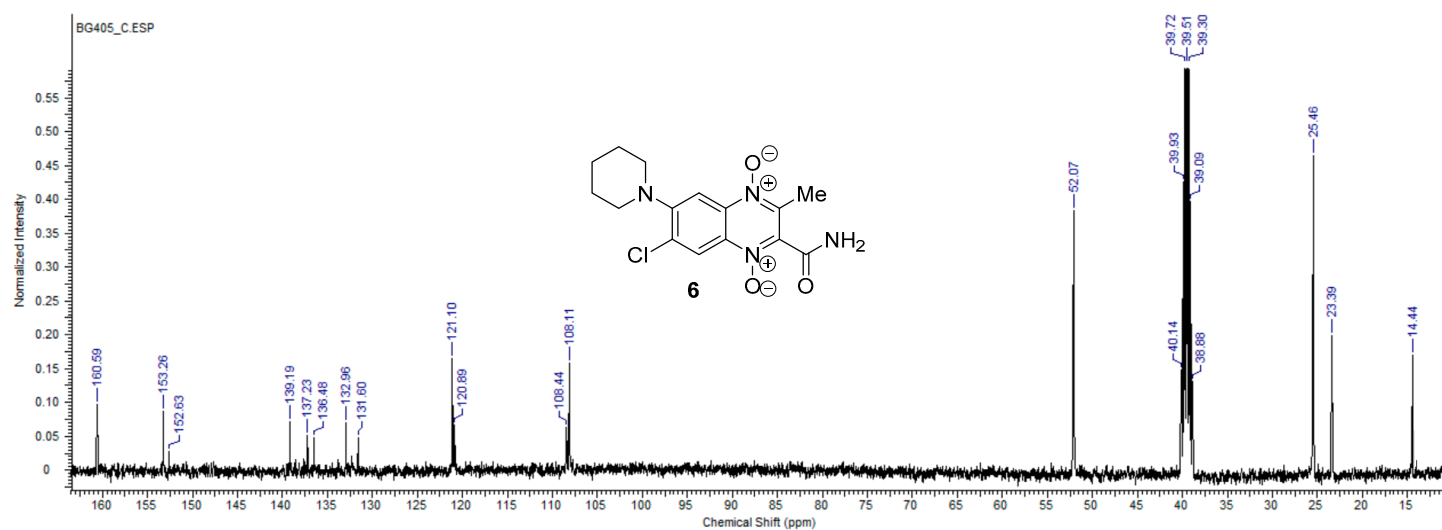


Figure S11. Copy of ^1H NMR spectrum of the derivative **7**.

BG-391 DMSO- d_6

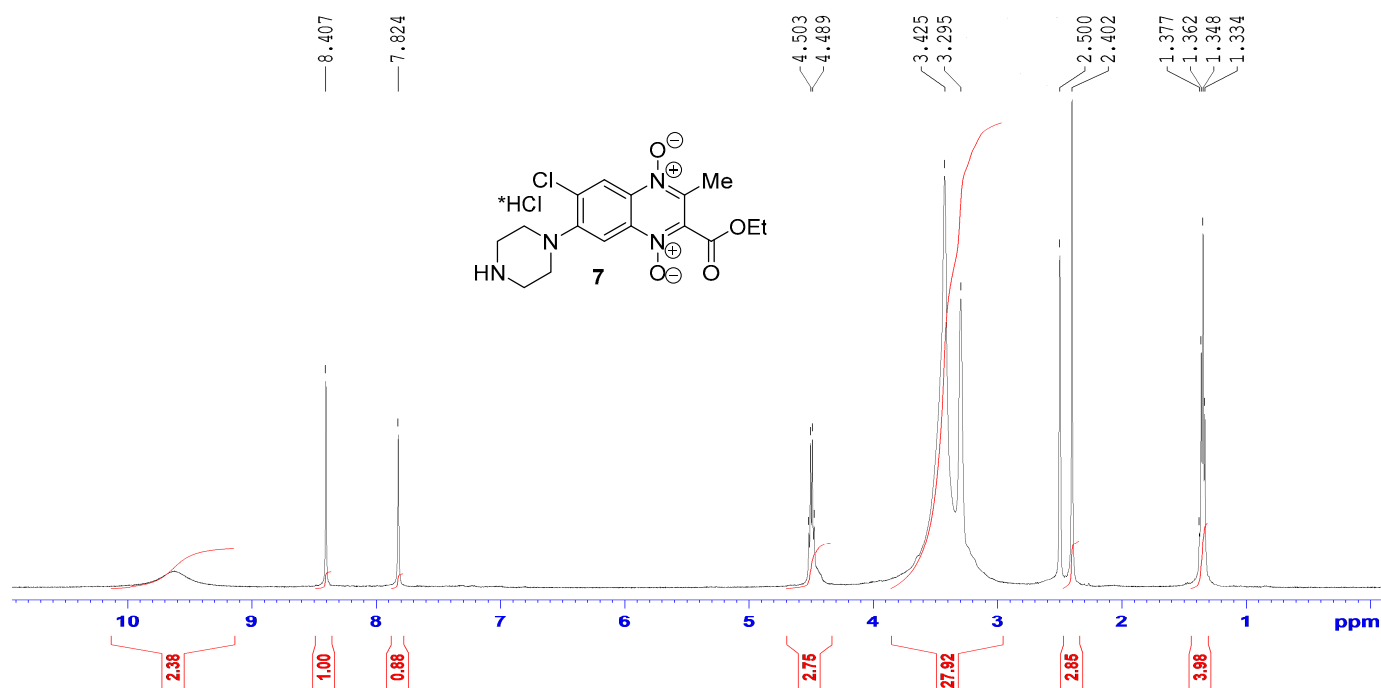


Figure S12. Copy of ^{13}C NMR spectrum of the derivative **7**.

BG-391 ^{13}C

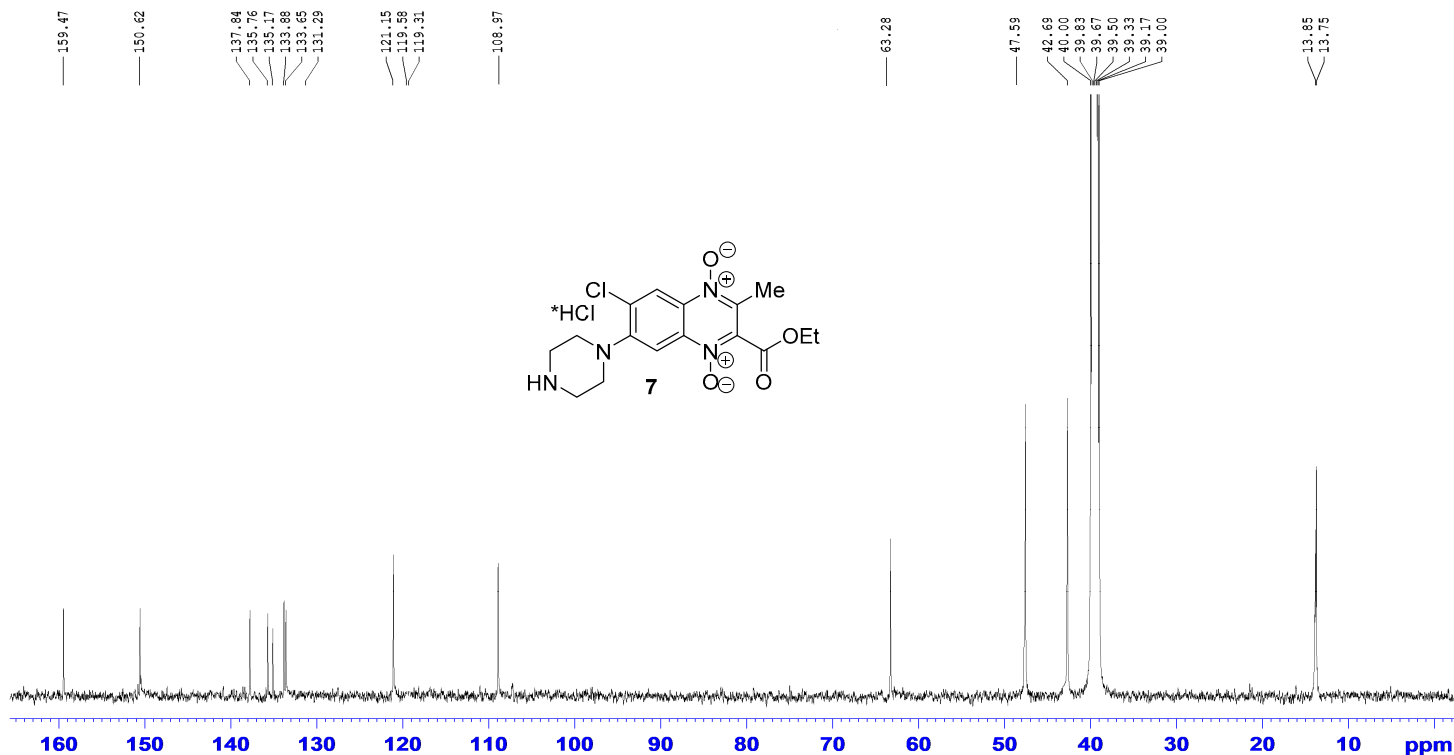


Figure S13. Copy of ^1H NMR spectrum of the derivative **8**.

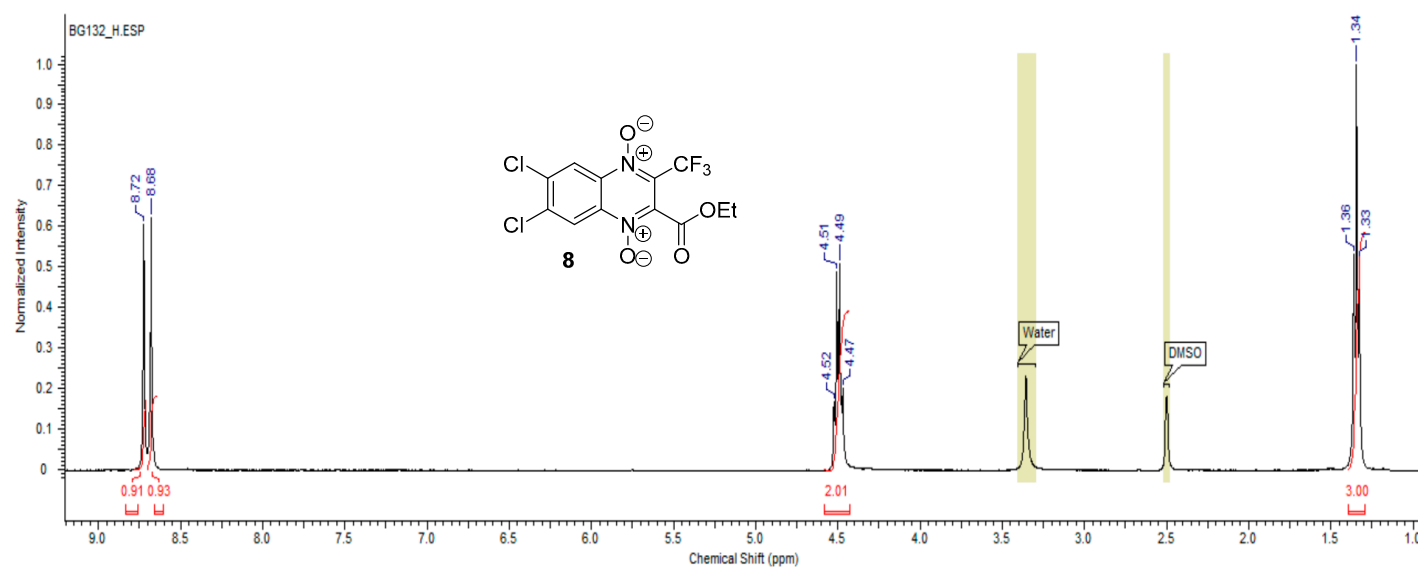


Figure S14. Copy of ^{13}C NMR spectrum of the derivative **8**.

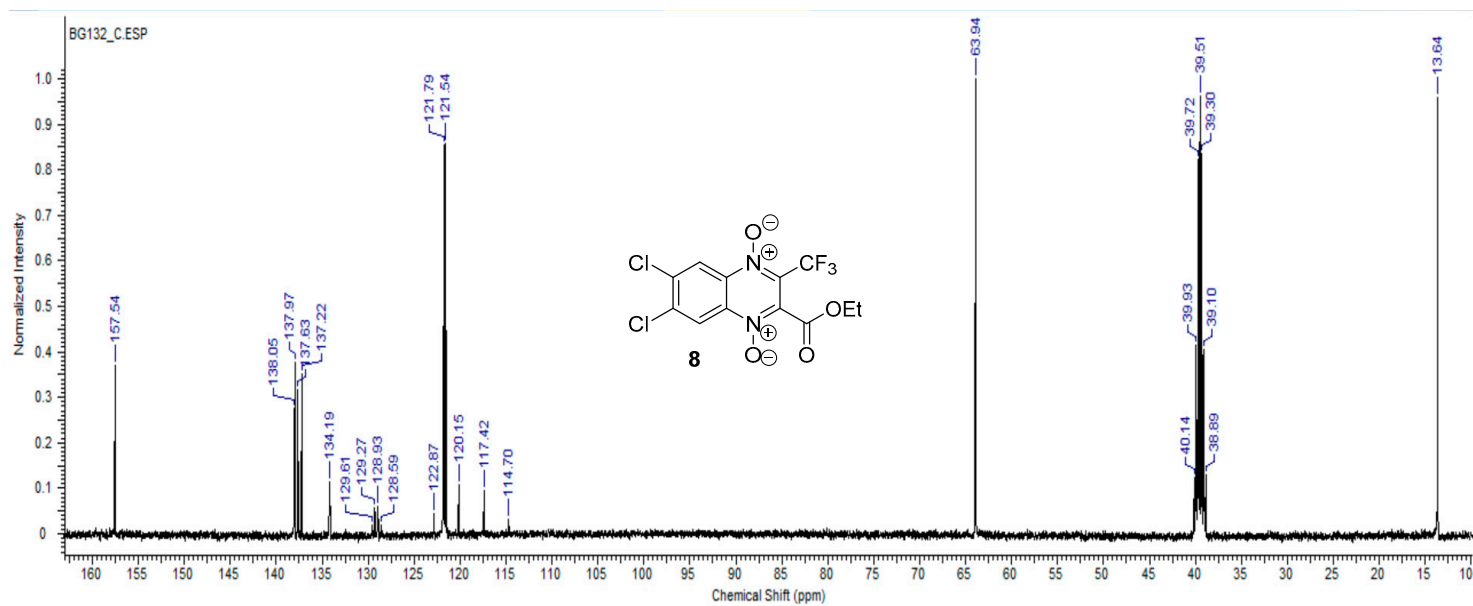


Figure S15. Copy of ^1H NMR spectrum of the 2-ethoxycarbonyl-3-methylquinoxaline 1,4-dioxide.

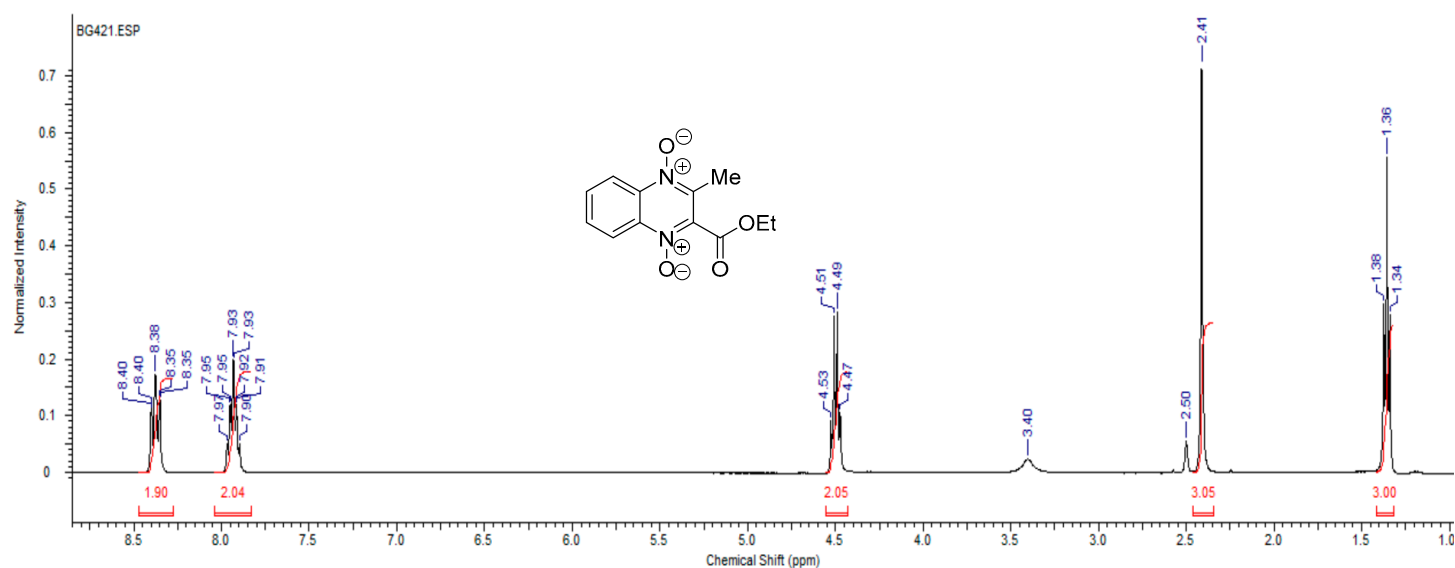
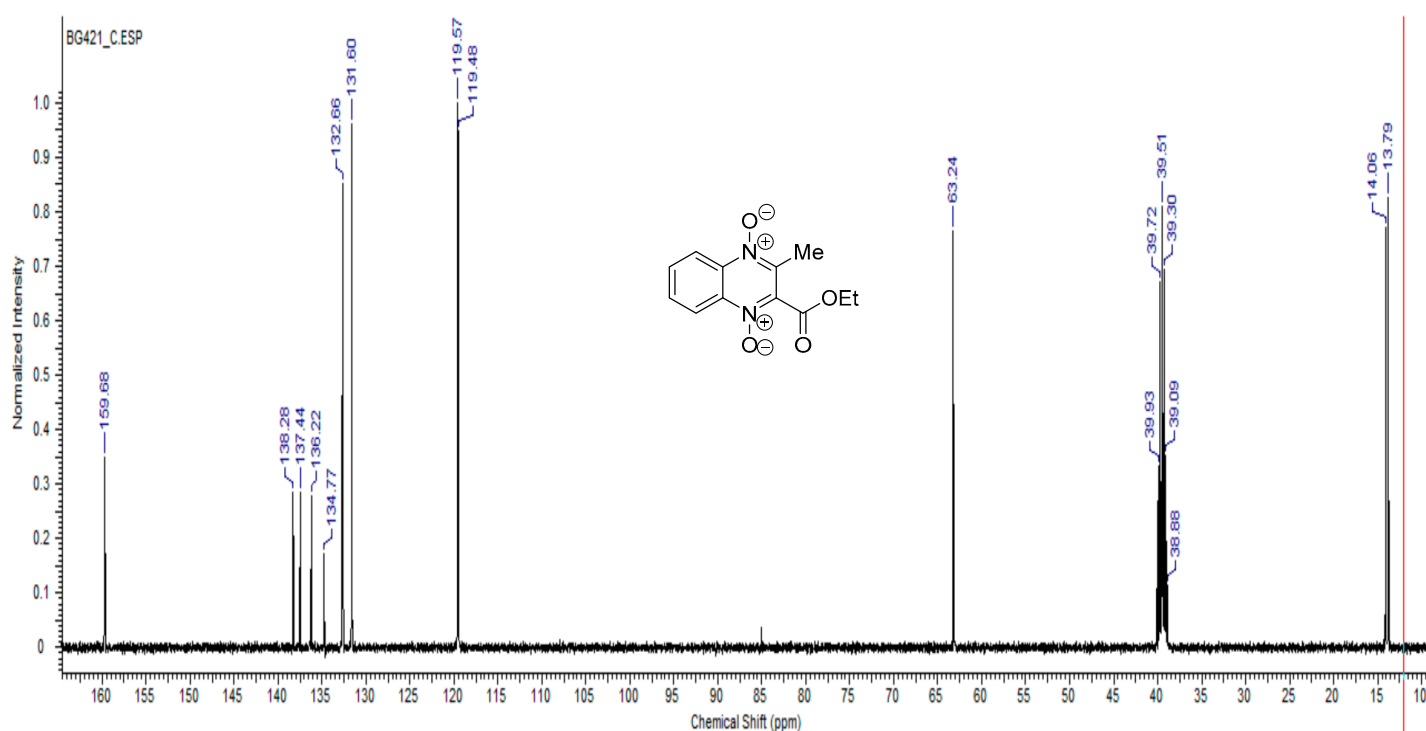
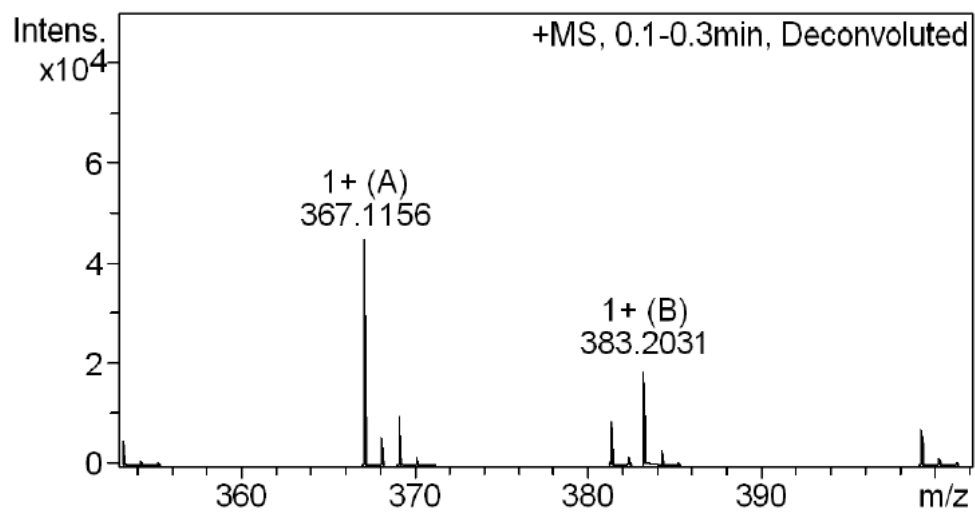


Figure S16. Copy of ^{13}C NMR spectrum of the derivative the 2-ethoxycarbonyl-3-methylquinoxaline 1,4-dioxide.



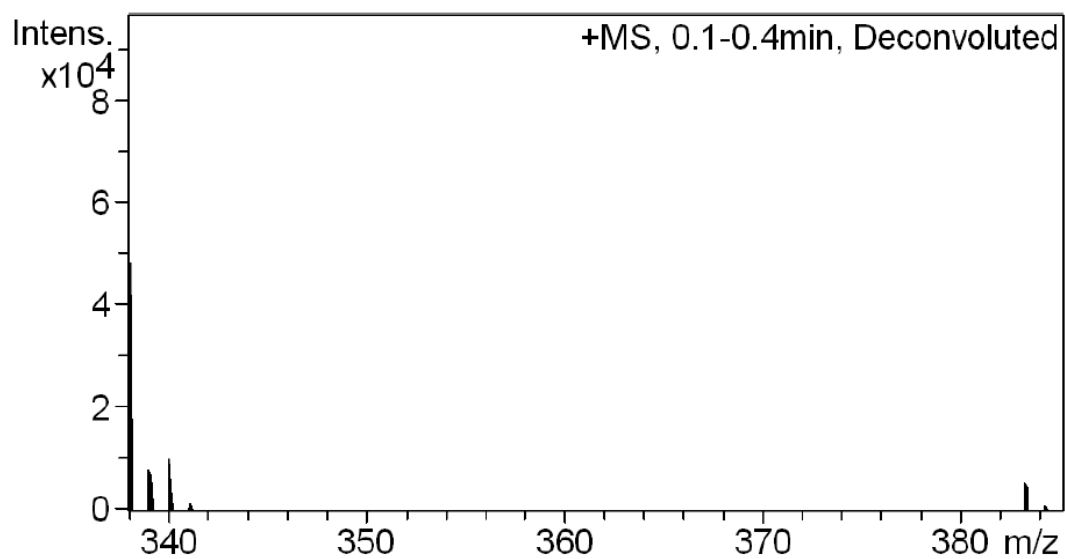
Copies of HRMS ESI Analysis

Figure S17. Copy of HRMS ESI analysis of the derivatives 4.



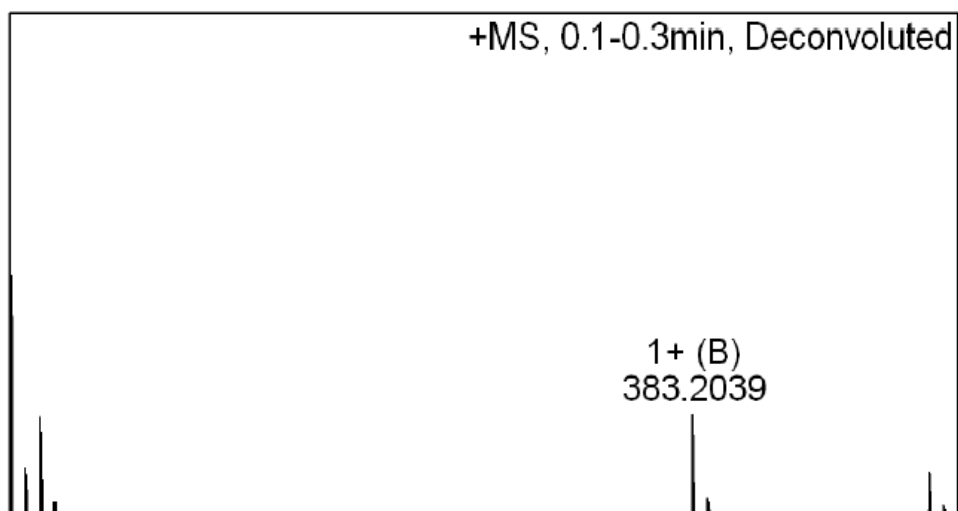
#	m/z	Res.	S/N	I	I %
1	353.2651			4980	10.9
2	367.1156			45857	100.0
3	369.1132			10487	22.9
4	381.2963			9106	19.9
5	383.2031			20309	44.3
6	399.1762			7620	16.6

Figure S18. Copy of HRMS ESI analysis of the derivatives **5**.



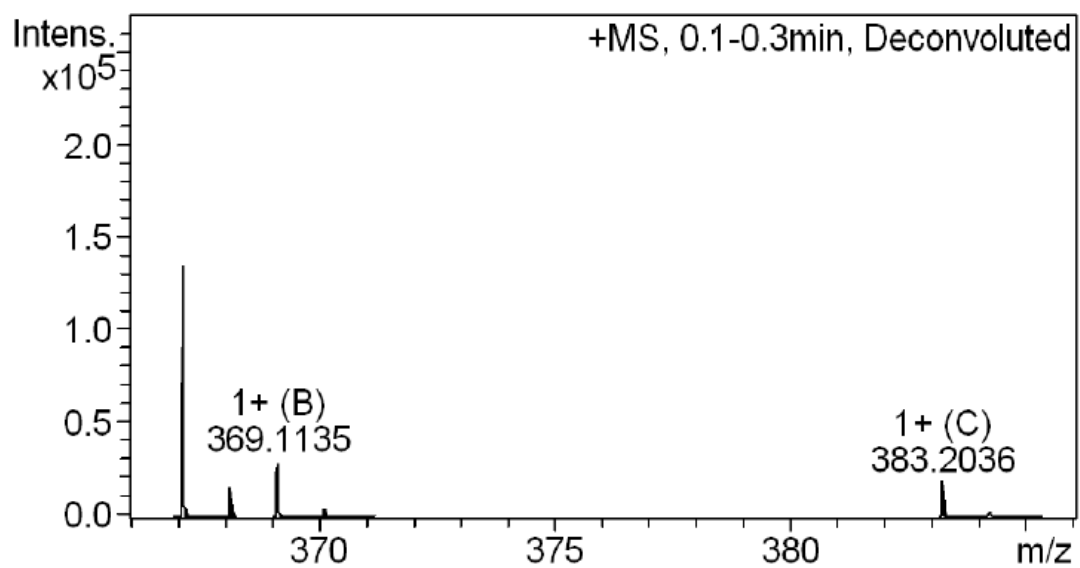
#	m/z	Res.	S/N	I	I %
1	338.1001			49185	100.0
2	340.0984			10435	21.2
3	383.2033			5443	11.1

Figure S19. Copy of HRMS ESI analysis of the derivatives **6**.



#	m/z	Res.	S/N	I	I %
1	337.1056			4991	100.0
2	339.1040			1938	38.8
3	383.2039			2001	40.1
4	399.1759			866	17.4

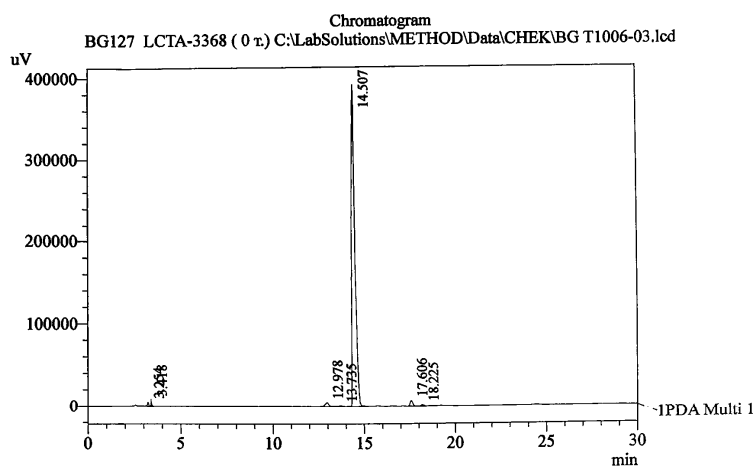
Figure S20. Copy of HRMS ESI analysis of the derivatives 7.



#	m/z	Res.	S/N	I	I %
1	367.1166			136969	100.0
2	369.1135			29731	21.7
3	383.2036			19119	14.0

Copies of HPLC Analysis

Figure S21. Copy HPLC analysis of the derivative 4.



1 PDA Multi 1 / 274nm 4nm

PDA Ch1 274nm 4nm

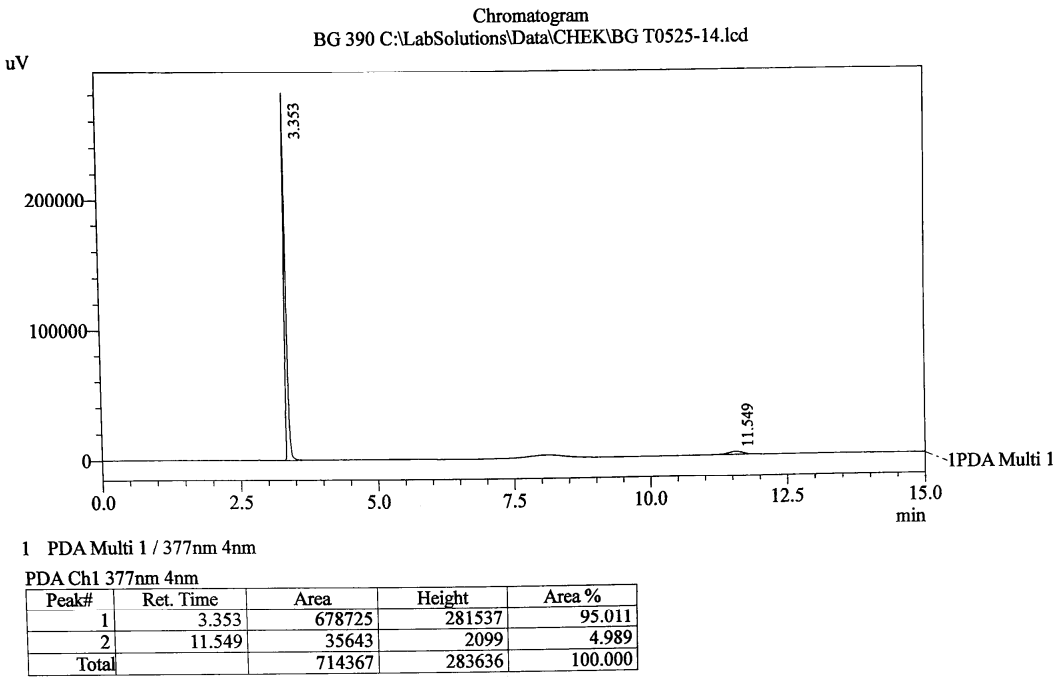
Peak#	Ret. Time	Area	Height	Area %
1	3.254	23293	4606	0.453
2	3.418	24715	8545	0.480
3	12.978	63092	4781	1.226
4	13.735	11958	1018	0.232
5	14.507	4937973	390981	95.948
6	17.606	68747	6733	1.336
7	18.225	16713	1648	0.325
Total		5146490	418312	100.000

Method Filename : FOS Cv.lcm 06.10.2023 14:12:28

Time	Unit	Command	Value
0.01	Pumps	B.Conc	10
30.00	Pumps	B.Conc	50
33.00	Pumps	B.Conc	10
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5µm. C-18, 4,6x250 mm. N 62511
Elution: A - H₃PO₄ 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 µl

Figure S22. Copy HPLC analysis of the derivative 5.

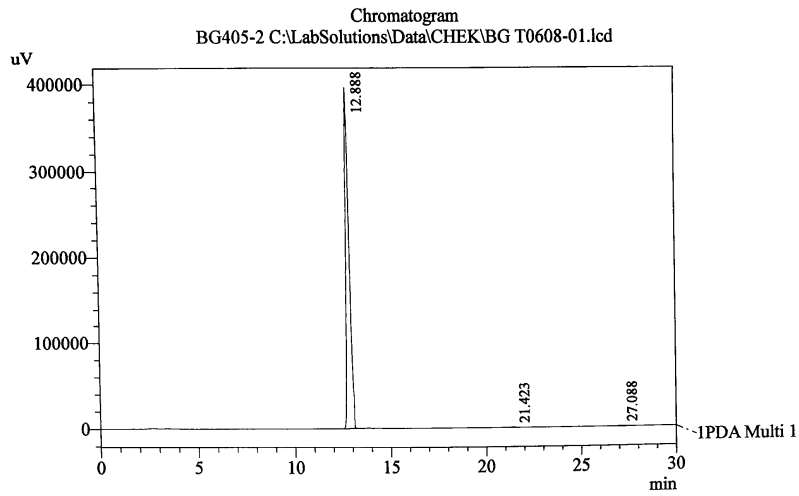


Method Filename : FRA02 vA.lcm 30.05.2023 13:58:19

Time	Unit	Command	Valu
0.01	Pumps	B.Conc	7
10.00	Pumps	B.Conc	7
30.00	Pumps	B.Conc	40
33.00	Pumps	B.Conc	7
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FRA 02 vA, Colon- Kromasil C-18, 4,6x250 mm. 5 mkm, N 59967
Elution: A - COOHNH4 0.2% pH 4.5; B - MeCN, fl - 1 ml/min, loop 20 mkl

Figure S23. Copy HPLC analysis of the derivative **6**.



PDA Ch1 375nm 4nm

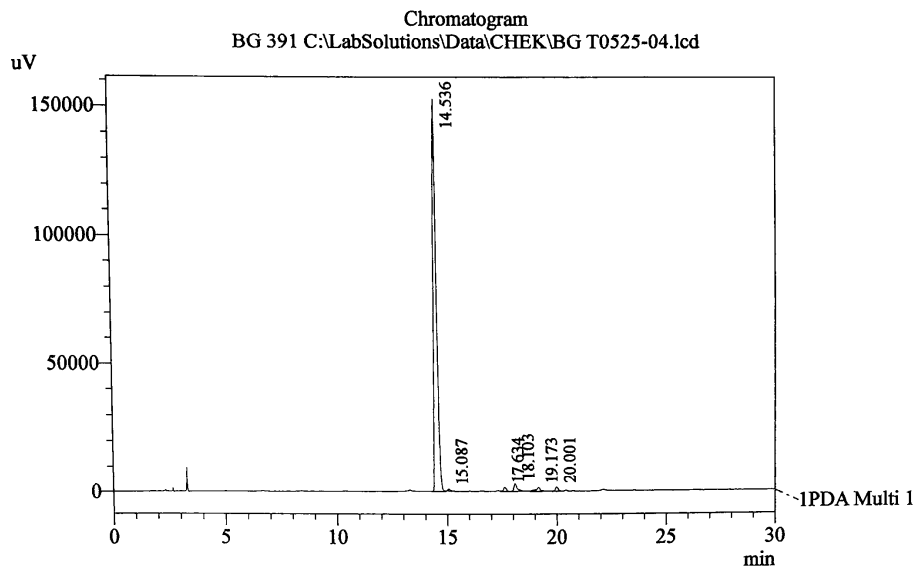
Peak#	Ret. Time	Area	Height	Area %
1	12.888	7646484	395884	99.746
2	21.423	10493	639	0.137
3	27.088	8982	528	0.117
Total		7665960	397051	100.000

Method Filename : FOS Av.lcm 08.06.2023 12:02:02

Time	Unit	Command	Valu
0.01	Pumps	B.Conc	30
30.00	Pumps	B.Conc	50
35.00	Pumps	B.Conc	30
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl

Figure S24. Copy HPLC analysis of the derivative 7.



1 PDA Multi 1 / 370nm 4nm

PDA Ch1 370nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	14.536	1563763	152604	94.708
2	15.087	6165	769	0.373
3	17.634	14574	1585	0.883
4	18.103	30405	2944	1.841
5	19.173	20295	1489	1.229
6	20.001	15942	1686	0.966
Total		1651144	161077	100.000

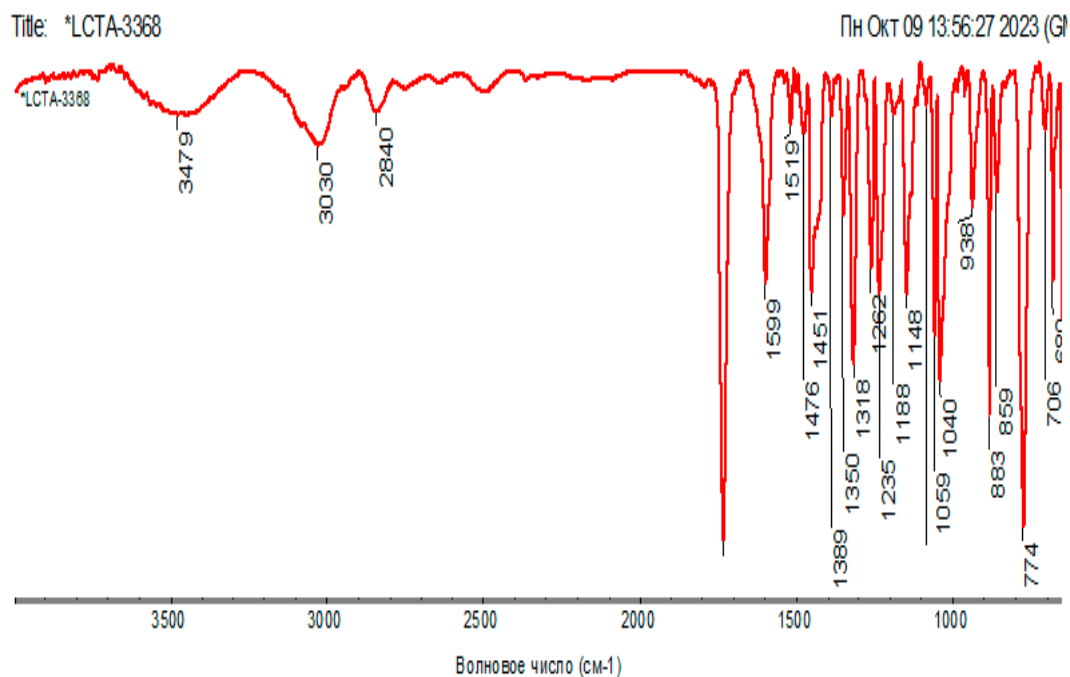
Method Filename : FOS Av.lcm 26.05.2023 12:25:18

Time	Unit	Command	Valu
0.01	Pumps	B.Conc	10
30.00	Pumps	B.Conc	50
35.00	Pumps	B.Conc	10
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5mkm. C-18, 4,6x250 mm. N 62511
Elution: A - H3PO4 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 mkl

Copies of IR Spectra

Figure S25. Copy of IR spectrum of the derivative **4**.



Expanded fingerprint region:

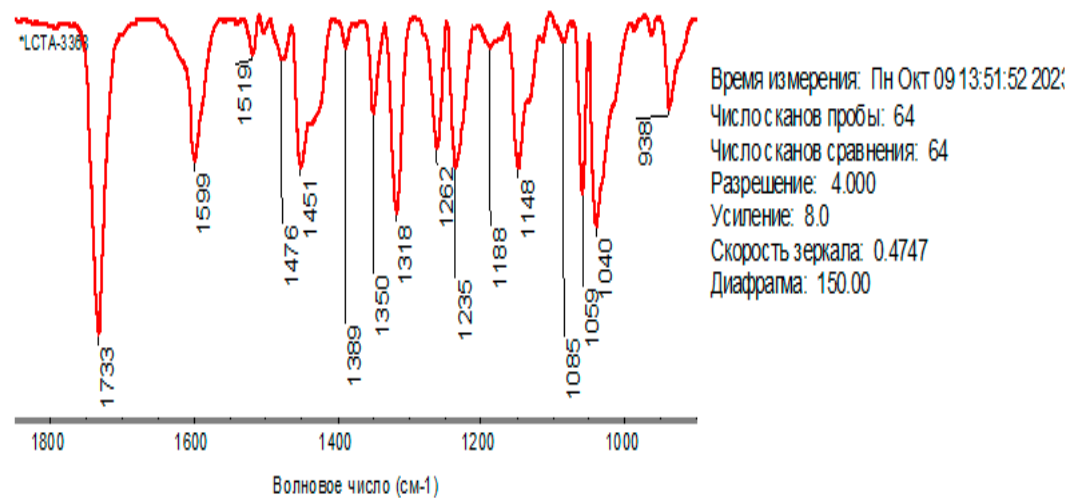
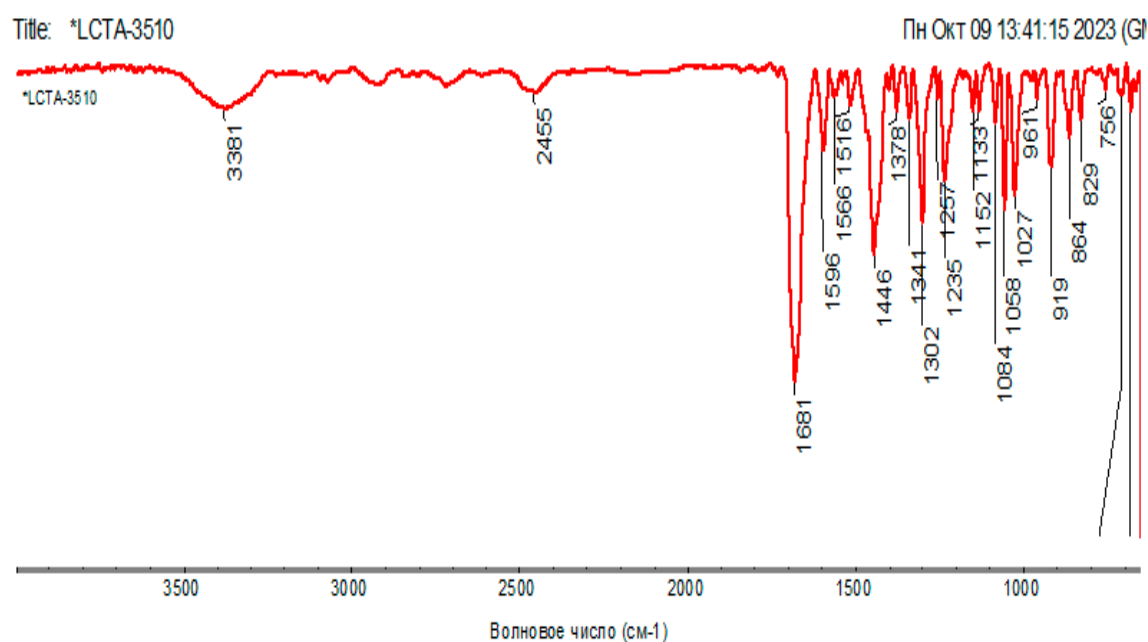


Figure S26. Copy of IR spectrum of the derivative **5**.



Expanded fingerprint region:

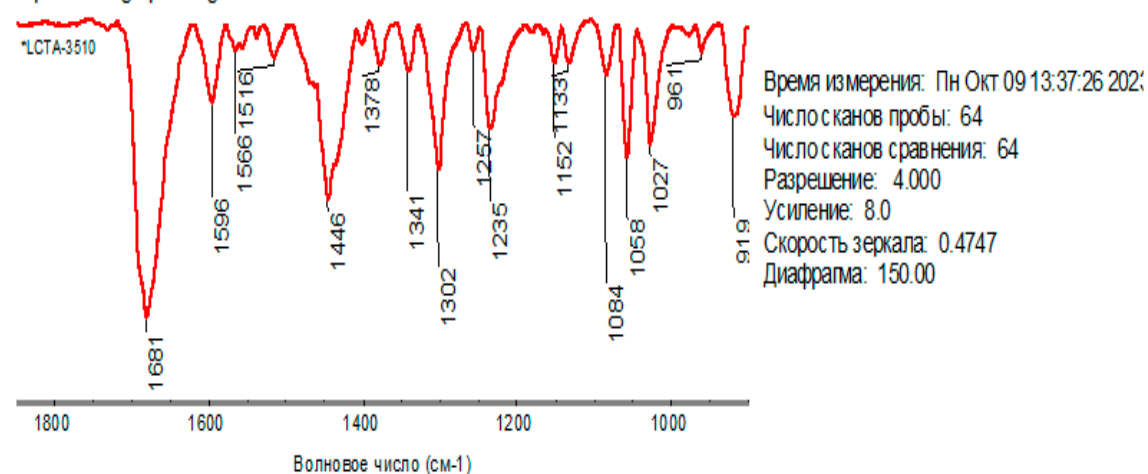


Figure S27. Copy of IR spectrum of the derivative **6**.

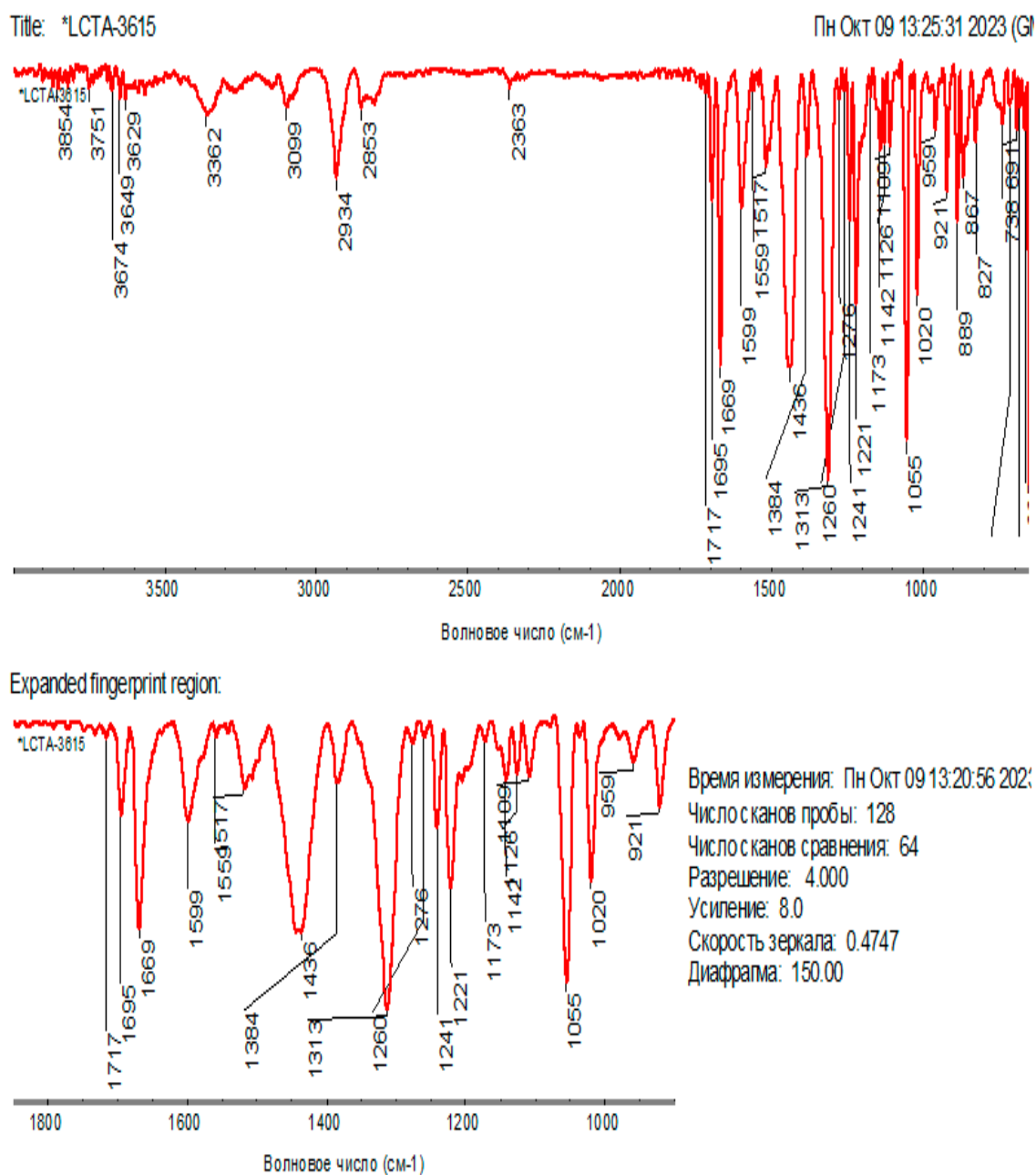
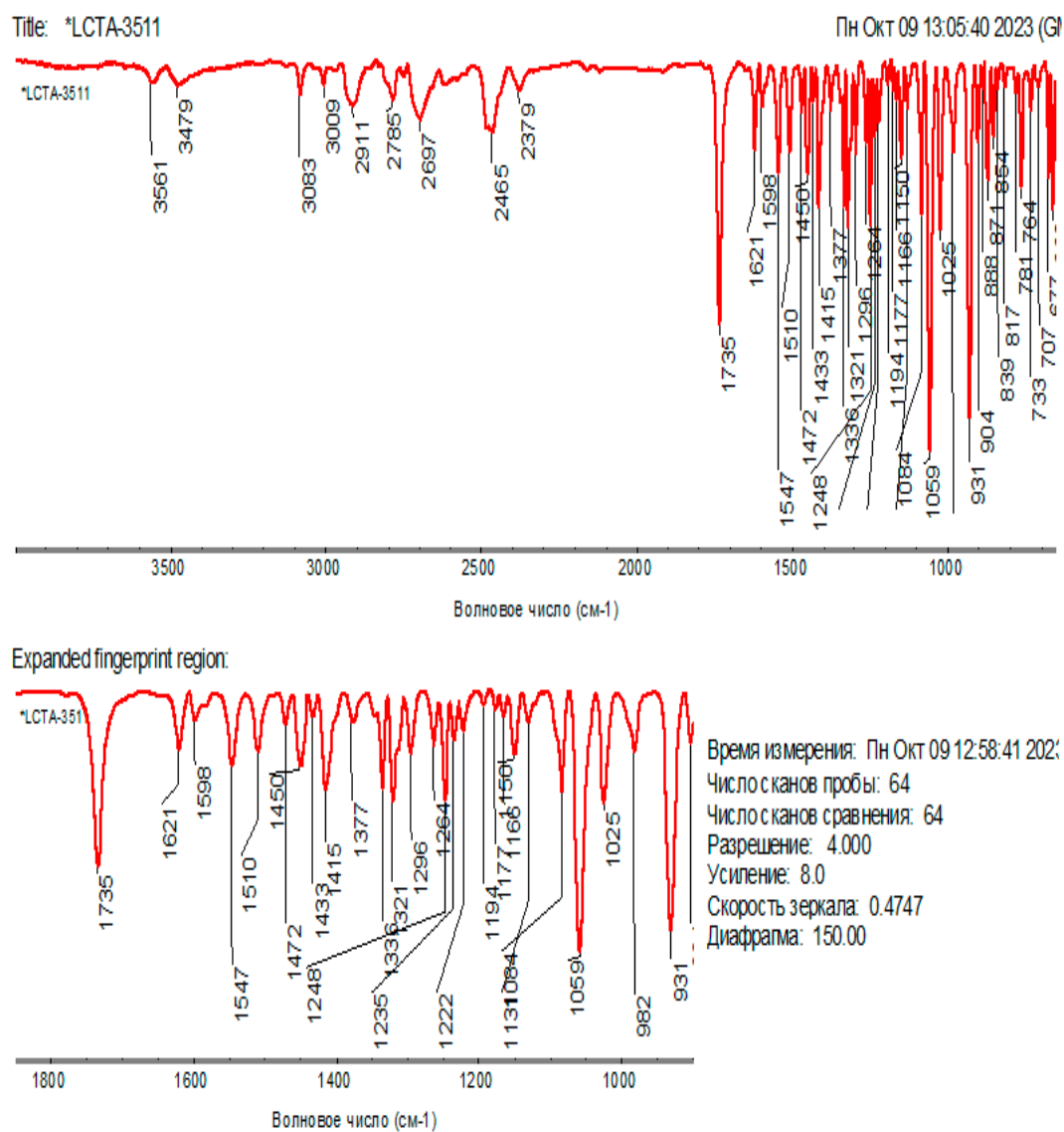


Figure S28. Copy of IR spectrum of the derivative 7.



Copies of 2D NMR Spectra of 4 and 7.

Figure S29. ^1H - ^{13}C HSQC spectrum for compound 4.

HSQC DMSO

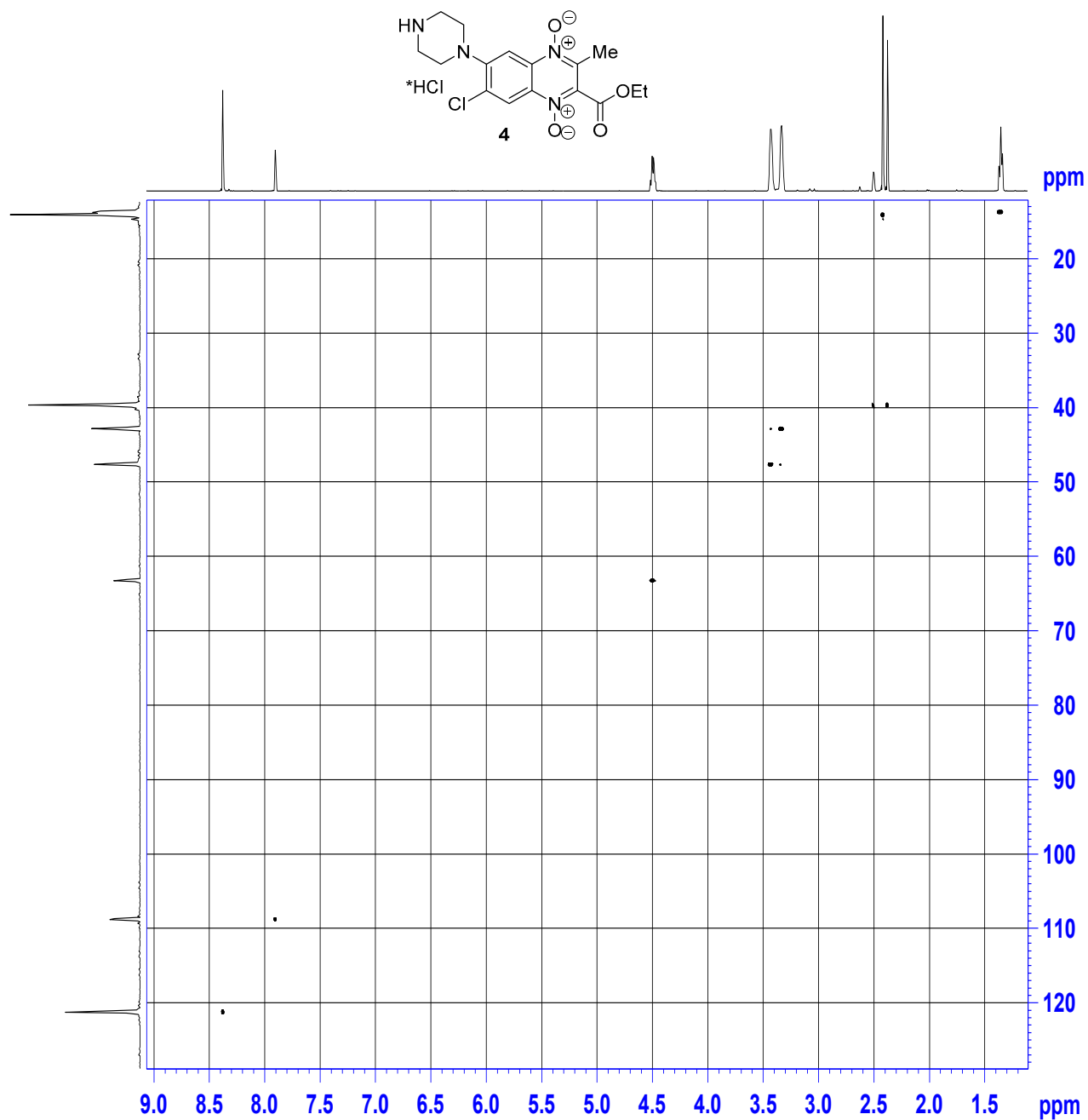


Figure S30. HMBC spectrum for compound **4**.

BG-127 DMSO-d₆ HMBC

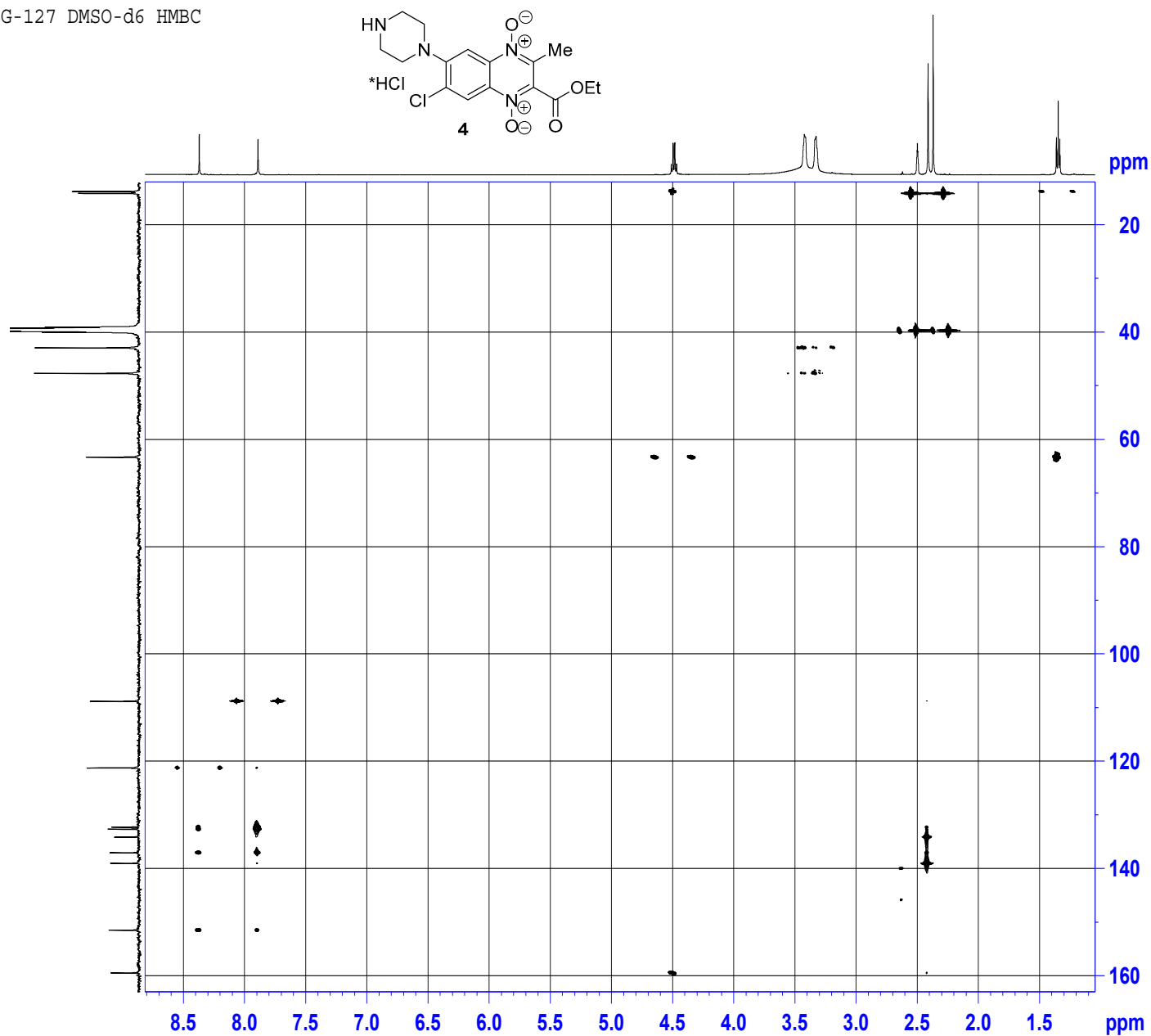


Figure S31. HMBC spectrum (fragment) for compound **4**.

BG-127 DMSO-d6 HMBC

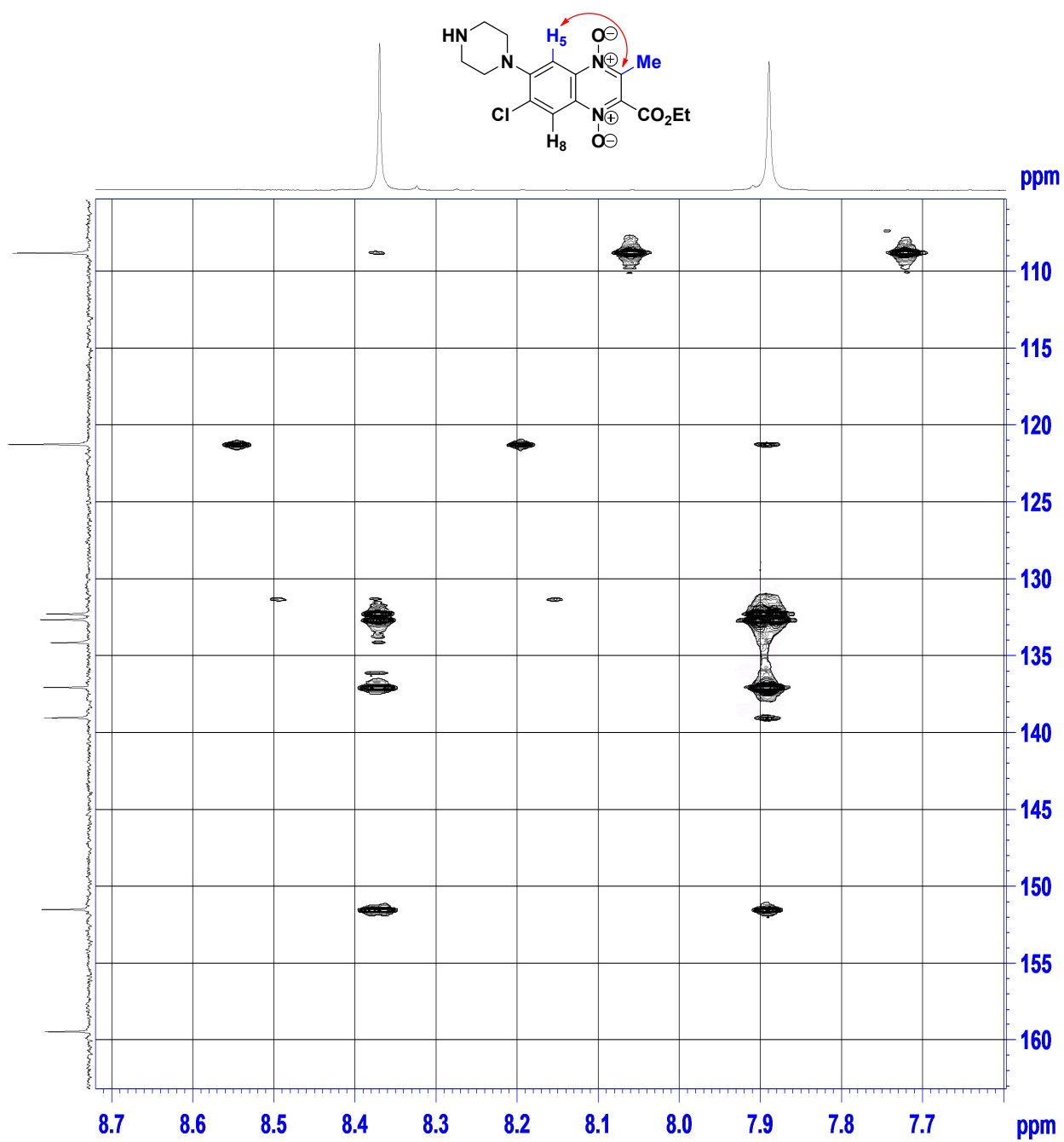


Figure S32. ^1H 2D NOESY spectrum of compound **4** in $\text{DMSO-}d_6$ at 500 MHz.

BG-121, NOESY, Tm=500m

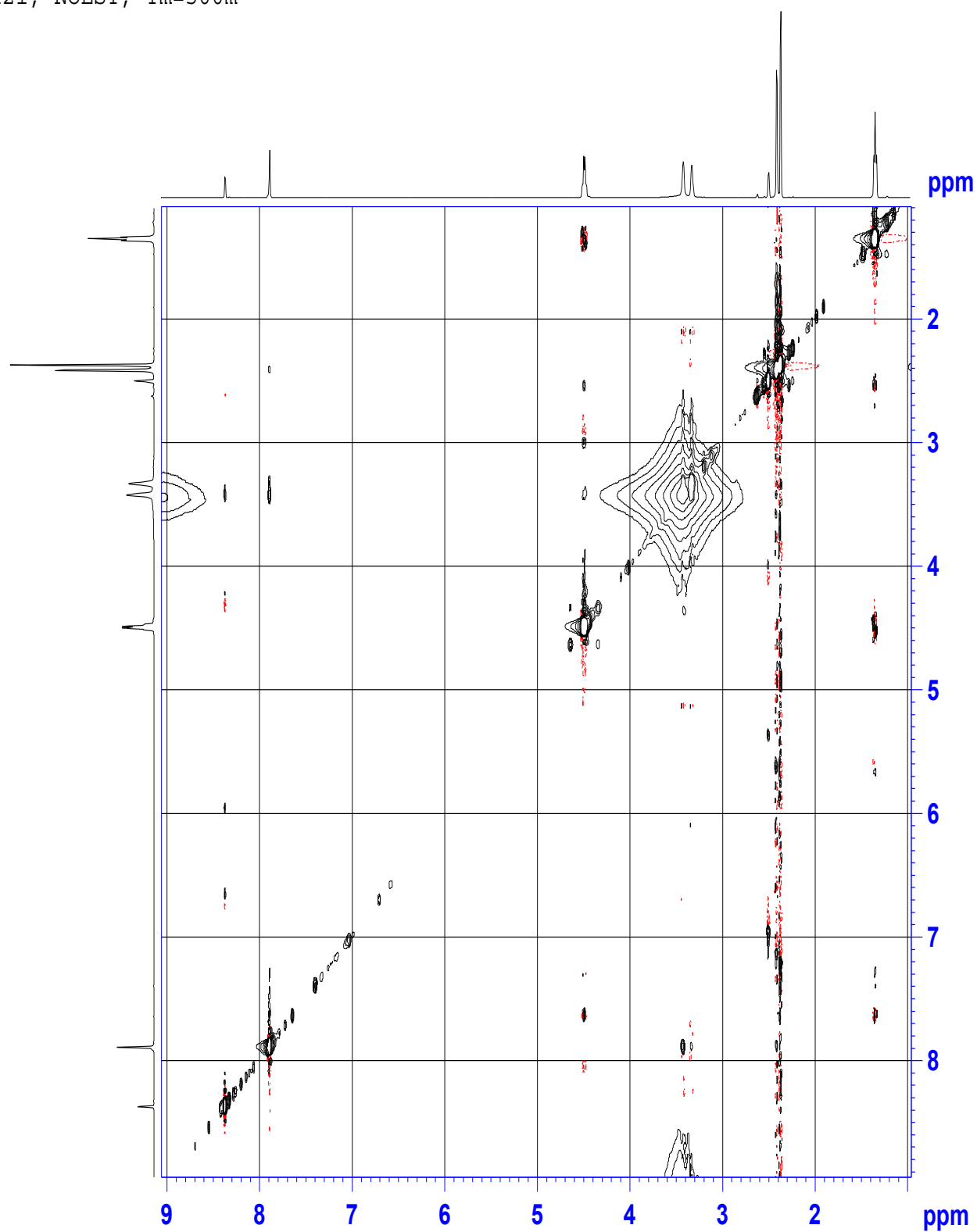


Figure S33. Selective NOE spectrum at CH₃ at 2.402 ppm for compound **4**.

BG-127 DMSO-d₆ Selective NOESY from CH₃- (3)

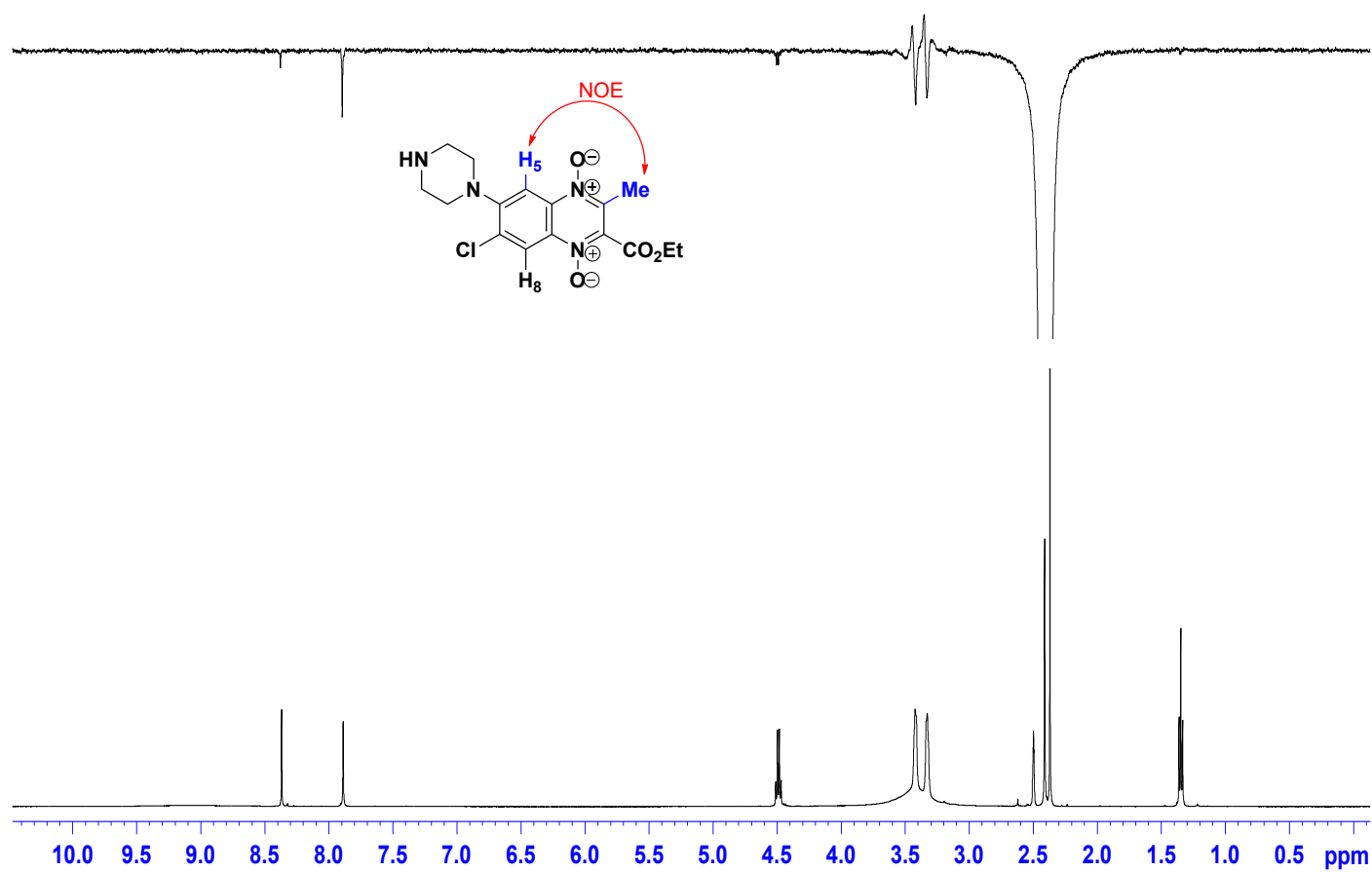


Figure S34. ^1H - ^{13}C HSQC spectrum for compound **7**.

BG-391 DMSO- d_6 HSQC

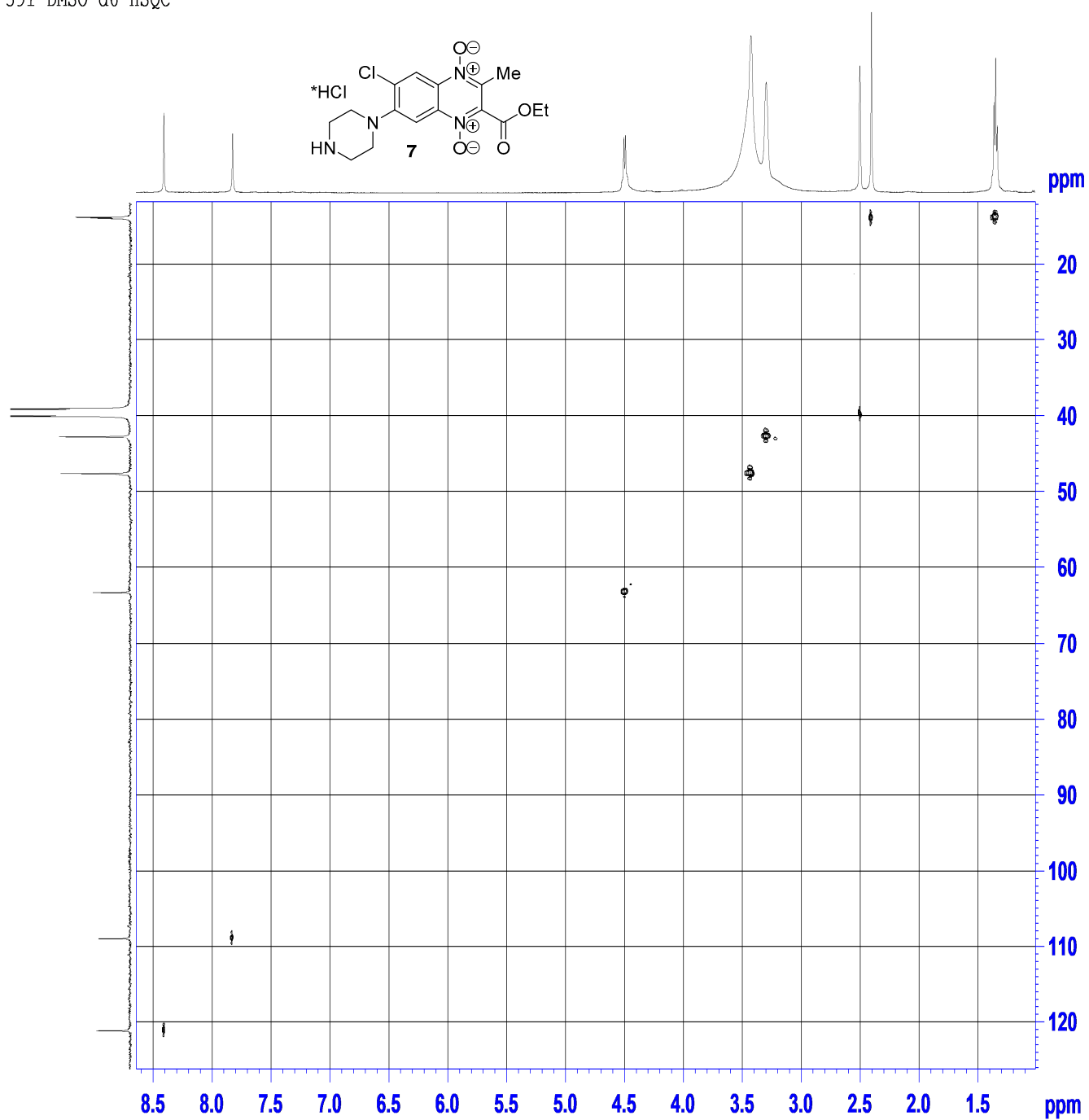


Figure S35. HMBC spectrum for compound **7**.

BG-391 DMSO-d6 HMBC

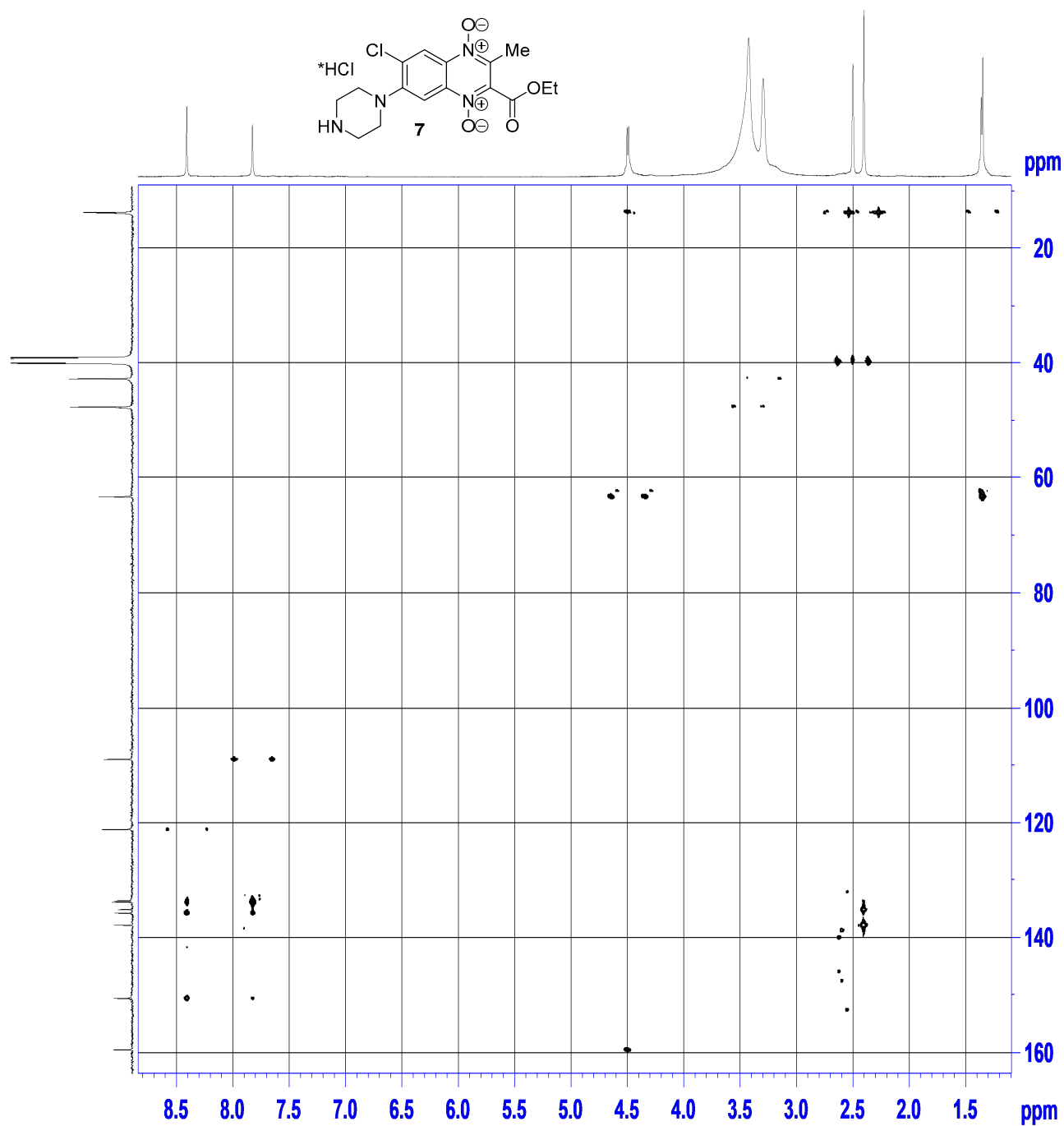


Figure S36. HMBC spectrum (fragment) for compound 7.

BG-391 DMSO-d6 HMBC

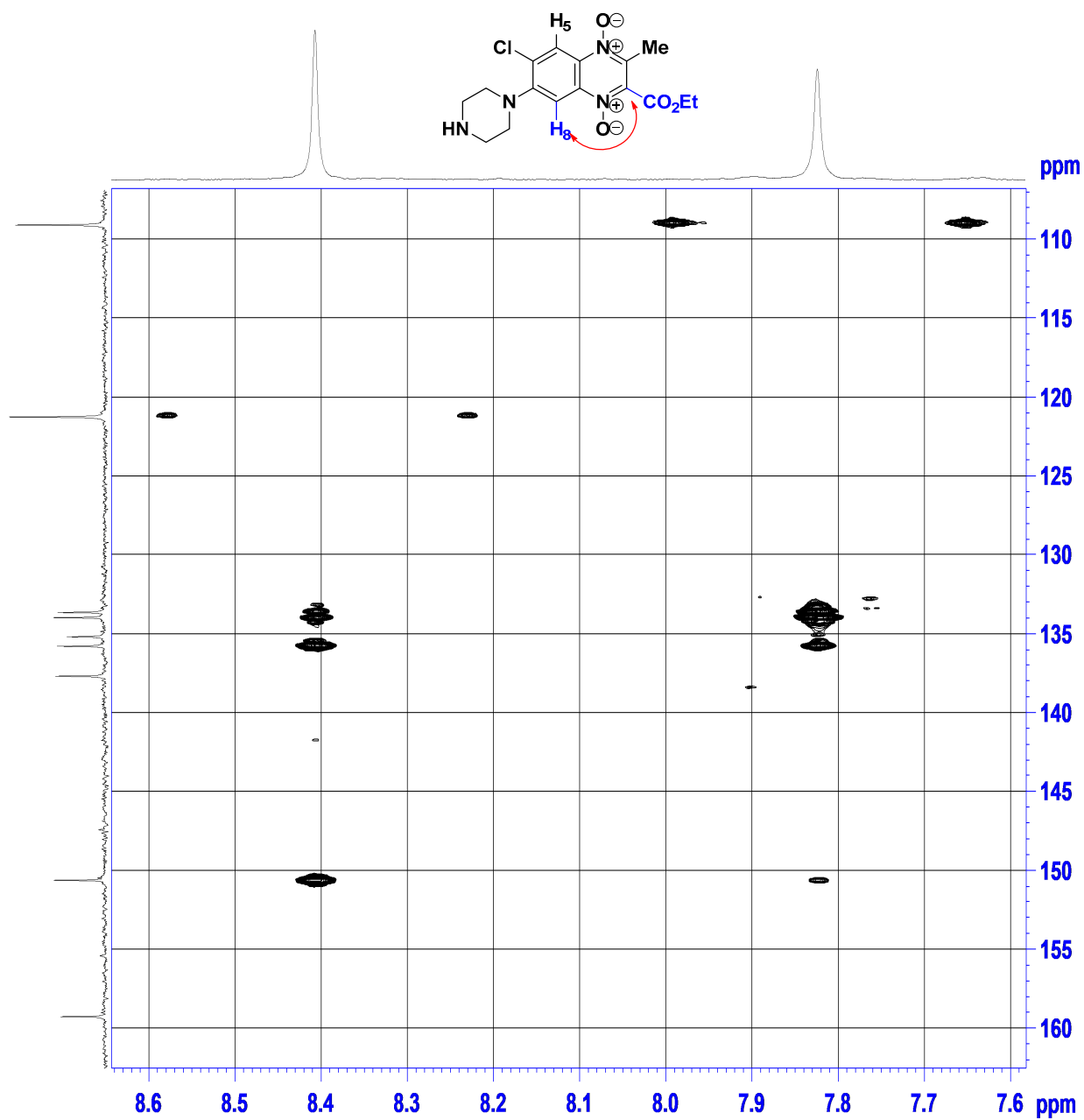


Figure S37. ^1H 2D NOESY spectrum of compound **7** in $\text{DMSO-}d_6$ at 500 MHz.

BG-391 DMSO- d_6 NOESY, $T_m=400\text{m}$

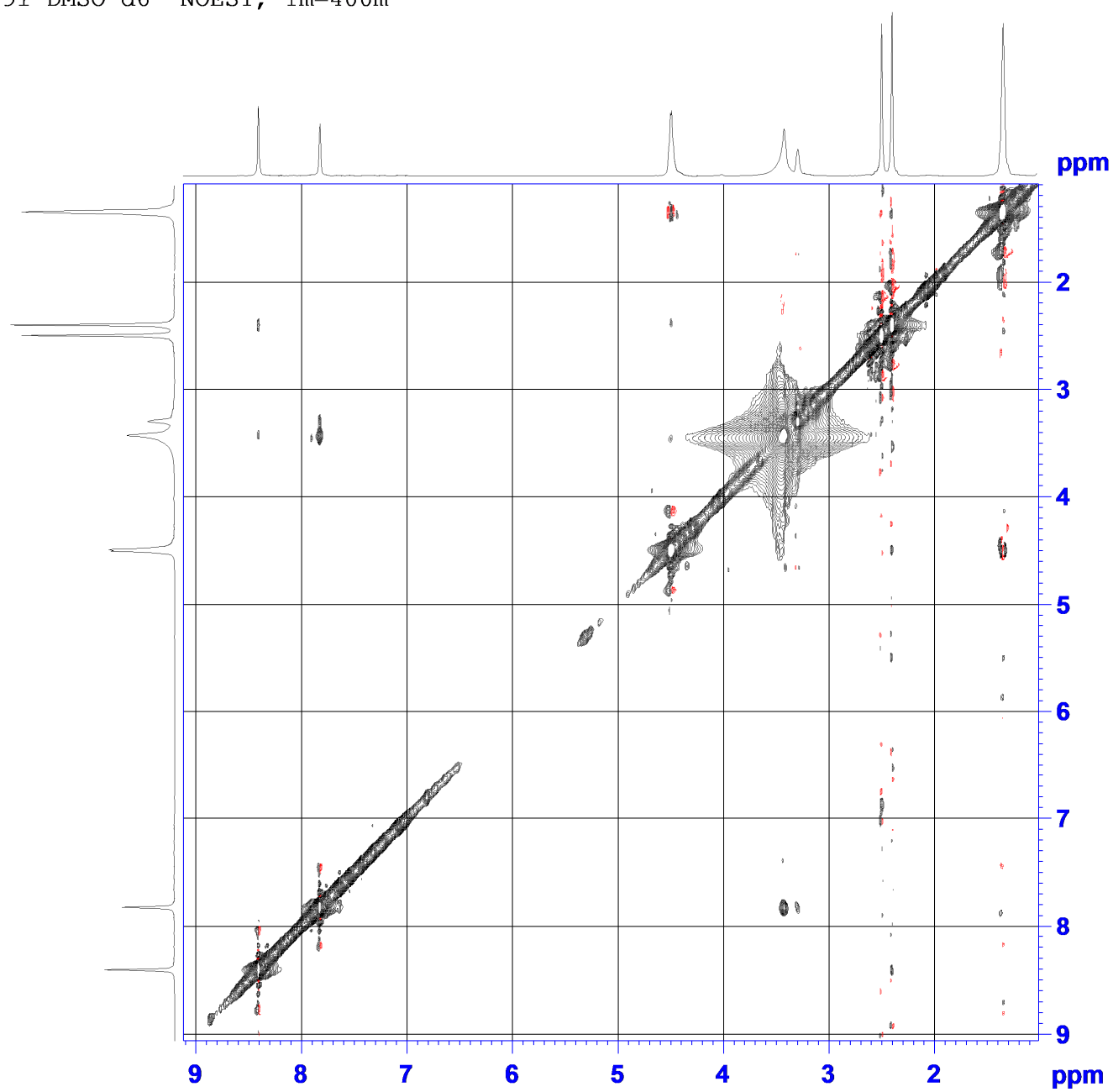


Figure S38. Selective NOE spectrum at CH₃ at 2.402 ppm for compound 7.

BG-391 DMSO-d₆ Te=25°C Sel. NOE at CH₃ at 2.402 ppm

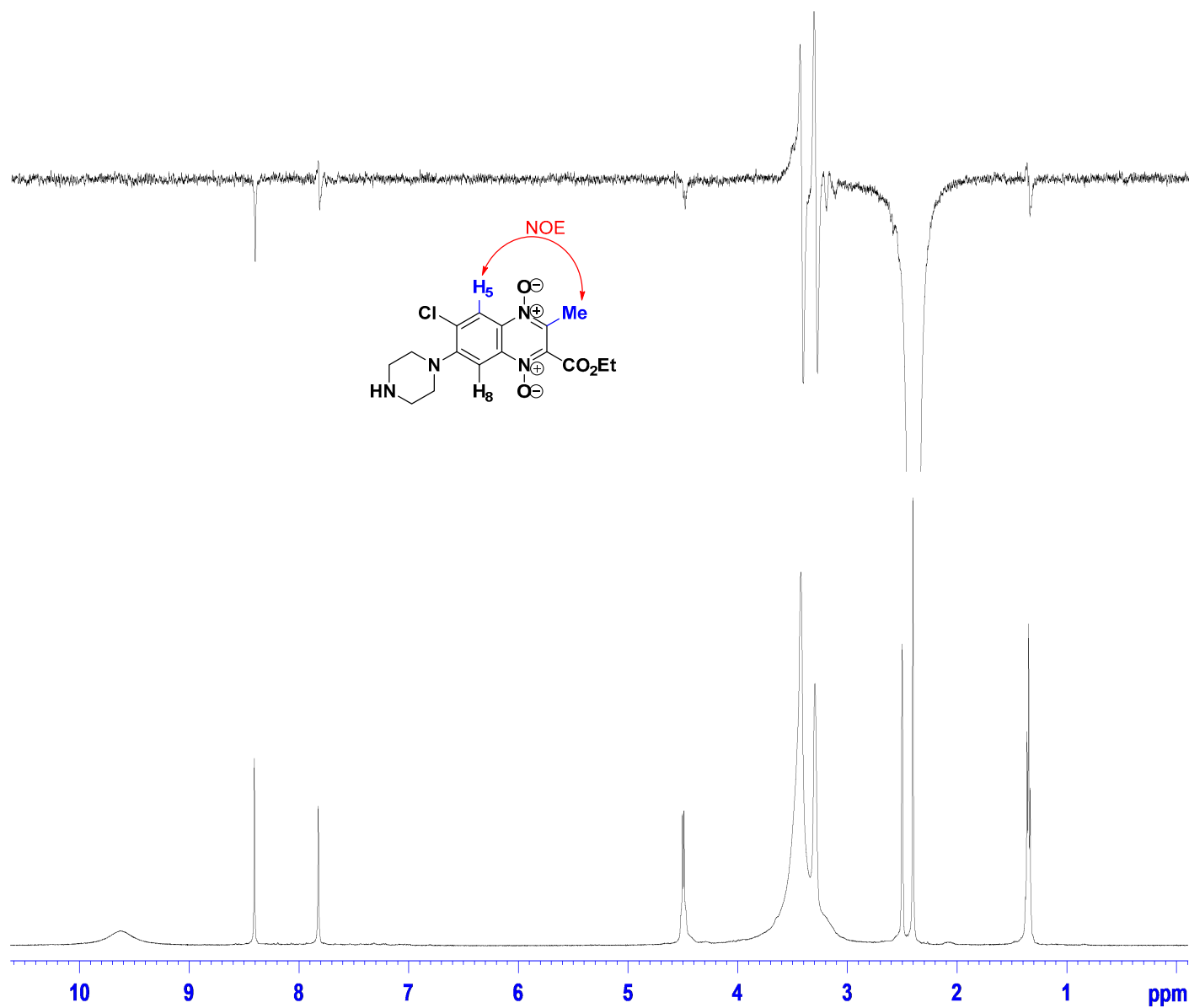


Table S1. ^{13}C chemical shifts (δ_{C} , ppm) and characteristic increments (I^{C}) for the ^{13}C chemical shift differences (relative to 2-ethoxycarbonyl-3-methylquinoxaline 1,4-dioxide) for the piperazine group for regioisomers **4** and **7**.

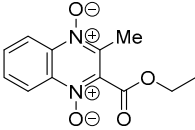
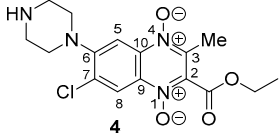
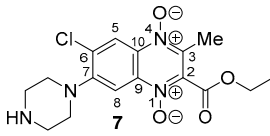
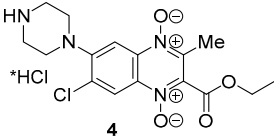
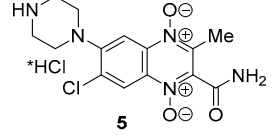
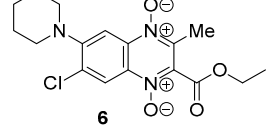
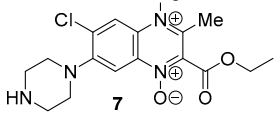
Position			I^{C}		I^{C}
	δ_{C}	δ_{C}		δ_{C}	
C-2	134.8	134.1	−0.7	135.2	+0.4
C-3	138.3	139.0	+0.7	137.8	−0.5
C-9	137.4	132.3	−5.1	135.8	−1.6
C-10	136.2	137.0	+0.8	133.7	−2.5

Table S2. Stability of aqueous solutions of derivatives **4-7** after 7 days storage at 37 °C.

Compound	HPLC analysis (purity, %)	
	0 day	7 day
 4	95.9	94.7
 5	95.0	24.9
 6	99.7	97.6
 7	94.7	84.9

>MSMEG_4883
 ATGAGCATATCGCTGCTGCTCGAGATGGCATCGTCGGGAGATCCCGACCGCACCGCGGTGGTTTCCGACG
 ACACCCGGCTCACCAGGCGAGTTGAGCACATTGGCCGACGGGGCAGCAGGCGTCATCGCCGGGTCAGG
 CGCGGCACACGTGCCTACGTGGGTACCGGTGGCG**CGCTGCTGCCGCTGCTGCT**GTTTCGCCTCGGCACGC
 GCGGCGATCCCCTTCACCCCCCTGAACTACCGTCTCAGCGCCGAAGGTCTGCGCGAGCTGGTCGACCGGT
 TGCCACACCGCTGGTGATCGCCGACGGCGAGTACGCCGGCATGCTCGCCGGAGCGGGCAGGCCGGTGCT
 CACCTCCGAGGAGTTCCTGTCCCAGGCCCCGACGGCCGATCCGGCCGCAGAGTTCGCCGACCCCGACGCG
 GTCGCGGTGGTGCTGTTACCTCGGGCACCACATCGCGCCCCAAGGCCGTGAACTCACCCACAACAACC
 TCACGAGCTACATCACCGGGACCGTCGAATTCGGTTCGGCCGCACCGGAGGACGCCGCGCTGATCTGTGT
 GCCGCCGTACCACATCGCGGGTGTCAGCGCGGCGATGTCCAACCTGTACGCCGGCCGGAAGATGGTGTAC
 CTGCGCAACTTCGACGCACACCGCTGGGTGAGTTGGTGCGCACCGAGGGCGTCACGTCTGCCACCGTGG
 TGCCGACCATGCTCGACCGTATCGTCACCGCACTTGAGACCACGCGCGCCGAGCTGCCGACCCTGCGCAA
 CCTCGCCTACGGCGGATCCAAGGTCGCGCTGCCCCTGGTCCGCAAGGCGCTGGAGCTGATGCCGAACGTC
 GGATTCGTCAACGCCTACGGTCTCACCGAAACCAGCTCCACCATCGCGGTCTTCGGACCCGACGACCACC
 GGGCCGCGCTGGCCTCCGACGACCCCGGTGTGACCCGCCGCCTCGGGTCGGTGGGACAGGTGGTGCCCGG
 GATCGAGGTGCAGATCCGCGGCGAGGACGGCACCGTGCTGGGGCCCGGCGAGACCGGTGAGCTGTTCTGTG
 CGCGGCGAGCAGGTGTCCGGCCGGTACACCGAGATCGGGTCGGTGCTCGACGAGGACGGCTGGTTCCCCA
 CCAAAGACGTTGCGATGCTTGACCAGGACGGCTATCTGTTTCATCGGCGGCCGGTCGGACGACACCATCAT
 CCGCGGCGGCGAGAACATCGTCTCCGCGGAGATCGAGGACGTTCTCGTGGAACATCCCGACGTGCGCGAC
 GTCGCGGTGGTCGGCCCCGAGGACCCCGAGTGGGGCCAGATCATCGTCGCGGTCTGTGGTGCCCGCCGACG
 GCGCCGAACCCGACGCCGACGTACTCCGCGAGCACGTCCGCAAACACCTGCGCGGATCCCGCACCCCGA
 CCGCGTGGTCTTCCGCGCCGAACTGCCCACCAACGCCACCGGCAAGGTGCTGCGCCGTCAACTCGTCGAC
 GAACTCCAGCCCATCTCGTAG

Figure S39. Nucleotide sequence of MSMEG_4883. The 9 bp repeats are underlined, while the deletion region is highlighted as bold.

Table S3. Unique SNPs in quinoxaline-resistant *M. smegmatis* mutants.

<i>M. smegmatis qdr1</i>					
<i>Locus tag</i>	Protein ID	annotation	Codon	SNP	Amino acid substitution
<i>MSMEG_0210</i>	YP_884625.1	LprO protein	codon=45	CTG>CTT	L>L
<i>MSMEG_0210</i>	YP_884625.1	LprO protein	codon=45	CTG>CCG	L>P
<i>MSMEG_0229</i>	YP_884644.1	dihydroxy-acid dehydratase	codon=38	ATG>ATT	M>I
<i>MSMEG_0232</i>	YP_884647.1	sugar transporter family protein	codon=349	GGC>GAC	G>D
<i>MSMEG_0234</i>	YP_884649.1	metallopeptidase	codon=158	CTG>CCG	L>P
<i>MSMEG_0318</i>	YP_884733.1	AMP-dependent synthetase/ligase	codon=23	CCT>CCA	P>P
<i>MSMEG_0613</i>	YP_885024.1	hypothetical protein	codon=148	ATG>ACG	M>T
<i>MSMEG_0705</i>	YP_885112.1	permease of the major facilitator superfamily protein	codon=119	CTG>CGG	L>R
<i>MSMEG_0706</i>	YP_885113.1	4-carboxy-4-hydroxy-2-oxoadipate aldolase	codon=38	GGC>AGC	G>S
<i>MSMEG_1240</i>	YP_885631.1	hypothetical protein	codon=253	CAT>CGT	H>R
<i>MSMEG_1328</i>	YP_885718.1	exodeoxyribonuclease V subunit gamma	codon=236	ACT>GCT	T>A
<i>MSMEG_1380</i>	YP_885766.1	transcriptional regulator	-	-	-
<i>MSMEG_1684</i>	YP_886060.1	hypothetical protein	codon=207	GAG>CAG	E>Q
<i>MSMEG_1775</i>	YP_886147.1	cytochrome P450 monooxygenase	Intergenic mutation		
<i>MSMEG_1930</i>	YP_886296.1	DEAD/DEAH box helicase	Intergenic mutation		
<i>MSMEG_2257</i>	YP_886609.1	cytochrome P450-terp	codon=394	GCC>GGC	A>G
<i>MSMEG_4378</i>	YP_888653.1	two-component system response regulator	codon=109	GTG>GGG	V>G
<i>MSMEG_4648</i>	YP_888911.1	DNA-binding protein	codon=49	CAG>CCG	Q>P
<i>MSMEG_4702</i>	YP_888963.1	ABC transporter permease	codon=73	GCG>GGG	A>G
<i>MSMEG_4712</i>	YP_888972.1	pyruvate dehydrogenase E1 component subunit alpha	codon=160	CAG>CGG	Q>R
<i>MSMEG_4846</i>	YP_889102.1	enoyl-CoA hydratase	Intergenic mutation		
<i>MSMEG_4861</i>	YP_889117.1	cyclase	Intergenic mutation		
<i>MSMEG_5122</i>	YP_889369.1	ferredoxin	Intergenic		

			mutation		
			Intergenic		
			mutation		
<i>MSMEG_5122</i>	YP_889369.1	ferredoxin			
<i>MSMEG_5348</i>	YP_889592.1	medium-chain fatty acid-CoA ligase	codon=254	CCC>CGC	P>R
<i>MSMEG_5351</i>	YP_889595.1	hypothetical protein	codon=43	GCG>GGG	A>G
<i>MSMEG_5437</i>	YP_889676.1	serine/threonine protein kinase	codon=272	CAT>TAT	H>Y
<i>MSMEG_5600</i>	YP_889834.1	hypothetical protein		Intergenic mutation	
<i>MSMEG_5757</i>		tRNA-Glu	codon=22	GTT>GCT	V>A
<i>MSMEG_6041</i>	YP_890265.1	acyl-CoA dehydrogenase	codon=281	ATC>GTC	I>V
<i>MSMEG_6232</i>	YP_890451.1	catalase KatA	codon=115	GGG>CGG	G>R
<i>MSMEG_6241</i>	YP_890460.1	ATPase AAA	codon=194	GTG>GCG	V>A
<i>MSMEG_6317</i>	YP_890535.1	lipolytic protein G-D-S-L	codon=132	CCC>CCA	P>P
<i>MSMEG_6628</i>	YP_890837.1	TetR family transcriptional regulator		Intergenic mutation	
<i>MSMEG_6858</i>	YP_891062.1	epoxide hydrolase 1	codon=163	TCG>TTG	S>L

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<i>Locus tag</i>	Protein ID	annotation	Codon	SNP	Amino acid substitution
<i>MSMEG_0001</i>	YP_884424.1	DNA polymerase III subunit beta	codon=152	GCG>GGG	A>G
<i>MSMEG_0312</i>	YP_884726.1	2-dehydro-3-deoxy-phosphogluconate aldolase	codon=99	ATG>ACG	M>T
<i>MSMEG_0576</i>	YP_884987.1	MmpL4 protein	codon=377	GTG>GTT	V>V
<i>MSMEG_0634</i>	YP_885043.1	PAP2 superfamily protein	codon=37	GAC>GGC	D>G
<i>MSMEG_0660</i>	YP_885069.1	extracellular solute-binding protein	codon=158	TTG>TTA	L>L
<i>MSMEG_0719</i>	YP_885126.1	flavoheomprotein	codon=175	CAG>CGG	Q>R
<i>MSMEG_1080</i>	YP_885476.1	large subunit of N,N-dimethylformamidase	codon=490	ACA>ACG	T>T
<i>MSMEG_1111</i>	YP_885505.1	hypothetical protein	codon=6	GCC>GGC	A>G
<i>MSMEG_1119</i>	YP_885513.1	glutamine amidotransferase	codon=114	CGA>AGA	R>R
<i>MSMEG_1211</i>	YP_885603.1	Fatty acid desaturase		Intergenic mutation	
<i>MSMEG_1380</i>	YP_885766.1	transcriptional regulator	-	-	-
		signal peptide peptidase SppA, 67K type			
<i>MSMEG_1476</i>	YP_885858.1		codon=232	GAG>GGG	E>G

<i>MSMEG_1476</i>	YP_885858.1	signal peptide peptidase SppA, 67K type	codon=420	AAA>AAC	K>N
<i>MSMEG_1641</i>	YP_886018.1	hypothetical protein	codon=181	GCC>GCT	A>A
<i>MSMEG_1644</i>	YP_886021.1	hypothetical protein	codon=247	GTG>ATG	V>M
<i>MSMEG_2077</i>	YP_886438.1	acyl-CoA dehydrogenase	codon=145	GTC>CTC	V>L
<i>MSMEG_2512</i>	YP_886850.1	lactate 2-monooxygenase	codon=241	ACC>ACG	T>T
<i>MSMEG_2968</i>	YP_887287.1	hypothetical protein	codon=144	AAC>AAT	N>N
<i>MSMEG_3159</i>	YP_887474.1	methylmalonyl-CoA mutase	codon=28	CCC>CCG	P>P
<i>MSMEG_3975</i>	YP_888263.1	regulatory protein	codon=396	GAG>GAC	E>D
<i>MSMEG_4044</i>	YP_888330.1	GAF domain-containing protein	codon=467	CAG>CGG	Q>R
<i>MSMEG_4723</i>	YP_888983.1	hypothetical protein	codon=365	GTG>GCG	V>A
<i>MSMEG_4853</i>	YP_889109.1	peptidase, M24 family protein	codon=10	CGG>CGC	R>R
<i>MSMEG_4872</i>	YP_889128.1	short chain dehydrogenase	Intergenic mutation		
<i>MSMEG_5122</i>	YP_889369.1	ferredoxin	codon=5	ATT>ACT	I>T
<i>MSMEG_5122</i>	YP_889369.1	ferredoxin	codon=29	CAT>TAT	H>Y
<i>MSMEG_5152</i>	YP_889397.1	hypothetical protein	codon=29	CAT>TAT	H>Y
<i>MSMEG_5423</i>	YP_889663.1	transcription-repair coupling factor	codon=906	ATC>ATT	I>I
<i>MSMEG_5619</i>	YP_889853.1	acyl-CoA dehydrogenase	codon=166	GAC>GGC	D>G
<i>MSMEG_5656</i>	YP_889889.1	histidinol dehydrogenase	codon=422	GCC>GCT	A>A
<i>MSMEG_6313</i>	YP_890531.1	queuine tRNA-ribosyltransferase	codon=349	ACG>CCG	T>P
<i>MSMEG_6341</i>	YP_890558.1	6-phosphogluconate dehydrogenase	codon=190	GTG>GTC	V>V

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<i>Locus tag</i>	Protein ID	annotation	Codon	SNP	Amino acid substitution
<i>MSMEG_0017</i>	YP_884437.1	ABC transporter permease	codon=535	AGT>CGT	S>R
<i>MSMEG_1186</i>	YP_885578.1	permease	codon=431	ATC>CTC	I>L
<i>MSMEG_1325</i>	YP_885716.1	exodeoxyribonuclease V subunit alpha	codon=419	GAA>AAA	E>K
<i>MSMEG_1380</i>	YP_885766.1	transcriptional regulator	codon=54	TAC>TCC	Y>S
<i>MSMEG_1469</i>	YP_885851.1	30S ribosomal protein S8	codon=58	AAG>ACG	K>T
<i>MSMEG_1515</i>	YP_885897.1	two-component sensor histidine kinase	codon=137	GGC>GAC	G>D
<i>MSMEG_2115</i>	YP_886471.1	hypothetical protein	codon=95	GAC>TAC	D>Y

<i>MSMEG_2115</i>	YP_886471.1	hypothetical protein	codon=95	GAC>GCC	D>A
<i>MSMEG_2139</i>	YP_886496.1	hypothetical protein	Intergenic mutation		
<i>MSMEG_2350</i>	YP_886693.1	hypothetical protein	codon=223	CTC>CCC	L>P
<i>MSMEG_2580</i>	YP_886917.1	4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase	codon=69	GTG>GTA	V>V
<i>MSMEG_2907</i>	YP_887226.1	oxidoreductase YeiQ	codon=443	GTC>CTC	V>L
<i>MSMEG_2950</i>	YP_887269.1	carbon monoxide dehydrogenase, medium chain	codon=5	CGG>GGG	R>G
<i>MSMEG_3673</i>	YP_887976.1	4-alpha-glucanotransferase	codon=272	GTG>GTA	V>V
<i>MSMEG_3741</i>	YP_888040.1	transcriptional regulator	codon=153	AAA>AAG	K>K
<i>MSMEG_4108</i>	YP_888390.1	NAD(P) transhydrogenase subunit beta	codon=370	CTG>CTC	L>L
<i>MSMEG_4109</i>	YP_888391.1	NAD(P) transhydrogenase subunit alpha	codon=408	GGA>GCA	G>A
<i>MSMEG_4259</i>	YP_888535.1	hypothetical protein	codon=280	CTG>CCG	L>P
<i>MSMEG_4383</i>	YP_888658.1	MmpL5 protein	codon=66	GTG>GGG	V>G
<i>MSMEG_4384</i>	YP_888659.1	penicillin binding protein transpeptidase domain-containing protein	codon=41	GTG>GTA	V>V
<i>MSMEG_4477</i>	YP_888750.1	hydrolase, alpha/beta hydrolase fold family protein	codon=236	CTC>CTG	L>L
<i>MSMEG_4641</i>	YP_888903.1	salicylate hydroxylase	codon=234	CGC>CCC	R>P
<i>MSMEG_4646</i>	YP_888909.1	pyruvate synthase	codon=652	TGA>TCA	*>S
<i>MSMEG_4917</i>	YP_889173.1	hypothetical protein	codon=73	GCC>TCC	A>S
<i>MSMEG_5585</i>	YP_889821.1	hypothetical protein	codon=39	GCC>GGC	A>G
<i>MSMEG_6749</i>	YP_890957.1	hypothetical protein	codon=11	AAG>AGG	K>R
<i>MSMEG_6934</i>	YP_891128.1	thioredoxin	codon=90	GTG>GGG	V>G

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<i>Locus tag</i>	Protein ID	annotation	Codon	SNP	Amino acid substitution
<i>MSMEG_0166</i>	YP_884582.1	GntR family transcriptional regulator	Intergenic mutation		
<i>MSMEG_0204</i>	YP_884619.1	hypothetical protein	codon=610	GCG>GTG	A>V
<i>MSMEG_0217</i>	YP_884632.1	alcohol dehydrogenase	Intergenic mutation		

<i>MSMEG_0635</i>	YP_885045.1	hypothetical protein	codon=93	ACC>AAC	T>N
		glutamyl-tRNA(Gln)/aspartyl-tRNA(Asn) amidotransferase subunit alpha		Intergenic mutation	
<i>MSMEG_1088</i>	YP_885483.1				
<i>MSMEG_1915</i>	YP_886281.1	anti-sigma factor, family protein	codon=55	TGC>TGG	C>W
<i>MSMEG_2401</i>	YP_886740.1	hypothetical protein	codon=170	CCG>GCG	P>A
<i>MSMEG_2531</i>	YP_886868.1	GntR family transcriptional regulator		Intergenic mutation	
<i>MSMEG_3598</i>	YP_887901.1	periplasmic sugar-binding proteins	codon=253	GAC>GTC	D>V
<i>MSMEG_3878</i>	YP_888169.1	precorrin-6Y C5,15-methyltransferase	codon=343	GCG>GCC	A>A
<i>MSMEG_4147</i>	YP_888427.1	major facilitator superfamily protein	codon=8	GTC>TTC	V>F
			Intergenic mutation		
<i>MSMEG_4290</i>	YP_888567.1	glutamine synthetase			
<i>MSMEG_4646</i>	YP_888909.1	pyruvate synthase	codon=95	AAC>CAC	N>H
<i>MSMEG_5117</i>	YP_889365.1	proline dehydrogenase	codon=184	GAG>CAG	E>Q
<i>MSMEG_5311</i>	YP_889557.1	hypothetical protein	codon=133	GCG>TCG	A>S
		phosphoribosylaminoimidazole synthetase			
<i>MSMEG_5798</i>	YP_890026.1		codon=336	TGG>CGG	W>R
<i>MSMEG_5836</i>	YP_890063.1	hypothetical protein	codon=141	CAC>TAC	H>Y
<i>MSMEG_6636</i>	YP_890845.1	[Mn] superoxide dismutase		Intergenic mutation	

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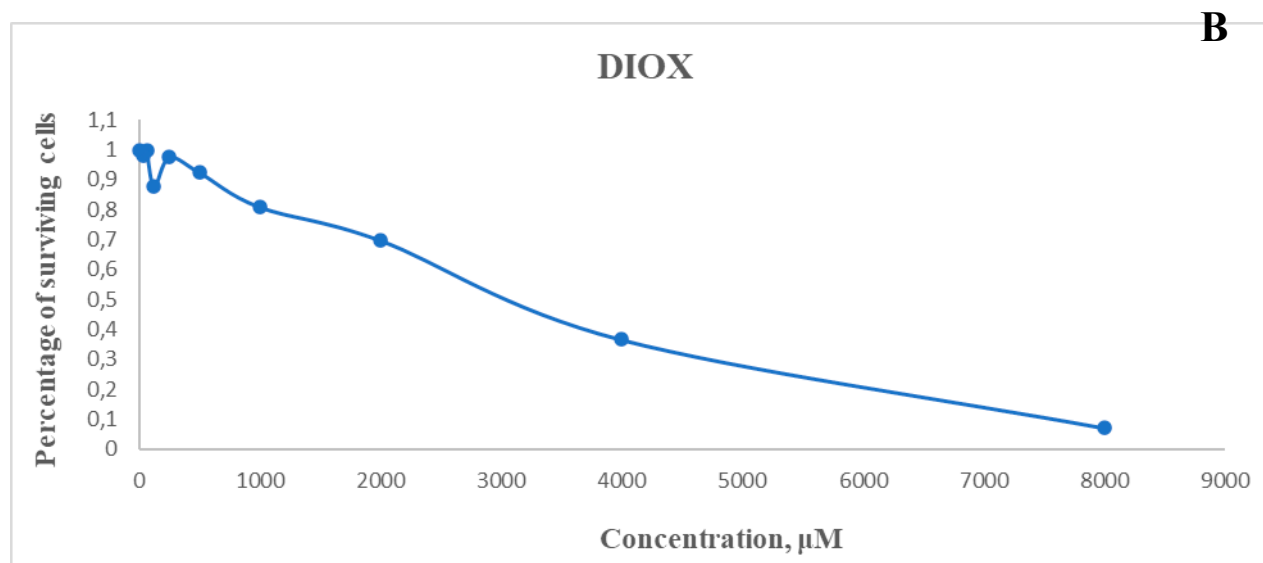
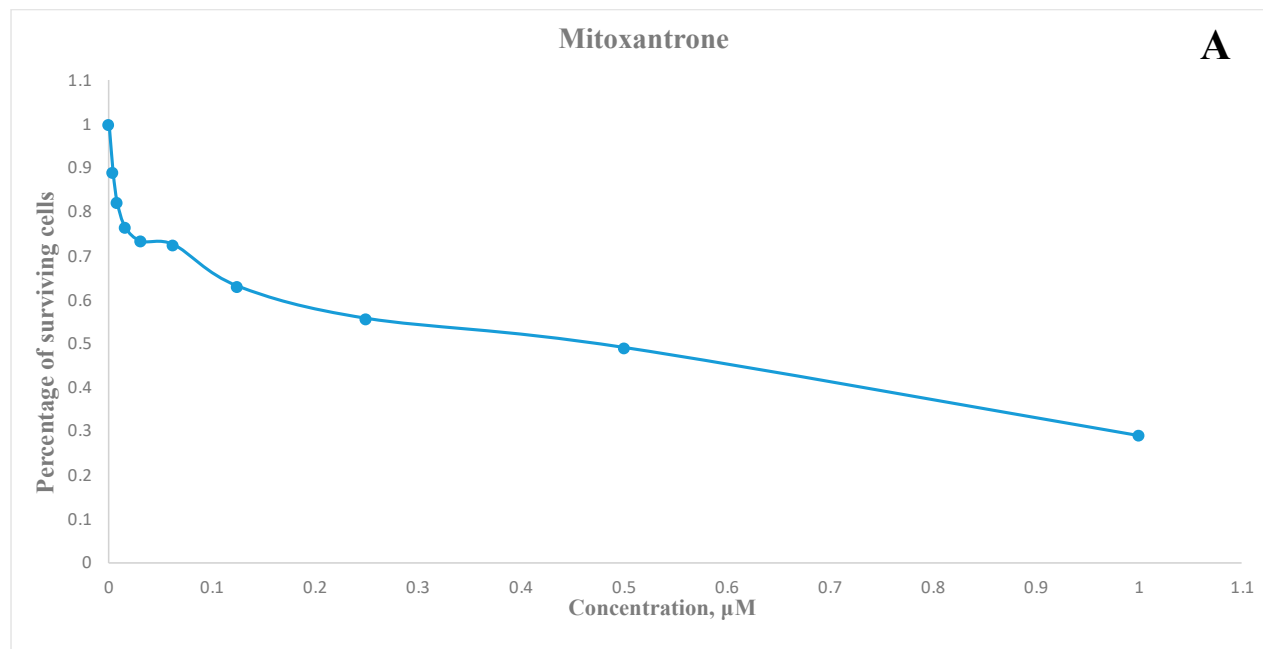
<i>Locus tag</i>	Protein ID	annotation	Codon	SNP	Amino acid substitution
<i>MSMEG_0070</i>	YP_884488.1	hypothetical protein		Intergenic mutation	
<i>MSMEG_0125</i>	YP_884540.1	integral membrane protein	codon=190	TCG>CCG	S>P
<i>MSMEG_0144</i>	YP_884561.1	HNH endonuclease	codon=417	GAC>GTC	D>V
<i>MSMEG_0354</i>	YP_884767.1	hypothetical protein	codon=104	GCA>CCA	A>P
<i>MSMEG_0516</i>	YP_884928.1	sugar transporter	codon=176	ATC>ATG	I>M
<i>MSMEG_0772</i>	YP_885178.1	phytase		Intergenic mutation	
<i>MSMEG_1380</i>	YP_885766.1	transcriptional regulator	codon=108	GGA>TGA	G>*
<i>MSMEG_1559</i>	YP_885939.1	phosphoglucosamine mutase	codon=148	CGG>CCG	R>P
		HNH endonuclease domain-containing protein			
<i>MSMEG_2148</i>	YP_886504.1			Intergenic mutation	

<i>MSMEG_2349</i>	YP_886692.1	glycosyl hydrolase family protein	codon=85	ATG>GTG	M>V
<i>MSMEG_2377</i>	YP_886719.1	P49 protein	codon=178	GTT>TTT	V>F
<i>MSMEG_3143</i>	YP_887458.1	aconitate hydratase	codon=835	GGC>GGG	G>G
<i>MSMEG_3183</i>	YP_887498.1	threonine dehydratase	codon=2	ACC>GCC	T>A
<i>MSMEG_3281</i>	YP_887592.1	spermidine/putrescine ABC transporter ATP-binding protein	codon=184	GGC>GGA	G>G
<i>MSMEG_3815</i>	YP_888107.1	drug efflux membrane protein	codon=29	GCC>GGC	A>G
<i>MSMEG_3839</i>	YP_888130.1	DNA polymerase I	codon=242	GGC>TGC	G>C
<i>MSMEG_3872</i>	YP_888163.1	precorrin-8X methylmutase	codon=44	GGC>GGA	G>G
<i>MSMEG_4516</i>	YP_888788.1	2,3-dihydroxybenzoate-AMP ligase	codon=359	CTG>CTC	L>L
<i>MSMEG_4646</i>	YP_888909.1	pyruvate synthase	codon=274	CCG>CTG	P>L
<i>MSMEG_4721</i>	YP_888981.1	permease of the major facilitator superfamily protein	codon=114	GTG>GGG	V>G
<i>MSMEG_4762</i>	YP_889019.1	ABC transporter	codon=112	TCG>TTG	S>L
<i>MSMEG_4793</i>	YP_889049.1	virulence factor Mce family protein tetracycline-resistance determinant	codon=69	GTT>GTC	V>V
<i>MSMEG_5187</i>	YP_889433.1	TetV	codon=82	AAC>AAG	N>K
<i>MSMEG_5253</i>	YP_889499.1	hypothetical protein	codon=2	ACC>ATC	T>I
<i>MSMEG_5450</i>	YP_889689.1	redox-sensitive transcriptional activator SoxR	codon=46	CTG>GTG	L>V
<i>MSMEG_5589</i>	YP_889824.1	manganese transporter MntH	codon=344	GCC>GAC	A>D
<i>MSMEG_5595</i>	YP_889830.1	MarR family transcriptional regulator major facilitator family protein	Intergenic mutation		
<i>MSMEG_5713</i>	YP_889945.1	transporter	codon=278	GGT>GTT	G>V
<i>MSMEG_5876</i>	YP_890101.1	H-N-H endonuclease F-TfIIIV	codon=107	GCC>TCC	A>S
<i>MSMEG_6646</i>	YP_890855.1	methylisocitrate lyase	codon=31	CCG>TCG	P>S
<i>MSMEG_6708</i>	YP_890916.1	epoxide hydrolase	codon=217	GCC>TCC	A>S
<i>MSMEG_6947</i>	YP_891139.1	chromosomal replication initiation protein	codon=232	AAG>AAT	K>N

* All Functionally annotated by BLAST search.

Table S4. Results of Dunnett's multiple comparison test for in vivo testing of lcta-3368.

Dunnett's multiple comparisons test	Mean Diff.	95.00% CI of diff.	Significant?	Summary	Adjusted P Value
RIF 10 vs. Solvent control	-0.2508	-0.4126 to -0.08905	Yes	***	0.0007
RIF 10 vs. LCTA 3368 30	-0.3010	-0.4628 to -0.1392	Yes	****	<0.0001
RIF 10 vs. LCTA 3368 100	-0.2463	-0.4081 to -0.08452	Yes	***	0.0009
RIF 10 vs. LCTA 3368 100 (I.P)	-0.2194	-0.3812 to -0.05765	Yes	**	0.0037
RIF 10 vs. LCTA 3368 200	-0.2899	-0.4517 to -0.1281	Yes	****	<0.0001



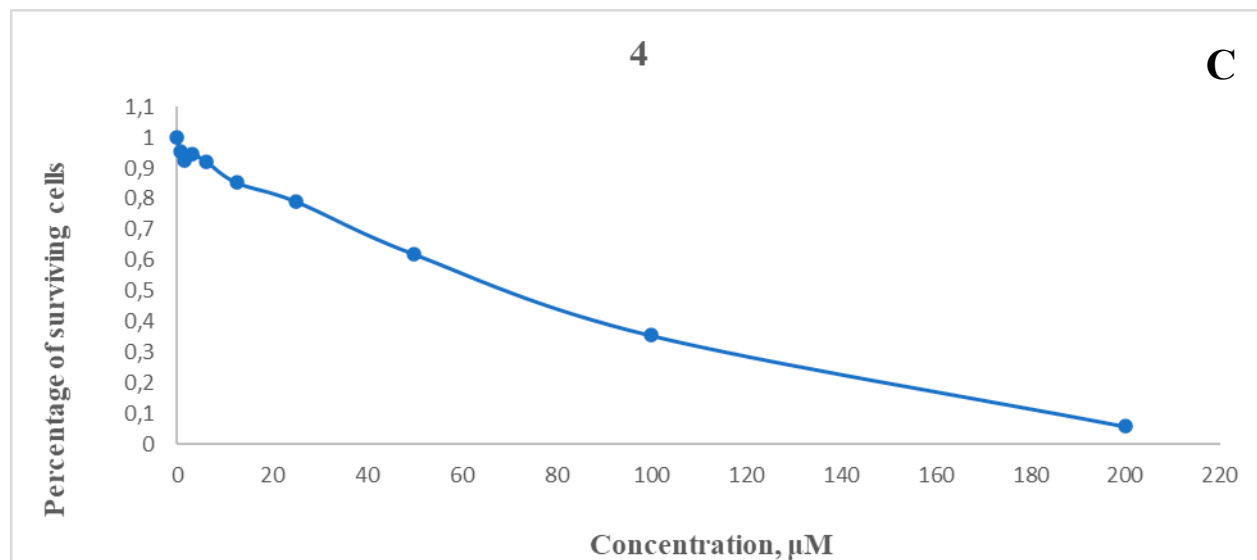


Figure S40. Results of MTT test of compounds on human fibroblasts. (A) Mitoxantrone was used as control. (B) Dioxidine (C) Tested 4.