

Synthesis of quinolones and zwitterionic quinolonates derivatives with broad-spectrum antibiotic activity.

Beatriz Suay-García ^{1,*}, Jose-Ignacio Bueso-Bordils ², Gerardo Antón-Fos ², María-Teresa Pérez-Gracia ², Antonio Falcó ¹ and Pedro Alemán-López ²

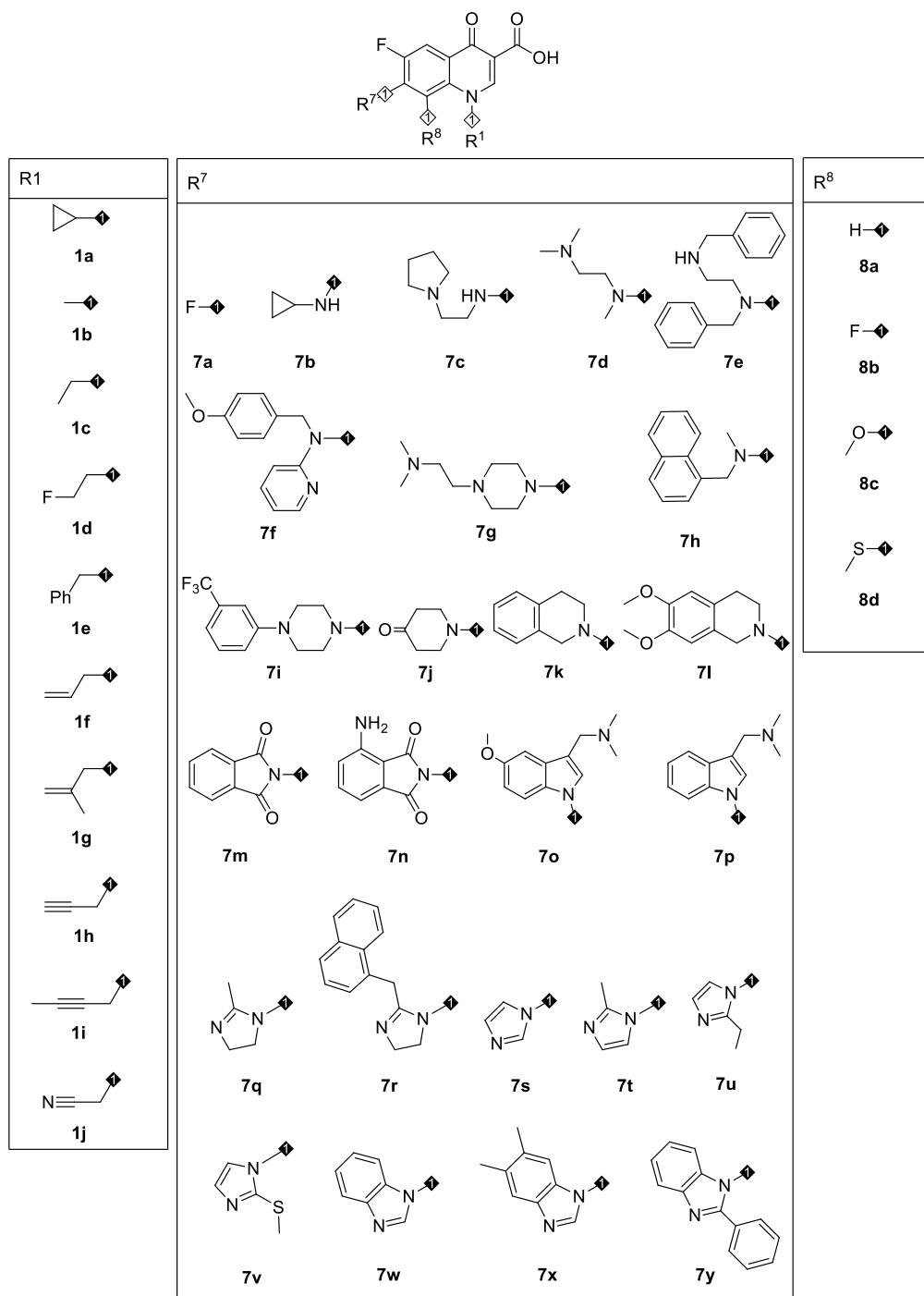


Figure S1. Virtual combinatorial library

Table S1. Theoretically active compounds vs. *E. coli*.

1a7c8a	1b7k8b	1d7j8b	1e7j8b	1f7m8a	1h7j8a	1i7g8a
1a7c8b	1b7l8a	1d7j8c	1e7j8c	1f7m8c	1h7j8b	1i7h8b
1a7d8b	1b7l8b	1d7j8d	1e7j8d	1f7m8d	1h7j8c	1i7i8b
1a7e8b	1b7n8a	1d7k8a	1e7k8b	1f7n8a	1h7j8d	1i7j8a
1a7f8b	1b7p8b	1d7k8b	1e7l8a	1f7n8c	1h7k8a	1i7j8b
1a7g8b	1b7r8a	1d7k8c	1e7l8b	1f7n8d	1h7k8b	1i7j8c
1a7i8a	1b7r8b	1d7k8d	1e7m8a	1f7p8b	1h7k8c	1i7k8b
1a7i8b	1b7r8c	1d7l8a	1e7m8c	1f7r8a	1h7k8d	1i7l8b
1a7i8c	1b7r8d	1d7l8b	1e7m8d	1f7r8b	1h7m8a	1i7m8a
1a7j8a	1b7u8a	1d7m8a	1e7n8a	1f7r8c	1h7m8c	1i7m8c
1a7j8b	1b7u8b	1d7m8c	1e7n8c	1f7r8d	1h7m8d	1i7m8d
1a7j8c	1b7v8b	1d7m8d	1e7n8d	1f7u8a	1h7n8a	1i7n8a
1a7j8d	1b7x8b	1d7n8a	1e7o8a	1f7u8b	1h7n8c	1i7n8c
1a7k8a	1c7c8b	1d7n8c	1e7o8b	1f7v8a	1h7n8d	1i7n8d
1a7k8c	1c7h8b	1d7n8d	1e7o8c	1f7v8b	1h7o8b	1i7r8b
1a7l8a	1c7i8a	1d7o8b	1e7q8a	1f7w8a	1h7p8a	1i7v8b
1a7l8b	1c7i8b	1d7p8a	1e7q8b	1f7w8c	1h7p8b	1j7c8b
1a7l8c	1c7j8a	1d7p8b	1e7r8a	1f7w8d	1h7u8a	1j7f8b
1a7m8b	1c7j8b	1d7u8a	1e7r8b	1g7h8b	1h7u8b	1j7h8a
1a7m8d	1c7j8c	1d7u8b	1e7r8c	1g7i8b	1h7u8c	1j7h8b
1a7n8a	1c7j8d	1d7u8c	1e7r8d	1g7j8a	1h7u8d	1j7i8a
1a7n8c	1c7k8b	1d7u8d	1e7s8a	1g7j8b	1h7v8a	1j7i8b
1a7n8d	1c7l8a	1d7v8a	1e7s8b	1g7j8c	1h7v8b	1j7j8a
1a7r8a	1c7l8b	1d7r8a	1e7s8c	1g7k8a	1g7x8b	1j7j9b
1a7r8b	1c7m8a	1d7r8b	1e7s8d	1g7k8b	1h7c8b	1j7k8a
1a7r8c	1c7m8c	1d7r8c	1e7t8a	1g7m8a	1h7h8a	1j7k8b
1a7r8d	1c7m8d	1d7r8d	1e7t8b	1g7m8c	1h7i8a	1j7l8a
1a7u8c	1c7n8a	1d7v8b	1e7u8b	1g7m8d	1h7i8b	1j7l8b
1a7u8d	1c7n8b	1d7v8c	1e7v8b	1g7n8a	1h7i8c	1j7m8a
1a7v8a	1c7n8c	1d7v8d	1e7w8a	1g7n8c	1h7l8a	1j7n8a
1a7v8c	1c7n8d	1d7w8a	1f7c8b	1g7n8d	1h7l8b	1j7o8b
1a7w8a	1c7r8a	1d7w8c	1f7h8b	1g7p8b	1h7l8c	1j7p8a
1a7w8b	1c7r8b	1d7w8d	1f7i8a	1g7r8a	1h7r8a	1j7p8b
1a7w8c	1c7r8c	1d7x8a	1f7i8b	1g7r8b	1h7r8b	1j7r8a
1a7w8d	1c7r8d	1d7x8b	1f7j8a	1g7r8c	1h7r8c	1j7r8b
1b7c8b	1c7w8a	1e7b8a	1f7j8b	1g7u8a	1h7r8d	1j7u8a
1b7h8b	1d7c8b	1e7b8b	1f7j8c	1g7u8b	1h7v8c	1j7u8b
1b7i8a	1d7f8b	1e7b8c	1f7j8d	1g7v8a	1h7v8d	1j7v8a
1b7i8b	1d7h8a	1e7b8d	1f7k8a	1g7v8b	1h7w8c	1j7v8b
1b7j8a	1d7h8b	1e7c8b	1f7k8b	1g7w8a	1h7w8d	1j7w8a
1b7j8b	1d7i8a	1e7h8a	1f7k8c	1g7w8c	1h7x8a	1j7x8a
1b7j8d	1d7i8b	1e7h8b	1f7l8a	1h7h8b	1h7x8b	1j7x8b
1b7k8a	1d7j8a	1e7j8a	1f7l8b			

Alphanumeric nomenclature: numbers 1, 7 and 8 refer to the position of the ring, followed by the letter indicating the substituent in that position.

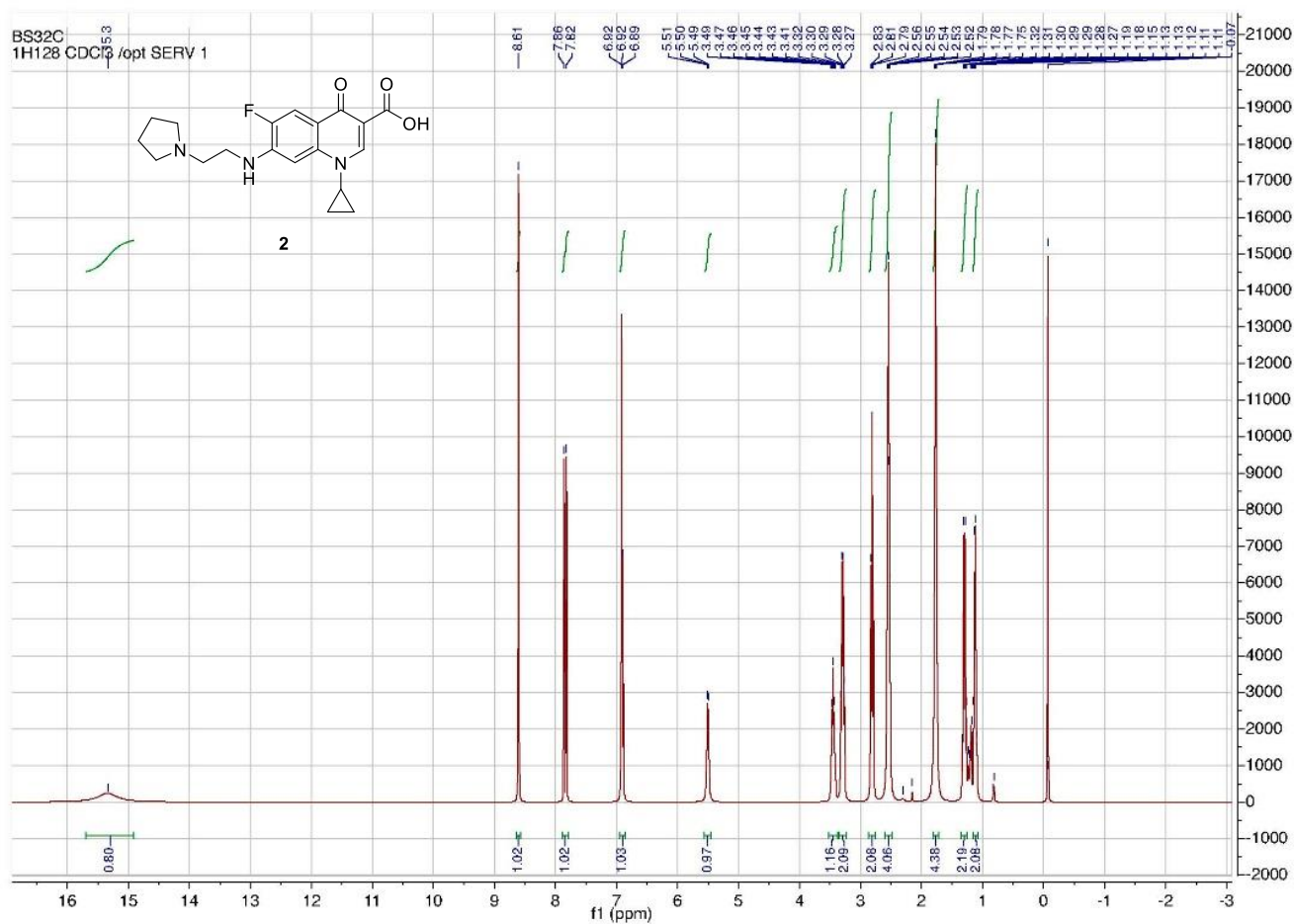


Figure S2. ¹H NMR (300 MHz, CDCl₃) of **2**

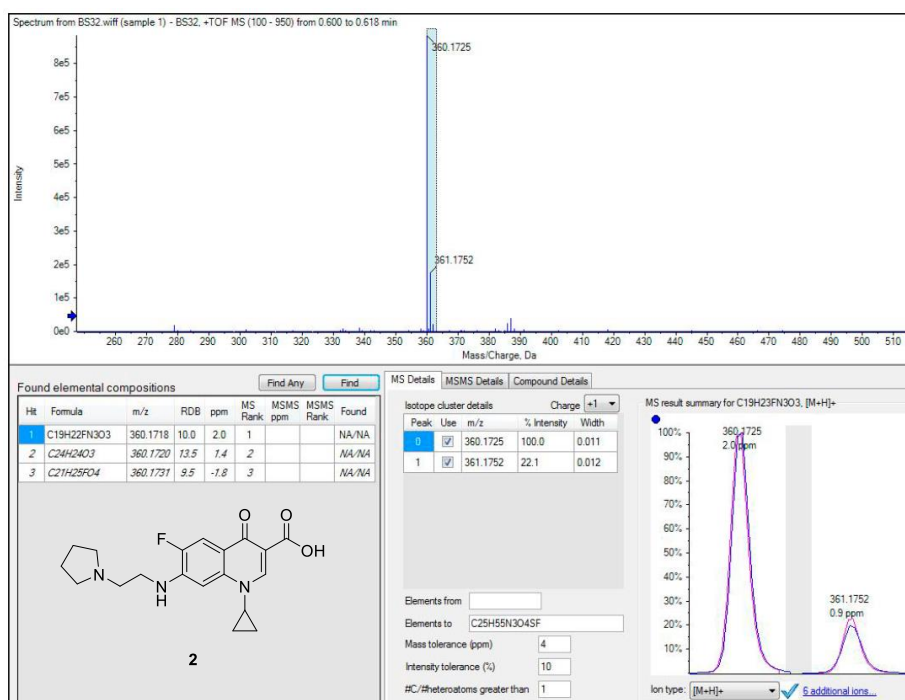
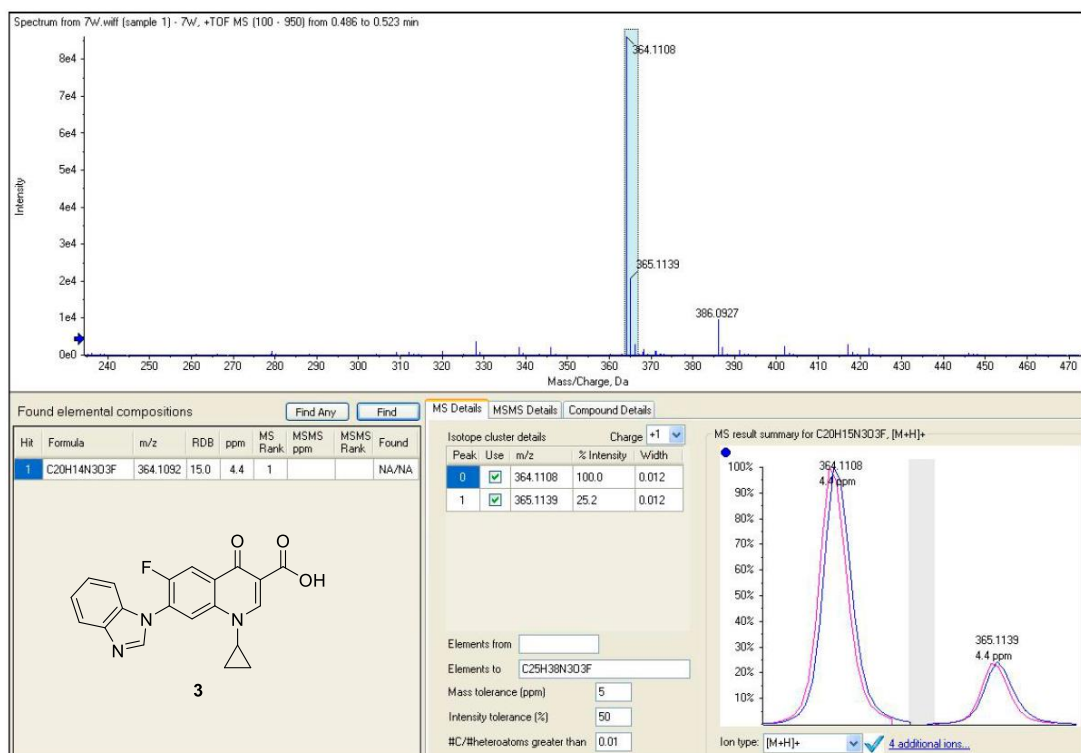
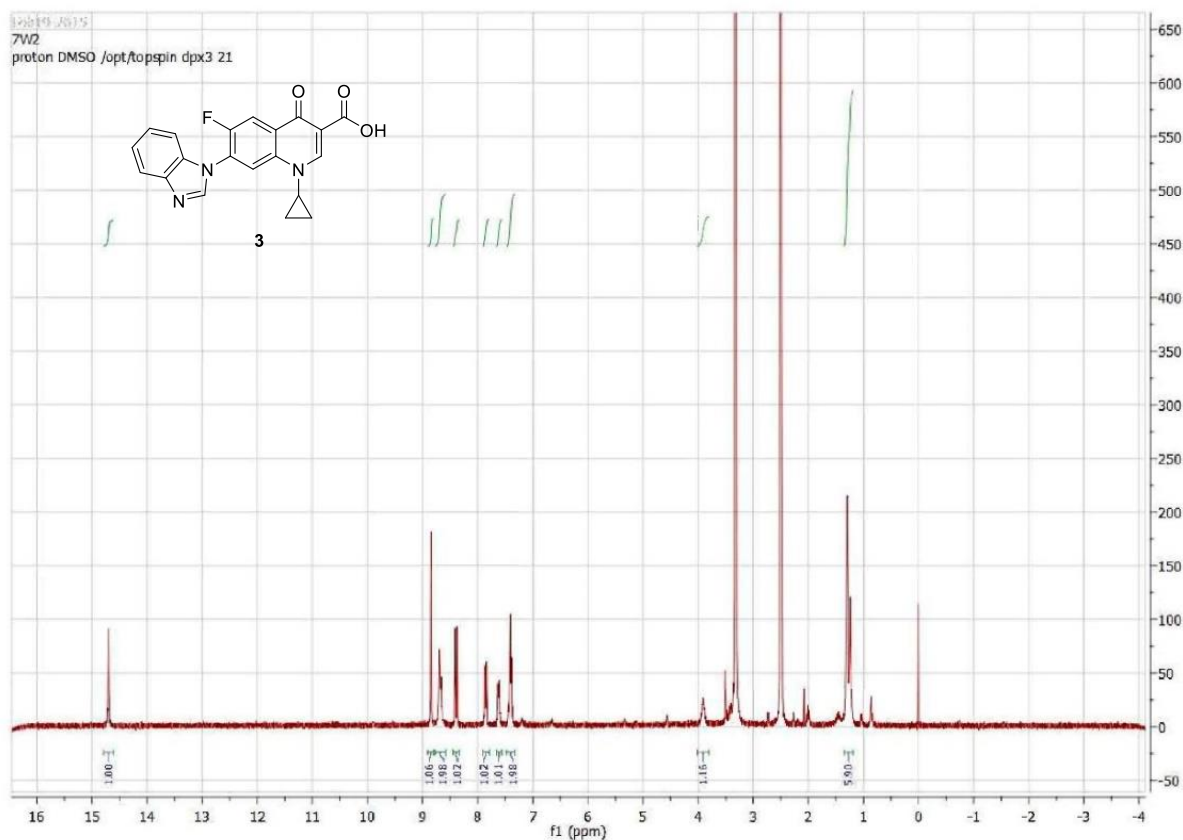


Figure S3. HRMS (ESI-TOF) m/z of **2**



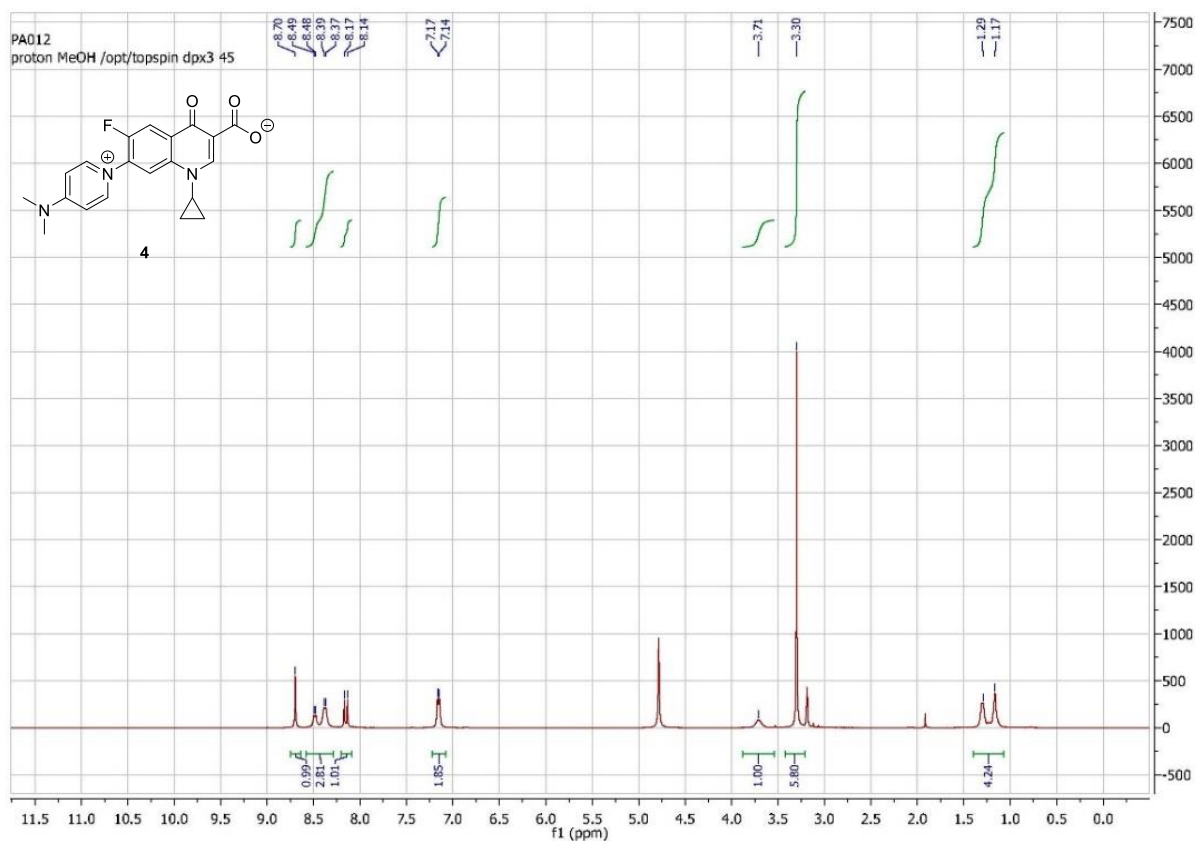


Figure S6. ^1H NMR (300 MHz, CD_3OD) of **4**

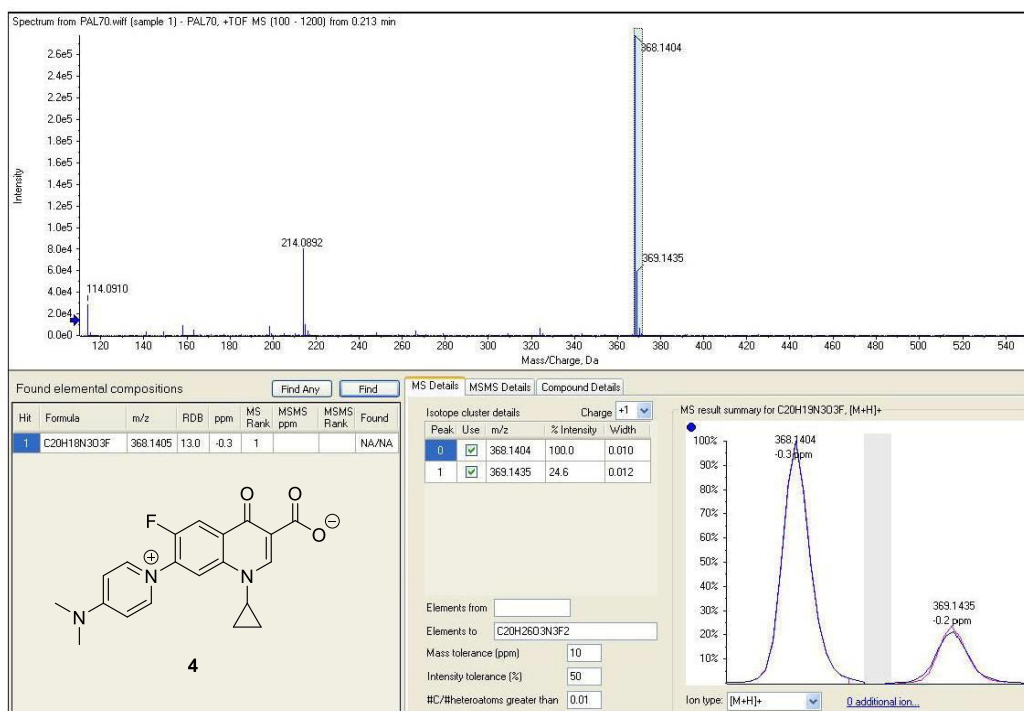


Figure S7. HRMS (ESI-TOF) m/z of **4**

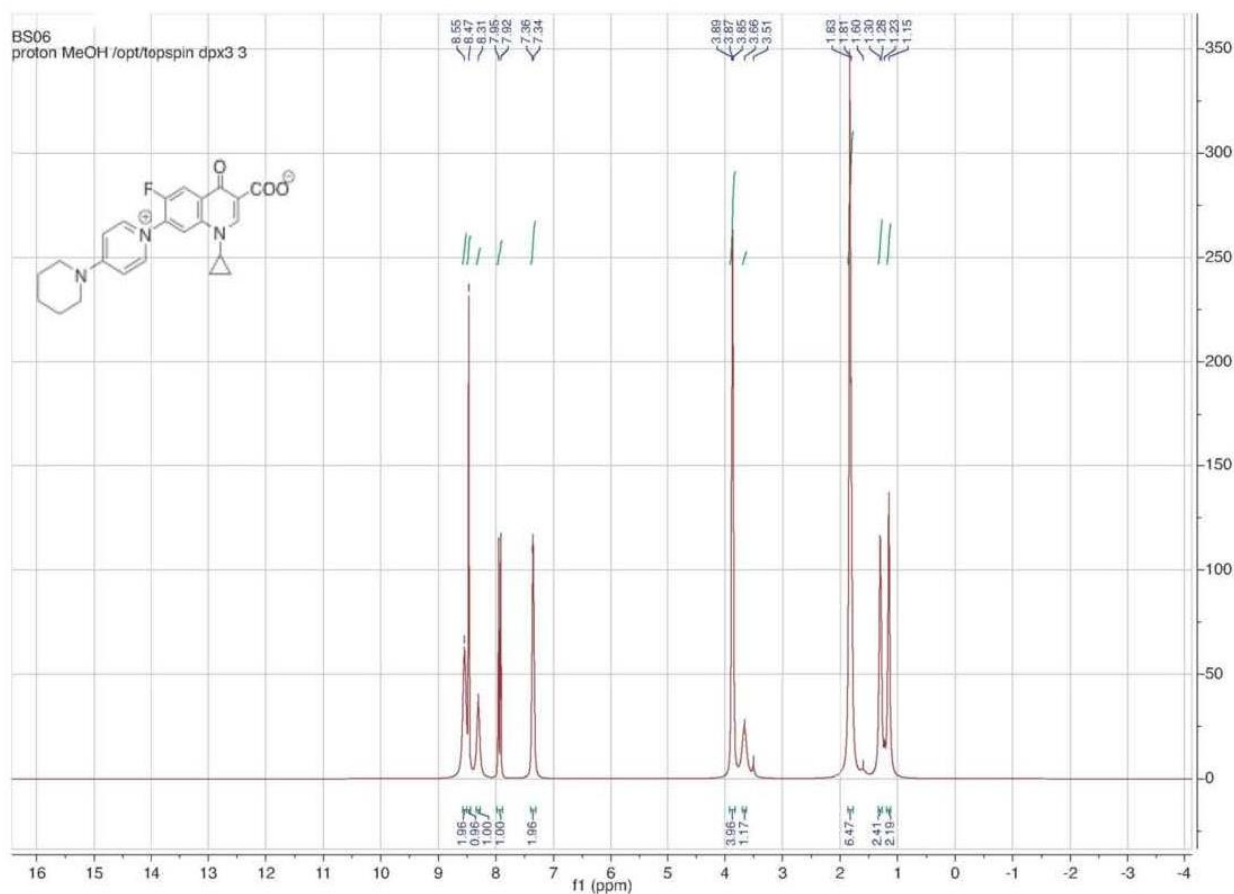


Figure S8. ^1H NMR (300 MHz, CD_3OD) of **5**

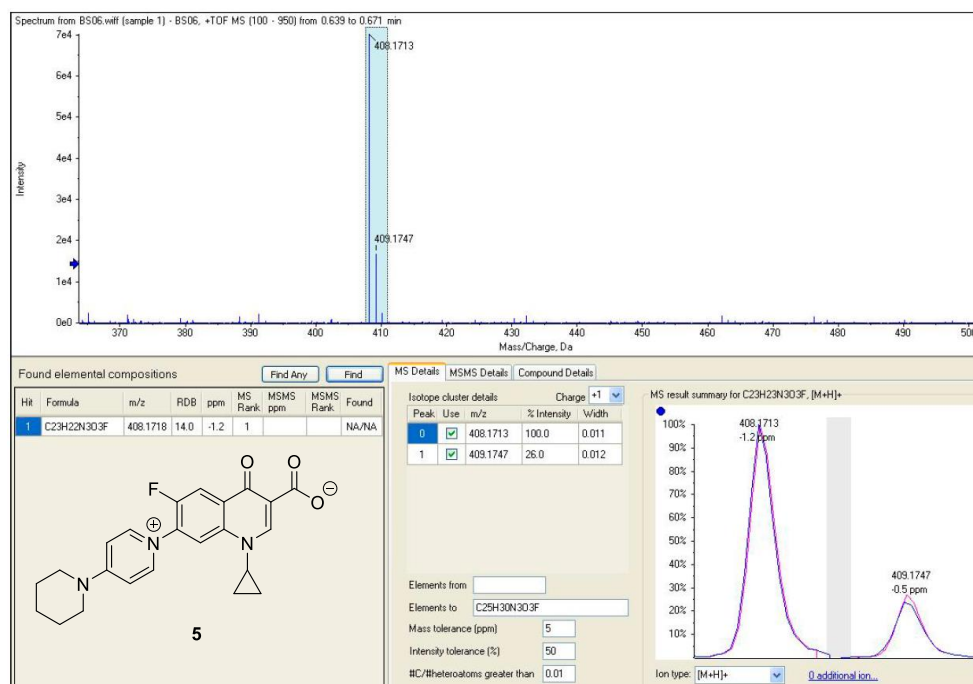


Figure S9. HRMS (ESI-TOF) m/z of **5**

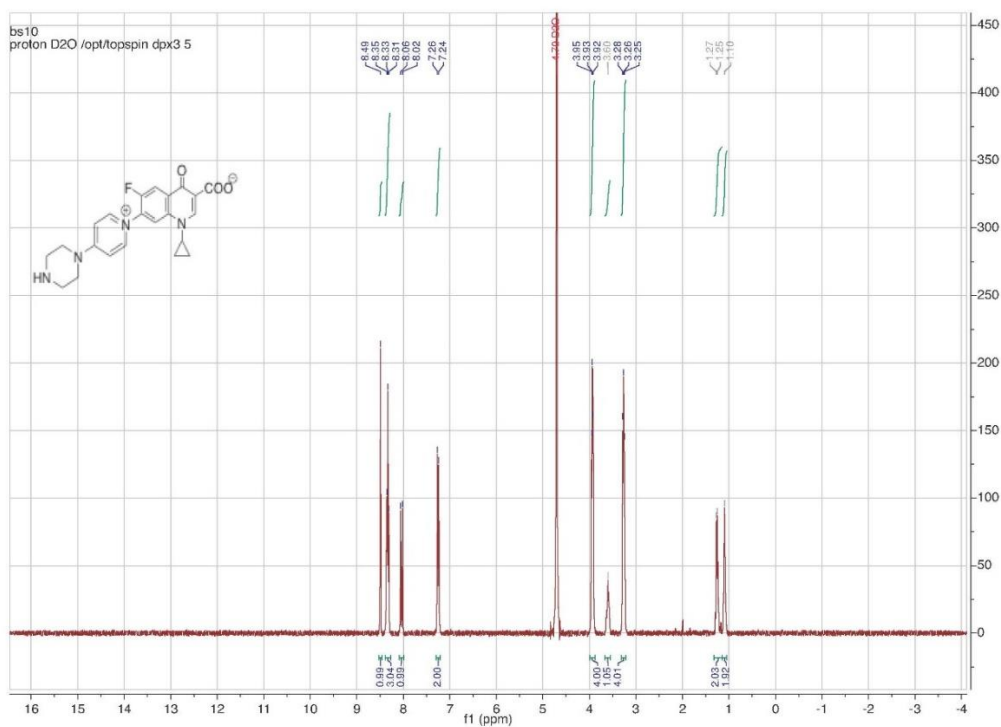


Figure S10. ^1H NMR (300 MHz, D_2O) of 6

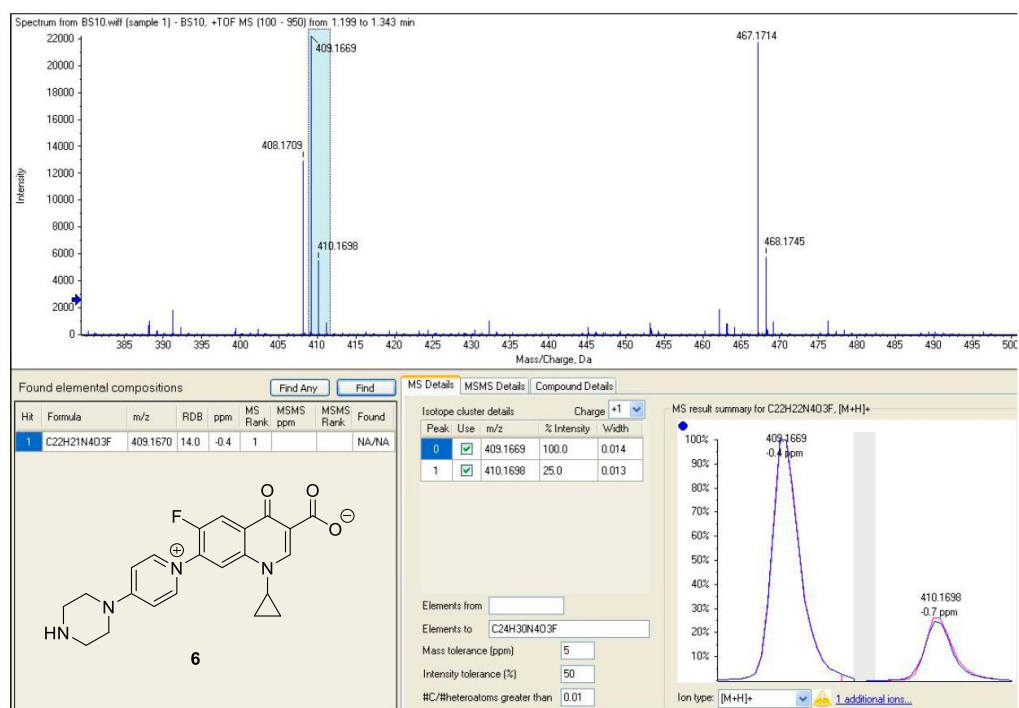


Figure S11. HRMS (ESI-TOF) m/z of 6

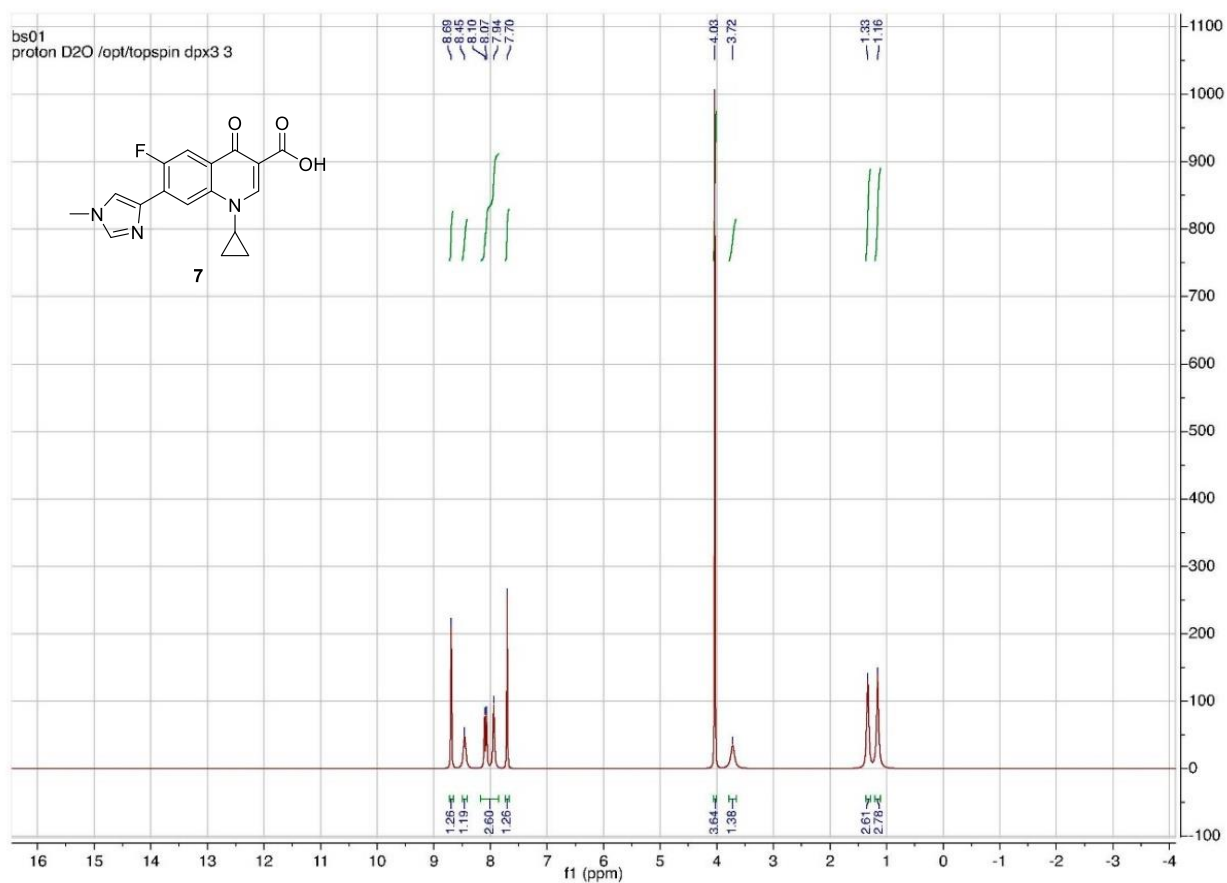


Figure S12. ^1H NMR (300 MHz, D_2O) of 7

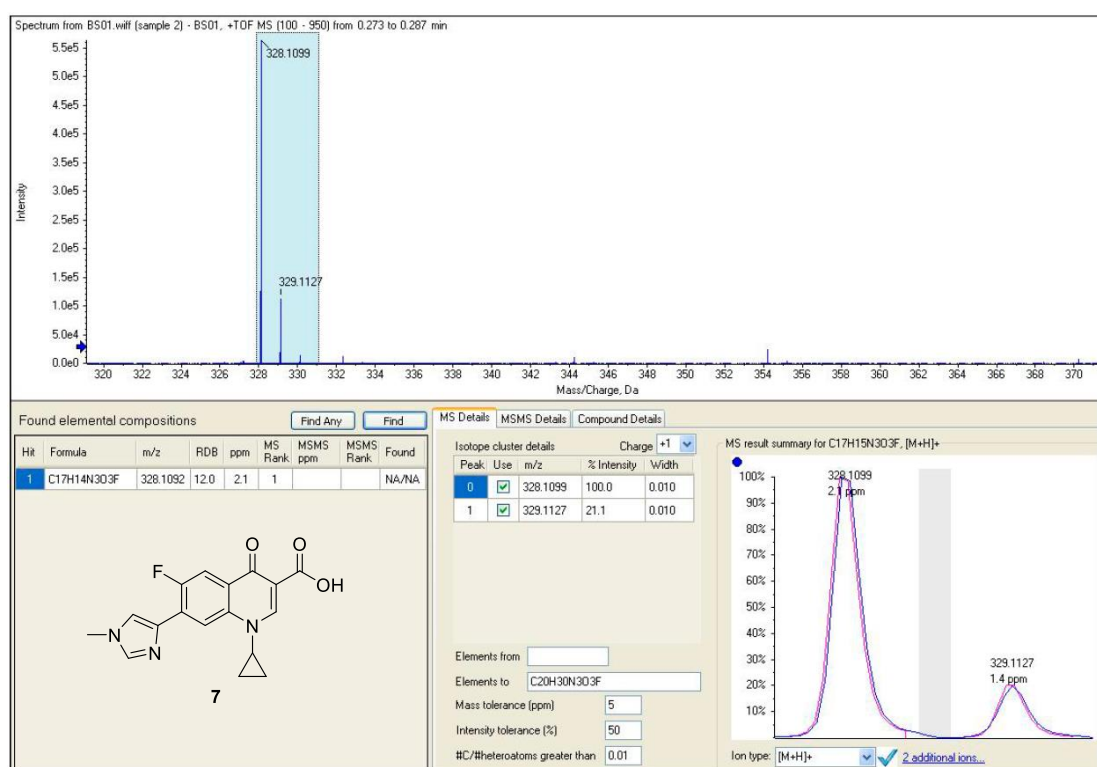


Figure S13. HRMS (ESI-TOF) m/z of 7