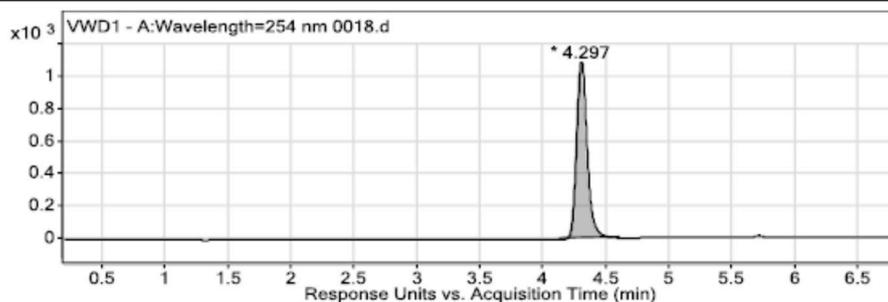


Data Filename	0018.d	Sample Name	
Sample Type	Sample	Position	Vial 38
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	3/12/2022 3:32:43 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.13	4.297	4.61	1087.31	6233.36	100

User Spectra

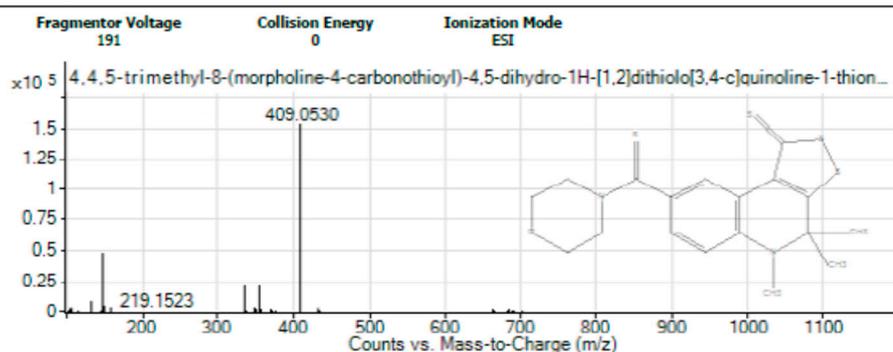
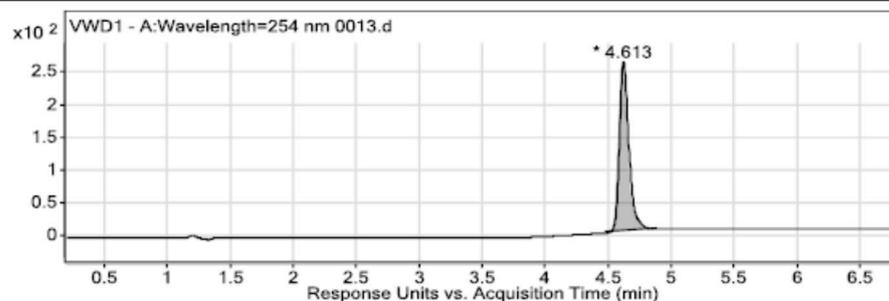


Figure S1: HPLC–HRMS–ESI spectra of 4,4,5-trimethyl-8-(morpholin-4-ylcarbonothioyl)-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione 2a

Data Filename	0013.d	Sample Name	
Sample Type	Sample	Position	Vial 33
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	3/12/2022 2:33:50 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.473	4.613	4.887	258.96	1372.07	100

User Spectra

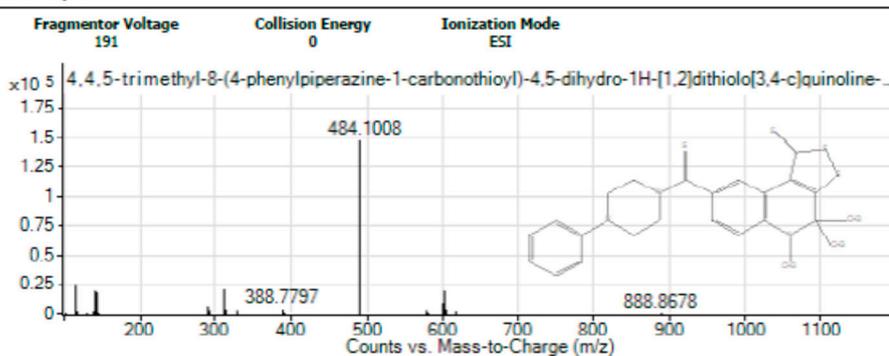
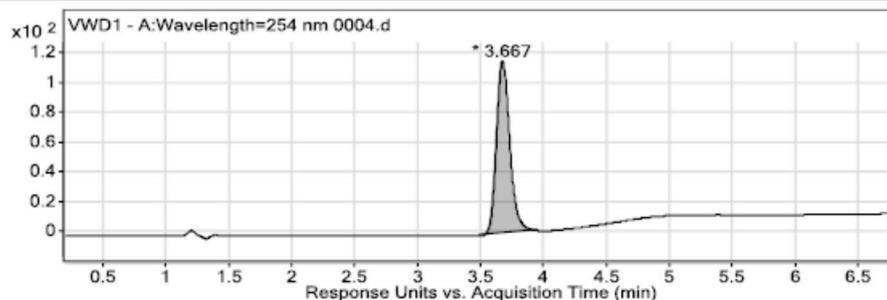


Figure S2: HPLC–HRMS–ESI spectra of 4,4,5-trimethyl-8-[(4-phenylpiperazin-1-yl)carbonothioyl]-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione 2b

Data Filename	0004.d	Sample Name	
Sample Type	Sample	Position	Vial 24
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	3/12/2022 12:41:37 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3.483	3.667	3.95	115.83	858.22	100

User Spectra

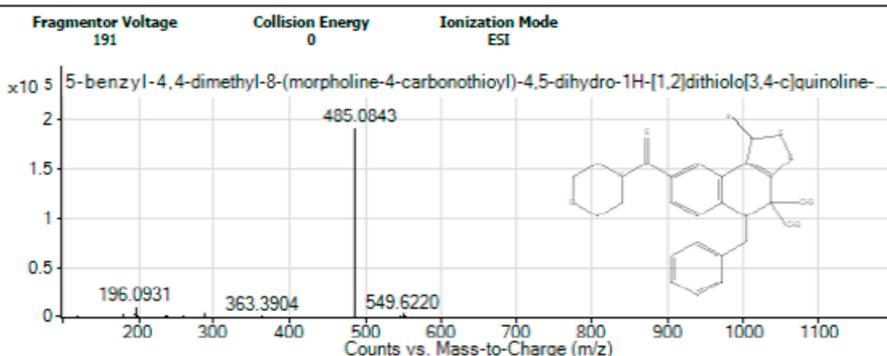
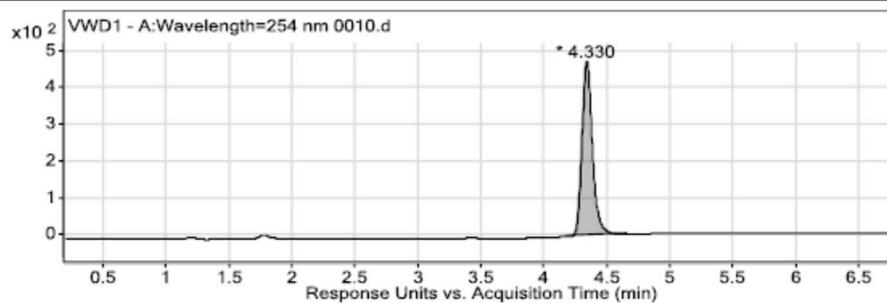


Figure S3: HPLC–HRMS–ESI spectra of 5-benzyl-4,4-dimethyl-8-(morpholin-4-ylcarbonothioyl)-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione 2c,

Data Filename	0010.d	Sample Name	
Sample Type	Sample	Position	Vial 30
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	3/12/2022 1:58:09 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.167	4.33	4.66	472.6	2709.3	100

User Spectra

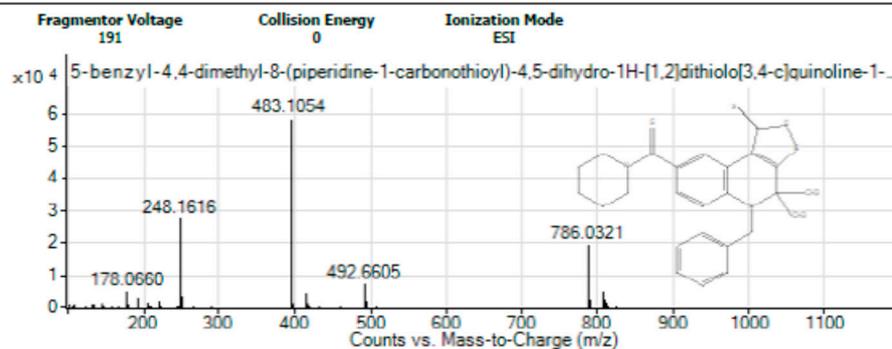
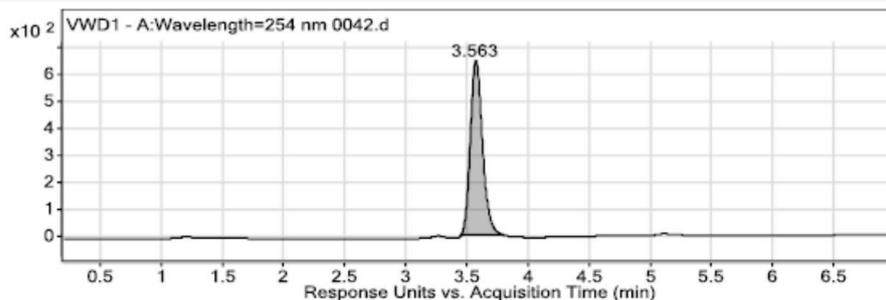


Figure S4: HPLC–HRMS–ESI spectra of 5-benzyl-4,4-dimethyl-8-(piperidin-1-ylcarbonothioyl)-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione 2d.,

Data Filename	0042.d	Sample Name	
Sample Type	Sample	Position	Vial 68
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	3/14/2022 2:00:55 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3.442	3.563	3.8	651.31	4529.68	100

User Spectra

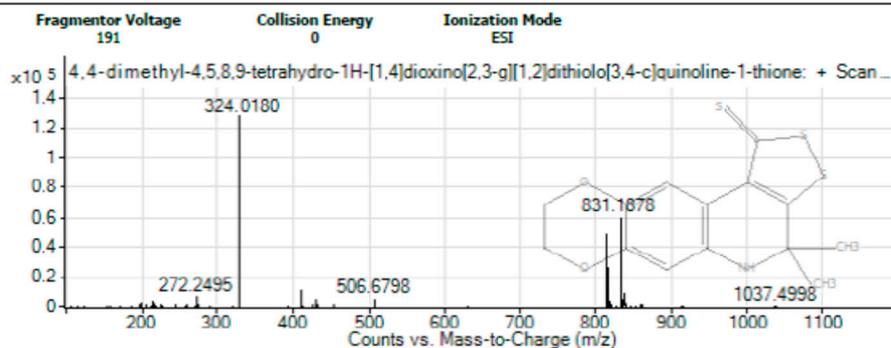
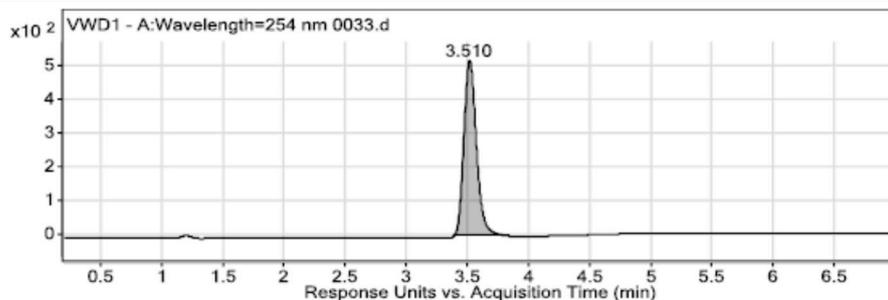


Figure S7: HPLC–HRMS–ESI spectra of 4,4-dimethyl-4,5,8,9-tetrahydro-1H-[1,4]dioxino[2,3-g][1,2]dithiolo[3,4-c]quinoline-1-thione 2h,

Data Filename	0033.d	Sample Name	
Sample Type	Sample	Position	Vial 59
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	3/14/2022 12:13:01 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3.382	3.51	3.842	518.95	3677.09	100

User Spectra

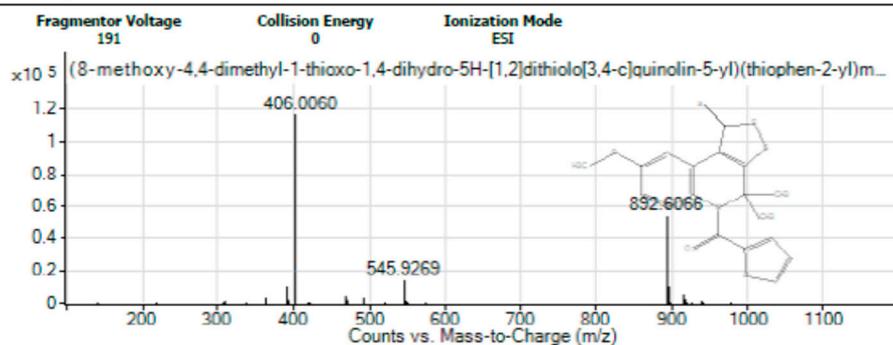


Figure S10: HPLC–HRMS–ESI spectra of 8-methoxy-4,4-dimethyl-5-(2-thienylcarbonyl)-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione 2i,

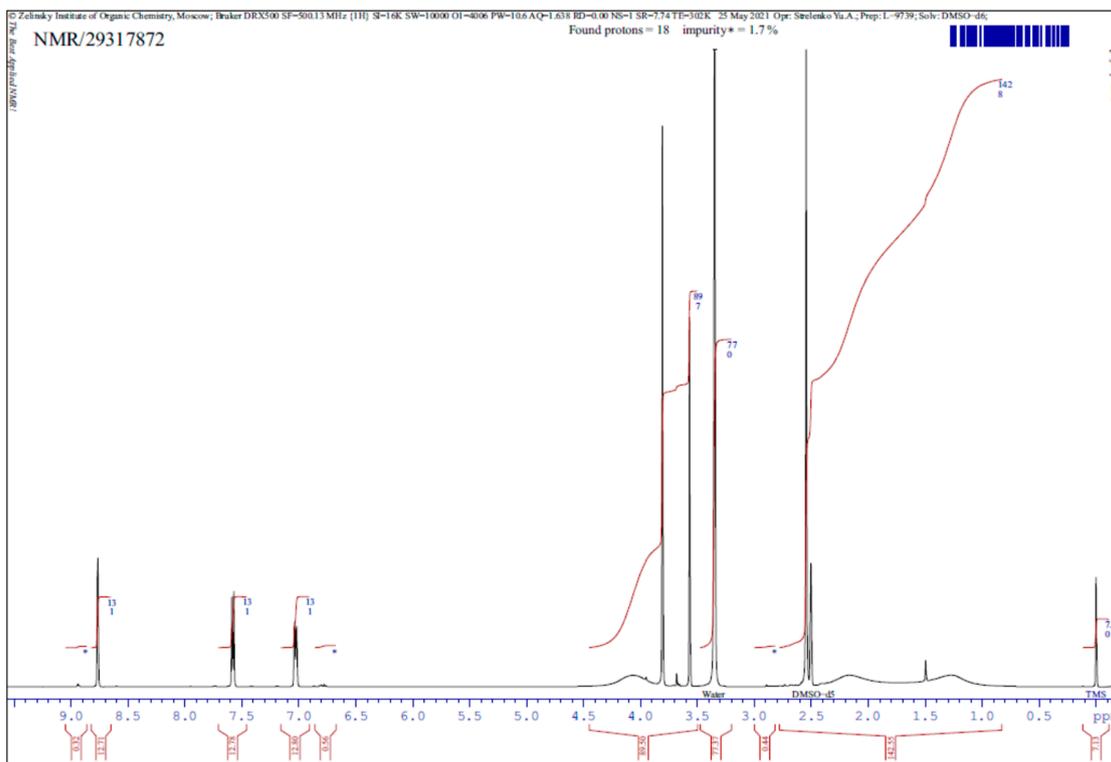


Figure S11: NMR ^1H spectra 1-[2-(8-methoxy-4,4-dimethyl-1-thioxo-1,4-dihydro-5H-[1,2]dithiolo[3,4-c]quinolin-5-yl)-2-oxoethyl]pyrrolidine-2,5-dione **2j**,

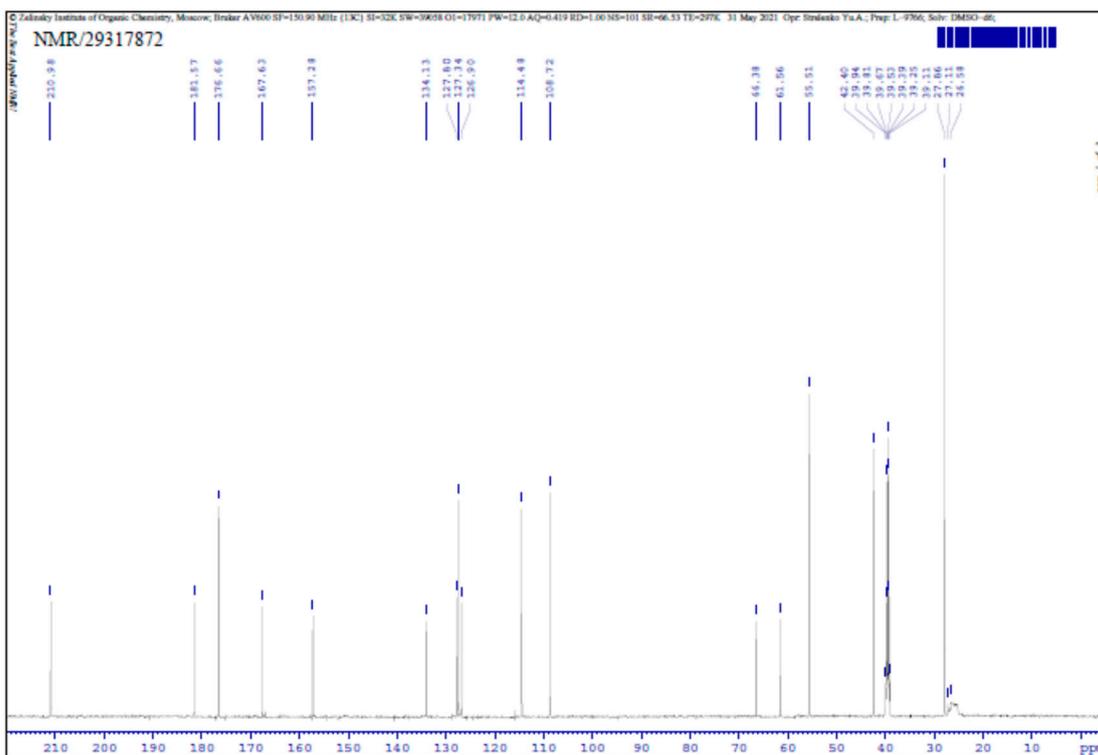
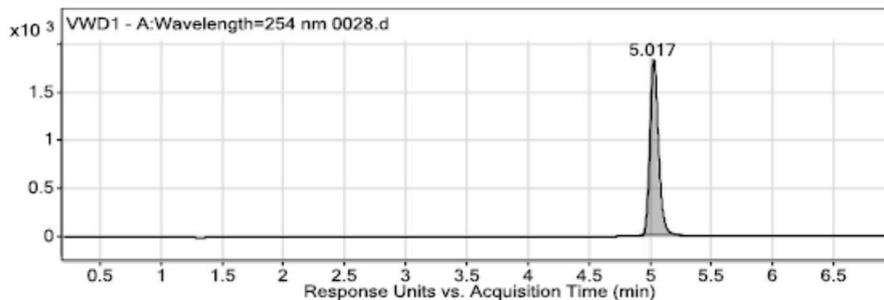


Figure S12: NMR ^{13}C spectra of 1-[2-(8-methoxy-4,4-dimethyl-1-thioxo-1,4-dihydro-5H-[1,2]dithiolo[3,4-c]quinolin-5-yl)-2-oxoethyl]pyrrolidine-2,5-dione **2j**,

Data Filename	0028.d	Sample Name	
Sample Type	Sample	Position	Vial 54
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	3/14/2022 11:13:07 AM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.913	5.017	5.26	1837.64	8894.43	100

User Spectra

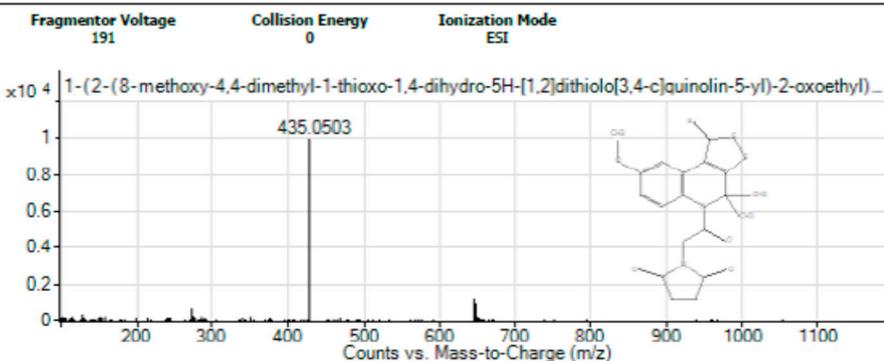


Figure S13: HPLC–HRMS–ESI spectra of 1-[2-(8-methoxy-4,4-dimethyl-1-thioxo-1,4-dihydro-5H-[1,2]dithiolo[3,4-c]quinolin-5-yl)-2-oxoethyl]pyrrolidine-2,5-dione 2j,

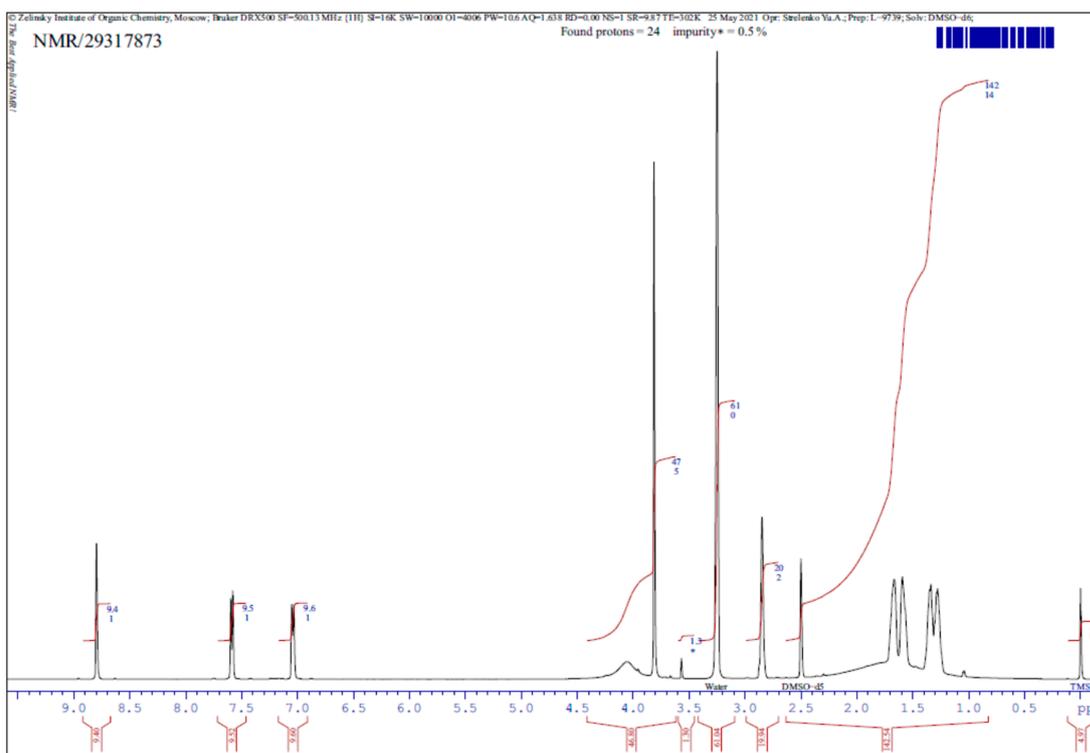


Figure S14: NMR ^1H spectra of 2-[2-(8-methoxy-4,4-dimethyl-1-thioxo-1,4-dihydro-5H-[1,2]dithiolo[3,4-c]quinolin-5-yl)-2-oxoethyl]hexahydro-1H-isoindole-1,3(2H)-dione 2k,

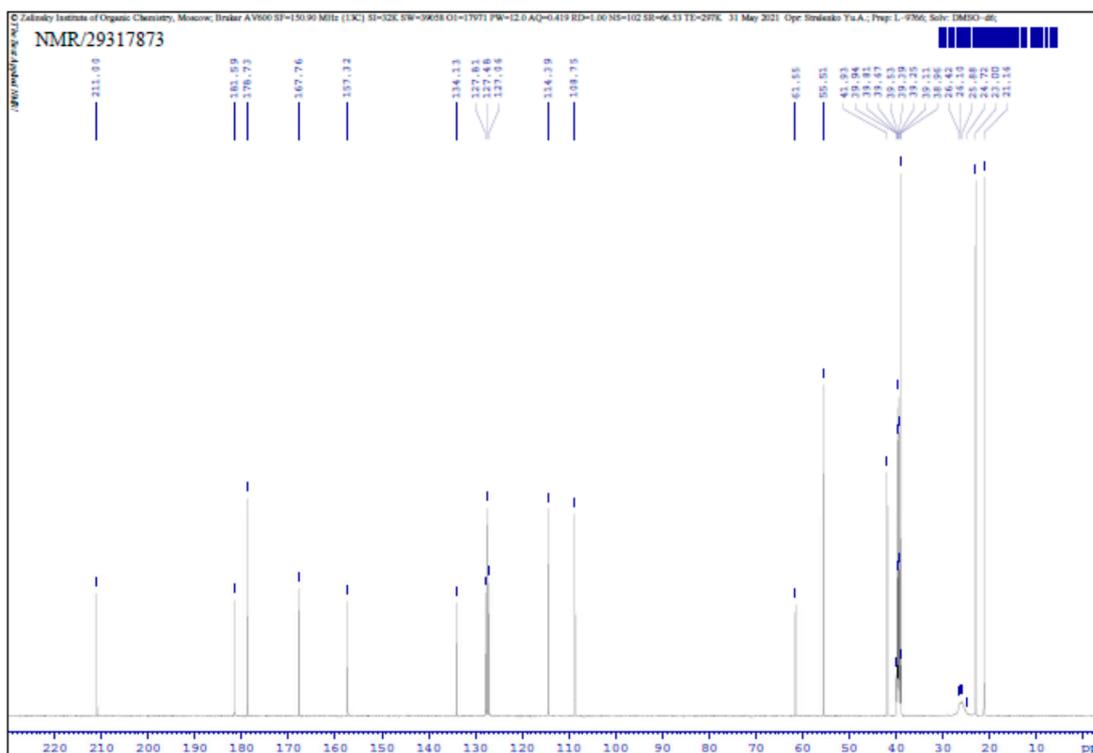
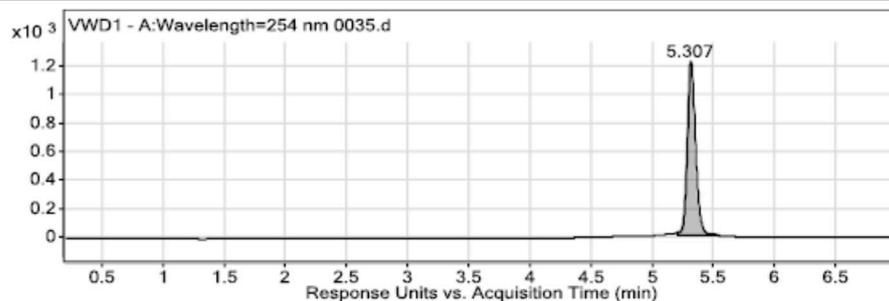


Figure S15: NMR ^{13}C spectra of 2-[2-(8-methoxy-4,4-dimethyl-1-thioxo-1,4-dihydro-5H-[1,2]dithiolo[3,4-c]quinolin-5-yl)-2-oxoethyl]hexahydro-1H-isoindole-1,3(2H)-dione 2k,

Data Filename	0035.d	Sample Name	
Sample Type	Sample	Position	Vial 61
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	3/14/2022 12:37:01 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	5.207	5.307	5.55	1227.8	5933.67	100

User Spectra

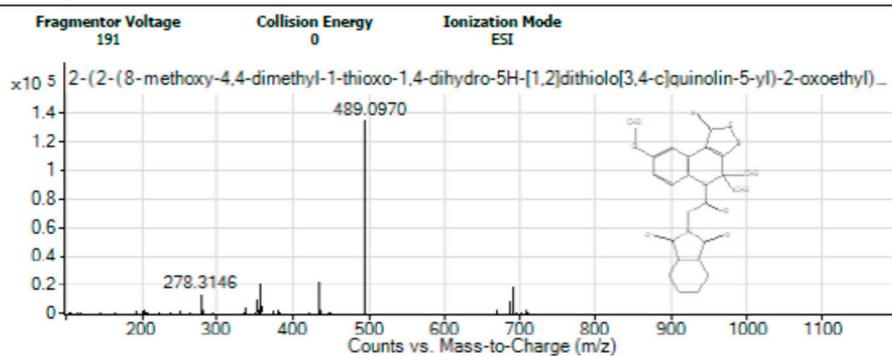


Figure S16: HPLC–HRMS–ESI spectra of 2-[2-(8-methoxy-4,4-dimethyl-1-thioxo-1,4-dihydro-5H-[1,2]dithiolo[3,4-c]quinolin-5-yl)-2-oxoethyl]hexahydro-1H-isoindole-1,3(2H)-dione 2k,

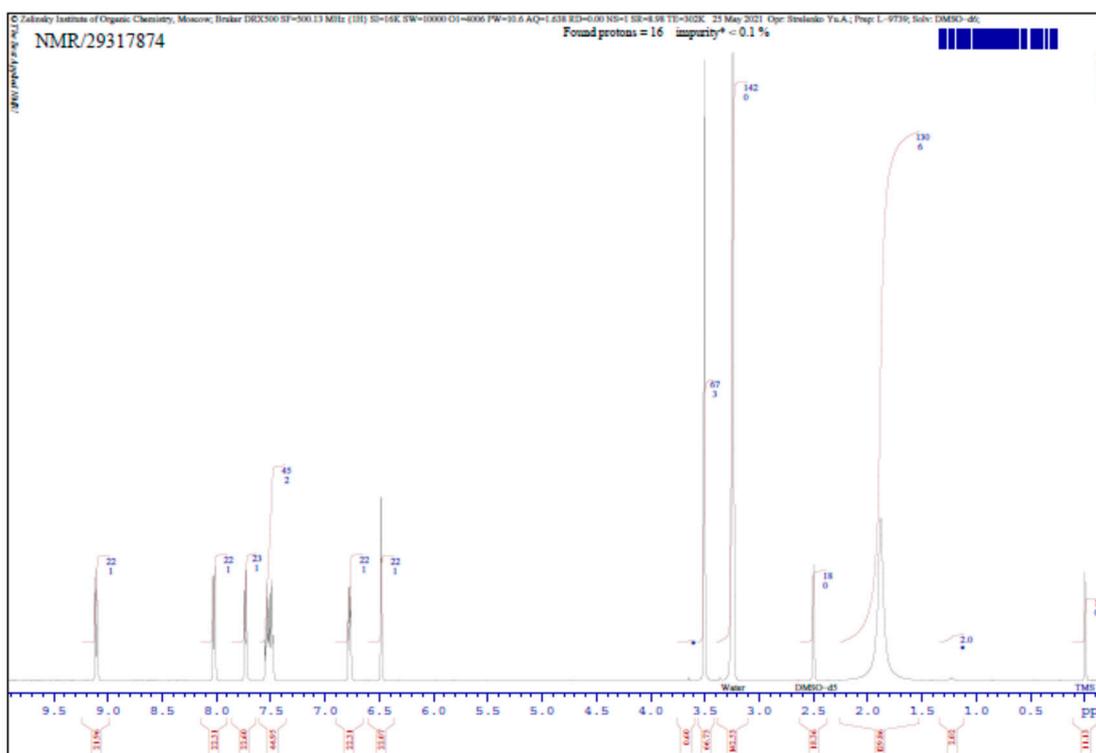


Figure S17: NMR ^1H spectra of 5-[(3-chloro-1-benzothien-2-yl)carbonyl]-7-methoxy-4,4-dimethyl-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione **2l**,

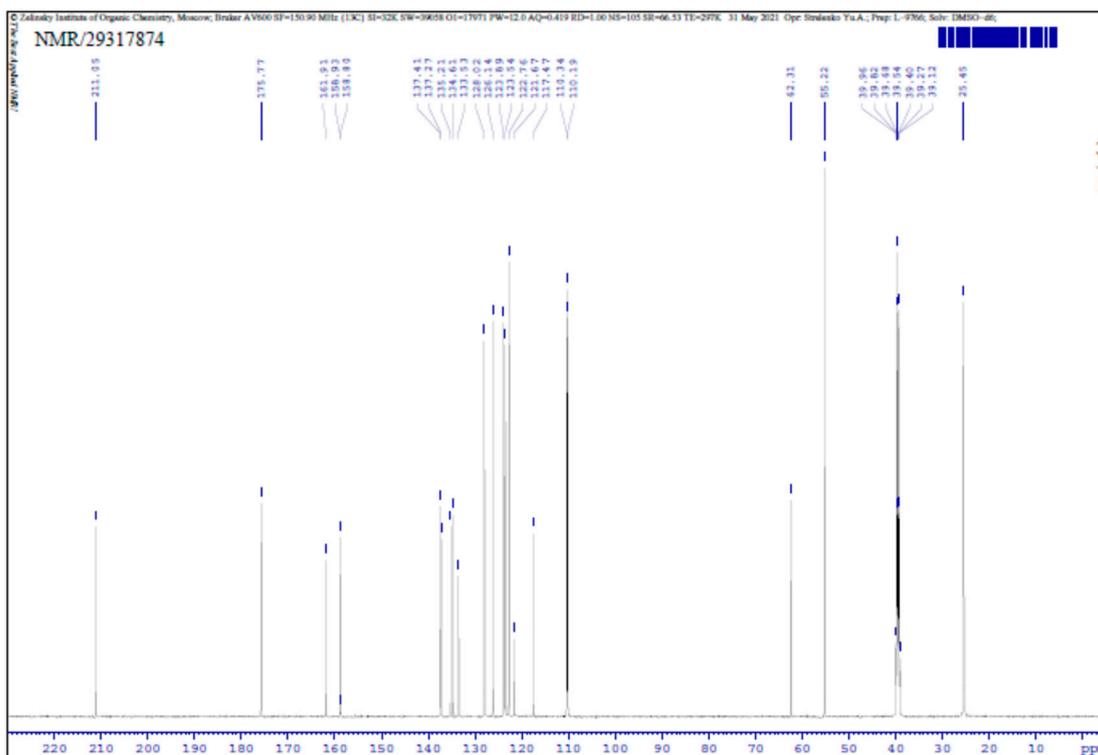
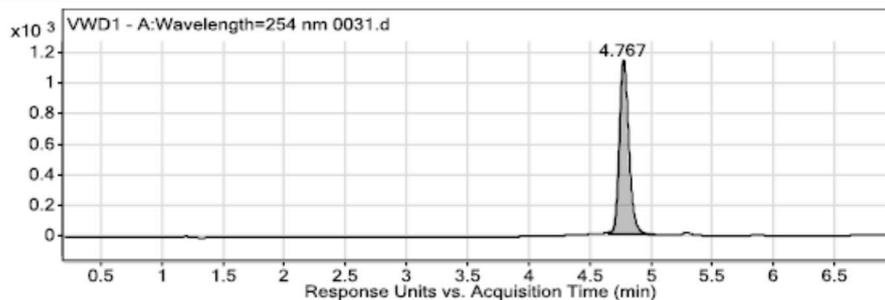


Figure S18: NMR ^{13}C spectra of 5-[(3-chloro-1-benzothien-2-yl)carbonyl]-7-methoxy-4,4-dimethyl-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione **2l**,

Data Filename	0031.d	Sample Name	
Sample Type	Sample	Position	Vial 57
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	3/14/2022 11:49:05 AM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.653	4.767	5.03	1143.6	6139.81	100

User Spectra

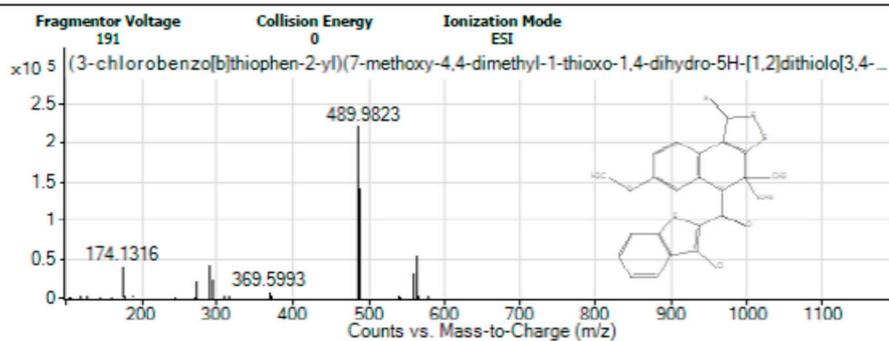
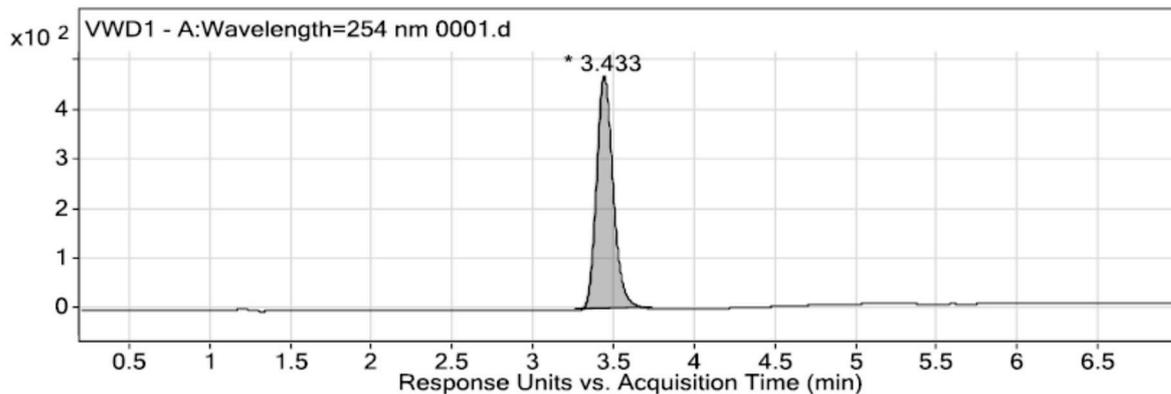


Figure S19: HPLC–HRMS–ESI spectra of 5-[(3-chloro-1-benzothien-2-yl)carbonyl]-7-methoxy-4,4-dimethyl-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione 2l,

Data Filename 0001.d **Sample Name**
Sample Type Sample **Position** Vial 21
Instrument Name Instrument 1 **User Name**
Acq Method ACN-H2O_60-40.m **Acquired Time** 3/12/2022 12:05:47 PM
IRM Calibration Status Success **DA Method** 111.m
Comment

Sample Group **Info.**
Stream Name LC 1 **Acquisition SW** 6200 series TOF/6500 series
Version Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3.26	3.433	3.74	469.81	3341.9	100

User Spectra

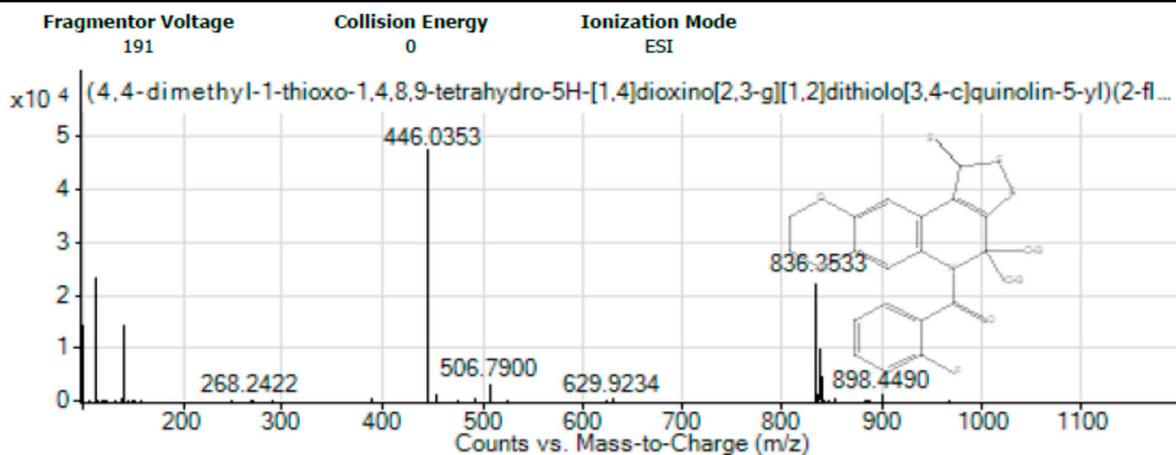


Figure S22: HPLC–HRMS–ESI spectra of 5-(2-fluorobenzoyl)-4,4-dimethyl-4,5,8,9-tetrahydro-1H-[1,4]dioxino[2,3-g][1,2]dithiolo[3,4-c]quinoline-1-thione 2m,

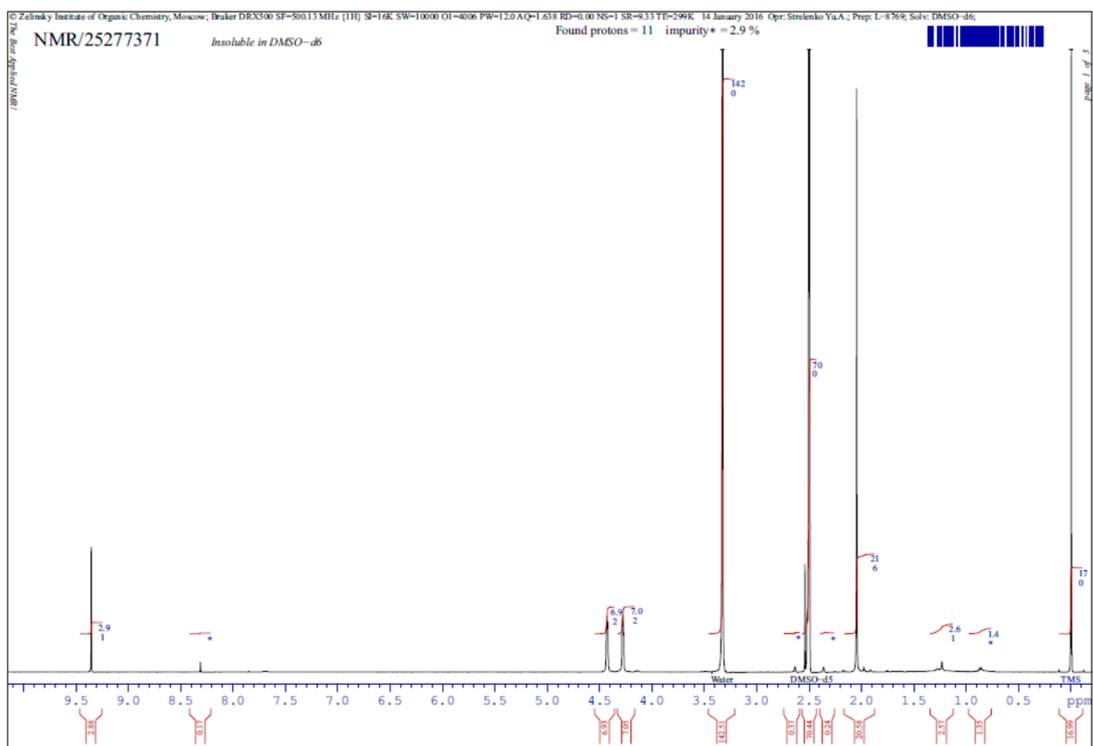
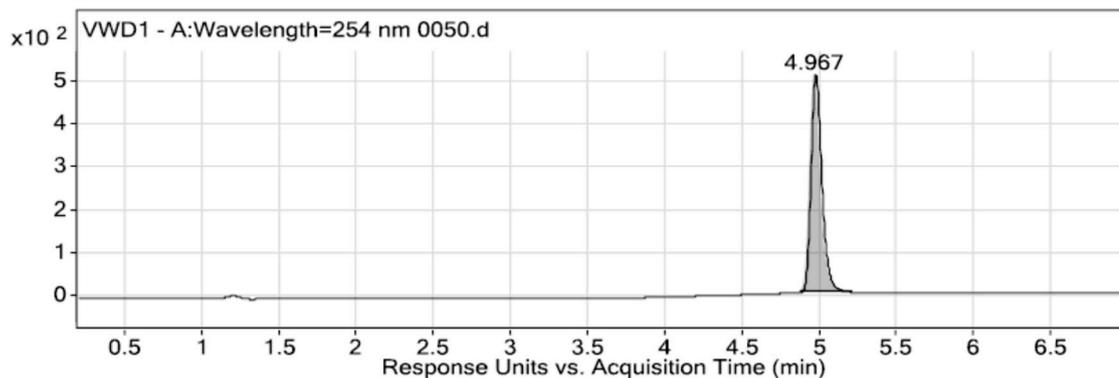


Figure S23: NMR 1H spectra of 8,8-dimethyl-11-thioxo-2,3,8,11-tetrahydro[1,4]dioxino[2,3-g][1,2]dithiolo[3,4-c]pyrrolo[3,2,1-ij]quinoline-5,6-dione 2n,

Data Filename	0050.d	Sample Name	
Sample Type	Sample	Position	Vial 76
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	3/14/2022 3:36:27 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.877	4.967	5.21	505.23	2480.1	100

User Spectra

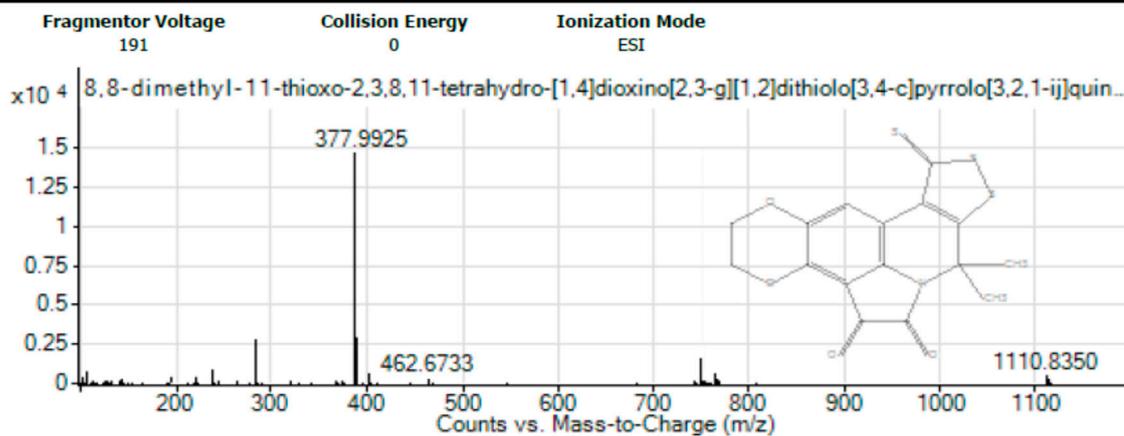


Figure S24: HPLC–HRMS–ESI spectra of 8,8-dimethyl-11-thioxo-2,3,8,11-tetrahydro[1,4]dioxino[2,3-g][1,2]dithiolo[3,4-c]pyrrolo[3,2,1-ij]quinoline-5,6-dione 2n,

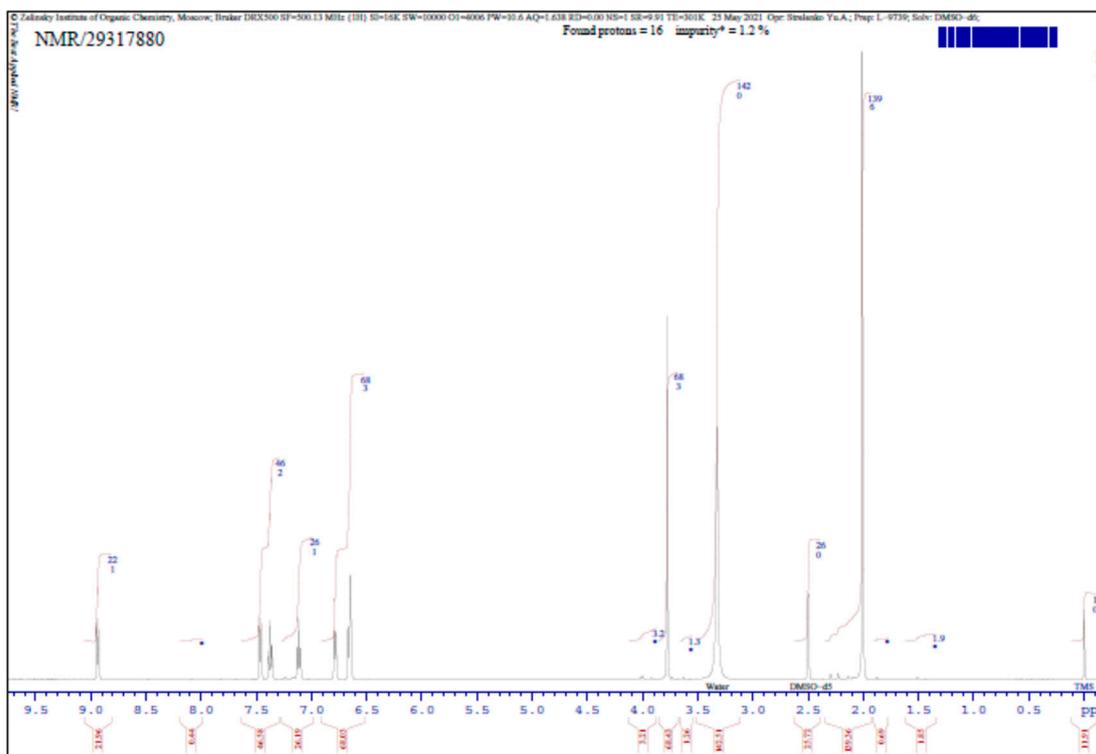


Figure S25: NMR ^1H spectra of 10-[(3-methoxyphenyl)imino]-7,7-dimethyl-7,10-dihydro[1,2]dithiolo[3,4-c]pyrrolo[3,2,1-ij]quinoline-4,5-dione **2q**,

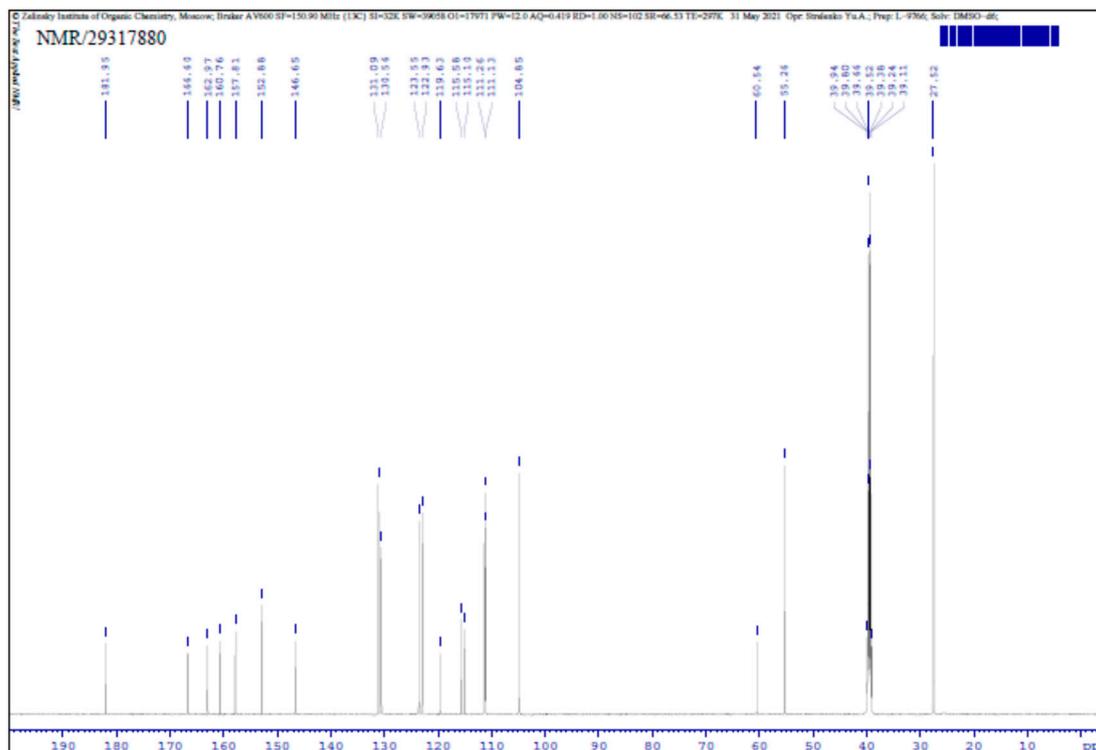
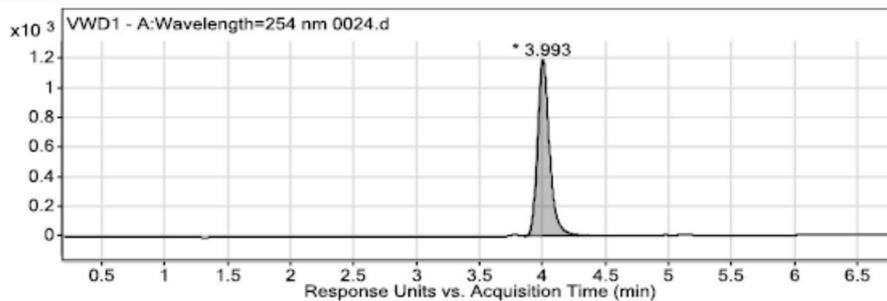


Figure S26: NMR ^{13}C spectra of 10-[(3-methoxyphenyl)imino]-7,7-dimethyl-7,10-dihydro[1,2]dithiolo[3,4-c]pyrrolo[3,2,1-ij]quinoline-4,5-dione **2q**,

Data Filename	0024.d	Sample Name	
Sample Type	Sample	Position	Vial 44
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	3/12/2022 4:44:26 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3.86	3.993	4.363	1198.81	8022.31	100

User Spectra

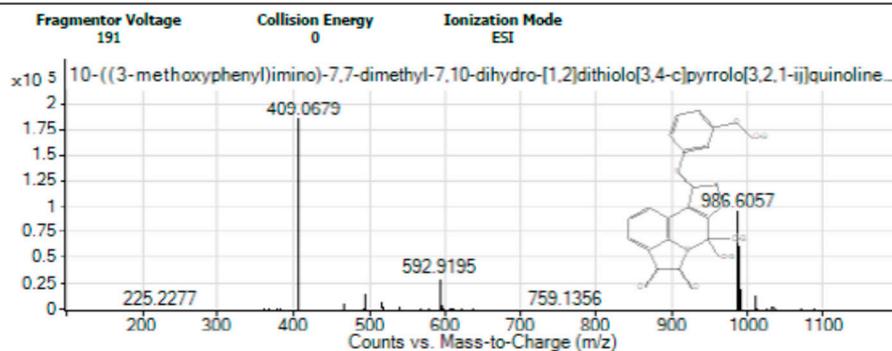


Figure S27: HPLC–HRMS–ESI spectra of 10-[(3-methoxyphenyl)imino]-7,7-dimethyl-7,10-dihydro[1,2]dithiolo[3,4-c]pyrrolo[3,2,1-ij]quinoline-4,5-dione 2q.