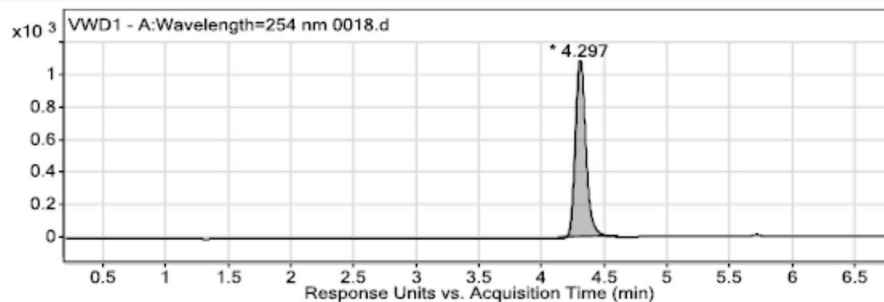


| | | | |
|-------------------------------|-----------------|-----------------------|-----------------------------|
| Data Filename | 0018.d | Sample Name | |
| Sample Type | Sample | Position | Vial 38 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | ACN-H2O_60-40.m | Acquired Time | 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

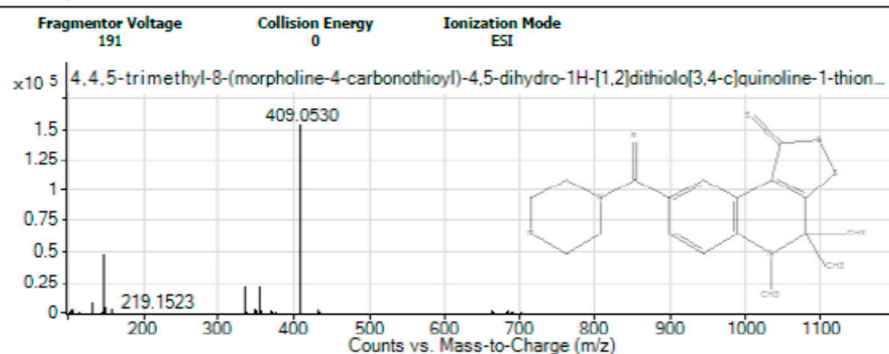
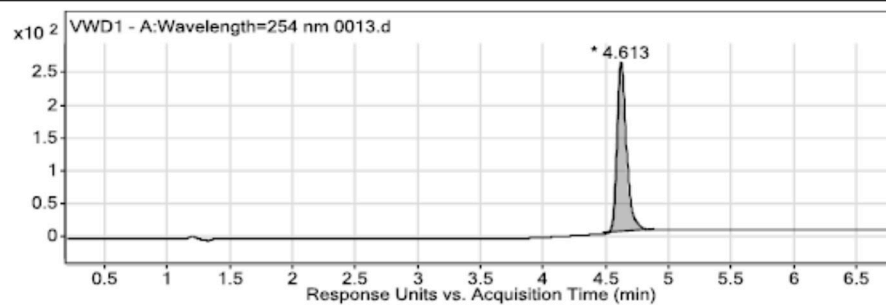


Figure S1: HPLC–HRMS–ESI spectra of 4,4,5-trimethyl-8-(morpholin-4-ylcarbonothioyl)-4,5-dihydro-1H-[1,2]dithiol[3,4-c]quinoline-1-thione 2a

| | | | |
|-------------------------------|-----------------|----------------------|----------------------|
| 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

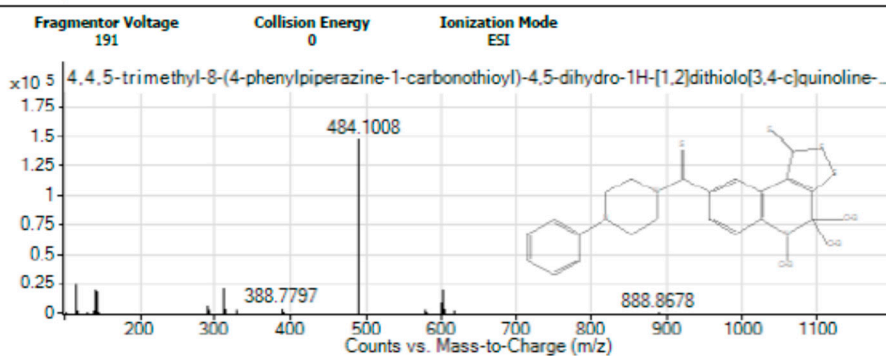
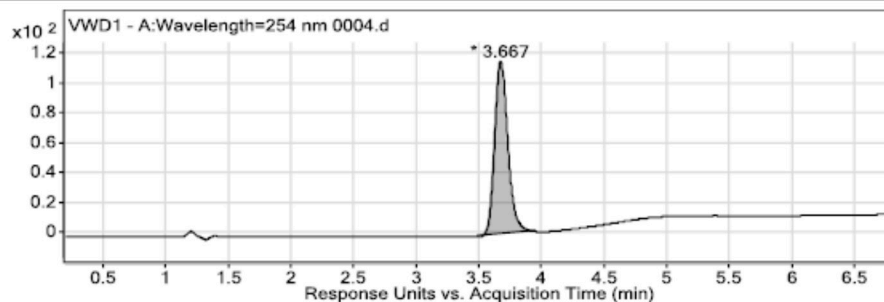


Figure S2: HPLC–HRMS–ESI spectra of 4,4,5-trimethyl-8-[(4-phenylpiperazin-1-yl)carbonothioyl]-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione 2b

| | | | |
|-------------------------------|-----------------|----------------------|-----------------------|
| 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

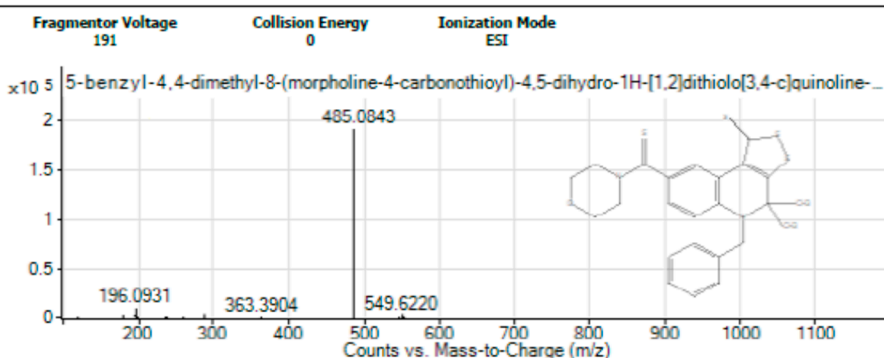
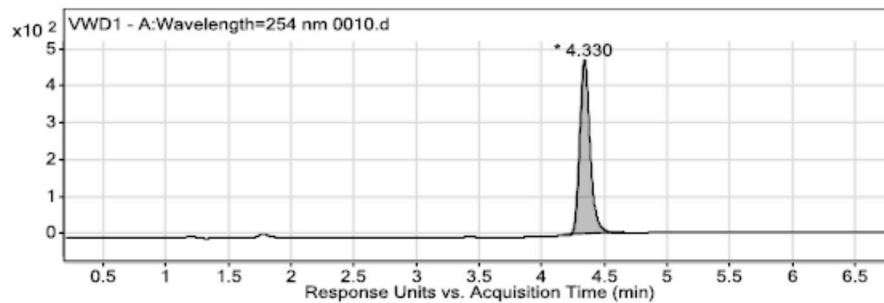


Figure S3: HPLC–HRMS–ESI spectra of 5-benzyl-4,4-dimethyl-8-(morpholin-4-ylcarbonothioyl)-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione 2c,

| | | | |
|-------------------------------|-----------------|-----------------------|-----------------------------|
| 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

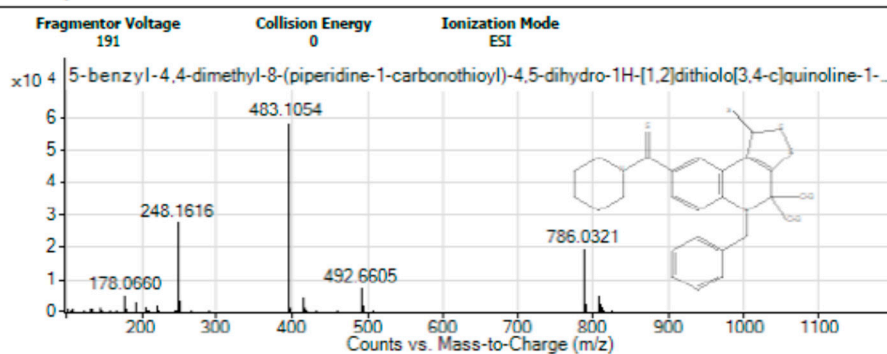


Figure S4: HPLC–HRMS–ESI spectra of 5-benzyl-4,4-dimethyl-8-(piperidin-1-ylcarbonothioyl)-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione 2d.,

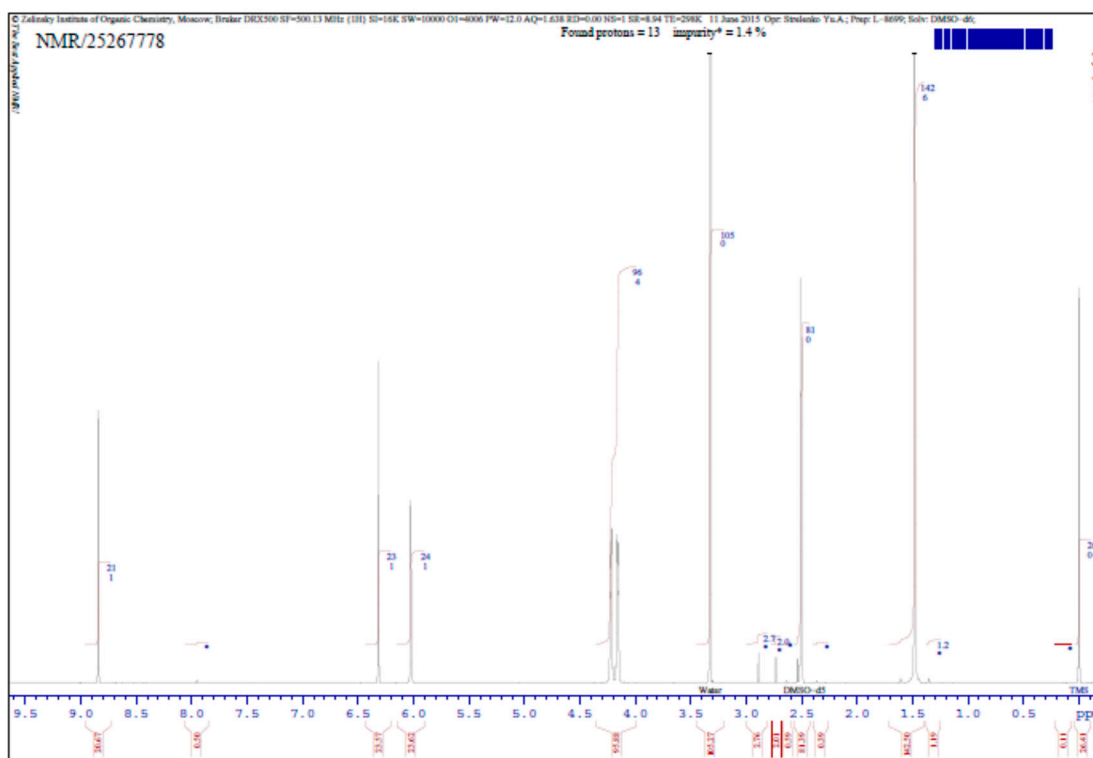


Figure S5: NMR ^1H spectra of 4,4-dimethyl-4,5,8,9-tetrahydro-1H-[1,4]dioxino[2,3-g][1,2]dithiolo[3,4-c]quinoline-1-thione 2h,

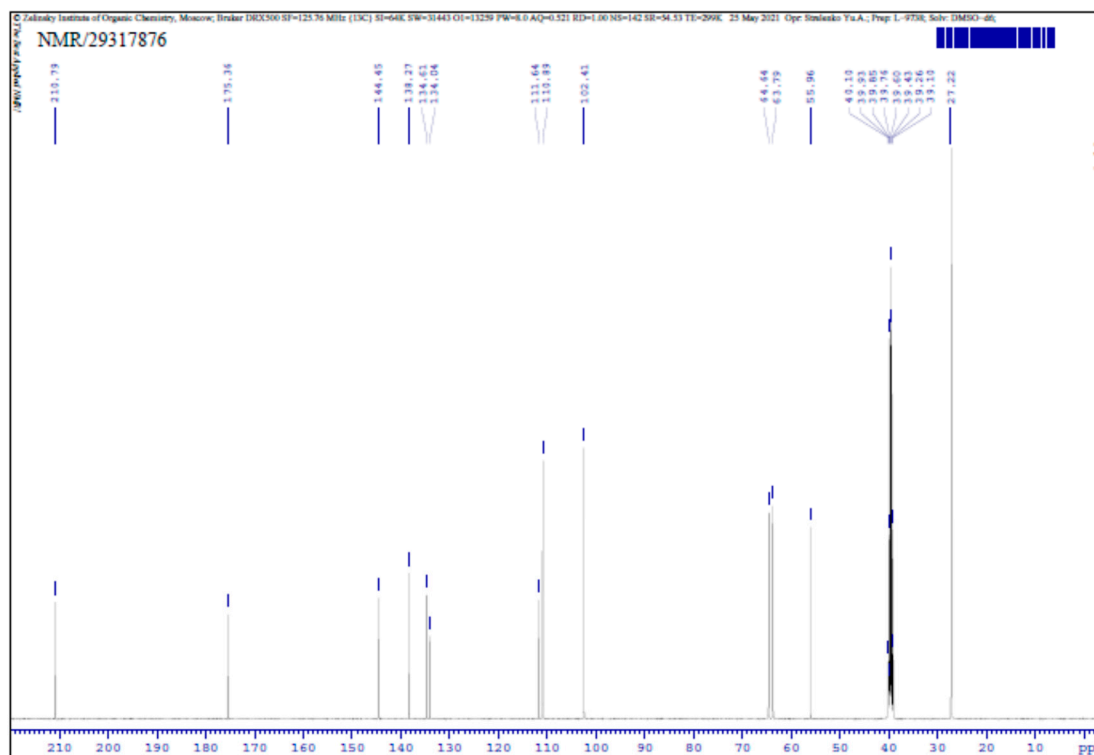
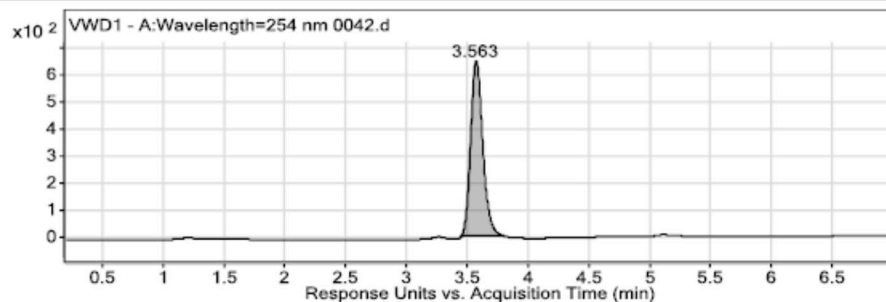


Figure S6: NMR ^{13}C spectra of 4,4-dimethyl-4,5,8,9-tetrahydro-1H-[1,4]dioxino[2,3-g][1,2]dithiolo[3,4-c]quinoline-1-thione 2h,

| | | | |
|-------------------------------|-----------------|----------------------|----------------------|
| Data Filename | 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

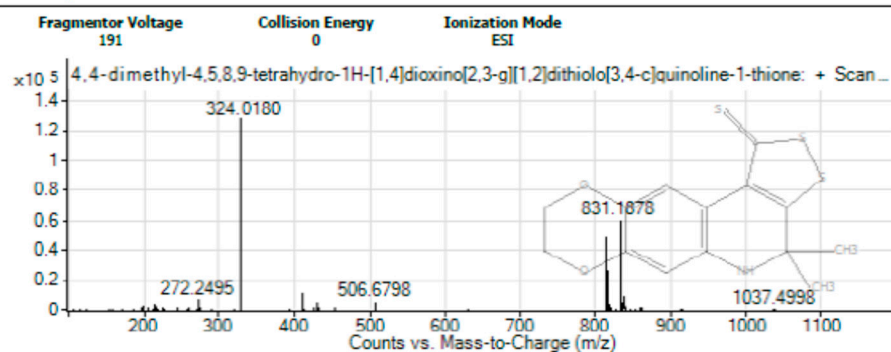


Figure S7: HPLC–HRMS–ESI spectra of 4,4-dimethyl-4,5,8,9-tetrahydro-1H-[1,4]dioxino[2,3-g][1,2]dithiolo[3,4-c]quinoline-1-thione 2h,

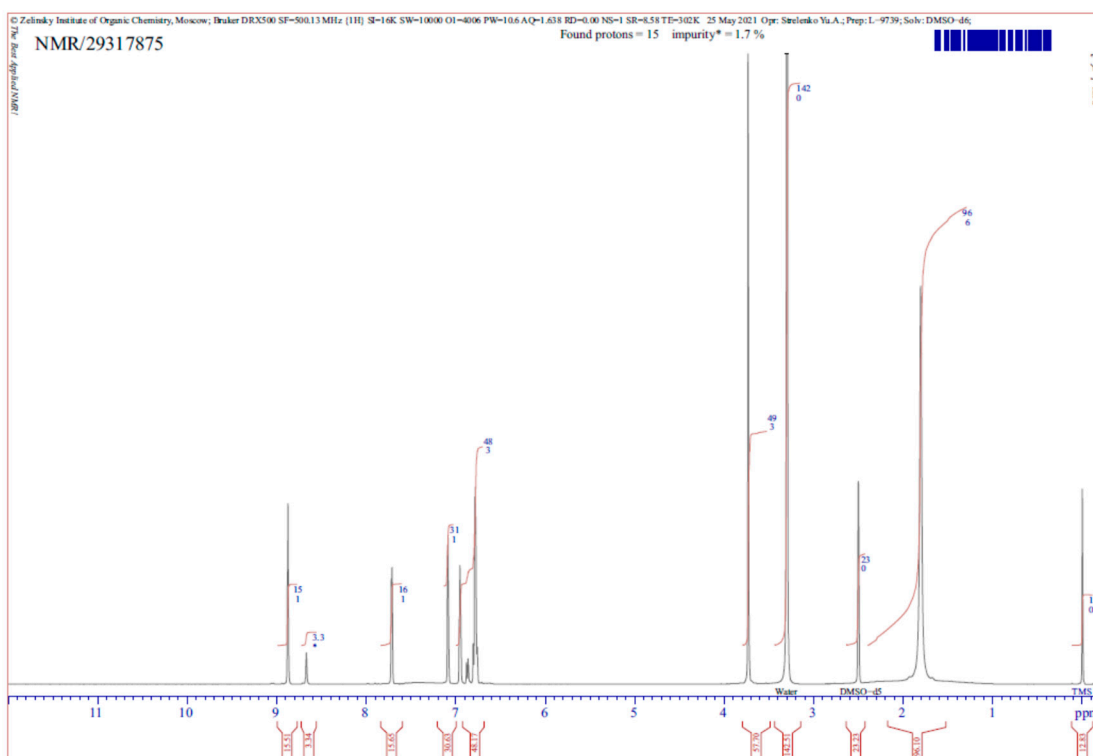


Figure S8: NMR ^1H spectra of 8-methoxy-4,4-dimethyl-5-(2-thienylcarbonyl)-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione **2i**,

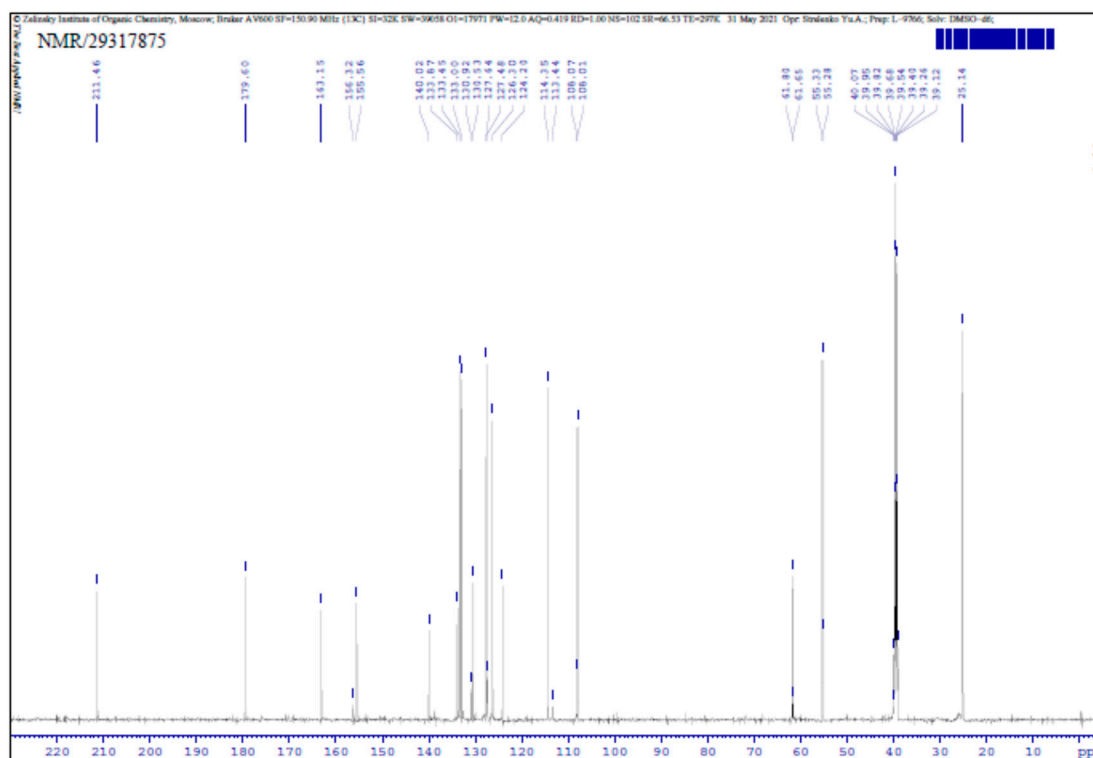
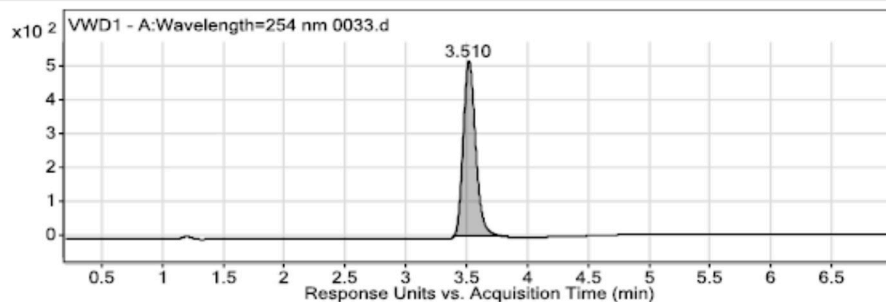


Figure S9: NMR ^{13}C spectra of 8-methoxy-4,4-dimethyl-5-(2-thienylcarbonyl)-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione **2i**,

| | | | |
|-------------------------------|-----------------|-----------------------|-----------------------------|
| 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

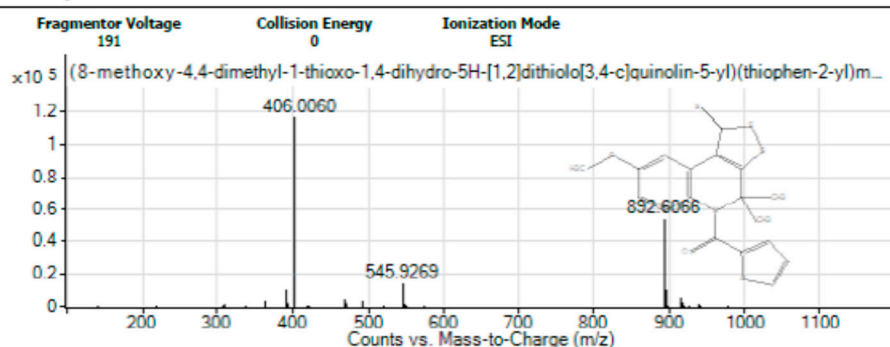


Figure S10: HPLC–HRMS–ESI spectra of 8-methoxy-4,4-dimethyl-5-(2-thienylcarbonyl)-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione 2i,

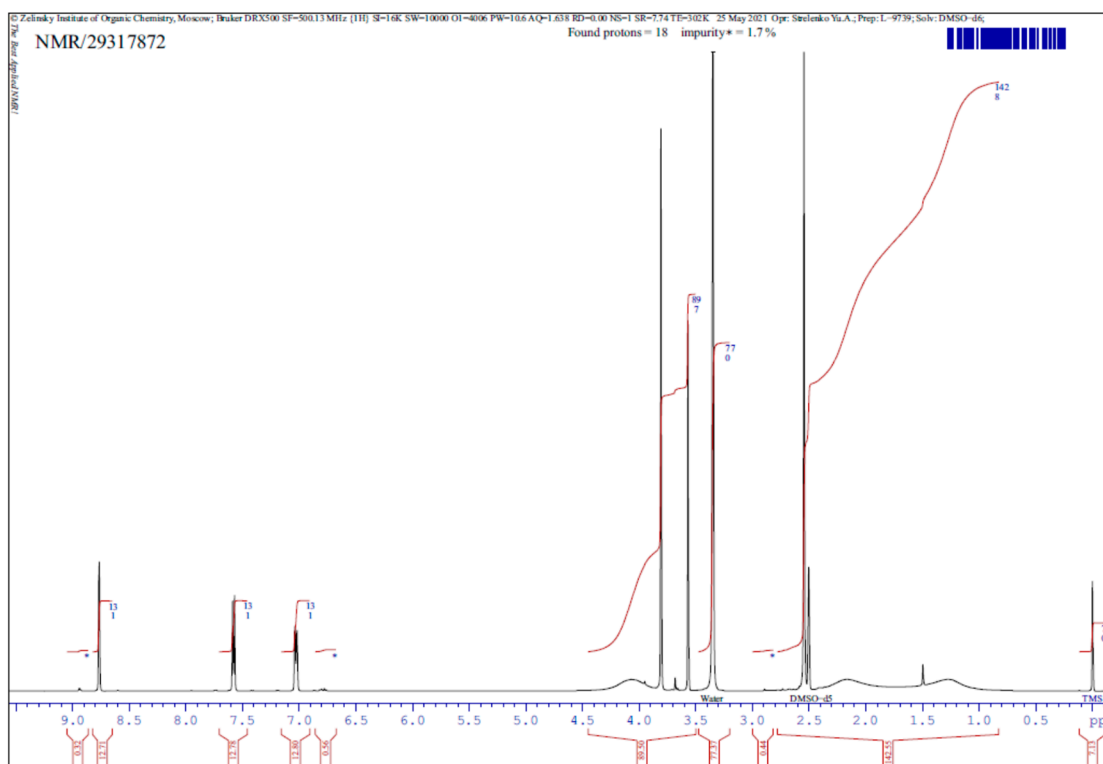


Figure S11: NMR ^1H spectra 1-[2-(8-methoxy-4,4-dimethyl-1-thioxo-1,4-dihydro-5H-[1,2]dithiolo[3,4-c]quinolin-5-yl)-2-oxoethyl]pyrrolidine-2,5-dione 2j,

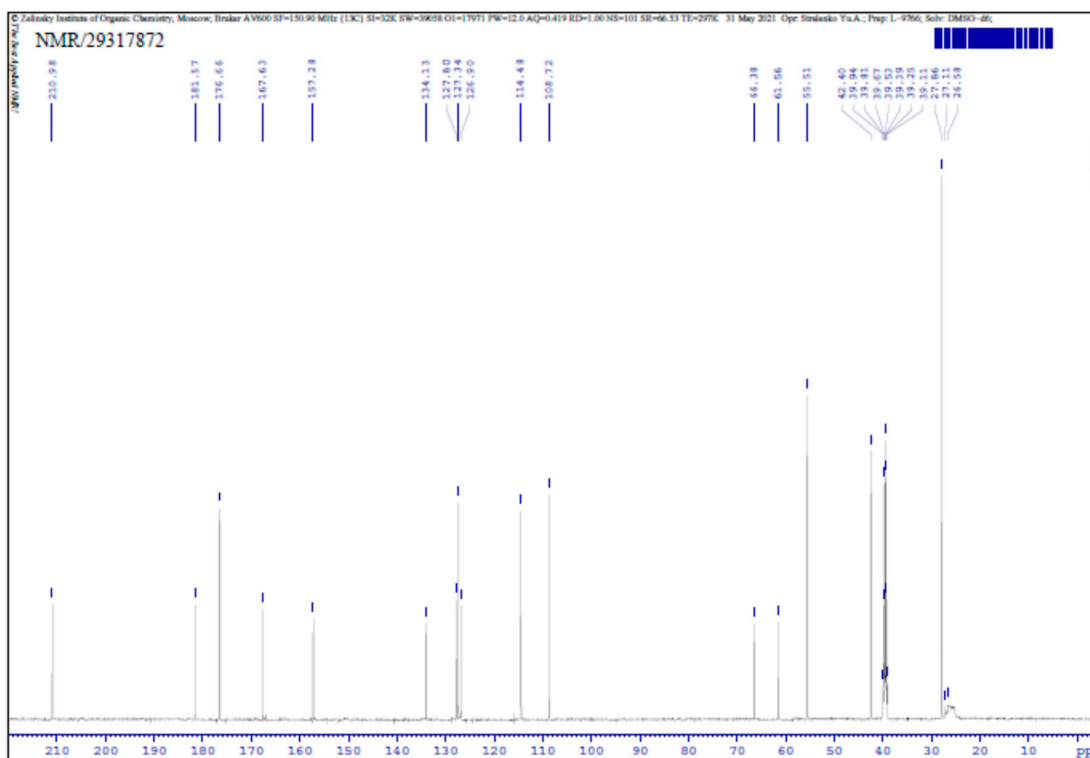
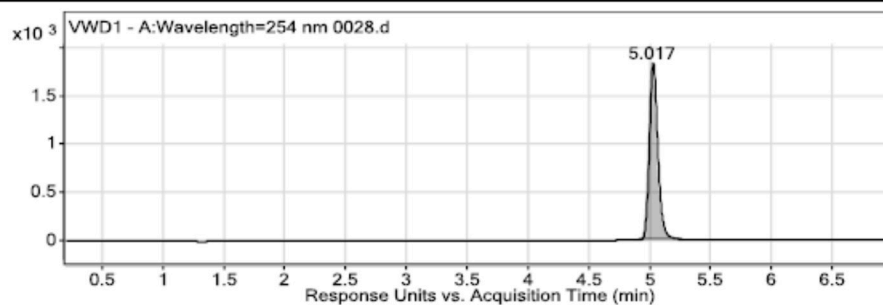


Figure S12: NMR ^{13}C spectra of 1-[2-(8-methoxy-4,4-dimethyl-1-thioxo-1,4-dihydro-5H-[1,2]dithiolo[3,4-c]quinolin-5-yl)-2-oxoethyl]pyrrolidine-2,5-dione 2j,

| | | | |
|-------------------------------|-----------------|-----------------------|-----------------------------|
| 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

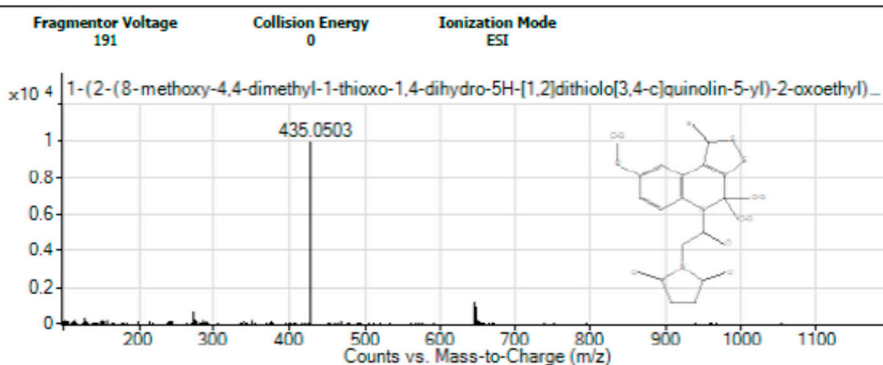


Figure S13: HPLC–HRMS–ESI spectra of 1-[2-(8-methoxy-4,4-dimethyl-1-thioxo-1,4-dihydro-5H-[1,2]dithiolo[3,4-c]quinolin-5-yl)-2-oxoethyl]pyrrolidine-2,5-dione 2j,

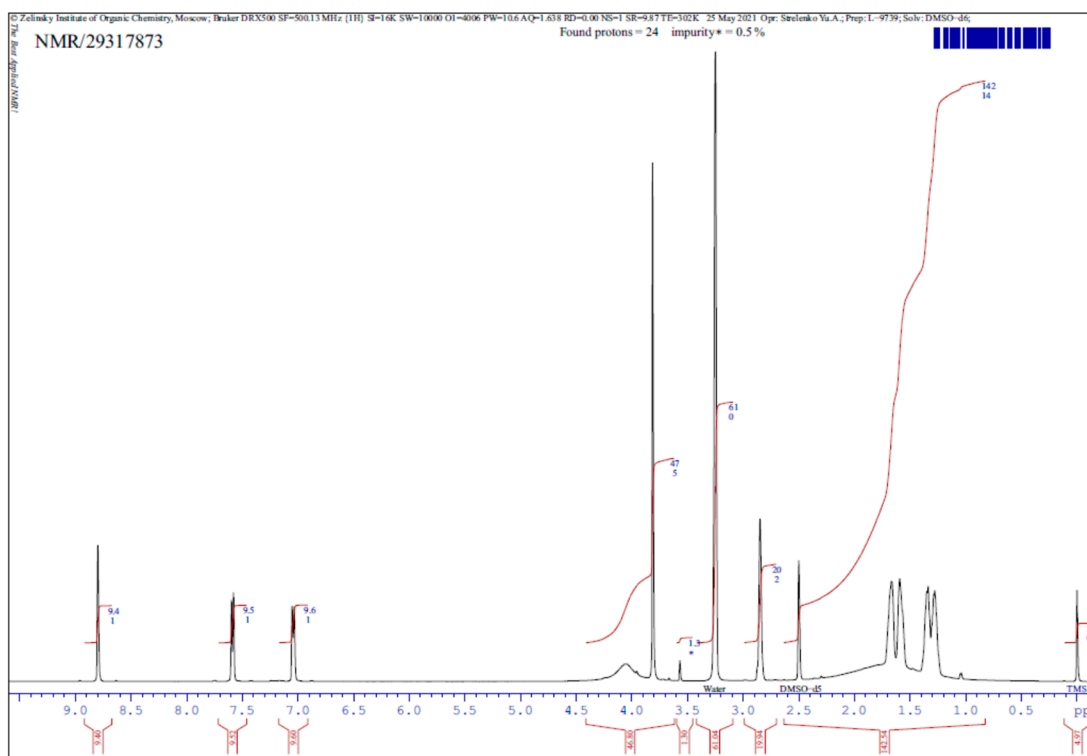


Figure S14: NMR ¹H spectra of 2-[2-(8-methoxy-4,4-dimethyl-1-thioxo-1,4-dihydro-5H-[1,2]dithiolo[3,4-c]quinolin-5-yl)-2-oxoethyl]hexahydro-1H-isoindole-1,3(2H)-dione 2k,

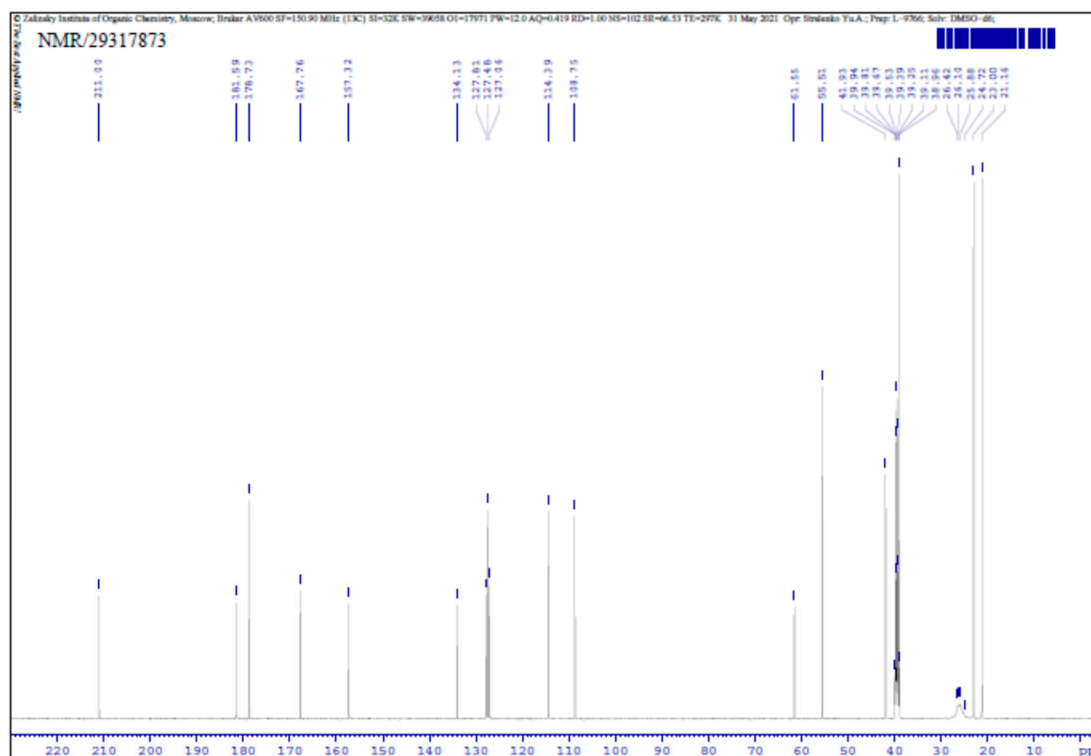
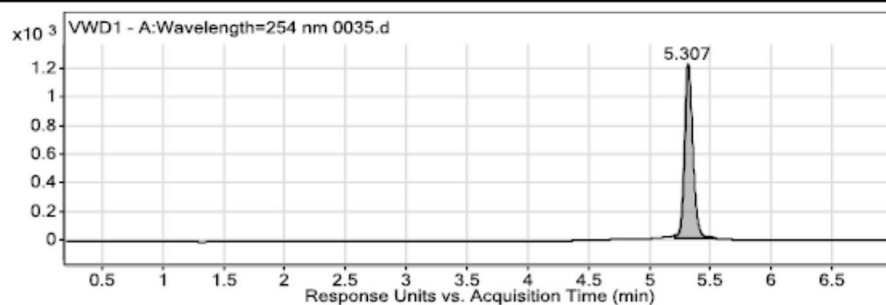


Figure S15: NMR ¹³C spectra of 2-[2-(8-methoxy-4,4-dimethyl-1-thioxo-1,4-dihydro-5H-[1,2]dithiolo[3,4-c]quinolin-5-yl)-2-oxoethyl]hexahydro-1H-isoindole-1,3(2H)-dione 2k,

| | | | |
|------------------------|-----------------|----------------|-----------------------------|
| 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 8.06.01 (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

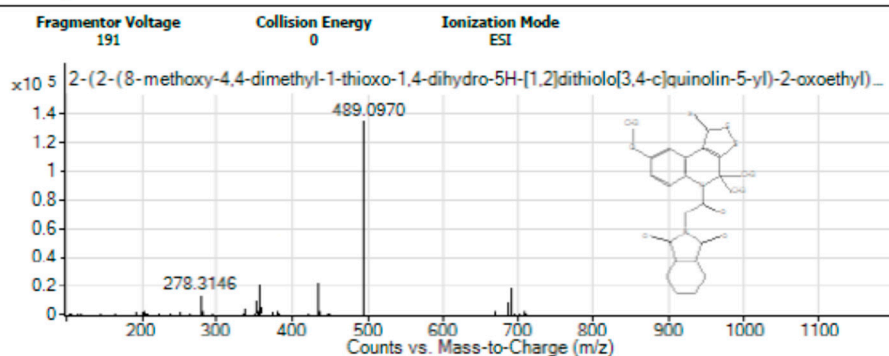


Figure S16: HPLC–HRMS–ESI spectra of 2-[2-(8-methoxy-4,4-dimethyl-1-thioxo-1,4-dihydro-5H-[1,2]dithiol[3,4-c]quinolin-5-yl)-2-oxoethyl]hexahydro-1H-isoindole-1,3(2H)-dione 2k,

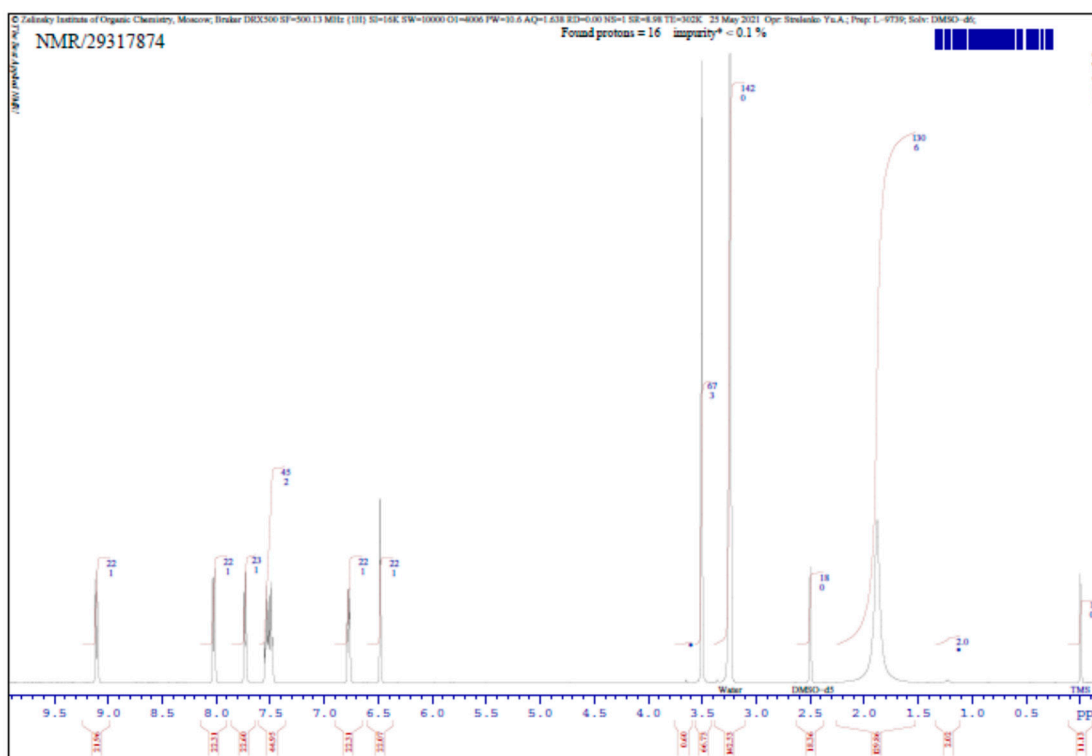


Figure S17: NMR ¹H spectra of 5-[(3-chloro-1-benzothien-2-yl)carbonyl]-7-methoxy-4,4-dimethyl-4,5-dihydro-1H-[1,2]dithiol[3,4-c]quinoline-1-thione 2l,

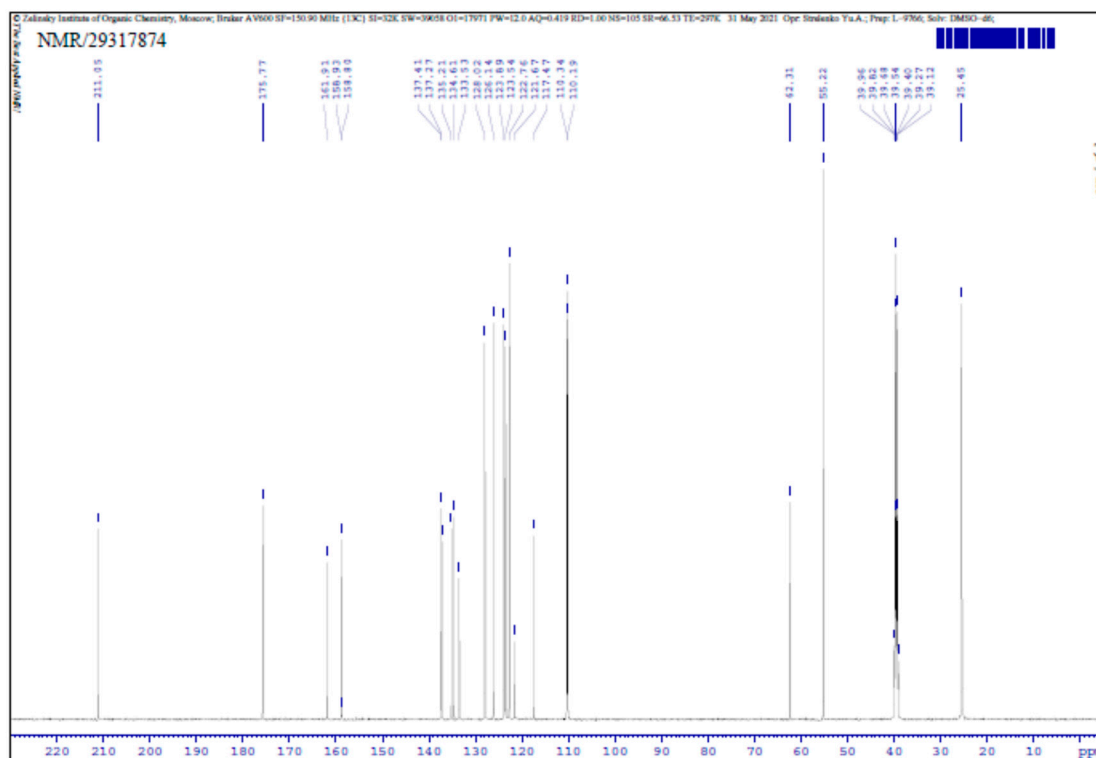
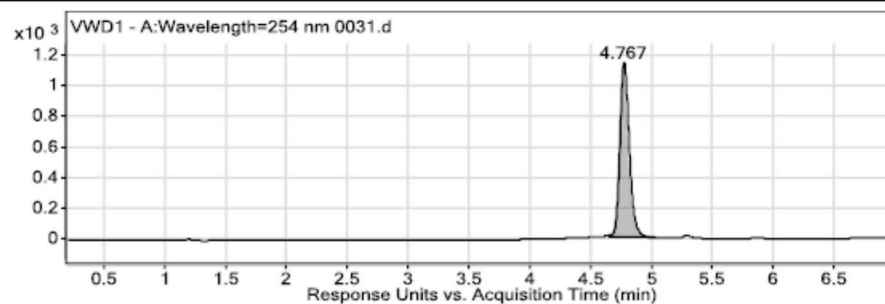


Figure S18: NMR ¹³C spectra of 5-[(3-chloro-1-benzothien-2-yl)carbonyl]-7-methoxy-4,4-dimethyl-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione 2l,

| | | | |
|------------------------|-----------------|---------------|-----------------------|
| 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

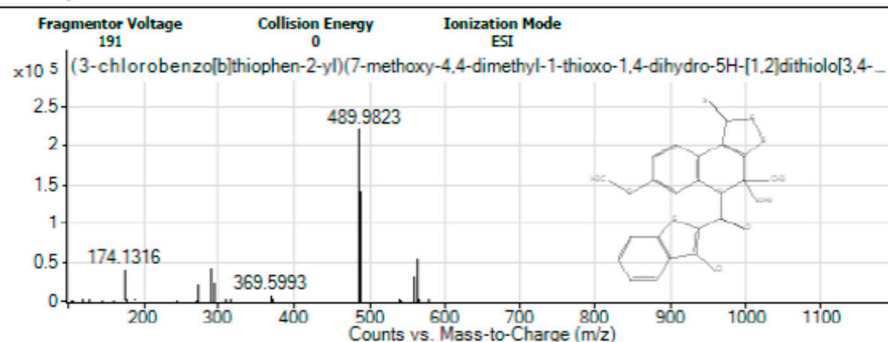


Figure S19: HPLC–HRMS–ESI spectra of 5-[(3-chloro-1-benzothien-2-yl)carbonyl]-7-methoxy-4,4-dimethyl-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione 2l,

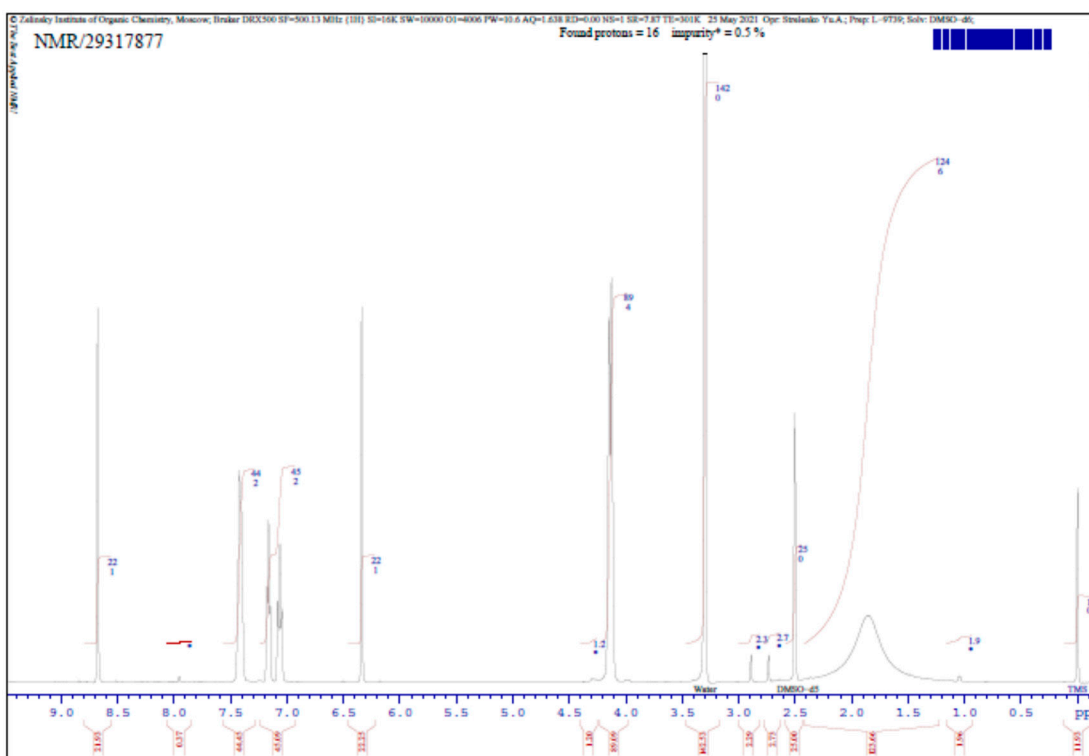


Figure S20: NMR ¹H spectra of 5-(2-fluorobenzoyl)-4,4-dimethyl-4,5,8,9-tetrahydro-1H-[1,4]dioxino[2,3-g][1,2]dithiolo[3,4-c]quinoline-1-thione 2m,

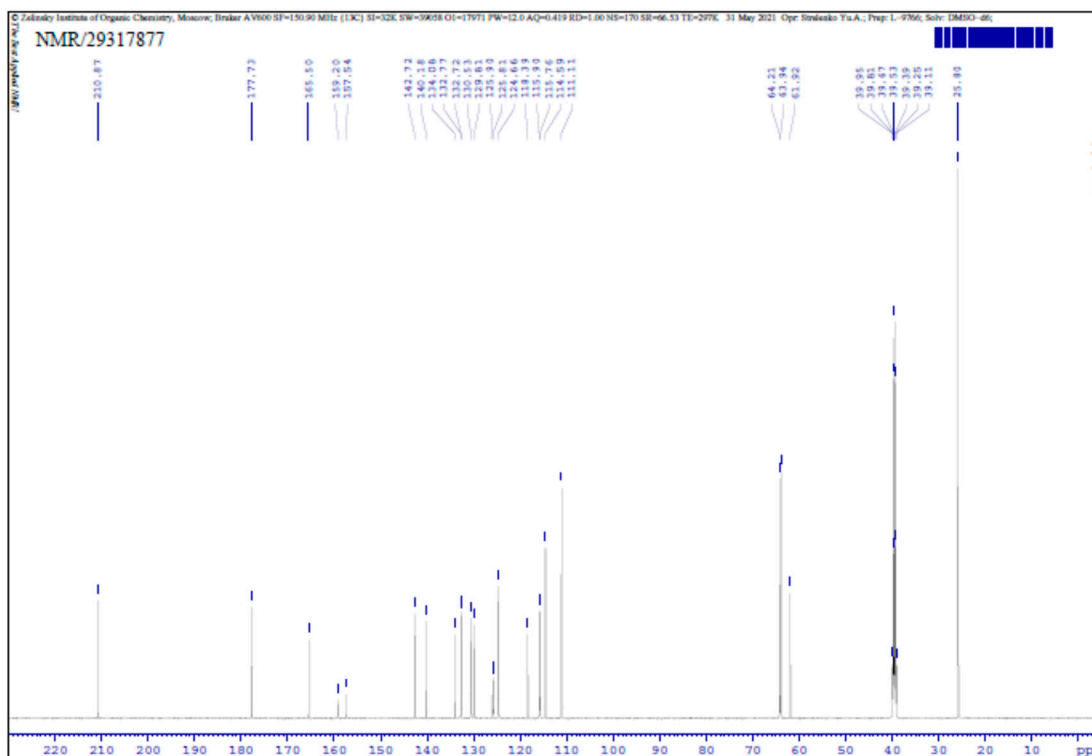
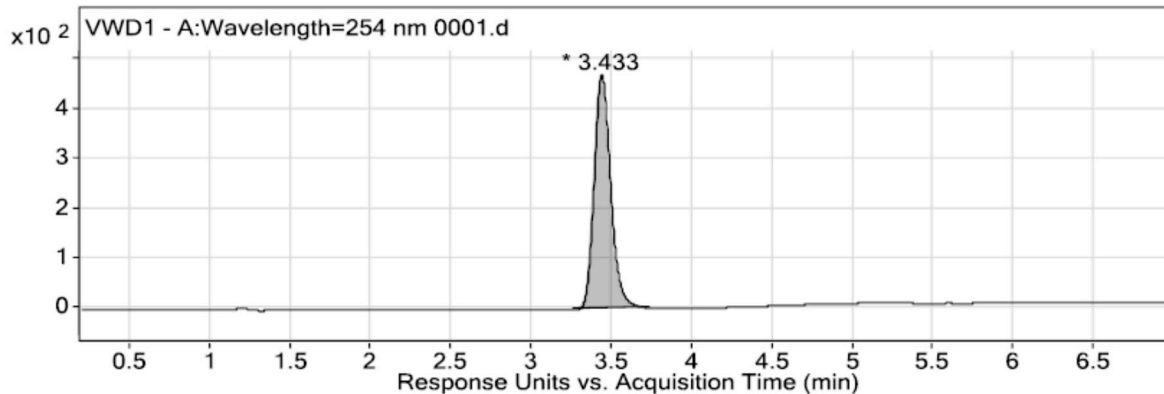


Figure S21: NMR ¹³C spectra of 5-(2-fluorobenzoyl)-4,4-dimethyl-4,5,8,9-tetrahydro-1H-[1,4]dioxino[2,3-g][1,2]dithiolo[3,4-c]quinoline-1-thione 2m,

| | | | |
|-------------------------------|-----------------|-----------------------|-----------------------------|
| 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

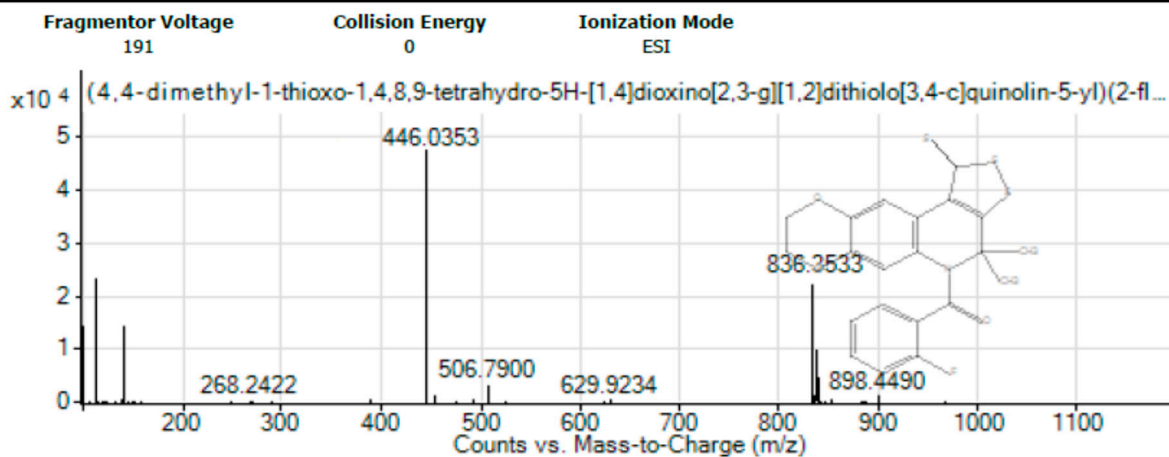


Figure S22: HPLC–HRMS–ESI spectra of 5-(2-fluorobenzoyl)-4,4-dimethyl-4,5,8,9-tetrahydro-1H-[1,4]dioxino[2,3-g][1,2]dithiolo[3,4-c]quinoline-1-thione 2m,

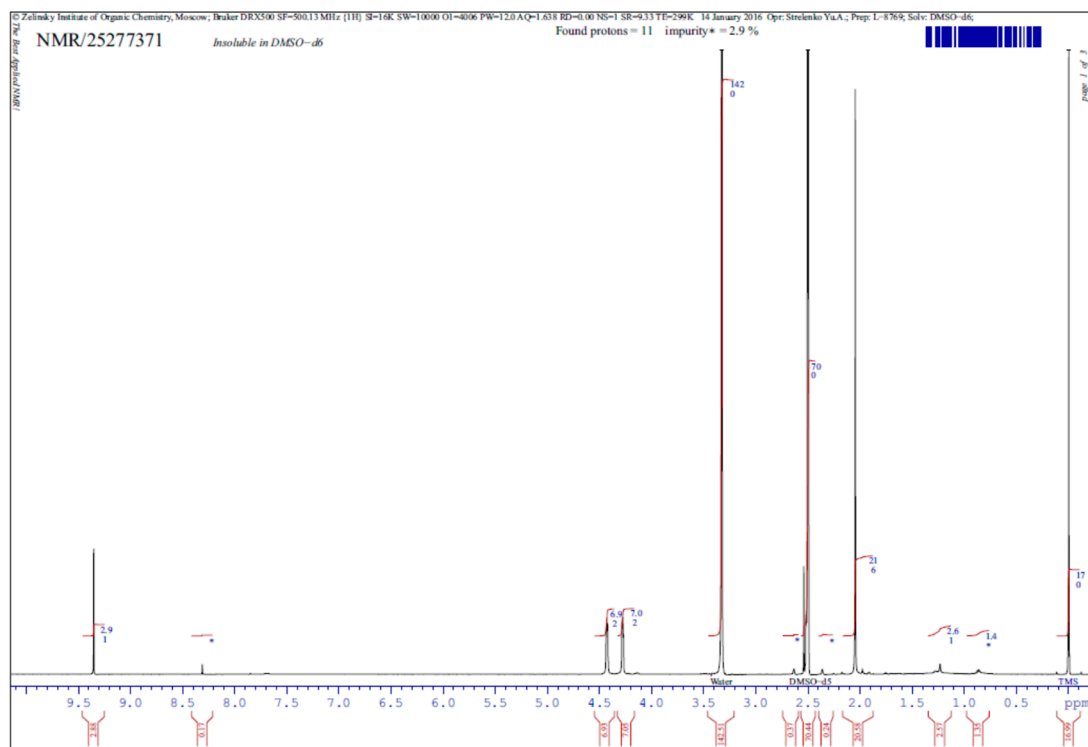
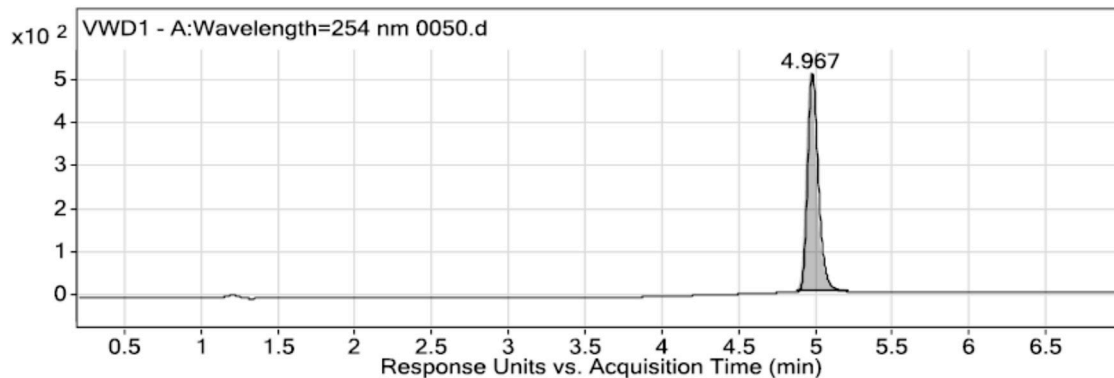


Figure S23: NMR ^1H spectra of 8,8-dimethyl-11-thioxo-2,3,8,11-tetrahydro[1,4]dioxino[2,3-g][1,2]dithiolo[3,4-c]pyrrolo[3,2,1-ij]quinoline-5,6-dione **2n**,

| | | | |
|------------------------|-----------------|----------------|-----------------------------|
| 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

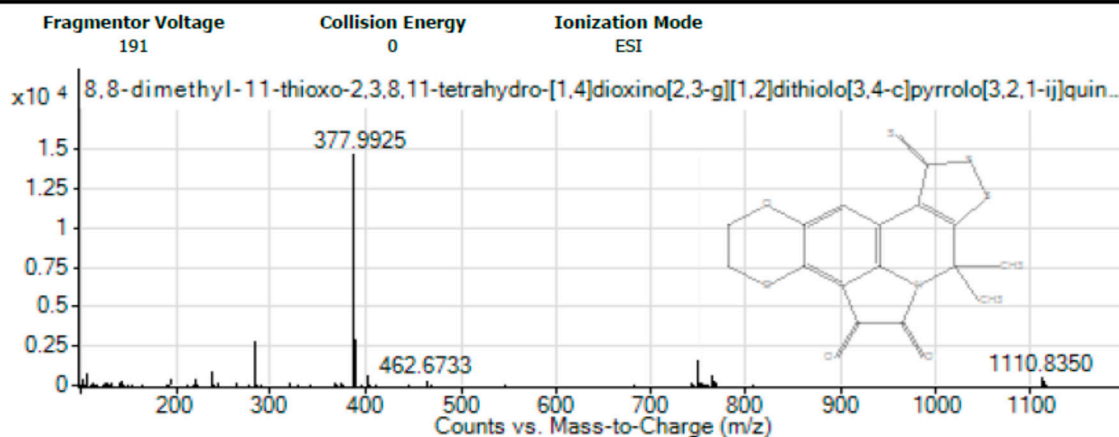


Figure S24: HPLC–HRMS–ESI spectra of 8,8-dimethyl-11-thioxo-2,3,8,11-tetrahydro[1,4]dioxino[2,3-g][1,2]dithiolo[3,4-c]pyrrolo[3,2,1-ij]quinoline-5,6-dione 2n,

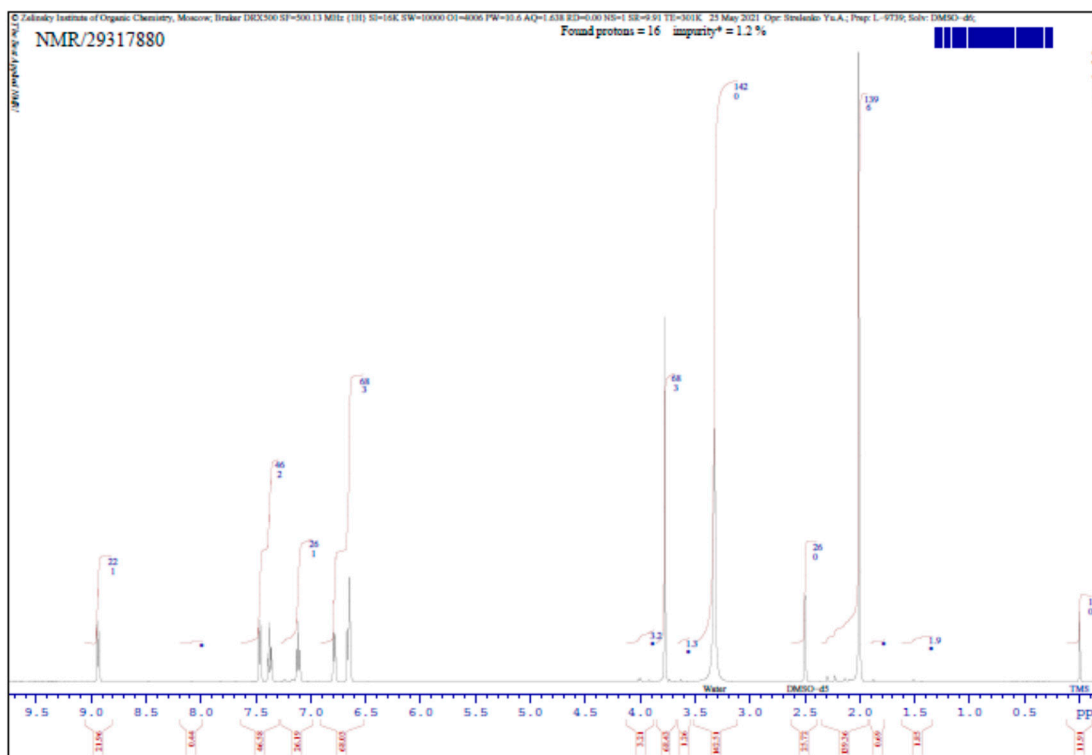


Figure S25: NMR ^1H spectra of 10-[(3-methoxyphenyl)imino]-7,7-dimethyl-7,10-dihydro[1,2]dithiolo[3,4-c]pyrrolo[3,2,1-ij]quinoline-4,5-dione **2q**,

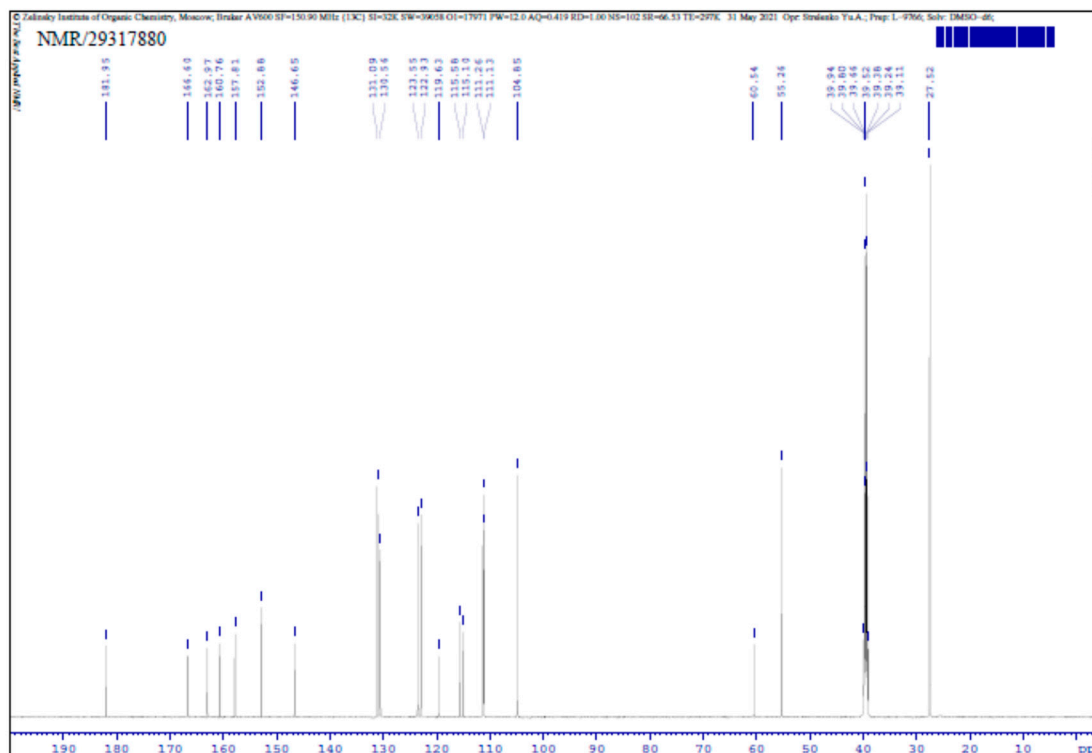
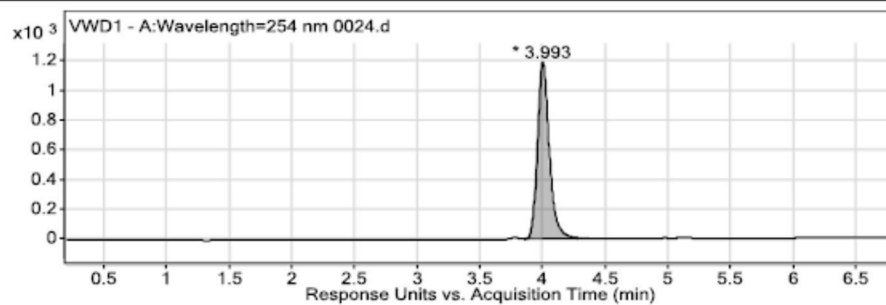


Figure S26: NMR ^{13}C spectra of 10-[(3-methoxyphenyl)imino]-7,7-dimethyl-7,10-dihydro[1,2]dithiolo[3,4-c]pyrrolo[3,2,1-ij]quinoline-4,5-dione **2q**,

| | | | |
|-------------------------------|-----------------|-----------------------|-----------------------------|
| 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

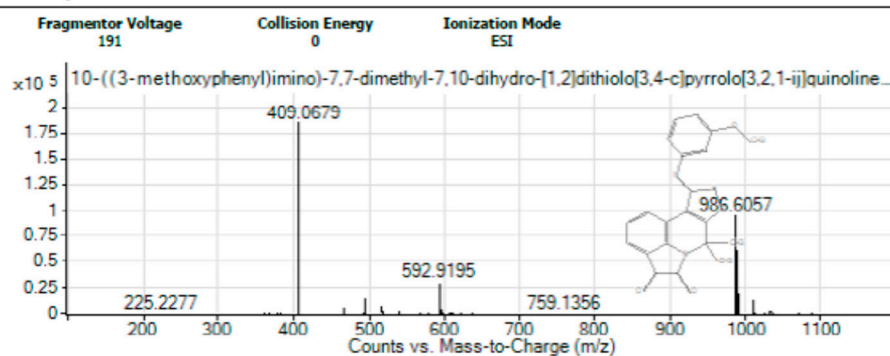


Figure S27: HPLC–HRMS–ESI spectra of 10-[(3-methoxyphenyl)imino]-7,7-dimethyl-7,10-dihydro[1,2]dithiolo[3,4-c]pyrrolo[3,2,1-ij]quinoline-4,5-dione 2q.