

5-(1*H*-Indole-3-ylmethyl)-4-oxo-2-thioxothiazolidin-3-yl)alkancarboxylic acids as antimicrobial agents. Synthesis, biological evaluation and molecular docking studies.

Horishny V.Ya.¹, Kartsev V.G.², Matychuk V.S.³, Geronikaki A⁴., Petrou⁴., Glamoclija J.⁵, Ciric A.⁵, Sokovic M.⁵

¹ *Danylo Halytsky Lviv National Medical University, 79010, Ukraine, Lviv, Pekarska 69*

² *InterBioScreen, Moscow, Russia*

³ *Aristotle University, School of Pharmacy, Thessaloniki, Greece*

⁴ *Ivan Franko National University of Lviv, 79005, Ukraine, Lviv, Kyryla i Mefodia 6.*

⁵ *Aristotle University of Thessaloniki, School of Pharmacy, Thessaloniki, 54124, Greece.*

⁶ *Mycological Laboratory, Institute of Biological Research Sinisa Stankovic, Belgrade University, Serbia*

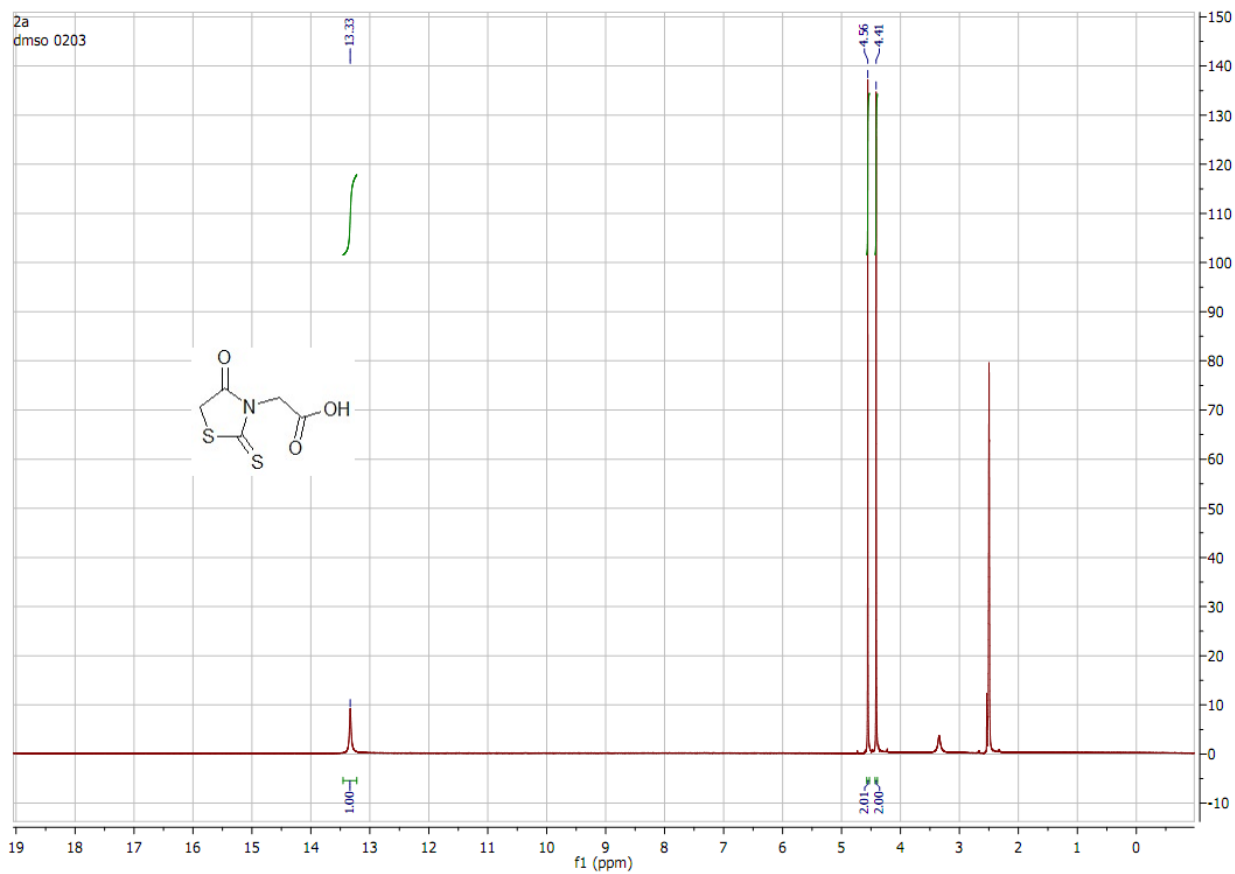


Figure S1. ^1H NMR spectrum (400 MHz, DMSO- d_6) of compound **2a**.

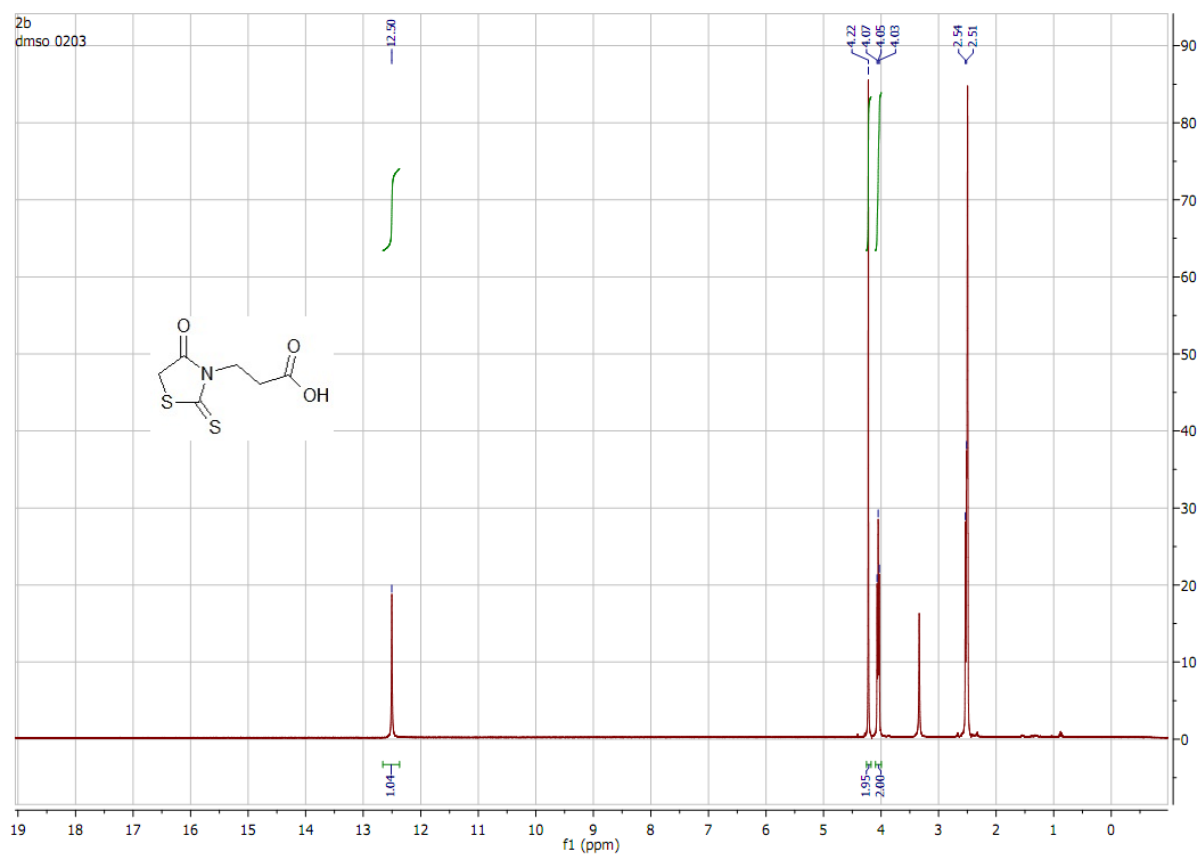


Figure S2. ^1H NMR spectrum (400 MHz, DMSO- d_6) of compound **2b**.

Figure S3. ^1H NMR spectrum (400 MHz, DMSO- d_6) of compound **2c**.

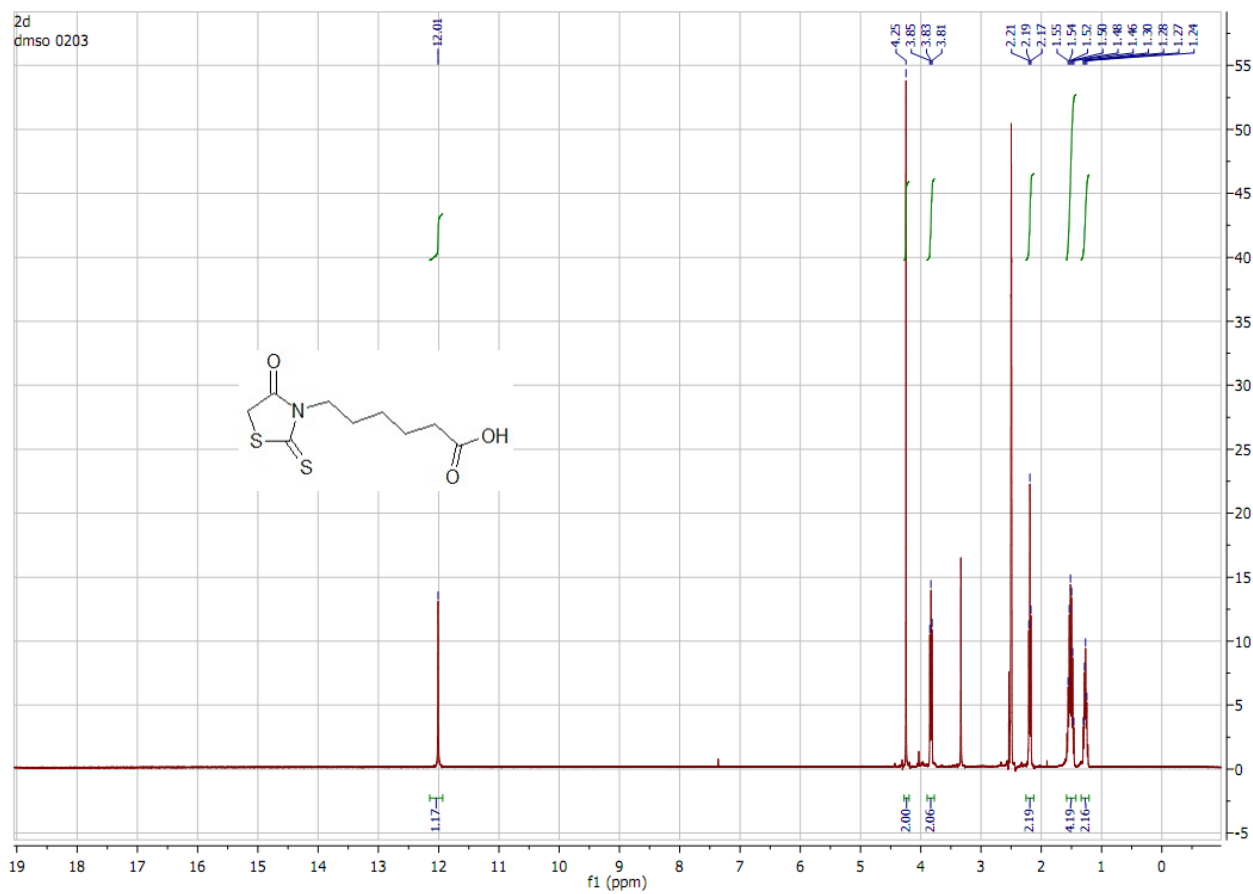


Figure S4. ^1H NMR spectrum (400 MHz, DMSO- d_6) of compound **2d**.

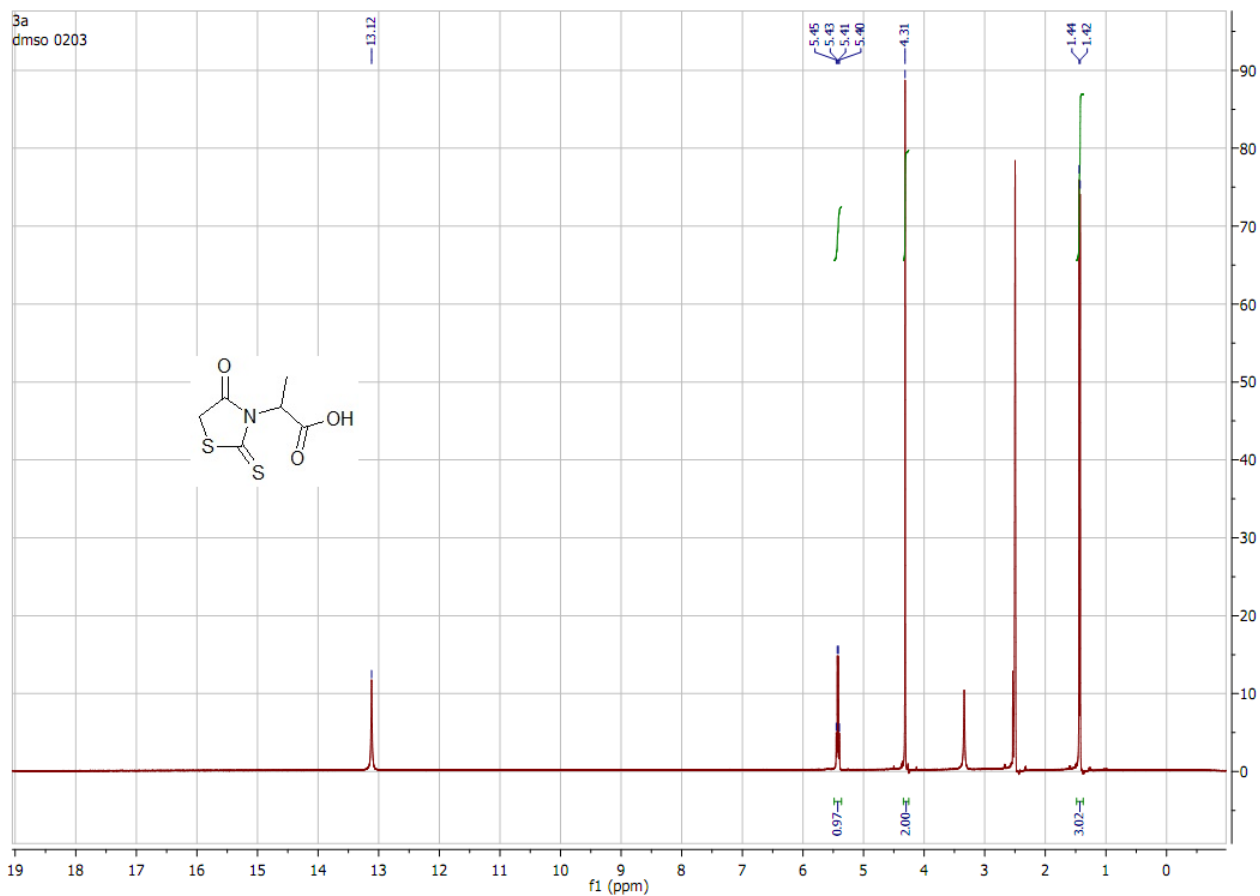


Figure S5. ^1H NMR spectrum (400 MHz, DMSO- d_6) of compound **3a**.

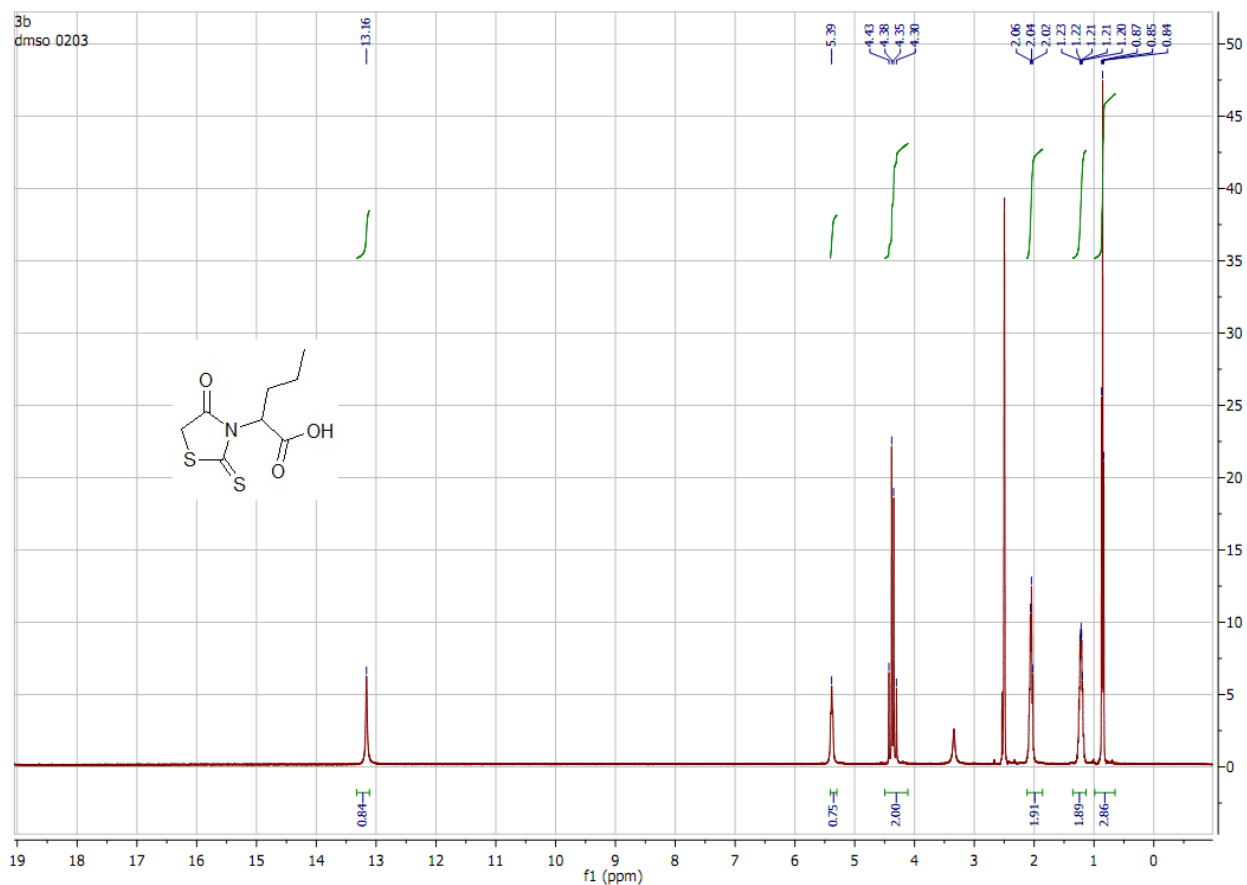


Figure S6. ^1H NMR spectrum (400 MHz, DMSO- d_6) of compound **3b**.

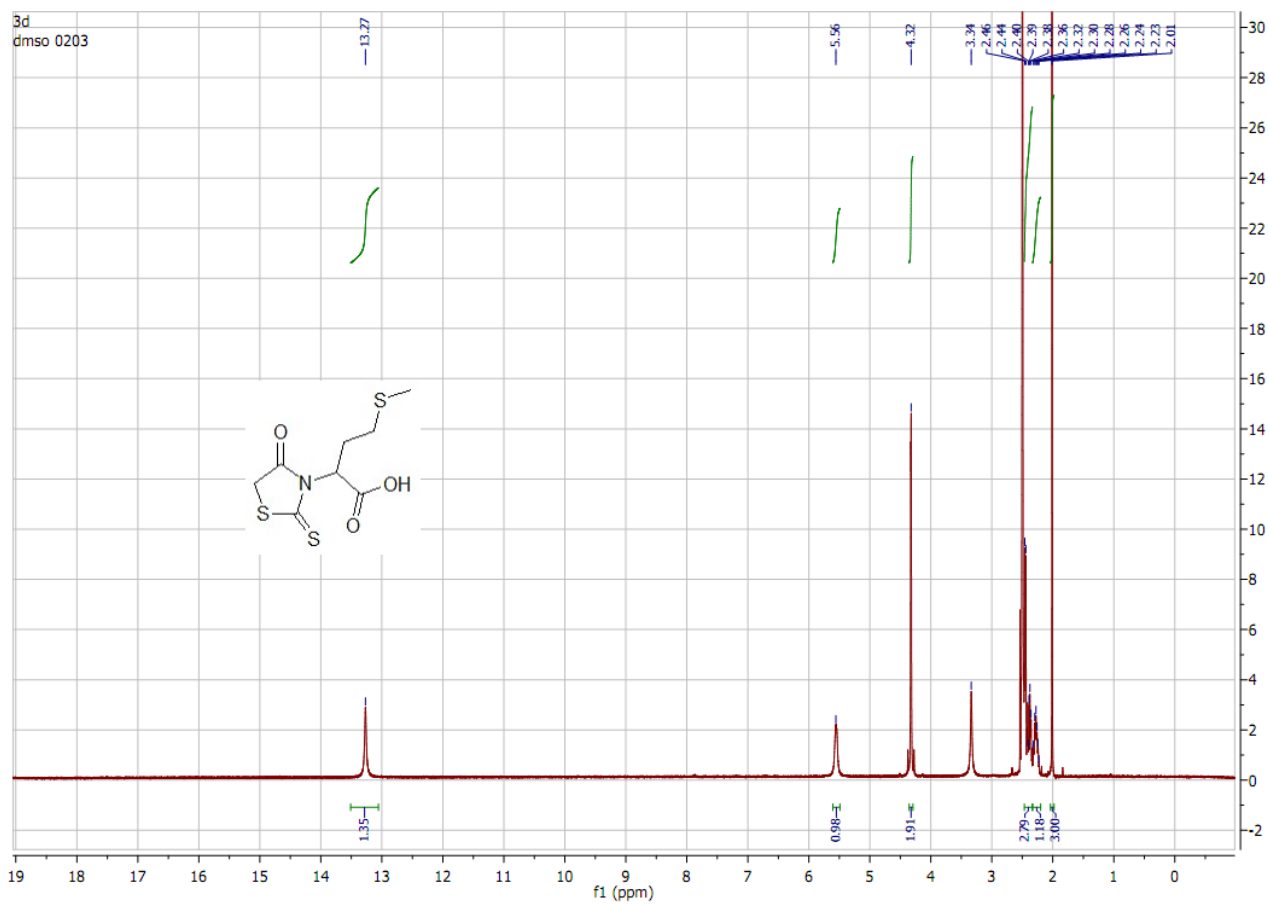


Figure S7. ^1H NMR spectrum (400 MHz, DMSO- d_6) of compound 3c.

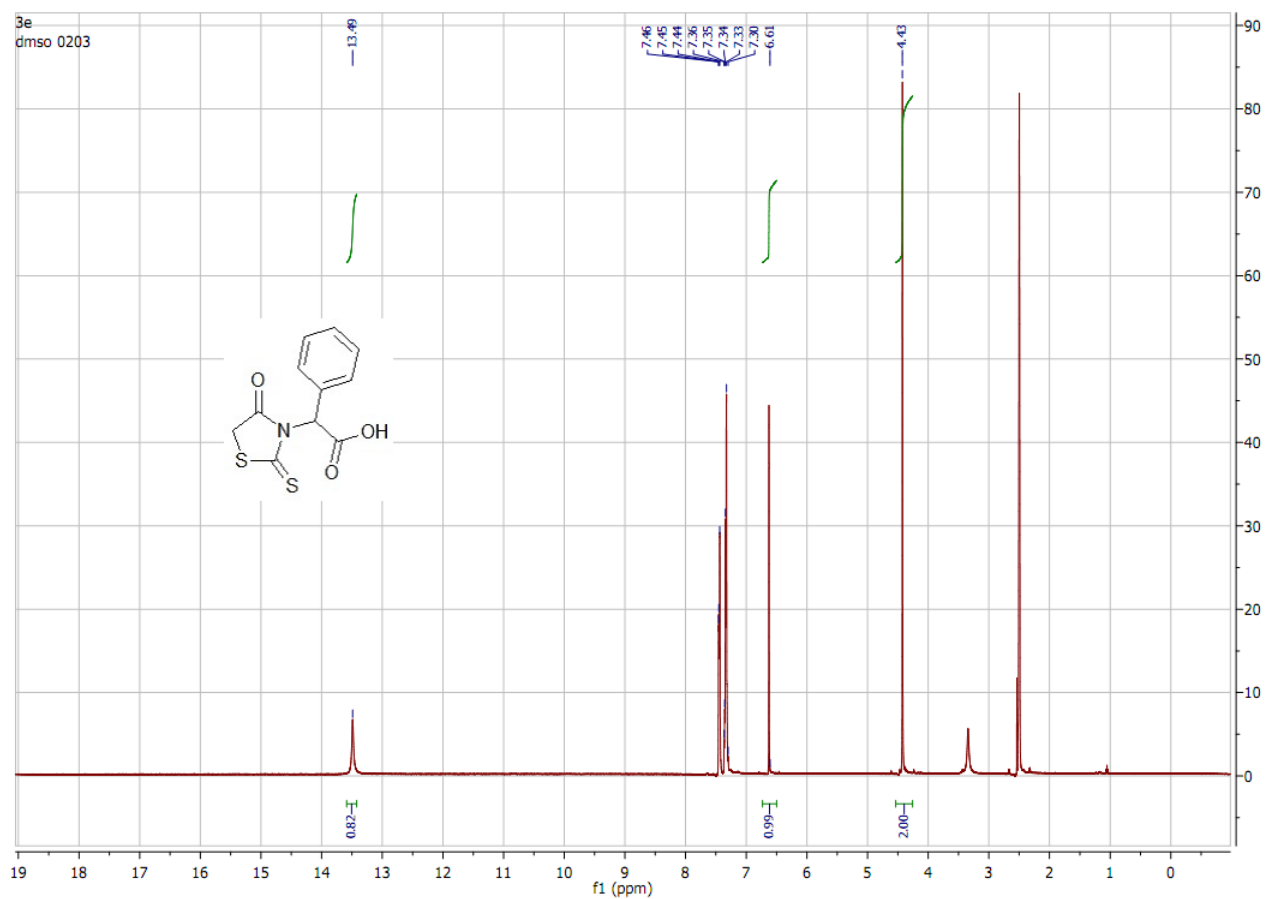


Figure S8. ^1H NMR spectrum (400 MHz, DMSO- d_6) of compound 3d.

Figure S9. ^1H NMR spectrum (400 MHz, DMSO-d_6) of compound **3e**

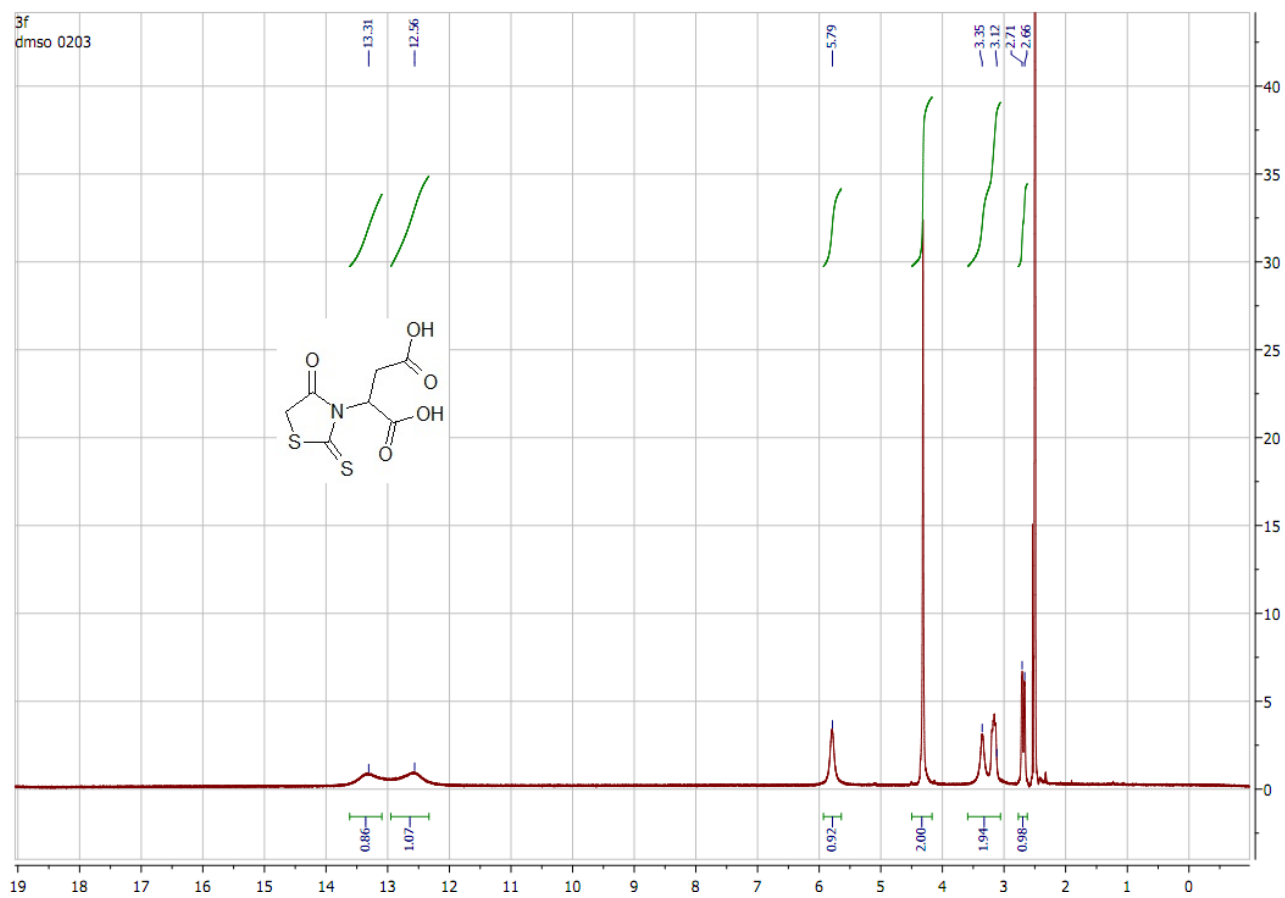


Figure S10. ^1H NMR spectrum (400 MHz, DMSO-d_6) of compound **3f**

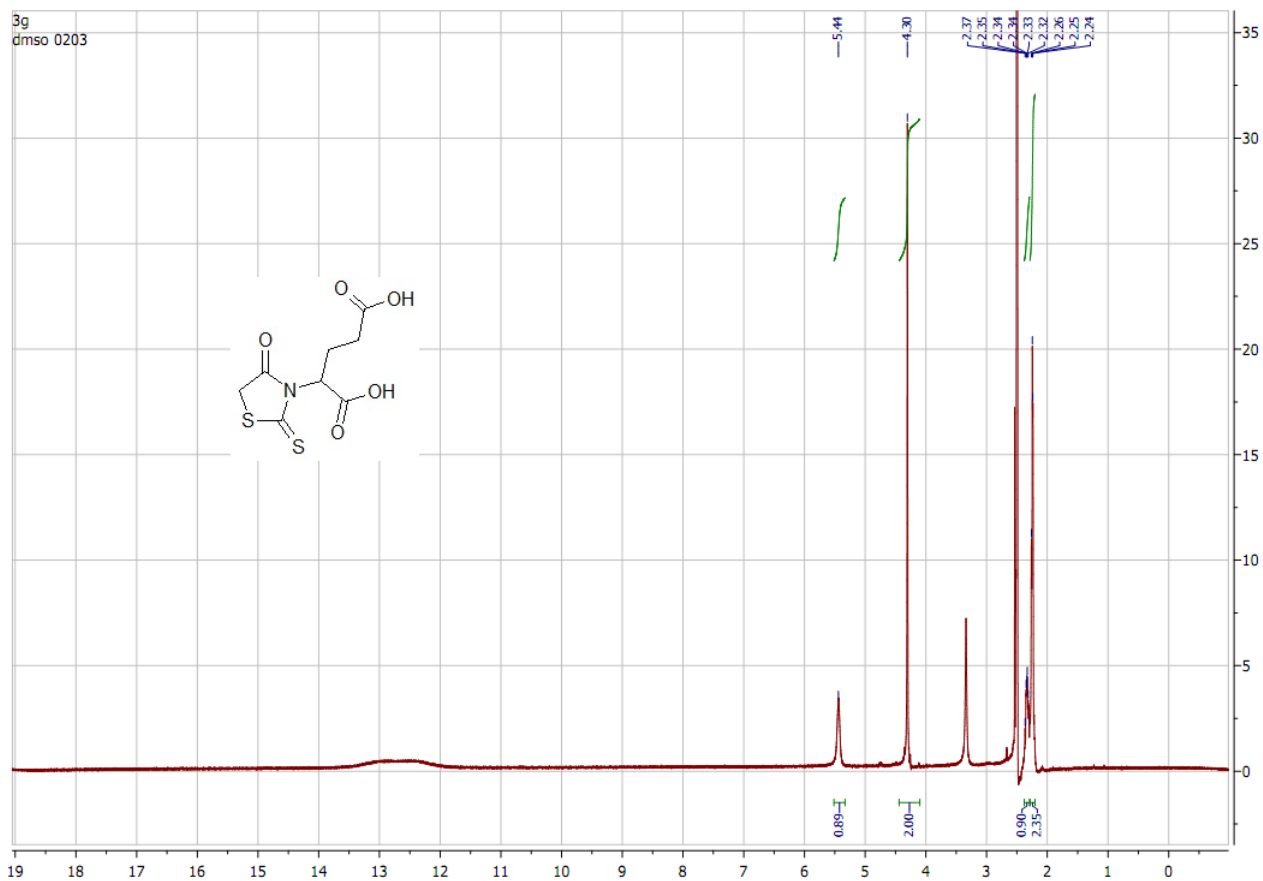


Figure S11. ^1H NMR spectrum (400 MHz, DMSO- d_6) of compound **3g**

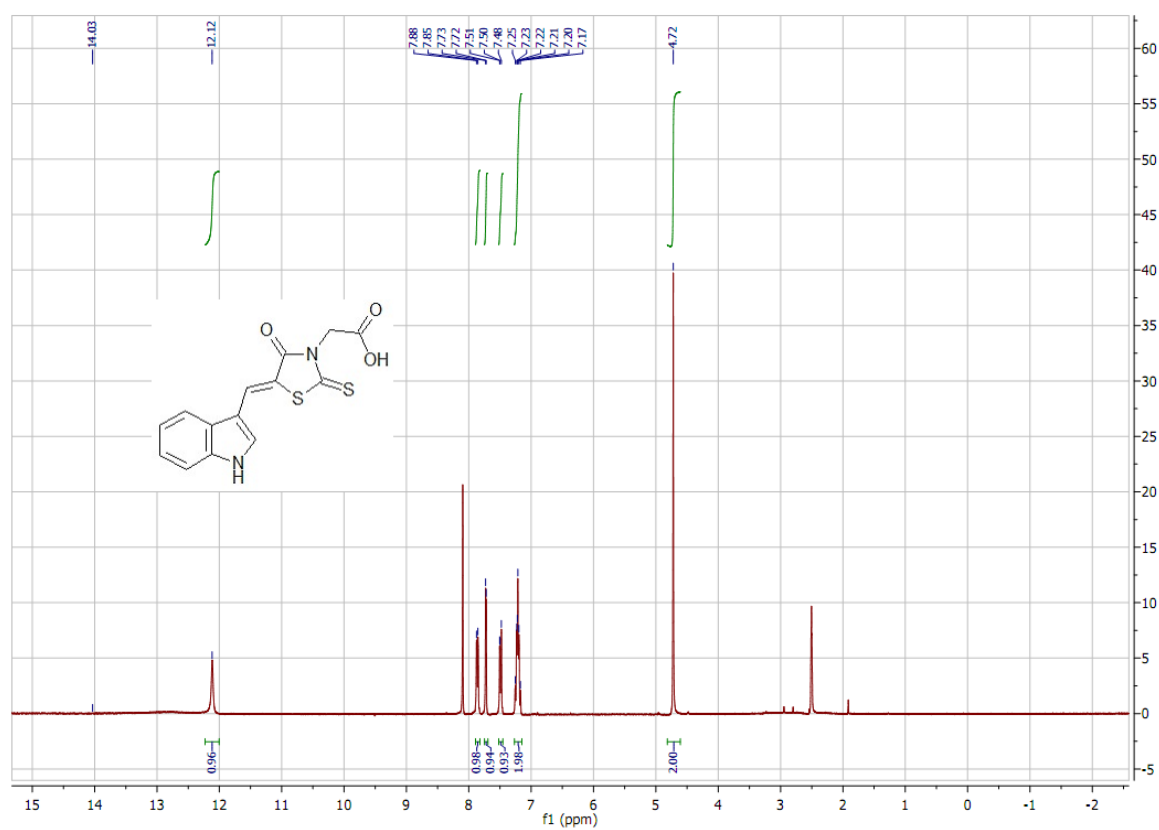


Figure S12. ^1H NMR spectrum (300 MHz, DMSO- d_6) of compound **4a**.

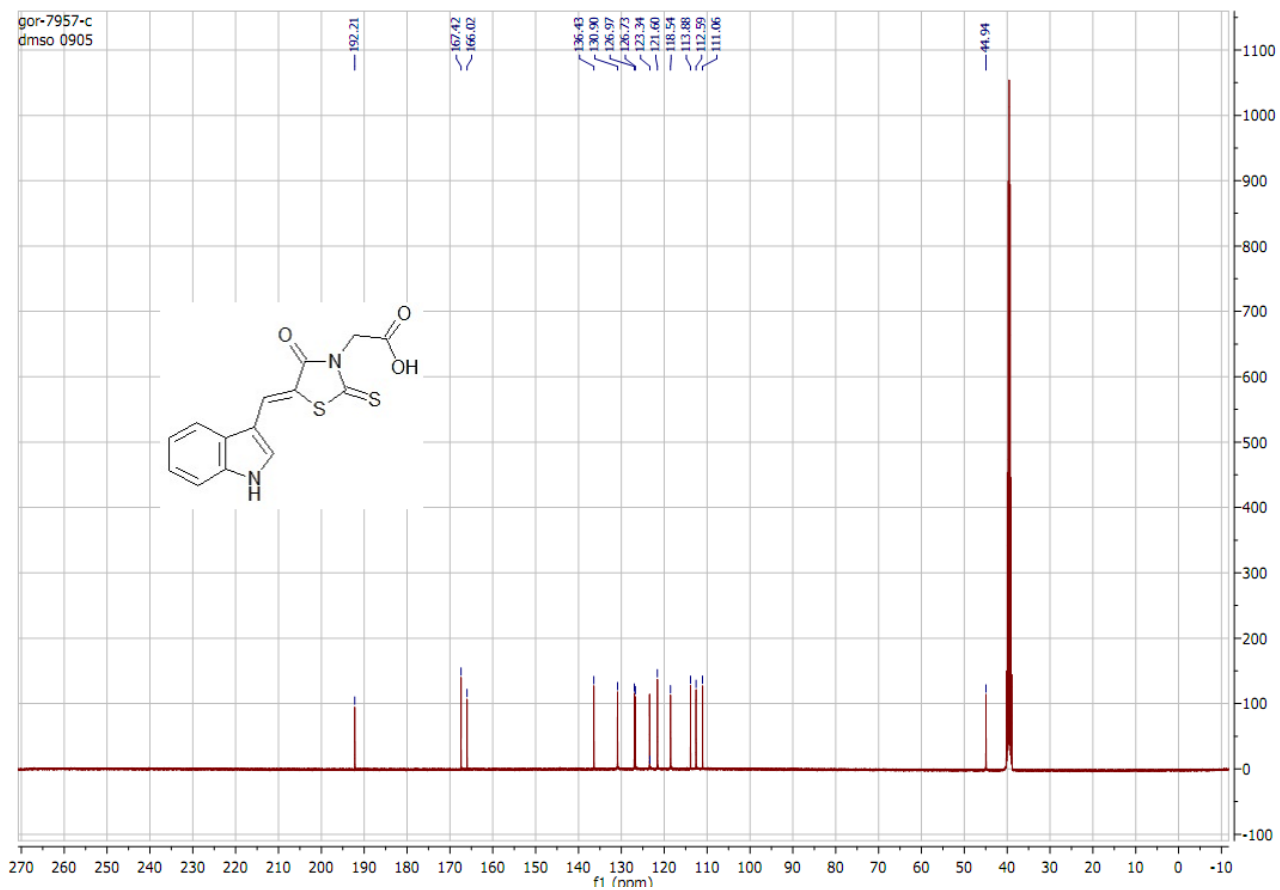
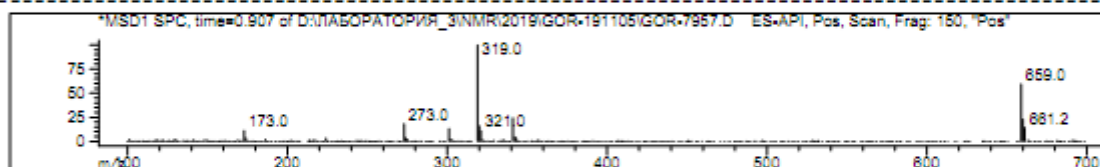
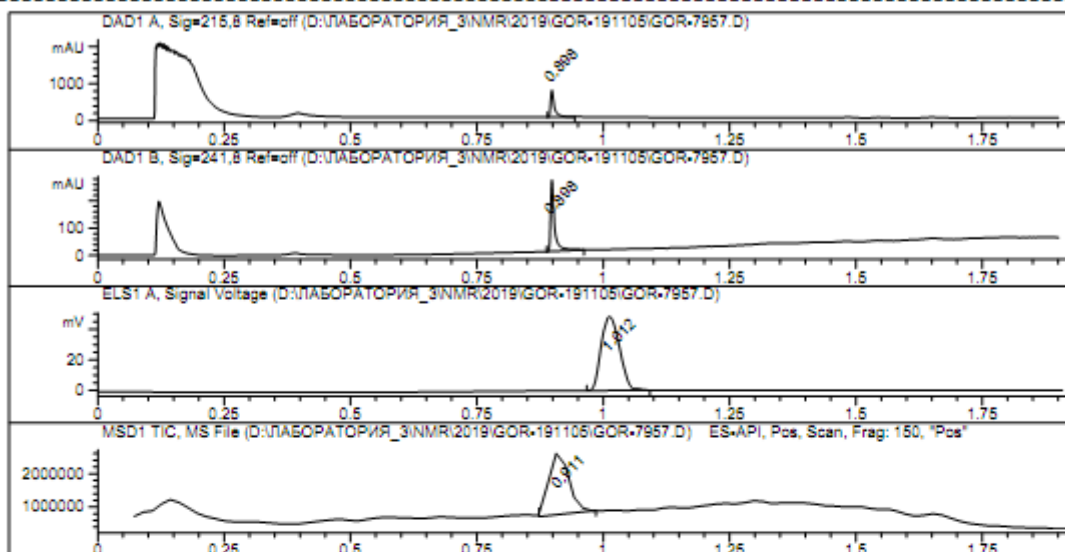


Figure S13. ^{13}C NMR spectrum (101 MHz, DMSO- d_6) of compound **4a**

-o.-Syntex Purity Report -o.-

System: Agilent 1200 LC/MSD SL
 Separation column: Rapid Resolution HT Cartige 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.898	100.000
1	DAD1 B, Sig=241,8 Ref=off	0.898	100.000
1	ELS1 A, Signal Voltage	1.012	100.000
1	MSD1 TIC, MS File	0.911	100.000

Inf. Data 05.11.2019

Figure S14. MS (ESI) spectrum of compound 4a.

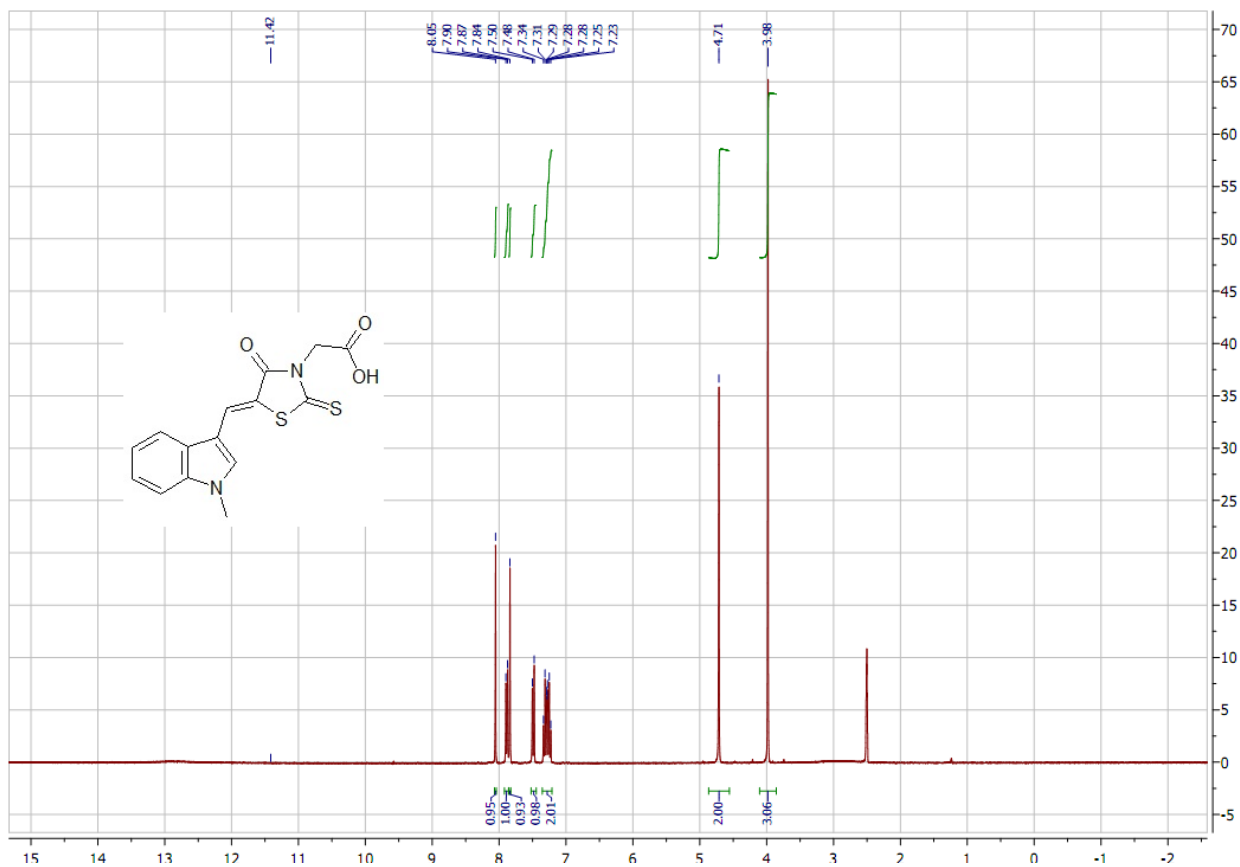


Figure S15. ¹H NMR spectrum (300 MHz, DMSO-d₆) of compound **4b**.

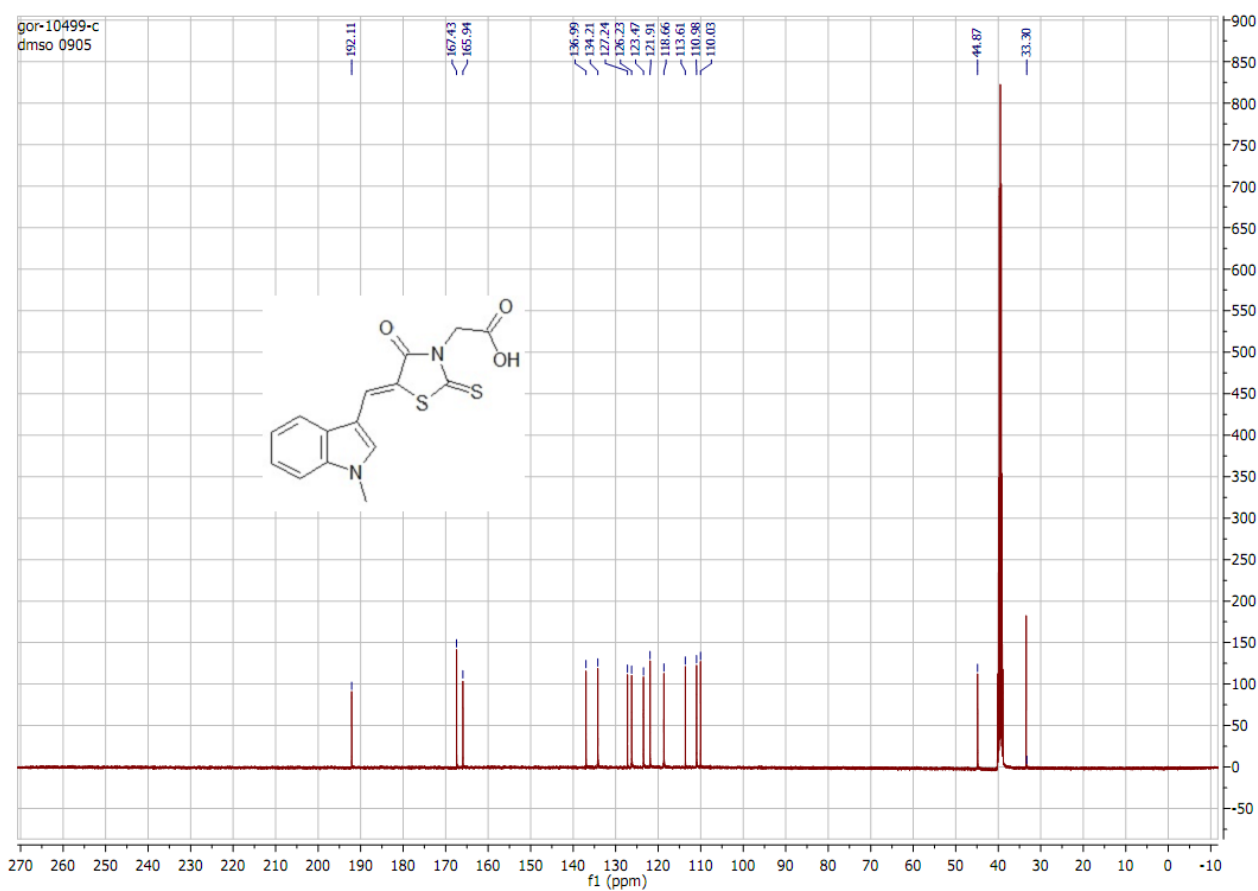
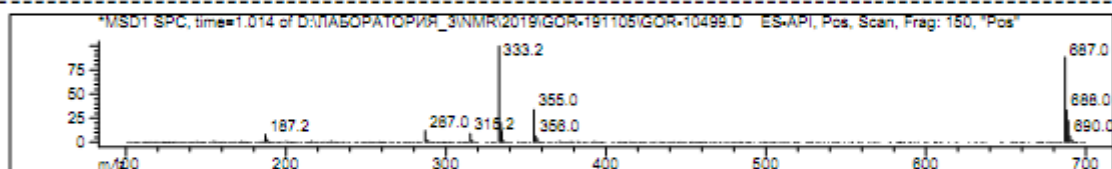
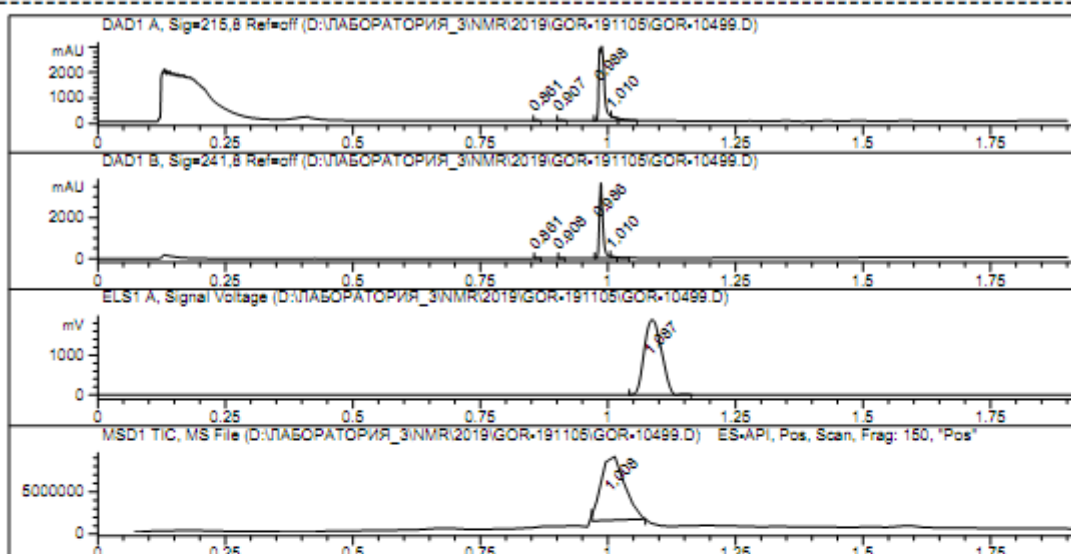


Figure S16. ¹³C NMR spectrum (101 MHz, DMSO-d₆) of compound **4b**.

System: Agilent 1200 LC/MSD SL
 Separation column: Rapid Resolutionn HT Cartige 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.861	0.187
2		0.907	0.508
3		0.988	99.236
4		1.010	0.069

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.861	0.311
2		0.908	0.340
3		0.986	98.967
4		1.010	0.382

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.087	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.008	100.000

Inj. Data 06.11.2019

Figure S17. MS (ESI) spectrum of compound **4b**.

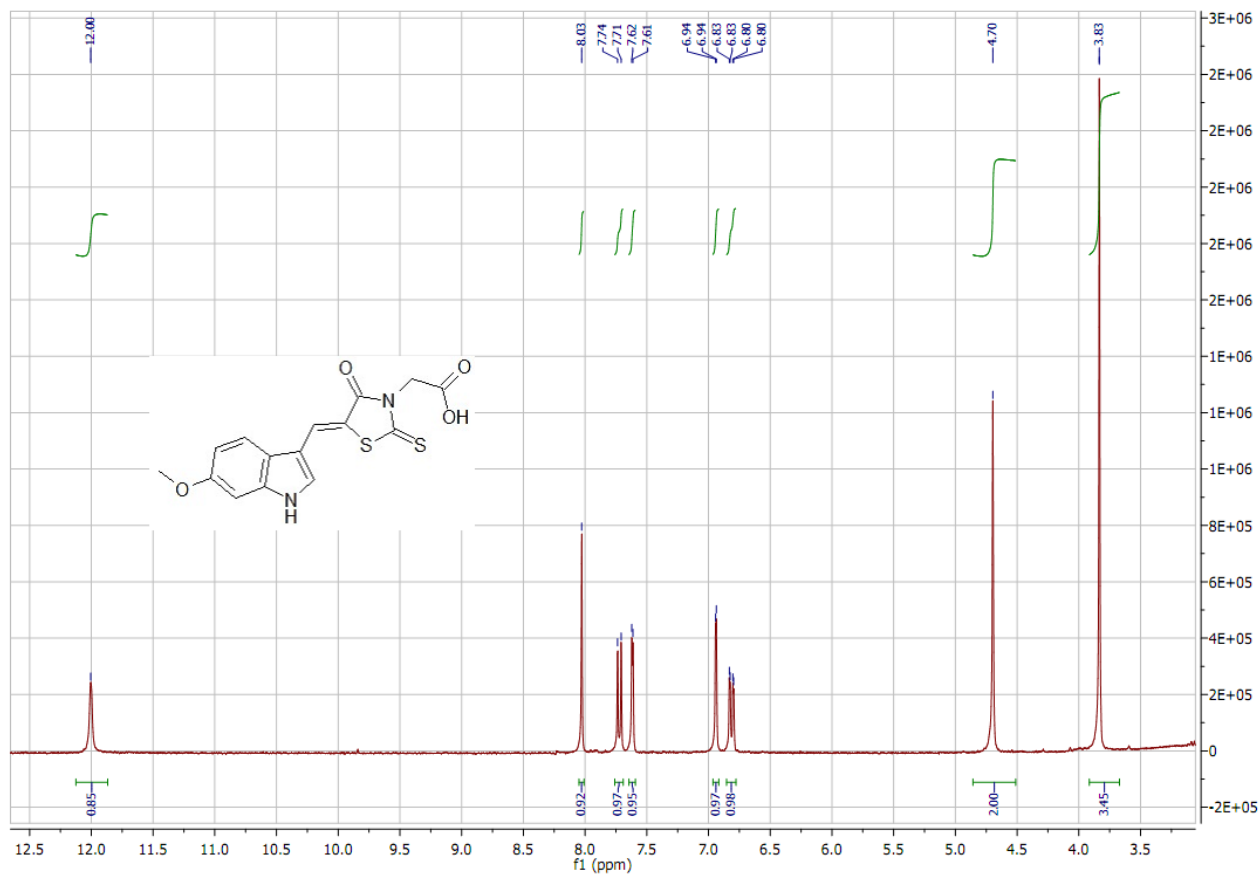


Figure S18. ^1H NMR spectrum (300 MHz, DMSO-d_6) of compound **4c**.

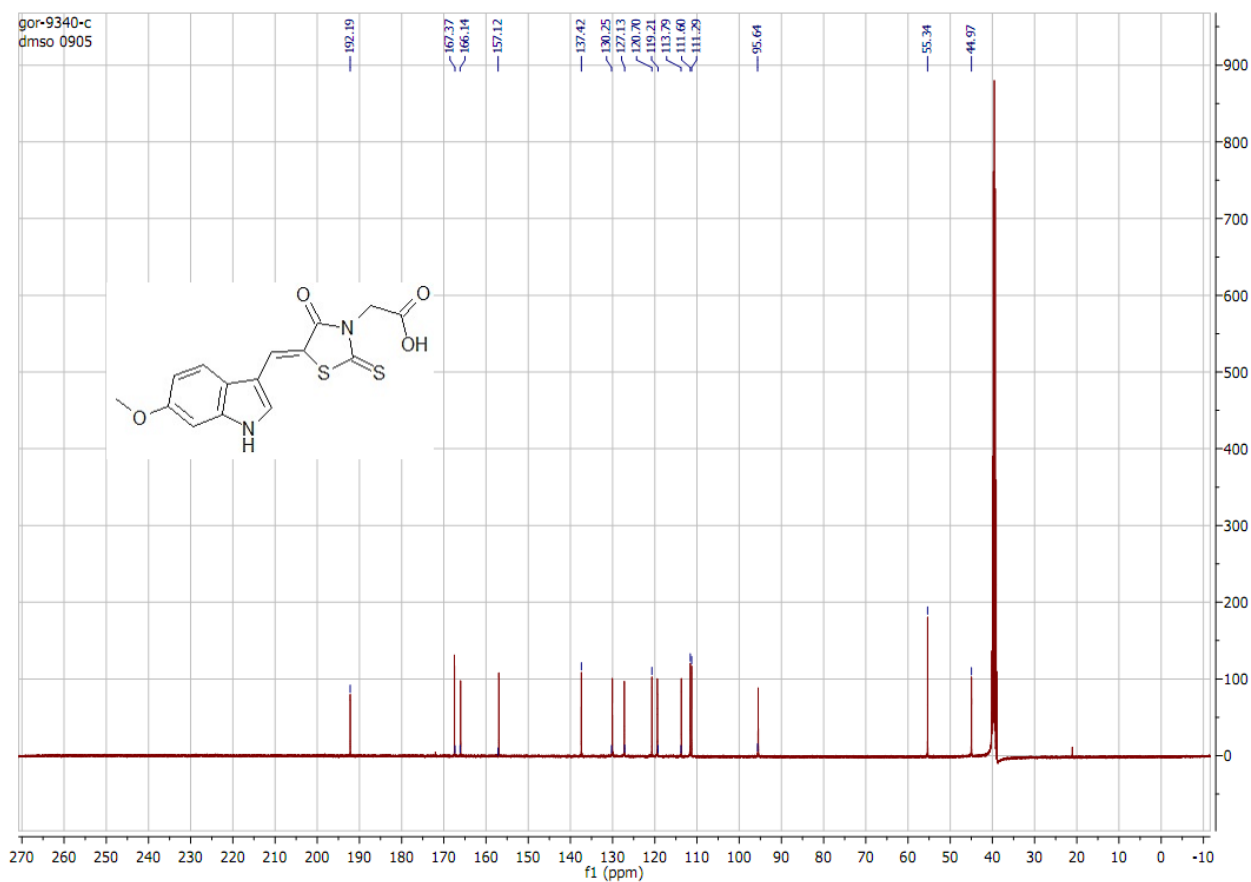
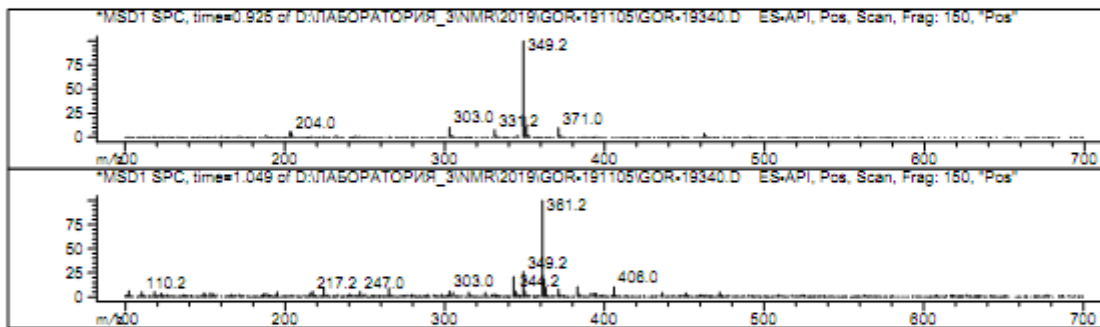
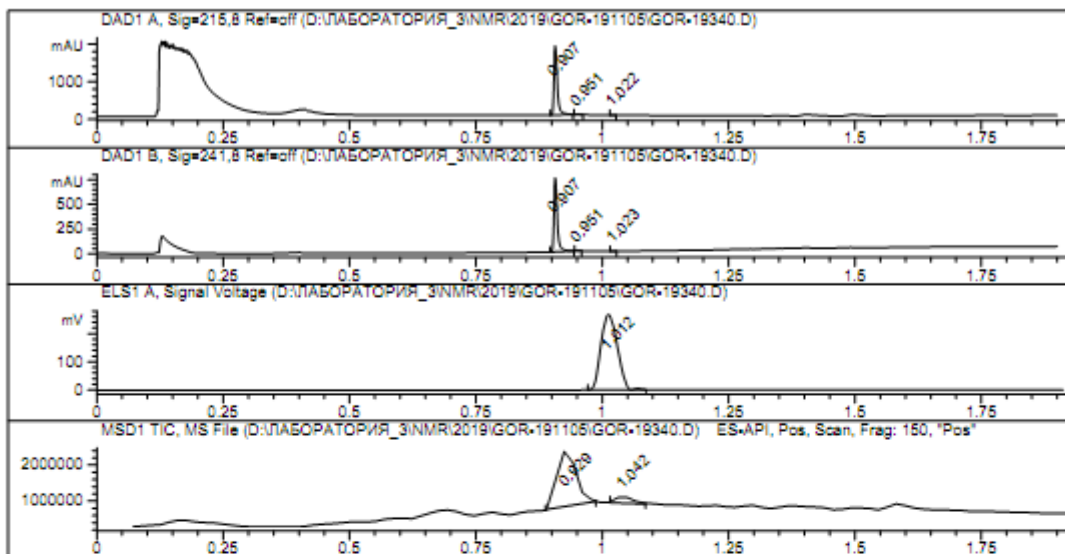


Figure S19. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of compound **4c**

System: Agilent 1200 LC/MSD SL
 Separation column: Rapid Resolution HT Cartige 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.907	98.924
2		0.951	0.692
3		1.022	0.384

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.907	99.157
2		0.951	0.412
3		1.023	0.431

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.012	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.929	91.946
2		1.042	8.054

Inj. Date 06.11.2019

Figure S20. MS (ESI) spectrum of compound **4c**.

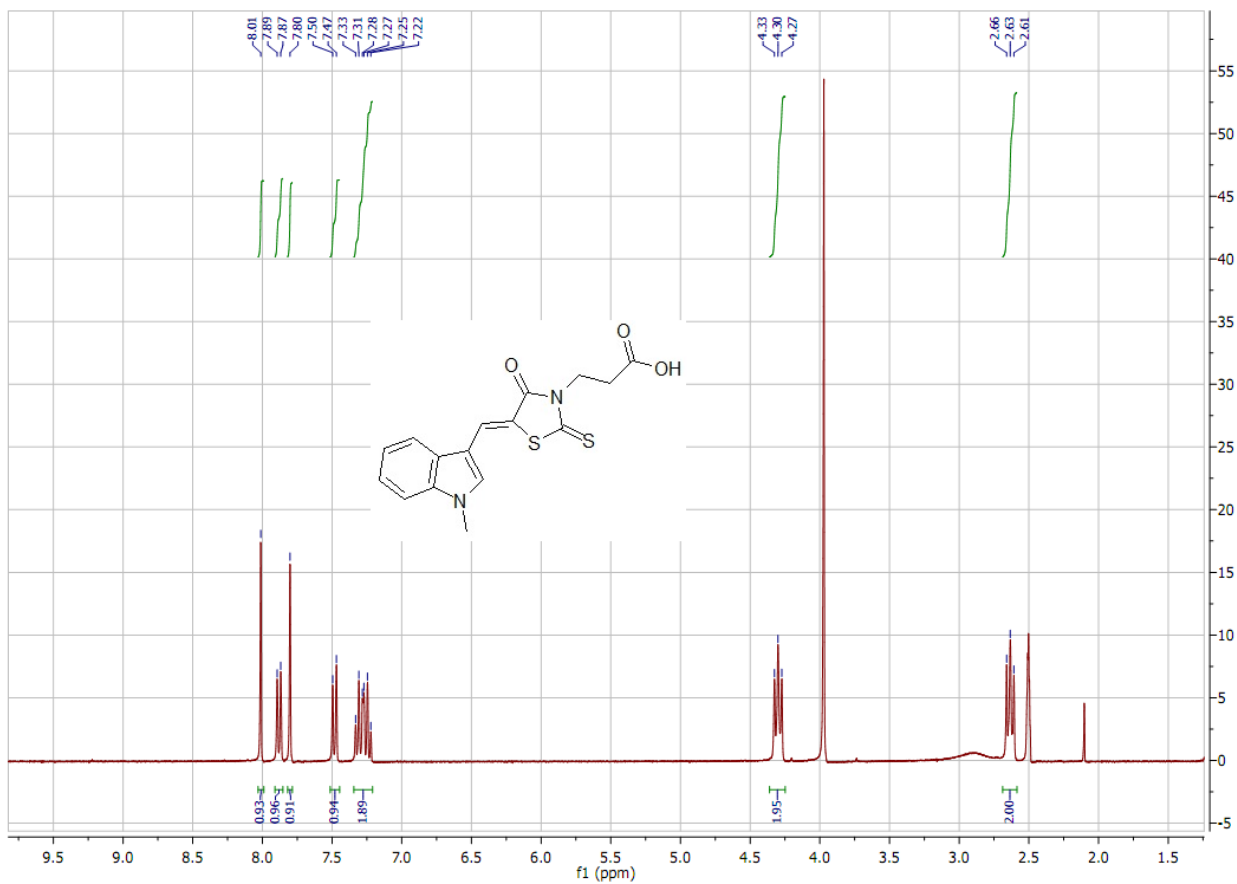


Figure S21. ^1H NMR spectrum (300 MHz, DMSO- d_6) of compound **4d**.

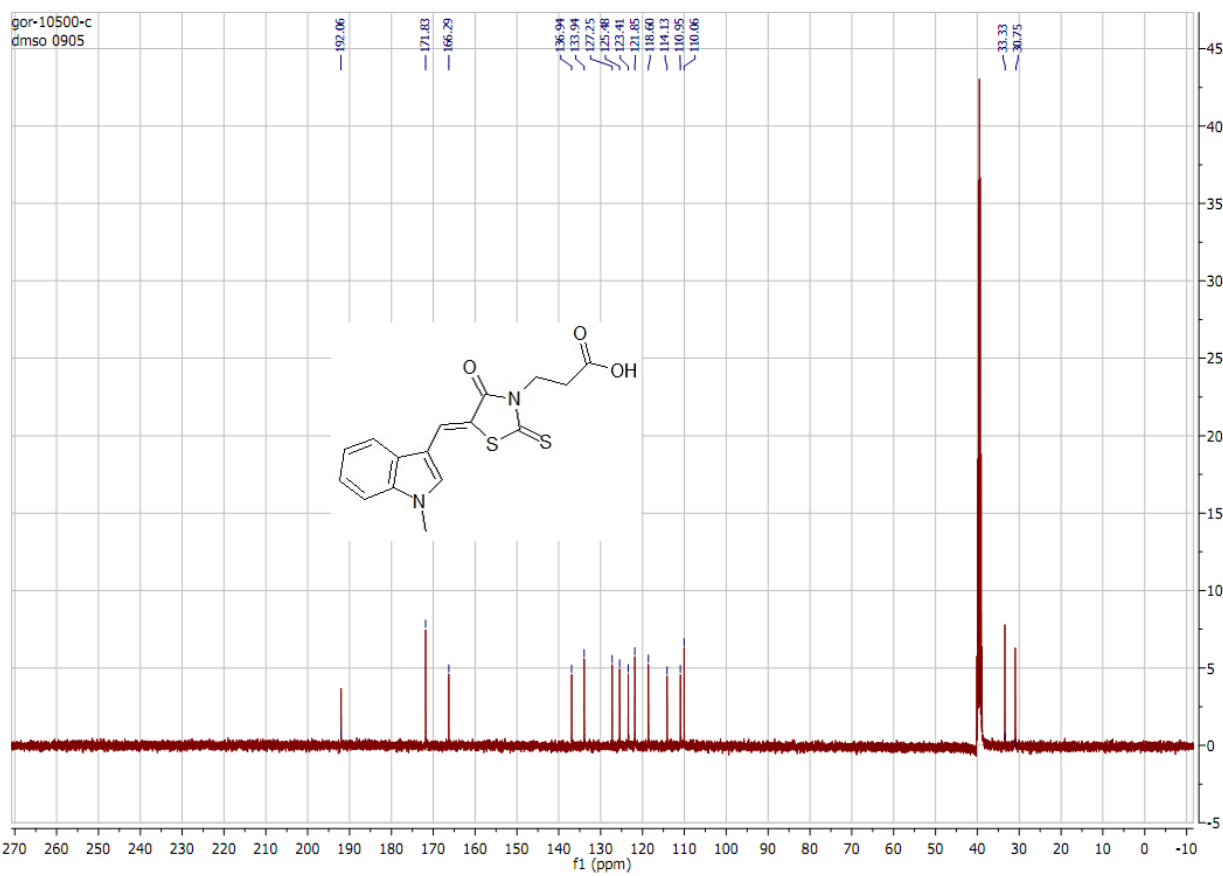
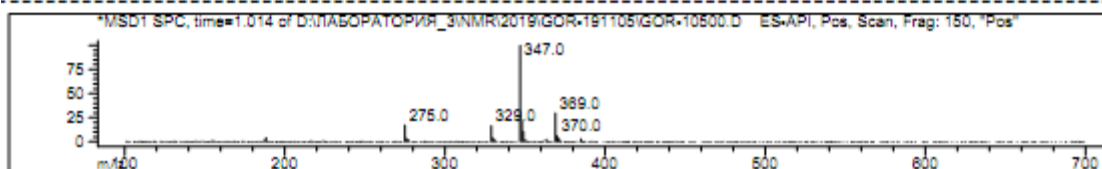
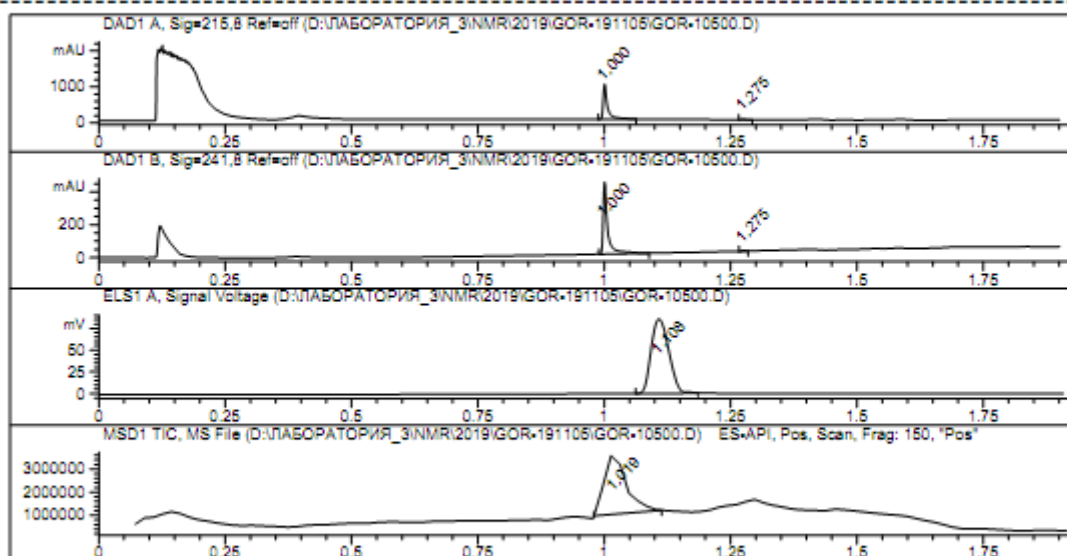


Figure S22. ^{13}C NMR spectrum (101 MHz, DMSO- d_6) of compound **4d**

-o.-Syntex Purity Report -o.-

System: Agilent 1200 LC/MSD SL

Separation column: Rapid Resolution HT Cartige 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	1.000	98.591
2		1.275	1.409
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	1.000	98.971
2		1.275	1.029
#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.108	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.019	100.000

inj. Data 05.11.2019

Figure S23. MS (ESI) spectrum of compound 4d.

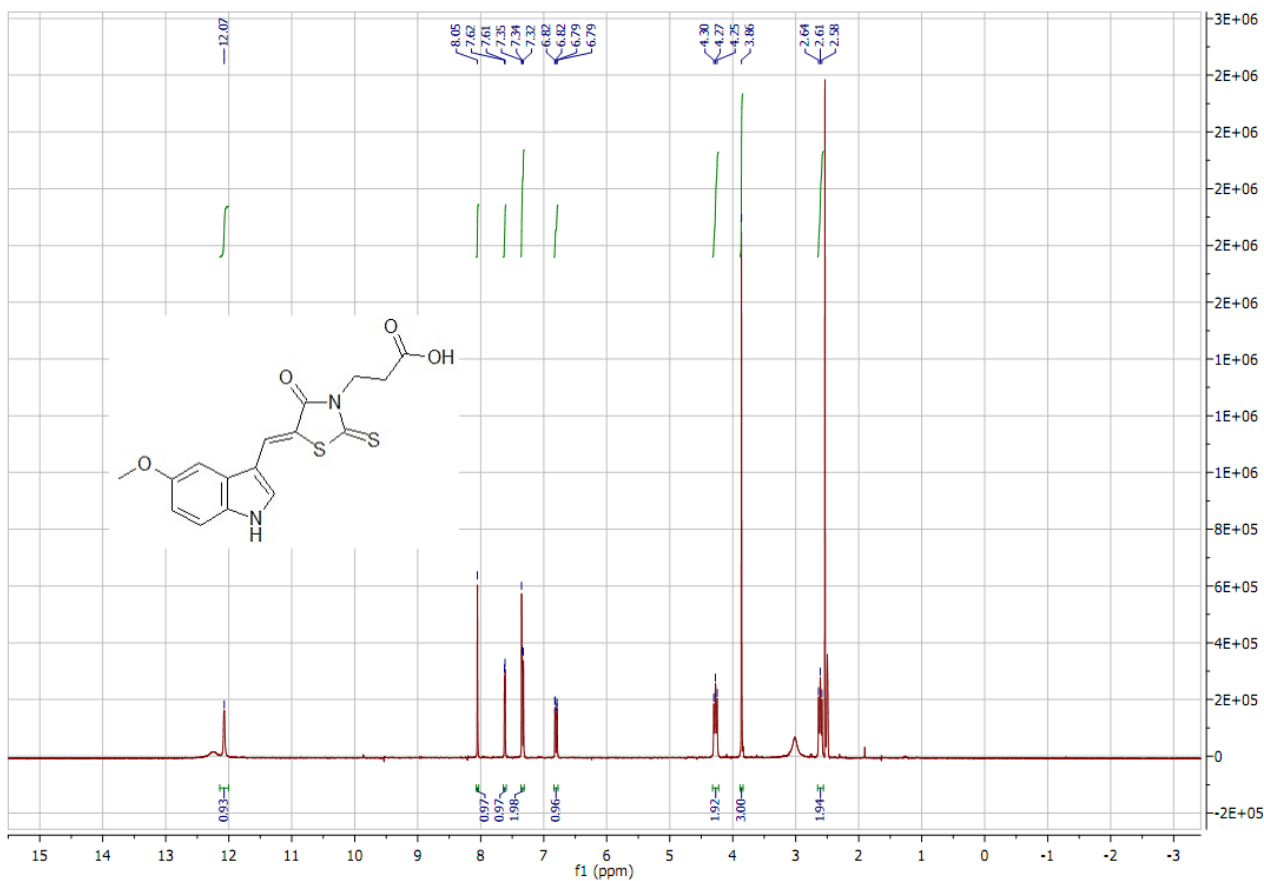


Figure S24. ^1H NMR spectrum (300 MHz, DMSO-d_6) of compound 4e.

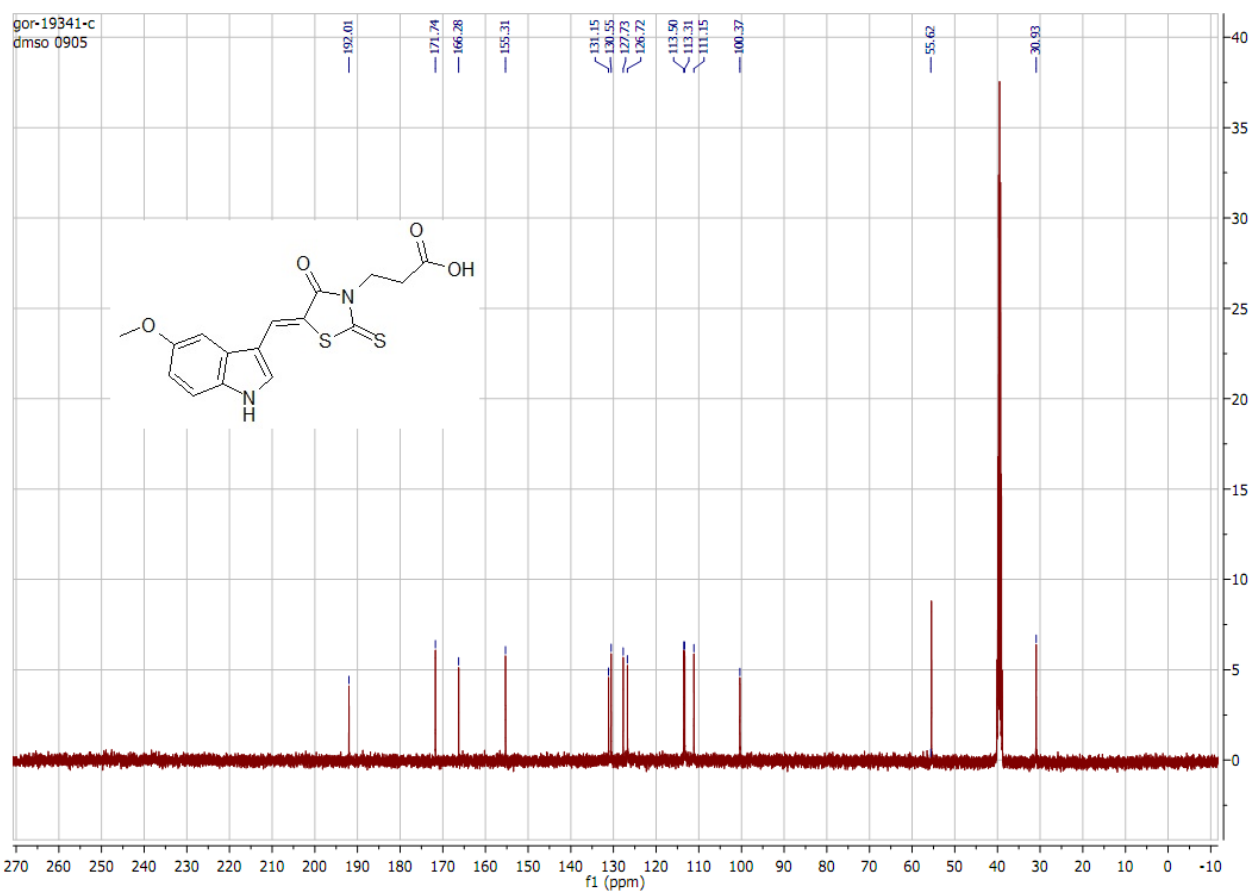
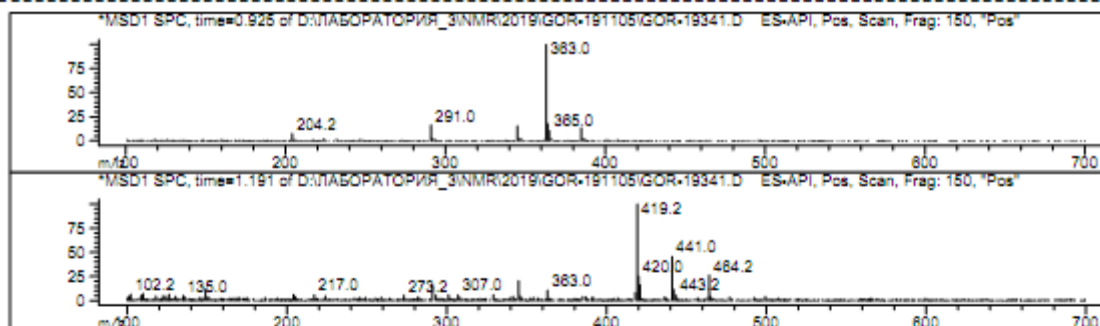
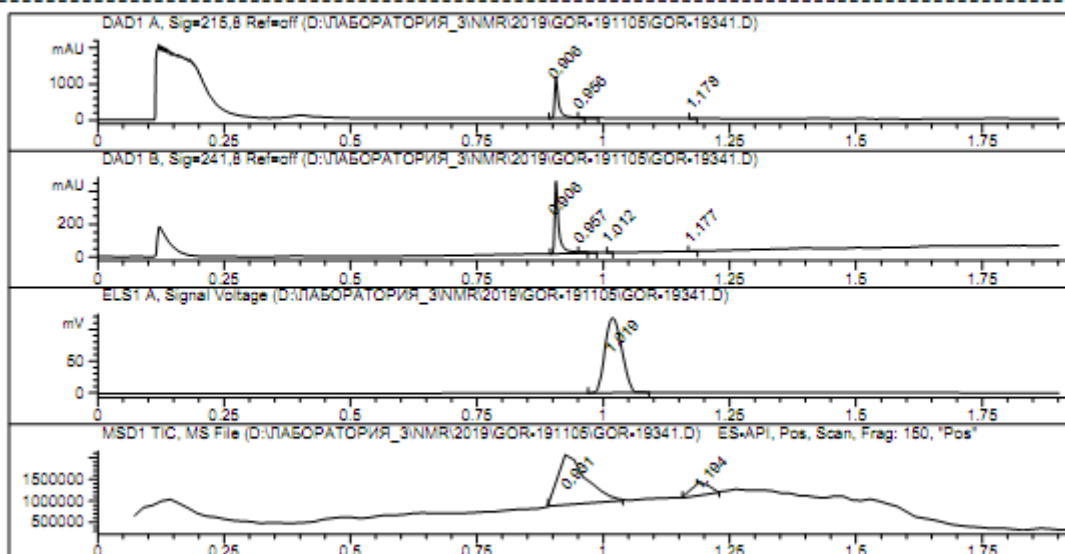


Figure S25. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of compound 4d

-o.-Synzetx Purity Report -o.-

System: Agilent 1200 LC/MSD SL
 Separation column: Rapid Resolution HT Cartige 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.906	98.540
2		0.956	0.434
3		1.178	1.026

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.906	98.127
2		0.957	0.795
3		1.012	0.310
4		1.177	0.768

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.019	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.931	86.775
2		1.194	13.225

Inj. Data 05.11.2019

Figure S26. MS (ESI) spectrum of compound 4e.

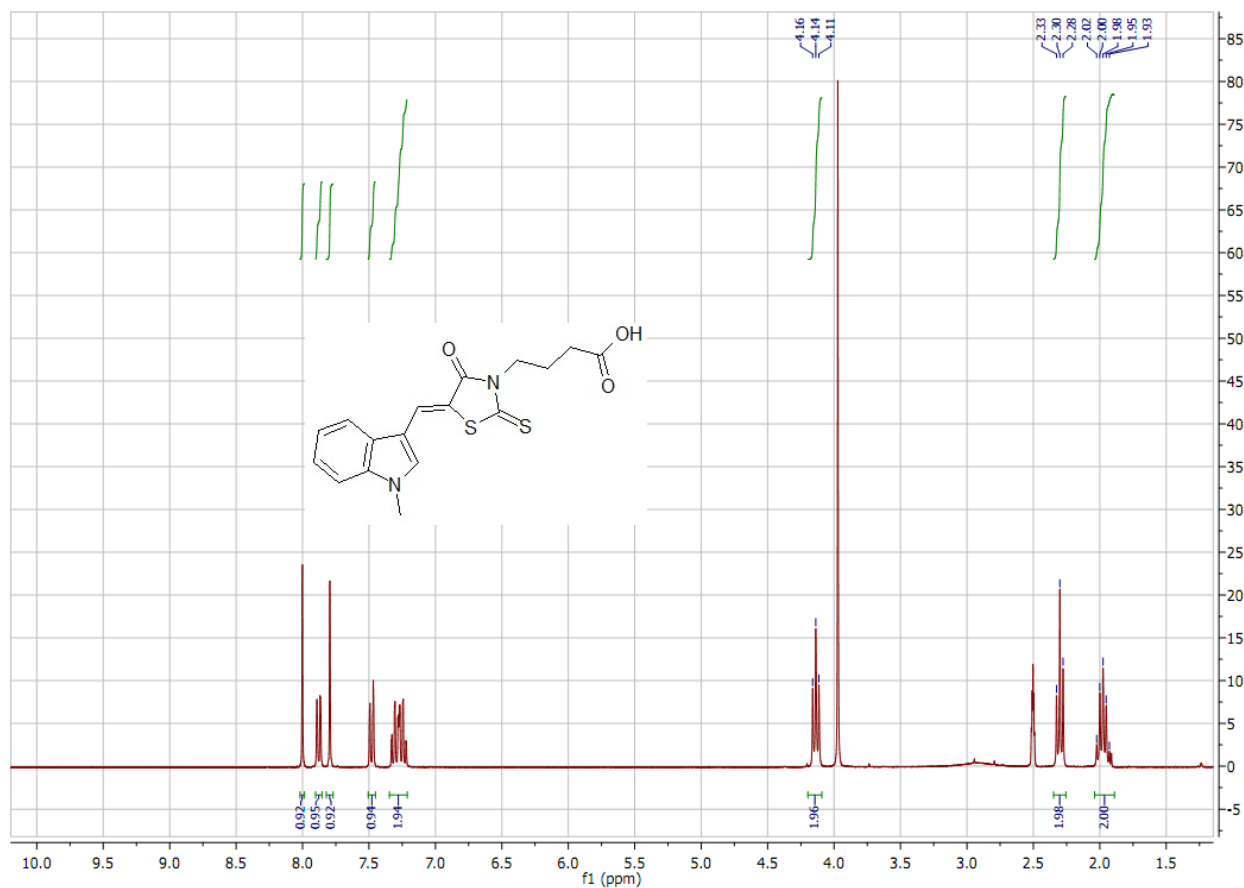


Figure S27. ^1H NMR spectrum (300 MHz, DMSO-d_6) of compound **4f**.

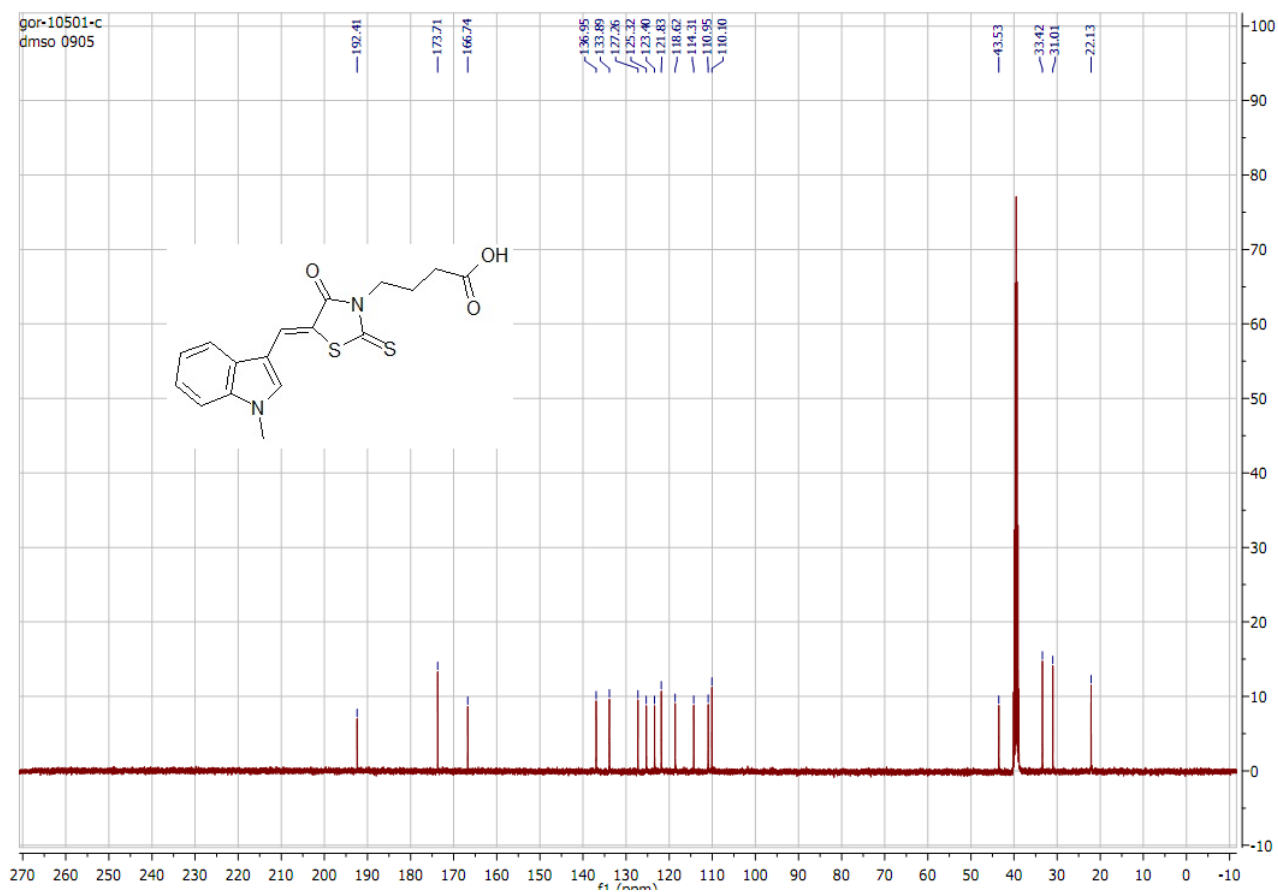
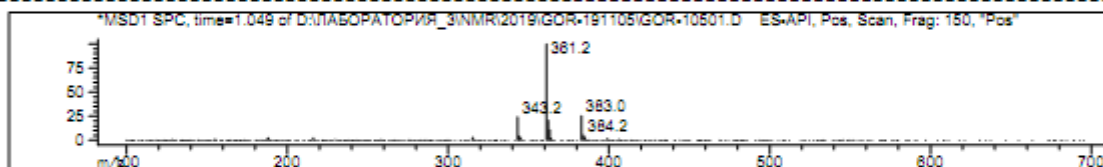
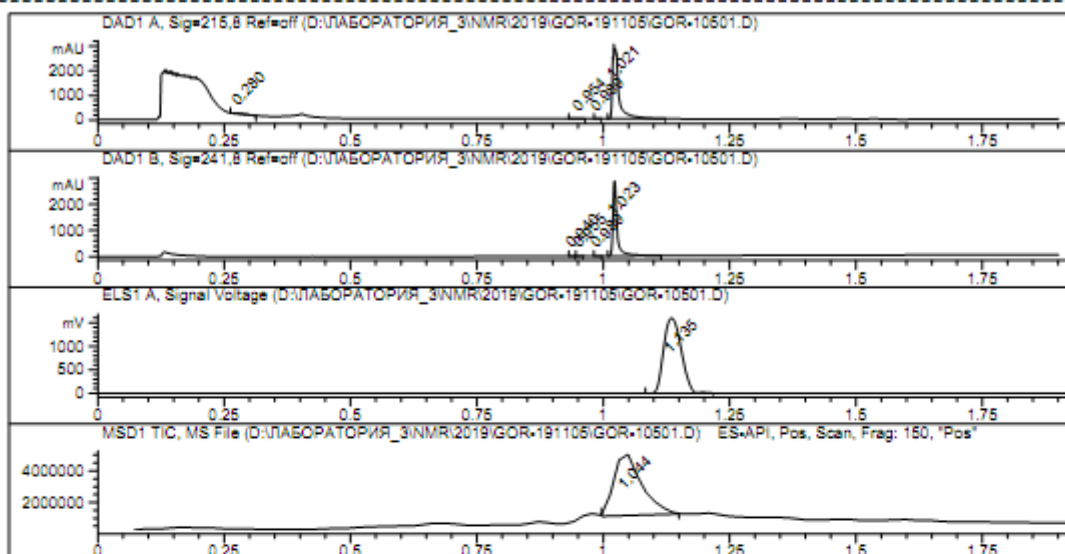


Figure S28. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of compound **4f**.

-o.-Syntex Purity Report -o.-

System: Agilent 1200 LC/MSD SL

Separation column: Rapid Resolution HT Cartige 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.280	1.868
2		0.954	0.299
3		0.989	0.128
4		1.021	97.706

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.940	0.068
2		0.955	0.092
3		0.989	0.139
4		1.023	99.701

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.135	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.044	100.000

Inj. Data 06.11.2019

Figure S29. MS (ESI) spectrum of compound **4f**.

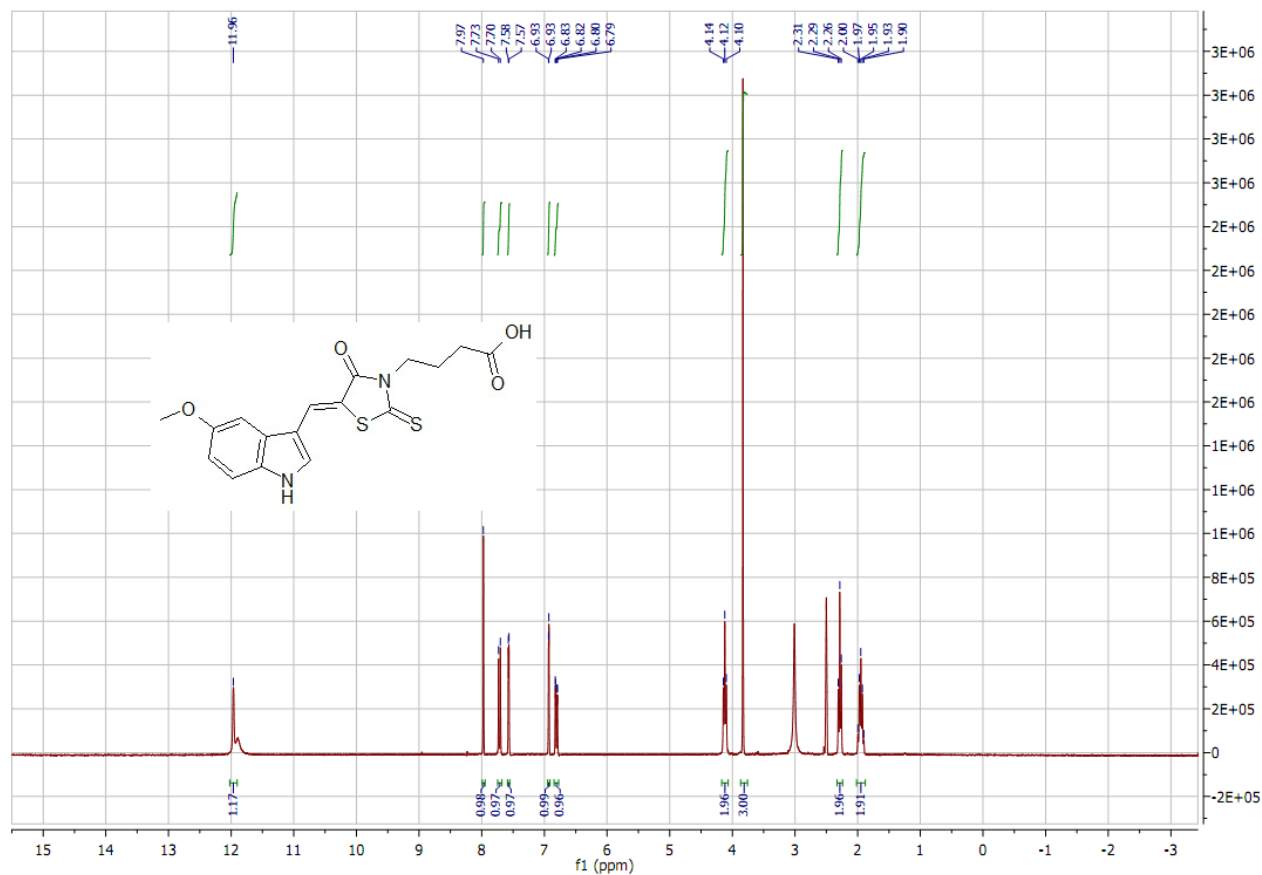


Figure S30. ^1H NMR spectrum (300 MHz, DMSO-d_6) of compound **4g**.

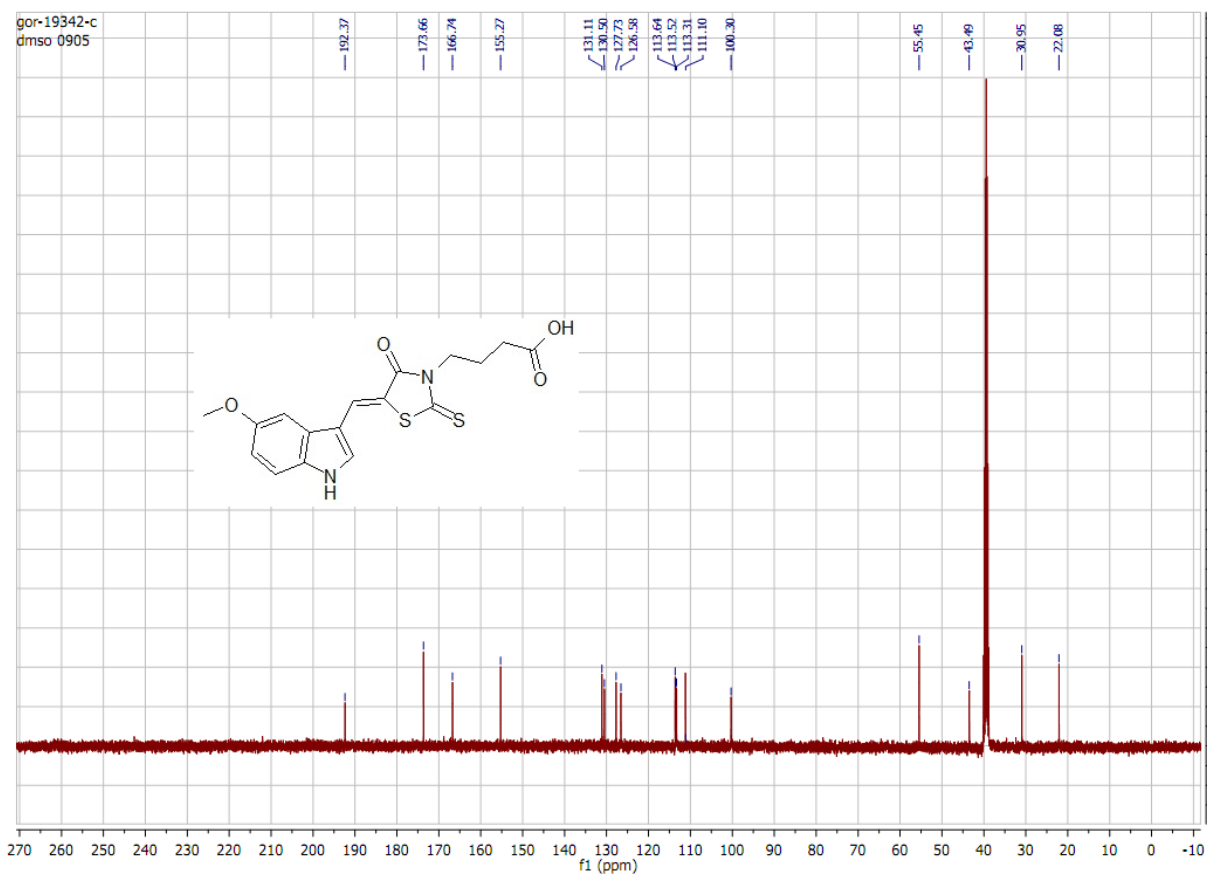
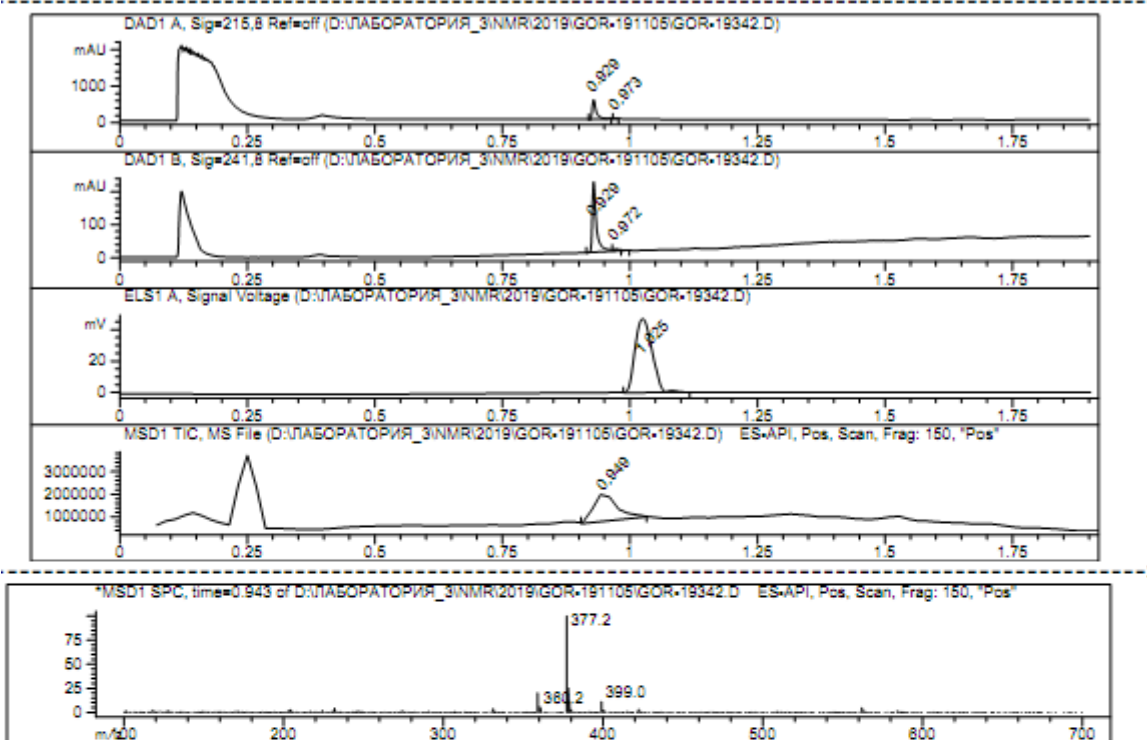


Figure S31. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of compound **4g**.

-o.-Synthes Purity Report -o.-

System: Agilent 1200 LC/MSD SL
 Separation column: Rapid Resolution HT Cartige 4.6x30mm, 1.8-Micron, Zorbax SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.929	99.533
2		0.973	0.467
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.929	98.942
2		0.972	1.058
#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.025	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.949	100.000

inj. Date 05.11.2019

Figure S32. MS (ESI) spectrum of compound 4g.

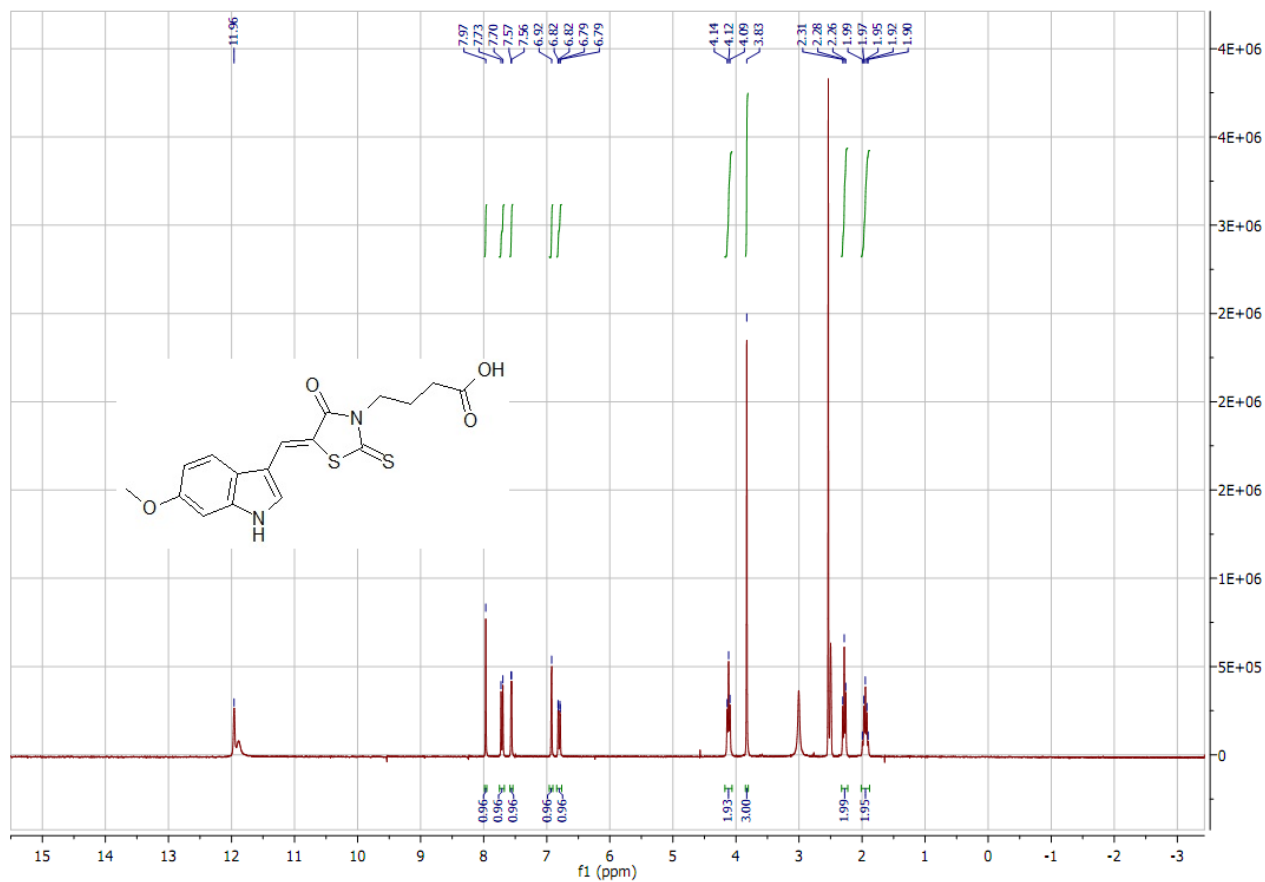


Figure S33. ^1H NMR spectrum (300 MHz, DMSO-d_6) of compound **4h**.

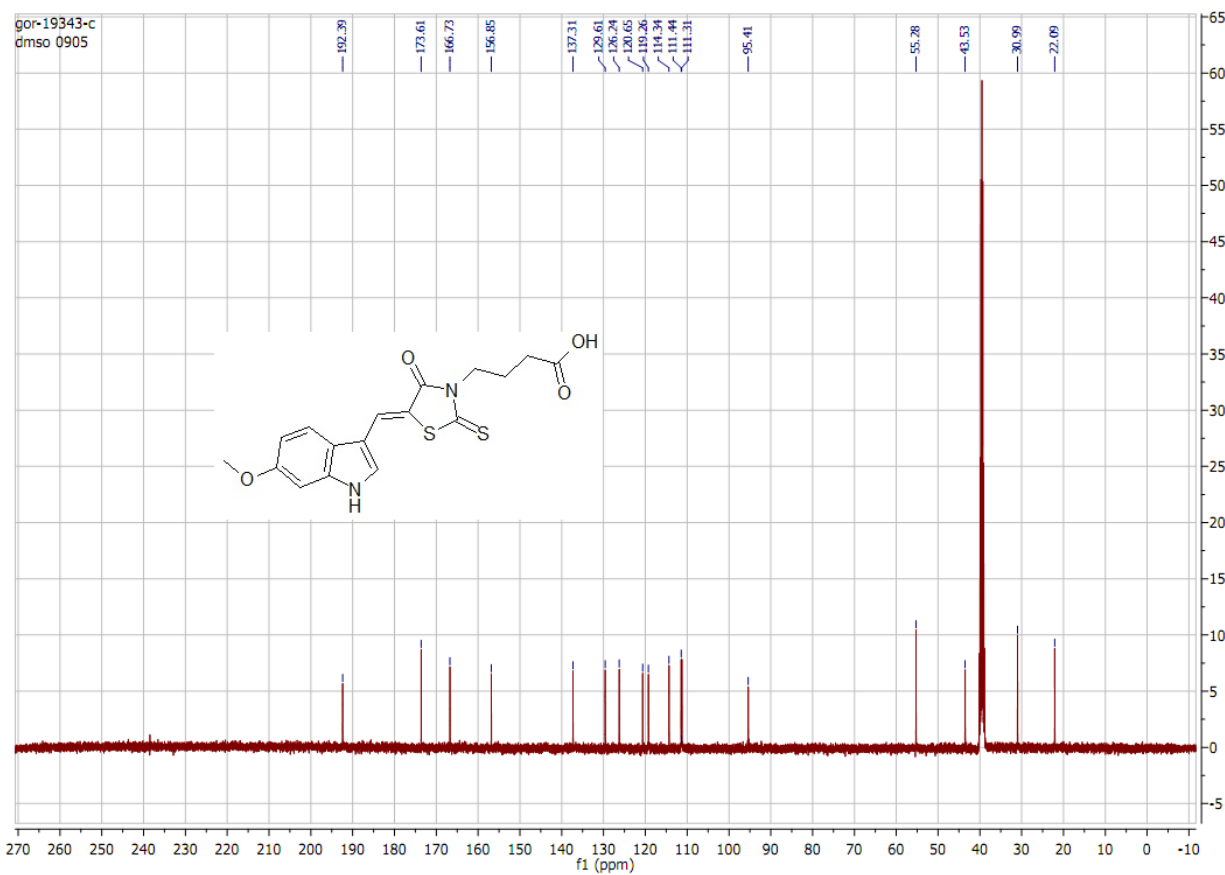
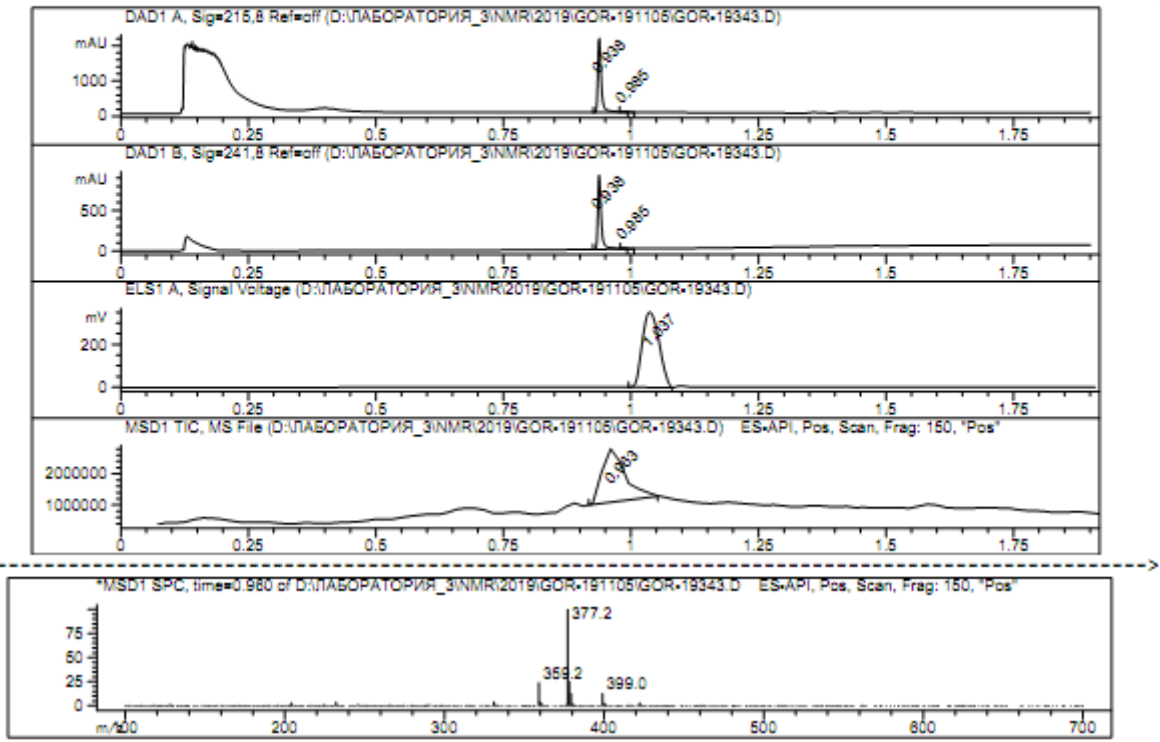


Figure S34. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of compound **4h**.

-o.-Syntez Purity Report -o.-

System: Agilent 1200 LC/MSD SL
 Separation column: Rapid Resolution HT Cartidge 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.938	99.403
2		0.985	0.597

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.938	99.433
2		0.985	0.567

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.037	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.963	100.000

Figure S35. MS (ESI) spectrum of compound 4h.

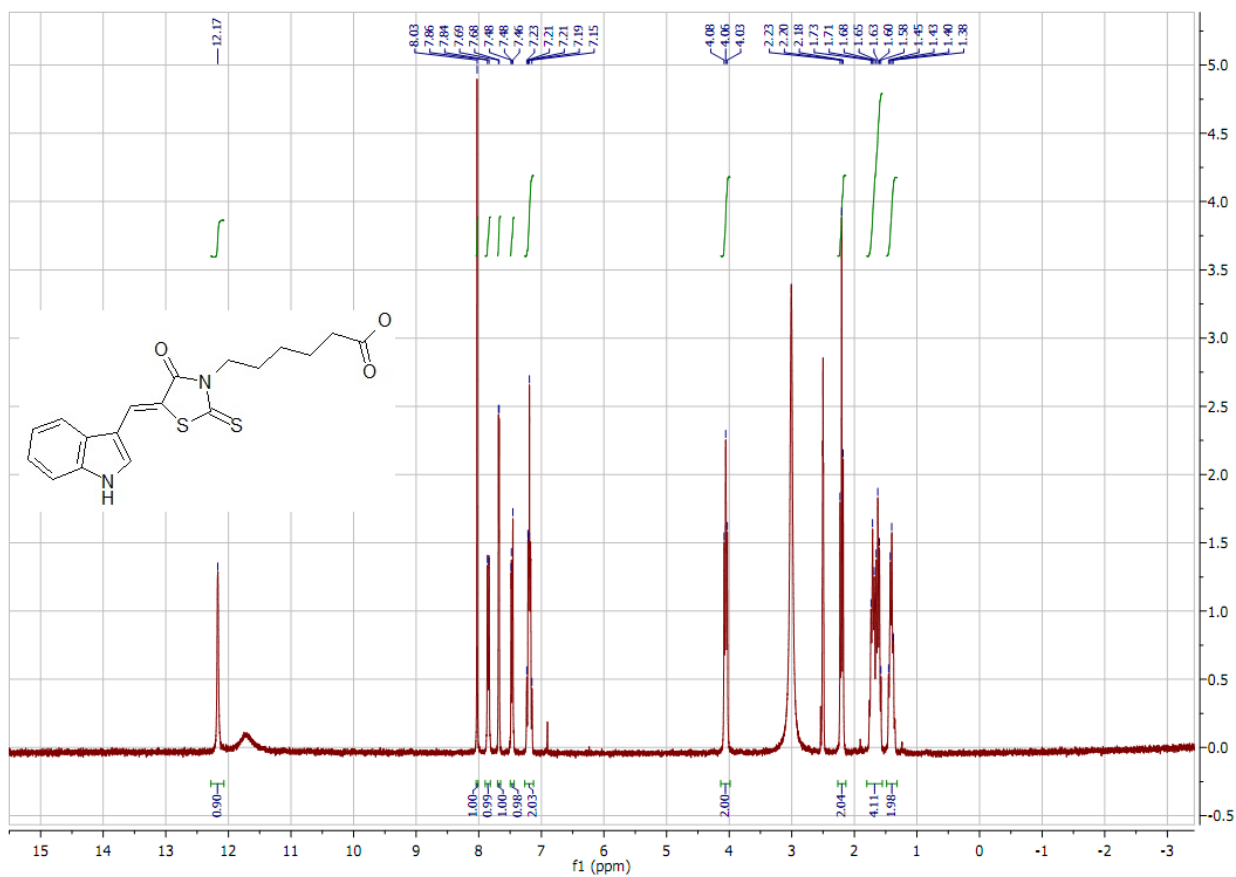


Figure S36. $^1\text{H NMR}$ spectrum (300 MHz, DMSO-d_6) of compound **4i**.

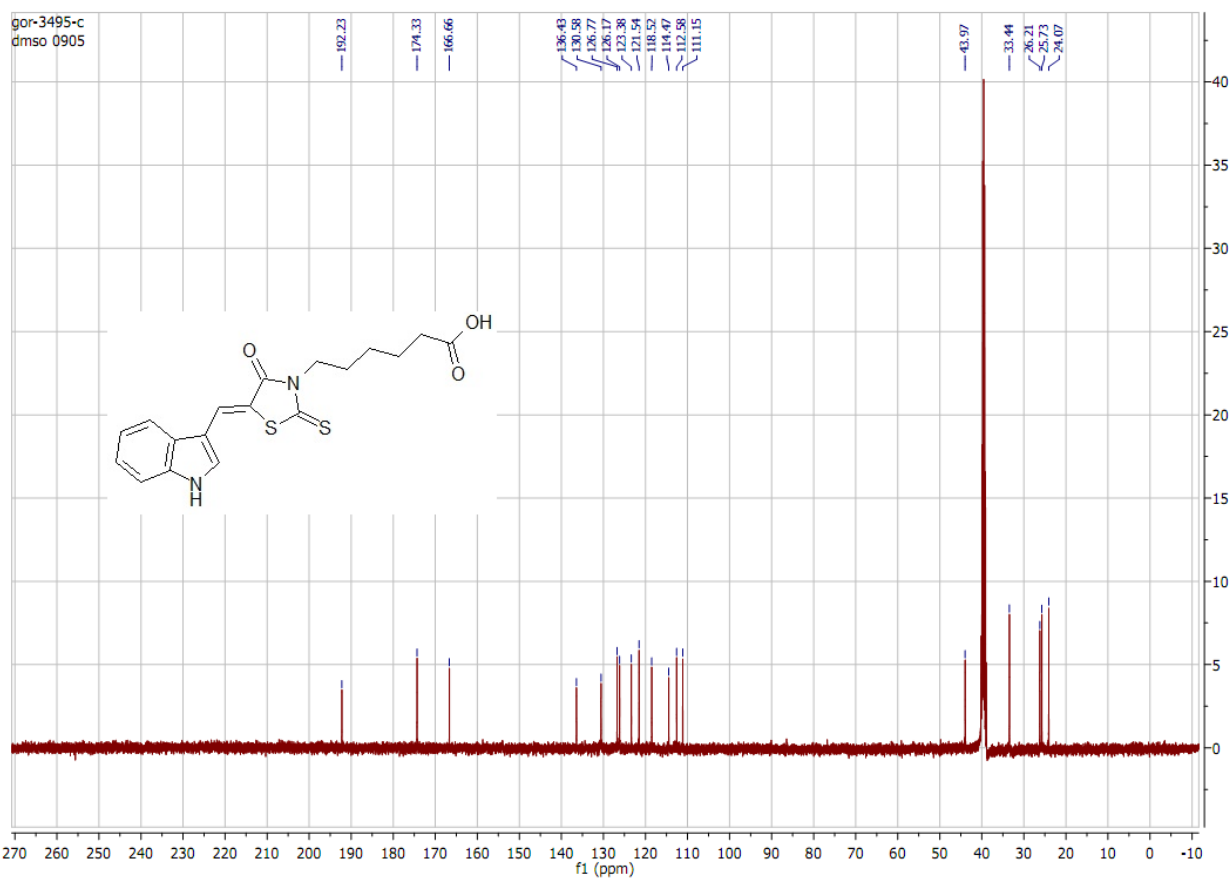
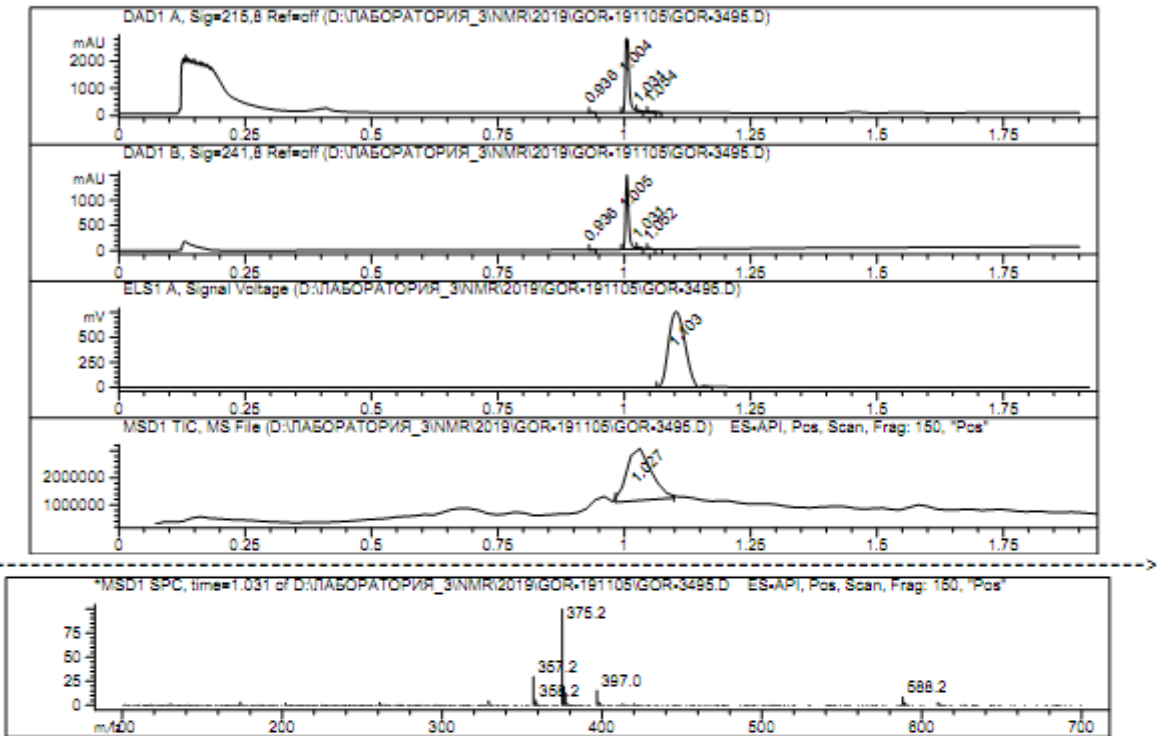


Figure S37. $^{13}\text{C NMR}$ spectrum (101 MHz, DMSO-d_6) of compound **4i**.

-o.-Syntez Purity Report -o.-

System: Agilent 1200 LC/MSD SL
 Separation column: Rapid Resolution HT Cartige 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.936	0.521
2		1.004	98.688
3		1.031	0.464
4		1.054	0.327

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.936	0.314
2		1.005	98.767
3		1.031	0.621
4		1.052	0.299

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.103	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.027	100.000

Inj. Data 06.11.2019

Figure S38. MS (ESI) spectrum of compound 4i.

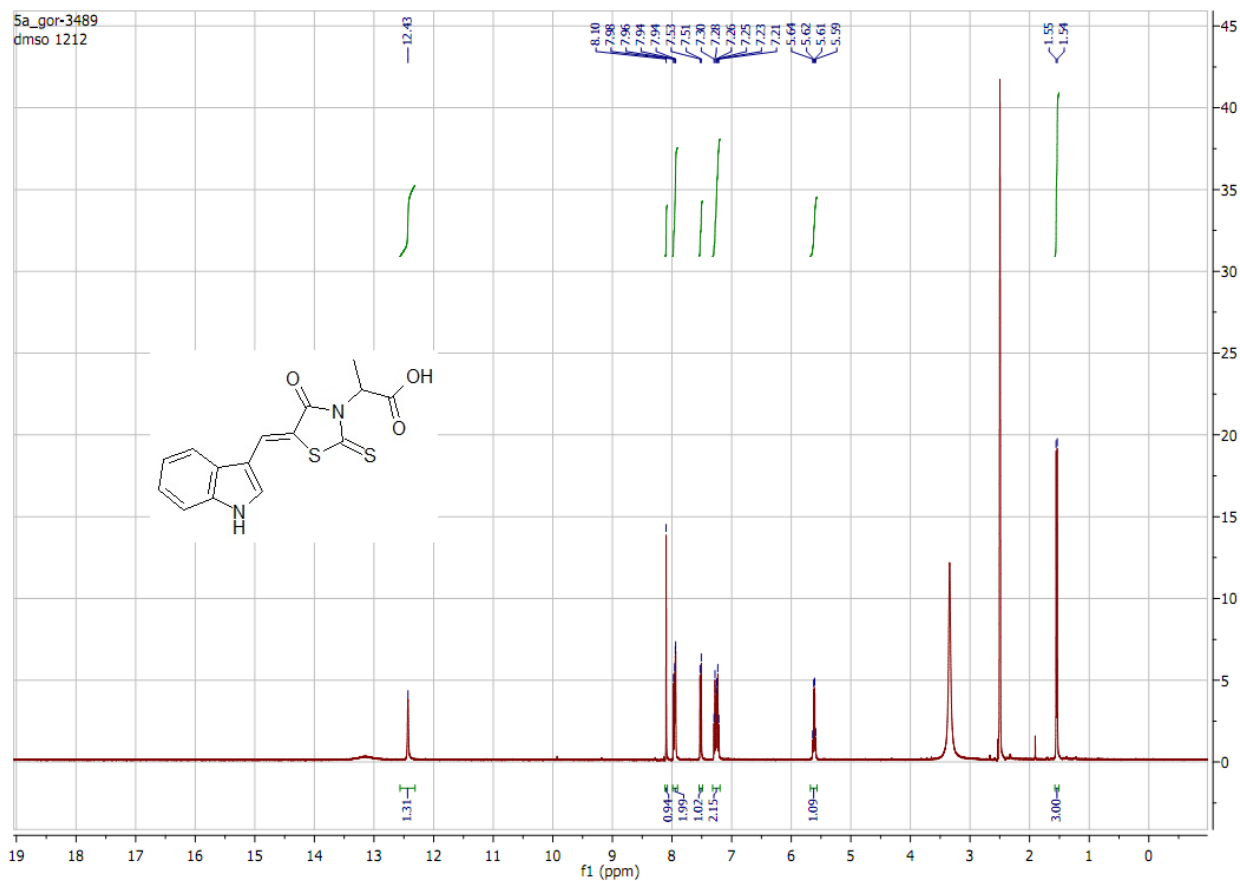


Figure S39. ^1H NMR spectrum (400 MHz, DMSO- d_6) of compound **5a**.

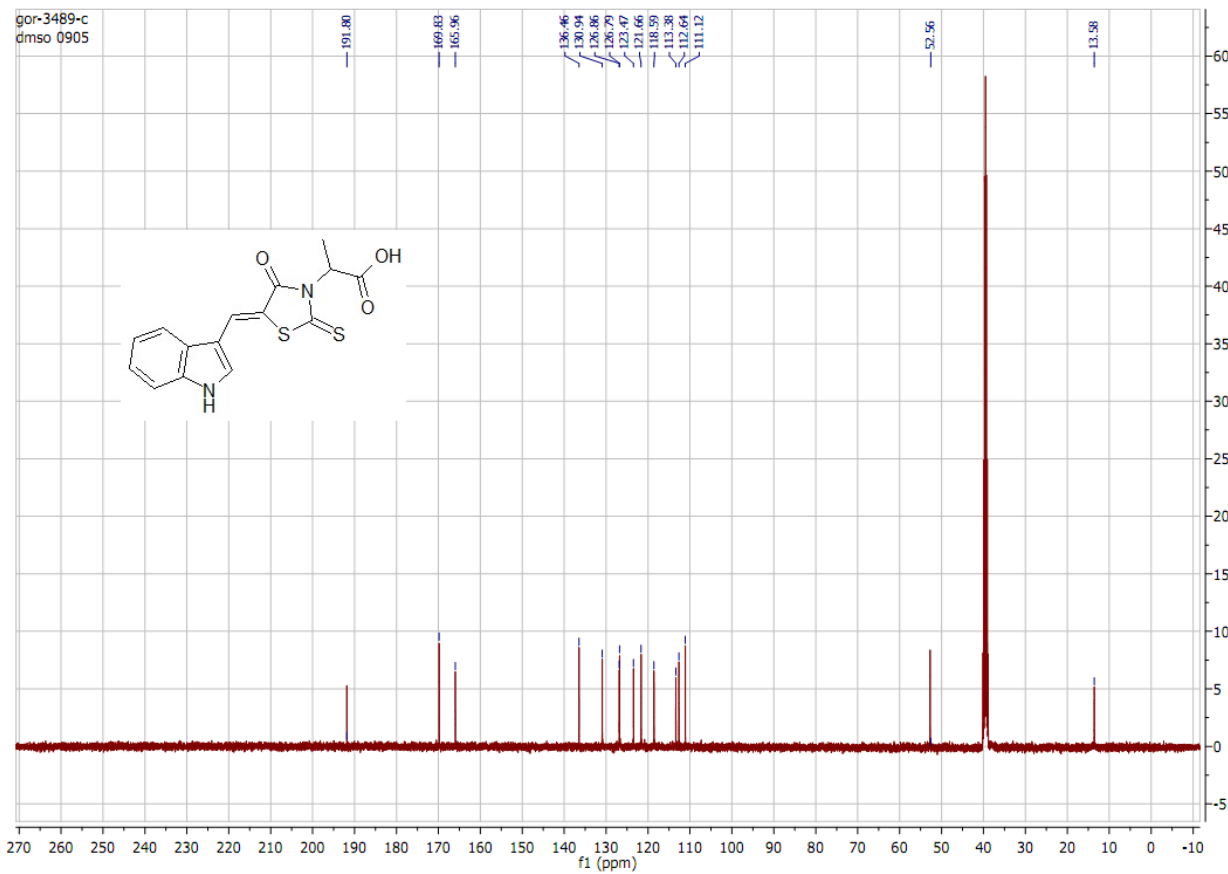
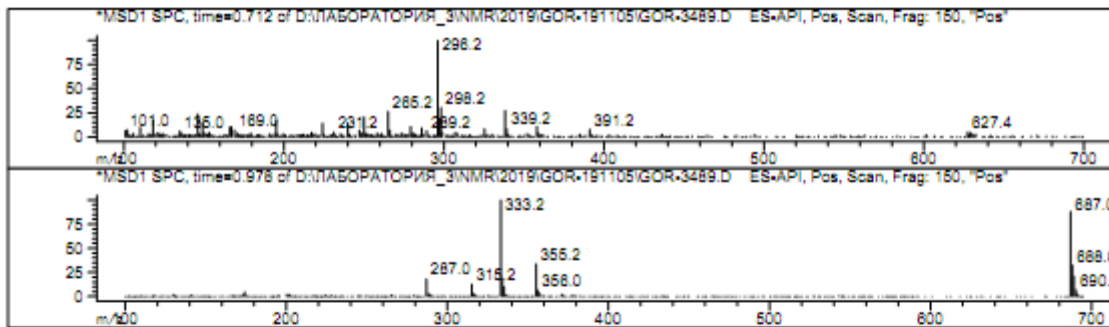
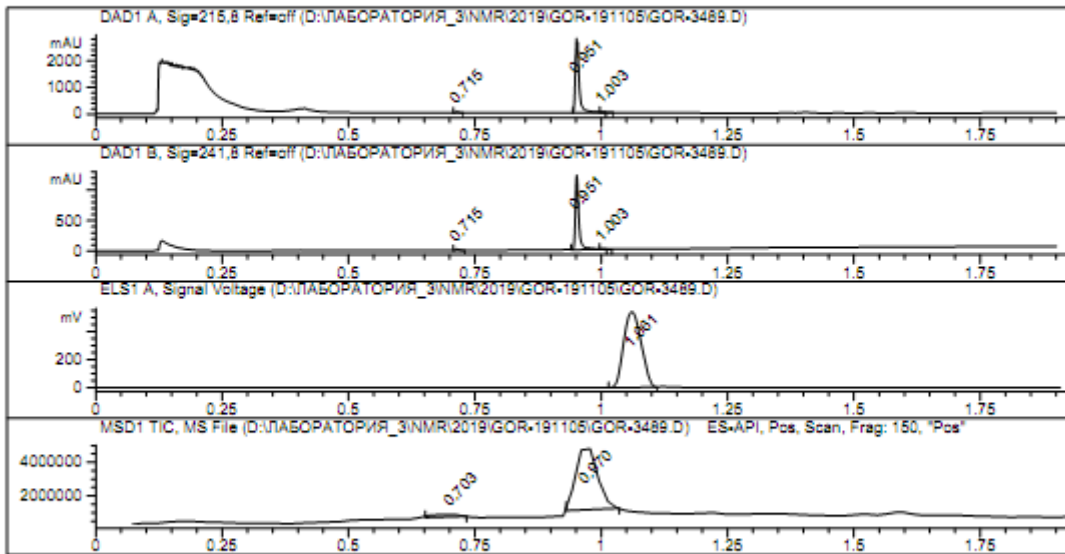


Figure S40. ^{13}C NMR spectrum (101 MHz, DMSO- d_6) of compound **5a**.

-o.-Syntex Purity Report -o.-

System: Agilent 1200 LC/MSD SL
 Separation column: Rapid Resolution HT Cartidge 4.6x30mm, 1.8-Micron, Zorbax SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.715	1.110
2		0.951	98.711
3		1.003	0.179

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.715	1.847
2		0.951	97.819
3		1.003	0.334

#	Signal	R.Time	Area %
1	ELSI A, Signal Voltage	1.061	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.703	4.220
2		0.970	95.780

Inj. Data 06.11.2019

Figure S41. MS (ESI) spectrum of compound 5a.

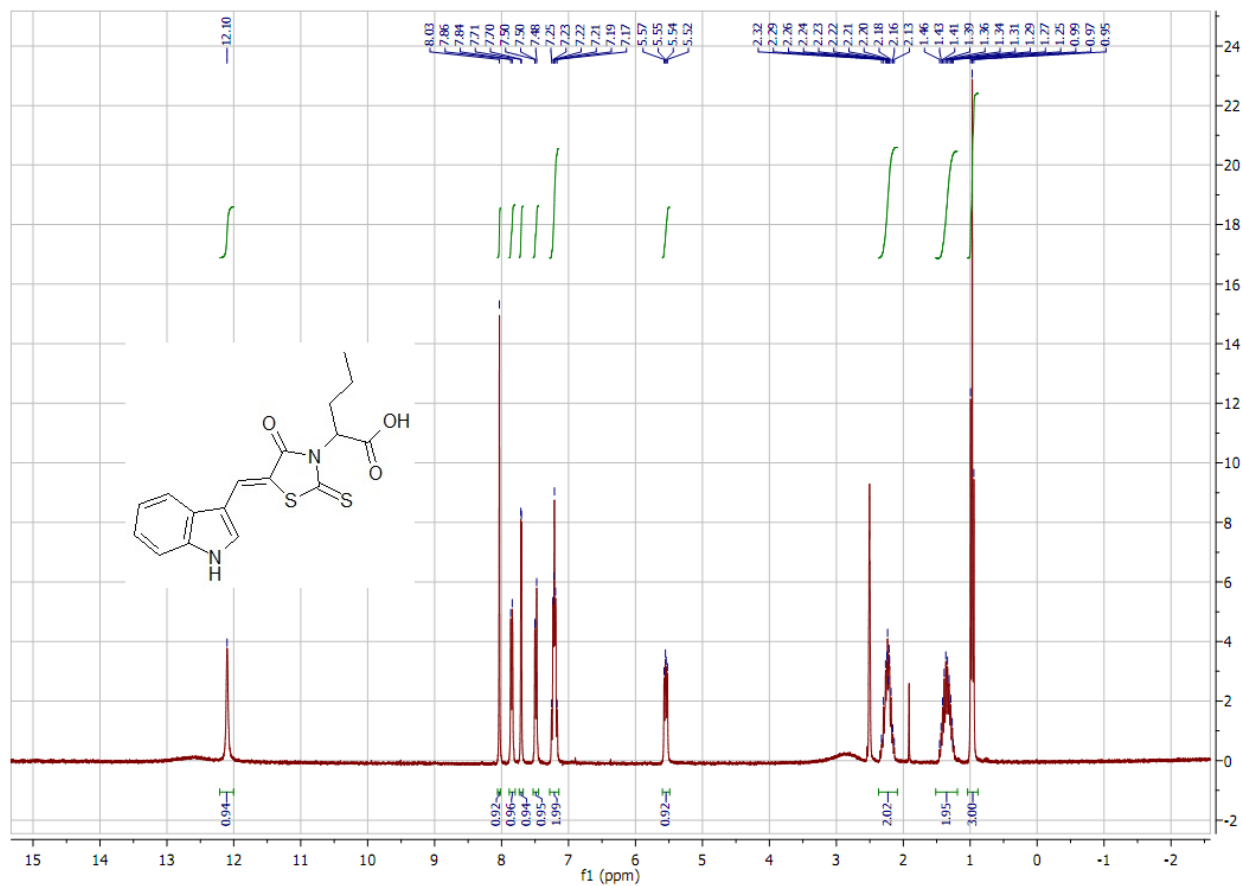


Figure S42. ^1H NMR spectrum (300 MHz, DMSO-d_6) of compound **5b**.

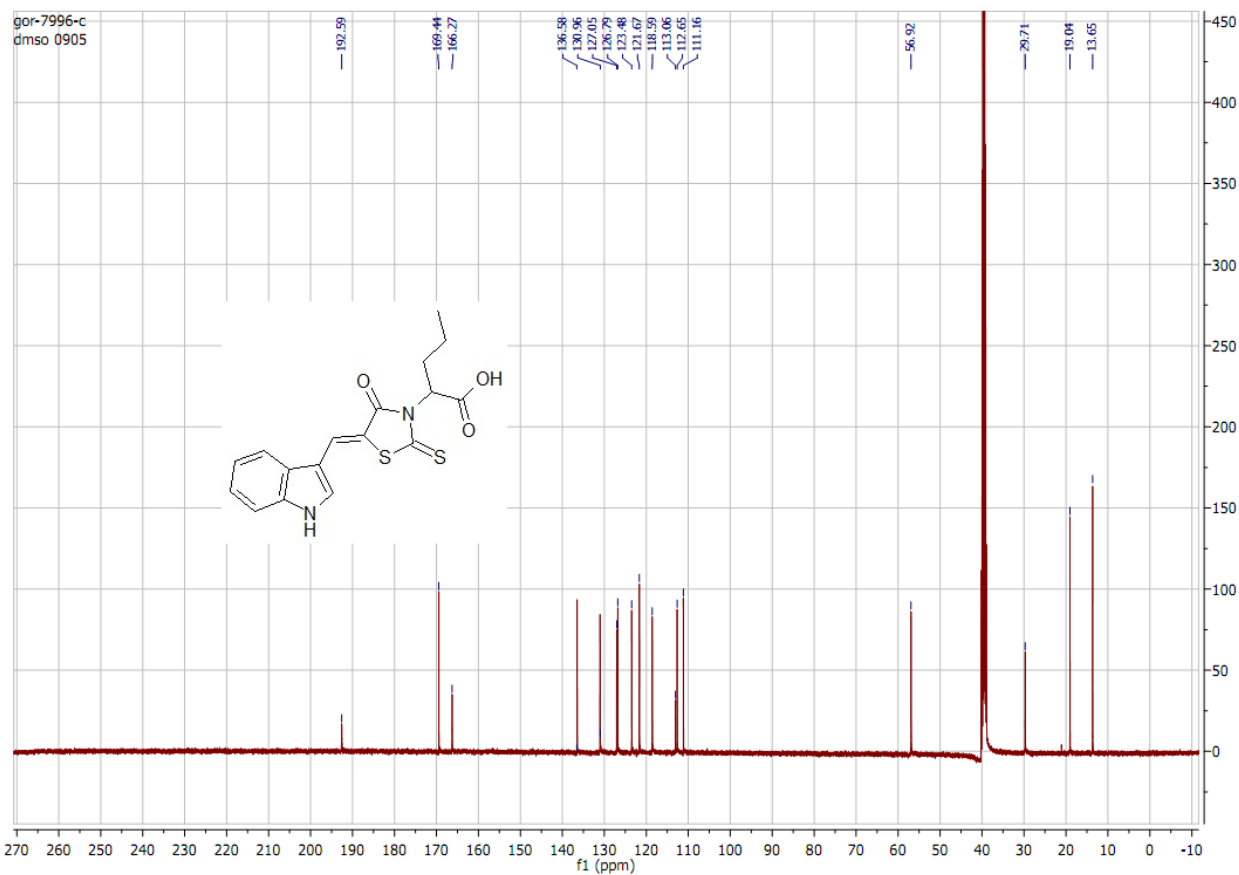
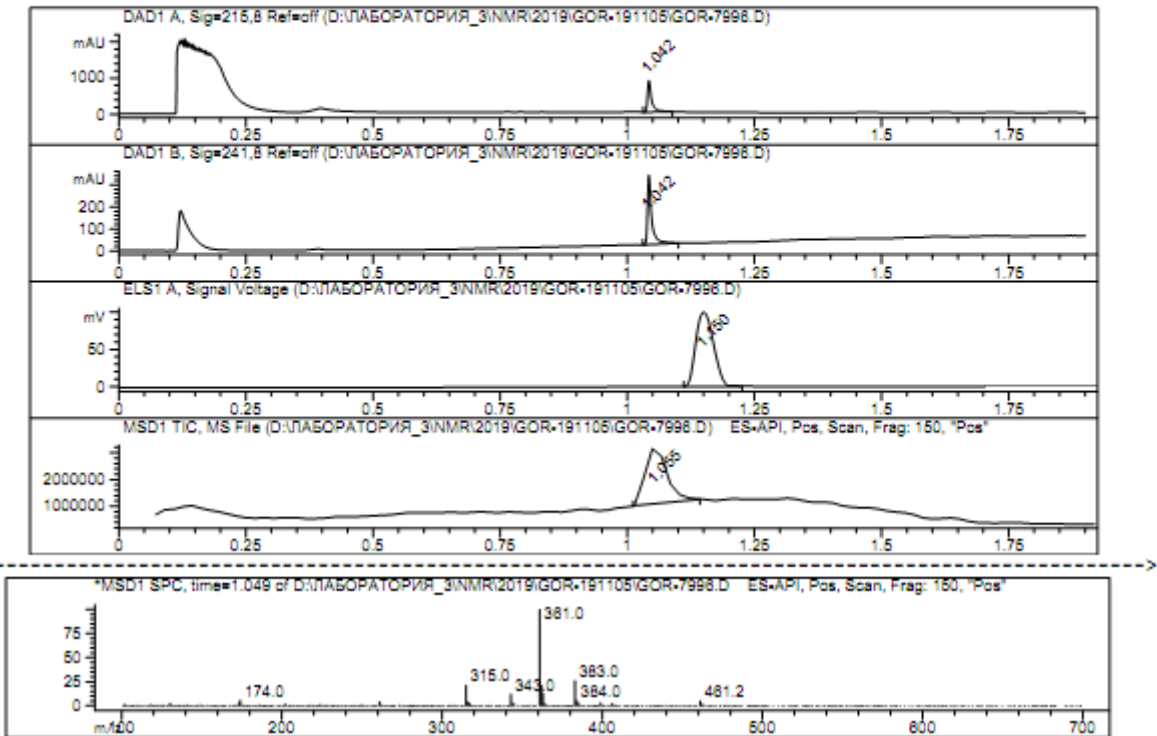


Figure S43. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of compound **5b**.

-o.-Syntez Purity Report -o.-

System: Agilent 1200 LC/MSD SL
 Separation column: Rapid Resolution HT Cartige 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	1.042	100.000
1	DAD1 B, Sig=241,8 Ref=off	1.042	100.000
1	ELS1 A, Signal Voltage	1.150	100.000
1	MSD1 TIC, MS File	1.055	100.000

Figure S44. MS (ESI) spectrum of compound 5b.

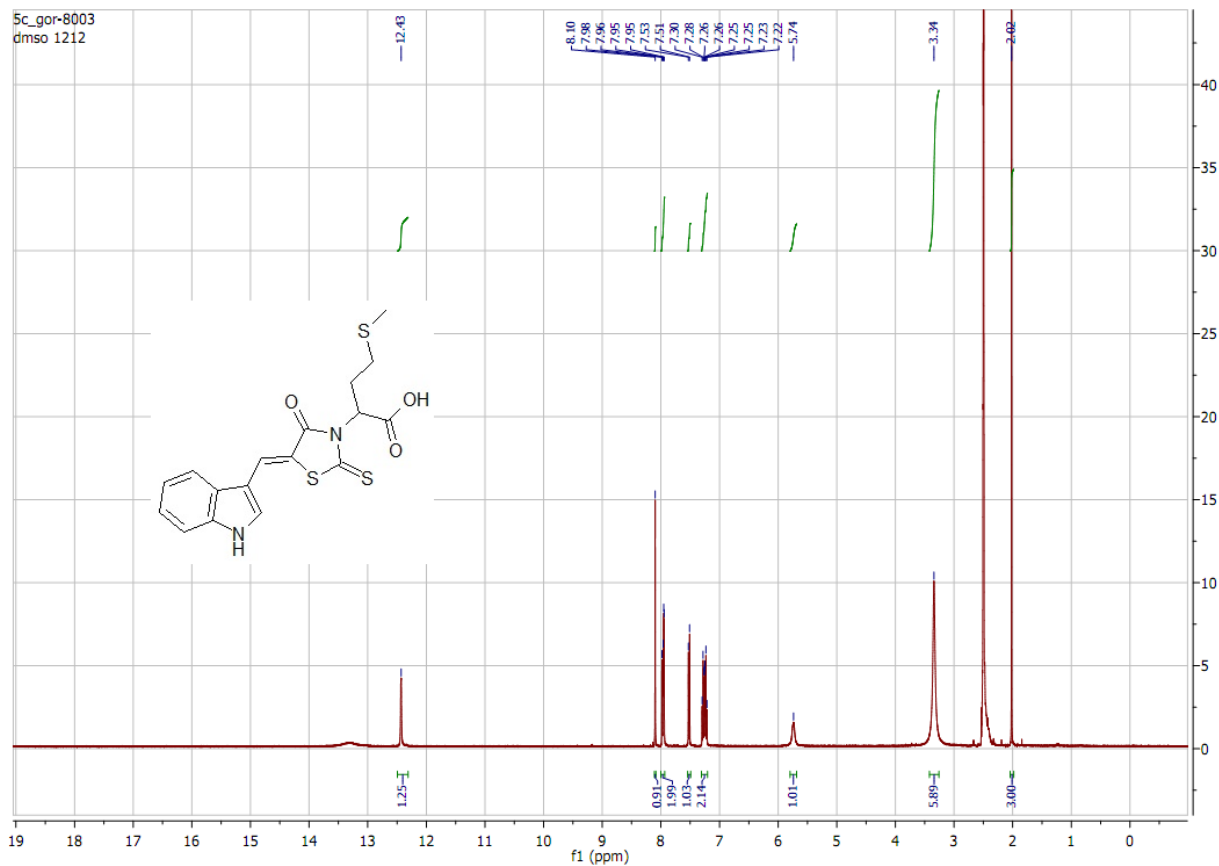


Figure S45. ^1H NMR spectrum (400 MHz, DMSO- d_6) of compound **5c**.

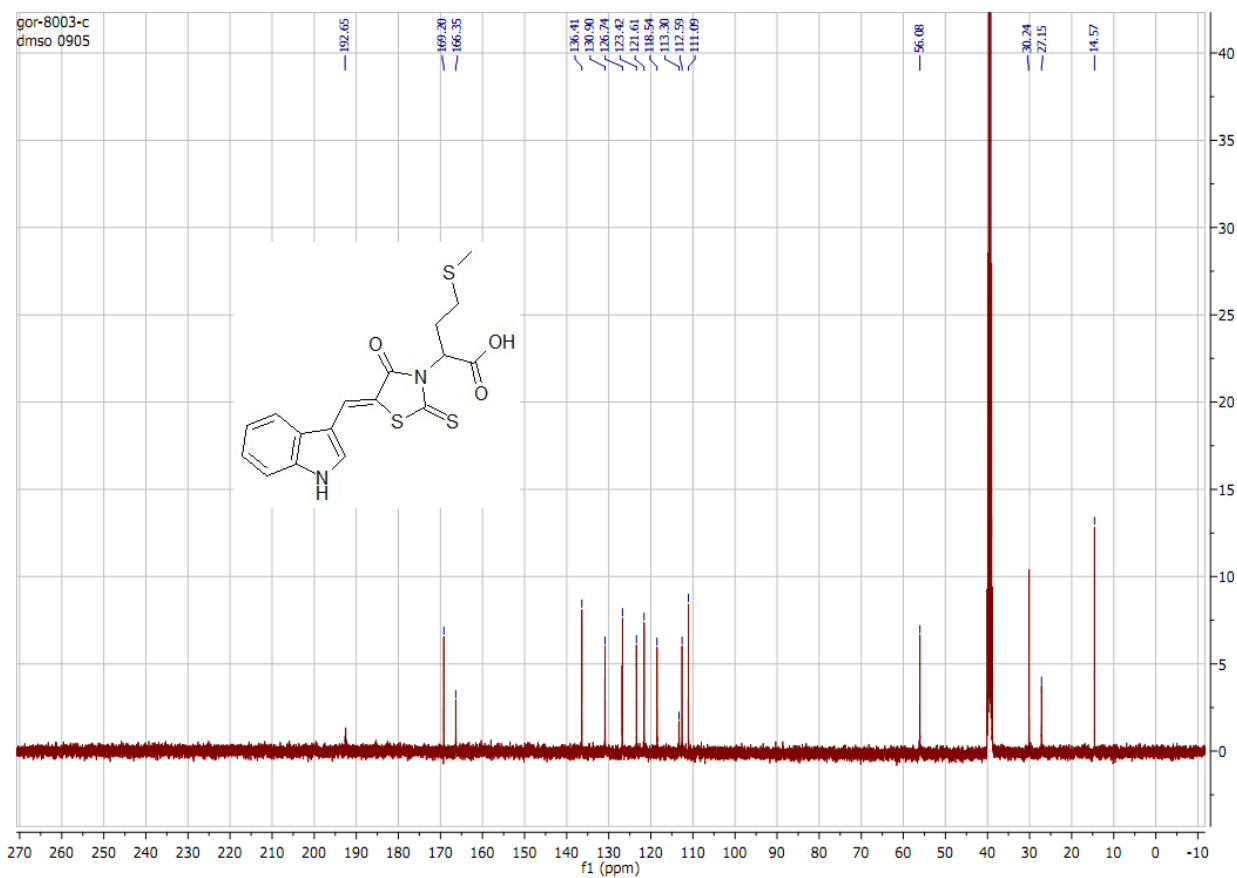
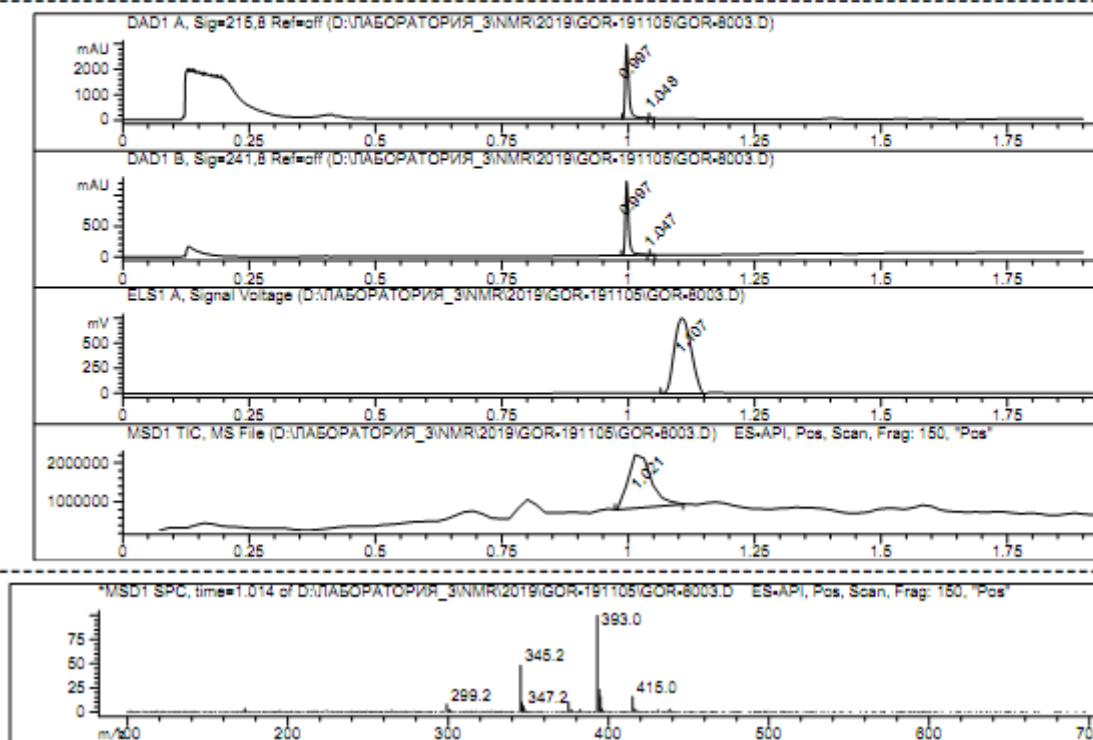


Figure S46. ^{13}C NMR spectrum (101 MHz, DMSO- d_6) of compound **5c**.

sample name: GOR-8003

-o.-Syntex Purity Report -o.-

System: Agilent 1200 LC/MSD SL
Separation column: Rapid Resolution HT Cartridge 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.997	99.691
2		1.048	0.309
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.997	99.552
2		1.047	0.448
#	Signal	R.Time	Area %
1	ELSI A, Signal Voltage	1.107	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.021	100.000

Inj. Data 06.11.2019

Figure S47. MS (ESI) spectrum of compound 5c.

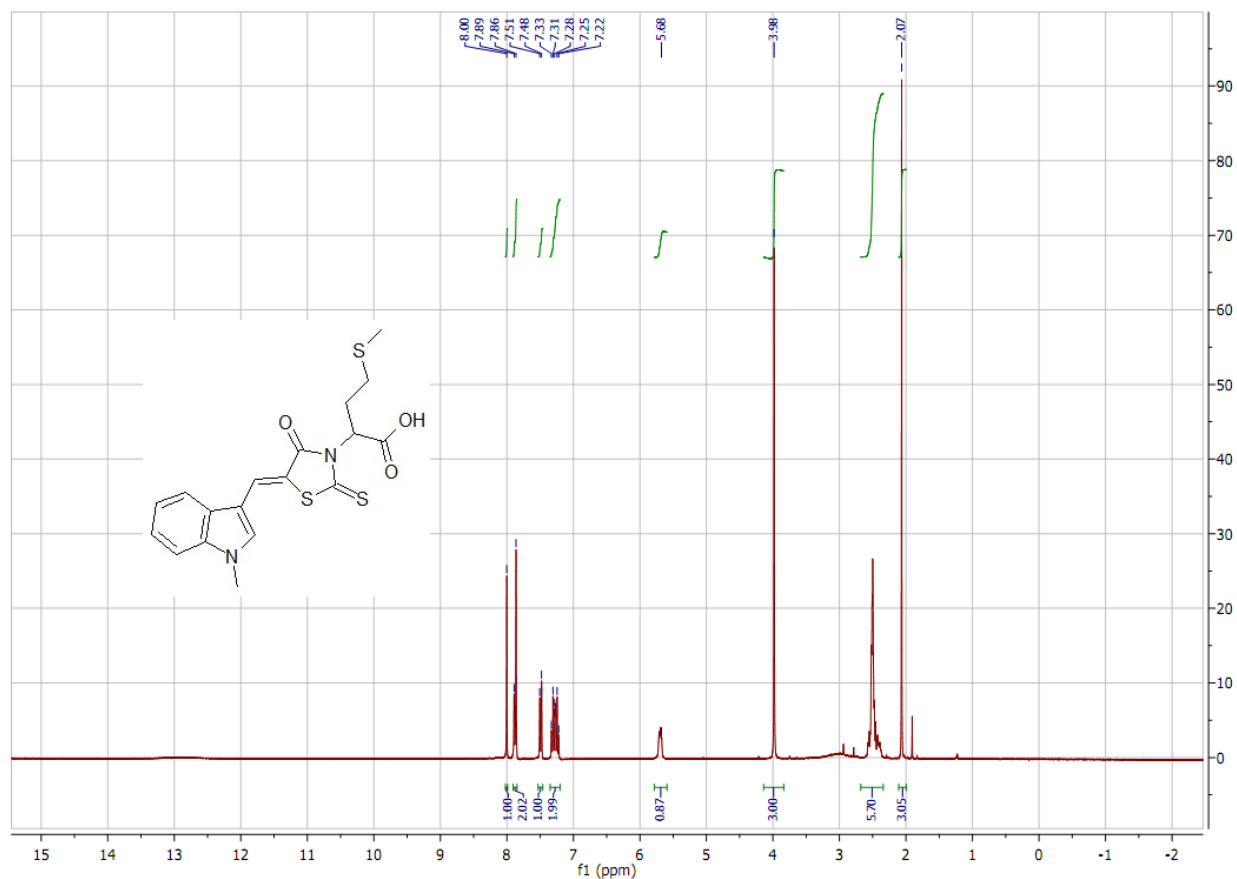


Figure S48. ¹H NMR spectrum (300 MHz, DMSO-d₆) of compound **5d**.

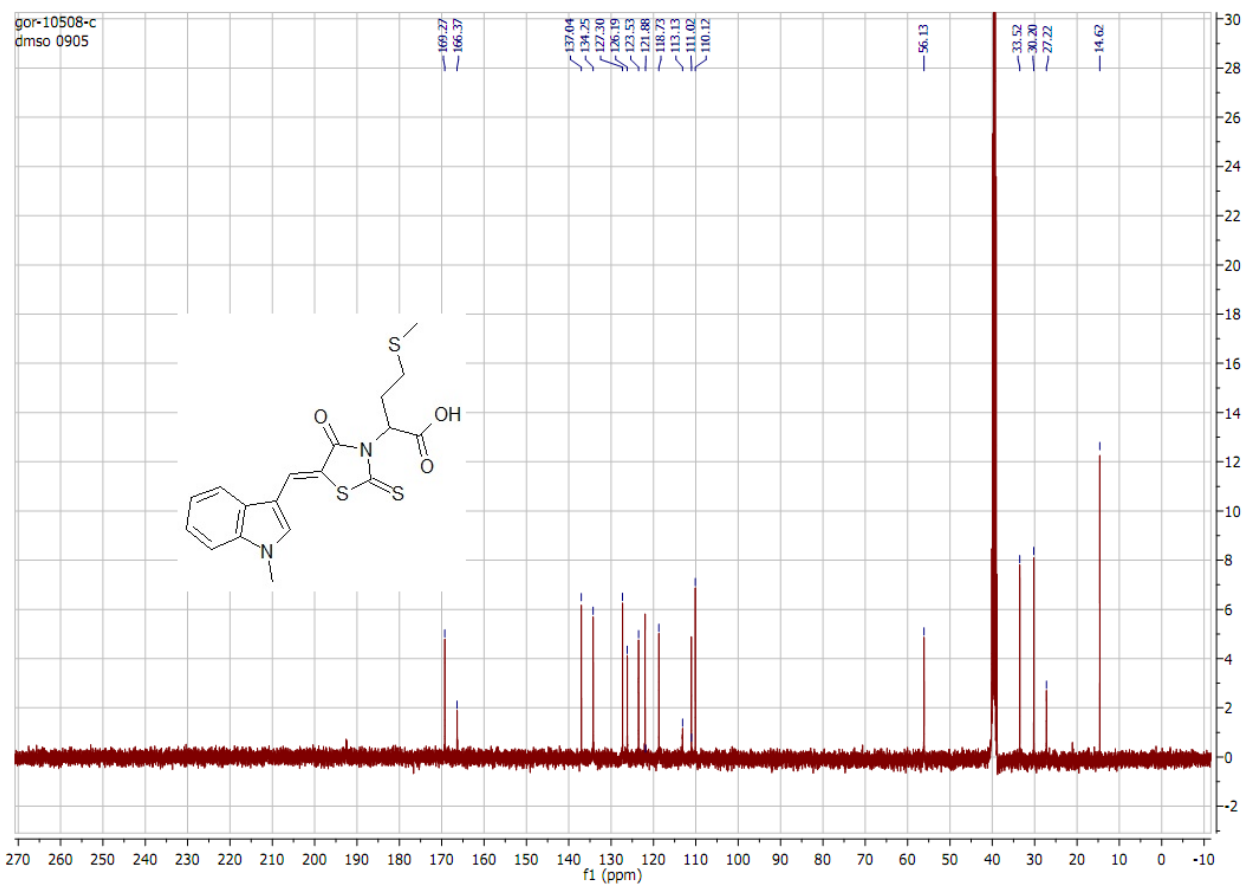
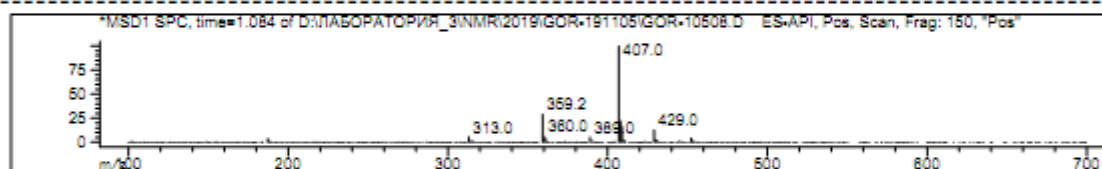
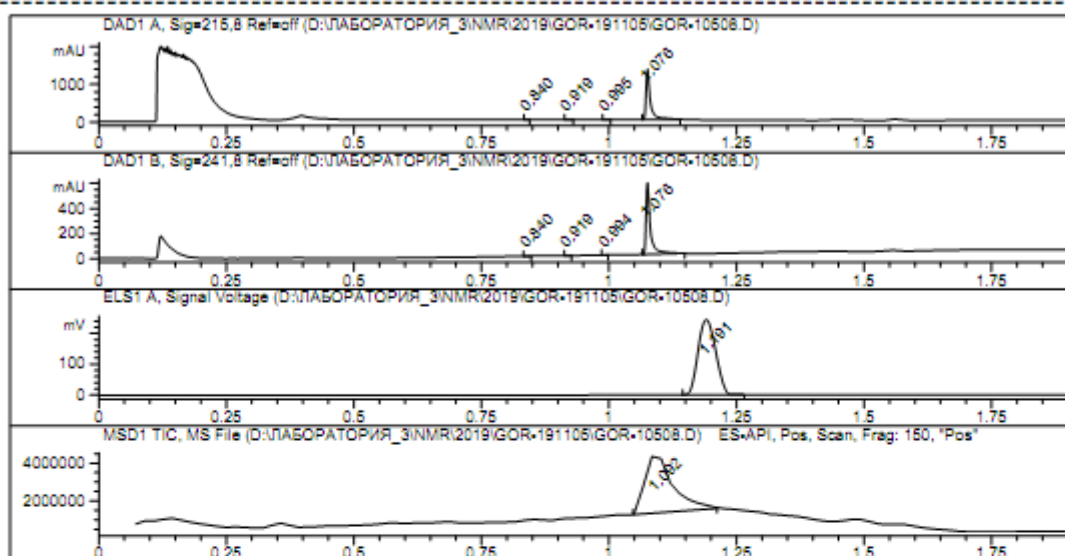


Figure S49. ¹³C NMR spectrum (101 MHz, DMSO-d₆) of compound **5d**.

-o.-Syntex Purity Report -o.-

System: Agilent 1200 LC/MSD SL

Separation column: Rapid Resolution HT Cartridge 4.6x30mm, 1.8-Micron, Zorbax SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.840	0.092
2		0.919	0.281
3		0.995	0.246
4		1.076	99.381
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.840	0.088
2		0.919	0.309
3		0.994	0.220
4		1.076	99.383
#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.191	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.092	100.000

Inj. Data 05.11.2019

Figure S50. MS (ESI) spectrum of compound 5d.

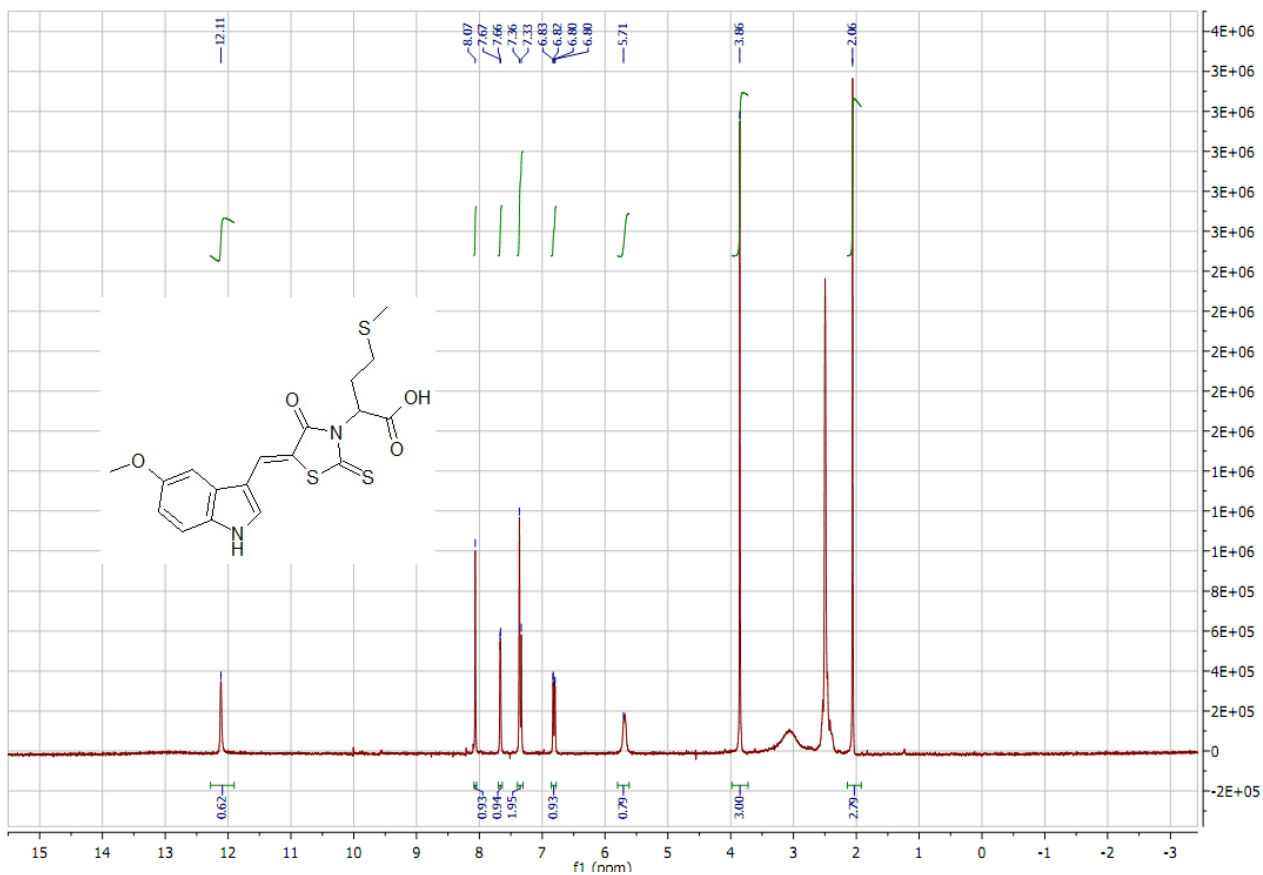


Figure S51. ^1H NMR spectrum (300 MHz, DMSO- d_6) of compound 5e.

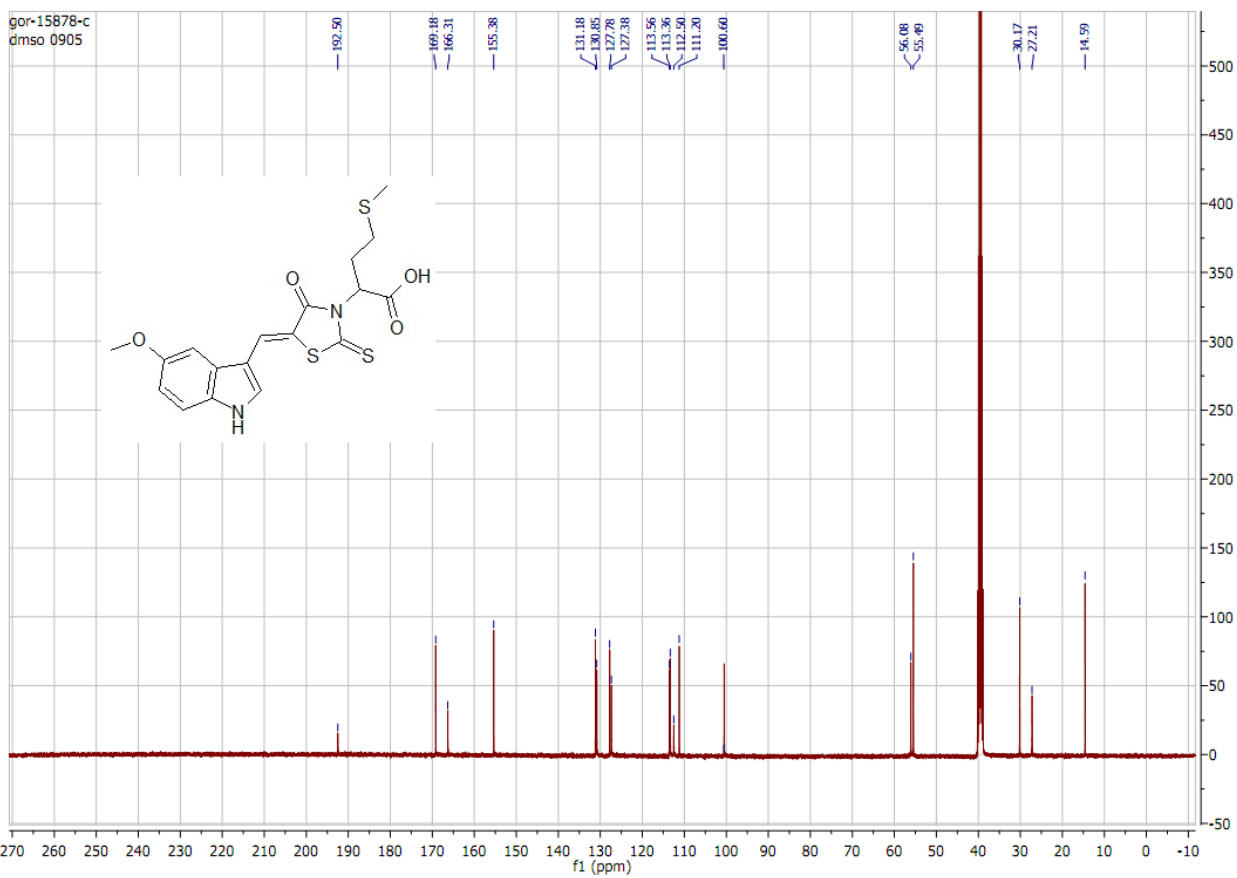
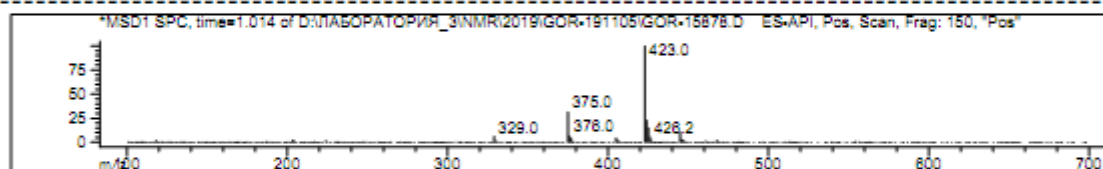
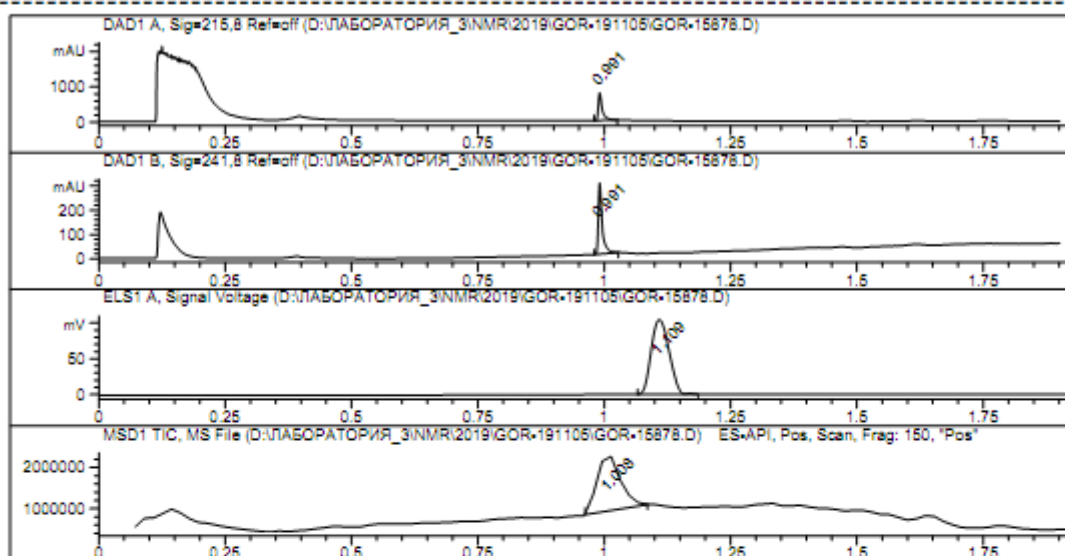


Figure S52. ^{13}C NMR spectrum (101 MHz, DMSO- d_6) of compound 5e.

-.o.-Syntex Purity Report -.o.-

System: Agilent 1200 LC/MSD SL

Separation column: Rapid Resolution HT Cartige 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.991	100.000
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.991	100.000
#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.109	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.008	100.000

Inj. Date 05.11.2019

Figure S53. MS (ESI) spectrum of compound 5e.

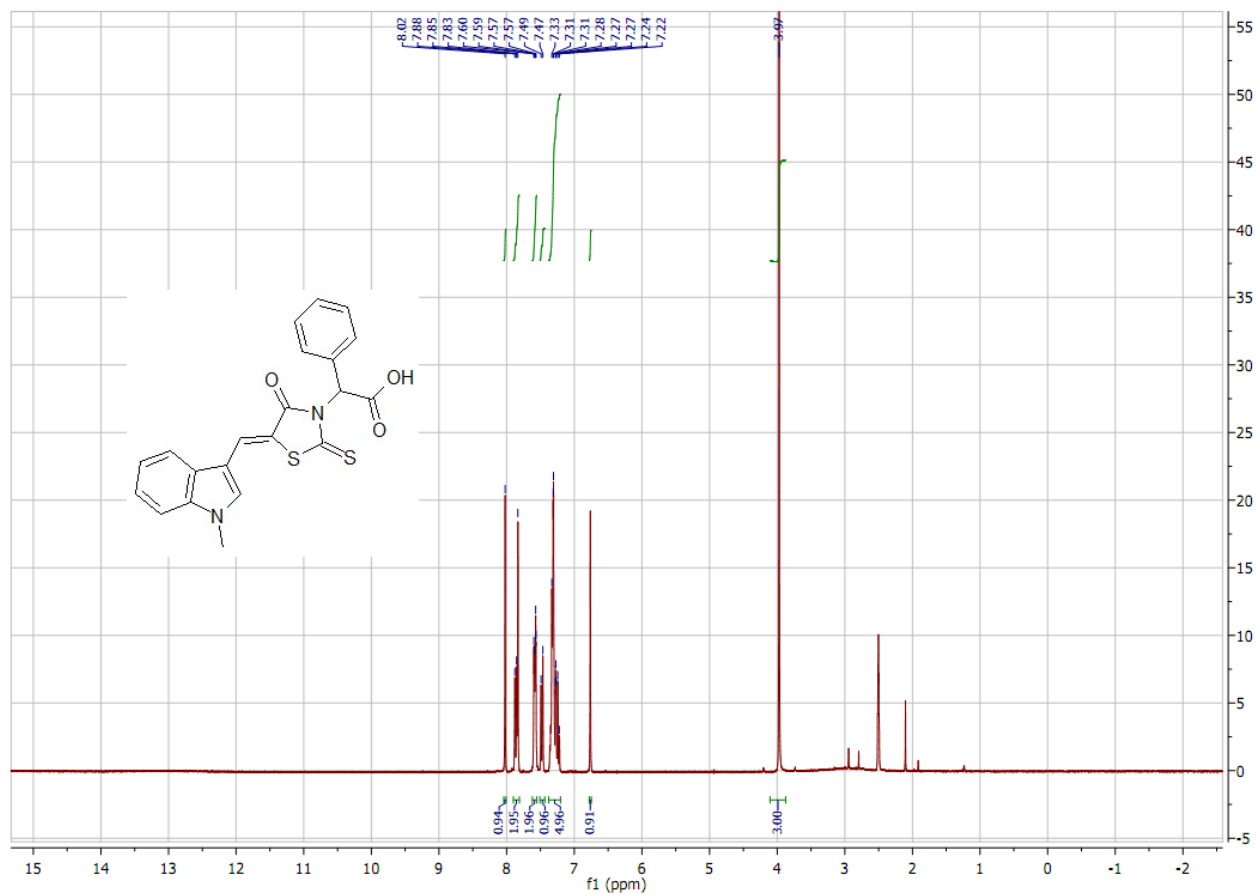


Figure S54. ¹H NMR spectrum (300 MHz, DMSO-d₆) of compound **5f**.

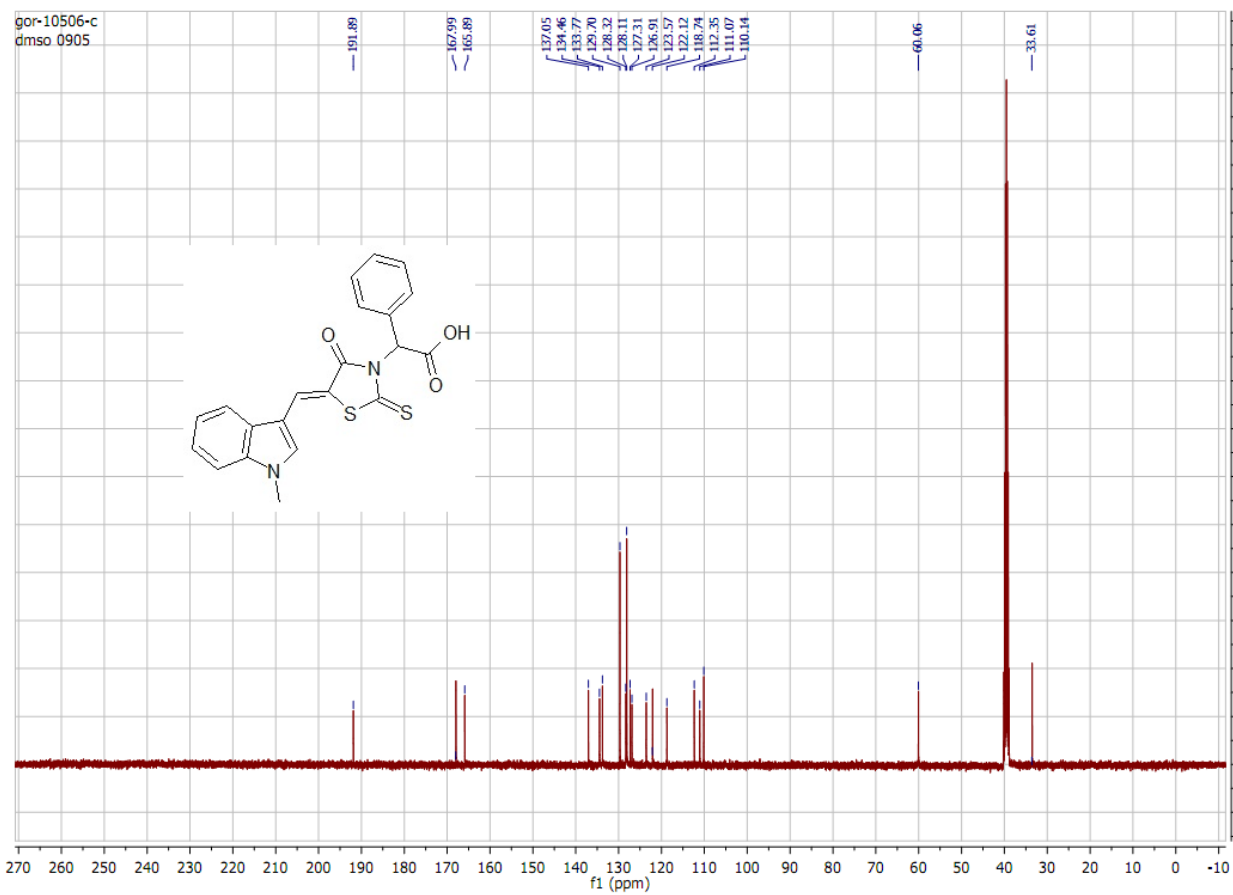
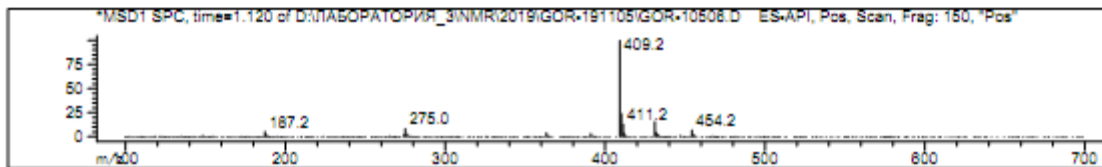
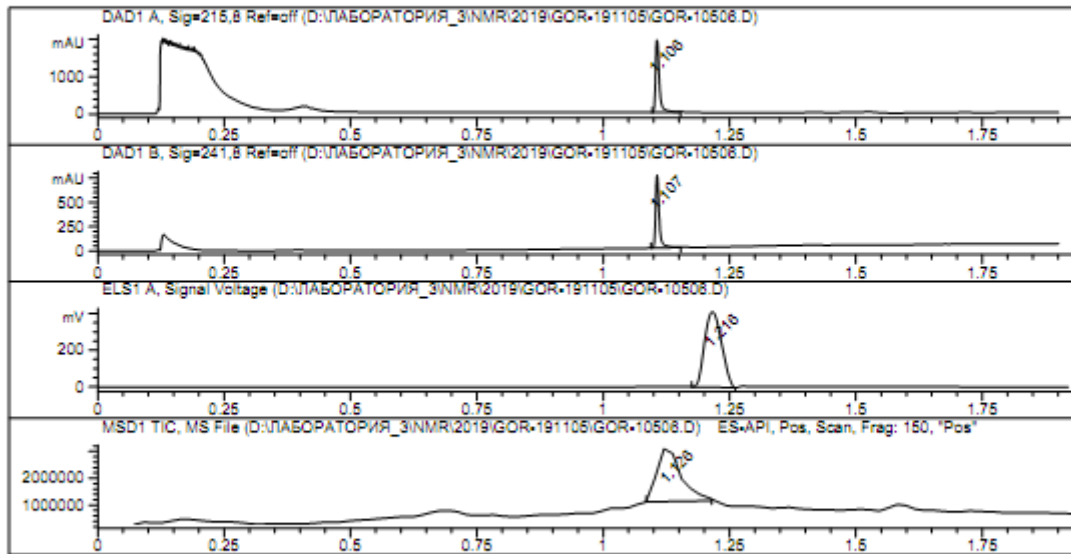


Figure S55. ¹³C NMR spectrum (101 MHz, DMSO-d₆) of compound **5f**.

-o.-Syntez Purity Report -o.-

System: Agilent 1200 LC/MSD SL
 Separation column: Rapid Resolution HT Cartige 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	1.106	100.000
1	DAD1 B, Sig=241,8 Ref=off	1.107	100.000
1	ELS1 A, Signal Voltage	1.216	100.000
1	MSD1 TIC, MS File	1.126	100.000

Inj. Data 06.11.2019

Figure S56. MS (ESI) spectrum of compound **5f**.

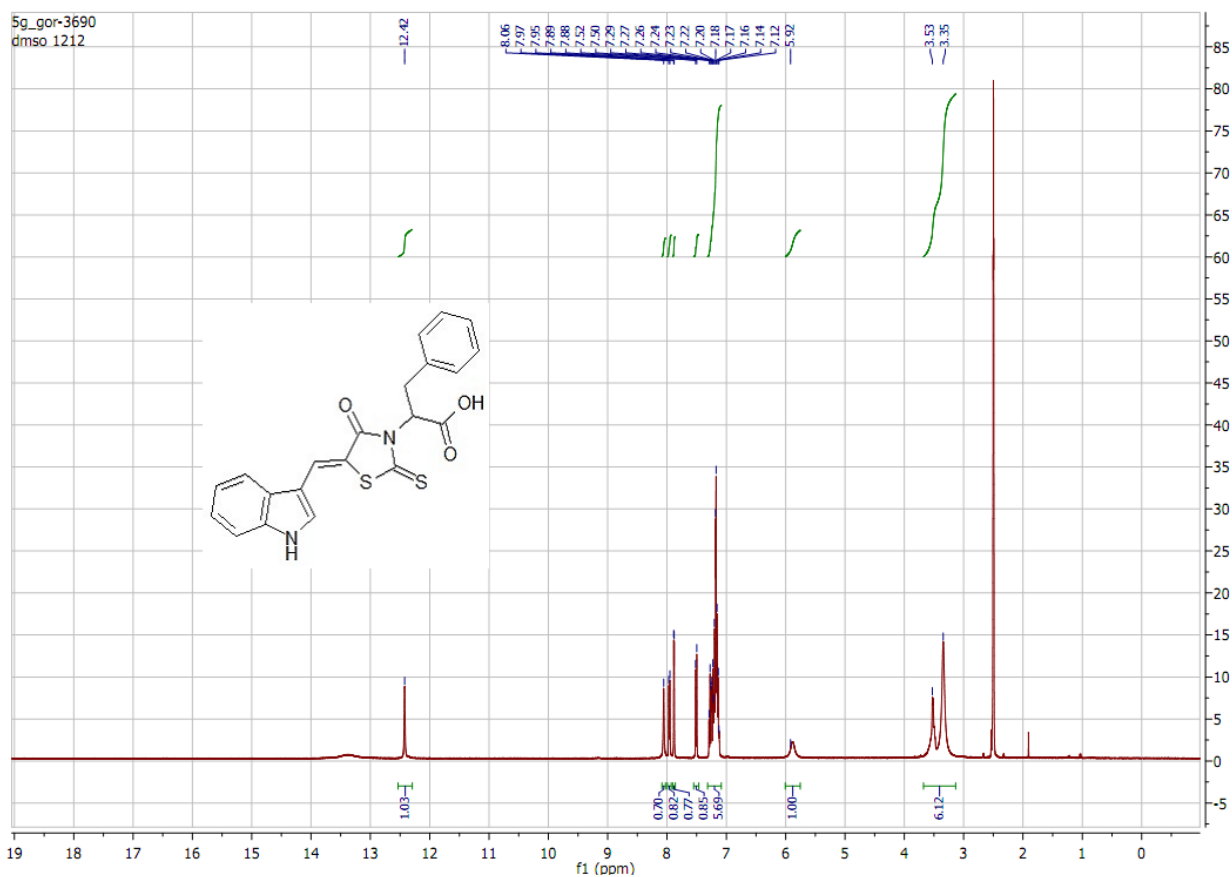


Figure S57. ^1H NMR spectrum (400 MHz, DMSO-d_6) of compound **5g**.

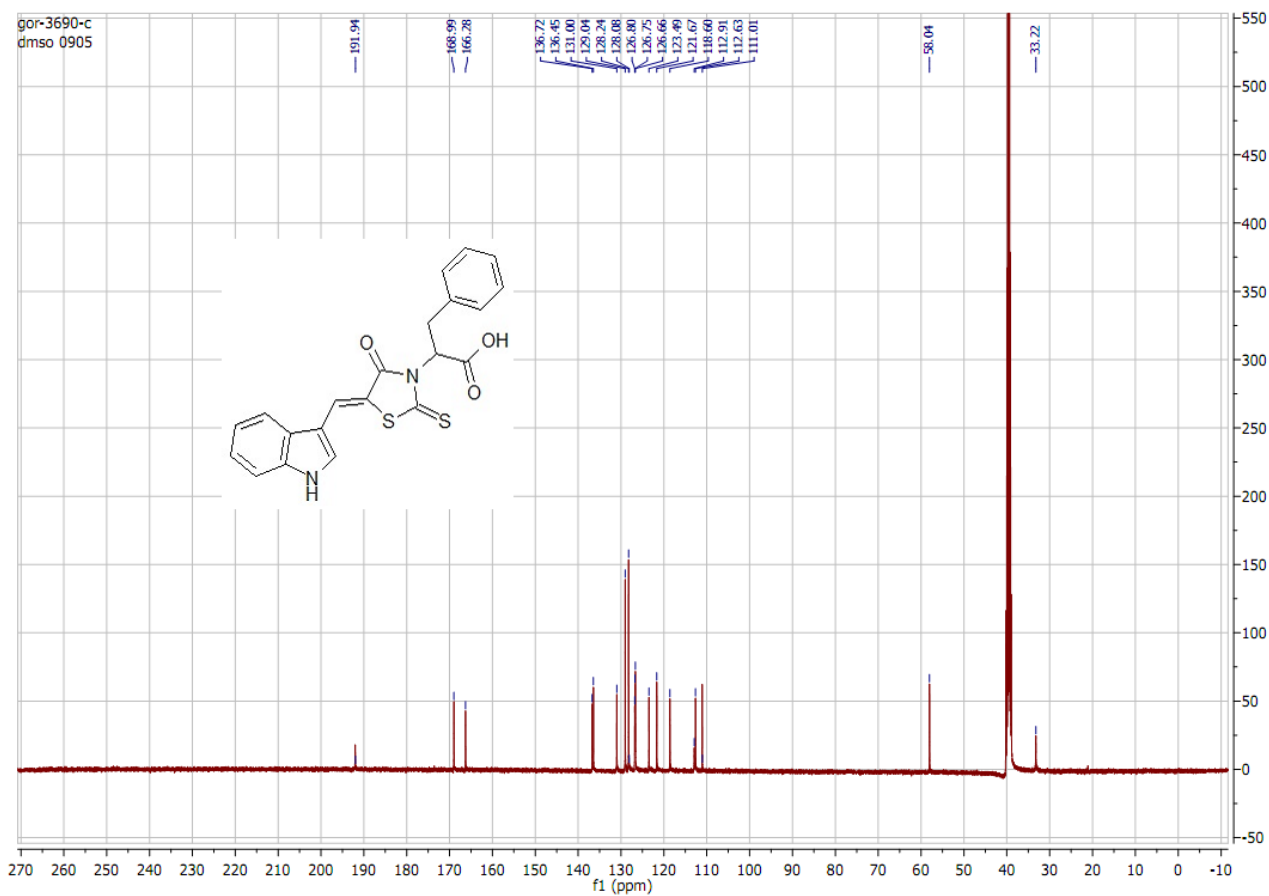
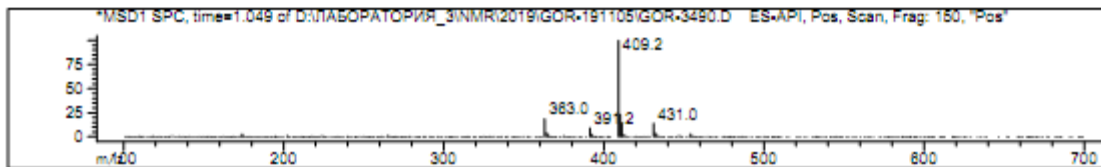
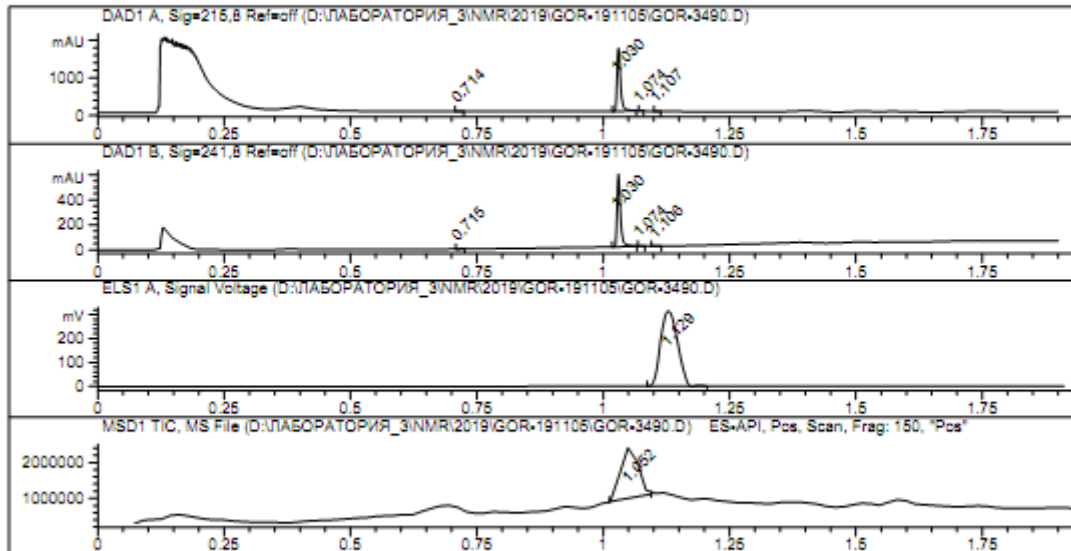


Figure S58. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of compound **5g**.

-o.-Syntez Purity Report -o.-

System: Agilent 1200 LC/MSD SL

Separation column: Rapid Resolutionn HT Cartige 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.714	0.604
2		1.030	98.747
3		1.074	0.358
4		1.107	0.291

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.715	0.925
2		1.030	98.497
3		1.074	0.230
4		1.106	0.349

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.129	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.052	100.000

Inj. Date 06.11.2019

Figure S59. MS (ESI) spectrum of compound 5g.

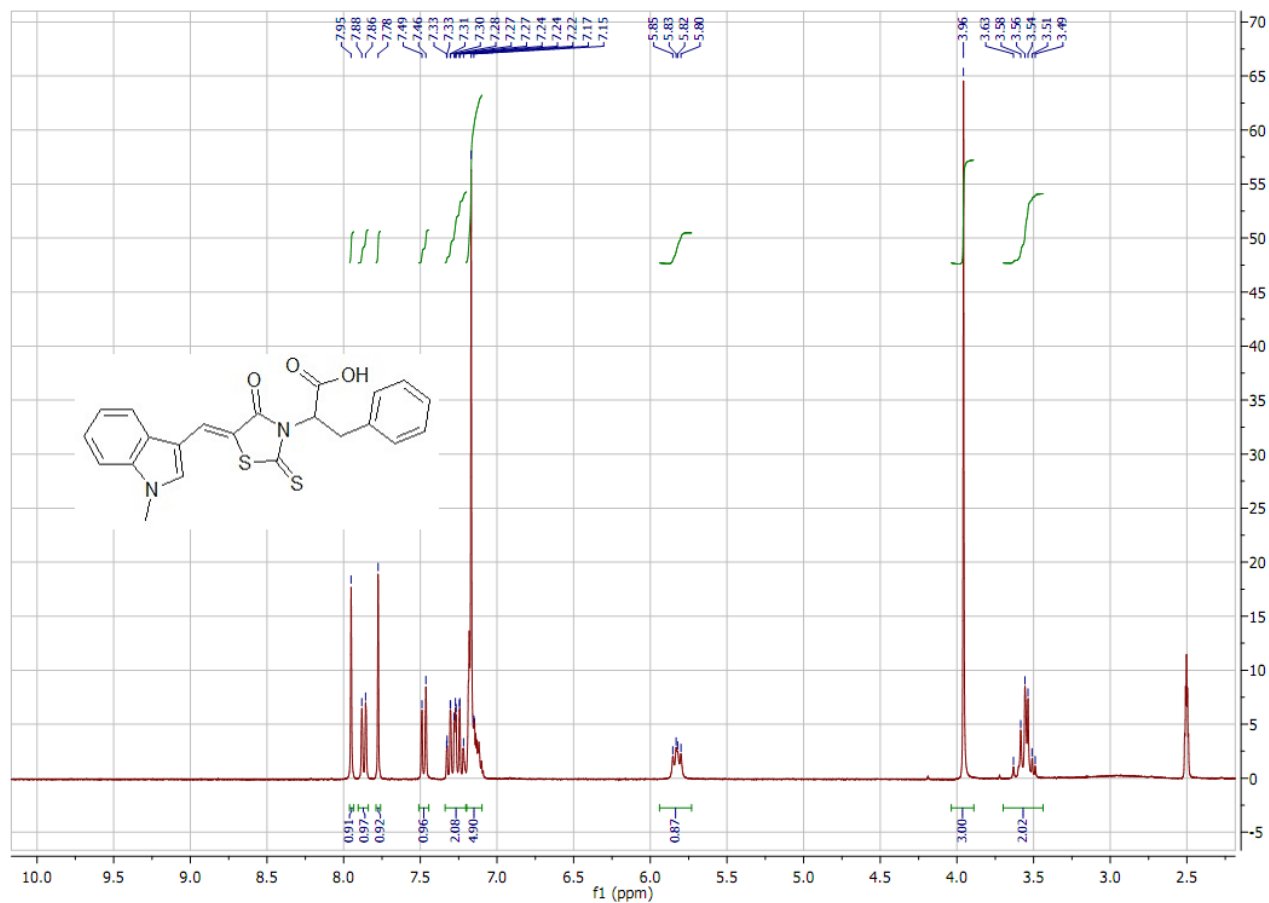


Figure S60. ¹H NMR spectrum (300 MHz, DMSO-d₆) of compound **5h**.

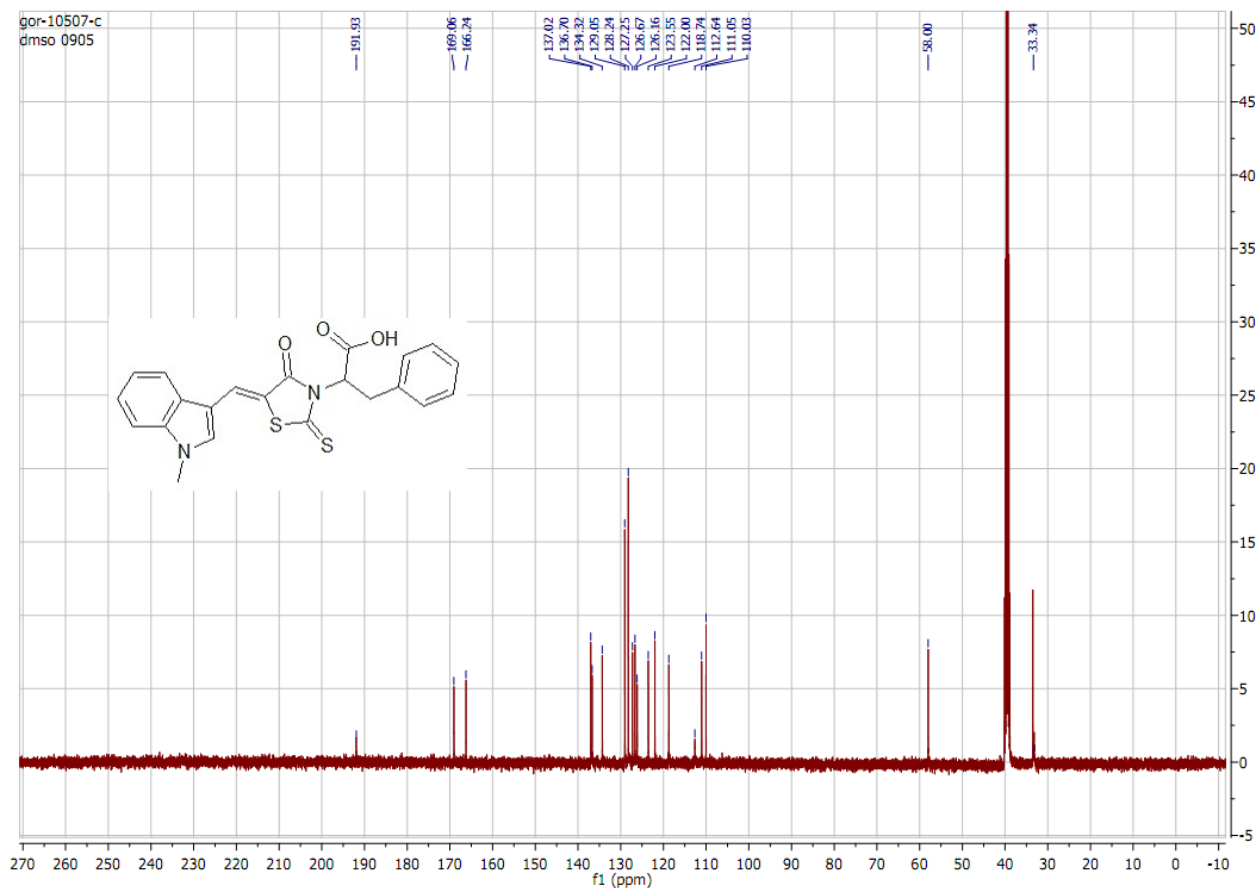
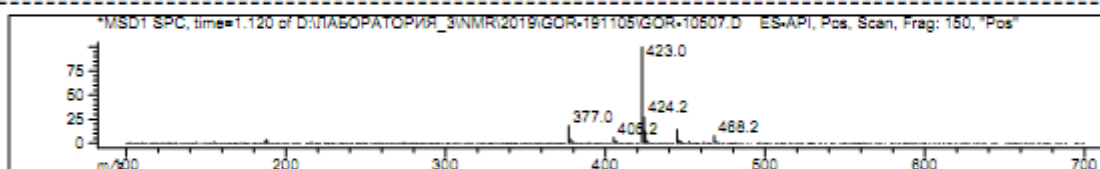
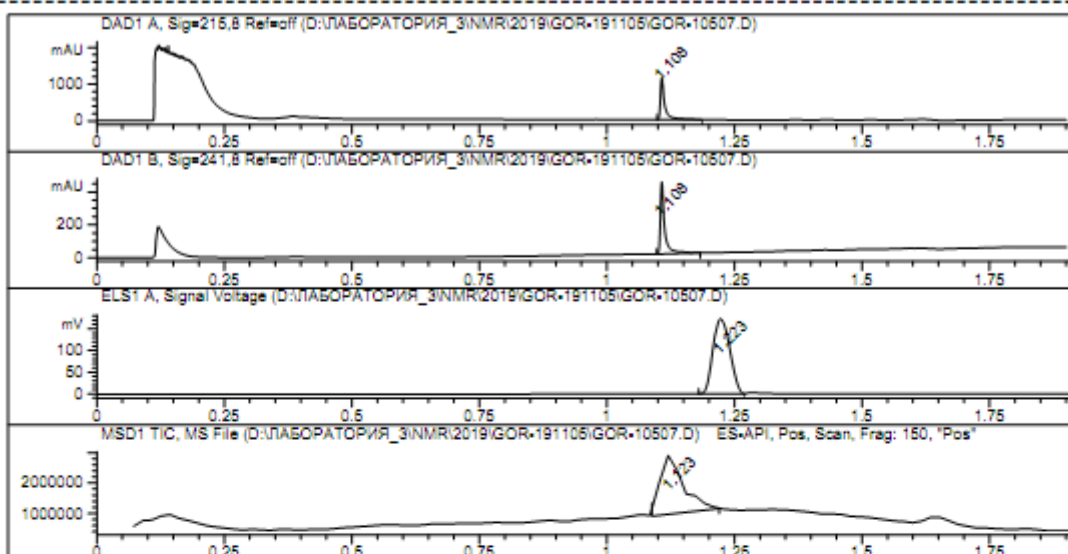


Figure S61. ¹³C NMR spectrum (101 MHz, DMSO-d₆) of compound **5h**.

-o.-Syntex Purity Report -o.-

System: Agilent 1200 LC/MSD SL
 Separation column: Rapid Resolution HT Cartige 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	1.108	100.000
1	DAD1 B, Sig=241,8 Ref=off	1.108	100.000
1	ELS1 A, Signal Voltage	1.223	100.000
1	MSD1 TIC, MS File	1.123	100.000

Inj. Date 05.11.2019

Figure S62. MS (ESI) spectrum of compound 5h.

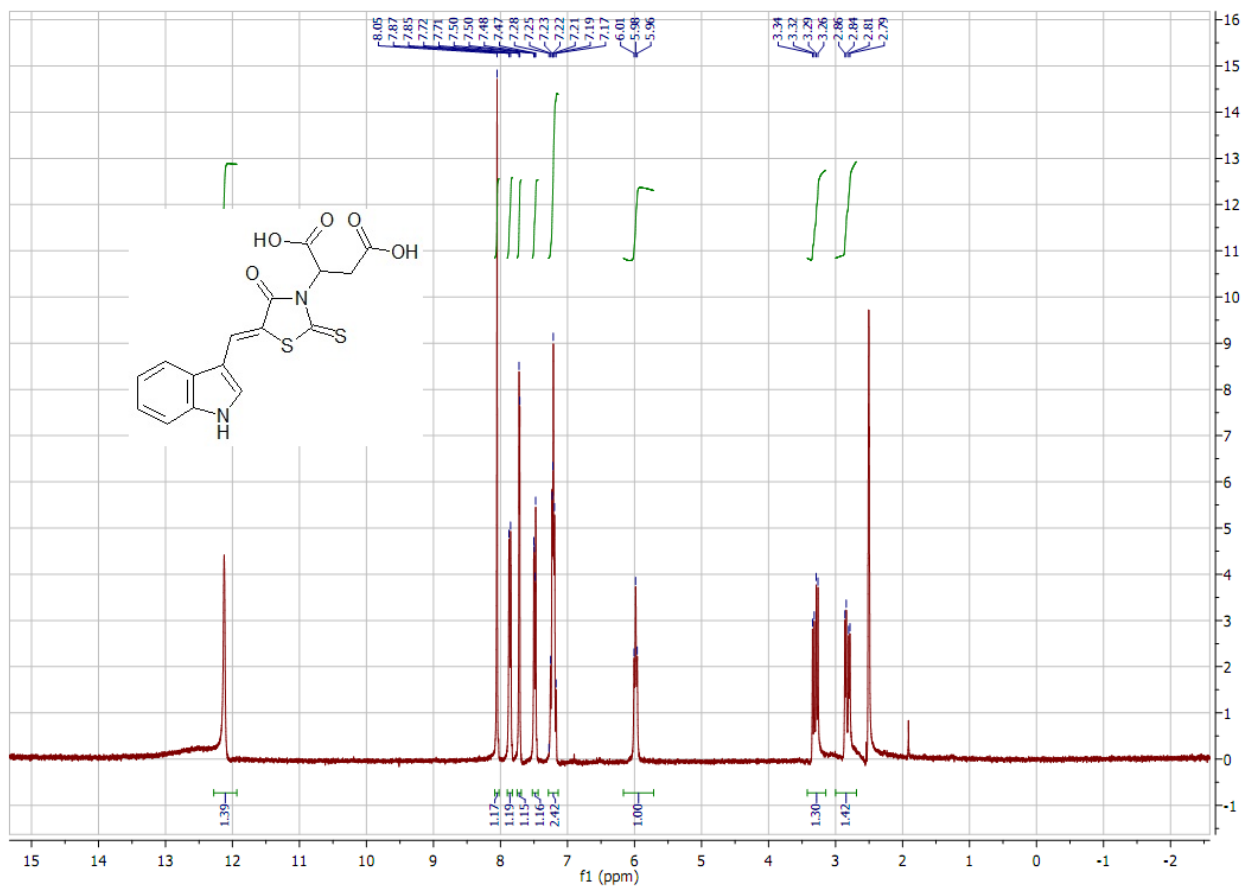


Figure S63. ^1H NMR spectrum (300 MHz, DMSO- d_6) of compound **5i**.

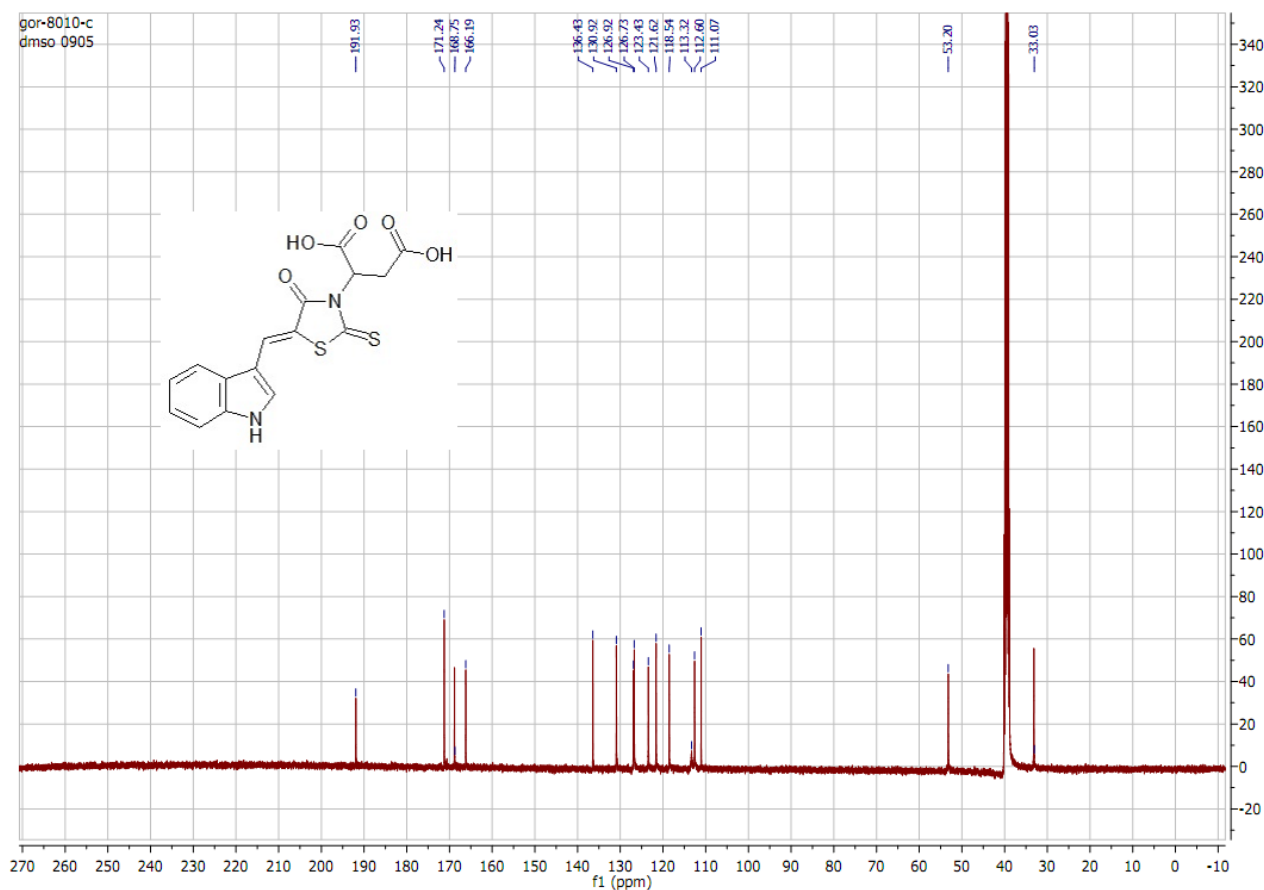
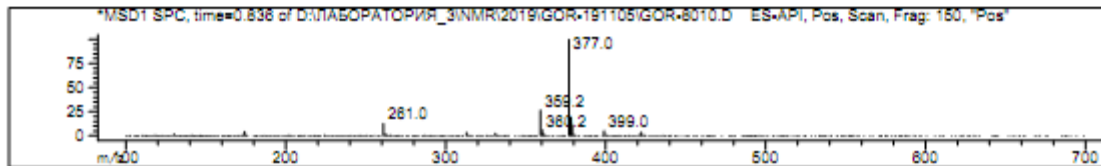
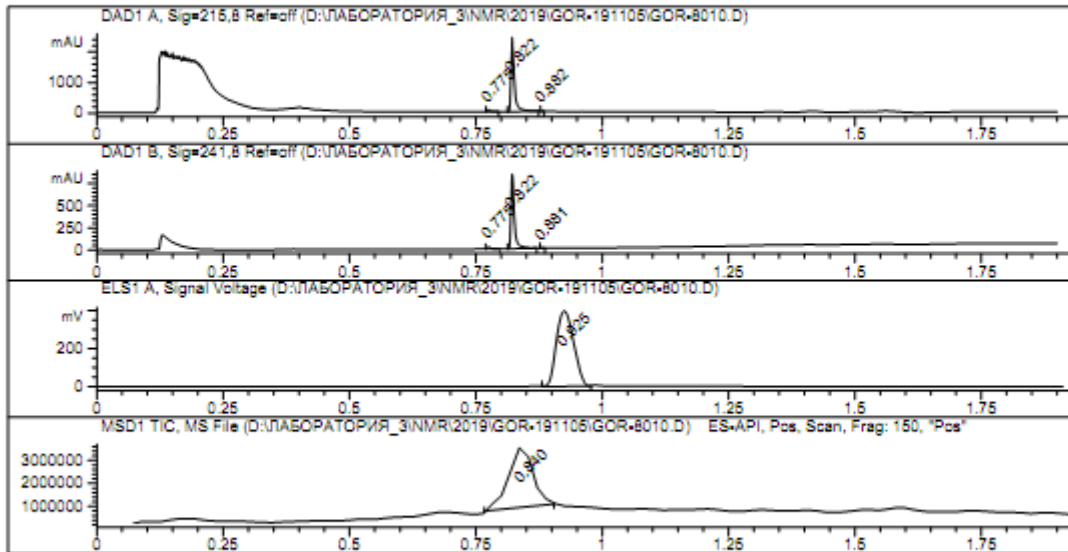


Figure S64. ^{13}C NMR spectrum (101 MHz, DMSO- d_6) of compound **5i**.

-o.-Syntez Purity Report -o.-

System: Agilent 1200 LC/MSD SL
 Separation column: Rapid Resolution HT Cartidge 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.775	3.142
2		0.822	96.774
3		0.882	0.085
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.775	2.670
2		0.822	97.100
3		0.881	0.230
#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	0.925	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.840	100.000

Inj. Data 06.11.2019

Figure S65. MS (ESI) spectrum of compound 5i.

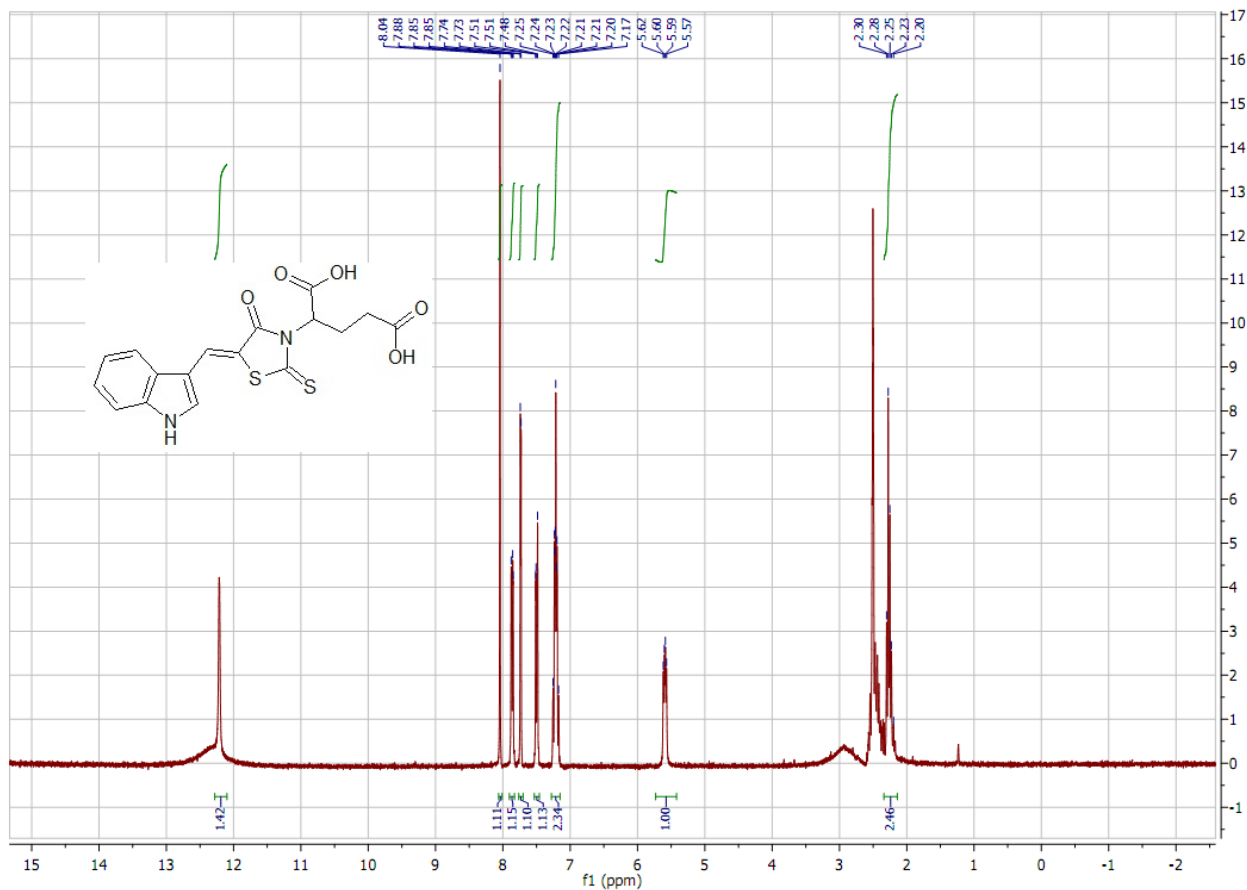


Figure S66. ¹H NMR spectrum (300 MHz, DMSO-d₆) of compound **5j**.

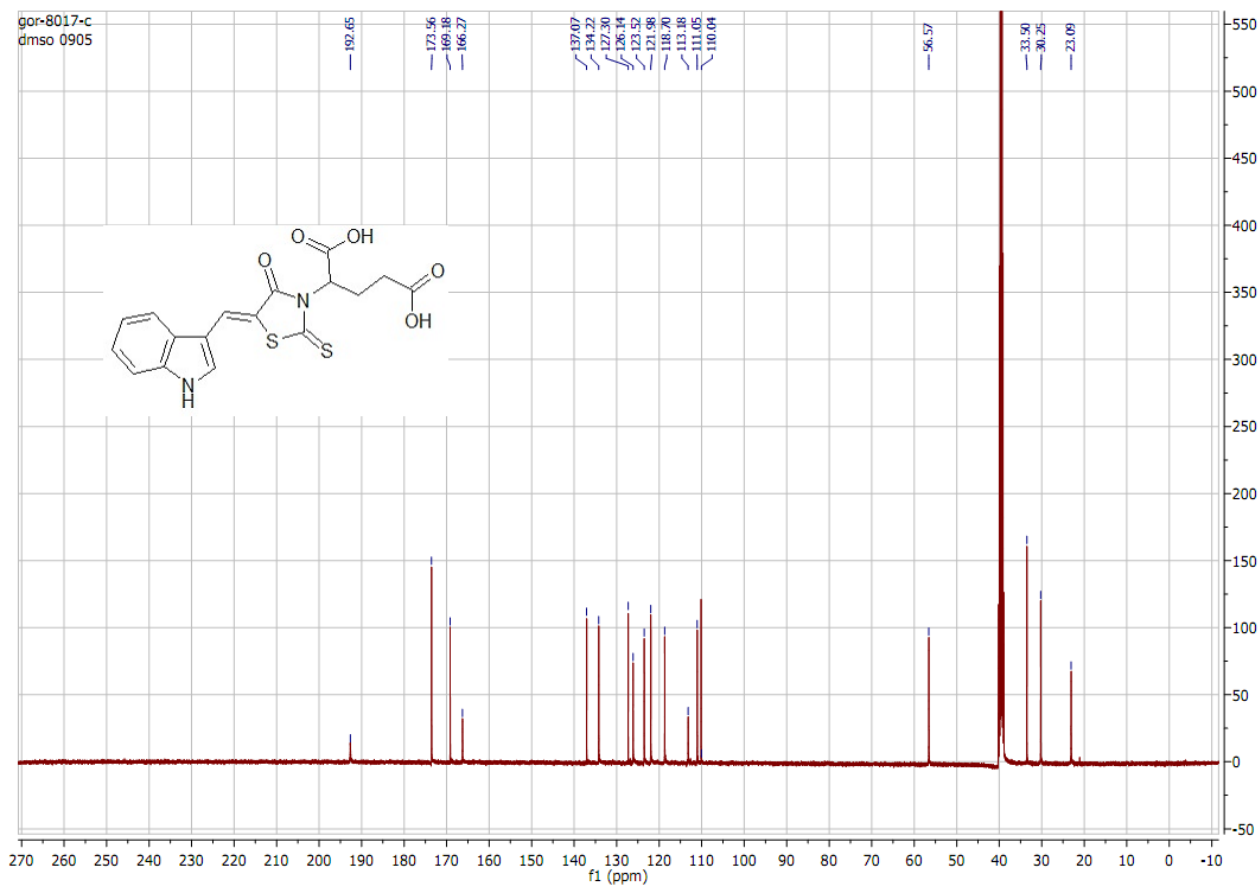
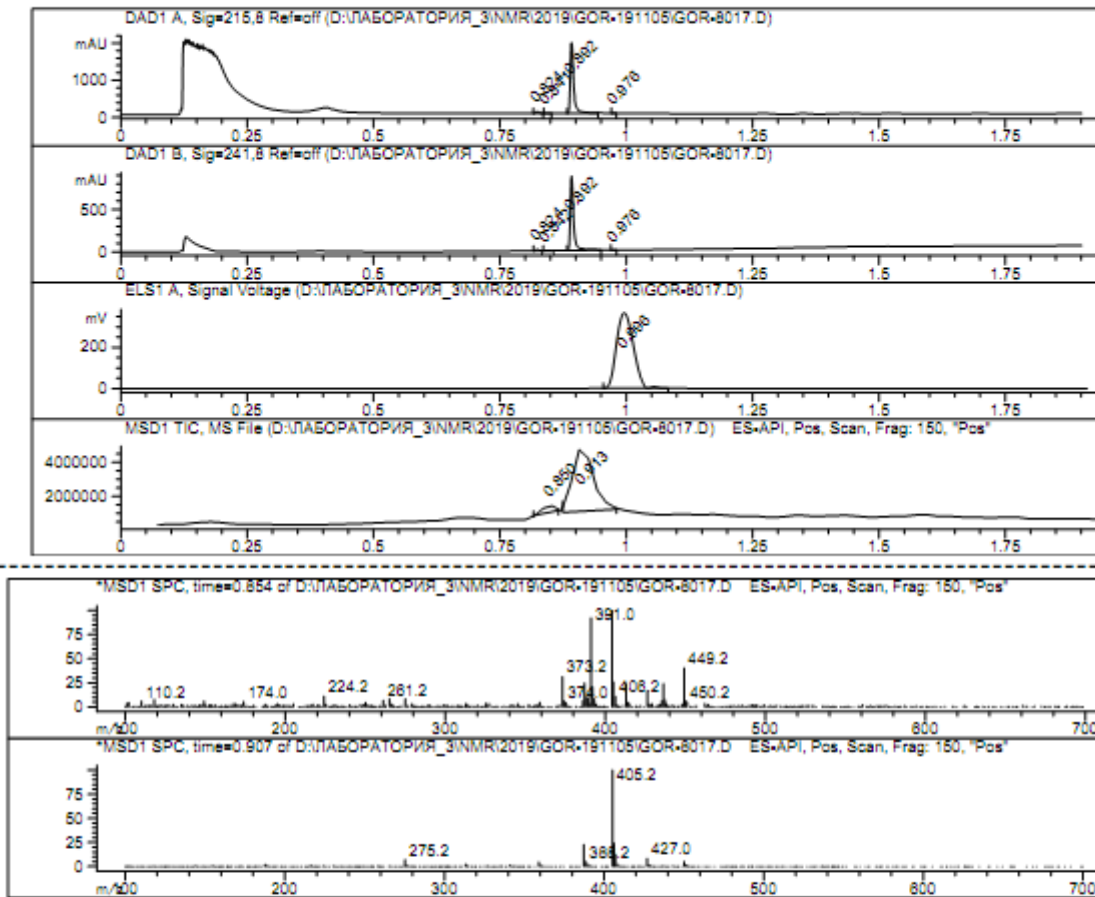


Figure S67. ¹³C NMR spectrum (101 MHz, DMSO-d₆) of compound **5j**.

-.o.-Syntez Purity Report -.o.-

System: Agilent 1200 LC/MSD SL
 Separation column: Rapid Resolutionn HT Cartige 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.824	2.024
2		0.841	0.377
3		0.892	97.395
4		0.976	0.204

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.824	1.643
2		0.842	0.513
3		0.892	97.629
4		0.976	0.215

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	0.996	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.850	6.581
2		0.913	93.419

Inj. Data 06.11.2019

Figure S68. MS (ESI) spectrum of compound 5j.

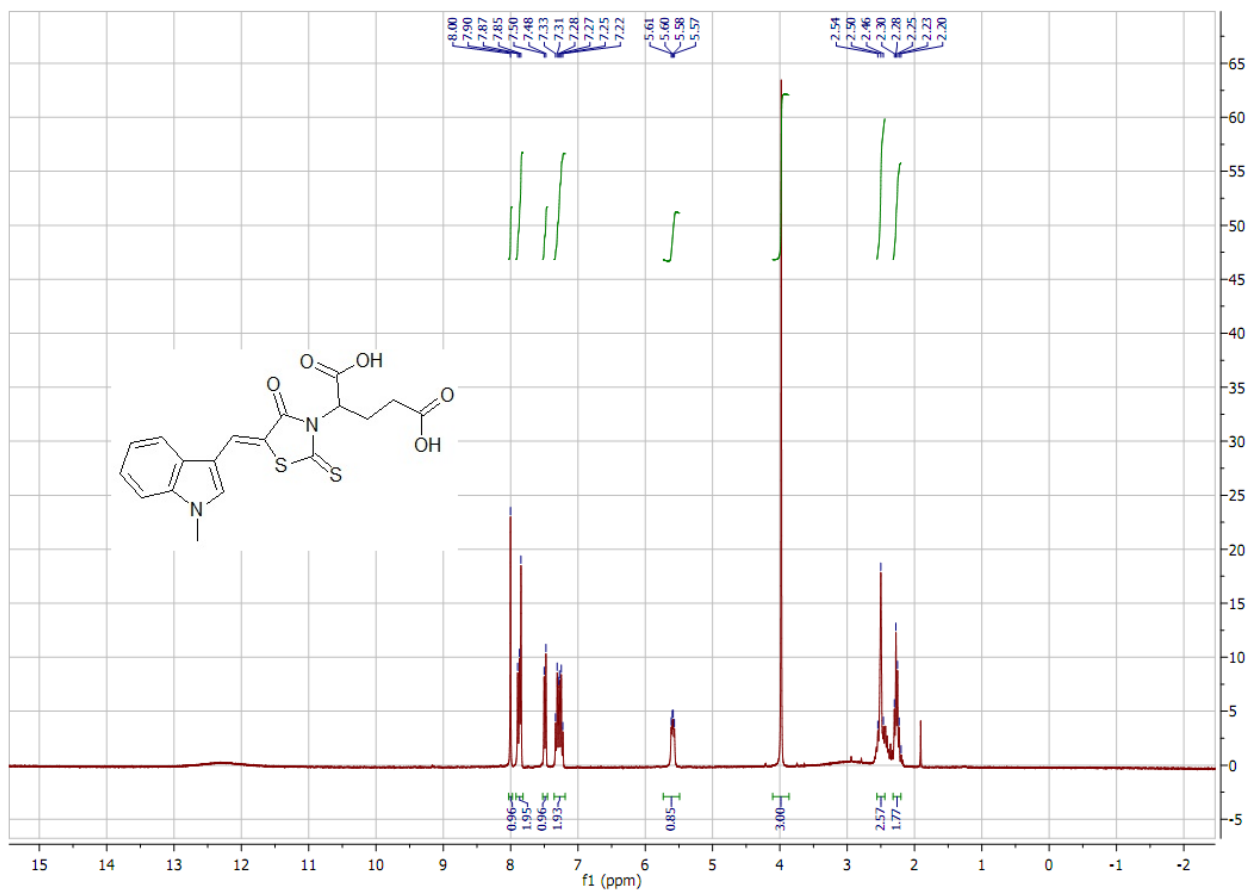


Figure S69. ¹H NMR spectrum (300 MHz, DMSO-d₆) of compound **5k**.

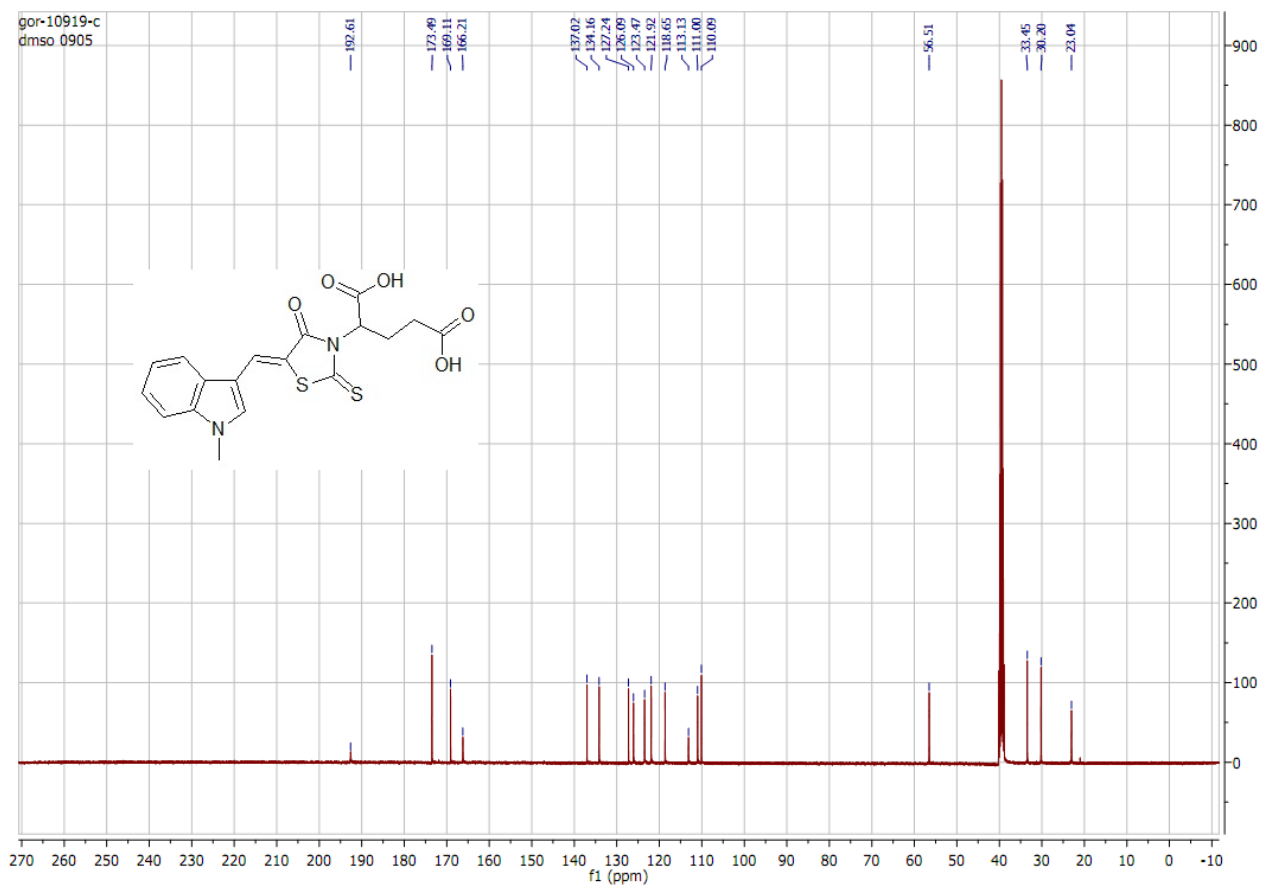
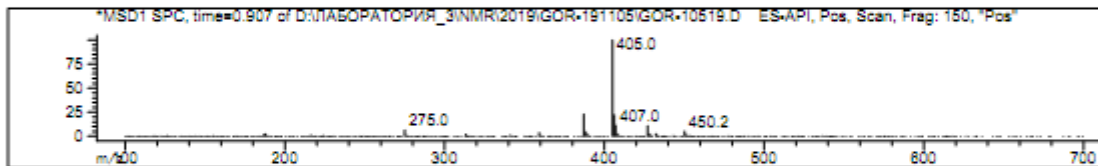
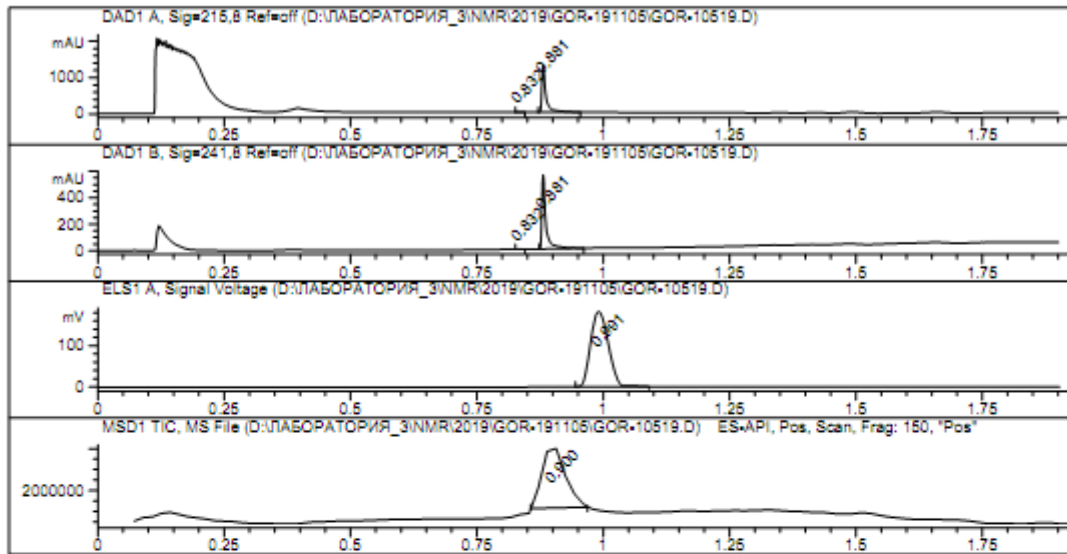


Figure S70. ¹³C NMR spectrum (101 MHz, DMSO-d₆) of compound **5k**.

-o.-SynTex Purity Report -o.-

System: Agilent 1200 LC/MSD SL
 Separation column: Rapid Resolution HT Cartige 4.6x30mm, 1.8-Micron, Zorbx SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.832	0.394
2		0.881	99.606
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.832	0.785
2		0.881	99.215
#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	0.991	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.900	100.000

Inj. Data 05.11.2019

Figure S71. MS (ESI) spectrum of compound **5k**.