

Figure S1. ¹H NMR spectrum (400 MHz, DMSO-d₆) of methyl 4-hydroxy-2-(methylthio)quinoline-3-carboxylate **3**.

Figure S2. ¹³C NMR spectrum (100 MHz, DMSO-d₆) of methyl 4-hydroxy-2-(methylthio)quinoline-3-carboxylate **3**.

Figure S3. LC/MS data for methyl 4-hydroxy-2-(methylthio)quinoline-3-carboxylate **3**.

Figure S4. ¹H NMR spectrum (400 MHz, DMSO-d₆) of pure methyl 4-methoxy-2-(methylthio)quinoline-3-carboxylate **4**.

Figure S5. ¹³C NMR spectrum (100 MHz, DMSO-d₆) of pure methyl 4-methoxy-2-(methylthio)quinoline-3-carboxylate **4**.

Figure S6. LC/MS data for pure methyl 4-methoxy-2-(methylthio)quinoline-3-carboxylate **4**.

Figure S7. ¹H NMR spectrum (400 MHz, DMSO-d₆) of pure methyl 1-methyl-2-(methylthio)-4-oxo-1,4-dihydroquinoline-3-carboxylate **5**.

Figure S8. ¹³C NMR spectrum (100 MHz, DMSO-d₆) of pure methyl 1-methyl-2-(methylthio)-4-oxo-1,4-dihydroquinoline-3-carboxylate **5**.

Figure S9. LC/MS data for pure methyl 1-methyl-2-(methylthio)-4-oxo-1,4-dihydroquinoline-3-carboxylate **5**.

Figure S10. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 1 (Table1).

Figure S11. LC/MS data for the reaction product of case 1 (Table1).

Figure S12. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 2 (Table1).

Figure S13. LC/MS data for the reaction product of case 2 (Table1).

Figure S14. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 3 (Table1).

Figure S15. LC/MS data for the reaction product of case 3 (Table1).

Figure S16. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 4 (Table1).

Figure S17. LC/MS data for the reaction product of case 4 (Table1).

Figure S18. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 5 (Table1).

Figure S19. LC/MS data for the reaction product of case 5 (Table1).

Figure S20. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 6 (Table1).

Figure S21. LC/MS data for the reaction product of case 6 (Table1).

Figure S22. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 7 (Table1).

Figure S23. LC/MS data for the reaction product of case 7 (Table1).

Figure S24. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 8 (Table1).

Figure S25. LC/MS data for the reaction product of case 8 (Table1).

Figure S26. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 9 (Table1).

Figure S27. LC/MS data for the reaction product of case 9 (Table1).

Figure S28. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 10 (Table1).

Figure S29. LC/MS data for the reaction product of case 10 (Table1).

Figure S30. ¹H NMR spectrum (400 MHz, DMSO-d₆) of 4-hydroxy-2-(methylthio)quinoline-3-carboxylic acid **6**.

Figure S31. ¹³C NMR spectrum (100 MHz, DMSO-d₆) of 4-hydroxy-2-(methylthio)quinoline-3-carboxylic acid **6**.

Figure S32. LC/MS data for 4-hydroxy-2-(methylthio)quinoline-3-carboxylic acid **6**.

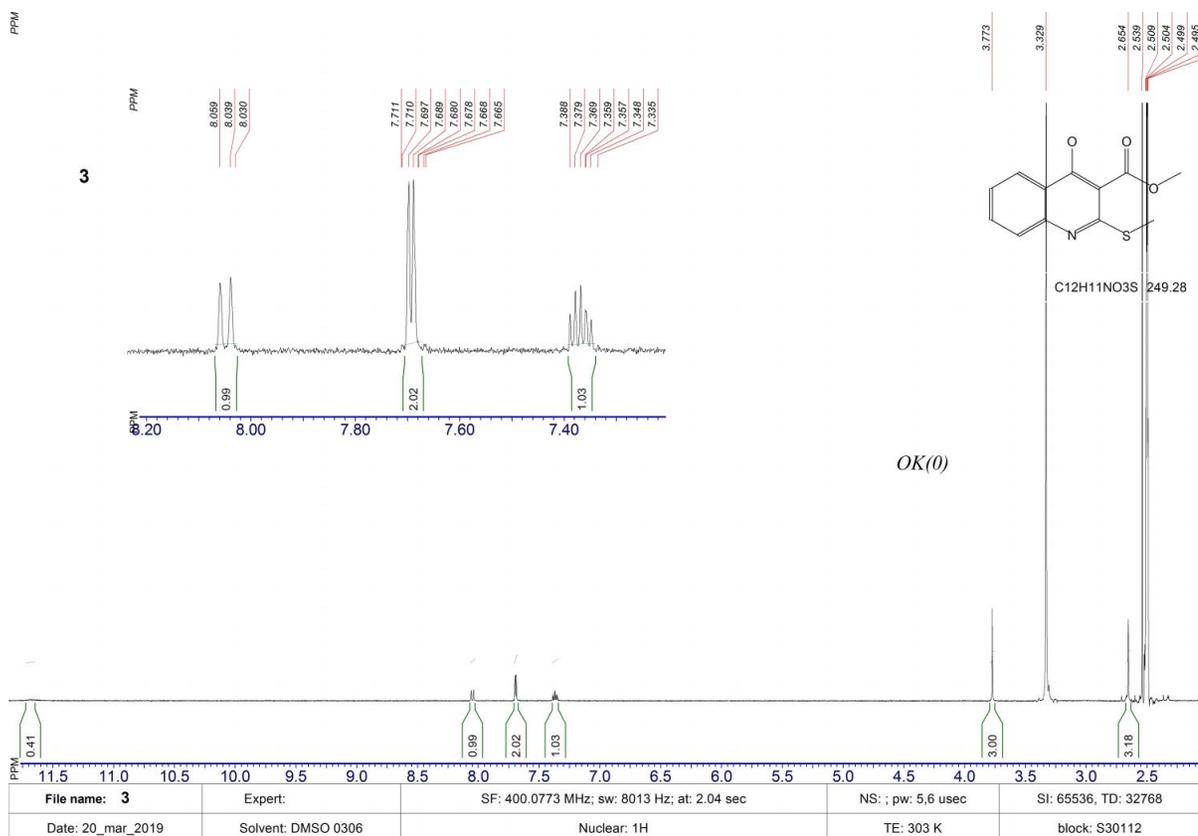


Figure S1. ^1H NMR spectrum (400 MHz, DMSO- d_6) of methyl 4-hydroxy-2-(methylthio)quinoline-3-carboxylate **3**.

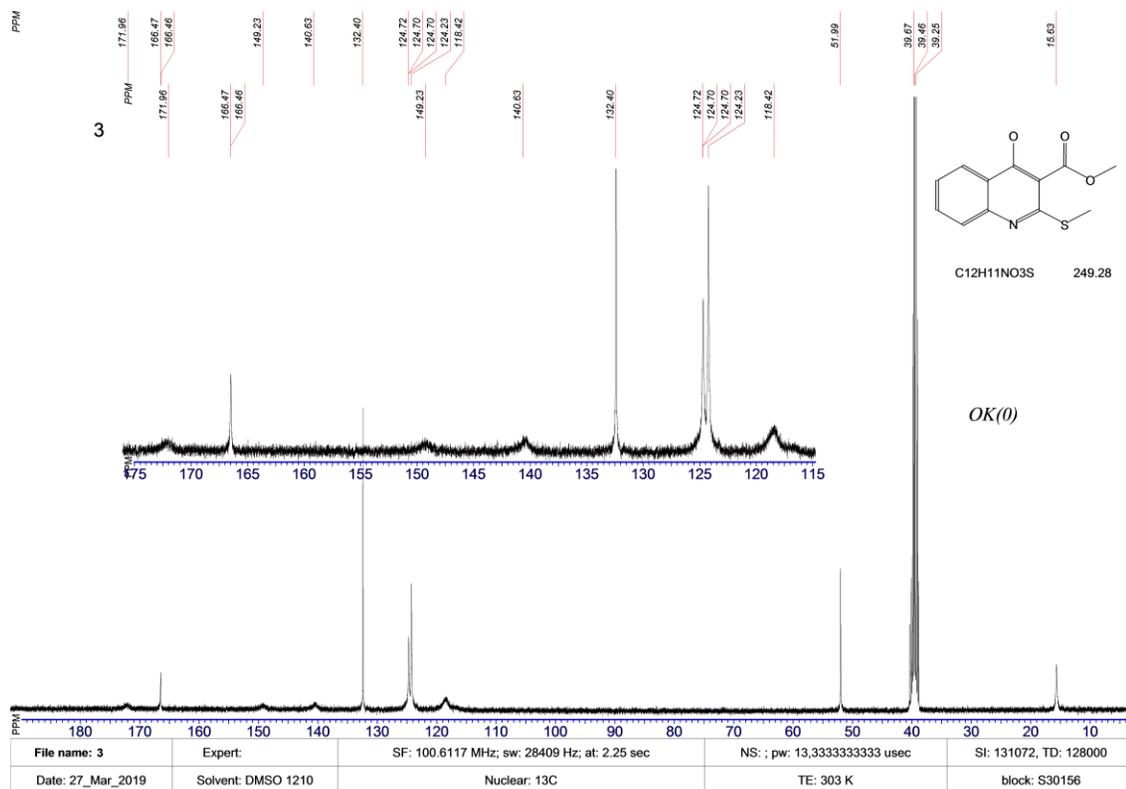
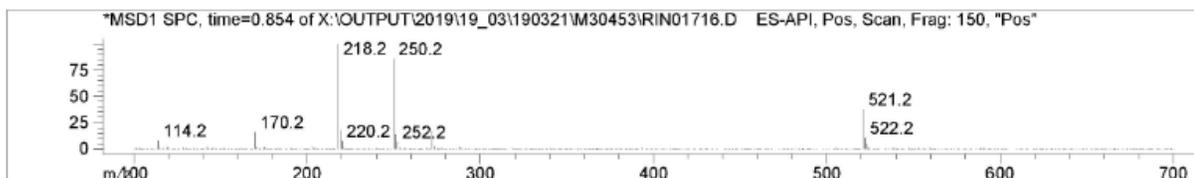
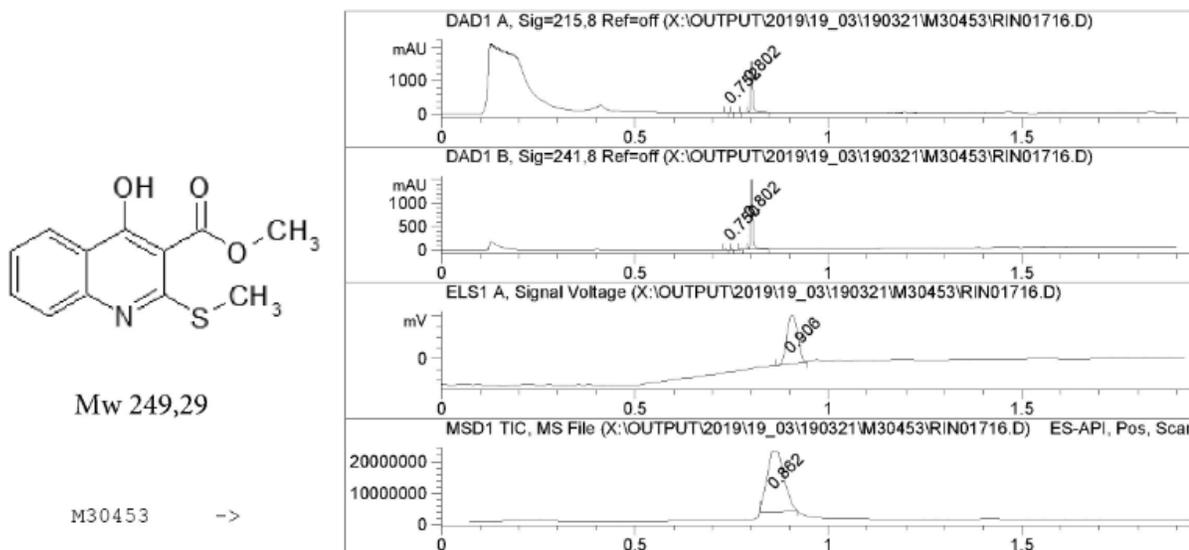


Figure S2. ^{13}C NMR spectrum (100 MHz, DMSO- d_6) of methyl 4-hydroxy-2-(methylthio)quinoline-3-carboxylate **3**.

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Agilent 1200 LC/MSD	Mobile Phase:A-H2O+0.1HCOOH;B-MeCN+0.1HCOOH
Diodearray G1315B (DAD1A-215nm; DAD1B-241nm)	Separation column: 99%
Mass Quad G6140A (MSD1-Pos, MSD2-Neg)	Rapid Resolutionn HT Cartige 4.6x30mm,
ELSD Altech 3300 (ADC1 A, ELSD)	1.8-Micron, Zorbax SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.733	0.251
2		0.752	0.216
3		0.773	0.180
4		0.802	99.353

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.734	0.312
2		0.750	0.145
3		0.773	0.225
4		0.802	99.318

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	0.906	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.862	100.000

Figure S3. LC/MS data for methyl 4-hydroxy-2-(methylthio)quinoline-3-carboxylate 3.

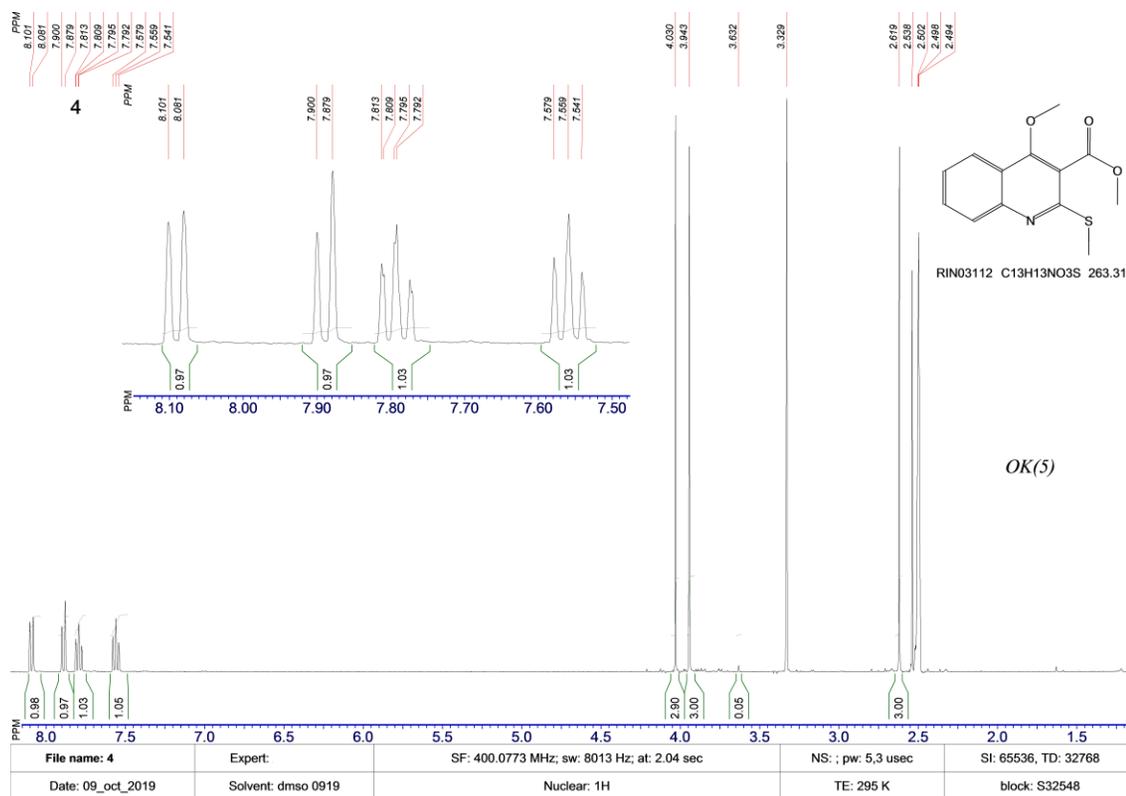


Figure S4. ^1H NMR spectrum (400 MHz, DMSO- d_6) of pure methyl 4-methoxy-2-(methylthio)quinoline-3-carboxylate **4**.

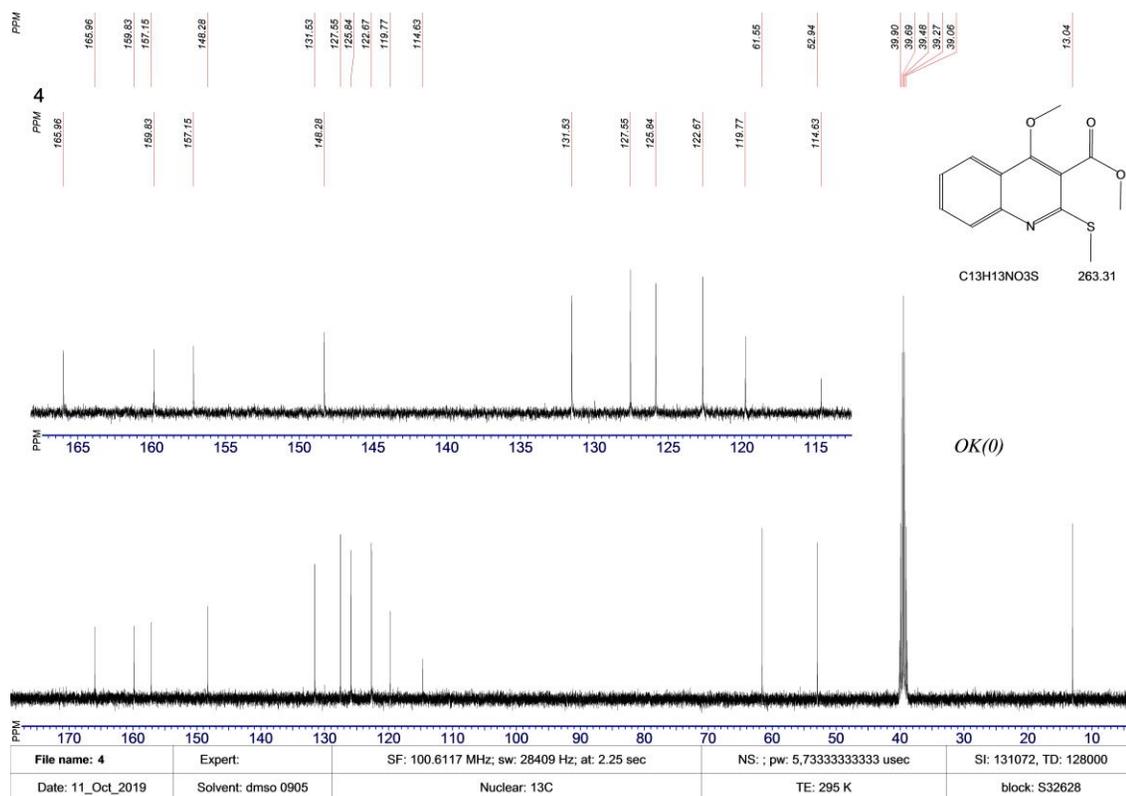
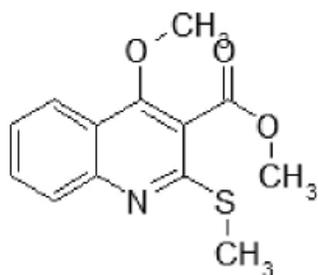


Figure S5. ^{13}C NMR spectrum (100 MHz, DMSO- d_6) of pure methyl 4-methoxy-2-(methylthio)quinoline-3-carboxylate **4**.

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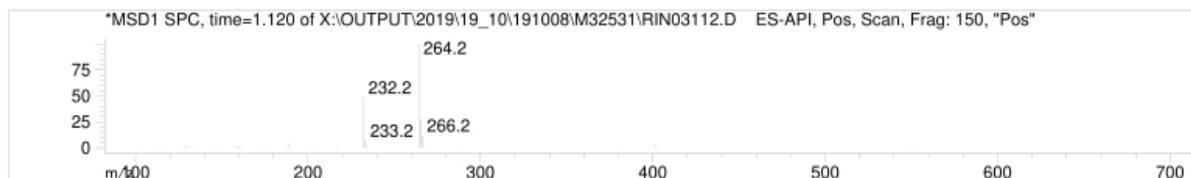
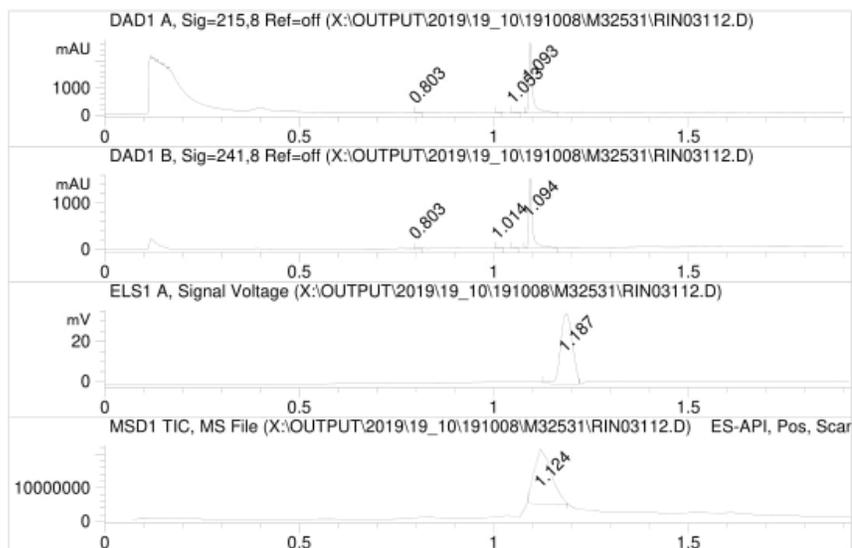
Agilent 1200 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-241nm)
 Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H₂O+0.1HCOOH;B-MeCN+0.1HCOOH
 Separation column: **96%**
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18



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M32531 →



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.803	0.805
2		1.014	0.809
3		1.053	0.717
4		1.093	97.668

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.803	0.897
2		1.014	1.152
3		1.053	1.705
4		1.094	96.246

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.187	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.124	100.000

Figure S6. LC/MS data for pure methyl 4-methoxy-2-(methylthio)quinoline-3-carboxylate **4**.

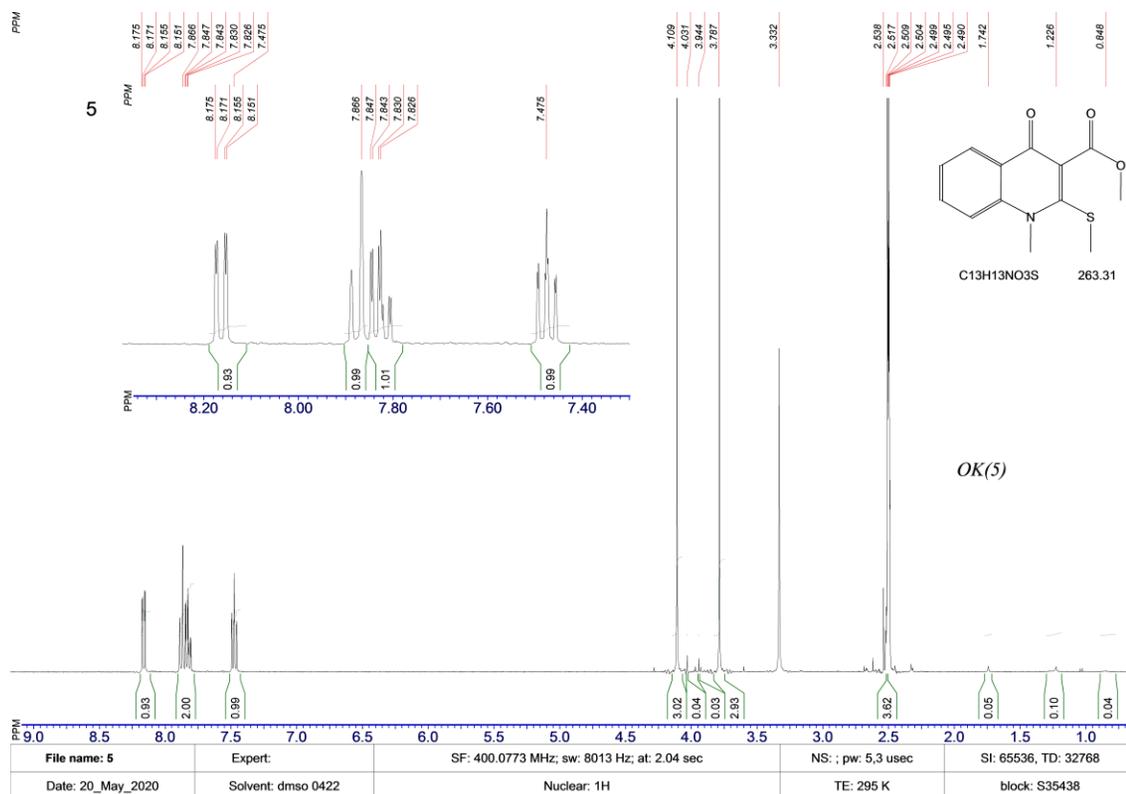


Figure S7. ¹H NMR spectrum (400 MHz, DMSO-d₆) of pure methyl 1-methyl-2-(methylthio)-4-oxo-1,4-dihydroquinoline-3-carboxylate 5.

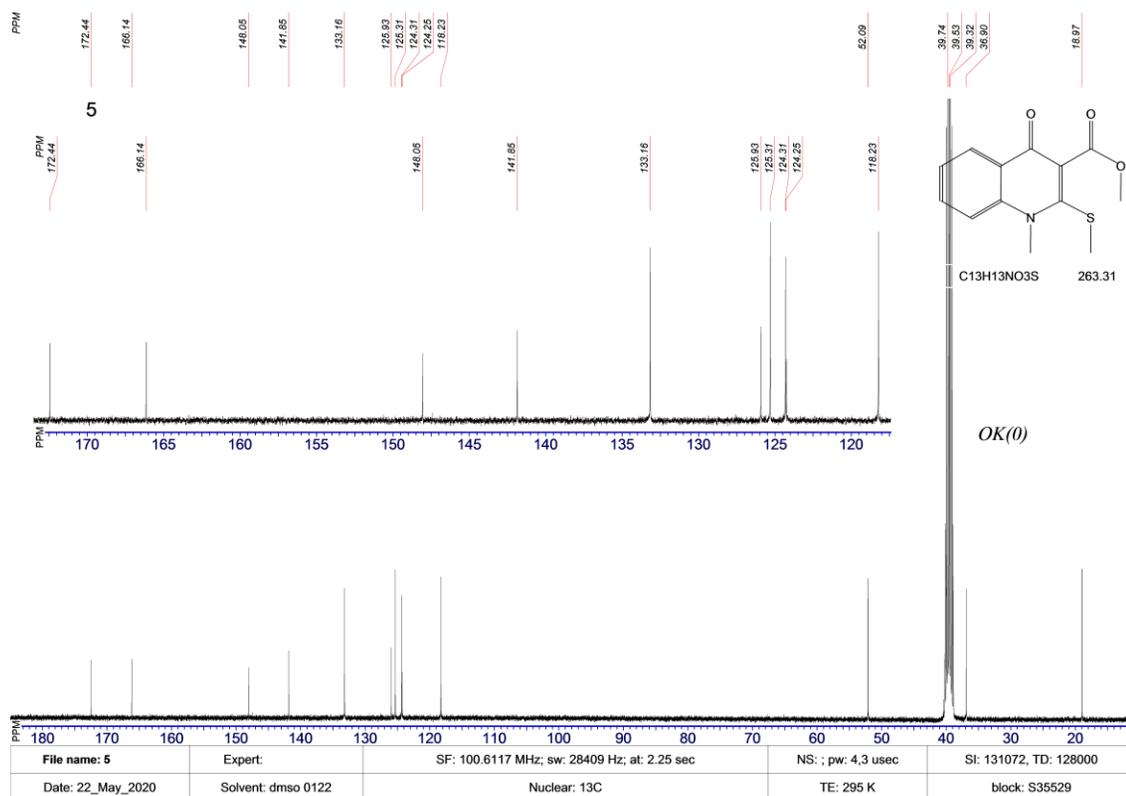
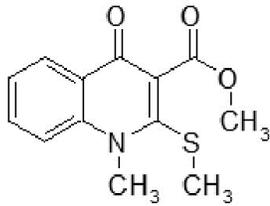


Figure S8. ¹³C NMR spectrum (100 MHz, DMSO-d₆) of pure methyl 1-methyl-2-(methylthio)-4-oxo-1,4-dihydroquinoline-3-carboxylate 5.

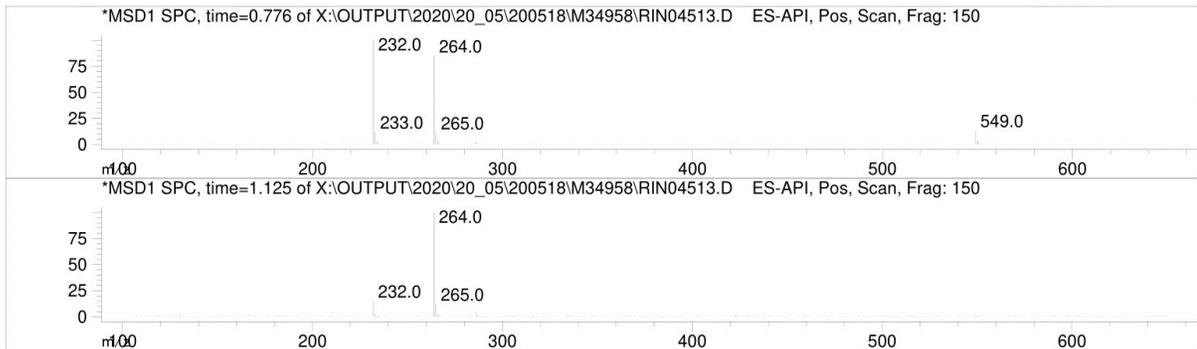
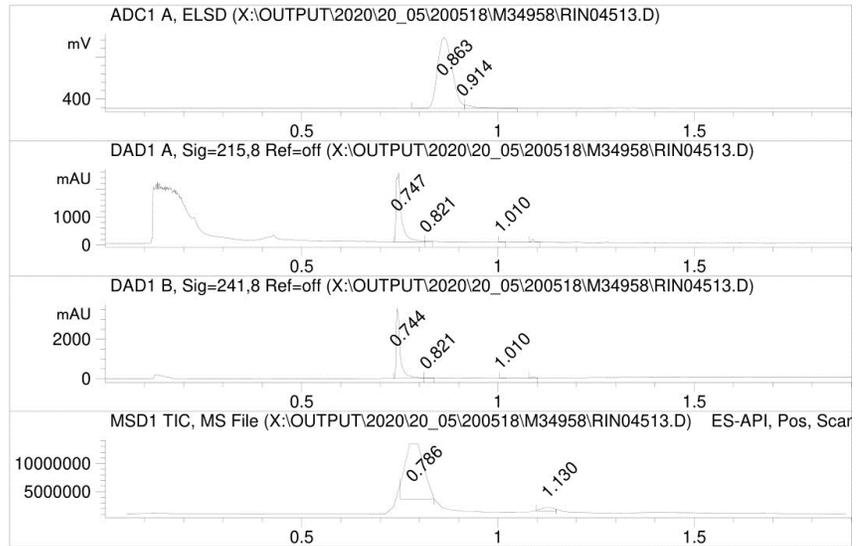
-.o.-Syntez Purity Report -.o.-

Agilent 1100 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H2O+0.1HCOOH;B-MeCN+0.1HCOOH
 Separation column:
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18



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#	Signal	R.Time	Area %
1	ADC1 A, ELSD	0.863	97.326
2		0.914	2.674
#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.747	97.015
2		0.821	0.701
3		1.010	0.281
4		1.088	2.003
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.744	97.694
2		0.821	0.674
3		1.010	0.491
4		1.088	1.141
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.786	94.739
2		1.130	5.261

Figure S9. LC/MS data for pure methyl 1-methyl-2-(methylthio)-4-oxo-1,4-dihydroquinoline-3-carboxylate 5.

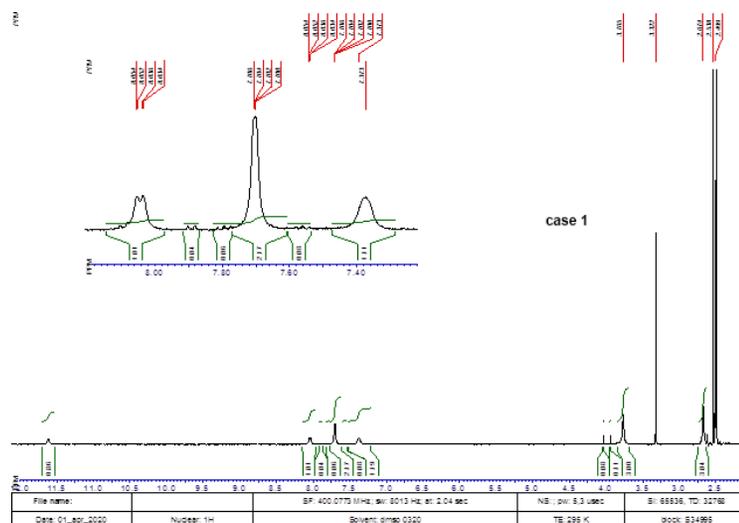
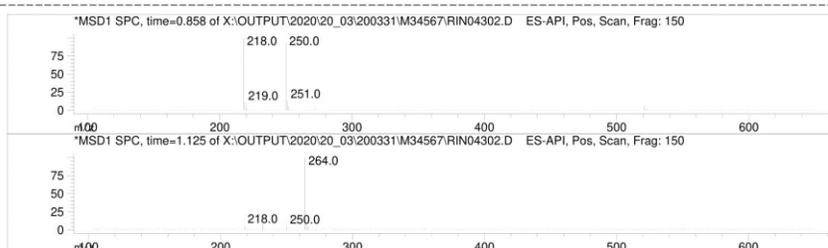
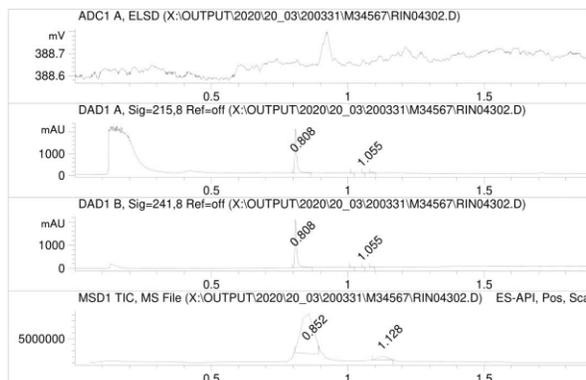


Figure S10. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 1 (Table 1).

-.o.-Syntez Purity Report -.o.-
 Agilent 1100 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H2O+0.1HCOOH;B-MeCN+0.1HCOOH
 Separation column:
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18

case 1



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.808	96.191
2		1.014	0.399
3		1.055	0.331
4		1.086	3.079
1	DAD1 B, Sig=241,8 Ref=off	0.808	97.406
2		1.014	0.768
3		1.055	0.265
4		1.086	1.561
1	MSD1 TIC, MS File	0.852	93.840
2		1.128	6.160

Figure S11. LC/MS data for the reaction product of case 1 (Table 1).

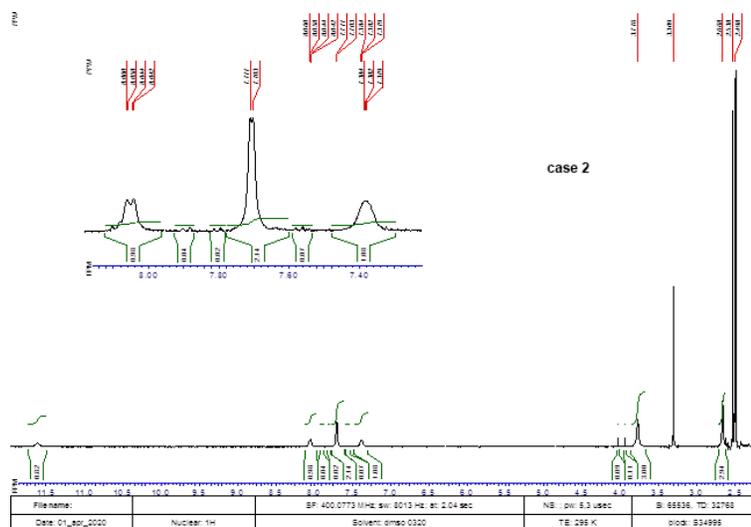
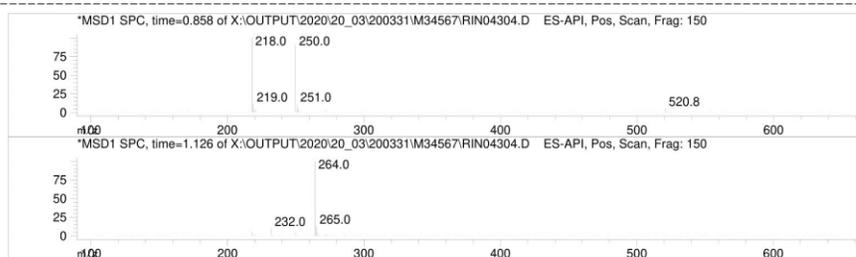
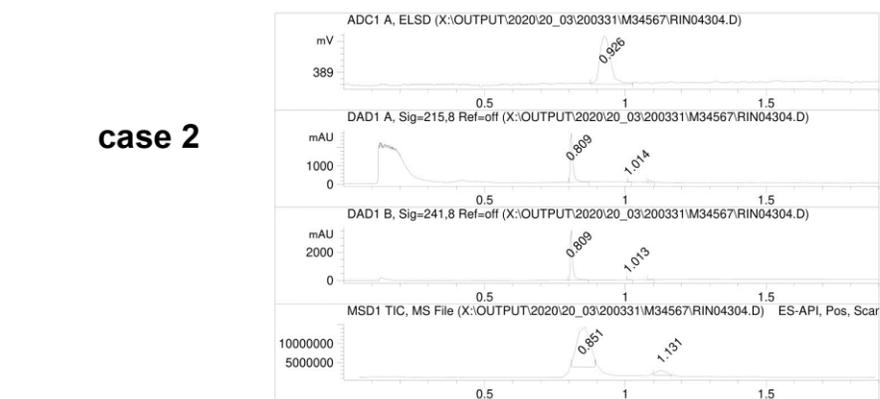


Figure S12. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 2 (Table 1).

-.o.-Synitez Purity Report -.o.-
 Agilent 1100 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H2O+0.1HCOOH;B-MeCN+0.1HCOOH
 Separation column:
 Rapid Resolutionn HT Cartidge 4.6x30mm,
 1.8-Micron, Zorbax SB-C18



#	Signal	R.Time	Area %
1	ADC1 A, ELSD	0.926	100.000

#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.809	96.060
2		1.014	0.353
3		1.086	3.587

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.809	97.616
2		1.013	0.577
3		1.086	1.807

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.851	92.305
2		1.131	7.695

Figure S13. LC/MS data for the reaction product of case 2 (Table 1).

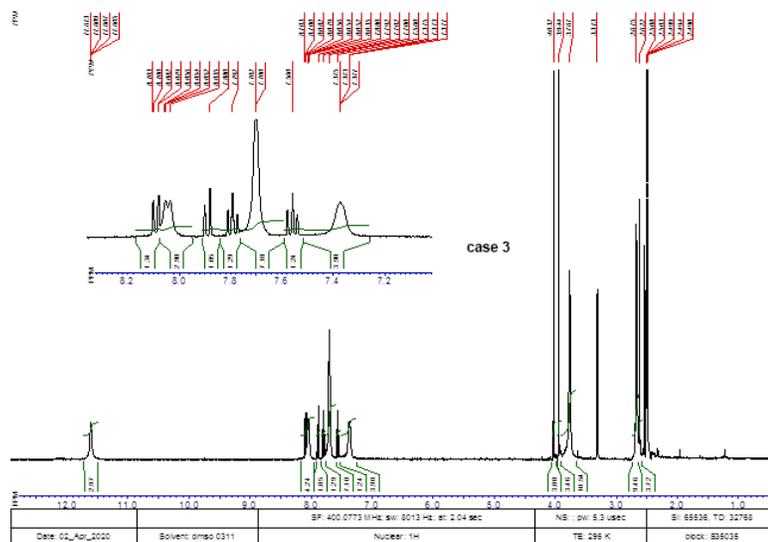


Figure S14. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 3 (Table 1).

-.o.-Syntex Purity Report -.o.-
 Agilent 1100 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H2O+0.1HCOOH;B-MeCN+0.1HCOOH
 Separation column:
 Rapid Resolutionn HT Cartidge 4.6x30mm,
 1.8-Micron, Zorbax SB-C18

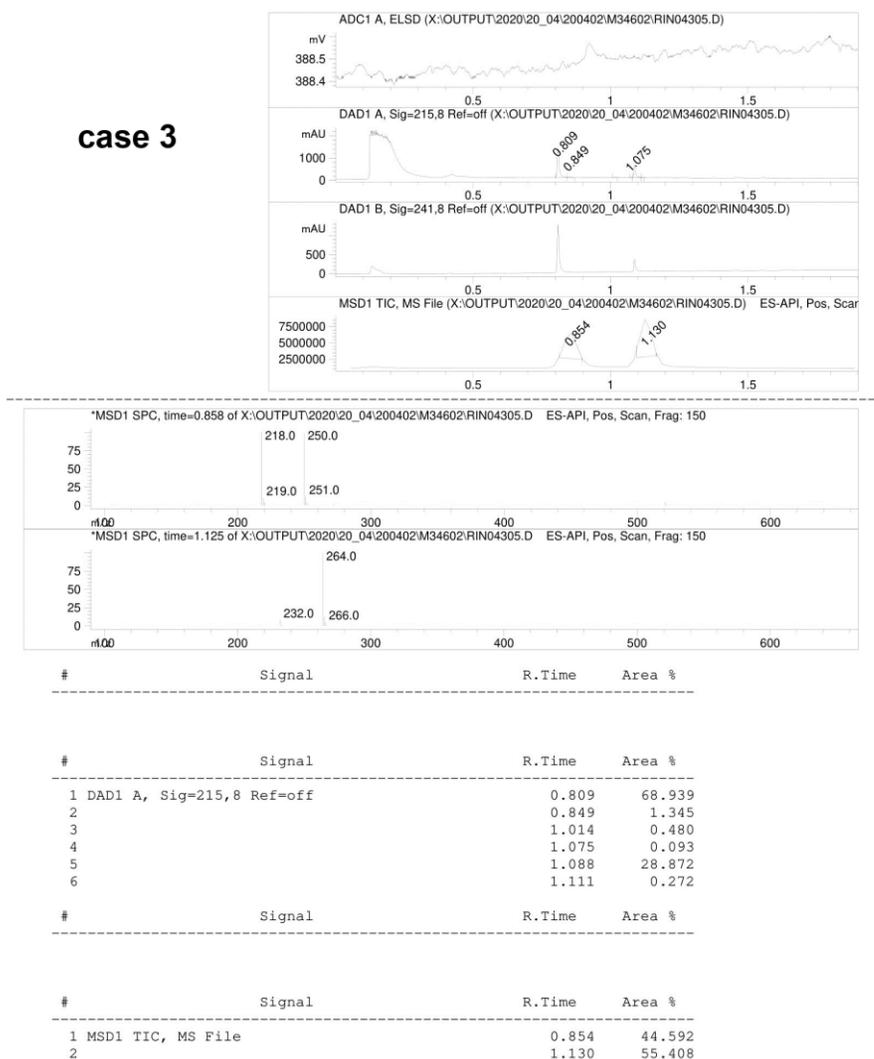


Figure S15. LC/MS data for the reaction product of case 3 (Table 1).

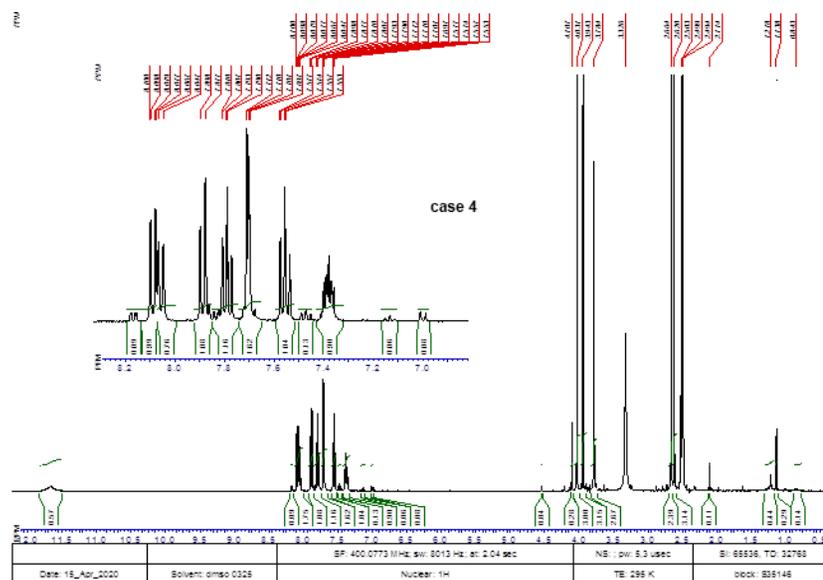
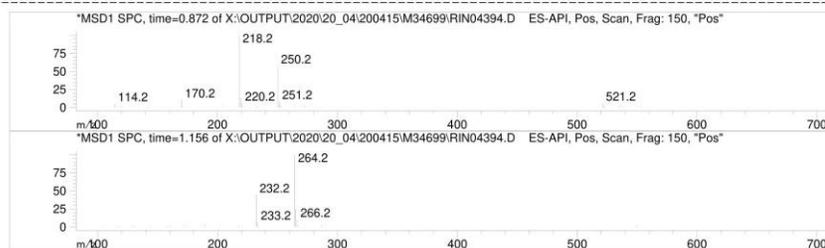
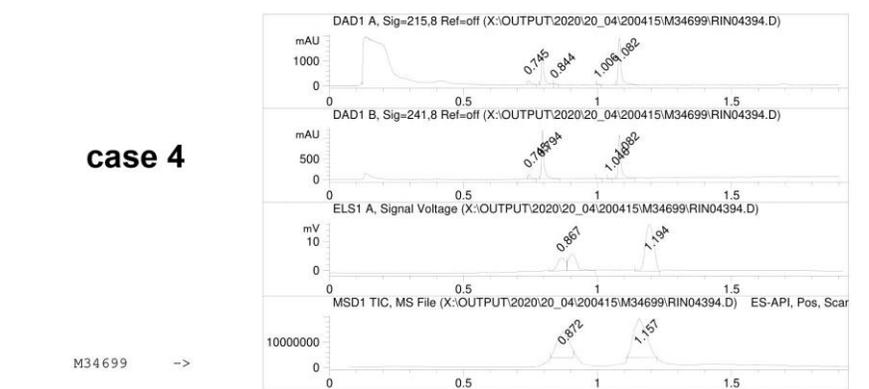


Figure S16. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 4 (Table 1).

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

Agilent 1200 LC/MSD	Mobile Phase:A-H2O+0.1HCOOH;B-MeCN+0.1HCOOH
Diodearray G1315B (DAD1A-215nm; DAD1B-241nm)	Separation column:
Mass Quad G6140A (MSD1-Pos, MSD2-Neg)	Rapid Resolutionn HT Cartige 4.6x30mm,
ELSD Altech 3300 (ADC1 A, ELSD)	1.8-Micron, Zorbax SB-C18



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.745	4.213
2		0.794	34.183
3		0.844	0.151
4		1.006	0.391
5		1.082	61.062

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.745	4.701
2		0.794	48.401
3		1.005	0.641
4		1.046	0.211
5		1.082	46.046

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	0.867	16.012
2		0.905	21.208
3		1.194	62.779

Figure S17. LC/MS data for the reaction product of case 4 (Table 1).

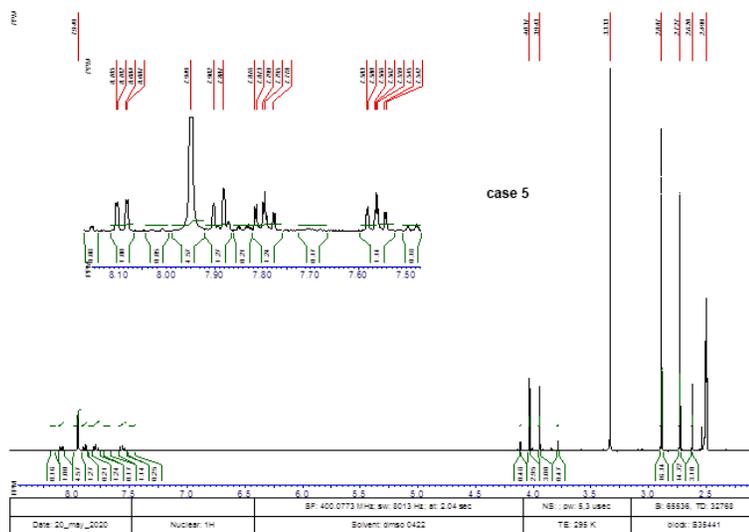


Figure S18. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 5 (Table 1).

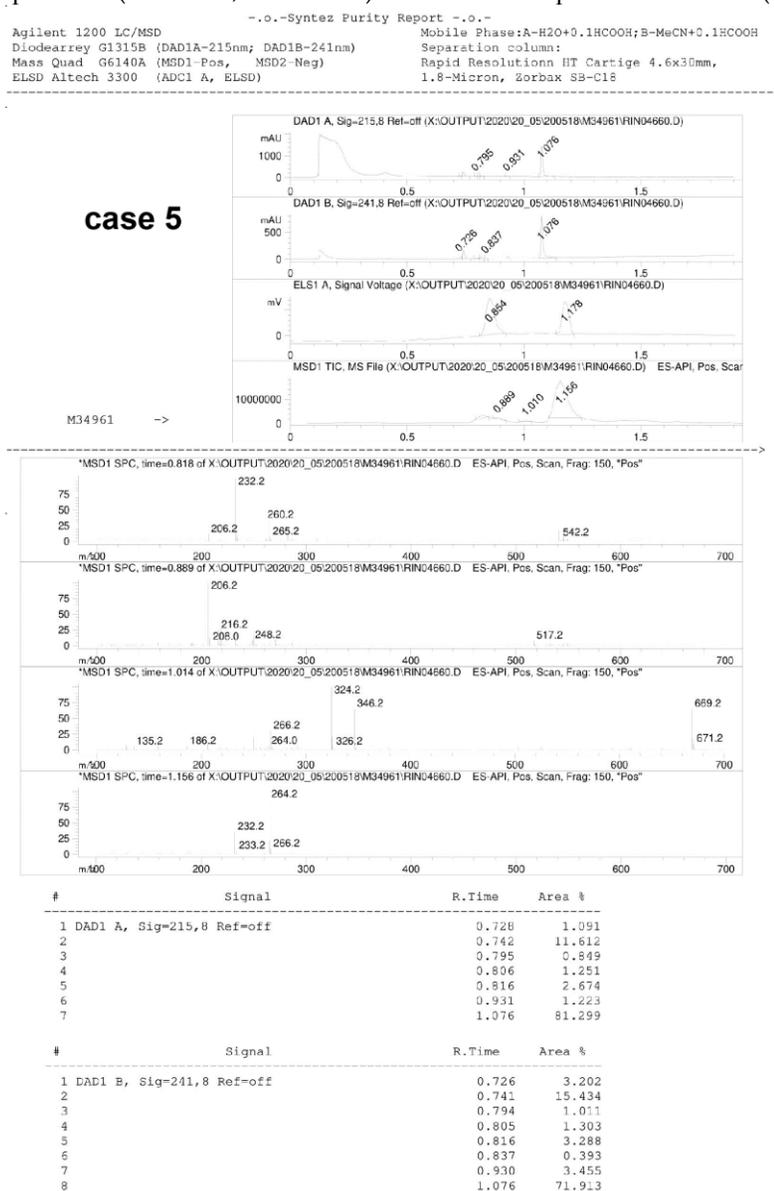


Figure S19. LC/MS data for the reaction product of case 5 (Table 1).

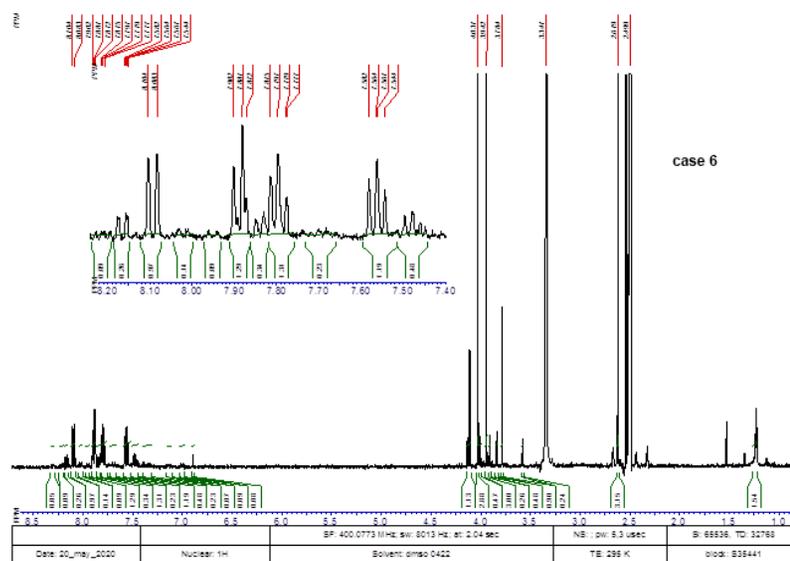


Figure S20. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 6 (Table 1).

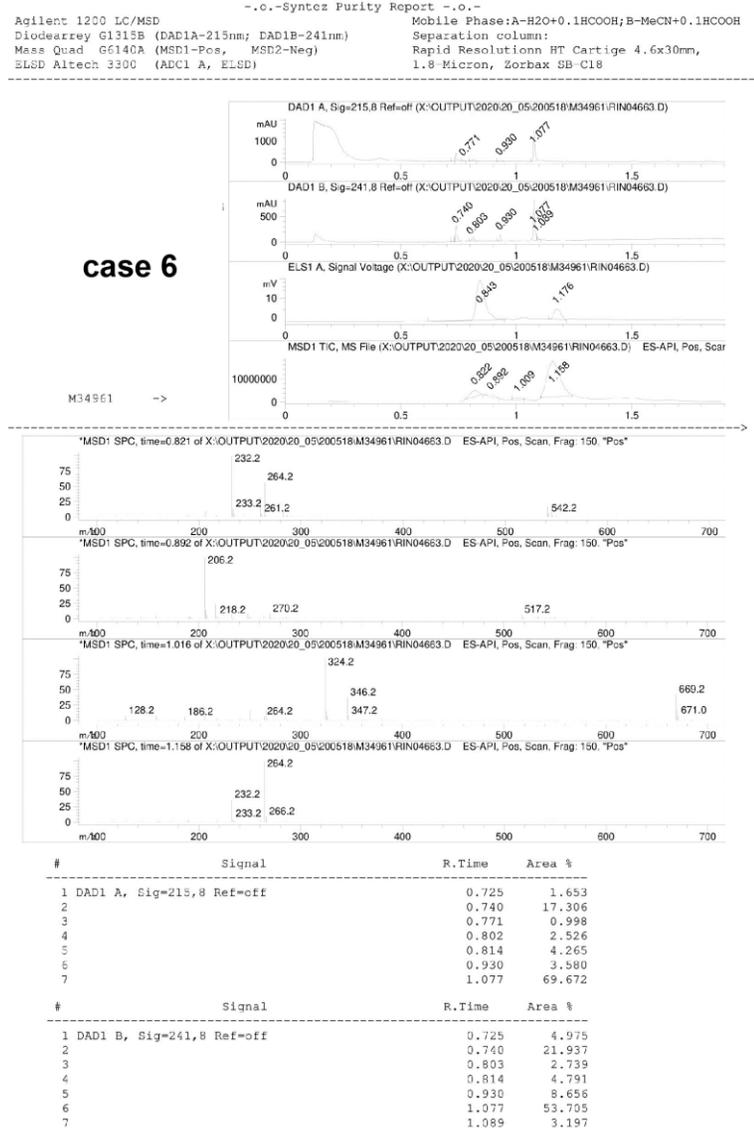


Figure S21. LC/MS data for the reaction product of case 6 (Table 1).

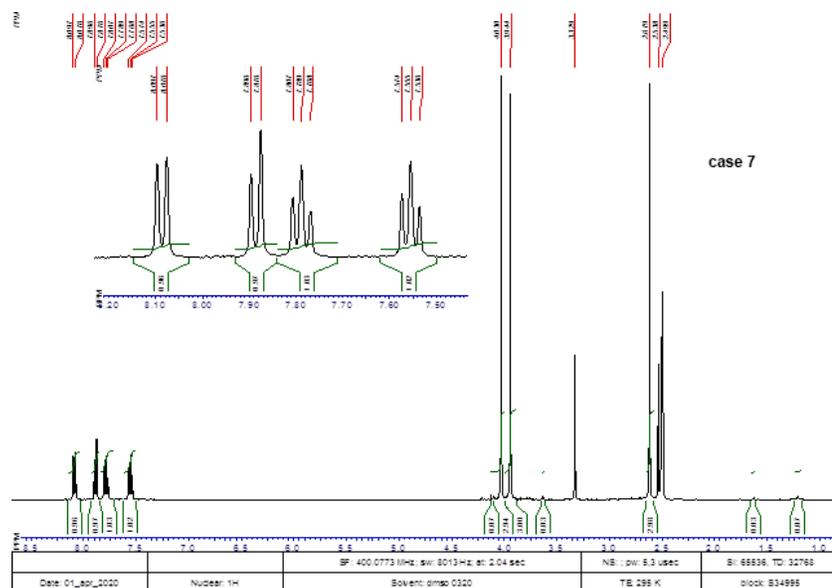


Figure S22. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 7 (Table 1).

-.o.-Synzetx Purity Report -.o.-
 Agilent 1100 LC/MSD Mobile Phase: A=H₂O+0.1HCOOH; B=MeCN+0.1HCOOH
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm) Separation column: **96%**
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg) Rapid Resolutionn HT Cartridge 4.6x30mm,
 ELSD Altech 3300 (ADC1 A, ELSD) 1.8-Micron, Zorbax SB-C18

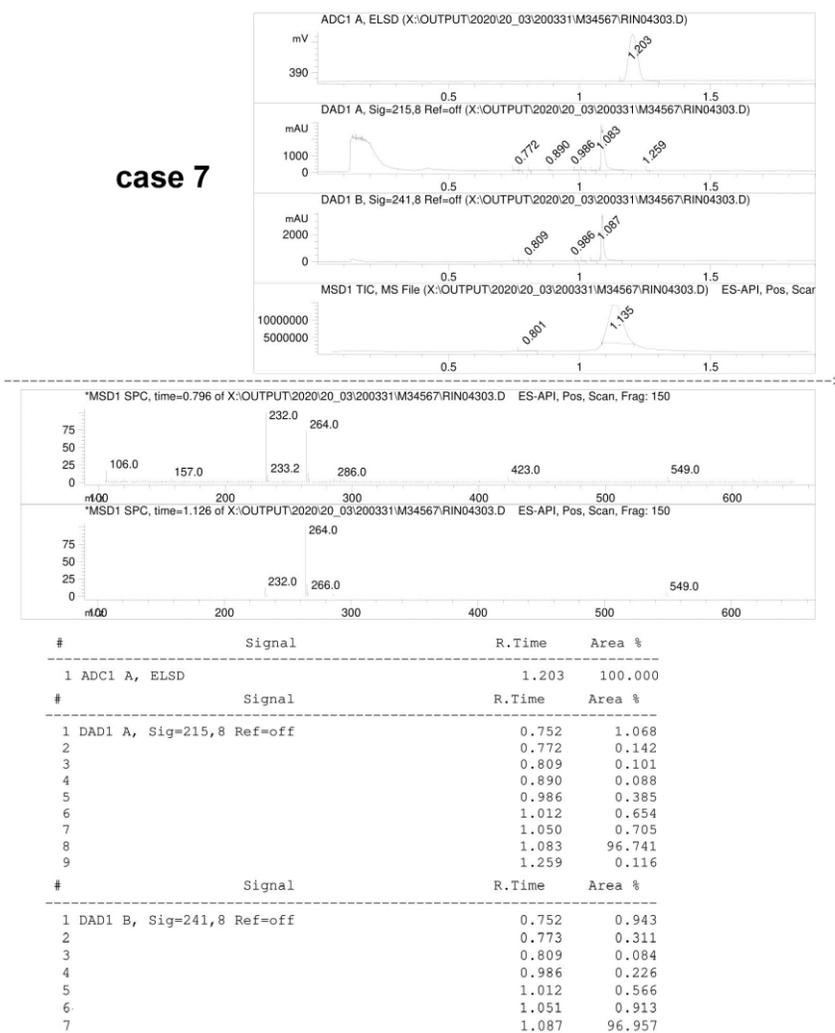


Figure S23. LC/MS data for the reaction product of case 7 (Table 1).

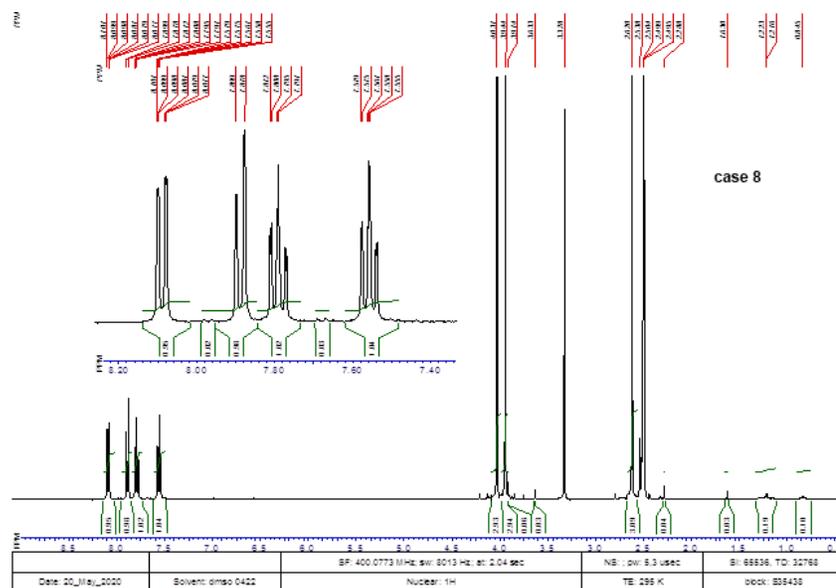


Figure S24. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 8 (Table 1).

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

Agilent 1100 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H2O+0.1HCOOH;B-MeCN+0.1HCOOH
 Separation column: **96%**
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18

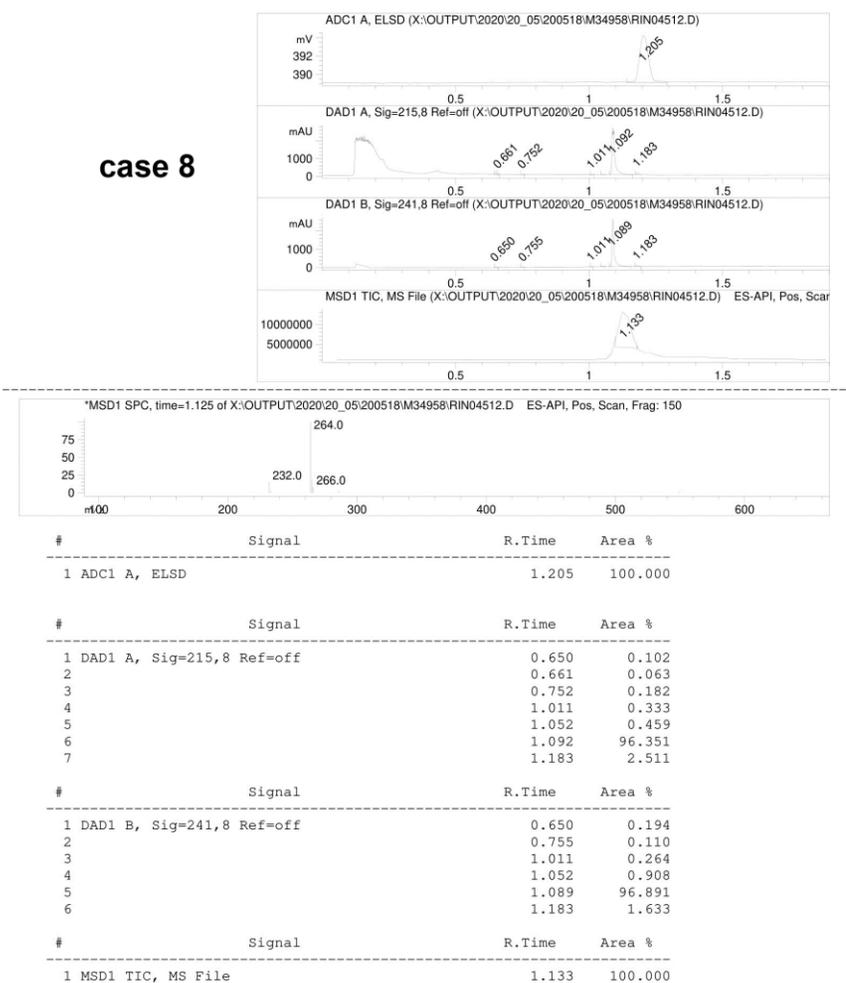


Figure S25. LC/MS data for the reaction product of case 8 (Table 1).

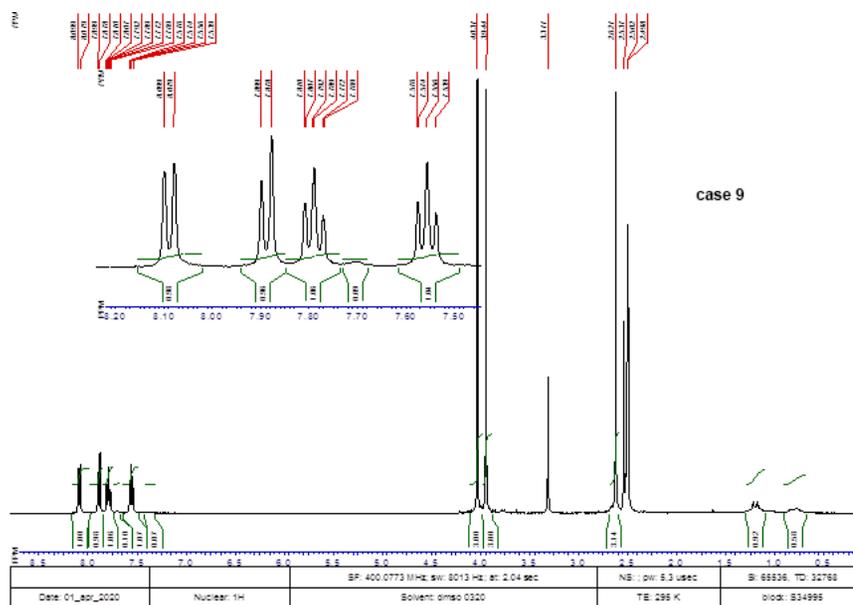


Figure S26. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 9 (Table 1).

Agilent 1100 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase: A-H₂O+0.1HCOOH; B-MeCN+0.1HCOOH
 Separation column: 95%
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18

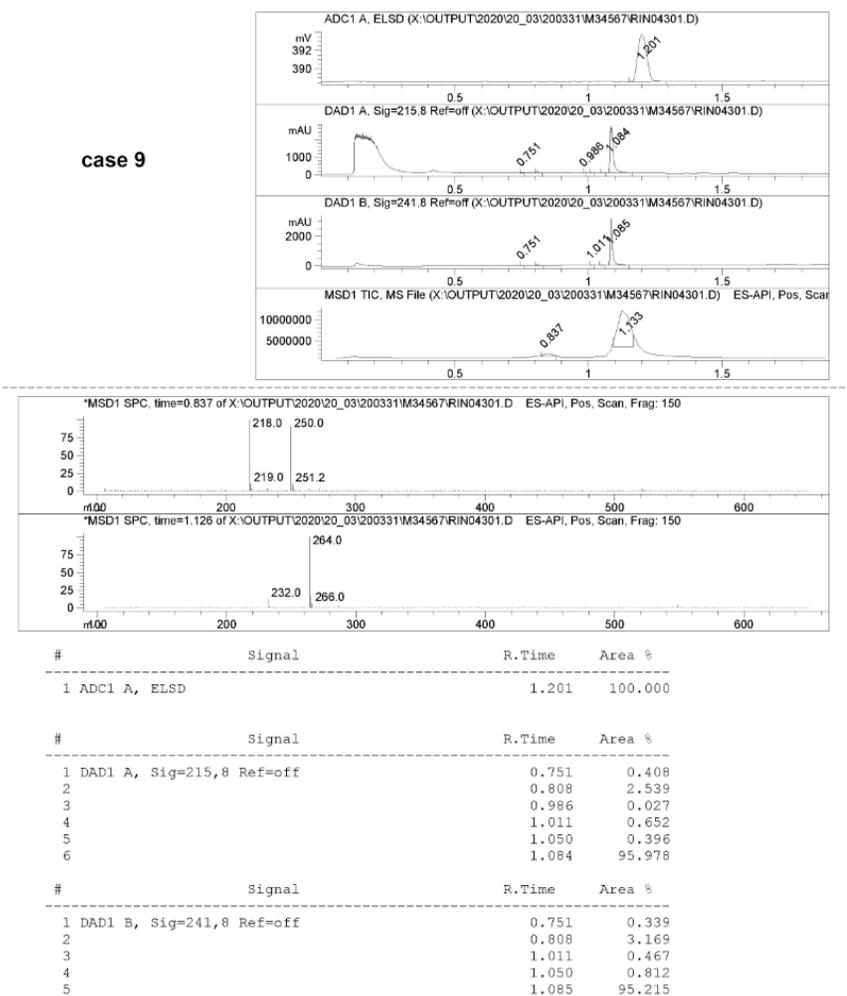


Figure S27. LC/MS data for the reaction product of case 9 (Table 1).

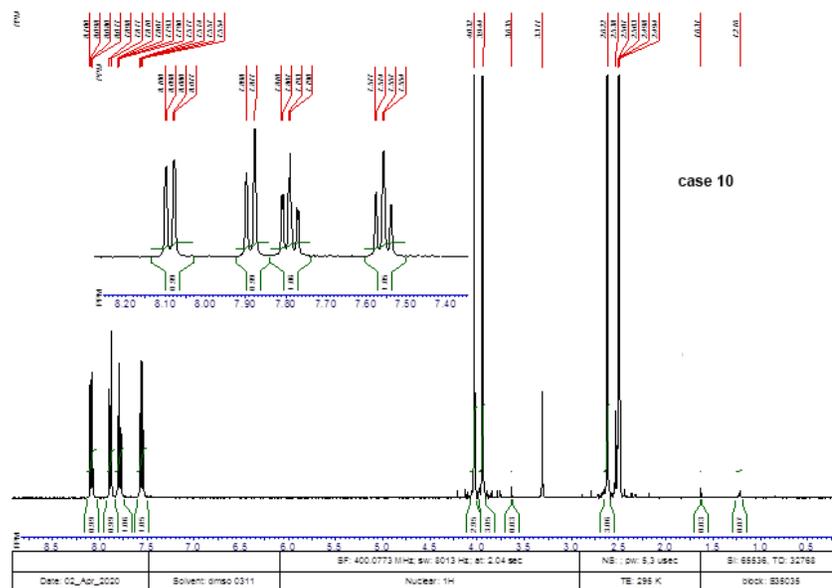
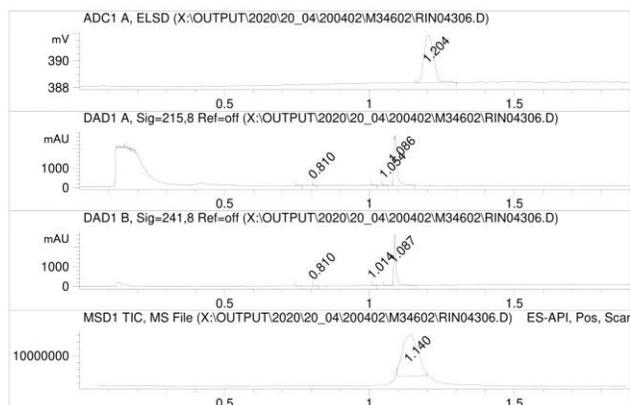


Figure S28. ¹H NMR spectrum (400 MHz, DMSO-d₆) of the reaction product of case 10 (Table 1).

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

Agilent 1100 LC/MSD	Mobile Phase: A-H ₂ O+0.1HCOOH; B-MeCN+0.1HCOOH
Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)	Separation column: 97%
Mass Quad G1956B (MSD1-Pos, MSD2-Neg)	Rapid Resolutionn HT Cartridge 4.6x30mm,
ELSD Altech 3300 (ADC1 A, ELSD)	1.8-Micron, Zorbax SB-C18

case 10



#	Signal	R.Time	Area %
1	ADC1 A, ELSD	1.204	100.000
#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.753	0.541
2		0.810	0.250
3		1.014	0.572
4		1.054	0.660
5		1.086	97.976
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.753	0.595
2		0.810	0.150
3		1.014	0.545
4		1.052	1.323
5		1.087	97.386
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.140	100.000

Figure S29. LC/MS data for the reaction product of case 10 (Table 1).

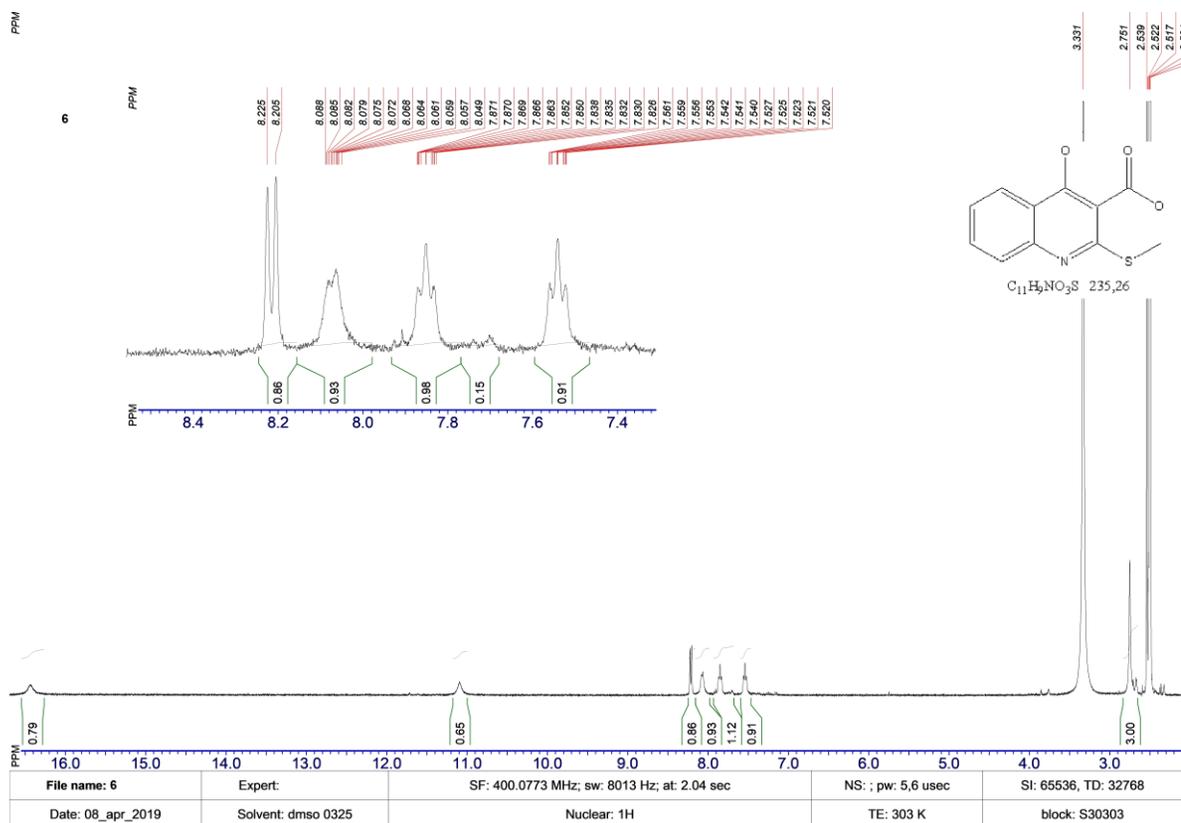


Figure S30. 1H NMR spectrum (400 MHz, DMSO- d_6) of 4-hydroxy-2-(methylthio)quinoline-3-carboxylic acid 6.

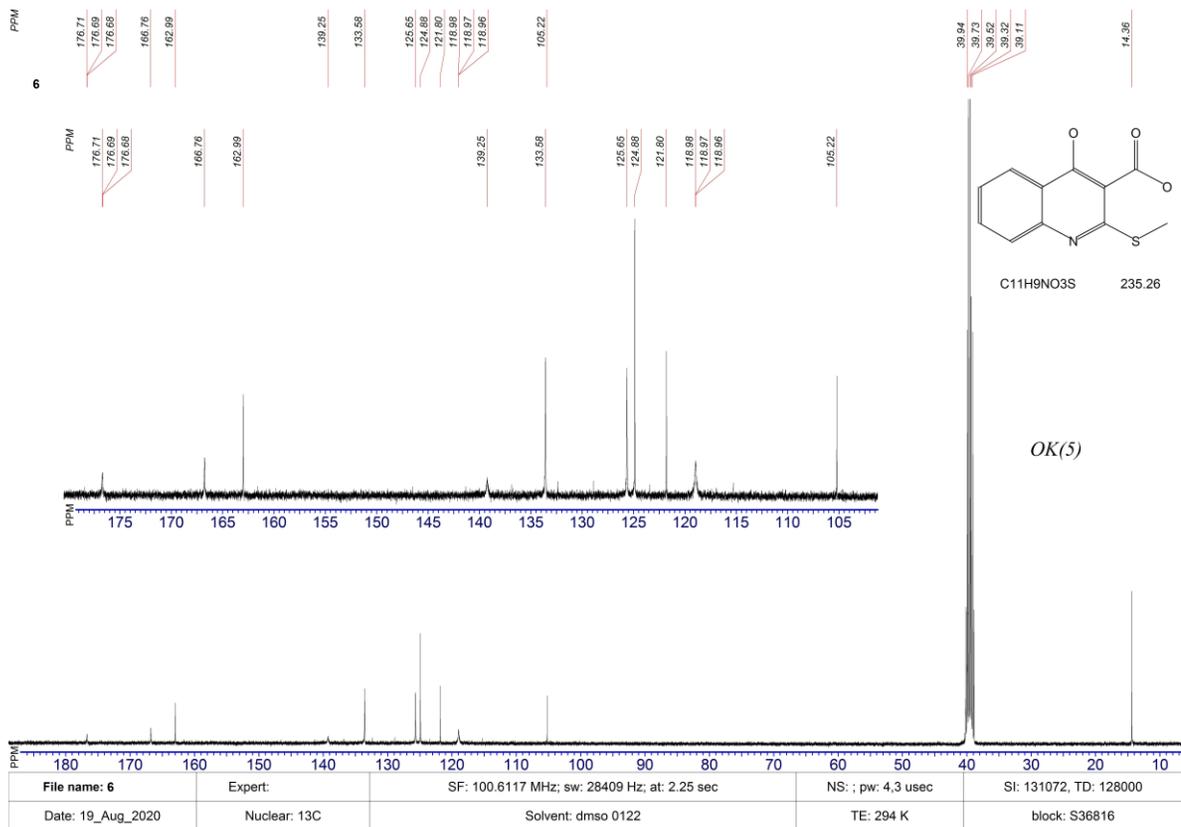
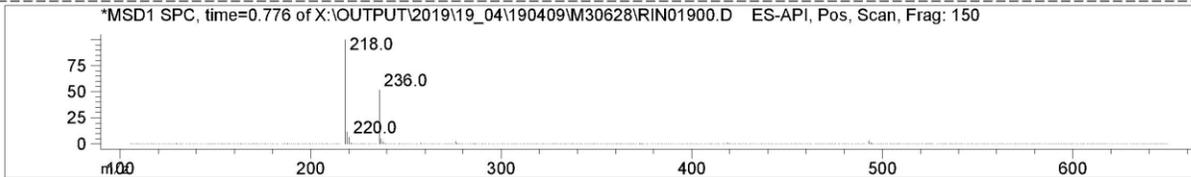
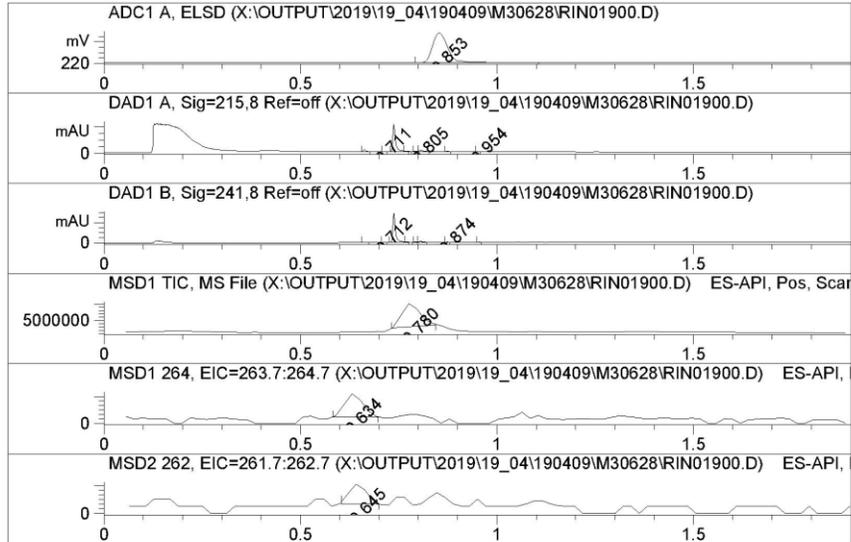
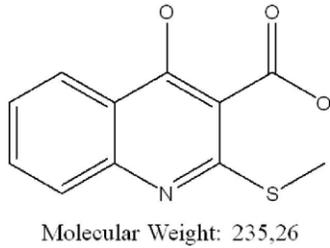


Figure S31. ^{13}C NMR spectrum (100 MHz, DMSO- d_6) of 4-hydroxy-2-(methylthio)quinoline-3-carboxylic acid 6.

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Agilent 1100 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-241nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H₂O+0.1HCOOH;B-MeCN+0.1HCOOH
 Separation column:
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18



#	Signal	R.Time	Area %
1	ADC1 A, ELSD	0.853	100.000

#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,8 Ref=off	0.663	6.440
2		0.711	0.628
3		0.738	84.932
4		0.769	0.457
5		0.792	0.747
6		0.805	5.532
7		0.874	1.005
8		0.954	0.261

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,8 Ref=off	0.663	1.292
2		0.712	0.613
3		0.738	92.563
4		0.768	0.417
5		0.793	0.826
6		0.805	3.586
7		0.874	0.215
8		0.954	0.488

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.780	100.000

Figure S32. LC/MS data for 4-hydroxy-2-(methylthio)quinoline-3-carboxylic acid 6.