A Novel Series of [1,2,4]Triazolo[4,3-a]pyridine Sulfonamides as Potential Antimalarial Agents: *In Silico* Studies, Synthesis and *In Vitro* Evaluation

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SUPPLEMENTARY MATERIAL

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Figure S118. LC/MS data for 1-(3-(4-fluorobenzylthio)-[1,2,4]triazolo[4,3-a]pyridin-8-ylsulfonyl)-1,2,3,4-tetrahydroquinoline **15f**.

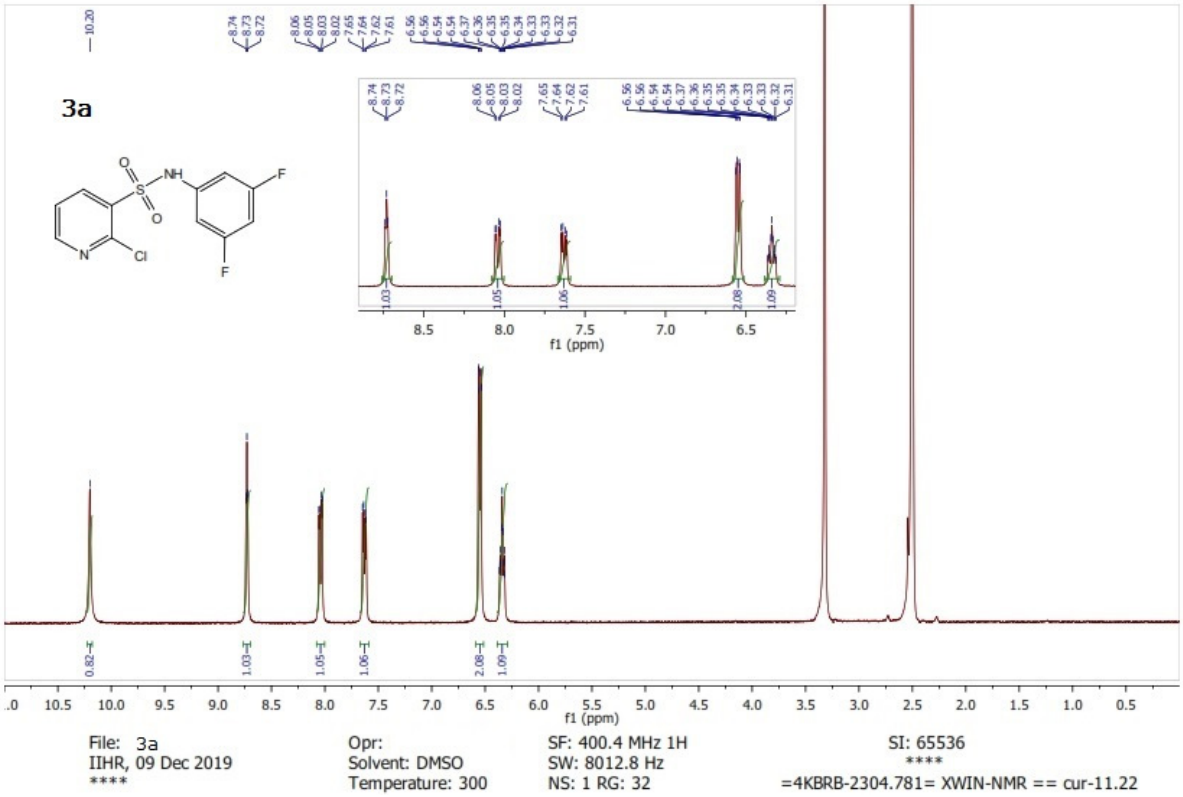


Figure S1. ^{1}H NMR spectrum (400 MHz, DMSO-d6) of 2-chloro-N-(3,5-difluorophenyl) pyridine-3-sulfonamide **3a**.

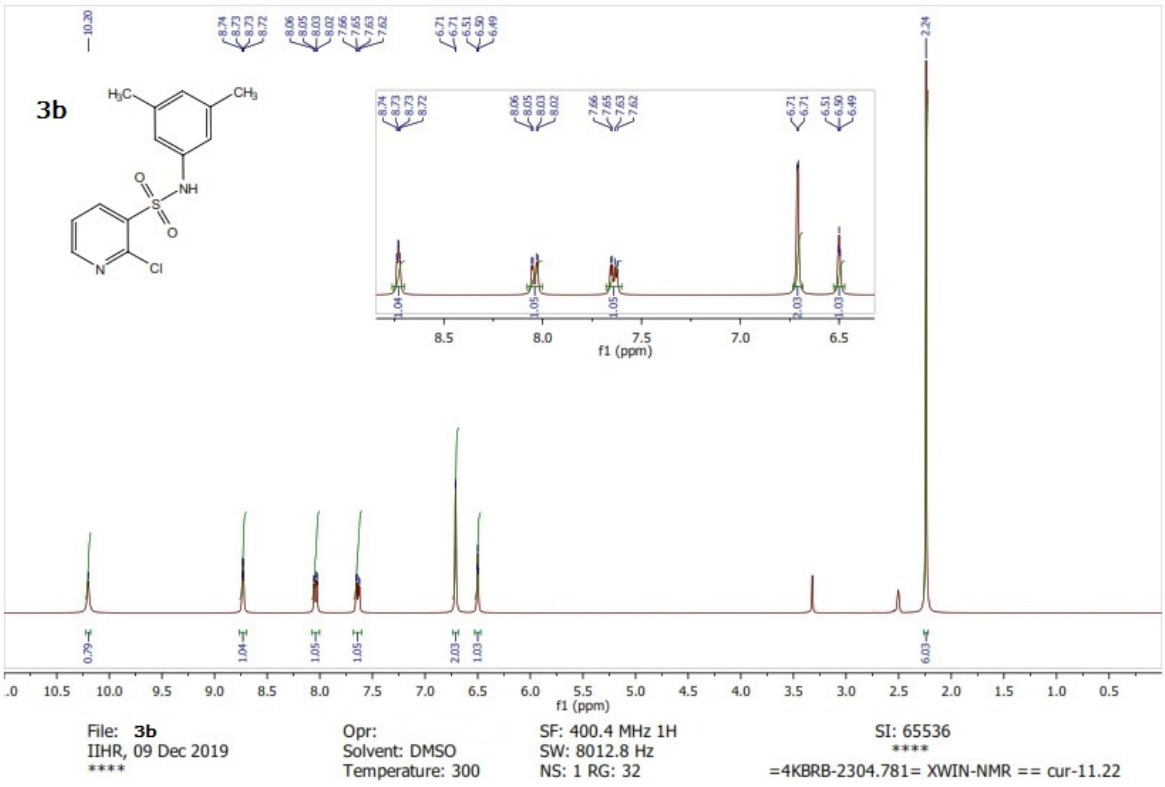


Figure S2. ^{1}H NMR spectrum (400 MHz, DMSO-d6) of 2-chloro-N-(3,5-dimethylphenyl) pyridine-3-sulfonamide **3b**.

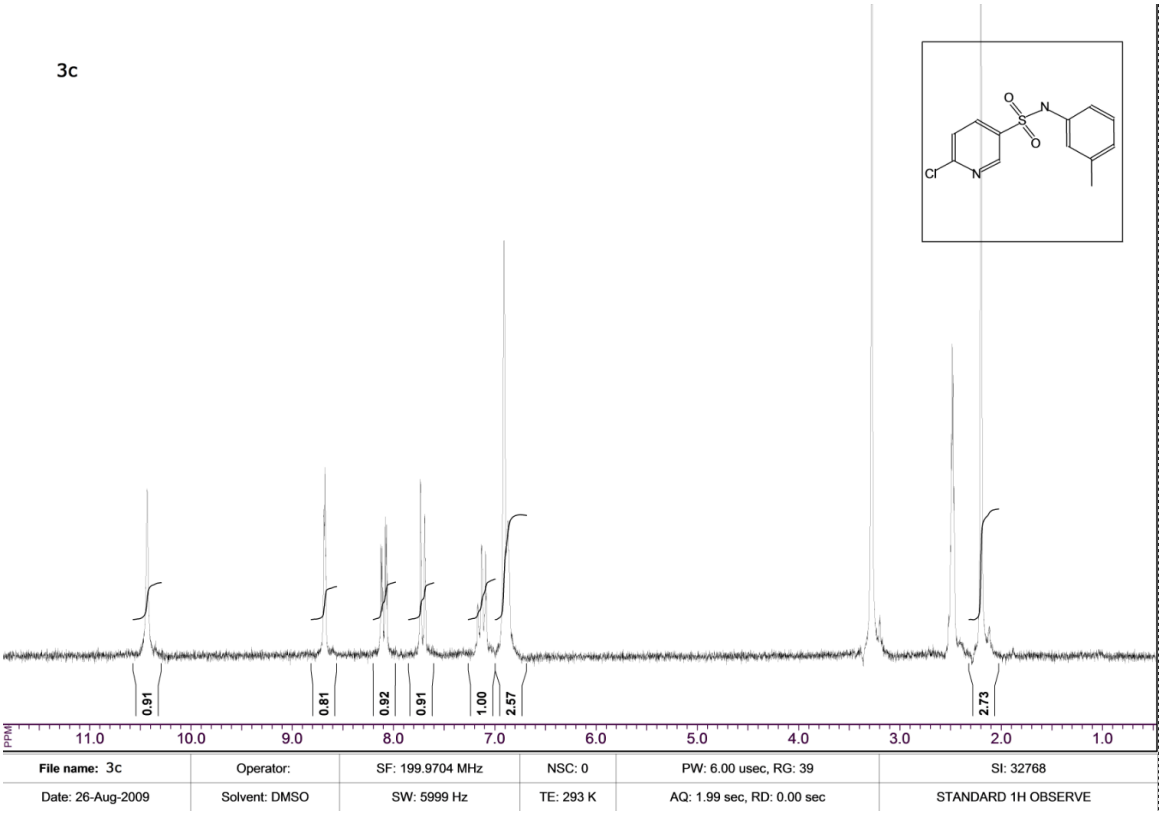


Figure S3. [1]H NMR spectrum (200 MHz, DMSO-d6) of 2-chloro-N-(3-methylphenyl) pyridine-5-sulfonamide **3c**.

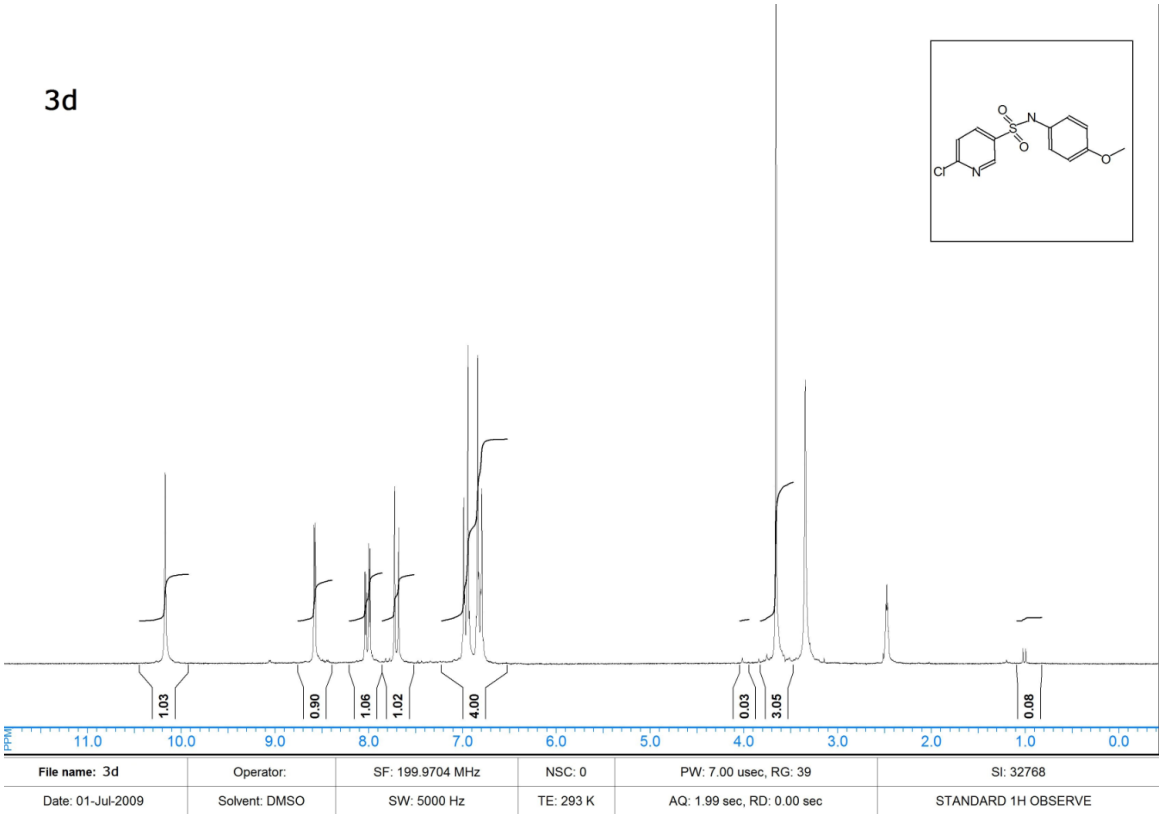


Figure S4. [1]H NMR spectrum (200 MHz, DMSO-d6) of 2-Chloro-N-(4-methoxyphenyl) pyridine-5-sulfonamide **3d**.

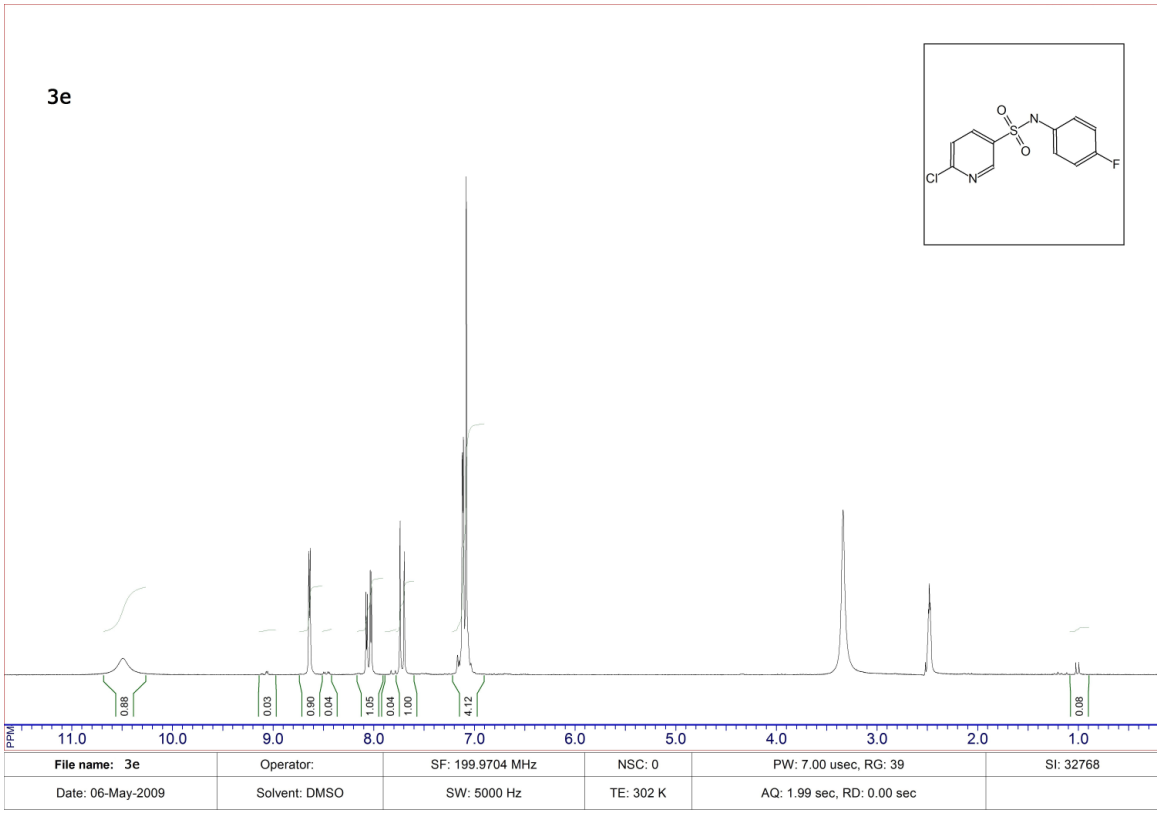


Figure S5. [1]H NMR spectrum (200 MHz, DMSO-d6) of 2-Chloro-N-(4-fluorophenyl) pyridine-5-sulfonamide **3e**.

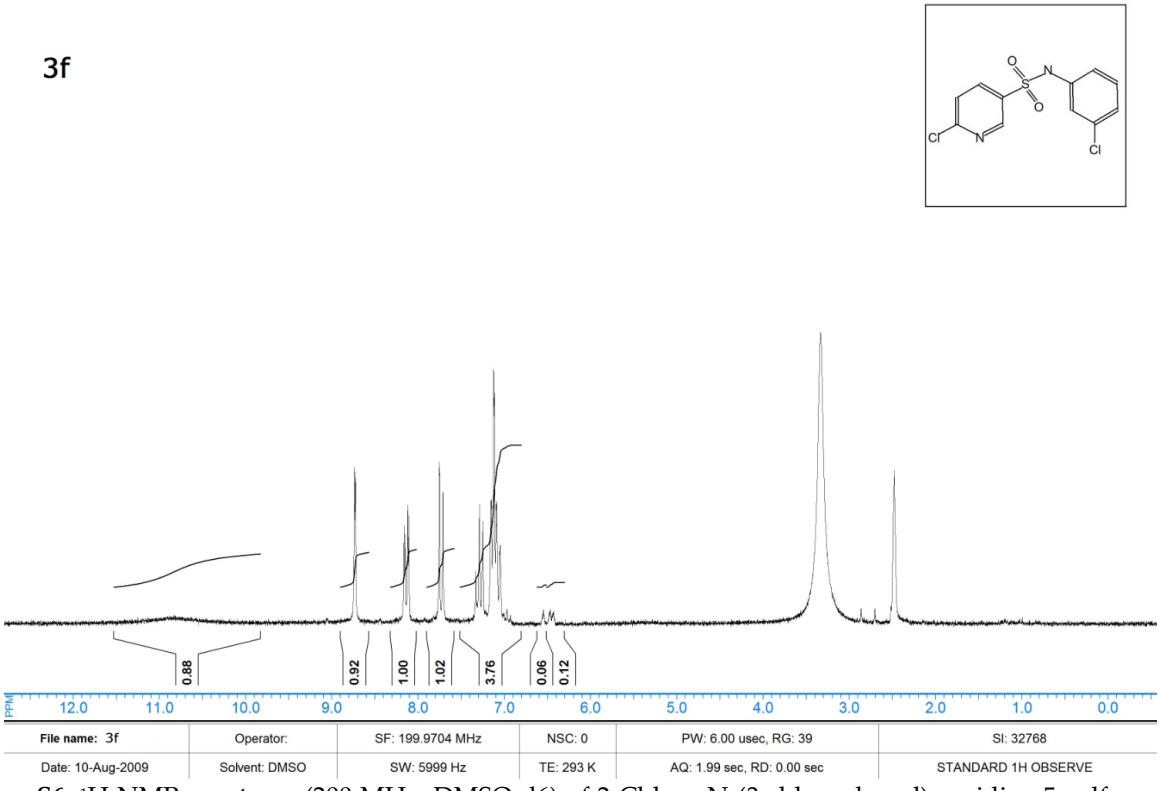


Figure S6. [1]H NMR spectrum (200 MHz, DMSO-d6) of 2-Chloro-N-(3-chlorophenyl) pyridine-5-sulfonamide **3f.**

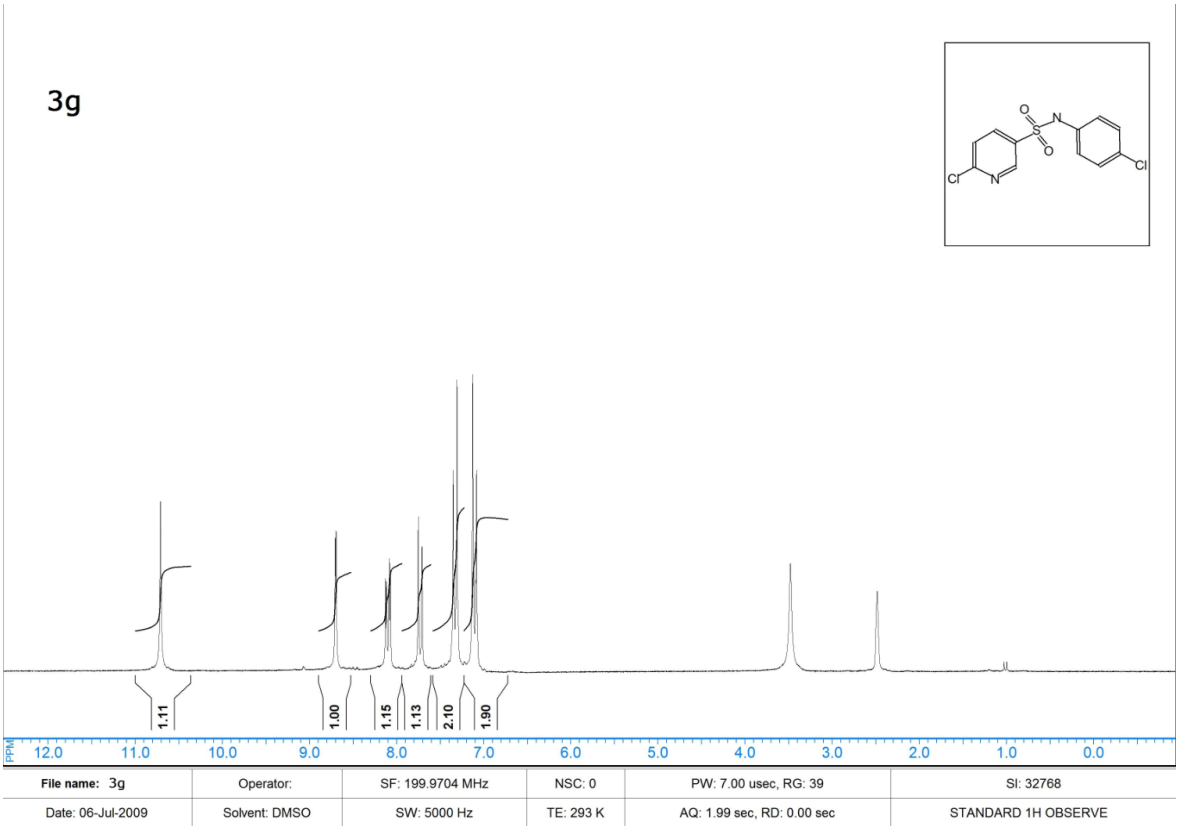


Figure S7. [1]H NMR spectrum (200 MHz, DMSO-d6) of 2-Chloro-N-(4-chlorophenyl) pyridine-5-sulfonamide **3g**.

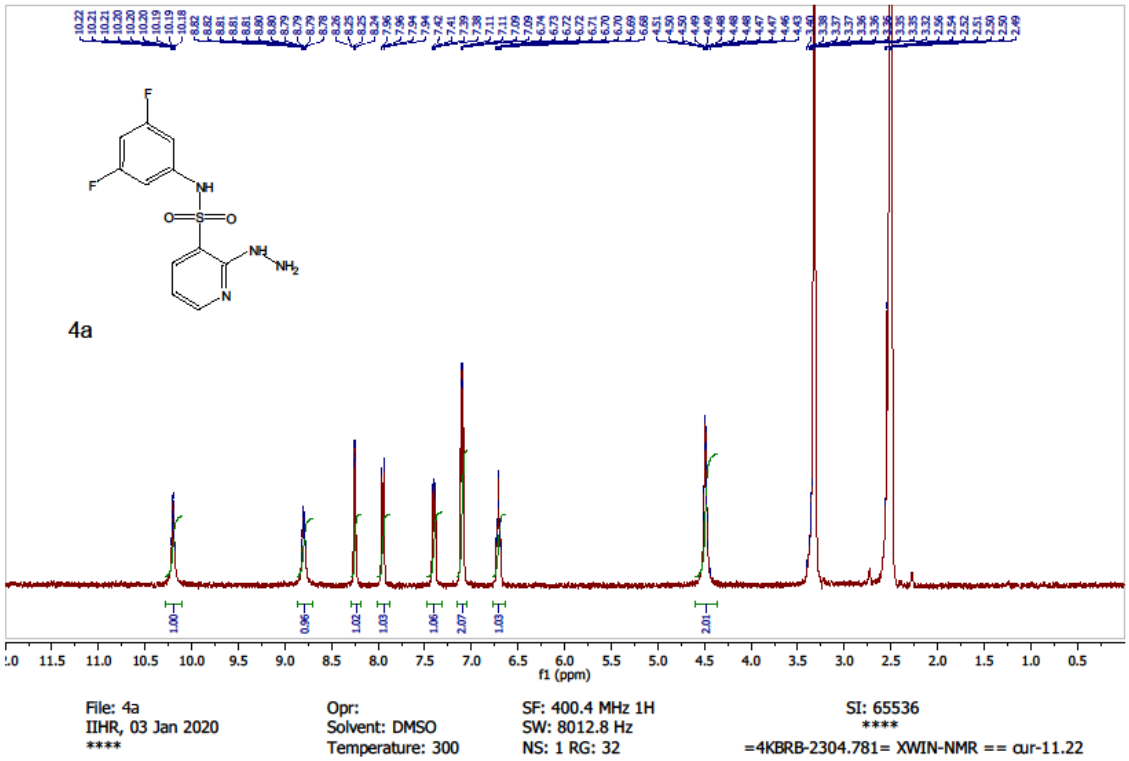


Figure S8. [1]H NMR spectrum (400 MHz, DMSO-d6) of N-(3,5-difluorophenyl)-2-hydrazinylpyridine-3-sulfonamide **4a**.

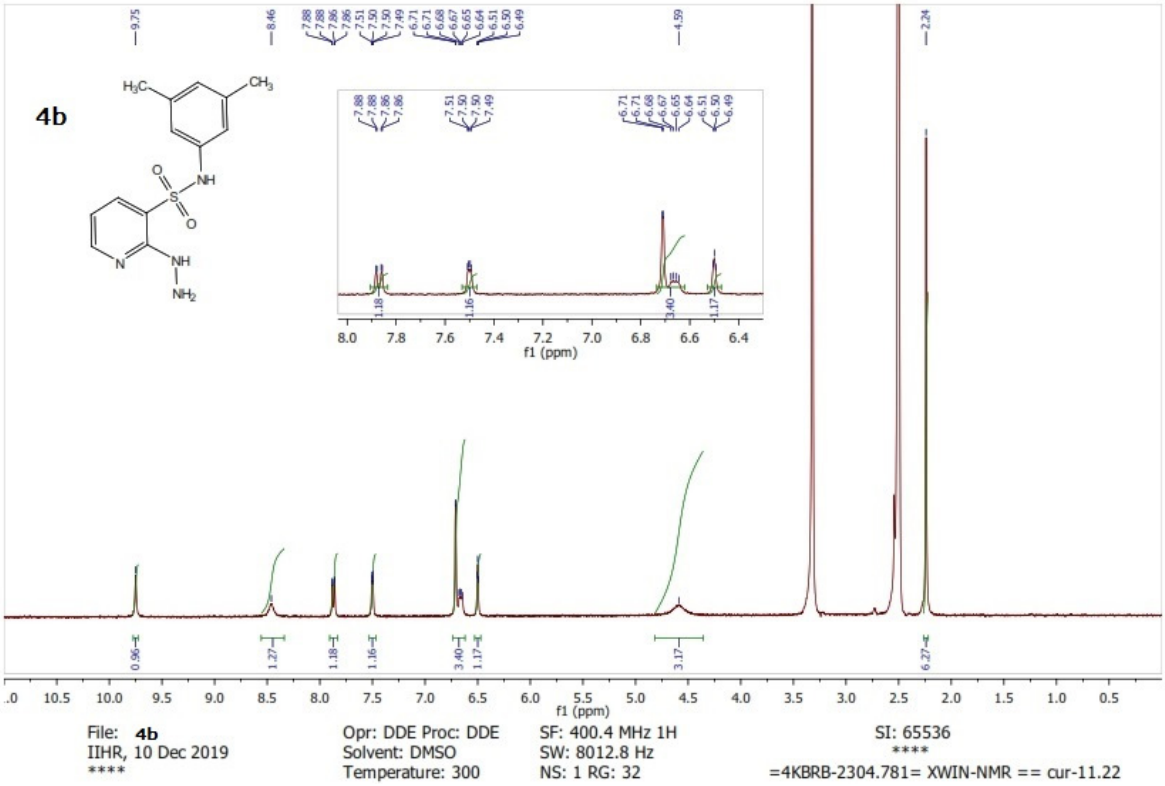


Figure S9. [1]H NMR spectrum (400 MHz, DMSO-d6) of N-(3,5-dimethylphenyl)-2-hydrazinylpyridine-3-sulfonamide **4b**.

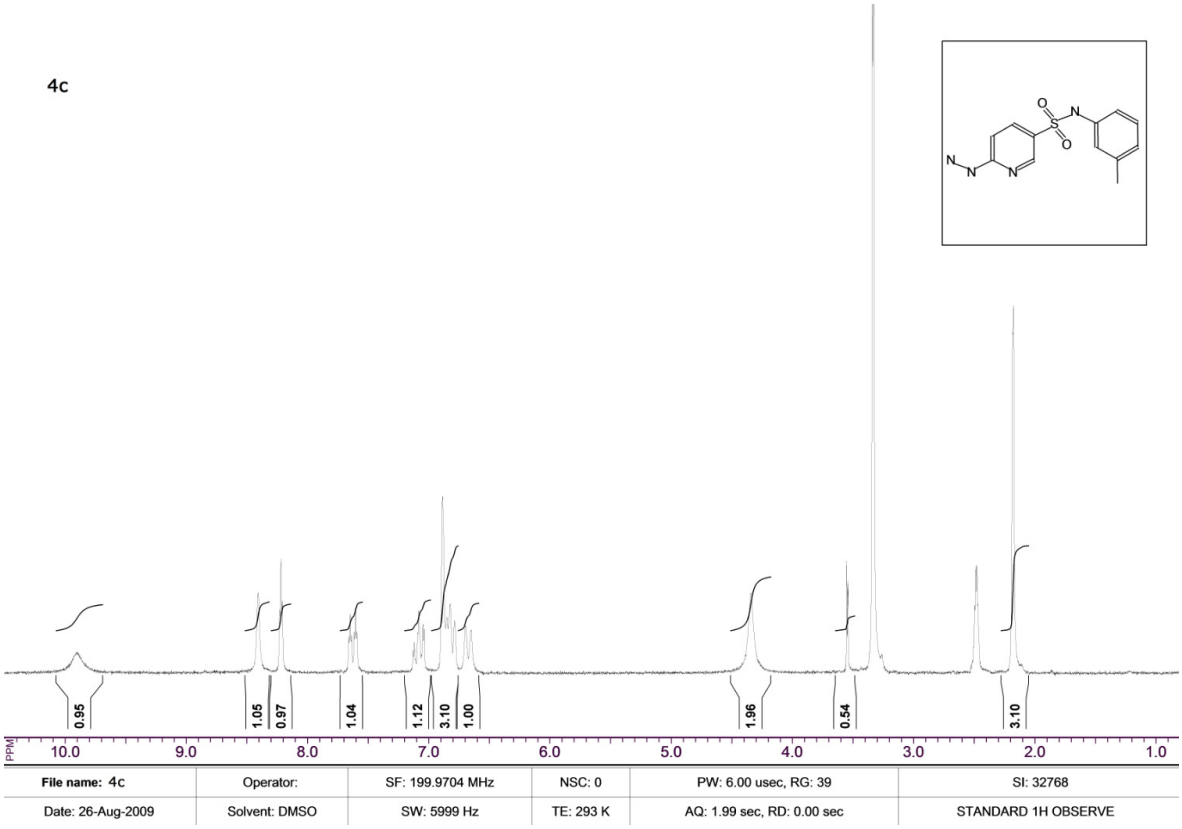


Figure S10. [1]H NMR spectrum (200 MHz, DMSO-d6) of 2-hydrazinyl-N-(3-methylphenyl) pyridine-5-sulfonamide **4c**.

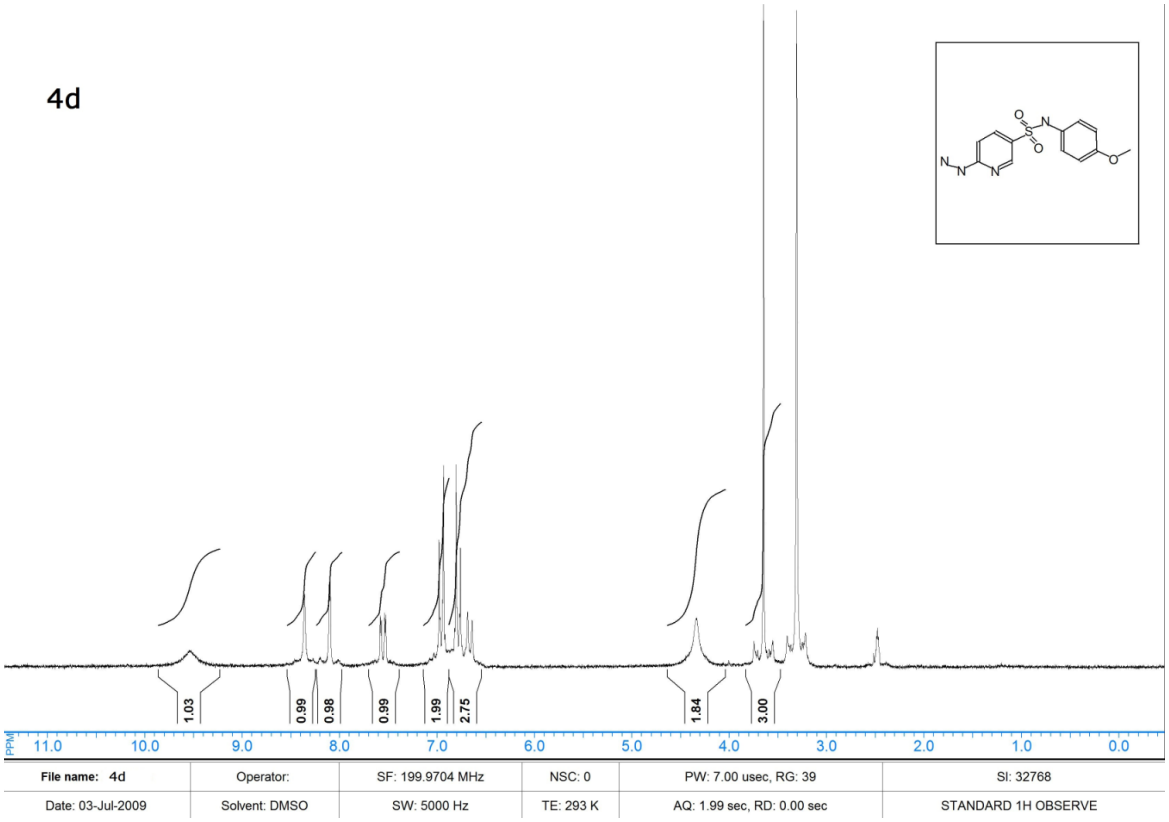


Figure S11. [1]H NMR spectrum (200 MHz, DMSO-d6) of 2-hydrazinyl-N-(4-methoxyphenyl) pyridine-5-sulfonamide **4d**.

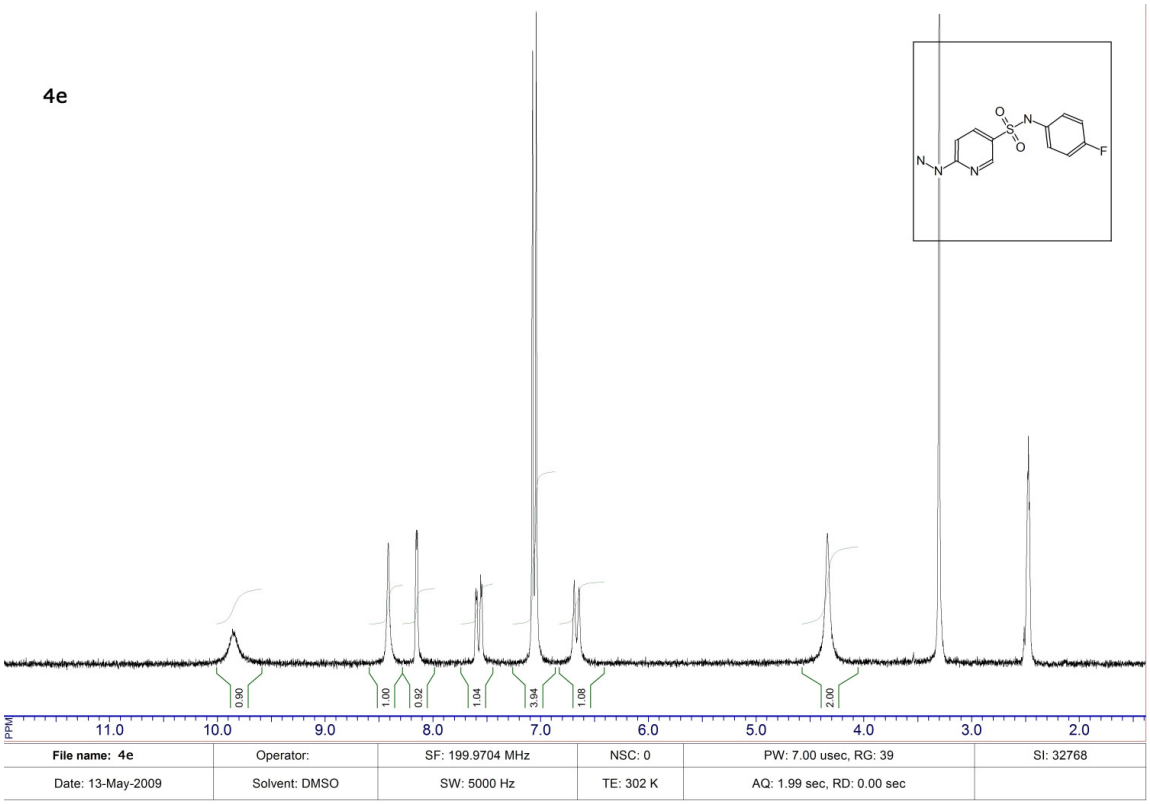


Figure S12. [1]H NMR spectrum (200 MHz, DMSO-d6) of N-(4-fluorophenyl)-2-hydrazinylpyridine-5-sulfonamide **4e**.

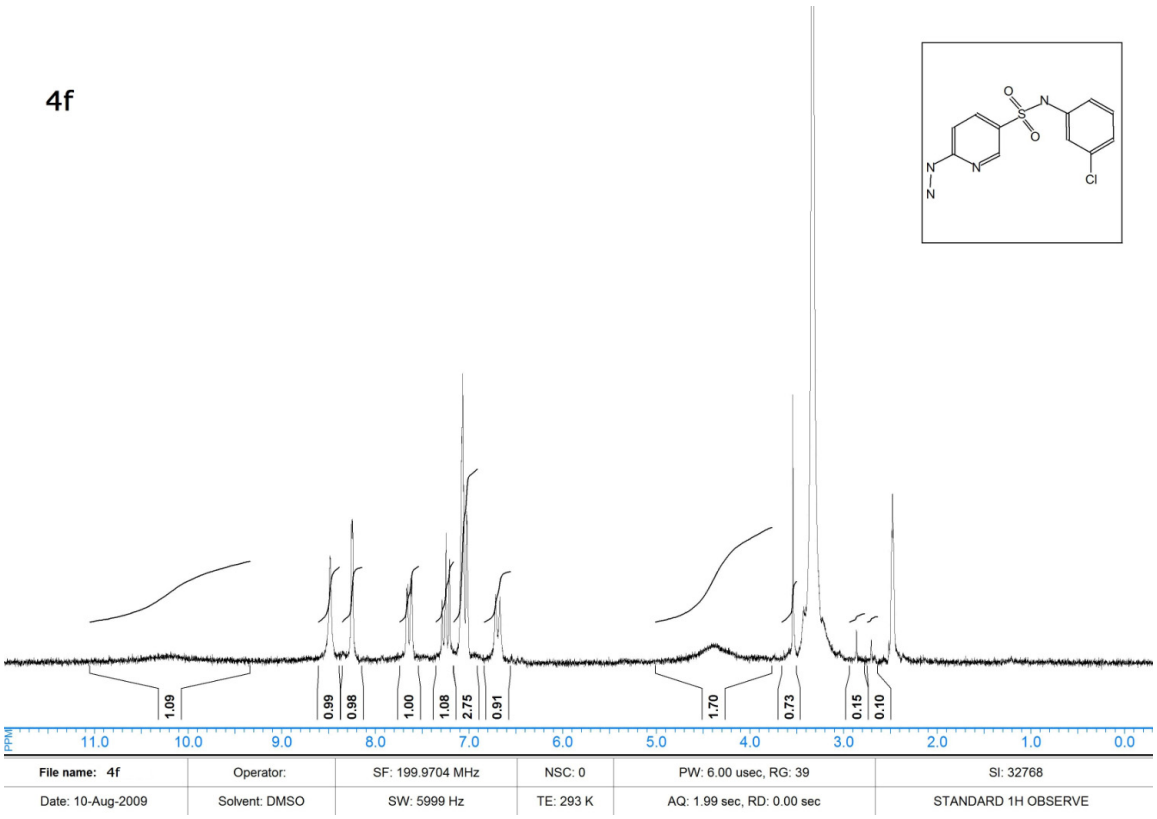


Figure S13. [1]H NMR spectrum (200 MHz, DMSO-d6) of N-(3-chlorophenyl)-2-hydrazinylpyridine-5-sulfonamide **4f**.

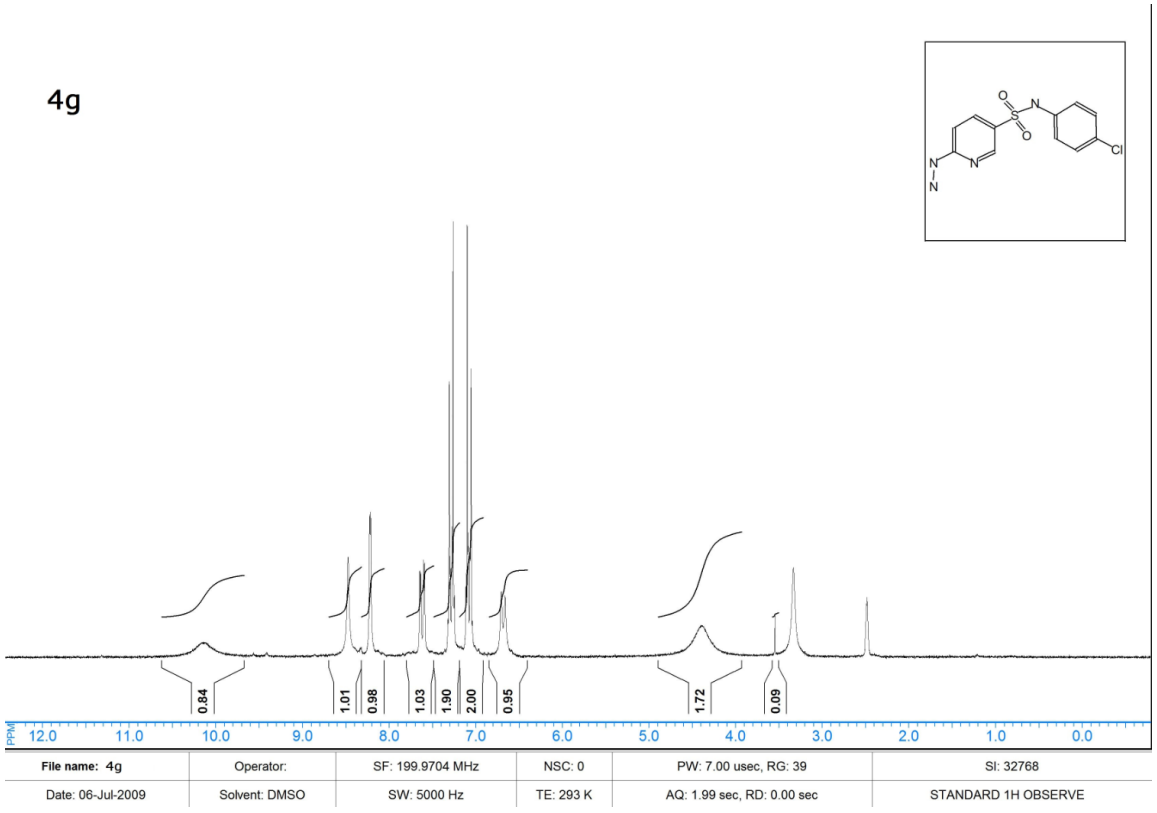


Figure S14. [1]H NMR spectrum (200 MHz, DMSO-d6) of N-(4-chlorophenyl)-2-hydrazinylpyridine-5-sulfonamide **4g**.

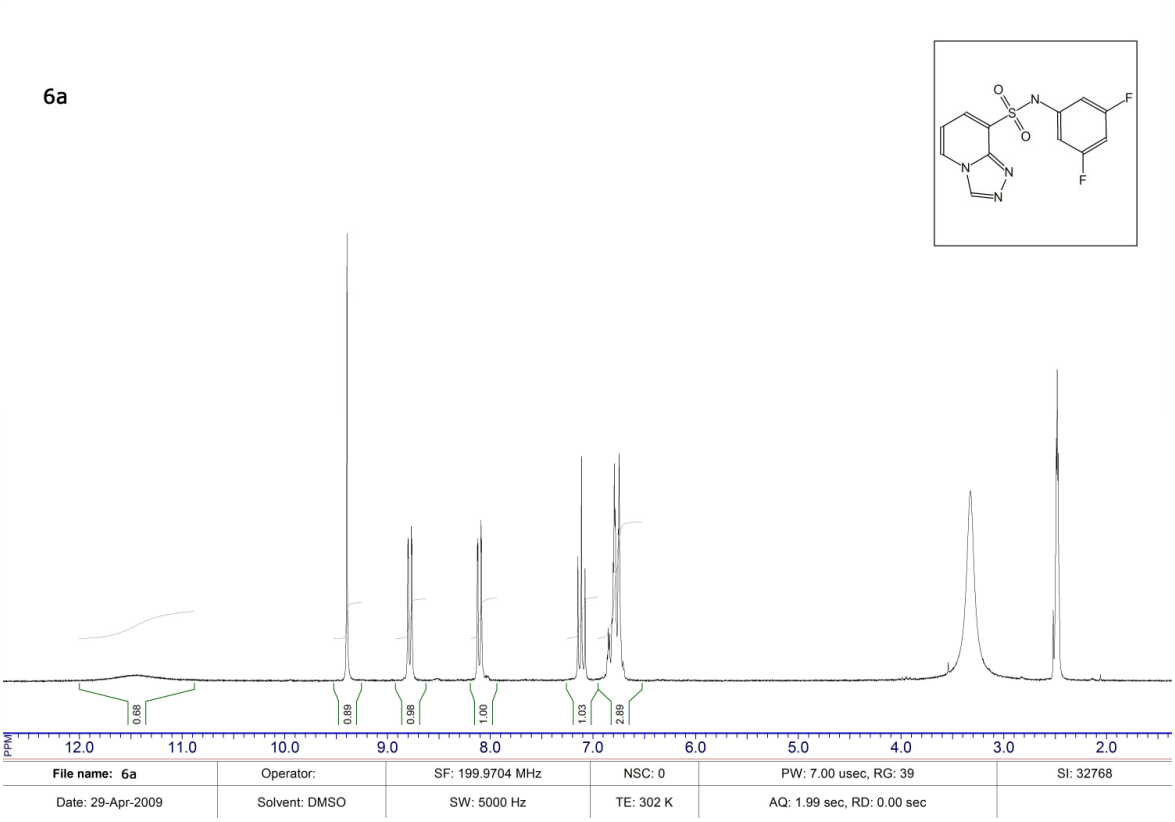


Figure S15. [1]H NMR spectrum (200 MHz, DMSO-d6) of N-(3,5-difluorophenyl)-[1,2,4]triazolo[4,3-a]pyridine-8-sulfonamide **6a**.

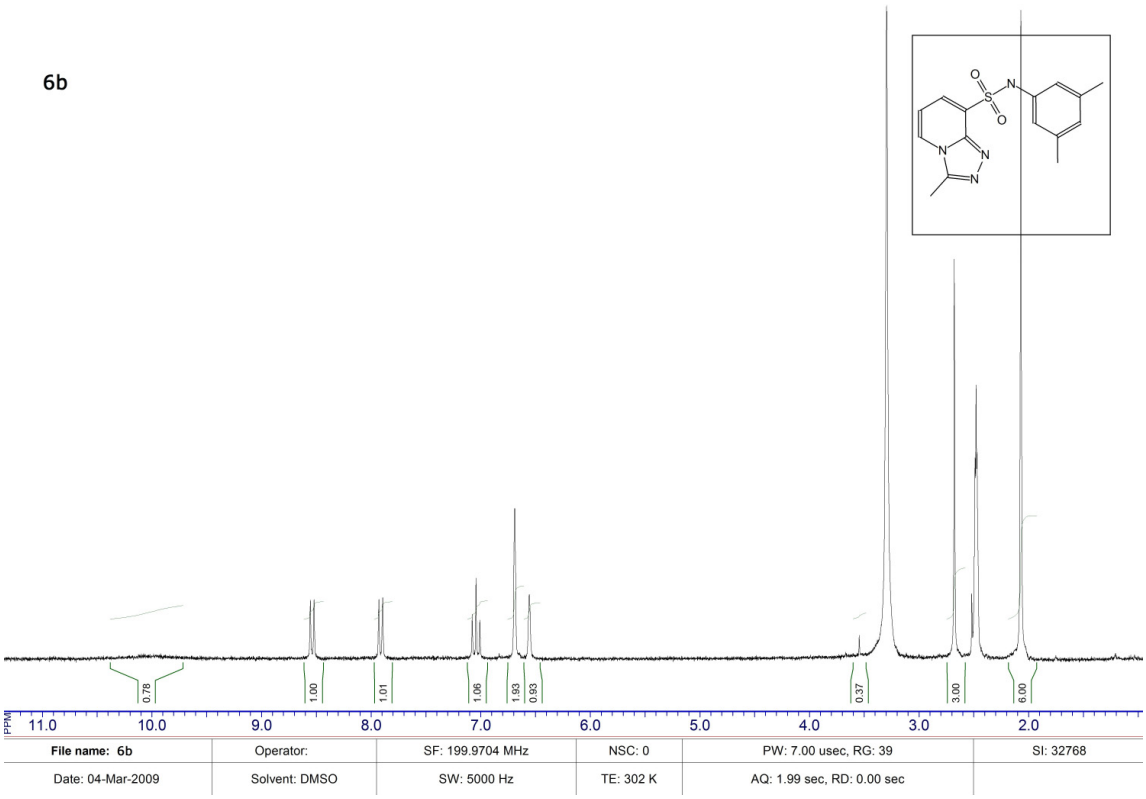


Figure S16. [1]H NMR spectrum (200 MHz, DMSO-d6) of N-(3,5-dimethylphenyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-8-sulfonamide **6b**.

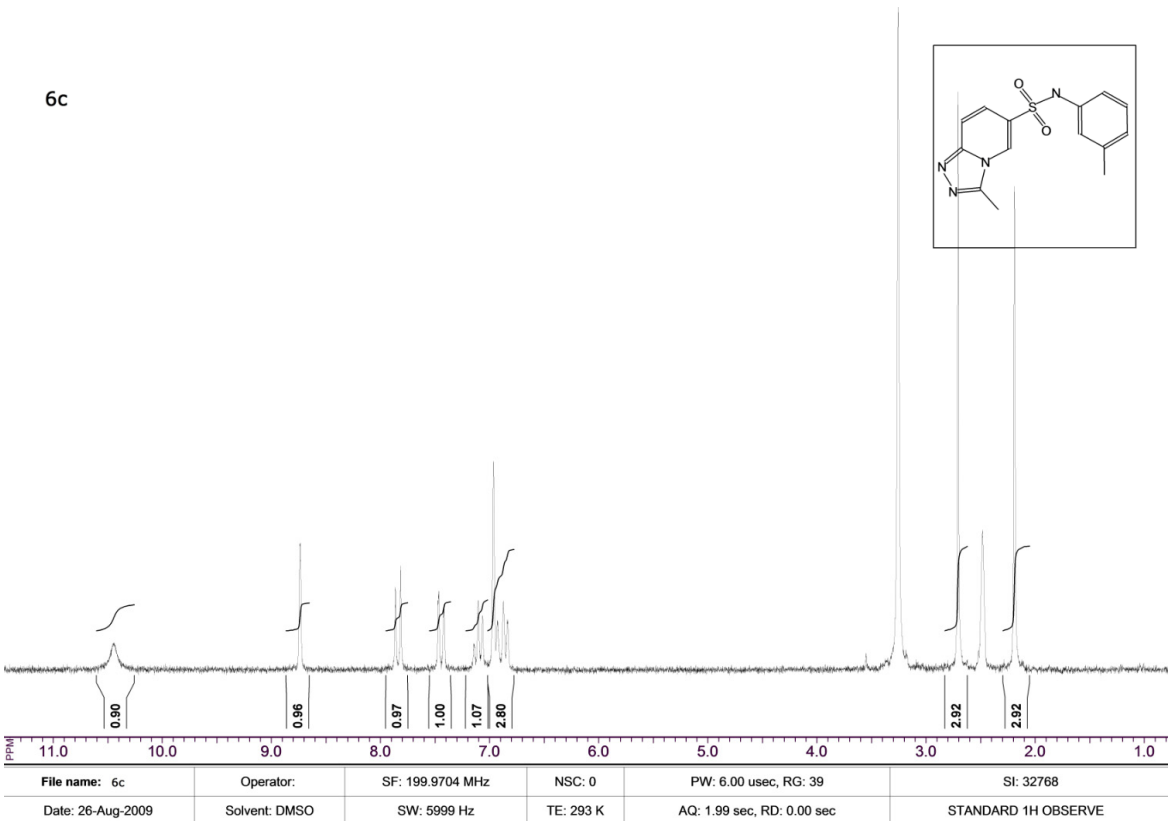


Figure S17. [1]H NMR spectrum (200 MHz, DMSO-d6) of 3-methyl-N-(3-methyphenyl)-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **6c**.

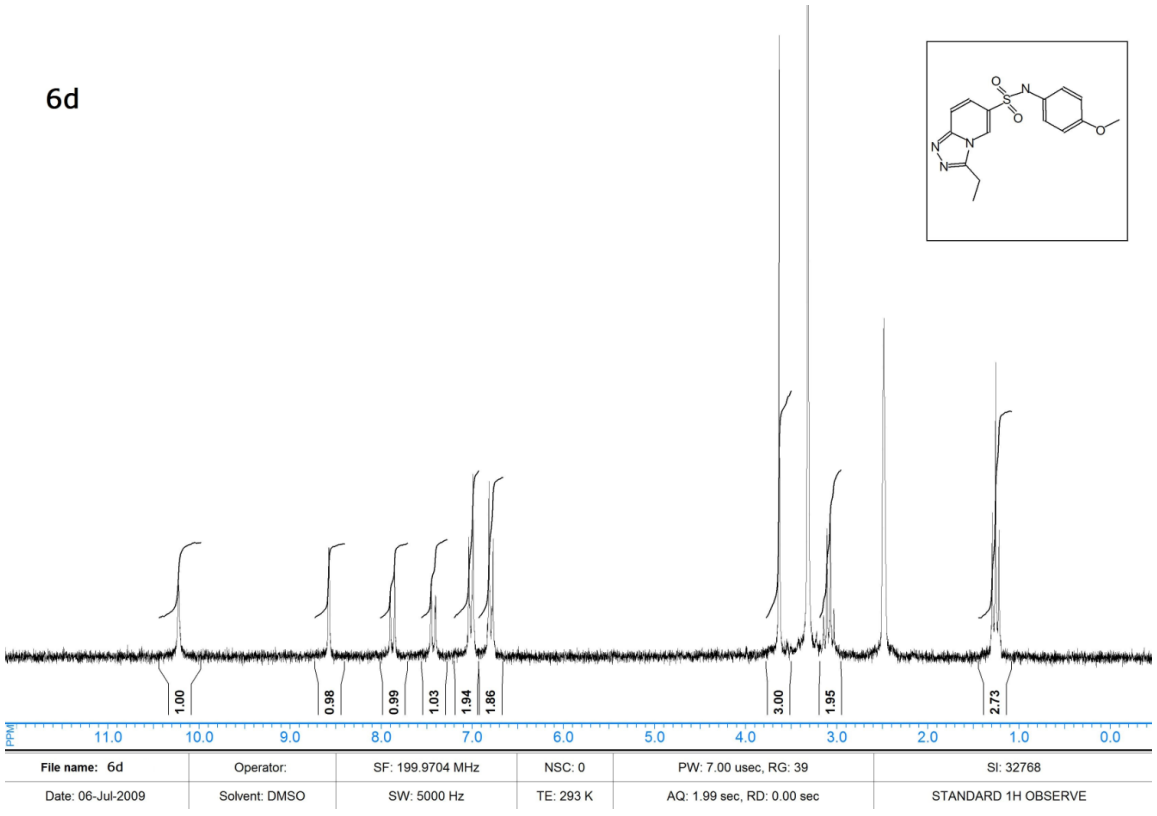


Figure S18. [1]H NMR spectrum (200 MHz, DMSO-d6) of 3-ethyl-N-(4-methoxyphenyl)-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **6d**.

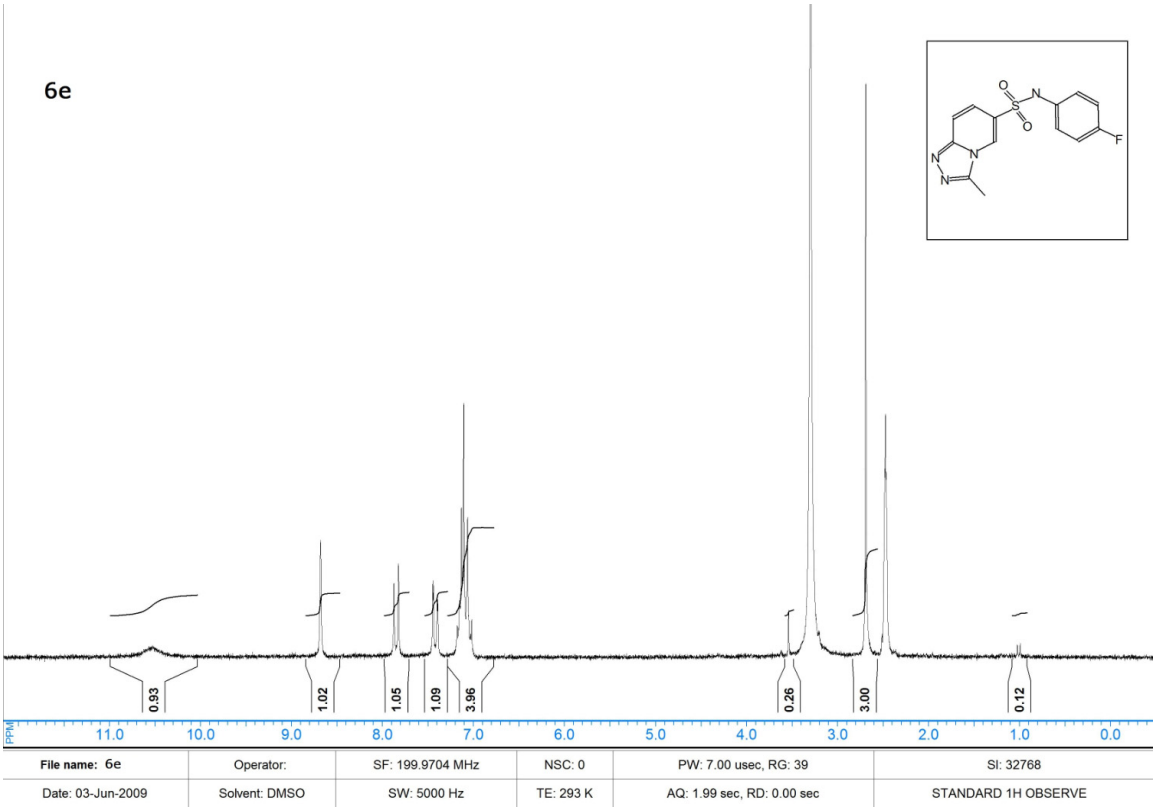


Figure S19. ^{1}H NMR spectrum (200 MHz, DMSO-d6) of N-(4-fluorophenyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **6e**.

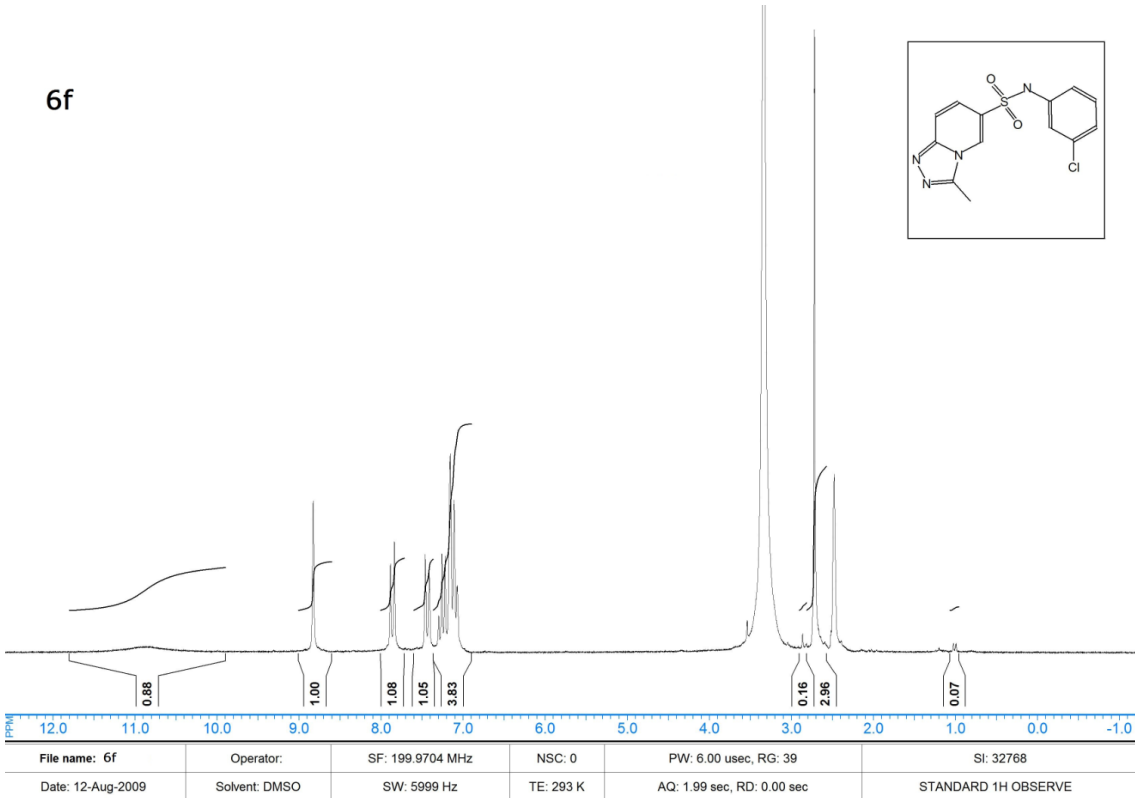


Figure S20. ^{1}H NMR spectrum (200 MHz, DMSO-d6) of N-(3-chlorophenyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **6f**.

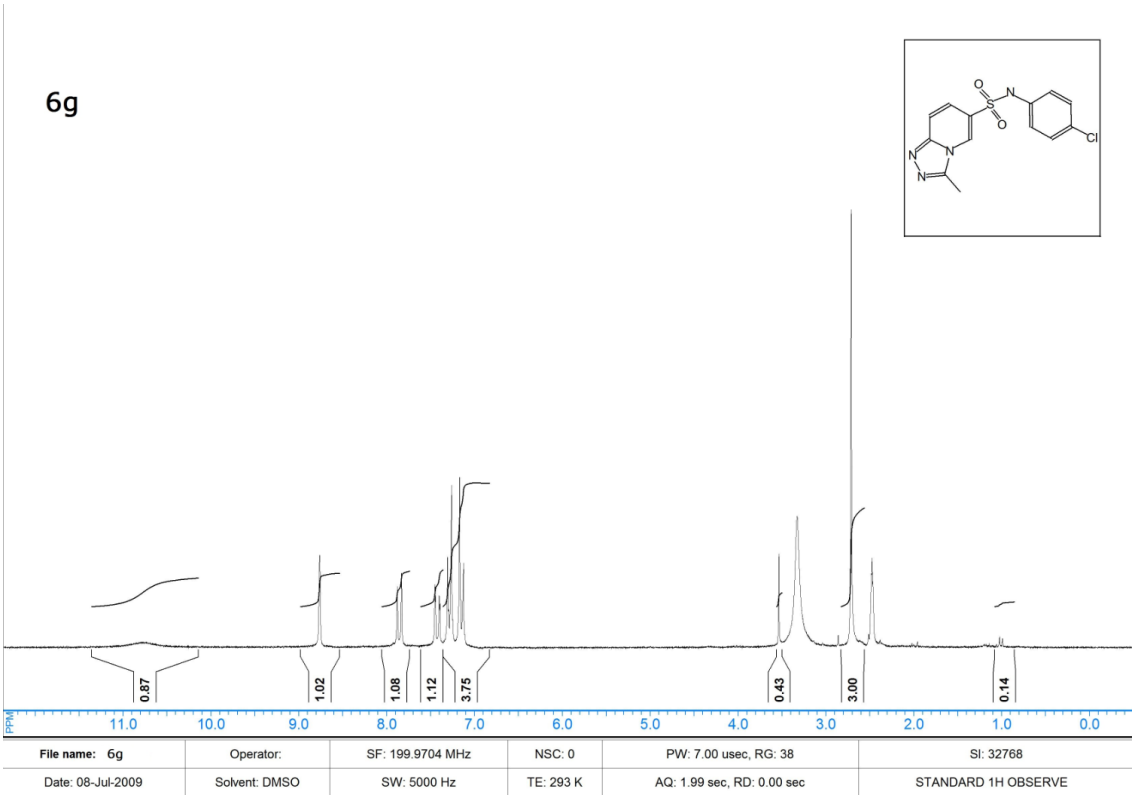


Figure S21. [1]H NMR spectrum (200 MHz, DMSO-d6) of N-(4-chlorophenyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **6g**.

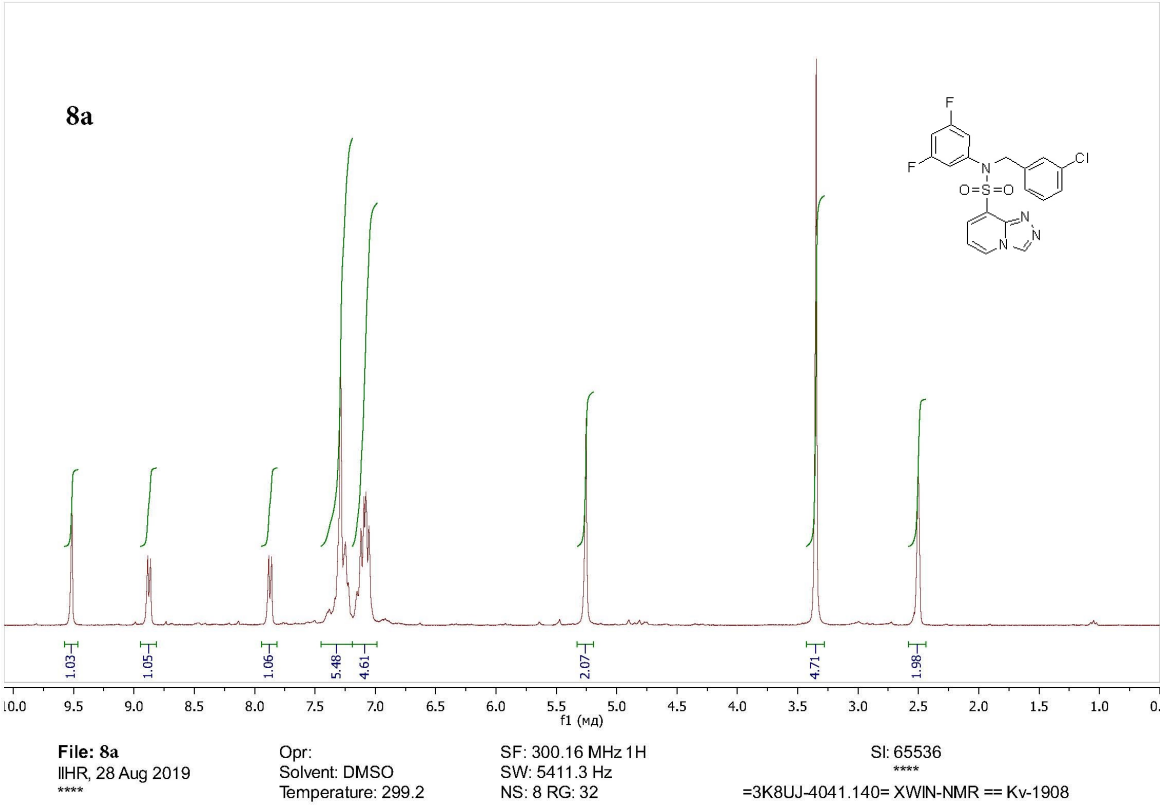


Figure S22. [1]H NMR spectrum (300 MHz, DMSO-d6) of N-(3-chlorobenzyl)-N-(3,5-difluorophenyl)-[1,2,4]triazolo[4,3-a]pyridine-8-sulfonamide **8a**.

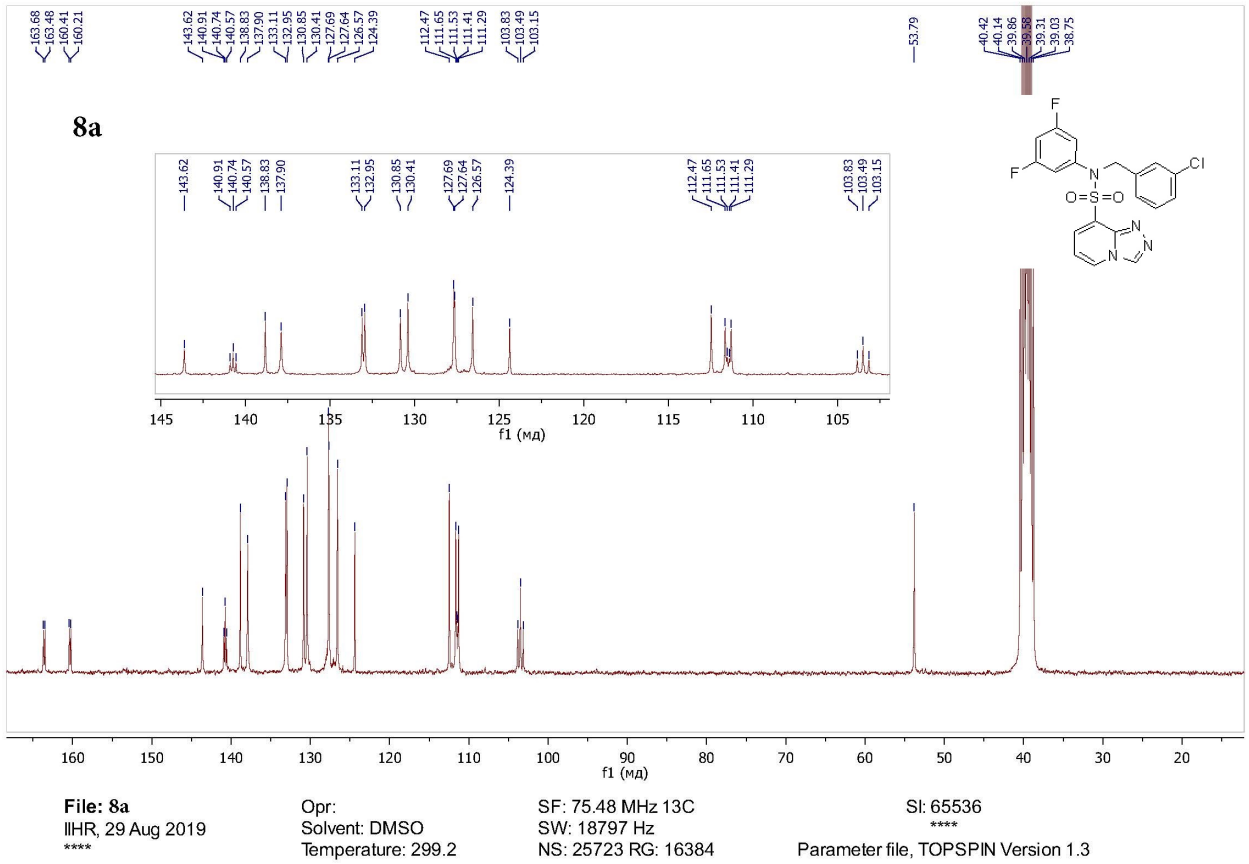


Figure S23. ^{13}C NMR spectrum (75 MHz, DMSO-d6) of N-(3-chlorobenzyl)-N-(3,5-difluorophenyl)-[1,2,4]triazolo[4,3-a]pyridine-8-sulfonamide **8a**.

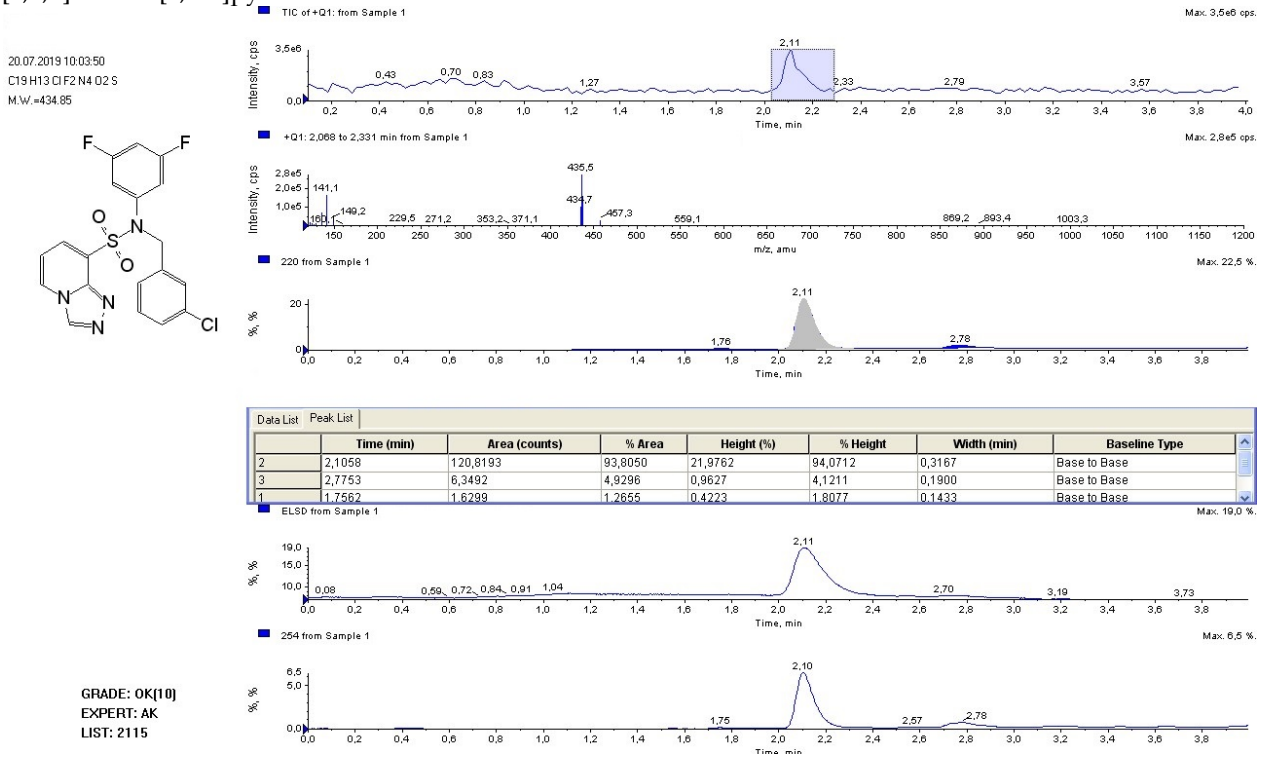


Figure S24. LC/MS data for N-(3-chlorobenzyl)-N-(3,5-difluorophenyl)-[1,2,4]triazolo[4,3-a]pyridine-8-sulfonamide **8a**.

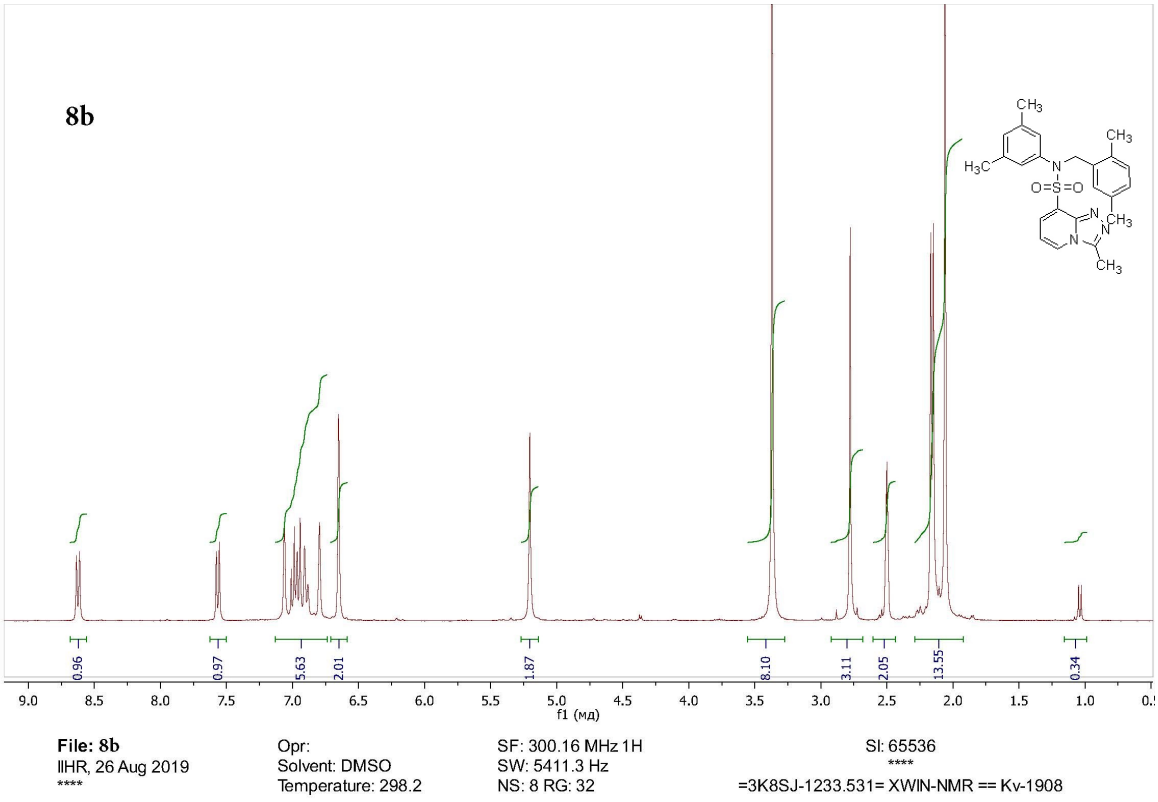


Figure S25. [1]H NMR spectrum (300 MHz, DMSO-d6) of N-(2,5-dimethylbenzyl)-N-(3,5-dimethylphenyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-8-sulfonamide **8b**.

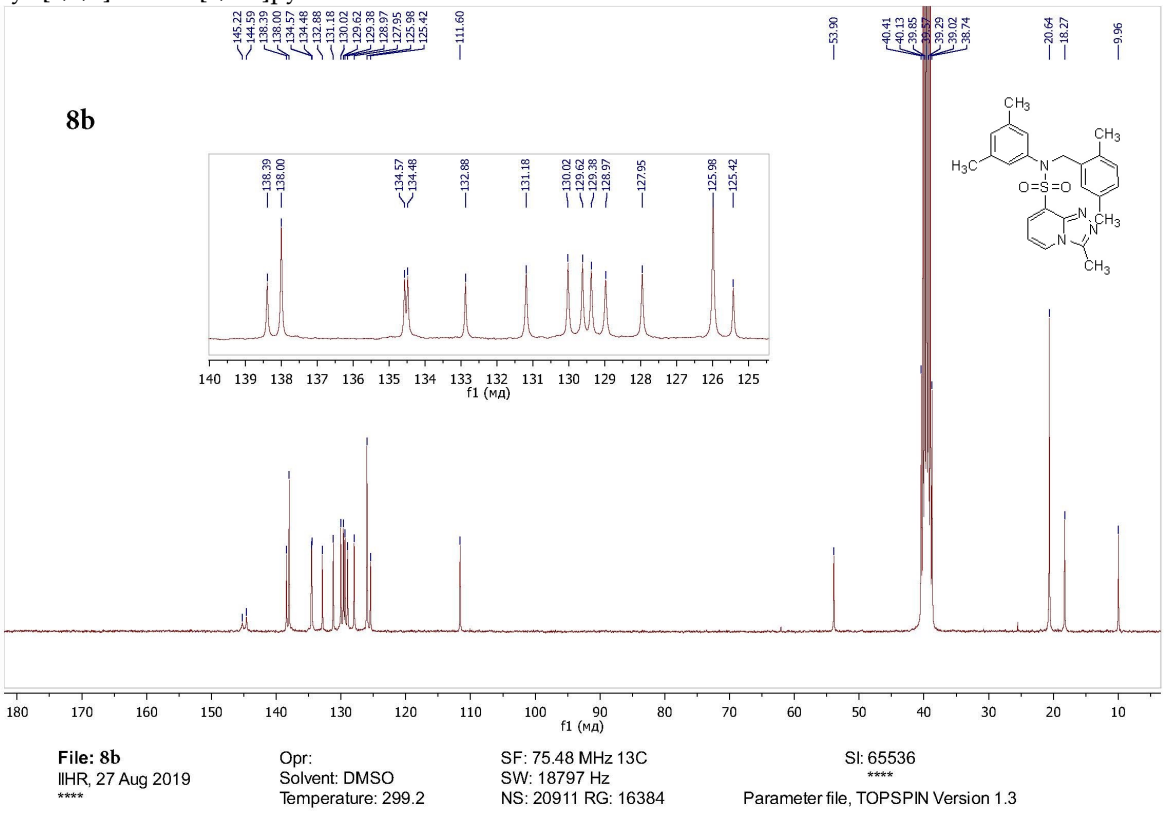


Figure S26. [13]C NMR spectrum (75 MHz, DMSO-d6) of N-(2,5-dimethylbenzyl)-N-(3,5-dimethylphenyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-8-sulfonamide **8b**.

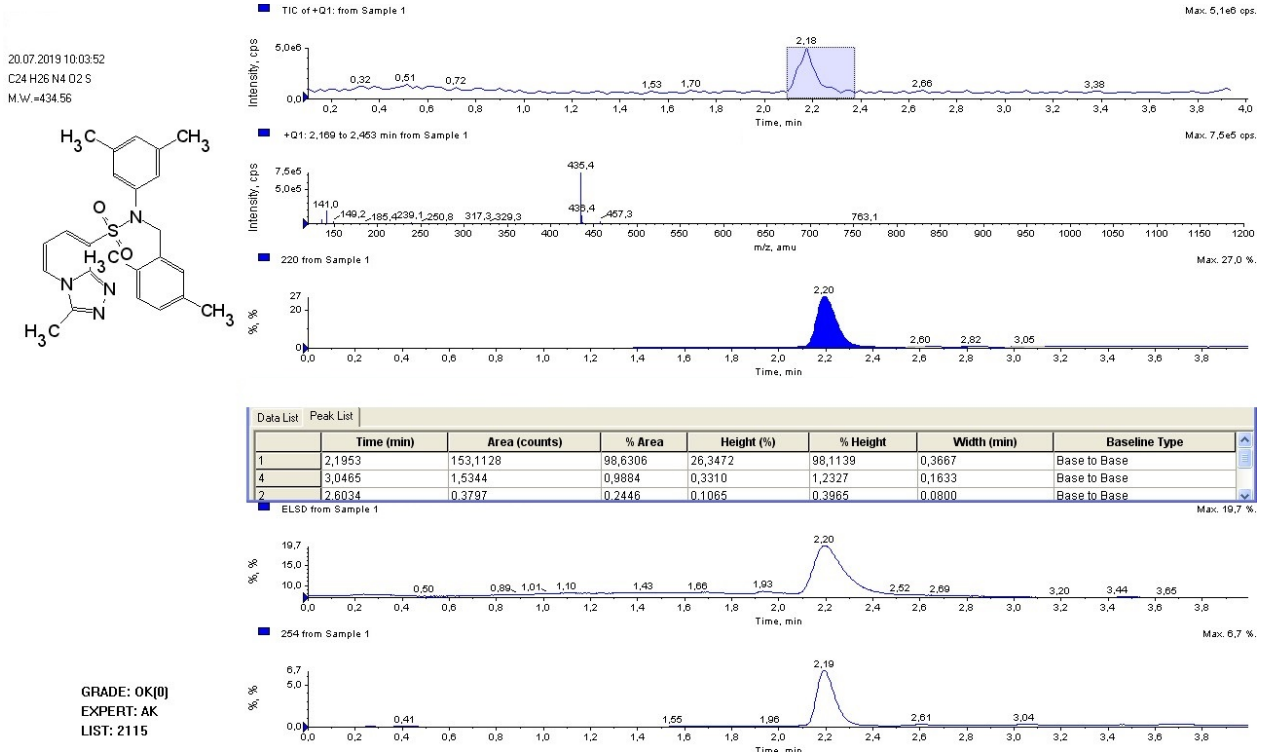


Figure S27. LC/MS data for N-(2,5-dimethylbenzyl)-N-(3,5-dimethylphenyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-8-sulfonamide **8b**.

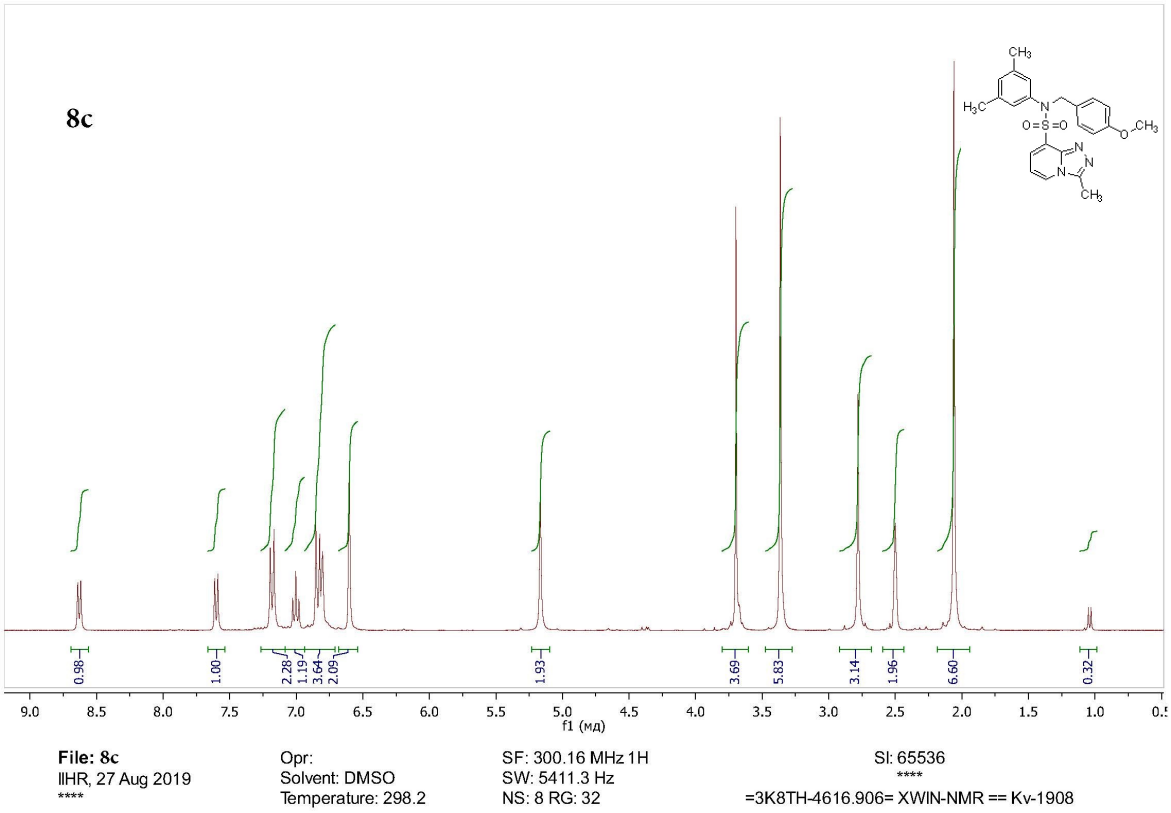


Figure S28. ^{1}H NMR spectrum (300 MHz, DMSO-d6) of N-(3,5-dimethylphenyl)-N-(4-methoxybenzyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-8-sulfonamide **8c**.

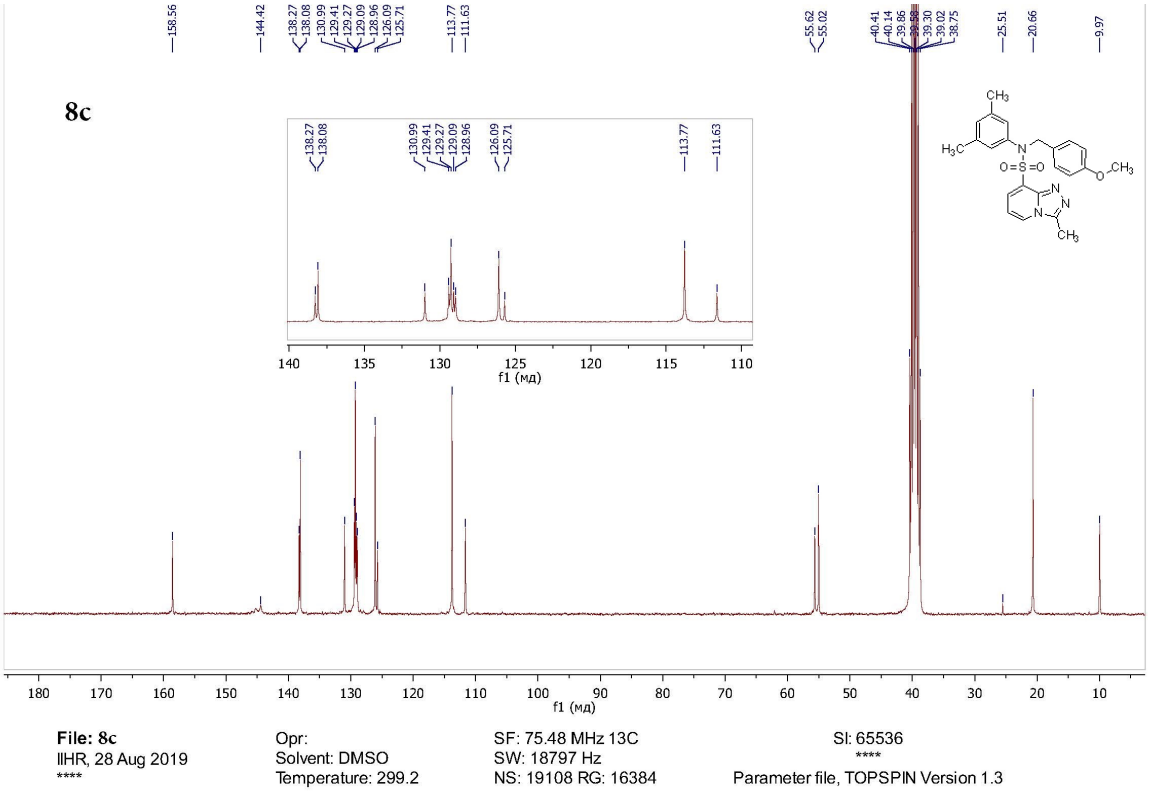


Figure S29. ^{13}C NMR spectrum (75 MHz, DMSO-d6) of N-(3,5-dimethylphenyl)-N-(4-methoxybenzyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-8-sulfonamide **8c**.

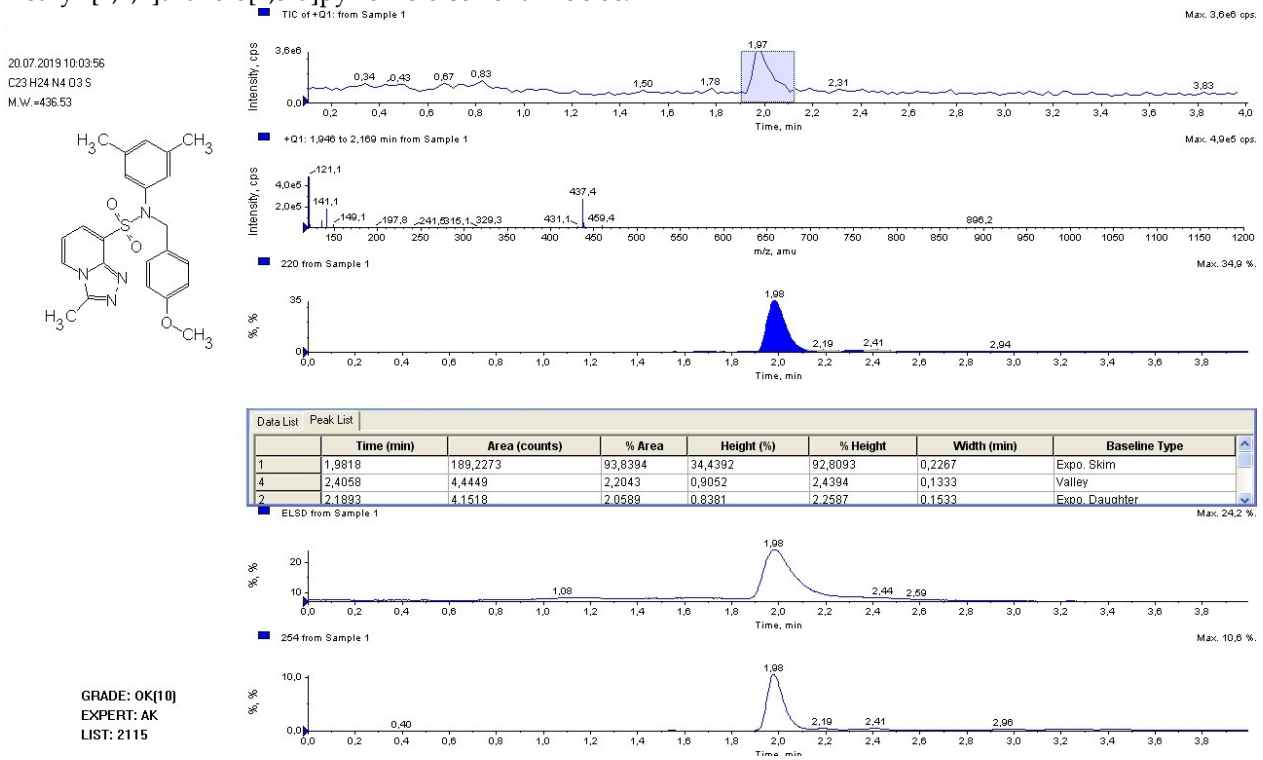


Figure S30. LC/MS data for N-(3,5-dimethylphenyl)-N-(4-methoxybenzyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-8-sulfonamide **8c**.

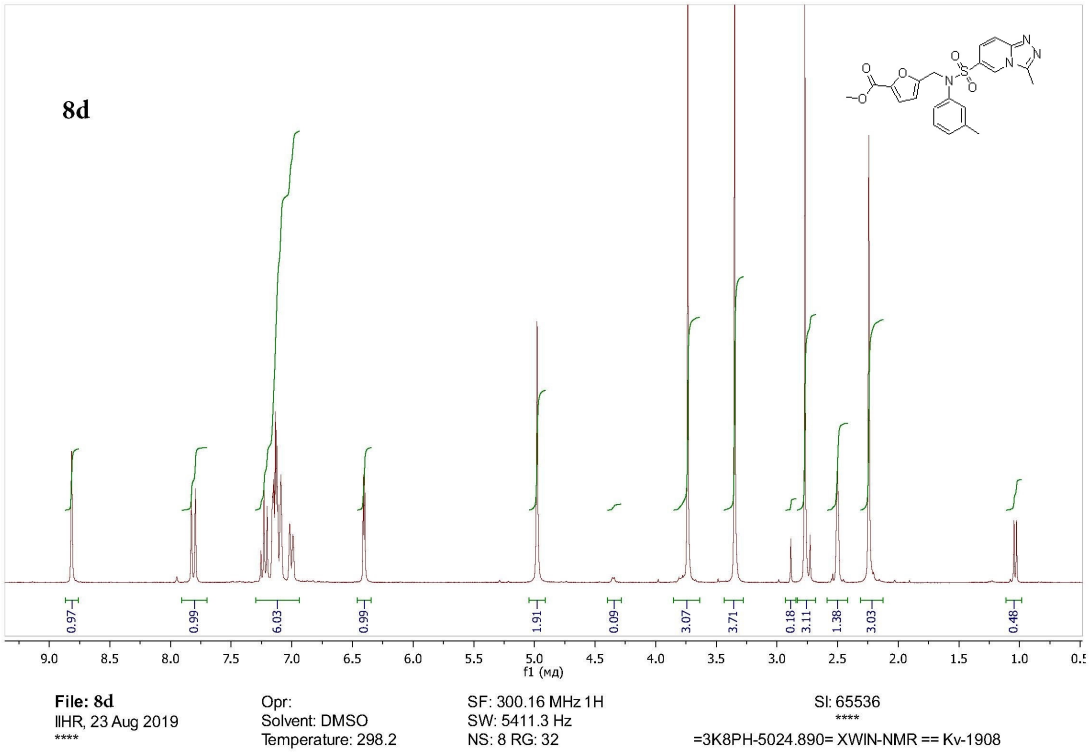


Figure S31. [1]H NMR spectrum (300 MHz, DMSO-d6) of Methyl 5-{[3-methyl-N-(3-methylphenyl)-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamido]methyl}furan-2-carboxylate **8d**.

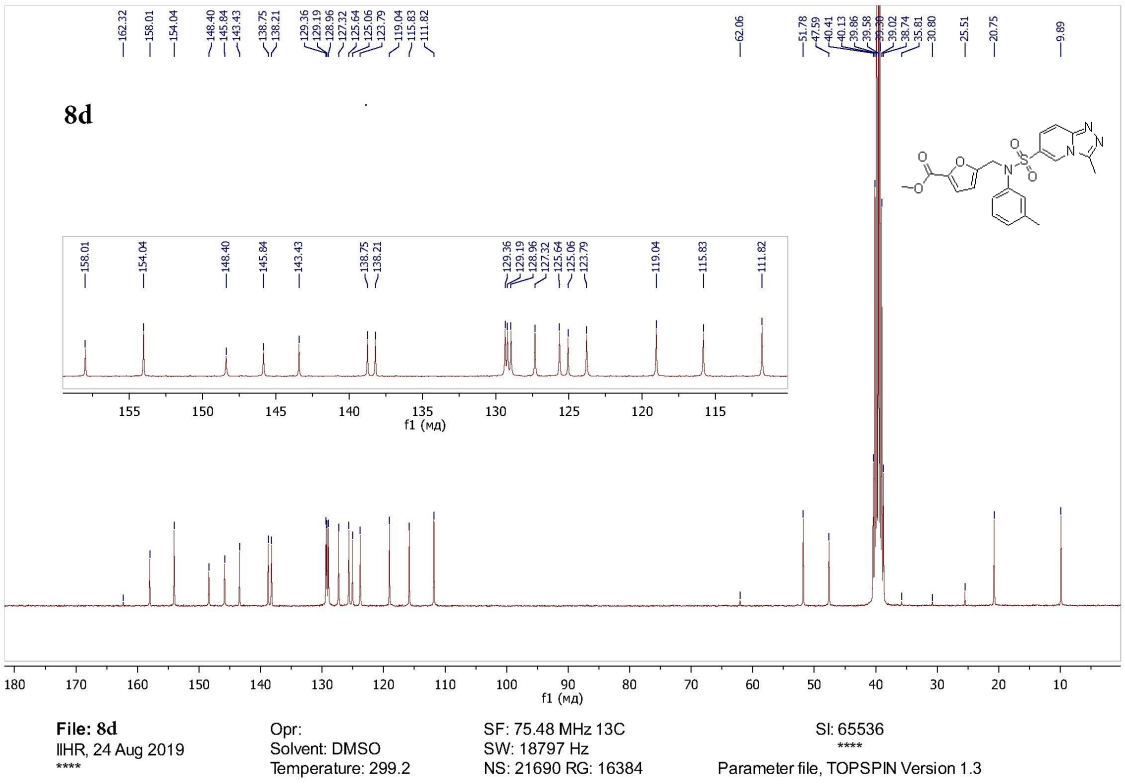


Figure S32. [13]C NMR spectrum (75 MHz, DMSO-d6) of Methyl 5-{[3-methyl-N-(3-methylphenyl)-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamido]methyl}furan-2-carboxylate **8d**.

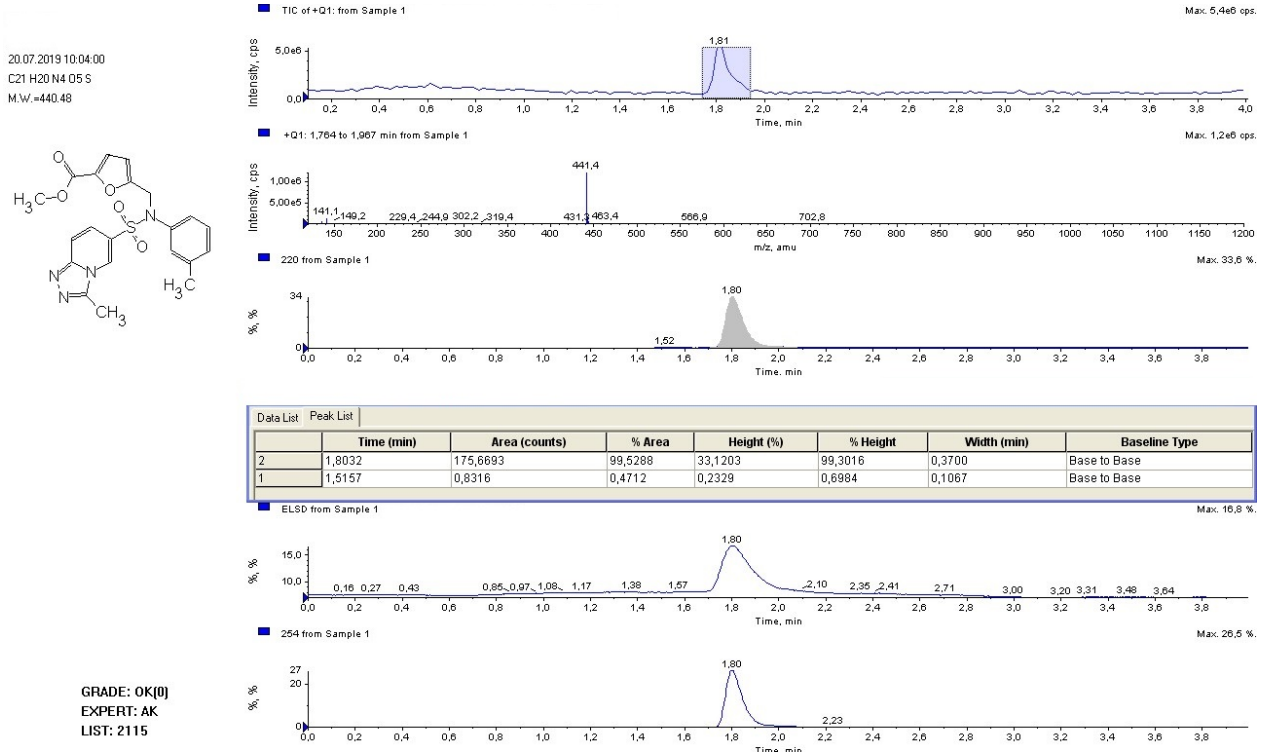


Figure S33. LC/MS data for Methyl 5-{[3-methyl-N-(3-methylphenyl)-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamido]methyl}furan-2-carboxylate **8d**.

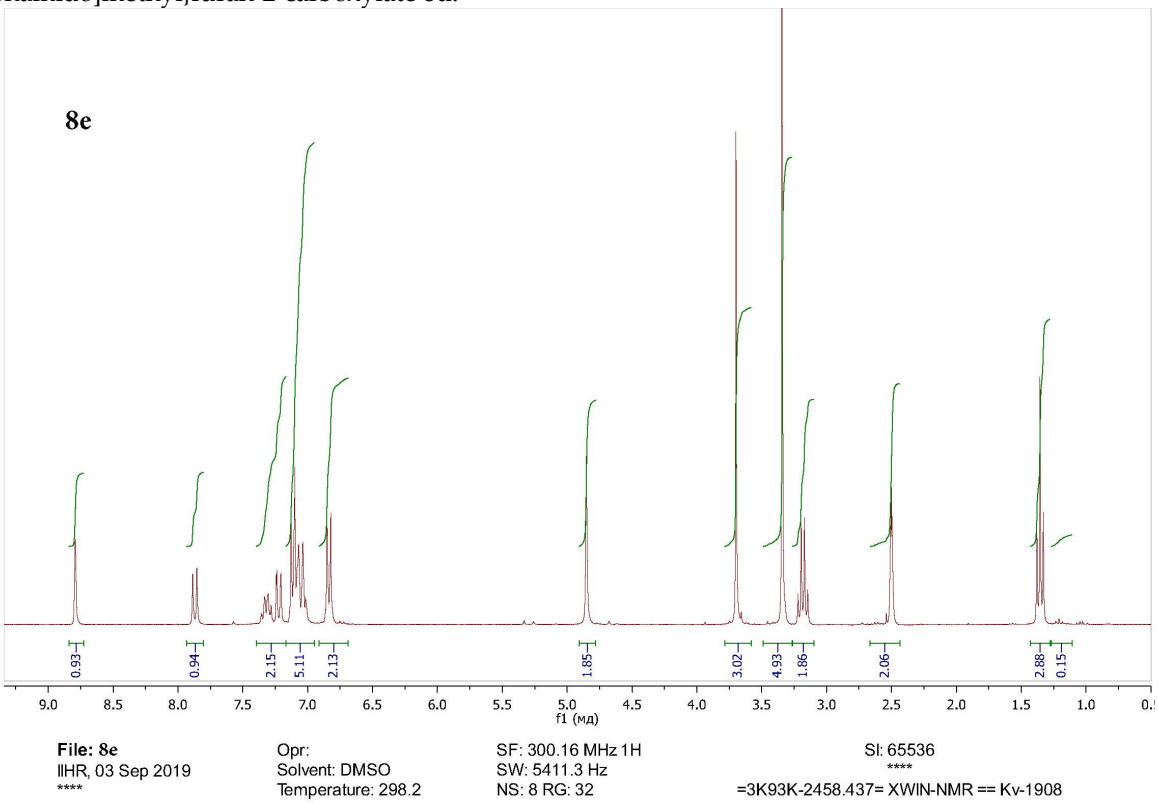


Figure S34. ^{1}H NMR spectrum (300 MHz, DMSO-d6) of 3-Ethyl-N-(3-fluorobenzyl)-N-(4-methoxyphenyl)-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8e**.

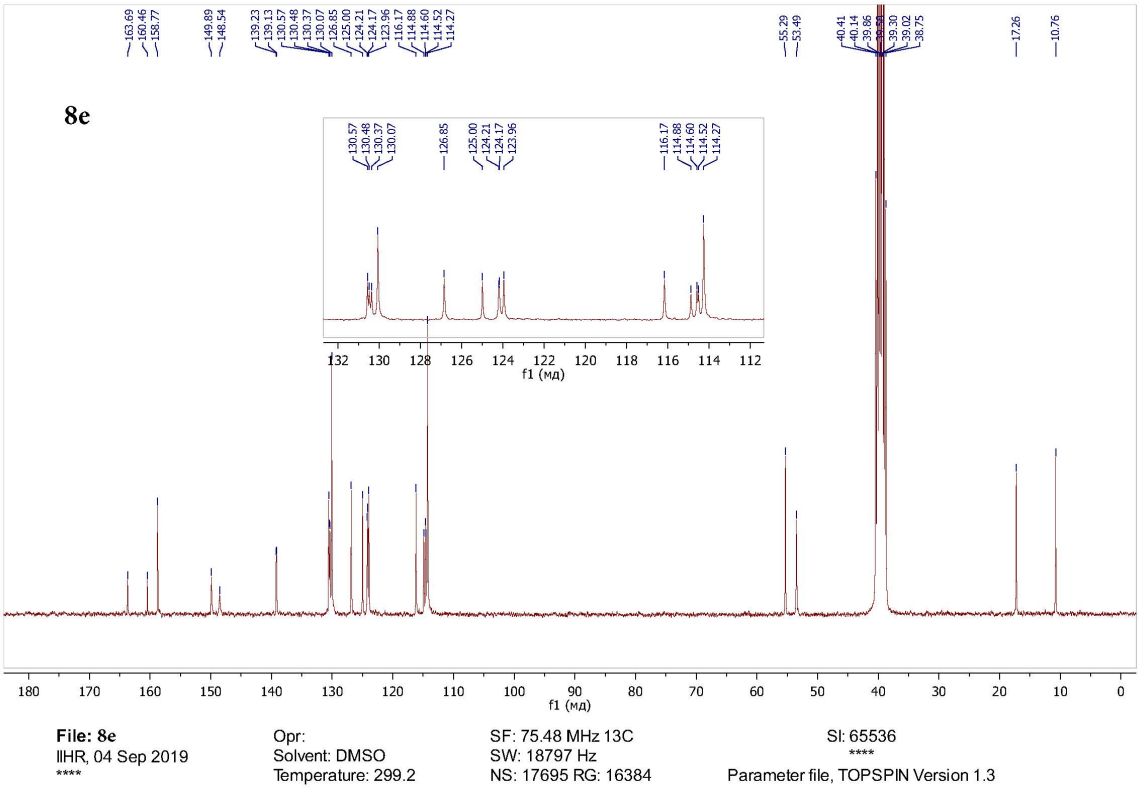
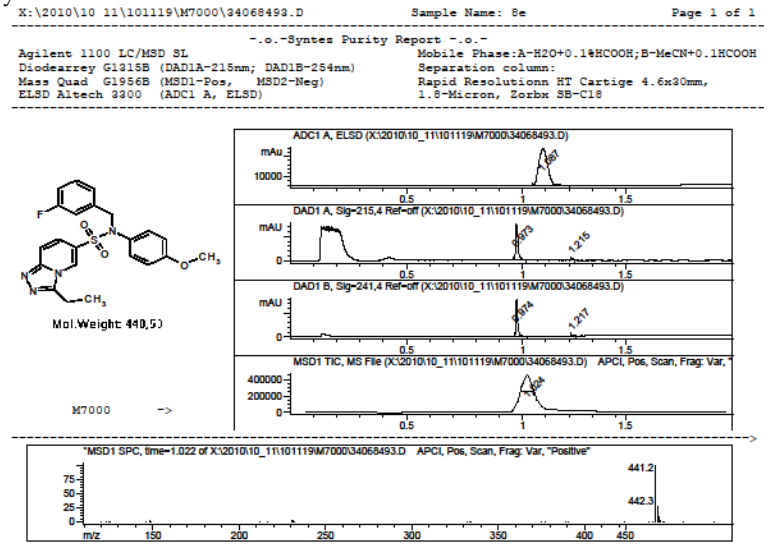


Figure S35. ^{13}C NMR spectrum (75 MHz, DMSO-d6) of 3-Ethyl-N-(3-fluorobenzyl)-N-(4-methoxyphenyl)-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8e**.



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2		1.217	2.177

#	Signal	R.Time	Area %
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Figure S36. LC/MS data for 3-Ethyl-N-(3-fluorobenzyl)-N-(4-methoxyphenyl)-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8e**.

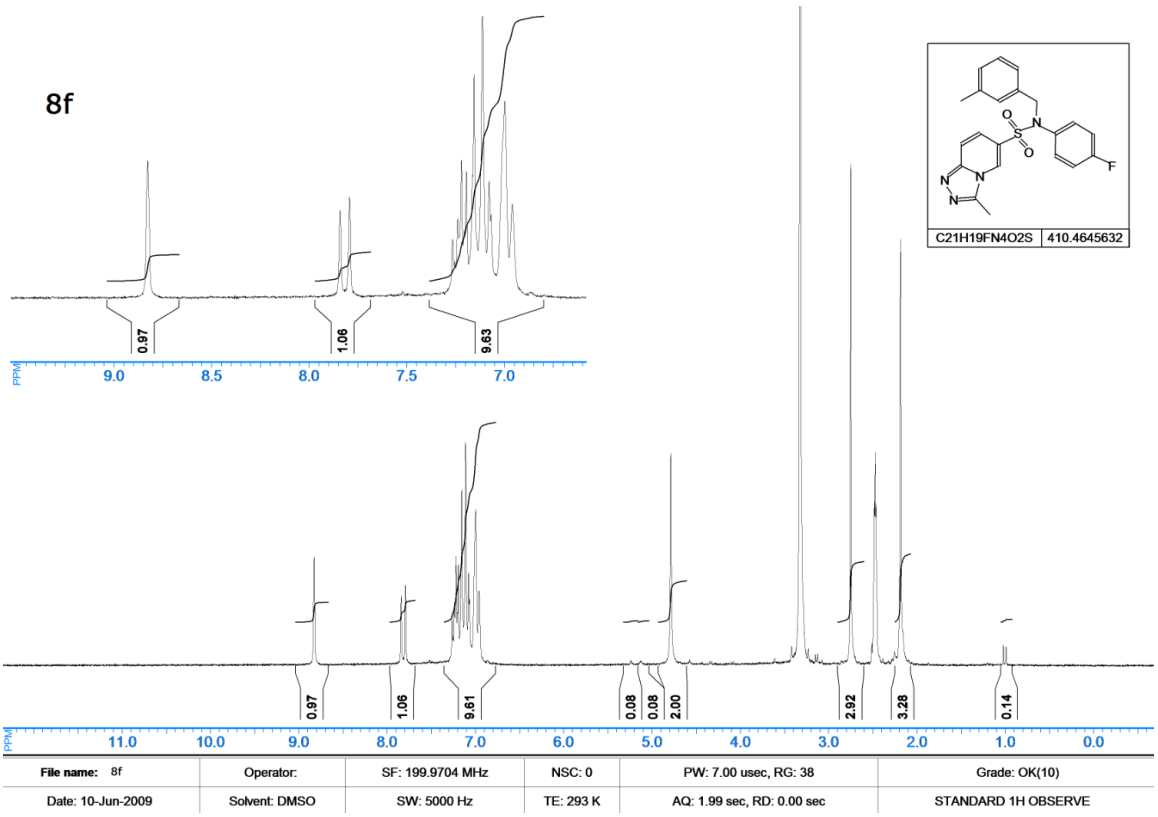

Figure S37. [1]H NMR spectrum (200 MHz, DMSO-d6) of N-(4-fluorophenyl)-3-methyl-N-(3-methylbenzyl)-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8f**.

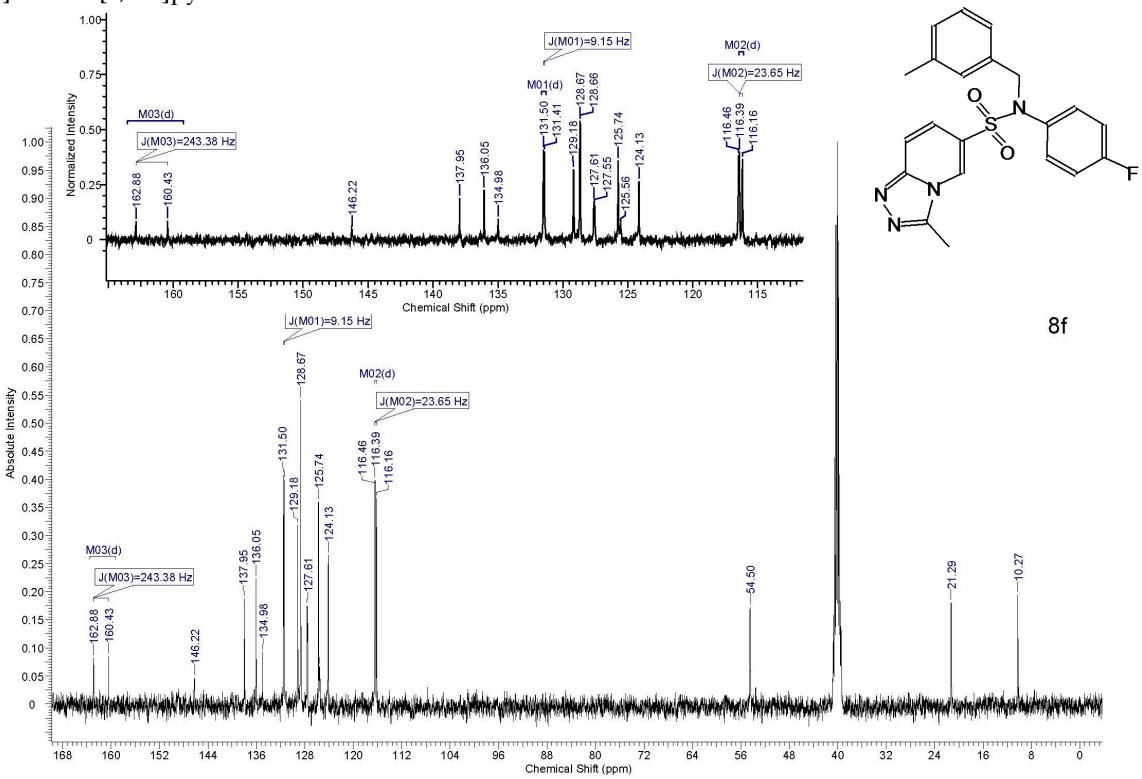

Figure S38. [13]C NMR spectrum (100 MHz, DMSO-d6) of N-(4-fluorophenyl)-3-methyl-N-(3-methylbenzyl)-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8f**.

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

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Diodearrey G1315B (DAD1A-215nm; DAD1B-254nm)
Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

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Separation column:
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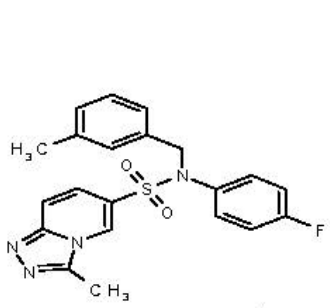
1.8-Micron, Zorbx SB-C18



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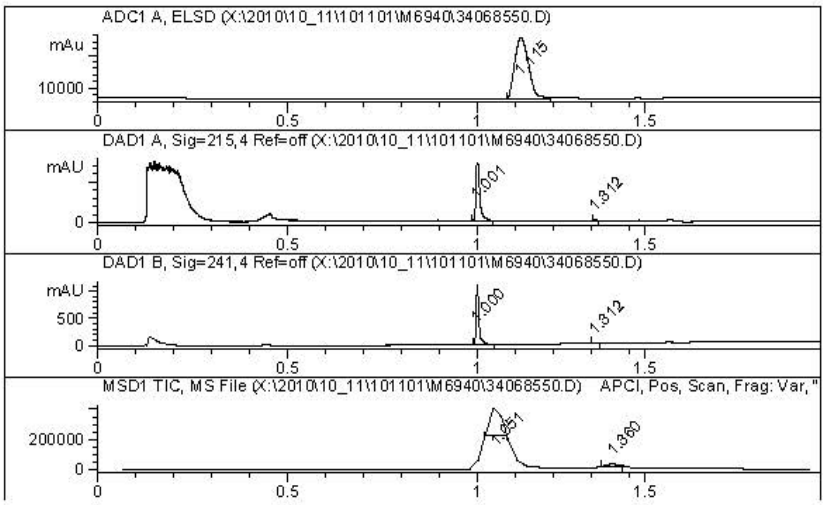

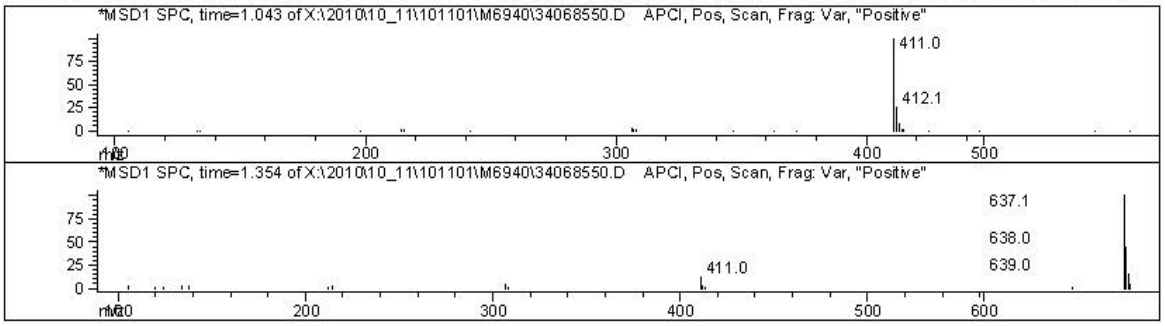

#	Signal	R.Time	Area %
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#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	1.001	98.000
2		1.312	2.000

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	1.000	98.392
2		1.312	1.608

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.051	91.905
2		1.360	8.095

Figure S39. LC/MS data for N-(4-fluorophenyl)-3-methyl-N-(3-methylbenzyl)-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8f**.

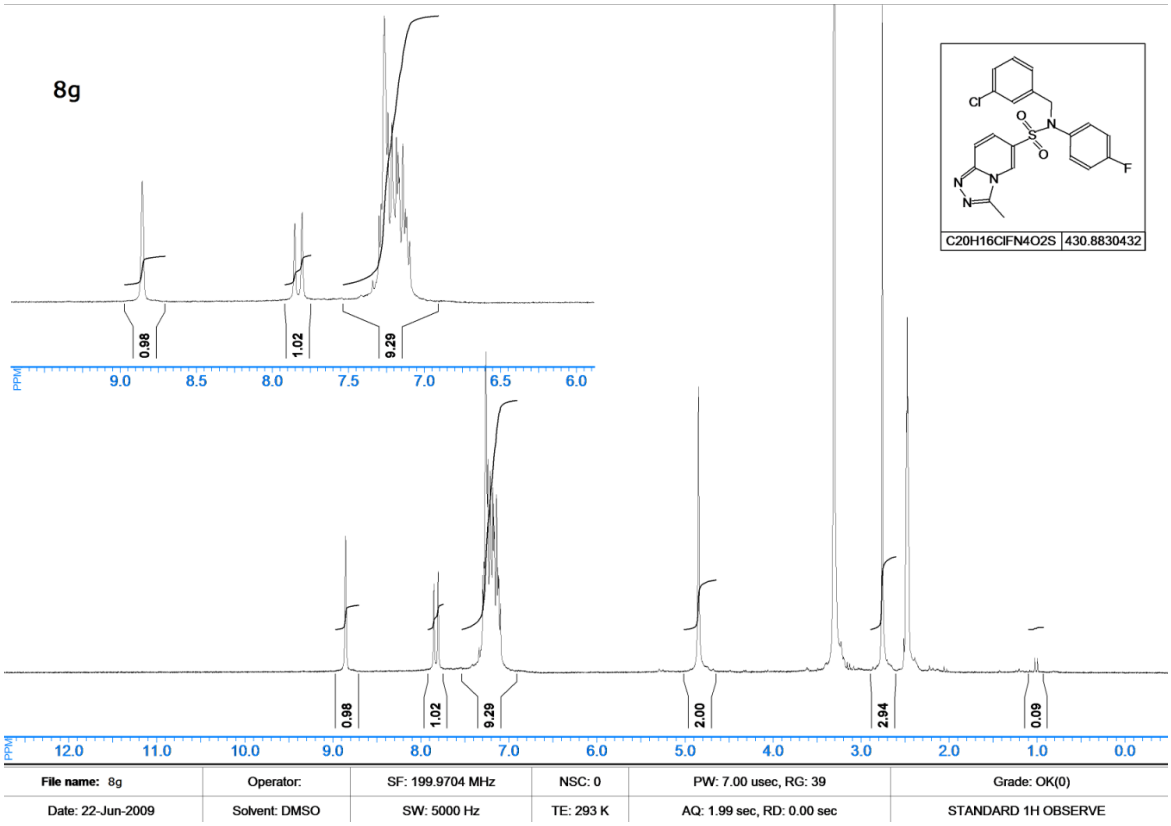


Figure S40. [1]H NMR spectrum (200 MHz, DMSO-d6) of N-(3-chlorobenzyl)-N-(4-fluorophenyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8g**.

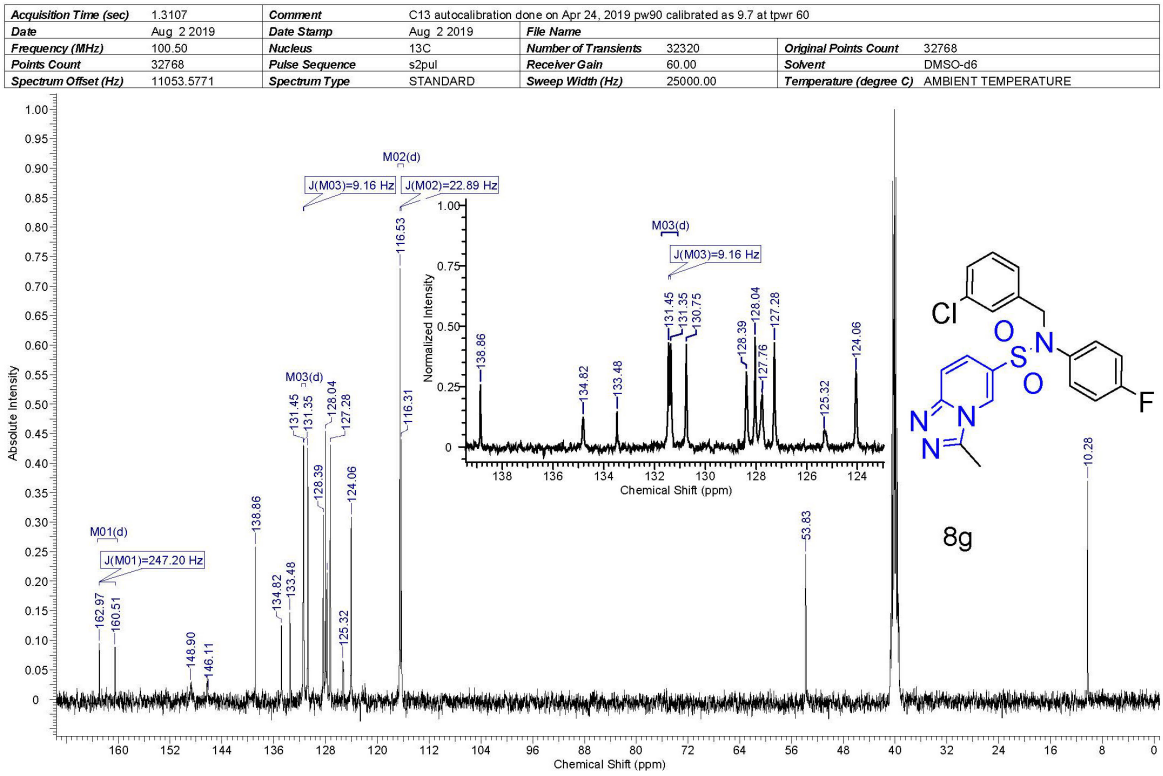


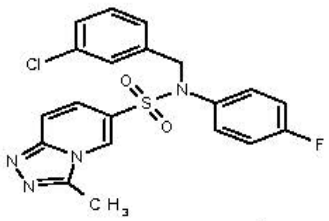
Figure S41. [13]C NMR spectrum (100 MHz, DMSO-d6) of N-(3-chlorobenzyl)-N-(4-fluorophenyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8g**.

X:\2010\10_11\101101\M6940\34068559.D Sample Name: 8g Page 1 of 1

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

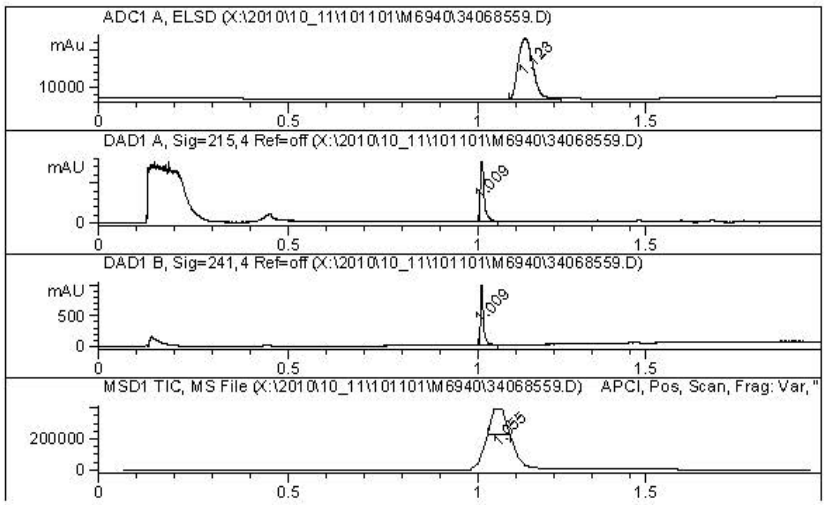
Agilent 1100 LC/MSD SL
Diodearrey G1315B (DAD1A-215nm; DAD1B-254nm)
Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

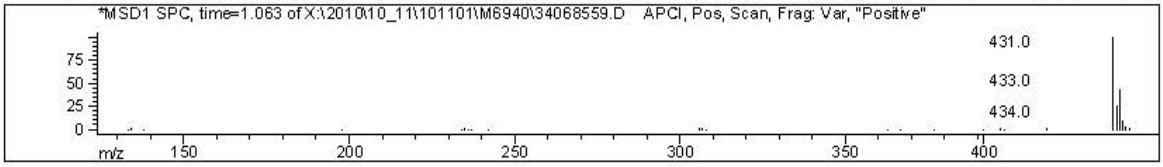
Mobile Phase:A-H2O+0.1%HCOOH;B-MeCN+0.1HCOOH
Separation column:
Rapid Resolutionn HT Cartige 4.6x30mm,
1.8-Micron, Zorbx SB-C18



Mol.Weight: 430,89

M6940 ->





#	Signal	R.Time	Area %
1	ADC1 A, ELSD	1.123	100.000

#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	1.009	100.000

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	1.009	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.055	100.000

Figure S42. LC/MS data for N-(3-chlorobenzyl)-N-(4-fluorophenyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8g**.

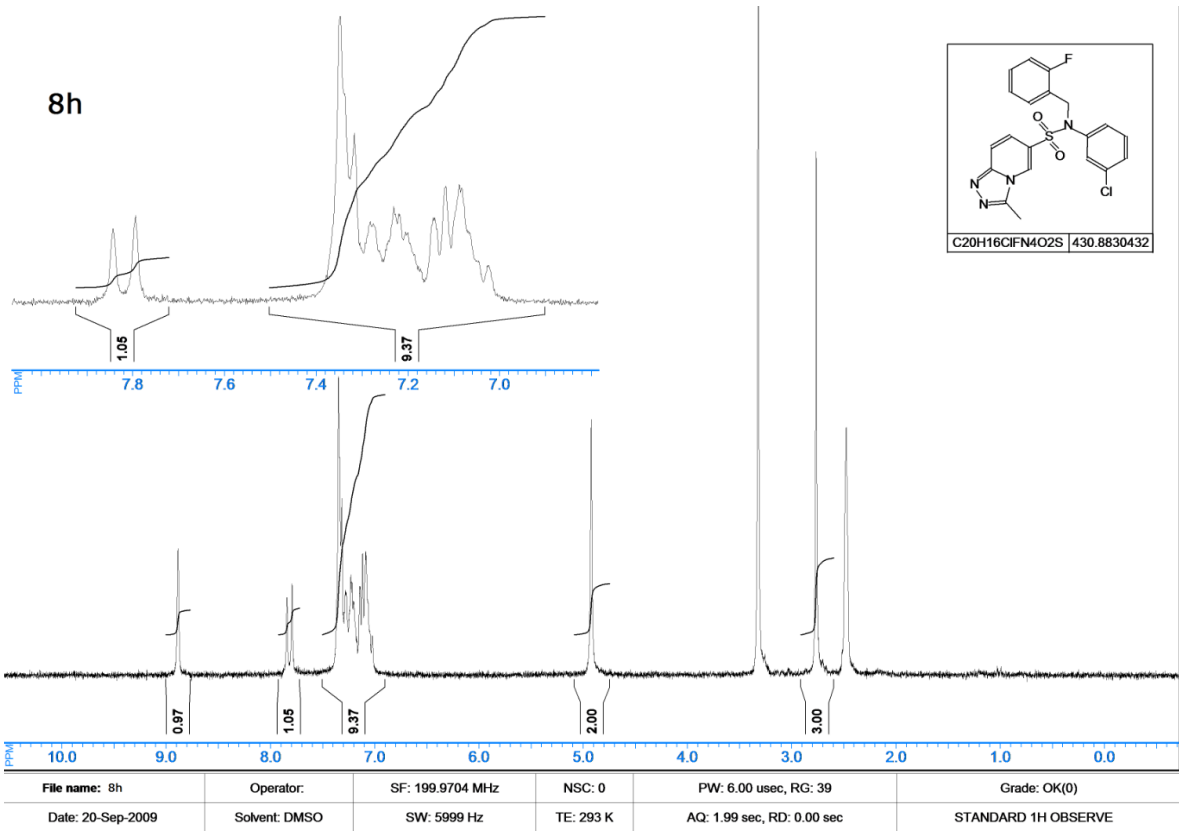


Figure S43. [1]H NMR spectrum (200 MHz, DMSO-d6) of N-(3-chlorophenyl)-N-(2-fluorobenzyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8h**.

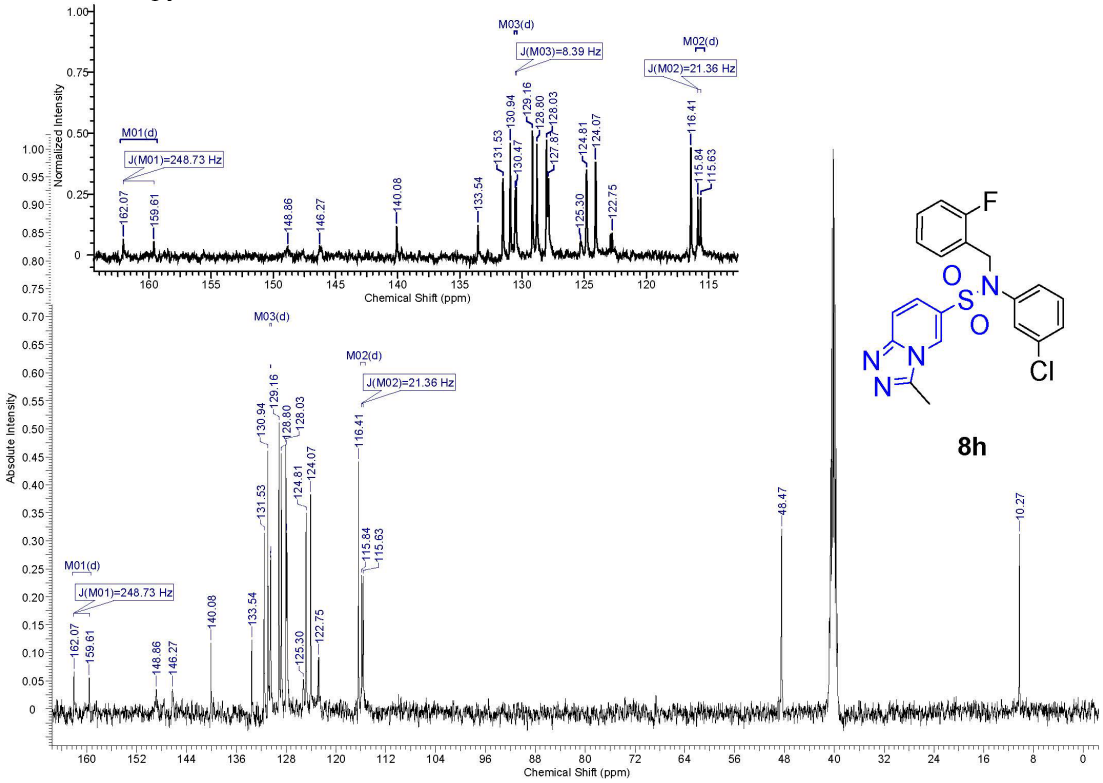


Figure S44. [13]C NMR spectrum (100 MHz, DMSO-d6) of N-(3-chlorophenyl)-N-(2-fluorobenzyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8h**.

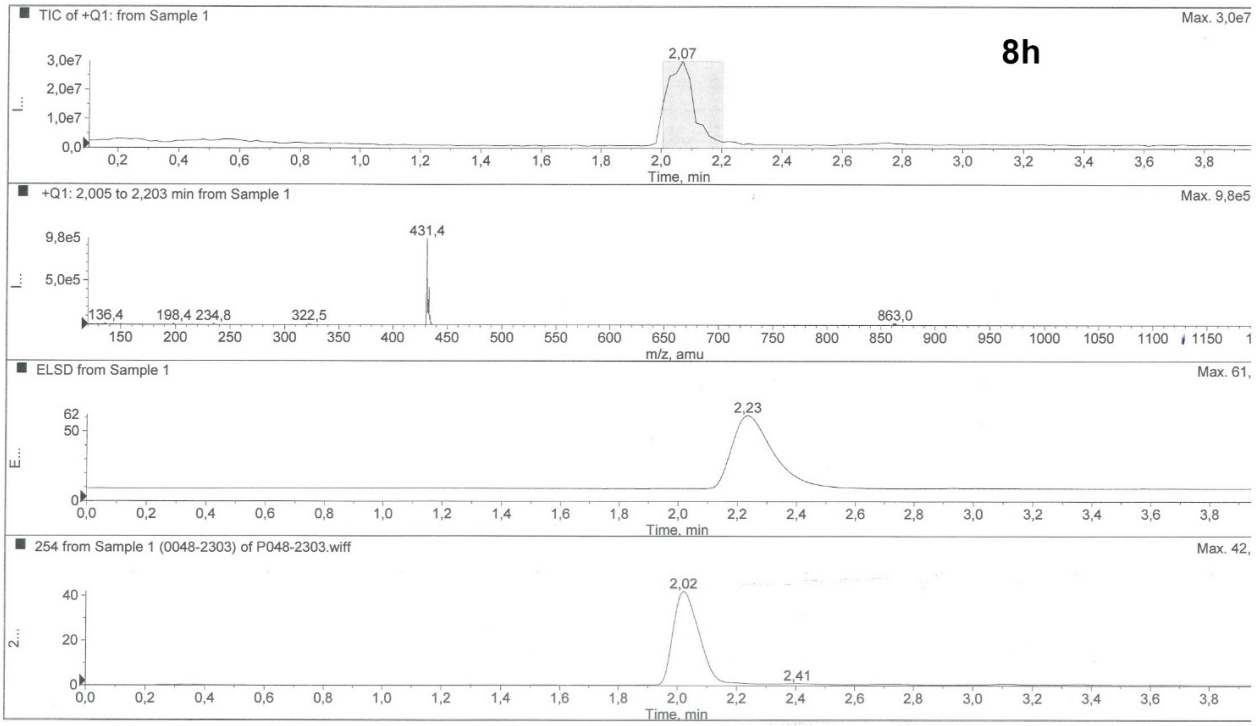


Figure S45. LC/MS data for N-(3-chlorophenyl)-N-(2-fluorobenzyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8h**.

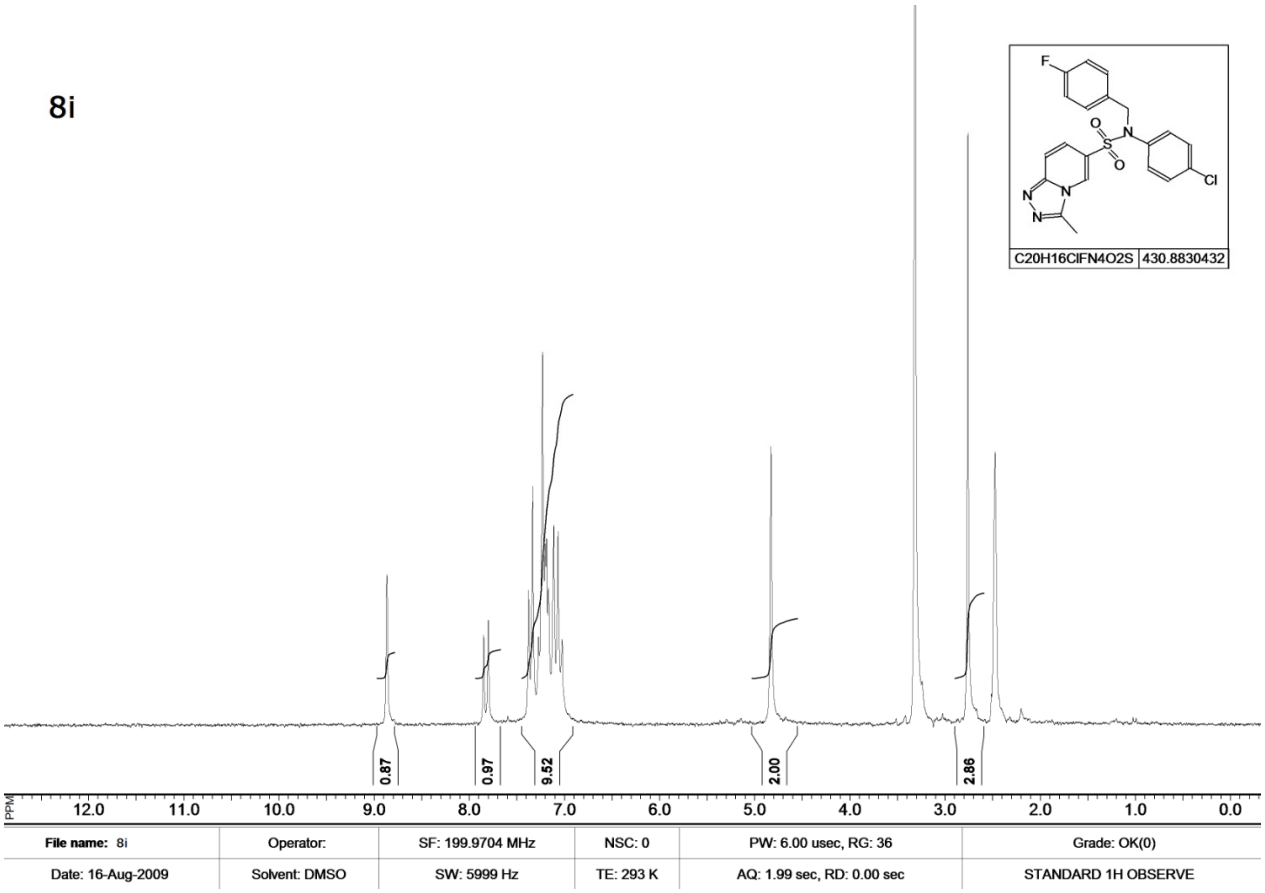


Figure S46. ^{1}H NMR spectrum (200 MHz, DMSO-d6) of N-(4-chlorophenyl)-N-(4-fluorobenzyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8i**.

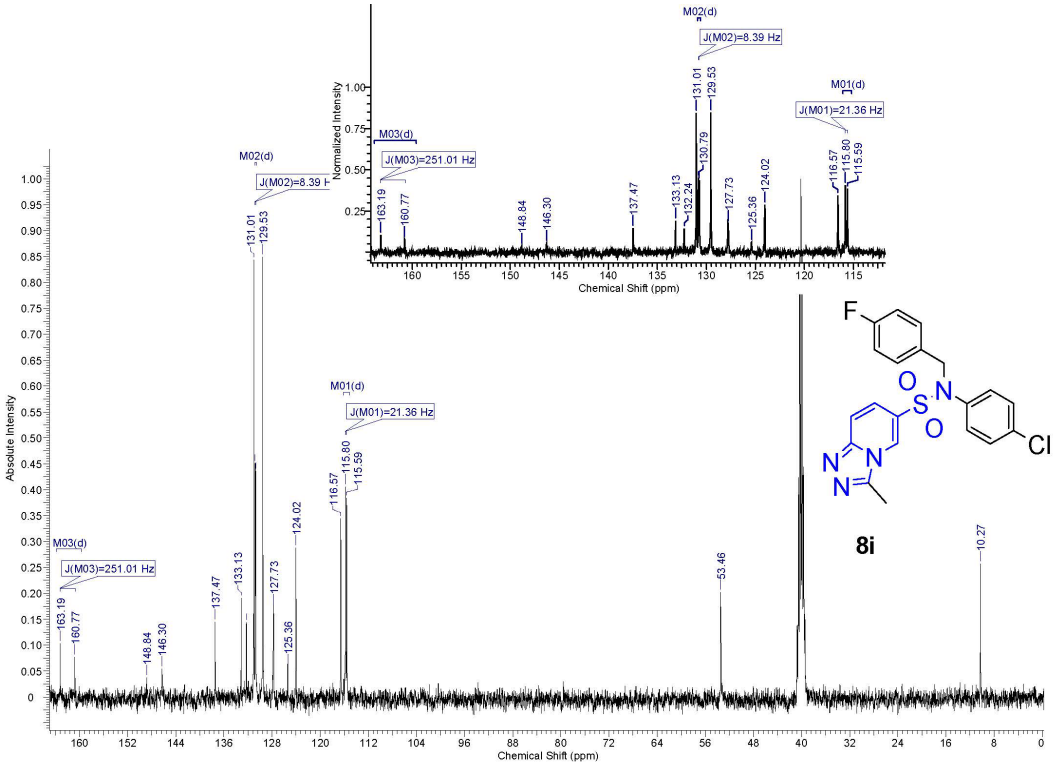
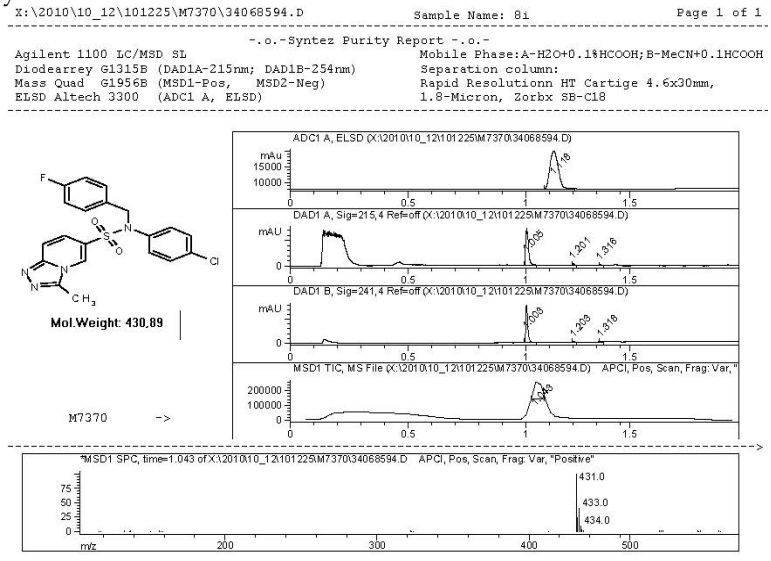


Figure S47. ^{13}C NMR spectrum (100 MHz, DMSO-d6) of N-(4-chlorophenyl)-N-(4-fluorobenzyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8i**



#	Signal	R.Time	Area %
1	ADC1 A, ELSD	1.118	100.000

#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	1.005	95.670
2		1.201	2.385
3		1.316	1.945

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	1.003	96.801
2		1.203	1.994
3		1.318	1.206

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.043	100.000

Figure S48. LC/MS data for N-(4-chlorophenyl)-N-(4-fluorobenzyl)-3-methyl-[1,2,4]triazolo[4,3-a]pyridine-6-sulfonamide **8i.**

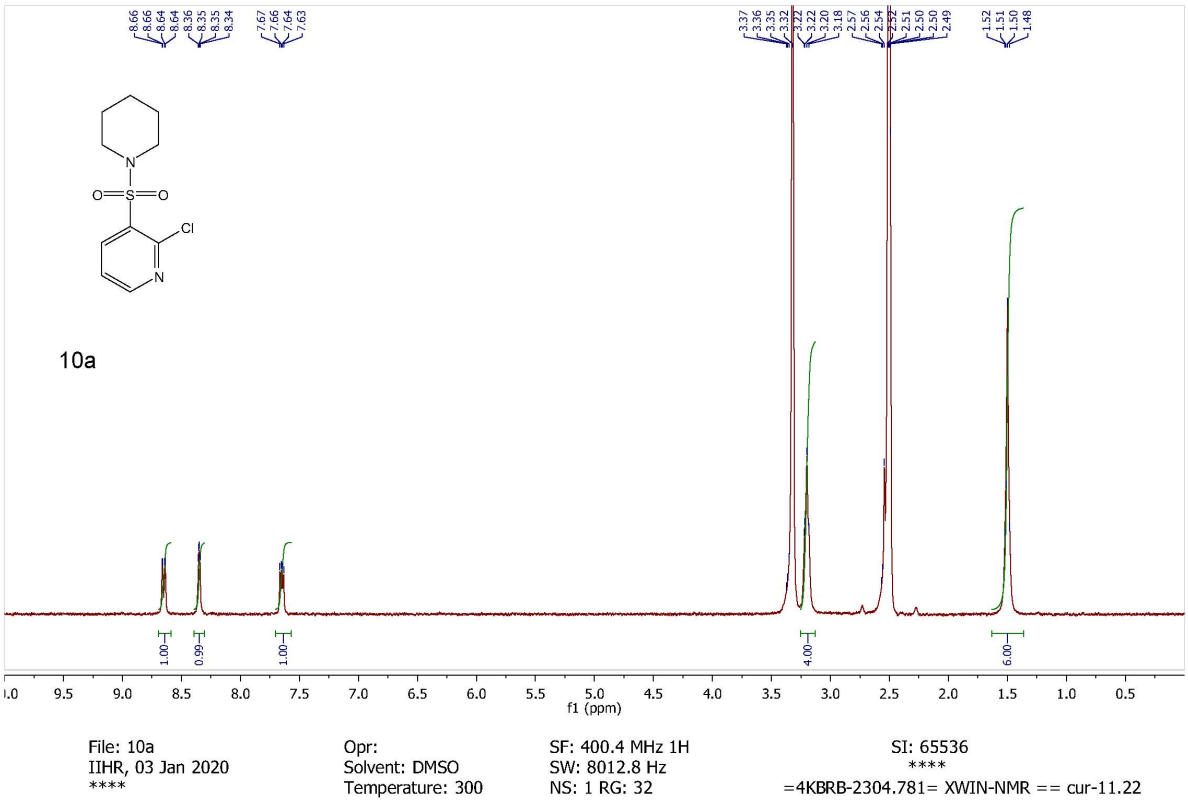


Figure S49. [1]H NMR spectrum (400 MHz, DMSO-d6) of 2-chloro-3-(piperidin-1-ylsulfonyl)pyridine **10a**.

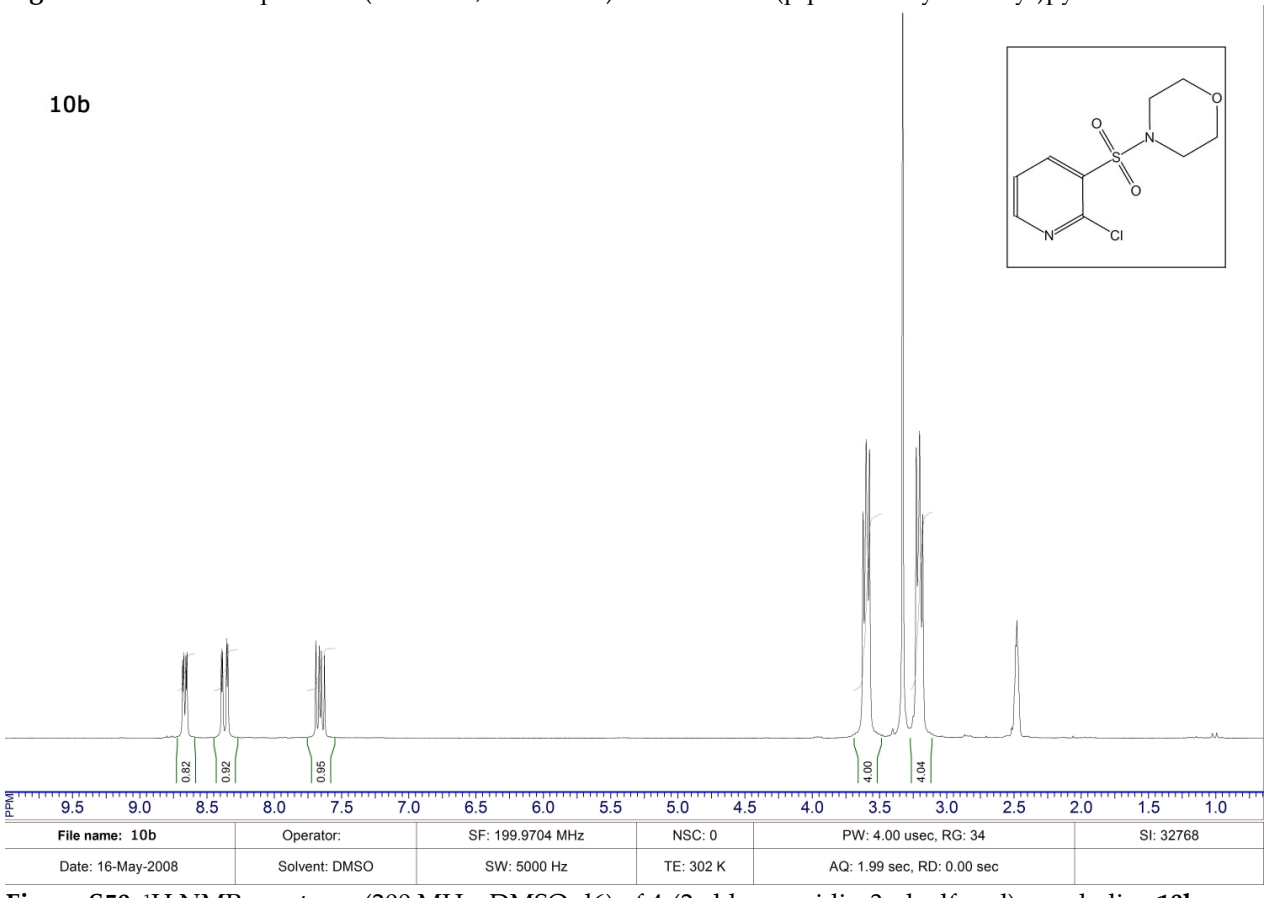


Figure S50. [1]H NMR spectrum (200 MHz, DMSO-d6) of 4-(2-chloropyridin-3-ylsulfonyl)morpholine **10b**.

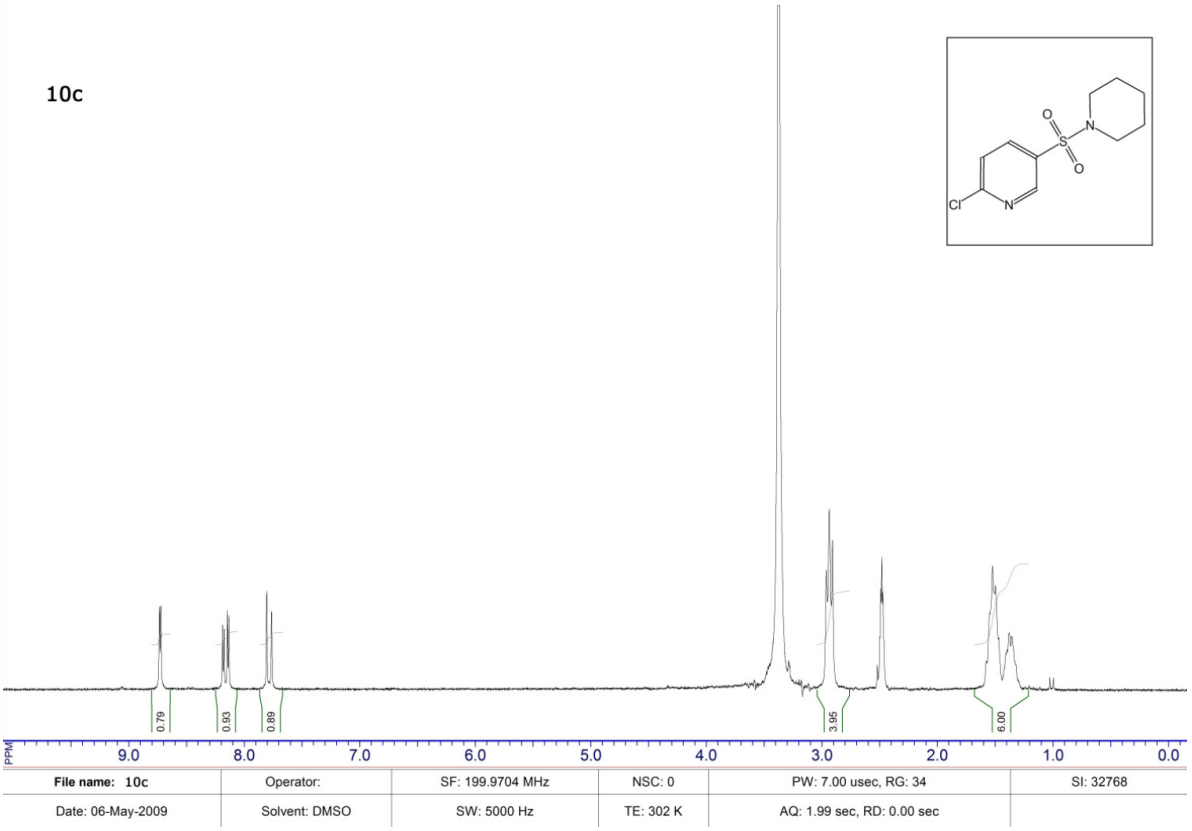


Figure S51. [1]H NMR spectrum (200 MHz, DMSO-d6) of 2-chloro-5-(piperidin-1-ylsulfonyl)pyridine **10c**.

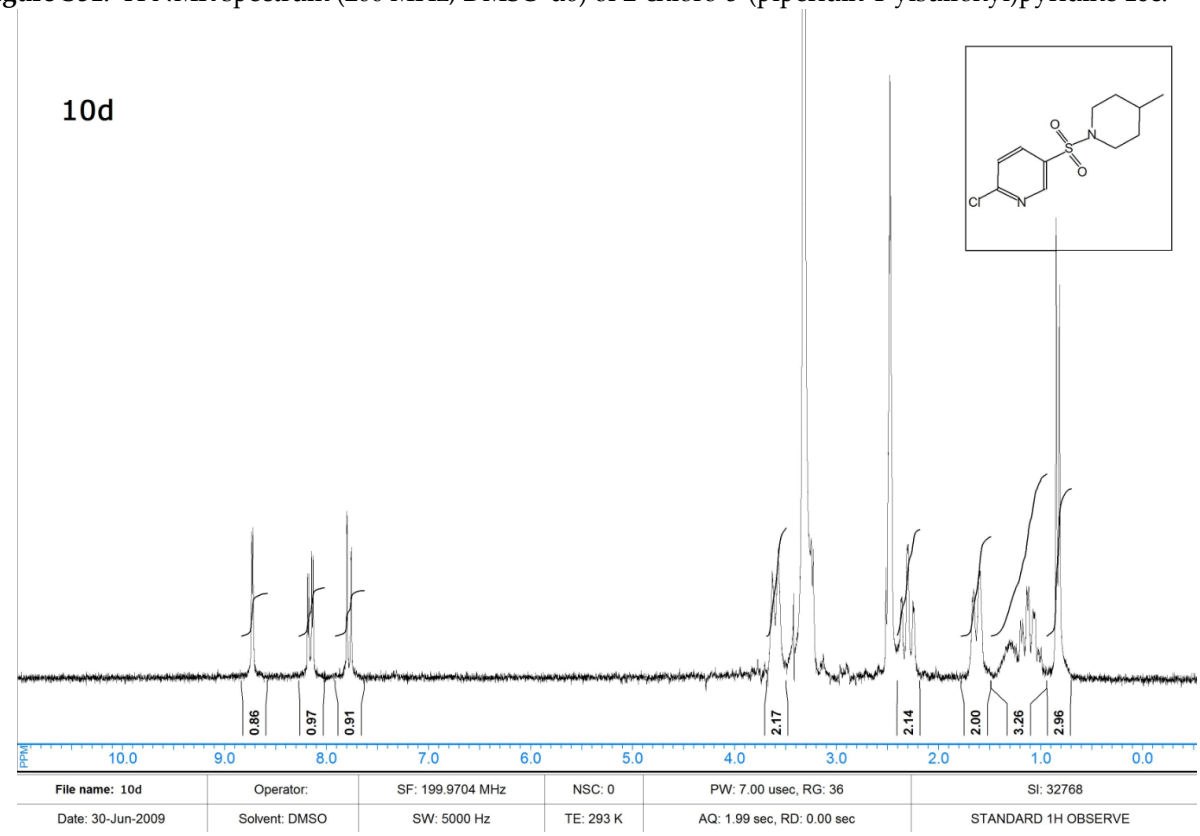


Figure S52. [1]H NMR spectrum (200 MHz, DMSO-d6) of 2-chloro-5-(4-methylpiperidin-1-ylsulfonyl)pyridine **10d**.

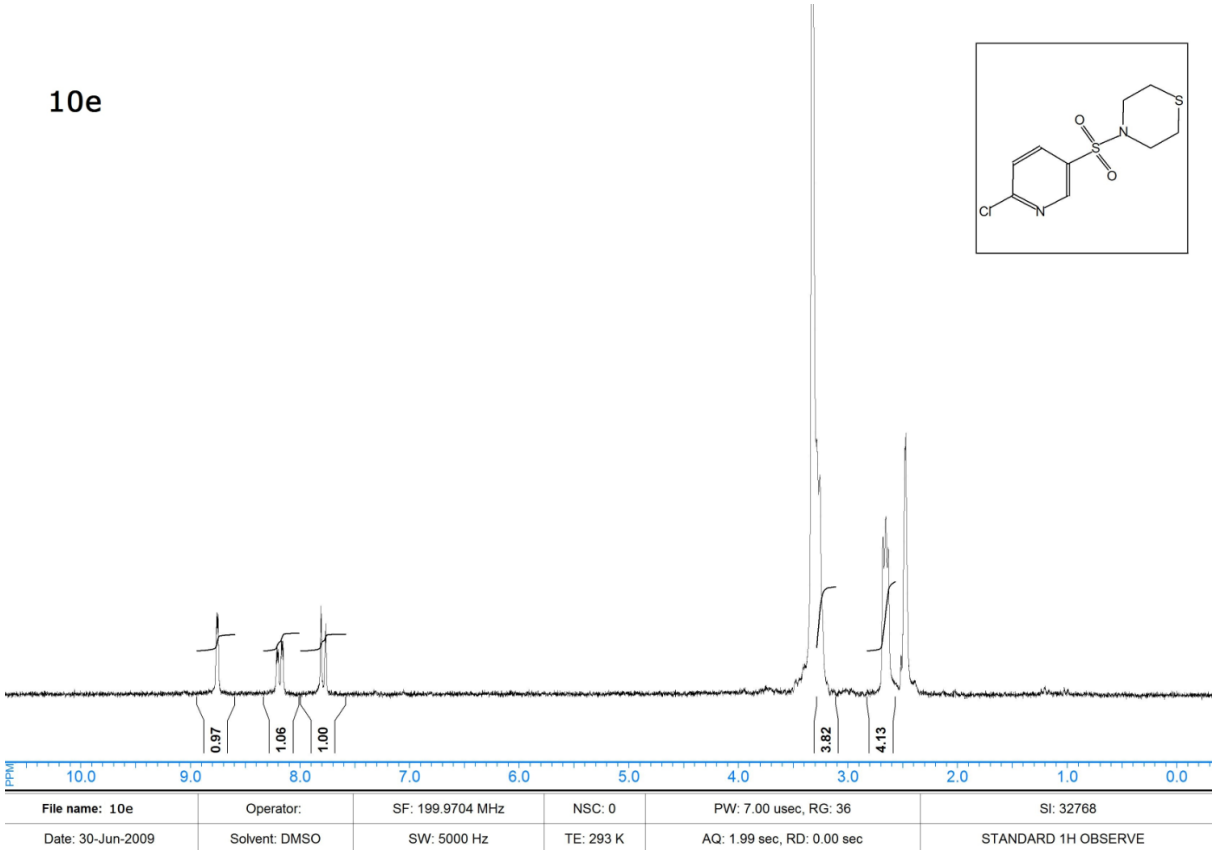


Figure S53. ^{1}H NMR spectrum (200 MHz, DMSO-d6) of 4-(6-chloropyridin-3-ylsulfonyl)thiomorpholine **10e**.

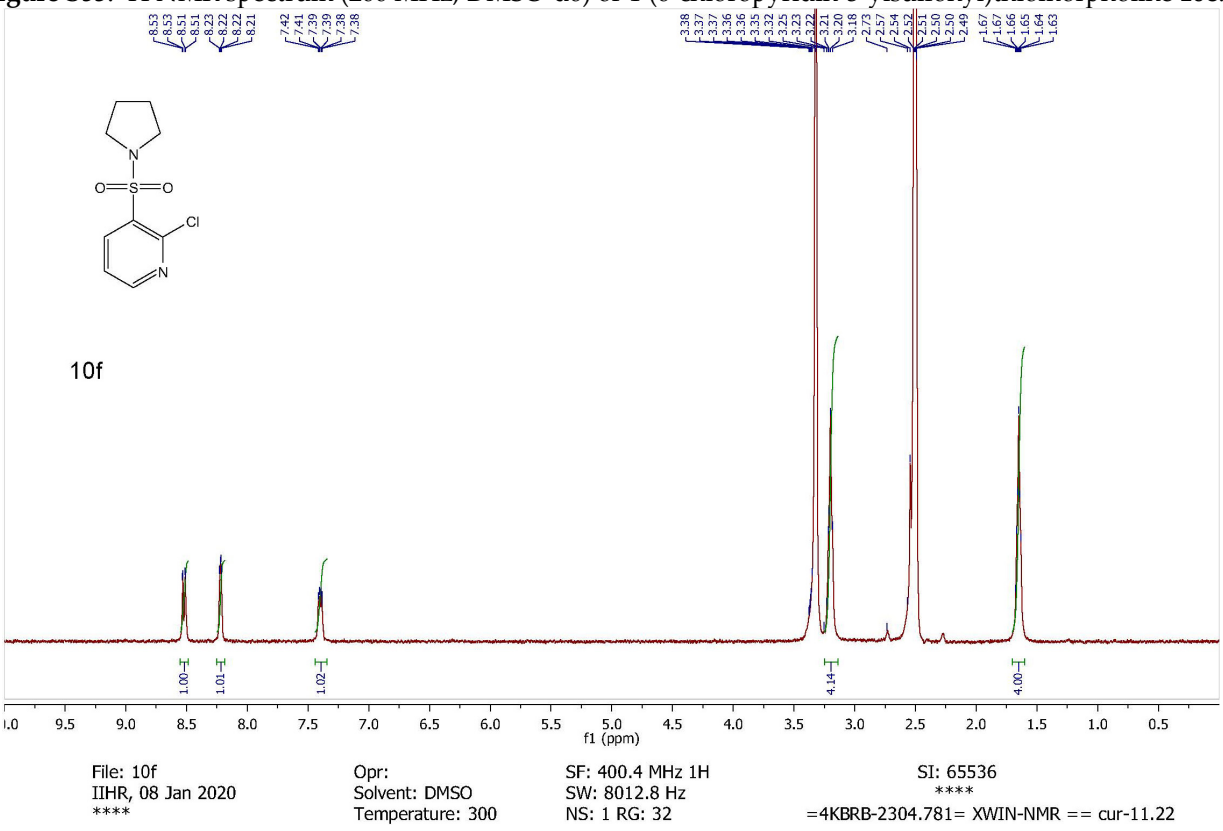


Figure S54. ^{1}H NMR spectrum (400 MHz, DMSO-d6) of 2-chloro-3-(pyrrolidin-1-ylsulfonyl)pyridine **10f.**

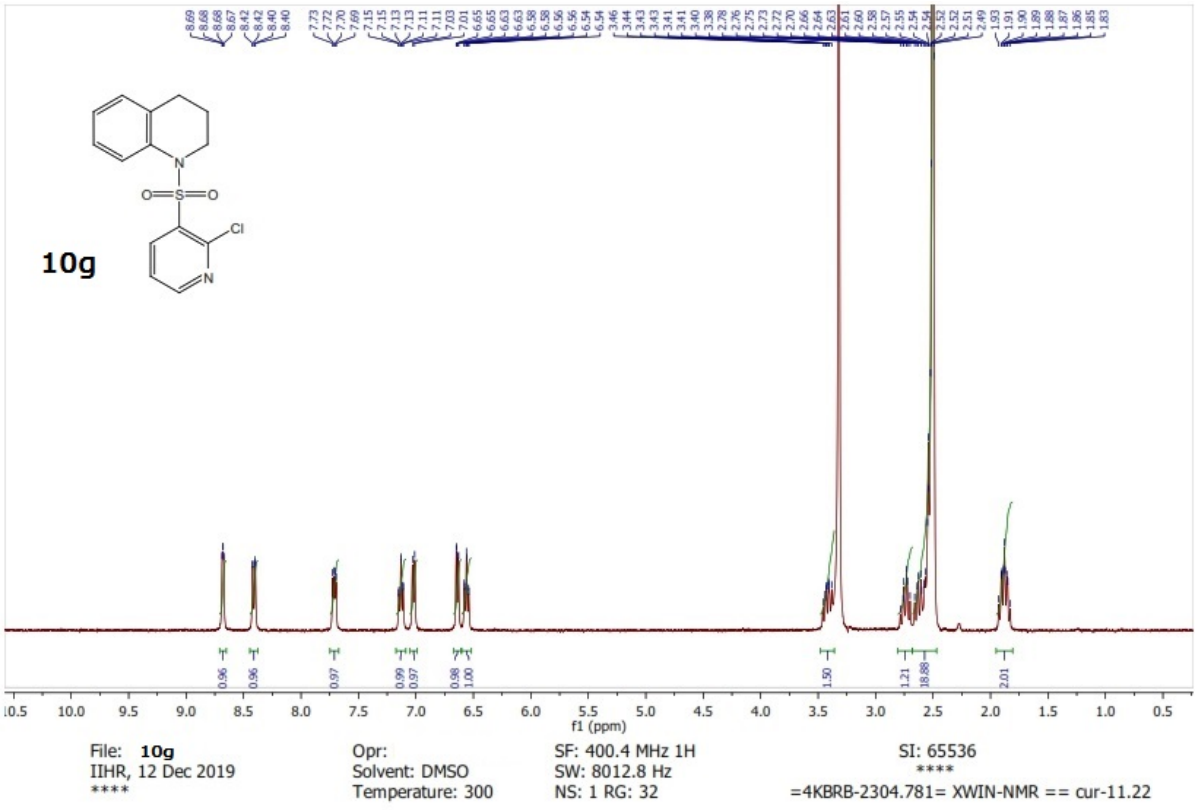


Figure S55. ^{1}H NMR spectrum (400 MHz, DMSO-d6) of 1-(2-chloropyridin-3-ylsulfonyl)-1,2,3,4-tetrahydroquinoline **10g**.

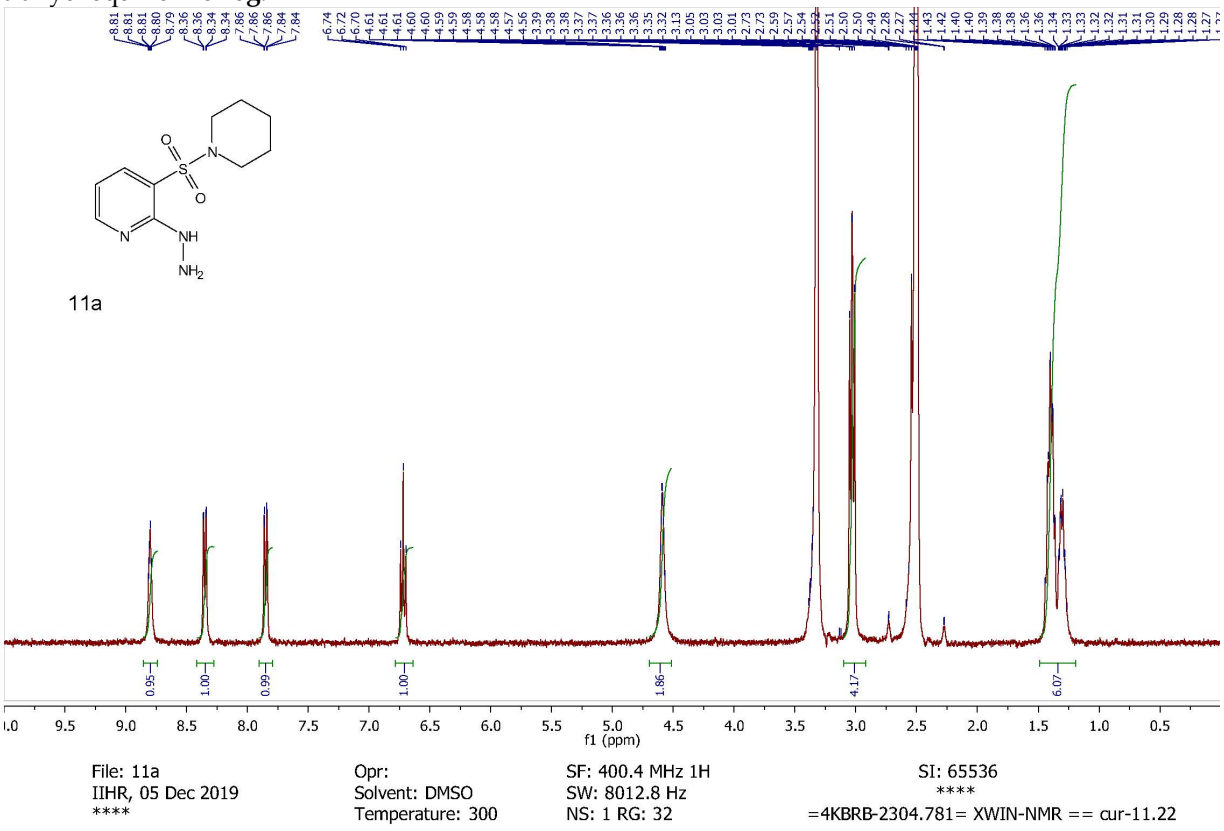


Figure S56. ^{1}H NMR spectrum (400 MHz, DMSO-d6) of 2-hydrazinyl-3-(piperidin-1-ylsulfonyl)pyridine **11a**.

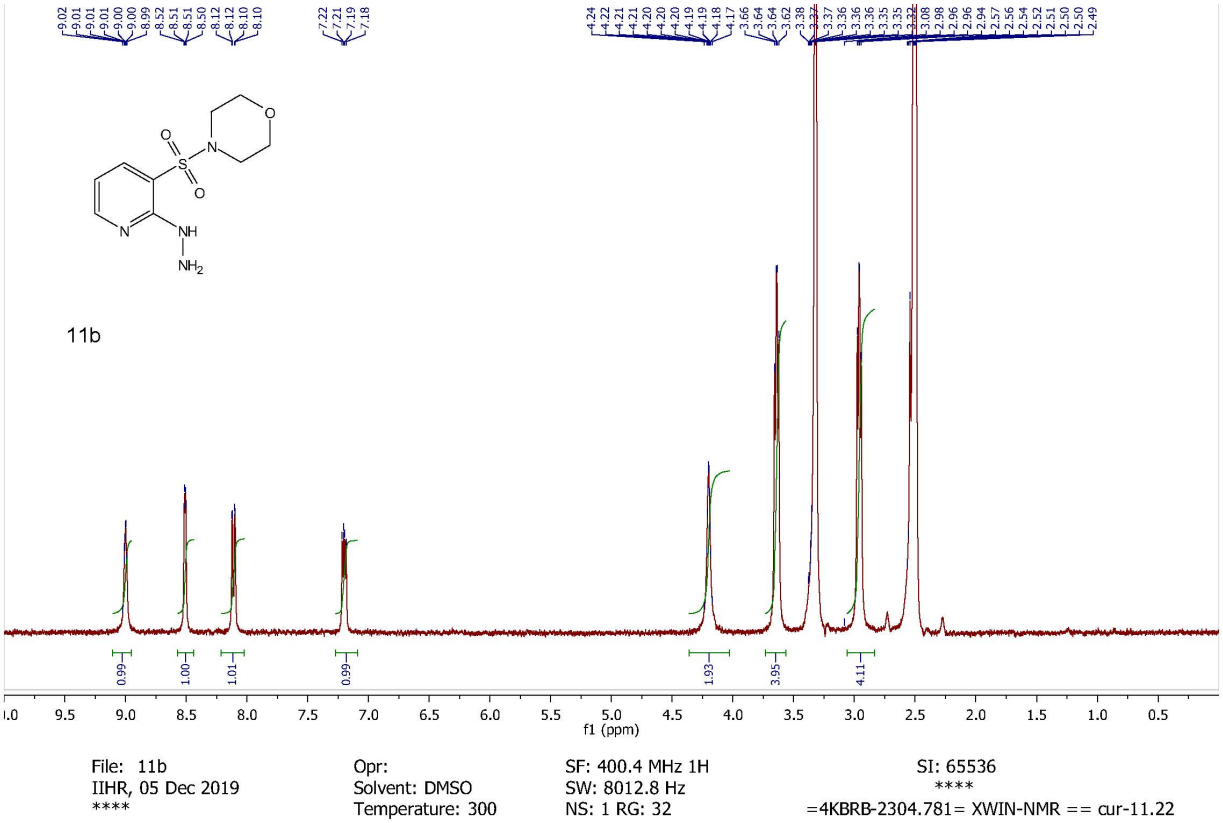


Figure S57. [1]H NMR spectrum (400 MHz, DMSO-d6) of 4-(2-hydrazinylpyridin-3-ylsulfonyl)morpholine **11b**.

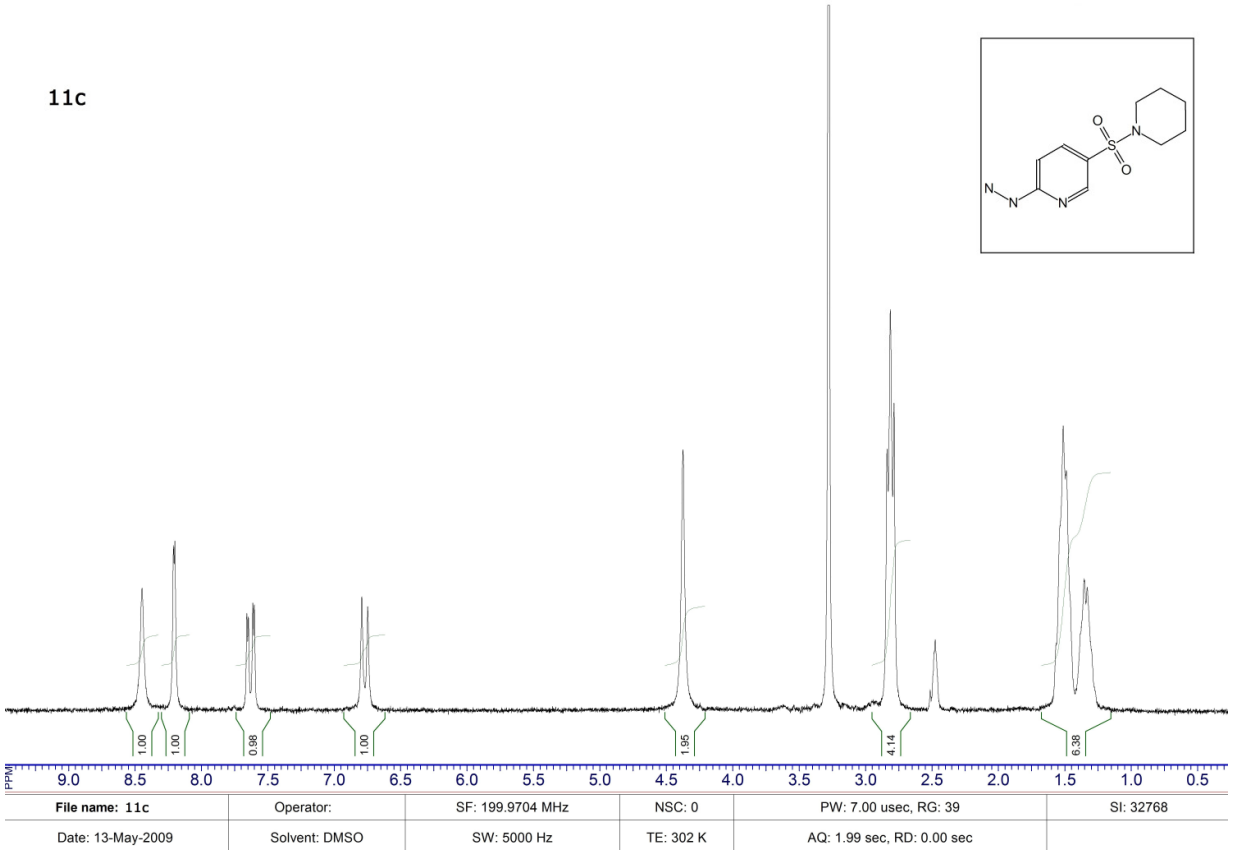


Figure S58. [1]H NMR spectrum (200 MHz, DMSO-d6) of 2-hydrazinyl-5-(piperidin-1-ylsulfonyl)pyridine **11c**.

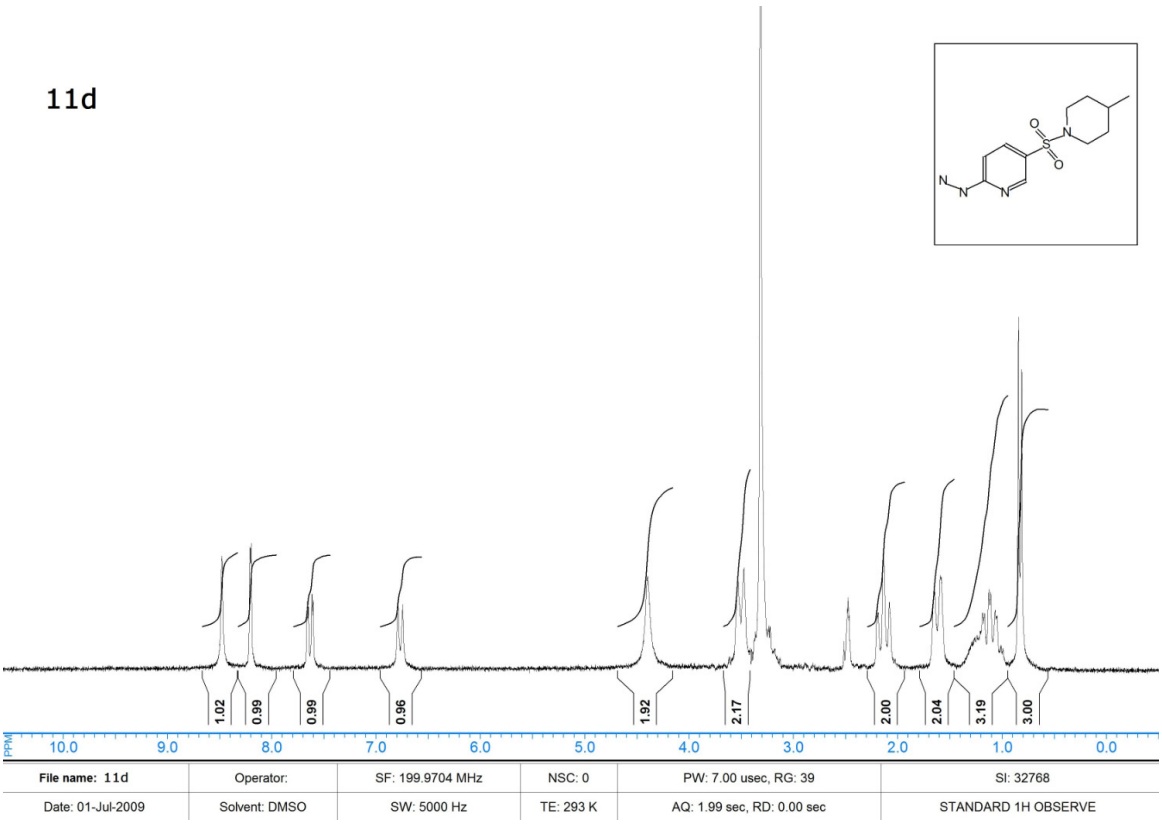


Figure S59. [1]H NMR spectrum (200 MHz, DMSO-d6) of 2-hydrazinyl-5-(4-methylpiperidin-1-ylsulfonyl)pyridine **11d**.

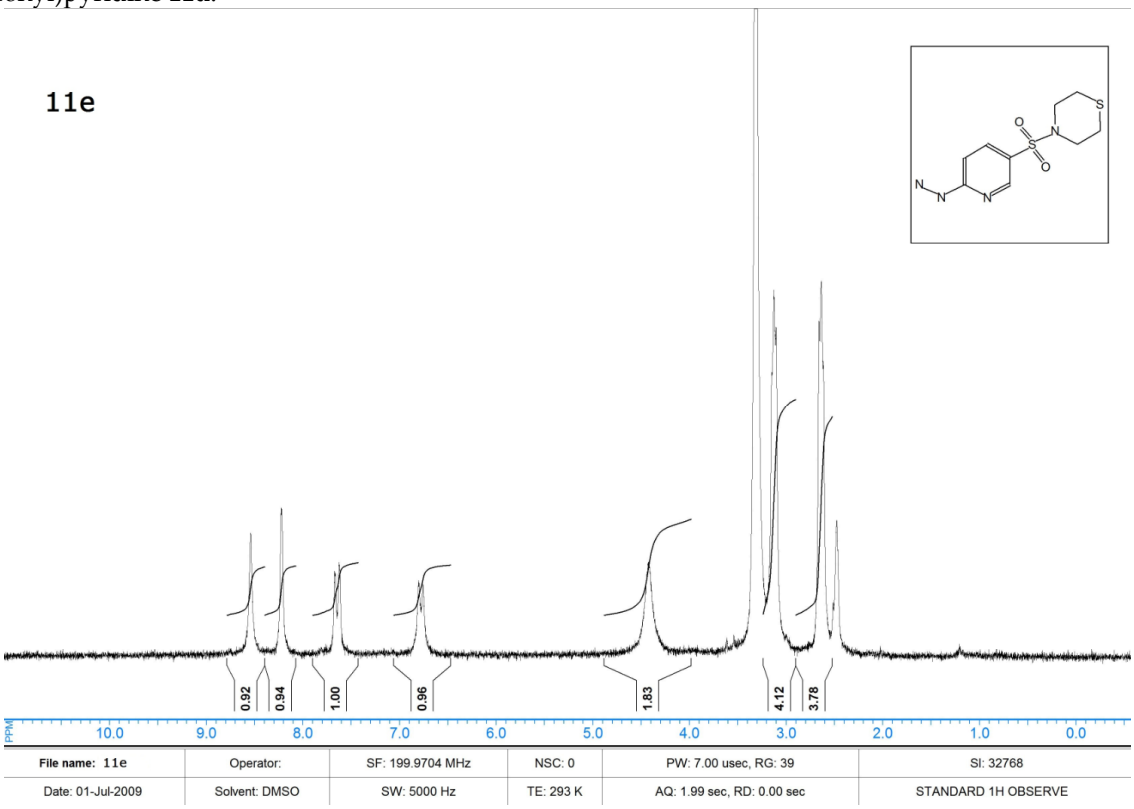


Figure S60. [1]H NMR spectrum (200 MHz, DMSO-d6) of 4-(6-hydrazinylpyridin-3-ylsulfonyl)thiomorpholine **11e.**

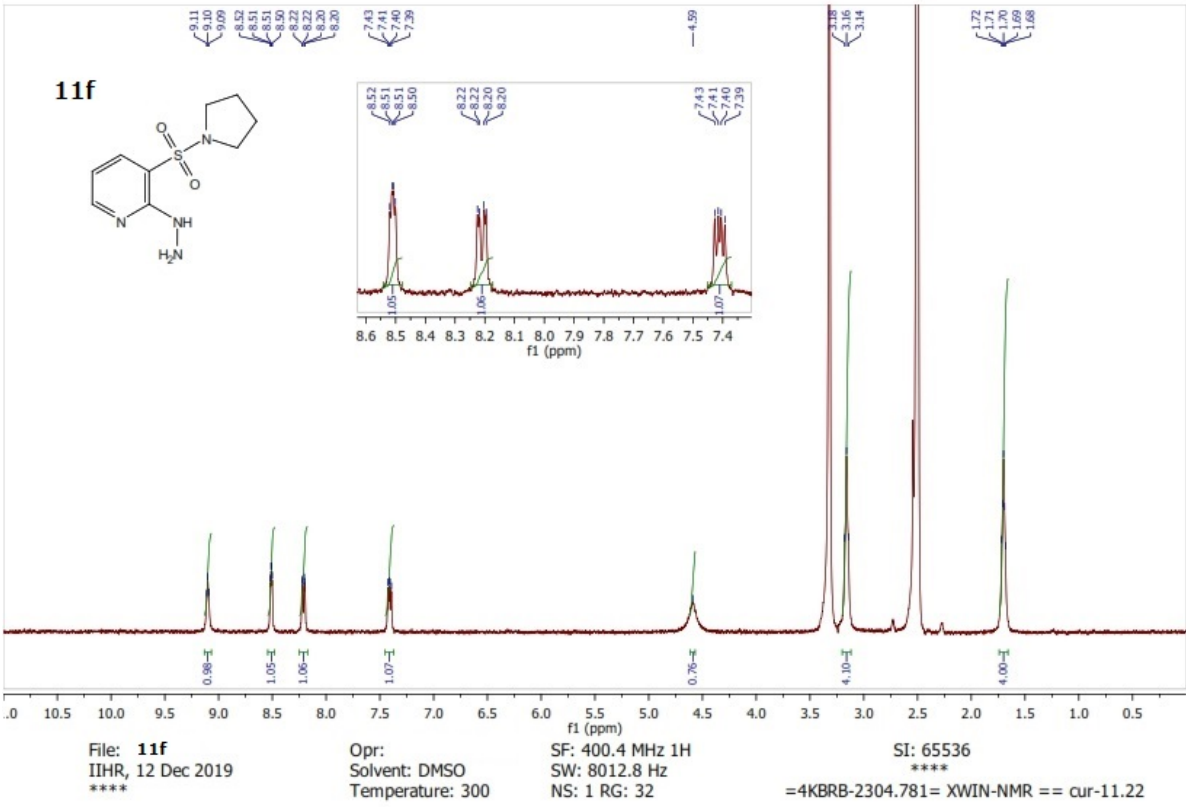


Figure S61. [1]H NMR spectrum (400 MHz, DMSO-d6) of 2-hydrazinyl-3-(pyrrolidin-1-ylsulfonyl)pyridine **11f.**

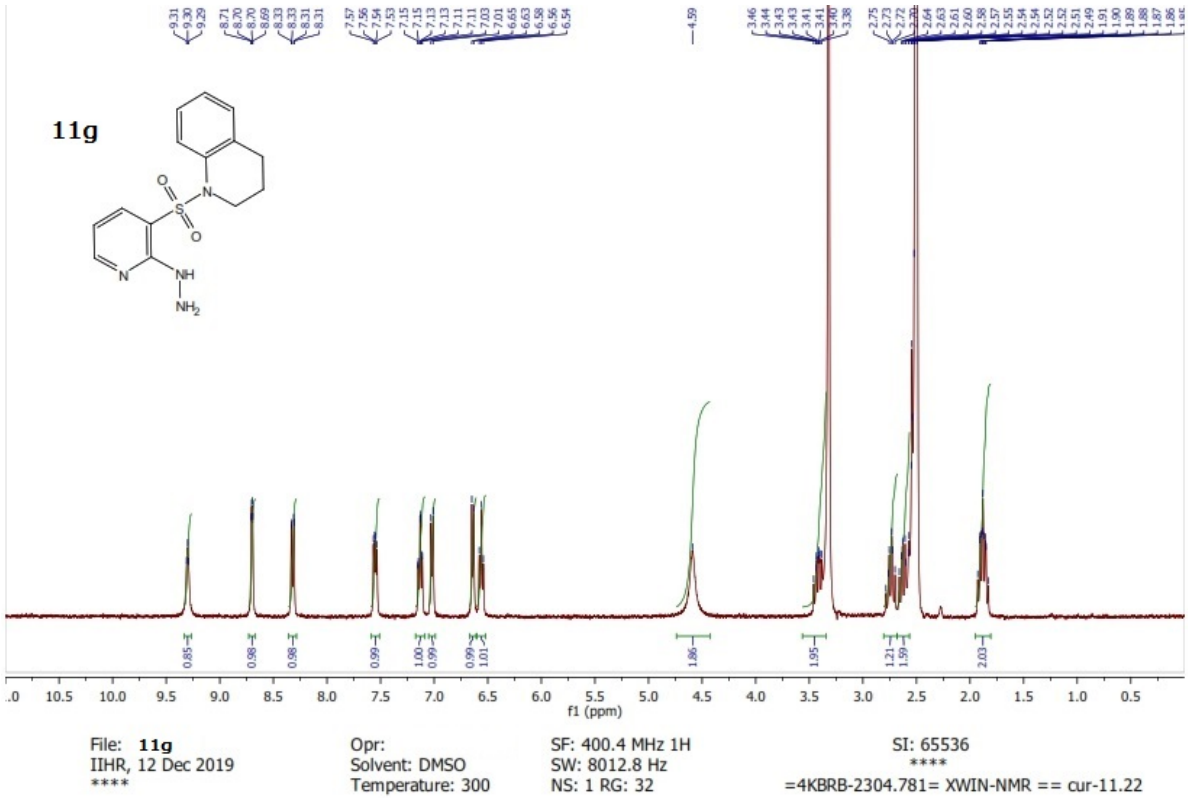


Figure S62. [1]H NMR spectrum (400 MHz, DMSO-d6) of 1-(2-hydrazinylpyridin-3-ylsulfonyl)-1,2,3,4-tetrahydroquinoline **11g**.

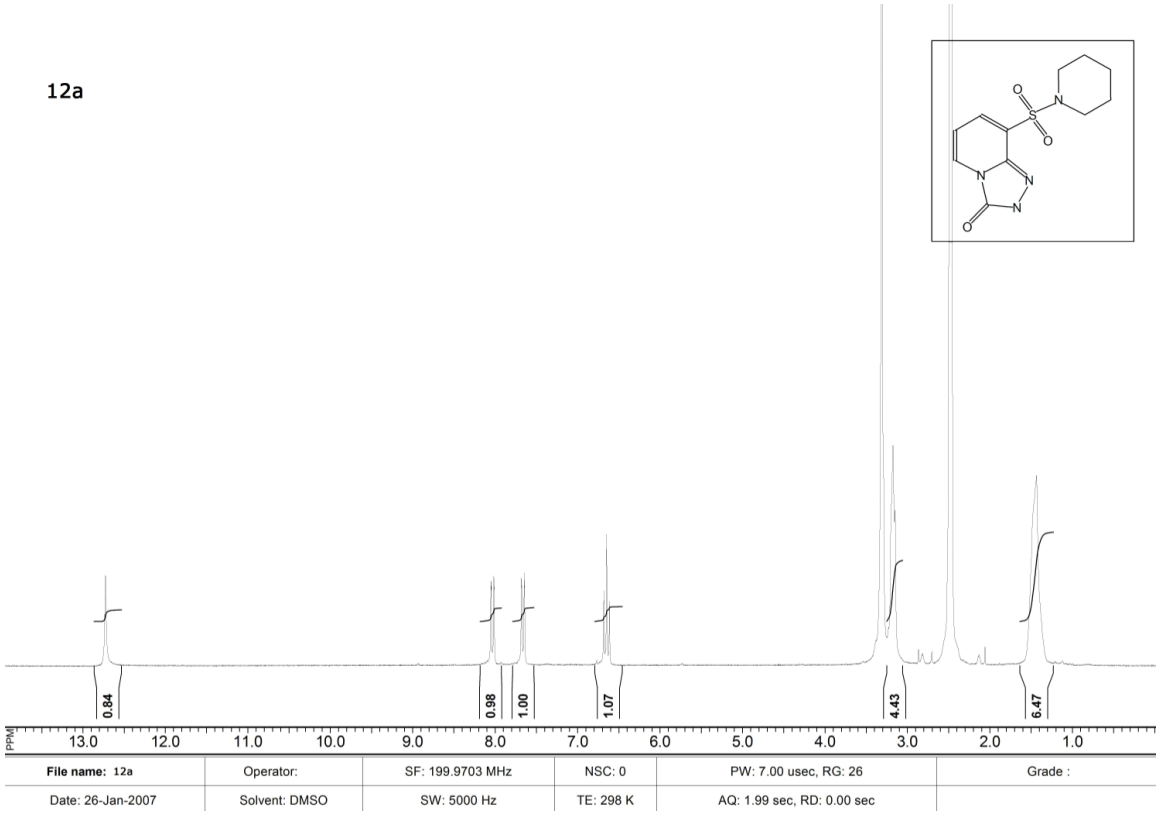


Figure S63. [1]H NMR spectrum (200 MHz, DMSO-d6) of 8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **12a.**

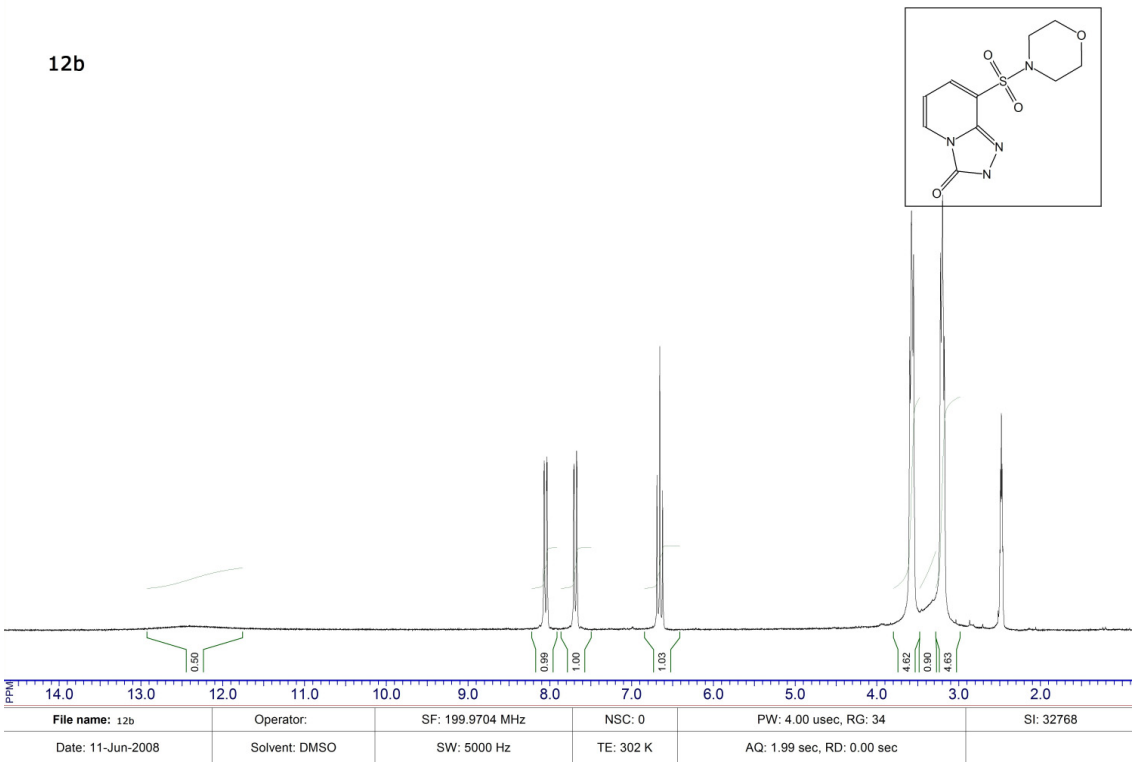


Figure S64. [1]H NMR spectrum (200 MHz, DMSO-d6) of 8-(morpholinosulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **12b**.

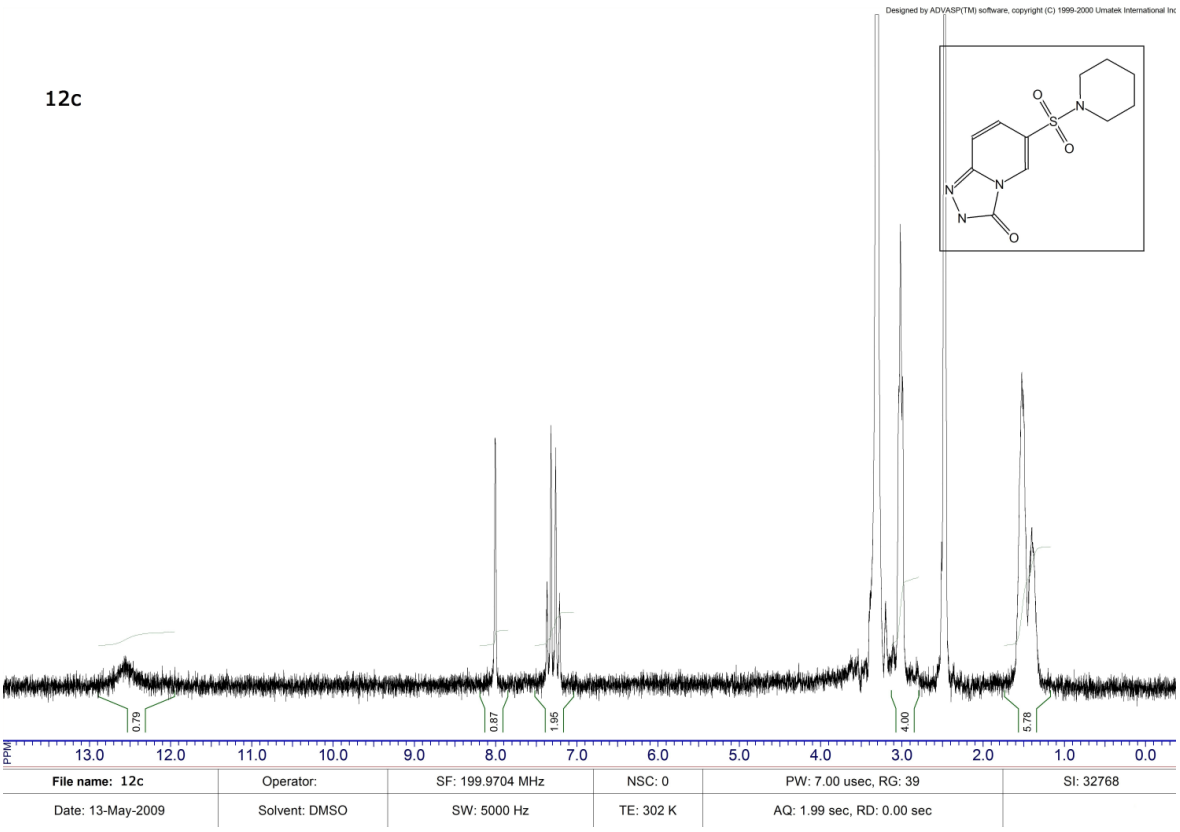


Figure S65. ^{1}H NMR spectrum (200 MHz, DMSO-d6) of 6-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **12c**.

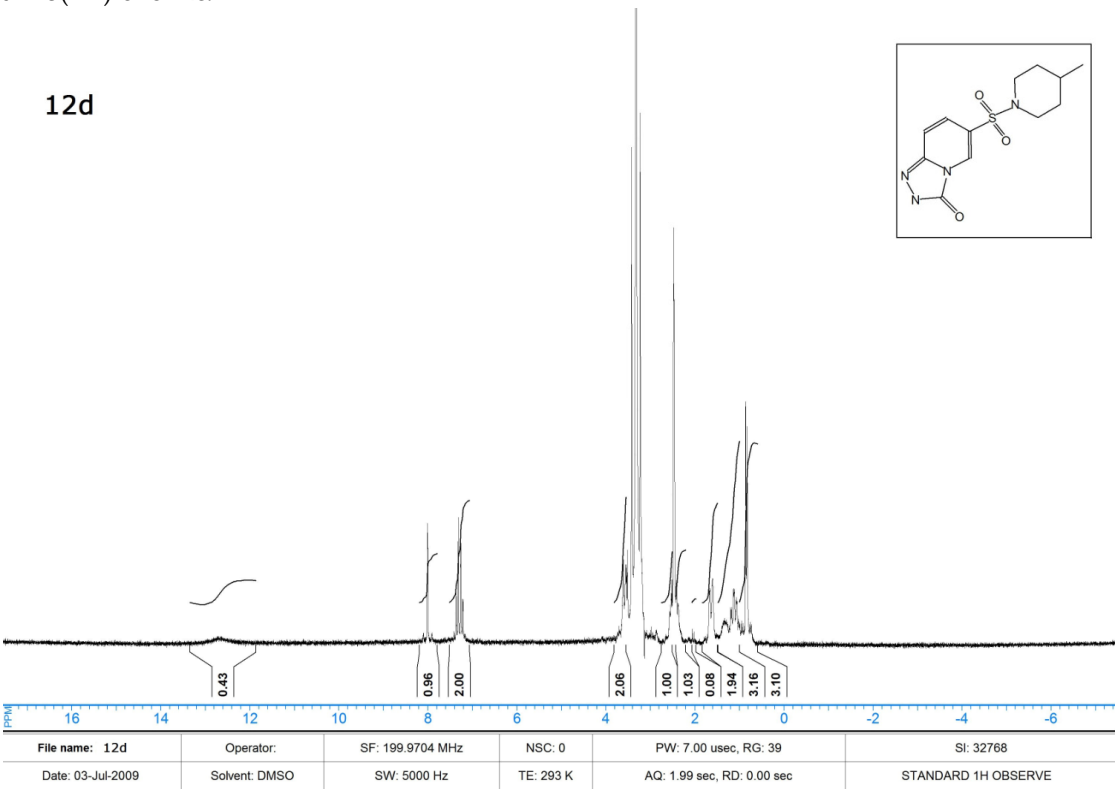


Figure S66. ^{1}H NMR spectrum (200 MHz, DMSO-d6) of 6-(4-methylpiperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **12d**.

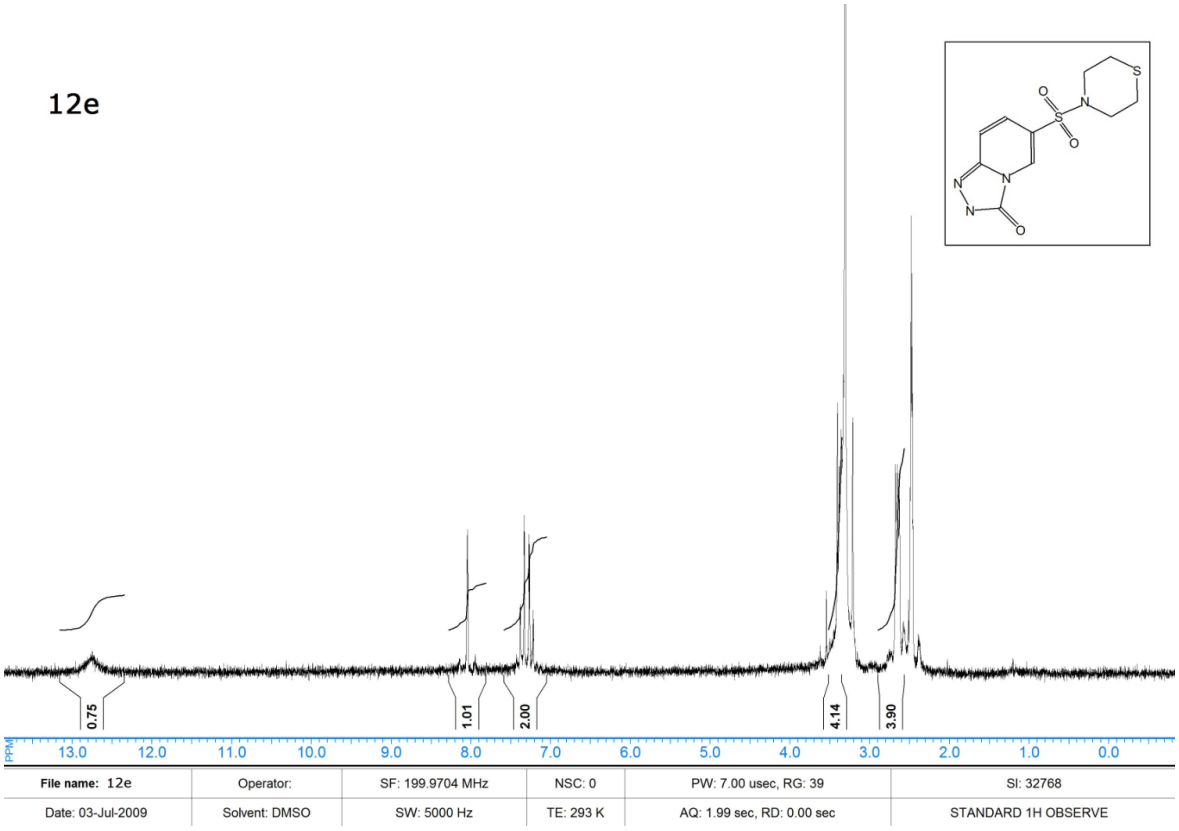


Figure S67. ^{1}H NMR spectrum (200 MHz, DMSO-d6) of 6-(thiomorpholinosulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **12e**.

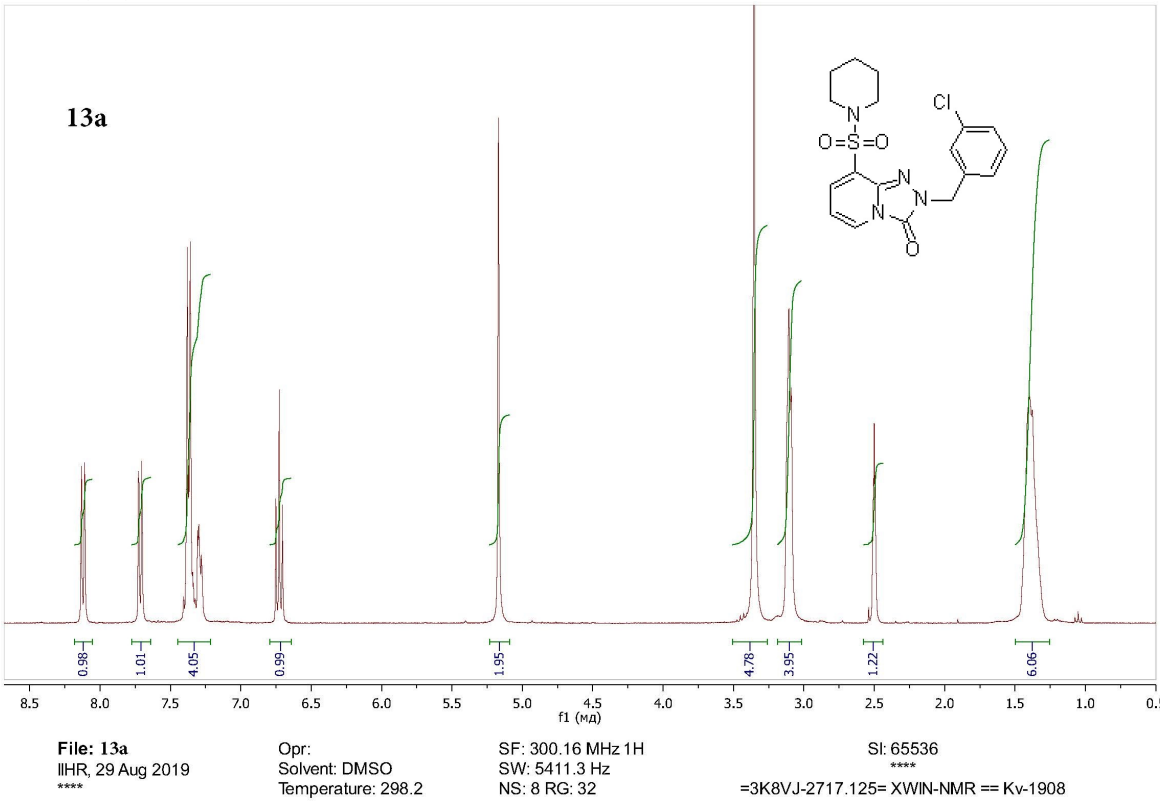


Figure S68. ^{1}H NMR spectrum (300 MHz, DMSO-d6) of 2-(3-chlorobenzyl)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13a**.

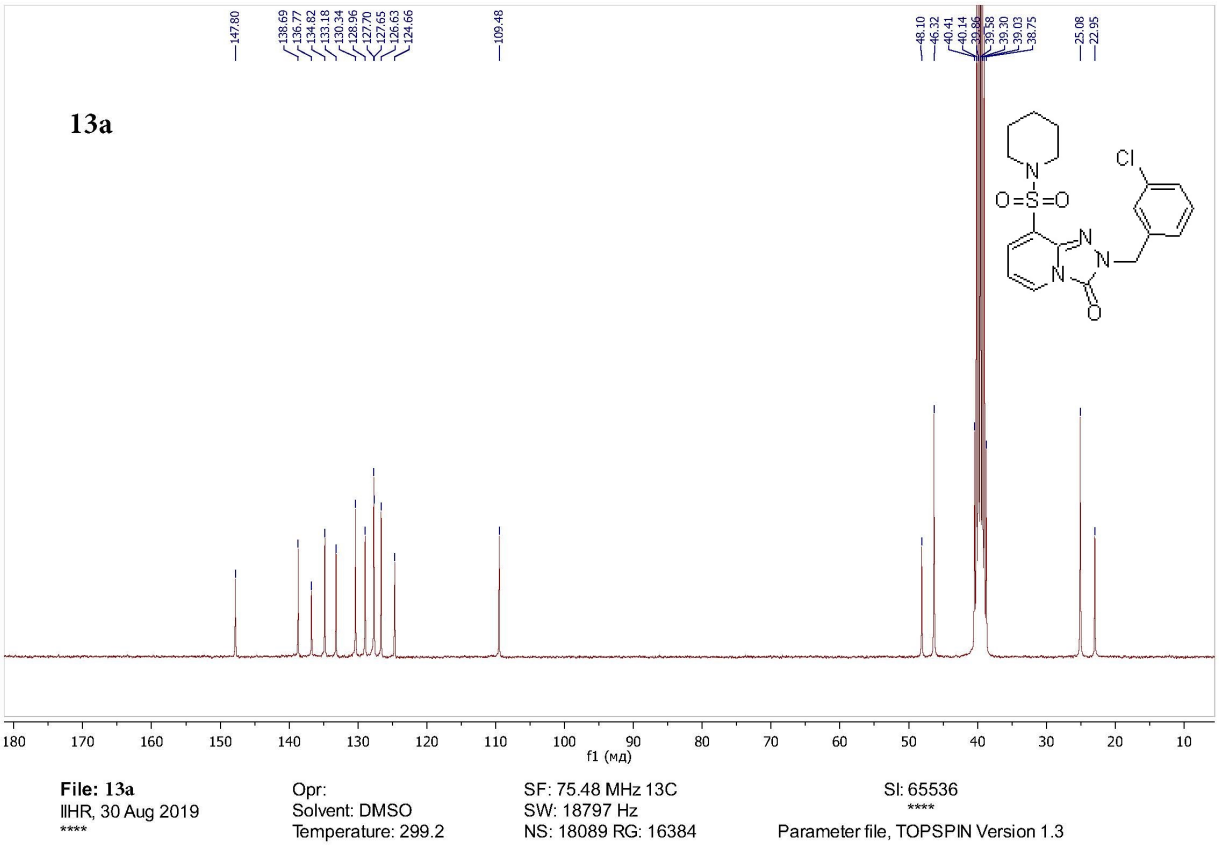


Figure S69. ^{13}C NMR spectrum (75 MHz, DMSO-d6) of 2-(3-chlorobenzyl)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13a**.

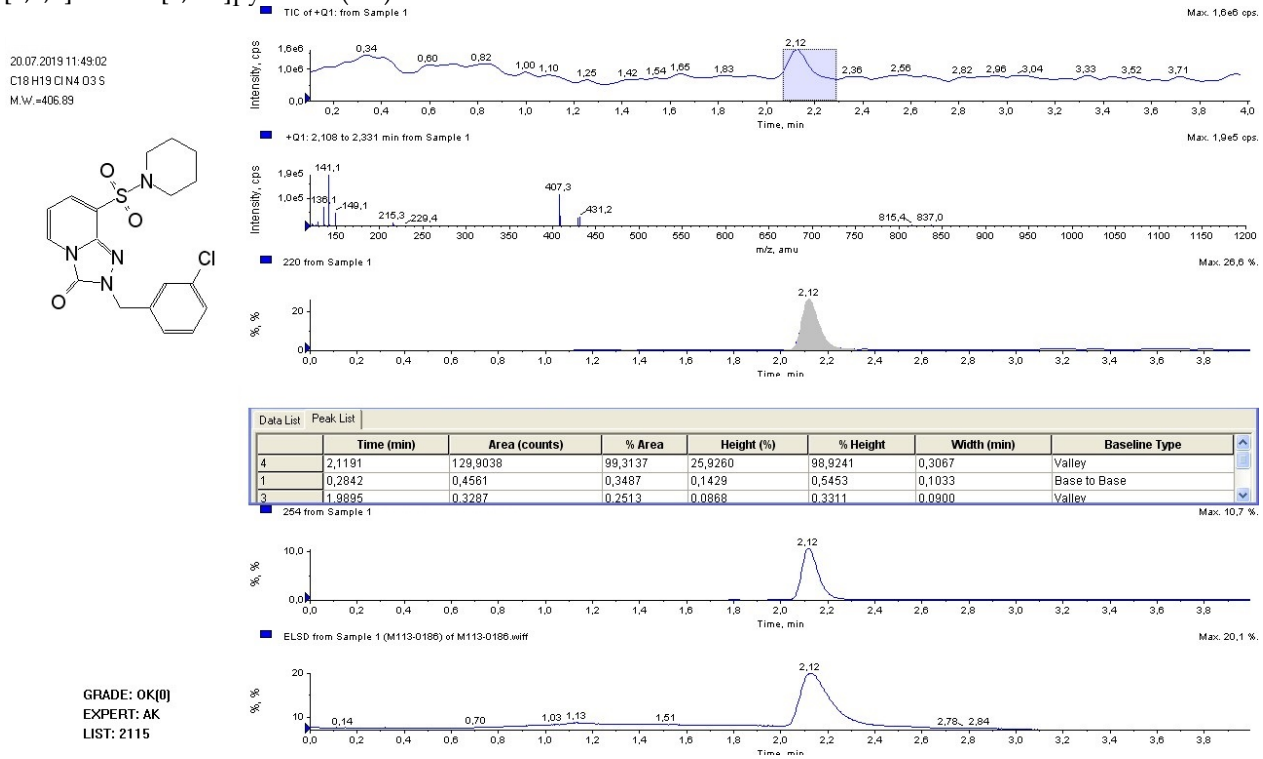


Figure S70. LC/MS data for 2-(3-chlorobenzyl)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13a**.

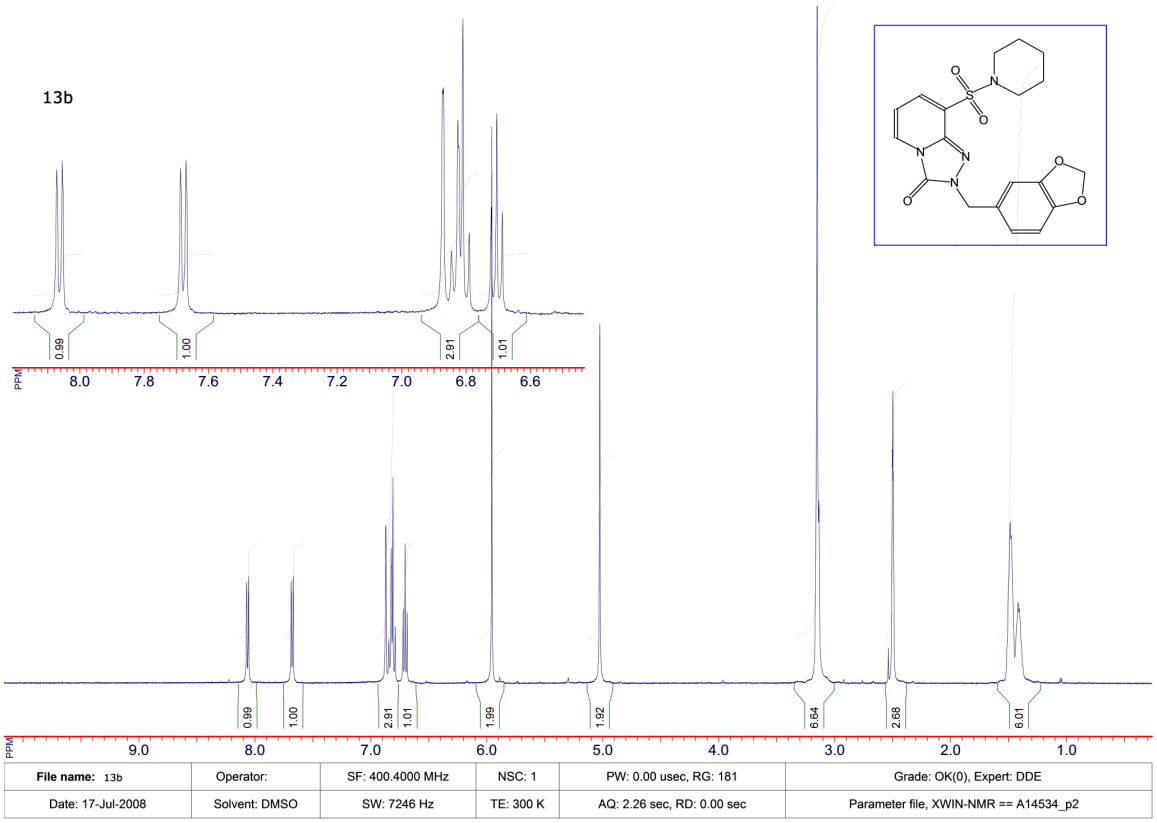


Figure S71. [1]H NMR spectrum (400 MHz, DMSO-d6) of 2-(benzo[d][1,3]dioxol-5-ylmethyl)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13b**.

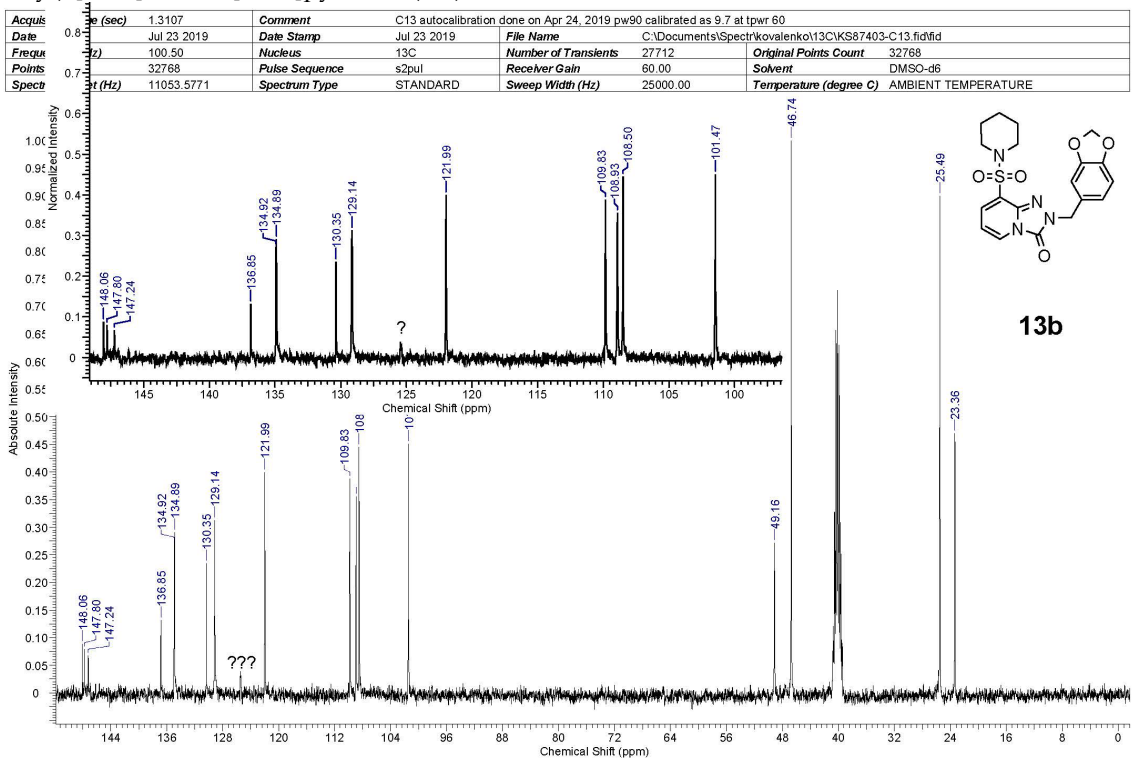


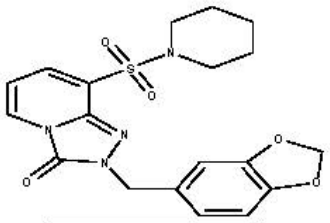
Figure S72. [13]C NMR spectrum (100 MHz, DMSO-d6) of 2-(benzo[d][1,3]dioxol-5-ylmethyl)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13b**.

X:\2010\10_10\101015\M6839\34063623.D Sample Name: 13b Page 1 of 1

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

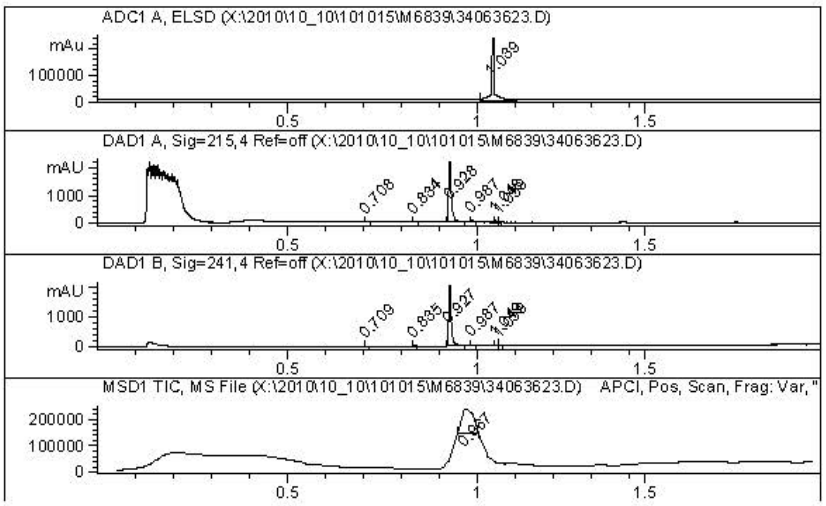
Agilent 1100 LC/MSD SL
Diodearrey G1315B (DAD1A-215nm; DAD1B-254nm)
Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

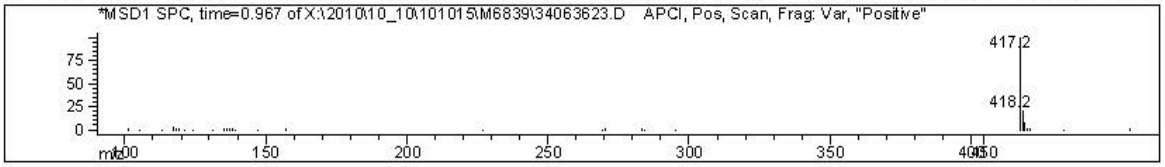
Mobile Phase:A-H2O+0.1%HCOOH;B-MeCN+0.1HCOOH
Separation column:
Rapid Resolutionn HT Cartige 4.6x30mm,
1.8-Micron, Zorbx SB-C18



Mol.Weight: 416,46

M6839 ->





#	Signal	R.Time	Area %
1	ADC1 A, ELSD	1.039	100.000

#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.708	0.839
2		0.834	0.495
3		0.928	94.038
4		0.987	1.715
5		1.048	2.056
6		1.059	0.857

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.709	0.404
2		0.835	0.390
3		0.927	95.723
4		0.987	1.516
5		1.049	1.278
6		1.059	0.689

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.967	100.000

Figure S73. LC/MS data for 2-(benzo[d][1,3]dioxol-5-ylmethyl)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13b**.

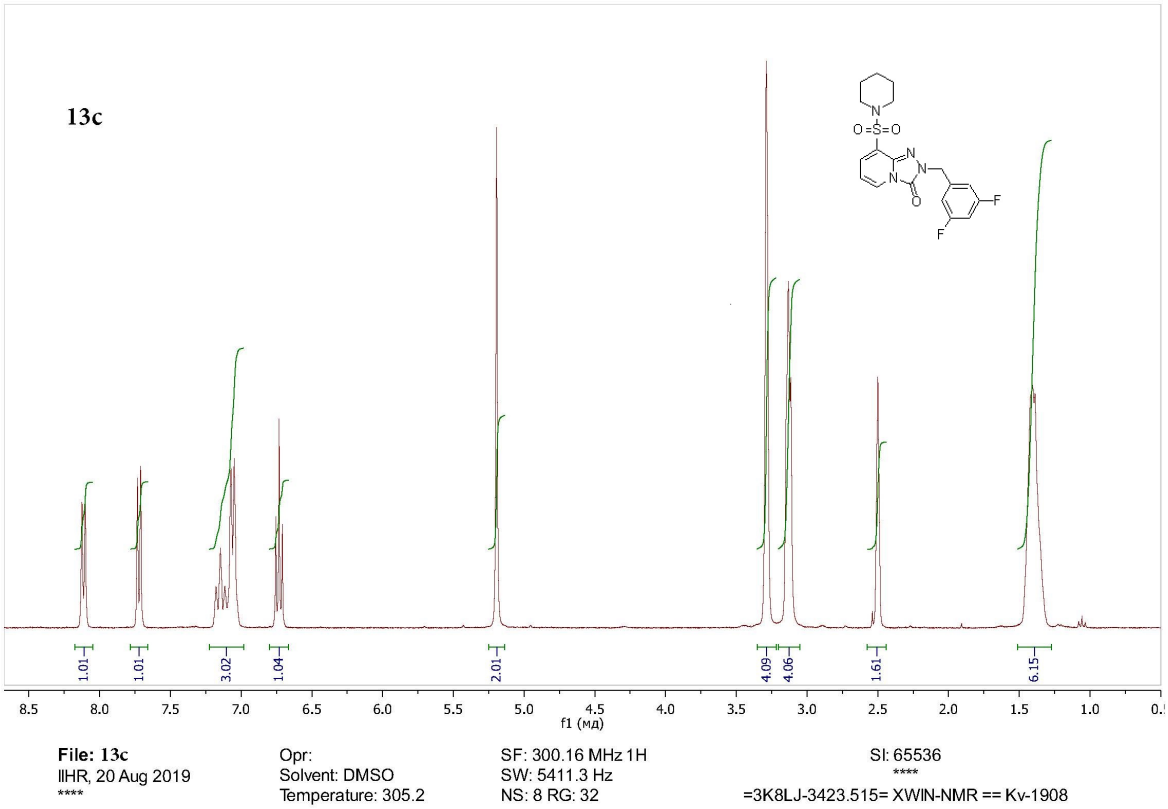


Figure S74. [1]H NMR spectrum (300 MHz, DMSO-d6) of 2-(3,5-difluorobenzyl)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13c**.

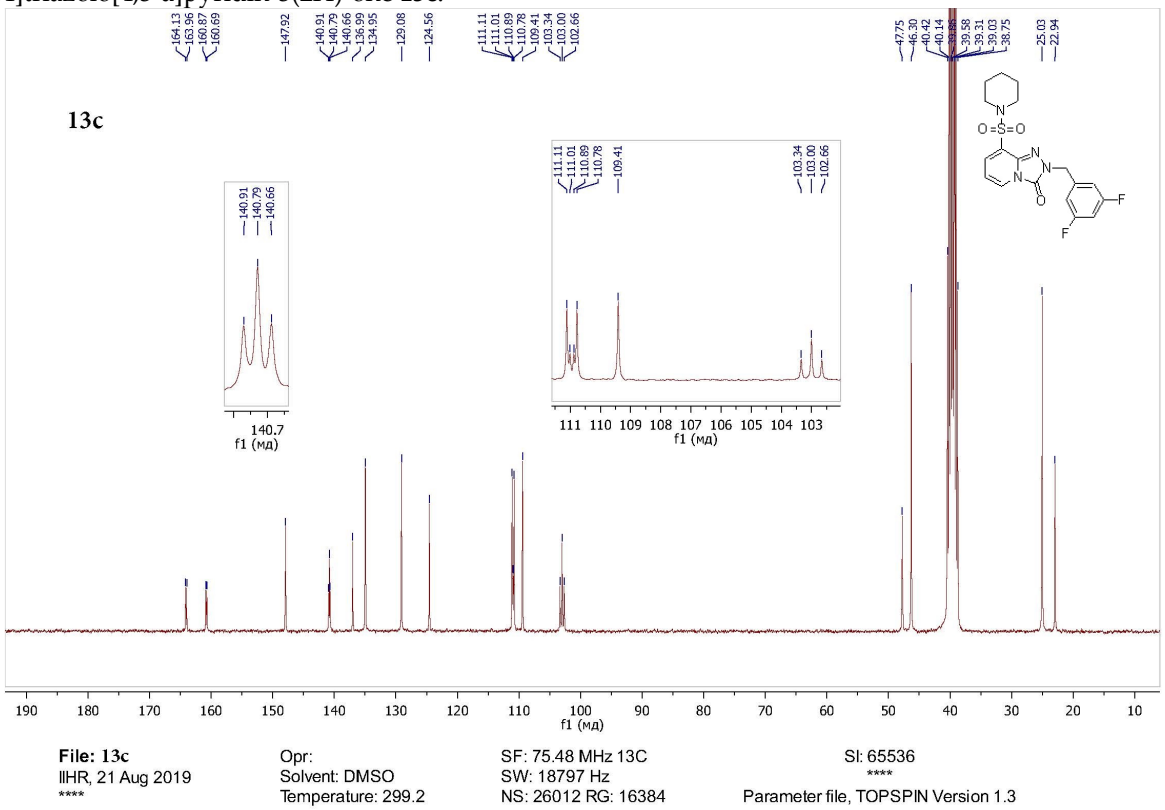


Figure S75. [13]C NMR spectrum (75 MHz, DMSO-d6) of 2-(3,5-difluorobenzyl)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13c**.

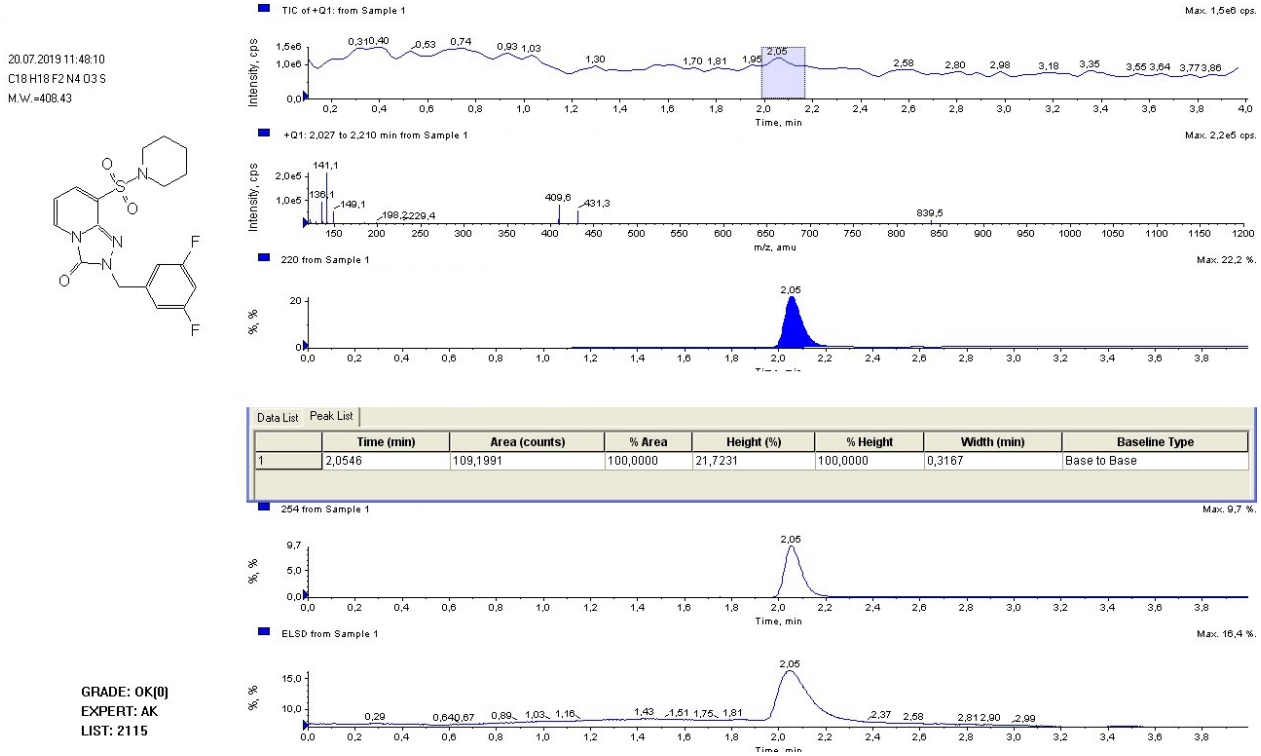


Figure S76. LC/MS data for 2-(3,5-difluorobenzyl)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13c**.

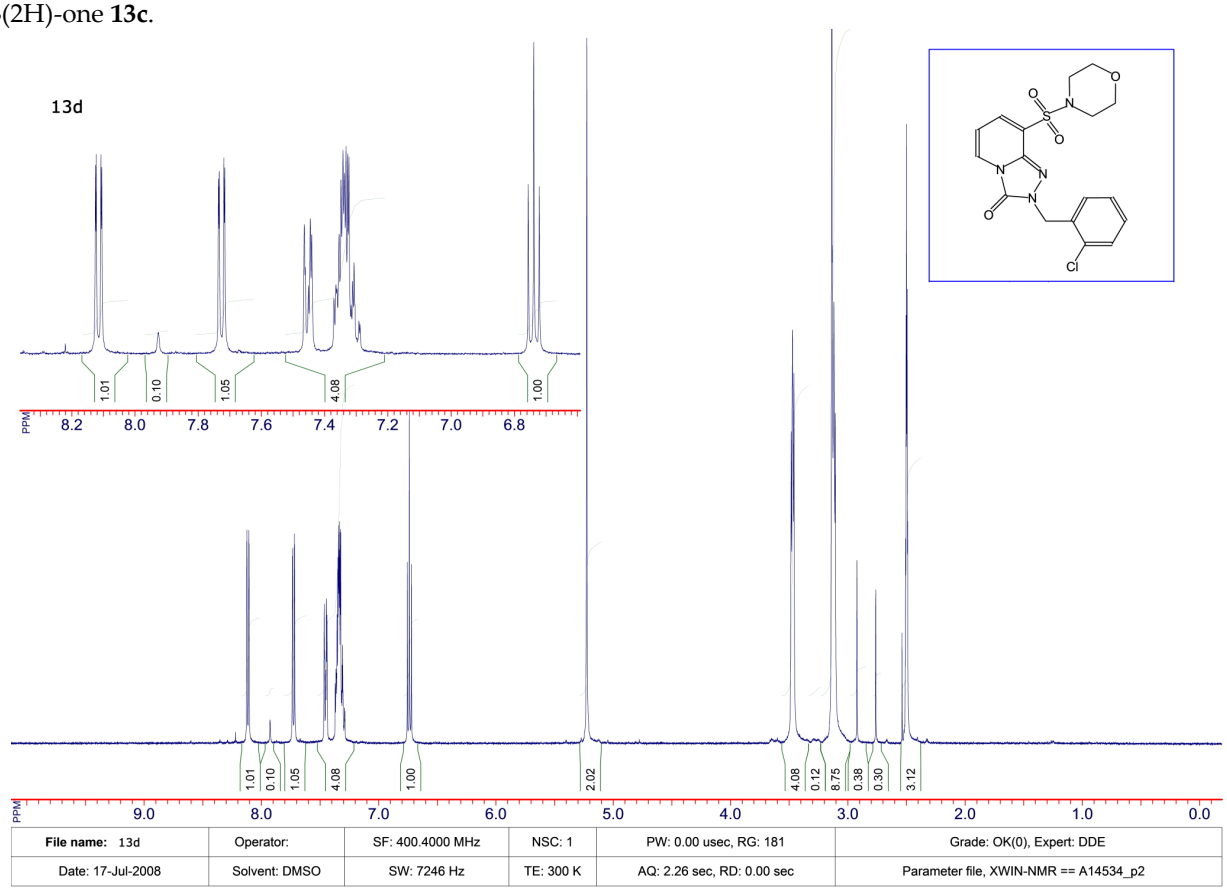


Figure S77. ^{1}H NMR spectrum (400 MHz, DMSO-d6) of 2-(2-chlorobenzyl)-8-(morpholinosulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13d**.

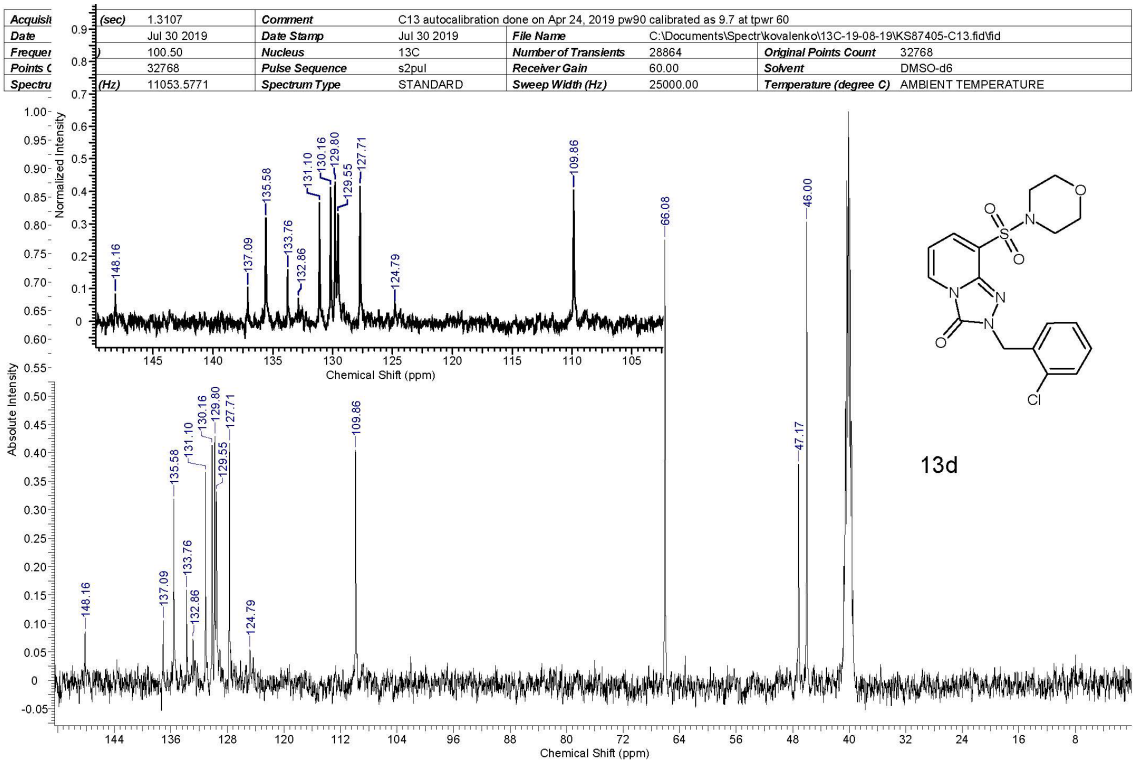
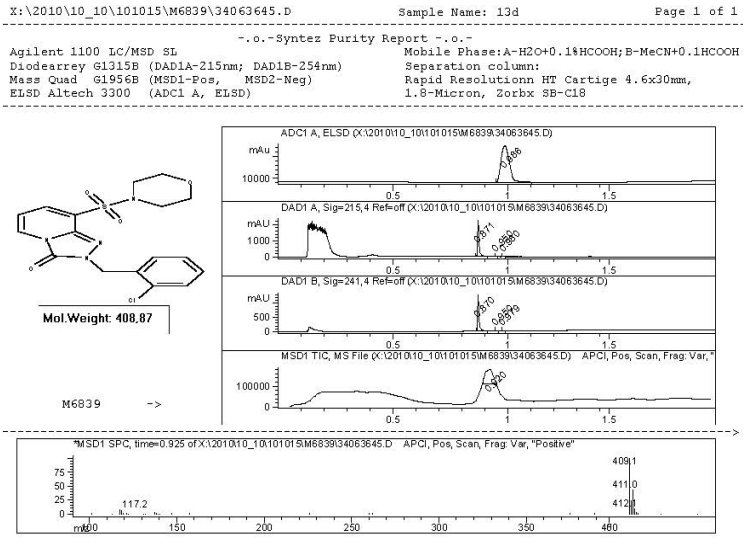


Figure S78. ^{13}C NMR spectrum (100 MHz, DMSO-d6) of 2-(2-chlorobenzyl)-8-(morpholinosulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13d**.



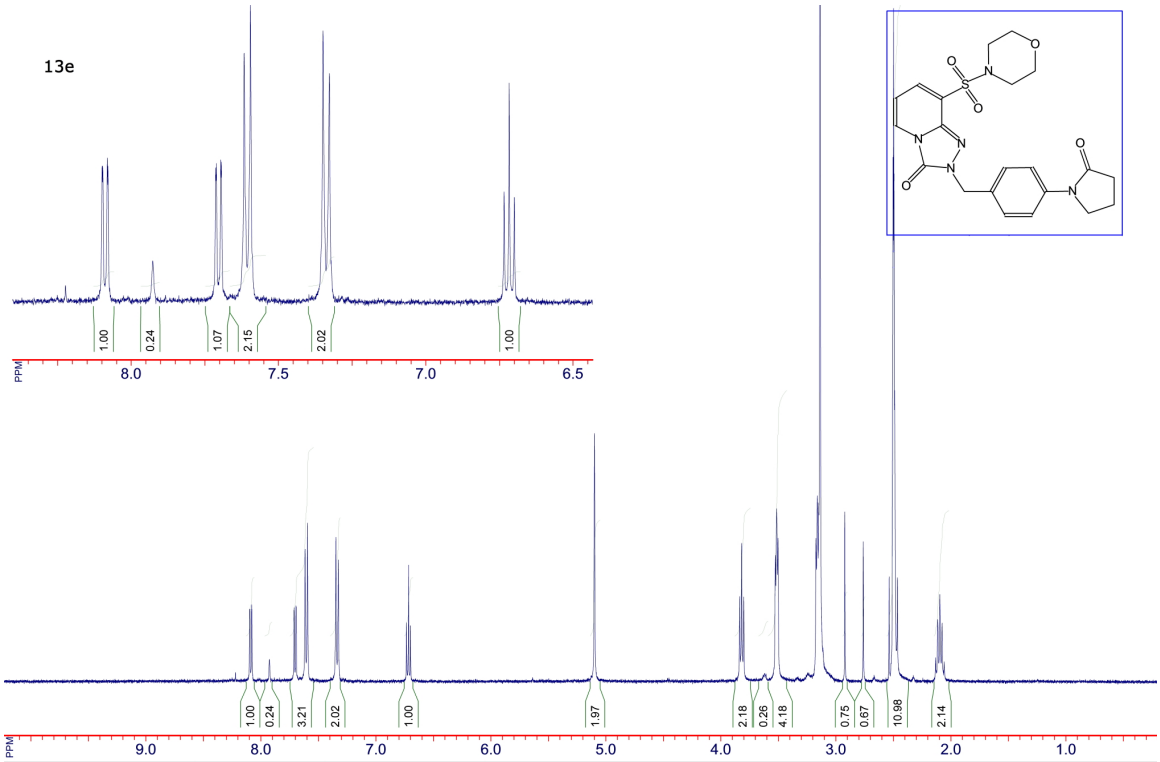
#	Signal	R.Time	Area %
1	ADC1 A, ELSD	0.986	100.000

#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.871	98.288
2		0.950	0.765
3		0.980	0.947

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.870	97.590
2		0.950	1.531
3		0.979	0.879

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.920	100.000

Figure S79. LC/MS data for 2-(2-chlorobenzyl)-8-(morpholinosulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13d**.



File name: 13e	Operator:	SF: 400.4000 MHz	NSC: 1	PW: 0.00 usec, RG: 181	Grade: OK(10), Expert: DDE
Date: 17-Jul-2008	Solvent: DMSO	SW: 7246 Hz	TE: 300 K	AQ: 2.26 sec, RD: 0.00 sec	Parameter file, XWIN-NMR == A14534_p2

Figure S80. [1]H NMR spectrum (400 MHz, DMSO-d6) of 8-(morpholinosulfonyl)-2-[4-(2-oxopyrrolidin-1-yl)benzyl]-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13e**.

Acquisiti	*(sec)* 1.3107	*Comment*	C13 autocalibration done on Apr 24, 2019 pw90 calibrated as 9.7 at tpwr 60		
Date	Aug 3 2019	*Date Stamp*	Aug 3 2019	*File Name*	C:\Documents\Spectr\kovalenko\13C-19-08-19\KS87404-C13.fid\fid
Frequen	100.50	*Nucleus*	13C	*Number of Transients*	69056	*Original Points Count*	32768
Points C	32768	*Pulse Sequence*	s2pul	*Receiver Gain*	60.00	*Solvent*	DMSO-d6
Spectrur	*Hz)* 11053.5771	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	25000.00	*Temperature (degree C)*	AMBIENT TEMPERATURE

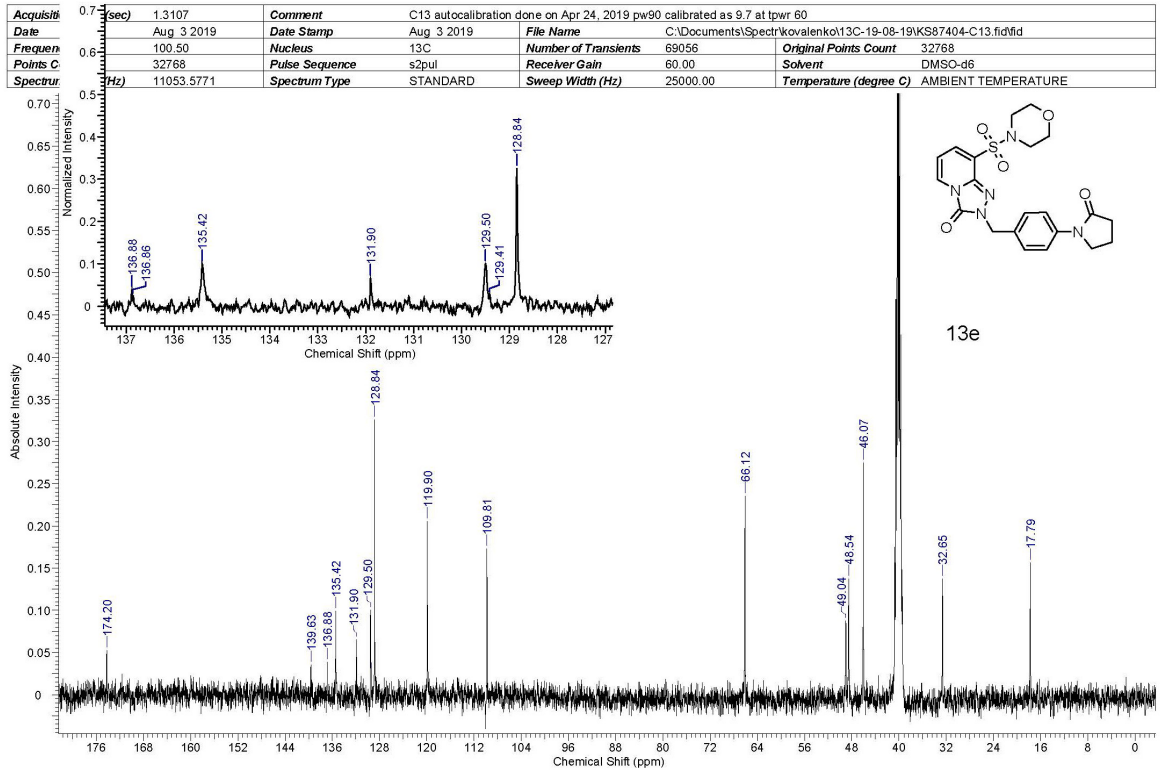


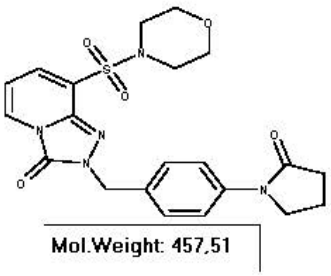
Figure S81. [13]C NMR spectrum (100 MHz, DMSO-d6) of 8-(morpholinosulfonyl)-2-[4-(2-oxopyrrolidin-1-yl)benzyl]-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13e**.

X:\2010\10_10\101015\M6839\34063644.D Sample Name: 13e Page 1 of 1

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

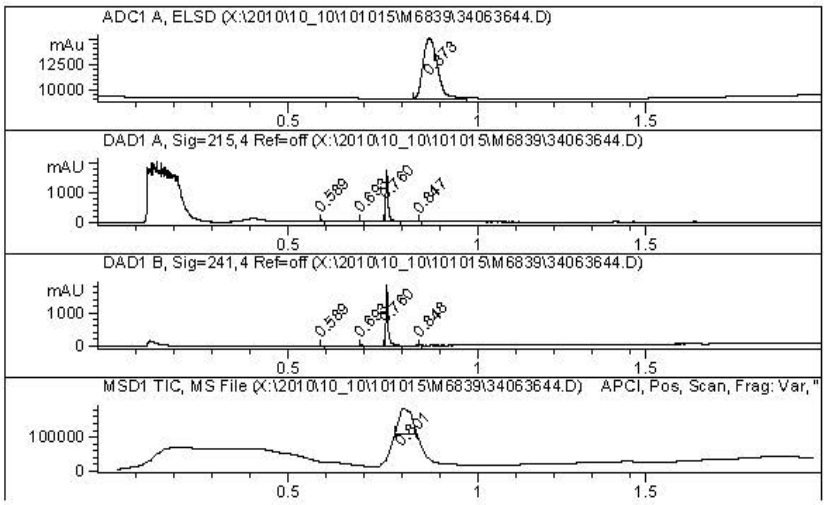
Agilent 1100 LC/MSD SL
Diodearrey G1315B (DAD1A-215nm; DAD1B-254nm)
Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

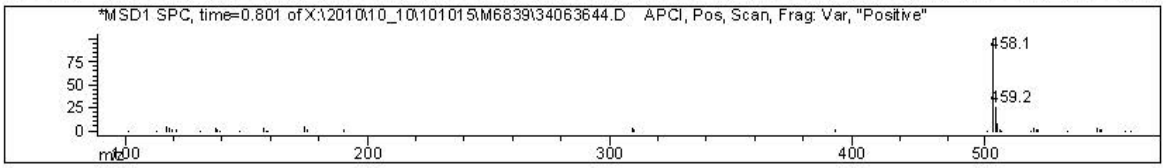
Mobile Phase:A-H2O+0.1%HCOOH;B-MeCN+0.1HCOOH
Separation column:
Rapid Resolutionn HT Cartige 4.6x30mm,
1.8-Micron, Zorbx SB-C18



Mol.Weight: 457.51

M6839 ->





#	Signal	R.Time	Area %
1	ADC1 A, ELSD	0.873	100.000

#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.589	1.990
2		0.693	1.011
3		0.760	96.705
4		0.847	0.293

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.589	0.537
2		0.693	1.114
3		0.760	98.030
4		0.848	0.319

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.801	100.000

Figure S82. LC/MS data for 8-(morpholinosulfonyl)-2-[4-(2-oxopyrrolidin-1-yl)benzyl]-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13e**.

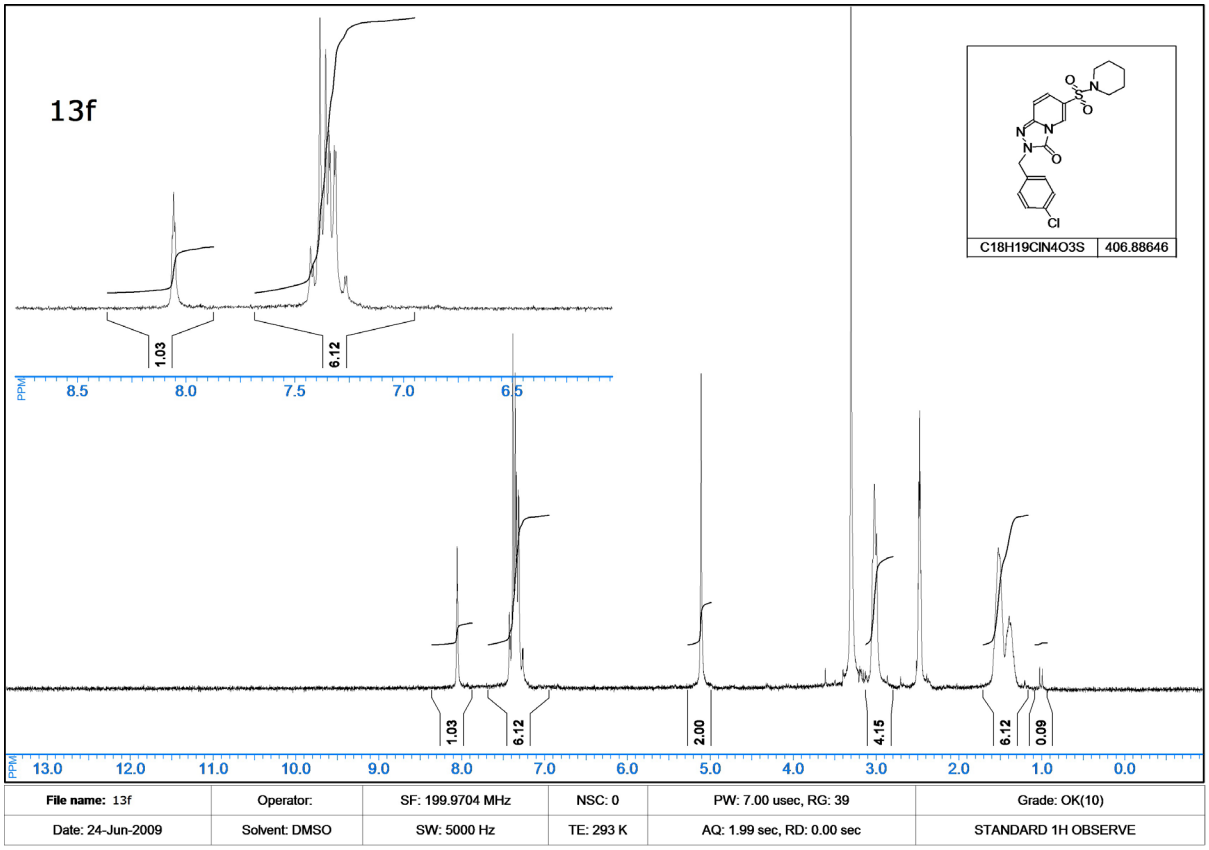


Figure S83. ^{1}H NMR spectrum (200 MHz, DMSO-d6) of 2-(4-chlorobenzyl)-6-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13f**.

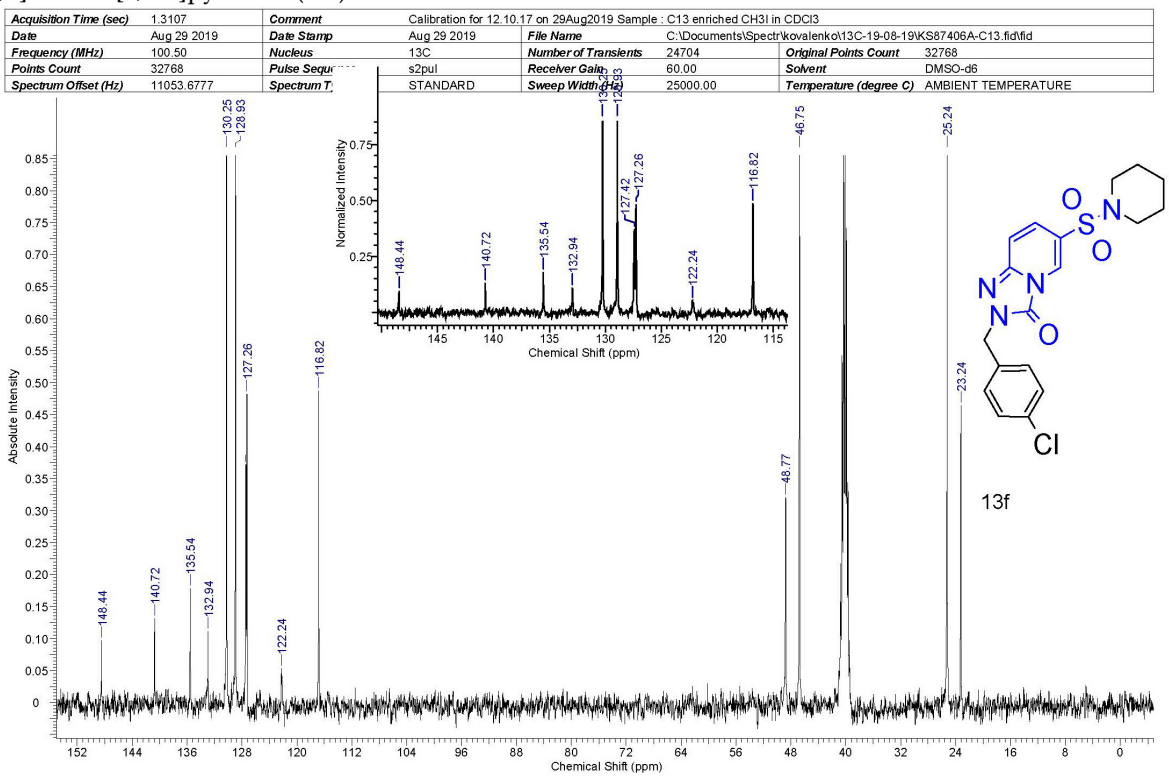


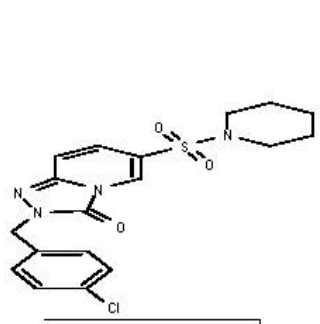
Figure S84. ^{13}C NMR spectrum (100 MHz, DMSO-d6) of 2-(4-chlorobenzyl)-6-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13f**.

X:\2010\10_10\101023\M6914\34068349.D Sample Name: 13f Page 1 of 1

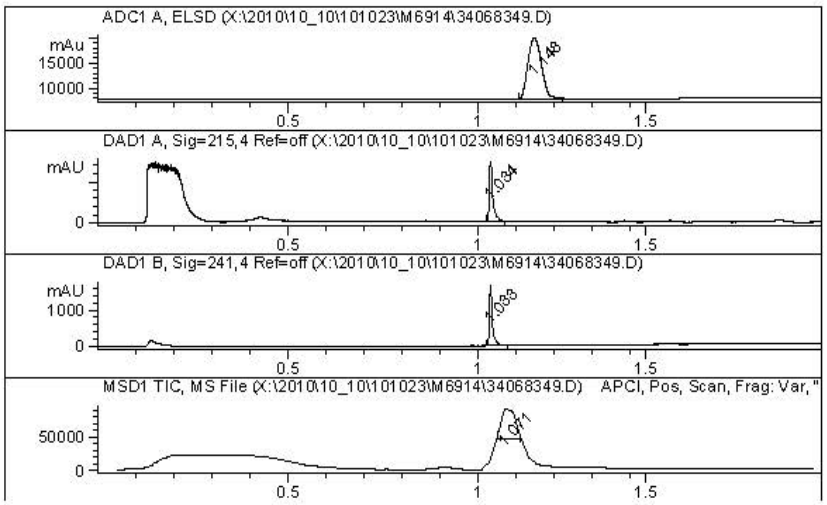
-.o.-Syntez Purity Report -.o.-

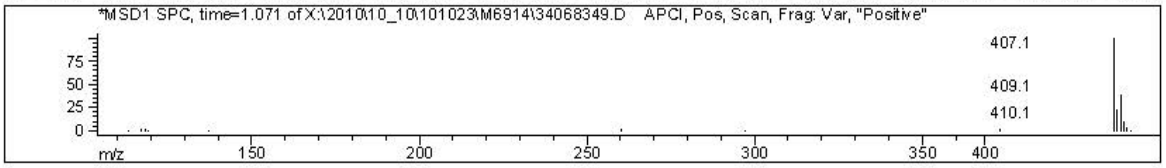
Agilent 1100 LC/MSD SL
Diodearrey G1315B (DAD1A-215nm; DAD1B-254nm)
Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

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



M6914 ->





#	Signal	R.Time	Area %
1	ADC1 A, ELSD	1.148	100.000

#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	1.034	100.000

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	1.033	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.071	100.000

Figure S85. LC/MS data for 2-(4-chlorobenzyl)-6-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13f**.

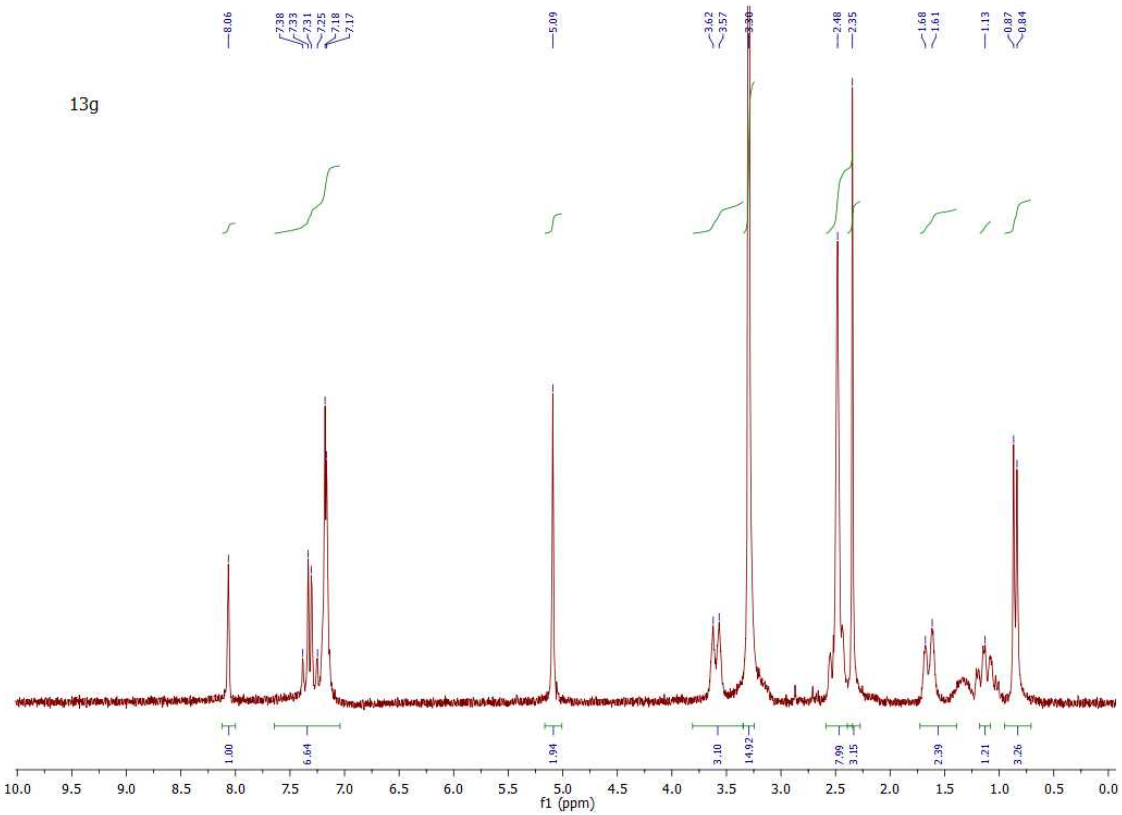


Figure S86. [1]H NMR spectrum (200 MHz, DMSO-d6) of 2-(3-methylbenzyl)-6-(4-methylpiperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13g**.

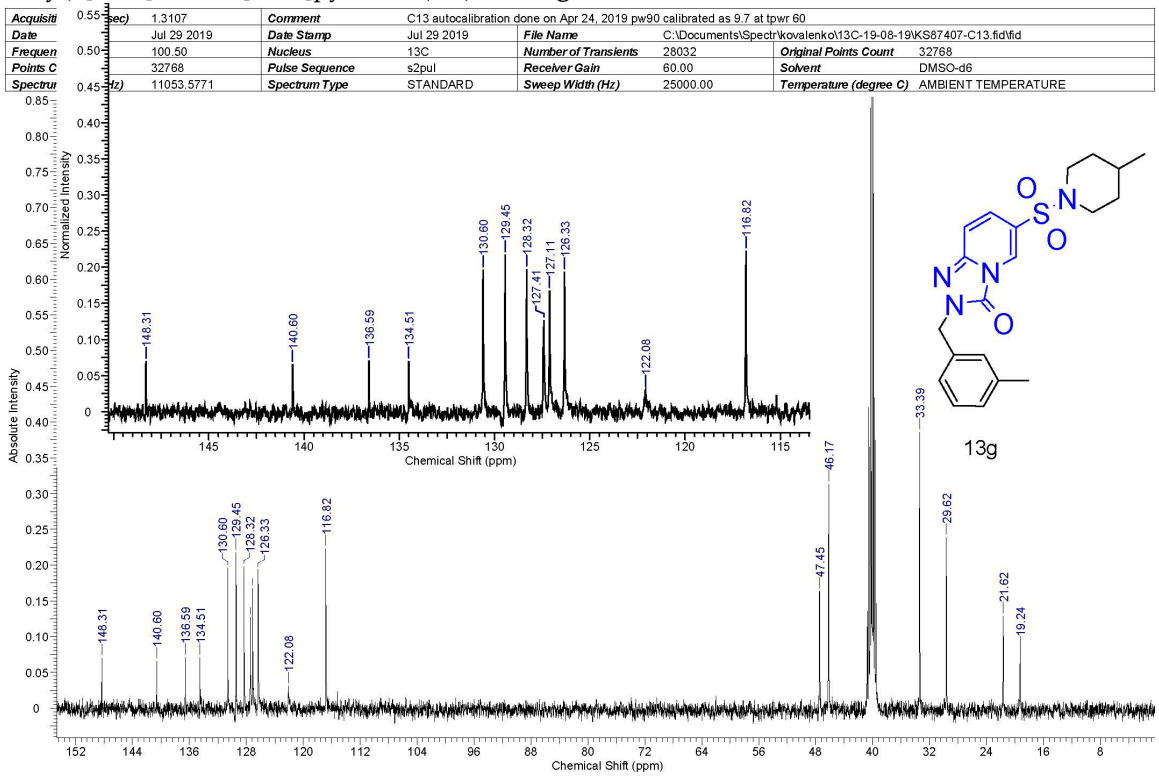


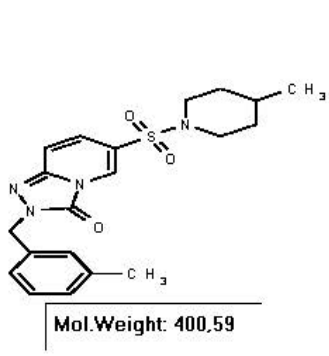
Figure S87. [13]C NMR spectrum (100 MHz, DMSO-d6) of 2-(3-methylbenzyl)-6-(4-methylpiperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13g**.

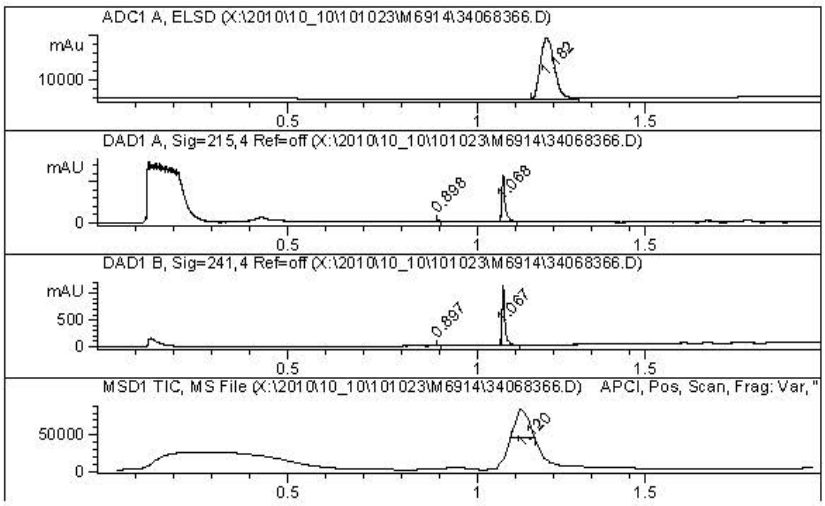
X:\2010\10_10\101023\M6914\34068366.D Sample Name: 13g Page 1 of 1

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

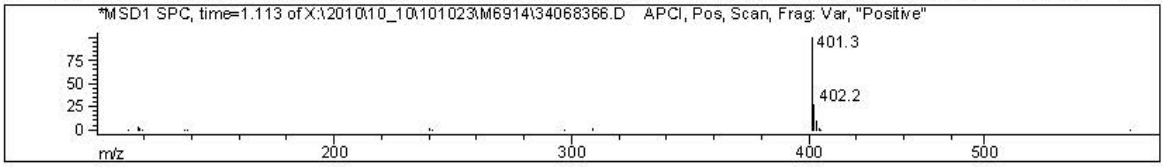
Agilent 1100 LC/MSD SL
Diodearrey G1315B (DAD1A-215nm; DAD1B-254nm)
Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

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





M6914 ->



#	Signal	R.Time	Area %
1	ADC1 A, ELSD	1.182	100.000

#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.898	1.457
2		1.068	98.543

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.897	0.761
2		1.067	99.239

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.120	100.000

Figure S88. LC/MS data for 2-(3-methylbenzyl)-6-(4-methylpiperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13g**.

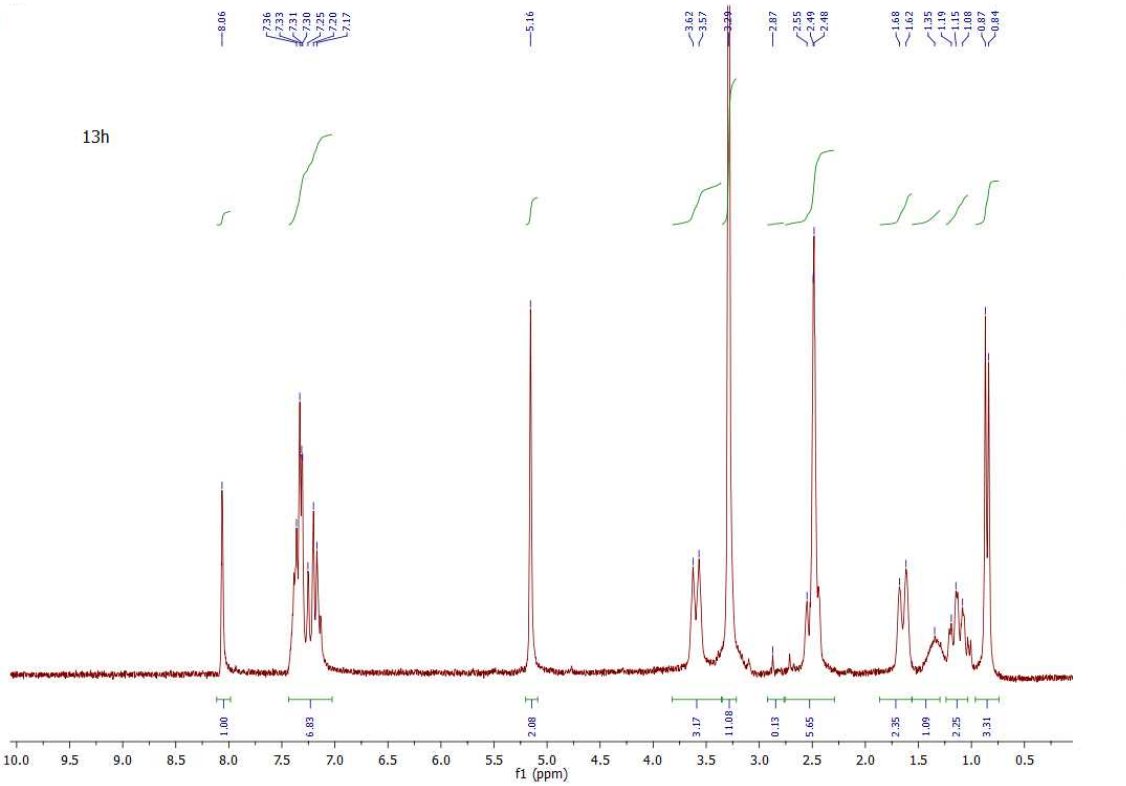


Figure S89. ^{1}H NMR spectrum (200 MHz, DMSO-d6) of 2-(2-fluorobenzyl)-6-(4-methylpiperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13h**.

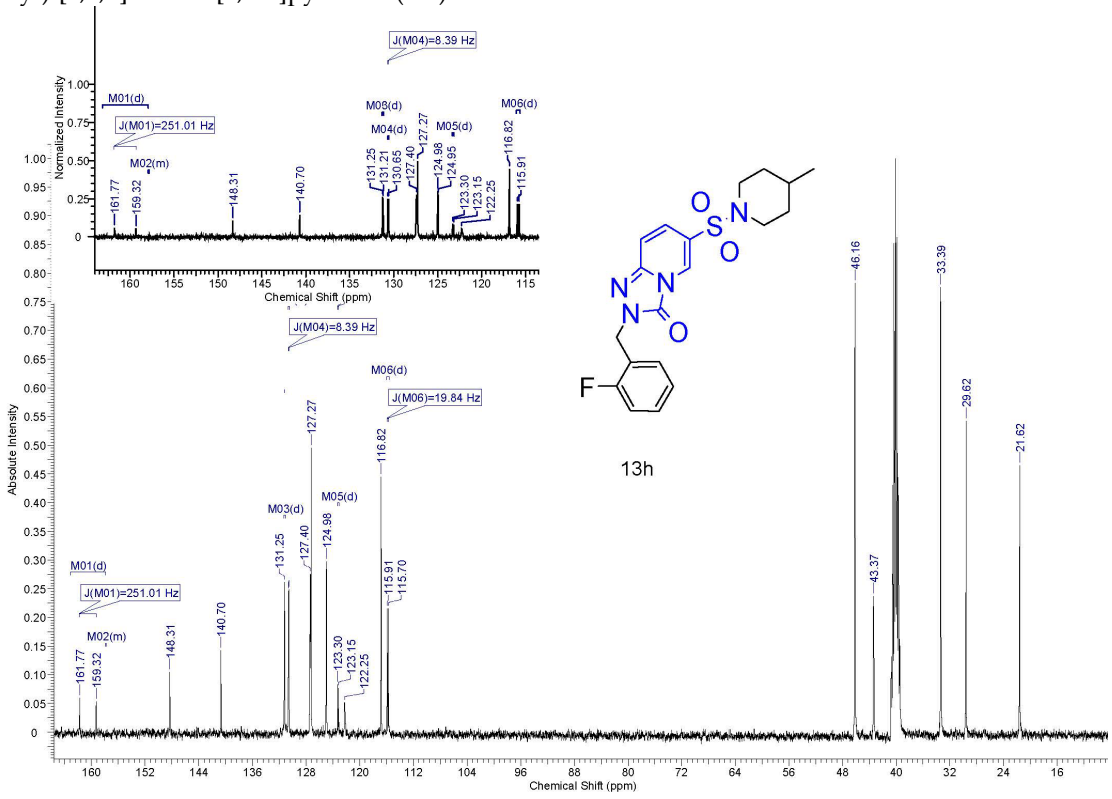


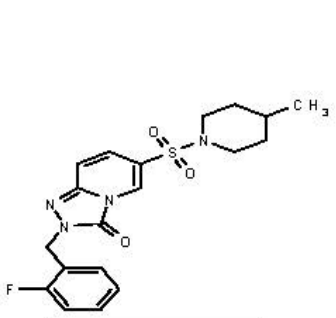
Figure S90. ^{13}C NMR spectrum (100 MHz, DMSO-d6) of 2-(2-fluorobenzyl)-6-(4-methylpiperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13h**.

X:\2010\10_10\101023\M6914\34068371.D Sample Name: 13h Page 1 of

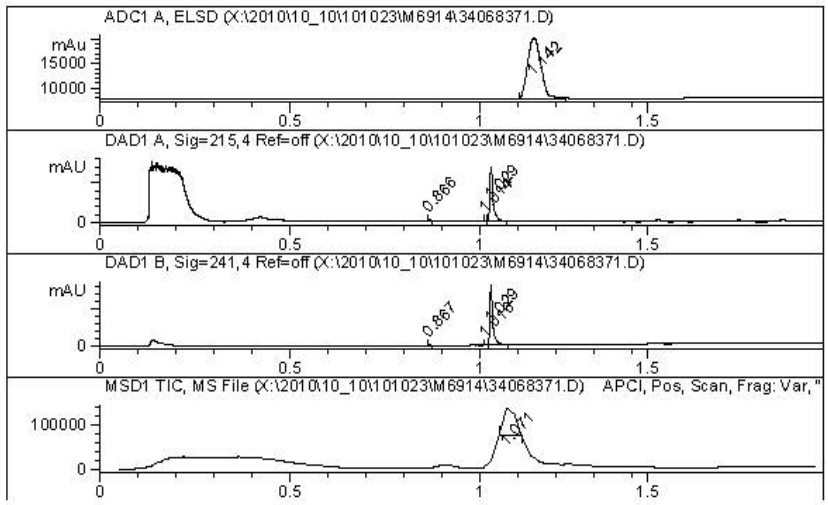
-.o.-Syntez Purity Report -.o.-

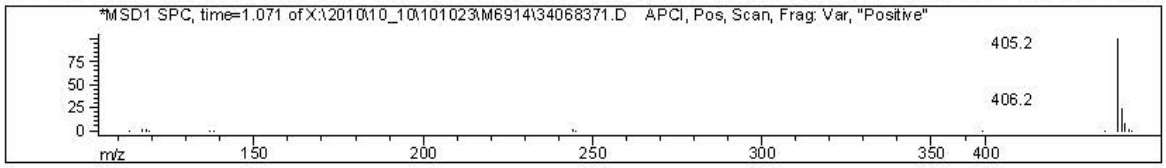
Agilent 1100 LC/MSD SL
Diodearrey G1315B (DAD1A-215nm; DAD1B-254nm)
Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

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



M6914 ->





#	Signal	R.Time	Area %
1	ADC1 A, ELSD	1.142	100.000

#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.866	1.103
2		1.014	0.597
3		1.029	98.300

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.867	0.713
2		1.016	0.493
3		1.029	98.793

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.071	100.000

Figure S91. LC/MS data for 2-(2-fluorobenzyl)-6-(4-methylpiperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13h**.

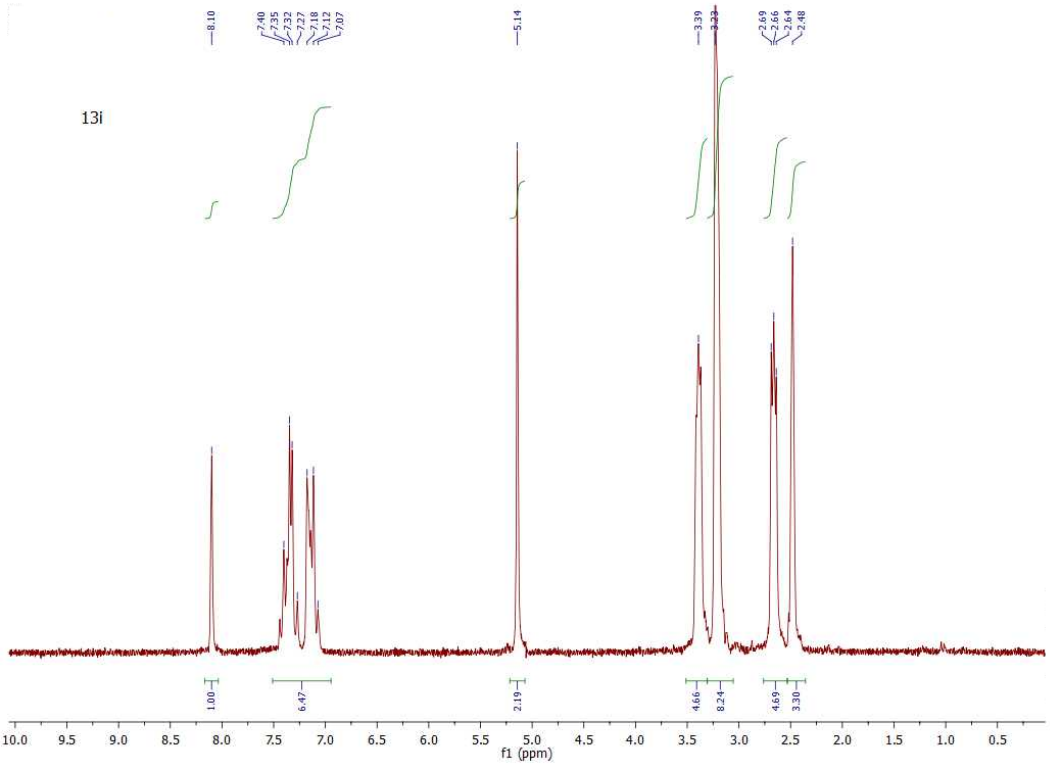


Figure S92. [1]H NMR spectrum (200 MHz, DMSO-d6) of 2-(3-fluorobenzyl)-6-(thiomorpholinosulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13i**.

Acquisition Time (sec)	1.3107	*Comment*	C13 autocalibration done on Apr 24, 2019 pw90 calibrated as 9.7 at tpwr 60				
Date	Jul 24 2019	*Date Stamp*	Jul 24 2019	*File Name*			
Frequency (MHz)	100.50	*Nucleus*	13C	*Number of Transients*	23744	*Original Points Count*	32768
Points Count	32768	*Pulse Sequence*	s2pul	*Receiver Gain*	60.00	*Solvent*	DMSO-d6
Spectrum Offset (Hz)	11053.5771	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	25000.00	*Temperature (degree C)*	AMBIENT TEMPERATURE

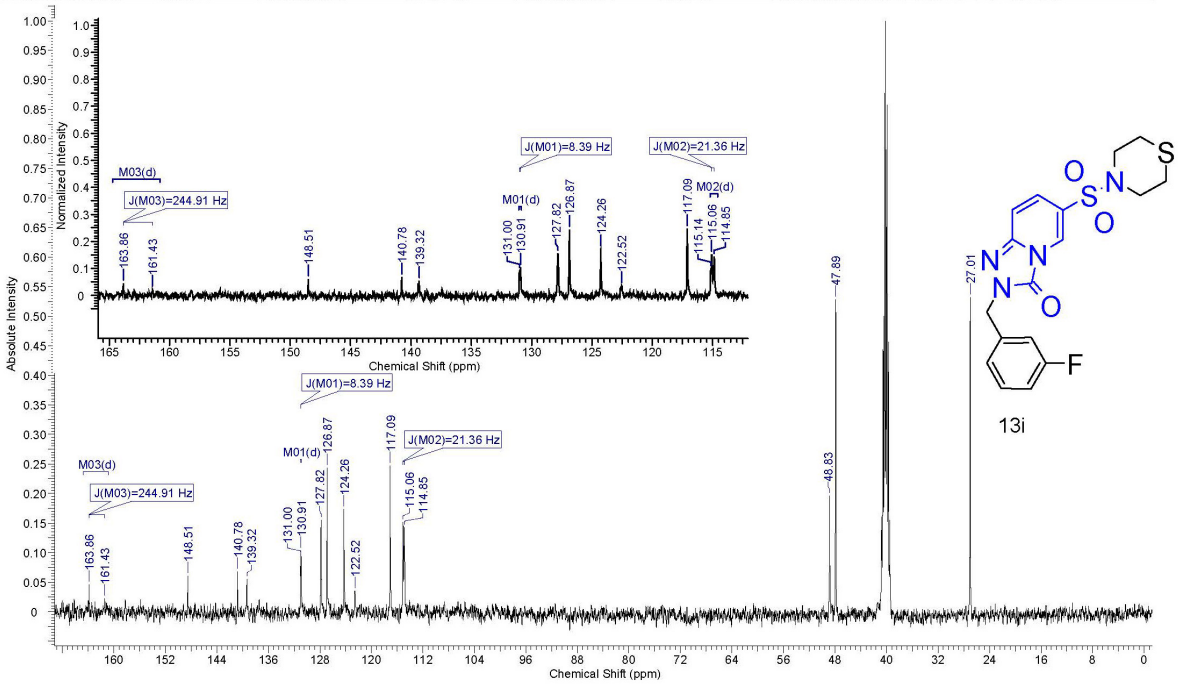


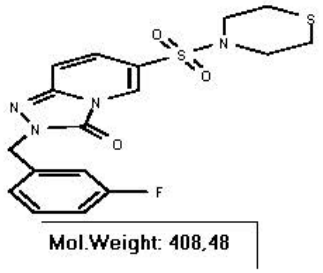
Figure S93. [13]C NMR spectrum (100 MHz, DMSO-d6) of 2-(3-fluorobenzyl)-6-(thiomorpholinosulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13i**.

X:\2010\10_10\101023\M6919\34068431.D Sample Name: 13i Page 1 of 1

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

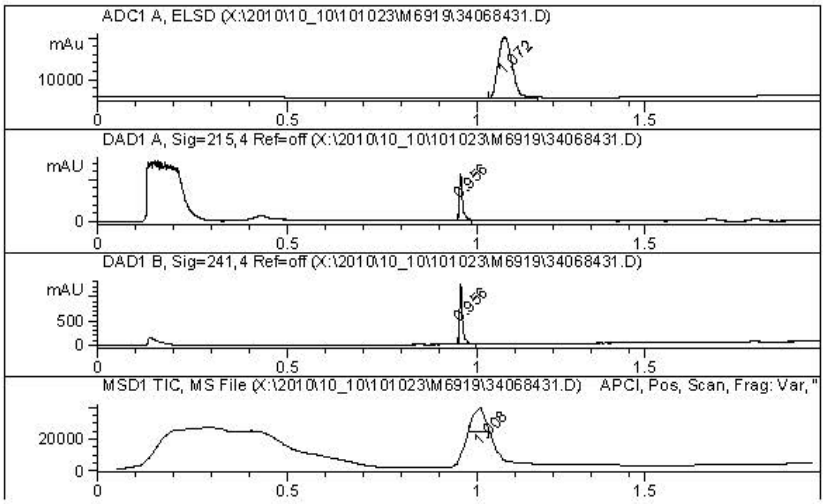
Agilent 1100 LC/MSD SL
Diodearrey G1315B (DAD1A-215nm; DAD1B-254nm)
Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

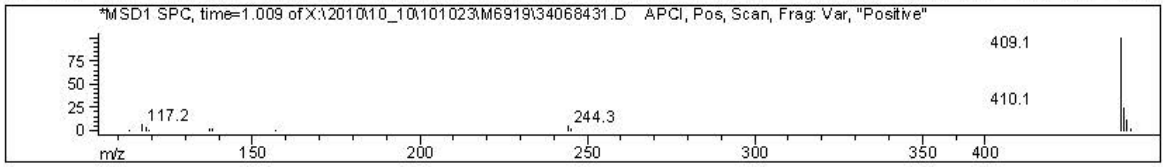
Mobile Phase:A-H2O+0.1%HCOOH;B-MeCN+0.1HCOOH
Separation column:
Rapid Resolutionn HT Cartige 4.6x30mm,
1.8-Micron, Zorbx SB-C18



Mol.Weight: 408,48

M6919 ->





#	Signal	R.Time	Area %
1	ADC1 A, ELSD	1.072	100.000

#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.956	100.000

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.956	100.000

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

Figure S94. LC/MS data for 2-(3-fluorobenzyl)-6-(thiomorpholinosulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13i**.

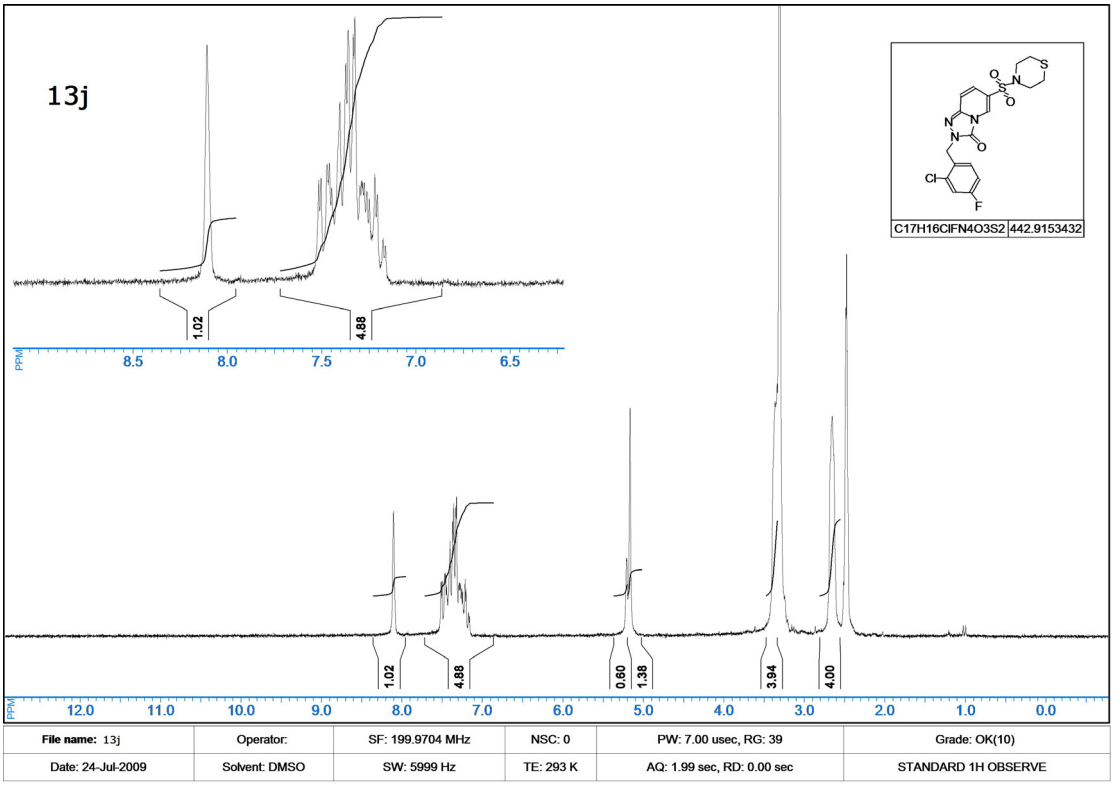


Figure S95. ^{1}H NMR spectrum (200 MHz, DMSO-d6) of 2-(2-chloro-4-fluorobenzyl)-6-(thiomorpholinosulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13j**.

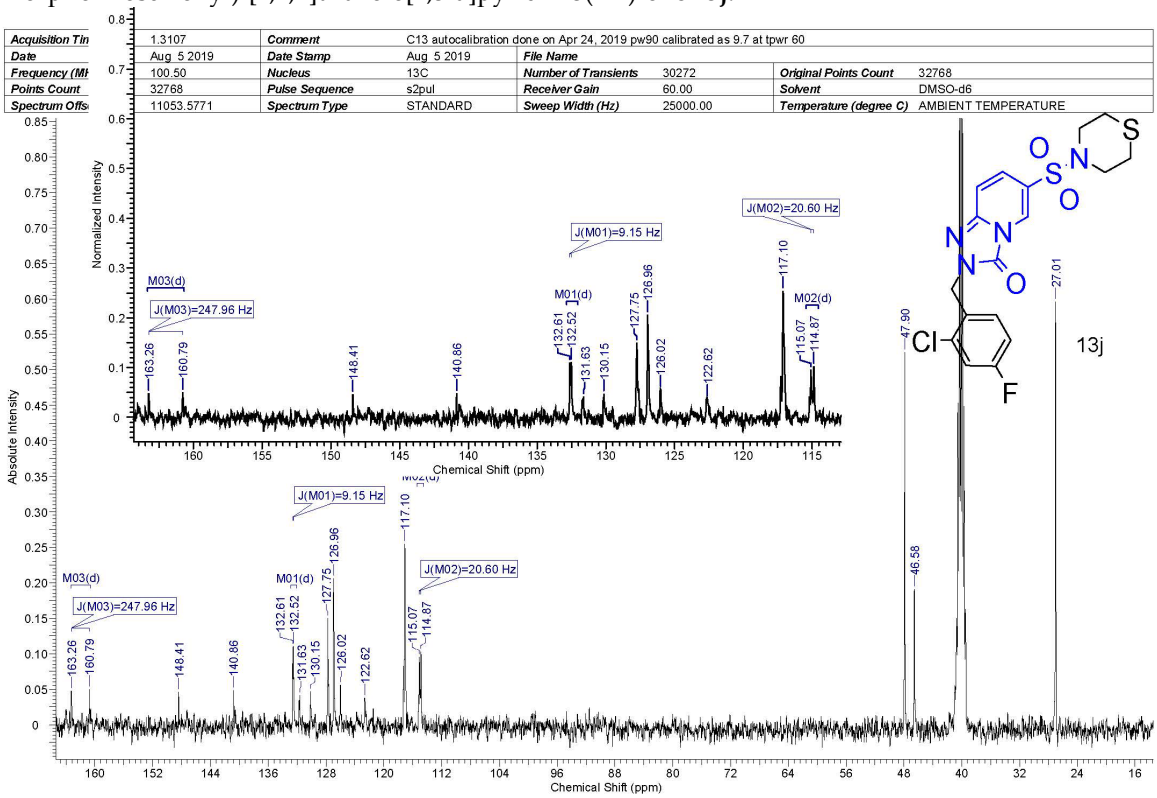


Figure S96. ^{13}C NMR spectrum (100 MHz, DMSO-d6) of 2-(2-chloro-4-fluorobenzyl)-6-(thiomorpholinosulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13j**.

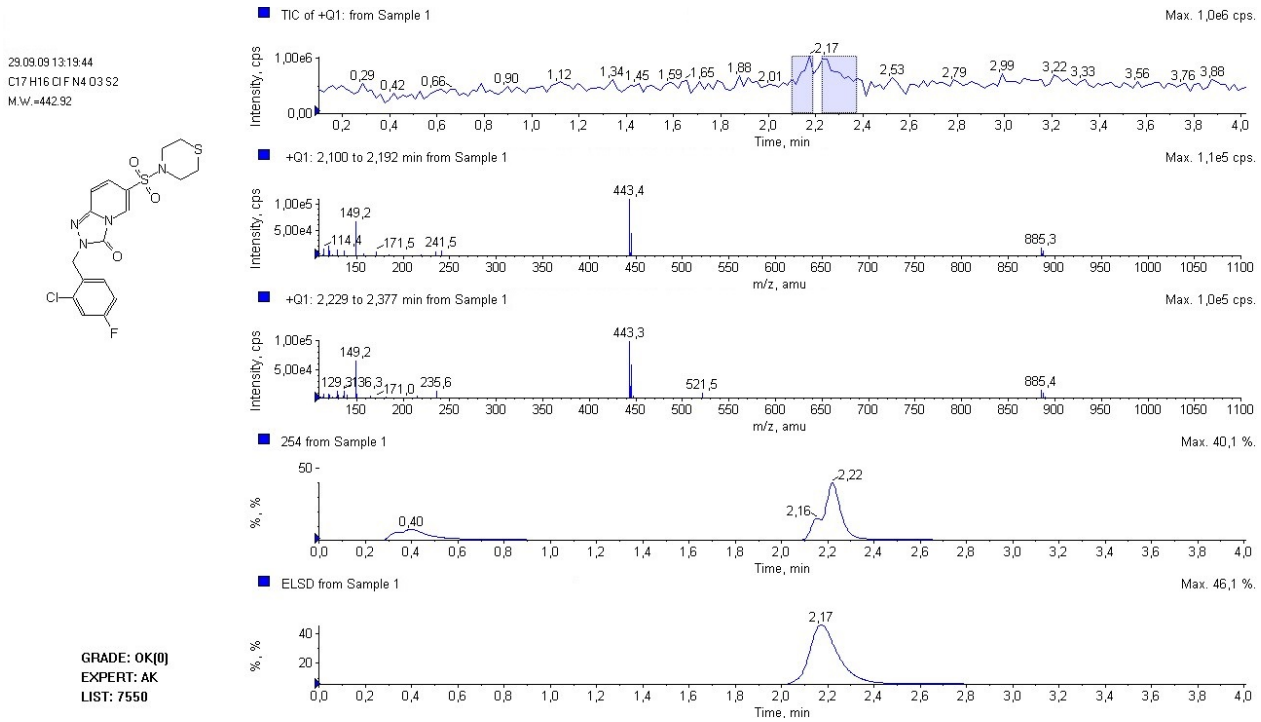


Figure S97. LC/MS data for 2-(2-chloro-4-fluorobenzyl)-6-(thiomorpholinosulfonyl)-[1,2,4]triazolo[4,3-a]pyridin-3(2H)-one **13j**.

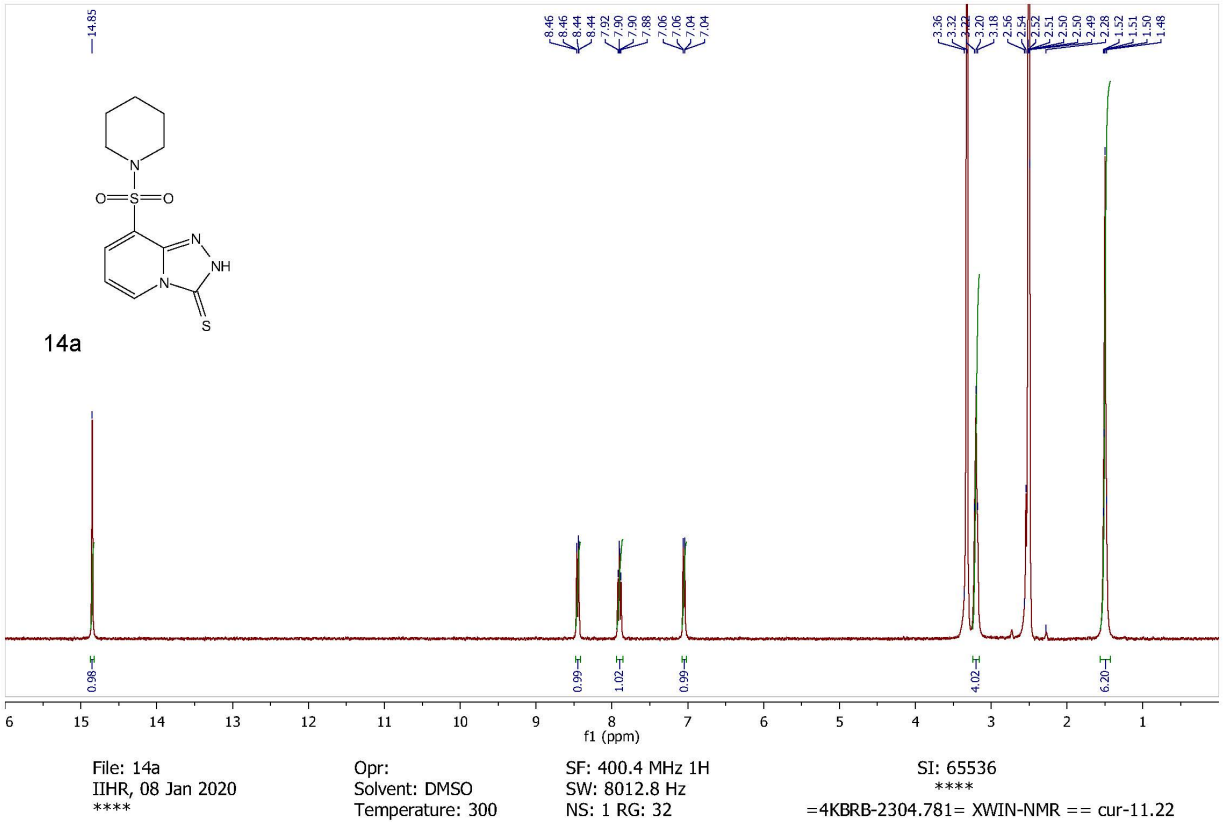


Figure S98. ^{1}H NMR spectrum (400 MHz, DMSO-d6) of 8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine-3(2H)-thione **14a**.

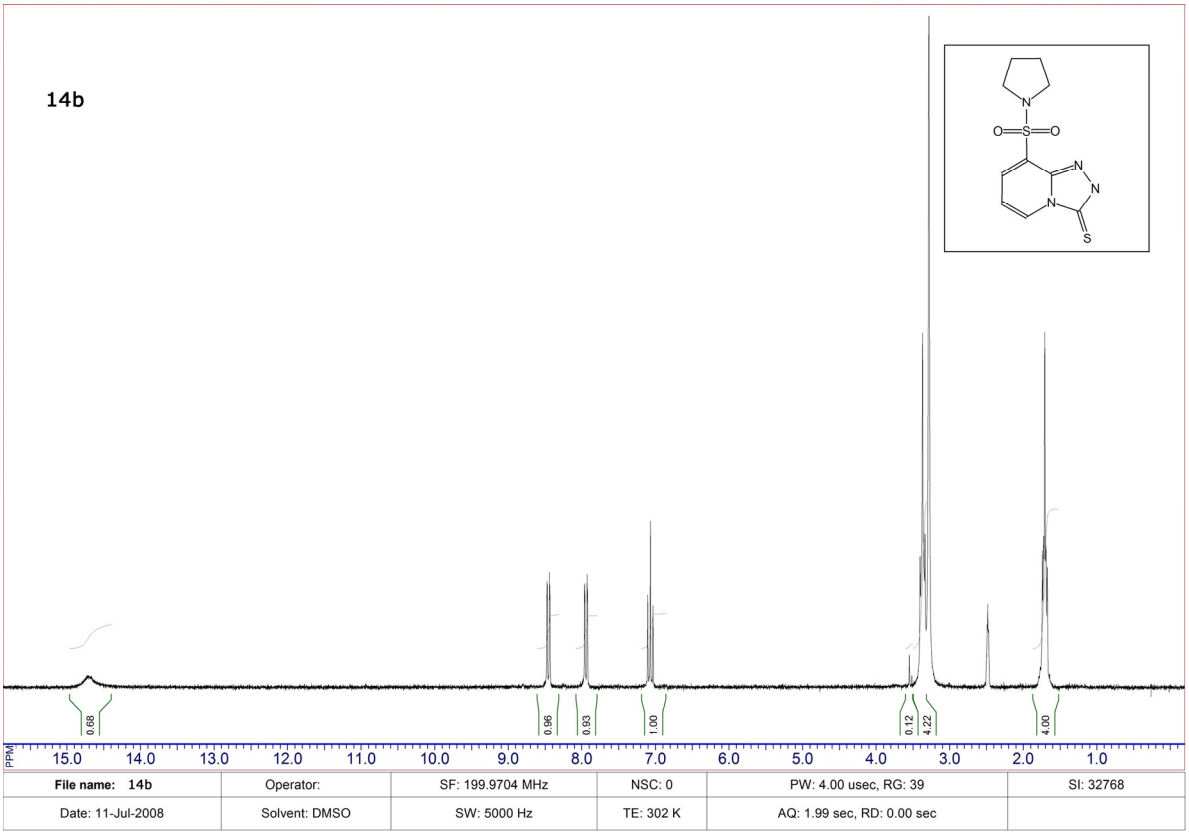


Figure S99. ^{1}H NMR spectrum (200 MHz, DMSO-d6) of 8-(pyrrolidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine-3(2H)-thione **14b**.

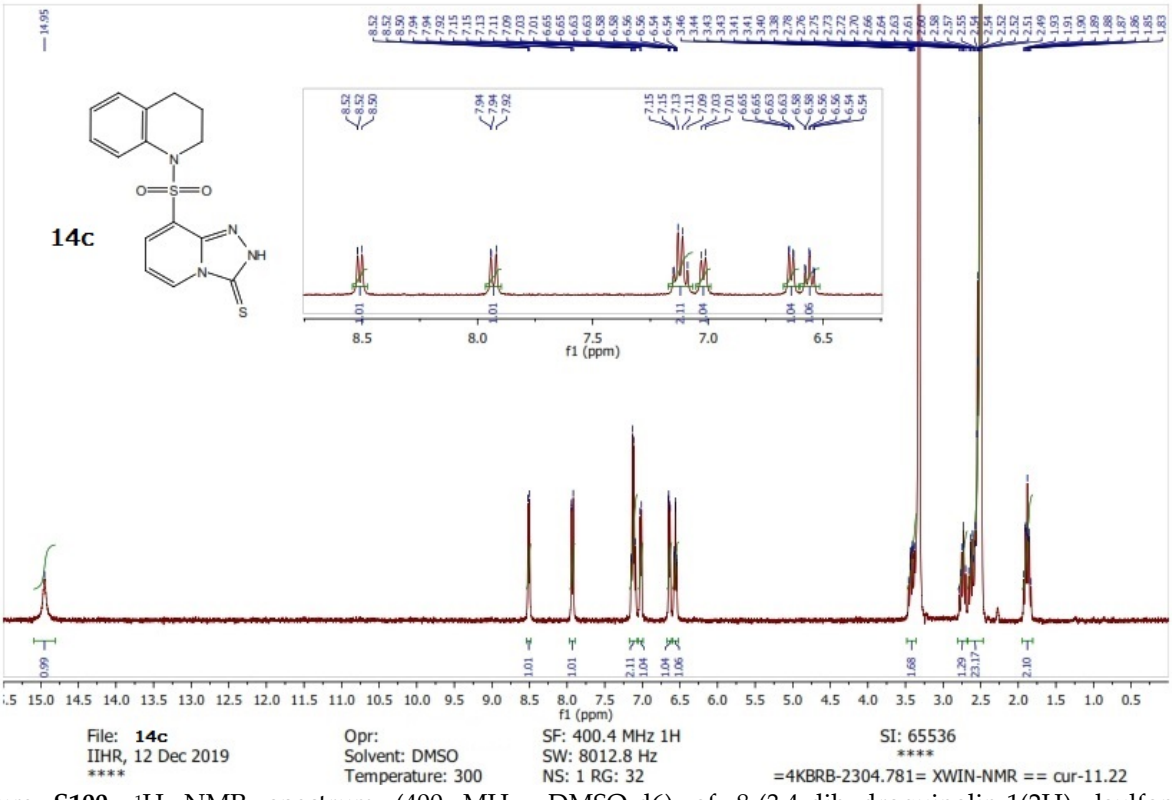


Figure S100. ^{1}H NMR spectrum (400 MHz, DMSO-d6) of 8-(3,4-dihydroquinolin-1(2H)-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine-3(2H)-thione **14c**.

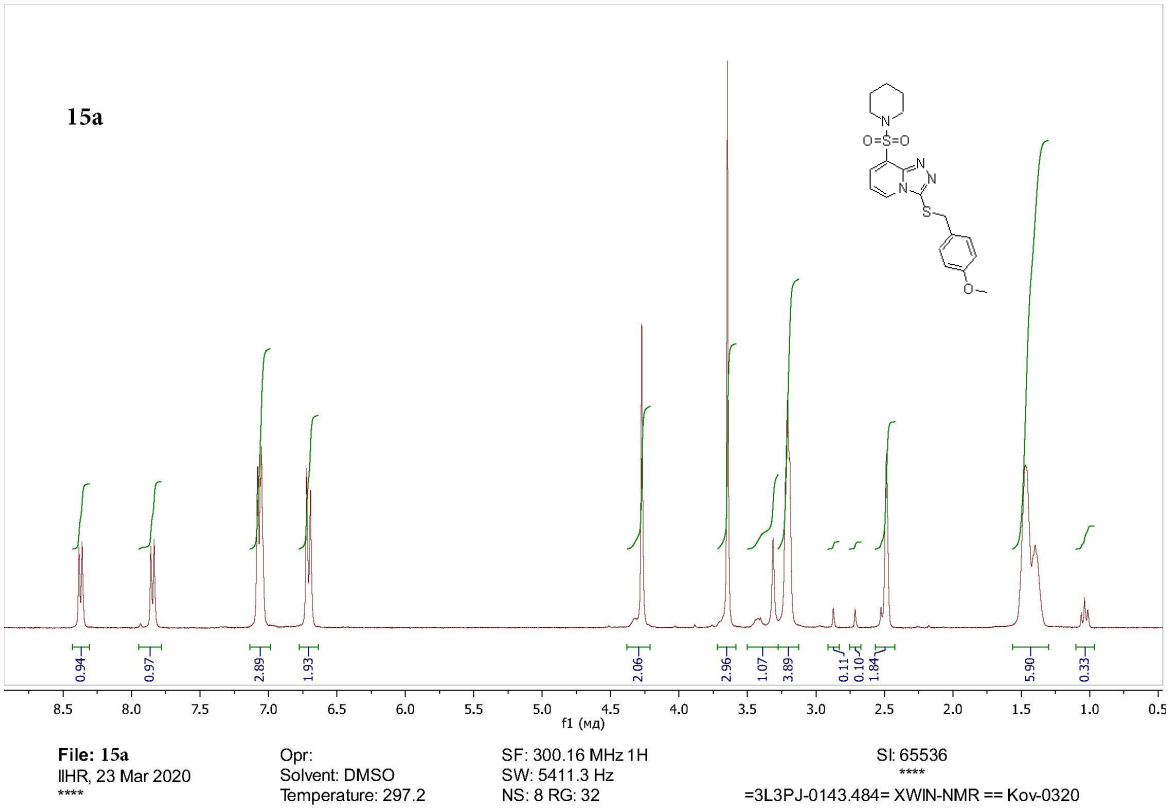


Figure S101. [1]H NMR spectrum (300 MHz, DMSO-d6) of 3-(4-methoxybenzylthio)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15a**.

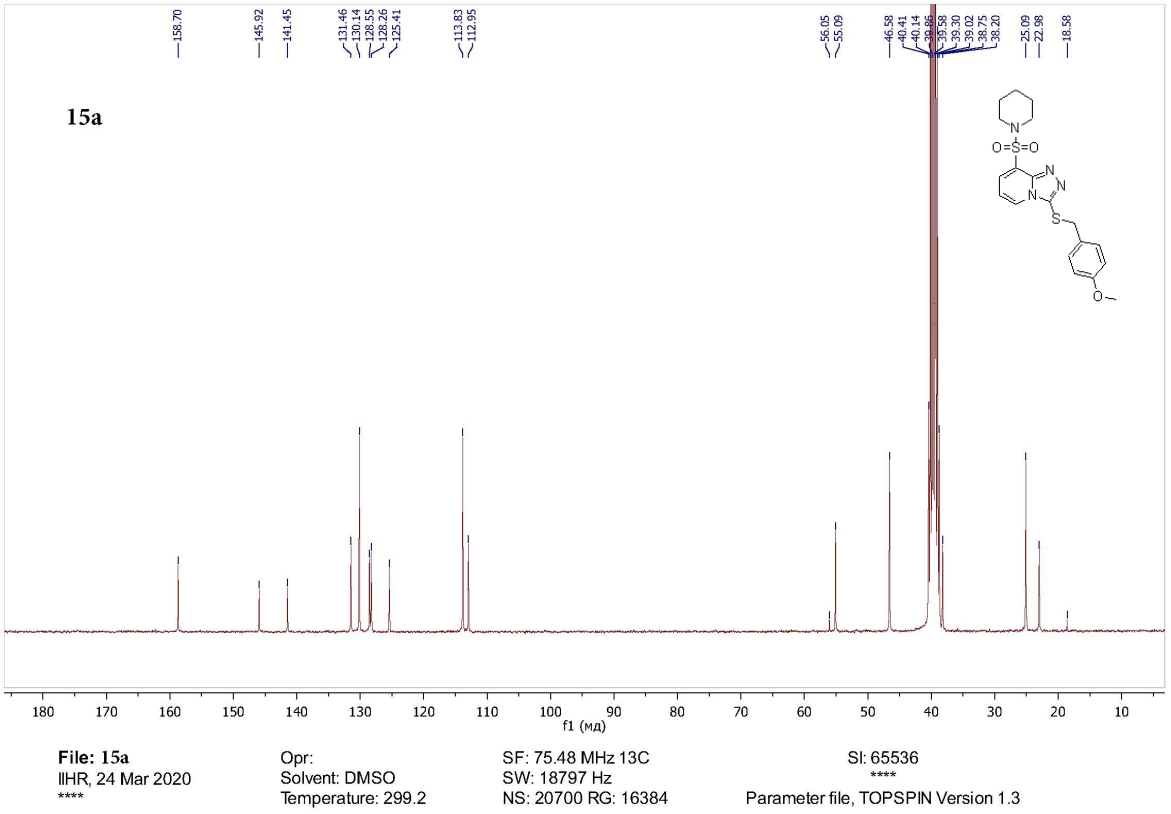


Figure S102. [13]C NMR spectrum (75 MHz, DMSO-d6) of 3-(4-methoxybenzylthio)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15a**.

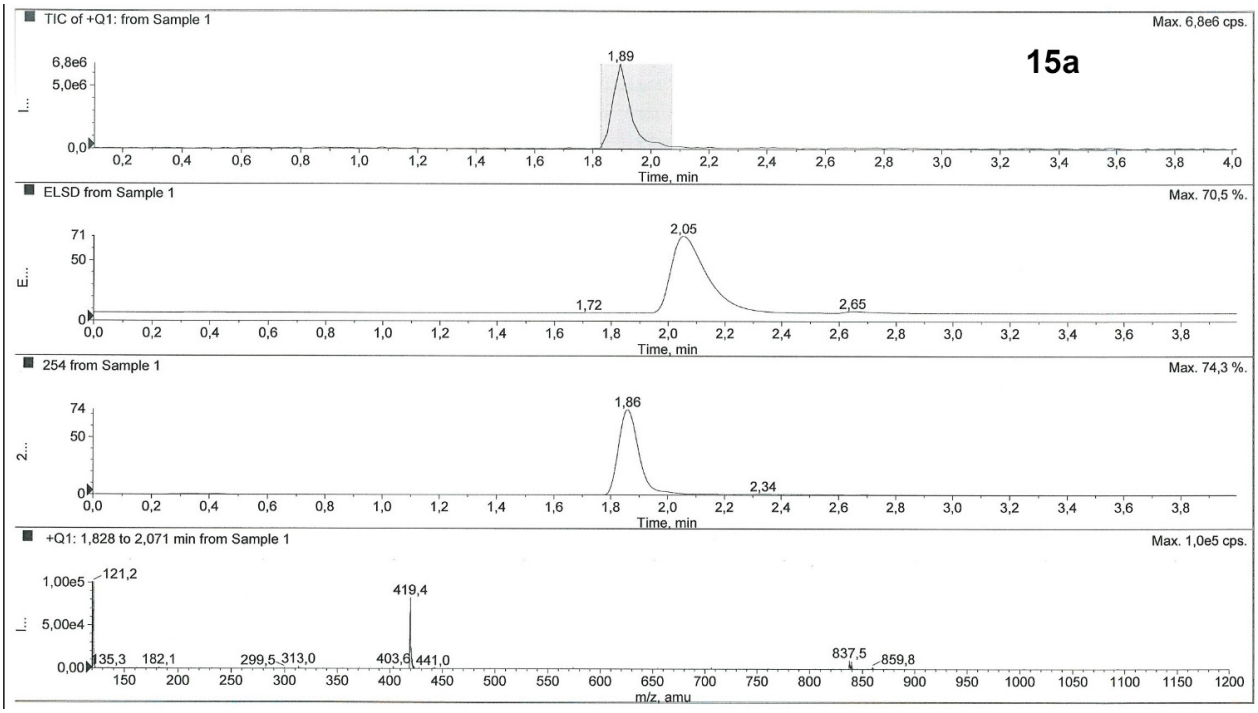


Figure S103. LC/MS data for 3-(4-methoxybenzylthio)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15a**.

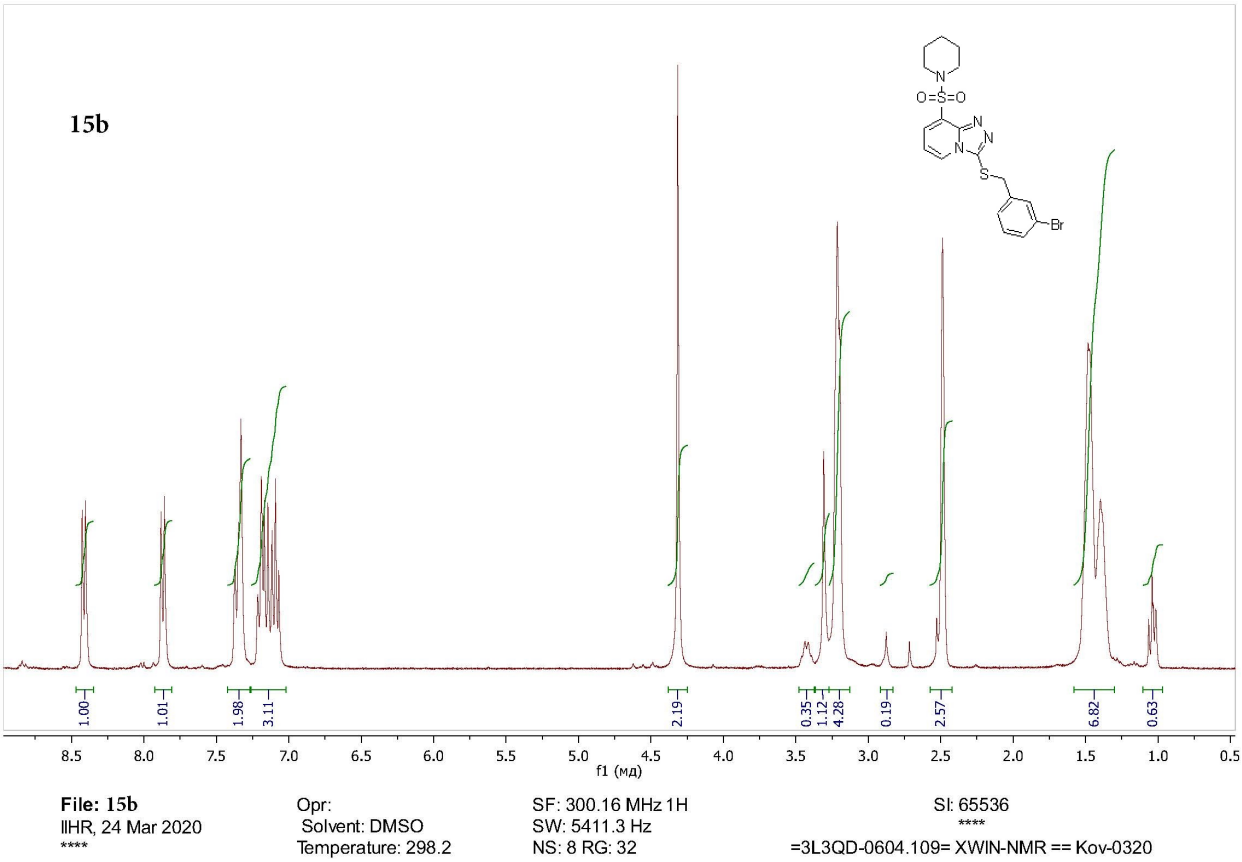


Figure S104. ^{1}H NMR spectrum (300 MHz, DMSO-d6) of 3-(3-bromobenzylthio)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15b**.

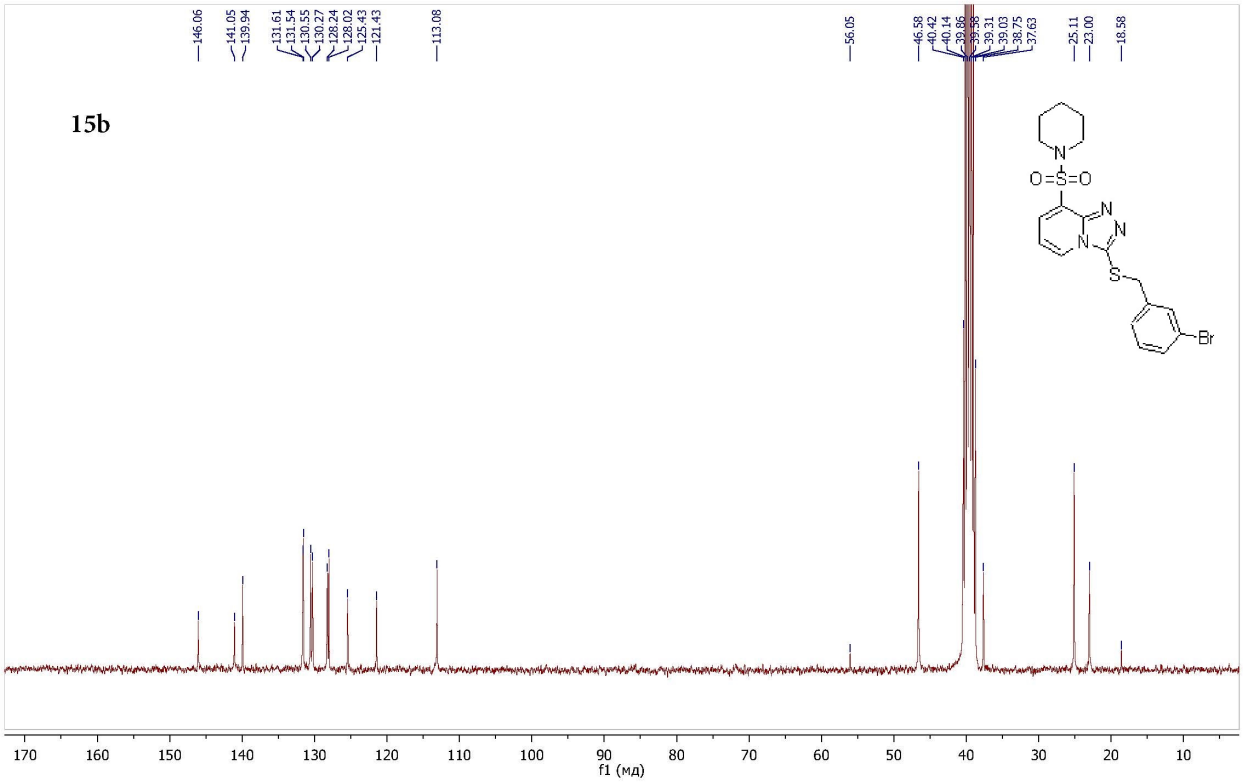


Figure S105. ^{13}C NMR spectrum (75 MHz, DMSO-d6) of 3-(3-bromobenzylthio)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15b**.

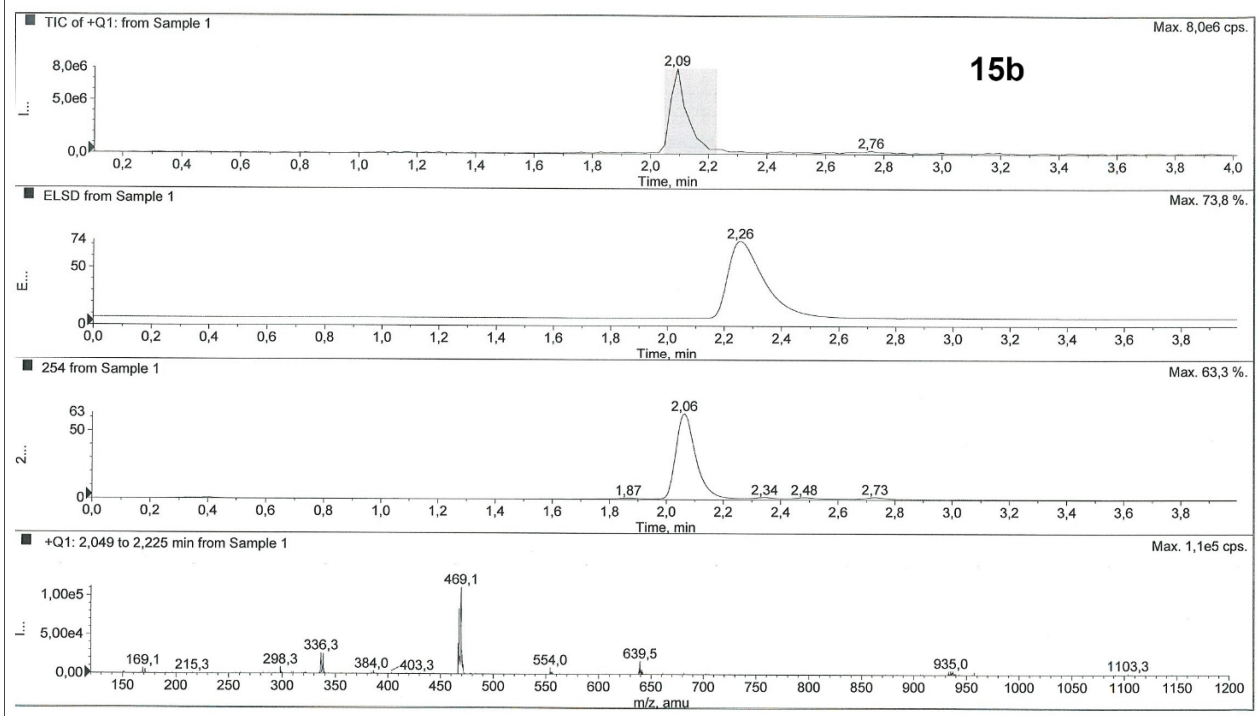


Figure S106. LC/MS data for 3-(3-bromobenzylthio)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15b**.

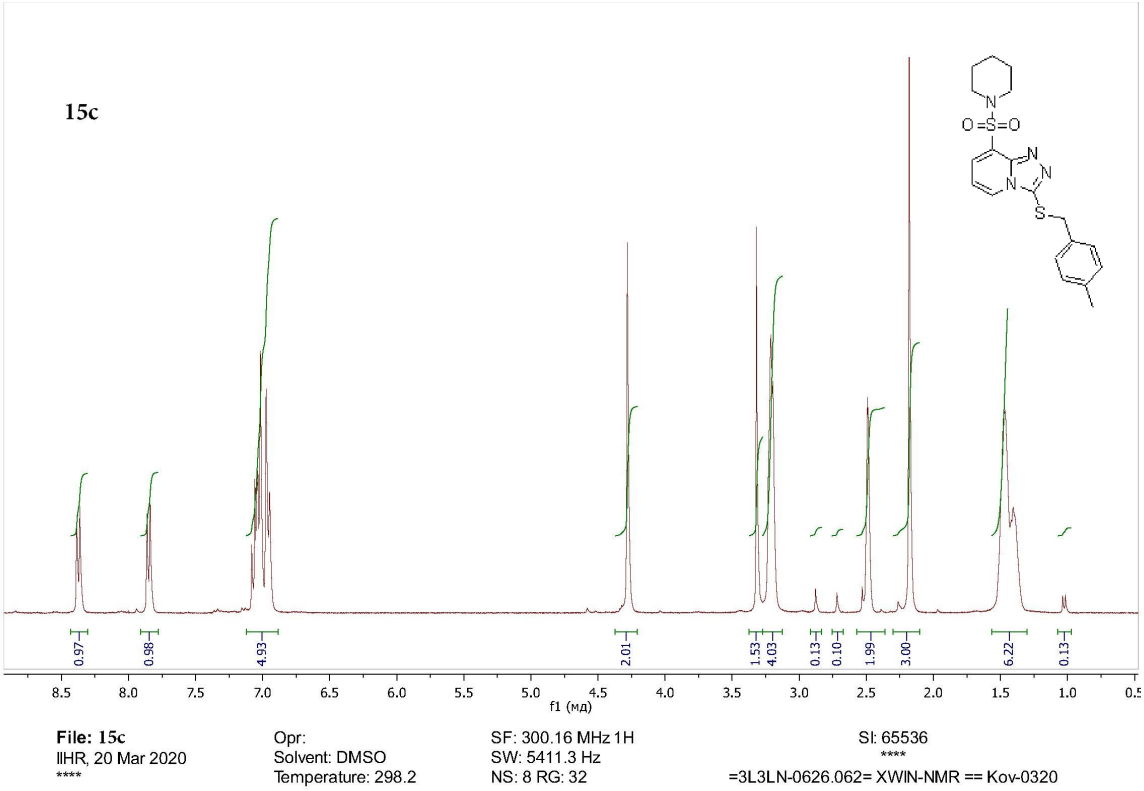


Figure S107. [1]H NMR spectrum (300 MHz, DMSO-d6) of 3-(4-methylbenzylthio)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15c**.

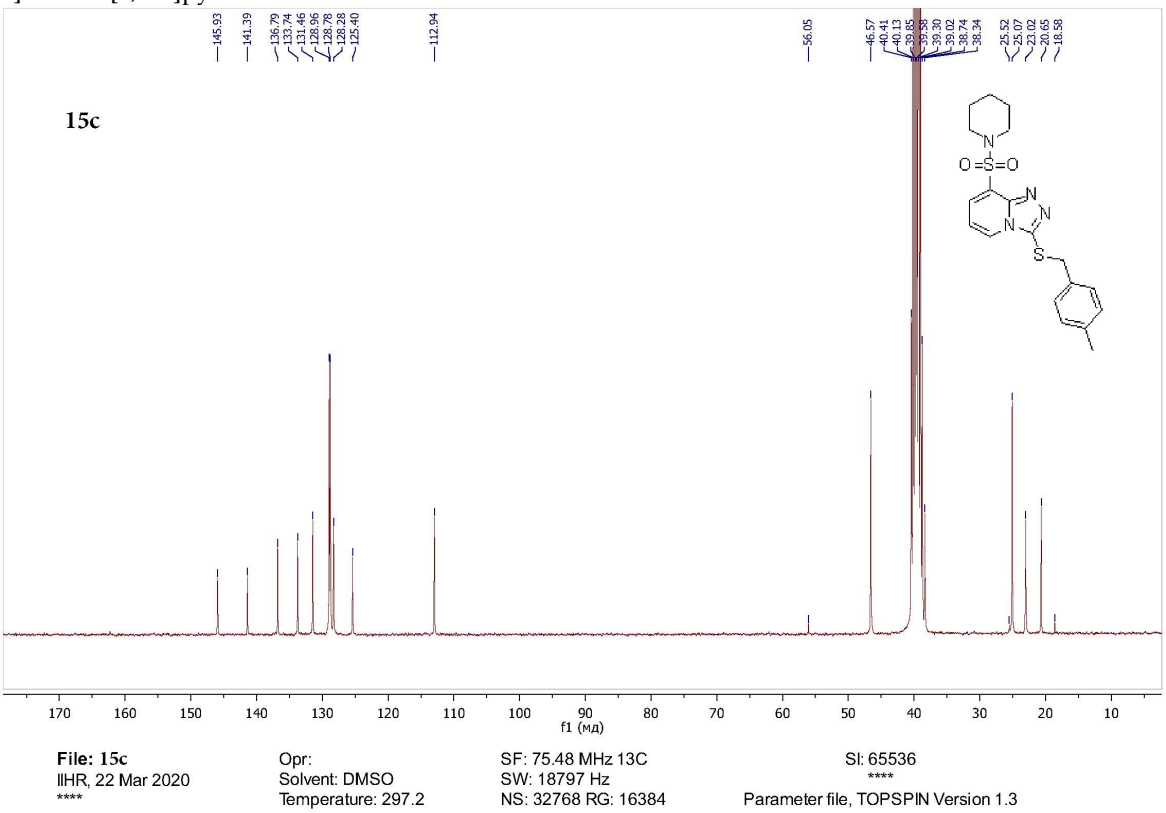


Figure S108. [13]C NMR spectrum (75 MHz, DMSO-d6) of 3-(4-methylbenzylthio)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15c**.

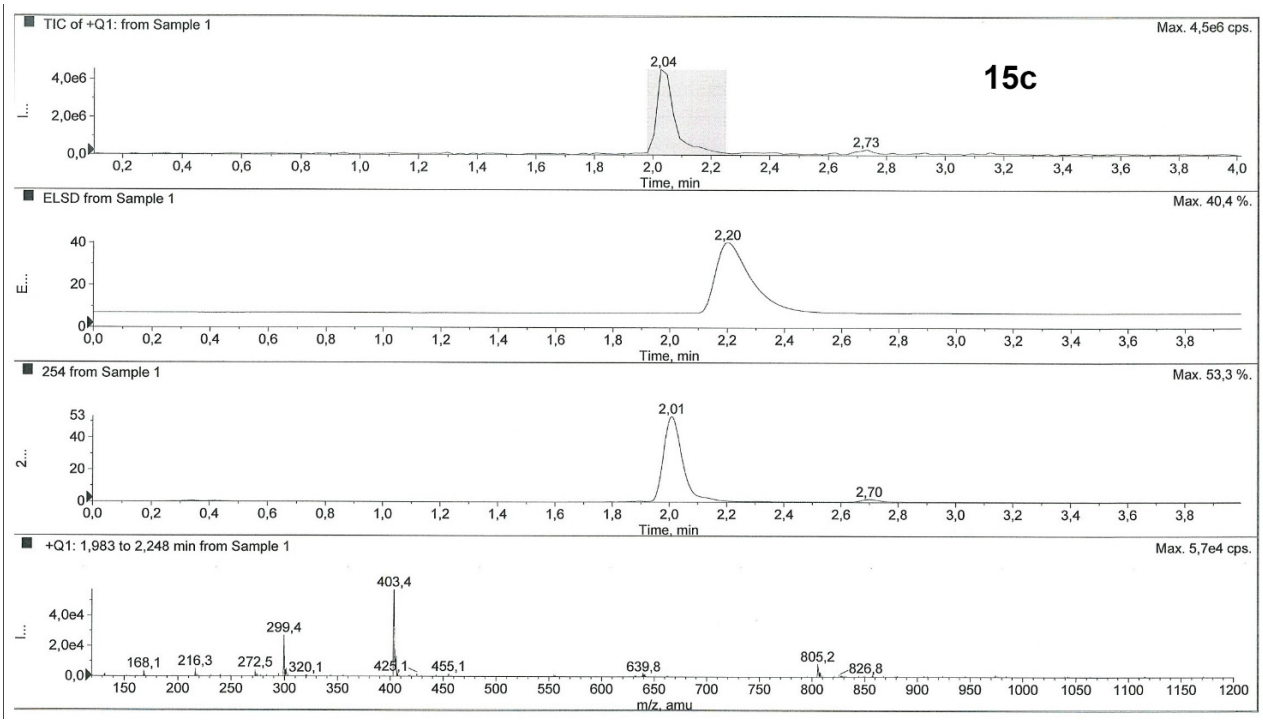


Figure S109. LC/MS data for 3-(4-methylbenzylthio)-8-(piperidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15c**.

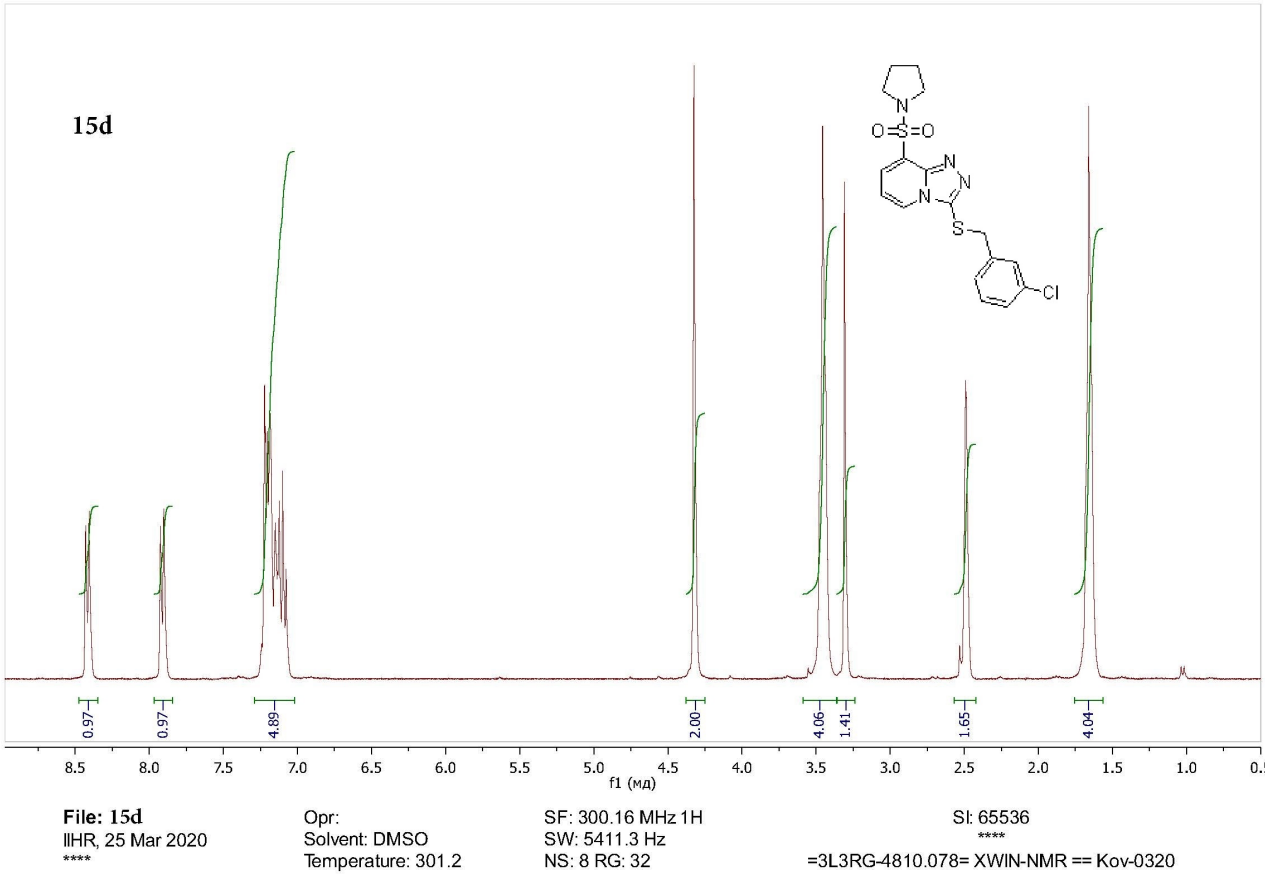


Figure S110. ^{1}H NMR spectrum (300 MHz, DMSO-d6) of 3-(3-chlorobenzylthio)-8-(pyrrolidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15d**.

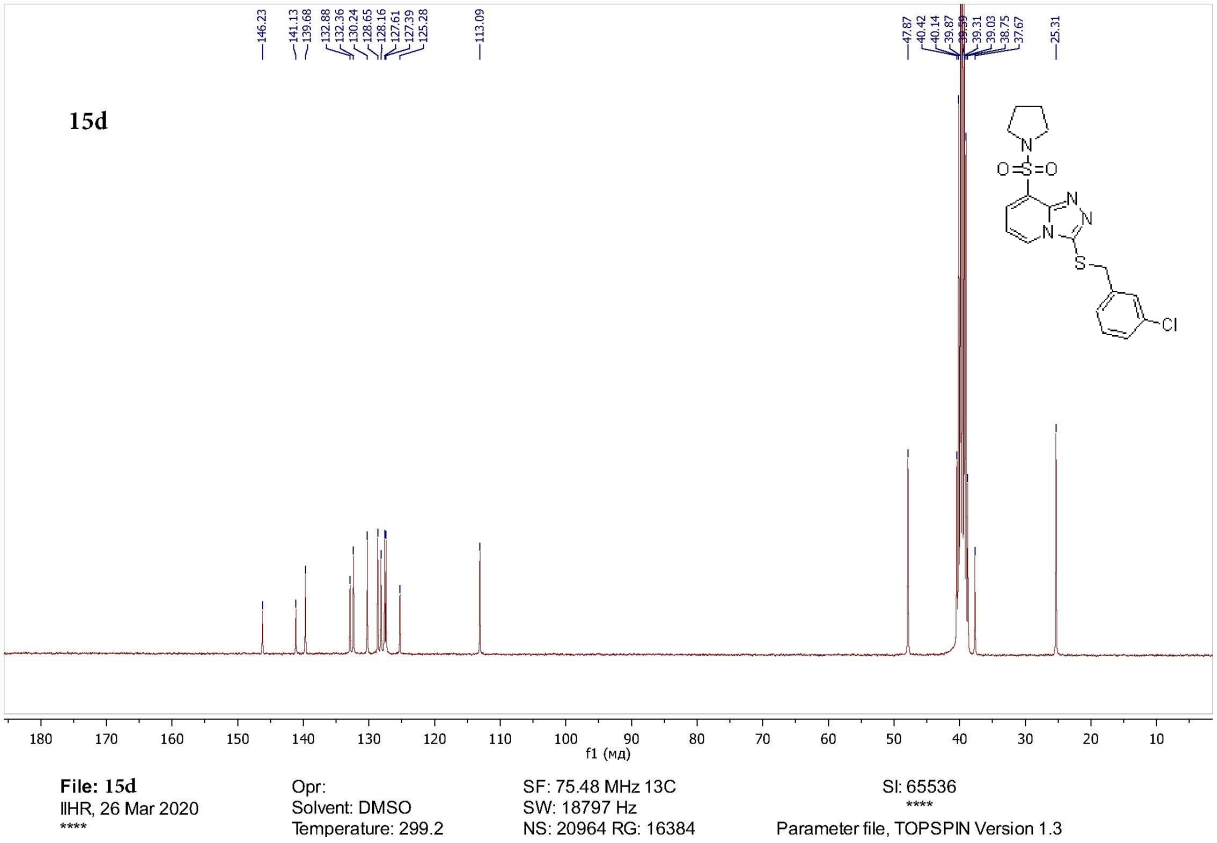


Figure S111. ^{13}C NMR spectrum (75 MHz, DMSO-d6) of 3-(3-chlorobenzylthio)-8-(pyrrolidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15d**.

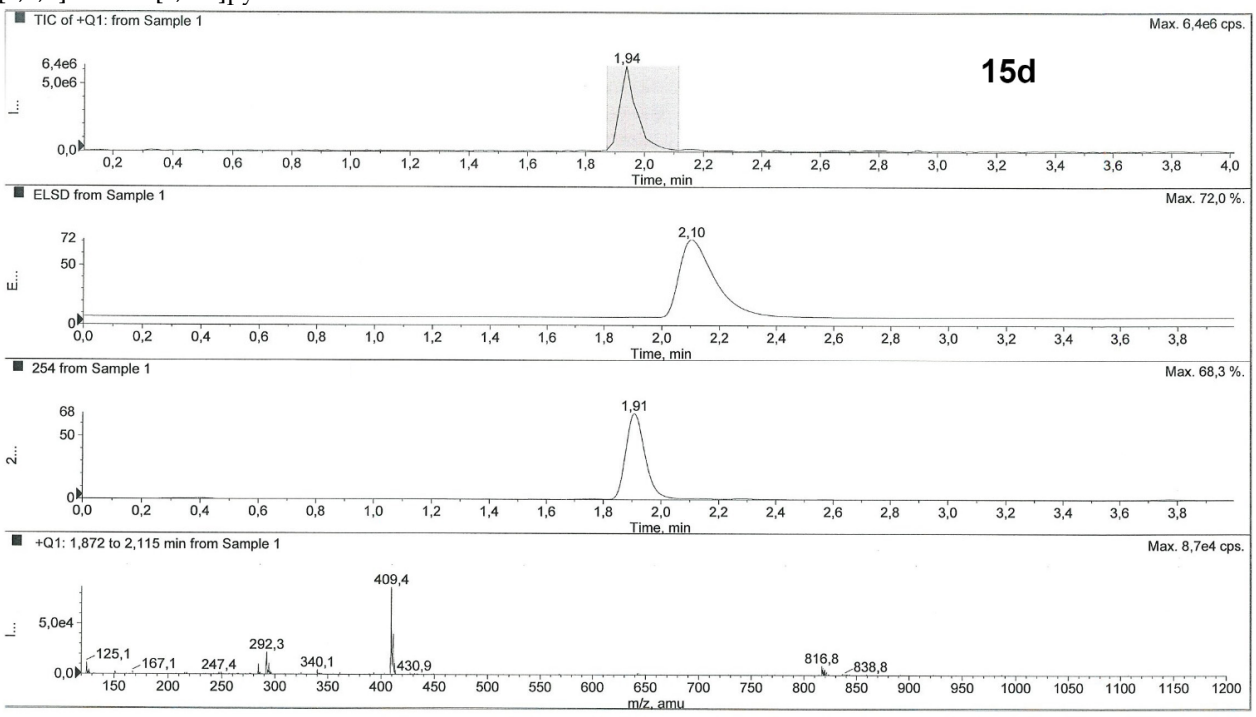


Figure S112. LC/MS data for 3-(3-chlorobenzylthio)-8-(pyrrolidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15d**.

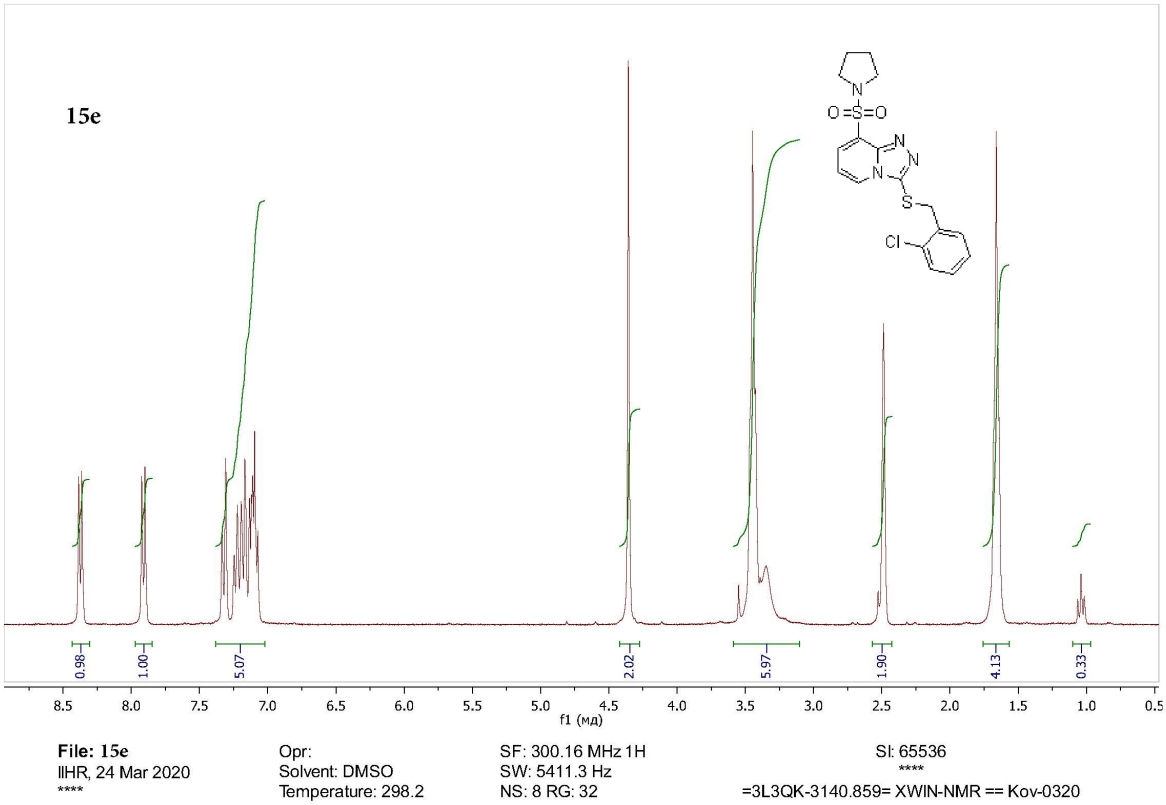


Figure S113. [1]H NMR spectrum (300 MHz, DMSO-d6) of 3-(2-chlorobenzylthio)-8-(pyrrolidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15e**.

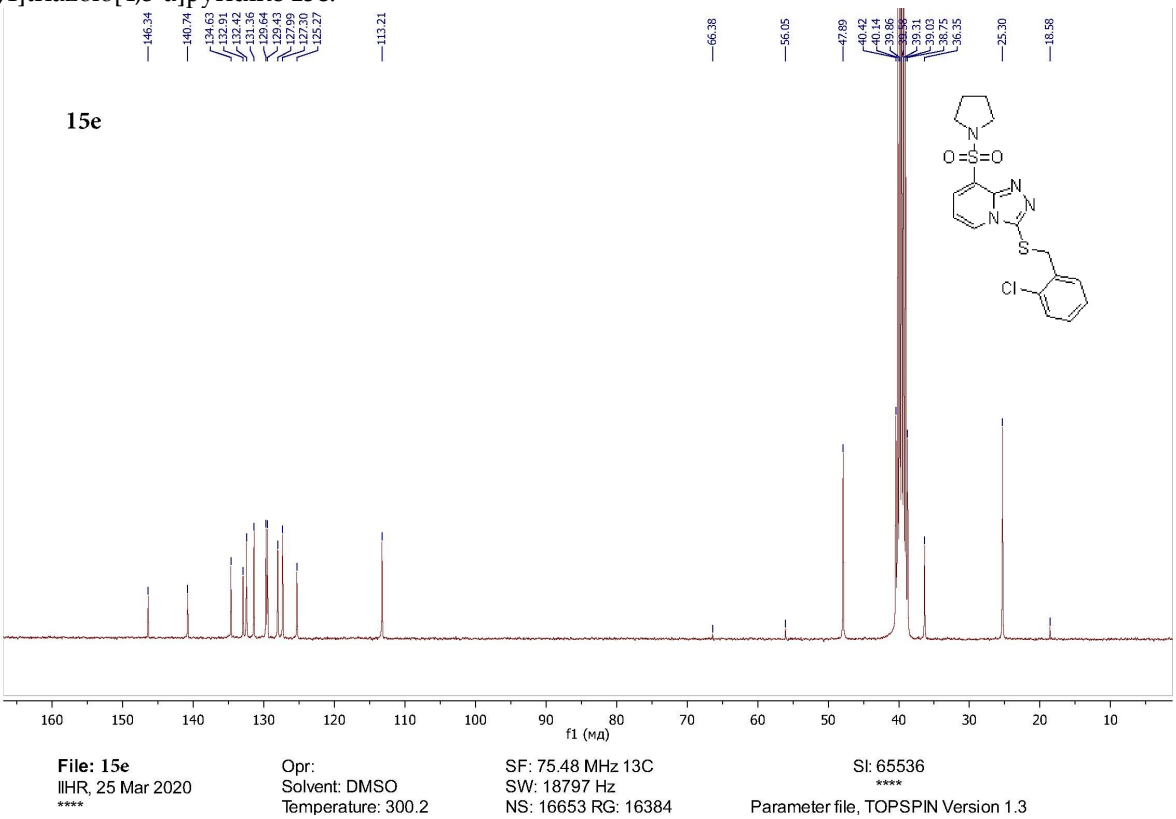


Figure S114. [13]C NMR spectrum (75 MHz, DMSO-d6) of 3-(2-chlorobenzylthio)-8-(pyrrolidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15e**.

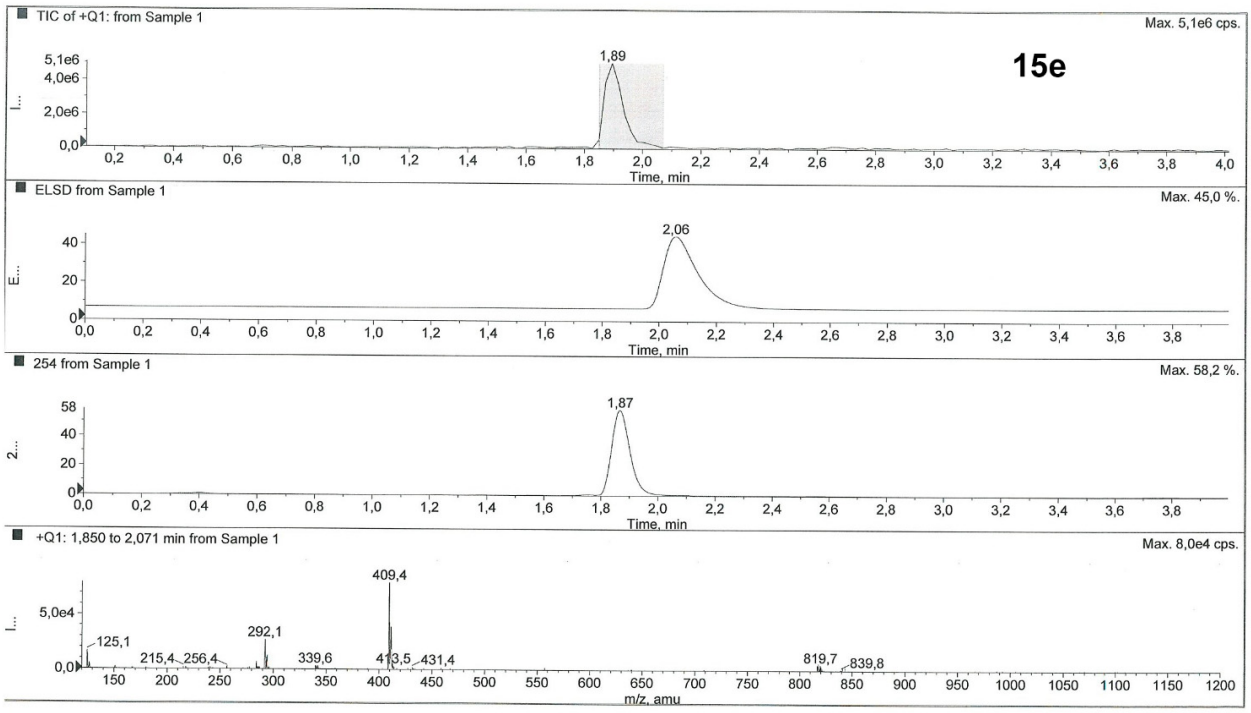


Figure S115. LC/MS data for 3-(2-chlorobenzylthio)-8-(pyrrolidin-1-ylsulfonyl)-[1,2,4]triazolo[4,3-a]pyridine **15e**.

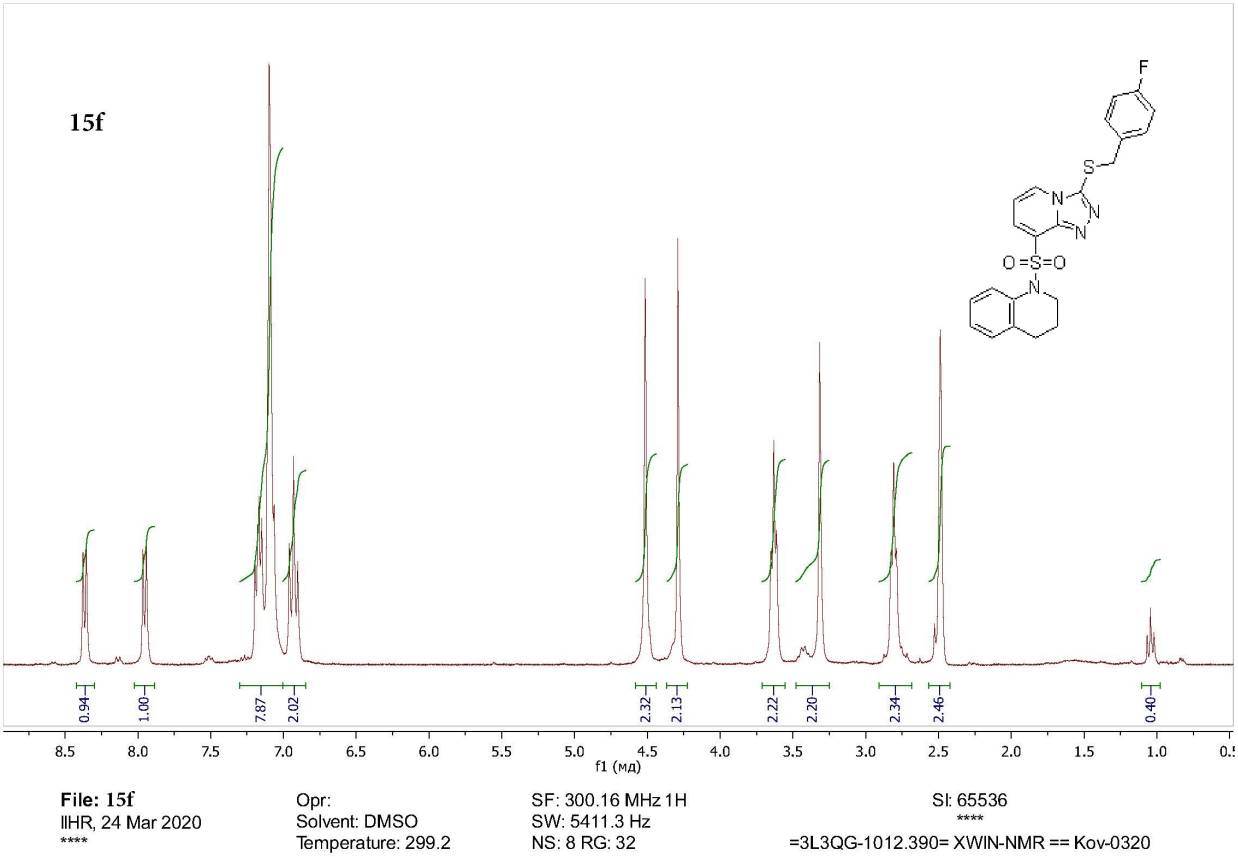


Figure S116. ^{1}H NMR spectrum (300 MHz, DMSO-d6) of 1-(3-(4-fluorobenzylthio)-[1,2,4]triazolo[4,3-a]pyridin-8-ylsulfonyl)-1,2,3,4-tetrahydroquinoline **15f**.

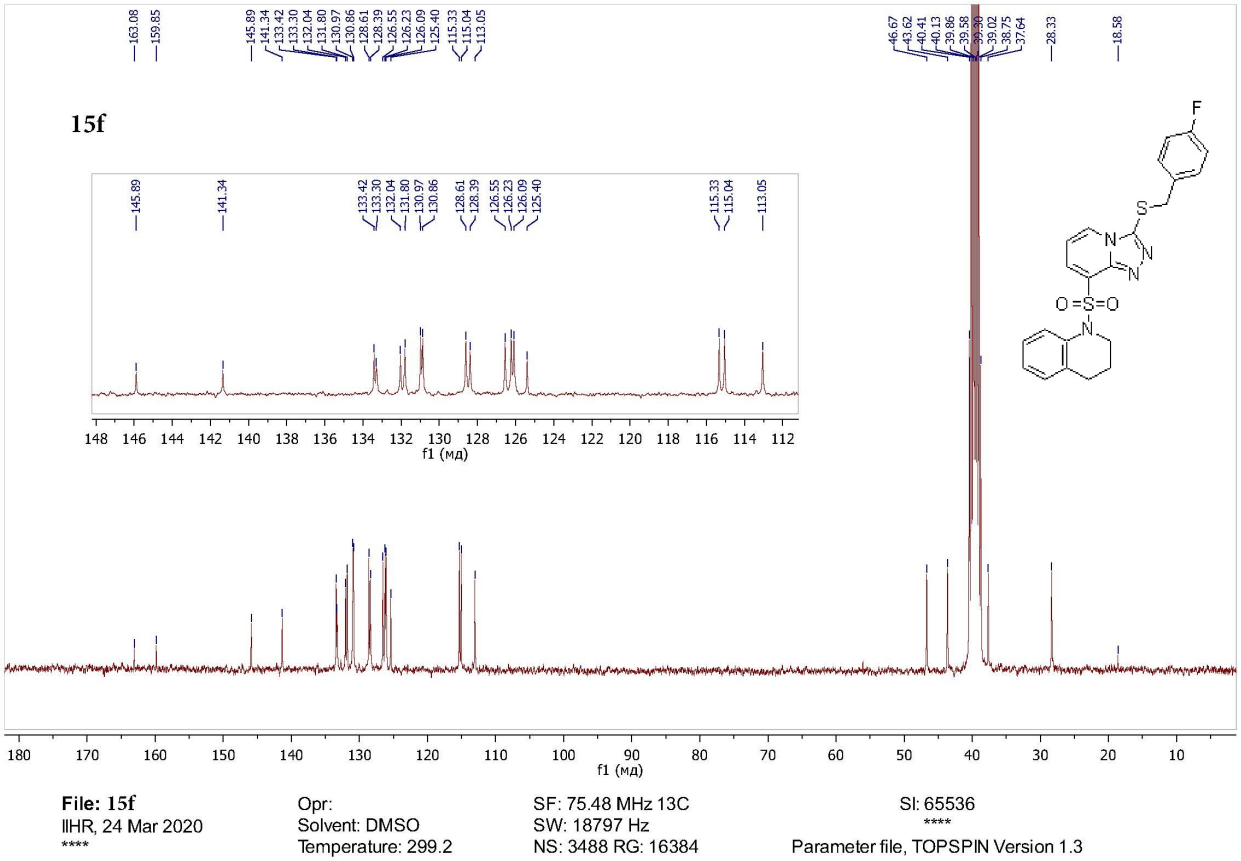


Figure S117. ^{13}C NMR spectrum (75 MHz, DMSO-d6) of 1-(3-(4-fluorobenzylthio)-[1,2,4]triazolo[4,3-a]pyridin-8-ylsulfonyl)-1,2,3,4-tetrahydroquinoline **15f**.

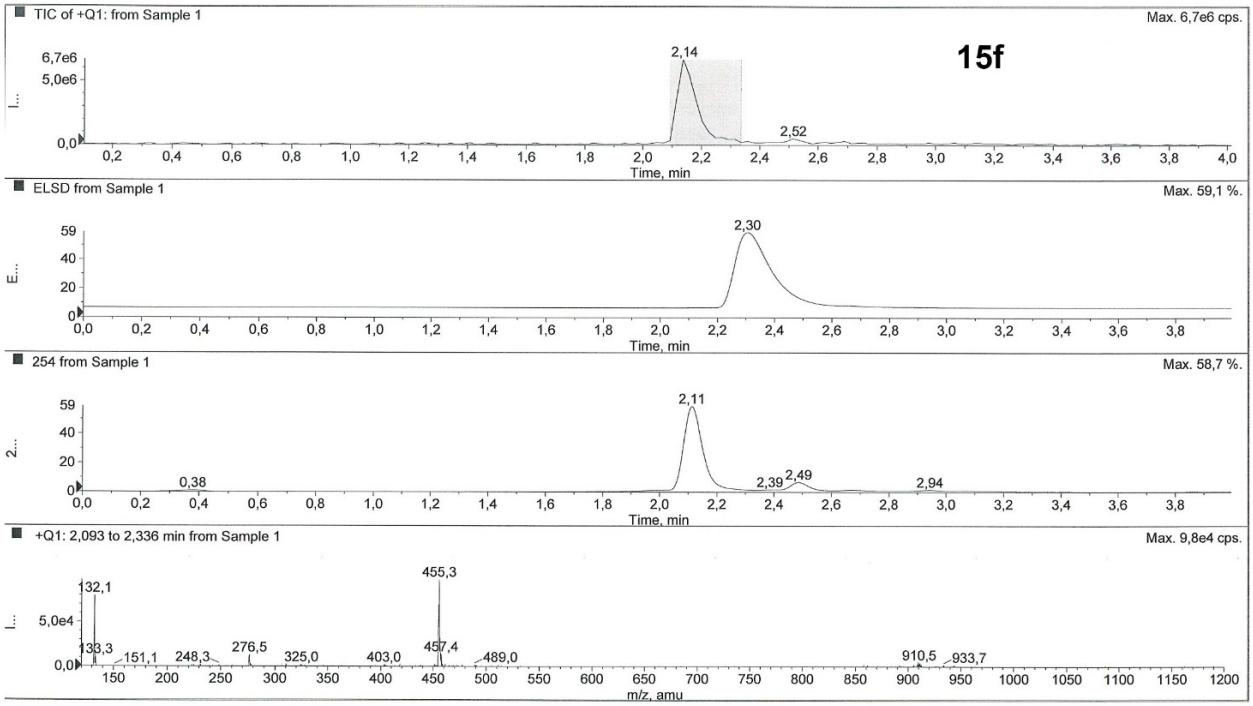


Figure S118. LC/MS data for 1-(3-(4-fluorobenzylthio)-[1,2,4]triazolo[4,3-a]pyridin-8-ylsulfonyl)-1,2,3,4-tetrahydroquinoline **15f**.