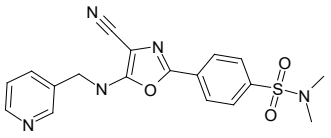
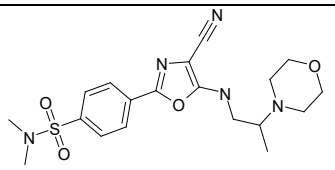
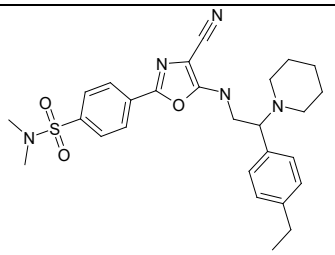
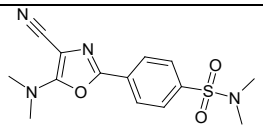
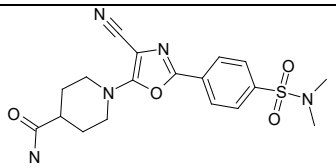
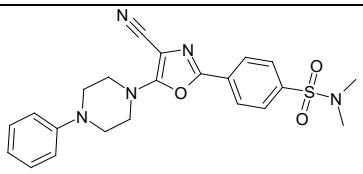
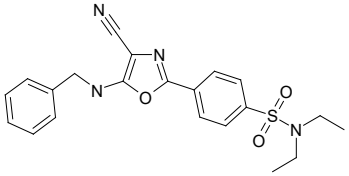
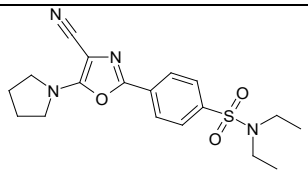
Supporting Information

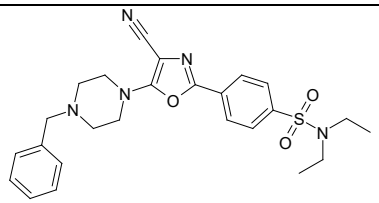
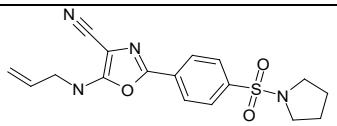
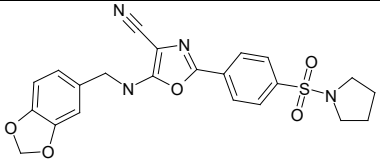
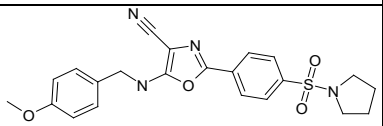
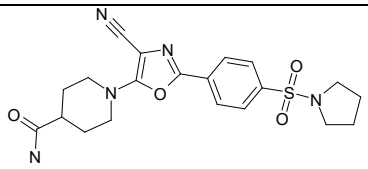
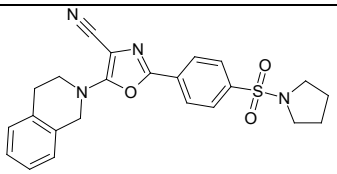
Design, Synthesis and Anticancer Activity of Novel 4-(5-amino-4-cyano-1,3-oxazol-2-yl)benzenesulfonamide derivatives

Oleksandr Severin, Stepan Pilyo, Ivan Semenyuta*, Maryna Kachaeva, Victor Zhirnov, Volodymyr Brovarets

Table of contents

Table S1. Chemical structures of synthesized compounds 1-14.

No	NSC number	Structure	Name
1	842150		4-[4-Cyano-5-(pyridin-3-ylmethylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide
2	842141		4-[4-Cyano-5-(2-morpholin-4-ylpropylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide
3	842142		4-[4-Cyano-5-[[2-(4-ethylphenyl)-2-piperidin-1-ylethyl]amino]-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide
4	842149		4-[4-Cyano-5-(dimethylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide
5	842148		1-[4-Cyano-2-[4-(dimethylsulfamoyl)phenyl]-1,3-oxazol-5-yl]piperidine-4-carboxamide
6	842147		4-[4-Cyano-5-(4-phenylpiperazin-1-yl)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide
7	842144		4-[5-(Benzylamino)-4-cyano-1,3-oxazol-2-yl]-N,N-diethylbenzenesulfonamide
8	842143		4-(4-Cyano-5-pyrrolidin-1-yl-1,3-oxazol-2-yl)-N,N-diethylbenzenesulfonamide

9	842145		4-[5-(4-Benzylpiperazin-1-yl)-4-cyano-1,3-oxazol-2-yl]-N,N-diethylbenzenesulfonamide
10	842594		5-(Prop-2-enylamino)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile
11	842596		5-(1,3-Benzodioxol-5-ylmethylamino)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile
12	842595		5-[(4-Methoxyphenyl)methylamino]-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile
13	842592		1-[4-Cyano-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazol-5-yl]piperidine-4-carboxamide
14	842593		5-(3,4-Dihydro-1H-isoquinolin-2-yl)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile

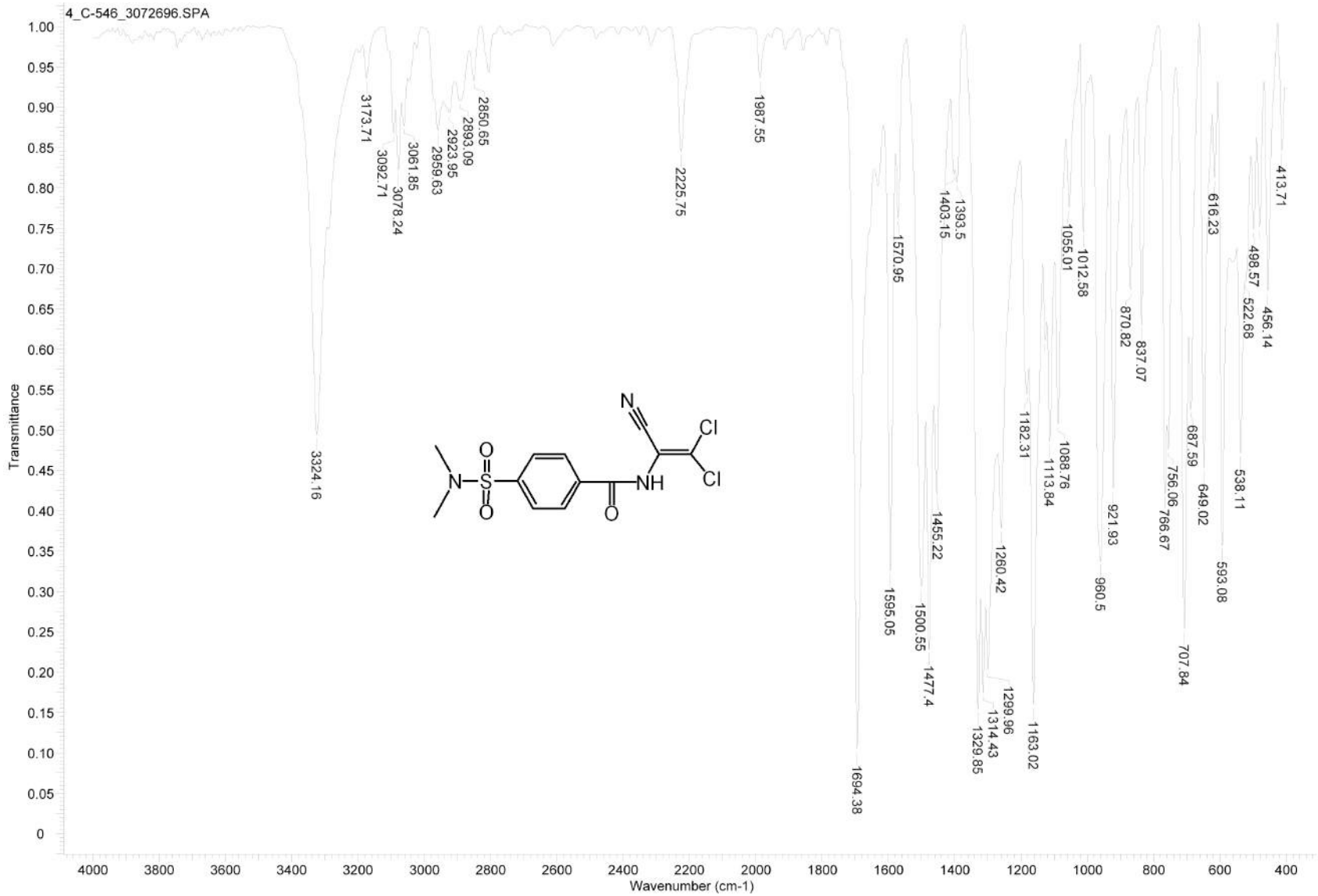


Fig. S1. IR spectrum of N-(2,2-dichloro-1-cyanoethenyl)-4-(dimethylsulfamoyl)benzamide VIIIa

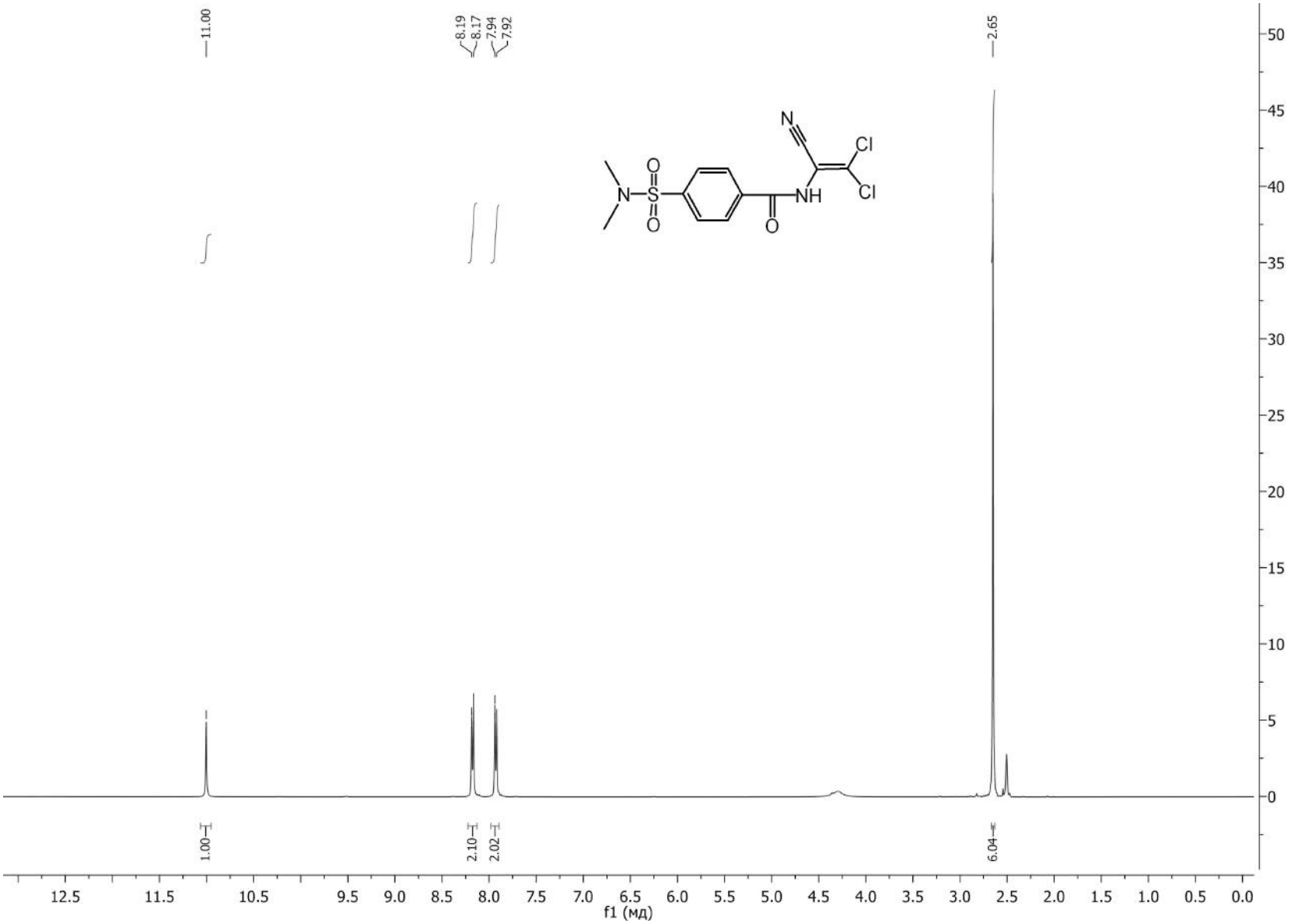


Fig. S2. [1]H NMR spectrum of N-(2,2-dichloro-1-cyanoethenyl)-4-(dimethylsulfamoyl)benzamide VIIIa

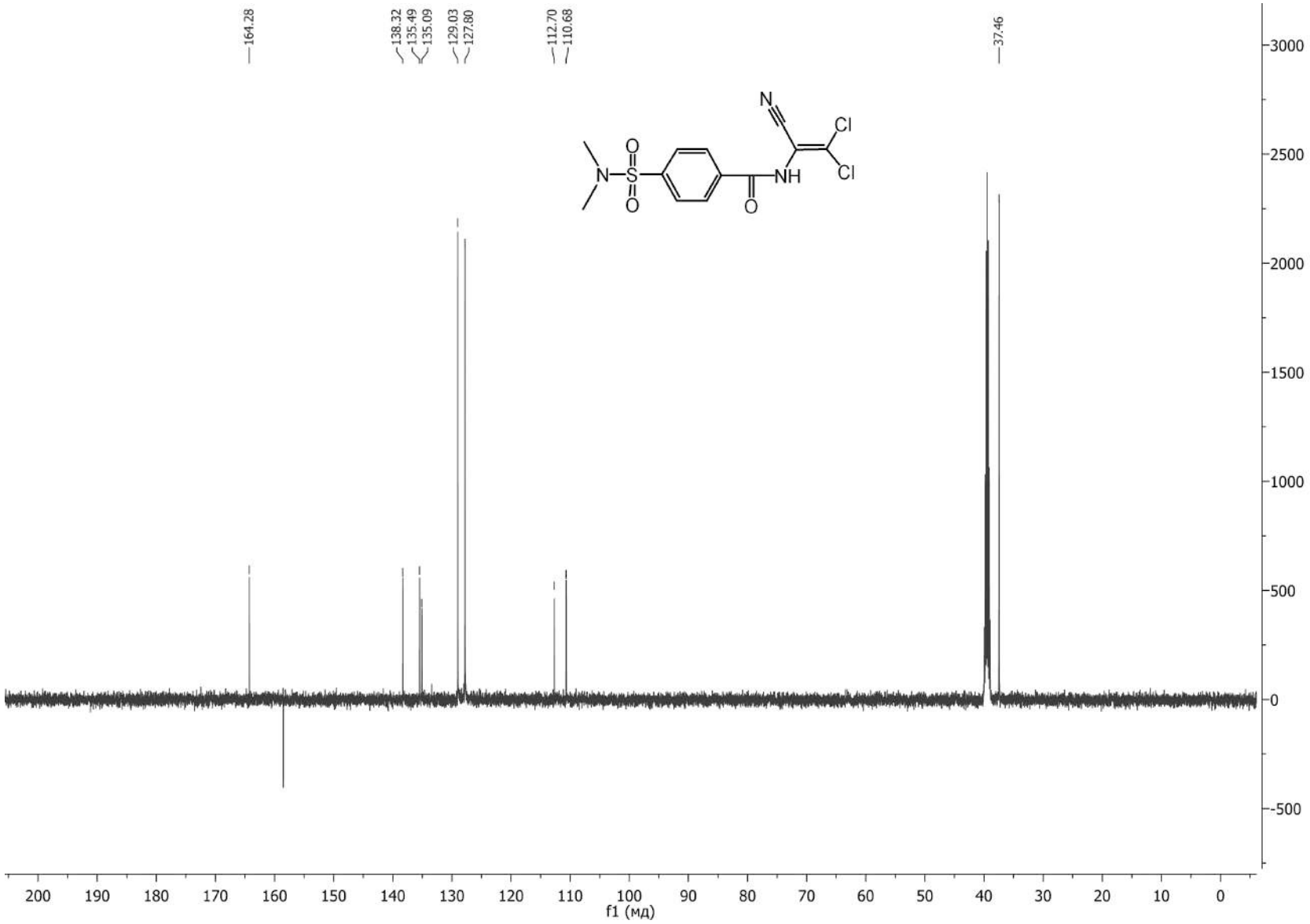


Fig. S3. ^{13}C NMR spectrum of N-(2,2-dichloro-1-cyanoethenyl)-4-(dimethylsulfamoyl)benzamide VIIIa

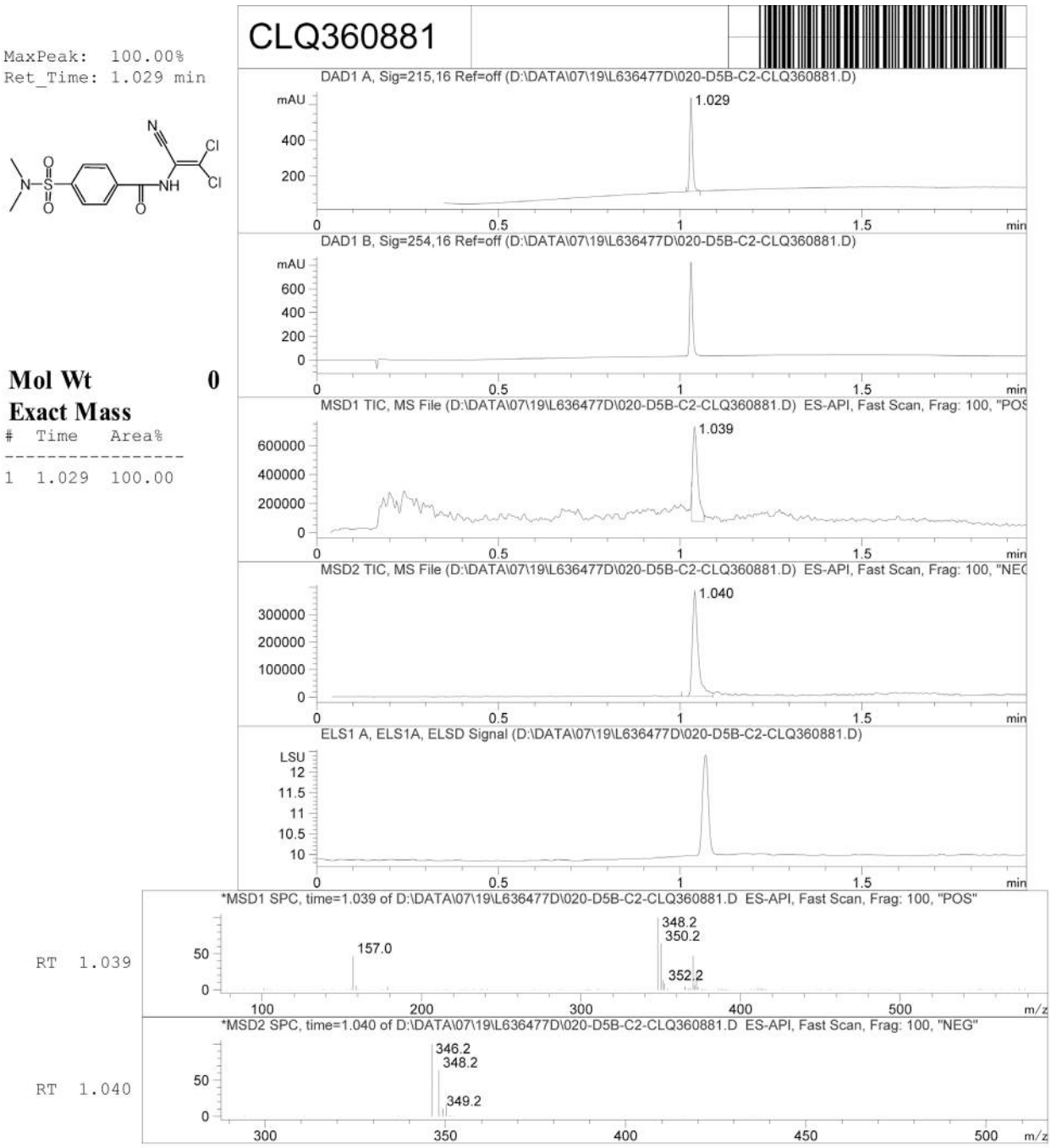


Fig. S4. LCMS spectrum of N-(2,2-dichloro-1-cyanoethenyl)-4-(dimethylsulfamoyl)benzamide VIIIa

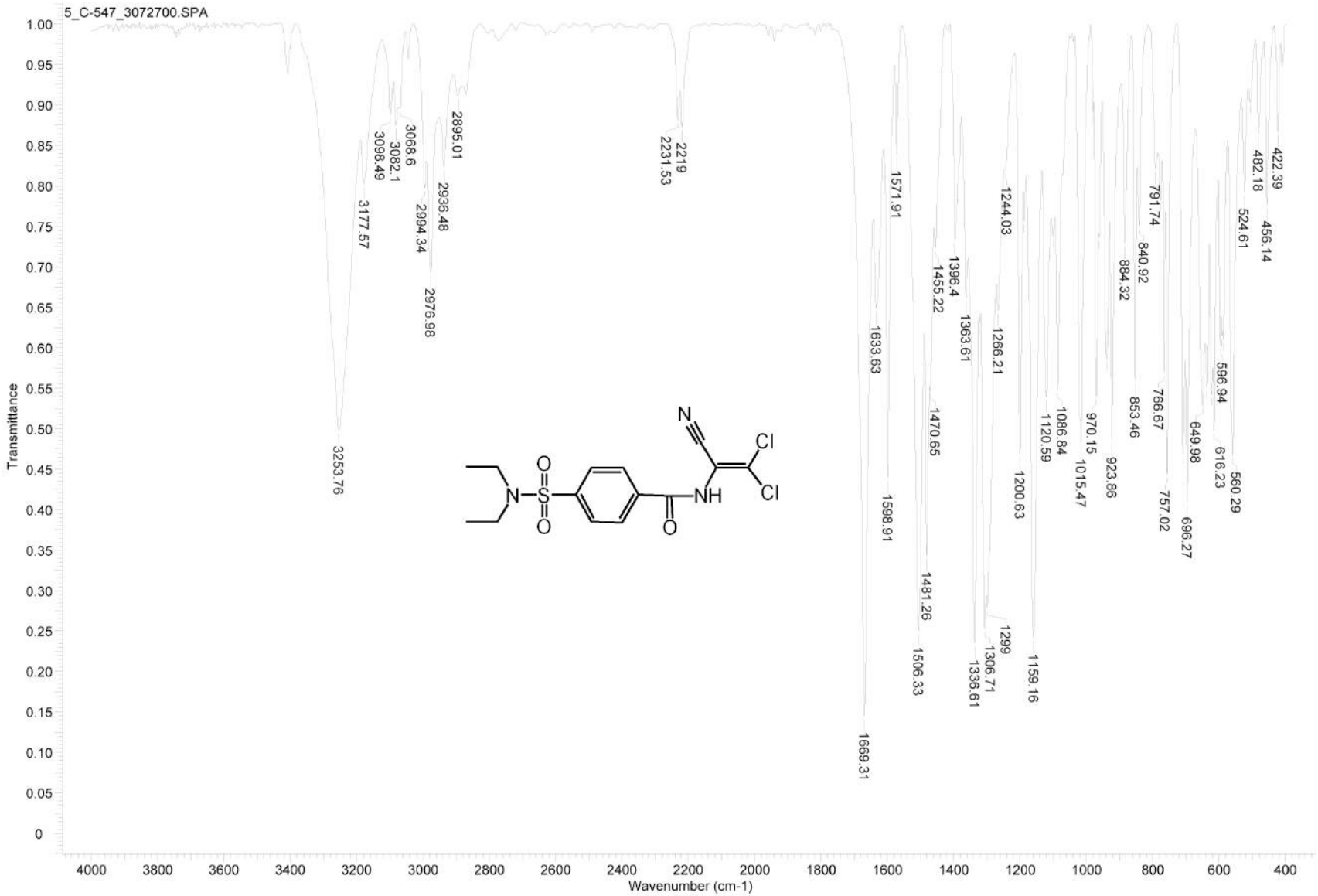


Fig. S5. IR spectrum of N-(2,2-dichloro-1-cyanoethenyl)-4-(diethylsulfamoyl)benzamide VIIIb

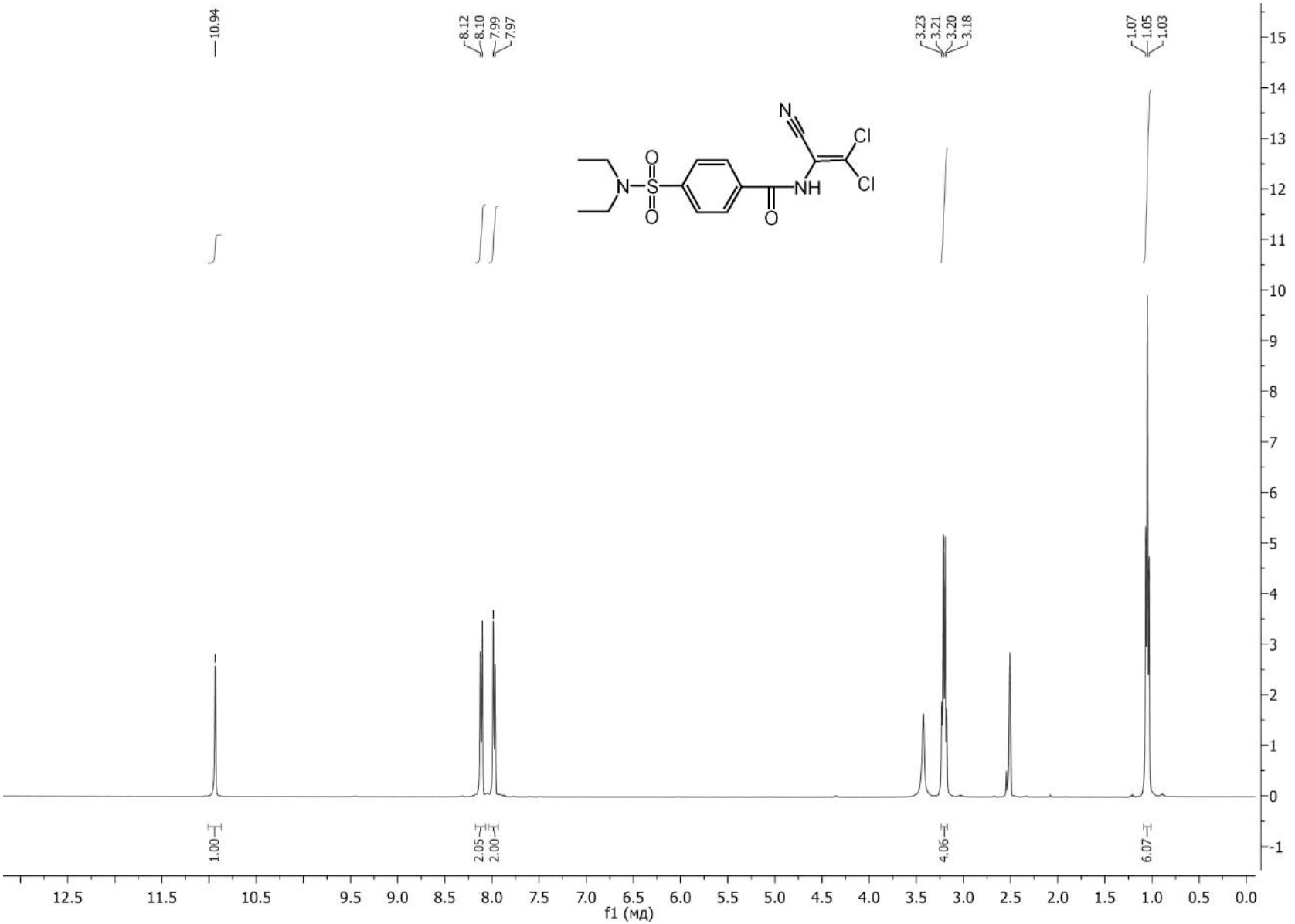


Fig. S6. [1]H NMR spectrum of N-(2,2-dichloro-1-cyanoethenyl)-4-(diethylsulfamoyl)benzamide VIIIb

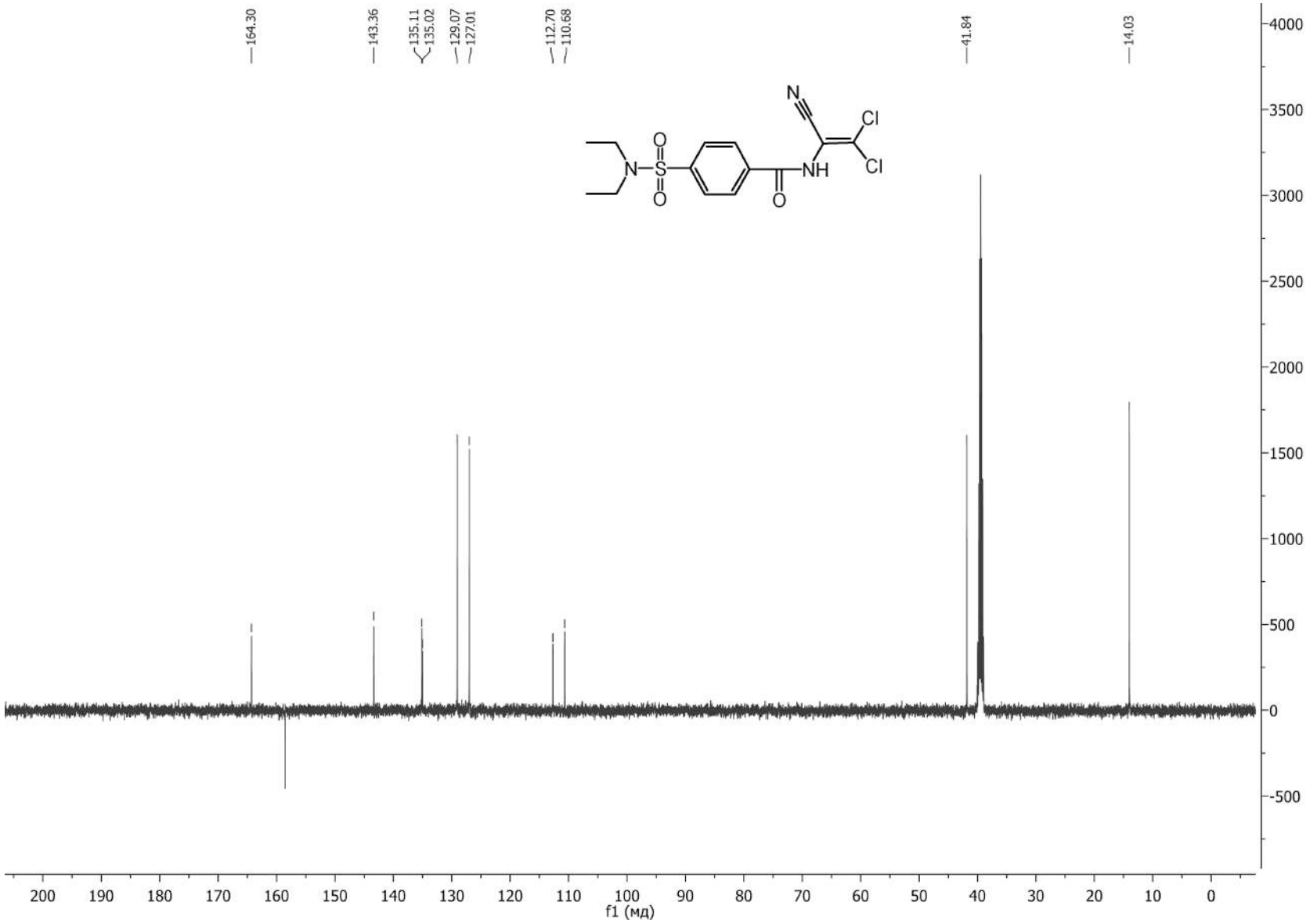


Fig. S7. ^{13}C NMR spectrum of N-(2,2-dichloro-1-cyanoethenyl)-4-(diethylsulfamoyl)benzamide VIIIb

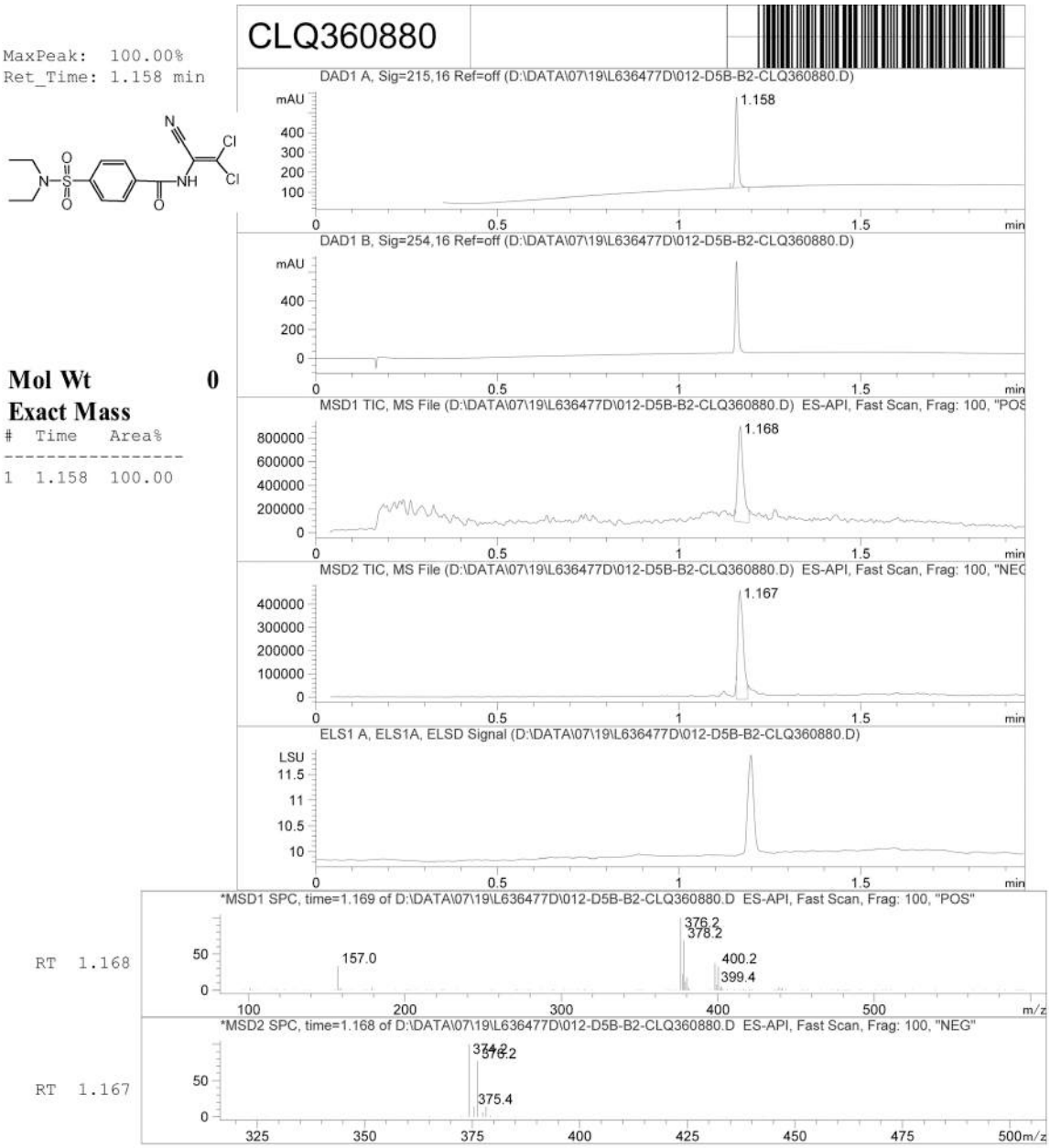


Fig. S8. LCMS spectrum of N-(2,2-dichloro-1-cyanoethenyl)-4-(diethylsulfamoyl)benzamide VIIIb

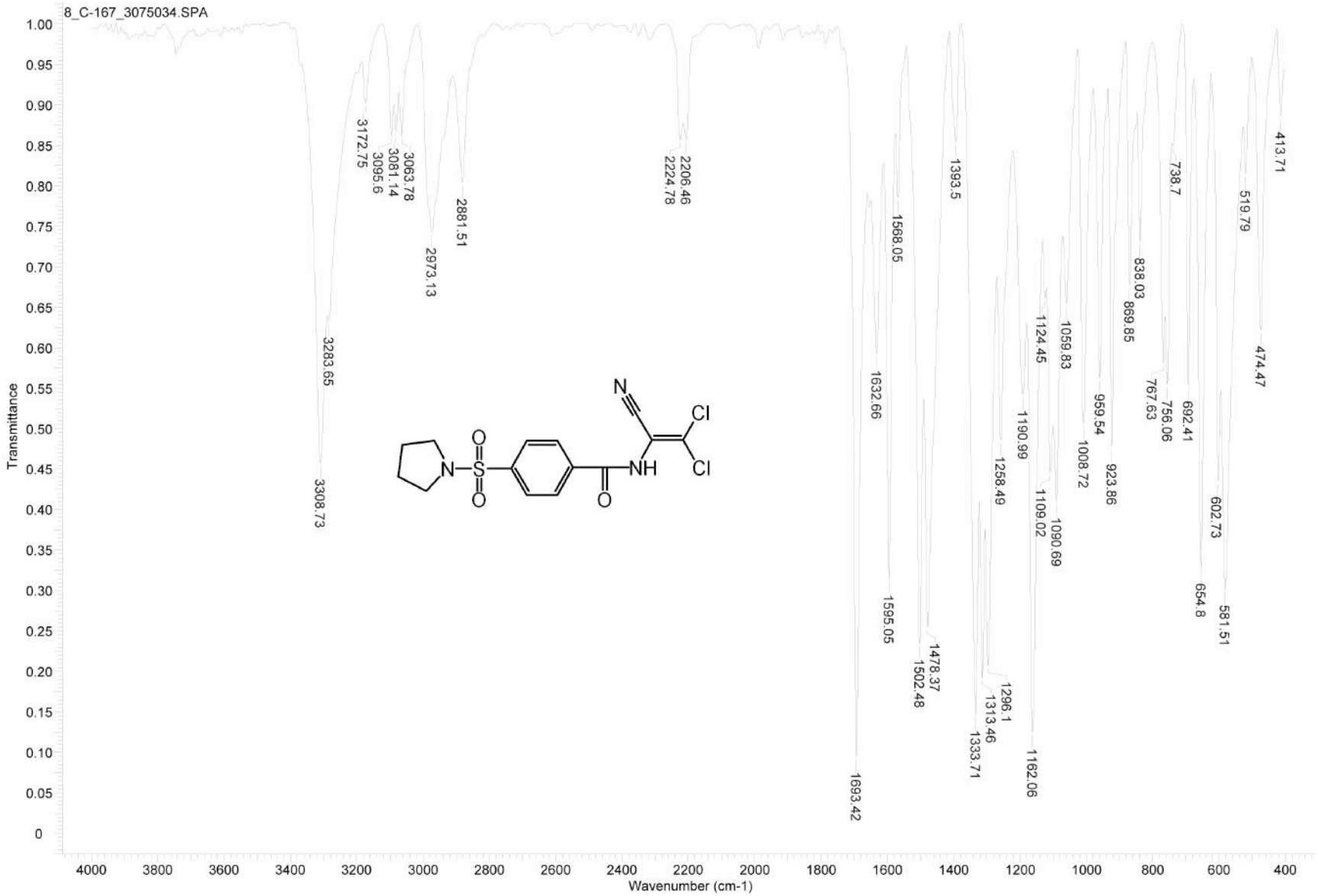


Fig. S9. IR spectrum of N-(2,2-dichloro-1-cyanoethenyl)-4-(pyrrolidin-1-ylsulfamoyl)benzamide VIIIc

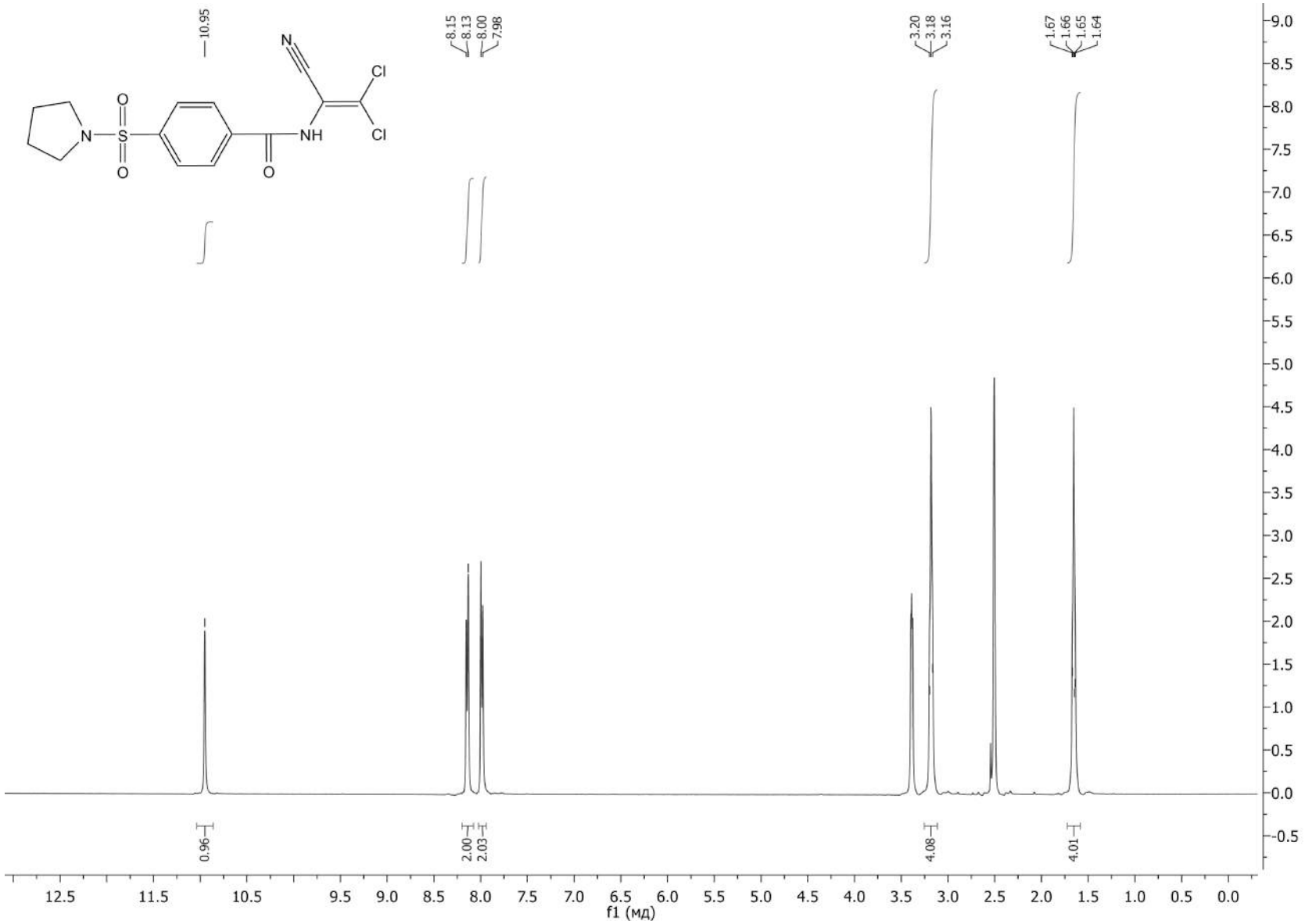


Fig. S10. [1]H NMR spectrum of N-(2,2-dichloro-1-cyanoethenyl)-4-(pyrrolidin-1-ylsulfamoyl)benzamide VIIIc

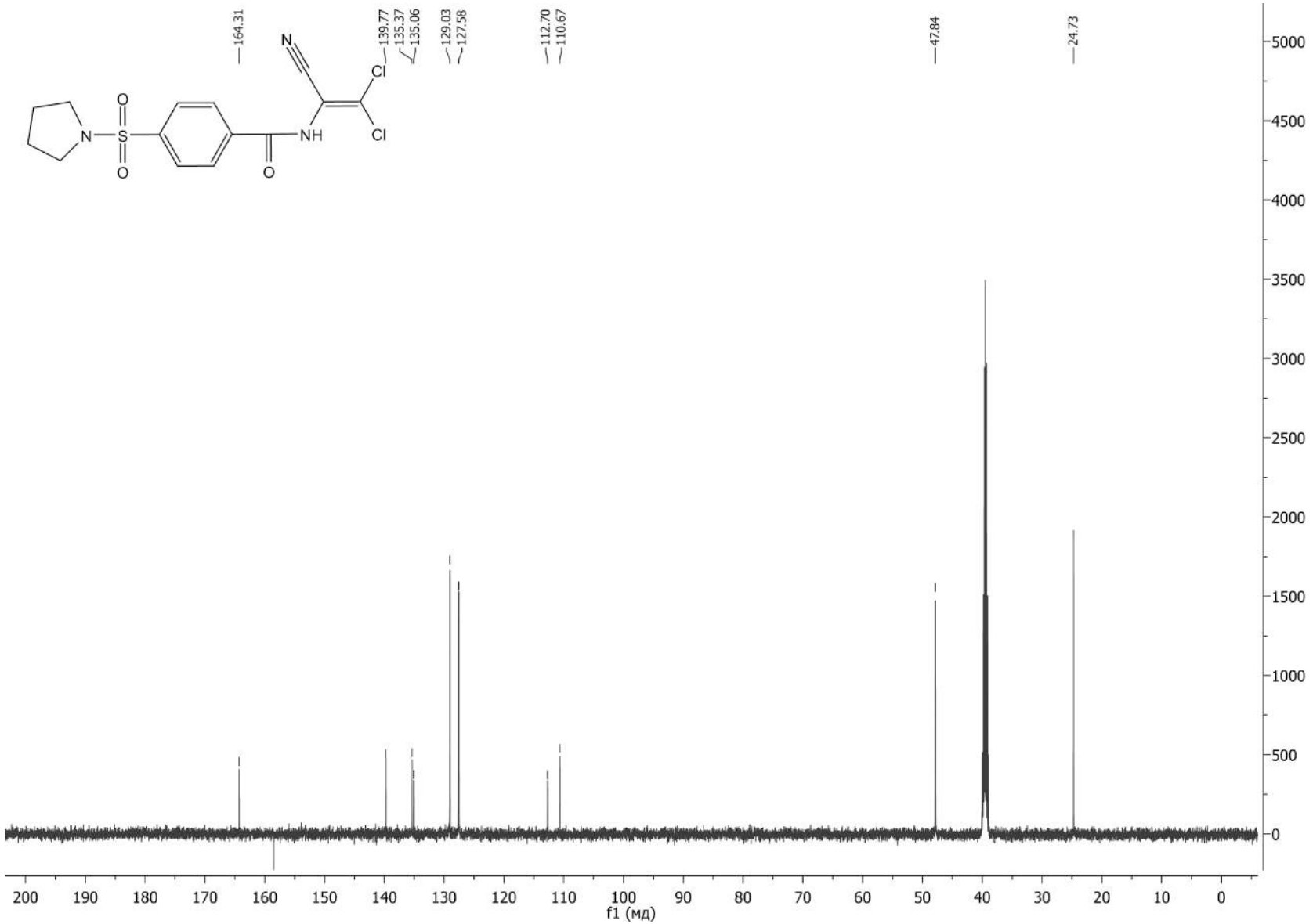


Fig. S11. ^{13}C NMR spectrum of N-(2,2-dichloro-1-cyanoethenyl)-4-(pyrrolidin-1-ylsulfamoyl)benzamide VIIIc

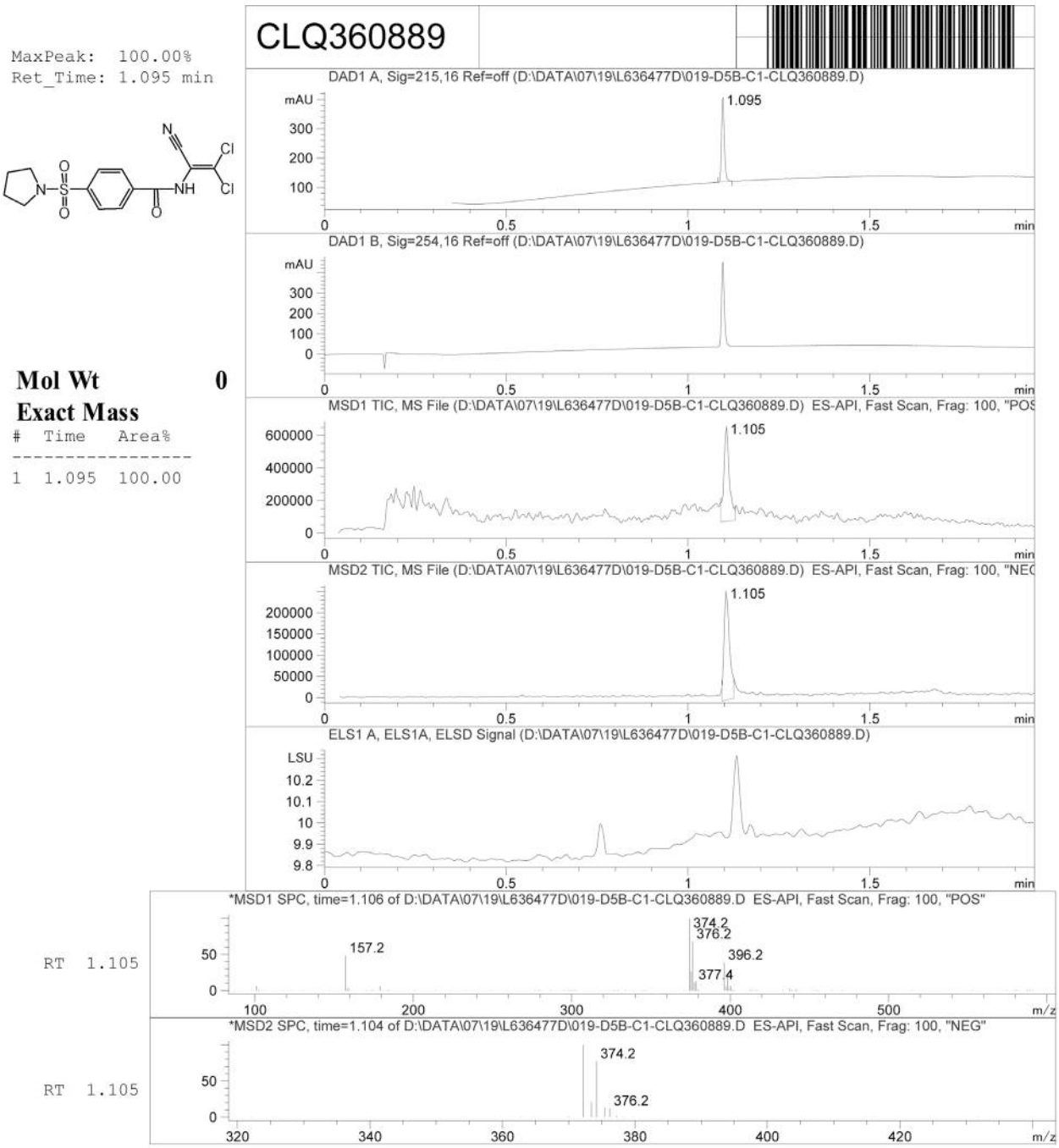


Fig. S12. LCMS spectrum of N-(2,2-dichloro-1-cyanoethenyl)-4-(pyrrolidin-1-ylsulfamoyl)benzamide VIIIc

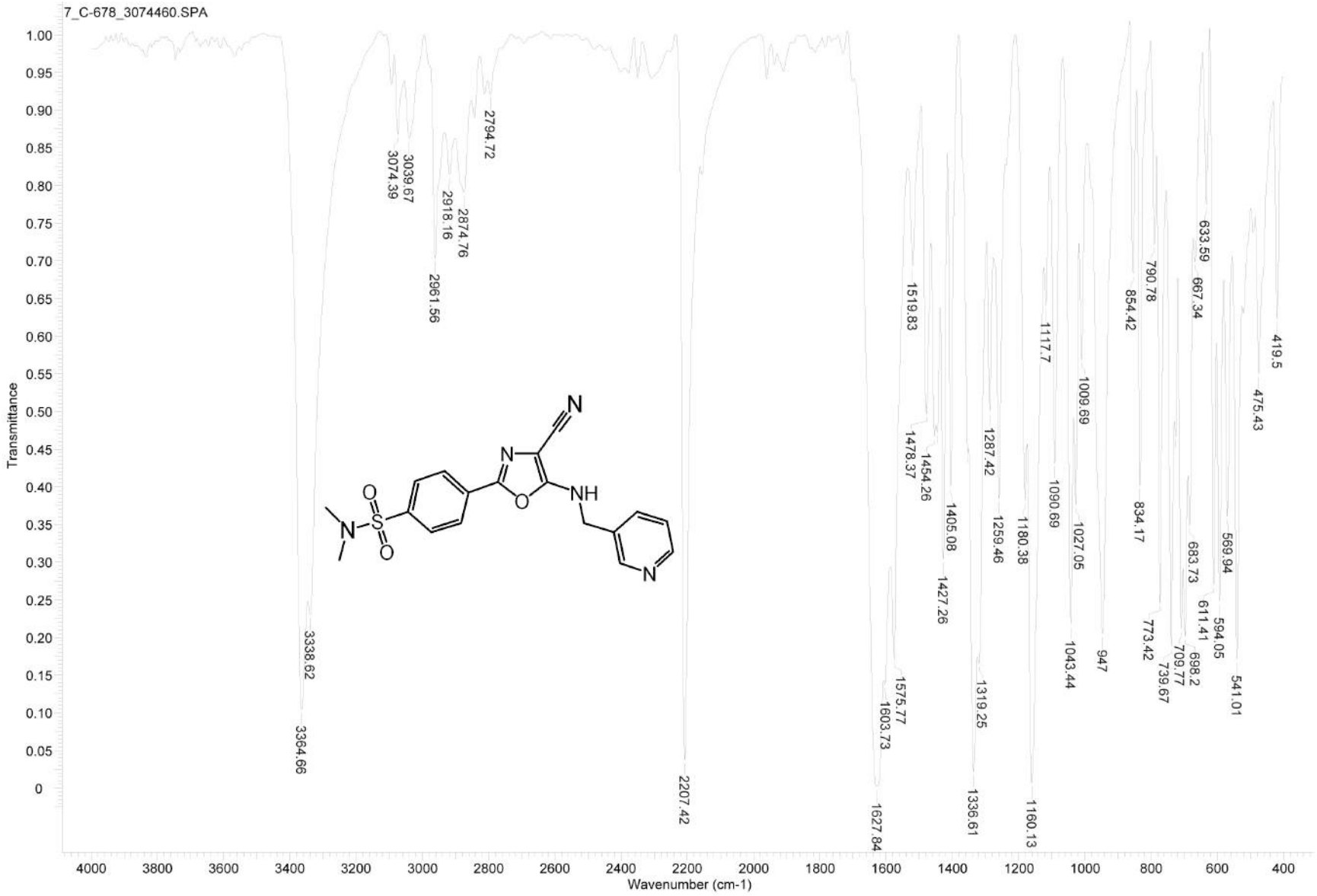


Fig. S13. IR spectrum of 4-[4-cyano-5-(pyridin-3-ylmethylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 1.

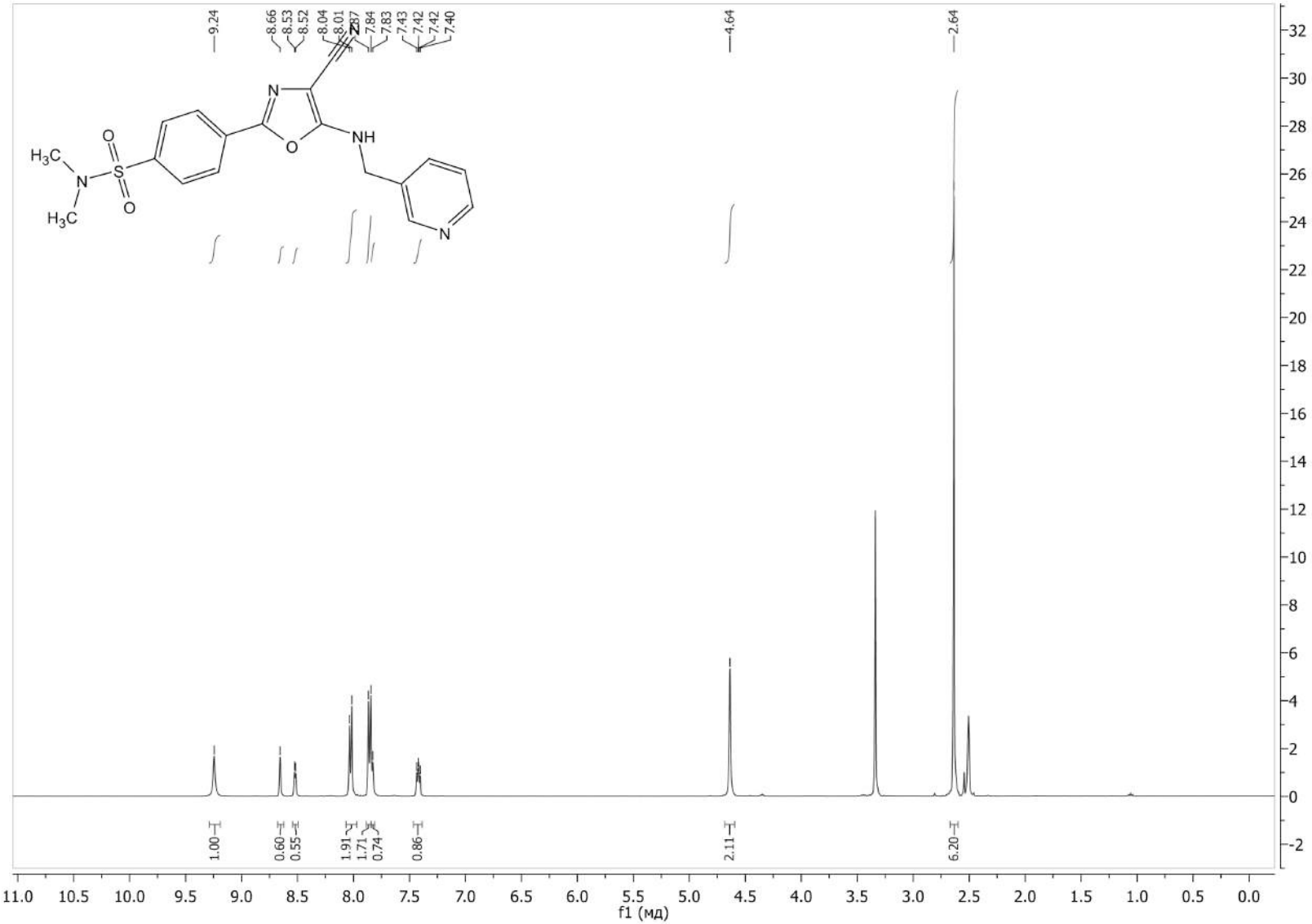


Fig. S14. [1]H NMR spectrum of 4-[4-cyano-5-(pyridin-3-ylmethylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 1.

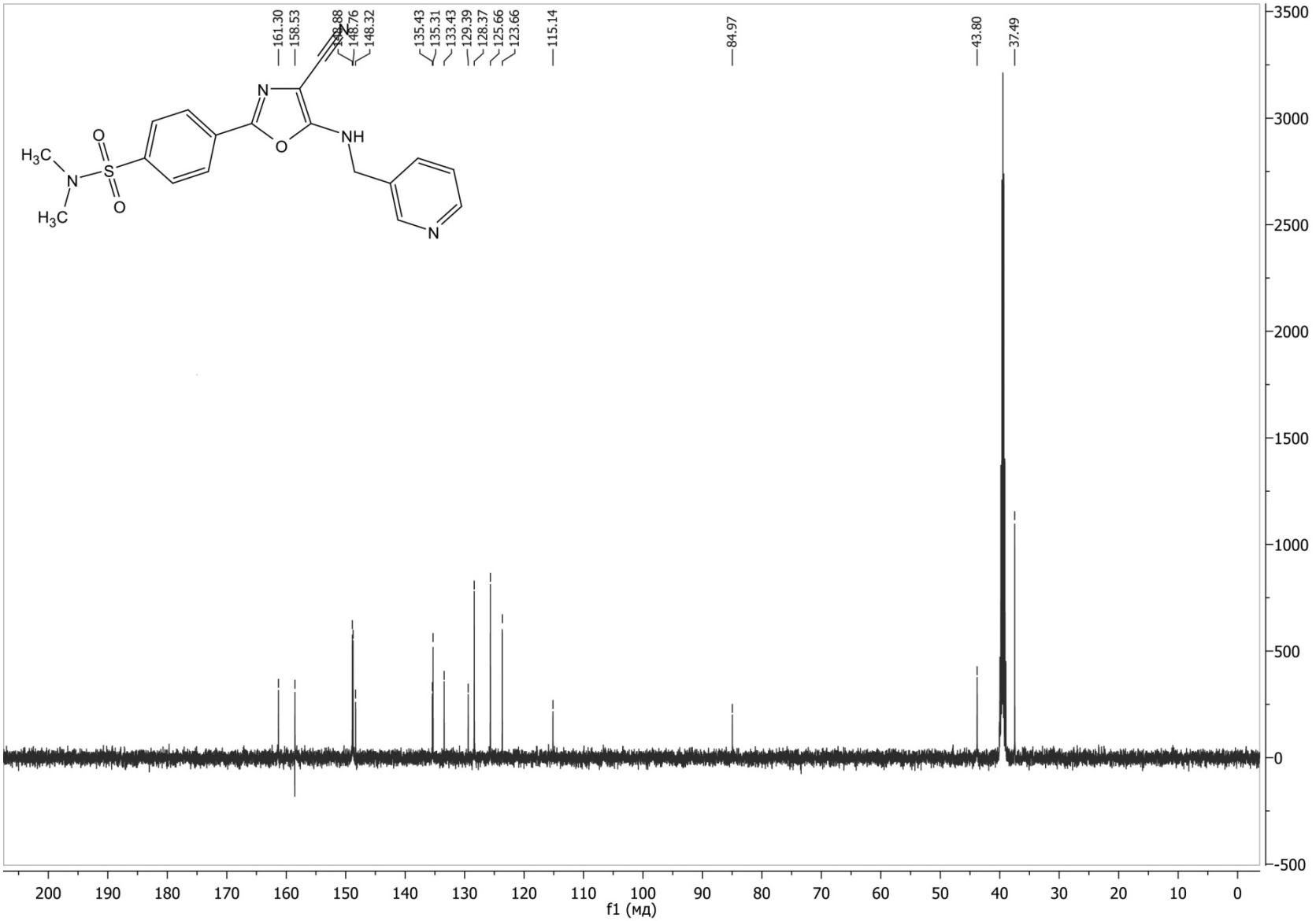


Fig. S15. ^{13}C NMR spectrum of 4-[4-cyano-5-(pyridin-3-ylmethylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 1.

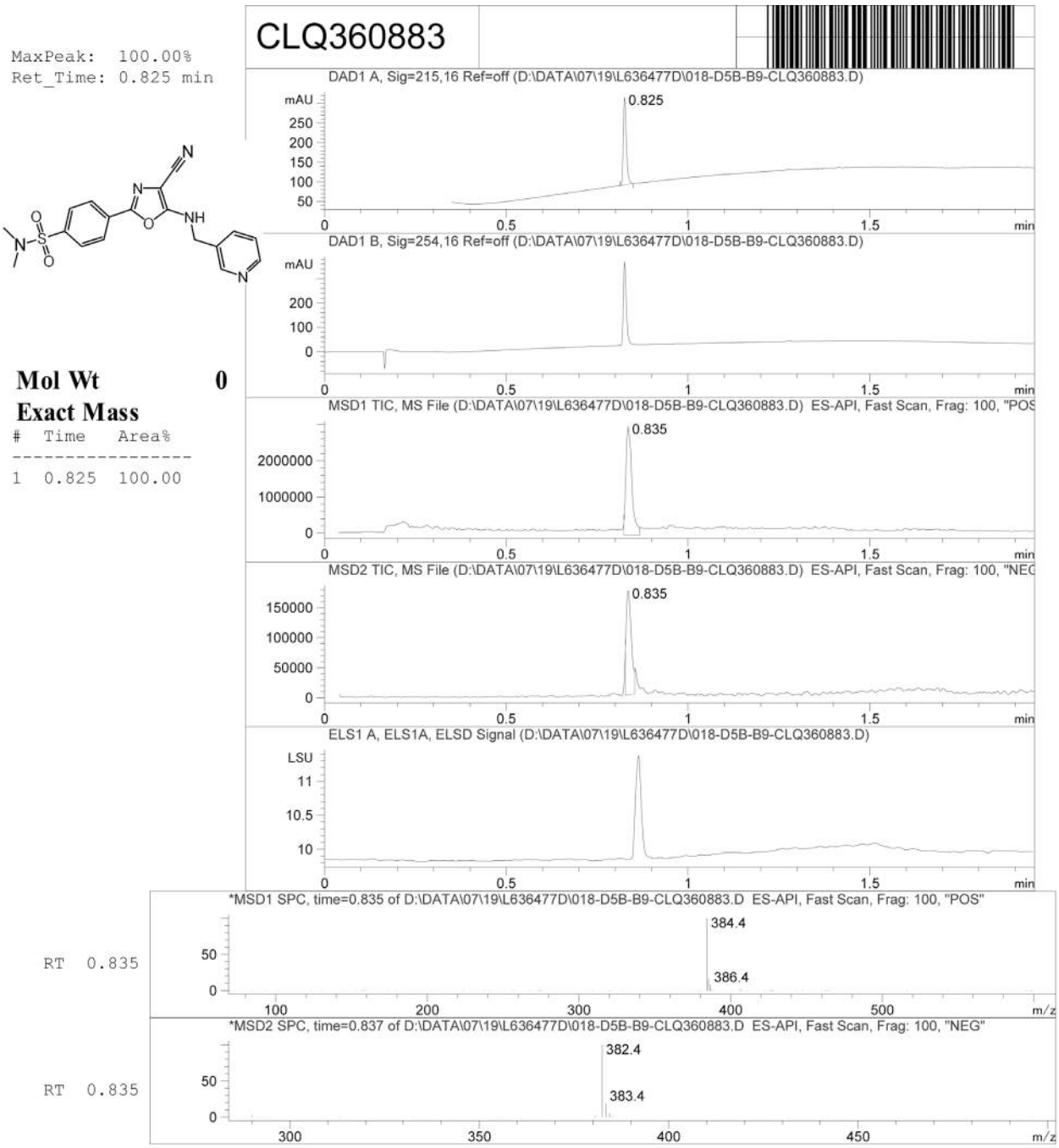


Fig. S16. LCMS spectrum of 4-[4-cyano-5-(pyridin-3-ylmethylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 1.

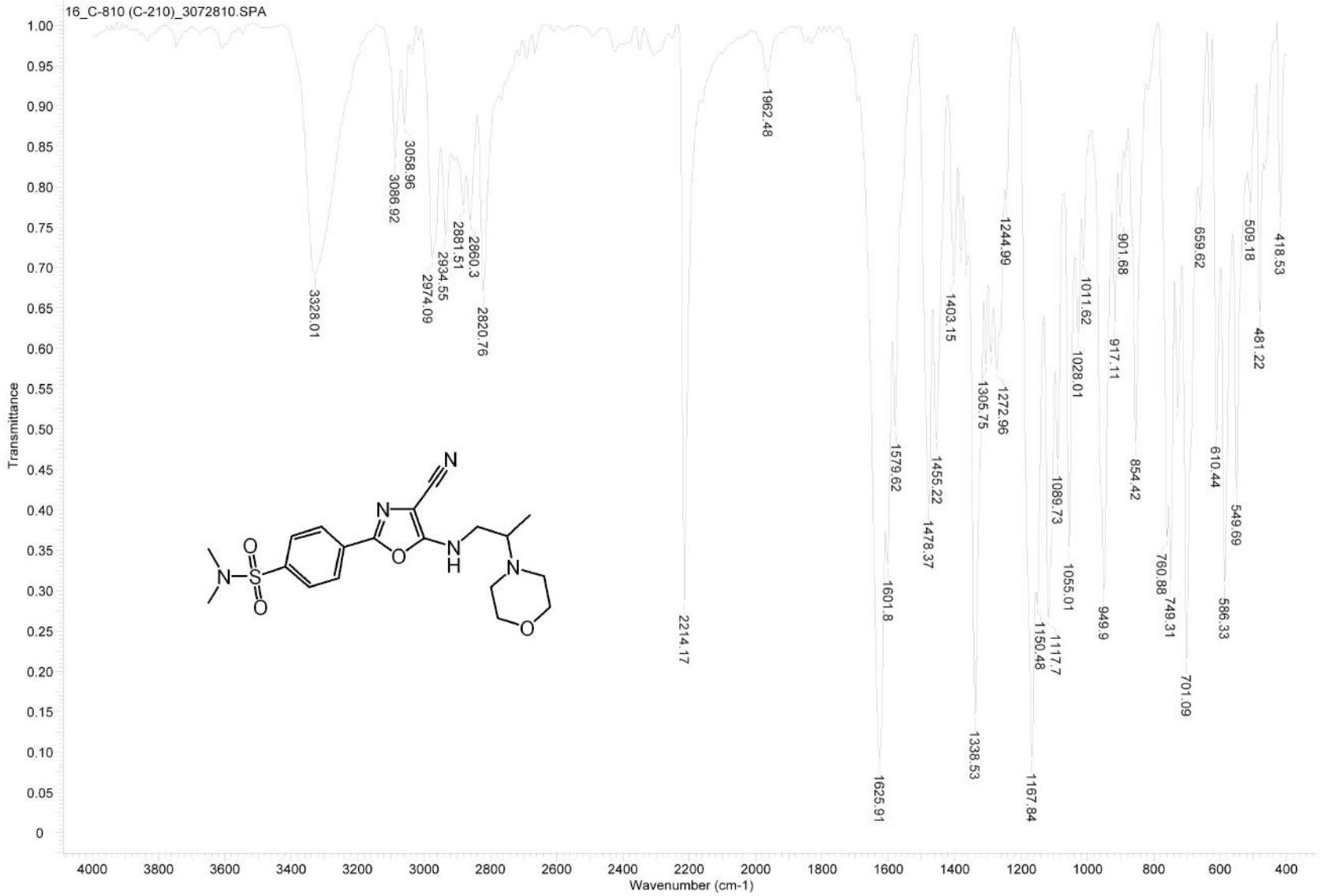


Fig. S17. IR spectrum of 4-[4-cyano-5-(2-morpholin-4-ylpropylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 2.

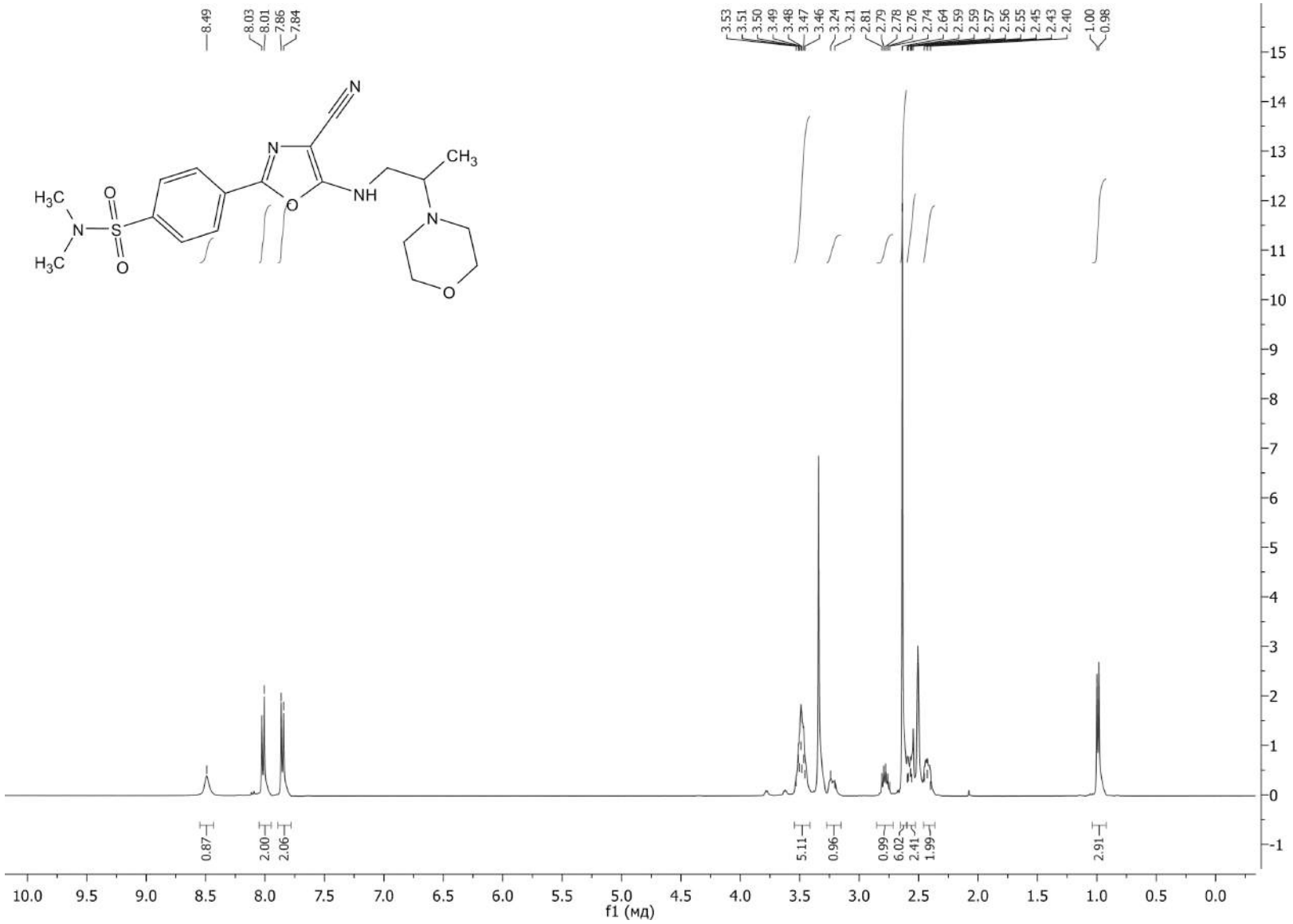


Fig. S18. [1]H NMR spectrum of 4-[4-cyano-5-(2-morpholin-4-ylpropylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 2.

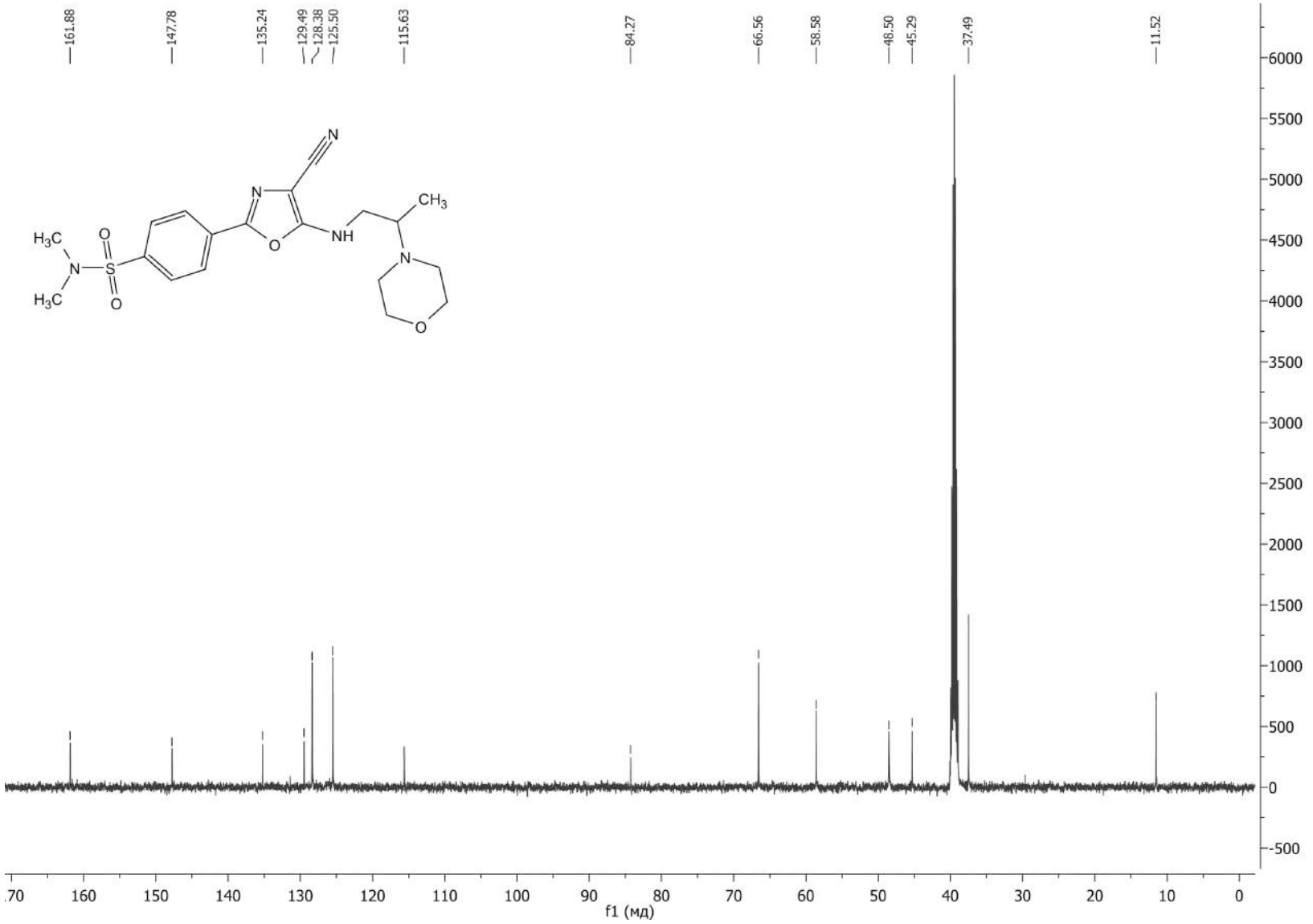


Fig. S19. ^{13}C NMR spectrum of 4-[4-cyano-5-(2-morpholin-4-ylpropylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 2.

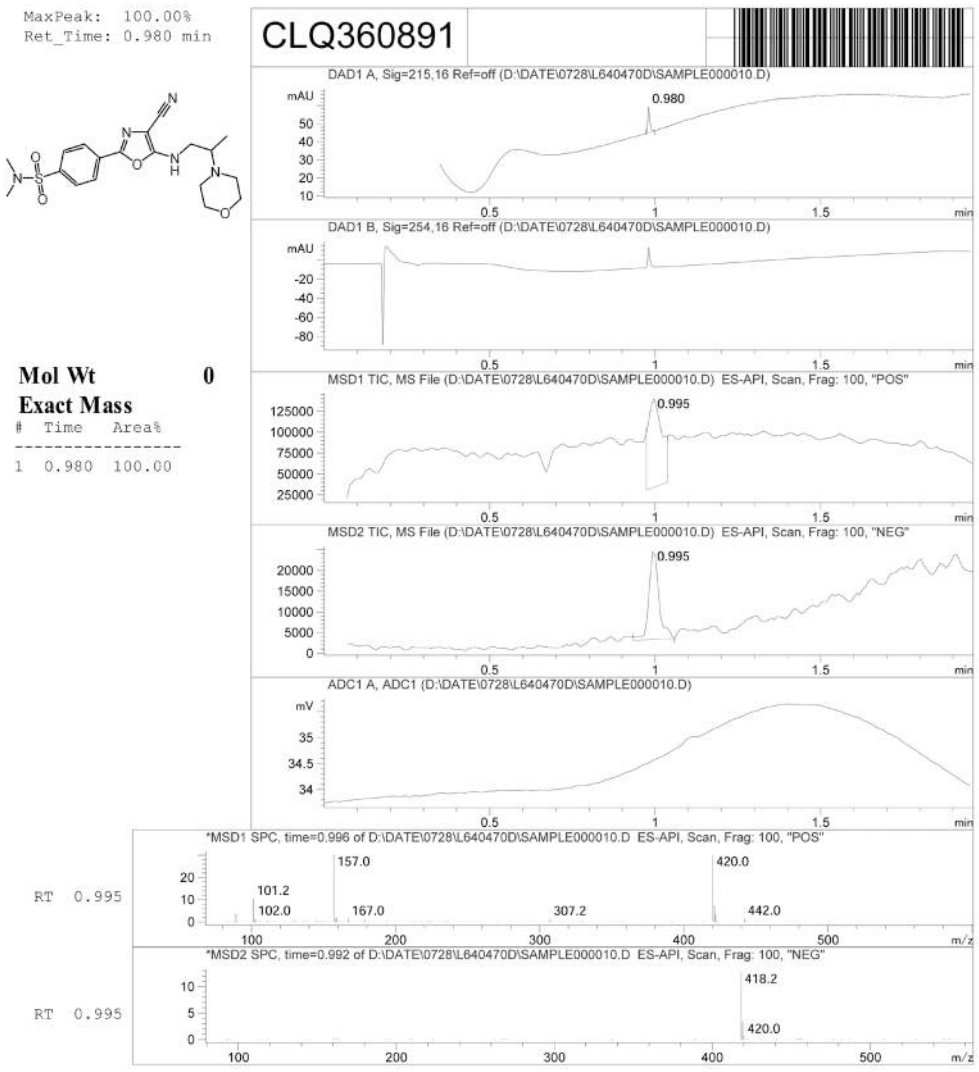


Fig. S20. LCMS spectrum of 4-[4-cyano-5-(2-morpholin-4-ylpropylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 2.

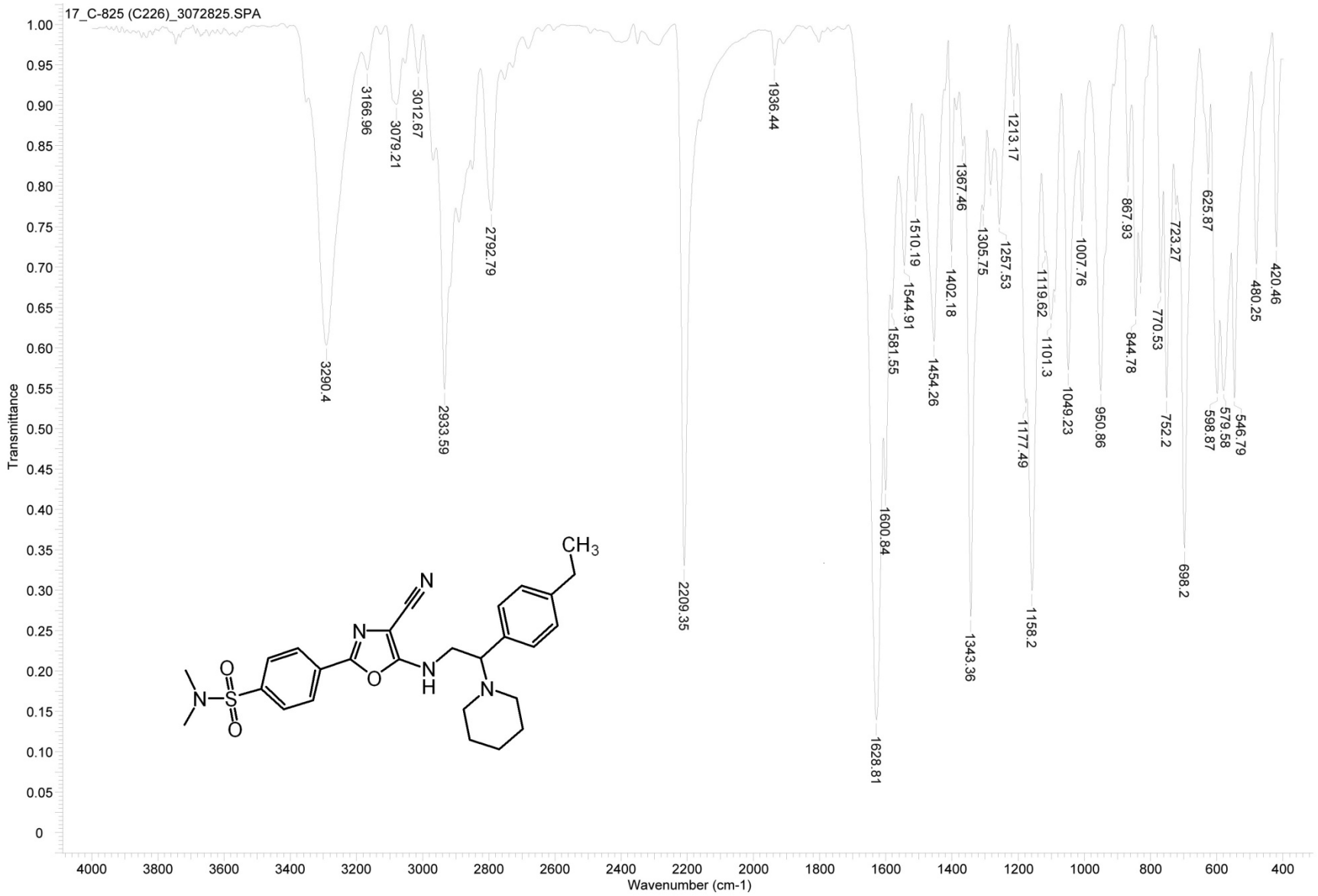


Fig. S21. IR spectrum of 4-[4-cyano-5-[[2-(4-ethylphenyl)-2-piperidin-1-ylethyl]amino]-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 3.

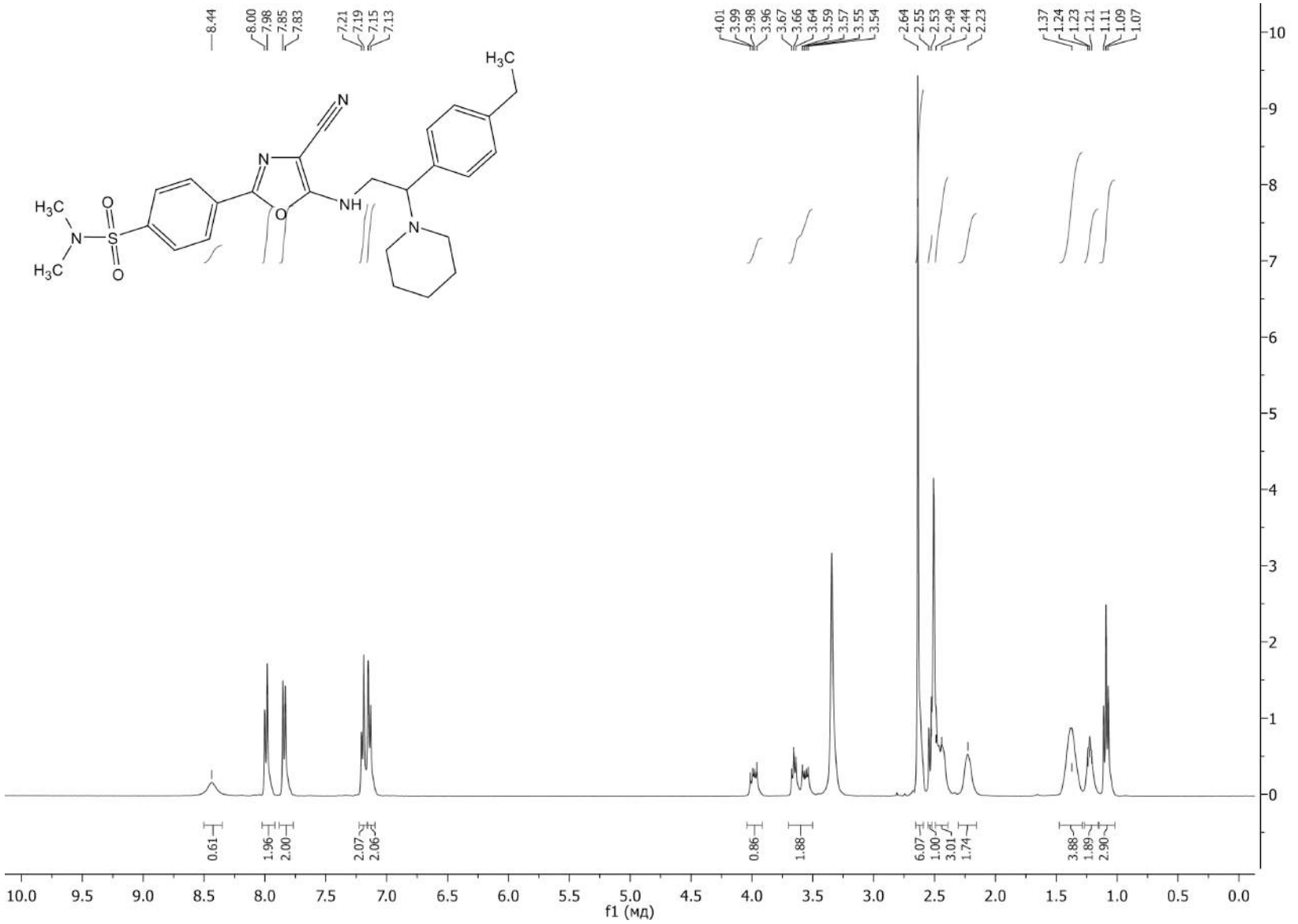


Fig. S22. ^{1}H NMR spectrum of 4-[4-cyano-5-[[2-(4-ethylphenyl)-2-piperidin-1-ylethyl]amino]-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 3.

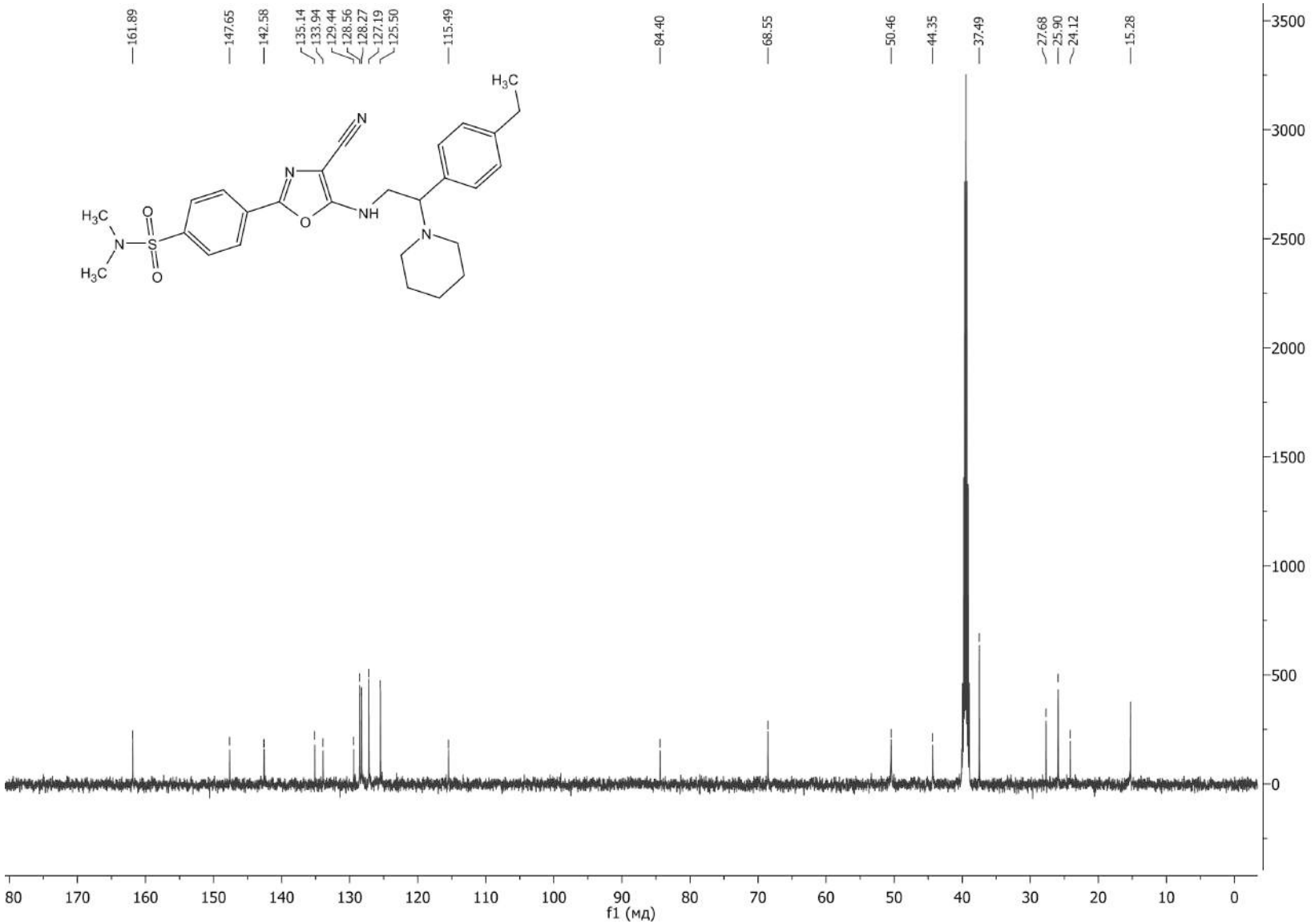


Fig. S23. ^{13}C NMR spectrum of 4-[4-cyano-5-[[2-(4-ethylphenyl)-2-piperidin-1-ylethyl]amino]-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 3.

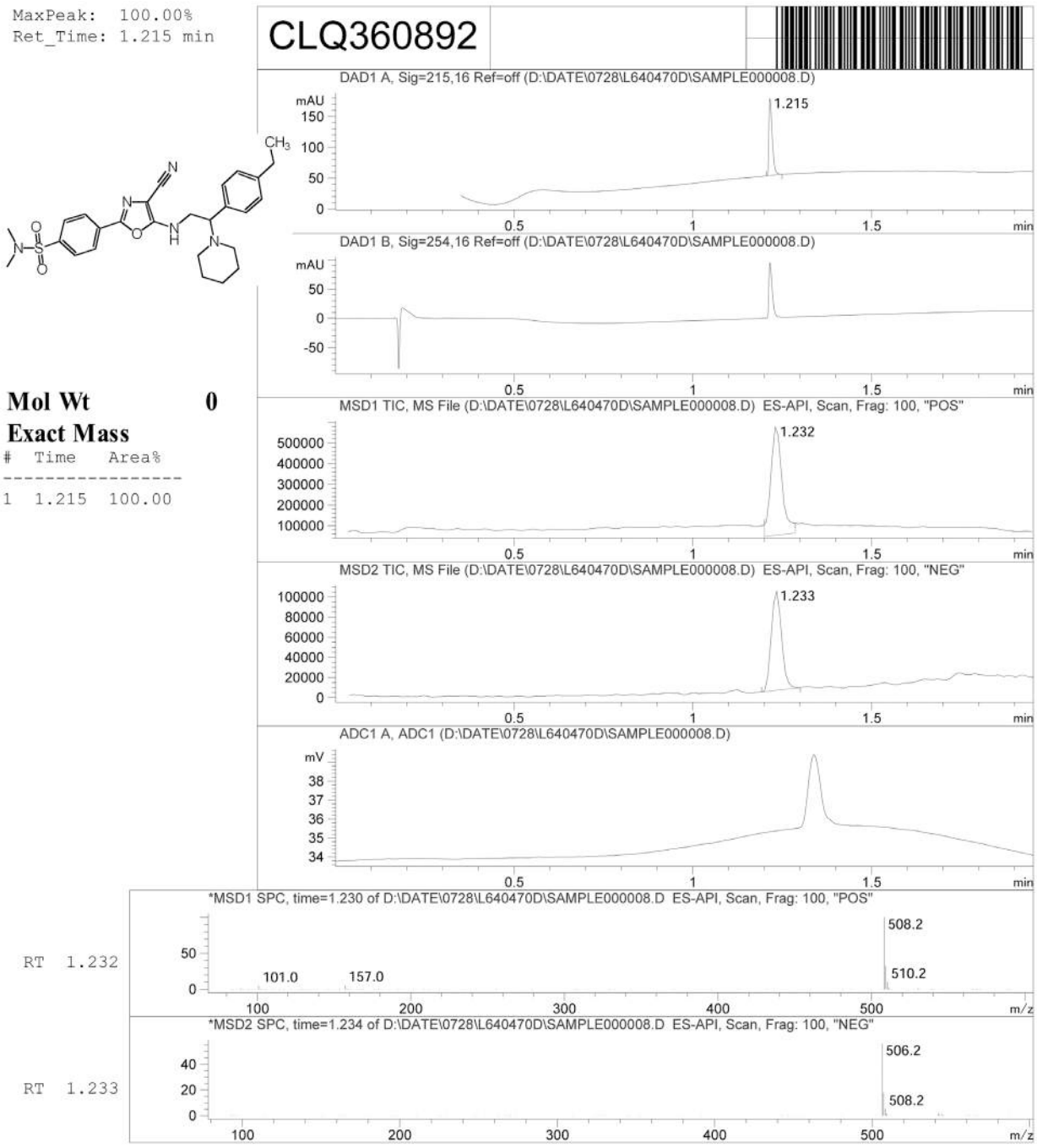


Fig. S24. LCMS spectrum of 4-[4-cyano-5-[[2-(4-ethylphenyl)-2-piperidin-1-ylethyl]amino]-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 3.

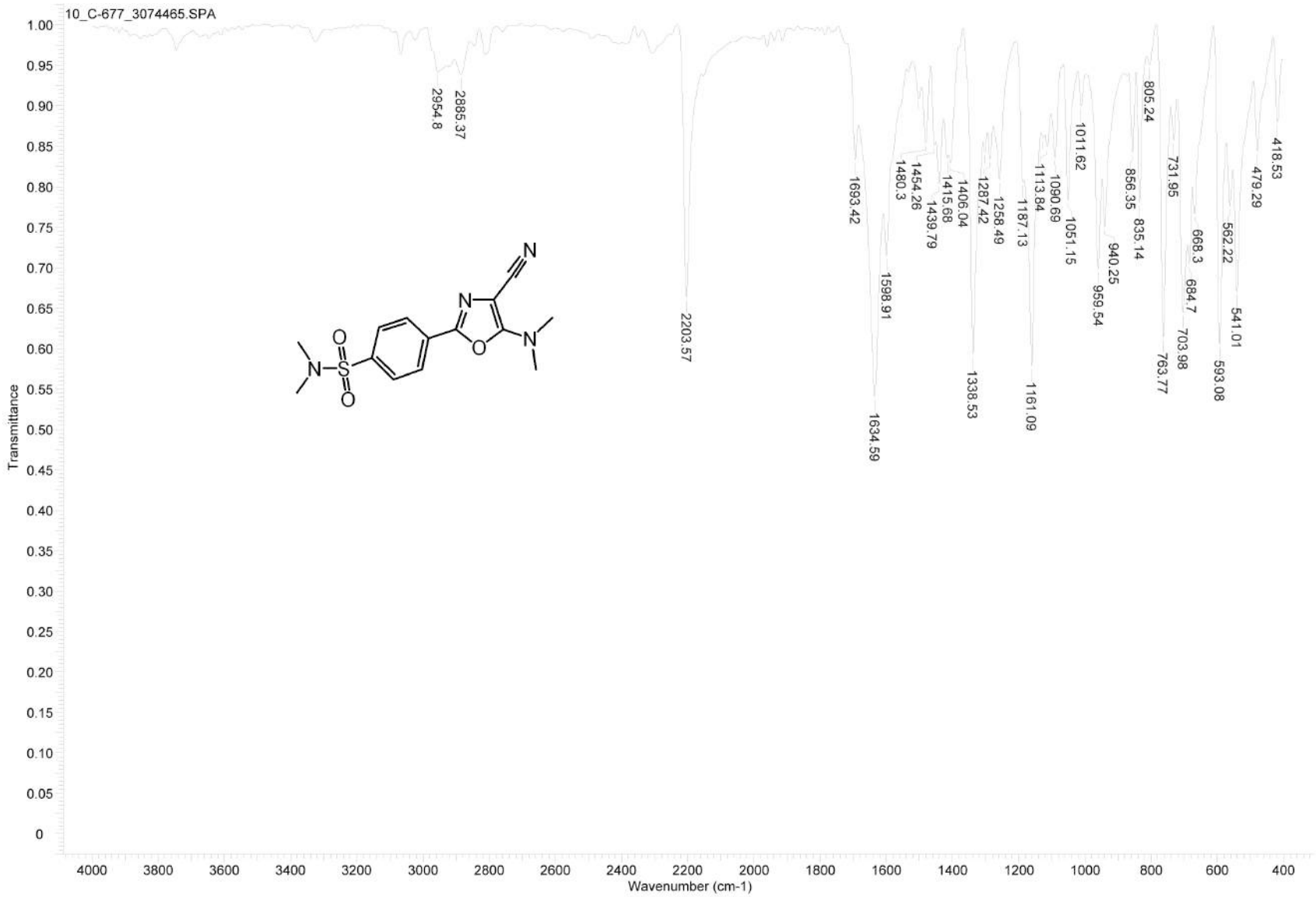


Fig. S25. IR spectrum of 4-[4-cyano-5-(dimethylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 4.

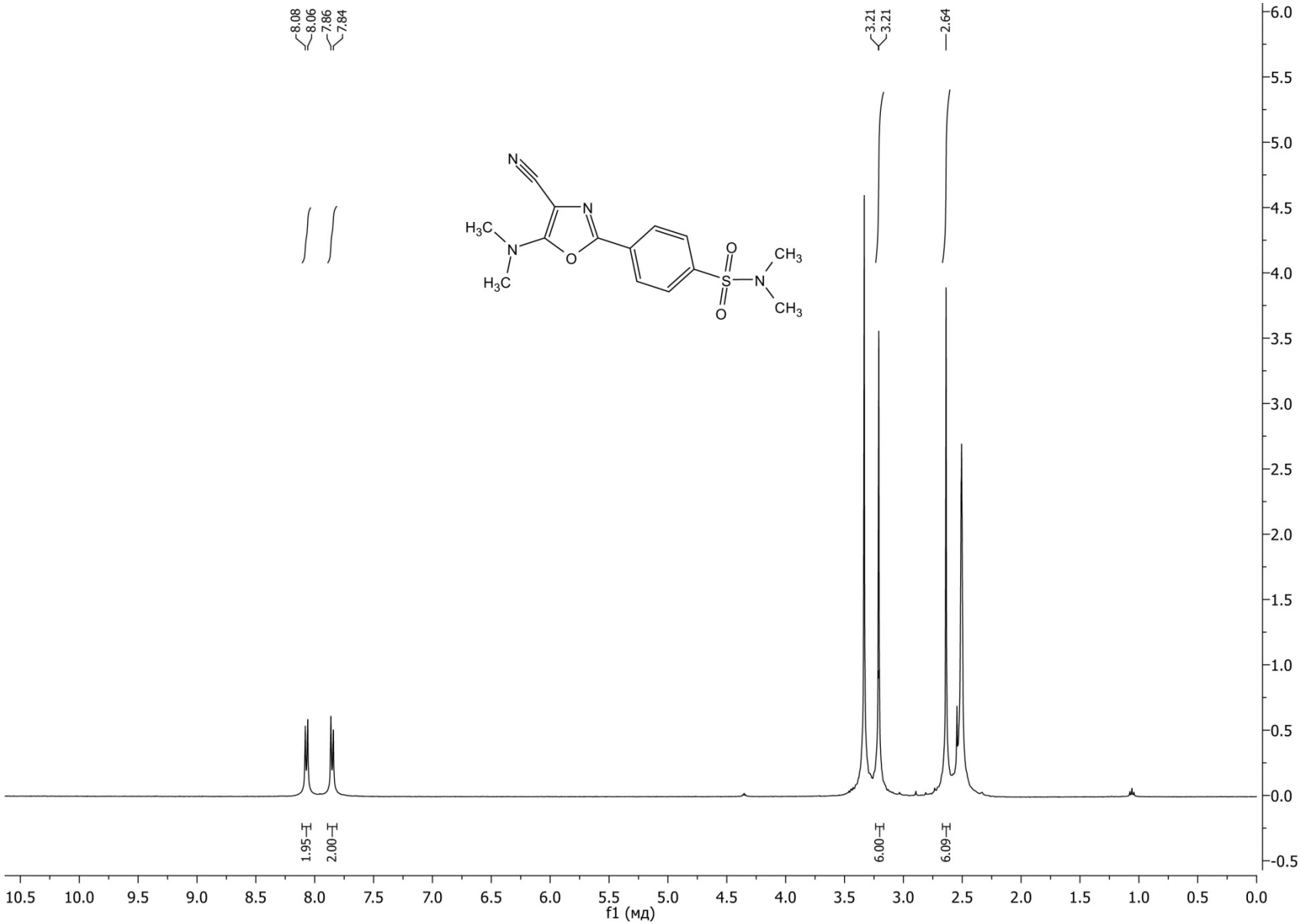


Fig. S26. ^{1}H NMR spectrum of 4-[4-cyano-5-(dimethylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 4.

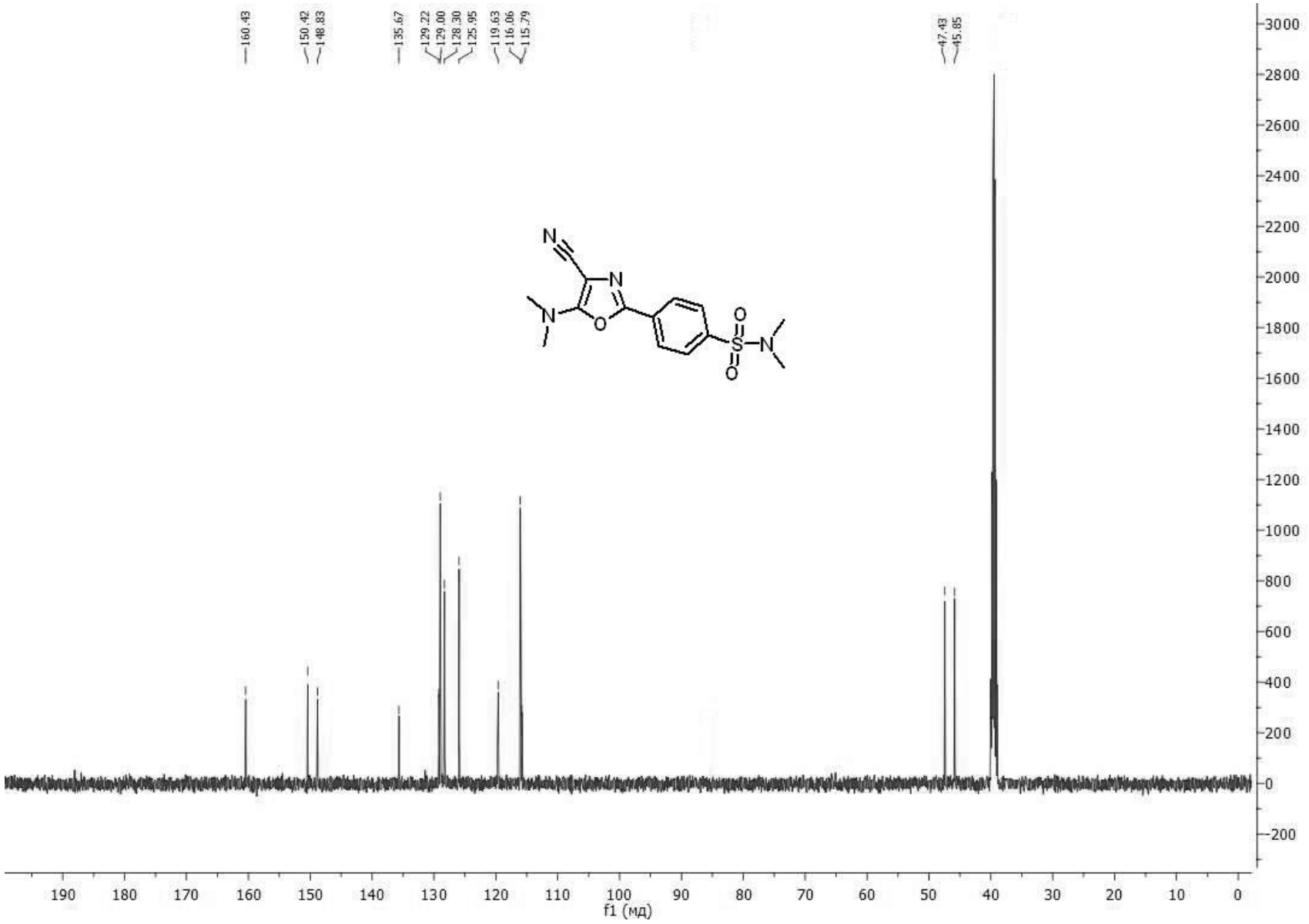


Fig. S27. ^{13}C NMR spectrum of 4-[4-cyano-5-(dimethylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 4.

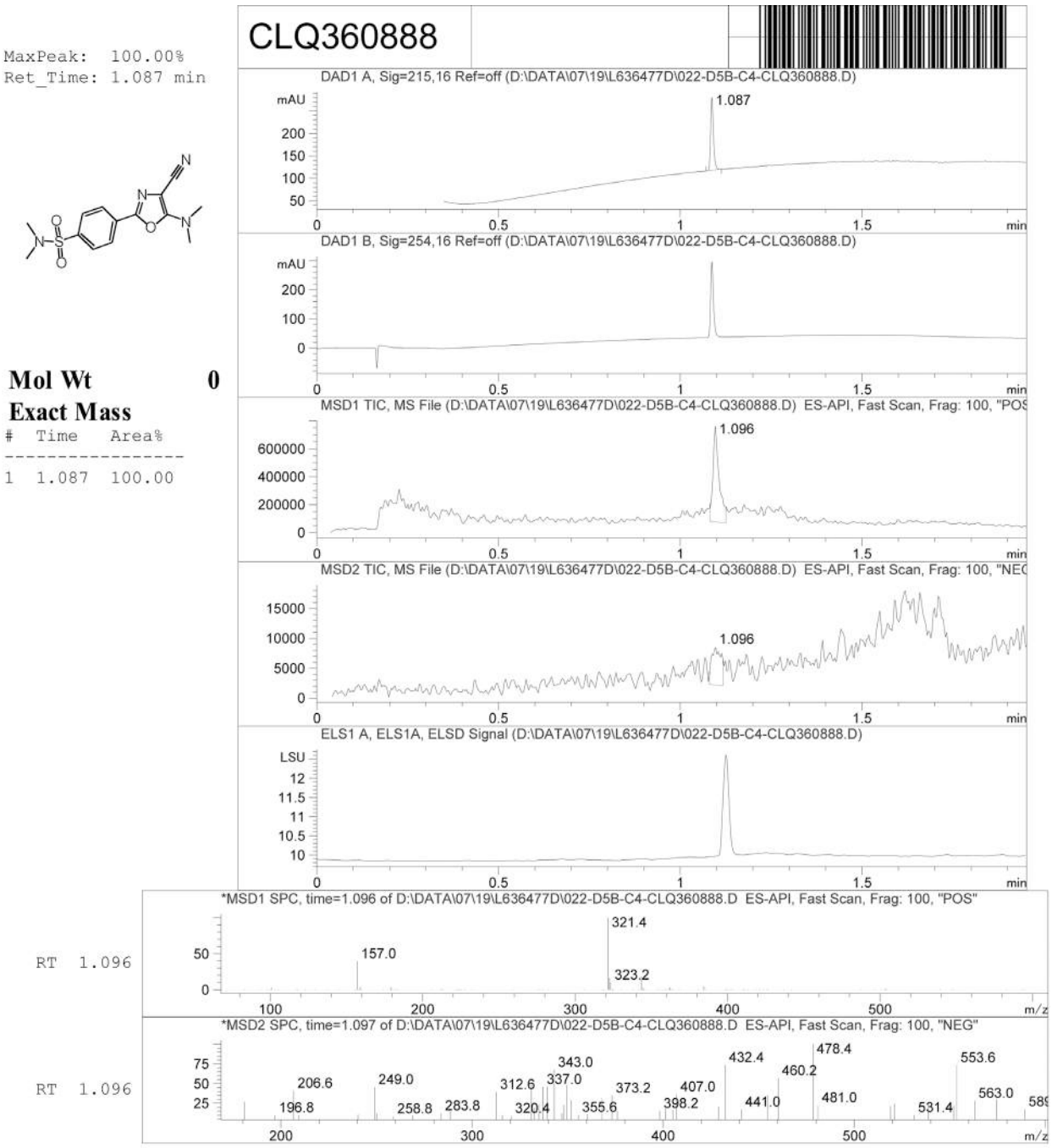


Fig. S28. LCMS spectrum of 4-[4-cyano-5-(dimethylamino)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 4.

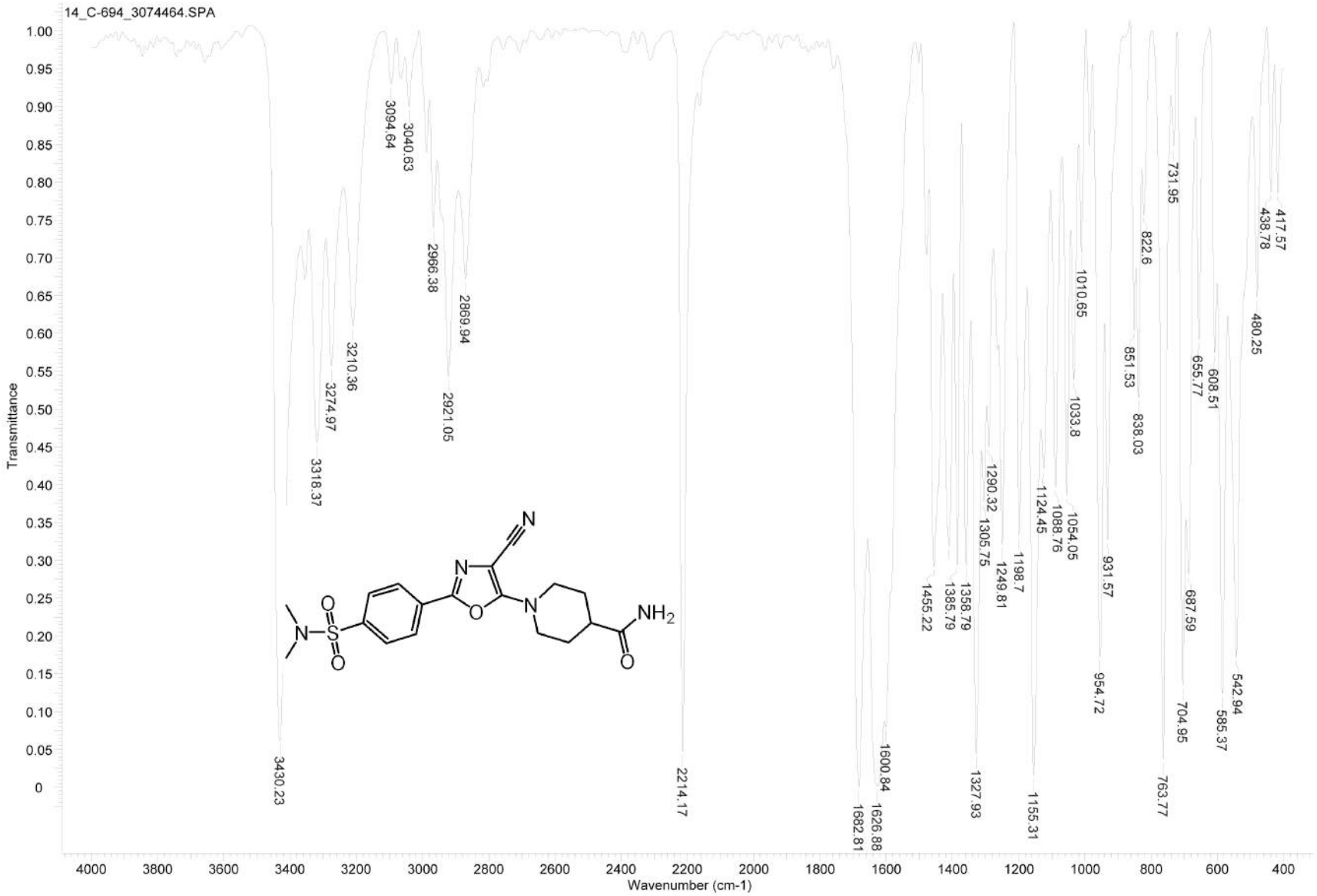


Fig. S29. IR spectrum of 1-[4-cyano-2-[4-(dimethylsulfamoyl)phenyl]-1,3-oxazol-5-yl]piperidine-4-carboxamide 5.

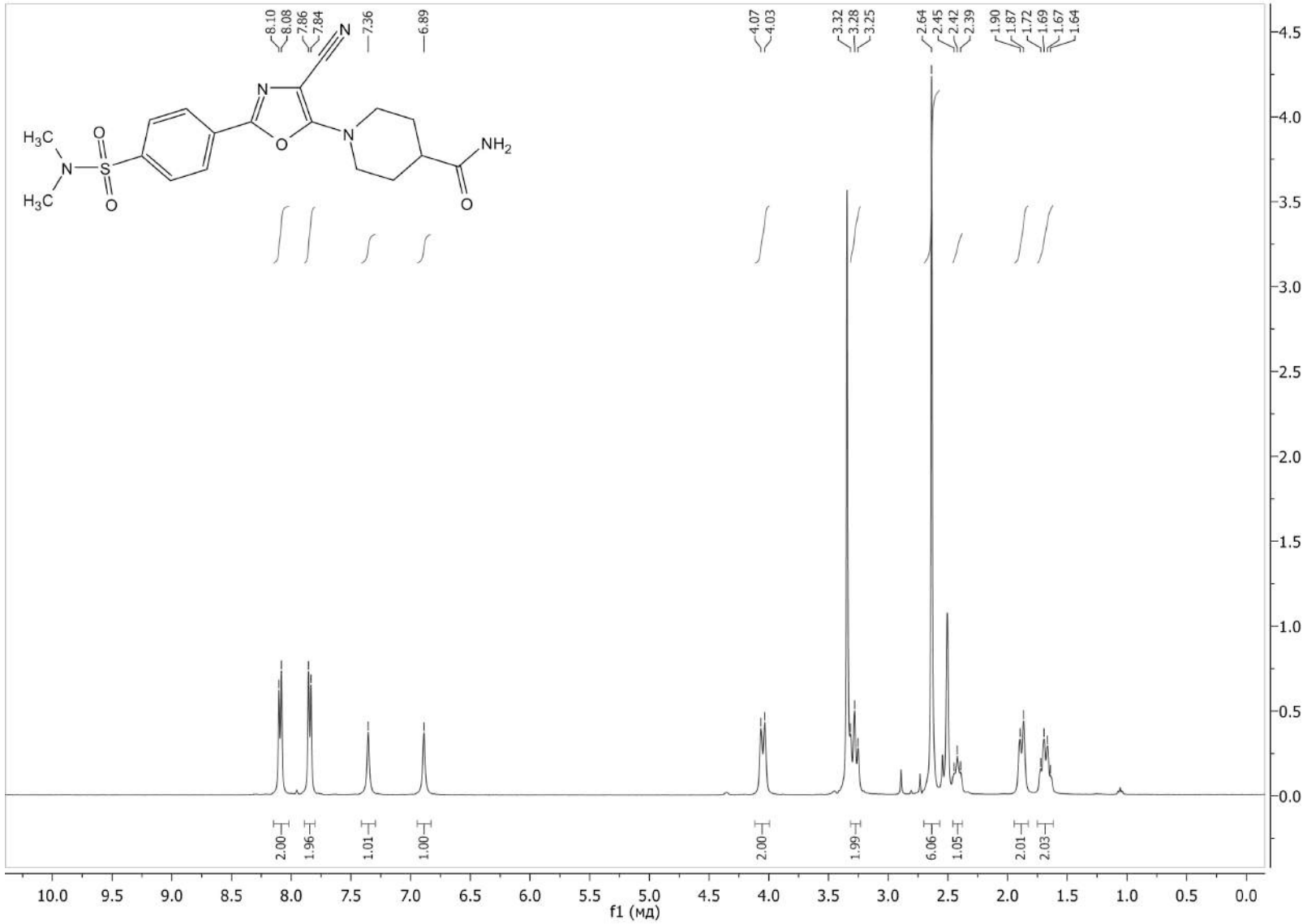


Fig. S30. [1]H NMR spectrum of 1-[4-cyano-2-[4-(dimethylsulfamoyl)phenyl]-1,3-oxazol-5-yl]piperidine-4-carboxamide 5.

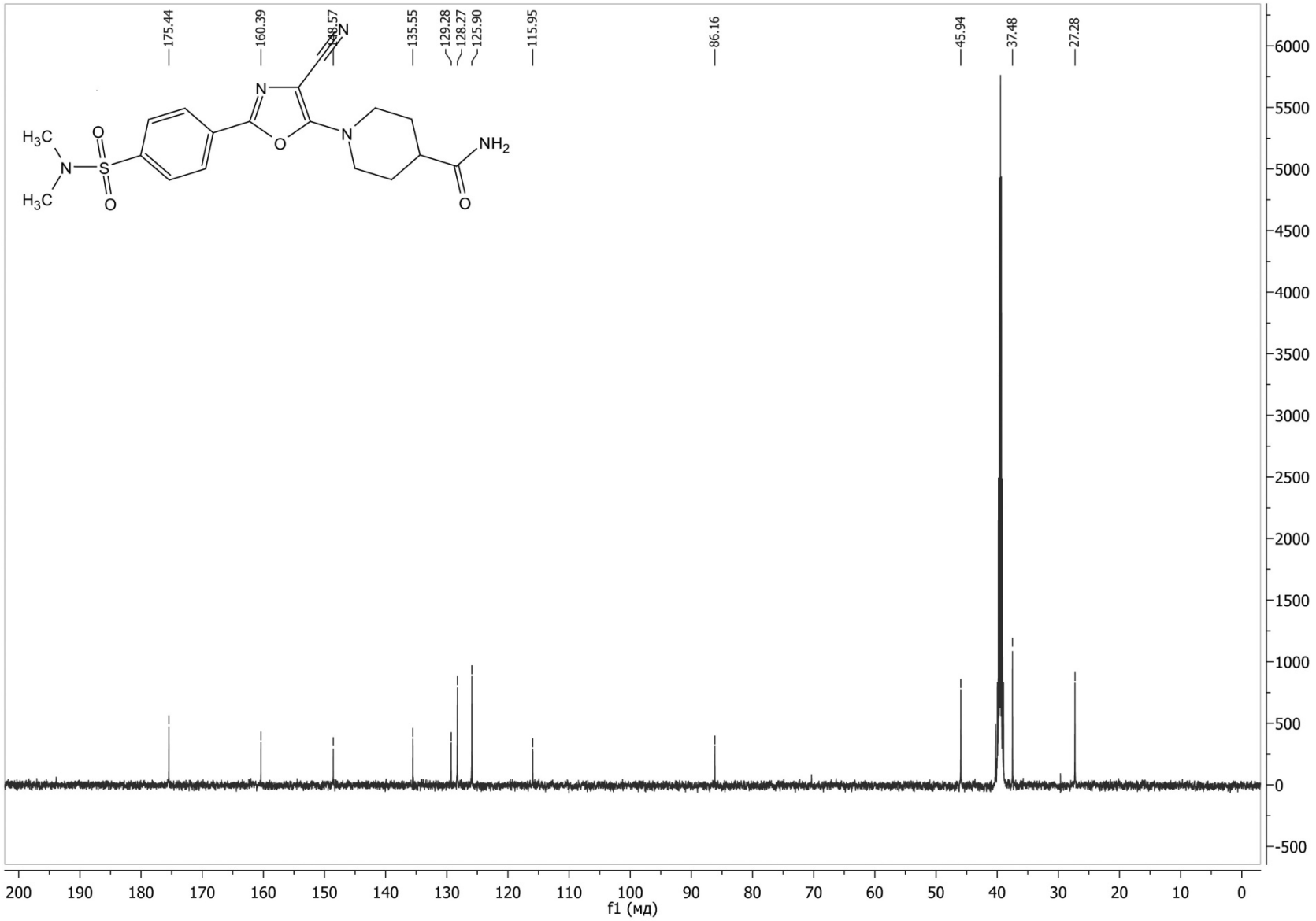


Fig. S31. ^{13}C NMR spectrum of 1-[4-cyano-2-[4-(dimethylsulfamoyl)phenyl]-1,3-oxazol-5-yl]piperidine-4-carboxamide 5.

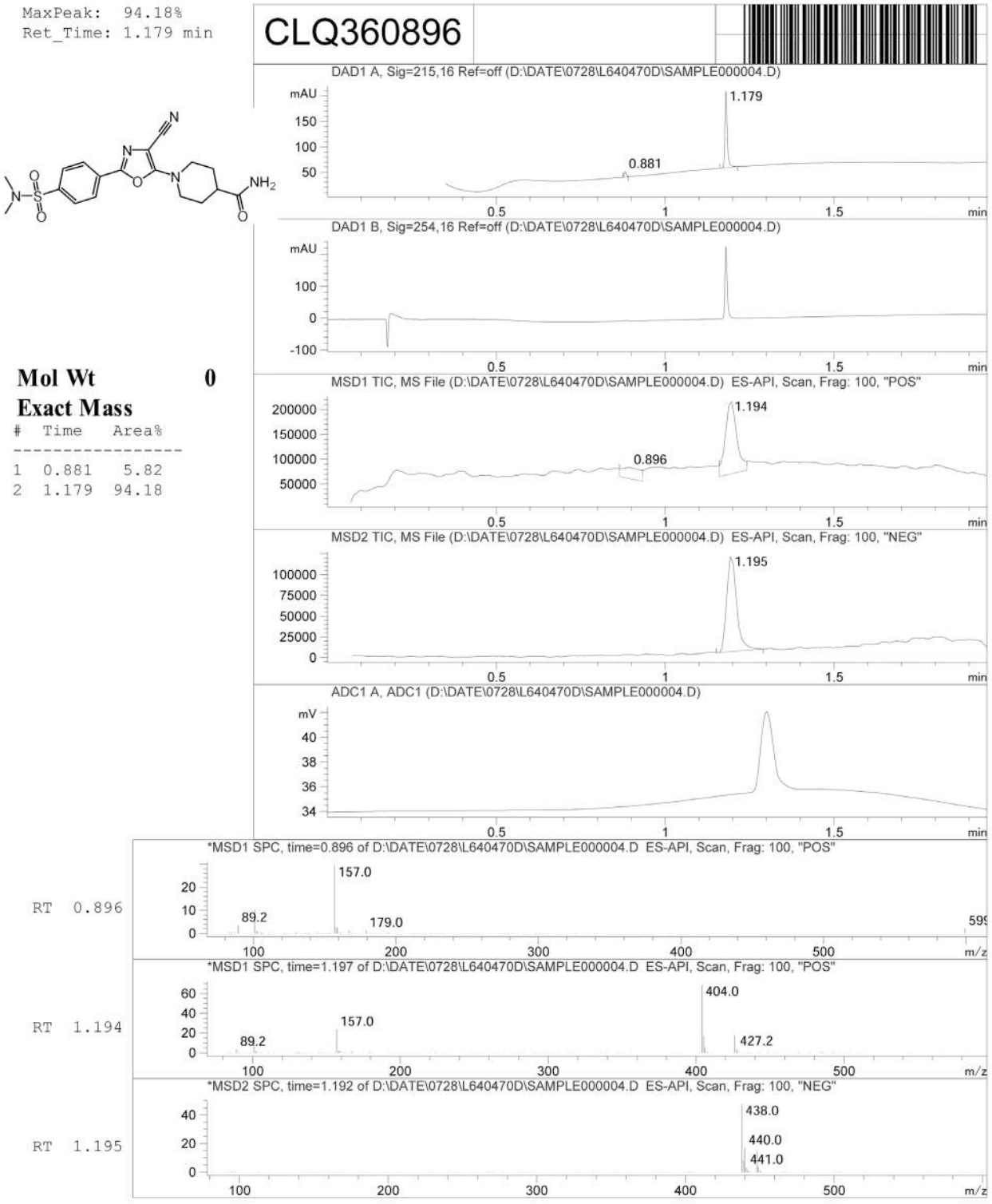


Fig. S32. LCMS spectrum of 1-[4-cyano-2-[4-(dimethylsulfamoyl)phenyl]-1,3-oxazol-5-yl]piperidine-4-carboxamide 5.

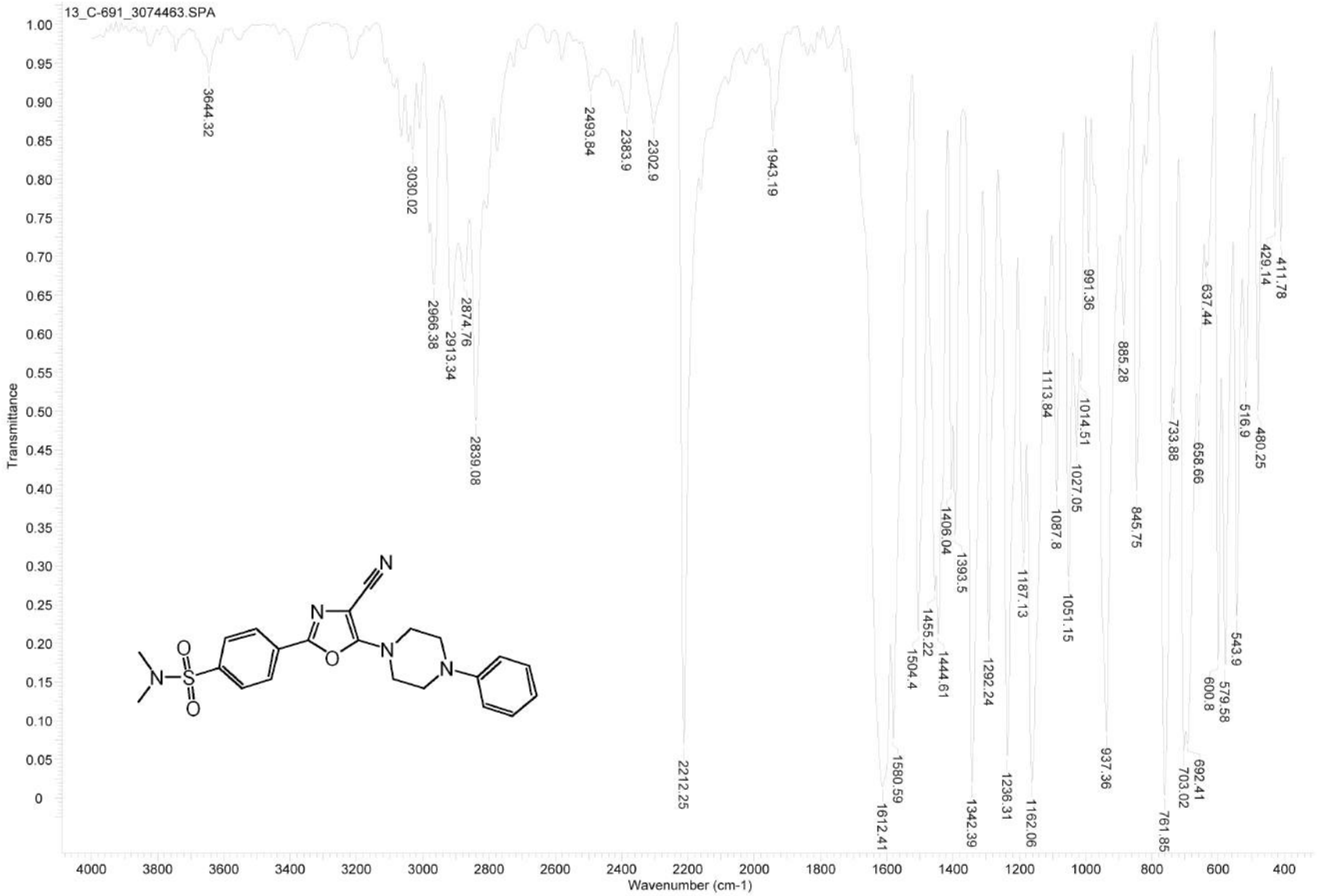


Fig. S33. IR spectrum of 4-[4-cyano-5-(4-phenylpiperazin-1-yl)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 6.

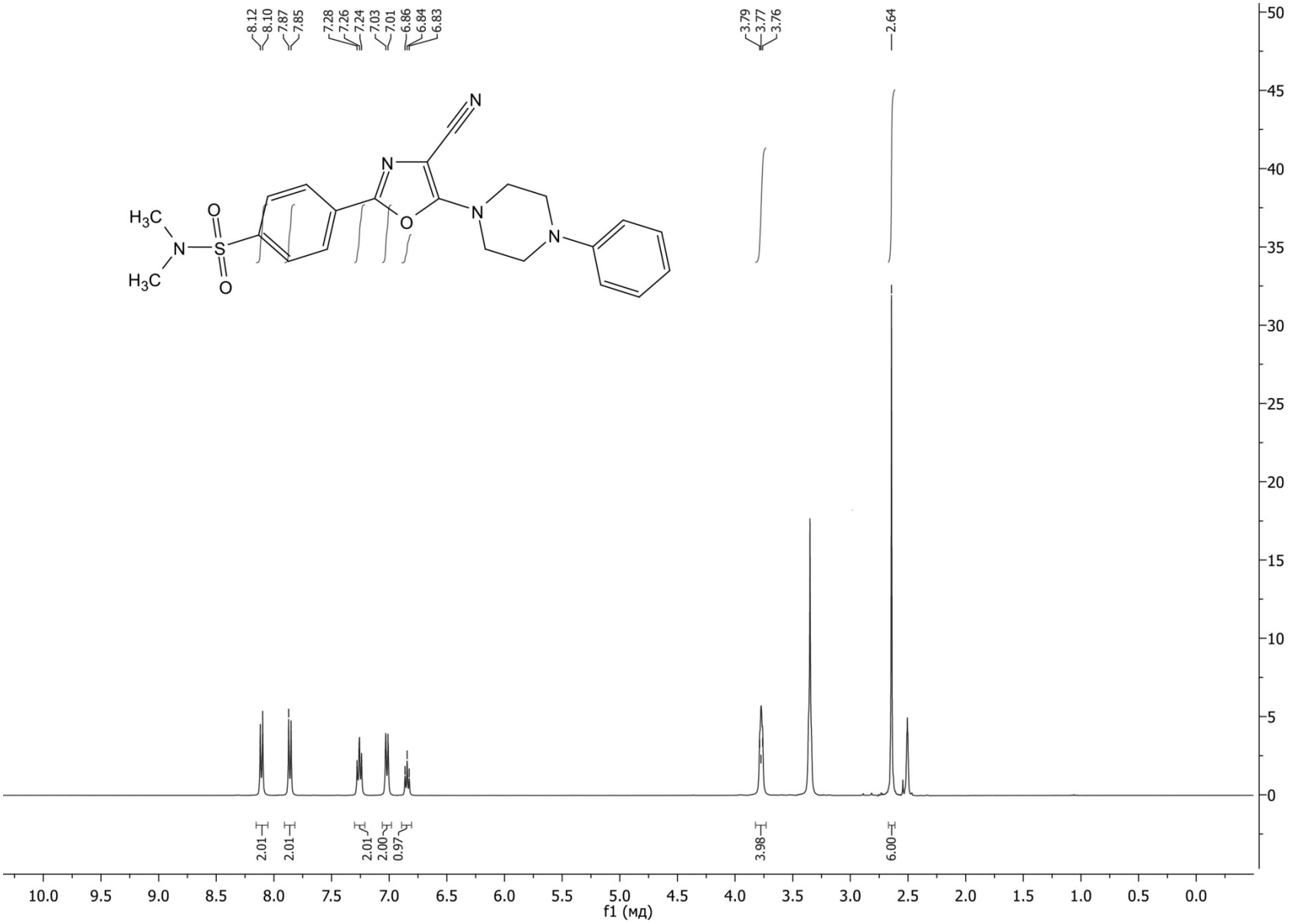


Fig. S34. [1]H NMR spectrum of 4-[4-cyano-5-(4-phenylpiperazin-1-yl)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 6.

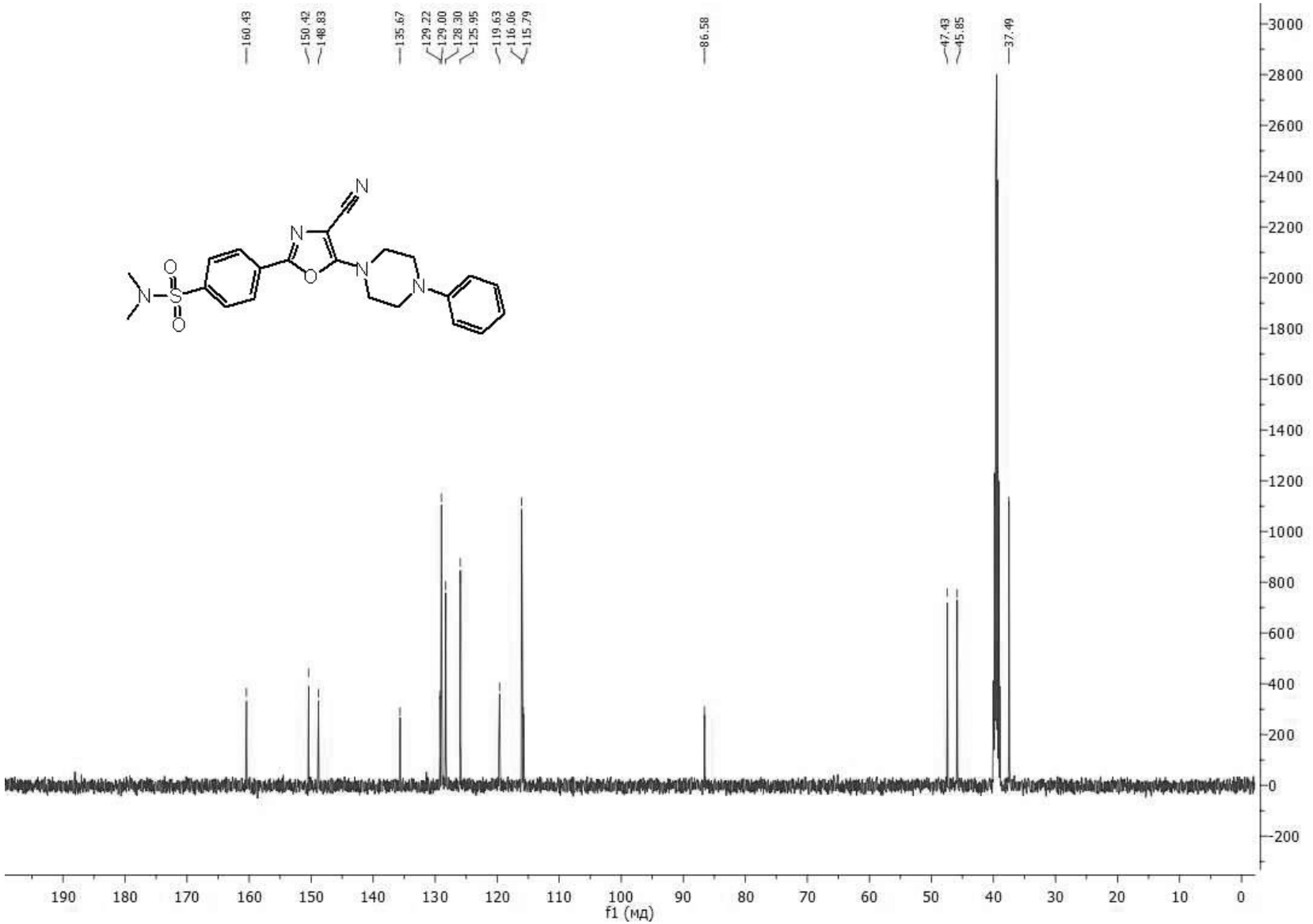
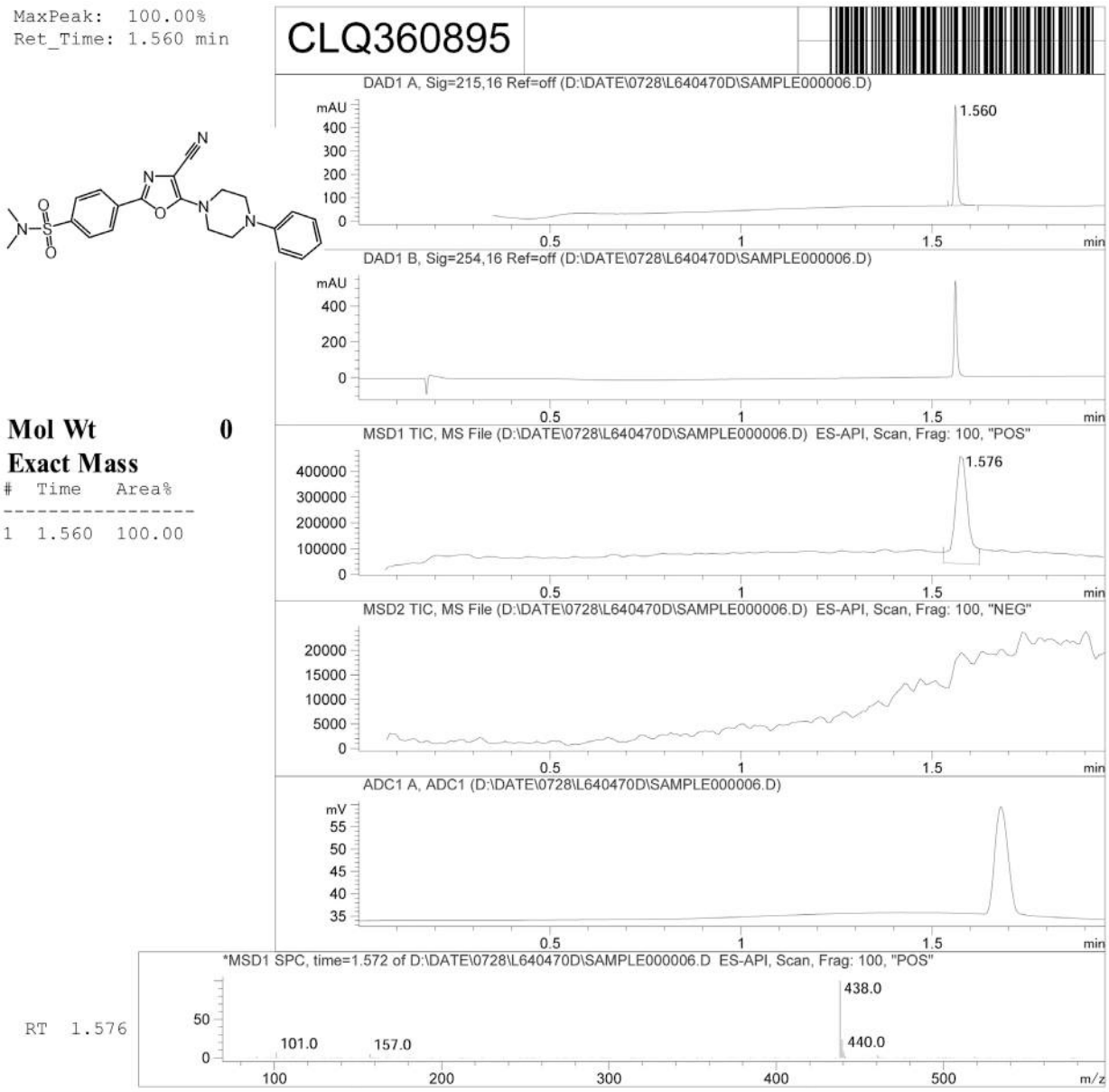


Fig. S35. ^{13}C NMR spectrum of 4-[4-cyano-5-(4-phenylpiperazin-1-yl)-1,3-oxazol-2-yl]-N,N-dimethylbenzenesulfonamide 6.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1.560
DAD1 B, Sig=254,16 Ref=off (D:\DATE\0728\L640470D\SAMPLE000006.D)
Mol Wt 0
Exact Mass
Time Area%
1 1.560 100.00
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1.576
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*MSD1 SPC, time=1.572 of D:\DATE\0728\L640470D\SAMPLE000006.D ES-API, Scan, Frag: 100, "POS"
RT 1.576
438.0
440.0
101.0
157.0
m/z

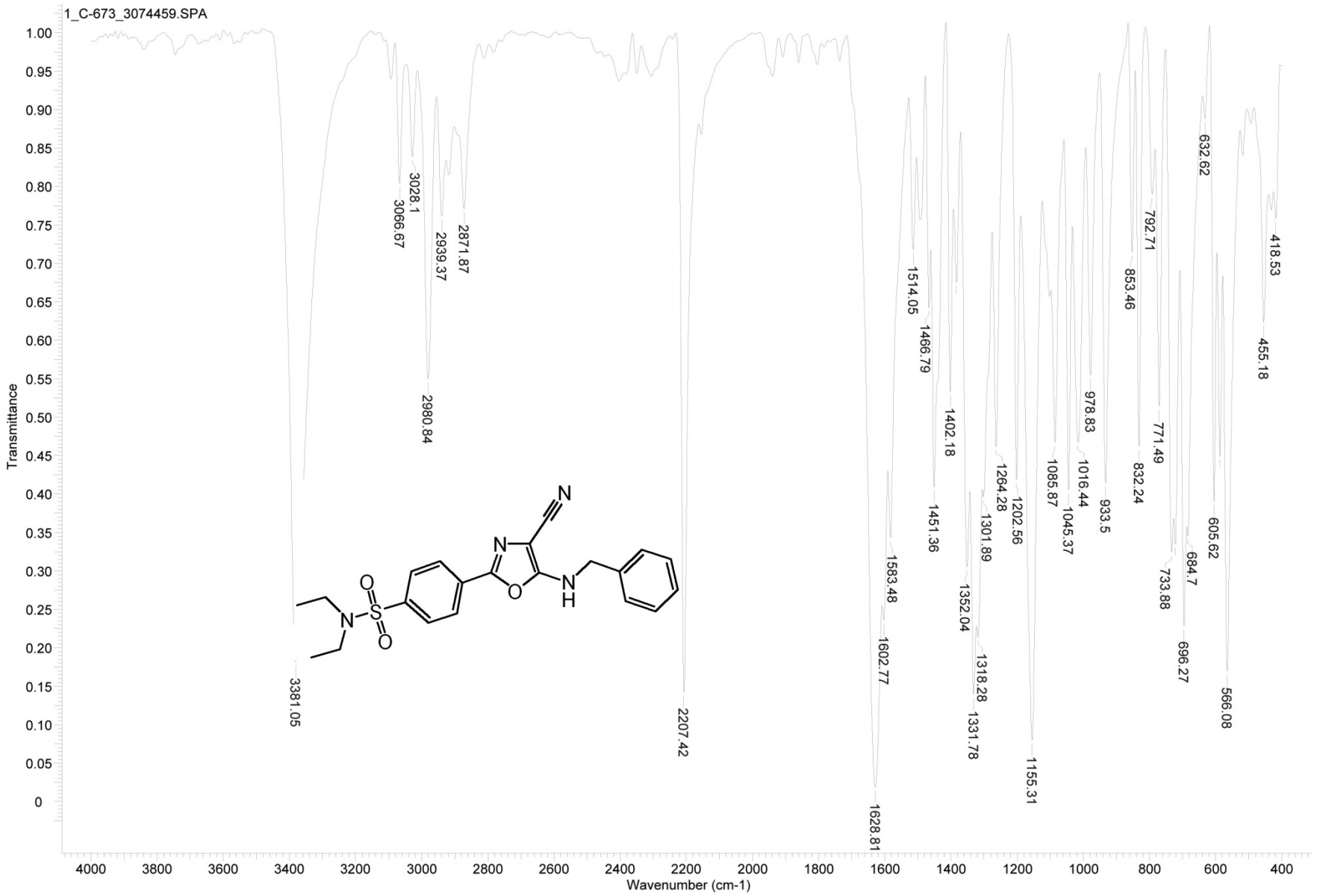

Fig. S37. IR spectrum of 4-[5-(benzylamino)-4-cyano-1,3-oxazol-2-yl]-N,N-diethylbenzenesulfonamide 7.

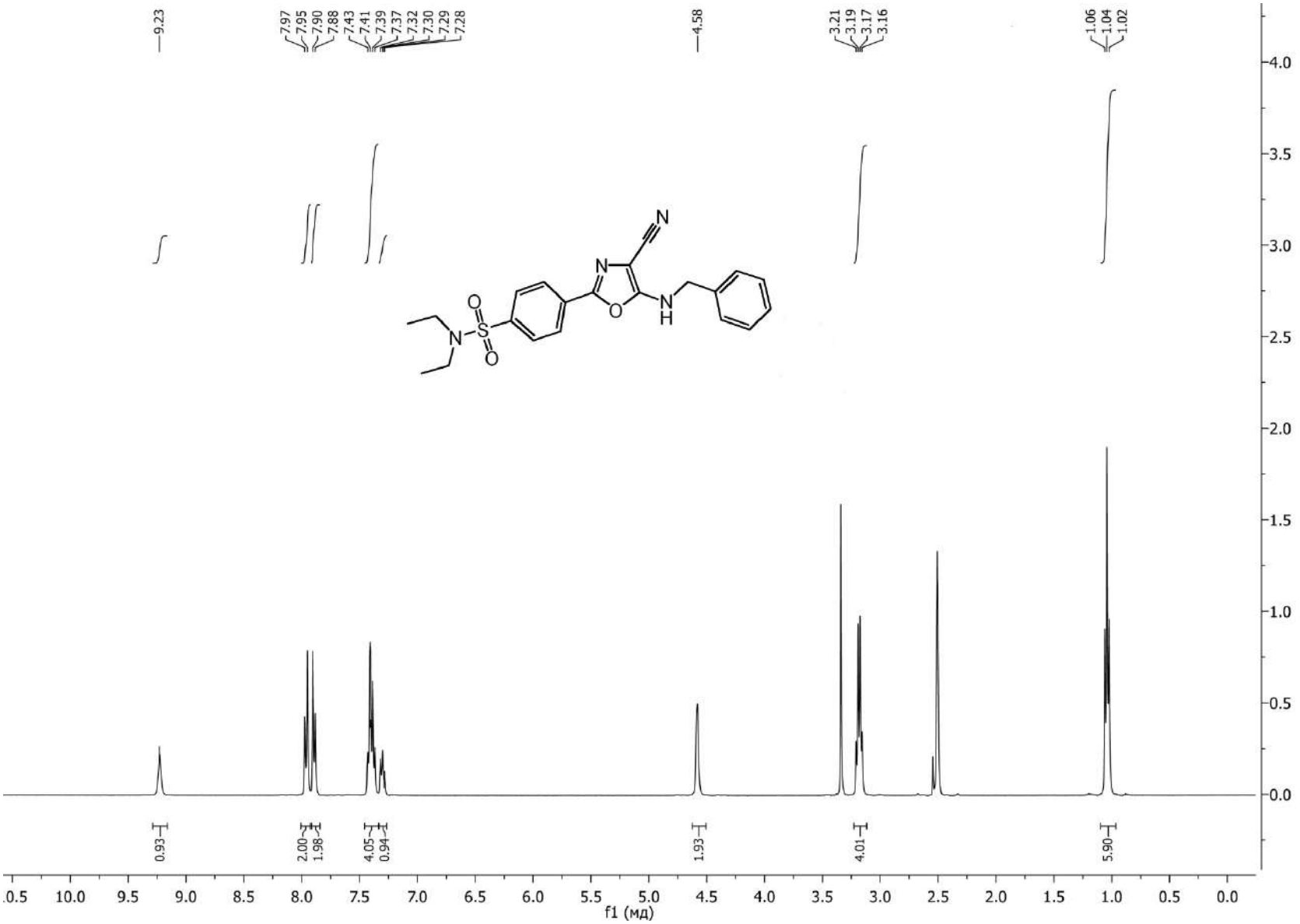

Fig. S38. [1]H NMR spectrum of 4-[5-(benzylamino)-4-cyano-1,3-oxazol-2-yl]-N,N-diethylbenzenesulfonamide 7.

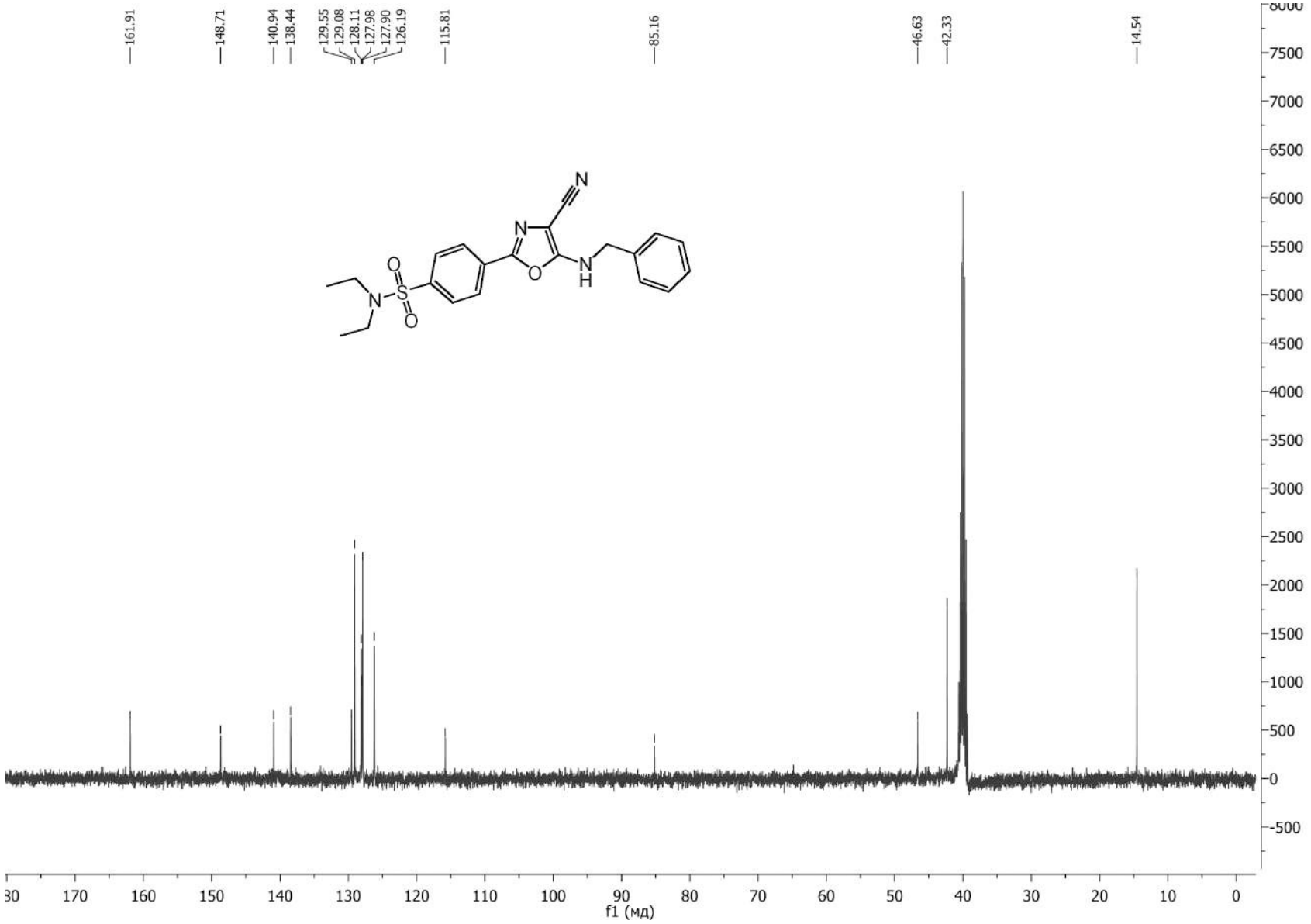

Fig. S39. ^{13}C NMR spectrum of 4-[5-(benzylamino)-4-cyano-1,3-oxazol-2-yl]-N,N-diethylbenzenesulfonamide 7.

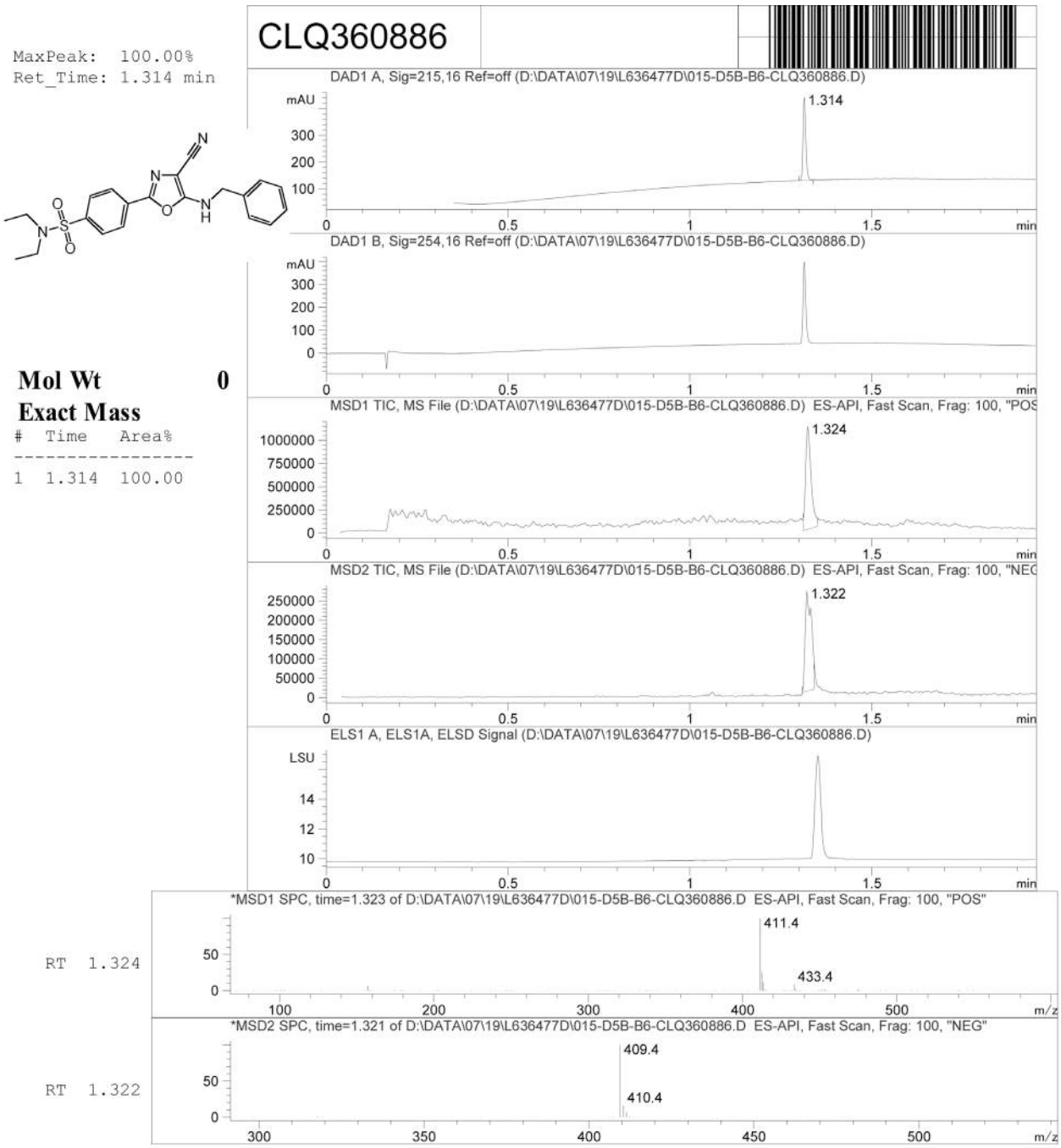

Fig. S40. LCMS spectrum of 4-[5-(benzylamino)-4-cyano-1,3-oxazol-2-yl]-N,N-diethylbenzenesulfonamide 7.

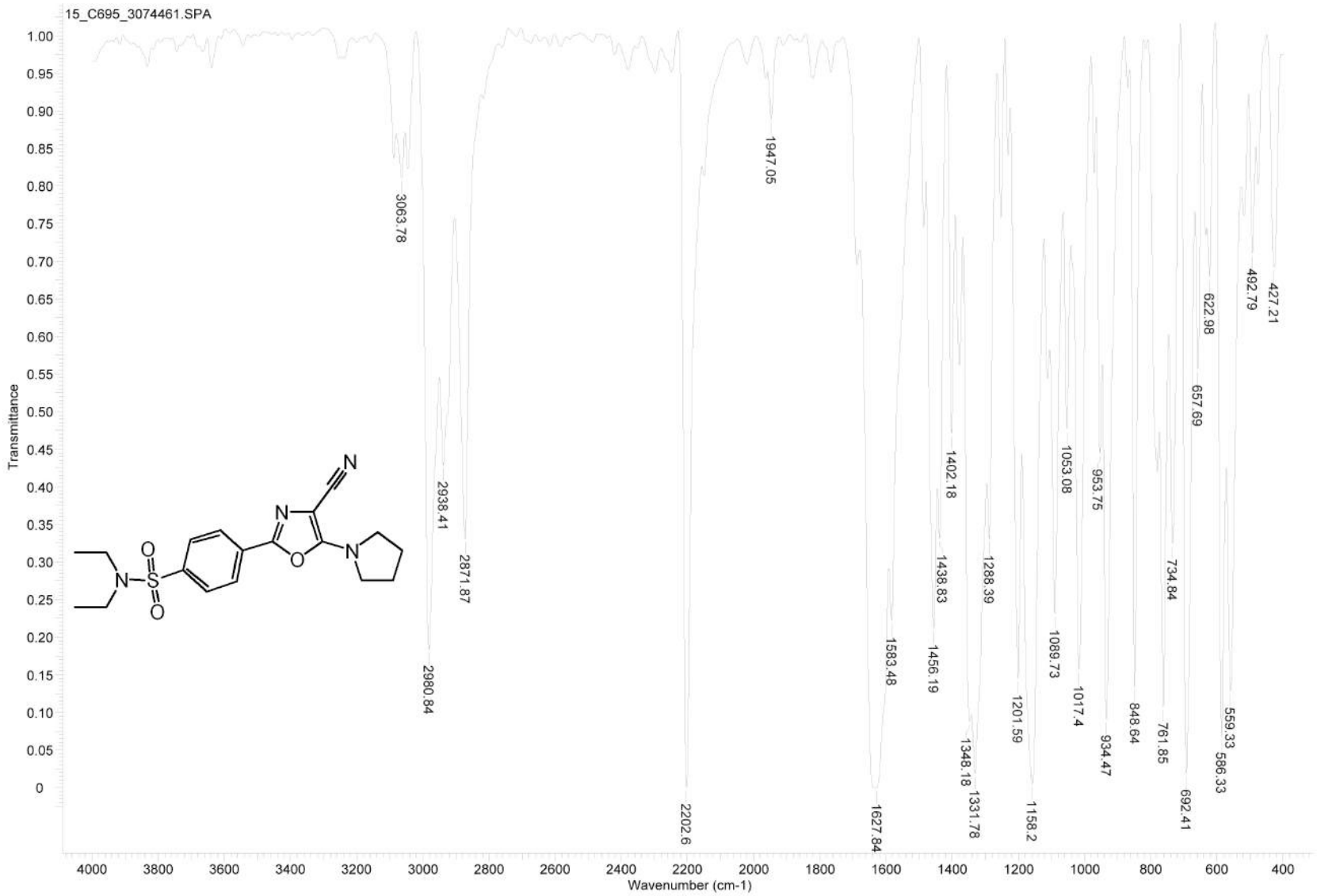

Fig. S41. IR spectrum of 4-(4-cyano-5-pyrrolidin-1-yl-1,3-oxazol-2-yl)-N,N-diethylbenzenesulfonamide 8.

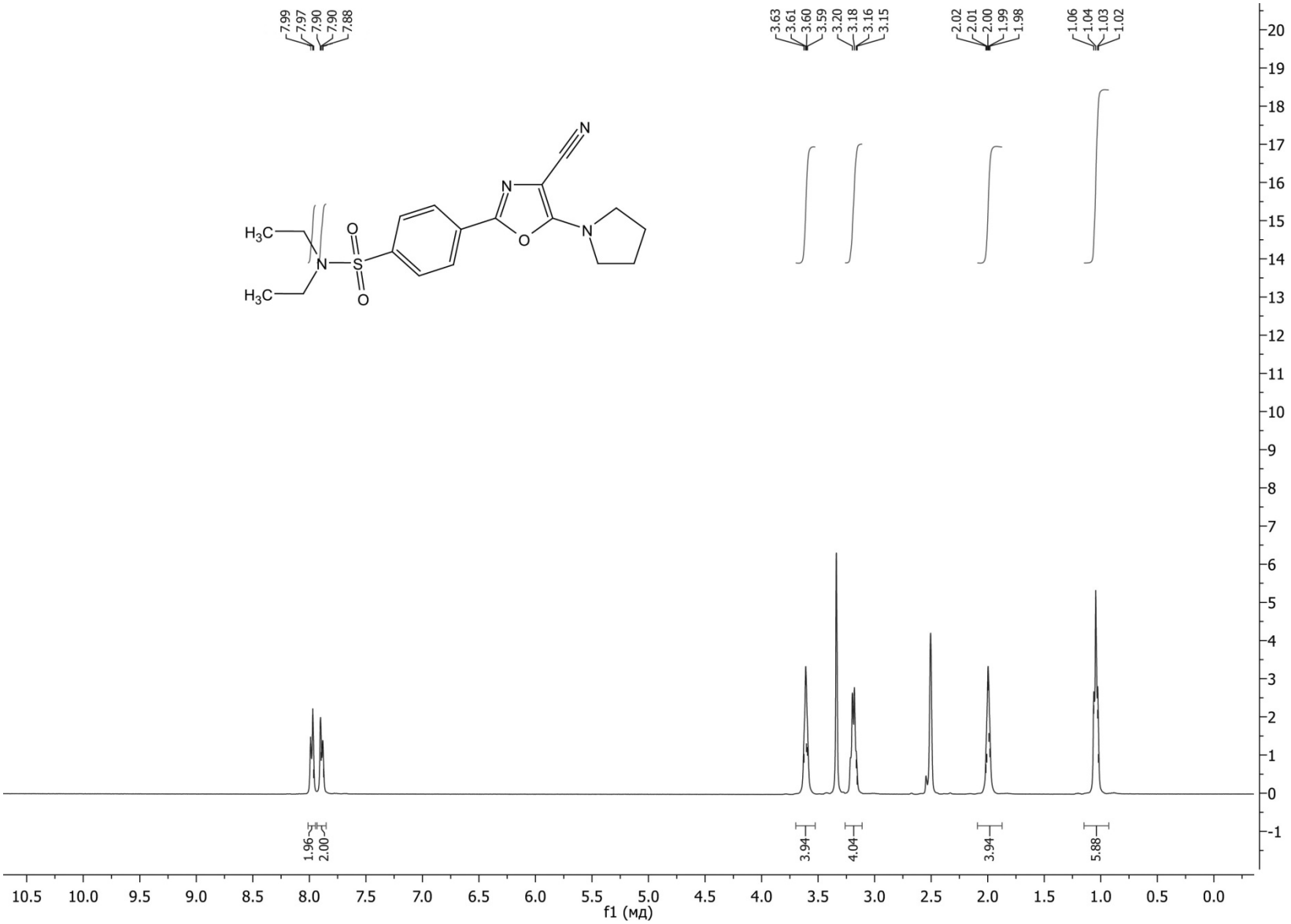

Fig. S42. ^{1}H NMR spectrum of 4-(4-cyano-5-pyrrolidin-1-yl-1,3-oxazol-2-yl)-N,N-diethylbenzenesulfonamide 8.

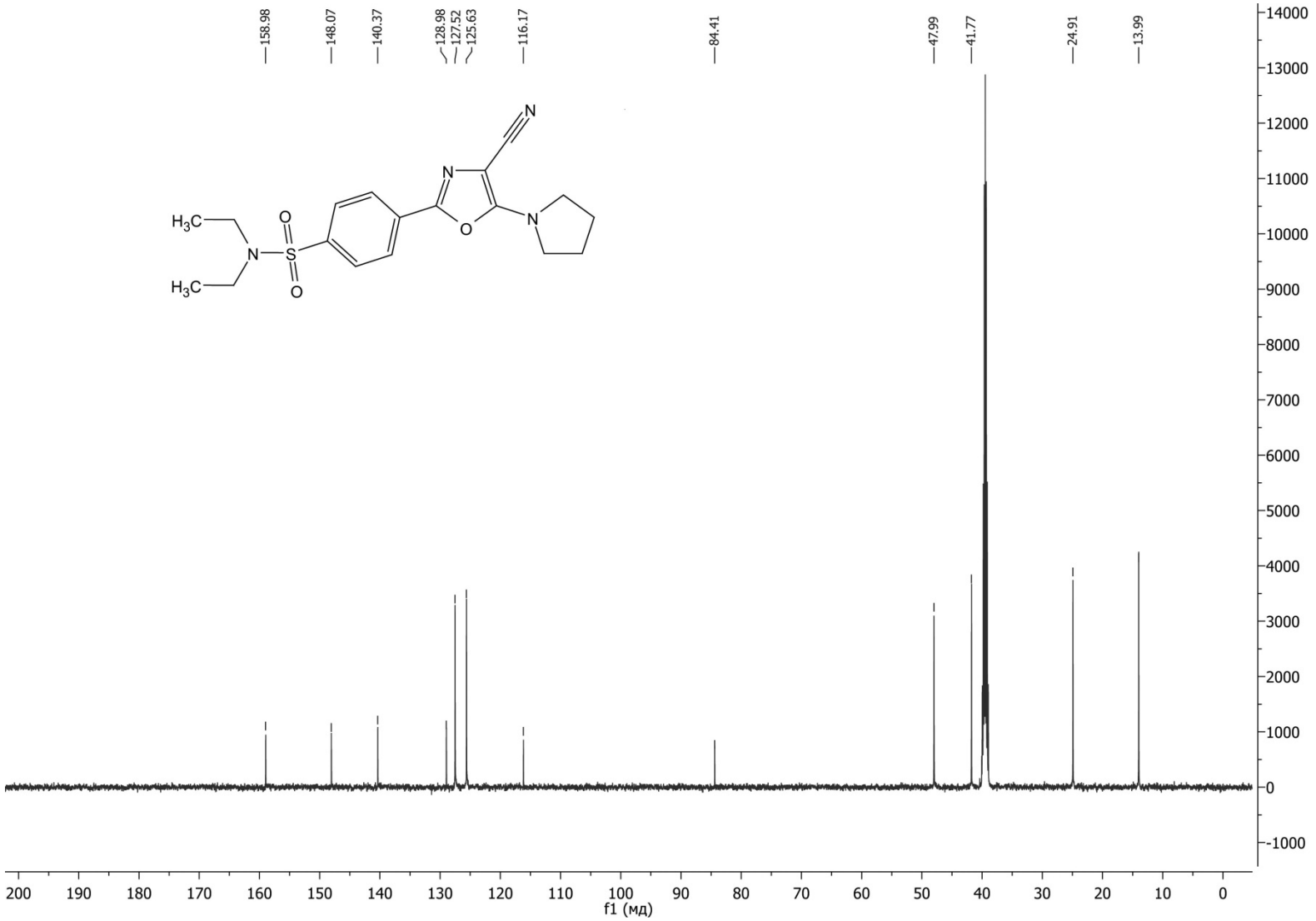

Fig. S43. ^{13}C NMR spectrum of 4-(4-cyano-5-pyrrolidin-1-yl-1,3-oxazol-2-yl)-N,N-diethylbenzenesulfonamide 8.

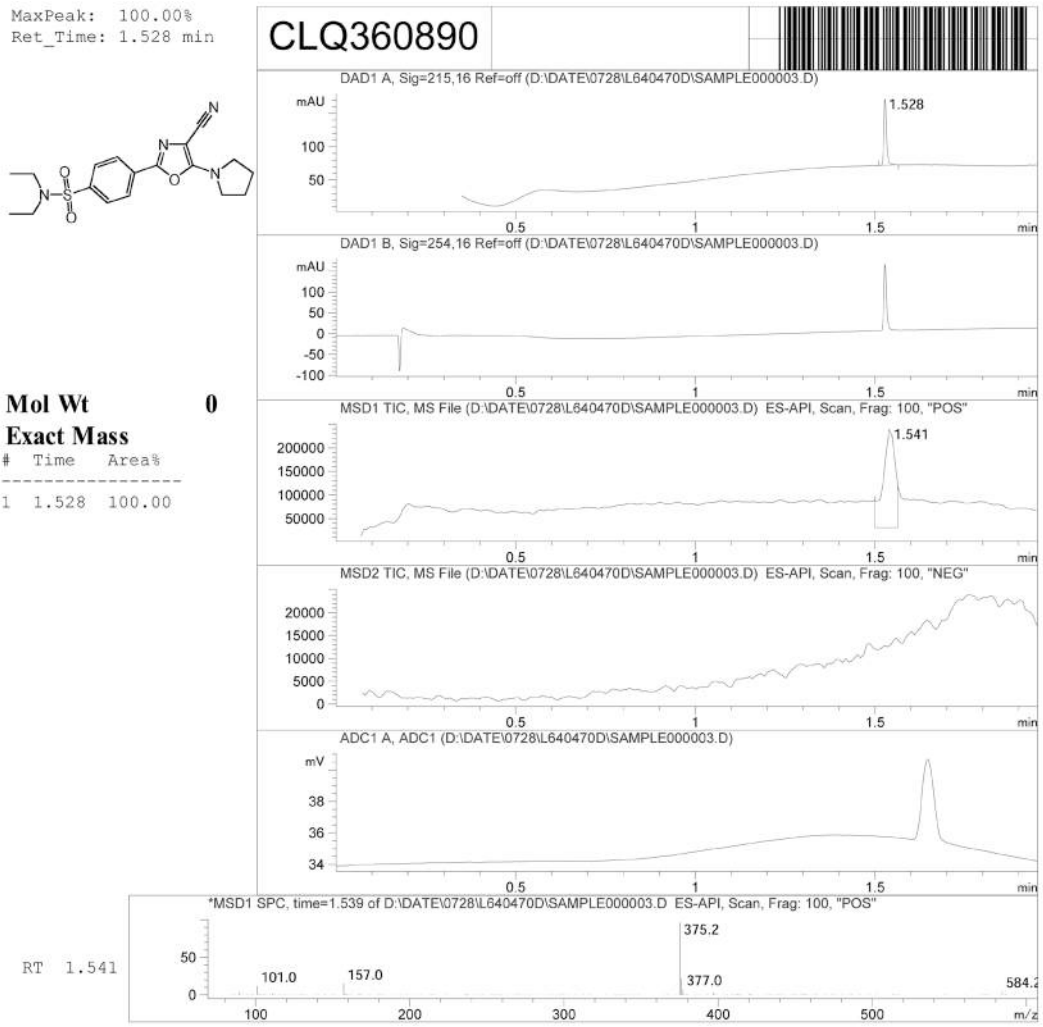

Fig. S44. LCMS spectrum of 4-(4-cyano-5-pyrrolidin-1-yl-1,3-oxazol-2-yl)-N,N-diethylbenzenesulfonamide 8.

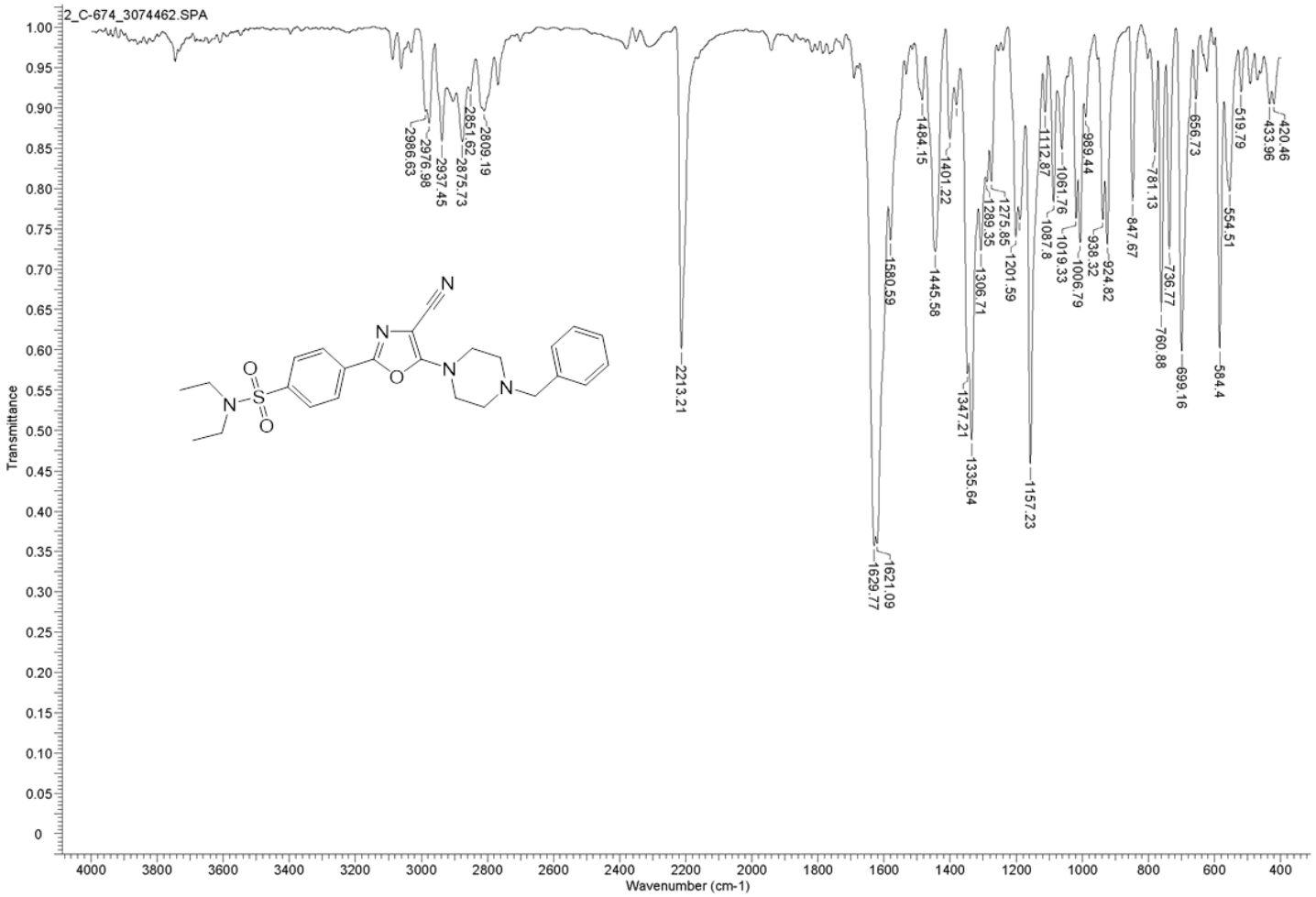

Fig. S45. IR spectrum of 4-[5-(4-benzylpiperazin-1-yl)-4-cyano-1,3-oxazol-2-yl]-N,N-diethylbenzenesulfonamide 9.

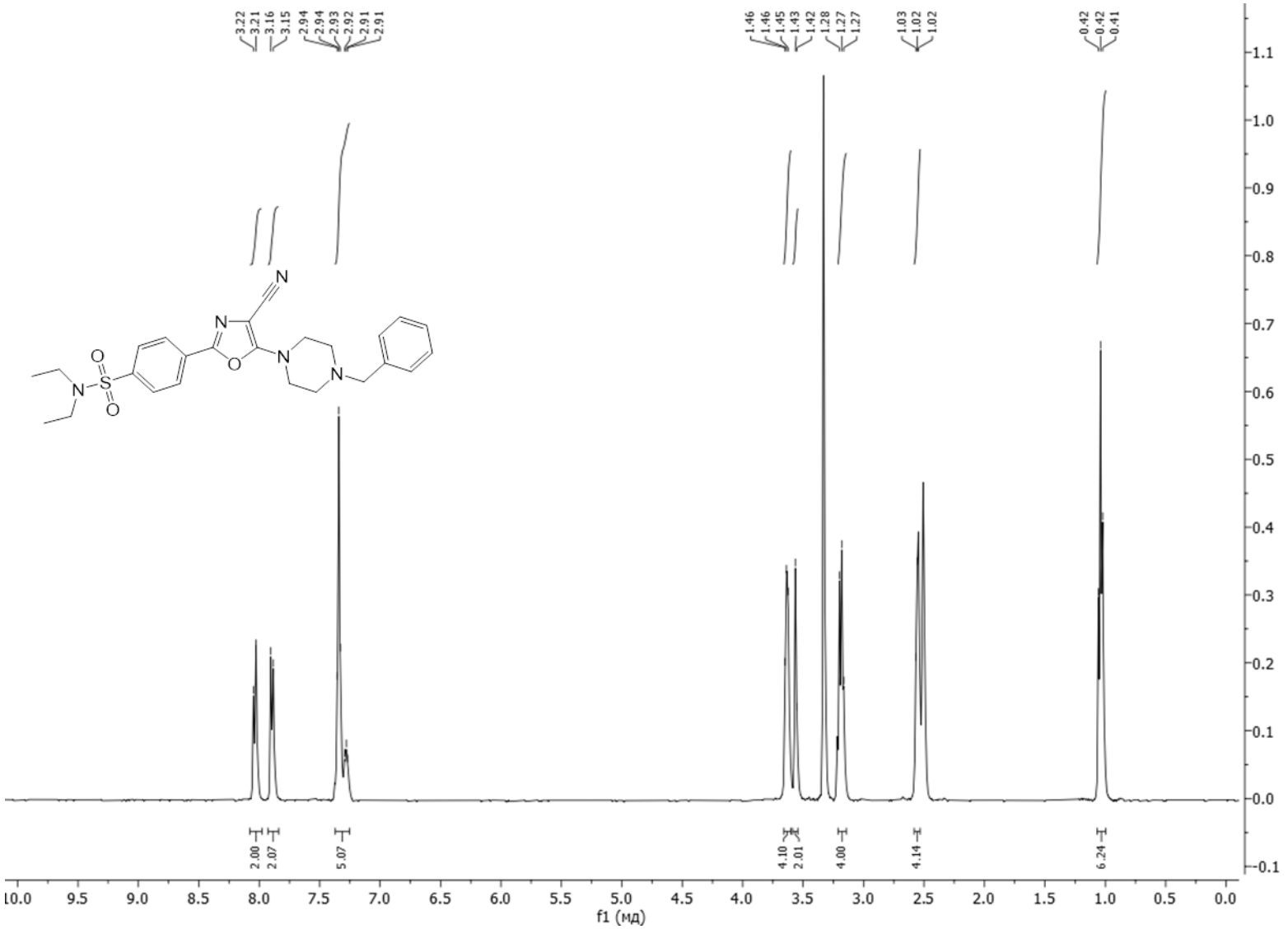

Fig. S46. [1]H NMR spectrum of 4-[5-(4-benzylpiperazin-1-yl)-4-cyano-1,3-oxazol-2-yl]-N,N-diethylbenzenesulfonamide 9.

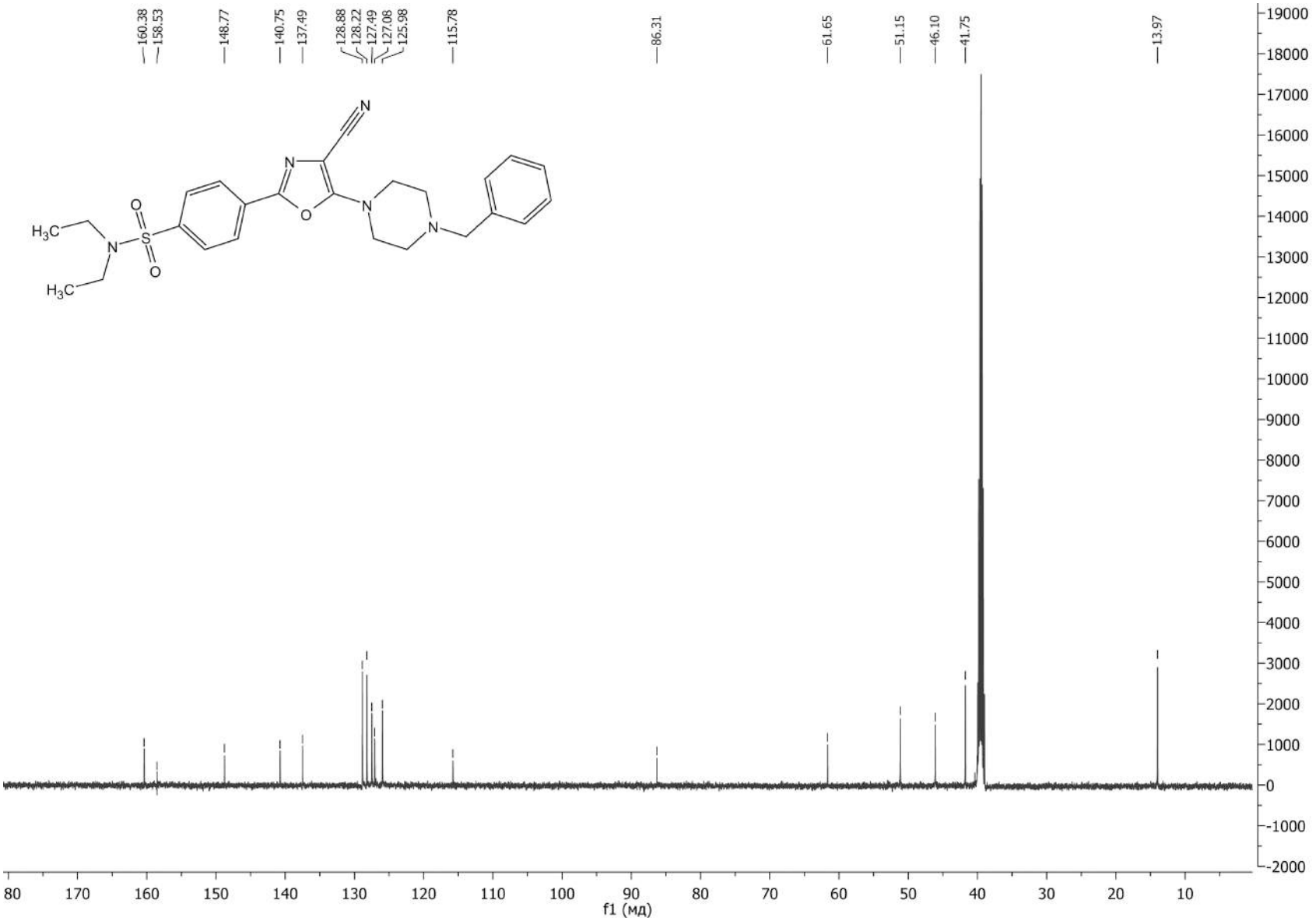

Fig. S47. ^{13}C NMR spectrum of 4-[5-(4-benzylpiperazin-1-yl)-4-cyano-1,3-oxazol-2-yl]-N,N-diethylbenzenesulfonamide 9.

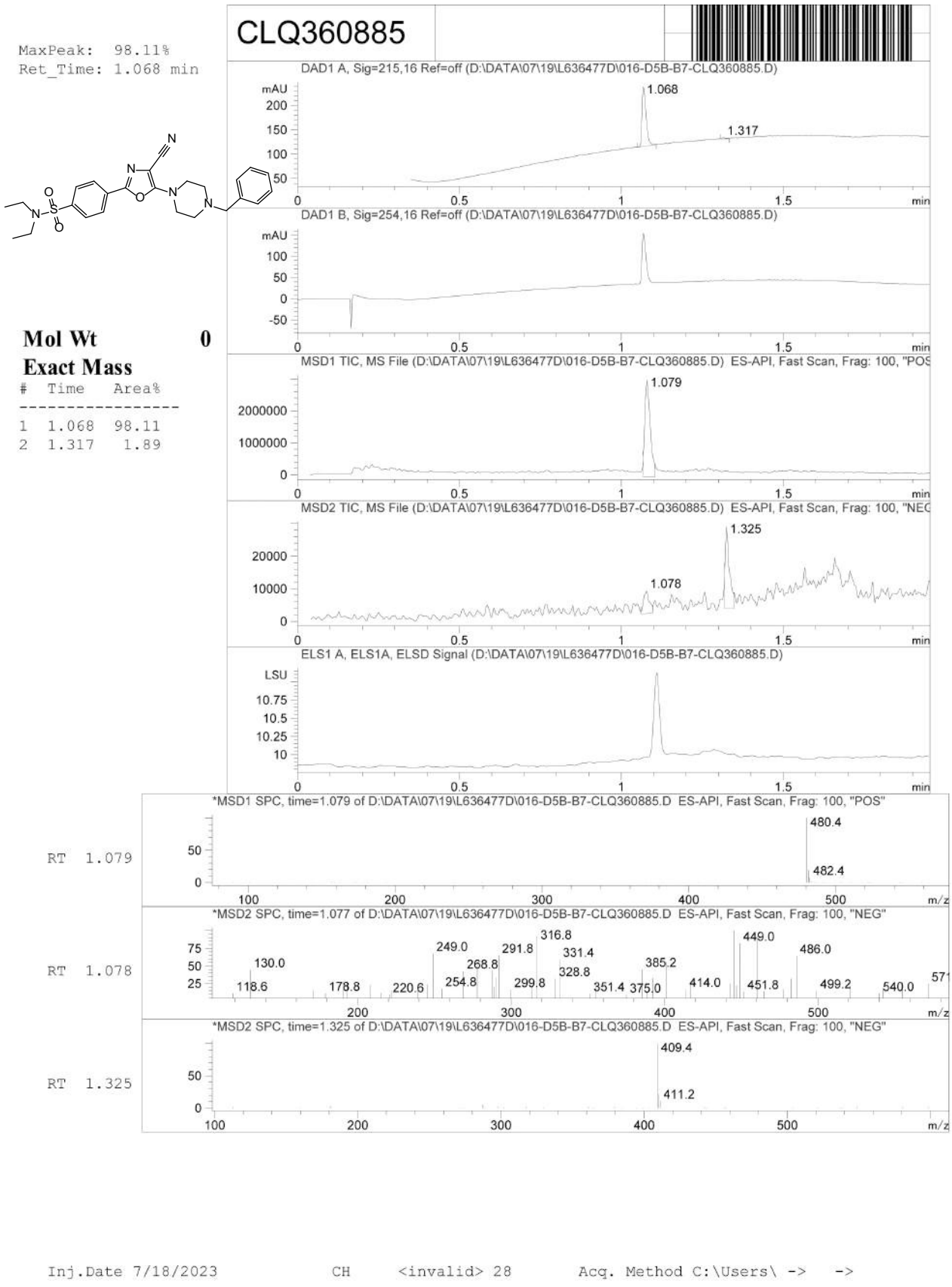

Fig. S48. LCMS spectrum of 4-[5-(4-benzylpiperazin-1-yl)-4-cyano-1,3-oxazol-2-yl]-N,N-diethylbenzenesulfonamide 9.

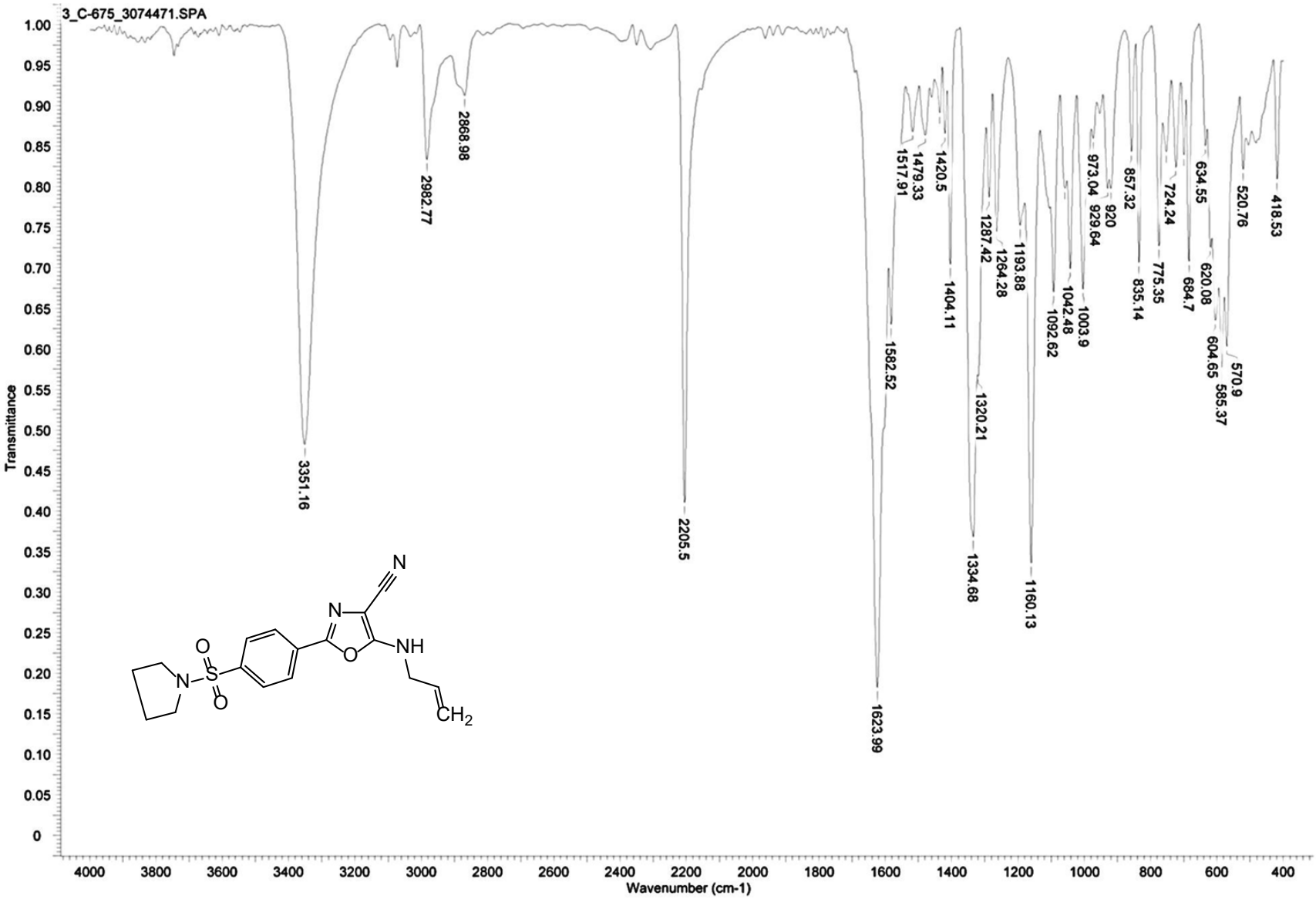

Fig. S49. IR spectrum of 5-(prop-2-enylamino)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 10.

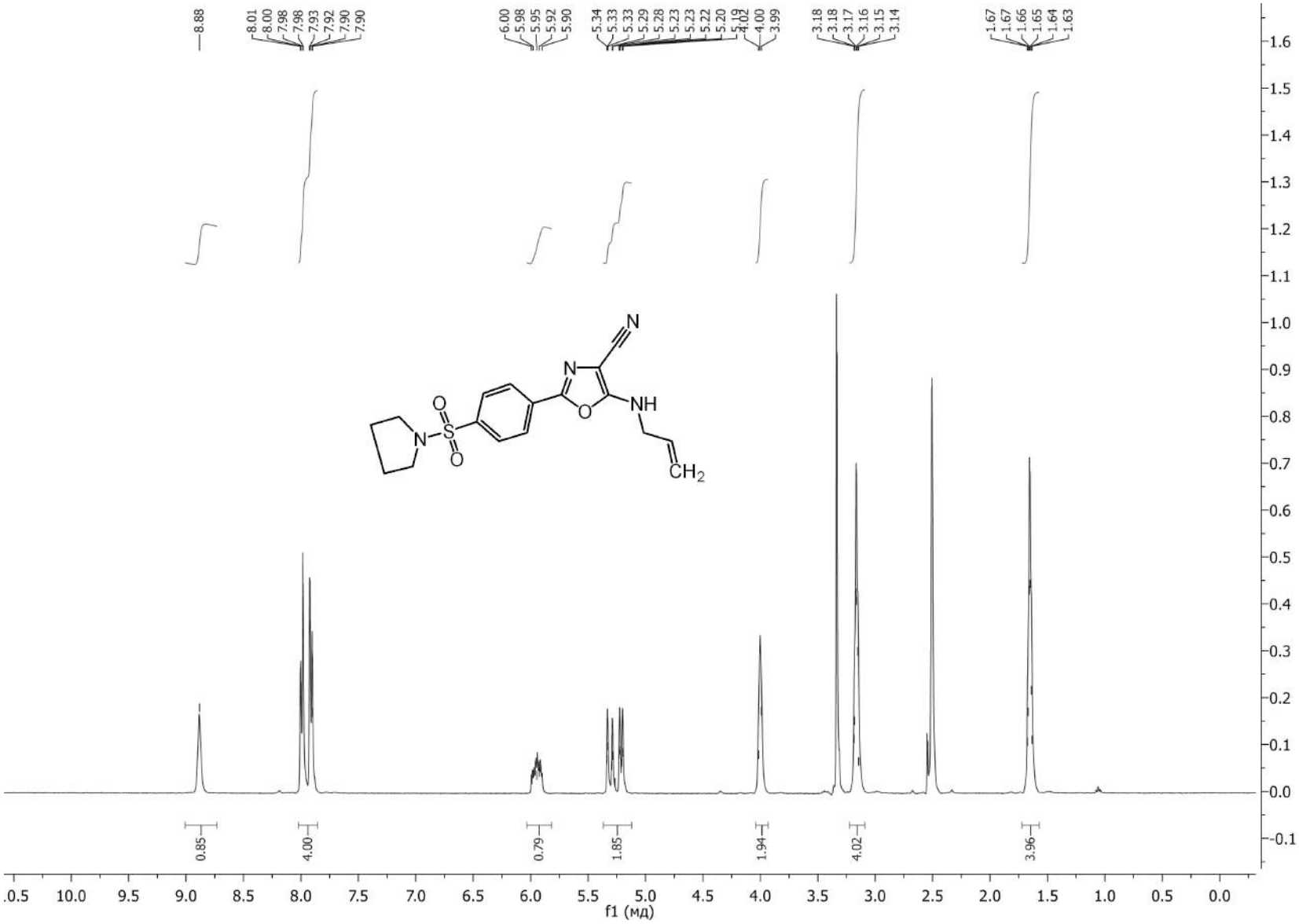

Fig. S50. [1]H NMR spectrum of 5-(prop-2-enylamino)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 10.

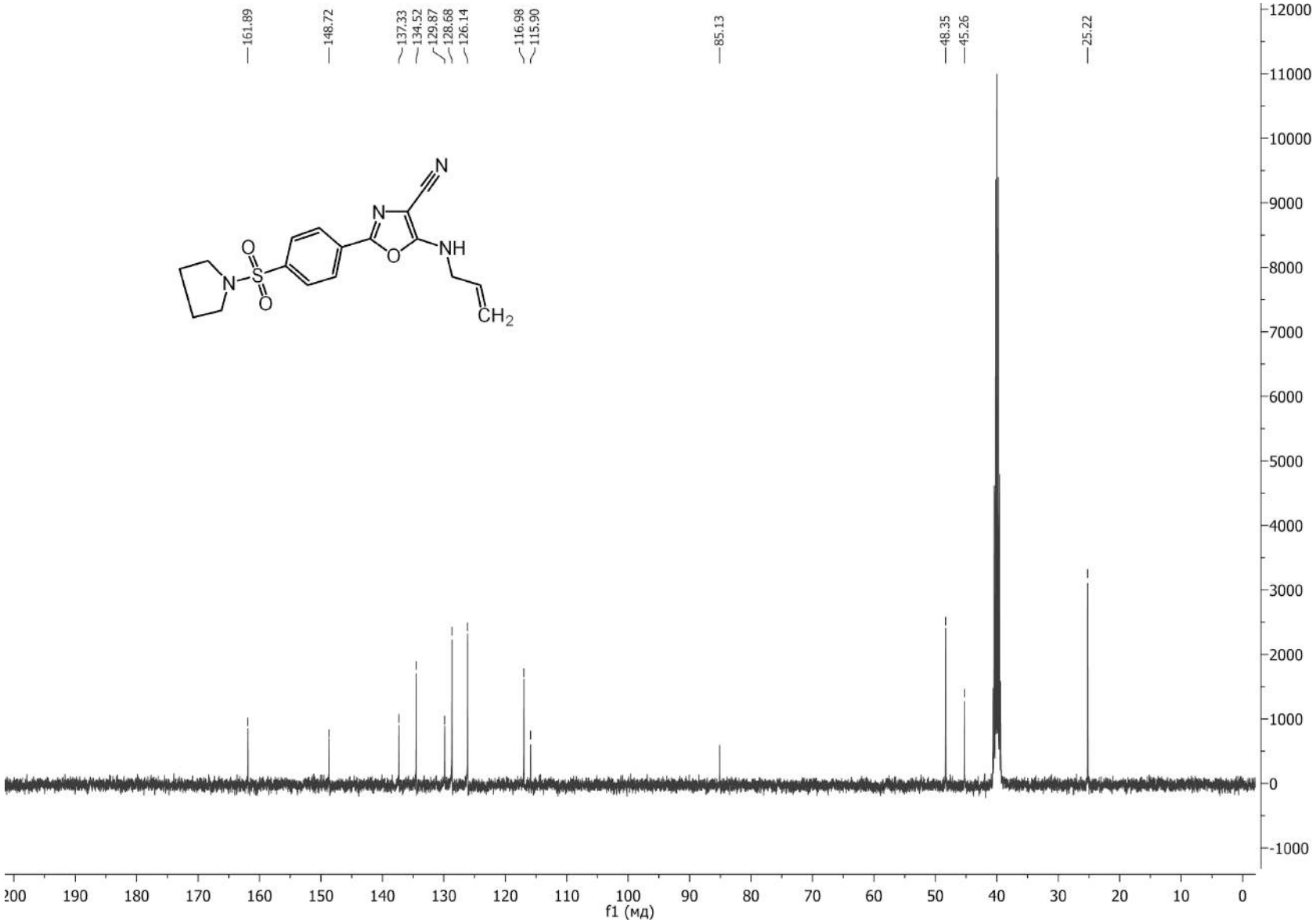

Fig. S51. ^{13}C NMR spectrum of 5-(prop-2-enylamino)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 10.

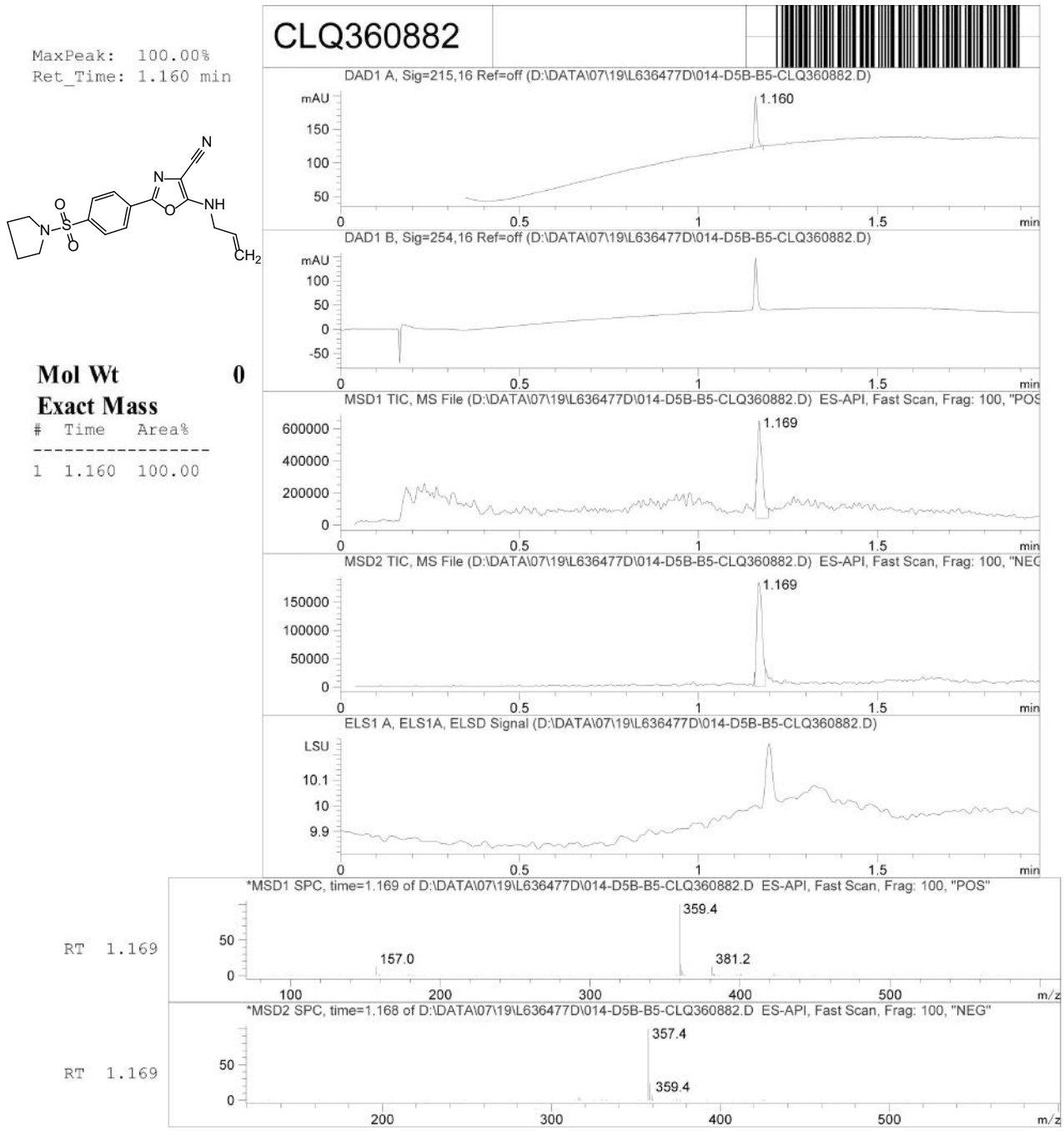

Fig. S52. LCMS spectrum of 5-(prop-2-enylamino)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 10.

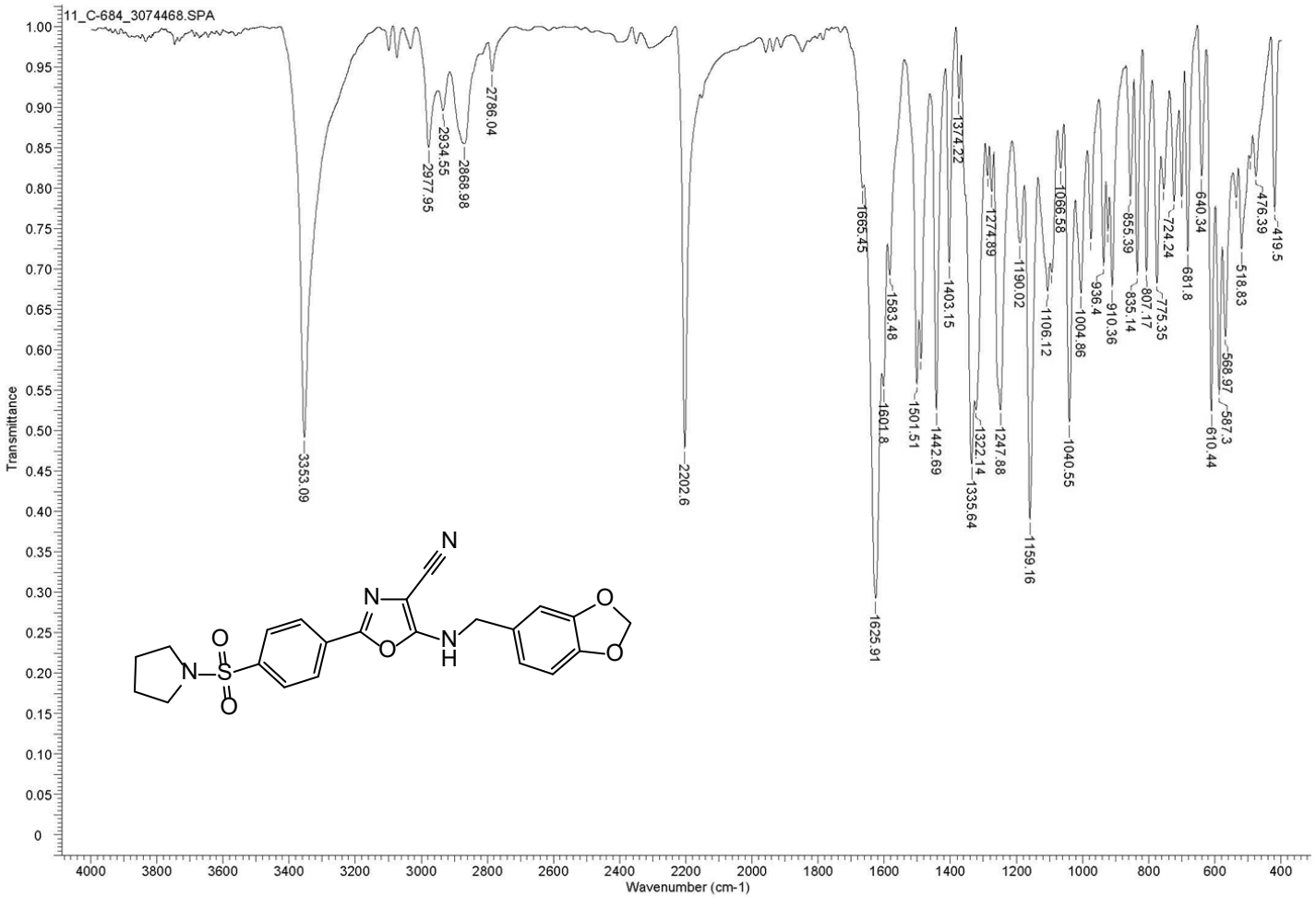

Fig. S53. IR spectrum of 5-(1,3-benzodioxol-5-ylmethylamino)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 11.

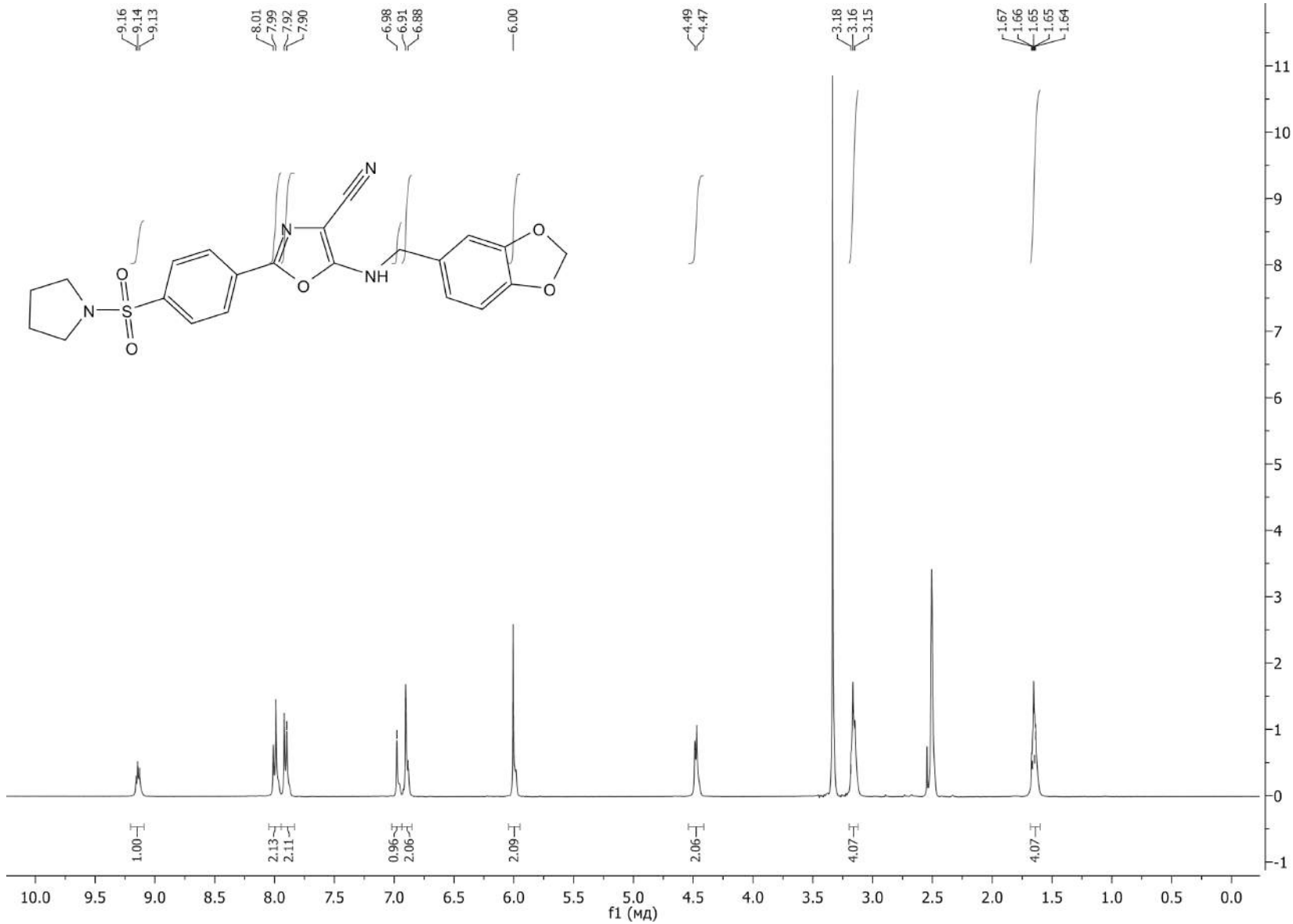

Fig. S54. [1]H NMR spectrum of 5-(1,3-benzodioxol-5-ylmethylamino)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 11.

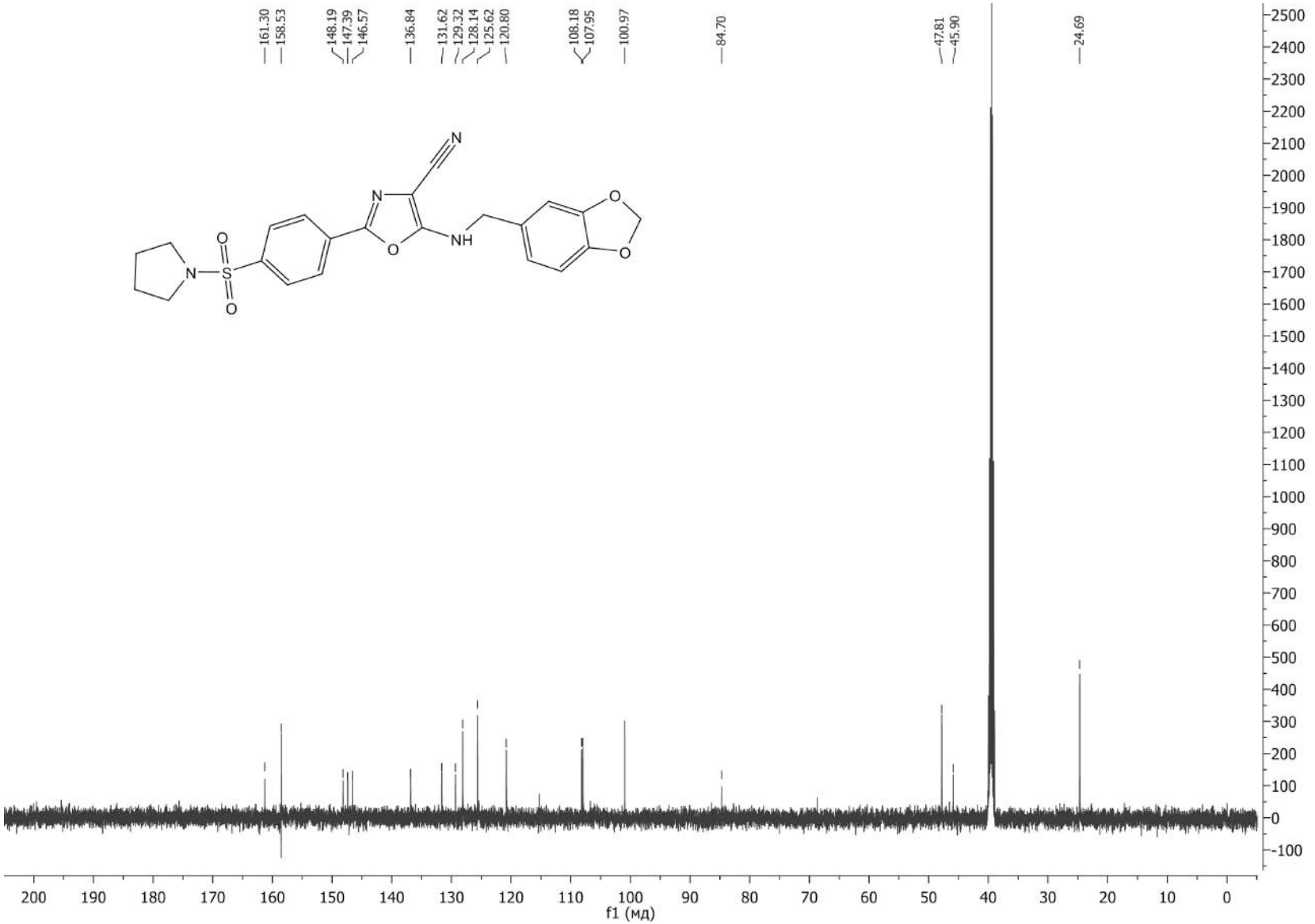

Fig. S55. ^{13}C NMR spectrum of 5-(1,3-benzodioxol-5-ylmethylamino)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 11.

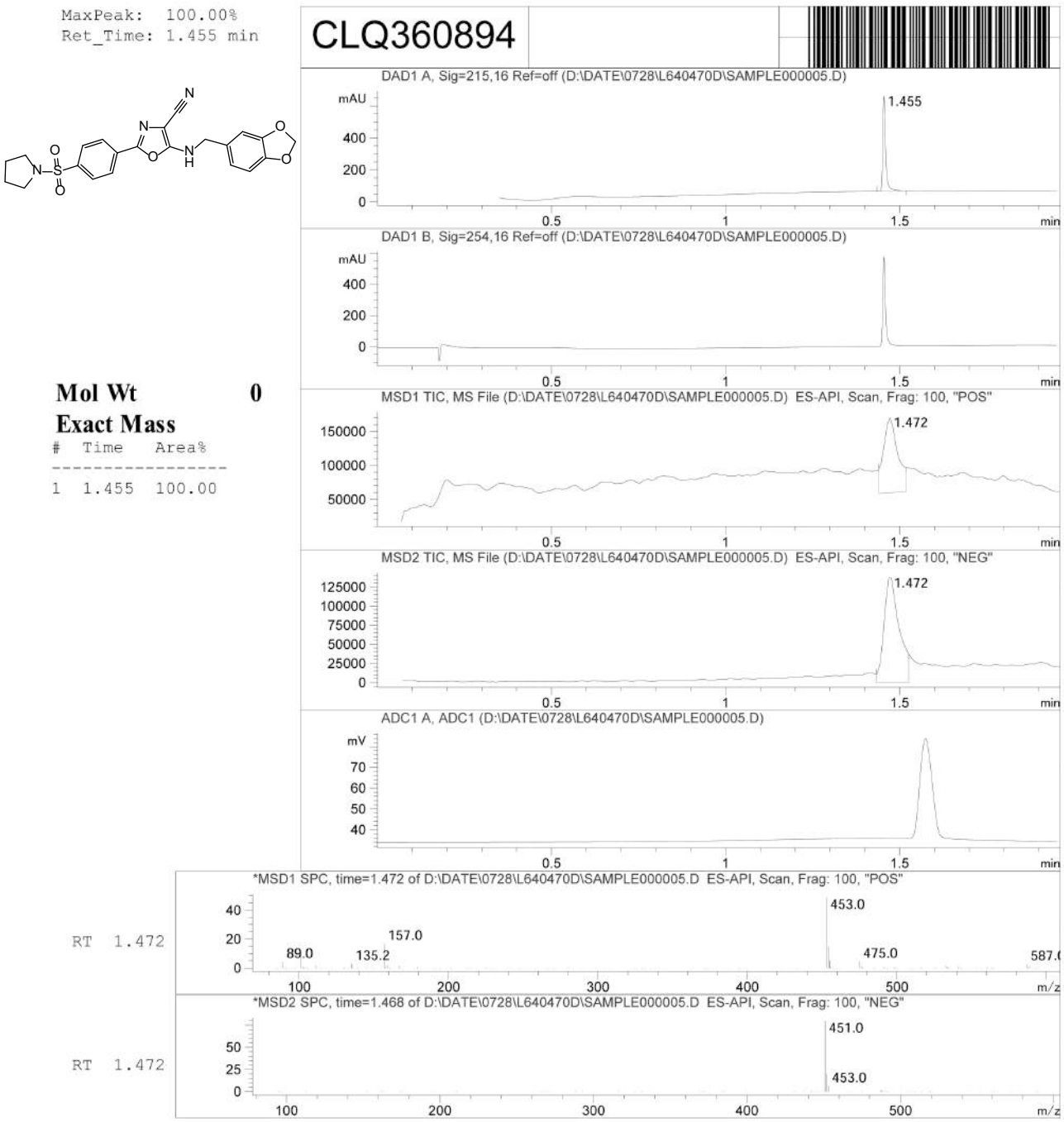

Fig. S56. LCMS spectrum of 5-(1,3-benzodioxol-5-ylmethylamino)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 11.

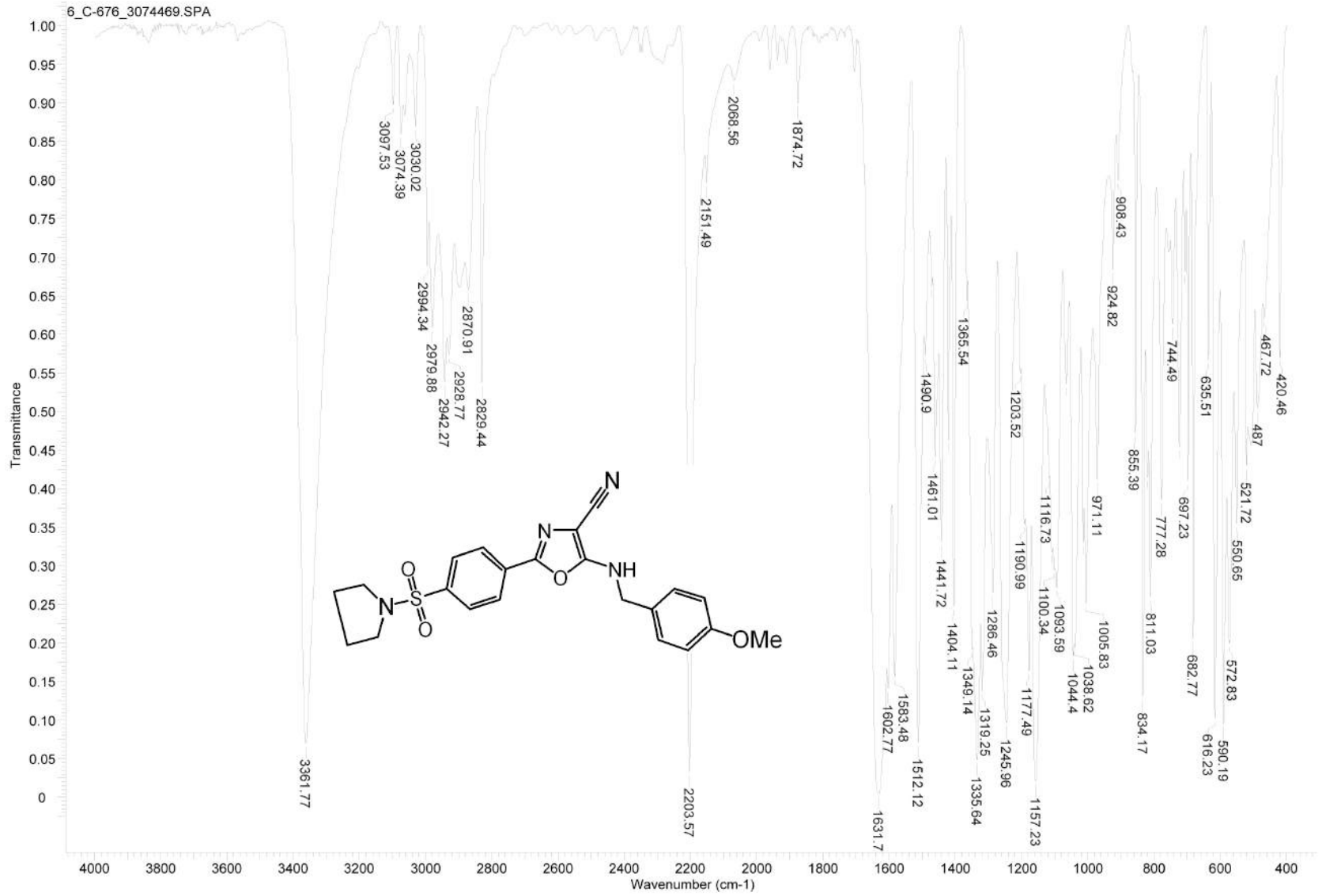

Fig. S57. IR spectrum of 5-[(4-methoxyphenyl)methylamino]-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 12.

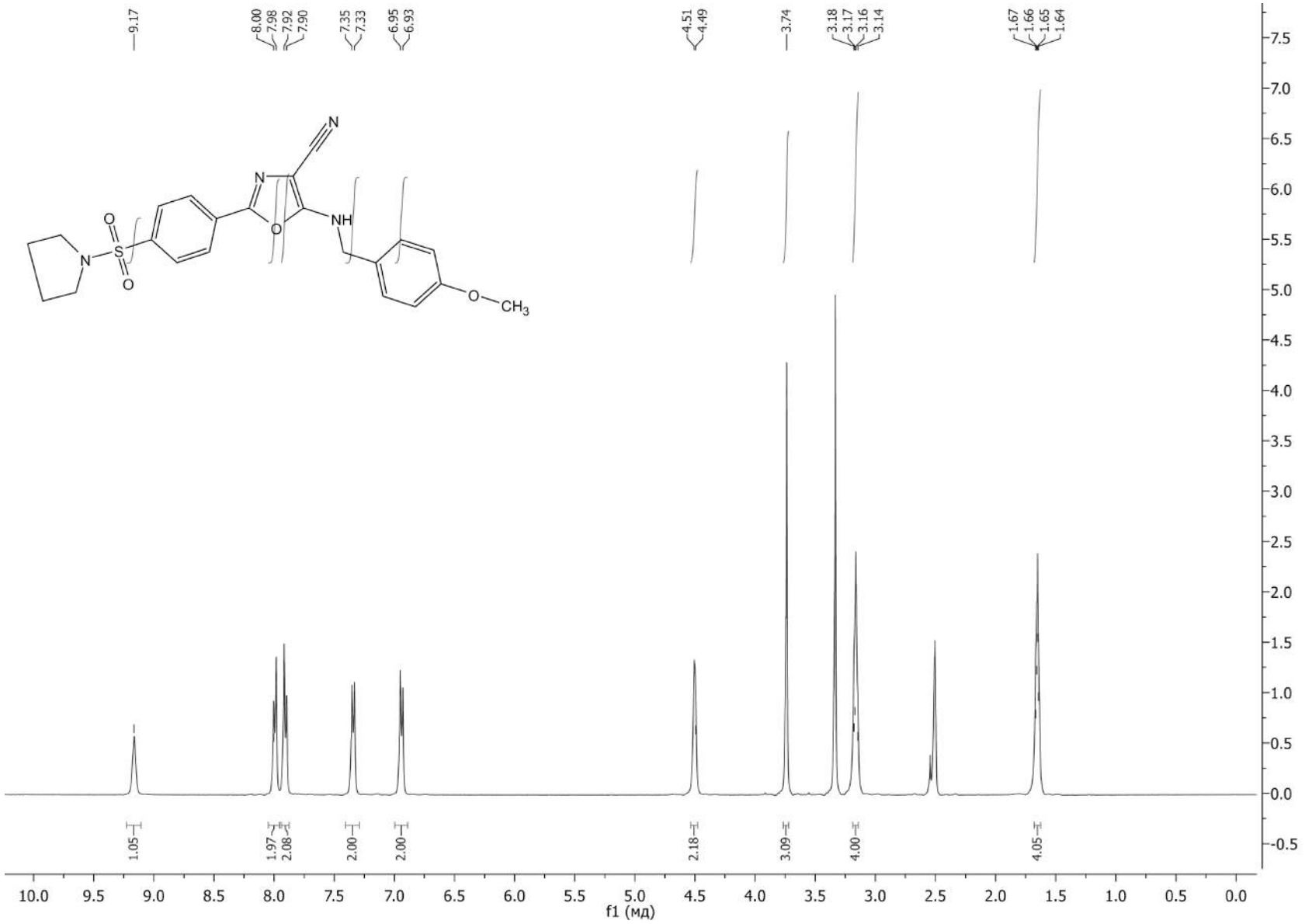

Fig. S58. [1]H NMR spectrum of 5-[(4-methoxyphenyl)methylamino]-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 12.

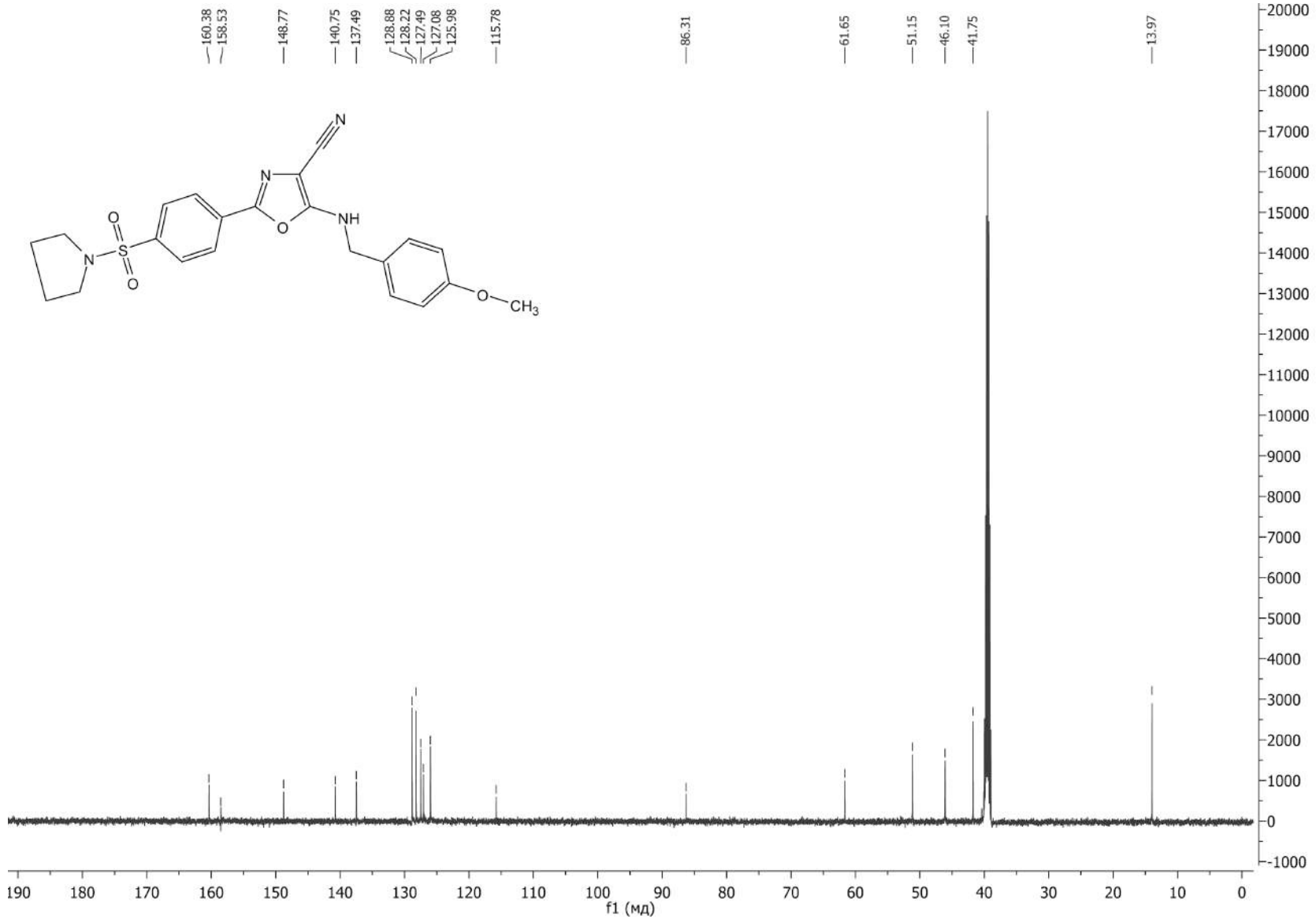

Fig. S59. ^{13}C NMR spectrum of 5-[(4-methoxyphenyl)methylamino]-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 12.

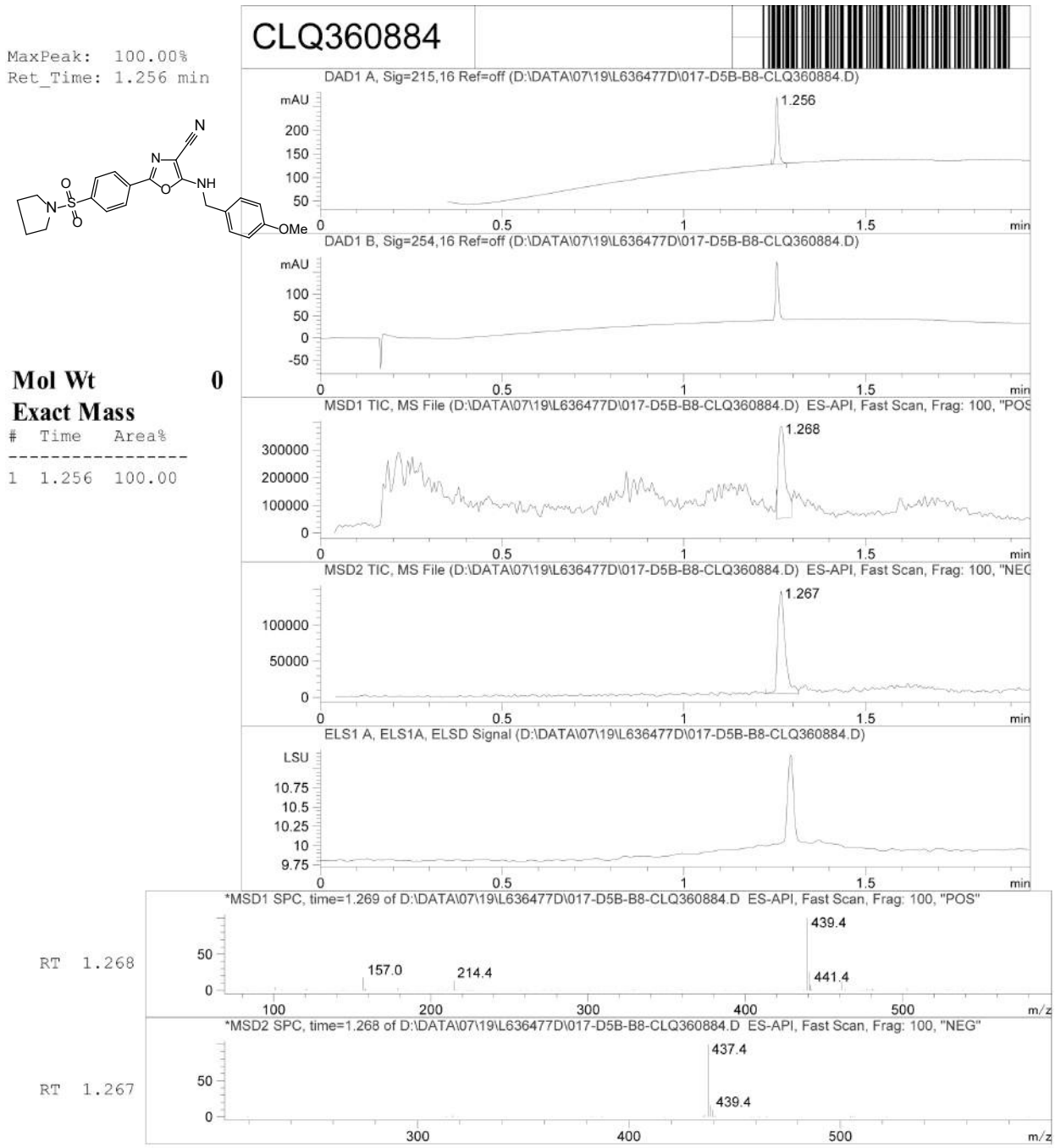

Fig. S60. LCMS spectrum of 5-[(4-methoxyphenyl)methylamino]-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 12.

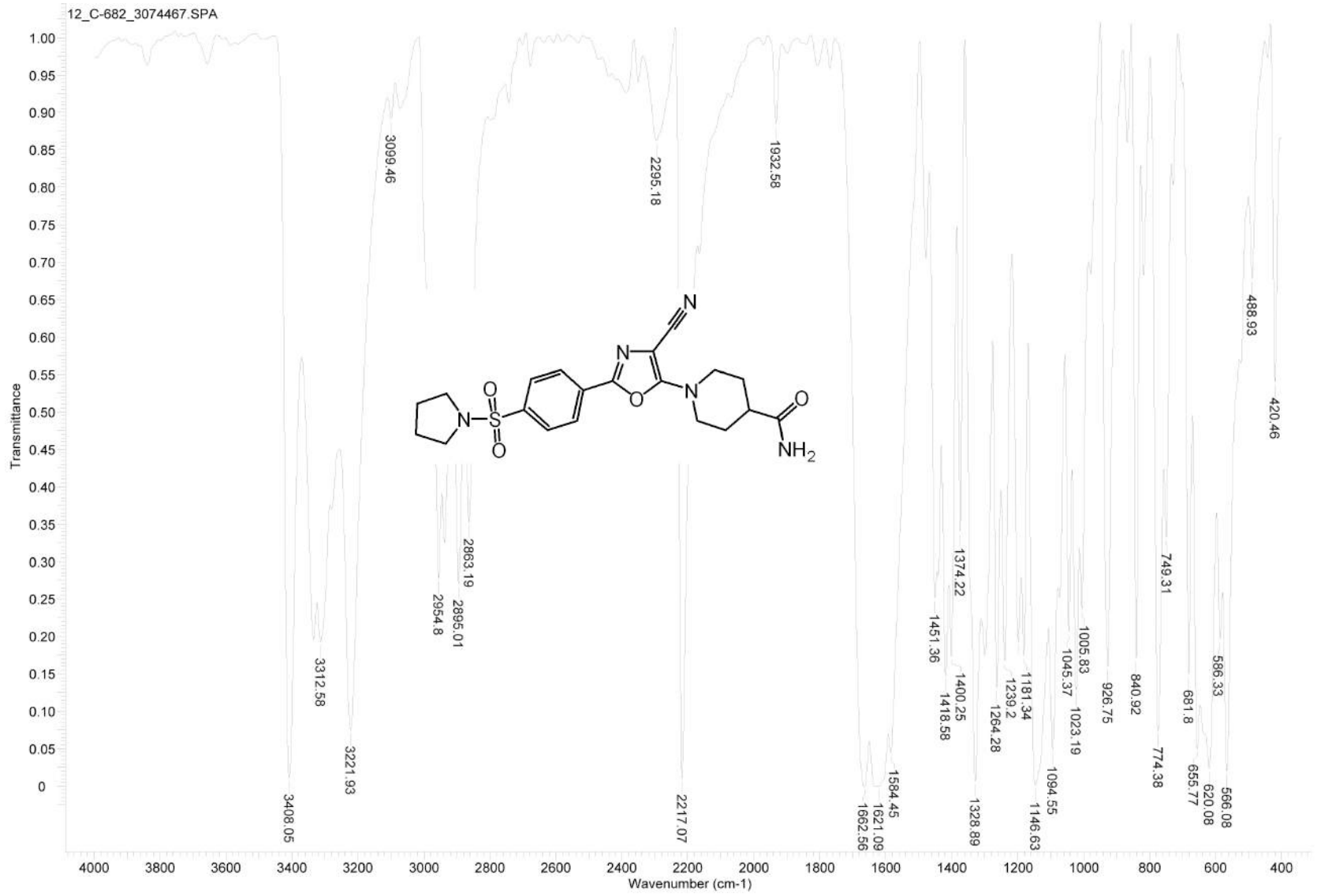

Fig. S61. IR spectrum of 1-[4-cyano-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazol-5-yl]piperidine-4-carboxamide 13.

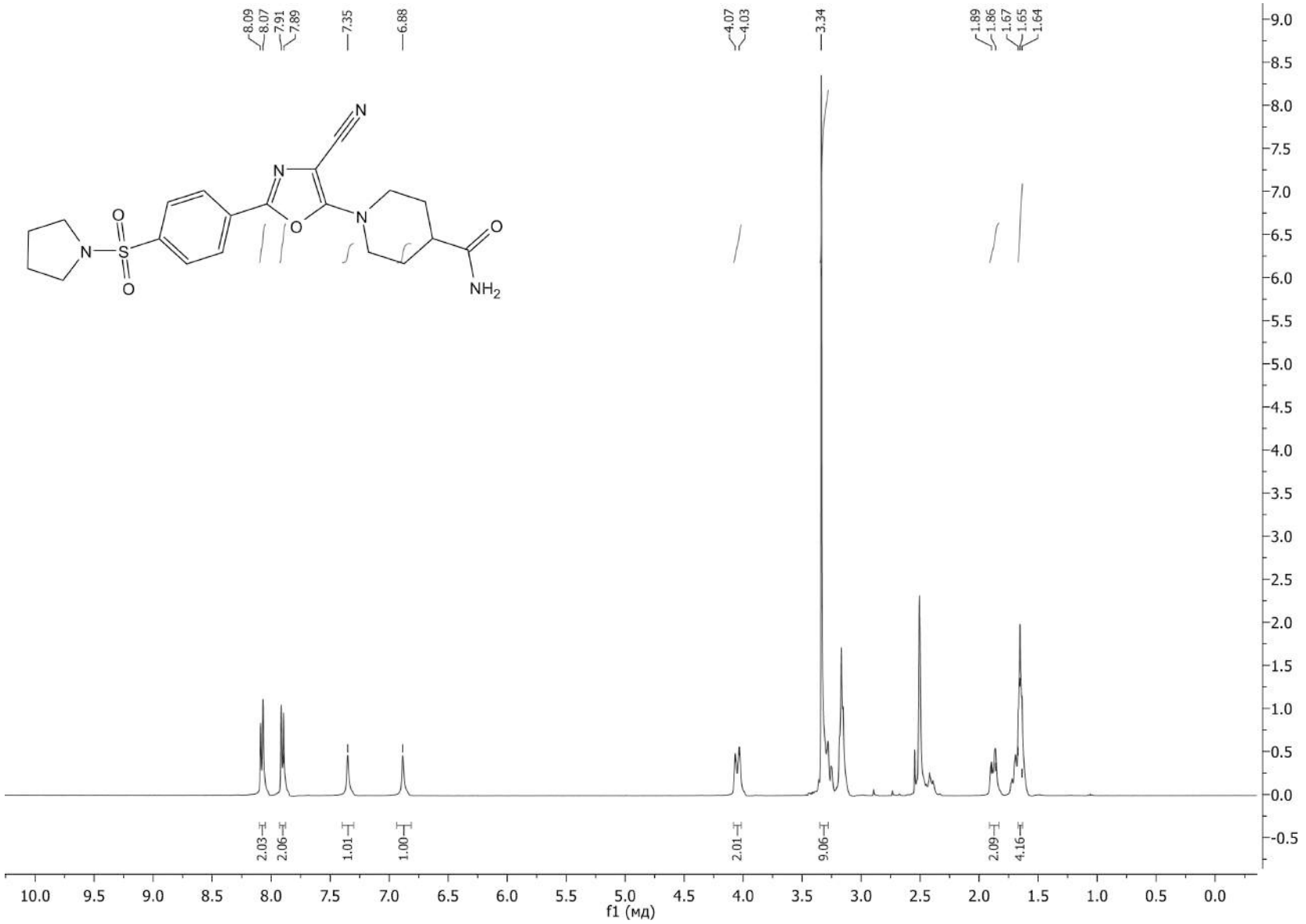

Fig. S62. ^{1}H NMR spectrum of 1-[4-cyano-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazol-5-yl]piperidine-4-carboxamide 13.

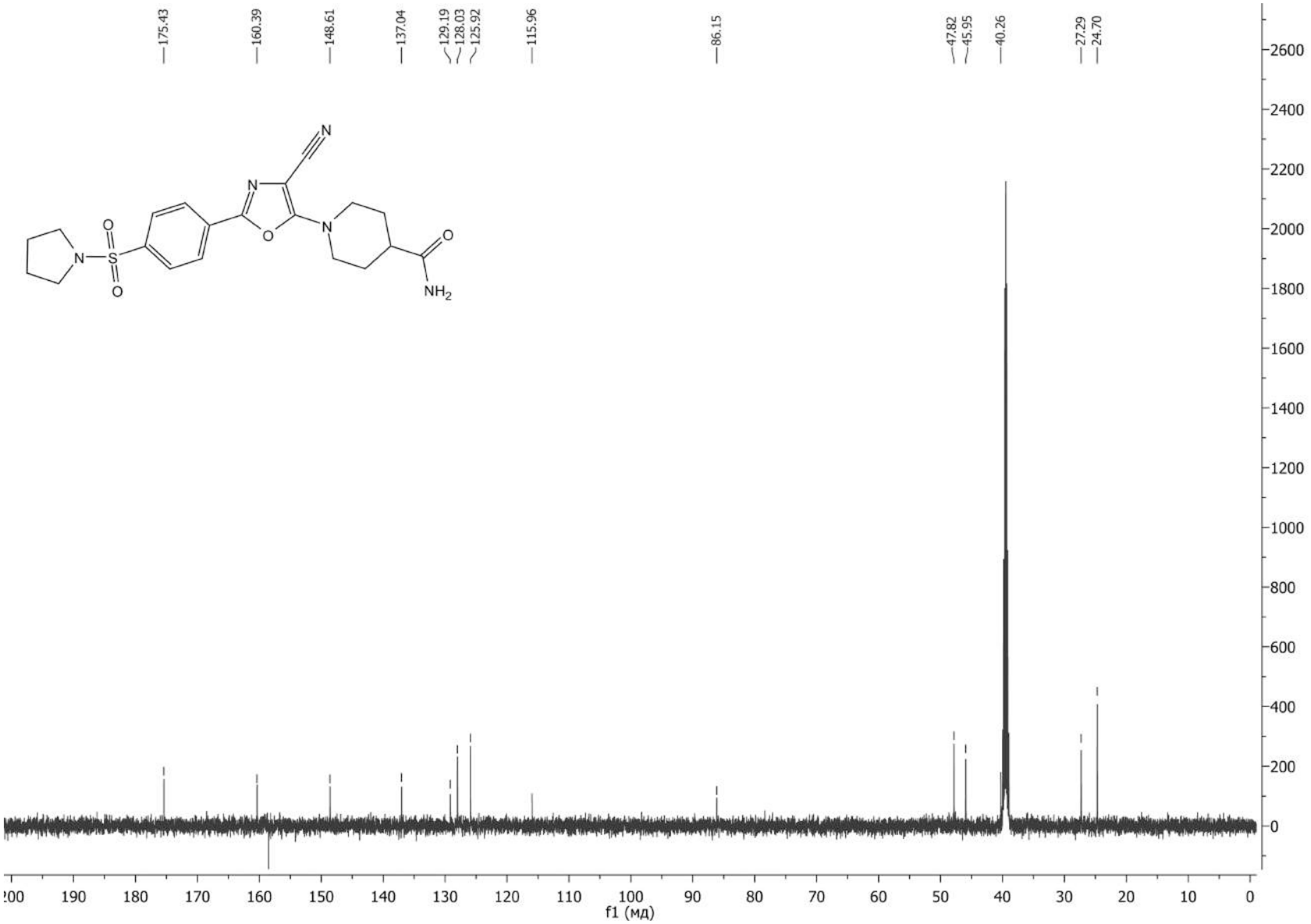

Fig. S63. ^{13}C NMR spectrum of 1-[4-cyano-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazol-5-yl]piperidine-4-carboxamide 13.

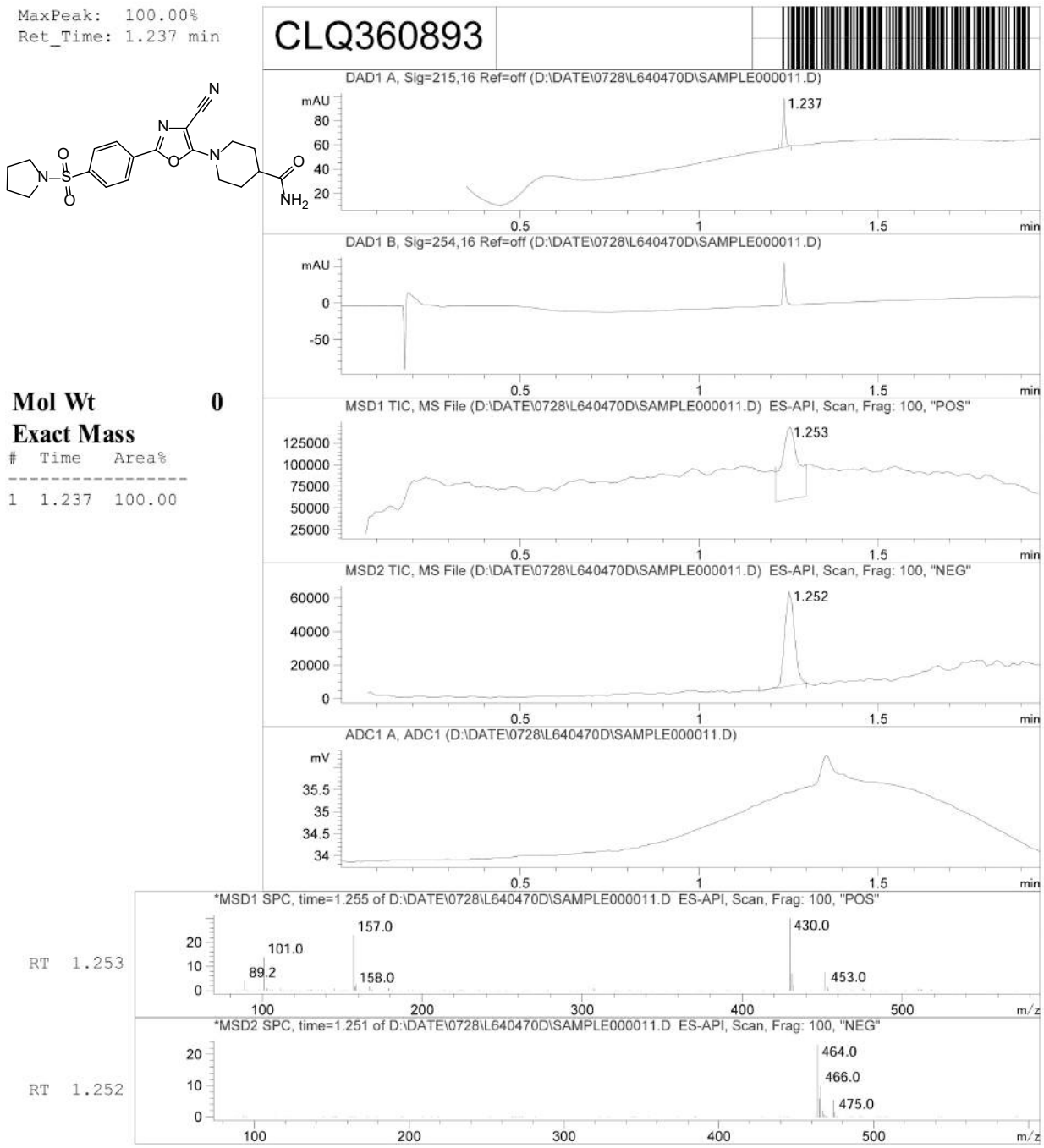

Fig. S64. LCMS spectrum of 1-[4-cyano-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazol-5-yl]piperidine-4-carboxamide 13.

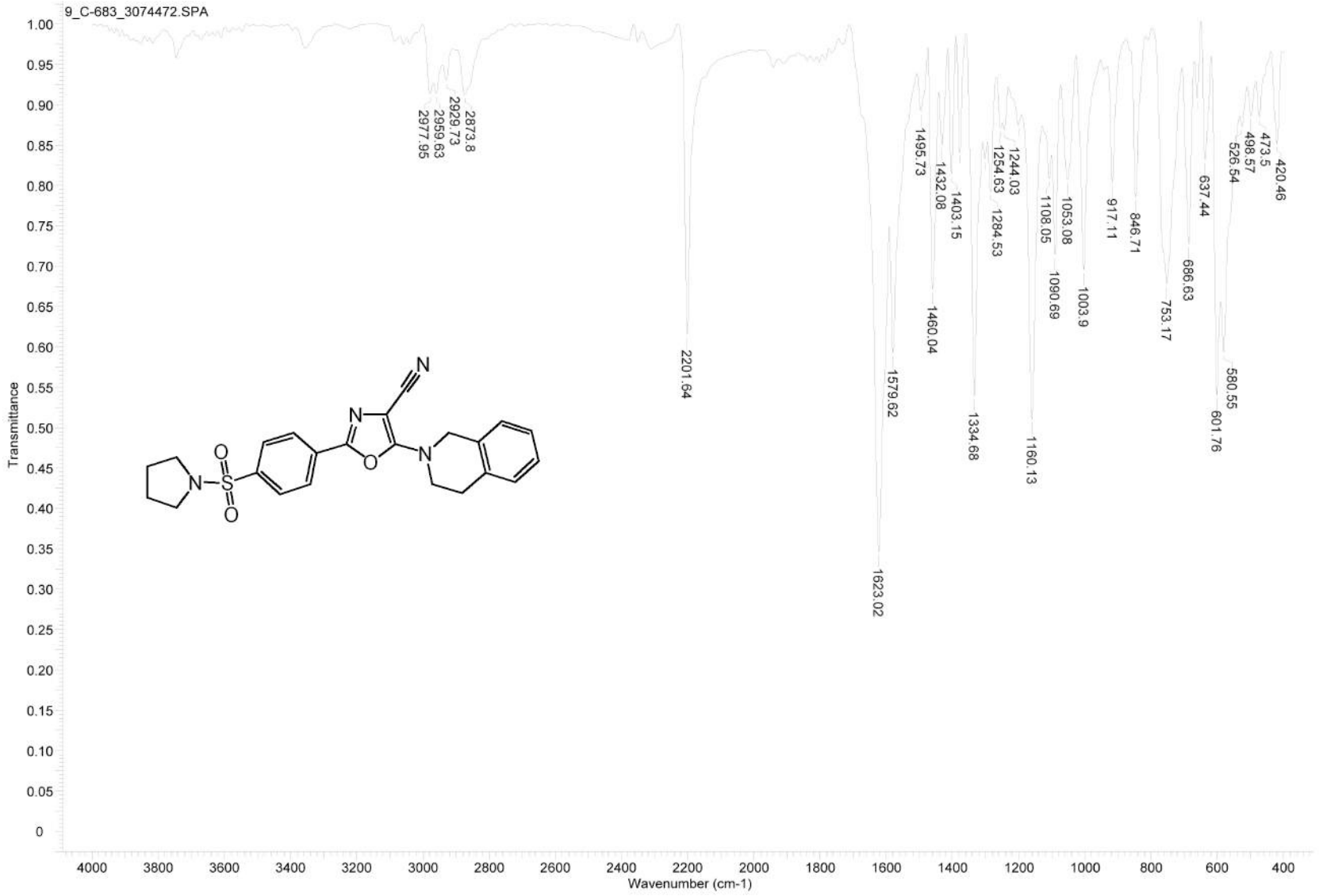

Fig. S65. IR spectrum of 5-(3,4-dihydro-1H-isoquinolin-2-yl)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 14.

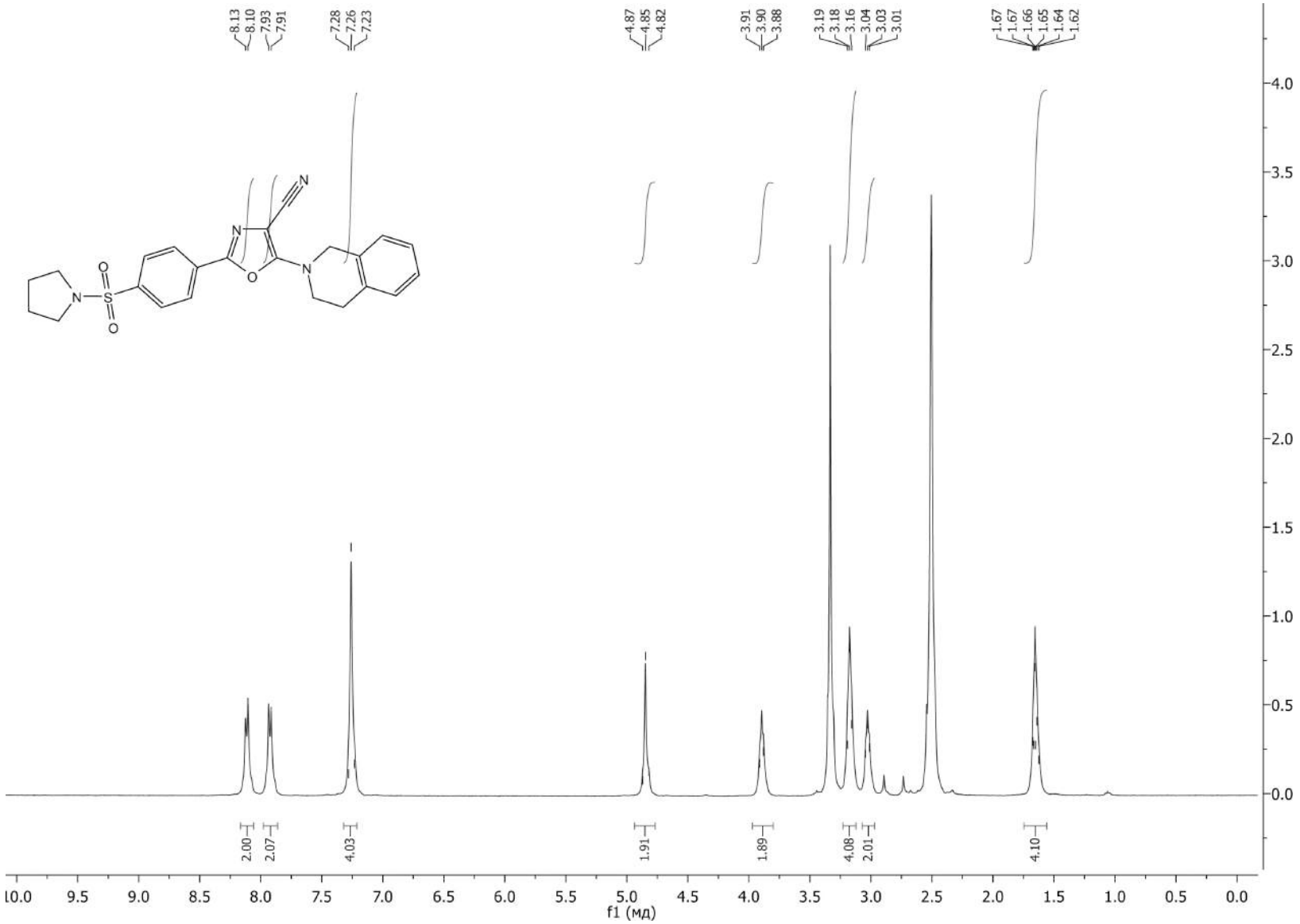

Fig. S66. [1]H NMR spectrum of 5-(3,4-dihydro-1H-isoquinolin-2-yl)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 14.

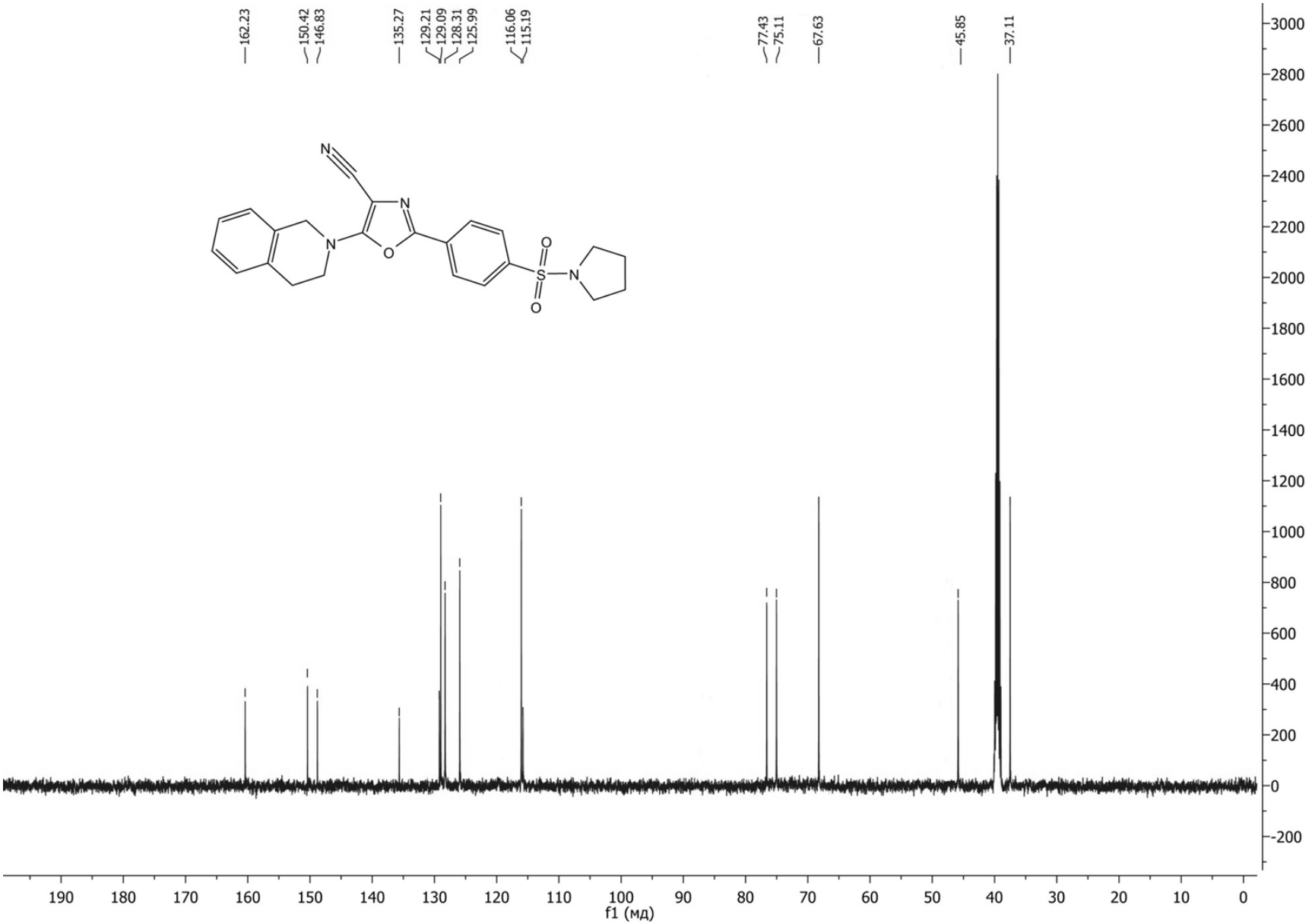

Fig. S67. ^{13}C NMR spectrum of 5-(3,4-dihydro-1H-isoquinolin-2-yl)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 14.

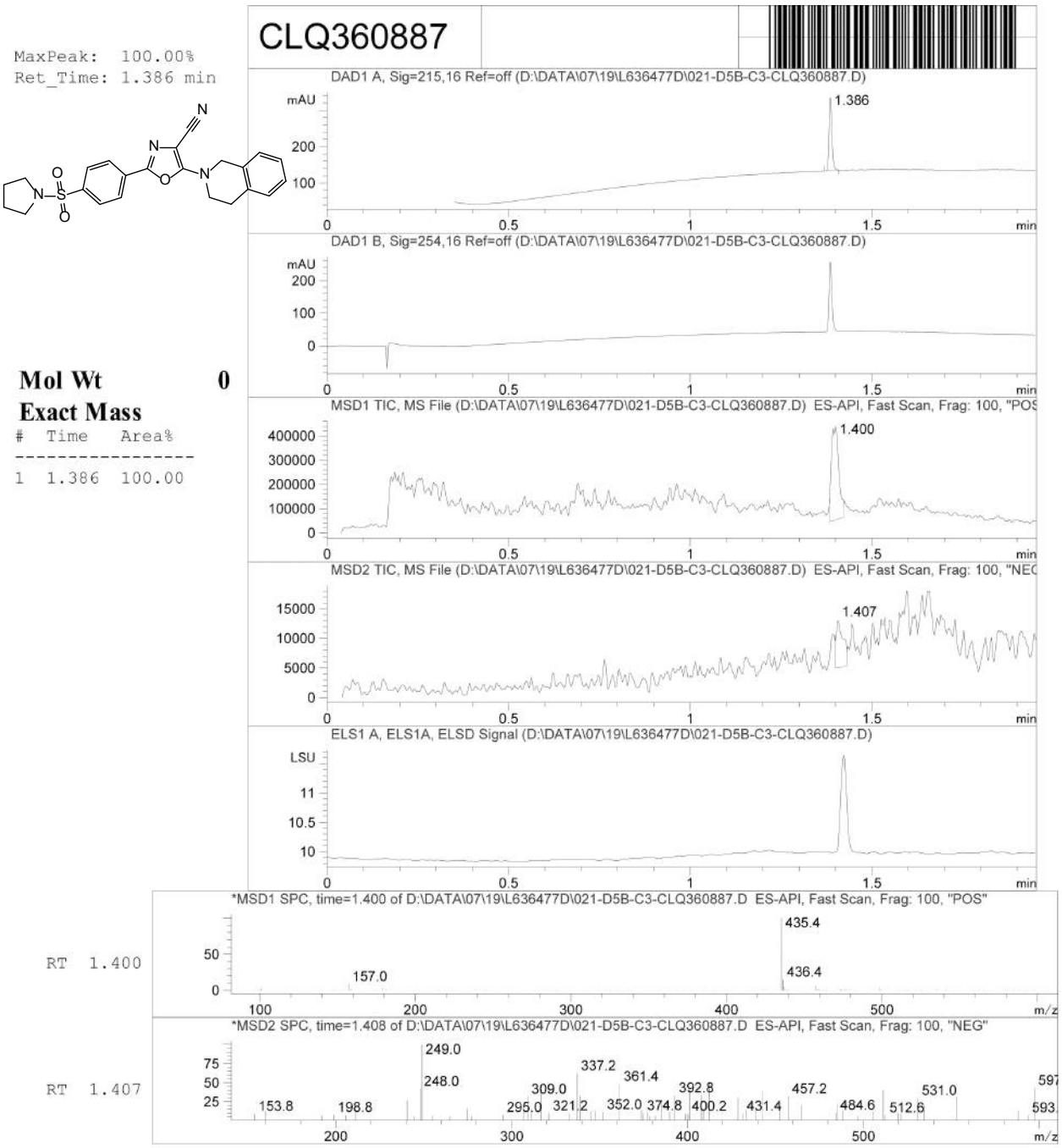

Fig. S68. LCMS spectrum of 5-(3,4-dihydro-1H-isoquinolin-2-yl)-2-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-oxazole-4-carbonitrile 14.

Table S2. Growth inhibition of NCI-60 cancer cell lines of tested compounds (*one-dose assay*), GI, %

Panel/Cell Line	**Compounds / GI, %**													
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**
Leukemia														
CCRF-CEM	84.74	106.53	56.79	82.19	79.73	76.19	105.25	107.60	51.04	96.71	101.26	97.53	96.30	94.96
HL-60(TB)	73.02	121.14	53.47	81.80	77.12	70.94	97.49	91.08	48.70	98.29	97.66	102.55	100.07	94.96
K-562	85.94	89.12	34.11	93.73	88.47	55.14	98.05	92.44	19.14	102.47	103.55	97.55	93.06	81.41
MOLT-4	75.42	124.28	54.91	83.18	81.98	66.63	108.14	107.91	45.32	106.51	110.62	104.55	107.19	93.47
RPMI-8226	90.11	100.39	37.50	86.94	90.05	56.04	98.50	97.08	27.54	99.34	99.93	99.84	99.08	92.52
SR	86.91	n/d	n/d	90.89	84.92	66.73	105.25	107.60	49.38	97.54	91.47	95.30	100.58	86.78
NSCLC														
A549/ATCC	102.06	99.17	64.87	99.07	97.13	76.68	96.05	97.98	74.77	91.59	76.63	82.52	98.34	82.52
EKVX	99.48	17.59	61.30	99.89	98.69	82.51	96.74	94.61	54.07	96.37	97.96	98.17	96.45	88.81
HOP-62	107.79	97.74	90.75	112.01	107.04	104.16	108.31	89.07	97.37	94.95	34.00	76.90	111.08	105.12
HOP-92	66.18	n/d	44.24	96.41	82.38	110.43	98.00	98.06	75.85	93.56	81.24	101.92	100.92	100.15
NCI-H226	96.48	13.55	66.41	107.97	96.15	76.89	95.62	77.59	65.82	100.65	90.45	97.41	105.51	104.96
NCI-H23	104.80	-1.30	64.62	103.78	99.63	93.36	87.27	90.24	65.13	100.17	105.15	97.16	96.24	92.41
NCI-H322M	92.48	88.96	95.83	96.66	97.45	104.24	90.15	90.14	91.42	116.14	105.46	106.61	124.13	131.91
NCI-H460	123.66	108.05	59.47	116.11	115.86	87.97	98.87	103.67	81.38	88.71	82.13	94.94	97.70	86.85
NCI-H522	91.09	95.82	70.81	92.58	90.84	73.57	97.84	92.40	59.01	91.59	76.63	82.52	98.34	82.52
Colon Cancer														
COLO 205	118.30	126.30	66.92	120.69	122.64	115.64	114.12	132.12	104.50	114.62	110.99	111.42	110.04	112.86
HCC-2998	108.34	-91.70	85.81	116.88	116.16	100.10	97.80	94.98	89.27	101.67	105.69	112.60	111.26	108.48
HCT-116	93.05	108.21	50.18	98.71	91.75	73.39	105.26	99.82	58.26	111.33	105.13	106.26	112.09	105.58
HCT-15	98.77	-22.61	51.80	99.08	96.83	77.31	98.23	96.76	62.18	94.61	100.20	95.05	97.56	83.37
HT29	106.10	99.08	51.13	95.29	99.34	75.53	104.89	99.86	70.99	116.88	109.82	113.31	118.10	93.64

KM12	102.76	107.33	83.12	100.40	98.03	90.21	100.34	108.45	63.72	106.39	103.37	96.83	103.80	109.10
SW-620	114.72	101.21	80.03	107.97	106.48	105.99	103.24	102.40	80.66	113.54	106.31	105.33	116.03	109.58
CNS Cancer														
SF-268	104.06	111.33	81.50	105.59	94.95	88.56	99.87	100.53	79.47	95.32	47.62	86.42	122.64	118.23
SF-295	95.37	15.83	63.41	95.82	96.95	72.63	90.91	86.73	56.68	98.93	97.90	102.26	91.85	94.67
SF-539	95.89	98.26	83.53	100.73	97.58	104.52	100.24	90.76	92.63	101.44	104.21	104.19	103.93	104.97
SNB-19	100.46	95.90	78.98	103.10	100.95	98.24	87.82	80.73	84.80	84.05	82.25	91.00	97.11	93.70
SNB-75	99.86	87.81	88.16	98.19	87.64	96.28	97.80	95.43	85.18	97.16	29.67	43.90	94.48	101.37
U251	94.44	101.53	71.96	100.81	100.36	94.90	104.13	98.83	88.53	97.03	77.09	97.40	97.19	98.29
Melanoma														
LOX IMVI	105.57	-94.07	78.82	112.75	99.69	97.85	81.30	94.03	81.72	101.73	100.69	90.78	99.41	106.08
MALME-3M	95.95	92.50	60.69	89.94	85.96	88.82	95.36	95.22	63.09	99.42	104.07	104.17	95.60	95.64
M14	104.78	125.58	68.87	100.49	96.33	91.60	105.52	96.65	70.89	109.02	103.89	102.99	105.68	104.11
MDA-MB-435	104.43	107.37	83.01	97.54	92.76	86.88	100.38	93.37	26.41	105.36	98.09	99.24	103.31	98.35
SK-MEL-2	114.35	103.74	95.91	113.67	112.58	95.42	108.32	116.11	49.98	117.07	90.95	106.98	122.00	114.81
SK-MEL-28	109.57	103.84	84.04	107.46	105.93	102.16	107.33	93.86	83.05	117.45	119.43	113.10	109.47	109.55
SK-MEL-5	74.44	-72.91	39.76	82.89	68.32	38.41	47.06	56.11	5.59	102.55	98.98	103.83	92.59	92.35
UACC-257	110.97	97.75	90.93	106.89	100.33	91.58	104.24	96.48	64.55	98.76	91.65	96.57	95.63	93.21
UACC-62	96.40	87.43	64.48	96.57	92.31	76.53	91.71	90.28	52.85	93.44	100.46	100.86	94.04	87.20
Ovarian Cancer														
IGROV1	117.84	102.93	95.31	118.59	116.64	117.65	104.99	111.25	45.35	108.48	103.27	103.42	112.64	109.64
OVCAR-3	114.06	118.75	95.50	113.37	107.53	110.53	112.50	113.09	84.64	131.14	106.55	115.50	132.65	140.66
OVCAR-4	102.50	109.64	71.73	106.33	104.86	75.87	113.69	99.30	59.15	107.60	102.92	109.84	102.67	106.00
OVCAR-5	98.40	98.82	88.86	108.33	101.81	104.39	92.96	95.98	94.79	107.31	119.20	116.61	107.03	100.11
OVCAR-8	101.09	99.51	81.91	106.56	106.68	97.24	100.90	93.53	85.88	86.86	74.02	65.61	96.16	92.35
NCI/ADR-RES	109.07	23.47	55.43	100.08	100.70	95.26	89.27	86.25	64.01	96.64	100.47	94.72	107.04	91.87
SK-OV-3	106.84	116.91	92.12	104.77	105.83	106.23	130.54	113.00	87.71	112.79	100.37	123.24	122.29	129.74
Renal Cancer														
786-0	103.50	101.72	68.08	89.72	95.57	88.14	116.14	109.82	83.24	109.87	104.71	112.23	104.45	93.37

A498	123.04	112.31	131.53	114.74	114.61	104.30	124.93	115.02	105.28	139.99	119.99	120.24	124.20	124.12
ACHN	105.65	100.60	89.75	108.32	104.34	99.25	99.69	90.09	81.98	106.42	111.55	110.06	112.70	115.18
CAKI-1	87.57	89.85	68.98	87.71	81.81	82.55	90.58	81.41	62.59	92.98	66.07	86.50	99.66	85.84
RXF 393	98.56	-20.46	42.38	120.11	103.91	97.59	93.86	89.93	79.67	104.50	95.14	104.34	111.43	110.39
SN12C	104.76	95.64	62.66	108.62	104.75	92.44	87.56	92.93	88.98	91.77	98.96	99.87	99.83	94.76
TK-10	109.50	100.71	90.69	96.80	98.35	91.38	108.60	100.74	80.75	111.15	100.30	117.59	107.20	98.61
UO-31	95.46	86.61	51.20	94.97	93.98	72.67	92.10	94.42	48.80	96.19	97.72	98.25	97.07	88.44
Prostate Cancer														
PC-3	94.53	101.72	37.93	99.04	92.13	73.24	111.78	110.12	50.54	98.39	100.88	94.66	93.86	91.75
DU-145	106.27	117.51	94.13	105.28	102.96	93.75	97.23	103.39	86.44	110.58	109.82	105.74	111.81	109.07
Breast Cancer														
MCF7	93.63	-6.95	56.47	99.13	94.26	79.27	89.83	87.53	64.67	85.07	82.47	72.93	84.05	84.23
MDA-MB-231/ATCC	95.73	90.11	84.09	108.23	98.10	106.30	85.58	93.27	76.85	97.92	97.72	91.80	101.72	104.99
HS 578T	99.46	90.43	65.29	119.17	106.93	108.44	91.01	96.49	82.44	105.16	56.52	69.20	109.67	99.69
BT-549	101.33	127.37	72.13	117.92	105.51	78.88	108.59	110.38	57.78	111.45	94.55	112.50	112.56	107.04
T-47D	99.98	97.01	69.08	109.86	103.60	66.24	106.96	100.70	67.72	110.24	90.63	108.28	101.37	102.10
MDA-MB-468	106.82	-33.89	28.85	104.30	104.23	74.04	93.97	74.49	7.11	109.03	100.01	112.63	101.99	104.71

Figure. S69. Anticancer activity of compound **2** against NCI-60 cancer cell lines (*five-dose assay*).

National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 842141 / 1	Experiment ID : 2307NS43	Test Type : 08	Units : Molar
Report Date : April 04, 2024	Test Date : July 10, 2023	QNS :	MC :
COMI : OXL0002060	Stain Reagent : SRB Dual-Pass Related	SSPL : 0Y5P	

		Log10 Concentration												
	Time	Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.418	1.813	1.943	1.999	1.891	1.812	1.265	109	113	106	100	61	> 1.00E-4	> 1.00E-4	> 1.00E-4
HL-60(TB)	0.393	1.709	1.664	1.716	1.524	1.505	1.084	97	101	86	84	52	> 1.00E-4	> 1.00E-4	> 1.00E-4
K-562	0.218	2.151	2.027	2.220	1.913	1.756	0.885	94	104	88	80	34	4.53E-5	> 1.00E-4	> 1.00E-4
MOLT-4	0.497	2.287	2.257	2.297	2.132	1.973	1.351	98	101	91	82	48	8.58E-5	> 1.00E-4	> 1.00E-4
RPMI-8226	0.736	2.794	2.728	2.801	2.702	2.519	1.747	97	100	96	87	49	9.48E-5	> 1.00E-4	> 1.00E-4
SR	0.438	2.464	2.431	2.443	2.302	2.282	1.219	98	99	92	91	39	6.04E-5	> 1.00E-4	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.509	2.679	2.416	2.551	2.365	2.341	1.927	88	94	85	84	65	> 1.00E-4	> 1.00E-4	> 1.00E-4
EKVX	0.807	1.898	1.797	1.819	1.800	1.717	1.438	91	93	91	83	58	> 1.00E-4	> 1.00E-4	> 1.00E-4
HOP-62	0.734	2.534	2.441	2.451	2.486	2.180	2.101	95	95	97	80	76	> 1.00E-4	> 1.00E-4	> 1.00E-4
HOP-92	1.384	1.818	1.821	1.840	1.714	1.543	1.531	101	105	76	37	34	4.56E-6	> 1.00E-4	> 1.00E-4
NCI-H226	0.974	1.597	1.483	1.549	1.575	1.418	1.273	82	92	96	71	48	8.18E-5	> 1.00E-4	> 1.00E-4
NCI-H23	0.837	2.064	1.994	2.057	1.951	1.856	1.763	94	99	91	83	75	> 1.00E-4	> 1.00E-4	> 1.00E-4
NCI-H322M	0.529	2.008	1.902	1.884	1.718	1.555	1.479	93	92	80	69	64	> 1.00E-4	> 1.00E-4	> 1.00E-4
NCI-H460	0.284	2.770	2.811	2.786	2.742	2.550	2.136	102	101	99	91	74	> 1.00E-4	> 1.00E-4	> 1.00E-4
NCI-H522	1.097	2.740	2.554	2.601	2.555	2.400	2.018	89	91	89	79	56	> 1.00E-4	> 1.00E-4	> 1.00E-4
Colon Cancer															
COLO 205	0.517	2.198	2.207	2.277	2.112	2.091	1.634	100	105	95	94	66	> 1.00E-4	> 1.00E-4	> 1.00E-4
HCC-2998	0.628	1.848	1.707	1.711	1.779	1.508	1.429	88	89	94	72	66	> 1.00E-4	> 1.00E-4	> 1.00E-4
HCT-116	0.186	1.837	1.584	1.986	1.831	1.651	1.243	85	109	100	89	64	> 1.00E-4	> 1.00E-4	> 1.00E-4
HCT-15	0.301	1.861	1.696	1.845	1.724	1.619	1.172	89	99	91	85	56	> 1.00E-4	> 1.00E-4	> 1.00E-4
HT29	0.324	2.154	2.153	2.140	2.088	1.918	1.439	100	99	96	87	61	> 1.00E-4	> 1.00E-4	> 1.00E-4
KM12	0.481	2.568	2.485	2.551	2.402	2.311	1.790	95	99	92	88	63	> 1.00E-4	> 1.00E-4	> 1.00E-4
SW-620	0.294	2.430	2.390	2.358	2.330	2.159	1.992	98	97	95	87	79	> 1.00E-4	> 1.00E-4	> 1.00E-4
CNS Cancer															
SF-268	1.122	3.138	3.049	3.158	2.944	2.725	2.662	96	101	90	79	76	> 1.00E-4	> 1.00E-4	> 1.00E-4
SF-295	0.657	2.215	2.057	2.151	2.090	1.889	1.638	90	96	92	79	63	> 1.00E-4	> 1.00E-4	> 1.00E-4
SF-539	0.796	2.636	2.592	2.568	2.575	2.403	2.222	98	96	97	87	77	> 1.00E-4	> 1.00E-4	> 1.00E-4
SNB-75	1.108	2.066	1.938	1.975	1.951	1.785	1.658	87	90	78	71	57	> 1.00E-4	> 1.00E-4	> 1.00E-4
U251	0.366	2.131	2.007	2.028	2.037	1.811	1.552	93	94	95	82	67	> 1.00E-4	> 1.00E-4	> 1.00E-4
Melanoma															
LOX IMVI	0.434	2.581	2.467	2.482	2.382	2.339	2.049	95	95	91	89	75	> 1.00E-4	> 1.00E-4	> 1.00E-4
MALME-3M	0.419	1.069	0.992	1.056	1.015	0.910	0.891	88	98	92	75	73	> 1.00E-4	> 1.00E-4	> 1.00E-4
M14	0.548	2.408	2.363	2.406	2.229	2.209	1.968	98	100	90	89	76	> 1.00E-4	> 1.00E-4	> 1.00E-4
MDA-MB-435	0.524	2.266	2.303	2.402	2.265	2.220	1.488	102	108	100	97	55	> 1.00E-4	> 1.00E-4	> 1.00E-4
SK-MEL-2	1.307	3.116	3.078	3.129	3.149	2.972	2.866	98	101	102	92	86	> 1.00E-4	> 1.00E-4	> 1.00E-4
SK-MEL-28	0.650	2.093	2.048	2.172	2.014	1.832	1.702	97	105	95	82	73	> 1.00E-4	> 1.00E-4	> 1.00E-4
SK-MEL-5	0.961	3.039	2.865	2.934	2.848	2.572	1.385	92	95	91	78	20	3.03E-5	> 1.00E-4	> 1.00E-4
UACC-257	1.082	2.627	2.565	2.599	2.523	2.444	2.287	96	98	93	88	78	> 1.00E-4	> 1.00E-4	> 1.00E-4
UACC-62	0.762	2.568	2.399	2.364	2.206	2.090	1.712	91	89	80	73	53	> 1.00E-4	> 1.00E-4	> 1.00E-4
Ovarian Cancer															
IGROV1	0.228	1.487	1.362	1.331	1.301	1.191	1.026	90	88	85	76	63	> 1.00E-4	> 1.00E-4	> 1.00E-4
OVCAR-3	0.589	2.305	2.234	2.240	2.149	1.849	1.651	96	96	91	73	62	> 1.00E-4	> 1.00E-4	> 1.00E-4
OVCAR-4	0.909	2.146	2.091	2.164	1.983	1.866	1.517	96	101	87	77	49	9.33E-5	> 1.00E-4	> 1.00E-4
OVCAR-5	0.511	1.687	1.653	1.565	1.663	1.382	1.361	97	90	98	74	72	> 1.00E-4	> 1.00E-4	> 1.00E-4
OVCAR-8	0.699	2.863	2.814	2.843	2.816	2.628	2.168	98	99	98	89	68	> 1.00E-4	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.445	1.388	1.387	1.441	1.343	1.265	1.030	100	106	95	87	62	> 1.00E-4	> 1.00E-4	> 1.00E-4
SK-OV-3	1.032	2.430	2.242	2.369	2.234	2.247	2.077	87	96	86	87	75	> 1.00E-4	> 1.00E-4	> 1.00E-4
Renal Cancer															
786-0	0.909	3.052	2.975	3.008	2.997	2.838	2.554	96	98	97	90	77	> 1.00E-4	> 1.00E-4	> 1.00E-4
A498	1.400	2.661	2.545	2.512	2.521	2.364	2.450	91	88	89	76	83	> 1.00E-4	> 1.00E-4	> 1.00E-4
ACHN	0.301	1.531	1.530	1.592	1.524	1.421	1.305	100	105	99	91	82	> 1.00E-4	> 1.00E-4	> 1.00E-4
CAKI-1	0.799	2.776	2.687	2.695	2.592	2.522	2.207	95	96	91	87	71	> 1.00E-4	> 1.00E-4	> 1.00E-4
RXF 393	0.921	1.516	1.431	1.476	1.469	1.324	1.206	86	93	92	68	48	7.78E-5	> 1.00E-4	> 1.00E-4
SN12C	0.640	2.443	2.437	2.345	2.117	1.986	1.682	100	95	82	75	58	> 1.00E-4	> 1.00E-4	> 1.00E-4
UO-31	0.571	2.060	1.789	1.821	1.780	1.689	1.419	82	84	81	75	57	> 1.00E-4	> 1.00E-4	> 1.00E-4
Prostate Cancer															
PC-3	0.621	2.226	2.085	2.087	1.985	1.842	1.505	91	91	85	76	55	> 1.00E-4	> 1.00E-4	> 1.00E-4
DU-145	0.467	2.344	2.428	2.258	2.156	2.041	1.837	104	95	90	84	73	> 1.00E-4	> 1.00E-4	> 1.00E-4
Breast Cancer															
MCF7	0.338	1.802	1.669	1.801	1.749	1.613	1.415	91	100	96	87	74	> 1.00E-4	> 1.00E-4	> 1.00E-4
MDA-MB-231/ATCC	0.524	1.255	1.260	1.268	1.192	1.127	1.052	101	102	91	82	72	> 1.00E-4	> 1.00E-4	> 1.00E-4
HS 578T	1.160	2.305	2.277	2.271	2.109	2.081	1.872	98	97	83	80	62	> 1.00E-4	> 1.00E-4	> 1.00E-4
BT-549	1.006	2.008	2.021	2.043	1.955	1.784	1.451	101	103	95	78	44	6.78E-5	> 1.00E-4	> 1.00E-4
T-47D	0.718	1.965	1.796	1.846	1.907	1.719	1.337	86	90	95	80	50	9.75E-5	> 1.00E-4	> 1.00E-4
MDA-MB-468	0.720	1.073	1.040	1.054	1.041	0.950	0.784	91	94	91	65	18	2.10E-5	> 1.00E-4	> 1.00E-4