

Supplementary Materials: Design, Synthesis and Biological Evaluation of Novel Benzothiazole Derivatives as Selective PI3K β Inhibitors

Shuang Cao, Ruiyuan Cao, Xialing Liu, Xiang Luo and Wu Zhong

Content

^1H -NMR, ^{13}C -NMR and HRMS spectra of compound 1–11.

1-(4-(2,4-Dimorpholinobenzo[d]thiazol-6-yl)phenyl)-3-ethylurea (1)

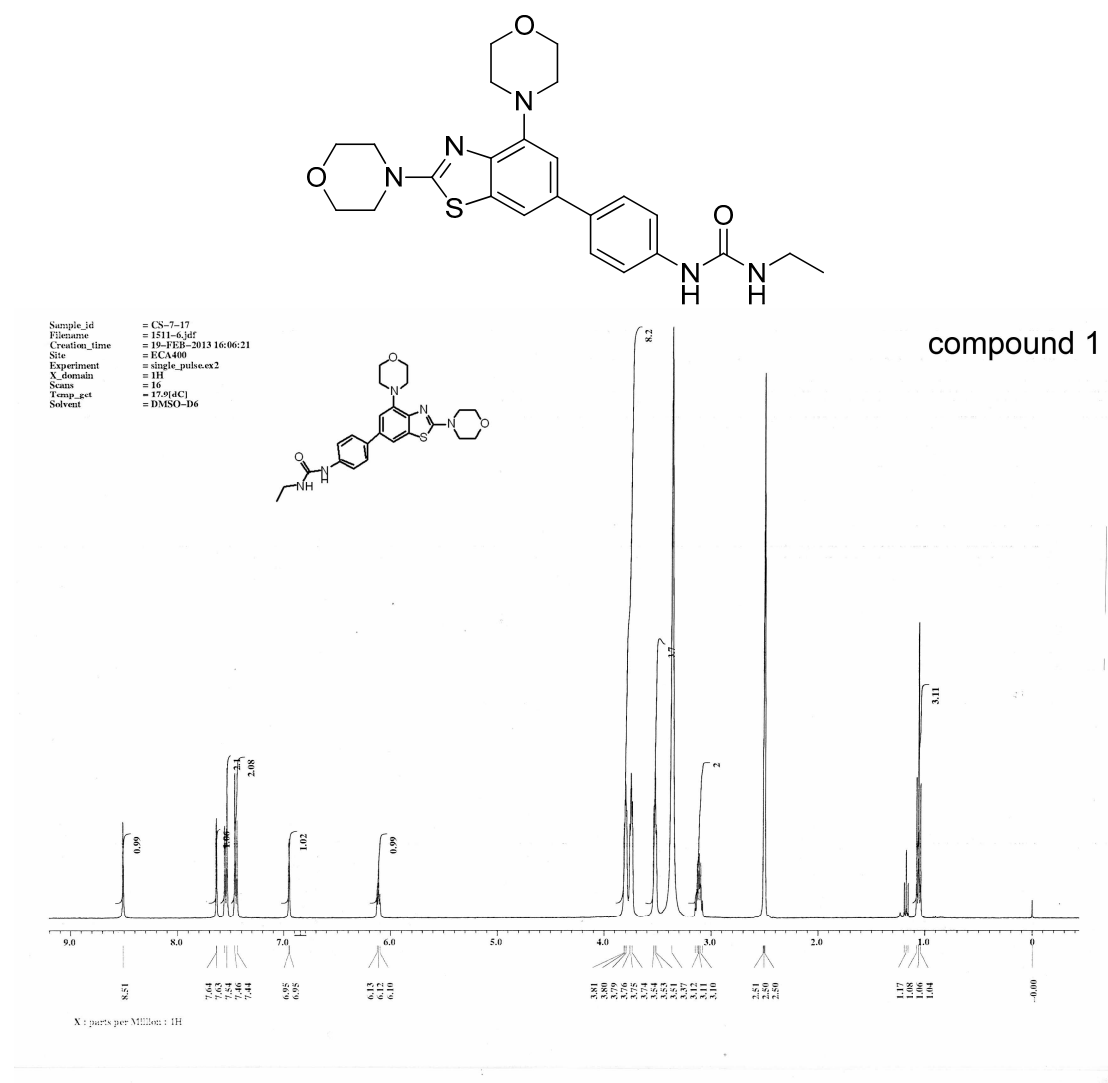
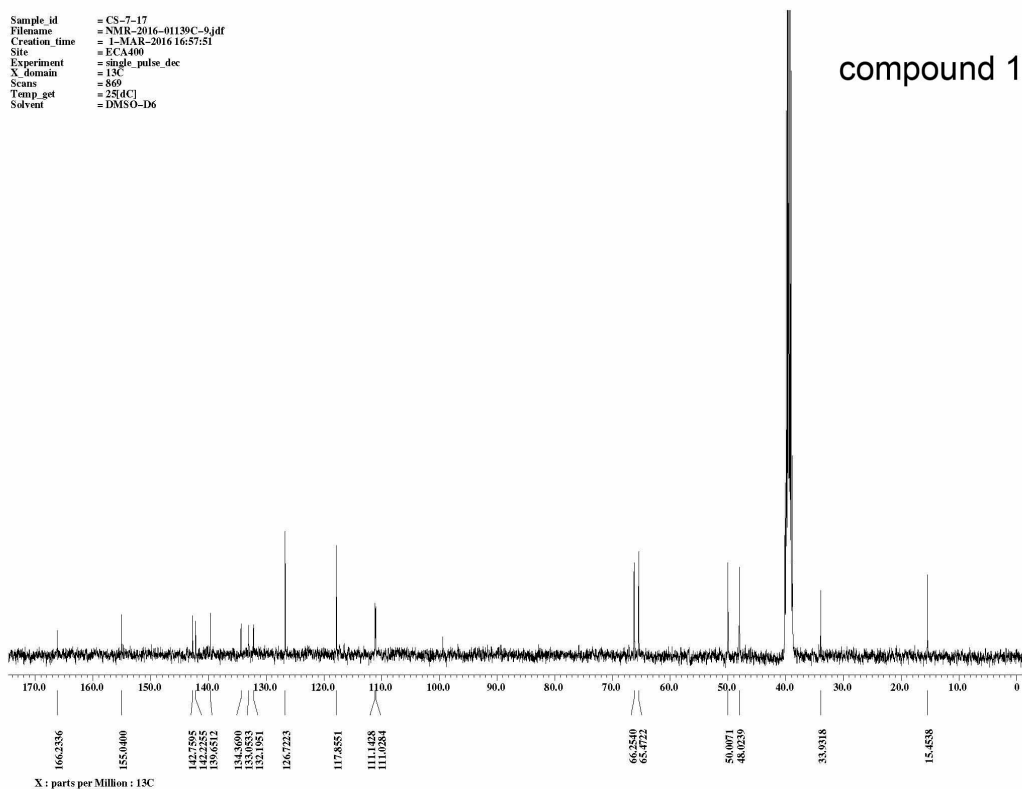


Figure S1. ^1H -NMR of compound 1.

Figure S2. ^{13}C -NMR of compound 1.

compound 1

Qualitative Analysis Report

Data Filename	0860.d	Sample Name	mTOR18
Instrument Name	TOF G6230A	Acquired Time	2016-03-23
Acq Method	YCLM	Acquired SW	6200 series TOF/6500 series
IRM Calibration Status	Success		
User Chromatograms			

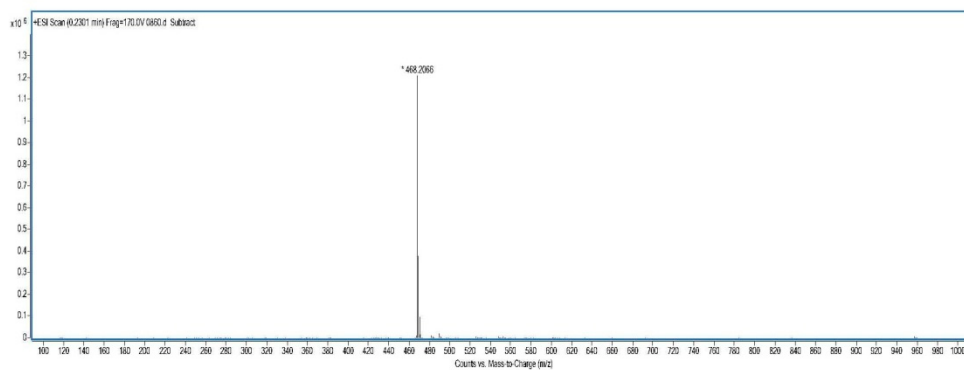
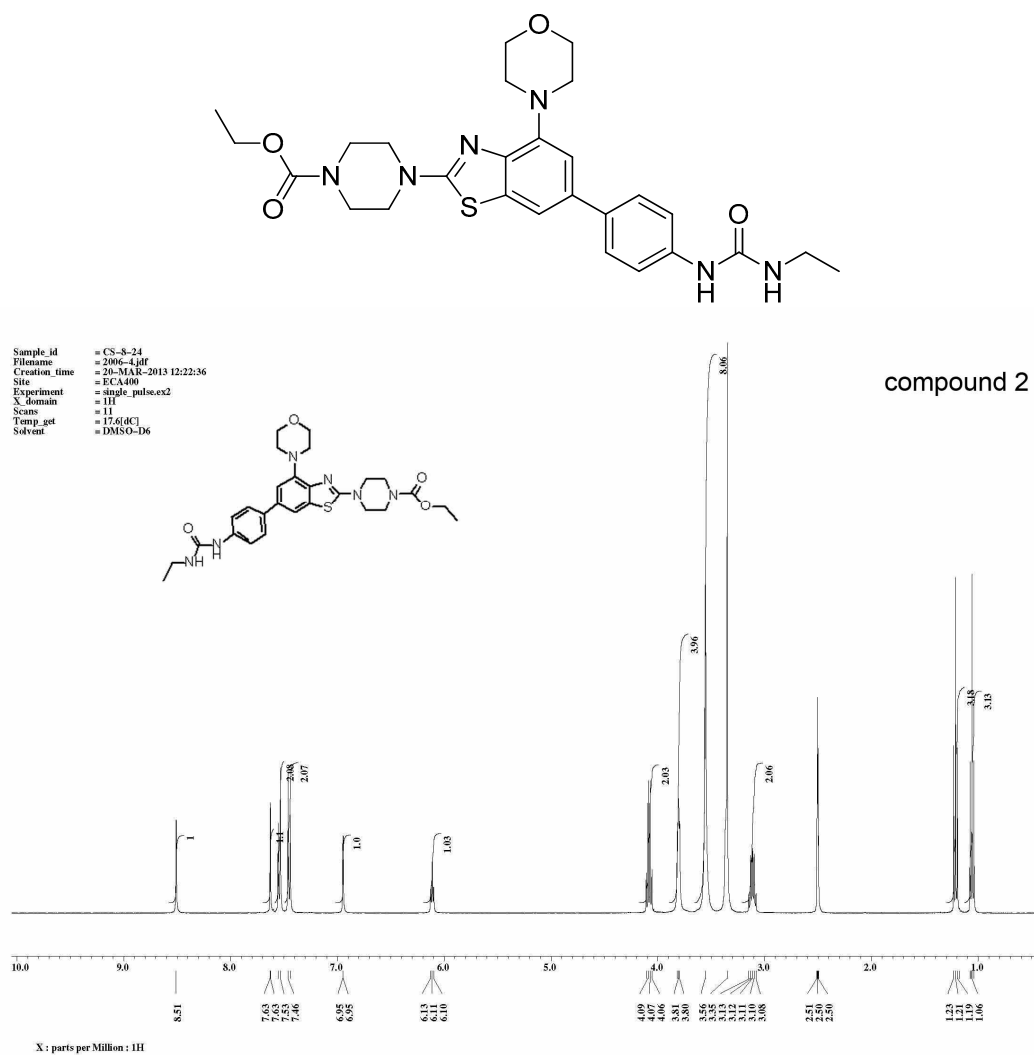
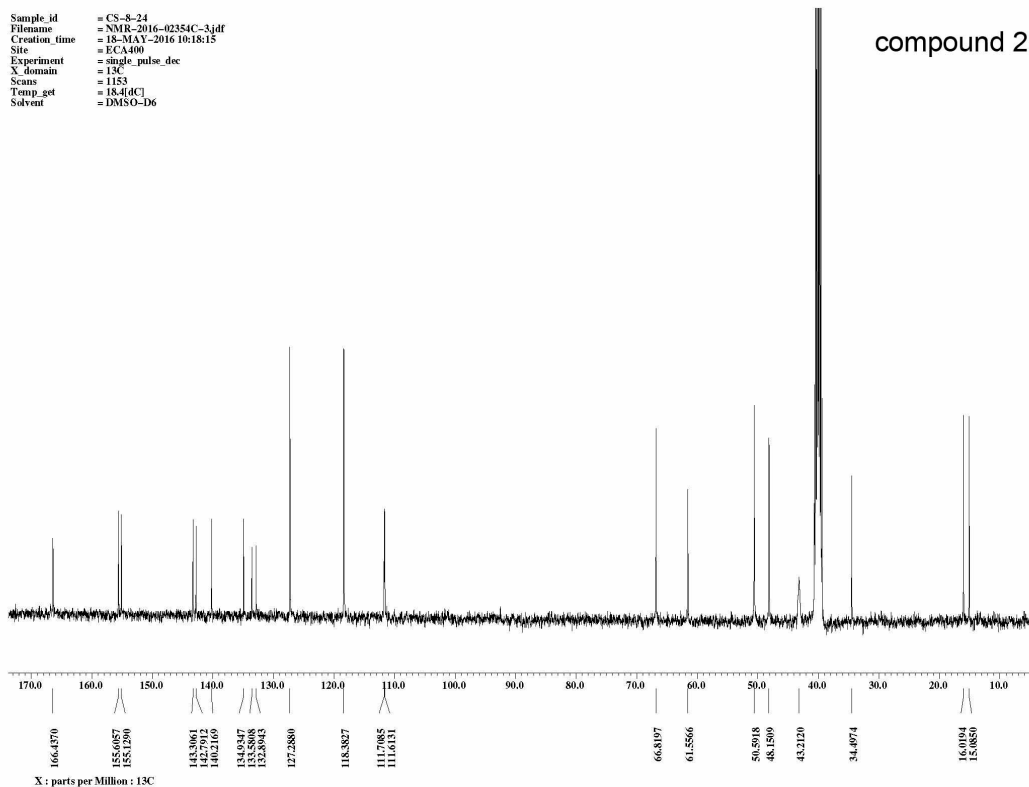


Figure S3. HRMS of compound 1.

Ethyl 4-(6-(4-(3-ethylureido)phenyl)-4-morpholinobenzo[d]thiazol-2-yl) piperazine-1-carboxylate (2)

Figure S4. ¹H-NMR of compound 2.

Figure S5. ^{13}C -NMR of compound 2.

compound 2

Qualitative Analysis Report

Data Filename	1416.d	Sample Name	CS-8-24
Instrument Name	TOF G6230A	Acquired Time	2016-05-24
Acq Method	YCLM	Acquired SW	6200 series TOF/6500 series
IRM Calibration Status	Success		
User Chromatograms			

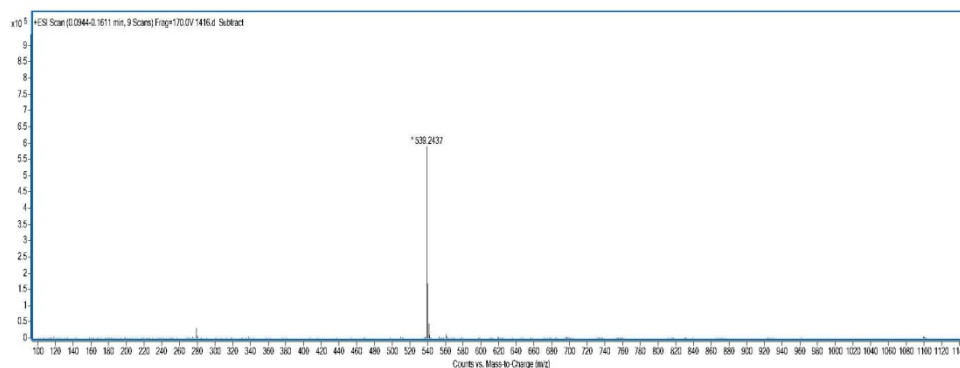
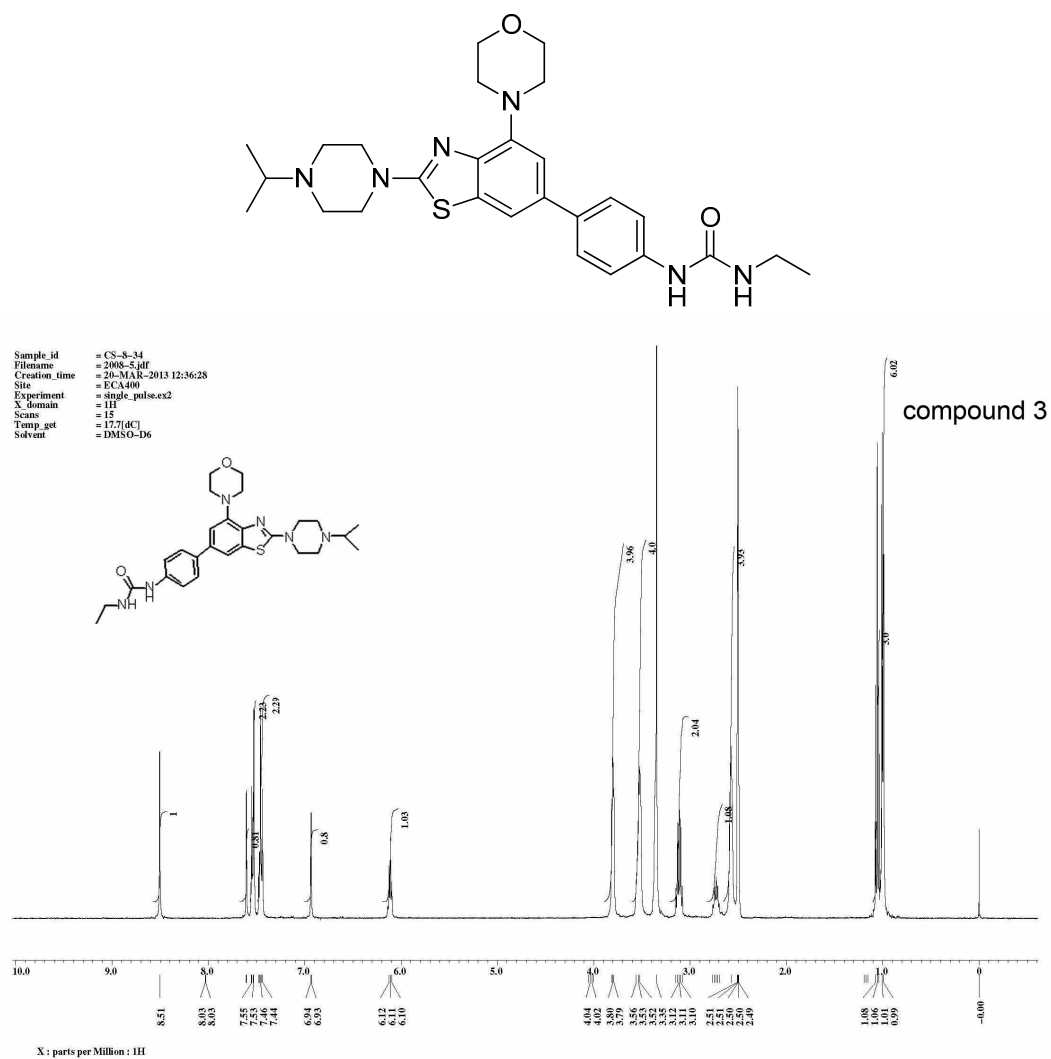
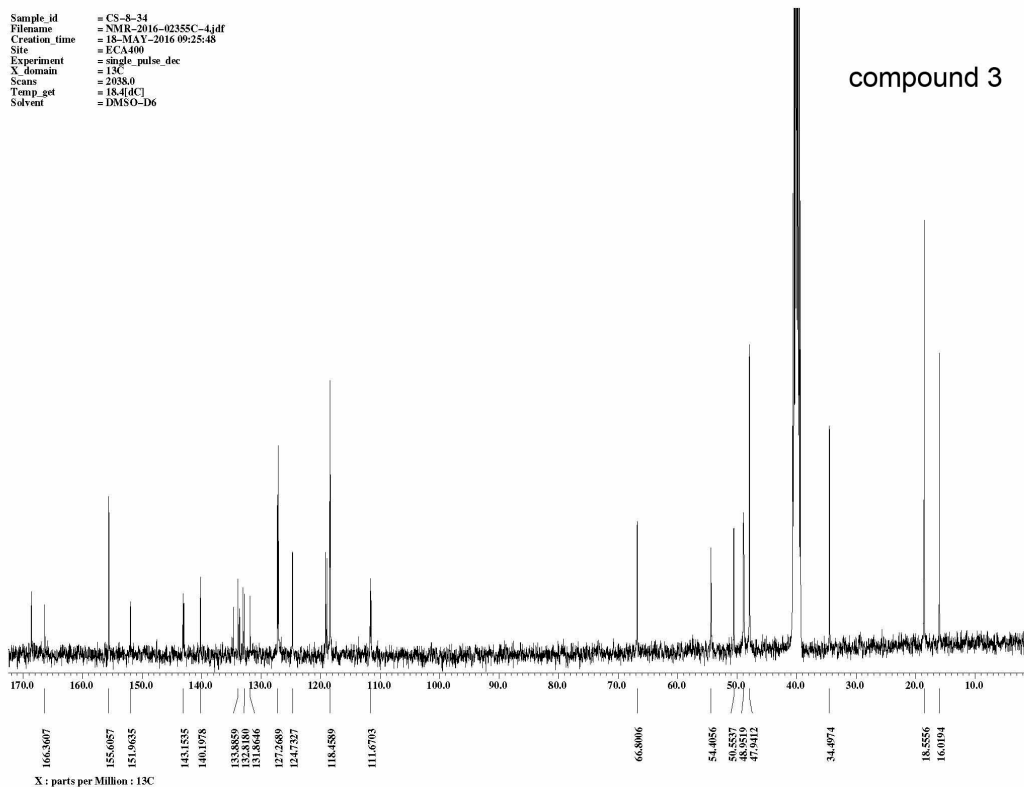


Figure S6. HRMS of compound 2.

1-Ethyl-3-(4-(2-(4-isopropylpiperazin-1-yl)-4-morpholinobenzo[d]thiazol-6-yl)phenyl)urea (3)

Figure S7. ¹H-NMR of compound 3.

Figure S8. ^{13}C -NMR of compound 3.

compound 3

Qualitative Analysis Report

Data Filename	1417.d	Sample Name	CS-8-34
Instrument Name	TOF G6230A	Acquired Time	2016-05-24
Acq Method	YCLM	Acquired SW	6200 series TOF/6500 series
IRM Calibration Status	Success		
User Chromatograms			

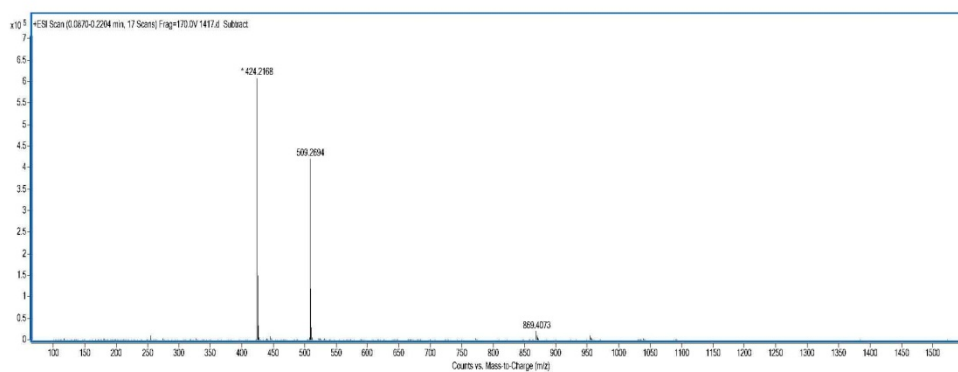
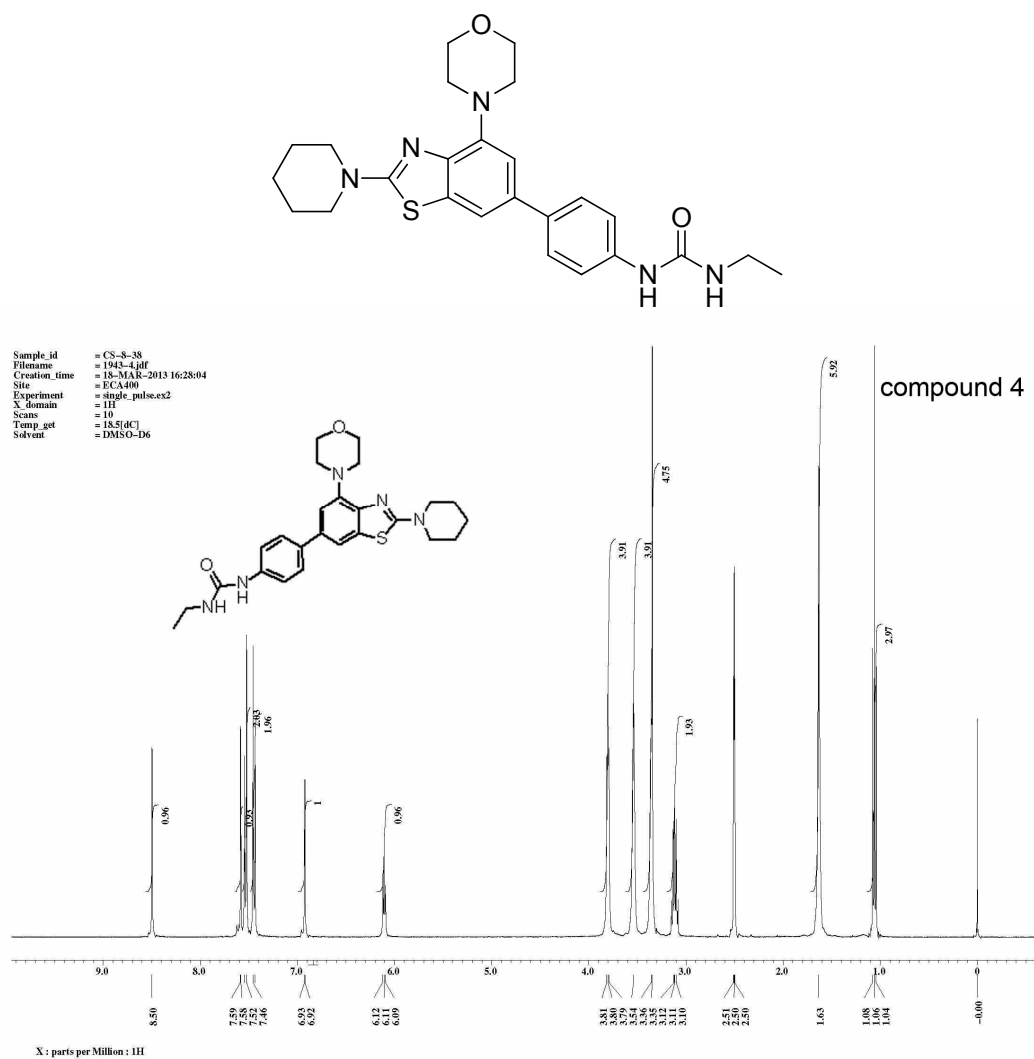
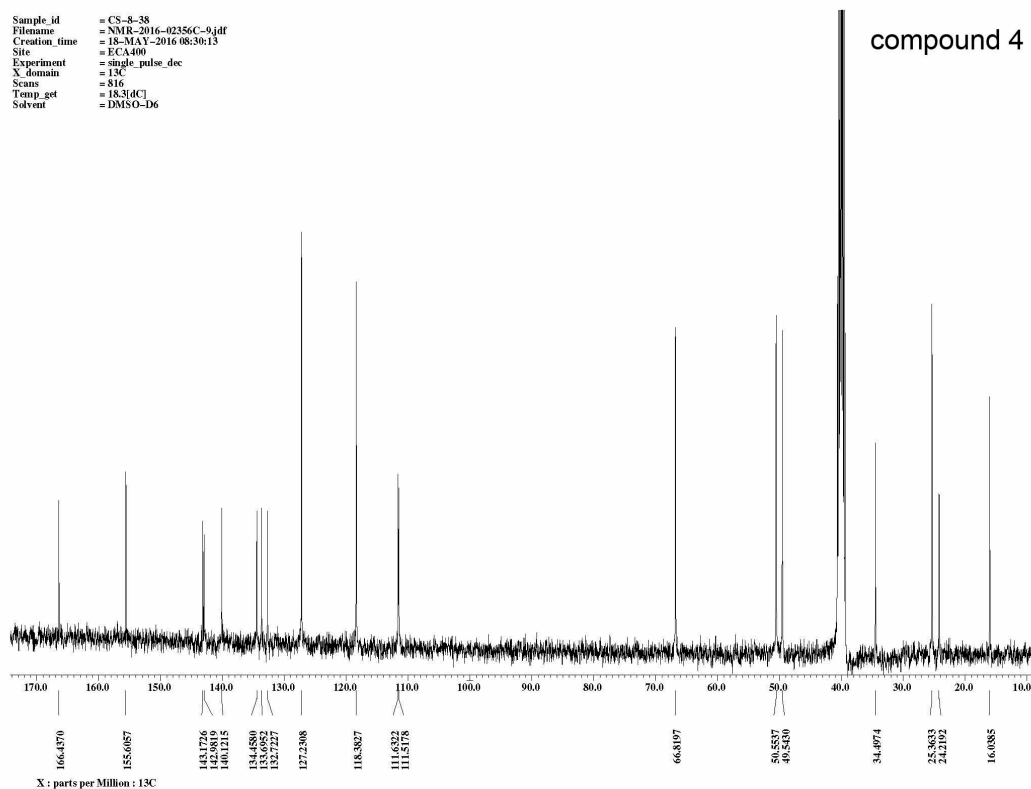


Figure S9. HRMS of compound 3.

1-Ethyl-3-(4-(4-morpholino-2-(piperidin-1-yl)benzo[d]thiazol-6-yl)phenyl)urea (**4**)Figure S10. ¹H-NMR of compound 4.

Figure S11. ^{13}C -NMR of compound 4.

compound 4

Qualitative Analysis Report

Data Filename	1418.d	Sample Name	CS-8-38
Instrument Name	TOF G6230A	Acquired Time	2016-05-24
Acq Method	YCLM	Acquired SW	6200 series TOF/6500 series
IRM Calibration Status	Success		
User Chromatograms			

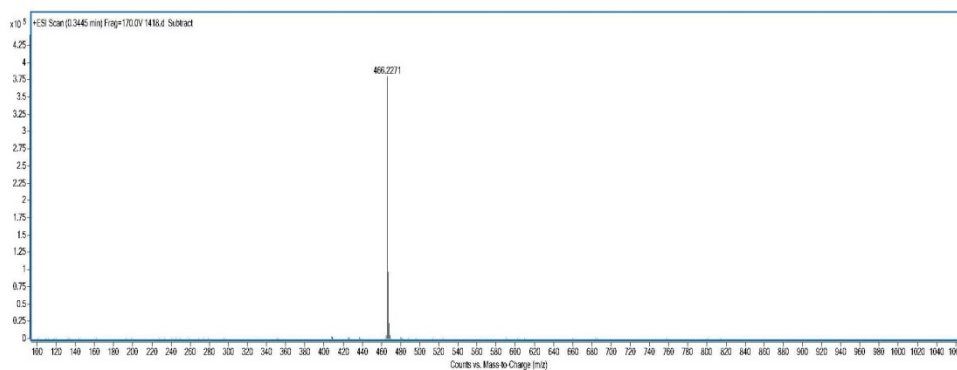
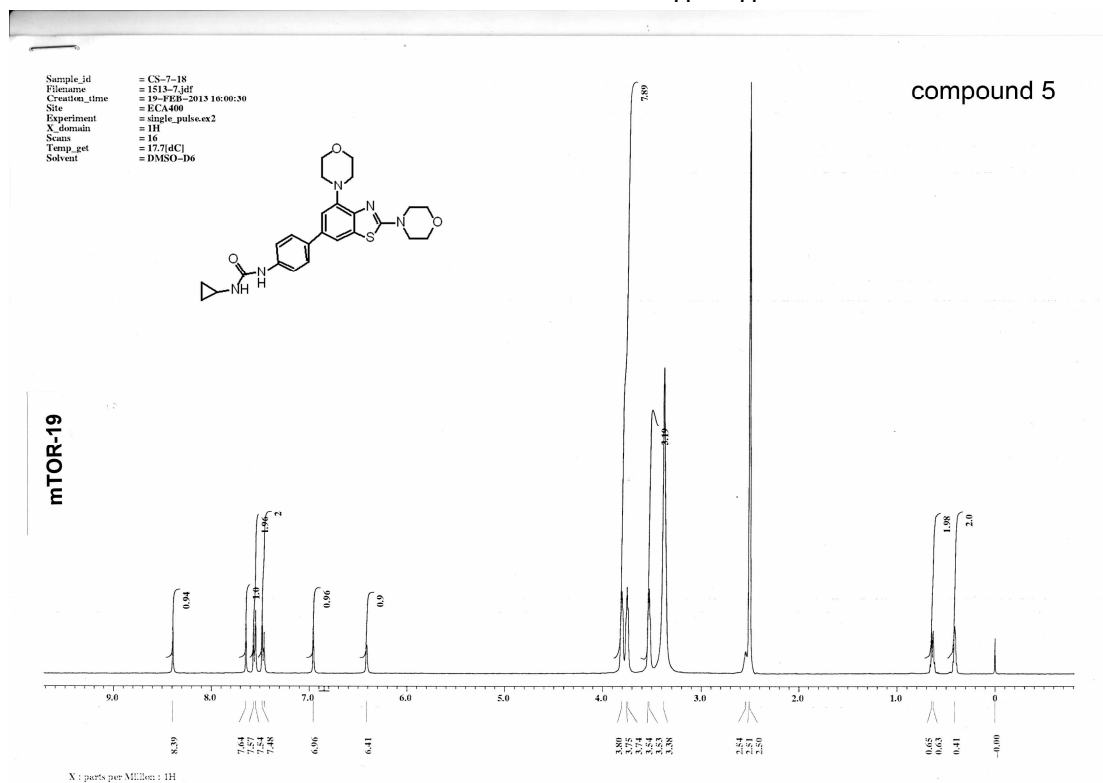
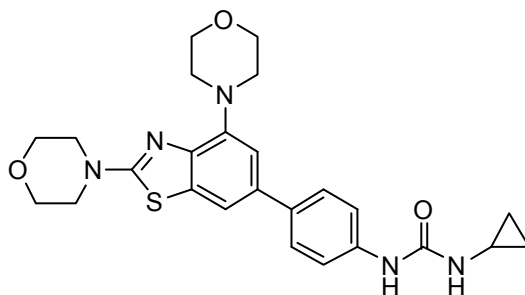
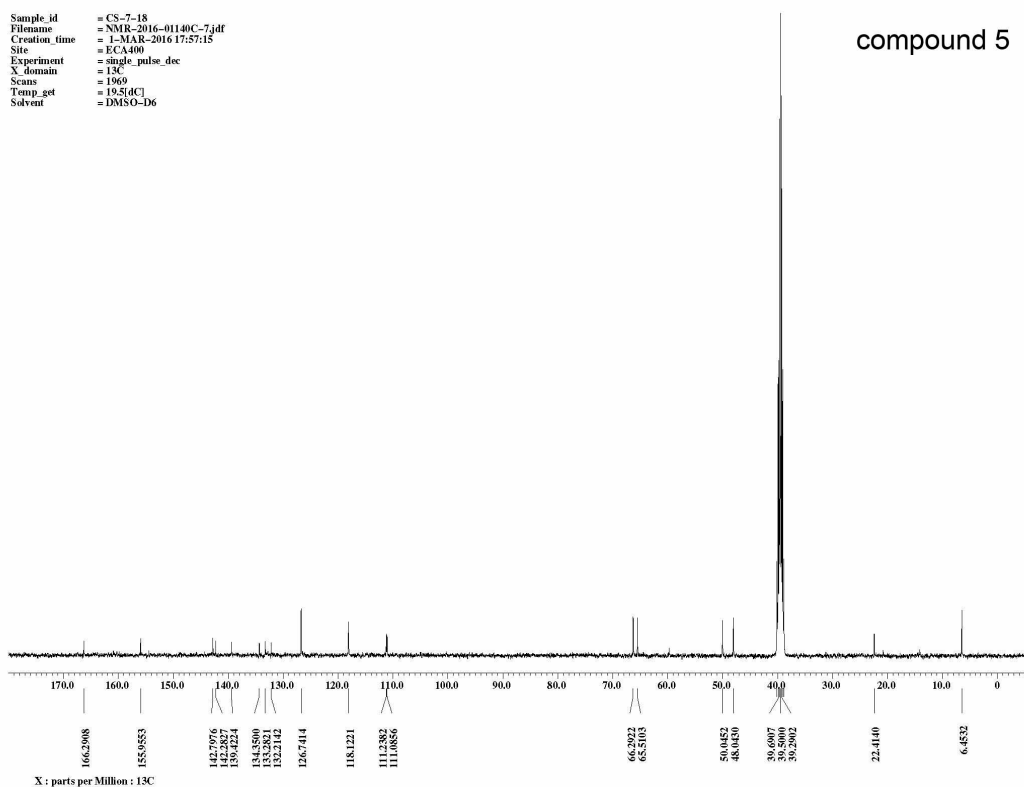


Figure S12. HRMS of compound 4.

1-Cyclopropyl-3-(4-(2,4-dimorpholinobenzo[d]thiazol-6-yl)phenyl)urea (5)

Figure S13. ¹H-NMR of compound 5.

Figure S14. ^{13}C -NMR of compound 5.

compound 5

Qualitative Analysis Report

Data Filename	1067.d	Sample Name	mTOR19
Instrument Name	TOF G6230A	Acquired Time	2016-04-07
Acq Method	YCLM	Acquired SW	6200 series TOF/6500 series
IRM Calibration Status	Success		
User Chromatograms			

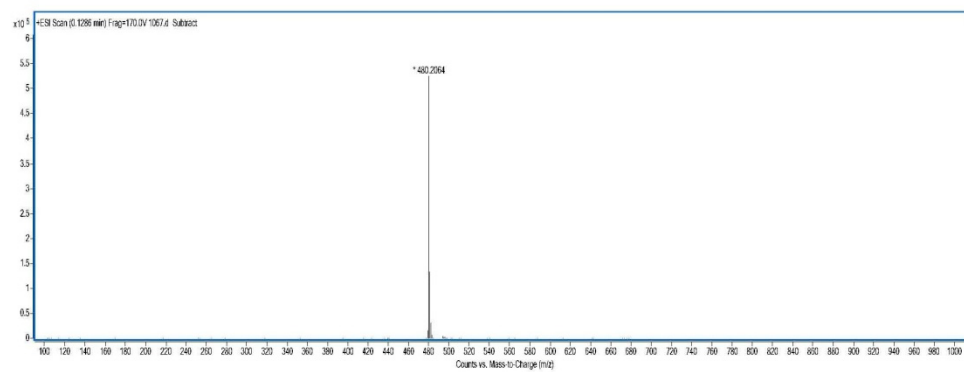
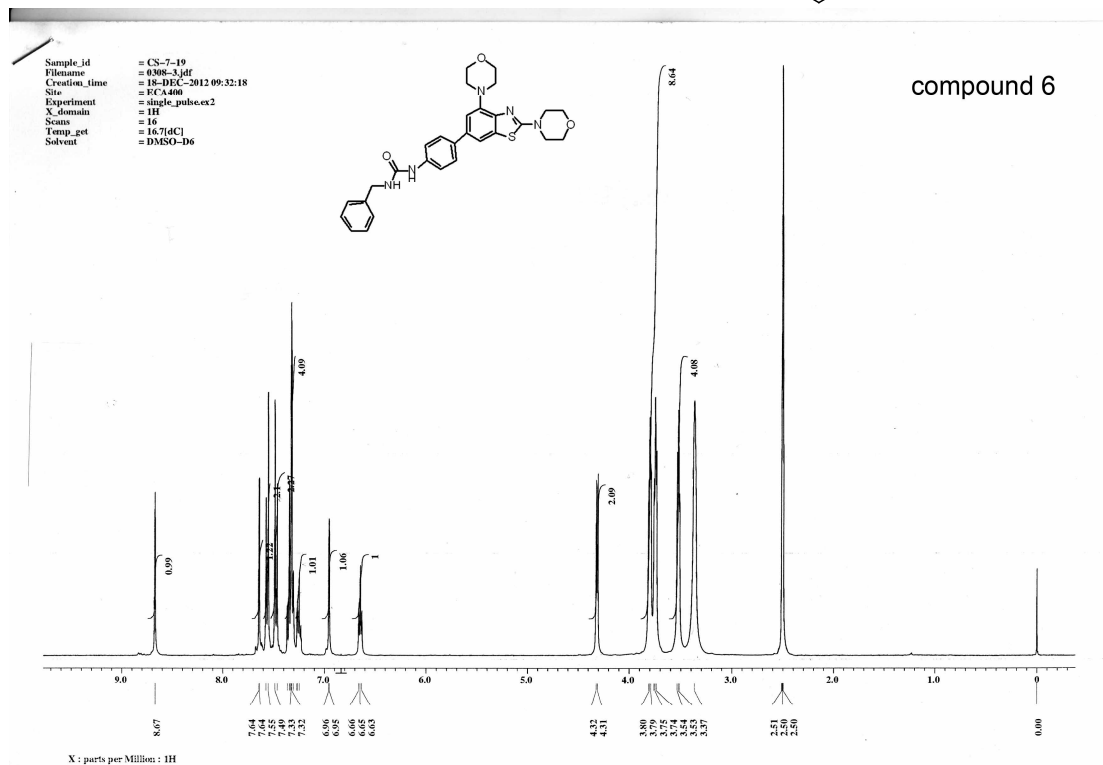
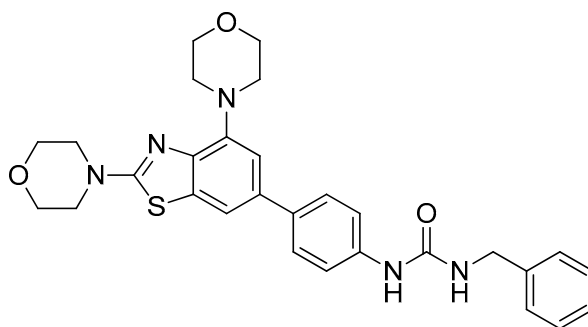
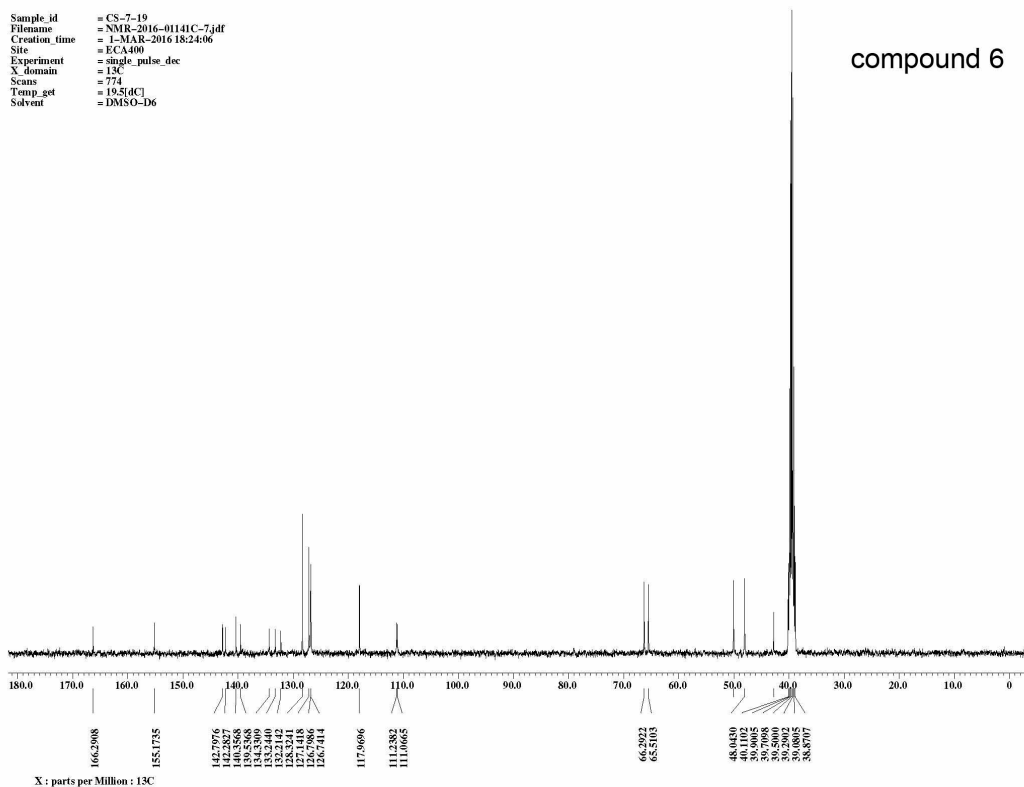


Figure S15. HRMS of compound 5.

1-Benzyl-3-(4-(2,4-dimorpholinobenzo[d]thiazol-6-yl)phenyl)urea (6)

Figure S16. ¹H-NMR of compound 6.

Figure S17. ^{13}C -NMR of compound 6.

compound 6

Qualitative Analysis Report

Data Filename	1419.d	Sample Name	CS-7-19
Instrument Name	TOF G6230A	Acquired Time	2016-05-24
Acq Method	YCLM	Acquired SW	6200 series TOF/6500 series
IRM Calibration Status	Success		
User Chromatograms			

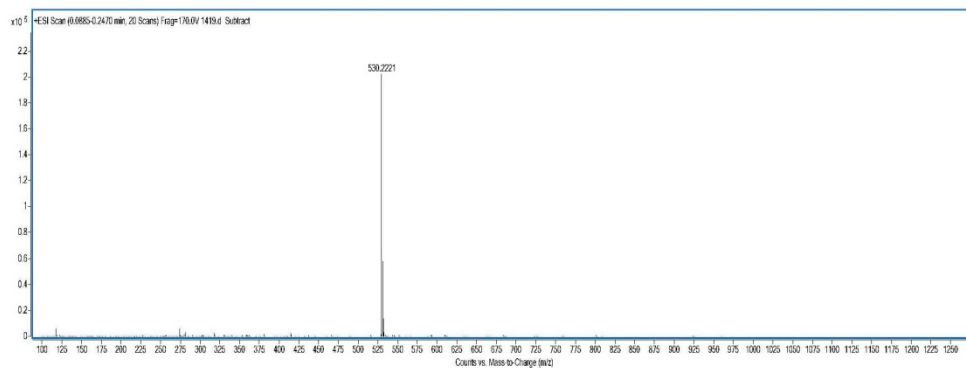
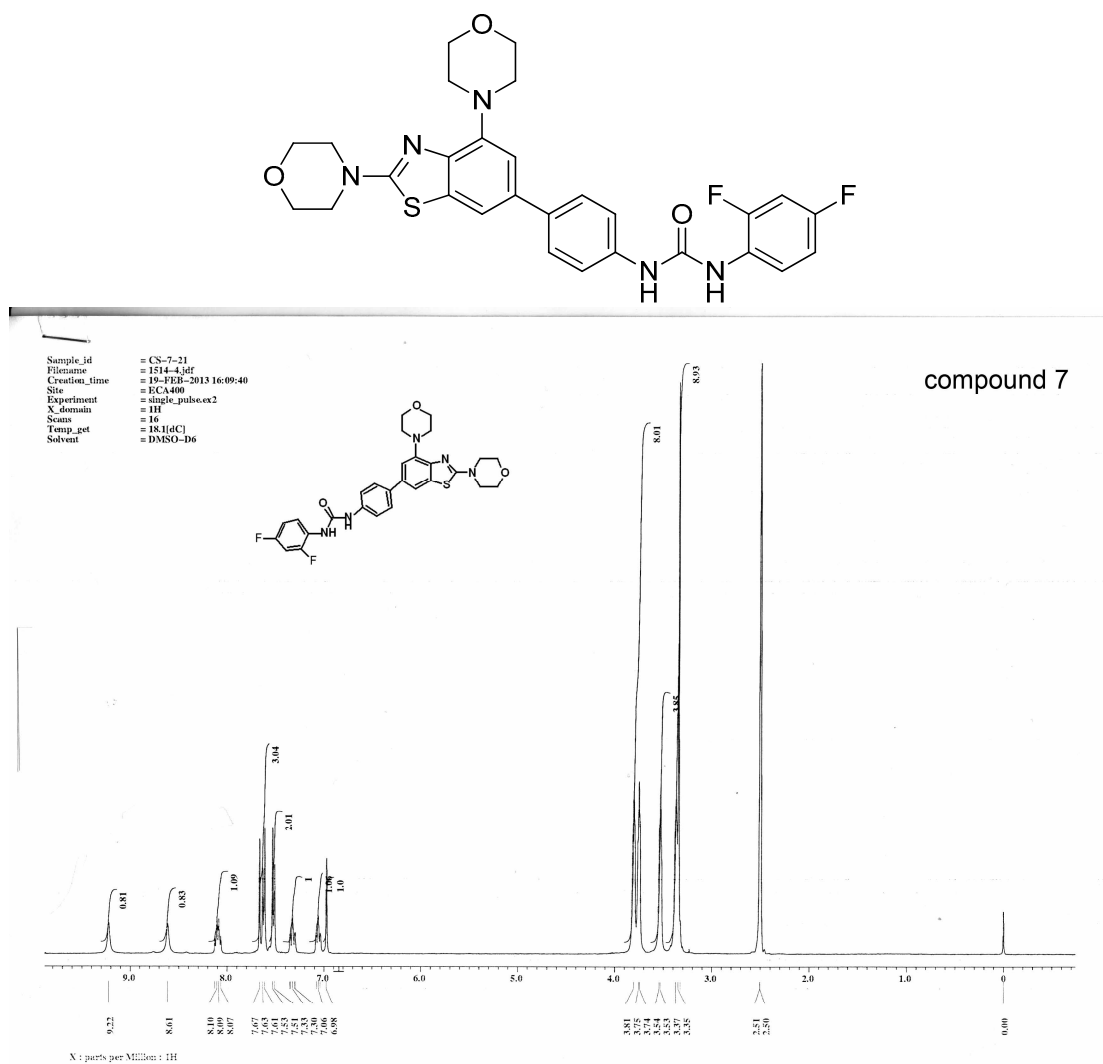
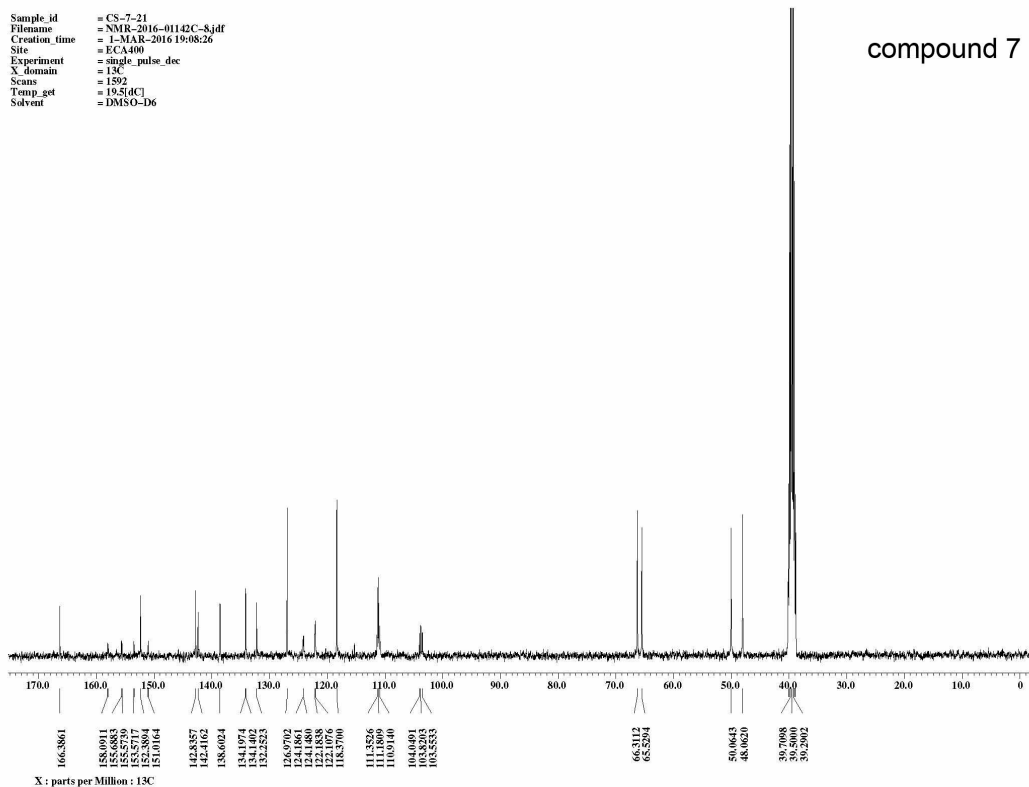


Figure S18. HRMS of compound 6.

1-(2,4-Difluorophenyl)-3-(4-(2,4-dimorpholinobenzo[d]thiazol-6-yl)phenyl)urea (7)

Figure S19. ¹H-NMR of compound 7.

Figure S20. ^{13}C -NMR of compound 7.

compound 7

Qualitative Analysis Report

Data Filename	1068.d	Sample Name	mTOR22
Instrument Name	TOF G6230A	Acquired Time	2016-04-07
Acq Method	YCLM	Acquired SW	6200 series TOF/6500 series
IRM Calibration Status	Success		
User Chromatograms			

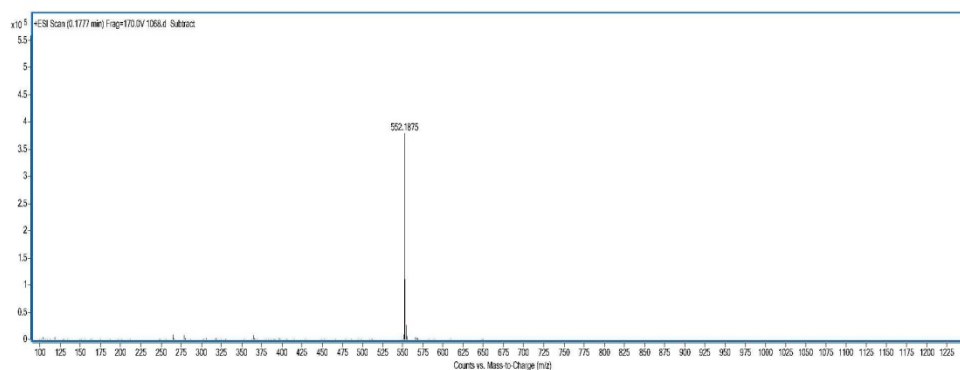


Figure S21. HRMS of compound 7.

1-(4-(2,4-Dimorpholinobenzo[d]thiazol-6-yl)phenyl)-3-methylurea (8)

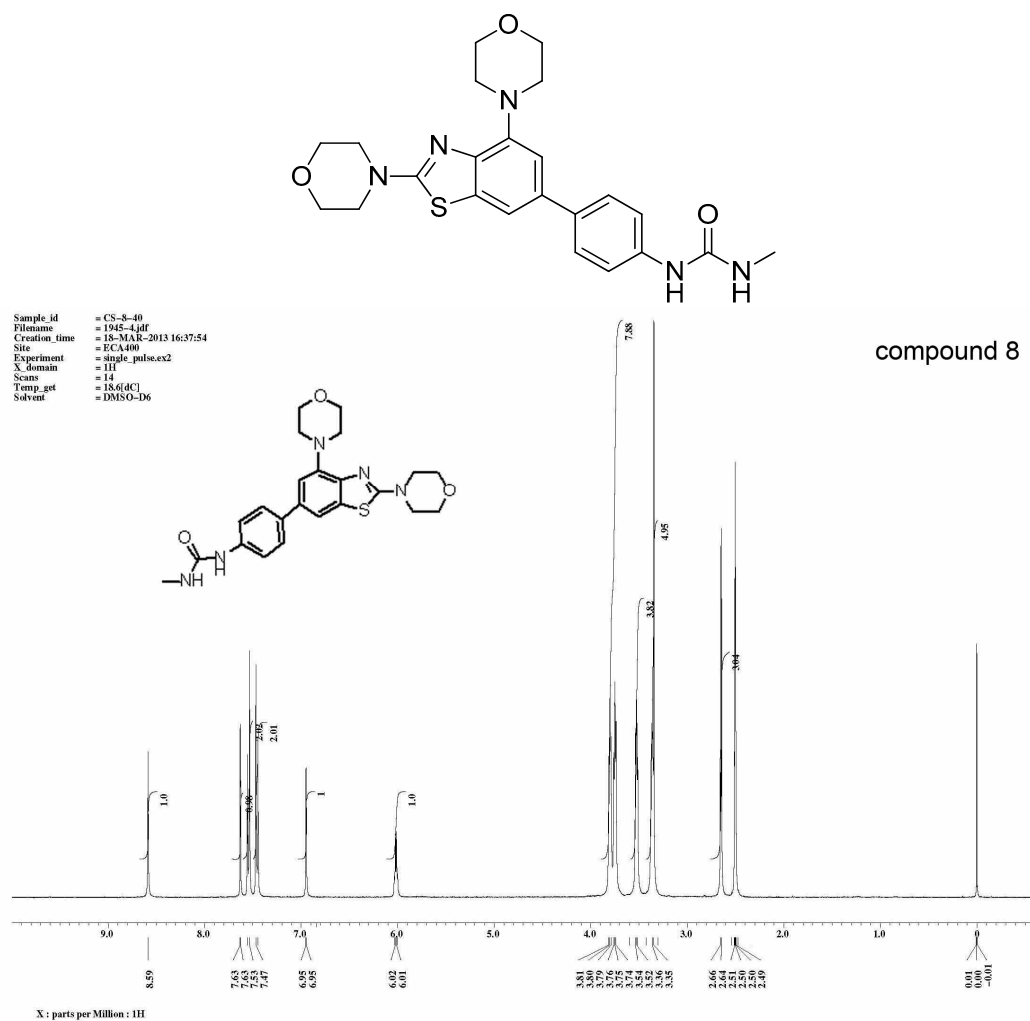
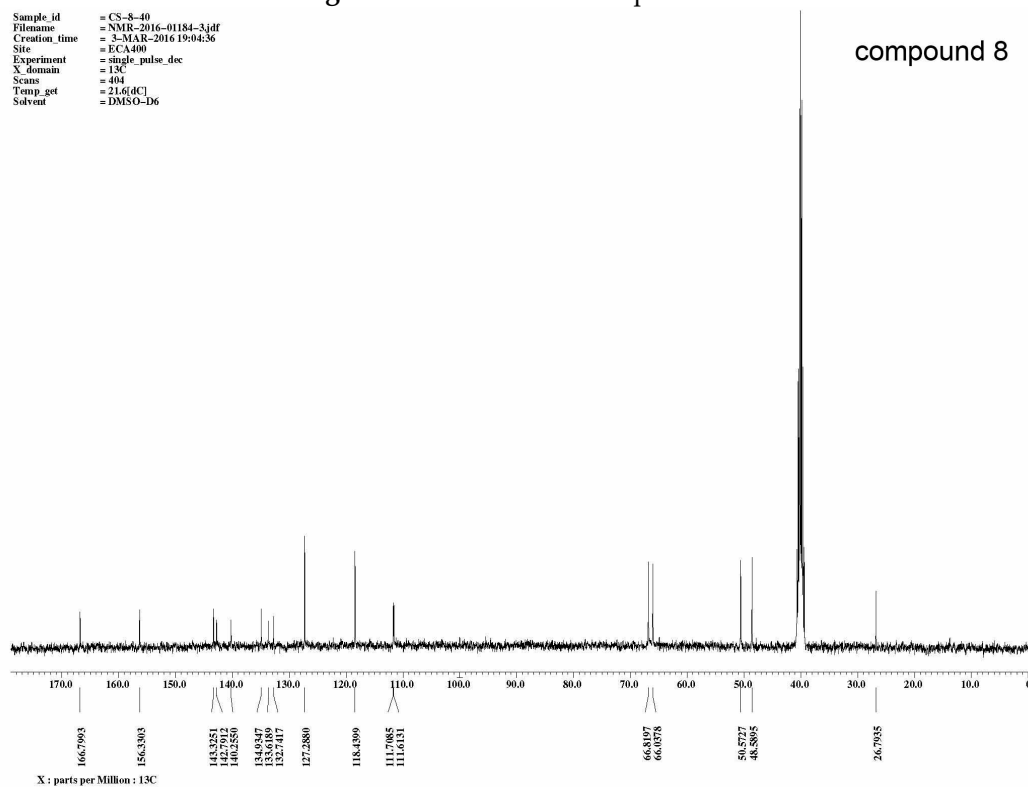
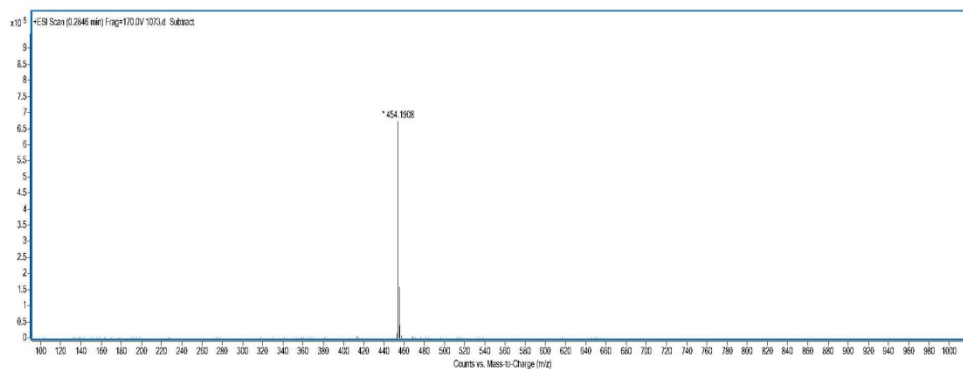
Figure S22. ¹H-NMR of compound 8.

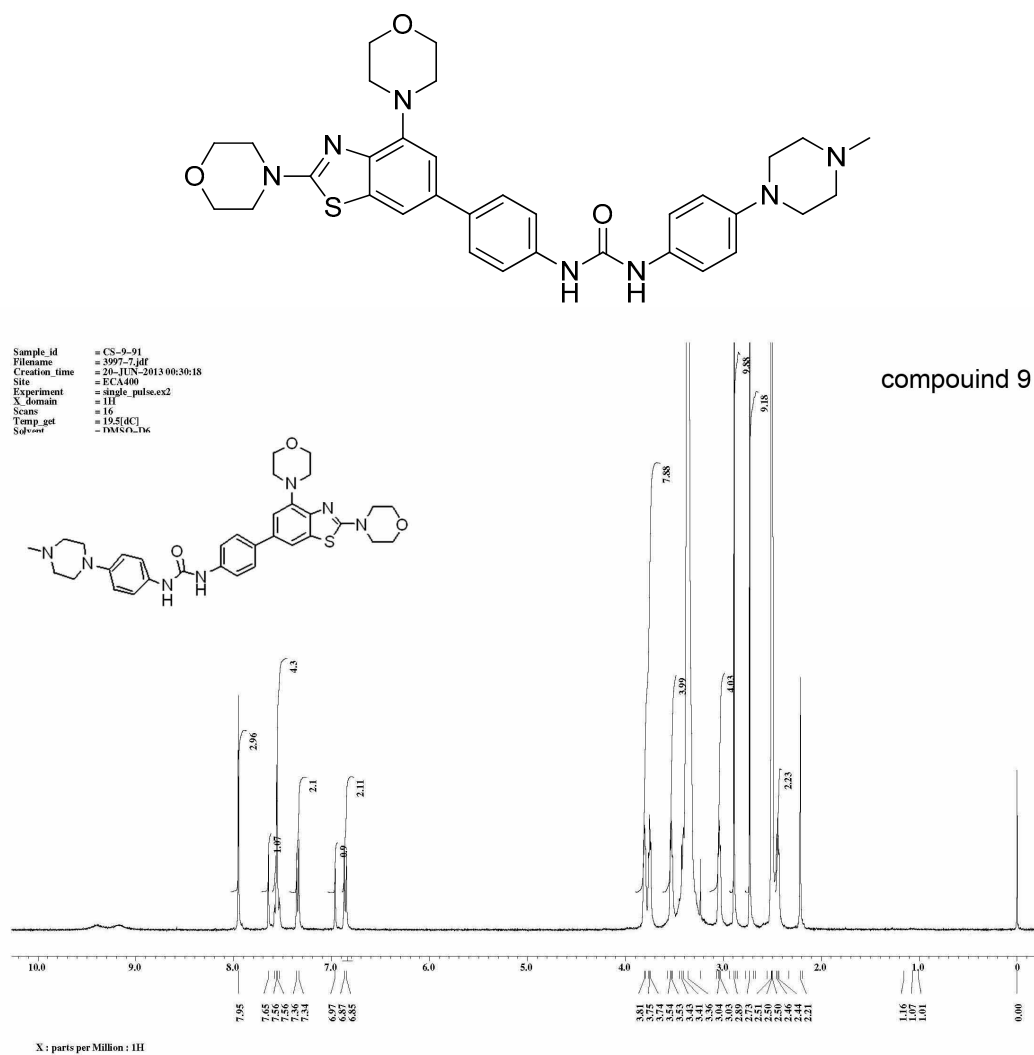
Figure S23. ^{13}C -NMR of compound 8.

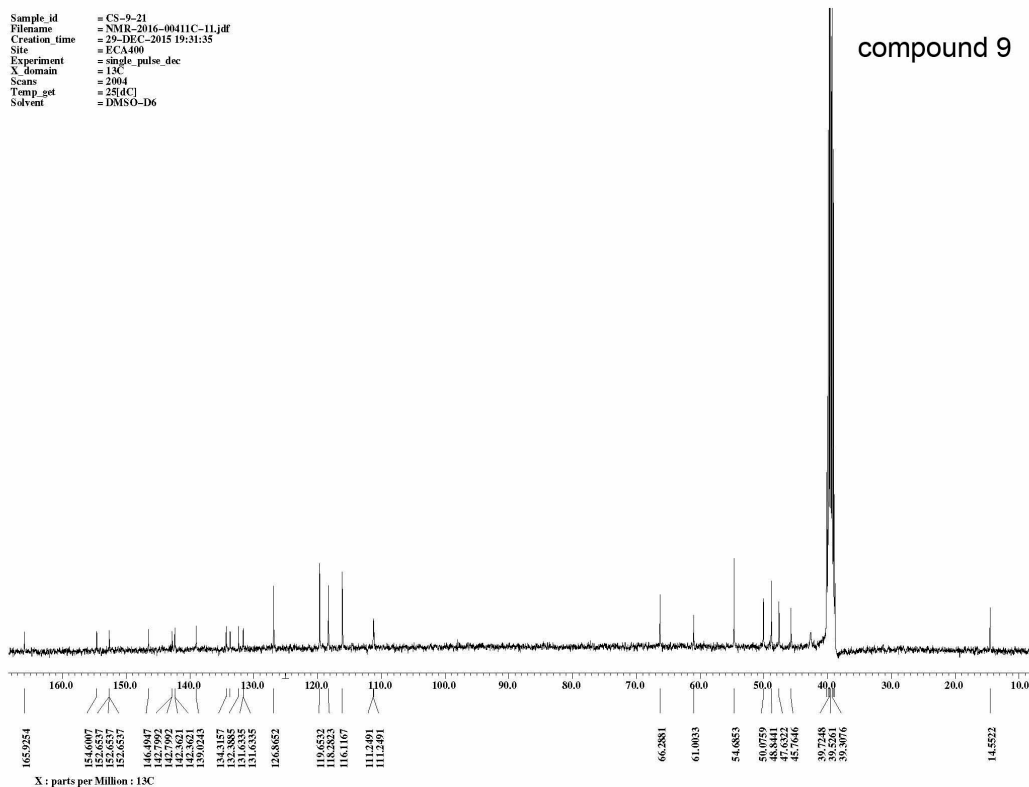
compound 8

Qualitative Analysis Report			
Data Filename	1073.d	Sample Name	mTOR44
Instrument Name	TOF G6230A	Acquired Time	2016-04-07
Acq Method	YCLM	Acquired SW	6200 series TOF/6500 series
IRM Calibration Status	Success		
User Chromatograms			

**Figure S24.** HRMS of compound 8.

1-(4-(2,4-Dimorpholinobenzo[d]thiazol-6-yl)phenyl)-3-(4-(4-methylpiperazin-1-yl)phenyl)urea (9)

Figure S25. ¹H-NMR of compound 9.

Figure S26. ^{13}C -NMR of compound 9.

compound 9

Qualitative Analysis Report

Data Filename	1420.d	Sample Name	CS-9-9A
Instrument Name	TOF G6230A	Acquired Time	2016-05-24
Acq Method	YCLIM	Acquired SW	6200 series TOF/6500 series
IRM Calibration Status	Success		
User Chromatograms			

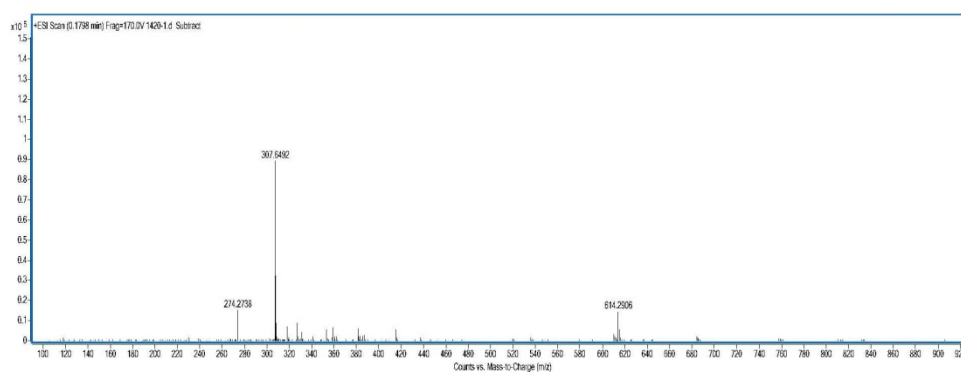
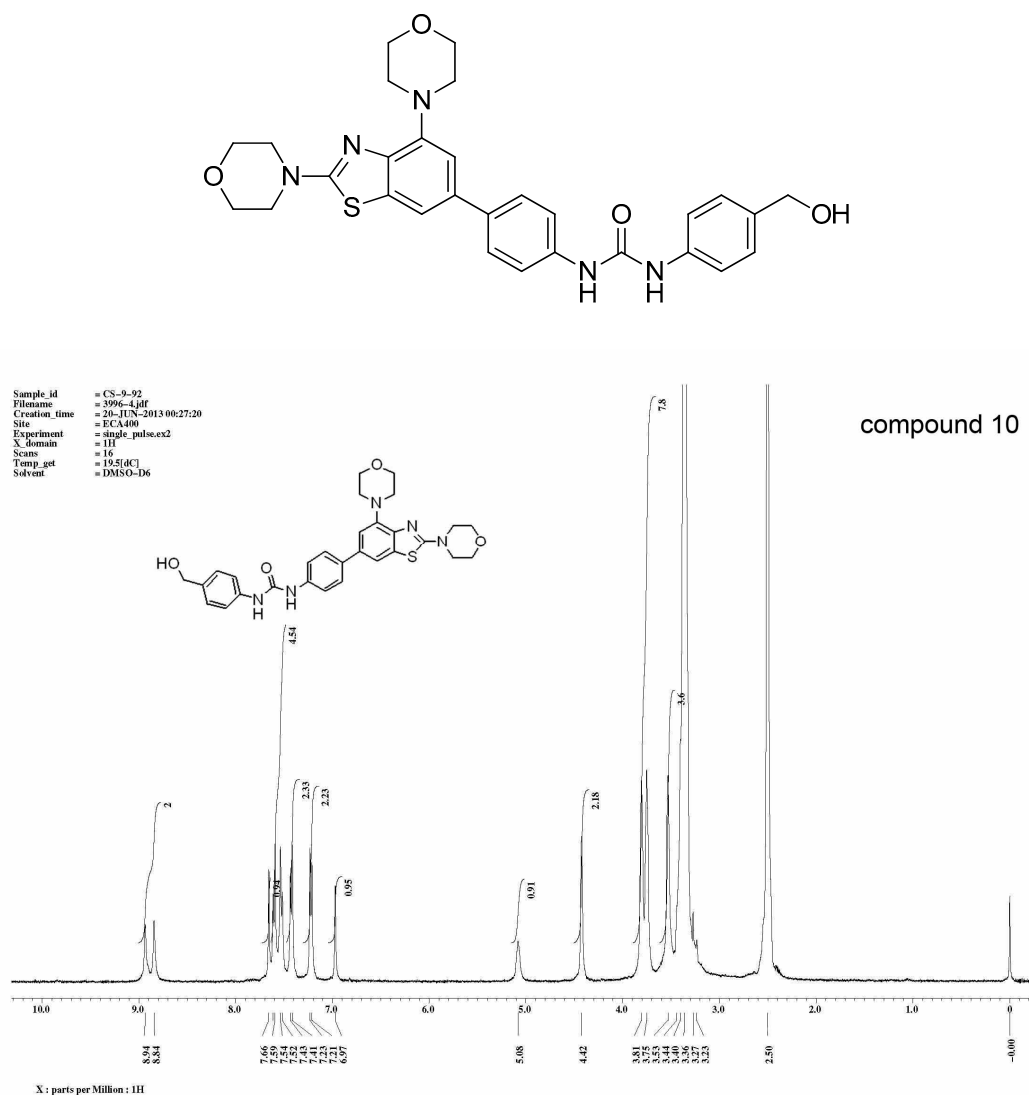
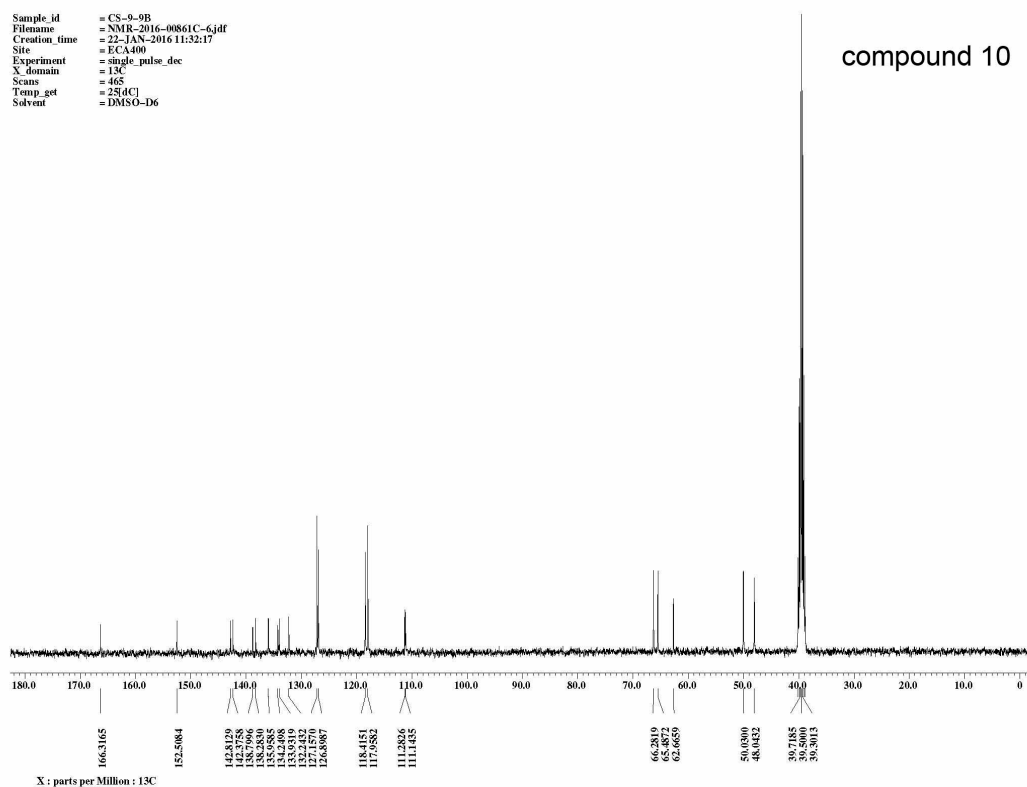


Figure S27. HRMS of compound 9.

1-(4-(2,4-Dimorpholinobenzo[d]thiazol-6-yl)phenyl)-3-(4-(hydroxymethyl)phenyl)urea (10)

Figure S28. ¹H-NMR of compound 10.

Figure S29. ^{13}C -NMR of compound 10.

compound 10

Qualitative Analysis Report

Data Filename	1076.d	Sample Name	mTOR46
Instrument Name	TOF G6230A	Acquired Time	2016-04-07
Acq Method	YCLM	Acquired SW	6200 series TOF/6500 series
IRM Calibration Status	Success		
User Chromatograms			

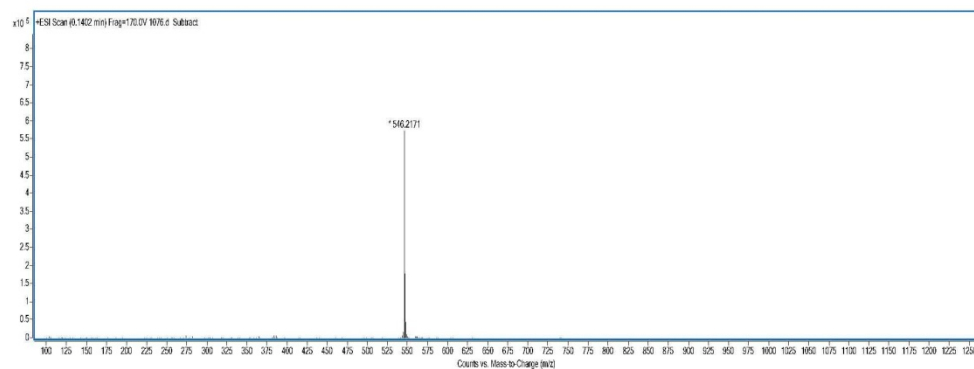
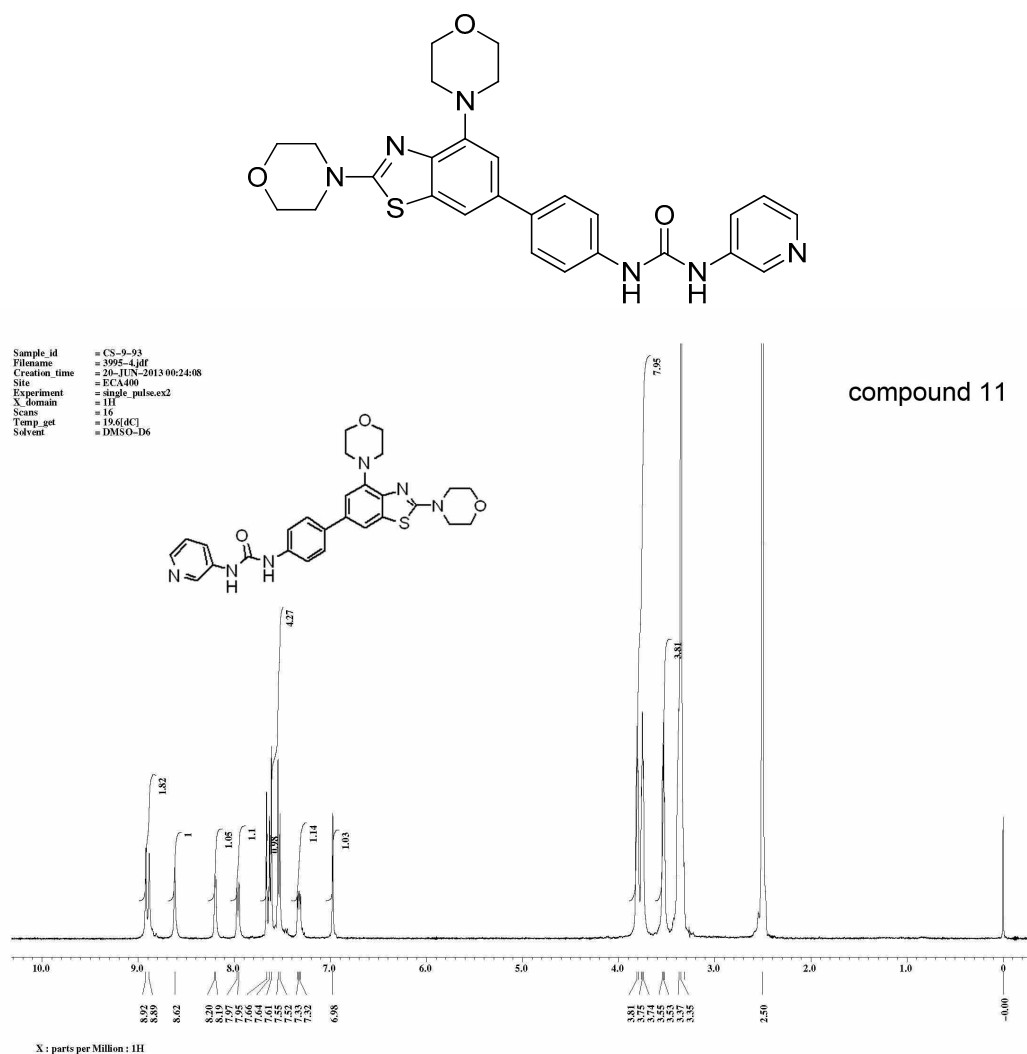
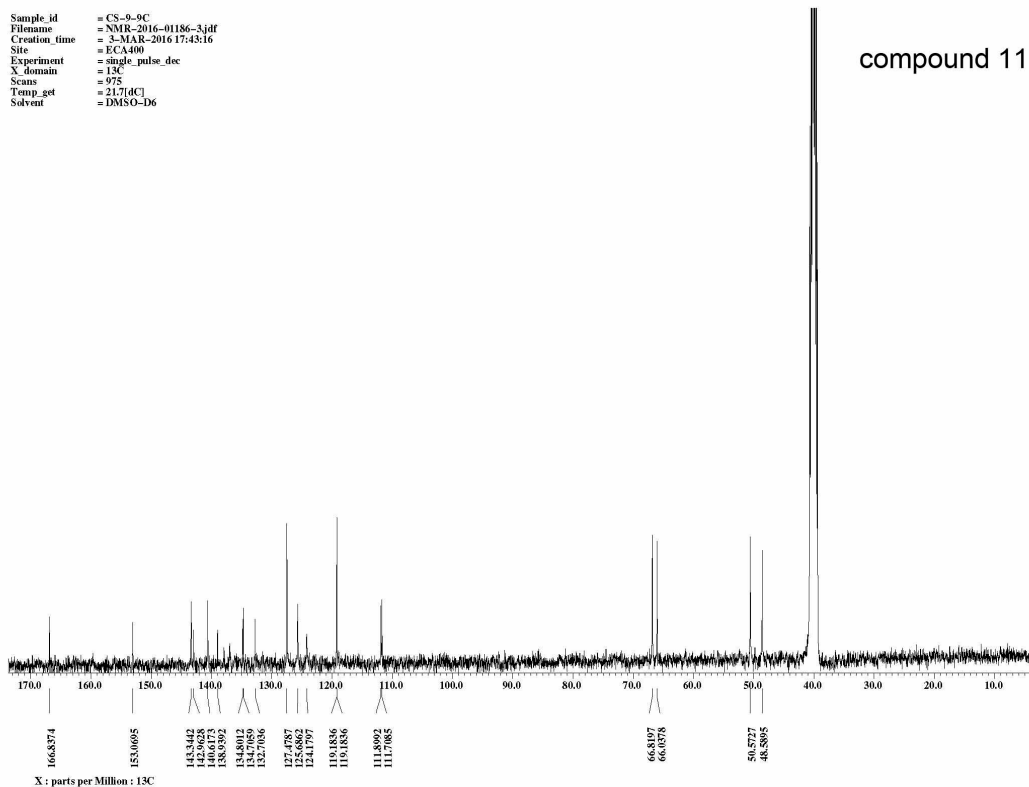


Figure S30. HRMS of compound 10.

1-(4-(2,4-Dimorpholinobenzo[d]thiazol-6-yl)phenyl)-3-(pyridin-3-yl)urea (11)

Figure S31. ¹H-NMR of compound 11.

Figure S32. ^{13}C -NMR of compound 11.

compound 11

Qualitative Analysis Report

Data Filename	1078.d	Sample Name	mTOR47
Instrument Name	TOF G6230A	Acquired Time	2016-04-07
Acq Method	YCLM	Acquired SW	6200 series TOF/6500 series
IRM Calibration Status	Success		
User Chromatograms			

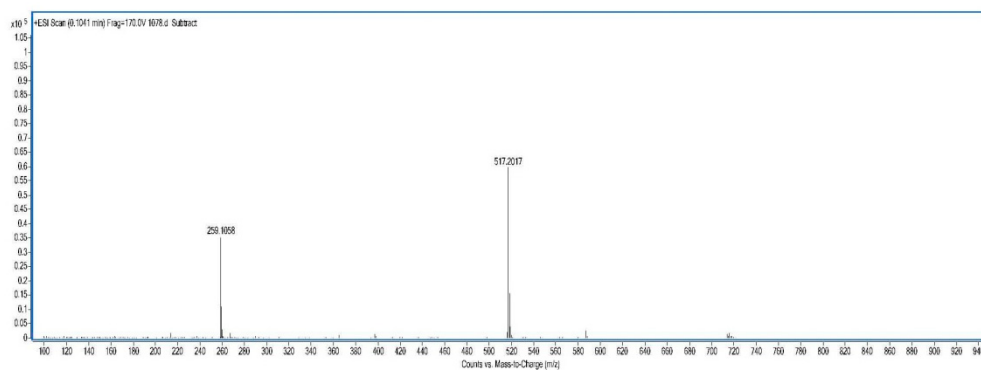


Figure S33. HRMS of compound 11.