

Supporting Information

SAR Studies on 1,2,4-Triazolo[3,4-b]-1,3,4-thiadiazoles as Inhibitors of *Mtb* Shikimate

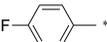
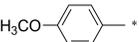
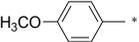
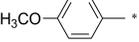
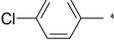
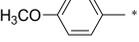
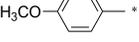
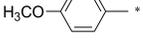
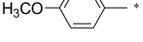
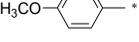
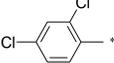
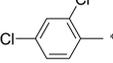
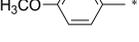
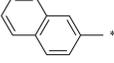
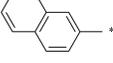
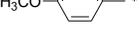
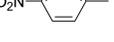
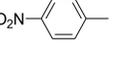
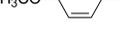
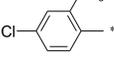
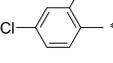
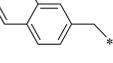
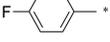
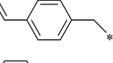
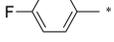
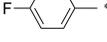
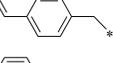
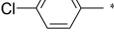
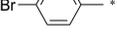
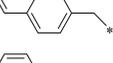
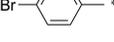
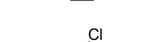
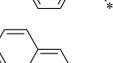
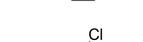
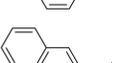
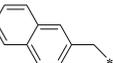
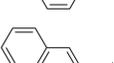
Dehydrogenase for the Development of Novel Antitubercular Agents

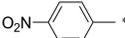
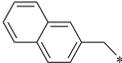
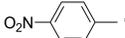
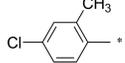
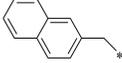
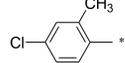
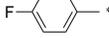
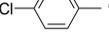
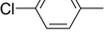
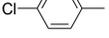
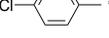
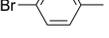
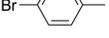
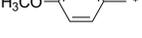
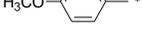
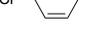
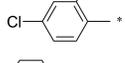
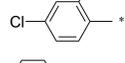
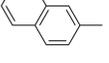
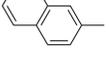
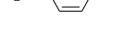
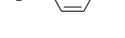
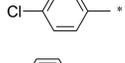
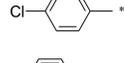
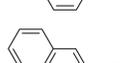
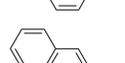
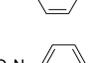
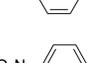
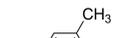
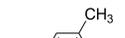
Ziqiang Li,^a Yishuang Liu,^a Xiaoguang Bai,^a Qi Deng,^a Juxian Wang,^a Guoning Zhang,^a Chunling Xiao,^a
Yaning Mei^{*,b} and Yucheng Wang^{*,a}

^a Institute of Medicinal Biotechnology, Chinese Academy of Medical Science & Peking Union Medical College, Beijing 100050, China. E-mail address: wyc9999@gmail.com; Tel: +86-10-63165263.

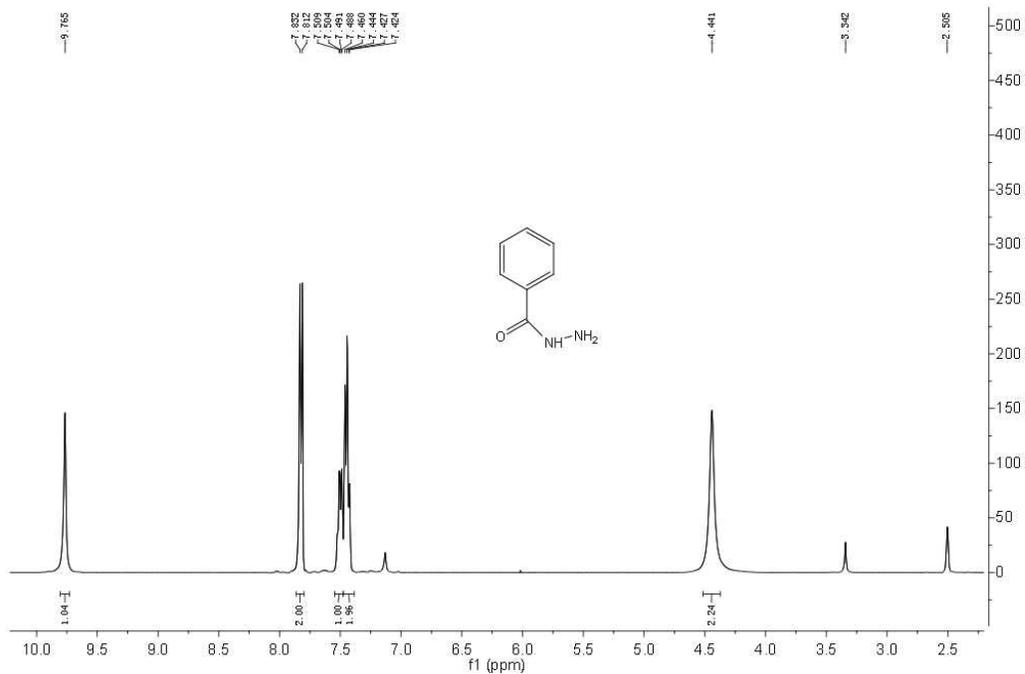
^b Department of Laboratory Medicine, the First Affiliated Hospital of Nanjing Medical University, Nanjing 210029, China. E-mail address: myn303@163.com; Tel: +86-25-68136287.

Table 1 Antibacterial activity of triazolothiadiazoles **6** against *Mtb* H37Rv strain (MIC, $\mu\text{g/mL}$)

compound	R ¹	R ²	<i>Mtb</i>		compound	R ¹	R ²	<i>Mtb</i>	
			H37Rv	MIC				H37Rv	MIC
1			8		6e-1			>8	
6a-1			>8		6e-2			>8	
6a-2			>8		6e-3			>8	
6a-3			>8		6e-4			>8	
6a-4			>8		6e-5			>8	
6a-5			>8		6e-6			>8	
6a-6			>8		6e-7			>8	
6a-7			>8		6e-8			>8	
6a-8			>8		6e-9			>8	
6a-9			>8		6f-1			>8	
6b-2			>8		6f-2			<8	
6b-3			>8		6f-3			>8	
6b-4			>8		6f-4			>8	
6b-5			<8		6f-5			>8	
6b-6			>8		6f-6			>8	
6b-7			<8		6f-7			>8	

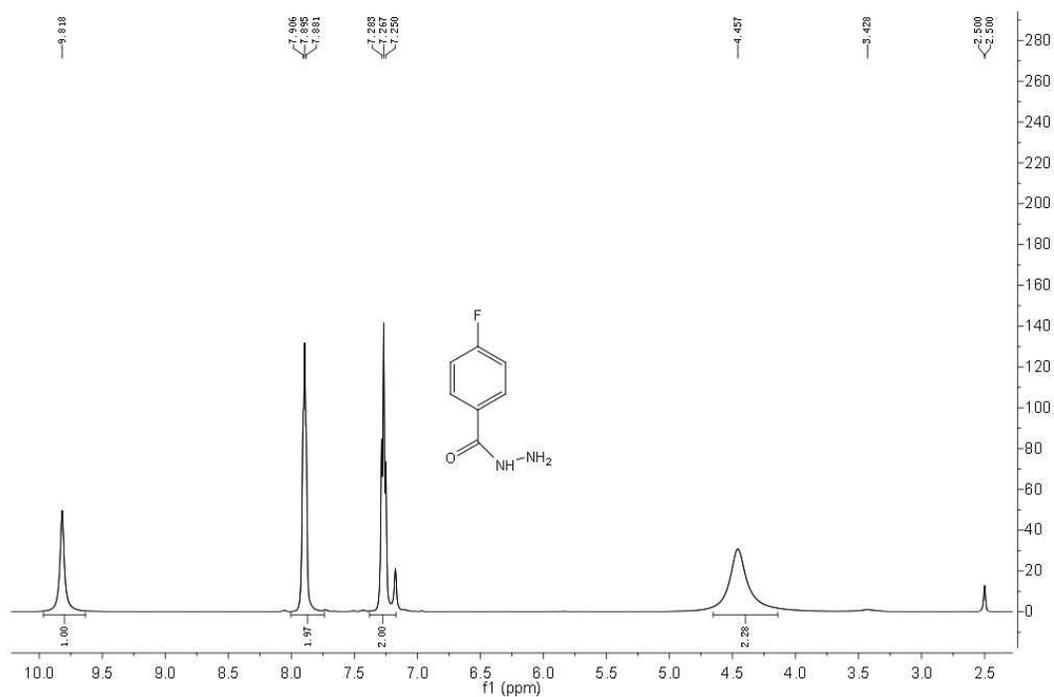
6b-8			>8	6f-8			<8
6b-9			>8	6f-9			>8
6c-1			>8	6g-1			>8
6c-2			<8	6g-2			>8
6c-3			>8	6g-3			>8
6c-4			<8	6g-4			>8
6c-5			>8	6g-5			>8
6c-6			>8	6g-6			>8
6c-7			<8	6g-7			>8
6c-8			<8	6g-8			>8
6c-9			>8	6g-9			>8
6d-1			>8	6h-1			<8
6d-2			<8	6h-2			>8
6d-3			<8	6h-3			>8
6d-4			<8	6h-4			>8
6d-5			<8	6h-5			>8
6d-6			<8	6h-6			<8
6d-7			>8	6h-7			>8
6d-8			<8	6h-8			>8
6d-9			<8	6h-9			>8

Mecury 400 1HNMR ATD131118.3 in DMSO



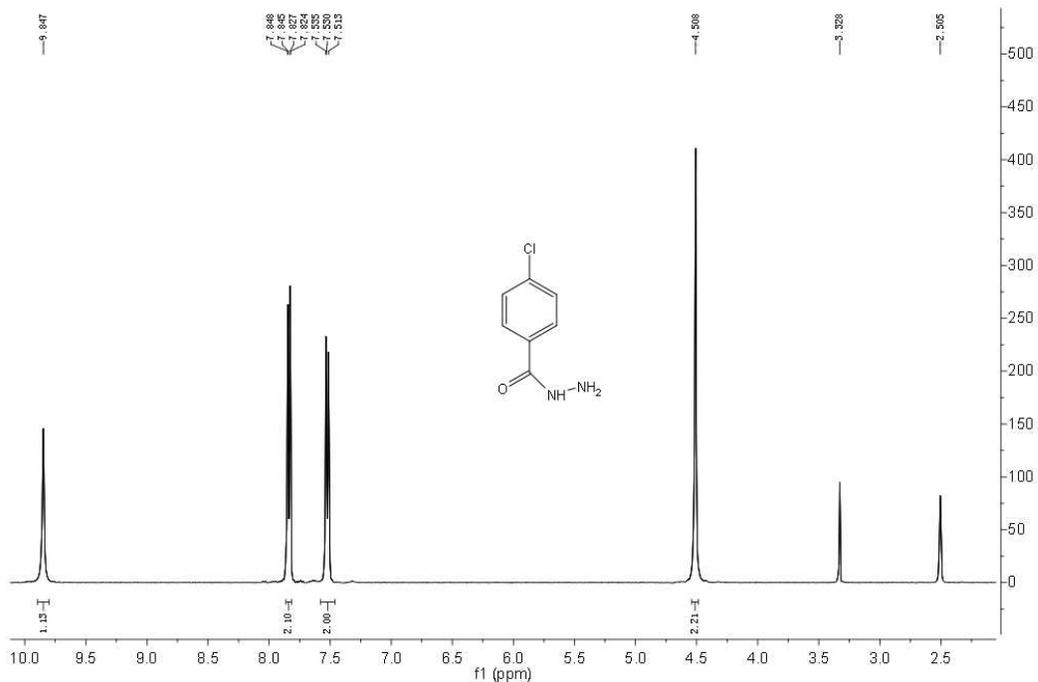
¹H NMR spectra of compound benzohydrazide (3a)

BRUKER AV-III-500 ¹H-NMR ATD-130928 IN DMSO



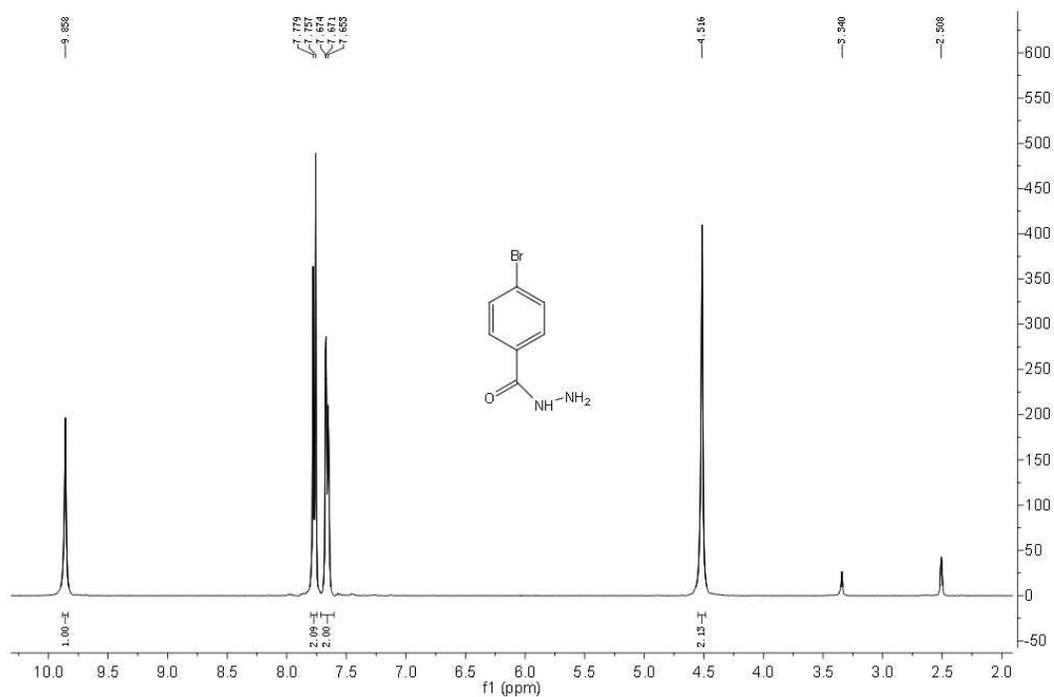
¹H NMR spectra of compound 4-fluorobenzohydrazide (3b)

Mecury 400 1H NMR ATD-131118-1 in DMSO



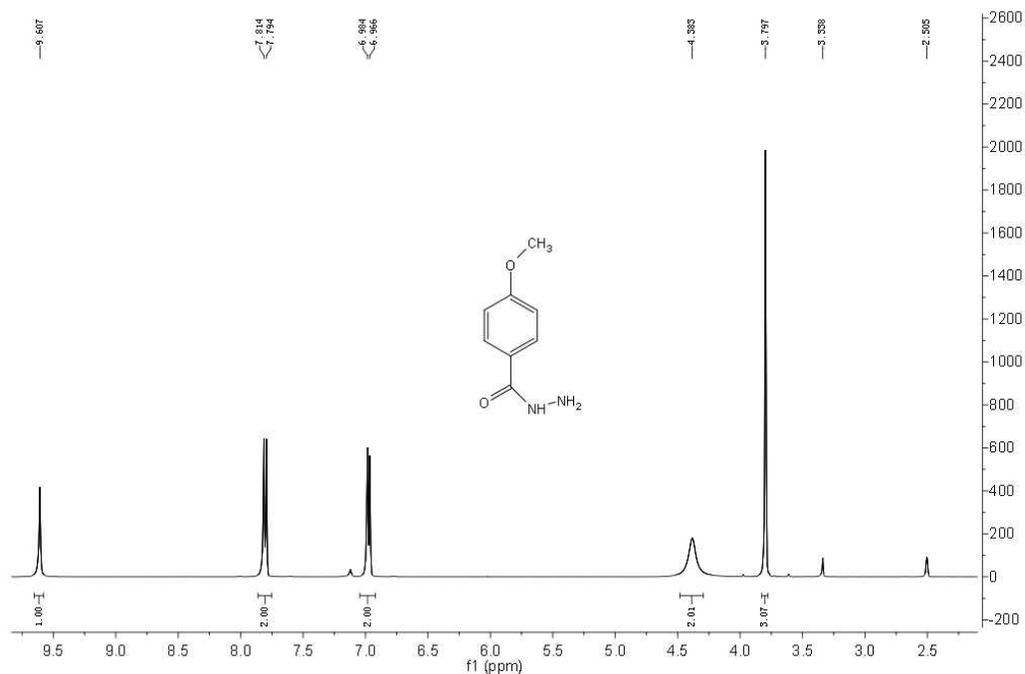
¹H NMR spectra of compound 4-chlorobenzohydrazide (3c)

MERCURY-400 H1NMR ATD-131127-1 IN DMSO



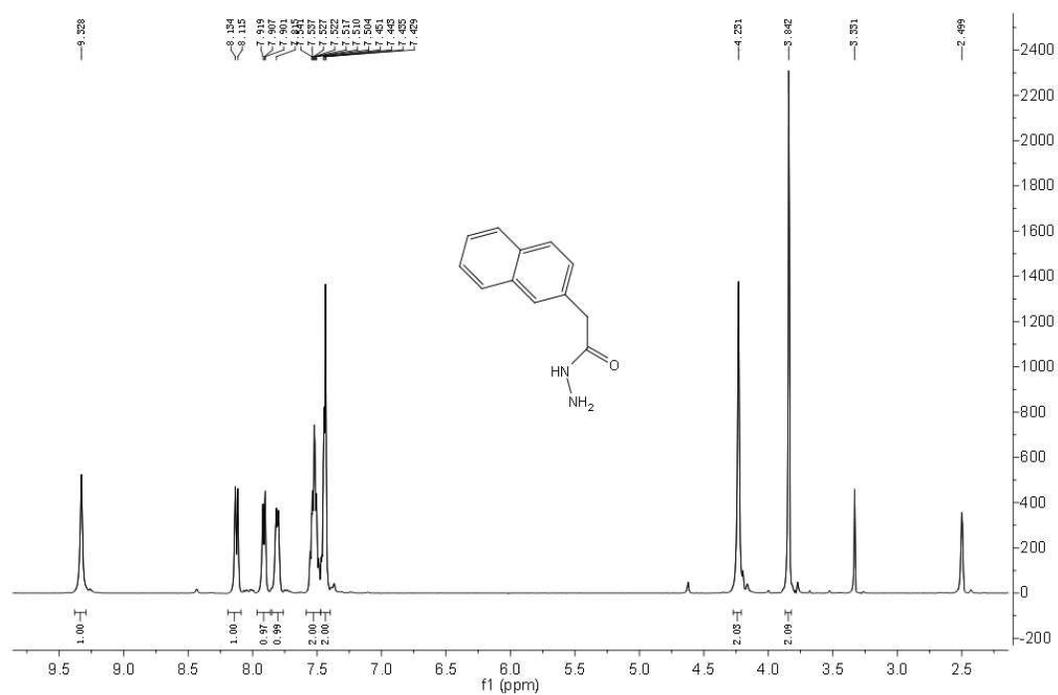
¹H NMR spectra of compound 4-bromobenzohydrazide (3d)

Mecury 400 1HNMR ATD-131118-2 IN DMSO



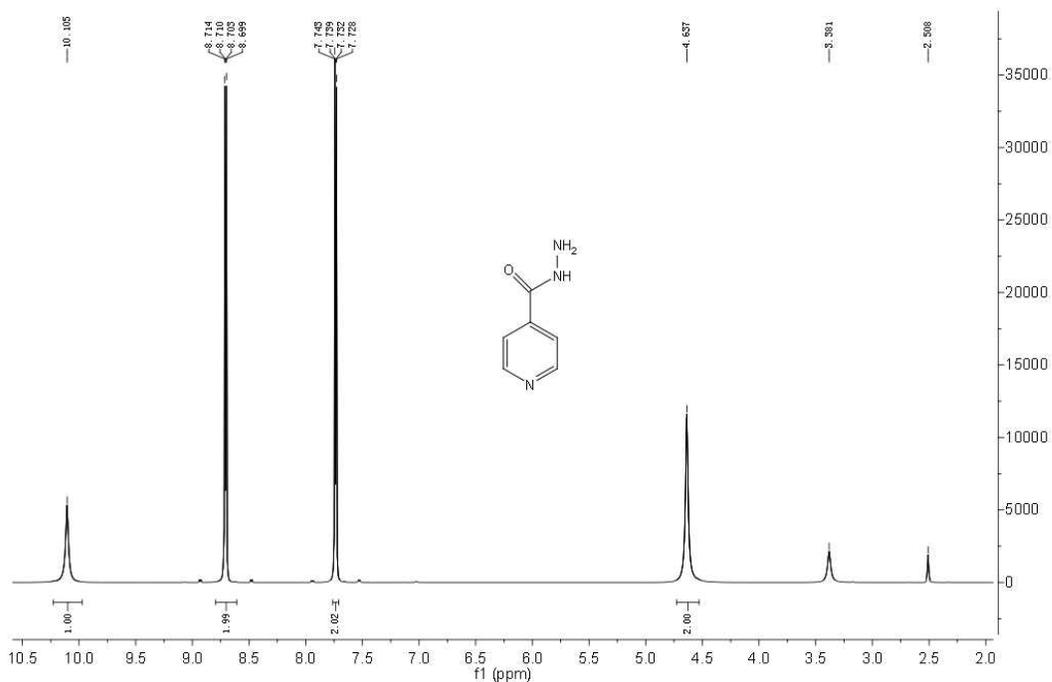
¹H NMR spectra of compound 4-methoxybenzohydrazide (3e)

Mecury 400 1HNMR ATD131127-3 IN DMSO

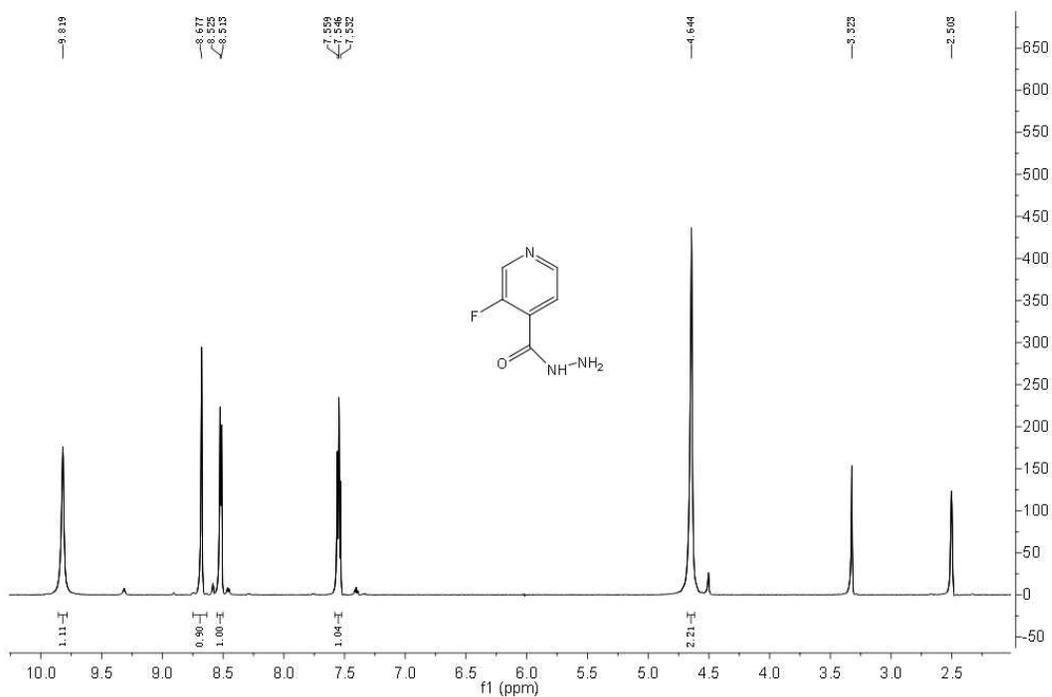


¹H NMR spectra of compound 2-(naphthalen-2-yl)acetohydrazide (3f)

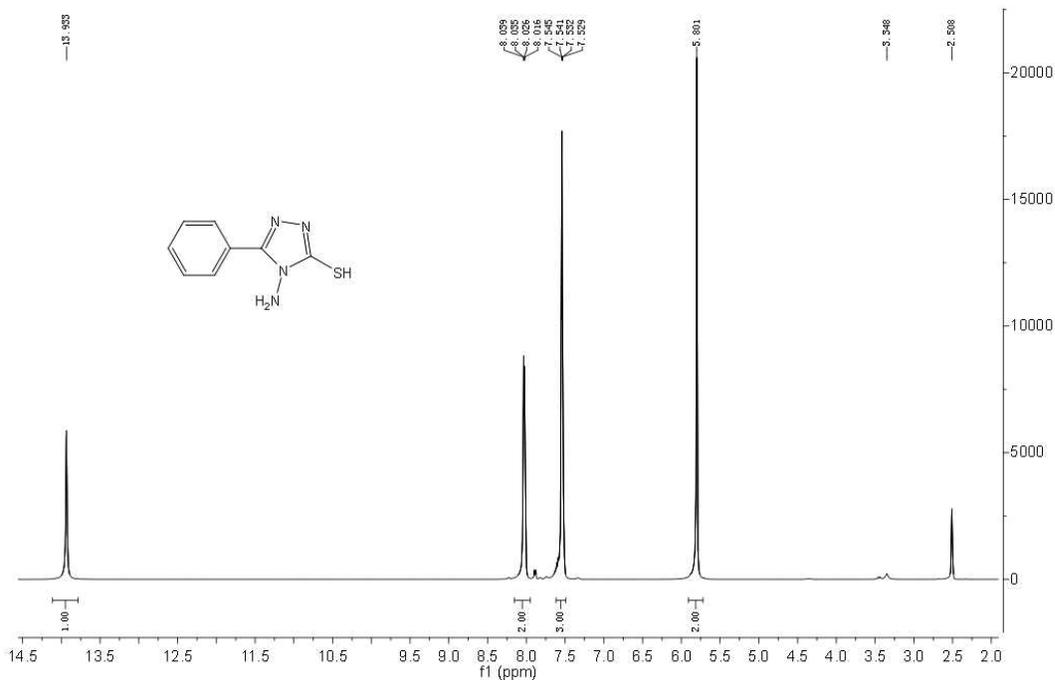
ATD-130926 Bruker AVANCE III 400 PROTON2 DMSO



BRUKER AV-III-400 ¹H-NMR ATD-140304-1 IN DMSO

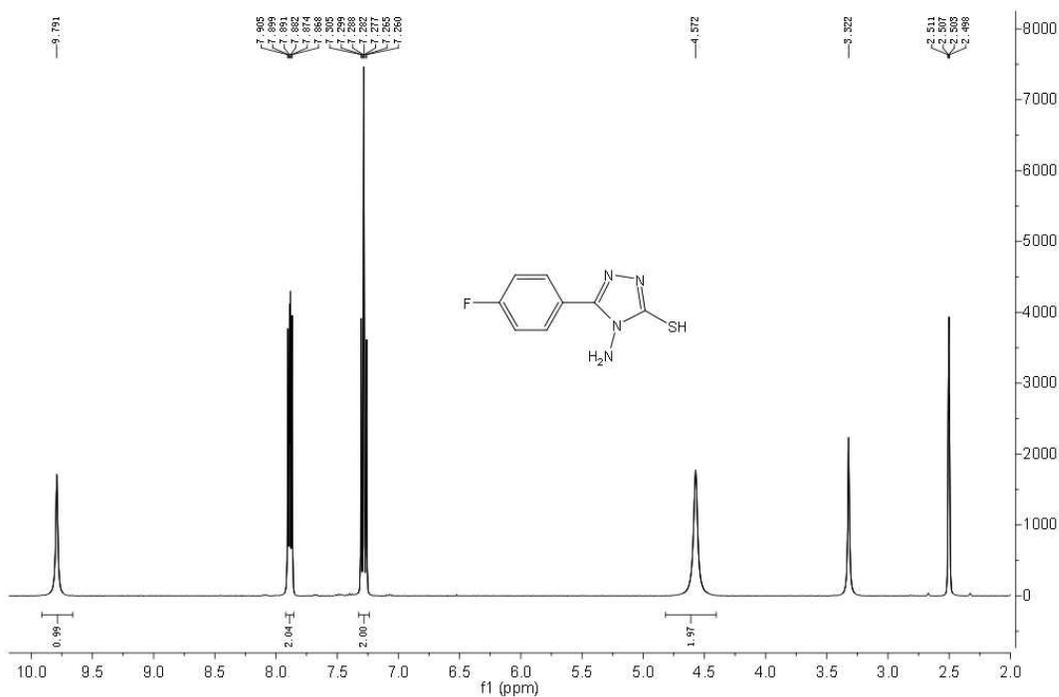


ATD-131125-3 Bruker AVANCE III 400 PROTON2 DMSO



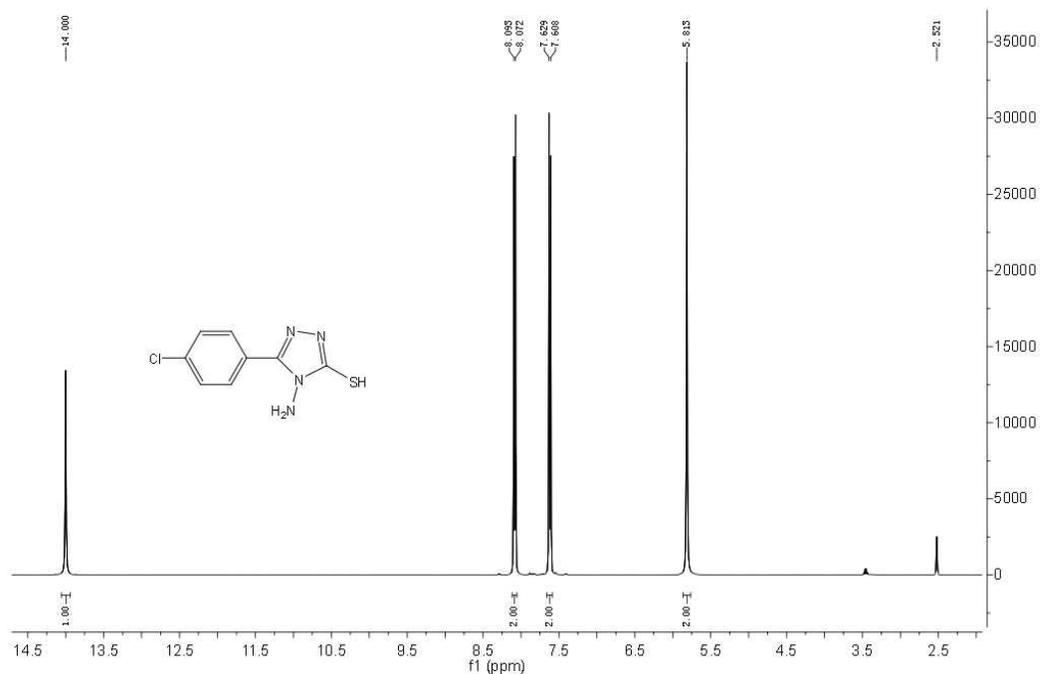
¹H NMR spectra of compound 4-amino-5-phenyl-3-mercapto-1,2,4-triazole (5a)

Bruker AVANCE III 400 20130701,ATD-130626-1 PROTON2 DMSO



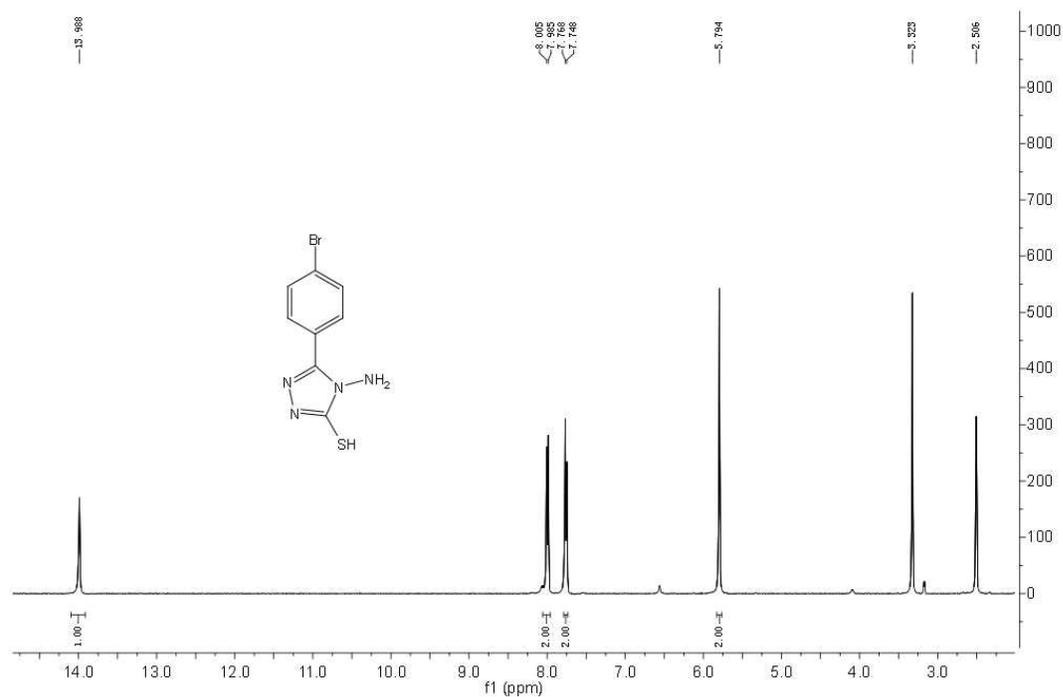
¹H NMR spectra of compound 4-amino-5-(4-fluorophenyl)-3-mercapto-1,2,4-triazole (5b)

ATD-131125-1 Bruker AVANCE III 400 PROTON2 DMSO

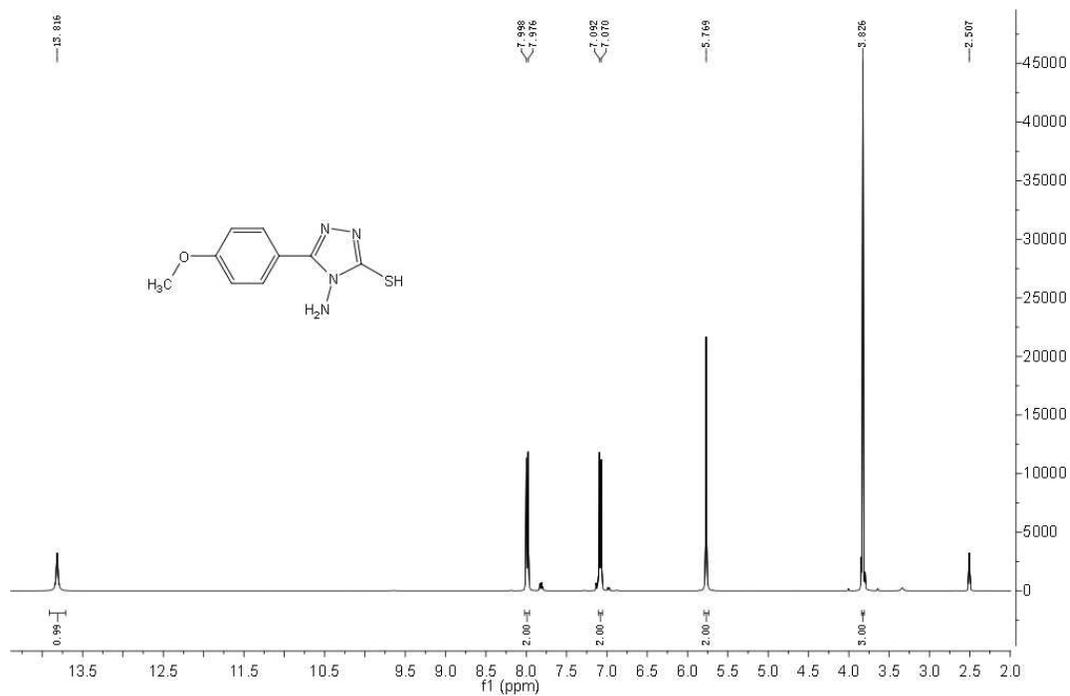


¹H NMR spectra of compound 4-amino-5-(4-chlorophenyl)-3-mercapto-1,2,4-triazole (5c)

ATD-131207-1 400 1HNMR ATD-131207-1 in DMSO

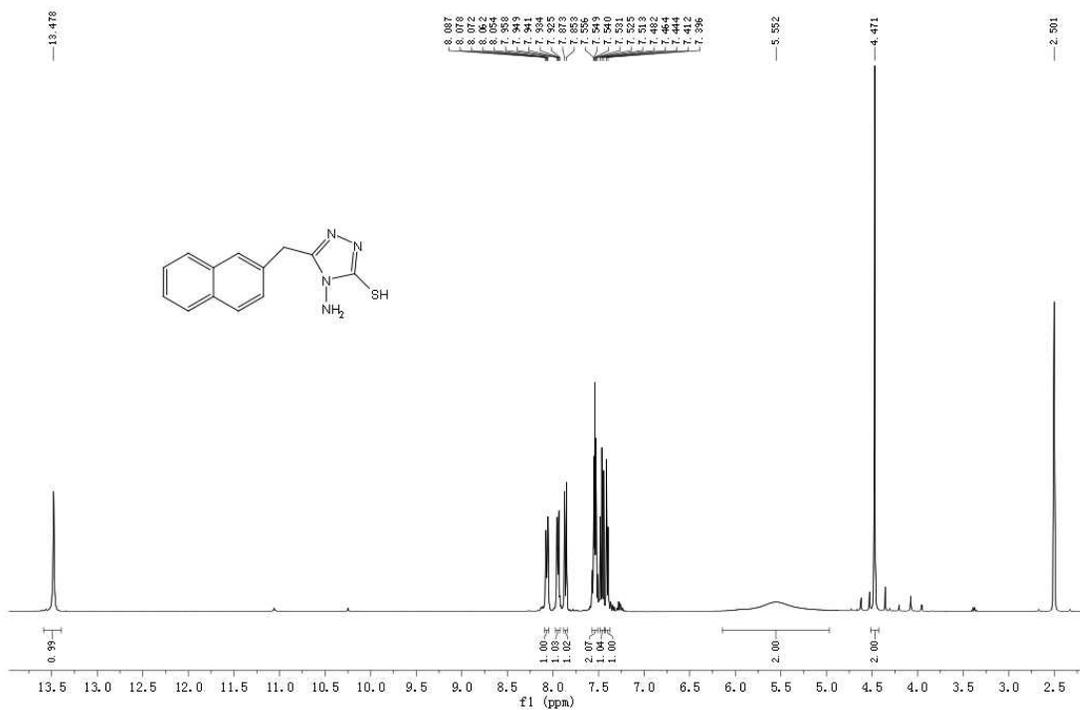


¹H NMR spectra of compound 4-amino-5-(4-bromophenyl)-3-mercapto-1,2,4-triazole (5d)



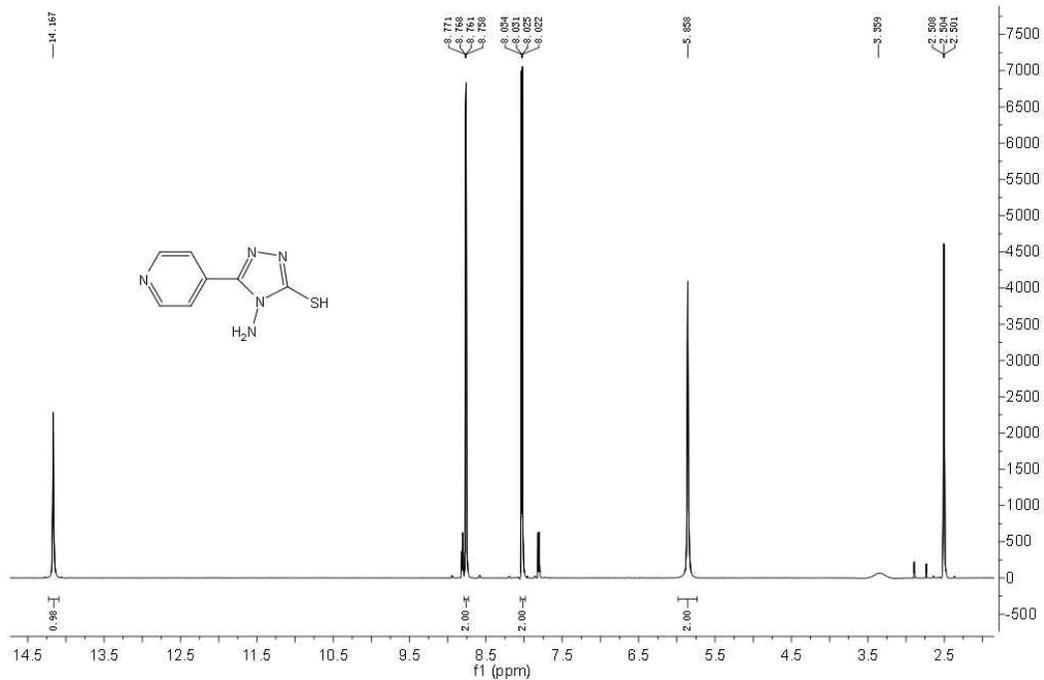
¹H NMR spectra of compound 4-amino-5-(4-methoxyphenyl)-3-mercapto-1,2,4-triazole (5e)

ATD-131207-3 Bruker AVANCE III 400 PROTON2 DMSO



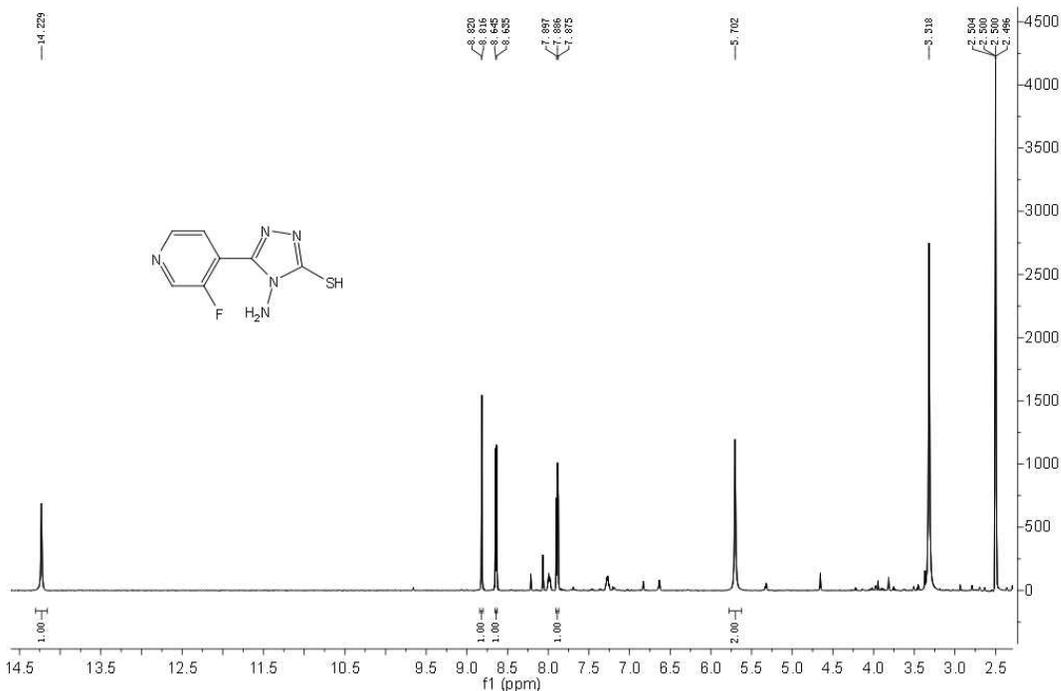
¹H NMR spectra of compound 4-amino-5-(naphthalen-2-ylmethyl)-3-mercapto-1,2,4-triazole (5f)

BRUKER AV-III-500 1H-NMR ATD-131001 IN DMSO PROTON DMSO



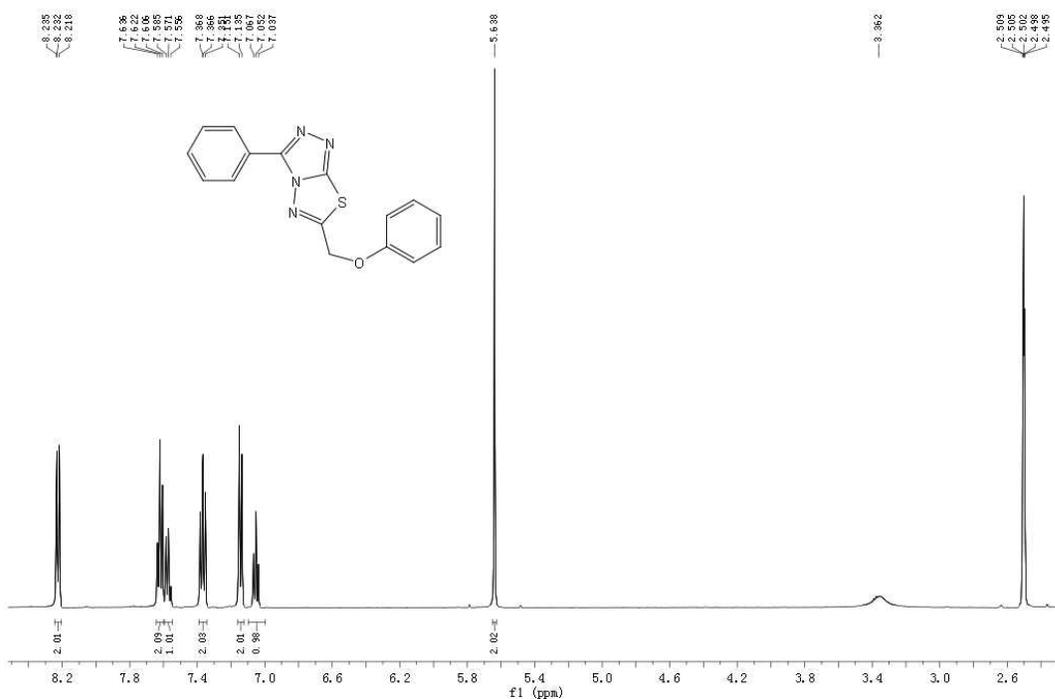
¹H NMR spectra of compound 4-amino-5-(pyridin-4-yl)-3-mercapto-1,2,4-triazole (5g)

ATD-140309-1 BRUKER AV-III-500 1H-NMR IN DMSO



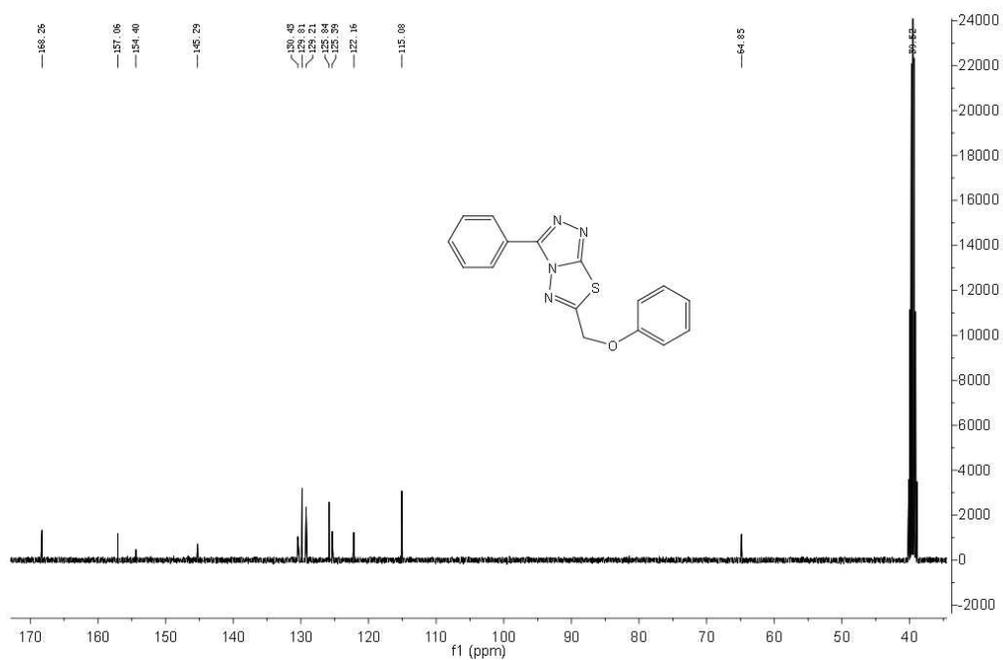
¹H NMR spectra of compound 4-amino-5-(3-fluoropyridin-4-yl)-3-mercapto-1,2,4-triazole (5h)

BRUKER AV-III-500 1H-NMR ATD-131213-3 IN DMSO



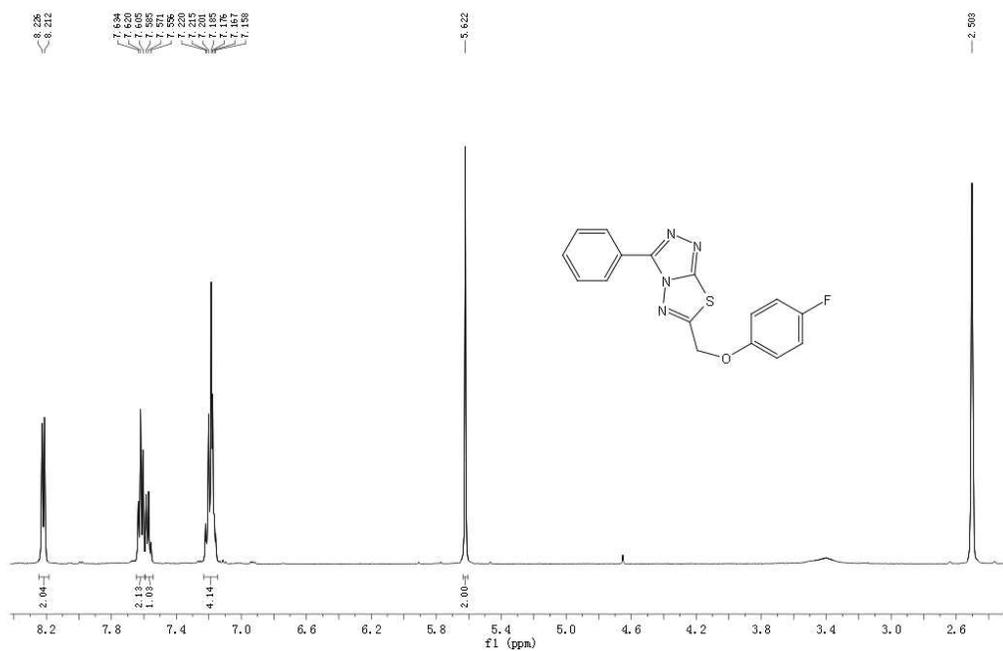
¹H NMR spectra of compound 6-(phoxymethyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-1)

BRUKER AV-III-400 ¹³C-NMR ATD-131213-3 IN DMSO



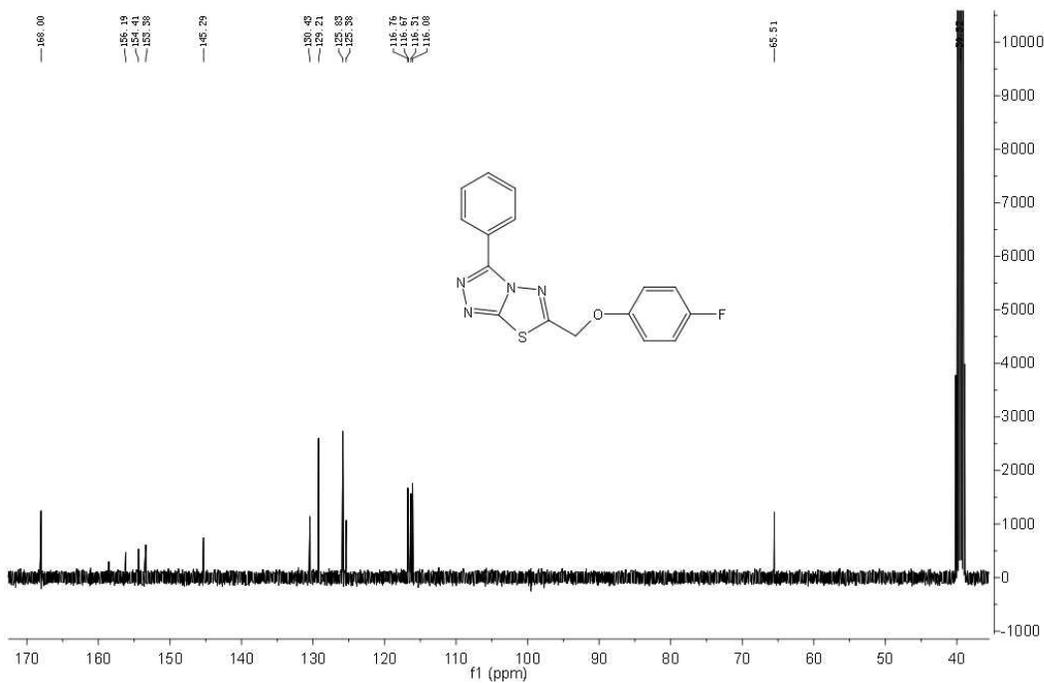
¹³C NMR spectra of compound 6-(phoxymethyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-1)

BRUKER AV-III-500 1H-NMR ATD-131223-1 IN DMSO PROTON DMSO



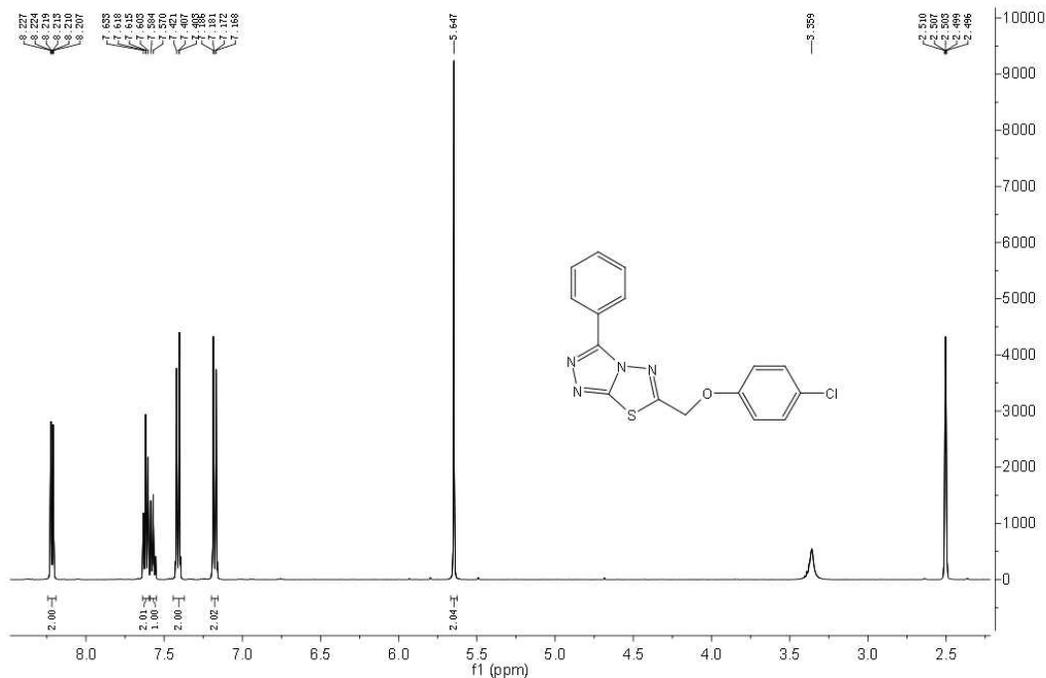
¹H NMR spectra of compound 6-((4-fluorophenoxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-2)

BRUKER AV-III-400 ¹³C-NMR ATD-131223-1 IN DMSO



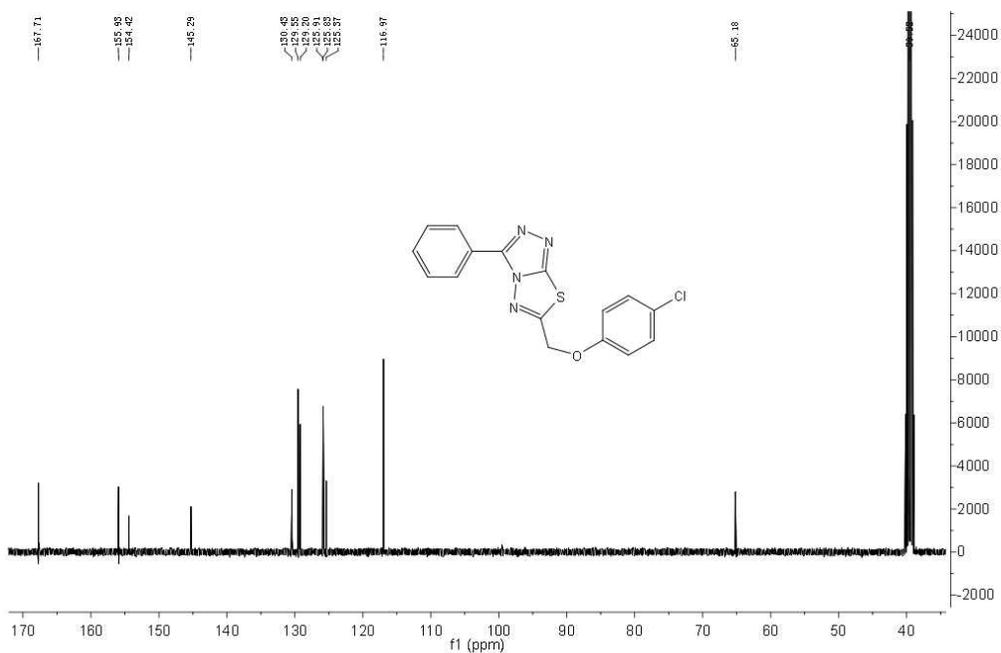
¹³C NMR spectra of compound 6-((4-fluorophenoxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-2)

BRUKER AV-III-500 1H-NMR ATD-131214-3 IN DMSO



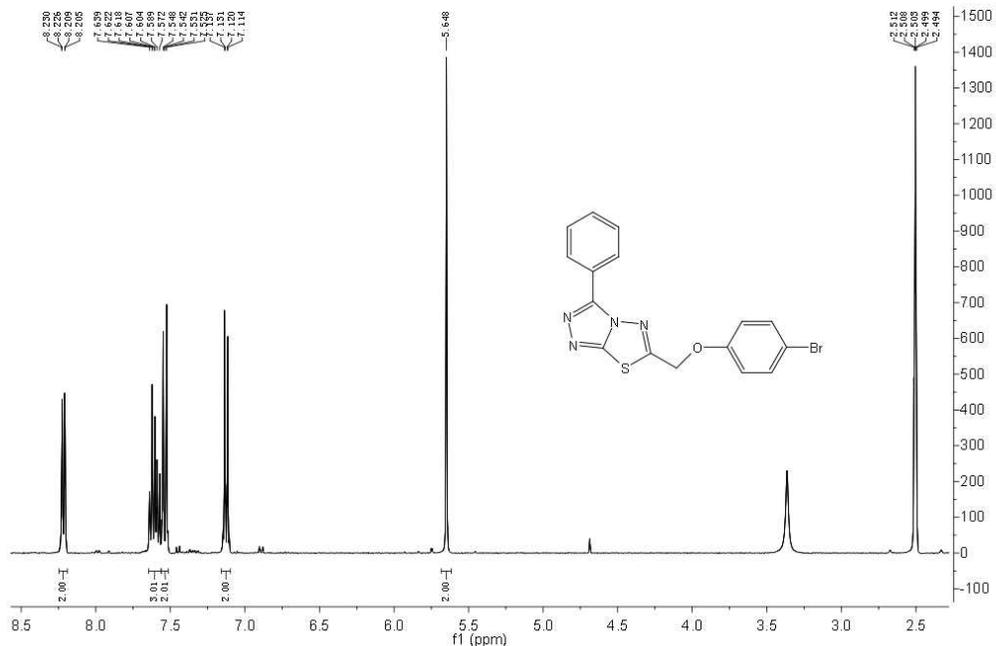
¹H NMR spectra of compound 6-((4-chlorophenoxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-3)

BRUKER AV-III-400 ¹³C-NMR ATD-131214-3 IN DMSO



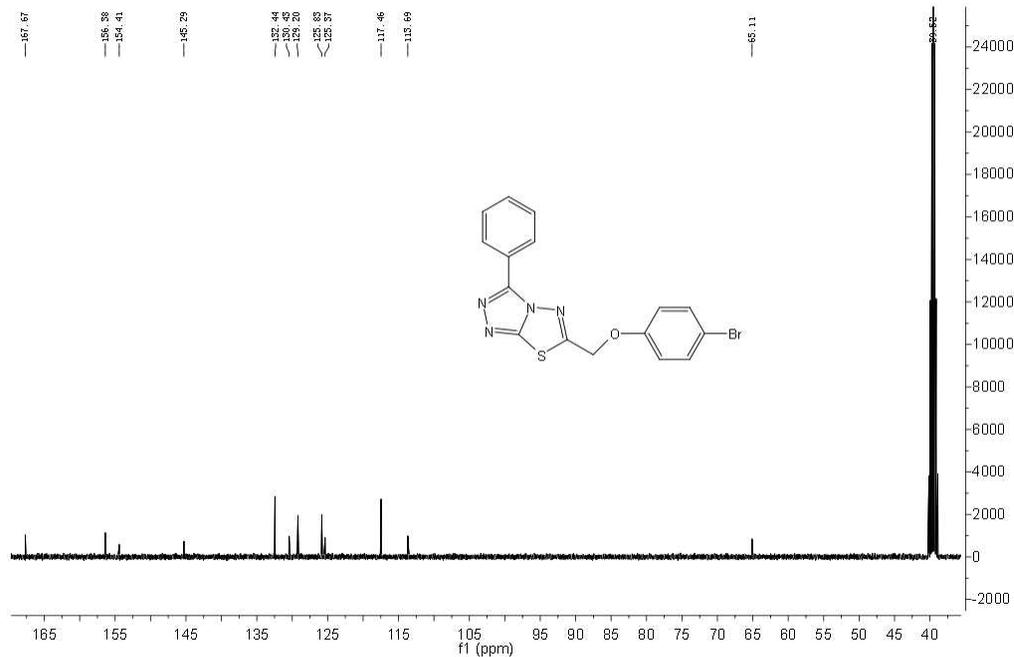
¹³C NMR spectra of compound 6-((4-chlorophenoxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-3)

BRUKER AV-III-400 1H-NMR ATD-131221-2 IN DMSO



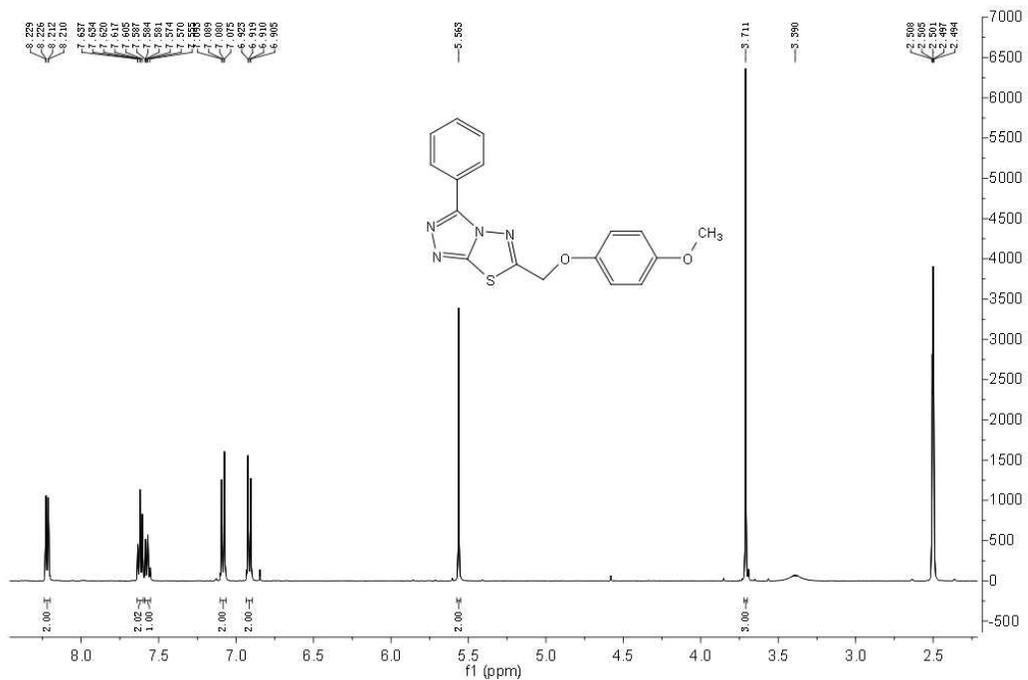
¹H NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]Thiadiazole (6a-4)

BRUKER AV-III-400 ¹³C-NMR ATD-131221-2 IN DMSO



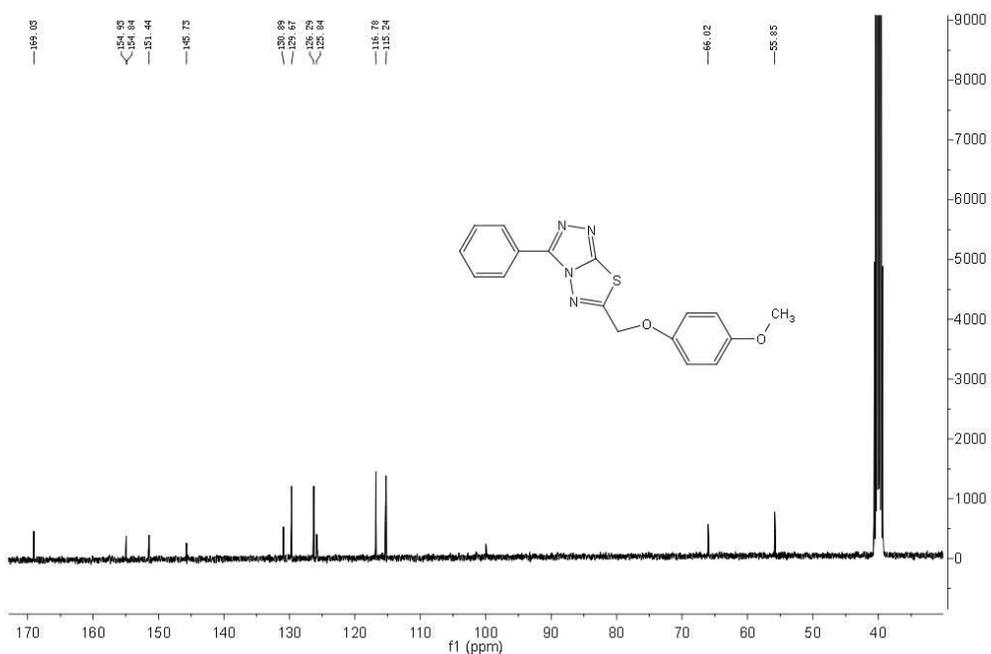
¹³C NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]Thiadiazole (6a-4)

BRUKER AV-III-500 1H-NMR ATD-131231-1 IN DMSO



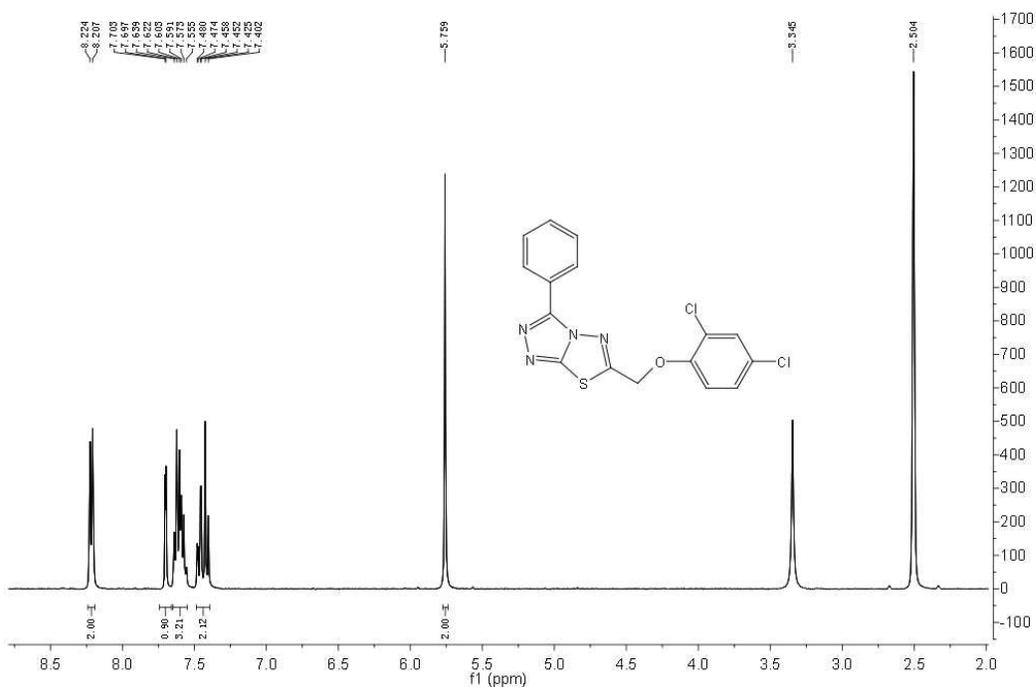
¹H NMR spectra of compound 6-((4-methoxyphenoxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-5)

BRUKER AV-III-400 ¹³C-NMR ATD-131231-1 IN DMSO



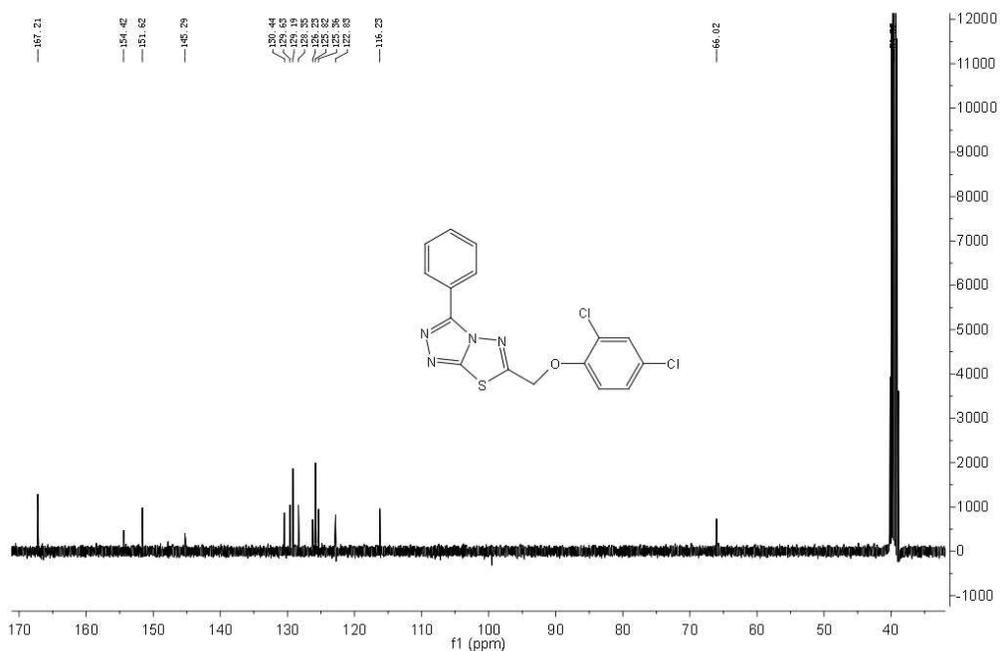
¹³C NMR spectra of compound 6-((4-methoxyphenoxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-5)

BRUKER AV-III-400 1H-NMR ATD-131221-1 IN DMSO



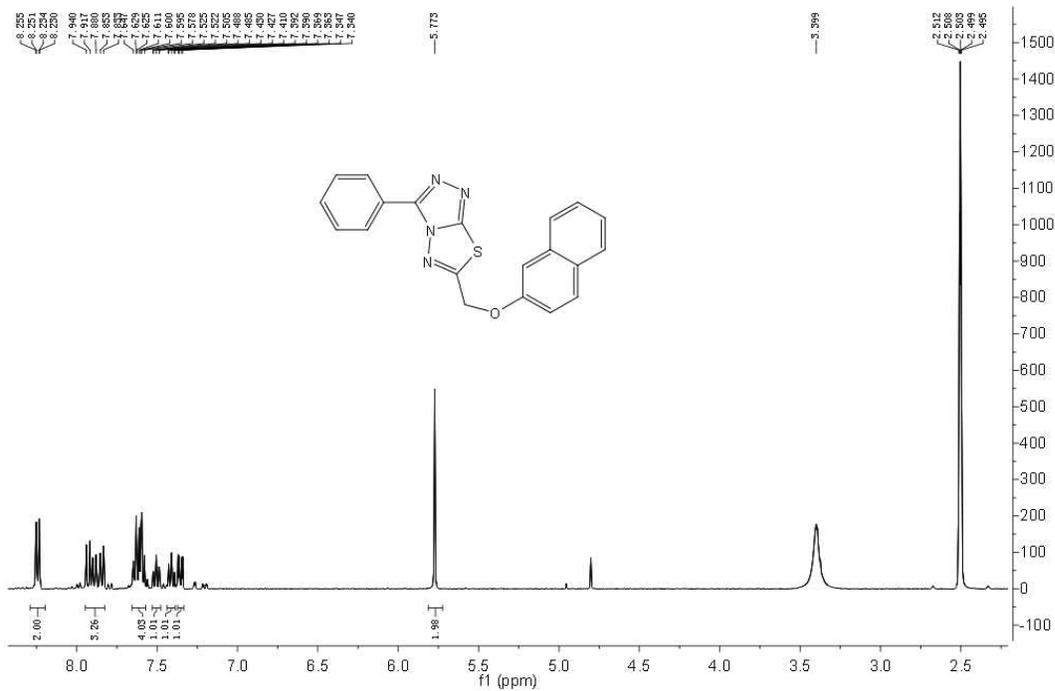
¹H NMR spectra of compound 6-((2,4-dichlorophenoxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-6)

BRUKER AV-III-400 ¹³C-NMR ATD-131221-1 IN DMSO



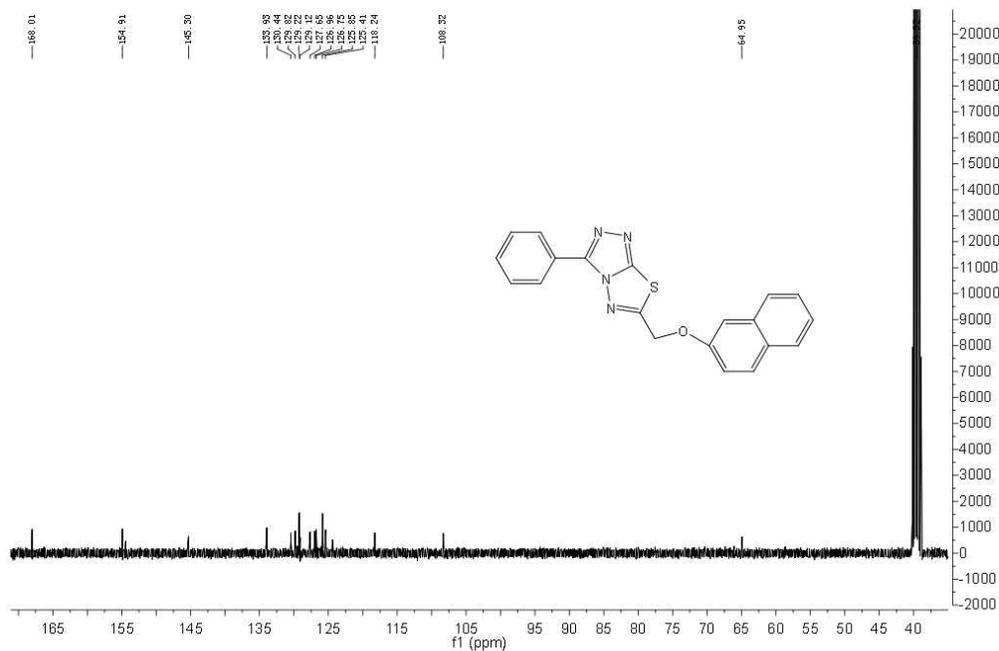
¹³C NMR spectra of compound 6-((2,4-dichlorophenoxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-6)

BRUKER AV-II-400 1H-NMR ATD-131223-2 IN DMSO



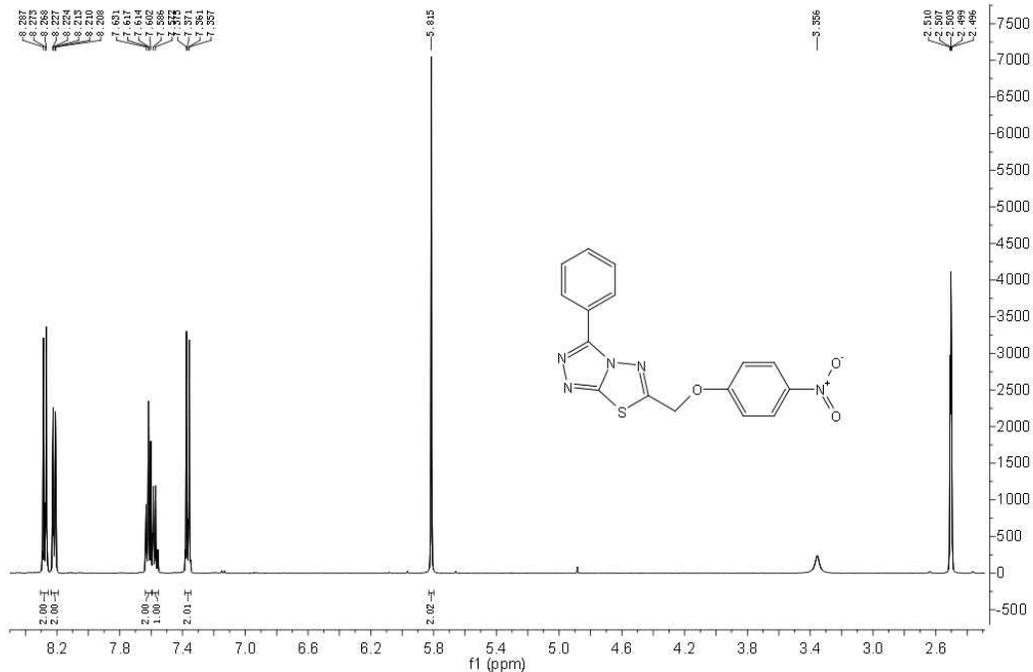
¹H NMR spectra of compound 6-((2-naphthyloxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-7)

BRUKER AV-III-400 ¹³C-NMR ATD-131223-2 IN DMSO



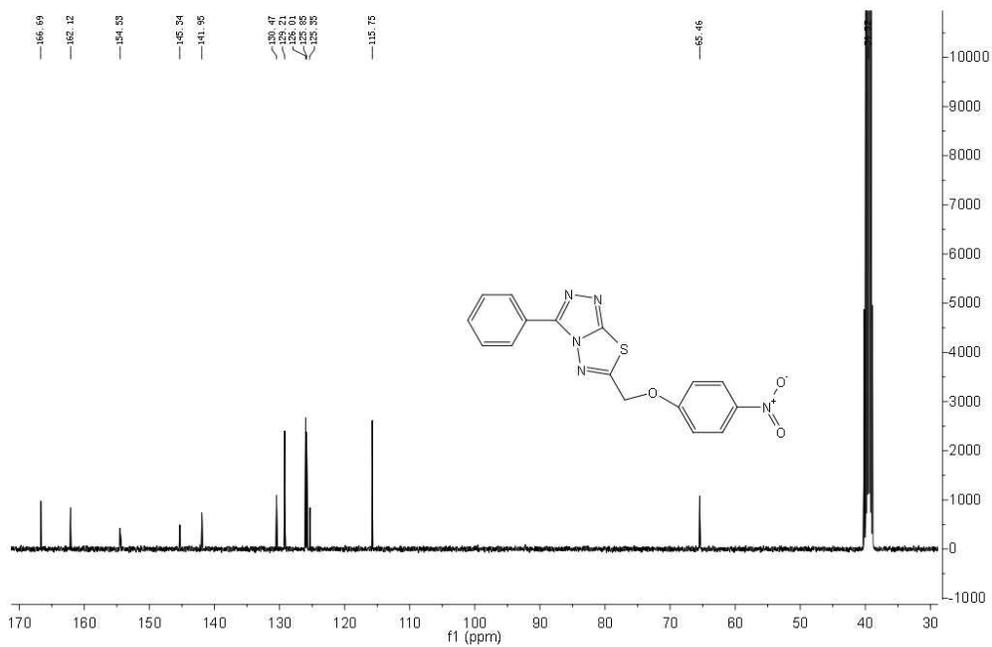
¹³C NMR spectra of compound 6-((2-naphthyloxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-7)

BRUKER AV-III-500 1H-NMR ATD-131231-3 IN DMSO



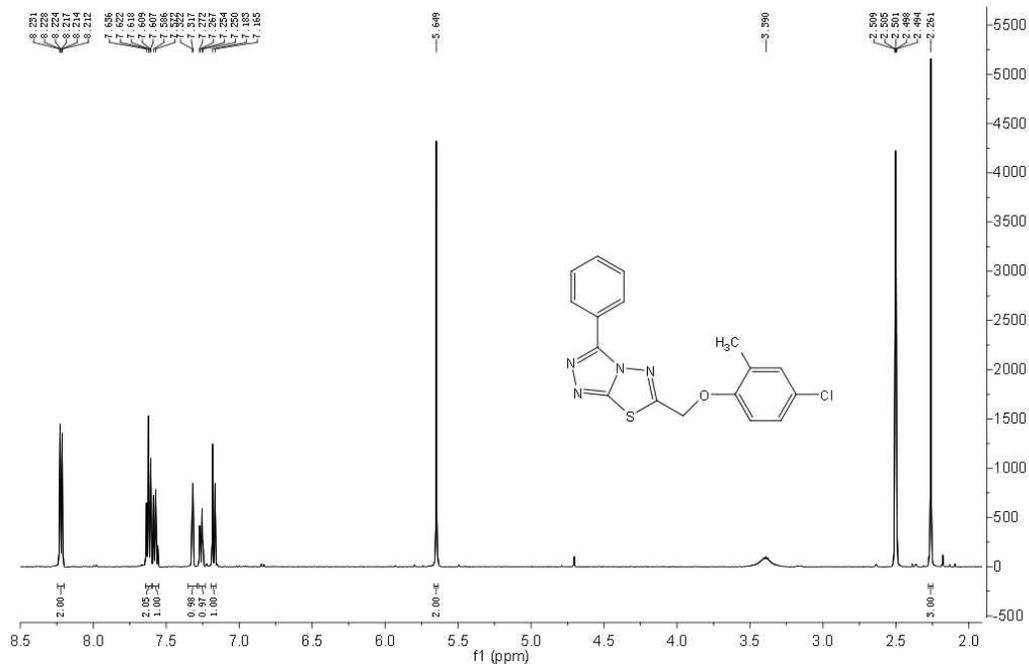
¹H NMR spectra of compound 6-((4-nitrophenoxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-8)

BRUKER AV-III-400 ¹³C-NMR ATD-131231-3 IN DMSO



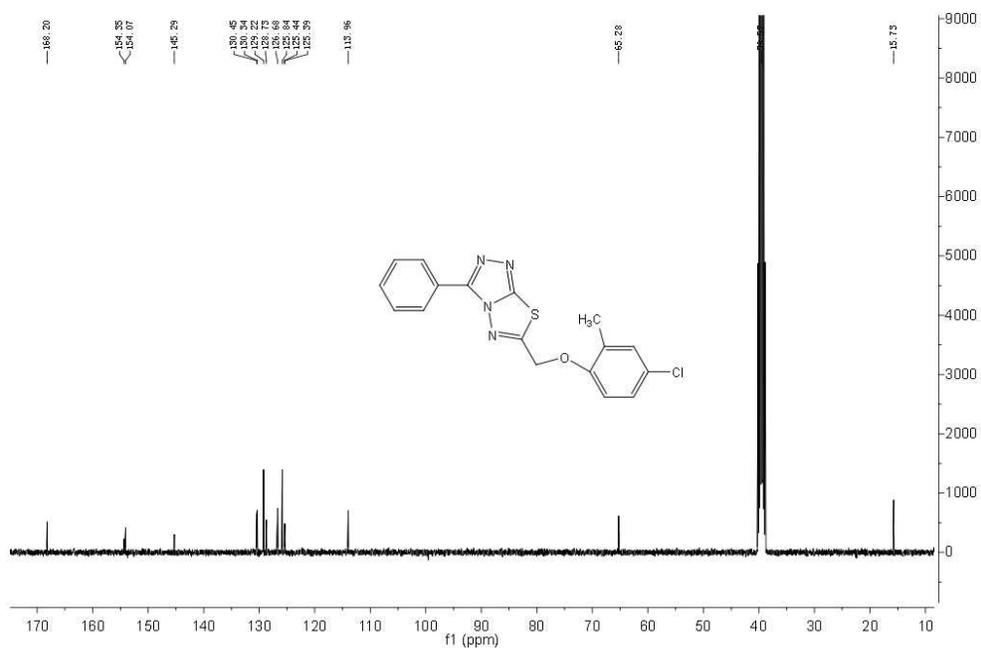
¹³C NMR spectra of compound 6-((4-nitrophenoxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-8)

BRUKER AV-III-500 1H-NMR ATD-131231-2 IN DMSO



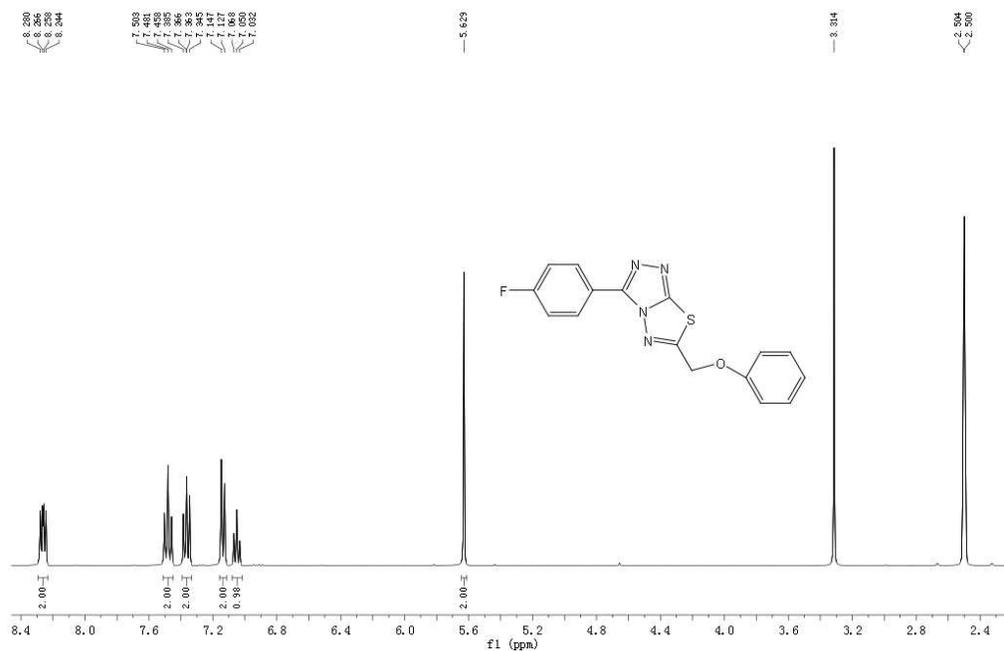
¹H NMR spectra of compound 6-((2-methyl-4-chlorophenoxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-9)

BRUKER AV-III-400 ¹³C-NMR ATD-131231-2 IN DMSO



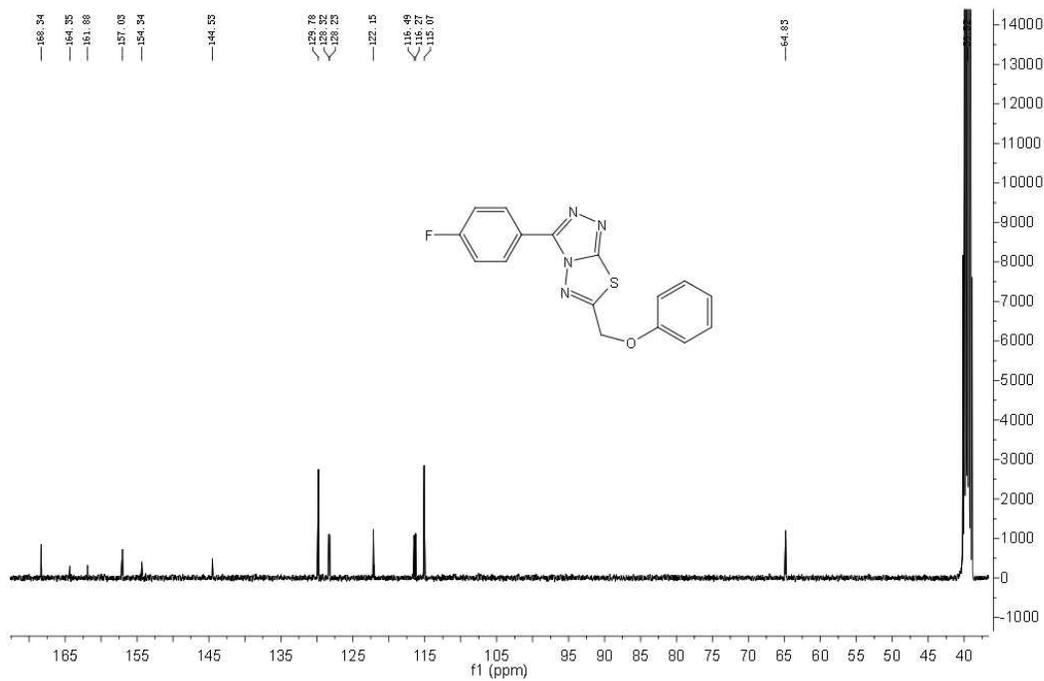
¹³C NMR spectra of compound 6-((2-methyl-4-chlorophenoxy)methyl)-3-phenyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6a-9)

ATD-130726 Bruker AVANCEIII 400 20140426PROTON2 DMSO



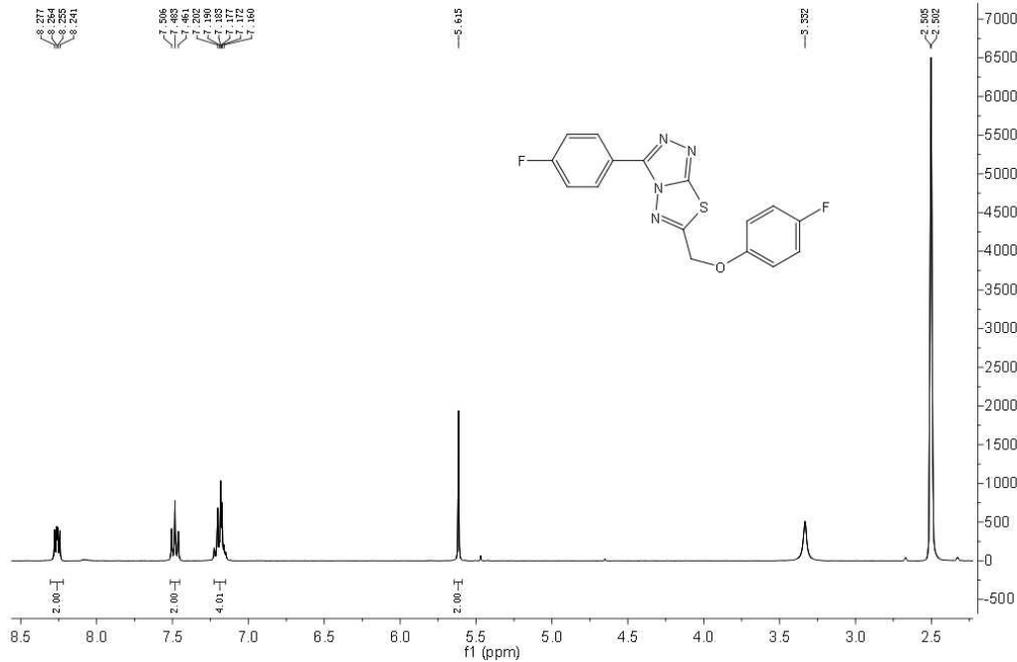
¹H NMR spectra of compound 3-(4-fluorophenyl)-6-(phenoxymethyl)-1,2,4-triazolo[3,4-b][1,3,4]thiadiazole (6b-1)

BRUKER AV-III-400 ¹³C-NMR ATD-130726 IN DMSO



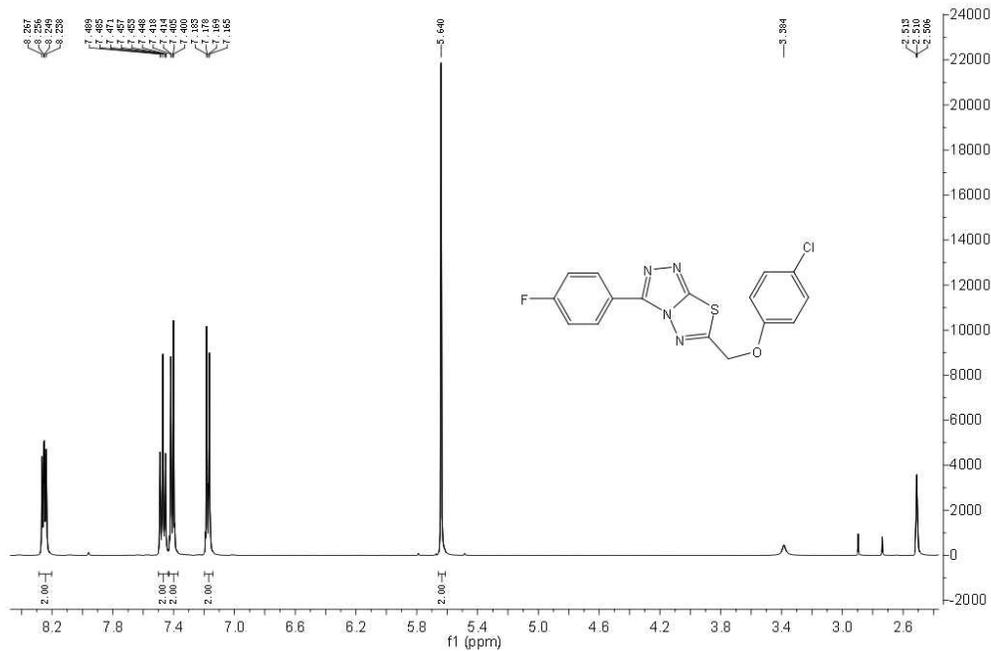
¹³C NMR spectra of compound 3-(4-fluorophenyl)-6-(phenoxymethyl)-1,2,4-triazolo[3,4-b][1,3,4]thiadiazole (6b-1)

ATD-140109-2 Bruker AVANCEIII 400 PROTON2 DMSO



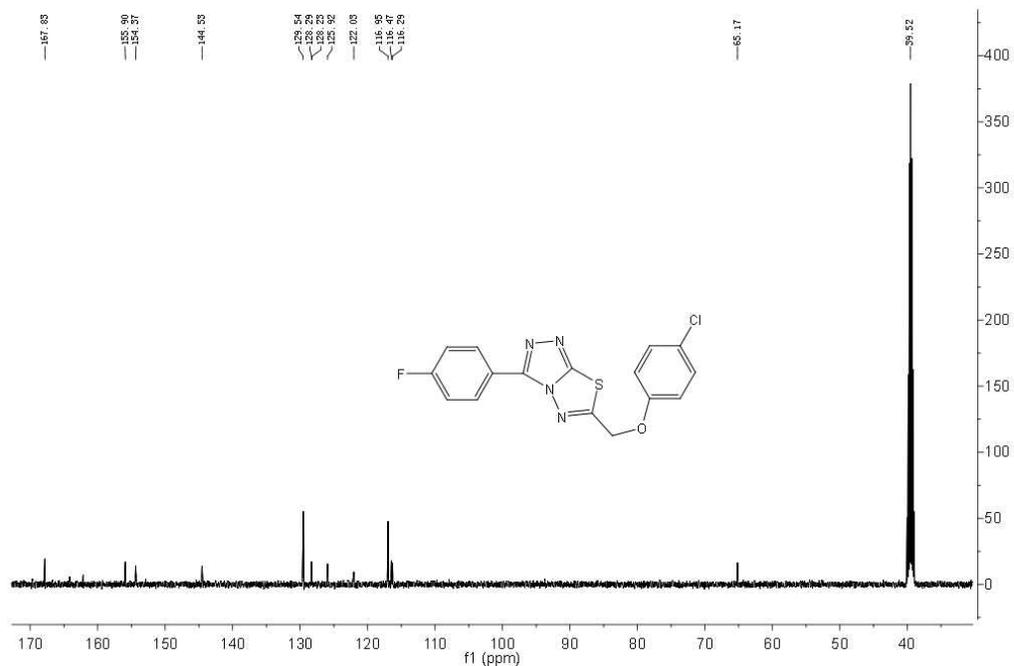
¹H NMR spectra of compound 6-((4-fluorophenoxy)methyl)-3-(4-fluorophenyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6b-2)

BROKER AV-III-500 1H-NMR SWF-131012 IN DMSO



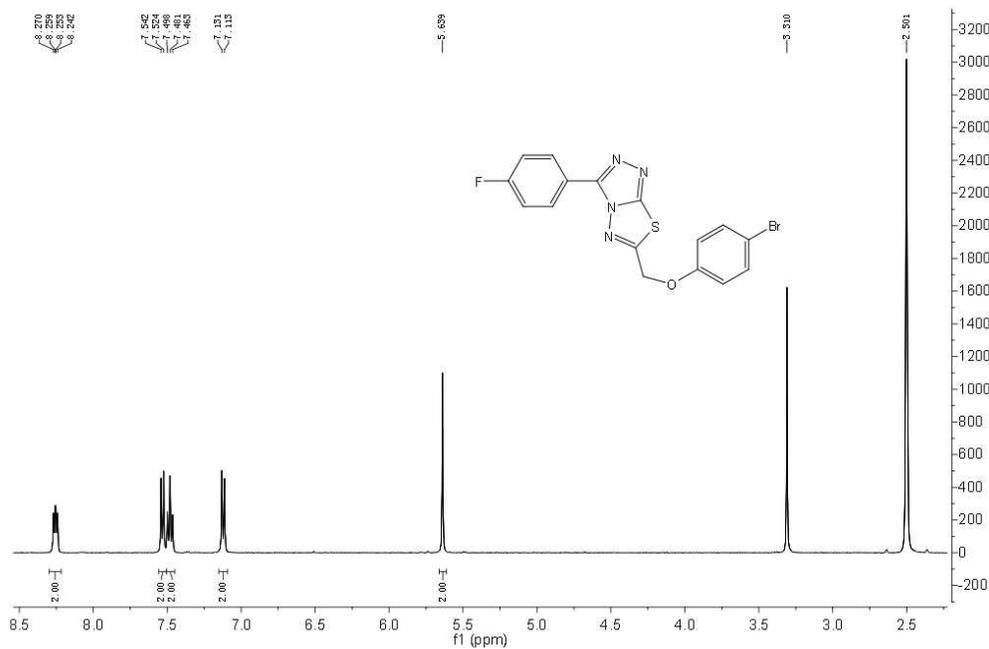
¹H NMR spectra of compound 6-((4-chlorophenoxy)methyl)-3-(4-fluorophenyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6b-3)

BRUKER AV-III-500 ¹³C-NMR ATD-131012 IN DMSO



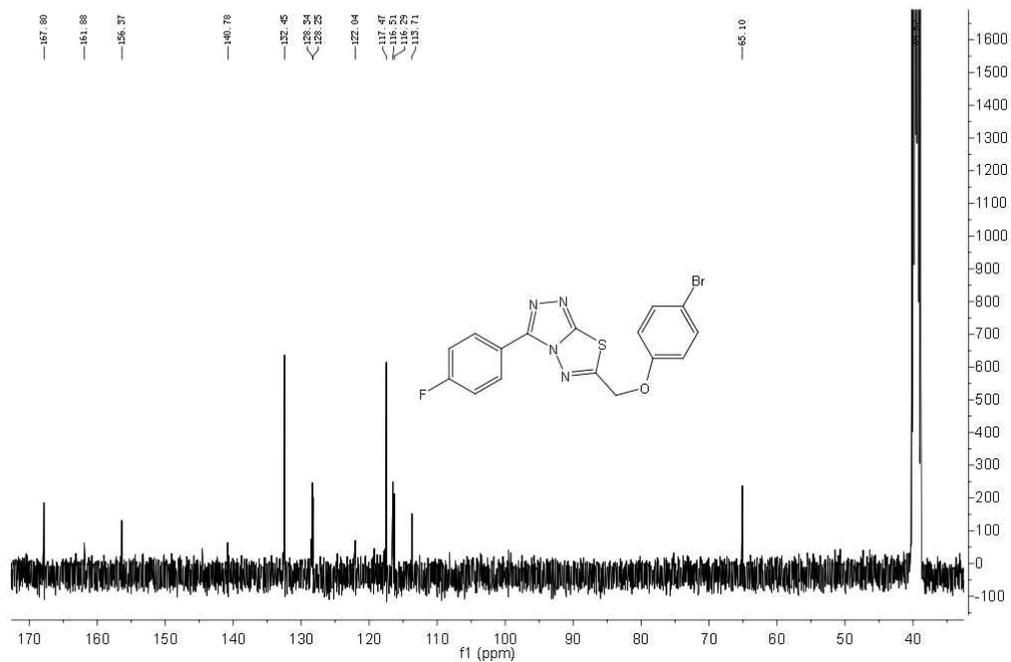
¹³C NMR spectra of compound 6-((4-chlorophenoxy)methyl)-3-(4-fluorophenyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6b-3)

BRUKER AV-III-500 ¹H-NMR ATD-140109-1 IN DMSO



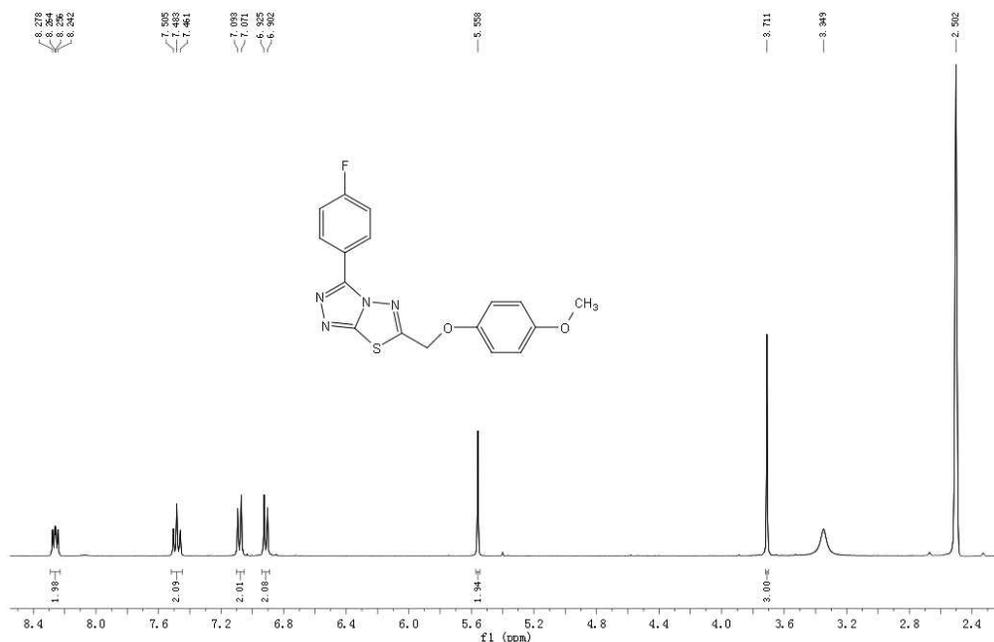
¹H NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-(4-fluorophenyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6b-4)

BRUKER AV-III-400 ¹³C-NMR ATD-140109-1 IN DMSO



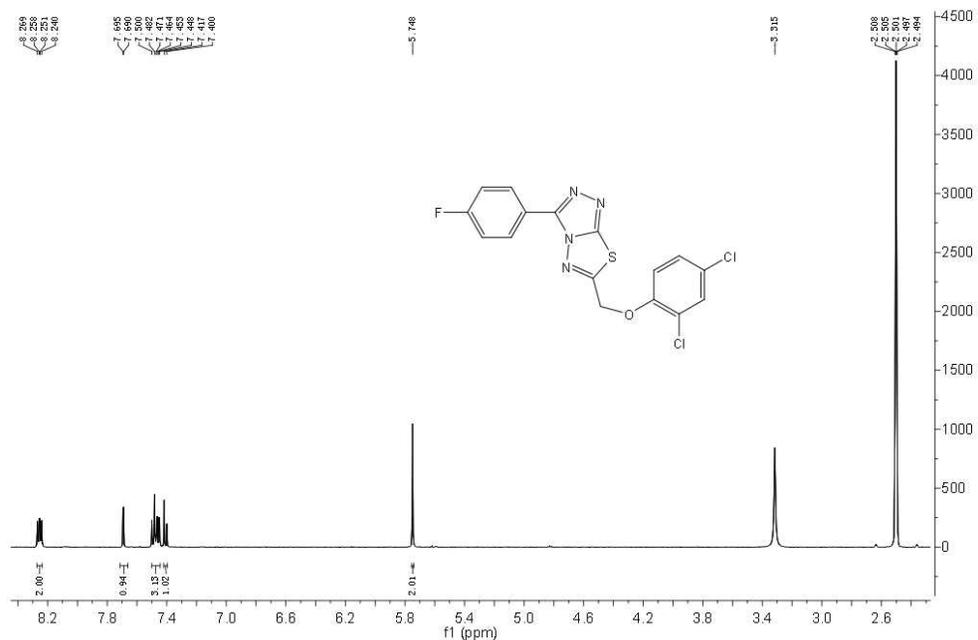
¹³C NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-(4-fluorophenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6b-4)

ATD-140110-2 Bruker AVANCEIII 400 PROTON2 DMSO



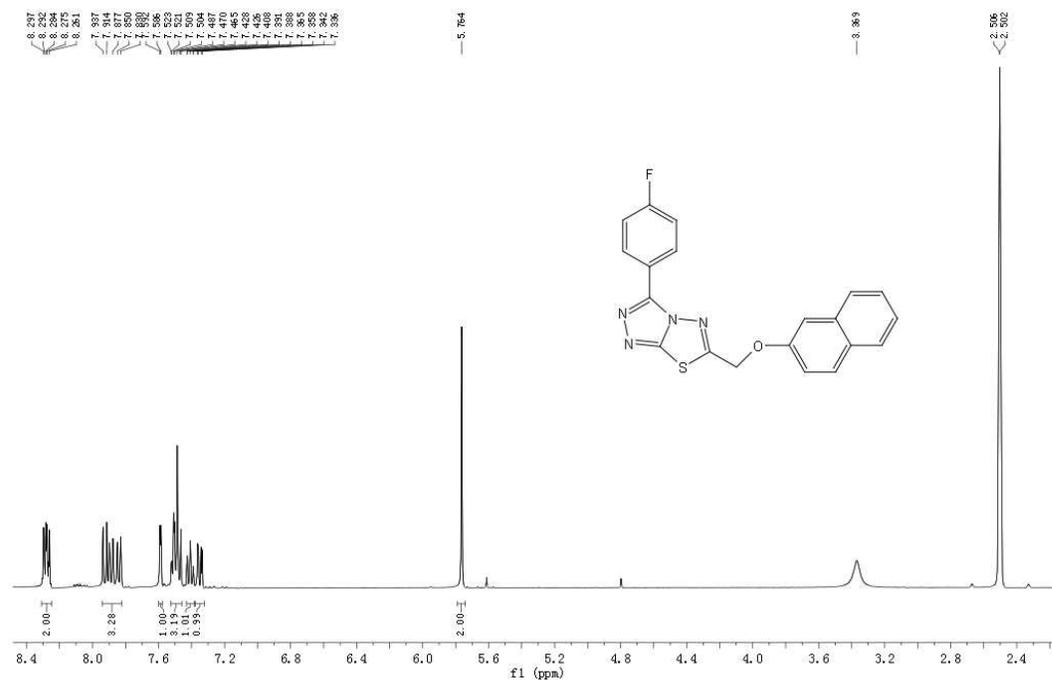
¹H NMR spectra of compound 3-(4-fluorophenyl)-6-((4-methoxyphenoxy)methyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6b-5)

BRUKER AV-III-500 1H-NMR ATD-140108-2 IN DMSO



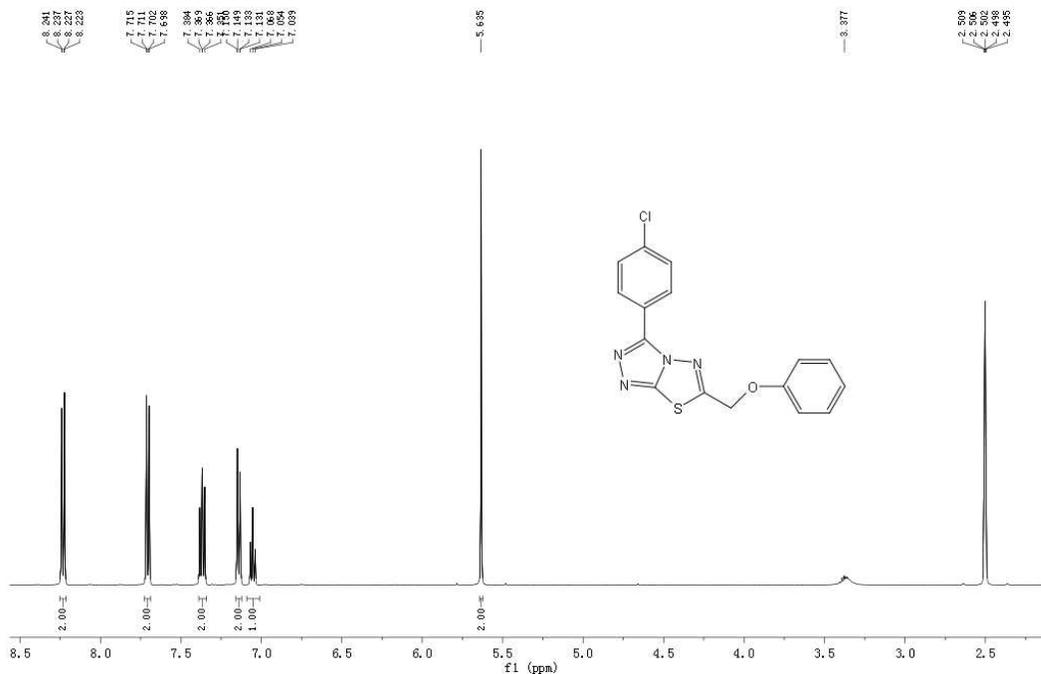
¹H NMR spectra of compound 6-((2,4-dichlorophenoxy)methyl)-3-(4-fluorophenyl)-[1,2,4]thiazolo [3,4-b][1,3,4]thiadiazole (6b-6)

MATD-140110-1 Bruker AVANCEIII 400 PROTON2 DMSO



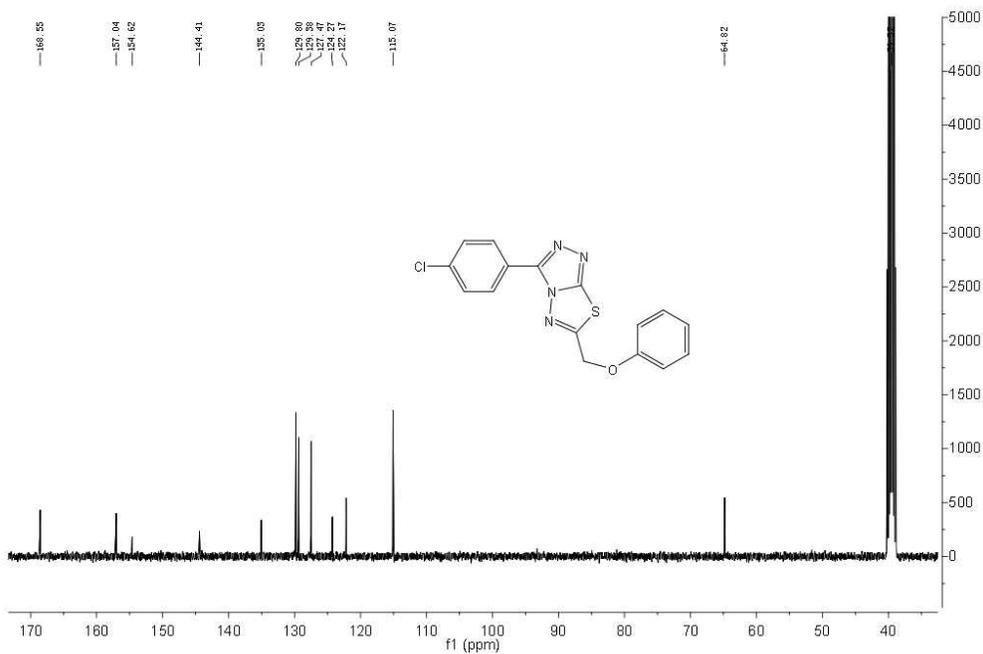
¹H NMR spectra of compound 3-(4-fluorophenyl)-6-((2-naphthyloxy)methyl)-[1,2,4]thiazolo[3,4-b] [1,3,4]thiadiazole (6b-7)

BRUKER AV-III-500 1H-NMR ATD-131214-1 IN DMSO



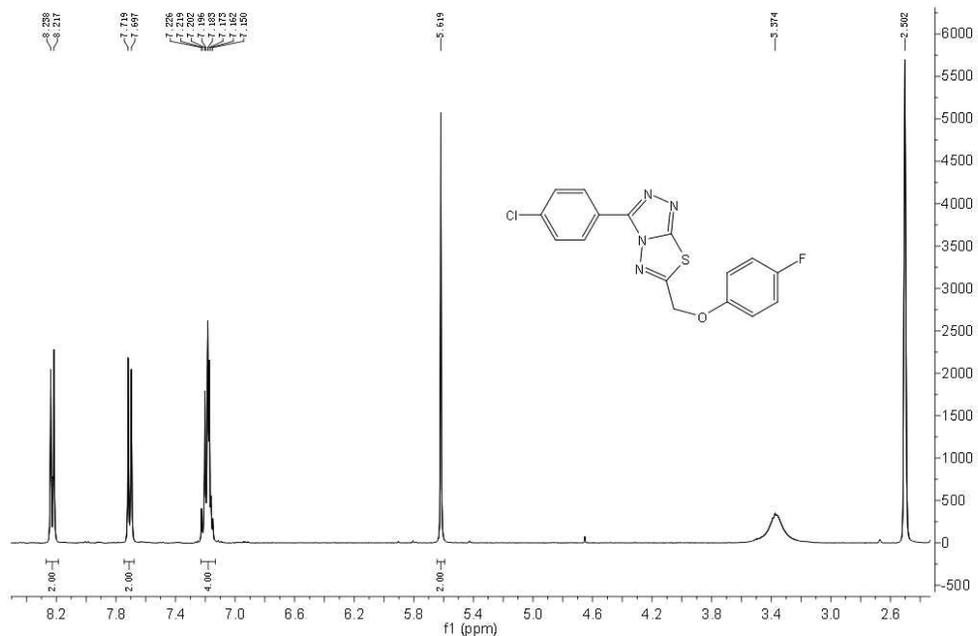
¹H NMR spectra of compound 3-(4-chlorophenyl)-6-(phoxymethyl)-1,2,4-triazolo[3,4-b][1,3,4]thiadiazole (6c-1)

BRUKER AV-III-400 ¹³C-NMR ATD-131214-1 IN DMSO



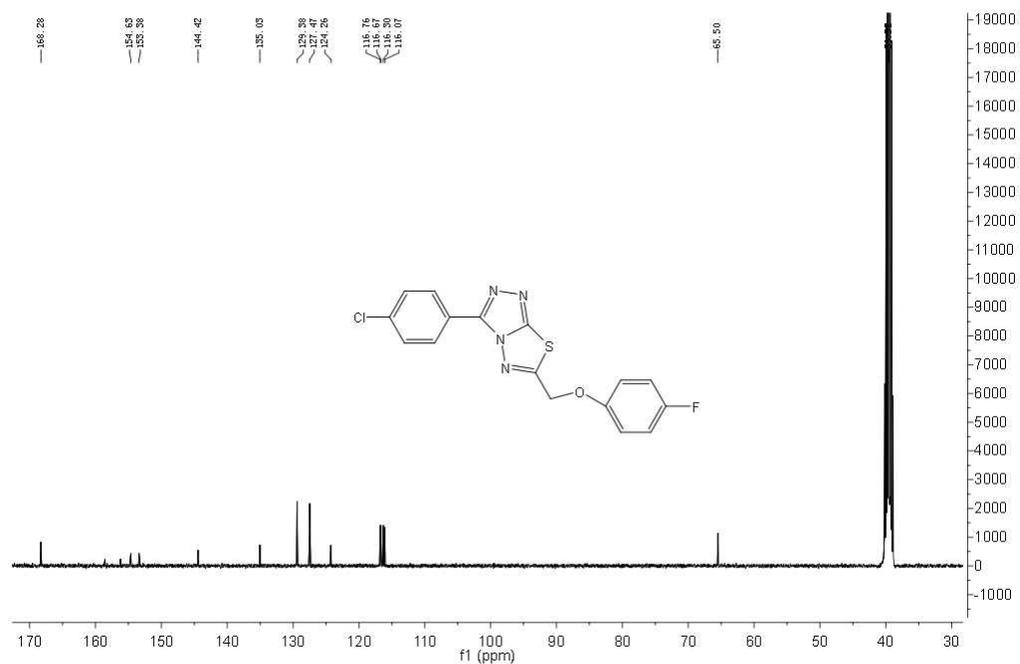
¹³C NMR spectra of compound 3-(4-chlorophenyl)-6-(phoxymethyl)-1,2,4-triazolo[3,4-b][1,3,4]thiadiazole (6c-1)

ATD-140113-3 Bruker AVANCEIII 400 PROTON2 DMSO



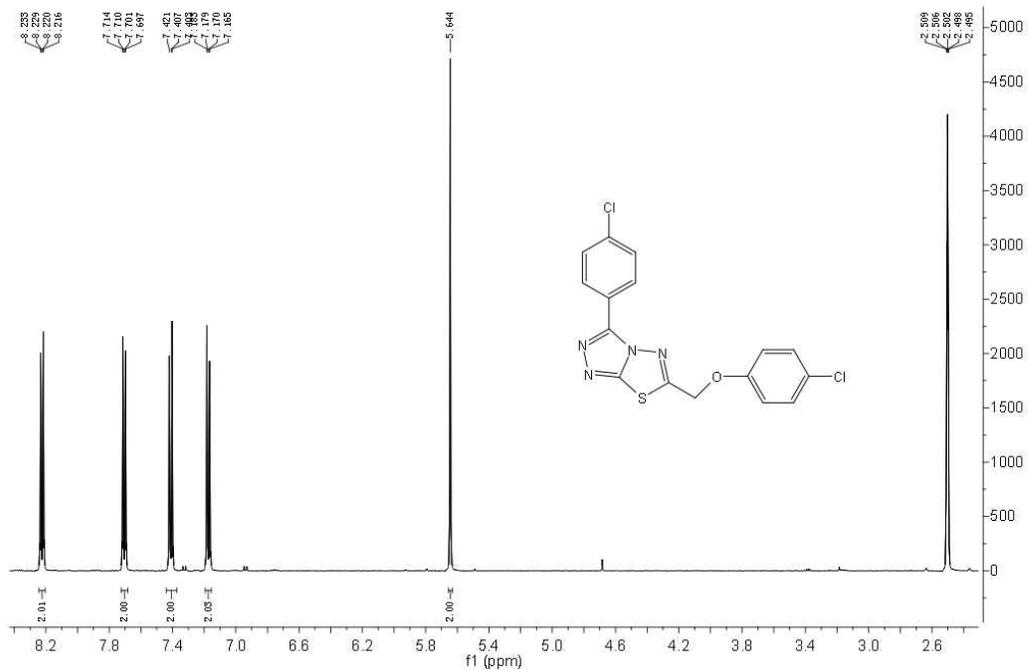
¹H NMR spectra of compound 3-(4-chlorophenyl)-6-((4-fluorophenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6c-2)

BRUKER AV-III-400 ¹³C-NMR ATD-140113-3 IN DMSO



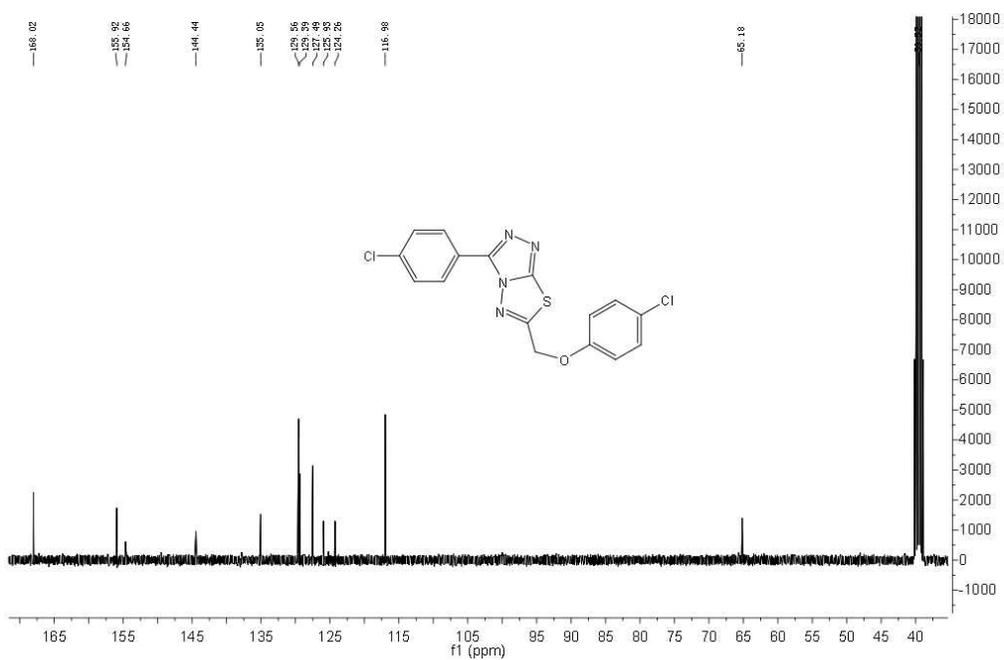
¹³C NMR spectra of compound 3-(4-chlorophenyl)-6-((4-fluorophenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6c-2)

BRUKER AV-III-500 1H-NMR ATD-131214-4 IN DMSO



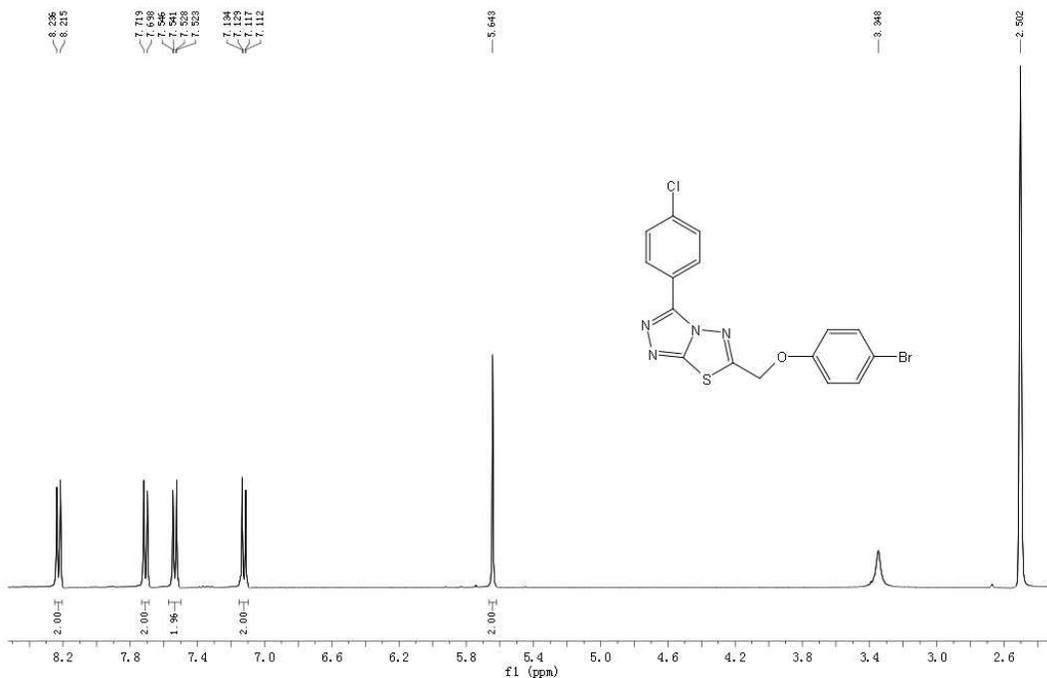
¹H NMR spectra of compound 6-((4-chlorophenoxy)methyl)-3-(4-chlorophenyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6c-3)

BRUKER AV-III-400 ¹³C-NMR ATD-131214-4 IN DMSO



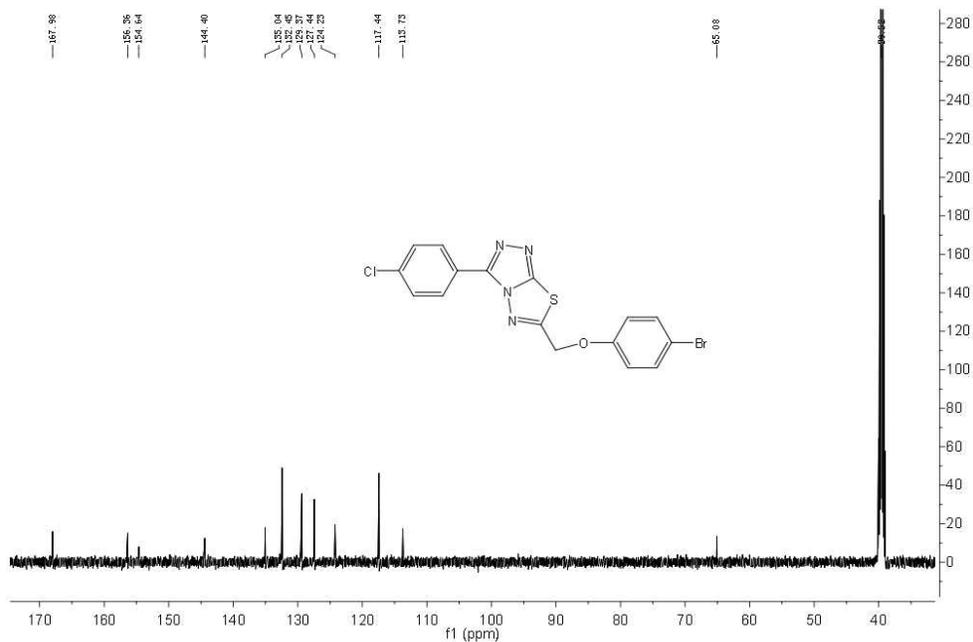
¹³C NMR spectra of compound 6-((4-chlorophenoxy)methyl)-3-(4-chlorophenyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6c-3)

ATD-140113-2 Bruker AVANCEIII 400 PROTON2 DMSO



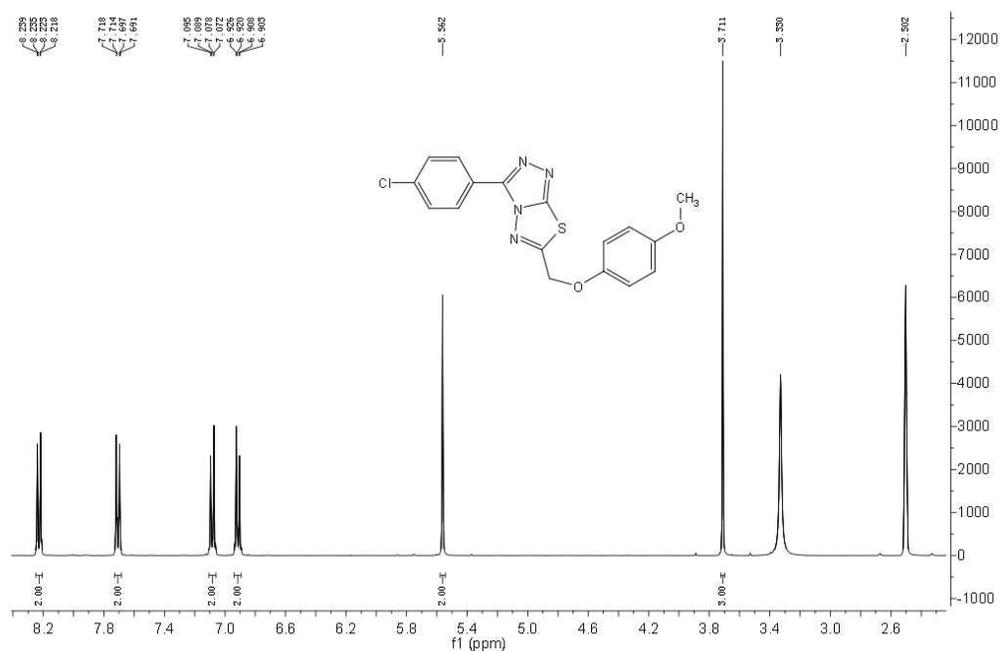
¹H NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-(4-chlorophenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6c-4)

BRUKER AV-III-500 ¹³C-NMR ATD-140113-2 IN DMSO

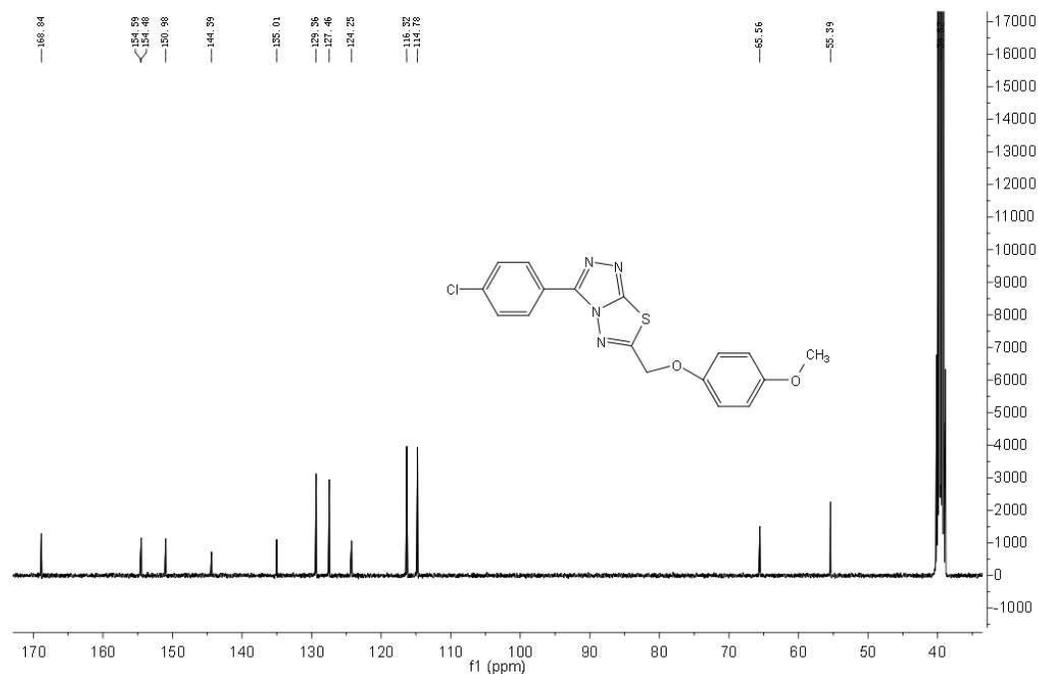


¹³C NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-(4-chlorophenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6c-4)

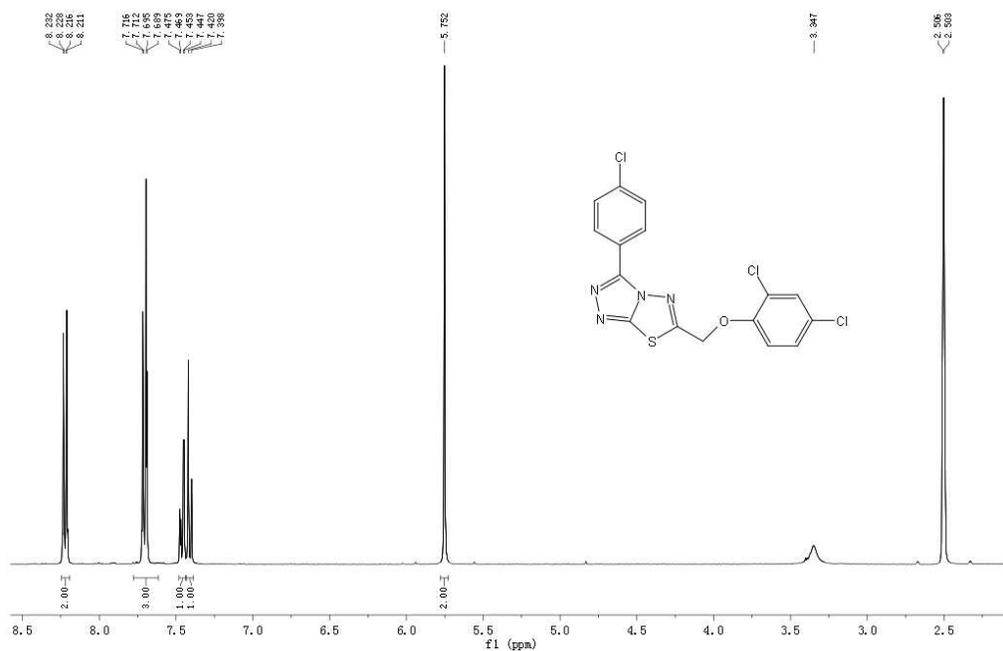
ATD-140114-2 Bruker AVANCEIII 400 PROTON2 DMSO



BRUKER AV-III-400 ¹³C-NMR ATD-140114-2 IN DMSO

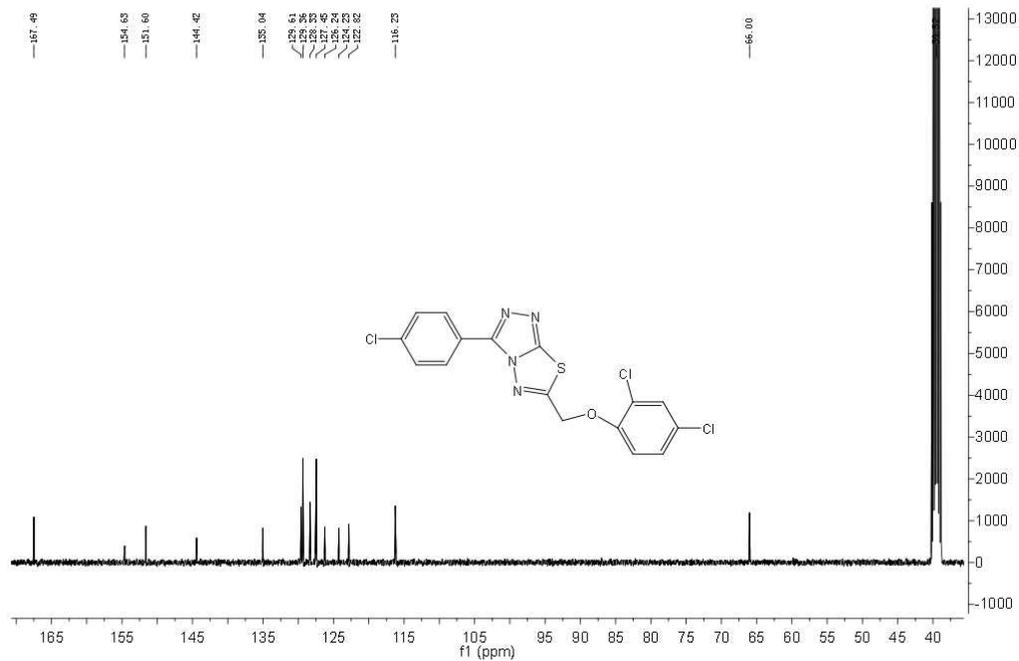


ATD-140113-1 Bruker AVANCEIII 400 PROTON2 DMSO



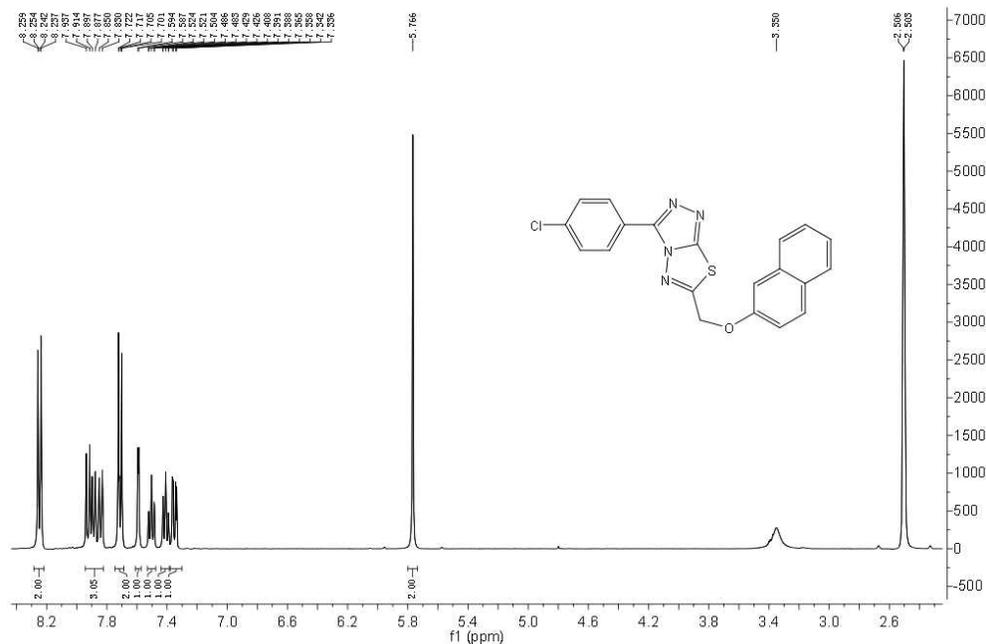
¹H NMR spectra of compound 3-(4-chlorophenyl)-6-((2,4-dichlorophenoxy)methyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6c-6)

BRUKER AV-III-400 ¹³C-NMR ATD-140113-1 IN DMSO

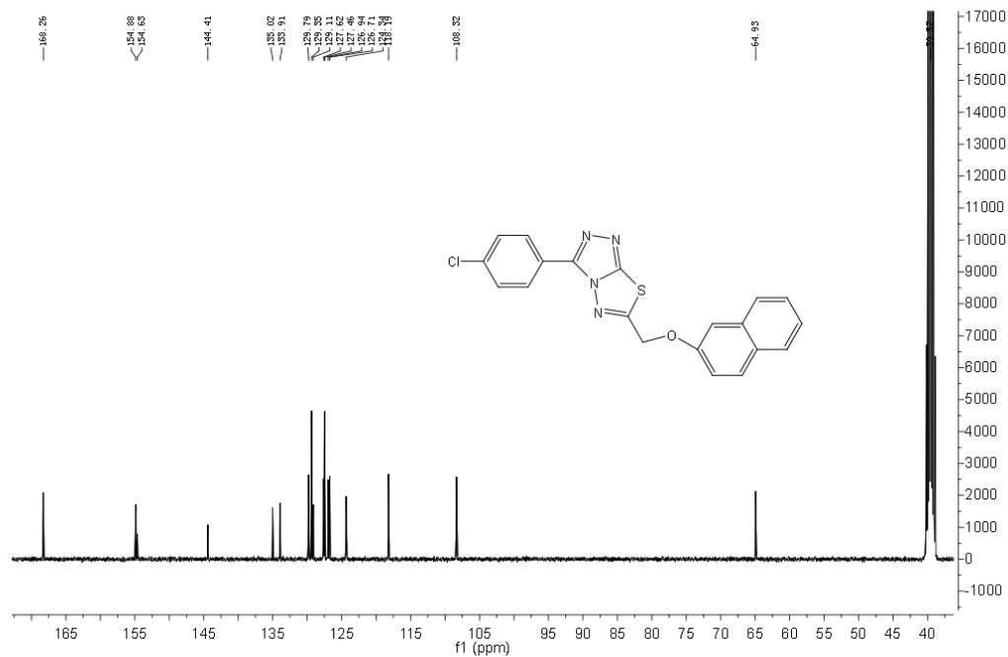


¹³C NMR spectra of compound 3-(4-chlorophenyl)-6-((2,4-dichlorophenoxy)methyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6c-6)

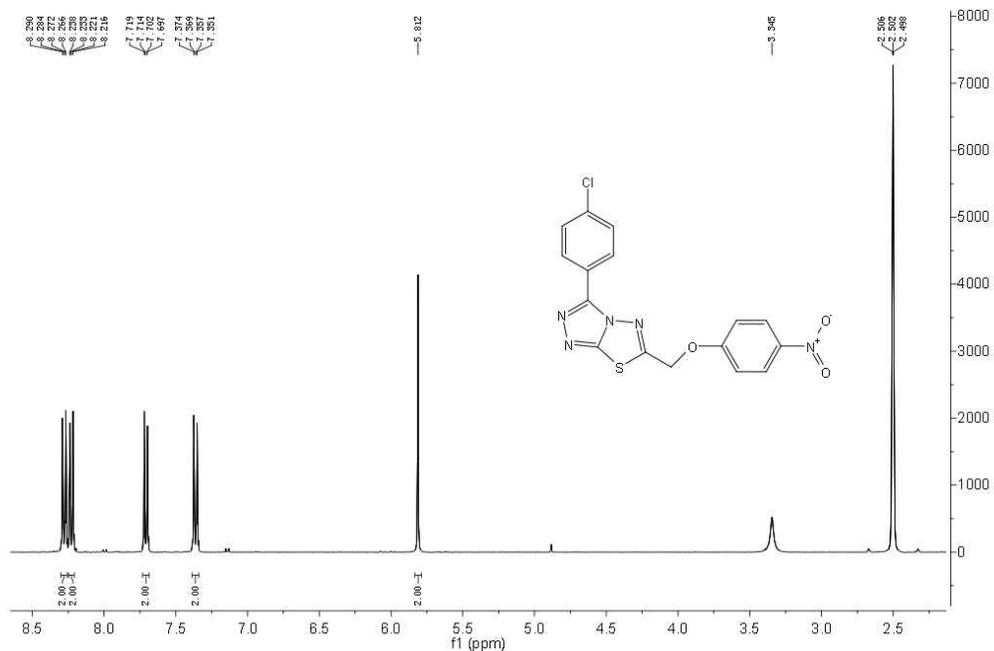
ATD-140114-1 Bruker AVANCEIII 400 PROTON2 DMSO



BRUKER AV-III-400 ¹³C-NMR ATD-140114-1 IN DMSO

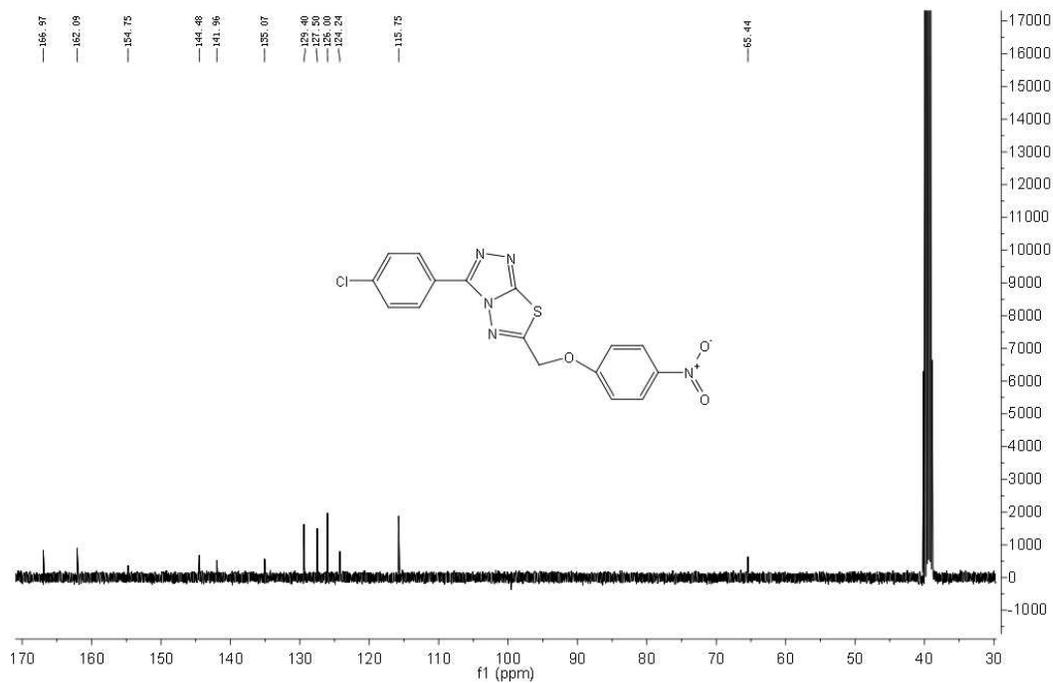


ATD-140116-1 Bruker AVANCEIII 400 PROTON2 DMSO



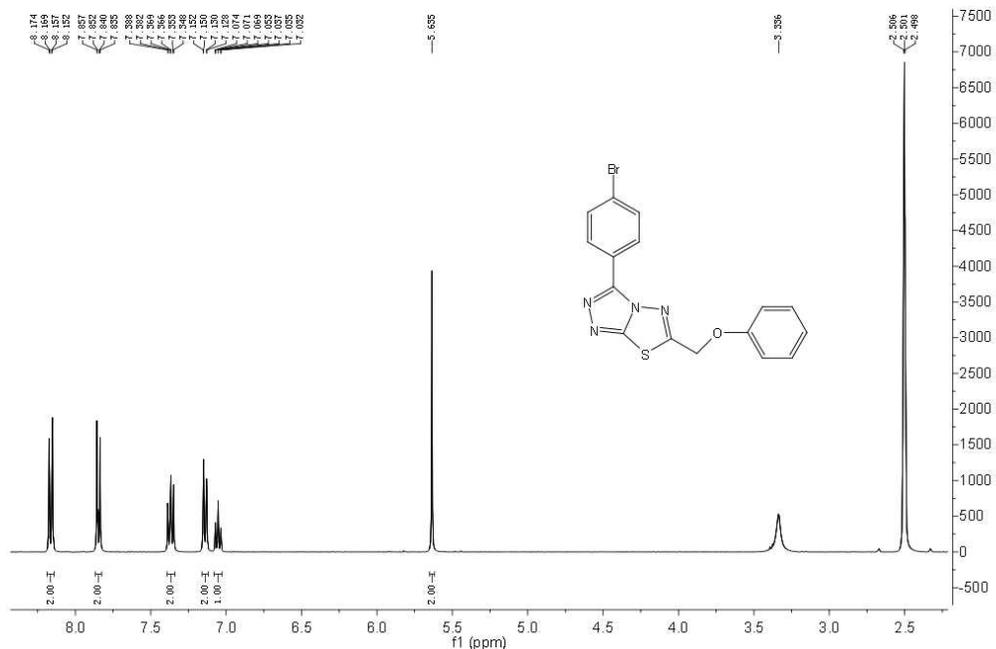
¹H NMR spectra of compound 3-(4-chlorophenyl)-6-((4-nitrophenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6c-8)

BRUKER AV-III-400 ¹³C-NMR ATD-140116-1 IN DMSO



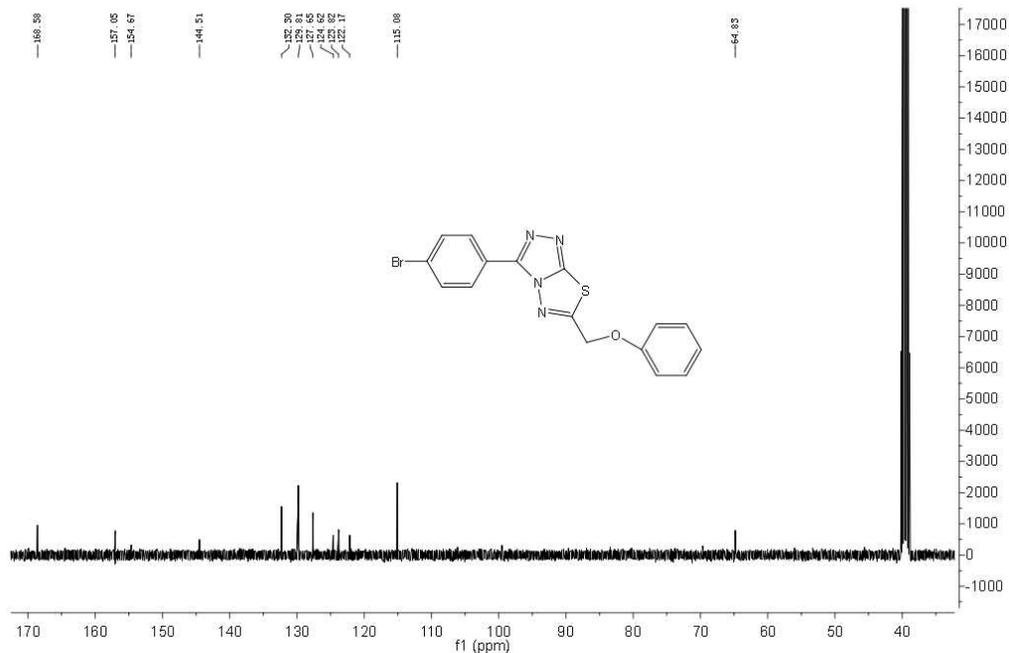
¹³C NMR spectra of compound 3-(4-chlorophenyl)-6-((4-nitrophenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6c-8)

ATD-140116-2 Bruker AVANCEIII 400 PROTON2 DMSO



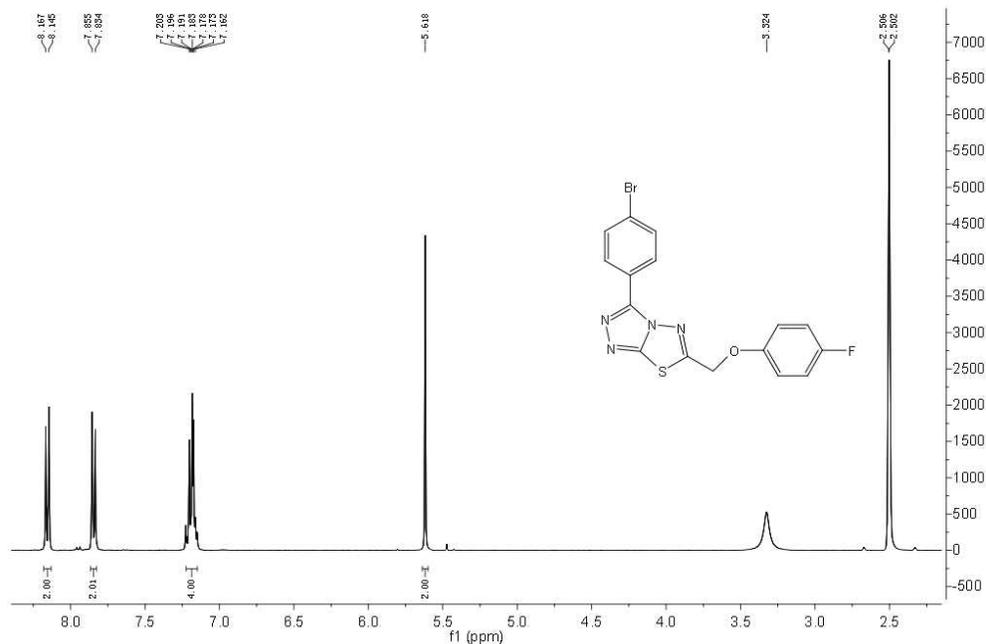
¹H NMR spectra of compound 3-(4-bromophenyl)-6-(phoxymethyl)-[1,2,4]thiazolo[3,4-b][1,3,4]Thiadiazole (6d-1)

BRUKER AV-III-400 ¹³C-NMR ATD-140116-2 IN DMSO



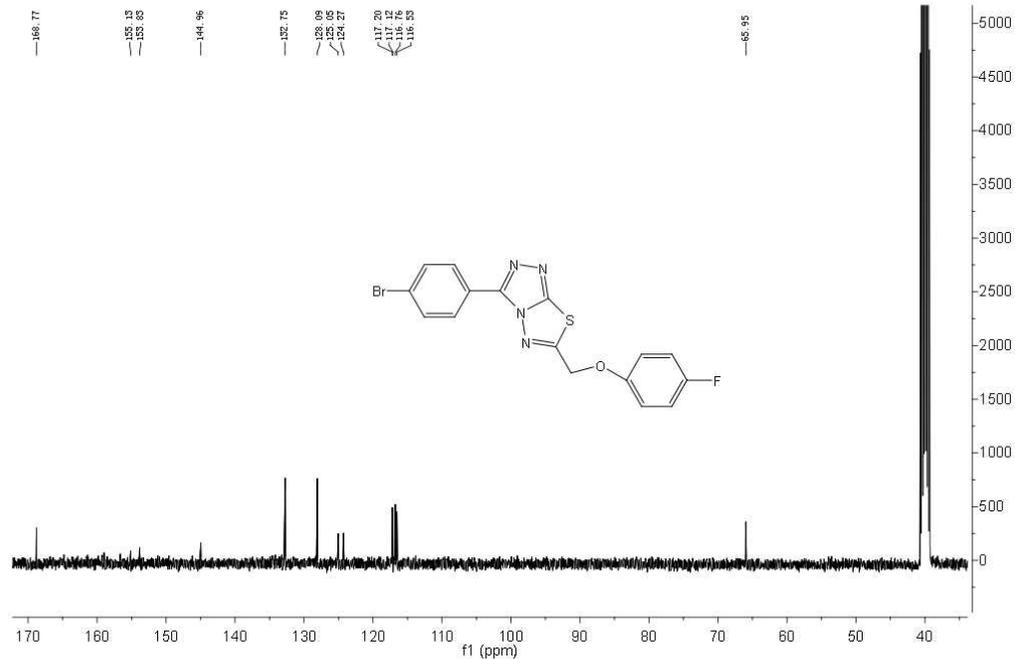
¹³C NMR spectra of compound 3-(4-bromophenyl)-6-(phoxymethyl)-[1,2,4]thiazolo[3,4-b][1,3,4]Thiadiazole (6d-1)

ATD-140218-2 Bruker AVANCEIII 400 PROTON2 DMSO



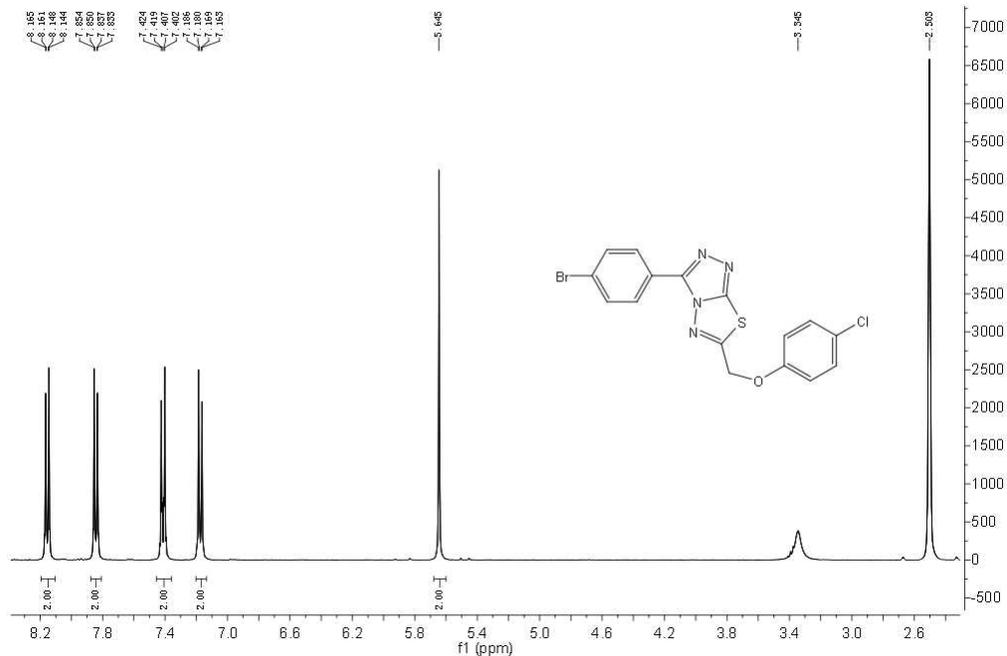
¹H NMR spectra of compound 3-(4-bromophenyl)-6-((4-fluorophenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6d-2)

BRUKER AV-III-400 ¹³C-NMR ATD-140218-2 IN DMSO



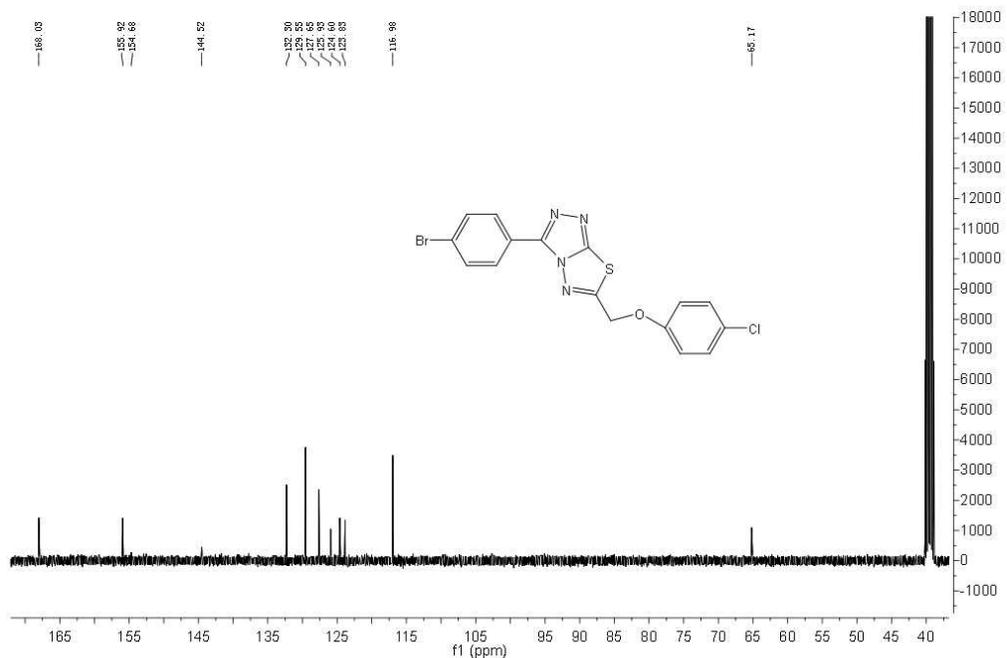
¹³C NMR spectra of compound 3-(4-bromophenyl)-6-((4-fluorophenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6d-2)

ATD-140217-2 Bruker AVANCEIII 400 PROTON2 DMSO



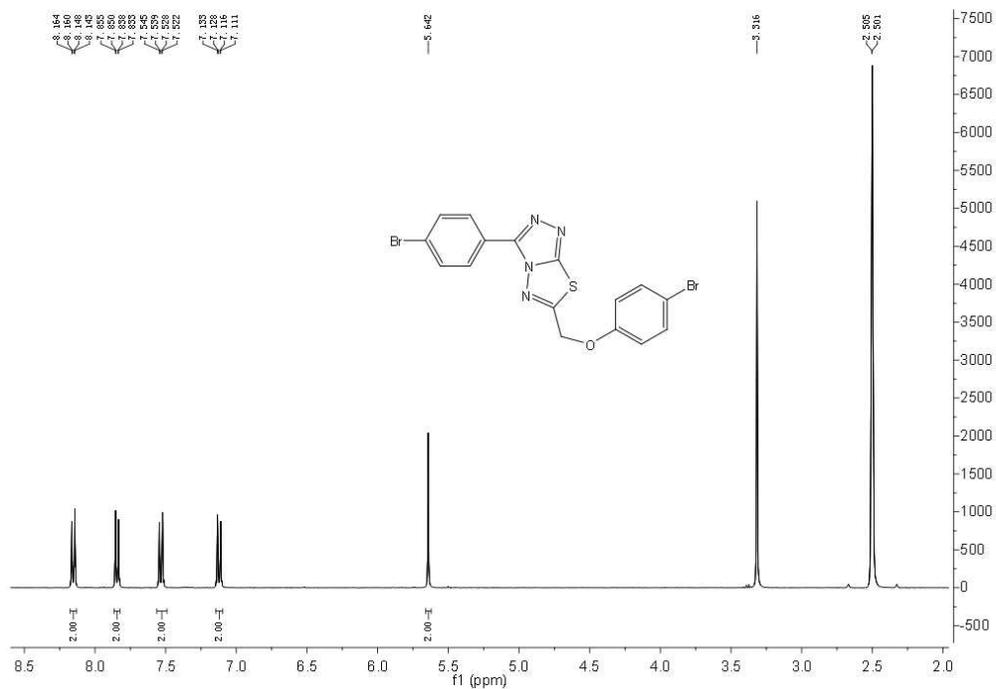
¹H NMR spectra of compound 3-(4-bromophenyl)-6-((4-chlorophenoxy)methyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6d-3)

BRUKER AV-III-400 ¹³C-NMR ATD-140217-2 IN DMSO



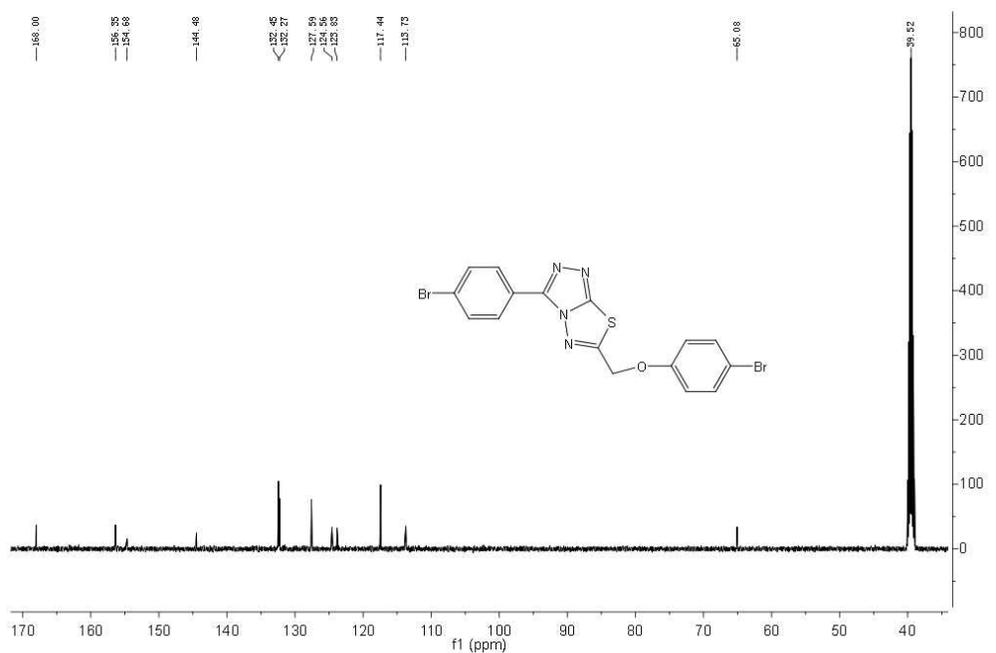
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ATD-140218-1 Bruker AVANCEIII 400 PROTON2 DMSO



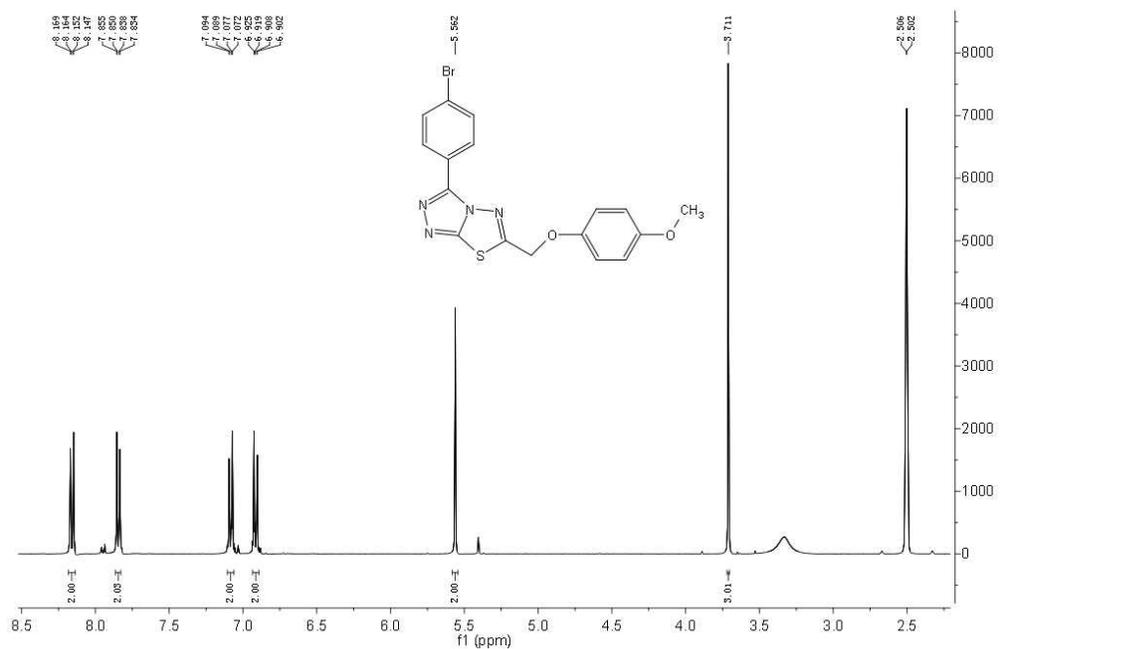
¹H NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-(4-bromophenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6d-4)

BRUKER AV-III-500 ¹³C-NMR ATD-140218-1 IN DMSO



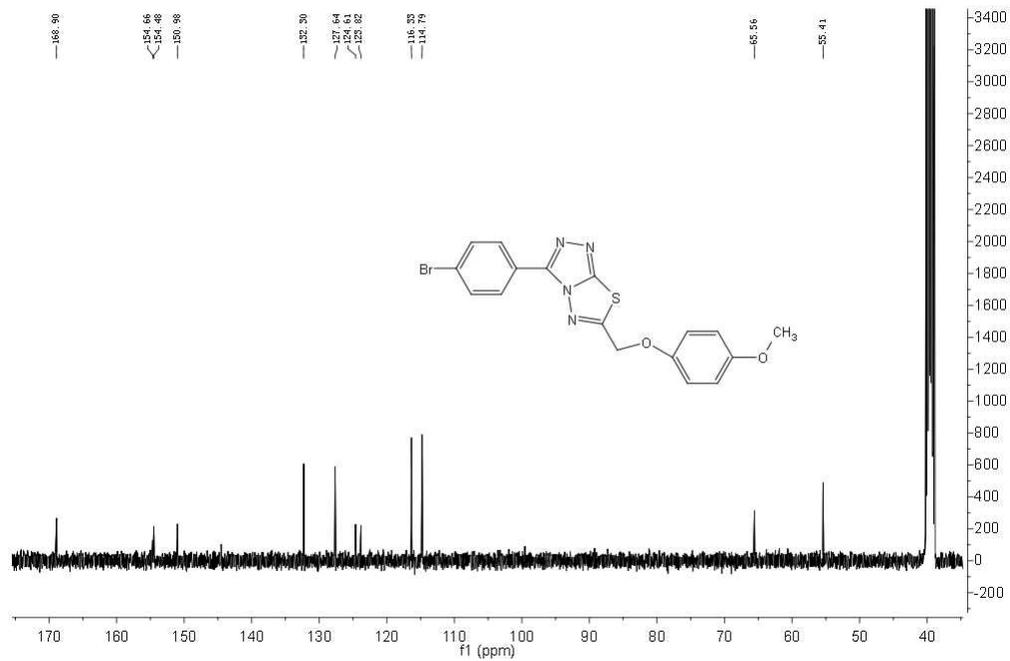
¹³C NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-(4-bromophenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6d-4)

ATD-140219-1 Bruker AVANCEIII 400 PROTON2 DMSO



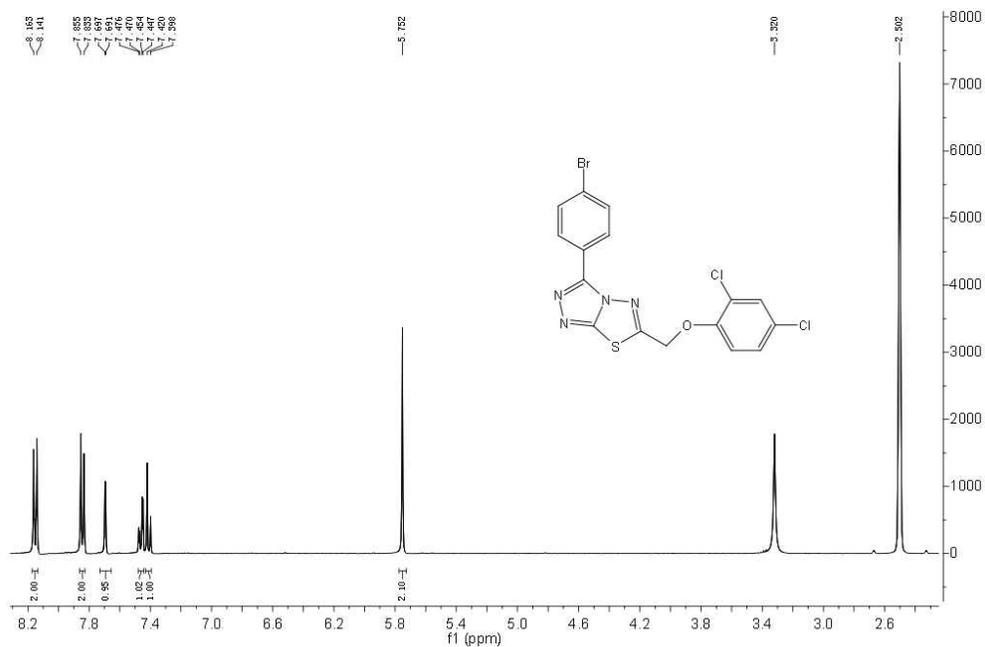
¹H NMR spectra of compound 3-(4-bromophenyl)-6-((4-methoxyphenoxy)methyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6d-5)

BRUKER AV-III-400 ¹³C-NMR ATD-140219-1 IN DMSO

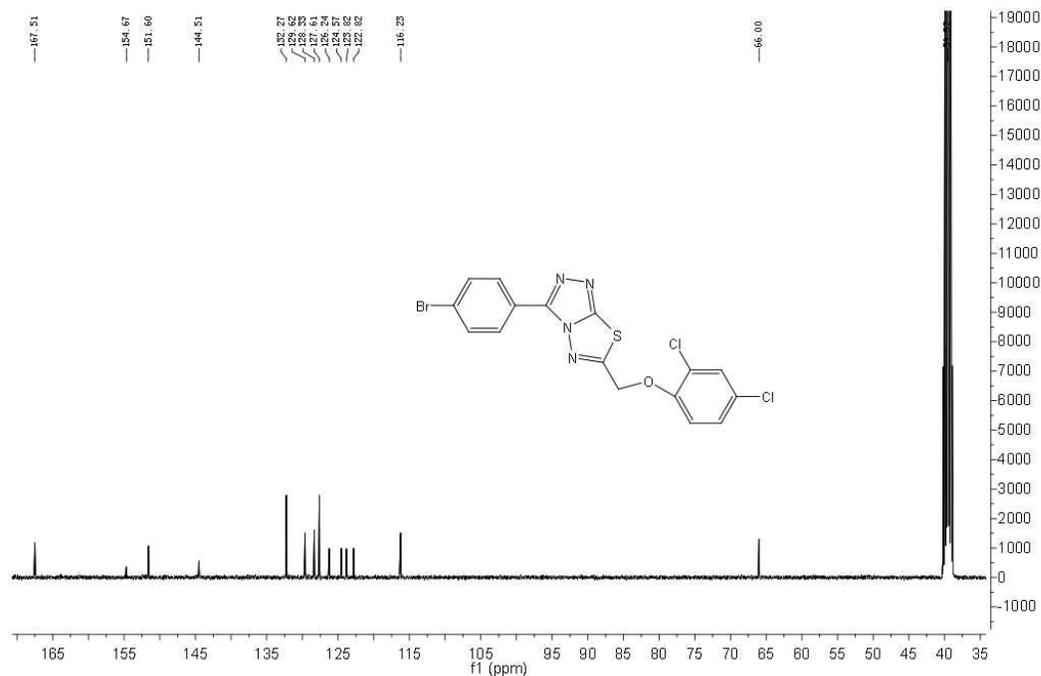


¹³C NMR spectra of compound 3-(4-bromophenyl)-6-((4-methoxyphenoxy)methyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6d-5)

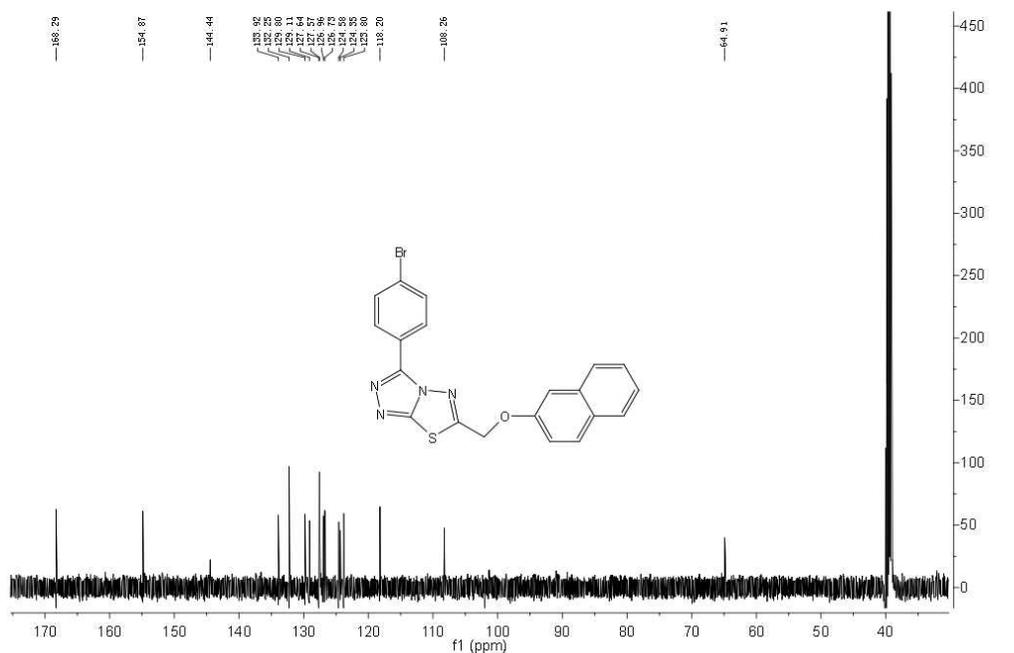
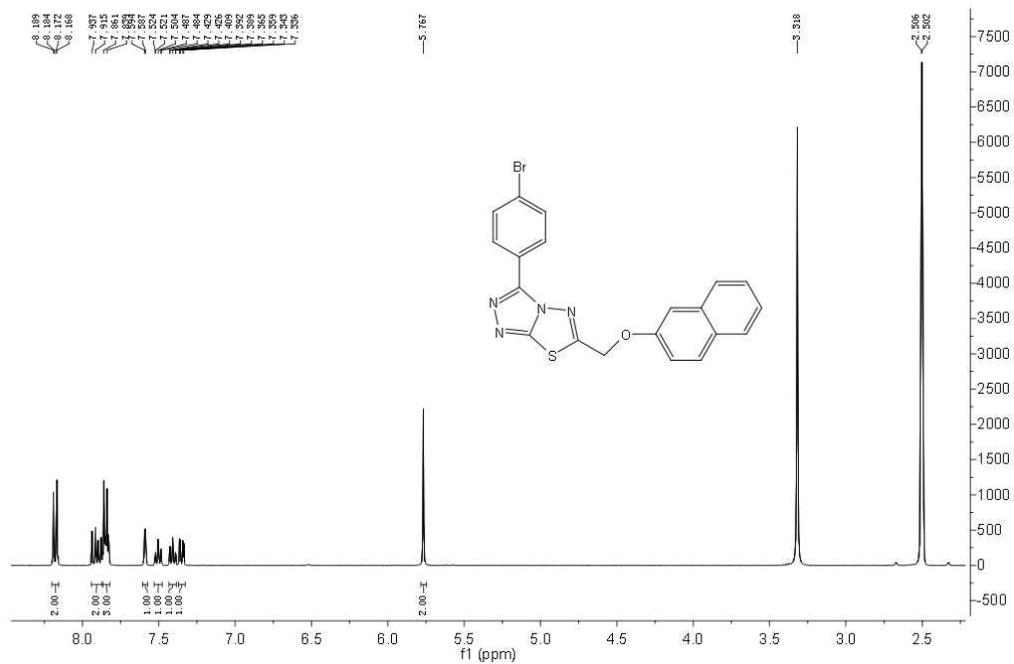
ATD-140217-1 Bruker AVANCEIII 400 PROTON2 DMSO



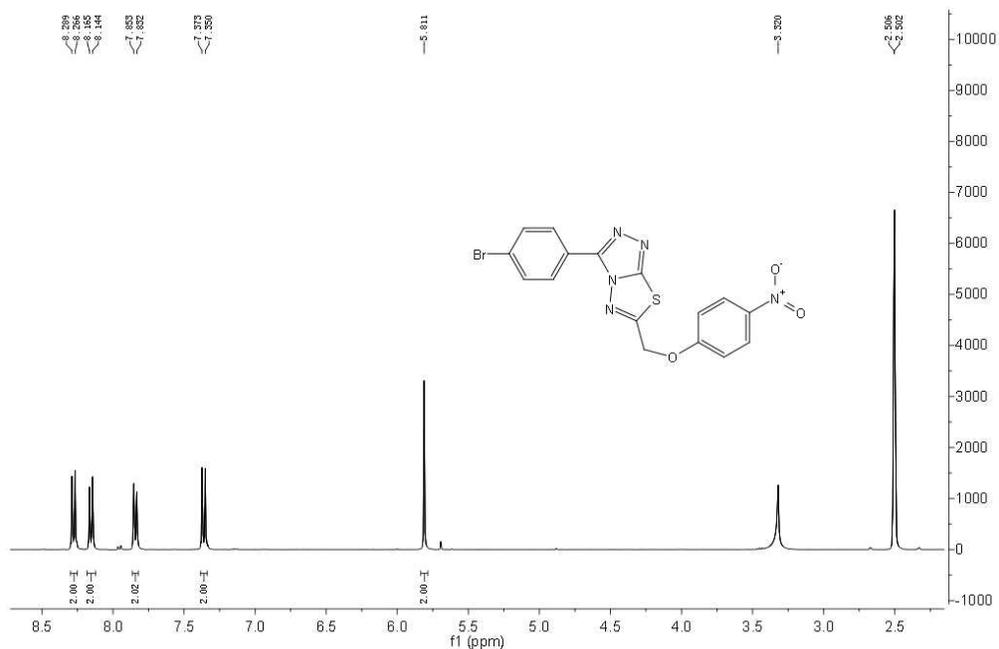
BRUKER AV-III-400 ¹³C-NMR ATD-140217-1 IN DMSO



ATD-140218-3 Bruker AVANCEIII 400 PROTON2 DMSO

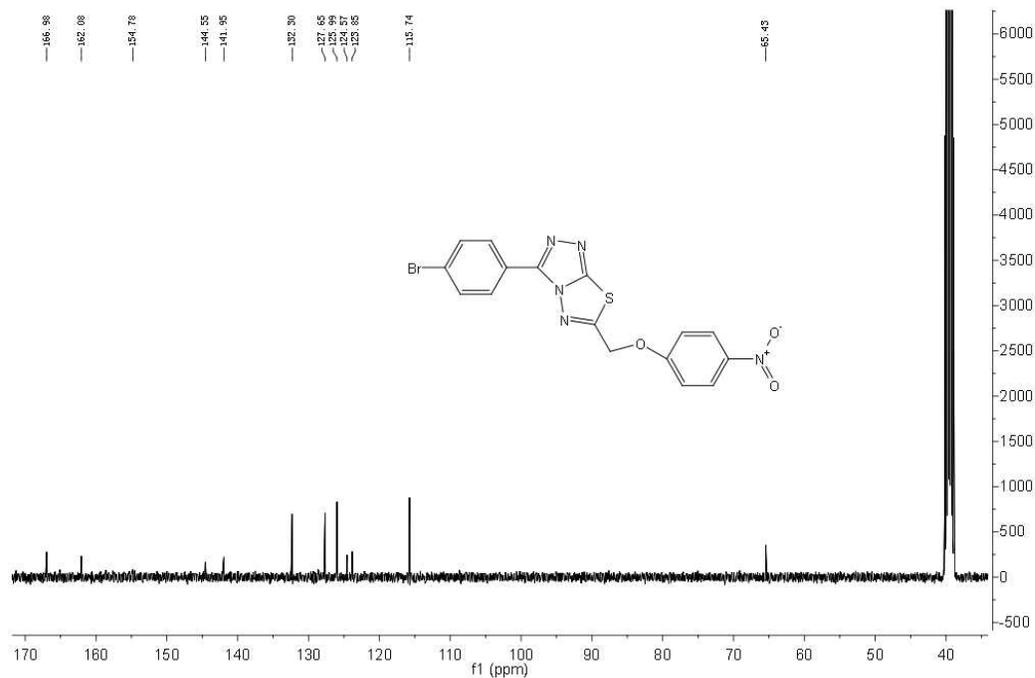


ATD-140219-3 Bruker AVANCEIII 400 PROTON2 DMSO



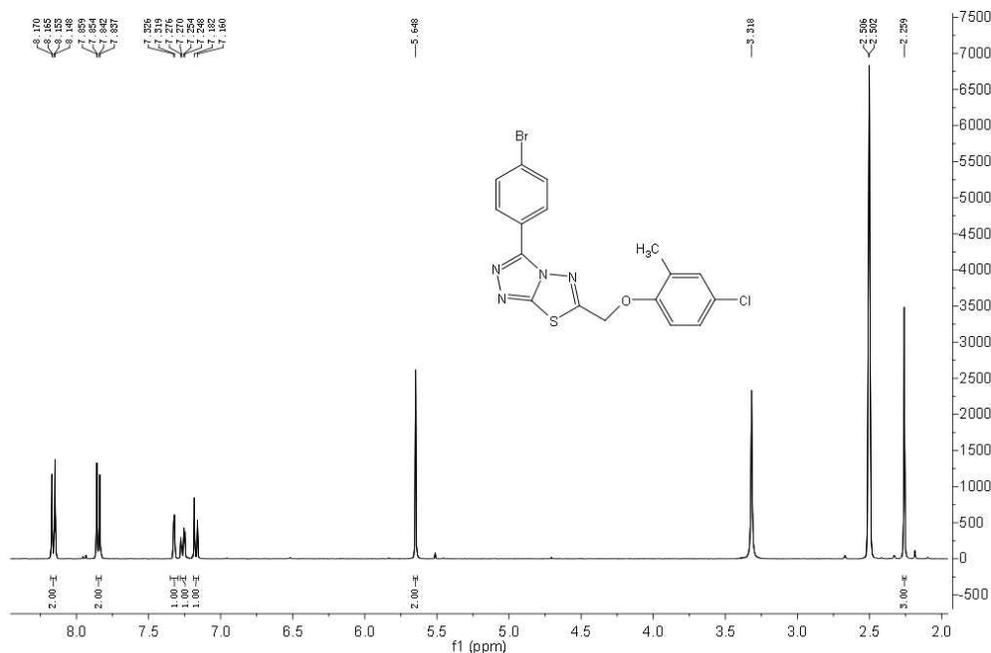
¹H NMR spectra of compound 3-(4-bromophenyl)-6-((4-nitrophenoxy)methyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6d-8)

BRUKER AV-III-400 ¹³C-NMR ATD-140219-3 IN DMSO



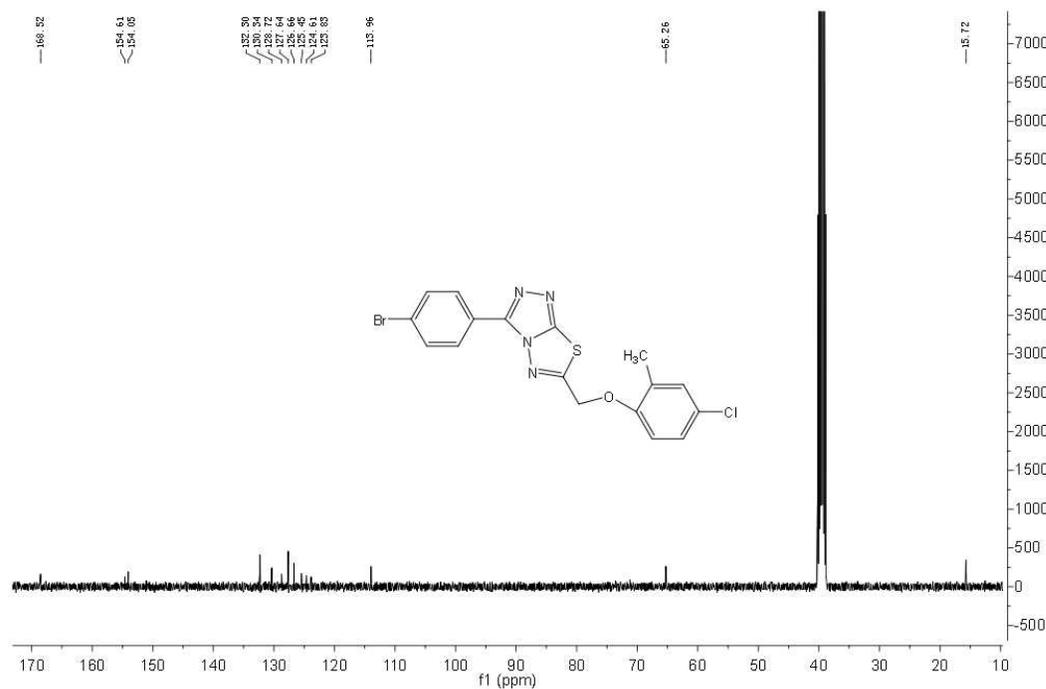
¹³C NMR spectra of compound 3-(4-bromophenyl)-6-((4-nitrophenoxy)methyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6d-8)

ATD-140219-2 Bruker AVANCEIII 400 PROTON2 DMSO



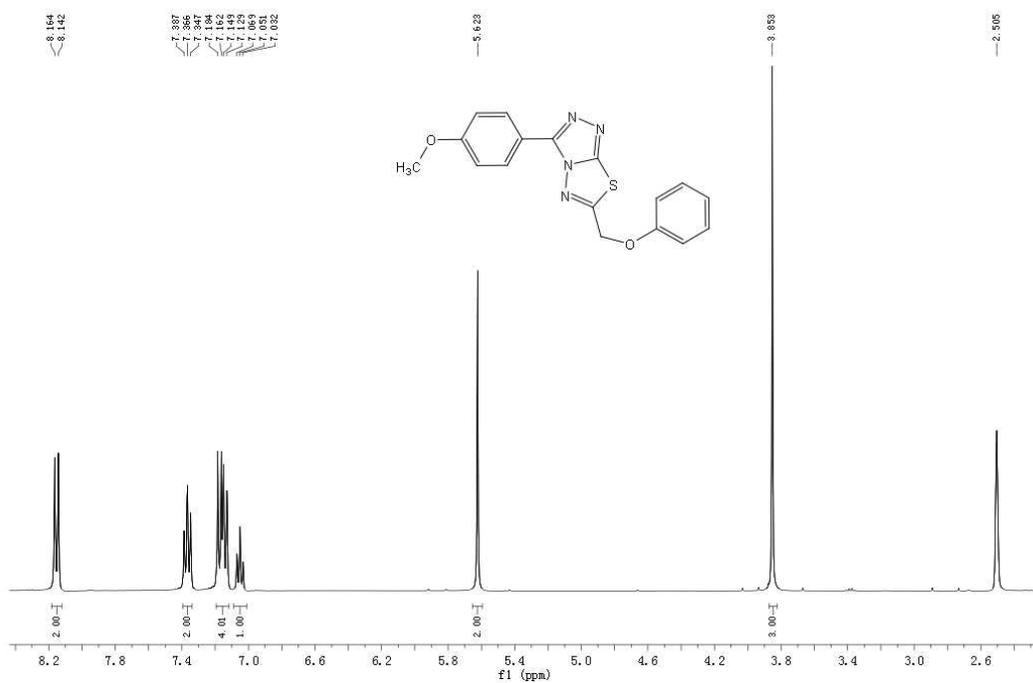
¹H NMR spectra of compound 3-(4-bromophenyl)-6-((2-methyl-4-chlorophenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6d-9)

BRUKER AV-III-400 ¹³C-NMR ATD-140219-2 IN DMSO



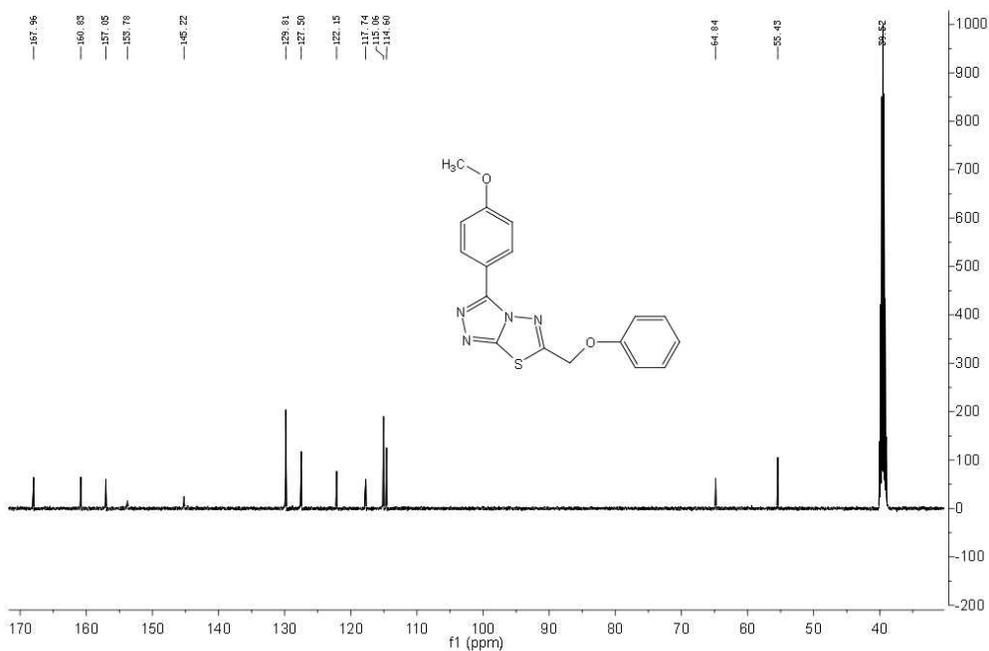
¹³C NMR spectra of compound 3-(4-bromophenyl)-6-((2-methyl-4-chlorophenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6d-9)

ATD-131211 Bruker AVANCE III 400 PROTON2 DMSO



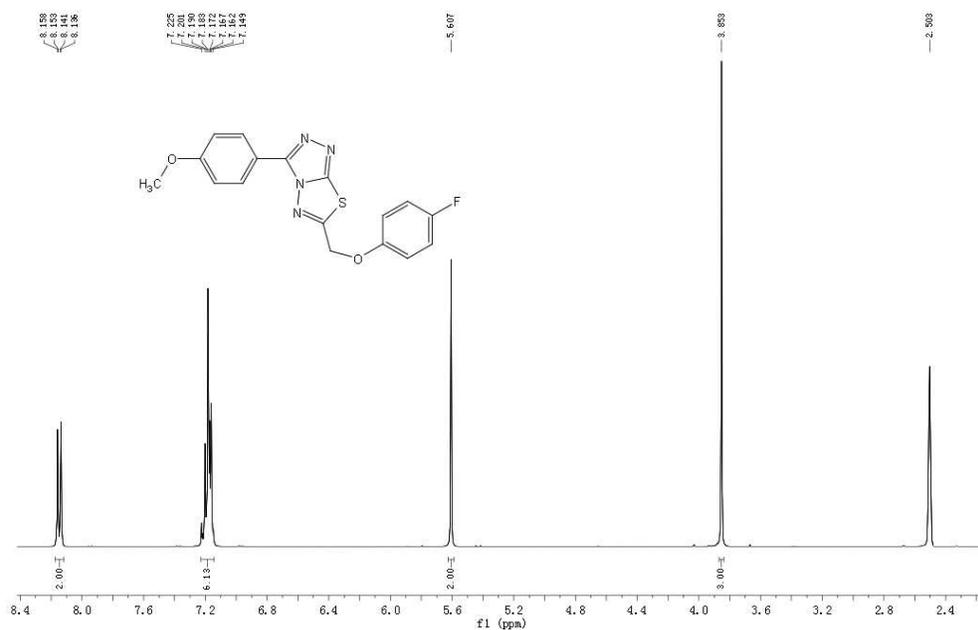
¹H NMR spectra of compound 3-(4-methoxyphenyl)-6-(phoxymethyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6e-1)

BRUKER AV-III-500 ¹³C-NMR ATD-131211 IN DMSO



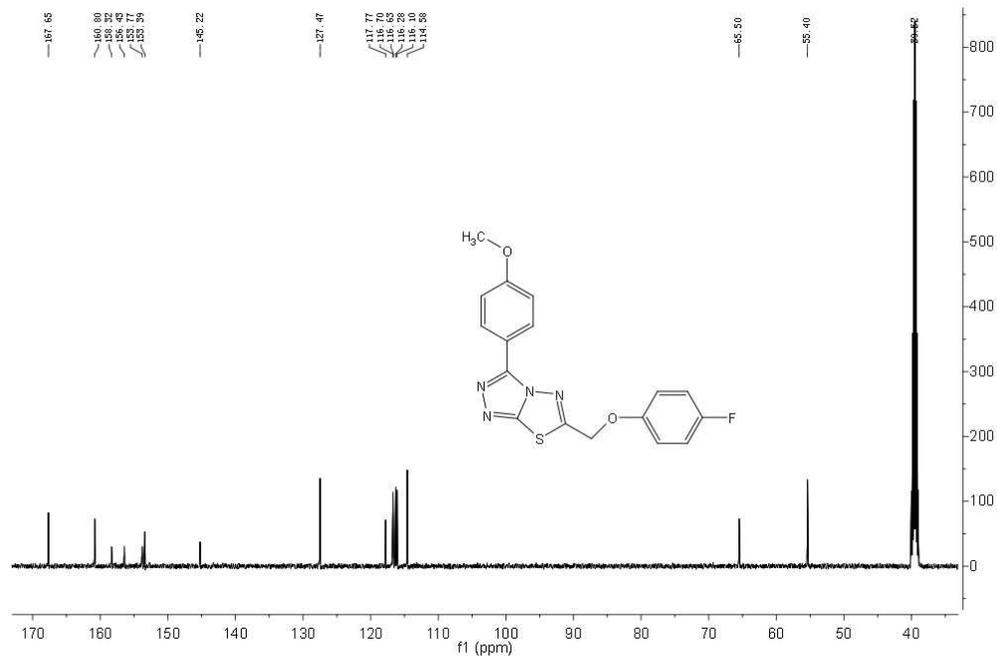
¹³C NMR spectra of compound 3-(4-methoxyphenyl)-6-(phoxymethyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6e-1)

ATD-131220-2 Bruker AVANCE III 400 PROTON2 DMSO



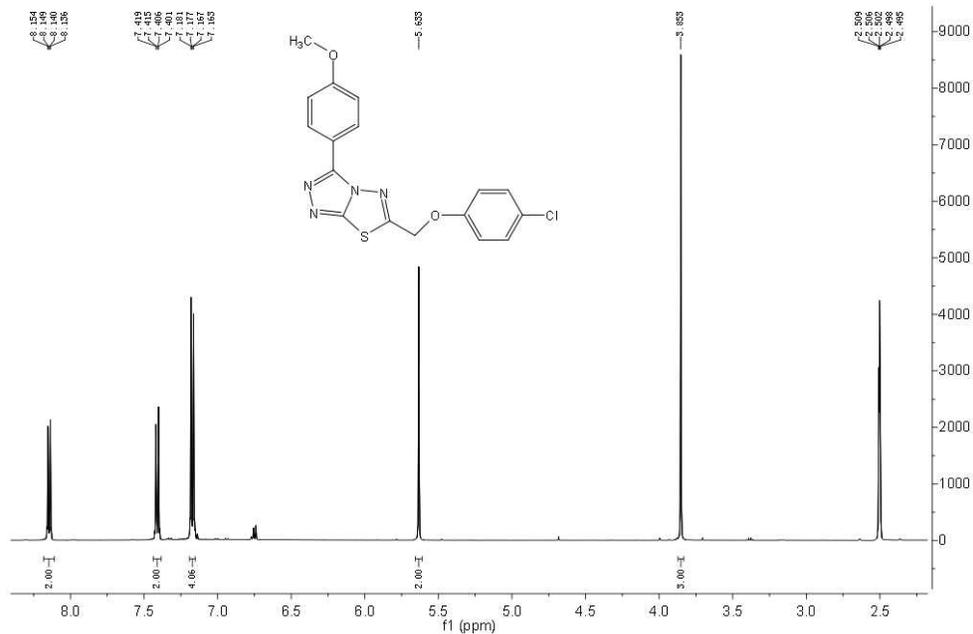
¹H NMR spectra of compound 6-((4-fluorophenoxy)methyl)-3-(4-methoxyphenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6e-2)

BRUKER AV-III-500 ¹³C-NMR ATD-131220-2 IN DMSO



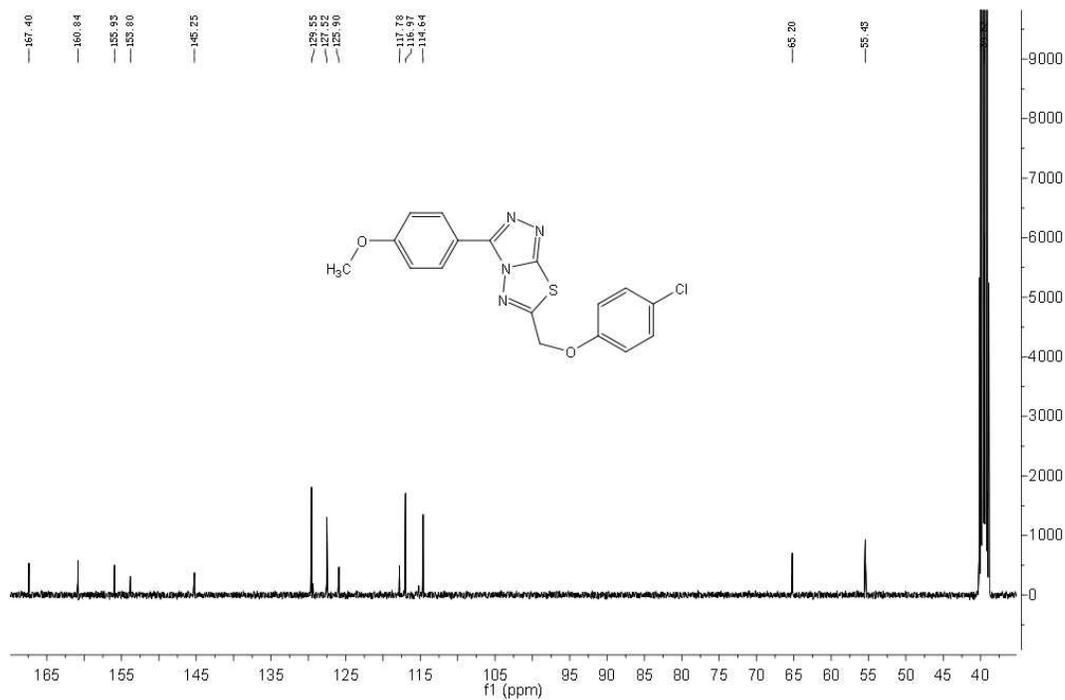
¹³C NMR spectra of compound 6-((4-fluorophenoxy)methyl)-3-(4-methoxyphenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6e-2)

BRUKER AV-III-500 1H-NMR ATD-131214-2 IN DMSO

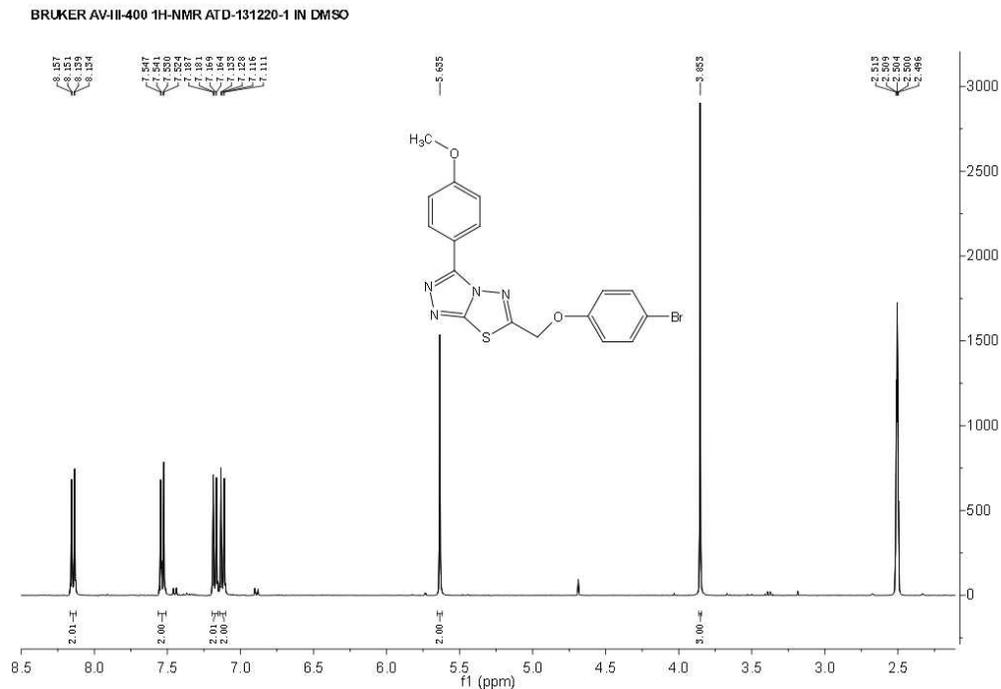


¹H NMR spectra of compound 6-((4-chlorophenoxy)methyl)-3-(4-methoxyphenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6e-3)

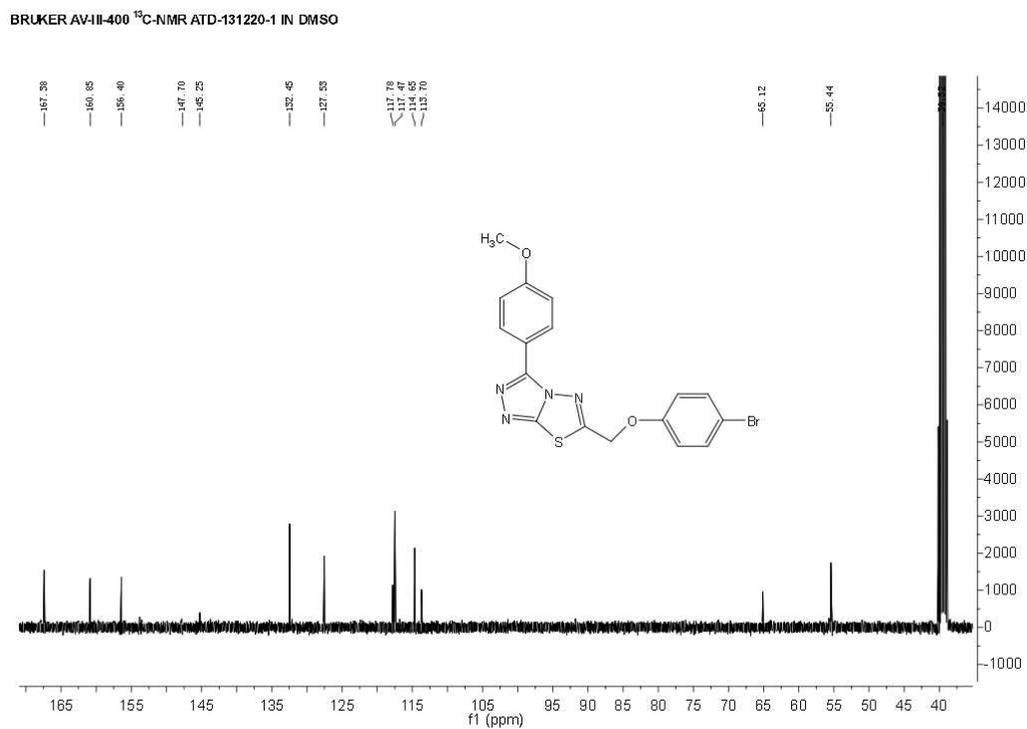
BRUKER AV-III-400 ¹³C-NMR ATD-131214-2 IN DMSO



¹³C NMR spectra of compound 6-((4-chlorophenoxy)methyl)-3-(4-methoxyphenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6e-3)

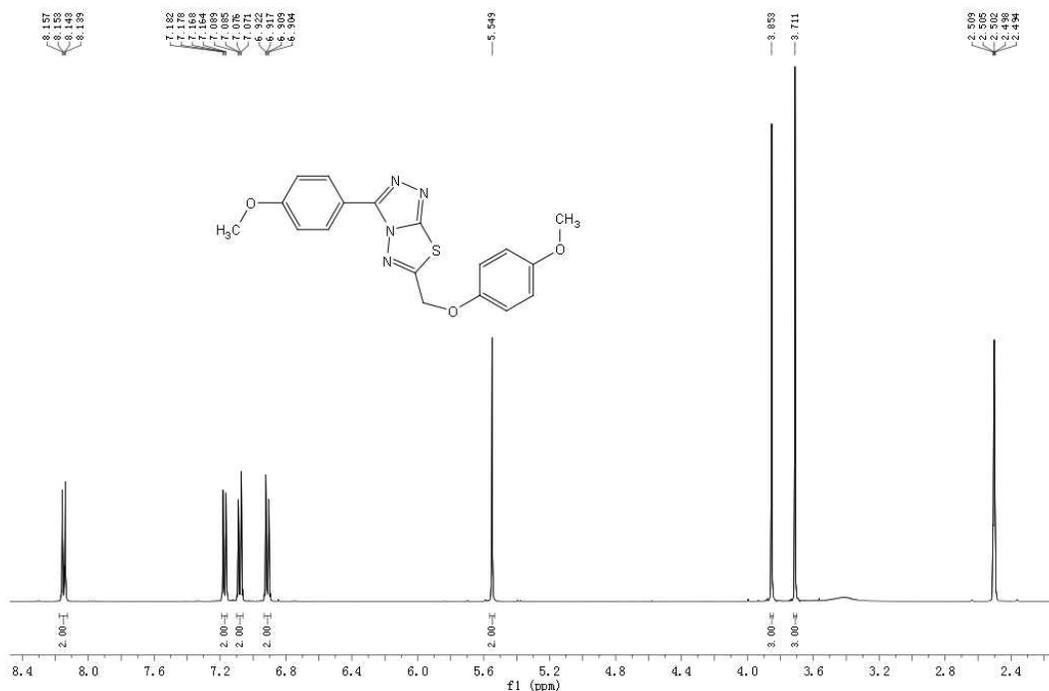


¹H NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-(4-methoxyphenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6e-4)



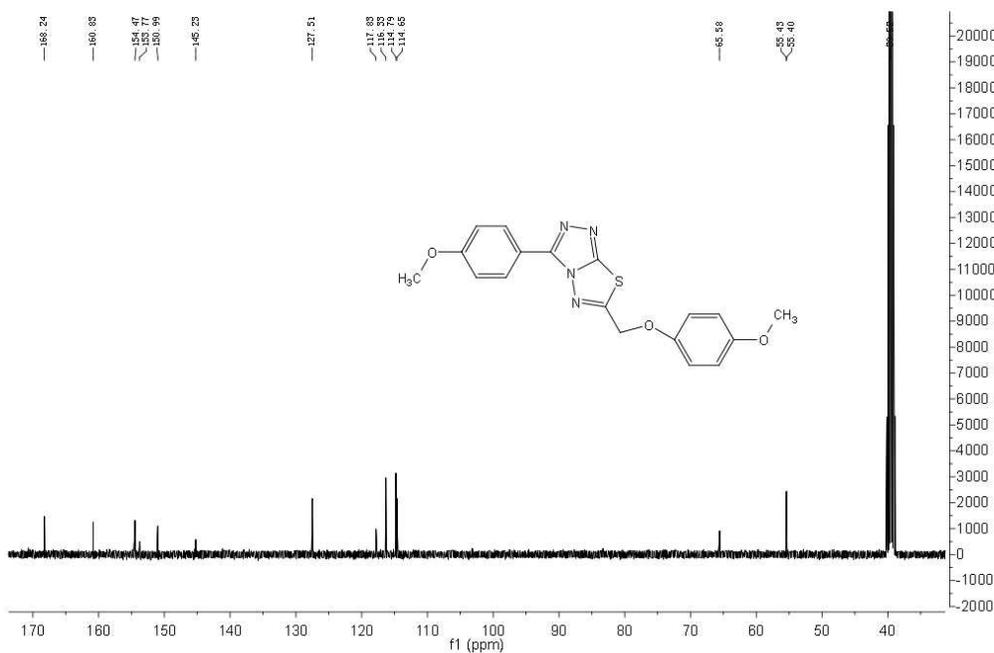
¹³C NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-(4-methoxyphenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6e-4)

BRUKER AV-III-500 1H-NMR ATD-131229-1 IN DMSO



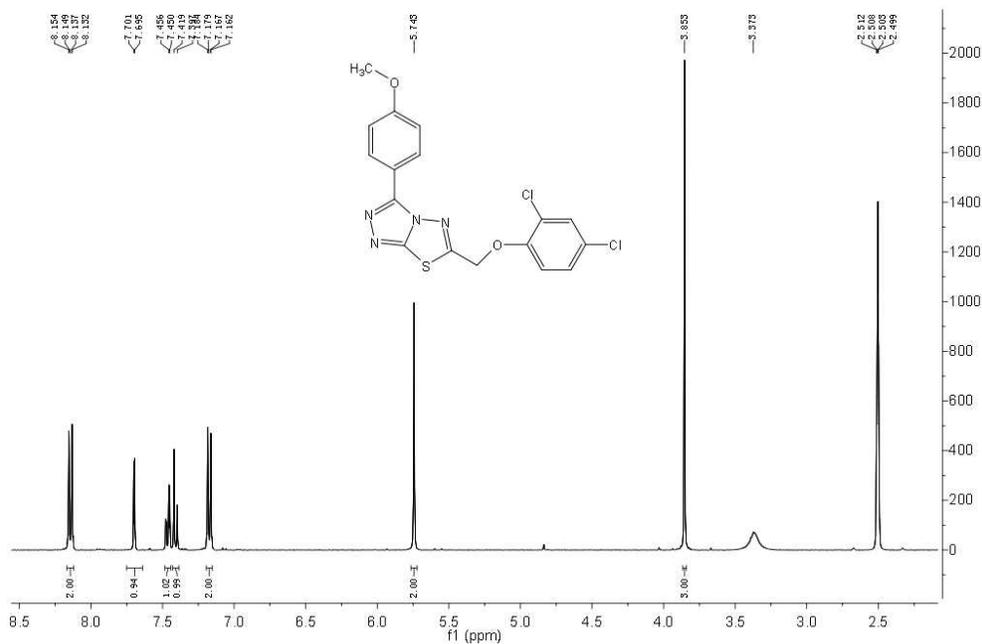
¹H NMR spectra of compound 6-((4-methoxyphenoxy)methyl)-3-(4-methoxyphenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6e-5)

BRUKER AV-III-400 ¹³C-NMR ATD-131229-1 IN DMSO



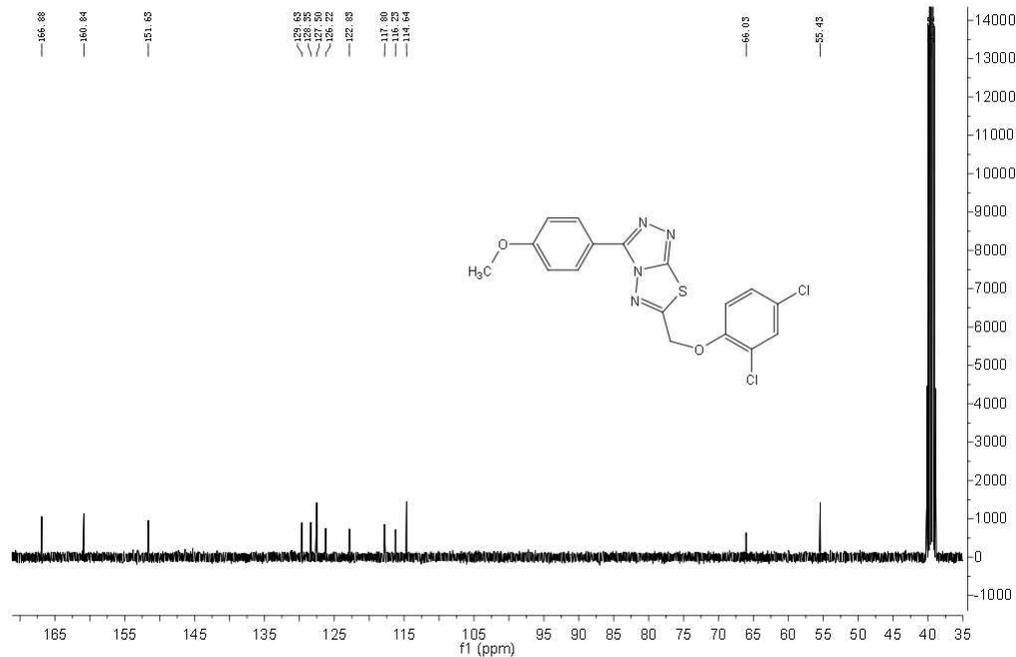
¹³C NMR spectra of compound 6-((4-methoxyphenoxy)methyl)-3-(4-methoxyphenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6e-5)

BRUKER AV-III-400 1H-NMR ATD-131219-1 IN DMSO



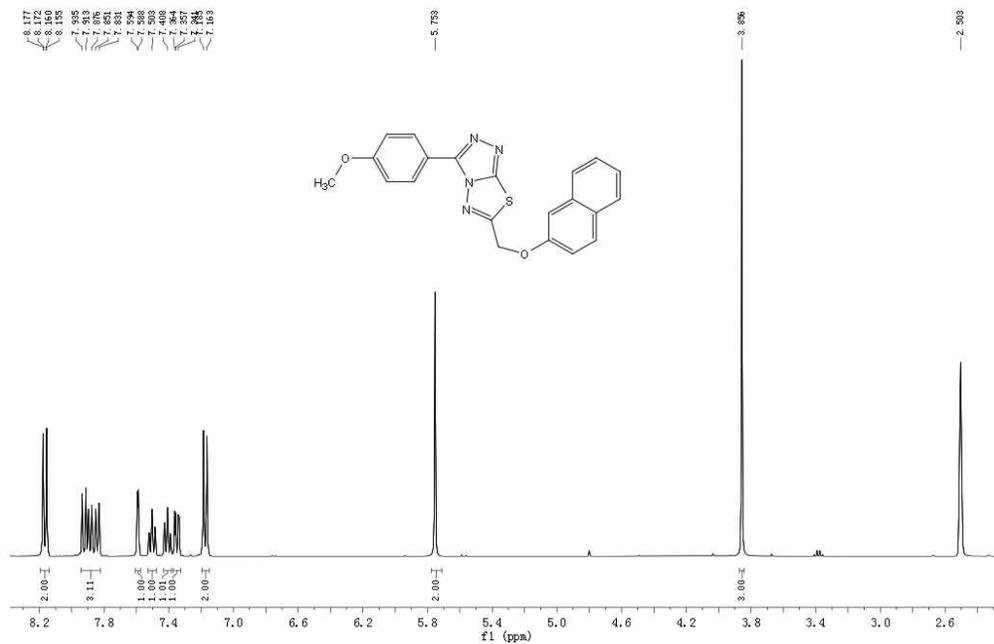
¹H NMR spectra of compound 6-((2,4-dichlorophenoxy)methyl)-3-(4-methoxyphenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6e-6)

BRUKER AV-III-400 ¹³C-NMR ATD-131219-1 IN DMSO



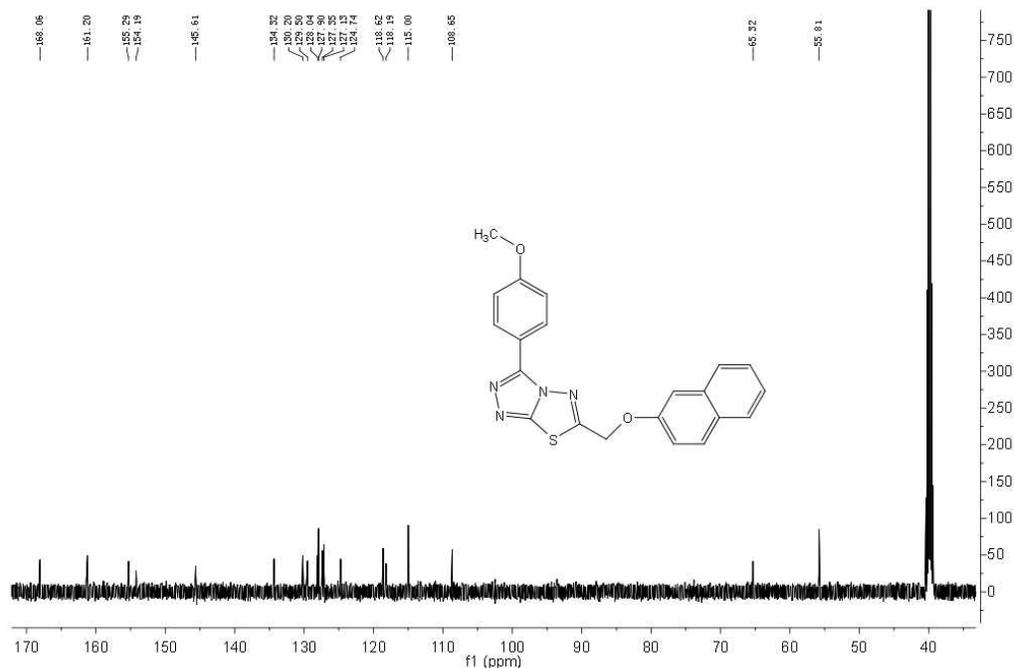
¹³C NMR spectra of compound 6-((2,4-dichlorophenoxy)methyl)-3-(4-methoxyphenyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6e-6)

ATD-131220-3 Bruker AVANCE III 400 PROTON2 DMSO



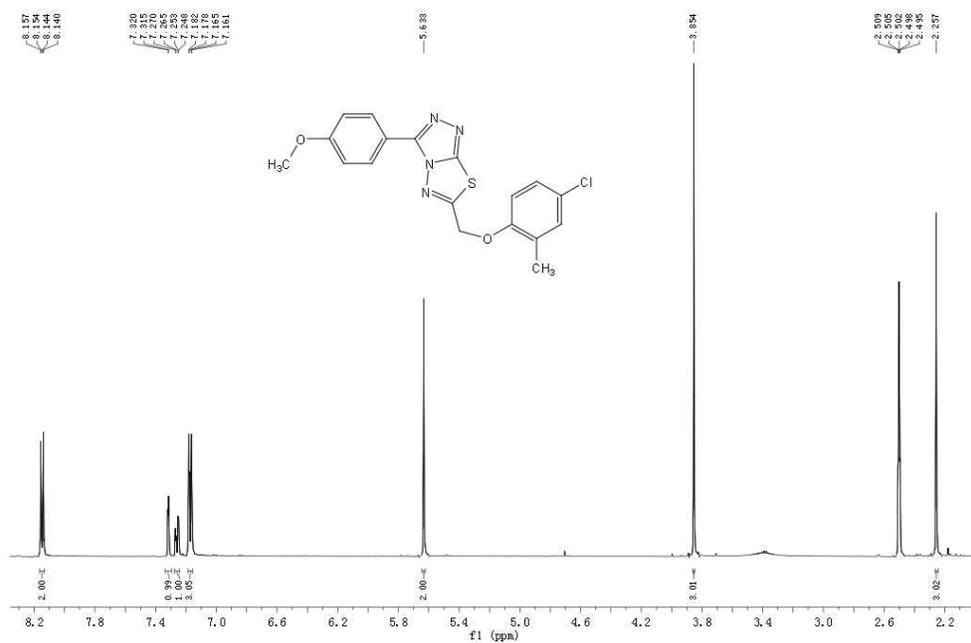
¹H NMR spectra of compound 3-(4-methoxyphenyl)-6-((2-naphthyloxy)methyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6e-7)

BRUKER AV-III-500 ¹³C-NMR ATD-131220-3 IN DMSO



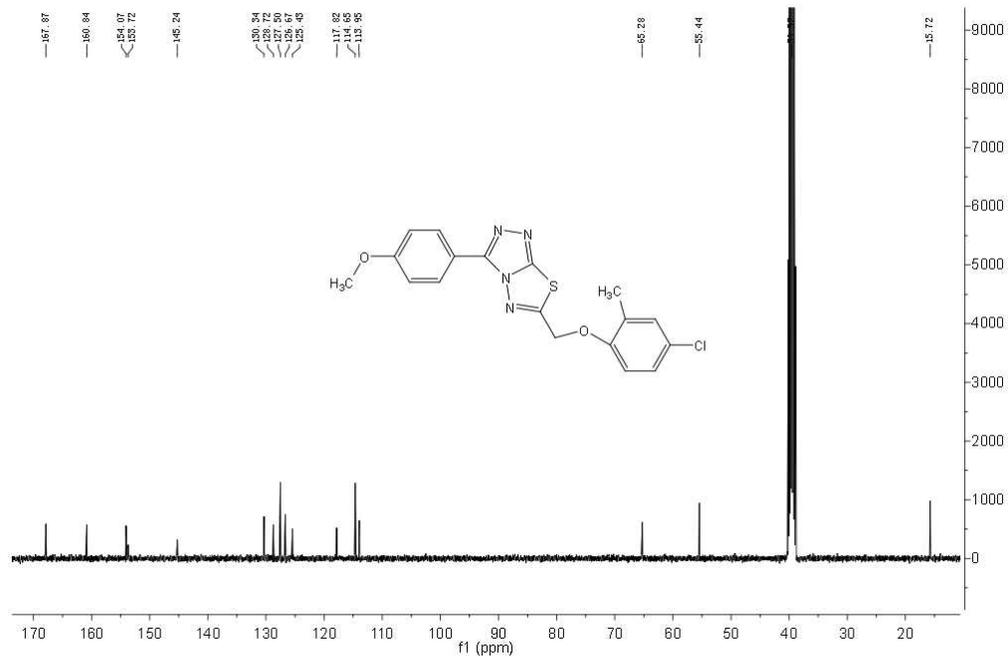
¹³C NMR spectra of compound 3-(4-methoxyphenyl)-6-((2-naphthyloxy)methyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6e-7)

BRUKER AV-III-500 1H-NMR ATD-131229-2 IN DMSO



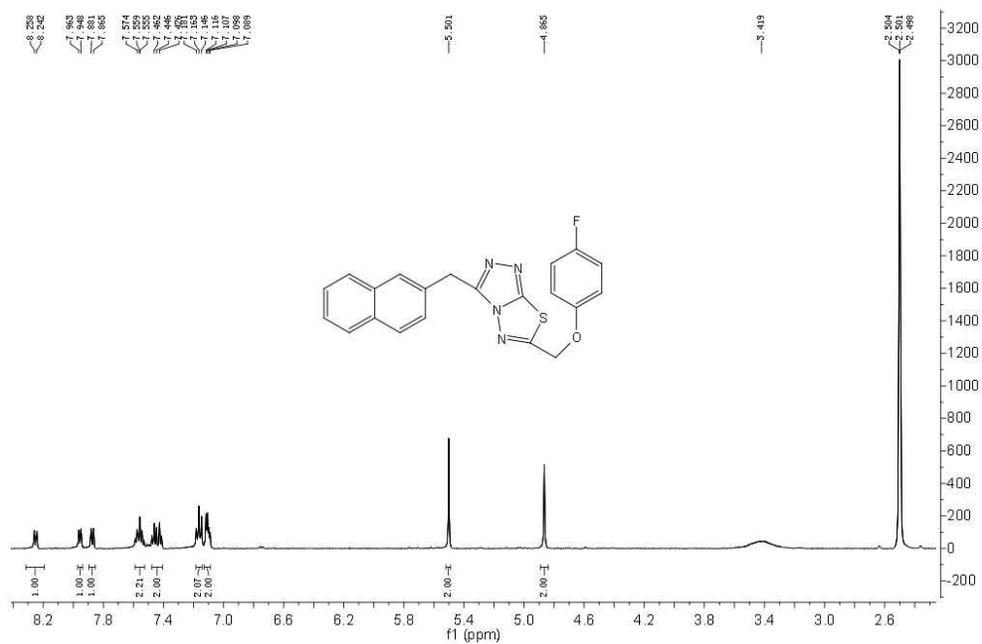
¹H NMR spectra of compound 3-(4-methoxyphenyl)-6-((2-methyl-4-chlorophenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6e-9)

BRUKER AV-III-400 ¹³C-NMR ATD-131219-2 IN DMSO



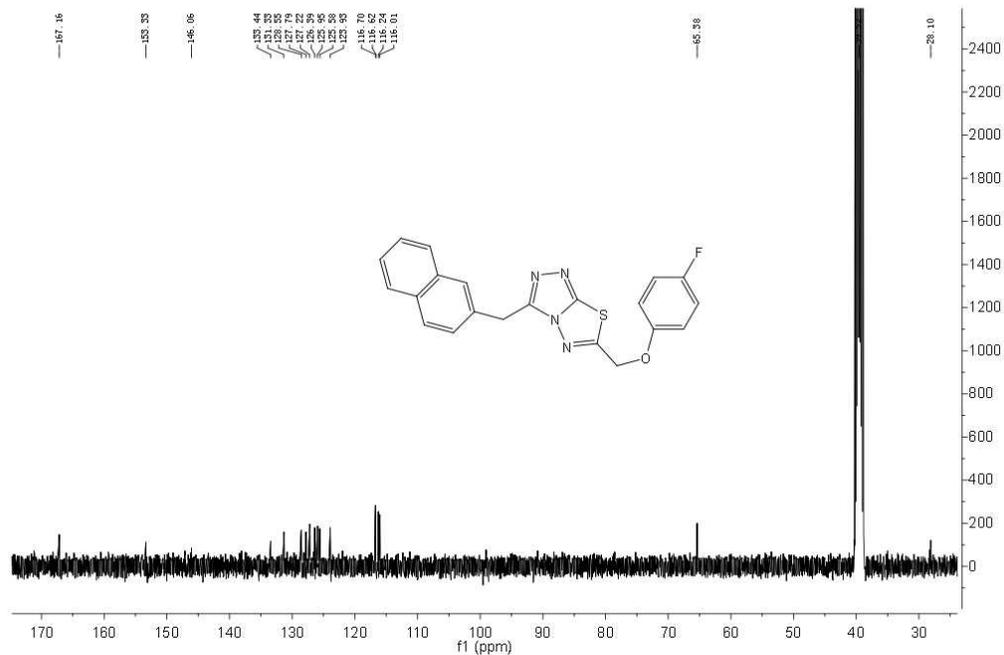
¹³C NMR spectra of compound 3-(4-methoxyphenyl)-6-((2-methyl-4-chlorophenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6e-9)

BRUKER AV-III-500 1H-NMR ATD-140108-1 IN DMSO



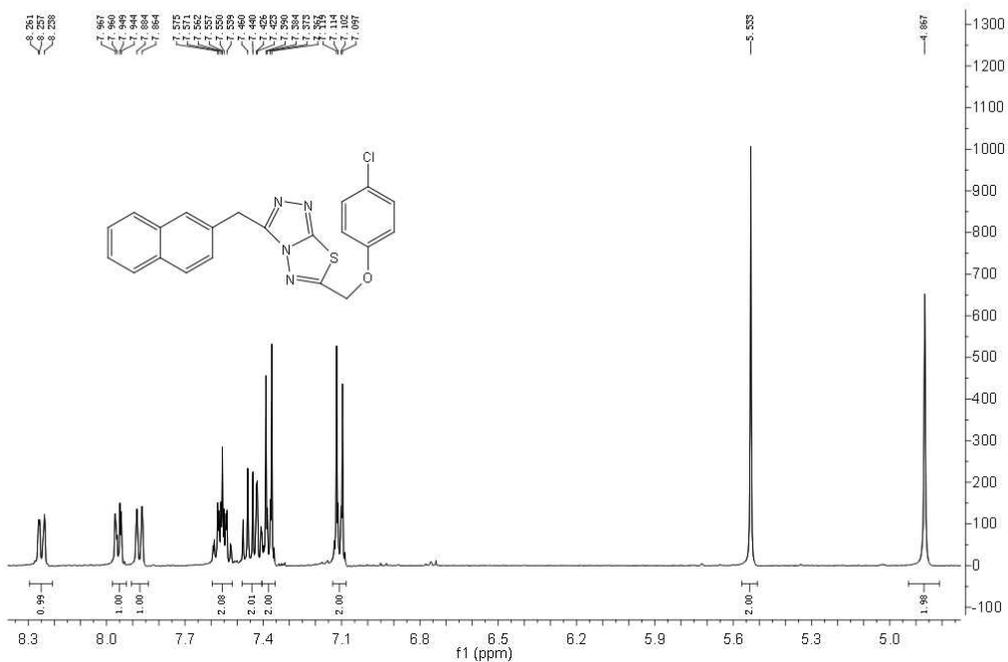
¹H NMR spectra of compound 6-((4-Fluorophenoxy)methyl)-3-(β-naphthylmethyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6f-2)

BRUKER AV-III-400 ¹³C-NMR ATD-140108-1 IN DMSO



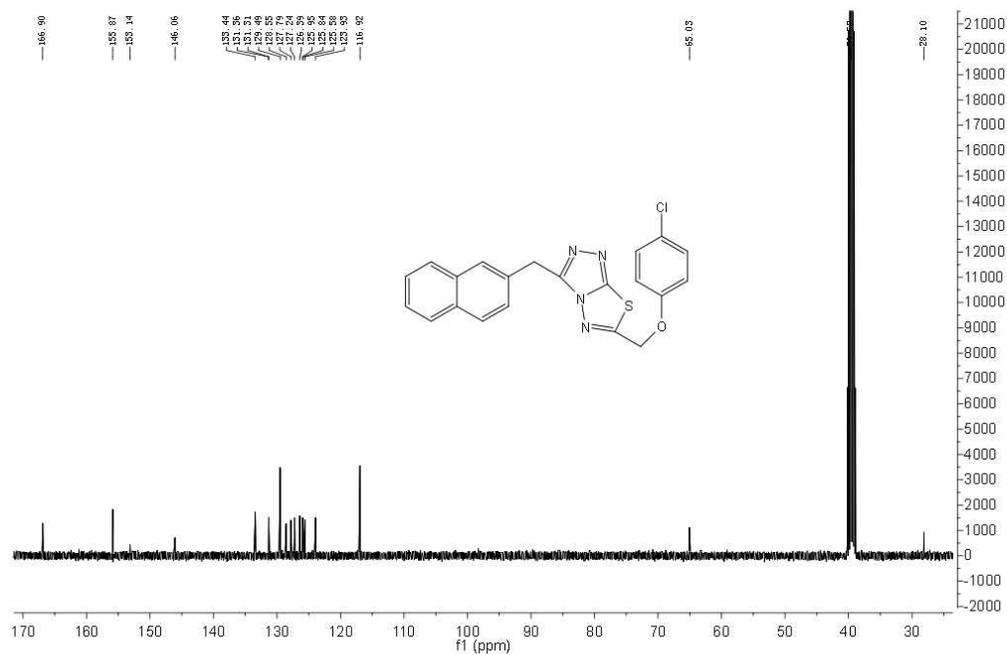
¹³C NMR spectra of compound 6-((4-Fluorophenoxy)methyl)-3-(β-naphthylmethyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6f-2)

ATD-131217-2 Bruker AVANCE III 400 20131223 PROTON2 DMSO



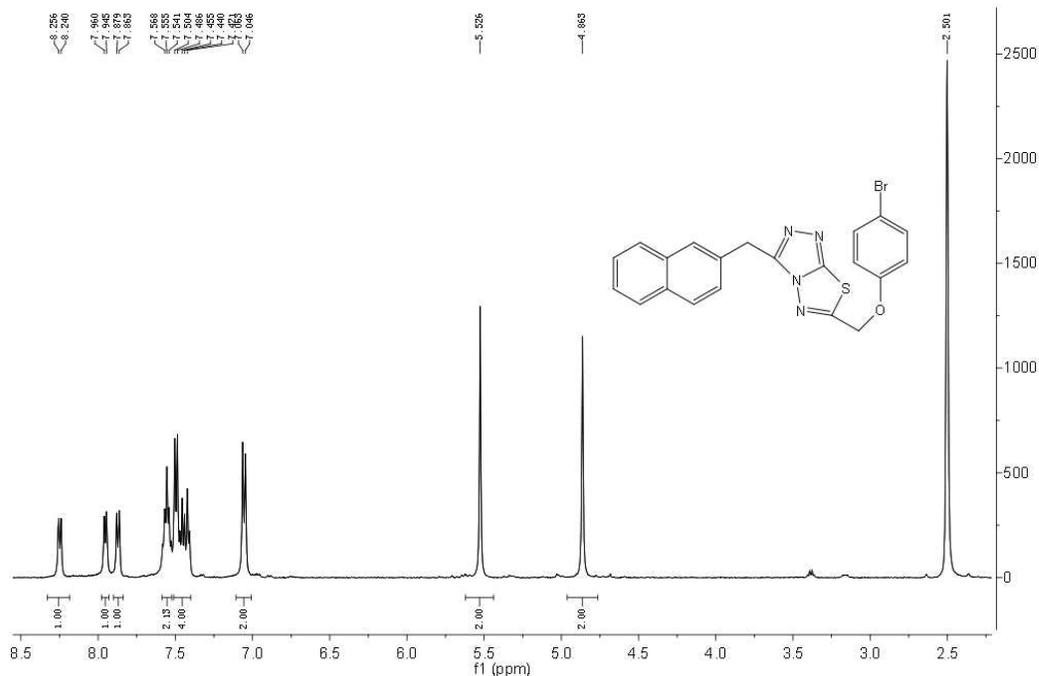
¹H NMR spectra of compound 6-((4-chlorophenoxy)methyl)-3-(6-naphthylmethyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6f-3)

BRUKER AV-III-400 ¹³C-NMR ATD-131217-2 IN DMSO



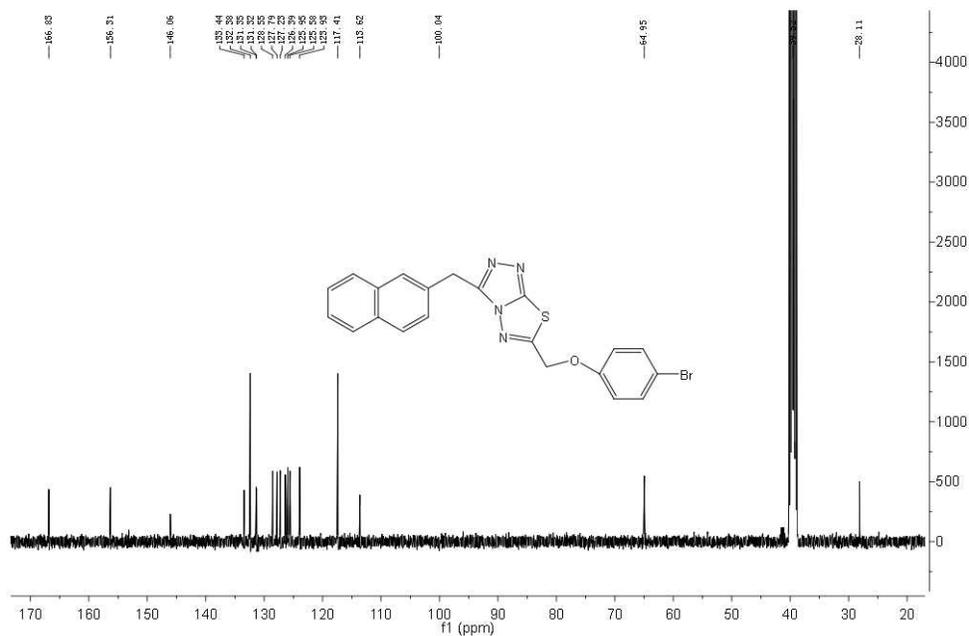
¹³C NMR spectra of compound 6-((4-chlorophenoxy)methyl)-3-(6-naphthylmethyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6f-3)

BRUKER AV-III-500 1H-NMR ATD-140101-3 IN DMSO

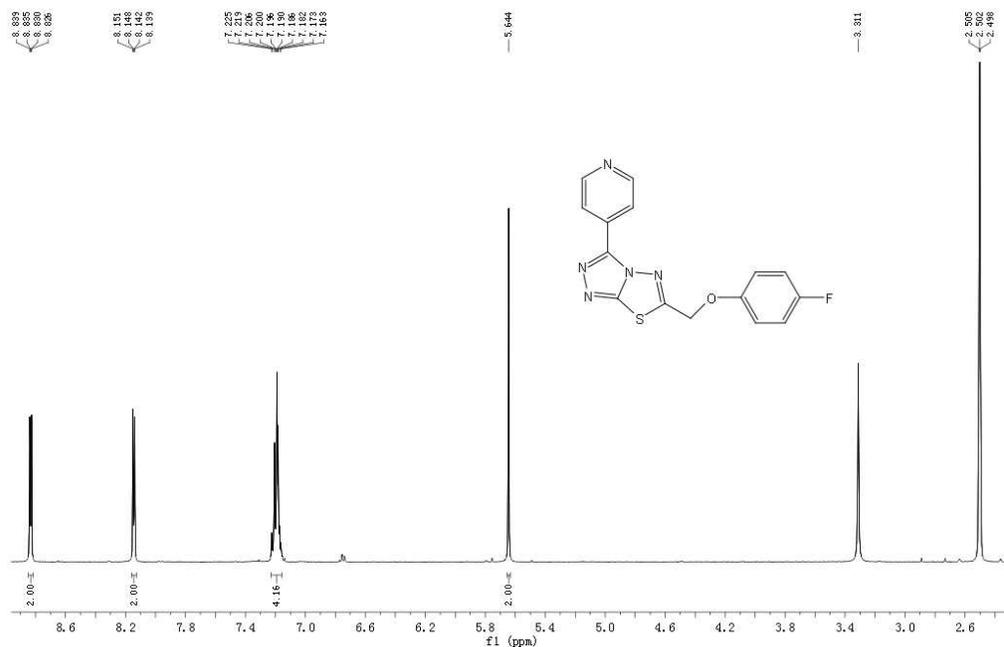


¹H NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-(8-naphthylmethyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6f-4)

BRUKER AV-III-400 ¹³C-NMR ATD-140101-3 IN DMSO

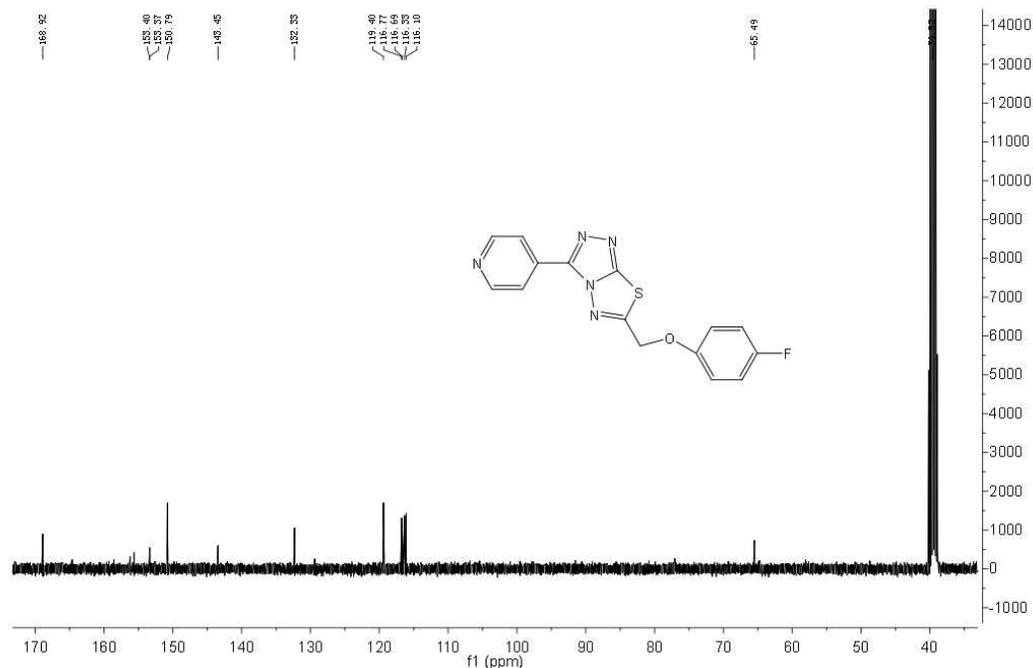


BRUKER AV-III-500 1H-NMR ATD-131224-3 IN DMSO



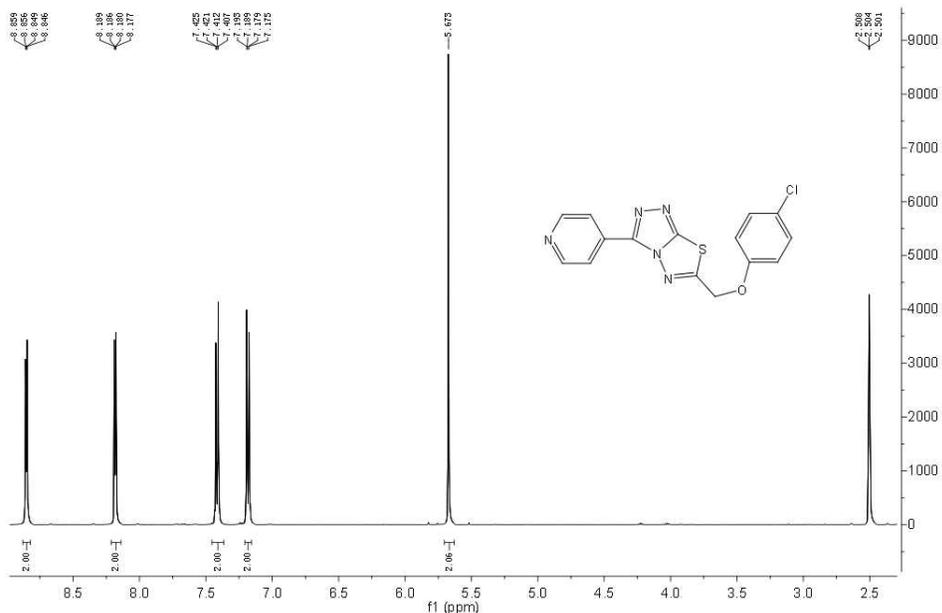
¹H NMR spectra of compound 6-((4-fluorophenoxy)methyl)-3-(pyridin-4-yl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6g-2)

BRUKER AV-III-400 ¹³C-NMR ATD-131224-3 IN DMSO

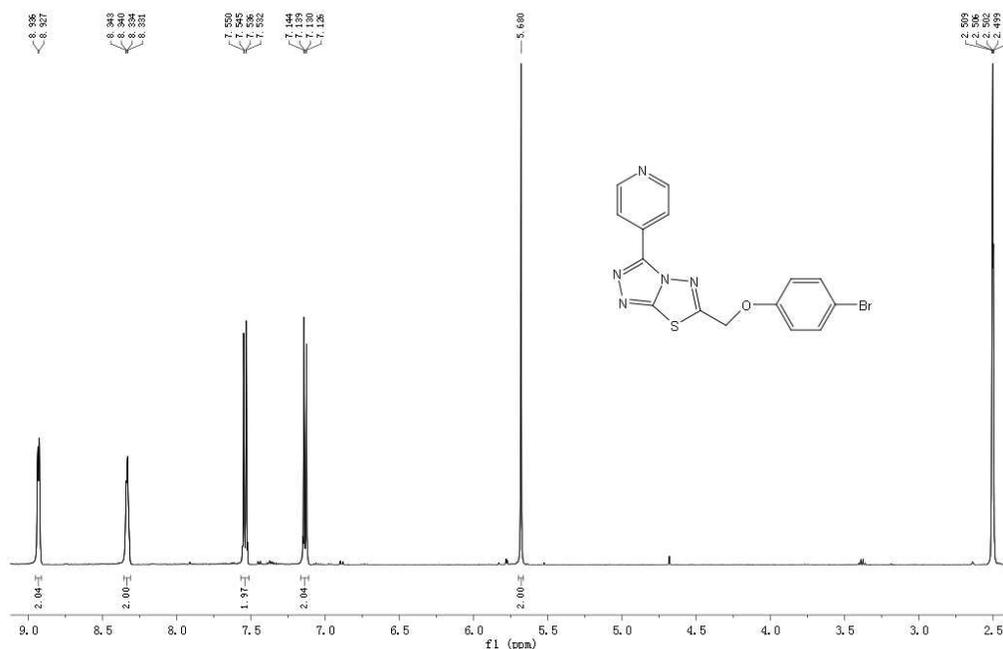


¹³C NMR spectra of compound 6-((4-fluorophenoxy)methyl)-3-(pyridin-4-yl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6g-2)

BRUKER AV-III-500 1H-NMR SMF-131027 IN DMSO

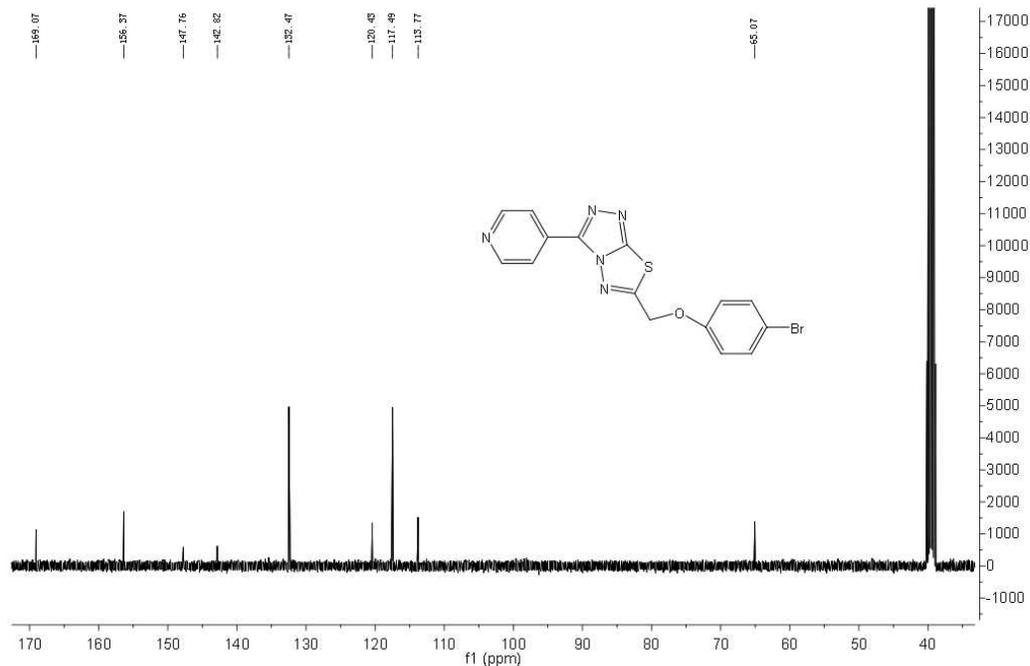


BRUKER AV-III-500 1H-NMR ATD-131224-2 IN DMSO



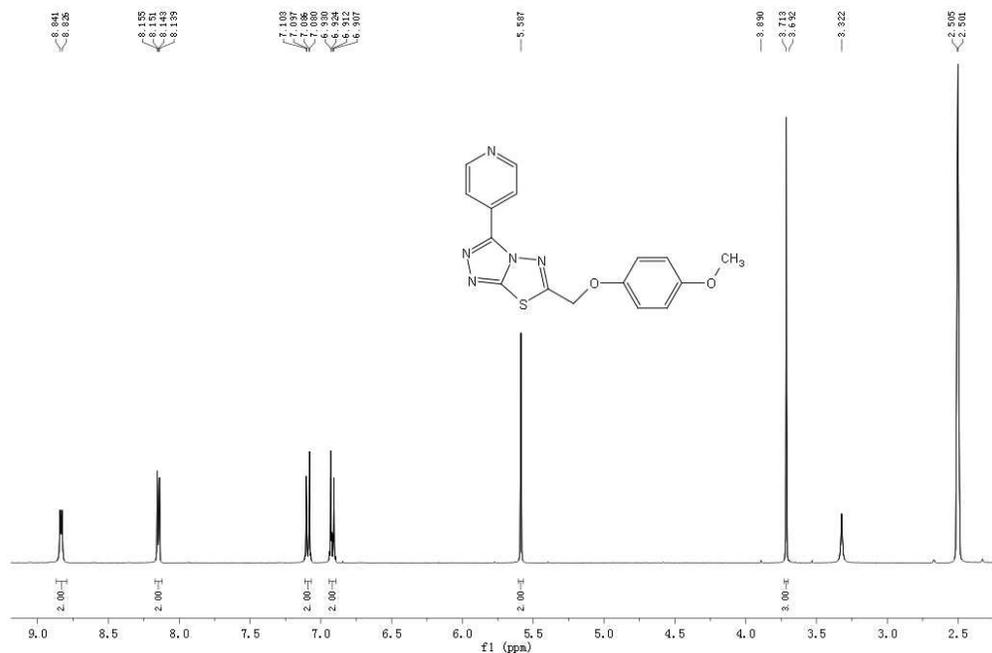
¹H NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-(pyridin-4-yl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6g-4)

BRUKER AV-III-400 ¹³C-NMR ATD-131224-2 IN DMSO



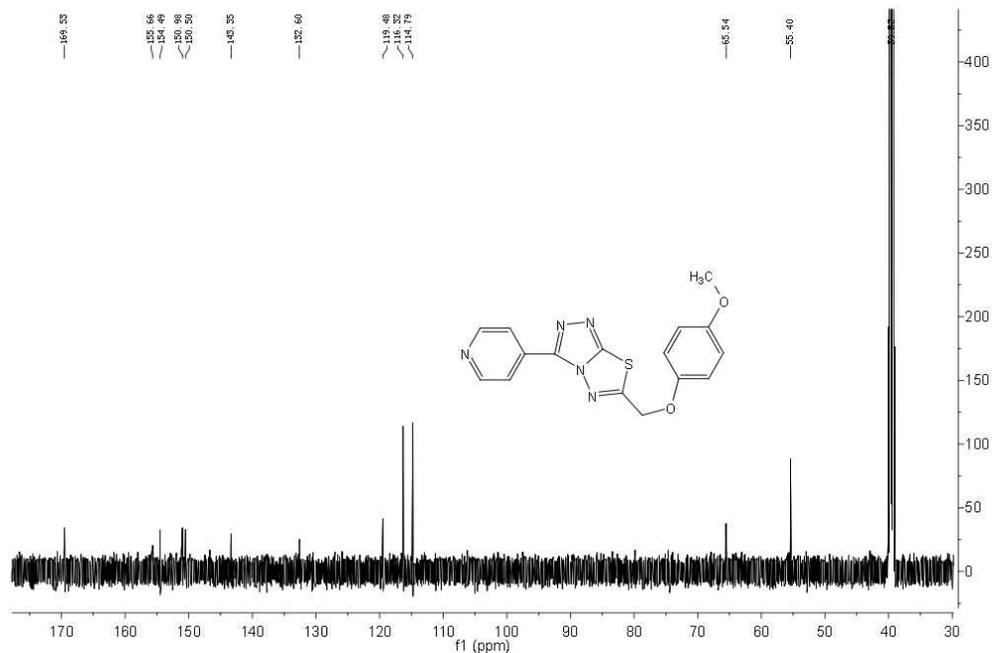
¹³C NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-(pyridin-4-yl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6g-4)

ATD-131226-3 Bruker AVANCE III 400 PROTON2 DMSO



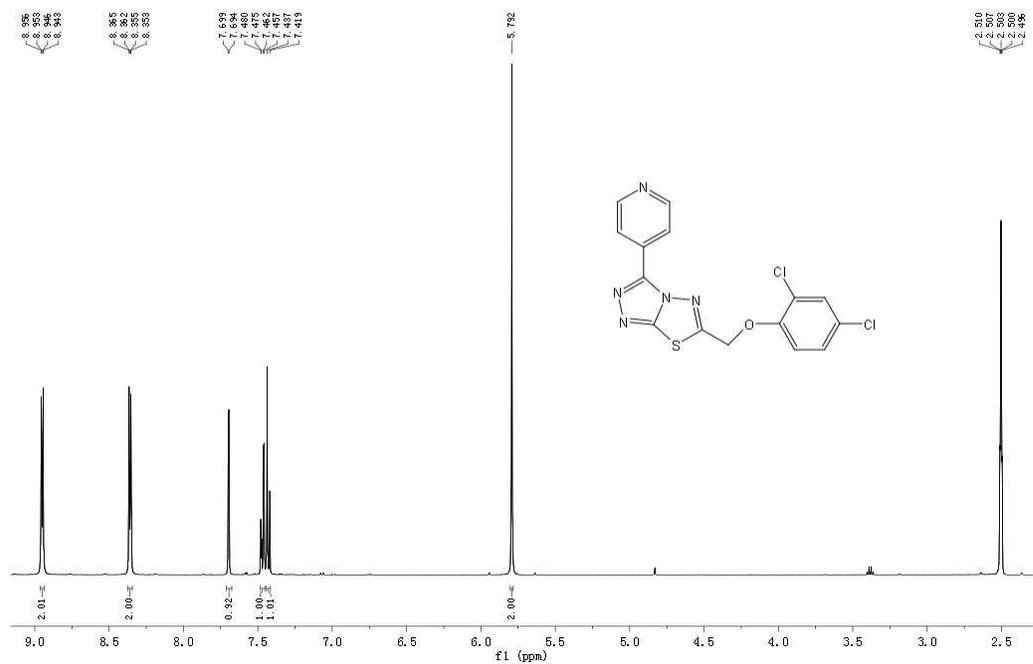
¹H NMR spectra of compound 6-((4-methoxyphenoxy)methyl)-3-(pyridin-4-yl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6g-5)

BRUKER AV-III-500 ¹³C-NMR ATD-131226-3 IN DMSO



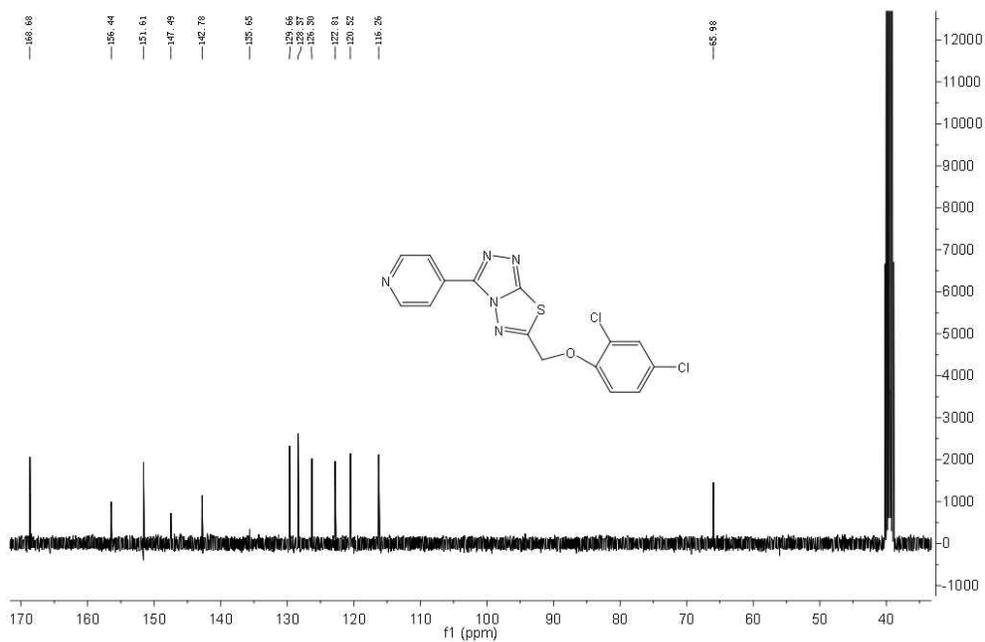
¹³C NMR spectra of compound 6-((4-methoxyphenoxy)methyl)-3-(pyridin-4-yl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6g-5)

BRUKER AV-III-500 1H-NMR ATD-131224-1 IN DMSO



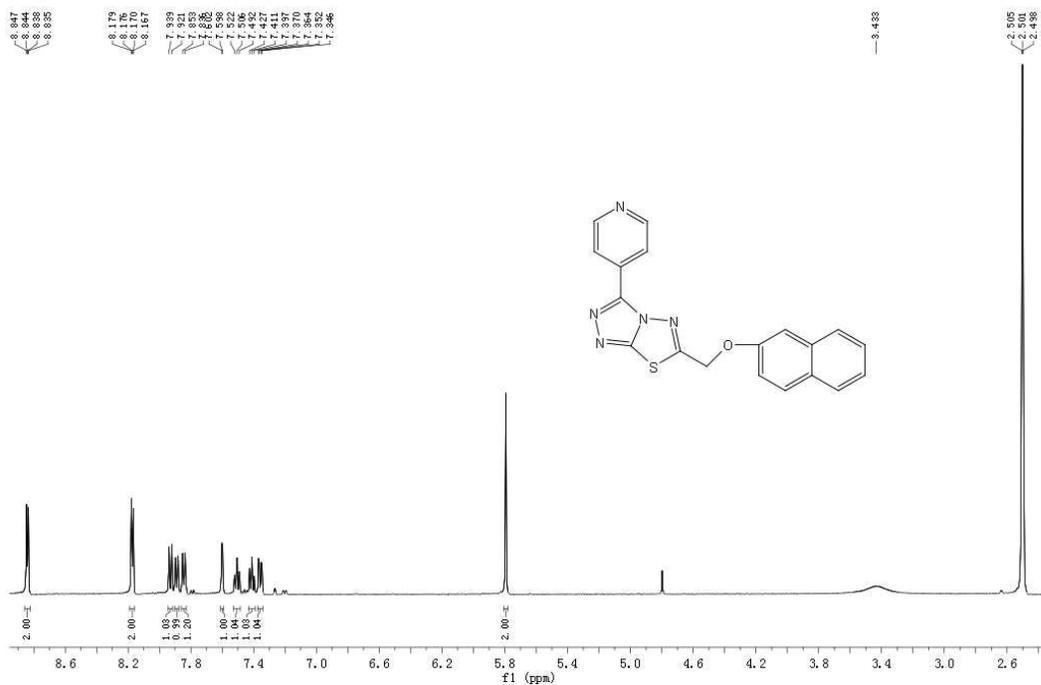
¹H NMR spectra of compound 6-((2,4-dichlorophenoxy)methyl)-3-(pyridin-4-yl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6g-6)

BRUKER AV-III-400 ¹³C-NMR ATD-131224-1 IN DMSO

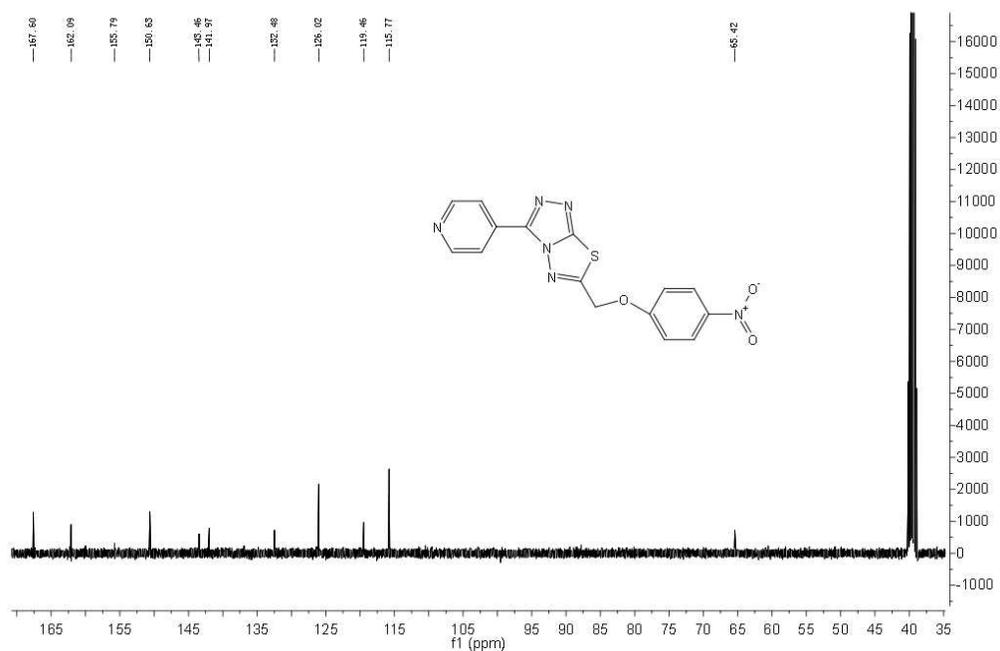


¹³C NMR spectra of compound 6-((2,4-dichlorophenoxy)methyl)-3-(pyridin-4-yl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6g-6)

BRUKER AV-III-500 1H-NMR ATO-131226-1 IN DMSO

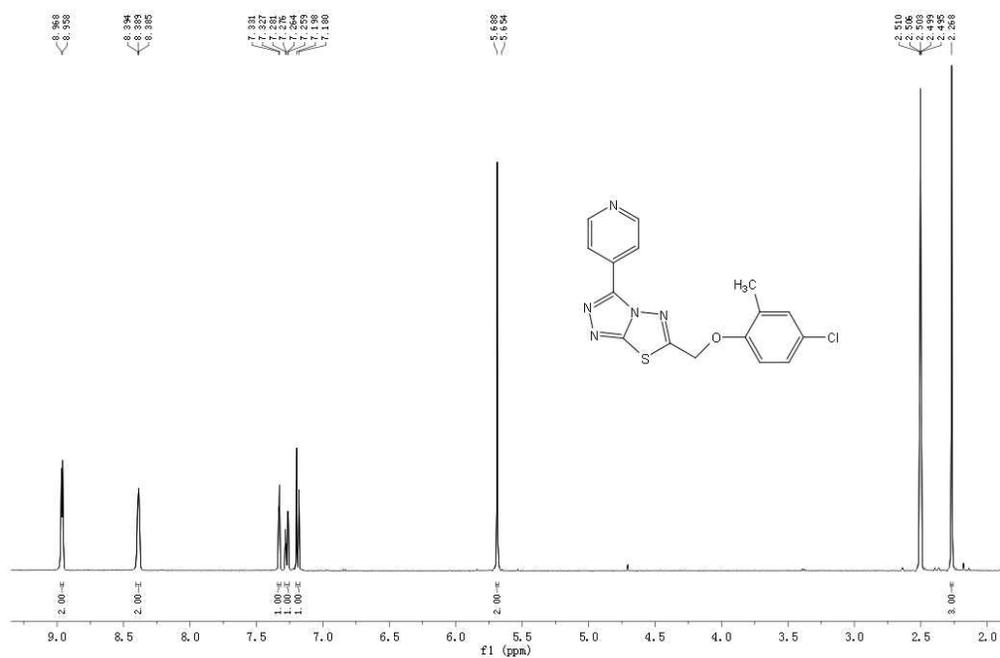


BRUKER AV-III-400 ¹³C-NMR ATD-131228-2 IN DMSO

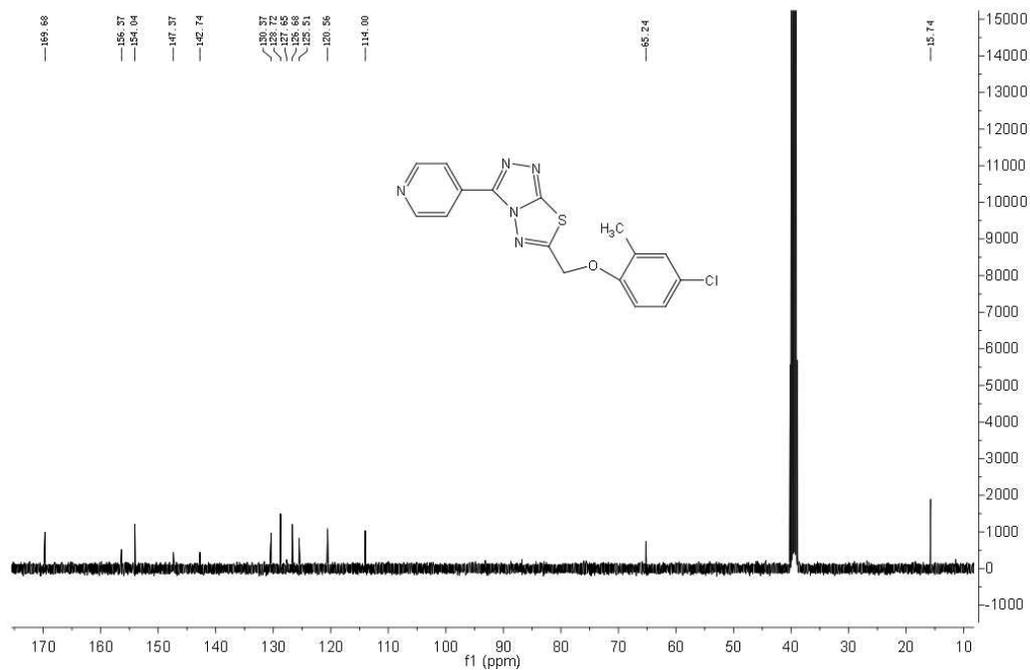


¹³C NMR spectra of compound 6-((4-nitrophenoxy)methyl)-3-(pyridin-4-yl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6g-8)

BRUKER AV-III-500 ¹H-NMR ATD-131228-1 IN DMSO

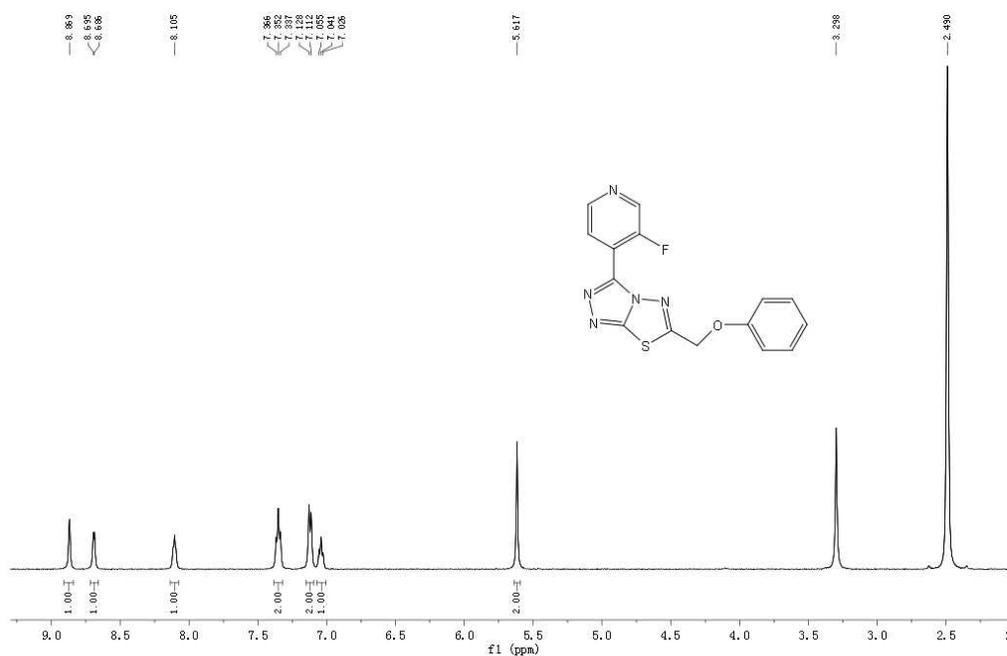


BRUKER AV-III-400 ¹³C-NMR ATD-131228-1 IN DMSO



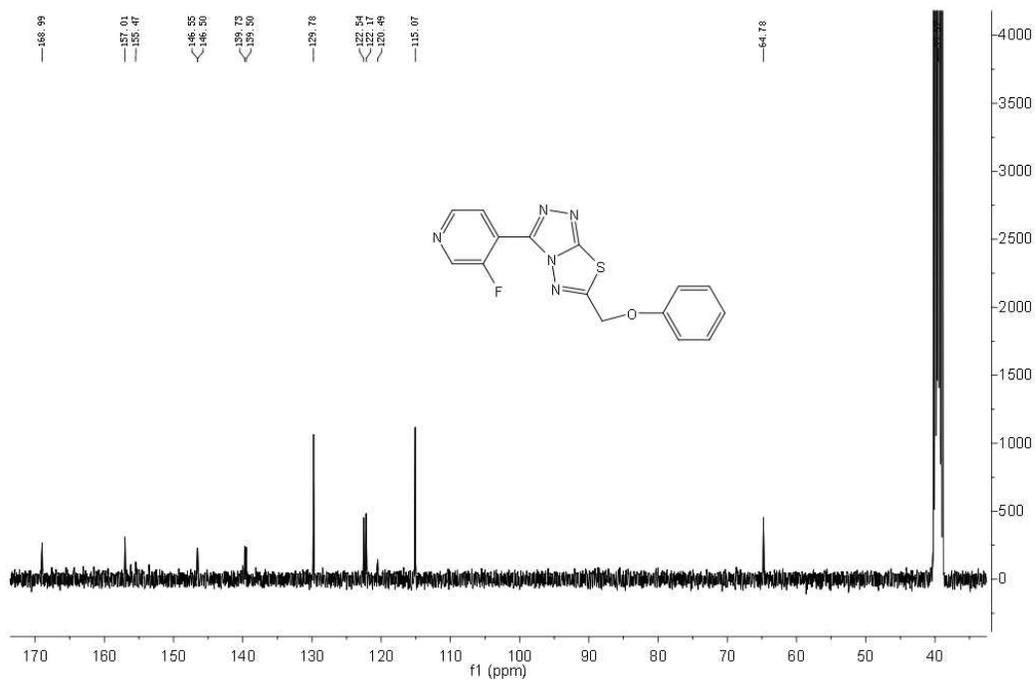
¹³C NMR spectra of compound 6-((2-methyl-4-chlorophenoxy)methyl)-3-(pyridin-4-yl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6g-9)

ATD-140318-1 BRUKER AV-III-500 ¹H-NMR ATD-140318-1 IN DMSO



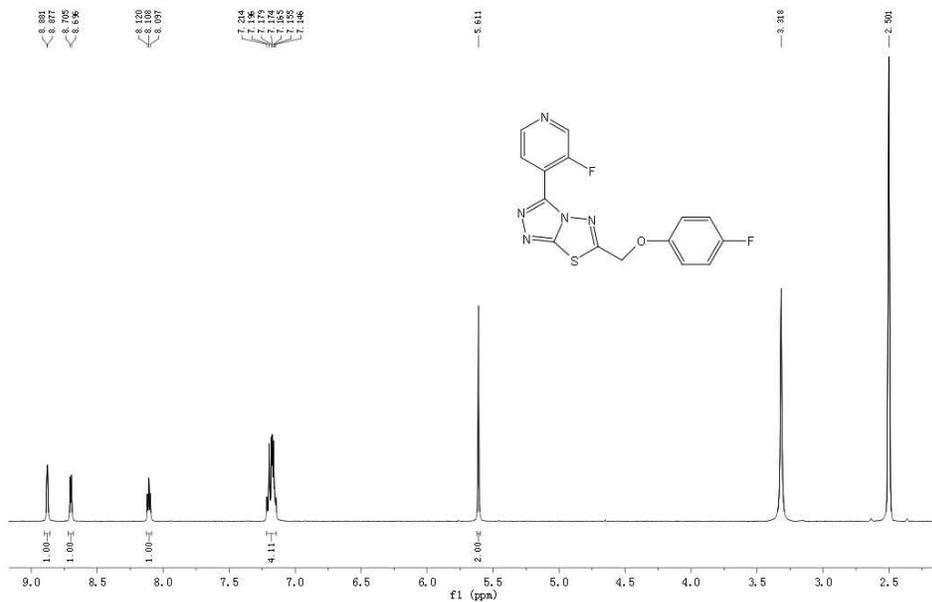
¹H NMR spectra of compound 3-(3-fluoropyridin-4-yl)-6-(phenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6h-1)

BRUKER AV-III-400 ¹³C-NMR ATD-140318-1 IN DMSO



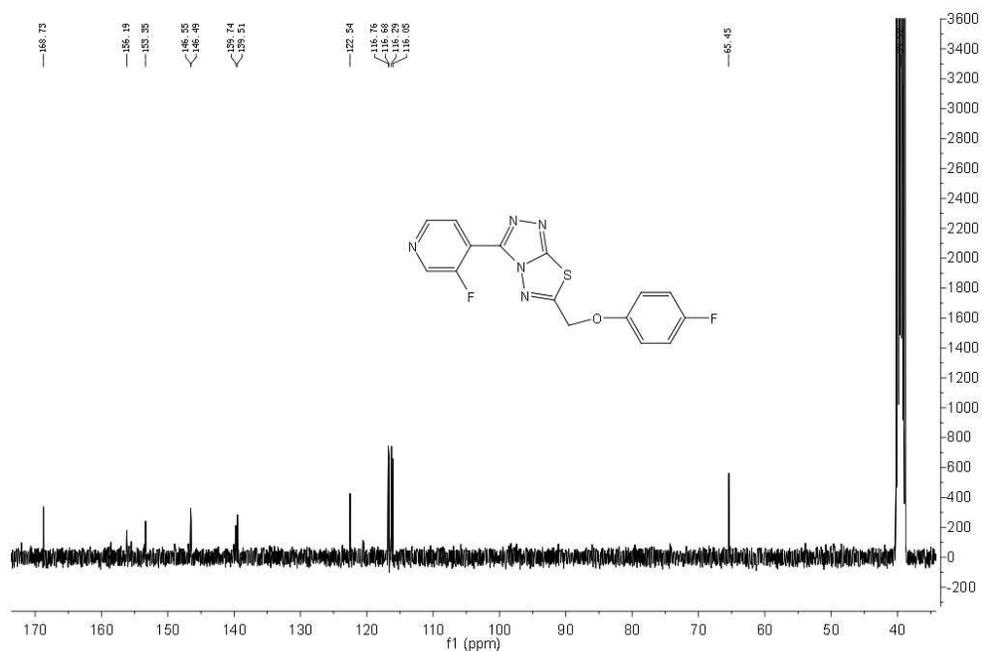
¹³C NMR spectra of compound 3-(3-fluoropyridin-4-yl)-6-(phenoxymethyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6h-1)

BRUKER AV-III-500 ¹H-NMR ATD-140323-1 IN DMSO



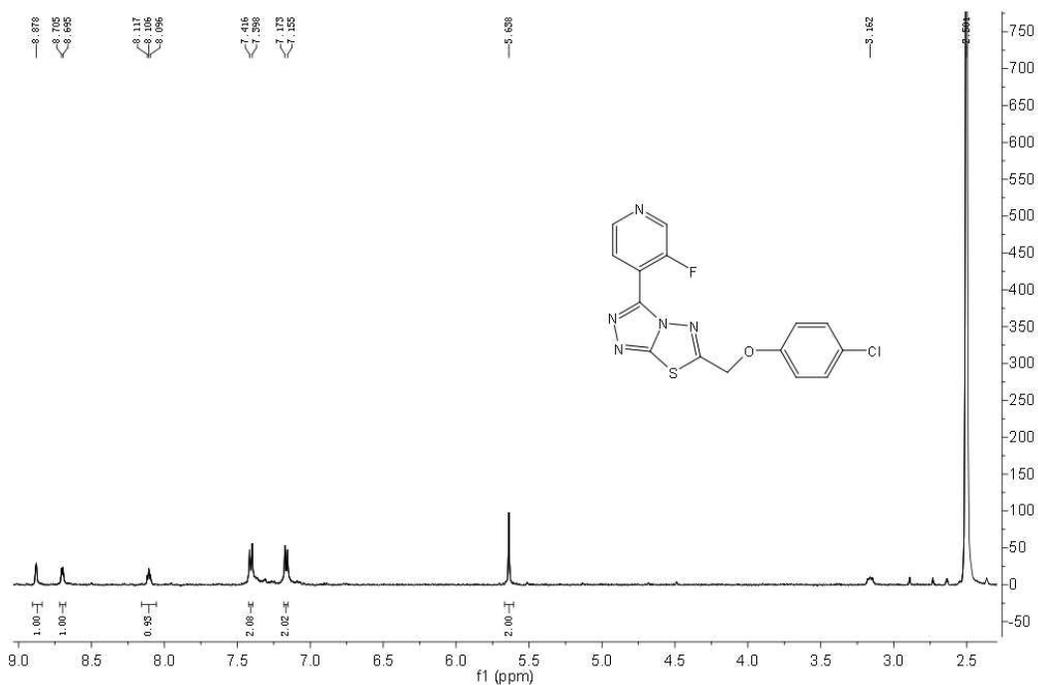
¹H NMR spectra of compound 6-((4-fluorophenoxy)methyl)-3-(3-fluoropyridin-4-yl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6h-2)

BRUKER AV-III-400 ¹³C-NMR ATD-140323-1 IN DMSO



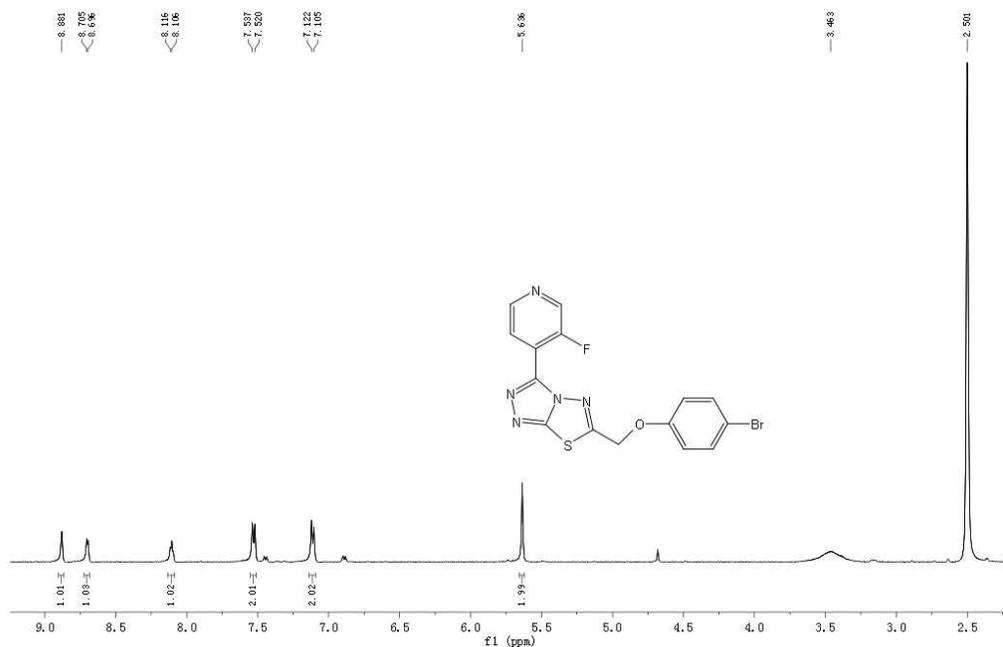
¹³C NMR spectra of compound 6-((4-fluorophenoxy)methyl)-3-(3-fluoropyridin-4-yl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6h-2)

BRUKER AV-III-500 ¹H-NMR ATD-140320-2 IN DMSO



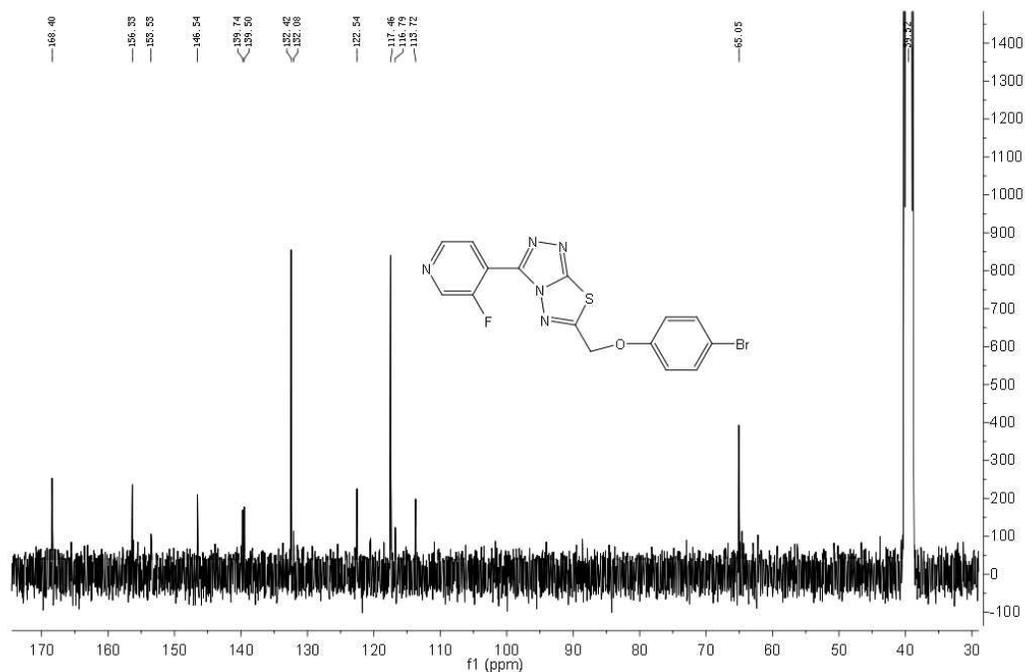
¹H NMR spectra of compound 6-((4-chlorophenoxy)methyl)-3-(3-fluoropyridin-4-yl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6h-3)

BRUKER AV-III-500 1H-NMR ATD-140320-3 IN DMSO



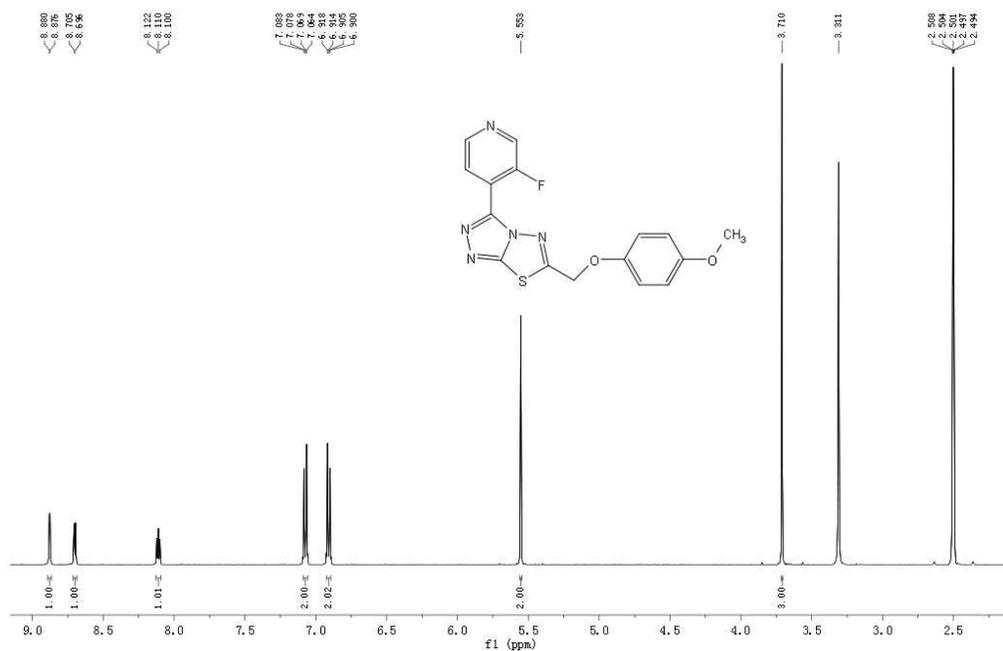
¹H NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-(3-fluoropyridin-4-yl)-[1,2,4]thiazolo [3,4-b][1,3,4]thiadiazole (6h-4)

BRUKER AV-III-400 ¹³C-NMR ATD-140320-3 IN DMSO



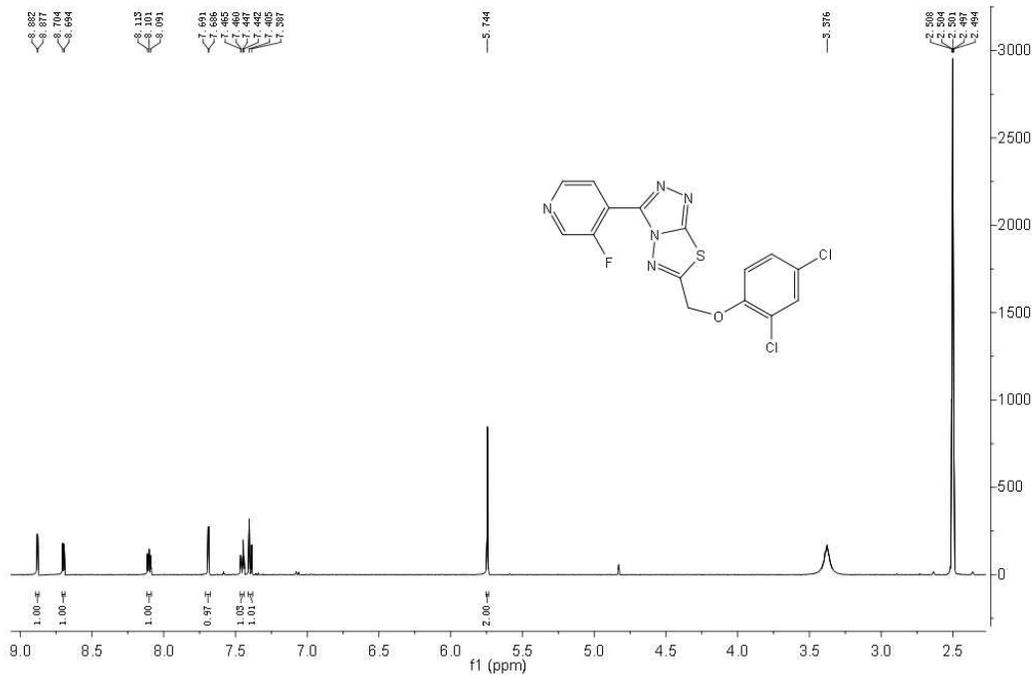
¹³C NMR spectra of compound 6-((4-bromophenoxy)methyl)-3-(3-fluoropyridin-4-yl)-[1,2,4]thiazolo [3,4-b][1,3,4]thiadiazole (6h-4)

BRUKER AV-III-500 1H-NMR ATD-140323-3 IN DMSO



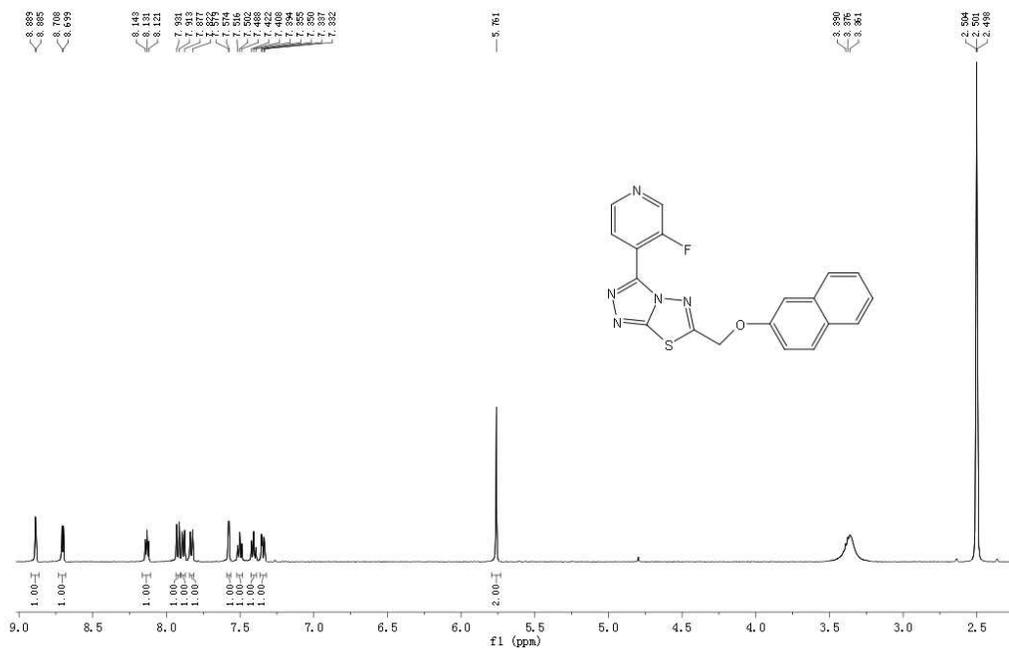
¹H NMR spectra of compound 3-(3-fluoropyridin-4-yl)-6-((4-methoxyphenoxy)methyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6h-5)

BRUKER AV-III-500 1H-NMR ATD-140320-1 IN DMSO



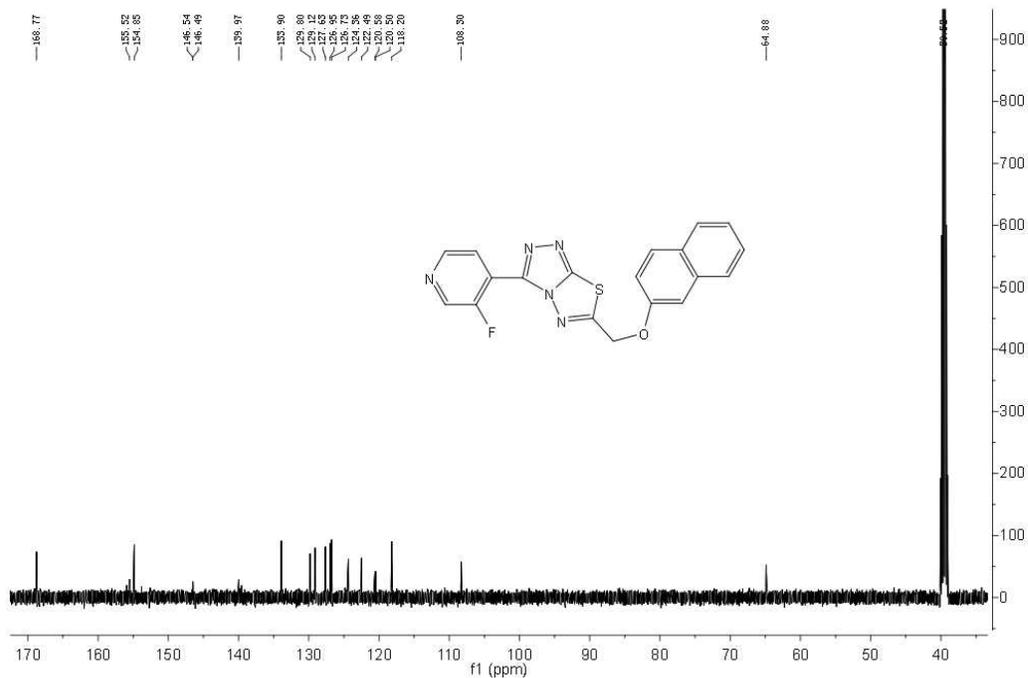
¹H NMR spectra of compound 6-((2,4-dichlorophenoxy)methyl)-3-(3-fluoropyridin-4-yl)-[1,2,4] triazolo[3,4-b][1,3,4]thiadiazole (6h-6)

BRUKER AV-III-500 1H-NMR ATD-140323-2 IN DMSO



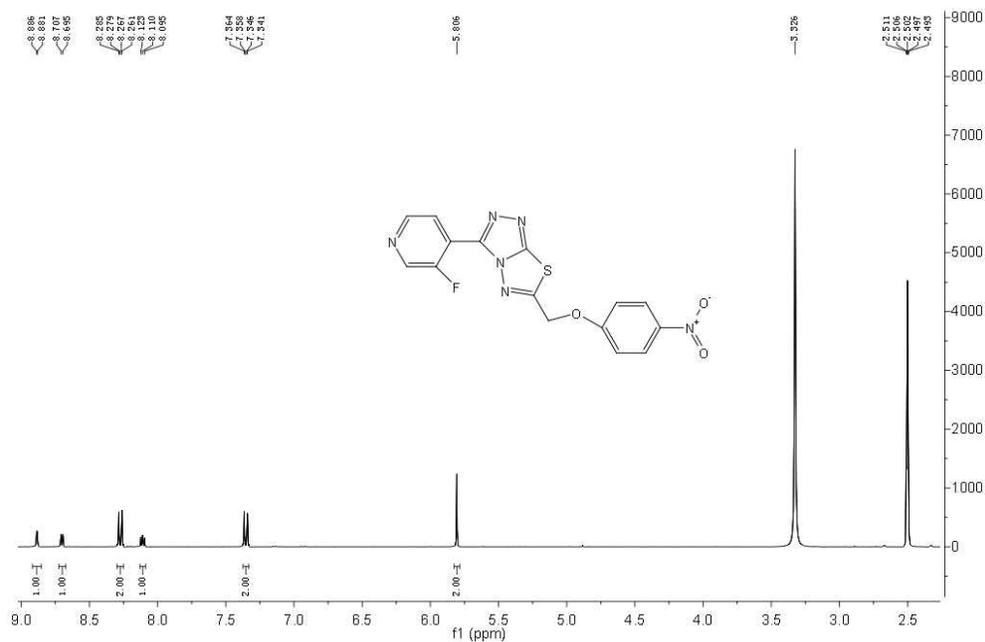
¹H NMR spectra of compound 3-(3-fluoropyridin-4-yl)-6-((2-naphthyloxy)methyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6h-7)

BRUKER AV-III-500 ¹³C-NMR ATD-140323-2 IN DMSO



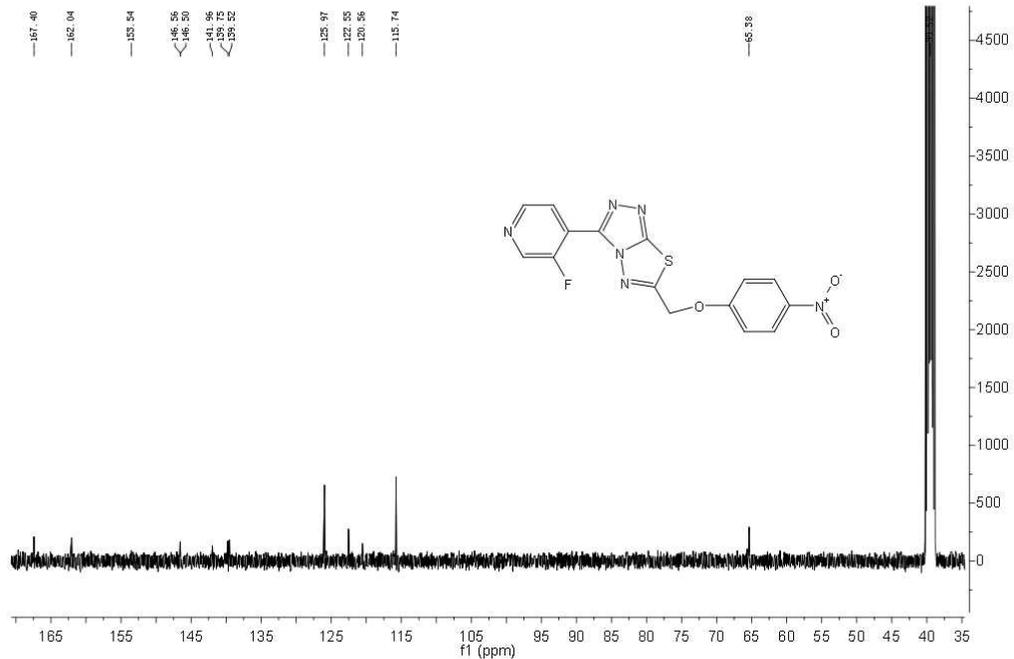
¹³C NMR spectra of compound 3-(3-fluoropyridin-4-yl)-6-((2-naphthyloxy)methyl)-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazole (6h-7)

BRUKER AV-III-400 1H-NMR ATD-140324-2 IN DMSO



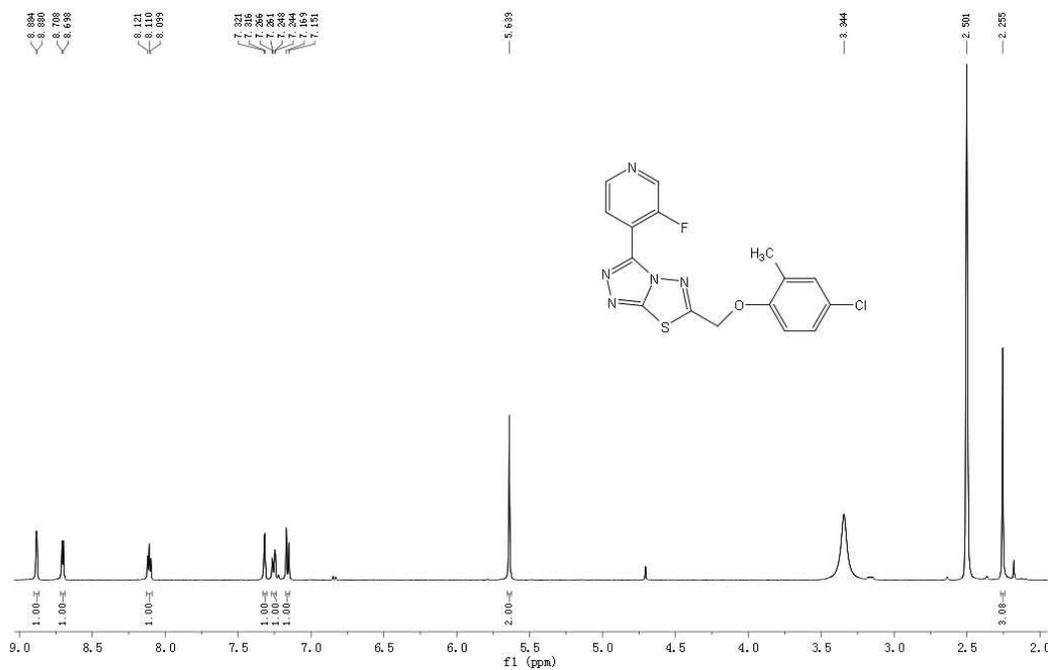
¹H NMR spectra of compound 3-(3-fluoropyridin-4-yl)-6-((4-nitrophenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6h-8)

BRUKER AV-III-400 ¹³C-NMR ATD-140324-2 IN DMSO



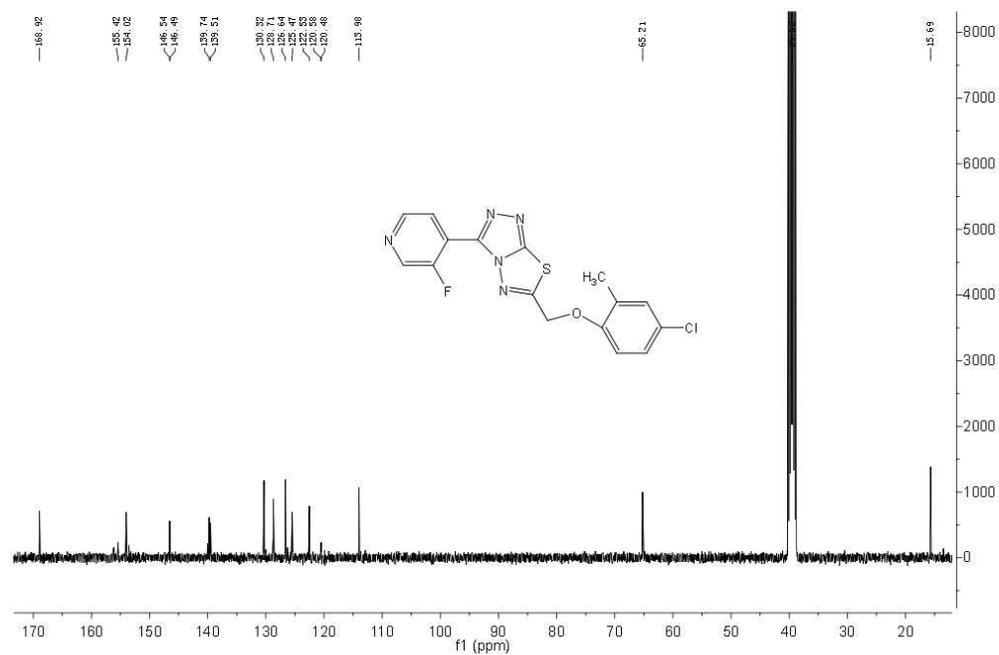
¹³C NMR spectra of compound 3-(3-fluoropyridin-4-yl)-6-((4-nitrophenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6h-8)

BRUKER AV-III-500 1H-NMR ATD-140324-1 IN DMSO



¹H NMR spectra of compound 3-(3-fluoropyridin-4-yl)-6-((2-methyl-4-chlorophenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6h-9)

BRUKER AV-III-400 ¹³C-NMR ATD-140324-1 IN DMSO



¹³C NMR spectra of compound 3-(3-fluoropyridin-4-yl)-6-((2-methyl-4-chlorophenoxy)methyl)-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (6h-9)