DOPNALAB

	Item	Value
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	Spectrum name	GS-BOS1
	Sample name	GS-BOS
	Sample ID	
	Option	
	Comment	
	No. of Scans	10
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

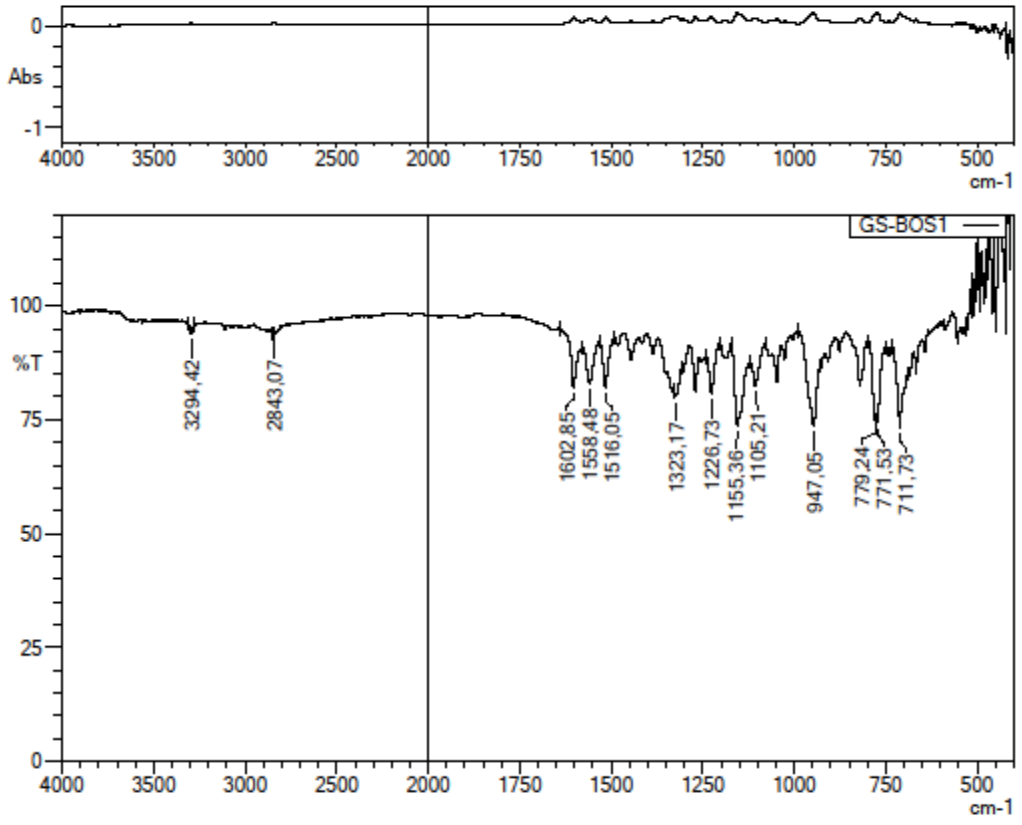

Figure S1. IR spectra of compound **3a**.

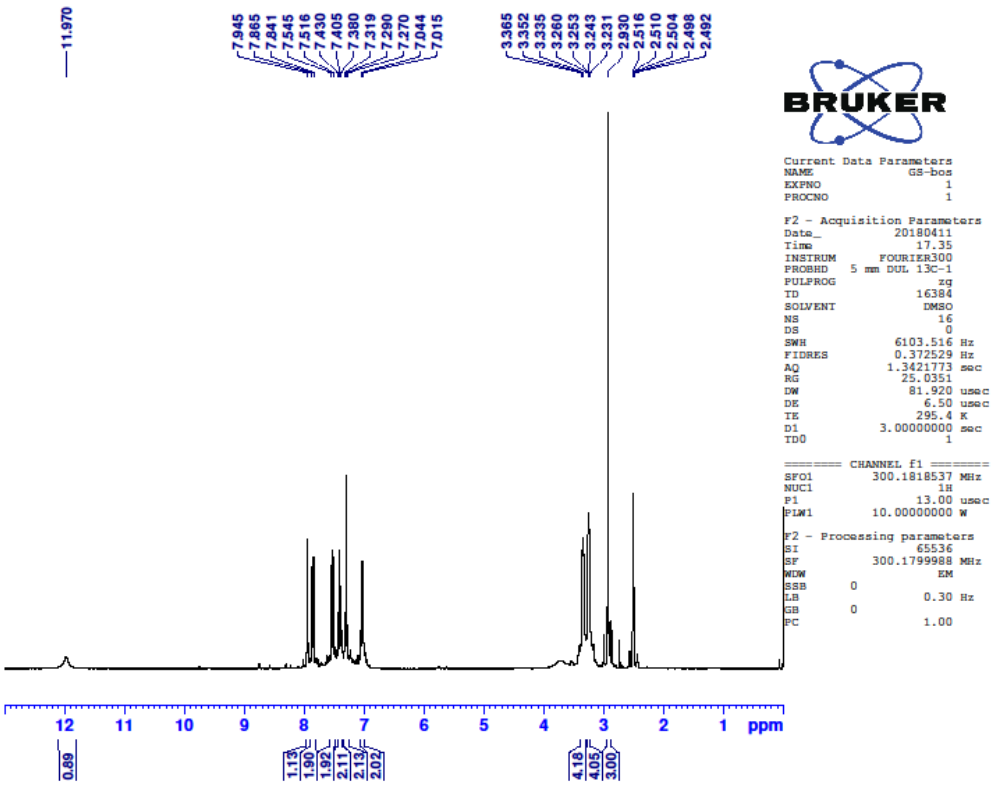

Figure S2. [1]H-NMR spectra of compound **3a**.

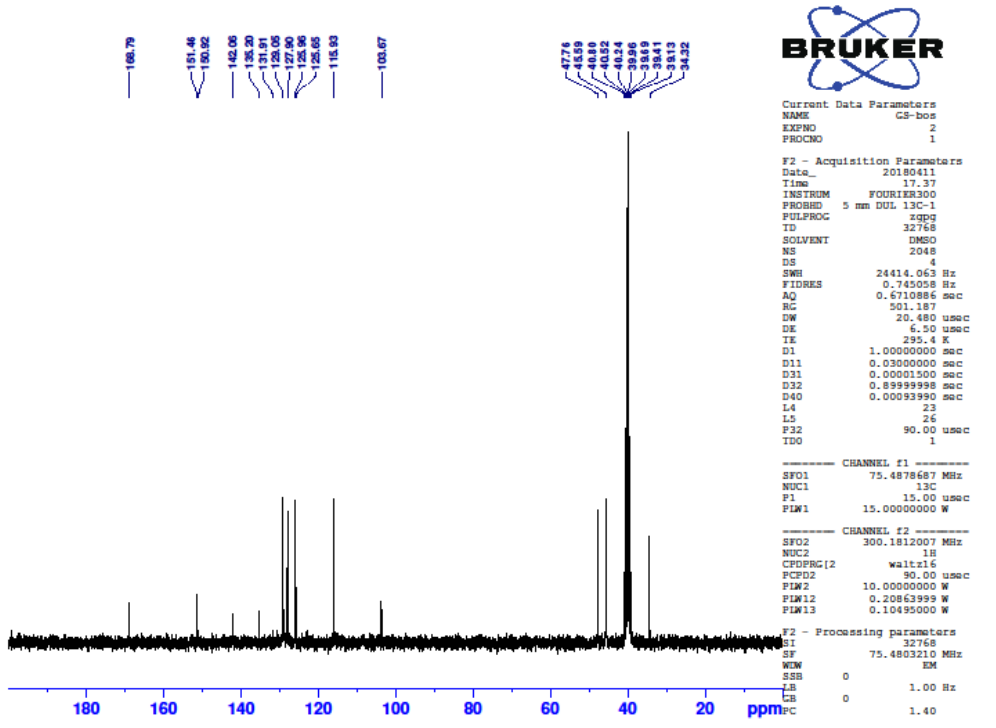

Figure S3. [13]C-NMR spectra of compound **3a**.

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: GS-Bos
Sample ID	:
Vail #	: 5
Injection Volume	: 0.3 uL
Data File Name	: GS-Bos_19.lcd
Method File Name	: genel.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 19.04.2018 12:52:35
Data Processed	: 19.04.2018 13:03:39

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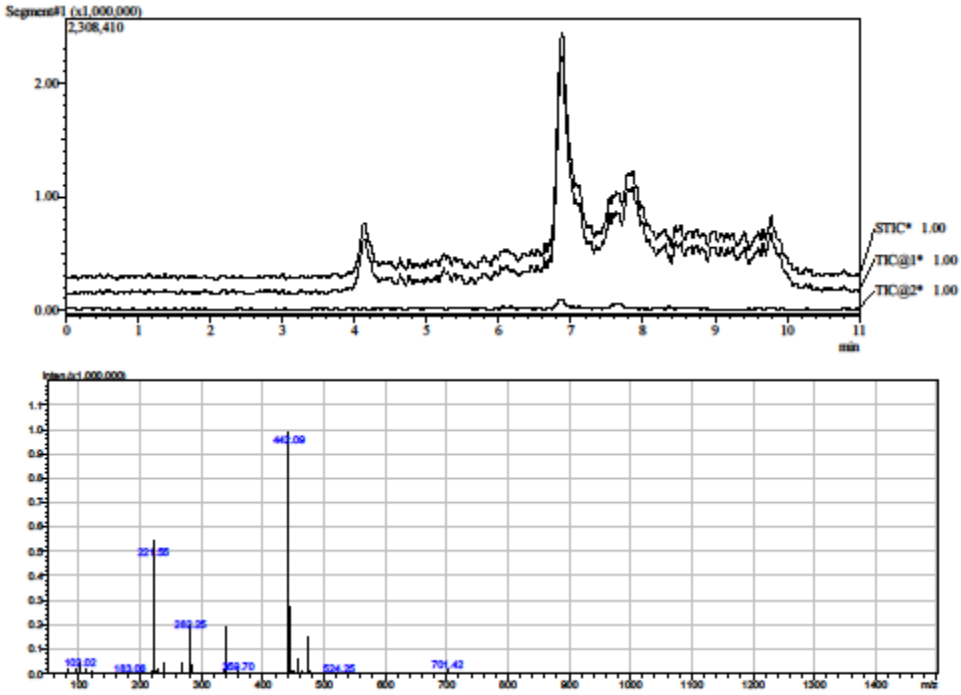

Figure S4. LCMSMS spectra of compound **3a**.

DOPNALAB

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	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\derya\ahmet osman tokay\GS-ME1.ispd
	Spectrum name	GS-ME1
	Sample name	GS-ME
	Sample ID	
	Option	
	Comment	
	No. of Scans	10
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

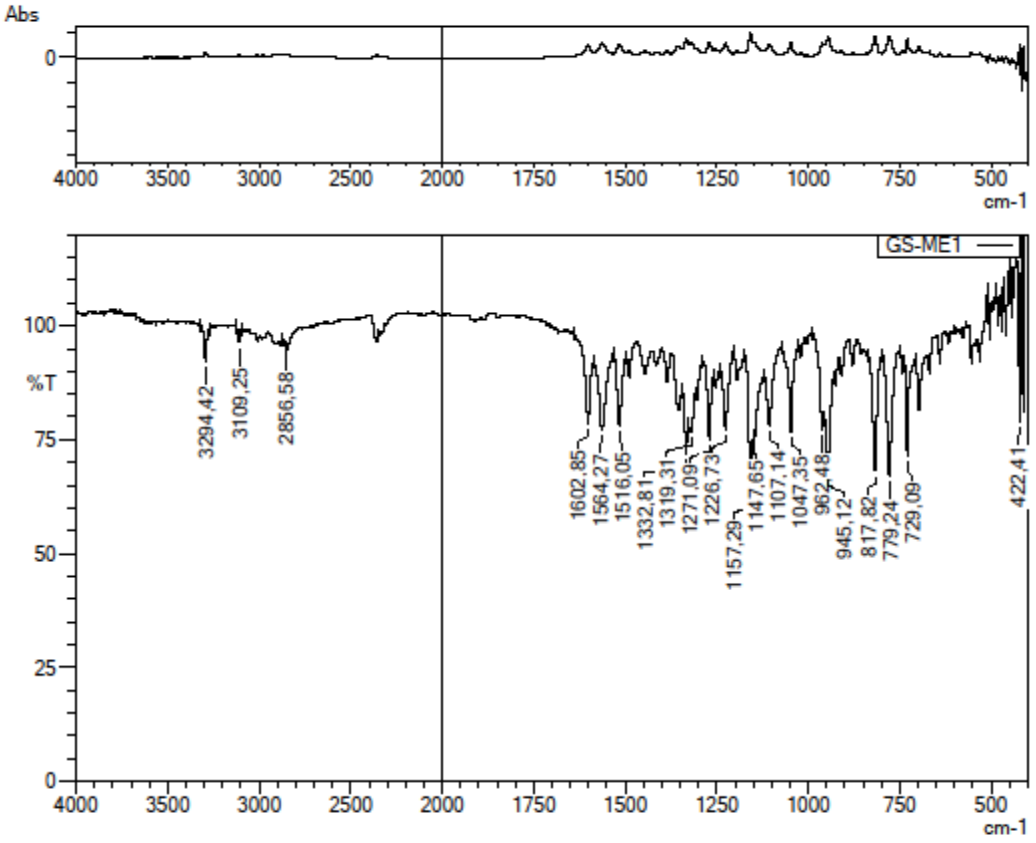

Figure S5. IR spectra of compound **3b**.

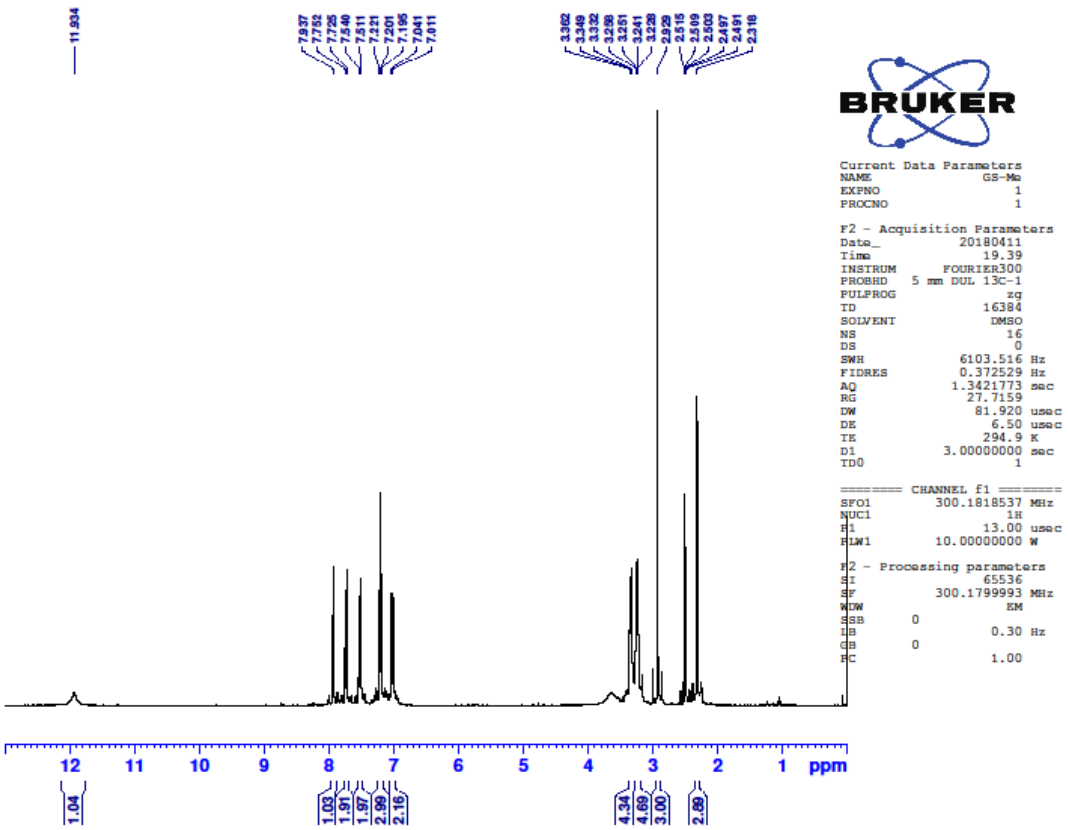

Figure S6. [1]H-NMR spectra of compound **3b**.

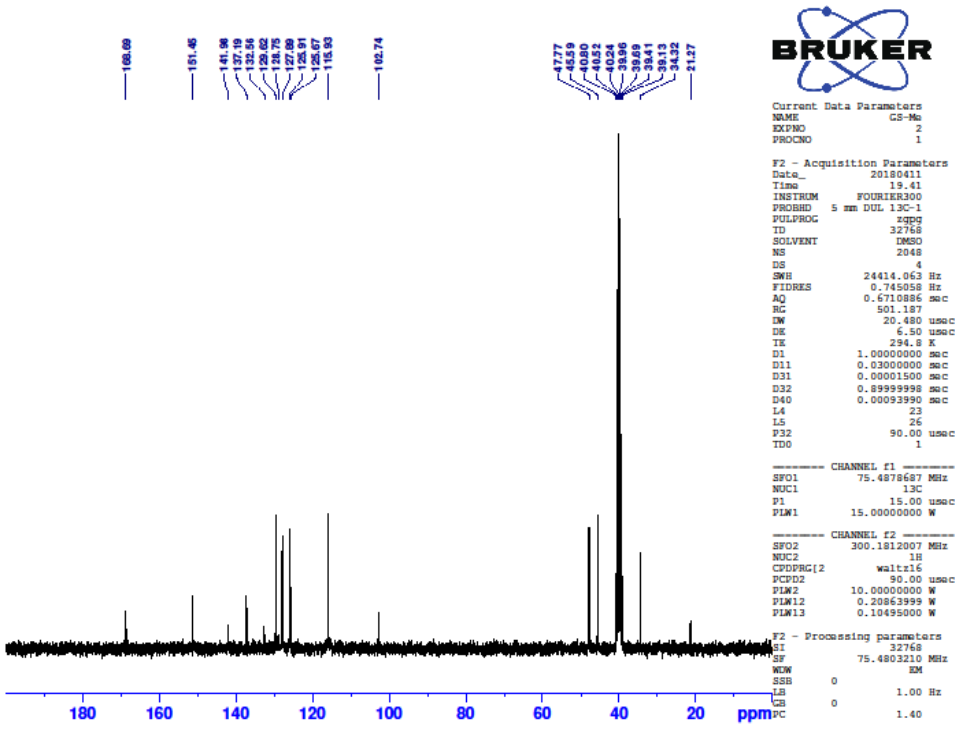

Figure S7. [13]C-NMR spectra of compound **3b**.

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: GS-Me
Sample ID	:
Vail #	: 6
Injection Volume	: 0.3 uL
Data File Name	: GS-Me_20.lcd
Method File Name	: genel.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 19.04.2018 13:04:10
Data Processed	: 19.04.2018 13:15:12

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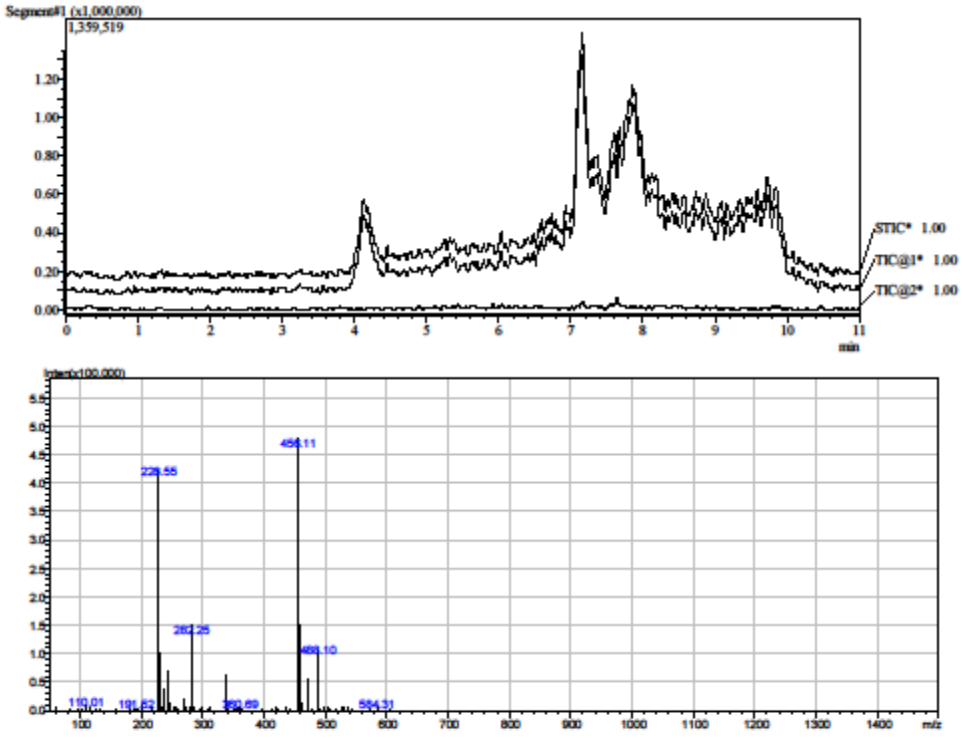

C:\LabSolutions\Data\Analiz\derya\GS-Me_20.lcd

Figure S8. LCMSMS spectra of compound **3b**.

DOPNALAB

	Item	Value
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	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\derya\ahmet osman tokay\GS-OME1.ispd
	Spectrum name	GS-OME1
	Sample name	GS-OME
	Sample ID	
	Option	
	Comment	
	No. of Scans	10
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

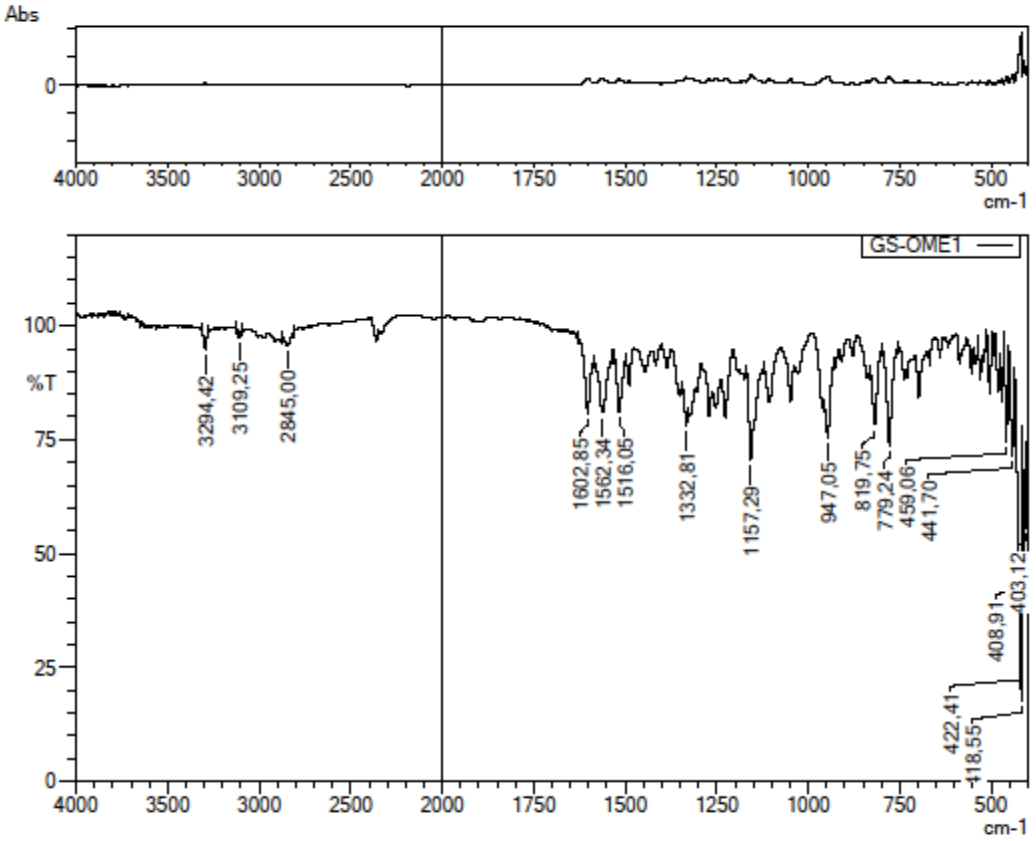

Figure S9. IR spectra of compound **3c**.

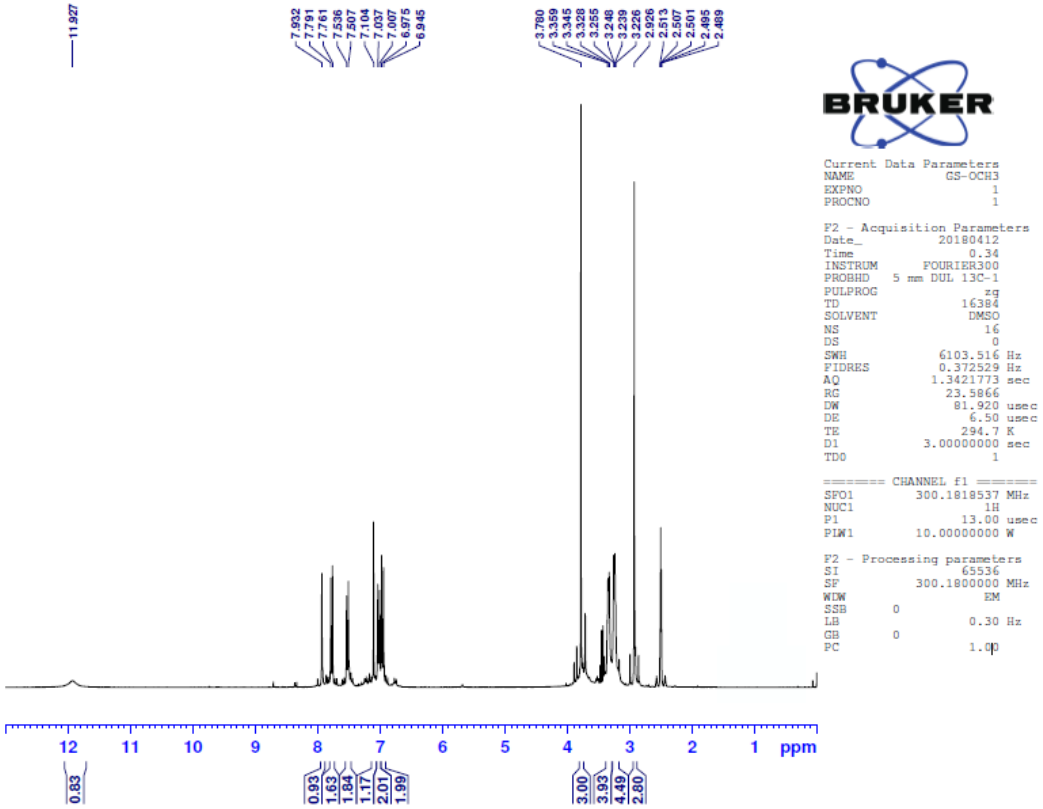

Figure S10. [1]H-NMR spectra of compound **3c**.

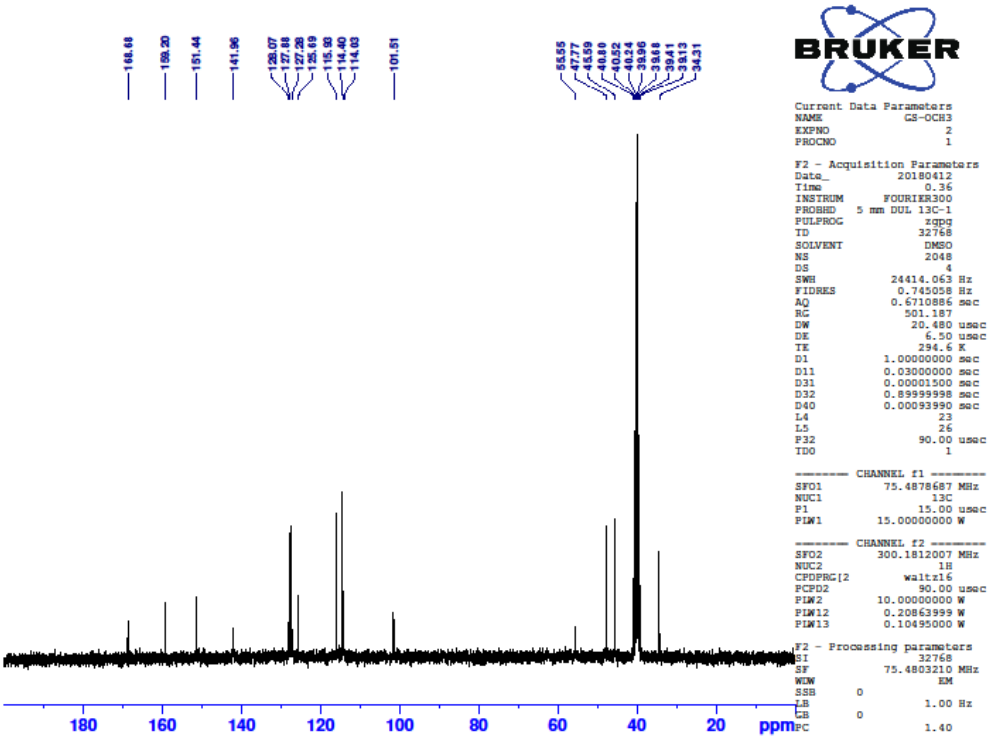

Figure S11. [13]C-NMR spectra of compound **3c**.

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: GS-OCH3
Sample ID	:
Vail #	: 1
Injection Volume	: 0.3 uL
Data File Name	: GS-OCH3_15.lcd
Method File Name	: genel.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 19.04.2018 12:06:21
Data Processed	: 19.04.2018 12:17:24

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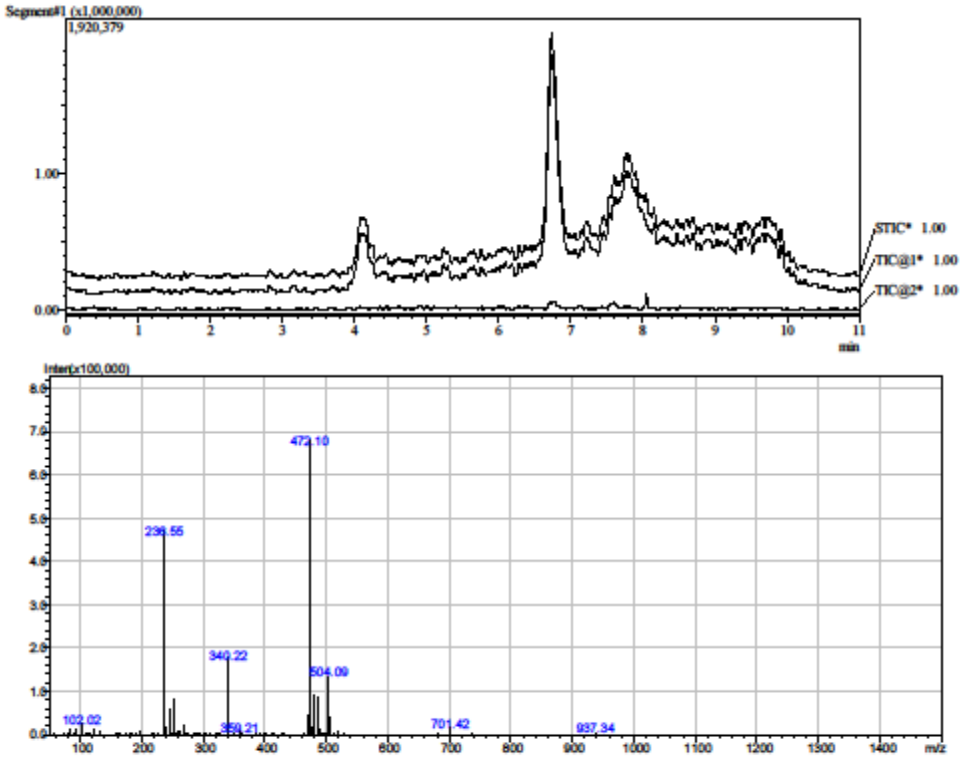

Figure S12. LCMSMS spectra of compound **3c**.

DOPNALAB

	Item	Value
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	Acquired by	System Administrator
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	Spectrum name	GS-CN1
	Sample name	GS-CN
	Sample ID	
	Option	
	Comment	
	No. of Scans	10
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

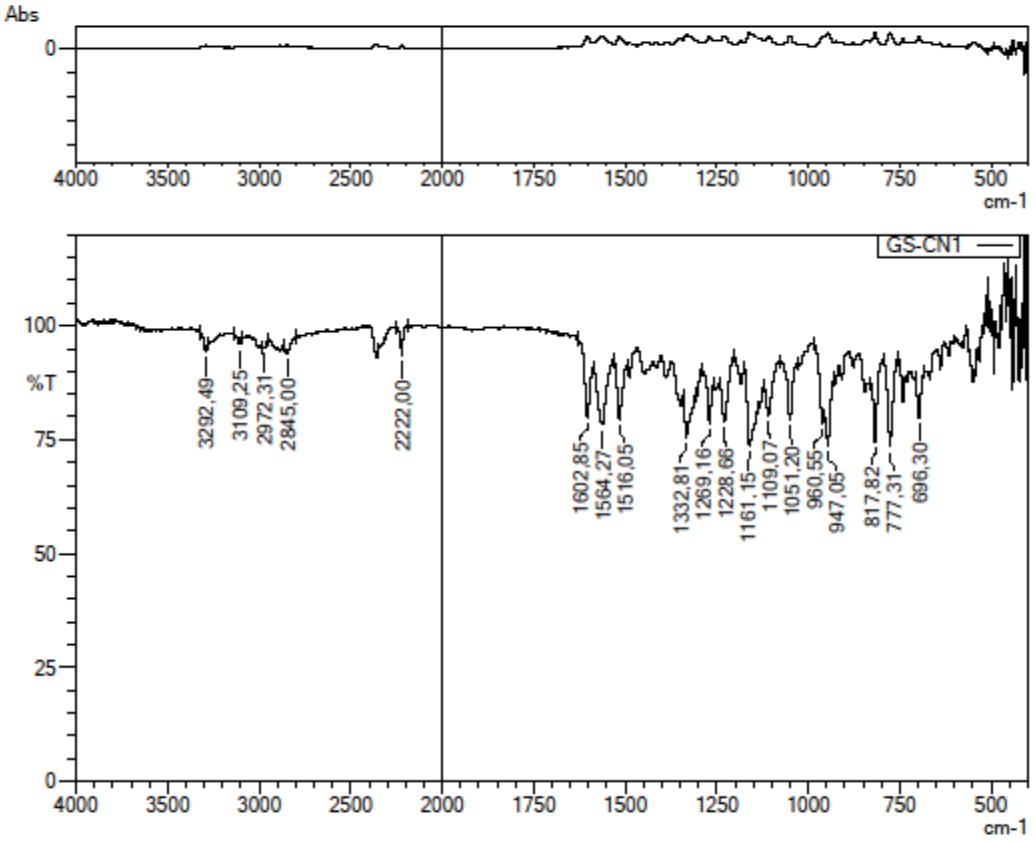

Figure S13. IR spectra of compound **3d**.

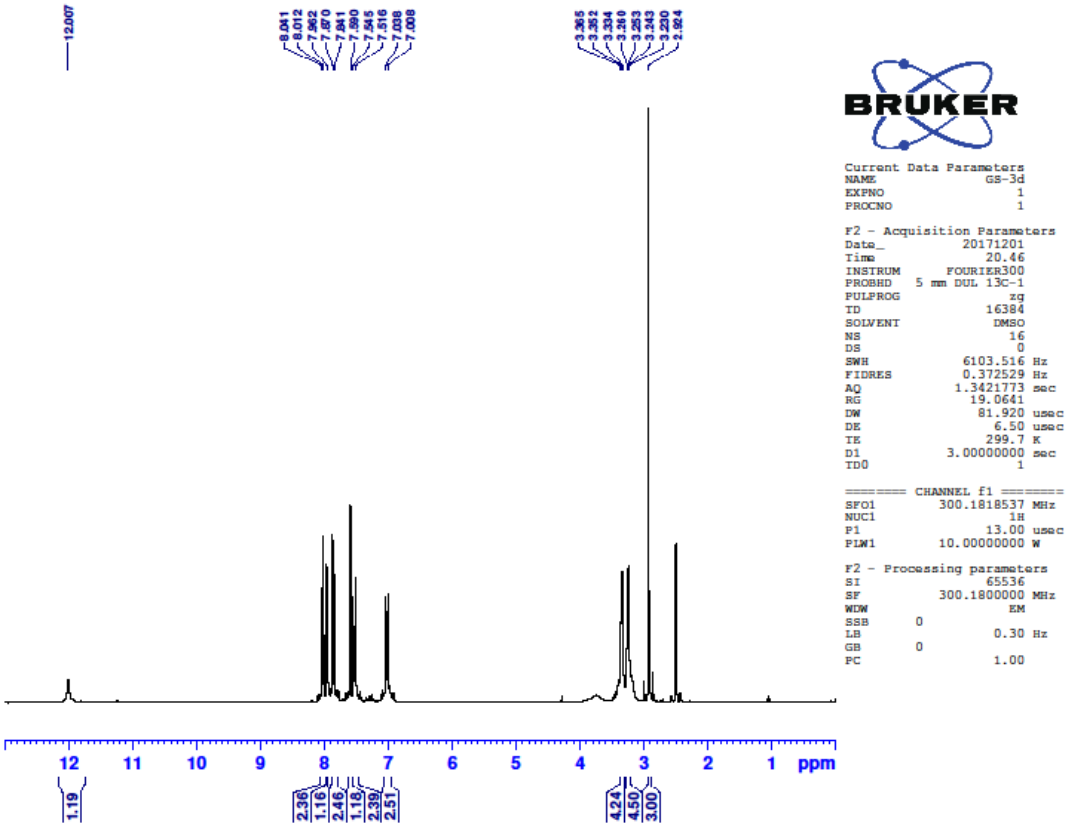

Figure S14. [1]H-NMR spectra of compound **3d**.

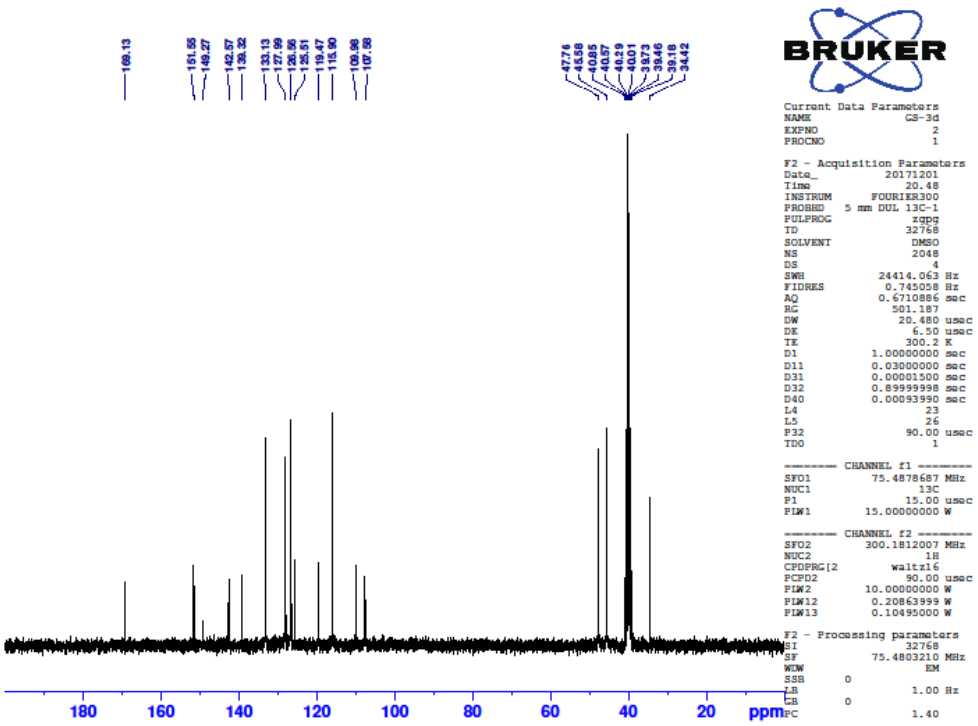

Figure S15. [13]C-NMR spectra of compound **3d**.

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: GS-CN
Sample ID	:
Vail #	: 7
Injection Volume	: 0.3 uL
Data File Name	: GS-CN_21.lcd
Method File Name	: genel.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 19.04.2018 13:15:42
Data Processed	: 19.04.2018 13:26:44

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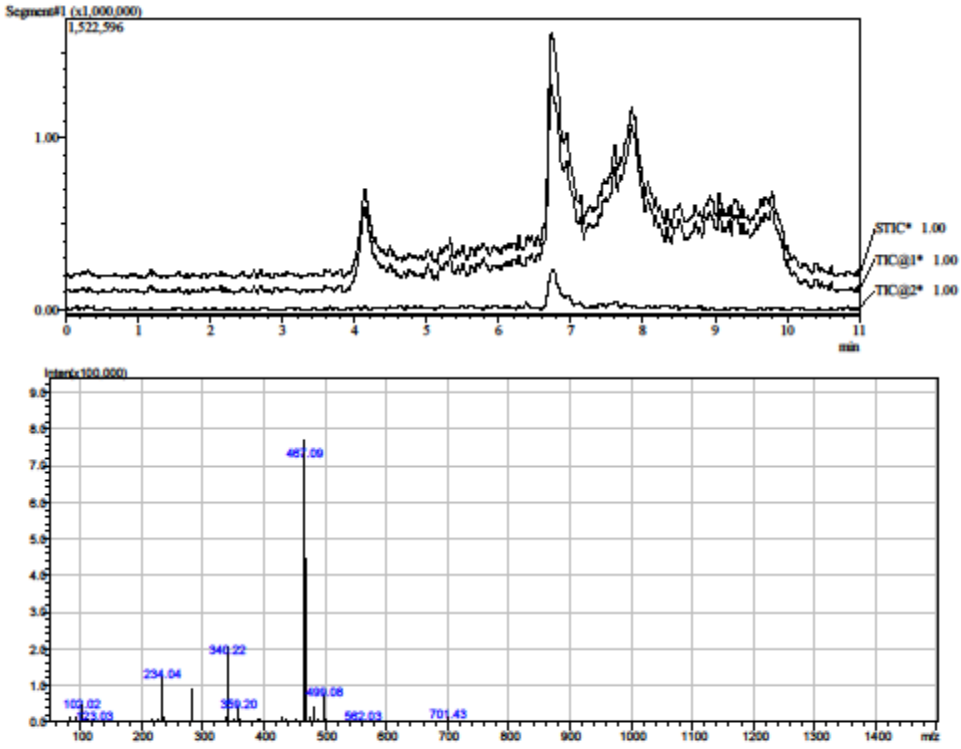

Figure S16. LCMSMS spectra of compound **3d**.

DOPNALAB

	Item	Value
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	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\derya\ahmet osman tokay\GS-NO21.lspd
	Spectrum name	GS-NO21
	Sample name	GS-NO2
	Sample ID	
	Option	
	Comment	
	No. of Scans	10
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

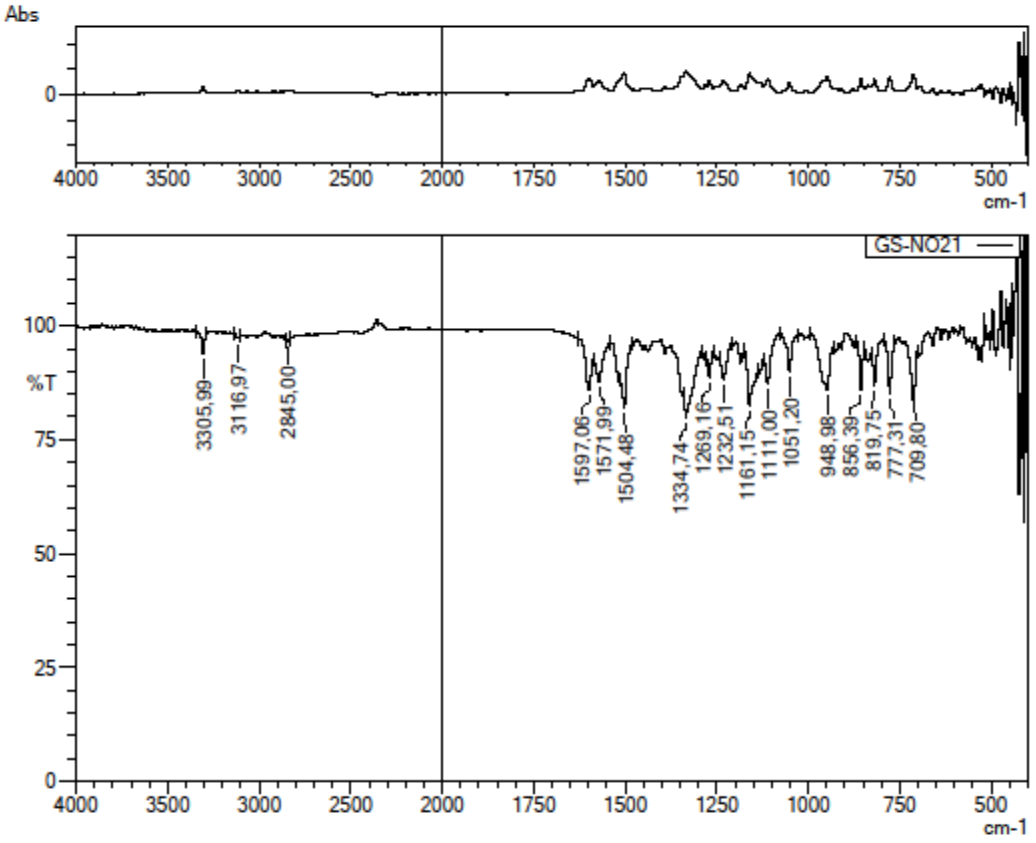

Figure S17. IR spectra of compound **3e**.

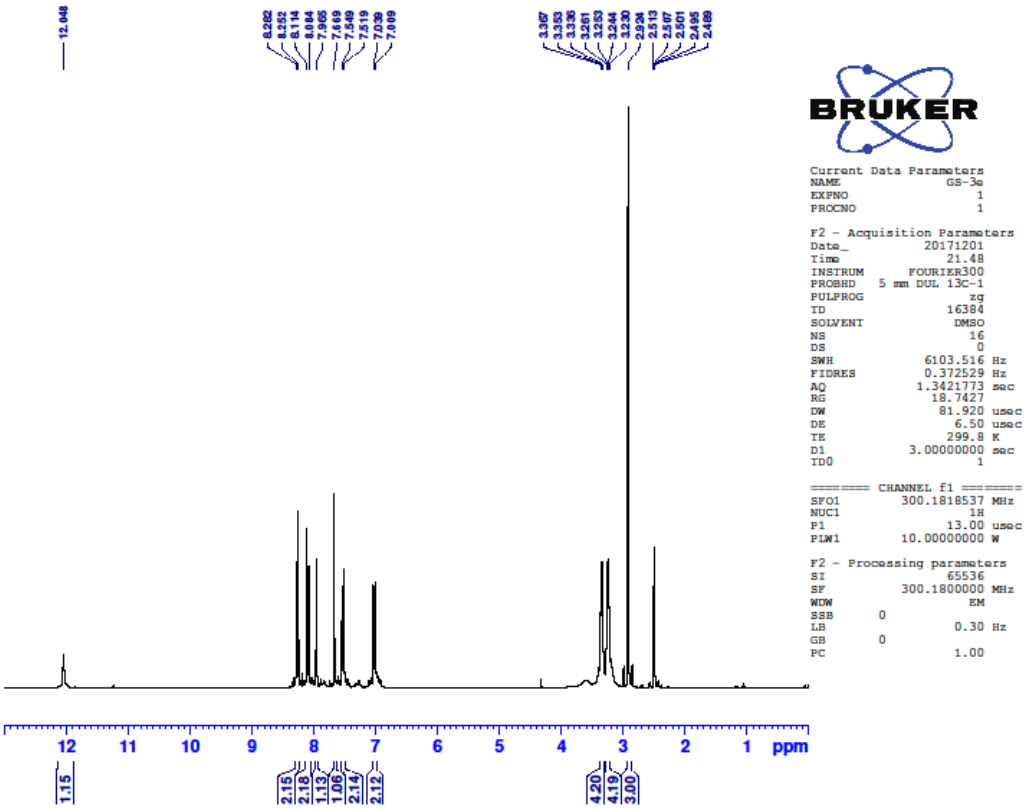

Figure S18. [1]H-NMR spectra of compound **3e**.

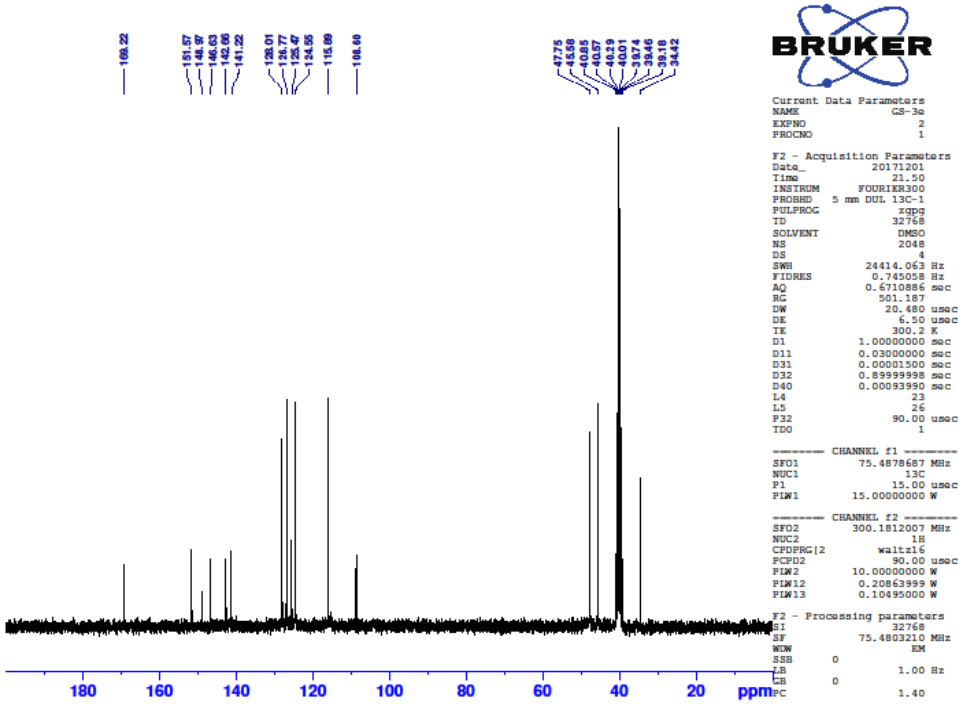

Figure S19. [13]C-NMR spectra of compound **3e**.

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: GS-NO2
Sample ID	:
Vail #	: 2
Injection Volume	: 0.3 uL
Data File Name	: GS-NO2_16.lcd
Method File Name	: genel.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
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Data Processed	: 19.04.2018 12:28:59

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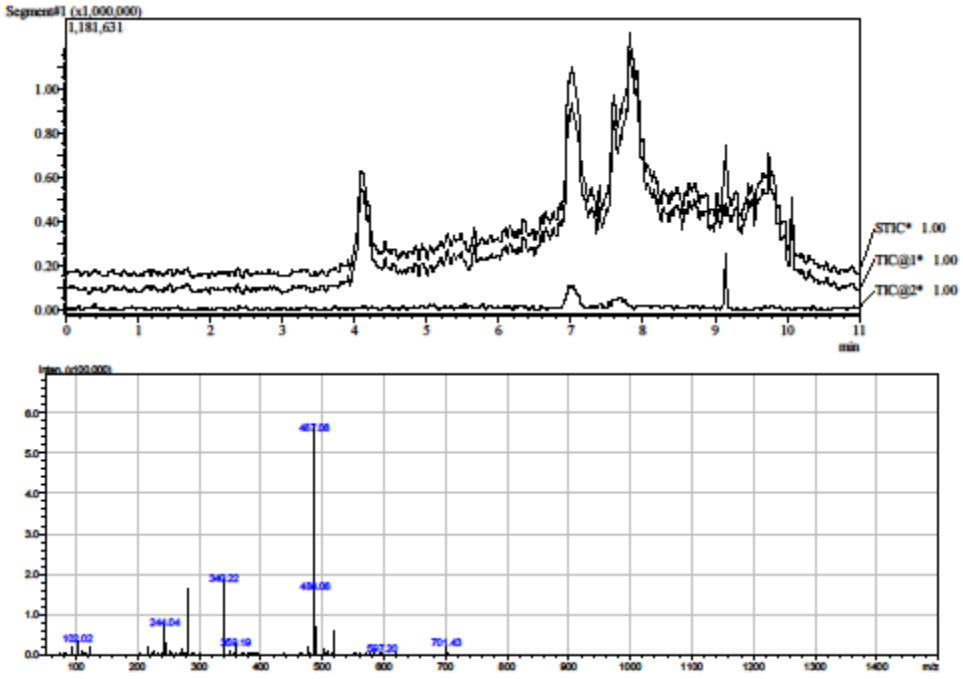

C:\LabSolutions\Data\Analiz\derya\GS-NO2_16.lcd

Figure S20. LCMSMS spectra of compound **3e**.

DOPNALAB

	Item	Value
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	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\derya\ahmet osman tokay\GS-F1.ispd
	Spectrum name	GS-F1
	Sample name	GS-F
	Sample ID	
	Option	
	Comment	
	No. of Scans	10
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

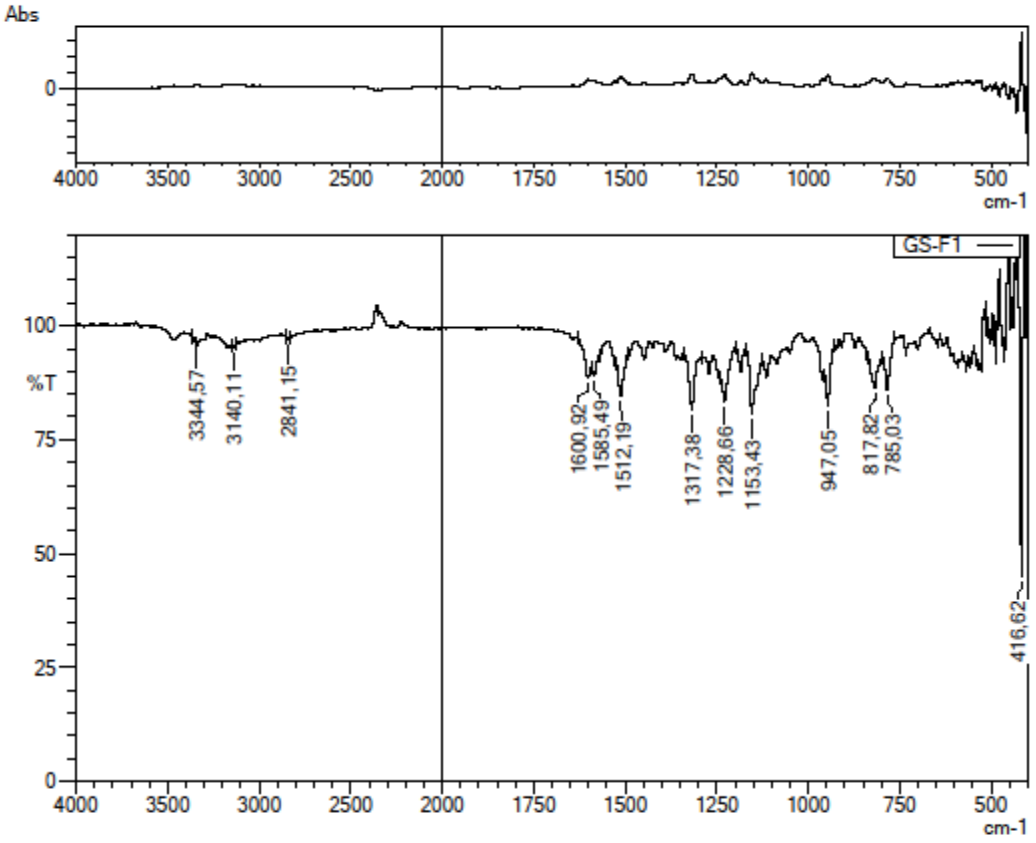

Figure S21. IR spectra of compound **3f**.

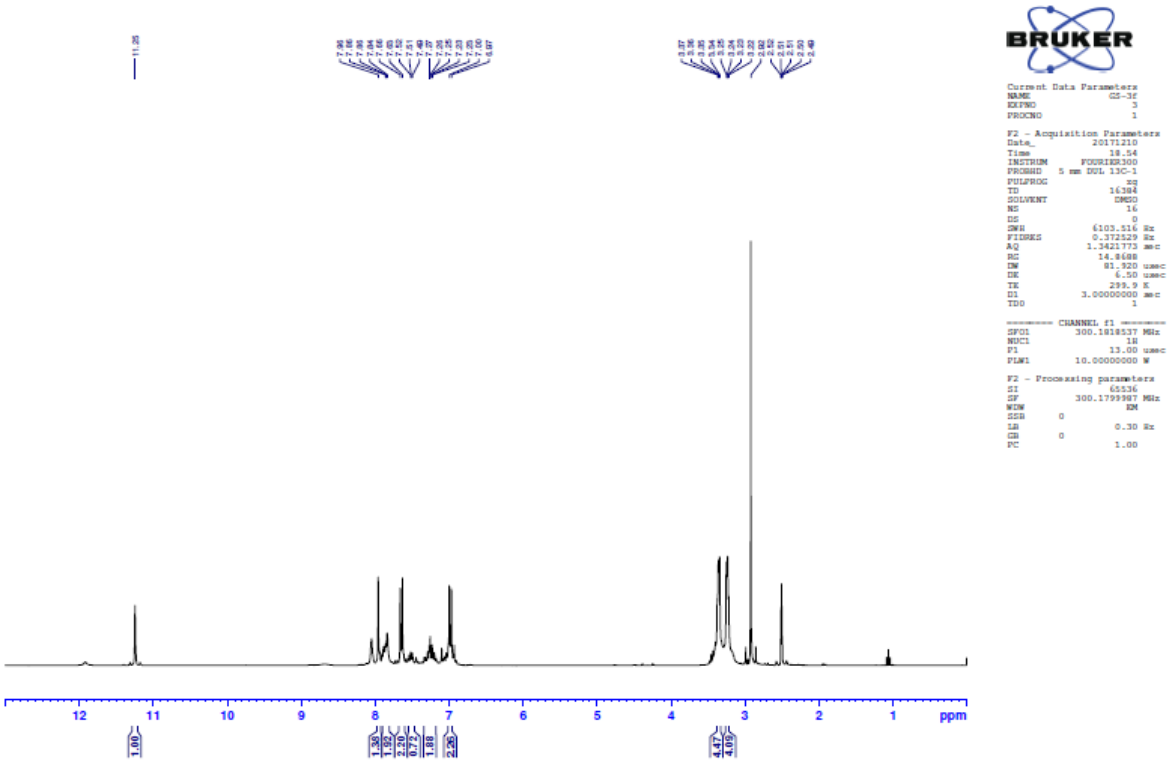

Figure S22. [1]H-NMR spectra of compound **3f**.

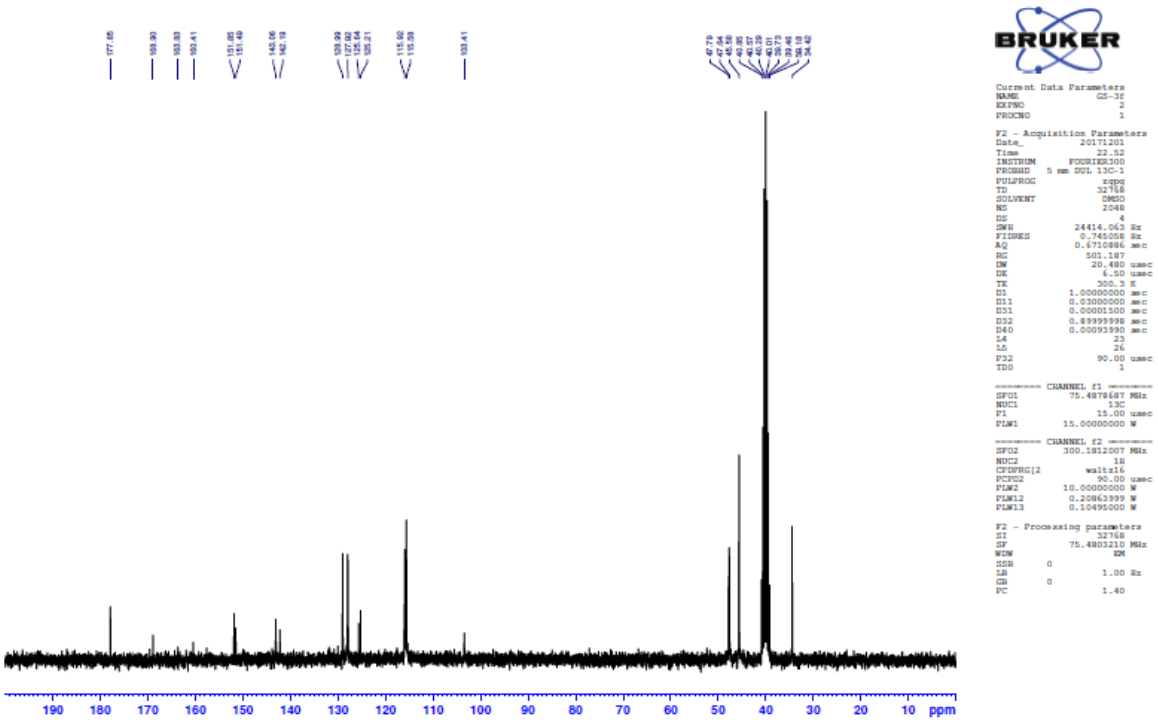

Figure S23. [13]C-NMR spectra of compound **3f**.

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	:Admin
Sample Name	:GS-F
Sample ID	
Vail #	:15
Injection Volume	:0.3 µL
Data File Name	:GS-F_22.lcd
Method File Name	:genel.lcm
Batch File Name	:batch.lcb
Report File Name	:DefaultLCMS.lcr
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Data Processed	:27.04.2021 10.46:14

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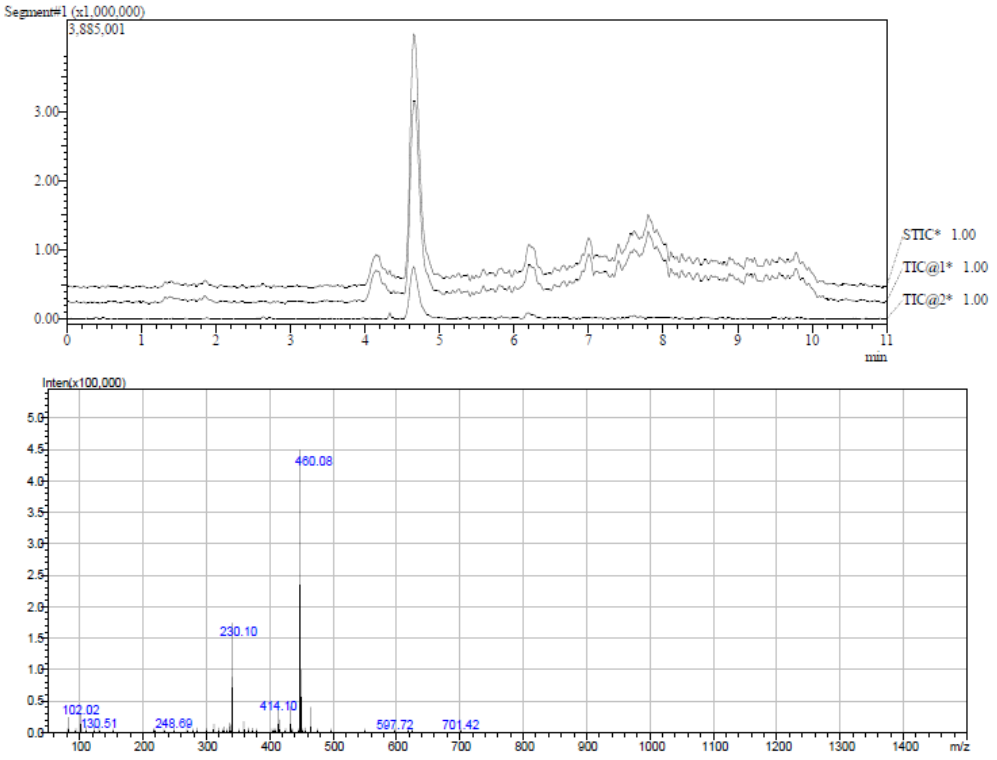

C:\LabSolutions\Data\Analiz\derya\GS-F_22.lcd

Figure S24. LCMSMS spectra of compound **3f**.

DOPNALAB

	Item	Value
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	Acquired by	System Administrator
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	Spectrum name	GS-Cl1
	Sample name	GS-Cl
	Sample ID	
	Option	
	Comment	
	No. of Scans	10
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

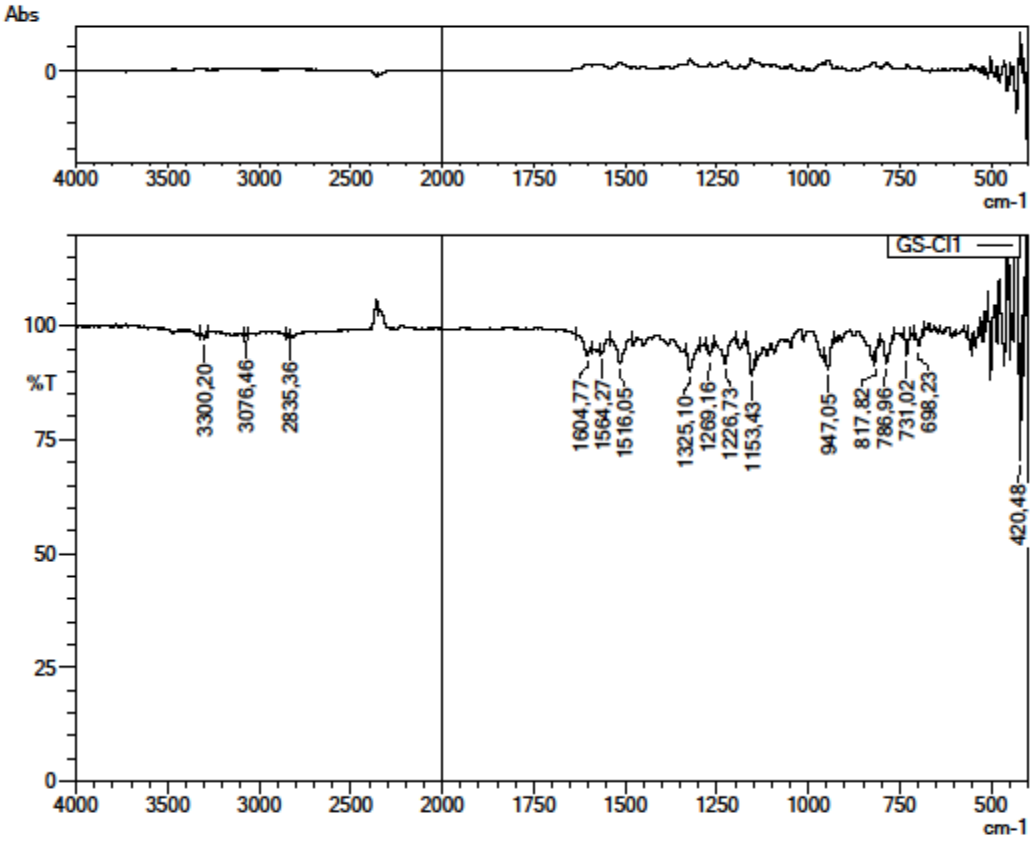

Figure S25. IR spectra of compound **3g**.

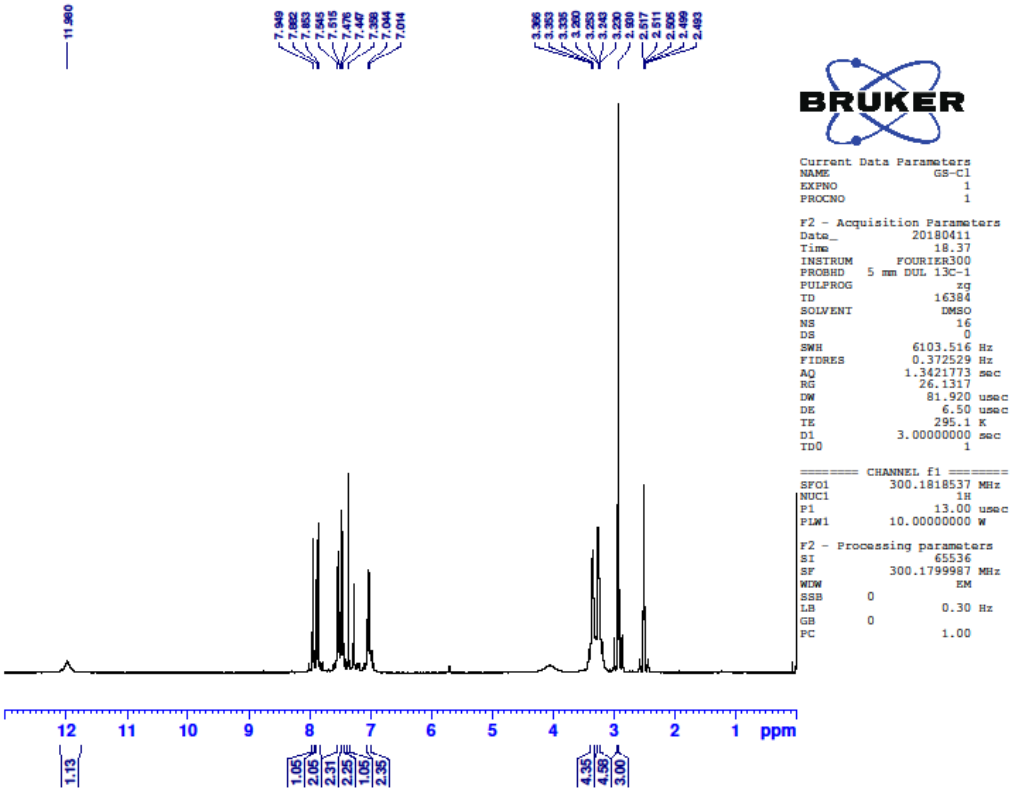

Figure S26. [1]H-NMR spectra of compound **3g**.

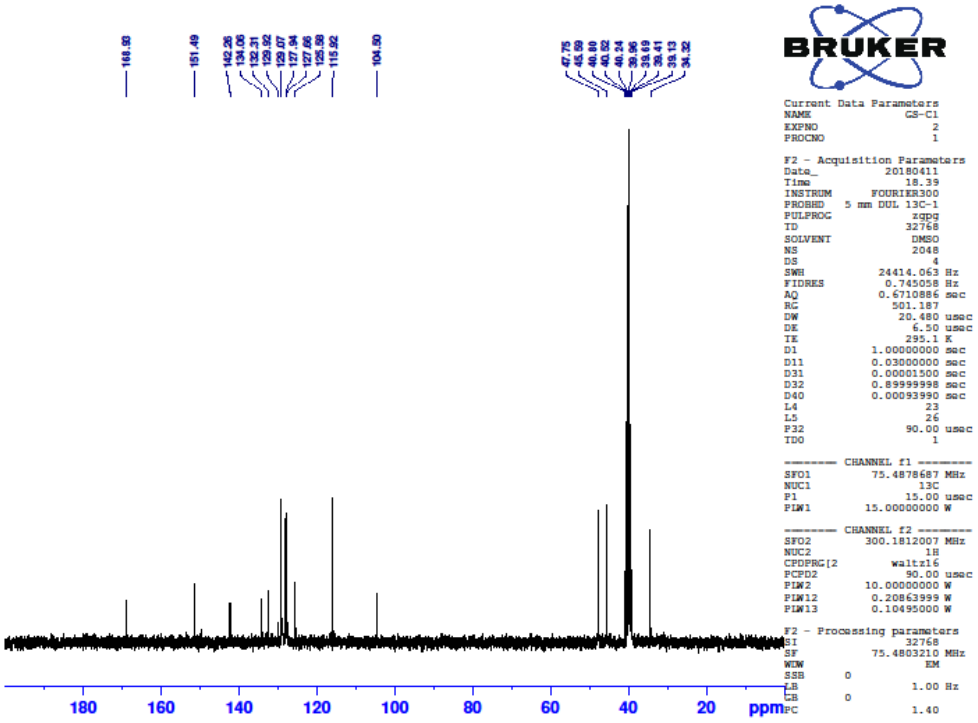

Figure S27. [13]C-NMR spectra of compound **3g**.

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: GS-Cl
Sample ID	:
Vail #	: 4
Injection Volume	: 0.3 uL
Data File Name	: GS-Cl_18.lcd
Method File Name	: genel.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 19.04.2018 12:41:02
Data Processed	: 19.04.2018 12:52:05

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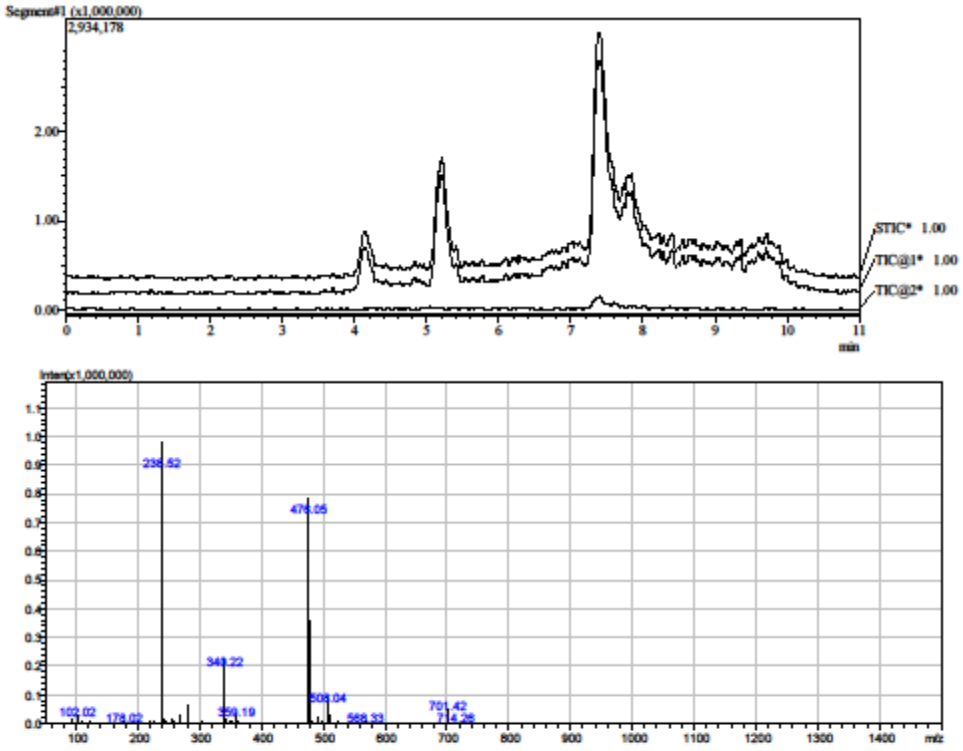


C:\LabSolutions\Data\Analiz\derya\GS-Cl_18.lcd

Figure S28. LCMSMS spectra of compound **3g**.

DOPNALAB

	Item	Value
	Acquired Date&Time	13.04.2018 15:21:58
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\derya\ahmet osman tokay\GS-CF31.lspd
	Spectrum name	GS-CF31
	Sample name	GS-CF3
	Sample ID	
	Option	
	Comment	
	No. of Scans	10
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

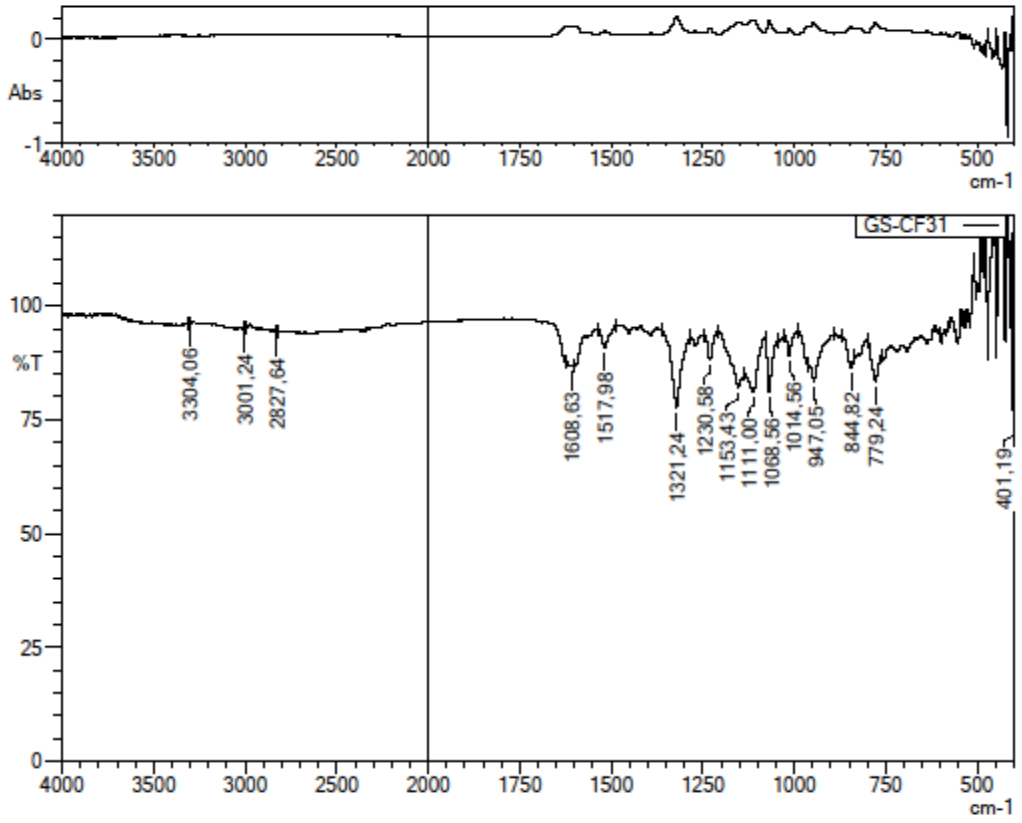


Figure S29. IR spectra of compound **3h**.

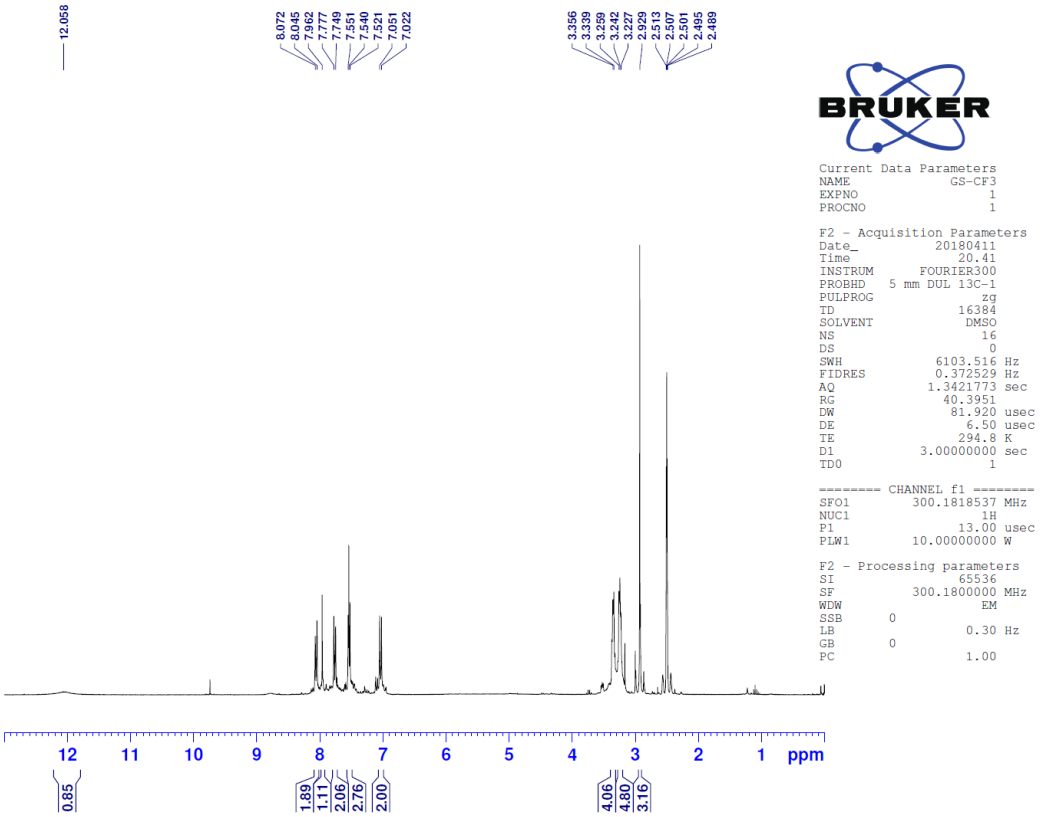


Figure S30. [1]H-NMR spectra of compound **3h**.

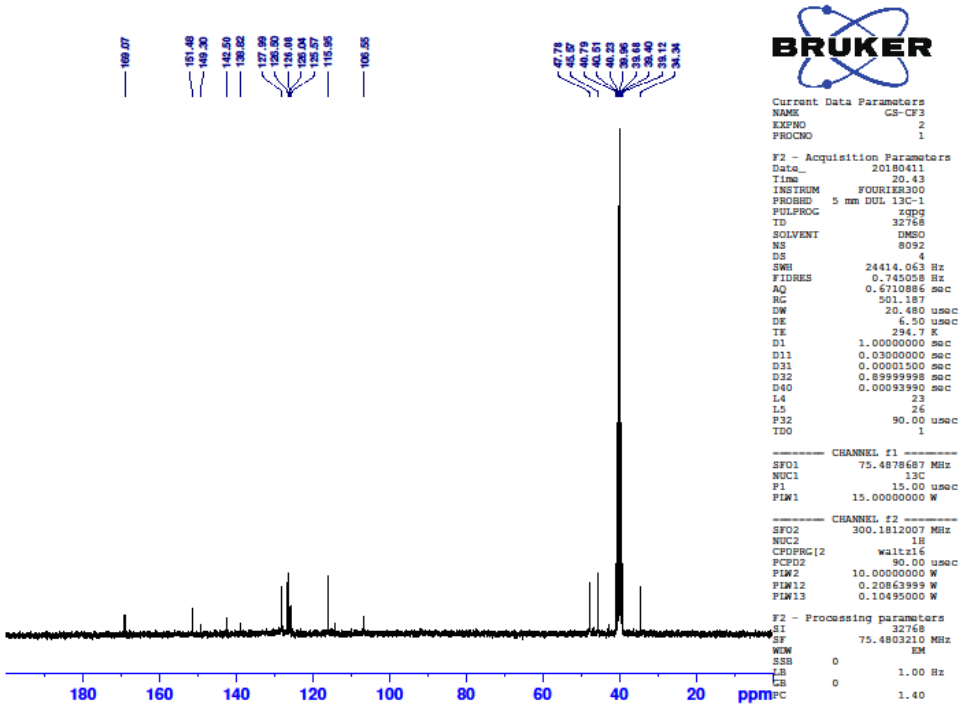
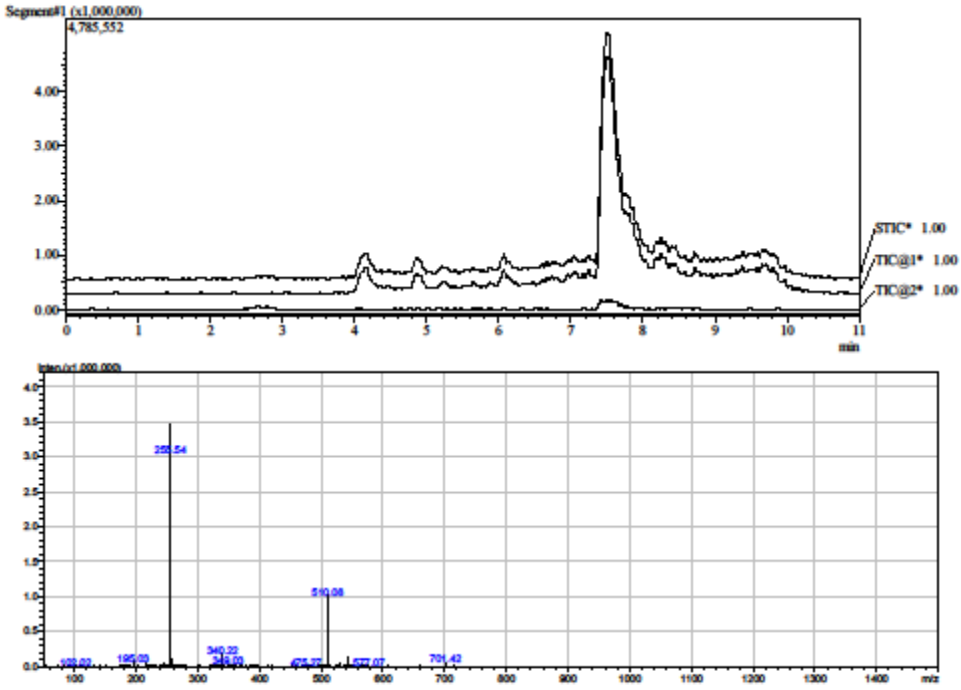


Figure S31. [13]C-NMR spectra of compound **3h**.

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by	: Admin
Sample Name	: GS-CF3
Sample ID	:
Vail #	: 3
Injection Volume	: 0.3 uL
Data File Name	: GS-CF3_17.lcd
Method File Name	: genel.lcm
Batch File Name	: batch.lcb
Report File Name	: DefaultLCMS.lcr
Data Acquired	: 19.04.2018 12:29:29
Data Processed	: 19.04.2018 12:40:32

<Chromatogram>



C:\LabSolutions\Data\Analiz\derya\GS-CF3_17.lcd

Figure S32. LCMSMS spectra of compound **3h**.

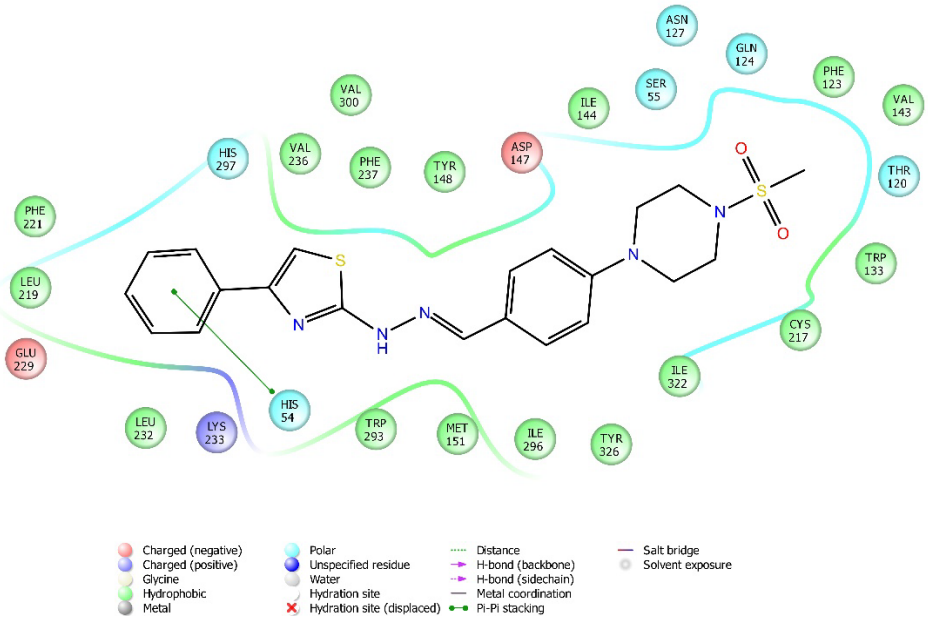


Figure S33. The two-dimensional interacting mode of compound **3a** in the active region of μ-opioid receptor (PDB Code: 5C1M).

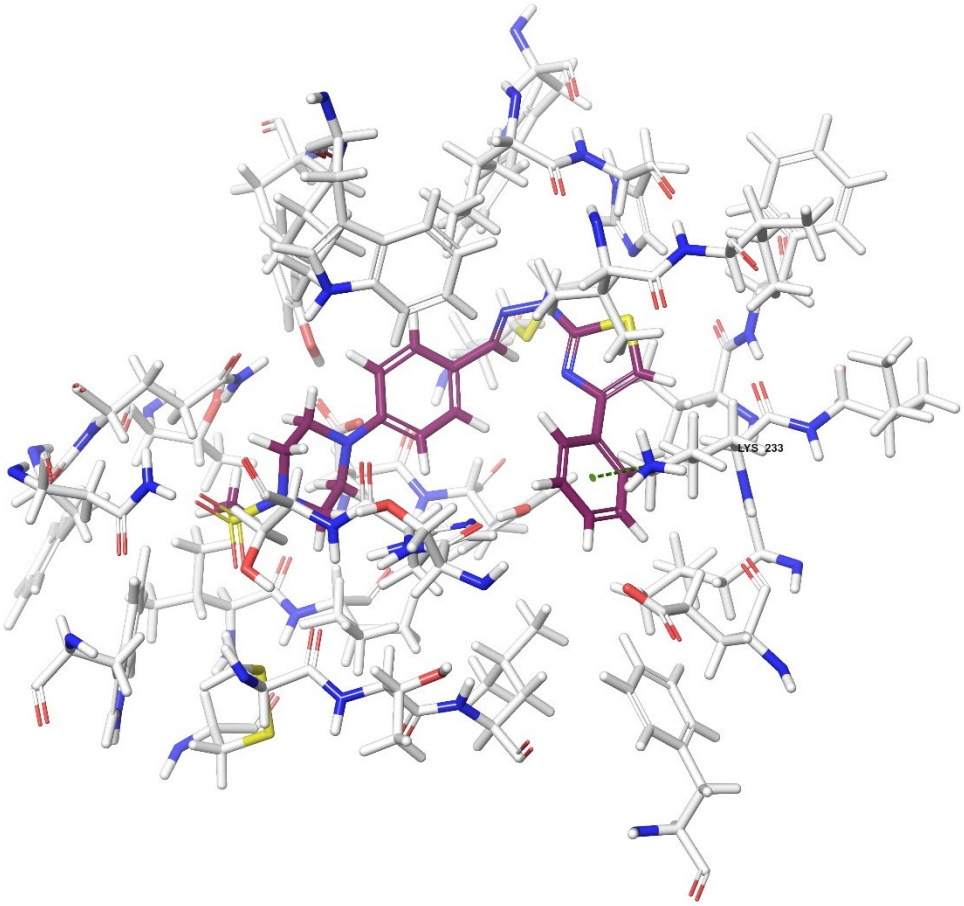


Figure S34. The three-dimensional interacting mode of compound **3a** in the active region of μ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with purple and white, respectively (PDB Code: 5C1M).

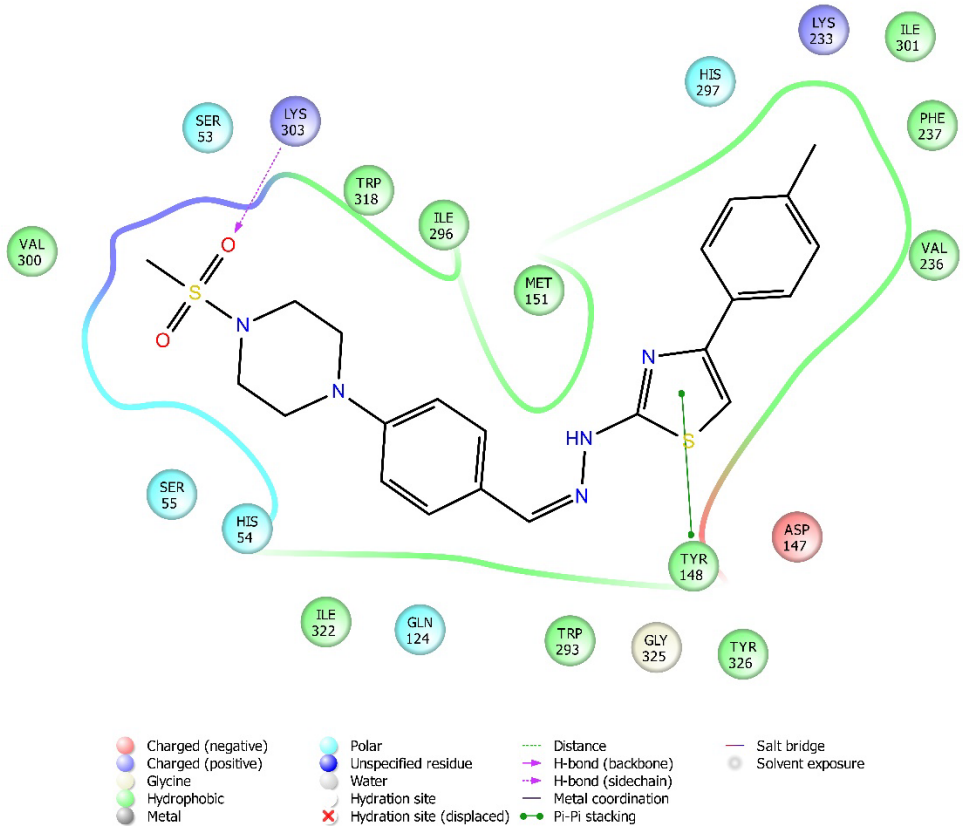


Figure S35. The two-dimensional interacting mode of compound **3b** in the active region of μ-opioid receptor (PDB Code: 5C1M).

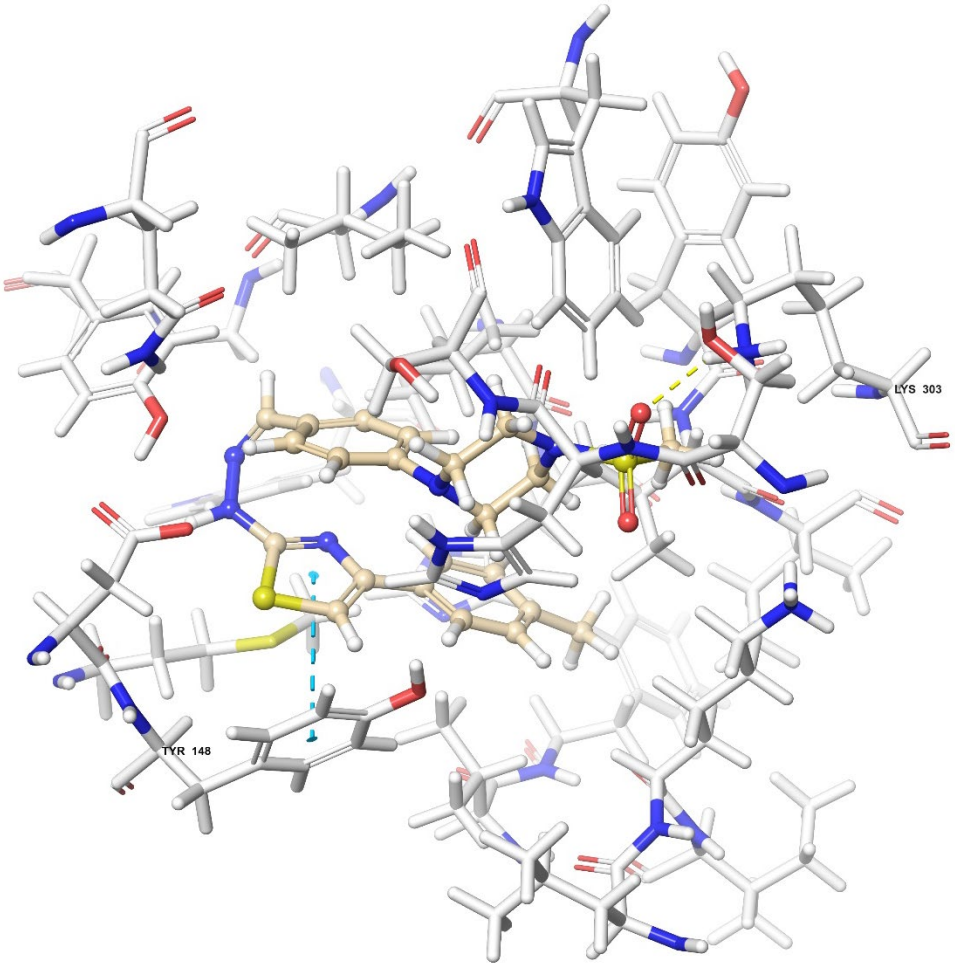


Figure S36. The three-dimensional interacting mode of compound **3b** in the active region of μ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with orange and white, respectively (PDB Code: 5C1M).

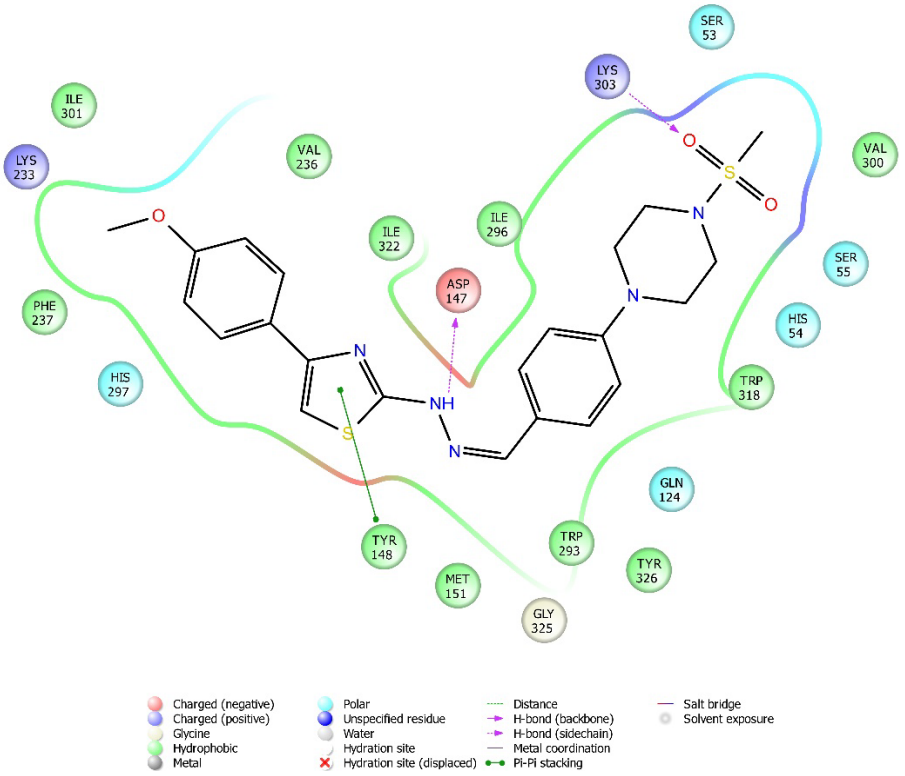


Figure S37. The two-dimensional interacting mode of compound **3c** in the active region of μ-opioid receptor (PDB Code: 5C1M).

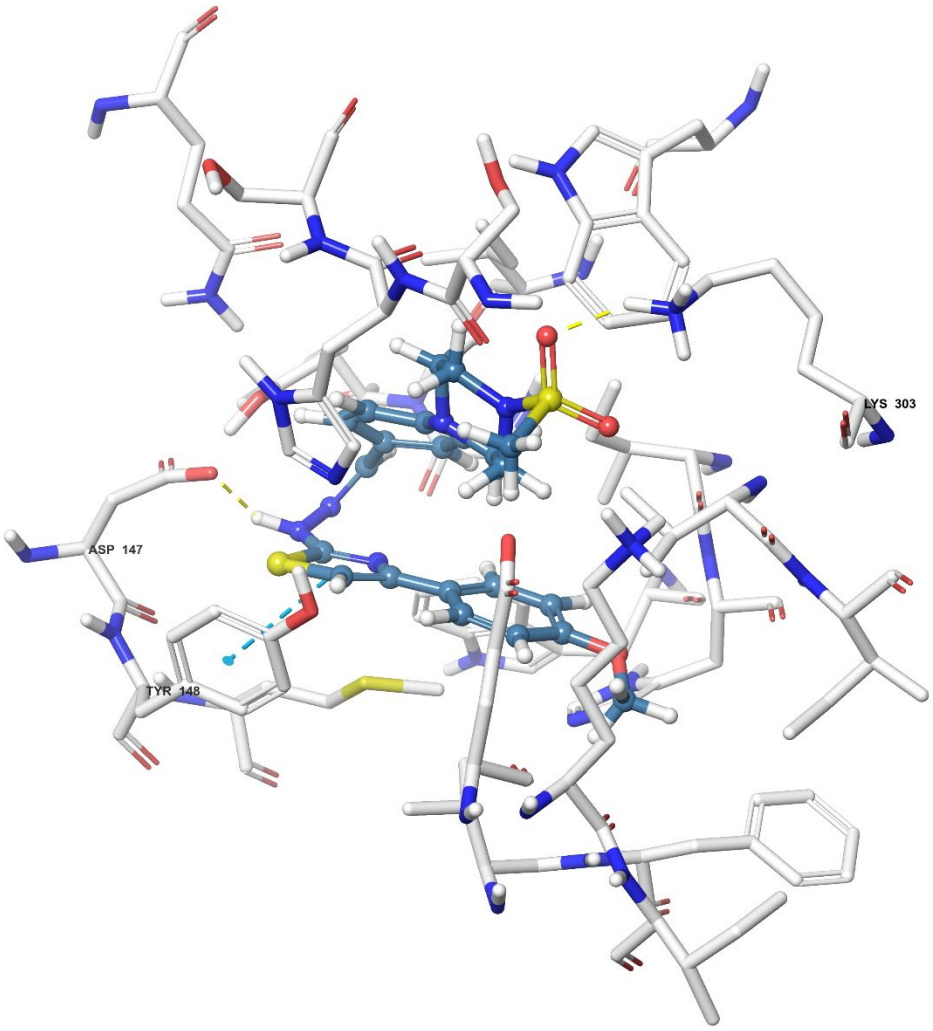


Figure S38. The three-dimensional interacting mode of compound **3c** in the active region of μ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with blue and white, respectively (PDB Code: 5C1M).

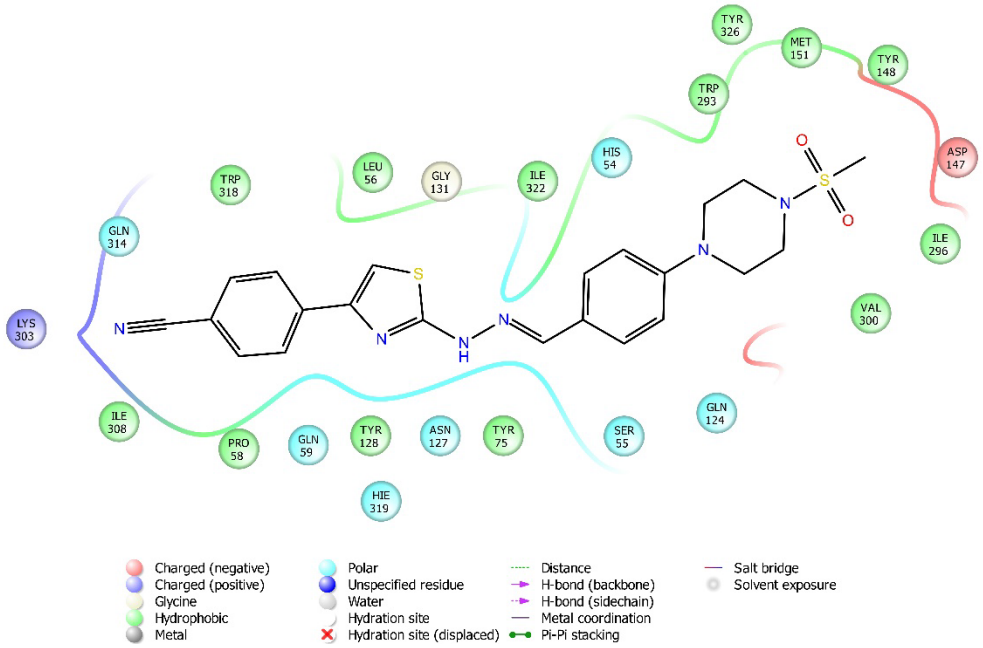


Figure S39. The two-dimensional interacting mode of compound **3d** in the active region of μ-opioid receptor (PDB Code: 5C1M).

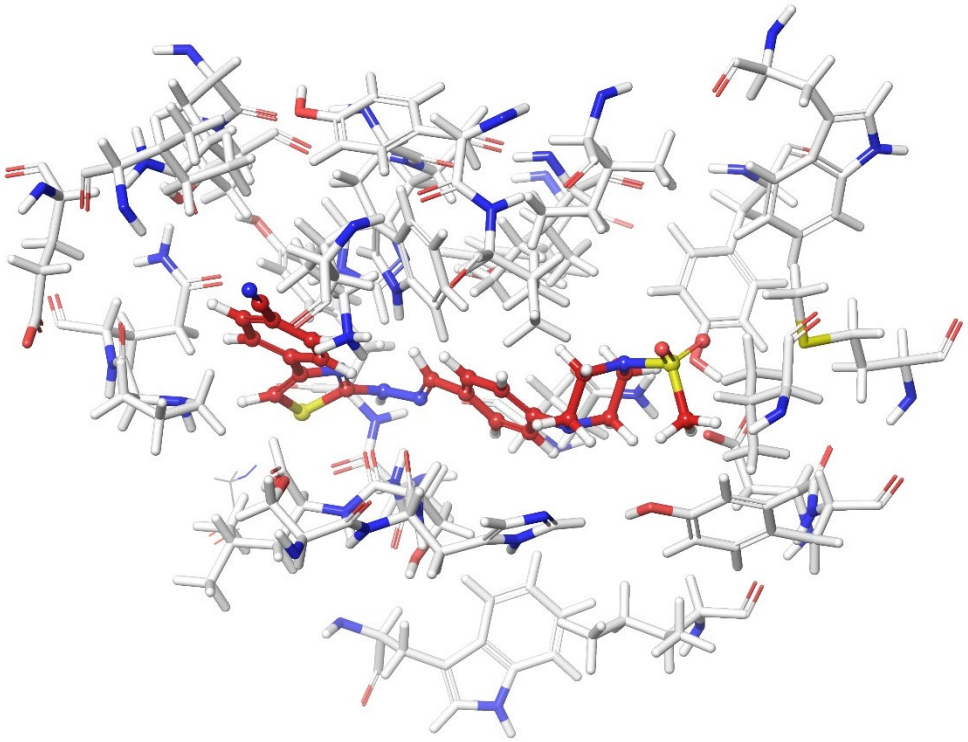


Figure S40. The three-dimensional interacting mode of compound **3d** in the active region of μ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with red and white, respectively (PDB Code: 5C1M).

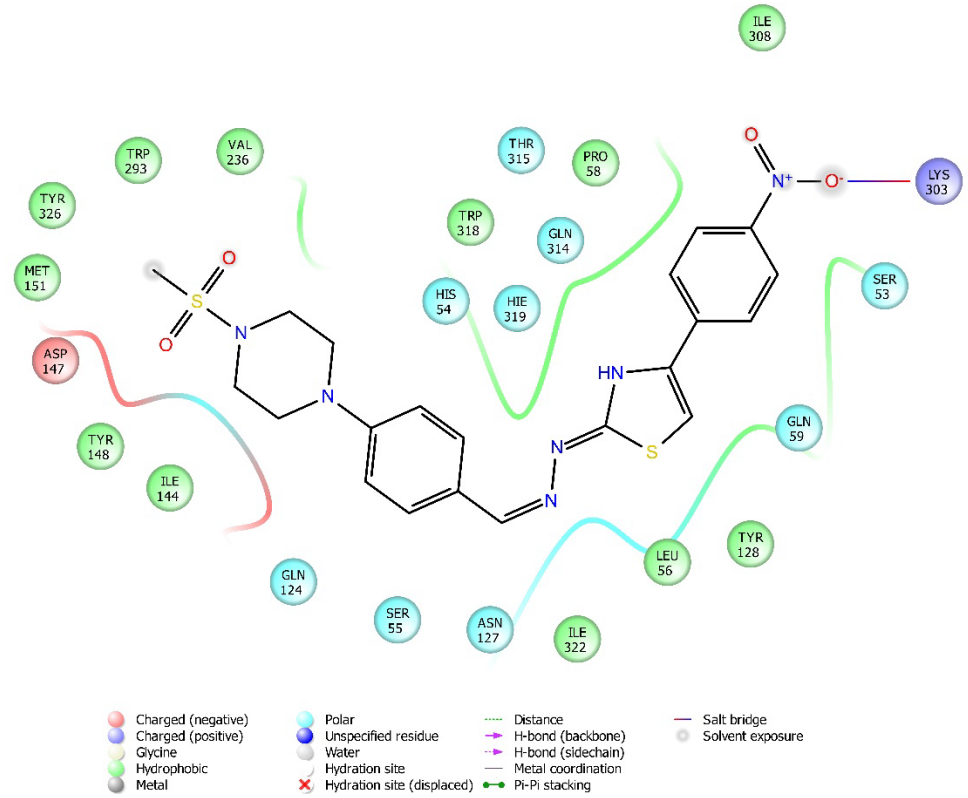


Figure S41. The two-dimensional interacting mode of compound **3e** in the active region of μ-opioid receptor (PDB Code: 5C1M).

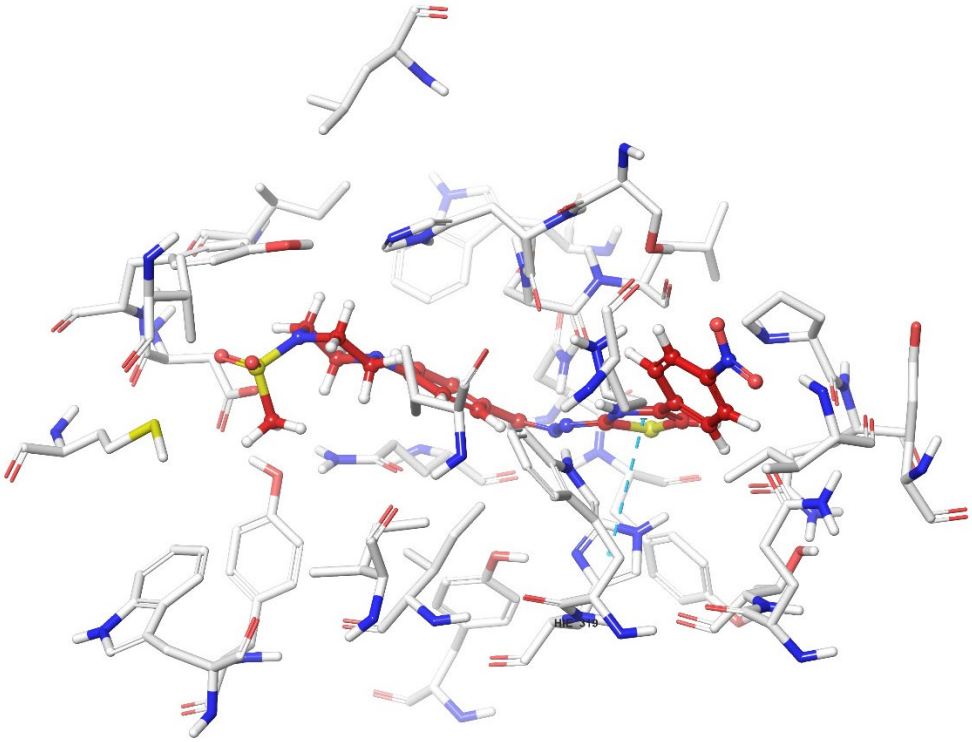


Figure S42. The three-dimensional interacting mode of compound **3e** in the active region of μ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with red and white, respectively (PDB Code: 5C1M).

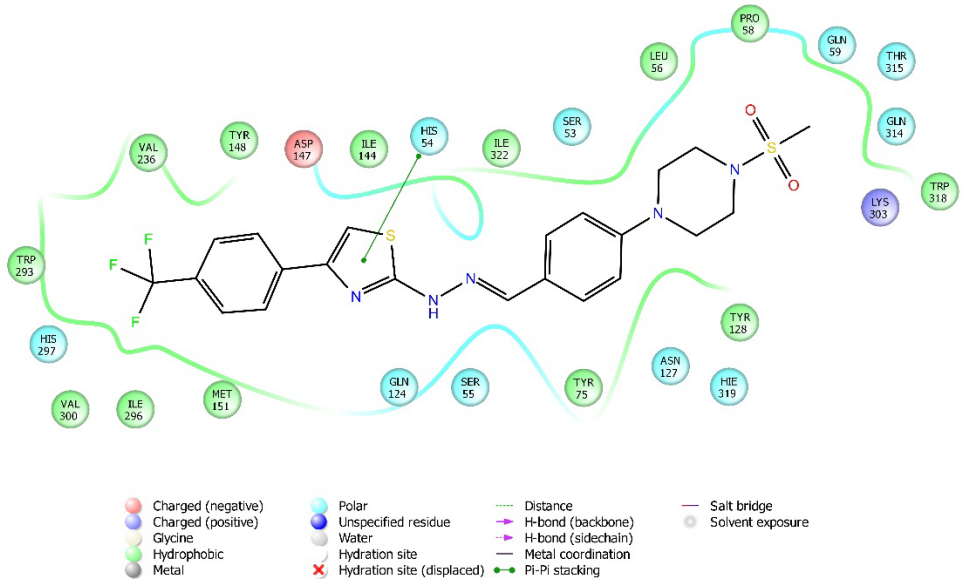


Figure S43. The two-dimensional interacting mode of compound **3h** in the active region of μ-opioid receptor (PDB Code: 5C1M).

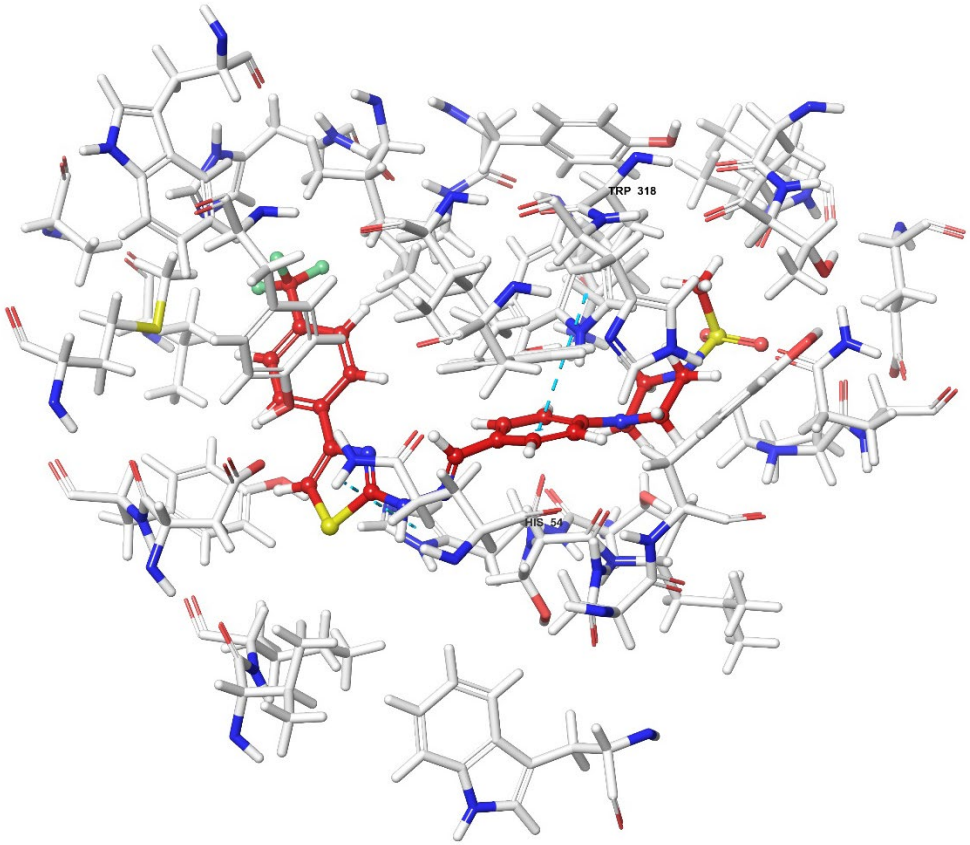


Figure S44. The three-dimensional interacting mode of compound **3h** in the active region of μ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with red and white, respectively (PDB Code: 5C1M).

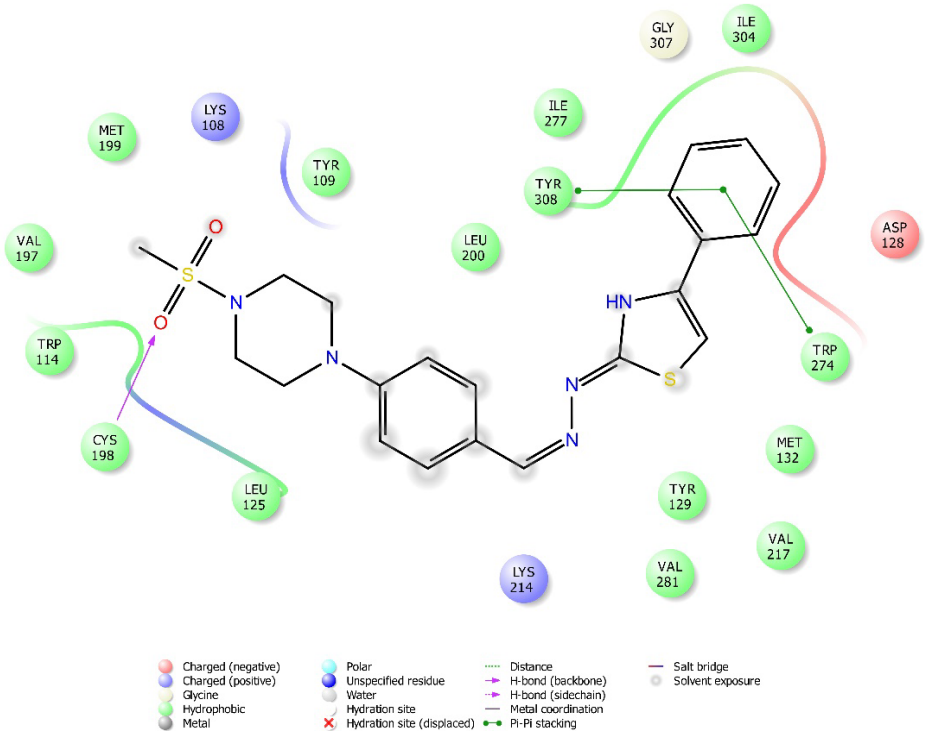


Figure S45. The two-dimensional interacting mode of compound **3a** in the active region of δ-opioid receptor (PDB Code: 4N6H).

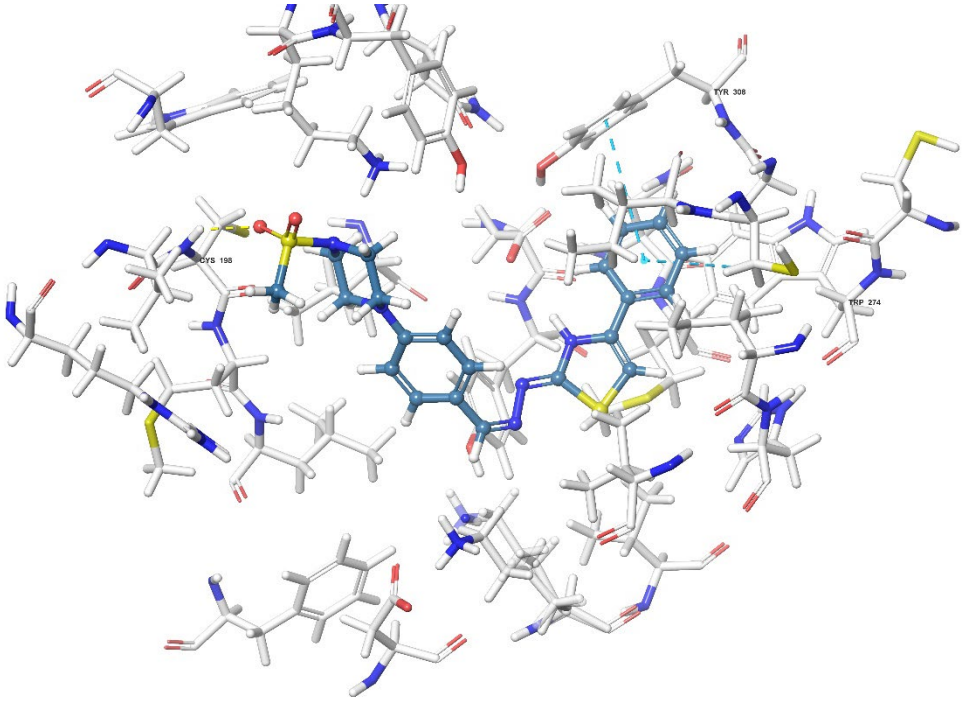


Figure S46. The three-dimensional interacting mode of compound **3a** in the active region of δ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with blue and white, respectively (PDB Code: 4N6H).

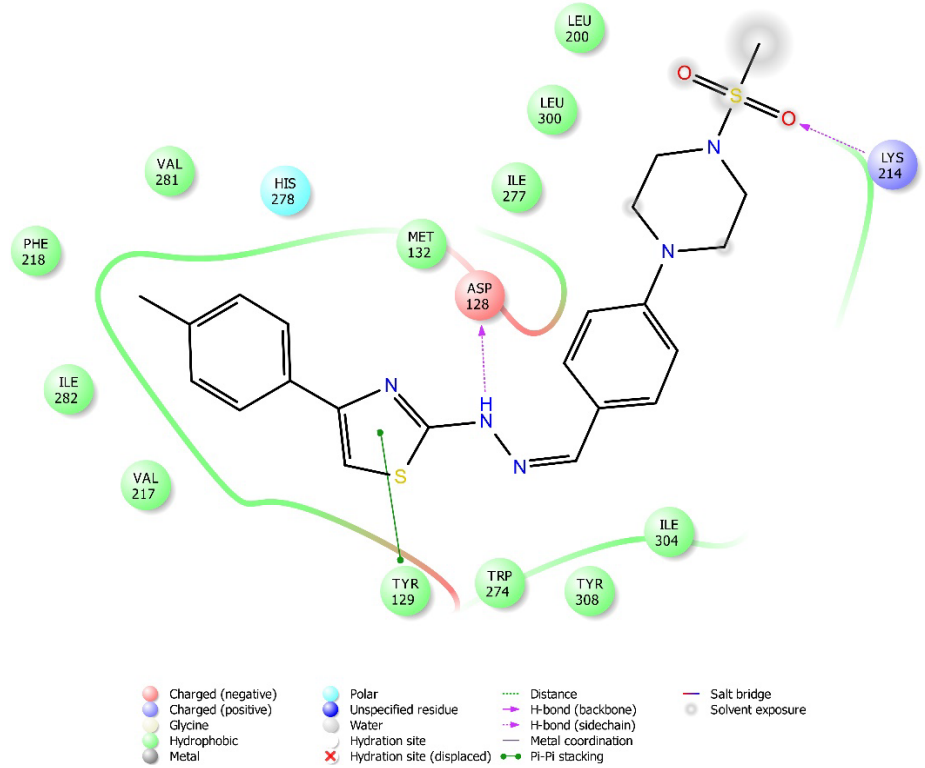


Figure S47. The two-dimensional interacting mode of compound **3b** in the active region of δ-opioid receptor (PDB Code: 4N6H).

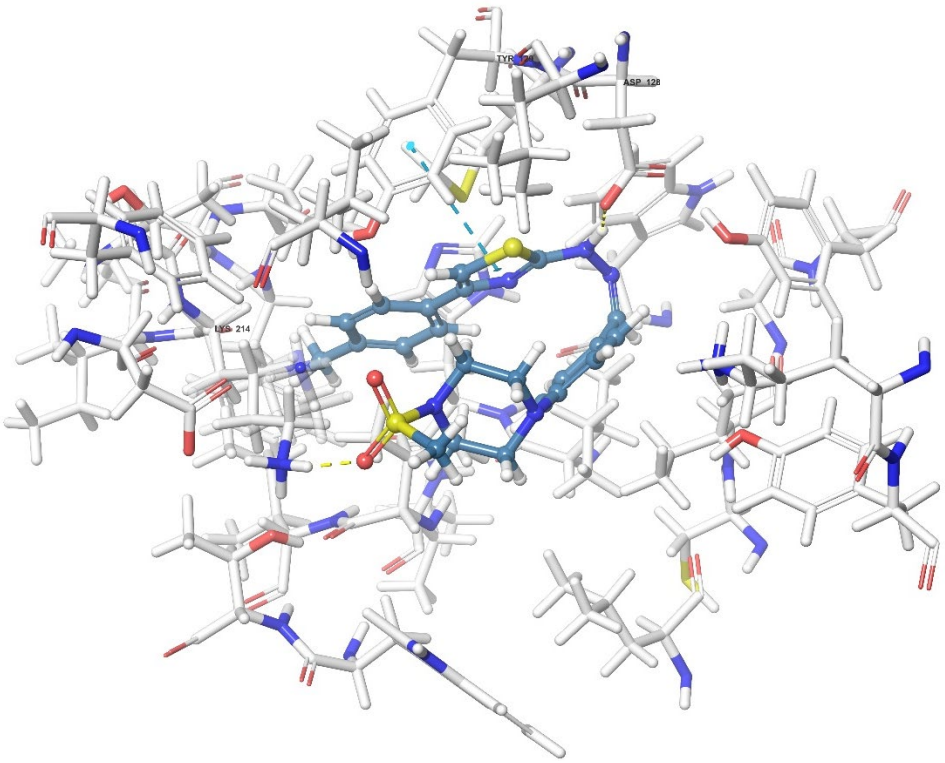


Figure S48. The three-dimensional interacting mode of compound **3b** in the active region of δ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with blue and white, respectively (PDB Code: 4N6H).

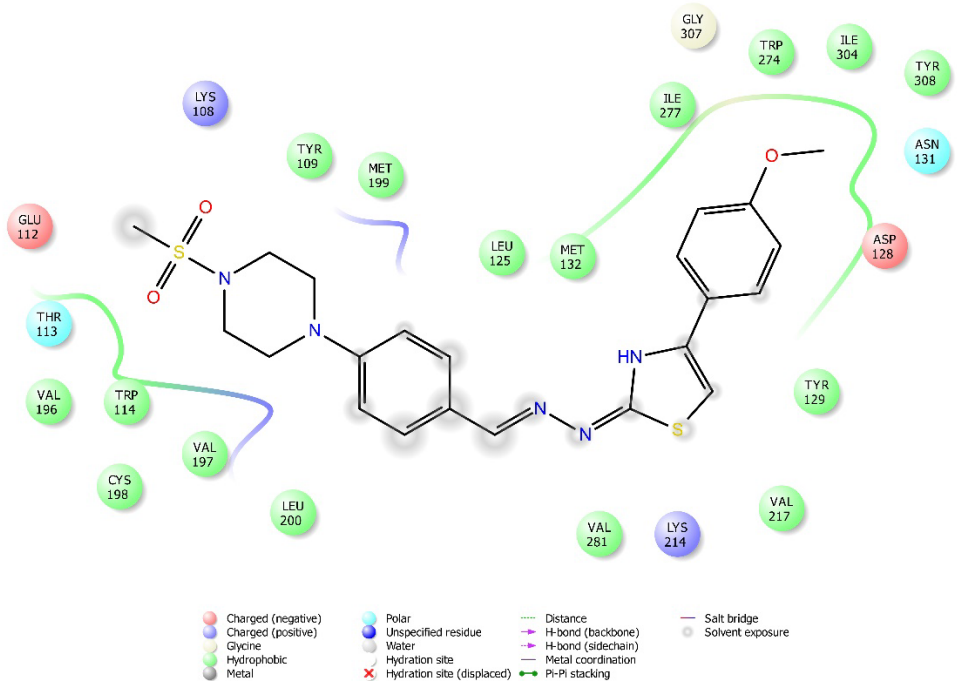


Figure S49. The two-dimensional interacting mode of compound **3c** in the active region of δ-opioid receptor (PDB Code: 4N6H).

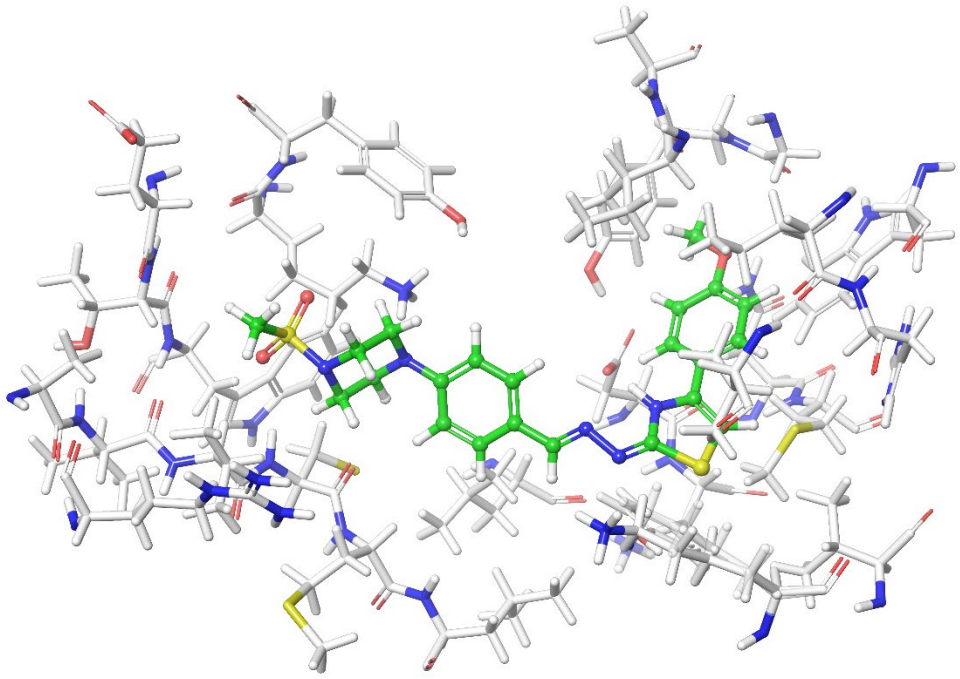


Figure S50. The three-dimensional interacting mode of compound **3c** in the active region of δ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with green and white, respectively (PDB Code: 4N6H).

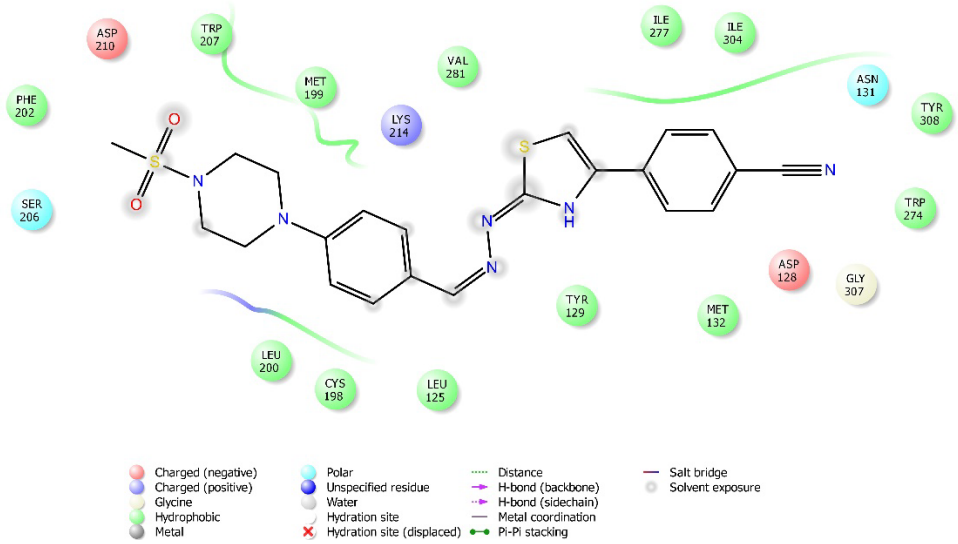


Figure S51. The two-dimensional interacting mode of compound **3d** in the active region of δ-opioid receptor (PDB Code: 4N6H).

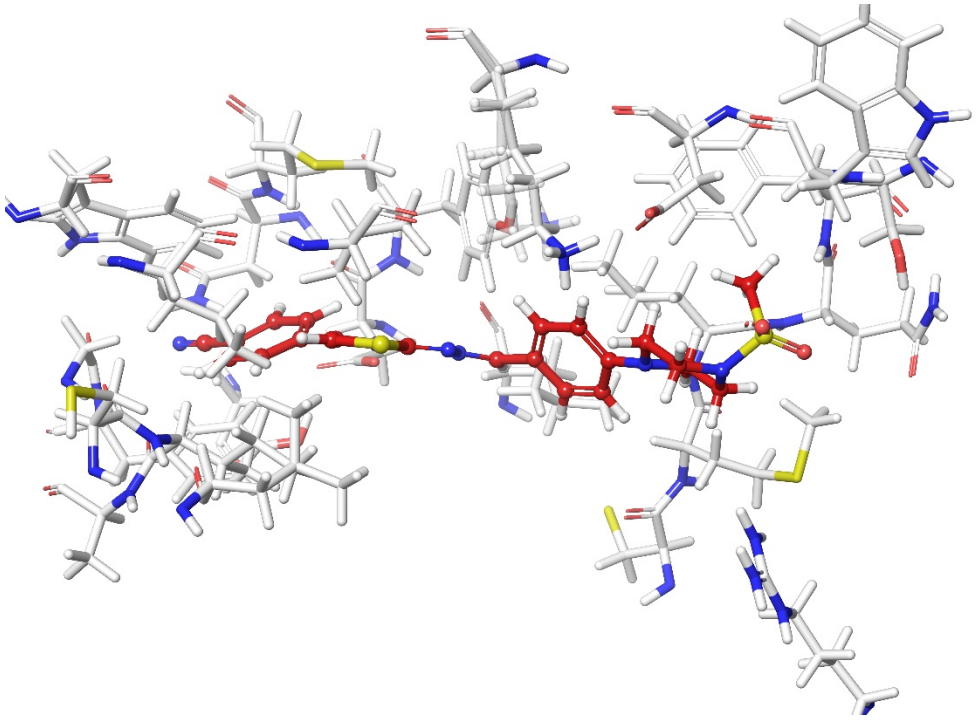


Figure S52. The three-dimensional interacting mode of compound **3d** in the active region of δ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with red and white, respectively (PDB Code: 4N6H).

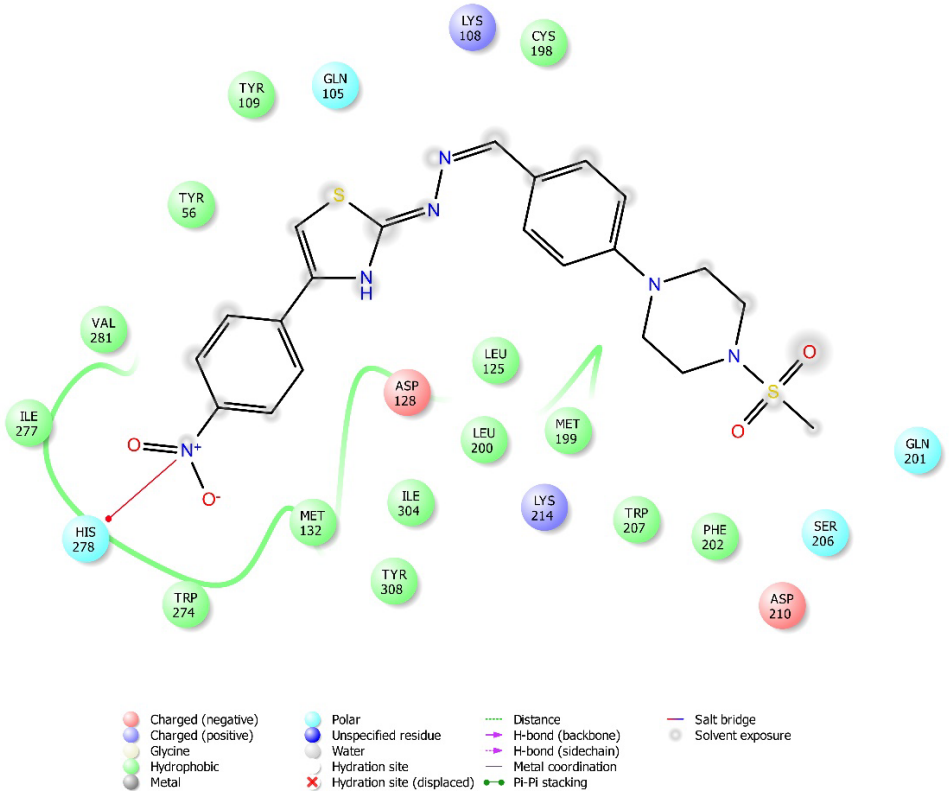


Figure S53. The two-dimensional interacting mode of compound **3e** in the active region of δ-opioid receptor (PDB Code: 4N6H).

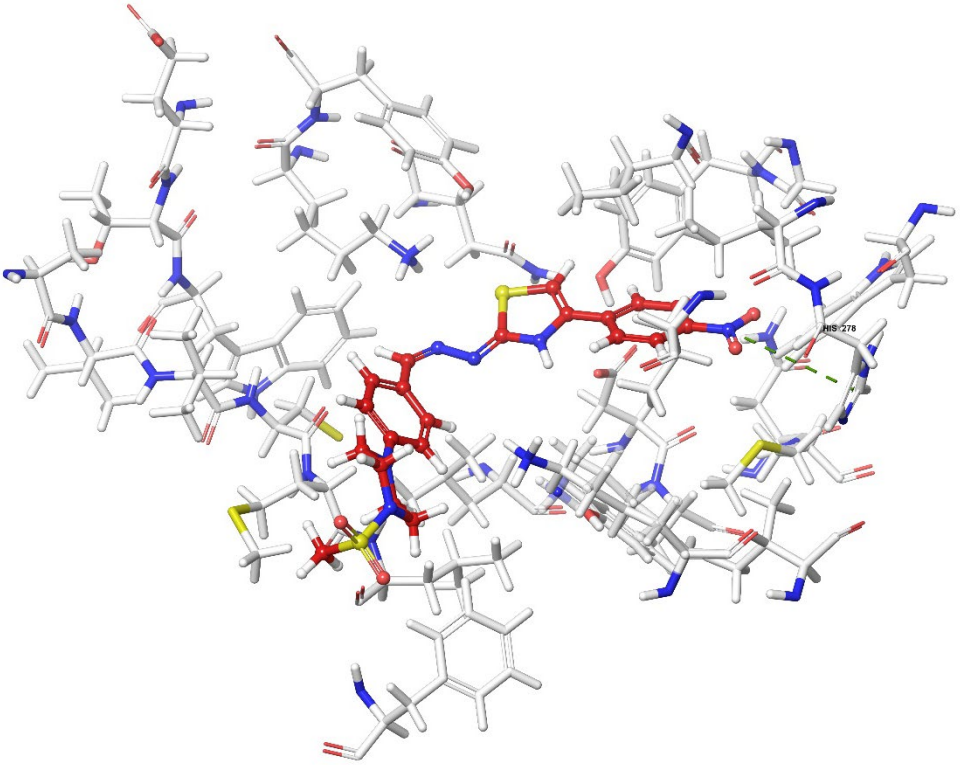


Figure S54. The three-dimensional interacting mode of compound **3e** in the active region of δ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with red and white, respectively (PDB Code: 4N6H).

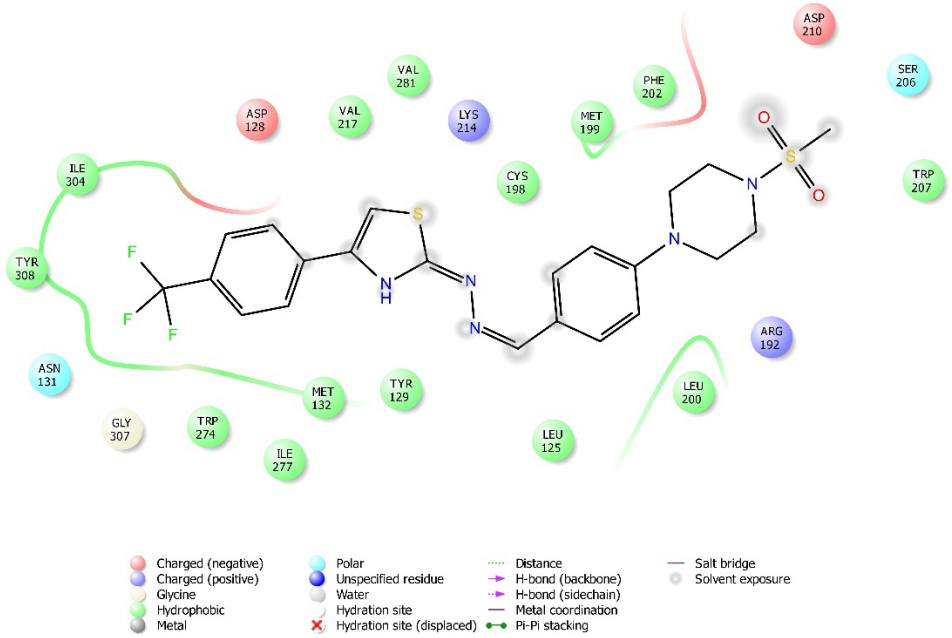


Figure S55. The two-dimensional interacting mode of compound **3h** in the active region of δ-opioid receptor (PDB Code: 4N6H).

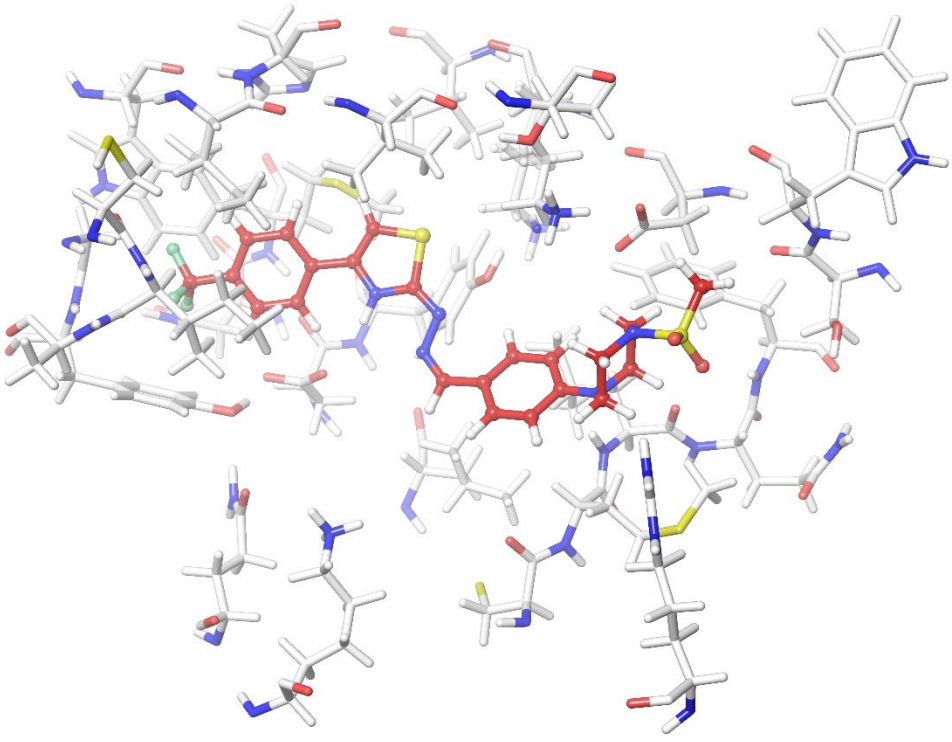


Figure S56. The three-dimensional interacting mode of compound **3h** in the active region of δ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with red and white, respectively (PDB Code: 4N6H).

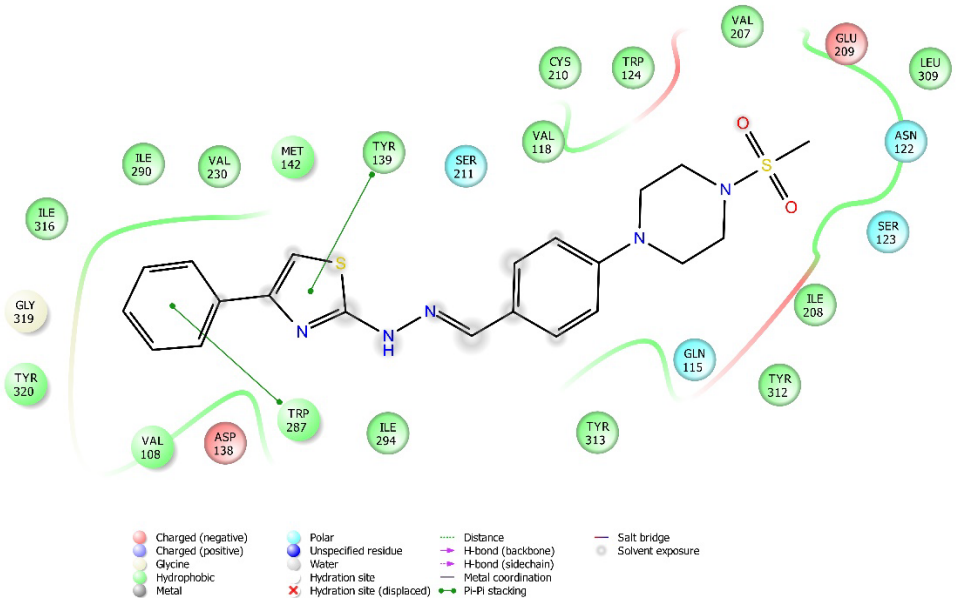


Figure S57. The two-dimensional interacting mode of compound **3a** in the active region of κ-opioid receptor (PDB Code: 6B73).

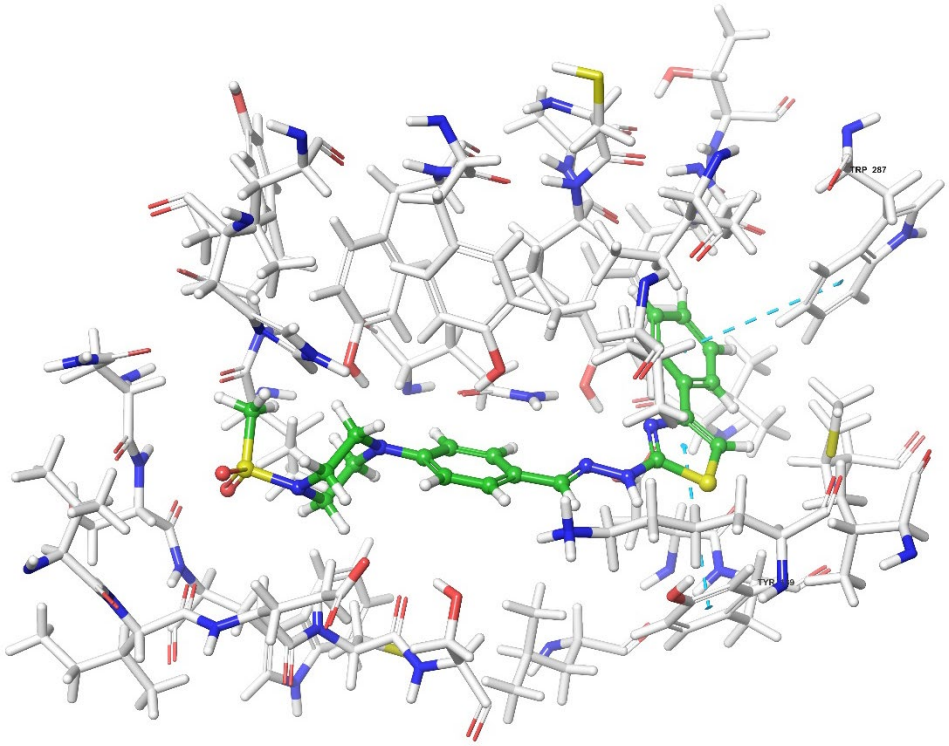


Figure S58. The three-dimensional interacting mode of compound **3a** in the active region of κ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with green and white, respectively (PDB Code: 6B73).

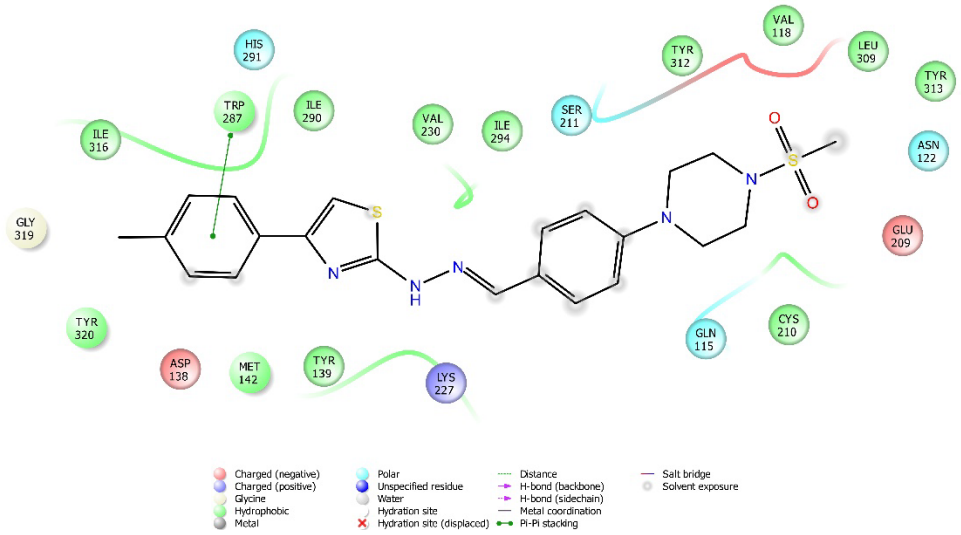


Figure S59. The two-dimensional interacting mode of compound **3b** in the active region of κ-opioid receptor (PDB Code: 6B73).

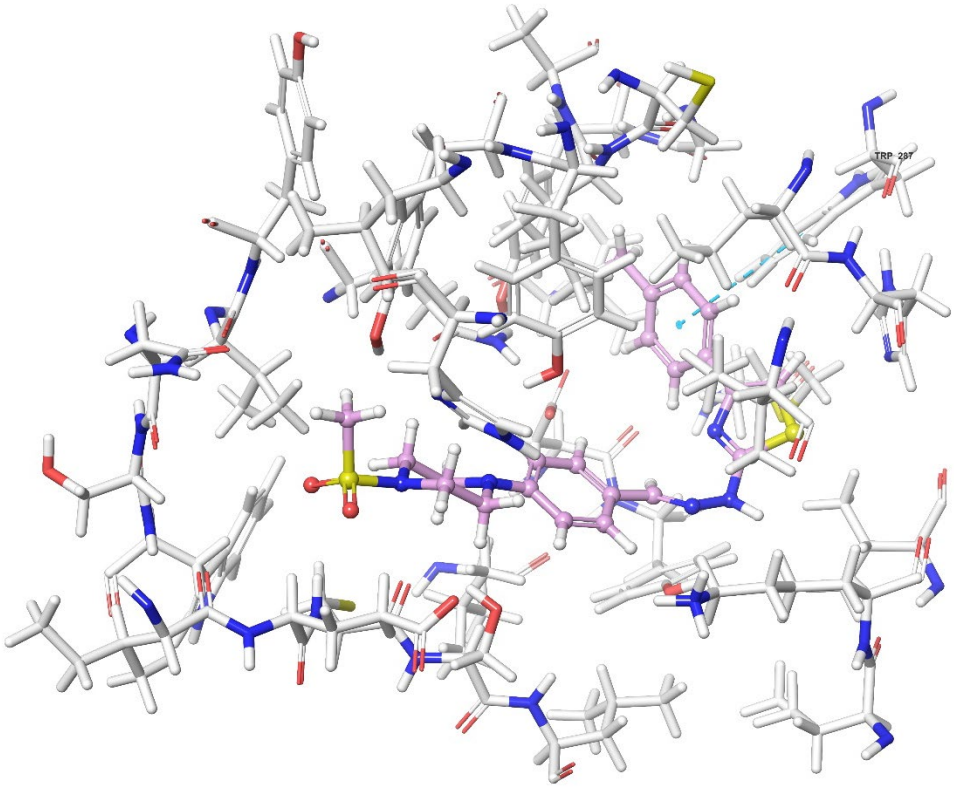


Figure S60. The three-dimensional interacting mode of compound **3b** in the active region of κ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with pink and white, respectively (PDB Code: 6B73).

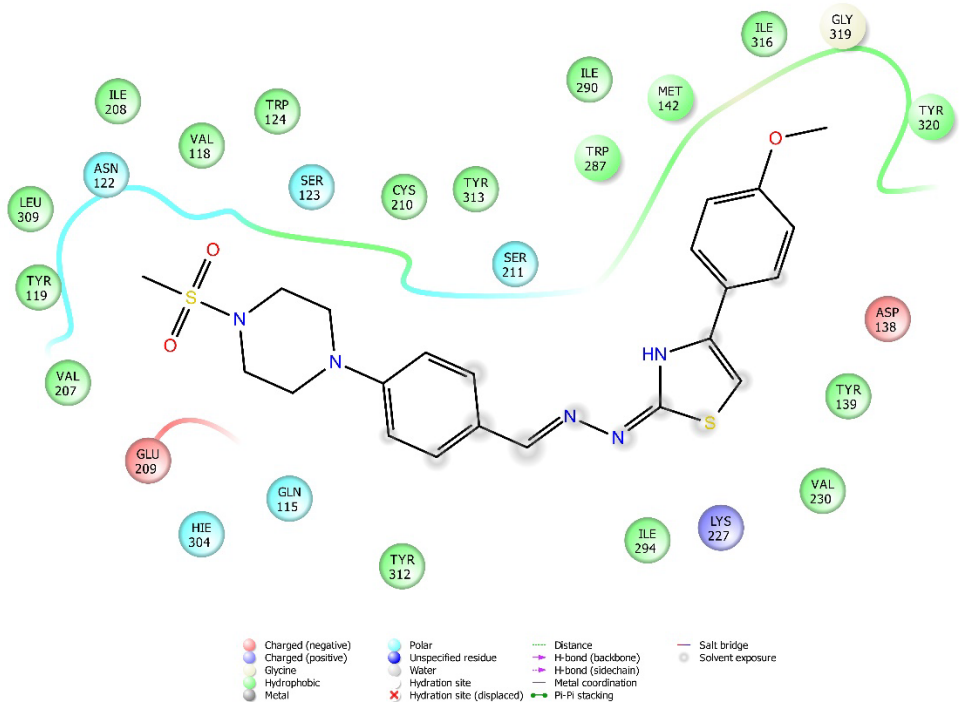


Figure S61. The two-dimensional interacting mode of compound **3c** in the active region of κ-opioid receptor (PDB Code: 6B73).

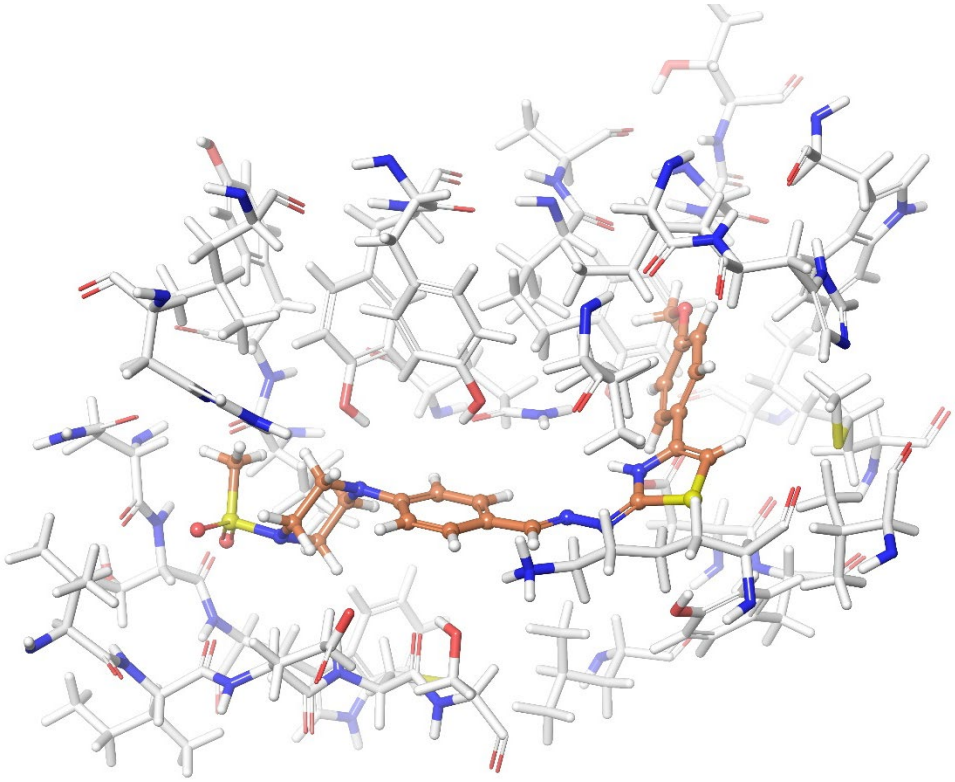


Figure S62. The three-dimensional interacting mode of compound **3c** in the active region of κ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with orange and white, respectively (PDB Code: 6B73).

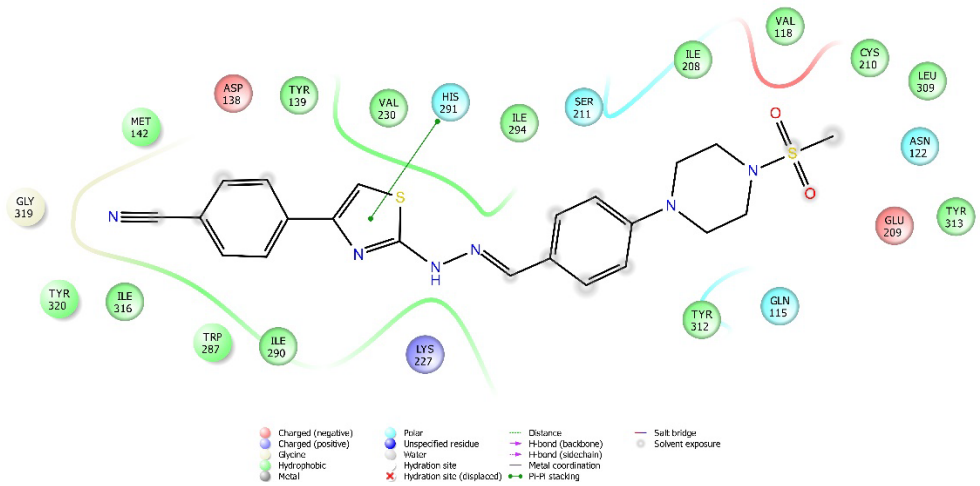


Figure S63. The two-dimensional interacting mode of compound **3d** in the active region of κ-opioid receptor (PDB Code: 6B73).

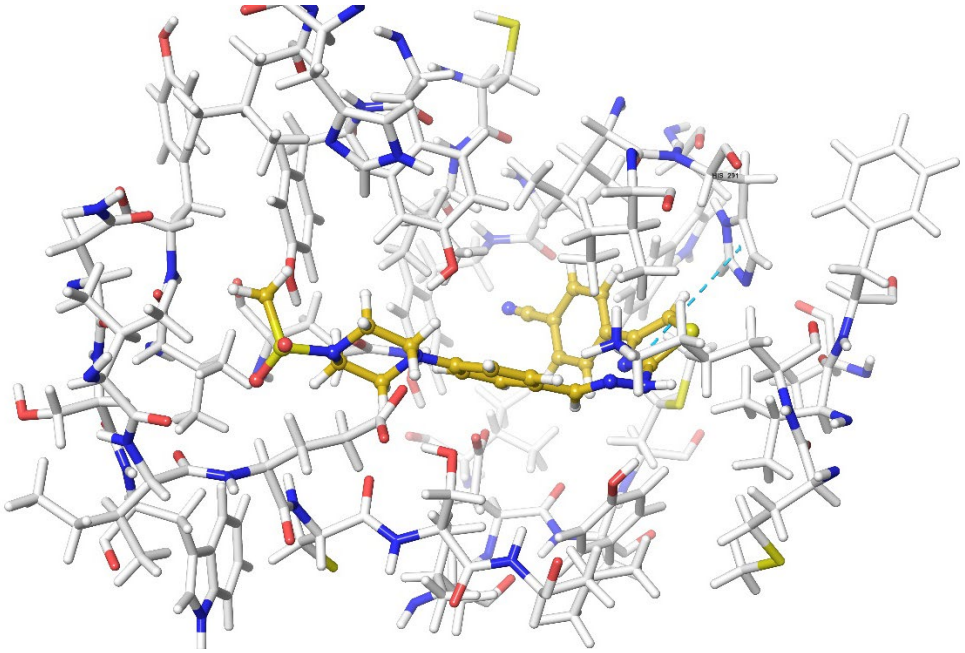


Figure S64. The three-dimensional interacting mode of compound **3d** in the active region of κ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with yellow and white, respectively (PDB Code: 6B73).

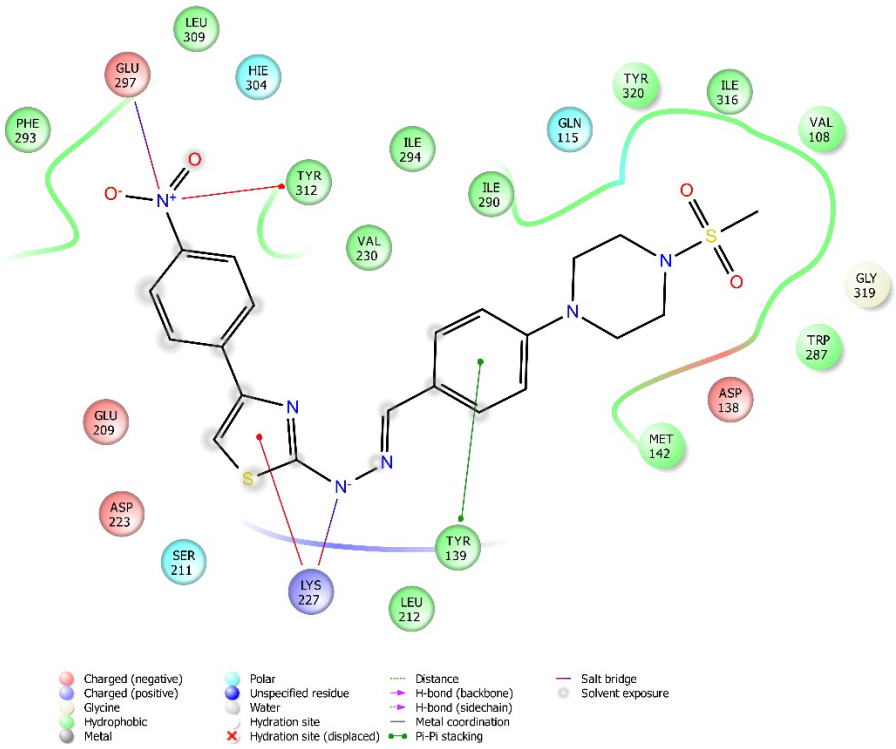


Figure S65. The two-dimensional interacting mode of compound **3e** in the active region of κ-opioid receptor (PDB Code: 6B73).

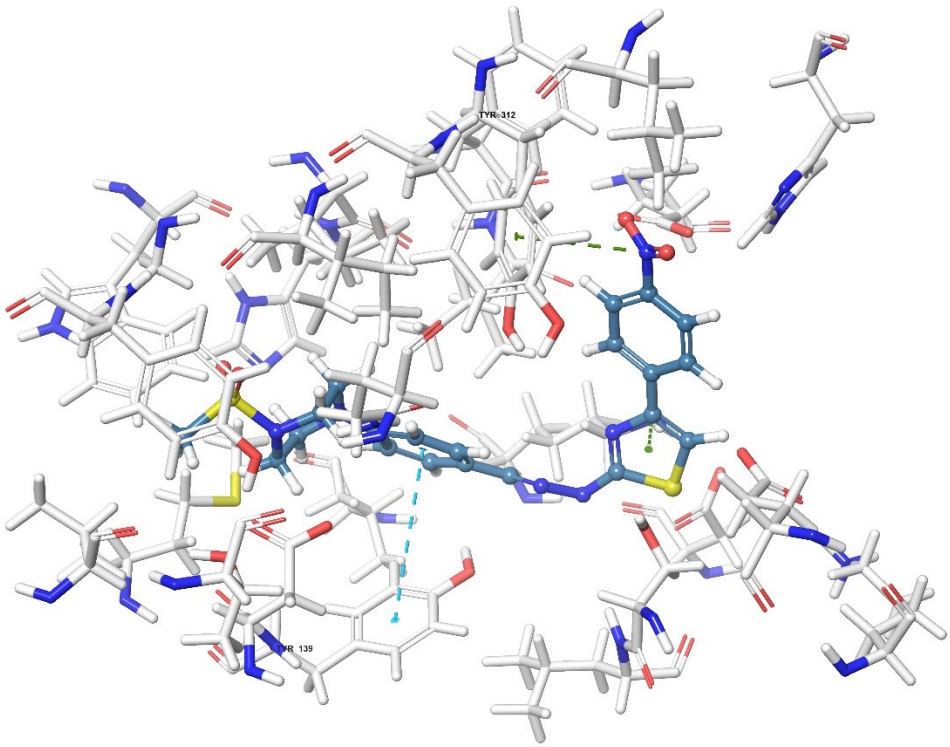


Figure S66. The three-dimensional interacting mode of compound **3e** in the active region of κ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with blue and white, respectively (PDB Code: 6B73).

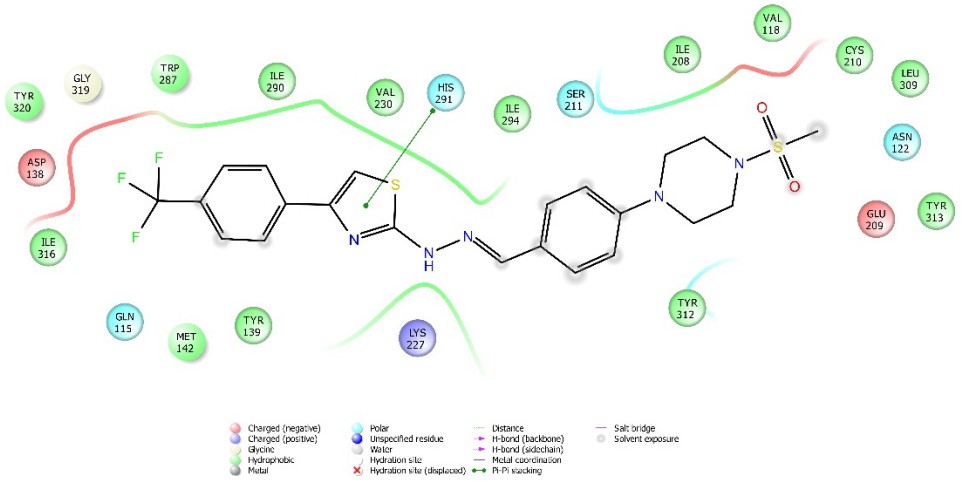


Figure S67. The two-dimensional interacting mode of compound **3h** in the active region of κ-opioid receptor (PDB Code: 6B73).

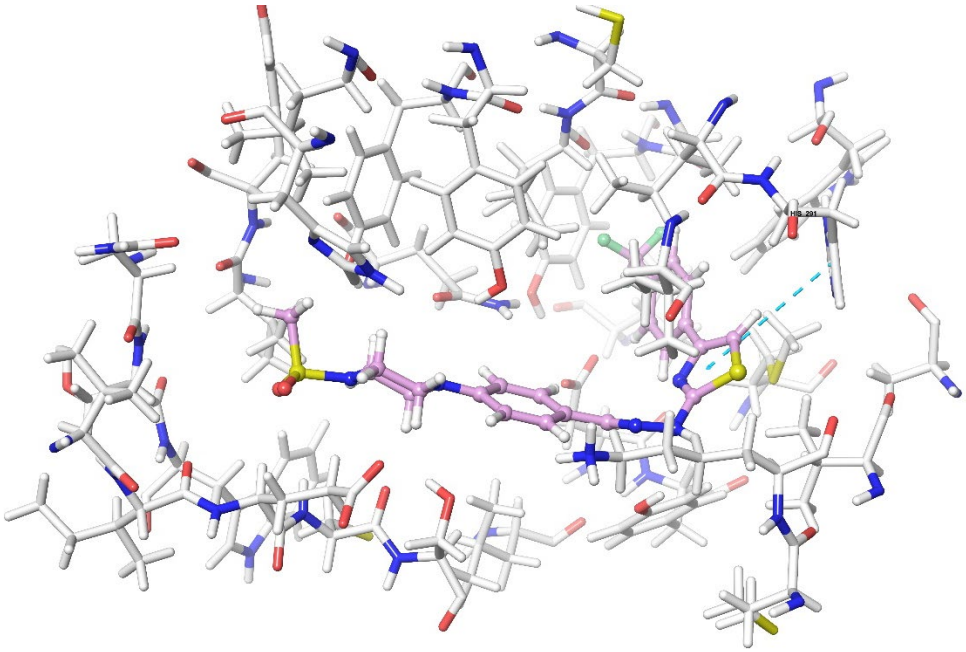


Figure S68. The three-dimensional interacting mode of compound **3h** in the active region of κ-opioid receptor. The ligand and significant residues of the active site of the receptor are presented by a tube model colored with pink and white, respectively (PDB Code: 6B73).