Supporting Information

Synthesis of Chiral 1,4-Oxazepane-5-Carboxylic Acids from Polymer-Supported Homoserine

Petra Králová,[1] Barbora Lemrová,[1] Michal Maloň,[2] and Miroslav Soural[1,3*]

[1] Department of Organic Chemistry, Faculty of Science, Palacký University, 771 46 Olomouc, Czech Republic
[2] JEOL (U.K.) Ltd., JEOL House, Silver Court, Watchmead, Welwyn Garden City, Hertfordshire AL7 1LT, United Kingdom
[3] Institute of Molecular and Translational Medicine, Faculty of Medicine and Dentistry, Palacký University, Hněvotínská 5, 779 00 Olomouc, Czech Republic

*Corresponding author. E-mail: miroslav.soural@upol.cz

Content

Analytical Data (NMR, IR, HRMS and optical rotation) of Prepared Derivatives

(-)-(*S*)-2-nitro-*N*-(2-oxo-2-phenethyl)-*N*-(2-oxotetrahydrofuran-3-yl)benzenesulfonamide 5a

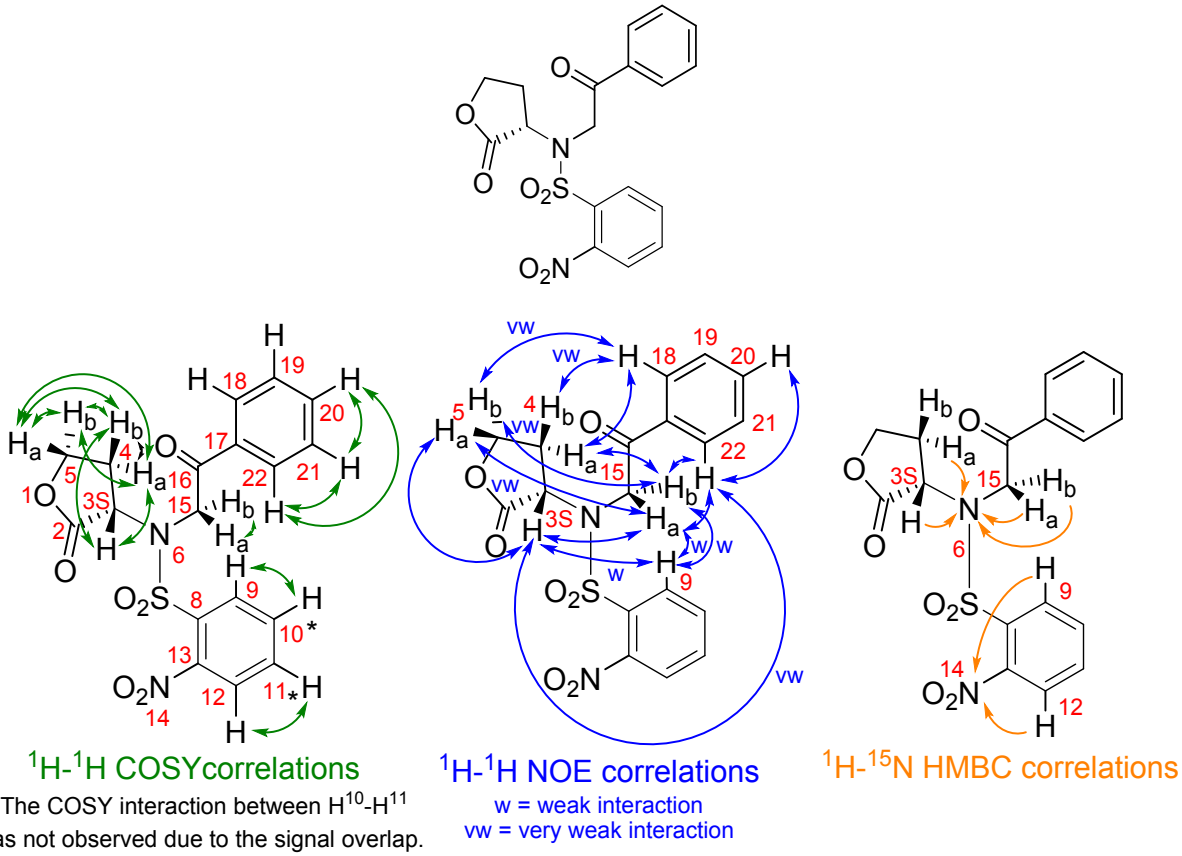


Figure S1. Detailed COSY, NOE and ^{1}H-^{15}N HMBC NMR analysis of lactone **5a**

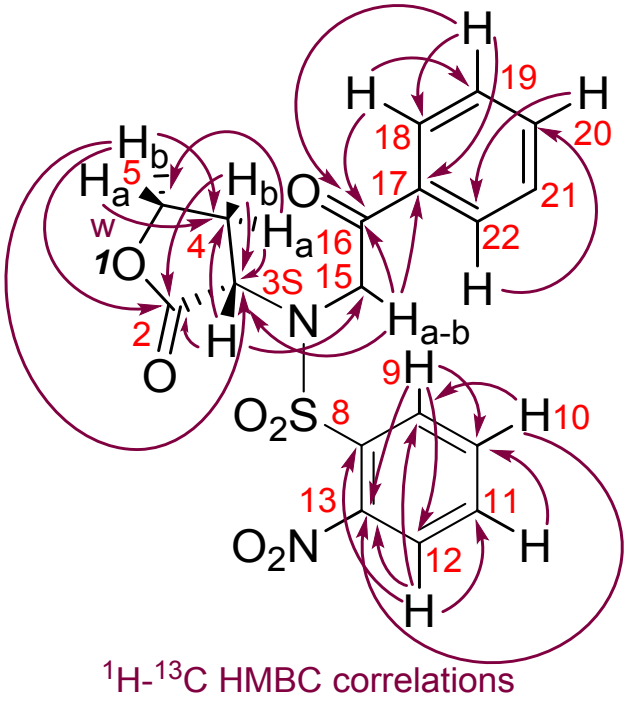


Figure S2. Detailed ^{1}H-^{13}C HMBC NMR analysis of lactone **5a**

Table S1. ^{1}H NMR (500 MHz) and ^{13}C{^{1}H} NMR (126 MHz) data, including detailed COSY, ^{1}H-^{13}C HMBC and NOE correlations for lactone **5a**[a]

position	^{1}H NMR δ_H [ppm][b]	splitting pattern, J [Hz], integration	^{13}C{^{1}H} NMR δ_C [ppm]	COSY correlations	^{1}H-^{13}C HMBC correlations	NOE correlations
2	-	-	174.4	-	-	-
3	5.05	dd, J = 12.4, 8.7 Hz, 1H	58.6	H_a^4, H_b^4	28.4, 53.2, 174.4	H_a^5, H^9 (weak int.), H_a^{15}, $H^{18,22}$ (very weak int.)
4	H_a : 2.29	dddd, J = 12.5, 12.5, 11.2, 9.0 Hz, 1H	28.4	H^3, H_a^5, H_b^5	58.6, 66.2	H_b^{15}, $H^{18,22}$
	H_b: 2.57	dddd, J = 12.7, 8.7, 5.8, 1.0 Hz, 1H		H^3, H_a^5, H_b^5 (weak int.)	58.6, 174.4	$H^{18,22}$ (very weak int.)
5	H_a : 4.24	ddd, J = 11.2, 9.0, 5.8 Hz, 1H	66.7	H_a^4, H_b^4, H_b^5 H_a^4, H_b^4 (weak int.), H_a^5	28.4 (weak int.)	H^3, H_a^{15}
	H_b: 4.31	ddd, J = 9.0, 9.0, 1.0 Hz, 1H		H_a^5,	28.4, 58.6, 174.4	H_a^{15} (very weak int.), $H^{18,22}$ (very weak int.)
8	-	-	133.8	-	-	-
9	8.26	dd, J = 7.7, 1.6 Hz, 1H	131.6	H^{10}	125.4, 135.4, 148.9	H^{11}, H^{12}
10	7.81	m, 1H	125.1	H^9	131.6, 148.9	H^{12}
11	7.77	m, 1H	133.3	H^{12}	125.4	H^9
12	7.75	m, 1H	135.4	H^{11}	131.6, 133.3, 133.8, 148.9	H^9, H^{10}
13	-	-	148.9	-		
15	H_a : 5.25	J = 19.2 Hz, 1H	53.2	H_b^{15}	58.6, 135.5, 194.7	H^3, H_a^5 (very weak int.), H^9 (weak int.), $H^{18,22}$
	H_b: 4.60	d, J = 19.2 Hz, 1H		H_a^{15}	58.6, 135.5, 194.7	H_a^4, H_b^5 (very weak int.), H^9 (weak int.), $H^{18,22}$
16	-	-	194.7	-	-	-
17	-	-	135.5	-	-	-
18,22	7.94-7.96	m, 2H	128.9	$H^{19,21}$	129.8, 134.9, 194.7	H^{20}
19,21	7.50-7.54	m, 2H	129.8	$H^{18,22}$, H^{20}	128.9, 135.5, 194.7	-
20	7.63-7.67	m, 1H	134.9	H^{21}	128.9	$H^{18,22}$

[a]Assignments are based on extensive 1D and 2D NMR analysis (^{1}H-^{1}H COSY, ^{1}H-^{13}C HMQC, ^{1}H-^{13}C HMBC and ^{1}H-^{1}H NOESY); measured in MeCN-d_3; int. = interaction.

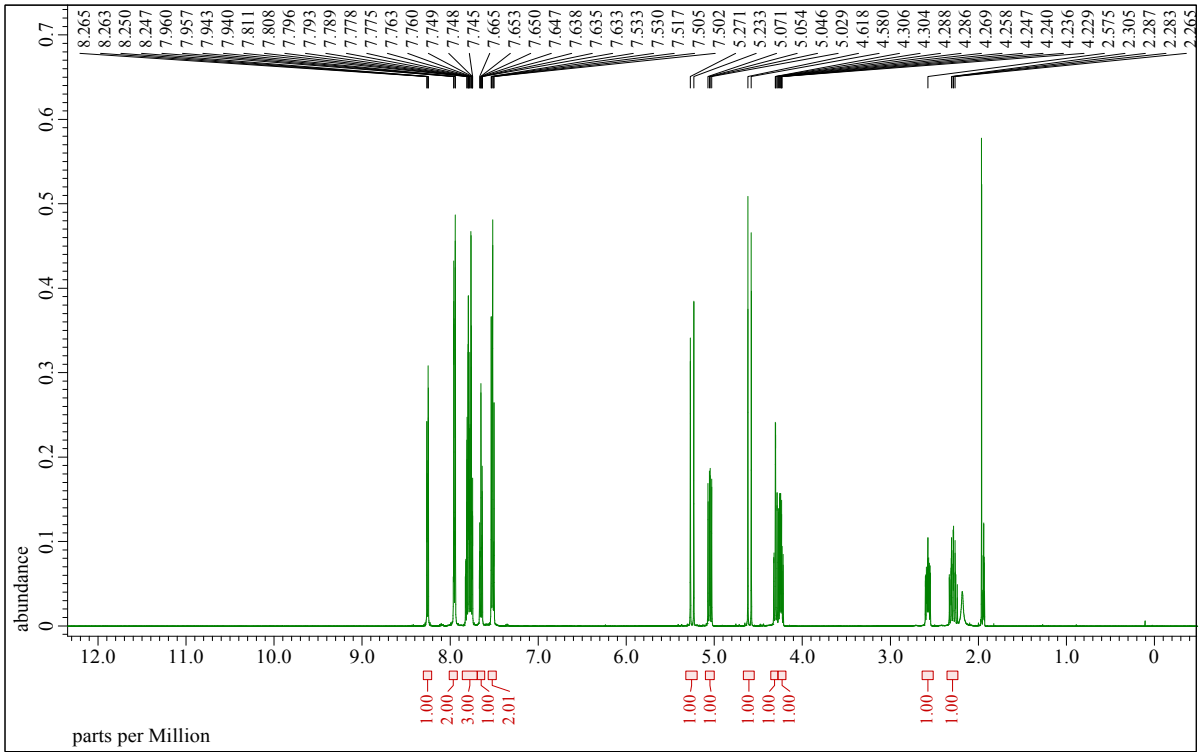


Figure S3. ^{1}H NMR spectrum of **5a** (500 MHz, MeCN-d_3); note: the signal of non-deuterated MeCN at 1.96 ppm and MeCN-d_3 at 1.94 ppm in ratio 62:38 in ^{1}H NMR

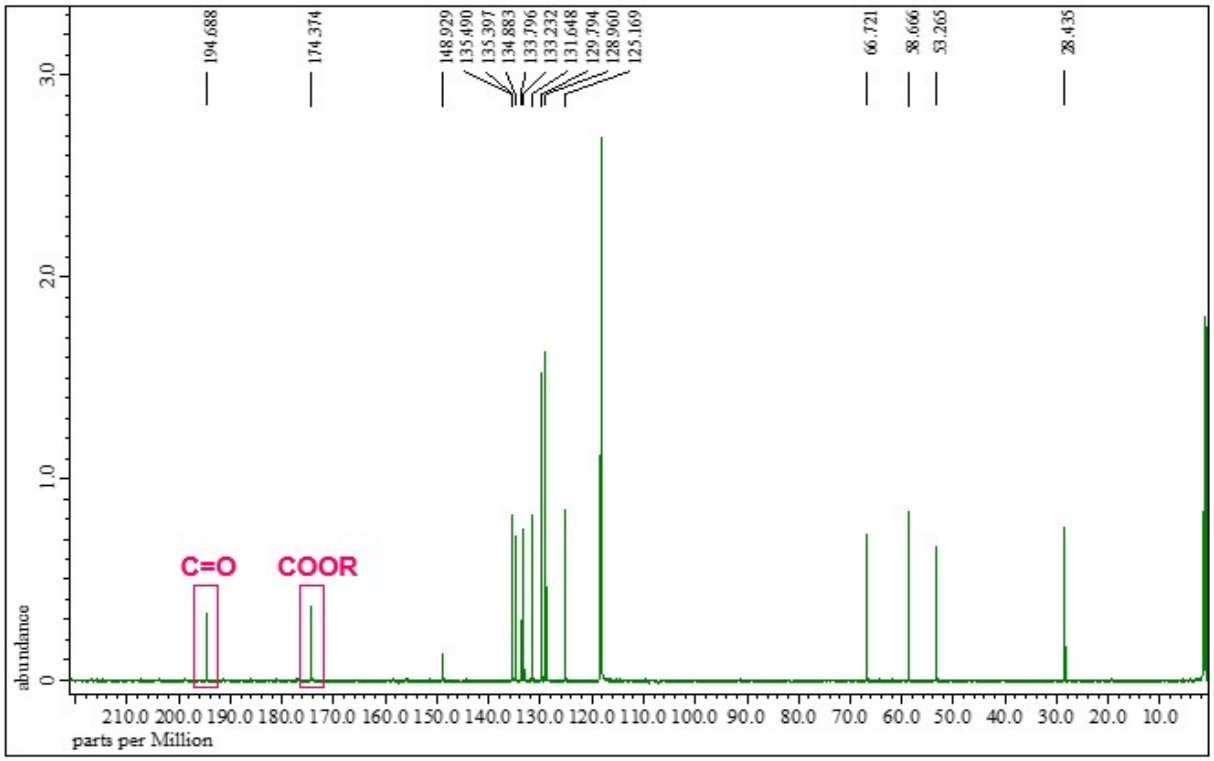


Figure S4. ^{13}C{^{1}H} NMR spectrum of **5a** (126 MHz, MeCN-d_3)

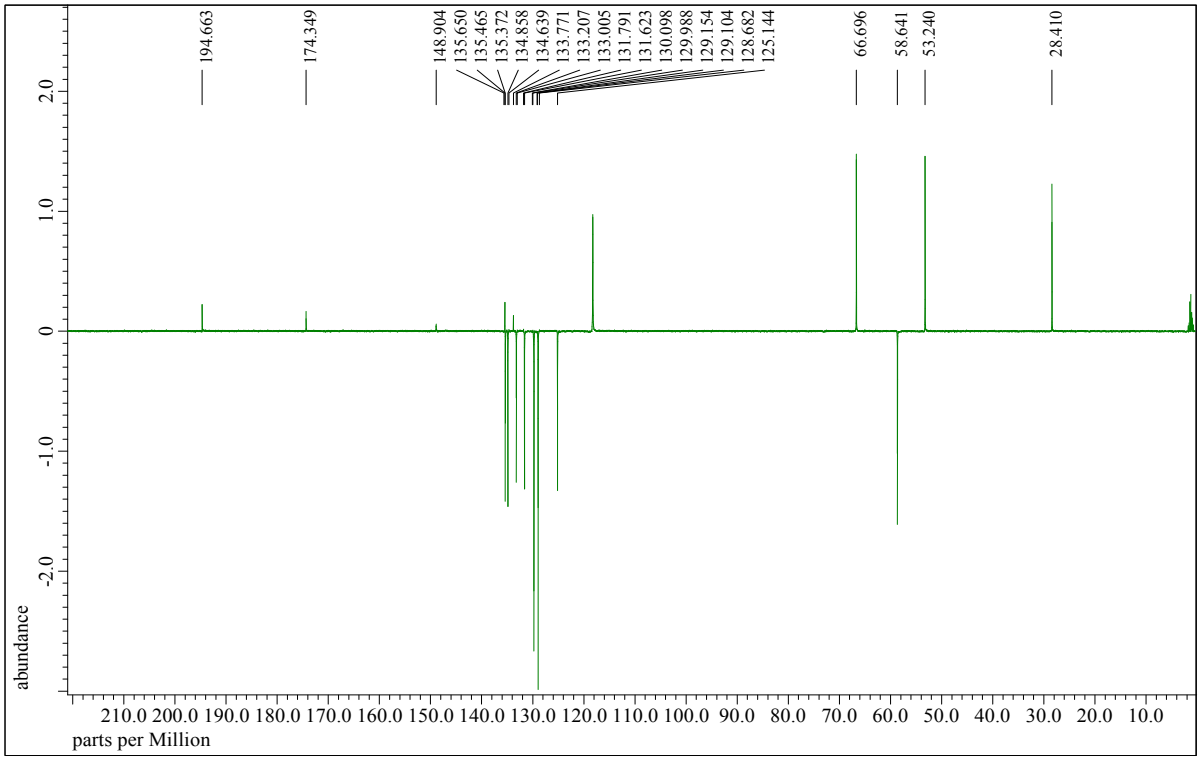


Figure S5. ^{13}C APT NMR spectrum of **5a** (126 MHz, MeCN-d_3)

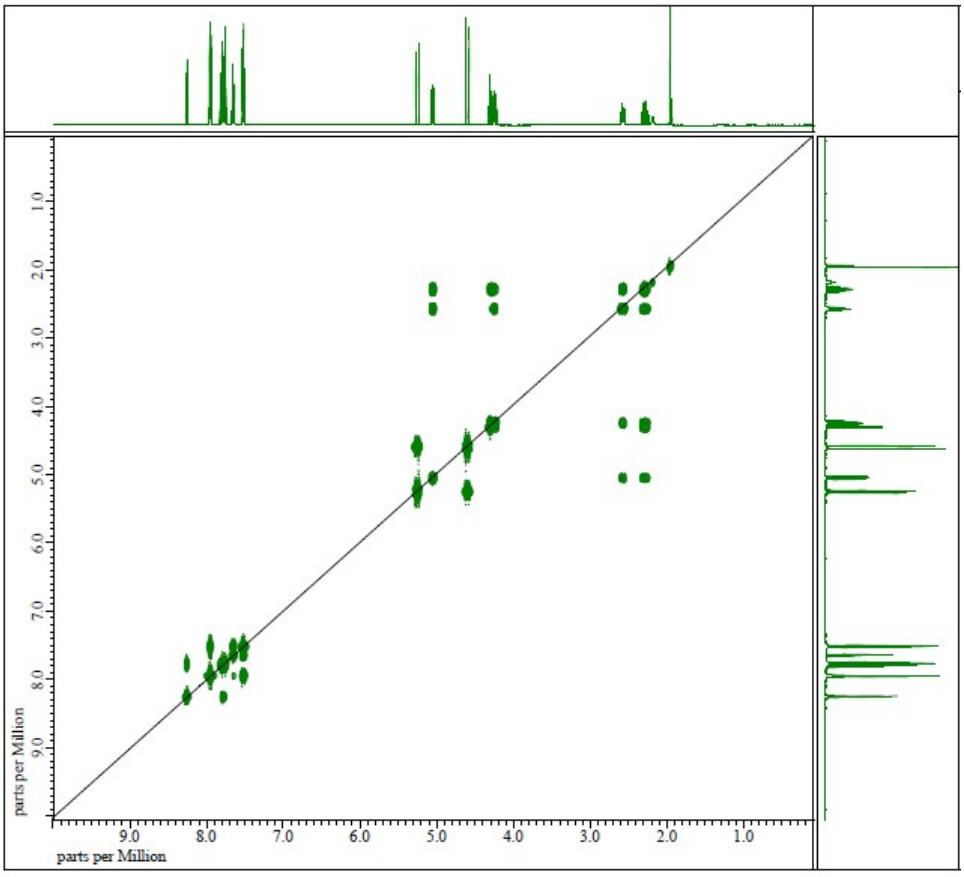


Figure S6. ^{1}H-^{1}H COSY NMR spectrum of **5a** (500 MHz, MeCN-d_3)

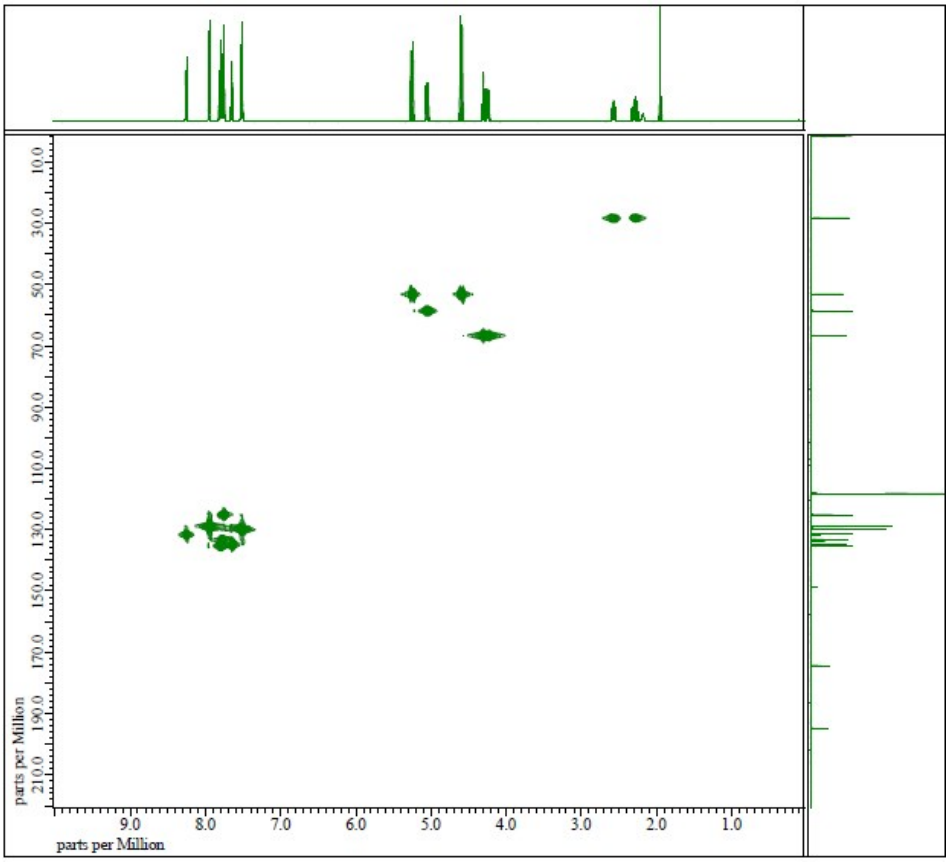


Figure S7. ^{1}H-^{13}C HMQC NMR spectrum of **5a** (MeCN-d_3)

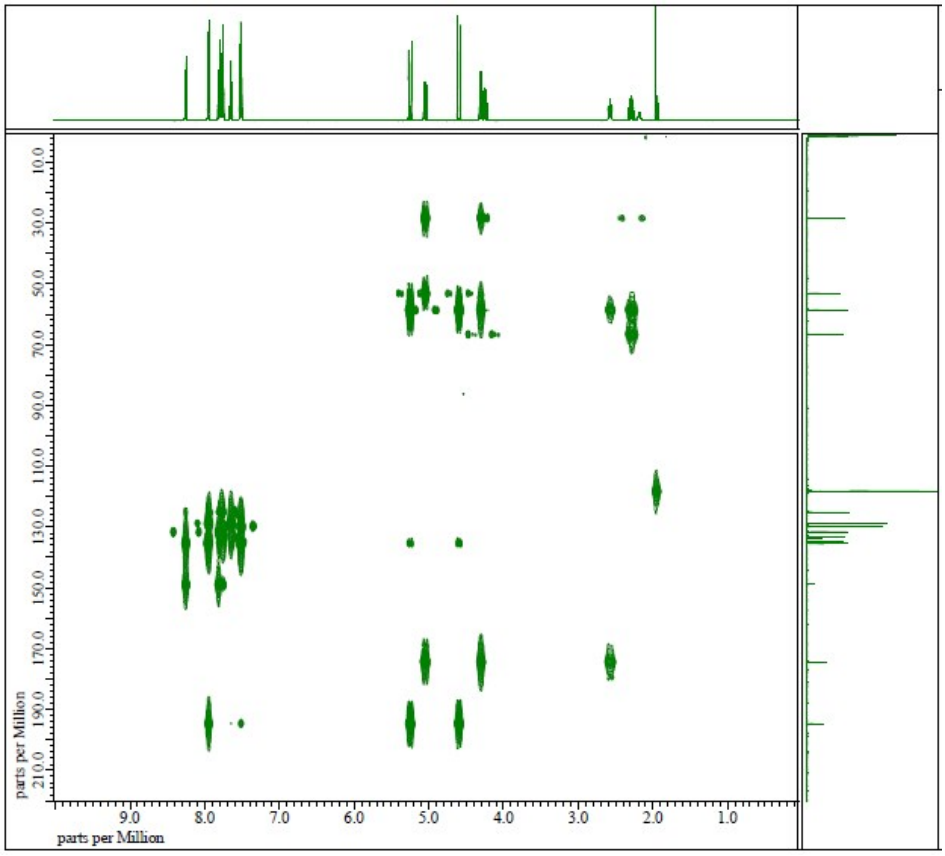


Figure S8. ^{1}H-^{13}C HMBC NMR spectrum of **5a** (MeCN-d_3)

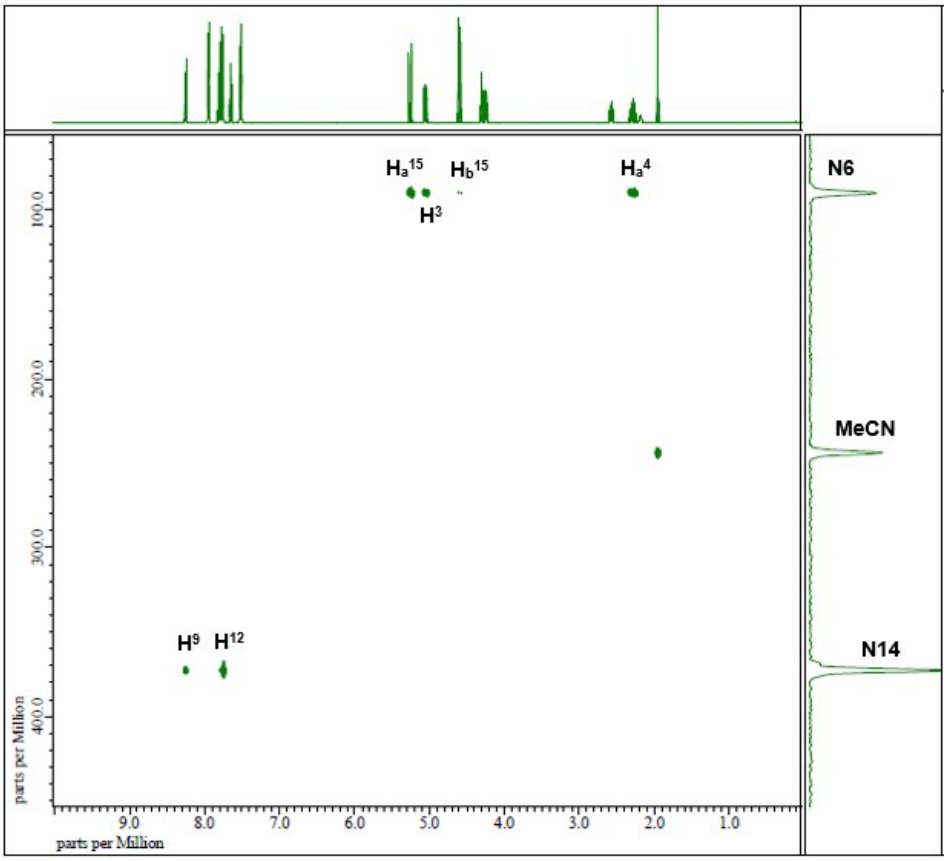


Figure S9. ^{1}H-^{15}N HMBC NMR spectrum of **5a** (MeCN-d_3)

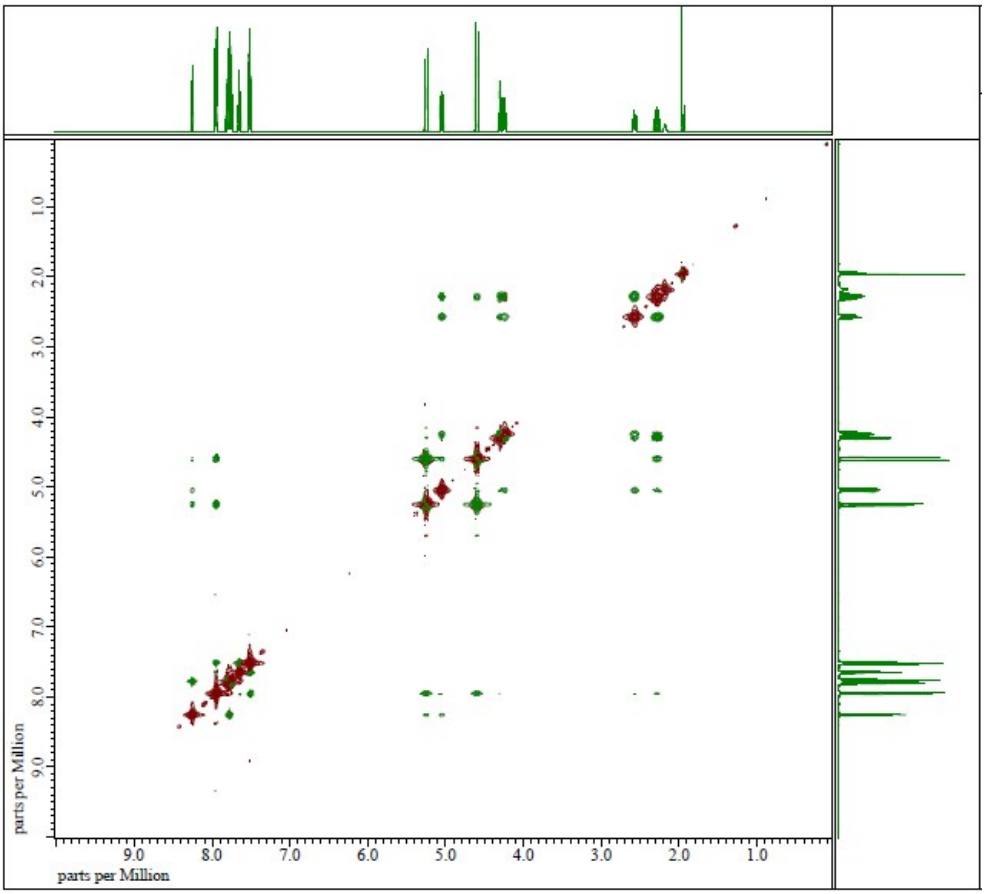


Figure S10. ^{1}H-^{1}H NOESY NMR spectrum of **5a** (MeCN-d_3)

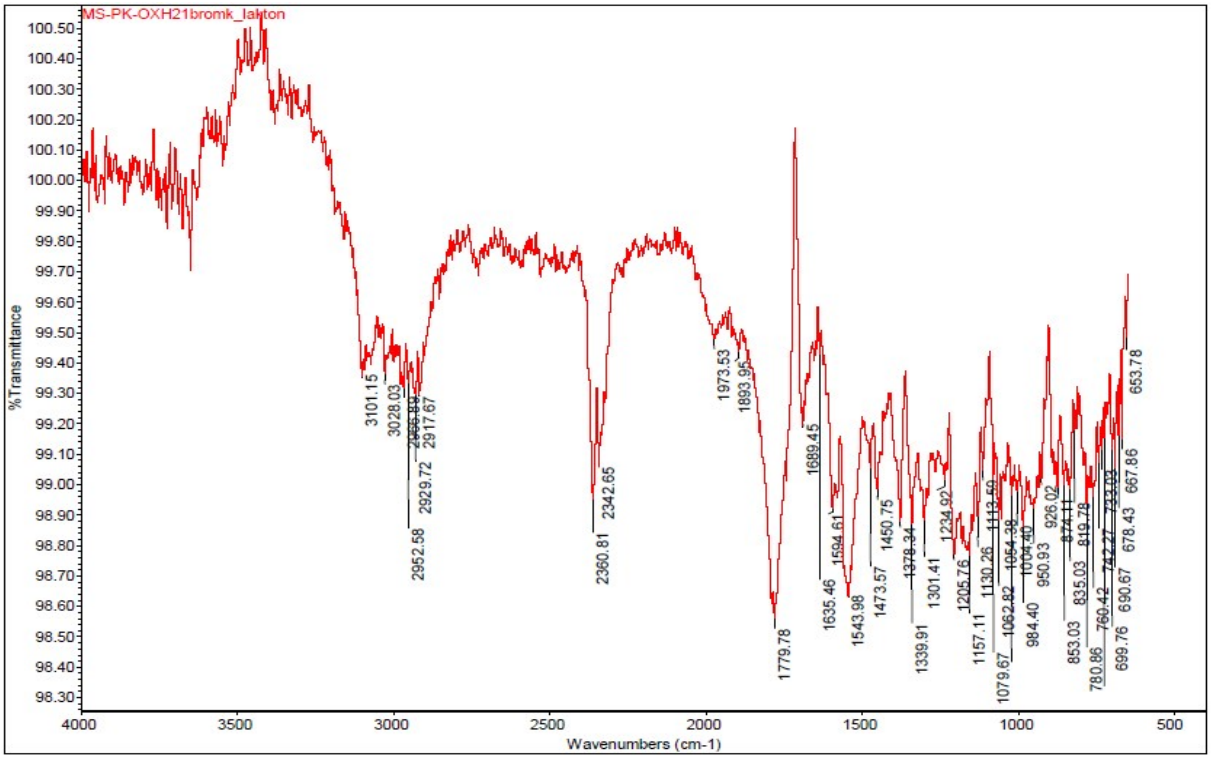


Figure S11. IR spectrum of **5a**

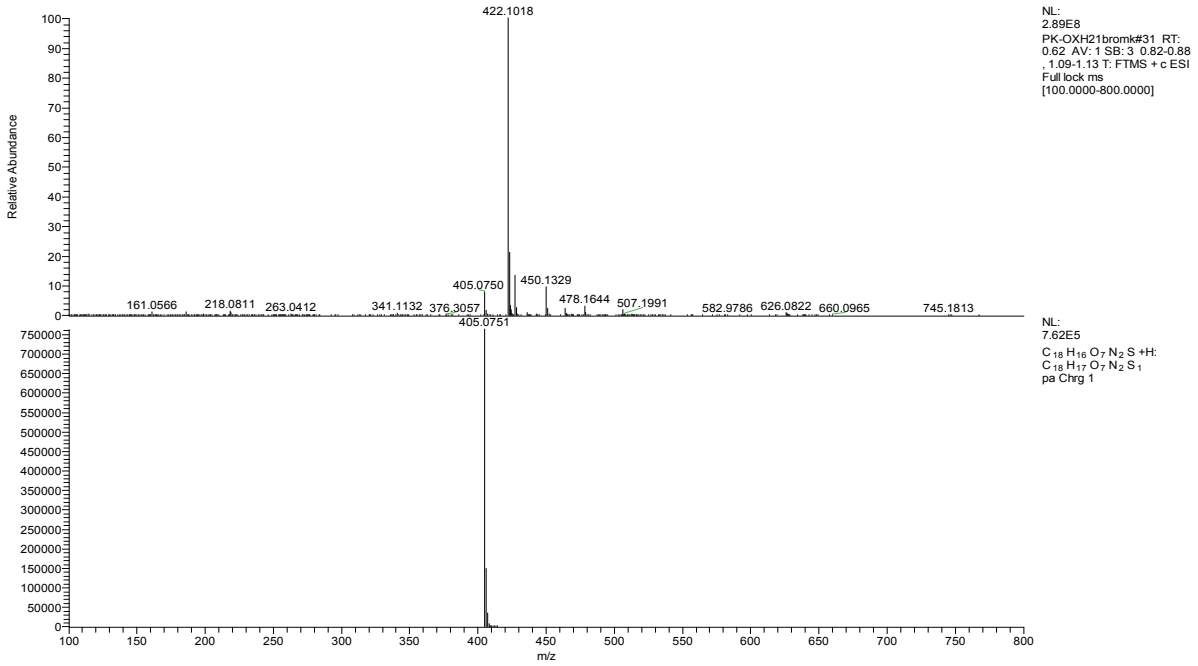
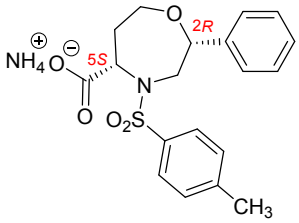


Figure S12. HRMS spectrum of **5a**. Note: ion 422 belongs to the ammonium adduct originating from mobile phase.

(-)-ammonium (2*R*,5S)-2-phenyl-4-tosyl-1,4-oxazepane-5-carboxylate 6g



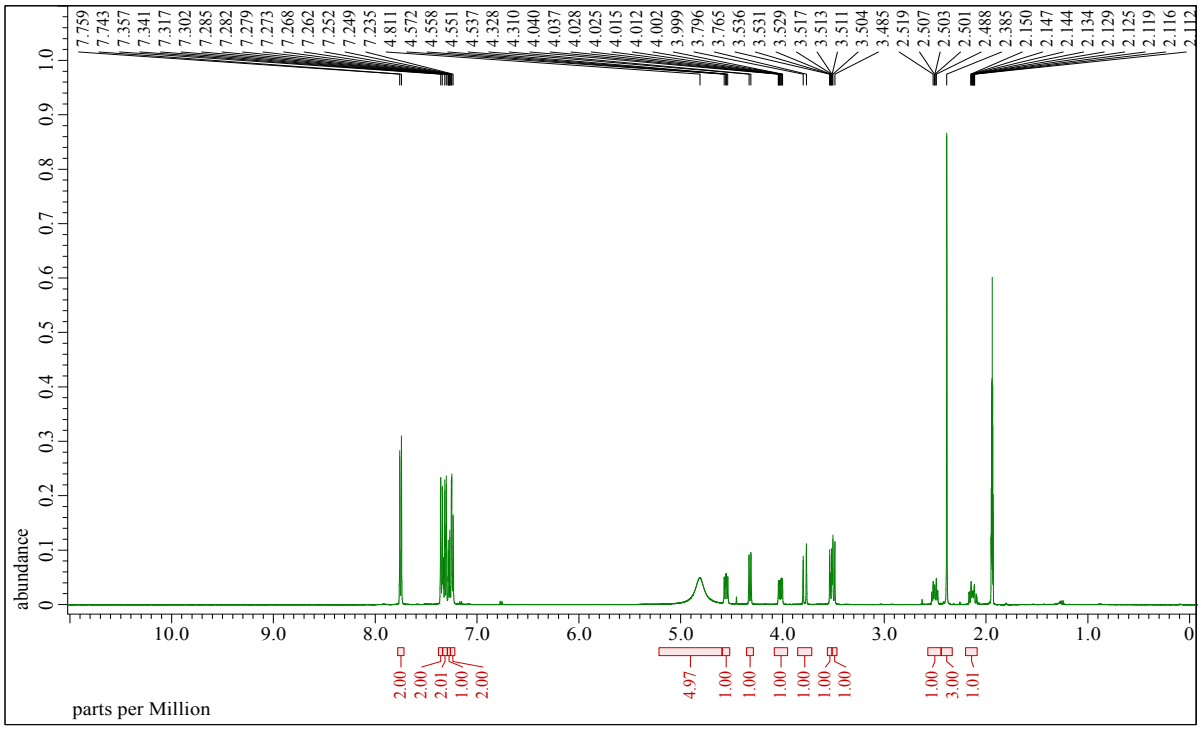


Figure S13. ^{1}H NMR spectrum of **6g** (500 MHz, MeCN-d_3). Note: The broad signal observed at 4.81 ppm represents ammonium ion and residual water.

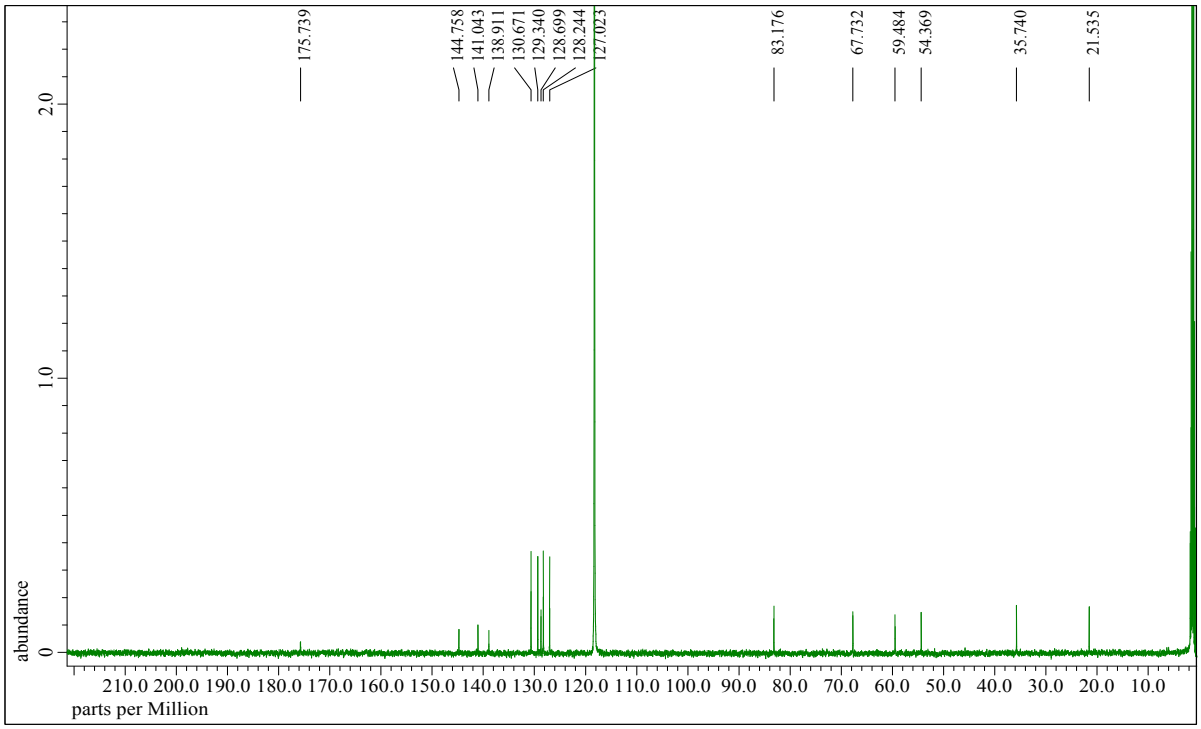


Figure S14. ^{13}C{^{1}H} NMR spectrum of **6g** (126 MHz, MeCN-d_3)

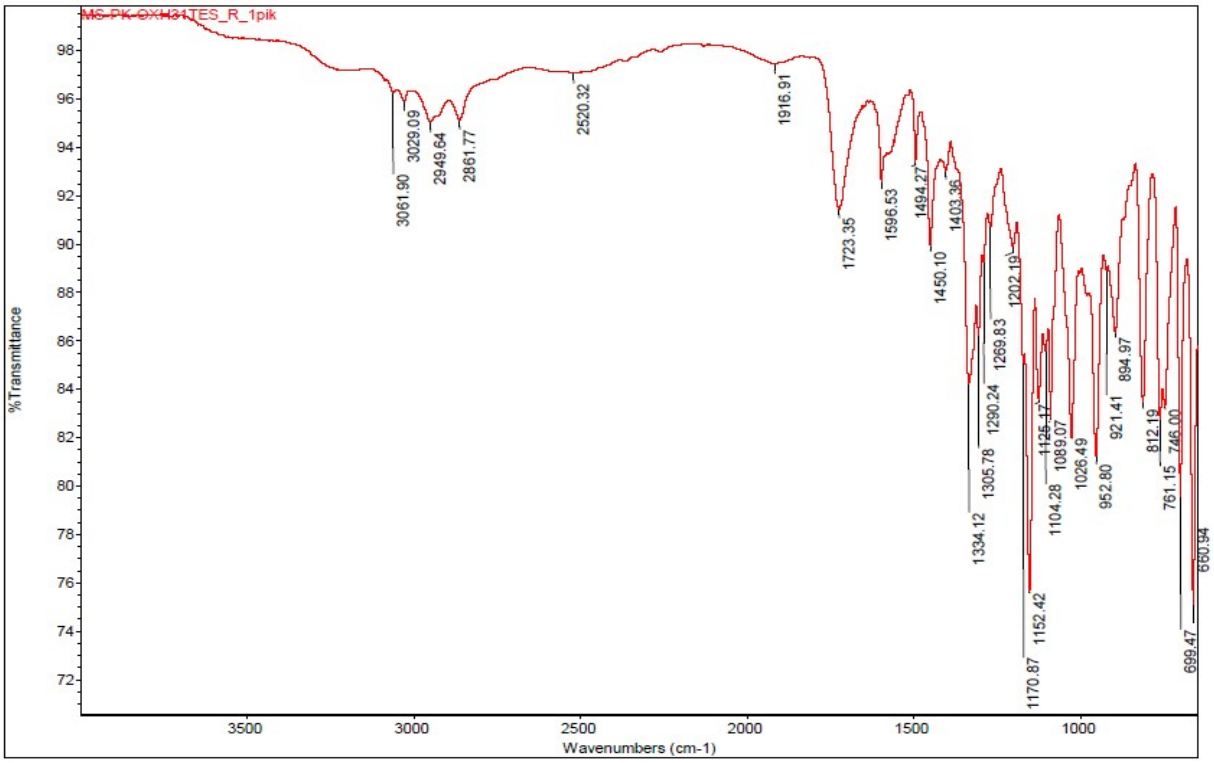


Figure S15. IR spectrum of **6g**

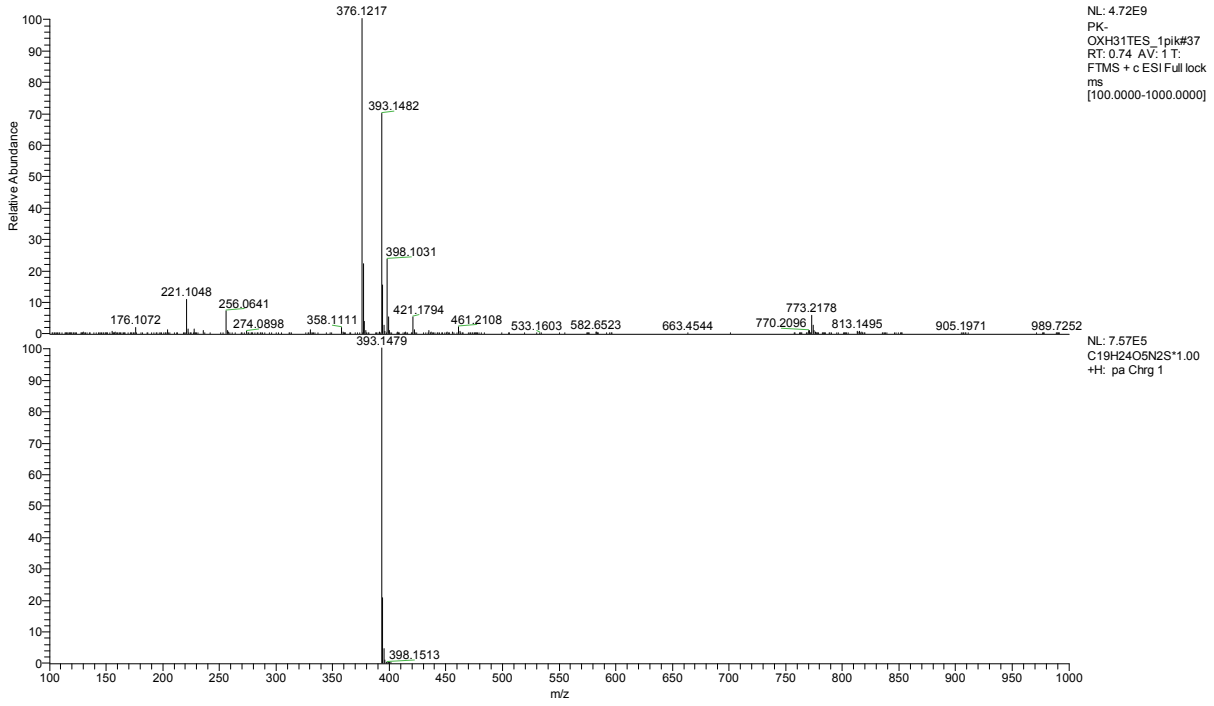


Figure S16. HRMS spectrum of **6g**

(-)-(2R,5S)-4-((2-aminophenyl)sulfonyl)-2-phenyl-1,4-oxazepane-5-carboxylic acid 7a

The analytical data are identical for **7a** prepared from Wang resin or Wang-piperazine resin.

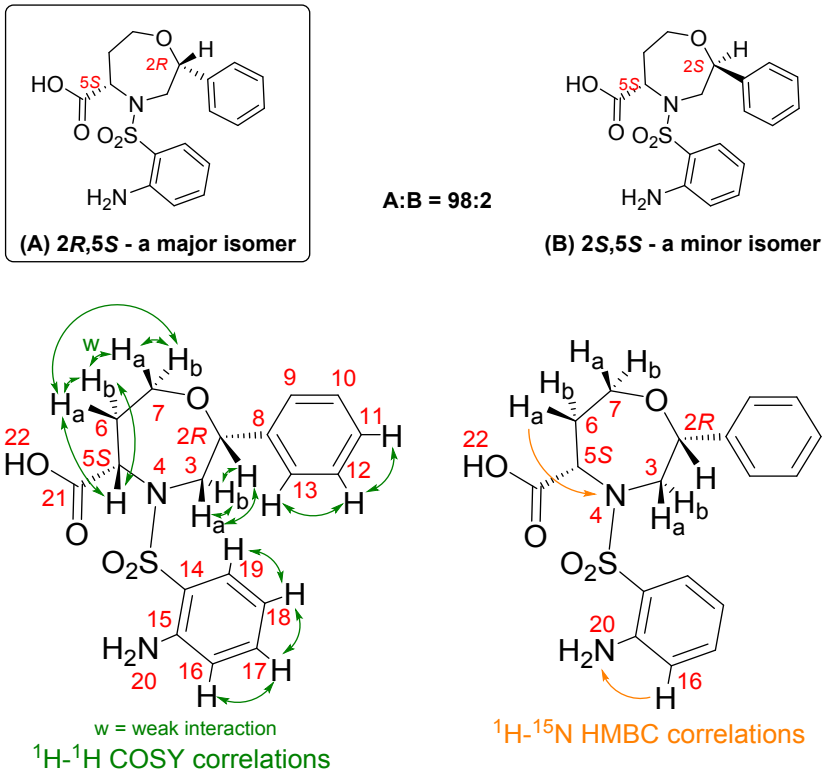


Figure S17. Detailed COSY and ^{1}H-^{15}N HMBC NMR analysis of 1,4-oxazepane **7a**

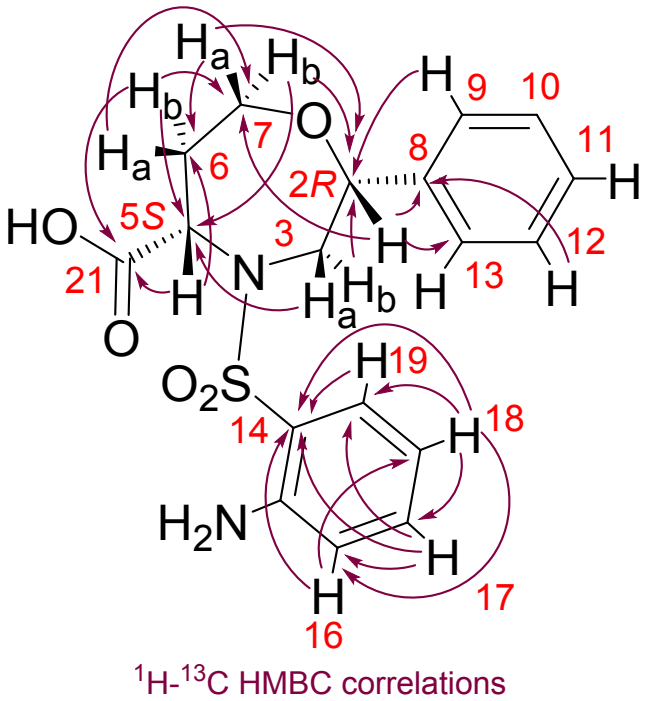


Figure S18. Detailed ^{1}H-^{13}C HMBC NMR analysis of 1,4-oxazepane **7a**

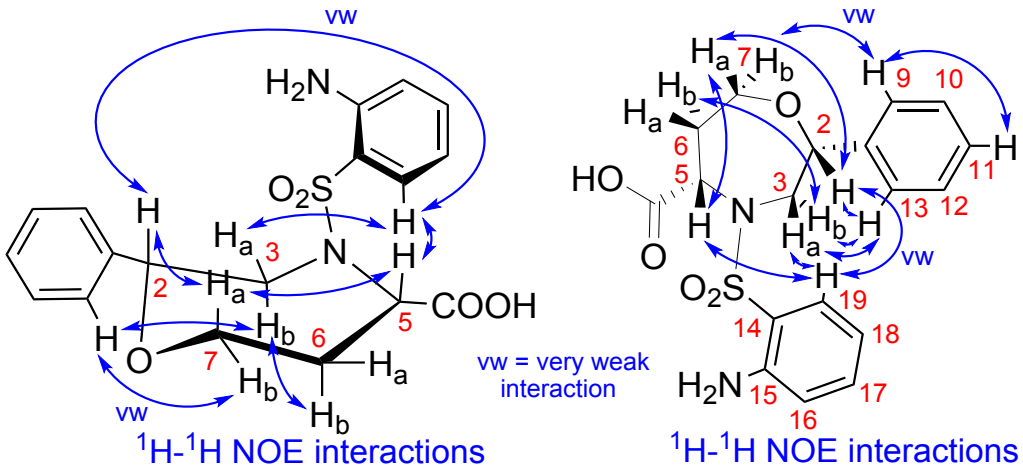


Figure S19. Detailed ^{1}H-^{1}H NOE NMR analysis of 1,4-oxazepane **7a**

Table S2. ^{1}H NMR (500 MHz) and ^{13}C{^{1}H} NMR (126 MHz) data, including detailed COSY, ^{1}H-^{13}C HMBC and NOE correlations for 1,4-oxazepane **7a**[a]

position	^{1}H NMR δ_H [ppm][b]	splitting pattern, J [Hz], integration	^{13}C{^{1}H} NMR δ_C [ppm]	COSY correlations	^{1}H-^{13}C HMBC correlations	NOE correlations
2	4.16	d, J = 9.5 Hz, 1H	82.7	H_b^3	67.5, 127.1, 141.0	H_a^7, $H^{9,13}$, H^{19} (weak int.)
3	H_a: 3.70	d, J = 16.1 Hz, 1H,	54.1	H_b^3	59.1	$H^{9,13}$, H^{19}
	H_b: 3.50	dd, J = 16.1, 9.5 Hz, 1H		H^2, H_a^3	59.1 (weak int.), 82.7	H_b^6, $H^{9,13}$
5	4.66	dd, J = 10.4, 7.1 Hz, 1H	59.1	H_a^6, H_b^6	35.6, 174.8	H_a^7, H^{19}
6	H_a: 2.54	ddd, J = 15.4, 7.1, 6.3 Hz, 1H	35.6	H^5, H_b^6, H_b^7	67.5	-
	H_b: 2.16	dddd, J = 15.4, 10.4, 8.9, 1.1 Hz, 1H		H^5, H_a^6, H_a^7	59.1, 67.5, 174.8	H_b^3
7	H_a: 3.65	dd, J = 12.7, 8.9 Hz, 1H	67.5	H_b^6, H_b^7	35.6, 59.1, 82.7	H^2, H^5,
	H_b: 4.02	ddd, J = 12.7, 6.3, 1.1 Hz, 1H		H_a^6, H_a^7	59.1, 82.7	$H^{9,13}$ (very weak int.)
8	-	-	141.0	-	-	
9,13	7.15	m, 2H	127.1	$H^{10,12}$	82.7, 128.7, 129.3	H^2, H_a^3, H_b^3, H_b^7 (very weak int.)
10,12	7.27-7.31	m, 2H	129.3	$H^{9,13}$, H^{11}	127.1, 128.7, 141.0	-
11	7.23-7.27	m, 1H	128.7	$H^{10,12}$	127.1, 129.3	-
14	-	-	121.9	-	-	-
15	-	-	147.5	-	-	-
16	6.84	dd, J = 8.3, 1.0 Hz, 1H	118.6	H^{17}	117.7, 121.9	-
17	7.34	ddd, J = 8.3, 7.2, 1.5 Hz, 1H	135.4	H^{16}, H^{18},	118.6, 131.0, 147.5	-
18	6.75	ddd, J = 8.1, 7.2, 1.0 Hz, 1H	117.7	H^{17}, H^{19}	121.9, 131.0, 135.4	-
19	7.66	dd, J = 8.1, 1.5 Hz, 1H	131.0	H^{18}	135.4, 147.5	H^2 (very weak int.), H_a^3, H^5
21	-	-	174.8	-	-	-

[a]Assignments are based on extensive 1D and 2D NMR analysis (^{1}H-^{1}H COSY, ^{1}H-^{13}C HMQC, ^{1}H-^{13}C HMBC and ^{1}H-^{1}H NOESY); measured in MeCN-d_3; int. = interaction.

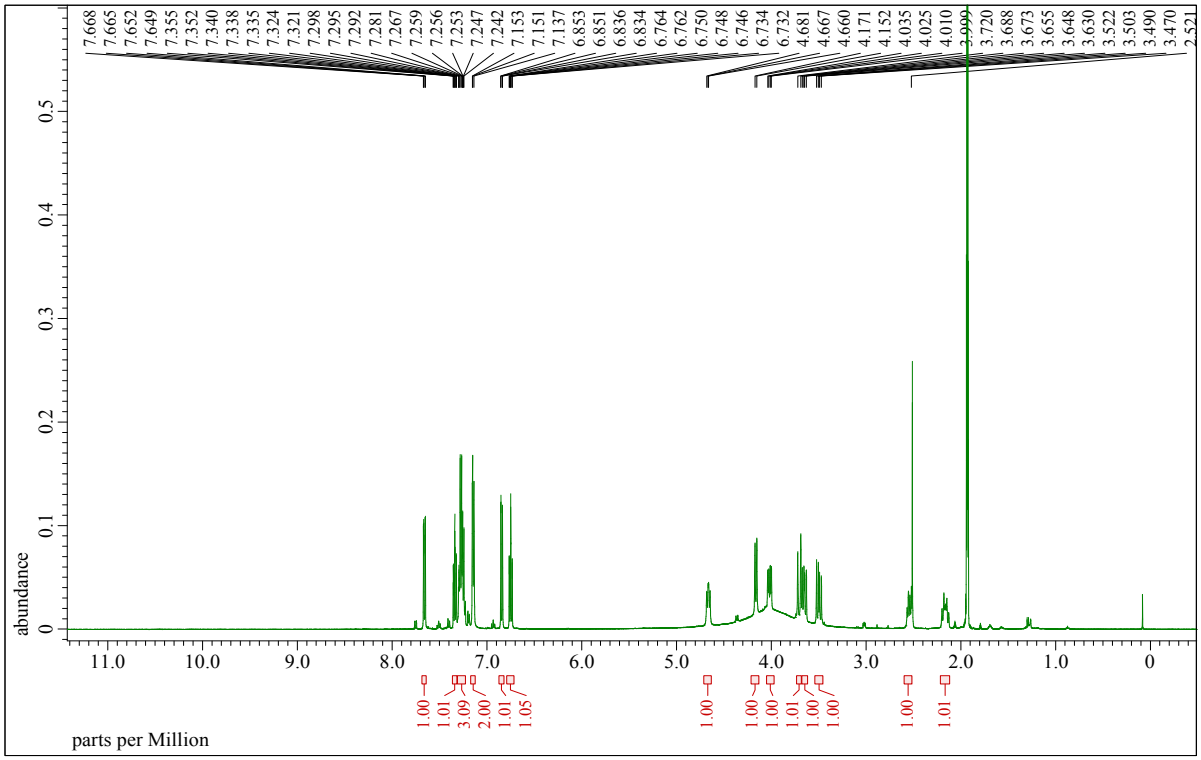


Figure S20. ^{1}H NMR spectrum of **7a** (500 MHz, MeCN-d_3)

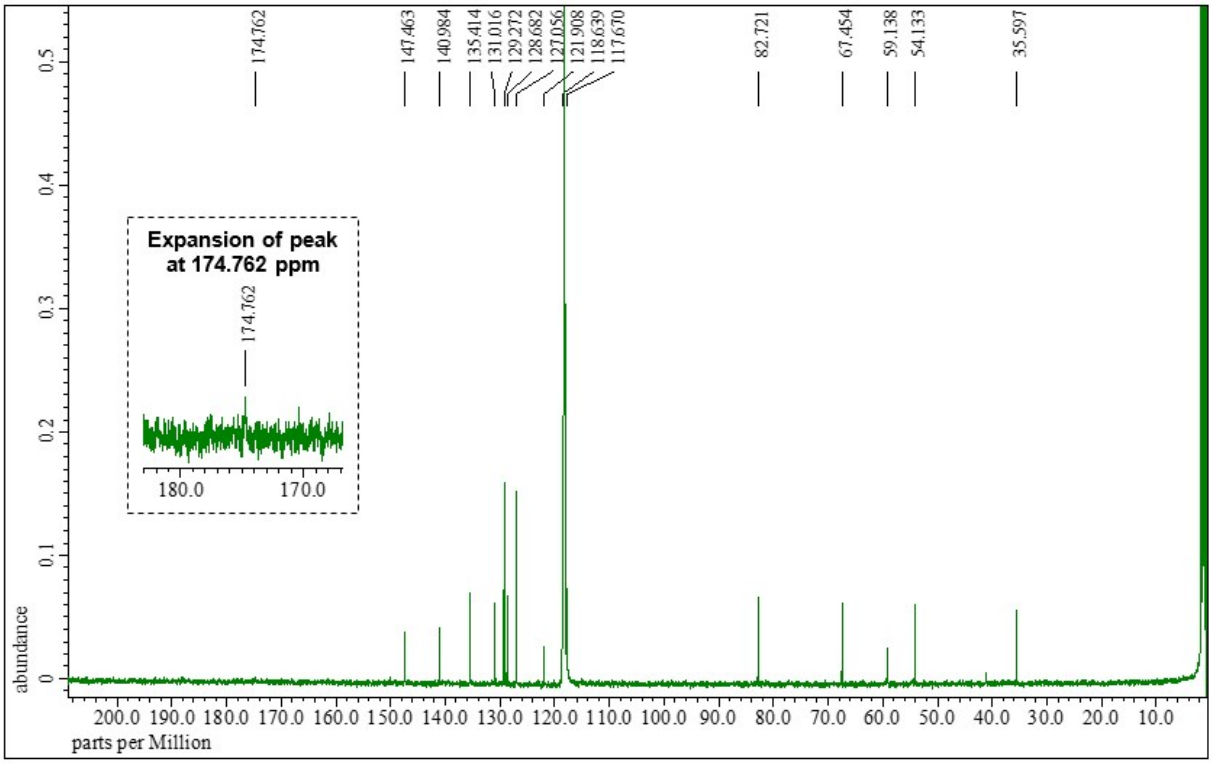


Figure S21. ^{13}C{^{1}H} NMR spectrum of **7a** (126 MHz, MeCN-d_3)

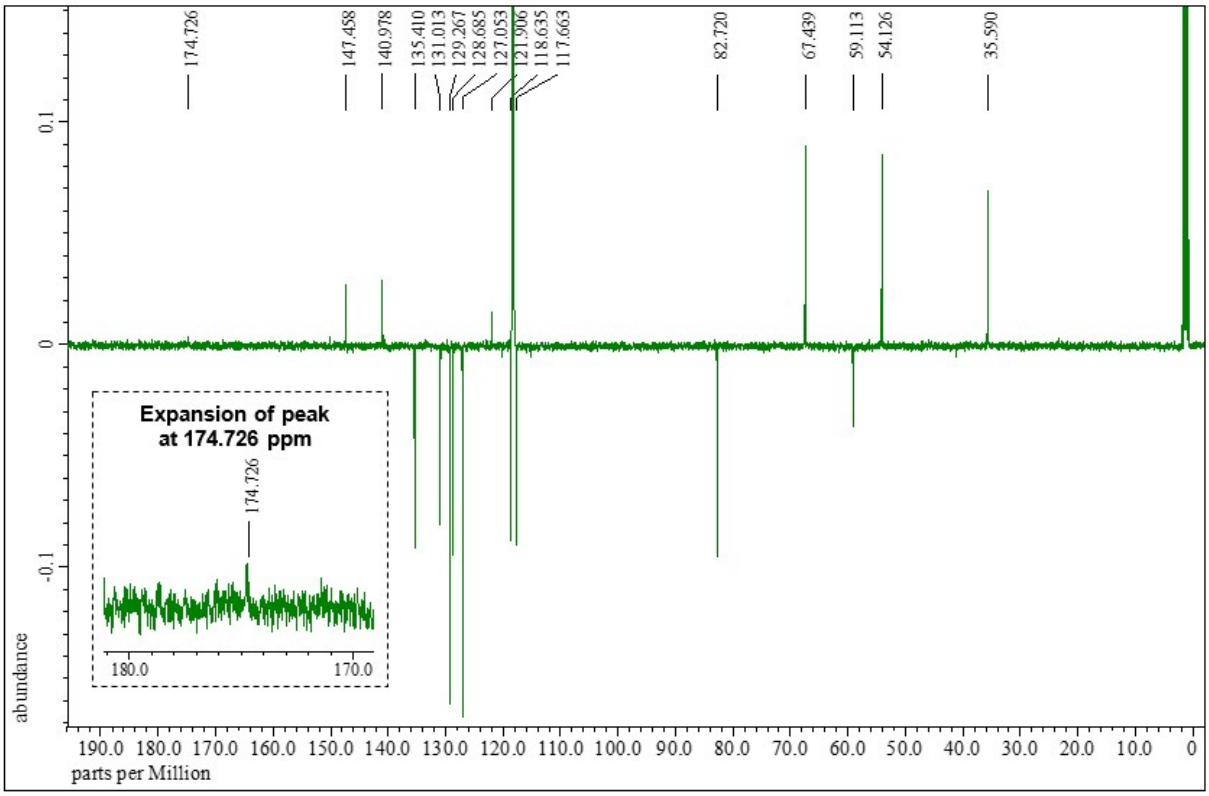


Figure S22. ^{13}C APT NMR spectrum of **7a** (126 MHz, MeCN-d_3)

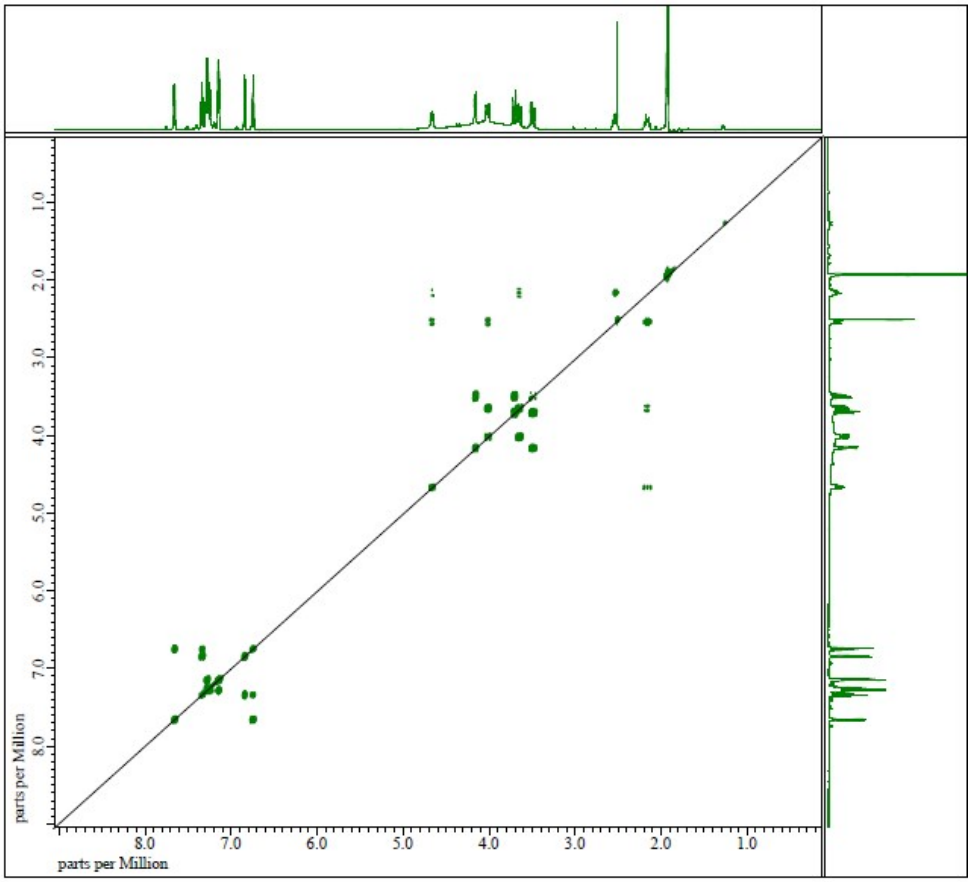


Figure S23. ^{1}H-^{1}H COSY NMR spectrum of **7a** (500 MHz, MeCN-d_3)

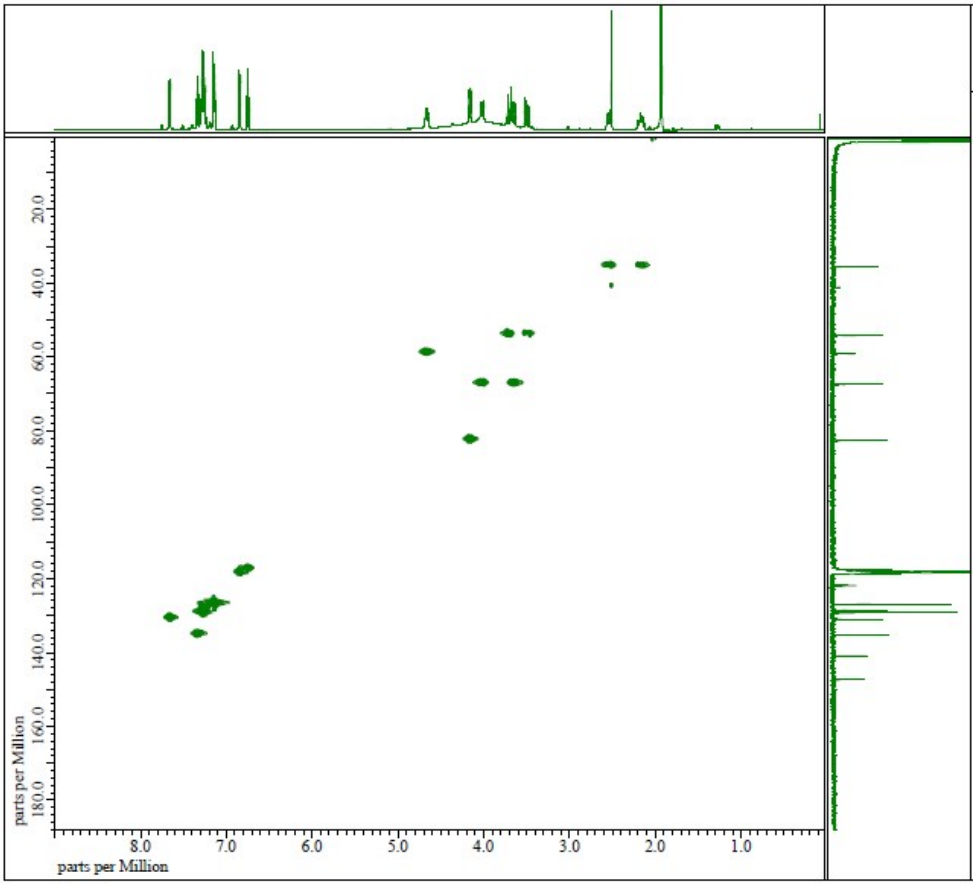


Figure S24. ^{1}H-^{13}C HMQC NMR spectrum of **7a** (MeCN-d_3)

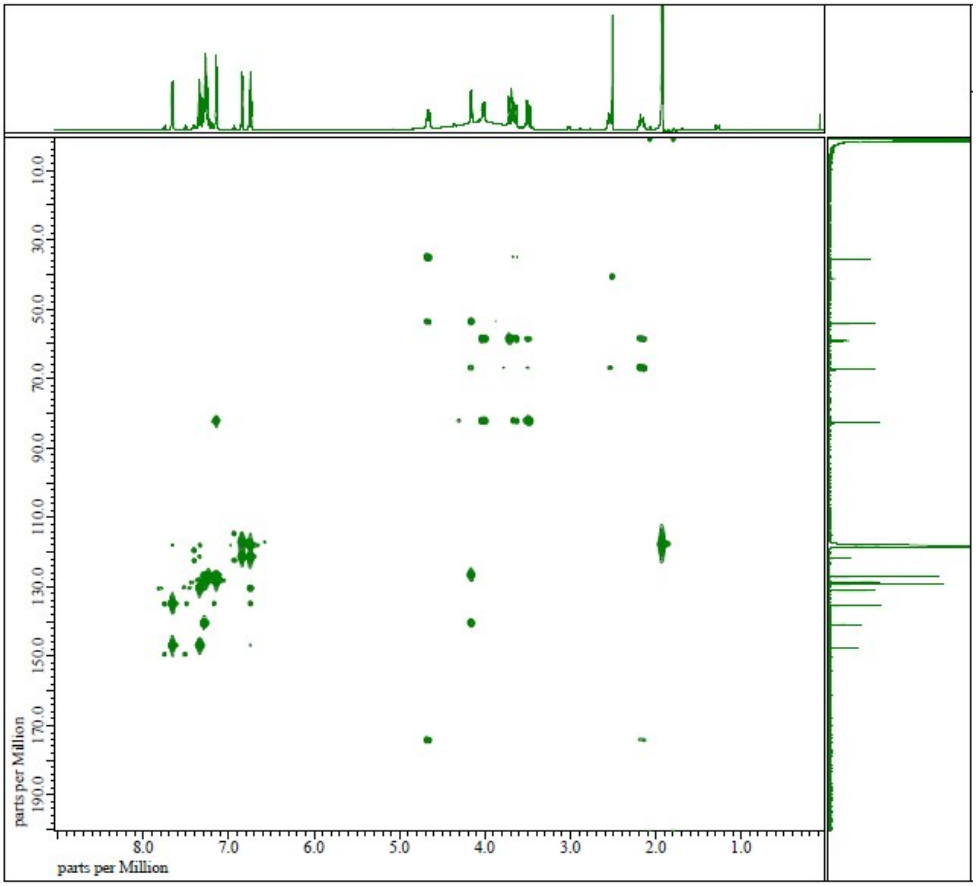


Figure S25. ^{1}H-^{13}C HMBC NMR spectrum of **7a** (MeCN-d_3)

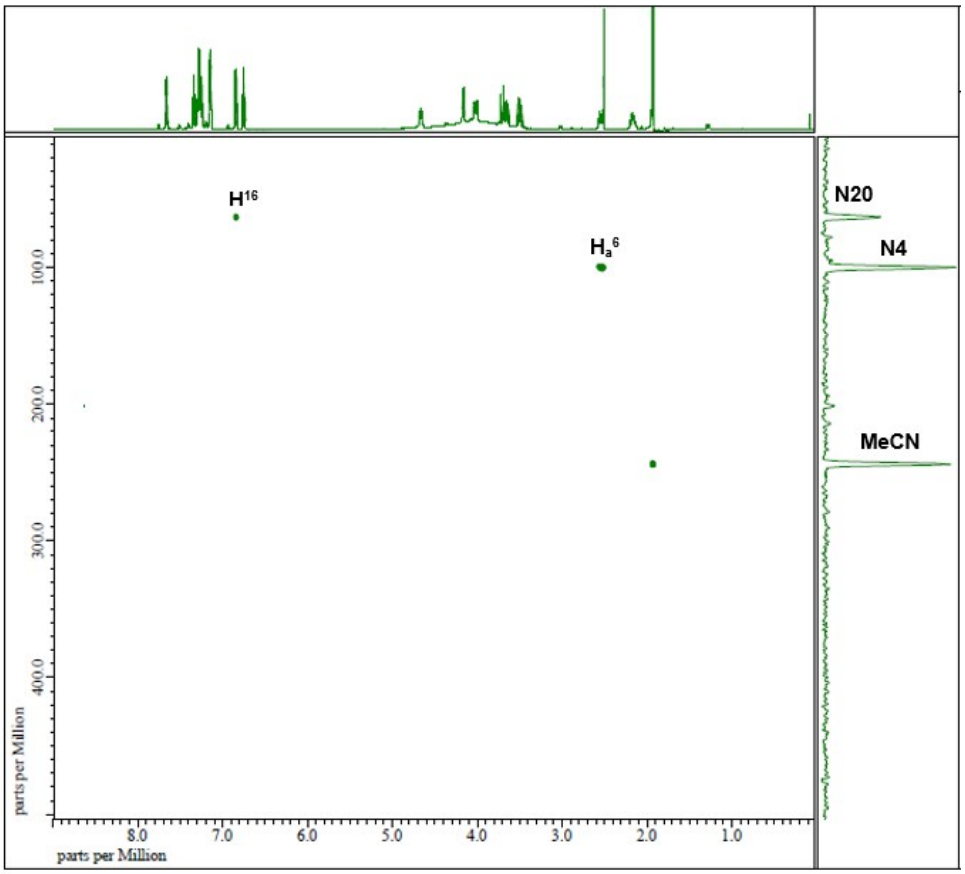


Figure S26. ^{1}H-^{15}N HMBC NMR spectrum of **7a** (MeCN-d_3)

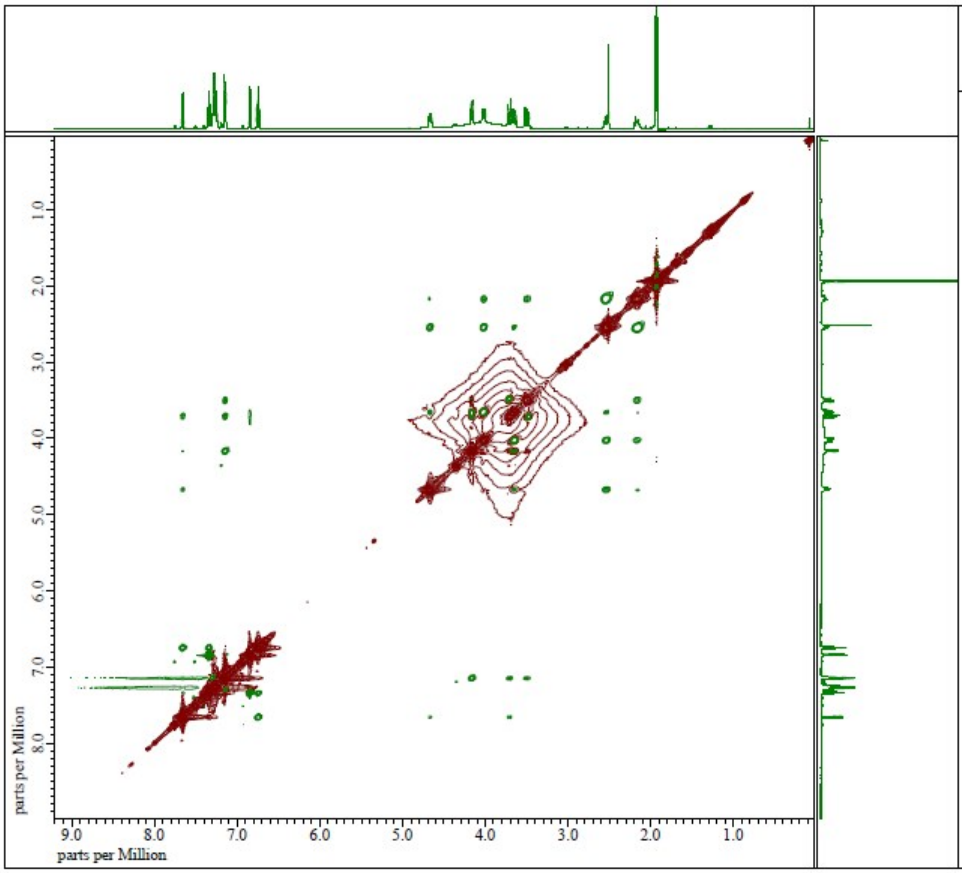


Figure S27. ^{1}H-^{1}H NOESY NMR spectrum of **7a** (MeCN-d_3)

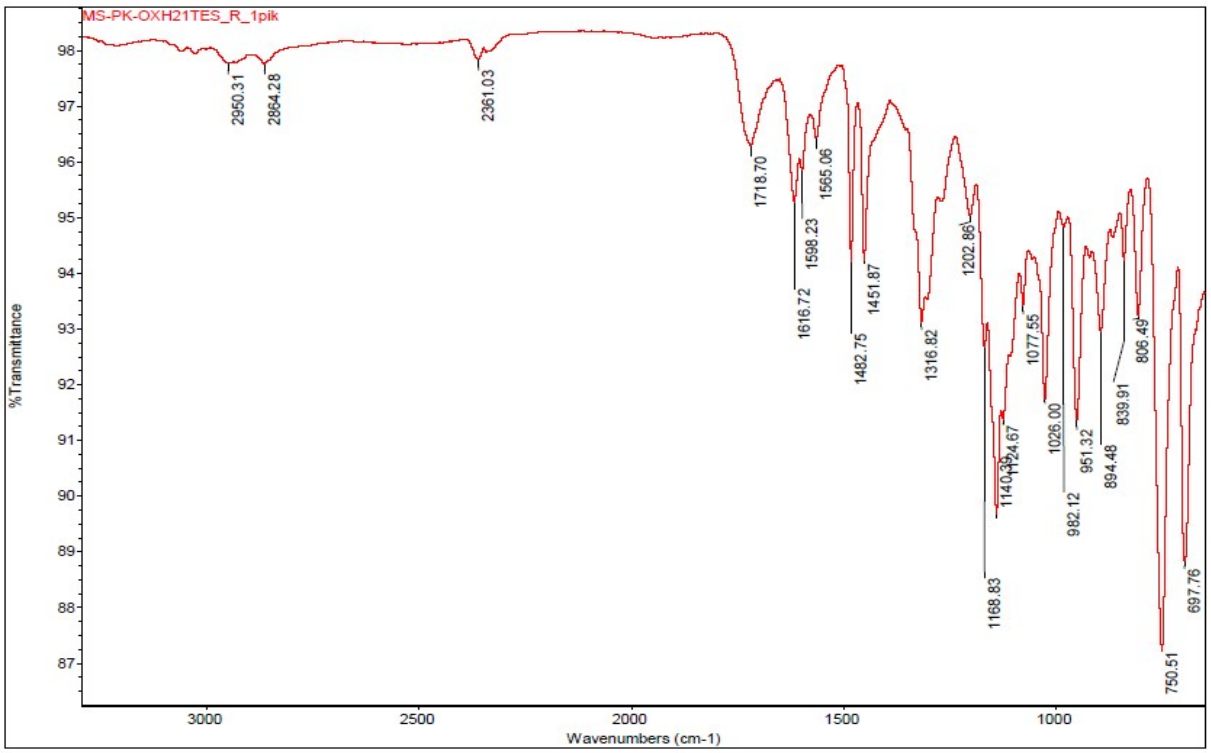


Figure S28. IR spectrum of **7a**

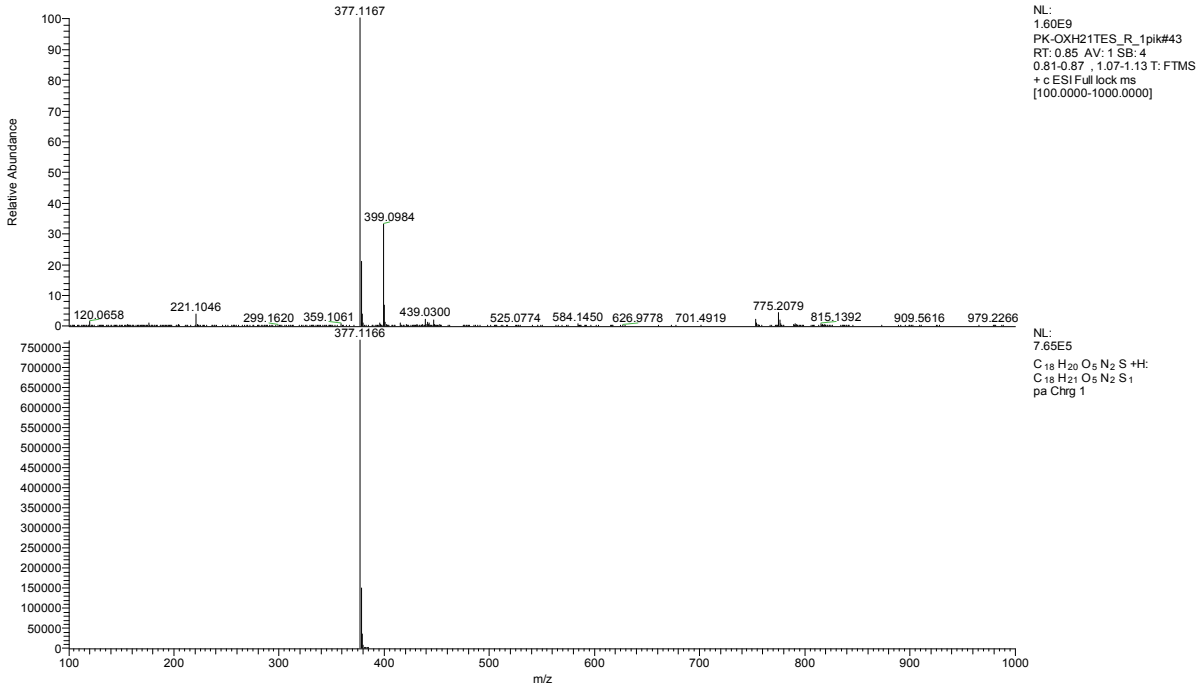
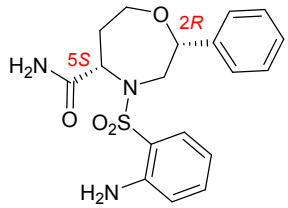


Figure S29. HRMS spectrum of **7a**

(-)-(2*R*,5S)-4-((2-aminophenyl)sulfonyl)-2-phenyl-1,4-oxazepane-5-carboxamide 7b^{2R}



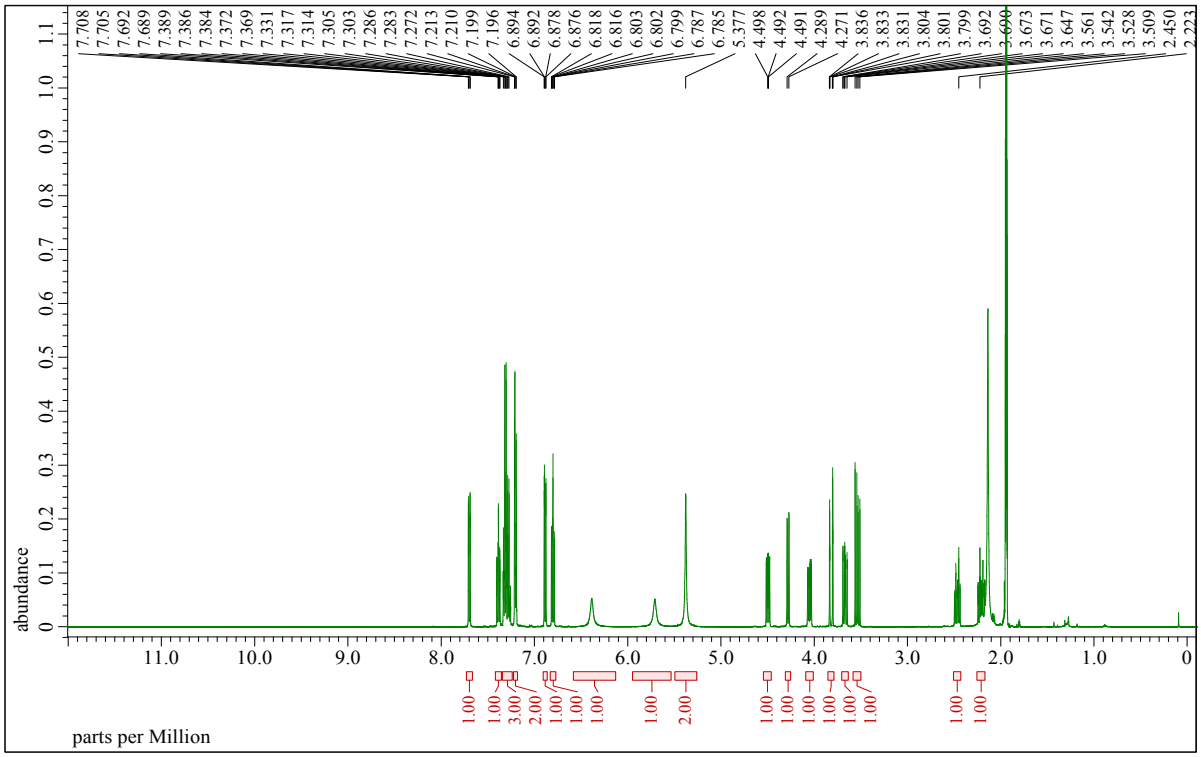


Figure S30. ^{1}H NMR spectrum of **7b^{2R}** (500 MHz, MeCN-d_3)

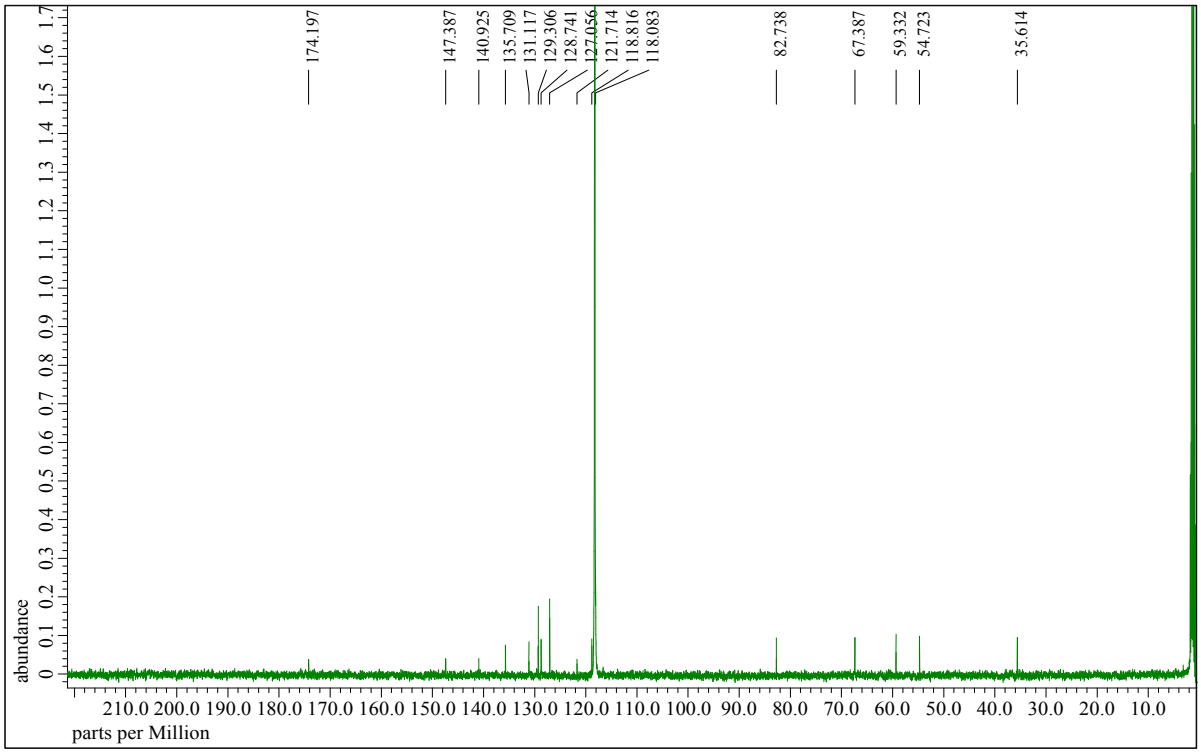


Figure S31. ^{13}C{^{1}H} NMR spectrum of **7b^{2R}** (126 MHz, MeCN-d_3)

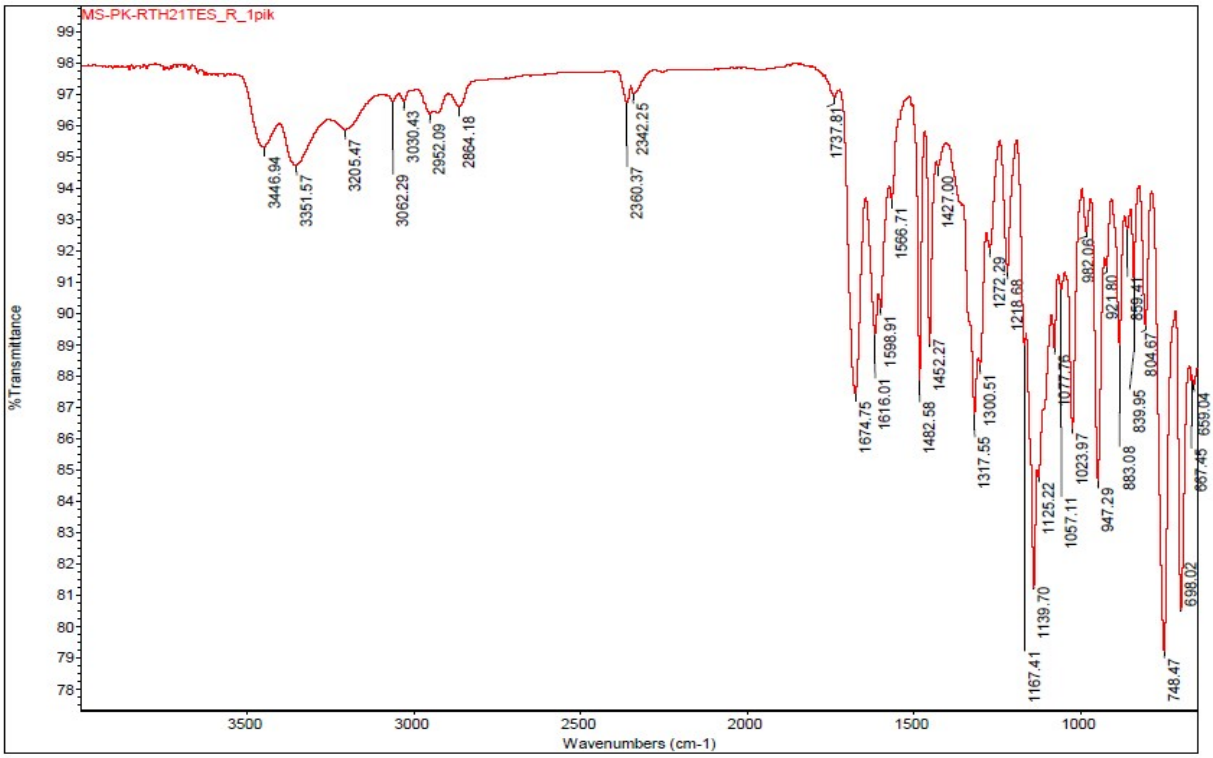


Figure S32. IR spectrum of **7b**^{2R}

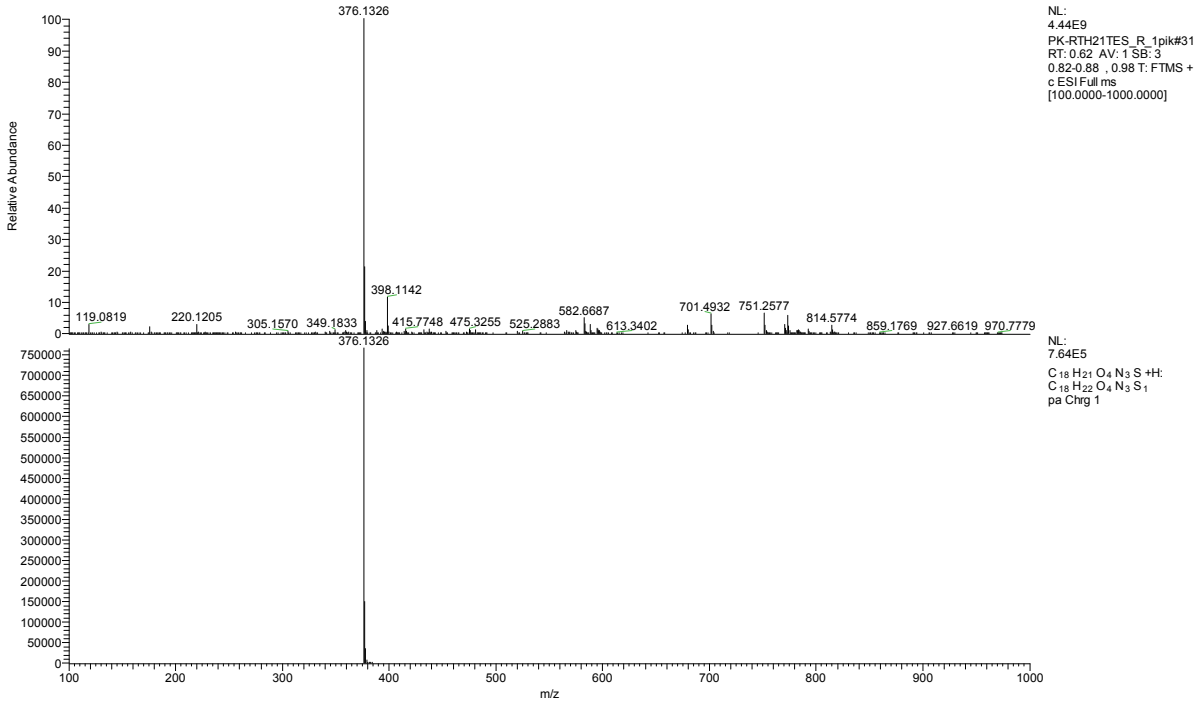


Figure S33. HRMS spectrum of **7b**^{2R}

(+)-(2*S*,5S)-4-((2-aminophenyl)sulfonyl)-2-phenyl-1,4-oxazepane-5-carboxamide 7b^{2S}

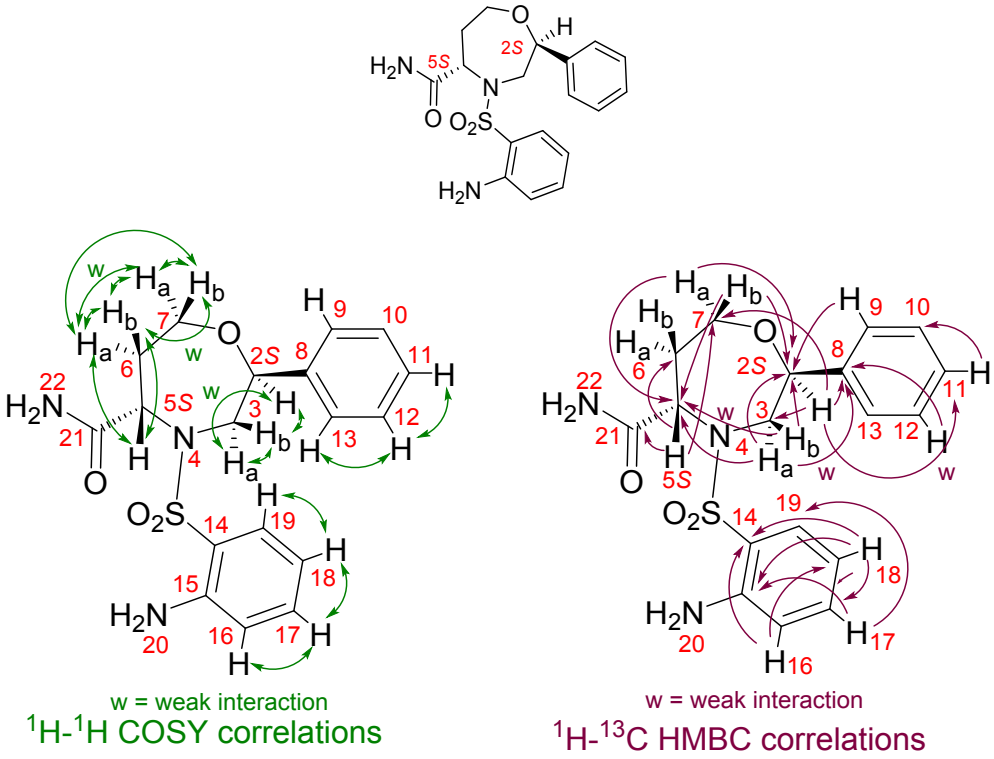


Figure S34. Detailed COSY and ^{1}H-^{13}C HMBC NMR analysis of 1,4-oxazepane **7b^{2S}**

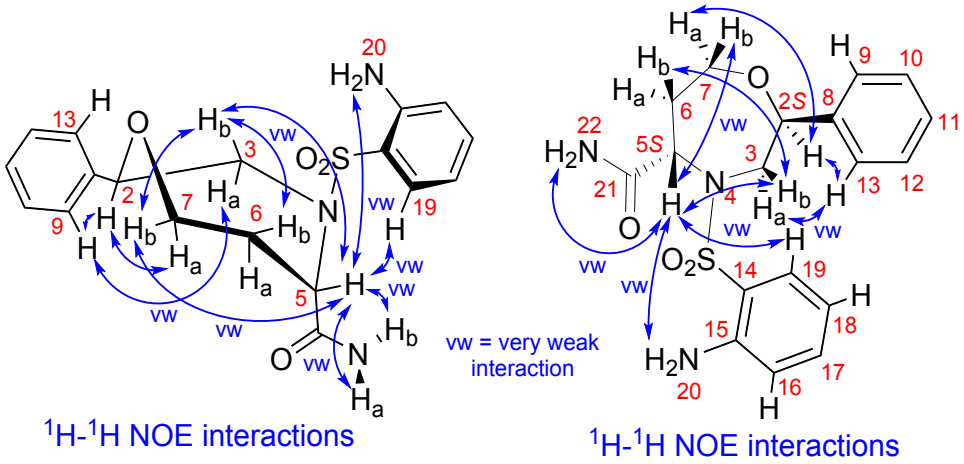


Figure S35. Detailed ^{1}H-^{1}H NOE NMR analysis of 1,4-oxazepane **7b^{2S}**

Table S3. ^{1}H NMR (500 MHz) and ^{13}C{^{1}H} NMR (126 MHz) spectral data, including detailed COSY, ^{1}H-^{13}C HMBC and NOE correlations for 1,4-oxazepane **7b**^{2S}[a]

position	^{1}H NMR δ_H [ppm][b]	splitting pattern, J [Hz], integration	^{13}C{^{1}H} NMR δ_C [ppm]	COSY correlations	^{1}H-^{13}C HMBC correlations	NOE correlations
2	4.64	dd, J = 8.7, 1.6 Hz, 1H	81.4	H_a^3, H_b^3	56.8, 126.6, 128.6 (weak int.), 141.9	H_a^7, $H^{9,13}$
3	H_a : 3.63	dd, J = 14.2, 1.6 Hz, 1H,	56.8	H^2, H_b^3	59.4, 81.4	$H^{9,13}$ (very weak int.)
	H_b: 3.43	dd, J = 14.2, 8.7 Hz, 1H		H^2, H_a^3	59.4 (weak int.), 81.4, 141.9 (weak int.)	H^5, H_b^6
5	4.59	dd, J = 4.5, 4.5 Hz, 1H	59.4	H_a^6, H_b^6	33.0 (weak int.), 66.9, 174.3	H_b^3, H_b^7 (very weak int.), H^{19} (very weak int.), H^{20}, H^{22} (very weak int.)
6	H_a : 2.30	dddd, J = 15.8, 4.9, 4.5, 1.6 Hz, 1H	33.0	H^5, H_b^6, H_a^7 (weak int.), H_b^7	-	-
	H_b: 2.10	dddd, J = 15.8, 11.0, 4.5, 3.0 Hz, 1H		H^5, H_a^6, H_a^7, H_b^7 (weak int.)	-	H_b^3
7	H_a : 3.78	ddd, J = 12.8, 11.0, 1.6 Hz, 1H	67.0	H_a^6 (weak int.), H_b^6, H_b^7	59.4, 81.4	H^2
	H_b: 3.94	ddd, J = 12.8, 4.5, 3.0 Hz, 1H		H_a^6, H_b^6 (weak int.), H_a^7	59.4, 81.4	H^5 (very weak int.)
8	-	-	141.9	-	-	-
9,13	7.18-7.19	m, 2H	126.6	$H^{10,12}$	81.4, 128.6	H^2, H_a^3 (weak int.)
10,12	7.27-7.30	m, 2H	129.3	$H^{9,13}$, H^{11}	141.9	-
11	7.24-7.27	m, 1H	128.6	$H^{10,12}$	126.6, 129.3	-
14	-	-	119.1	-	-	-
15	-	-	148.0	-	-	-
16	6.85	dd, J = 8.5, 1.1 Hz, 1H	118.7	H^{17}	117.5, 119.1	-
17	7.35	ddd, J = 8.5, 7.2, 1.6 Hz, 1H	135.7	H^{16}, H^{18},	131.3, 148.0	-
18	6.70	ddd, J = 8.2, 7.2, 1.1 Hz, 1H	117.5	H^{17}, H^{19}	118.7, 119.1, 148.0	-
19	7.58	dd, J = 8.1, 1.6 Hz, 1H	131.3	H^{18}	135.7	H^5 (very weak int.)
20	5.62	br. s, 2H	-	-	-	H^5
21	-	-	174.4	-	-	-
22	H_a : 5.99	br. s, 1H	-	-	-	H^5 (very weak int.)
	H_b: 6.75	br.s, 1H				H^5 (very weak int.)

[a]Assignments are based on extensive 1D and 2D NMR analysis (^{1}H-^{1}H COSY, ^{1}H-^{13}C HMQC, ^{1}H-^{13}C HMBC and ^{1}H-^{1}H NOESY); measured in MeCN-d_3; int. = interaction.

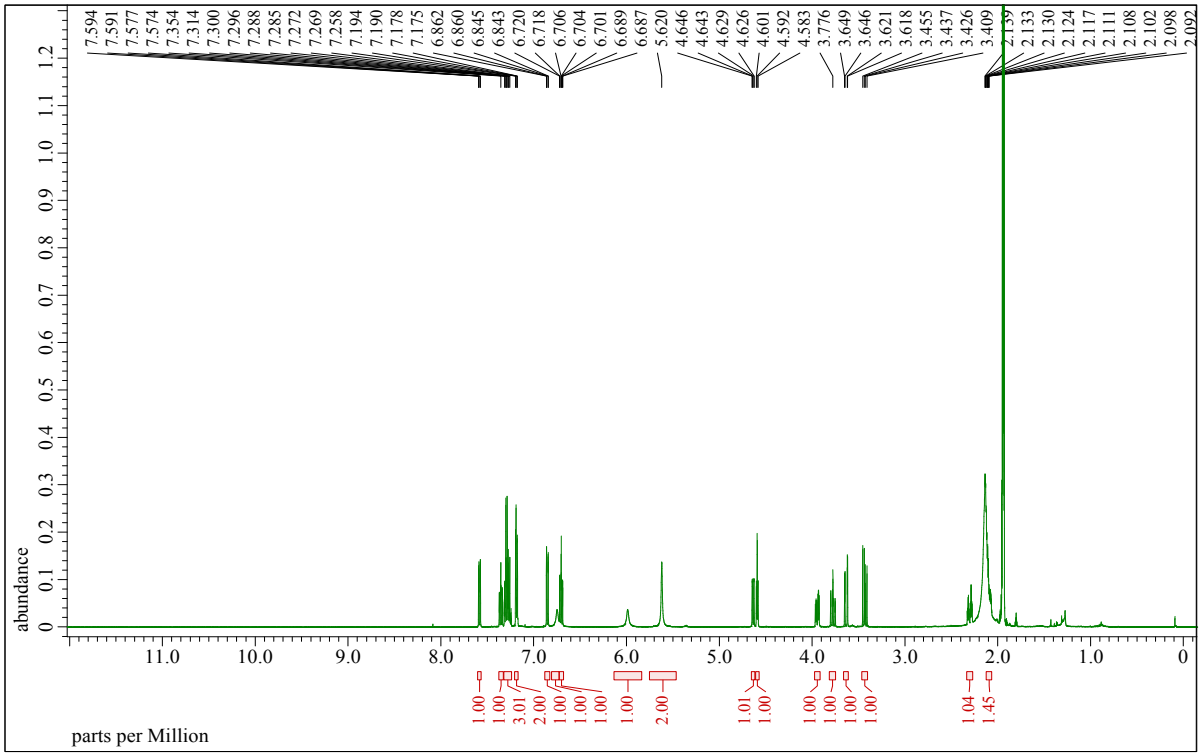


Figure S36. ^{1}H NMR spectrum of **7b^{2S}** (500 MHz, MeCN-d_3)

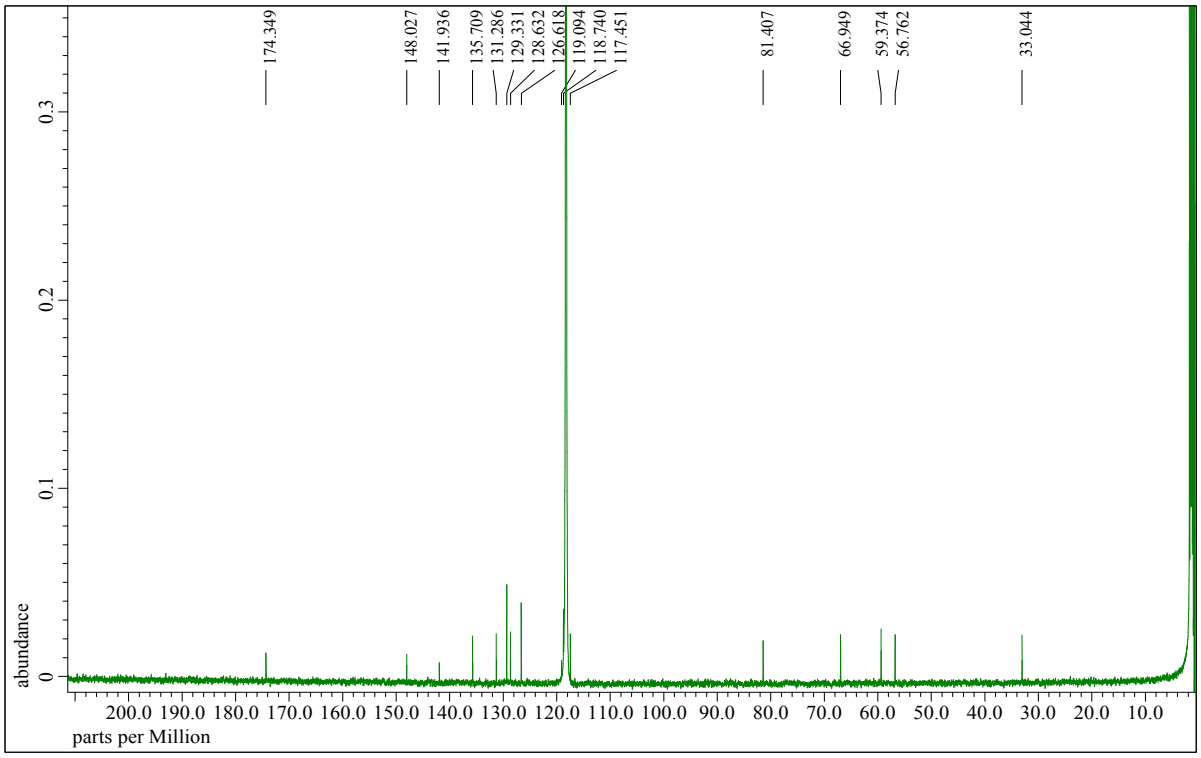


Figure S37. ^{13}C{^{1}H} NMR spectrum of **7b^{2S}** (126 MHz, MeCN-d_3)

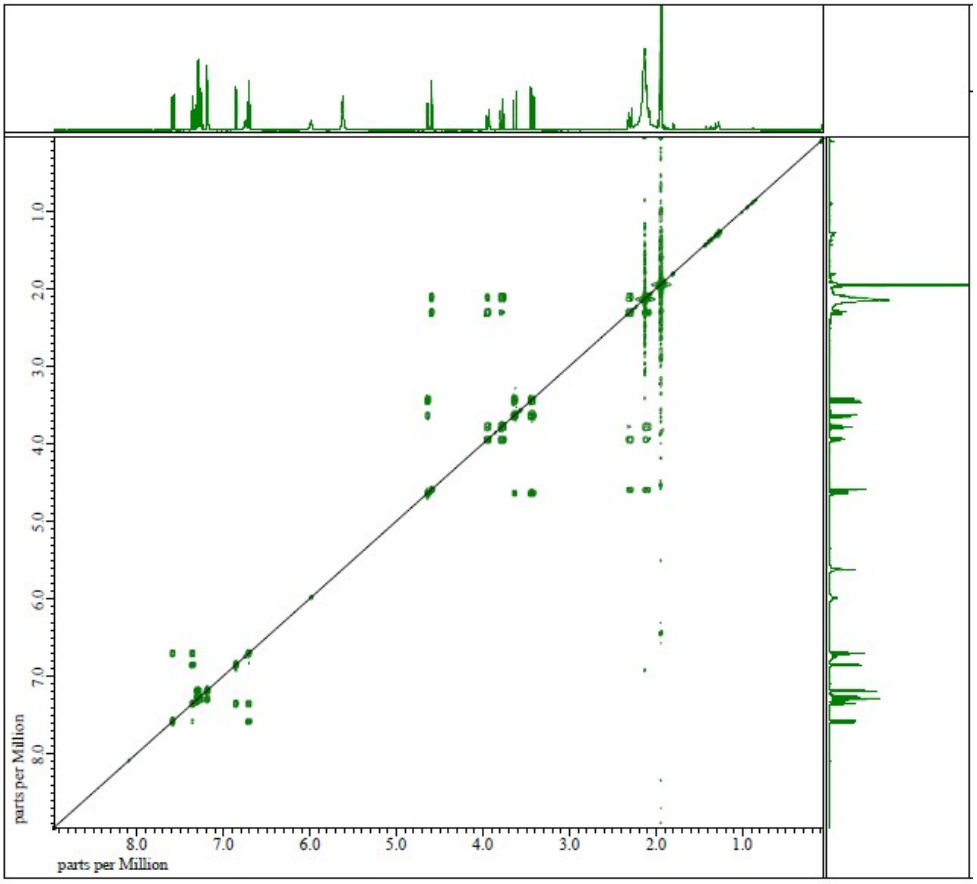


Figure S38. ^{1}H-^{1}H COSY NMR spectrum of **7b**^{2S} (500 MHz, MeCN-d_3)

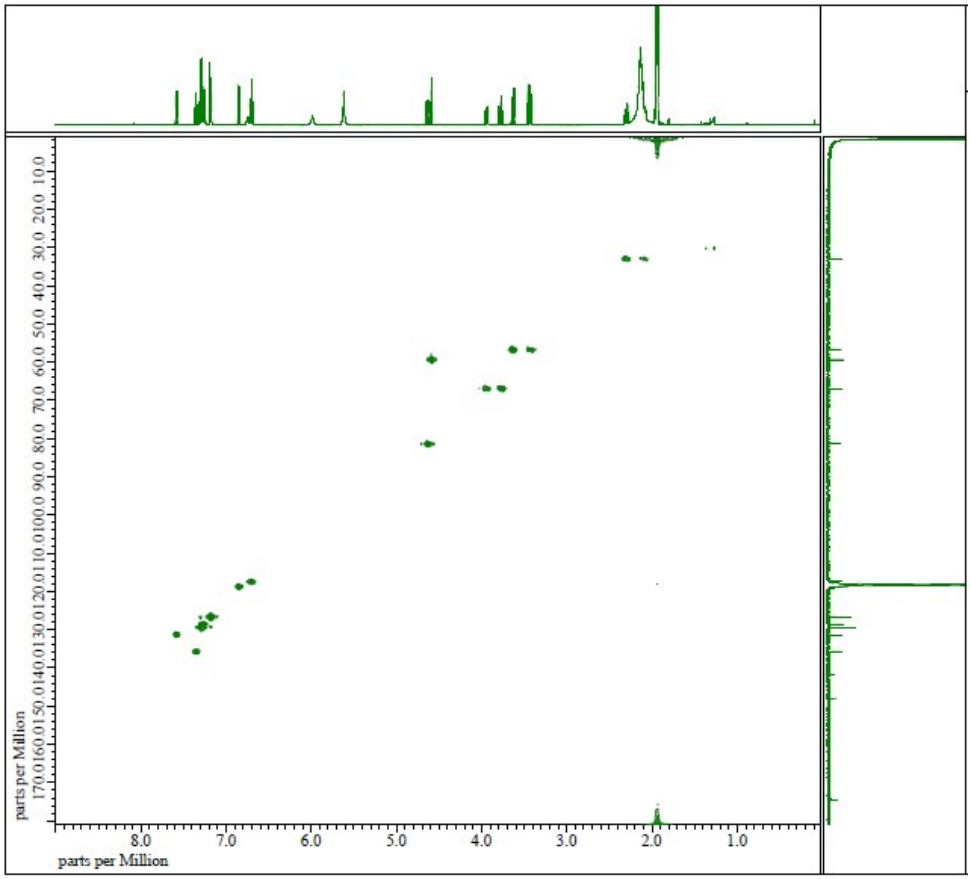


Figure S39. ^{1}H-^{13}C HMQC NMR spectrum of **7b**^{2S} (MeCN-d_3)

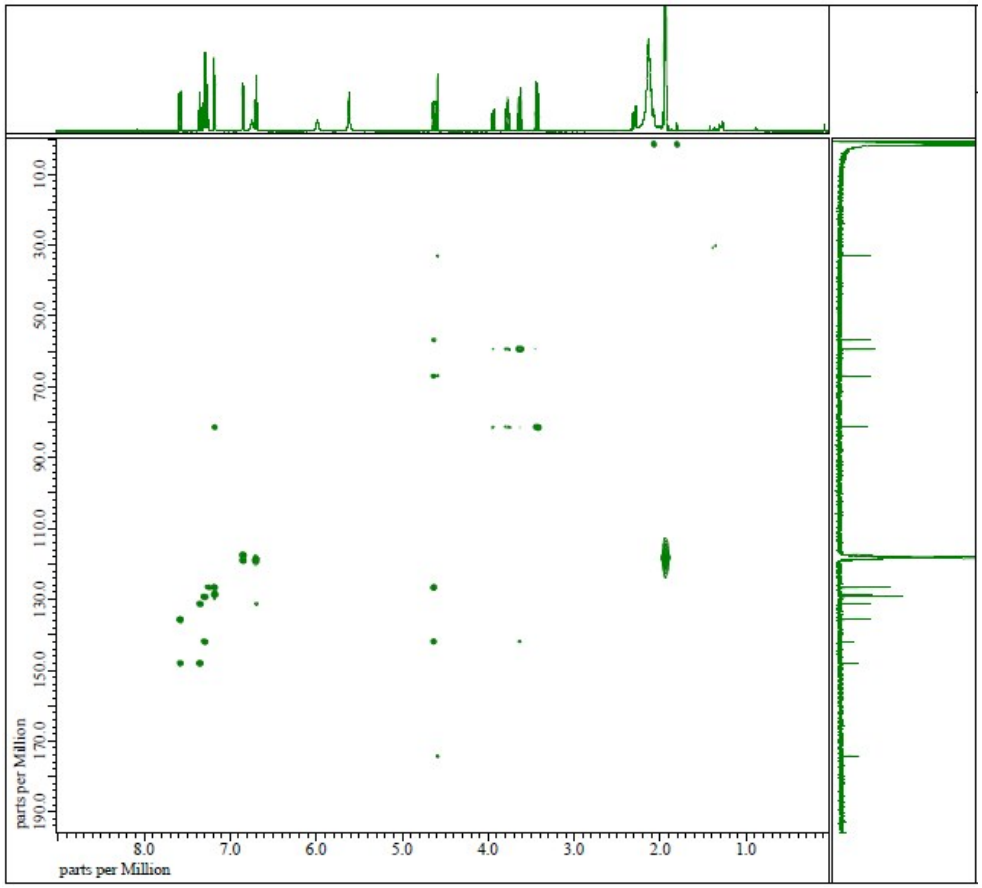


Figure S40. ^{1}H-^{13}C HMBC NMR spectrum of **7b^{2S}** (MeCN-d_3)

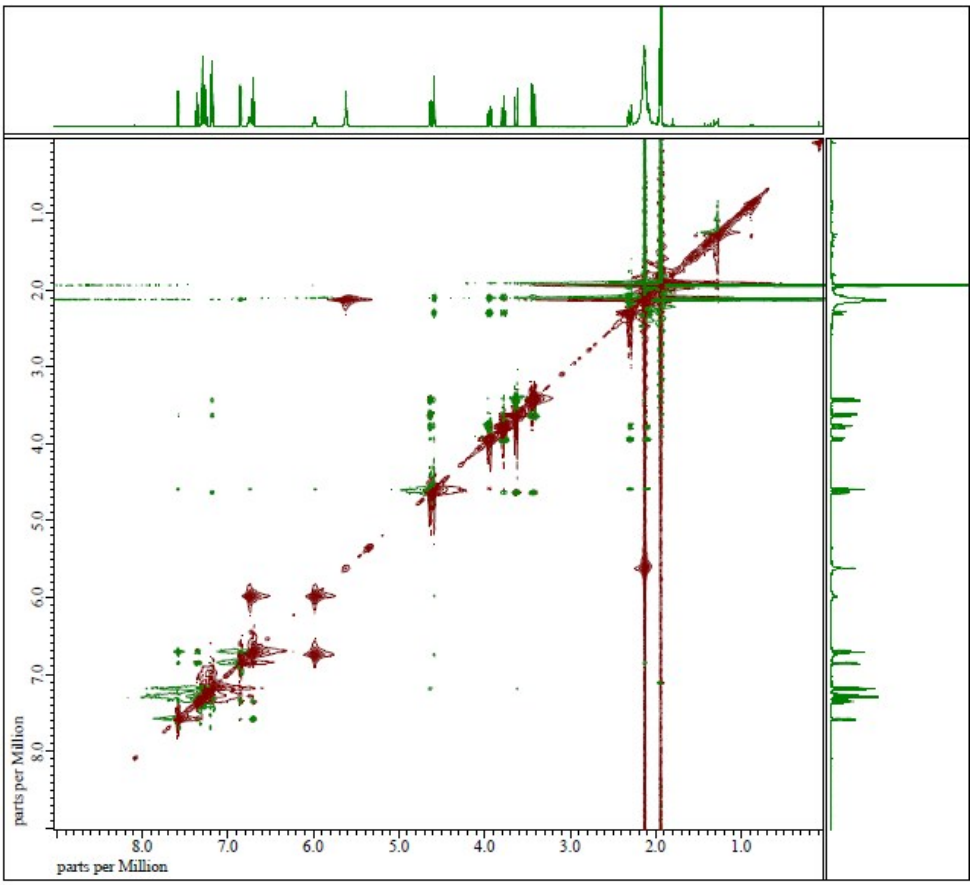


Figure S41. ^{1}H-^{1}H NOESY NMR spectrum of **7b^{2S}** (MeCN-d_3)

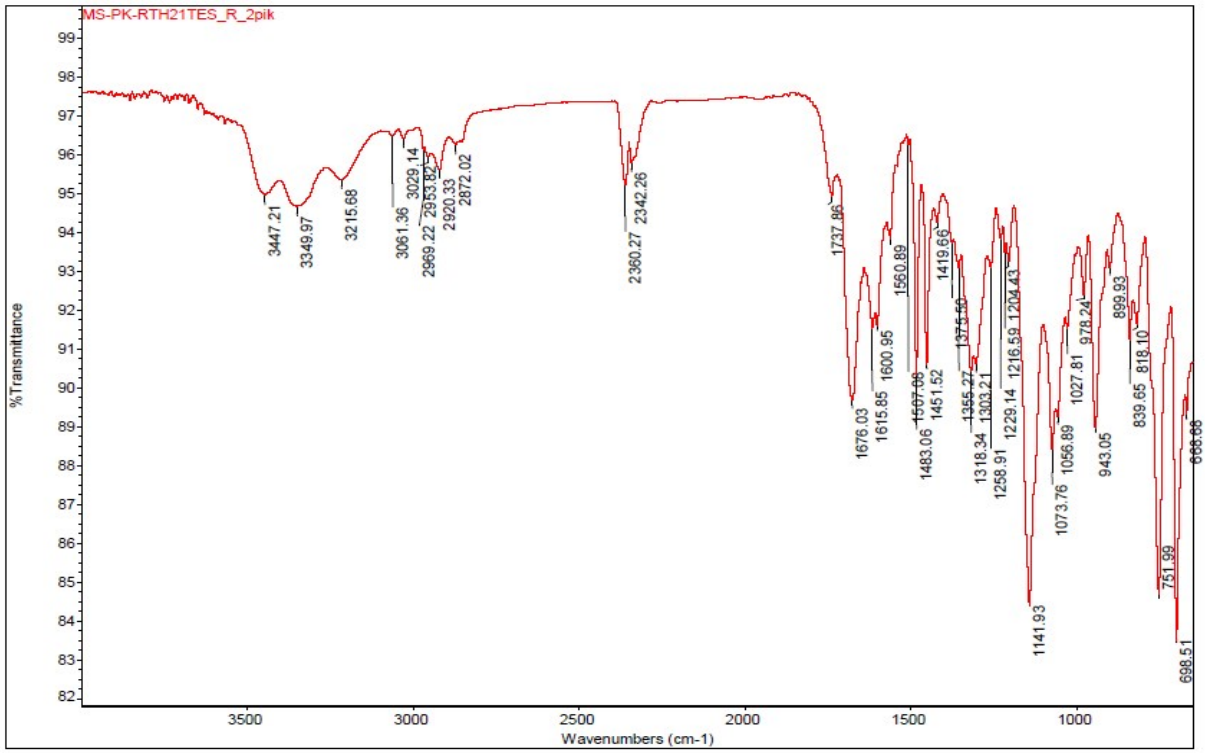


Figure S42. IR spectrum of **7b**^{2S}

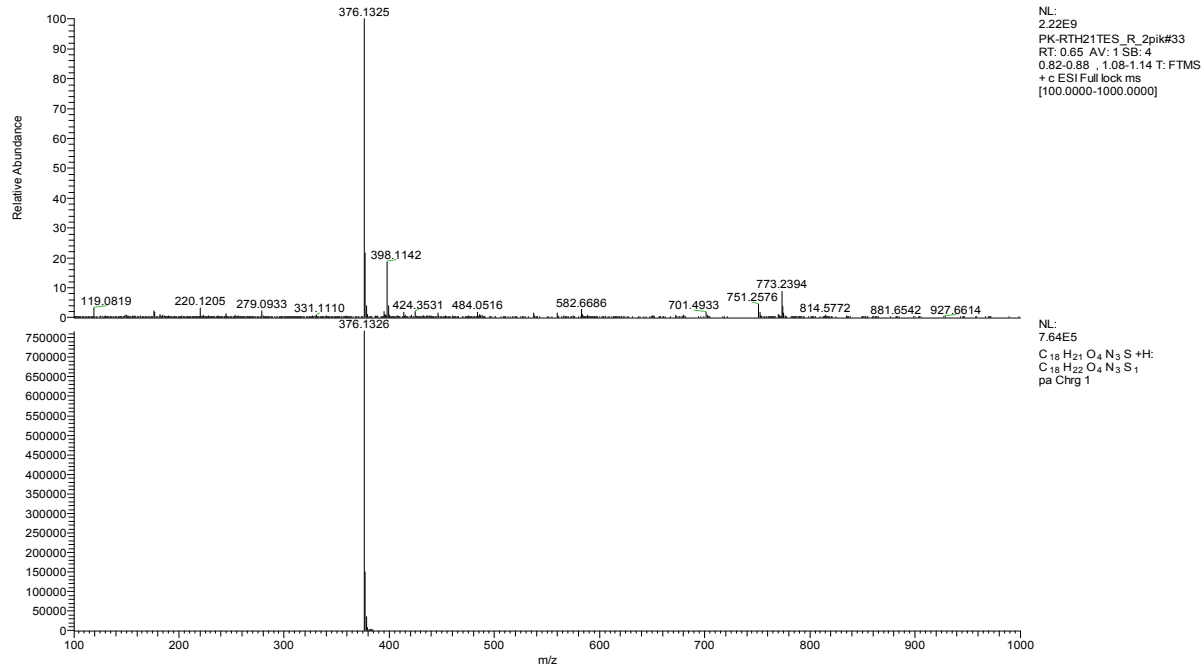
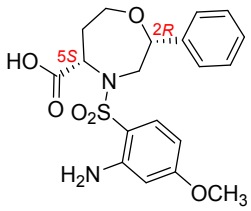


Figure S43. HRMS spectrum of **7b**^{2S}

(-)-(2*R*,5S)-4-((2-amino-4-methoxyphenyl)sulfonyl)-2-phenyl-1,4-oxazepane-5-carboxylic acid 7e



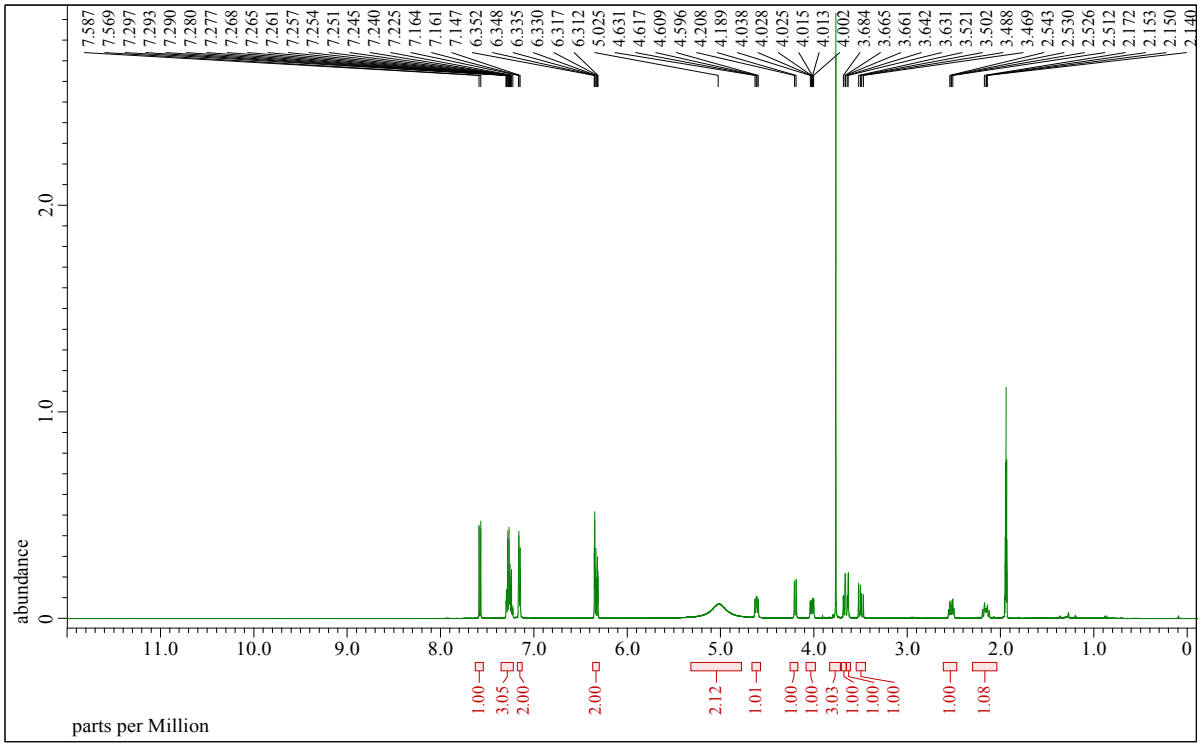


Figure S44. ^{1}H NMR spectrum of **7e** (500 MHz, MeCN-d_3)

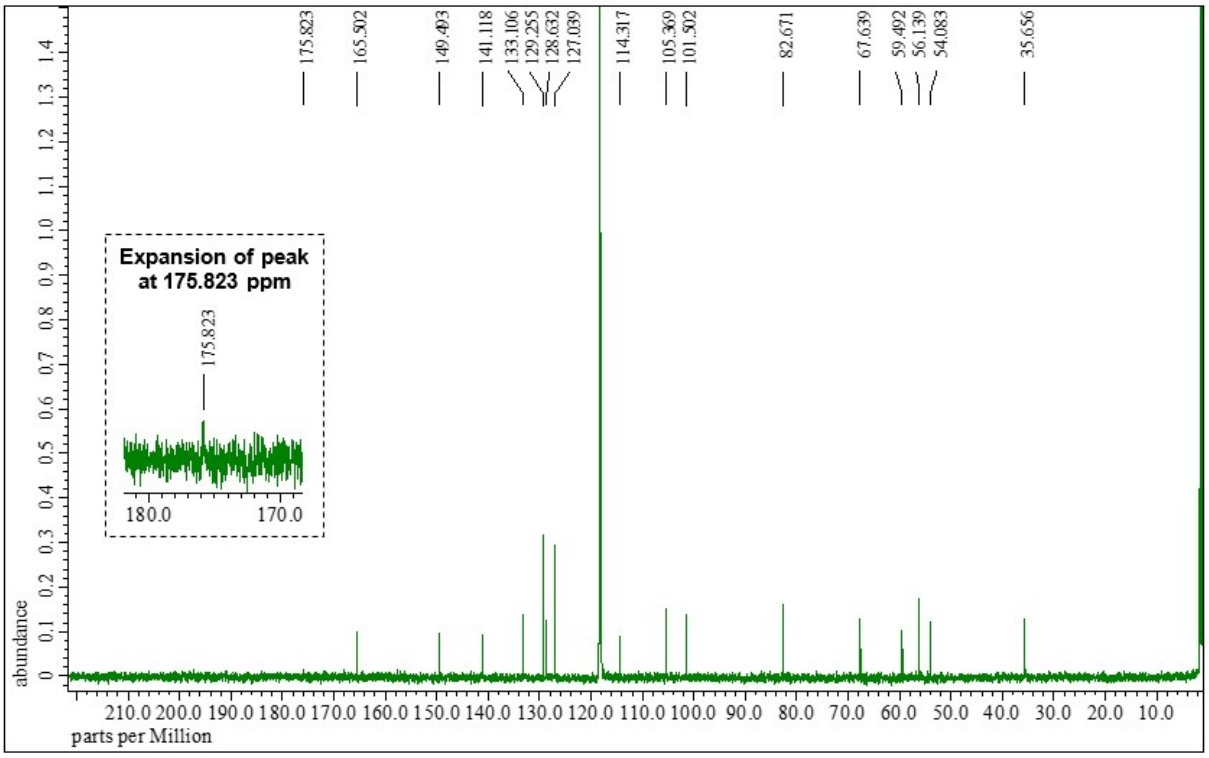


Figure S45. ^{13}C{^{1}H} NMR spectrum of **7e** (126 MHz, MeCN-d_3)

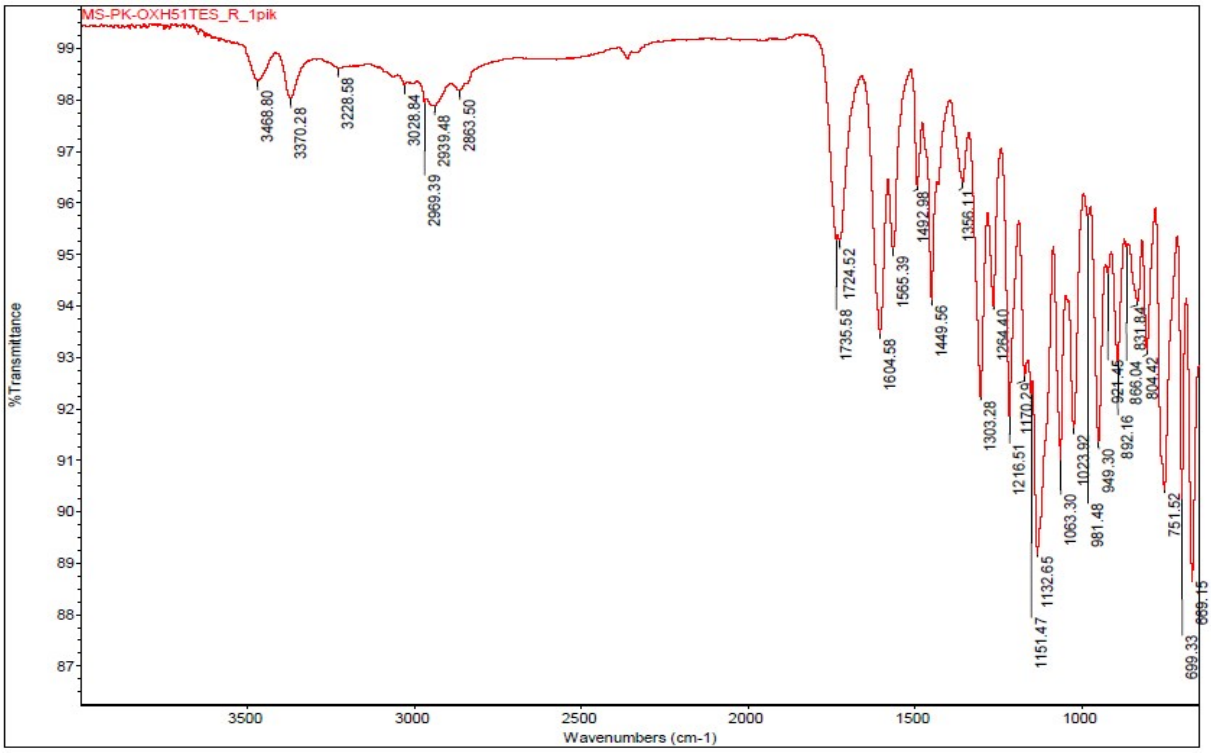


Figure S46. IR spectrum of **7e**

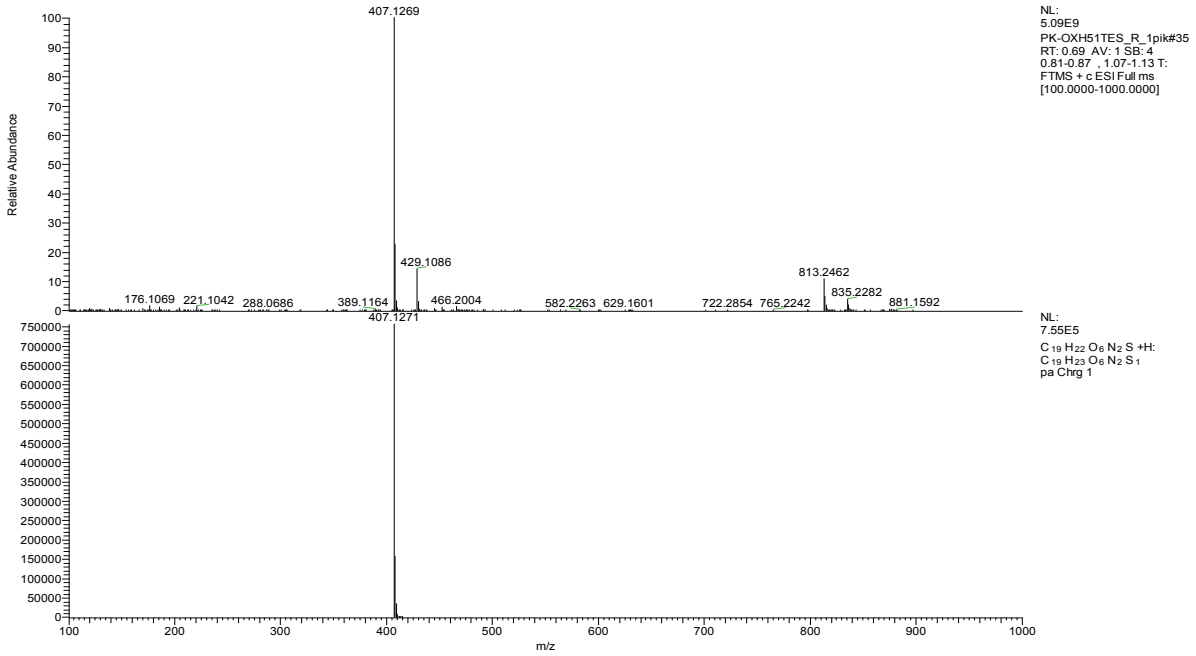
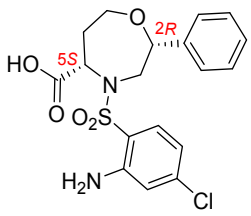


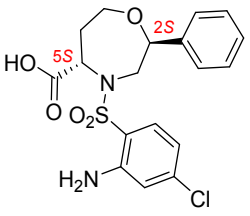
Figure S47. HRMS spectrum of **7e**

(-)-(2*RS*,5S)-4-((2-amino-4-chlorophenyl)sulfonyl)-2-phenyl-1,4-oxazepane-5-carboxylic acid 7f[2RS]



(A) 5*S*, *2R* isomer

A:B = 78:22



(B) 5*S*, *2S* isomer

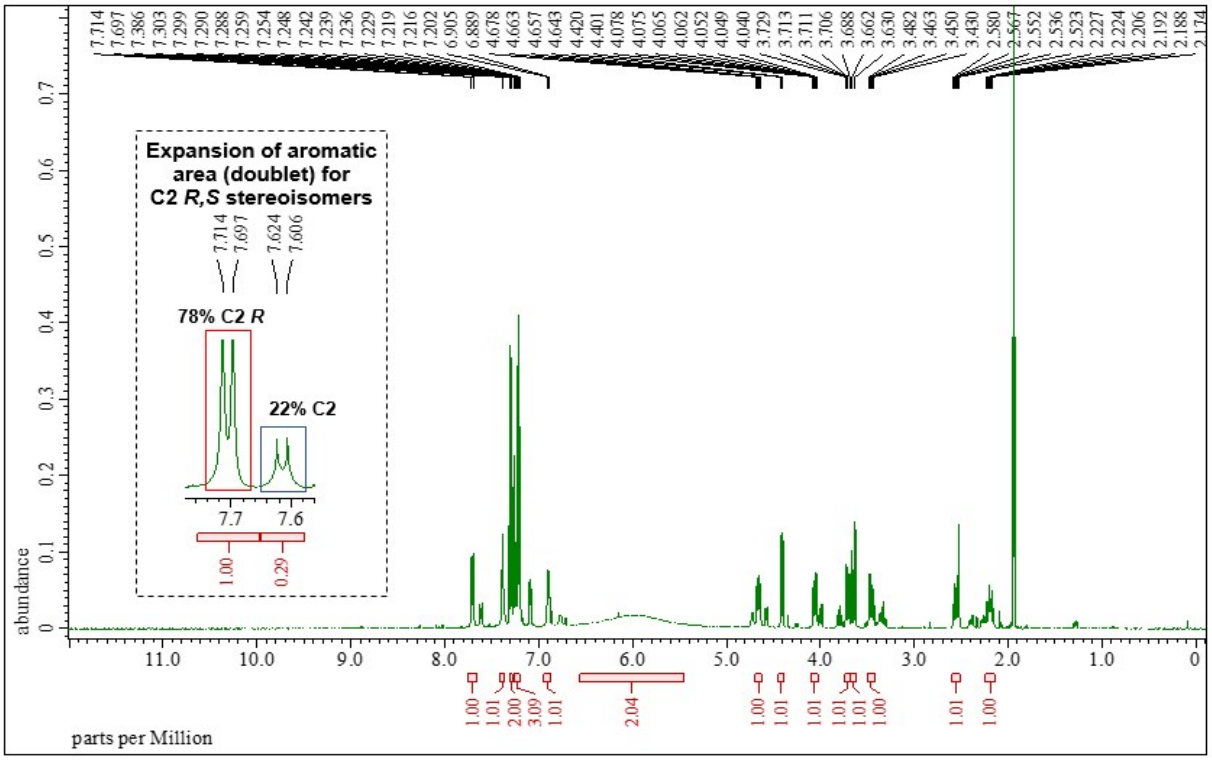


Figure S48. ^{1}H NMR spectrum of **7f^{2RS}** (500 MHz, MeCN-d_3). Note: Only the signals belonging to the major diastereomer were analyzed.

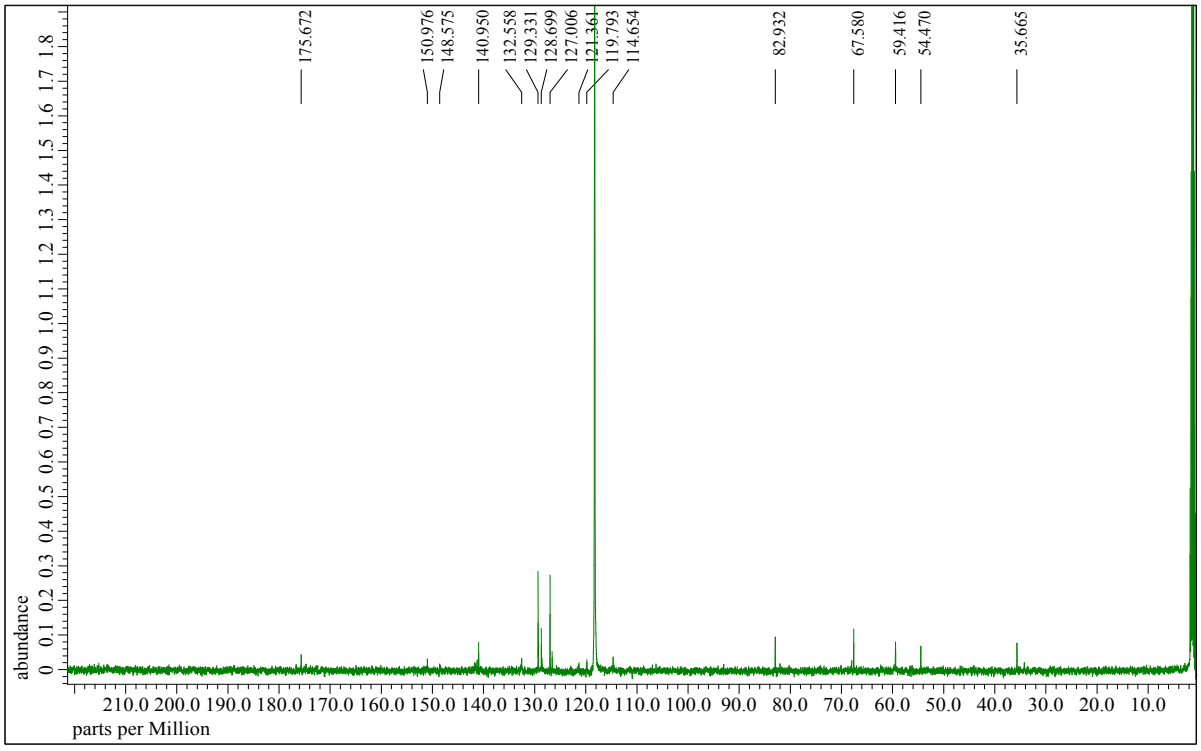


Figure S49. ^{13}C{^{1}H} NMR spectrum of **7f^{2RS}** (126 MHz, MeCN-d_3). Note: Only the signals belonging to the major diastereomer were analyzed.

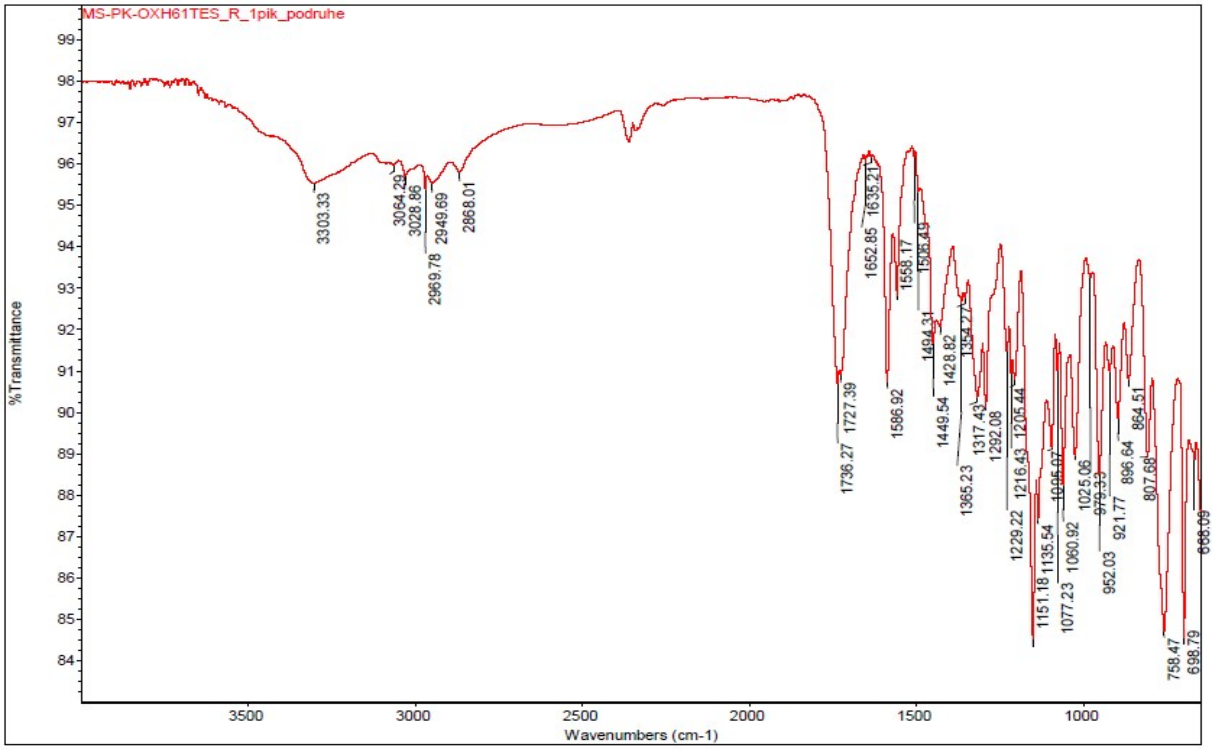


Figure S50. IR spectrum of **7f**^{2RS}

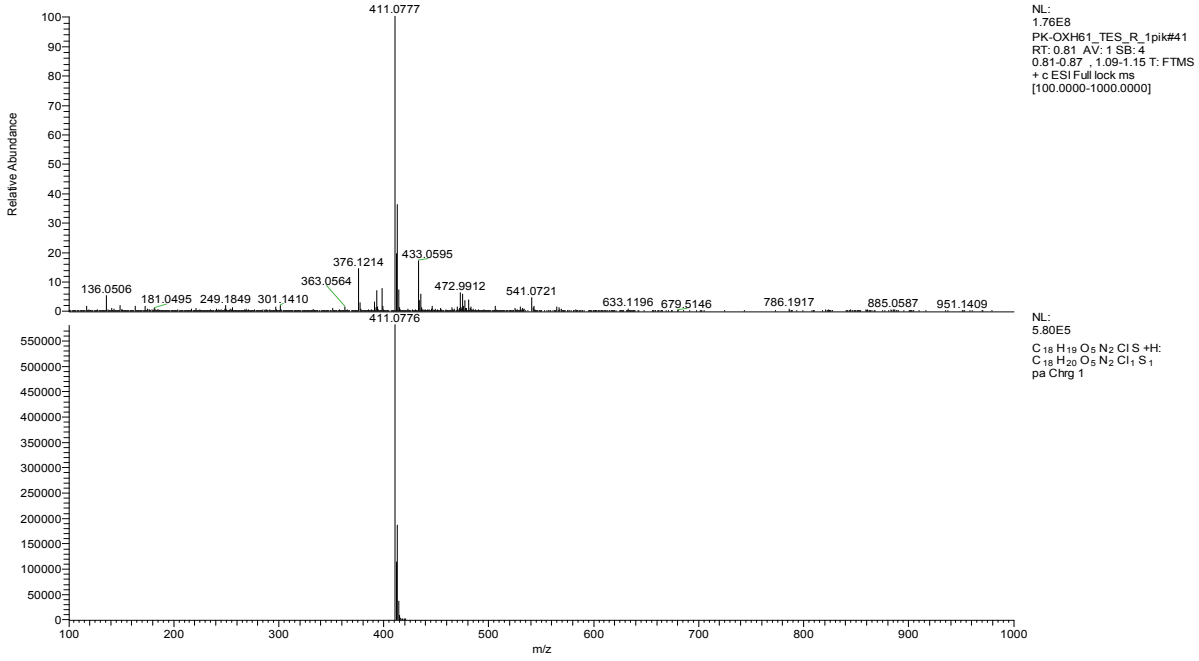
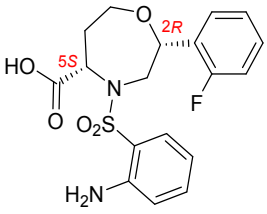


Figure S51. HRMS spectrum of **7f**^{2RS}

(-)-(2*R*,5S)-4-((2-aminophenyl)sulfonyl)-2-(2-fluorophenyl)-1,4-oxazepane-5-carboxylic acid 7i^{2R}



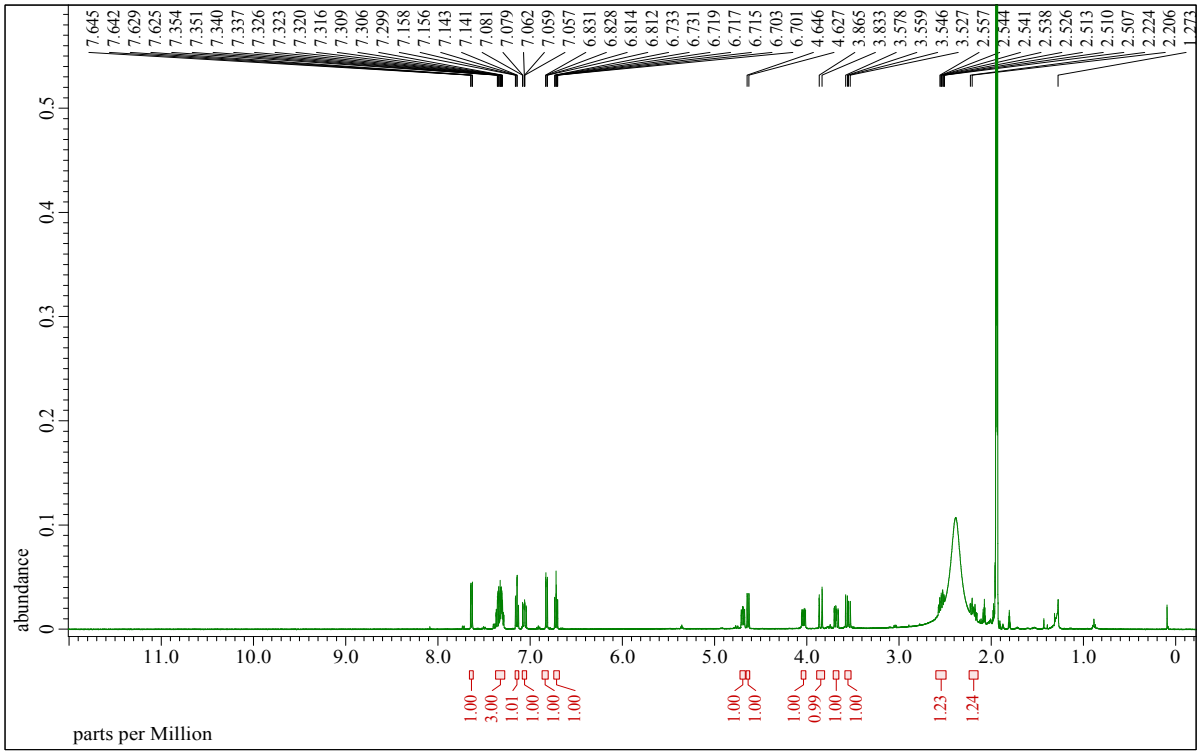


Figure S52. ^{1}H NMR spectrum of **7i^{2R}** (500 MHz, MeCN-d_3)

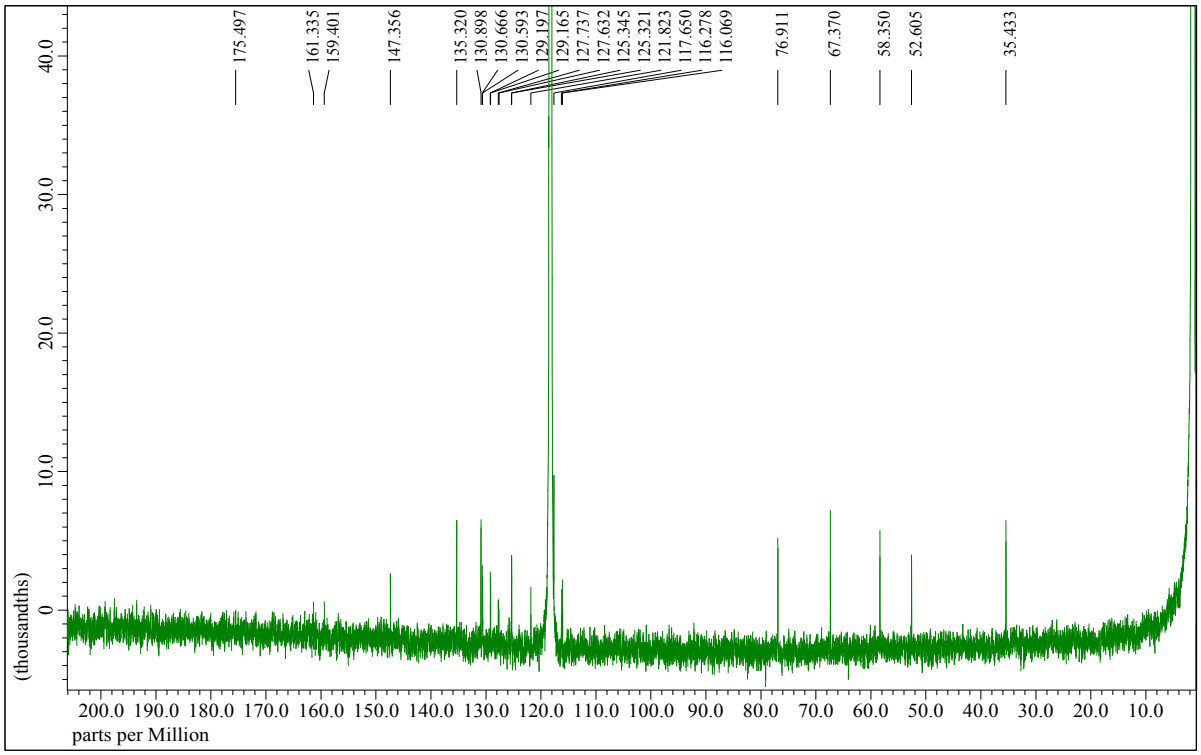


Figure S53. ^{13}C{^{1}H} NMR spectrum of **7i^{2R}** (126 MHz, MeCN-d_3)

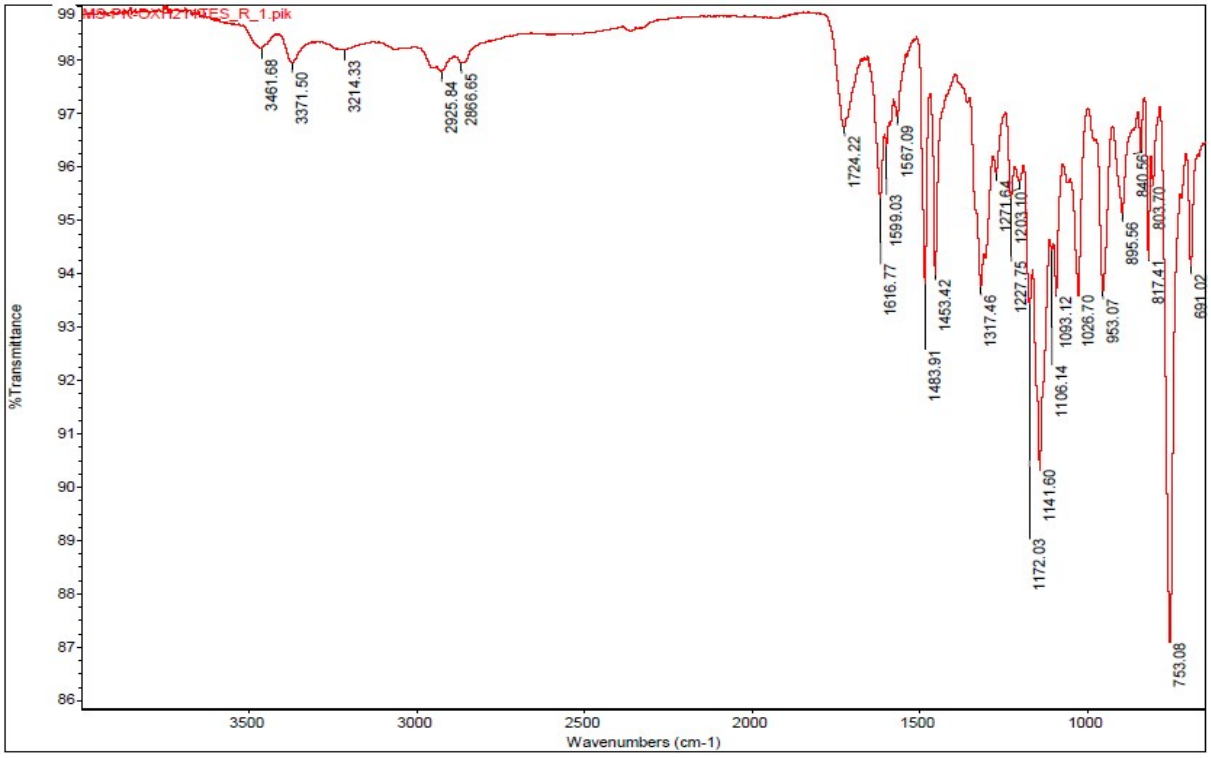


Figure S54. IR spectrum of **7i**^{2R}

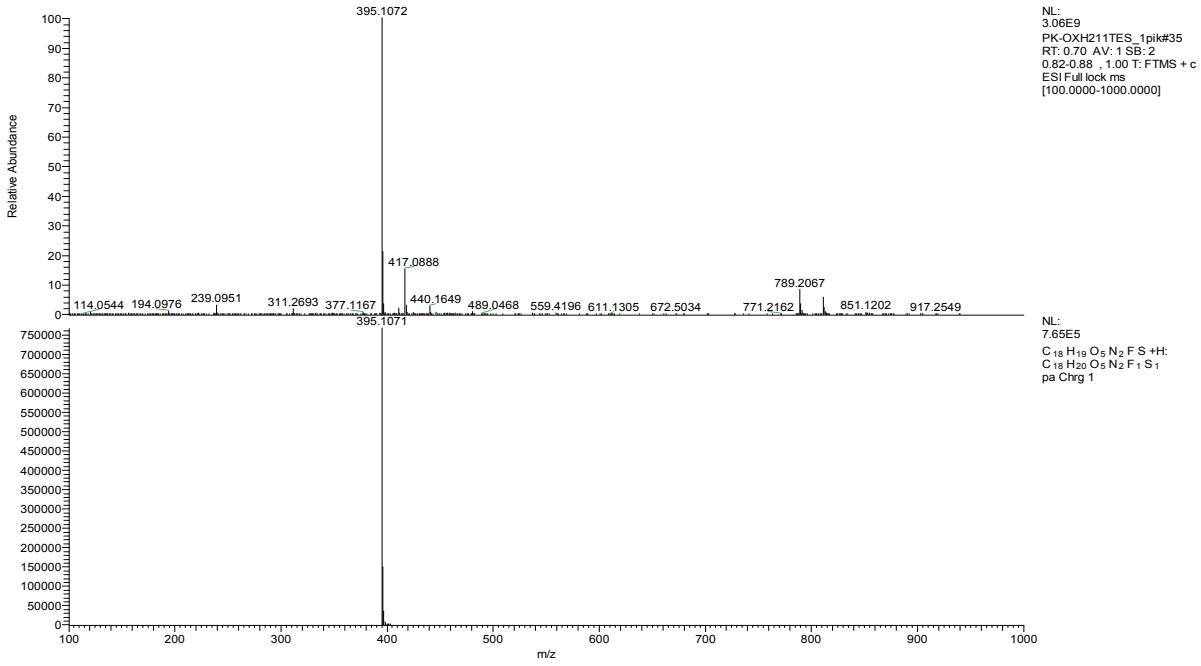
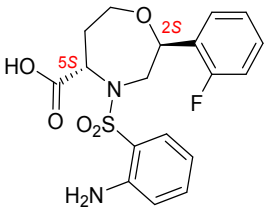


Figure S55. HRMS spectrum of **7i**^{2R}

(-)-(2*S*,5S)-4-((2-aminophenyl)sulfonyl)-2-(2-fluorophenyl)-1,4-oxazepane-5-carboxylic acid 7i^{2S}



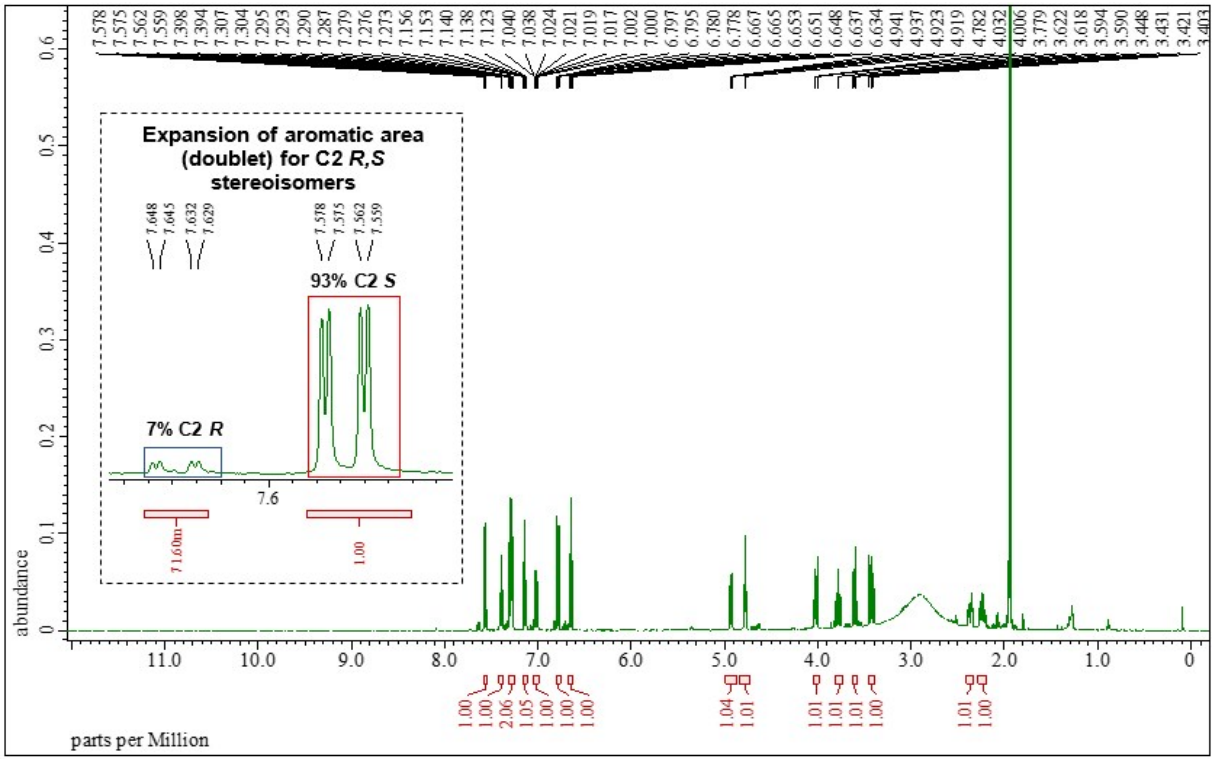


Figure S56. ^{1}H NMR spectrum of **7i^{2S}** (500 MHz, MeCN-d_3). Note: Only the signals belonging to the major diastereomer were analyzed.

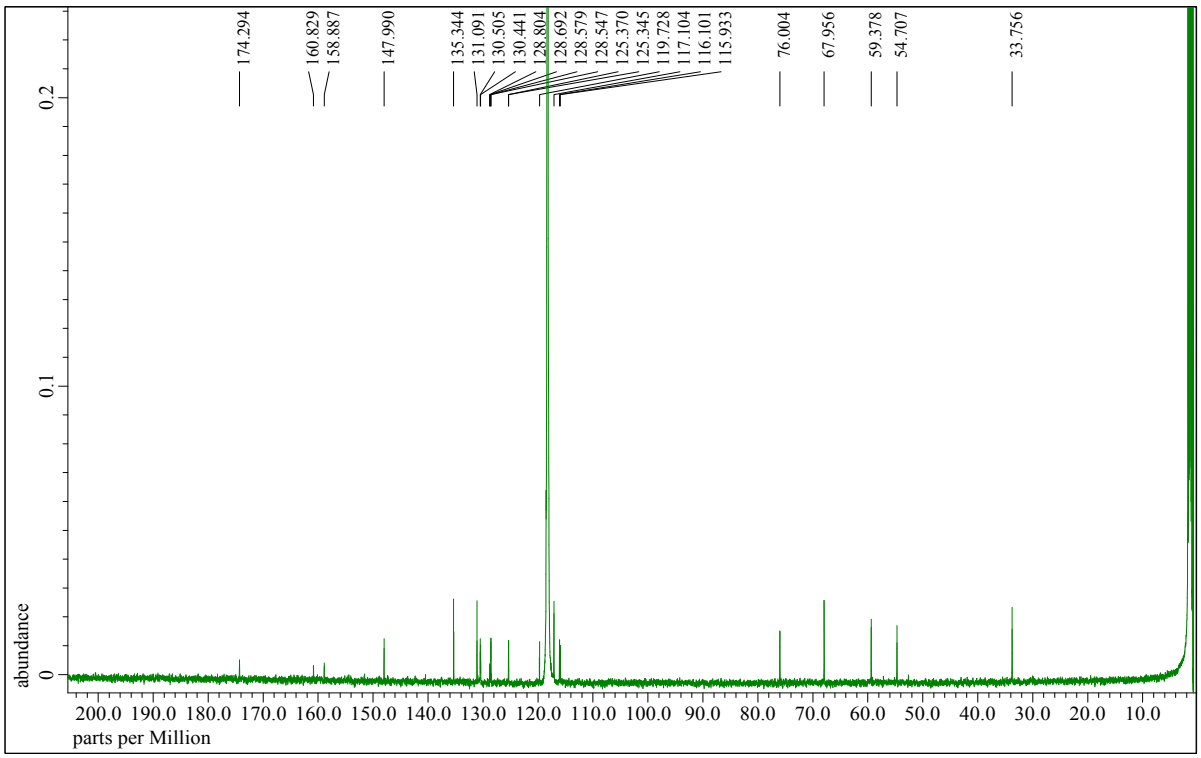


Figure S57. ^{13}C{^{1}H} NMR spectrum of **7i^{2S}** (126 MHz, MeCN-d_3). Note: Only the signals belonging to the major diastereomer were analyzed.

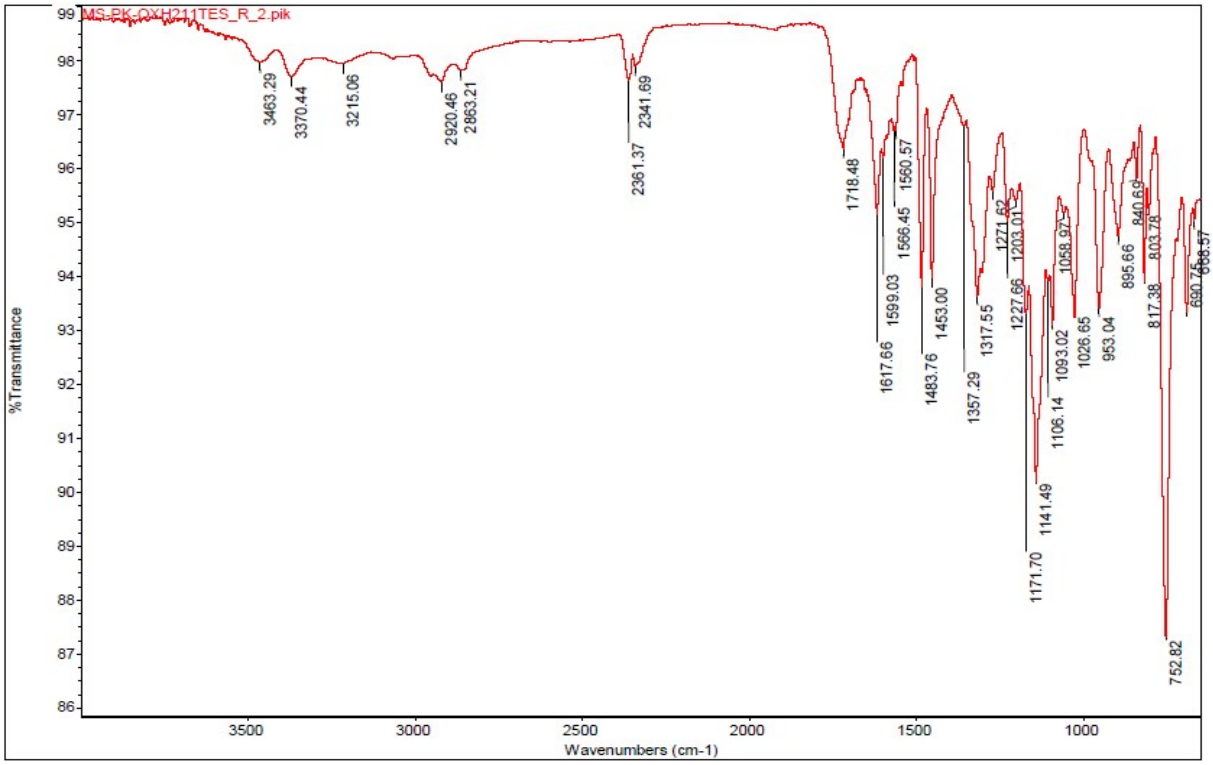


Figure S58. IR spectrum of **7i*2S***

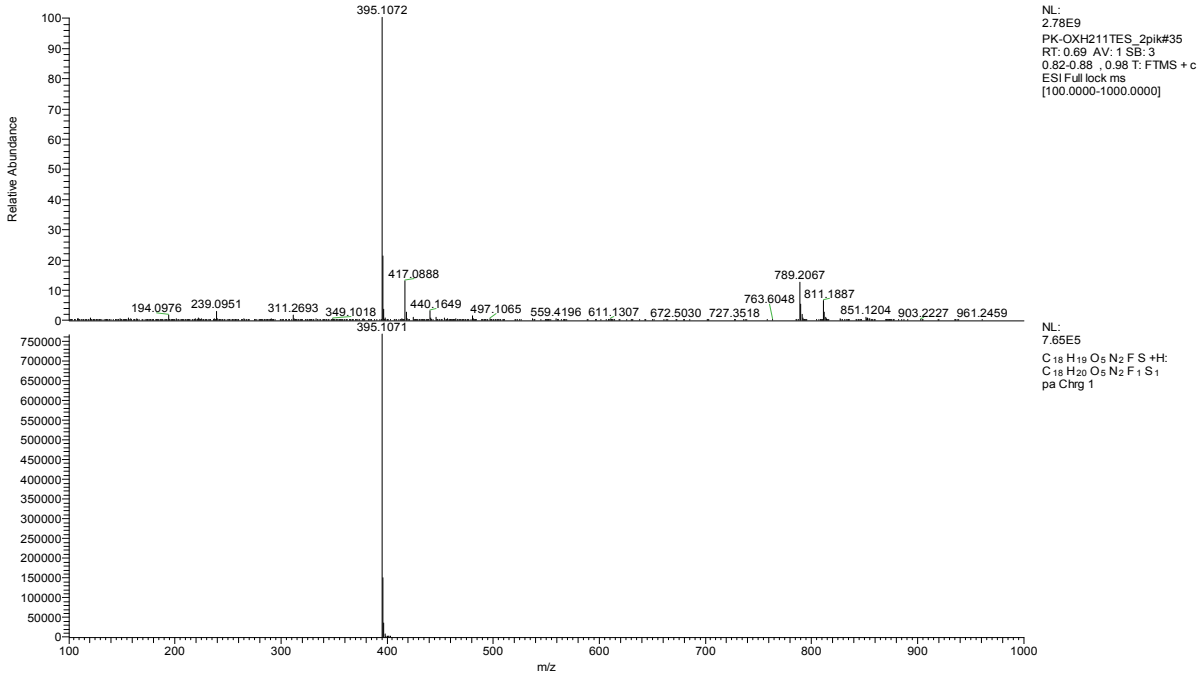
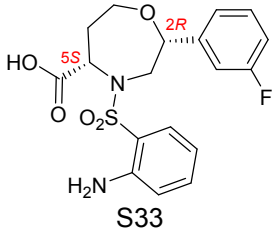


Figure S59. HRMS spectrum of **7i*2S***

(-)-(2*R*,5S)-4-((2-aminophenyl)sulfonyl)-2-(3-fluorophenyl)-1,4-oxazepane-5-carboxylic acid 7k



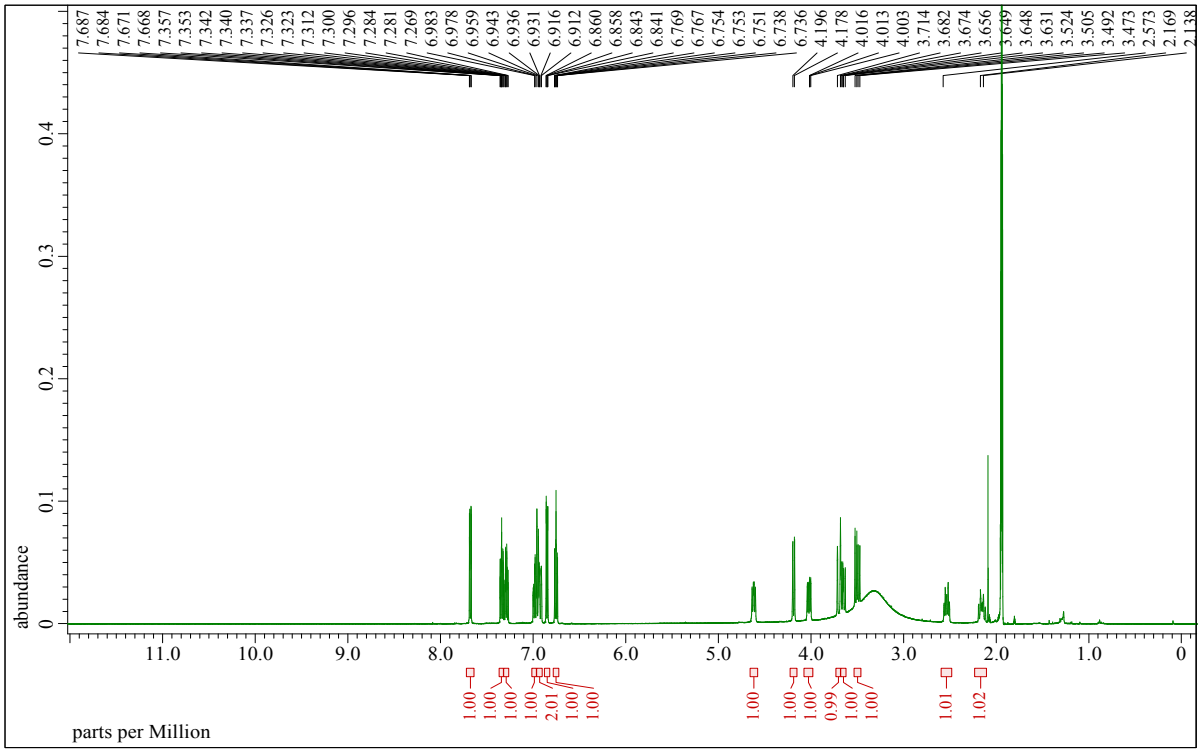


Figure S60. ^{1}H NMR spectrum of **7k** (500 MHz, MeCN-d_3)

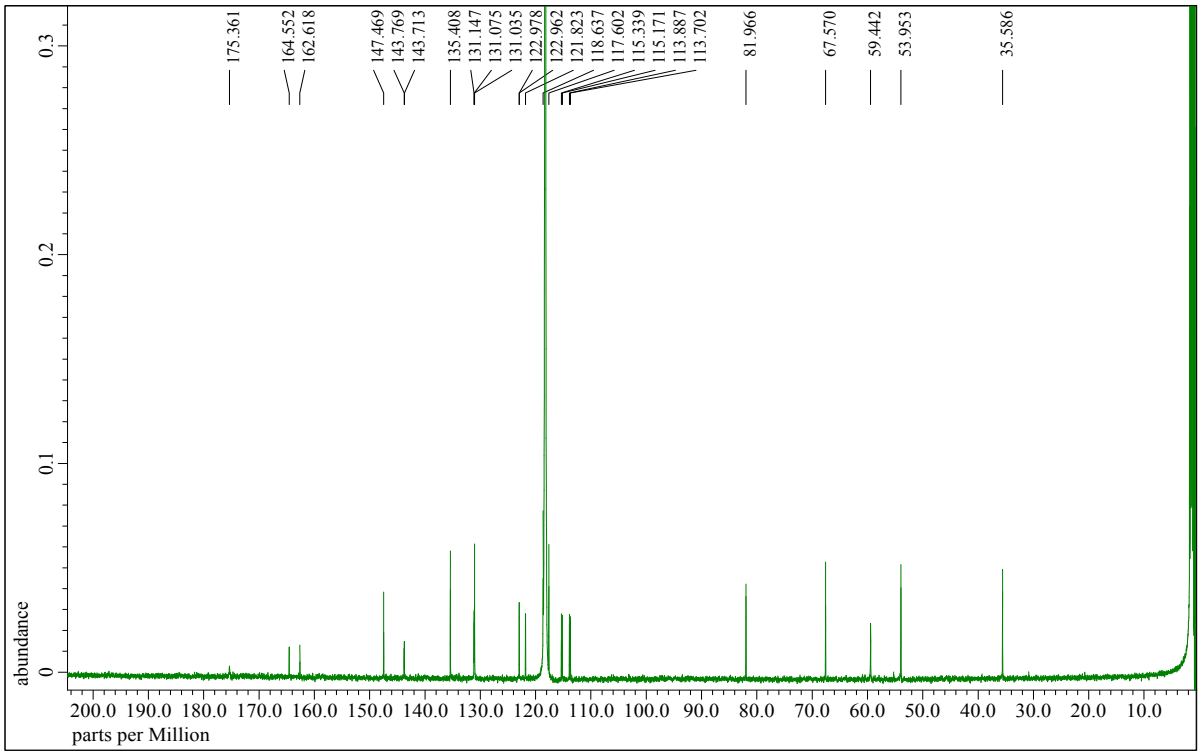


Figure S61. ^{13}C{^{1}H} NMR spectrum of **7k** (126 MHz, MeCN-d_3)

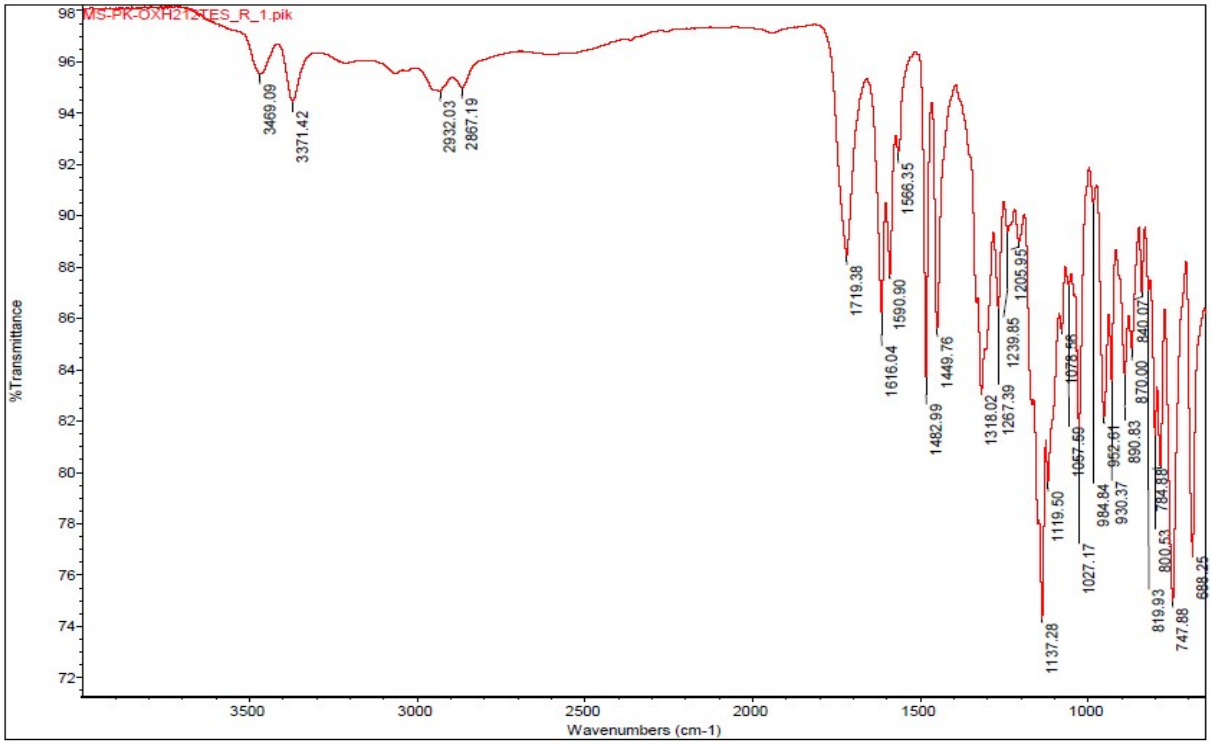


Figure S62. IR spectrum of **7k**

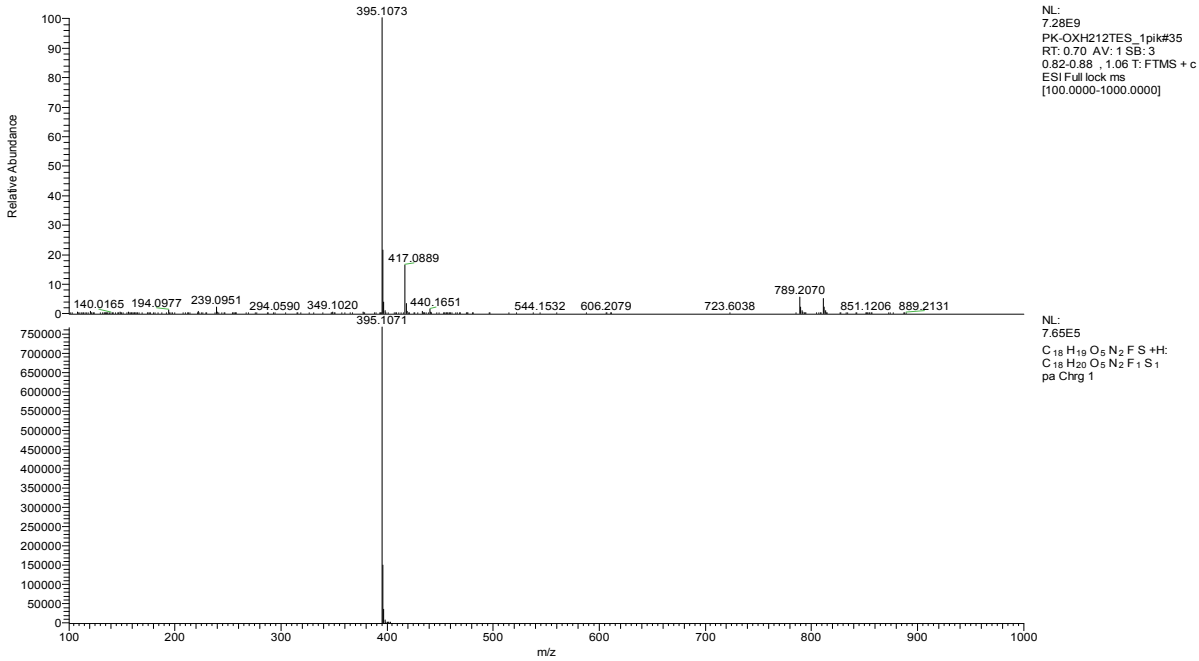
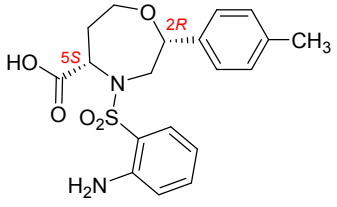


Figure S63. HRMS spectrum of **7k**

(+)-(2*R*,5S)-4-((2-aminophenyl)sulfonyl)-2-(*p*-tolyl)-1,4-oxazepane-5-carboxylic acid 7m



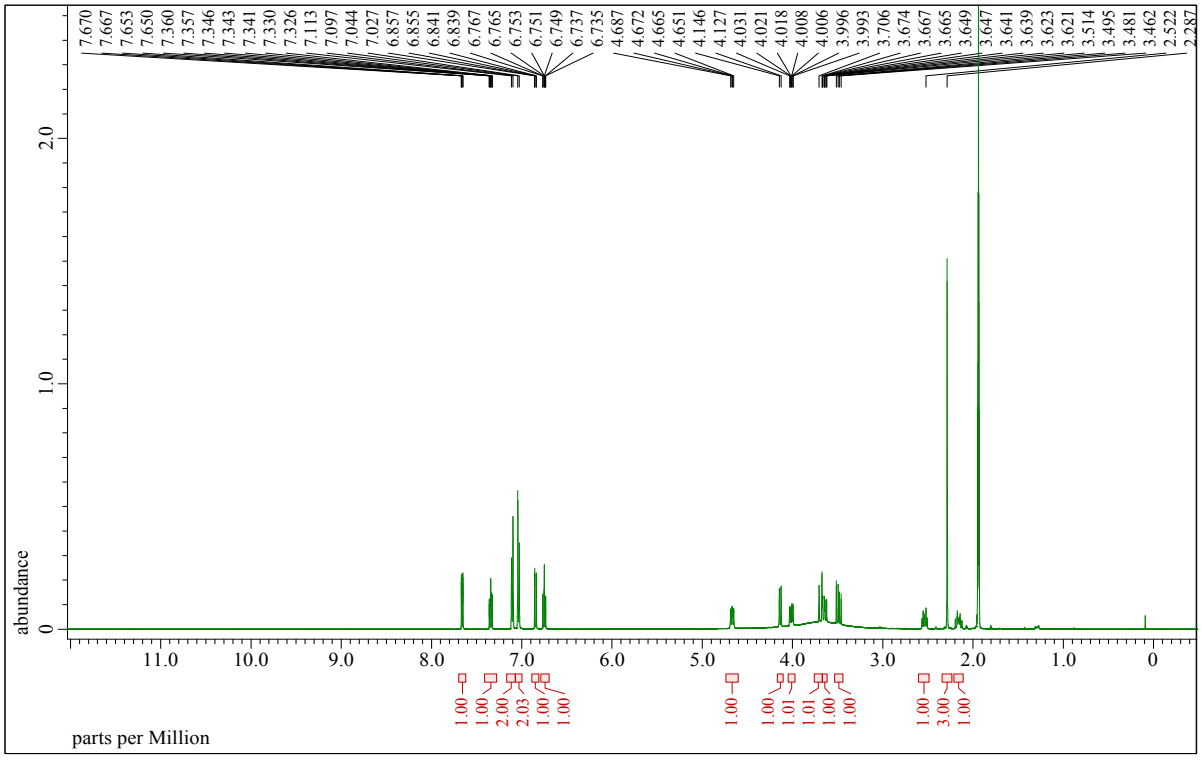


Figure S64. ^{1}H NMR spectrum of **7m** (500 MHz, MeCN-d_3)

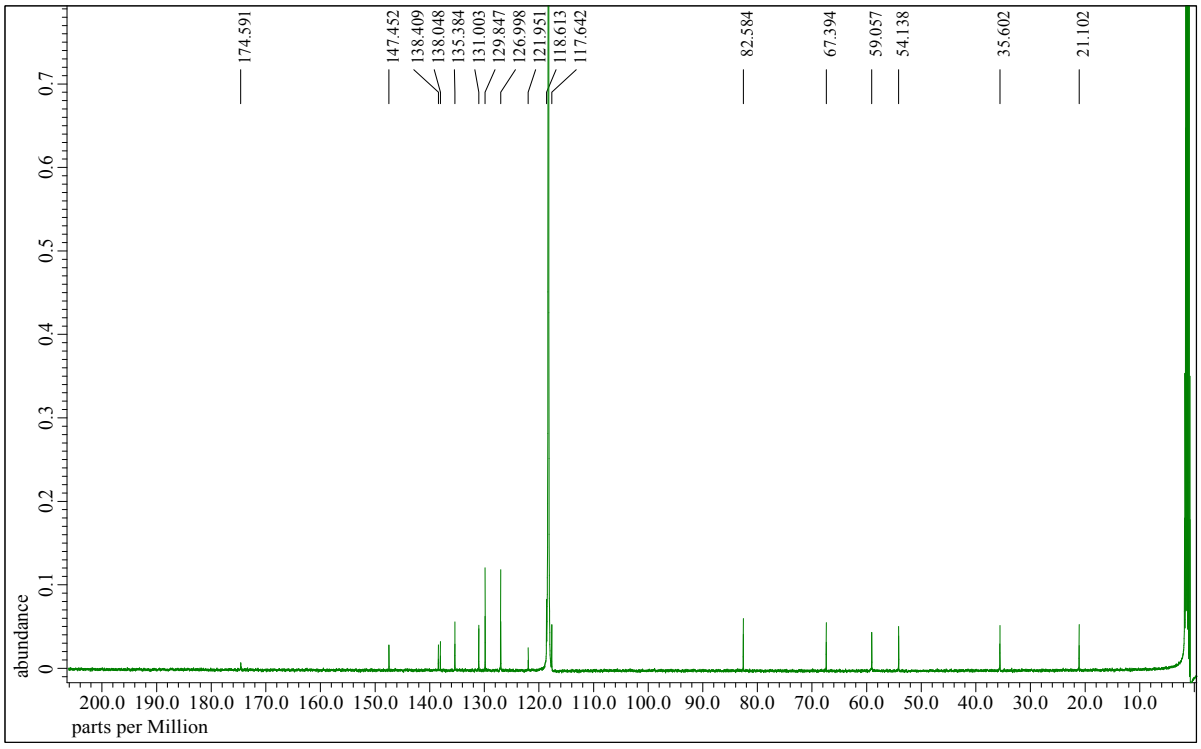


Figure S65. ^{13}C{^{1}H} NMR spectrum of **7m** (126 MHz, MeCN-d_3)

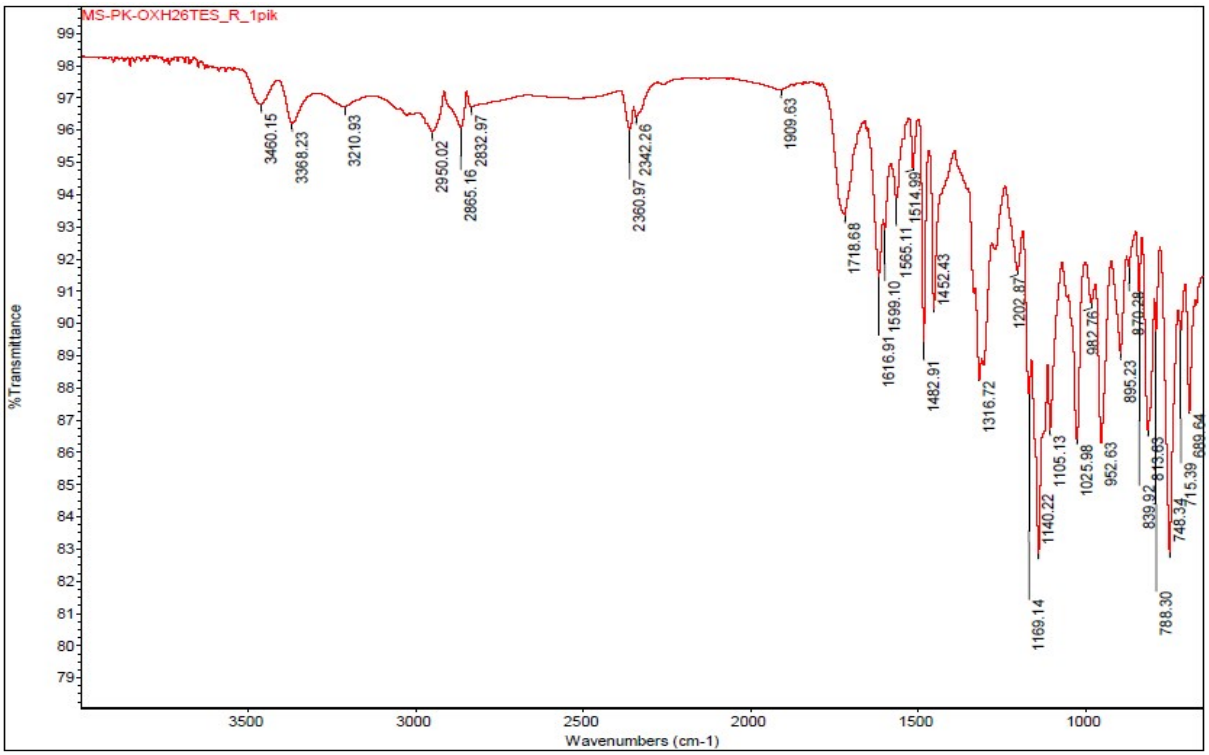


Figure S66. IR spectrum of **7m**

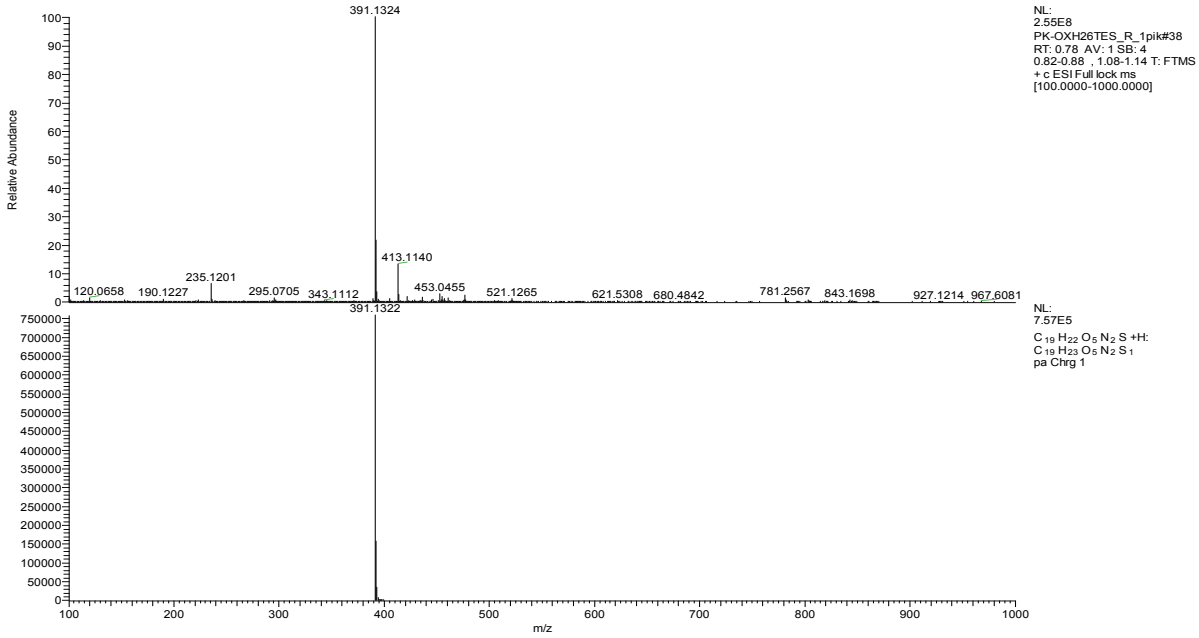
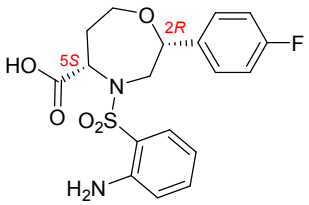


Figure S67. HRMS spectrum of **7m**

(+)-(2*R*,5S)-4-((2-aminophenyl)sulfonyl)-2-(4-fluorophenyl)-1,4-oxazepane-5-carboxylic acid 7o



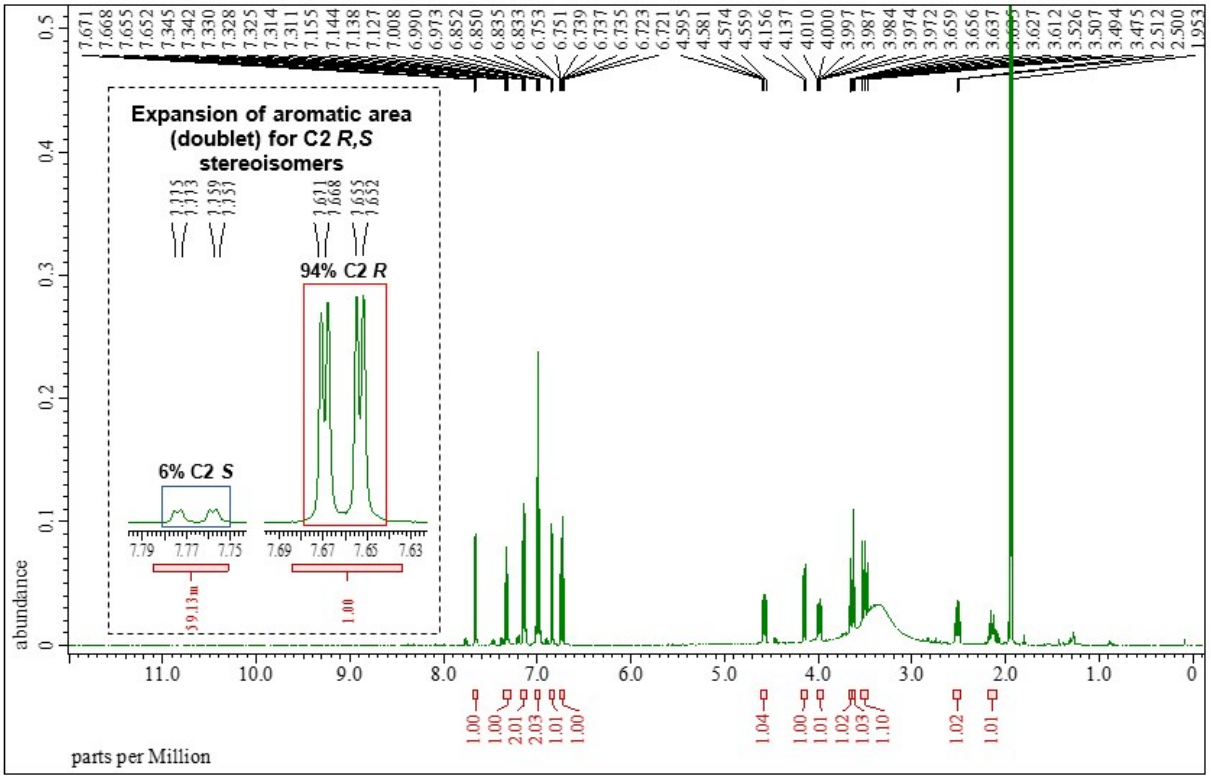


Figure S68. ^{1}H NMR spectrum of **7o** (500 MHz, MeCN-d_3). Note: Only the signals belonging to the major diastereomer were analyzed.

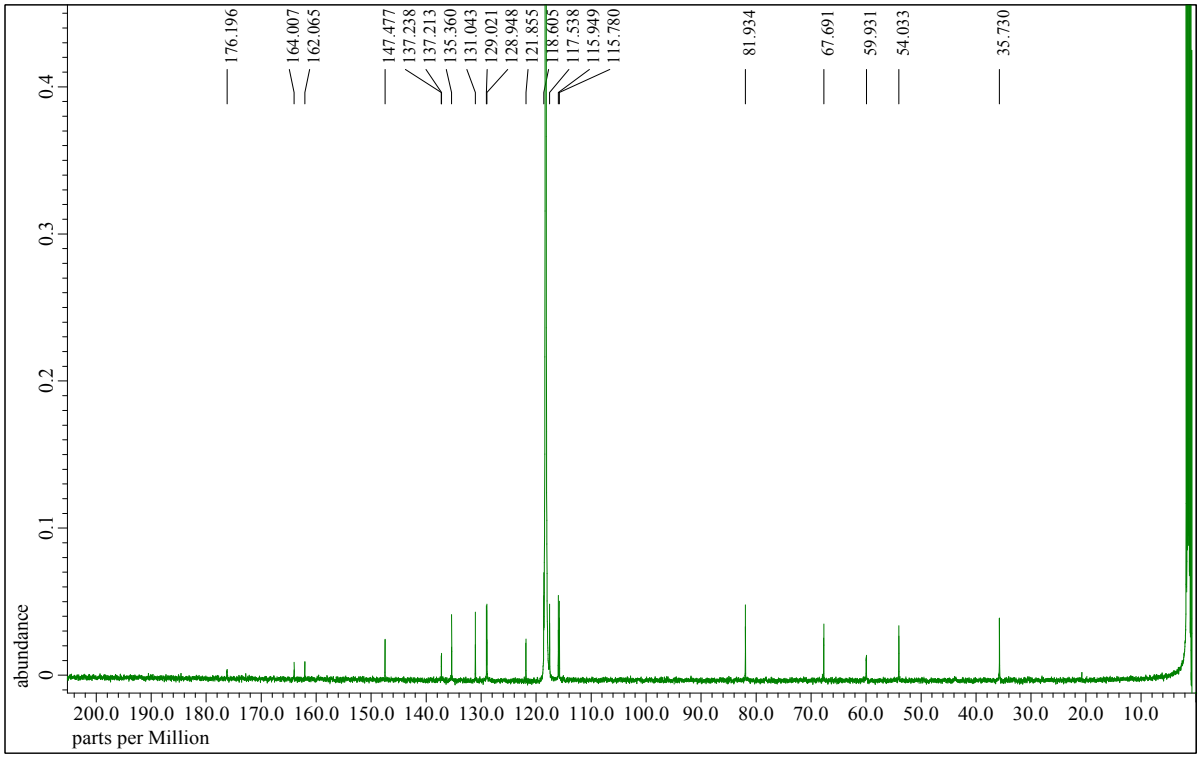


Figure S69. ^{13}C{^{1}H} NMR spectrum of **7o** (126 MHz, MeCN-d_3). Note: Only the signals belonging to the major diastereomer were analyzed.

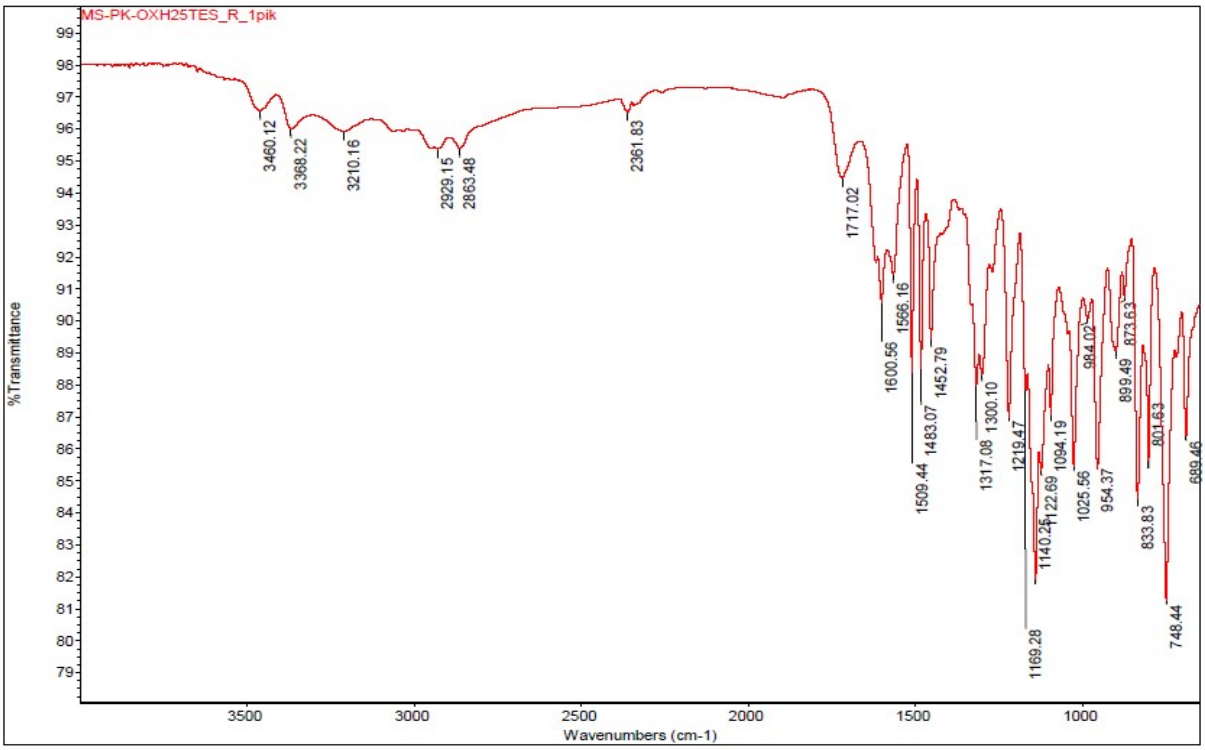


Figure S70. IR spectrum of **7o**

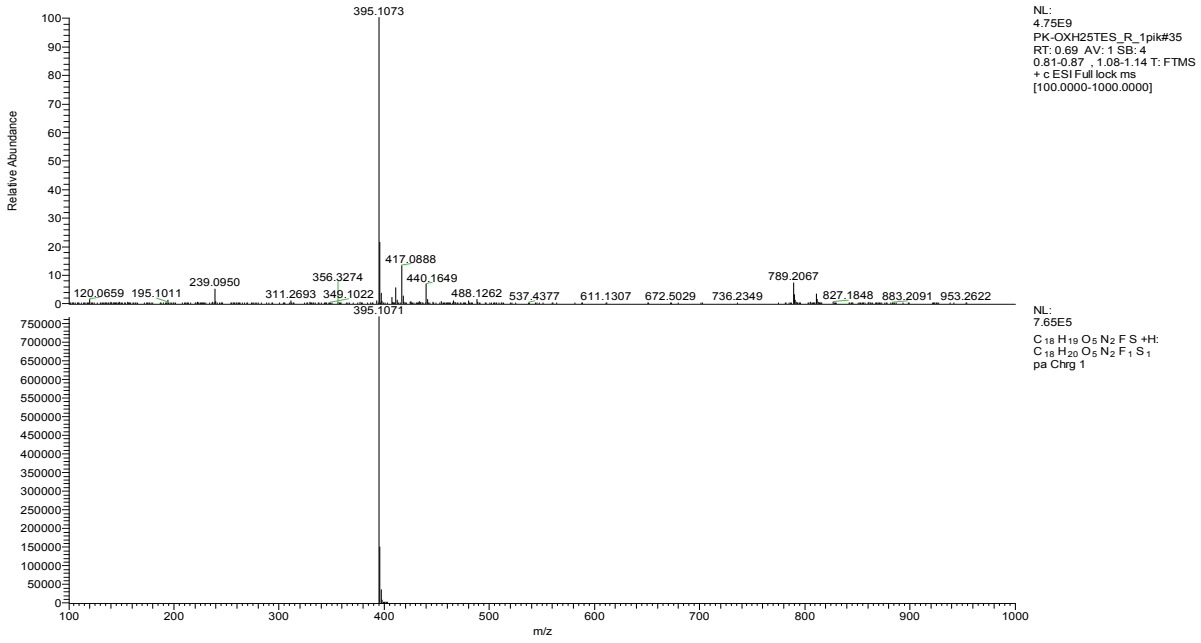
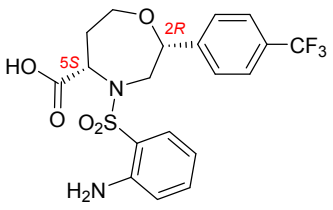


Figure S71. HRMS spectrum of **7o**

(-)-(2*R*,5S)-4-((2-aminophenyl)sulfonyl)-2-(4-(trifluoromethyl)phenyl)-1,4-oxazepane-5-carboxylic acid 7q



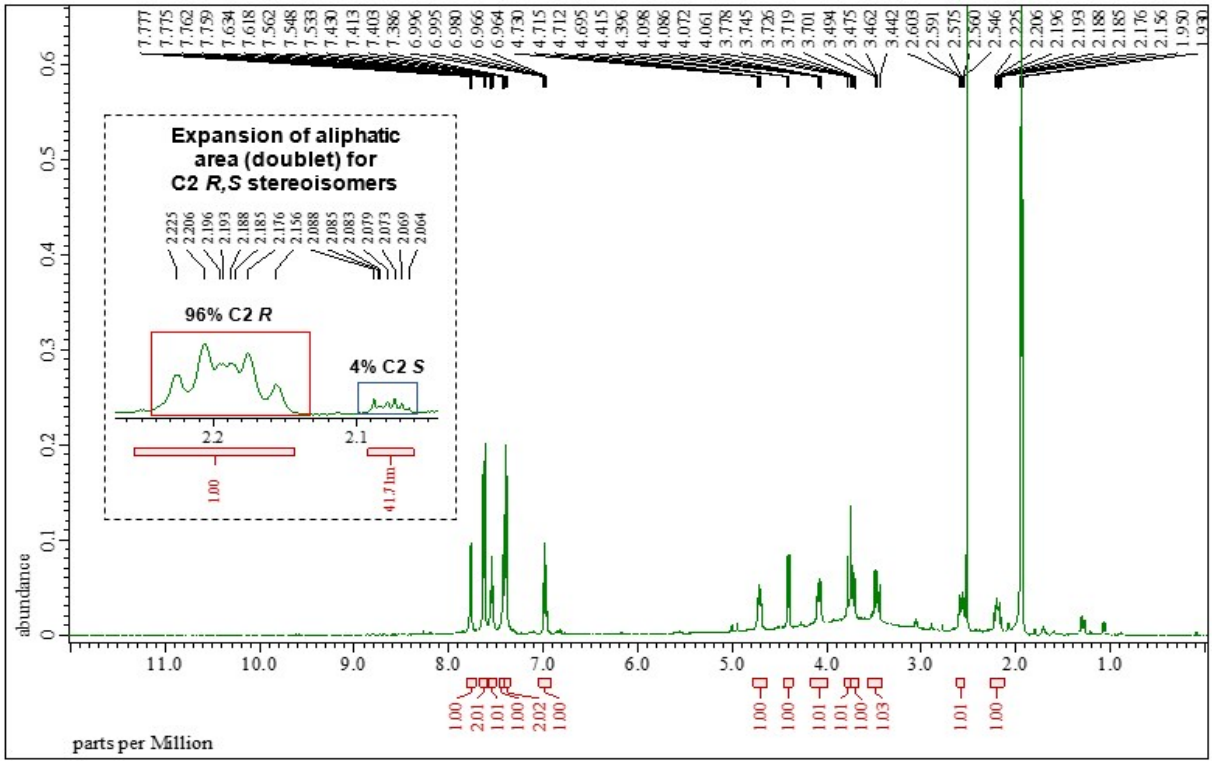


Figure S72. ^{1}H NMR spectrum of **7q** (500 MHz, MeCN-d_3). Note: Only the signals belonging to the major diastereomer were analyzed.

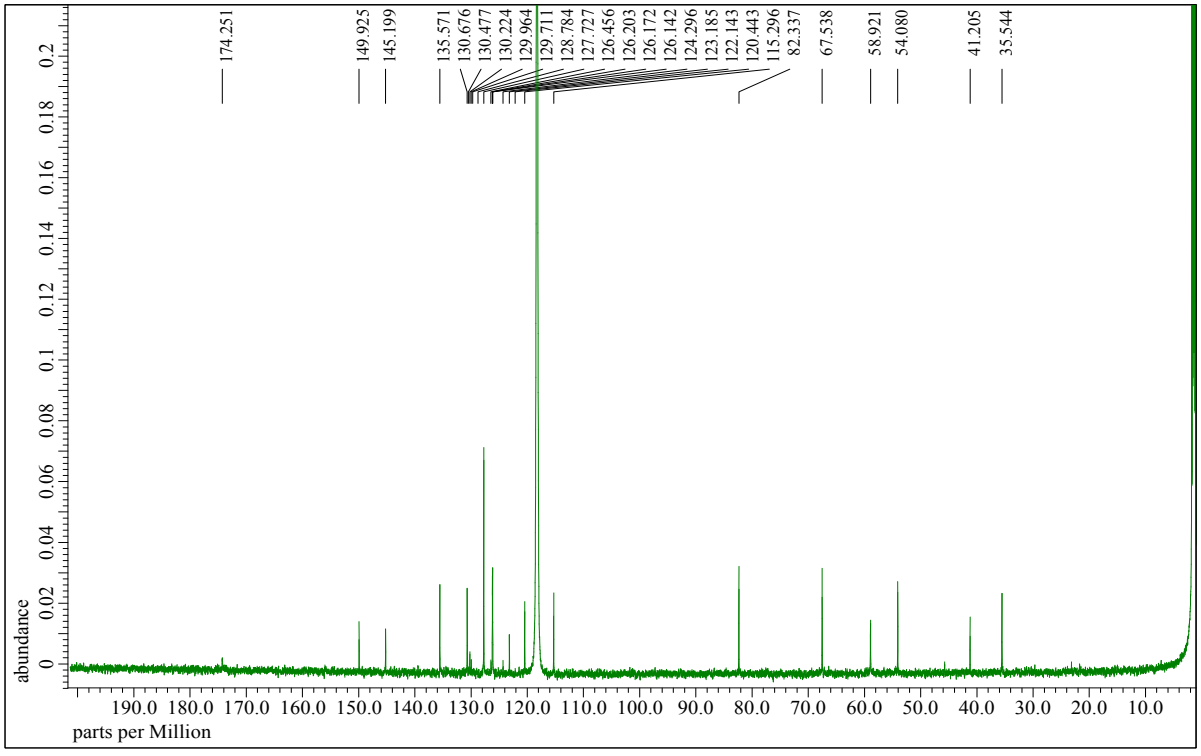


Figure S73. ^{13}C{^{1}H} NMR spectrum of **7q** (126 MHz, MeCN-d_3). Note: Only the signals belonging to the major diastereomer were analyzed.

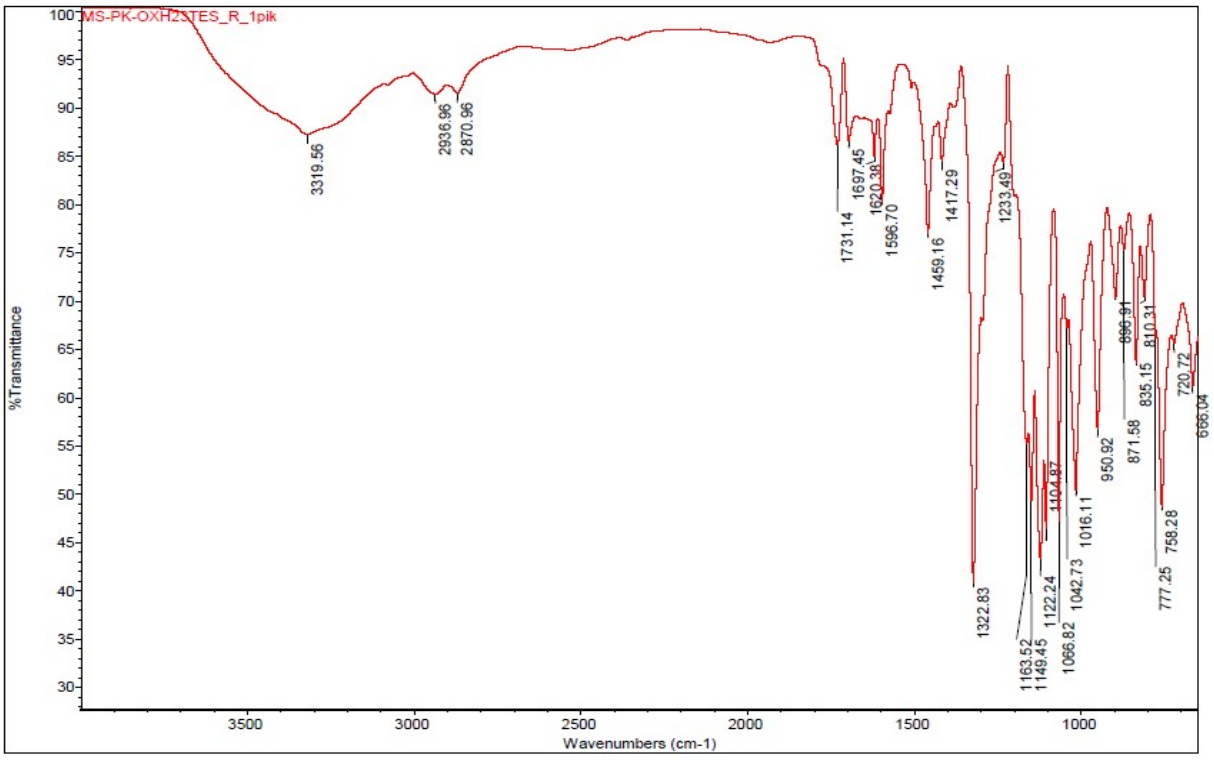


Figure S74. IR spectrum of **7q**

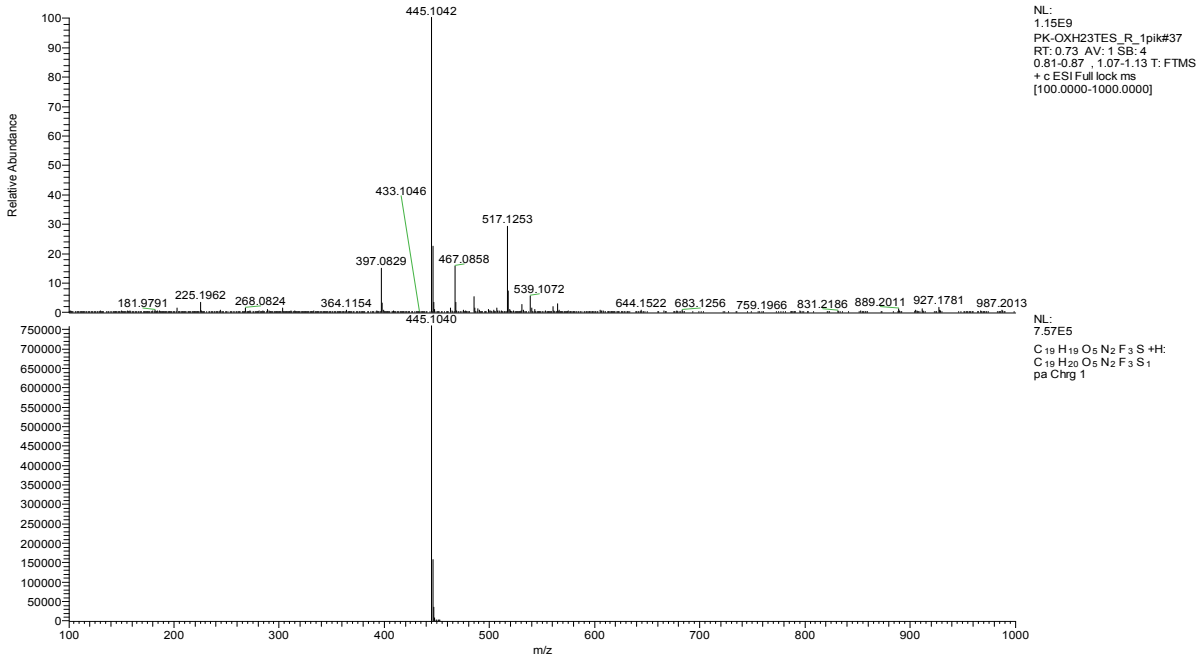
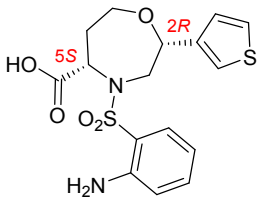


Figure S75. HRMS spectrum of **7q**

(-)-(2*R*,5S)-4-((2-aminophenyl)sulfonyl)-2-(thiophen-3-yl)-1,4-oxazepane-5-carboxylic acid 7t



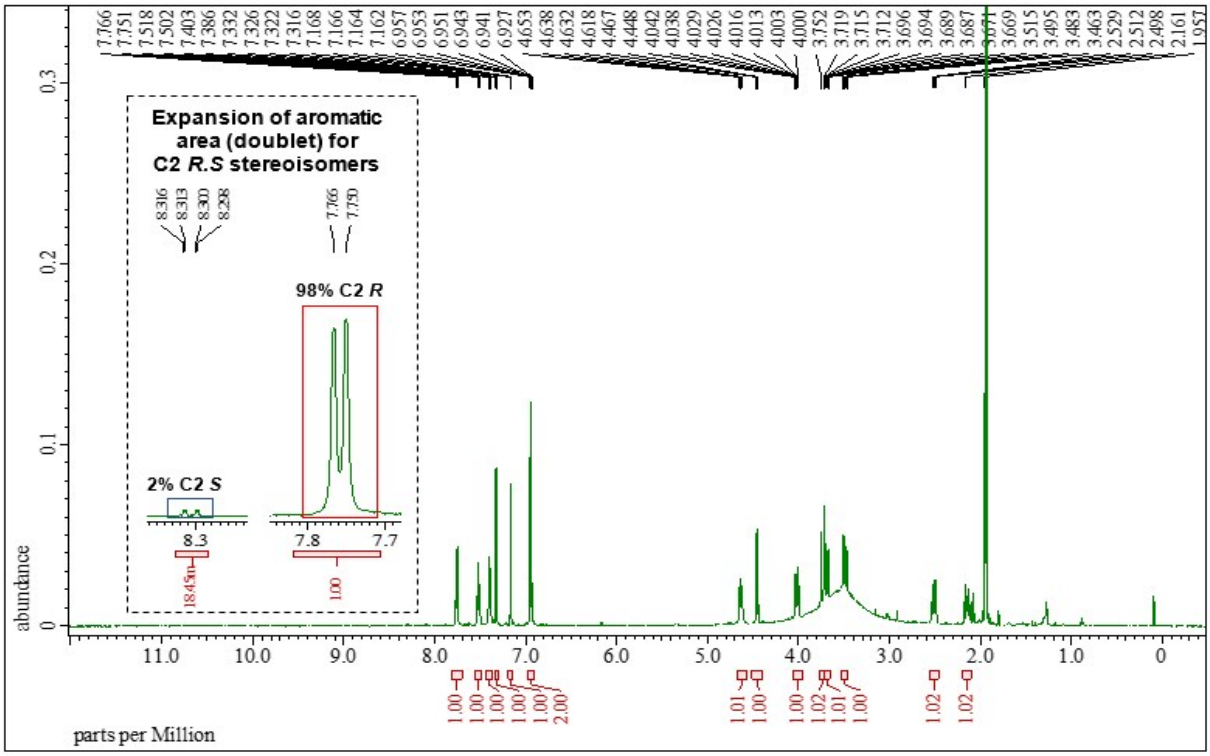


Figure S76. ^{1}H NMR spectrum of **7t** (500 MHz, MeCN-d_3)

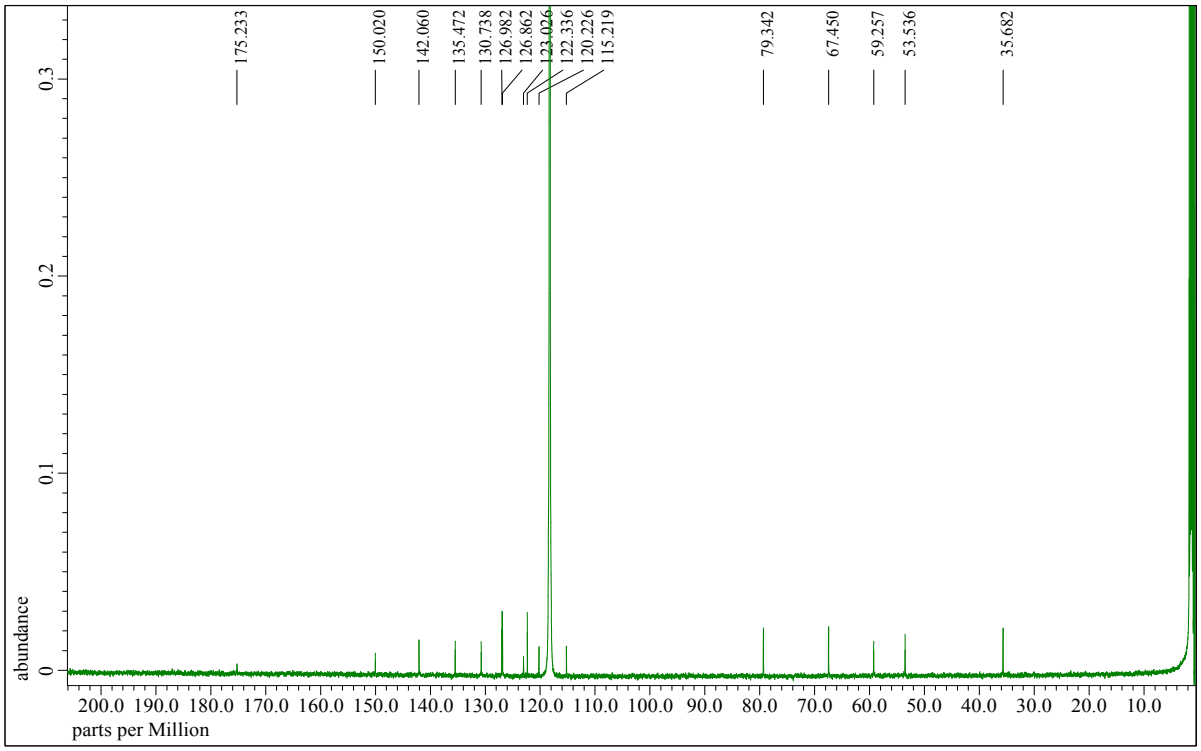


Figure S77. ^{13}C{^{1}H} NMR spectrum of **7t** (126 MHz, MeCN-d_3)

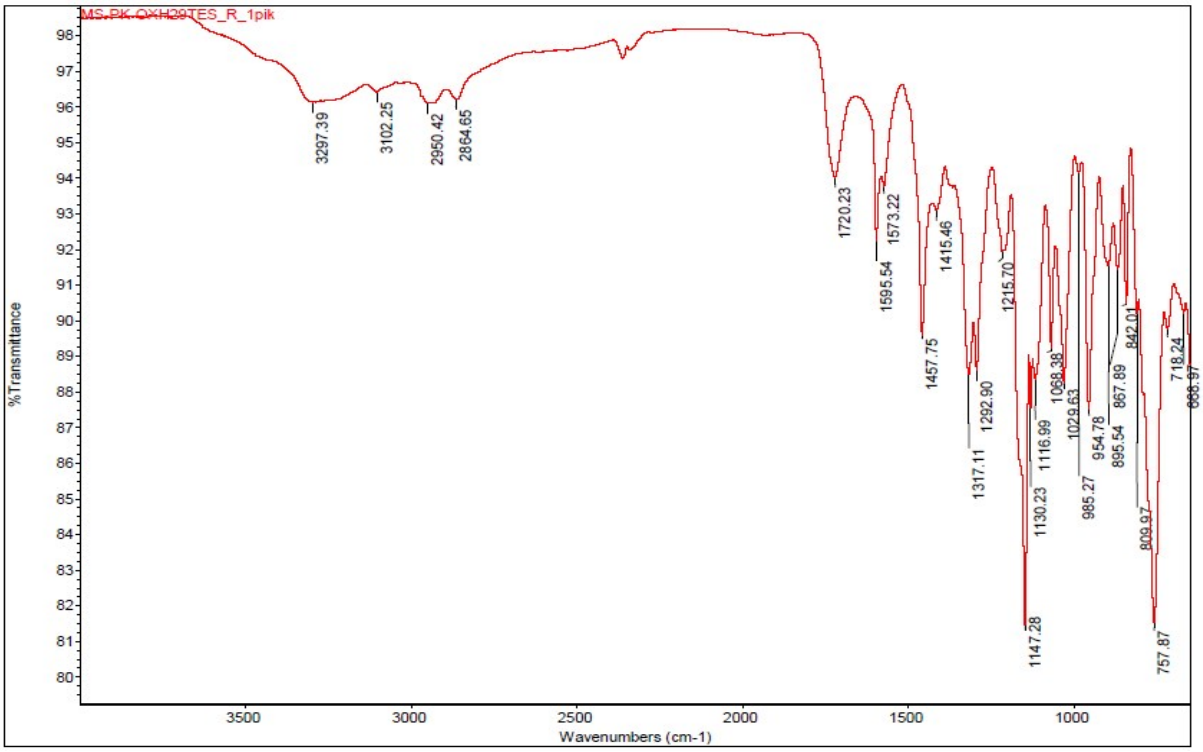


Figure S78. IR spectrum of **7t**

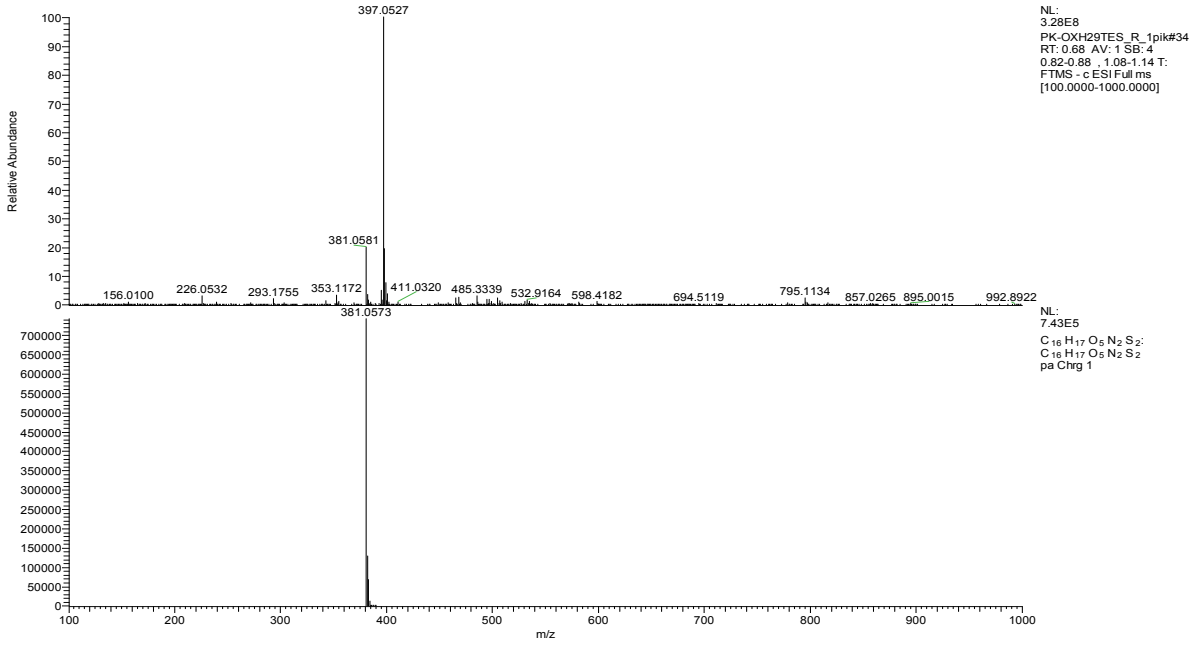
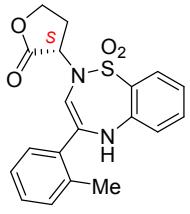


Figure S79. HRMS spectrum of **7t**. Note: ion 397 belongs to the ammonium adduct originating from mobile phase.

(-)-(*S*)-3-(1,1-dioxo-4-(*o*-tolyl)benzo[*f*][1,2,5]thiadiazepin-2(5*H*)-yl)dihydrofuran-2(3*H*)-one 9h



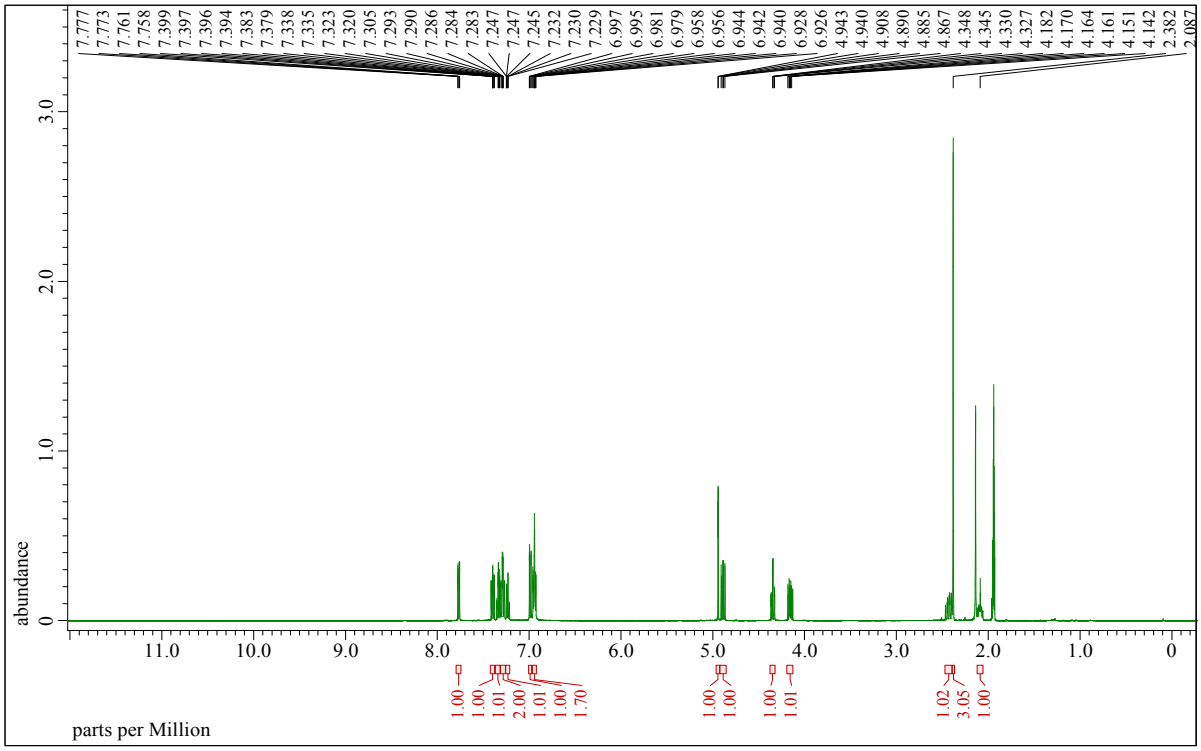


Figure S80. ^{1}H NMR spectrum of **9h** (500 MHz, MeCN-d_3)

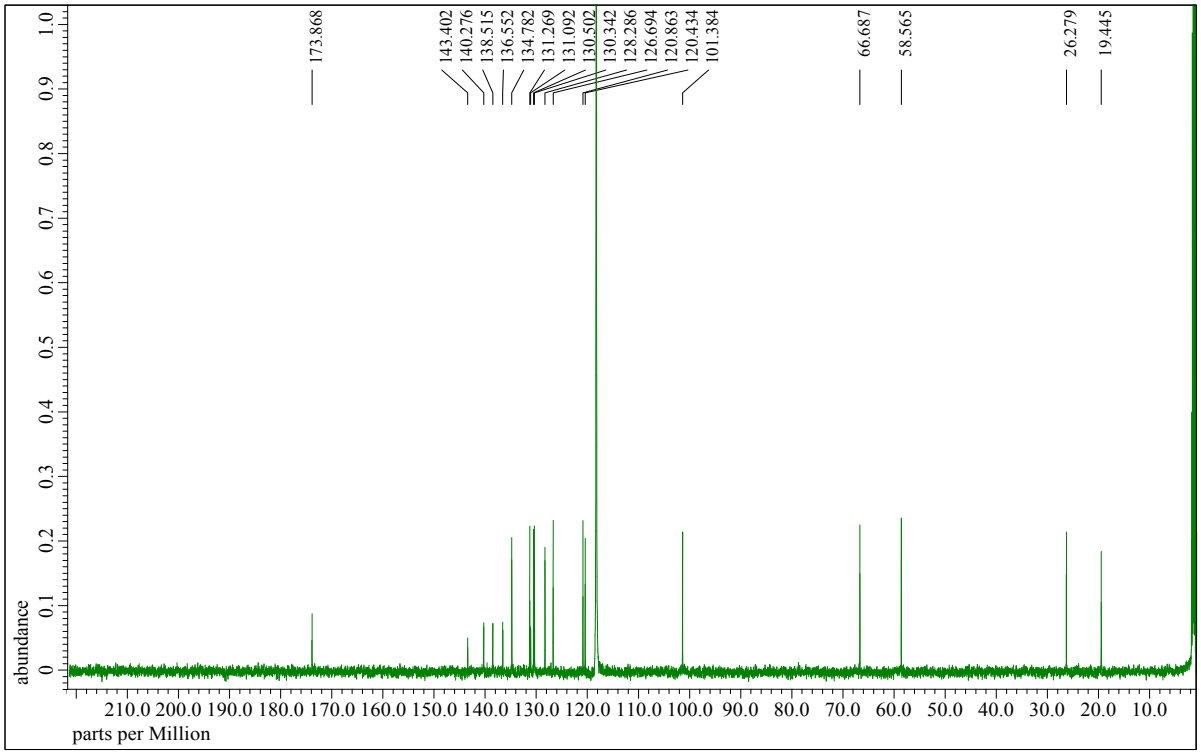


Figure S81. ^{13}C{^{1}H} NMR spectrum of **9h** (126 MHz, MeCN-d_3)

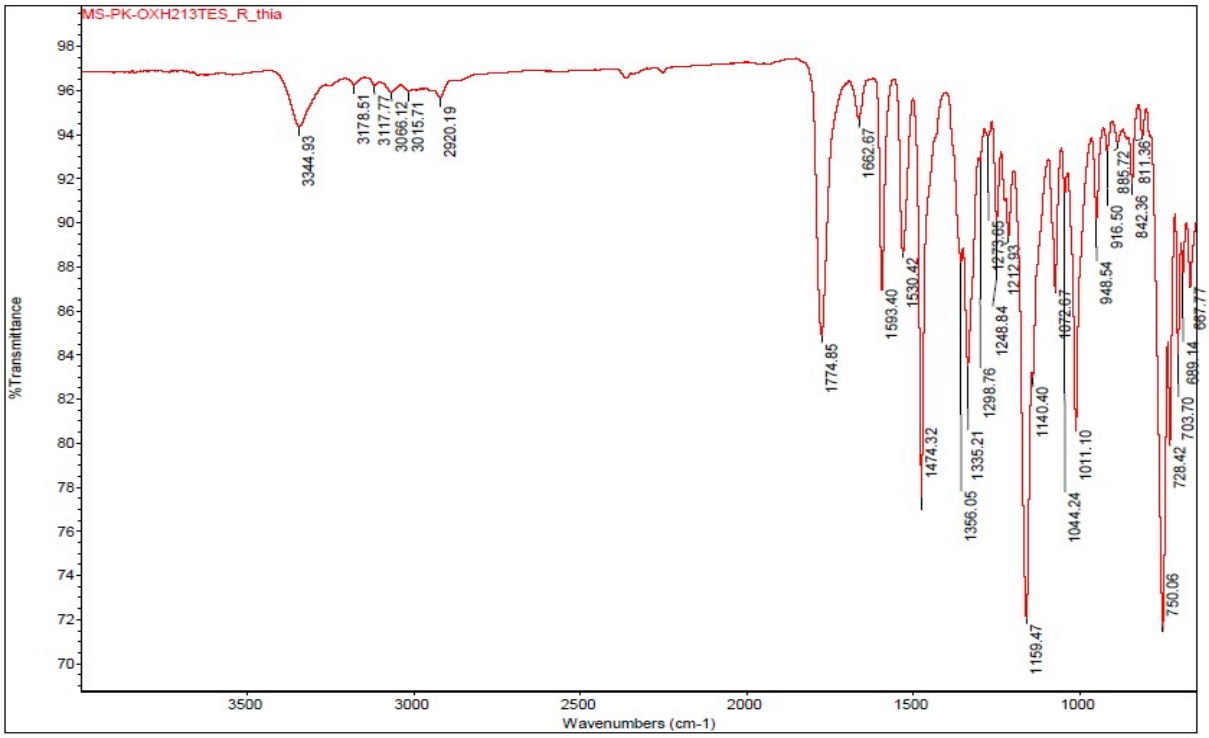


Figure S82. IR spectrum of **9h**

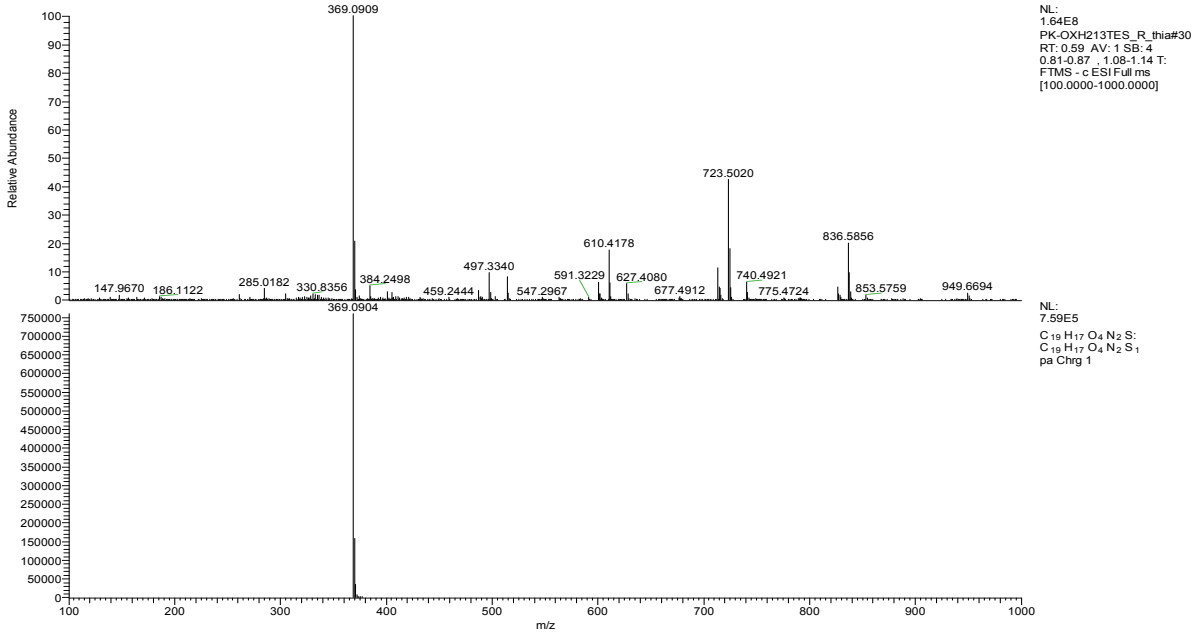
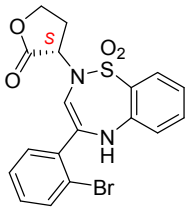


Figure S83. HRMS spectrum of **9h**

(-)-(*S*)-3-(4-(2-bromophenyl)-1,1-dioxobenzo[*f*][1,2,5]thiadiazepin-2(5*H*)-yl)dihydrofuran-2(3*H*)-one 9j



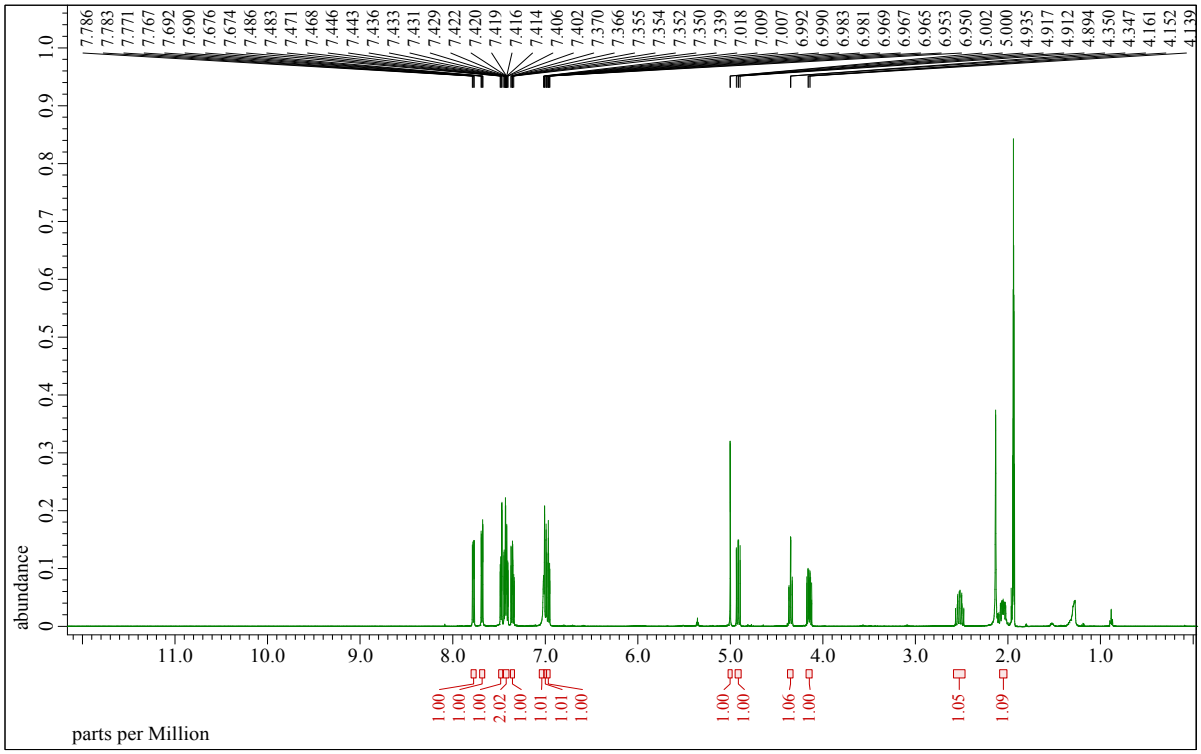


Figure S84. ^{1}H NMR spectrum of **9j** (500 MHz, MeCN-d_3)

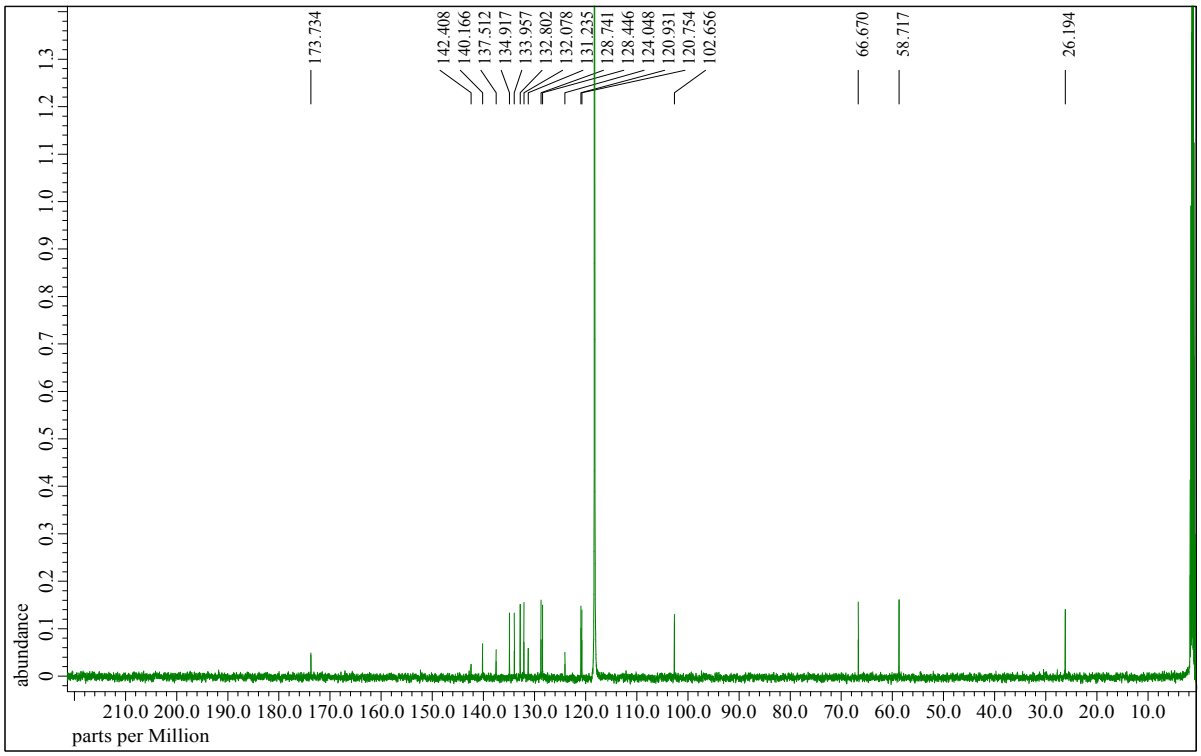


Figure S85. ^{13}C{^{1}H} NMR spectrum of **9j** (126 MHz, MeCN-d_3)

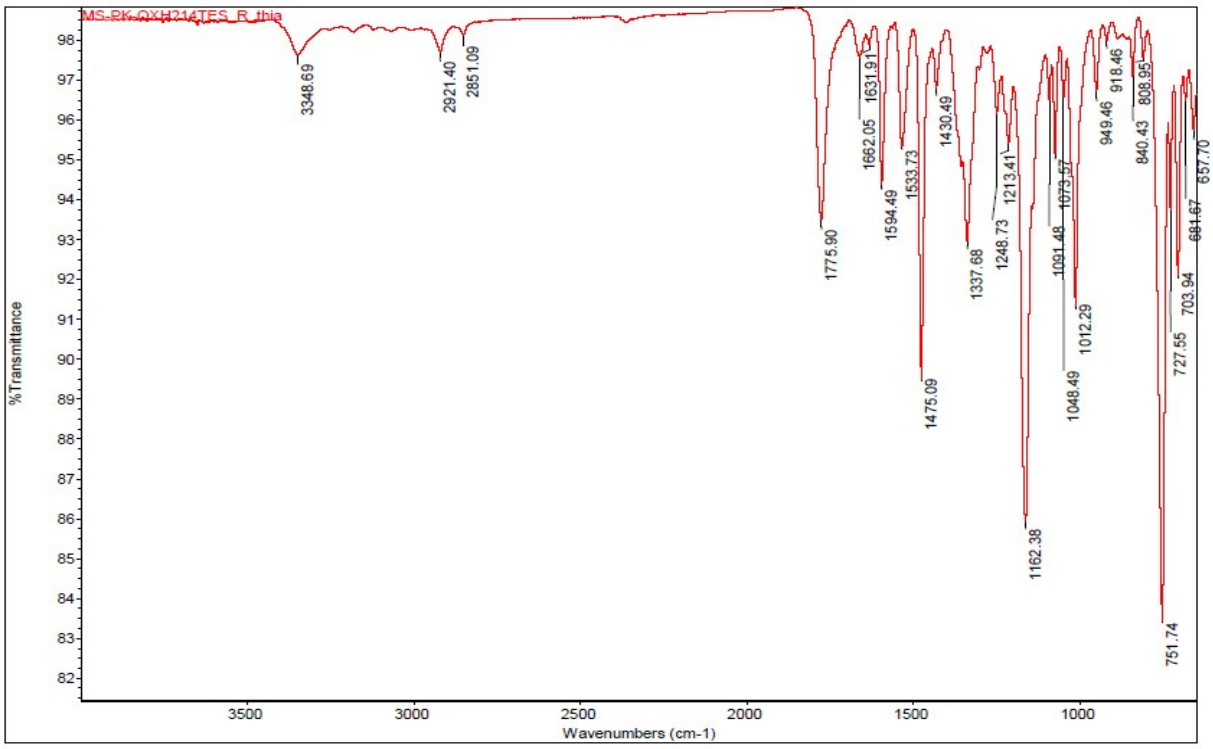


Figure S86. IR spectrum of **9j**

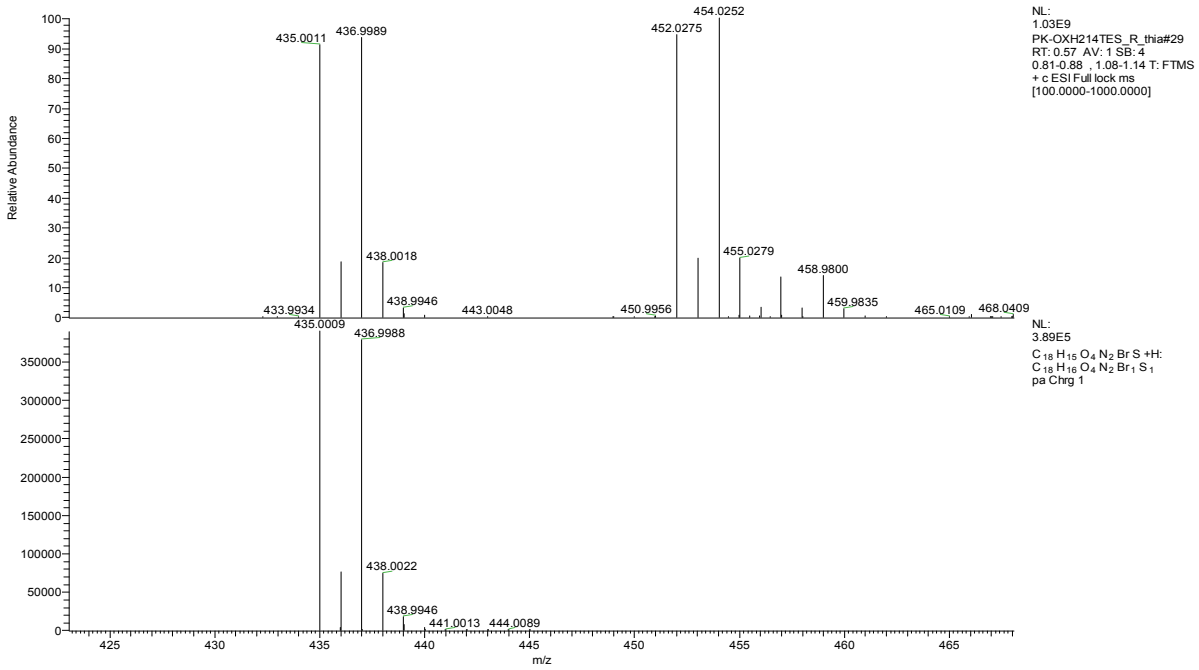
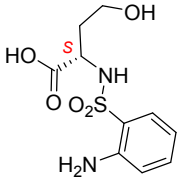


Figure 87. HRMS spectrum of **9j**. Note: ions 452 and 454 belongs to the ammonium adduct originating from mobile phase.

(+)-(*S*)-((2-aminophenyl)sulfonyl)-*L*-homoserine 10r



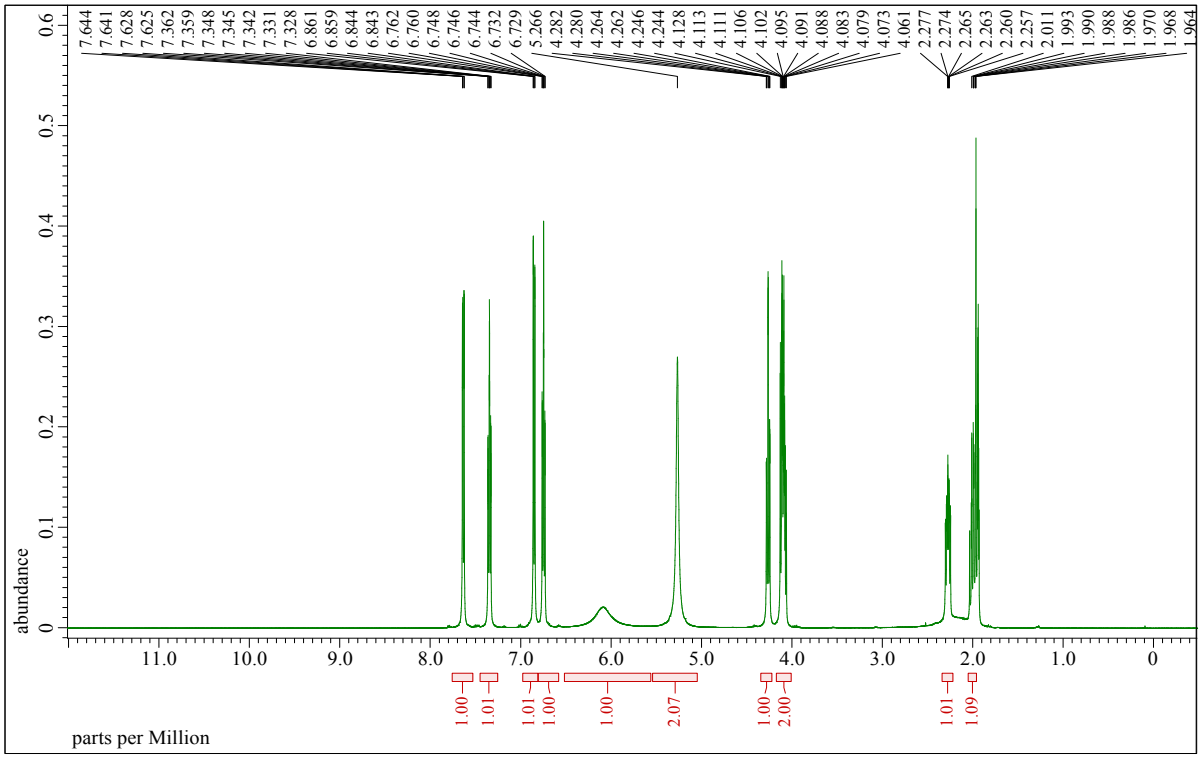


Figure S88. ^{1}H NMR spectrum of **10r** (500 MHz, MeCN-d_3)

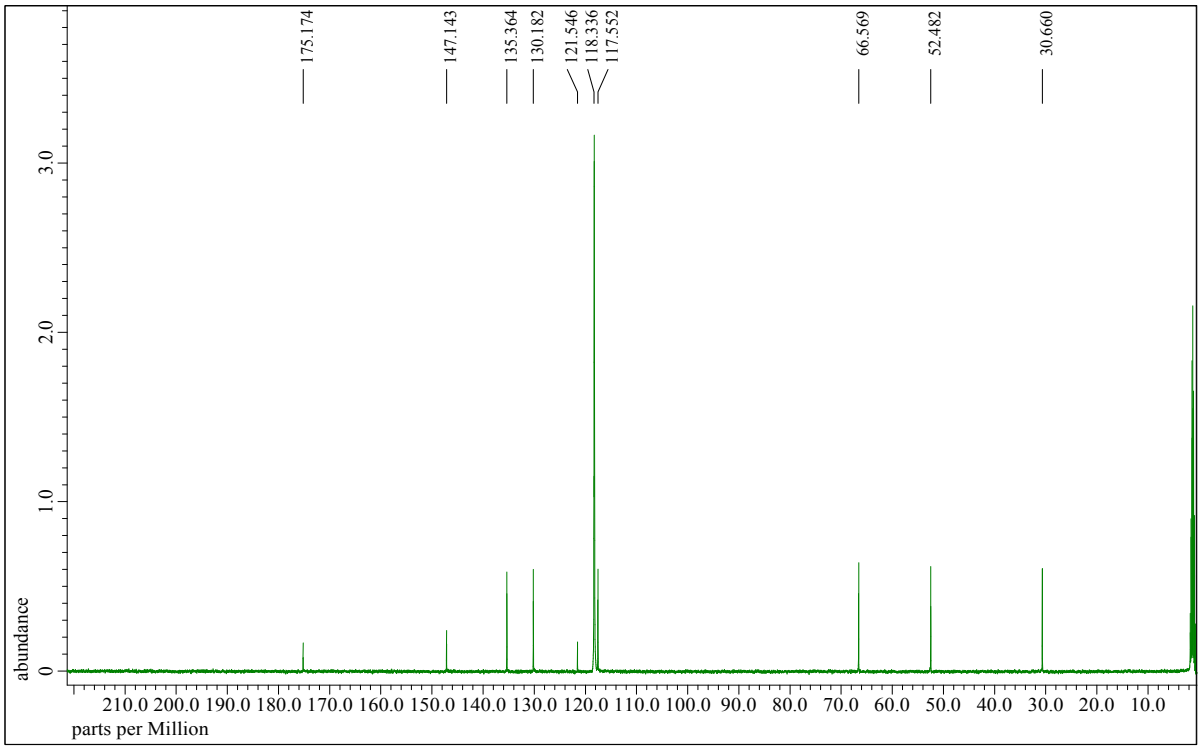


Figure S89. ^{13}C{^{1}H} NMR spectrum of **10r** (126 MHz, MeCN-d_3)

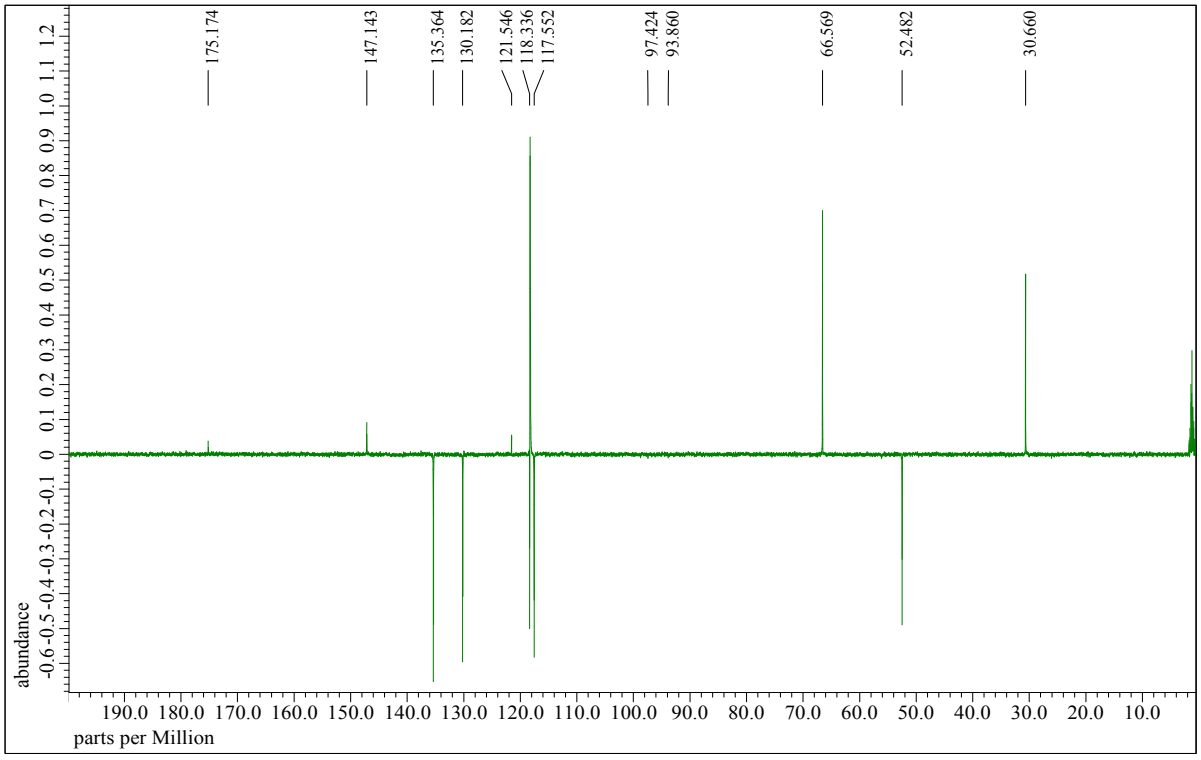


Figure S90. ^{13}C APT NMR spectrum of **10r** (126 MHz, MeCN-d_3)

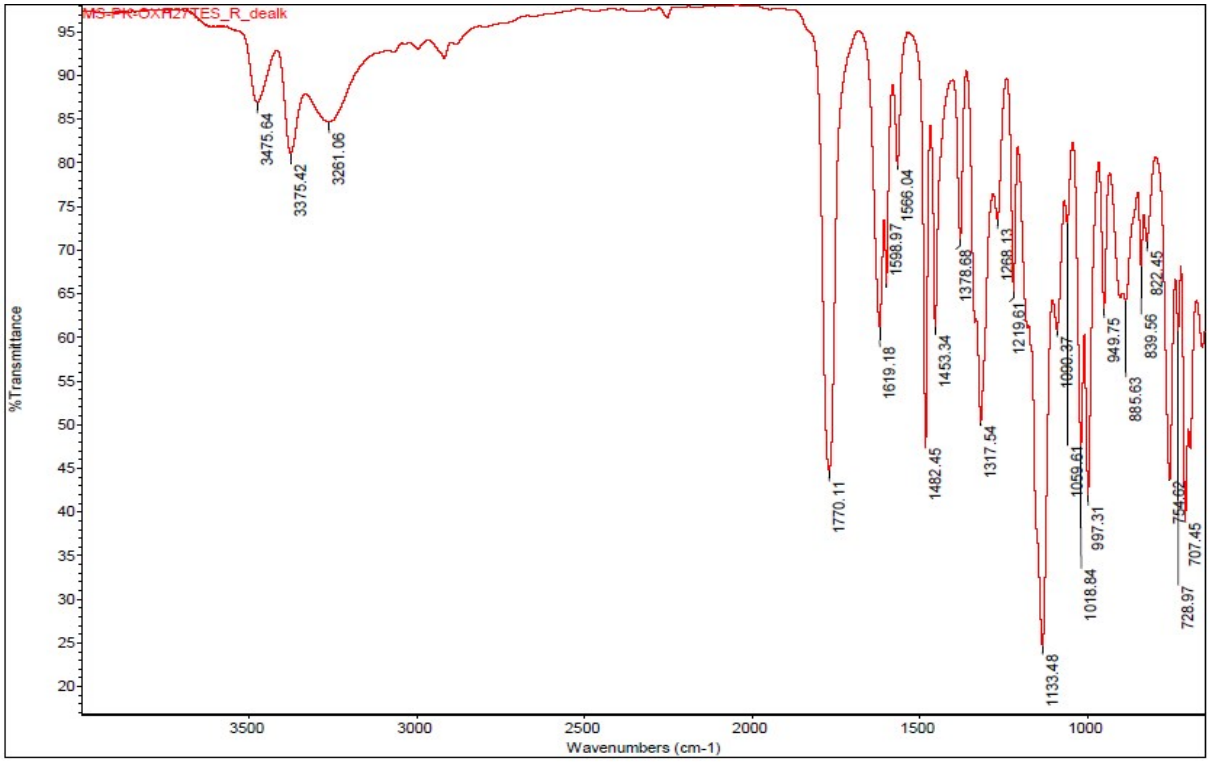


Figure S91. IR spectrum of **10r**

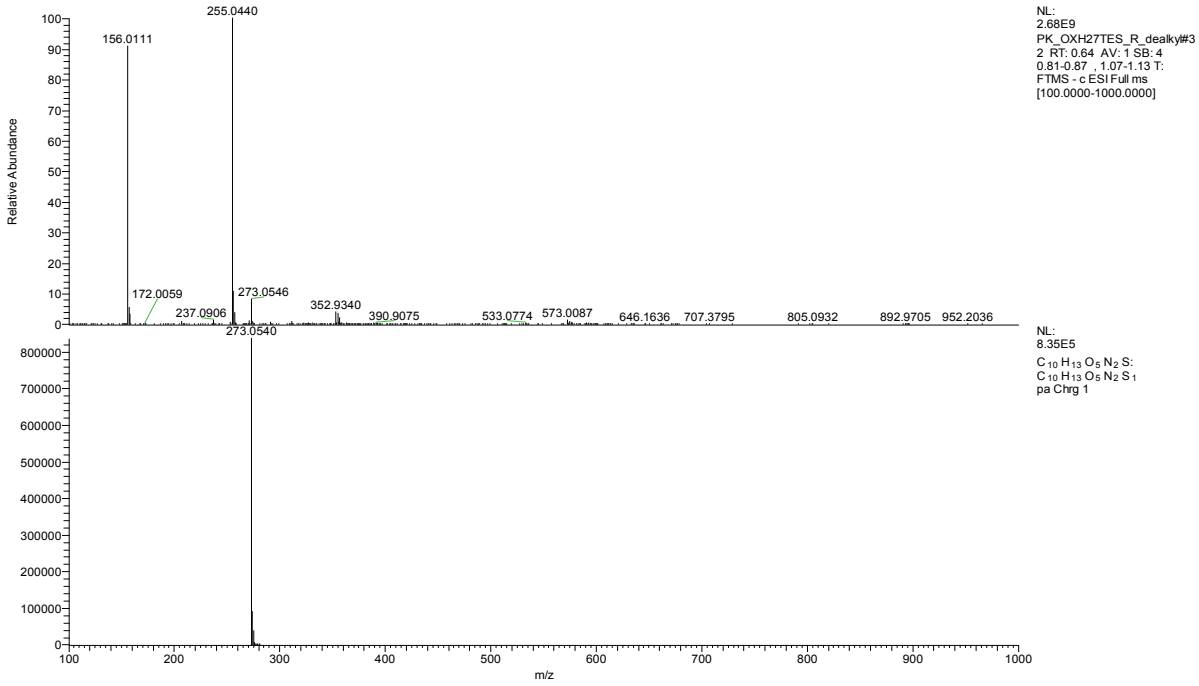
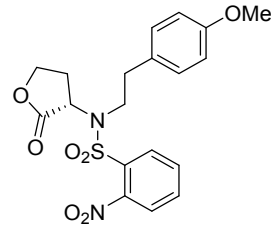


Figure S92. HRMS spectrum of **10r**

(-)-(*S*)-*N*-(4-methoxyphenethyl)-2-nitro-*N*-(2-oxotetrahydrofuran-3-yl)benzenesulfonamide 11n



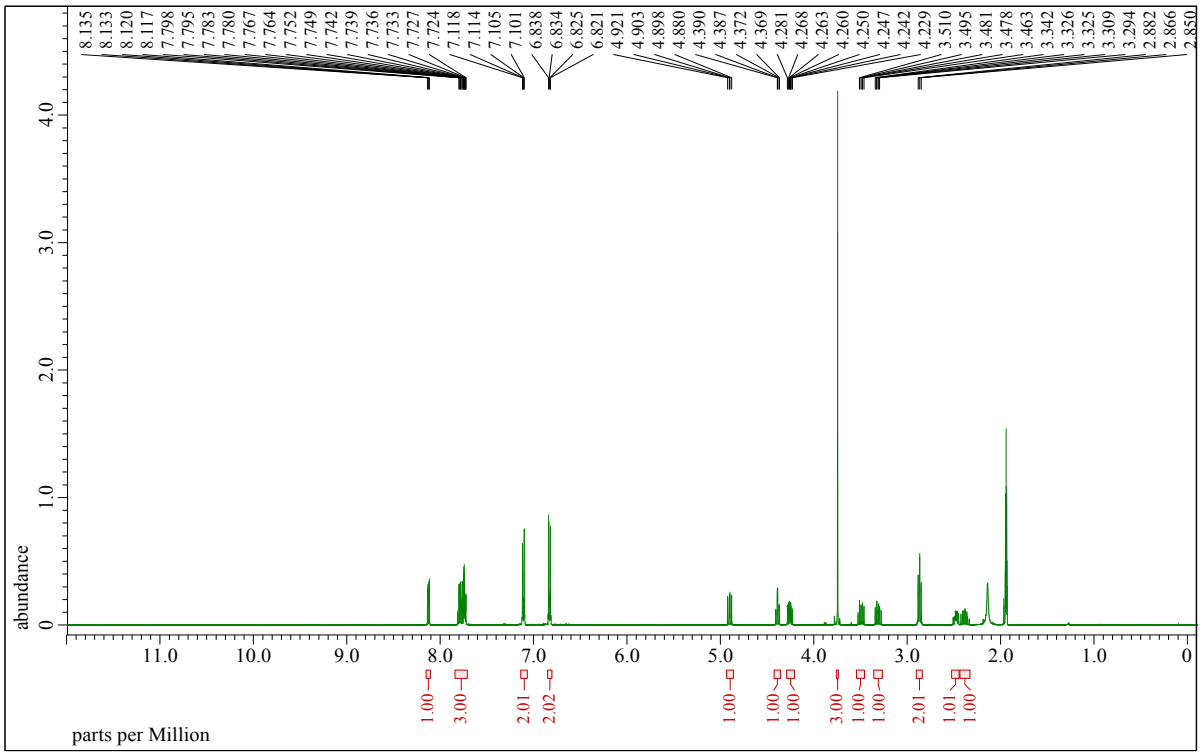


Figure S93. ^{1}H NMR spectrum of **11n** (500 MHz, MeCN-d_3)

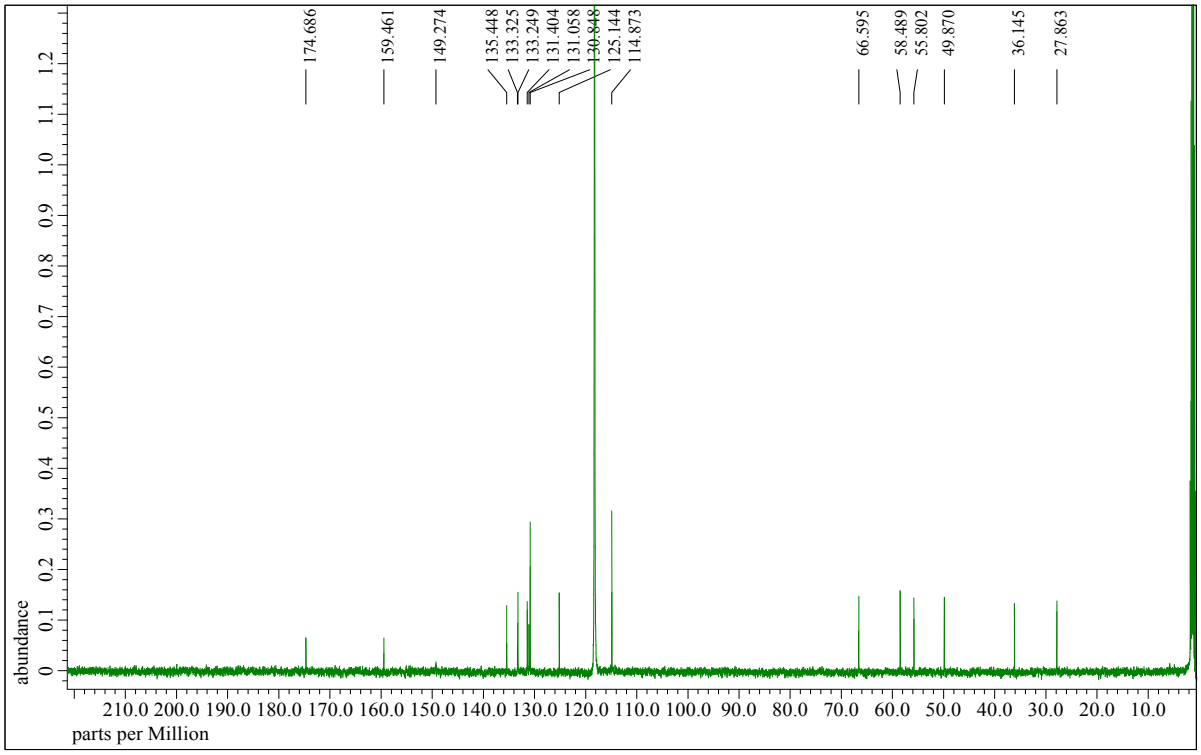


Figure S94. $^{13}C\{^{1}H\}$ NMR spectrum of **11n** (126 MHz, MeCN-d_3)

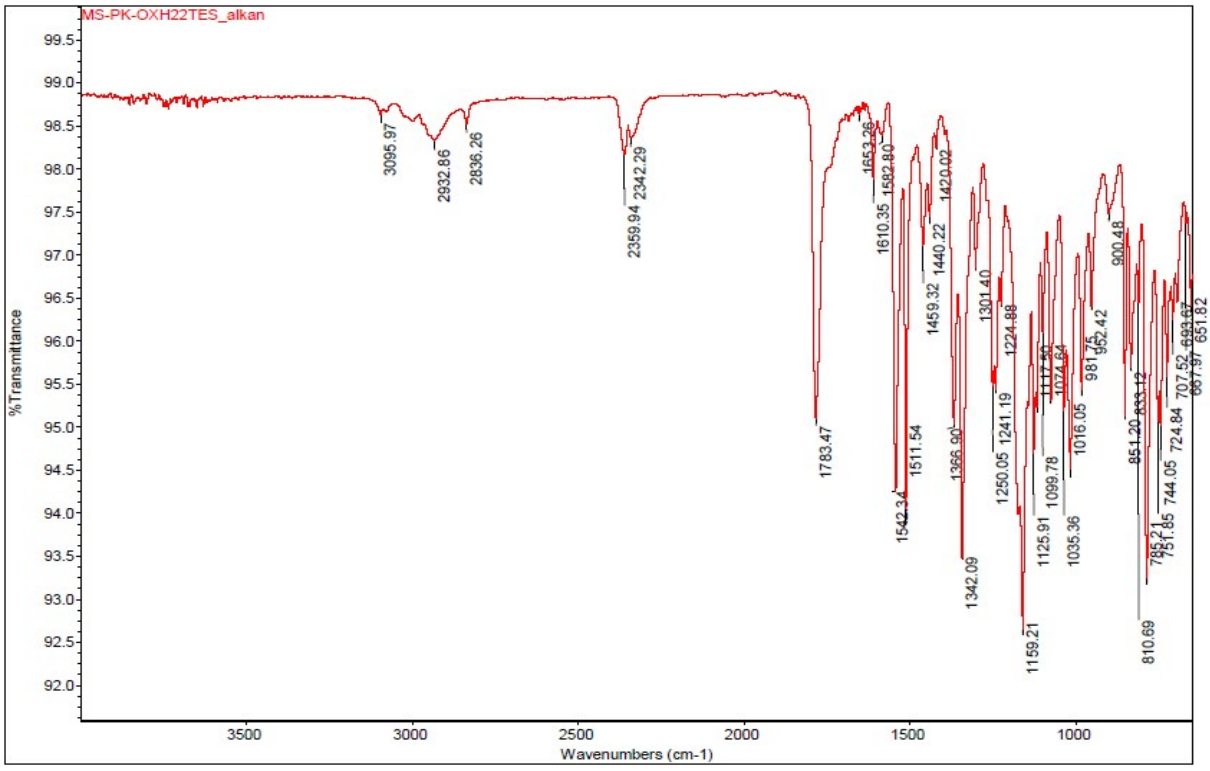


Figure S95. IR spectrum of **11n**

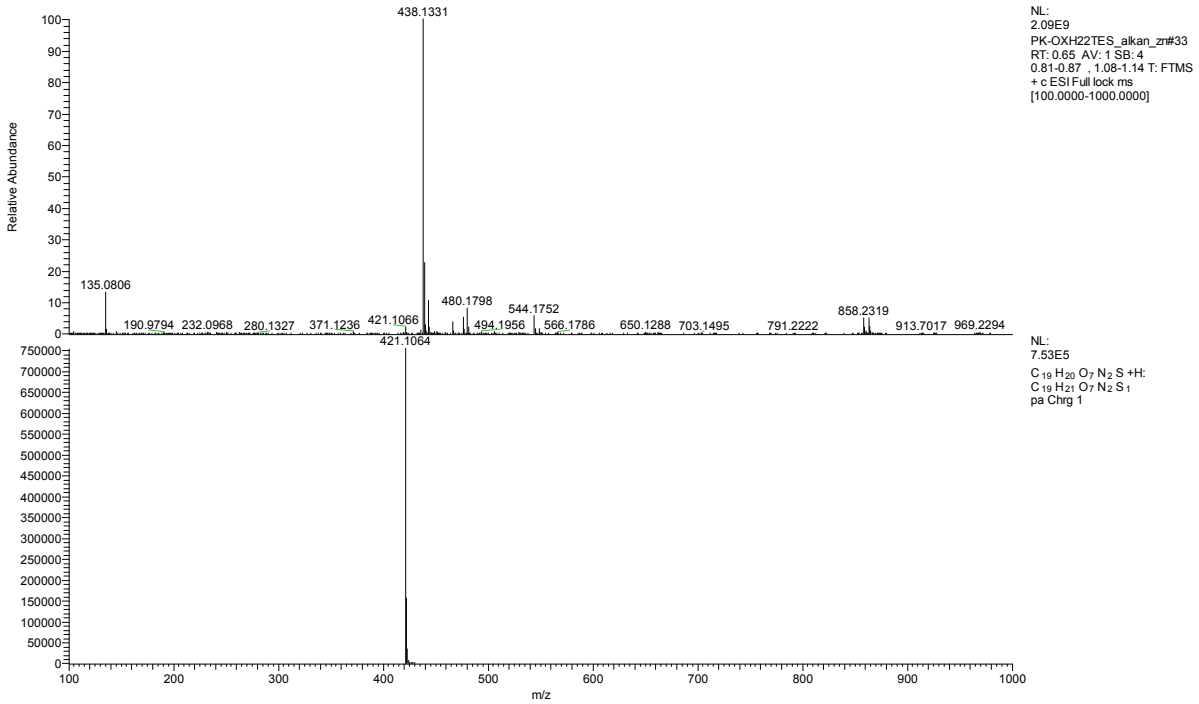


Figure S96. HRMS spectrum of **11n**. Note: ion 438 belongs to the ammonium adduct originating from mobile phase.