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J. Serb. Chem. Soc. 87 (10) S331–S353 (2022) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Synthesis of novel fluorinated 1,5-benzothiazepine derivatives and their biological evaluation as anticancer and antibacterial agents

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SPECTROSCOPIC DATA

*2-(3,4-difluorophenyl)-4-phenyl-2,3-dihydrobenzo[*b*][1,4]thiazepine (**4a**)*

Yellow solid, Yield: 91 %, M.P. = 145-147 °C, IR (υ_{max}/cm^{-1}): 2918 (C-H), 1605 (C=N), 1322 (C-N), 685 (C-S-C). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.04 (dd, *J*= 7.6, 1.7 Hz, 2H, Ar-H), 7.60 (dd, *J*= 7.7, 0.9 Hz, 1H, Ar-H), 7.49 (dt, *J*= 8.7, 4.3 Hz, 4H, Ar-H), 7.31 (dd, *J*= 7.9, 1.0 Hz, 1H, Ar-H), 7.21- 6.97 (m, 4H, Ar-H), 4.92 (dd, J_{ax}= 12.5, J_{ab}= 4.7 Hz, 1H, CH), 3.28 (dd, J_{bx}= 12.9, J_{ab}= 4.8 Hz, 1H, CH_2), 2.97 (t, J_{ab}= 12.7 Hz, 1H, CH_2). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 168.51, 152.39, 150.23 (dd, $^1J_{FC}$= 249.2, 12.8 Hz), 149.74 (dd, $^1J_{FC}$= 248.8, 12.5 Hz), 141.77- 139.95 (m), 137.49, 134.99, 131.25, 130.08, 128.83, 127.37, 125.48, 122.08 (t, *J* = 4.9 Hz), 117.43 (d, $^2J_{FC}$= 17.4 Hz), 115.25 (d, $^2J_{FC}$= 17.8 Hz), 59.28 (CH), 37.52 (CH_2). MS (ESI) *m/z*: 352.5 $(M+1)^+$. Elemental analysis for $C_{21}H_{15}F_2NS$: C, 71.78; H, 4.30; N, 3.99; S, 9.12; found: C, 71.65; H, 4.28; N, 3.82; S, 9.09.

*2-(3,4-difluorophenyl)-4-(p-tolyl)-2,3-dihydrobenzo[*b*][1,4]thiazepine (**4b**)*

Yellow solid, Yield: 93 %, M.P.= 157-159 °C, IR (υ_{max}/cm^{-1}): 2901 (C-H), 1604 (C=N),1319 (C-N), 684 (C-S-C). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.93 (d, J= 8.1 Hz, 2H, Ar-H), 7.58 (d, *J*= 7.6 Hz, 1H, Ar-H), 7.47 (t, *J*= 7.6 Hz, 1H, Ar-H), 7.29 (d, *J*= 8.0 Hz, 3H, Ar-H), 7.08 (ddd, *J*= 14.7, 11.3, 6.0 Hz, 4H, Ar-H), 4.89 (dd, J_{ax}= 12.5, J_{ab}= 4.7 Hz, 1H, CH), 3.26 (dd, J_{bx}= 12.9, J_{ab}= 4.8 Hz, 1H, CH_2), 2.95 (t, J_{ab}= 12.7 Hz, 1H, CH_2), 2.43 (s, 3H, CH_3). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 168.33, 152.52, 150.22 (dd, $^1J_{FC}$= 249.0, 12.8 Hz), 149.72 (dd, $^1J_{FC}$= 248.8, 12.6 Hz), 141.74, 141.12, 134.96, 134.74, 130.04, 129.55, 127.37, 125.38 (d, $^3J_{FC}$= 9.7 Hz), 122.07 (t, *J*= 4.8 Hz), 117.40 (d, $^2J_{FC}$=17.5 Hz), 115.24 (d, $^2J_{FC}$=17.7 Hz), 59.24 (CH), 37.42 (CH_2), 21.47 (CH_3). MS (ESI) *m/z*: 366.5 $(M+1)^+$. Elemental analysis for $C_{22}H_{17}F_2NS$: C, 72.31; H, 4.69; N, 3.83; S, 8.77; found: C, 72.20; H, 4.54; N, 3.63; S, 8.68.

*4-(4-chlorophenyl)-2-(3,4-difluorophenyl)-2,3-dihydrobenzo[*b*][1,4]thiazepine (**4c**)*

Yellow solid, Yield: 90 %, M.P. = 149-151 °C, IR (υ_{max}/cm^{-1}): 2902 (C-H), 1605 (C=N), 1321 (C-N), 685 (C-S-C). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.96 (d, *J*= 8.7 Hz, 2H, Ar-H),

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7.59 (dd, *J*= 7.7, 1.2 Hz, 1H, Ar-H), 7.53-7.40 (m, 3H, Ar-H), 7.29 (dd, *J*= 7.9, 1.2 Hz, 1H, Ar-H), 7.22- 6.93 (m, 4H, Ar-H), 4.89 (dd, J_{ax}= 12.4, J_{ab}= 4.8 Hz, 1H, CH), 3.22 (dd, J_{bx}= 13.0, J_{ab}= 4.9 Hz, 1H, CH_2), 2.96 (t, J_{ab}= 12.7 Hz, 1H, CH_2). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 167.26, 152.16, 150.23 (dd, $^1J_{FC}$= 249.0, 12.8 Hz), 149.77 (dd, $^1J_{FC}$=248.9, 12.7 Hz), 141.30-140.18 (m), 137.48, 135.90, 135.03, 130.15, 129.03, 128.69, 125.57 (d, J= 16.1 Hz), 122.07 (dd, *J*= 6.0, 3.2 Hz), 117.48 (d, $^2J_{FC}$= 17.4 Hz), 115.23 (d, $^2J_{FC}$= 17.8 Hz), 59.27 (CH), 37.36 (CH_2). MS (ESI) *m/z*: 385.7 $(M)^+$. Elemental analysis for $C_{21}H_{14}ClF_2NS$: C, 65.37; H, 3.66; N, 3.63; S, 8.31; found: C, 65.29; H, 3.58; N, 3.50; S, 8.23.

*2-(3,4-difluorophenyl)-4-(4-fluorophenyl)-2,3-dihydrobenzo[*b*][1,4]thiazepine (**4d**)*

Yellow solid, Yield: 89 %, M.P. = 143-145 °C, IR (υ_{max}/cm^{-1}): 2905 (C-H), 1601 (C=N), 1311 (C-N), 683 (C-S-C). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.12- 7.92 (m, 2H, Ar-H), 7.59 (d, *J*= 7.6 Hz, 1H, Ar-H), 7.48 (dd, *J*= 11.0, 4.3 Hz, 1H, Ar-H), 7.29 (d, *J*= 7.8 Hz, 1H, Ar-H), 7.22- 6.88 (m, 6H, Ar-H), 4.89 (dd, J_{ax}= 12.4, J_{ab}= 4.8 Hz, 1H, CH), 3.23 (dd, J_{bx}= 13.0, J_{ab}= 4.8 Hz, 1H, CH_2), 2.96 (t, J_{ab}= 12.7 Hz, 1H, CH_2). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 167.21, 164.76 (d, $^1J_{FC}$= 252.3 Hz), 152.25, 150.23 (dd, $^1J_{FC}$= 249.3, 12.8 Hz), 149.76 (dd, $^1J_{FC}$= 248.9, 12.7 Hz), 141.87- 139.82 (m), 135.01, 133.71 (d, *J*= 3.1 Hz), 130.14, 129.55 (d, $^3J_{FC}$= 8.7 Hz), 125.50 (d,$^3J_{FC}$=8.6 Hz), 122.08 (dd, *J*= 7.2, 4.5 Hz), 117.46 (d, $^2J_{FC}$=17.3 Hz), 115.84 (d, *J*= 21.8 Hz), 115.25 (d, $^2J_{FC}$= 17.8 Hz), 59.21 (CH), 37.42 (CH_2). MS (ESI) *m/z*: 370.4 (M+1) $^+$. Elemental analysis for $C_{21}H_{14}F_3NS$: C, 68.28; H, 3.82; N, 3.79; S, 8.68; found: C, 68.20; H, 3.75; N, 3.70; S, 8.52.

*4-(4-bromophenyl)-2-(3,4-difluorophenyl)-2,3-dihydrobenzo[*b*][1,4]thiazepine (**4e**)*

Yellow solid, Yield: 90 %, M.P. = 164-166 °C, IR (υ_{max}/cm^{-1}): 2901 (C-H), 1604 (C=N),1320 (C-N), 684 (C-S-C). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.89 (d, *J*= 8.3 Hz, 2H, Ar-H), 7.66-7.54 (m, 3H, Ar-H), 7.48 (t, *J*= 7.6 Hz, 1H, Ar-H), 7.29 (d, *J*= 7.8 Hz, 1H, Ar-H), 7.21-6.91 (m, 4H, Ar-H), 4.88 (dd, J_{ax}= 12.4, J_{ab}= 4.6 Hz, 1H, CH), 3.21 (dd, J_{bx}= 13.0, J_{ab}= 4.8 Hz, 1H, CH_2), 2.95 (t, J_{ab}= 12.7 Hz, 1H, CH_2). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 167.27, 152.24, 150.28 (dd, $^1J_{FC}$= 248.9, 12.6 Hz), 149.82 (dd, $^1J_{FC}$= 248.5, 12.7 Hz), 140.75, 136.50, 134.97, 131.98, 130.08, 128.88, 125.92, 125.53 (d, $^3J_{FC}$=11.1 Hz), 122.09, 117.44 (d, $^2J_{FC}$= 17.2 Hz), 115.26 (d, $^2J_{FC}$=17.9 Hz), 59.33 (CH), 37.31 (CH_2). MS (ESI) *m/z:* 430.2 $(M+1)^+$. Elemental analysis for $C_{21}H_{14}BrF_2NS$: C, 58.62; H, 3.28; N, 3.26; S, 7.45; found: C, 58.40; H, 3.25; N, 3.08; S, 7.30.

*2-(3,4-*difluorophenyl*)-4-(4-methoxyphenyl)-2,3-dihydro benzo[*b*][1,4]thiazepine (**4f**)*

Yellow solid, Yield: 92 %, M. P.= 137-139 ºC, IR (υ_{max}/cm^{-1}): 2844 (C-H), 1595 (C=N), 1322 (C-N), 684 (C-S-C). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.00 (d, *J*= 8.9 Hz, 2H, Ar-H), 7.58 (dd, *J*= 7.7, 1.2 Hz, 1H, Ar-H), 7.47 (td, *J*= 7.8, 1.4 Hz, 1H, Ar-H), 7.29 (dd, *J*= 7.9, 1.2 Hz, 1H, Ar-H), 7.20- 7.06 (m, 3H, Ar-H), 7.06- 6.94 (m, 3H, Ar-H), 4.89 (dd, J_{ax}= 12.4, J_{ab}= 4.7 Hz, 1H, CH), 3.87 (d, *J*= 6.6 Hz, 3H, OCH_3), 3.25 (dd, J_{bx}= 12.9, J_{ab}= 4.8 Hz, 1H, CH_2), 2.95 (t, J_{ab}= 12.7 Hz, 1H, CH_2). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 167.65, 162.22, 152.64, 150.23 (dd, $^1J_{FC}$= 251.1, 10.9 Hz), 149.71 (dd, $^1J_{FC}$= 248.7, 12.7 Hz), 141.15 (d, $^4J_{FC}$= 4.3 Hz), 141.09 (d, $^4J_{FC}$= 4.6 Hz), 134.95, 130.05, 129.13, 125.43, 125.16, 122.12 (d, $^3J_{FC}$= 9.5 Hz), 122.04, 117.41 (d, $^2J_{FC}$= 17.1 Hz), 115.25 (d, $^2J_{FC}$= 17.7 Hz), 114.14, 59.18 (CH), 55.47 (OCH_3), 37.26 (CH_2).MS (ESI) *m/z*: 382.8 (M+1) $^+$. Elemental analysis for $C_{22}H_{17}F_2NOS$: C, 69.27; H, 4.49; N, 3.67; S, 8.40; found: C, 69.15; H, 4.33; N, 3.59; S, 8.37.

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*2-(3,4-difluorophenyl)-4-(furan-2-yl)-2,3-dihydrobenzo[*b*][1,4]thiazepine (**4g**)*

Yellow solid, Yield: 88 %, M.P. = 125-127 °C, IR (υ_{max}/cm^{-1}): 3105 (C-H), 1605 (C=N), 1319 (C-N), 681 (C-S-C). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.66-7.57 (m, 2H, Ar-H), 7.54-7.43 (m, 1H, Ar-H), 7.37-7.30 (m, 1H, Ar-H), 7.22- 6.99 (m, 5H, Ar-H), 6.68- 6.50 (m, 1H, Ar-H), 4.96 (dd, J_{ax}= 11.8, J_{ab}= 5.1 Hz, 1H, CH), 3.19 (dd, J_{bx}= 12.9, J_{ab}= 5.1 Hz, 1H, CH_2), 2.88 (t, J_{ab}= 12.4 Hz, 1H, CH_2). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 159.26, 152.45, 150.29 (d, $^1J_{FC}$= 249.2 Hz), 149.71 (dd, $^1J_{FC}$= 248.7, 12.7 Hz), 145.75, 140.80, 135.04, 130.14, 125.74 (d, J= 23.6 Hz), 122.64, 122.20 (dd, J= 6.3, 3.6 Hz), 117.40 (d, $^2J_{FC}$= 17.3 Hz), 115.36 (d, $^2J_{FC}$= 17.9 Hz), 113.93, 112.48, 59.38 (CH), 37.52 (CH_2). MS (ESI) *m/z*: 342.1 $(M+1)^+$. Elemental analysis for $C_{19}H_{13}F_2NOS$: C, 66.85; H, 3.84; N, 4.10; S, 9.39; found: C, 66.82; H, 3.75; N, 4.06; S, 9.25.

*2-(3,4-difluorophenyl)-4-(thiophen-2-yl)-2,3-dihydrobenzo[*b*][1,4]thiazepine (**4h**)*

Yellow solid, Yield: 87 %, M.P. = 149-151 °C, IR (υ_{max}/cm^{-1}): 2917 (C-H), 1599 (C=N),1322 (C-N), 688 (C-S-C). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.66-7.53 (m, 2H, Ar-H), 7.53- 7.40 (m, 2H, Ar-H), 7.37-7.27 (m, 1H, Ar-H), 7.24-6.99 (m, 5H, Ar-H), 4.99 (dd, J_{ax}= 11.9, J_{ab}= 5.0 Hz, 1H, CH), 3.23 (dd, J_{bx}= 13.0, J_{ab}= 5.0 Hz, 1H, CH_2), 2.99 (t, J_{ab}= 12.5 Hz, 1H, CH_2). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 163.24, 151.53, 150.12 (d, $^1J_{FC}$= 242.5 Hz), 140.80, 134.96, 131.46, 130.10, 128.83, 127.91, 125.75, 125.57, 122.62, 122.12, 117.45 (d, $^2J_{FC}$= 17.4 Hz), 115.37 (d, $^2J_{FC}$= 17.9 Hz), 59.18 (CH), 38.46 (CH_2). MS (ESI) *m/z*: 359.7 $(M+2)^+$. Elemental analysis for $C_{19}H_{13}F_2NS_2$: C, 63.85; H, 3.67; N, 3.92; S, 17.94; found: C, 63.75; H, 3.56; N, 3.88; S, 17.81.

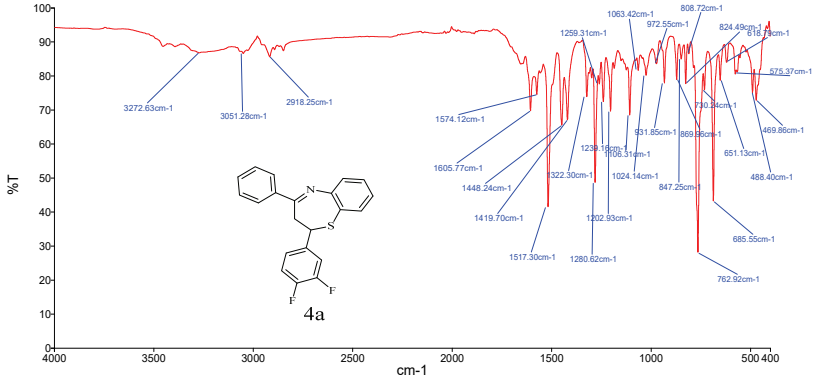

Fig. S-1. FTIR Spectrum of Compound **4a**

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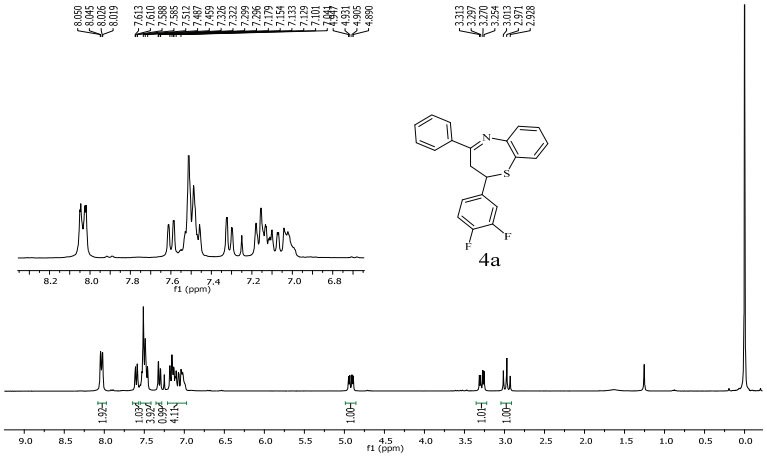

Fig. S-2. ^{1}H-NMR spectrum of compound **4a** (300 MHz, $CDCl_3$)

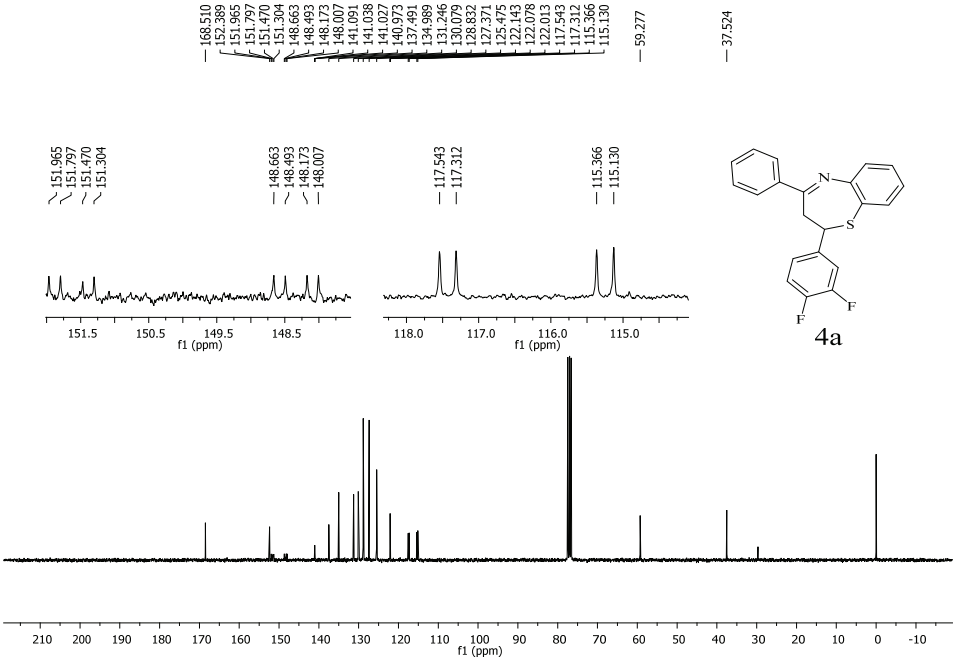

Fig. S-3. ^{13}C-NMR spectrum of compound **4a** (75 MHz, $CDCl_3$)

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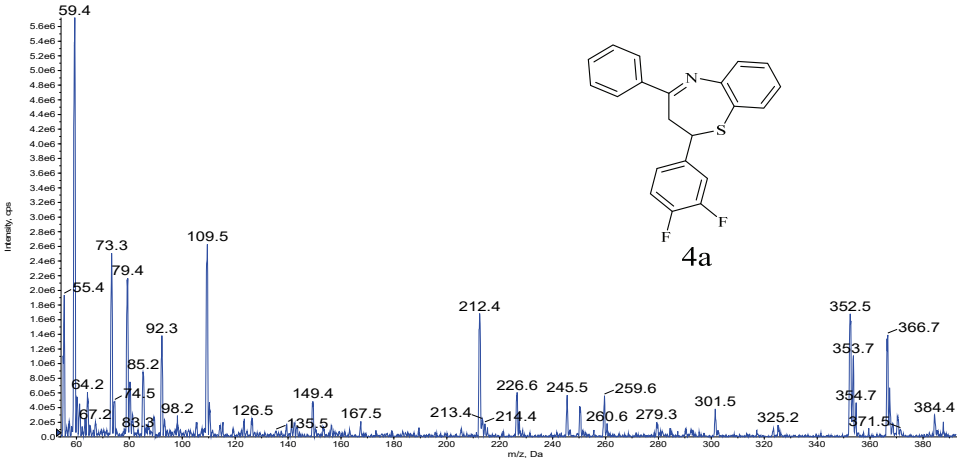

Fig. S-4. Mass spectrum of compound **4a**

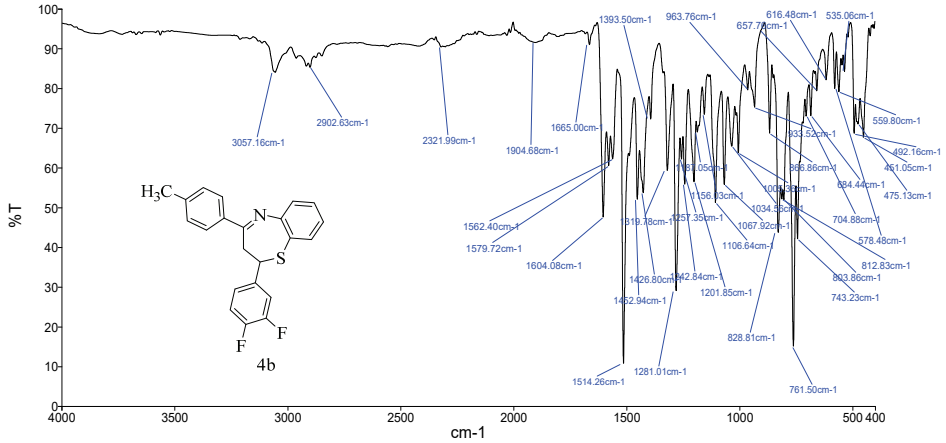

Fig. S-5. FTIR Spectrum of Compound **4b**

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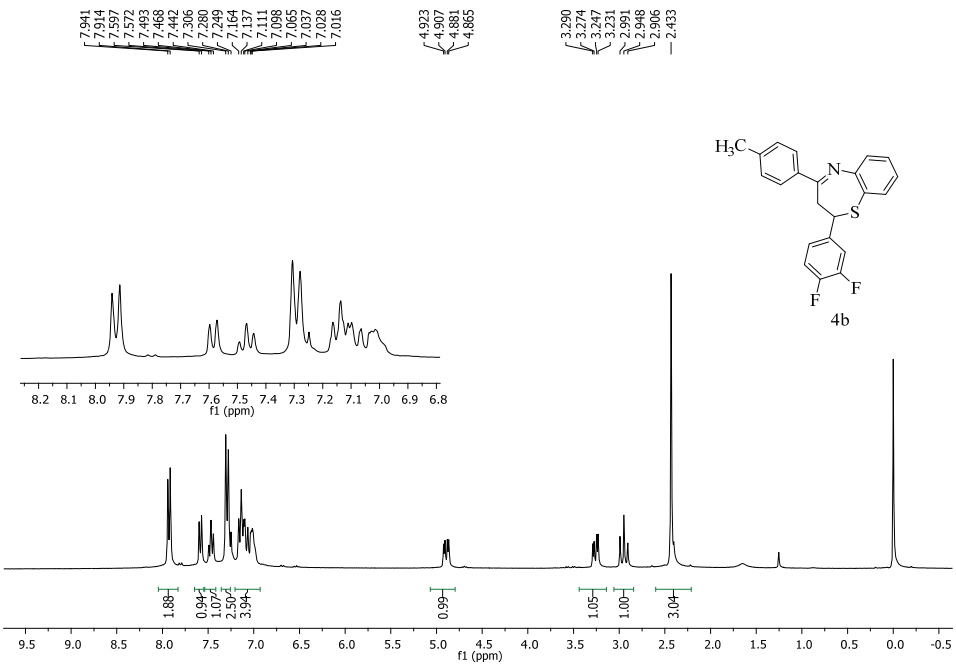

Fig. S-6. ^{1}H-NMR spectrum of compound **4b** (300 MHz, $CDCl_3$)

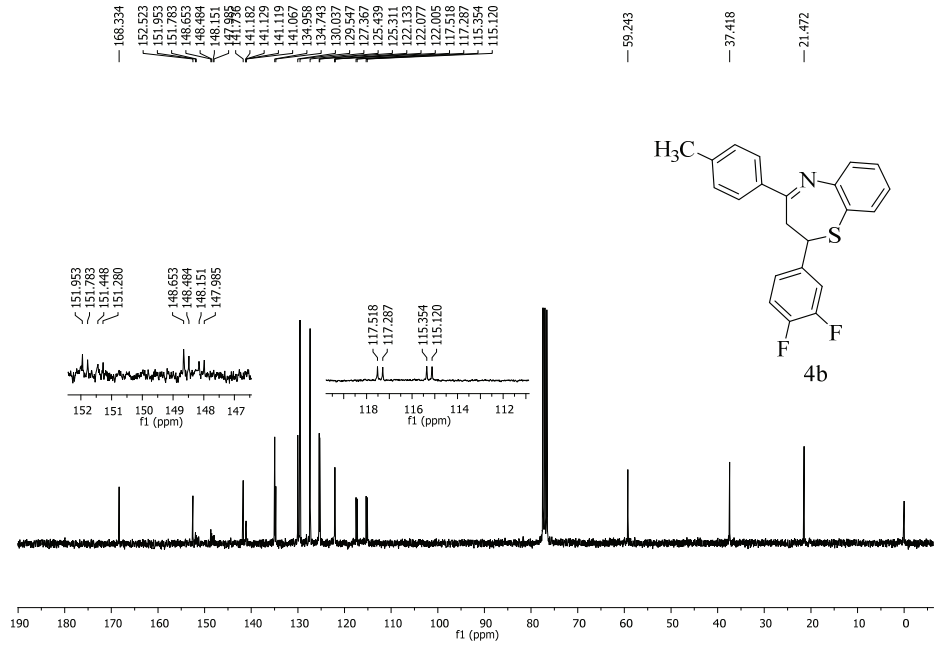

Fig. S-7. ^{13}C-NMR spectrum of compound **4b** (75 MHz, $CDCl_3$)

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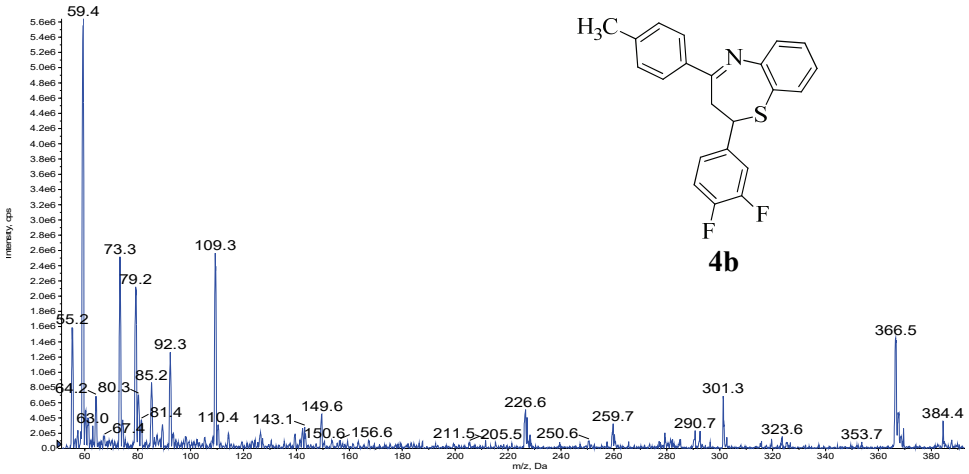

Fig. S-8. Mass spectrum of compound **4b**

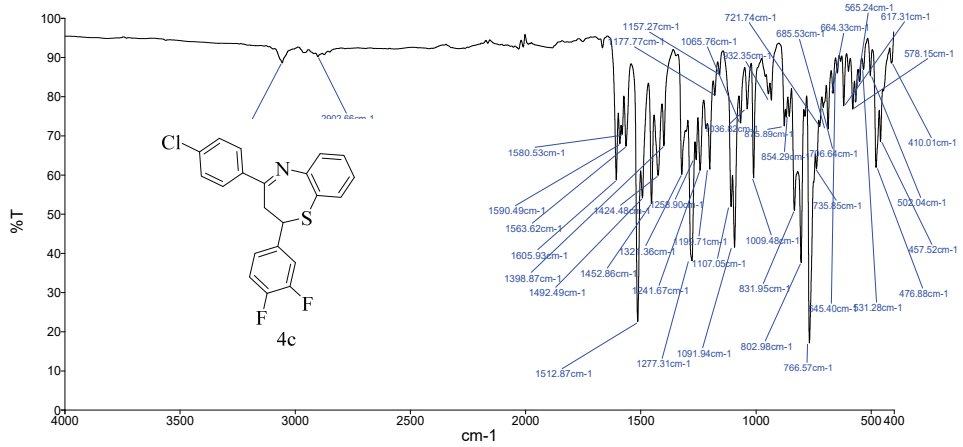

Fig. S-9. FTIR spectrum of compound **4c**

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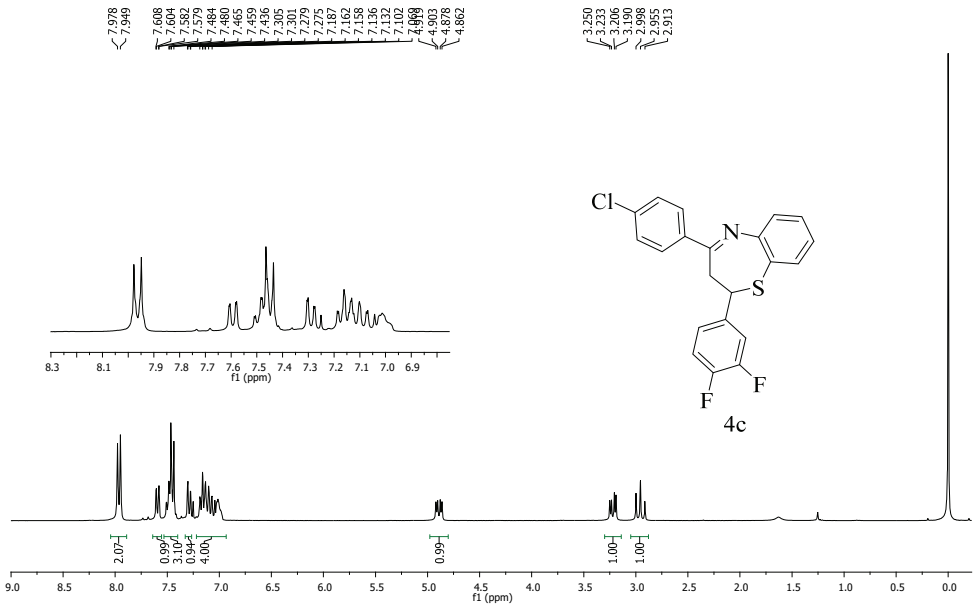

Fig. S-10. ^{1}H-NMR spectrum of compound **4c** (300 MHz, $CDCl_3$)

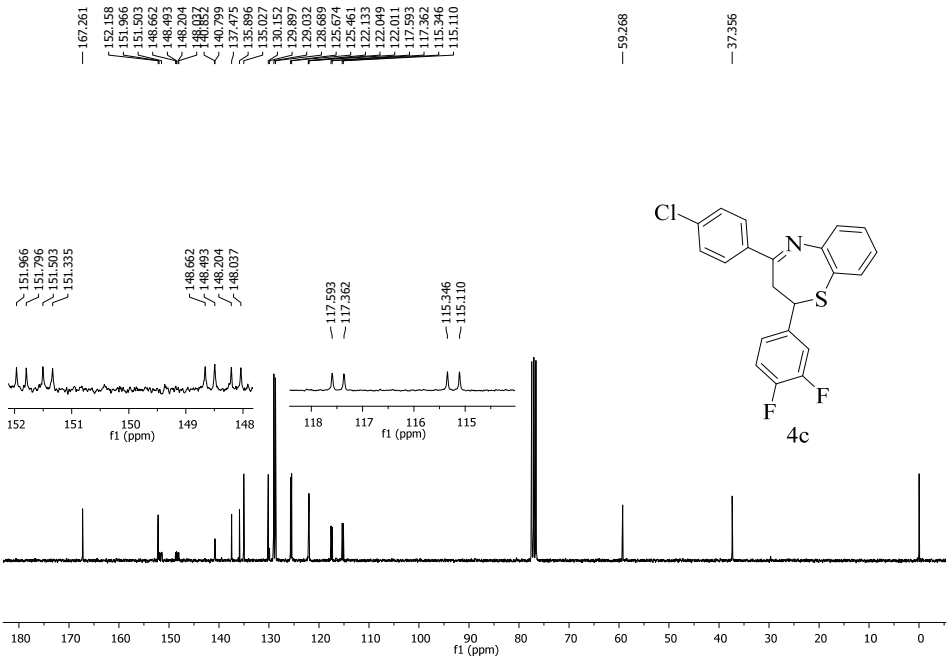

Fig. S-11. ^{13}C-NMR spectrum of compound **4c** (75 MHz, $CDCl_3$)

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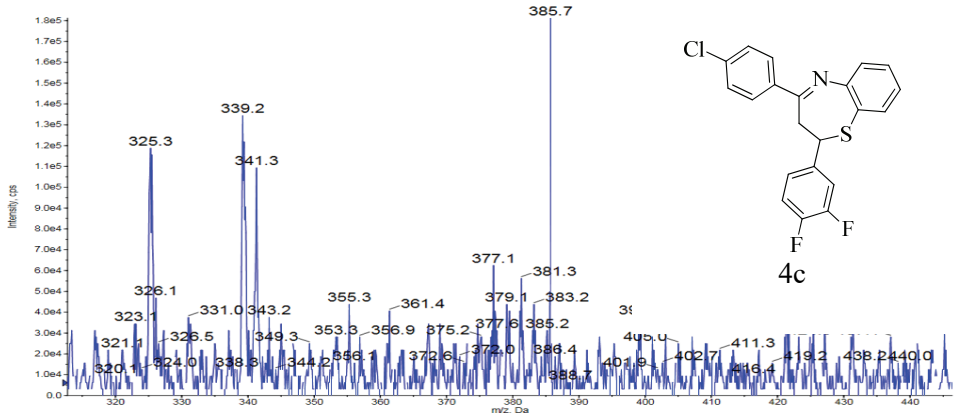

Fig. S-12. Mass spectrum of compound **4c**

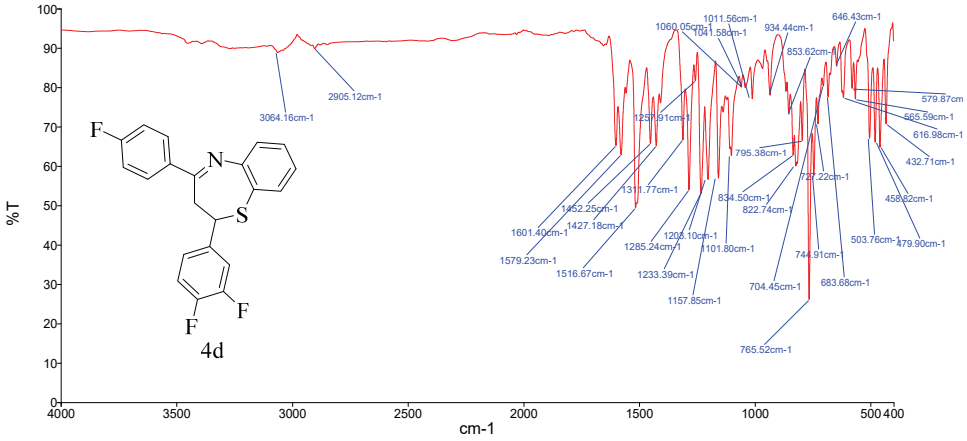

Fig. S-13. FTIR spectrum of Compound **4d**

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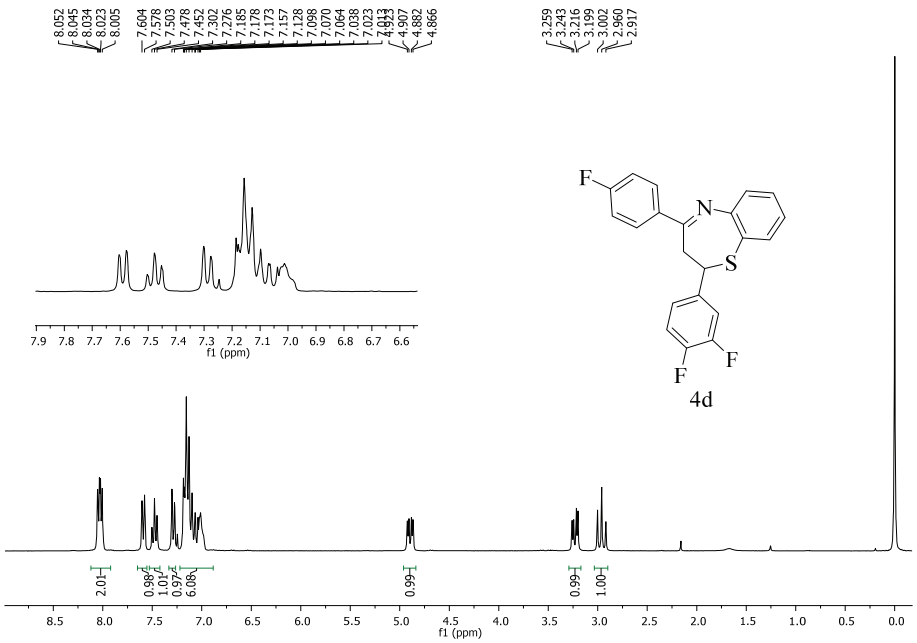

Fig. S-14. ^{1}H-NMR spectrum of compound 4d (300 MHz, $CDCl_3$)

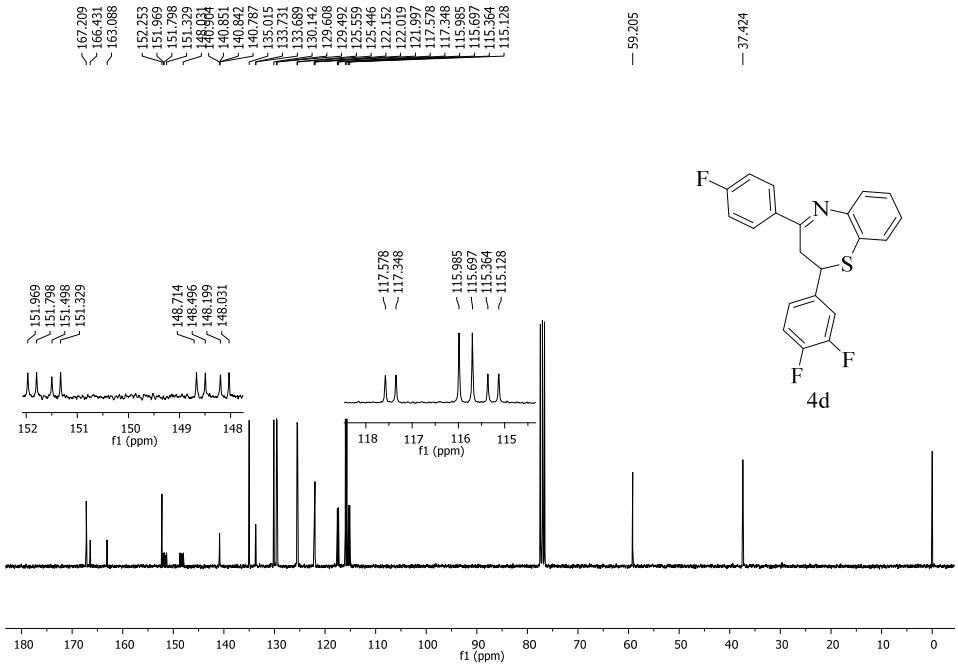

Fig. S-15. ^{13}C-NMR spectrum of compound **4d** (75 MHz, $CDCl_3$)

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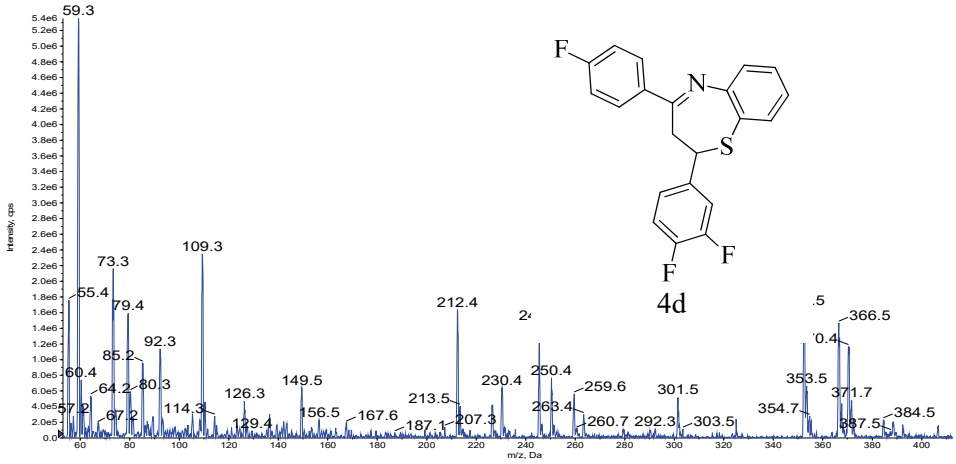

Fig. S-16. Mass spectrum of compound **4d**

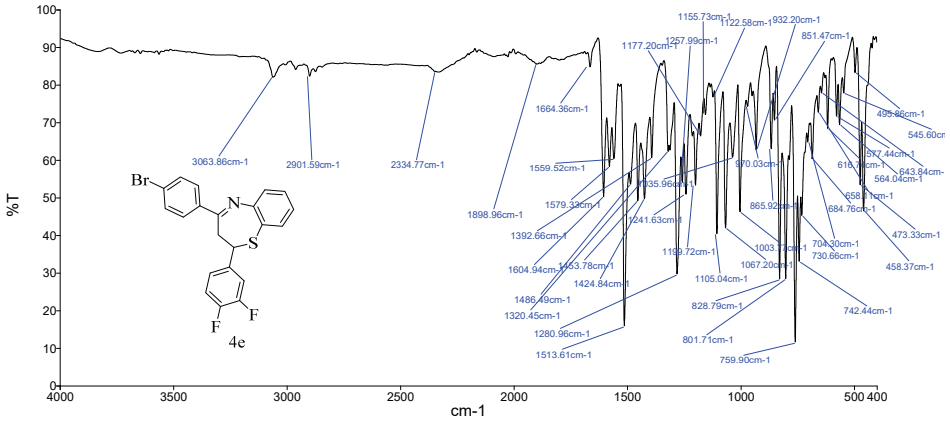

Fig. S-17. FTIR spectrum of compound **4e**

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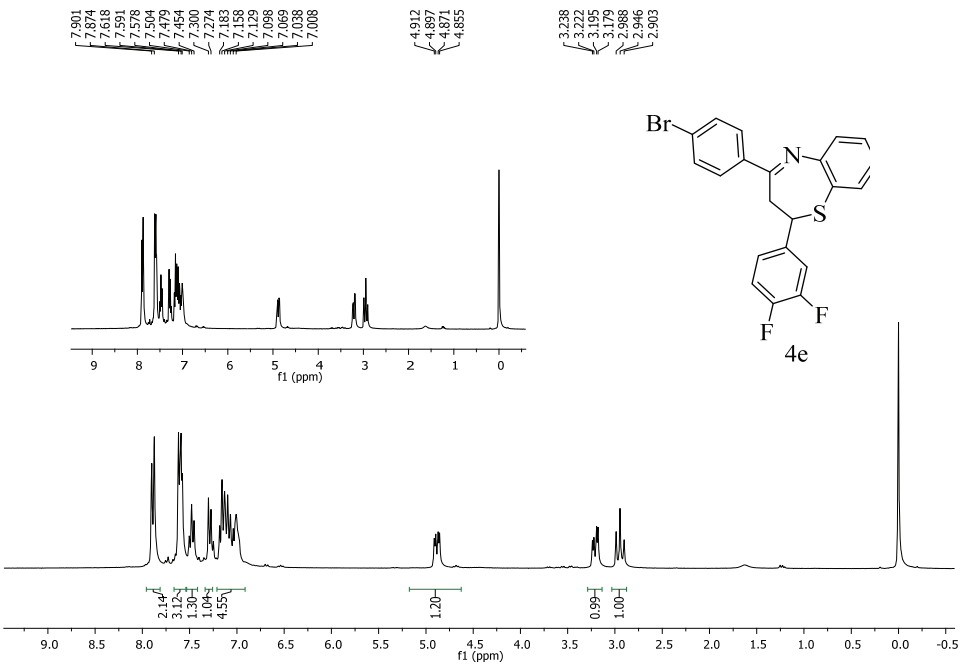

Fig. S-18. ^{1}H-NMR spectrum of compound **4e** (300 MHz, $CDCl_3$)

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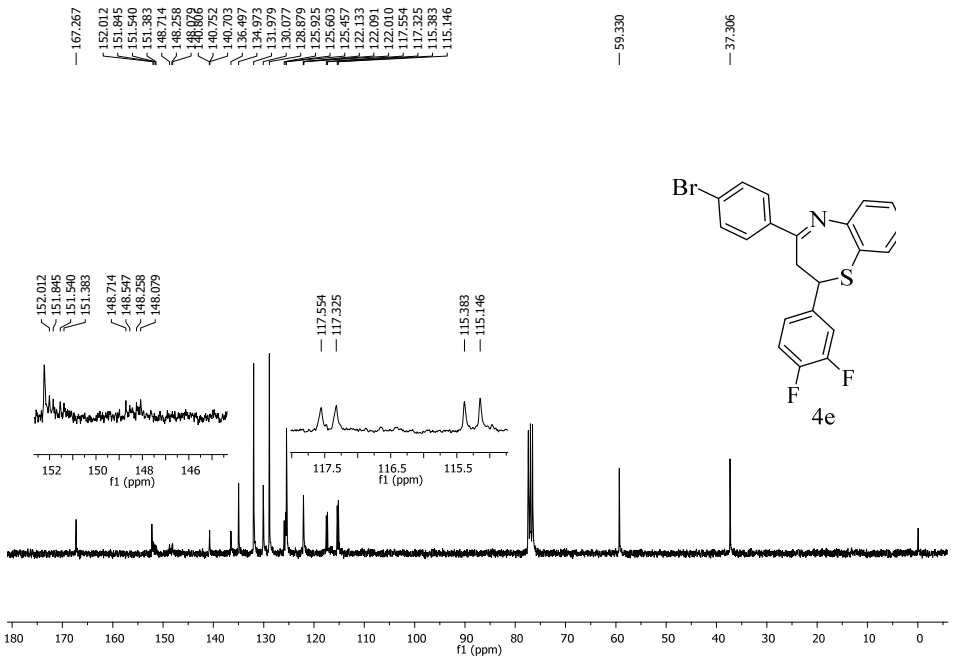

Fig. S-19. ^{13}C-NMR spectrum of compound 4e (75 MHz, $CDCl_3$)

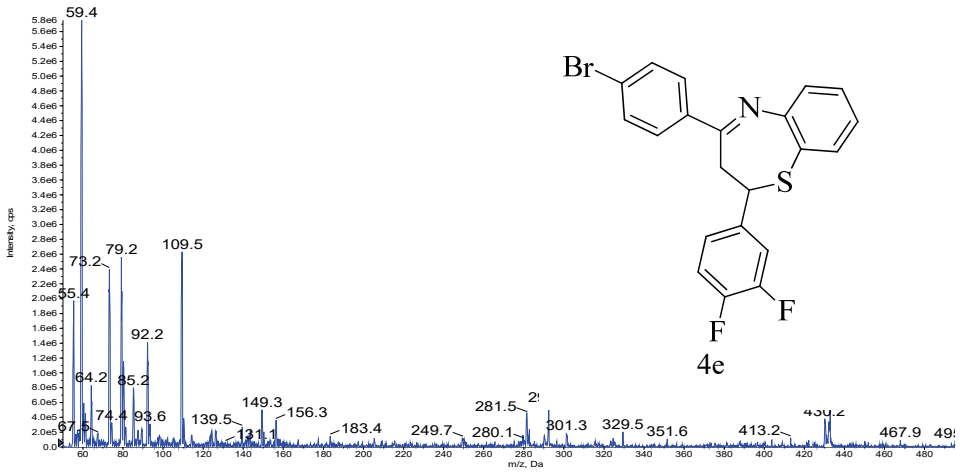

Fig. S-20. Mass spectrum of compound **4e**

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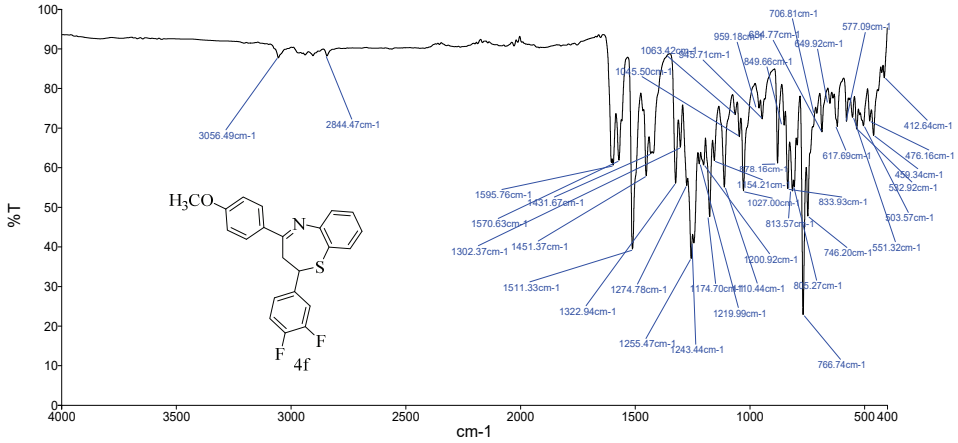

Fig. S-21. FTIR spectrum of compound 4f

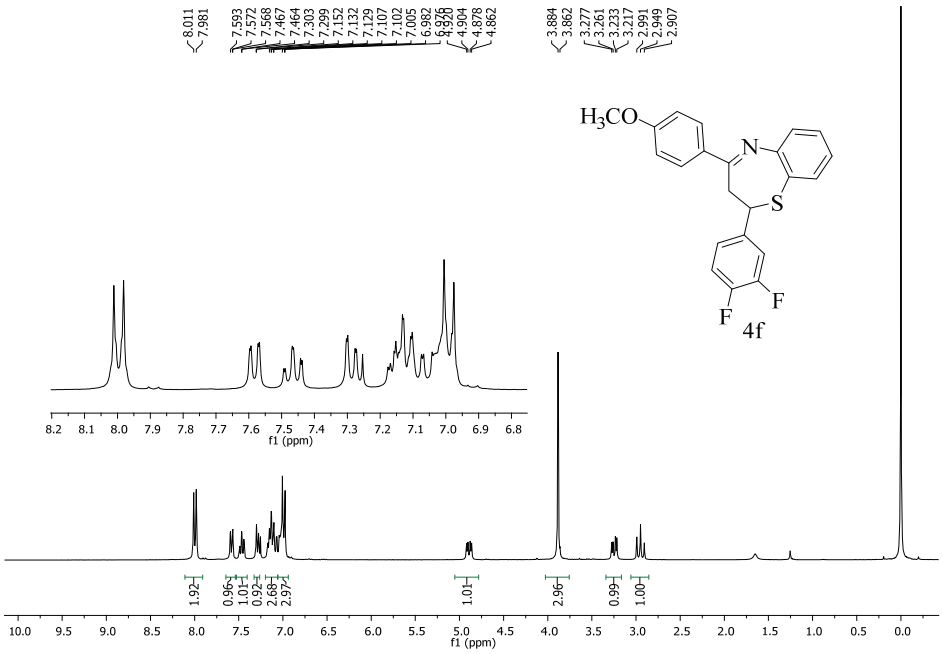

Fig. S-22. ^{1}H-NMR spectrum of compound **4f** (300 MHz, $CDCl_3$)

(CC) 2022 SCS.

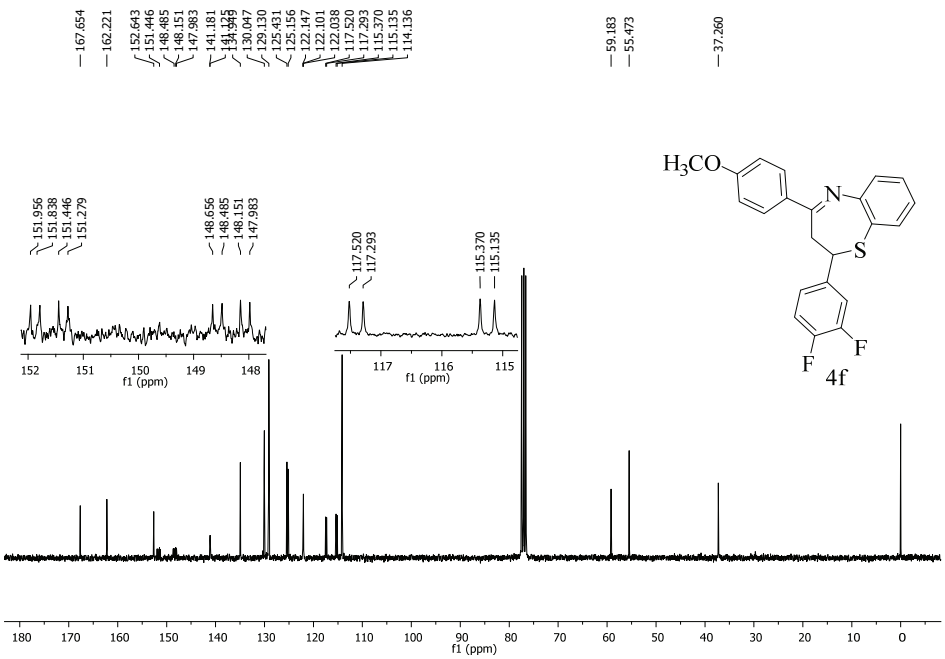

Fig. S-23. ^{13}C-NMR spectrum of compound **4f** (75 MHz, $CDCl_3$)

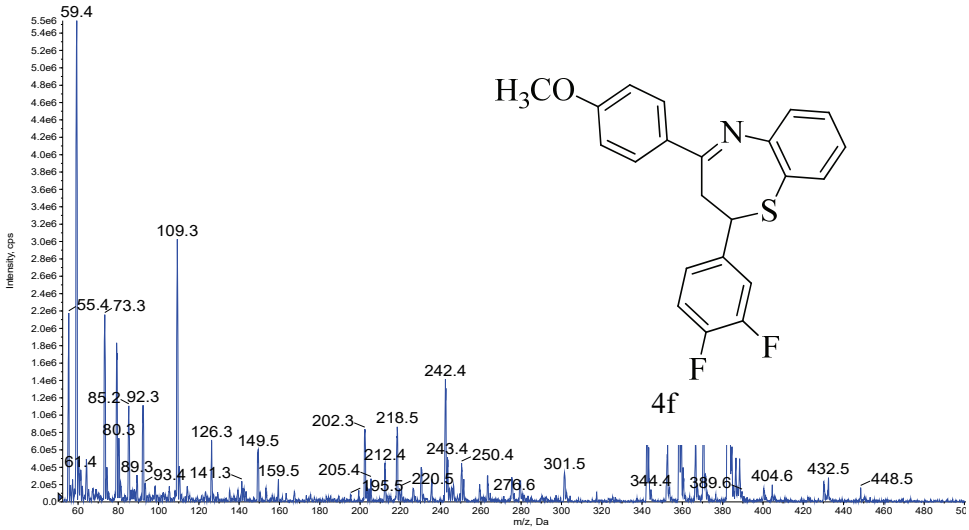

Fig. S-24. Mass spectrum of compound **4f**

(CC) 2022 SCS.

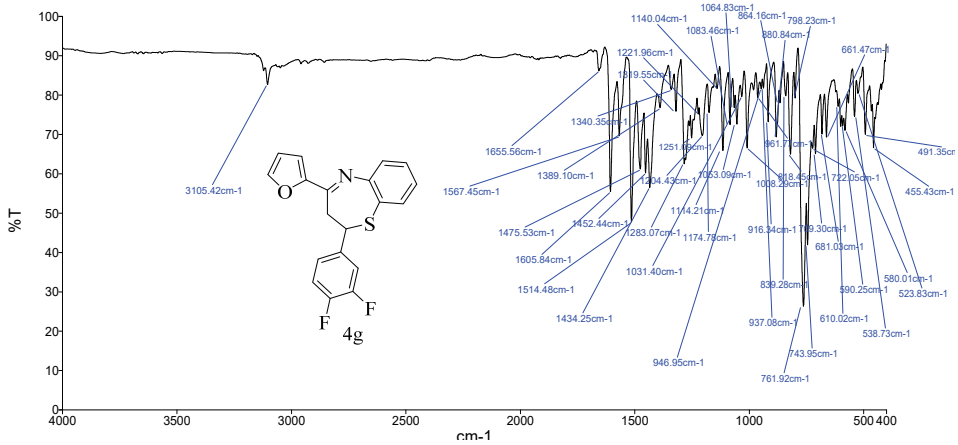

Fig. S-25. FTIR spectrum of compound **4g**

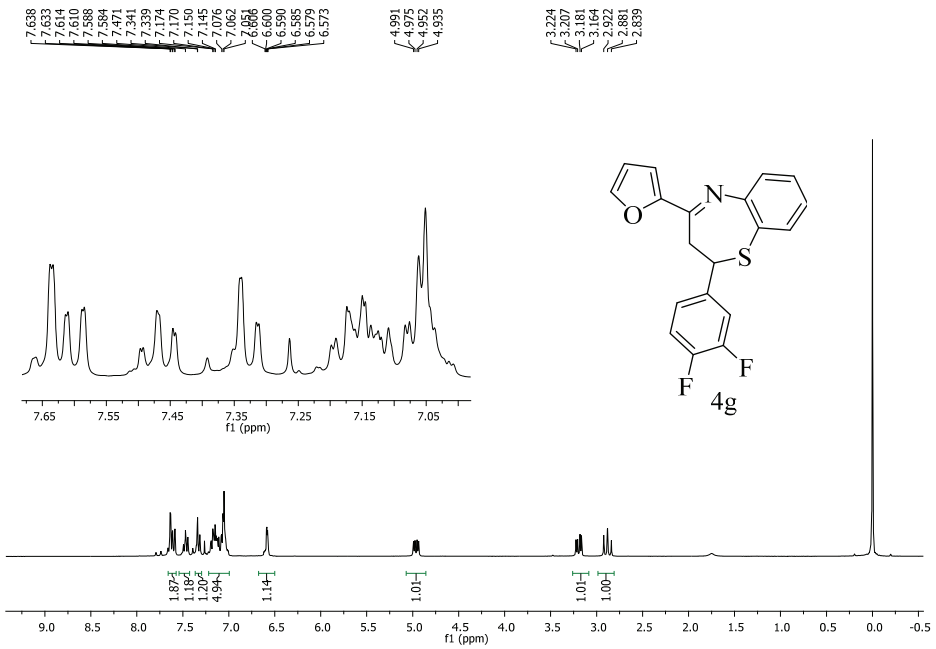

Fig. S-26. ^{1}H-NMR spectrum of compound **4g** (300 MHz, $CDCl_3$)

(CC) 2022 SCS.

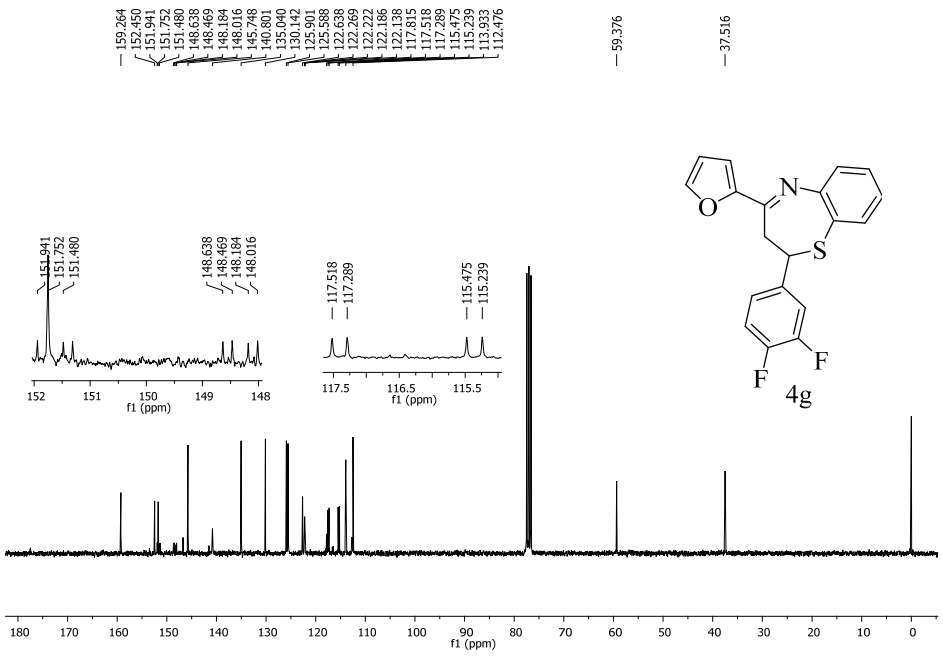

Fig. S-27. ^{13}C-NMR spectrum of compound **4g** (75 MHz, $CDCl_3$)

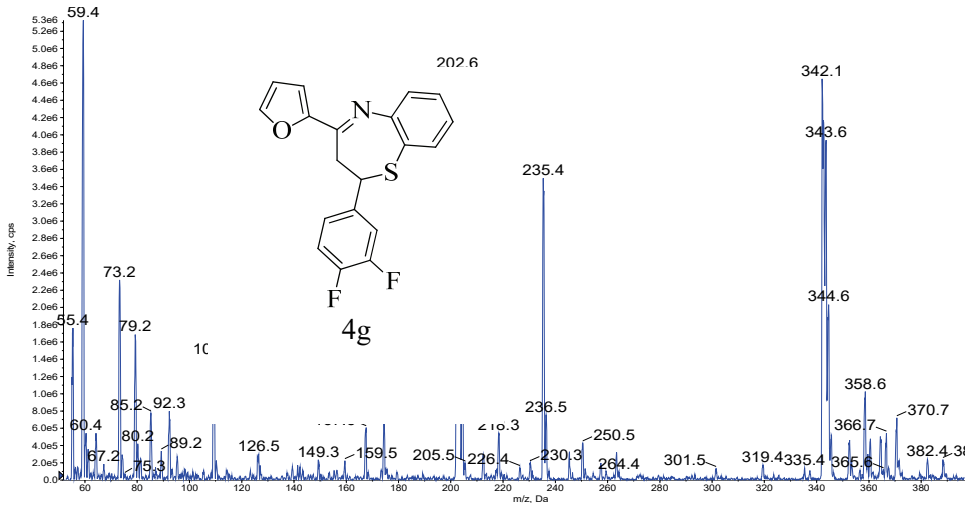

Fig. S-28. Mass spectrum of compound **4g**

(CC) 2022 SCS.

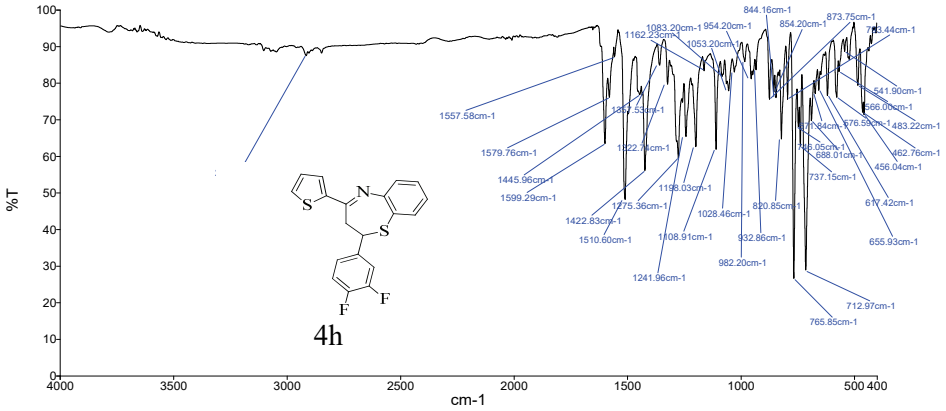

Fig. S-29. FTIR Spectrum of compound **4h**

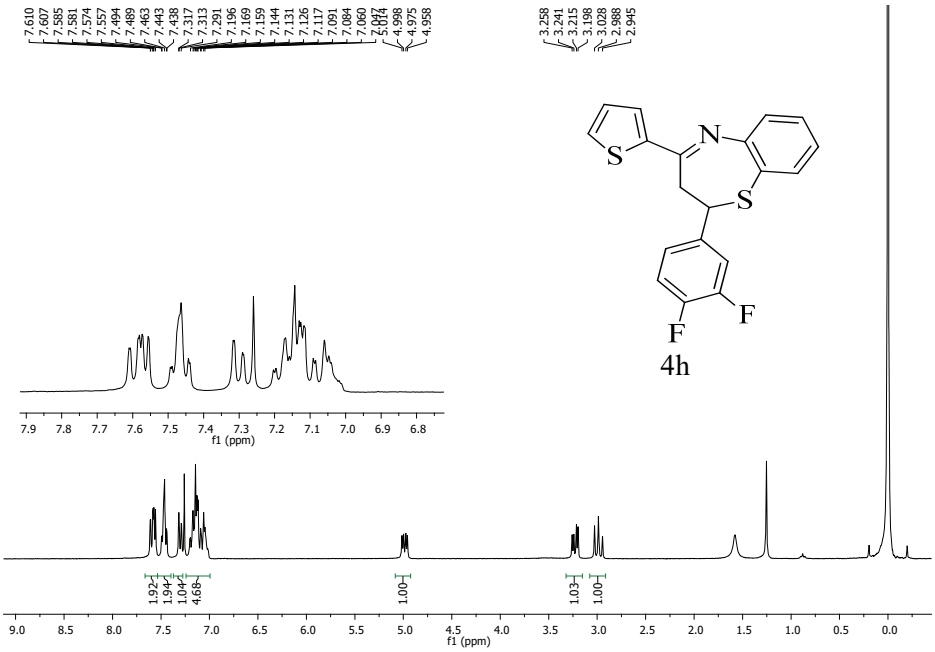

Fig. S-30. ^{1}H-NMR spectrum of compound **4h** (300 MHz, $CDCl_3$)

(CC) 2022 SCS.

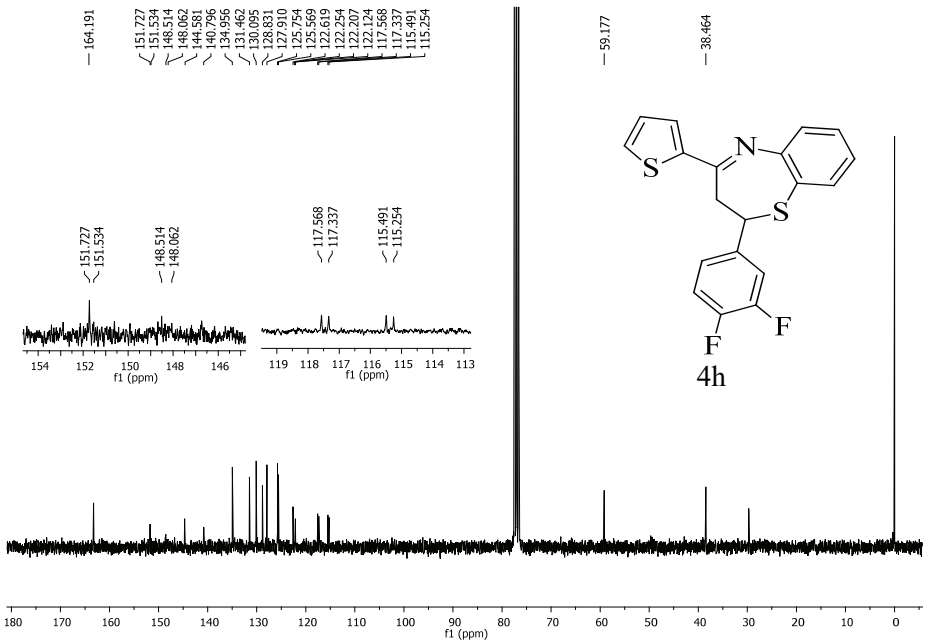

Fig. S-31. ^{13}C-NMR spectrum of compound **4h** (75 MHz, $CDCl_3$)

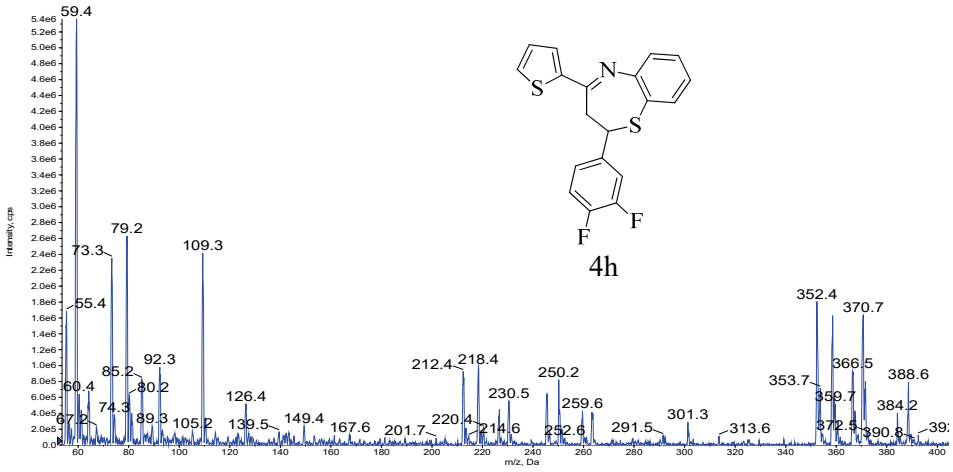

Fig. S-32. Mass spectrum of compound **4h**

(CC) 2022 SCS.

Anticancer activity

Table S-I. Control growth against human lung cancer cell line A549

Compound	Experiment 1				Experiment 2				Experiment 3			
	Control growth, %											
	10	20	40	80	10	20	40	80	10	20	40	80
	Drug concentration, μg ml^{-1}											
4a	79.8	69.7	54.9	28.2	89.9	80.8	72.7	35.1	96.7	91.9	85.1	46.2
4b	92.5	80.7	46.9	11.5	75.7	56.6	27.3	8.1	80.2	71.5	30.5	10.1
4c	59.7	24.6	3.6	-10.4	71.3	30.3	4.8	-18.1	84.4	41.1	9.3	-24.6
4d	51.2	18.3	1.7	-42.3	36.1	10.9	0.9	-30.7	24.6	9.5	3.1	-19.4
4e	72.5	52.2	48.5	1.6	65.4	37.1	33.7	1.2	81.4	67.9	58.2	0.5
4f	91.3	86.9	61.2	-12.2	87.5	78.6	55.1	-5.8	78.6	69.7	37.3	-1.5
4g	26.3	13.9	-11.2	-43	12.5	4.2	-3.5	-36	5.9	1.4	-1.2	-11
4h	40.1	24.4	15.8	-12.7	18.9	10.8	5.4	-5.8	10.3	6.2	2.5	-1.9
ADR	12.6	0.7	-16.9	-50	8.5	1.0	-12.3	-41	4.1	1.6	-6.2	-35

Table S-II. Average control growth against human lung cancer cell line A549

Compound	Average control growth, %				GI_{50} / μg ml^{-1}
	10	20	40	80	
	Drug concentration, μg ml^{-1}				
4a	88.8	80.8	70.9	36.5	69.23
4b	82.8	69.6	34.9	9.9	27.88
4c	71.8	32.0	5.9	-17.7	<10
4d	37.3	12.9	1.9	-30.8	<10
4e	73.1	52.4	46.8	1.1	22.07
4f	85.8	78.4	51.2	-6.5	32.33
4g	14.9	6.5	-5.3	-30	<10
4h	23.1	13.8	7.9	-6.8	<10
ADR	8.4	1.1	-11.8	-42	<10

Table S-III. Control growth against human breast cancer cell line MCF-7

Compound	Experiment 1				Experiment 2				Experiment 3			
	Control growth, %											
	10	20	40	80	10	20	40	80	10	20	40	80
	Drug concentration, μg ml^{-1}											
4a	109.9	91.1	70.1	55.8	95.7	82.6	58.6	42.3	89.9	70.5	46.2	30.6
4b	95.6	93.8	83.1	37.1	75.9	74.5	70.2	14.1	61.6	60.9	55.2	8.8
4c	60.7	26.3	11.5	-18.9	52.4	16.3	5.7	-11.1	24.9	6.9	2.3	-7.2
4d	49.8	18.9	-9.2	-56.2	25.1	11.9	-3.8	-41.1	11.2	7.6	-1.1	-35.6
4e	65.3	32.4	17.3	11.7	50.1	15.2	11.2	7.5	42.4	9.7	4.2	2.1
4f	82.5	70.2	64.5	51.5	62.2	55.4	50.1	42.2	50.9	42.1	36.3	30.5
4g	42.7	30.1	27.7	-15.2	29.5	16.4	14.5	-6.7	12.1	9.3	4.9	-2.4
4h	51.4	31.4	10.5	-41.2	42.6	19.9	4.3	-26.4	15.2	10.8	1.1	-14.6
ADR	14.3	1.6	-15.3	-43.4	8.3	1.1	-11.5	-29.1	5.3	0.9	-7.1	-17.8

(CC) 2022 SCS.

Table S-IV. Average control growth against human breast cancer cell line MCF-7

Compound	Average control growth, %				GI_{50}/μg ml^{-1}
	10	20	40	80	
	Drug concentration, μg ml^{-1}				
4a	98.5	81.4	58.3	42.9	68.59
4b	77.7	76.4	69.5	20	48.23
4c	46	16.5	6.5	-12.4	<10
4d	28.7	12.8	-4.7	-44.3	<10
4e	52.6	19.1	10.9	7.1	<10
4f	83.6	51.8	47.9	37.3	35.05
4g	28.1	18.6	15.7	-8.1	<10
4h	36.4	20.7	5.3	-27.4	<10
ADR	9.3	1.2	-11.3	-30.1	<10

Table S-V. Control growth against human liver cancer cell line HEPG2

Compound	Experiment 1				Experiment 2				Experiment 3			
	Control growth, %											
	10	20	40	80	10	20	40	80	10	20	40	80
	Drug concentration, μg ml^{-1}											
4a	95.4	88.3	70.7	49.3	87.3	79.1	56.9	41.1	76.2	64.5	45.8	30.2
4b	89.8	69.7	60.1	52.9	77.8	57.2	41.6	39.5	70.9	37.8	23.7	22.2
4c	69.1	46.5	20.3	-17.2	52.9	31.6	12.1	-10.2	45.7	24.2	5.4	-4.1
4d	30.6	16.2	-50.7	-48.1	20.1	6.7	-38.5	-34.8	16.5	3.8	-29.9	-14.9
4e	94.2	65.5	62.1	49.5	82.7	50.6	51.8	36.5	73.9	39.3	29.8	25.9
4f	79.6	70.2	46.2	-11.2	68.4	61.1	32.1	-8.6	57.5	31.6	14.1	-2.1
4g	59.2	40.4	21.9	-36.3	48.6	31.1	13.3	-27.8	34.4	19.7	8.9	-16.3
4h	21.8	9.1	-12.3	1.1	17.3	7.2	-10.1	0.7	10.1	2.3	-6.1	2.1
ADR	11.9	9.1	-5.3	-30.9	8.7	5.2	-3.2	-21.6	4.3	1.3	-1.4	-10.2

Table S-VI. Average control growth against human liver cancer cell line HEPG2

Compound	Average control growth, %				GI_{50}/μg ml^{-1}
	10	20	40	80	
	Drug concentration, μg ml^{-1}				
4a	86.3	77.3	57.8	40.2	57.69
4b	79.5	54.9	41.8	38.2	32.6
4c	55.9	34.1	12.6	-10.5	<10
4d	22.4	8.9	-39.7	-32.6	<10
4e	68.5	54.3	30.8	-7.3	16.98
4f	65.2	55.9	50.3	41.4	33.46
4g	47.4	30.4	14.7	-26.8	<10
4h	16.4	6.2	-9.5	1.3	<10
ADR	8.3	5.2	-3.3	-20.9	<10

(CC) 2022 SCS.

Table S-VII. Control growth against human prostate cancer cell line PC-3

Compound	Experiment 1				Experiment 2				Experiment 3			
	Control growth, %											
	10	20	40	80	10	20	40	80	10	20	40	80
	Drug concentration, μg ml^{-1}											
4a	109.2	90.5	88.7	60.1	100.7	81.2	70.9	50.3	89.8	69.8	61.8	33.9
4b	90.2	63.2	51.5	42.8	74.9	47.9	46.1	30.9	67.1	36.2	32.9	21.1
4c	45.3	41.1	31	22.4	36.4	24.7	19	14.2	25.1	13.4	10	5.1
4d	40.2	35.6	4.2	-12.4	25.2	20.4	2.8	-9.1	17.4	11.2	1.1	-3.1
4e	70.2	31.8	9.4	-39.4	54.1	23.5	7.2	-27.2	46.1	11.3	3.5	-18.6
4f	58.1	52	43.5	11.8	45.9	41	29.2	7.2	39.1	27	17.6	2.3
4g	39.1	32.4	22.8	15.2	30.4	20.5	11.1	8.9	20.2	13.7	6.3	5.6
4h	59.6	40.9	15.5	-11.2	45.8	32.6	11.7	-7.9	37.7	16.5	3.1	-2.2
ADR	13.6	1.1	-12.1	-28.8	9.2	0.7	-7.5	-22.1	5.1	1.8	-5.3	-11.8

Table S-VIII. Average control growth against human prostate cancer cell line PC-3

Compound	Average control growth, %				GI_{50} /μg ml^{-1}
	10	20	40	80	
	Drug concentration, μg ml^{-1}				
4a	99.9	80.5	73.8	48.1	92.93
4b	77.4	49.1	43.5	31.6	28.19
4c	35.6	26.4	20	13.9	<10
4d	27.6	22.4	2.7	-8.2	<10
4e	56.8	22.2	6.7	-28.4	<10
4f	47.7	40	30.1	7.1	11.59
4g	29.9	22.2	13.4	9.9	<10
4h	47.7	30	10.1	-7.1	<10
ADR	9.3	1.2	-8.3	-20.9	<10

Antibacterial activity

Gram positive

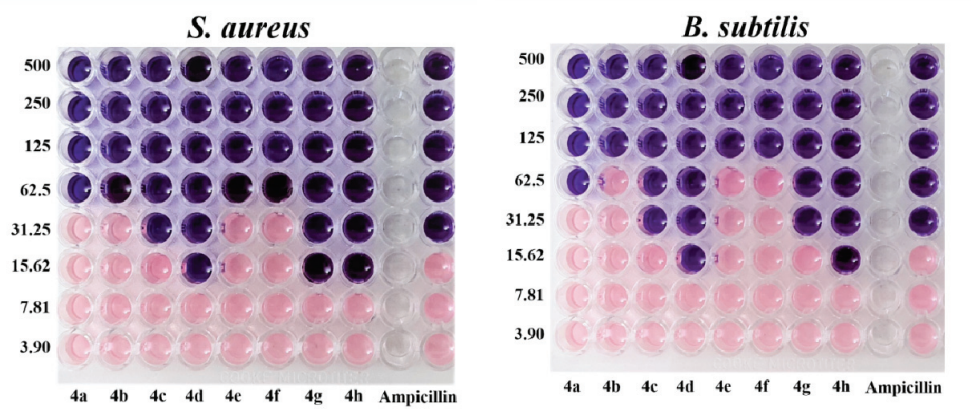

Fig. S-33. Antibacterial activity of synthesized compounds against gram positive strains

(CC) 2022 SCS.

Gram negative

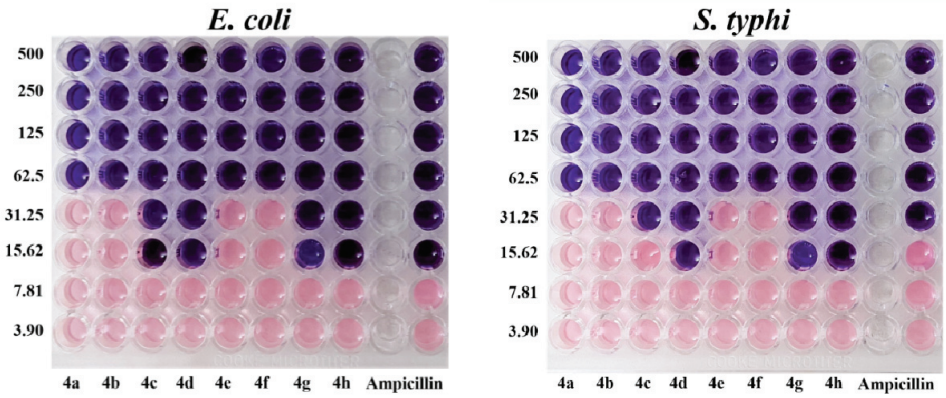

Fig. S-34. Antibacterial activity of synthesized compounds against gram negative strains

(CC) 2022 SCS.