Supplementary Material

Novel strigolactone mimics that modulate photosynthesis and biomass accumulation in *Chlorella sorokiana*

by Daria Gabriela Popa, Florentina Georgescu, Florea Dumitrascu, Sergiu Shova, Diana Constantinescu-Aruxandei, Constantin Draghici, Lucian Vladulescu, Florin Oancea

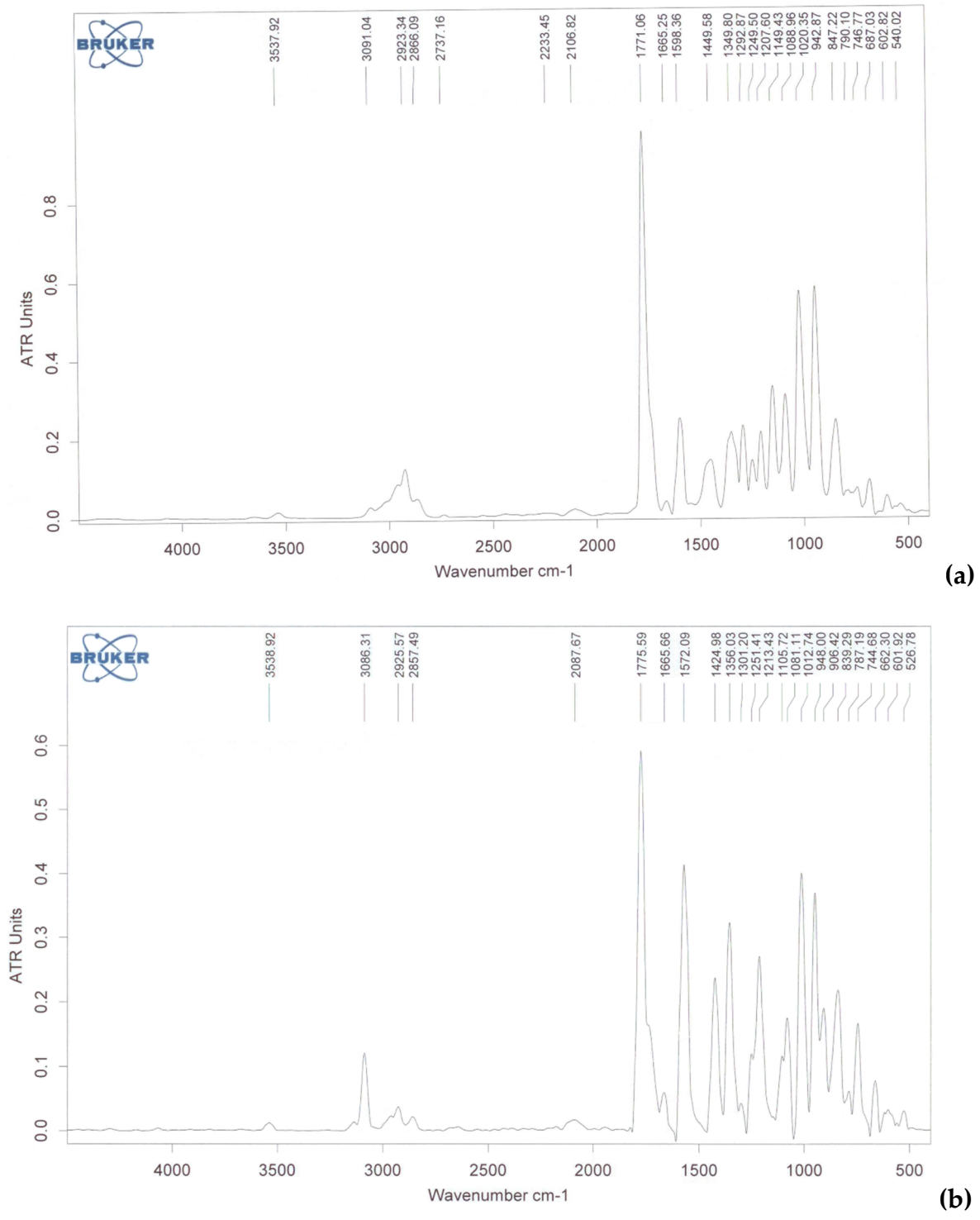
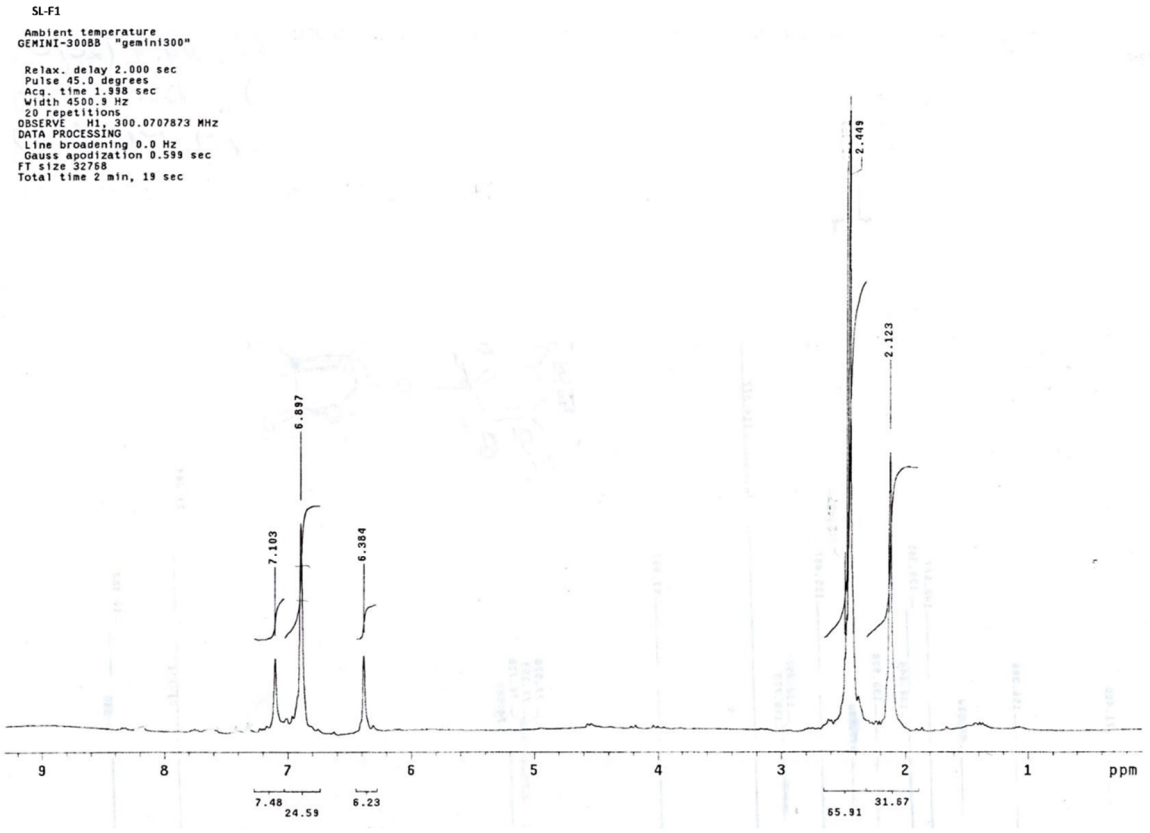
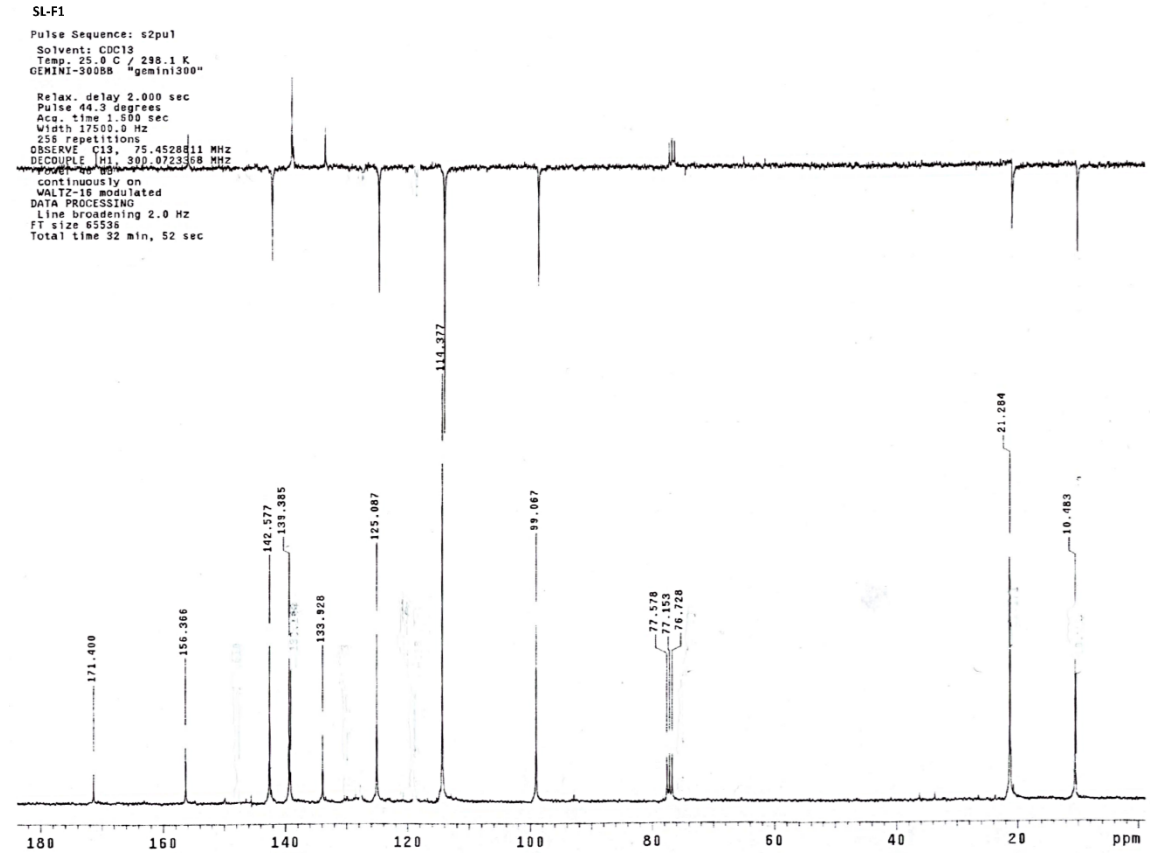


Figure S1. IR spectrum of (a) compound **3** (SL-F1) and (b) compound **4** (SL-F2)

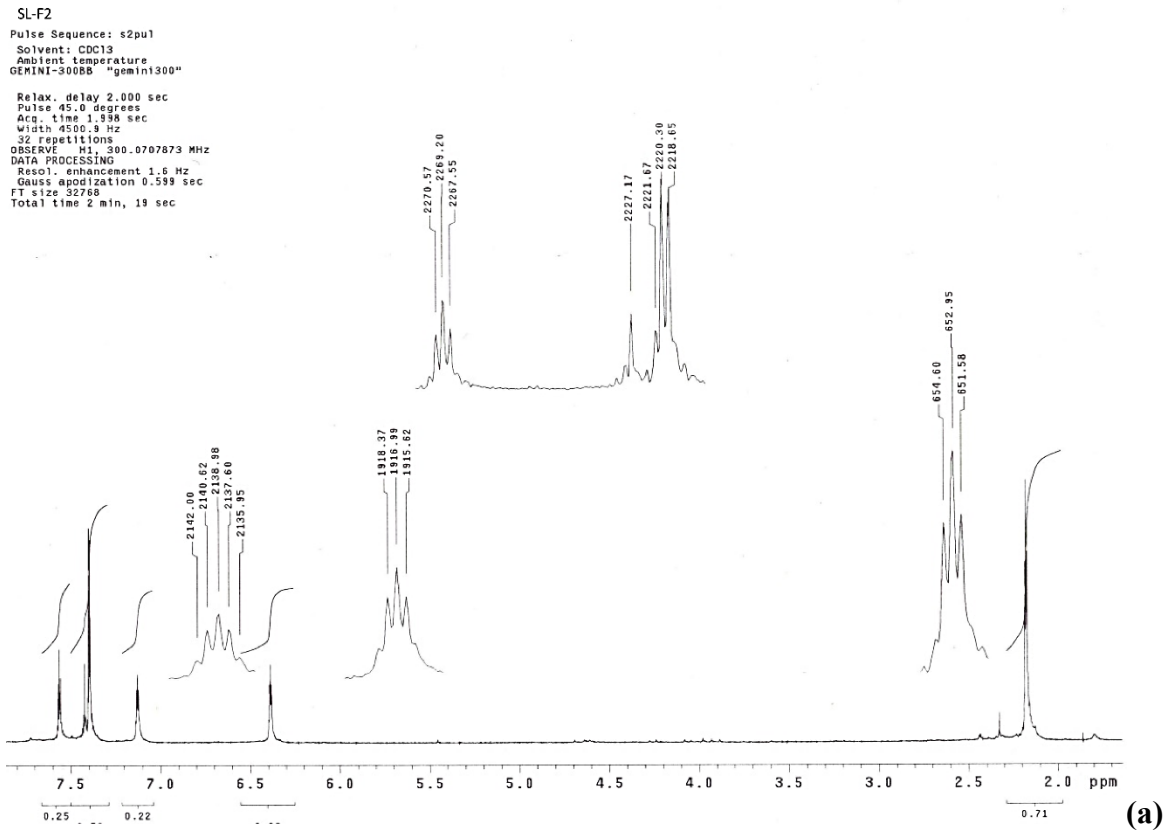


(a)

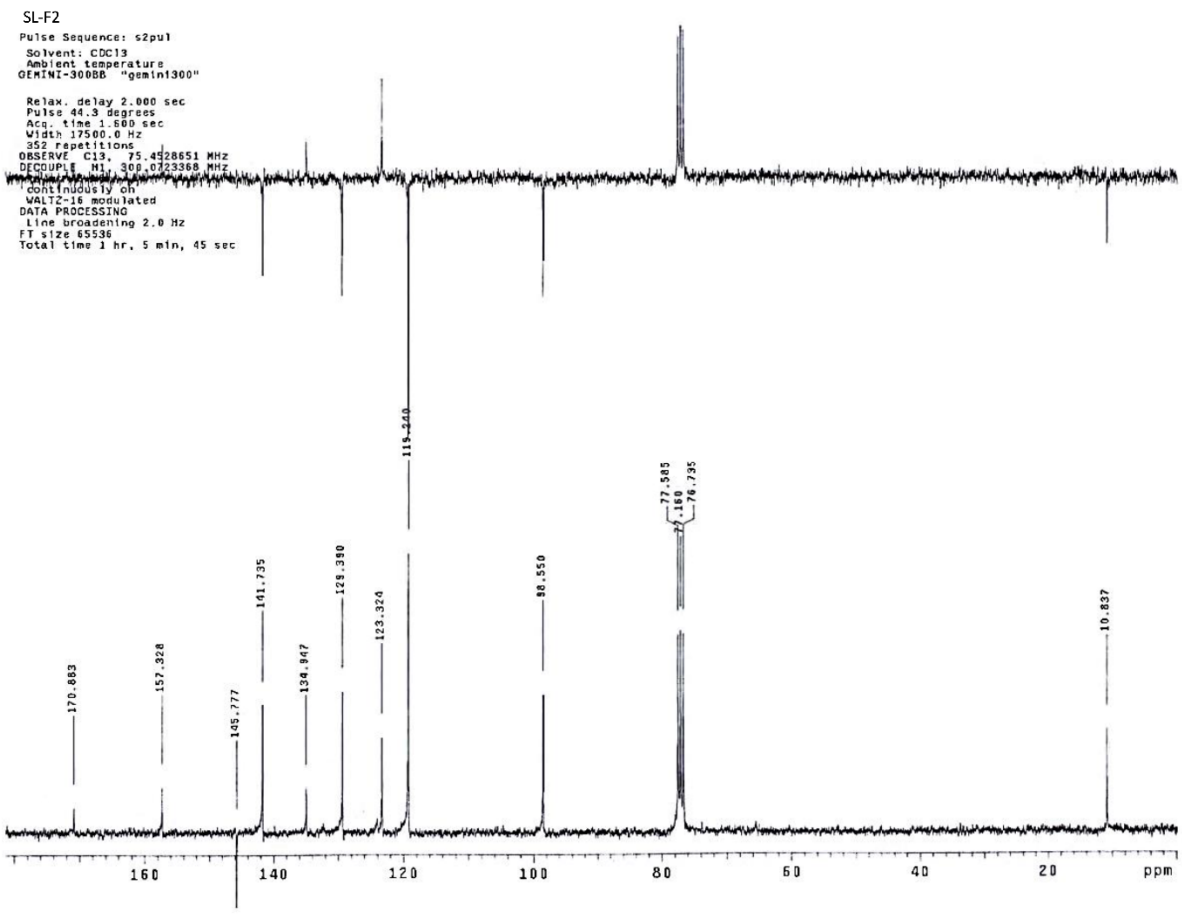


(b)

Figure S2. (a) The ^{1}H NMR spectrum for compound **3** (SL-F1), recorded in $CDCl_3$; (b) The ^{13}C NMR spectrum for compound **3** (SL-F1), recorded in $CDCl_3$.

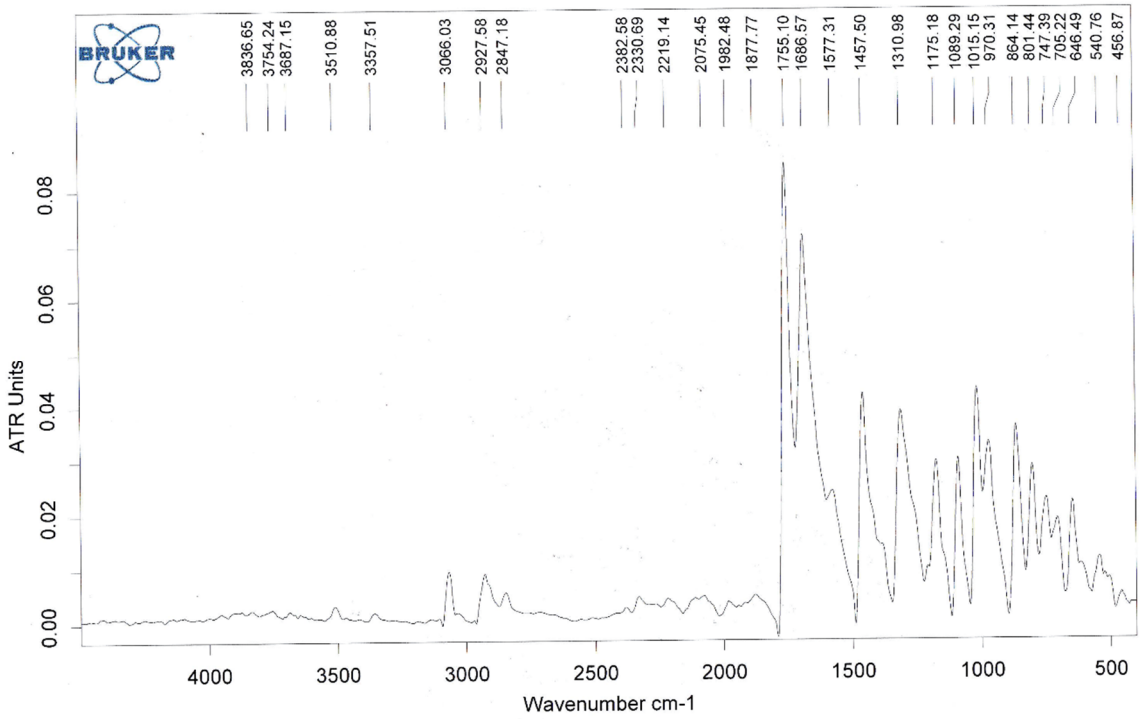


(a)



(b)

Figure S3. (a) The ^{1}H NMR spectrum for compound **4** (SL-F2) recorded in $CDCl_3$; (b) The ^{13}C NMR spectrum for compound **4** (SL-F2) recorded in $CDCl_3$.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3357.51
3066.03
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2847.18
2382.58
2330.69
2219.14
2075.45
1982.48
1877.77
1755.10
1686.57
1577.31
1457.50
1310.98
1175.18
1089.29
1015.15
970.31
864.14
801.44
747.39
705.22
646.49
540.76
456.87
ATR Units
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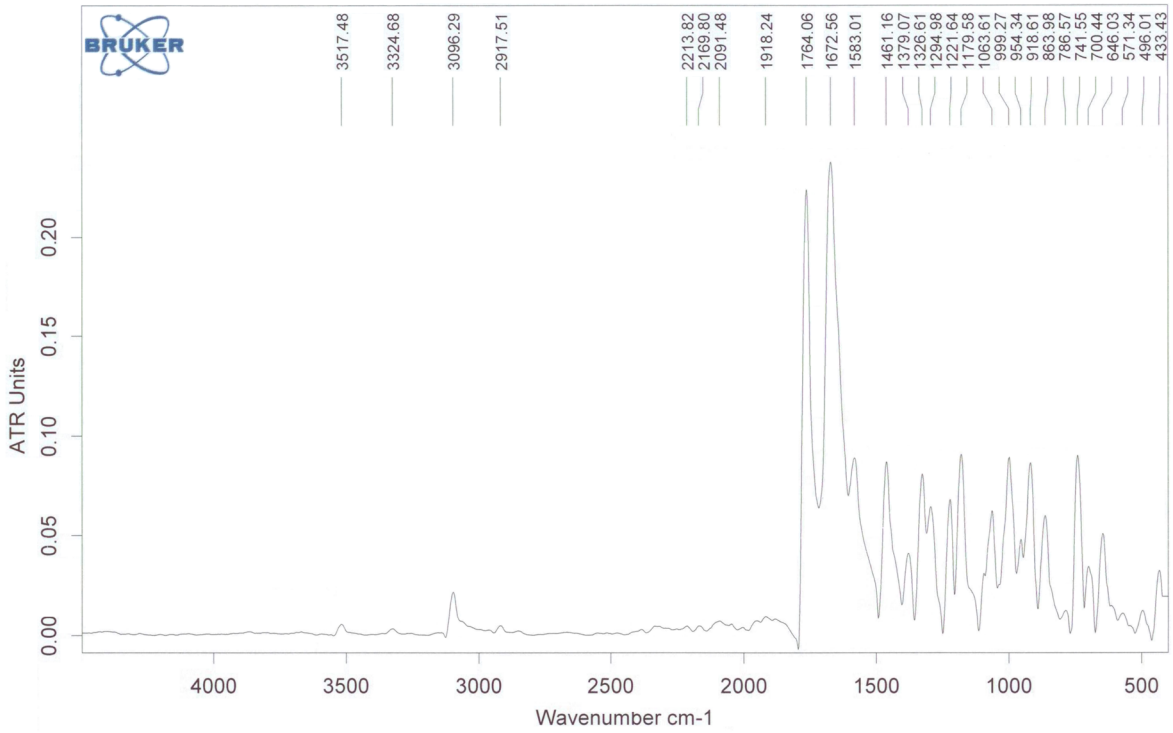
0.02
0.04
0.06
0.08
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

(a)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3096.29
2917.51
2213.82
2169.80
2091.48
1918.24
1764.06
1672.56
1583.01
1461.16
1379.07
1326.61
1294.98
1221.64
1179.58
1063.61
999.27
954.34
918.61
863.98
786.57
741.55
700.44
646.03
571.34
496.01
433.43
ATR Units
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0.05
0.10
0.15
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4000
3500
3000
2500
2000
1500
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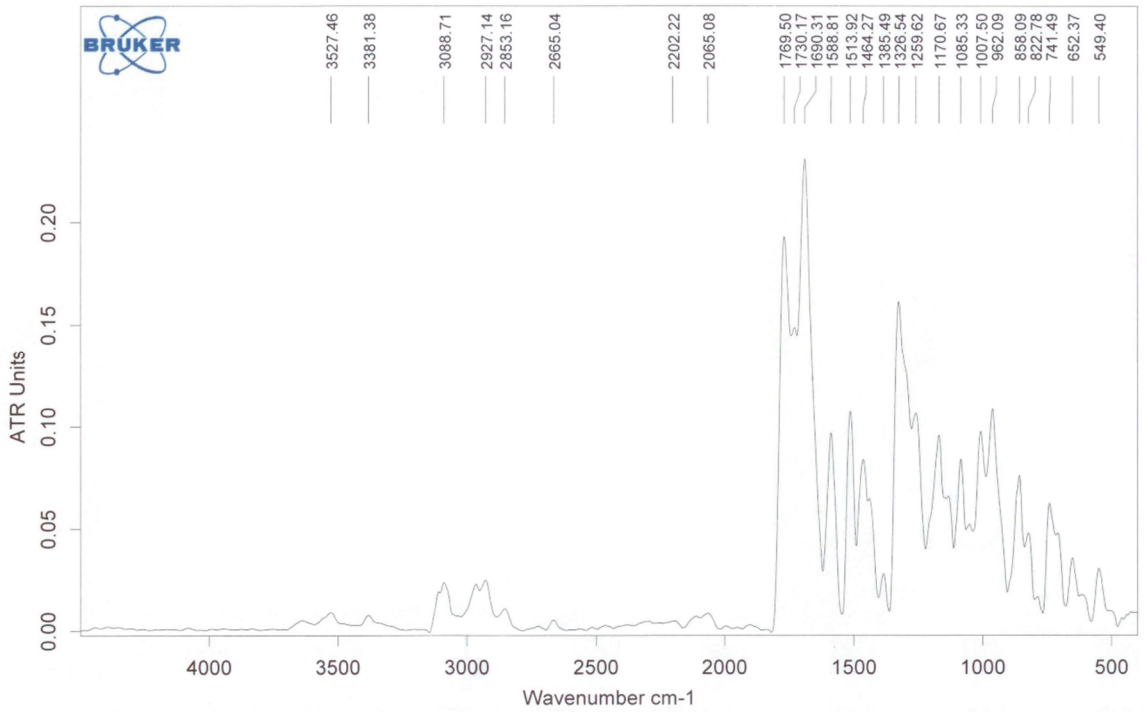
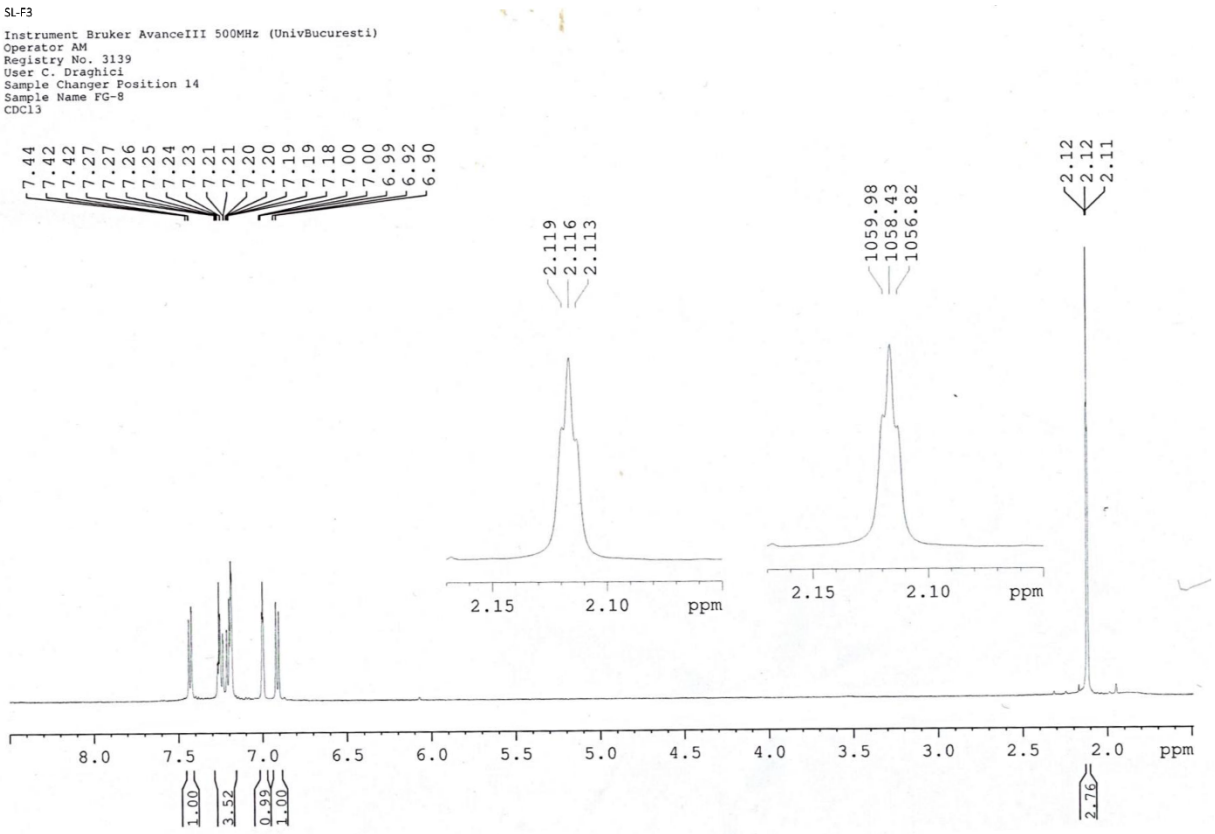
Wavenumber cm-1

(b)

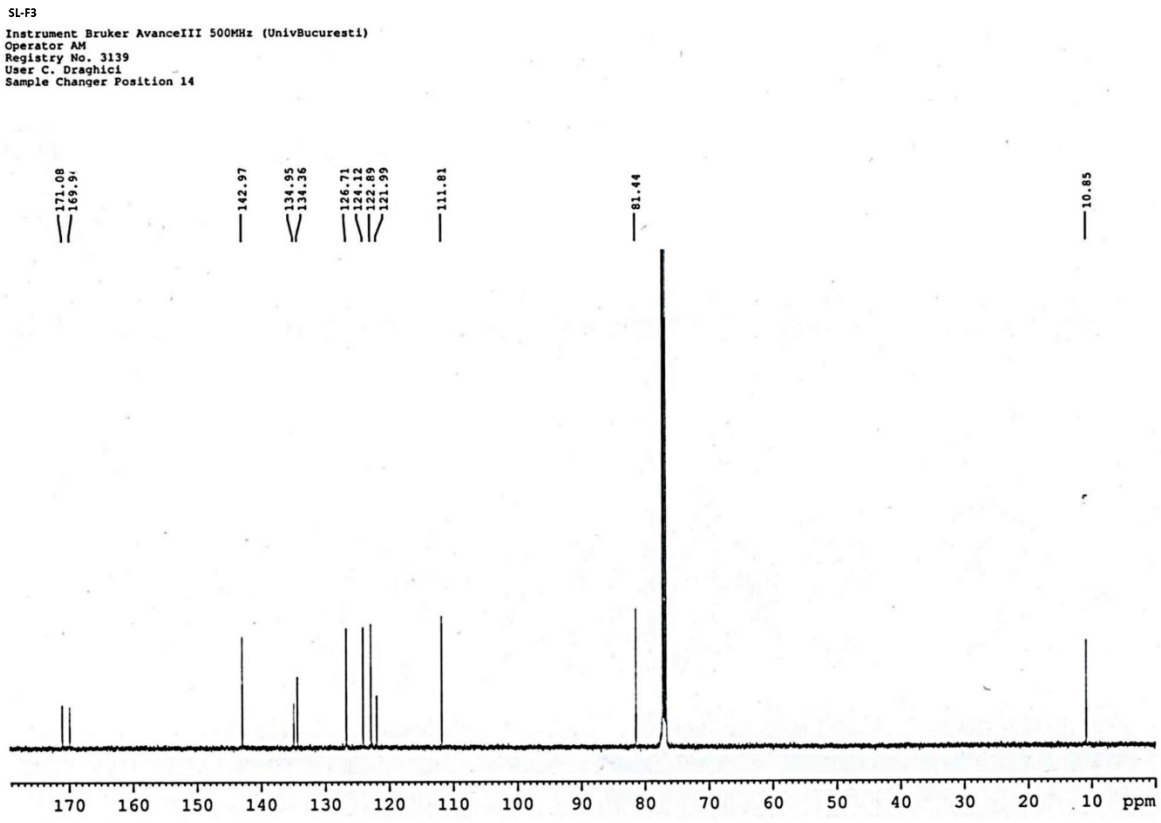


(c)

Figure S4. (a) IR spectrum of (a) compound **7** (SL-F3); (b) IR spectrum of (a) compound **9** (SL-F5); (c) IR spectrum of (a) compound **11** (SL-F6).

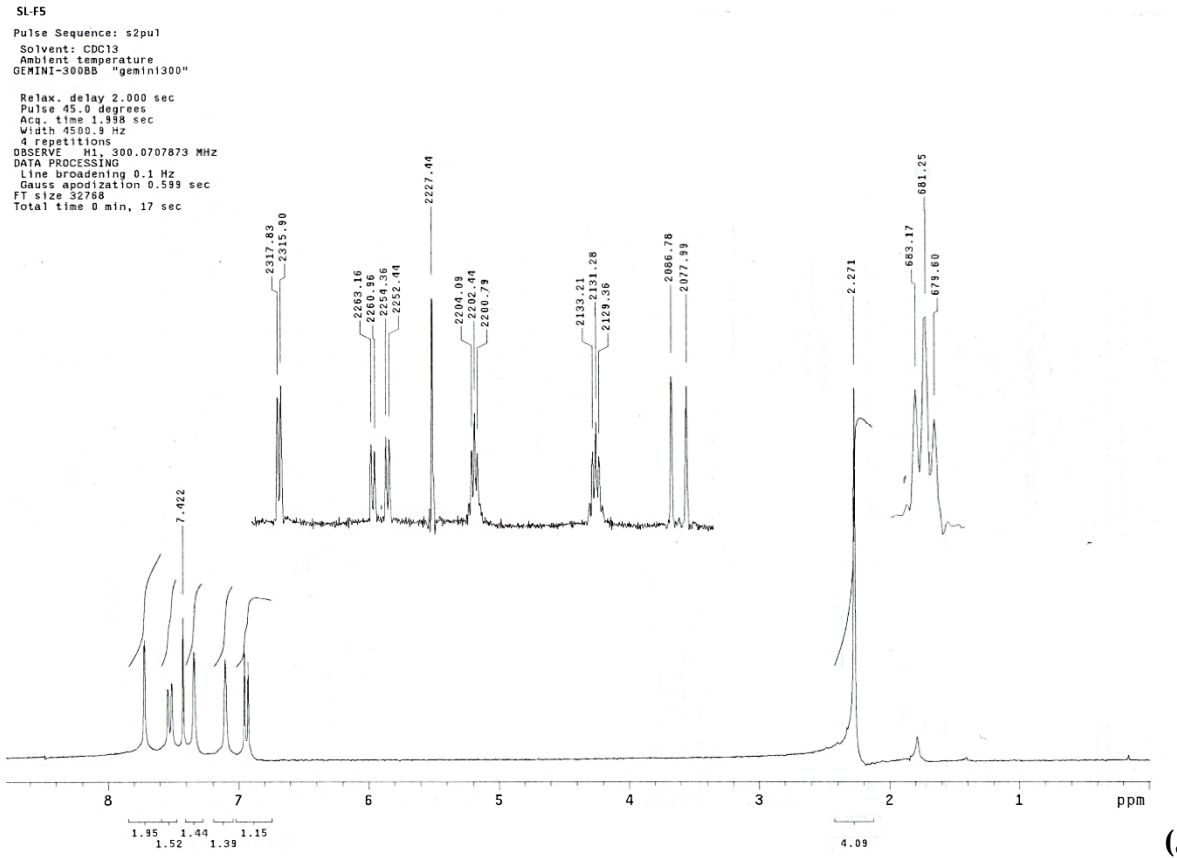


(a)

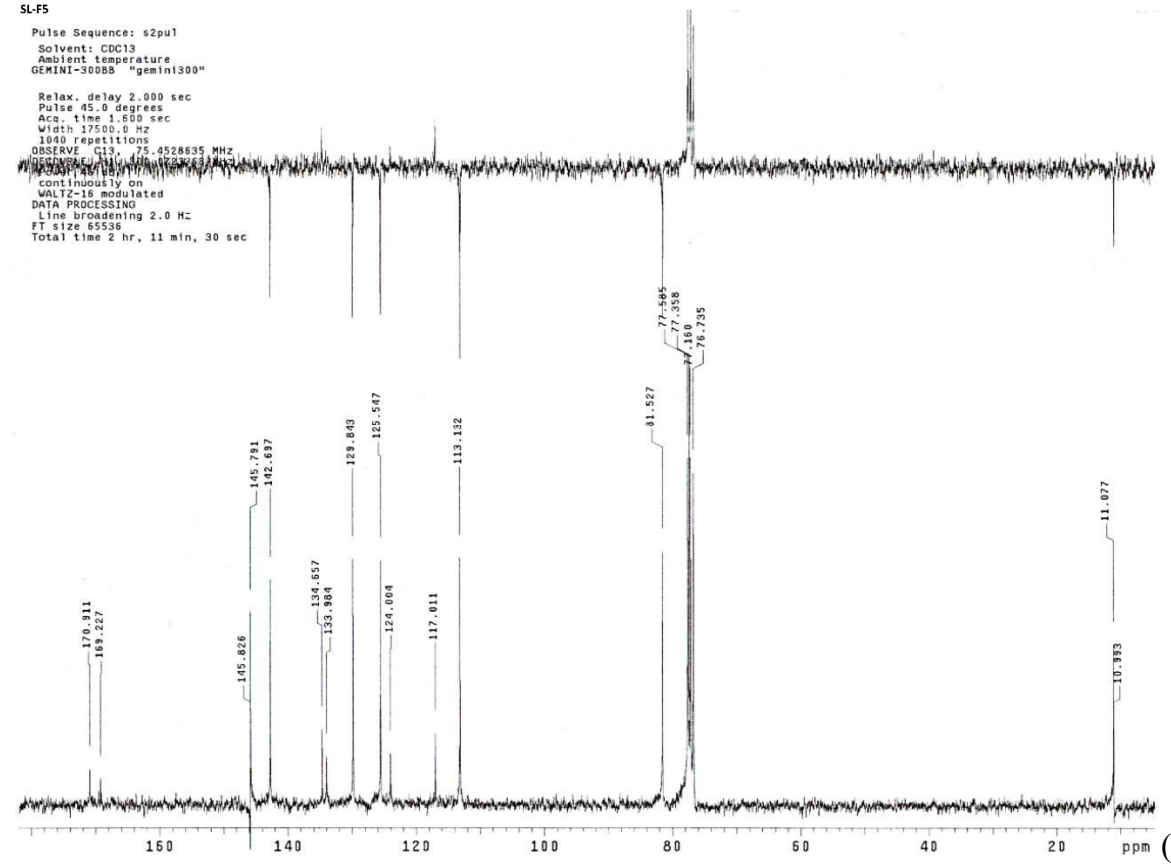


(b)

Figure S5. (a) The ^{1}H NMR spectrum for compound **7** (SL-F3) recorded in $CDCl_3$; (b) The ^{13}C NMR spectrum for compound **7** (SL-F3) recorded in $CDCl_3$.

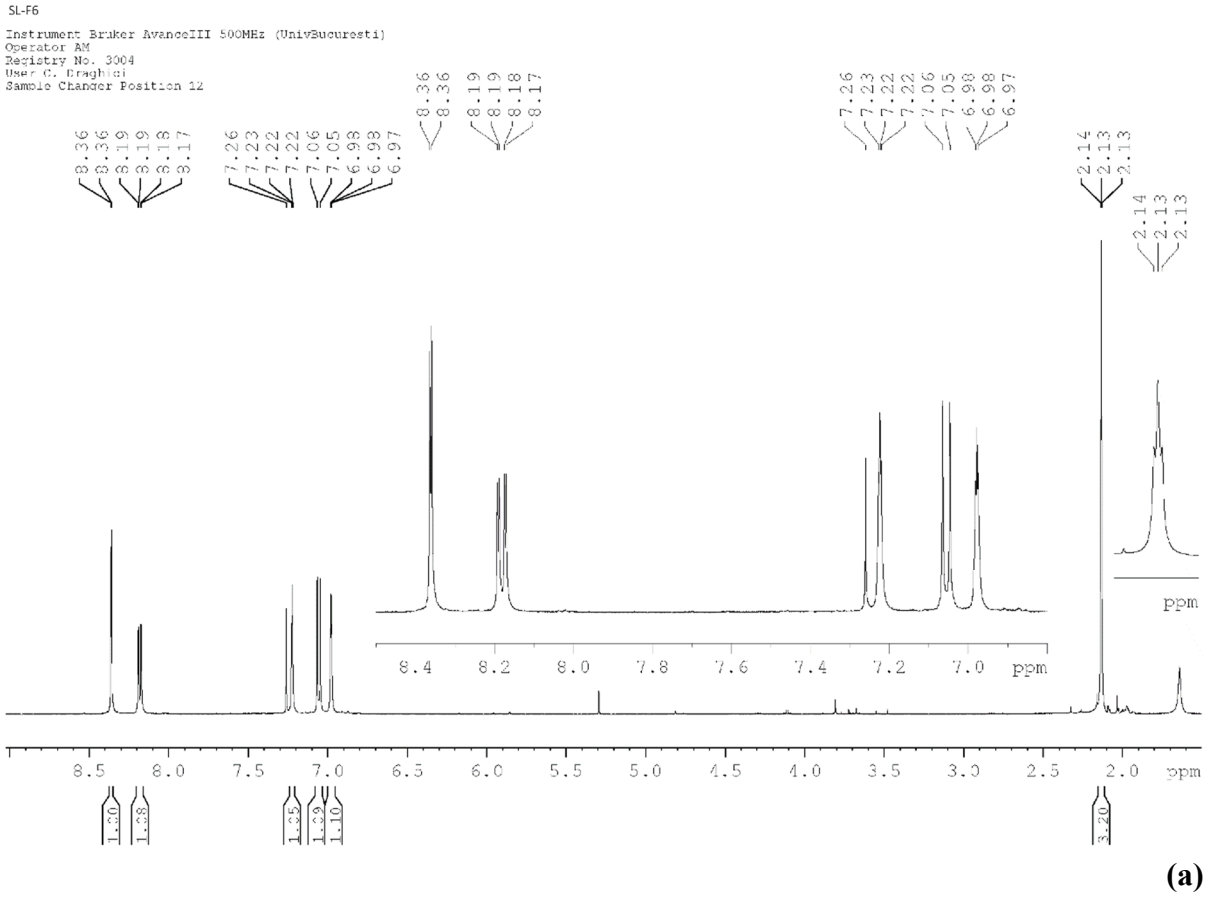


(a)

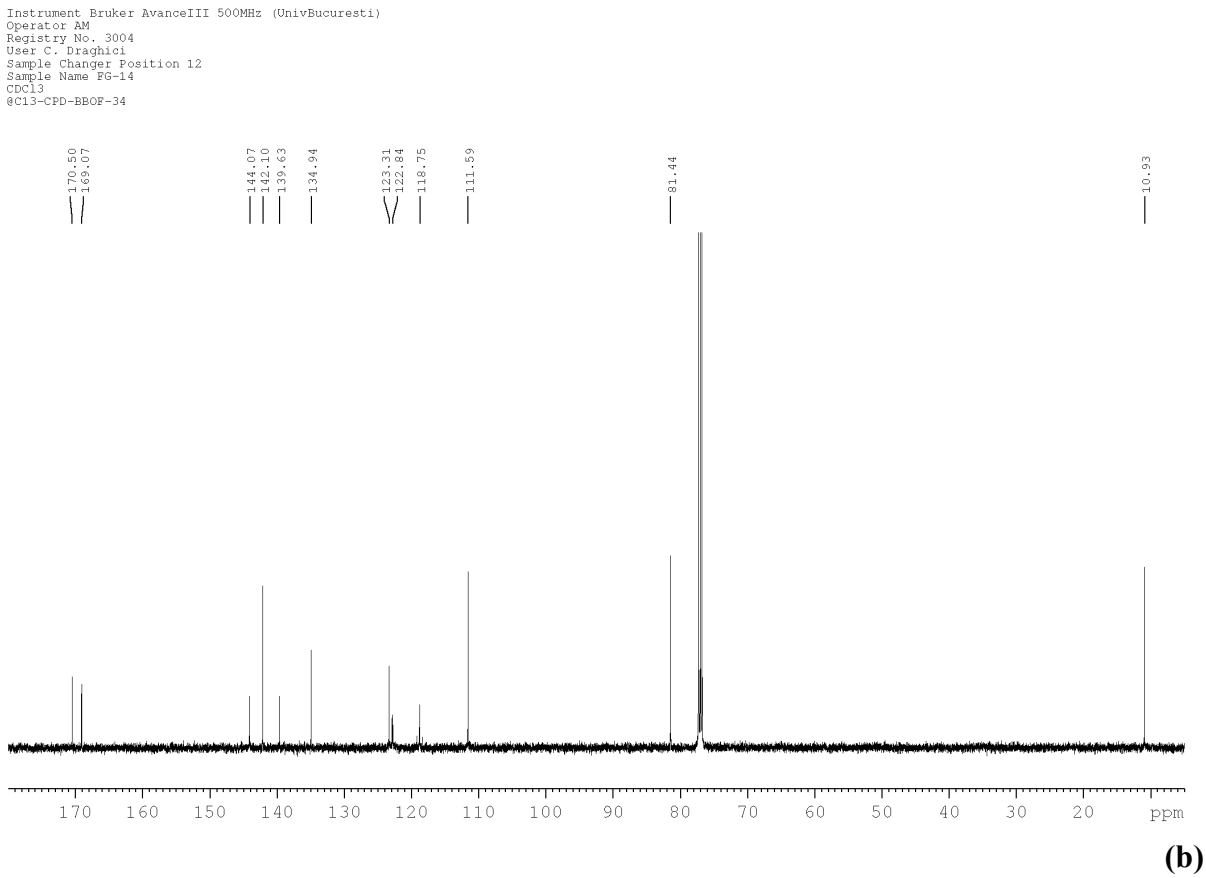


(b)

Figure S6. (a**)** The ^{1}H NMR spectrum for compound **9** (SL-F5) recorded in $CDCl_3$. (b) The ^{13}C NMR spectrum for compound **9** (SL-F5) recorded in $CDCl_3$.



(a)



(b)

Figure S7. (a) The ^{1}H NMR spectrum for compound **11** (SL-F6) recorded in $CDCl_3$. (b) The ^{13}C NMR spectrum for compound **11** (SL-F6) recorded in $CDCl_3$.

Crystallographic data

Table S1. Crystal data and details of data collection.

	7 [SL-FL3]	**8**
empirical formula	$C_{12}H_9NO_3S$	C_7H_4BrNOS
Fw	247.26	230.08
space group	*I*2/*a*	*C*2/*c*
	28.065(2)	16.8477(14)
b [Å]	4.0890(3)	3.9602(3)
c [Å]	18.9725(13)	23.005(3)
α [°]	90	90
β [°]	94.700(6)	98.437(10)
γ [°]	90	90
V [Å^3]	2169.9(3)	1518.3(3)
Z	8	8
r_{calcd} [g cm^{-3}]	1.514	2.013
Crystal size [mm]	0.35 × 0.05 × 0.05	0.40 × 0.10 × 0.02
T [K]	293	293
μ [mm^{-1}]	0.292	5.620
2Θ range [°]	4.308 to 59.116	3.58 to 57.986
Reflections collected	9289	4178
Independent reflections	2636[R_{int}=0.0413]	1717[R_{int}=0.0368]
Data/restraints/parameters	2636/0/155	1717/0/100
R_1[a]	0.0505	0.0538
wR_2[b]	0.1203	0.1075
GOF[c]	1.029	1.076
Largest diff. peak/hole [e Å^{-3}]	0.24/-0.36	0.34/-0.69
CCDC	2109012	2109011

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$. [c] GOF = $\{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$, where n is the number of reflections and p is the total number of parameters refined.

Table S2. Bond distances (Å) and angles (°) of compound **8**

Bond	Distance (Å)	Bond	Distance (Å)	Bonds	Angle (°)	Bonds	Angle (°)
Br1-C3	1.893(5)	C1-C2	1.371(6)	C1-S1-C7	91.4(2)	C3-C4-C5	119.9(4)
S1-C1	1.756(4)	C1-C6	1.391(6)	C7-N1-C6	115.4(4)	C6-C5-C4	118.6(5)
S1-C7	1.778(5)	C2-C3	1.381(6)	C2-C1-S1	128.7(3)	C1-C6-N1	113.3(4)
O1-C7	1.217(6)	C3-C4	1.385(6)	C2-C1-C6	121.1(4)	C5-C6-N1	126.0(4)
N1-C6	1.397(6)	C4-C5	1.388(7)	C6-C1-S1	110.2(4)	C5-C6-C1	120.7(5)
N1-C7	1.358(6)	C5-C6	1.378(6)	C1-C2-C3	118.0(4)	O1-C7-S1	124.4(4)
				C2-C3-Br1	118.6(4)	O1-C7-N1	125.9(5)
				C2-C3-C4	121.7(5)	N1-C7-S1	109.7(4)
				C4-C3-Br1	119.7(4)		

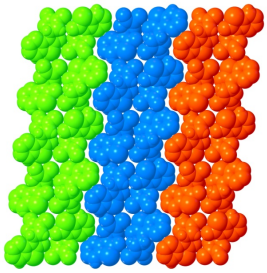


Figure S8. Space filling representation of the crystal structure **7** showing the packing of 2D layers.

Table S3. Bond distances (Å) and angles (°) of compound **7** (SL-F3)

Bond	Distance (Å)	Bonds	Angle (°)	Bonds	Angle (°)
S1-C1	1.746(2)	C1-S1-C7	91.82(11)	O2-C8-C9	104.66(18)
S1-C7	1.764(2)	C11-O2-C8	108.45(16)	N1-C8-C9	117.44(19)
O1-C7	1.212(3)	C6-N1-C8	121.04(18)	C10-C9-C8	109.9(2)
O2-C8	1.437(3)	C7-N1-C6	114.77(19)	C9-C10-C11	107.9(2)
O2-C11	1.374(3)	C7-N1-C8	124.18(19)	C9-C10-C12	131.3(2)
O3-C11	1.196(3)	C2-C1-S1	128.10(19)	C11-C10-C12	120.8(2)
N1-C6	1.409(3)	C2-C1-C6	120.7(2)	O2-C11-C10	108.80(19)
N1-C7	1.383(3)	C6-C1-S1	111.17(17)	O3-C11-O2	120.7(2)
N1-C8	1.443(3)	C3-C2-C1	118.1(2)	O3-C11-C10	130.5(2)
C1-C2	1.379(3)	C4-C3-C2	121.2(2)		
C1-C6	1.393(3)	C3-C4-C5	121.2(2)		
C2-C3	1.379(4)	C6-C5-C4	117.9(2)		
C3-C4	1.375(3)	C1-C6-N1	112.4(2)		
C4-C5	1.383(3)	C5-C6-N1	126.7(2)		
C5-C6	1.379(3)	C5-C6-C1	120.9(2)		
C8-C9	1.491(3)	O1-C7-S1	124.32(19)		
C9-C10	1.320(3)	O1-C7-N1	126.0(2)		
C10-C11	1.469(3)	N1-C7-S1	109.71(16)		
C10-C12	1.492(3)	O2-C8-N1	109.37(16)		