Electronic Supplementary Information (ESI):

Nonlinear Optical Properties of Diaromatic Stilbene, Butadiene and Thiophene Derivatives

Esa Kukkonen,[†] Elmeri Lahtinen,[†] Pasi Myllyperkiö,[‡] Matti Haukka,[†] and Jari Konu *[,†]

† Department of Chemistry and ‡ Nanoscience Center, University of Jyväskylä, P.O. Box 35, FI-40014 Jyväskylä, Finland.

Table S1. Crystallographic data for compounds **1a**·centro,[a] **1a**·non-centro,[a] **1b**,[a] and **1c**[a].

	1a·centro	**1a**·non-centro	**1b**	**1c**
emp. formula	$C_{16}H_{14}ClNO_4$	$C_{16}H_{14}ClNO_4$	$C_{14}H_9BrN_2O_5$	$C_{15}H_{13}NO_3$
Fw	319.73	319.73	365.14	255.26
cryst. system	Monoclinic	Monoclinic	Monoclinic	Triclinic
space group	$P2_1/c$	$P2_1$	Cc	P-1
a, Å	7.9071(2)	4.2178(2)	3.2836(1)	11.6720(2)
b, Å	28.2960(6)	16.5839(6)	26.8722(5)	11.8172(2)
c, Å	7.1173(2)	10.2700(4)	13.2409(2)	14.7910(2)
α, deg.	90	90	90	109.528(1)
β, deg.	115.383(4)	93.821(4)	93.319(2)	103.389(1)
γ, deg.	90	90	90	90.949(1)
V, Å^3	1438.69(8)	716.76(5)	1358.20(5)	1860.67(5)
Z	4	2	4	6
T, °C	-150	-150	-150	-150
ρ_{calcd}, g/cm^3	1.476	1.481	1.786	1.367
μ, mm^{-1}	2.524	2.533	4.397	0.787
cryst. size, mm^3	0.31×0.15×0.10	0.39×0.07×0.07	0.61×0.07×0.02	0.25×0.21×0.16
F(000)	664	332	728	804
Θ range, deg	6.20-76.83	4.32-76.87	3.29-76.74	3.28-76.98
reflns collected	5734	2847	5023	72195
unique reflns	2655	1977	1997	7134
R_{int}	0.0235	0.0321	0.0220	0.0297
reflns [$I>2\sigma(I)$]	2946	2072	2021	7769
R_1 [$I>2\sigma(I)$]	0.0345	0.0391	0.0296	0.0390
wR_2 (all data)	0.0940	0.1061	0.0826	0.1103
GOF on F^2	1.050	1.077	1.050	1.059
completeness	0.997	0.997	0.998	0.999

[a] λ (CuKα) = 1.54184 Å.

Table S2. Crystallographic data for compounds **1d**,[a] **1e**,[b] **4**·Pcell,[b] and **4**·Ccell[b].

	1d	**1e**	**4**·Pcell	**4**·Ccell
emp. formula	$C_{16}H_{15}NO_4$	$C_{16}H_{16}N_2O_2$	$C_{32}H_{28}Cl_2N_2O_8$	$C_{32}H_{28}Cl_2N_2O_8$
Fw	285.29	268.31	639.46	639.46
cryst. system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	$P2_1/c$	$P2_1$	$P2_1/n$	$C2/c$
a, Å	13.242(2)	5.9378(4)	11.5166(2)	14.6720(3)
b, Å	7.6505(7)	7.3721(7)	12.8669(2)	10.3954(2)
c, Å	14.519(1)	15.357(1)	19.7897(3)	18.9716(3)
α, deg.	90	90	90	90
β, deg.	111.61(1)	96.42(1)	90.467(2)	93.264(2)
γ, deg.	90	90	90	90
V, Å^3	1367.4(3)	668.02(9)	2932.40(9)	2888.88(9)
Z	4	2	4	4
T, °C	-150	-150	-150	-150
ρ_{calcd}, g/cm^3	1.386	1.334	1.448	1.470
μ, mm^{-1}	0.100	0.719	2.476	2.514
cryst. size, mm^3	0.26×0.15×0.10	0.13×0.05×0.03	0.25×0.10×0.05	0.11×0.07×0.02
F(000)	600	284	1328	1328
Θ range, deg	2.86-29.21	2.83-76.76	4.10-76.51	4.67-76.76
reflns collected	5843	3947	12694	4692
unique reflns	1633	1671	5148	2707
R_{int}	0.0564	0.0322	0.0288	0.0139
reflns [$I>2\sigma(I)$]	3149	2194	6015	2910
R_1 [$I>2\sigma(I)$]	0.0802	0.0855	0.0356	0.0355
wR_2 (all data)	0.2551	0.2602	0.0958	0.0981
GOF on F^2	1.030	1.101	1.021	1.052
completeness	0.994	0.997	0.999	0.993

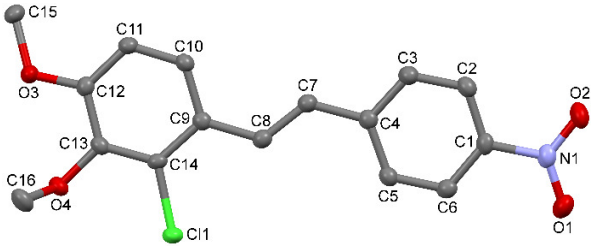
[a] λ (MoKα) = 0.71073 Å. [b] λ (CuKα) = 1.54184 Å.

Table S3. Crystallographic data for **2a**,[a] **3a**·mono,[a] **3a**·ortho,[a] **3b,**[b] and **3c**[a].

	2a	**3a**·mono	**3a**·ortho	**3b**	**3c**
emp. formula	$C_{16}H_{12}FNO_2$	$C_{12}H_8BrNO_2S$	$C_{12}H_8BrNO_2S$	$C_{13}H_{11}NO_2S$	$C_{13}H_{11}NO_2S_2$
Fw	269.27	310.16	310.16	245.29	277.35
cryst. system	monoclinic	Monoclinic	Orthorhombic	Monoclinic	Monoclinic
space group	Pc	$P2_1/c$	Pbca	$P2_1/n$	$P2_1/n$
a, Å	7.1272(2)	10.1458(5)	7.579(2)	11.2659(2)	7.903(2)
b, Å	12.8757(4)	15.8649(6)	11.453(2)	7.5074(1)	7.321(2)
c, Å	7.3763(3)	14.8141(7)	27.652(6)	27.4441(4)	22.042(4)
α, deg.	90	90	90	90	90
β, deg.	104.703(4)	102.260(5)	90	92.743(2)	90.25(3)
γ, deg.	90	90	90	90	90
V, Å^3	654.74(4)	2330.1(2)	2400.4(8)	2318.50(6)	1275.3(4)
Z	2	8	8	8	4
T, °C	-150	-150	-120	-150	-120
ρ_{calcd}, g/cm^3	1.366	1.768	1.717	1.405	1.445
μ, mm^{-1}	0.832	3.694	3.586	2.390	0.409
cryst. size, mm^3	0.53×0.22×0.13	0.28×0.19×0.16	0.20×0.10×0.04	0.20×0.10×0.06	0.50×0.30×0.04
F(000)	280	1232	1232	1024	576
Θ range, deg	3.43-85.30	2.40-28.36	2.95-25.02	3.22-76.83	2.73-27.47
reflns collected	4854	10991	8985	9641	10689
unique reflns	1777	3951	2112	4115	2189
R_{int}	0.0182	0.0342	0.0944	0.0230	0.0388
reflns [$I>2\sigma(I)$]	1881	5067	1734	4756	2912
R_1 [$I>2\sigma(I)$]	0.0334	0.0375	0.0945	0.0338	0.0497
wR_2 (all data)	0.0962	0.0823	0.1737	0.0929	0.1117
GOF on F^2	1.063	1.024	1.266	1.045	1.126
completeness	0.994	0.999	0.997	0.995	0.998

[a] λ (MoKα) = 0.71073 Å. [b] λ (CuKα) = 1.54184 Å.

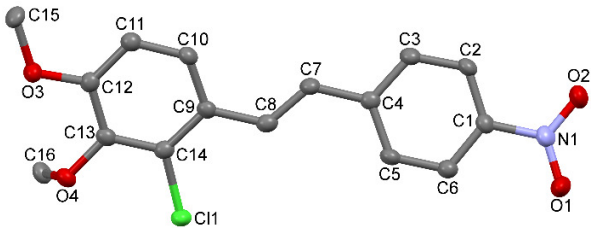
Table S4. Bond lengths and angles in compound **1a**·centro (H atoms removed for clarity).



Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C14	1.7395(14)	C4	C5	1.401(2)
O1	N1	1.2268(18)	C4	C7	1.463(2)
O2	N1	1.2288(18)	C5	C6	1.386(2)
O3	C12	1.3528(17)	C7	C8	1.333(2)
O3	C15	1.4389(18)	C8	C9	1.4633(19)
O4	C13	1.3717(16)	C9	C10	1.403(2)
O4	C16	1.4381(19)	C9	C14	1.4067(19)
N1	C1	1.4656(18)	C10	C11	1.385(2)
C1	C2	1.384(2)	C11	C12	1.396(2)
C1	C6	1.386(2)	C12	C13	1.406(2)
C2	C3	1.383(2)	C13	C14	1.387(2)
C3	C4	1.403(2)			

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C12	O3	C15	117.22(11)	C7	C8	C9	125.43(13)
C13	O4	C16	113.71(11)	C10	C9	C8	122.33(13)
O1	N1	O2	123.60(13)	C10	C9	C14	115.87(13)
O1	N1	C1	118.54(13)	C14	C9	C8	121.79(13)
O2	N1	C1	117.86(13)	C11	C10	C9	122.38(13)
C2	C1	N1	118.31(13)	C10	C11	C12	120.13(13)
C2	C1	C6	122.20(13)	O3	C12	C11	125.12(13)
C6	C1	N1	119.49(13)	O3	C12	C13	115.52(12)
C3	C2	C1	118.24(13)	C11	C12	C13	119.36(13)
C2	C3	C4	121.63(14)	O4	C13	C12	120.01(13)
C3	C4	C7	118.13(13)	O4	C13	C14	121.00(12)
C5	C4	C3	118.21(13)	C14	C13	C12	118.86(13)
C5	C4	C7	123.66(13)	C9	C14	Cl1	120.05(11)
C6	C5	C4	120.93(13)	C13	C14	Cl1	116.73(10)
C1	C6	C5	118.79(13)	C13	C14	C9	123.22(13)
C8	C7	C4	127.08(14)				

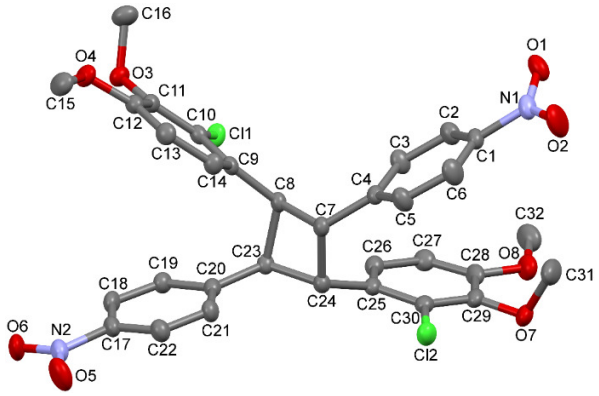
Table S5. Bond lengths and angles in compound **1a**·noncentro (H atoms removed for clarity).



Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C14	1.730(3)	C4	C5	1.404(5)
O1	N1	1.236(5)	C4	C7	1.466(5)
O2	N1	1.223(4)	C5	C6	1.389(5)
O3	C12	1.367(4)	C7	C8	1.333(5)
O3	C15	1.428(4)	C8	C9	1.466(5)
O4	C13	1.365(4)	C9	C10	1.394(5)
O4	C16	1.434(4)	C9	C14	1.406(5)
N1	C1	1.473(4)	C10	C11	1.391(5)
C1	C2	1.389(5)	C11	C12	1.387(5)
C1	C6	1.383(5)	C12	C13	1.409(5)
C2	C3	1.376(5)	C13	C14	1.403(5)
C3	C4	1.398(5)			

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C12	O3	C15	116.6(3)	C7	C8	C9	125.9(3)
C13	O4	C16	113.0(3)	C10	C9	C8	121.6(3)
O1	N1	C1	117.7(3)	C10	C9	C14	116.9(3)
O2	N1	O1	123.3(3)	C14	C9	C8	121.5(3)
O2	N1	C1	119.0(3)	C11	C10	C9	122.5(3)
C2	C1	N1	119.0(3)	C12	C11	C10	119.7(3)
C6	C1	N1	118.2(3)	O3	C12	C11	124.4(3)
C6	C1	C2	122.8(3)	O3	C12	C13	115.5(3)
C3	C2	C1	117.6(3)	C11	C12	C13	120.0(3)
C2	C3	C4	122.2(3)	O4	C13	C12	120.3(3)
C3	C4	C5	118.1(3)	O4	C13	C14	121.0(3)
C3	C4	C7	119.3(3)	C14	C13	C12	118.7(3)
C5	C4	C7	122.5(3)	C9	C14	Cl1	121.5(3)
C6	C5	C4	121.0(3)	C13	C14	Cl1	116.4(2)
C1	C6	C5	118.2(3)	C13	C14	C9	122.1(3)
C8	C7	C4	125.4(3)				

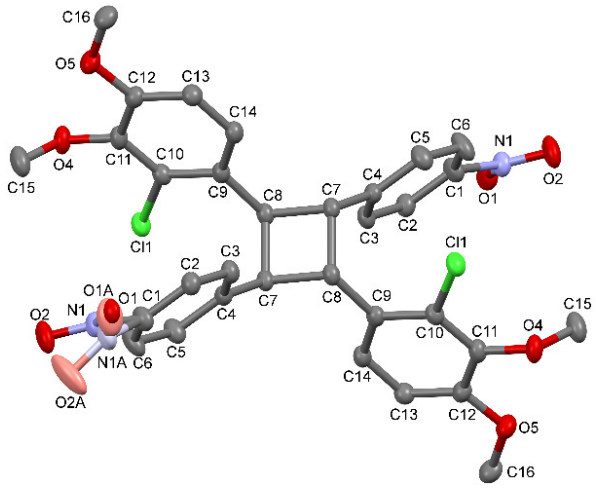
Table S6. Bond lengths and angles in compound **4**·Pcell (H atoms removed for clarity).



Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C10	1.7386(15)	C7	C24	1.597(2)
Cl2	C30	1.7380(17)	C8	C9	1.5035(19)
O1	N1	1.228(2)	C8	C23	1.583(2)
O2	N1	1.222(2)	C9	C10	1.399(2)
O3	C11	1.3707(19)	C9	C14	1.390(2)
O3	C16	1.434(2)	C10	C11	1.392(2)
O4	C12	1.3613(18)	C11	C12	1.409(2)
O4	C15	1.434(2)	C12	C13	1.384(2)
O5	N2	1.223(2)	C13	C14	1.396(2)
O6	N2	1.228(2)	C17	C18	1.380(3)
O7	C29	1.368(2)	C17	C22	1.381(2)
O7	C31	1.436(2)	C18	C19	1.388(2)
O8	C28	1.3702(19)	C19	C20	1.397(2)
O8	C32	1.426(3)	C20	C21	1.391(2)
N1	C1	1.465(2)	C20	C23	1.506(2)
N2	C17	1.472(2)	C21	C22	1.387(2)
C1	C2	1.377(2)	C23	C24	1.552(2)
C1	C6	1.379(2)	C24	C25	1.507(2)
C2	C3	1.381(2)	C25	C26	1.386(2)
C3	C4	1.392(2)	C25	C30	1.406(2)
C4	C5	1.393(2)	C26	C27	1.399(2)
C4	C7	1.508(2)	C27	C28	1.385(2)
C5	C6	1.386(2)	C28	C29	1.401(3)
C7	C8	1.544(2)	C29	C30	1.391(2)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C11	O3	C16	113.76(13)	O4	C12	C11	115.17(14)
C12	O4	C15	116.64(13)	O4	C12	C13	125.34(14)
C29	O7	C31	112.63(13)	C13	C12	C11	119.47(14)
C28	O8	C32	116.24(15)	C12	C13	C14	120.07(14)
O1	N1	C1	118.02(14)	C9	C14	C13	122.26(15)
O2	N1	O1	123.55(15)	C18	C17	N2	119.23(15)
O2	N1	C1	118.43(15)	C18	C17	C22	122.26(15)
O5	N2	O6	123.24(15)	C22	C17	N2	118.48(16)
O5	N2	C17	118.49(15)	C17	C18	C19	118.40(15)
O6	N2	C17	118.25(16)	C18	C19	C20	121.02(16)
C2	C1	N1	117.87(15)	C19	C20	C23	117.94(14)
C2	C1	C6	122.01(15)	C21	C20	C19	118.67(14)
C6	C1	N1	120.11(15)	C21	C20	C23	123.28(14)
C1	C2	C3	118.69(15)	C22	C21	C20	121.07(15)
C2	C3	C4	121.46(15)	C17	C22	C21	118.51(16)
C3	C4	C5	117.99(14)	C20	C23	C8	112.26(12)
C3	C4	C7	122.06(14)	C20	C23	C24	116.36(13)
C5	C4	C7	119.92(14)	C24	C23	C8	88.46(11)
C6	C5	C4	121.50(16)	C23	C24	C7	88.34(11)
C1	C6	C5	118.34(16)	C25	C24	C7	111.43(12)
C4	C7	C8	118.59(13)	C25	C24	C23	117.51(13)
C4	C7	C24	120.18(12)	C26	C25	C24	124.10(14)
C8	C7	C24	88.21(11)	C26	C25	C30	116.36(14)
C7	C8	C23	89.15(11)	C30	C25	C24	119.09(14)
C9	C8	C7	120.81(12)	C25	C26	C27	122.52(15)
C9	C8	C23	118.99(12)	C28	C27	C26	119.70(16)
C10	C9	C8	120.98(13)	O8	C28	C27	125.43(17)
C14	C9	C8	122.42(14)	O8	C28	C29	115.09(15)
C14	C9	C10	116.46(13)	C27	C28	C29	119.48(15)
C9	C10	Cl1	119.74(11)	O7	C29	C28	119.81(15)
C11	C10	Cl1	117.27(12)	O7	C29	C30	120.89(16)
C11	C10	C9	122.96(13)	C30	C29	C28	119.30(15)
O3	C11	C10	120.46(13)	C25	C30	Cl2	120.19(12)
O3	C11	C12	120.60(13)	C29	C30	Cl2	117.42(13)
C10	C11	C12	118.74(14)	C29	C30	C25	122.37(15)

Table S7. Bond lengths and angles in compound **4**·Ccell (H atoms removed for clarity).



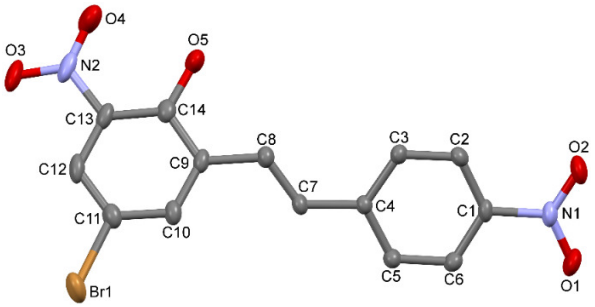
Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C10	1.7381(14)	C7	C8[1]	1.5884(19)
O4	C11	1.3743(18)	C7	C8	1.5558(18)
O4	C15	1.429(2)	C8	C9	1.5068(19)
O5	C12	1.3651(18)	C9	C10	1.4085(19)
O5	C16	1.4231(19)	C9	C14	1.383(2)
C1	C2	1.387(2)	C10	C11	1.389(2)
C1	C6	1.382(2)	C11	C12	1.401(2)
C1	N1	1.473(5)	C12	C13	1.386(2)
C1	N1A	1.486(6)	C13	C14	1.391(2)
C2	C3	1.381(2)	O1	N1	1.235(8)
C3	C4	1.396(2)	O2	N1	1.225(5)
C4	C5	1.395(2)	O1A	N1A	1.226(10)
C4	C7	1.5039(19)	O2A	N1A	1.226(7)
C5	C6	1.385(2)			

[1]1/2-X,3/2-Y,1-Z

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C11	O4	C15	114.08(12)	C10	C9	C8	119.96(12)
C12	O5	C16	116.96(12)	C14	C9	C8	123.79(13)
C2	C1	N1	119.6(2)	C14	C9	C10	116.23(13)
C2	C1	N1A	115.8(3)	C9	C10	Cl1	119.44(11)
C6	C1	C2	122.36(14)	C11	C10	Cl1	117.74(11)
C6	C1	N1	117.4(2)	C11	C10	C9	122.82(13)
C6	C1	N1A	121.3(3)	O4	C11	C10	120.31(13)
C3	C2	C1	118.06(14)	O4	C11	C12	120.76(13)
C2	C3	C4	121.50(14)	C10	C11	C12	118.88(13)
C3	C4	C7	121.38(13)	O5	C12	C11	115.80(13)
C5	C4	C3	118.50(13)	O5	C12	C13	124.76(14)
C5	C4	C7	120.01(13)	C13	C12	C11	119.44(13)
C6	C5	C4	121.10(14)	C12	C13	C14	120.14(14)
C1	C6	C5	118.42(15)	C9	C14	C13	122.47(14)
C4	C7	C8[1]	116.55(11)	O1	N1	C1	116.6(7)
C4	C7	C8	116.73(12)	O2	N1	C1	120.4(4)
C8	C7	C8[1]	89.66(11)	O2	N1	O1	122.9(8)
C7	C8	C7[1]	90.34(11)	O1A	N1A	C1	118.4(10)
C9	C8	C7[1]	117.97(11)	O1A	N1A	O2A	124.4(9)
C9	C8	C7	119.69(12)	O2A	N1A	C1	116.8(5)

[1]1/2-X,3/2-Y,1-Z

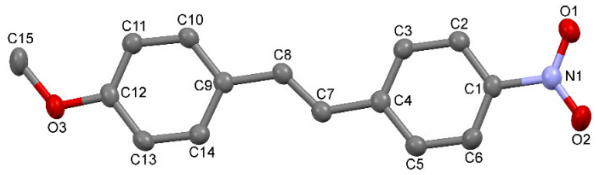
Table S8. Bond lengths and angles in compound **1b** (H atoms removed for clarity).



Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C11	1.897(4)	C4	C5	1.406(4)
O1	N1	1.236(5)	C4	C7	1.460(5)
O2	N1	1.224(5)	C5	C6	1.388(5)
O3	N2	1.223(6)	C7	C8	1.342(5)
O4	N2	1.231(7)	C8	C9	1.463(5)
O5	C14	1.345(6)	C9	C10	1.395(6)
N1	C1	1.463(4)	C9	C14	1.416(6)
N2	C13	1.458(6)	C10	C11	1.395(5)
C1	C2	1.390(5)	C11	C12	1.377(6)
C1	C6	1.385(6)	C12	C13	1.392(7)
C2	C3	1.382(5)	C13	C14	1.402(6)
C3	C4	1.400(5)			

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O1	N1	C1	117.8(4)	C8	C7	C4	126.4(3)
O2	N1	O1	123.3(3)	C7	C8	C9	122.6(4)
O2	N1	C1	119.0(3)	C10	C9	C8	121.8(4)
O3	N2	O4	122.8(4)	C10	C9	C14	118.5(4)
O3	N2	C13	118.3(5)	C14	C9	C8	119.7(4)
O4	N2	C13	118.8(4)	C11	C10	C9	121.0(4)
C2	C1	N1	118.8(3)	C10	C11	Br1	119.2(3)
C6	C1	N1	118.6(3)	C12	C11	Br1	119.3(3)
C6	C1	C2	122.5(3)	C12	C11	C10	121.5(4)
C3	C2	C1	118.4(3)	C11	C12	C13	117.6(4)
C2	C3	C4	121.1(3)	C12	C13	N2	116.7(4)
C3	C4	C5	118.8(3)	C12	C13	C14	122.9(4)
C3	C4	C7	123.2(3)	C14	C13	N2	120.3(4)
C5	C4	C7	118.0(3)	O5	C14	C9	117.2(4)
C6	C5	C4	120.9(3)	O5	C14	C13	124.3(4)
C1	C6	C5	118.3(3)	C13	C14	C9	118.4(4)

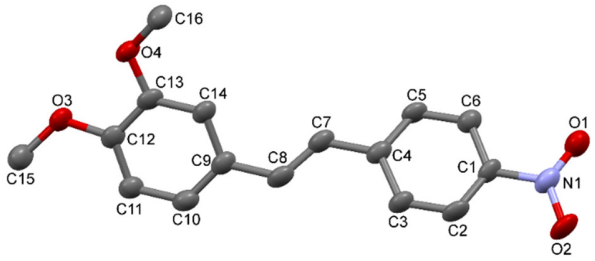
Table S9. Bond lengths and angles in compound **1c** (only one of the three discrete molecules, H atoms removed for clarity).



Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	N1	1.2297(13)	C4	C7	1.4678(15)
O2	N1	1.2305(13)	C5	C6	1.3837(16)
O3	C12	1.3604(13)	C7	C8	1.3399(16)
O3	C15	1.4327(16)	C8	C9	1.4618(15)
N1	C1	1.4631(14)	C9	C10	1.3964(16)
C1	C2	1.3848(16)	C9	C14	1.4048(16)
C1	C6	1.3837(16)	C10	C11	1.3885(16)
C2	C3	1.3811(16)	C11	C12	1.3923(16)
C3	C4	1.4029(16)	C12	C13	1.3952(17)
C4	C5	1.4018(16)	C13	C14	1.3765(16)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C12	O3	C15	117.54(9)	C5	C6	C1	118.29(11)
O1	N1	O2	123.08(10)	C8	C7	C4	126.29(11)
O1	N1	C1	118.65(10)	C7	C8	C9	127.45(11)
O2	N1	C1	118.27(10)	C10	C9	C8	119.77(10)
C2	C1	N1	118.62(10)	C10	C9	C14	116.96(10)
C6	C1	N1	119.32(10)	C14	C9	C8	123.27(10)
C6	C1	C2	122.06(10)	C11	C10	C9	122.63(10)
C3	C2	C1	118.91(10)	C10	C11	C12	119.11(10)
C2	C3	C4	121.10(10)	O3	C12	C11	124.94(11)
C3	C4	C7	122.90(10)	O3	C12	C13	115.78(10)
C5	C4	C3	118.00(10)	C11	C12	C13	119.27(10)
C5	C4	C7	119.10(10)	C14	C13	C12	120.91(10)
C6	C5	C4	121.65(11)	C13	C14	C9	121.11(11)

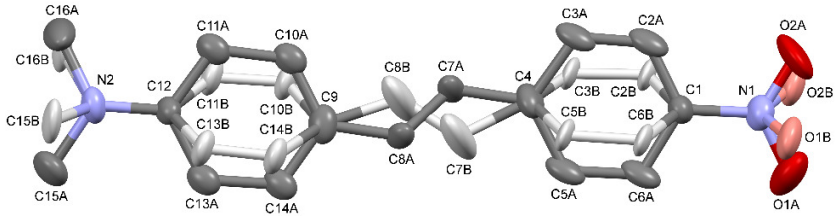
Table S10. Bond lengths and angles in compound **1d** (H atoms removed for clarity).



Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	N1	1.223(4)	C4	C5	1.393(4)
O2	N1	1.234(3)	C4	C7	1.461(4)
O3	C12	1.371(4)	C5	C6	1.379(4)
O3	C15	1.426(4)	C7	C8	1.330(5)
O4	C13	1.369(4)	C8	C9	1.459(4)
O4	C16	1.429(4)	C9	C10	1.387(5)
N1	C1	1.460(4)	C9	C14	1.411(4)
C1	C2	1.380(5)	C10	C11	1.397(4)
C1	C6	1.379(4)	C11	C12	1.380(5)
C2	C3	1.370(4)	C12	C13	1.400(5)
C3	C4	1.406(4)	C13	C14	1.382(4)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C12	O3	C15	117.8(3)	C8	C7	C4	128.1(3)
C13	O4	C16	117.8(2)	C7	C8	C9	125.7(3)
O1	N1	O2	122.7(3)	C10	C9	C8	120.3(3)
O1	N1	C1	119.4(3)	C10	C9	C14	118.0(3)
O2	N1	C1	117.9(3)	C14	C9	C8	121.7(3)
C2	C1	N1	120.1(3)	C9	C10	C11	121.5(3)
C6	C1	N1	118.5(3)	C12	C11	C10	119.8(3)
C6	C1	C2	121.4(3)	O3	C12	C11	125.2(3)
C3	C2	C1	119.5(3)	O3	C12	C13	115.0(3)
C2	C3	C4	120.8(3)	C11	C12	C13	119.7(3)
C3	C4	C7	122.7(3)	O4	C13	C12	115.3(3)
C5	C4	C3	118.0(3)	O4	C13	C14	124.5(3)
C5	C4	C7	119.3(3)	C14	C13	C12	120.2(3)
C6	C5	C4	121.5(3)	C13	C14	C9	120.7(3)
C5	C6	C1	118.7(3)				

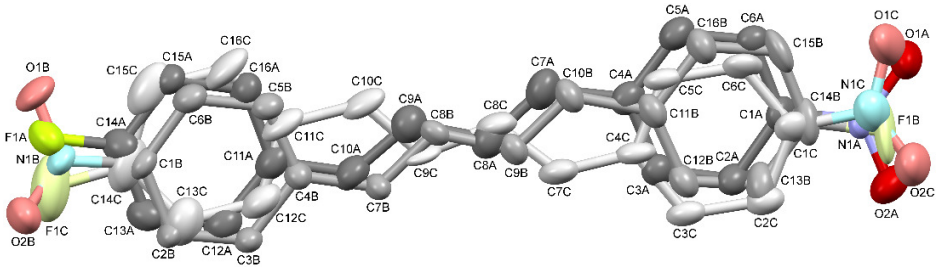
Table S11. Bond lengths and angles in compound **1e** (60:40 site occupancies, bond parameters of only the main component A are listed in the table, H atoms removed for clarity).



Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	O1A	1.233(10)	C6A	C1	1.399(9)
N1	O2A	1.209(10)	C7A	C8A	1.304(7)
N1	C1	1.460(4)	C7A	C4	1.467(6)
N2	C15A	1.439(12)	C8A	C9	1.436(6)
N2	C16A	1.451(14)	C10A	C11A	1.421(12)
N2	C12	1.379(4)	C10A	C9	1.342(10)
C2A	C3A	1.342(13)	C11A	C12	1.397(9)
C2A	C1	1.357(10)	C13A	C14A	1.408(12)
C3A	C4	1.440(9)	C13A	C12	1.422(10)
C5A	C6A	1.388(13)	C14A	C9	1.351(10)
C5A	C4	1.435(11)			

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O1A	N1	C1	118.1(6)	C14A	C13A	C12	120.8(7)
O2A	N1	O1A	122.4(7)	C9	C14A	C13A	122.1(8)
O2A	N1	C1	119.4(6)	C2A	C1	N1	118.5(5)
C15A	N2	C16A	117.2(7)	C2A	C1	C6A	122.3(6)
C12	N2	C15A	119.6(6)	C6A	C1	N1	119.2(5)
C12	N2	C16A	119.8(6)	C3A	C4	C7A	117.2(6)
C3A	C2A	C1	120.4(7)	C5A	C4	C3A	117.2(6)
C2A	C3A	C4	121.3(8)	C5A	C4	C7A	125.6(6)
C6A	C5A	C4	119.8(6)	C10A	C9	C8A	125.3(6)
C5A	C6A	C1	118.9(8)	C10A	C9	C14A	117.6(6)
C8A	C7A	C4	127.7(5)	C14A	C9	C8A	117.2(6)
C7A	C8A	C9	127.2(5)	N2	C12	C11A	122.3(5)
C9	C10A	C11A	124.0(7)	N2	C12	C13A	121.4(5)
C12	C11A	C10A	119.3(7)	C11A	C12	C13A	116.3(6)

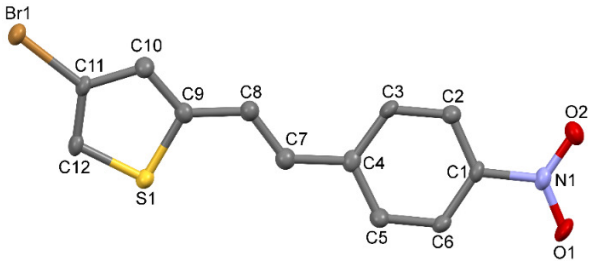
Table S12. Bond lengths and angles in compound **2a** (40:40:20 site occupancies, bond parameters of only the main component A are listed in the table, H atoms removed for clarity).



Atom	Atom	Length/Å	Atom	Atom	Length/Å
F1A	C14A	1.304(11)	C7A	C8A	1.283(15)
O1A	N1A	1.296(13)	C8A	C9A	1.433(12)
O2A	N1A	1.215(12)	C9A	C10A	1.313(13)
N1A	C1A	1.448(11)	C10A	C11A	1.399(11)
C1A	C2A	1.418(10)	C11A	C12A	1.388(15)
C1A	C6A	1.371(9)	C11A	C16A	1.366(11)
C2A	C3A	1.326(10)	C12A	C13A	1.353(12)
C3A	C4A	1.381(10)	C13A	C14A	1.310(11)
C4A	C5A	1.420(11)	C14A	C15A	1.439(10)
C4A	C7A	1.488(10)	C15A	C16A	1.343(10)
C5A	C6A	1.334(11)			

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O1A	N1A	C1A	120.9(7)	C7A	C8A	C9A	125.7(13)
O2A	N1A	O1A	121.9(9)	C10A	C9A	C8A	127.9(11)
O2A	N1A	C1A	117.1(9)	C9A	C10A	C11A	129.7(9)
C2A	C1A	N1A	119.5(7)	C12A	C11A	C10A	119.9(10)
C6A	C1A	N1A	116.3(8)	C16A	C11A	C10A	118.9(10)
C6A	C1A	C2A	124.1(8)	C16A	C11A	C12A	121.1(9)
C3A	C2A	C1A	117.8(7)	C13A	C12A	C11A	121.8(9)
C2A	C3A	C4A	120.0(7)	C14A	C13A	C12A	116.6(7)
C3A	C4A	C5A	120.6(7)	F1A	C14A	C13A	116.5(8)
C3A	C4A	C7A	119.2(8)	F1A	C14A	C15A	119.5(7)
C5A	C4A	C7A	120.2(7)	C13A	C14A	C15A	124.0(8)
C6A	C5A	C4A	120.8(7)	C16A	C15A	C14A	118.2(7)
C5A	C6A	C1A	116.7(8)	C15A	C16A	C11A	118.3(8)
C8A	C7A	C4A	129.8(10)				

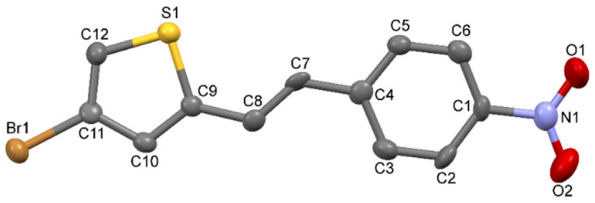
Table S13. Bond lengths and angles in compound **3a**·mono (only one of the two discrete molecules shown, H atoms removed for clarity).



Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C11	1.886(3)	C3	C4	1.405(4)
S1	C9	1.731(3)	C4	C5	1.397(4)
S1	C12	1.712(3)	C4	C7	1.461(4)
O1	N1	1.230(3)	C5	C6	1.378(4)
O2	N1	1.224(3)	C7	C8	1.333(4)
N1	C1	1.464(3)	C8	C9	1.444(4)
C1	C2	1.385(4)	C9	C10	1.361(4)
C1	C6	1.379(4)	C10	C11	1.407(4)
C2	C3	1.378(4)	C11	C12	1.351(4)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C12	S1	C9	92.25(14)	C6	C5	C4	121.3(3)
O1	N1	C1	118.1(3)	C5	C6	C1	118.5(3)
O2	N1	O1	123.2(2)	C8	C7	C4	128.1(3)
O2	N1	C1	118.7(3)	C7	C8	C9	124.5(3)
C2	C1	N1	119.5(3)	C8	C9	S1	121.6(2)
C6	C1	N1	118.1(3)	C10	C9	S1	110.5(2)
C6	C1	C2	122.4(3)	C10	C9	C8	127.9(3)
C3	C2	C1	118.5(3)	C9	C10	C11	112.5(3)
C2	C3	C4	121.0(3)	C10	C11	Br1	123.4(2)
C3	C4	C7	123.9(3)	C12	C11	Br1	122.4(2)
C5	C4	C3	118.4(3)	C12	C11	C10	114.2(3)
C5	C4	C7	117.7(3)	C11	C12	S1	110.6(2)

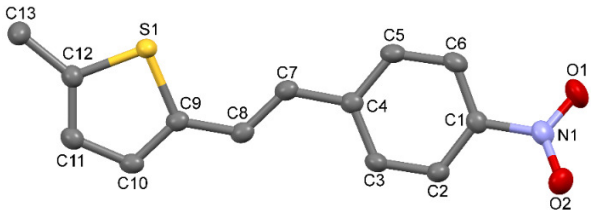
Table S14. Bond lengths and angles in compound **3a**·ortho (H atoms removed for clarity).



Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C11	1.897(10)	C3	C4	1.431(14)
S1	C9	1.749(10)	C4	C5	1.399(14)
S1	C12	1.714(10)	C4	C7	1.469(13)
O1	N1	1.220(12)	C5	C6	1.387(13)
O2	N1	1.227(12)	C7	C8	1.339(14)
N1	C1	1.476(12)	C8	C9	1.462(13)
C1	C2	1.383(14)	C9	C10	1.363(13)
C1	C6	1.397(14)	C10	C11	1.414(13)
C2	C3	1.387(13)	C11	C12	1.352(14)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C12	S1	C9	91.5(5)	C6	C5	C4	122.0(9)
O1	N1	O2	123.9(10)	C5	C6	C1	118.3(10)
O1	N1	C1	118.3(9)	C8	C7	C4	128.7(9)
O2	N1	C1	117.8(9)	C7	C8	C9	125.3(9)
C2	C1	N1	119.6(9)	C8	C9	S1	120.6(7)
C2	C1	C6	122.0(9)	C10	C9	S1	110.3(7)
C6	C1	N1	118.4(9)	C10	C9	C8	129.1(9)
C1	C2	C3	119.5(9)	C9	C10	C11	113.1(9)
C2	C3	C4	120.3(10)	C10	C11	Br1	123.7(7)
C3	C4	C7	122.8(9)	C12	C11	Br1	123.1(7)
C5	C4	C3	117.9(9)	C12	C11	C10	113.1(9)
C5	C4	C7	119.3(9)	C11	C12	S1	111.9(8)

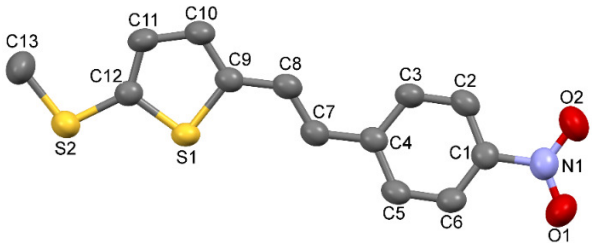
Table S15. Bond lengths and angles in compound **3b** (only one of the two discrete molecules shown, H atoms removed for clarity).



Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	C9	1.7352(14)	C5	C6	1.383(2)
S1	C12	1.7317(16)	C7	C8	1.342(2)
O1	N1	1.2299(19)	C8	C9	1.444(2)
O2	N1	1.2259(19)	C9	C10	1.370(2)
N1	C1	1.4612(19)	C10	C11	1.417(2)
C1	C2	1.385(2)	C11	C12	1.365(2)
C1	C6	1.382(2)	C12	C13	1.496(2)
C2	C3	1.376(2)	S2	C22	1.7399(14)
C3	C4	1.405(2)	S2	C25	1.7315(15)
C4	C5	1.407(2)	O3	N2	1.2252(19)
C4	C7	1.460(2)	O4	N2	1.2323(18)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C12	S1	C9	92.39(7)	C6	C5	C4	121.55(14)
O1	N1	C1	117.97(14)	C1	C6	C5	118.09(14)
O2	N1	O1	123.50(14)	C8	C7	C4	125.78(13)
O2	N1	C1	118.51(13)	C7	C8	C9	126.14(13)
C2	C1	N1	118.30(13)	C8	C9	S1	122.87(11)
C6	C1	N1	119.23(14)	C10	C9	S1	110.12(11)
C6	C1	C2	122.47(14)	C10	C9	C8	126.90(13)
C3	C2	C1	118.74(13)	C9	C10	C11	113.65(13)
C2	C3	C4	121.20(14)	C12	C11	C10	113.07(14)
C3	C4	C5	117.91(14)	C11	C12	S1	110.77(11)
C3	C4	C7	122.93(14)	C11	C12	C13	128.98(15)
C5	C4	C7	119.16(13)	C13	C12	S1	120.22(12)

Table S16. Bond lengths and angles in compound **3c** (H atoms removed for clarity).



Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	C9	1.739(3)	C3	C4	1.402(3)
S1	C12	1.728(3)	C4	C5	1.400(3)
S2	C12	1.740(3)	C4	C7	1.456(4)
S2	C13	1.783(3)	C5	C6	1.374(4)
O1	N1	1.222(3)	C7	C8	1.333(3)
O2	N1	1.226(3)	C8	C9	1.438(4)
N1	C1	1.461(3)	C9	C10	1.360(4)
C1	C2	1.378(4)	C10	C11	1.410(4)
C1	C6	1.377(3)	C11	C12	1.365(3)
C2	C3	1.371(4)			

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C12	S1	C9	92.14(12)	C6	C5	C4	121.5(2)
C12	S2	C13	101.69(14)	C5	C6	C1	118.8(2)
O1	N1	O2	123.1(3)	C8	C7	C4	126.8(2)
O1	N1	C1	118.1(2)	C7	C8	C9	127.0(2)
O2	N1	C1	118.8(3)	C8	C9	S1	121.53(19)
C2	C1	N1	119.1(2)	C10	C9	S1	110.0(2)
C6	C1	N1	119.2(2)	C10	C9	C8	128.5(2)
C6	C1	C2	121.7(3)	C9	C10	C11	114.2(2)
C3	C2	C1	119.0(2)	C12	C11	C10	112.8(2)
C2	C3	C4	121.3(2)	S1	C12	S2	117.46(14)
C3	C4	C7	122.8(2)	C11	C12	S1	110.9(2)
C5	C4	C3	117.6(2)	C11	C12	S2	131.7(2)
C5	C4	C7	119.6(2)				

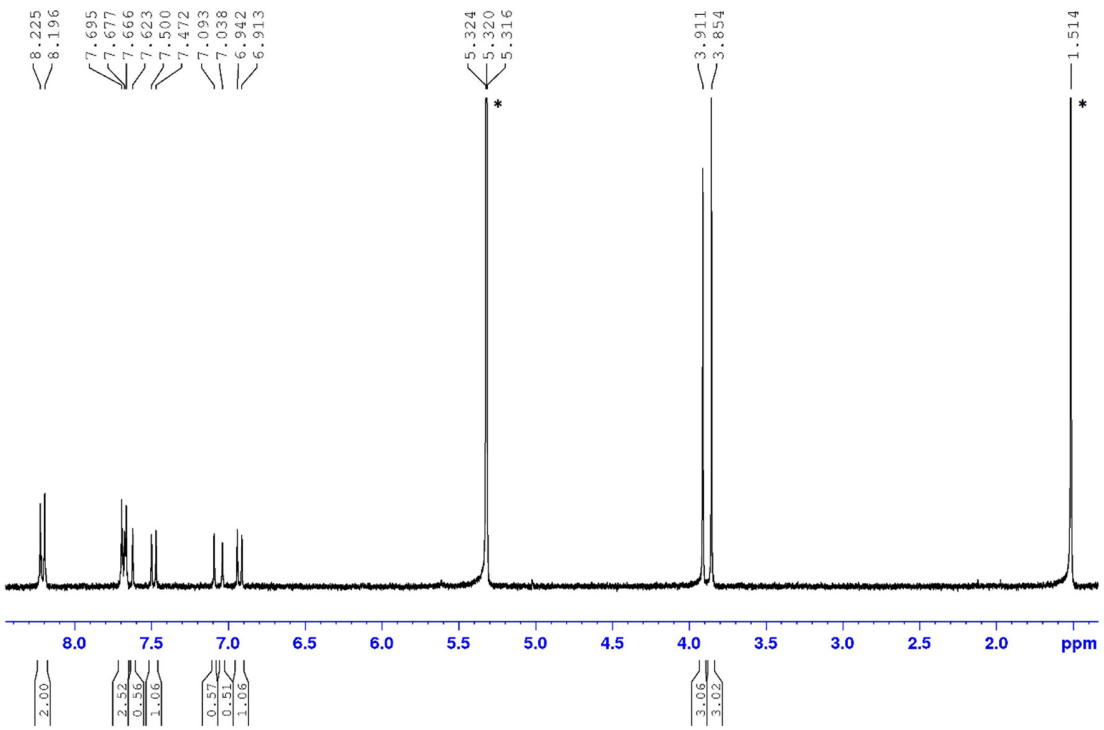


Figure S1. ^{1}H NMR spectrum of compound **1a** (*solvent and solvent impurity peaks).

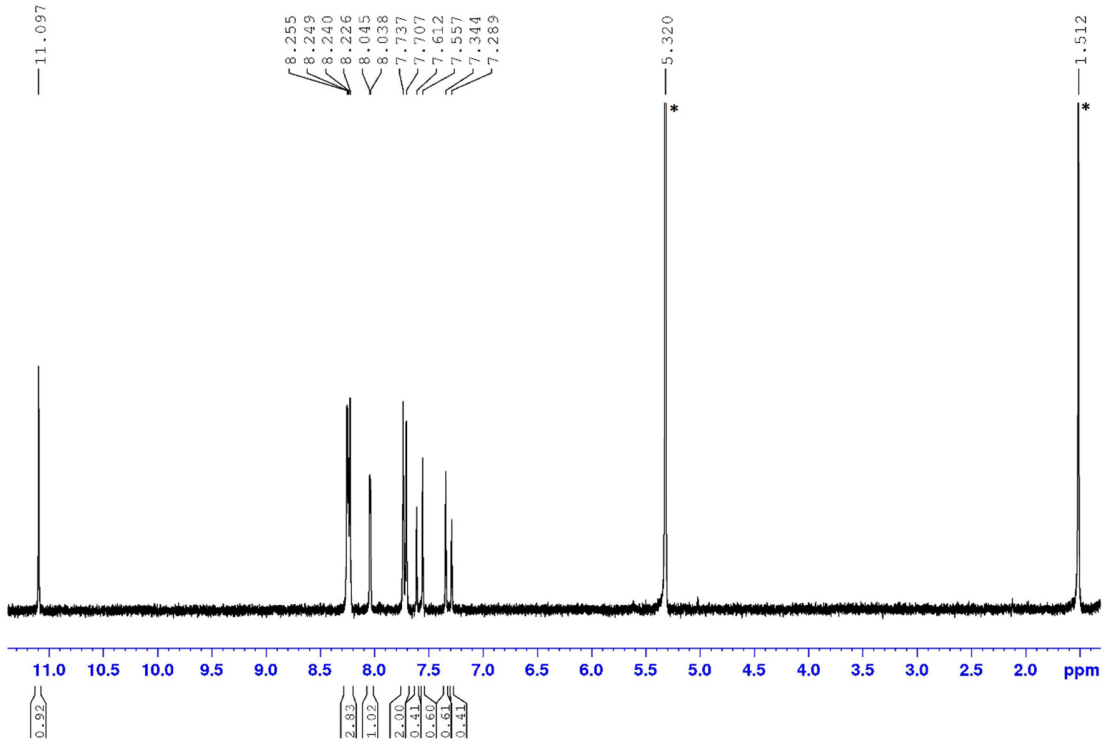


Figure S2. ^{1}H NMR spectrum of compound **1b** (*solvent and solvent impurity peaks).

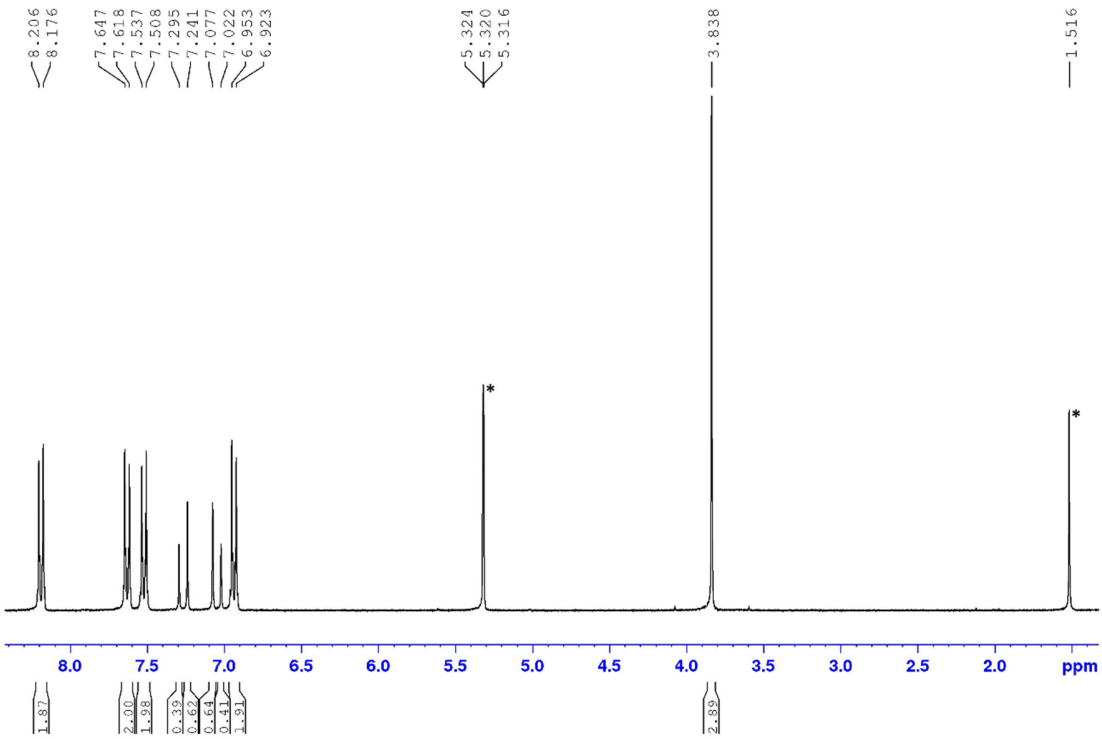


Figure S3. ^{1}H NMR spectrum of compound **1c** (*solvent and solvent impurity peaks).

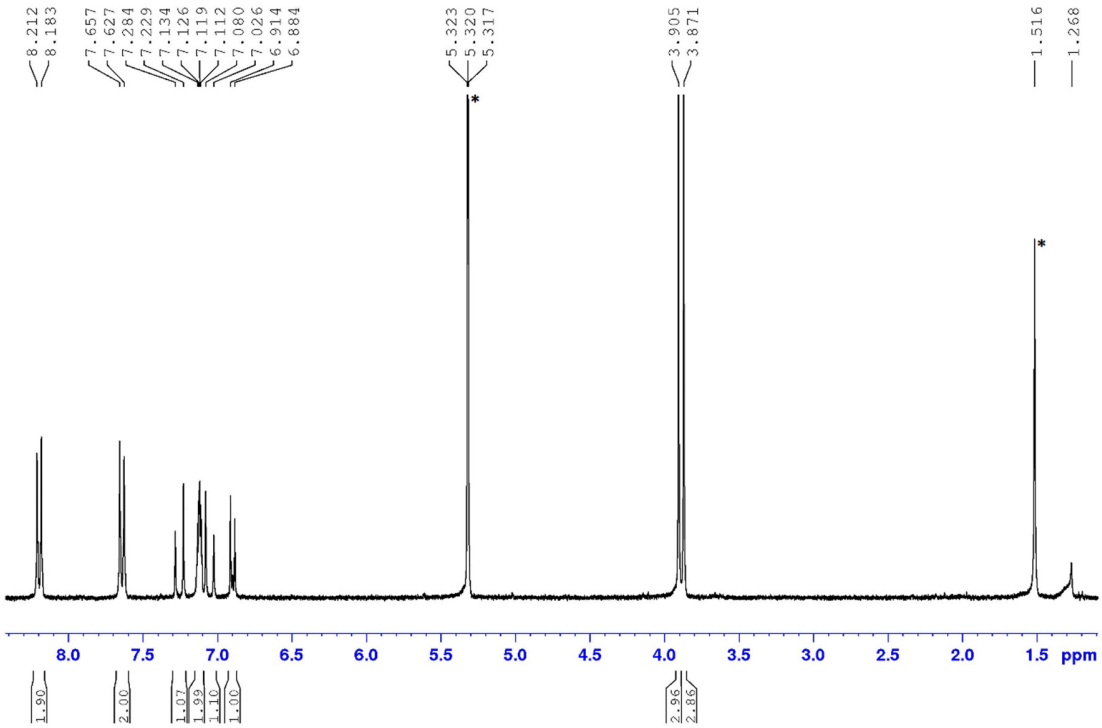


Figure S4. ^{1}H NMR spectrum of compound **1d** (*solvent and solvent impurity peaks).

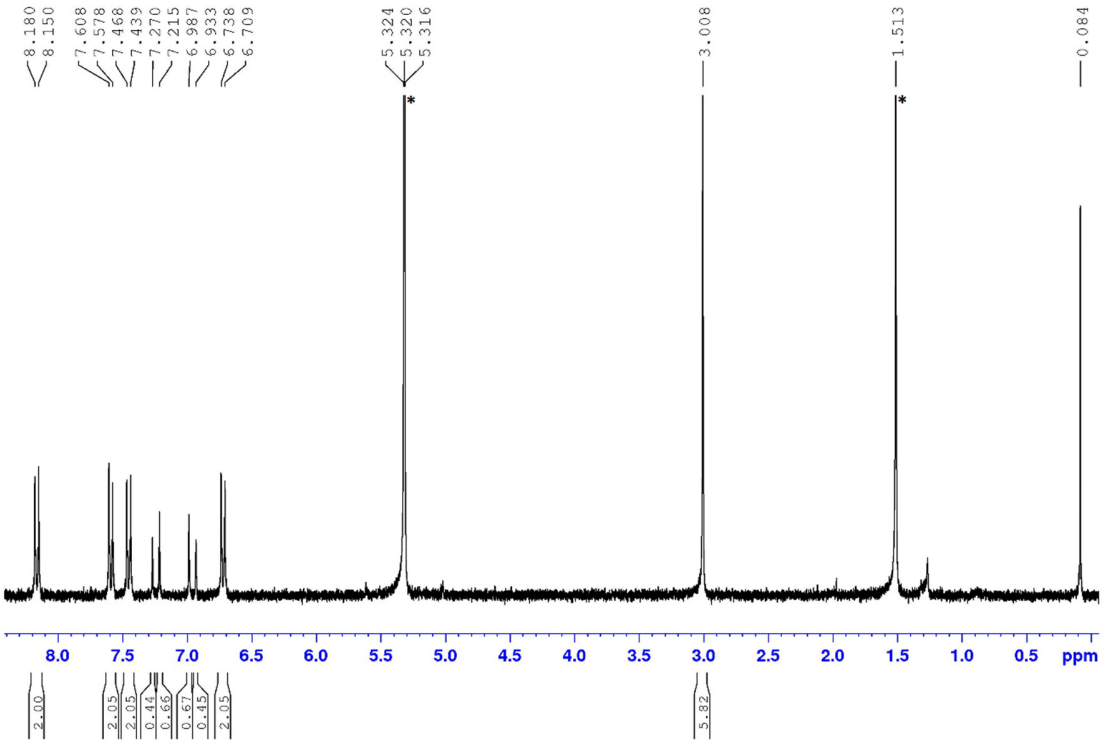


Figure S5. ^{1}H NMR spectrum of compound **1e** (*solvent and solvent impurity peaks).

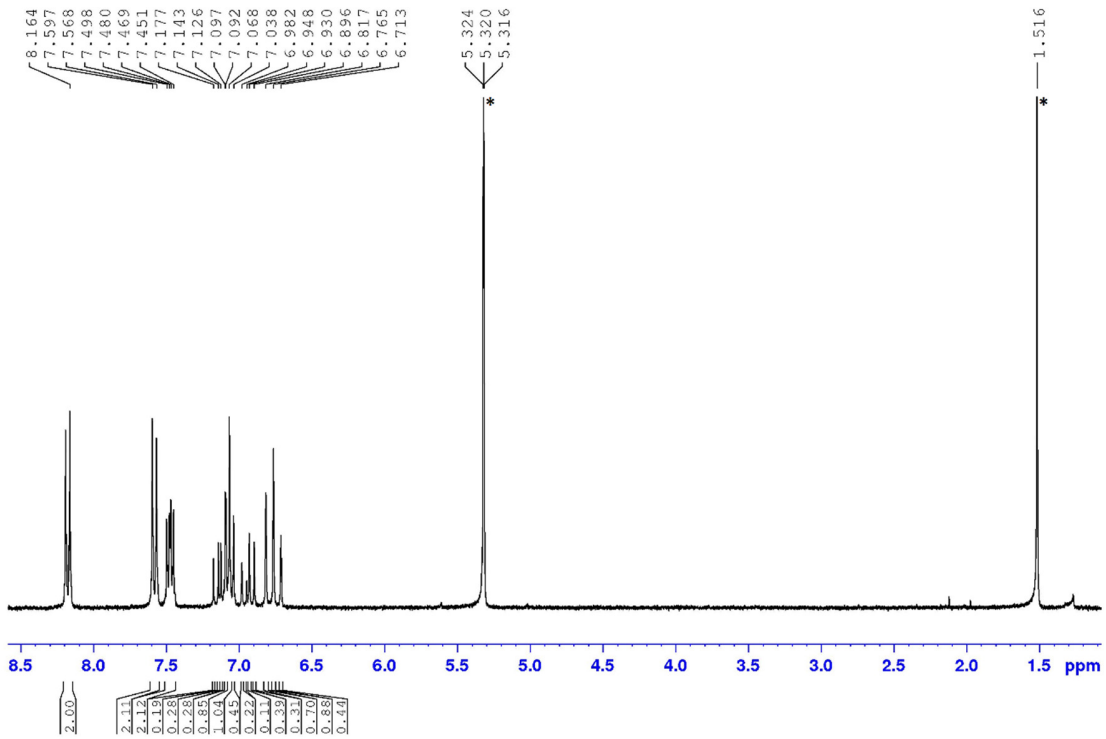


Figure S6. ^{1}H NMR spectrum of compound **2a** (*solvent and solvent impurity peaks).

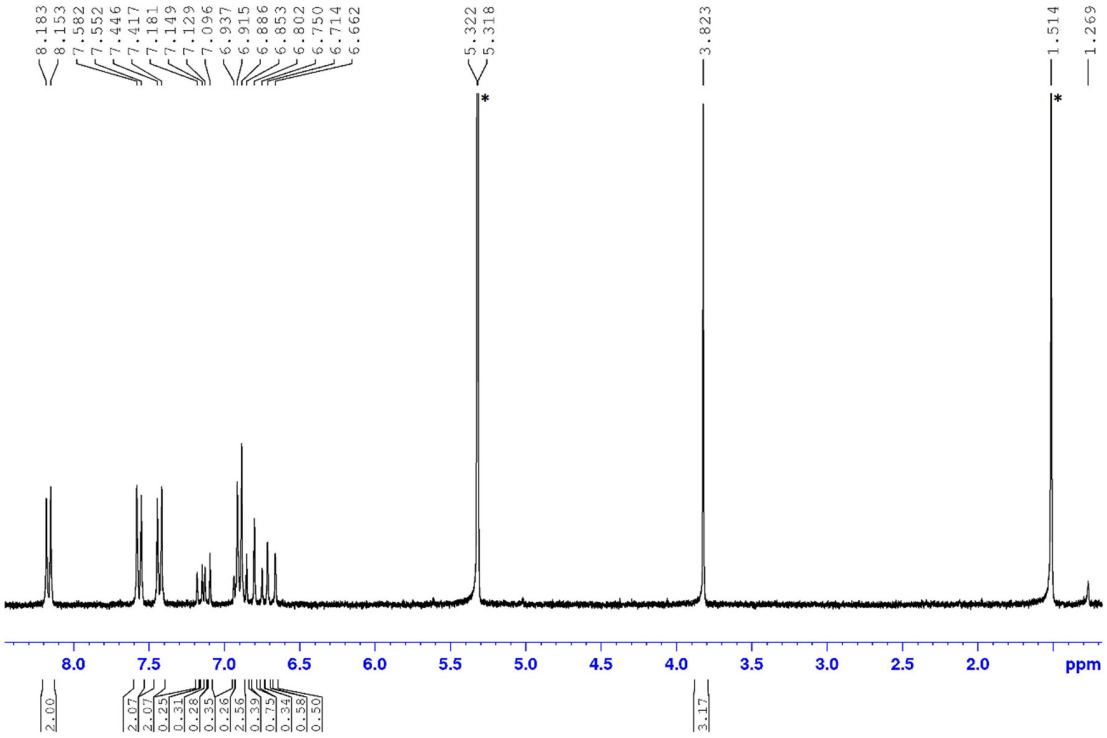


Figure S7. [1]H NMR spectrum of compound **2b** (*solvent and solvent impurity peaks).

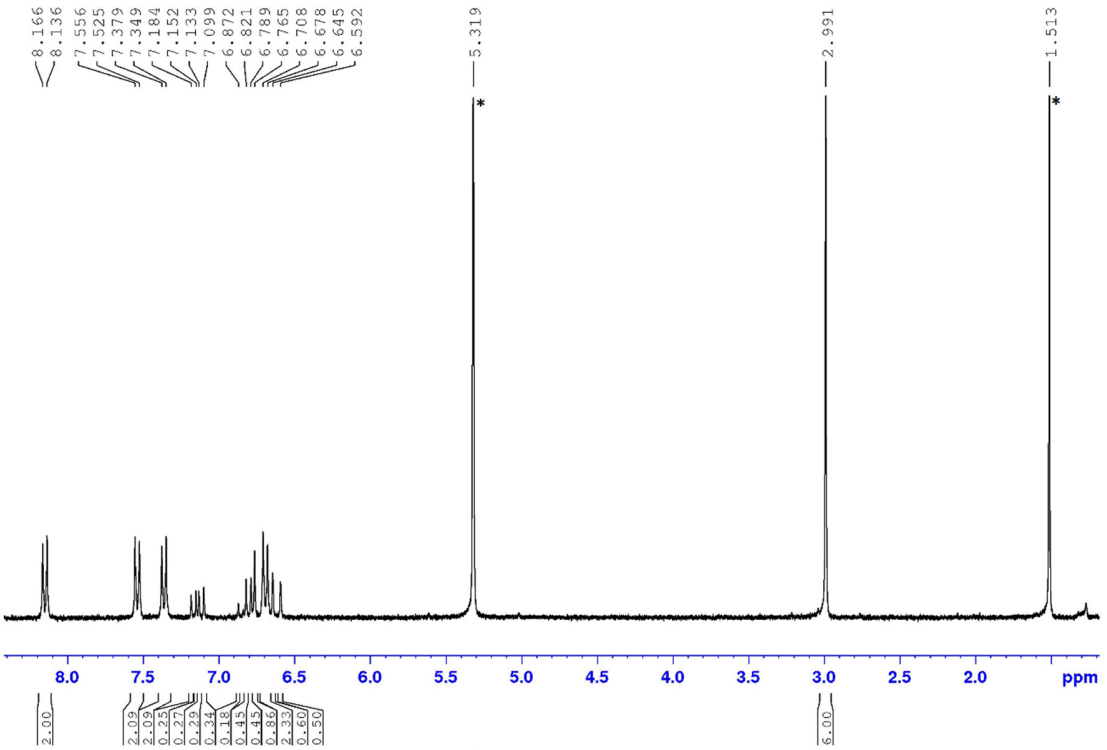


Figure S8. [1]H NMR spectrum of compound **2c** (*solvent and solvent impurity peaks).

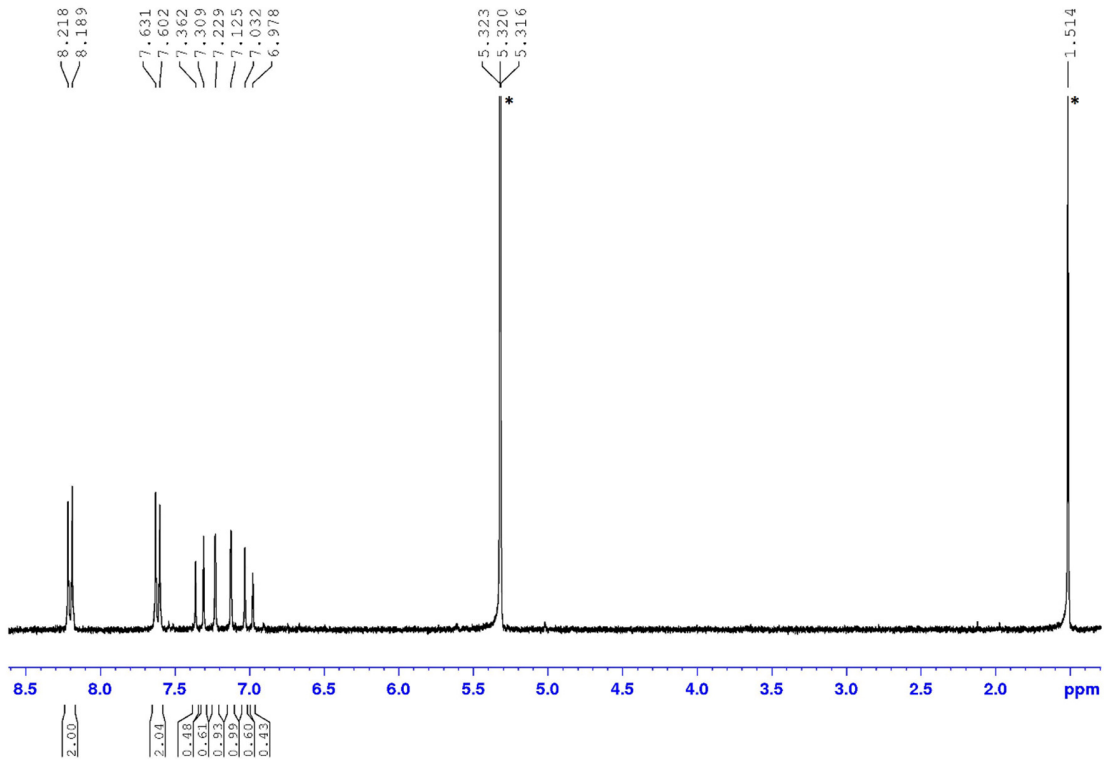


Figure S9. ^{1}H NMR spectrum of compound **3a** (*solvent and solvent impurity peaks).

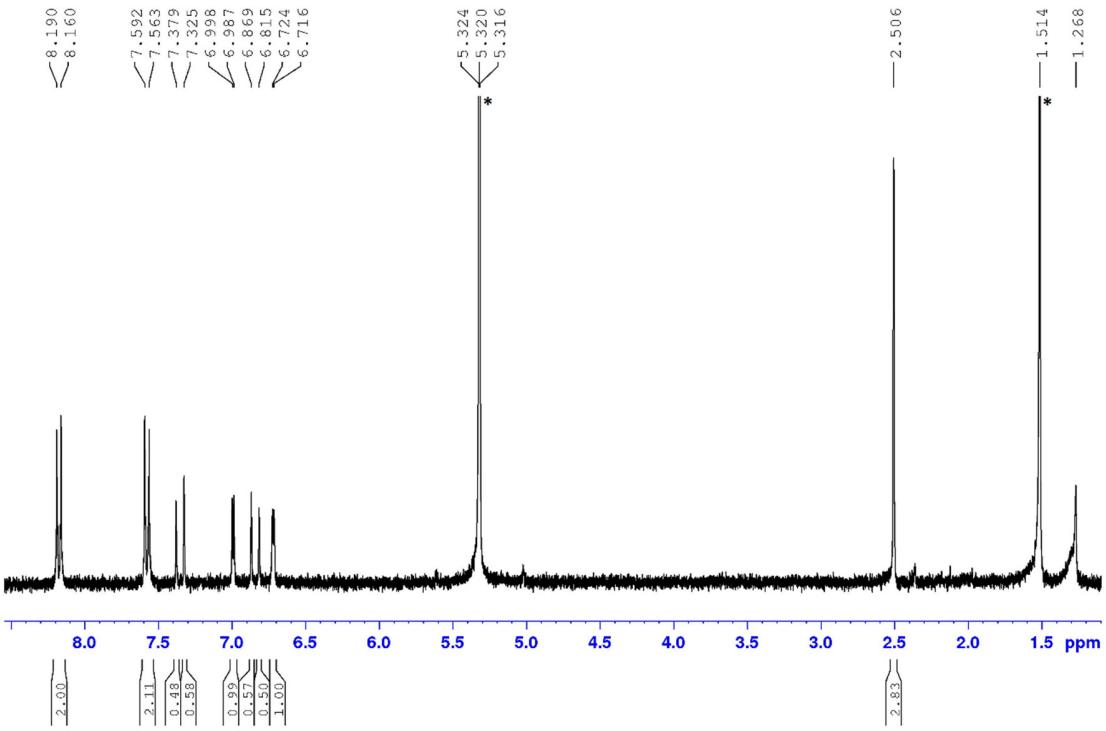


Figure S10. ^{1}H NMR spectrum of compound **3b** (*solvent and solvent impurity peaks).

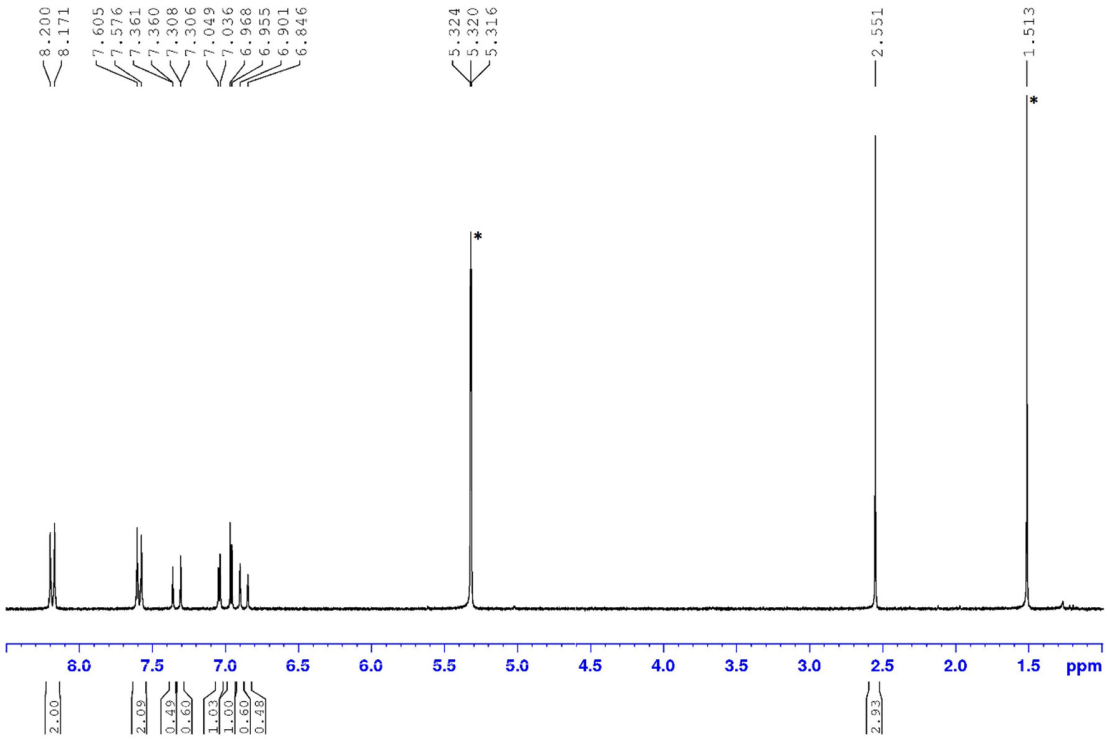


Figure S11. ^{1}H NMR spectrum of compound **3c** (*solvent and solvent impurity peaks).

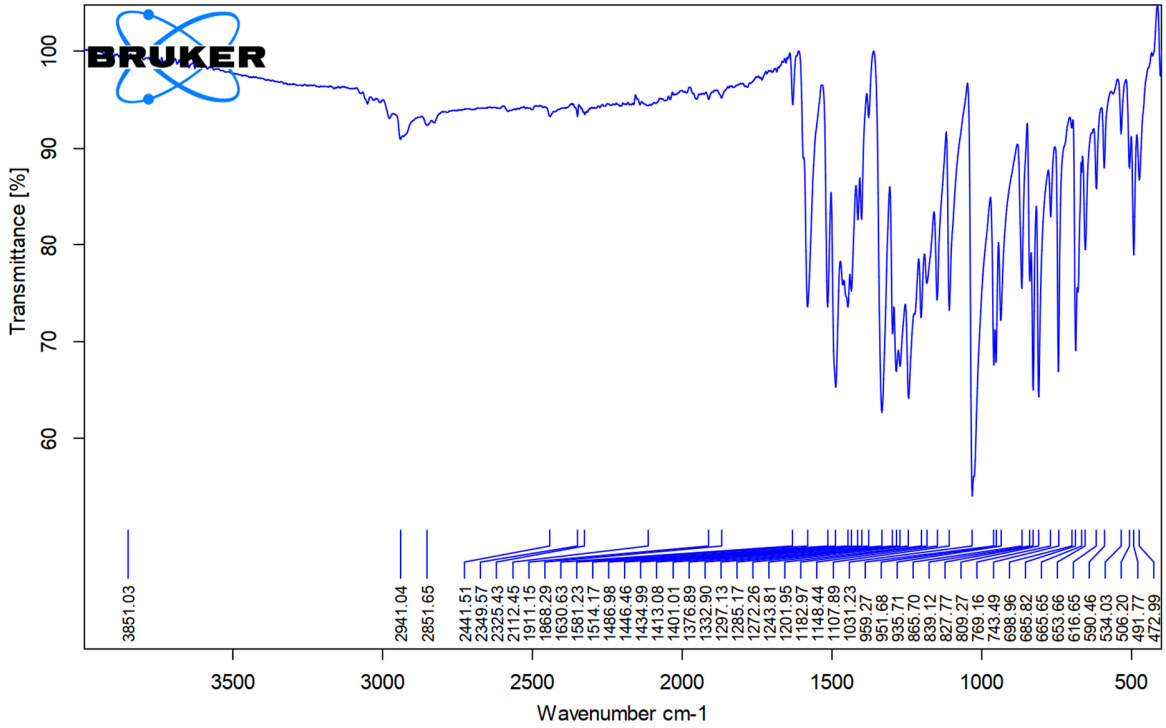


Figure S12. IR spectrum of compound **1a**.

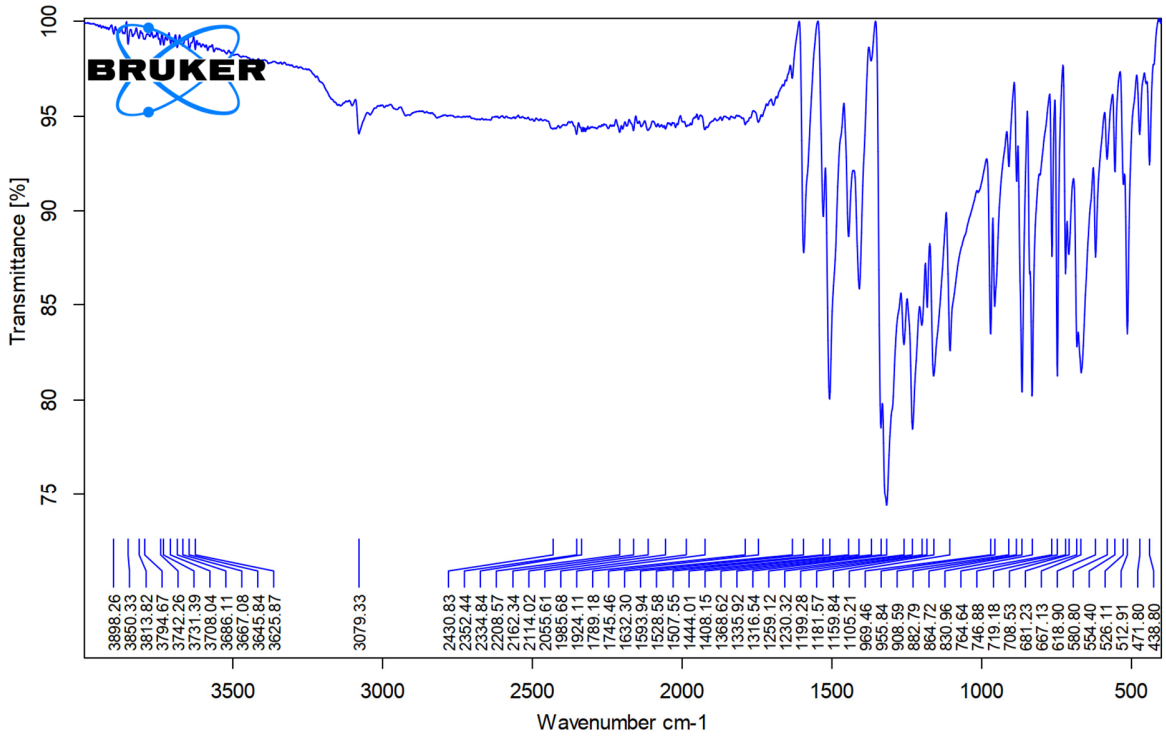


Figure S13. IR spectrum of compound **1b**.

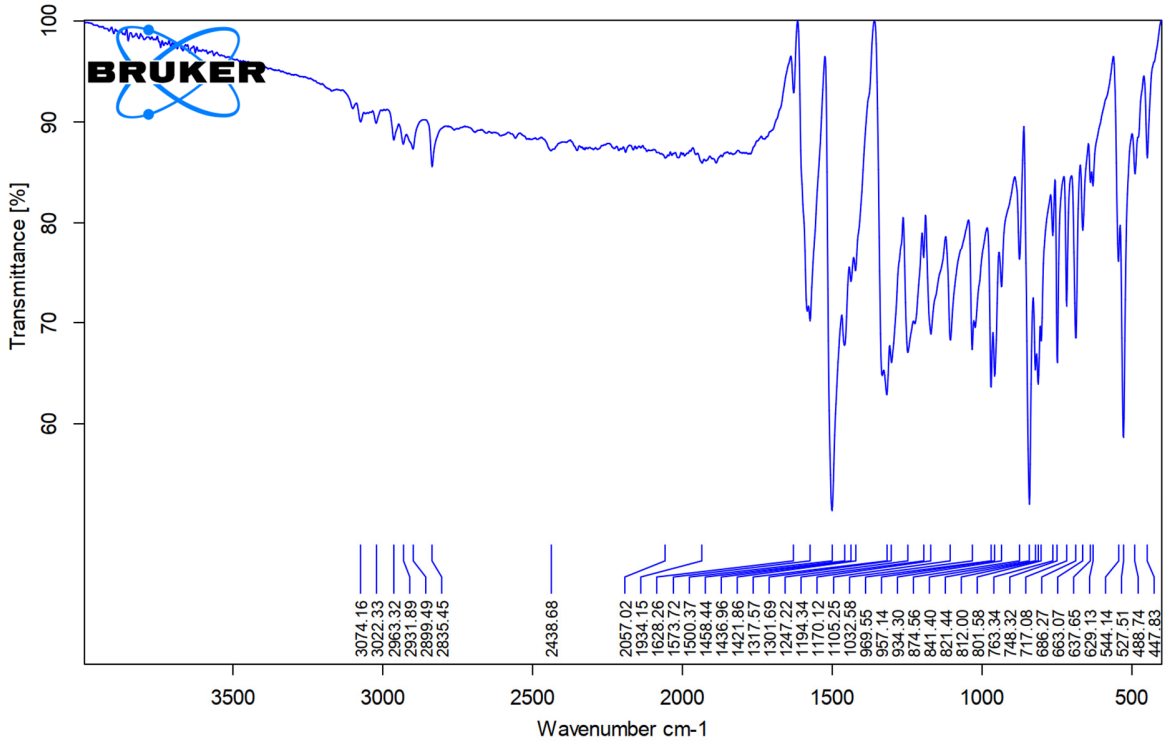


Figure S14. IR spectrum of compound **1c**.

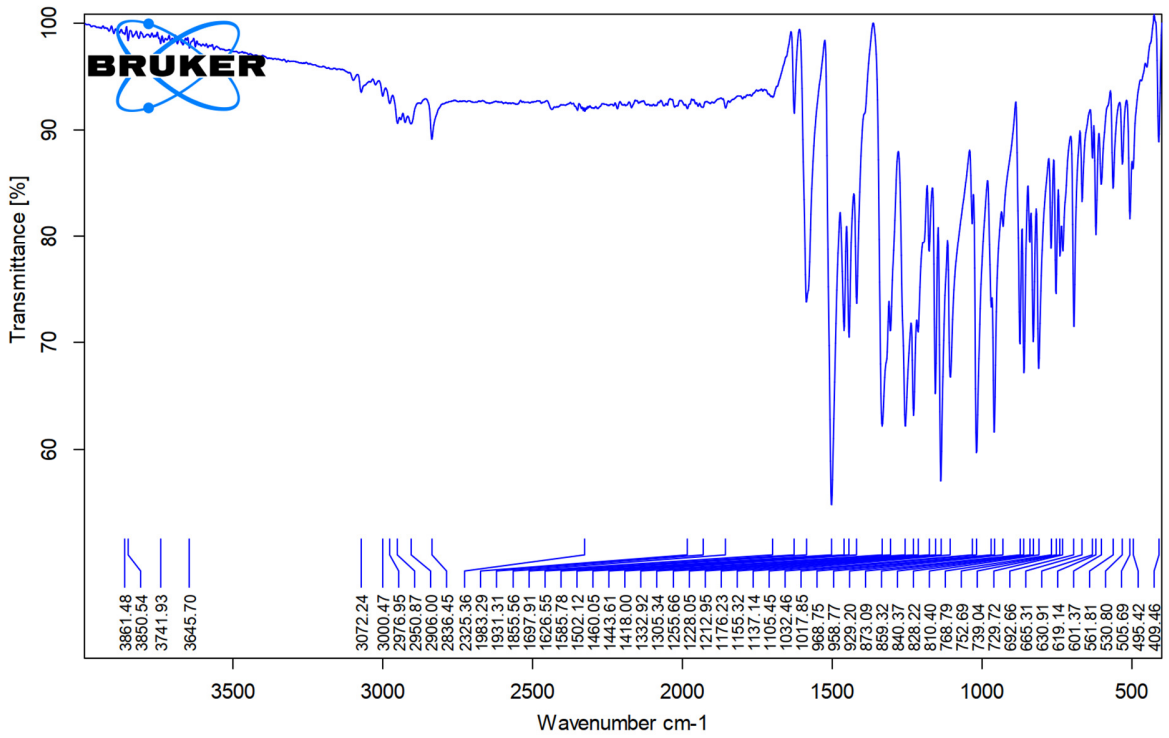


Figure S15. IR spectrum of compound **1d**.

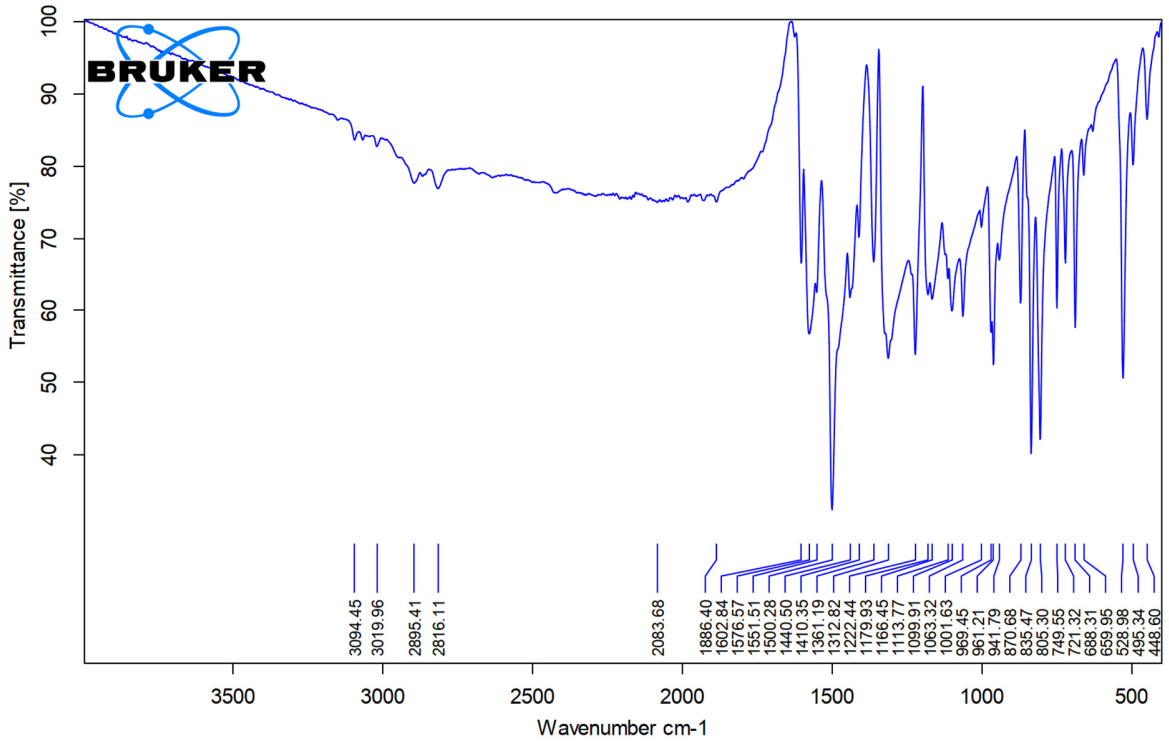


Figure S16. IR spectrum of compound **1e**.

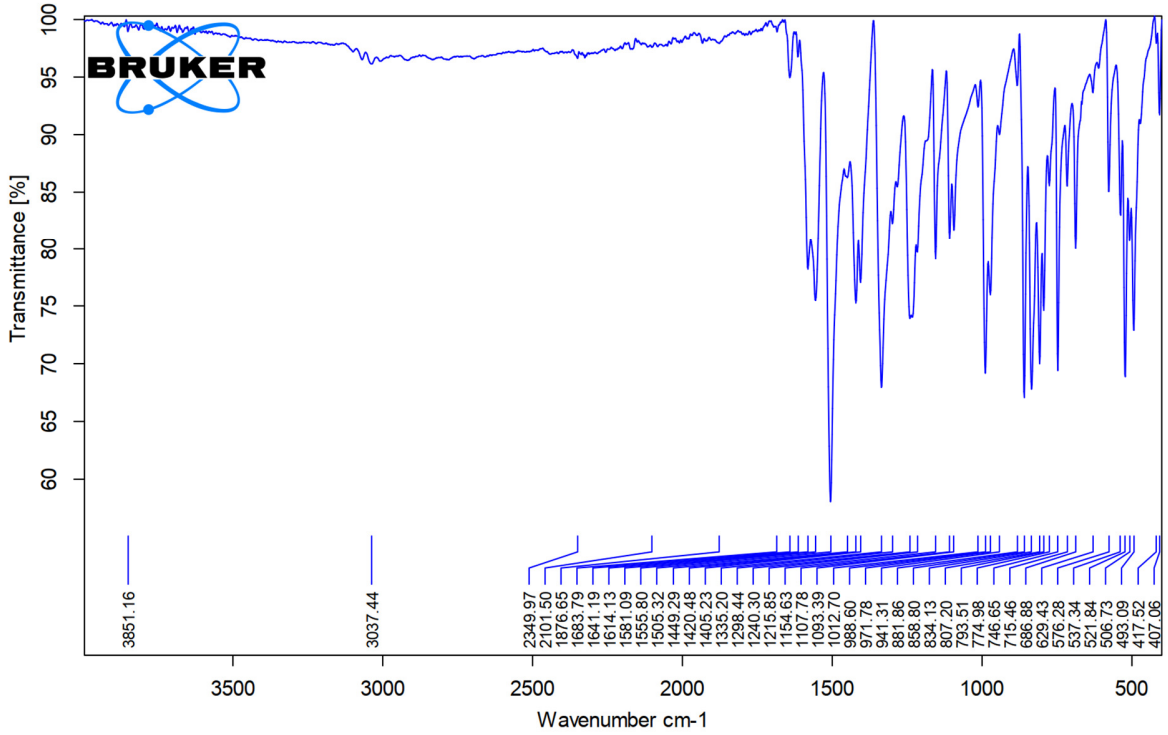


Figure S17. IR spectrum of compound **2a**.

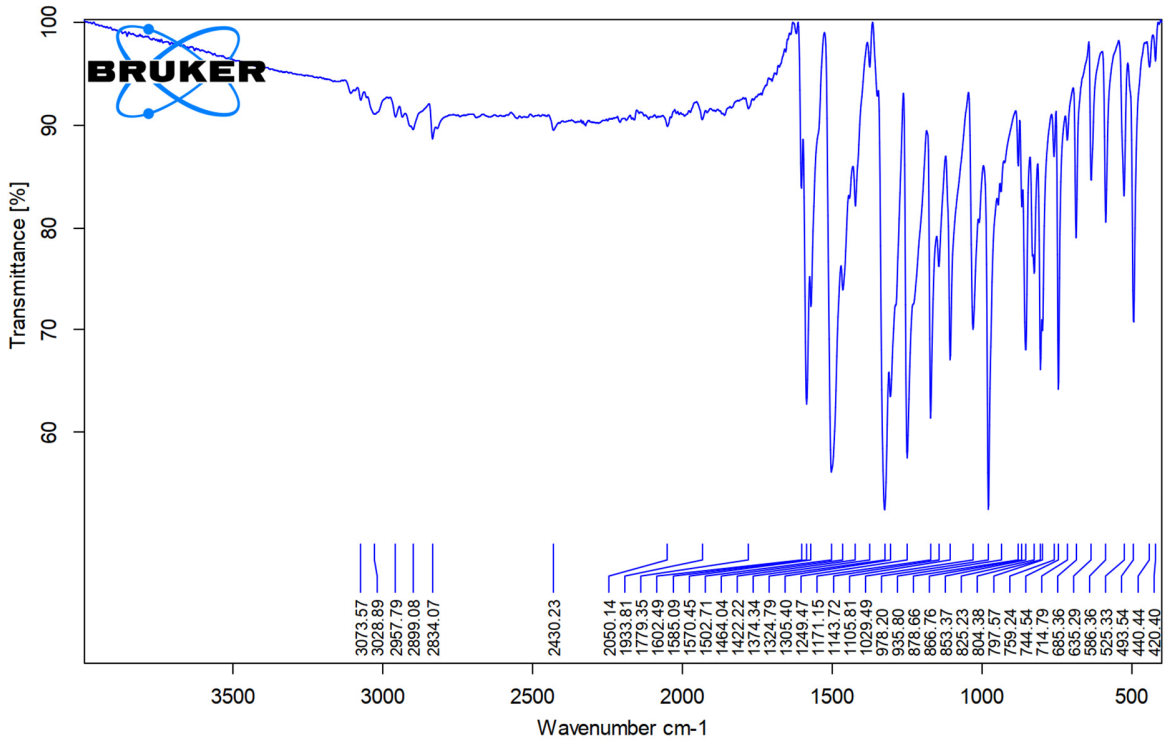


Figure S18. IR spectrum of compound **2b**.

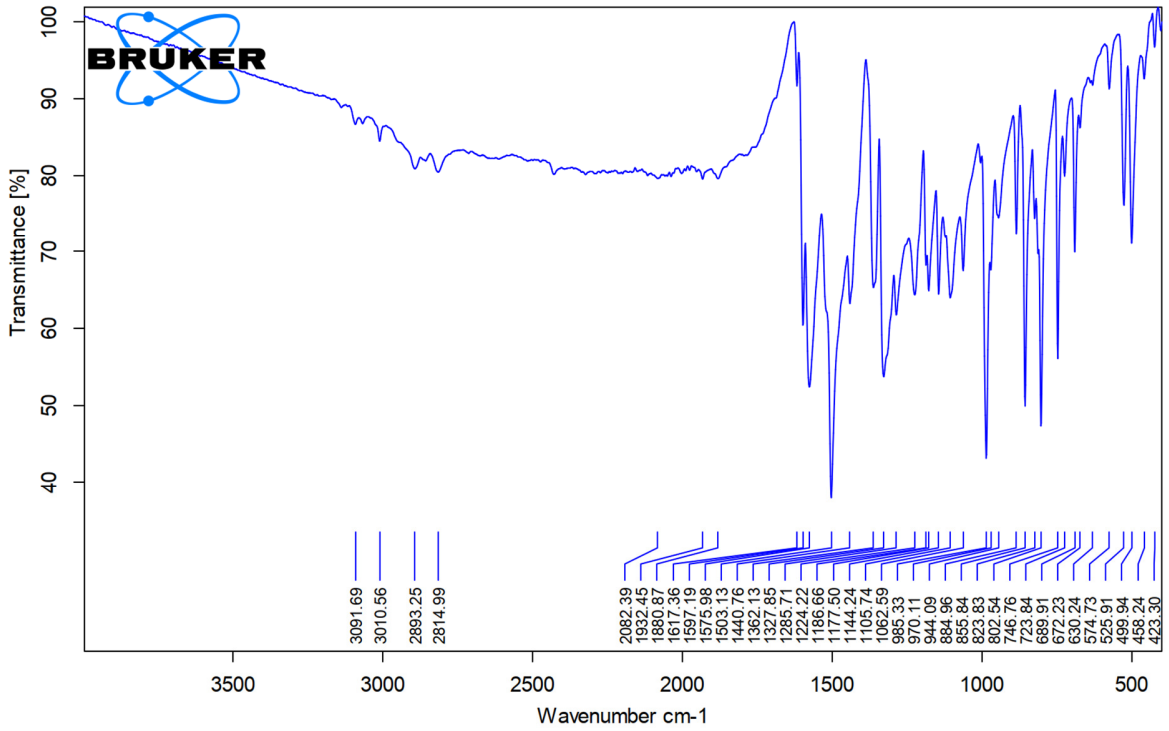


Figure S19. IR spectrum of compound **2c**.

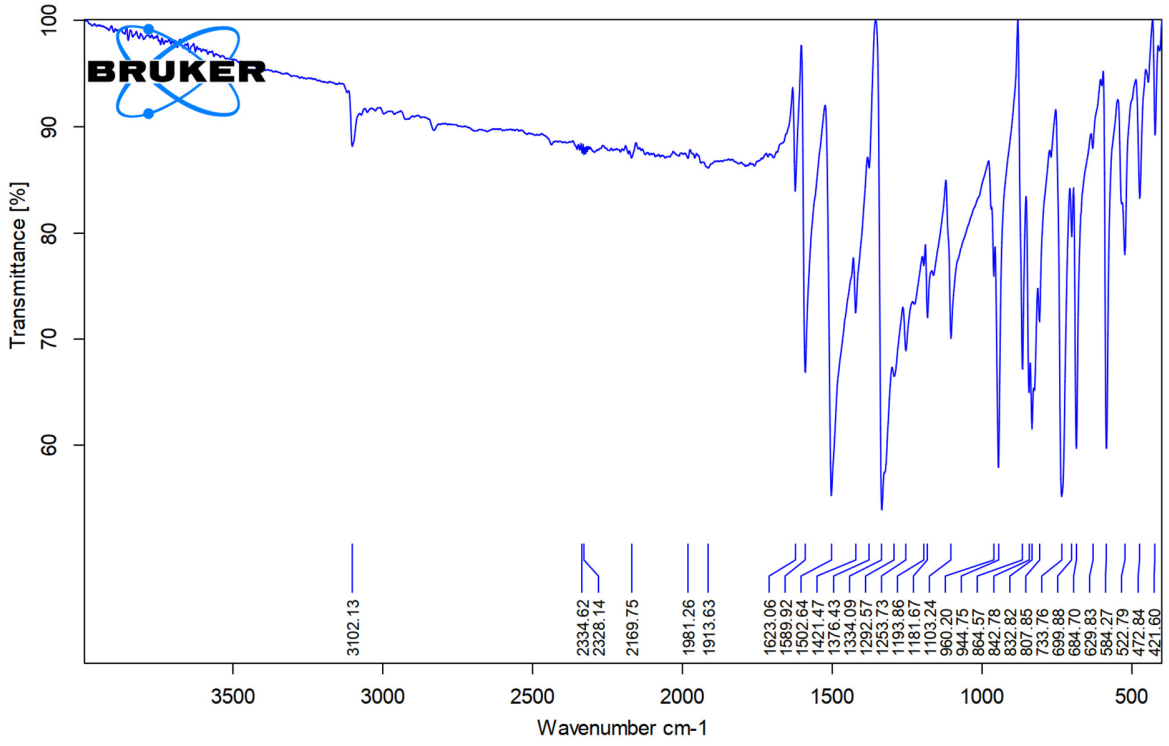


Figure S20. IR spectrum of compound **3a**.

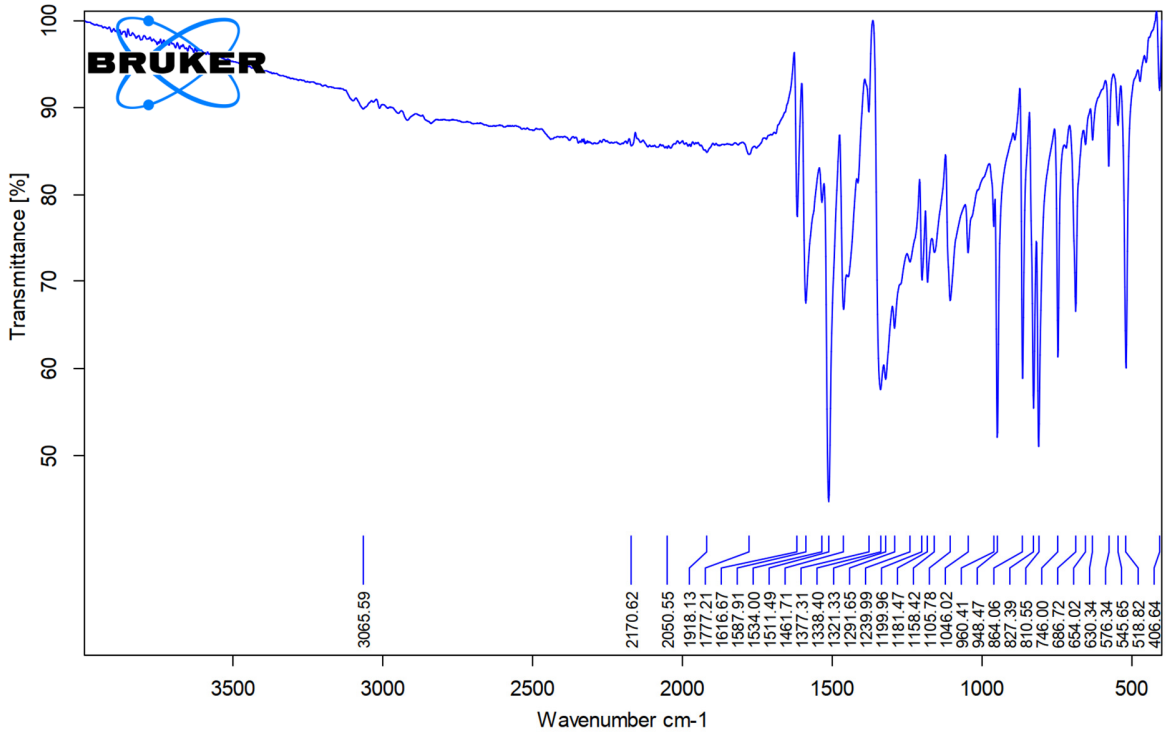


Figure S21. IR spectrum of compound **3b**.

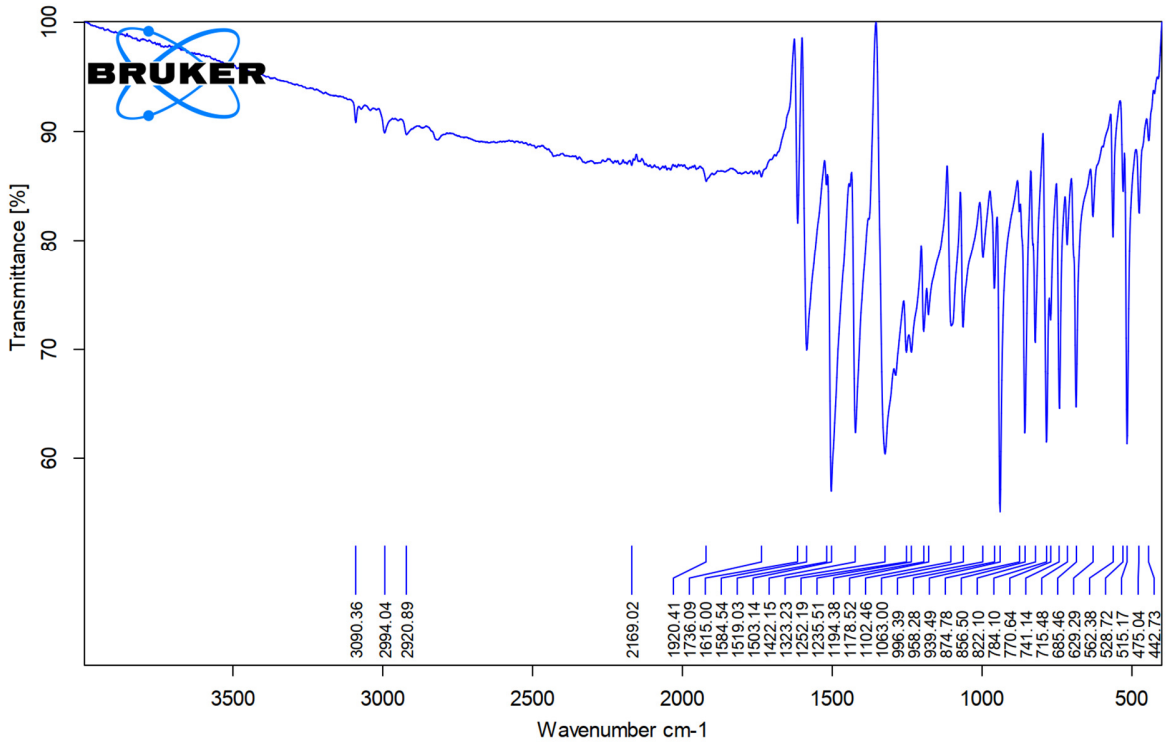


Figure S22. IR spectrum of compound **3c**.