Supporting Information

Microwave assisted, $BF_3 \cdot OEt_2$ catalyzed efficient synthesis of tosylhydrazones and SC-XRD study of two of the synthesized tosylhydrazones

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1. Spectral data of synthesized compounds

N'-(diphenylmethylene)-4-methylbenzenesulfonohydrazide (**3a**). ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.44 (s, 1H), 7.81 (d, J = 8 Hz, 2H), 7.52-7.5 (m, 3H), 7.43 (d, J =8 Hz, 2H), 7.38- 7.31 (m, 3H), 7.25- 7.20 (m, 4H), 2.39 (s, 3H).^{13}C NMR (100 MHz, DMSO-d_6) δ 153.2, 143.4, 136.7, 136.1, 131.9, 131.1, 129.5, 128.4, 127.7, 21.1. HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{20}H_{18}N_2O_2S$ 350.1089; found 350.1085.

N'-(4-chlorophenyl(phenyl)methylene)-4-methylbenzenesulfonohydrazide (**3b**). ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.58 (s, 1H), 7.83 (d, J =8.4 Hz, 2H), 7.54-7.52 (m, 3H), 7.43-7.40 (m, 4H), 7.28-7.21 (m, 4H), 2.38 (s, 3H).^{13}C NMR (100 MHz, DMSO-d_6) δ 153.2, 143.4, 136.0, 134.5, 132.1, 130.9, 129.6, 128.9, 128.8, 128.5, 127.7, 127.2, 21.1. HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{20}H_{17}ClN_2O_2S$ 383.0699; found 383.0695.

N'-(bis(4-chlorophenyl)methylene)-4-methylbenzenesulfonohydrazide (**3c**). ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.71 (s, 1H), 7.82 (d, J =8.4 Hz, 2H), 7.58 (d, J =12 Hz, 2H), 7.43-7.39 (m, 4H), 7.29- 7.25 (m, 4H), 2.37 (s, 3H).^{13}C NMR (100 MHz, DMSO-d_6) δ 151.8, 143.5, 136.0, 135.6, 134.6, 134.4, 130.9, 129.6, 129.1, 128.8, 128.6, 127.6, 21.1. HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{20}H_{16}ClN_2O_2S$ 418.0310; found 418.0313.

N'-(4-bromophenyl(phenyl)methylene)-4-methylbenzenesulfonohydrazide (**3d**). ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.60 (s, 1H), 7.80 (d, J =8.4 Hz, 2H), 7.72 (d, J =8 Hz, 2H), 7.43 (d, J =8.4 Hz, 2H), 7.39-7.32 (m, 3H), 7.26 (d, J =6.8 Hz, 2H), 7.17 (d, J =8.4 Hz, 2H), 2.39 (s, 3H).^{13}C NMR (100 MHz, DMSO-d_6) δ 153.1, 143.4, 136.7, 136.1, 131.9, 131.1, 129.5, 128.4, 127.7, 127.2, 122.9, 21.1. HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{20}H_{17}BrN_2O_2S$ 428.0194; found 428.0192.

N'-(bis(4-methoxyphenyl)methylene)-4-methylbenzenesulfonohydrazide (**3e**). ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.03 (s, 1H), 7.75 (d, J =8.4 Hz, 2H), 7.36 (d, J =8.4 Hz, 2H), 7.15 (d, J =8.8 Hz, 2H), 7.07-7.00 (m, 4H), 6.81 (d, J =8.8 Hz, 2H), 3.76 (s, 3H), 3.67(s, 3H), 2.31(s, 3H).^{13}C NMR (100 MHz, DMSO-d_6) δ 161.3, 160.6, 155.7, 144.5, 136.4,131.0, 130.5, 130.3,129.7, 128.5, 125.2, 115.0, 114.4, 55.9, 21.7. HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{22}H_{22}N_2O_4S$ 410.1300; found 410.1300.

4-methyl-N'-(1-phenylethylidene)benzenesulfonohydrazide (**3g**). ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.51 (s, 1H), 7.81 (d, J = 8 Hz, 2H), 7.63-7.61 (m, 2H), 7.41 (d, J = 8.4 Hz, 2H), 7.38-7.36 (m, 5H), 2.37 (s, 3H), 2.17 (s, 3H).^{13}C NMR (100 MHz, DMSO-d_6) δ 153.3, 143.5, 137.4, 136.3, 129.4, 128.4, 127.6, 125.9, 21.0, 14.3. HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{15}H_{17}N_2O_2S$ 289.1011; found 289.1013.

N'-(1-(2-aminophenyl)ethylidene)-4-methylbenzenesulfonohydrazide (**3i**). ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.52 (s, 1H), 7.78 (d, J = 8.4, 2H), 7.40 (d, J = 8.4 Hz, 2H), 7.29 (d, J = 9.6 Hz, 1H), 7.03-6.99 (m, 1H), 6.64 (d, J = 8.4, 1H), 6.52-6.48 (m, 1H).^{13}C NMR (100 MHz, DMSO-d_6) δ 157.0, 147.1, 143.5, 136.0, 129.7, 129.6, 129.1, 127.4, 117.5, 116.0, 114.8, 21.0, 15.4. HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{15}H_{17}N_3O_2S$ 303.1041; found 303.1043.

4-methyl-N'-(propan-2-ylidene)benzenesulfonohydrazide (**3j**). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.98 (s, 1H), 7.72 (d, J = 8.4 Hz, 2H), 7.37 (d, J = 8.4 Hz, 2H), 2.36 (s, 3H), 1.78 (s, 6H).^{13}C NMR (100 MHz, DMSO-d_6) δ 147.2, 143.5, 136.0, 127.4, 116.0, 26.1, 21.0, 18.2. HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{10}H_{15}N_2O_2S$ 227.0854; found 227.0851.

N'-benzylidene-4-methylbenzenesulfonohydrazide (**3k**). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.45(s, 1H), 7.91(s, 1H), 7.69(d, J = 8.4 Hz, 1H), 7.56-7.54 (m, 2H), 7.41-7.37(m, 6H), 2.35(s, 3H).^{13}C NMR (100 MHz, DMSO-d_6) δ 147.0, 143.5, 136.1, 135.1, 133.7, 130.1, 129.7, 129.5, 128.8, 127.7, 127.2, 126.7, 21.0. HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{14}H_{15}N_2O_2S$ 275.0854; found 275.0853.

N'-(4-chlorobenzylidene)-4-methylbenzenesulfonohydrazide (**3l**). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.55(s, 1H), 7.90(s, 1H) 7.75(d, J = 8.8 Hz, 2H), 7.40(d, J= 8 Hz, 2H), 2.36 (s, 3H).^{13}C NMR (100 MHz, DMSO-d_6) δ 145.7, 143.6, 136.1, 134.5, 132.6, 129.7, 128.9, 128.4, 127.2, 21.0. HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{14}H_{14}ClN_2O_2S$ 309.0470; found 309.0472.

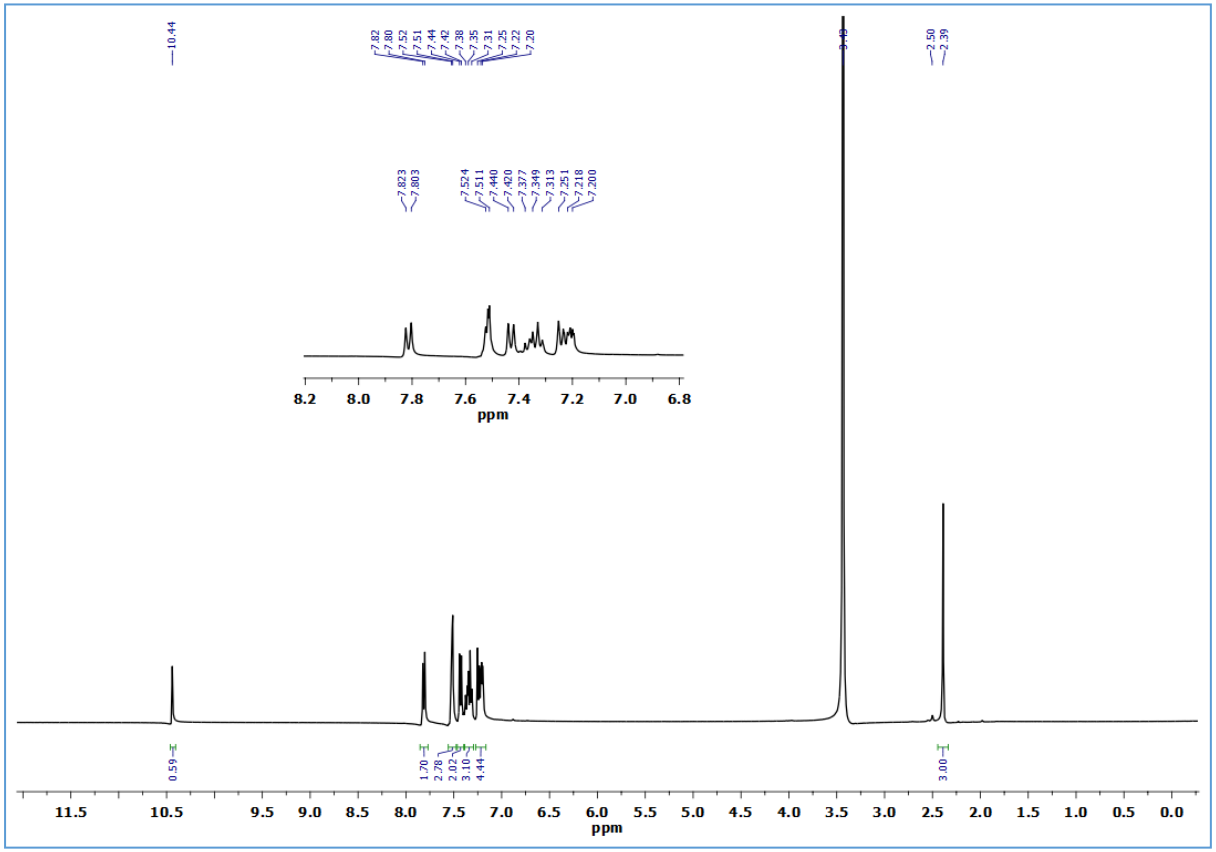
N'-(4-dimethylamino)benzylidene)-4-methylbenzenesulfonohydrazide (**3n**). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.03(s, 1H), 7.76-7.73 (m, 3H), 7.39-7.34 (m, 4H), 6.66 (d, J = 8.8 Hz, 2H), 2.91 (s, 6H), 2.34 (s, 3H).^{13}C NMR (100 MHz, DMSO-d_6) δ 148.6, 145.1, 143.5, 139.4, 137.2, 129.7, 127.2, 122.2, 119.3, 45.4, 21.0. HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{16}H_{20}N_3O_2S$ 318.1282; found 318.1280.

N'-(4-methoxybenzylidene)-4-methylbenzenesulfonohydrazide (**3o**). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.25 (s, 1H), 7.86 (s, 1H) 7.77 (d, J = 8.4 Hz, 2H), 7.50 (d, J = 8.8 Hz, 2H), 7.39 (d, J = 8.4 Hz, 2H), 6.94 (d, J = 8.8 Hz, 2H), 3.75 (s, 3H), 2.34 (s, 1H).^{13}C NMR (100 MHz, DMSO-d_6) δ 160.9, 147.0, 143.3, 136.2, 129.6, 128.4, 127.3, 126.3, 114.1, 56.3, 21.0. HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{15}H_{16}N_2O_3S$ 304.0882; found 304.0883.

4-methyl-N'-(napthalen-1-ylmethylene)benzenesulfonohydrazide (**3p**). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.61(s, 1H), 8.59 (d, J = 8 Hz, 1H), 8.53 (s, 1H), 7.93 (d, J = 8 Hz, 2H), 7.87 (d, J = 8 Hz, 2H), 7.72 (d, J = 6.8 Hz, 1H), 7.61-7.48 (m, 3H) 7.40 (d, J = 8.4 Hz, 2H), 2.29 (1s, 3H).^{13}C NMR (100 MHz, DMSO-d_6) δ 147.4, 143.6, 136.1, 133.4, 130.6, 129.7, 129.5, 128.9, 128.7, 128.2, 127.7, 127.4, 125.4, 124.2, 21.0. HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{18}H_{17}N_2O_2S$ 325.1011; found 325.1012.

N'-(furan-2-ylmethylene)-4-methylbenzenesulfonohydrazide (**3q**). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.43 (s, 1H), 7.78-7.72 (m, 4H), 7.40 (d, J = 8 Hz, 2H), 6.79 (d, J = 3.2 Hz, 1H) 6.56-6.54 (m, 1H), 2.35 (s, 3H).^{13}C NMR (100 MHz, DMSO-d_6) δ 148.6, 145.1, 143.5, 136.9, 136.1, 129.7, 127.2, 113.9, 112.0, 21.0. HRMS (ESI-TOF) m/z: $[M + H]^+$calcd for $C_{12}H_{13}N_2O_3S$ 265.0652; found 265.0651.

2. ^{1}H &^{13}C NMR and mass spectra of synthesized compounds:



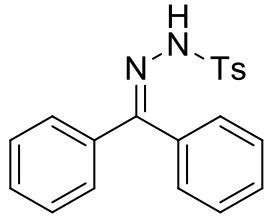
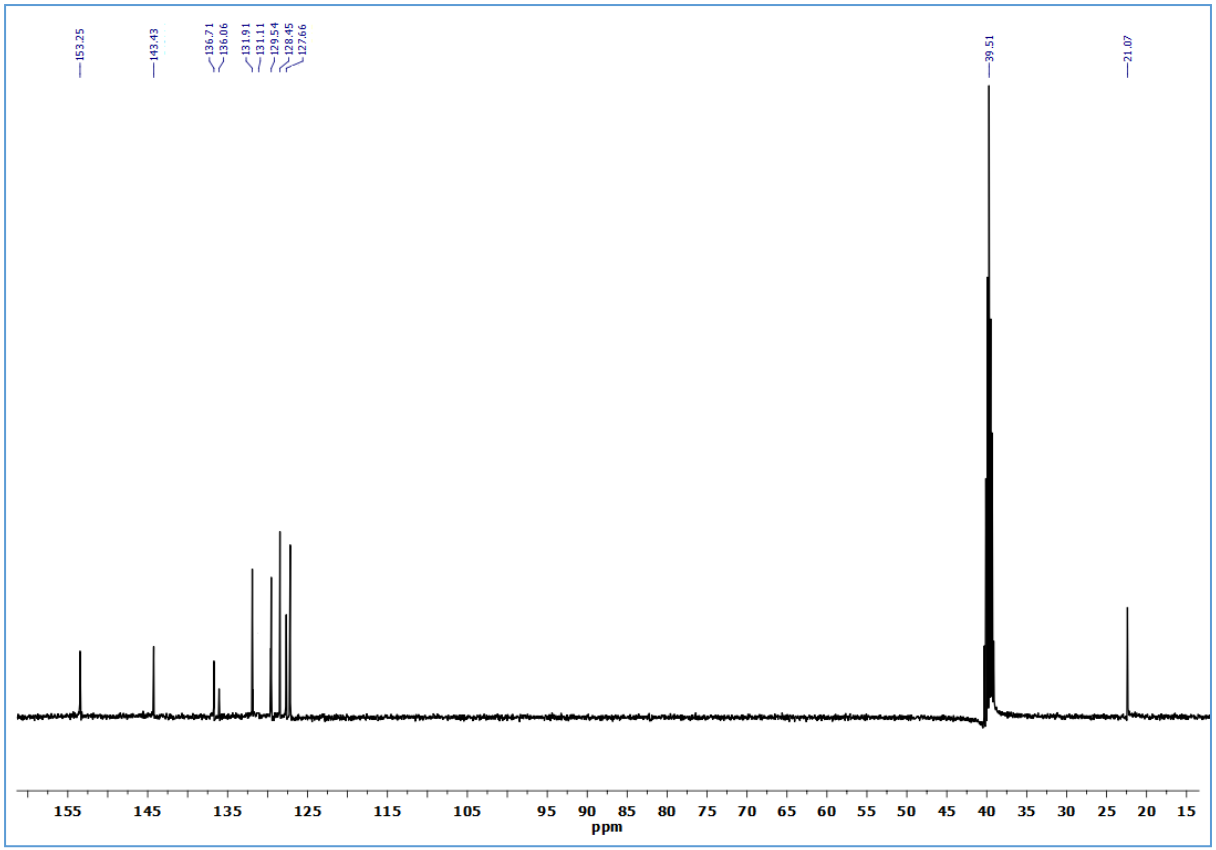


Fig. 1: ^{1}H NMR spectrum of **3a**



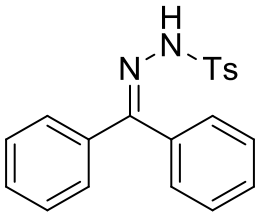
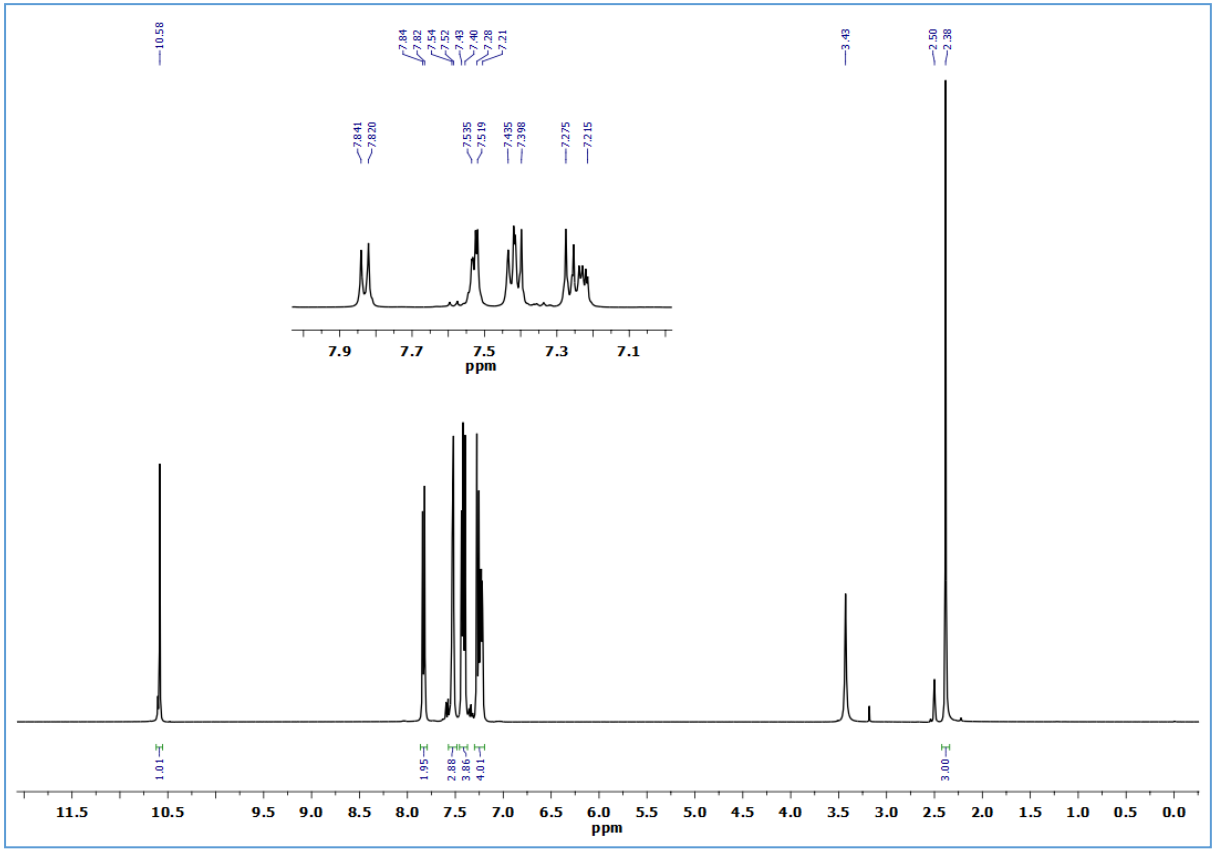


Fig. 2: ^{13}C NMR spectrum of **3a**



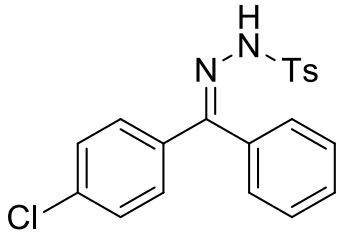
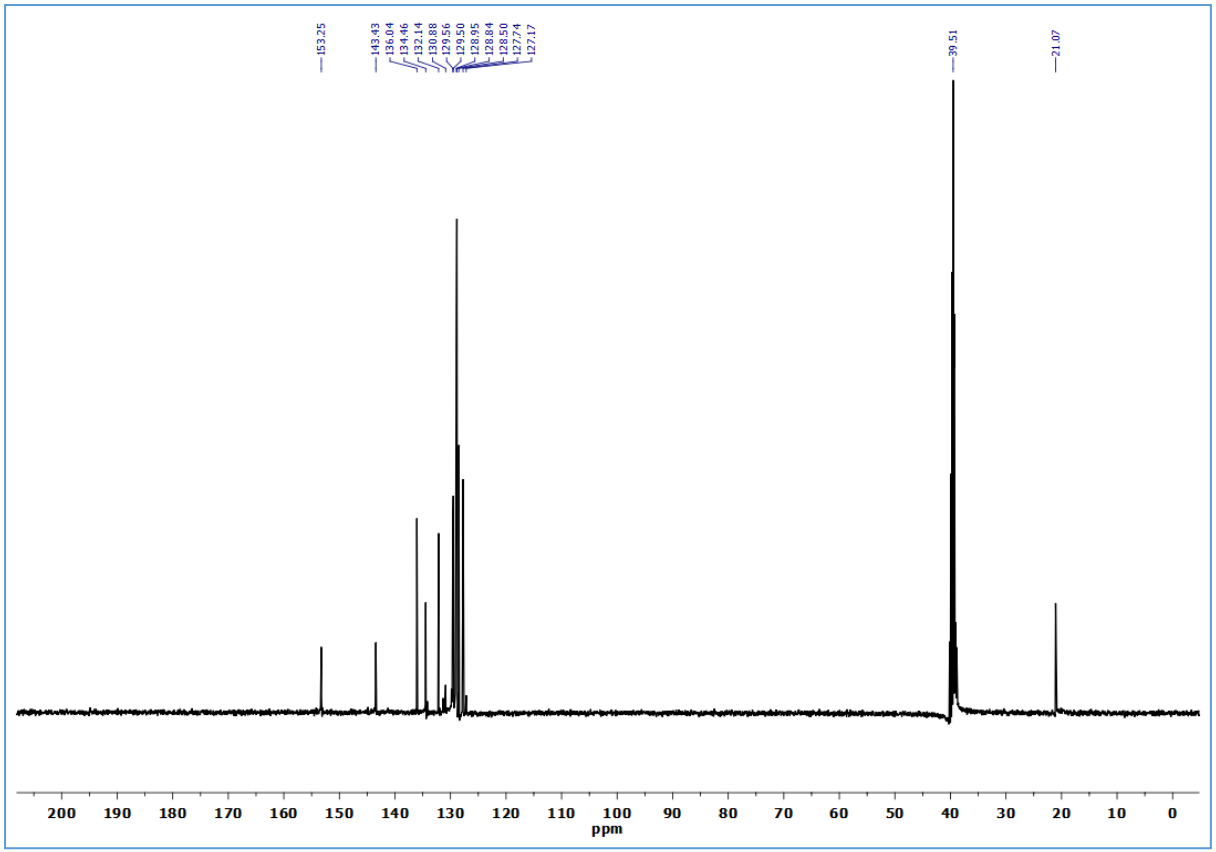


Fig. 3: ^{1}H NMR spectrum of **3b**



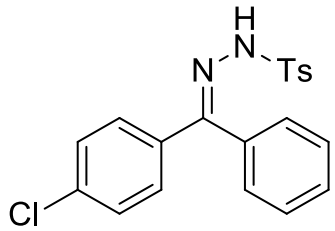
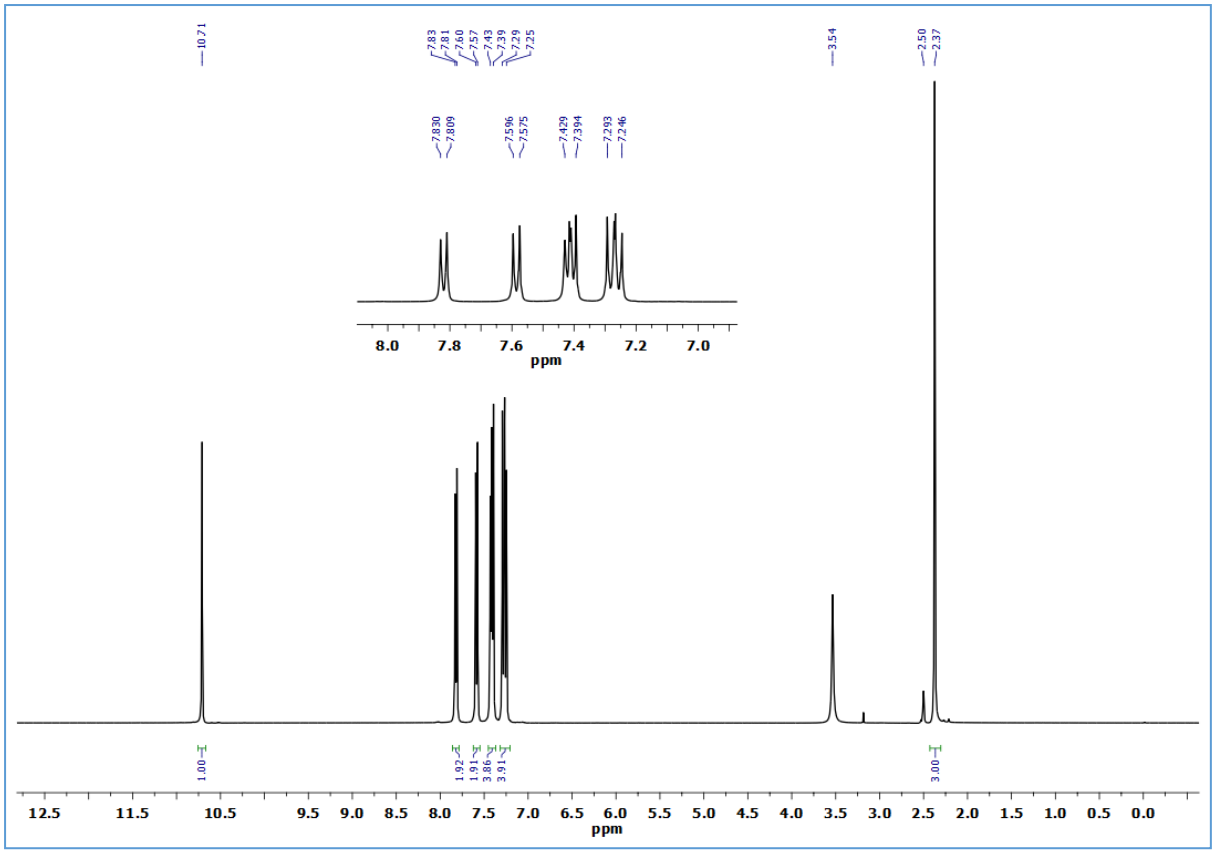


Fig. 4: ^{13}C NMR spectrum of **3b**



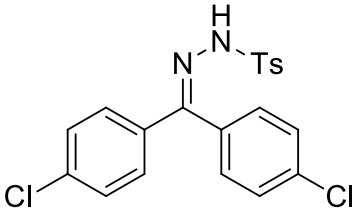
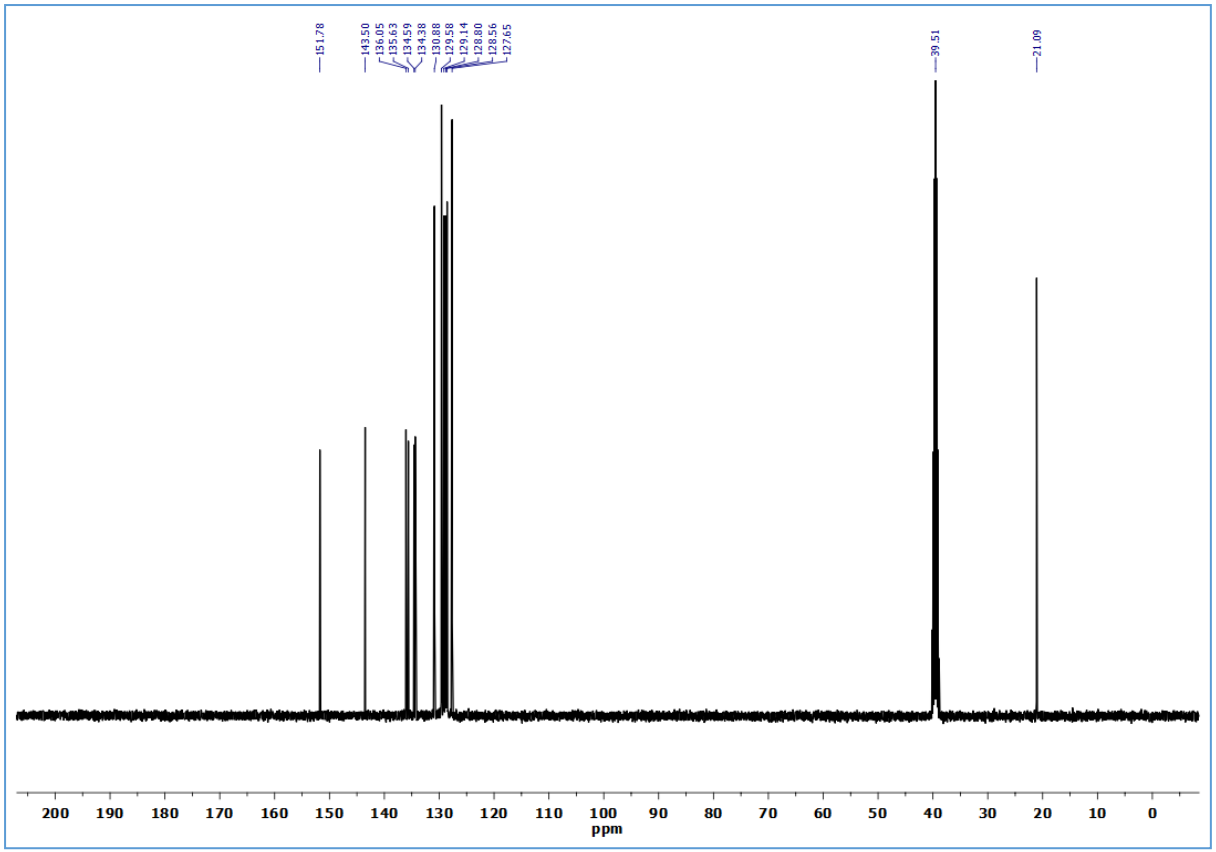


Fig. 5: ^{1}H NMR spectrum of **3c**



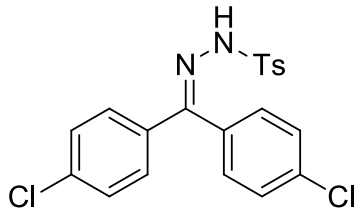
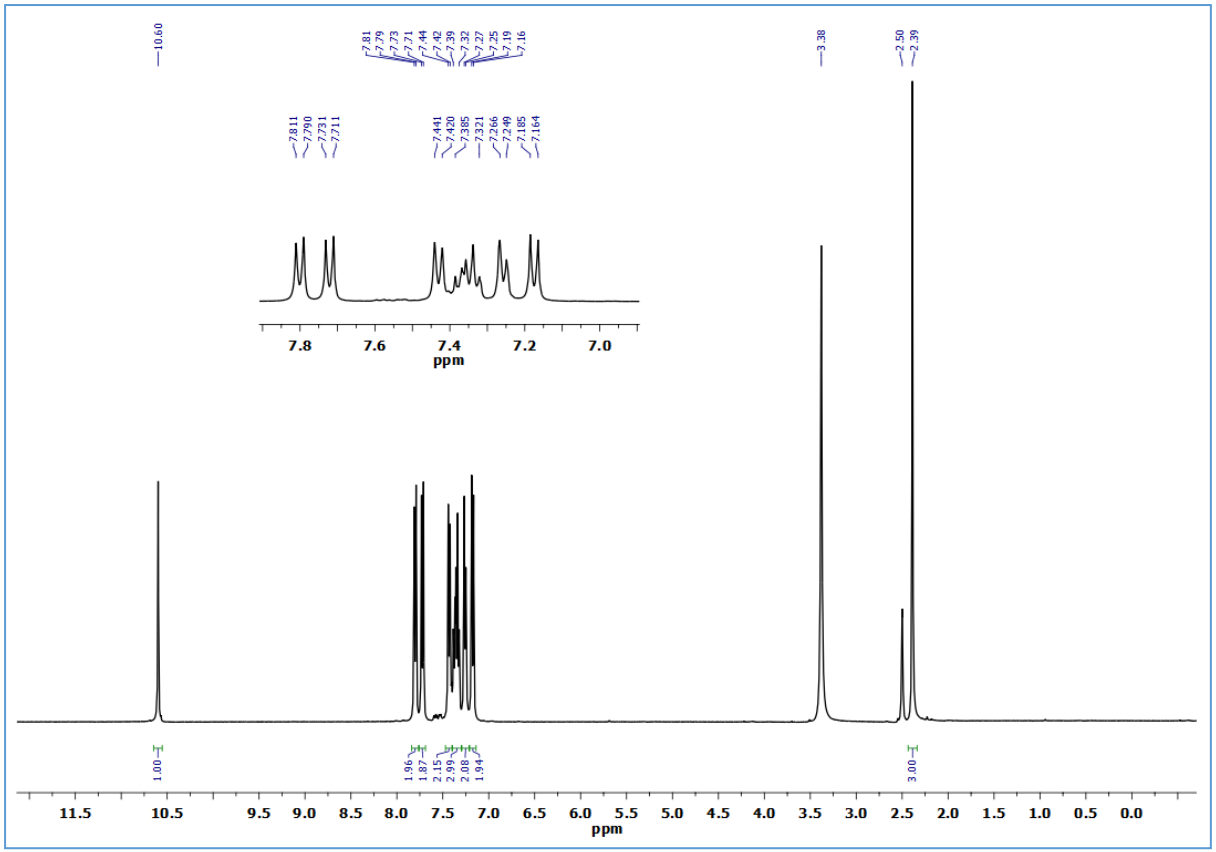


Fig. 6: ^{13}C NMR spectrum of **3c**



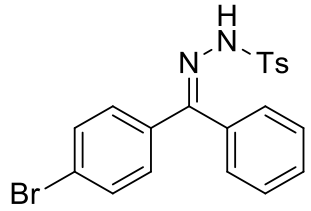
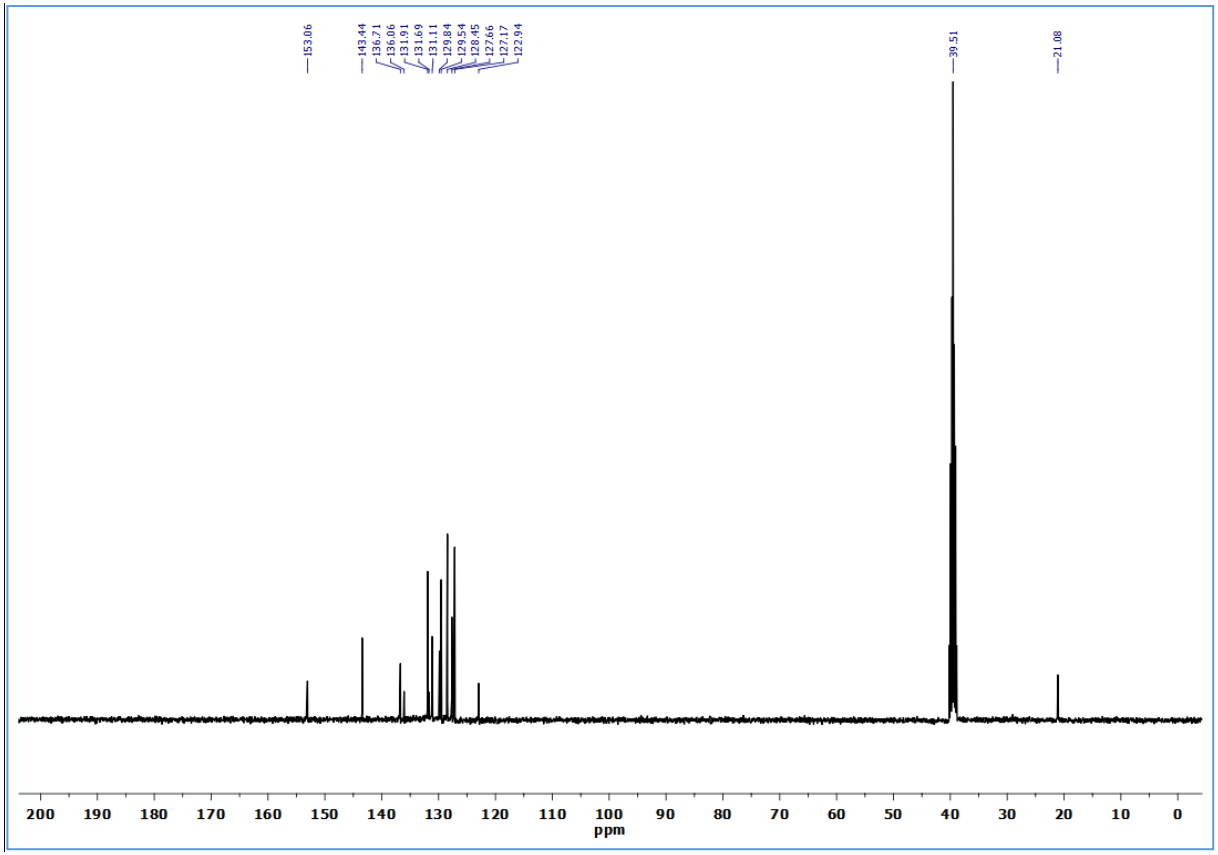


Fig. 7:^{1}H NMR spectrum of **3d**



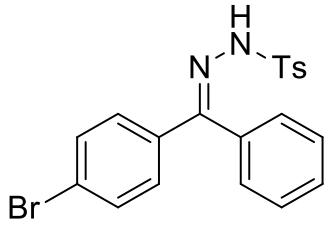
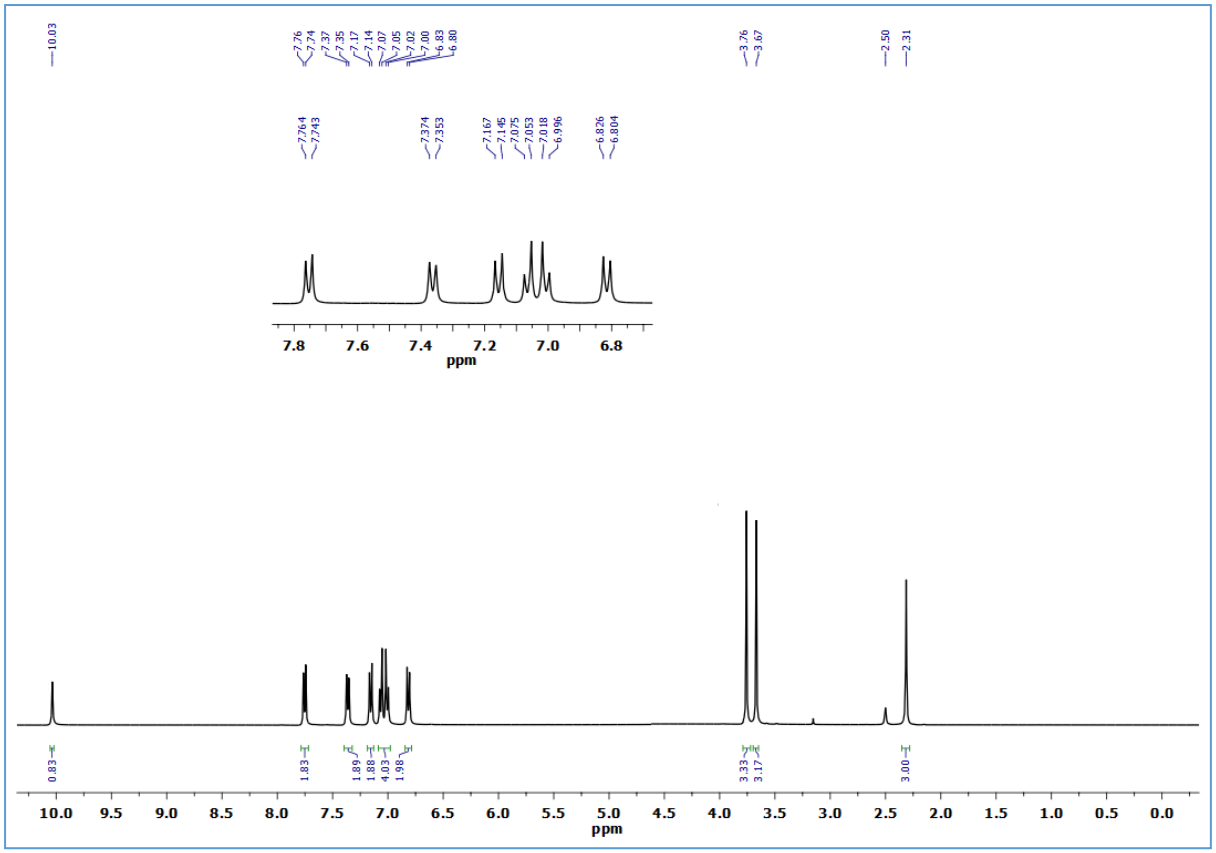


Fig. 8: ^{13}C NMR spectrum of **3d**



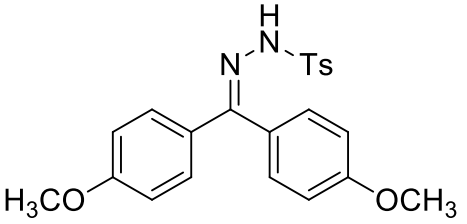
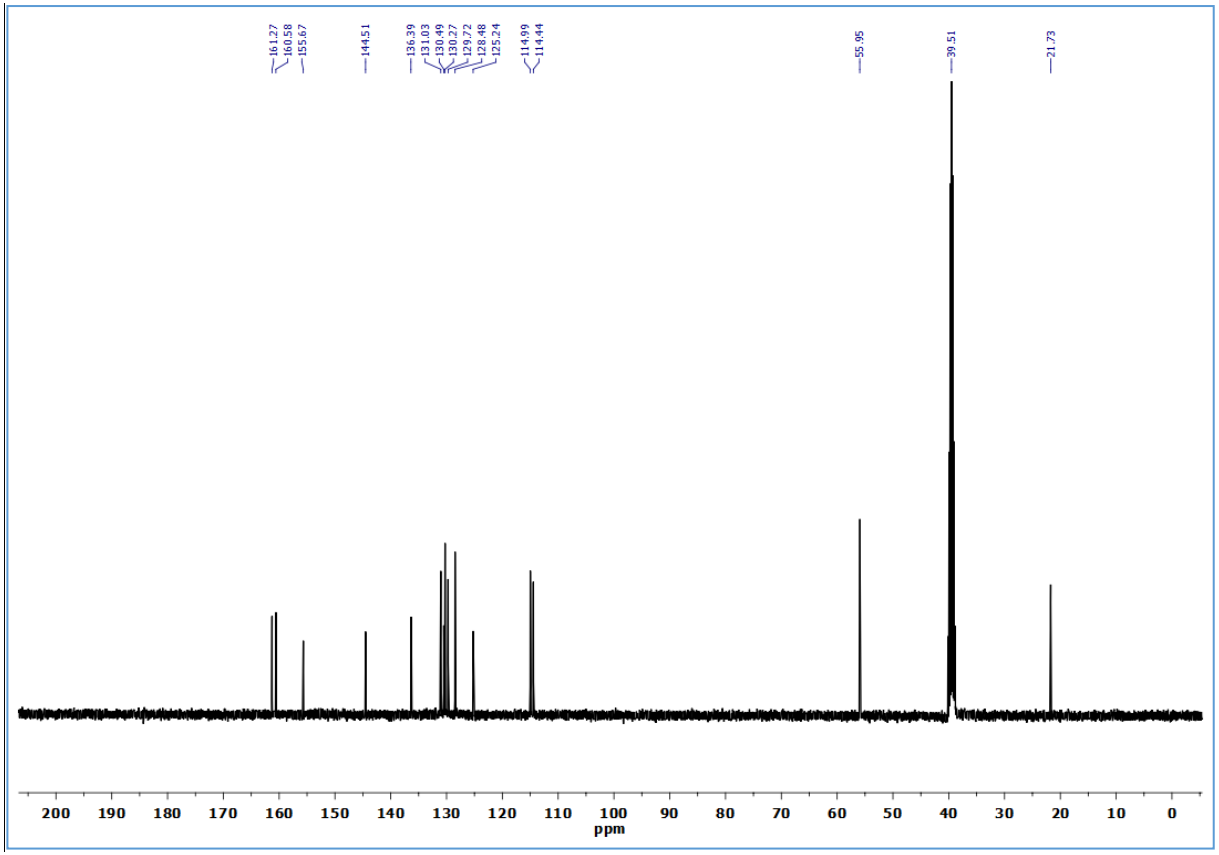


Fig. 9: ^{1}H NMR spectrum of **3e**



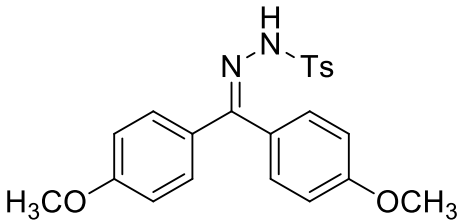
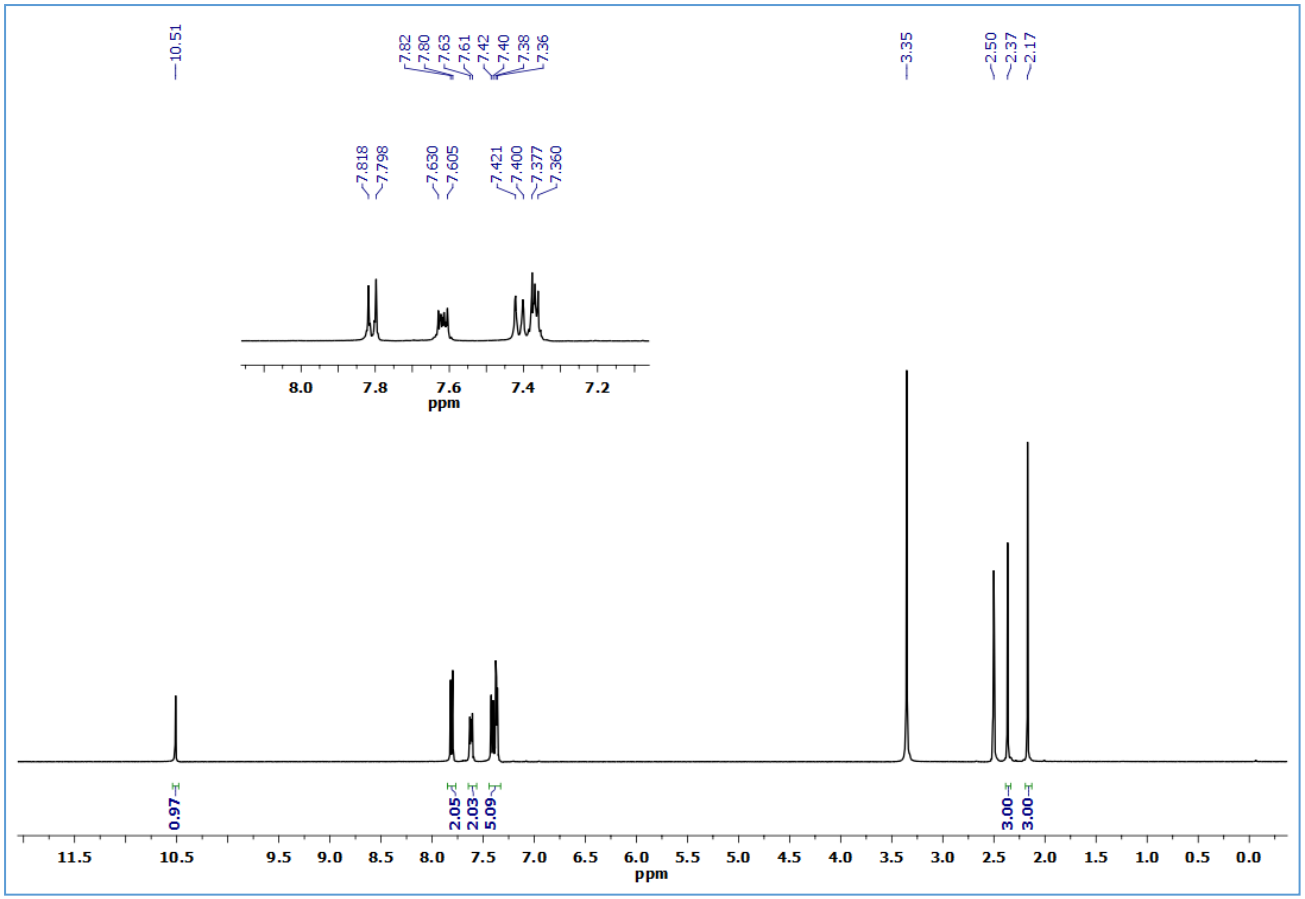


Fig. 10: ^{13}C NMR spectrum of **3e**



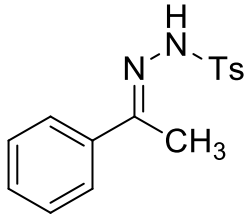


Fig. 11: ^{1}H NMR spectrum of **3g**

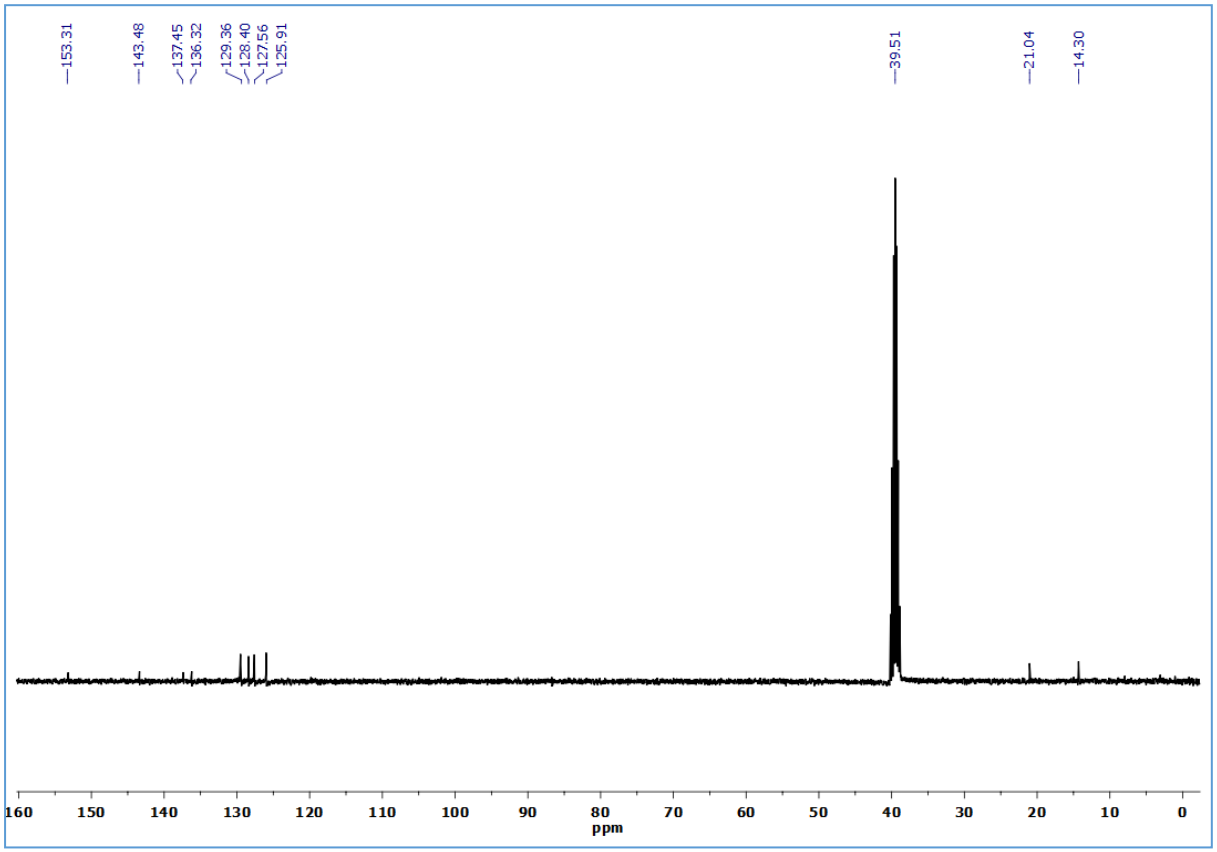
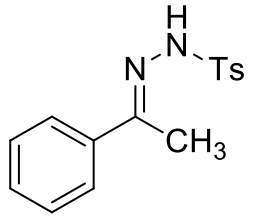


Fig. 12: ^{13}C NMR spectrum of **3g**



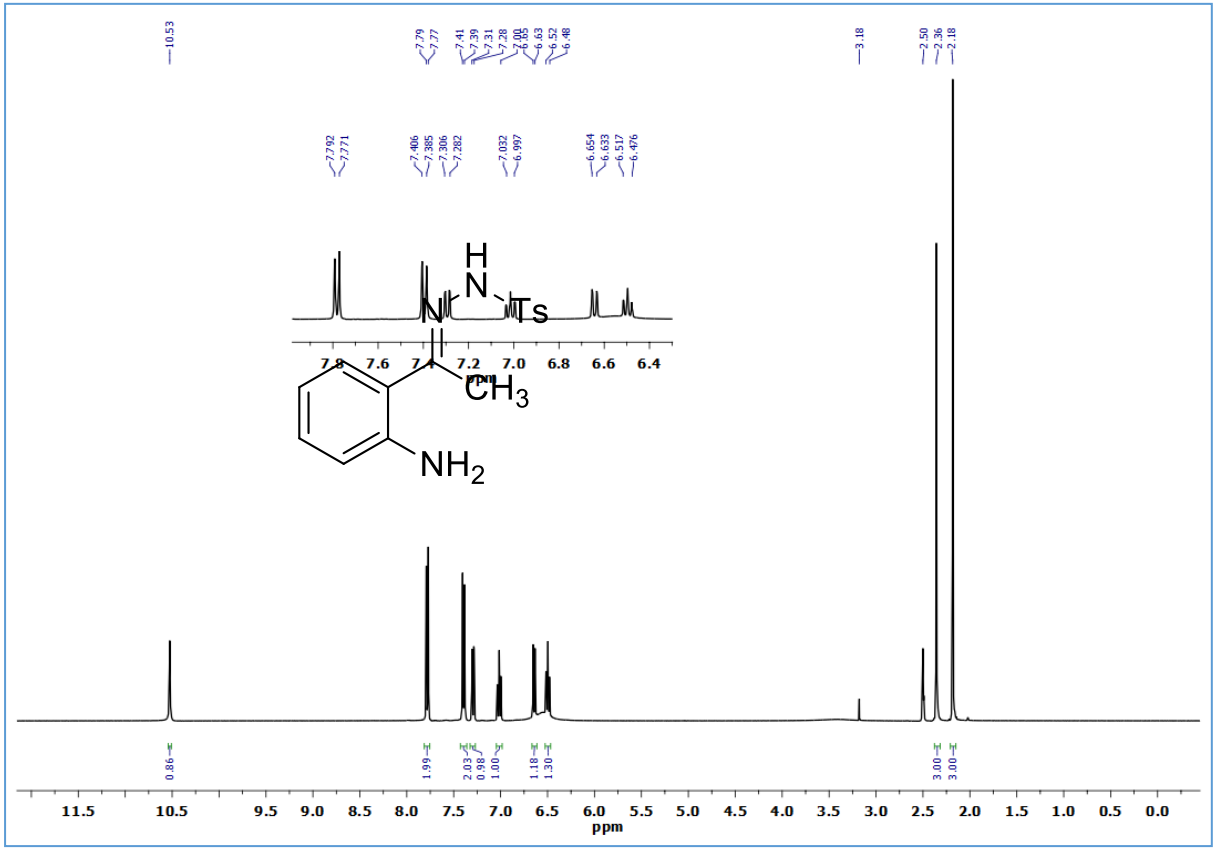
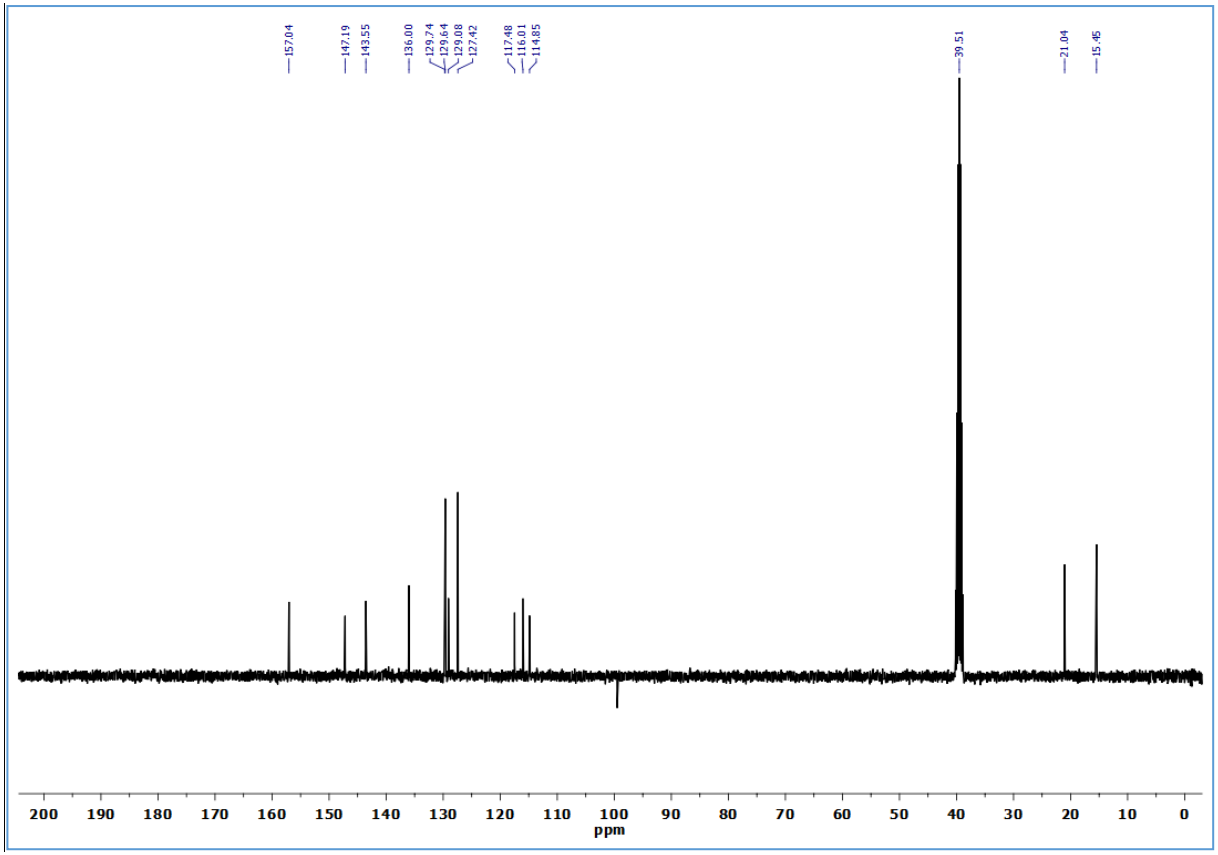


Fig. 13: ^{1}H NMR spectrum of **3i**



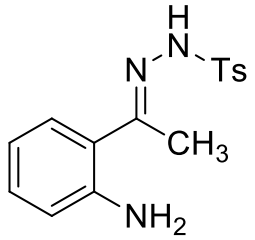
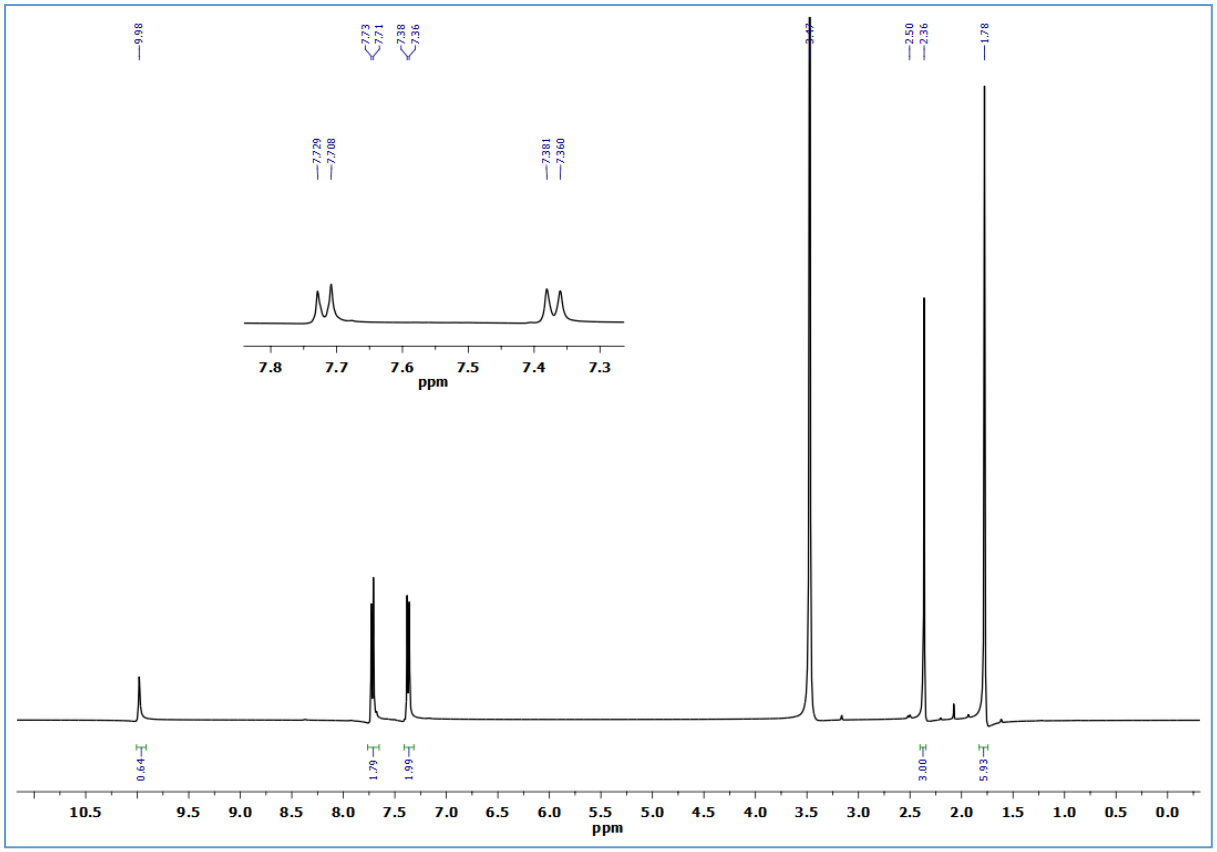


Fig. 14: ^{13}C NMR spectrum of **3i**



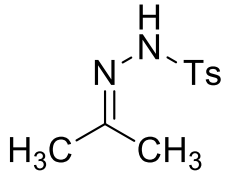


Fig. 15: ^{1}H NMR spectrum of **3j**

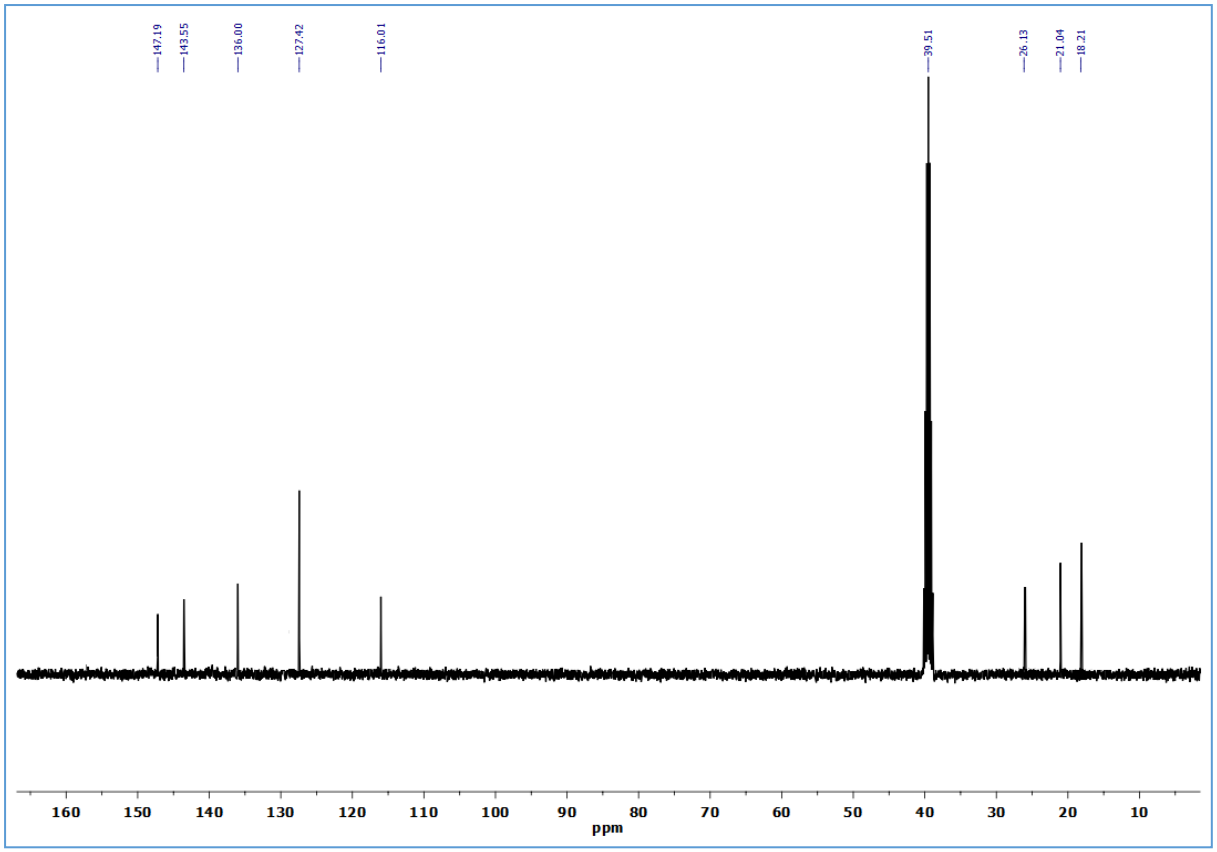
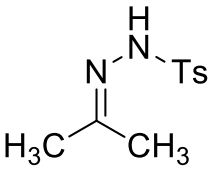
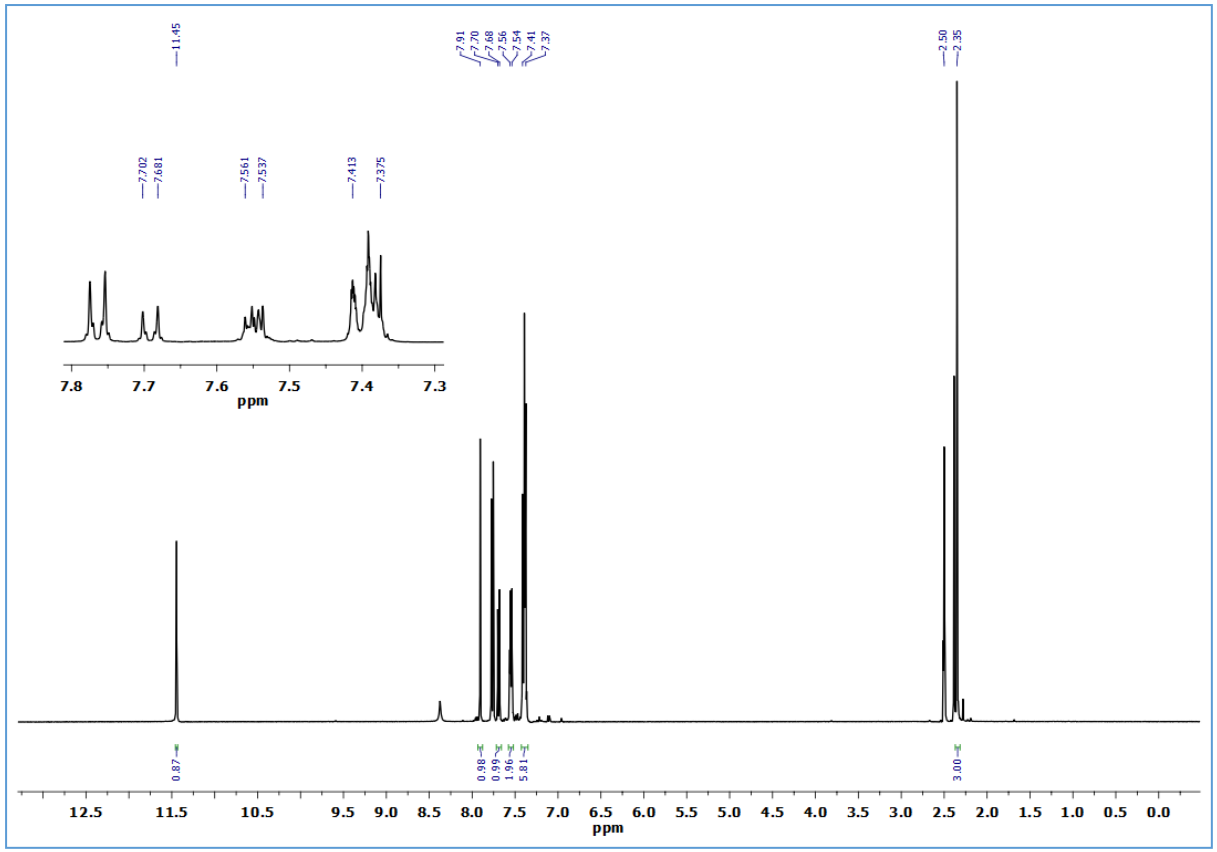


Fig. 16: ^{13}C NMR spectrum of **3j**





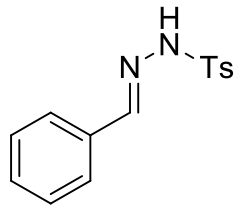
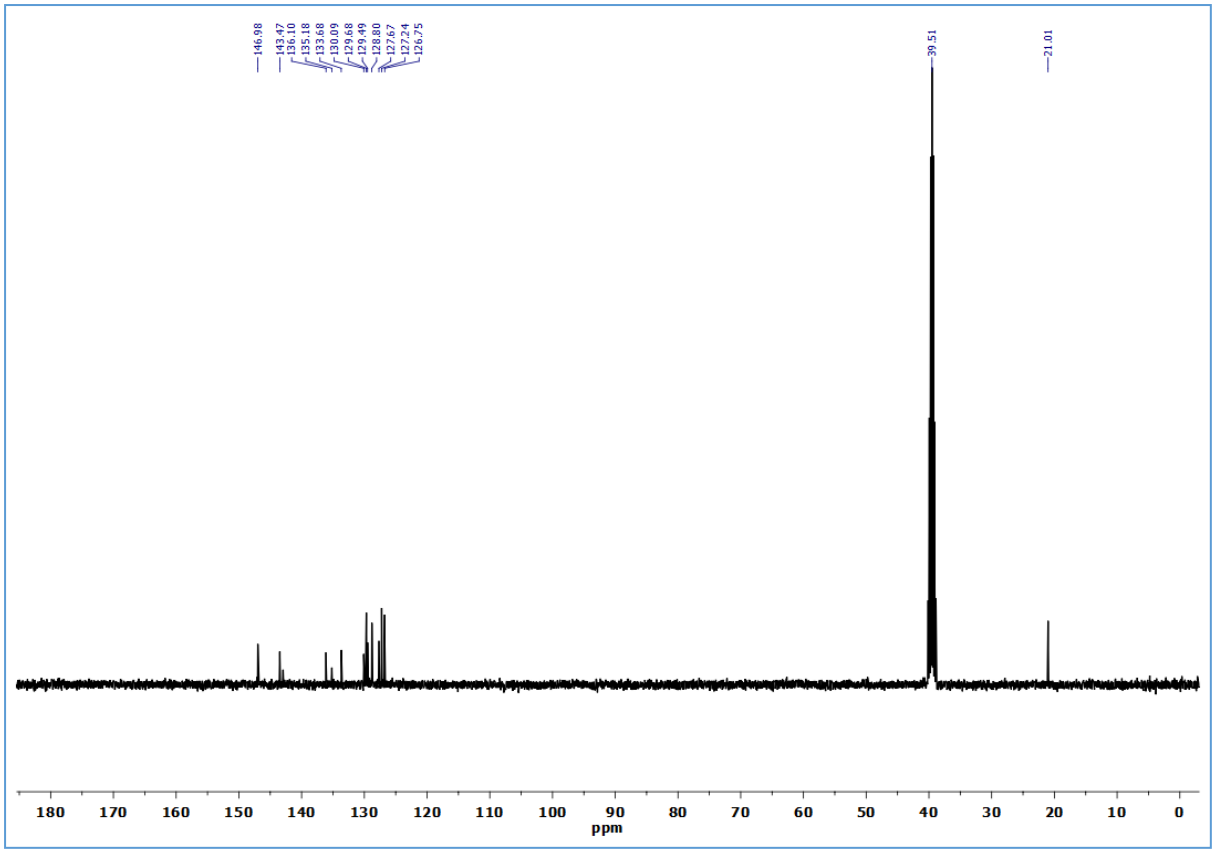


Fig. 17: ^{1}H NMR spectrum of **3k**



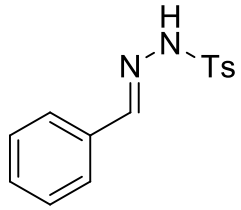
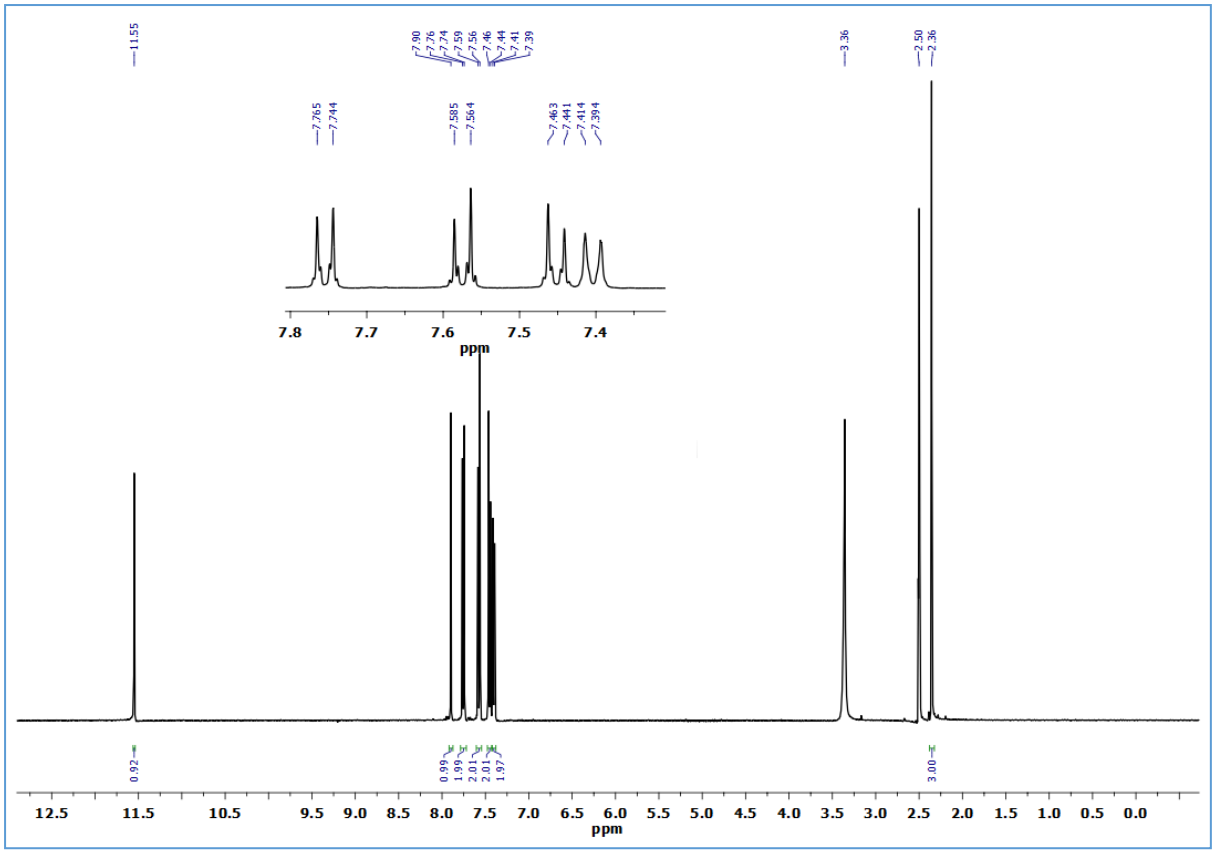


Fig. 18: ^{13}C NMR spectrum of **3k**



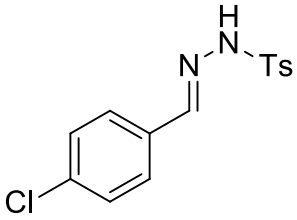


Fig. 19: ^{1}H NMR spectrum of **3l**

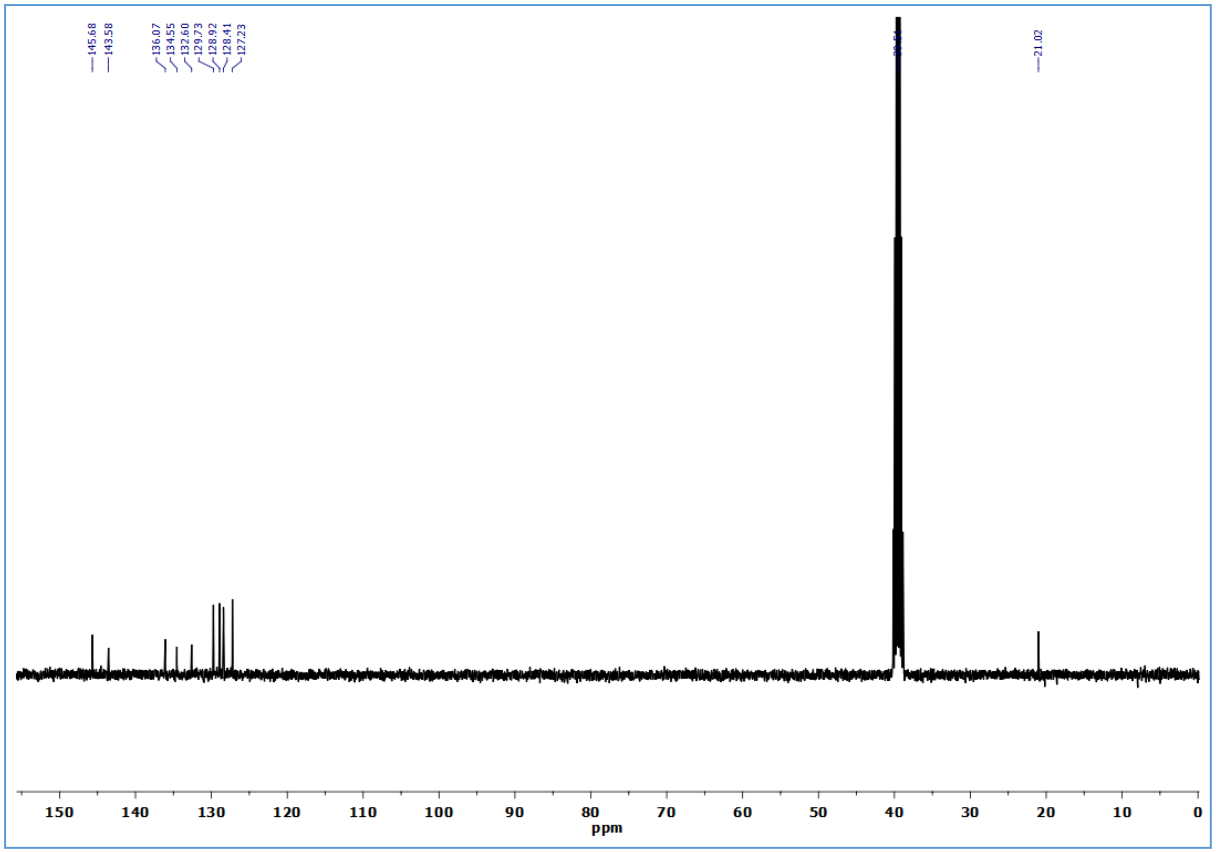
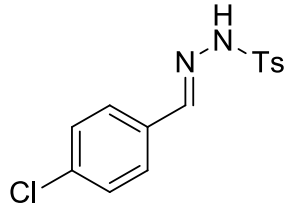
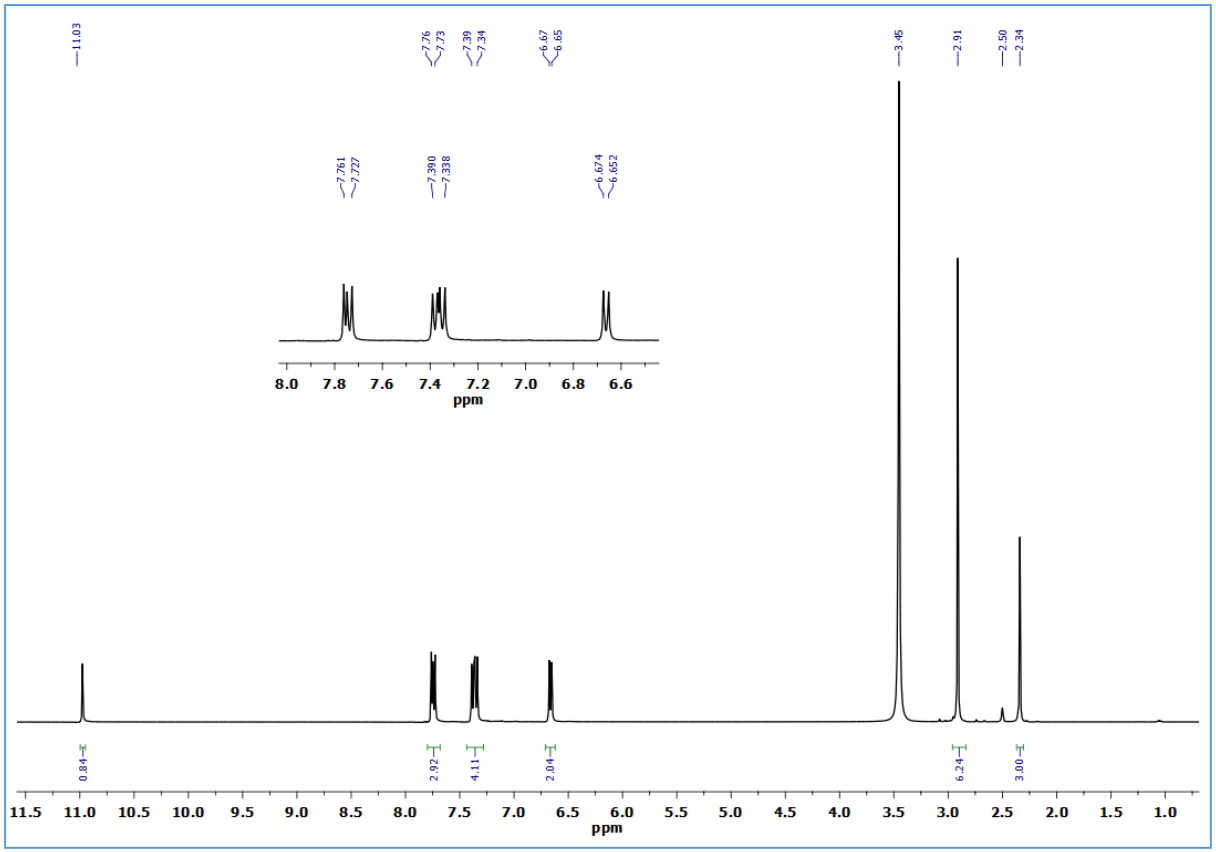


Fig. 20: ^{13}C NMR spectrum of **3l**





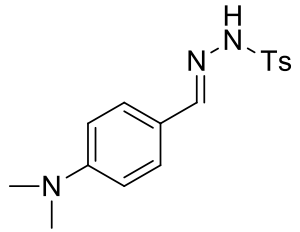
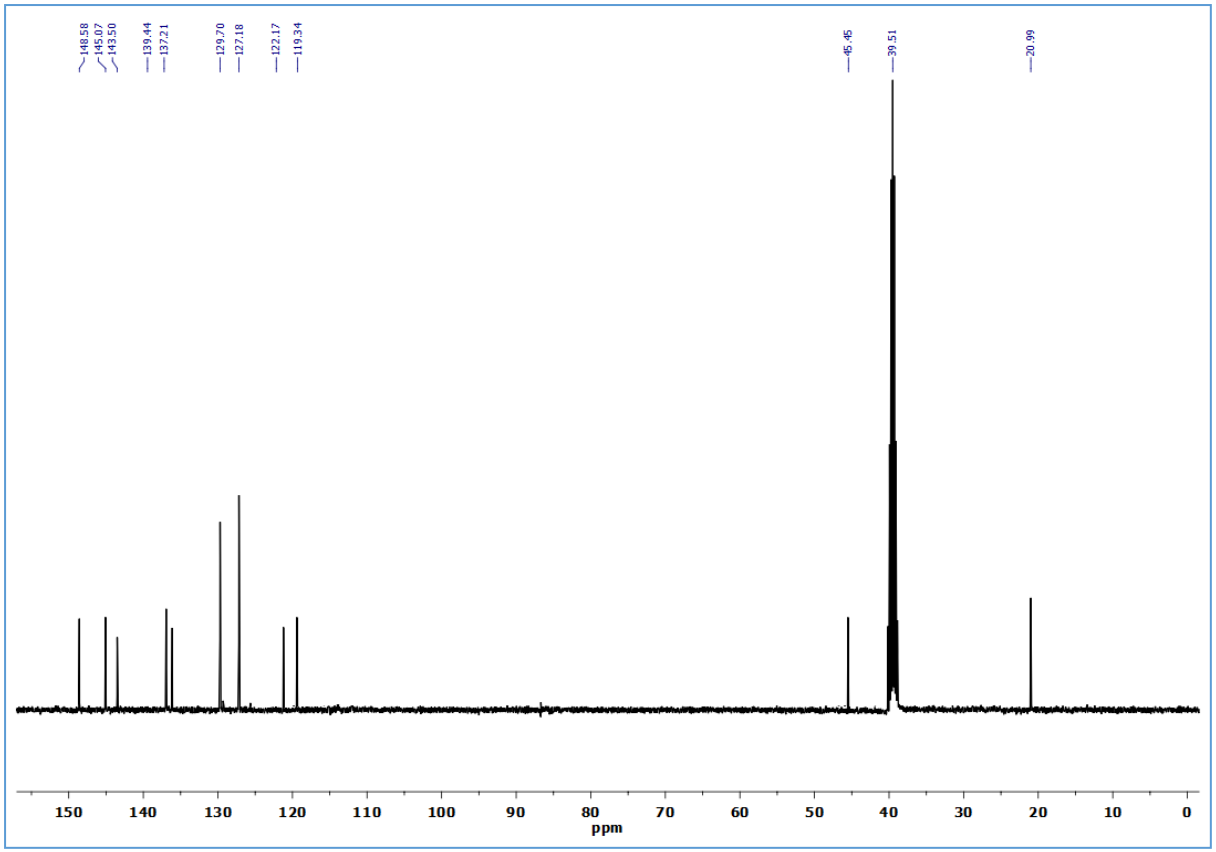


Fig. 21: ^{1}H NMR spectrum of **3n**



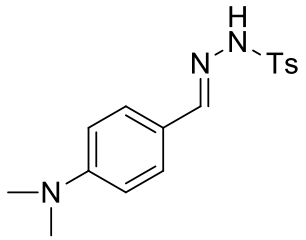
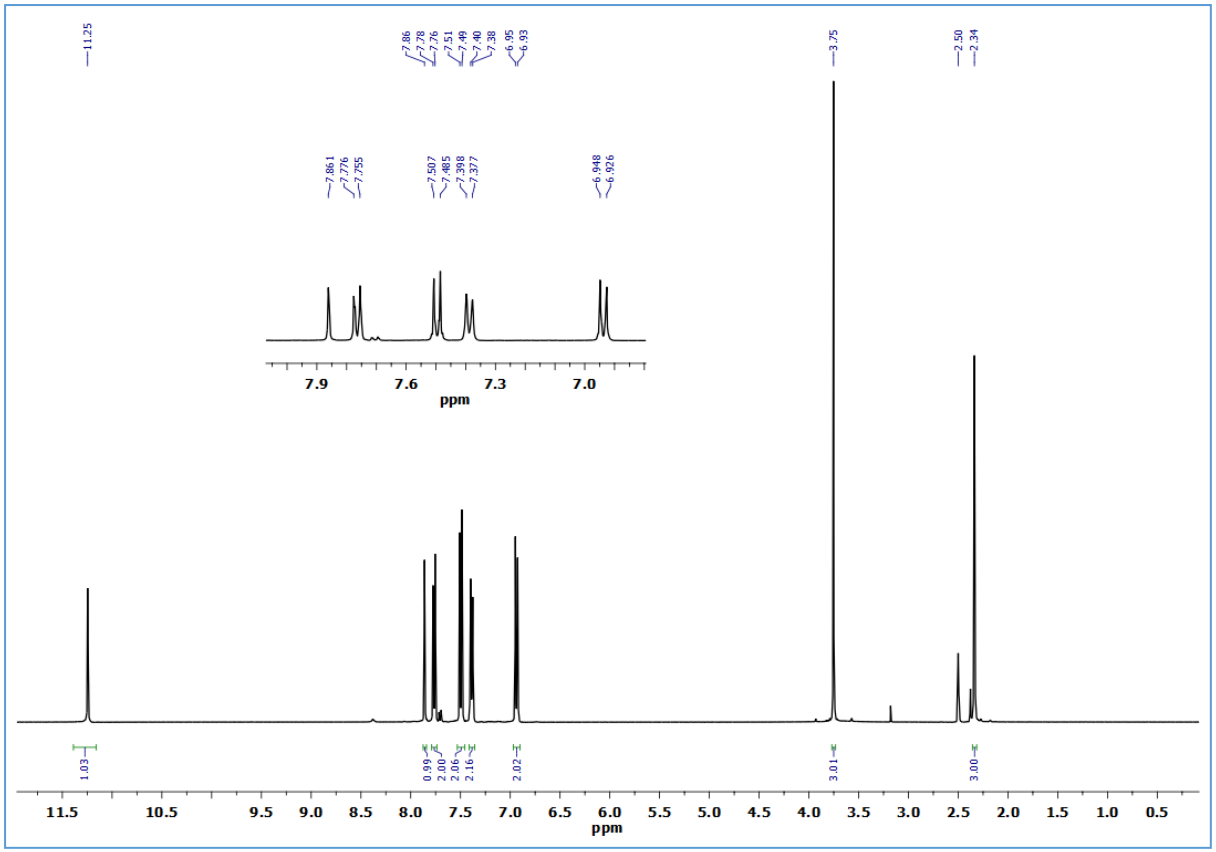


Fig. 22: ^{13}C NMR spectrum of **3n**



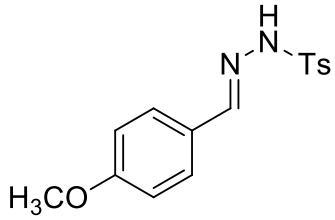
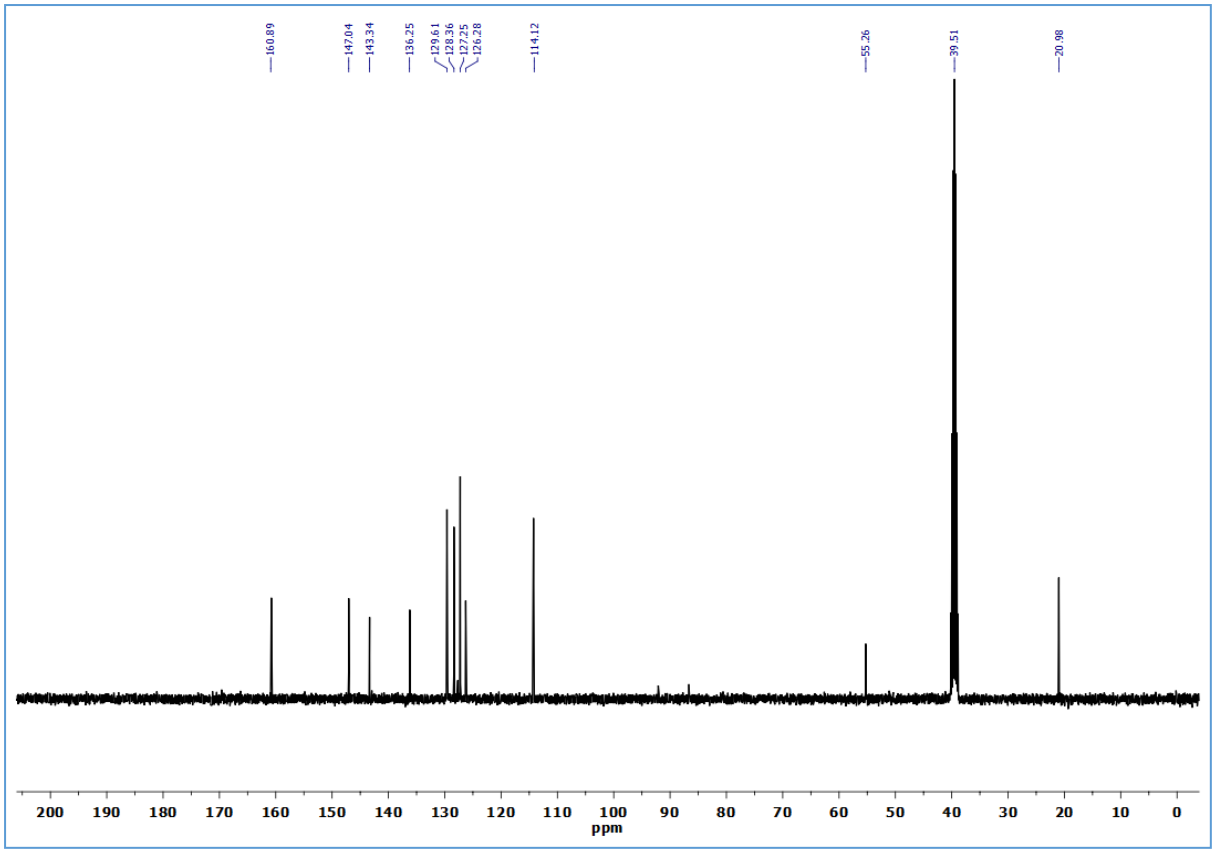


Fig. 23: ^{1}H NMR spectrum of **3o**



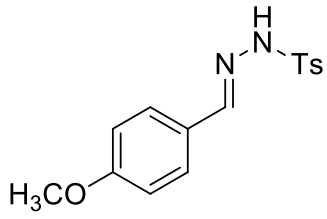
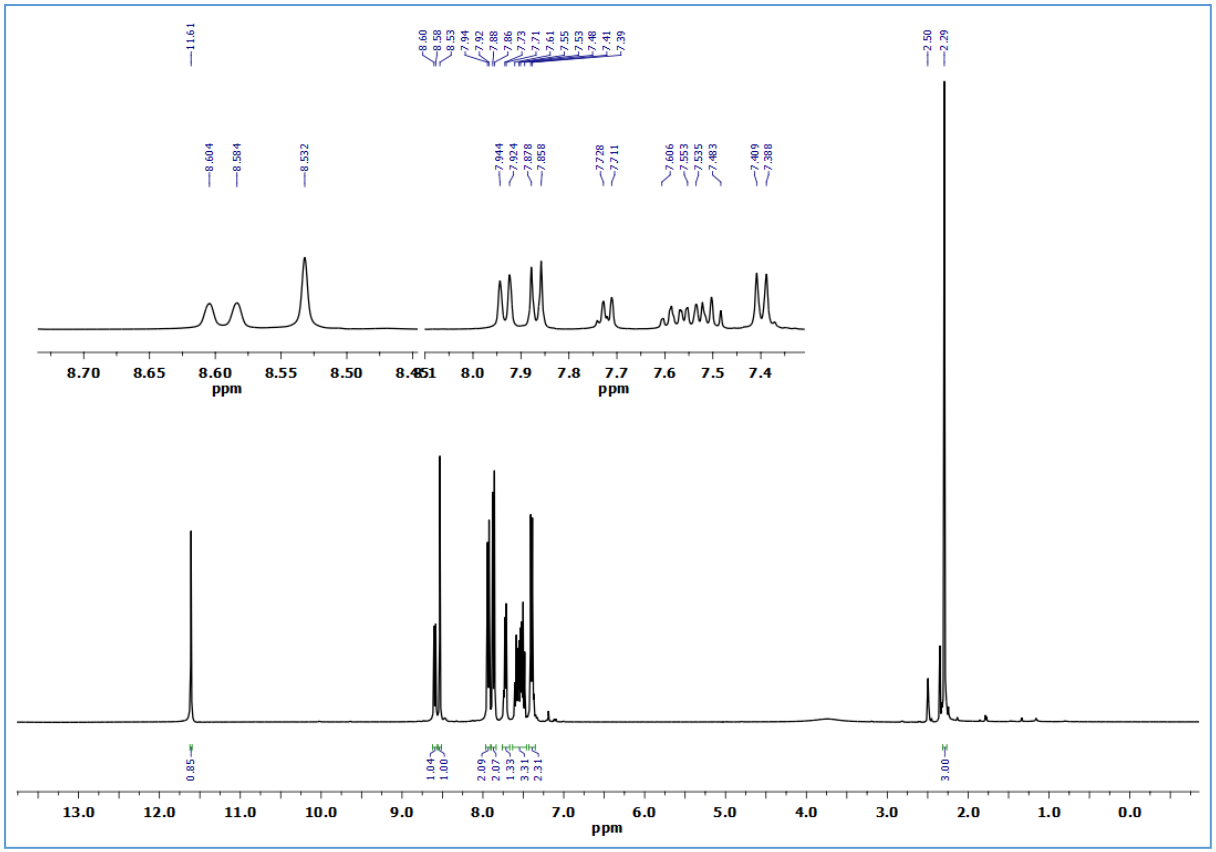


Fig. 24: ^{13}C NMR spectra of **3o**



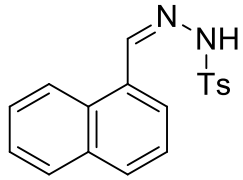
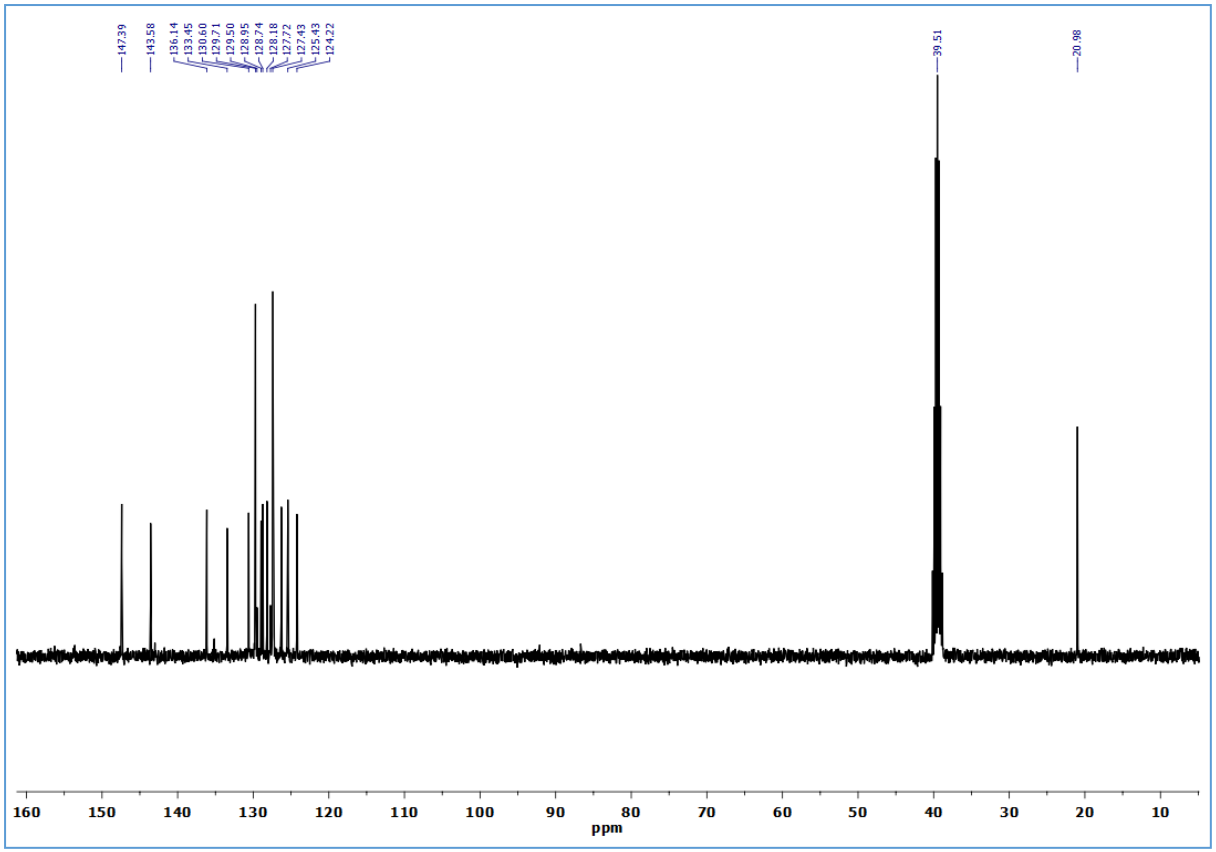


Fig. 25: ^{1}H NMR spectrum of **3p**



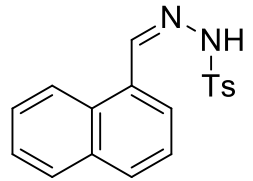
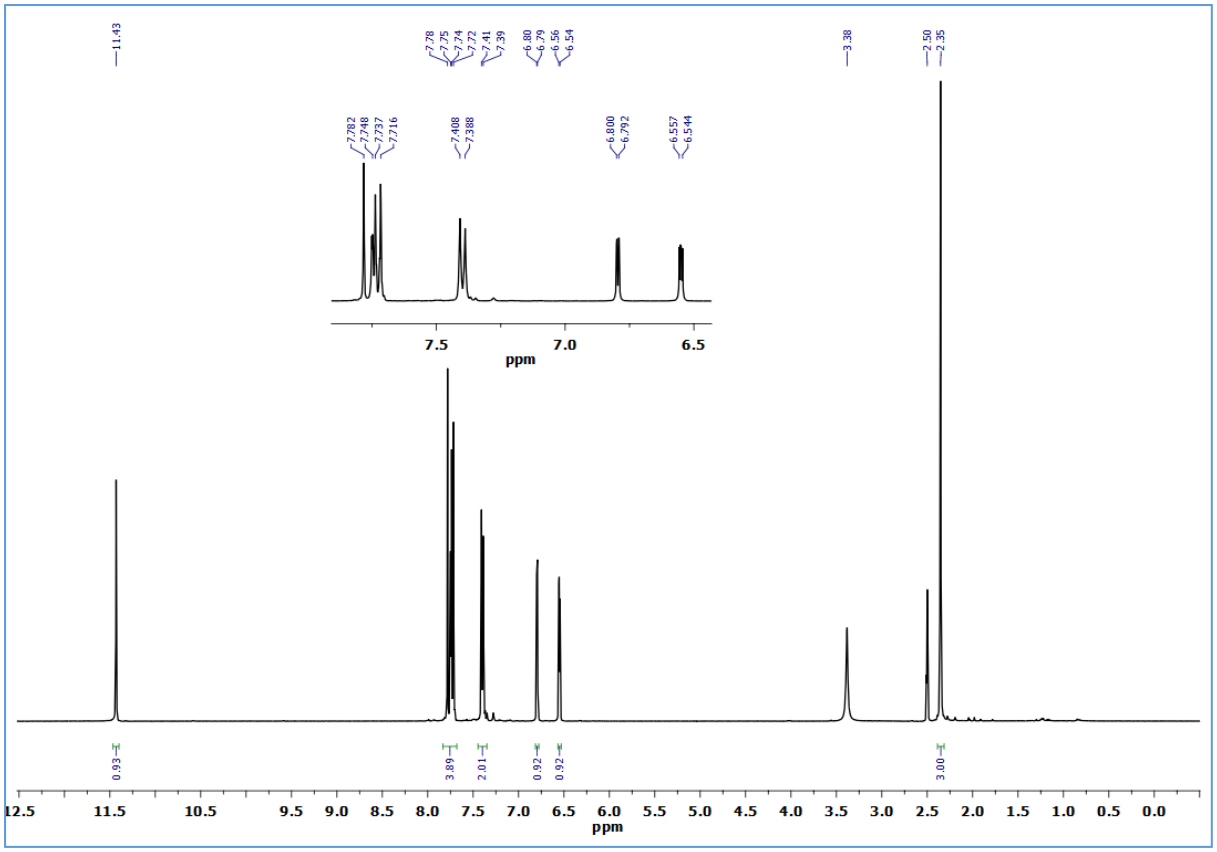


Fig. 26: ^{13}C NMR spectrum of **3p**



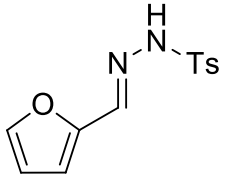


Fig. 27: ^{1}H NMR spectrum of **3q**

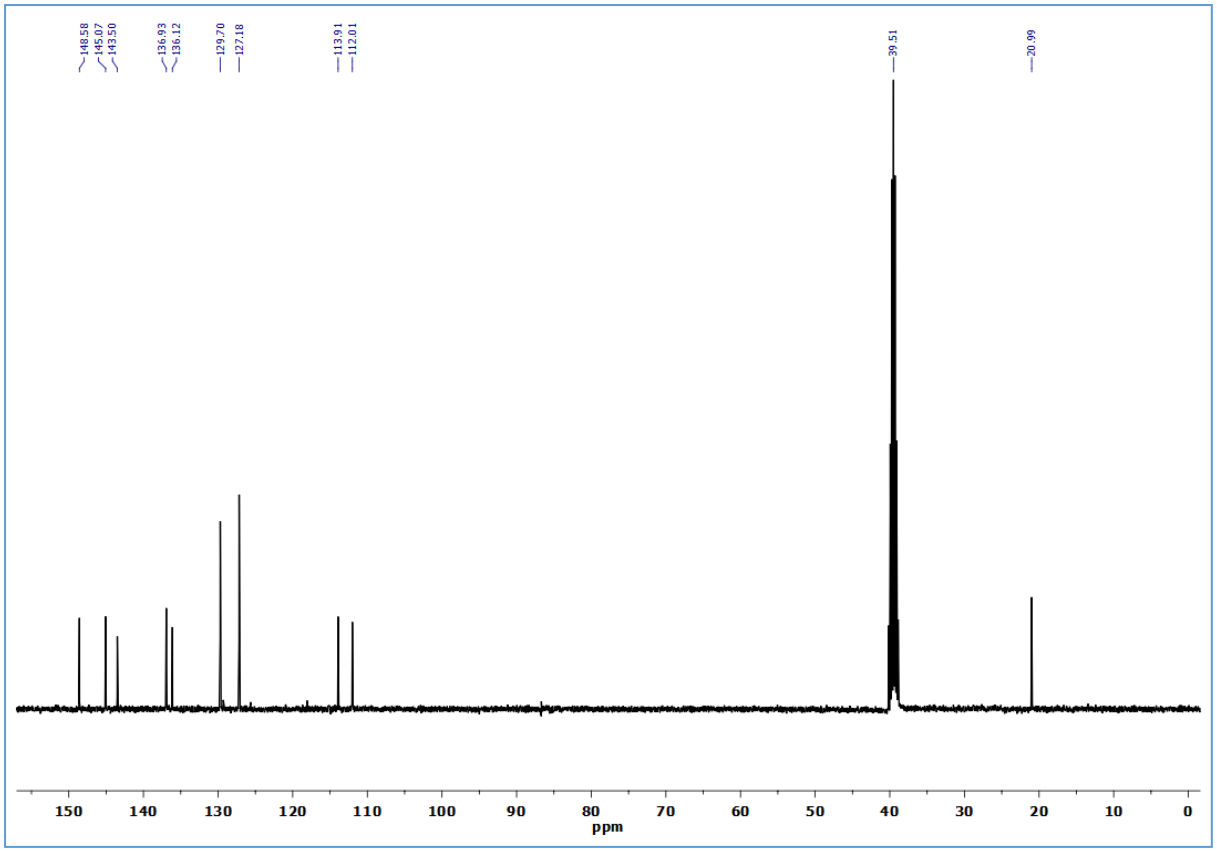
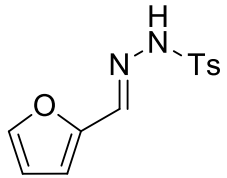


Fig. 28: ^{13}C NMR spectrum of **3q**



3. X-ray Crystallographic Procedures

Suitable transparent single crystals were mounted on glass fibers for intensity data collection at room temperature (296 K) using graphite-monochromatized Mo-Kα radiation (λ = 0.71073 Å) on a Bruker SMART APEX II CCD diffractometer.[1] Cell parameters were determined using SMART software and refined using SAINT on all observed reflections. Data reduction was performed using the SAINT software which corrects for Lorentz, polarization and decay effects. Absorption corrections were done by using SADABS. The structures are solved by the direct method using SHELXS-2013 and refined on F^2 using full-matrix least-squares techniques (SHELXL-2013)[2] incorporated in WinGX-Version 2014.1[3] and olex2[4] platform available for personal computers. All non-hydrogen atoms were refined with anisotropic displacement parameters. The structural illustrations have been drawn using Mercury,[5] and Diamond 3.[6]

Table 1 Bond Lengths for 3i

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S4	O7	1.430(8)	C41	C42	1.366(16)
S4	O8	1.419(7)	C41	N9	1.374(14)
S4	C46	1.805(9)	C40	C45	1.406(15)
S4	N10	1.638(9)	C45	C44	1.327(15)
S1	O2	1.446(8)	N5	N4	1.436(11)
S1	N1	1.638(8)	N5	C23	1.262(13)
S1	C1	1.716(10)	C43	C42	1.430(18)
S1	O1	1.434(7)	C43	C44	1.383(18)
S3	O5	1.444(8)	C23	C24	1.517(15)
S3	O6	1.425(8)	C23	C25	1.508(14)
S3	N7	1.642(9)	C6	C1	1.398(13)
S3	C31	1.804(12)	C6	C5	1.369(14)
S2	O3	1.420(8)	C1	C2	1.406(13)
S2	O4	1.443(8)	C3	C2	1.403(14)
S2	C16	1.716(12)	C3	C4	1.343(15)
S2	N4	1.634(9)	C54	C53	1.530(14)

N1	N2	1.394(11)	N10	N11	1.411(12)
C46	C51	1.381(13)	N11	C53	1.299(13)
C46	C47	1.373(14)	C25	C30	1.382(15)
C51	C50	1.390(14)	C25	C26	1.400(15)
C50	C49	1.398(15)	C53	C55	1.468(15)
C20	C19	1.383(16)	C4	C5	1.386(15)
C20	C21	1.407(16)	C4	C7	1.543(13)
C48	C49	1.435(15)	C30	C29	1.443(15)
C48	C47	1.370(14)	C30	N6	1.379(14)
C49	C52	1.467(14)	C29	C28	1.316(19)
C16	C21	1.421(15)	C27	C26	1.418(16)
C16	C17	1.373(15)	C27	C28	1.376(19)
C19	C18	1.386(17)	C37	C34	1.538(17)
C19	C22	1.476(16)	C35	C34	1.400(17)
N2	C8	1.288(12)	C11	C10	1.425(14)
C8	C9	1.481(14)	C11	C12	1.389(19)
C8	C10	1.493(15)	N3	C15	1.437(14)
C17	C18	1.441(18)	C15	C10	1.377(15)
N7	N8	1.379(11)	C15	C14	1.395(15)
N8	C38	1.308(13)	C12	C13	1.37(2)
C38	C39	1.501(15)	C13	C14	1.410(17)
C38	C40	1.456(14)	N12	C56	1.367(14)
C33	C32	1.319(18)	C56	C55	1.441(14)
C33	C34	1.387(18)	C56	C57	1.413(16)
C31	C32	1.397(14)	C55	C60	1.390(14)
C31	C36	1.361(15)	C60	C59	1.369(17)
C36	C35	1.345(17)	C57	C58	1.329(18)
C41	C40	1.462(14)	C59	C58	1.376(19)

Table 2 Bond Angles for 3i

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O7	S4	C46	107.1(5)	N9	C41	C40	118.5(10)
O7	S4	N10	104.5(4)	C38	C40	C41	124.6(10)
O8	S4	O7	120.4(5)	C45	C40	C38	121.7(9)
O8	S4	C46	108.6(5)	C45	C40	C41	113.8(10)
O8	S4	N10	107.7(5)	C44	C45	C40	126.4(12)
N10	S4	C46	107.9(4)	C23	N5	N4	118.2(9)
O2	S1	N1	103.6(5)	C44	C43	C42	118.2(11)
O2	S1	C1	109.1(5)	C41	C42	C43	121.4(11)
N1	S1	C1	107.5(4)	N5	N4	S2	112.9(7)
O1	S1	O2	119.2(4)	C45	C44	C43	119.8(12)
O1	S1	N1	108.2(5)	N5	C23	C24	124.2(10)
O1	S1	C1	108.7(4)	N5	C23	C25	117.2(10)
O5	S3	N7	108.4(5)	C25	C23	C24	118.6(10)
O5	S3	C31	108.0(5)	C5	C6	C1	121.7(10)
O6	S3	O5	120.3(5)	C6	C1	S1	120.4(7)
O6	S3	N7	104.5(5)	C6	C1	C2	117.0(9)
O6	S3	C31	108.4(5)	C2	C1	S1	122.5(8)
N7	S3	C31	106.5(5)	C4	C3	C2	121.6(9)
O3	S2	O4	119.2(5)	C3	C2	C1	119.8(10)
O3	S2	C16	107.5(5)	N11	N10	S4	112.8(6)
O3	S2	N4	107.2(5)	C53	N11	N10	118.3(8)
O4	S2	C16	109.8(5)	C30	C25	C23	121.7(10)
O4	S2	N4	103.9(5)	C30	C25	C26	120.7(10)
N4	S2	C16	108.8(5)	C26	C25	C23	117.6(10)
N2	N1	S1	113.6(6)	N11	C53	C54	121.0(10)

C51	C46	S4	117.9(7)	N11	C53	C55	117.9(9)
C47	C46	S4	118.2(8)	C55	C53	C54	121.1(9)
C47	C46	C51	123.8(9)	C3	C4	C5	119.3(9)
C46	C51	C50	116.9(9)	C3	C4	C7	121.3(10)
C51	C50	C49	122.6(10)	C5	C4	C7	119.3(10)
C19	C20	C21	119.8(11)	C25	C30	C29	116.8(11)
C47	C48	C49	121.2(9)	N6	C30	C25	126.8(10)
C50	C49	C48	116.8(9)	N6	C30	C29	116.3(11)
C50	C49	C52	122.1(10)	C6	C5	C4	120.5(11)
C48	C49	C52	121.0(9)	C28	C29	C30	122.2(12)
C21	C16	S2	120.2(8)	C28	C27	C26	118.4(12)
C17	C16	S2	121.6(8)	C25	C26	C27	119.9(11)
C17	C16	C21	118.2(11)	C29	C28	C27	122.0(12)
C20	C19	C18	121.3(12)	C36	C35	C34	122.7(12)
C20	C19	C22	120.3(12)	C33	C34	C37	123.4(12)
C18	C19	C22	118.3(12)	C33	C34	C35	114.6(12)
C48	C47	C46	118.5(10)	C35	C34	C37	122.0(12)
C20	C21	C16	120.7(10)	C12	C11	C10	120.3(13)
C8	N2	N1	116.6(8)	C10	C15	N3	123.6(9)
N2	C8	C9	124.7(9)	C10	C15	C14	122.4(11)
N2	C8	C10	115.6(9)	C14	C15	N3	113.9(11)
C9	C8	C10	119.8(9)	C11	C10	C8	117.9(10)
C16	C17	C18	121.7(10)	C15	C10	C8	124.5(9)
N8	N7	S3	114.1(7)	C15	C10	C11	117.6(10)
C38	N8	N7	118.3(9)	C13	C12	C11	121.1(13)
N8	C38	C39	121.6(10)	C12	C13	C14	119.5(12)
N8	C38	C40	117.0(9)	C15	C14	C13	119.0(13)
C40	C38	C39	121.4(9)	N12	C56	C55	123.2(9)
C32	C33	C34	125.3(11)	N12	C56	C57	120.1(11)

C32	C31	S3	119.1(8)	C57	C56	C55	116.6(11)
C36	C31	S3	119.5(8)	C56	C55	C53	122.4(9)
C36	C31	C32	121.4(11)	C60	C55	C53	120.6(9)
C19	C18	C17	118.2(11)	C60	C55	C56	116.9(10)
C33	C32	C31	117.1(11)	C59	C60	C55	124.0(12)
C35	C36	C31	118.9(11)	C58	C57	C56	123.3(14)
C42	C41	C40	120.4(11)	C60	C59	C58	118.1(12)
C42	C41	N9	121.0(10)	C57	C58	C59	120.8(13)

Table 3 Bond Lengths for 3f.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	O1	1.4288(19)	C3	C4	1.375(4)
S1	N1	1.651(2)	C15	C14	1.382(4)
S1	O2	1.4313(19)	C12	C13	1.379(4)
S1	C10	1.754(3)	C12	C11	1.382(4)
N1	N2	1.411(3)	C13	C14	1.383(4)
N2	C1	1.285(3)	C13	C16	1.514(4)
C10	C15	1.384(4)	C8	C7	1.395(5)
C10	C11	1.381(4)	C4	C5	1.378(4)
C1	C3	1.481(4)	C6	C7	1.351(5)
C1	C2	1.505(4)	C6	C5	1.369(4)
C3	C8	1.387(4)	C6	C9	1.516(5)

Table 4 Bond Angles for 3f.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°

O1	S1	N1	107.01(12)	C4	C3	C8	115.8(3)
O1	S1	O2	119.93(12)	C14	C15	C10	119.2(3)
O1	S1	C10	108.05(12)	C13	C12	C11	121.4(3)
N1	S1	C10	108.65(11)	C12	C13	C14	117.9(3)
O2	S1	N1	103.75(12)	C12	C13	C16	121.1(3)
O2	S1	C10	108.97(12)	C14	C13	C16	121.1(3)
N2	N1	S1	113.83(16)	C10	C11	C12	119.8(3)
C1	N2	N1	116.1(2)	C3	C8	C7	121.6(3)
C15	C10	S1	119.2(2)	C15	C14	C13	121.8(3)
C11	C10	S1	121.0(2)	C3	C4	C5	121.4(3)
C11	C10	C15	119.8(3)	C7	C6	C5	116.2(3)
N2	C1	C3	116.3(2)	C7	C6	C9	123.0(3)
N2	C1	C2	123.4(2)	C5	C6	C9	120.8(4)
C3	C1	C2	120.2(2)	C6	C7	C8	122.0(3)
C8	C3	C1	122.8(3)	C6	C5	C4	123.0(3)
C4	C3	C1	121.4(2)				

4. References

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