Electronic Supplementary Material (ESI) for RSC Advances.

One-pot and facile synthesis of novel *N*-benzimidazolyl-*a*-arylnitrones catalyzed by salts of transition metals

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Supporting Information

Experimental

All the consumed chemicals were purchased from companies Merck or Fluka. By using an Electro-thermal digital apparatus, melting points were determined and are uncorrected. A Galaxy Series FT-IR 5000 spectrometer (using KBr discs) was used for recording of IR spectra. ^{1}H- and ^{13}C NMR spectra were performed in DMSO-d_6 on a Bruker (300 and 500 MHz) spectrometer. Chemical shifts (δ) were presented in ppm using tetramethyl silane (TMS) as internal standard. The Mass spectra were recorded on an Agilent model: 5975C VL MSD with Tripe-Axis Detector spectrometer at 70 eV. Reactions were monitored by thin layer chromatography (TLC) using silica gel F_{254} aluminum sheets (Merck).

General preparation of nitrones 3a-j

To a solution of 2-aminobenzimidazole (1 mmol) and corresponding aromatic aldehyde (1 mmol) in ethanol (5 mL), the $Mn(NO_3)_2$. $6H_2O$ (10 mol%, 0.027 gr) was added. The reaction mixture was stirred using a magnetically at room temperature. Then, *m*-CPBA (1.2 mmol) is added to it. The reaction progress was pursued by TLC (petroleum ether: ethyl acetate 2:1). After completing of the reaction, to the mixture was added aqueous $NaHCO_3$ (10%, 15 mL) and the resulting precipitate was filtrated to give pure nitrones **3a-j**. For further purity, these products can be crystallized by the mixture of ether: *n*-hexane (1:1). Also, the increase of HCl (10%) to the filtrate causes the *m*-chlorobenzoic acid to precipitate which by filtrating, the acid extraneous product is separated off.

Spectroscopic data for nitrones 3a-j

***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-phenyl nitrone (3a).** Light yellow solid. IR (KBr, υ_{max}): 3269 (N-H), 3095 (C-H), 1683, 1608 (C=N), 1535 (-C=N-O), 1419, 1222 (C=C), 1382 (H-C=N), 1263 (C-N), 1029 (N-O), 898, 759 (C-H), 619 cm^{-1}; ^{1}H NMR (300 MHz, DMSO-d_6): δ_H 11.07 (br, 1H, NH, The NH protons disappeared upon D_2O addition), 8.68 (s br, 1H, H-C=N^{+}-O^{-}), 7.98 (s br, 2H, H-Ar), 7.49-7.08 (t br, 6H, H-Ar) ppm, ^{13}C NMR (DMSO-d_6, 75 MHz): δ_C 170.1, 153.6, 139.2, 133.2, 132.4, 130.8, 130.2, 129.3, 1^{28}.1, 122.2, 111.5 ppm; MS (m/z, %): 237.2 (M^{+}, 5), 156.0 (75), 133.1 (100), 111.1 (58), 85.2 (40), 71.2 (46), 57.2 (62), 43.2 (43).

***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(2-chlorophenyl) nitrone (3b)**. Gray solid. IR (KBr, υ_{max}): 3377 (N-H), 1666, 1631 (C=N), 1579 (-C=N-O), 1519, 1435, 1298, 1273 (C=C), 1456 (H-C=N), 1176 (C-N), 1143, 1020 (N-O), 866 (C-Cl), 744 (C-H) cm^{-1}; ^{1}H NMR (DMSO-d_6, 300 MHz): δ_H 12.27 (br, 1H, NH), 7.68 (d, J = 5.91 Hz, 1H, H-C=N^{+}-O^{-}), 7.55-7.45 (m, 6H, H-Ar), 7.12 (s br, 2H, H-Ar) ppm, ^{13}C NMR (DMSO-d_6, 125 MHz): δ_C 167.2, 147.3, 135.8, 135.2, 131.4, 130.2, 129.7, 129.3, 127.0, 121.4, 119.9, 113.8 ppm, MS (m/z, %): 271.1 (M^{+}, 46), 236.1 (52), 208.1 (48), 139.1 (100), 111.1 (71), 75.1 (34).

***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(3-chlorophenyl) nitrone (3c)**. Gray solid. IR (KBr, υ_{max}): 3307 (N-H), 1624, 1604 (C=N), 1575 (-C=N-O), 1596, 1344 (C=C), 1473 (H-C=N), 1263 (C-N), 1024 (N-O), 918 (C-Cl), 758 (C-H), 740 cm^{-1}; ^1H NMR (DMSO-d_6, 300 MHz): δ_H 12.22 (br, 1H, NH), 7.68 (d, J = 5.49 Hz, 1H, H-C=N^+-O^-), 7.55-7.48 (t br, 6H, H-Ar), 7.14 (s, 2H, H-Ar) ppm, ^{13}C NMR (DMSO-d_6, 75 MHz): δ_C 167.2, 147.2, 135.6, 135.0, 131.2, 129.9, 129.5, 129.0, 126.9, 124.0, 121.2, 113.6 ppm, MS (m/z, %): 271.1 (M^+, 21), 243.1 (18), 160.1 (28), 139.1 (100), 111.1 (71), 75.1 (`27).

***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(4-chlorophenyl) nitrone (3d).** Gray solid. IR (KBr, υ_{max}): 3348 (N-H), 1653, 1641 (C=N), 1571 (-C=N-O), 1591, 1523, 1435 (C=C), 1462 (H-C=N), 1271 (C-N), 1093 (N-O), 844 (C-Cl), 750 (C-H) cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ_H 12.33 (br, 1H, NH, The NH protons disappeared upon D_2O addition), 8.15 (s br, 1H, H-C=N^+-O^-), 7.89 (s br, 2H, H-Ar), 7.65-7.53 (t br, 4H, H-Ar), 7.15 (s, 2H, H-Ar) ppm; ^{13}C NMR (DMSO-d_6, 125 MHz): δ_C 168.8, 150.1, 136.8, 136.4, 134.3, 132.8, 131.0, 130.2, 128.2, 121.8, 119.6, 112.7 ppm, MS (m/z, %): 271.1 (M+, 48), 236.2 (51), 208.2 (41), 139.2 (100), 111.2 (45), 75.2 (17).

***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(4-bromophenyl) nitrone (3e)**. Gray solid. IR (KBr, υ_{max}): 3311 (N-H), 1660, 1624 (C=N), 1550 (-C=N-O), 1571, 1394 (C=C), 1340 (H-C=N), 1273 (C-N), 1012 (N-O), 808 (C-Br), 769 (C-H), 736 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ_H 12.36 (br, 1H, NH), 8.07 (s br, 2H, H-C=N^+-O^- and H-Ar), 7.70 (br, 2H, H-Ar), 7.44 (br, 2H, H-Ar), 7.14 (br, 3H, H-Ar) ppm, ^{13}C NMR (DMSO-d_6, 125 MHz): δ_C 169.1, 150.2, 134.8, 132.7, 131.1, 130.4, 129.3, 128.3, 127.7, 125.5, 121.8, 119.0, 112.7 ppm, MS (m/z, %): 315.2 (M^+, 57), 287. 1 (53), 185. 1 (100), 155.1 (50), 132 (14), 105. 2 (28), 76. 2 (28).

***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(3-nitrophenyl) nitrone (3f)**. Red solid. IR (KBr, υ_{max}): 3317 (N-H), 1705, 1618 (C=N), 1581 (-C=N-O), 1531, 1348 (-NO_2), 1597, 1469, 1419 (C=C), 1400 (H-C=N), 1263 (C-N), 1080 (N-O), 923, 752 (C-H), 731, 715 cm^{-1}; ^1H NMR (300 MHz, DMSO-d_6): δ_H (the NH proton exchange with deuterium of D_2O, which is present in DMSO-d_6), 8.96 (s, 1H, H-C=N^+-O^-), 8.57-8.50 (m, 1H, H-Ar), 8.36 (d, J = 6.66 Hz, 1H, H-Ar), 7.91-7.74 (m, 2H, H-Ar), 7.34 (d, J = 7.50 Hz, 2H, H-Ar), 7.15 (br, 2H, H-Ar) ppm; ^{13}C NMR (DMSO-d_6, 75 MHz): δ_C 170.1, 137.6, 135.3, 135.0, 131.9, 131.4, 130.1, 128.9, 125.7, 124.4, 123.4, 122.4, 112.5 ppm, MS (m/z, %): 282.1 (M^+, 50), 160.1 (50), 132.1 (100), 105.1 (50), 76.1 (37).

***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(4-nitrophenyl) nitrone (3g)**. Red solid. IR (KBr, υ_{max}): 3346 (N-H), 1670, 1651 (C=N), 1575 (-C=N-O), 1521, 1352 (-NO_2), 1597, 1309 (C=C), 1462 (H-C=N), 1278 (C-N), 1103 (N-O), 850, 740 (C-H), 715 cm^{-1}; ^1H NMR (DMSO-d_6, 300 MHz): δ_H 12.56 (br, 1H, NH), 8.34 (d, J = 6.99 Hz, 3H, H-C=N^+-O^- and H-Ar), 8.13 (d, J = 8.07 Hz, 2H, H-Ar), 7.44-7.18 (d br, 4H, H-Ar) ppm; ^{13}C NMR (DMSO-d_6,75 MHz): δ_C 170.6, 152.4, 151.0, 149.4, 143.3, 140.4,

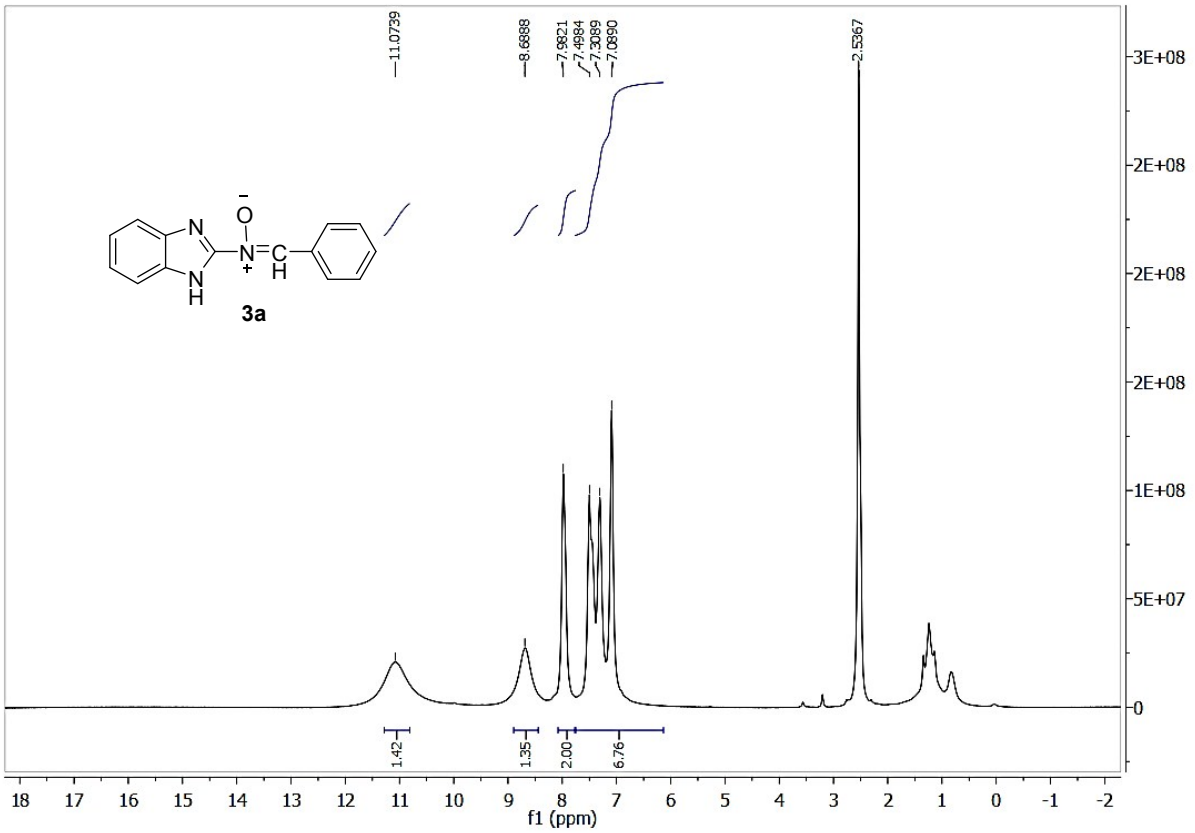
131.0, 130.1, 124.6, 123.7, 122.8, 112.5 ppm; MS (m/z, %): 282 (M^+, 100), 254 (57), 235 (12), 219 (12), 160 (99), 121, 104 (77).

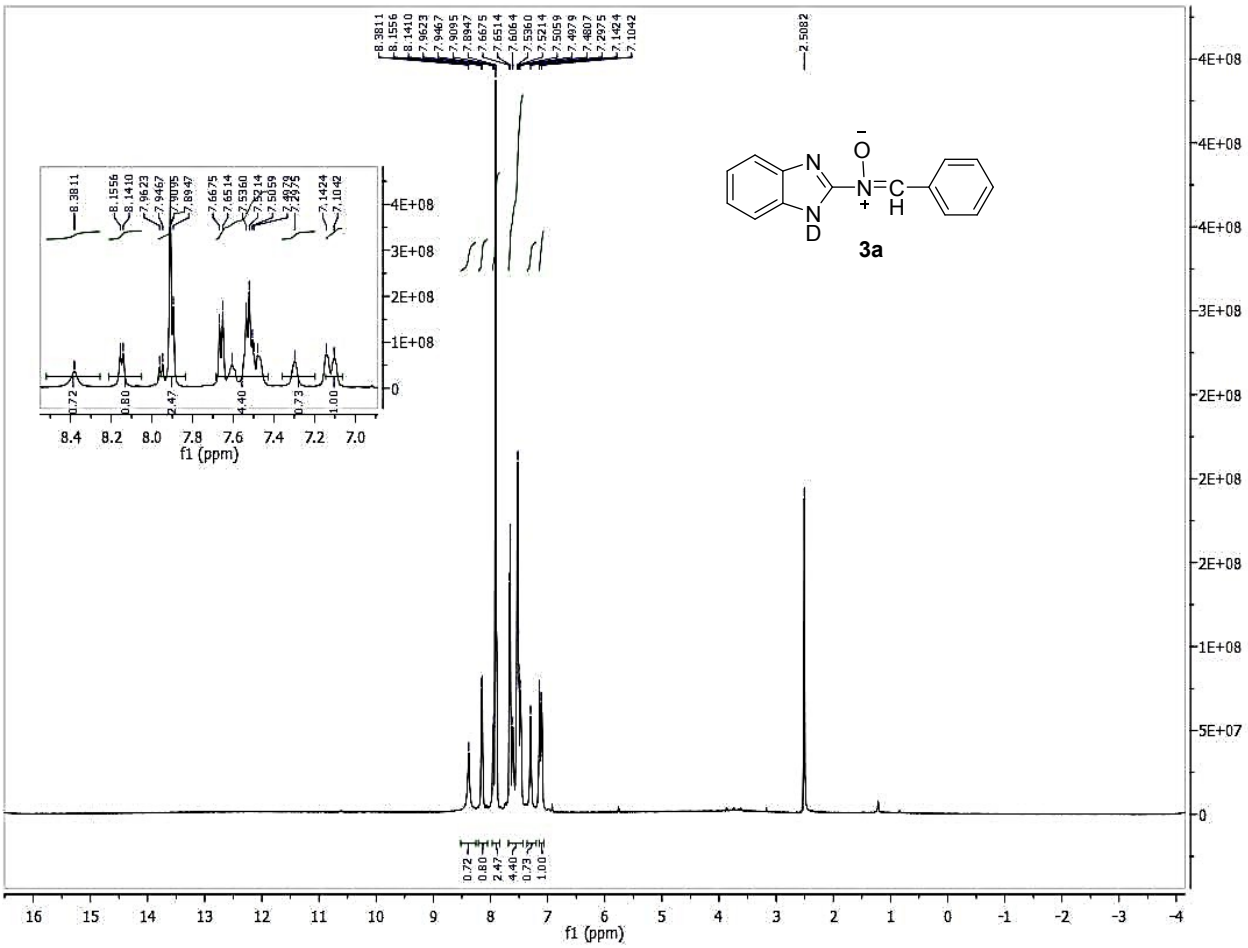
***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(*p*-tolyl) nitrone (3h).** Gray solid. IR (KBr, υ_{max}): 3396 (N-H), 2924 (C-H), 1658, 1633 (C=N), 1573 (-C=N-O), 1527, 1456, 1313, 1257 (C=C), 1431 (H-C=N), 1168 (C-N), 1020 (N-O), 842, 767, 750 (C-H), 611 cm^{-1}; ^1H NMR (300 MHz, DMSO-d_6): δ_H (the NH proton exchange with deuterium of D_2O, which is present in DMSO-d_6), 8.08 (d, J = 7.50 Hz, 2H, H-C=N^+-O^- and H-Ar), 7.08-7.42 (m, 7H, H-Ar), 2.36 (s, 3H, CH_3) ppm; ^{13}C NMR (DMSO-d_6, 75 MHz): δ_C 168.8, 151.1, 142. 0, 135.7, 133.0, 129.2, 128.8, 121.3, 113.7 ppm, MS (m/z, %): 251.2 (M^+, 96), 223.2 (56), 119.1 (100), 91.1 (87), 65.1 (25).

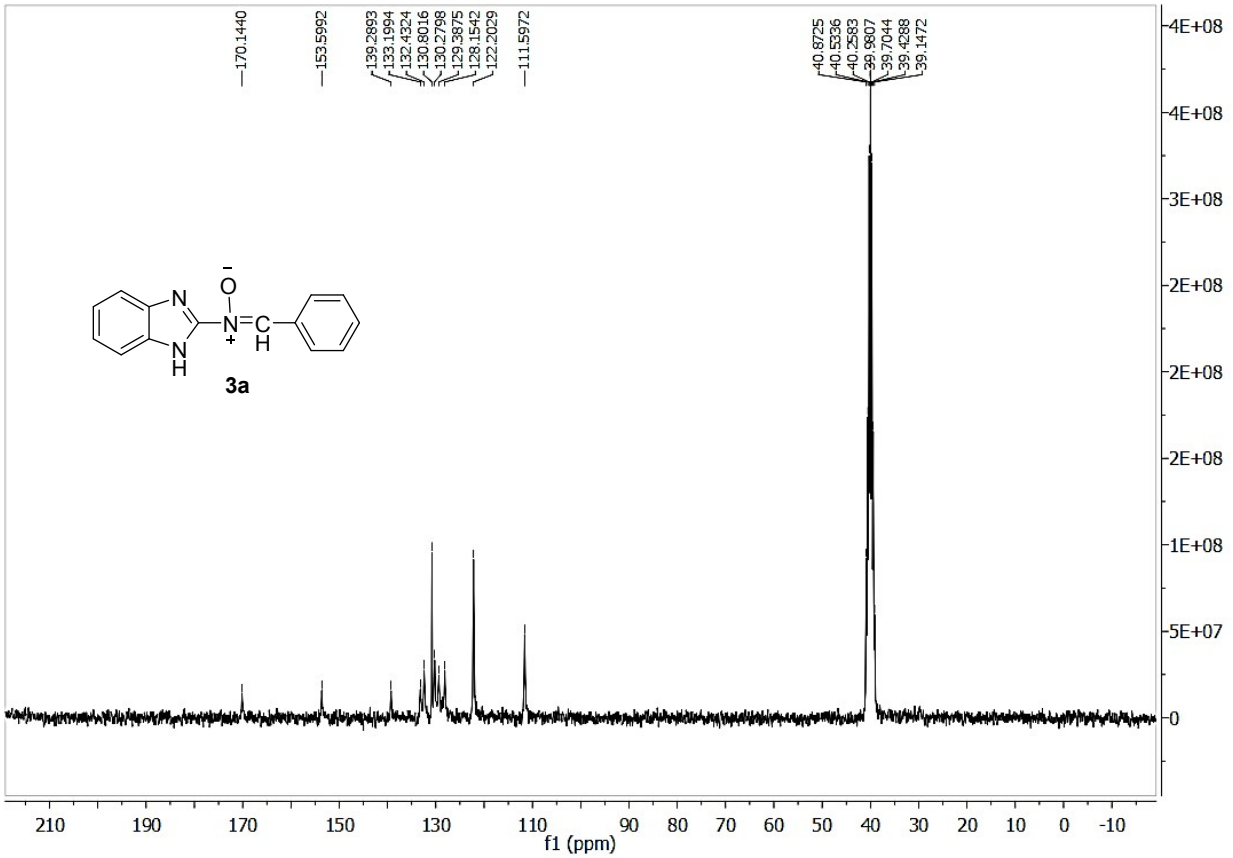
***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(4-methoxyphenyl) nitrone (3i).** Gray solid. IR (KBr, υ_{max}): 3327 (N-H), 1660, 1624 (C=N), 1556 (-C=N-O), 1602, 1573, 1458, 1519 (C=C), 1346 (H-C=N), 1286 (C-O), 1273 (C-N), 1020 (N-O), 910, 767 (C-H), 731 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ_H 12.18 (br, 1H, NH), 8.12 (d, J = 6.55 Hz, 1H, H-C=N^+-O^-), 7.87 (t, J = 8.55 Hz, 1H, H-Ar), 7.66 (d, J = 7.75 Hz, 1H, H-Ar), 7.53-7.44 (q br, 2H, H-Ar), 7.12-6.90 (m, 4H, H-Ar), 3.83 (s, 3H, OMe) ppm; ^{13}C NMR (DMSO-d_6, 125 MHz,): δ_C 166.9, 162.3, 148.5, 134.7, 131.6, 130.2, 125.8, 121.1, 114.4, 113.5, 55.3 ppm; MS (m/z, %): 267.1 (M^+, 13), 263.1 (14), 220.1 (72), 133.1 (54), 105.1 (27), 77.1 (25), 44 (100).

***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(2-hydroxyphenyl) nitrone (3j)**. Gray solid. IR (KBr, υ_{max}): 3369 (N-H), 1683, 1635 (C=N), 1560 (-C=N-O) 1580, 1381 (C=C), 1458 (H-C=N), 1290 (C-O), 1273 (C-N), 1047 (N-O), 744 (C-H) cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz,): δ_H 11.95 (br, 1H, NH), 11.04 (br, 1H, OH), 8.11 (s, 1H, H-C=N^+-O^-), 7.85 (s, 1H, H-Ar), 7.37-7.28 (d br, 2H, H-Ar), 6.97 (t br, 2H, H-Ar), 6.87-6.78 (m, 5H, H-Ar) ppm; ^{13}C NMR (DMSO-d_6, 125 MHz,): δ_C 169.5, 154.0, 138.6, 133.68, 133.63, 133.2, 131.0, 130.3, 129.3, 128.1, 121.7, 111.6 ppm; EIMS (m/z, %): 253.1 (M^+, 22), 225.1 (13), 160.0 (17), 121.1 (100), 93.1 (54), 65.1 (82).

***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-phenyl nitrone (3a)**



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39.7044
39.4288
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4E+08
4E+08
3E+08
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1E+08
5E+07
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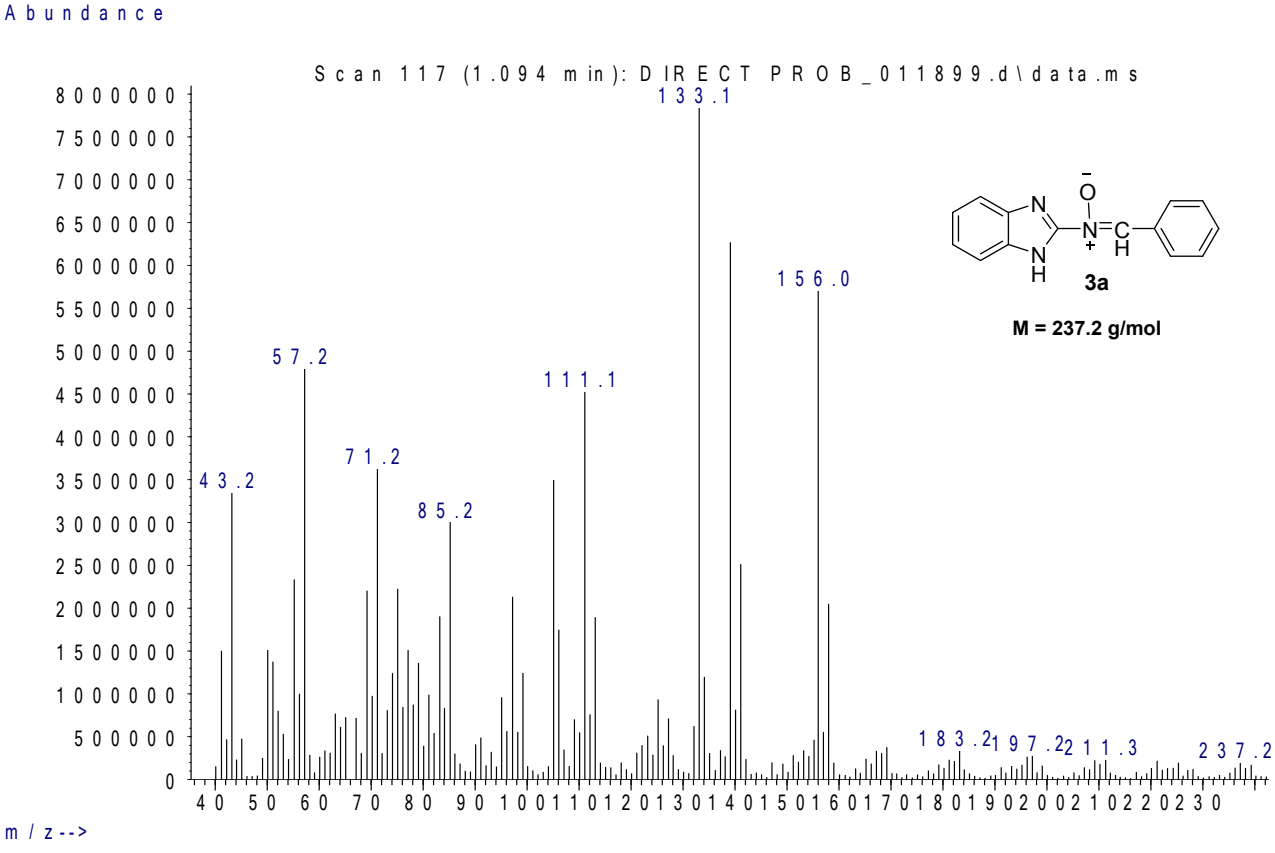
f1 (ppm)
3a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197.2
211.3
237.2
3a
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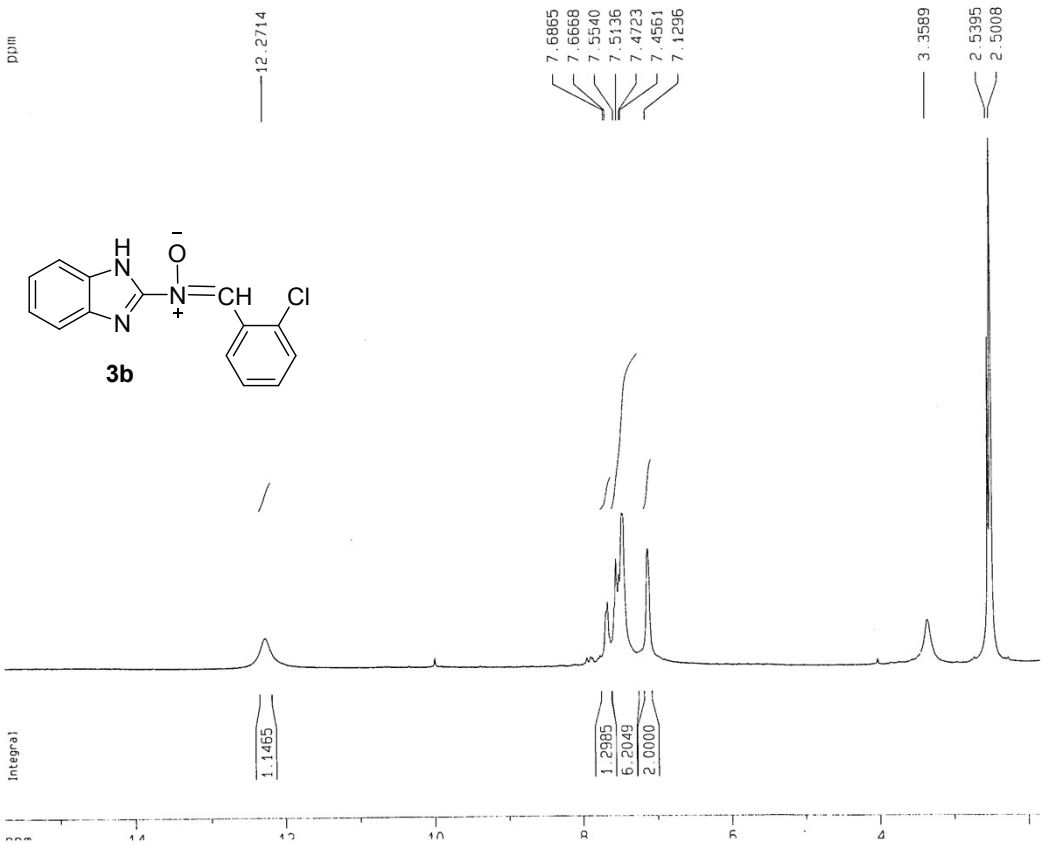
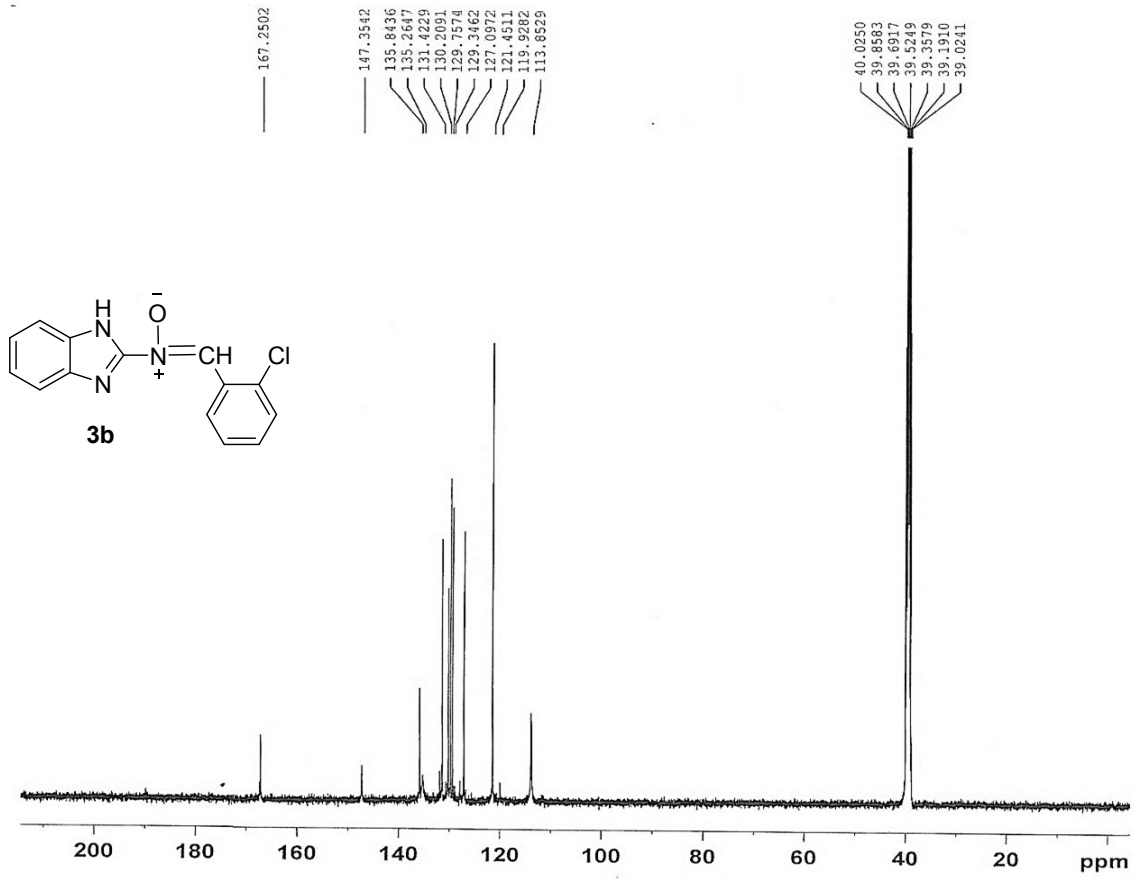
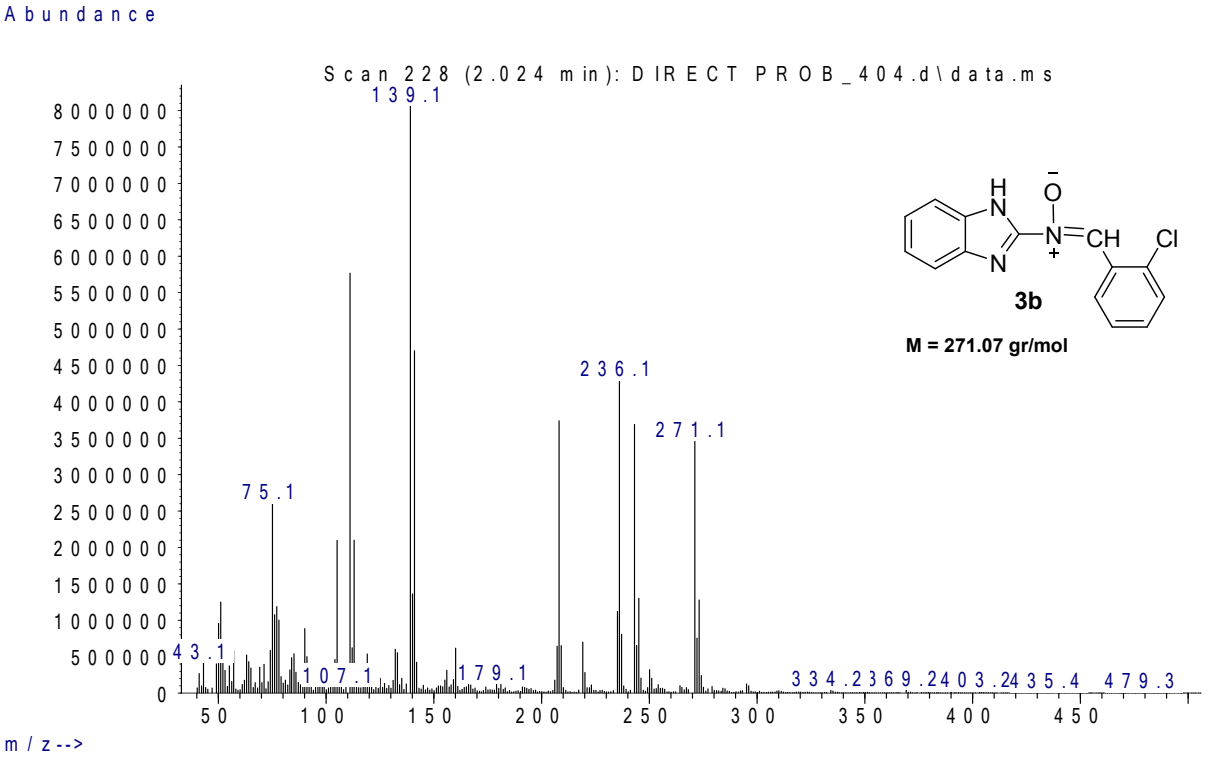
m/z-->

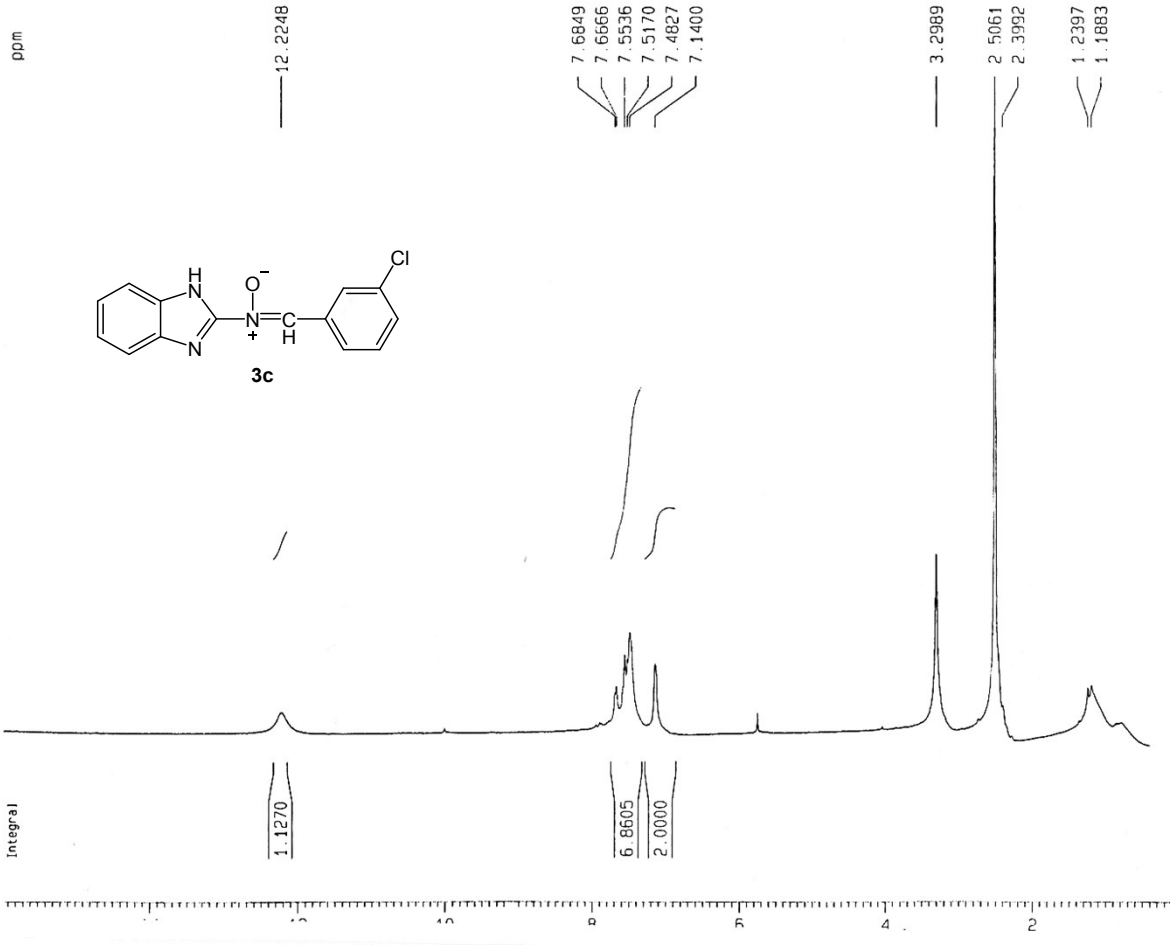
***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(2-chlorophenyl) nitrone (3b)**

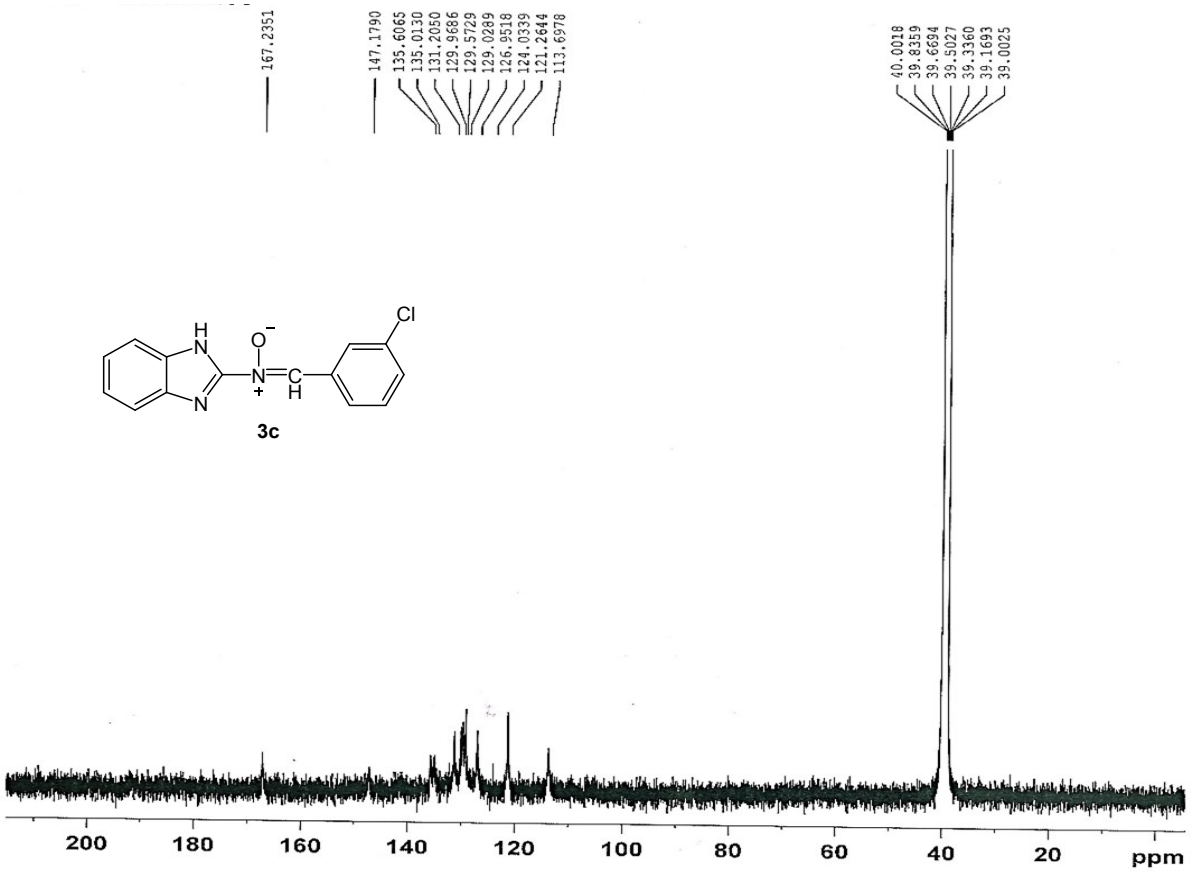




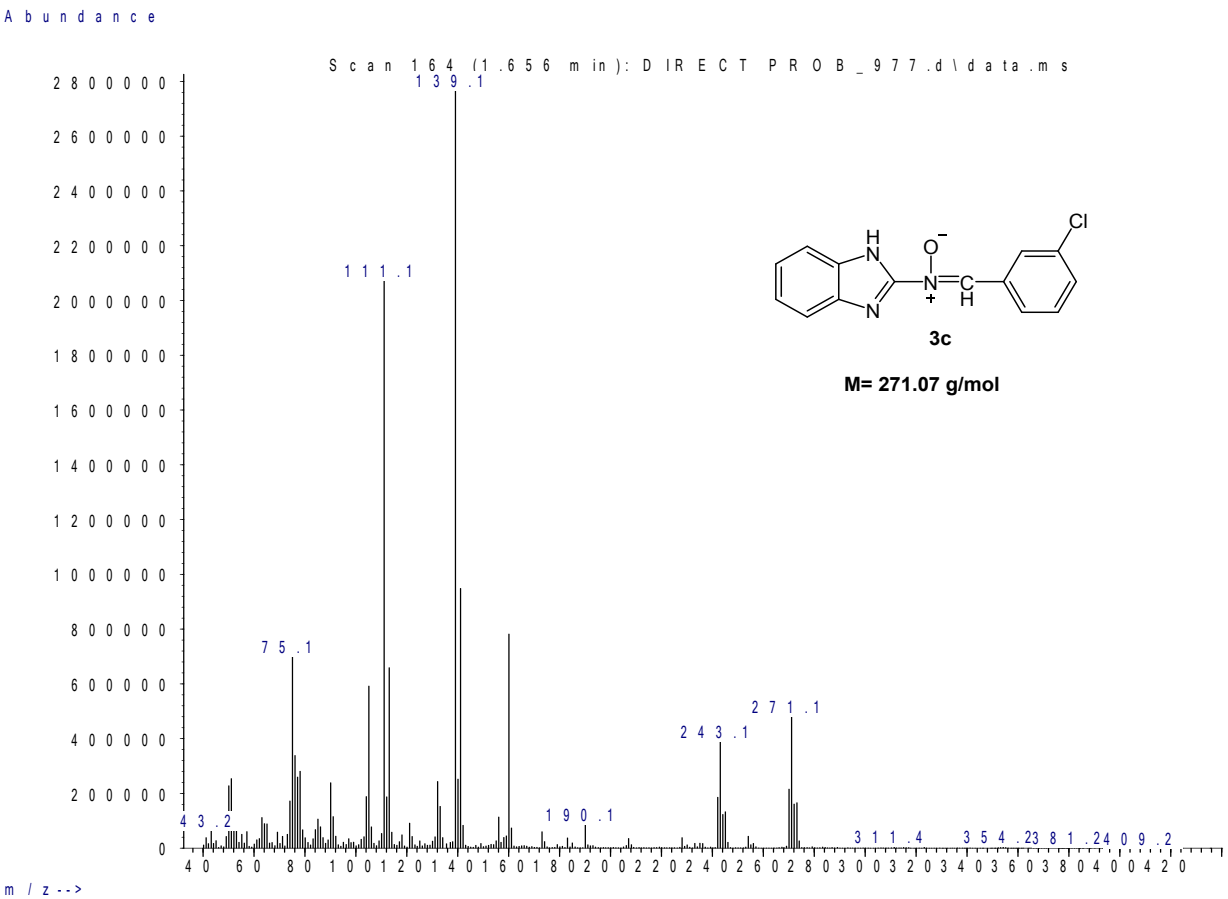


N-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(3-chlorophenyl) nitrone (3c)





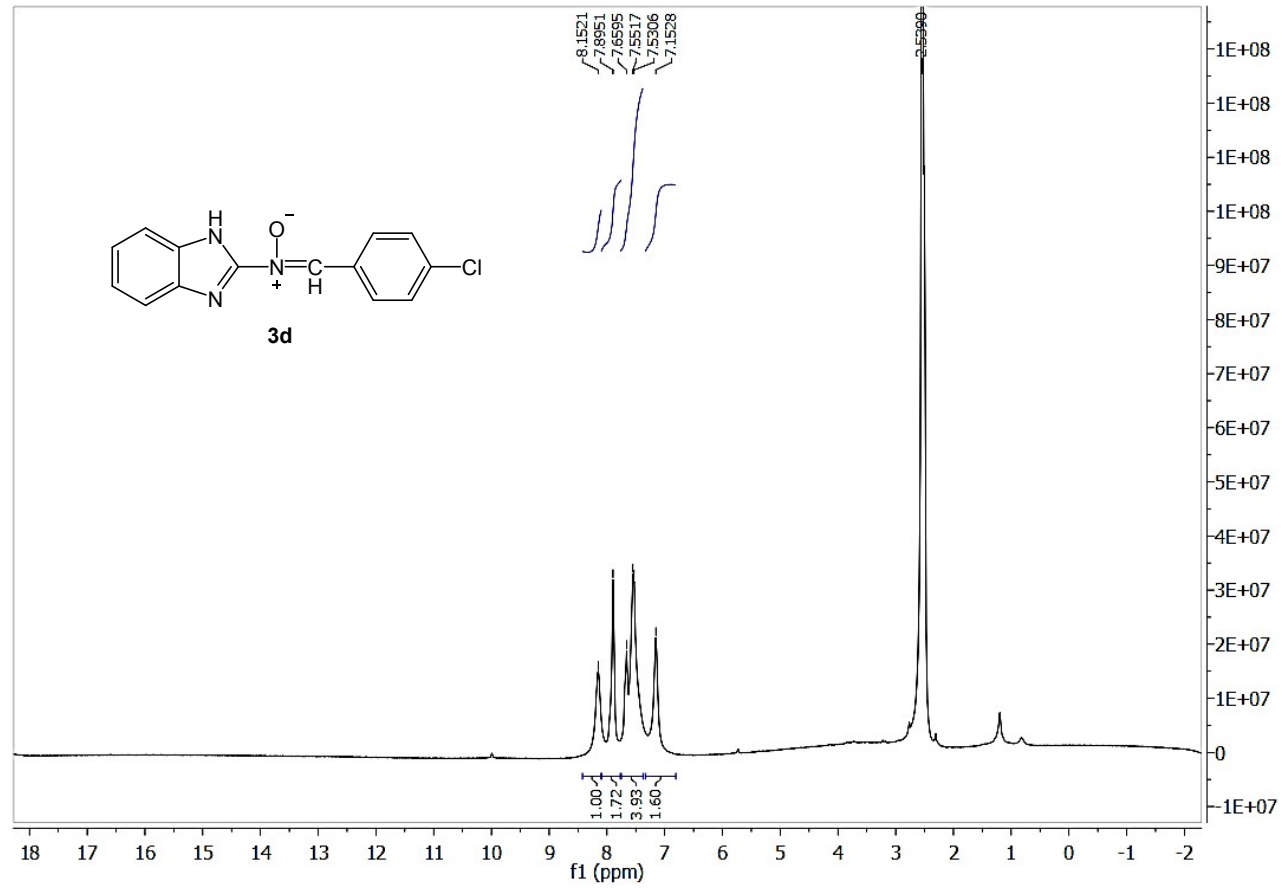
3c

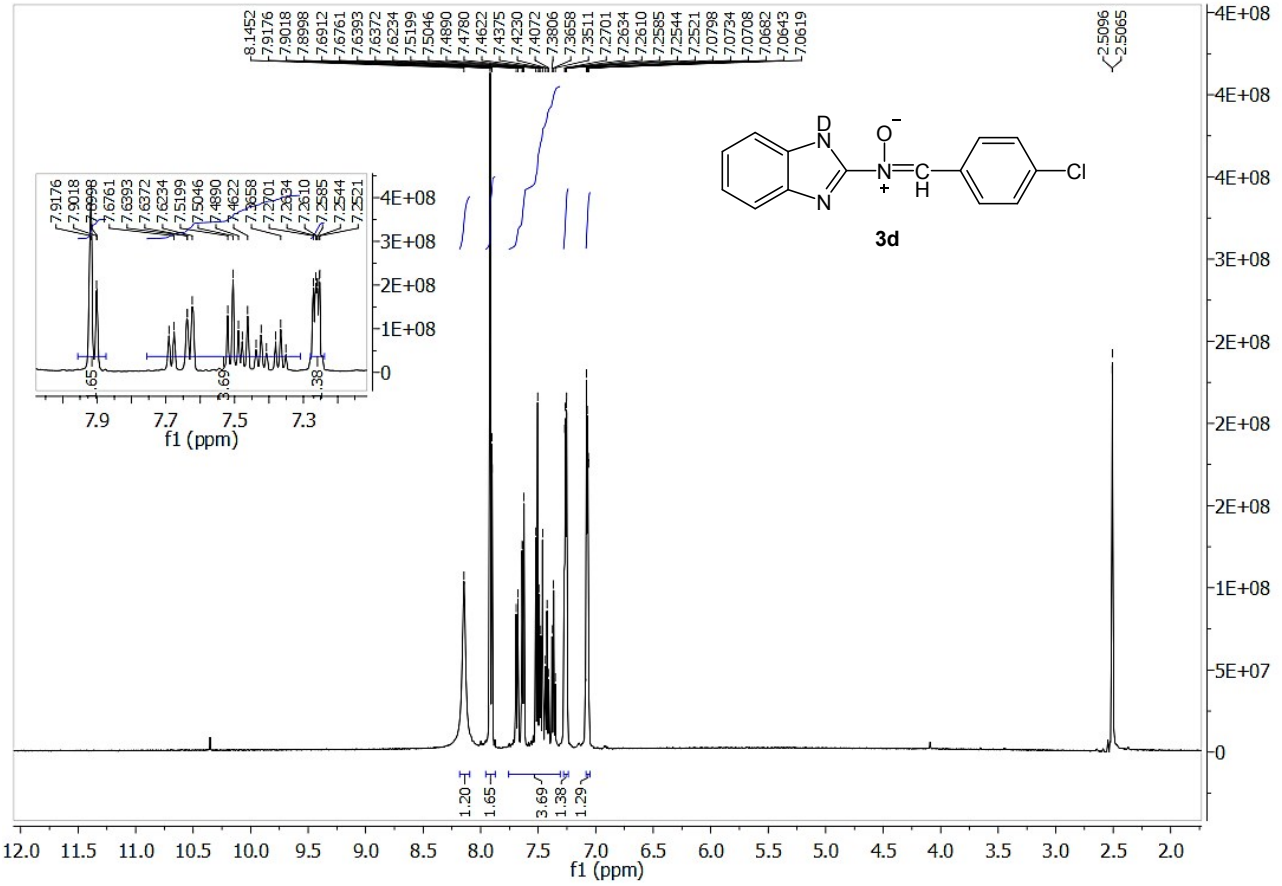


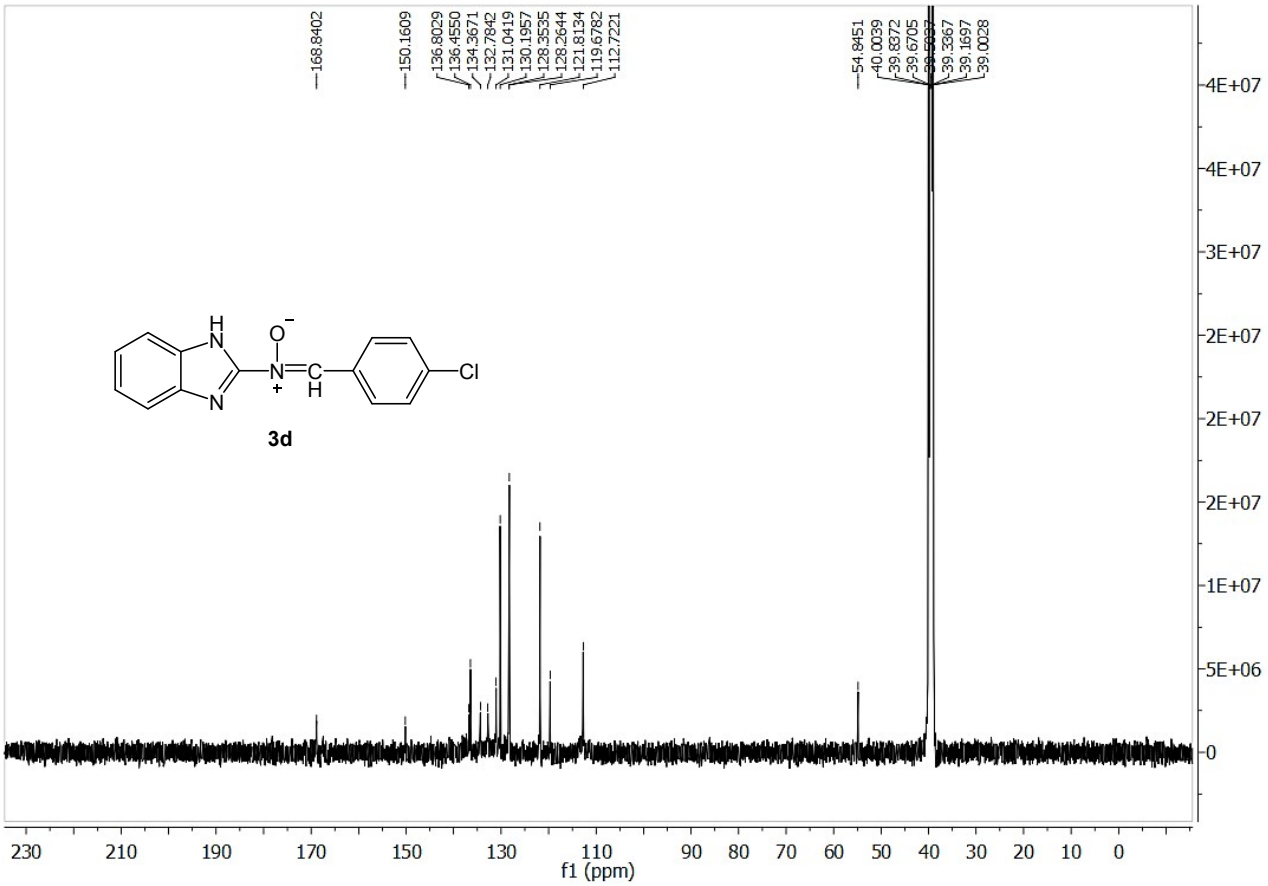
3c

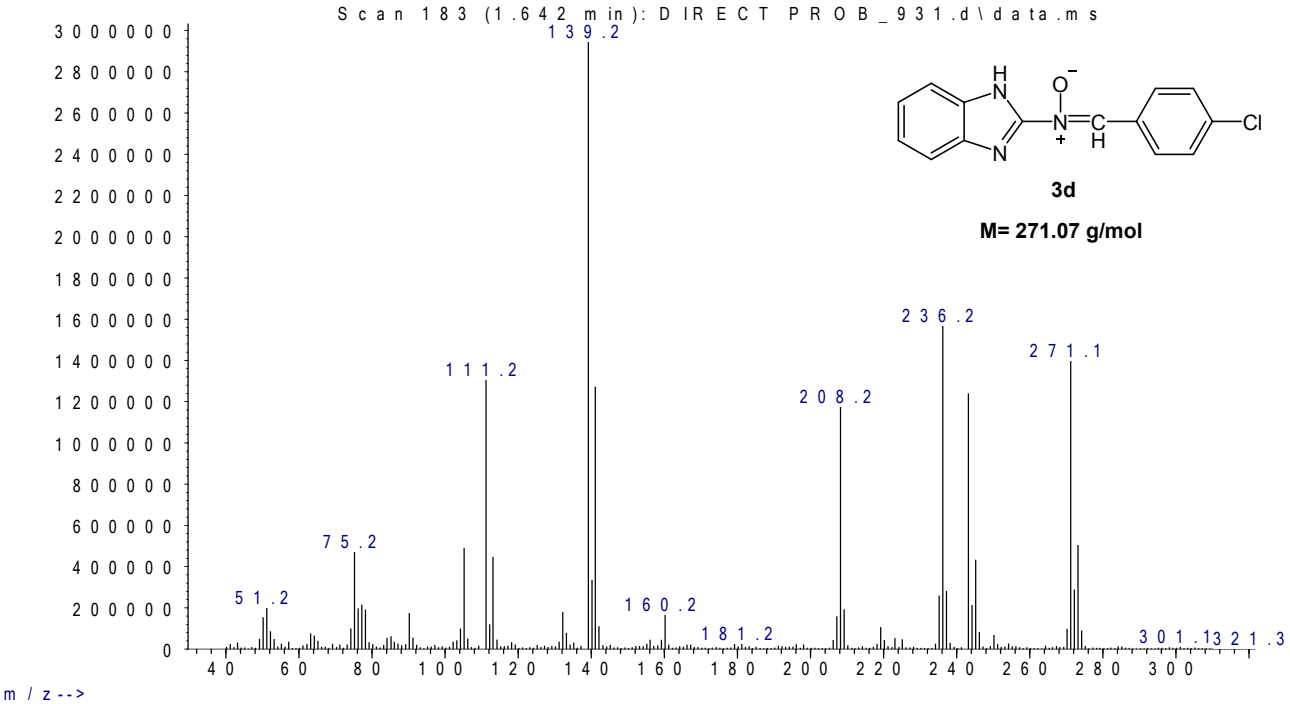
M= 271.07 g/mol

***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(4-chlorophenyl) nitrone (3d)**

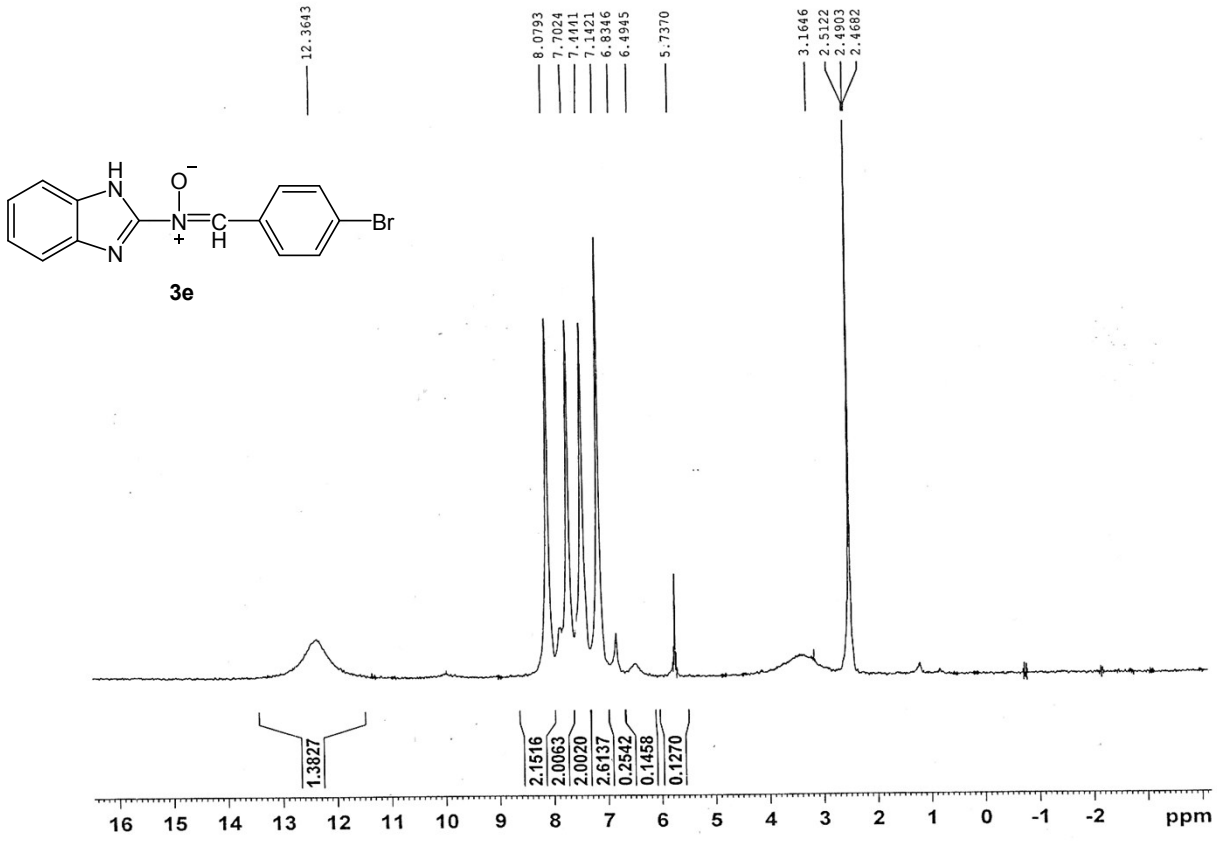








_N_-(1_H_-benzo[_d_]imidazol-2-yl)-_a_-(4-bromophenyl) nitrone (3e)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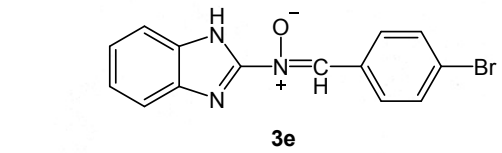
H
N
O
N
C
H
Br

3e

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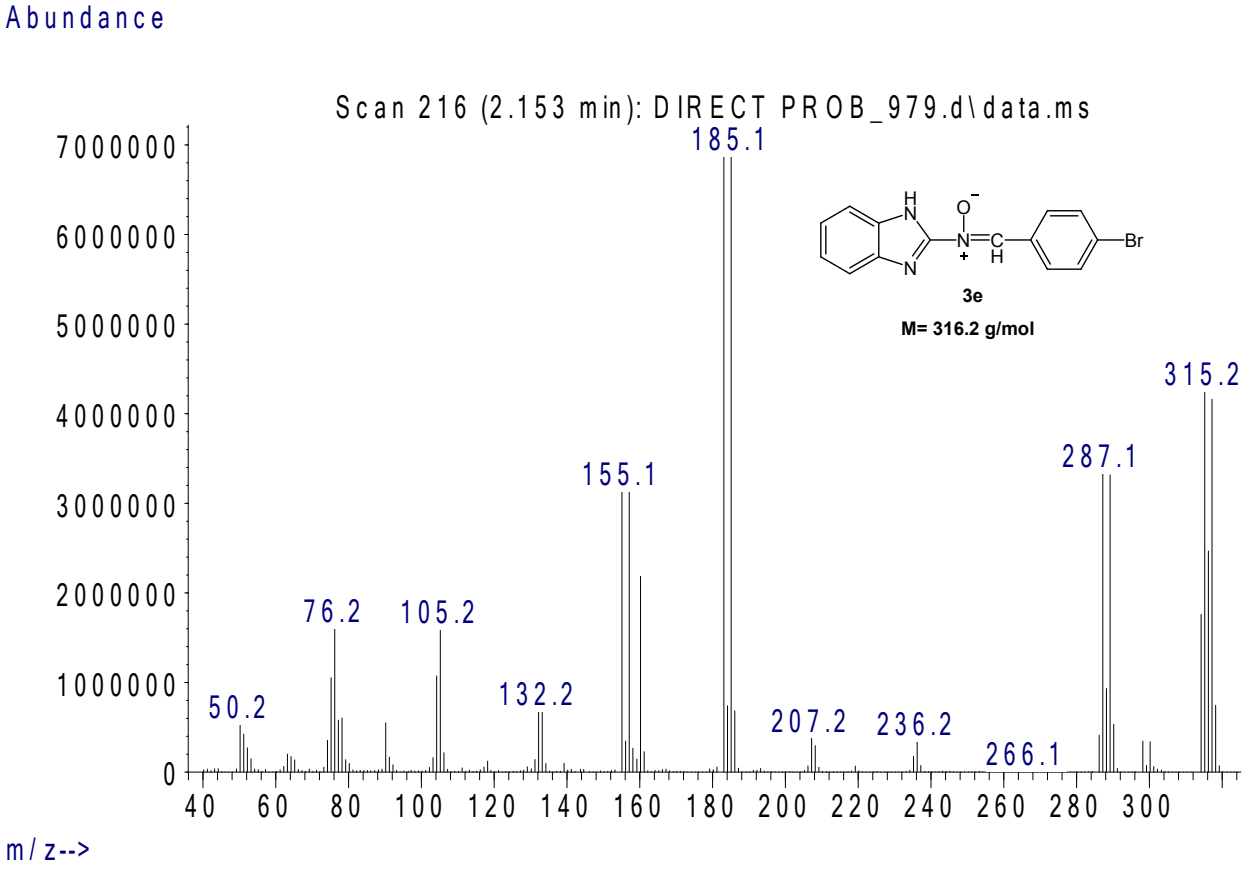
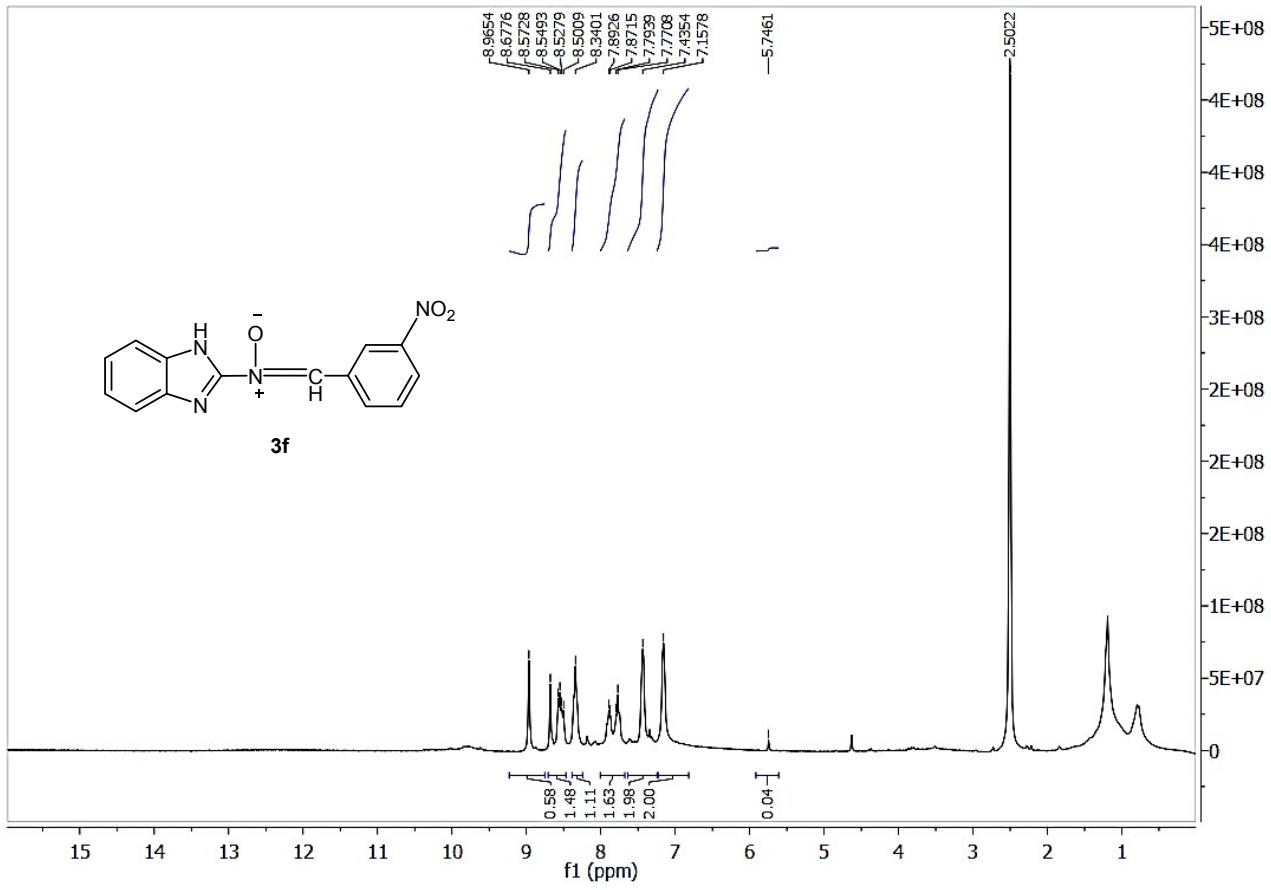
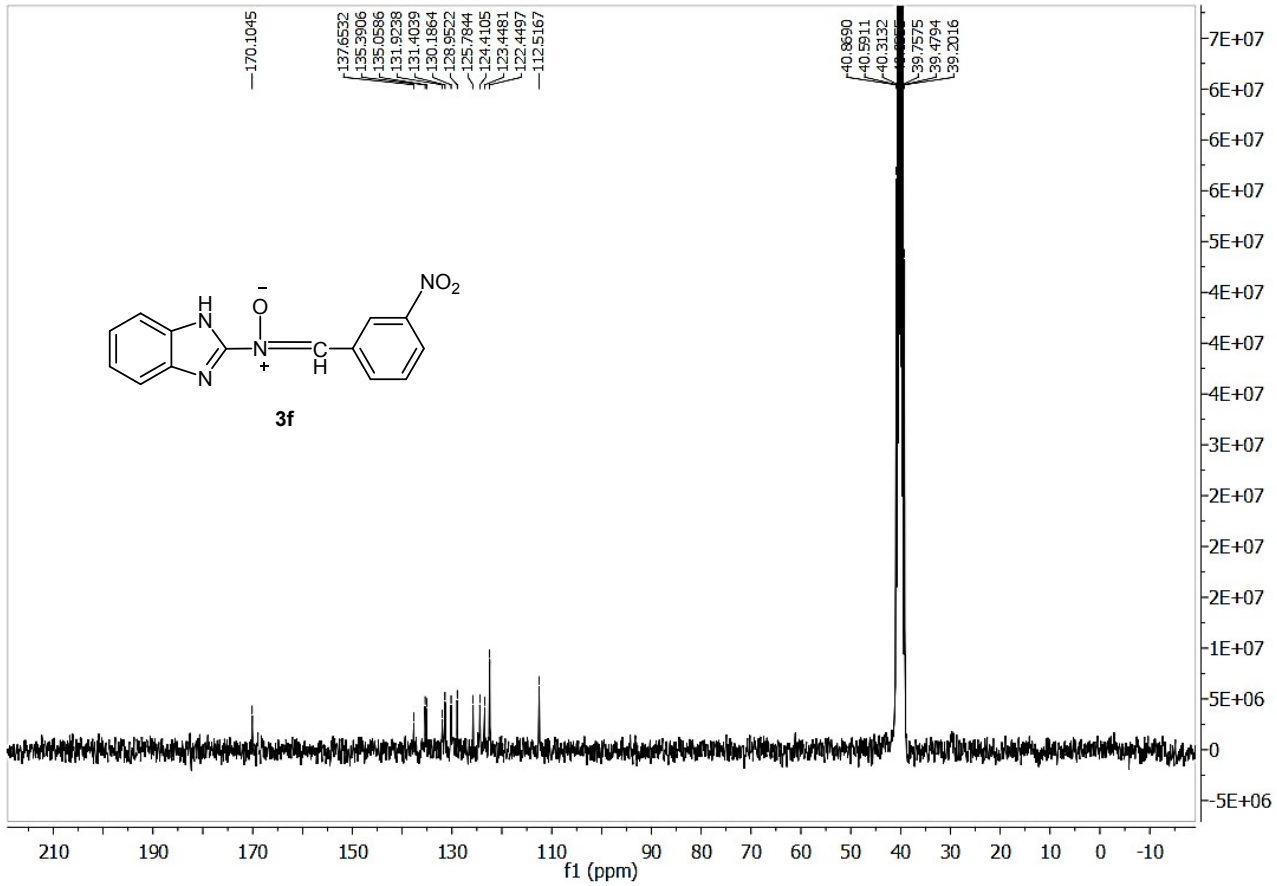
ppm

3e



***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(3-nitrophenyl) nitrone (3f)**

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5E+07
4E+07
4E+07
4E+07
3E+07
2E+07
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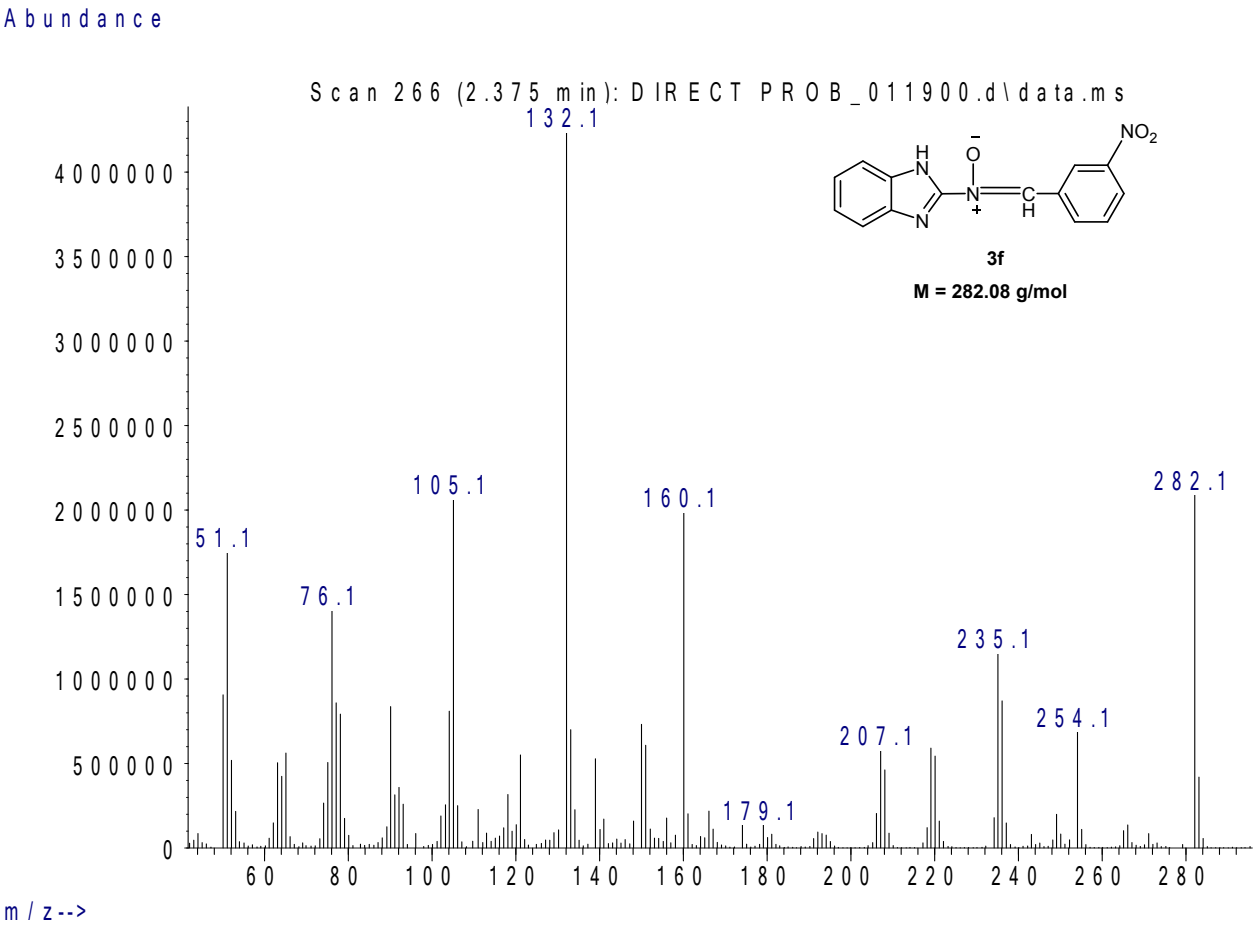
f1 (ppm)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2500000
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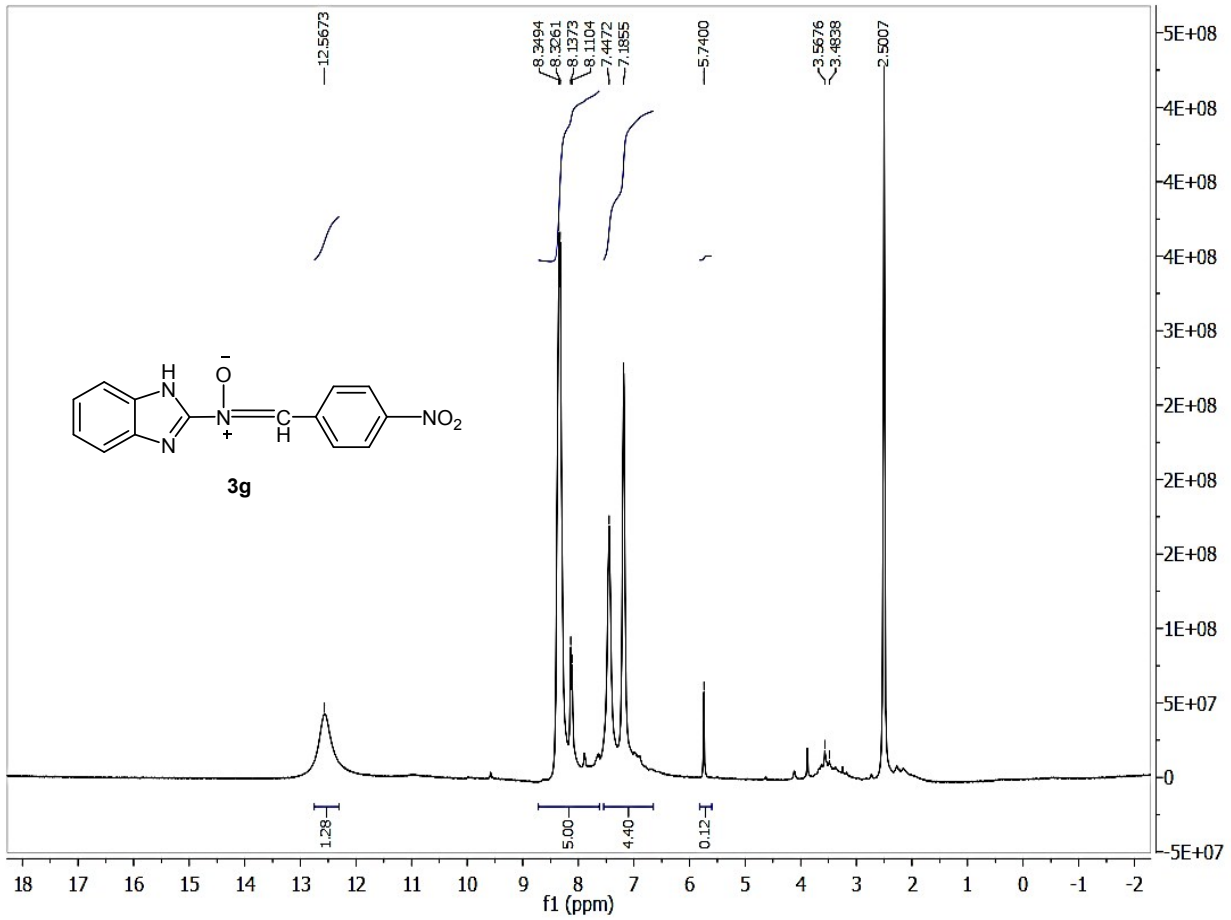
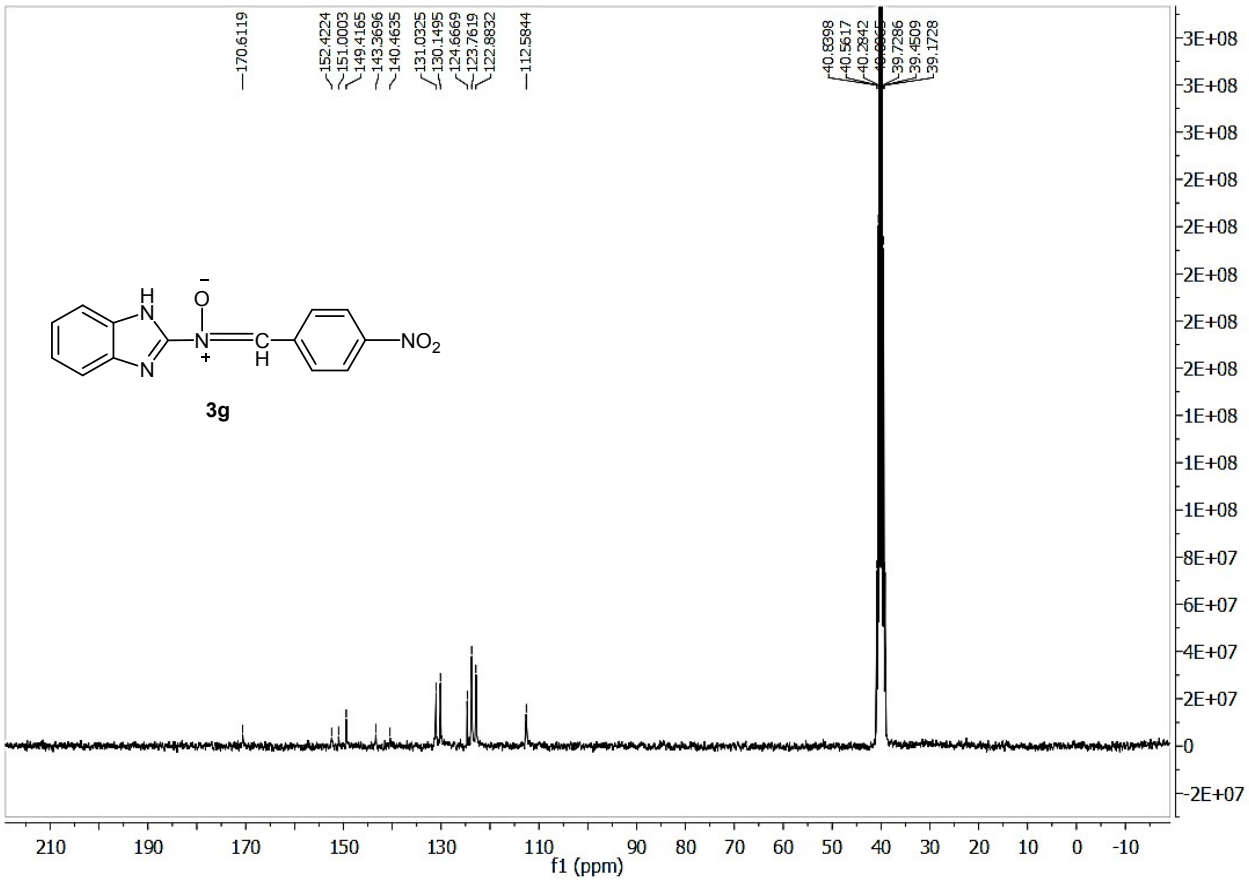
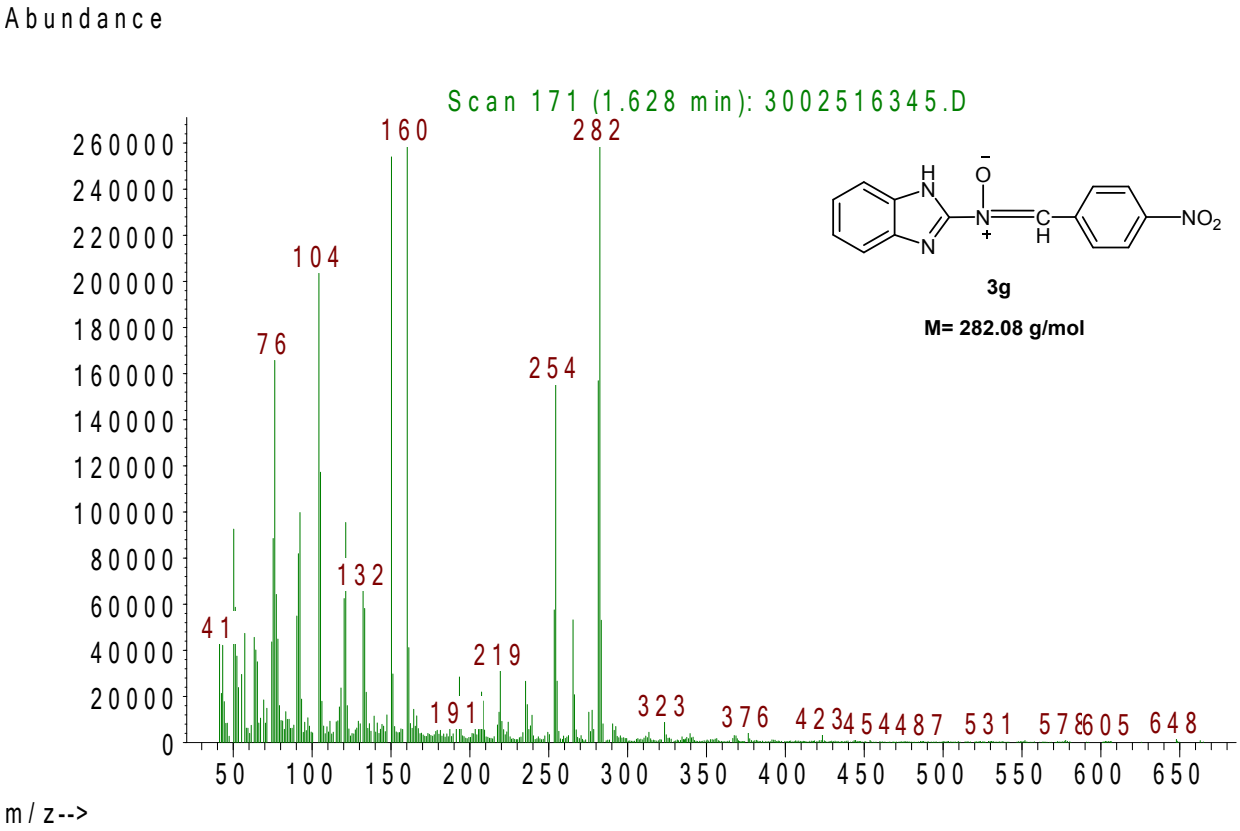
160.1
282.1
51.1
76.1
235.1
254.1
207.1
179.1
60 80 100 120 140 160 180 200 220 240 260 280
m/z-->

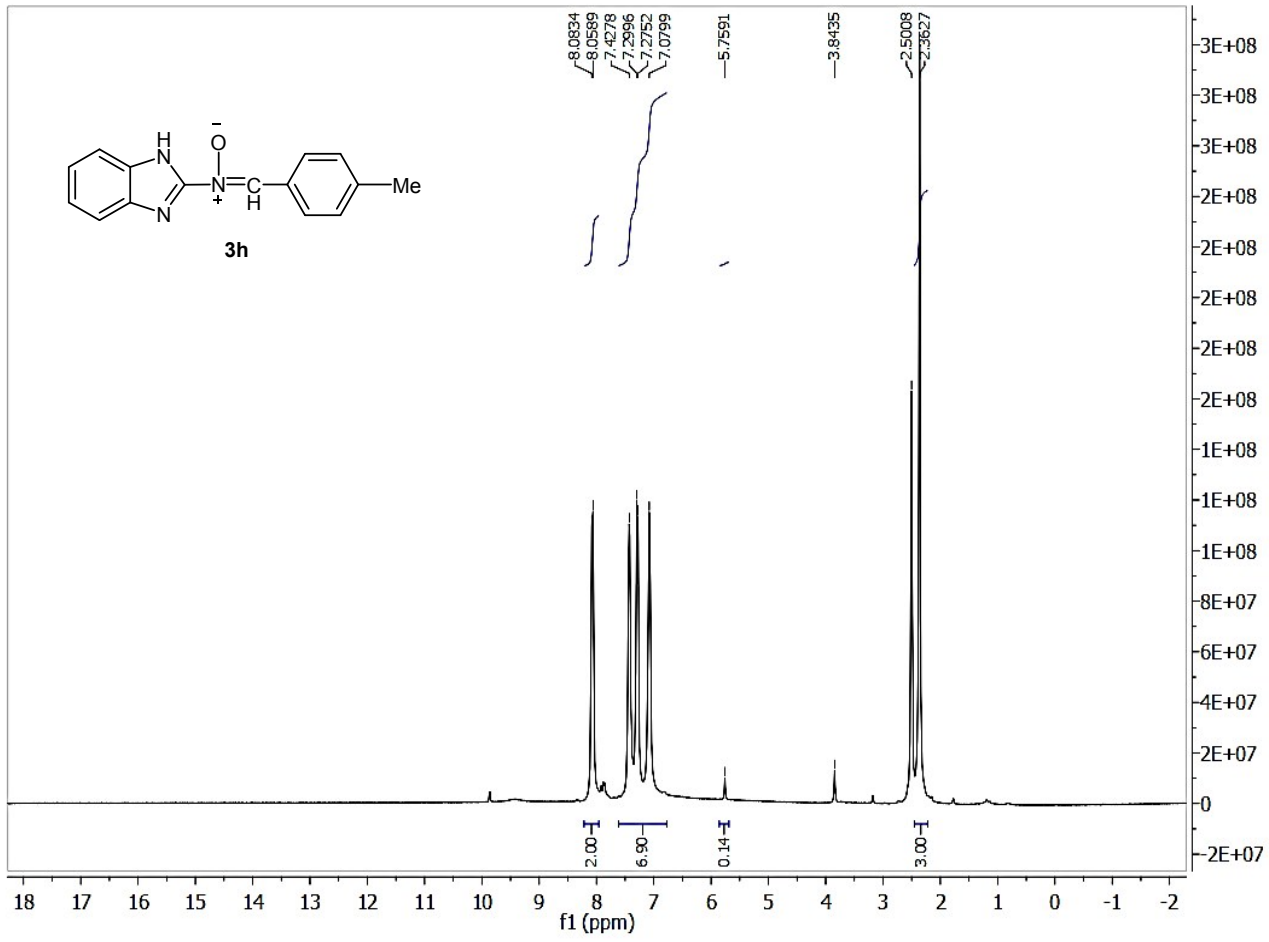
***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(4-nitrophenyl) nitrone (3g)**

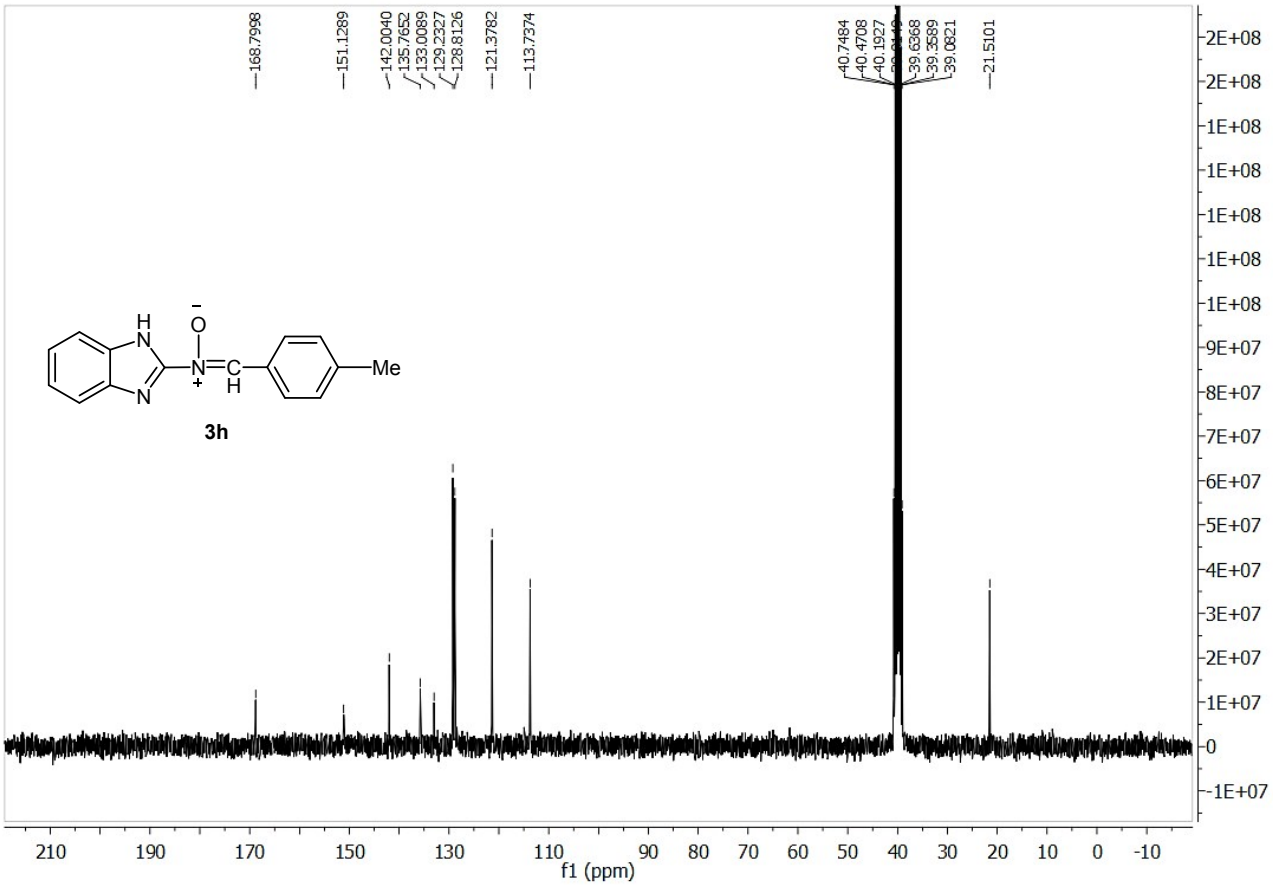






_N_-(1_H_-benzo[_d_]imidazol-2-yl)-_a_-(_p_-tolyl) nitrone (3h)

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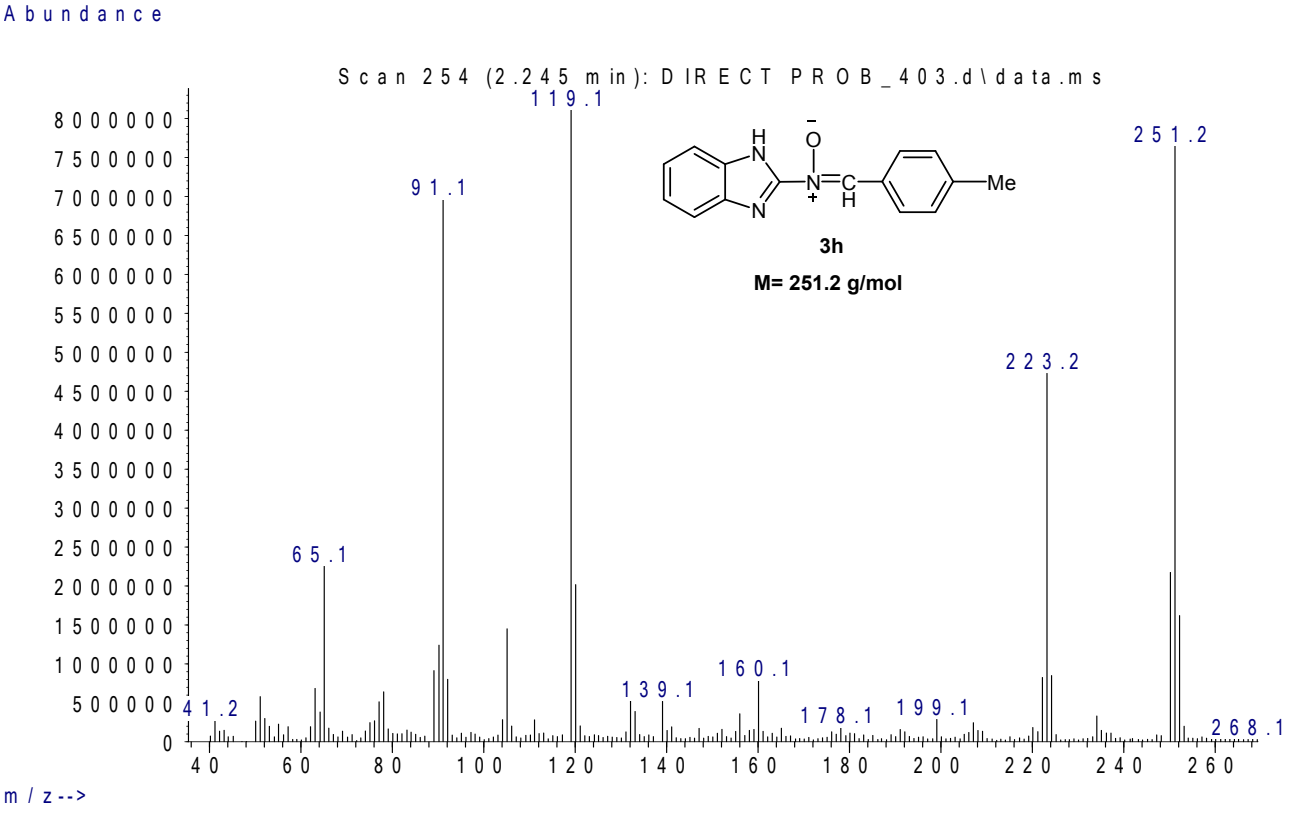
39.0821
21.5101
Me
3h
f1 (ppm)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251.2
223.2
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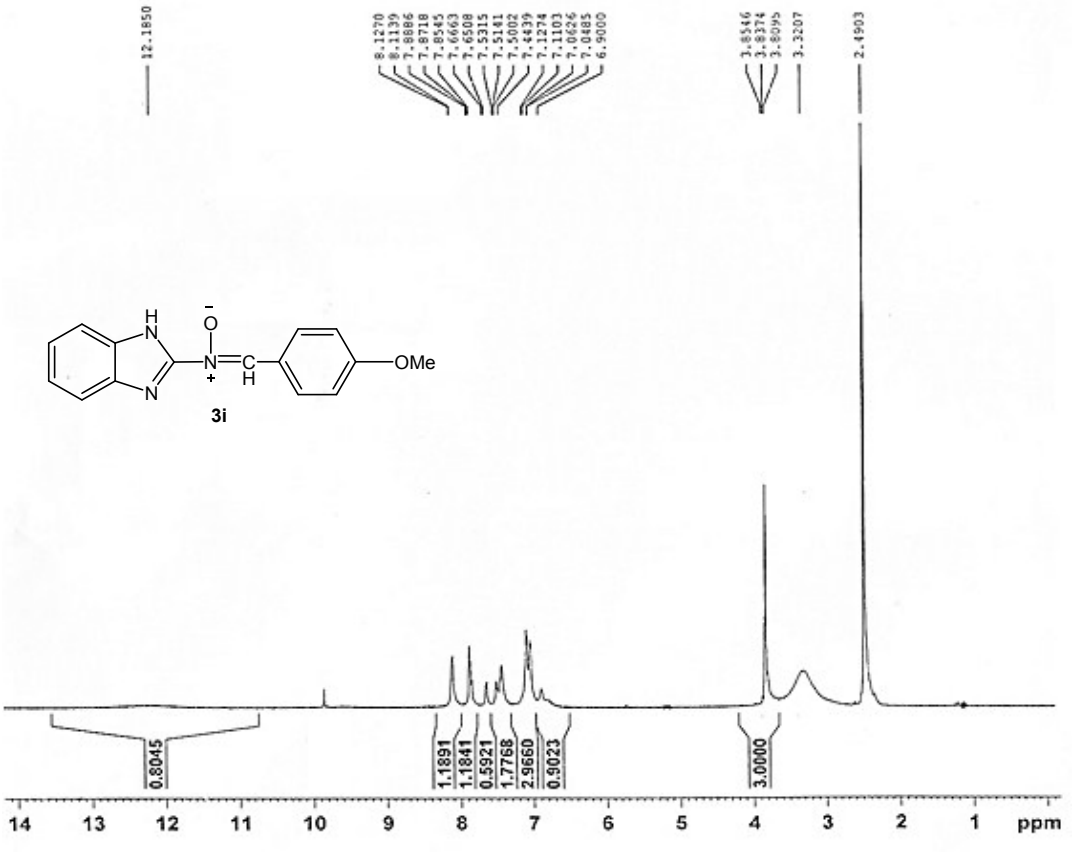
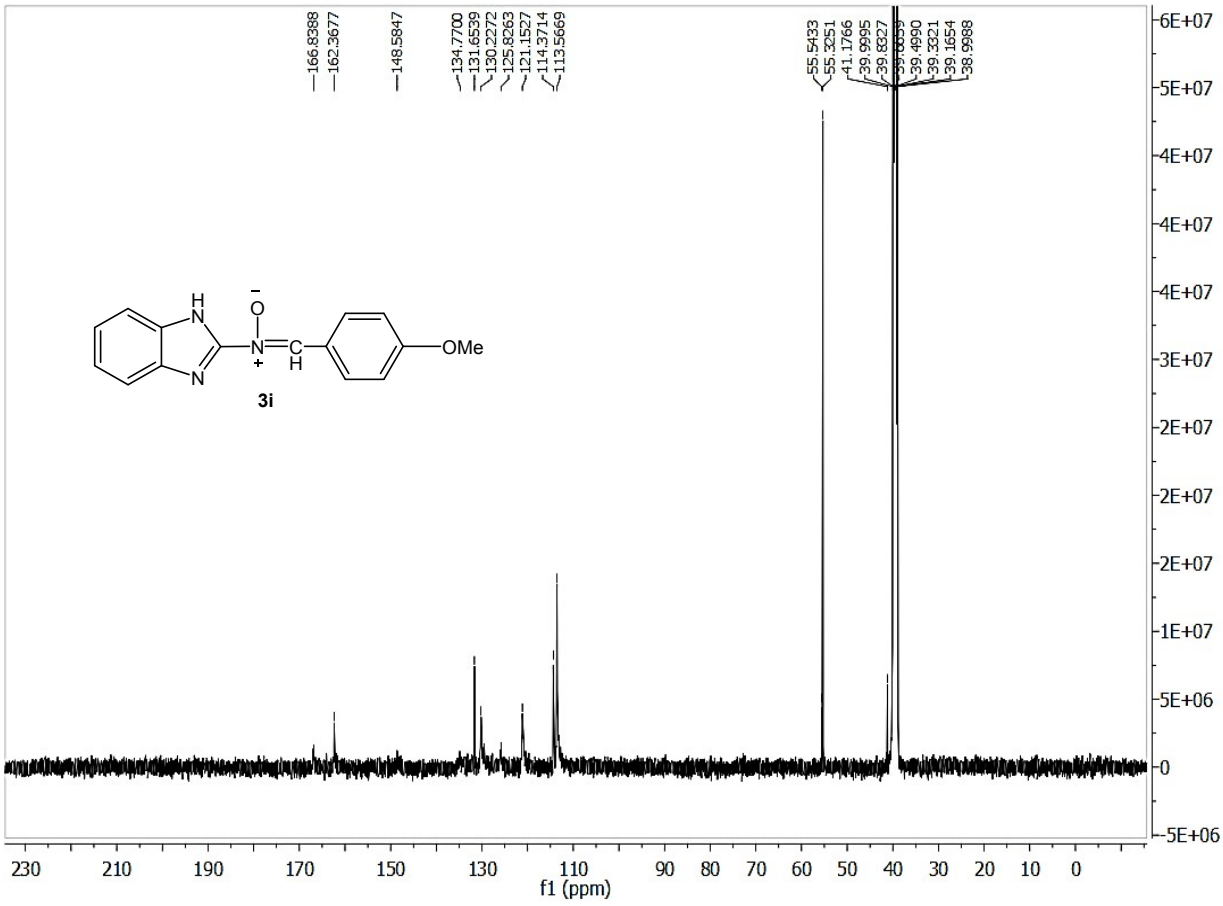
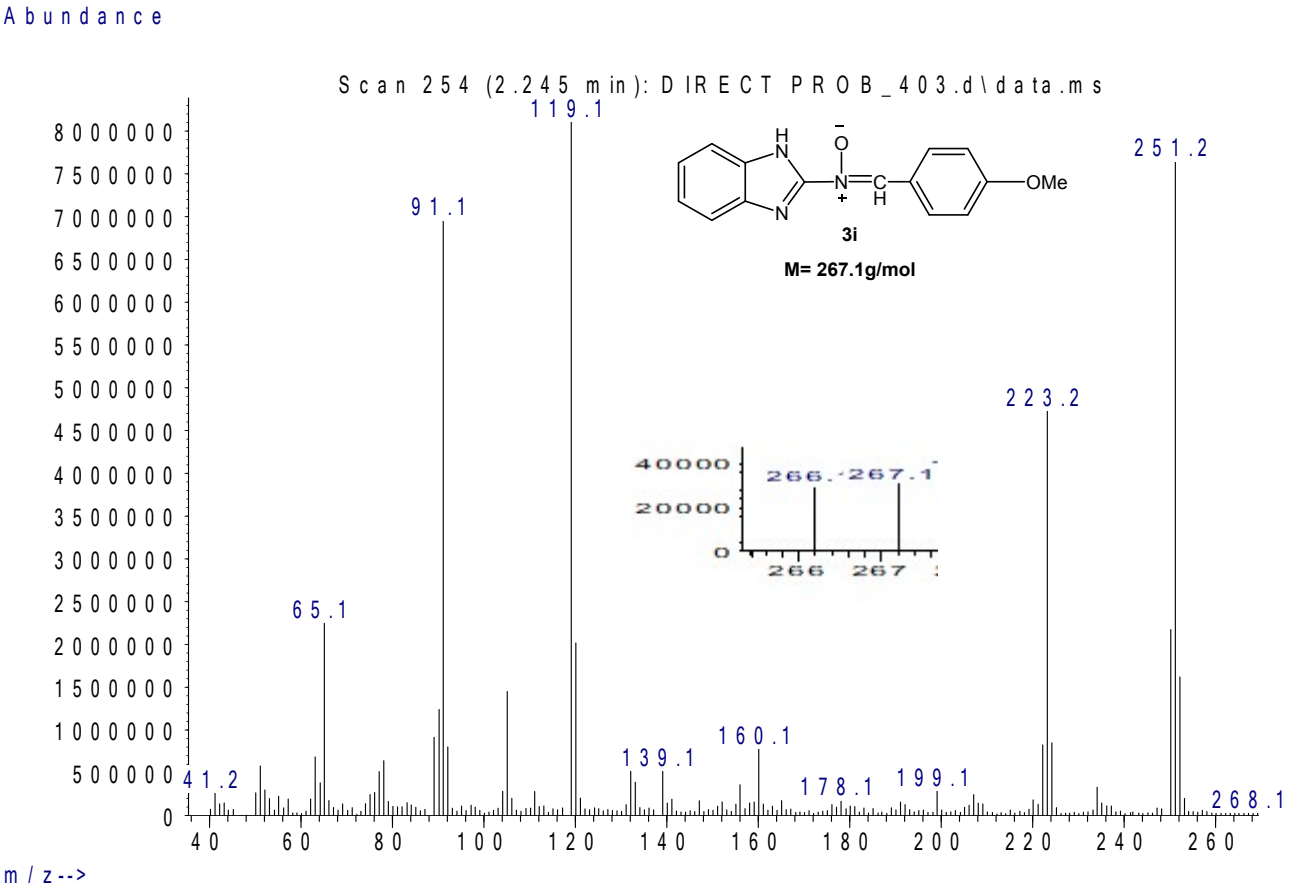
178.1
199.1
41.2
268.1
Me
3h
M= 251.2 g/mol
m/z-->

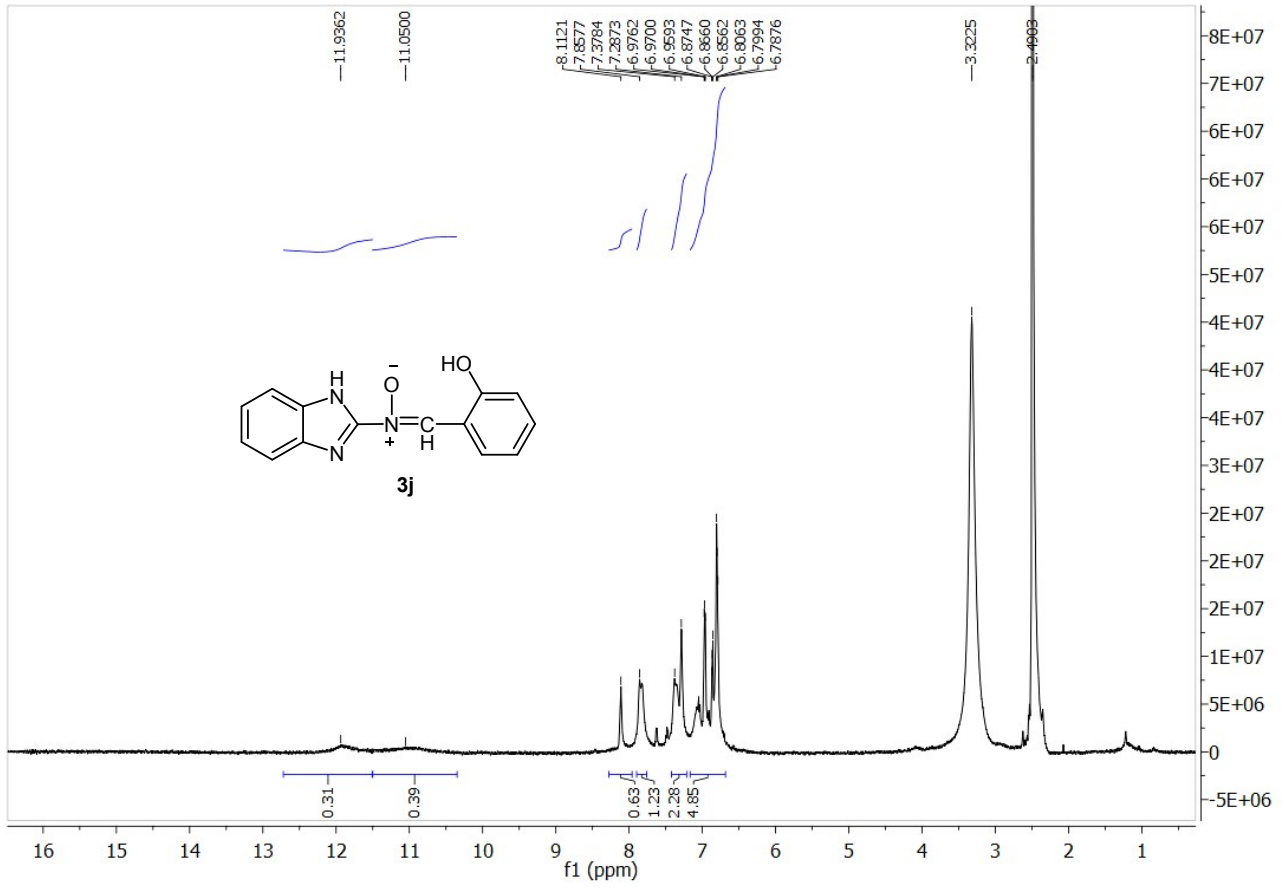
***N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(4-methoxyphenyl) nitrone (3i)**

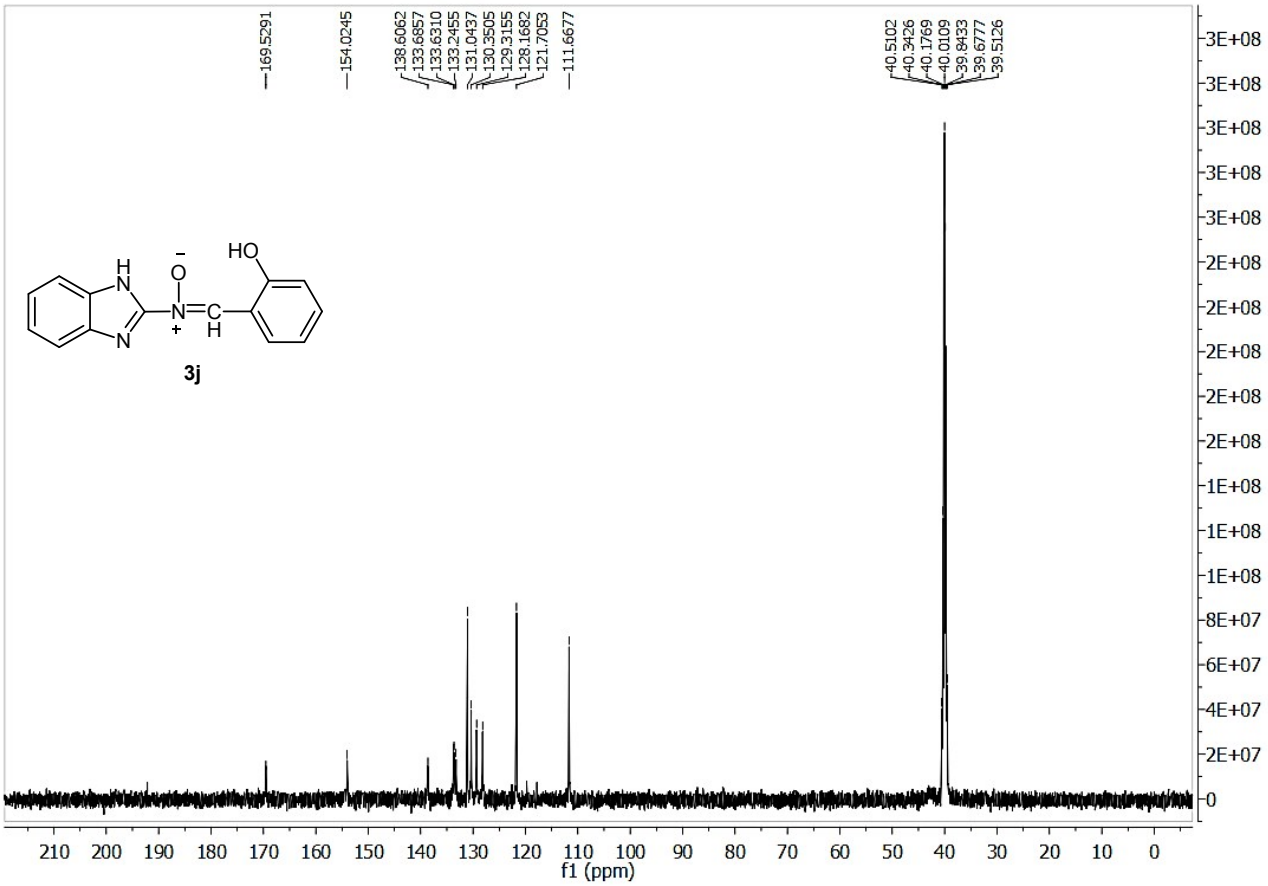




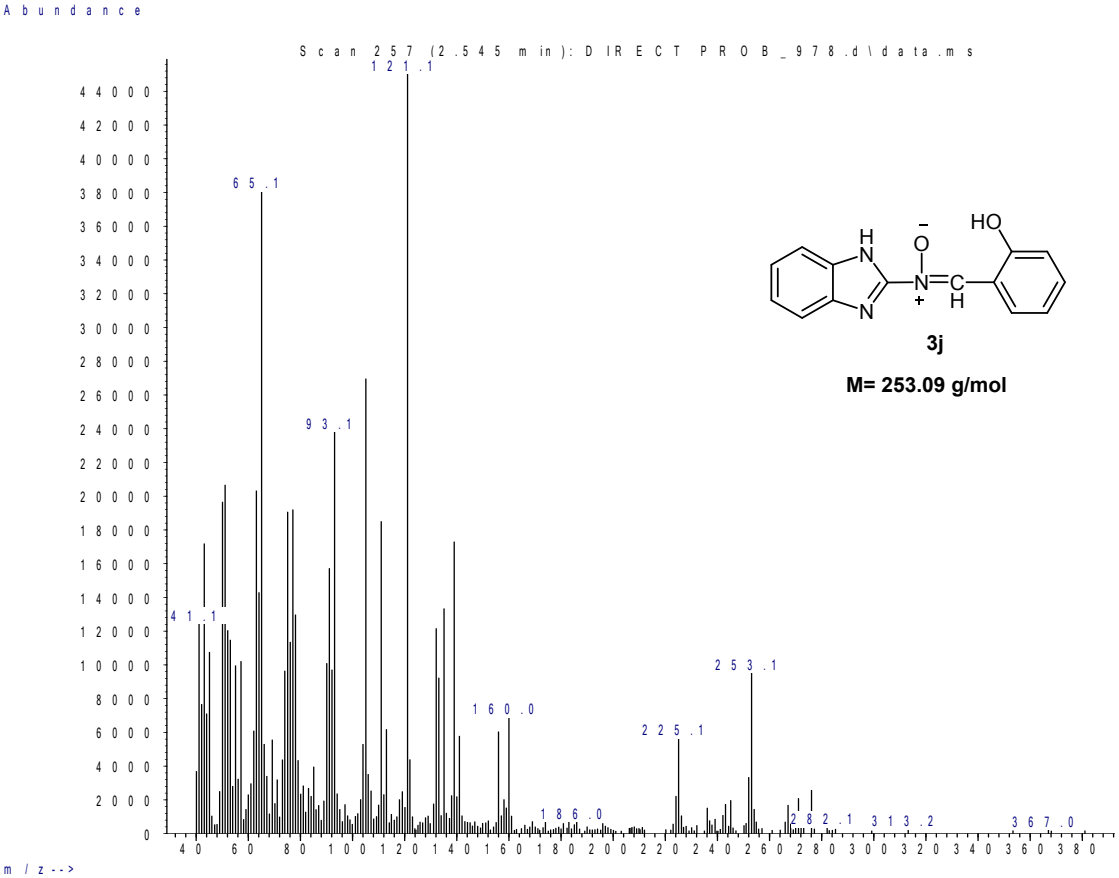


N-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-(2-hydroxyphenyl) nitrone (3j)





3j



3j

M= 253.09 g/mol

Computational data of compound 3a

(*E*)-*N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-phenyl nitrone (3a$_E$)

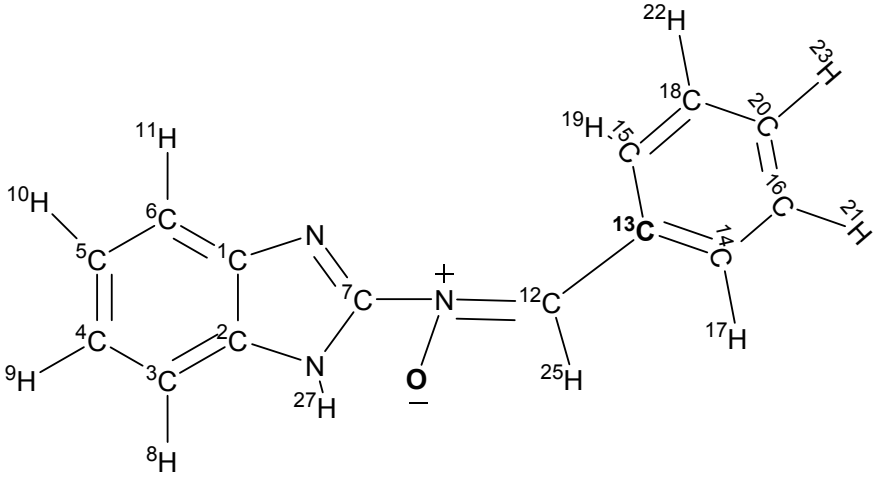
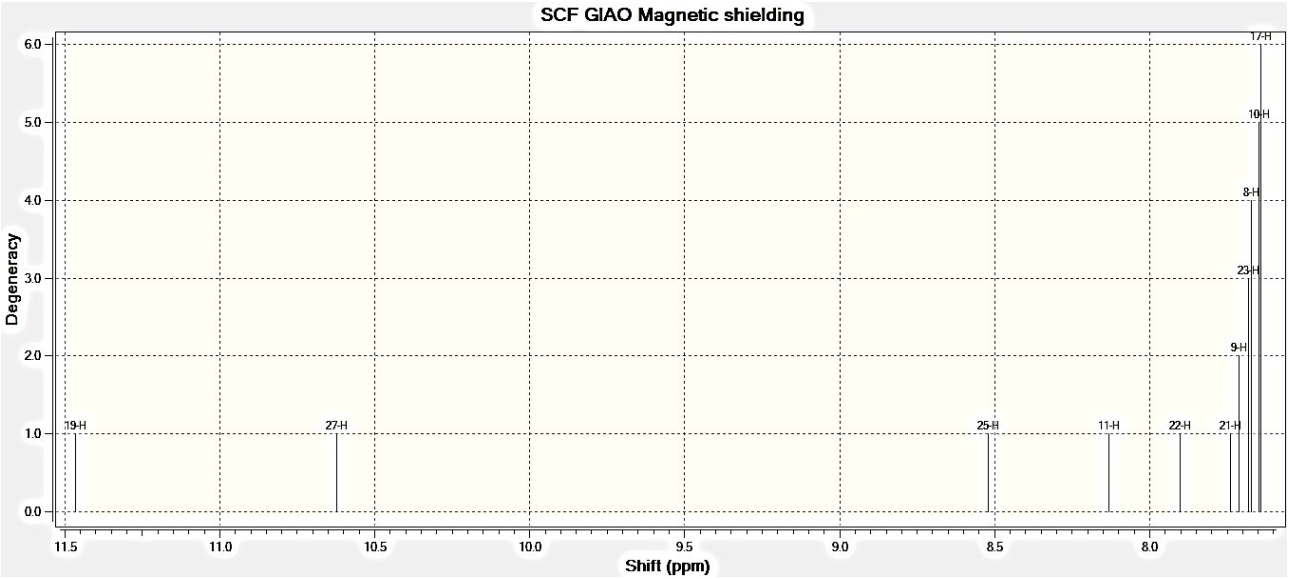
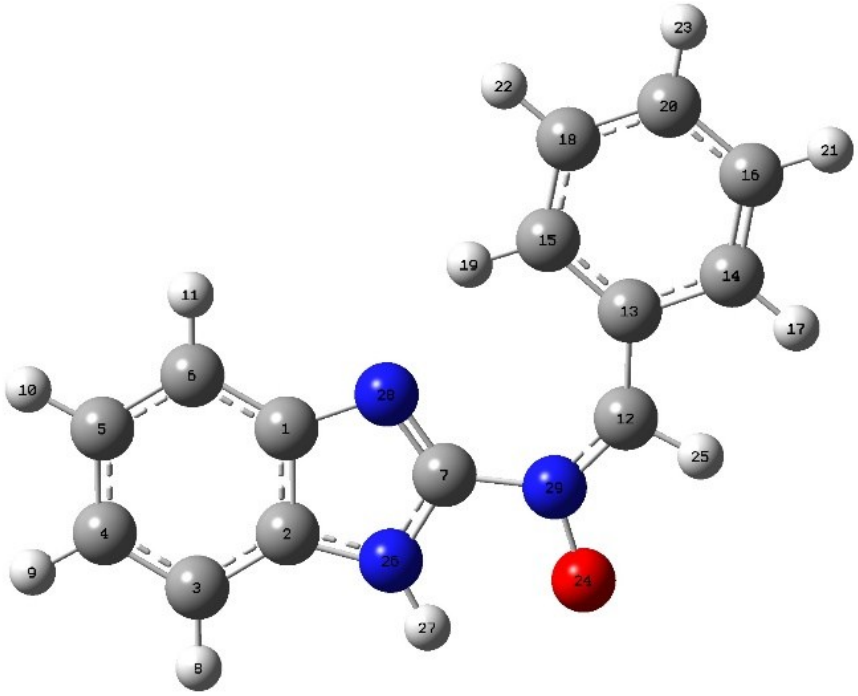


Table 1. Principal geometrical parameters including bond lengths (r, Å), bond angles and dihedral angles for nitrone (**3a$_E$**) at B3LYP/6-311+G*.

variable	B3lyp/6-311g(d)	variable	B3lyp/6-311g(d)	variable	B3lyp/6-311g(d)
Bond length(A°)		Bond angle(°)		dihedral angle(°)	
C_1–C_2	1.42	A(1,2,3)	122.32	D(1,2,3,4)	-0.00
C_2–C_3	1.40	A(2,3,4)	116.69	D(2,3,4,5)	0.00
C_3–C_4	1.39	A(3,4,5)	121.67	D(3,4,5,6)	0.00
C_4–C_5	1.41	A(4,5,6)	121.48	D(4,5,6,1)	0.00
C_5–C_6	1.39	A(1,6,5)	117.85	D(5,6,1,28)	179.99
C_1–N_{28}	1.39	A(6,1,28)	129.90	D(6,1,28,7)	-179.99
C_2–N_{26}	1.38	A(1,28,7)	104.40	D(6,1,2,26)	179.99
N_{28}–C_7	1.30	A(3,2,26)	133.06	D(1,2,26,7)	0.00
N_{26}–H_{27}	1.01	A(1,2,26)	104.61	D(1,28,7,29)	-179.99
N_{26}–C_7	1.36	A(2,26,7)	106.65	D(1,28,7,26)	0.00
C_7–N_{29}	1.43	A(2,26,27)	132.06	D(27,26,7,28)	-179.99
N_{29}–O_{24}	1.30	A(27,26,7)	121.29	D(27,26,7,29)	0.00
N_{29}–C_{12}	1.33	A(26,7,29)	115.45	D(28,7,29,24)	-179.98
C_{12}–H_{25}	1.08	A(28,7,29)	130.33	D(26,7,29,24)	0.01
C_{12}–C_{13}	1.45	A(7,29,24)	111.95	D(7,29,12,13)	0.02
C_{13}–C_{15}	1.41	A(24,29,12)	119.21	D(24,29,12,13)	-179.98
C_{13}–C_{14}	1.42	A(29,12,25)	107.25	D(29,12,13,15)	-0.04
C_{14}–C_{16}	1.39	A(29,12,13)	137.99	D(29,12,13,14)	179.97
C_{15}–C_{18}	1.39	A(13,15,18)	120.36	D(12,13,14,16)	179.99
C_{18}–C_{20}	1.39	A(15,13,14)	117.52	D(25,12,13,15)	179.97
C_{16}–C_{20}	1.39	A(12,13,14)	113.26	D(12,13,14,17)	-0.00
C_{15}–H_{19}	1.08	A(13,14,16)	121.63	D(13,14,16,20)	-0.00
C_{14}–H_{17}	1.09	A(14,16,20)	119.96	D(21,16,20,18)	179.99
C_3–H_8	1.08	A(16,20,18)	119.28	D(13,15,18,20)	0.00
C_6–H_{11}	1.08	A(20,18,15)	121.25		

Figure 1. The Computational [1]H-NMR Spectrum Data for nitrone (**3a$_E$**) at B3LYP/6-311+G*.





19-H	**27-H N-H**	**25-H C-H**	11-H	22-H	21-H	9-H	23-H	8-H	10-H	17-H
11.64	**10.62**	**8.52**	8.13	7.90	7.74	7.71	7.68	7.67	7.64	7.64

(*Z*)-*N*-(1*H*-benzo[*d*]imidazol-2-yl)-*a*-phenyl nitrone ($3a_Z$)

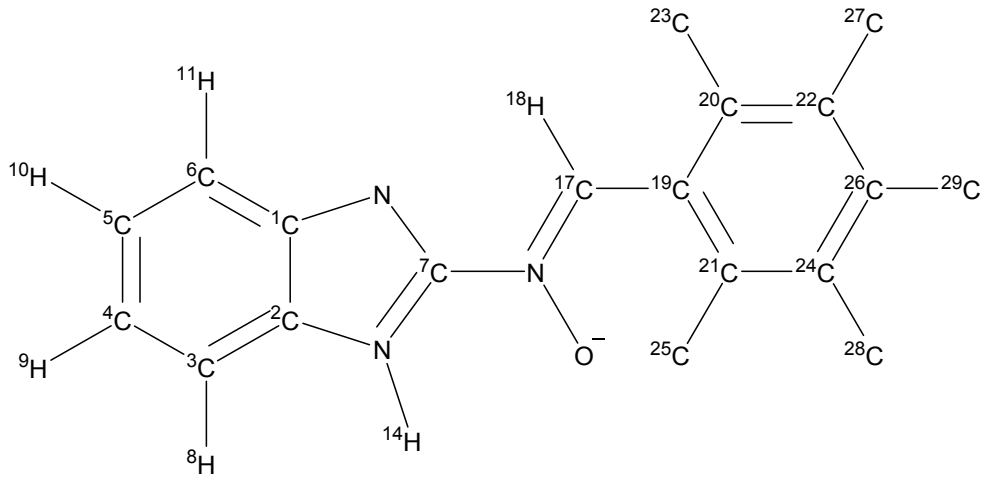
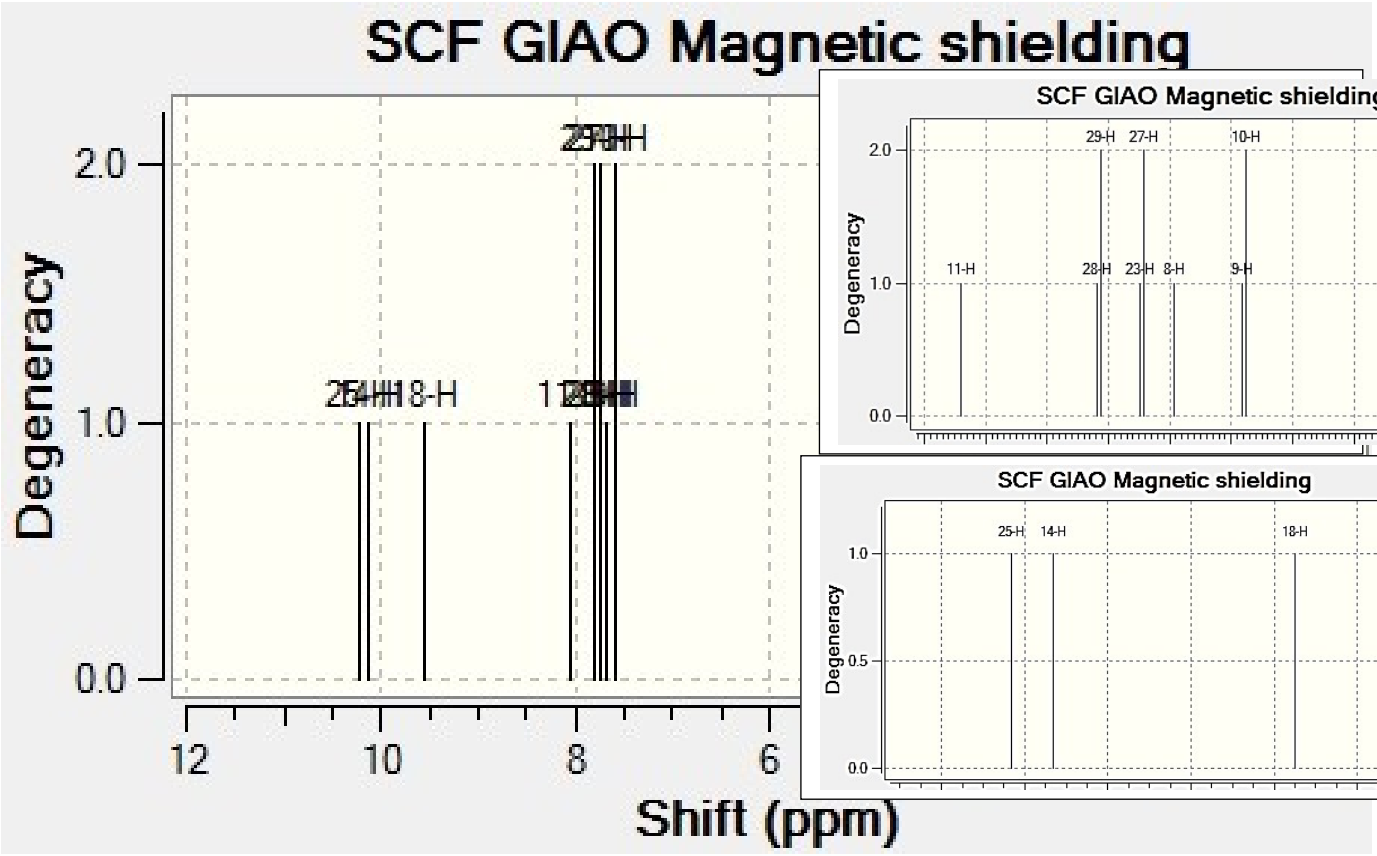
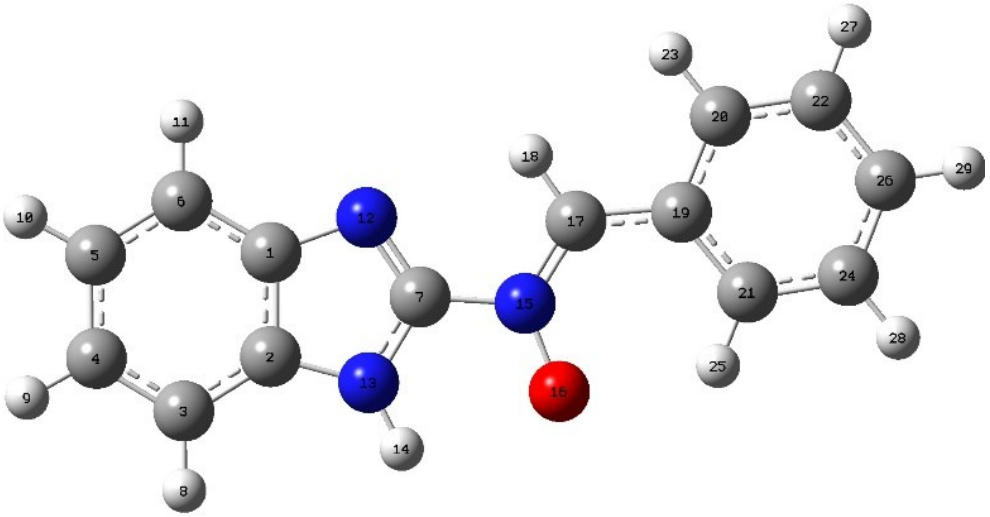


Table 2. Principal geometrical parameters including bond lengths (r, Å), bond angles and dihedral angles for nitrone (**$3a_Z$**) at B3LYP/6-311+G*.

variable	B3lyp/6-311g(d)	variable	B3lyp/6-311g(d)	variable	B3lyp/6-311g(d)
Bond length(A°)		∠Bond angle(°)		∠dihedral angle(°)	
C_1–C_2	1.42	A(1,2,3)	122.41	D(1,2,3,4)	0.00
C_2–C_3	1.39	A(2,3,4)	116.71	D(2,3,4,5)	0.00
C_3–C_4	1.39	A(3,4,5)	121.61	D(3,4,5,6)	0.00
C_4–C_5	1.41	A(4,5,6)	121.49	D(4,5,6,1)	0.00
C_5–C_6	1.39	A(1,6,5)	117.96	D(5,6,1,12)	180.00
C_1–N_{12}	1.39	A(6,1,12)	129.88	D(6,1,12,7)	180.00
C_2–N_{13}	1.38	A(1,12,7)	103.81	D(6,1,2,13)	180.00
N_{12}–C_7	1.30	A(3,2,13)	133.01	D(1,2,13,7)	0.00
N_{13}–H_{14}	1.01	A(1,2,13)	104.57	D(1,12,7,15)	-180.00
N_{13}–C_7	1.36	A(2,13,7)	106.09	D(1,12,7,13)	0.00
C_7–N_{15}	1.43	A(2,13,14)	131.32	D(14,13,7,12)	179.99
N_{15}–O_{16}	1.29	A(14,13,7)	122.58	D(14,13,7,15)	0.00
N_{15}–C_{17}	1.32	A(13,7,15)	117.44	D(12,7,15,16)	-179.99
C_{17}–H_{18}	1.08	A(12,7,15)	127.35	D(13,7,15,16)	0.01
C_{17}–C_{19}	1.44	A(7,15,16)	114.64	D(7,15,17,19)	-179.99
C_{19}–C_{20}	1.41	A(16,15,17)	127.10	D(16,15,17,19)	-0.00
C_{19}–C_{21}	1.41	A(15,17,18)	113.54	D(15,17,19,20)	180.00
C_{20}–C_{22}	1.39	A(15,17,19)	126.49	D(15,17,19,21)	0.00
C_{22}–C_{26}	1.40	A(19,20,22)	120.96	D(17,19,21,24)	-180.00
C_{26}–C_{24}	1.39	A(20,19,21)	118.54	D(18,17,19,20)	0.00
C_{24}–C_{21}	1.39	A(21,19,17)	124.65	D(17,19,21,25)	0.00
C_{21}–H_{25}	1.08	A(19,21,24)	119.93	D(19,21,24,26)	0.00
C_{20}–H_{23}	1.09	A(20,22,26)	119.96	D(21,24,26,22)	0.00
C_3–H_8	1.08	A(22,26,24)	119.74	D(19,20,22,26)	0.00
C_6–H_{11}	1.08	A(26,24,21)	120.87		

Figure 2. The Computational [1]H-NMR Spectrum Data for nitrone (**3a$_Z$**) at B3LYP/6-311+G*.





25-H	**14-H** **N-H**	**18-H** **C-H**	11-H	28-H	29-H	23-H	27-H	8-H	9-H	10-H
10.23	**10.13**	**9.55**	8.04	7.81	7.81	7.74	7.74	7.69	7.58	7.57

2-(1*H*-benzo[d]imidazol-2-yl)-3-phenyl-1,2-oxaziridine (4)

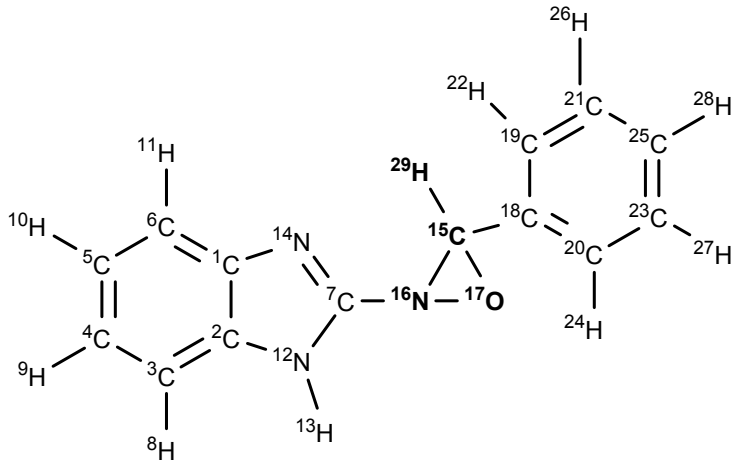
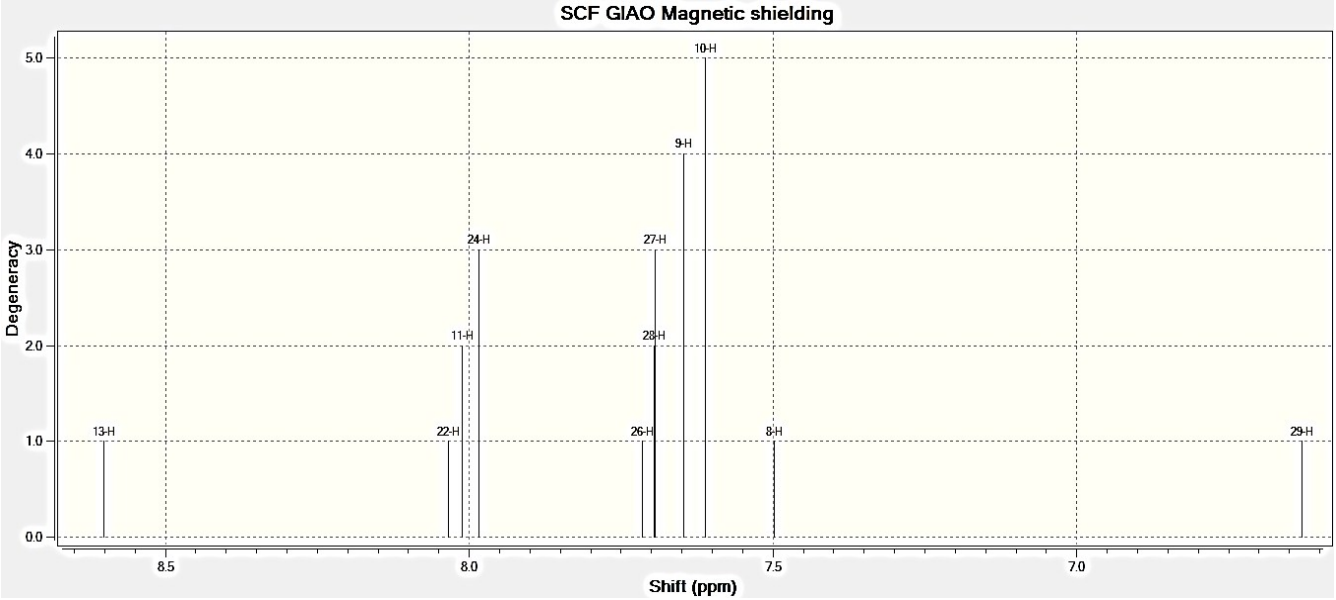


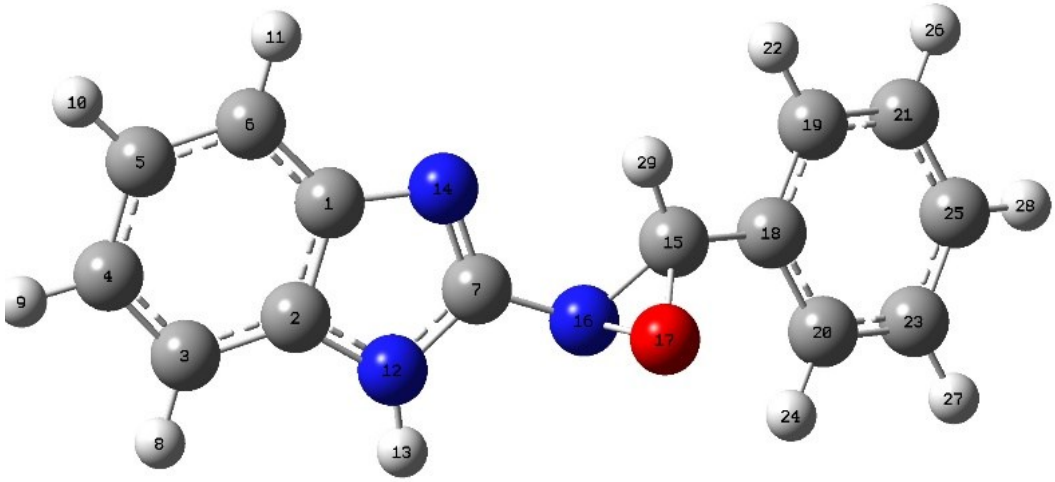
Table 3. Principal geometrical parameters including bond lengths (r, Å), bond angles and dihedral angles for the oxaziridine **(4)** at B3LYP/6-311+G*.

variable	B3lyp/6-311g(d)	variable	B3lyp/6-311g(d)	variable	B3lyp/6-311g(d)
Bond length (A°)		Bond angle (°)		dihedral angle (°)	
C_1–C_2	1.42	A(1,2,3)	122.41	D(1,2,3,4)	0.05
C_2–C_3	1.39	A(2,3,4)	116.73	D(2,3,4,5)	-0.02
C_3–C_4	1.39	A(3,4,5)	121.61	D(3,4,5,6)	0.05
C_4–C_5	1.41	A(4,5,6)	121.41	D(4,5,6,1)	-0.11
C_5–C_6	1.39	A(1,6,5)	118.06	D(5,6,1,14)	-179.96
C_1–N_{14}	1.38	A(6,1,14)	129.88	D(6,1,14,7)	-179.83
C_2–N_{12}	1.38	A(1,14,7)	104.74	D(6,1,2,12)	179.66
N_{14}–C_7	1.31	A(3,2,12)	133.15	D(1,2,12,7)	0.33
N_{12}–H_{13}	1.01	A(1,2,12)	104.43	D(1,14,7,16)	176.95
N_{12}–C_7	1.37	A(2,12,7)	106.86	D(1,14,7,12)	0.15
C_7–N_{16}	1.41	A(2,12,13)	128.27	D(13,12,7,14)	179.11
N_{16}–O_{17}	1.53	A(13,12,7)	124.87	D(13,12,7,16)	1.94
N_{16}–C_{15}	1.44	A(12,7,16)	117.86	D(14,7,16,17)	78.10
C_{15}–H_{29}	1.09	A(14,7,16)	128.46	D(12,7,16,17)	-105.21
C_{15}–C_{18}	1.49	A(7,16,17)	110.14	D(7,16,15,18)	-150.56
C_{18}–C_{19}	1.39	A(17,16,15)	56.65	D(17,16,15,18)	110.56
C_{18}–C_{20}	1.40	A(16,15,29)	115.43	D(16,15,18,19)	134.63
C_{20}–C_{23}	1.40	A(16,15,18)	118.25	D(17,15,18,20)	29.37
C_{19}–C_{21}	1.39	A(18,19,21)	120.31	D(15,18,20,23)	179.84
C_{21}–C_{25}	1.39	A(19,18,20)	119.64	D(29,15,18,19)	-8.86
C_{23}–C_{25}	1.39	A(15,18,20)	120.85	D(15,18,20,24)	-0.44
C_{19}–H_{22}	1.09	A(18,20,23)	120.01	D(18,20,23,25)	0.11

C_{20}–H_{24}	1.08	A(20,23,25)	120.21	D(27,23,25,21)	-179.69
C_3–H_8	1.08	A(23,25,21)	119.95	D(18,19,21,25)	-0.38
C_6–H_{11}	1.08	A(19,21,25)	119.87		

Figure 3. The Computational ^{1}H-NMR Spectrum Data for oxaziridine (**4**) at B3LYP/6-311+G*





13-H N-H	22-H	11-H	24-H	22-H	26-H	28-H	27-H	9-H	10-H	8-H	**29-H C-H**

8.60	8.03	8.01	7.98	7.90	7.71	7.69	7.69	7.64	7.61	7.64	**6.62**