Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

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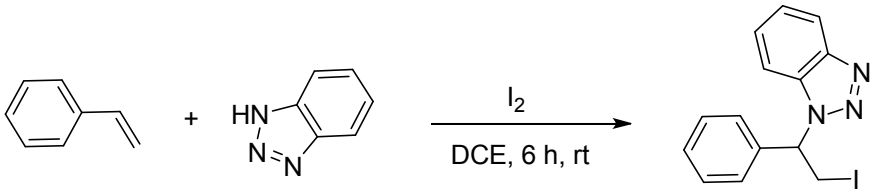
I. General Remarks:

Unless otherwise stated, all commercial reagents and solvents were used without additional purification. All the reactions were carried out under air atmosphere. ^{1}H NMR spectra were recorded at 25 ºC on a Bruker Ascend™ 400 spectrometer (Germany), ^{13}C NMR spectra were recorded at 25 ºC on a Bruker 100 MHz, and TMS as internal standard. Melting points were obtained with a micro melting point XT4A Beijing Keyi electrooptic apparatus and are uncorrected. HRMS data were obtained on a Waters LCT Premierxe™ (USA). All reactions were monitored by TLC with Taizhou GF254 silica gel coated plates. Flash column chromatography was carried out using 300-400 mesh silica gel at increased pressure.

II. General procedure for the preparation of 3 (**1a** as an example).



1a **2a** **3a**

Styrene **1a** (52.0 mg, 0.5 mmol), 1*H*-benzo[*d*][1,2,3]triazole **2a** (119.1 mg, 1.0 mmol), I_2 (126.9 mg, 0.5mmol) were added to DCE (2 mL). The mixture was stirred at 20 ºC for 6.0 h (monitored by TLC), quenched with water (10 mL), extracted with dichloromethane (5×3 mL), and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure, and the residue was purified by a shot flash silica gel column chromatography (EtOAc/petro ether = 1 : 6) to give compound **3a** as a white solid (155.3 mg, 89%).

III. Crystallographic data for 3a

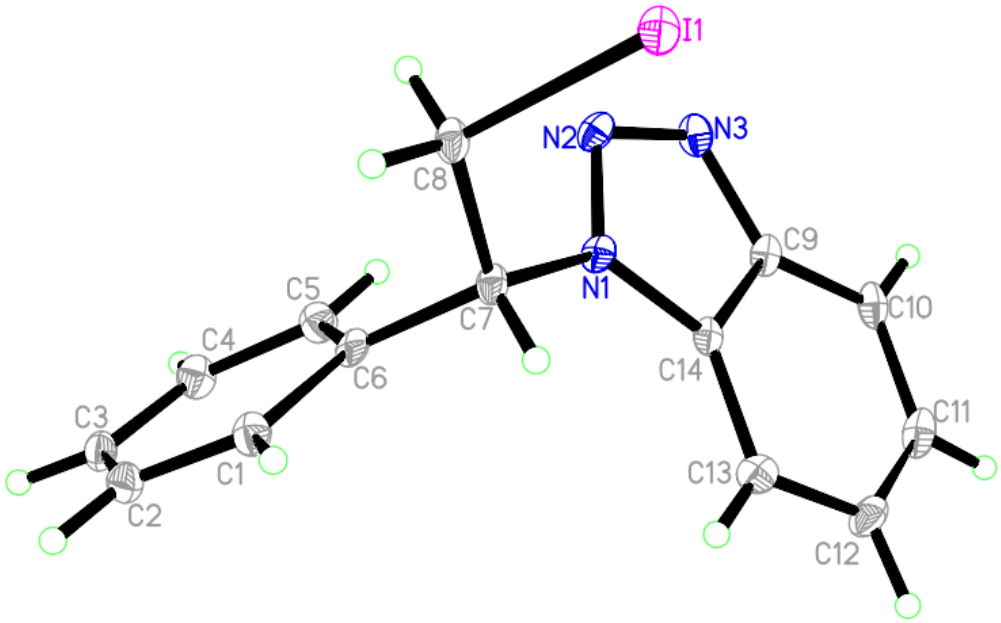


Table 1. Crystal data and structure refinement for **3a**.

Identification code	**3a**
Empirical formula	$C_{14}H_{12}IN_3$
Formula weight	349.17
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 8.7065(17) Å alpha = 90 deg.
	b = 13.352(3) Å beta = 99.24(3) deg.
	c = 11.519(2) Å gamma = 90 deg.
Volume	1321.7(5) Å 3
Z	4
Calculated density	1.755 Mg/m^3
Absorption coefficient	2.408 mm^{-1}
F(000)	680
Crystal size	0.20 x 0.20 x 0.20 mm
Theta range for data collection	2.35 to 25.01 deg.
Limiting indices	-10<=h<=8, -11<=k<=15, -8<=l<=13
Reflections collected / unique	4771 / 2315 [R(int) = 0.0262]
Completeness to theta = 25.01	99.4 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2315 / 0 / 163
Goodness-of-fit on F^2	1.014
Final R indices [I>2sigma(I)]	R1 = 0.0355, wR2 = 0.1164
R indices (all data)	R1 = 0.0382, wR2 = 0.1197
Largest diff. peak and hole	1.676 and -1.418 e. $Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **3a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	7122(1)	724(1)	7827(1)	23(1)
N(1)	9148(3)	2868(2)	8121(3)	18(1)
N(2)	9108(3)	2858(2)	6932(3)	21(1)
C(4)	14114(4)	2853(3)	8933(3)	26(1)
C(14)	8402(4)	3702(3)	8435(3)	17(1)
C(2)	13922(4)	1786(3)	10543(3)	25(1)
C(1)	12364(4)	1725(3)	10242(3)	23(1)
C(7)	9859(4)	2064(3)	8875(3)	19(1)

C(11)	6856(5)	5483(3)	8419(4)	27(1)
C(10)	7093(4)	5107(3)	7346(4)	22(1)
C(8)	9569(4)	1053(3)	8291(3)	21(1)
C(6)	11604(4)	2213(3)	9226(3)	18(1)
C(12)	7335(4)	4970(3)	9472(4)	28(1)
C(13)	8138(5)	4070(3)	9528(4)	22(1)
C(5)	12491(4)	2779(3)	8567(3)	25(1)
N(3)	8364(3)	3648(3)	6466(3)	22(1)
C(3)	14808(4)	2335(3)	9902(3)	24(1)
C(9)	7900(4)	4187(3)	7369(4)	18(1)

Table 3. Bond lengths [Å] and angles [deg] for **3a**.

I(1)-C(8)	2.157(4)
N(1)-N(2)	1.364(4)
N(1)-C(14)	1.367(5)
N(1)-C(7)	1.455(5)
N(2)-N(3)	1.308(4)
C(4)-C(3)	1.368(5)
C(4)-C(5)	1.412(5)
C(4)-H(4A)	0.9300
C(14)-C(9)	1.395(6)
C(14)-C(13)	1.404(5)
C(2)-C(1)	1.348(5)
C(2)-C(3)	1.364(5)
C(2)-H(2A)	0.9300
C(1)-C(6)	1.408(5)
C(1)-H(1A)	0.9300
C(7)-C(8)	1.512(5)
C(7)-C(6)	1.522(5)
C(7)-H(7A)	0.9800
C(11)-C(10)	1.381(6)
C(11)-C(12)	1.397(6)
C(11)-H(11A)	0.9300
C(10)-C(9)	1.413(5)
C(10)-H(10A)	0.9300
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(6)-C(5)	1.390(5)
C(12)-C(13)	1.386(6)
C(12)-H(12A)	0.9300
C(13)-H(13A)	0.9300

C(5)-H(5A)	0.9300
N(3)-C(9)	1.377(5)
C(3)-H(3A)	0.9300

N(2)-N(1)-C(14)	109.7(3)
N(2)-N(1)-C(7)	122.1(3)
C(14)-N(1)-C(7)	128.1(3)
N(3)-N(2)-N(1)	109.5(3)
C(3)-C(4)-C(5)	119.8(4)
C(3)-C(4)-H(4A)	120.1
C(5)-C(4)-H(4A)	120.1
N(1)-C(14)-C(9)	103.9(3)
N(1)-C(14)-C(13)	132.5(4)
C(9)-C(14)-C(13)	123.6(4)
C(1)-C(2)-C(3)	121.7(4)
C(1)-C(2)-H(2A)	119.1
C(3)-C(2)-H(2A)	119.1
C(2)-C(1)-C(6)	120.4(4)
C(2)-C(1)-H(1A)	119.8
C(6)-C(1)-H(1A)	119.8
N(1)-C(7)-C(8)	111.6(3)
N(1)-C(7)-C(6)	111.9(3)
C(8)-C(7)-C(6)	108.8(3)
N(1)-C(7)-H(7A)	108.1
C(8)-C(7)-H(7A)	108.1
C(6)-C(7)-H(7A)	108.1
C(10)-C(11)-C(12)	122.2(4)
C(10)-C(11)-H(11A)	118.9
C(12)-C(11)-H(11A)	118.9
C(11)-C(10)-C(9)	116.4(4)
C(11)-C(10)-H(10A)	121.8
C(9)-C(10)-H(10A)	121.8
C(7)-C(8)-I(1)	112.3(2)
C(7)-C(8)-H(8A)	109.1
I(1)-C(8)-H(8A)	109.1
C(7)-C(8)-H(8B)	109.1
I(1)-C(8)-H(8B)	109.1
H(8A)-C(8)-H(8B)	107.9
C(5)-C(6)-C(1)	118.5(3)
C(5)-C(6)-C(7)	123.0(3)
C(1)-C(6)-C(7)	118.5(3)
C(13)-C(12)-C(11)	122.9(4)
C(13)-C(12)-H(12A)	118.5
C(11)-C(12)-H(12A)	118.5

C(12)-C(13)-C(14)	114.6(4)
C(12)-C(13)-H(13A)	122.7
C(14)-C(13)-H(13A)	122.7
C(6)-C(5)-C(4)	119.5(4)
C(6)-C(5)-H(5A)	120.3
C(4)-C(5)-H(5A)	120.3
N(2)-N(3)-C(9)	107.3(3)
C(2)-C(3)-C(4)	120.0(3)
C(2)-C(3)-H(3A)	120.0
C(4)-C(3)-H(3A)	120.0
N(3)-C(9)-C(14)	109.5(3)
N(3)-C(9)-C(10)	130.1(4)
C(14)-C(9)-C(10)	120.3(4)

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **3a**. The anisotropic displacement factor exponent takes the form: [$h^2 a^{*2} U^{11}$ + ... + 2 h k a* b* U^{12}]

	U11	U22	U33	U23	U13	U12
I(1)	19(1)	15(1)	35(1)	0(1)	5(1)	-2(1)
N(1)	19(2)	9(2)	26(2)	-1(1)	5(1)	-1(1)
N(2)	23(2)	14(2)	27(2)	0(1)	10(1)	0(1)
C(4)	20(2)	26(2)	33(2)	1(2)	7(2)	-4(2)
C(14)	12(2)	9(2)	29(2)	-1(1)	4(1)	-3(1)
C(2)	25(2)	20(2)	26(2)	-1(2)	-1(2)	6(2)
C(1)	22(2)	16(2)	29(2)	0(2)	3(2)	0(2)
C(7)	17(2)	15(2)	25(2)	1(2)	3(1)	3(1)
C(11)	21(2)	11(2)	51(3)	0(2)	11(2)	-1(2)
C(10)	14(2)	17(2)	36(2)	8(2)	6(2)	-2(2)
C(8)	15(2)	15(2)	33(2)	1(2)	2(2)	0(2)
C(6)	23(2)	7(2)	25(2)	0(1)	4(2)	4(1)
C(12)	27(2)	21(2)	37(2)	-11(2)	11(2)	1(2)
C(13)	25(2)	15(2)	28(2)	-3(2)	5(2)	-5(2)
C(5)	25(2)	21(2)	27(2)	2(2)	3(2)	1(2)
N(3)	21(2)	20(2)	26(2)	7(1)	3(1)	2(1)
C(3)	17(2)	24(2)	30(2)	-5(2)	2(2)	3(2)
C(9)	15(2)	10(2)	29(2)	5(1)	8(2)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **3a**.

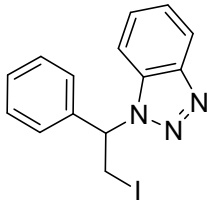
	x	y	z	U(eq)
H(4A)	14710	3253	8517	31
H(2A)	14406	1445	11206	29
H(1A)	11788	1359	10707	27
H(7A)	9388	2062	9593	23
H(11A)	6361	6098	8442	33
H(10A)	6740	5440	6645	27
H(8A)	10058	539	8819	26
H(8B)	10047	1038	7586	26
H(12A)	7105	5244	10166	33
H(13A)	8475	3738	10232	27
H(5A)	12019	3106	7890	29
H(3A)	15882	2357	10122	29

Table 6. Torsion angles [deg] for **3a**.

C(14)-N(1)-N(2)-N(3)	-0.2(4)
C(7)-N(1)-N(2)-N(3)	178.0(3)
N(2)-N(1)-C(14)-C(9)	0.5(4)
C(7)-N(1)-C(14)-C(9)	-177.6(3)
N(2)-N(1)-C(14)-C(13)	-178.9(4)
C(7)-N(1)-C(14)-C(13)	3.0(6)
C(3)-C(2)-C(1)-C(6)	1.6(6)
N(2)-N(1)-C(7)-C(8)	-37.2(4)
C(14)-N(1)-C(7)-C(8)	140.7(3)
N(2)-N(1)-C(7)-C(6)	85.1(4)
C(14)-N(1)-C(7)-C(6)	-97.0(4)
C(12)-C(11)-C(10)-C(9)	-2.3(6)
N(1)-C(7)-C(8)-I(1)	-58.8(3)
C(6)-C(7)-C(8)-I(1)	177.2(2)
C(2)-C(1)-C(6)-C(5)	-1.9(5)
C(2)-C(1)-C(6)-C(7)	175.8(3)
N(1)-C(7)-C(6)-C(5)	-24.1(5)
C(8)-C(7)-C(6)-C(5)	99.7(4)
N(1)-C(7)-C(6)-C(1)	158.3(3)
C(8)-C(7)-C(6)-C(1)	-77.9(4)
C(10)-C(11)-C(12)-C(13)	2.8(6)
C(11)-C(12)-C(13)-C(14)	-1.4(6)
N(1)-C(14)-C(13)-C(12)	179.0(4)
C(9)-C(14)-C(13)-C(12)	-0.3(5)

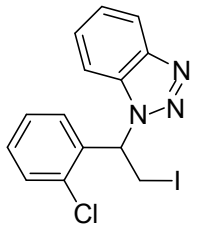
C(1)-C(6)-C(5)-C(4)	-0.3(5)
C(7)-C(6)-C(5)-C(4)	-177.9(3)
C(3)-C(4)-C(5)-C(6)	2.8(6)
N(1)-N(2)-N(3)-C(9)	-0.2(4)
C(1)-C(2)-C(3)-C(4)	0.9(6)
C(5)-C(4)-C(3)-C(2)	-3.1(6)
N(2)-N(3)-C(9)-C(14)	0.5(4)
N(2)-N(3)-C(9)-C(10)	178.5(4)
N(1)-C(14)-C(9)-N(3)	-0.6(4)
C(13)-C(14)-C(9)-N(3)	178.9(3)
N(1)-C(14)-C(9)-C(10)	-178.8(3)
C(13)-C(14)-C(9)-C(10)	0.7(5)
C(11)-C(10)-C(9)-N(3)	-177.2(4)
C(11)-C(10)-C(9)-C(14)	0.6(5)

IV. Analytical data of products obtained in this study



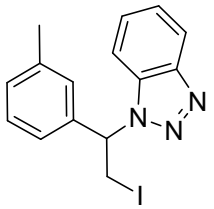
1-(2-iodo-1-phenylethyl)-1*H*-benzo[*d*][1,2,3]triazole 3a

White solid. Mp: 82-83 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.04 (q, J = 5.2, 1H), 4.47 (t, J = 10.4, 1H), 5.57 (q, J = 5.2, 1H), 7.34-7.45 (m, 8H), 8.09 (d, J = 8.0, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 5.1, 65.5, 109.3, 120.2, 124.2, 126.8, 127.6, 129.2, 133.1, 137.5, 146.0. HRMS (ESI-TOF) Calcd for $C_{14}H_{13}IN_3$, $[M+H]^+$ 350.0152; Found 350.0157.



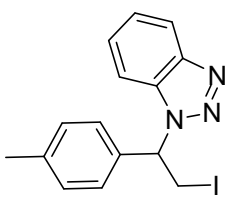
1-(1-(2-chlorophenyl)-2-iodoethyl)-1*H*-benzo[*d*][1,2,3]triazole 3b

White solid. Mp: 103-104 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.03 (q, J = 5.2, 1H), 4.37 (t, J = 10.4, 1H), 6.50 (q, J = 5.2, 1H), 7.19-7.50 (m, 7H), 8.09 (d, J = 8.0, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 3.5, 61.1, 109.4, 120.1, 124.4, 127.8, 127.9, 129.9, 130.3, 132.6, 133.3, 135.4, 145.8. HRMS (ESI-TOF) Calcd for $C_{14}H_{12}ICIN_3$, $[M+H]^+$ 383.9764; Found 383.9760.



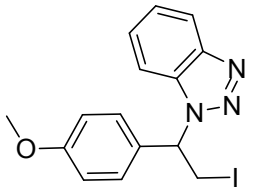
1-(2-iodo-1-(m-tolyl)ethyl)-1*H*-benzo[*d*][1,2,3]triazole 3c

White solid. Mp: 80-81 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.31 (s, 3H), 4.02 (q, J = 5.2, 1H), 4.47 (t, J = 10.4, 1H), 5.96 (q, J = 5.2, 1H), 7.13 (d, J = 6.4, 1H), 7.23 (d, J = 6.4, 3H), 7.36 (t, J = 4.2, 1H), 7.44-7.45 (m, 1H), 8.08 (d, J = 8.4, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 5.3, 21.4, 65.6, 109.4, 120.1, 123.9, 124.2, 127.3, 127.6, 129.0, 129.3, 129.9, 133.1, 137.4, 139.1, 146.0. HRMS (ESI-TOF) Calcd for $C_{15}H_{15}IN_3$, $[M+H]^+$ 364.0309; Found 364.0314.



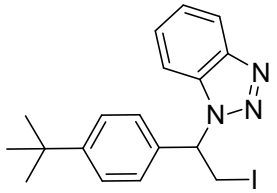
1-(2-iodo-1-(p-tolyl)ethyl)-1*H*-benzo[*d*][1,2,3]triazole 3d

White solid. Mp: 85-87 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.31 (s, 3H), 4.02 (q, J = 5.2, 1H), 4.46 (t, J = 10.4, 1H), 5.96 (q, J = 5.2, 1H), 7.15 (d, J = 8.0, 1H), 7.30 (d, J = 8.0, 2H), 7.35-7.44 (m, 3H), 8.08 (d, J = 8.0, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 5.3, 21.2, 65.3, 109.4, 120.1, 124.1, 126.7, 127.6, 129.8, 133.0, 134.5, 139.1, 146.1. HRMS (ESI-TOF) Calcd for $C_{15}H_{15}IN_3$, $[M+H]^+$ 364.0309; Found 364.0315.



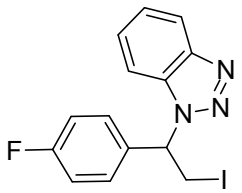
1-(2-iodo-1-(4-methoxyphenyl)ethyl)-1*H*-benzo[*d*][1,2,3]triazole 3e

White solid. Mp: 98-99 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.74 (s, 3H), 3.99 (q, J = 5.2, 1H), 4.43 (t, J = 10.4, 1H), 5.96 (q, J = 5.2, 1H), 6.84 (d, J = 8.8, 2H), 7.33 (t, J = 8.4, 3H), 7.42 (d, J = 4.4, 2H), 8.06 (d, J = 8.0, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 5.7, 55.3, 64.9, 109.5, 114.5, 120.1, 124.1, 127.6, 128.1, 129.5, 132.9, 146.0, 160.0. HRMS (ESI-TOF) Calcd for $C_{15}H_{15}ION_3$, $[M+H]^+$ 380.0260; Found 380.0265.



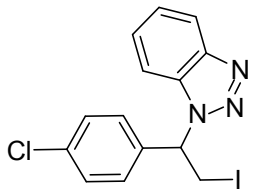
1-(1-(4-(tert-butyl)phenyl)-2-iodoethyl)-1*H*-benzo[*d*][1,2,3]triazole 3f

White solid. Mp: 85-86 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.28 (s, 9H), 4.00 (q, J = 4.8, 1H), 4.48 (t, J = 10.4, 1H), 5.96 (q, J = 5.2, 1H), 7.37-7.45 (m, 7H), 8.09 (d, J = 8.4, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 5.3, 31.2, 34.6, 65.3, 109.4, 120.2, 124.1, 126.1, 126.4, 127.5, 133.1, 134.5, 146.0, 152.3. HRMS (ESI-TOF) Calcd for $C_{18}H_{21}IN_3$, $[M+H]^+$ 406.0780; Found 406.0774.



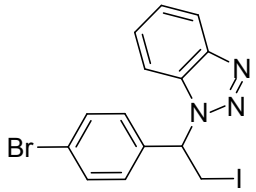
1-(1-(4-fluorophenyl)-2-iodoethyl)-1*H*-benzo[*d*][1,2,3]triazole 3g

White solid. Mp: 91-92 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.01 (q, J = 5.2, 1H), 4.34 (t, J = 10.4, 1H), 5.96 (q, J = 5.2, 1H), 7.05 (d, J = 8.8, 2H), 7.40-7.45 (m, 5H), 8.09 (d, J = 8.4, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 4.9, 64.7, 109.1, 116.1, 116.3, 120.3, 124.3, 127.8, 128.7, 128.8, 132.9, 133.3, 133.4, 146.0, 161.7, 164.2. HRMS (ESI-TOF) Calcd for $C_{14}H_{13}IFN_3$, $[M+H]^+$ 368.0062; Found 368.0067.



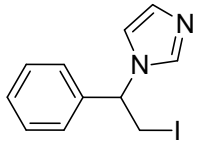
1-(1-(4-chlorophenyl)-2-iodoethyl)-1*H*-benzo[*d*][1,2,3]triazole 3h

White solid. Mp: 118-120 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.01 (q, J = 5.2, 1H), 4.42 (t, J = 10.4, 1H), 5.94 (q, J = 5.2, 1H), 7.33-7.49 (m, 7H), 8.10 (d, J = 8.0, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 4.6, 64.8, 109.1, 120.3, 124.3, 127.8, 129.4, 132.9, 135.2, 135.9, 146.0. HRMS (ESI-TOF) Calcd for $C_{14}H_{12}ICIN_3$, $[M+H]^+$ 383.9764; Found 383.9769.



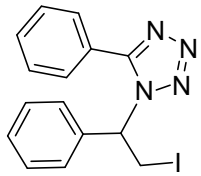
1-(1-(4-bromophenyl)-2-iodoethyl)-1*H*-benzo[*d*][1,2,3]triazole 3i

Yellow solid. Mp: 125-126 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.40 (t, J = 5.2, 1H), 4.39 (d, J = 10.4, 1H), 5.96 (q, J = 5.2, 1H), 7.33-7.50 (m, 7H), 8.12 (d, J = 8.4, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 4.7, 64.8, 109.2, 120.3, 123.4, 124.4, 127.9, 128.6 132.1, 132.9, 136.5, 145.9. HRMS (ESI-TOF) Calcd for $C_{14}H_{12}IBrN_3$, $[M+H]^+$ 427.9254; Found 427.9259.



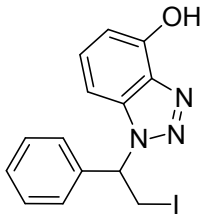
1-(2-iodo-1-phenylethyl)-1H-imidazole 3j

White solid. Mp: 70-71 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.78 (q, J = 5.2, 1H), 4.17 (t, J = 10.4, 1H), 5.49 (q, J = 5.2, 1H), 7.33-7.46 (m, 6H), 7.64 (d, J = 1.6, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 4.7, 67.8, 105.6, 126.8, 128.7, 129.5, 138.8, 140.0. HRMS (ESI-TOF) Calcd for $C_{11}H_{12}IN_2$, $[M+H]^+$ 299.0044; Found 299.0048.



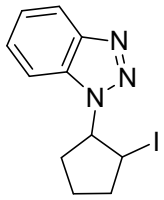
1-(2-iodo-1-phenylethyl)-5-phenyl-1*H*-tetrazole 3k

Yellow solid. Mp: 87-88 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.03 (q, J = 5.2, 1H), 4.47 (t, J = 10.4, 1H), 5.98 (q, J = 5.2, 1H), 7.34-7.45 (m, 8H), 8.09 (d, J = 8.4, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 5.1, 65.5, 109.3, 120.2, 124.2, 126.8, 127.6, 129.2, 133.1, 137.5, 146.1. HRMS (ESI-TOF) Calcd for $C_{15}H_{14}IN_4$, $[M+H]^+$ 377.0264; Found 377.0268.



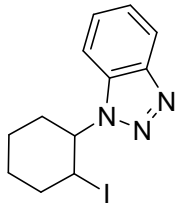
1-(2-iodo-1-phenylethyl)-1*H*-benzo[*d*][1,2,3]triazol-4-ol 3l

Yellow solid. Mp: 97-98 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.03 (q, J = 5.2, 1H), 4.47 (t, J = 10.4, 1H), 5.98 (q, J = 5.2, 1H), 7.35-7.44 (m, 6H), 8.09 (d, J = 8.4, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 4.9, 65.6, 109.3, 120.2, 126.1, 126.8, 127.6, 128.2, 133.1, 137.5, 146.1. HRMS (ESI-TOF) Calcd for $C_{14}H_{13}ION_3$, $[M+H]^+$ 366.0104; Found 366.0112.



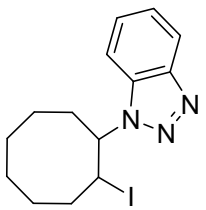
1-(2-iodocyclopentyl)-1*H*-benzo[*d*][1,2,3]triazole 3m

Yellow liquid. ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.09-2.31 (m, 3H), 2.46-2.59 (m, 3H), 4.63 (t, J = 6.8, 1H), 5.34 (t, J = 8.0, 1H), 7.39 (d, J = 7.6, 1H), 7.52 (d, J = 6.8, 1H), 7.59 (d, J = 8.0, 1H), 8.07 (d, J = 8.0, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 23.8, 26.9, 30.5, 38.0, 69.6, 105.5, 120.1, 124.1, 127.4, 133.2, 145.7. HRMS (ESI-TOF) Calcd for $C_{11}H_{13}IN_3$, $[M+H]^+$ 314.0154; Found 314.0150.



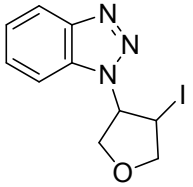
1-(2-iodocyclohexyl)-1*H*-benzo[*d*][1,2,3]triazole 3n

Yellow liquid. ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.26-1.77 (m, 4H), 2.09-2.31 (m, 4H), 2.78 (d, J = 13.6, 1H), 4.77 (q, J = 4.0, 1H), 4.87 (t, J = 4.4, 1H), 7.40 (t, J = 7.2, 1H), 7.52-7.58 (m, 2H), 8.09 (d, J = 8.4, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 25.2, 27.9, 31.5, 34.3, 40.2, 65.4, 109.4, 120.2, 123.9, 127.2, 133.2, 145.7. HRMS (ESI-TOF) Calcd for $C_{12}H_{15}IN_3$, $[M+H]^+$ 328.0311; Found 328.0317.



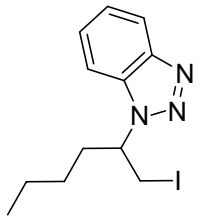
1-(2-iodocyclooctyl)-1*H*-benzo[*d*][1,2,3]triazole 3o

Yellow solid. Mp: 106-108 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.56-1.91 (m, 8H), 2.04-2.49 (m, 4H), 5.24 (t, J = 8.4, 1H), 5.33 (q, J = 3.2, 1H), 7.36 (q, J = 4.4, 1H), 7.38-7.53 (m, 2H), 8.07 (d, J = 8.0, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 25.4, 25.6, 27.1, 27.8, 33.7, 33.9, 38.1, 67.8, 109.4, 120.1, 123.9, 127.2, 132.4, 145.8. HRMS (ESI-TOF) Calcd for $C_{14}H_{19}IN_3$, $[M+H]^+$ 356.0621; Found 356.0626.



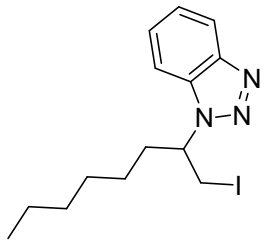
1-(4-iodotetrahydrofuran-3-yl)-1*H*-benzo[*d*][1,2,3]triazole 3p

Yellow liquid. ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.26 (t, J = 8.4, 1H), 4.51 (d, J = 6.0, 2H), 4.65 (d, J = 6.0, 2H), 5.68 (t, J = 4.4, 1H), 7.44 (d, J = 8.0, 1H), 7.56 (q, J = 7.2, 1H), 7.66 (d, J = 8.4, 1H), 8.11 (d, J = 8.4, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 20.1, 69.1, 70.6, 76.7, 109.3, 120.5, 124.5, 128.0, 132.2, 146.3. HRMS (ESI-TOF) Calcd for $C_{10}H_{11}ION_3$, $[M+H]^+$ 315.9945; Found 313.9939.



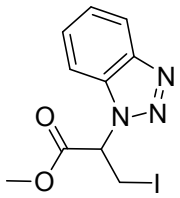
1-(1-iodohexan-2-yl)-1*H*-benzo[*d*][1,2,3]triazole 3q

Yellow liquid. ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.04-1.31 (m, 7H), 2.22-2.37 (m, 2H), 3.74-3.88 (m, 2H), 4.91 (t, J = 4.8, 1H), 7.38-7.41 (m, 1H), 7.51 (d, J = 6.0, 2H), 8.10 (d, J = 8.4, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 20.1, 69.1, 70.6, 76.7, 109.3, 120.5, 124.5, 128.0, 132.2, 146.3. HRMS (ESI-TOF) Calcd for $C_{12}H_{17}IN_3$, $[M+H]^+$ 330.0465; Found 330.0461.



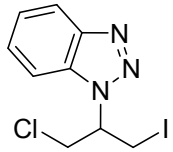
1-(1-iodooctan-2-yl)-1*H*-benzo[*d*][1,2,3]triazole 3r

Yellow liquid. ^{1}H NMR (400 MHz; $CDCl_3$): δ = 0.86 (t, J = 6.8, 3H), 1.24-1.40 (m, 7H), 1.63-1.83 (m, 4H), 4.61 (dd, J_1 = 1.6, J_2 = 8.8, 2H), 5.03 (q, J = 6.8, 1H), 7.42 (t, J = 7.2, 1H), 7.55 (q, J = 6.8, 2H), 8.06 (d, J = 8.4, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 13.9, 22.5, 28.2, 29.7, 30.8, 31.5, 37.1, 55.9, 109.3, 120.2, 124.1, 127.6, 133.2, 145.7. HRMS (ESI-TOF) Calcd for $C_{14}H_{21}IN_3$, $[M+H]^+$ 358.0780; Found 358.0774.



methyl 2-(1*H*-benzo[*d*][1,2,3]triazol-1-yl)-3-iodopropanoate 3s

Yellow liquid. ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.68 (s, 3H), 4.99-5.11 (m, 2H), 5.21 (q, J = 8.8, 1H), 7.38 (t, J = 7.2, 1H), 7.53 (d, J = 0.8, 1H), 7.64 (q, J = 8.4, 1H), 8.05 (d, J = 8.4, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 13.9, 22.5, 28.2, 29.7, 30.8, 31.5, 37.1, 55.9, 109.3, 120.2, 124.1, 127.6, 133.2, 145.7. HRMS (ESI-TOF) Calcd for $C_{10}H_{11}IO_2N_3$, $[M+H]^+$ 331.9896; Found 331.9890.

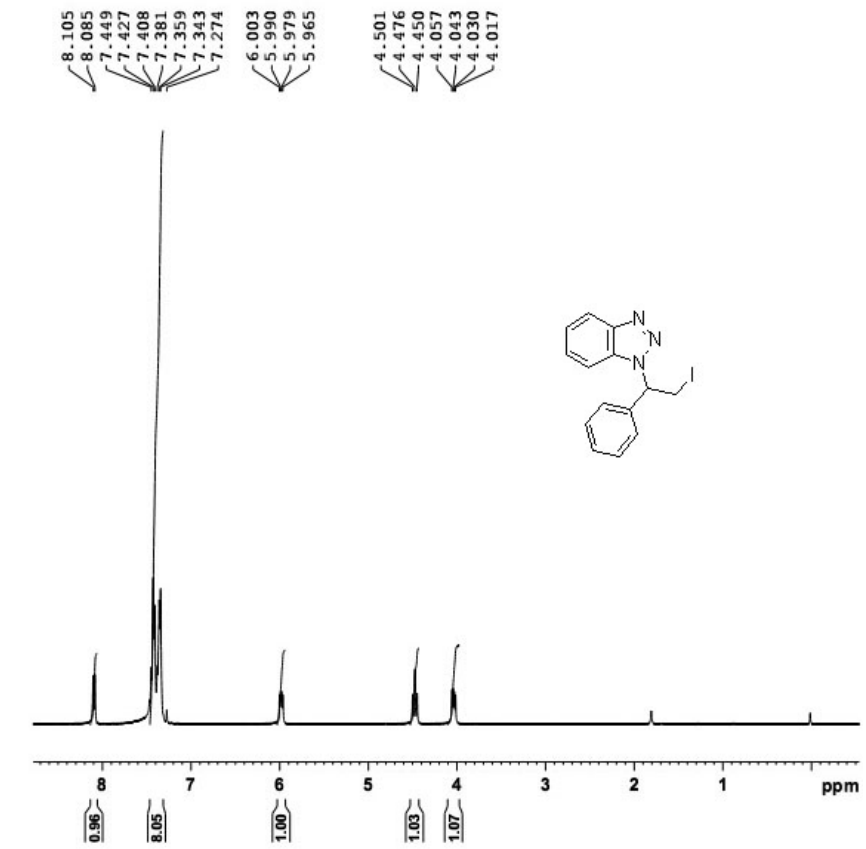


1-(1-chloro-3-iodopropan-2-yl)-1*H*-benzo[*d*][1,2,3]triazole 3t

Yellow liquid. ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.94 (t, J = 8.0, 2H), 4.86 (q, J = 4.8, 1H), 5.08 (t, J = 6.8, 1H), 5.19 (q, J = 8.4, 1H), 7..42 (t, J = 8.0, 1H), 7.56 (t, J = 8.4, 1H), 7.64 (d, J = 8.4, 1H), 8.11 (d, J = 8.4, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 25.2, 47.7, 52.3, 62.5, 109.3, 120.2, 124.2, 127.9, 133.3, 145.7. HRMS (ESI-TOF) Calcd for $C_9H_{10}ICIN_3$, $[M+H]^+$ 321.9606; Found 321.9601.

V. ^{1}H NMR and ^{13}C NMR spectra copies of compounds 3

Compound 3a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7.343
7.274
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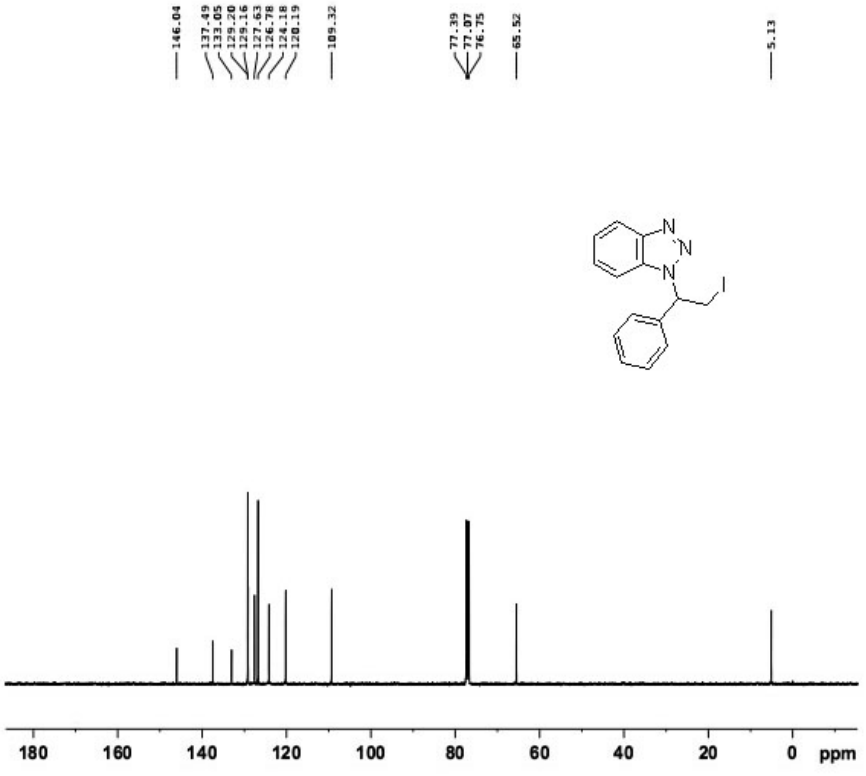
5.965
4.501
4.476
4.450
4.057
4.043
4.030
4.017
N
N
N
I
8
7
6
5
4
3
2
1
ppm
0.96
8.05
1.00
1.03
1.07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127.63
126.78
124.18
120.19
109.32
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77.07
76.75
65.52
5.13
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N
N
I
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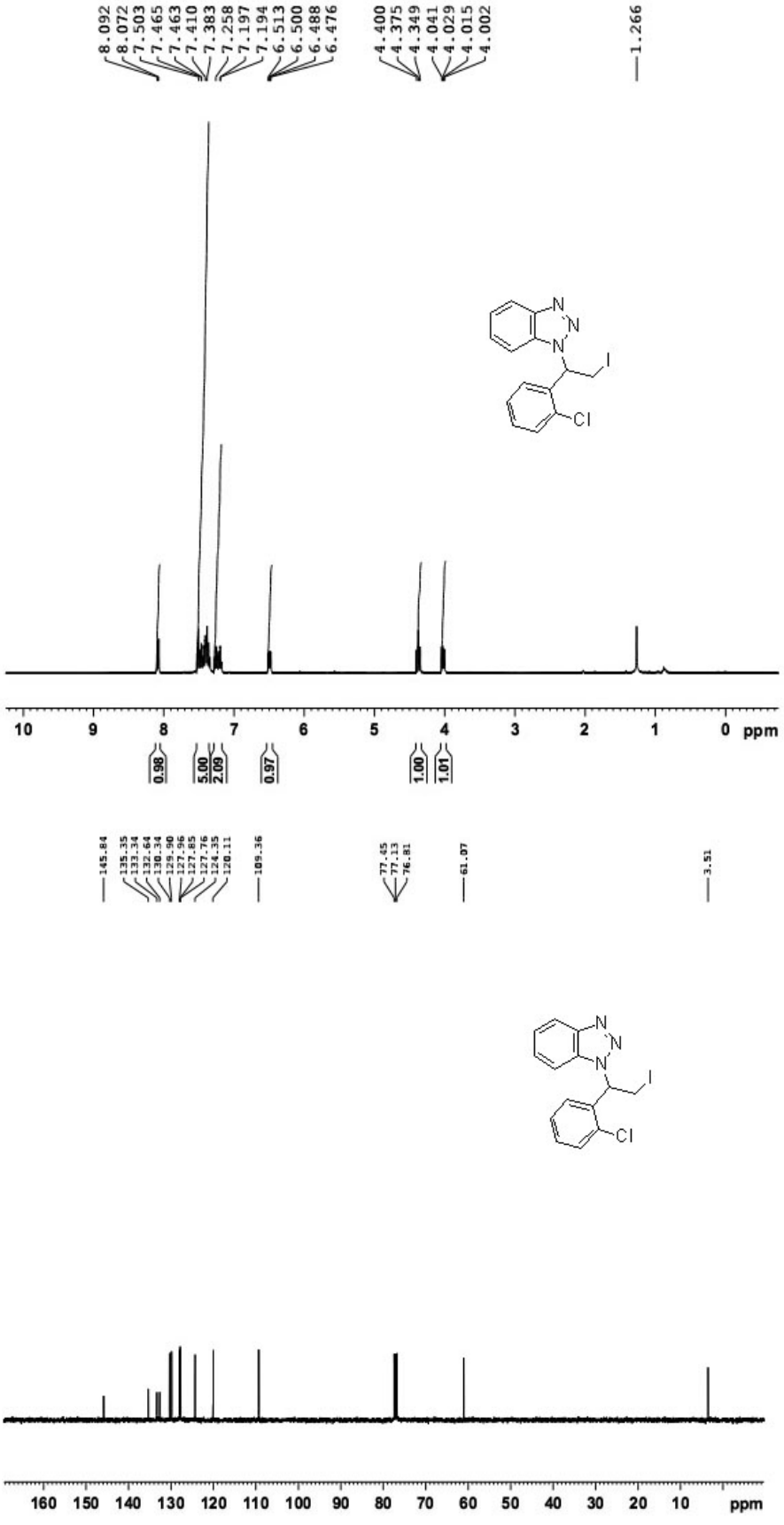
160
140
120
100
80
60
40
20
0
ppm

Compound 3b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7.465
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7.258
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6.476
4.400
4.375
4.349
4.041
4.029
4.015
4.002
1.266
N
N
N
I
Cl
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5.00
2.09
0.97
1.00
1.01
145.84
135.35
133.34
132.64
130.34
129.90
127.96
127.85
127.76
124.35
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61.07
3.51
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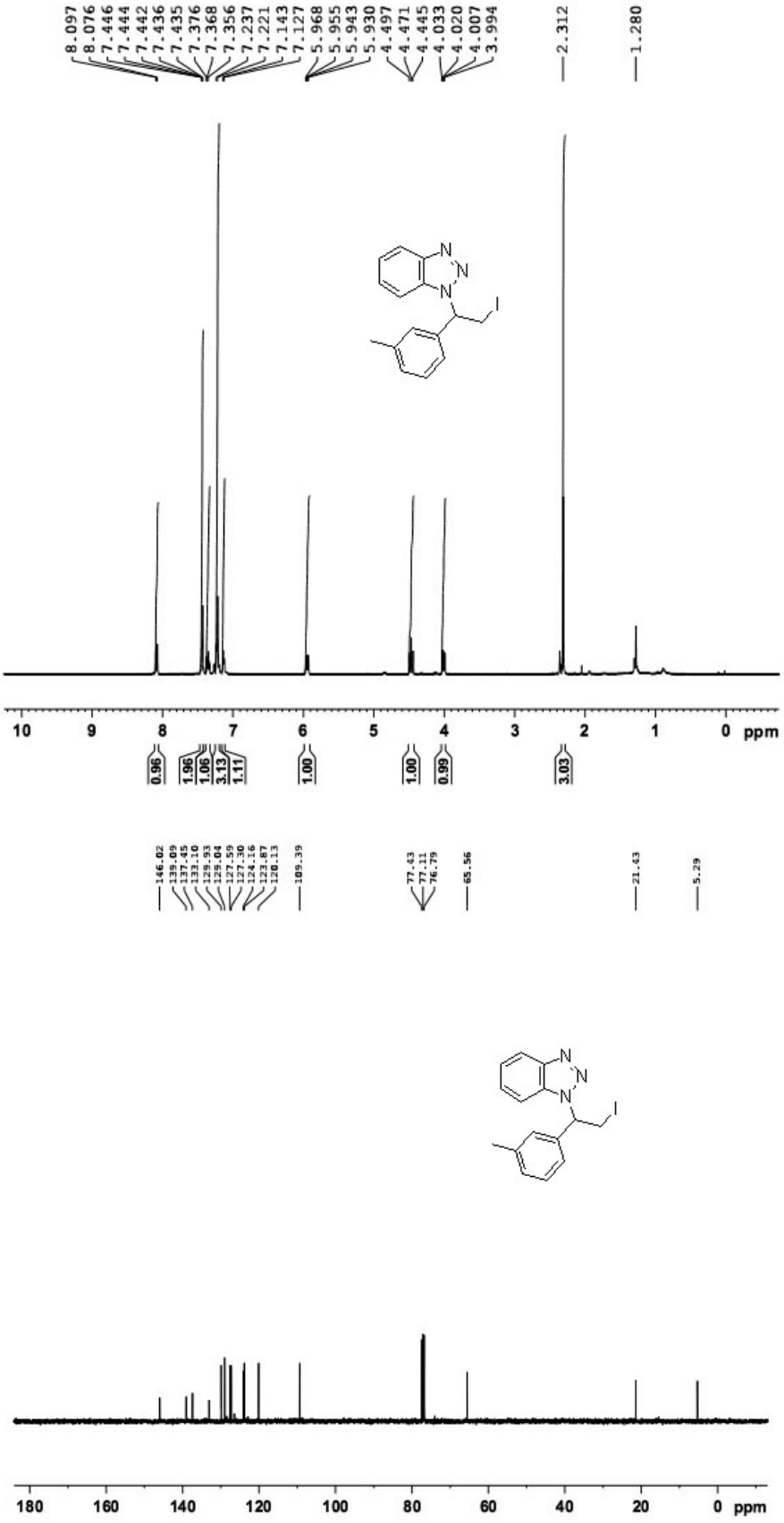
Compound 3c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7.442
7.436
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7.376
7.368
7.356
7.237
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7.143
7.127
5.968
5.955
5.943
5.930
4.497
4.471
4.445
4.033
4.020
4.007
3.994
2.312
1.280
N
N
N
I
10 9 8 7 6 5 4 3 2 1 0 ppm
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1.96
1.06
3.13
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1.00
1.00
0.99
3.03
146.02
139.09
137.45
133.10
129.93
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127.59
127.30
124.16
123.87
120.13
109.39
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5.29
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N
I
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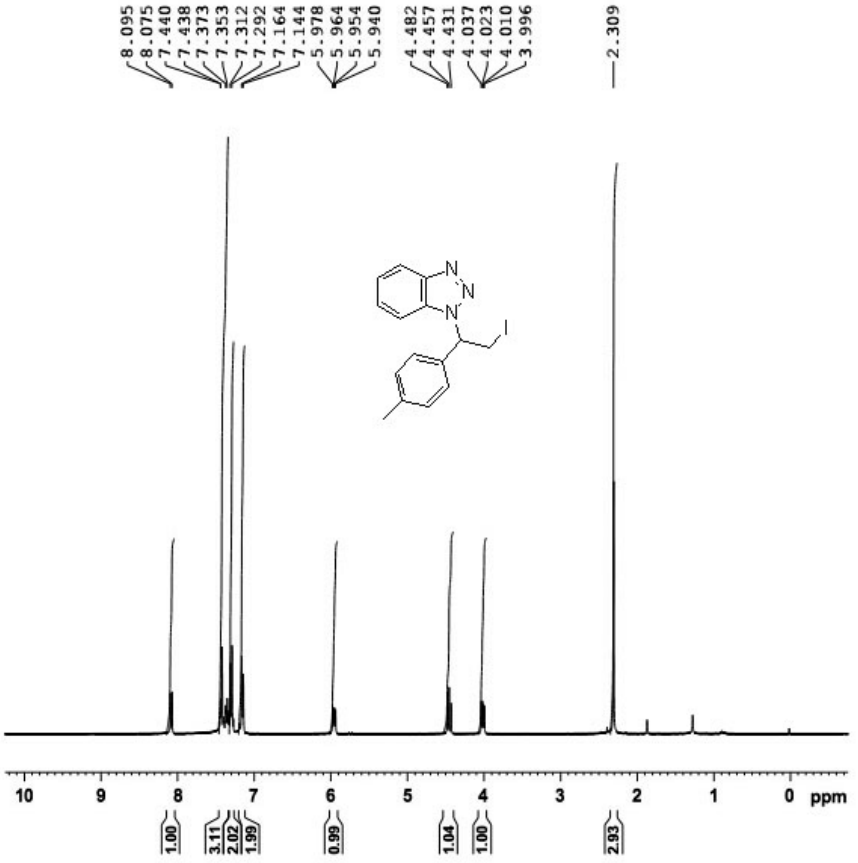
Compound 3d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4.037
4.023
4.010
3.996
2.309
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3.11
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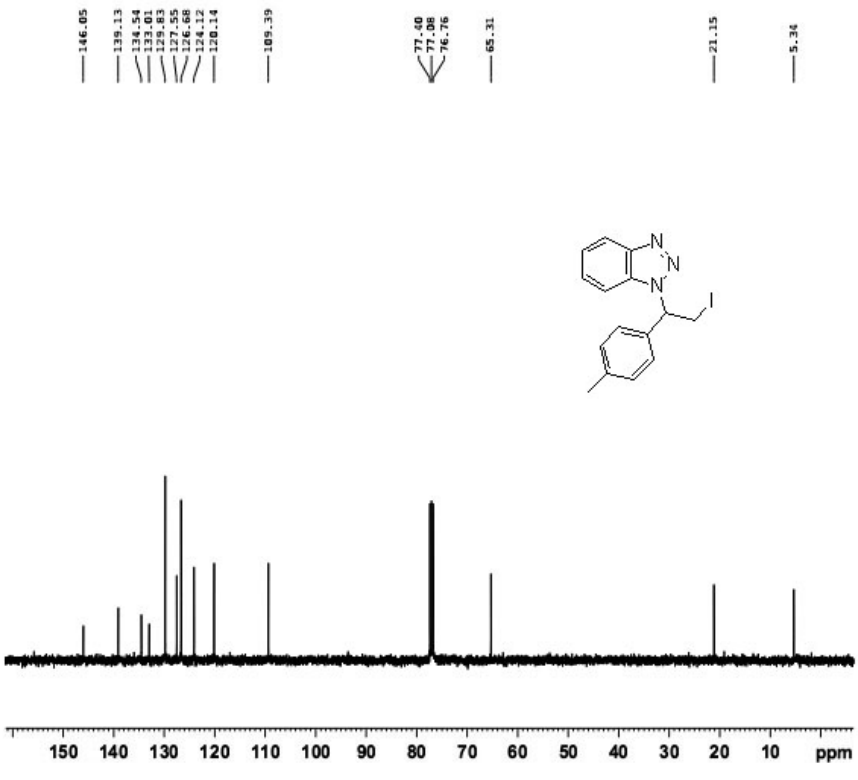
1.99
0.99
1.04
1.00
2.93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139.13
134.54
133.01
129.83
127.55
126.68
124.12
120.14
109.39
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77.08
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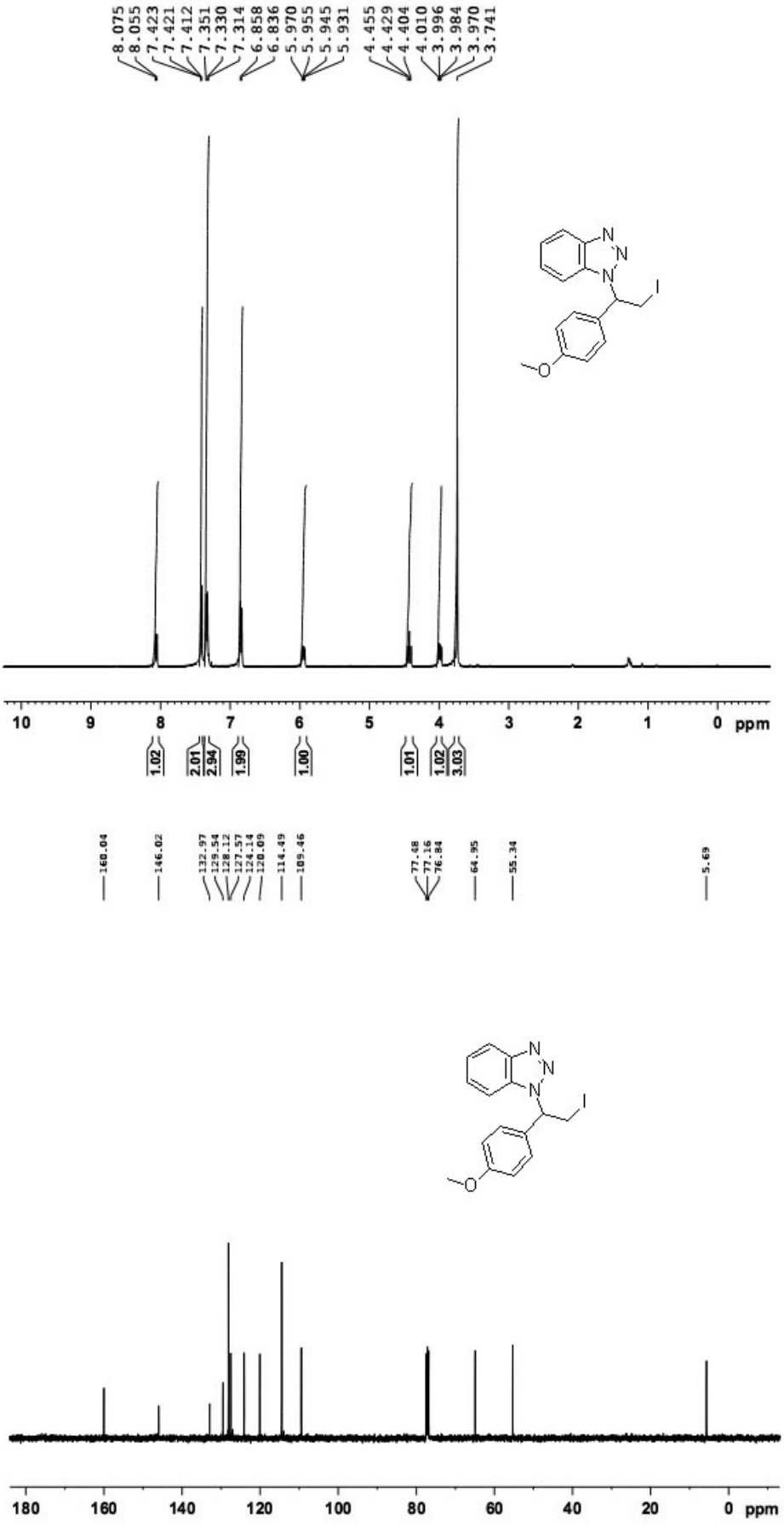
5.34
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Compound 3e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3.970
3.741
N
N
N
I
O
10
9
8
7
6
5
4
3
2
1
0 ppm
1.02
2.01
2.94
1.99
1.00
1.01
1.02
3.03
160.04
146.02
132.97
129.54
128.12
127.57
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77.16
76.84
64.95
55.34
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N
N
I
O
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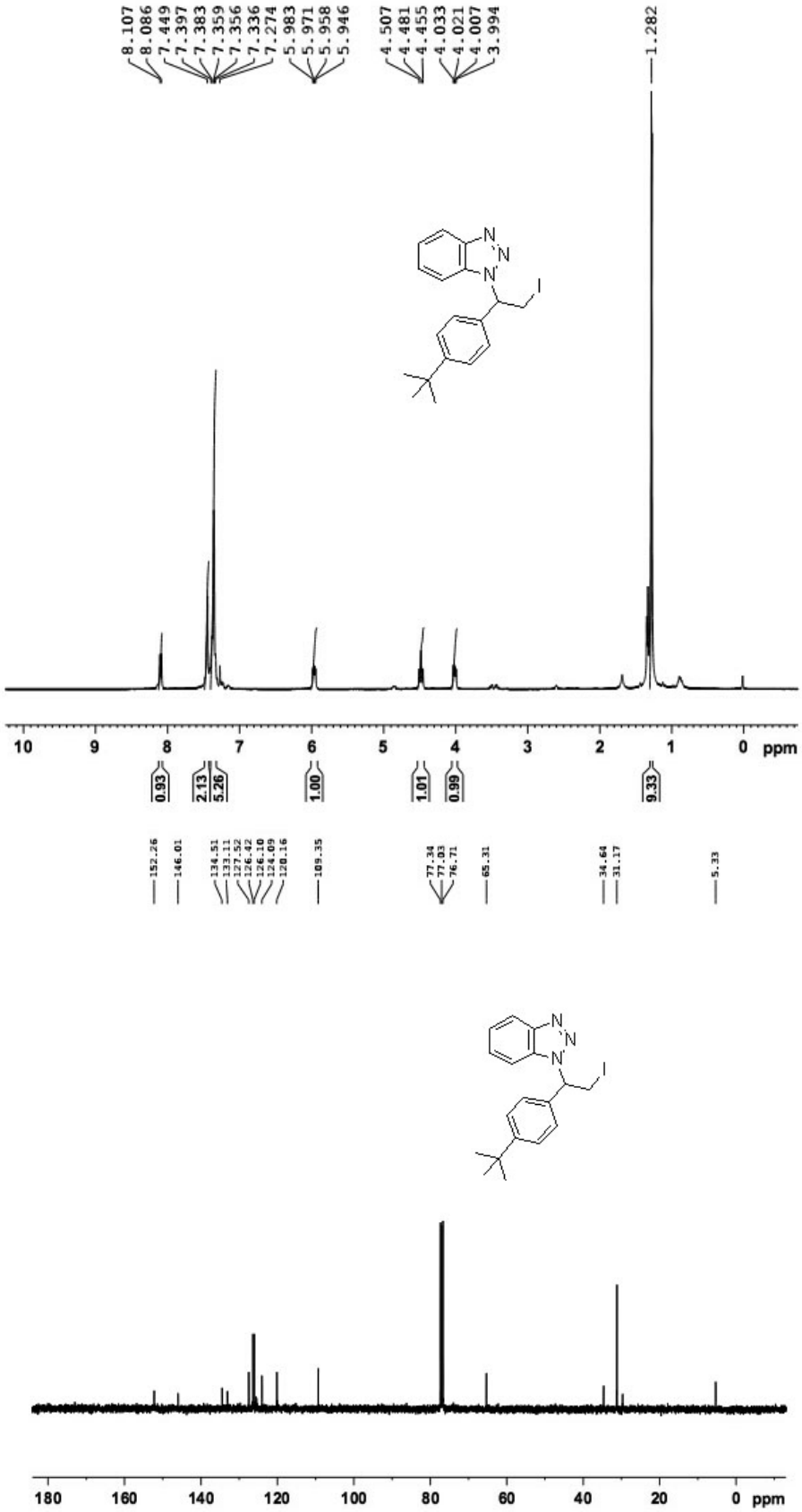
160
140
120
100
80
60
40
20
0 ppm

Compound 3f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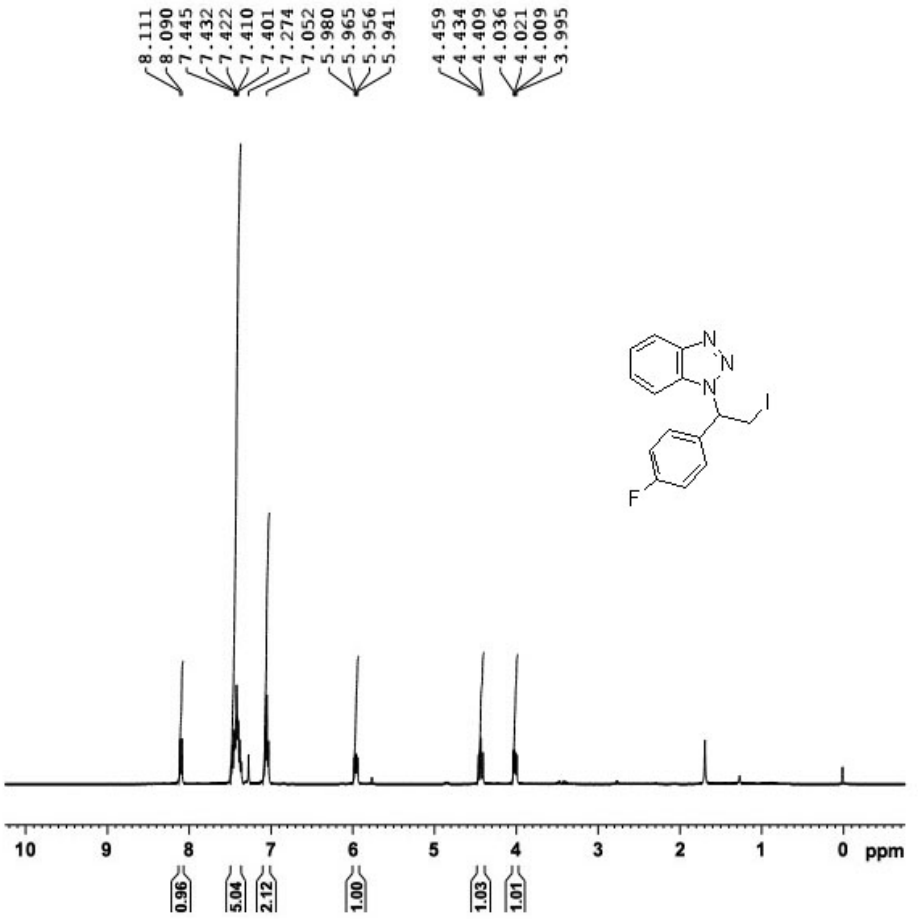
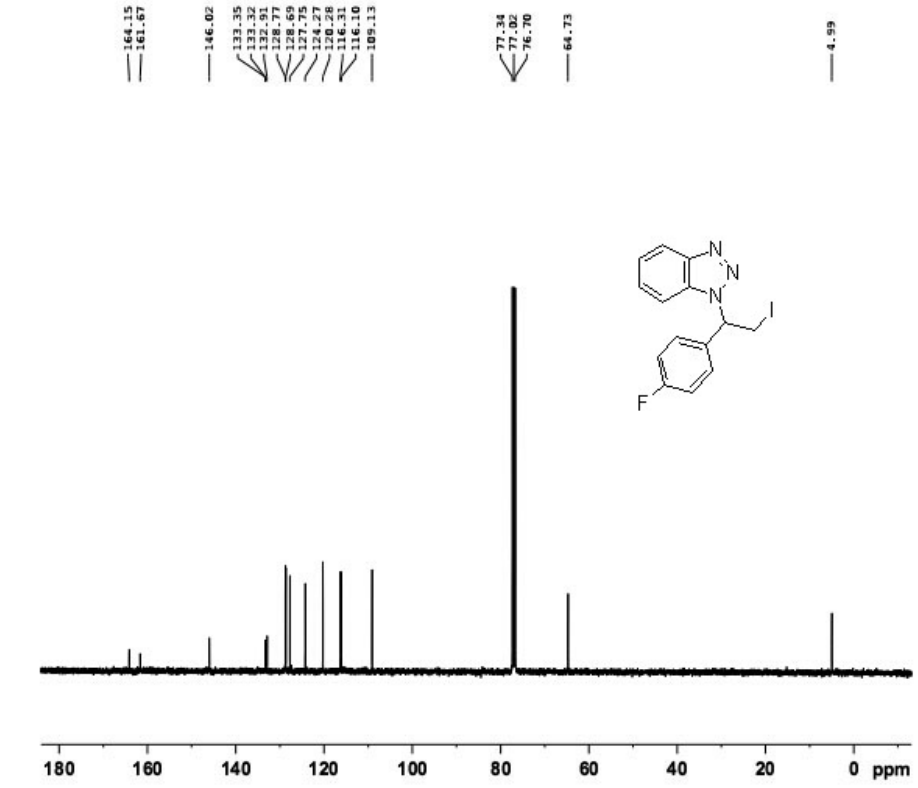
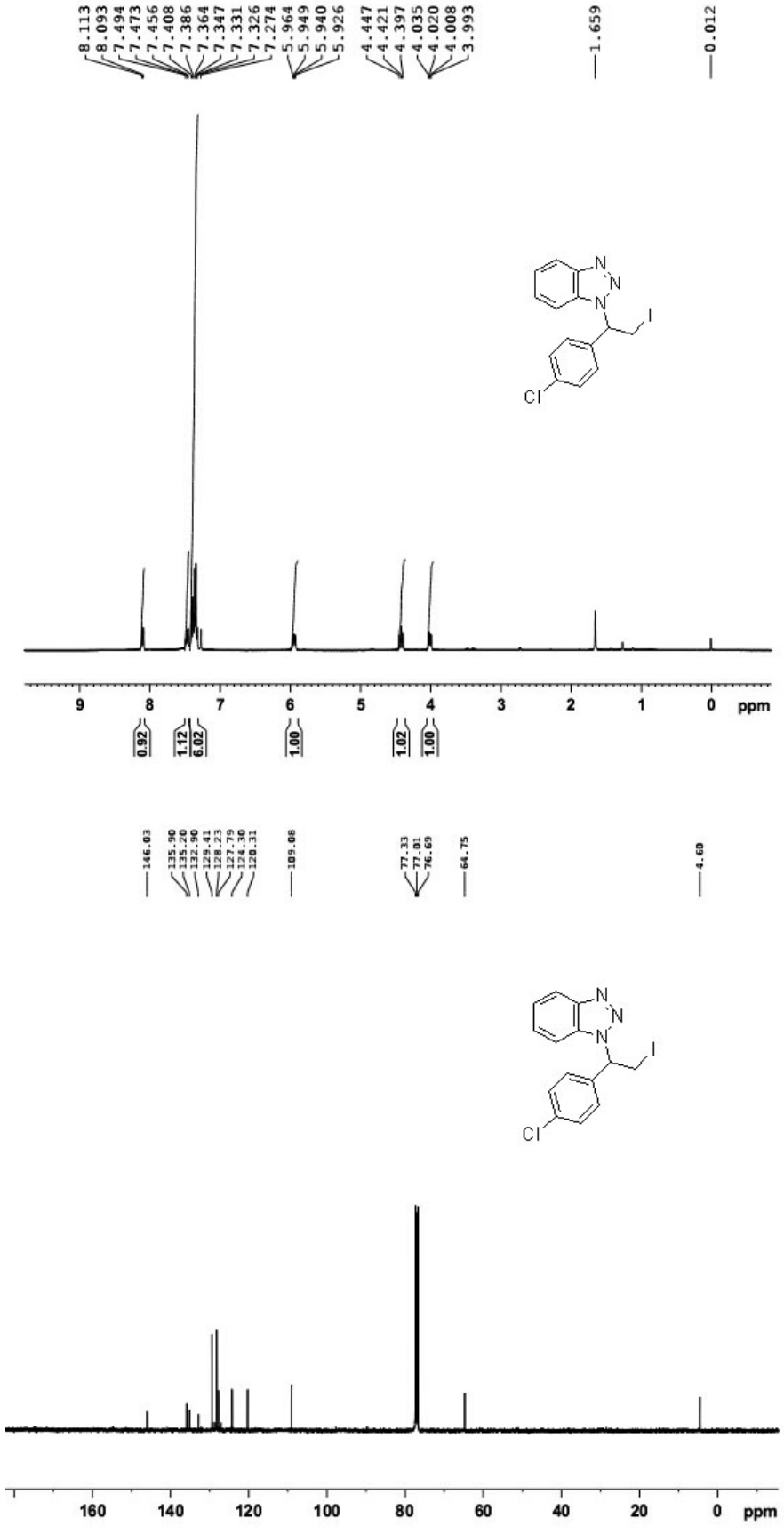
7.397
7.383
7.359
7.356
7.336
7.274
5.983
5.971
5.958
5.946
4.507
4.481
4.455
4.033
4.021
4.007
3.994
1.282
N
N
N
I
10
9
8
7
6
5
4
3
2
1
0
ppm
0.93
2.13
5.26
1.00
1.01
0.99
9.33
152.26
146.01
134.51
133.11
127.52
126.42
125.10
124.09
120.16
109.35
77.34
77.03
76.71
65.31
34.64
31.17
5.33
N
N
N
I
180
160
140
120
100
80
60
40
20
0
ppm

Compound 3g

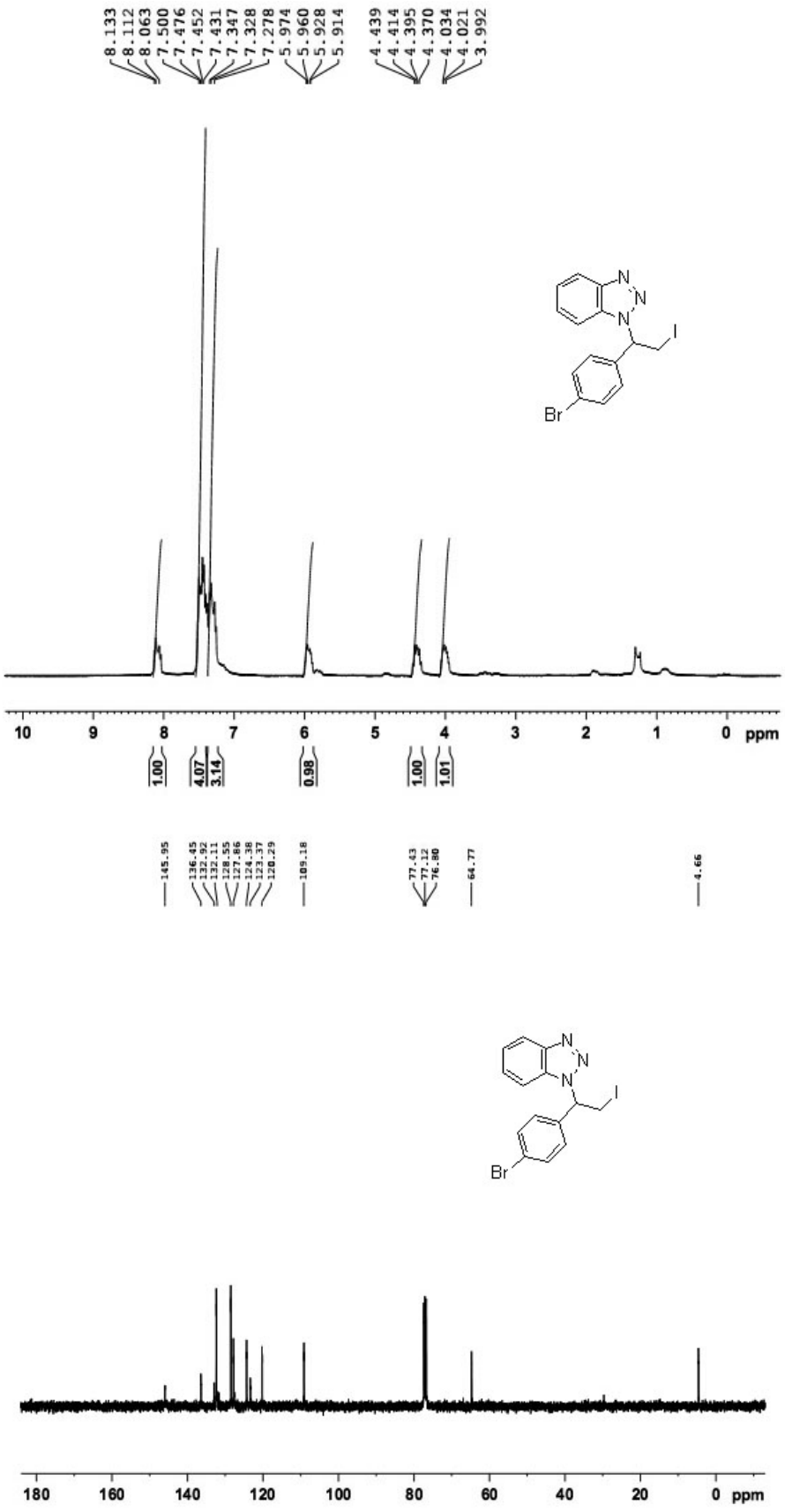

8.111
8.090
7.445
7.432
7.422
7.410
7.401
7.274
7.052
5.980
5.965
5.956
5.941
4.459
4.434
4.409
4.036
4.021
4.009
3.995
N
N
N
I
F
10
9
8
7
6
5
4
3
2
1
0 ppm
0.96
5.04
2.12
1.00
1.03
1.01


164.15
161.67
146.02
133.35
133.32
132.91
128.77
128.69
127.75
124.27
120.28
116.31
116.10
109.13
77.34
77.02
76.70
64.73
4.99
N
N
N
I
F
180
160
140
120
100
80
60
40
20
0 ppm

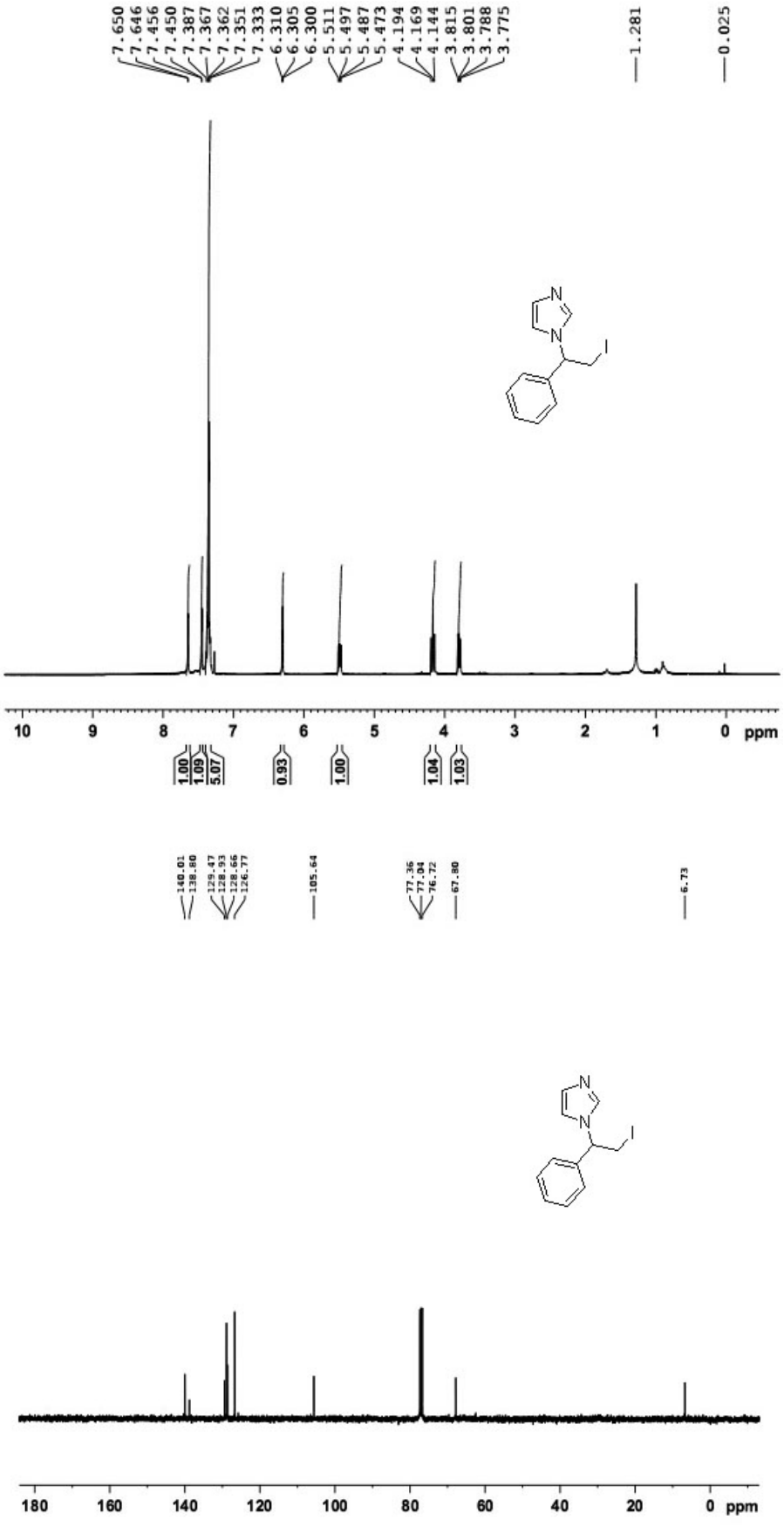
Compound 3h


8.113
8.093
7.494
7.473
7.456
7.408
7.386
7.364
7.347
7.331
7.326
7.274
5.964
5.949
5.940
5.926
4.447
4.421
4.397
4.035
4.020
4.008
3.993
1.659
0.012
N
N
N
I
Cl
9
8
7
6
5
4
3
2
1
0
ppm
0.92
1.12
6.02
1.00
1.02
1.00
146.03
135.90
135.20
132.90
129.41
128.23
127.79
124.30
120.31
109.08
77.33
77.01
76.69
64.75
4.69
160
140
120
100
80
60
40
20
0
ppm

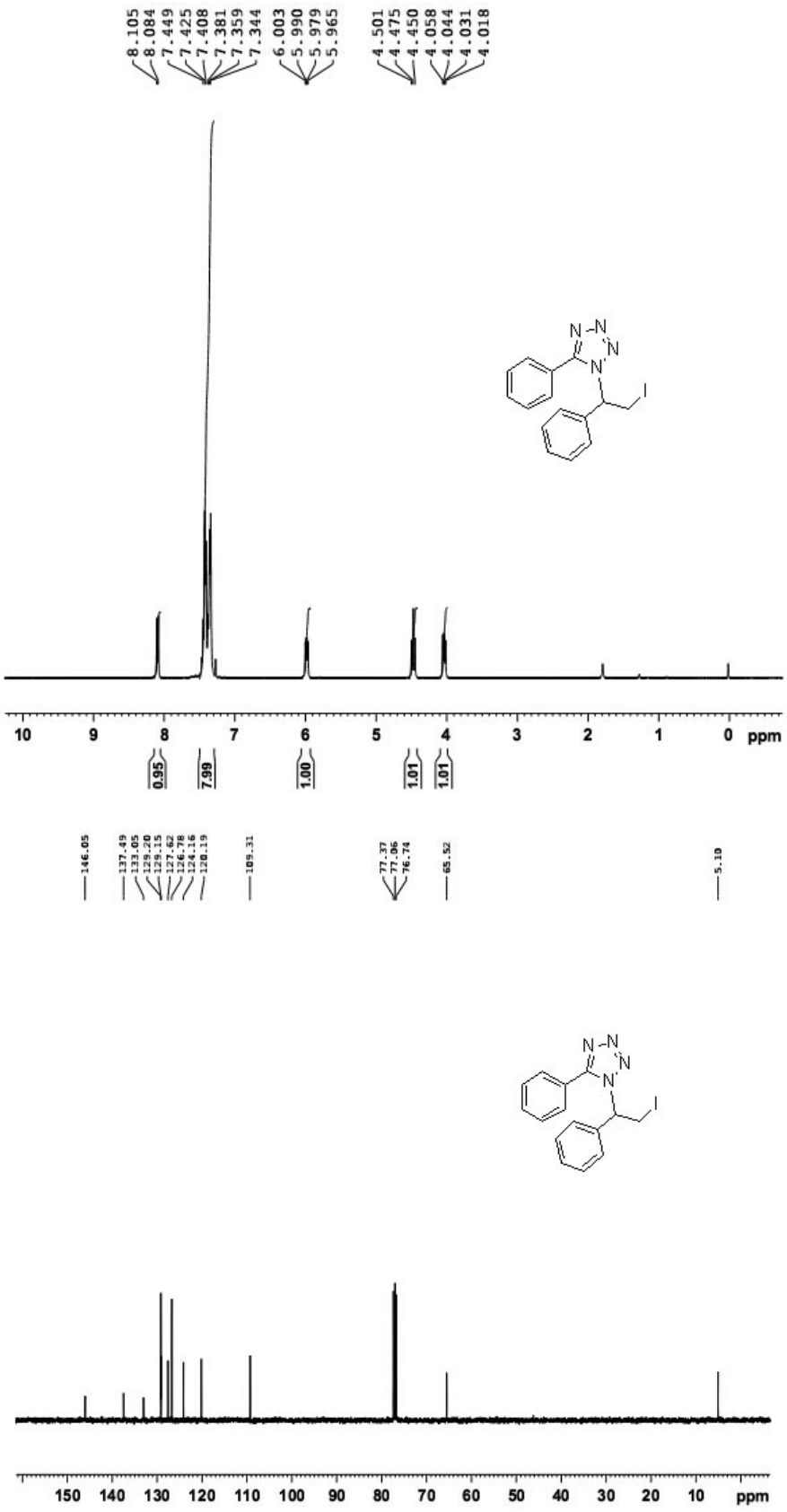
Compound 3i


8.133
8.112
8.063
7.500
7.476
7.452
7.431
7.347
7.328
7.278
5.974
5.960
5.928
5.914
4.439
4.414
4.395
4.370
4.034
4.021
3.992
N
N
N
I
Br
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
4.07
3.14
0.98
1.00
1.01
145.95
136.45
132.92
132.11
128.55
127.86
124.38
123.37
120.29
109.18
77.43
77.12
76.80
64.77
4.66
N
N
N
I
Br
180
160
140
120
100
80
60
40
20
0 ppm

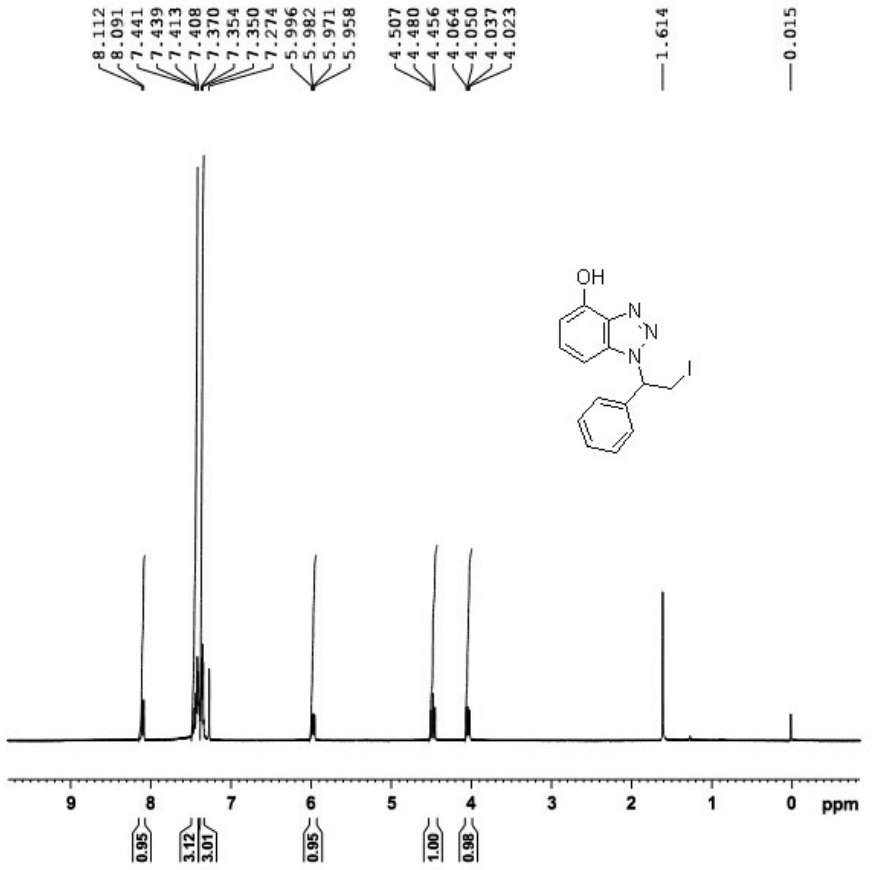
Compound 3j

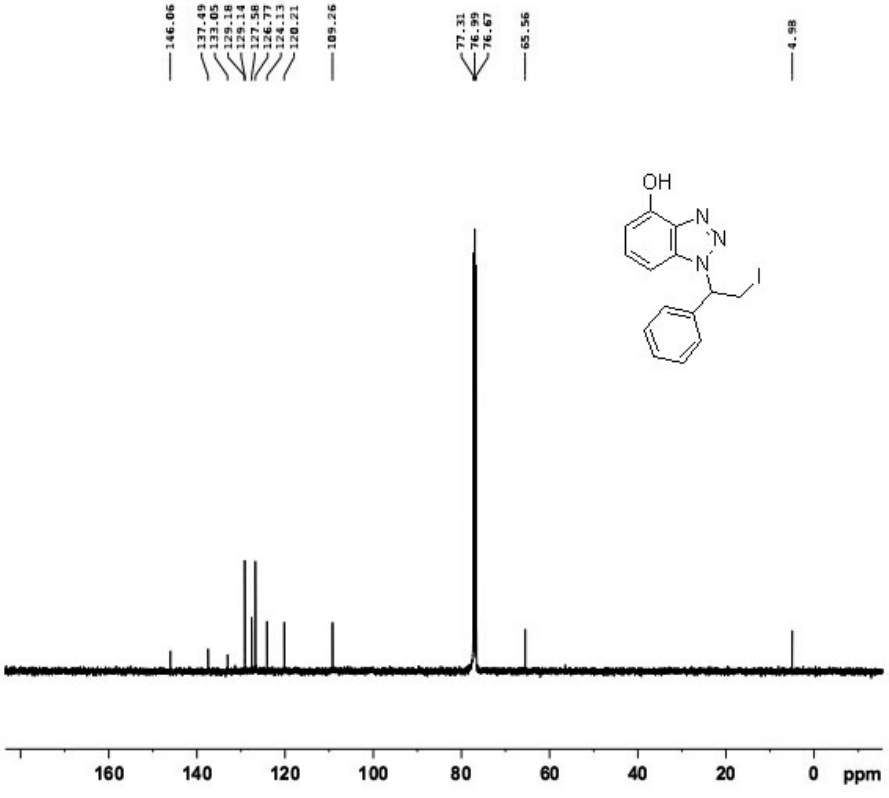

7.650
7.646
7.456
7.450
7.387
7.367
7.362
7.351
7.333
6.310
6.305
6.300
5.511
5.497
5.487
5.473
4.194
4.169
4.144
3.815
3.801
3.788
3.775
1.281
0.025
N
N
I
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.09
5.07
0.93
1.00
1.04
1.03
140.01
138.80
129.47
128.93
128.66
126.77
105.64
77.36
77.04
76.72
67.80
6.73
N
N
I
180 160 140 120 100 80 60 40 20 0 ppm

Compound 3k

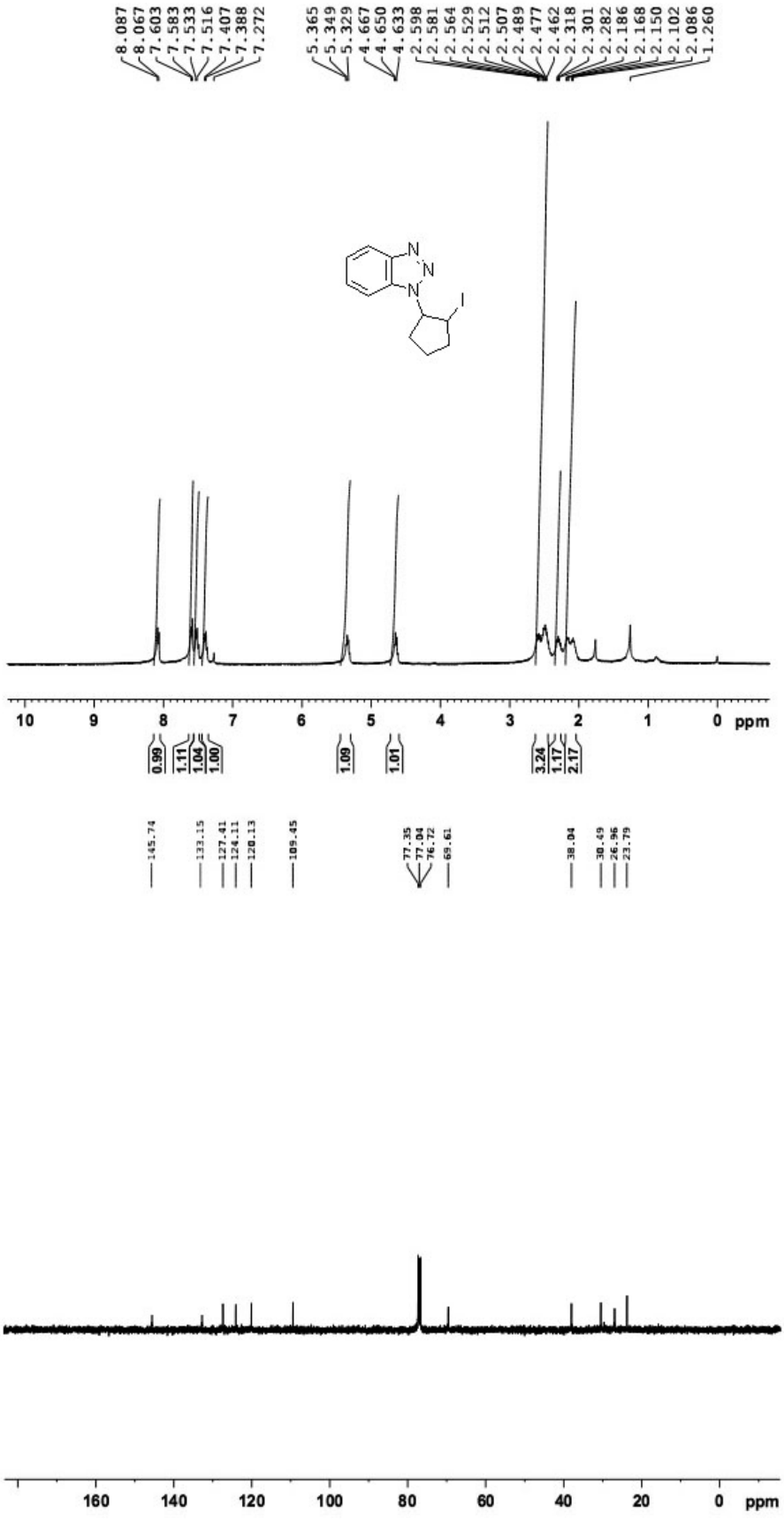

8.105
8.084
7.449
7.425
7.408
7.381
7.359
7.344
6.003
5.990
5.979
5.965
4.501
4.475
4.450
4.058
4.044
4.031
4.018
10 9 8 7 6 5 4 3 2 1 0 ppm
0.95
7.99
1.00
1.01
1.01
146.05
137.49
133.05
129.26
128.15
127.62
126.78
124.16
120.19
109.31
77.37
77.06
76.74
65.52
5.10
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Compound 3l

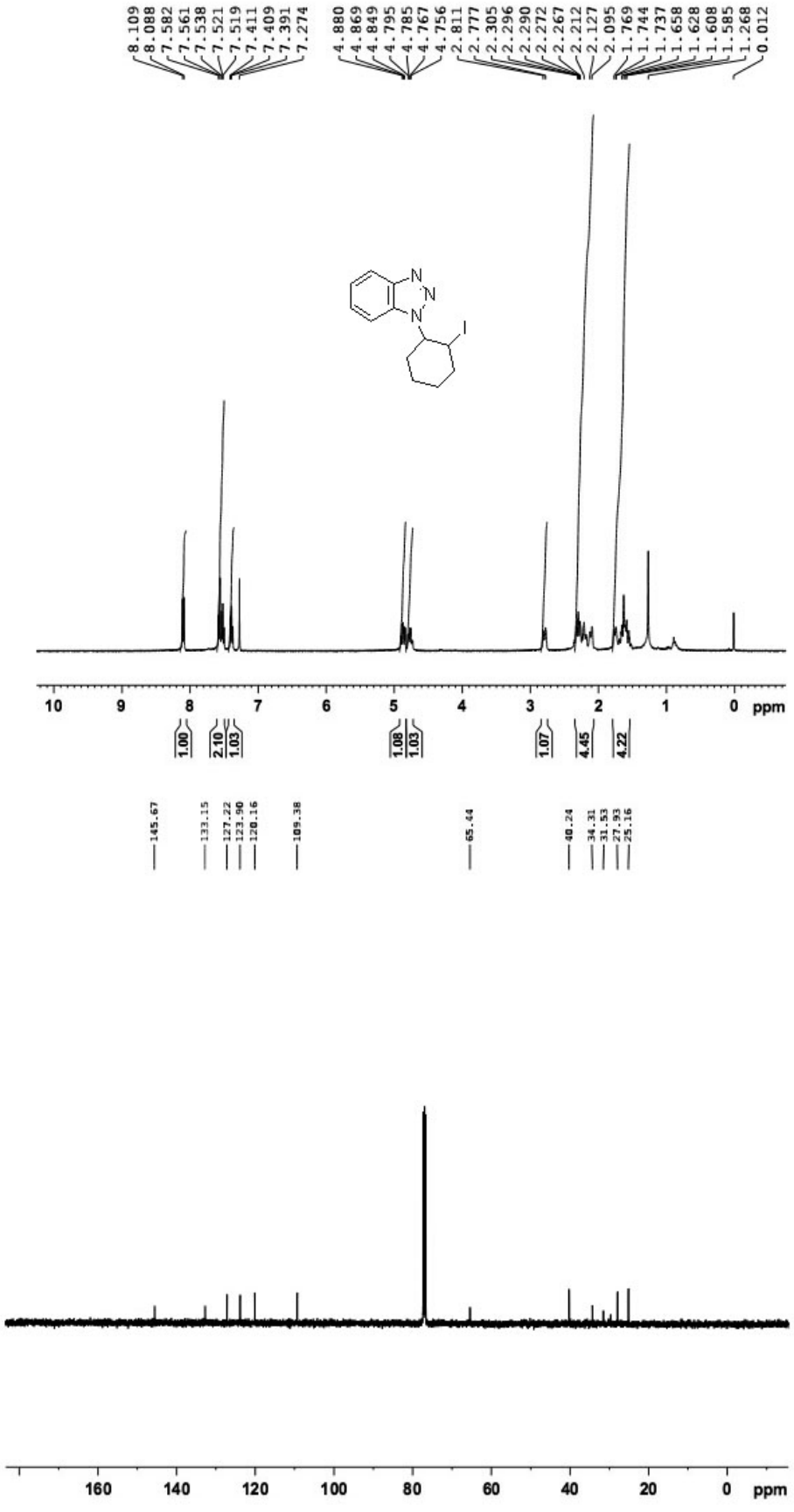

8.112
8.091
7.441
7.439
7.413
7.408
7.370
7.354
7.350
7.274
5.996
5.982
5.971
5.958
4.507
4.480
4.456
4.064
4.050
4.037
4.023
1.614
0.015
OH
N
N
N
I
9
8
7
6
5
4
3
2
1
0
ppm
0.95
3.12
3.01
0.95
1.00
0.98


146.06
137.49
133.65
129.18
128.14
127.58
126.77
124.13
120.21
109.26
77.31
76.99
76.67
65.56
4.98
OH
N
N
N
I
160
140
120
100
80
60
40
20
0
ppm

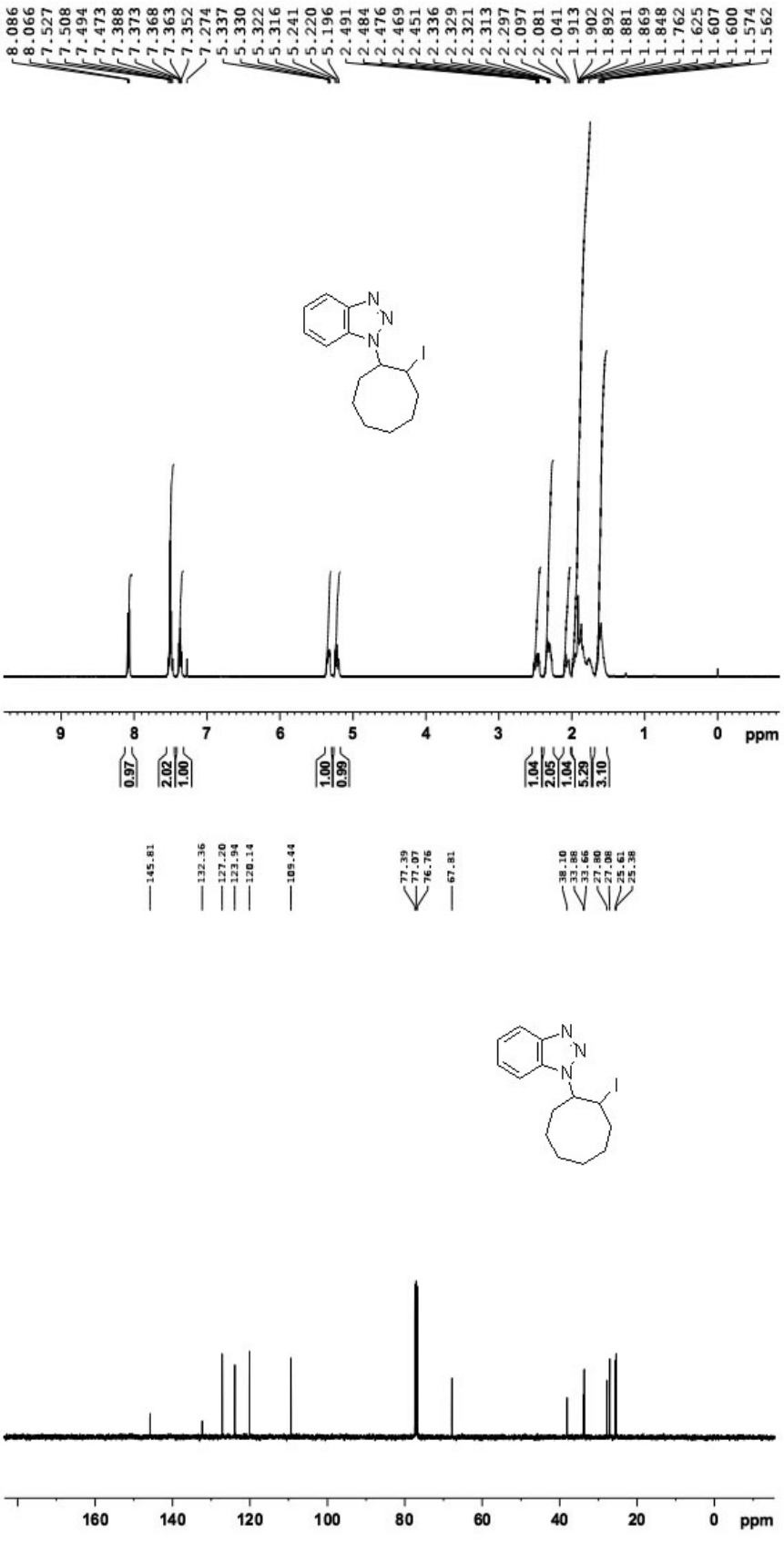
Compound 3m


8.087
8.067
7.603
7.583
7.533
7.516
7.407
7.388
7.272
5.365
5.349
5.329
4.667
4.650
4.633
2.598
2.581
2.564
2.529
2.512
2.507
2.489
2.477
2.462
2.318
2.301
2.282
2.186
2.168
2.150
2.102
2.086
1.260
N
N
N
I
10
9
8
7
6
5
4
3
2
1
0
ppm
0.99
1.11
1.04
1.00
1.09
1.01
3.24
1.17
2.17
145.74
133.15
127.41
124.11
120.13
109.45
77.35
77.04
76.72
69.61
38.04
30.49
26.96
23.79
160
140
120
100
80
60
40
20
0
ppm

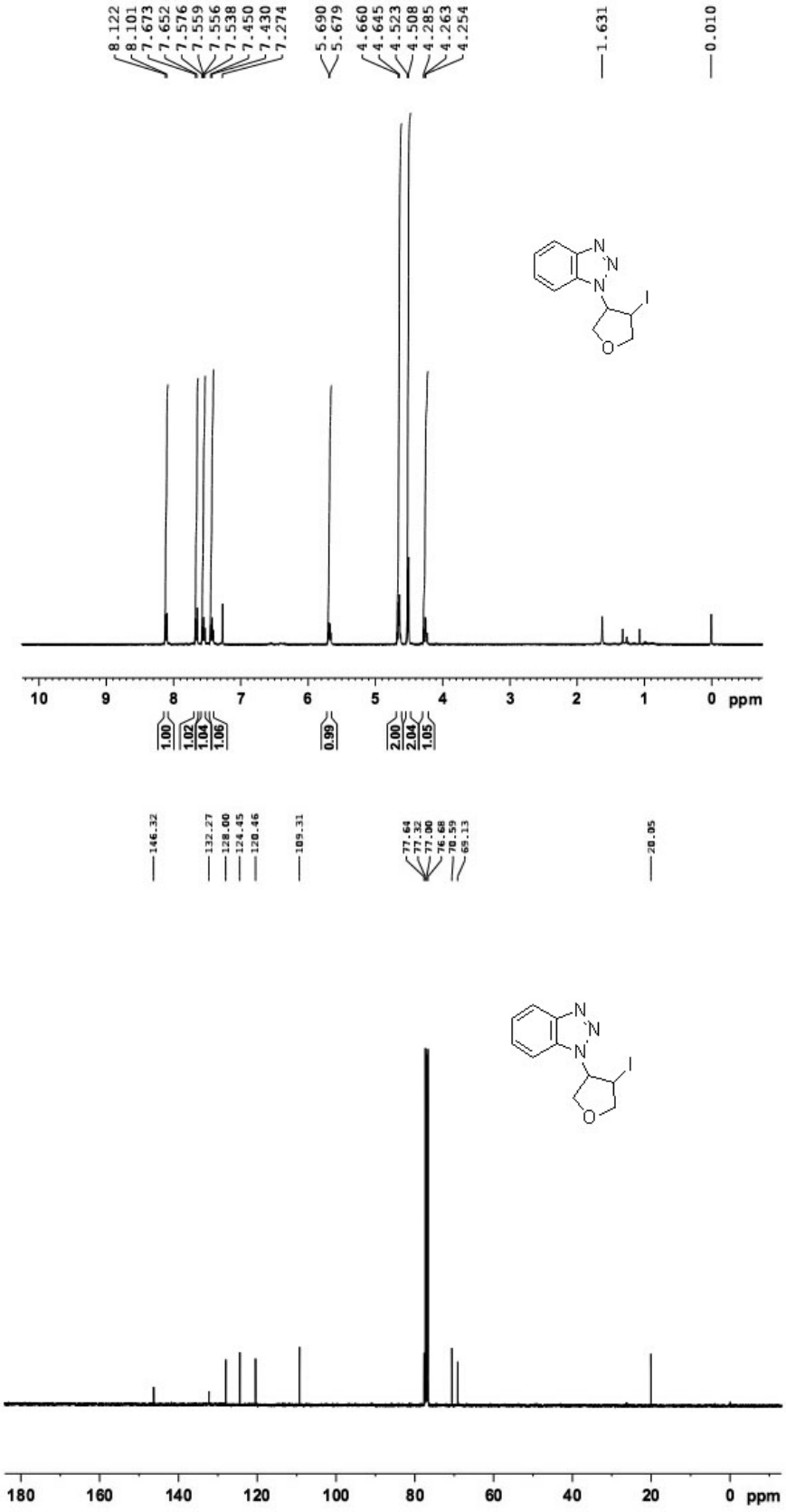
Compound 3n


8.109
8.088
7.582
7.561
7.538
7.521
7.519
7.411
7.409
7.391
7.274
4.880
4.869
4.849
4.795
4.785
4.767
4.756
2.811
2.777
2.305
2.296
2.290
2.272
2.267
2.212
2.127
2.095
1.769
1.744
1.737
1.658
1.628
1.608
1.585
1.268
0.012
N
N
N
I
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
2.10
1.03
1.08
1.03
1.07
4.45
4.22
145.67
133.15
127.22
123.90
120.16
109.38
65.44
40.24
34.31
31.53
27.93
25.16
160 140 120 100 80 60 40 20 0 ppm

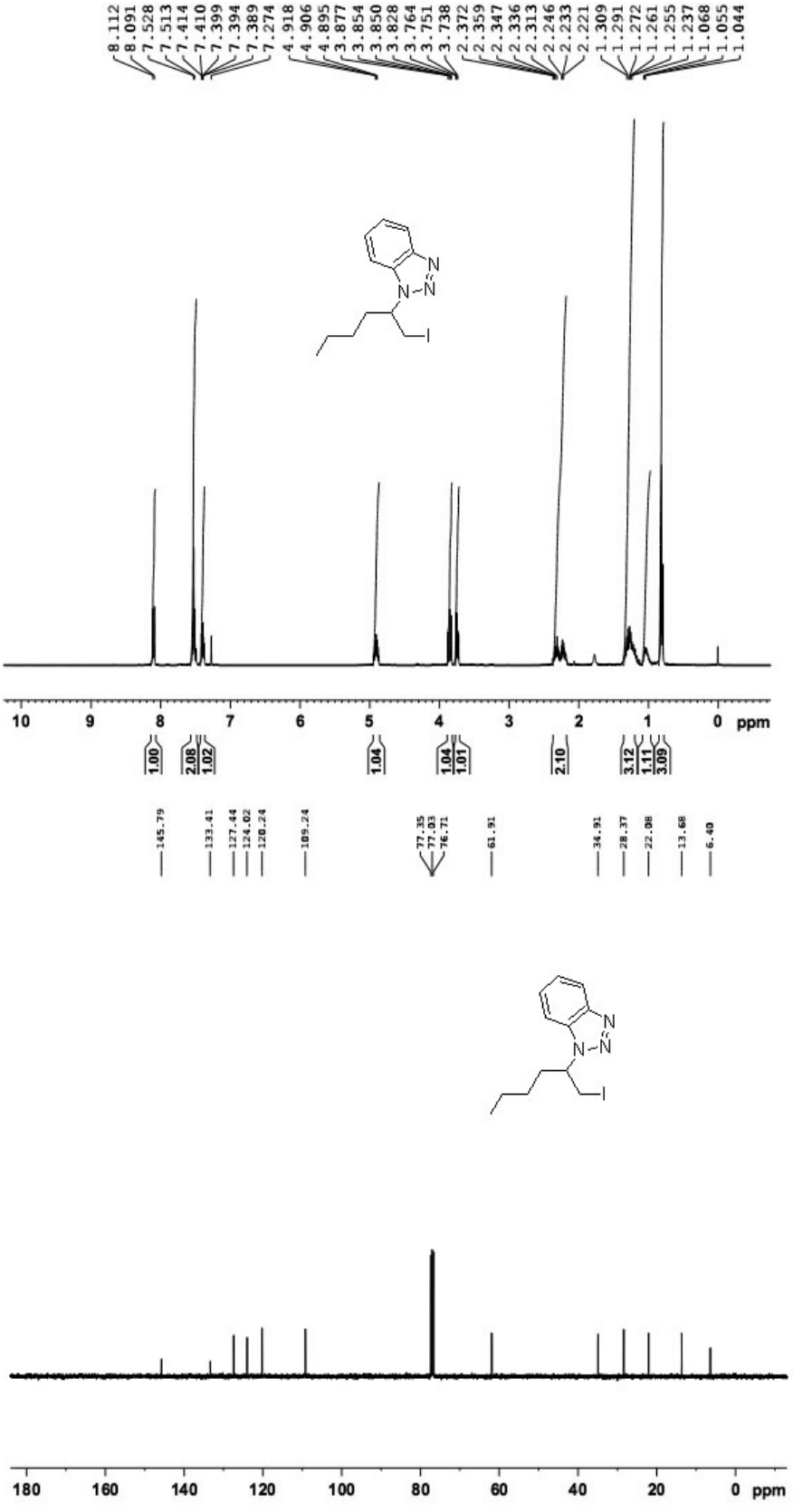
Compound 3o


8.086
8.066
7.527
7.508
7.494
7.473
7.388
7.373
7.368
7.363
7.352
7.274
5.337
5.330
5.322
5.316
5.241
5.220
5.196
2.491
2.484
2.476
2.469
2.451
2.336
2.329
2.321
2.313
2.297
2.097
2.081
2.041
1.913
1.902
1.892
1.881
1.869
1.848
1.762
1.625
1.607
1.600
1.574
1.562
N
N
N
I
9
8
7
6
5
4
3
2
1
0
ppm
0.97
2.02
1.00
1.00
0.99
1.04
2.05
1.04
5.29
3.10
145.81
132.36
127.20
123.94
120.14
109.44
77.39
77.07
76.76
67.81
38.10
33.88
33.66
27.80
27.08
25.61
25.38
N
N
N
I
160
140
120
100
80
60
40
20
0
ppm

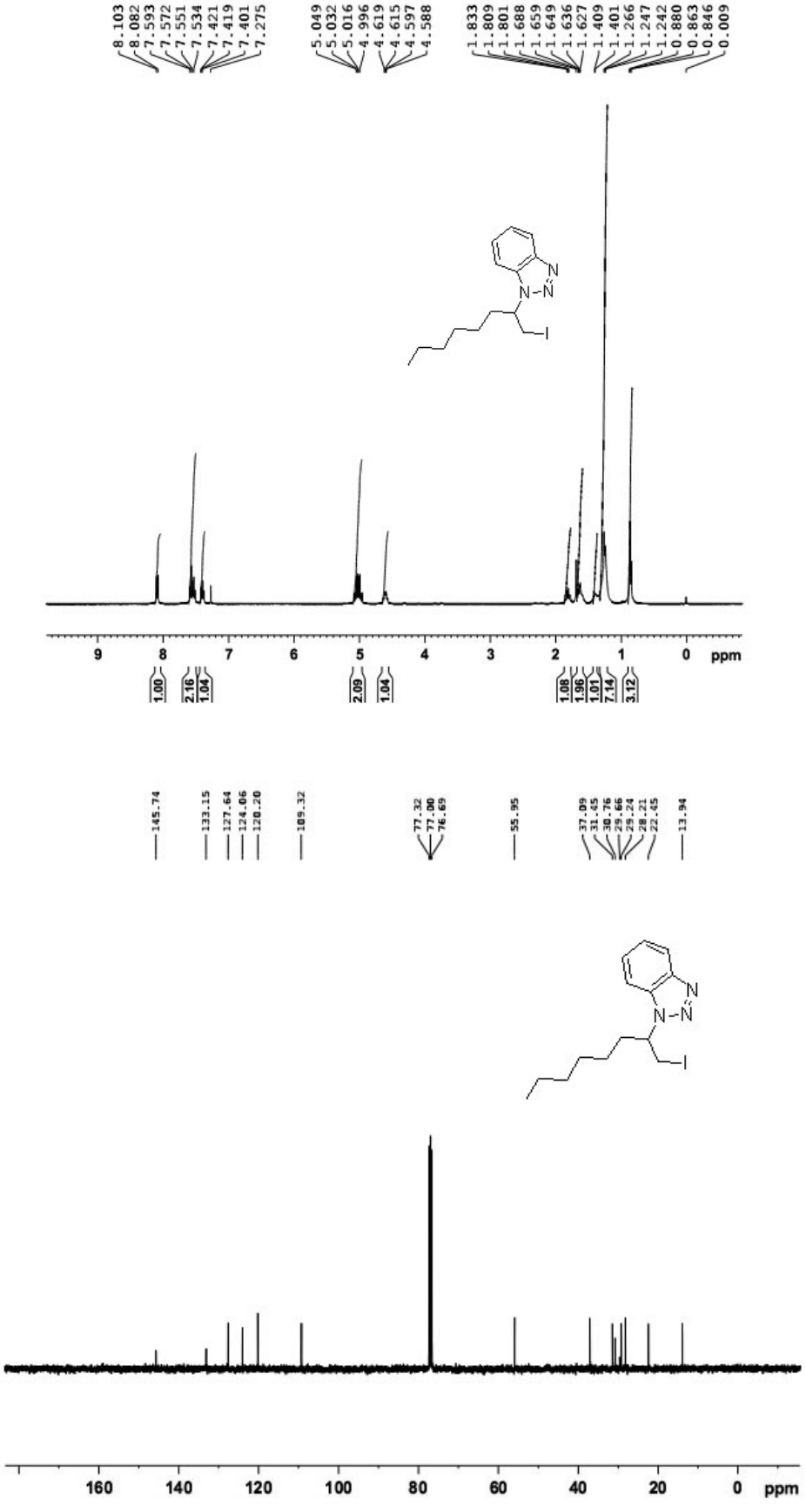
Compound 3p


8.122
8.101
7.673
7.652
7.576
7.559
7.556
7.538
7.450
7.430
7.274
5.690
5.679
4.660
4.645
4.523
4.508
4.285
4.263
4.254
1.631
0.010
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 1.02 1.04 1.06 0.99 2.00 2.04 1.05
146.32
132.27
128.00
124.45
120.46
109.31
77.64
77.32
77.00
76.68
70.59
69.13
20.05
180 160 140 120 100 80 60 40 20 0 ppm

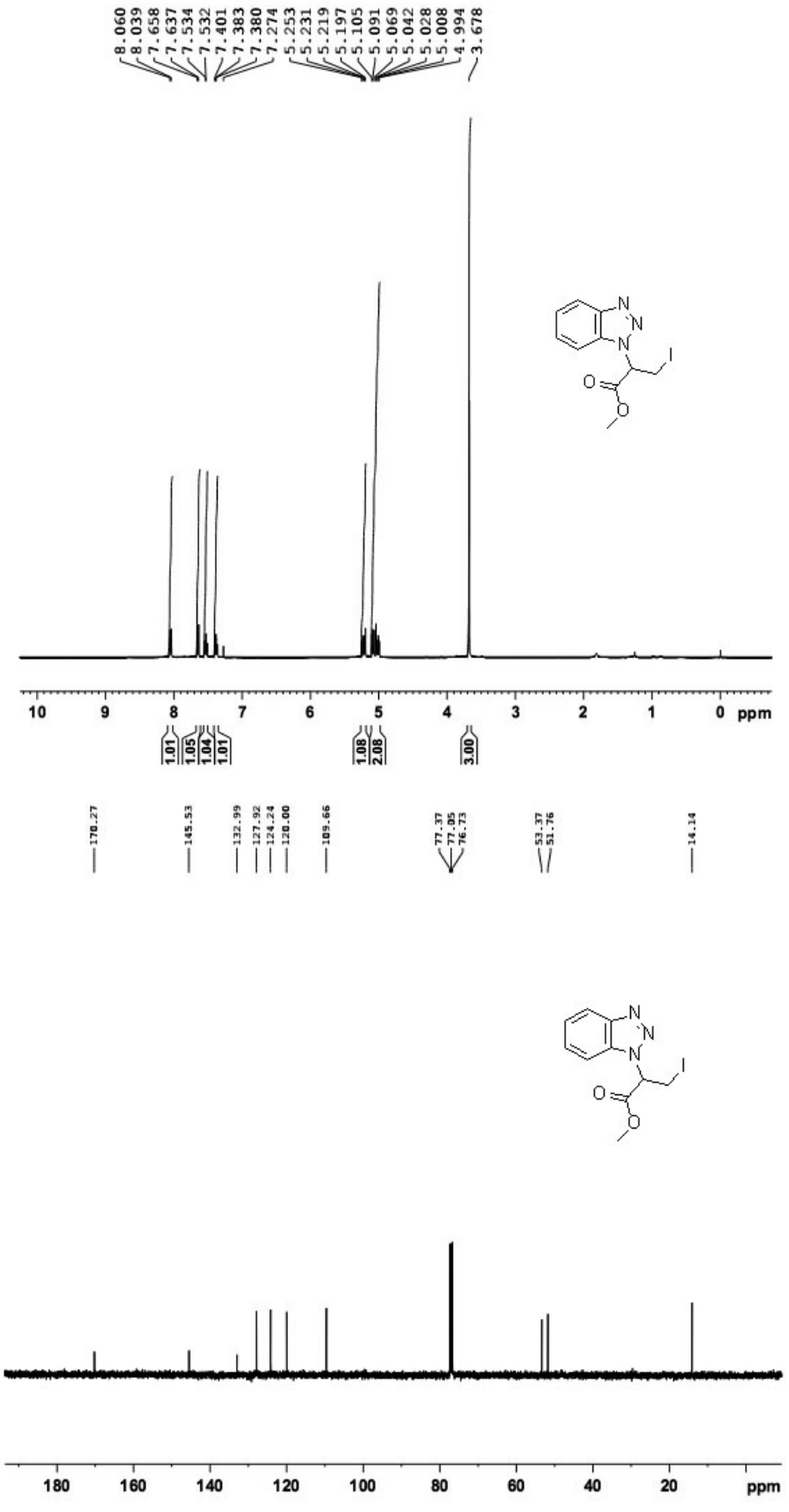
Compound 3q


8.112
8.091
7.528
7.513
7.414
7.410
7.399
7.394
7.389
7.274
4.918
4.906
4.895
3.877
3.854
3.850
3.828
3.764
3.751
3.738
2.372
2.359
2.347
2.336
2.313
2.246
2.233
2.221
1.309
1.291
1.272
1.261
1.255
1.237
1.068
1.055
1.044
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 2.08 1.02 1.04 1.04 1.01 2.10 3.12 1.11 3.09
145.79
133.41
127.44
124.02
120.24
109.24
77.35
77.03
76.71
61.91
34.91
28.37
22.08
13.68
6.40
180 160 140 120 100 80 60 40 20 0 ppm

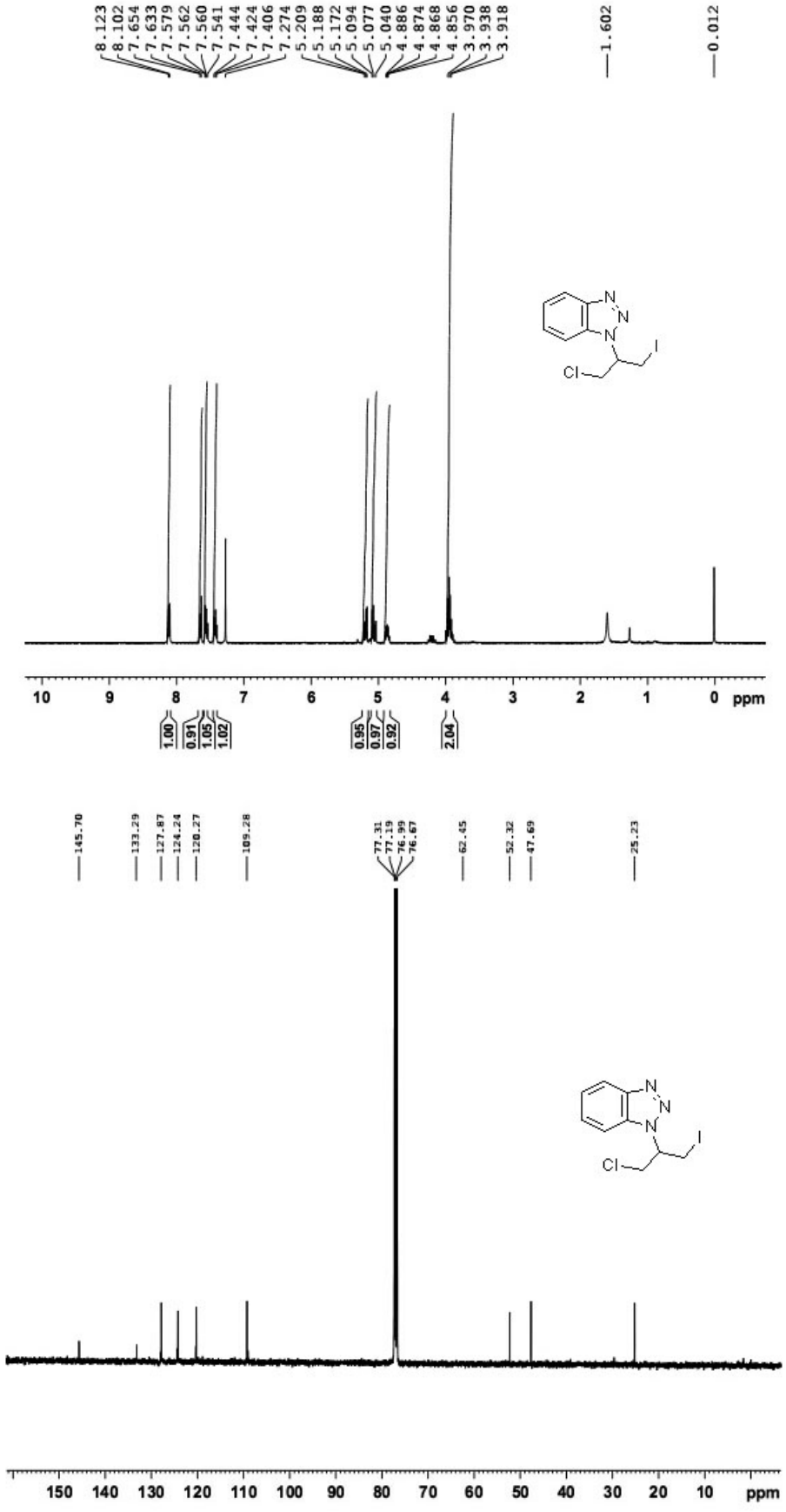
Compound 3r


8.103
8.082
7.593
7.572
7.551
7.534
7.421
7.419
7.401
7.275
5.049
5.032
5.016
4.996
4.619
4.615
4.597
4.588
1.833
1.809
1.801
1.688
1.659
1.649
1.636
1.627
1.409
1.401
1.266
1.247
1.242
0.880
0.863
0.846
0.009
N
N-N
I
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.16
1.04
2.09
1.04
1.08
1.96
1.01
7.14
3.12
145.74
133.15
127.64
124.06
120.20
109.32
77.32
77.00
76.69
55.95
37.09
31.45
30.76
29.66
29.24
28.21
22.45
13.94
160
140
120
100
80
60
40
20
0
ppm

Compound 3s


8.060
8.039
7.658
7.637
7.534
7.532
7.401
7.383
7.380
7.274
5.253
5.231
5.219
5.197
5.105
5.091
5.069
5.042
5.028
5.008
4.994
3.678
10 9 8 7 6 5 4 3 2 1 0 ppm
1.01
1.05
1.04
1.01
1.08
2.08
3.00
170.27
145.53
132.99
127.92
124.24
120.00
109.66
77.37
77.05
76.73
53.37
51.76
14.14
180 160 140 120 100 80 60 40 20 ppm

Compound 3t


8.123
8.102
7.654
7.633
7.579
7.562
7.560
7.541
7.444
7.424
7.406
7.274
5.209
5.188
5.172
5.094
5.077
5.040
4.886
4.874
4.868
4.856
3.970
3.938
3.918
1.602
0.012
N
N
N
I
Cl
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
0.91
1.05
1.02
0.95
0.97
0.92
2.04
145.70
133.29
127.87
124.24
120.27
109.28
77.31
77.19
76.99
76.67
62.45
52.32
47.69
25.23
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm