

Supporting information

Convenient Synthesis of Benzo[4,5]thiazolo [2,3-*c*][1,2,4]triazoles with 1 mol% CuCl₂•2H₂O as Catalyst in Water

Li-Rong Wen,* Shou-Lei Li, Jian Zhang, and Ming Li*

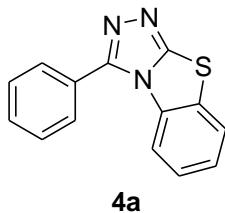
State Key Laboratory Base of Eco-Chemical Engineering, College of Chemistry and Molecular
Engineering, Qingdao University of Science and Technology, Qingdao 266042, P. R. China

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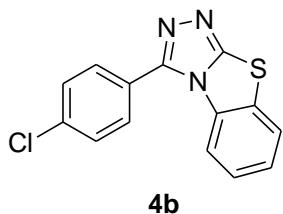
Characterization Data

3-Phenylbenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**4a**)¹



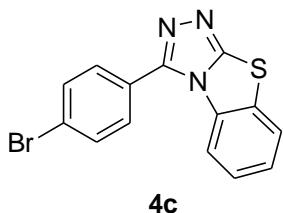
Yellow powder; Mp 145-146 °C; **IR** (KBr) ν : 3074, 1636, 1579, 1483, 773, 755, 704 cm⁻¹; **1H NMR** (DMSO-*d*₆, 500 MHz): δ = 8.09 (dd, *J* = 1.2, 8.0 Hz, 1H, ArH), 7.85–7.83 (m, 2H, ArH), 7.67–7.66 (m, 3H, ArH), 7.48–7.41 (m, 3H, ArH); **13C NMR** (DMSO-*d*₆, 125 MHz): δ = 132.3, 131.2, 130.2, 129.7, 129.6, 127.3, 126.9, 126.3, 114.4; **HRMS** (ESI-TOF⁺): *m/z* calcd for C₁₄H₁₀N₃S [(M + H)⁺], 252.0595; found, 252.0592.

3-(4-Chlorophenyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**4b**)



Cyan powder; Mp 198-199 °C; **IR** (KBr) ν : 3092, 3074, 1632, 1603, 1484, 843, 762 cm⁻¹; **1H NMR** (DMSO-*d*₆, 500 MHz): δ = 8.09 (d, *J* = 7.5 Hz, 1H, ArH), 7.89 (d, *J* = 8.4 Hz, 2H, ArH), 7.74 (d, *J* = 8.5 Hz, 2H, ArH), 7.51–7.42 (m, 3H, ArH); **13C NMR** (DMSO-*d*₆, 125 MHz): δ = 136.0, 132.2, 131.6, 130.2, 129.7, 127.4, 126.9, 126.2, 114.6; **HRMS** (ESI-TOF⁺): *m/z* calcd for C₁₄H₉ClN₃S [(M + H)⁺], 286.0206; found, 286.0210.

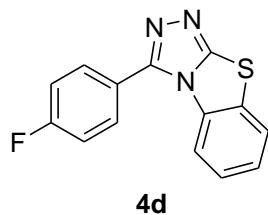
3-(4-Bromophenyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**4c**)



Yellow powder; Mp 198-200 °C; **IR** (KBr) ν : 3089, 3072, 1629, 1599, 1483, 830, 762

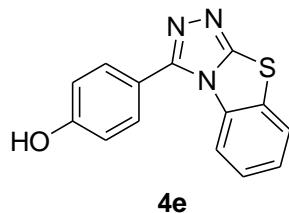
cm^{-1} ; **1H NMR** ($\text{DMSO}-d_6$, 500 MHz): $\delta = 8.09$ (d, $J = 7.3$ Hz, 1H, ArH), 7.87 (d, $J = 8.4$ Hz, 2H, ArH), 7.80 (d, $J = 8.4$ Hz, 2H, ArH), 7.51–7.42 (m, 3H, ArH); **13C NMR** ($\text{DMSO}-d_6$, 125 MHz): $\delta = 132.6, 132.2, 131.7, 130.2, 127.4, 126.9, 126.6, 126.2, 124.8, 114.6$; **HRMS** (ESI-TOF $^+$): m/z calcd for $\text{C}_{14}\text{H}_9\text{BrN}_3\text{S}$ [(M + H) $^+$], 329.9701; found, 329.9709.

3-(4-Fluorophenyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4d)



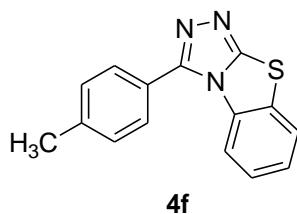
Gray powder; Mp 168–169 °C; **IR** (KBr) ν : 3069, 1609, 1486, 840, 765 cm^{-1} ; **1H NMR** (CDCl_3 , 500 MHz): $\delta = 7.80$ –7.78 (m, 2H, ArH), 7.71 (d, $J = 8.0$ Hz, 1H, ArH), 7.48 (d, $J = 8.1$ Hz, 1H, ArH), 7.41 (t, $J = 7.5$ Hz, 1H, ArH), 7.36–7.29 (m, 3H, ArH); **13C NMR** (CDCl_3 , 125 MHz): $\delta = 164.2$ (${}^1J_{\text{C-F}} = 247.6$ Hz), 132.6, 131.3 (${}^3J_{\text{C-F}} = 6.6$ Hz), 129.9, 126.4, 124.9, 123.1, 116.4 (${}^2J_{\text{C-F}} = 21.7$ Hz), 114.1; **HRMS** (ESI-TOF $^+$): m/z calcd for $\text{C}_{14}\text{H}_9\text{N}_3\text{OSF}$ [(M + H) $^+$], 270.0501; found, 270.0512.

4-(Benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazol-3-yl)phenol (4e)



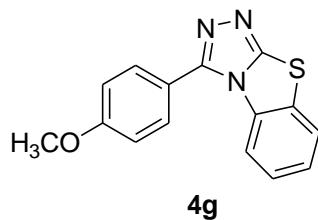
Gray powder; Mp 275–276 °C; **IR** (KBr) ν : 3056, 3013, 1613, 1589, 1494, 840, 750 cm^{-1} ; **1H NMR** ($\text{DMSO}-d_6$, 500 MHz): $\delta = 10.15$ (s, 1H, OH), 8.06 (t, $J = 4.5$ Hz, 1H, ArH), 7.62 (d, $J = 8.2$ Hz, 2H, ArH), 7.46–7.43 (m, 3H, ArH), 7.02–7.00 (d, $J = 8.3$ Hz, 2H, ArH); **13C NMR** ($\text{DMSO}-d_6$, 125 MHz): $\delta = 160.1, 131.3, 130.3, 127.3, 126.8, 126.2, 116.3, 114.4, 102.7$; **HRMS** (ESI-TOF $^+$): m/z calcd for $\text{C}_{14}\text{H}_{10}\text{N}_3\text{OS}$ [(M + H) $^+$], 268.0545; found, 268.0549.

3-(*p*-Tolyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4f)¹



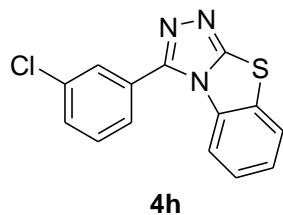
Brown powder; Mp 155-156 °C; **IR** (KBr) ν : 3066, 3031, 2919, 2850, 1609, 1579, 1486, 820, 748 cm⁻¹; **1H NMR** (DMSO-*d*₆, 500 MHz): δ = 8.07 (d, *J* = 7.9 Hz, 1H, ArH), 7.72 (d, *J* = 7.7 Hz, 2H, ArH), 7.47 (d, *J* = 7.7 Hz, 3H, ArH), 7.45–7.41 (m, 2H, ArH), 2.46 (s, 3H, CH₃); **13C NMR** (DMSO-*d*₆, 125 MHz): δ = 141.0, 132.3, 130.1, 129.6, 127.3, 126.9, 126.3, 124.5, 114.5, 21.6; **HRMS** (ESI-TOF⁺): *m/z* calcd for C₁₅H₁₂N₃S [(M + H)⁺], 266.0752; found, 266.0759.

3-(4-Methoxyphenyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4g)¹



Cyan powder; Mp 141-142 °C; **IR** (KBr) ν : 3088, 3056, 2999, 2922, 2841, 1614, 1575, 1483, 846, 747 cm⁻¹; **1H NMR** (CDCl₃, 500 MHz): δ = 7.72–7.69 (m, 3H, ArH), 7.54 (d, *J* = 8.1 Hz, 1H, ArH), 7.39 (t, *J* = 7.5 Hz, 1H, ArH), 7.33 (t, *J* = 7.7 Hz, 1H, ArH), 7.11 (d, *J* = 8.5 Hz, 2H, ArH), 3.93 (s, 3H, OCH₃); **13C NMR** (CDCl₃, 125 MHz): δ = 161.5, 132.7, 130.7, 130.3, 126.2, 124.8, 119.1, 114.5, 114.3, 55.5; **HRMS** (ESI-TOF⁺): *m/z* calcd for C₁₅H₁₂ON₃S [(M + H)⁺], 282.0701; found, 282.0709.

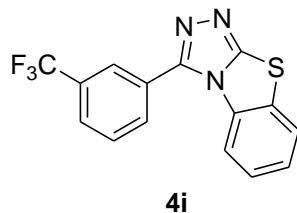
3-(3-Chlorophenyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4h)



Pink powder; Mp 168-169 °C; **IR** (KBr) ν : 3053, 3009, 1626, 1569, 1482, 775, 755, 708 cm⁻¹; **1H NMR** (CDCl₃, 500 MHz): δ = 7.83 (s, 1H, ArH), 7.74–7.69 (m, 2H, ArH),

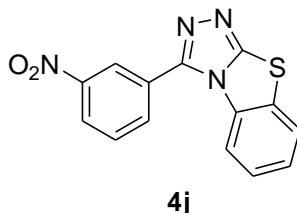
7.62–7.59 (m, 1H, ArH), 7.57 (d, J = 7.7, Hz, 1H, ArH), 7.54 (d, J = 7.9, Hz, 1H, ArH), 7.45–7.36 (m, 2H, ArH); **^{13}C NMR** (CDCl_3 , 125 MHz): δ = 156.6, 148.0, 135.2, 132.6, 130.9, 130.3, 129.8, 129.2, 128.6, 127.2, 126.6, 124.9, 114.2; **HRMS** (ESI-TOF $^+$): m/z calcd for $\text{C}_{14}\text{H}_9\text{N}_3\text{SCl}$ [(M + H) $^+$], 286.0206; found, 286.0213.

3-(3-(Trifluoromethyl)phenyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4i)



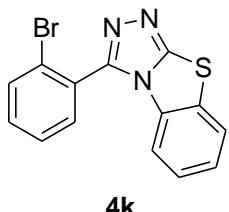
Gray powder; Mp 174–175 °C; **IR** (KBr) ν : 3083, 3046, 1622, 1581, 1482, 808, 747, 704 cm^{-1} ; **^1H NMR** (CDCl_3 , 500 MHz): δ = 8.11 (s, 1H, ArH), 8.03 (d, J = 7.5 Hz, 1H, ArH), 7.89 (d, J = 7.8 Hz, 1H, ArH), 7.79–7.74 (m, 2H, ArH), 7.48–7.43 (m, 2H, ArH), 7.39 (t, J = 7.7 Hz, 1H, ArH); **^{13}C NMR** (CDCl_3 , 125 MHz): δ = 132.8, 132.3, 131.7 ($^2J_{\text{C}-\text{F}} = 33.2$ Hz), 130.0, 129.7, 128.2, 127.4, 126.6, 126.5, 126.1, 125.0, 123.5 ($^1J_{\text{C}-\text{F}} = 271.3$ Hz), 114.1; **HRMS** (ESI-TOF $^+$): m/z calcd for $\text{C}_{15}\text{H}_9\text{N}_3\text{SF}_3$ [(M + H) $^+$], 320.0469; found, 320.0473.

3-(3-Nitrophenyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4j)



Gray powder; Mp 237–238 °C; **IR** (KBr) ν : 3097, 1624, 1579, 1483, 813, 754, 681 cm^{-1} ; **^1H NMR** (CDCl_3 , 500 MHz): δ = 8.72 (s, 1H, ArH), 8.49 (d, J = 7.5 Hz, 1H, ArH), 8.20 (d, J = 7.0 Hz, 1H, ArH), 7.85 (t, J = 7.6 Hz, 1H, ArH), 7.77 (d, J = 7.6 Hz, 1H, ArH), 7.51–7.40 (m, 3H, ArH); **^{13}C NMR** (CDCl_3 , 125 MHz): δ = 148.5, 134.8, 132.7, 130.4, 129.7, 128.9, 126.8, 126.7, 125.3, 125.2, 123.9, 113.9; **HRMS** (ESI-TOF $^+$): m/z calcd for $\text{C}_{14}\text{H}_9\text{N}_4\text{O}_2\text{S}$ [(M + H) $^+$], 297.0446; found, 297.0459.

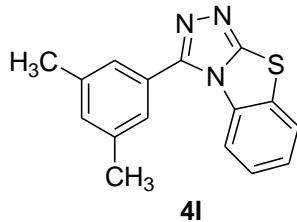
3-(2-Bromophenyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4k)



4k

Brown powder; Mp 145-146 °C; **IR** (KBr) ν : 3059, 1636, 1600, 1483, 770, 761, 682 cm⁻¹; **1H NMR** (CDCl₃, 500 MHz): δ = 7.82 (d, J = 7.7 Hz, 1H, ArH), 7.71 (d, J = 8.0 Hz, 1H, ArH), 7.66 (d, J = 2.8 Hz, 1H, ArH), 7.57–7.51 (m, 2H, ArH), 7.39 (t, J = 7.6 Hz, 1H, ArH), 7.31 (t, J = 7.7 Hz, 1H, ArH), 7.03 (d, J = 8.2 Hz, 1H, ArH); **13C NMR** (CDCl₃, 125 MHz): δ = 133.3, 132.8, 132.5, 129.7, 128.8, 127.9, 126.5, 126.4, 124.6, 124.3, 114.4; **HRMS** (ESI-TOF⁺): m/z calcd for C₁₄H₉N₃BrS [(M + H)⁺], 329.9701; found, 329.9710.

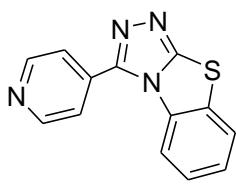
3-(3,5-Dimethylphenyl)benzo[4,5]thiazolo[2,3-c][1,2,4]triazole (4l)



4l

White powder; Mp 186-187 °C; **IR** (KBr) ν : 3052, 3006, 2917, 2850, 1602, 1483, 752, 720, 683 cm⁻¹; **1H NMR** (CDCl₃, 500 MHz): δ = 7.70 (d, J = 7.9 Hz, 1H, ArH), 7.56 (d, J = 8.0 Hz, 1H, ArH), 7.41–7.32 (m, 4H, ArH), 7.24 (s, 1H, ArH), 2.44 (s, 6H, CH₃); **13C NMR** (CDCl₃, 125 MHz): δ = 156.1, 149.7, 138.8, 132.7, 130.1, 126.8, 126.6, 126.3, 126.2, 124.7, 114.3, 40.9, 21.3; **HRMS** (ESI-TOF⁺): m/z calcd for C₁₆H₁₄N₃S [(M + H)⁺], 280.0908; found, 280.0913.

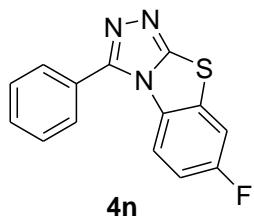
3-Benzylbenzo[4,5]thiazolo[2,3-c][1,2,4]triazole (4m)



4m

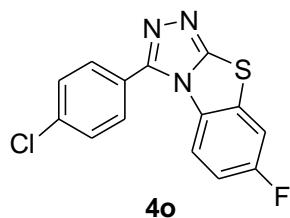
Brown powder; Mp 145–147 °C; **IR** (KBr) ν : 3059, 1632, 1600, 1489, 748, 727, 681 cm⁻¹; **¹H NMR** (CDCl₃, 500 MHz): δ = 8.90 (d, J = 4.3 Hz, 2H, ArH), 7.76–7.74 (m, 3H, ArH), 7.61 (d, J = 8.1 Hz, 1H, ArH), 7.46 (t, J = 7.7 Hz, 1H, ArH), 7.41 (t, J = 7.7 Hz, 1H, ArH); **¹³C NMR** (CDCl₃, 125 MHz): δ = 150.7, 134.7, 132.6, 129.6, 126.9, 126.7, 125.2, 123.4, 122.9, 114.3; **HRMS** (ESI-TOF⁺): m/z calcd for C₁₃H₈N₄S [(M + H)⁺], 253.0571; found, 253.0562.

7-Fluoro-3-phenylbenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**4n**)



White powder; Mp 181–182 °C; **IR** (KBr) ν : 3076, 1626, 1589, 1490, 799, 767, 699 cm⁻¹; **¹H NMR** (CDCl₃, 500 MHz): δ = 7.79–7.76 (m, 2H, ArH), 7.65–7.59 (m, 3H, ArH), 7.50 (dd, J = 4.4, 9.1 Hz, 1H, ArH), 7.44 (dd, J = 2.6, 7.7 Hz, 1H, ArH), 7.07–7.03 (m, 1H, ArH); **¹³C NMR** (CDCl₃, 125 MHz): δ = 160.3 ($^1J_{C-F}$ = 248.6 Hz), 159.3, 134.3 ($^3J_{C-F}$ = 10.0 Hz), 129.2, 129.1, 127.9, 127.8, 127.6, 126.6, 115.3 ($^3J_{C-F}$ = 8.9 Hz), 114.1 ($^2J_{C-F}$ = 24.3 Hz), 111.9 ($^2J_{C-F}$ = 27.1 Hz); **HRMS** (ESI-TOF⁺): m/z calcd for C₁₄H₉N₃SF [(M + H)⁺], 270.0501; found, 270.0512.

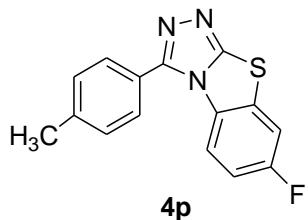
3-(4-Chlorophenyl)-7-fluorobenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**4o**)



Gray powder; Mp 264–265 °C; **IR** (KBr) ν : 3099, 3075, 1636, 1601, 1487, 853, 824, 719 cm⁻¹; **¹H NMR** (CDCl₃, 500 MHz): δ = 7.73 (d, J = 8.2 Hz, 2H, ArH), 7.60 (d, J = 8.2 Hz, 2H, ArH), 7.49–7.44 (m, 2H, ArH), 7.10–7.07 (m, 1H, ArH); **¹³C NMR** (CDCl₃, 125 MHz): δ = 160.3 ($^1J_{C-F}$ = 248.6 Hz), 137.2, 134.3 ($^3J_{C-F}$ = 10.0 Hz), 130.3, 129.6, 126.4, 125.1, 115.1 ($^3J_{C-F}$ = 8.9 Hz), 114.2 ($^2J_{C-F}$ = 24.5 Hz), 112.1 ($^2J_{C-F}$ = 27.0 Hz), 111.9; **HRMS** (ESI-TOF⁺): m/z calcd for C₁₄H₈N₃ClFS [(M + H)⁺], 304.0112;

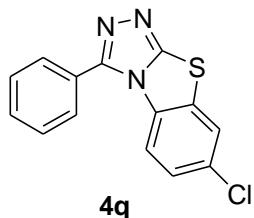
found, 304.0119.

7-Fluoro-3-(*p*-tolyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4p)



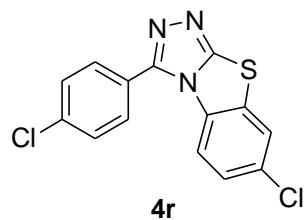
Pink powder; Mp 216-217 °C; **IR** (KBr) ν : 3073, 3029, 2920, 2851, 1636, 1585, 1491, 842, 825, 720 cm⁻¹; **¹H NMR** (CDCl₃, 500 MHz): δ = 7.67 (d, J = 8.0 Hz, 2H, ArH), 7.51 (dd, J = 4.4, 9.1 Hz, 1H, ArH), 7.44–7.41 (m, 3H, ArH), 7.07–7.03 (m, 1H, ArH), 2.50 (s, 3H, CH₃); **¹³C NMR** (CDCl₃, 125 MHz): δ = 160.2 ($^1J_{C-F}$ = 248.2 Hz), 156.0, 149.4, 141.2, 134.3 ($^3J_{C-F}$ = 10.0 Hz), 129.9, 128.9, 126.6, 123.6, 115.3 ($^3J_{C-F}$ = 8.7 Hz), 114.0 ($^2J_{C-F}$ = 24.0 Hz), 111.9 ($^2J_{C-F}$ = 27.2 Hz); **HRMS** (ESI-TOF⁺): m/z calcd for C₁₅H₁₁N₃FS [(M + H)⁺], 284.0658; found, 284.0649.

7-Chloro-3-phenylbenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4q)



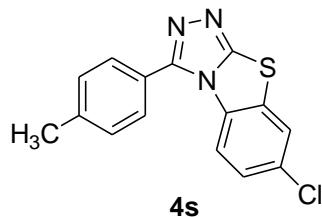
White powder; Mp 209-211 °C; **IR** (KBr) ν : 3083, 3072, 2992, 2851, 1716, 1528, 1481, 1466, 1447, 854, 792, 769, 717, 698, 623 cm⁻¹; **¹H NMR** (CDCl₃, 500 MHz): δ = 7.79–7.77 (m, 2H, ArH), 7.70 (d, J = 2.0 Hz, 1H, ArH), 7.64–7.59 (m, 3H, ArH), 7.47 (d, J = 8.9 Hz, 1H, ArH), 7.30 (dd, J = 2.0, 8.8 Hz, 1H, ArH); **¹³C NMR** (CDCl₃, 125 MHz): δ = 134.2, 132.1, 131.0, 129.1, 128.6, 126.8, 126.6, 115.0; **HRMS** (ESI-TOF⁺): m/z calcd for C₁₄H₉N₃SCl [(M + H)⁺], 286.0206; found, 286.0215.

7-Chloro-3-(4-chlorophenyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4r)



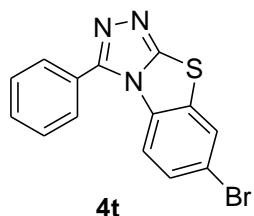
Brown powder; Mp 270-271 °C; **IR** (KBr) ν : 3092, 3069, 1735, 1519, 1484, 845, 824, 799, 743 cm⁻¹; **¹H NMR** (DMSO-*d*₆, 500 MHz): δ = 8.25 (s, 1H, ArH), 7.85 (d, *J* = 8.2 Hz, 2H, ArH), 7.72 (d, *J* = 8.3 Hz, 2H, ArH), 7.49 (d, *J* = 8.8 Hz, 1H, ArH), 7.38 (d, *J* = 8.8 Hz, 1H, ArH); **¹³C NMR** (CDCl₃, 125 MHz): δ = 137.3, 134.2, 132.3, 130.3, 129.6, 128.4, 126.9, 125.1, 124.7, 114.8; **HRMS** (ESI-TOF⁺): *m/z* calcd for C₁₄H₈N₃SCl₂ [(M + H)⁺], 319.9816; found, 319.9812.

7-Chloro-3-(p-tolyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4s)



Gray powder; Mp 230-231 °C; **IR** (KBr) ν : 3093, 3054, 2923, 2853, 1540, 1486, 856, 829, 816, 794 cm⁻¹; **¹H NMR** (CDCl₃, 500 MHz): δ = 7.68 (d, *J* = 1.8 Hz, 1H, ArH), 7.65 (d, *J* = 8.0 Hz, 2H, ArH), 7.46 (d, *J* = 8.9 Hz, 1H, ArH), 7.40 (d, *J* = 7.8 Hz, 2H, ArH), 7.28 (dd, *J* = 1.9, 8.7 Hz, 1H, ArH), 2.49 (s, 3H, CH₃); **¹³C NMR** (CDCl₃, 125 MHz): δ = 149.7, 141.3, 134.2, 131.9, 129.8, 128.9, 128.7, 126.7, 124.5, 123.6, 115.0, 21.5; **HRMS** (ESI-TOF⁺): *m/z* calcd for C₁₅H₁₁N₃SCl [(M + H)⁺], 300.0362; found, 300.0356.

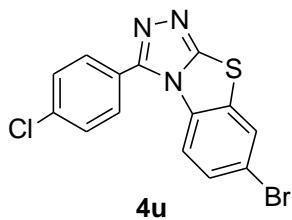
7-Bromo-3-phenylbenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4t)



White powder; Mp 224-225 °C; **IR** (KBr) ν : 3090, 1526, 1480, 828, 765, 716, 698, 622

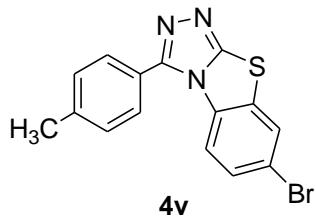
cm^{-1} ; **1H NMR** (CDCl_3 , 500 MHz): δ = 7.85 (d, J = 8.0 Hz, 2H, ArH), 7.78-7.76 (m, 2H, ArH), 7.62-7.60 (m, 3H, ArH), 7.45 (dd, J = 1.4, 8.8 Hz, 1H, ArH), 7.39 (d, J = 8.8 Hz, 1H, ArH); **13C NMR** (CDCl_3 , 125 MHz): δ = 134.7, 131.0, 129.7, 129.2, 127.3, 126.9, 119.3, 115.5; **HRMS** (ESI-TOF $^+$): m/z calcd for $\text{C}_{14}\text{H}_9\text{N}_3\text{SBr}$ [(M + H) $^+$], 329.9701; found, 329.9715.

7-Bromo-3-(4-chlorophenyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4u)



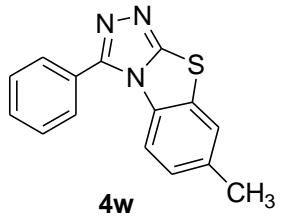
Brown powder; Mp 297-298 °C; **IR** (KBr) ν : 3064, 1726, 1602, 1485, 862, 842, 775, 669 cm^{-1} ; **1H NMR** ($\text{DMSO}-d_6$, 500 MHz): δ = 8.38 (s, 1H, ArH), 7.85 (d, J = 8.0 Hz, 2H, ArH), 7.72 (d, J = 8.0 Hz, 2H, ArH), 7.61 (d, J = 8.6 Hz, 1H, ArH), 7.32 (d, J = 8.7 Hz, 1H, ArH); **13C NMR** (CDCl_3 , 125 MHz): δ = 137.4, 134.6, 130.3, 129.8, 129.6, 128.9, 127.6, 125.1, 119.5, 115.3; **HRMS** (ESI-TOF $^+$): m/z calcd for $\text{C}_{14}\text{H}_9\text{N}_3\text{SBr}$ [(M + H) $^+$], 363.9311; found, 363.9320.

7-Bromo-3-(*p*-tolyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4v)



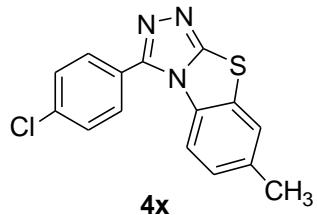
Brown powder; Mp 254-255 °C; **IR** (KBr) ν : 3098, 2921, 2852, 1724, 1484, 848, 829, 816, 771 cm^{-1} ; **1H NMR** (CDCl_3 , 500 MHz): δ = 7.83 (d, J = 1.6 Hz, 1H, ArH), 7.65 (d, J = 8.0 Hz, 2H, ArH), 7.45-7.43 (m, 1H, ArH), 7.42-7.41 (m, 2H, ArH), 7.40-7.39 (m, 1H, ArH), 2.50 (s, 3H, CH_3); **13C NMR** (CDCl_3 , 125 MHz): δ = 141.3, 134.5, 129.9, 129.5, 129.0, 128.9, 127.3, 123.5, 119.2, 115.3, 21.6; **HRMS** (ESI-TOF $^+$): m/z calcd for $\text{C}_{15}\text{H}_{11}\text{N}_3\text{SBr}$ [(M + H) $^+$], 343.9857; found, 343.9846.

7-Methyl-3-phenylbenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4w)



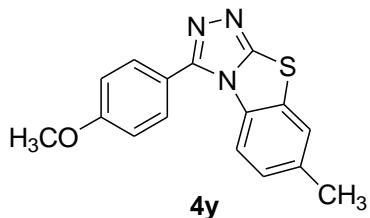
White powder; Mp 180-181 °C; **IR** (KBr) ν : 3025, 2920, 2851, 1636, 1584, 1493, 1385, 813, 762, 694 cm⁻¹; **¹H NMR** (CDCl₃, 500 MHz): δ = 7.80–7.79 (m, 2H, ArH), 7.61–7.59 (m, 3H, ArH), 7.50 (s, 1H, ArH), 7.42 (d, J = 8.5 Hz, 1H, ArH), 7.12 (d, J = 8.5 Hz, 1H, ArH), 2.45 (s, 3H, CH₃); **¹³C NMR** (CDCl₃, 125 MHz): δ = 136.7, 132.6, 130.6, 129.1, 128.9, 127.9, 127.2, 126.9, 124.8, 113.9, 21.3; **HRMS** (ESI-TOF⁺): *m/z* calcd for C₁₅H₁₂N₃S [(M + H)⁺], 266.0752; found, 266.0763.

3-(4-Chlorophenyl)-7-methylbenzo[4,5]thiazolo[2,3-c][1,2,4]triazole (4x)



Gray powder; Mp 222-223 °C; **IR** (KBr) ν : 3098, 3078, 2920, 2853, 1604, 1493, 1383, 827, 723, 698 cm⁻¹; **¹H NMR** (CDCl₃, 500 MHz): δ = 7.75 (d, J = 8.4 Hz, 2H, ArH), 7.58 (d, J = 8.5 Hz, 2H, ArH), 7.51 (s, 1H, ArH), 7.39 (d, J = 8.4 Hz, 1H, ArH), 7.14 (d, J = 8.3 Hz, 1H, ArH), 2.46 (s, 3H, CH₃); **¹³C NMR** (CDCl₃, 125 MHz): δ = 136.9 (J = 8.3 Hz), 136.8, 132.7, 130.4, 129.4, 127.8, 127.3, 125.6, 124.9, 113.8, 21.3; **HRMS** (ESI-TOF⁺): *m/z* calcd for C₁₅H₁₁N₃SCl [(M + H)⁺], 300.0362; found, 300.0375.

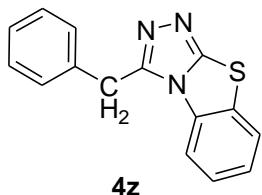
3-(4-Methoxyphenyl)-7-methylbenzo[4,5]thiazolo[2,3-c][1,2,4]triazole (4y)



White powder; Mp 161-162 °C; **IR** (KBr) ν : 3055, 2921, 2850, 1615, 1494, 1383, 840, 805, 731 cm⁻¹; **¹H NMR** (CDCl₃, 500 MHz): δ = 7.72 (d, J = 7.5 Hz, 2H, ArH), 7.48 (s,

1H, ArH), 7.42 (d, J = 8.0 Hz, 1H, ArH), 7.12 (d, J = 6.7 Hz, 3H, ArH), 3.90 (s, 3H, OCH₃), 2.45 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 125 MHz): δ = 161.4, 136.5, 132.7, 130.6, 128.0, 127.2, 124.8, 119.2, 114.4, 113.9, 55.5, 21.3; HRMS (ESI-TOF⁺): *m/z* calcd for C₁₆H₁₄N₃OS [(M + H)⁺], 296.0858; found, 298.0849.

3-Benzylbenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (4z)

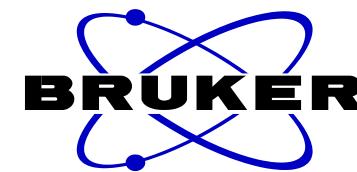
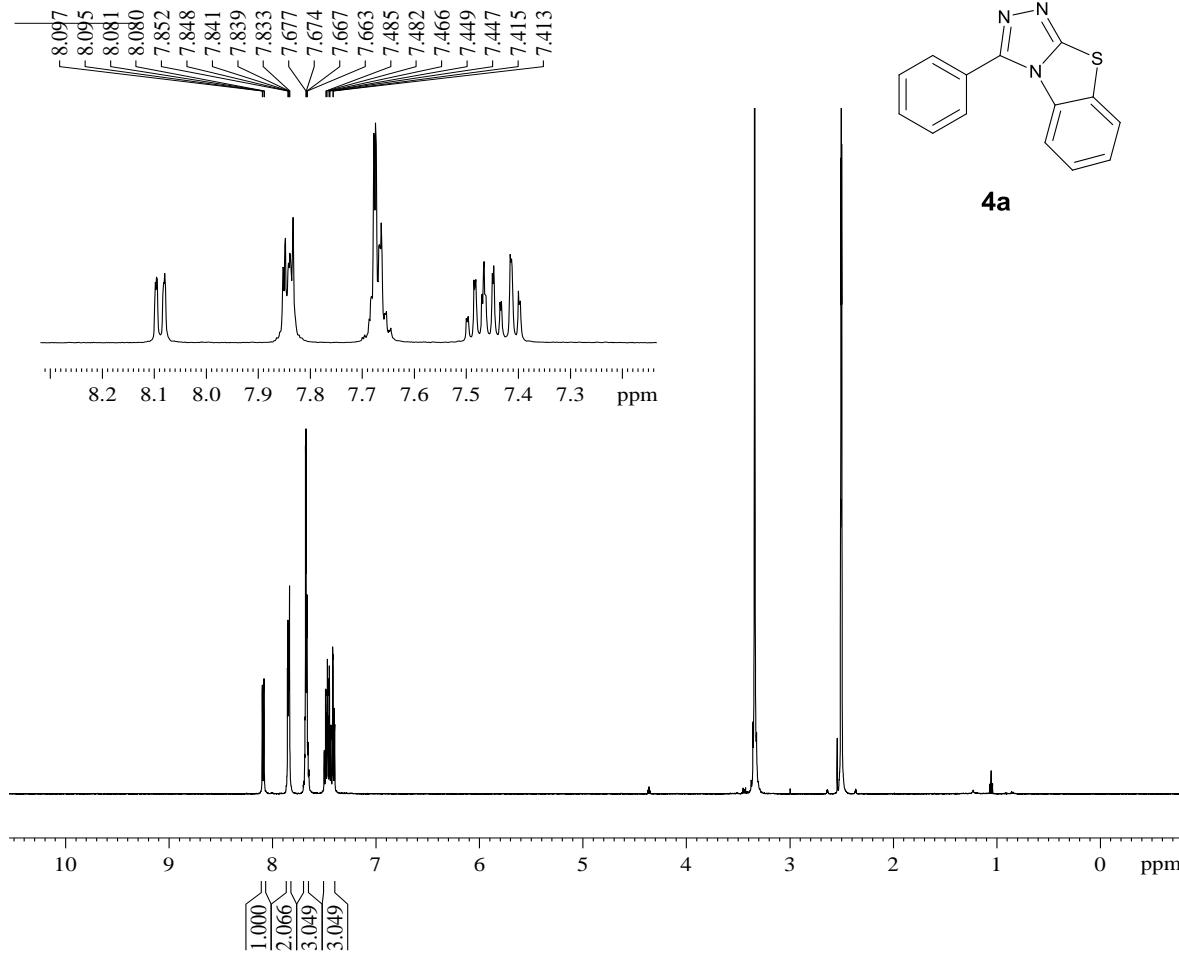


Cyan powder; Mp 170-171 °C; IR (KBr) ν : 3059, 2925, 1632, 1600, 1489, 748, 727, 681 cm⁻¹; ¹H NMR (CDCl₃, 500 MHz): δ = 7.64 (d, J = 6.4 Hz, 1H, ArH), 7.42 (d, J = 6.3 Hz, 1H, ArH), 7.34-7.31 (m, 4H, ArH), 7.28-7.26 (m, 3H, ArH), 4.65 (s, 2H, CH₂); ¹³C NMR (CDCl₃, 125 MHz): δ = 134.5, 132.4, 129.1, 128.1, 127.4, 126.6, 126.0, 124.6, 114.1, 32.5; HRMS (ESI-TOF⁺): *m/z* calcd for C₁₅H₁₂N₃S [(M + H)⁺], 266.0752; found, 266.0741.

References

1. G. Jayanthi, S. Muthusamy, R. Paramasivam, V. T. Ramakrishnan, N. Ramasamy, P. Ramamurthy, *J. Org. Chem.*, 1997, **62**, 5766-5770.

¹H and ¹³C NMR spectra of compound 4



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PROCNO    1
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PULPROG  zg30
TD        32768
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FIDRES   0.305176 Hz
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DW        50.000 usec
DE        6.00 usec
TE        296.1 K
D1        2.0000000 sec
TD0        1

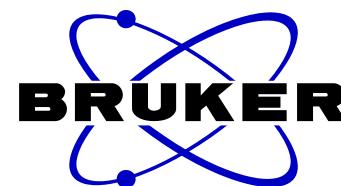
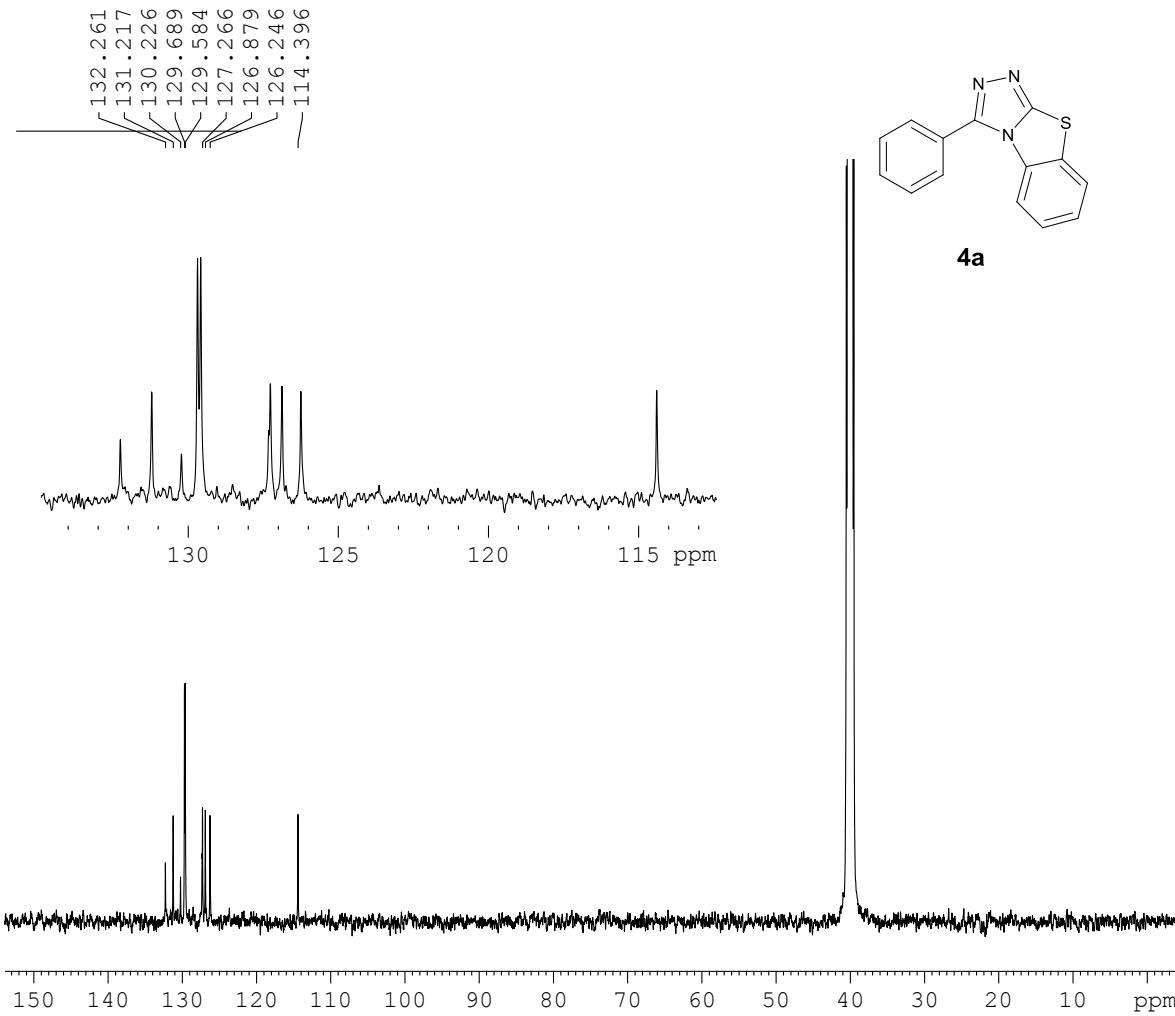
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PC        2.00

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LM-2-1B 13C 1D 2011 11 03



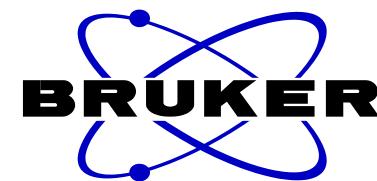
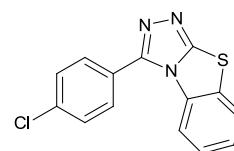
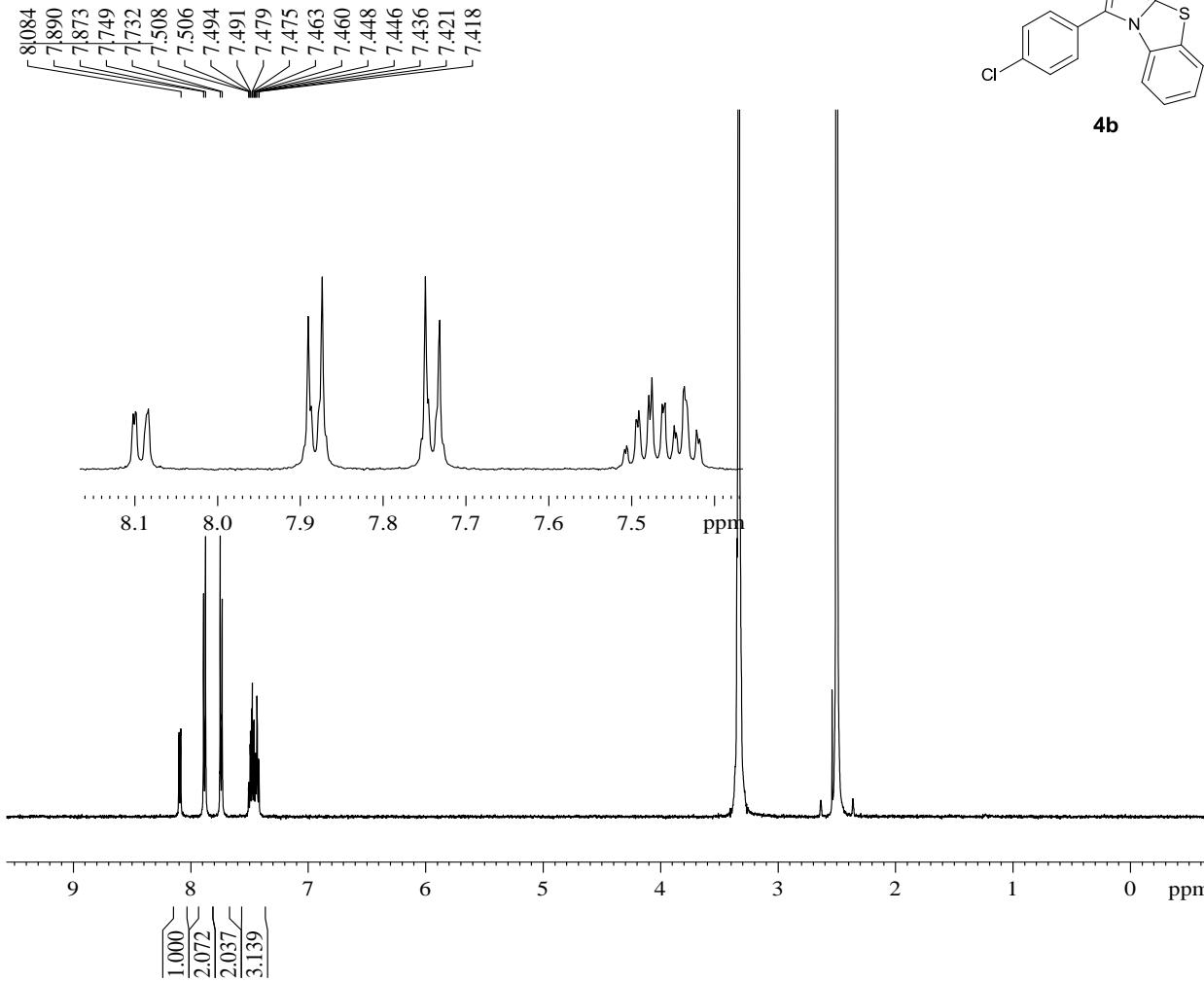
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SOLVENT DMSO
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FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 3640
DW 15.300 usec
DE 6.00 usec
TE 298.3 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999998 sec
TDO 1

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SFO1	125.7464750 MHz

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PL12	17.66 dB
PL13	17.66 dB
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SI	32768
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WDW	EM
SSB	0
LB	6.00 Hz
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EXPNO     1
PROCNO    1
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Time   19.59
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PROBHD  5 mm PABBO BB-
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TD      32768
SOLVENT  DMSO
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DS       1
SWH     10000.000 Hz
FIDRES  0.305176 Hz
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RG      575
DW      50.000 usec
DE      6.00 usec
TE      296.0 K
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TD0      1

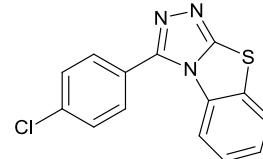
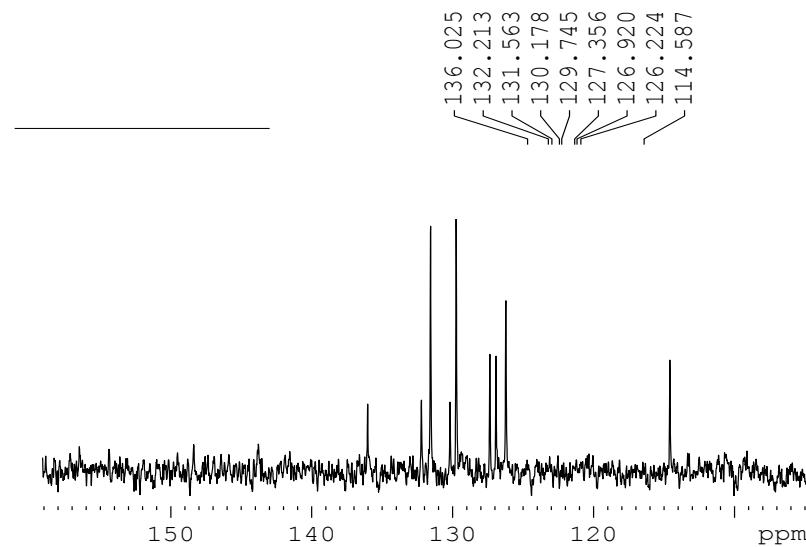
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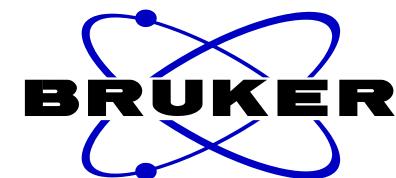
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LM-2-2B 13C 1D 2011 11 21



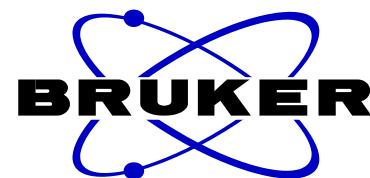
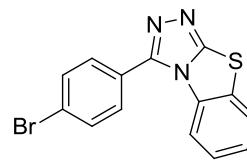
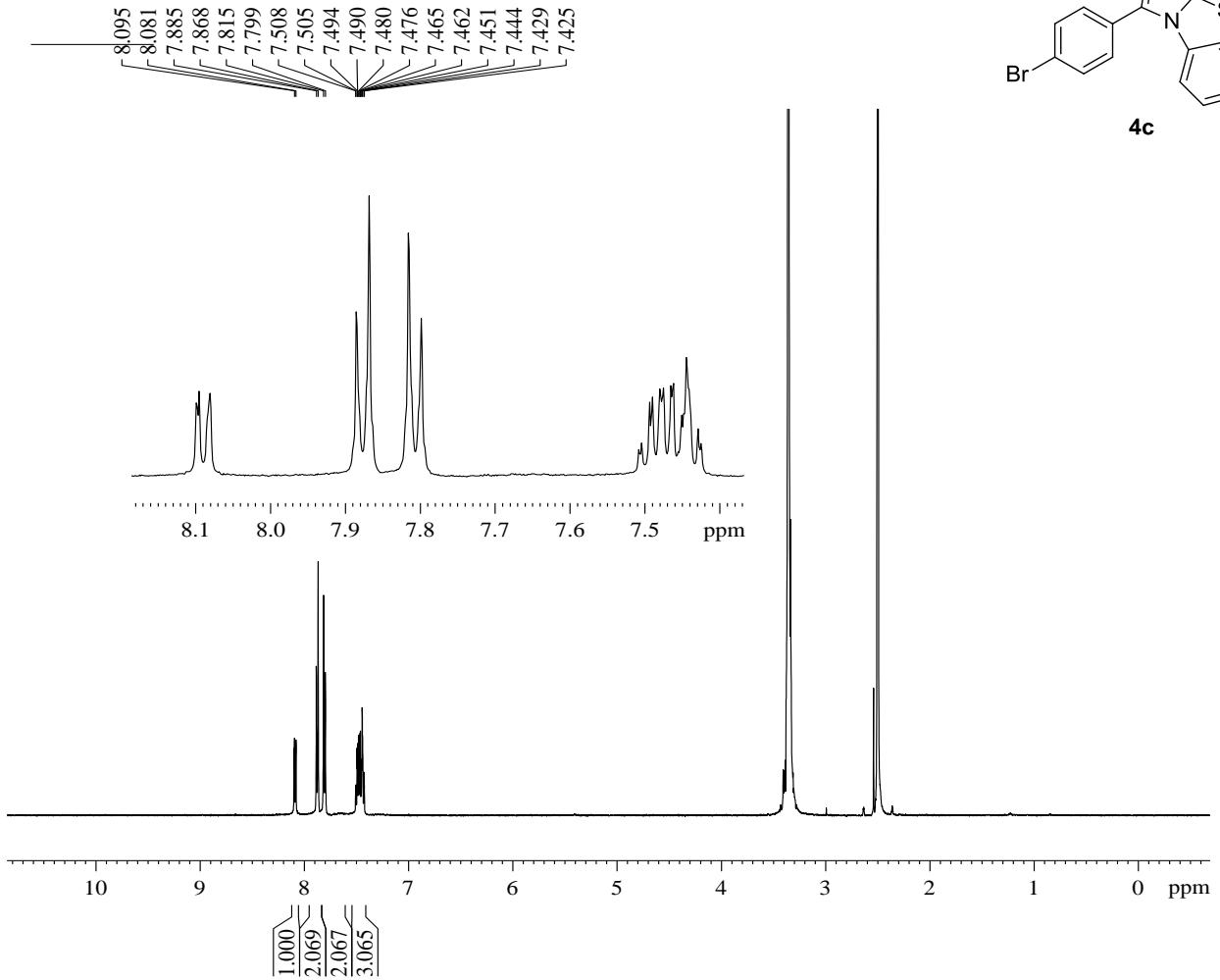
4b



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TD 65536
SOLVENT DMSO
NS 2167
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
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DW 15.300 usec
DE 6.00 usec
TE 295.3 K
D1 2.00000000 sec
d11 0.03000000 sec
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TDO 1

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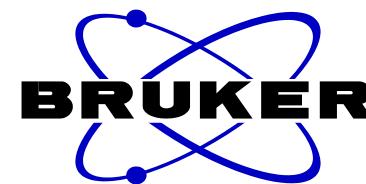
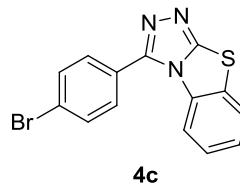
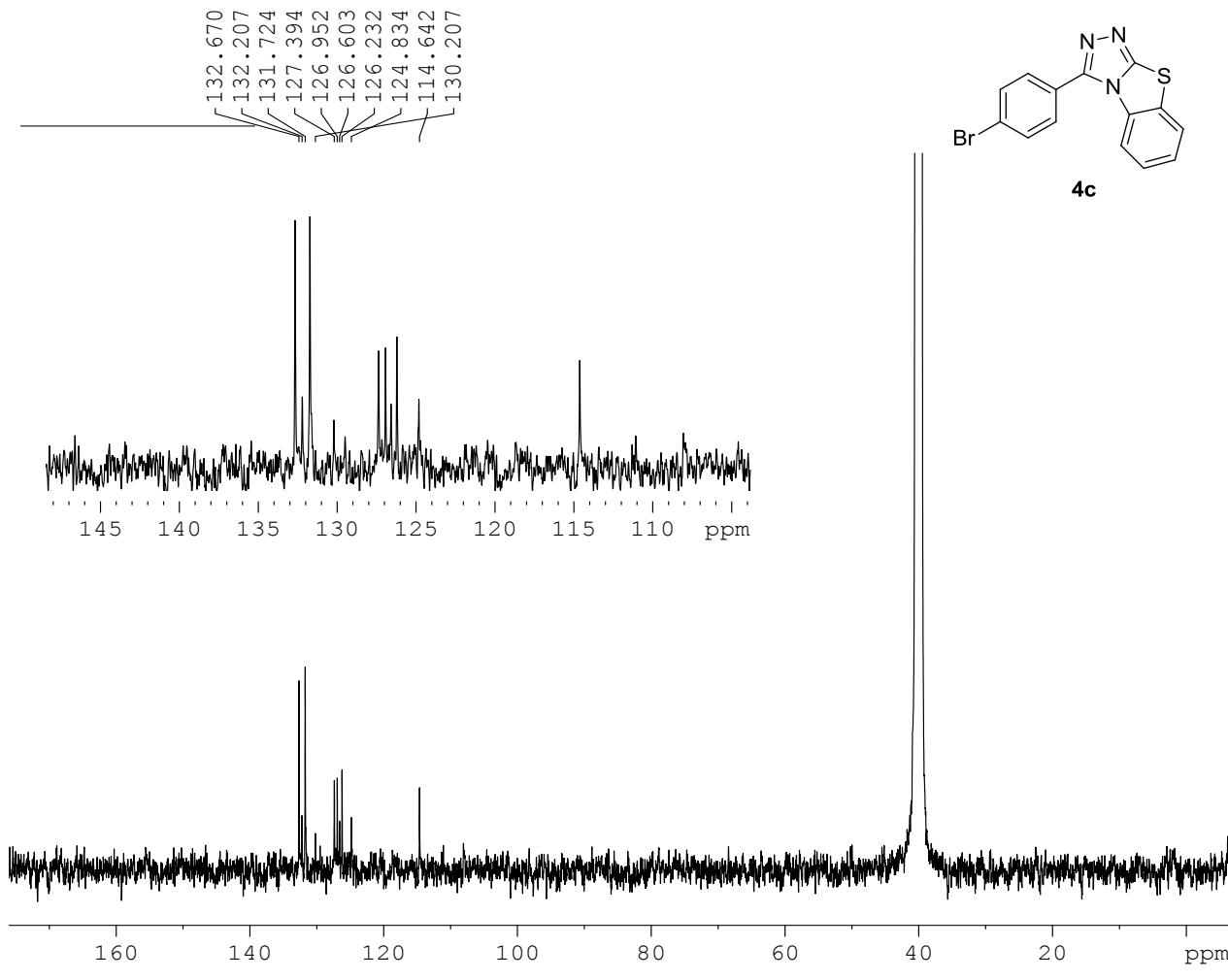
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SFO2 500.0355000 MHz
SI 32768
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SSB 0
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GB 0
PC 2.00



NAME Lm-3B
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 PROCNO 1
 Date_ 20111122
 Time 16.01
 INSTRUM av500
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
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 DS 1
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 RG 322
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 TD0 1

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 SFO1 500.0335010 MHz
 SI 16384
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LM-2-3B 13C 1D 2011 11 29



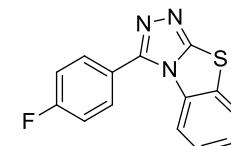
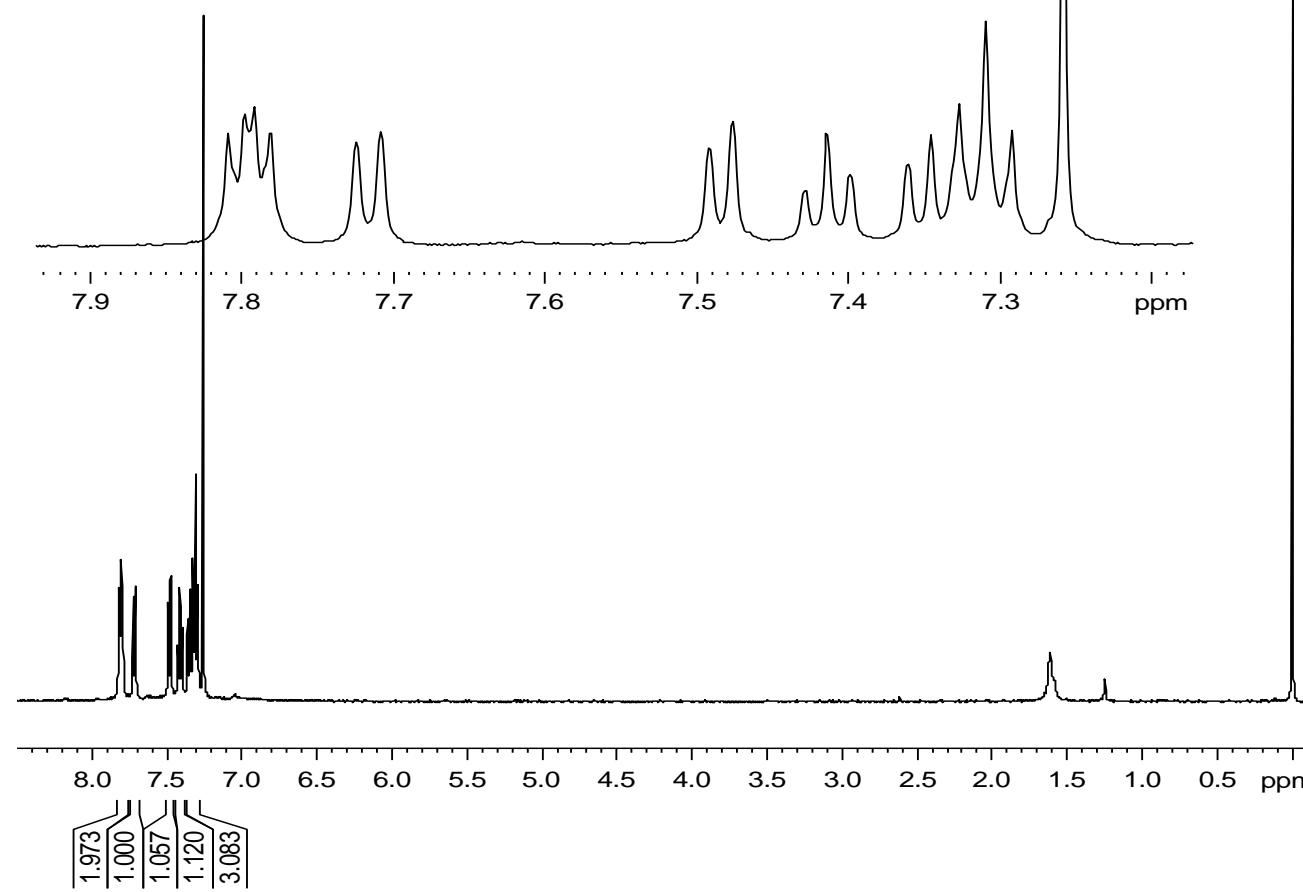
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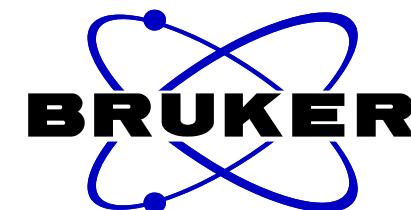
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—lm-2-7b 1H 2011 12 14

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4d

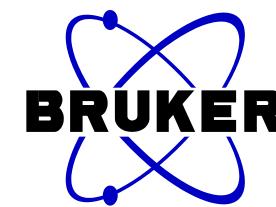
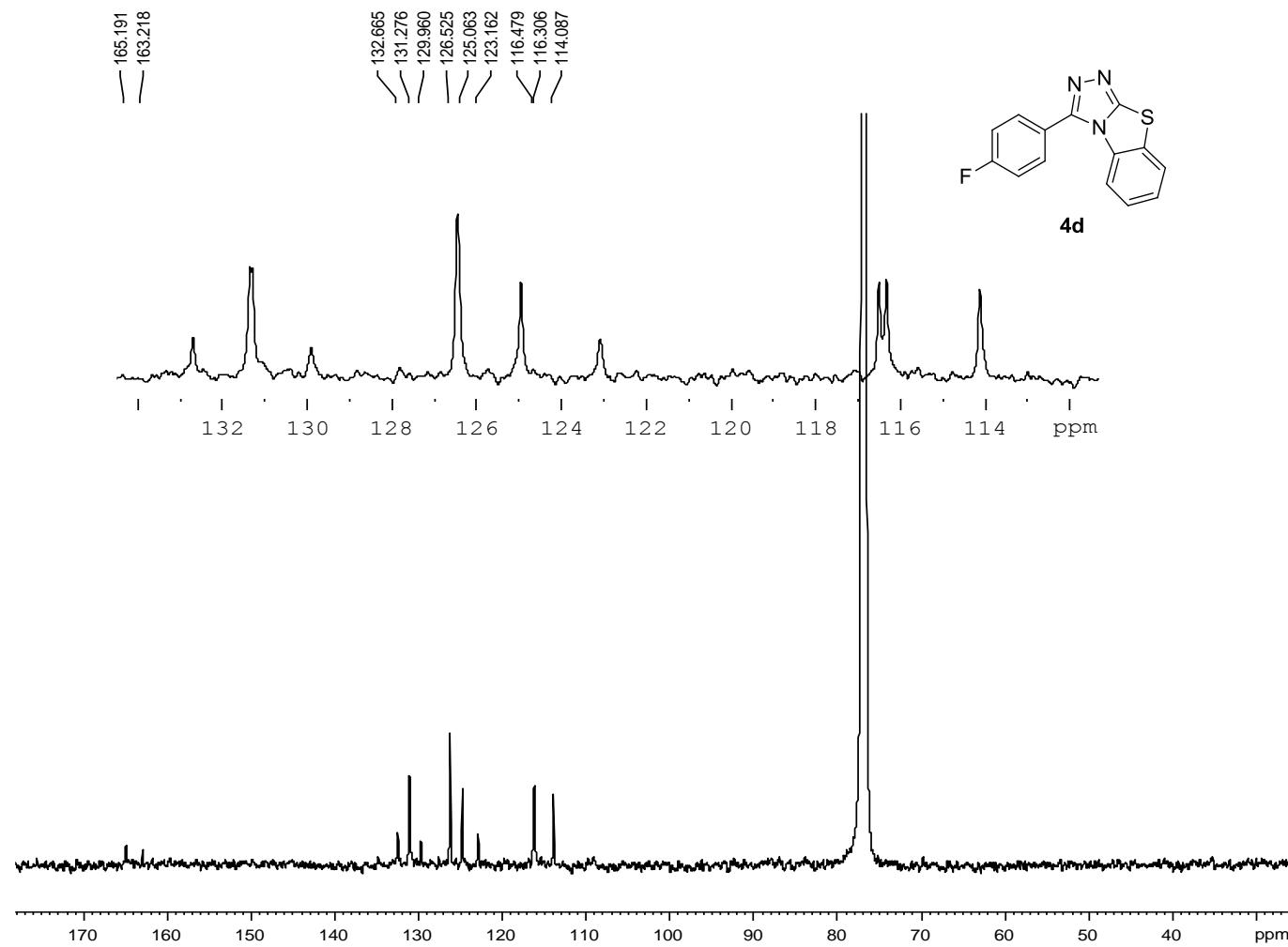


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RG 812
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D1 2.00000000 sec
TDO 1

===== CHANNEL f1 ======

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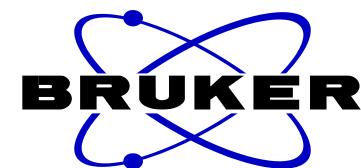
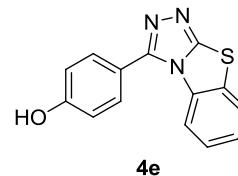
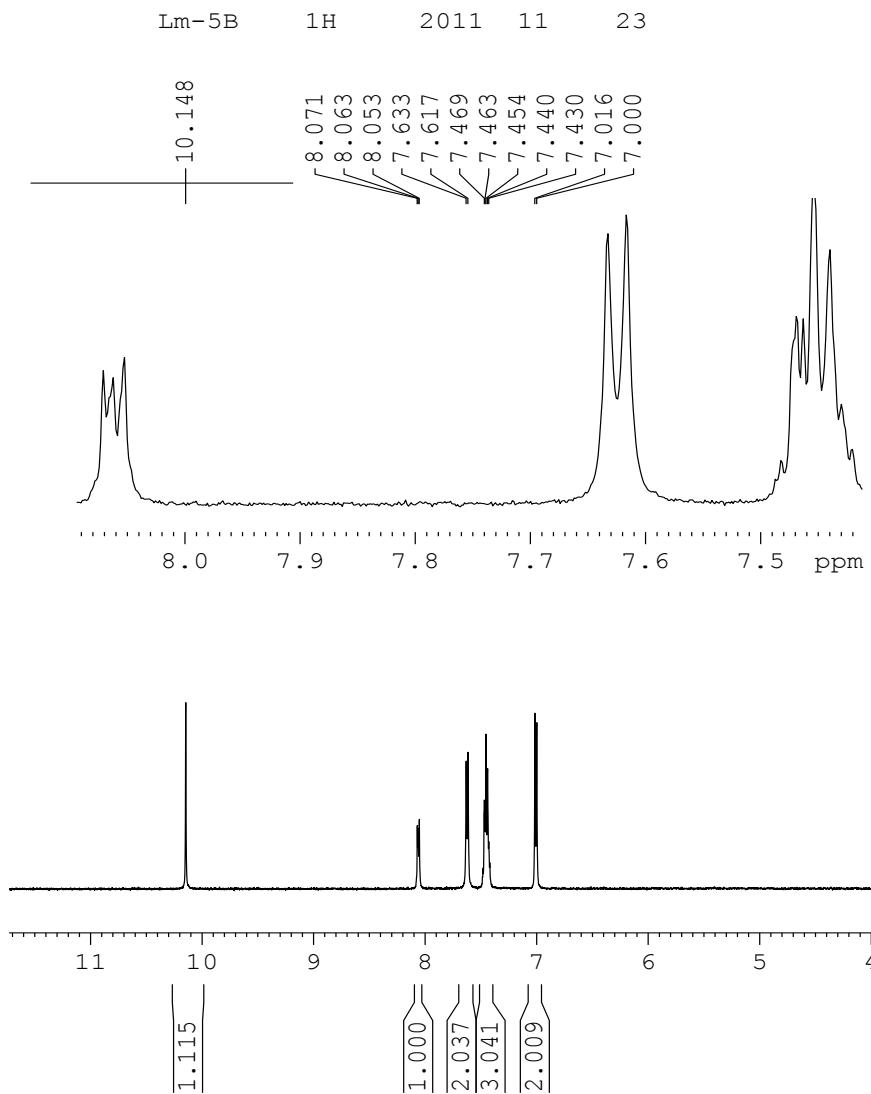
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TD 65536
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AQ 1.0027661 sec
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DW 15.300 usec
DE 6.00 usec
TE 294.5 K
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d11 0.03000000 sec
DELTA 1.8999999 sec
TDO 1

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SFO1 125.7464750 MHz

===== CHANNEL f2 =====
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PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326472 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 2 00

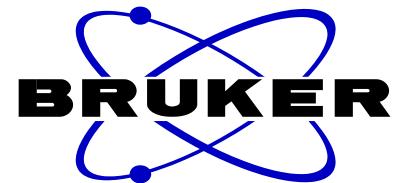
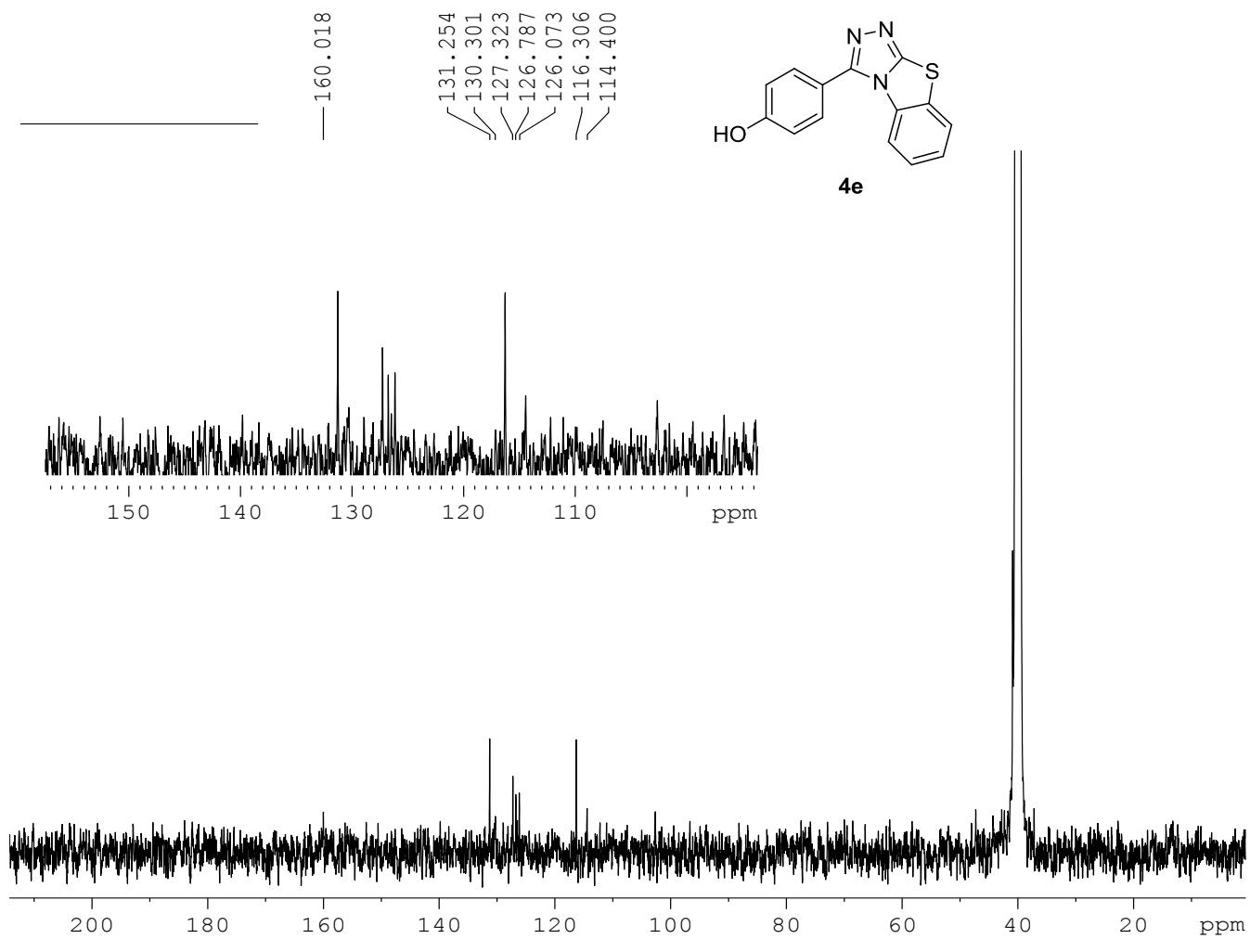


NAME	Lm-5B
EXPNO	1
PROCNO	1
Date	20111122
Time	16.10
INSTRUM	av500
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	8
DS	1
SWH	10000.000 Hz
FIDRES	0.305176 Hz
AQ	1.6385000 sec
RG	322
DW	50.000 usec
DE	6.00 usec
TE	294.8 K
D1	2.00000000 sec
TDO	1
===== CHANNEL f1 =====	
NUC1	1H
P1	13.50 usec
PL1	2.20 dB
SFO1	500.0335010 MHz
SI	16384
SF	500.0300015 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

LM-2-5B

13C 1D

2011 12 07



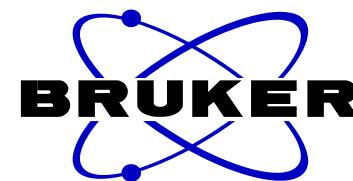
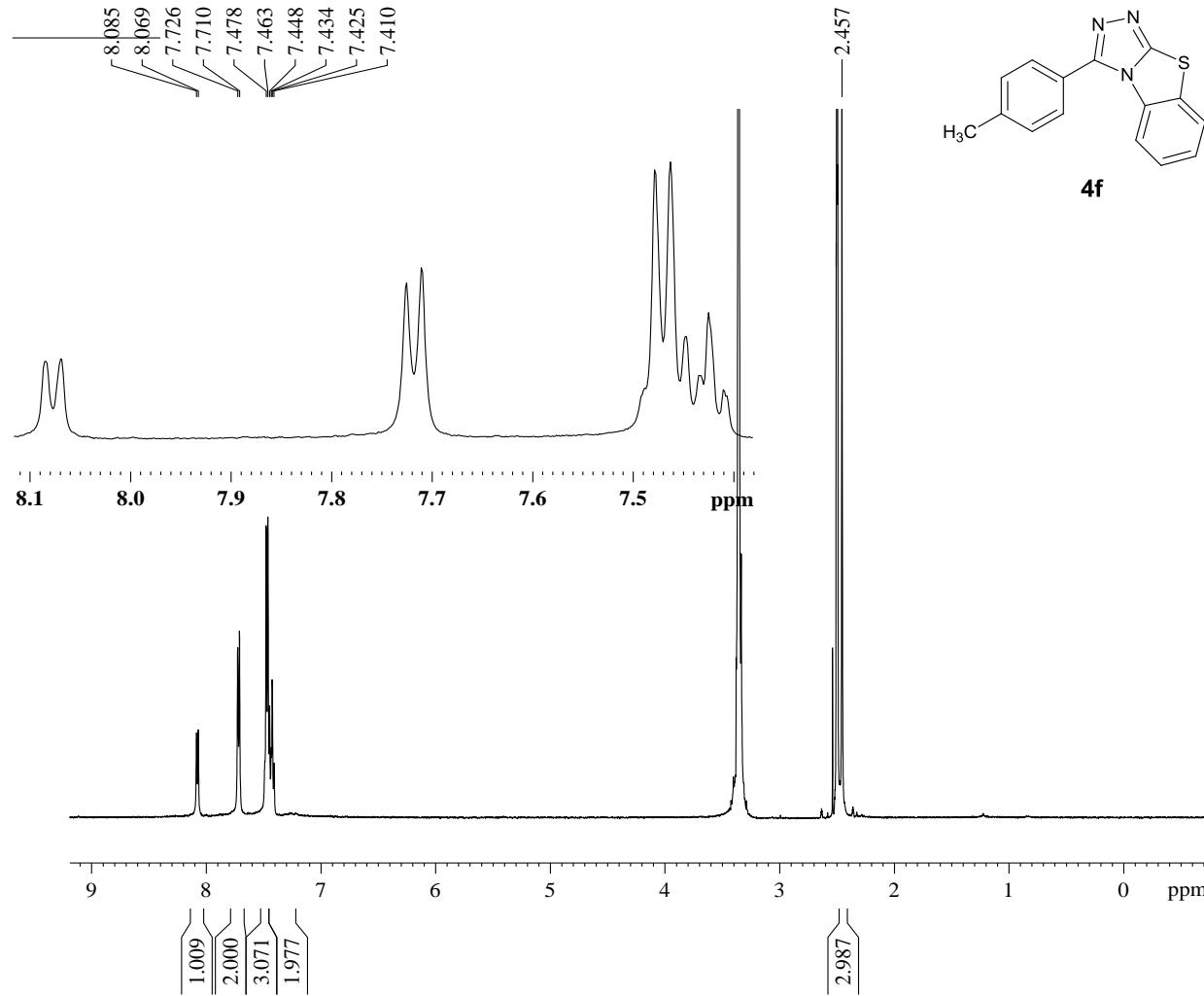
NAME LM-2-5B
 EXPNO 2
 PROCNO 1
 Date_ 2011207
 Time_ 13.58
 INSTRUM av500
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 932
 DS 2
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 18400
 DW 15.300 usec
 DE 6.00 usec
 TE 296.8 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 sec
 TDO 1

===== CHANNEL f1 =====

NUC1 13C
 P1 9.60 usec
 PL1 2.00 dB
 SFO1 125.7464750 MHz

===== CHANNEL f2 =====

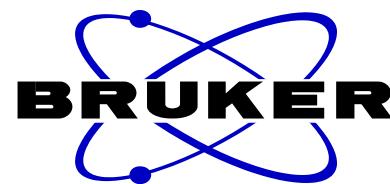
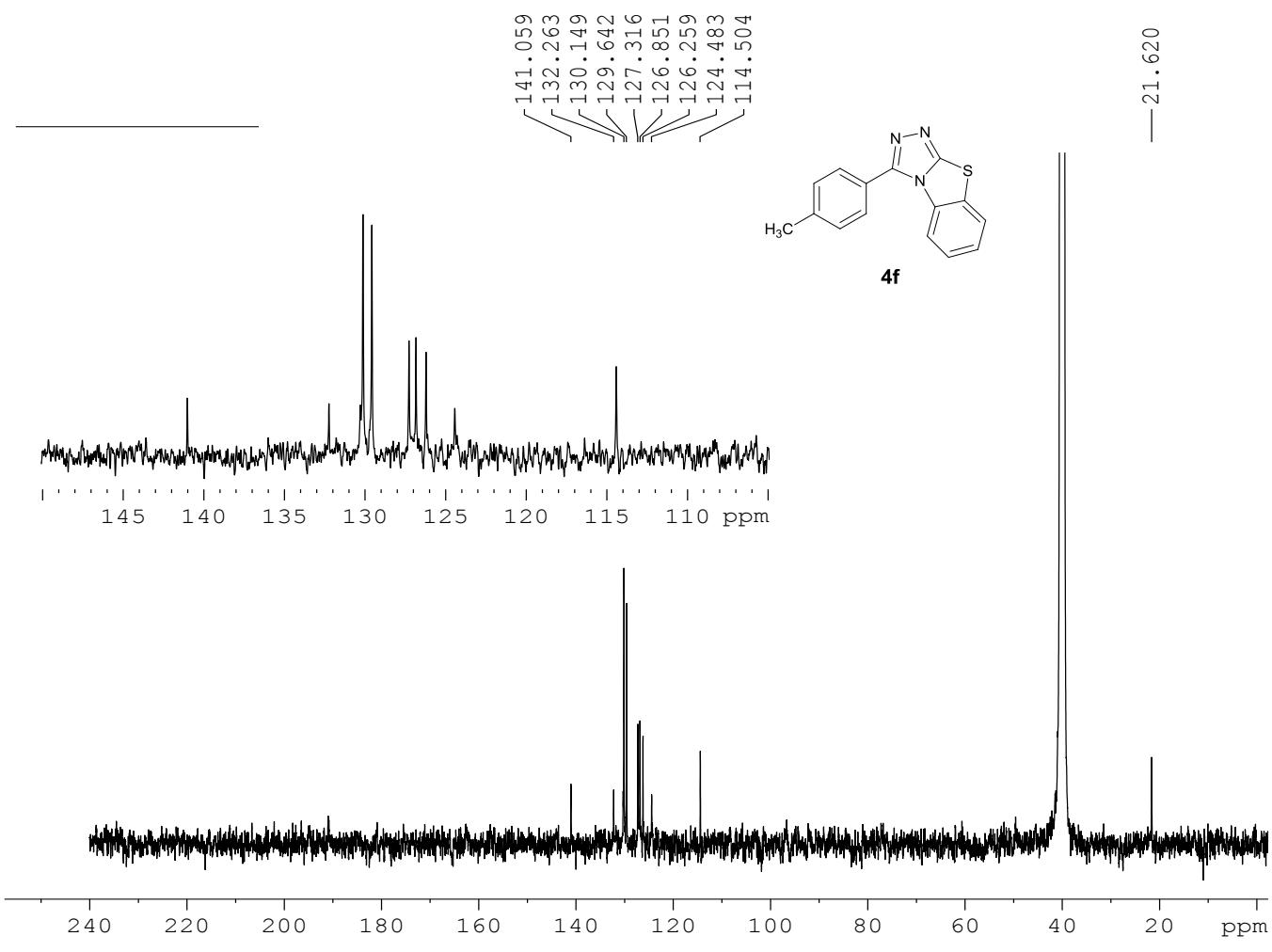
CPDPFG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.20 dB
 PL12 17.66 dB
 PL13 17.66 dB
 SFO2 500.0355000 MHz
 SI 32768
 SF 125.7326387 MHz
 WDW EM
 SSB 0
 LB 6.00 Hz
 GB 0
 PC 2.00



NAME Lm-4B
 EXPNO 1
 PROCNO 1
 Date 20111122
 Time 16.06
 INSTRUM av500
 PROBH 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 8
 DS 1
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6385000 sec
 RG 322
 DW 50.000 usec
 DE 6.00 usec
 TE 294.8 K
 D1 2.0000000 sec
 TD0 1

===== CHANNEL f1 ======
 NUC1 1H
 P1 13.50 usec
 PL1 2.20 dB
 SFO1 500.0335010 MHz
 SI 16384
 SF 500.0300015 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 2.00

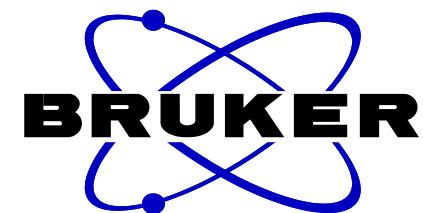
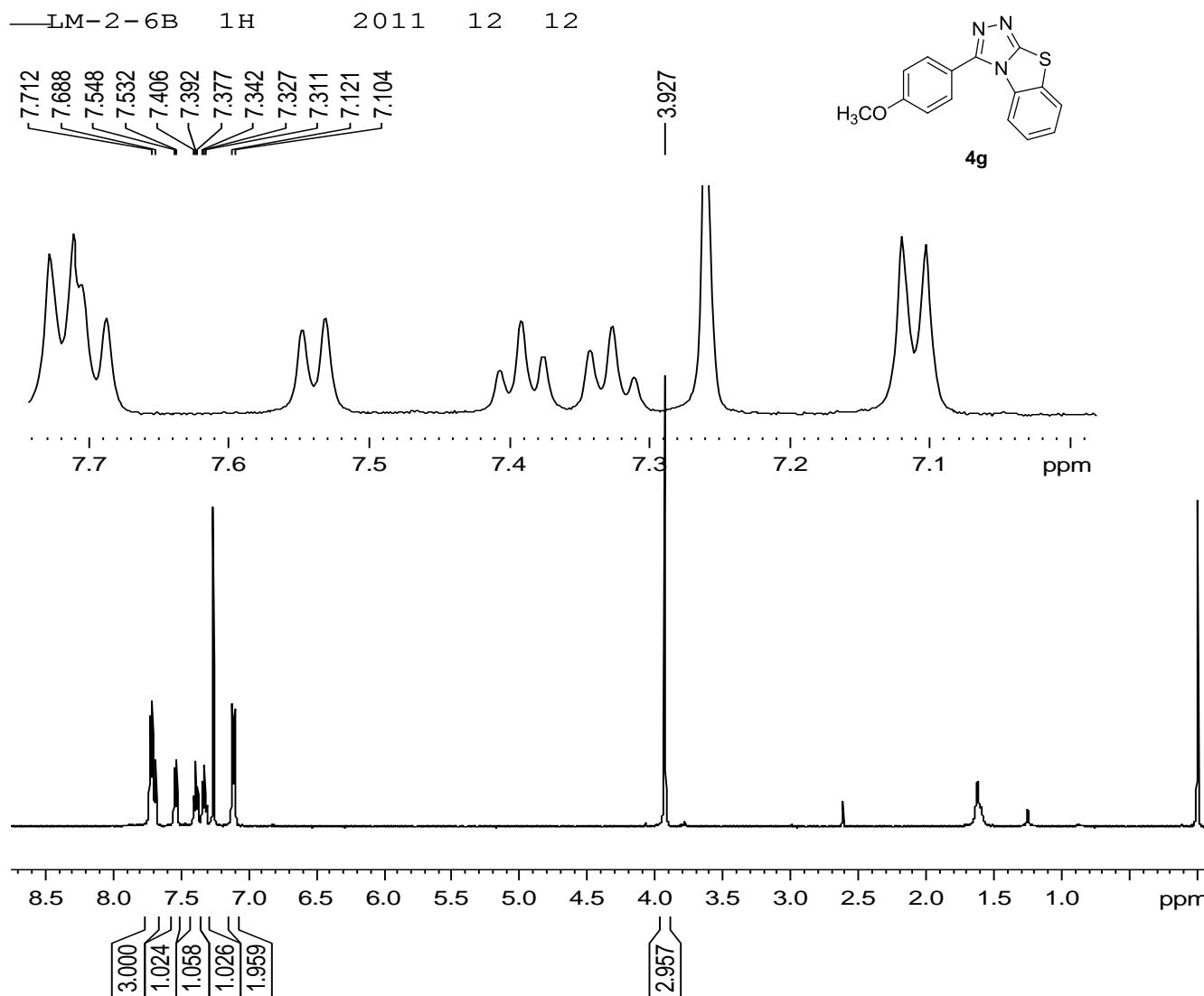
Lm-2-4B 13C 1D 2011 11 29



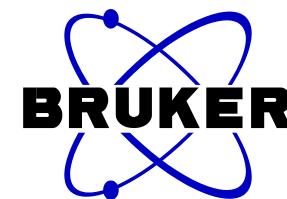
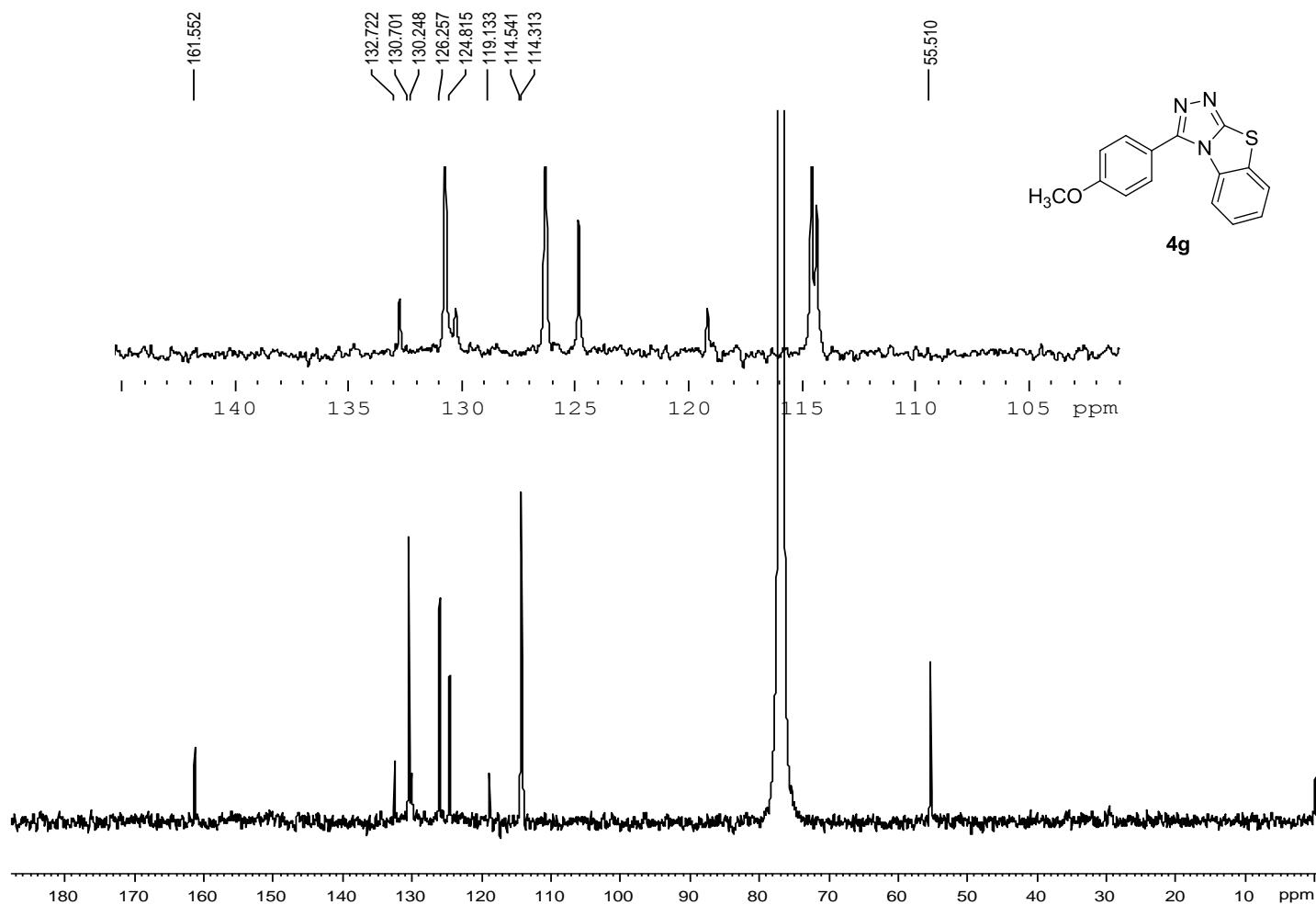
NAME Lm-2-4B
EXPNO 2
PROCNO 1
Date 20111129
Time 18.15
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1883
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 512
DW 15.300 usec
DE 6.00 usec
TE 297.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

===== CHANNEL f2 =====
CPDPG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.20 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326387 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 2.00



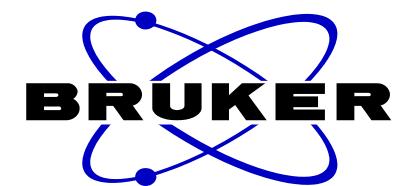
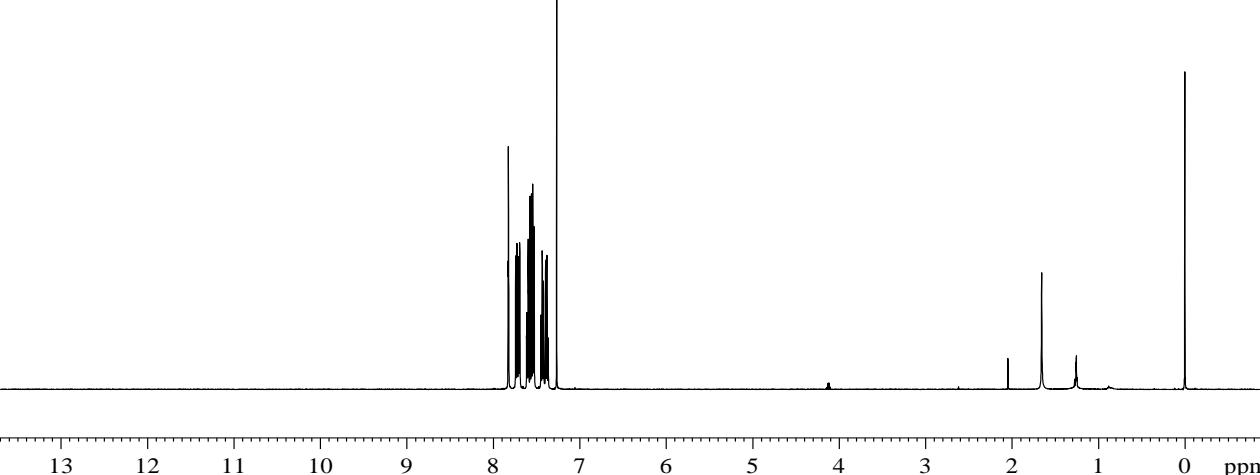
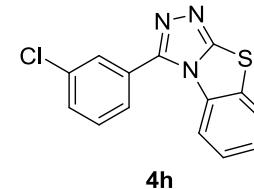
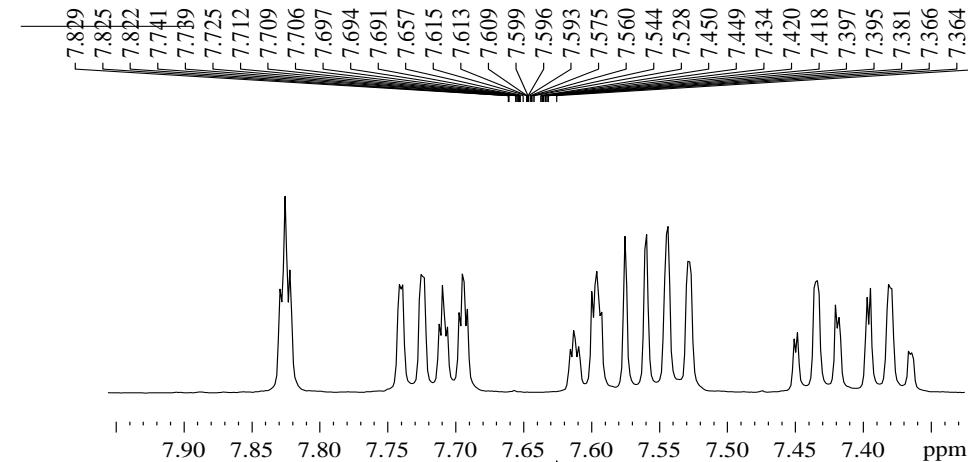
— Lm-2-BB 13C 1D 2011 12 14



NAME Lm-2-BB
EXPNO 2
PROCNO 1
Date_ 20111214
Time 21.57
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 11361
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 2050
DW 15.300 usec
DE 6.00 usec
TE 295.6 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.8999998 sec
TD0 1

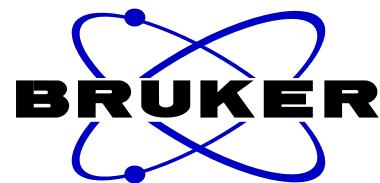
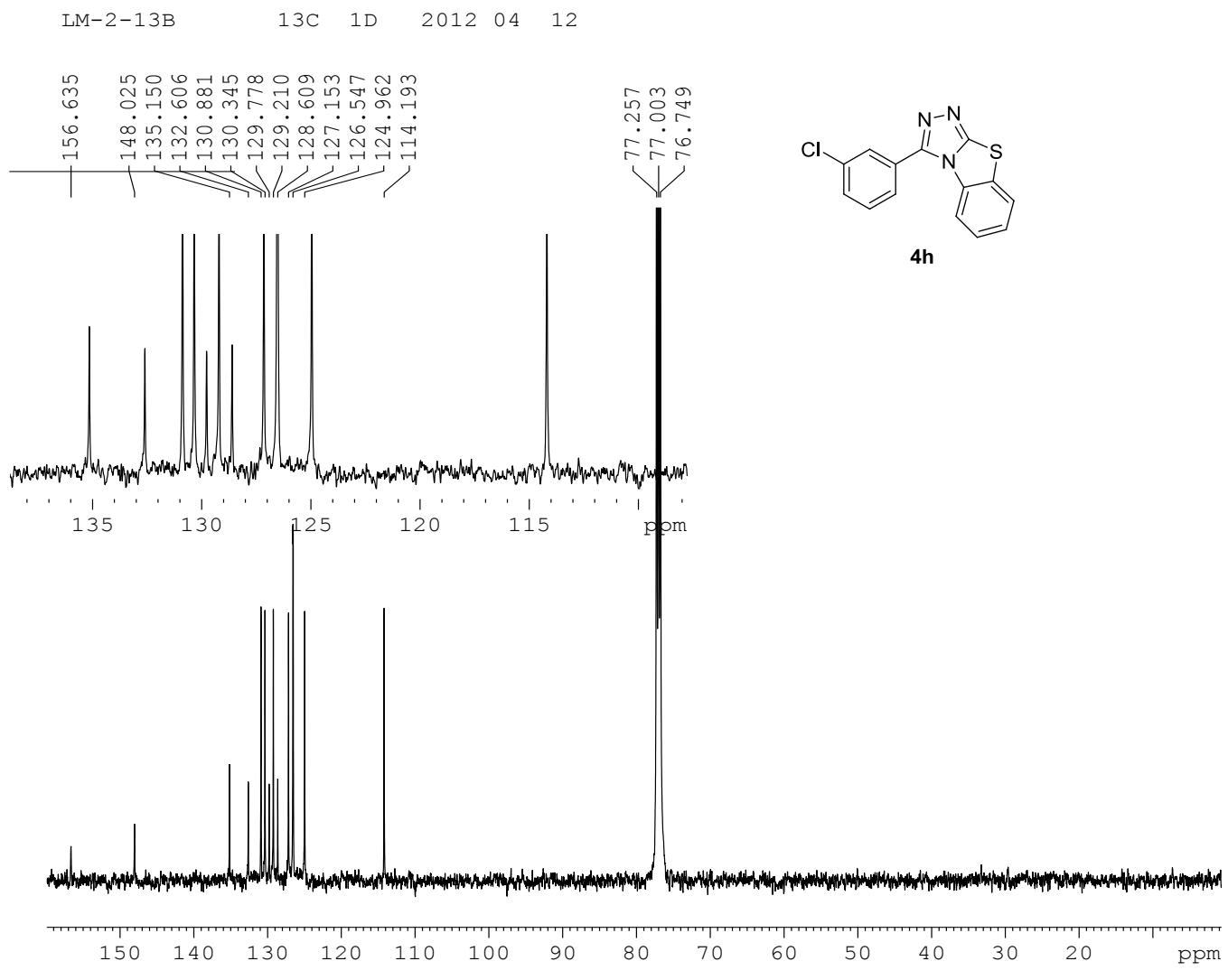
===== CHANNEL f1 =====
NUC1 ¹³C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

===== CHANNEL f2 =====
CPDPRG2 w_waltz16
NUC2 ¹H
PCPD2 80.00 usec
PL2 2.60 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326395 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 2.00



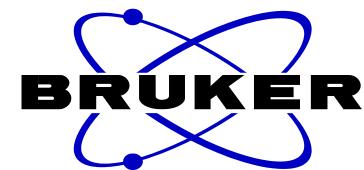
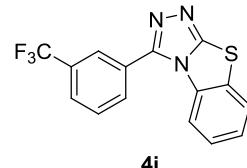
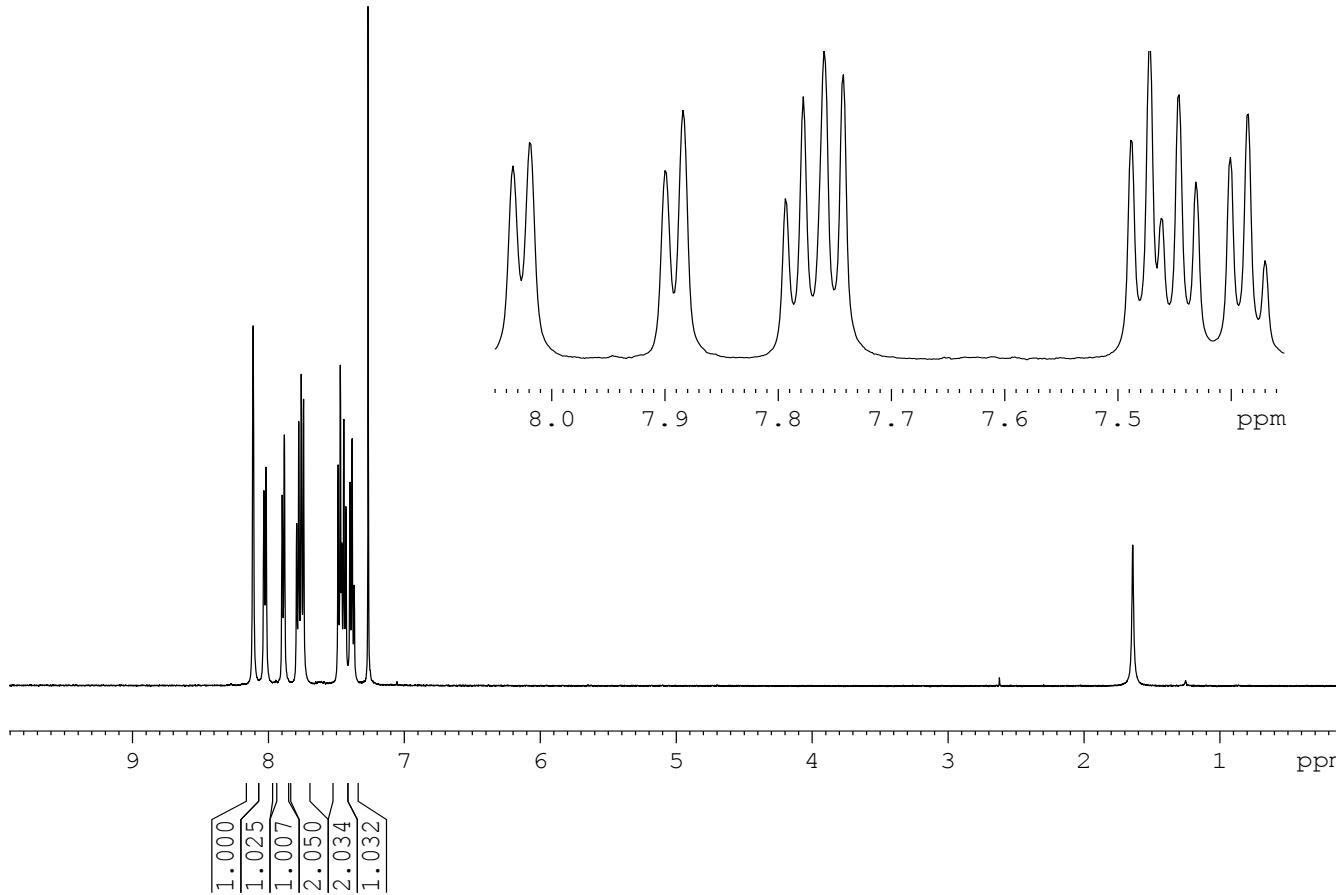
NAME LM-2-13B
 EXPNO 1
 PROCNO 1
 Date_ 20120411
 Time 21.56
 INSTRUM av500
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 8
 DS 1
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6385000 sec
 RG 645
 DW 50.000 usec
 DE 6.00 usec
 TE 297.8 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 ======
 NUC1 ¹H
 P1 13.50 usec
 PL1 2.20 dB
 SFO1 500.0335010 MHz
 SI 16384
 SF 500.0300064 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 2.00



LM-2-15B 1H 2012 04 12

8.114
8.034
8.019
7.899
7.884
7.793
7.778
7.759
7.743
7.488
7.472
7.461
7.446
7.431
7.401
7.385
7.370



NAME	LM-2-15B
EXPNO	1
PROCNO	1
Date	20120412
Time	10.14
INSTRUM	av500
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	CDCl ₃
NS	8
DS	1
SWH	10000.000 Hz
FIDRES	0.305176 Hz
AQ	1.6385000 sec
RG	645
DW	50.000 usec
DE	6.00 usec
TE	293.1 K
D1	2.00000000 sec
TDO	1

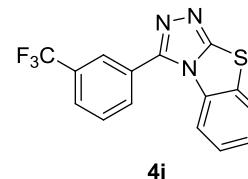
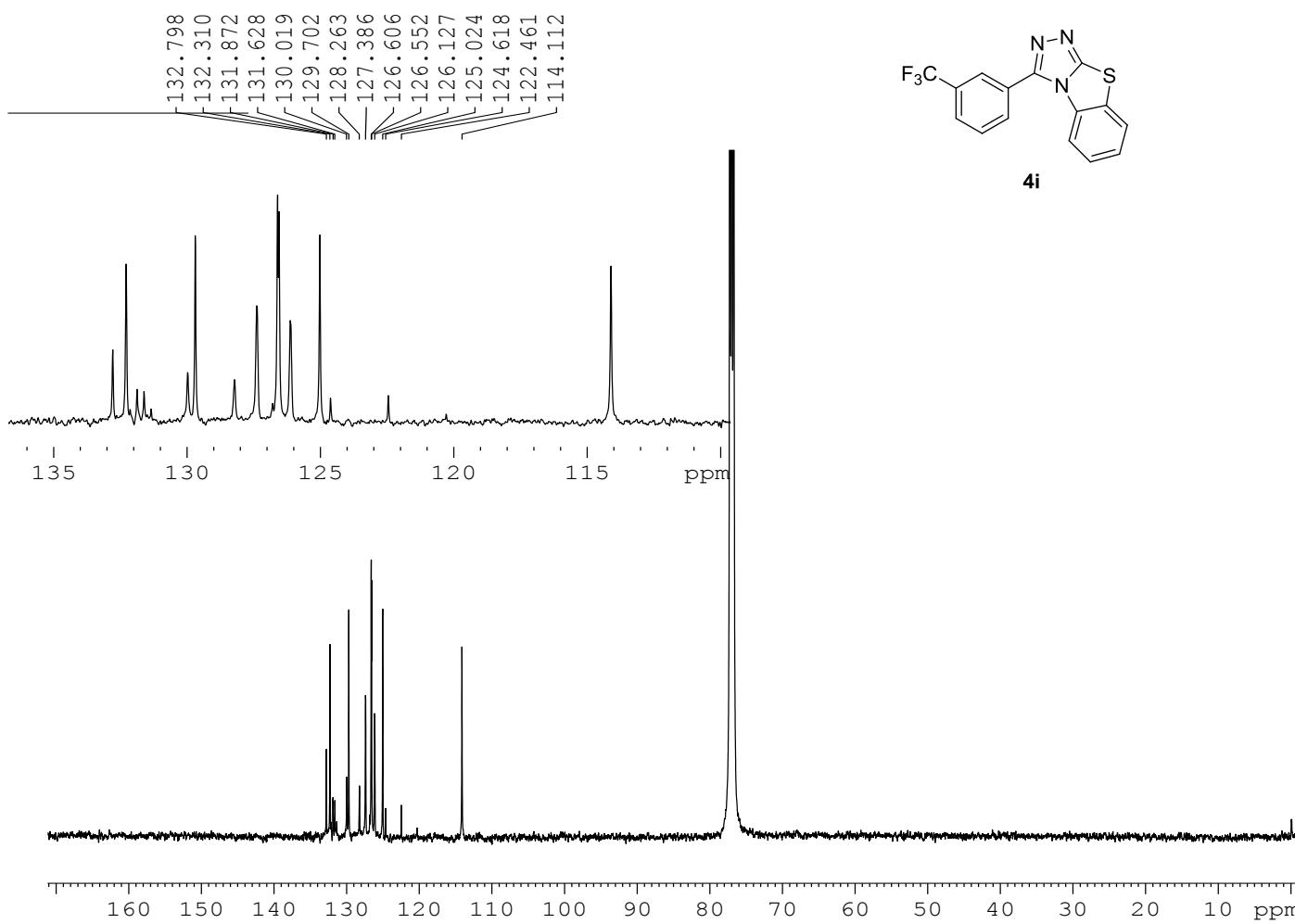
===== CHANNEL f1 =====

NUC1	1H
P1	13.50 usec
PL1	2.20 dB
SFO1	500.0335010 MHz
SI	16384
SF	500.0300064 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

LM-2-15B

13C 1D

2012 04 14



NAME LM-2-15B
 EXPNO 2
 PROCNO 1
 Date 20120415
 Time 6.58
 INSTRUM av500
 PROBHD 5 mm PABBO BB-
 PULPROG zgppg30
 TD 65536
 SOLVENT CDCl3
 NS 10716
 DS 2
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 812
 DW 15.300 usec
 DE 6.00 usec
 TE 298.1 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

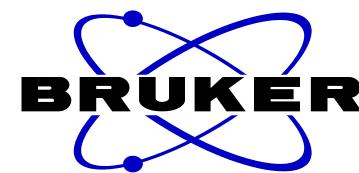
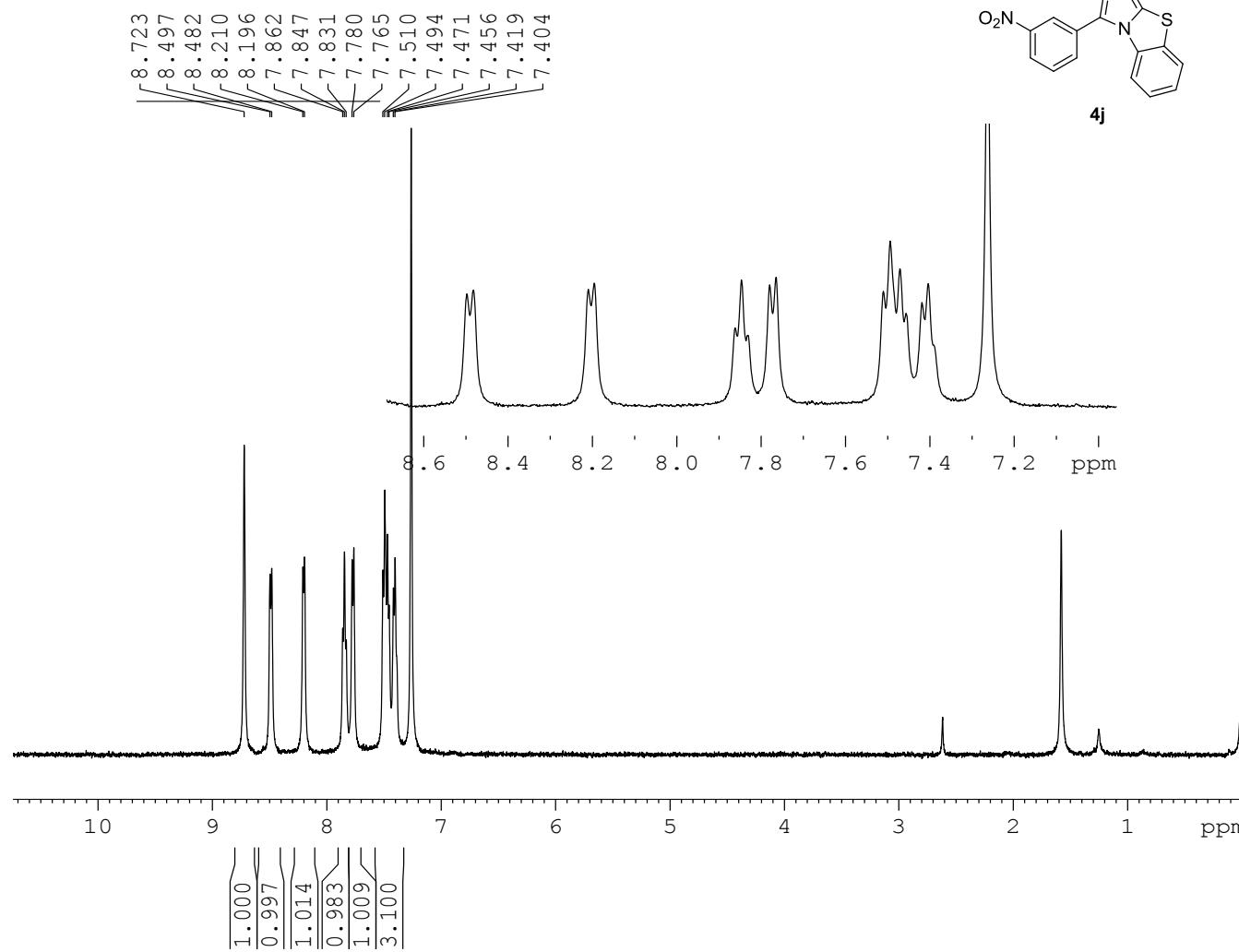
===== CHANNEL f1 =====

NUC1 13C
 P1 9.60 usec
 PL1 2.00 dB
 SFO1 125.7464750 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.60 dB
 PL12 17.66 dB
 PL13 17.66 dB
 SFO2 500.0355000 MHz
 SI 32768
 SF 125.7326482 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 2.00

LM-2-16B 1H 2012 04 17

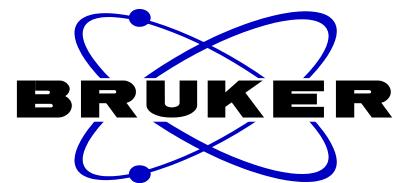
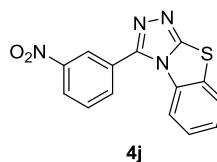
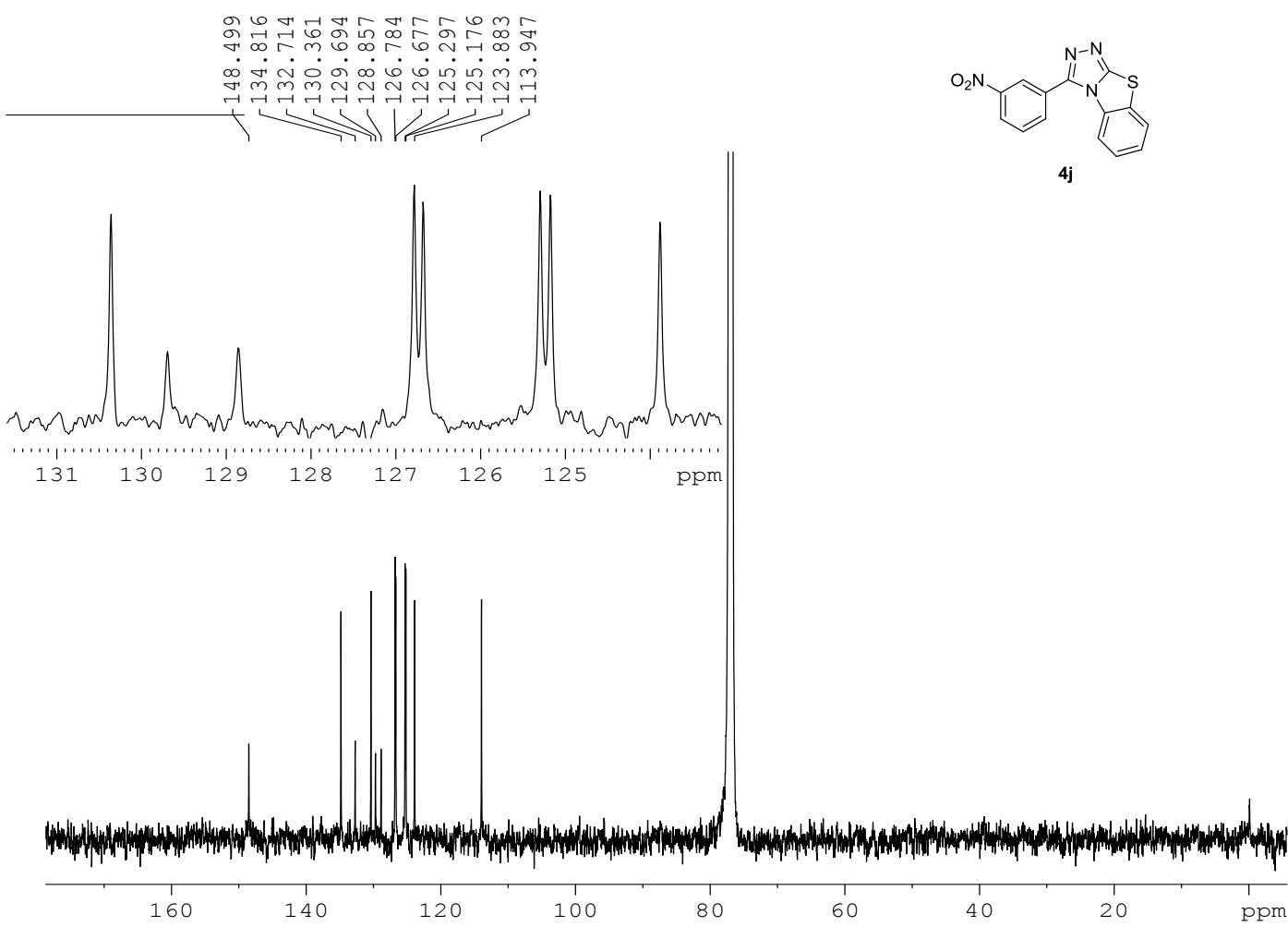


NAME LM-2-16B
EXPNO 1
PROCNO 1
Date_ 20120417
Time_ 16.53
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 8
DS 1
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6385000 sec
RG 645
DW 50.000 usec
DE 6.00 usec
TE 294.6 K
D1 2.000000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.50 usec
PL1 2.20 dB
SFO1 500.0335010 MHz
SI 16384
SF 500.0300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

LM-2-16B

13C 1D 2012 04 19



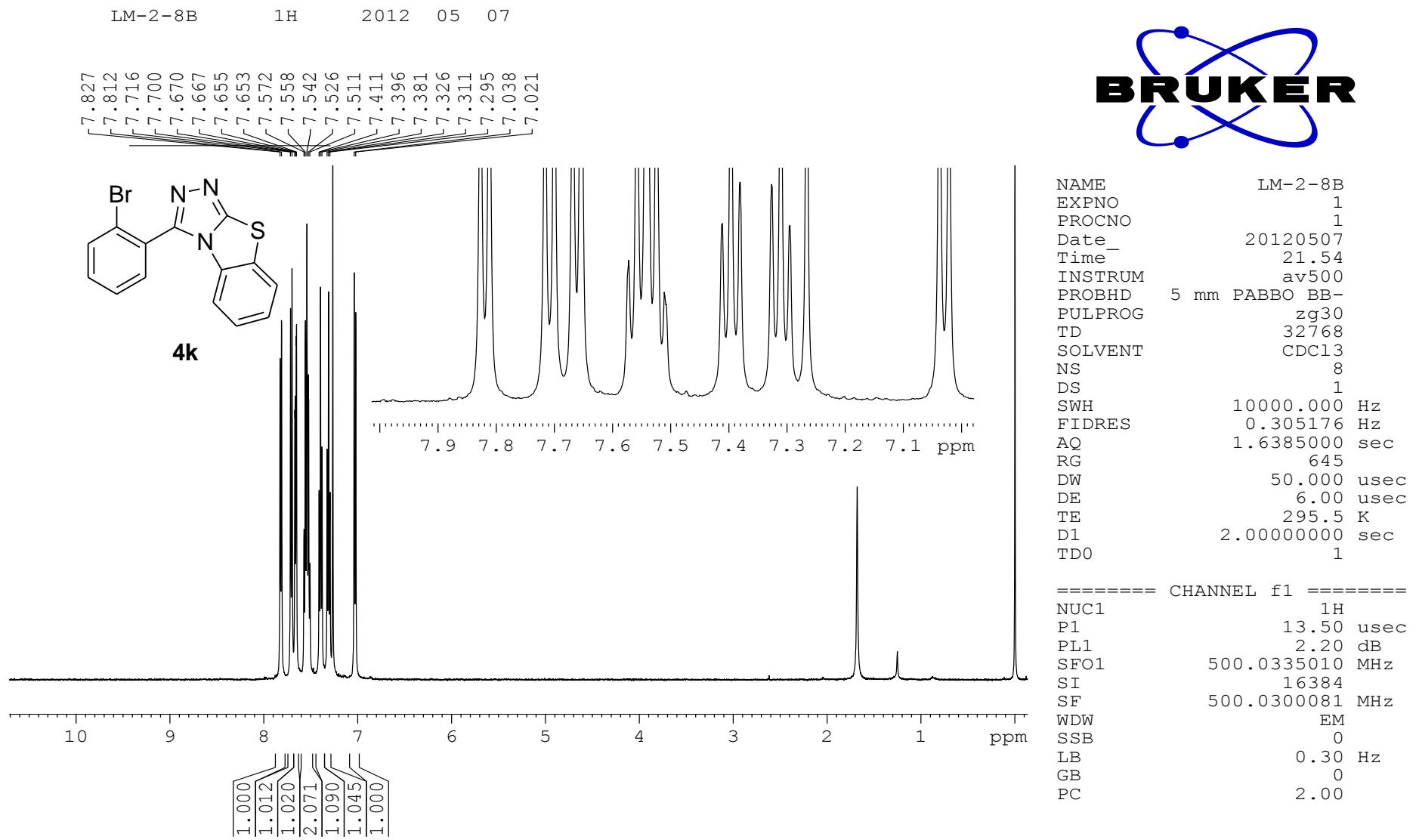
NAME LM-2-16B
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 PROCNO 1
 Date 20120419
 Time 11.24
 INSTRUM av500
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 4298
 DS 2
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 812
 DW 15.300 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====

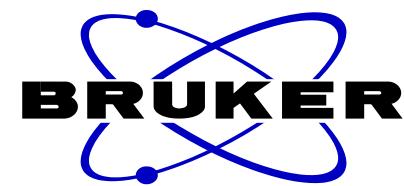
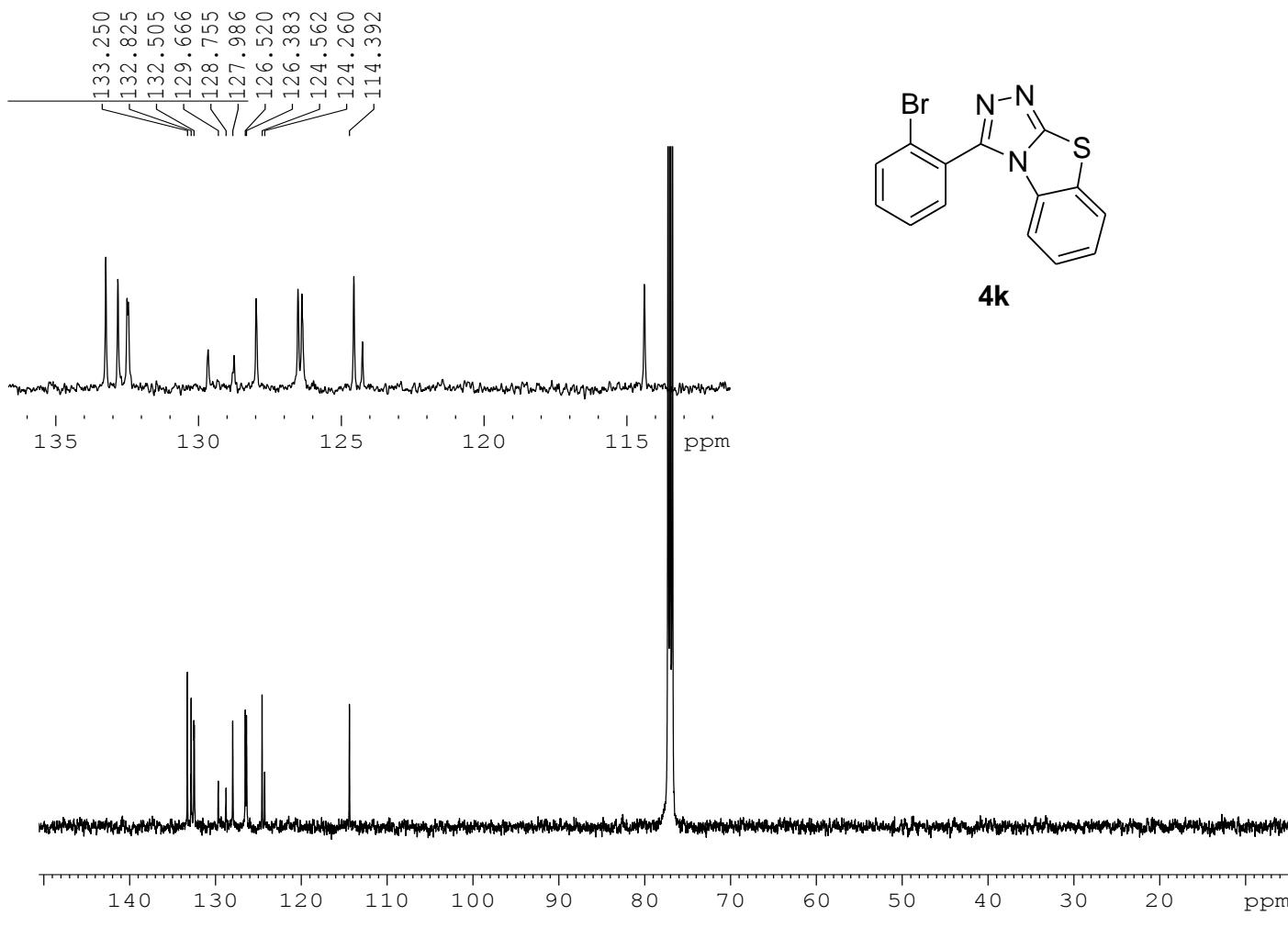
NUC1 13C
 P1 9.60 usec
 PL1 2.00 dB
 SFO1 125.7464750 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.60 dB
 PL12 17.66 dB
 PL13 17.66 dB
 SFO2 500.0355000 MHz
 SI 32768
 SF 125.7326482 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 2.00



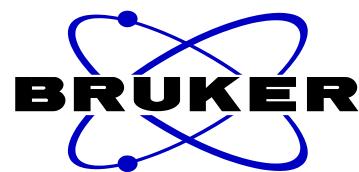
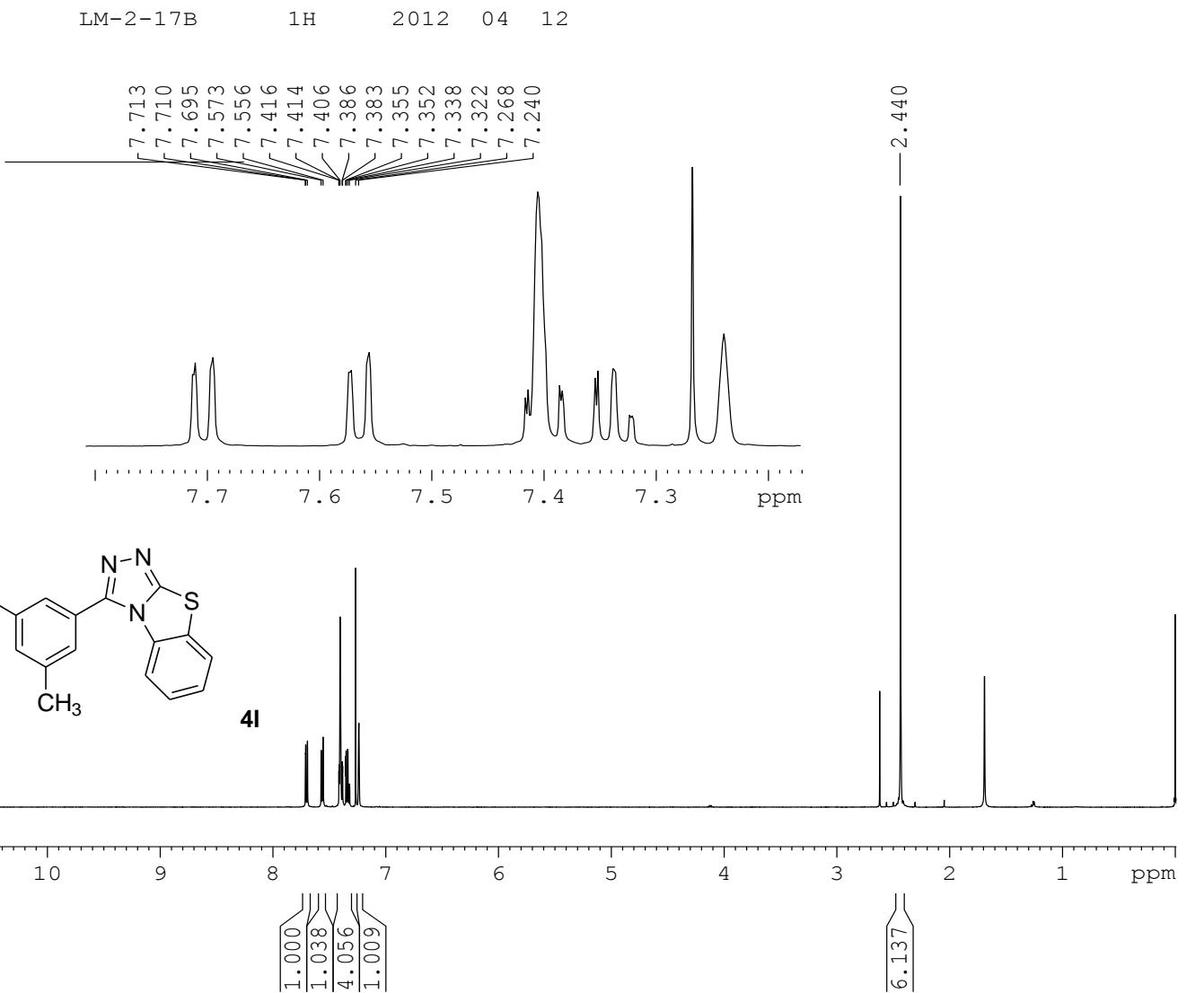
LM-2-8B 13C 1D 2012 05 09



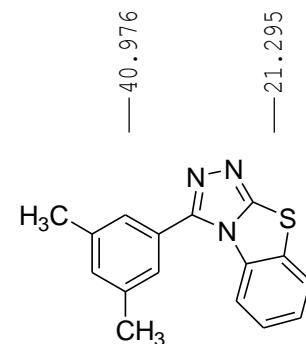
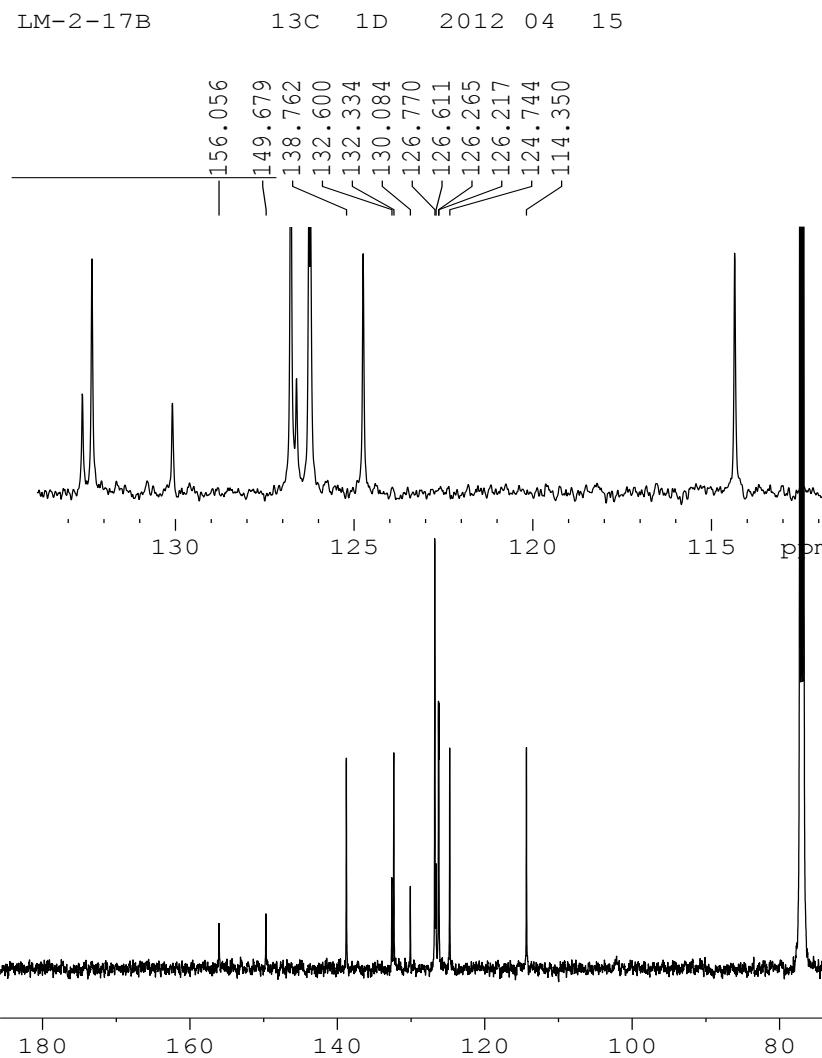
NAME LM-2-8B
EXPNO 2
PROCNO 1
Date 20120509
Time 18.45
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 612
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 11500
DW 15.300 usec
DE 6.00 usec
TE 301.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 ======
NUC1 ¹³C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

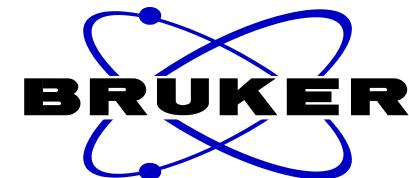
===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.60 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326440 MHz
WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 2.00



LM-2-17B



4



NAME	LM-2-17B
EXPNO	2
PROCNO	1
Date	20120415
Time	18.47
INSTRUM	av500
PROBHDI	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	1713
DS	2
SWH	32679.738 Hz
FIDRES	0.498653 Hz
AQ	1.0027661 sec
RG	812
DW	15.300 usec
DE	6.00 usec
TE	296.5 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TDO	1

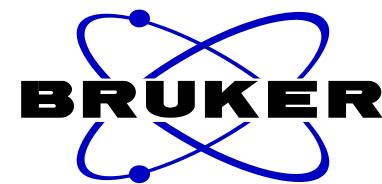
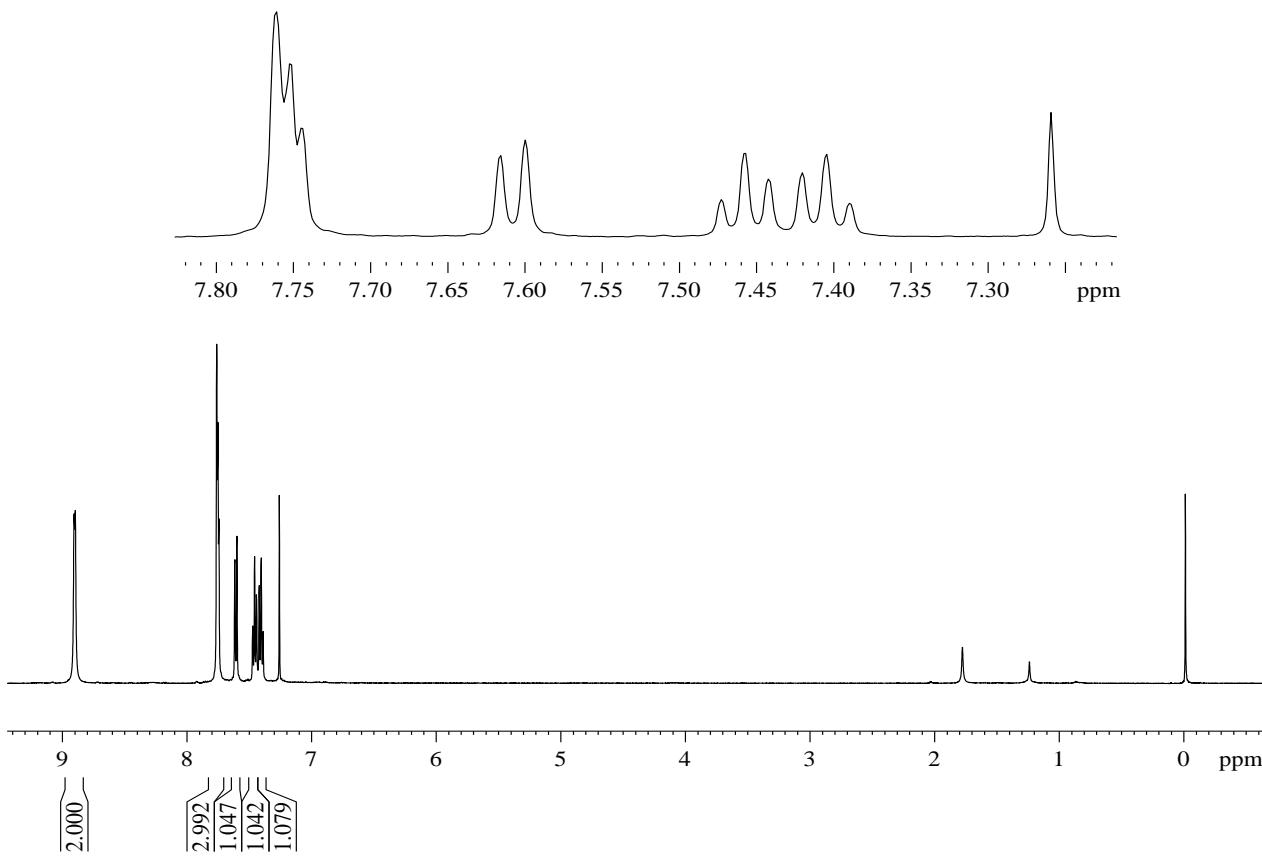
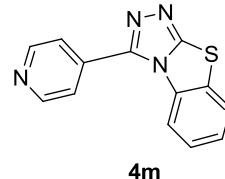
===== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

```

===== CHANNEL f2 =====
CPDPRG2          waltz16
NUC2              1H
PCPD2            80.00 usec
PL2               2.60 dB
PL12              17.66 dB
PL13              17.66 dB
SFO2             500.0355000 MHz
SI                32768
SF                125.7326482 MHz
WDW               EM
SSB               0
LB                5.00 Hz
GB               0
PC                2.00

```

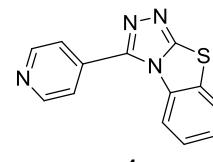
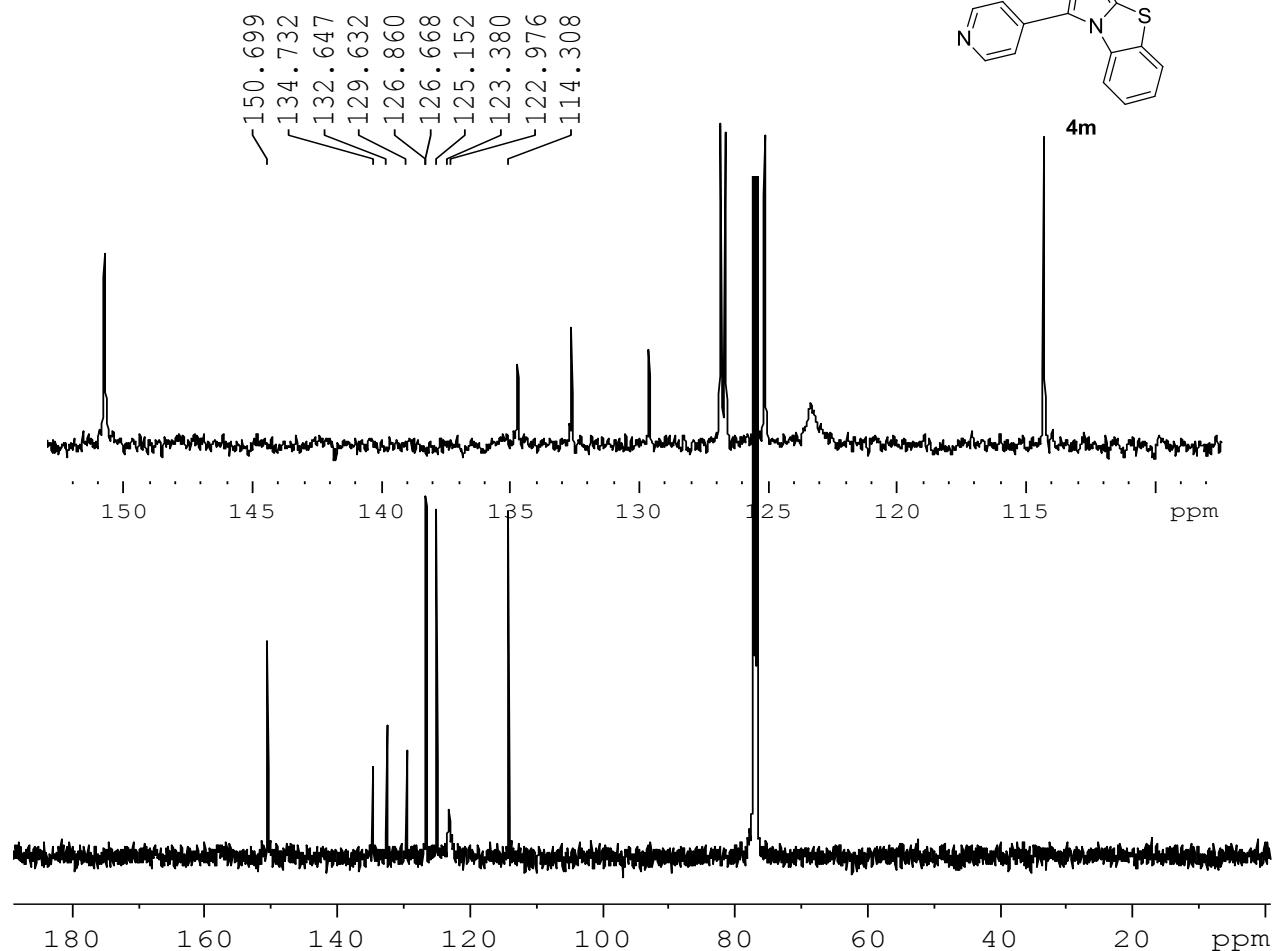
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7.616
7.600
7.442
7.420
7.405
7.390
7.259



NAME LM-2-18B-2
EXPNO 1
PROCNO 1
Date 20121207
Time 19.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 8
DS 1
SWH 10000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8193000 sec
RG 645
DW 50.000 usec
DE 8.00 usec
TE 292.4 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.00 usec
PL1 2.00 dB
SFO1 500.0338500 MHz
SI 16384
SF 500.0300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 5.00

LM-2-18B-2 13C 1D 2012 12 12

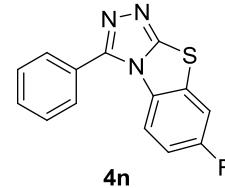
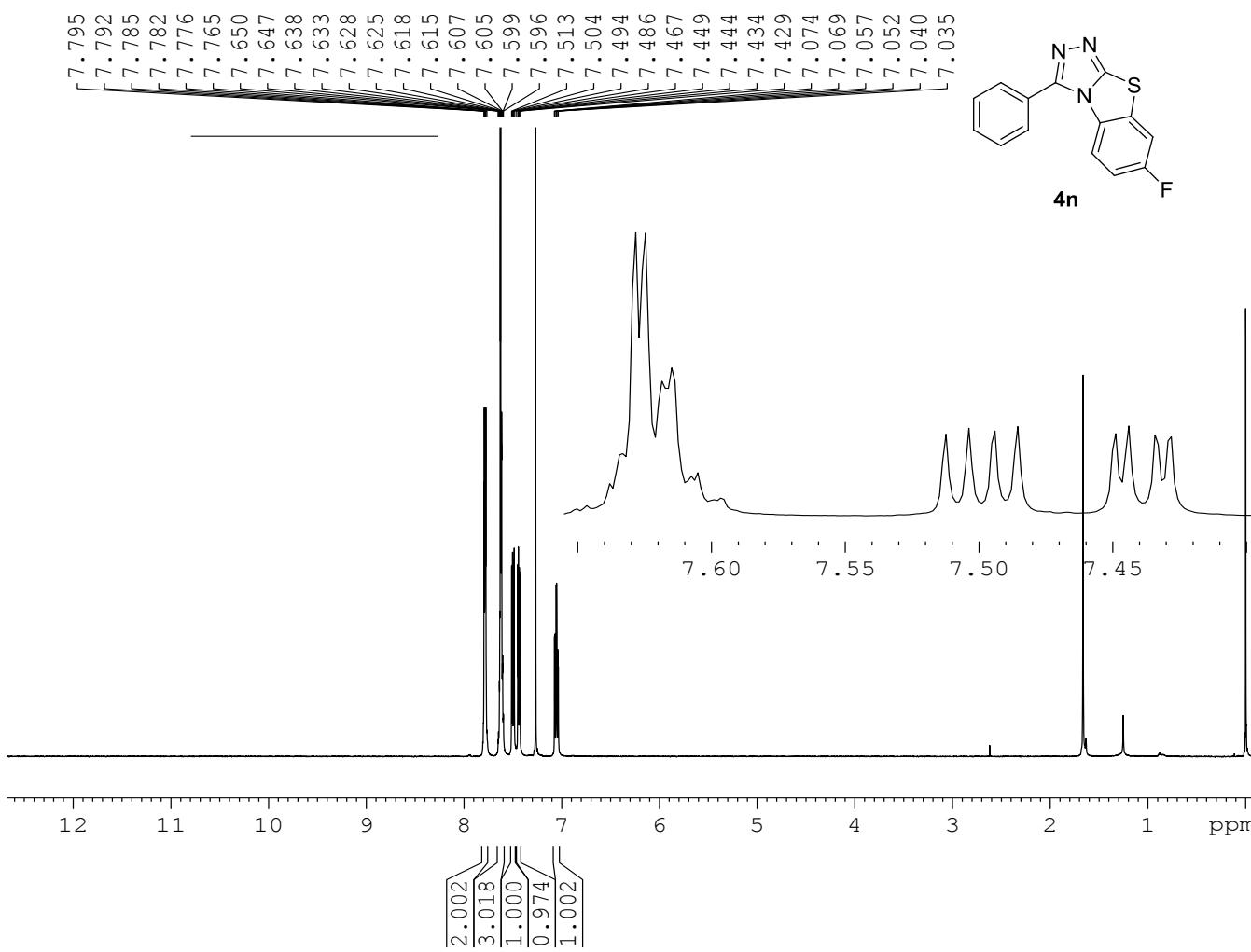


NAME LM-2-18B-2
EXPNO 2
PROCNO 1
Date_ 20121212
Time_ 12.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 556
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 1150
DW 15.300 usec
DE 6.00 usec
TE 292.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 10

===== CHANNEL f1 =====
NUC1 ¹³C
P1 12.20 usec
PL1 3.00 dB
SFO1 125.7464750 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.70 dB
PL13 17.70 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326455 MHz
WDW EM
SSB 0

LM-2-10B 1H 2012 03 29



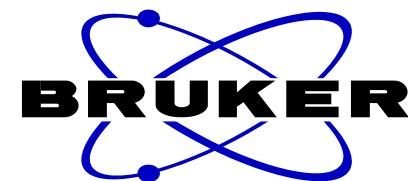
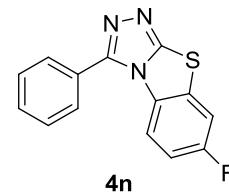
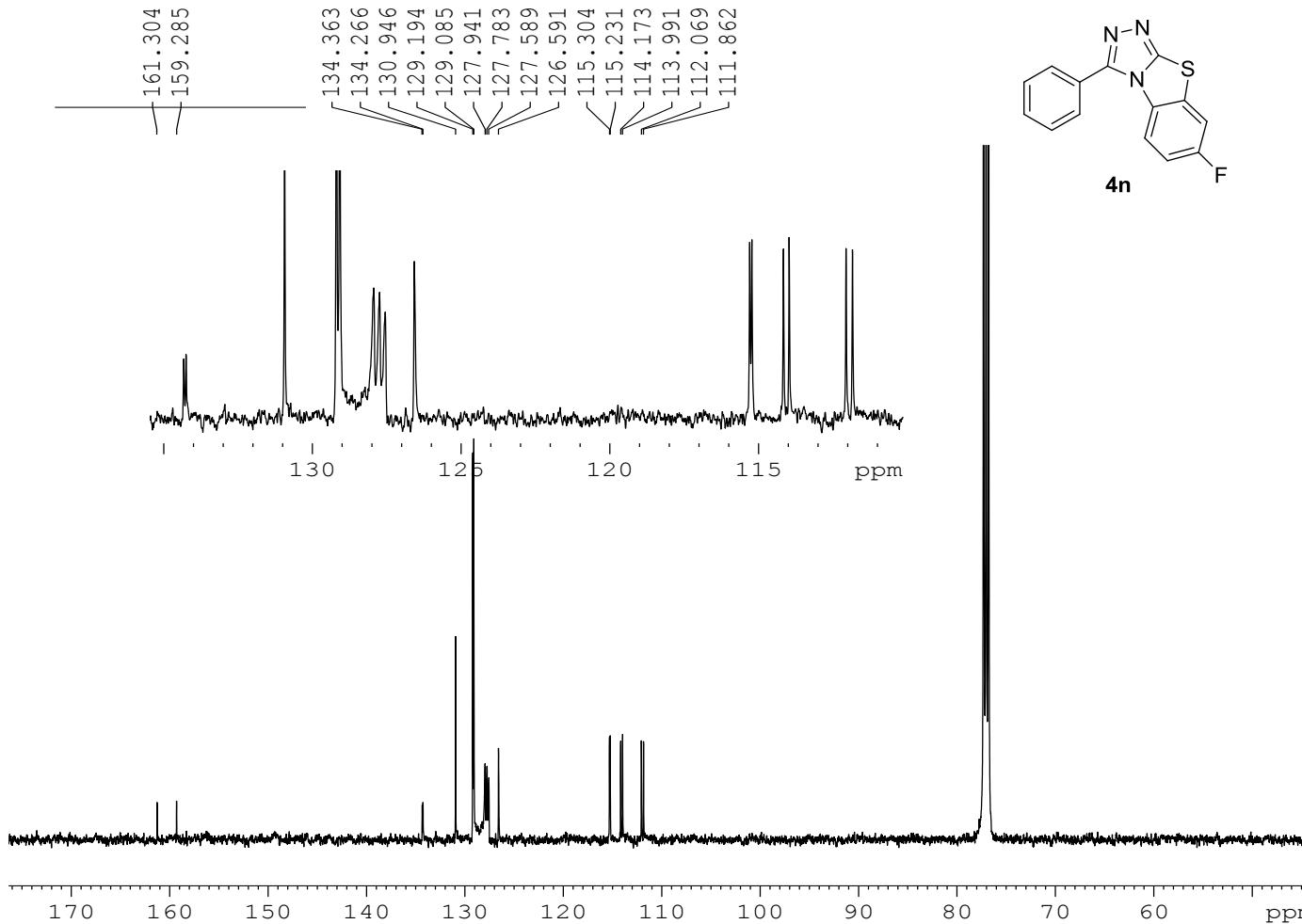
The Bruker logo consists of the word "BRUKER" in a bold, black, sans-serif font. A blue stylized atomic orbital path is drawn over the letters, with two small blue dots representing electrons at specific points on the orbitals.

NAME	LM-2-10B
EXPNO	1
PROCNO	1
Date _	20120329
Time	19.18
INSTRUM	av500
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	CDC13
NS	8
DS	1
SWH	10000.000 Hz
FIDRES	0.305176 Hz
AQ	1.6385000 sec
RG	645
DW	50.000 usec
DE	6.00 usec
TE	292.7 K
PPM	
D1	2.00000000 sec
TDO	1
===== CHANNEL f1 =====	
NUC1	1H
P1	13.50 usec
PL1	2.20 dB
SFO1	500.0335010 MHz
SI	16384
SF	500.0300068 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

LM-2-10B

13C 1D

2012 04 05



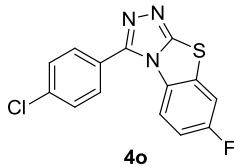
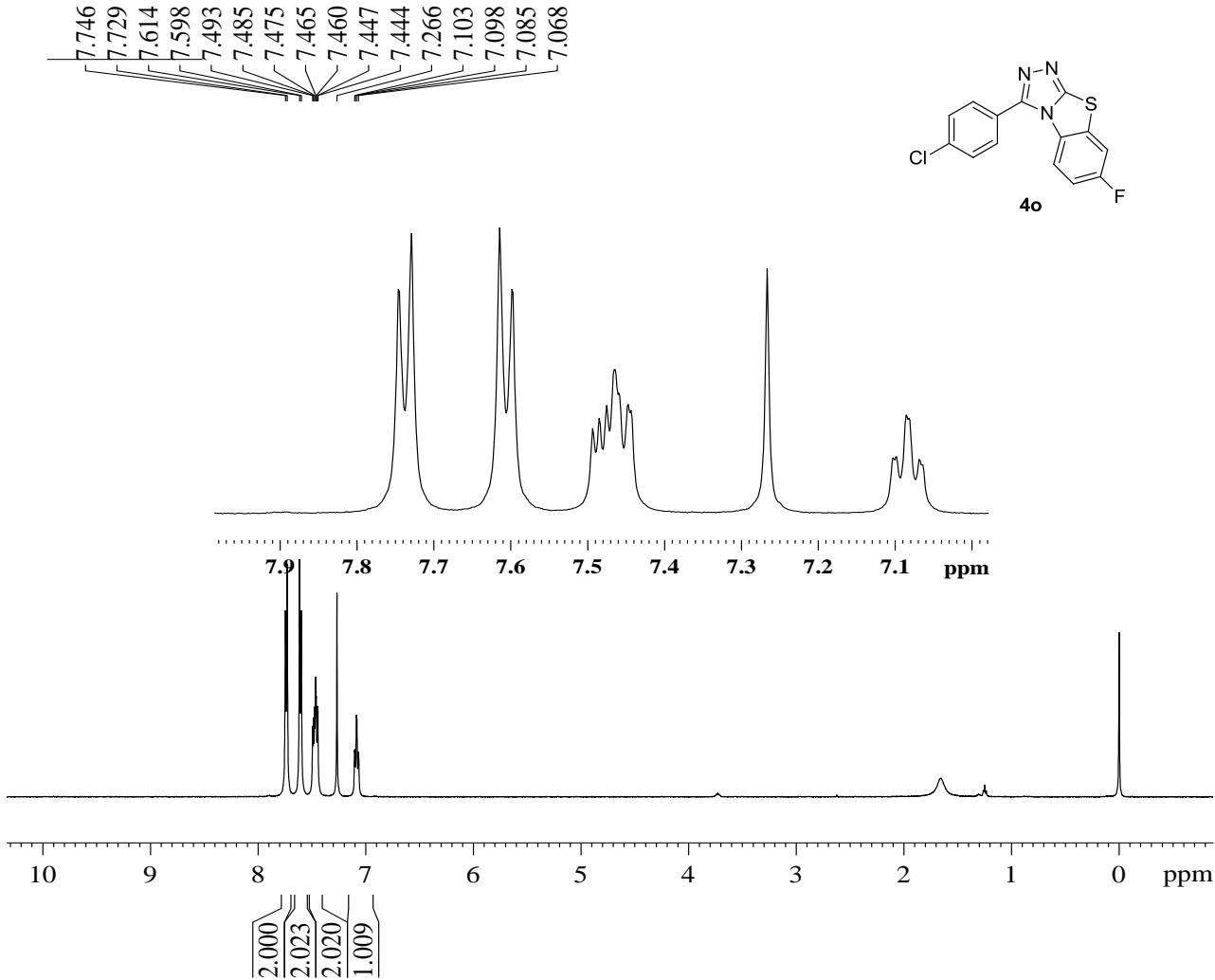
NAME LM-2-10B
 EXPNO 2
 PROCNO 11
 Date_ 20120405
 Time 10.43
 INSTRUM av500
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 2203
 DS 2
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 3250
 DW 15.300 usec
 DE 6.00 usec
 TE 294.1 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====

NUC1	13C
P1	9.60 usec
PL1	2.00 dB
SFO1	125.7464750 MHz

===== CHANNEL f2 =====

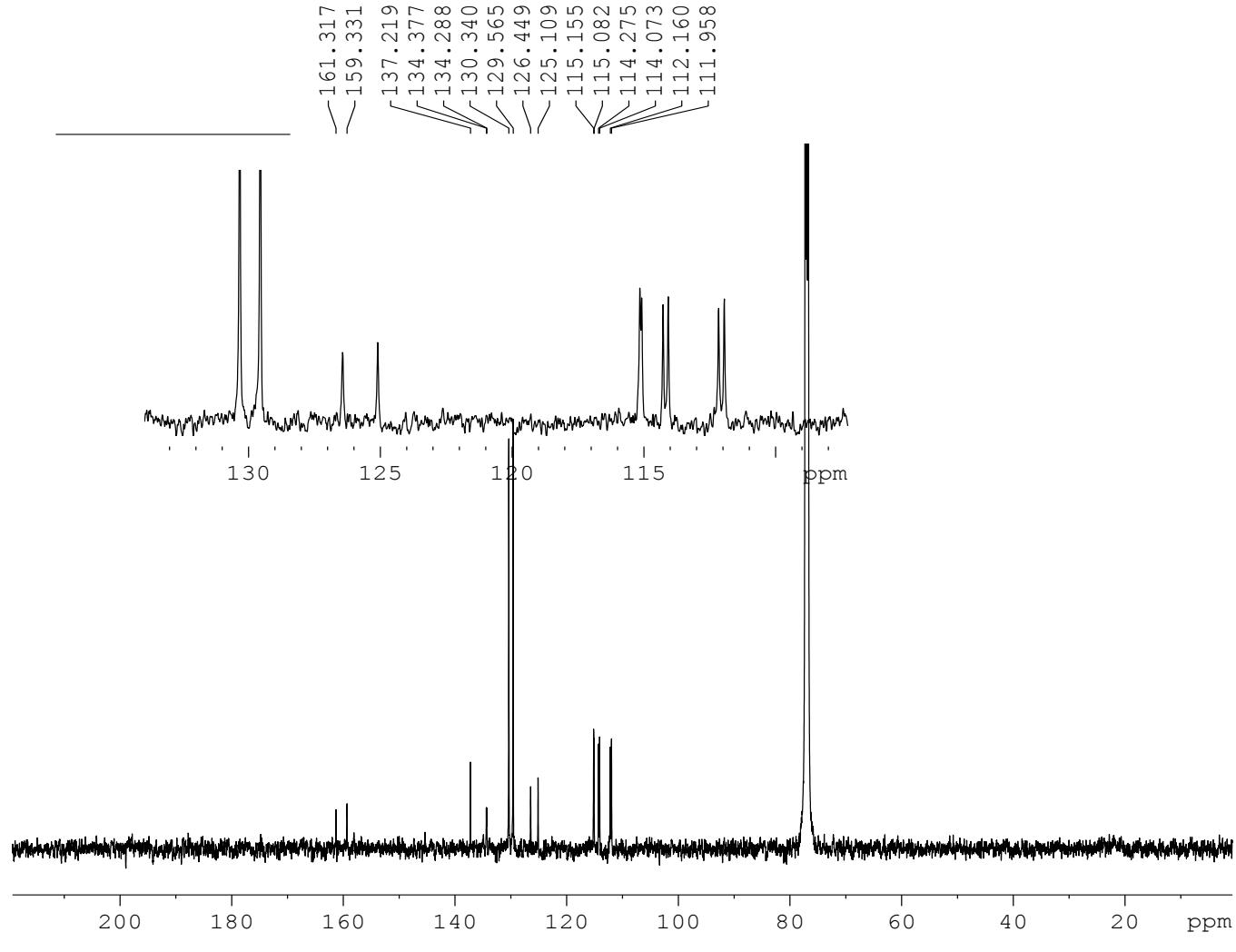
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.20 dB
PL12	17.66 dB
PL13	17.66 dB
SFO2	500.0355000 MHz
SI	32768
SF	125.7326435 MHz
WWDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	2.00



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NAME LM-2-11B
 EXPNO 1
 PROCNO 1
 Date_ 20120329
 Time 19.22
 INSTRUM av500
 PROBHDI 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 1
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6385000 sec
 RG 645
 DW 50.000 usec
 DE 6.00 usec
 TE 292.7 K
 D1 2.0000000 sec
 TD0 1

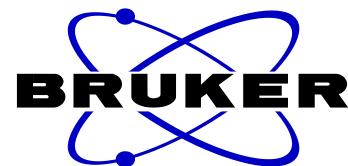
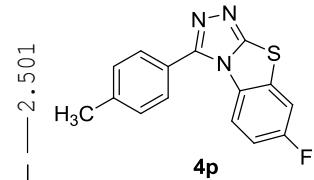
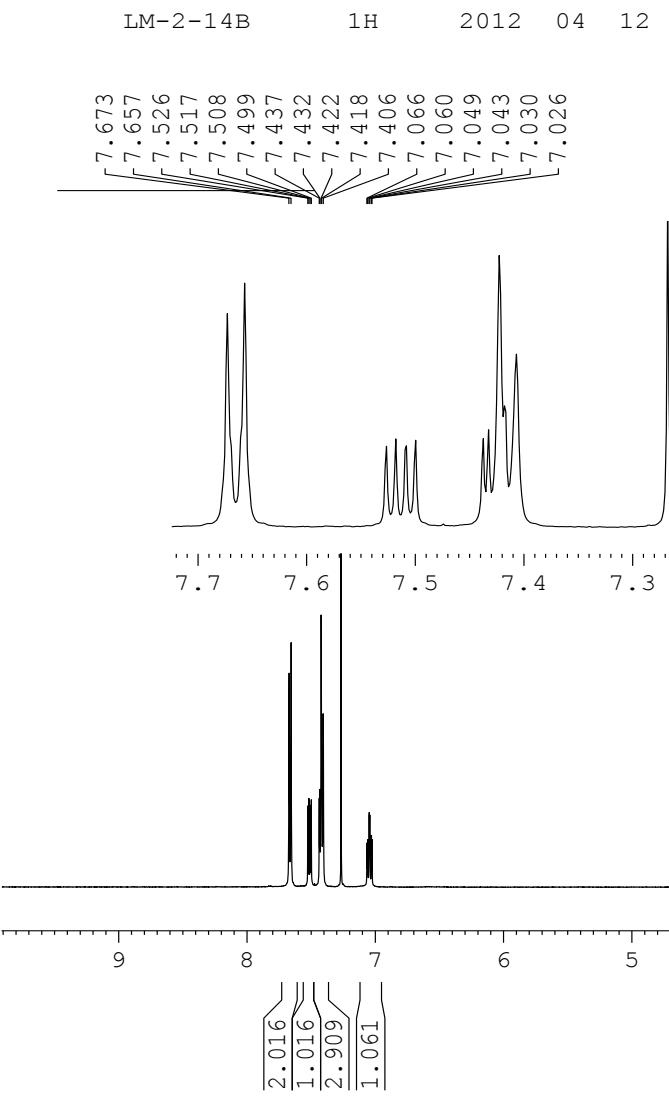
===== CHANNEL f1 =====
NUC1 1H
P1 13.50 usec
PL1 2.20 dB
SFO1 500.0335010 MHz
SI 16384
SF 500.0300064 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

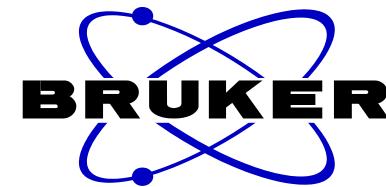
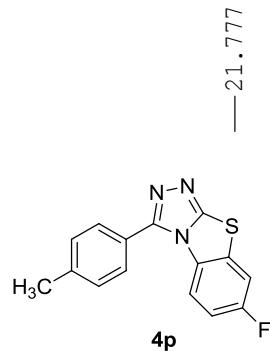
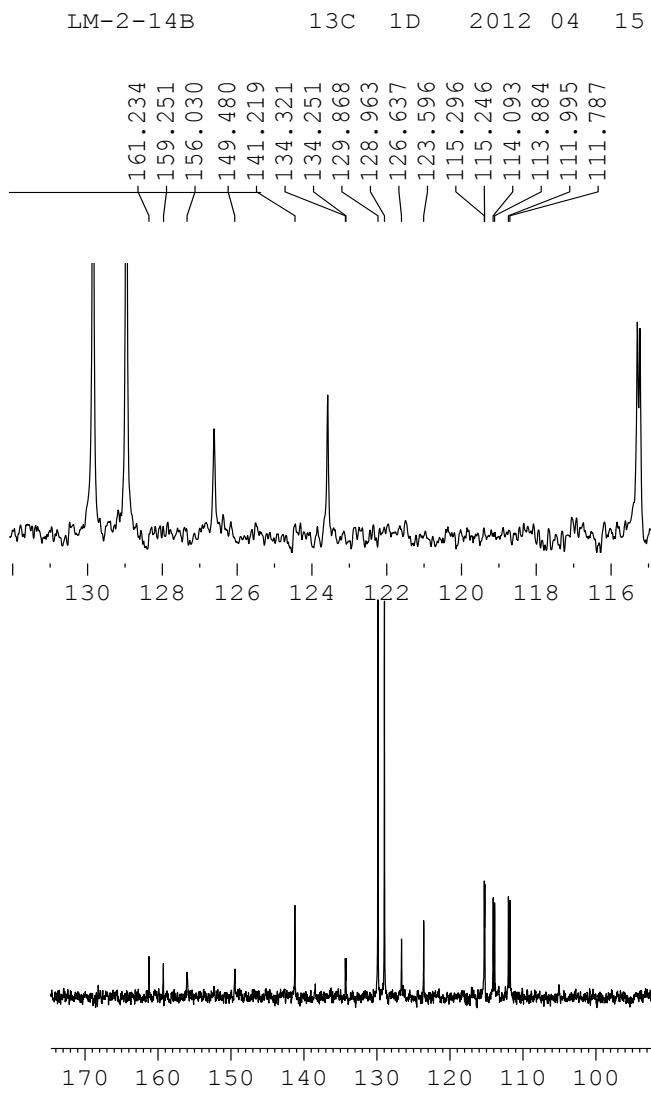


NAME LM-2-11B
 EXPNO 2
 PROCN0 1
 Date_ 20120405
 Time_ 11.42
 INSTRUM av500
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 3024
 DS 2
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 3250
 DW 15.300 usec
 DE 6.00 usec
 TE 293.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 2.00 dB
 SFO1 125.7464750 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.60 dB
 PL12 17.66 dB
 PL13 17.66 dB
 SFO2 500.0355000 MHz
 SI 32768
 SF 125.7326482 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 2.00





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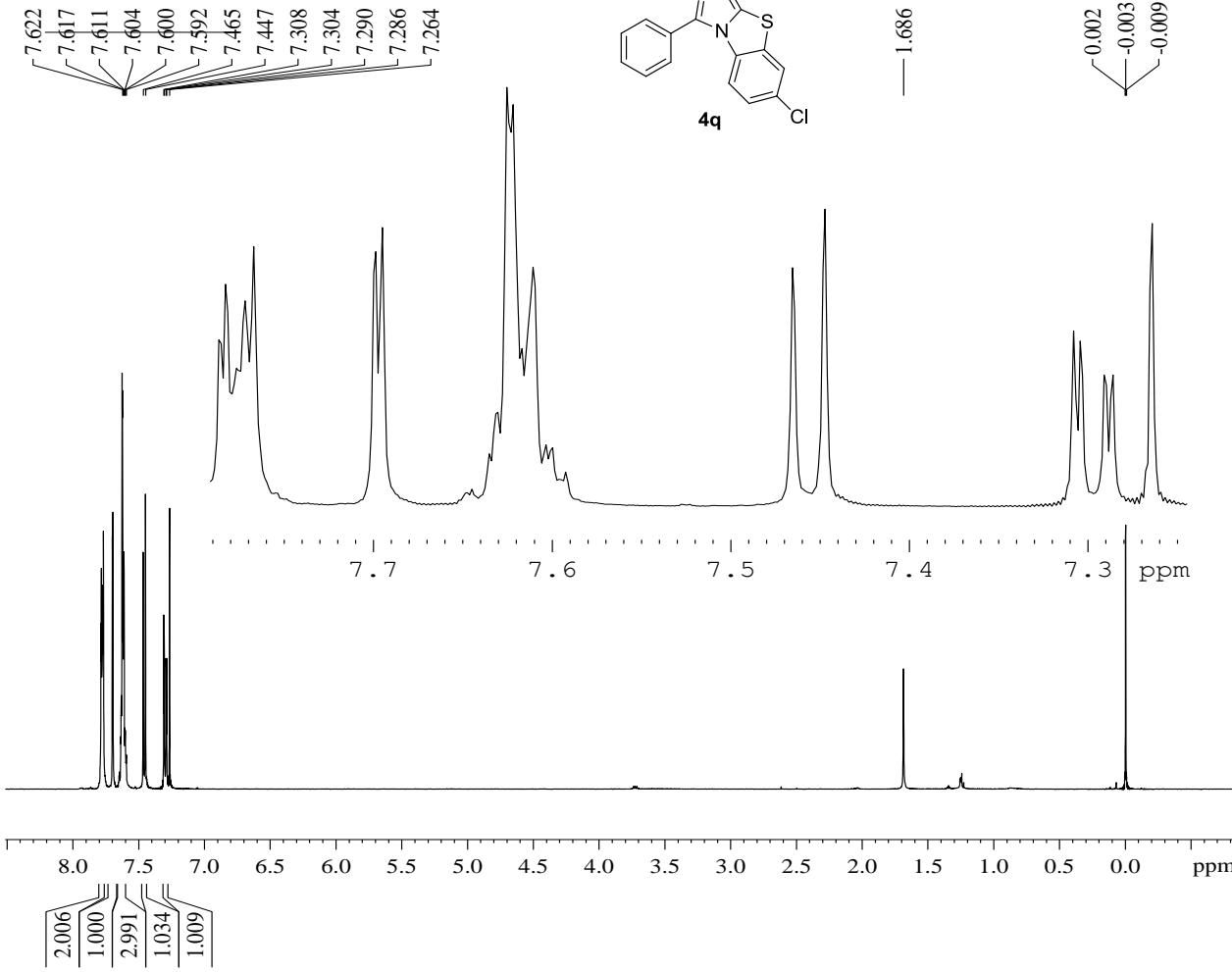
NAME          LM-2-14B
EXPNO         21
PROCNO        1
Date_         20120415
Time_          13.31
INSTRUM       av500
PROBHD        5 mm PABBO BB-
PULPROG      zgpg30
TD             65536
SOLVENT        CDC13
NS              1727
DS              2
SWH            32679.738 Hz
FIDRES        0.498653 Hz
AQ             1.0027661 sec
RG              812
DW             15.300 usec
DE              6.00 usec
TE              296.2 K
D1           2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                 1

===== CHANNEL f1 =====
NUC1            13C
P1              9.60 usec
PL1             2.00 dB
SFO1        125.7464750 MHz

===== CHANNEL f2 =====
CPDPRG2        waltz16
NUC2              1H
PCPD2          80.00 usec
PL2              2.60 dB
PL12             17.66 dB
PL13             17.66 dB
SFO2        500.0355000 MHz
SI                32768
SF           125.7326440 MHz
WDW                  EM
SSB                   0
LB              5.00 Hz
GB                   0
PC                2.00

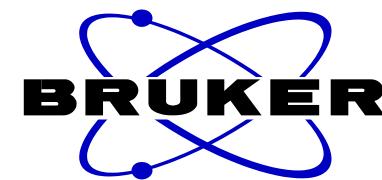
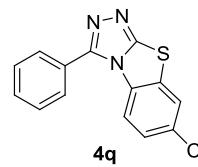
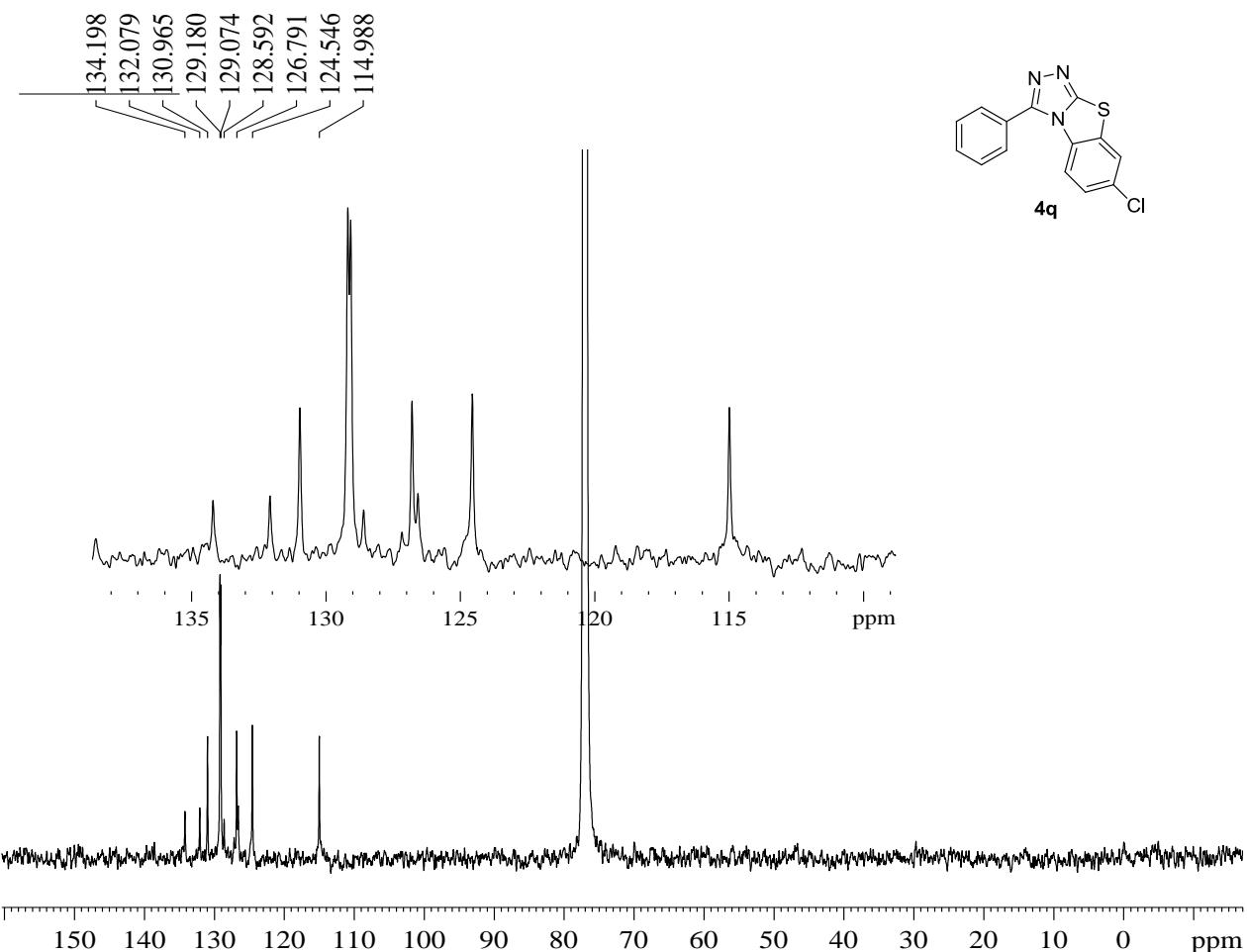
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LSL-2-22b 1H 1D 2013 12 27



NAME LSL-2-22b
EXPNO 1
PROCNO 1
Date_ 20131227
Time 16.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 8
DS 1
SWH 10000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8193000 sec
RG 512
DW 50.000 usec
DE 8.00 usec
TE 293.6 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.00 usec
PL1 2.00 dB
SFO1 500.0338500 MHz
SI 16384
SF 500.0300087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00



```

NAME      lm-2-22b
EXPNO     2
PROCNO    1
Date_     20130620
Time      15.21
INSTRUM   spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT   CDCl3
NS        2111
DS        2
SWH      32679.738 Hz
FIDRES   0.498653 Hz
AQ        1.0027661 sec
RG        5160
DW        15.300 usec
DE        6.00 usec
TE        301.6 K
D1        2.0000000 sec
d11       0.03000000 sec
DELTA    1.89999998 sec
TD0        20

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===== CHANNEL f1 =====
NUC1      13C
P1        9.60 usec
PL1       2.00 dB
SFO1     125.7464750 MHz

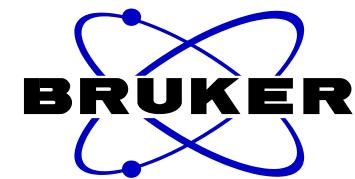
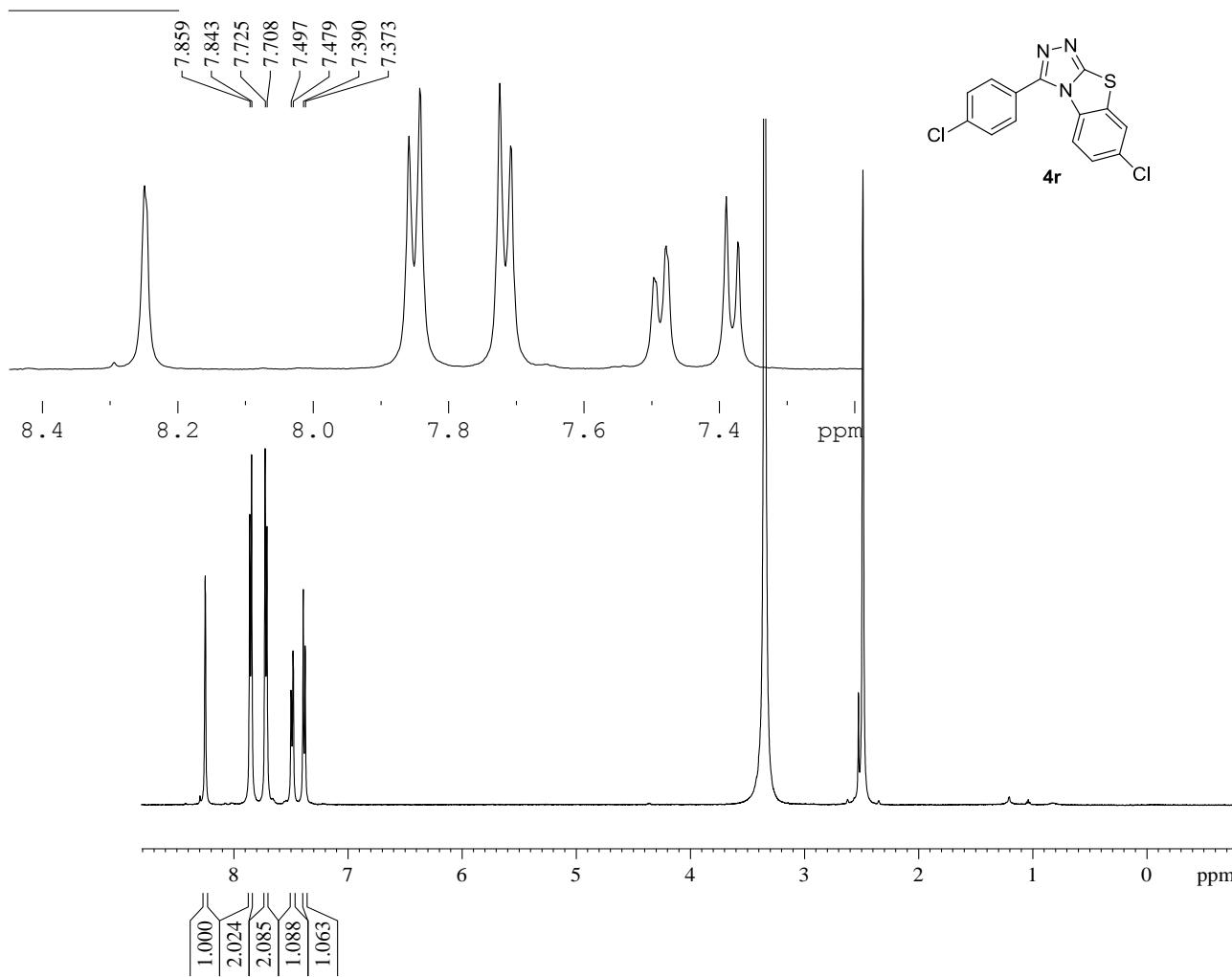
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===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        2.60 dB
PL12      17.66 dB
PL13      17.66 dB
SFO2     500.0355000 MHz
SI         32768
SF      125.7326440 MHz
WDW       EM

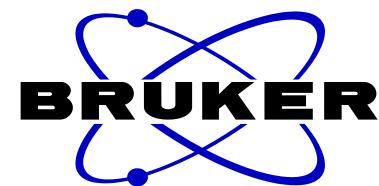
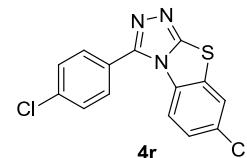
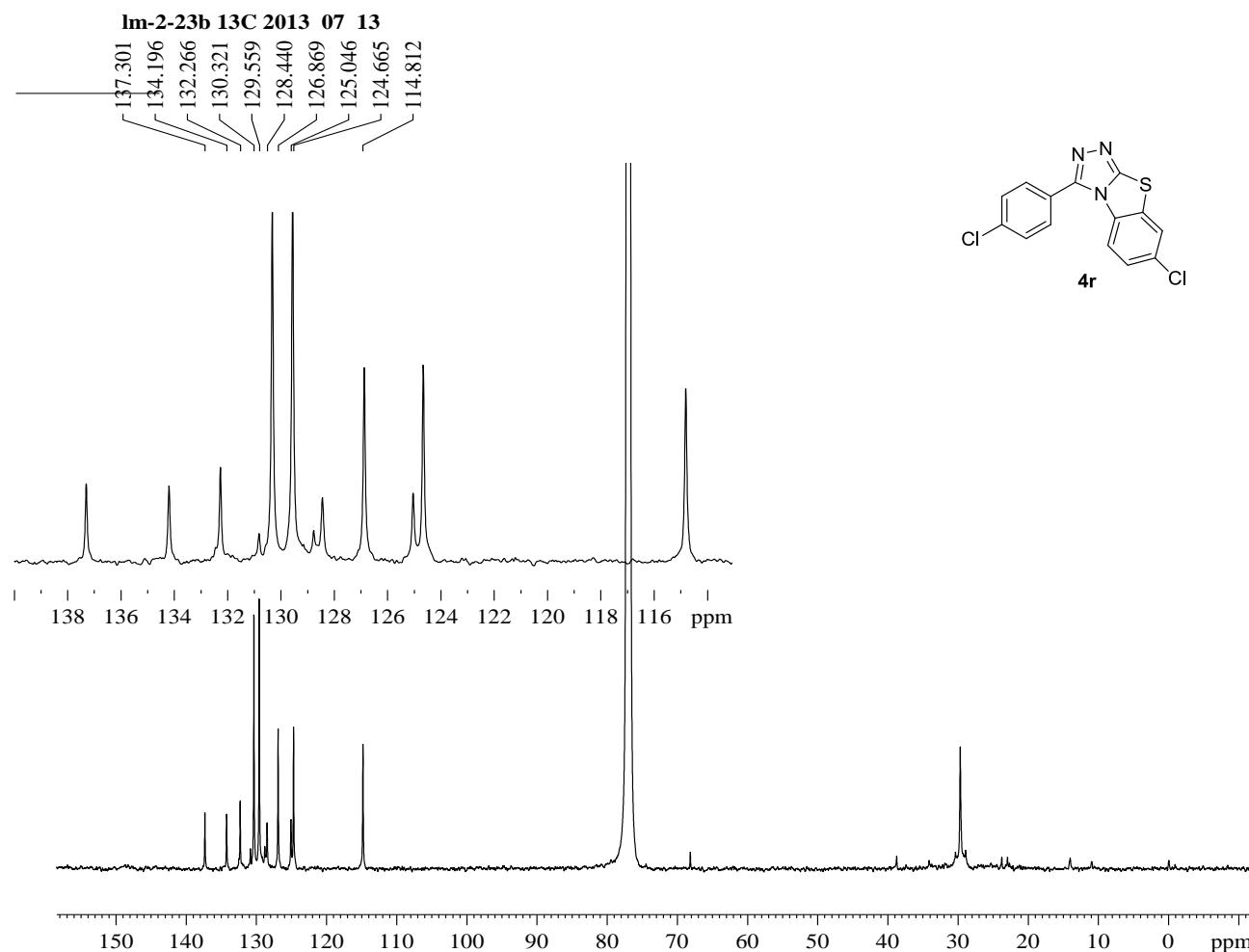
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lm-2-23b-1 1H 1D 2013 12 31



NAME lm-2-23b-1
EXPNO 1
PROCNO 1
Date_ 20131231
Time 16.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT DMSO
NS 8
DS 1
SWH 10000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8193000 sec
RG 322
DW 50.000 usec
DE 8.00 usec
TE 293.4 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.00 usec
PL1 2.00 dB
SFO1 500.0338500 MHz
SI 16384
SF 500.0300085 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 4.00



NAME lm-2-23b
 EXPNO 21
 PROCNO 1
 Date 20130713
 Time 21.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 17784
 DS 2
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 1820
 DW 15.300 usec
 DE 6.00 usec
 TE 673.2 K
 D1 2.0000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 T0D 40

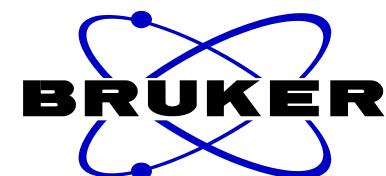
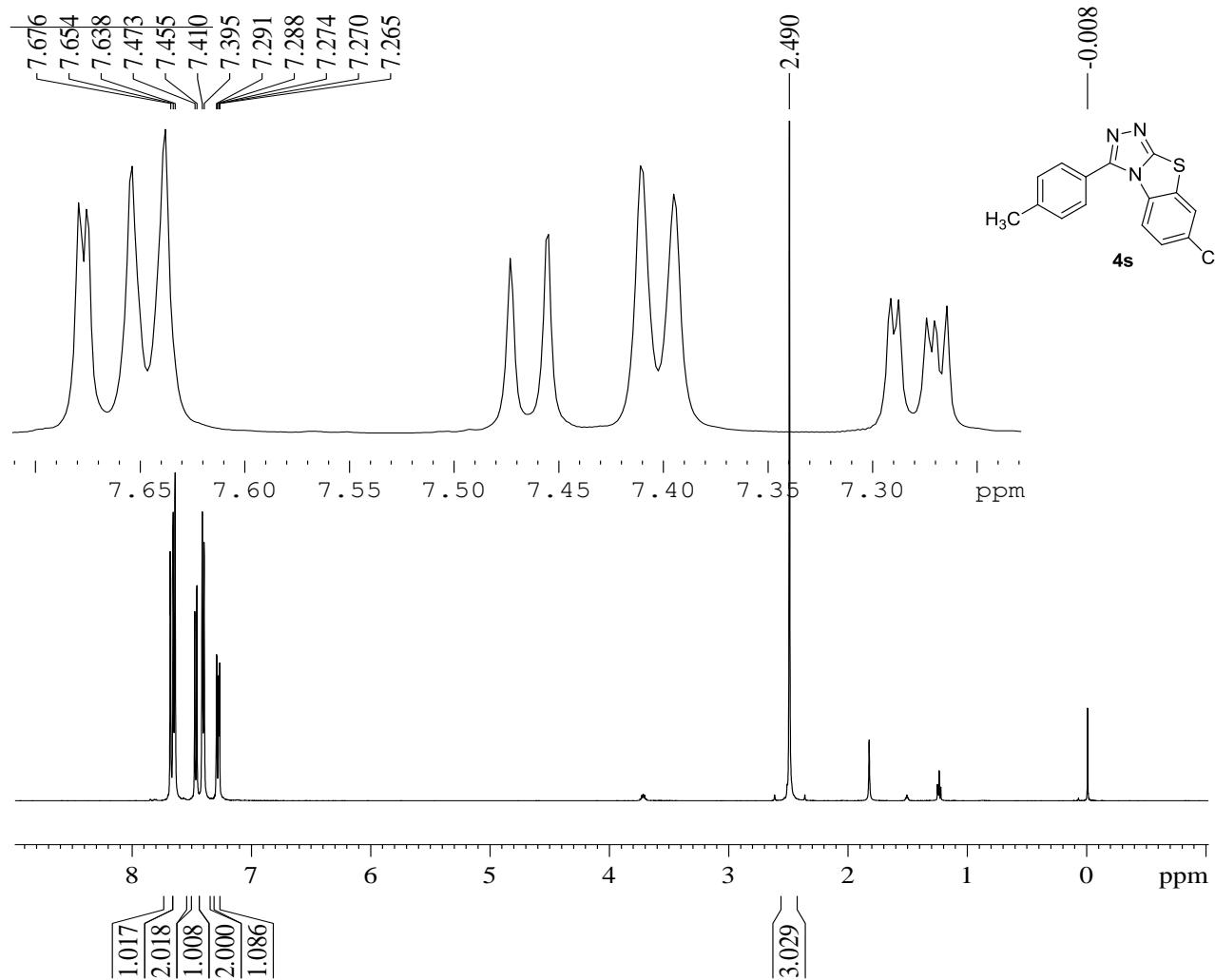
===== CHANNEL f1 =====

NUC1 13C
 P1 12.20 usec
 PL1 3.00 dB
 SFO1 125.7464750 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.00 dB
 PL12 17.70 dB
 PL13 17.70 dB
 SFO2 500.0355000 MHz
 SI 32768
 SF 125.7326466 MHz
 WDW EM

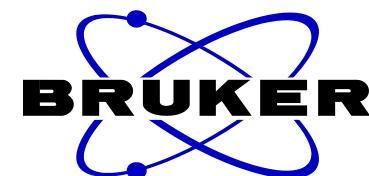
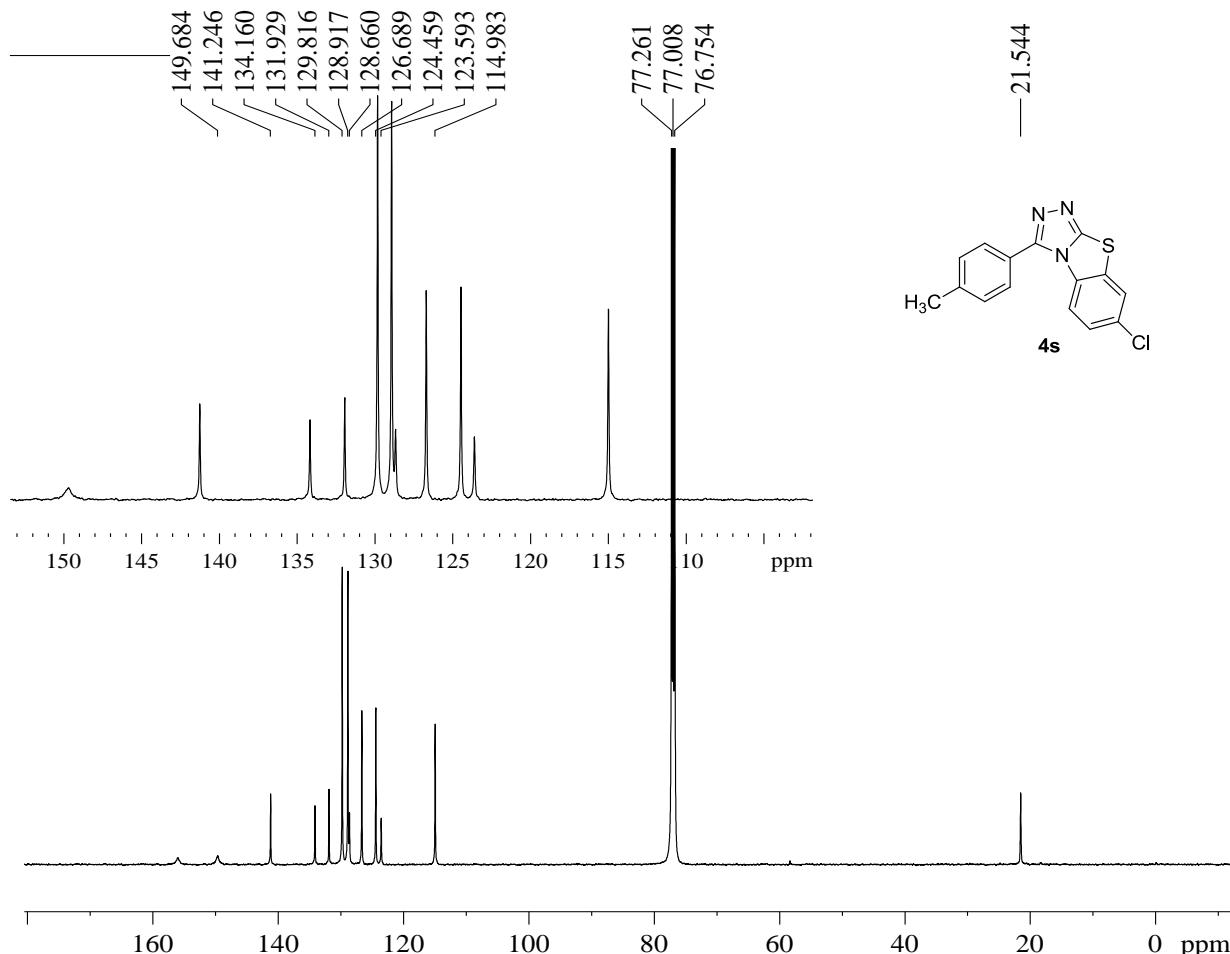
lm-2-24b-1 1H 1D 2013 12 31



NAME lm-2-24b-1
EXPNO 1
PROCNO 1
Date_ 20131231
Time 17.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl₃
NS 8
DS 1
SWH 10000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8193000 sec
RG 322
DW 50.000 usec
DE 8.00 usec
TE 293.5 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.00 usec
PL1 2.00 dB
SFO1 500.0338500 MHz
SI 16384
SF 500.0300085 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 4.00

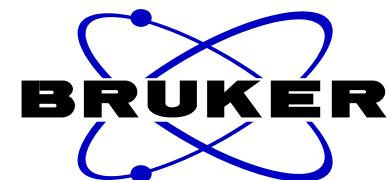
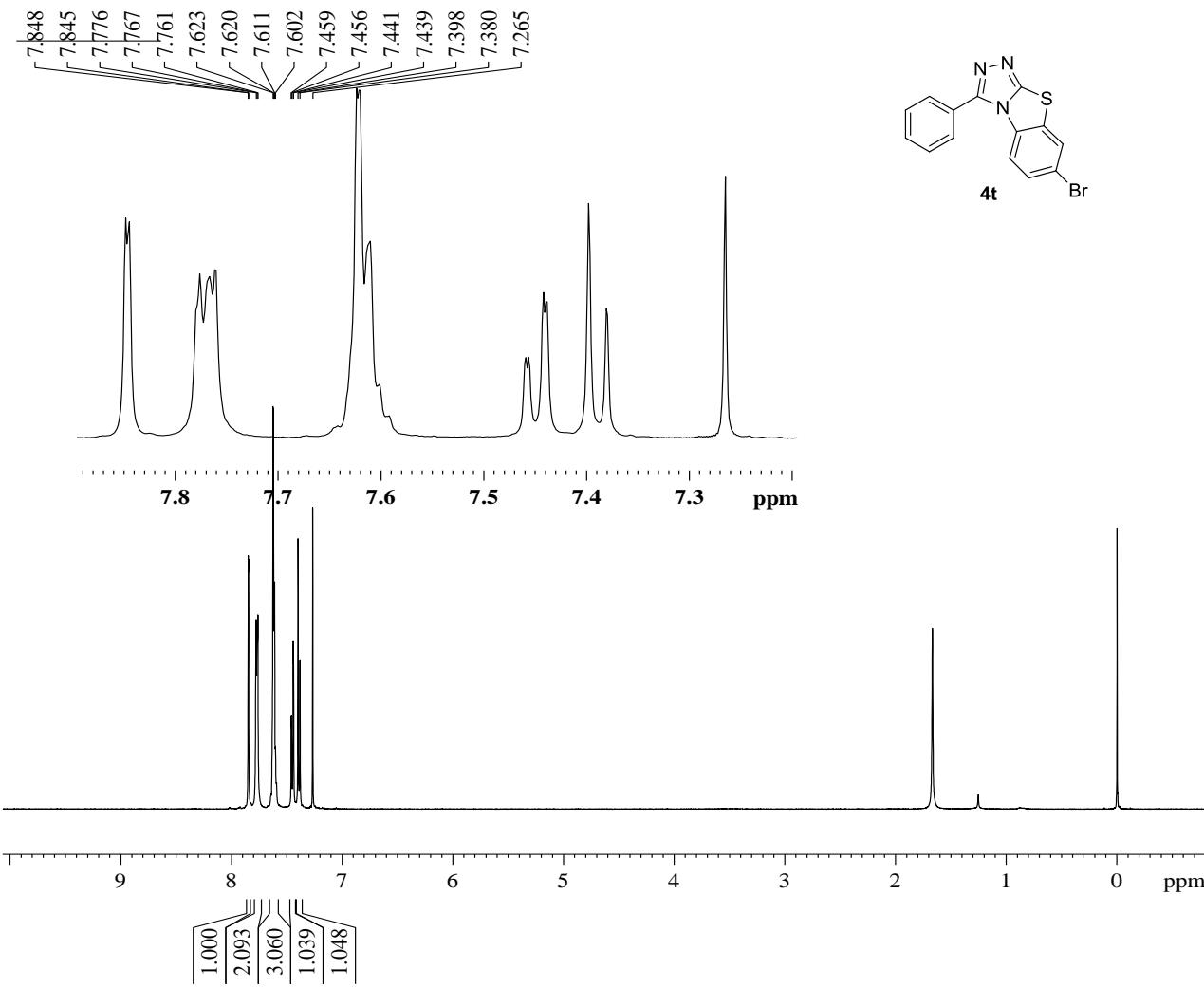
lm-2-24B-2 13C 2013 12 31



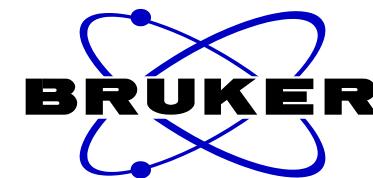
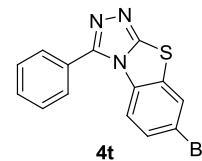
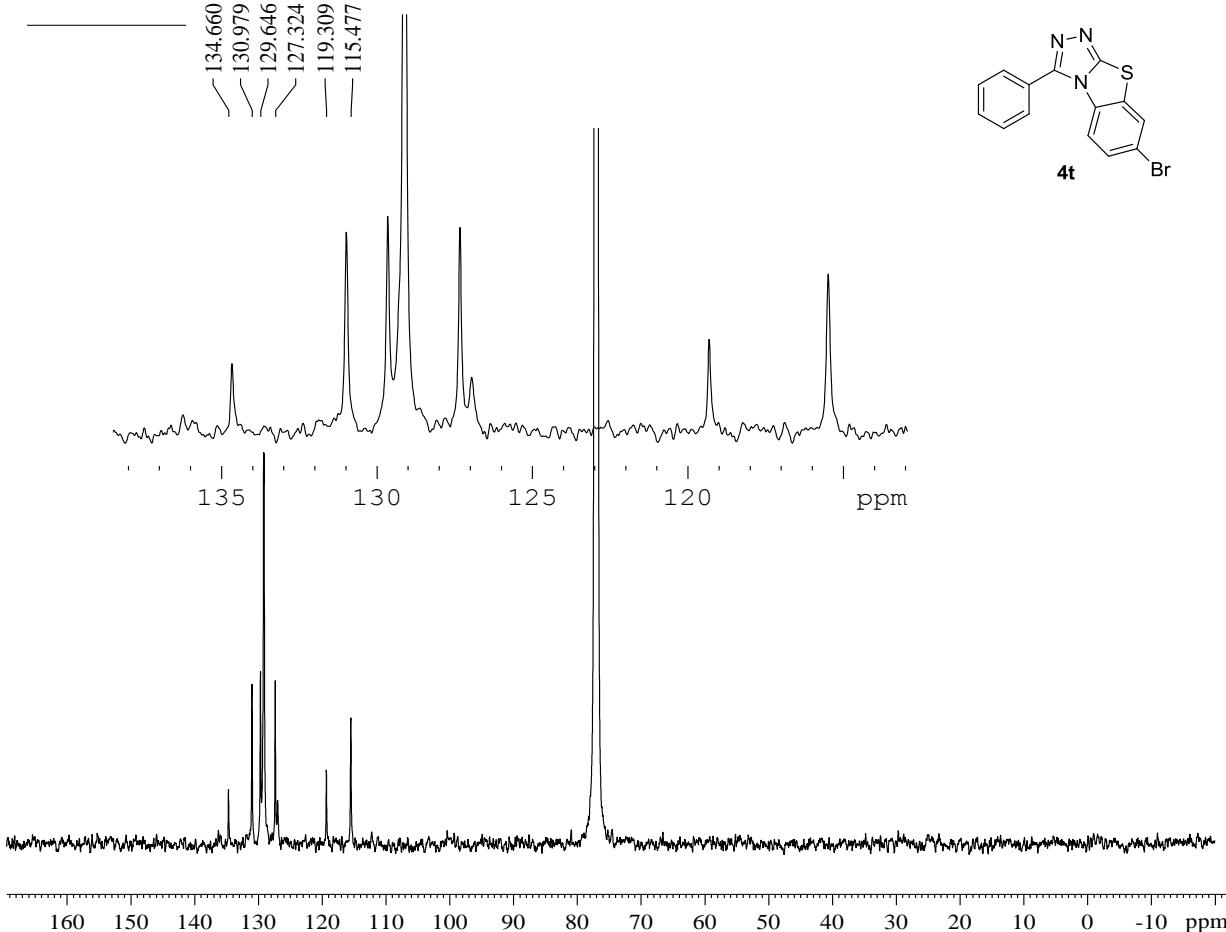
NAME lm-2-24b-2
EXPNO 2
PROCNO 1
Date_ 20131231
Time 18.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 16164
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 1820
DW 15.300 usec
DE 6.00 usec
TE 296.6 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.8999998 sec
TDO 40

===== CHANNEL f1 ======
NUC1 ¹³C
P1 12.20 usec
PL1 3.00 dB
SFO1 125.7464750 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.70 dB
PL13 17.70 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326472 MHz
WDW EM



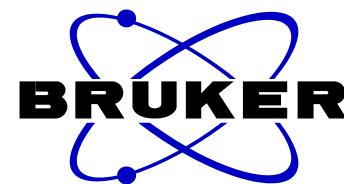
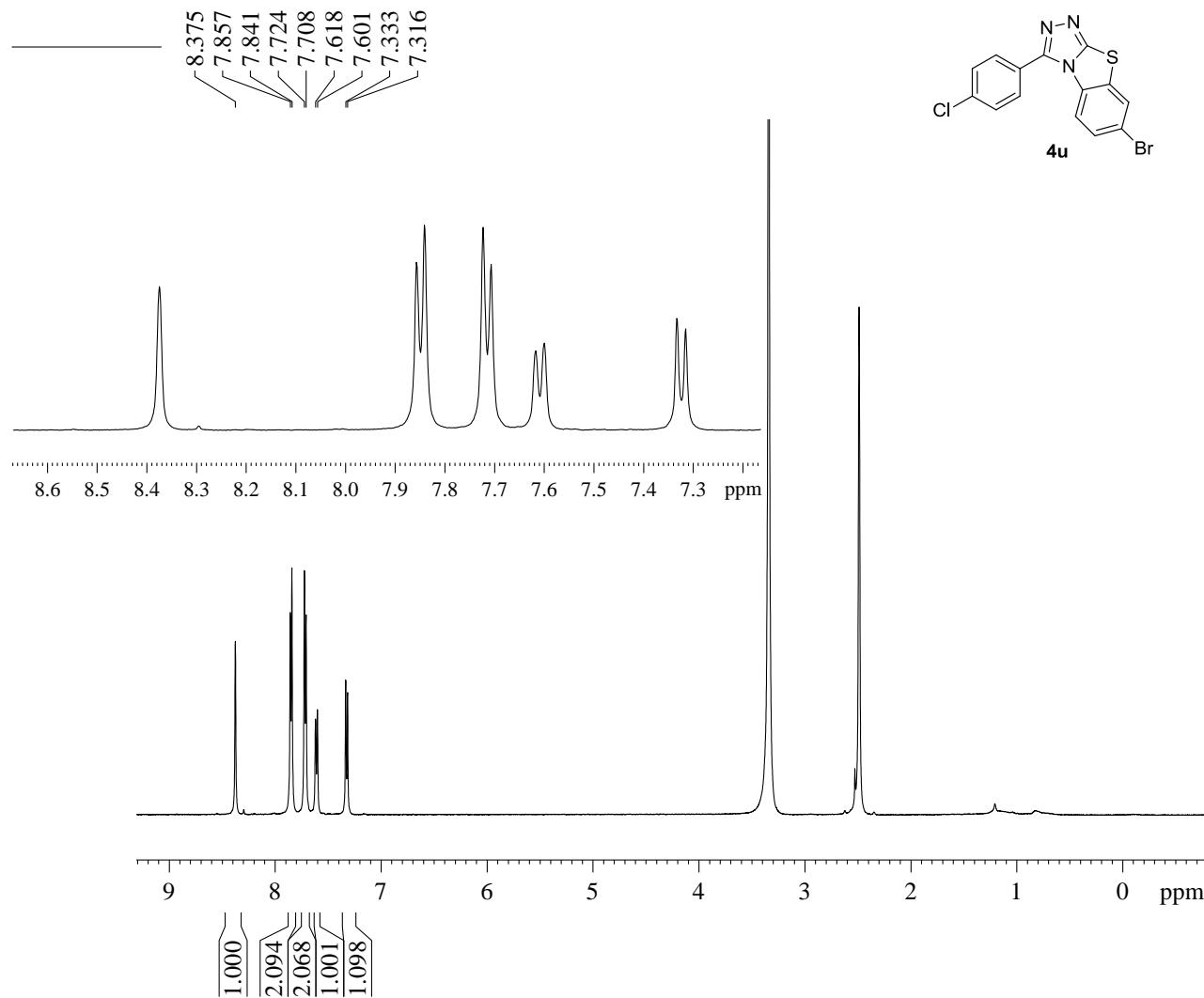
lm-2-25b 13C 2013 06 20

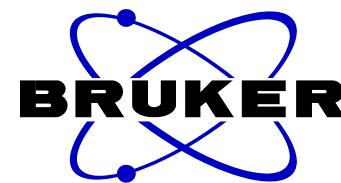
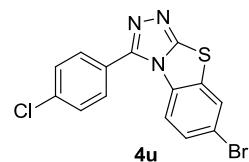
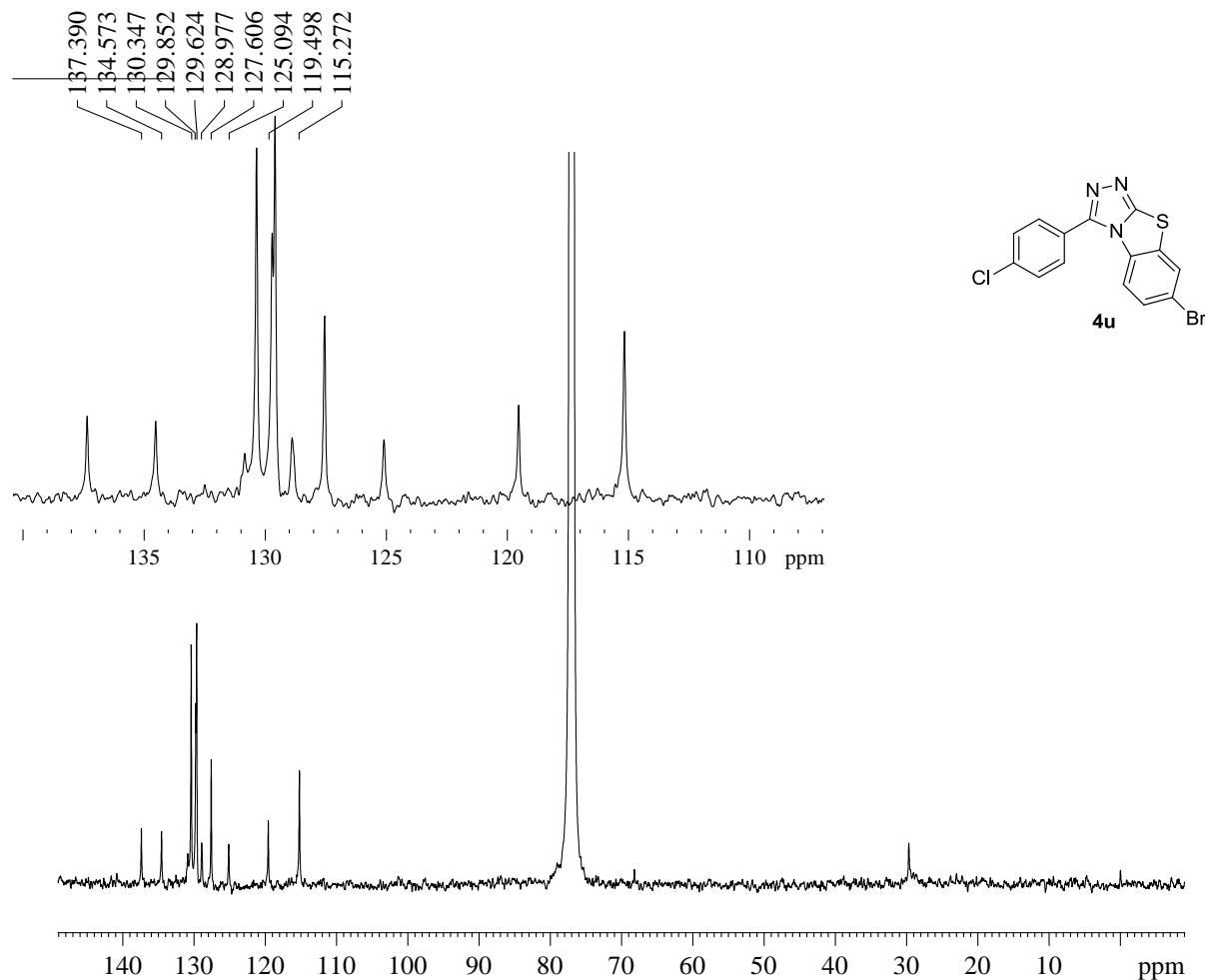


NAME lm-2-25b
EXPNO 2
PROCNO 1
Date 20130620
Time 17.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 1493
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 5160
DW 15.300 usec
DE 6.00 usec
TE 299.4 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.8999998 sec
TD0 40

===== CHANNEL f1 =====
NUC1 ¹³C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.60 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326472 MHz
WDW EM





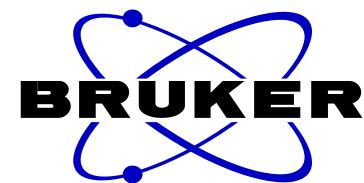
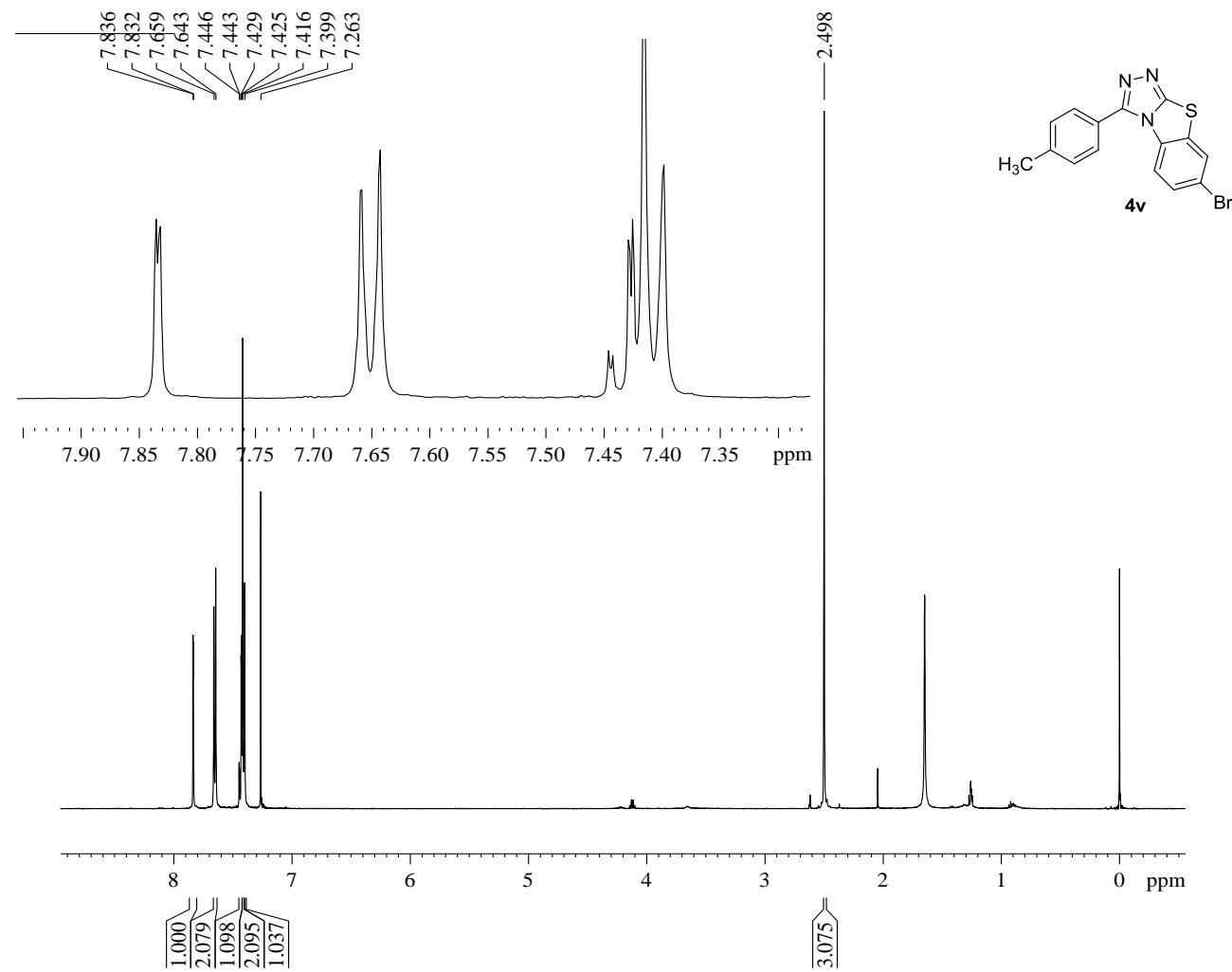
NAME lm-2-26b
 EXPNO 2
 PROCNO 1
 Date_ 20130623
 Time 22.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 11125
 DS 2
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 5160
 DW 15.300 usec
 DE 6.00 usec
 TE 299.6 K
 D1 2.0000000 sec
 d11 0.03000000 sec
 DELTA 1.8999998 sec
 TD0 40

===== CHANNEL f1 =====

NUC1 13C
 P1 9.60 usec
 PL1 2.00 dB
 SFO1 125.7464750 MHz

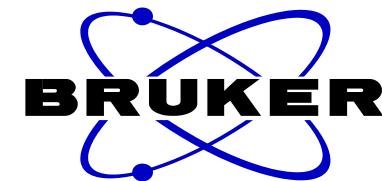
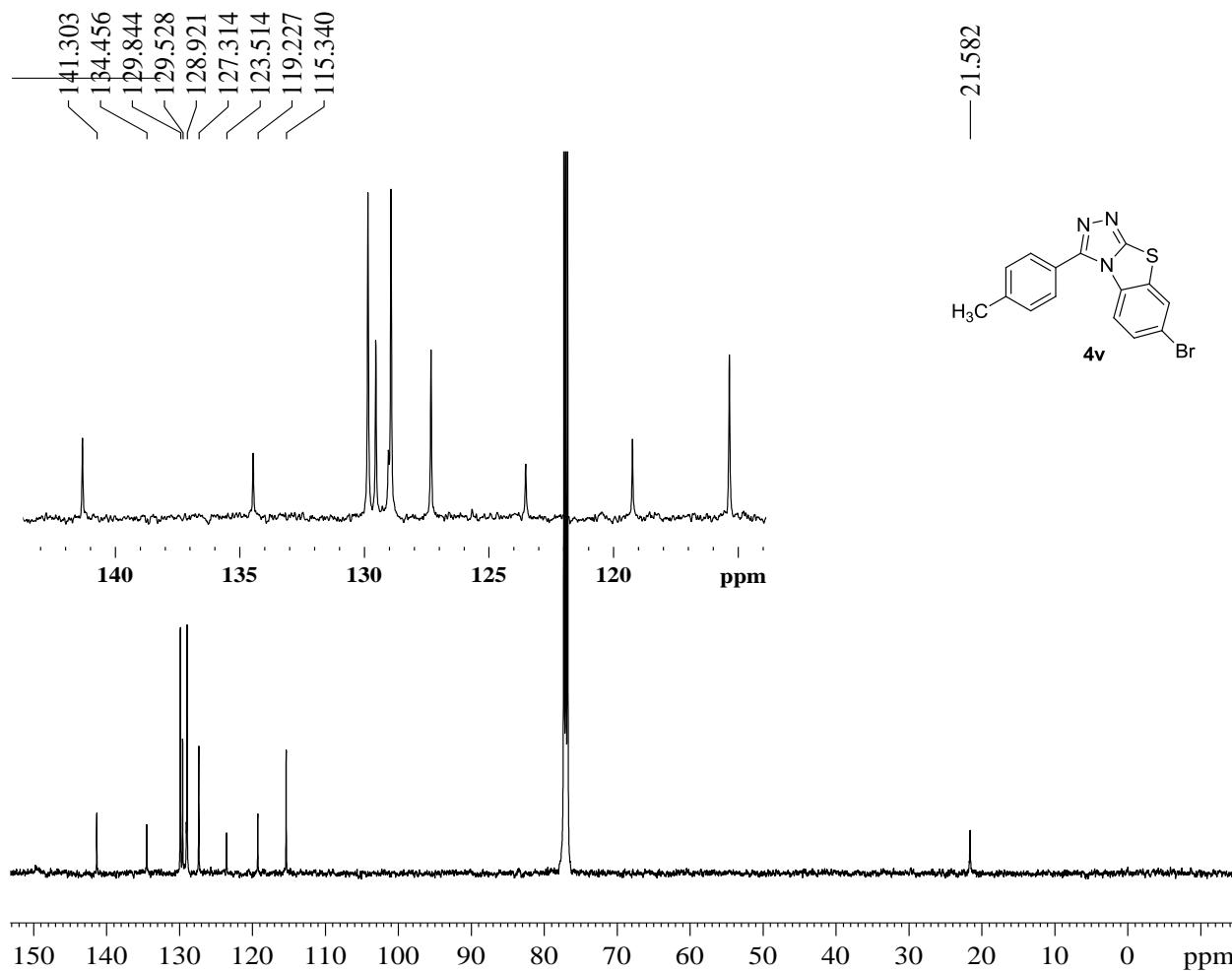
===== CHANNEL f2 =====

CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.60 dB
 PL12 17.66 dB
 PL13 17.66 dB
 SFO2 500.0355000 MHz
 SI 32768
 SF 125.7326422 MHz
 WDW EM



NAME lm-2-27b
 EXPNO 1
 PROCNO 1
 Date 20130702
 Time 17.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 16384
 SOLVENT CDCl₃
 NS 8
 DS 1
 SWH 10000.000 Hz
 FIDRES 0.610352 Hz
 AQ 0.8193000 sec
 RG 724
 DW 50.000 usec
 DE 8.00 usec
 TE 297.9 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 13.00 usec
 PL1 2.00 dB
 SFO1 500.0338500 MHz
 SI 16384
 SF 500.0300085 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 2.00



NAME lm-2-27b
 EXPNO 2
 PROCNO 1
 Date_ 20130705
 Time 12.18
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 2500
 DS 2
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 1820
 DW 15.300 usec
 DE 6.00 usec
 TE 298.0 K
 D1 2.0000000 sec
 d11 0.03000000 sec
 DELTA 1.8999998 sec
 TDO 5

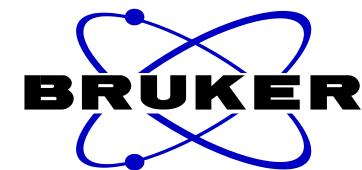
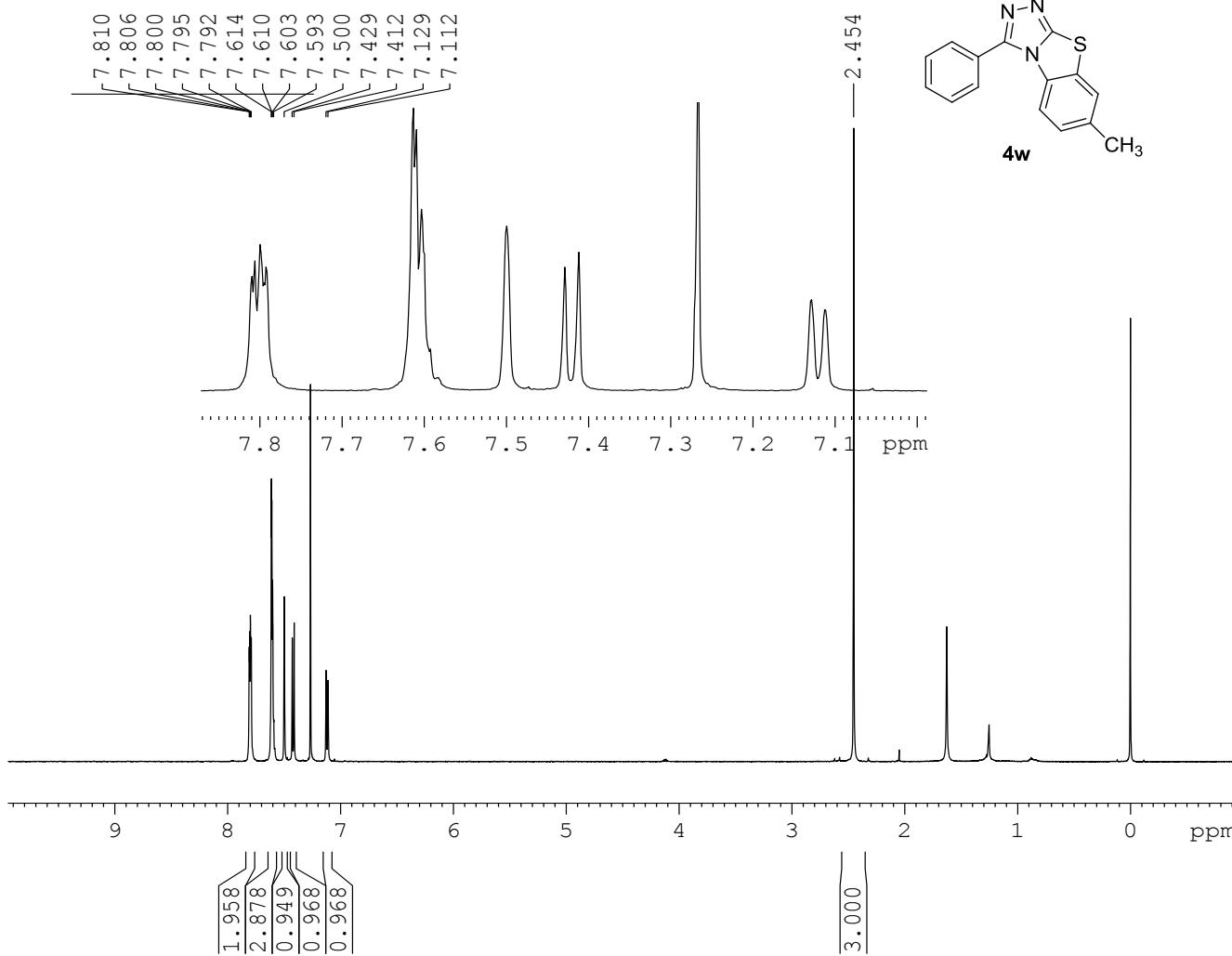
===== CHANNEL f1 =====

NUC1 ¹³C
 P1 12.20 usec
 PL1 3.00 dB
 SFO1 125.7464750 MHz

===== CHANNEL f2 =====

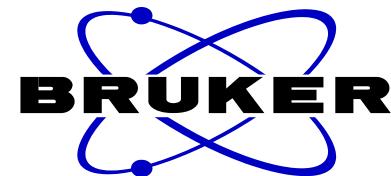
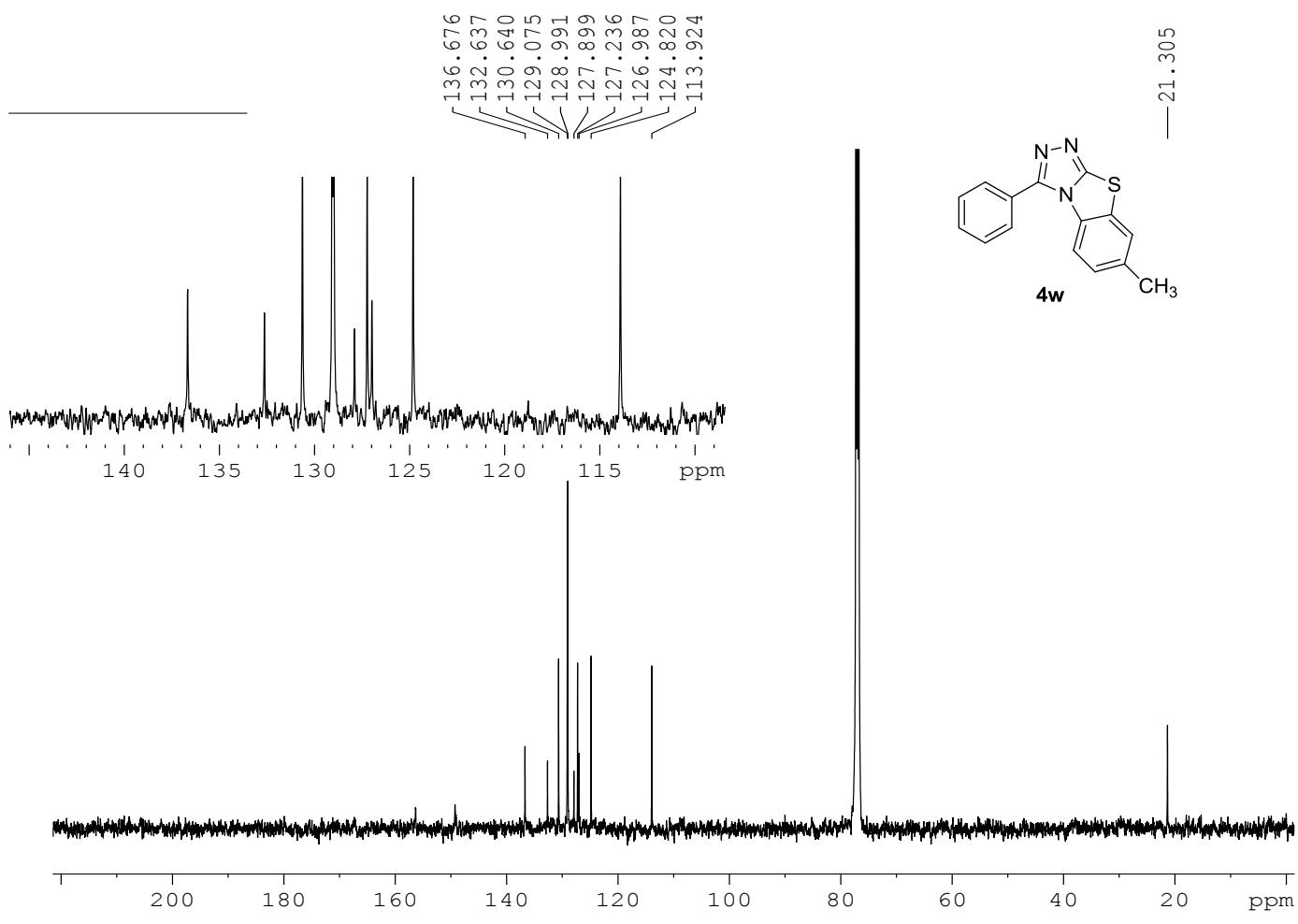
CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.00 dB
 PL12 17.70 dB
 PL13 17.70 dB
 SFO2 500.0355000 MHz
 SI 32768
 SF 125.7326466 MHz
 WDW EM

LM-2-12B 1H 2012 04 12



LM-2-12B

13C 1D 2012 04 12



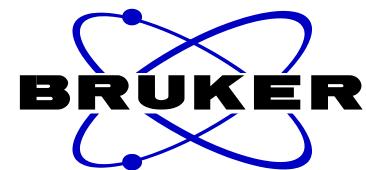
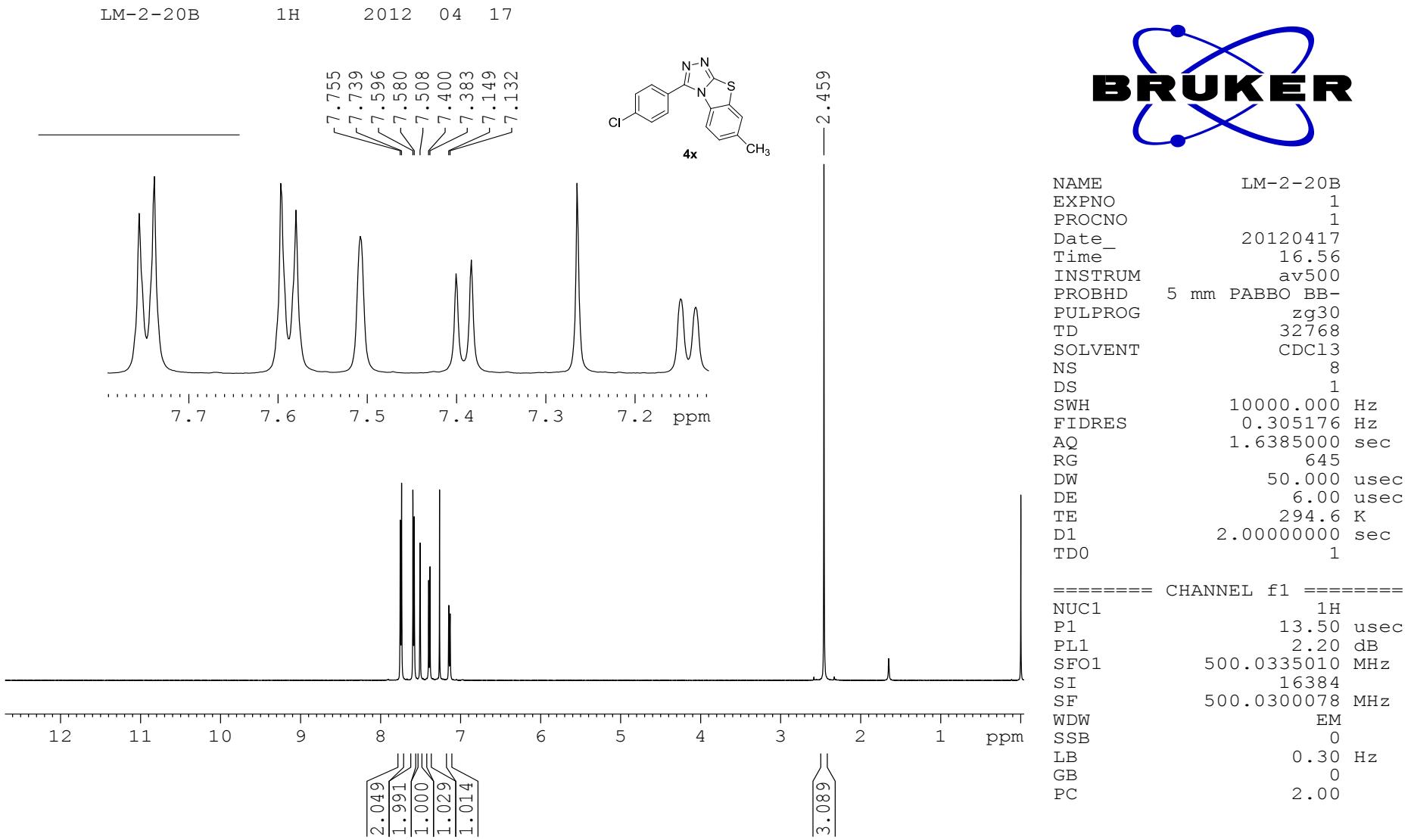
NAME	LM-2-12B
EXPNO	2
PROCNO	1
Date	20120414
Time	12.13
INSTRUM	av500
PROBHDL	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	2707
DS	2
SWH	32679.738 Hz
FIDRES	0.498653 Hz
AQ	1.0027661 sec
RG	812
DW	15.300 usec
DE	6.00 usec
TE	295.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TDO	1

```
===== CHANNEL f1 ======  
NUC1          13C  
P1           9.60  usec  
PL1          2.00  dB  
SFO1        125.7464750 MHz
```

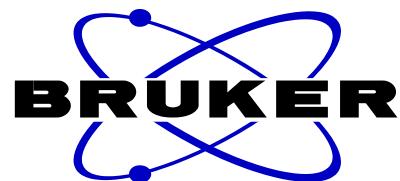
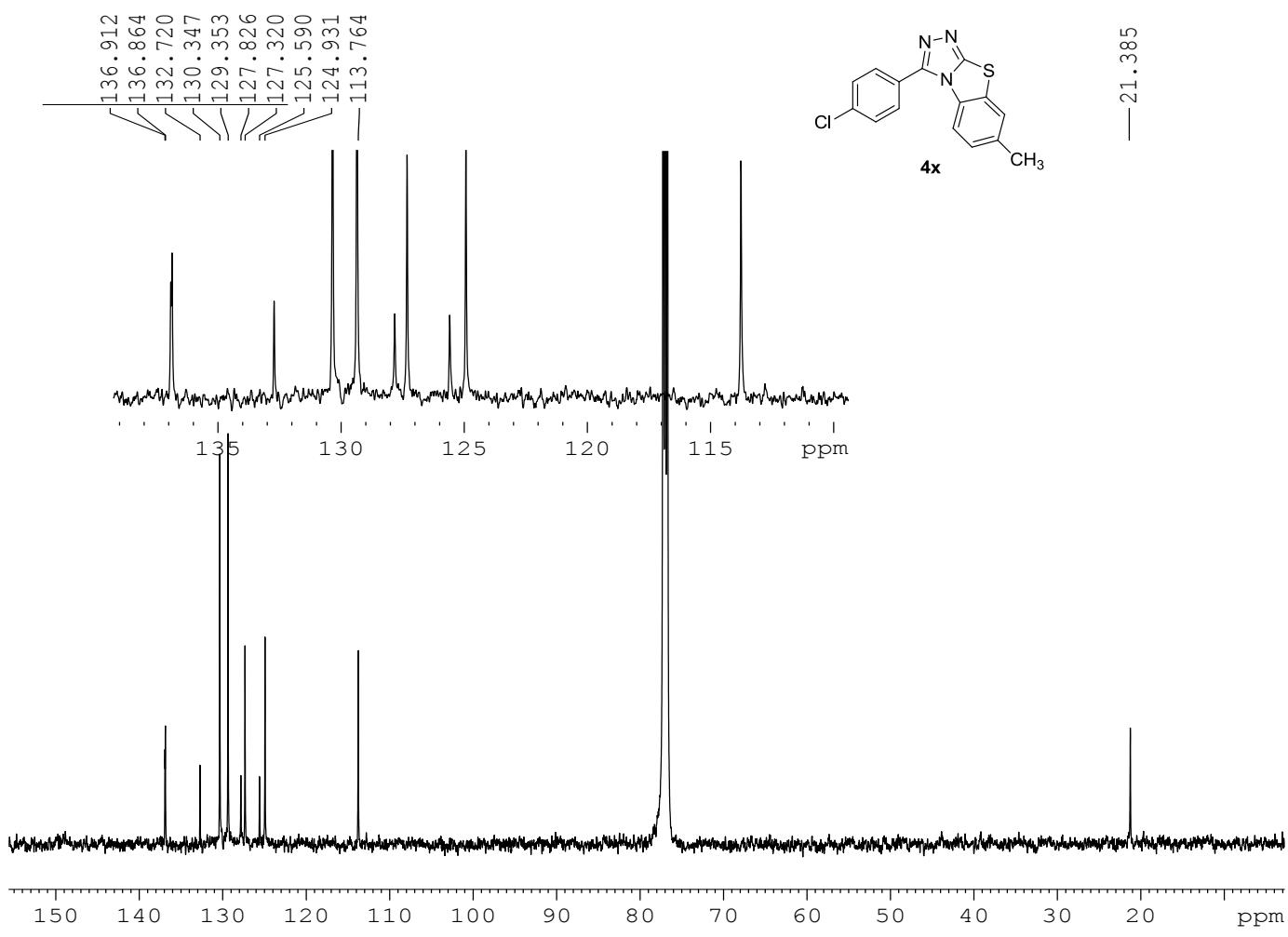
```

===== CHANNEL f2 =====
CPDPRG2          waltz16
NUC2              1H
PCPD2            80.00  usec
PL2               2.60  dB
PL12              17.66 dB
PL13              17.66 dB
SFO2             500.0355000 MHz
SI                32768
SF                125.7326482 MHz
WDW               EM
SSB               0
LB                5.00  Hz
GB               0
PC               2.00

```



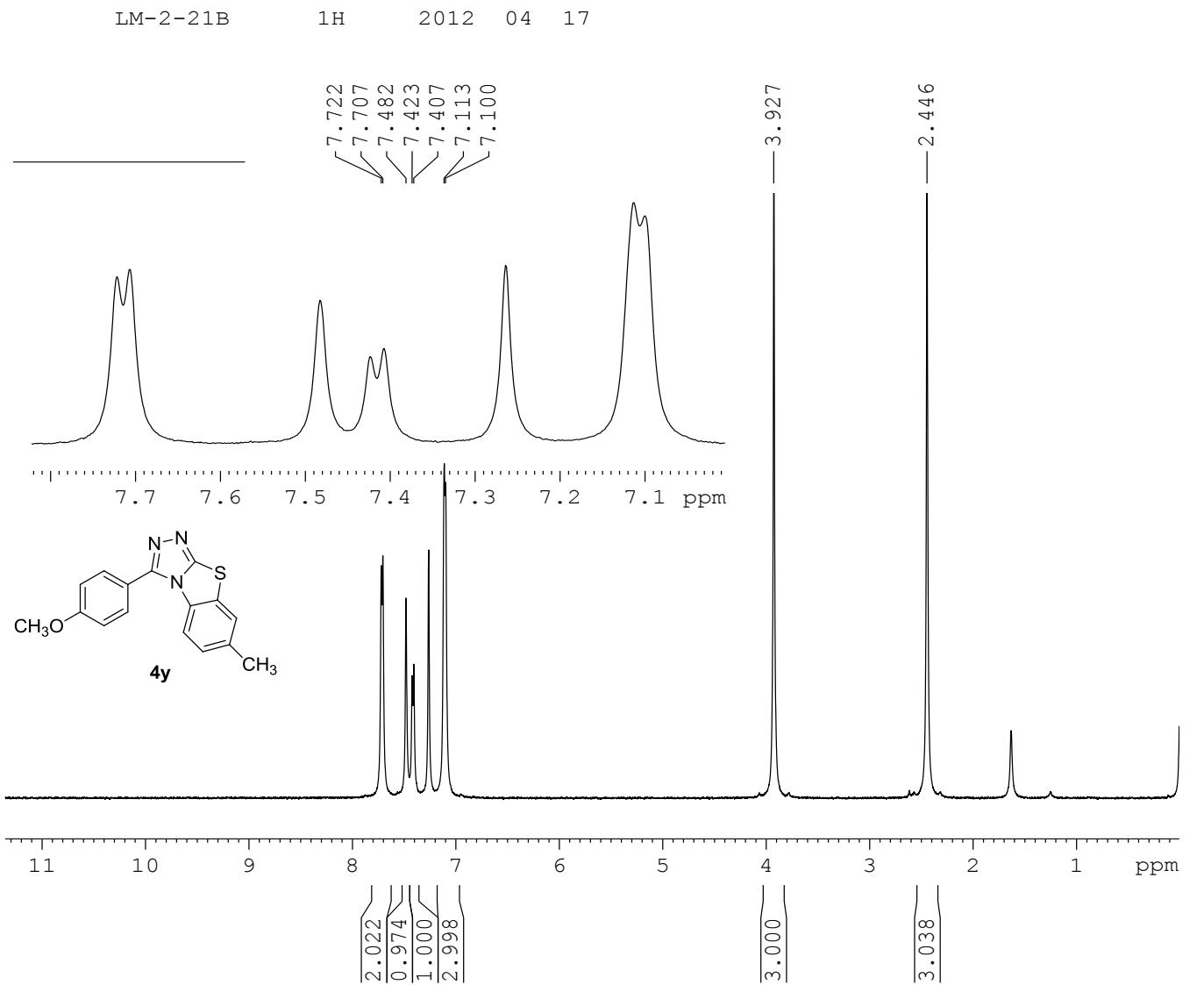
LM-2-20B 13C 1D 2012 04 19

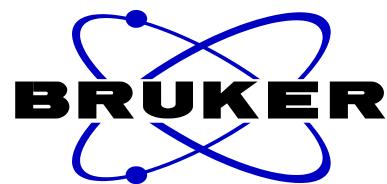
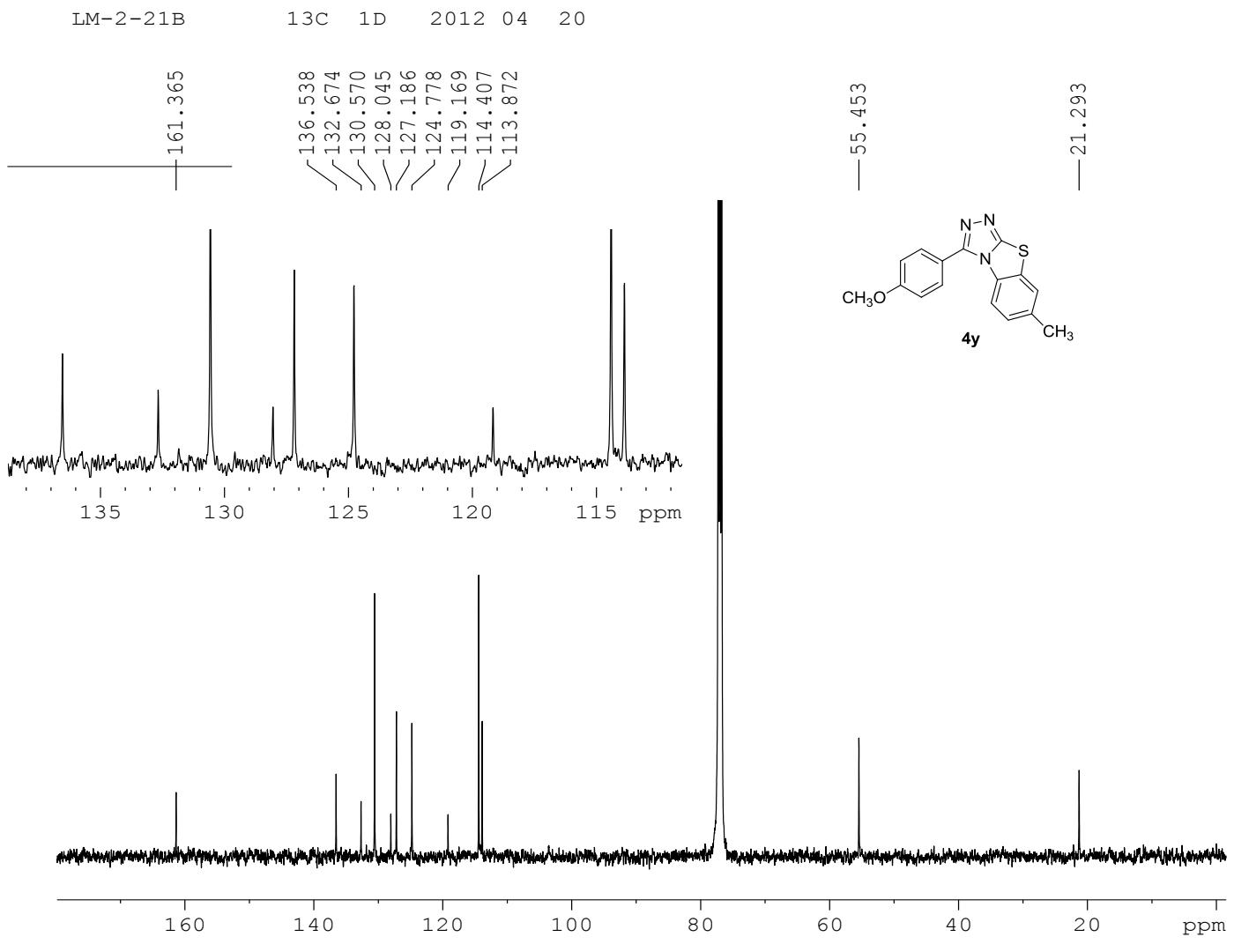


NAME LM-2-20B
EXPNO 2
PROCNO 1
Date_ 20120419
Time_ 13.48
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2000
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 812
DW 15.300 usec
DE 6.00 usec
TE 298.7 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 ======
NUC1 13C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

===== CHANNEL f2 ======
CPDPG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.60 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326482 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 2.00





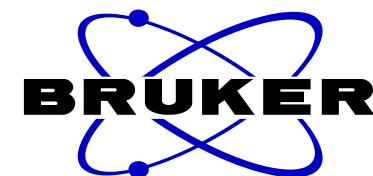
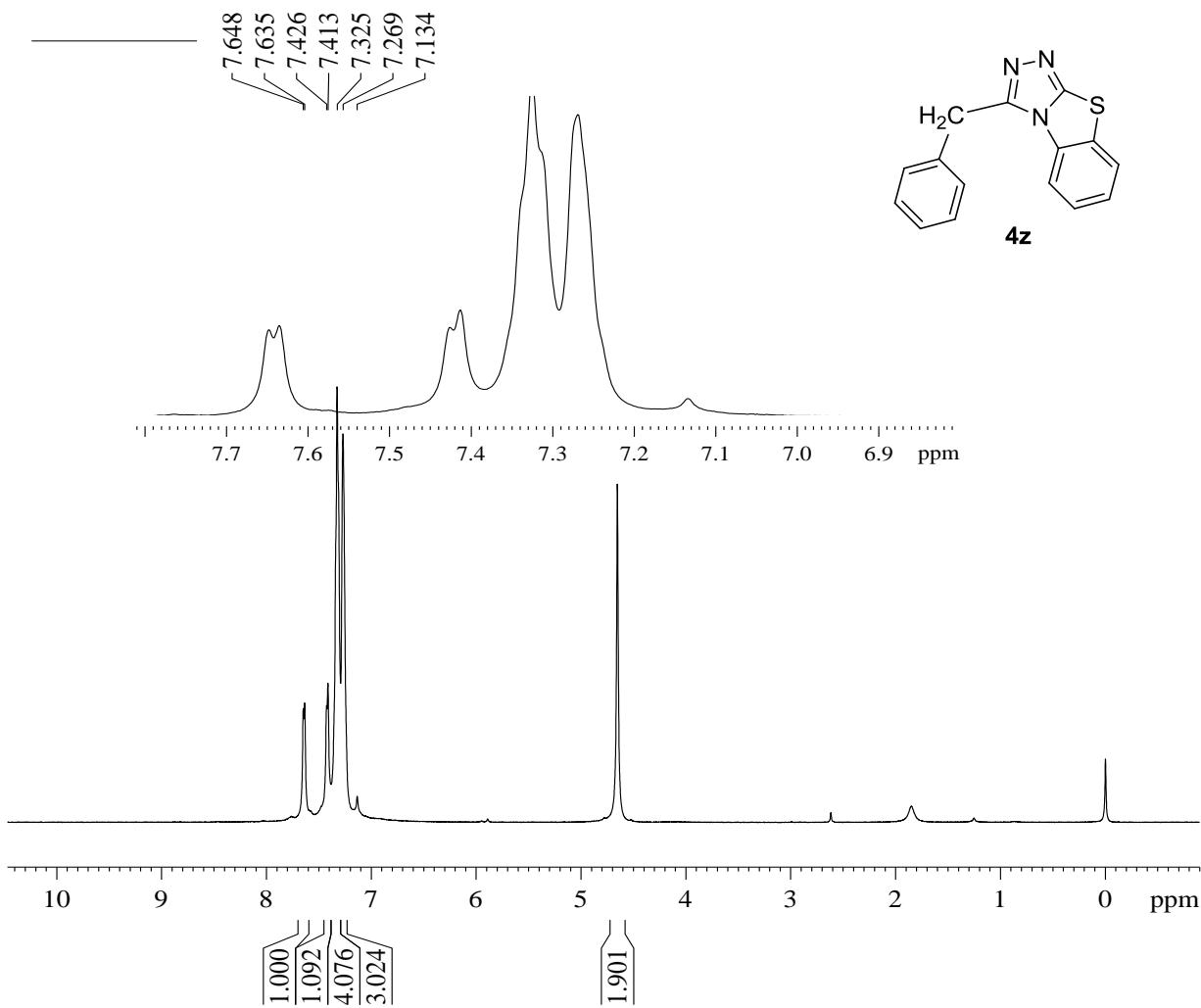
NAME LM-2-21B
 EXPNO 2
 PROCNO 1
 Date 20120420
 Time 10.14
 av500
 INSTRUM PABBO BB-
 PROBHD 5 mm PABBO BB-
 PULPROG zgppg30
 TD 65536
 SOLVENT CDCl3
 NS 2000
 DS 2
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 812
 DW 15.300 usec
 DE 6.00 usec
 TE 295.6 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====

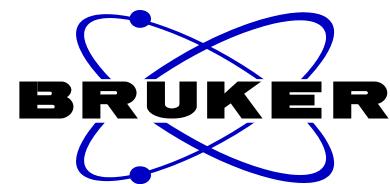
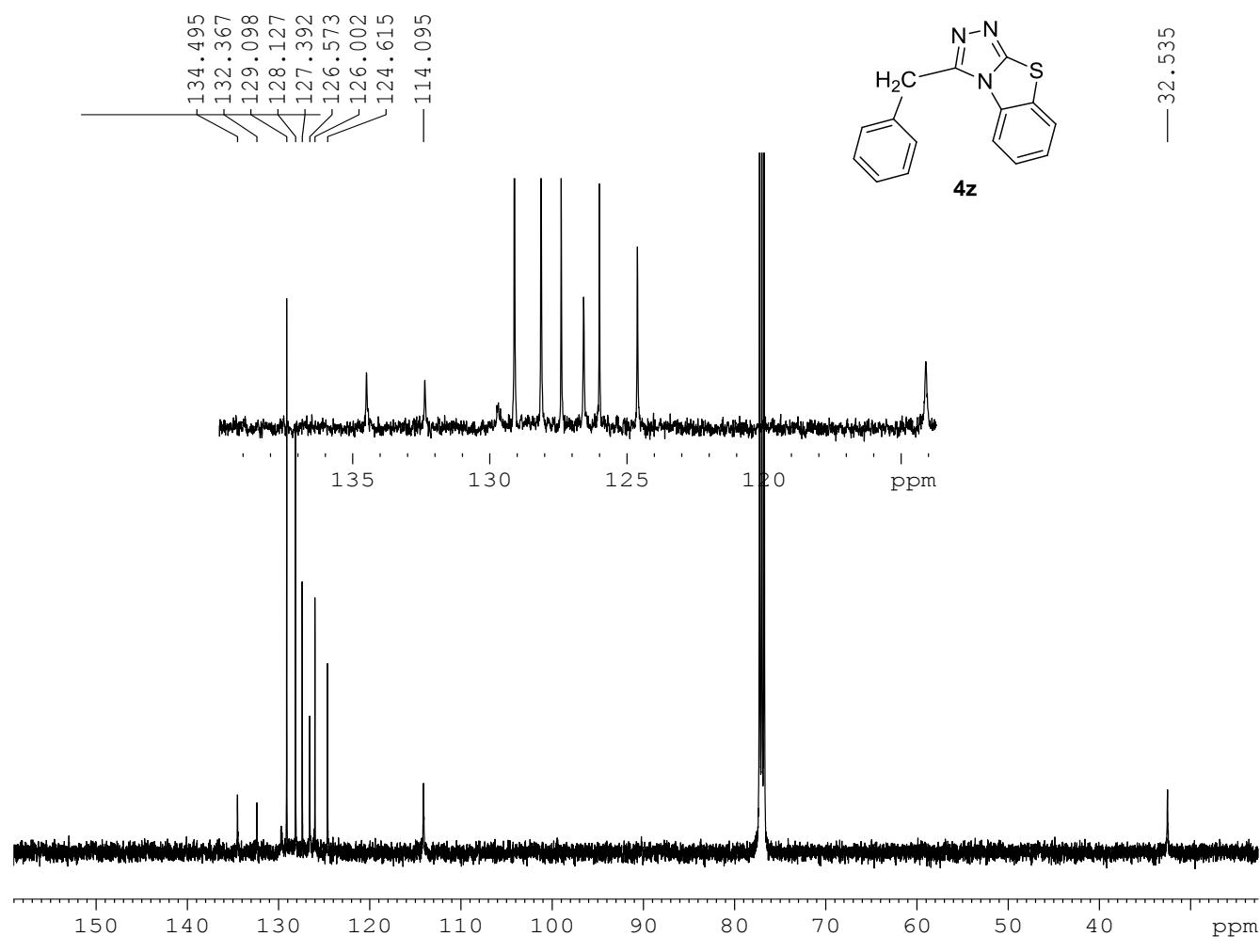
NUC1 13C
 P1 9.60 usec
 PL1 2.00 dB
 SFO1 125.7464750 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.60 dB
 PL12 17.66 dB
 PL13 17.66 dB
 SFO2 500.0355000 MHz
 SI 32768
 SF 125.7326482 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 2.00



LM-2-9B 13C 1D 2012 04 06



NAME LM-2-9B
EXPNO 2
PROCNO 1
Date 20120406
Time 13.38
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 1200
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 4100
DW 15.300 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1
===== CHANNEL f1 =====
NUC1 ¹³C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz
===== CHANNEL f2 =====
CPDPG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.60 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326513 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00