

Supplementary Material for

Systematic Color Tuning of a Family of Luminescent Azole-Based Organoboron Compounds for OLED applications.

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TDDFT Calculation for 5

B3LYP

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.2647 eV 379.77 nm f=0.2248
98 -> 99 0.66905

This state for optimization and/or second-order correction.

Total Energy, E(RPA) = -1193.82763139

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.5980 eV 344.59 nm f=0.0056
96 -> 99 -0.11310
97 -> 99 0.69504

Excited State 3: Singlet-A 3.7313 eV 332.28 nm f=0.0060
96 -> 99 0.69427
97 -> 99 0.11296

Excited State 4: Singlet-A 3.8139 eV 325.08 nm f=0.0103
94 -> 99 0.14194
95 -> 99 0.68859

Excited State 5: Singlet-A 3.9154 eV 316.66 nm f=0.0004
94 -> 99 0.69089
95 -> 99 -0.14148

Excited State 6: Singlet-A 4.2017 eV 295.08 nm f=0.4226
93 -> 99 0.65652
98 ->102 -0.10464

Excited State 7: Singlet-A 4.5168 eV 274.50 nm f=0.0303
92 -> 99 0.62899
98 ->100 0.24707

Excited State 8: Singlet-A 4.7482 eV 261.12 nm f=0.0218
91 -> 99 -0.13748
92 -> 99 -0.21577
98 ->100 0.62955

Excited State 9: Singlet-A 4.9169 eV 252.16 nm f=0.0809
91 -> 99 0.66308
98 ->100 0.11309
98 ->102 -0.11238

Excited State 10: Singlet-A 5.0522 eV 245.40 nm f=0.0060
95 ->100 -0.11233
97 ->100 0.63861
98 ->101 -0.12554

Excited State 11: Singlet-A 5.0573 eV 245.16 nm f=0.0376
90 -> 99 -0.20850
92 -> 99 0.10009

97 ->100 0.14881
98 ->101 0.56431
98 ->102 0.27956

Excited State 12: Singlet-A 5.1305 eV 241.66 nm f=0.0104

95 ->100 -0.17670
95 ->103 -0.10983
95 ->105 -0.10073
96 ->100 0.57842
98 ->102 0.10440

Excited State 13: Singlet-A 5.1336 eV 241.51 nm f=0.1073

90 -> 99 -0.13717
91 -> 99 0.10546
96 ->100 -0.10477
98 ->101 -0.32341
98 ->102 0.51120
98 ->103 0.16382

Excited State 14: Singlet-A 5.2079 eV 238.07 nm f=0.0031

90 -> 99 0.13621
94 ->103 -0.13372
95 ->100 0.38054
95 ->105 0.11071
95 ->106 -0.10677
96 ->100 0.17178
97 ->100 0.20138
97 ->102 0.18115
97 ->103 0.11363
97 ->105 -0.15261
97 ->106 -0.11440
98 ->103 0.25983

Excited State 15: Singlet-A 5.2269 eV 237.20 nm f=0.0010

90 -> 99 0.20272
95 ->100 -0.37636
96 ->100 -0.18834
98 ->103 0.46603

Excited State 16: Singlet-A 5.2710 eV 235.22 nm f=0.0099

90 -> 99 0.11660
94 ->100 -0.15565
94 ->102 0.10007
94 ->103 0.16640
95 ->100 0.38156
95 ->103 -0.11574
95 ->105 -0.19499
97 ->102 -0.21508
97 ->103 -0.14411
97 ->105 0.14826
98 ->103 0.17198
98 ->105 -0.12968

Excited State 17: Singlet-A 5.2744 eV 235.07 nm f=0.0043

94 ->106	-0.15072
96 ->100	-0.22763
96 ->103	-0.18016
96 ->105	0.11998
96 ->106	-0.14204
97 ->102	0.11392
97 ->106	-0.10152
97 ->108	-0.11824
97 ->109	0.12398
98 ->103	-0.17038
98 ->104	0.32335
98 ->105	-0.25611
98 ->106	-0.11039

Excited State 18: Singlet-A 5.3071 eV 233.62 nm f=0.0015

94 ->106	0.10157
95 ->103	0.10484
95 ->105	0.11793
96 ->100	0.14281
96 ->103	0.12897
96 ->105	-0.12773
97 ->108	0.10098
98 ->103	0.10767
98 ->104	0.49458
98 ->106	-0.11946
98 ->107	-0.13678

Excited State 19: Singlet-A 5.3171 eV 233.18 nm f=0.0066

88 -> 99	0.23749
89 -> 99	0.61032
98 ->104	0.13034

Excited State 20: Singlet-A 5.3372 eV 232.30 nm f=0.0051

94 ->100	0.66138
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Excited State 21: Singlet-A 5.3503 eV 231.73 nm f=0.0005

90 -> 99	-0.24831
98 ->104	0.16877
98 ->106	0.56472
98 ->107	-0.11801

Excited State 22: Singlet-A 5.3798 eV 230.46 nm f=0.0495

90 -> 99	-0.21692
97 ->101	0.50480
97 ->102	-0.19730
98 ->103	0.14557
98 ->105	0.21590
98 ->106	-0.12205

Excited State 23: Singlet-A 5.3911 eV 229.98 nm f=0.1362

90 -> 99	0.33496
93 ->101	-0.12153
97 ->101	0.40197
98 ->102	0.14768

98 ->103	-0.18872
98 ->106	0.29273
Excited State 24: Singlet-A	5.3952 eV 229.80 nm f=0.0194
90 -> 99	0.17176
97 ->101	-0.13006
97 ->102	0.17508
98 ->104	0.15179
98 ->105	0.53068
98 ->107	-0.16625
Excited State 25: Singlet-A	5.4554 eV 227.27 nm f=0.0120
93 ->100	0.21716
96 ->101	0.38205
96 ->102	-0.16941
97 ->101	0.13061
97 ->102	0.42138
97 ->105	0.12819
Excited State 26: Singlet-A	5.4905 eV 225.81 nm f=0.0242
95 ->101	-0.15386
96 ->101	0.49635
97 ->101	-0.13751
97 ->102	-0.30073
97 ->103	0.12069
97 ->105	-0.14450
Excited State 27: Singlet-A	5.5219 eV 224.53 nm f=0.0324
92 ->101	-0.24890
93 ->100	0.54692
96 ->101	-0.21189
Excited State 28: Singlet-A	5.5523 eV 223.30 nm f=0.0016
95 ->101	0.66659
96 ->101	0.16474
Excited State 29: Singlet-A	5.5876 eV 221.89 nm f=0.0031
96 ->102	-0.23145
96 ->105	-0.12951
97 ->103	0.50288
97 ->104	-0.20095
97 ->105	0.24359
Excited State 30: Singlet-A	5.6012 eV 221.35 nm f=0.0019
98 ->104	0.18997
98 ->105	0.14828
98 ->107	0.60324
Excited State 31: Singlet-A	5.6076 eV 221.10 nm f=0.0079
94 ->102	0.21865
94 ->103	0.10196
96 ->102	0.53414
96 ->103	-0.11825
97 ->102	0.11007

97 ->103 0.14410
97 ->105 0.14358
98 ->107 0.13310
98 ->108 0.15100
98 ->109 -0.10509

Excited State 32: Singlet-A 5.6225 eV 220.51 nm f=0.0273

96 ->102 -0.16591
98 ->105 -0.10455
98 ->108 0.50442
98 ->109 -0.36700

Excited State 33: Singlet-A 5.6530 eV 219.33 nm f=0.0034

94 ->101 0.67459

Excited State 34: Singlet-A 5.6655 eV 218.84 nm f=0.0070

94 ->102 0.15616
95 ->102 0.56378
96 ->102 -0.13103
97 ->103 0.11128
97 ->104 0.17385
97 ->106 0.16105

Excited State 35: Singlet-A 5.6845 eV 218.11 nm f=0.0049

95 ->102 -0.23342
97 ->103 0.20572
97 ->104 0.51189
97 ->108 0.12808
97 ->109 0.14717
97 ->110 0.16568
98 ->109 0.10053

Excited State 36: Singlet-A 5.7401 eV 216.00 nm f=0.0134

88 -> 99 0.30498
89 -> 99 -0.12548
94 ->102 -0.25283
95 ->102 0.11587
96 ->103 -0.31268
96 ->105 -0.10596
97 ->103 -0.15165
97 ->105 0.24109
97 ->106 -0.18720

Excited State 37: Singlet-A 5.7491 eV 215.66 nm f=0.0013

88 -> 99 0.54251
89 -> 99 -0.21727
94 ->102 0.15060
95 ->102 -0.12934
96 ->103 0.21677

Excited State 38: Singlet-A 5.7669 eV 214.99 nm f=0.0097

95 ->102 0.13234
95 ->103 -0.24008
95 ->105 0.16910

96 ->103	0.27590
96 ->105	0.12767
96 ->108	0.16433
97 ->105	0.30285
97 ->106	-0.19141
97 ->109	0.14904
98 ->109	-0.16241

Excited State 39: Singlet-A 5.7754 eV 214.68 nm f=0.0049

94 ->102	0.15002
95 ->105	0.13894
96 ->103	0.16604
96 ->104	-0.20073
97 ->104	-0.13236
98 ->108	0.33047
98 ->109	0.42783
98 ->112	-0.11716

Excited State 40: Singlet-A 5.8038 eV 213.62 nm f=0.0057

94 ->110	0.11242
95 ->104	0.15762
96 ->104	0.53402
96 ->108	0.12066
96 ->109	0.15156
98 ->108	0.13447
98 ->109	0.17611

TDDFT Calculation for **6**

B3LYP

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.0959 eV 400.47 nm f=0.2170
102 ->103 0.66850

This state for optimization and/or second-order correction.

Total Energy, E(RPA) = -1516.80925887

Copying the excited state density for this state as the 1-particle RhoCl density.

Excited State 2: Singlet-A 3.4389 eV 360.53 nm f=0.0051
100 ->103 -0.12140
101 ->103 0.69314

Excited State 3: Singlet-A 3.5444 eV 349.80 nm f=0.0033
100 ->103 0.69313
101 ->103 0.12160

Excited State 4: Singlet-A 3.6442 eV 340.23 nm f=0.0058
98 ->103 -0.14575
99 ->103 0.68793

Excited State 5: Singlet-A 3.7543 eV 330.25 nm f=0.0004
98 ->103 0.68992
99 ->103 0.14456

Excited State 6: Singlet-A 3.9603 eV 313.07 nm f=0.2978
96 ->103 -0.15969
97 ->103 0.64633

Excited State 7: Singlet-A 4.1005 eV 302.36 nm f=0.1214
96 ->103 0.64696
97 ->103 0.15464
102 ->104 0.11431

Excited State 8: Singlet-A 4.5938 eV 269.89 nm f=0.0284
95 ->103 -0.19138
102 ->104 0.64781

Excited State 9: Singlet-A 4.7112 eV 263.17 nm f=0.0596
95 ->103 0.65789
102 ->104 0.18425

Excited State 10: Singlet-A 4.7921 eV 258.73 nm f=0.0059
102 ->105 0.66238

Excited State 11: Singlet-A 4.9440 eV 250.78 nm f=0.0016
99 ->104 0.14115
100 ->104 0.17806
101 ->104 0.64934

Excited State 12: Singlet-A 4.9695 eV 249.49 nm f=0.0137

99 ->104	0.12708
100 ->104	0.61873
101 ->104	-0.21227
102 ->106	0.11069
Excited State 13: Singlet-A 4.9913 eV 248.40 nm f=0.0182	
94 ->103	0.43228
100 ->104	-0.13247
102 ->106	0.29357
102 ->107	0.41877
Excited State 14: Singlet-A 5.0395 eV 246.03 nm f=0.0115	
92 ->103	0.12762
93 ->103	0.63110
102 ->106	0.20465
Excited State 15: Singlet-A 5.0456 eV 245.73 nm f=0.0258	
93 ->103	-0.23256
94 ->103	-0.18158
96 ->104	-0.14640
102 ->106	0.54646
102 ->107	-0.17919
Excited State 16: Singlet-A 5.0899 eV 243.59 nm f=0.0085	
99 ->104	0.65428
100 ->104	-0.17203
101 ->104	-0.10242
Excited State 17: Singlet-A 5.1337 eV 241.51 nm f=0.1102	
94 ->103	-0.36779
96 ->104	-0.12809
96 ->106	-0.12940
102 ->107	0.44163
102 ->108	0.20379
Excited State 18: Singlet-A 5.1848 eV 239.13 nm f=0.0115	
98 ->104	0.62424
100 ->104	0.11125
Excited State 19: Singlet-A 5.2238 eV 237.35 nm f=0.0061	
94 ->103	0.12673
98 ->104	0.22988
98 ->107	-0.13377
98 ->108	-0.13203
99 ->104	-0.12327
99 ->110	0.15230
100 ->107	0.13672
100 ->110	0.10835
100 ->113	-0.12510
101 ->107	0.11439
102 ->108	0.35790
102 ->109	0.22622
Excited State 20: Singlet-A 5.2386 eV 236.68 nm f=0.0125	

94 ->103	0.11179
98 ->107	0.15458
98 ->111	0.14244
99 ->108	0.16282
99 ->109	0.11955
100 ->104	0.11733
100 ->107	-0.13784
100 ->108	-0.17187
100 ->110	-0.22476
101 ->107	0.11258
101 ->111	0.14828
101 ->113	0.18297
102 ->108	0.19392
102 ->110	0.27527

Excited State 21: Singlet-A 5.2602 eV 235.70 nm f=0.0059

98 ->104	-0.12599
98 ->108	0.13319
99 ->110	-0.14620
99 ->111	0.10754
100 ->111	-0.11400
100 ->113	0.10982
101 ->106	0.15905
101 ->107	-0.24553
101 ->108	-0.12179
101 ->110	-0.13474
101 ->111	-0.13117
101 ->113	-0.11139
102 ->108	0.34327
102 ->109	0.15997
102 ->110	0.13582
102 ->111	-0.12430

Excited State 22: Singlet-A 5.2991 eV 233.97 nm f=0.0016

96 ->105	0.13655
97 ->104	0.18054
100 ->105	-0.18074
101 ->105	0.60309

Excited State 23: Singlet-A 5.3127 eV 233.37 nm f=0.0155

97 ->104	0.10049
102 ->108	-0.20540
102 ->109	0.61730

Excited State 24: Singlet-A 5.3266 eV 232.77 nm f=0.0148

94 ->103	-0.10881
96 ->105	0.12674
96 ->106	0.15753
97 ->104	0.46988
97 ->106	-0.10945
100 ->106	-0.16377
101 ->105	-0.27957
102 ->108	0.14953

Excited State 25: Singlet-A 5.3667 eV 231.02 nm f=0.0444
97 ->105 0.10445
100 ->105 0.21517
101 ->106 0.40475
102 ->110 -0.26958
102 ->111 0.33885

Excited State 26: Singlet-A 5.3723 eV 230.78 nm f=0.0041
100 ->106 -0.12118
101 ->106 0.35607
102 ->108 -0.18000
102 ->110 0.49810

Excited State 27: Singlet-A 5.3906 eV 230.00 nm f=0.0243
96 ->105 0.10431
100 ->105 -0.39097
100 ->106 -0.11373
101 ->106 -0.10820
101 ->107 -0.16980
102 ->111 0.45114
102 ->113 0.10009

Excited State 28: Singlet-A 5.4016 eV 229.53 nm f=0.0069
97 ->104 0.23143
100 ->105 0.37140
101 ->105 0.11688
101 ->106 -0.34239
102 ->110 0.16123
102 ->111 0.26179

Excited State 29: Singlet-A 5.4205 eV 228.73 nm f=0.0055
96 ->105 0.26372
97 ->105 -0.20708
99 ->106 0.14153
100 ->106 0.52812

Excited State 30: Singlet-A 5.4518 eV 227.42 nm f=0.0096
96 ->105 -0.16429
97 ->105 0.18680
99 ->105 0.10018
100 ->105 -0.20594
100 ->106 0.15599
100 ->107 -0.15508
101 ->107 0.46272
101 ->110 -0.13246
102 ->111 0.12774

Excited State 31: Singlet-A 5.4692 eV 226.69 nm f=0.0227
96 ->104 -0.12375
96 ->105 0.20333
96 ->106 -0.11031
97 ->105 -0.22638
97 ->106 0.14613
99 ->105 -0.12253

100 ->105	0.22475
100 ->106	-0.26546
101 ->107	0.29193
101 ->110	-0.13793

Excited State 32: Singlet-A 5.4932 eV 225.71 nm f=0.0107

96 ->104	-0.10678
98 ->105	-0.15693
99 ->105	0.57364
99 ->106	0.25292
100 ->106	-0.15846

Excited State 33: Singlet-A 5.5337 eV 224.05 nm f=0.0215

98 ->105	0.16087
99 ->105	-0.22519
99 ->106	0.59306

Excited State 34: Singlet-A 5.5710 eV 222.55 nm f=0.1069

92 ->103	0.22001
96 ->104	-0.33345
97 ->104	0.11223
97 ->105	0.31321
97 ->106	0.12178
98 ->105	-0.25620
98 ->106	-0.16128
99 ->105	-0.14190
99 ->107	-0.11166
100 ->107	0.13864

Excited State 35: Singlet-A 5.5776 eV 222.29 nm f=0.0824

92 ->103	-0.22082
96 ->104	0.22420
97 ->104	-0.11578
97 ->106	-0.18161
98 ->105	-0.26684
98 ->106	-0.14952
98 ->107	0.12628
99 ->106	0.10743
100 ->107	0.36673

Excited State 36: Singlet-A 5.5838 eV 222.04 nm f=0.0089

92 ->103	0.54403
93 ->103	-0.12120
96 ->104	0.14008
97 ->105	-0.10098
100 ->107	0.16242
102 ->113	0.25233

Excited State 37: Singlet-A 5.6032 eV 221.27 nm f=0.0589

96 ->104	-0.12281
96 ->105	-0.14569
97 ->105	-0.17490
97 ->106	0.14059
98 ->105	0.28178

98 ->106	-0.25713
98 ->107	0.17537
99 ->105	0.13564
99 ->106	-0.11273
100 ->107	0.31224
101 ->108	-0.10367
102 ->113	-0.18561

Excited State 38: Singlet-A 5.6189 eV 220.66 nm f=0.0267

92 ->103	-0.16464
96 ->105	-0.17673
97 ->105	-0.14776
98 ->105	-0.11356
98 ->106	-0.32629
102 ->113	0.46194

Excited State 39: Singlet-A 5.6247 eV 220.43 nm f=0.0217

92 ->103	-0.14752
96 ->104	-0.11240
96 ->105	0.18533
97 ->105	0.19264
98 ->105	0.26378
98 ->106	0.29317
98 ->107	0.17427
100 ->107	0.16526
102 ->113	0.33732

Excited State 40: Singlet-A 5.6420 eV 219.75 nm f=0.0041

98 ->107	0.10975
101 ->107	-0.10821
101 ->108	0.54988
101 ->110	-0.16161
102 ->112	-0.20293

TDDFT Calculation for **7a**

B3LYP

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.7675 eV 447.99 nm f=0.0487
111 ->112 0.67122

This state for optimization and/or second-order correction.

Total Energy, E(RPA) = -1347.52212958

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.3801 eV 366.81 nm f=0.0073
108 ->112 -0.13020
109 ->112 -0.12799
110 ->112 0.68041

Excited State 3: Singlet-A 3.4936 eV 354.89 nm f=0.3149
108 ->112 -0.32554
109 ->112 0.59661

Excited State 4: Singlet-A 3.5372 eV 350.51 nm f=0.4362
108 ->112 0.60453
109 ->112 0.26067
110 ->112 0.15659

Excited State 5: Singlet-A 3.5988 eV 344.52 nm f=0.0196
106 ->112 -0.15196
107 ->112 0.68685

Excited State 6: Singlet-A 3.7028 eV 334.83 nm f=0.0020
106 ->112 0.68776
107 ->112 0.15264

Excited State 7: Singlet-A 4.3052 eV 287.99 nm f=0.1951
103 ->112 -0.12696
105 ->112 -0.29560
111 ->113 0.59779

Excited State 8: Singlet-A 4.3485 eV 285.12 nm f=0.1410
104 ->112 -0.18370
105 ->112 0.58644
109 ->114 0.12075
111 ->113 0.25961

Excited State 9: Singlet-A 4.4940 eV 275.89 nm f=0.0436
103 ->112 0.41387
104 ->112 -0.17639
109 ->113 -0.26207
110 ->113 -0.10132
111 ->114 0.40099
111 ->115 0.13624

Excited State 10: Singlet-A 4.5636 eV 271.68 nm f=0.2406

103 ->112 -0.12737
104 ->112 0.55398
105 ->112 0.11854
111 ->114 0.34874

Excited State 11: Singlet-A 4.6864 eV 264.56 nm f=0.0218

103 ->112 -0.16529
104 ->112 -0.22085
109 ->113 0.16507
109 ->114 -0.10512
111 ->114 0.39838
111 ->115 -0.38722
111 ->120 0.12887

Excited State 12: Singlet-A 4.7867 eV 259.02 nm f=0.2902

102 ->112 0.18552
103 ->112 0.44937
104 ->112 0.15430
109 ->113 0.24159
110 ->113 0.20595
111 ->115 -0.27409

Excited State 13: Singlet-A 4.8245 eV 256.99 nm f=0.0136

109 ->113 -0.18270
110 ->113 0.65213
111 ->115 0.13876

Excited State 14: Singlet-A 4.8999 eV 253.04 nm f=0.0386

102 ->112 -0.25279
109 ->113 0.48203
111 ->115 0.35463

Excited State 15: Singlet-A 4.9510 eV 250.42 nm f=0.0237

101 ->112 -0.14882
102 ->112 -0.42355
108 ->113 0.46232
111 ->115 -0.10706

Excited State 16: Singlet-A 4.9559 eV 250.18 nm f=0.0525

101 ->112 0.12721
102 ->112 0.29838
108 ->113 0.47360
109 ->114 -0.14257
111 ->115 0.25212
111 ->116 -0.11127
111 ->120 0.12845

Excited State 17: Singlet-A 5.0167 eV 247.15 nm f=0.0004

107 ->113 0.61842
107 ->114 0.10130
110 ->114 -0.13871
111 ->116 -0.16734

Excited State 18: Singlet-A 5.0281 eV 246.58 nm f=0.0016

107 ->113	0.21627
111 ->116	0.61054
111 ->117	0.13787
111 ->120	0.13926

Excited State 19: Singlet-A 5.0657 eV 244.75 nm f=0.0089

111 ->116	-0.10078
111 ->117	0.58629
111 ->118	0.19257
111 ->119	0.11099
111 ->120	-0.15688
111 ->121	-0.21511

Excited State 20: Singlet-A 5.0723 eV 244.43 nm f=0.0392

106 ->113	0.13139
107 ->113	0.15003
110 ->114	0.60183

Excited State 21: Singlet-A 5.1038 eV 242.93 nm f=0.0444

101 ->112	0.12719
102 ->112	0.11226
105 ->115	-0.11615
106 ->113	-0.11673
107 ->113	-0.11107
109 ->114	0.49457
111 ->117	0.10736
111 ->118	-0.11750
111 ->119	-0.26673
111 ->120	-0.10898

Excited State 22: Singlet-A 5.1185 eV 242.23 nm f=0.0103

106 ->113	0.55281
107 ->114	0.10210
111 ->119	-0.31901
111 ->121	-0.10032

Excited State 23: Singlet-A 5.1252 eV 241.91 nm f=0.0543

102 ->112	0.11481
106 ->113	0.36281
108 ->114	0.10986
109 ->114	0.23159
111 ->119	0.42877

Excited State 24: Singlet-A 5.1605 eV 240.26 nm f=0.0028

101 ->112	0.14848
106 ->114	0.10180
106 ->116	-0.14839
107 ->116	-0.11558
107 ->118	-0.15877
108 ->114	0.46660
108 ->116	-0.12629
108 ->118	0.10181
111 ->118	0.15114
111 ->119	-0.11670

111 ->121 0.13312

Excited State 25: Singlet-A 5.1694 eV 239.84 nm f=0.0185

100 ->112 0.13481

101 ->112 0.55058

102 ->112 -0.18677

111 ->118 -0.12880

111 ->119 0.25259

111 ->121 -0.10597

Excited State 26: Singlet-A 5.1904 eV 238.87 nm f=0.0950

108 ->114 -0.17860

109 ->114 0.16443

111 ->118 0.53357

111 ->120 0.20674

111 ->121 0.12207

111 ->123 -0.11246

Excited State 27: Singlet-A 5.2329 eV 236.93 nm f=0.1776

101 ->112 -0.15203

108 ->114 0.20077

111 ->118 -0.11442

111 ->120 0.42393

111 ->121 -0.34684

Excited State 28: Singlet-A 5.2779 eV 234.91 nm f=0.0281

106 ->116 0.12677

106 ->119 0.15399

107 ->119 -0.15258

108 ->115 -0.11719

108 ->119 -0.16623

108 ->123 -0.10383

109 ->114 -0.15137

110 ->114 0.24019

110 ->116 0.29242

110 ->118 -0.21540

110 ->123 0.14335

111 ->120 -0.10177

Excited State 29: Singlet-A 5.2979 eV 234.02 nm f=0.0051

106 ->114 -0.10600

107 ->114 0.55528

108 ->114 0.27478

110 ->115 -0.15407

Excited State 30: Singlet-A 5.3174 eV 233.17 nm f=0.0011

111 ->116 -0.11116

111 ->117 0.29106

111 ->118 -0.19207

111 ->120 0.30075

111 ->121 0.43886

111 ->124 -0.22823

111 ->125 -0.10967

Excited State 31: Singlet-A 5.3206 eV 233.03 nm f=0.0021
106 ->114 0.18184
106 ->116 -0.15134
107 ->114 0.36647
107 ->116 -0.11864
107 ->118 -0.18270
108 ->114 -0.23665
108 ->116 -0.12228
108 ->118 0.13506
110 ->115 0.27615

Excited State 32: Singlet-A 5.3348 eV 232.41 nm f=0.0089
106 ->114 -0.16637
108 ->114 0.17851
109 ->115 -0.19488
110 ->115 0.57506

Excited State 33: Singlet-A 5.4096 eV 229.19 nm f=0.0016
106 ->114 0.36327
108 ->115 -0.30617
108 ->116 0.10139
109 ->115 0.24833
110 ->115 0.10446
111 ->122 -0.25448
111 ->123 0.21649

Excited State 34: Singlet-A 5.4129 eV 229.05 nm f=0.0289
106 ->114 0.36225
111 ->122 0.41972
111 ->123 -0.33040

Excited State 35: Singlet-A 5.4225 eV 228.65 nm f=0.0693
106 ->114 0.34834
107 ->115 -0.16398
108 ->115 0.34148
109 ->115 -0.35610
111 ->122 -0.13892

Excited State 36: Singlet-A 5.4519 eV 227.41 nm f=0.0048
111 ->122 0.33120
111 ->123 0.47019
111 ->124 -0.11947
111 ->125 -0.16945
111 ->126 0.29552

Excited State 37: Singlet-A 5.4619 eV 227.00 nm f=0.0901
105 ->113 0.14555
108 ->115 0.46953
109 ->115 0.39816
111 ->123 0.10577

Excited State 38: Singlet-A 5.5040 eV 225.26 nm f=0.0019
107 ->115 0.66694
108 ->115 0.14908

Excited State 39: Singlet-A 5.5622 eV 222.90 nm f=0.0064
100 ->112 0.65972
101 ->112 -0.16766

Excited State 40: Singlet-A 5.5733 eV 222.46 nm f=0.0027
111 ->117 0.13764
111 ->120 0.11564
111 ->121 0.12688
111 ->123 0.13717
111 ->124 0.57785
111 ->125 0.17209
111 ->127 -0.12306

TDDFT Calculation for **7b**

B3LYP

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.6454 eV 468.69 nm f=0.0370
115 ->116 0.67434

This state for optimization and/or second-order correction.

Total Energy, E(RPA) = -1670.50208778

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.2544 eV 380.98 nm f=0.0114
112 ->116 -0.14253
113 ->116 0.41798
114 ->116 0.54784

Excited State 3: Singlet-A 3.3351 eV 371.76 nm f=0.4386
112 ->116 0.21315
113 ->116 0.54024
114 ->116 -0.34222

Excited State 4: Singlet-A 3.3829 eV 366.51 nm f=0.2611
112 ->116 0.65111
114 ->116 0.21138

Excited State 5: Singlet-A 3.4675 eV 357.56 nm f=0.0280
110 ->116 -0.14712
111 ->116 0.68703

Excited State 6: Singlet-A 3.5803 eV 346.29 nm f=0.0056
110 ->116 0.68847
111 ->116 0.14752

Excited State 7: Singlet-A 3.9305 eV 315.44 nm f=0.0492
109 ->116 0.67531

Excited State 8: Singlet-A 4.2727 eV 290.18 nm f=0.2906
107 ->116 -0.18598
108 ->116 -0.11618
115 ->117 0.62408

Excited State 9: Singlet-A 4.3679 eV 283.85 nm f=0.0571
107 ->116 -0.40785
108 ->116 0.51390
113 ->117 0.11610
114 ->117 -0.12687

Excited State 10: Singlet-A 4.4113 eV 281.06 nm f=0.0173
108 ->116 0.12674
115 ->117 0.15711
115 ->118 0.66894

Excited State 11: Singlet-A 4.5213 eV 274.22 nm f=0.0277
107 ->116 0.29214
108 ->116 0.38267
113 ->117 -0.15569
114 ->117 0.18517
115 ->118 -0.10806
115 ->120 -0.30842
115 ->125 -0.16618

Excited State 12: Singlet-A 4.6575 eV 266.20 nm f=0.2532
106 ->116 0.28325
107 ->116 0.35498
113 ->117 0.17634
114 ->117 -0.23922
115 ->119 0.29307
115 ->120 0.19323

Excited State 13: Singlet-A 4.6672 eV 265.65 nm f=0.0162
107 ->116 -0.14735
114 ->117 0.11720
115 ->119 0.61383
115 ->120 -0.22851

Excited State 14: Singlet-A 4.7584 eV 260.56 nm f=0.0537
105 ->116 -0.25637
106 ->116 0.52912
107 ->116 -0.13812
113 ->117 -0.14881
114 ->117 0.24053

Excited State 15: Singlet-A 4.8009 eV 258.25 nm f=0.0081
113 ->117 0.48295
114 ->117 0.48655

Excited State 16: Singlet-A 4.8548 eV 255.39 nm f=0.0414
106 ->116 -0.12827
109 ->120 0.11456
112 ->117 -0.16007
113 ->117 -0.30048
113 ->118 -0.23244
114 ->117 0.16401
114 ->118 0.32536
115 ->120 0.30175

Excited State 17: Singlet-A 4.9013 eV 252.96 nm f=0.0013
112 ->117 0.53088
112 ->118 0.19119
114 ->118 0.35123

Excited State 18: Singlet-A 4.9106 eV 252.48 nm f=0.1136
105 ->116 0.11412
112 ->117 0.18234
112 ->118 0.13527

113 ->117	-0.12659
113 ->118	0.12652
114 ->118	-0.36842
115 ->120	0.38755
115 ->122	-0.10328
115 ->124	-0.10512
115 ->125	-0.17270

Excited State 19: Singlet-A 4.9316 eV 251.41 nm f=0.0071

111 ->117	0.16478
112 ->117	-0.26662
113 ->118	0.54926
114 ->118	0.21691

Excited State 20: Singlet-A 4.9756 eV 249.18 nm f=0.0290

105 ->116	0.49437
106 ->116	0.20607
111 ->117	0.12388
112 ->118	0.24733
113 ->118	-0.11487
114 ->119	-0.11905
115 ->120	-0.10770
115 ->124	0.13911

Excited State 21: Singlet-A 4.9865 eV 248.64 nm f=0.0033

105 ->116	-0.27120
106 ->116	-0.13242
111 ->117	0.40249
111 ->118	0.14859
112 ->117	-0.14731
112 ->118	0.34595
113 ->118	-0.18410

Excited State 22: Singlet-A 5.0144 eV 247.26 nm f=0.0078

111 ->117	0.46989
112 ->117	0.11445
112 ->118	-0.43099

Excited State 23: Singlet-A 5.0237 eV 246.80 nm f=0.0261

111 ->117	-0.12332
115 ->121	0.64039
115 ->123	-0.13249

Excited State 24: Singlet-A 5.0530 eV 245.37 nm f=0.0016

105 ->116	0.11498
112 ->119	0.13548
113 ->119	-0.36968
113 ->120	0.10670
114 ->119	0.46929
114 ->120	-0.12545

Excited State 25: Singlet-A 5.0725 eV 244.42 nm f=0.0157

115 ->122	0.59361
115 ->123	0.19523

115 ->125	-0.19685
115 ->126	0.12205
Excited State 26: Singlet-A	5.0778 eV 244.17 nm f=0.0032
110 ->117	0.49344
110 ->118	0.11662
111 ->118	0.44197
Excited State 27: Singlet-A	5.1159 eV 242.35 nm f=0.0100
115 ->124	0.61066
115 ->125	-0.23897
Excited State 28: Singlet-A	5.1262 eV 241.86 nm f=0.0231
110 ->117	-0.41659
110 ->118	-0.16230
111 ->117	-0.15152
111 ->118	0.46778
112 ->118	-0.14855
Excited State 29: Singlet-A	5.1725 eV 239.70 nm f=0.0067
110 ->118	-0.21469
115 ->122	-0.20408
115 ->123	0.53642
115 ->126	0.14340
Excited State 30: Singlet-A	5.2046 eV 238.22 nm f=0.0077
110 ->117	-0.17305
110 ->118	0.56314
115 ->122	-0.10029
115 ->123	0.24268
Excited State 31: Singlet-A	5.2292 eV 237.10 nm f=0.0128
110 ->118	-0.16290
110 ->121	0.11386
110 ->124	-0.11545
111 ->123	0.11235
111 ->124	0.16286
112 ->124	-0.15930
113 ->119	0.25958
113 ->120	0.19624
113 ->121	-0.14168
113 ->123	0.12450
113 ->124	-0.10185
114 ->119	0.20758
114 ->120	0.14467
114 ->121	-0.17015
114 ->123	0.10256
Excited State 32: Singlet-A	5.2388 eV 236.67 nm f=0.4190
114 ->119	0.12955
115 ->121	0.13279
115 ->122	0.10988
115 ->124	0.18583
115 ->125	0.44122

115 ->127 0.19024
115 ->131 0.12615

Excited State 33: Singlet-A 5.2671 eV 235.39 nm f=0.0282

110 ->117 0.13615
110 ->118 -0.20109
110 ->119 -0.14557
110 ->121 0.17711
110 ->124 0.11998
111 ->119 -0.12983
111 ->121 0.15219
111 ->122 -0.15173
111 ->123 0.13023
112 ->118 0.10104
112 ->119 0.20297
112 ->120 0.12313
112 ->121 -0.19335
112 ->123 0.19771
113 ->127 0.10971
114 ->120 -0.10653
115 ->123 0.15628

Excited State 34: Singlet-A 5.2929 eV 234.25 nm f=0.0802

109 ->117 -0.18450
109 ->118 -0.22089
113 ->120 -0.22275
114 ->119 0.17279
114 ->120 0.45030

Excited State 35: Singlet-A 5.3241 eV 232.87 nm f=0.0019

112 ->119 -0.19625
113 ->119 0.36999
113 ->120 -0.21348
114 ->119 0.34512
114 ->120 -0.27084

Excited State 36: Singlet-A 5.3311 eV 232.57 nm f=0.0094

111 ->124 -0.10791
112 ->120 -0.16022
112 ->124 0.10576
113 ->119 0.14255
113 ->120 0.47245
114 ->120 0.25156
114 ->121 0.10362

Excited State 37: Singlet-A 5.3626 eV 231.20 nm f=0.0001

115 ->123 -0.12035
115 ->126 0.53587
115 ->128 -0.29062
115 ->129 0.20793
115 ->130 0.12979

Excited State 38: Singlet-A 5.3749 eV 230.67 nm f=0.0338

111 ->120 0.12854

112 ->120	0.45603
113 ->120	0.19230
115 ->127	0.35647

Excited State 39: Singlet-A 5.3905 eV 230.01 nm f=0.0239

104 ->116	0.12483
109 ->119	0.11874
110 ->119	-0.10182
112 ->119	-0.26145
112 ->120	-0.34791
113 ->119	-0.12252
115 ->125	-0.12144
115 ->127	0.34341
115 ->128	-0.12036

Excited State 40: Singlet-A 5.3954 eV 229.80 nm f=0.0220

109 ->117	0.15083
109 ->119	-0.23795
110 ->119	0.11661
112 ->119	0.38668
112 ->120	-0.20623
113 ->119	0.26616
115 ->127	0.25846

TDDFT Calculation for **8a**

B3LYP

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.0429 eV 407.46 nm f=0.3277
111 ->112 0.66009

This state for optimization and/or second-order correction.

Total Energy, E(RPA) = -1347.51710933

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.6424 eV 340.39 nm f=0.0048
110 ->112 0.69717

Excited State 3: Singlet-A 3.7599 eV 329.75 nm f=0.0011
109 ->112 0.69543

Excited State 4: Singlet-A 3.8481 eV 322.19 nm f=0.0157
107 ->112 0.14299
108 ->112 0.67788
111 ->113 0.10486

Excited State 5: Singlet-A 3.8740 eV 320.04 nm f=0.0171
106 ->112 -0.45833
107 ->112 0.14215
108 ->112 -0.13207
111 ->113 0.47120

Excited State 6: Singlet-A 3.9576 eV 313.28 nm f=0.0011
106 ->112 0.14977
107 ->112 0.67340
108 ->112 -0.11863

Excited State 7: Singlet-A 4.0996 eV 302.43 nm f=0.6797
105 ->112 -0.16408
106 ->112 0.45963
111 ->113 0.43174

Excited State 8: Singlet-A 4.3780 eV 283.20 nm f=0.1707
104 ->112 -0.12236
105 ->112 0.49034
111 ->114 0.45348

Excited State 9: Singlet-A 4.4684 eV 277.47 nm f=0.2063
103 ->112 0.13719
104 ->112 -0.13909
105 ->112 -0.41210
106 ->112 -0.10902
106 ->113 0.16319
111 ->114 0.46977

Excited State 10: Singlet-A 4.5943 eV 269.87 nm f=0.0421
104 ->112 0.57917
111 ->114 0.16493
111 ->115 -0.31087

Excited State 11: Singlet-A 4.7193 eV 262.72 nm f=0.0040
110 ->113 0.68962

Excited State 12: Singlet-A 4.7550 eV 260.74 nm f=0.0335
103 ->112 -0.11682
104 ->112 0.26694
106 ->113 -0.14817
110 ->113 0.12846
111 ->114 0.10909
111 ->115 0.54669
111 ->116 -0.11486

Excited State 13: Singlet-A 4.8448 eV 255.91 nm f=0.0033
109 ->113 0.69357

Excited State 14: Singlet-A 4.9014 eV 252.96 nm f=0.0068
111 ->116 0.68378

Excited State 15: Singlet-A 4.9251 eV 251.74 nm f=0.0015
107 ->113 0.12460
108 ->113 0.68537

Excited State 16: Singlet-A 4.9896 eV 248.49 nm f=0.0071
103 ->112 -0.17973
106 ->113 0.18779
111 ->117 0.53082
111 ->118 -0.28346
111 ->119 -0.10902
111 ->120 0.11693

Excited State 17: Singlet-A 4.9940 eV 248.27 nm f=0.0249
102 ->112 -0.17897
103 ->112 0.54687
106 ->113 -0.20488
107 ->113 0.14890
111 ->117 0.18573
111 ->118 -0.11370

Excited State 18: Singlet-A 5.0267 eV 246.65 nm f=0.0093
107 ->113 0.51945
108 ->113 -0.11636
111 ->117 0.21111
111 ->118 0.20504
111 ->119 0.20456
111 ->120 0.11931

Excited State 19: Singlet-A 5.0317 eV 246.41 nm f=0.0080
106 ->113 0.22964
107 ->113 0.40353

111 ->117 -0.24356
111 ->118 -0.29188
111 ->119 -0.23752
111 ->120 -0.14588

Excited State 20: Singlet-A 5.0725 eV 244.43 nm f=0.0068

111 ->118 -0.33139
111 ->119 0.58898

Excited State 21: Singlet-A 5.1060 eV 242.82 nm f=0.0016

108 ->114 0.10174
109 ->119 -0.11204
110 ->114 0.56546
110 ->116 -0.10824
110 ->118 0.10318
111 ->118 0.12960
111 ->121 0.14721

Excited State 22: Singlet-A 5.1081 eV 242.72 nm f=0.0372

105 ->113 0.17295
106 ->113 0.24128
110 ->114 -0.27256
111 ->115 0.12615
111 ->118 0.30165
111 ->119 0.15119
111 ->121 0.24176
111 ->122 0.12587
111 ->123 -0.21105
111 ->124 0.13274

Excited State 23: Singlet-A 5.1539 eV 240.56 nm f=0.0057

102 ->112 0.54776
105 ->113 0.15839
106 ->113 -0.13594
109 ->114 -0.26168

Excited State 24: Singlet-A 5.1589 eV 240.33 nm f=0.0097

102 ->112 0.26816
107 ->116 0.13144
108 ->114 -0.15683
108 ->116 -0.11040
108 ->118 -0.13508
109 ->114 0.49159
109 ->116 -0.12377
111 ->118 -0.12349

Excited State 25: Singlet-A 5.2497 eV 236.17 nm f=0.0062

107 ->116 -0.16917
108 ->114 0.33498
108 ->118 0.13126
108 ->119 -0.13268
109 ->114 0.20251
109 ->119 -0.12498
109 ->121 0.10398

110 ->114	-0.26934
110 ->115	0.13609
110 ->116	-0.21038
110 ->118	0.15403
110 ->119	0.10483
111 ->120	-0.10828
111 ->121	0.11313

Excited State 26: Singlet-A 5.2562 eV 235.88 nm f=0.0012

111 ->117	-0.20035
111 ->118	-0.11945
111 ->120	0.63317

Excited State 27: Singlet-A 5.2892 eV 234.41 nm f=0.0080

107 ->119	0.13153
108 ->114	0.41993
108 ->119	0.11415
109 ->114	0.27162
109 ->116	0.14537
109 ->119	0.16351
110 ->115	-0.13605
110 ->116	0.13388
110 ->118	-0.13297
110 ->121	-0.13606
111 ->121	-0.13516
111 ->123	-0.10415

Excited State 28: Singlet-A 5.3043 eV 233.74 nm f=0.0128

107 ->116	0.17503
107 ->119	-0.10602
108 ->114	0.33795
108 ->116	-0.15193
108 ->118	-0.20674
109 ->114	-0.22163
109 ->115	0.13092
109 ->116	-0.19243
109 ->118	0.15899
109 ->119	-0.10373
110 ->121	0.12797
111 ->121	-0.24094

Excited State 29: Singlet-A 5.3188 eV 233.11 nm f=0.0252

106 ->113	-0.11471
107 ->116	0.12208
108 ->114	0.19958
108 ->118	-0.11670
110 ->115	-0.10353
110 ->116	0.12941
111 ->121	0.47417
111 ->122	0.19264
111 ->123	0.19310

Excited State 30: Singlet-A 5.3688 eV 230.94 nm f=0.1714

103 ->112	-0.17450
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105 ->113	0.30720
106 ->113	-0.27363
106 ->114	0.12298
107 ->114	-0.21658
111 ->122	0.29391
111 ->123	-0.10430
111 ->124	0.14041
111 ->127	0.11549

Excited State 31: Singlet-A 5.3748 eV 230.68 nm f=0.0250

105 ->113	-0.14783
106 ->113	0.12418
107 ->114	0.25665
111 ->121	-0.21665
111 ->122	0.48170
111 ->124	0.12650
111 ->125	0.17417
111 ->126	0.13433

Excited State 32: Singlet-A 5.3784 eV 230.52 nm f=0.0995

104 ->113	0.10406
104 ->115	-0.10531
105 ->113	0.15426
106 ->113	-0.14587
107 ->114	0.55665
111 ->122	-0.11008
111 ->123	-0.18483

Excited State 33: Singlet-A 5.4252 eV 228.53 nm f=0.0344

100 ->112	-0.21050
101 ->112	-0.32417
104 ->115	0.11411
105 ->113	0.14448
106 ->114	0.36519
107 ->114	0.17569
111 ->123	0.29201
111 ->124	-0.10707

Excited State 34: Singlet-A 5.4355 eV 228.10 nm f=0.0026

100 ->112	0.26364
101 ->112	0.36685
102 ->112	-0.11907
104 ->113	-0.12543
104 ->115	0.11289
106 ->114	0.39208
107 ->114	0.10474
110 ->115	-0.13560

Excited State 35: Singlet-A 5.4580 eV 227.16 nm f=0.0053

109 ->115	-0.10431
110 ->115	0.63868
110 ->116	0.15791

Excited State 36: Singlet-A 5.5056 eV 225.20 nm f=0.0027

105 ->113	0.12068
109 ->115	0.10627
111 ->122	-0.18337
111 ->123	0.27170
111 ->124	0.47827
111 ->125	0.22241
111 ->126	-0.13210

Excited State 37: Singlet-A 5.5114 eV 224.96 nm f=0.0143

100 ->112	0.14553
101 ->112	0.13979
102 ->112	-0.11424
105 ->113	0.25391
108 ->115	-0.10662
109 ->115	0.38020
111 ->123	0.18378
111 ->124	-0.26419
111 ->125	-0.10534

Excited State 38: Singlet-A 5.5302 eV 224.20 nm f=0.0241

105 ->113	-0.20295
106 ->114	0.17906
108 ->115	-0.10890
109 ->115	0.49956
109 ->116	0.11060
110 ->116	0.17131
111 ->123	-0.15552

Excited State 39: Singlet-A 5.5715 eV 222.53 nm f=0.0072

107 ->116	-0.12189
108 ->115	0.15123
109 ->116	0.11344
110 ->116	0.46038
110 ->117	-0.10392
110 ->118	0.29833
111 ->123	0.16426
111 ->125	-0.16465

Excited State 40: Singlet-A 5.5816 eV 222.13 nm f=0.0187

105 ->113	0.11904
110 ->116	0.11150
111 ->123	-0.13819
111 ->124	-0.26424
111 ->125	0.52472
111 ->126	-0.14561
111 ->127	0.11266

TDDFT Calculation for **8b**

B3LYP

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8948 eV 428.30 nm f=0.3478
115 ->116 0.65968

This state for optimization and/or second-order correction.

Total Energy, E(RPA) = -1670.49812825

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.4868 eV 355.58 nm f=0.0036
114 ->116 0.69824

Excited State 3: Singlet-A 3.5907 eV 345.29 nm f=0.0006
113 ->116 0.69787

Excited State 4: Singlet-A 3.6924 eV 335.78 nm f=0.0051
111 ->116 0.12839
112 ->116 0.68894

Excited State 5: Singlet-A 3.7657 eV 329.25 nm f=0.1186
110 ->116 0.51872
111 ->116 -0.30319
115 ->117 0.33654

Excited State 6: Singlet-A 3.8082 eV 325.57 nm f=0.0159
110 ->116 0.27638
111 ->116 0.62142
112 ->116 -0.13398
115 ->117 0.12222

Excited State 7: Singlet-A 4.0037 eV 309.68 nm f=0.4863
108 ->116 -0.17969
110 ->116 -0.32550
115 ->117 0.54458

Excited State 8: Singlet-A 4.0603 eV 305.36 nm f=0.0454
109 ->116 0.64777
115 ->118 0.21162

Excited State 9: Singlet-A 4.3080 eV 287.80 nm f=0.1428
107 ->116 -0.10749
108 ->116 0.53609
110 ->117 -0.11348
115 ->117 0.12132
115 ->118 0.36654

Excited State 10: Singlet-A 4.3828 eV 282.89 nm f=0.1681
108 ->116 -0.35714
109 ->116 -0.17536
115 ->118 0.54373

Excited State 11: Singlet-A 4.5201 eV 274.29 nm f=0.0052
110 ->117 0.10855
115 ->119 0.64061
115 ->120 0.19476

Excited State 12: Singlet-A 4.6409 eV 267.15 nm f=0.0067
107 ->116 -0.19386
110 ->117 -0.21057
114 ->117 0.21380
115 ->120 0.55768

Excited State 13: Singlet-A 4.6744 eV 265.24 nm f=0.0008
114 ->117 0.66987
115 ->120 -0.18067

Excited State 14: Singlet-A 4.7821 eV 259.27 nm f=0.0009
113 ->117 0.68486

Excited State 15: Singlet-A 4.8247 eV 256.98 nm f=0.0153
106 ->116 0.23713
107 ->116 0.56639
110 ->117 -0.23430
113 ->117 0.10192

Excited State 16: Singlet-A 4.8748 eV 254.34 nm f=0.0015
111 ->117 0.13684
112 ->117 0.67853

Excited State 17: Singlet-A 4.9006 eV 253.00 nm f=0.0001
115 ->121 0.62842
115 ->122 0.15773

Excited State 18: Singlet-A 4.9311 eV 251.43 nm f=0.0455
110 ->117 0.22466
115 ->119 -0.12703
115 ->120 0.20452
115 ->121 -0.25088
115 ->122 0.34065
115 ->123 -0.16095
115 ->124 0.31438
115 ->125 0.15056

Excited State 19: Singlet-A 4.9689 eV 249.52 nm f=0.0118
105 ->116 -0.13953
106 ->116 0.51730
107 ->116 -0.15200
109 ->117 -0.10554
111 ->117 -0.34147

Excited State 20: Singlet-A 4.9897 eV 248.48 nm f=0.0036
106 ->116 0.27384
107 ->116 -0.12581
110 ->117 0.12925
111 ->117 0.57529

112 ->117	-0.14369			
Excited State 21: Singlet-A	5.0015 eV	247.89 nm	f=0.0048	
112 ->118	-0.13051			
113 ->118	-0.17050			
114 ->118	0.58293			
115 ->123	-0.21039			
115 ->124	-0.12939			
Excited State 22: Singlet-A	5.0089 eV	247.53 nm	f=0.0050	
114 ->118	0.26724			
115 ->122	-0.11026			
115 ->123	0.55061			
115 ->124	0.24304			
Excited State 23: Singlet-A	5.0187 eV	247.04 nm	f=0.0179	
112 ->118	0.13166			
113 ->118	0.58955			
114 ->118	0.19893			
115 ->123	-0.13960			
115 ->124	0.11598			
Excited State 24: Singlet-A	5.0564 eV	245.20 nm	f=0.0044	
113 ->118	-0.16256			
115 ->122	-0.39689			
115 ->123	-0.25828			
115 ->124	0.45367			
Excited State 25: Singlet-A	5.0776 eV	244.18 nm	f=0.0366	
110 ->117	0.19219			
115 ->122	-0.34047			
115 ->124	-0.23519			
115 ->125	0.46592			
Excited State 26: Singlet-A	5.1506 eV	240.72 nm	f=0.0072	
112 ->118	0.64702			
113 ->118	-0.18739			
114 ->118	0.11143			
Excited State 27: Singlet-A	5.1957 eV	238.63 nm	f=0.0359	
104 ->116	0.18412			
105 ->116	0.57673			
106 ->116	0.13073			
109 ->117	-0.16668			
115 ->125	0.17274			
Excited State 28: Singlet-A	5.2172 eV	237.65 nm	f=0.0202	
105 ->116	0.18994			
106 ->116	0.14452			
109 ->117	0.36826			
110 ->118	-0.22456			
111 ->118	0.37972			
115 ->125	-0.14582			

Excited State 29: Singlet-A 5.2411 eV 236.56 nm f=0.0158

109 ->117	-0.37059
110 ->118	0.12166
111 ->118	0.42901
111 ->121	0.12322
112 ->122	0.10661
113 ->118	-0.13653
113 ->122	0.10619
115 ->125	0.11559

Excited State 30: Singlet-A 5.2515 eV 236.09 nm f=0.2226

108 ->117	0.10819
109 ->119	-0.10213
110 ->117	0.30674
110 ->118	0.27576
110 ->119	-0.12069
112 ->124	-0.10437
115 ->125	-0.23486
115 ->127	0.11533
115 ->128	-0.16307

Excited State 31: Singlet-A 5.2725 eV 235.15 nm f=0.0102

111 ->118	0.10810
111 ->121	-0.12594
111 ->124	-0.15528
112 ->121	0.14349
112 ->122	-0.18875
113 ->118	0.13151
113 ->120	0.10860
113 ->121	-0.22318
113 ->123	-0.11467
113 ->124	0.23648
114 ->118	0.10444
114 ->121	-0.14915
114 ->122	-0.18398
114 ->125	0.18703
114 ->127	-0.10108
114 ->128	0.17546

Excited State 32: Singlet-A 5.2767 eV 234.96 nm f=0.1102

108 ->117	0.15049
110 ->117	0.18066
110 ->118	0.15542
111 ->118	0.31584
111 ->121	-0.16831
112 ->118	0.14827
112 ->122	-0.10895
112 ->124	0.16083
113 ->122	-0.15055
113 ->128	-0.13948
114 ->119	-0.12189
114 ->121	0.18163
115 ->125	-0.10883

Excited State 33: Singlet-A 5.3057 eV 233.68 nm f=0.0113
109 ->119 -0.10502
110 ->118 0.10324
115 ->126 0.49130
115 ->127 0.35194
115 ->128 0.16086

Excited State 34: Singlet-A 5.3121 eV 233.40 nm f=0.0029
109 ->117 0.22483
109 ->119 -0.17566
110 ->118 0.22335
114 ->119 0.17994
115 ->126 -0.11072
115 ->127 -0.26746
115 ->128 0.41798

Excited State 35: Singlet-A 5.3250 eV 232.83 nm f=0.0712
108 ->117 0.30697
109 ->117 -0.15752
109 ->118 0.10985
109 ->119 0.12357
110 ->117 0.12425
110 ->118 -0.26708
114 ->119 -0.11231
115 ->126 0.13366
115 ->128 0.32484
115 ->132 0.10203

Excited State 36: Singlet-A 5.3500 eV 231.75 nm f=0.0022
115 ->123 -0.10329
115 ->126 -0.38071
115 ->127 0.46845
115 ->128 0.22213
115 ->130 0.12615
115 ->131 -0.16997

Excited State 37: Singlet-A 5.3525 eV 231.64 nm f=0.0007
109 ->117 -0.11696
110 ->118 -0.14782
114 ->119 0.62687

Excited State 38: Singlet-A 5.4196 eV 228.77 nm f=0.0327
108 ->117 0.18843
109 ->119 -0.14336
109 ->120 -0.11632
113 ->119 0.46202
114 ->120 0.32593
115 ->128 -0.13695

Excited State 39: Singlet-A 5.4253 eV 228.53 nm f=0.0156
108 ->117 -0.25466
109 ->119 0.13456
110 ->118 -0.11534
110 ->119 0.14477

113 ->119	0.41712
113 ->120	-0.19144
114 ->120	-0.15028
115 ->125	-0.14811
115 ->128	0.18848

Excited State 40: Singlet-A 5.4531 eV 227.37 nm f=0.0392

108 ->117	-0.23051
113 ->119	-0.12085
113 ->120	0.10561
114 ->120	0.53354
114 ->122	0.12641
115 ->125	-0.11991
115 ->128	0.12640
115 ->132	-0.11602

VModes Analysis for **5**

Number	Orbital	Energy, eV	Group Number					Total
	Index		Azole Ligand	Azole Hetero	Aryl Ligand	Boron	Biphenyl Ac	
79	(A)--O	-10.454	36.5	3.1	39.3	2.4	18.7	100
80	(A)--O	-10.358	20.3	2.2	36.4	2.3	38.7	100
81	(A)--O	-10.288	42.7	4	39.2	1.9	12.3	100
82	(A)--O	-10.081	40.2	12.1	24.5	1.5	21.6	100
83	(A)--O	-9.581	4.6	0.1	47.2	1.3	46.8	100
84	(A)--O	-9.479	6.1	0.5	8.6	0.7	84.1	100
85	(A)--O	-9.412	1.9	0	17.2	0.7	80.2	100
86	(A)--O	-8.907	1	0.1	8.9	2.3	87.8	100
87	(A)--O	-8.883	1.4	0.1	11	0.9	86.6	100
88	(A)--O	-8.627	2.4	0.2	41.9	7.8	47.8	100
89	(A)--O	-8.459	14	0.9	43.3	6.3	35.5	100
90	(A)--O	-8.126	50.2	0.4	46.3	0.3	2.9	100
91	(A)--O	-7.802	20.7	0.1	12.3	12.3	54.7	100
92	(A)--O	-7.464	67	11.7	5.9	2.2	13.2	100
93	(A)--O	-7.016	42	0.4	56.1	0.2	1.3	100
94	(A)--O	-6.53	3.3	0	1.2	0.6	94.9	100
95	(A)--O	-6.448	3.6	0.1	2.6	0.3	93.4	100
96	(A)--O	-6.399	3.4	0.2	5.2	0.5	90.8	100
97	(A)--O	-6.269	2	0	6.5	1.3	90.1	100
98	(A)--O	-6.107	15.9	0.5	59.4	1.3	22.9	100
99	(A)--V	-2.247	49.4	6.1	39.4	1.3	3.7	100
100	(A)--V	-0.799	80.6	3	9.6	2.4	4.5	100
101	(A)--V	-0.523	86	1	10.1	0.8	2.1	100
102	(A)--V	-0.29	5.6	0.5	82	2.2	9.6	100
103	(A)--V	-0.002	14.6	0.3	11.3	4.9	68.9	100
104	(A)--V	0.134	14.4	0.6	10.1	1.1	73.7	100
105	(A)--V	0.188	2.6	0.1	5.1	1	91.3	100
106	(A)--V	0.399	4.6	0.1	2.8	1.5	91	100
107	(A)--V	0.787	31.8	4	49.6	5.2	9.4	100
108	(A)--V	0.97	95.6	0.3	0.9	1.2	2	100
109	(A)--V	1.176	12.5	1.2	82.1	0.7	3.6	100
110	(A)--V	1.539	11.2	0.5	4.7	10.7	72.9	100
111	(A)--V	1.724	14.3	0.5	3.4	0.4	81.3	100
112	(A)--V	1.864	56.4	2.1	34.4	0.6	6.6	100
113	(A)--V	2.019	43.3	1.2	40.4	0.8	14.3	100
114	(A)--V	2.259	23.1	4.9	44.1	1.3	26.6	100
115	(A)--V	2.447	23.3	0	7.8	0.7	68.2	100
116	(A)--V	2.457	7.2	0.1	22	0.4	70.3	100
117	(A)--V	2.726	67.8	0	8.6	1.1	22.4	100
118	(A)--V	2.754	17.4	0.8	36.5	6.2	39.1	100
118	(A)--V	2.754	17.4	0.8	36.5	6.2	39.1	100

VModes Analysis for **6**

Number	Orbital	Energy, eV	Group				Total	
	Index		Azole Ligan	Azole Hetero	Aryl Ligand	Boron		Biphenyl Ac
83	(A)--O	-10.374	16.7	9.4	35.4	2.5	36	100
84	(A)--O	-10.204	57.2	3.2	32.1	1.3	6.2	100
85	(A)--O	-10.044	54.5	28.5	12.9	0.4	3.7	100
86	(A)--O	-9.559	5.6	0.7	46.6	1.3	45.9	100
87	(A)--O	-9.448	15.4	4.5	2.9	0.9	76.3	100
88	(A)--O	-9.405	2.3	0.2	17.6	0.8	79	100
89	(A)--O	-9.136	35.5	46	8.8	1.2	8.6	100
90	(A)--O	-8.896	1.5	0.9	4.4	2.2	91	100
91	(A)--O	-8.862	1.4	0.3	10.5	0.6	87.2	100
92	(A)--O	-8.616	2.7	0.5	32.8	9.3	54.7	100
93	(A)--O	-8.346	15.8	3.5	49.6	5	26.1	100
94	(A)--O	-8.08	53.1	1	42.6	0.3	3	100
95	(A)--O	-7.744	13.1	0.1	13.3	13.6	59.9	100
96	(A)--O	-7.138	57.2	26	6.2	1.1	9.5	100
97	(A)--O	-6.97	36.4	7.2	55	0.3	1.1	100
98	(A)--O	-6.52	3.5	0.2	1.9	0.5	93.9	100
99	(A)--O	-6.439	3.4	0.1	3.2	0.2	93.1	100
100	(A)--O	-6.362	4.5	0.3	4.5	0.2	90.4	100
101	(A)--O	-6.278	1.1	0.1	5.1	1.1	92.6	100
102	(A)--O	-6.088	16.4	1.5	60.6	1.3	20.2	100
103	(A)--V	-2.418	54	11.9	29	0.9	4.3	100
104	(A)--V	-0.949	84.9	6	2.7	2.8	3.6	100
105	(A)--V	-0.625	65.2	24.9	8.4	0.4	1.1	100
106	(A)--V	-0.485	79	7.4	10.4	0.9	2.2	100
107	(A)--V	-0.29	16.9	6.5	61.5	3.2	11.8	100
108	(A)--V	0.032	21.7	4.8	14.1	2.8	56.5	100
109	(A)--V	0.142	14.3	0.7	9.6	0.4	75	100
110	(A)--V	0.199	5	0.4	12.1	1.2	81.3	100
111	(A)--V	0.374	12.8	3.4	18.6	4.2	61	100
112	(A)--V	0.496	26.5	5	35.9	4.3	28.2	100
113	(A)--V	0.998	22.8	26.8	48.7	0.4	1.2	100
114	(A)--V	1.223	79.3	1.6	10.2	3.6	5.3	100
115	(A)--V	1.521	22.4	13.7	30.6	6.1	27.2	100
116	(A)--V	1.61	10.2	8	28.8	5.1	48	100
117	(A)--V	1.743	3.6	0.4	3.3	0.7	92	100
118	(A)--V	2.066	86.7	0.6	3.2	0.4	9	100
119	(A)--V	2.157	12.4	3.2	71.3	0.2	12.9	100
120	(A)--V	2.43	9.9	0.7	9.9	2	77.5	100
121	(A)--V	2.491	12.2	0.4	19.9	0.7	66.8	100
122	(A)--V	2.659	8.6	1.2	21.7	9	59.4	100

VModes Analysis for **7a**

Number	Orbital	Energy, eV	Group				Total	
	Index		Azole Ligan	Azole Heter	Aryl Ligand	Boron		Biphenyl Ac
92	(A)--O	-10.047	9.3	6.6	21.9	1.5	60.7	100
93	(A)--O	-9.978	4.2	0.1	88.7	0.2	6.9	100
94	(A)--O	-9.59	1.9	0.1	91.7	0.3	6	100
95	(A)--O	-9.46	6.8	0.3	10.7	0.3	81.9	100
96	(A)--O	-9.427	1.7	0.3	5.7	0.2	92.1	100
97	(A)--O	-9.07	11.4	0.7	59.1	2.8	26	100
98	(A)--O	-8.885	1.1	0	8.2	2.3	88.5	100
99	(A)--O	-8.839	1.5	0	12.1	0.5	85.9	100
100	(A)--O	-8.598	1.9	0.1	31	9.5	57.5	100
101	(A)--O	-8.414	14.4	0.7	59.2	4.3	21.4	100
102	(A)--O	-8.092	13.5	0.3	61.4	5.1	19.7	100
103	(A)--O	-7.744	50.3	1.2	31.6	2.7	14.2	100
104	(A)--O	-7.648	43.5	0.5	32.4	4	19.5	100
105	(A)--O	-7.461	45.4	9.3	15.7	4.2	25.4	100
106	(A)--O	-6.514	4.6	0.1	7.2	0.6	87.5	100
107	(A)--O	-6.504	29.3	0.8	51.4	1	17.5	100
108	(A)--O	-6.426	2.4	0.1	1.7	0.3	95.5	100
109	(A)--O	-6.375	6.3	0.2	4.9	0.4	88.3	100
110	(A)--O	-6.24	1.2	0	3.9	1	93.9	100
111	(A)--O	-5.827	2.6	0	84.3	1.2	11.9	100
112	(A)--V	-2.497	42.2	5.6	48.2	1.1	2.9	100
113	(A)--V	-1.064	44.3	0	52.7	0.2	2.8	100
114	(A)--V	-0.755	59	4.2	28.2	3.2	5.4	100
115	(A)--V	-0.577	72.8	0.8	23.9	0.8	1.8	100
116	(A)--V	0.003	15.5	0.4	12.1	4.5	67.5	100
117	(A)--V	0.086	18.2	0.8	44.7	3.2	33	100
118	(A)--V	0.193	3.8	0	18.5	0.9	76.8	100
119	(A)--V	0.195	15.2	0.9	30.1	0.8	53.1	100
120	(A)--V	0.405	4.4	0.2	7.1	1.6	86.7	100
121	(A)--V	0.614	19.3	2.1	66	2.1	10.5	100
122	(A)--V	0.94	95.4	0.3	1.4	1.1	1.8	100
123	(A)--V	1.178	6.2	0.5	92.5	0.1	0.7	100
124	(A)--V	1.525	9.8	2.6	24.4	7.9	55.3	100
125	(A)--V	1.537	11.6	0.5	81.1	1.6	5.2	100
126	(A)--V	1.719	18.7	0.5	13.1	0.4	67.4	100
127	(A)--V	1.89	57.1	1.3	27.2	0.3	14.1	100
128	(A)--V	2.011	37.9	2.9	39.5	0.9	18.9	100
129	(A)--V	2.307	19.6	1.7	35.8	0.8	42.2	100
130	(A)--V	2.461	20.3	0.2	3.6	0.5	75.4	100
131	(A)--V	2.588	24.5	0.6	48.4	2.2	24.3	100

VModes Analysis for **7b**

Number	Orbital	Energy, eV	Group				Total	
	Index		Azole Ligand	Azole Hetero	Aryl Ligand	Boron		Biphenyl Ac
96	(A)--O	-9.949	8.4	0.8	84.7	0.3	5.8	100
97	(A)--O	-9.564	1.8	1.1	92	0.3	4.8	100
98	(A)--O	-9.438	15.3	7.7	7.2	1.1	68.8	100
99	(A)--O	-9.426	1.9	0.1	3	0.2	94.8	100
100	(A)--O	-9.223	33.3	31.9	11.4	1.5	21.9	100
101	(A)--O	-8.966	15.6	15.9	44.8	1.9	21.9	100
102	(A)--O	-8.88	1.2	0.1	7.2	2.2	89.3	100
103	(A)--O	-8.815	2.8	0.9	15.6	0.3	80.4	100
104	(A)--O	-8.597	2.4	0.3	26.7	10.2	60.3	100
105	(A)--O	-8.318	15.4	2.5	63.2	3.6	15.2	100
106	(A)--O	-8.032	13.1	1.4	60	5.1	20.4	100
107	(A)--O	-7.695	44.3	0.7	39.9	2.6	12.6	100
108	(A)--O	-7.591	24.8	0.1	30.3	7.3	37.4	100
109	(A)--O	-7.166	50.6	26.8	9	1.4	12.2	100
110	(A)--O	-6.513	6	0.8	10.9	0.6	81.7	100
111	(A)--O	-6.47	24	3	46.3	0.6	26.1	100
112	(A)--O	-6.412	4.7	0.8	8.9	0.4	85.2	100
113	(A)--O	-6.341	7.8	0.3	4.9	0.2	86.8	100
114	(A)--O	-6.259	1.2	0	3.9	0.8	94.1	100
115	(A)--O	-5.813	2.9	0.1	85	1.4	10.6	100
116	(A)--V	-2.622	49	11.1	35.8	0.4	3.6	100
117	(A)--V	-1.068	43.4	2.4	51.9	0.2	2.2	100
118	(A)--V	-0.958	67.3	7.5	17.8	3.4	4	100
119	(A)--V	-0.629	62.3	24.9	10.8	0.6	1.4	100
120	(A)--V	-0.549	64.4	3	29.2	1.3	2.1	100
121	(A)--V	-0.045	29	5.3	41.6	2.9	21.2	100
122	(A)--V	0.056	22.5	2.5	19.9	6.5	48.6	100
123	(A)--V	0.153	14	0.8	14.4	0.3	70.5	100
124	(A)--V	0.194	3.7	1	18.7	0.7	75.9	100
125	(A)--V	0.393	5.6	0.3	20.4	1	72.7	100
126	(A)--V	0.537	13	2.1	64.8	1.2	18.9	100
127	(A)--V	0.979	22.7	26.3	49.2	0.7	1.1	100
128	(A)--V	1.201	71.9	1.4	21.5	2.1	3.1	100
129	(A)--V	1.334	16	11.6	71.6	0.3	0.5	100
130	(A)--V	1.569	9.6	0.2	10.8	11.6	67.8	100
131	(A)--V	1.73	6.4	1.1	37.9	0.5	54.1	100
132	(A)--V	1.786	6.1	3.3	74.3	0.1	16.2	100
133	(A)--V	2.044	87.1	0.4	2.2	0.5	9.7	100
134	(A)--V	2.348	11.4	2.7	61.3	0.7	23.9	100
135	(A)--V	2.412	9.7	2.7	13.8	2.7	71.2	100

VModes Analysis for **8a**

Number	Orbital	Energy, eV	Group				Total	
	Index		Azole Ligan	Azole Heter	Aryl Ligand	Boron		Biphenyl Ac
92	(A)--O	-10.014	12.1	8.6	22.6	1.1	55.7	100
93	(A)--O	-9.959	10.8	0.9	82.7	0.2	5.4	100
94	(A)--O	-9.626	1.3	0.1	86.1	0.5	12	100
95	(A)--O	-9.488	7.6	0.5	19.7	0.3	71.9	100
96	(A)--O	-9.464	1.4	0.3	8.8	0.3	89.3	100
97	(A)--O	-9.2	12.4	0.6	69.6	1.3	16.1	100
98	(A)--O	-8.939	1.4	0.1	18.3	2.2	78	100
99	(A)--O	-8.913	1.7	0.1	18.3	1.2	78.8	100
100	(A)--O	-8.7	3.7	0.3	56.3	4.6	35.1	100
101	(A)--O	-8.544	11.6	0.8	23.4	9.3	54.9	100
102	(A)--O	-8.012	12.8	0.3	43.9	7.8	35.3	100
103	(A)--O	-7.799	51.8	0	25	5	18.2	100
104	(A)--O	-7.453	74.8	10	14.2	0.1	0.8	100
105	(A)--O	-7.197	7.5	2.1	60.5	3.4	26.4	100
106	(A)--O	-6.827	34.4	0.3	59.8	0.6	4.8	100
107	(A)--O	-6.553	3.2	0	2.1	0.5	94.2	100
108	(A)--O	-6.467	2.8	0.1	2.7	0.3	94.1	100
109	(A)--O	-6.399	3.7	0.1	4.2	0.3	91.6	100
110	(A)--O	-6.297	1.2	0	6.1	0.9	91.8	100
111	(A)--O	-5.767	15.1	1	70.9	0.8	12.2	100
112	(A)--V	-2.204	42.1	5.2	46.2	1.6	4.9	100
113	(A)--V	-1.183	8.1	0.3	88.7	0.4	2.6	100
114	(A)--V	-0.753	76.8	2.5	14.2	2.3	4.3	100
115	(A)--V	-0.482	78.3	1.8	16.3	0.9	2.8	100
116	(A)--V	-0.053	14.6	0.1	17	5.9	62.4	100
117	(A)--V	0.082	15.8	0.7	20.7	1.2	61.6	100
118	(A)--V	0.171	5.3	0.4	9.5	0.9	83.8	100
119	(A)--V	0.278	22.4	2.2	43.8	1.4	30.1	100
120	(A)--V	0.399	7.1	0.4	8.7	0.8	83	100
121	(A)--V	0.722	10.3	1	82.1	2	4.5	100
122	(A)--V	1.013	94.8	0.3	1.3	1.4	2.3	100
123	(A)--V	1.237	4.4	0.5	89.3	1.1	4.7	100
124	(A)--V	1.487	10	0	46.7	5.7	37.5	100
125	(A)--V	1.572	14.2	2.1	63.4	1.8	18.5	100
126	(A)--V	1.705	11.8	0.4	7.6	0.5	79.8	100
127	(A)--V	1.932	58.1	1.1	32.7	0.6	7.6	100
128	(A)--V	2.078	26.1	2.8	55.8	1	14.3	100
129	(A)--V	2.267	10.2	1.3	49.7	0.6	38.1	100
130	(A)--V	2.407	12.2	0.1	7.6	1	79	100
131	(A)--V	2.566	18.3	0.3	28.6	4.4	48.4	100

VModes Analysis for **8b**

Number	Orbital	Energy, eV	Group Number					Total
	Index		Azole Ligand	Azole Hetero	Aryl Ligand	Boron	Biphenyl Ac	
96	(A)--O	-9.908	22.4	10.4	59.9	0.4	7	100
97	(A)--O	-9.6	2.4	0.1	87.4	0.4	9.6	100
98	(A)--O	-9.457	12.9	3.1	15	0.6	68.4	100
99	(A)--O	-9.451	3	0.9	7.6	0.5	88	100
100	(A)--O	-9.229	27.7	12.5	36	1.7	22.2	100
101	(A)--O	-9.012	23.7	35.2	34.1	1.2	5.7	100
102	(A)--O	-8.925	3.1	3.3	2	2	89.5	100
103	(A)--O	-8.877	1.5	0.8	16.3	0.6	80.8	100
104	(A)--O	-8.673	3.4	1.3	46.3	7.3	41.8	100
105	(A)--O	-8.441	14.1	3.5	40.6	6.4	35.3	100
106	(A)--O	-7.966	15.8	0.9	42.1	7.6	33.6	100
107	(A)--O	-7.761	48.7	0.3	24.1	5.5	21.5	100
108	(A)--O	-7.243	17.3	4.3	62.5	2	13.9	100
109	(A)--O	-7.048	46	23.4	12.3	1.8	16.4	100
110	(A)--O	-6.798	30.2	4.1	63.7	0.5	1.5	100
111	(A)--O	-6.541	3.4	0.1	1.9	0.5	94	100
112	(A)--O	-6.458	2.9	0.1	2.7	0.4	93.9	100
113	(A)--O	-6.377	4.8	0.2	3.9	0.2	90.8	100
114	(A)--O	-6.298	0.9	0	5.7	0.8	92.6	100
115	(A)--O	-5.752	14.8	2.5	71.5	0.7	10.4	100
116	(A)--V	-2.348	49	10.7	33.8	1.3	5.2	100
117	(A)--V	-1.208	9.4	3	84.9	0.3	2.4	100
118	(A)--V	-0.875	83	5.2	3.3	3.9	4.6	100
119	(A)--V	-0.561	65.2	21.9	10.9	0.6	1.5	100
120	(A)--V	-0.438	66.3	16.9	13.9	0.4	2.5	100
121	(A)--V	-0.027	21.2	4.3	17.1	6.2	51.2	100
122	(A)--V	0.03	34.7	3.2	36.5	3.6	22	100
123	(A)--V	0.116	13.7	1	17.4	0.3	67.6	100
124	(A)--V	0.216	5.8	0.8	13.9	0.8	78.7	100
125	(A)--V	0.39	5	0.4	3.1	0.7	90.8	100
126	(A)--V	0.672	10	7.9	75.8	2.2	4.2	100
127	(A)--V	1.096	25.1	26.5	46.8	0.6	1	100
128	(A)--V	1.256	53.5	1.2	33.2	4.2	7.9	100
129	(A)--V	1.373	29.6	8.1	57.3	0.7	4.3	100
130	(A)--V	1.553	7	1.1	23.4	8.2	60.3	100
131	(A)--V	1.717	4.6	0.9	17.9	0.5	76.2	100
132	(A)--V	1.801	8	6.4	75.3	0.4	9.9	100
133	(A)--V	2.093	86.1	0.4	2.6	0.8	10.1	100
134	(A)--V	2.309	6.1	1.2	58.6	0.8	33.3	100
135	(A)--V	2.374	11.5	3.1	18.3	2	65	100

NMR data for 3a

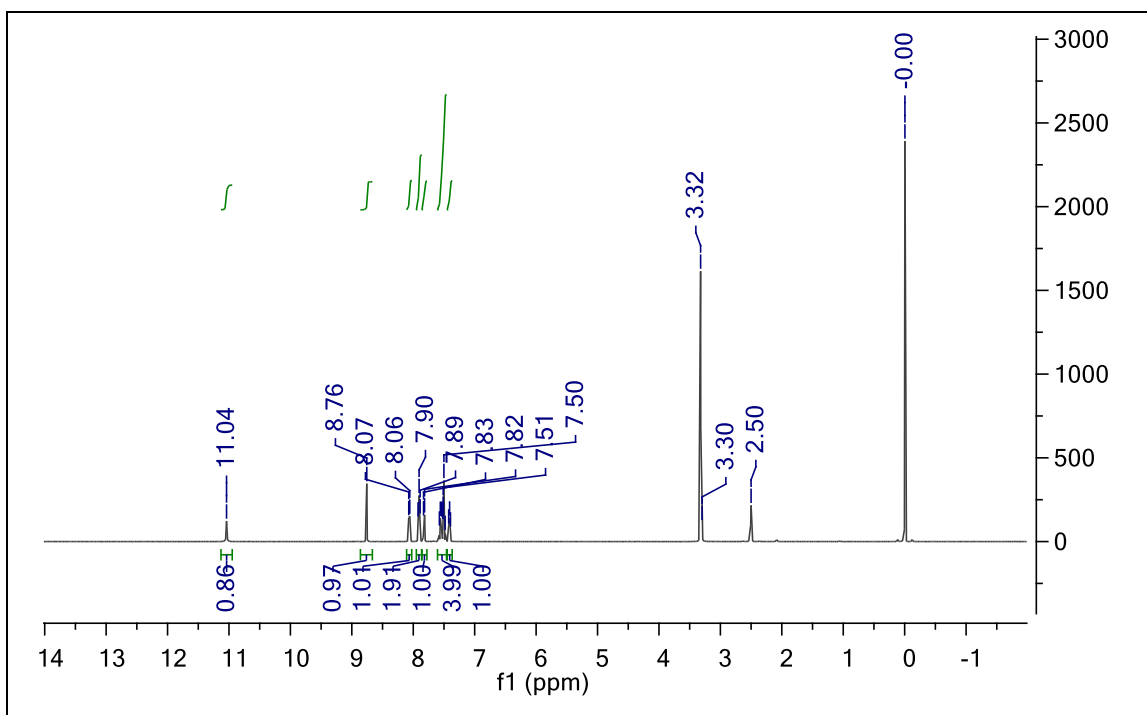


FIG 40 23HNBO_L, ¹H NMR (500 MHz, dmsol)

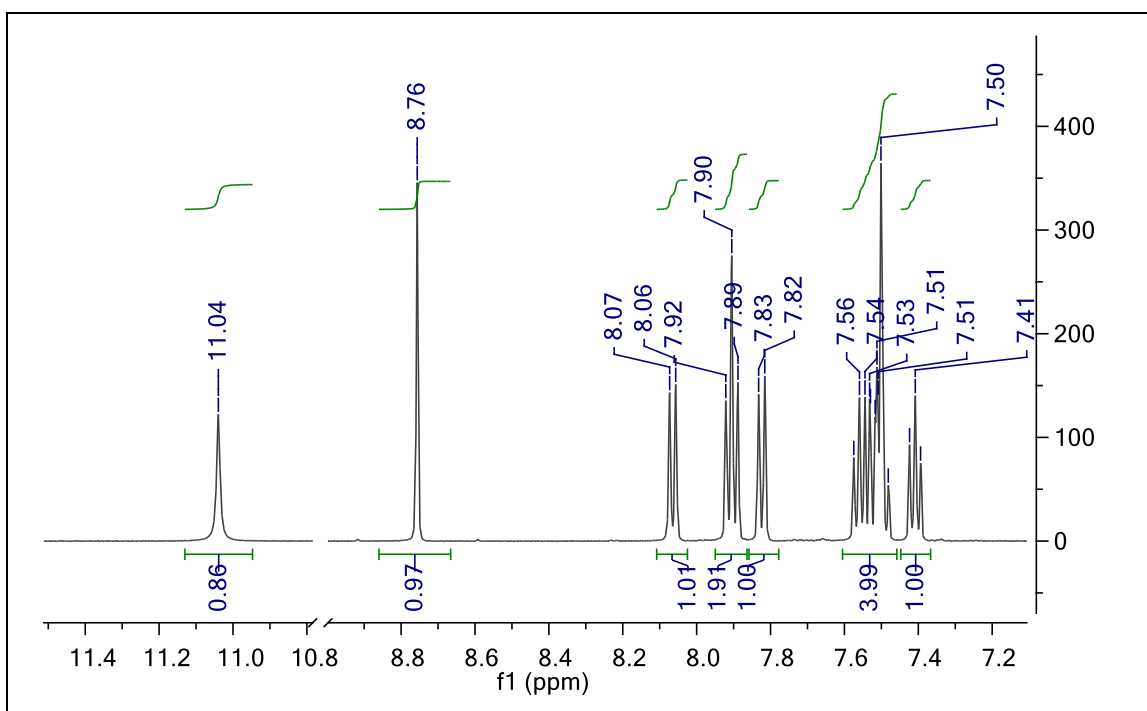


FIG 41 23HNBO_L, ¹H NMR (500 MHz, dmsol) δ 11.04, 8.76, 8.07, 8.06, 7.92, 7.90, 7.89, 7.83, 7.82, 7.57, 7.56, 7.54, 7.53, 7.52, 7.51, 7.51, 7.50, 7.48, 7.42, 7.41, 7.39, 3.32, 3.30, 2.50, -0.00.

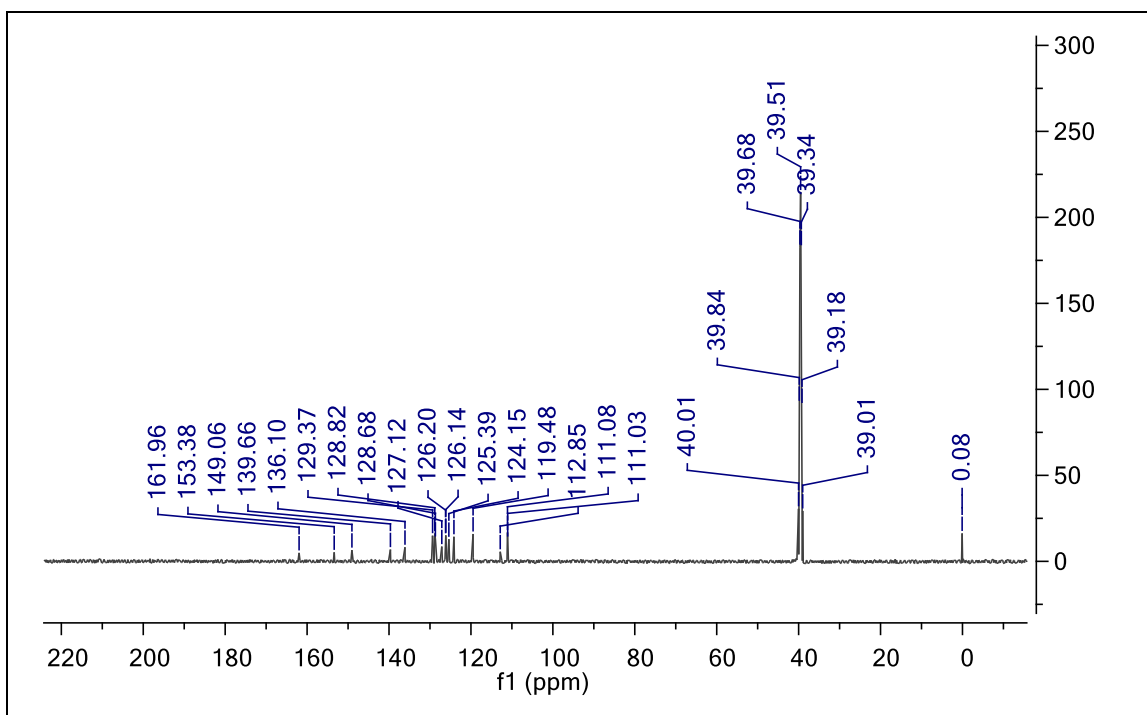


FIG 42 23HNBO_L, ^{13}C NMR (126 MHz, dmsol)

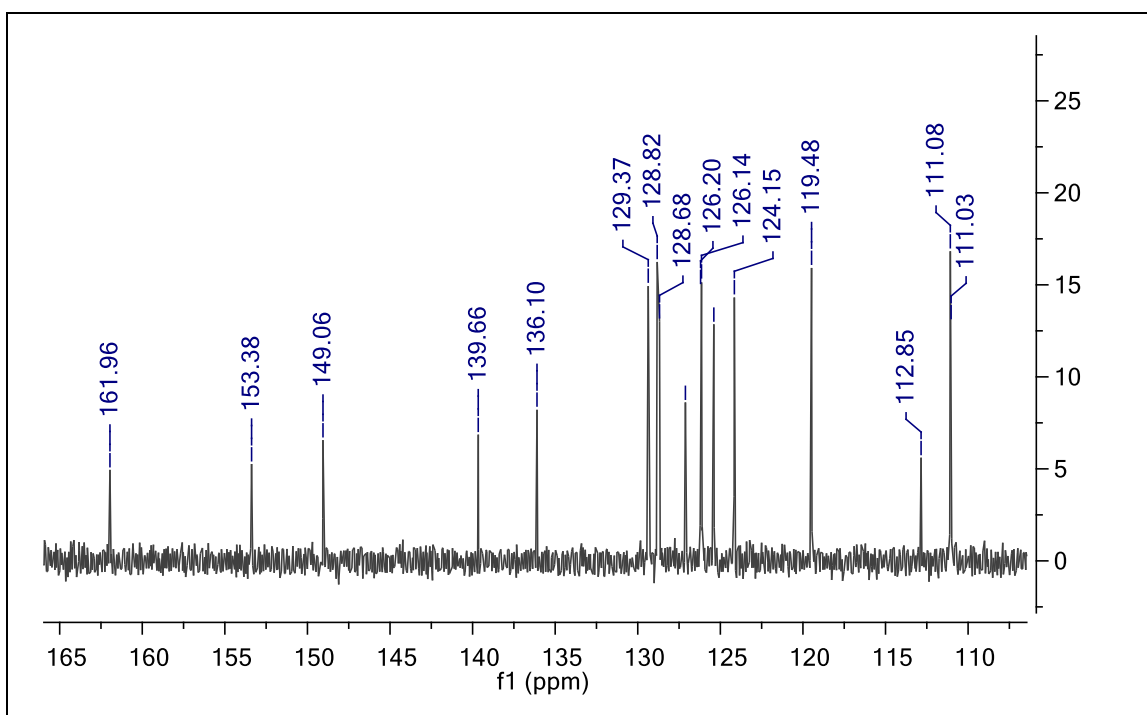


FIG 43 23HNBO_L, ^{13}C NMR (126 MHz, dmsol) δ 161.96, 153.38, 149.06, 139.66, 136.10, 129.37, 128.82, 128.68, 127.12, 126.20, 126.14, 125.39, 124.15, 119.48, 112.85, 111.08, 111.03, 40.01, 39.84, 39.68, 39.51, 39.34, 39.18, 39.01, 0.08.

NMR data for 3b

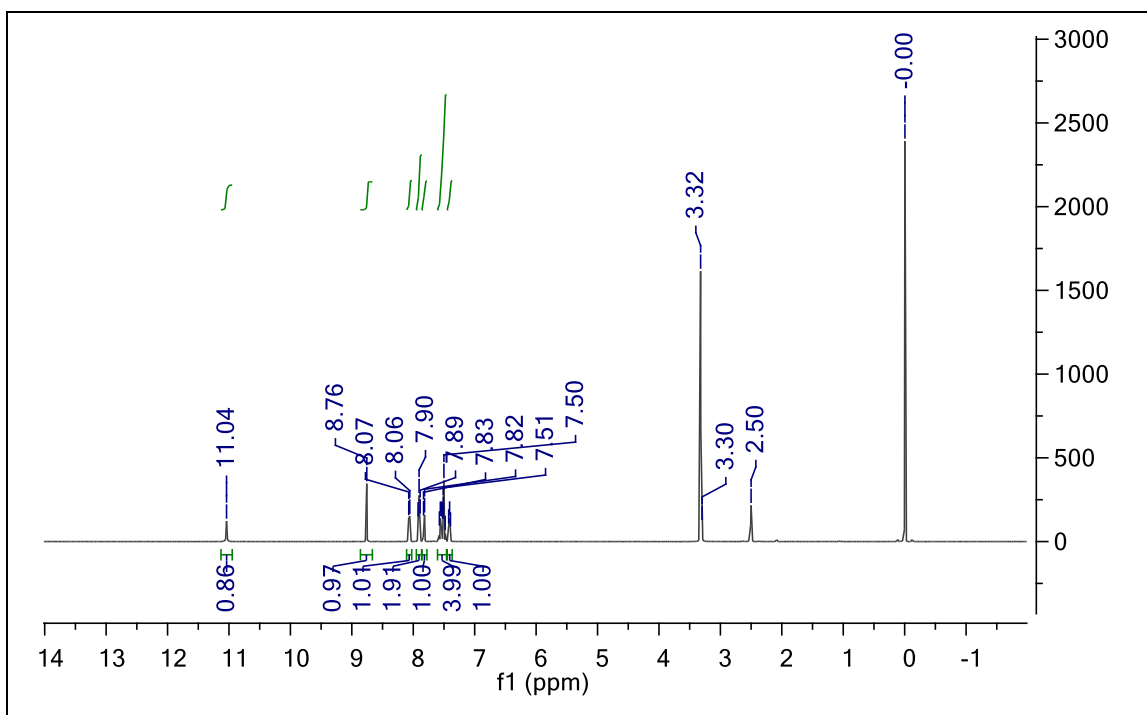


FIG 44 23HNBT_L, ¹H NMR (500 MHz, dmsol)

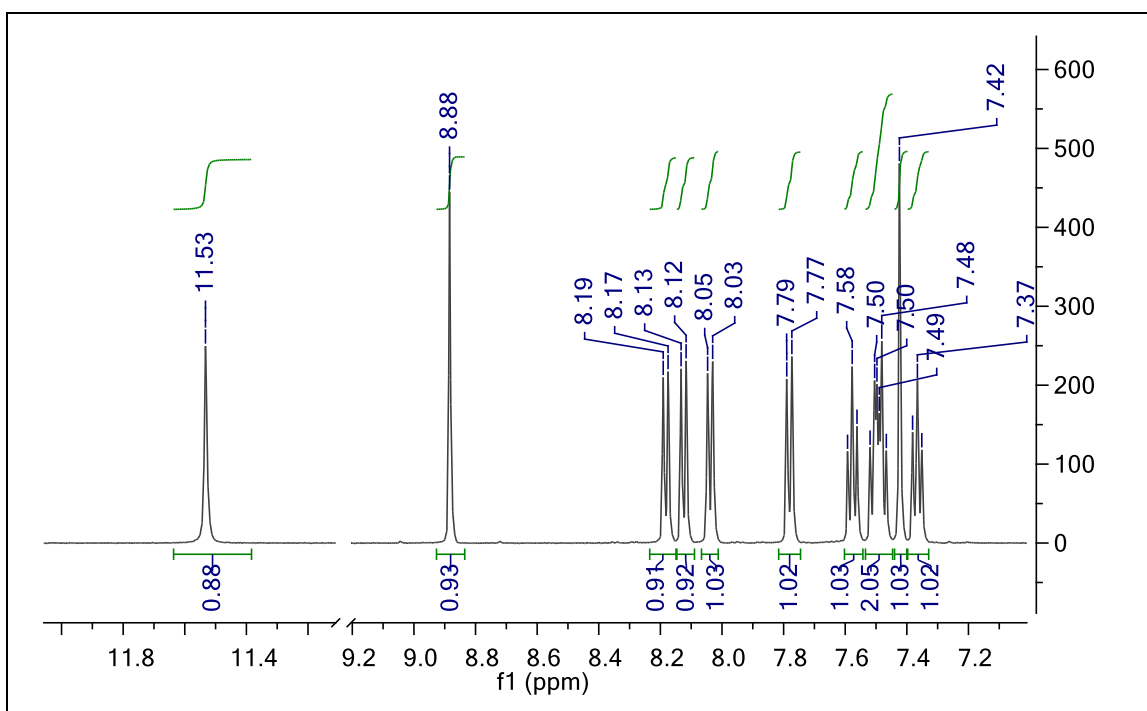


FIG 45 23HNBT_L, ¹H NMR (500 MHz, dmsol) δ 11.53, 8.88, 8.19, 8.17, 8.13, 8.12, 8.05, 8.03, 7.79, 7.77, 7.59, 7.58, 7.56, 7.52, 7.50, 7.50, 7.49, 7.48, 7.47, 7.42, 7.38, 7.37, 7.35, 3.33, 2.50, -0.01.

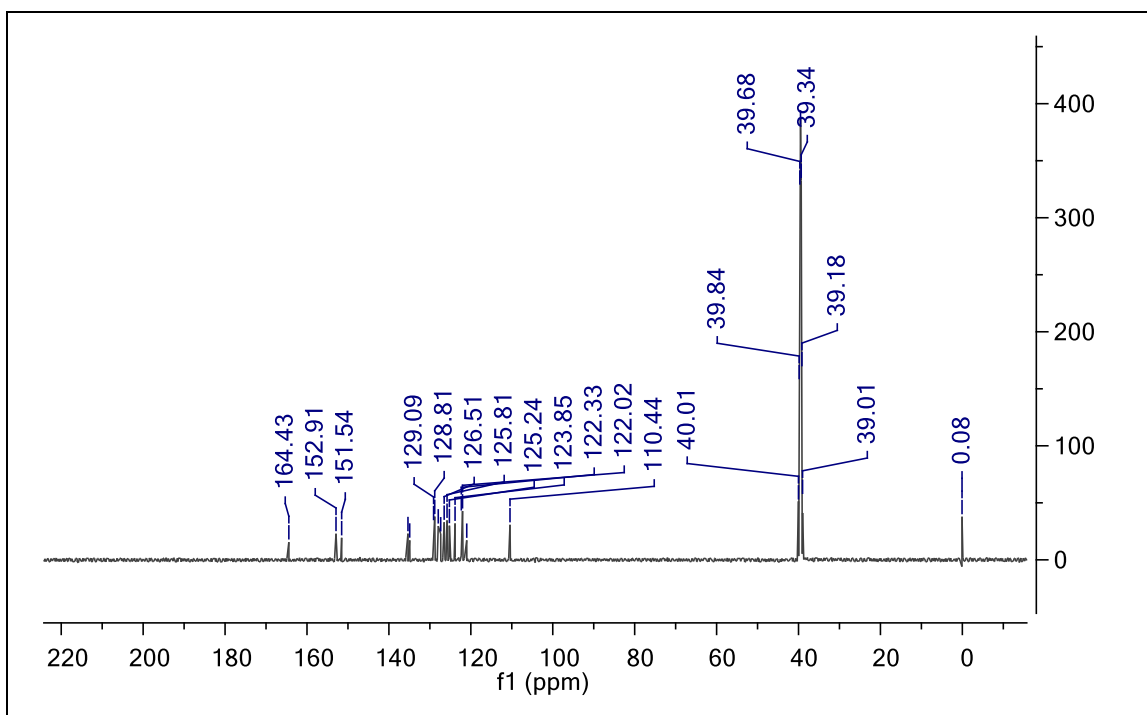


FIG 46 23HNBT_L, ^{13}C NMR (126 MHz, dmso)

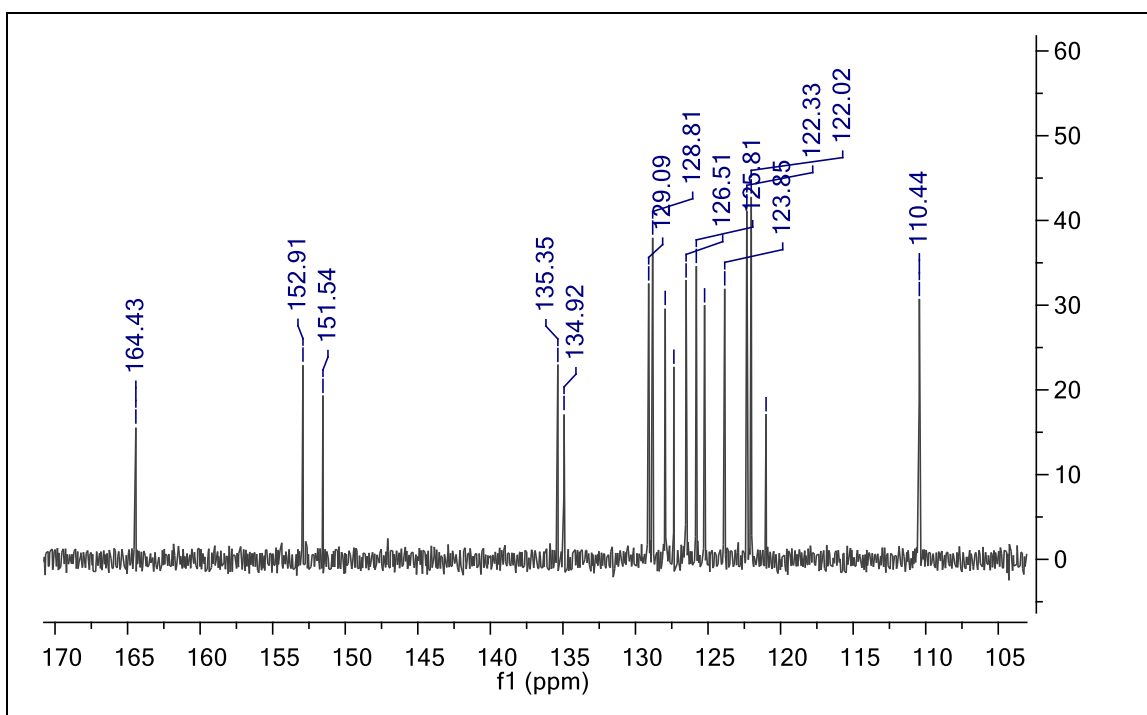


FIG 47 23HNBT_L, ^{13}C NMR (126 MHz, dmso) δ 164.43, 152.91, 151.54, 135.35, 134.92, 129.09, 128.81, 127.95, 127.35, 126.51, 125.81, 125.24, 123.85, 122.33, 122.02, 121.00, 110.44, 40.01, 39.84, 39.68, 39.51, 39.34, 39.18, 39.01.

NMR data for 4a

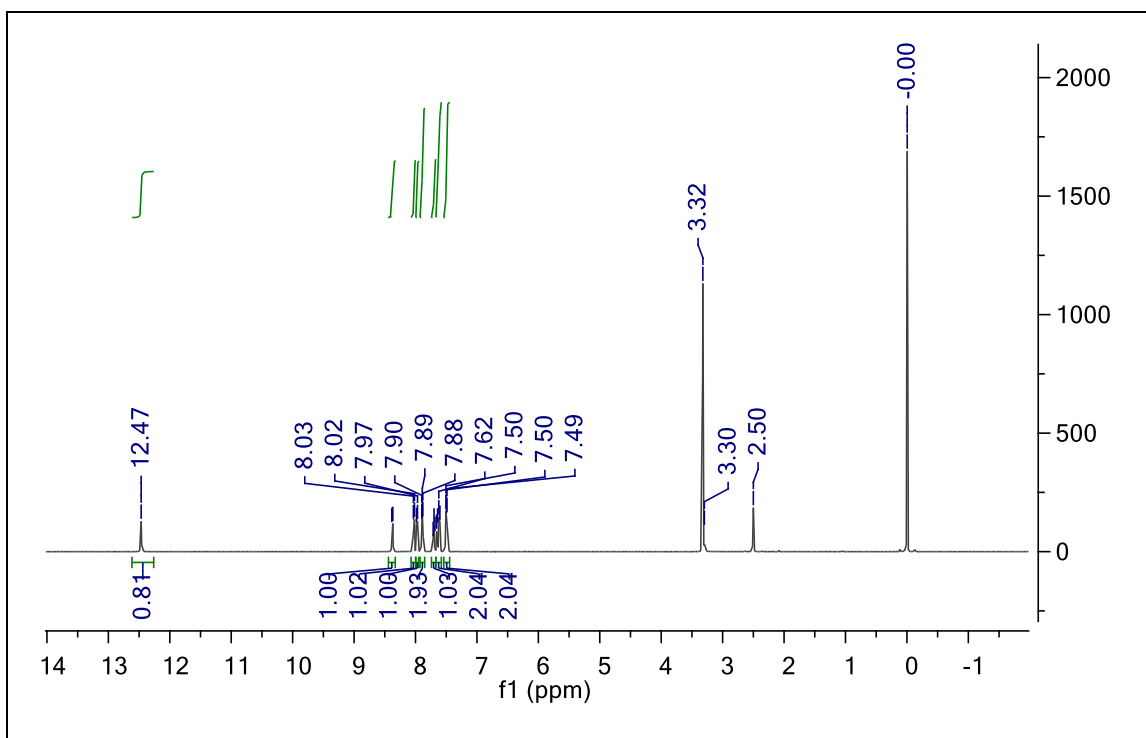


FIG 32 12HNBO_L, ¹H NMR (500 MHz, dmsol)

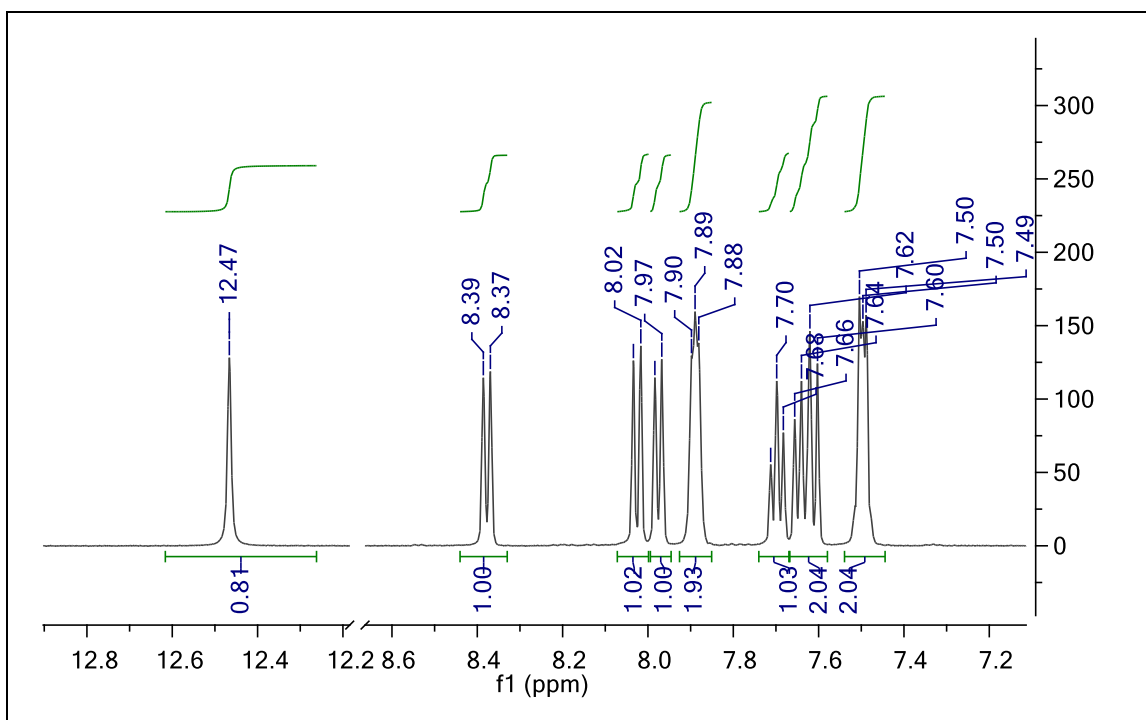


FIG 33 12HNBO_L, ¹H NMR (500 MHz, dmsol) δ 12.47, 8.39, 8.37, 8.03, 8.02, 7.98, 7.97, 7.90, 7.89, 7.88, 7.71, 7.70, 7.68, 7.66, 7.64, 7.62, 7.60, 7.50, 7.50, 7.49, 3.32, 3.30, 2.50, -0.00.

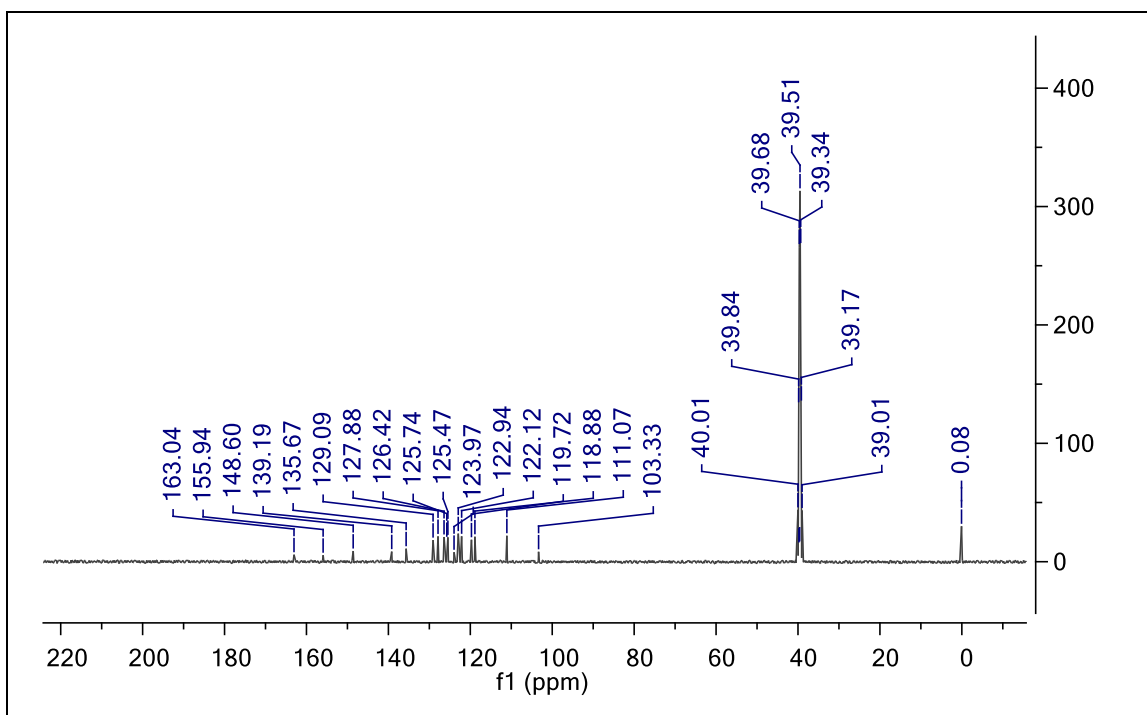


FIG 34 12HNBO_L, ^{13}C NMR (126 MHz, dmsol)

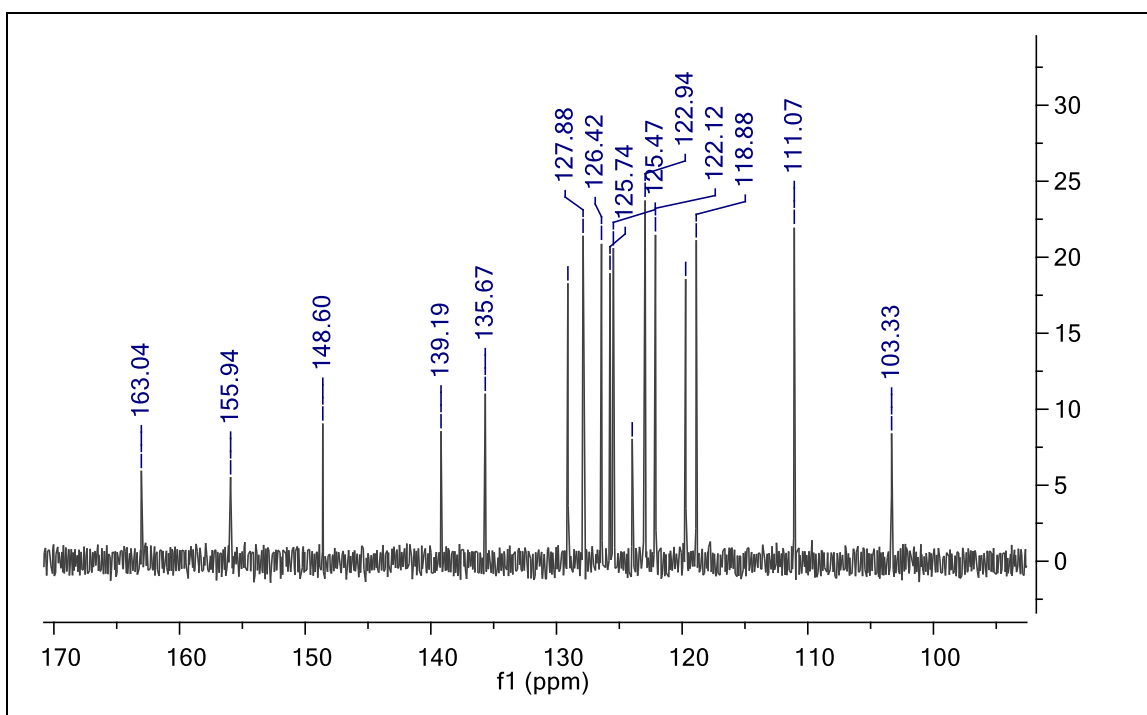


FIG 35 12HNBO_L, ^{13}C NMR (126 MHz, dmsol) δ 163.04, 155.94, 148.60, 139.19, 135.67, 129.09, 127.88, 126.42, 125.74, 125.47, 123.97, 122.94, 122.12, 119.72, 118.88, 111.07, 103.33, 40.01, 39.84, 39.77, 39.68, 39.60, 39.51, 39.34, 39.17, 39.01, 0.08.

NMR data for 4b

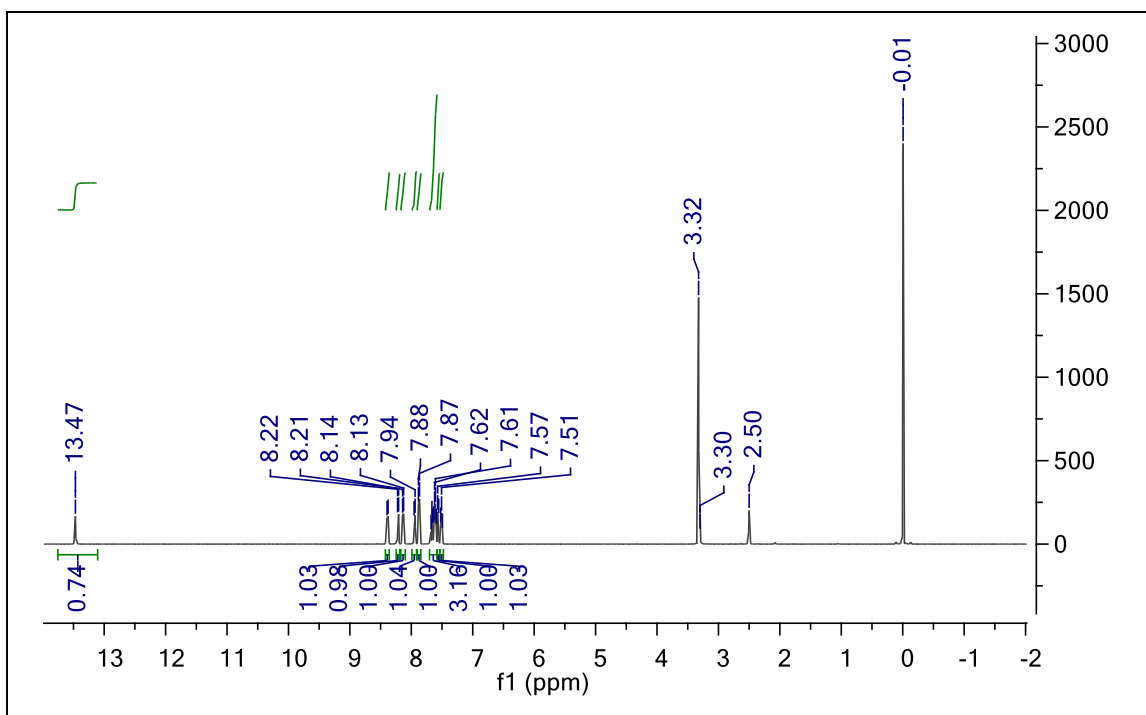


FIG 36 12HNBT_L, ¹H NMR (500 MHz, dmsol) δ

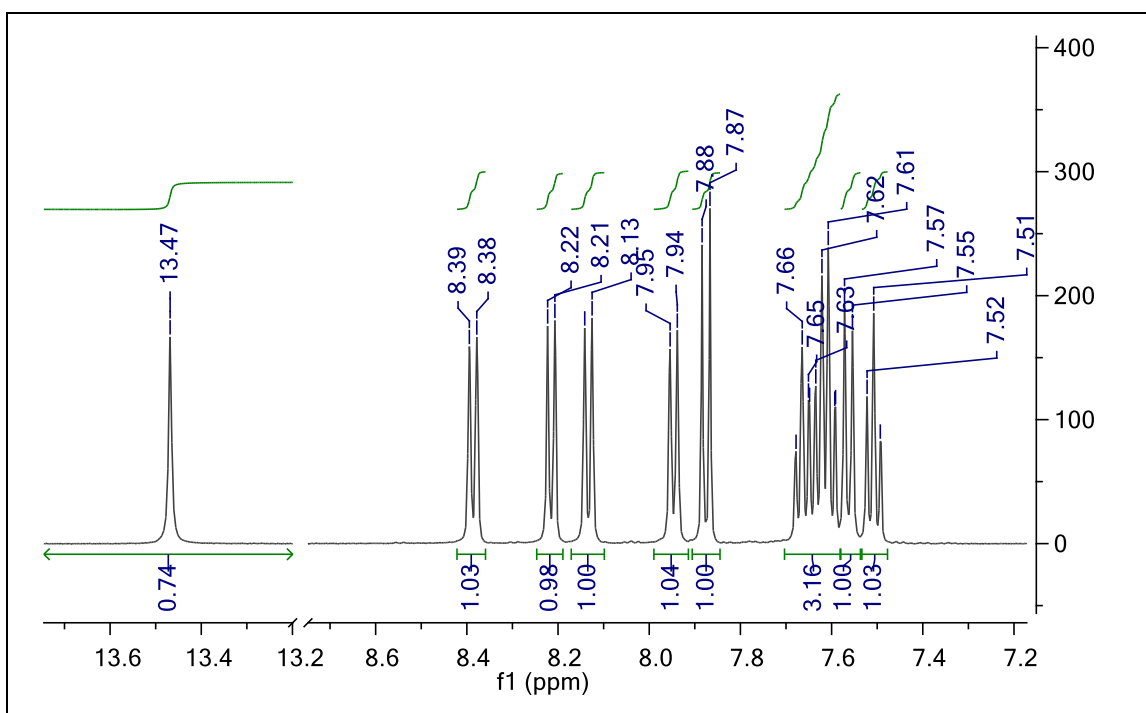


FIG 37 12HNBT_L, ¹H NMR (500 MHz, dmsol) δ 13.47, 8.39, 8.38, 8.22, 8.21, 8.14, 8.13, 7.95, 7.94, 7.88, 7.87, 7.68, 7.66, 7.65, 7.65, 7.63, 7.62, 7.61, 7.59, 7.59, 7.57, 7.55, 7.52, 7.51, 7.49, 3.32, 3.30, 2.50, -0.01.

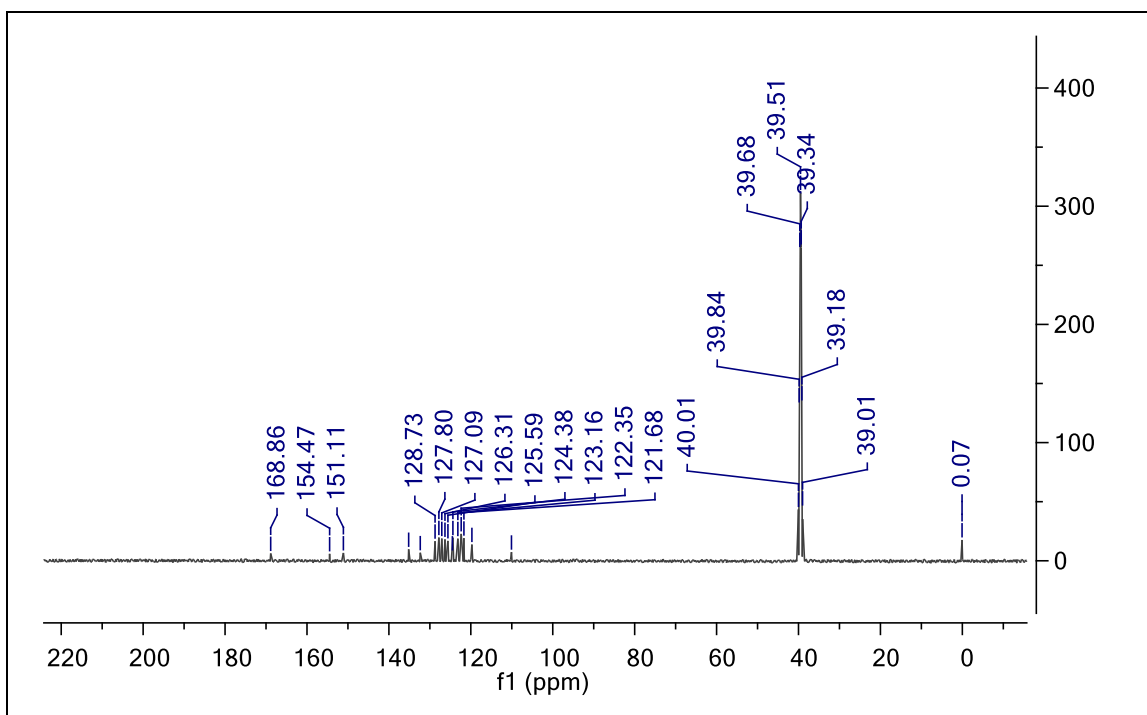


FIG 38 12HNBT_L, ^{13}C NMR (126 MHz, dmsol)

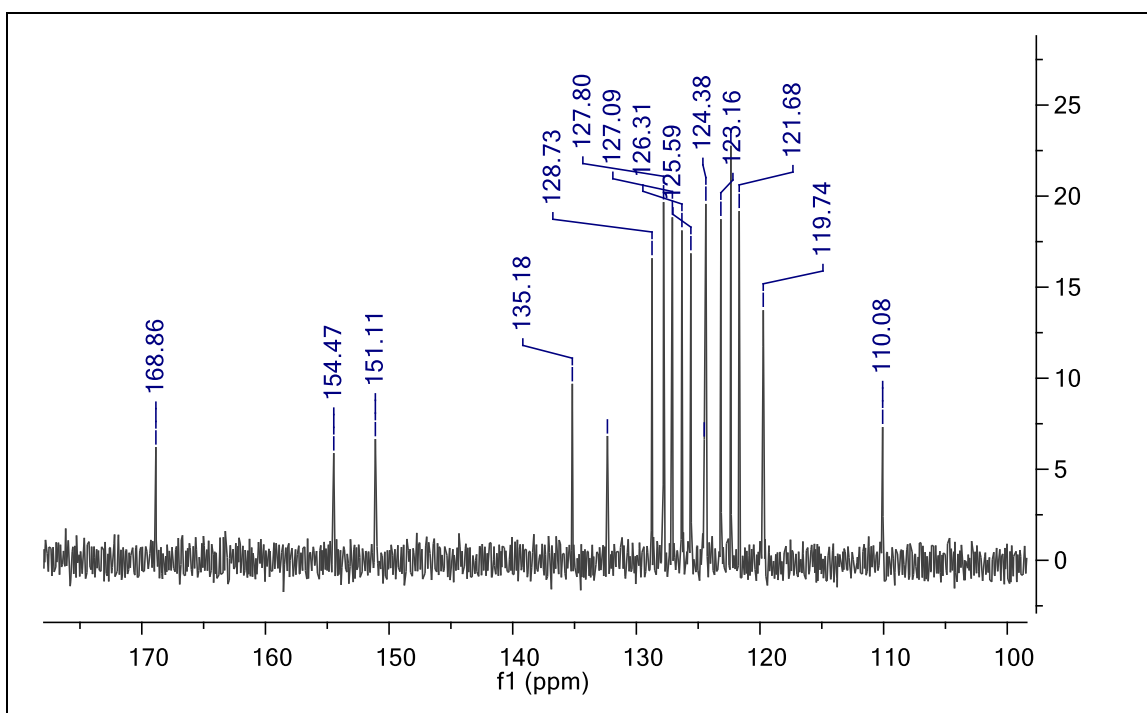


FIG 39 12HNBT_L, ^{13}C NMR (126 MHz, dmsol) δ 168.86, 154.47, 151.11, 135.18, 132.34, 128.73, 127.80, 127.09, 126.31, 125.59, 124.51, 124.38, 123.16, 122.35, 121.68, 119.74, 110.08, 40.01, 39.84, 39.68, 39.51, 39.34, 39.18, 39.01,

NMR data for 5

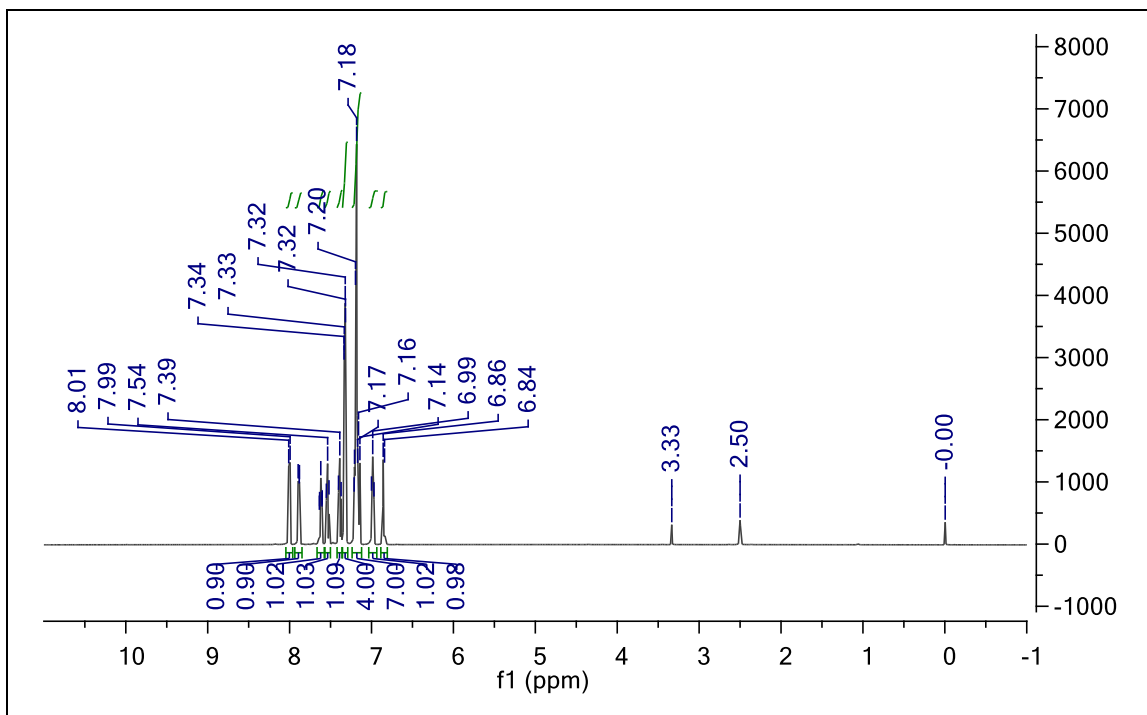


FIG 48 HPBO, ¹H NMR (500 MHz, dms)

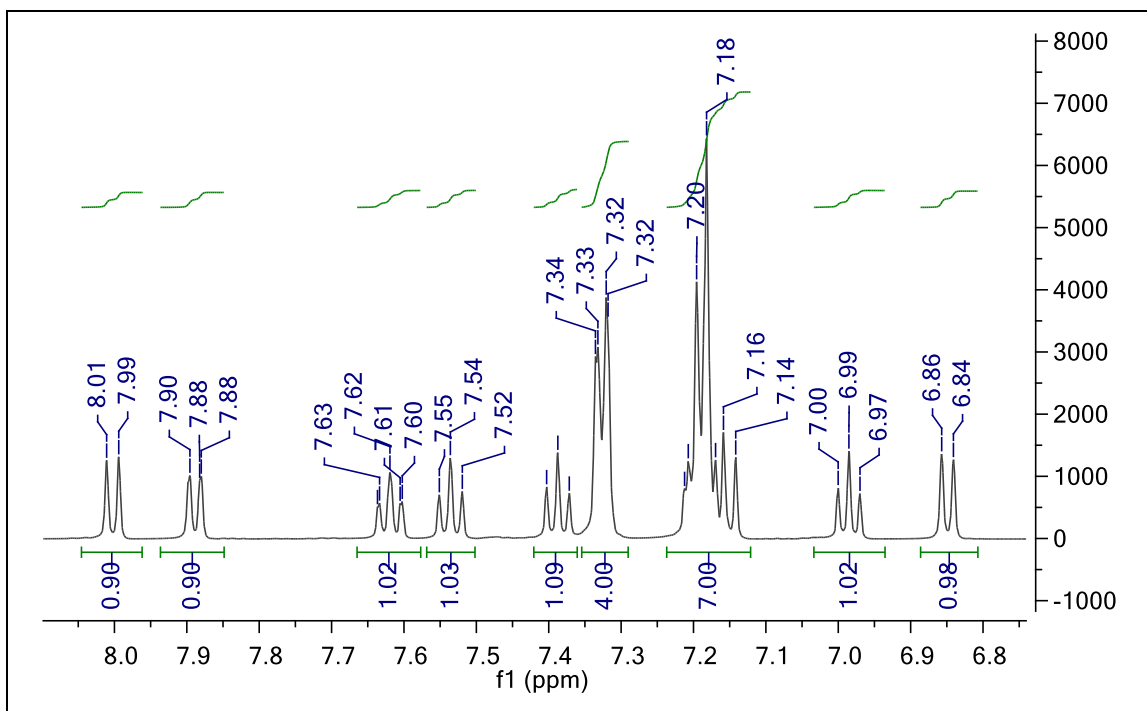


FIG 49 HPBO, ¹H NMR (500 MHz, dms) δ 8.01, 7.99, 7.90, 7.88, 7.88, 7.64, 7.63, 7.62, 7.61, 7.60, 7.55, 7.54, 7.52, 7.40, 7.39, 7.37, 7.34, 7.33, 7.32, 7.32, 7.21, 7.21, 7.20, 7.18, 7.17, 7.16, 7.14, 7.00, 6.99, 6.97, 6.86, 6.84, 3.33, 2.50, -0.00.

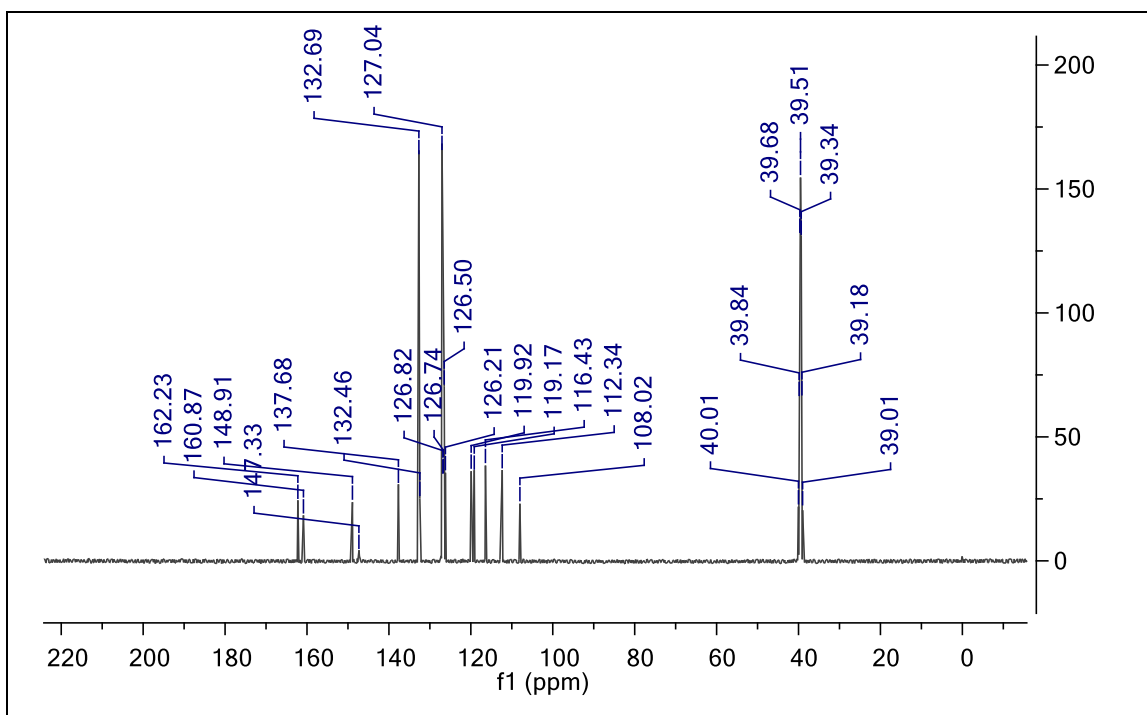


FIG 50 HPBO, ¹³C NMR (126 MHz, dmsol) δ

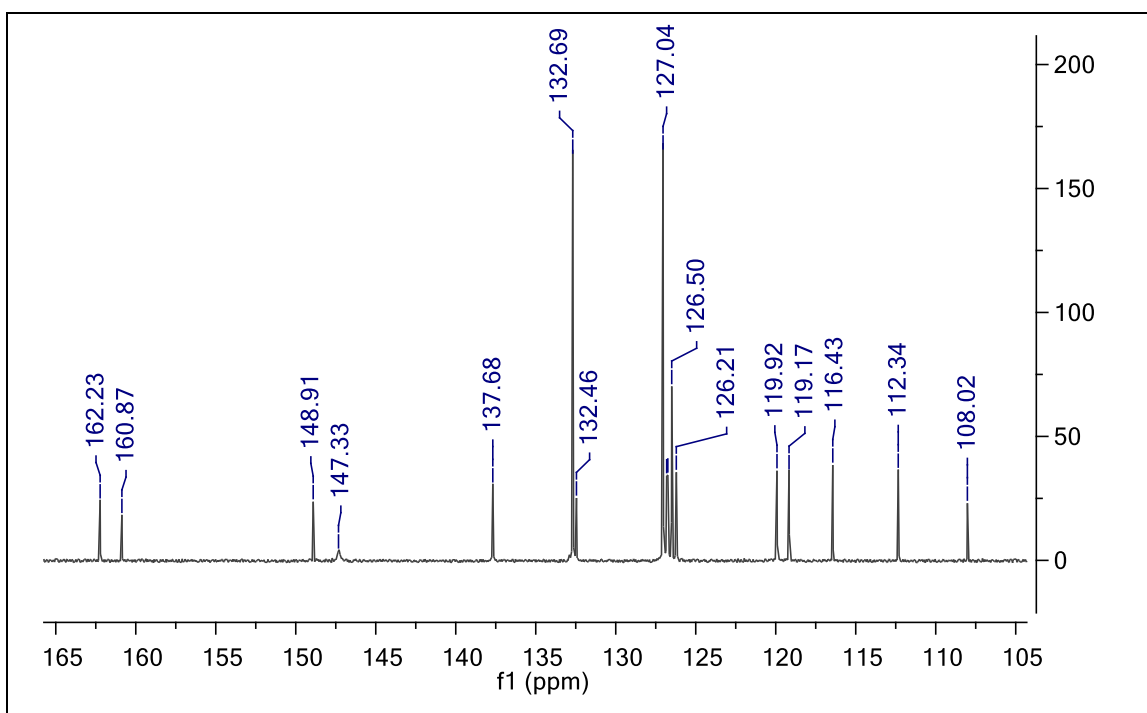
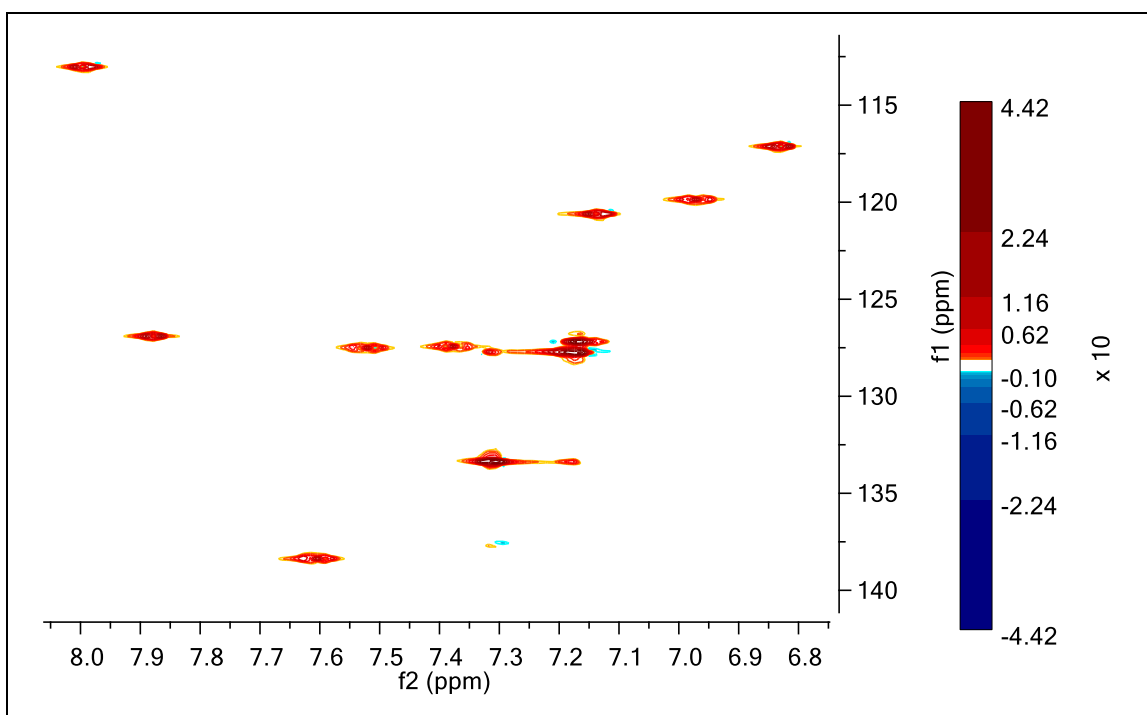
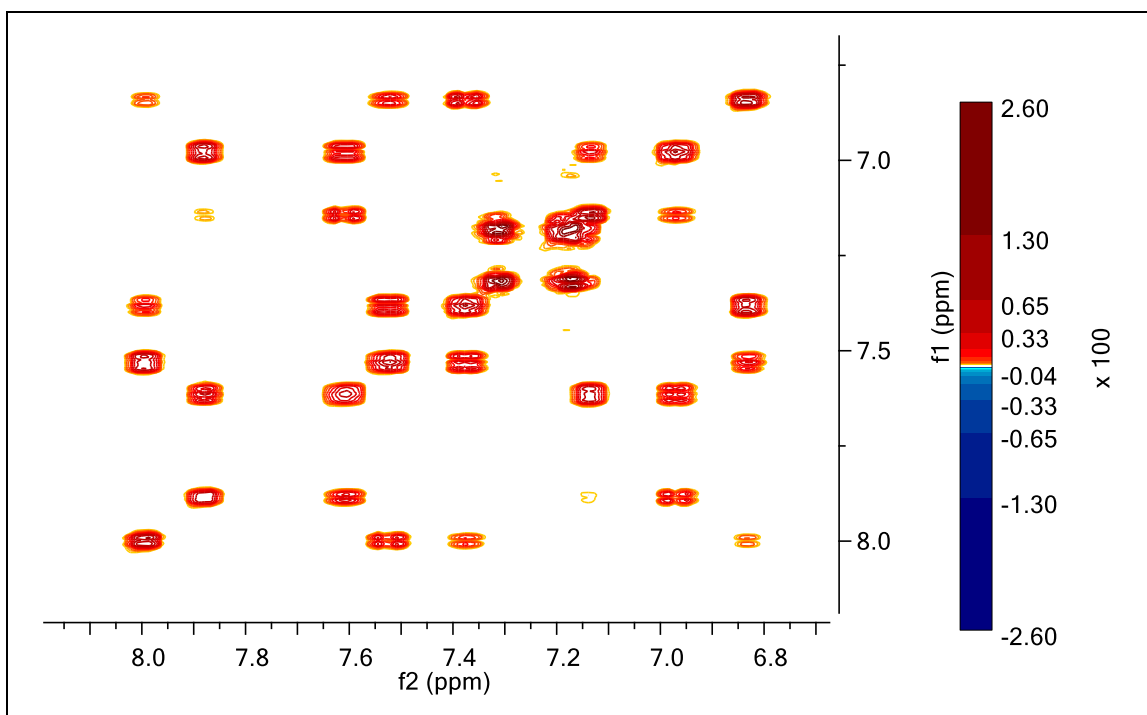


FIG 51 HPBO, ¹³C NMR (126 MHz, dmsol) δ 162.23, 160.87, 148.91, 147.33, 137.68, 132.69, 132.46, 127.04, 126.82, 126.74, 126.50, 126.21, 119.92, 119.17, 116.43, 112.34, 108.02, 40.01, 39.84, 39.68, 39.51, 39.34, 39.18, 39.01.



NMR data for 6

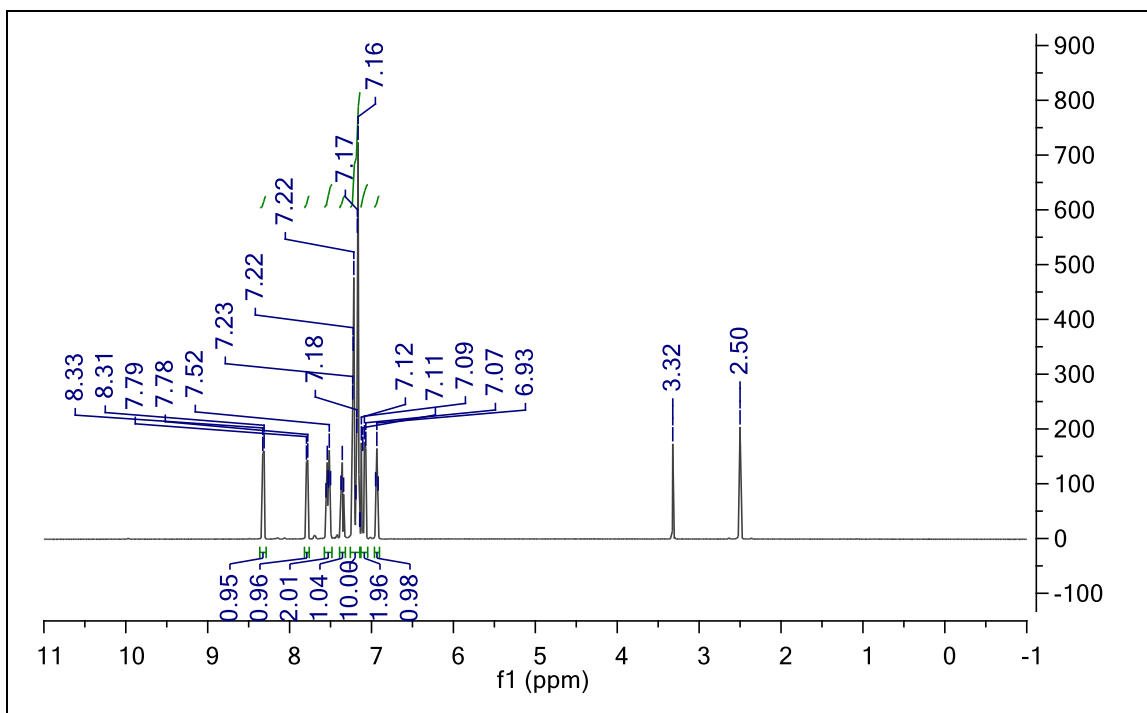


FIG 54 HPBT, ¹H NMR (500 MHz, dmsol)

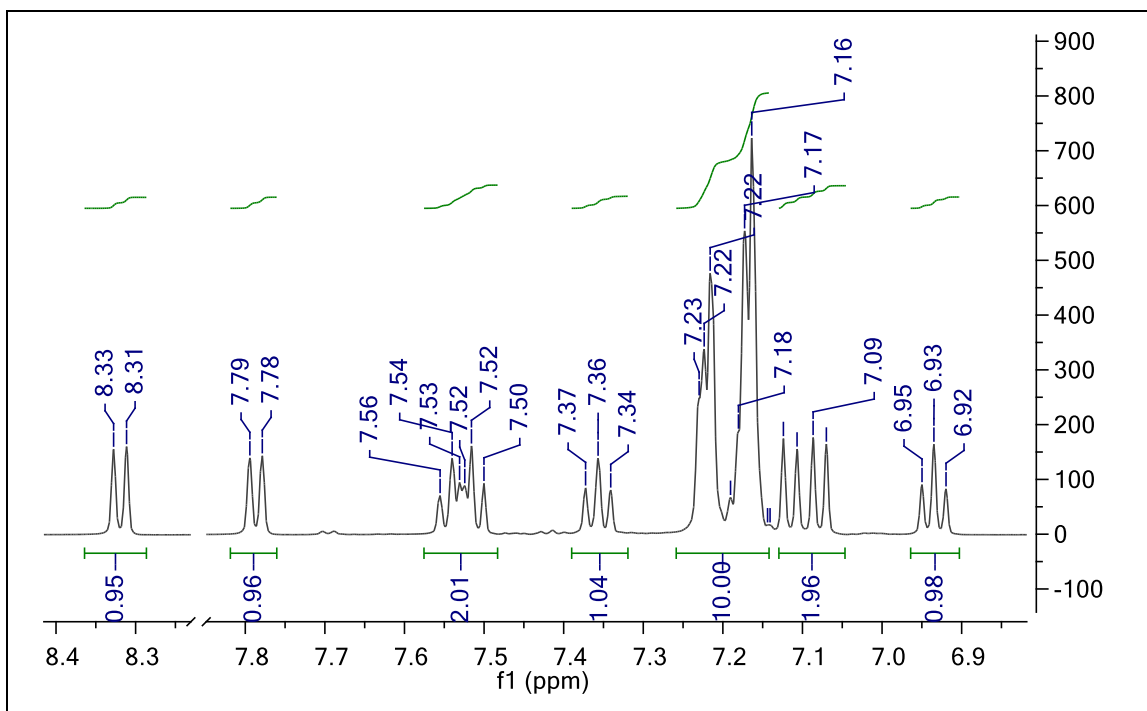


FIG 55 HPBT, ¹H NMR (500 MHz, dmsol) δ 8.33, 8.31, 7.79, 7.78, 7.56, 7.54, 7.53, 7.52, 7.52, 7.50, 7.37, 7.36, 7.34, 7.23, 7.22, 7.22, 7.19, 7.18, 7.17, 7.16, 7.14, 7.14, 7.12, 7.11, 7.09, 7.07, 6.95, 6.93, 6.92, 3.32, 2.50.

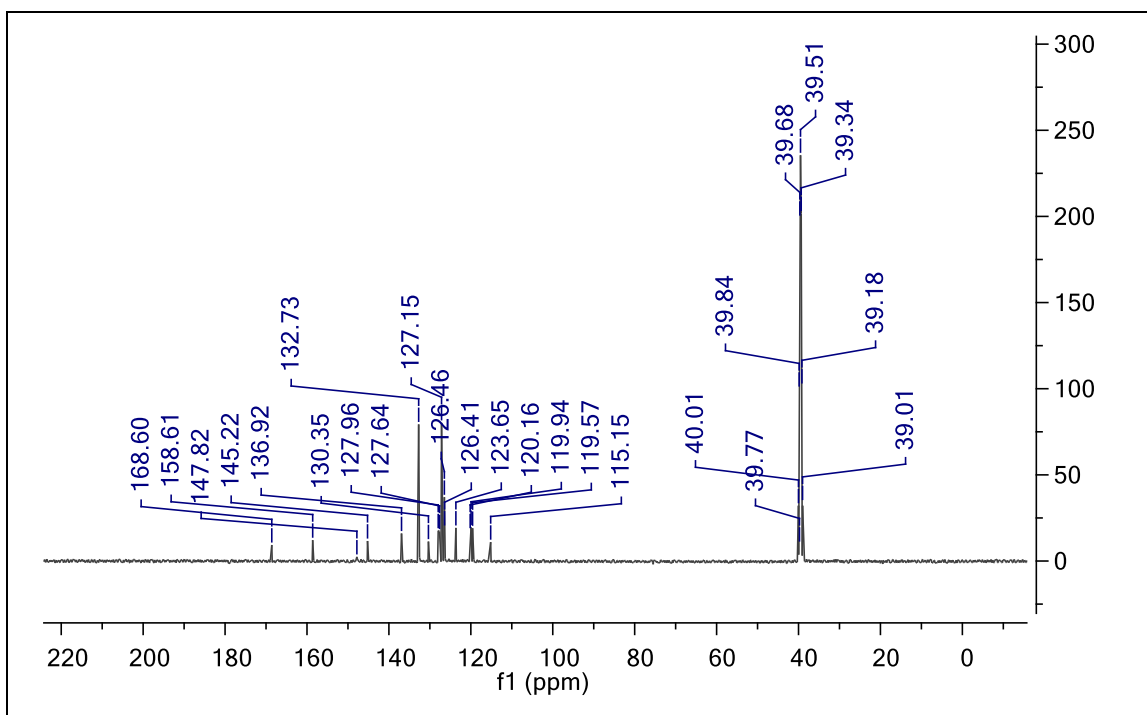


FIG 56 HPBT, ^{13}C NMR (126 MHz, dmsd)

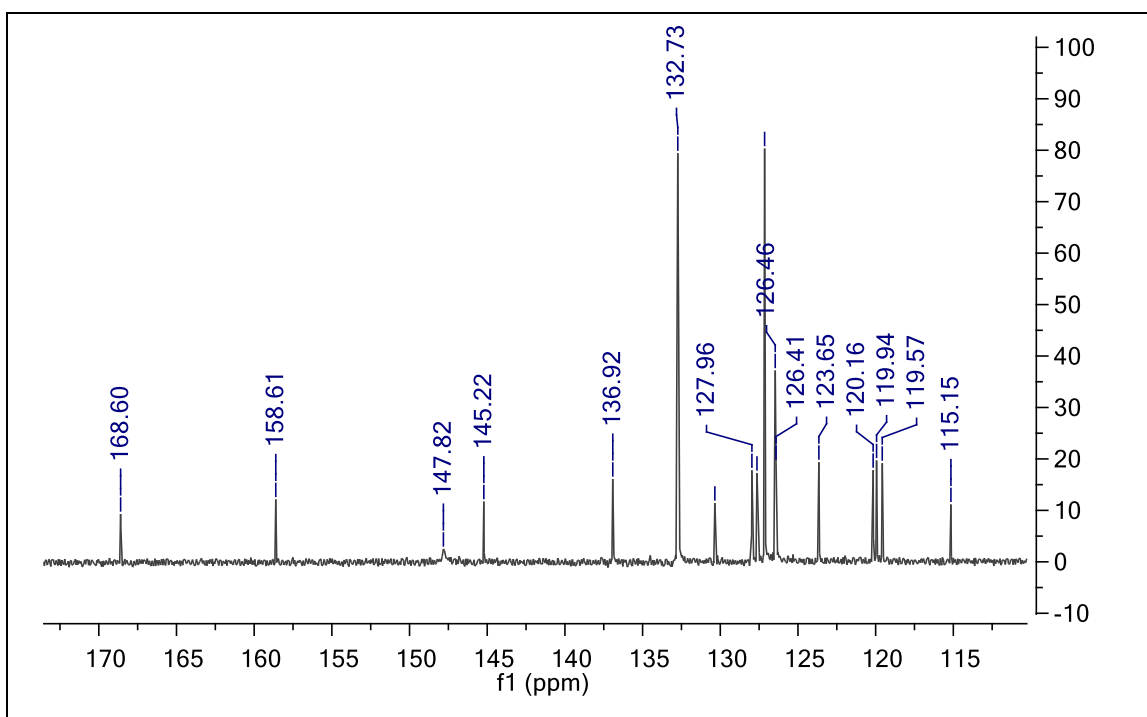


FIG 57 HPBT, ^{13}C NMR (126 MHz, dmsd) δ 168.60, 158.61, 147.82, 145.22, 136.92, 132.73, 130.35, 127.96, 127.64, 127.15, 126.46, 126.41, 123.65, 120.16, 119.94, 119.57, 115.15, 40.01, 39.84, 39.77, 39.68, 39.51, 39.34, 39.18, 39.01.

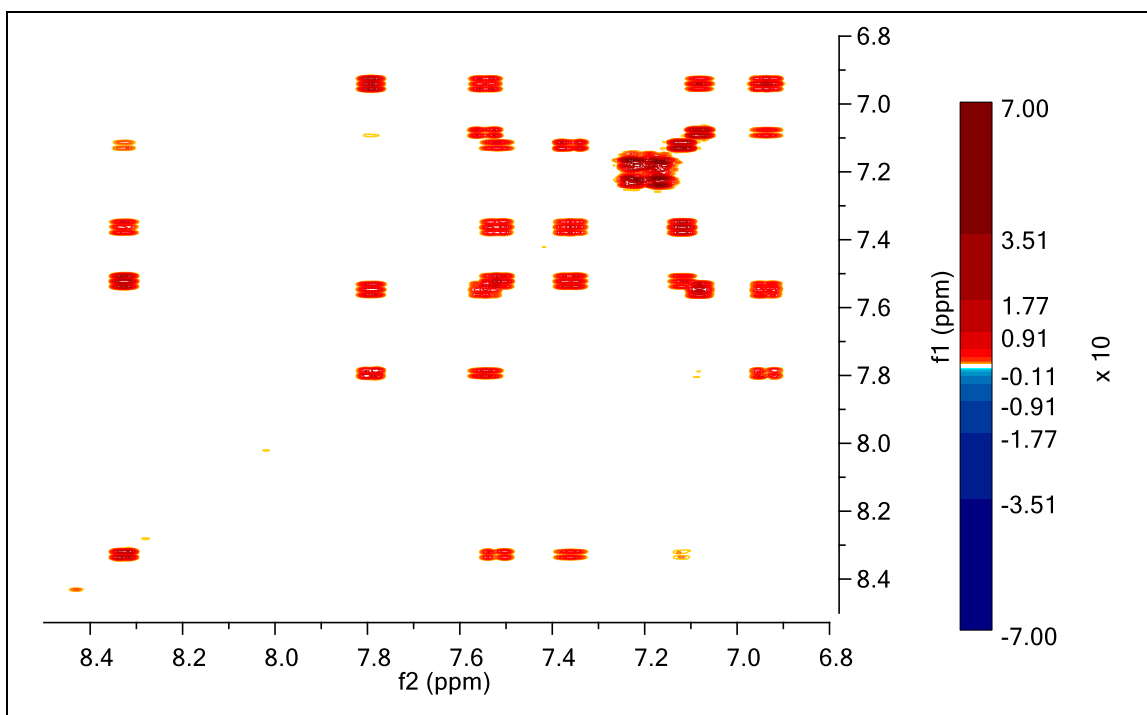


FIG 58 HPBT, G-COSY (dmsol)

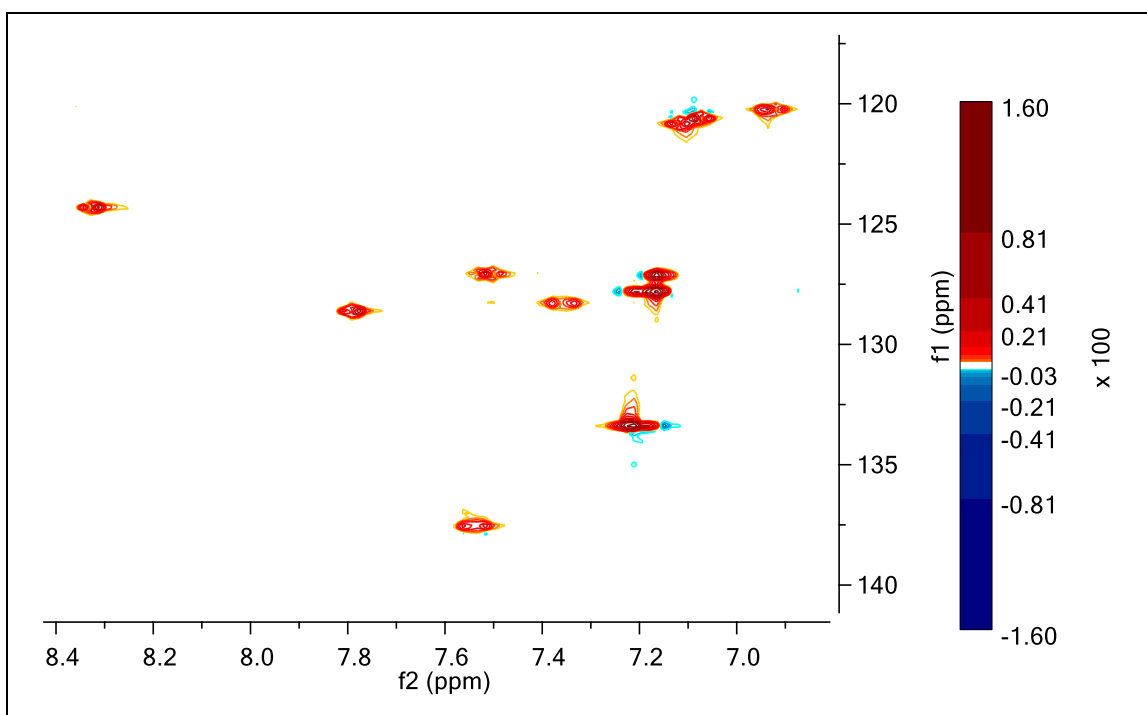


FIG 59 HPBT, G-HMQC (dmsol)

NMR data of 7a

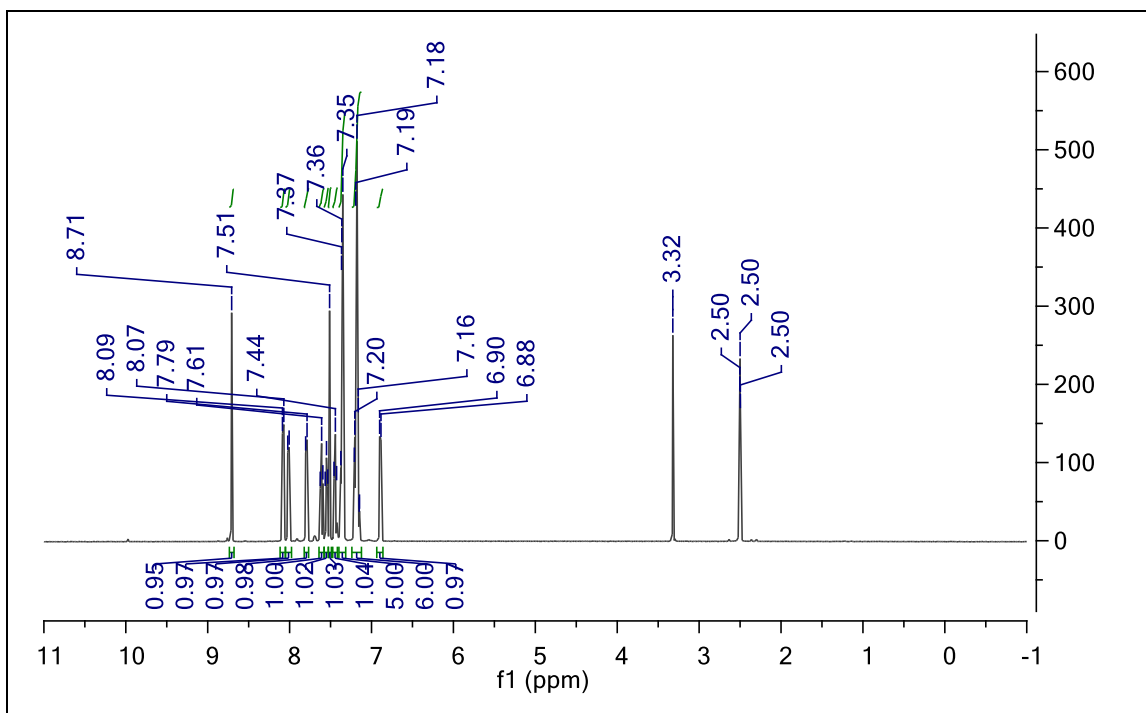


FIG 72 23HNBO, ¹H NMR (500 MHz, dmsol)

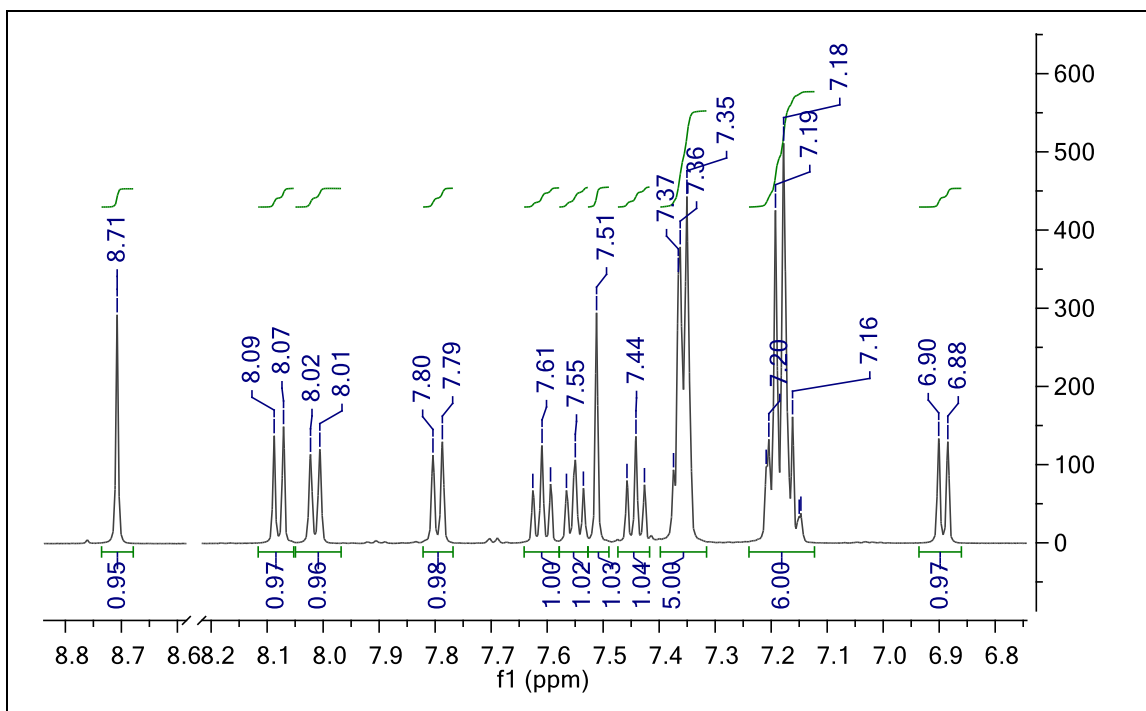


FIG 73 23HNBO, ¹H NMR (500 MHz, dmsol) δ 8.71, 8.09, 8.07, 8.02, 8.01, 7.80, 7.79, 7.63, 7.61, 7.59, 7.57, 7.55, 7.54, 7.51, 7.46, 7.44, 7.43, 7.37, 7.37, 7.36, 7.35, 7.21, 7.20, 7.19, 7.18, 7.16, 7.15, 7.15, 6.90, 6.88, 3.32, 2.50, 2.50, 2.50.

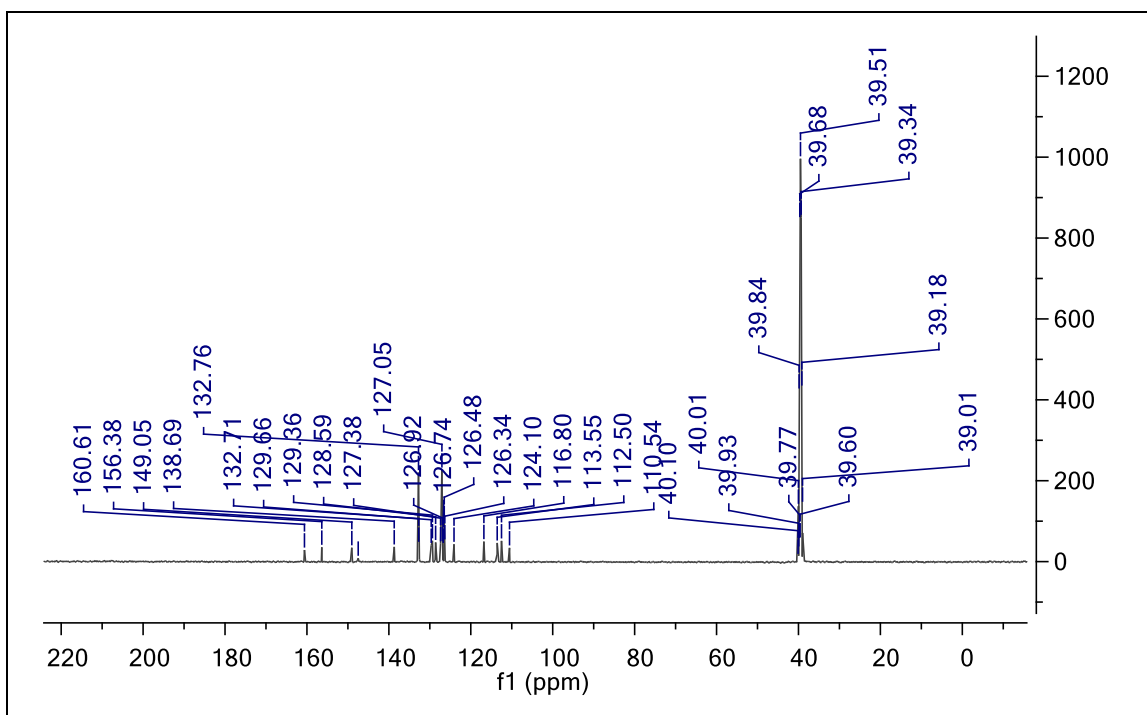


FIG 74 23HNBO, ^{13}C NMR (126 MHz, dmsol)

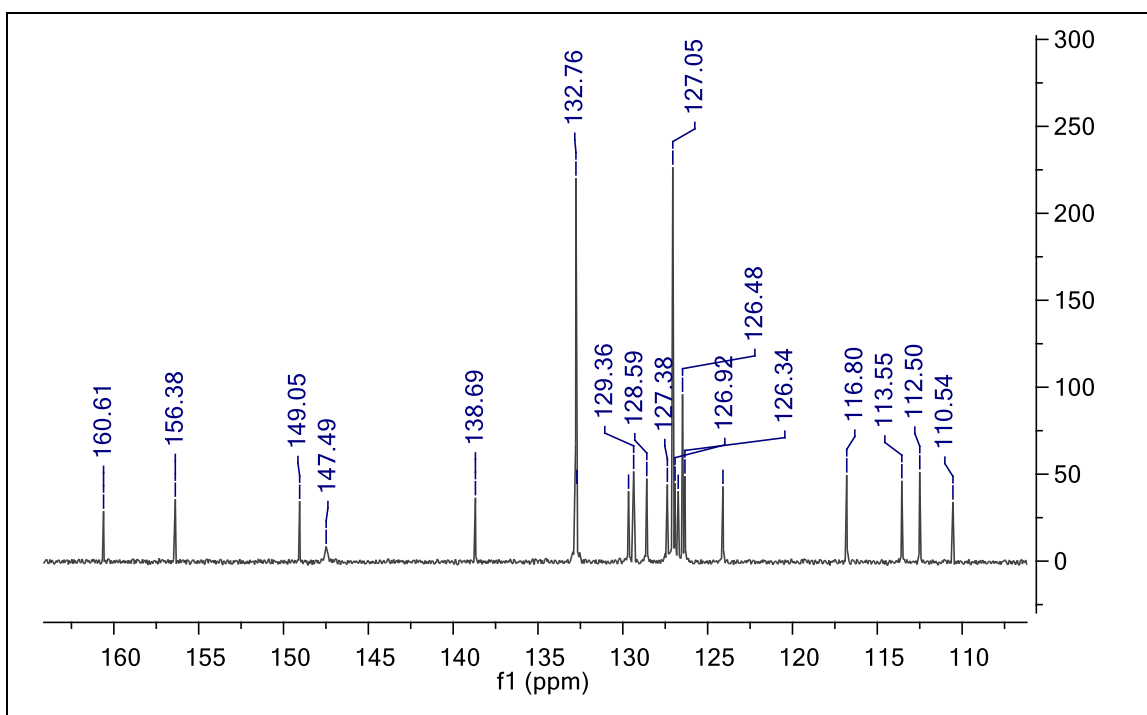


FIG 75 23HNBO, ^{13}C NMR (126 MHz, dmsol) δ 160.61, 156.38, 149.05, 147.49, 138.69, 132.76, 132.71, 129.66, 129.36, 128.59, 127.38, 127.05, 126.92, 126.74, 126.48, 126.34, 124.10, 116.80, 113.55, 112.50, 110.54, 40.10, 40.01, 39.93, 39.84, 39.77, 39.68, 39.60, 39.51, 39.34, 39.18, 39.01.

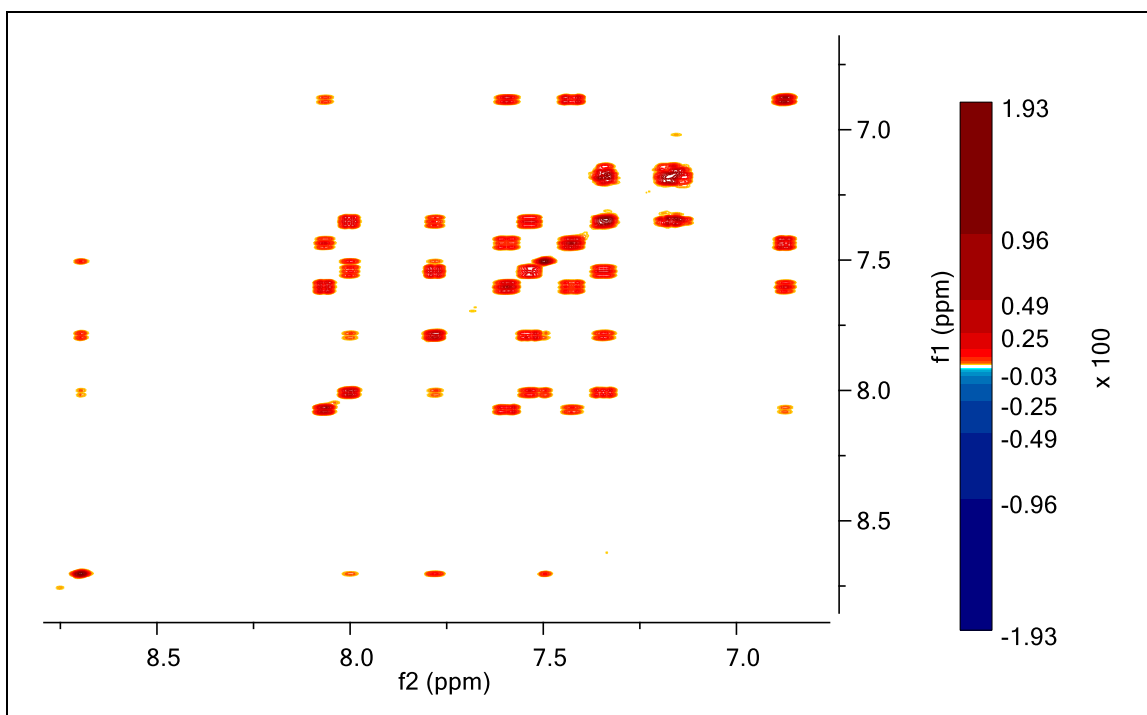


FIG 76 23HNBO, G-COSY (dmsol)

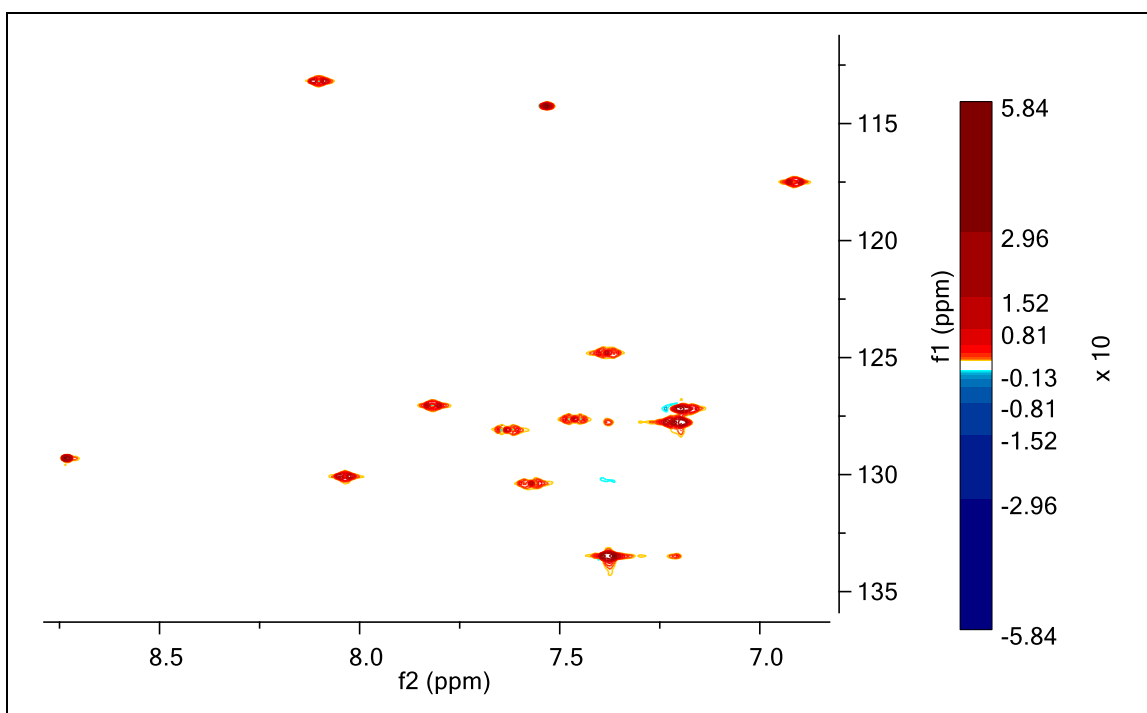


FIG 77 23HNBO, G-HMQC (dmsol)

NMR data of 7b

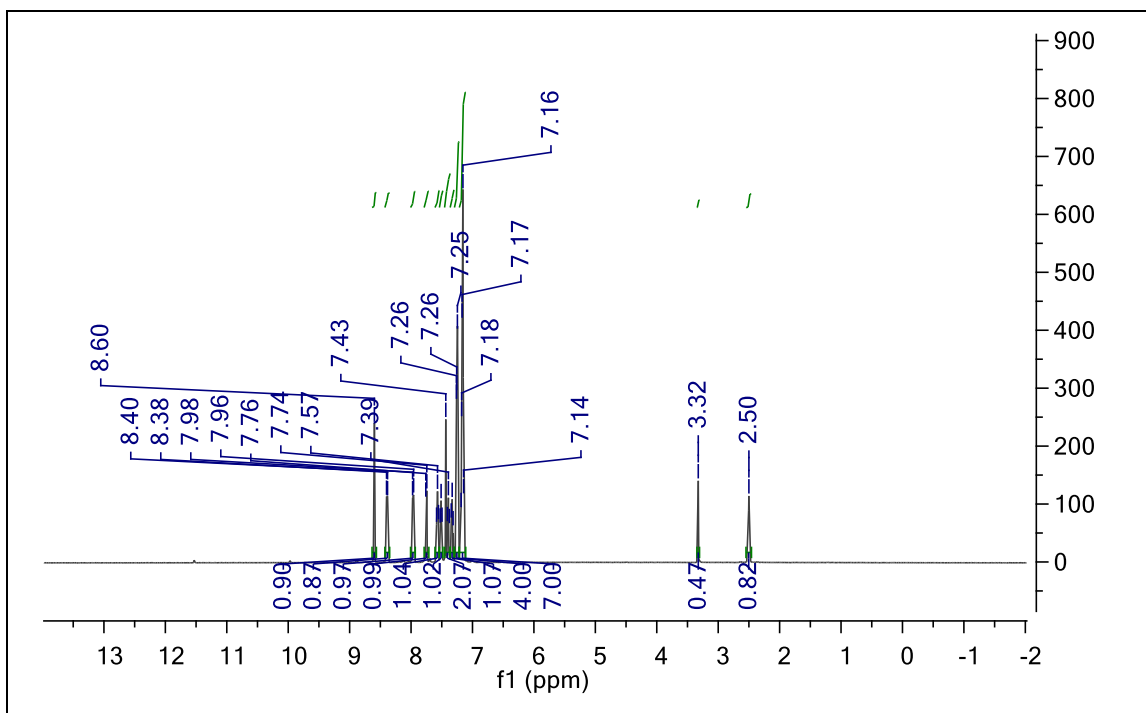


FIG 78 23HNBT, ¹H NMR (500 MHz, dmsol)

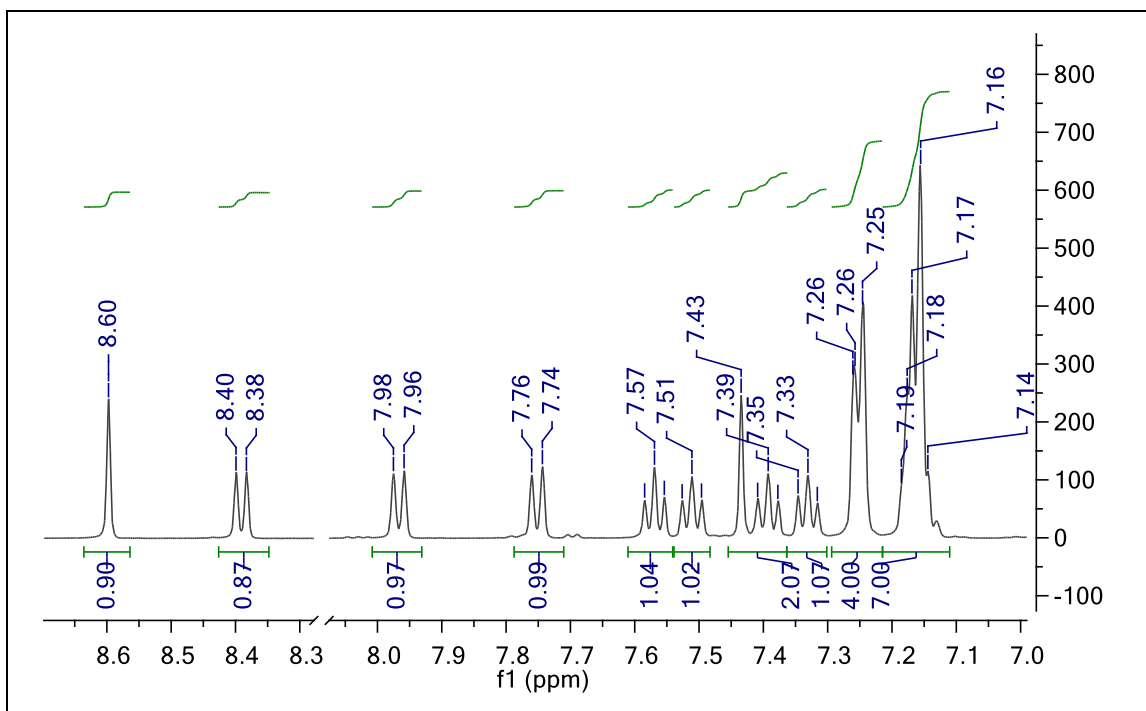


FIG 79 23HNBT, ¹H NMR (500 MHz, dmsol) δ 8.60, 8.40, 8.38, 7.98, 7.96, 7.76, 7.74, 7.58, 7.57, 7.55, 7.53, 7.51, 7.50, 7.43, 7.41, 7.39, 7.38, 7.35, 7.33, 7.32, 7.26, 7.26, 7.25, 7.19, 7.18, 7.17, 7.16, 7.14, 3.32, 2.50.

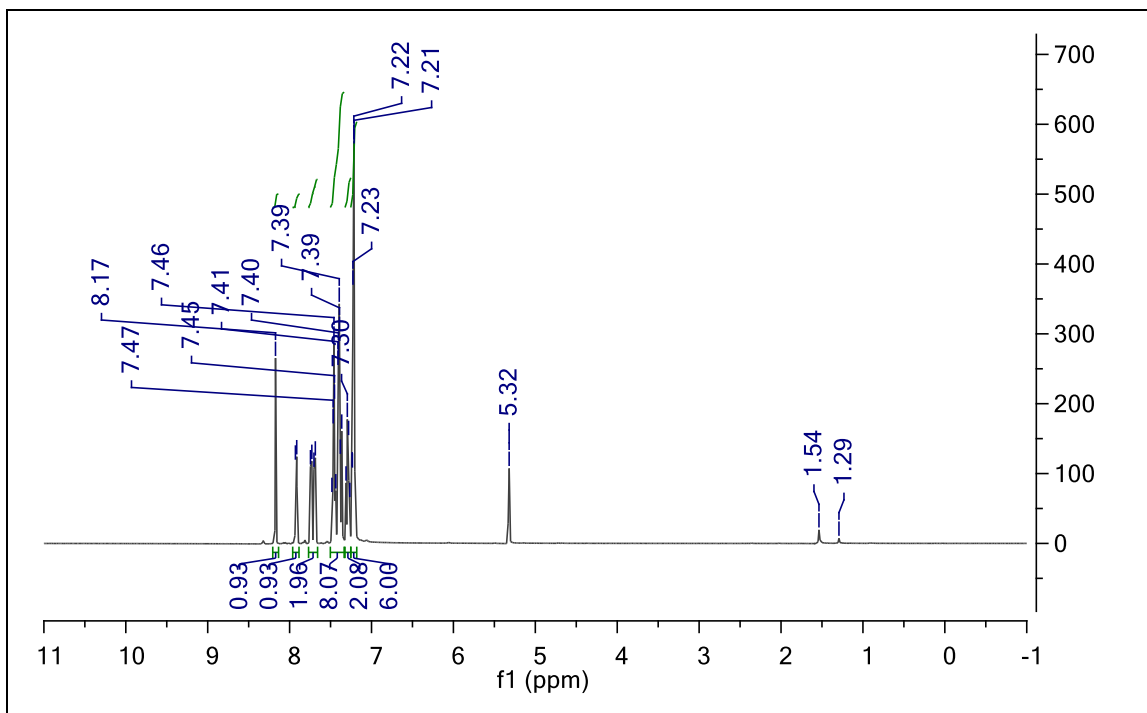


FIG 80 23HNBT, ^1H NMR (500 MHz, CD_2Cl_2)

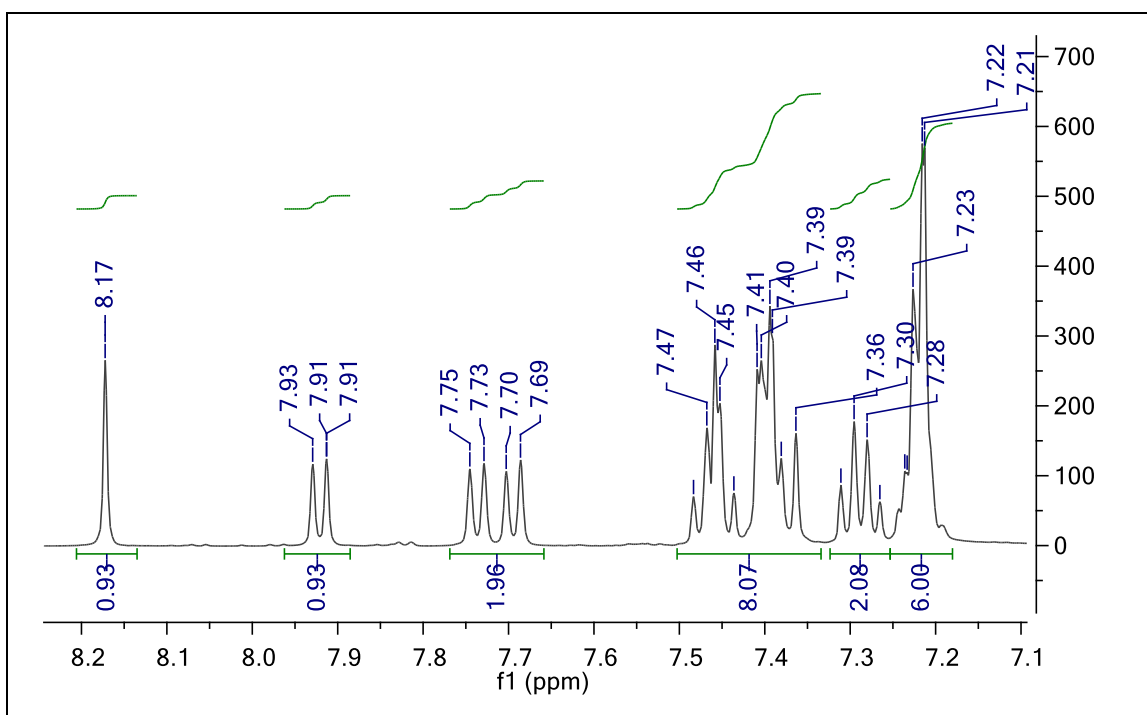


FIG 81 23HNBT, ^1H NMR (500 MHz, CD_2Cl_2) δ 8.17, 7.93, 7.91, 7.75, 7.73, 7.70, 7.69, 7.48, 7.47, 7.46, 7.45, 7.44, 7.41, 7.40, 7.39, 7.39, 7.38, 7.36, 7.31, 7.30, 7.28, 7.27, 7.24, 7.23, 7.23, 7.22, 7.21, 5.32, 1.54, 1.29.

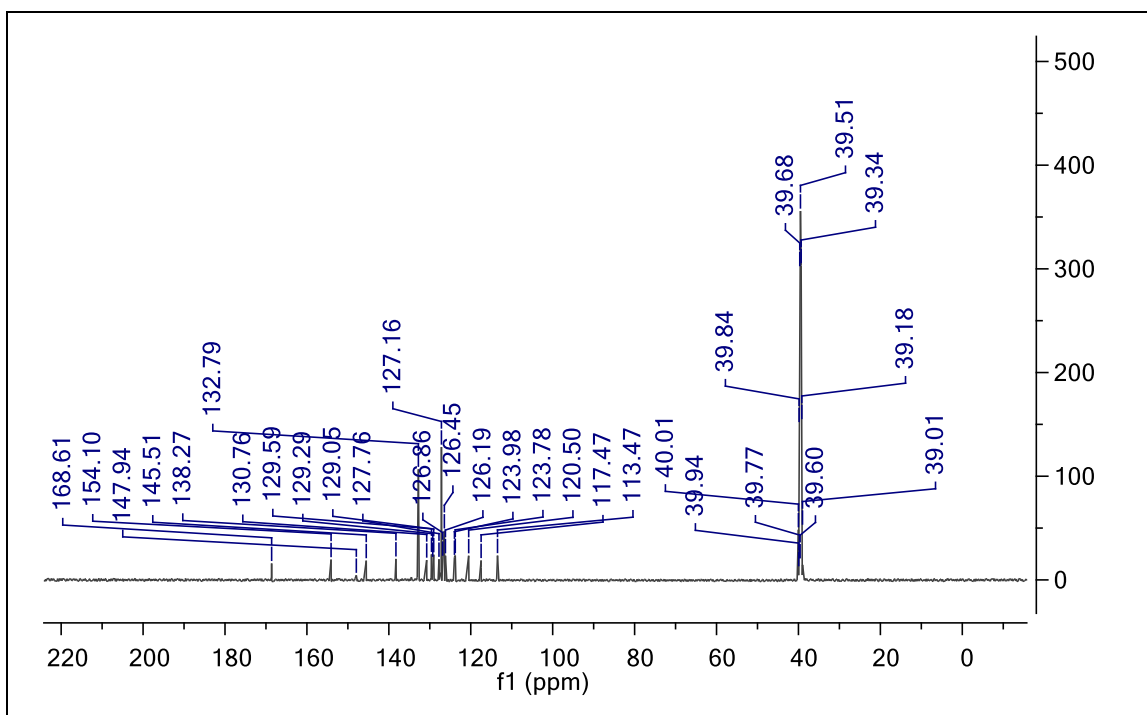


FIG 82 23HNBT, ¹³C NMR (126 MHz, dmsol)

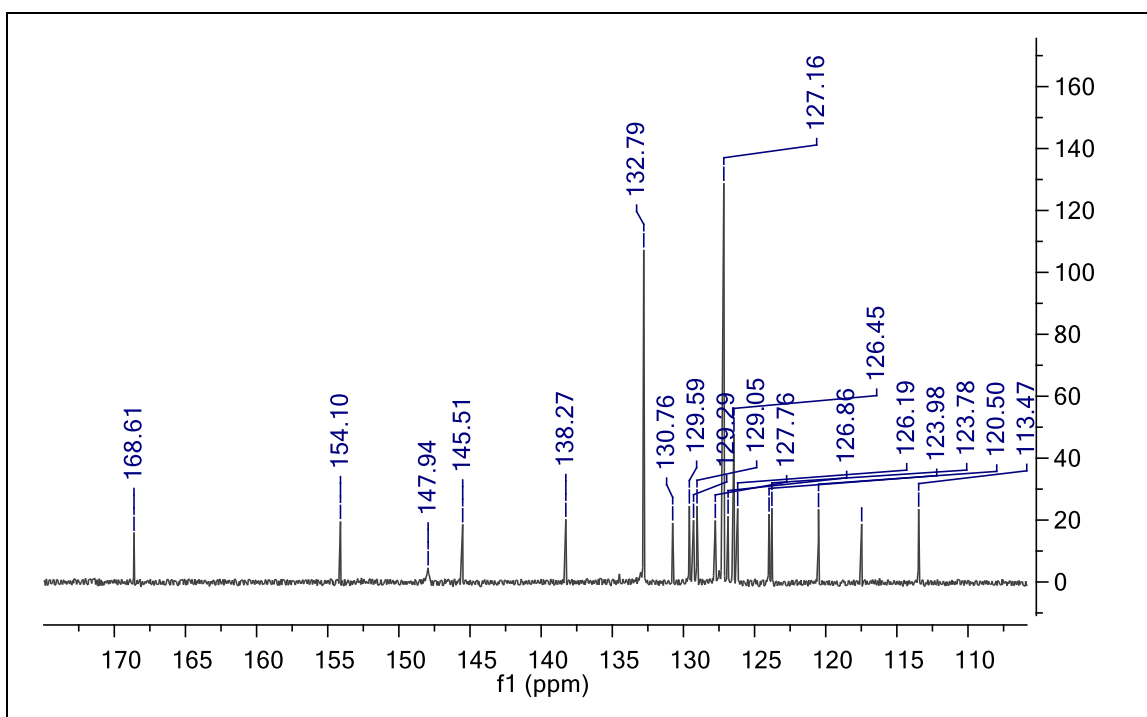


FIG 83 23HNBT, ¹³C NMR (126 MHz, dmsol) δ 168.61, 154.10, 147.94, 145.51, 138.27, 132.79, 130.76, 129.59, 129.29, 129.05, 127.76, **127.16**, **127.16**, 126.86, 126.45, 126.19, 123.98, 123.78, 120.50, 117.47, 113.47, 40.01, 39.94, 39.84, 39.77, 39.68, 39.60, 39.51, 39.34, 39.18, 39.01.

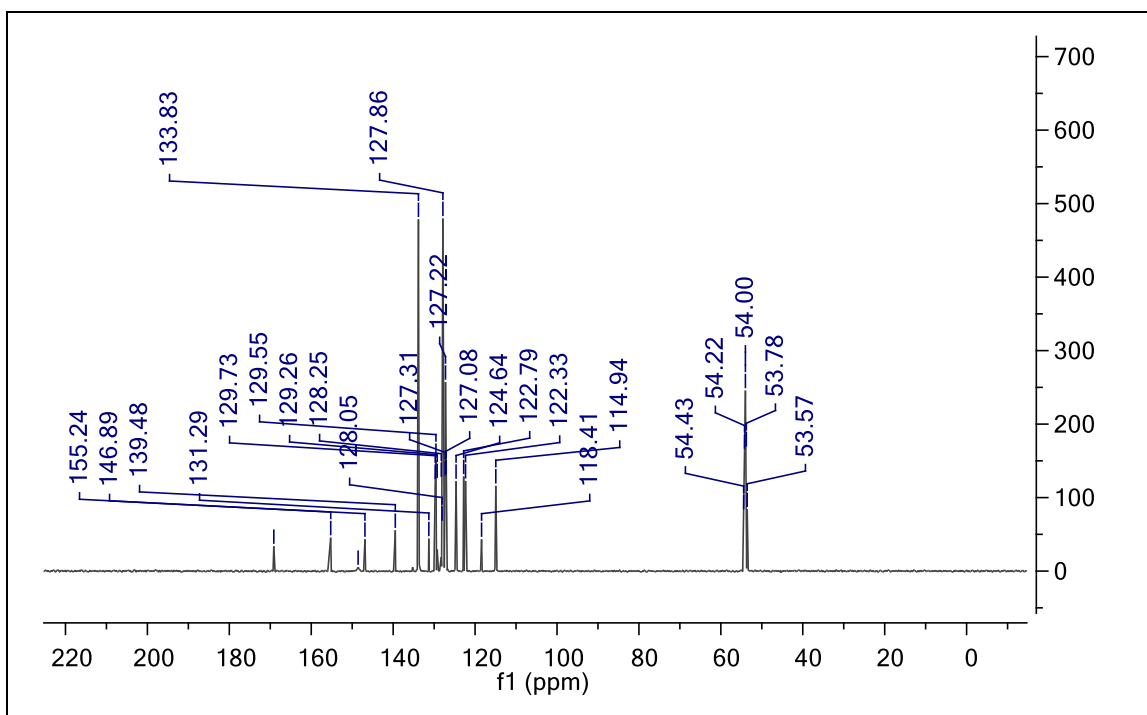


FIG 84 23HNBT, ^{13}C NMR (126 MHz, cd_2cl_2)

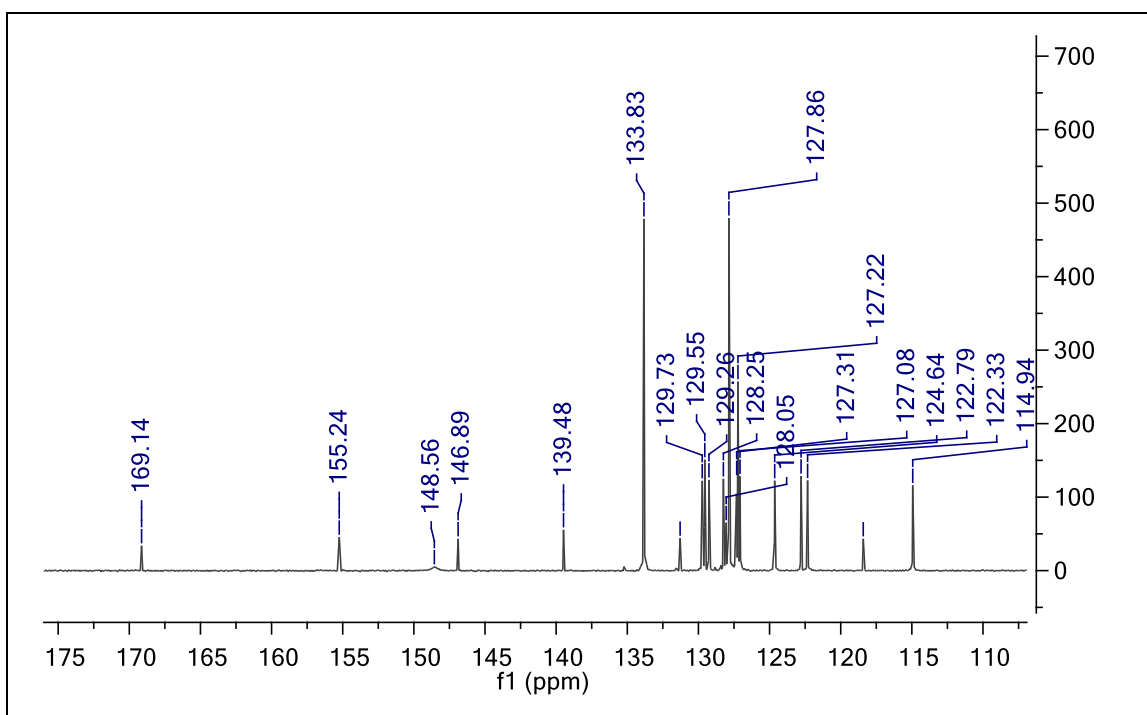


FIG 85 23HNBT, ^{13}C NMR (126 MHz, cd_2cl_2) δ 169.14, 155.24, 148.56, 146.89, 139.48, 133.83, 131.29, 129.73, 129.55, 129.26, 128.25, 128.05, 127.86, 127.31, 127.22, 127.08, 124.64, 122.79, 122.33, 118.41, 114.94, 54.43, 54.22, 54.00, 53.78, 53.57.

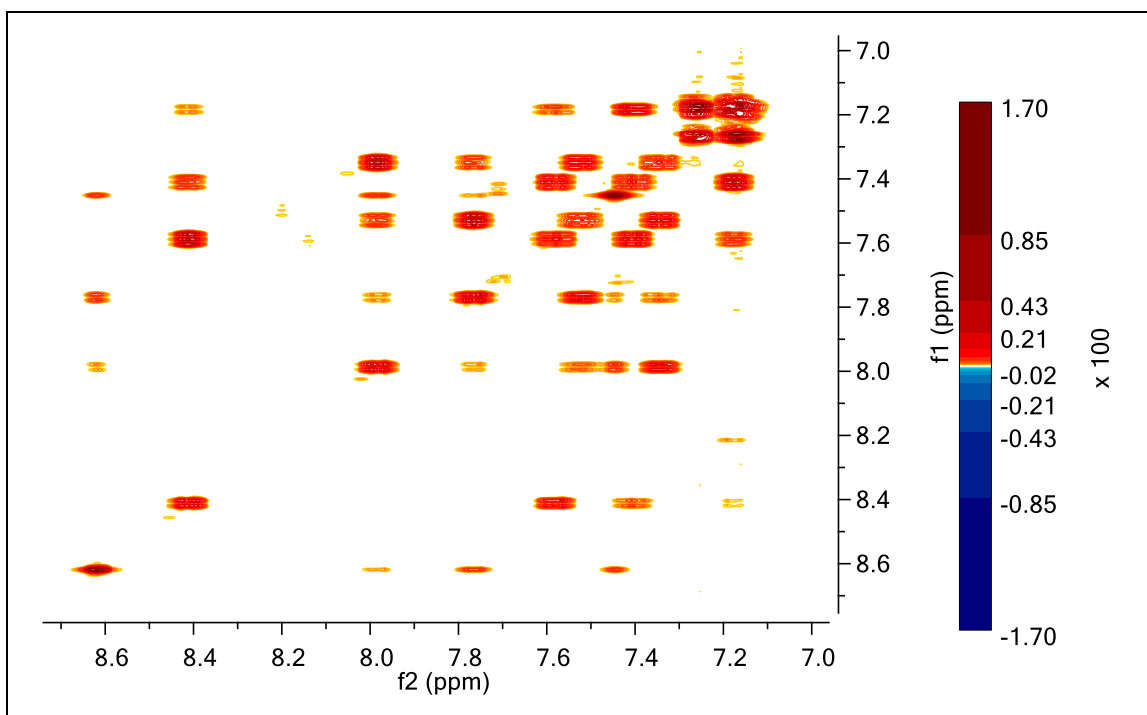


FIG 86 23HNBT, G-COSY (dmsol)

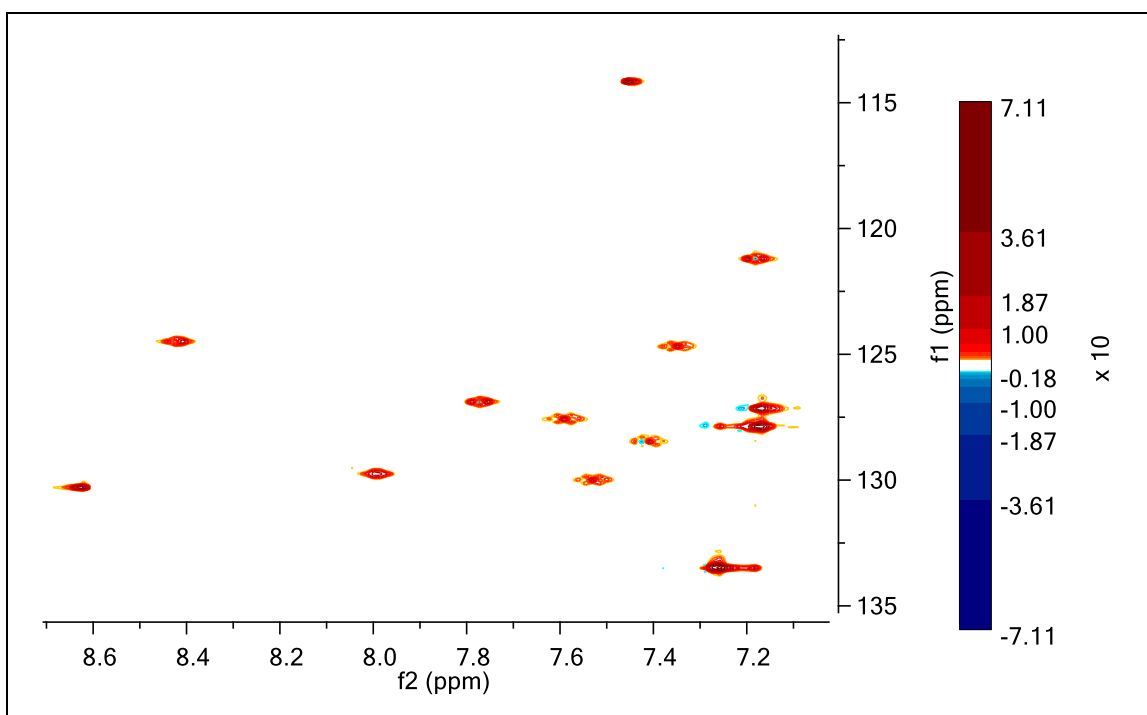


FIG 87 23HNBT, G-HMQC (dmsol)

NMR data of 8a

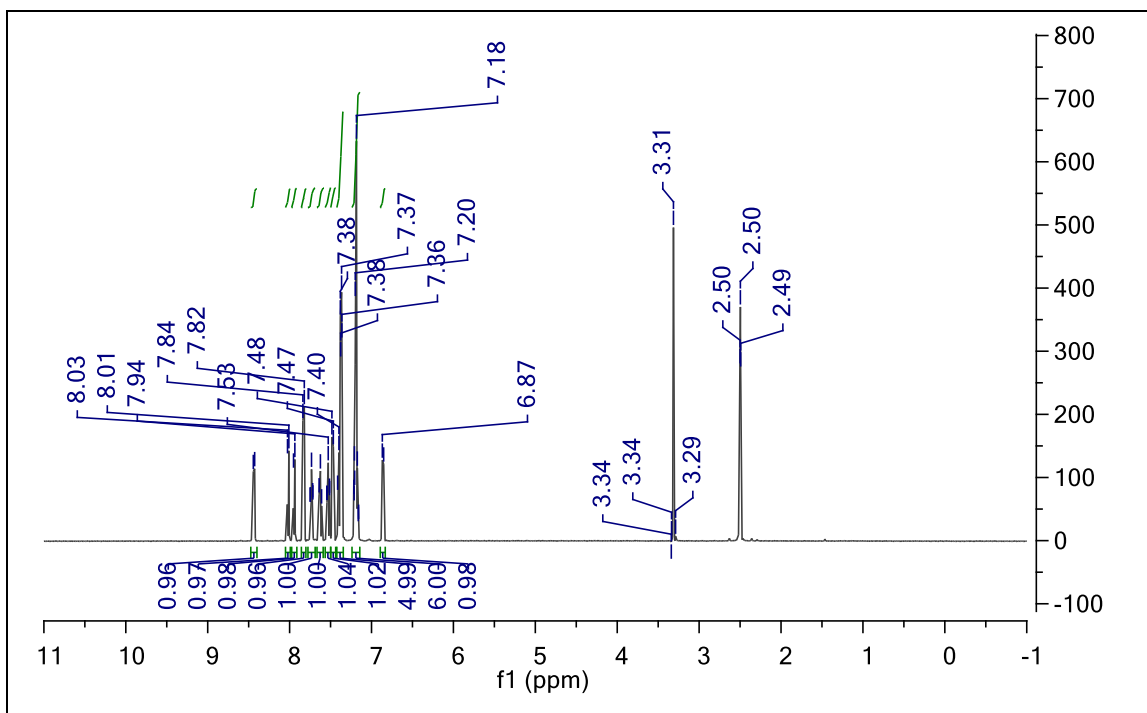


FIG 60 12HNBO, ¹H NMR (500 MHz, dmsol)

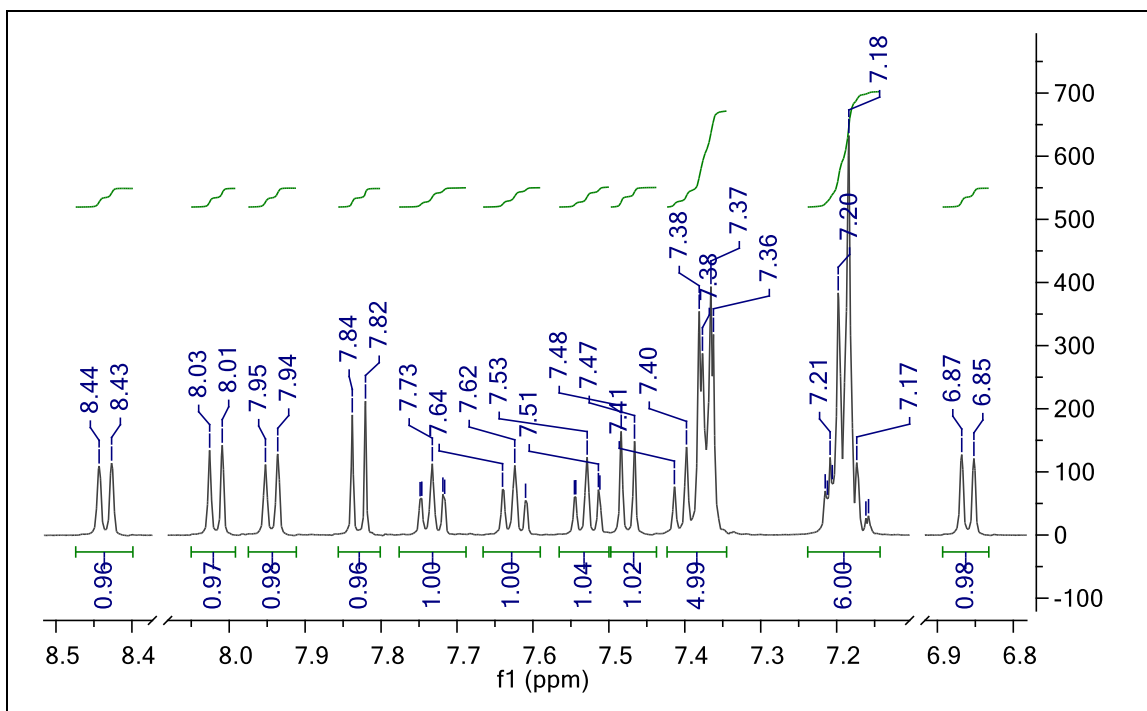


FIG 61 12HNBO, ¹H NMR (500 MHz, dmsol) δ 8.44, 8.43, 8.03, 8.01, 7.95, 7.94, 7.84, 7.82, 7.75, 7.75, 7.73, 7.72, 7.72, 7.64, 7.62, 7.61, 7.55, 7.54, 7.53, 7.51, 7.51, 7.48, 7.47, 7.41, 7.40, 7.38, 7.38, 7.37, 7.36, 7.22, 7.21, 7.21, 7.20, 7.18, 7.17, 7.16, 7.16, 6.87, 6.85, 3.34, 3.34, 3.31, 3.29, 2.50, 2.50, 2.49.

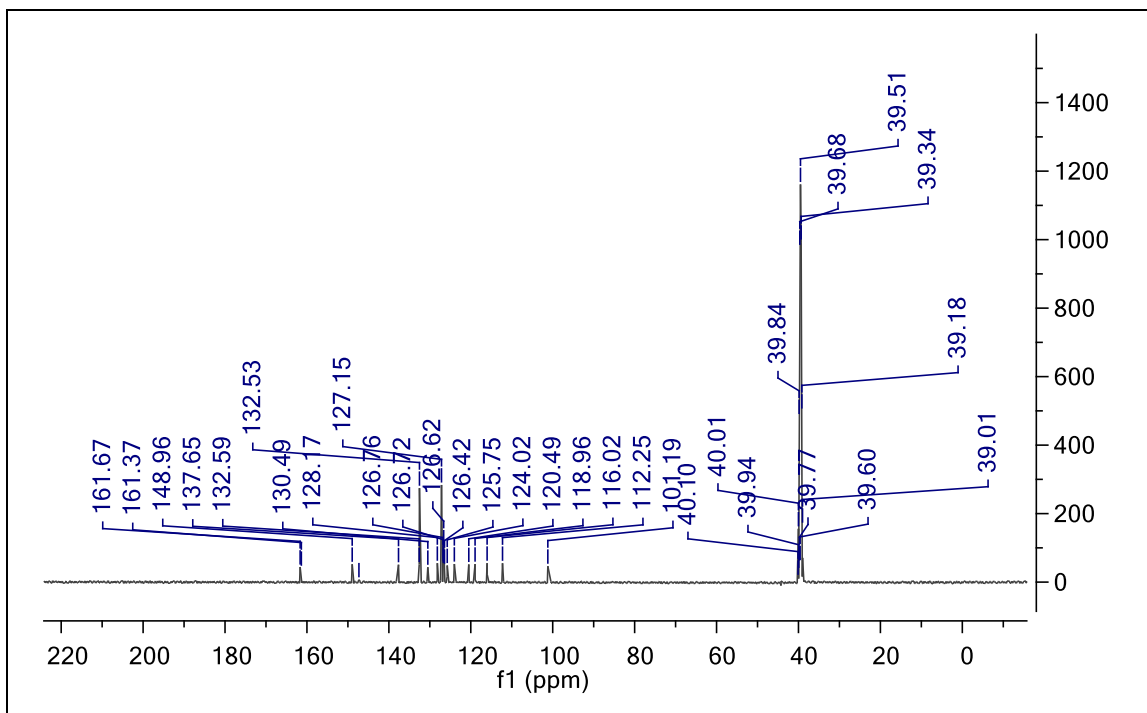


FIG 62 12HNBO, ^{13}C NMR (126 MHz, dmsol)

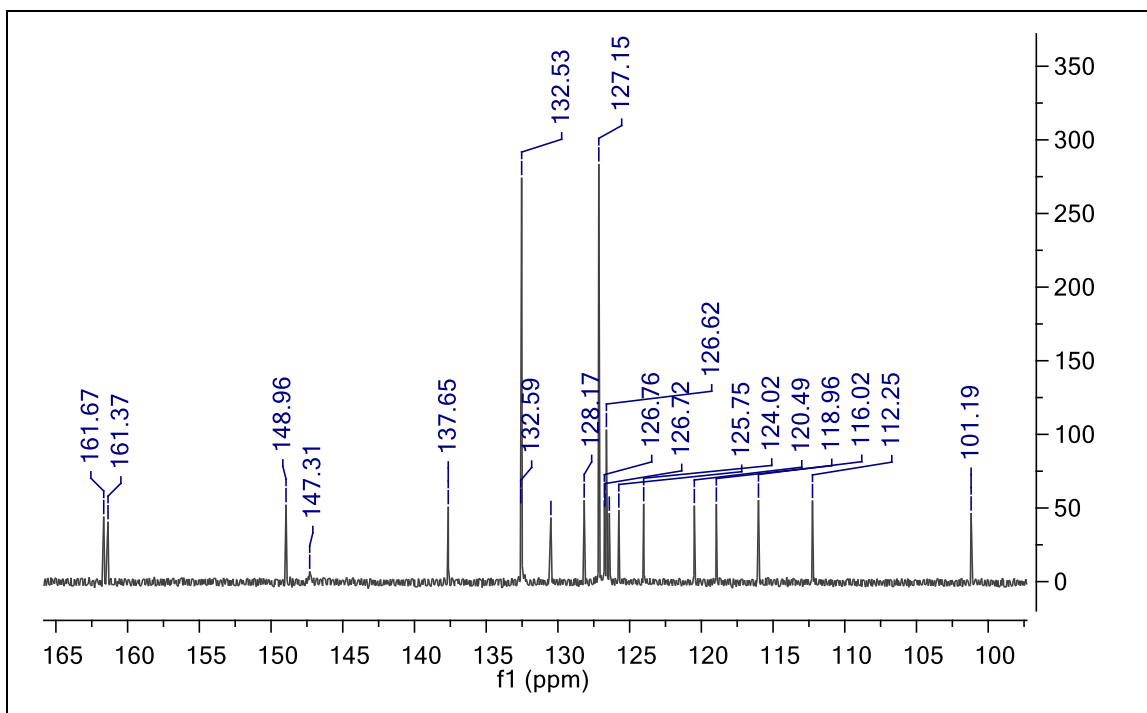


FIG 63 12HNBO, ^{13}C NMR (126 MHz, dmsol) δ 161.67, 161.37, 148.96, 147.31, 137.65, 132.59, 132.53, 130.49, 128.17, 127.15, 126.76, 126.72, 126.62, 126.42, 125.75, 124.02, 120.49, 118.96, 116.02, 112.25, 101.19, 40.10, 40.01, 39.94, 39.84, 39.77, 39.68, 39.60, 39.51, 39.34, 39.18, 39.01.

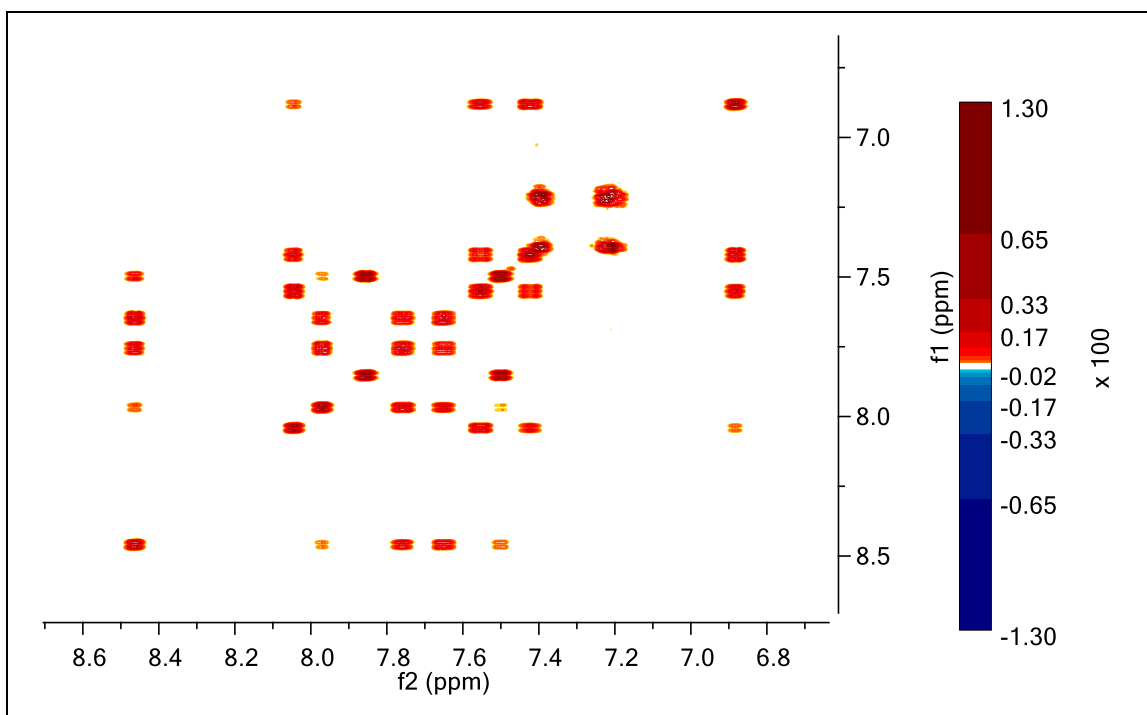


FIG 64 12HNBO, G-COSY (dmsol)

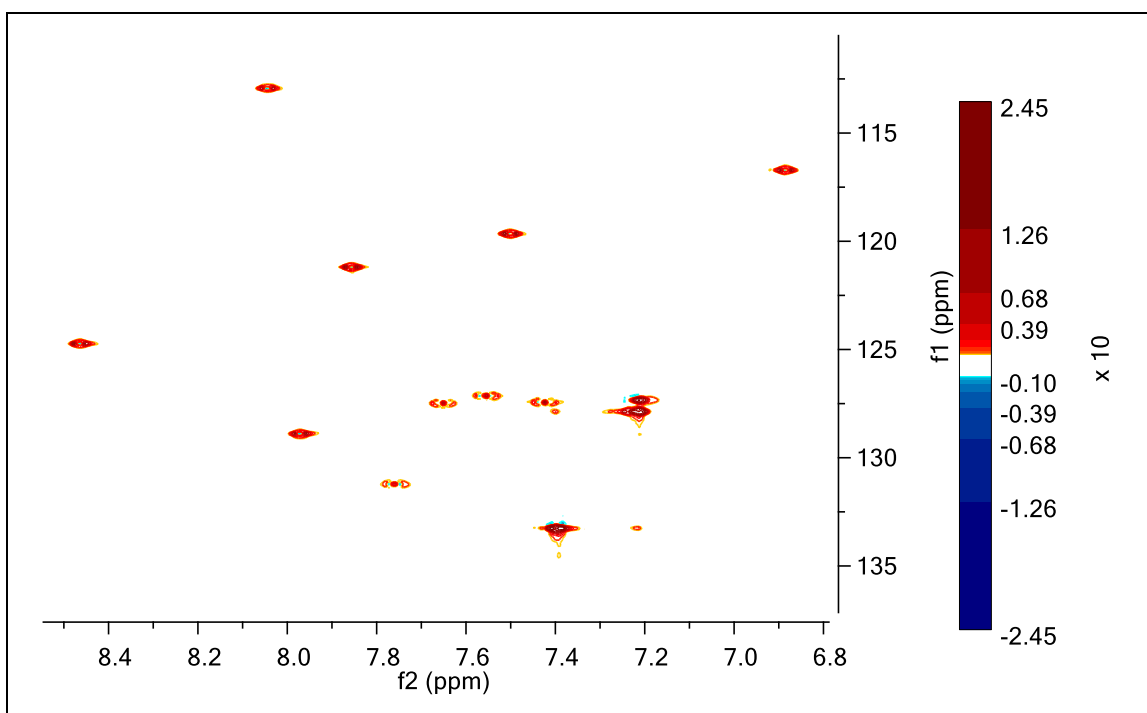


FIG 65 12HNBO, G-HMQC (dmsol)

NMR data of 8b

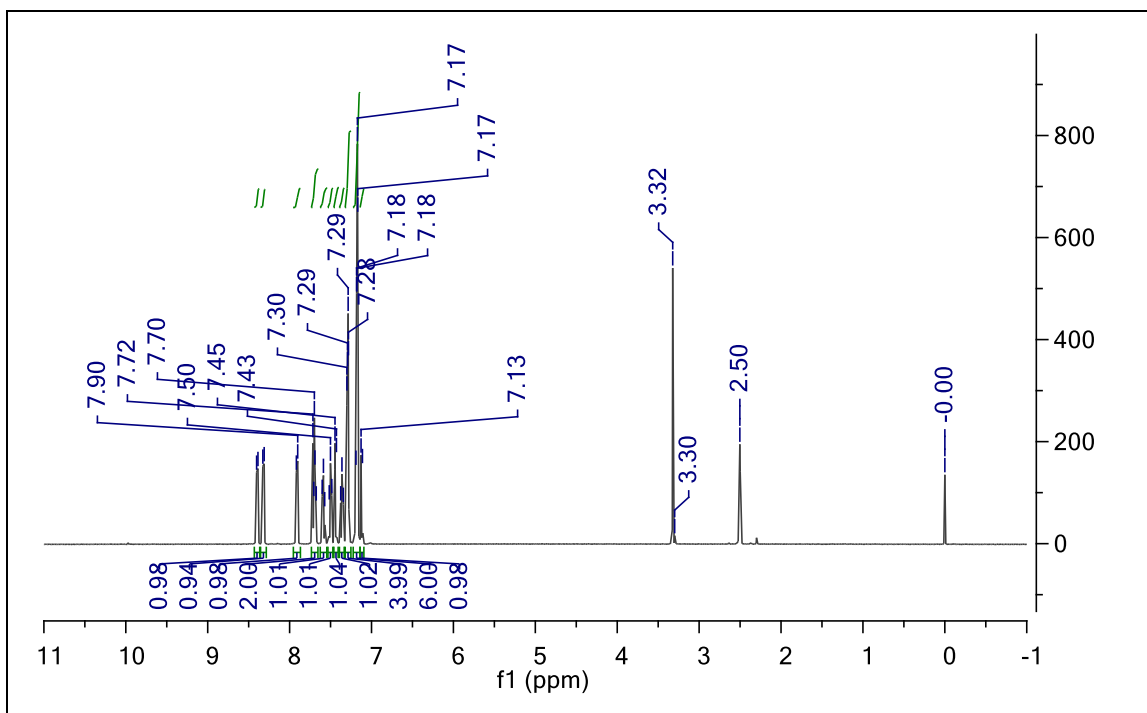


FIG 66 12HNBT, ¹H NMR (500 MHz, dmsol)

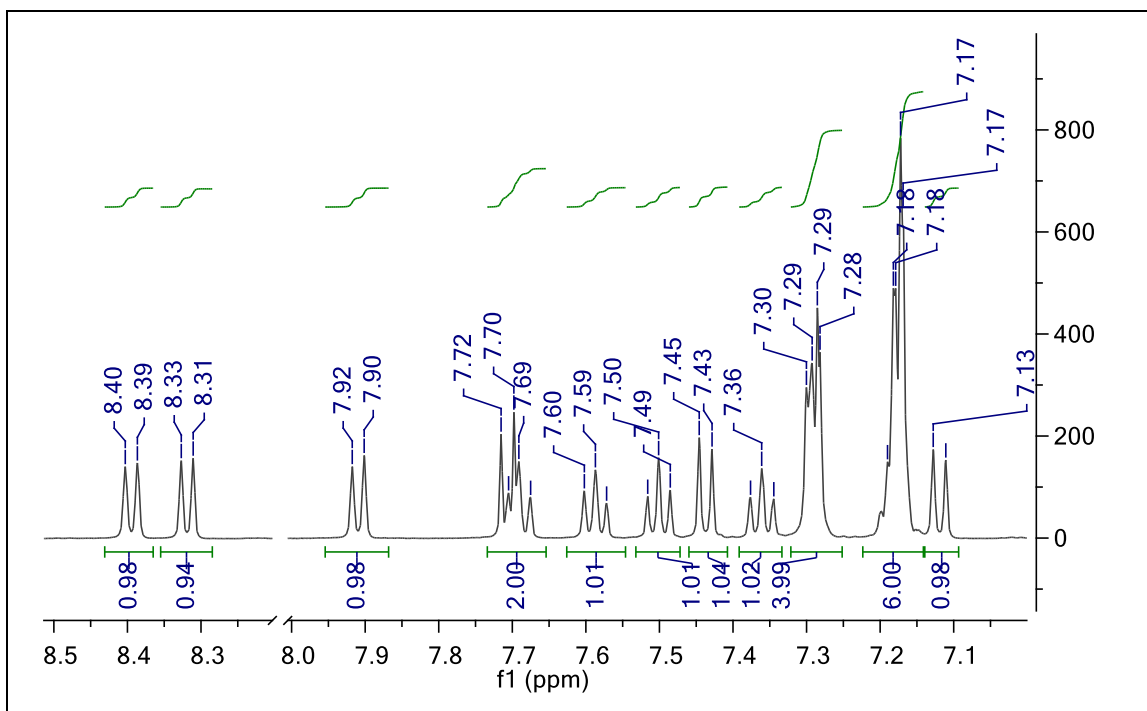


FIG 67 12HNBT, ¹H NMR (500 MHz, dmsol) δ 8.40, 8.39, 8.33, 8.31, 7.92, 7.90, 7.72, 7.71, 7.70, 7.69, 7.68, 7.60, 7.59, 7.57, 7.52, 7.50, 7.49, 7.45, 7.43, 7.38, 7.36, 7.34, 7.30, 7.29, 7.29, 7.28, 7.19, 7.18, 7.18, 7.17, 7.17, 7.13, 7.11, 3.32, 3.30, 2.50, -0.00.

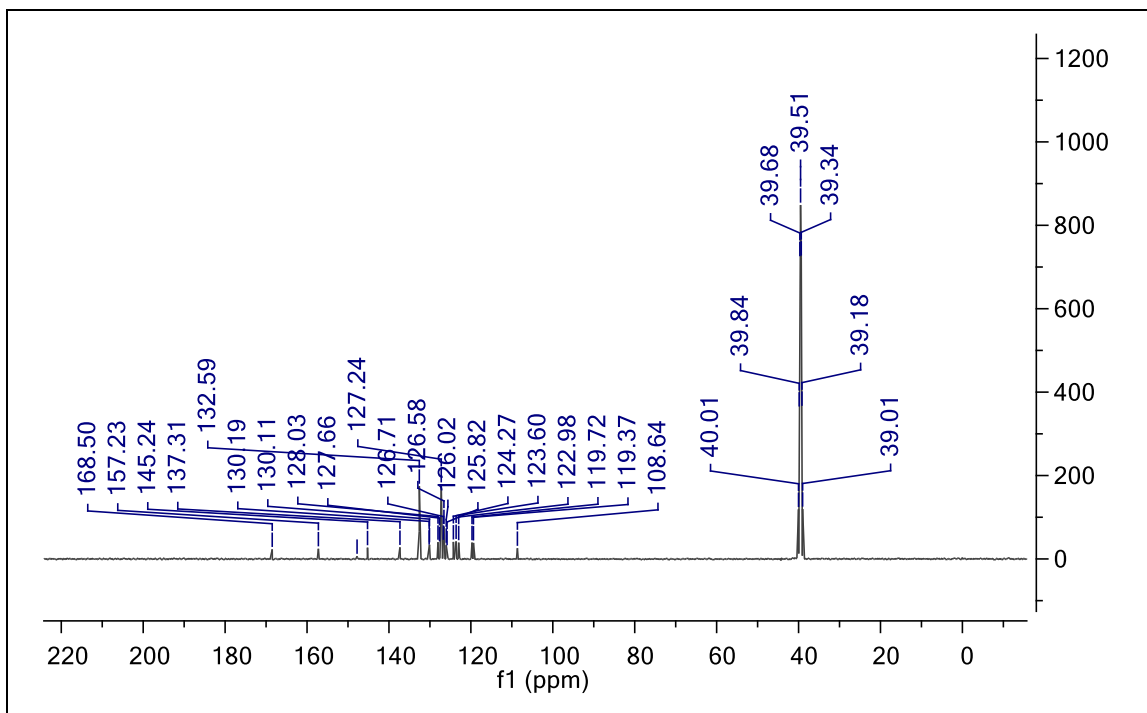


FIG 68 12HNBT, ^{13}C NMR (126 MHz, dmsol)

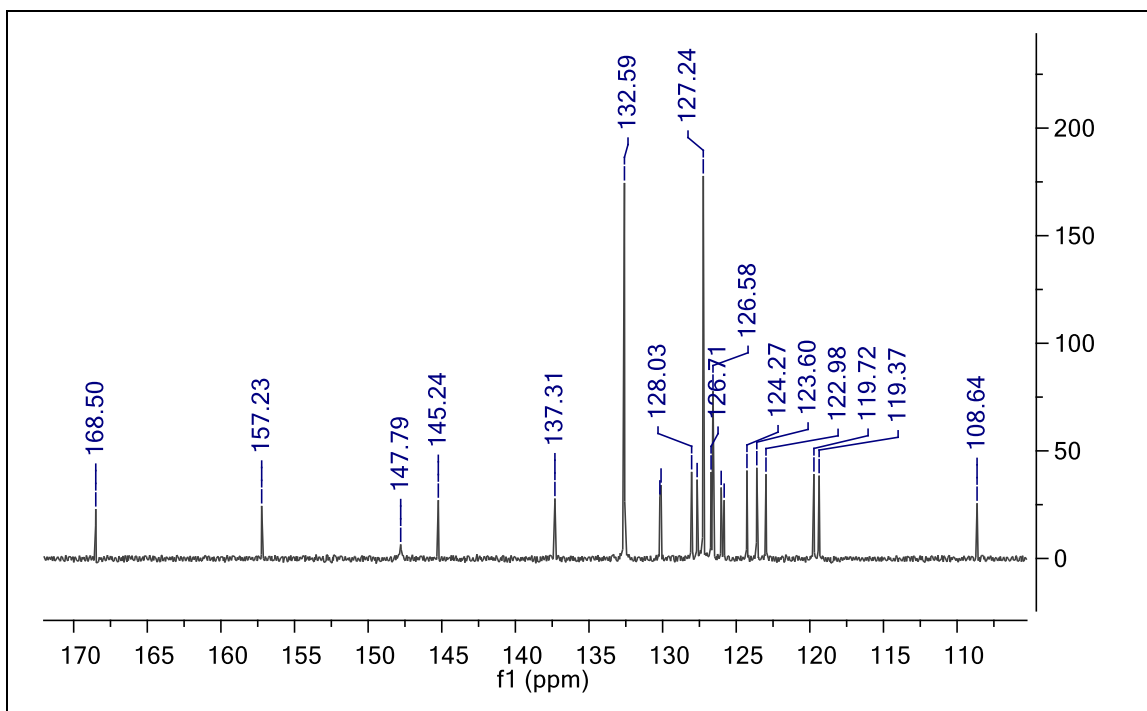


FIG 69 12HNBT, ^{13}C NMR (126 MHz, dmsol) δ 168.50, 157.23, 147.79, 145.24, 137.31, 132.59, 130.19, 130.11, 128.03, 127.66, 127.24, 126.71, 126.58, 126.02, 125.82, 124.27, 123.60, 122.98, 119.72, 119.37, 108.64, 40.01, 39.84, 39.68, 39.51, 39.34, 39.18, 39.01.

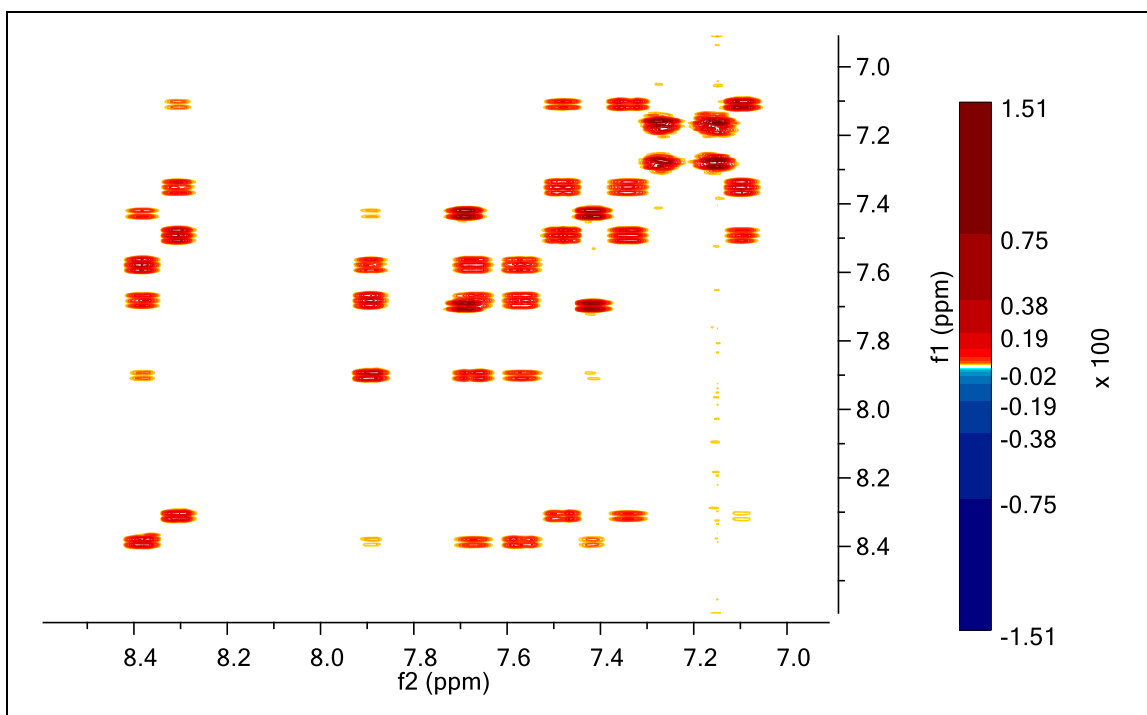


FIG 70 12HNBT, G-COSY (dmsol)

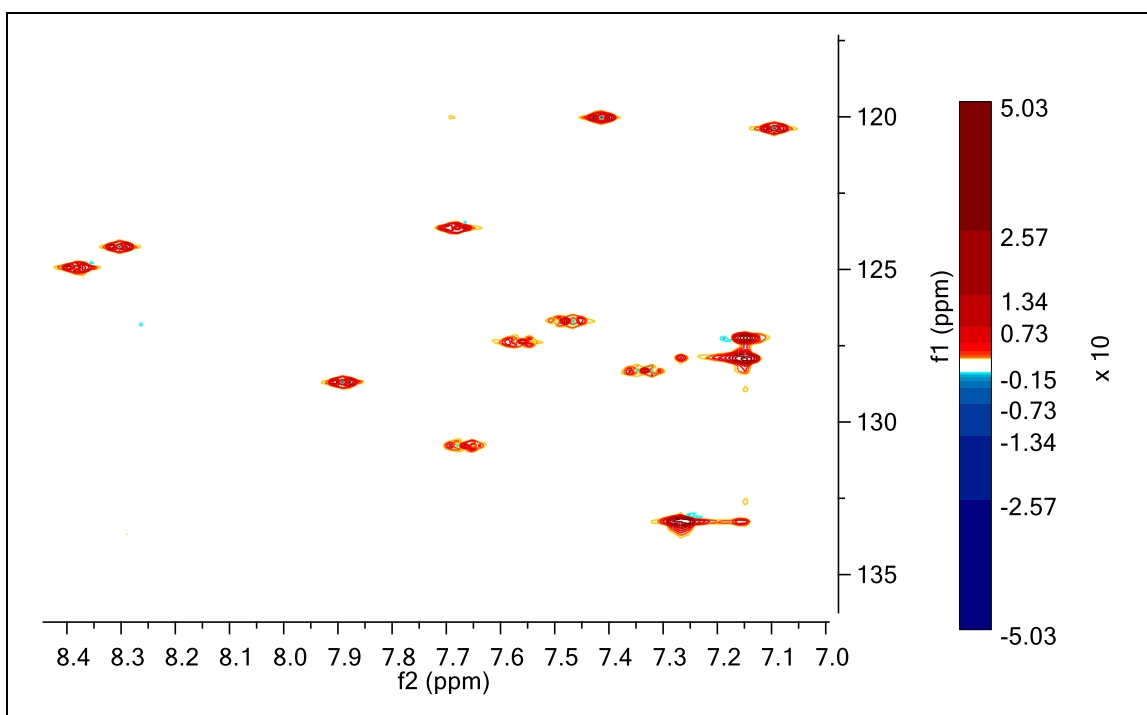


FIG 71 12HNBT, G-HMQC (dmsol)

