Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Configurations dependent optical properties and acid susceptibility of azulene compounds

Tao Tang,[a,b] Tingting Lin,[b] Fuat Erden,[a,b] Fuke Wang,*[b] and Chaobin He*[a, b]

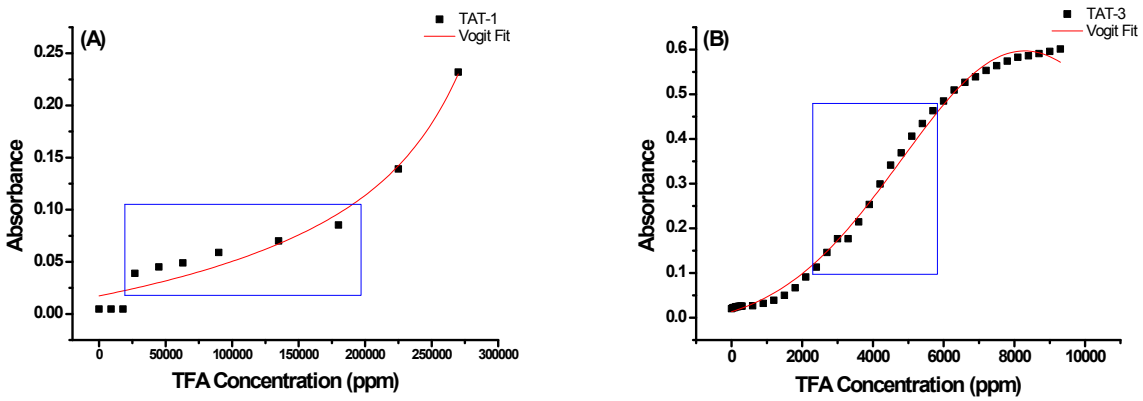
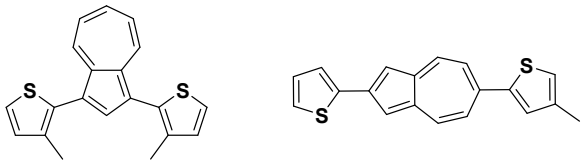


Figure S1. UV-vis-NIR spectra at the fixed wavelength of the **TAT-1** (A: 513 nm) and **TAT-3** (B: 546 nm)) in chloroform solution as a function of TFA concentration.

Tabel S1. Excitation energies and oscillator strenghts from the ground-state structures (S_0) of **TAT-1** and **TAT-3** in neutral and protonated states.



TAT-1 **TAT-3**

Model compound

TAT-1

Excited State 1: Singlet-A 2.0958 eV 591.60 nm f=0.0074 <S**2>=0.000

84 -> 85 0.70213

Excited State 2: Singlet-A 3.1154 eV 397.97 nm f=0.0737 <S**2>=0.000

83 -> 85 -0.47240

84 -> 86 0.52238

Excited State 3: Singlet-A 3.3850 eV **366.28** nm f=**0.2159** <S**2>=0.000

80 -> 85 -0.18553

81 -> 85 0.15430

83 -> 85 0.50176

84 -> 86 0.43200

Excited State 4: Singlet-A 3.7770 eV 328.26 nm f=0.0303 <S**2>=0.000

79 -> 85 -0.21199

82 -> 85 0.52282

83 -> 86 -0.41115

Excited State 5: Singlet-A 3.8707 eV 320.32 nm f=0.0600 <S**2>=0.000

82 -> 85 0.44286

83 -> 86 0.51134

84 -> 87 0.18491

Excited State 6: Singlet-A 3.9023 eV 317.72 nm f=0.0322 <S**2>=0.000

80 -> 85 0.20814

81 -> 85 0.66459

Excited State 7: Singlet-A 4.0371 eV **307.12** nm f=**0.1952** <S**2>=0.000

79 -> 85 -0.43820

82 -> 85 -0.14459

84 -> 87 0.52992

Excited State 8: Singlet-A 4.0566 eV **305.64** nm f=**0.3087** <S**2>=0.000

79 -> 85 0.48672

83 -> 86 -0.24484

84 -> 87 0.41774

Excited State 9: Singlet-A 4.2431 eV **292.20** nm f=**0.2788** <S**2>=0.000

80 -> 85 0.48447

84 -> 86 0.11559

84 -> 88 -0.47511

Protonated **TAT-1**

Excited State 1: Singlet-A 2.1490 eV 576.93 nm f=0.0054 <S**2>=0.000

84 -> 85 0.69340

Excited State 2: Singlet-A 2.3048 eV 537.94 nm f=0.0146 <S**2>=0.000

84 -> 86 0.69706

Excited State 3: Singlet-A 2.4692 eV 502.12 nm f=0.0073 <S**2>=0.000

83 -> 85 0.69732

Excited State 4: Singlet-A 2.6211 eV 473.02 nm f=0.0077 <S**2>=0.000

83 -> 86 0.70513

Excited State 5: Singlet-A 2.7169 eV 456.34 nm f=0.0016 <S**2>=0.000

81 -> 85 -0.13531

82 -> 85 0.69260

Excited State 6: Singlet-A 2.7850 eV 445.19 nm f=0.0038 <S**2>=0.000

81 -> 85 0.69119

82 -> 85 0.13313

Excited State 7: Singlet-A 2.8892 eV 429.13 nm f=0.0085 <S**2>=0.000

82 -> 86 0.70018

Excited State 8: Singlet-A 2.9429 eV 421.30 nm f=0.0029 <S**2>=0.000

81 -> 86 0.69983

Excited State 9: Singlet-A 3.8317 eV **323.58** nm f=**0.1070** <S**2>=0.000

79 -> 86 0.10052

80 -> 85 0.53048

80 -> 86 0.44005

Excited State 10: Singlet-A 3.9307 eV **315.43** nm f=**0.1735** <S**2>=0.000

79 -> 86 -0.14506

80 -> 85 -0.41171

80 -> 86 0.52432

84 -> 87 -0.11576

TAT-3

Excited State 1: Singlet-A 2.2499 eV 551.07 nm f=0.0083 <S**2>=0.000

79 -> 81 0.68689

80 -> 81 -0.11683

80 -> 82 -0.10393

Excited State 2: Singlet-A 2.7318 eV **453.86** nm f=**1.0576** <S**2>=0.000

79 -> 81 0.11549

79 -> 82 0.15118

80 -> 81 0.68091

Excited State 3: Singlet-A 3.5829 eV 346.04 nm f=0.0799 <S**2>=0.000

78 -> 81 0.67812

79 -> 82 -0.11085

80 -> 83 -0.12542

Excited State 4: Singlet-A 3.7694 eV 328.92 nm f=0.0457 <S**2>=0.000

74 -> 81 0.11692

79 -> 81 0.10006

80 -> 82 0.67674

Excited State 5: Singlet-A 3.9477 eV 314.07 nm f=0.0243 <S**2>=0.000

77 -> 81 0.69608

Excited State 6: Singlet-A 4.0829 eV **303.67** nm f=**1.0351** <S**2>=0.000

75 -> 81 0.19670

76 -> 81 0.24907

78 -> 81 0.11477

79 -> 82 0.58655

80 -> 81 -0.12910

80 -> 84 -0.10531

Excited State 7: Singlet-A 4.1339 eV **299.92** nm f=**0.1691** <S**2>=0.000

76 -> 81 0.65554

79 -> 82 -0.21034

Protonated **TAT-3**

Excited State 1: Singlet-A 2.4538 eV **505.28** nm f=**1.1928** <S**2>=0.000

80 -> 81 0.69615

Excited State 2: Singlet-A 2.5623 eV 483.88 nm f=0.0774 <S**2>=0.000

80 -> 82 0.69305

Excited State 3: Singlet-A 3.0906 eV **401.17** nm f=**0.2085** <S**2>=0.000

79 -> 81 0.52656

79 -> 82 -0.45750

Excited State 4: Singlet-A 3.1790 eV 390.01 nm f=0.0390 <S**2>=0.000

78 -> 81 -0.19486

78 -> 82 -0.10296

79 -> 81 0.41619

79 -> 82 0.51583

Excited State 5: Singlet-A 3.3339 eV 371.89 nm f=0.0009 <S**2>=0.000

78 -> 81 0.66768

78 -> 82 -0.13668

79 -> 81 0.12381

79 -> 82 0.11488

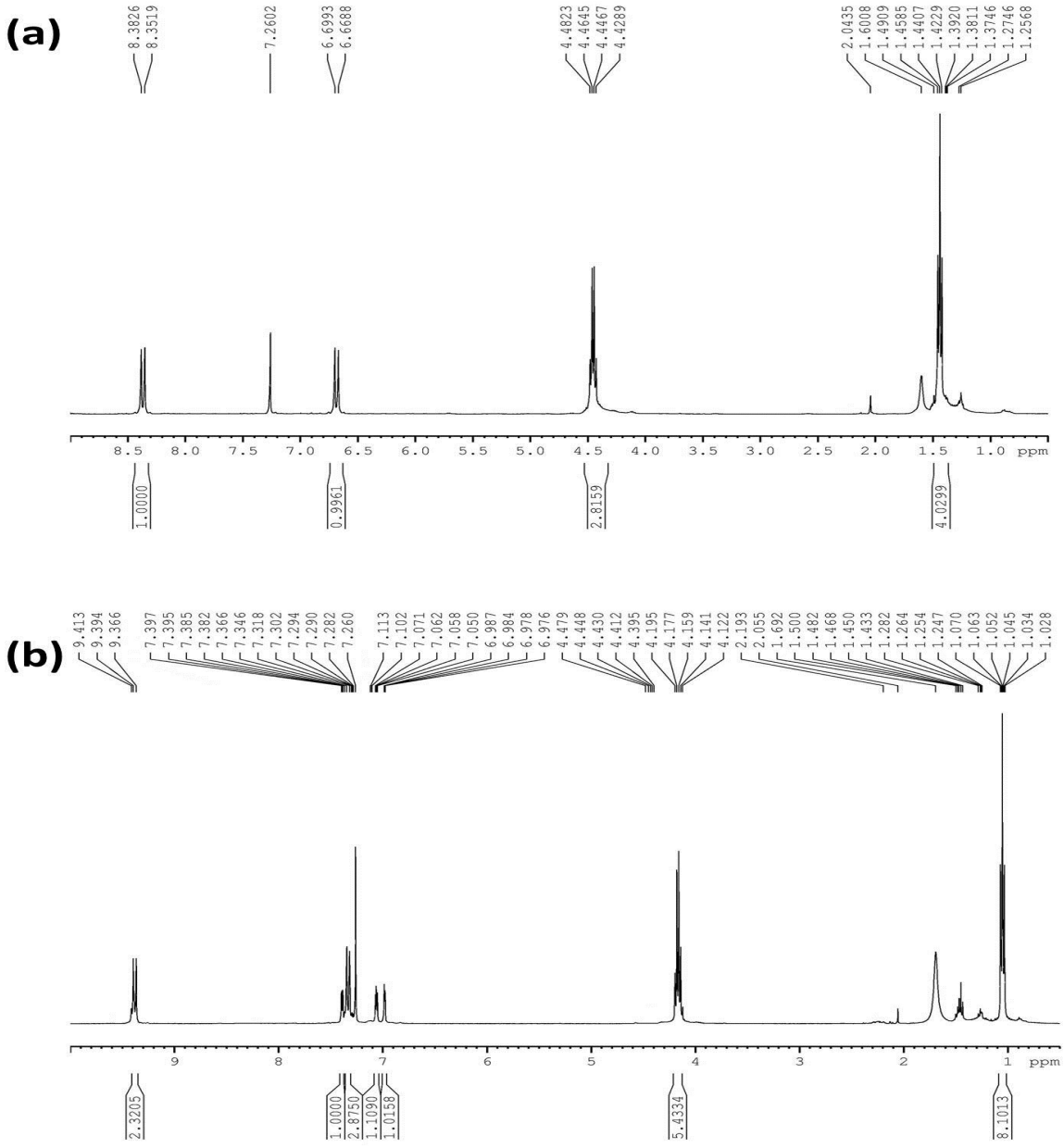
Excited State 6: Singlet-A 3.5160 eV 352.63 nm f=0.0153 <S**2>=0.000

77 -> 81 0.69758

Excited State 7: Singlet-A 3.5427 eV **349.97** nm f=**0.1435** <S**2>=0.000

78 -> 82 0.67732

79 -> 81 0.12585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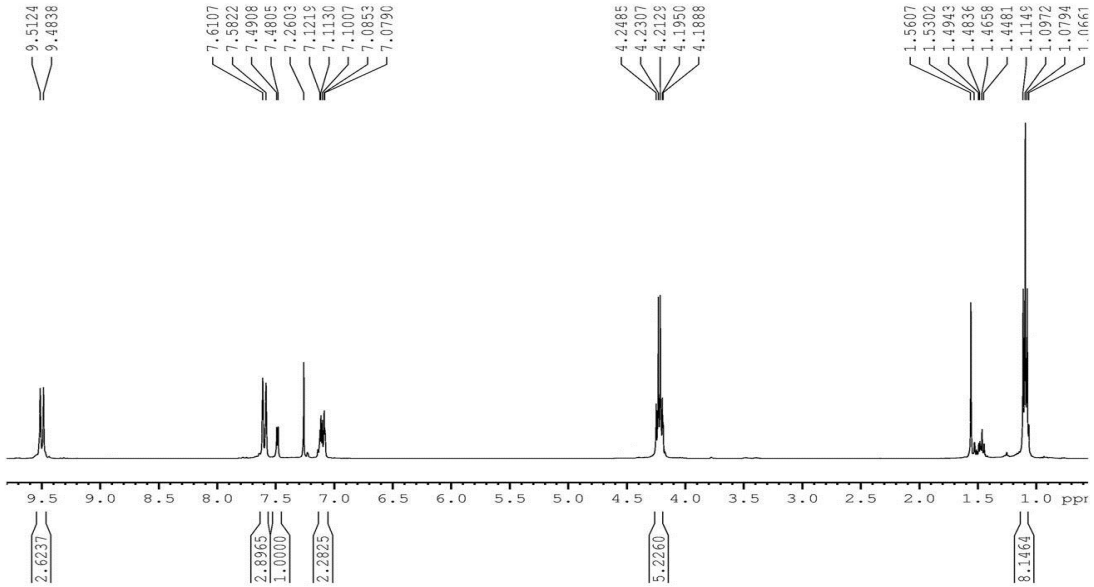
8.3519
7.2602
6.6993
6.6688
4.4823
4.4645
4.4467
4.4289
2.0435
1.6008
1.4909
1.4585
1.4407
1.4229
1.3920
1.3811
1.3746
1.2746
1.2568
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.0000
0.9961
2.8159
4.0299
(b)
9.413
9.394
9.366
7.397
7.395
7.385
7.382
7.366
7.346
7.318
7.302
7.294
7.290
7.282
7.260
7.113
7.102
7.071
7.062
7.058
7.050
6.987
6.984
6.978
6.976
4.479
4.448
4.430
4.412
4.395
4.195
4.177
4.159
4.141
4.122
2.193
2.055
1.692
1.500
1.482
1.468
1.450
1.433
1.282
1.264
1.254
1.247
1.070
1.063
1.052
1.045
1.034
1.028
9 8 7 6 5 4 3 2 1 ppm
2.3205
1.0000
2.8750
1.1090
1.0158
5.4334
8.1013

(c)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9.4838
7.6107
7.5822
7.4908
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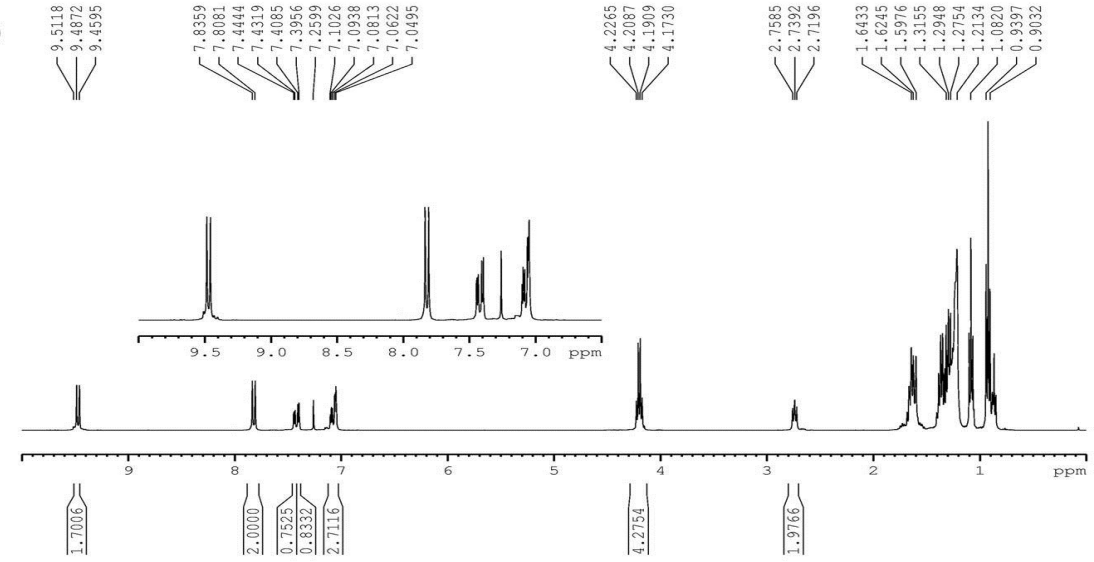
7.1130
7.1007
7.0853
7.0790
4.2485
4.2307
4.2123
4.1950
4.1888
1.5607
1.5302
1.4943
1.4836
1.4658
1.4481
1.1149
1.0972
1.0794
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppr
2.6237
2.8965
1.0000
2.2825
5.2260
8.1464

(d)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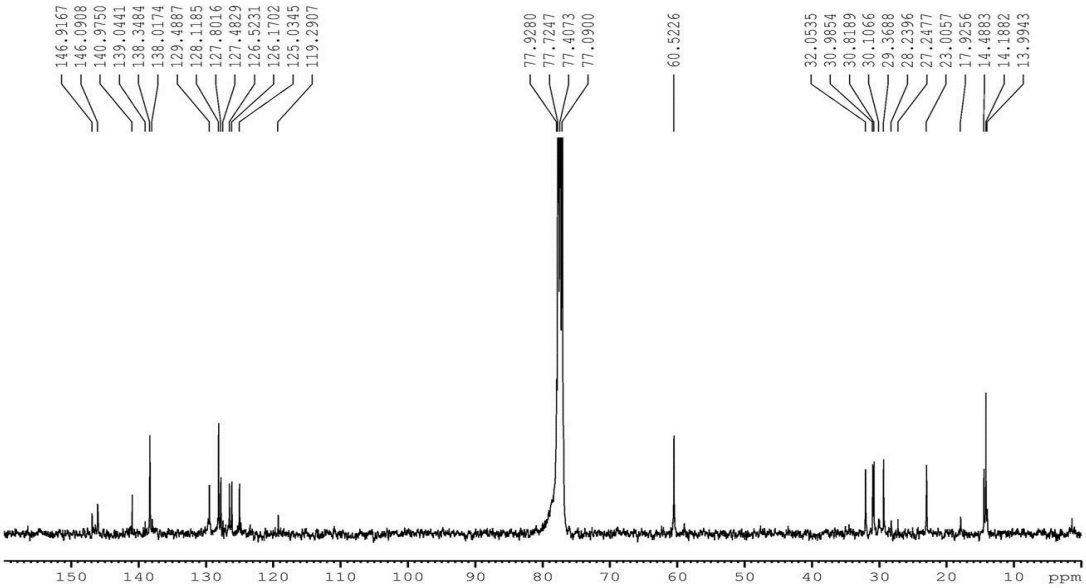
9.4872
9.4595
7.8359
7.8081
7.4444
7.4319
7.4085
7.3956
7.2599
7.1026
7.0938
7.0813
7.0622
7.0495
4.2265
4.2087
4.1909
4.1730
2.7585
2.7392
2.7196
1.6433
1.6245
1.5976
1.3155
1.2948
1.2754
1.2134
1.0820
0.9397
0.9032
9.5 9.0 8.5 8.0 7.5 7.0 ppm
9 8 7 6 5 4 3 2 1 ppm
1.7006
2.0000
0.7525
0.8332
2.7116
4.2754
1.9766

(e)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139.0441
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127.8016
127.4829
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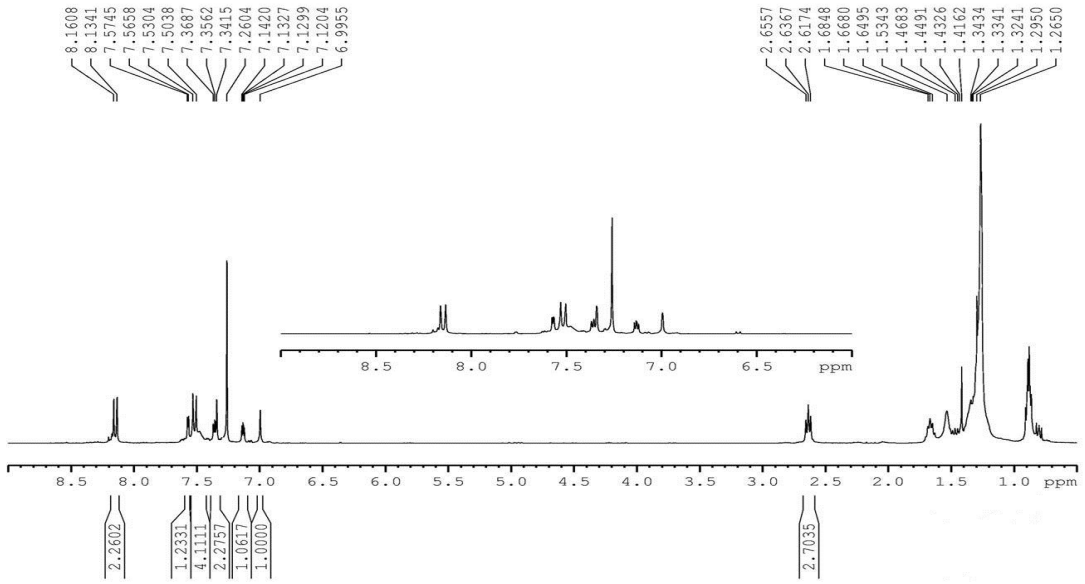
126.1702
125.0345
119.2907
77.9280
77.7247
77.4073
77.0900
60.5226
32.0535
30.9854
30.8189
30.1066
29.3688
28.2396
27.2477
23.0057
17.9256
14.4883
14.1882
13.9943
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

(f)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8.1341
7.5745
7.5658
7.5304
7.5038
7.3687
7.3562
7.3415
7.2604
7.1420
7.1327
7.1299
7.1204
6.9955
2.6557
2.6367
2.6174
1.6848
1.6680
1.6495
1.5343
1.4683
1.4491
1.4326
1.4162
1.3434
1.3341
1.3241
1.2950
1.2650
8.5 8.0 7.5 7.0 6.5 ppm
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
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1.0617
1.0000
2.7035

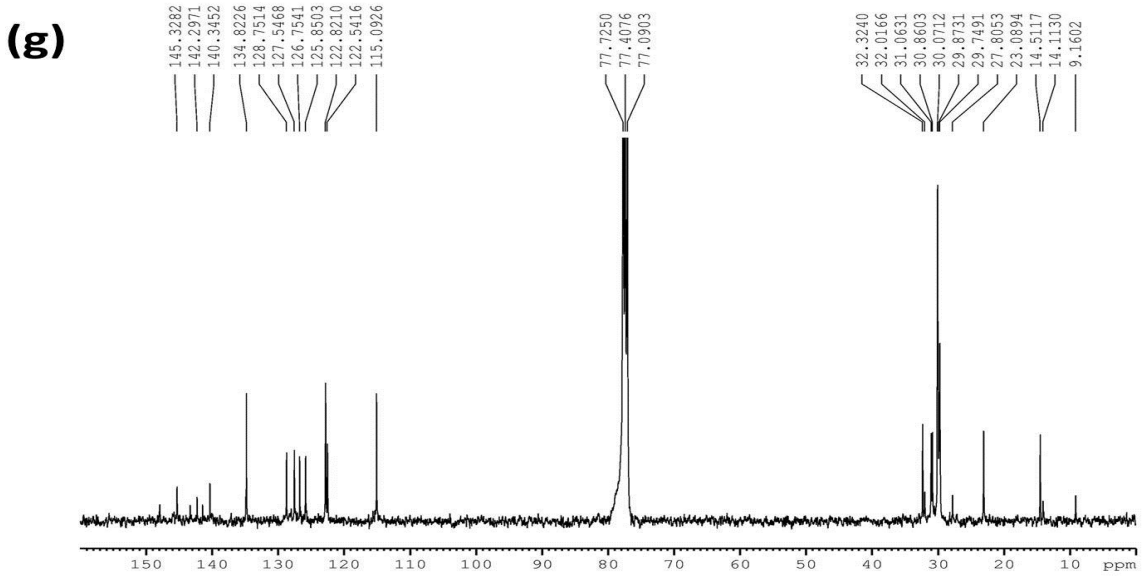

Figure S2. NMR spectra of synthesized compounds. ^{1}H-NMR in $CDCl_3$: (a) compound **5**; (b) compound **6** and (c) compound **7**; (d) and (e), ^{1}H-NMR and ^{13}C-NMR spectra of **TAT-2** in $CDCl_3$; (f) and (g), ^{1}H-NMR and ^{13}C-NMR spectra of **TAT-3** in $CDCl_3$;

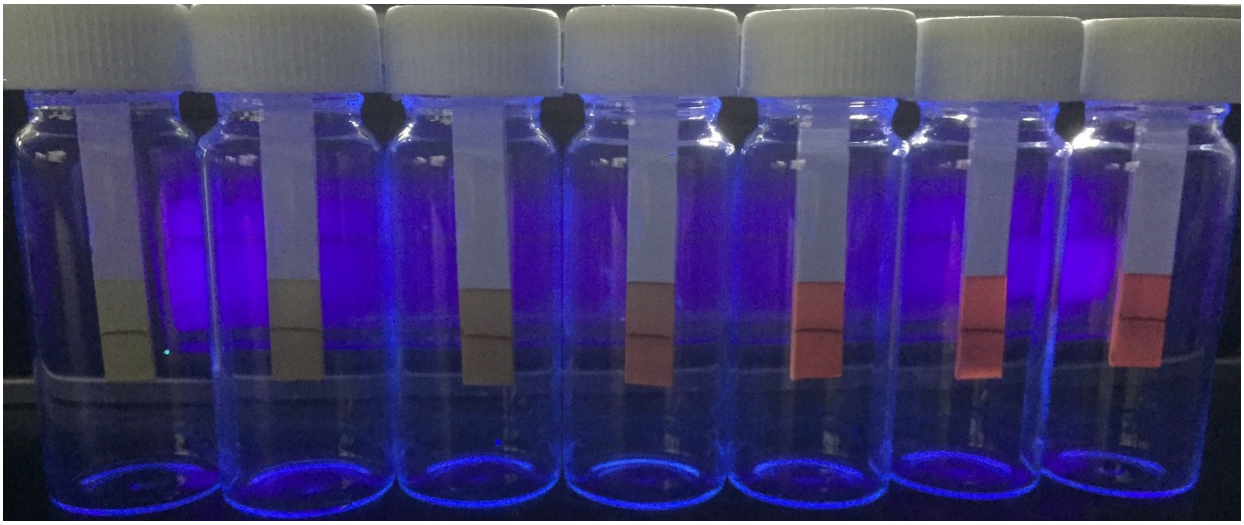

Figure S3. Fluoresence change of TAT-3 film when exposure to various TFA concentration.