Electronic Supplementary Information for:

Anion-dependent fluorescence in bis(anilinoethynyl)pyridine derivatives: switchable ON-OFF *and* OFF-ON responses

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Experimental Details

General. ^{1}H and ^{13}C NMR spectra were obtained on a Varian 300 MHz spectrometer (^{1}H 299.95 Hz, ^{13}C 75.43 Hz) or Inova 500 MHz spectrometer (^{1}H 500.10 MHz, ^{13}C 125.75 MHz). Chemical shifts (∂) are expressed in ppm downfield from tetramethylsilane (TMS) using non-deuterated solvent present in the bulk deuterated solvent ($CDCl_3$: ^{1}H 7.26 ppm, ^{13}C 77.0 ppm; DMSO-d_6: ^{1}H 2.54 ppm ^{13}C 40.45 ppm). Unless otherwise specified, solvents were obtained from distillation using published literature procedures directly before use. Mass spectra were acquired on a Thermo Finnigan LCQ Deca XP Plus electrospray ionization spectrometer in positive mode in MeOH solvent. UV-Vis spectra were acquired with a Hewlett-Packard 8453 UV-Visible spectrophotometer equipped with a 250 nm cutoff filter. Fluorescence data was acquired with a Horiba Jobin-Yvon FluoroMax-4 fluorescence spectrophotometer equipped with an integrating sphere. Absolute photoluminescence quantum yields were taken in O_2-containing (no inert gas purging) $CHCl_3$. All slit widths (ex/em) were held constant at 5 nm/5 nm. Dianiline **1** and parent phenylurea **2** were prepared as previously described.[1]

Methoxyphenyl urea 3a. Dianiline **1** (100 mg, 0.238 mmol) was reacted in a flame-dried round bottom flask with *p*-methoxyphenyl isocyanate (88.6 mg, 0.594 mmol) in freshly distilled toluene (5 mL). The crude reaction was diluted with pentane, filtered through a sintered glass funnel and the crude solid collected. Trituration with chloroform furnished **3a** (160 mg, 93%) as an off-white solid. Recrystallization by diffusion (pentane/chloroform) yielded colorless crystals. Mp: 178-180 °C. ^{1}H NMR (300 MHz, DMSO-d_6): ∂ 9.37 (br s, 2H), 8.32 (br s, 2H), 8.12 (d, J = 9 Hz, 2H), 8.10 (t, J = 7.8 Hz, 1H), 7.91 (d, J = 7.8 Hz, 2 H), 7.63 (d, J = 2.1 Hz, 2H), 7.57 (dd, J = 6.3, 2.1 Hz, 2H), 7.47 (d, J = 8.7 Hz, 4H), 6.97 (d, J = 8.7 Hz, 4H), 3.82 (s, 6H), 1.40 (s, 18 H). ^{13}C NMR (300 MHz, DMSO-d_6): ∂ 151.08, 148.83, 140.99, 139.29, 134.93, 133.90, 128.88,

125.49, 124.07. 123.73, 116.63, 116.35, 110.51, 106.44, 89.93, 82.33, 51.61, 30.41, 27.43. MS (ESI pos) *m/z* (%): 744.8 ($M+Na^+$+2, 10) 743.8 ($M+Na^+$+1, 40), 742.7 ($M+Na^+$, 100), 741.1 (10), 740.1 (8); $C_{45}H_{45}N_5O_4$ (719.35), $C_{45}H_{45}N_5O_4Na$ (742.34).

Nitrophenyl urea 3b. Dianiline **1** (100 mg, 0.238 mmol) was reacted in a flame-dried round bottom flask with *p*-nitrophenyl isocyanate (97.5 mg, 0.594 mmol) in freshly distilled toluene (5 mL). The crude reaction was diluted with pentane, filtered through a sintered glass funnel and the crude solid collected. Trituration with chloroform afforded **3b** (166 mg, 92%) as a pale yellow solid. Recrystallization by diffusion (pentane/chloroform) yielded pale yellow crystals. Mp: 186 °C (decomp). ^{1}H NMR (300 MHz, DMSO-d_6): ∂ 10.13 (br s, 2H), 8.54 (br s, 2H), 8.19 (d, *J* = 9 Hz, 4H), 8.02-7.98 (m, 3H), 7.82 (d, *J* = 7.8 Hz, 2H), 7.71 (d, *J* = 9 Hz, 4H), 7.57 (d, *J* = 2.1 Hz, 2H), 7.51 (dd, *J* = 6.6, 2.1 Hz, 2H), 1.30 (s, 18 Hz). ^{13}C NMR (300 MHz, DMSO-d_6): ∂ 152.49, 146.81, 146.28, 143.45, 141.85, 138.22, 129.94, 128.44, 128.12, 125.92, 121.19, 118.26, 111.68, 94.27, 86.40, 34.77, 31.64. MS (ESI pos) *m/z* (%): 774.9 ($M+Na^+$+3, 31), 774 ($M+Na^+$+2, 65), 773.2 ($M+Na^+$+1, 98), 772.4 ($M+Na^+$, 100); $C_{43}H_{39}N_7O_6$ (749.81), $C_{43}H_{39}N_7O_6Na$ (772.8).

Methoxyphenyl sulfonamide 4a. Dianiline **1** (110 mg, 0.26 mmol) was reacted in a flame-dried round bottom flask with *p*-methoxybenzenesulfonyl chloride (268 mg, 1.3 mmol) in freshly distilled pyridine (5 mL) under inert atmosphere (N_2). Following concentration *in vacuo*, the crude product was filtered through a 2.5 cm silica plug with EtOAc. Purification by chromatography (20:1 CH_2Cl_2:EtOAc) afforded **4a** (185 mg, 93%) as a white crystalline solid. Recrystallization by diffusion (hexanes:CH_2Cl_2) yielded colorless crystals. Mp: 141-143 °C. ^{1}H

NMR (300 MHz, $CDCl_3$): δ 7.77 (d, *J* = 9 Hz, 4H), 7.72 (t, *J* = 7.7 Hz, 1H), 7.54-7.44 (m, 8H), 7.33 (dd, *J* = 9.2, 2.4 Hz, 2H), 6.81 (d, *J* = 9 Hz, 4H), 3.72 (s, 6H), 1.24 (s, 18H). ^{13}C NMR (75 MHz, $CDCl_3$): ∂ 163.06, 147.62, 142.93, 136.75, 135.70, 130.85, 129.60, 129.43, 127.85, 126.44, 120.64, 114.09, 113.02, 93.28, 85.33, 55.45, 34.31, 31.03. MS (ESI pos) *m/z* (%): 765.5 (6), 764.5 (18), 763.5 (36), 762.6 (MH^+, 100); $C_{43}H_{43}N_3O_6S_2$ (761.95); 786.3 ($M+Na^+$ +2, 4), 785.3 ($M+Na^+$+1, 9), 784.33 ($M+Na^+$, 20); $C_{43}H_{43}N_3O_6S_2Na$ (784.85).

Nitrophenyl sulfonamide 4b. Dianiline **1** (150 mg, 0.36 mmol) was reacted in a flame-dried round bottom flask with *p*-nitrobenzenesulfonyl chloride (180 mg, 0.81 mmol) in freshly distilled pyridine (5 mL) under inert atmosphere (N_2). Following concentration *in vacuo*, the crude product was filtered through a 2.5 cm silica plug with EtOAc. Purification by chromatography (20:1 CH_2Cl_2:EtOAc) afforded **4b** (265 mg, 92%) as a yellow solid. Recrystallization by diffusion (hexanes:CH_2Cl_2) yielded pale yellow crystals. Mp: 137-139 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.15 (d, *J* = 8.7 Hz, 4H), 8.03 (d, *J* = 8.7 Hz, 4H), 7.74 (t, *J* = 7.8 Hz, 1H), 7.55 (d, *J* = 8.7 Hz, 2H), 7.48-7.38 (m, 6H), 1.29 (s, 18H). ^{13}C NMR (75 MHz, $CDCl_3$): ∂ 150.10, 149.33, 145.32, 142.68, 137.20, 134.63, 129.82, 128.68, 128.28, 126.31, 124.12, 123.31, 114.59, 92.68, 85.71, 34.51, 31.05 MS (ESI pos) *m/z* (%): 795.5 (M^++3, 6) 794.5 (M^++2, 16), 793.5 (MH^+, 33), 792.5 (M^+, 59), 608 (18), 607 (46); $C_{41}H_{37}N_5O_8S_2$ (791.89); 816.2 ($M+Na^+$+2, 20), 815.2 ($M+Na^+$+1, 39), 814.2 ($M+Na^+$, 100); $C_{41}H_{37}N_5O_8S_2Na$ (814.88).

NMR and Mass spectra

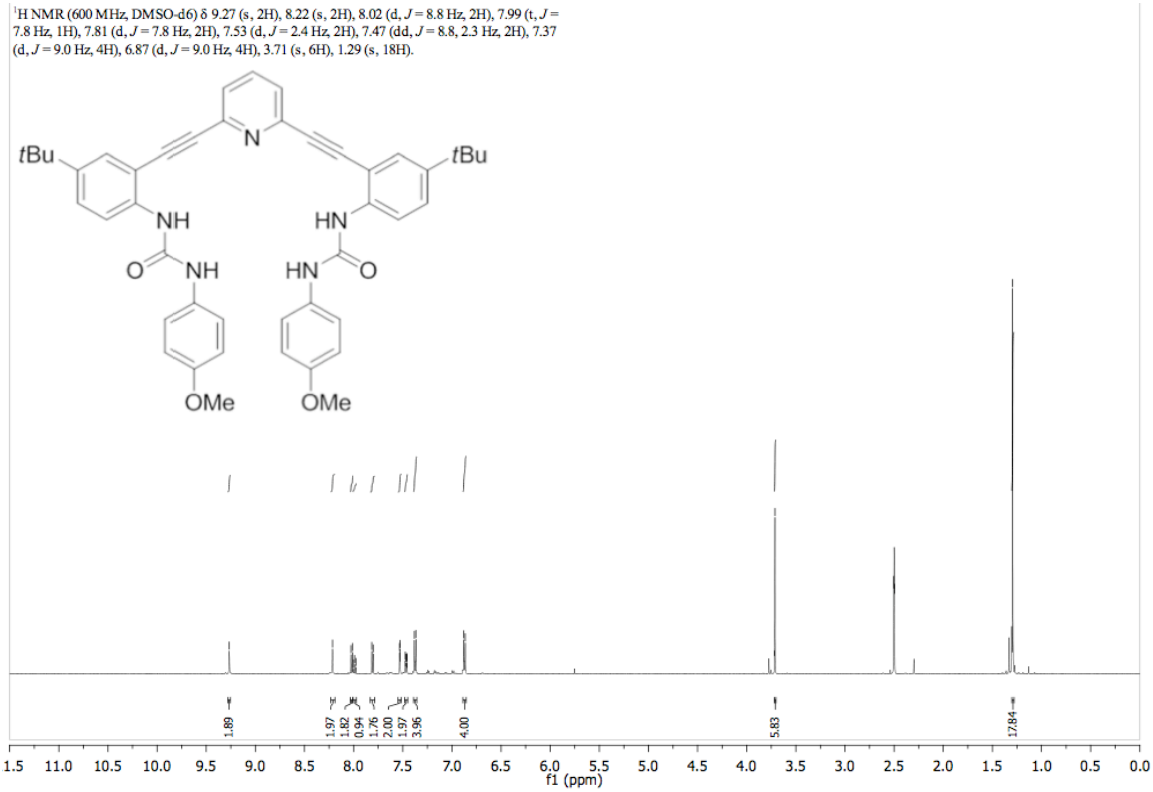


Fig. S1a [1]H-NMR spectrum of **3a**

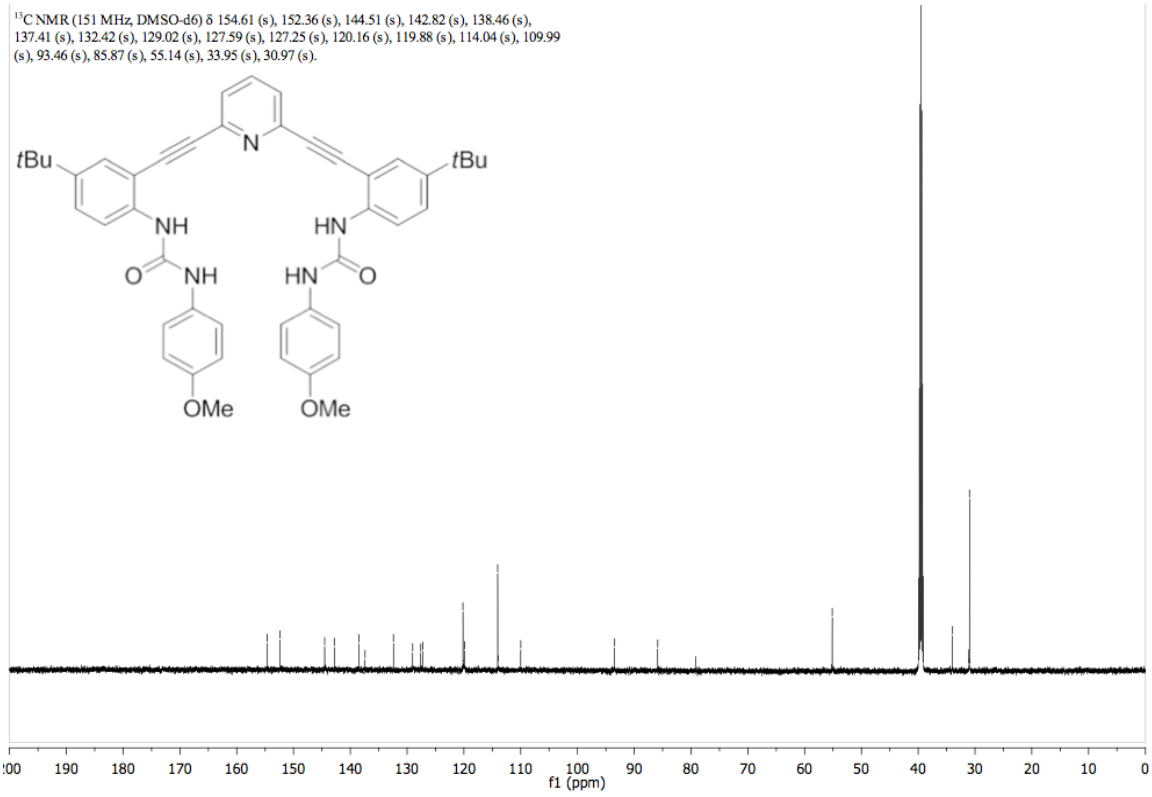


Fig. S1b [13]C-NMR spectrum of **3a**

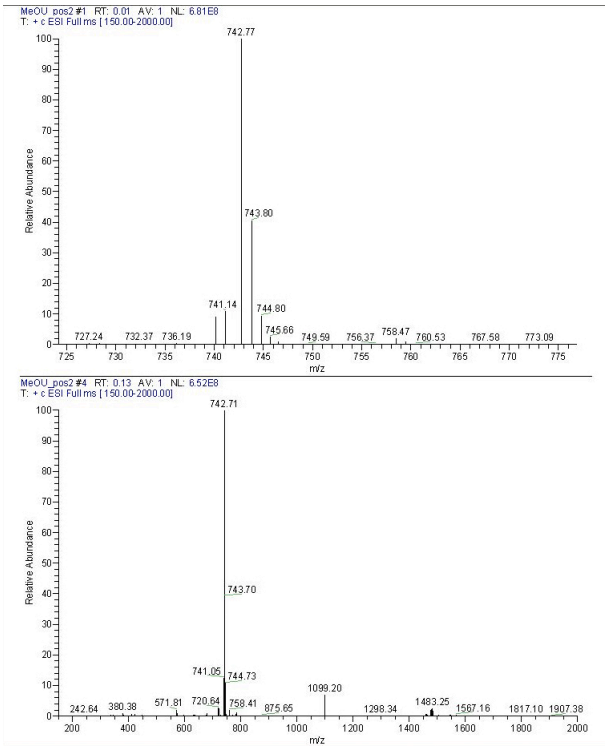


Fig. S1c Mass spectrum of **3a** (ESI pos)

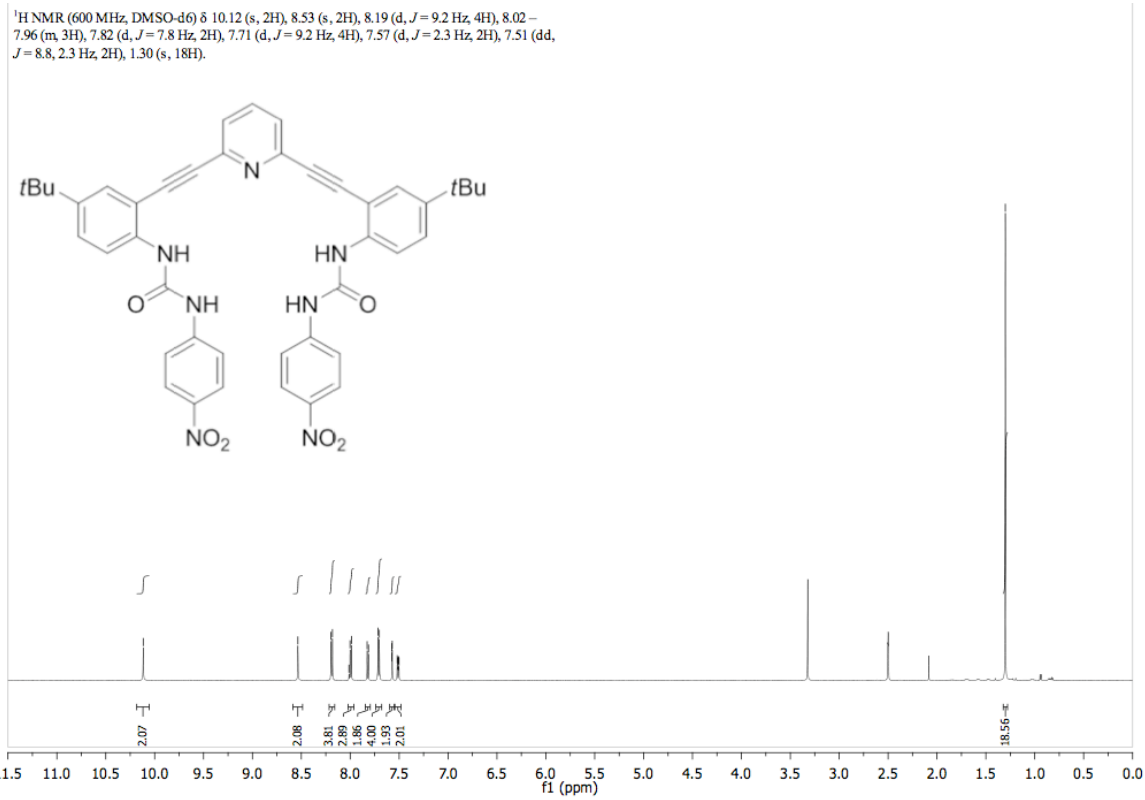


Fig. S2a ^{1}H-NMR spectrum of **3b**

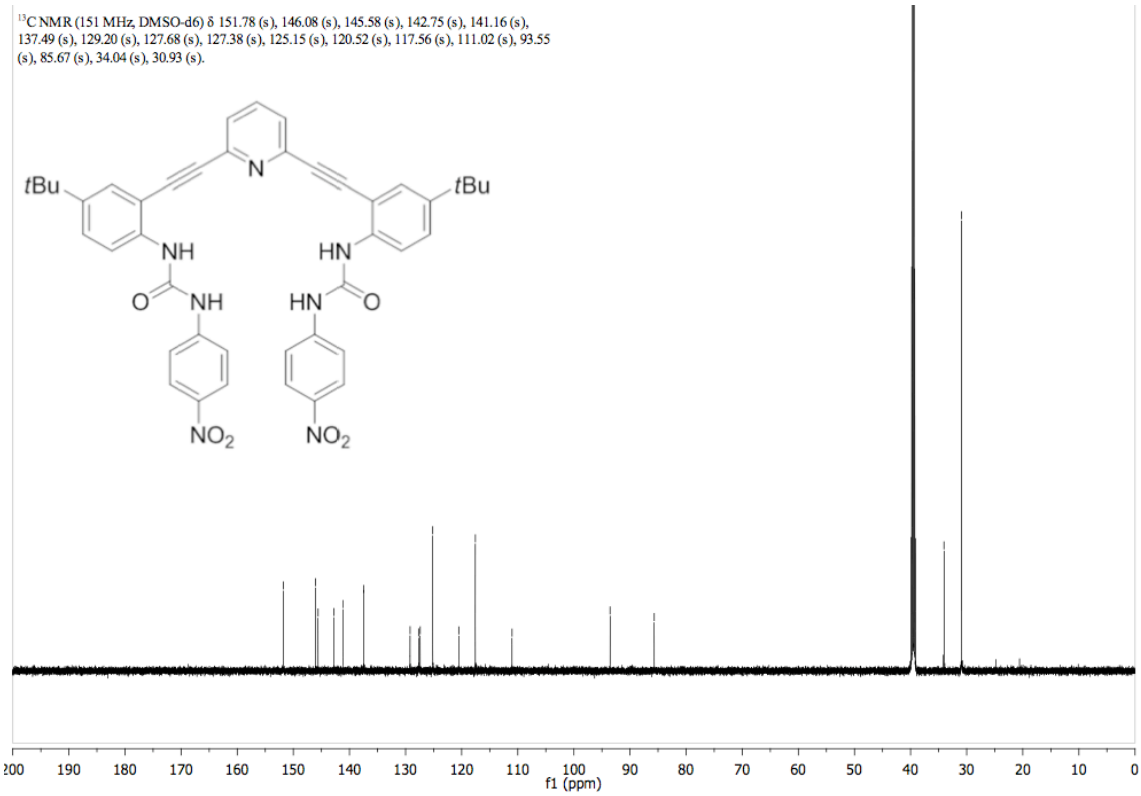


Fig. S2b ^{13}C-NMR spectrum of **3b**

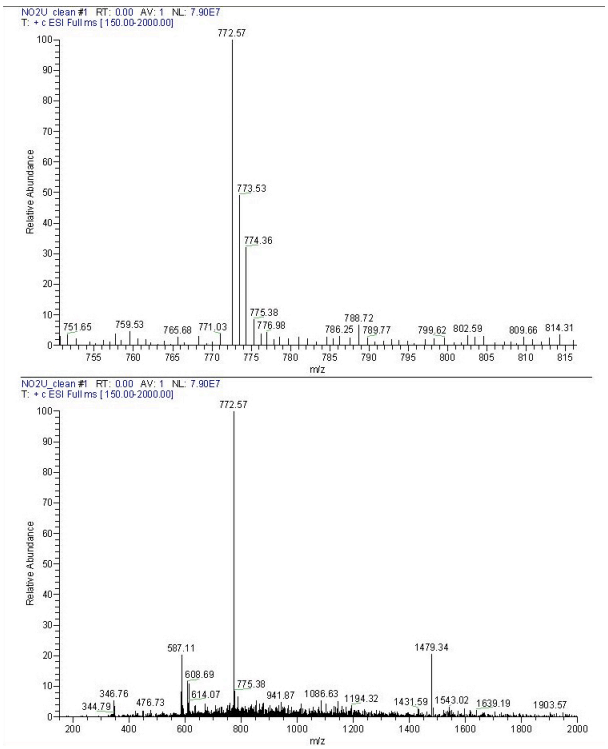


Fig. S2c Mass spectrum of **3b** (ESI pos)

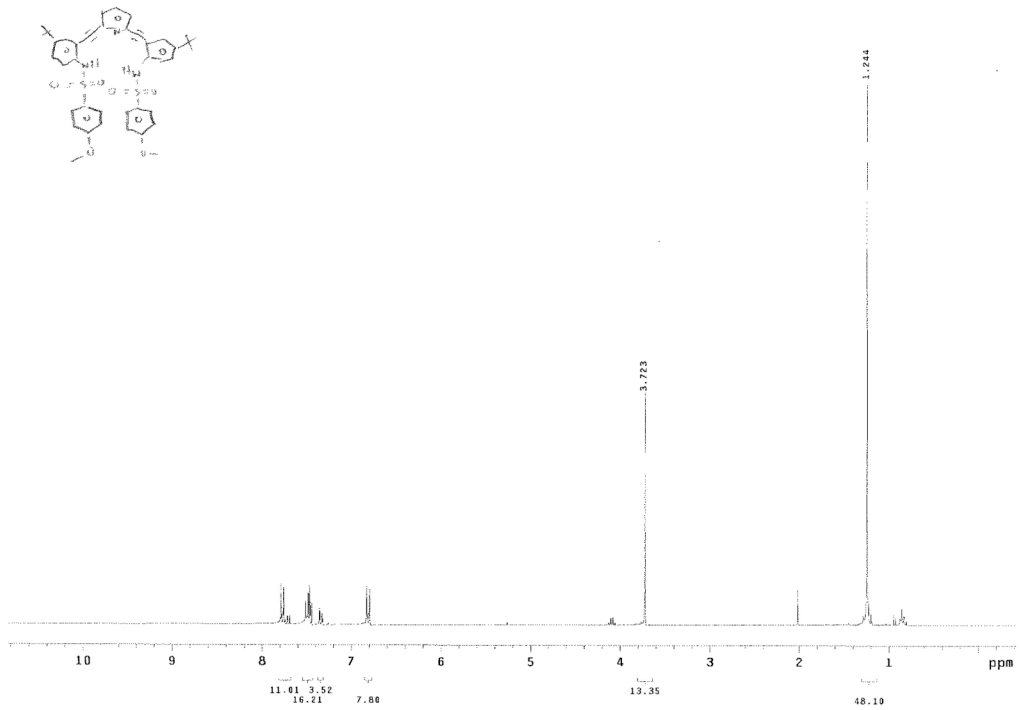
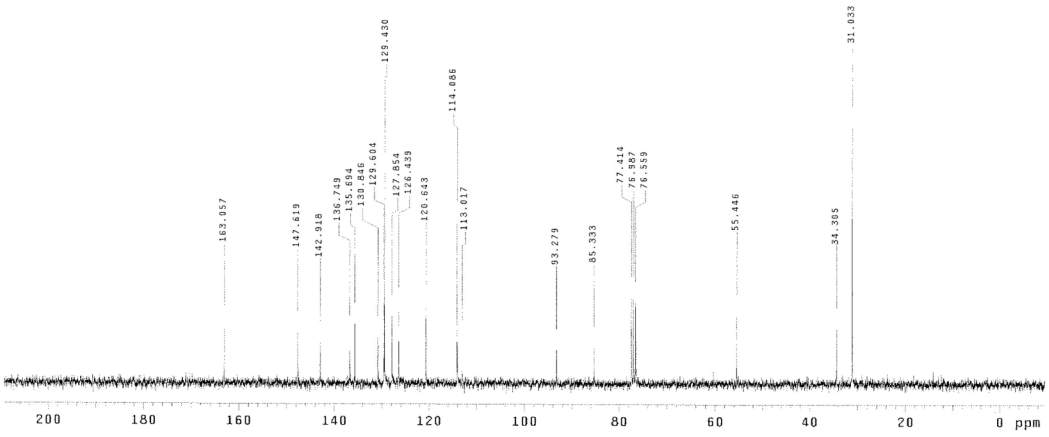


Fig. S3a ^{1}H-NMR spectrum of **4a**



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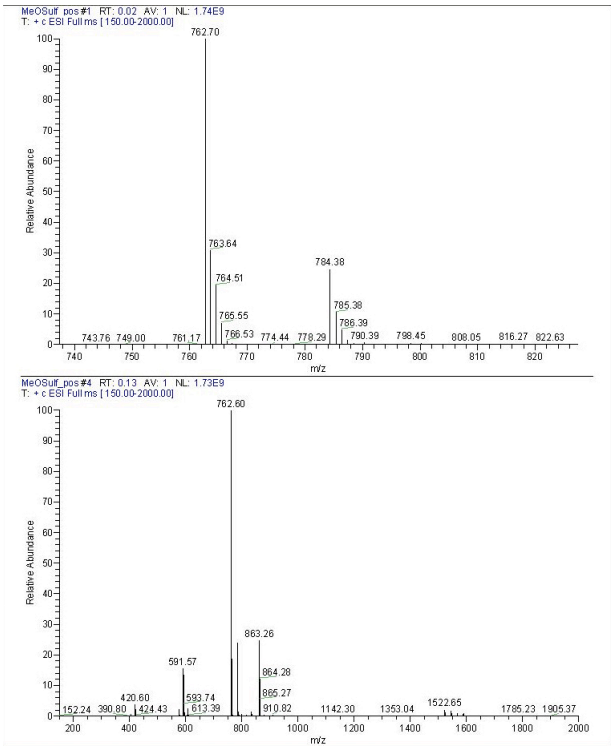

Fig. S3c Mass spectrum of **4a** (ESI pos)

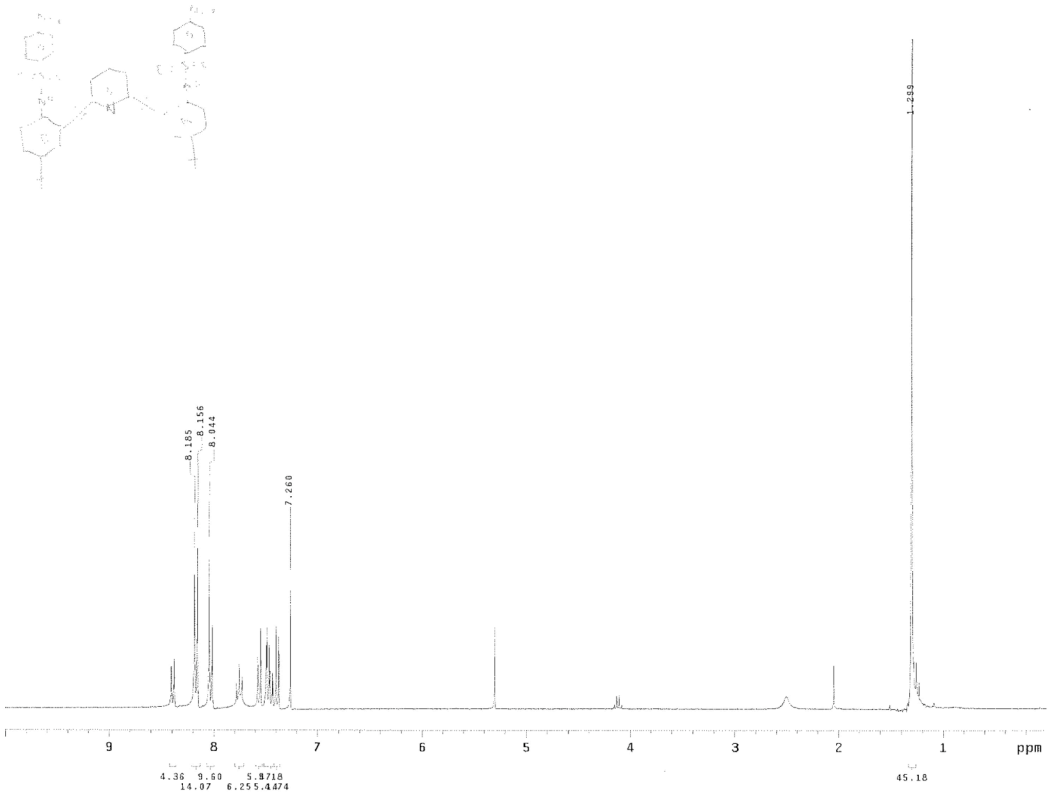

Fig. S4a ^{1}H-NMR spectrum of **4b**

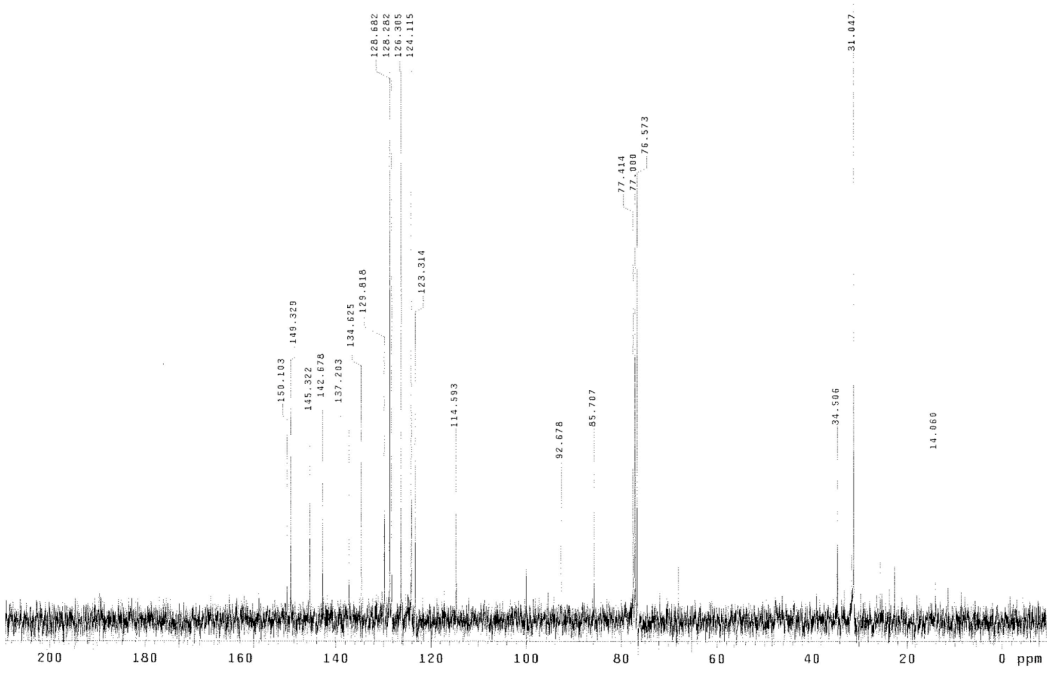

Fig. S4b ^{13}C-NMR spectrum of **4b**

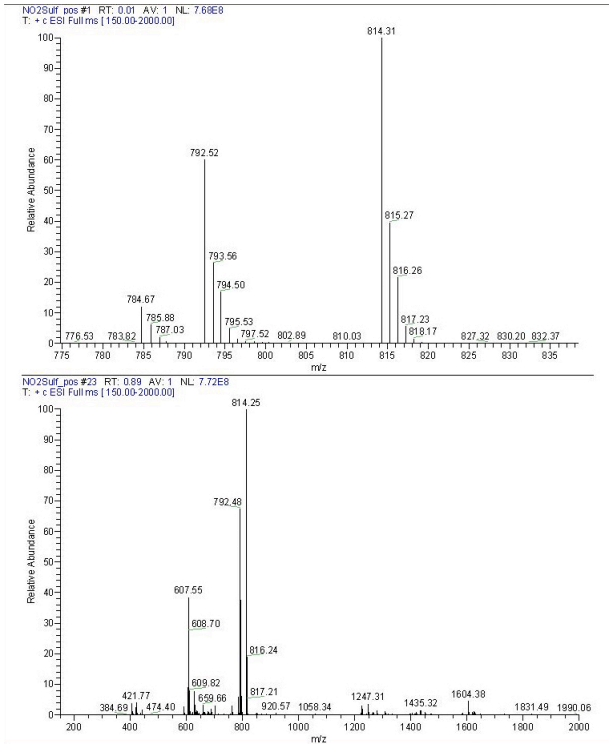

Fig. S4c Mass spectrum of **4b** (ESI pos)

UV-visible and fluorescence excitation spectra

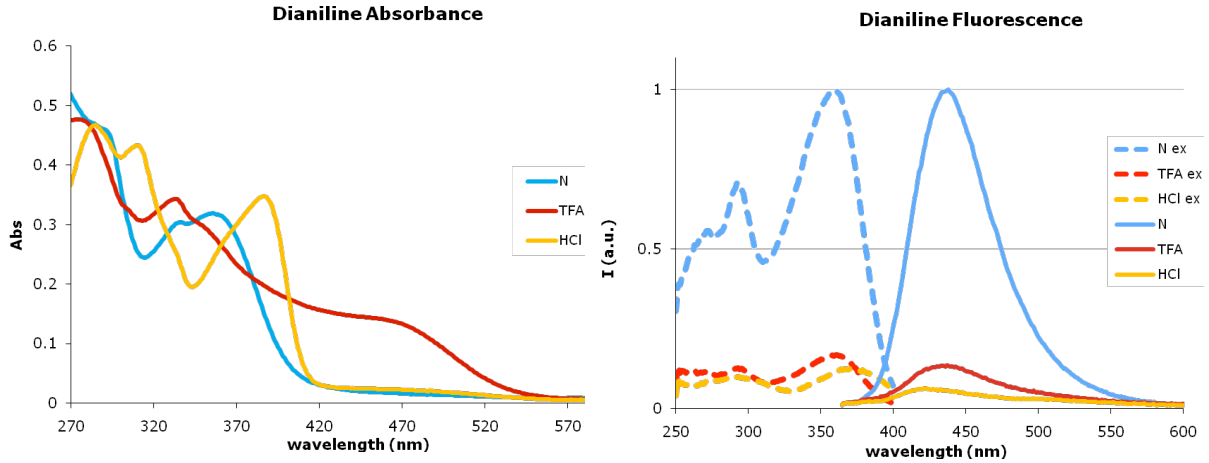

Fig. S5 UV-visible and fluorescence spectra for **1**, **1•TFA** and **1•HCl**

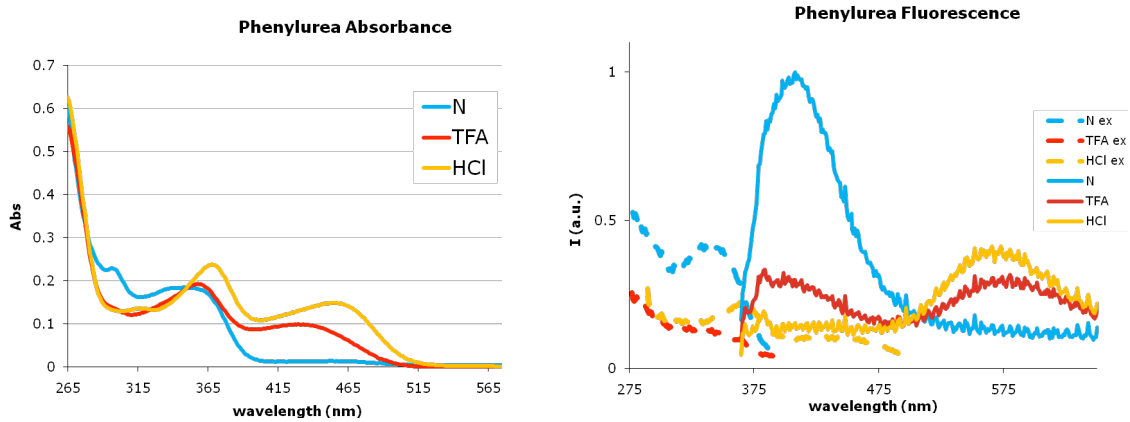

Fig. S6 UV-visible and fluorescence spectra for **2**, **2•TFA** and **2•HCl**

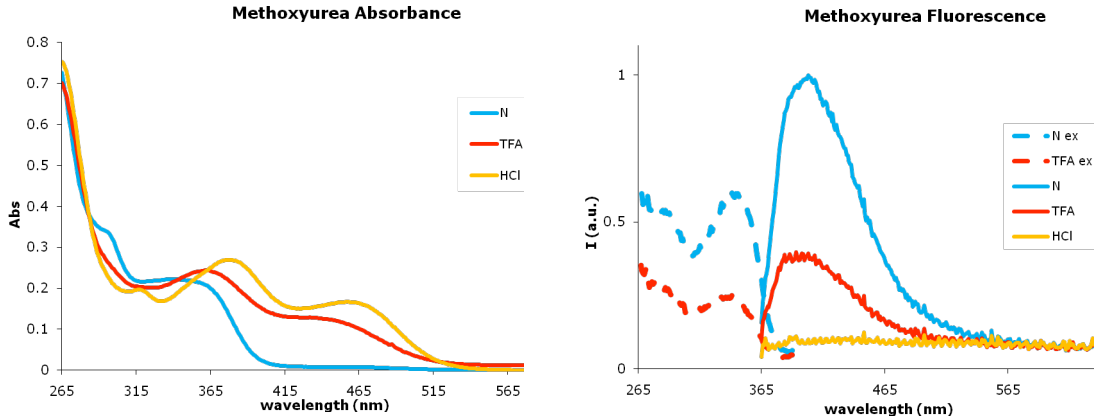

Fig. S7 UV-visible and fluorescence spectra for **3a**, **3a•TFA** and **3a•HCl.** HCl protonation results in a fully non-fluorescent species at any of the absorbing wavelengths, thus no excitation spectrum was recorded.

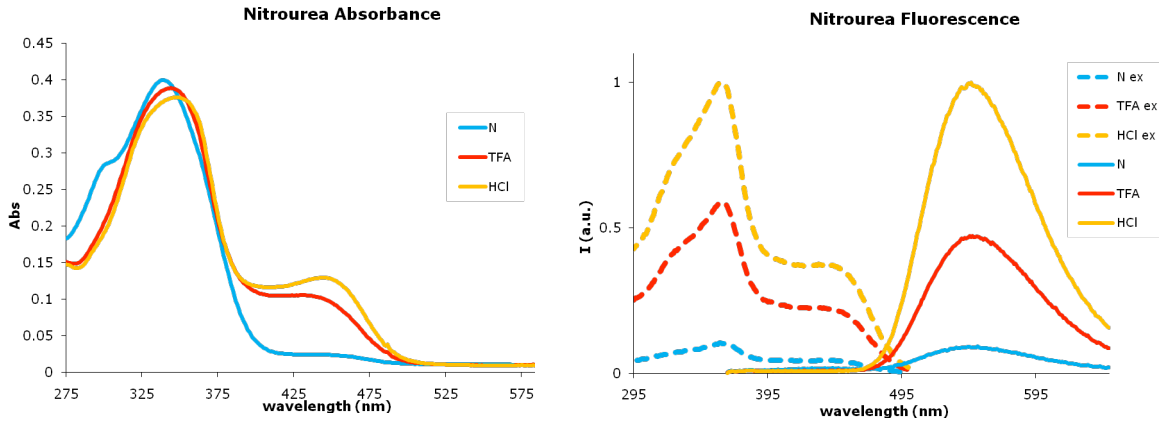

Fig. S8 UV-visible and fluorescence spectra for **3b**, **3b•TFA** and **3b•HCl**

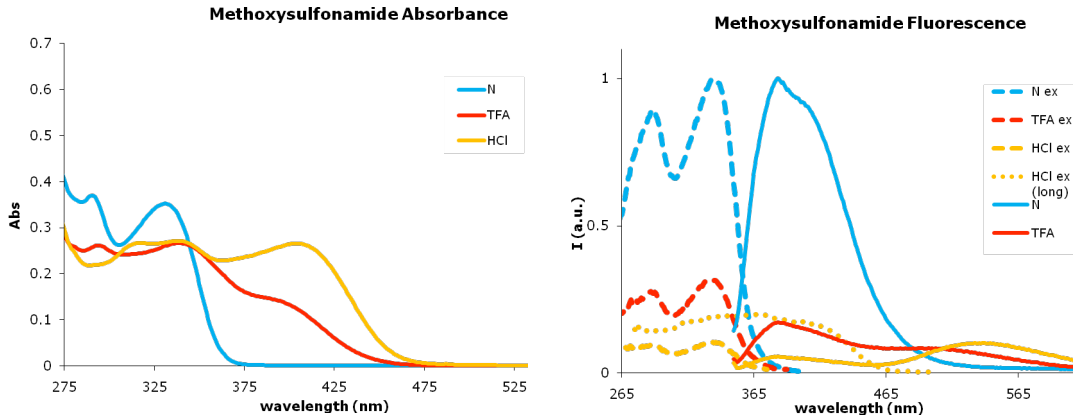

Fig. S9 UV-visible and fluorescence spectra for **4a**, **4a•TFA** and **4a•HCl**. The dotted "HCl ex (long)" trace is the excitation spectrum when monitoring emission at 535 nm.

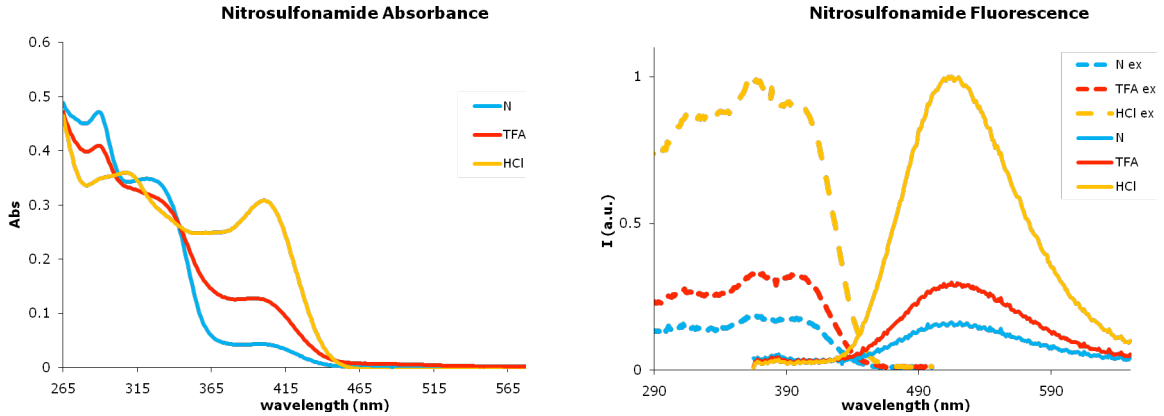

Fig. S10 UV-visible and fluorescence spectra for **4b**, **4b•TFA** and **4b•HCl**

HBr protonated fluorescence emission

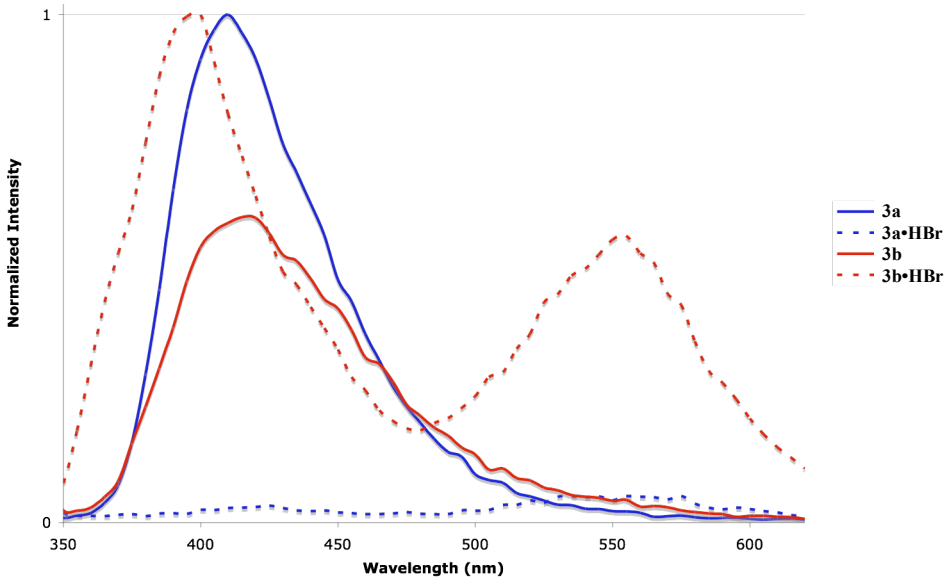

Fig. S11 Fluorescence emission in $CHCl_3$ of **3a** and **3b** with HBr. The dual emission in **3b•HBr** is possibly from incomplete protonation of the receptor, although treatment with an excess of HBr exhibited no further change in the spectra.

Calculations

Computational Methods. Computations for **3a,b** were calculated using the SPARTAN '08 Quantum Mechanics Program: (PC/x86) Release 131v4[2] at the B3LYP/6-31G* level of theory.[3] Computations for **4a,b** were calculated using the Gaussian 03 suite[4] of programs at the B3LYP/ 6-31G* level of theory[5] (opt=loose). All stationary points were confirmed by harmonic frequency analysis and checked for stability for triplet and SCF convergence. The energies of the stationary points were determined, including zero point energies, at the same level of theory.

Methoxyphenyl Urea **3a**
B3LYP/6-31G* = -2080.617890 au

1 C C0 1.1940237 -0.3882307 -0.6274487
2 C C1 1.1357013 0.9933314 -0.3559783
3 N N2 -0.0245955 1.6603171 -0.2057209
4 C C3 -1.1716675 0.9648448 -0.3257965
5 C C4 -1.2029340 -0.4178893 -0.5957503
6 C C5 0.0022835 -1.0944958 -0.7464891
7 C C6 2.3402705 1.7534275 -0.2314747
8 C C7 -2.3906757 1.6952902 -0.1696799
9 C C8 -3.4156340 2.3423928 -0.0489185
10 C C9 3.3532210 2.4233706 -0.1364423
11 C C10 -4.6237030 3.0811264 0.0806850
12 C C11 4.5465746 3.1906106 -0.0384069
13 C C12 -5.8747990 2.4097094 0.1479862
14 C C13 -7.0454619 3.1737177 0.2569466
15 C C14 -6.9677513 4.5617563 0.3009208
16 C C15 -5.7446520 5.2494752 0.2424844
17 C C16 -4.5854230 4.4880568 0.1340293
18 C C17 4.4786340 4.5973887 -0.0227610
19 C C18 5.6223376 5.3857874 0.0532986
20 C C19 6.8603471 4.7258189 0.1175817
21 C C20 6.9673367 3.3391439 0.1106584
22 C C21 5.8121987 2.5479619 0.0344745
23 C C22 -5.6946536 6.7587792 0.2887021
24 C C23 5.5416099 6.8942669 0.0603066
25 N N24 5.8197064 1.1481520 0.0455075
26 N N25 -5.8521879 1.0103472 0.1213371
27 C C26 -6.9316481 0.1333340 0.0731914
28 O O27 -8.1005375 0.4881963 0.0022226
29 N N28 -6.5182585 -1.1879870 0.1112608
30 C C29 -7.3172495 -2.3537050 0.0706498
31 C C30 6.9181538 0.2941259 0.0180559
32 N N31 6.5349160 -1.0344370 0.0961891
33 O O32 8.0785307 0.6725477 -0.0685462

34 C C33 7.3613458 -2.1817673 0.0915561
35 C C34 -8.7011294 -2.3463022 -0.1770482
36 C C35 -9.4018592 -3.5448826 -0.2143677
37 C C36 -8.7577111 -4.7727156 -0.0127778
38 C C37 -7.3813244 -4.7846727 0.2315791
39 C C38 -6.6765821 -3.5806448 0.2713331
40 C C39 8.7433162 -2.1500668 -0.1648175
41 C C40 9.4730611 -3.3318571 -0.1625704
42 C C41 8.8602377 -4.5667644 0.0877504
43 C C42 7.4856835 -4.6031059 0.3395519
44 C C43 6.7517969 -3.4158295 0.3397210
45 O O44 -9.5514039 -5.8854025 -0.0736099
46 O O45 9.6810206 -5.6611986 0.0649170
47 C C46 -8.9421664 -7.1472664 0.1342926
48 C C47 9.1038149 -6.9289001 0.3236023
49 H H1 2.1541799 -0.8785955 -0.7494891
50 H H2 -2.1535550 -0.9320766 -0.6919919
51 H H3 0.0126719 -2.1596918 -0.9600618
52 H H4 -7.9995153 2.6683096 0.3001338
53 H H5 -7.8926335 5.1283631 0.3864579
54 H H6 -3.6150720 4.9732454 0.0835690
55 H H7 3.4975334 5.0600371 -0.0762913
56 H H8 7.7737265 5.3140673 0.1776791
57 H H9 7.9321038 2.8548882 0.1572681
58 H H10 -6.1993641 7.1494605 1.1806228
59 H H11 -4.6625339 7.1222969 0.3028493
60 H H12 -6.1914332 7.2037624 -0.5827551
61 H H13 6.0407357 7.3182156 0.9404632
62 H H14 6.0273098 7.3263784 -0.8240430
63 H H15 4.5022698 7.2373951 0.0683924
64 H H16 4.8936506 0.7408285 -0.0058345
65 H H17 -4.9178871 0.6251547 0.0520659
66 H H18 -5.5405300 -1.3614570 0.2993102
67 H H19 5.5623142 -1.2242408 0.2944314
68 H H20 -9.2119486 -1.4060805 -0.3288542
69 H H21 -10.4710940 -3.5476670 -0.4026393
70 H H22 -6.8453114 -5.7130489 0.3932273
71 H H23 -5.6050030 -3.6060798 0.4636625
72 H H24 9.2302605 -1.2038538 -0.3532824
73 H H25 10.5411275 -3.3154326 -0.3565940
74 H H26 6.9735647 -5.5377954 0.5376312
75 H H27 5.6821845 -3.4603734 0.5390985
76 H H28 -9.7419309 -7.8855420 0.0505671
77 H H29 -8.1756528 -7.3575085 -0.6243450
78 H H30 -8.4871646 -7.2179264 1.1319346
79 H H31 9.9210818 -7.6502424 0.2637748
80 H H32 8.6549590 -6.9725270 1.3256292
81 H H33 8.3394337 -7.1863356 -0.4226326

Nitrophenyl Urea **3b**
B3LYP/6-31G* = -2260.583526 au

1 C C0 1.1573938 -0.3113823 -0.6020548
2 C C1 1.0914459 1.0730354 -0.3488388
3 N N2 -0.0701580 1.7279383 -0.1628531
4 C C3 -1.2115565 1.0165208 -0.2271220
5 C C4 -1.2353841 -0.3706595 -0.4717540
6 C C5 -0.0285713 -1.0349929 -0.6603508
7 C C6 2.2889316 1.8525929 -0.2823578
8 C C7 -2.4309065 1.7394077 -0.0388887
9 C C8 -3.4504195 2.3896029 0.1067663
10 C C9 3.2893892 2.5455455 -0.2355007
11 C C10 -4.6480135 3.1413355 0.2610602
12 C C11 4.4668337 3.3423391 -0.1880241
13 C C12 -5.9062060 2.4872492 0.3365424
14 C C13 -7.0665971 3.2606954 0.4666056
15 C C14 -6.9720128 4.6476494 0.5264900
16 C C15 -5.7414339 5.3204236 0.4624043
17 C C16 -4.5921930 4.5465891 0.3304823
18 C C17 4.3676930 4.7465379 -0.2226797
19 C C18 5.4957120 5.5612835 -0.1929920
20 C C19 6.7487427 4.9322103 -0.1200567
21 C C20 6.8859201 3.5483787 -0.0783931
22 C C21 5.7473168 2.7336067 -0.1125980
23 C C22 -5.6721708 6.8280653 0.5246892
24 C C23 5.3833264 7.0665723 -0.2446112
25 N N24 5.7858199 1.3311651 -0.0528276
26 N N25 -5.8986215 1.0834636 0.2986226
27 C C26 -6.9839259 0.2270631 0.2505082
28 O O27 -8.1497149 0.5838367 0.1819338
29 N N28 -6.5836183 -1.1113005 0.2929548
30 C C29 -7.3890578 -2.2541196 0.2396296
31 C C30 6.8968867 0.5087129 -0.1030779
32 N N31 6.5442814 -0.8378123 0.0193584
33 O O32 8.0464864 0.8990244 -0.2347422
34 C C33 7.3848108 -1.9558043 -0.0096041
35 C C34 -8.7749820 -2.2223548 -0.0051254
36 C C35 -9.4911866 -3.4118798 -0.0522631
37 C C36 -8.8383377 -4.6284947 0.1401616
38 C C37 -7.4655688 -4.6799913 0.3822107
39 C C38 -6.7491120 -3.4951976 0.4298518
40 C C39 8.7631988 -1.8904066 -0.2879502
41 C C40 9.5166590 -3.0575581 -0.3028506
42 C C41 8.9083514 -4.2851337 -0.0448185
43 C C42 7.5434246 -4.3699621 0.2302076
44 C C43 6.7898667 -3.2076261 0.2453373
45 H H1 2.1180164 -0.7912685 -0.7579626
46 H H2 -2.1816714 -0.8989854 -0.5201159
47 H H3 -0.0123255 -2.1035572 -0.8555532
48 H H4 -8.0271972 2.7682332 0.5150718

49 H H5 -7.8889470 5.2235054 0.6300238
50 H H6 -3.6167690 5.0203980 0.2748740
51 H H7 3.3760973 5.1859337 -0.2776371
52 H H8 7.6491408 5.5420358 -0.0921319
53 H H9 7.8623226 3.0885767 -0.0261154
54 H H10 -6.2004638 7.2171354 1.4031908
55 H H11 -4.6363996 7.1777076 0.5746013
56 H H12 -6.1350946 7.2863198 -0.3584239
57 H H13 5.9141585 7.5360675 0.5923772
58 H H14 5.8195793 7.4680305 -1.1680631
59 H H15 4.3388890 7.3909626 -0.2031289
60 H H16 4.8667951 0.9040734 -0.0616780
61 H H17 -4.9678152 0.6896166 0.2234948
62 H H18 -5.6088206 -1.2944391 0.4892120
63 H H19 5.5807566 -1.0434499 0.2465026
64 H H20 -9.2709992 -1.2736128 -0.1475559
65 H H21 -10.5581830 -3.4068652 -0.2384764
66 H H22 -6.9833173 -5.6384240 0.5296513
67 H H23 -5.6779753 -3.5266363 0.6180290
68 H H24 9.2243200 -0.9329470 -0.4801669
69 H H25 10.5785149 -3.0266571 -0.5141405
70 H H26 7.0955559 -5.3359413 0.4282736
71 H H27 5.7246320 -3.2653692 0.4589052
72 N N1 -9.6020879 -5.8743842 0.0886940
73 O O1 -10.8143699 -5.7978605 -0.1185624
74 O O2 -8.9879156 -6.9309390 0.2552579
75 N N3 9.7112444 -5.5071278 -0.0608919
76 O O3 9.1365392 -6.5742651 0.1675596
77 O O4 10.9150598 -5.4012578 -0.3019290

Methoxyphenyl Sulfonamide **4a**
B3LYP/6-31G* = -2840.34476156 au
B3LYP/6-31G* Zero Point Corrected Energy = -2839.737133 au
NIMAG = 0

C	0.43845200	5.83212900	0.51685500
C	0.61495100	4.47338700	0.19190500
N	-0.41172000	3.64277300	-0.07467300
C	-1.65805700	4.15048300	-0.02535300
C	-1.92742700	5.49499000	0.29643300
C	-0.85593800	6.33918100	0.56903300
C	1.92594000	3.90698700	0.13349200
C	-2.72986500	3.25744800	-0.33754300
C	3.04258800	3.42675400	0.07792500
C	-3.65628100	2.52068500	-0.61976100
C	4.29628700	2.75953600	0.01481700
C	-4.69311800	1.62107900	-0.98996600
C	5.49257800	3.47574800	-0.18241200
C	6.72816700	2.83880600	-0.24972600
C	6.74582900	1.44007600	-0.12663500

C	5.58129800	0.70324400	0.05465800
C	4.34119400	1.34681500	0.13877600
C	-4.37204700	0.35424700	-1.54287700
C	-5.41561400	-0.49708100	-1.93086600
C	-6.73955100	-0.11388000	-1.74622900
C	-7.08347600	1.13269700	-1.19892600
C	-6.04520900	1.98678100	-0.83894300
C	8.00729800	3.61729100	-0.45042000
C	-8.52972800	1.53295500	-1.02386200
N	3.13290100	0.64308900	0.28906100
S	2.91697000	-0.72350900	1.28435100
C	3.08550800	-2.10565700	0.17108700
O	1.51175400	-0.60970300	1.69456300
O	3.99509600	-0.80484900	2.27146700
C	4.13007200	-3.00758800	0.35844700
C	4.25441400	-4.11149100	-0.48696500
C	3.32022500	-4.30500900	-1.51366000
C	2.26230300	-3.39354100	-1.68468200
C	2.14010300	-2.29809400	-0.84672500
N	-3.01666700	0.02120300	-1.74477700
S	-2.33498400	-1.51254700	-1.45151100
O	-3.11320000	-2.48715400	-2.21773300
O	-0.90916800	-1.29241400	-1.70947000
C	-2.55169000	-1.87600100	0.28103800
C	-3.66901500	-2.59857600	0.70040100
C	-3.85044000	-2.86931400	2.05633800
C	-2.90365000	-2.41668600	2.98717300
C	-1.77628300	-1.69873800	2.55242700
C	-1.60060800	-1.42314000	1.20616900
H	1.30203300	6.45512300	0.72317600
H	-2.95197600	5.85012700	0.32209600
H	-1.02802800	7.38232600	0.81915200
H	5.43141100	4.55604600	-0.27979100
H	7.69496600	0.91170200	-0.18230800
H	5.63406400	-0.37589100	0.13325200
H	-5.17701700	-1.44916300	-2.38869900
H	-7.52836100	-0.79657900	-2.05468700
H	-6.26611100	2.96511100	-0.42147400
H	7.80944600	4.68872800	-0.55410600
H	8.54056900	3.28835700	-1.35103600
H	8.69350900	3.48628800	0.39570800
H	-8.61684900	2.52423100	-0.56824900
H	-9.06765200	0.82306200	-0.38331200
H	-9.05706300	1.56107800	-1.98565800
H	2.29851300	1.22611200	0.33421200
H	4.83564900	-2.85119300	1.16735200
H	5.06996700	-4.80783200	-0.33159400
H	1.54162900	-3.56750300	-2.47666700
H	1.31016700	-1.61334000	-0.98377800
H	-2.35704200	0.75169700	-1.48023600
H	-4.38209000	-2.96589900	-0.02896500

H	-4.71837000	-3.43649800	2.37110200
H	-1.04040200	-1.37643700	3.28120100
H	-0.71584500	-0.88718800	0.88333400
O	-2.98142000	-2.62997000	4.32659400
O	3.34617600	-5.34143500	-2.39126700
C	-4.08597600	-3.36322200	4.83695600
H	-3.93840000	-3.40883300	5.91710300
H	-5.03724800	-2.86001700	4.62110100
H	-4.11391500	-4.38245900	4.43073400
C	4.38227500	-6.30651800	-2.27375500
H	4.34687000	-6.81771300	-1.30321000
H	4.20525500	-7.03073000	-3.07041500
H	5.37200700	-5.85178100	-2.40904700

Nitrophenyl Sulfonamide **4b**
B3LYP/6-31G* = -3020.29175256 au
B3LYP/6-31G* Zero Point Corrected Energy = -3019.745012 au
NIMAG = 0

C	-0.11683600	5.82238700	0.25609000
C	0.18141100	4.48422200	-0.06503200
N	-0.76256400	3.57667100	-0.38088100
C	-2.04568100	3.98643500	-0.38935200
C	-2.43547000	5.30260000	-0.07653600
C	-1.44790900	6.22630100	0.25035400
C	1.53655600	4.02867600	-0.07167800
C	-3.02472100	3.01152500	-0.75731300
C	2.68631200	3.63185400	-0.08517200
C	-3.85775000	2.18201000	-1.07039600
C	4.00840600	3.11110600	-0.14127400
C	-4.76436300	1.16522700	-1.47753200
C	5.11750500	3.95934700	-0.32393900
C	6.41793700	3.46494700	-0.38129600
C	6.59540600	2.07688800	-0.26505300
C	5.51794000	1.21331400	-0.10268800
C	4.21569500	1.71468100	-0.02754900
C	-4.27106400	-0.10267600	-1.87685500
C	-5.17513300	-1.07896100	-2.31177100
C	-6.54119600	-0.81499800	-2.31540600
C	-7.05678200	0.43046300	-1.92170500
C	-6.15096800	1.40792400	-1.51752400
C	7.60180900	4.38478100	-0.56599500
C	-8.54260700	0.70046000	-1.95371000
N	3.09215800	0.86522300	0.10364000
S	2.98072800	-0.37183800	1.26234100
C	3.33228200	-1.86523600	0.32034100
O	1.55944000	-0.39420300	1.62460900
O	4.03261900	-0.23030300	2.26696900
C	4.49411100	-2.58228800	0.61127400
C	4.76366800	-3.75246800	-0.09579000

C	3.85656800	-4.16802800	-1.06705800
C	2.68699000	-3.46430400	-1.35212400
C	2.41841400	-2.29507200	-0.64595700
N	-2.87110700	-0.32147400	-1.88564700
S	-2.11750000	-1.69677700	-1.24668200
O	-2.75171600	-2.87159100	-1.84008200
O	-0.68897800	-1.41979000	-1.40920600
C	-2.48373400	-1.72053600	0.51616000
C	-3.66272700	-2.33093000	0.95706900
C	-3.96002400	-2.32512700	2.31660800
C	-3.06440900	-1.71668300	3.19468000
C	-1.88120900	-1.12031100	2.76522500
C	-1.58830900	-1.11820700	1.40299900
H	0.68427100	6.50961800	0.50558200
H	-3.48487100	5.57599200	-0.09801100
H	-1.71250500	7.25087400	0.49568200
H	4.93685900	5.02627100	-0.41746000
H	7.59881900	1.66075700	-0.31441800
H	5.68811600	0.14467600	-0.03822300
H	-4.79782100	-2.03587000	-2.65126500
H	-7.22287900	-1.59201200	-2.65349900
H	-6.50792000	2.38843900	-1.21598700
H	7.28480000	5.42682500	-0.67085400
H	8.17895300	4.11979900	-1.46037100
H	8.28783000	4.32933900	0.28828900
H	-8.77418600	1.70442900	-1.58532800
H	-9.09283600	-0.01829400	-1.33445700
H	-8.94080400	0.61881100	-2.97264500
H	2.19375100	1.34521400	0.04969200
H	5.16601600	-2.23130600	1.38657000
H	5.65241000	-4.34066200	0.09544500
H	2.00442400	-3.83186300	-2.10814000
H	1.50569500	-1.74345900	-0.84443600
H	-2.31477700	0.50858800	-1.68045200
H	-4.32416900	-2.81765200	0.25005400
H	-4.85982400	-2.78695900	2.70310000
H	-1.20279700	-0.67651700	3.48299500
H	-0.66229800	-0.67938300	1.05066300
N	-3.38175000	-1.71382000	4.63671300
O	-2.58202200	-1.16902600	5.39420600
O	-4.42894100	-2.25480300	4.98907700
N	4.14349500	-5.40699700	-1.81760700
O	3.32786600	-5.75891800	-2.66672500
O	5.18195200	-6.00774000	-1.54624700

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