Color-tunable single-benzene fluorophore-based sensor for sensitive detection of palladium in solution and living cells

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Supplementary figures:

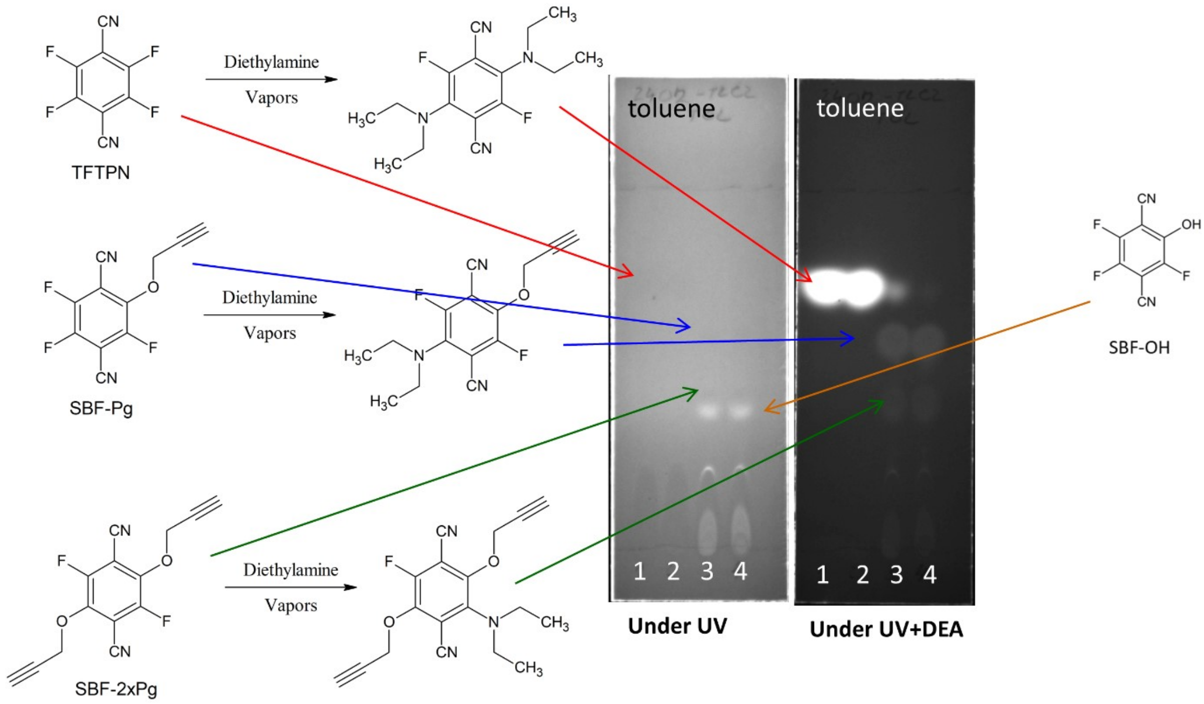


Fig. S1. TLC plate developed using diethylamine. The samples were separated on TLC with toluene as mobile phase and visualised under UV. The plate was then developed by incubation with diethylamine vapors. The position of individual compounds and diethylamine modified counterparts are indicated by arrows.

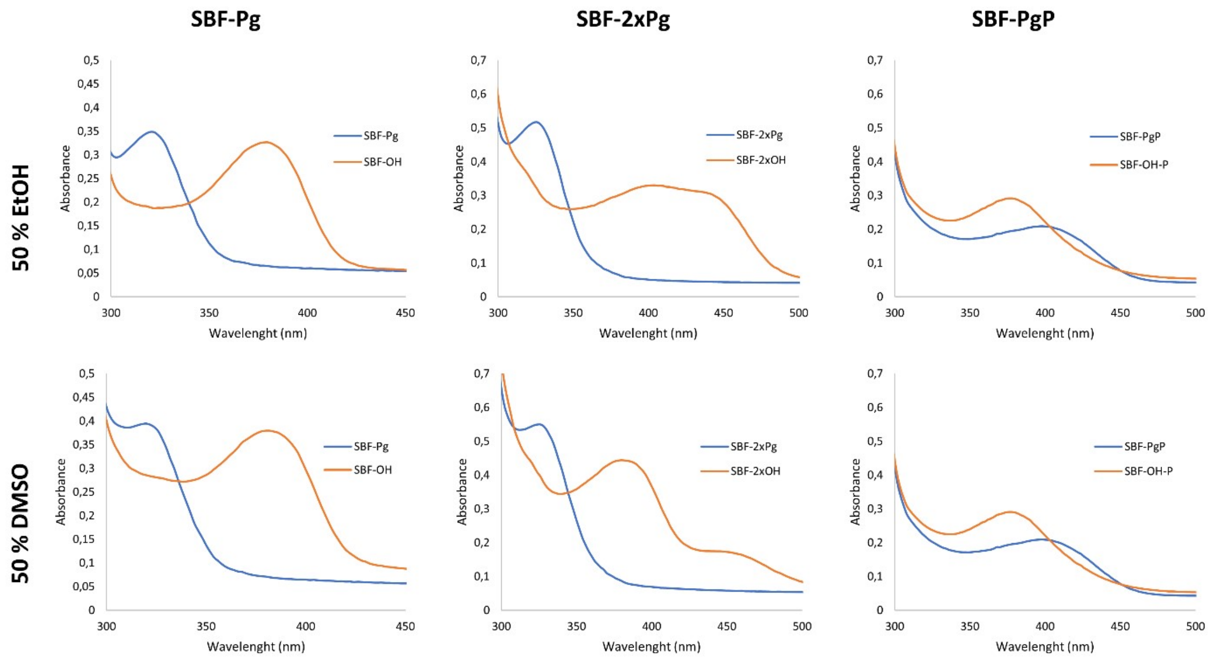


Fig. S2. Absorption scans of the SBF probes and depropargylated fluorophores.

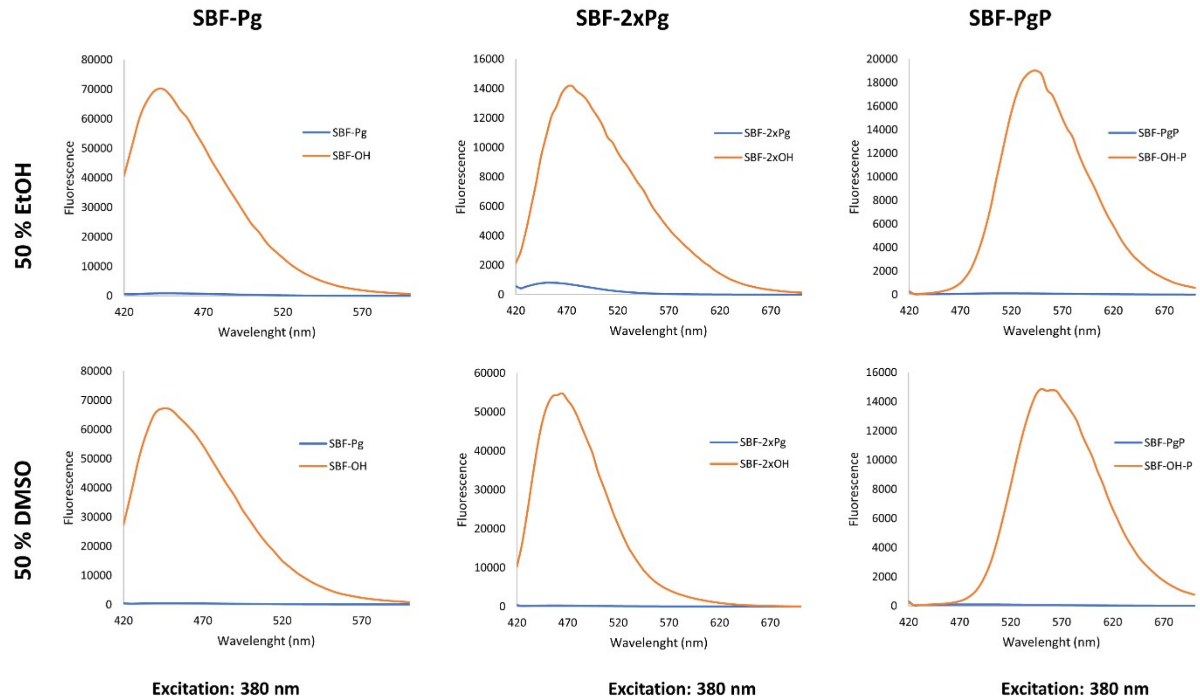


Fig. S3. Emission spectra of the SBF probes and depropargylated fluorophores.

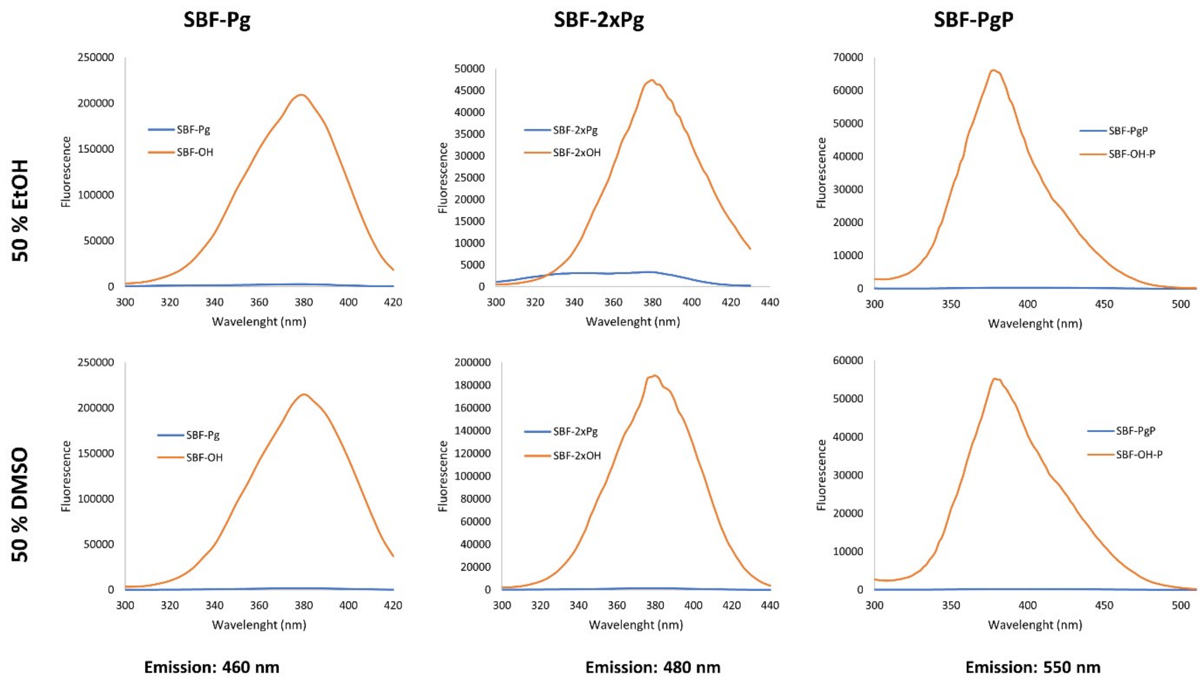


Fig. S4. Excitation spectra of the SBF probes and depropargylated fluorophores.

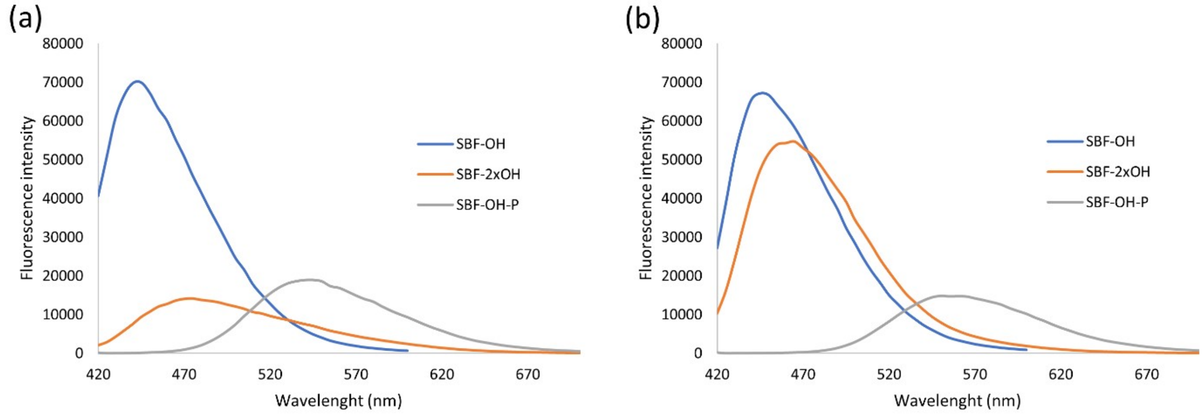
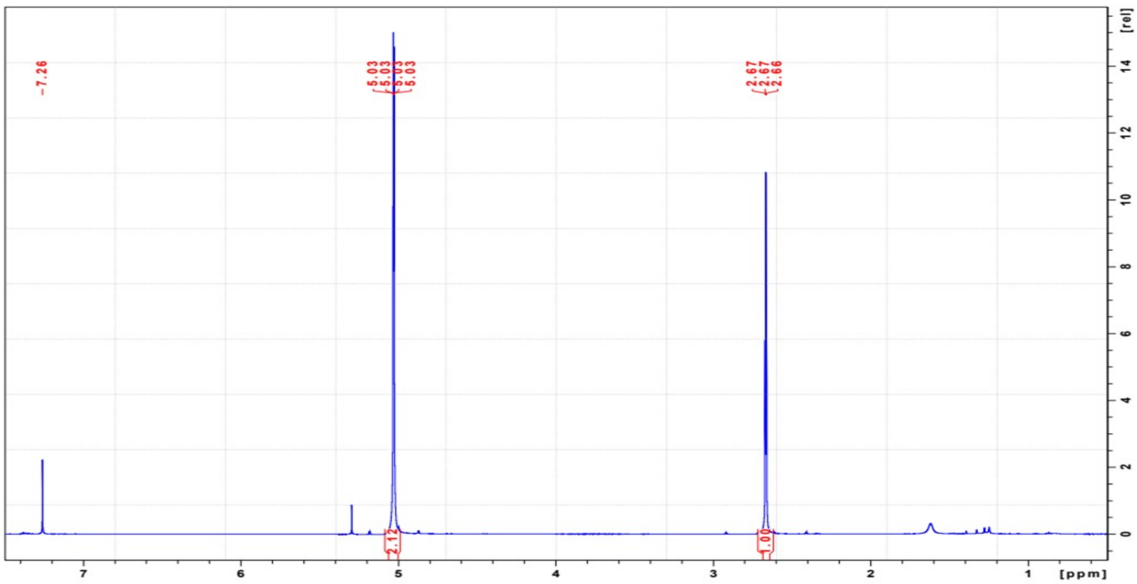
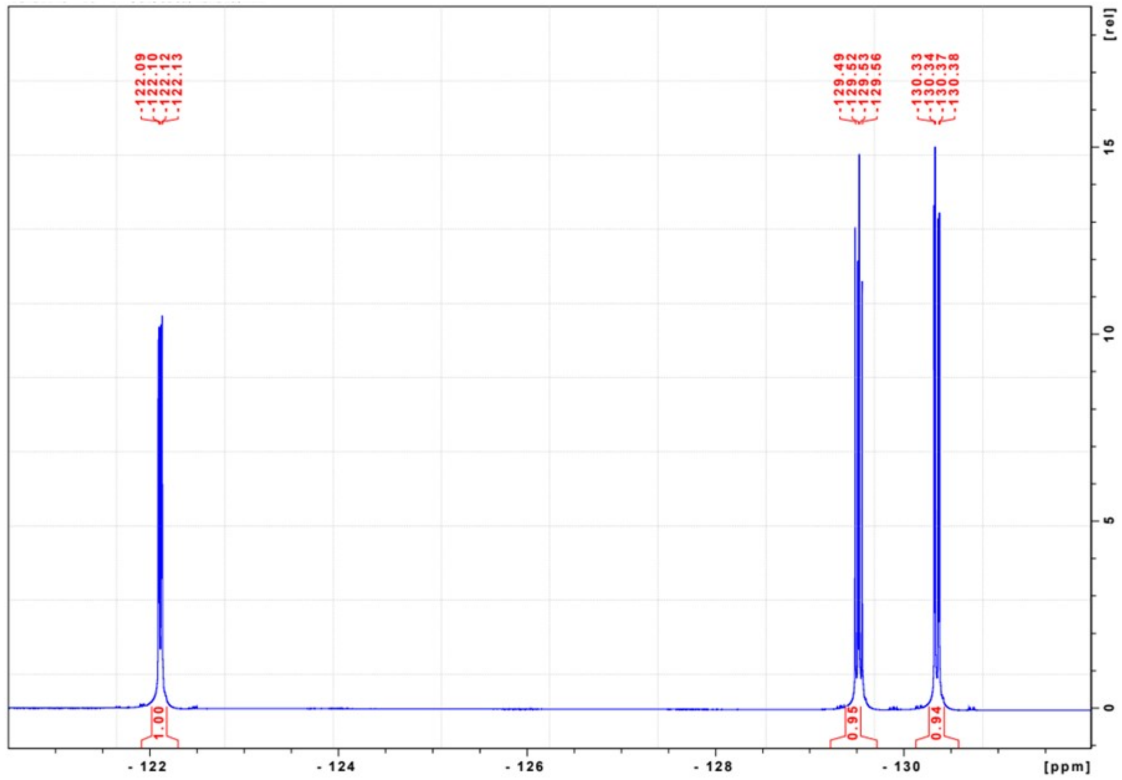


Fig. S5. Emission spectra of the deprotected fluorophores in 50 % EtOH (**a**) and 50 % DMSO (**b**)

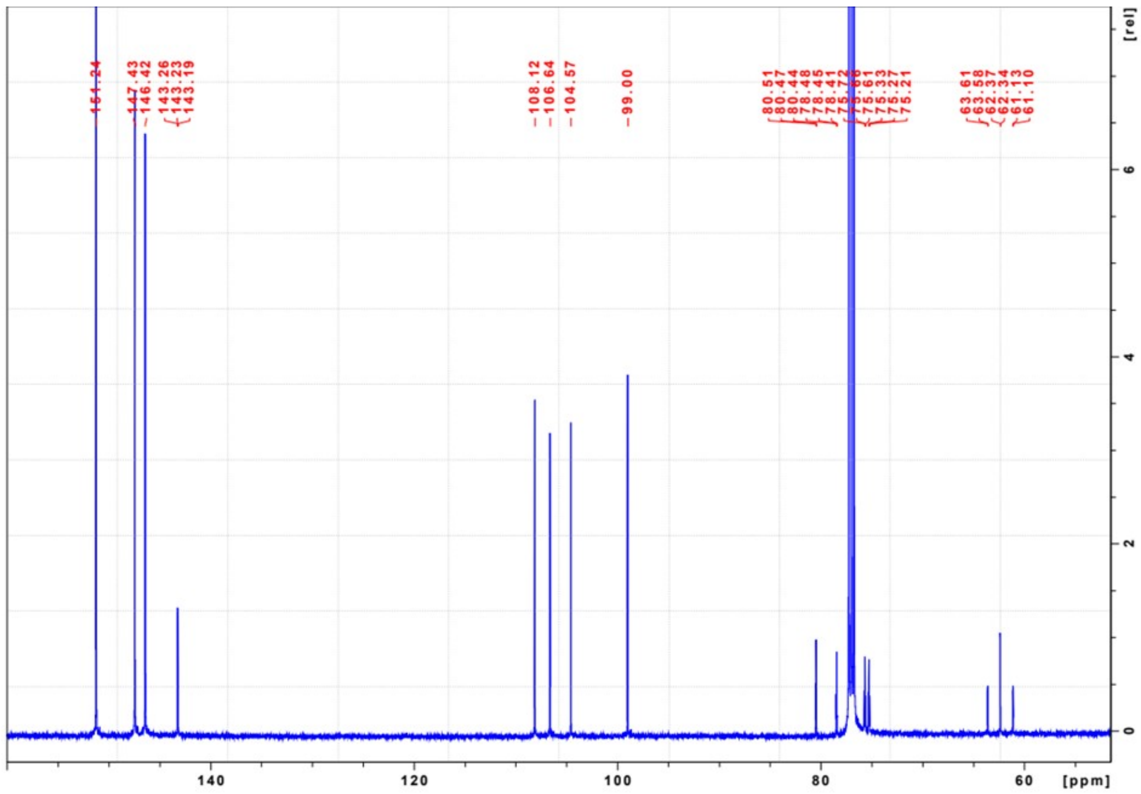
NMR spectra of isolated compounds:



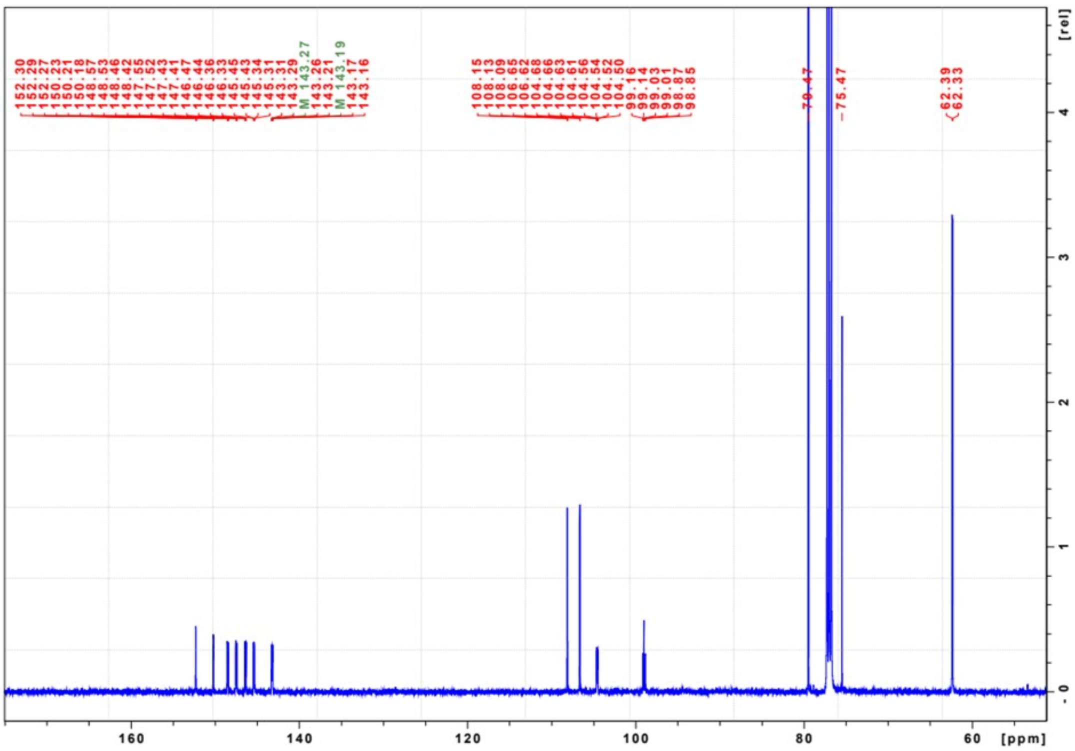
SBF-Pg **^{1}H NMR** (500 MHz, $CDCl_3$) δ ppm: 2.67 (t, 1 H); 5.03 (dd, 2 H).



SBF-Pg ^{19}F NMR (471 MHz, $CDCl_3$) δ ppm: -122.11 (dd, 1 F); -129.53 (dd, 1 F); -130.36 (dd, 1 F).



SBF-Pg: ^{13}C NMR with ^{19}F decoupling (signals 1,2,3 and 4 are splitted due to interactions with ^{1}H). ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm: 62.36 (td, 1 C); 75.47 (dt, 1 C); 79.47 (dt, 1 C); 99.00 (1 C); 104.57 (1 C); 106.64 (1 C); 108.12 (1 C); 143.23 (t, 1 C); 146.42 (1 C); 147.43 (1 C); 151.24 (1 C).



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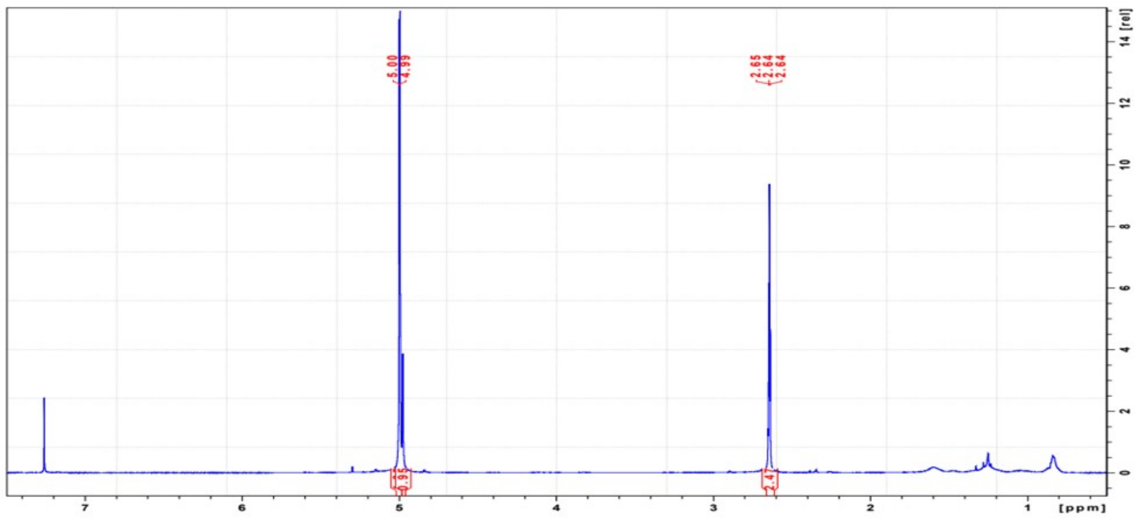
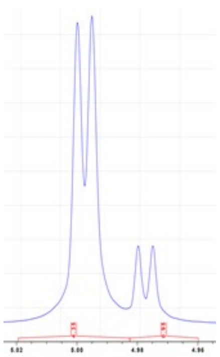
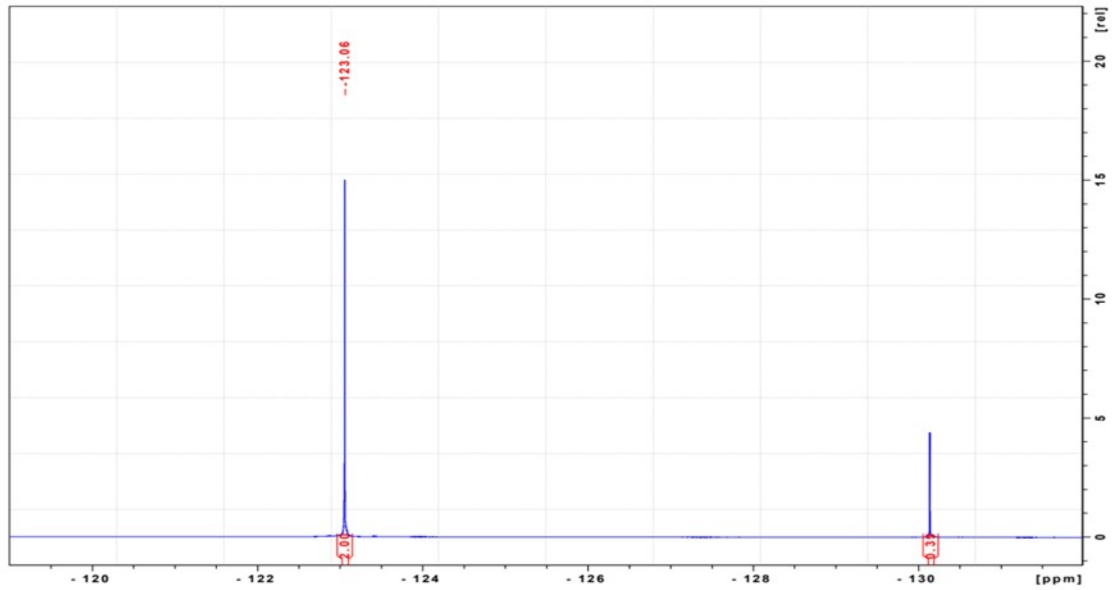
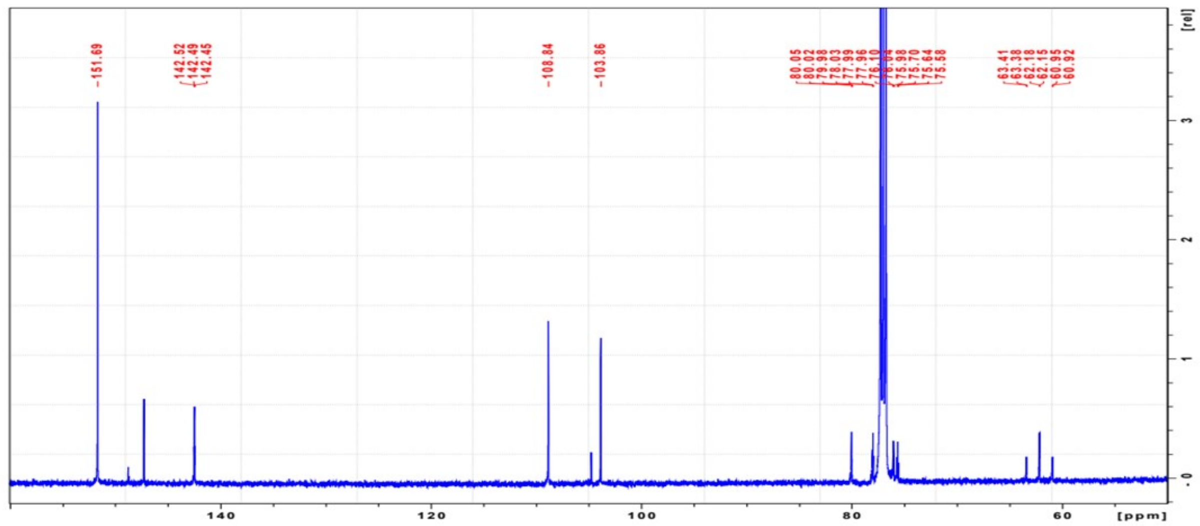




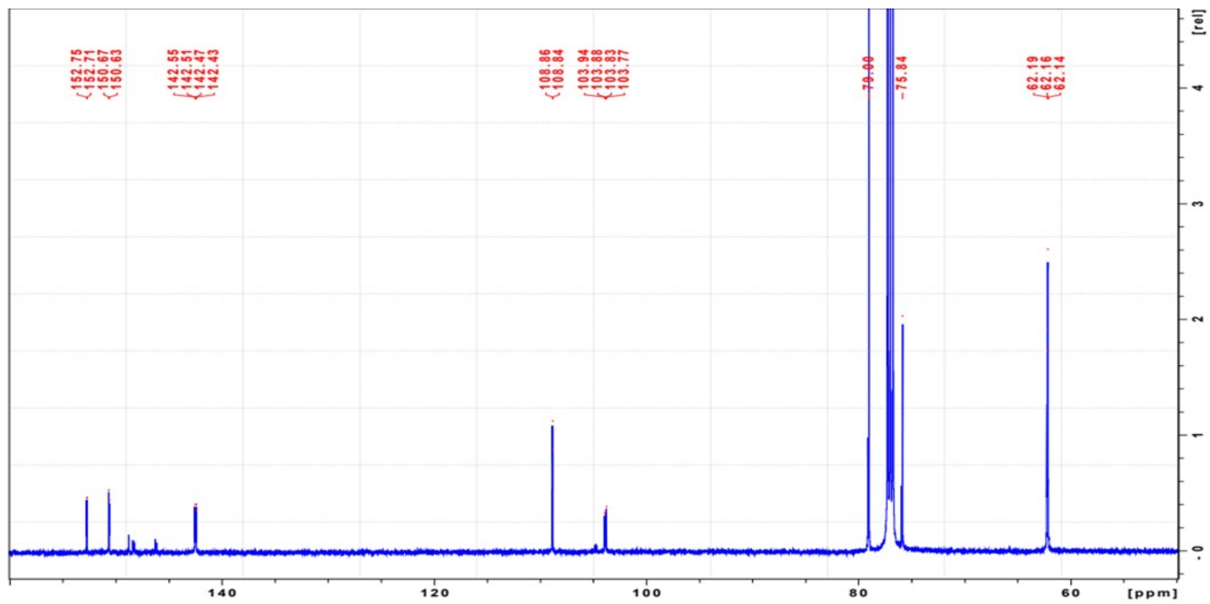
SBF-2×Pg: ^{1}H NMR ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm: 2.64 (t, 2 H); 5.00 (d, 4 H). Aside from the major component, a minor structure appeared in the spectrum. According to the integrals, the amount of the minor component is up to 20% (4 : 1, 2 : 0.5). Structure of this minority was not determined.



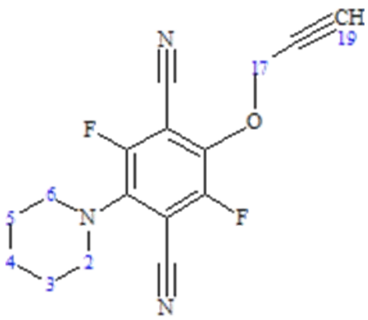
SBF-2×Pg: ^{19}F NMR (471 MHz, $CDCl_3$) δ ppm: -123.06 (s, 2 F). The minor structure was visible also in the ^{19}F spectrum. The integral also indicated that the amount is no more than 20%.

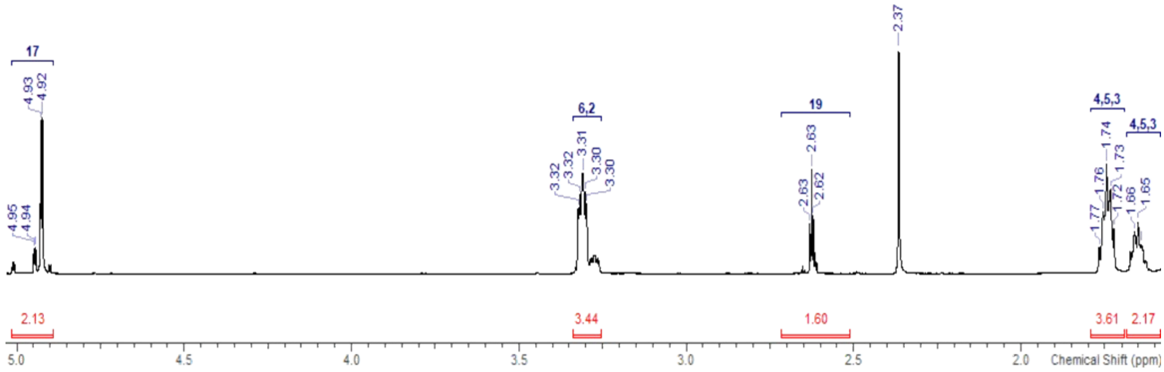


SBF-2×Pg: ^{13}C NMR with ^{19}F decoupling (signals 1,2,3 and 4 are splitted due to interactions with ^{1}H). ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm: 62.16 (td, 2 C); 75.84 (dt, 2 C); 79.00 (dt, 2 C); 103.86 (2 C); 108.84 (2 C); 142.49 (t, 2 C); 151.69 (2 C). In this spectrum, several signals of the minor component are visible.

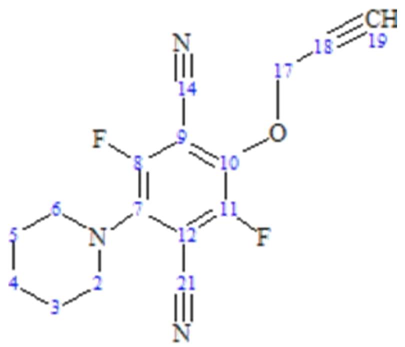


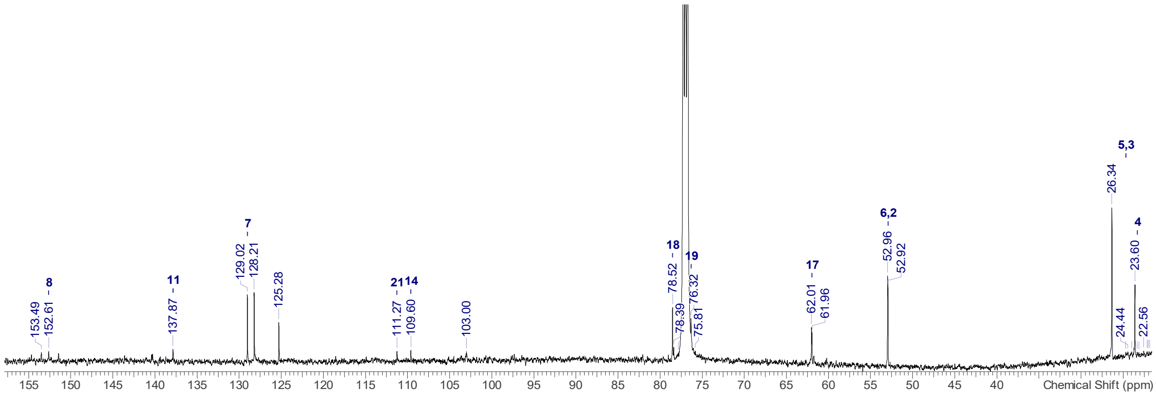
SBF-2×Pg: ^{13}C NMR with ^{1}H decoupling (signals are splitted due to interactions with ^{19}F). ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm: 62.16 (t, 2 C); 75.84 (2 C); 79.00 (2 C); 103.86 (dd, 2 C); 108.85 (d, 2 C); 142.49 (dd, 2 C); 151.69 (dd, 2 C). In this spectrum, several signals of the minor component are also visible.



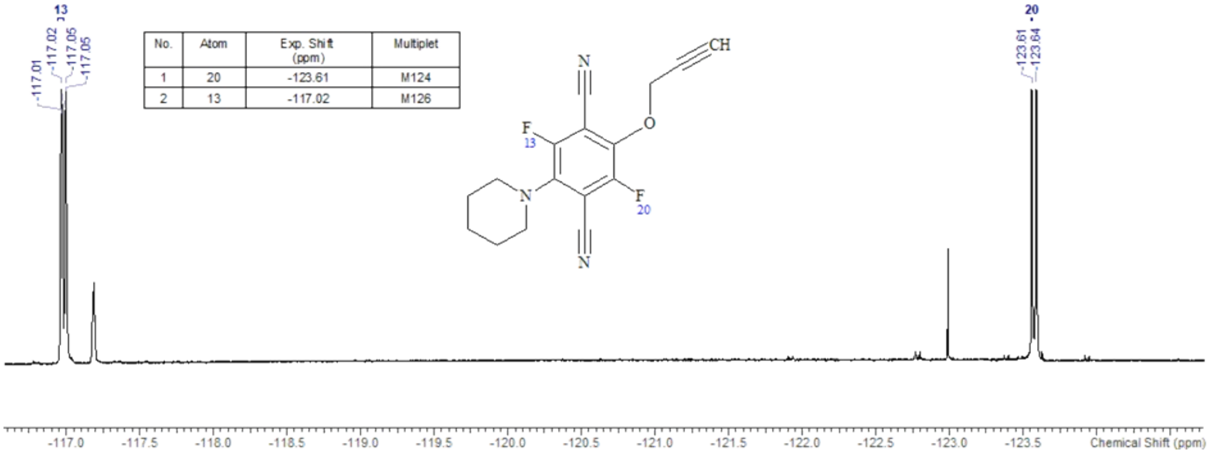


SBF-PgP: ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 1.65 (br t, *J*=5.34 Hz, 2 H) 1.74 (quin, *J*=5.53 Hz, 4 H) 2.63 (t, *J*=2.44 Hz, 2 H) 3.25 - 3.34 (m, 3 H) 4.89 - 5.01 (m, 2 H).





SBF-PgP: ^{13}C NMR ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 6.01 (s, 1 C) 6.14 (s, 1 C) 6.31 (s, 1 C) 6.58 (s, 1 C) 6.70 (s, 1 C) 7.17 (s, 1 C) 7.47 (s, 1 C) 7.82 (s, 1 C) 8.07 (s, 1 C) 8.88 (br dd, *J*=48.26, 27.12 Hz, 1 C) 10.16 (br dd, *J*=74.92, 58.37 Hz, 1 C) 10.43 (s, 1 C) 10.84 (s, 1 C) 11.64 (br dd, *J*=87.32, 37.69 Hz, 1 C) 11.62 (s, 1 C) 12.33 (s, 1 C) 12.76 (s, 1 C) 12.90 (s, 1 C) 13.28 (s, 1 C) 13.96 (br dd, *J*=56.07, 19.30 Hz, 1 C) 14.76 (s, 1 C) 15.39 (s, 1 C) 16.18 (br dd, *J*=94.22, 43.66 Hz, 1 C) 16.59 (s, 1 C) 16.84 (s, 1 C) 17.27 (s, 1 C) 17.44 (s, 1 C) 17.67 (s, 1 C) 18.07 (s, 1 C) 18.44 (s, 1 C) 18.63 (s, 1 C) 20.03 (br dd, *J*=182.92, 91.00 Hz, 1 C) 19.43 (s, 1 C) 19.77 (s, 1 C) 19.90 (s, 1 C) 20.10 (s, 1 C) 20.78 (s, 1 C) 21.45 (s, 1 C) 21.86 (s, 1 C) 22.02 (s, 1 C) 22.17 (s, 1 C) 22.56 (s, 1 C) 23.14 (s, 1 C) 23.32 (s, 1 C) 23.60 (s, 1 C) 23.99 (s, 1 C) 24.44 (s, 1 C) 24.68 (s, 1 C) 26.34 (s, 1 C) 52.92 (s, 1 C) 52.96 (s, 1 C) 61.96 (s, 1 C) 62.01 (s, 1 C) 75.81 (s, 1 C) 76.32 (s, 1 C) 77.84 (s, 1 C) 78.39 (s, 1 C) 78.52 (s, 1 C) 103.00 (s, 1 C) 109.60 (s, 1 C) 111.27 (s, 1 C) 125.28 (s, 1 C) 128.21 (s, 1 C) 129.02 (s, 1 C) 137.87 (s, 1 C) 152.61 (s, 1 C) 153.49 (s, 1 C).



SBF-PgP: ^{19}F NMR.