Supporting information for

Phosphorus Corrole Complexes: From Property Tuning to Applications in Photocatalysis and Triplet-Triplet Annihilation Upconversion

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† These authors contribute equally to this work.

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1. ^{1}H-NMR, ^{19}F-NMR and HR-MS Spectra

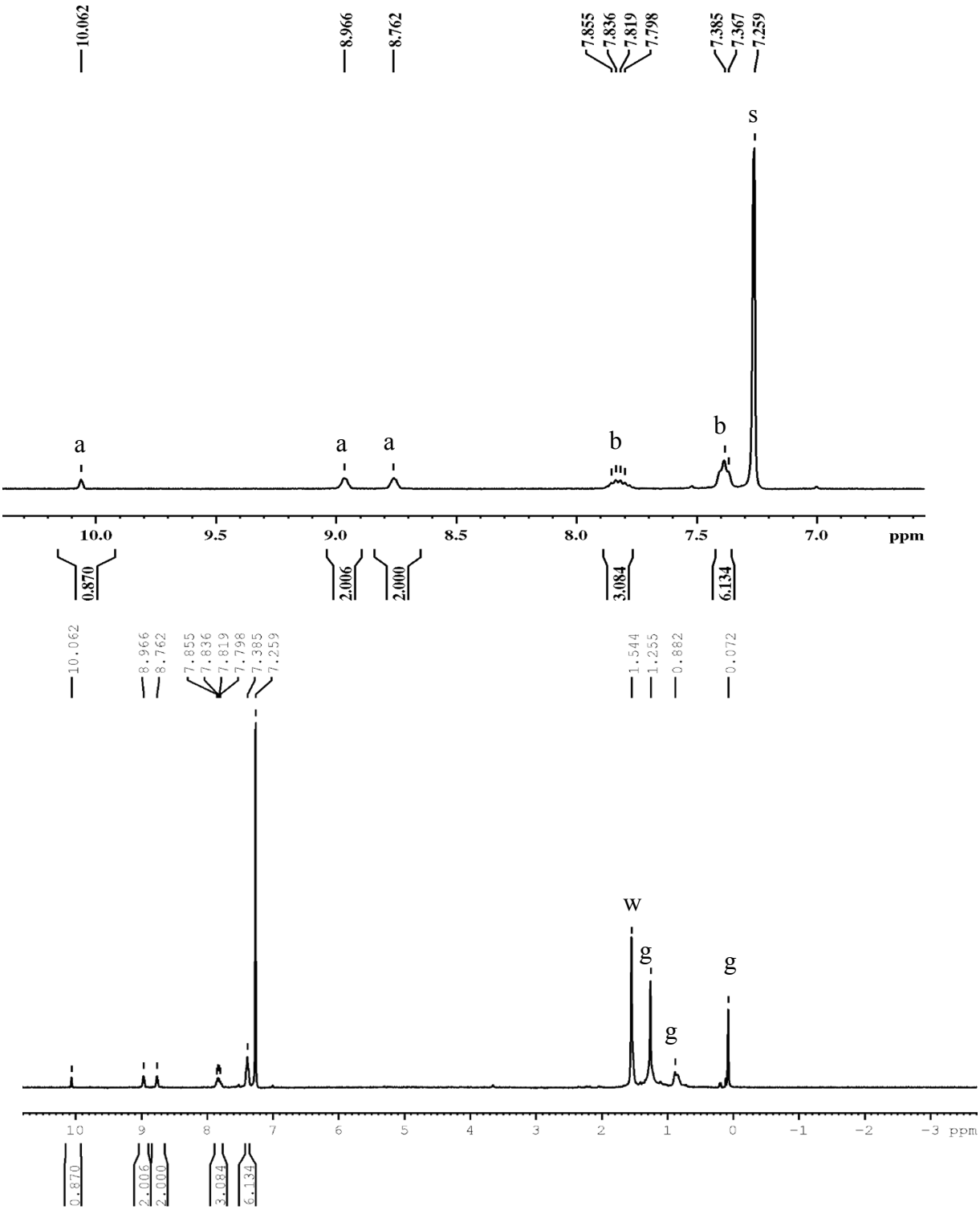


Figure S1. ^{1}H NMR spectrum of **$2PF_2$-I_3** (400 MHz, Chloroform-*d*), 25 °C (residual solvents: s = $CHCl_3$, w = water, g = grease). a = β-pyrrole-H, b = aryl-H.

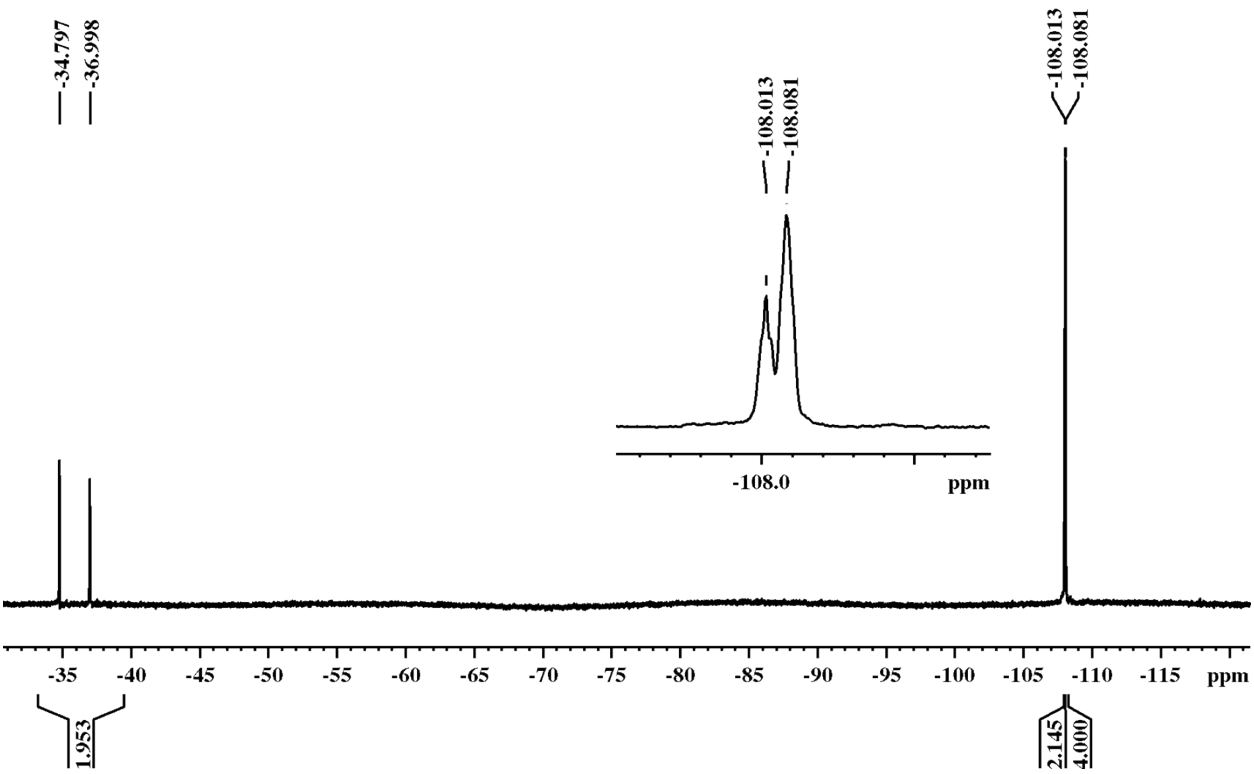


Figure S2. ^{19}F NMR spectrum of **2PF$_2$-I$_3$** (377 MHz, Chloroform-*d*), 25 °C.

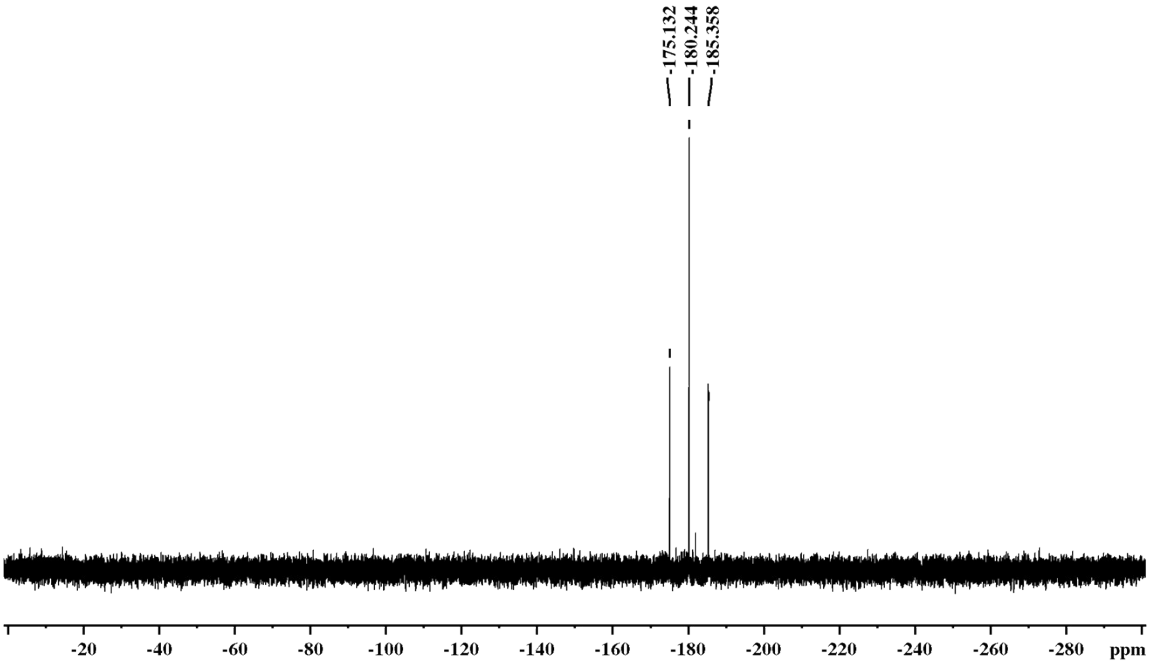


Figure S3. ^{31}P NMR spectrum of **2PF$_2$-I$_3$** (162 MHz, , Chloroform-*d*), 25 °C.

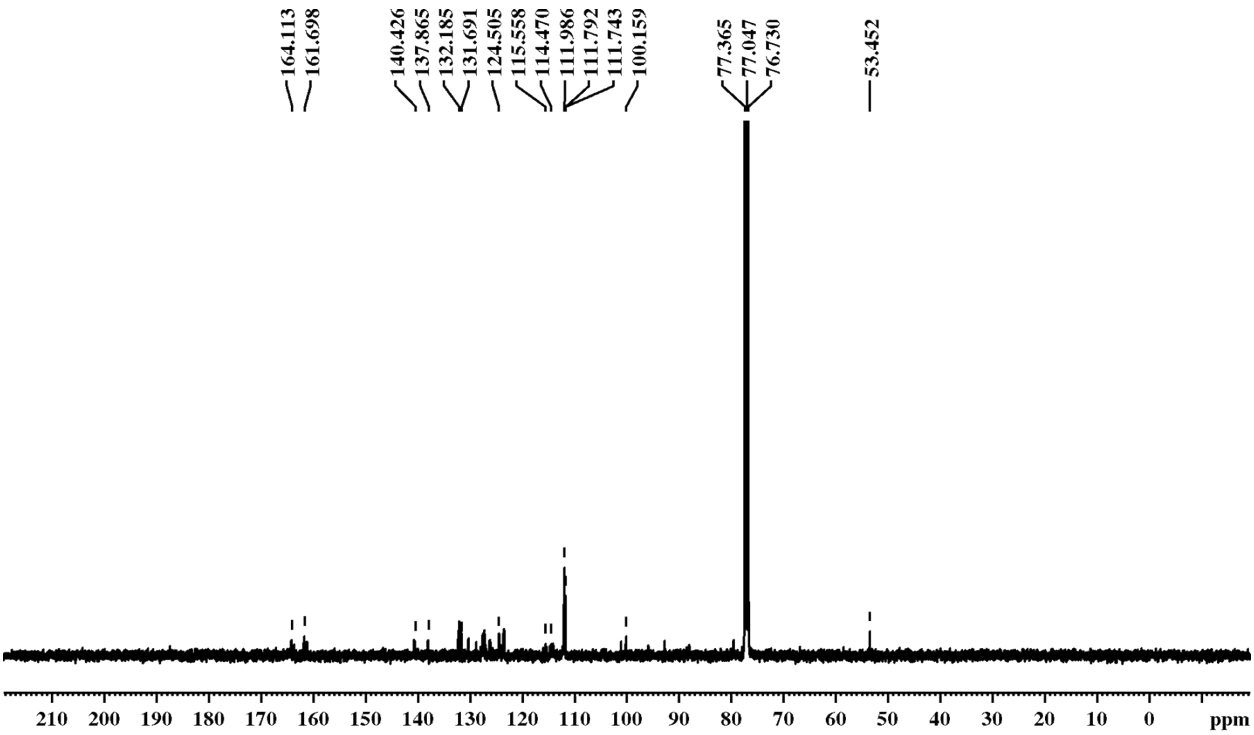


Figure S4. ^{13}C NMR spectrum of **2PF$_2$-I$_3$** (100.7 MHz, Chloroform-*d*), 25 °C**.**

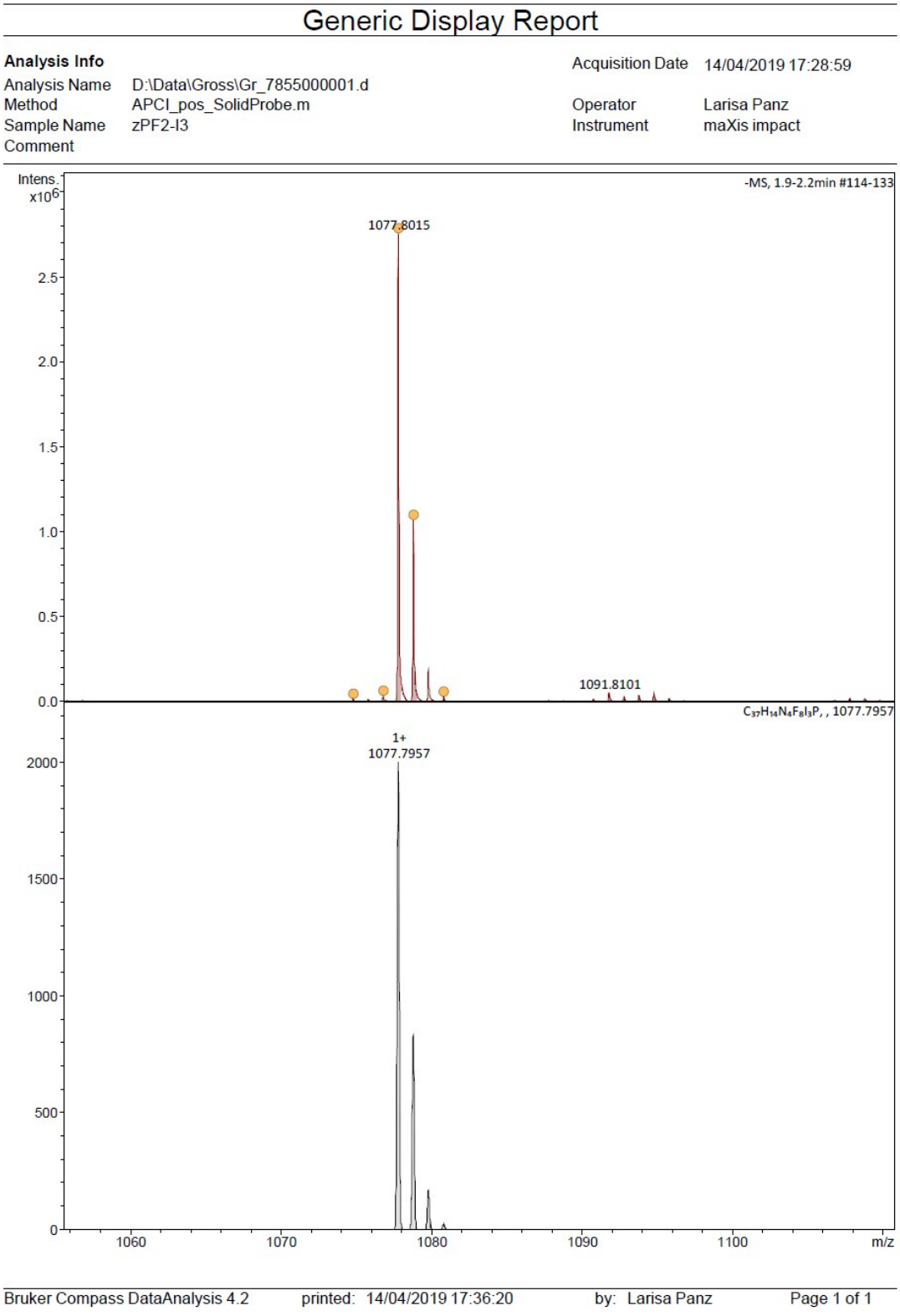


Figure S5. High resolution APCI⁺ mass spectrum of compound **$2PF_2$-I_3**.

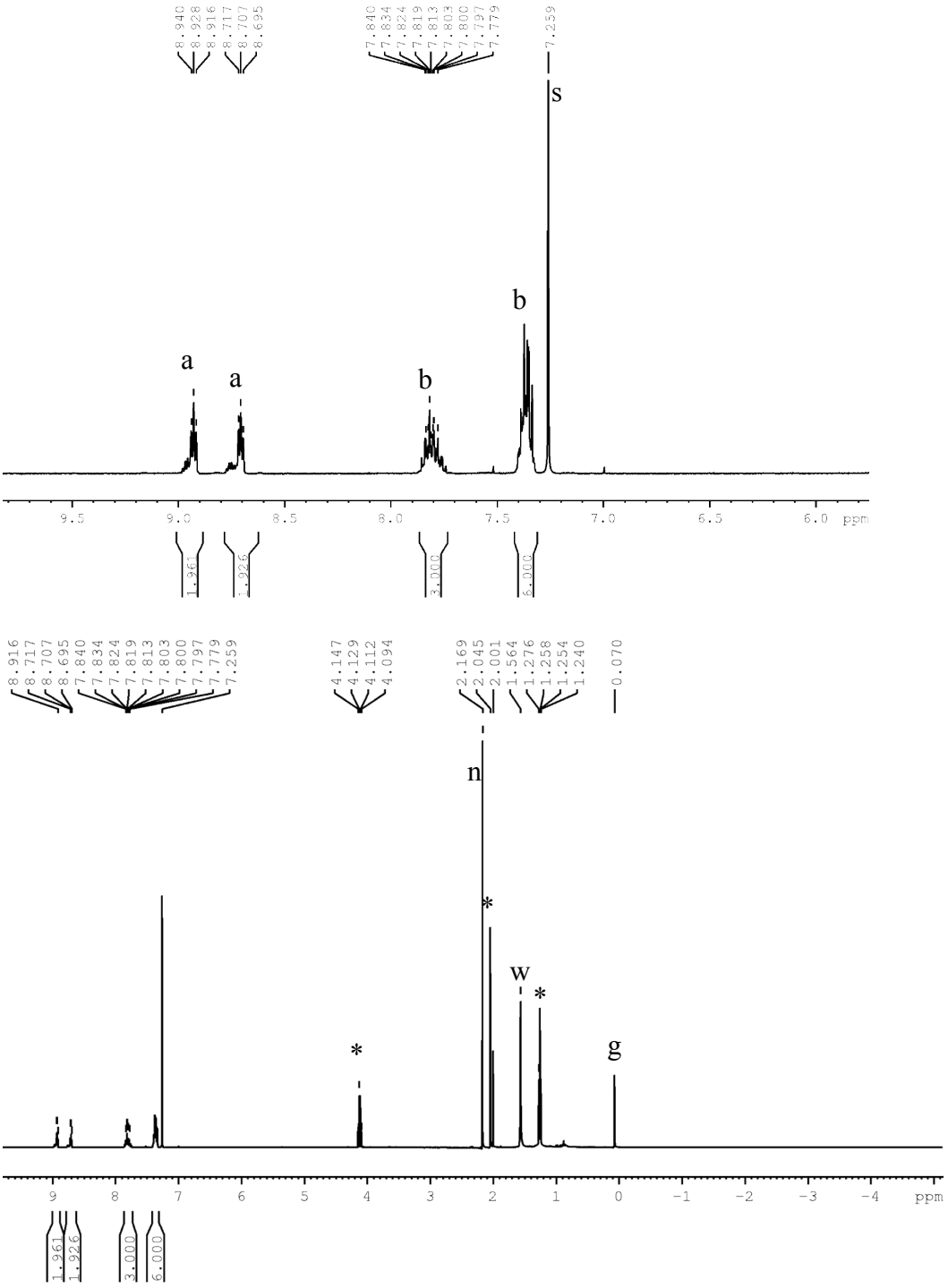


Figure S6. ^{1}H NMR spectrum of **2PF$_2$-I$_4$** (400 MHz, Chloroform-*d*), 25 °C (residual solvents: s = $CHCl_3$, *= ethyl acetate, n = acetone, w = water, g = grease). a = β-pyrrole-H, b = aryl-H.

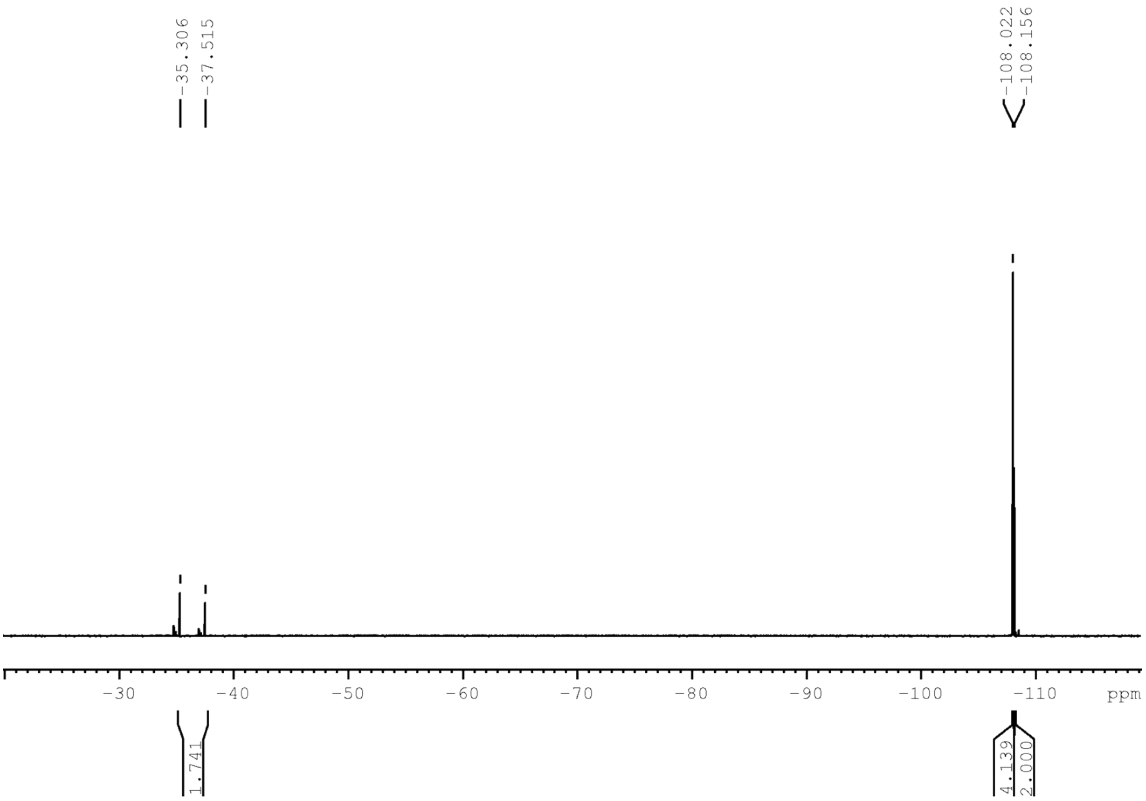


Figure S7. ^{19}F NMR spectrum of **2PF$_2$-I$_4$** (377 MHz, Chloroform-*d*), 25 °C**.**

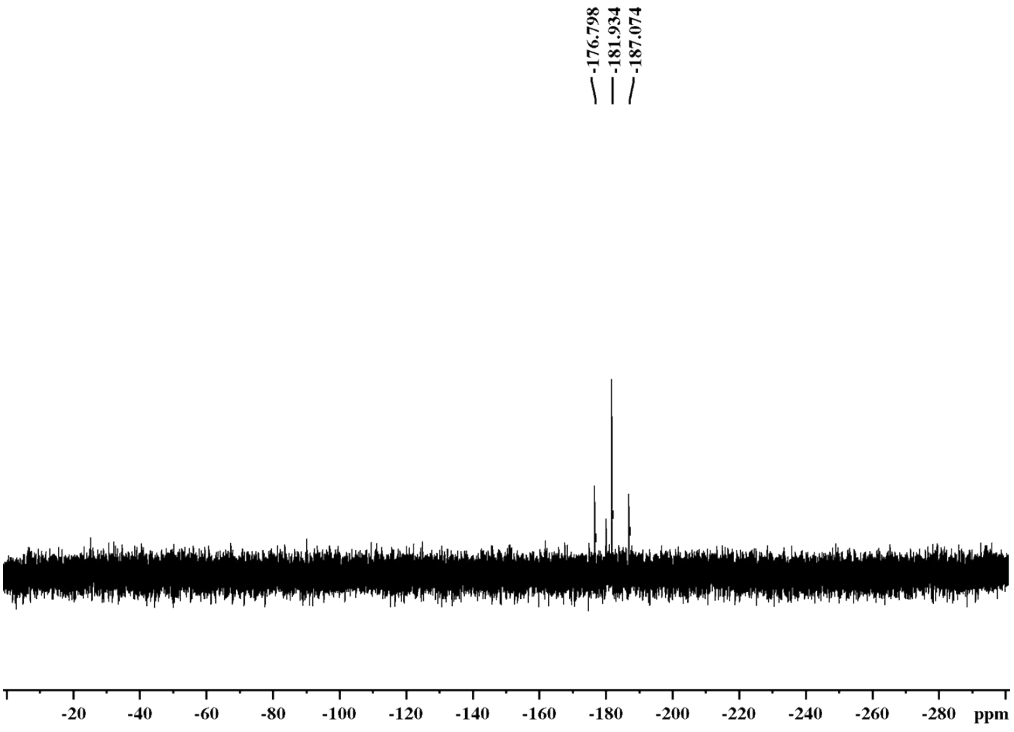


Figure S8. ^{31}P NMR spectrum of **2PF$_2$-I$_4$** (162 MHz, , Chloroform-*d*), 25 °C**.**

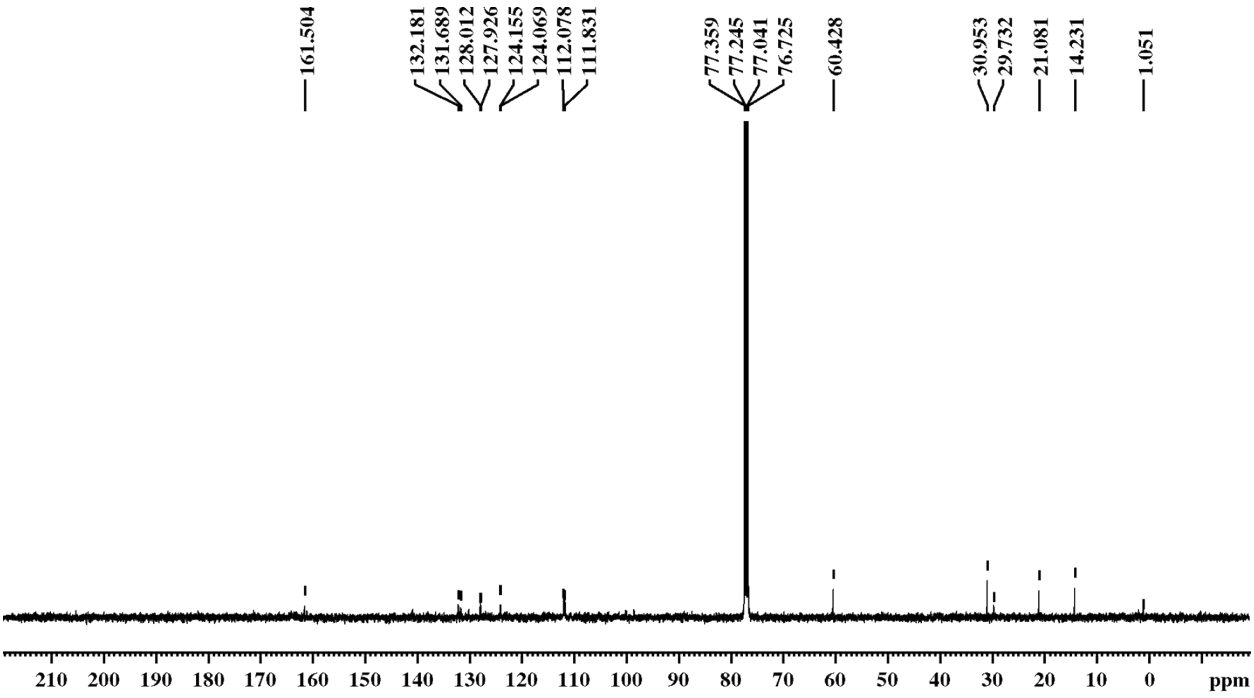


Figure S9. ^{13}C NMR spectrum of **2PF$_2$-I$_4$** (100.7 MHz, Chloroform-*d*), 25 °C**.**

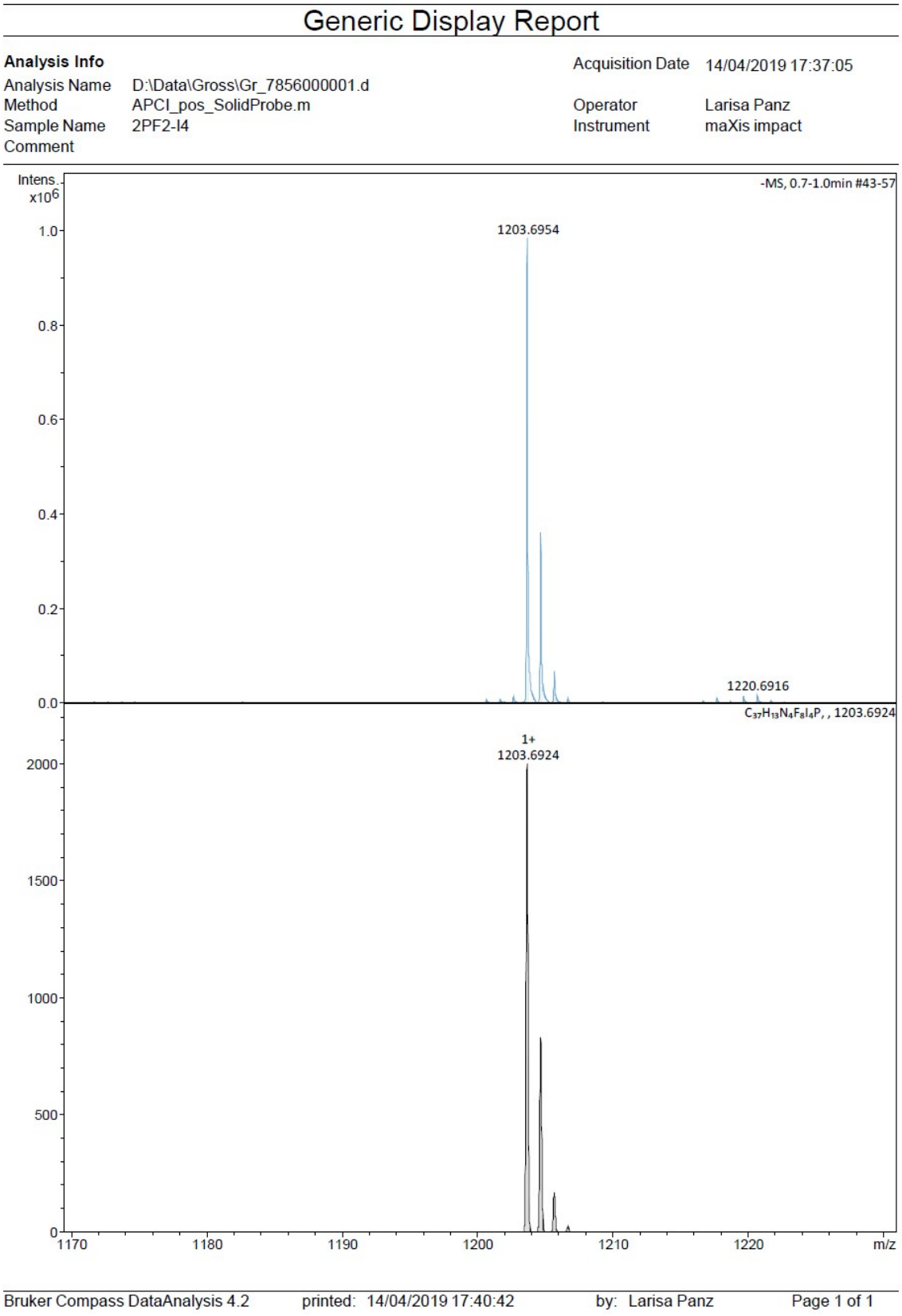


Figure S10. High resolution APCI$^+$ mass spectrum of compound **2PF$_2$-I$_4$**.

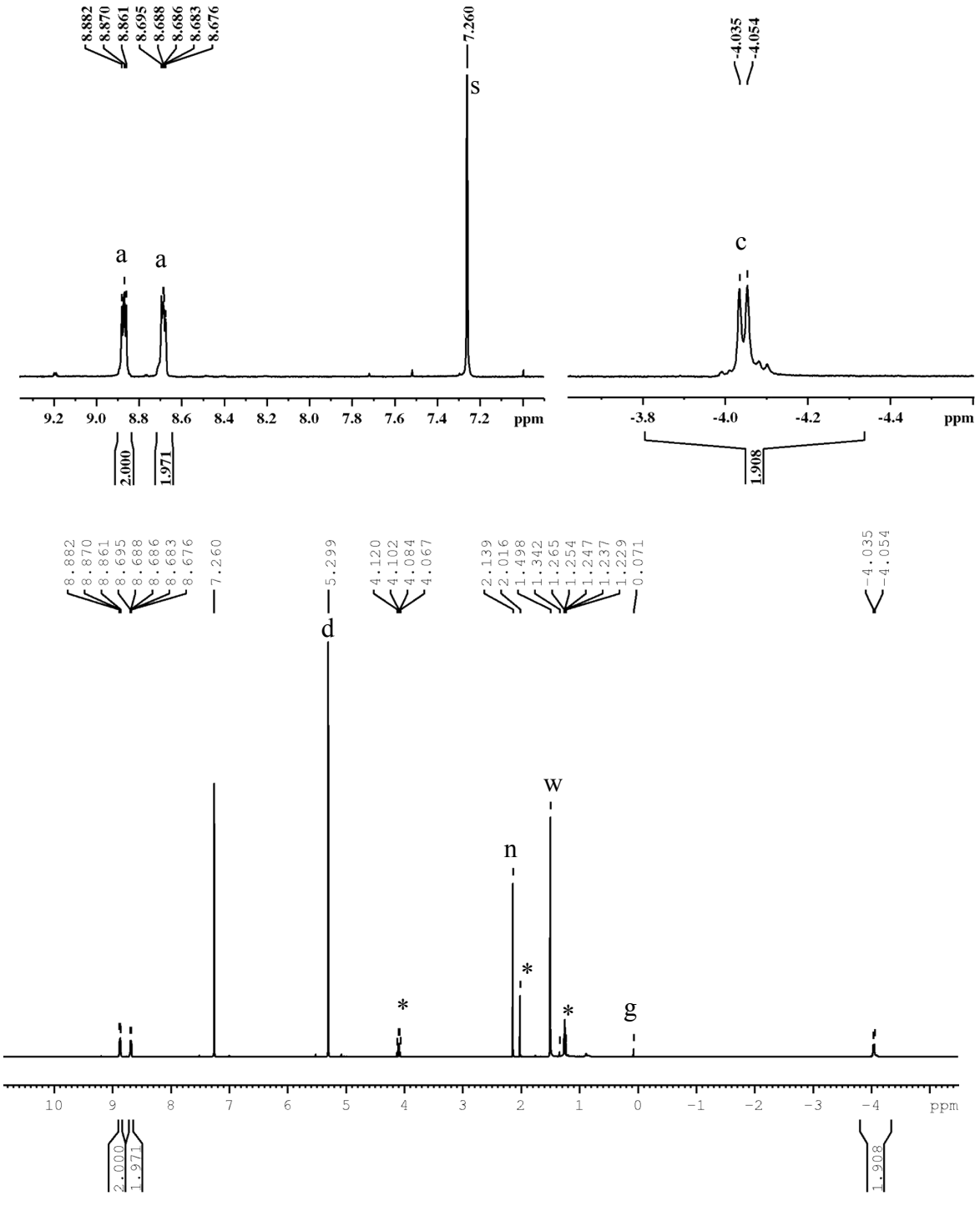


Figure S11. ^{1}H NMR spectrum of **1P(OH)$_2$-I$_4$** (400 MHz, Chloroform-*d*), 25 °C (residual solvents: s = $CHCl_3$, *= ethyl acetate, n = acetone, w = water, g = grease). a = β-pyrrole-H, c = OH axial ligands.

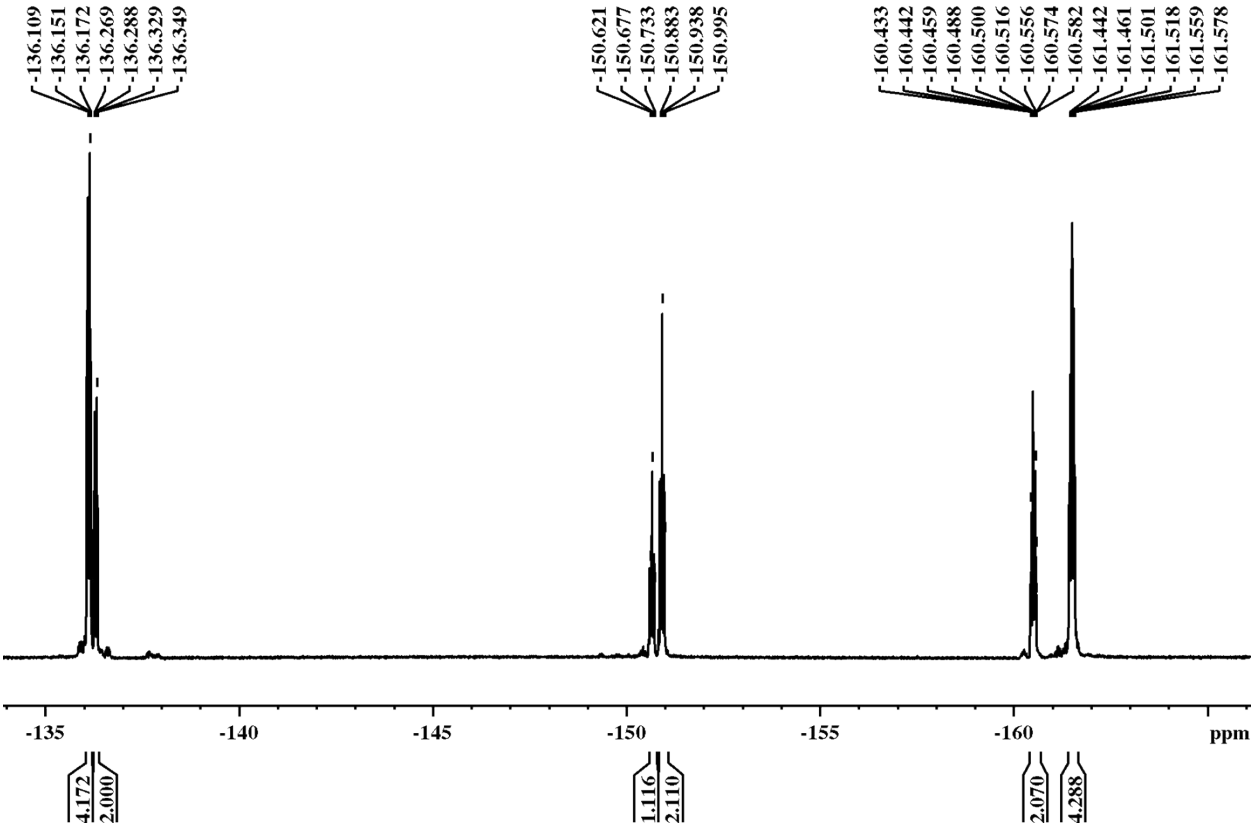


Figure S12. ^{19}F NMR spectrum of **1P(OH)$_2$-I$_4$** (377 MHz, , Chloroform-*d*), 25 °C**.**

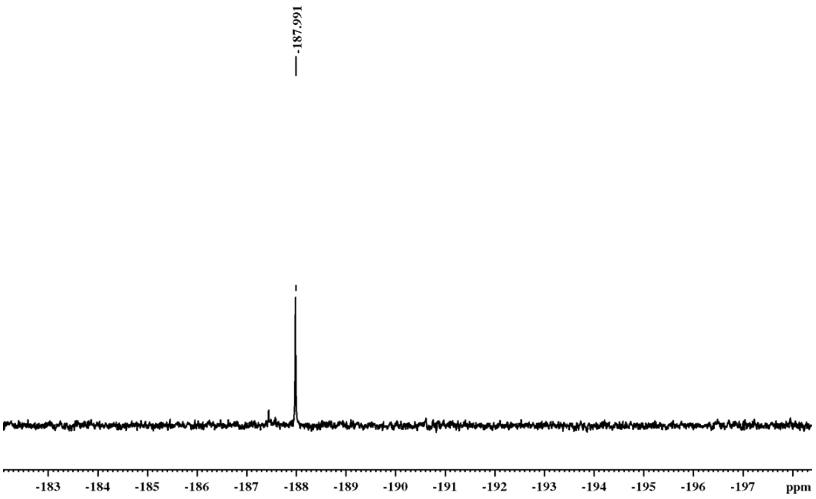


Figure S13. ^{31}P NMR spectrum of **1P(OH)$_2$-I$_4$** (162 MHz, , Chloroform-*d*), 25 °C**.**

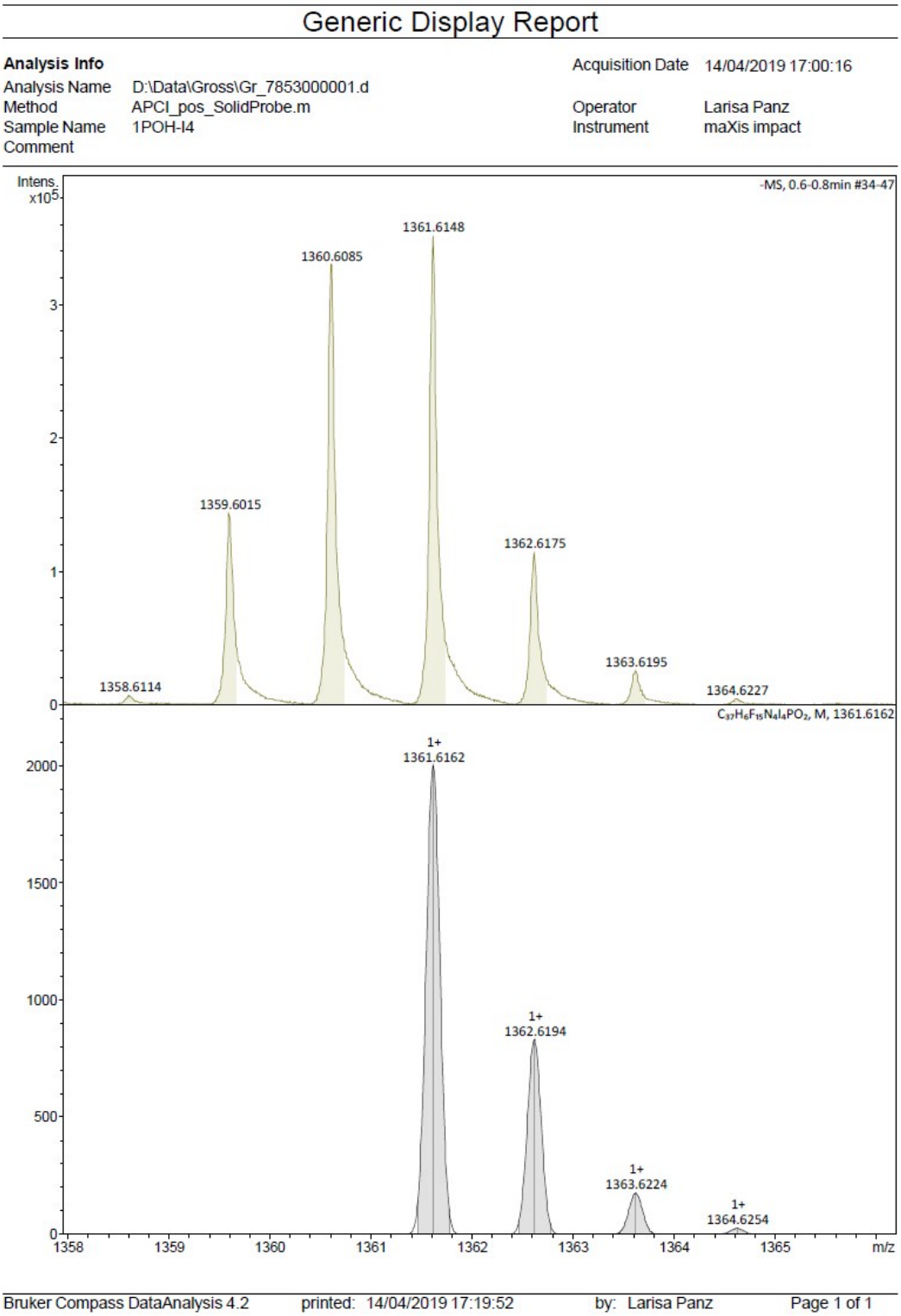


Figure S14. MR-MS High resolution APCI⁺ mass spectrum of compound **1P(OH)$_2$-I$_4$**.

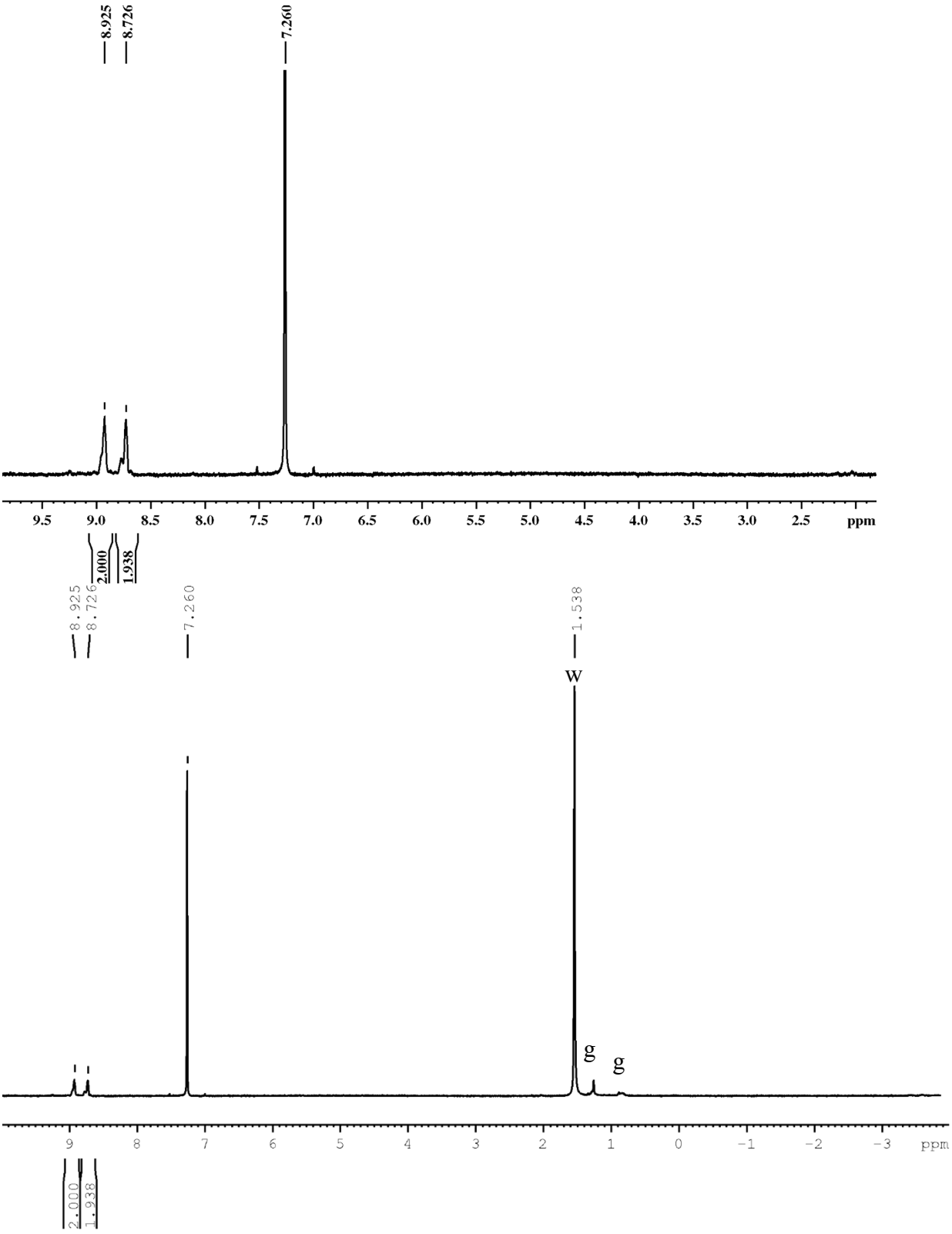


Figure S15. ^{1}H NMR spectrum of **1PF$_2$-I$_4$** (400 MHz, Chloroform-*d*), 25 °C (residual solvents: w = water, g = grease).

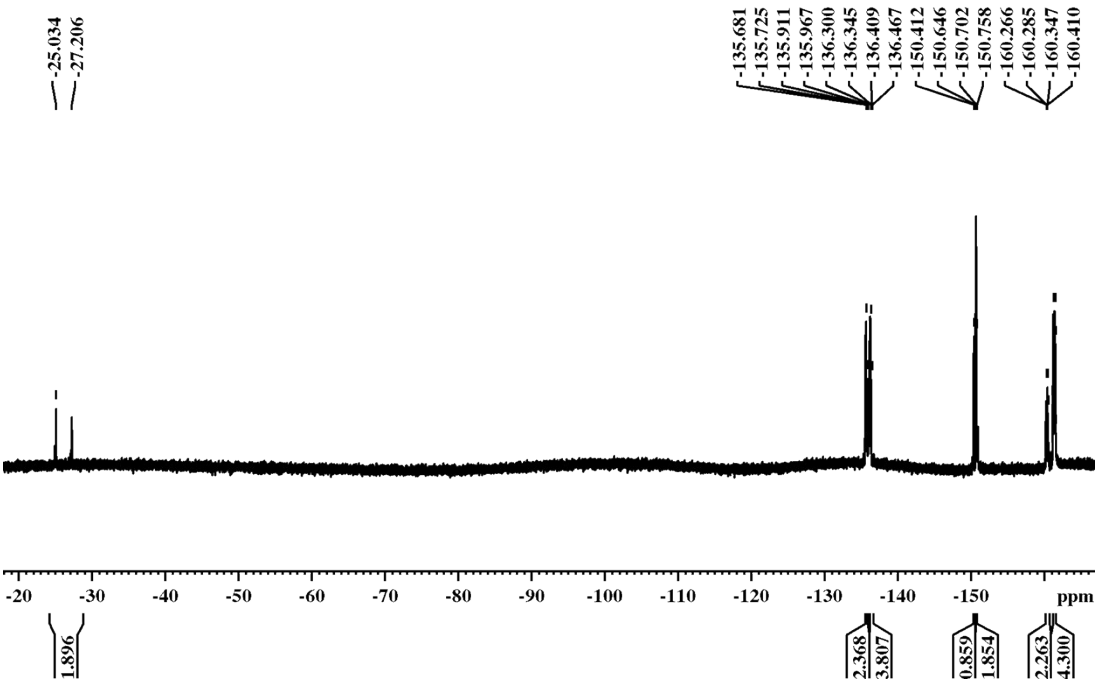


Figure S16. ^{19}F NMR spectrum of **$1PF_2$-I_4** (377 MHz, Chloroform-*d*), 25 °C.

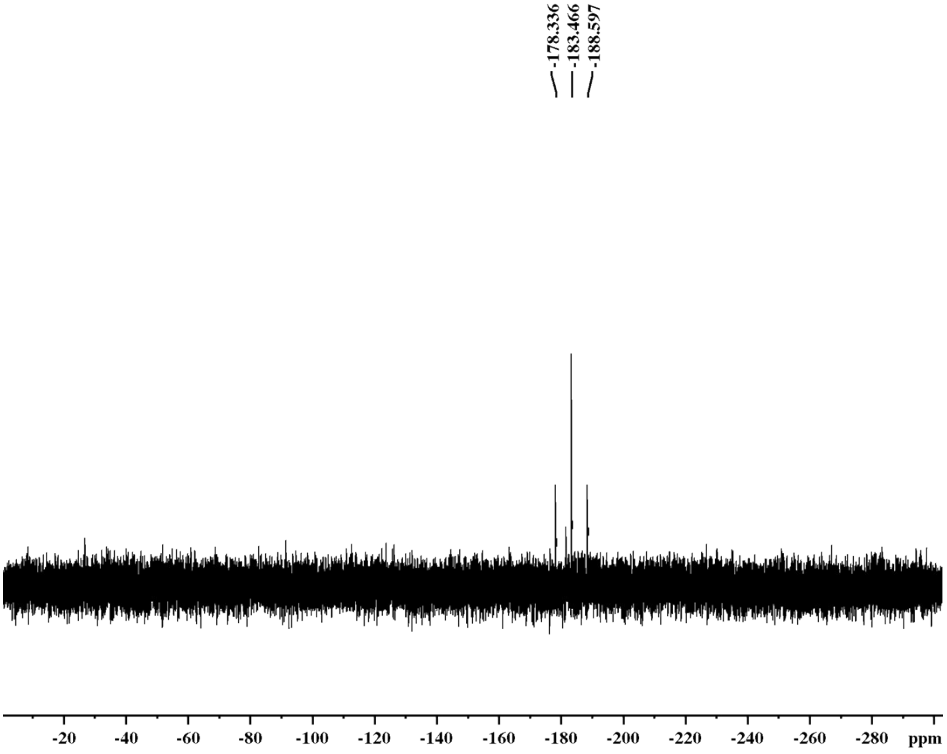


Figure S17. ^{31}P NMR spectrum of **$1PF_2$-I_4** (162 MHz, , Chloroform-*d*), 25 °C.

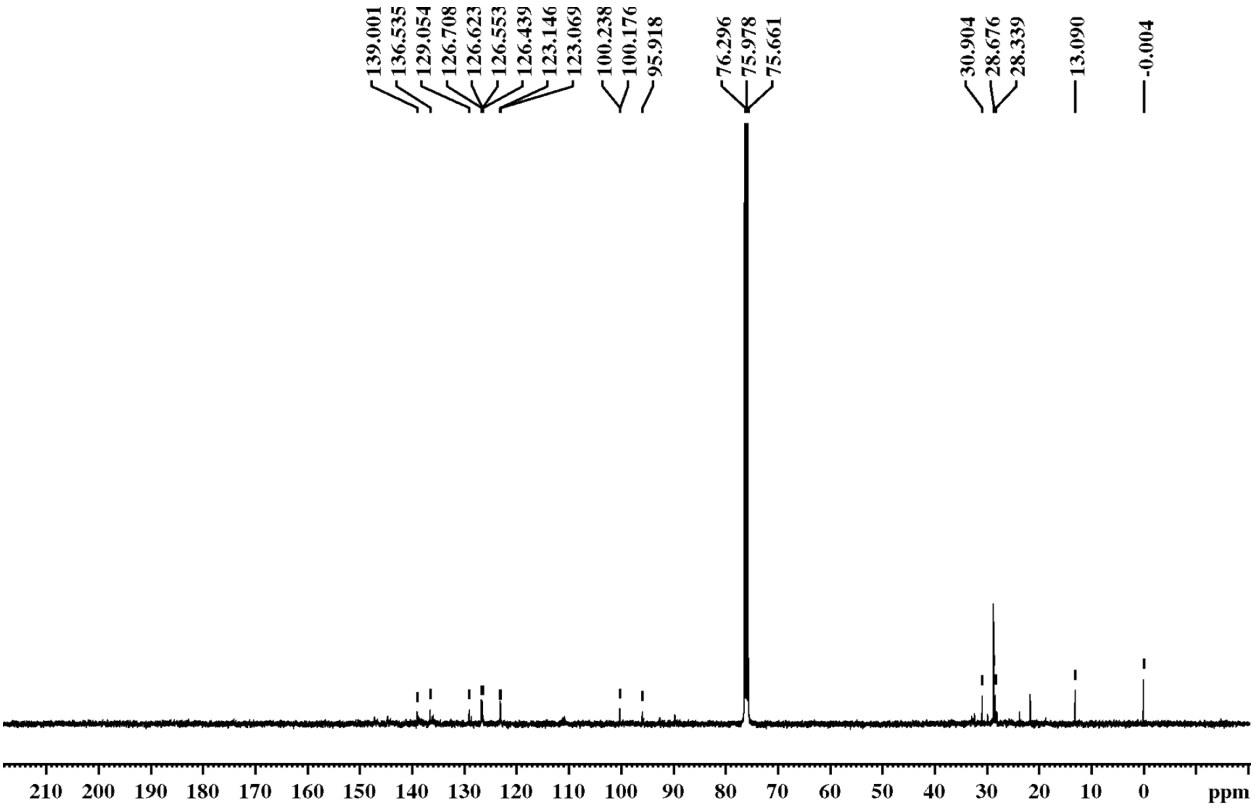


Figure S18. ^{13}C NMR spectrum of **1PF$_2$-I$_4$** (100.7 MHz, Chloroform-*d*), 25 °C**.**

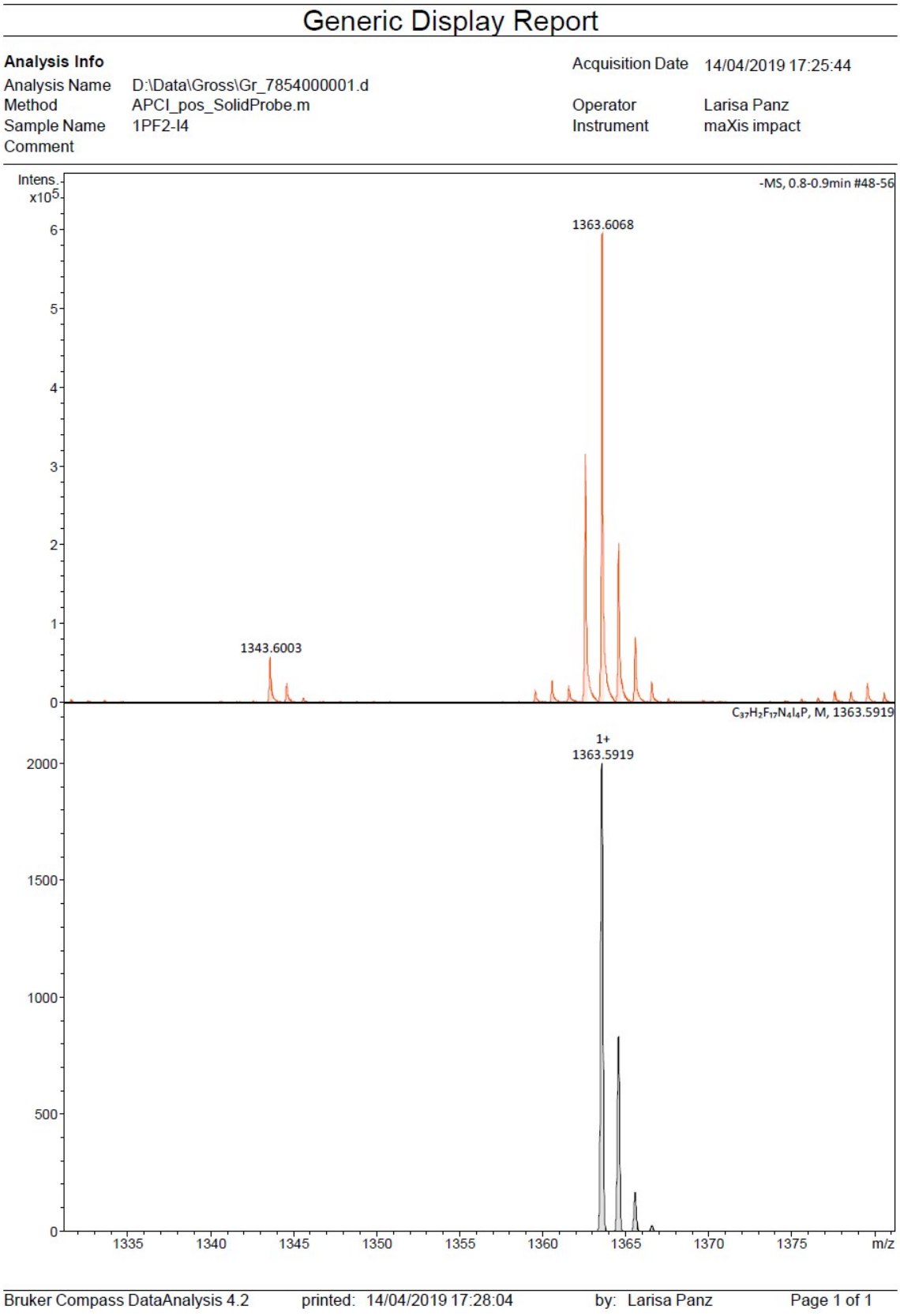


Figure S19. High resolution APCI⁺ mass spectrum of compound **1PF$_2$-I$_4$**.

2. HPLC separation

HPLC Column details:
HiCHROM; Packing: LiChrospher RP18-5 Endcapped; Length: 25 cm; i.d.: 4.6 mm; o.d. ¼").

Test Conditions:
Mobile phase: Acetonitrile/ water; Wavelength: 409 nm; Flow rate: 1.0 mL/min.

Time	Acetonitrile %	Water
0	20	80
3	100	0
5.5	100	0
5.6	20	80
13	20	80

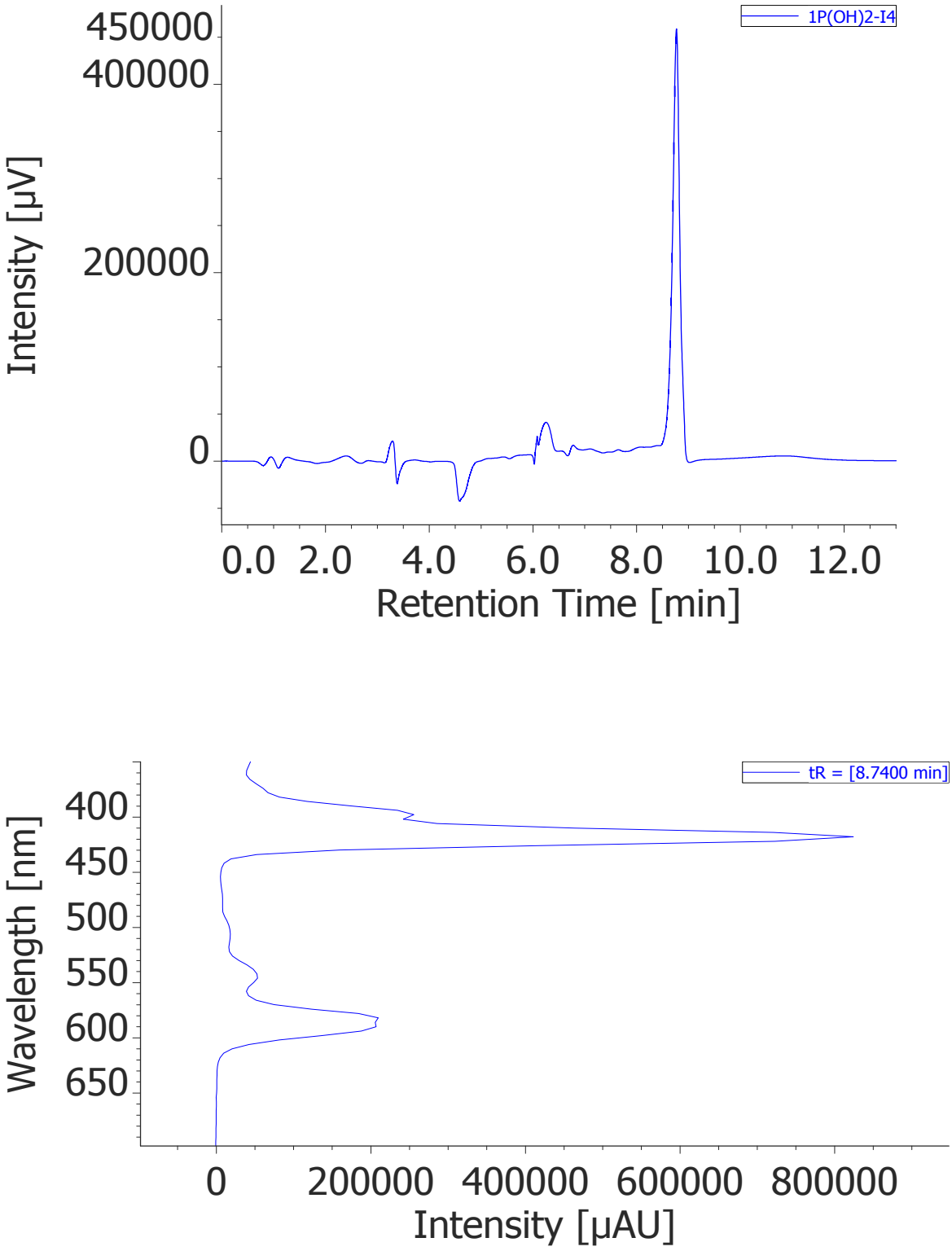


Figure S20. HPLC chromatogram of **1P(OH)$_2$-I$_4$** and the UV-vis spectrum recorded at the elution time 8.74 min.

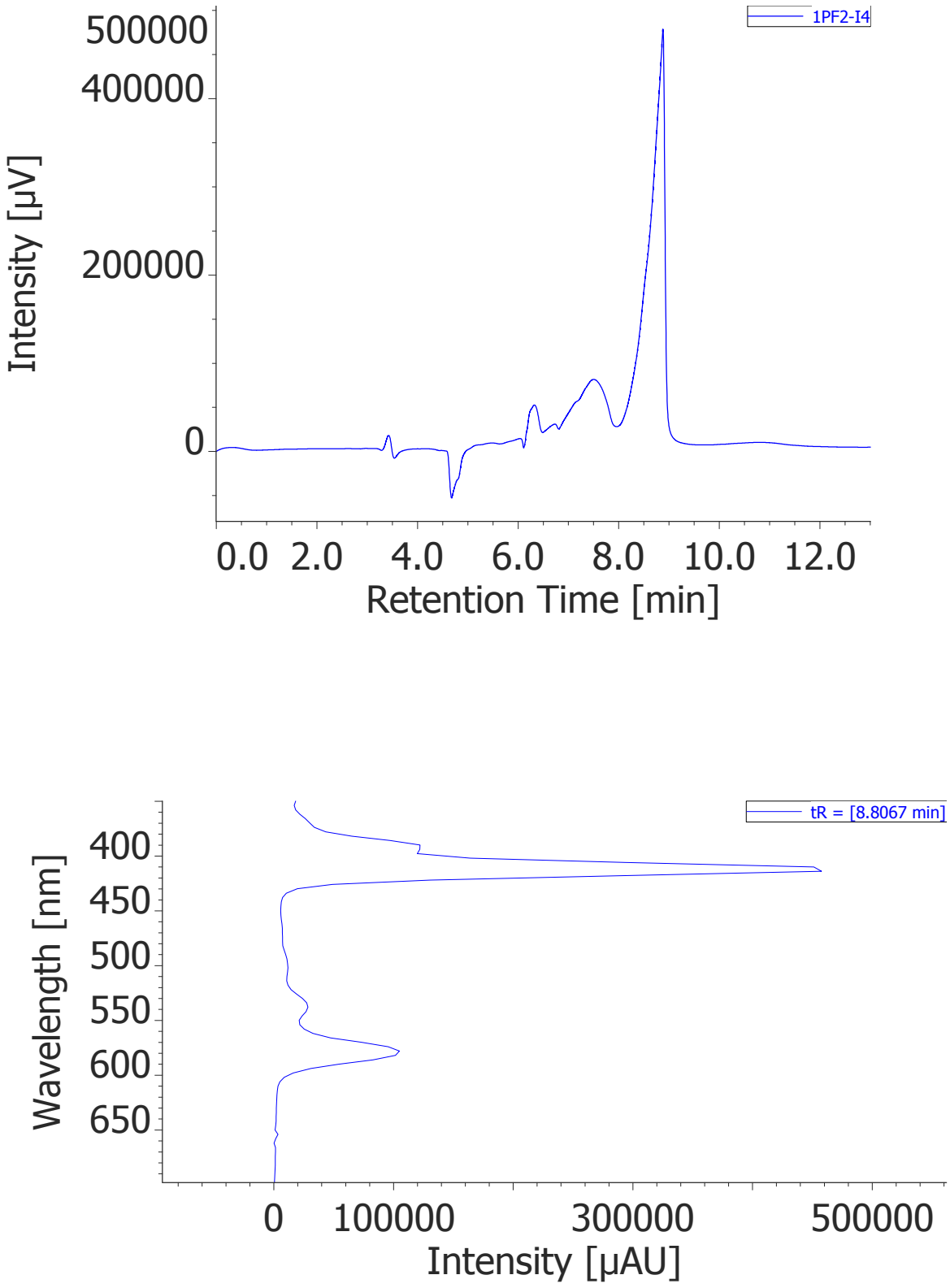
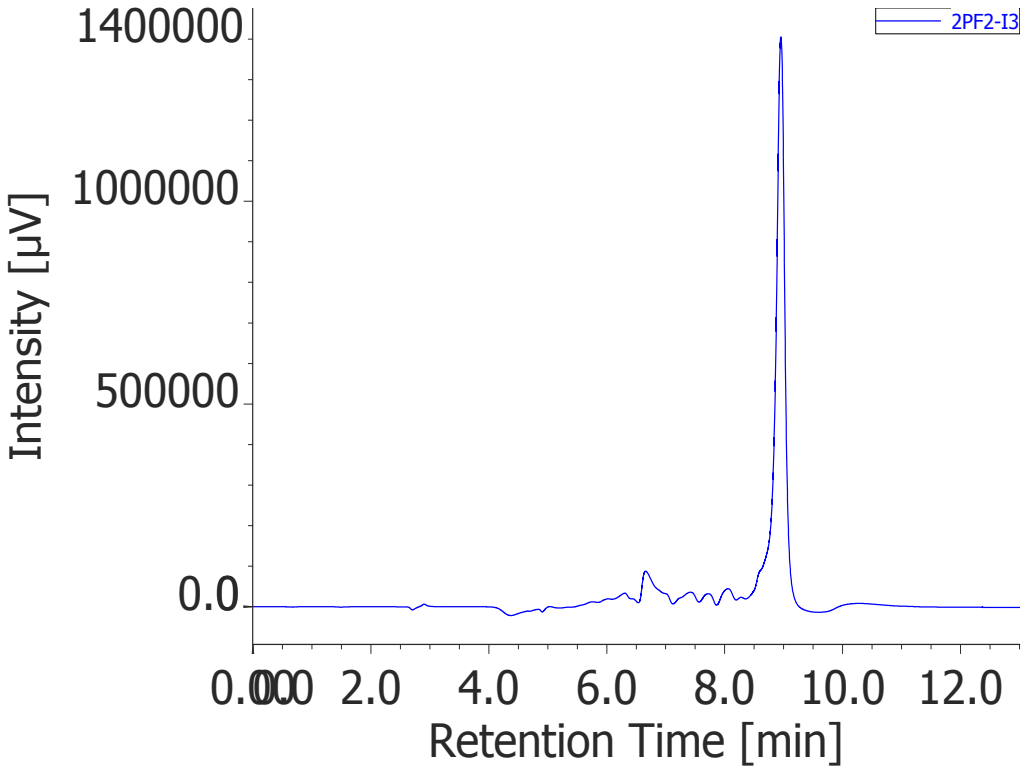


Figure S21. HPLC chromatogram of **1PF$_2$-I$_4$** and the UV-vis spectrum recorded at the elution time 8.80 min.



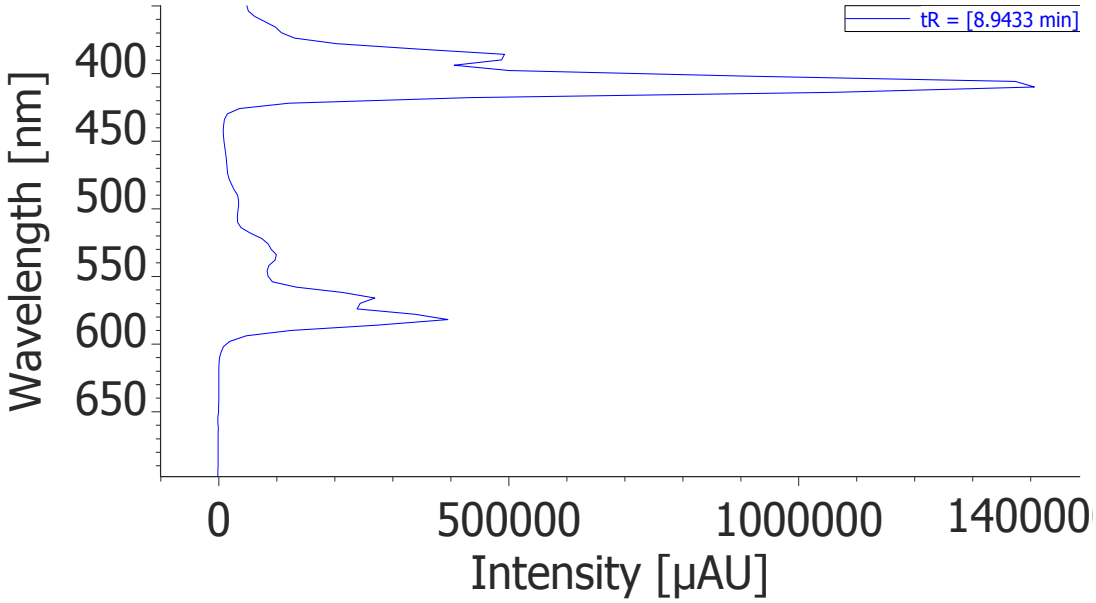


Figure S22. HPLC chromatogram of **$2PF_2$-I_3** and the UV-vis spectrum recorded at the elution time 8.94 min.

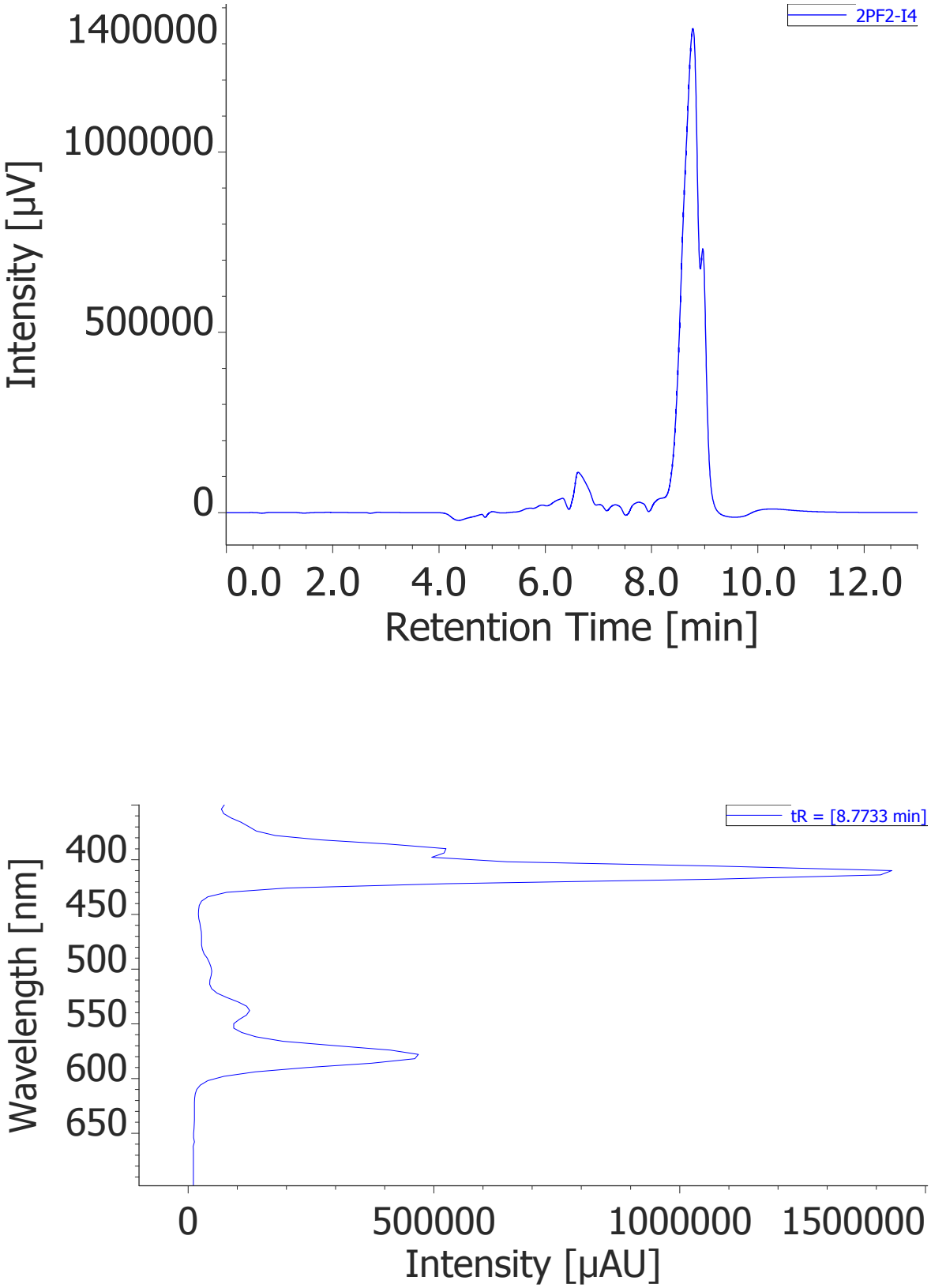


Figure S23. HPLC chromatogram of **$2PF_2$-I_4** and the UV-vis spectrum recorded at the elution time 8.77 min.

3. Stead-state UV–vis Absorption and Emission Spectra Measurement

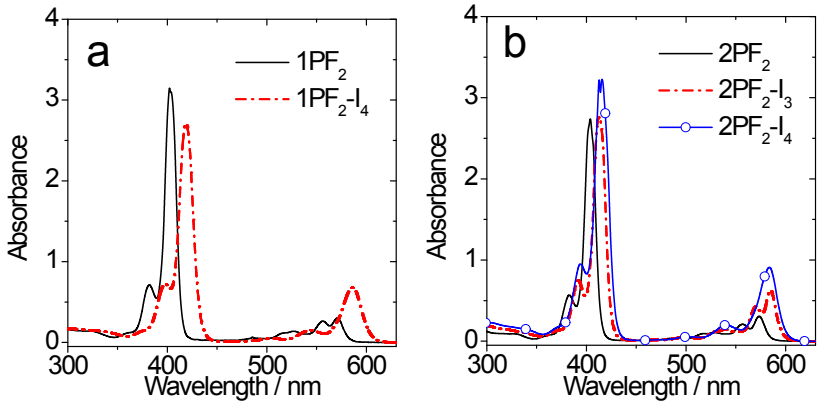


Figure S24. UV–Vis absorption spectra of (a) **$1BF_2$** and **$1BF_2$-I_4**; (b) **$2BF_2$, $2BF_2$-I_3** and **$2BF_2$-I_4** in DCM; $c = 1\times10^{-5}$ M, 20 °C.

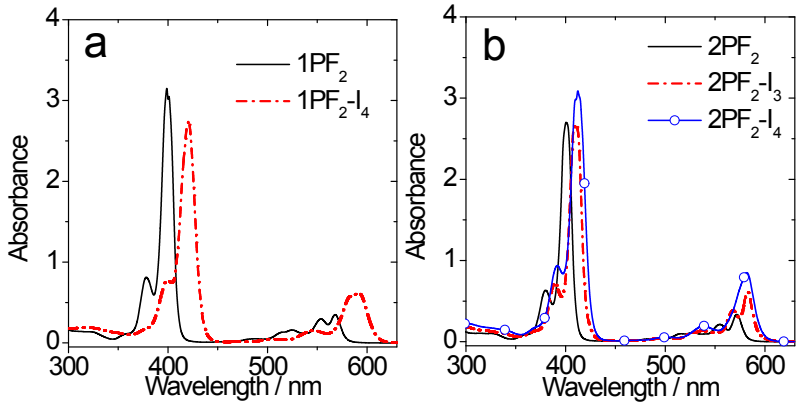


Figure S25. UV–Vis absorption spectra of (a) **$1BF_2$** and **$1BF_2$-I_4**; (b) **$2BF_2$, $2BF_2$-I_3** and **$2BF_2$-I_4** in MeOH; $c = 1\times10^{-5}$ M, 20 °C.

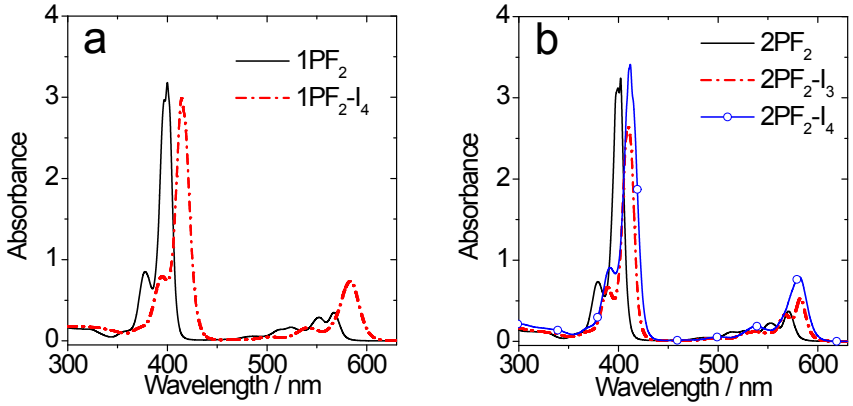


Figure S26. UV–Vis absorption spectra of (a) **$1BF_2$** and **$1BF_2$-I_4**; (b) **$2BF_2$, $2BF_2$-I_3** and **$2BF_2$-I_4** in CH_3CN; $c = 1\times10^{-5}$ M, 20 °C.

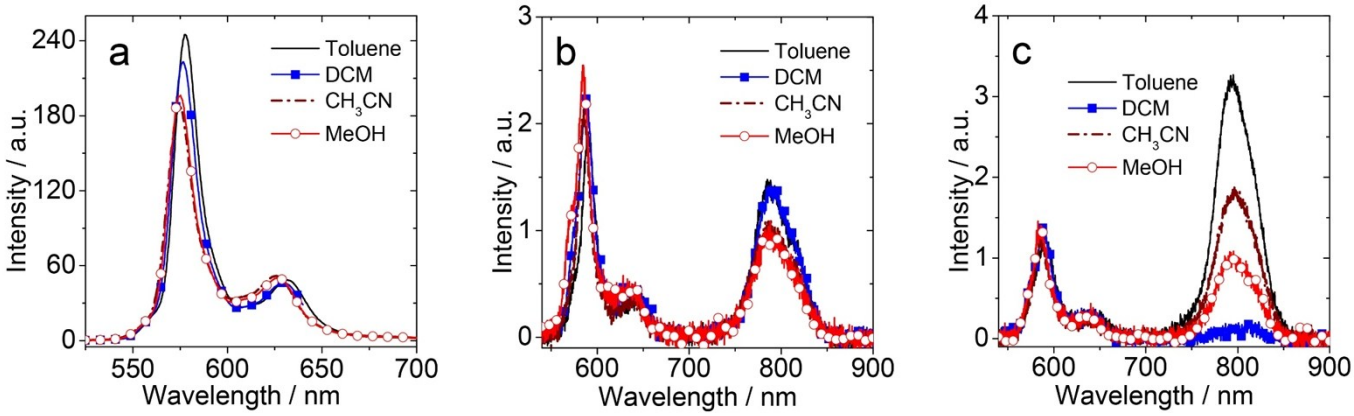


Figure S27. Fluorescence emission spectra of (a) **$2PF_2$**; (b) **$2PF_2$-I_3**; (c) **$2PF_2$-I_4** in different deaerated solvents. $A = 0.454$; $\lambda_{ex} = 410$ nm; Optically matched solutions were used, 20 °C.

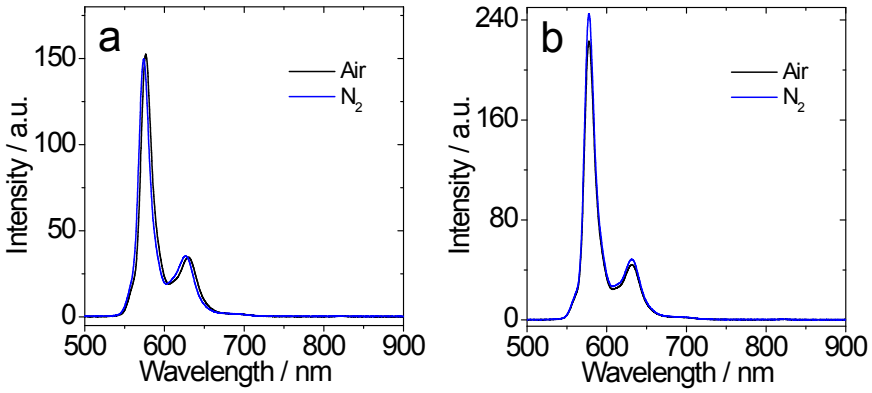


Figure S28. Fluorescence emission spectra of (a) **1PF$_2$**; (b) **2PF$_2$** in air and nitrogen saturated toluene. A = 0.454; λ_{ex} = 410 nm; Optically matched solutions were used, 20 °C.

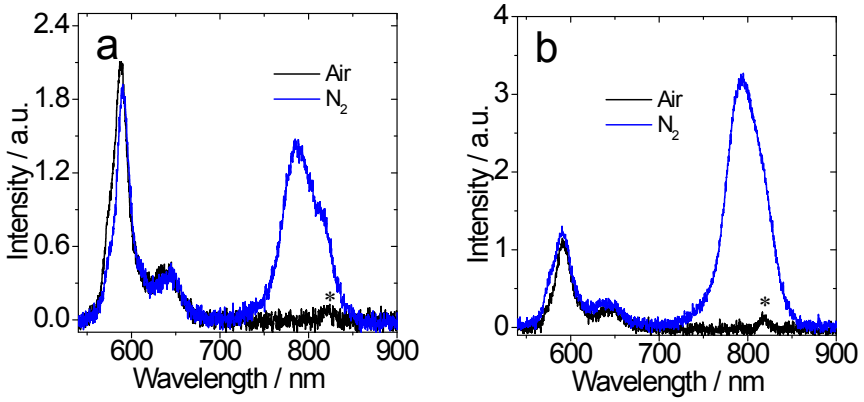


Figure S29. Fluorescence emission spectra of (a) **2PF$_2$-I$_3$**; (b) **2PF$_2$-I$_4$** in air and nitrogen saturated toluene. A = 0.454; λ_{ex} = 410 nm; "∗" was labeled as frequency doubling of excitation wavelength, optically matched solutions were used, 20 °C.

4. Luminescence Lifetimes and Fluorescence Decay Kinetics of the Compounds

Table S1. Luminescence lifetimes of the compounds [a]

	τ_L [b]	τ_L [c]	τ_L [d]	τ_L [e]
1PF$_2$	3.2 [f]	3.3 [f]	3.6 [f]	3.0 [f]
1PF$_2$-I$_4$	0.065 (64%), 3.0 (36%) [f]; 412 [g]	0.074 (37%), 3.0 (63%) [f]; 411 [g]	0.060 (99%), 5.5 (1%) [f]; 322 [g]	0.036 (45%), 3.4 (55%) [f]; 323 [g]
2PF$_2$	3.8 [f]	3.7 [f]	4.0 [f]	1.9 [f]
2PF$_2$-I$_3$	0.056 (86%), 3.1 (14%) [f]; 338 [g]	0.050 (97%), 3.4 (3%) [f]; 335 [g]	0.040 (98%), 3.9 (2%) [f]; 250 [g]	0.053 (96%), 3.6 (4%) [f]; 269 [g]
2PF$_2$-I$_4$	0.039 (97%), 4.1 (3%) [f]; 530 [g]	0.25 (87%), 4.1 (13%) [f]; 505 [g]	0.050 (67%), 3.5 (33%) [f]; 325 [g]	0.048 (96%), 3.4 (4%) [f]; 429 [g]

[a] $c = 1.0 \times 10^{-5}$ M, RT. [b] In toluene. [c] In DCM. [d] In CH_3CN. [e] In MeOH. [f] Fluorescence lifetimes (ns), in aerated solutions. [g] Phosphorescence lifetimes (μs), in deaerated solutions.

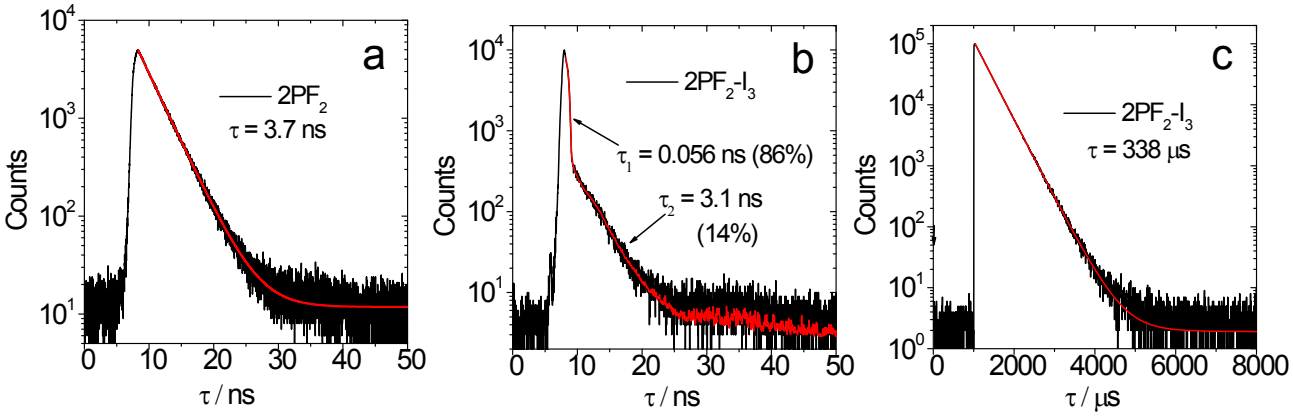


Figure S30. Decay traces of the luminescence of (a) **$2PF_2$** at 577 nm (fluorescence peak) in toluene; (b) **$2PF_2$-I_3** at 591 nm (fluorescence peak) in toluene; (c) **$2PF_2$-I_3** at 786 nm (phosphorescence peak) in deaerated toluene. Excited with picoseconds pulsed laser for fluorescence peak and λ_{ex} = 405 nm, excited with microseconds pulsed laser for phosphorescence peak and λ_{ex} = 420 nm, $c = 1.0 \times 10^{-5}$, 20 °C.

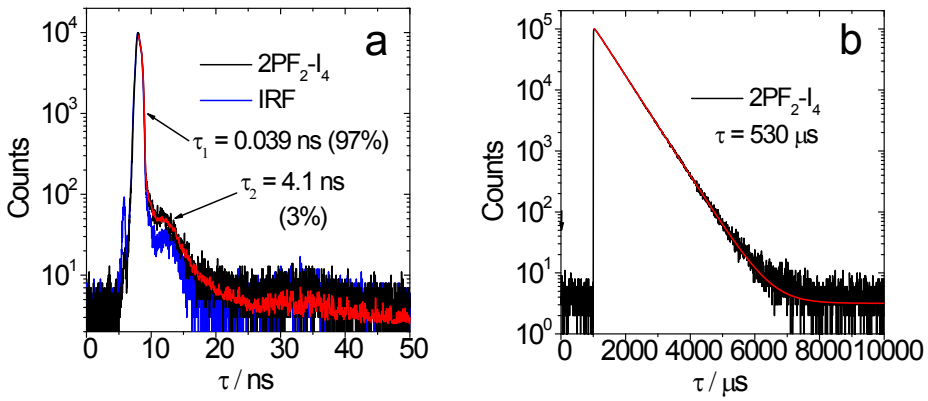


Figure S31. Decay traces of the luminescence of (a) **$2PF_2$-I_4** at 591 nm (fluorescence peak) in toluene; (c) **$2PF_2$-I_4** at 795 nm (phosphorescence peak) in deaerated toluene. Excited with picoseconds pulsed laser for fluorescence peak and λ_{ex} = 405 nm, excited with microseconds pulsed laser for phosphorescence peak and λ_{ex} = 420 nm, c = 1.0 × 10^{-5}, 20 °C.

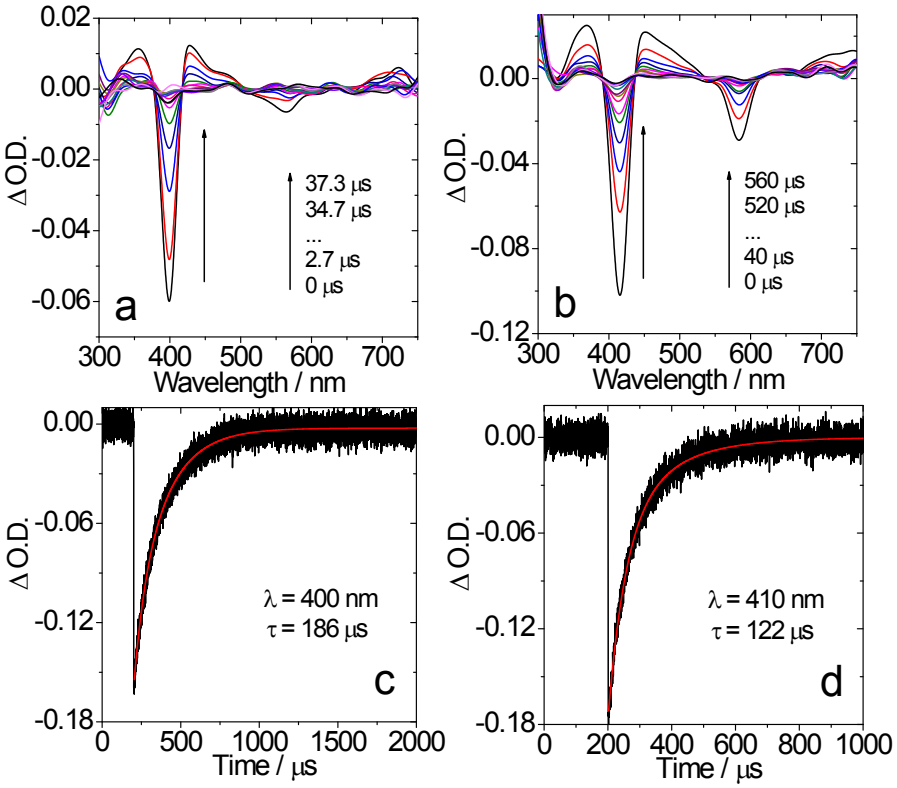


Figure S32. Nanosecond transient absorption spectra of (a) **1PF$_2$** (λ_{ex} = 556 nm), (b) **1PF$_2$-I$_4$** (λ_{ex} = 589 nm); Decay trace of (c) **1PF$_2$** at 400 nm, (d) **PF$_2$-I$_4$** at 410 nm. $c = 2.5 \times 10^{-6}$ M in deaerated CH_3CN, 20 °C.

5. Nanosecond Transient Absorption Spectra

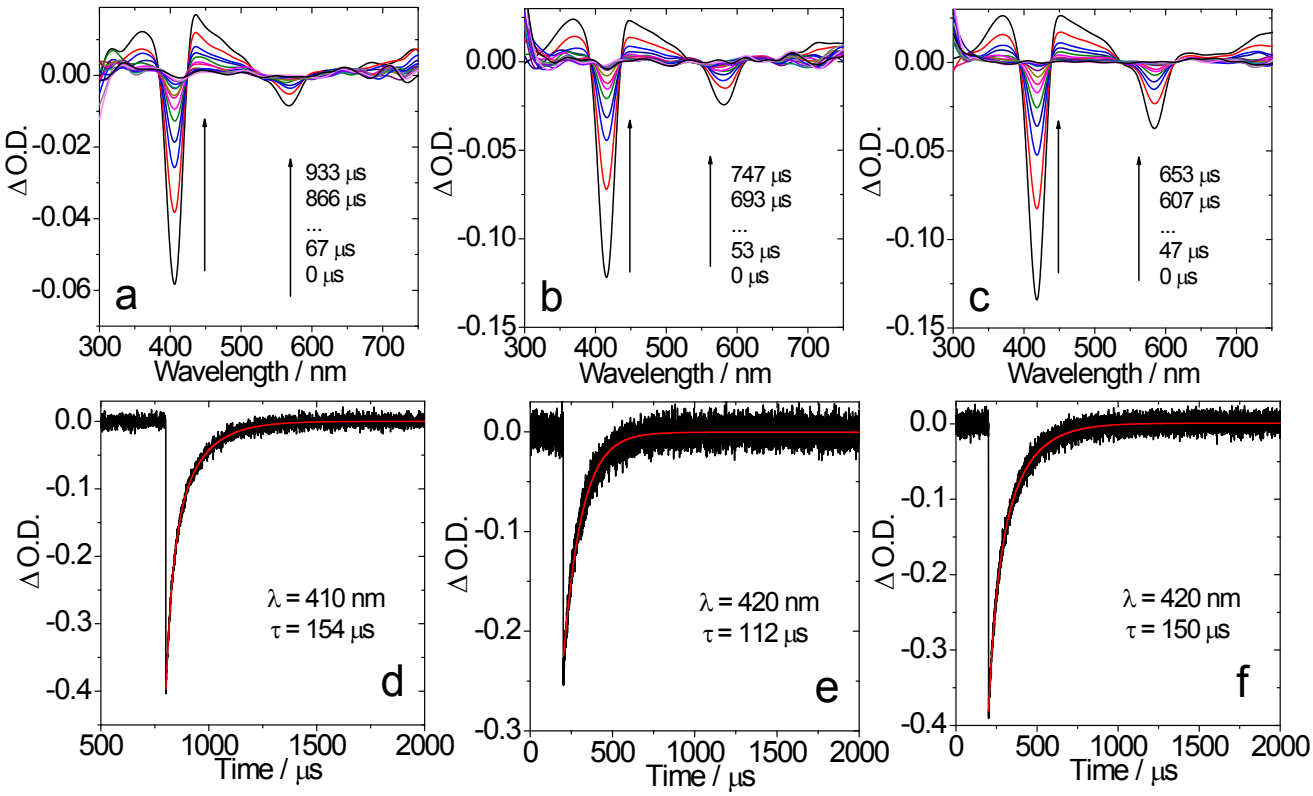


Figure S33. Nanosecond transient absorption spectra of (a) **2PF$_2$** (λ_{ex} = 576 nm), (b) **2PF$_2$-I$_3$** (λ_{ex} = 587 nm), (c) **2PF$_2$-I$_4$** (λ_{ex} = 587 nm); Decay trace of (d) **2PF$_2$** at 410 nm, (e) **2PF$_2$-I$_3$** at 420 nm, (f) **2PF$_2$-I$_4$** at 420 nm, c = 2.5 × 10^{-6} M in deaerated toluene, 20 °C.

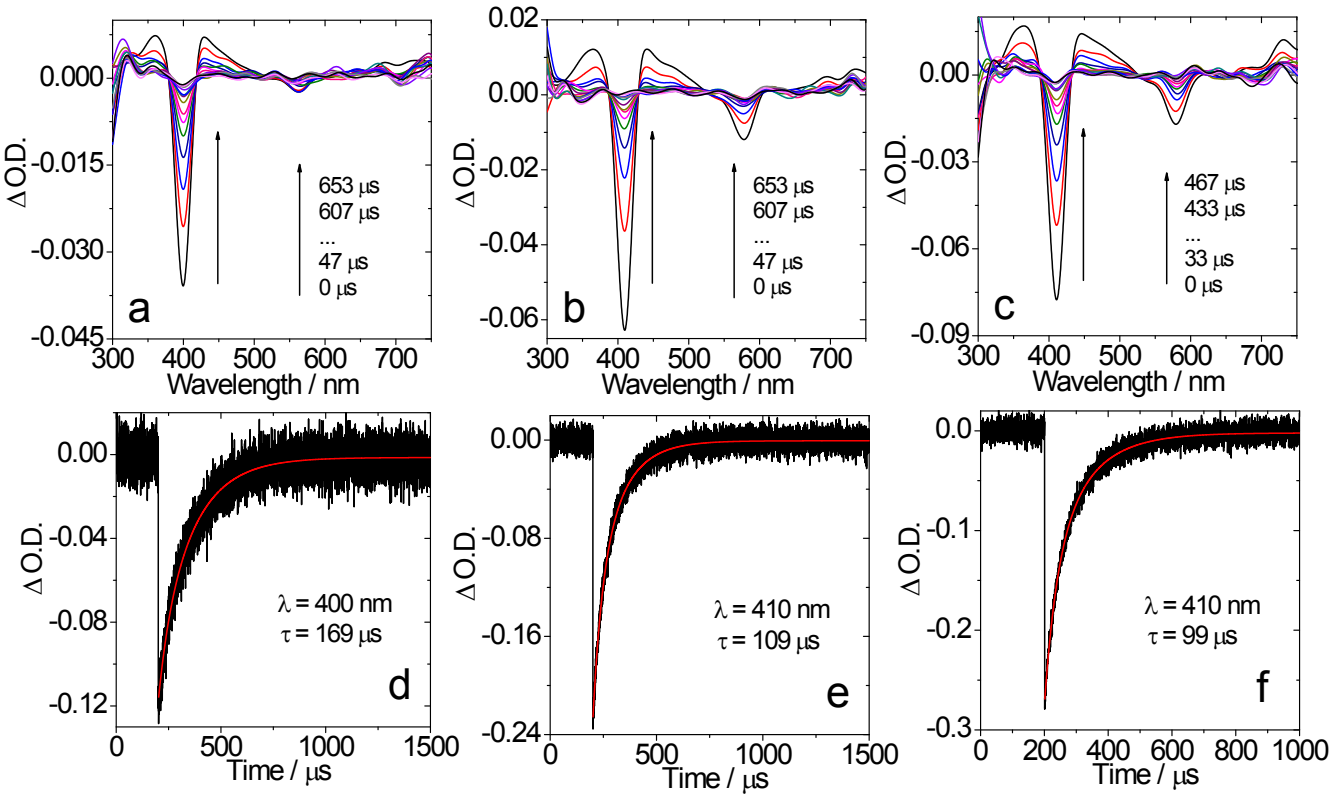


Figure S34. Nanosecond transient absorption spectra of (a) **2PF$_2$** (λ_{ex} = 576 nm), (b) **2PF$_2$-I$_3$** (λ_{ex} = 587 nm), (c) **2PF$_2$-I$_4$** (λ_{ex} = 587 nm); Decay trace of (d) **2PF$_2$** at 400 nm, (e) **2PF$_2$-I$_3$** at 420 nm, (f) **2PF$_2$-I$_4$** at 420 nm, c = 2.5 × 10^{-6} M in deaerated CH_3CN, 20 °C.

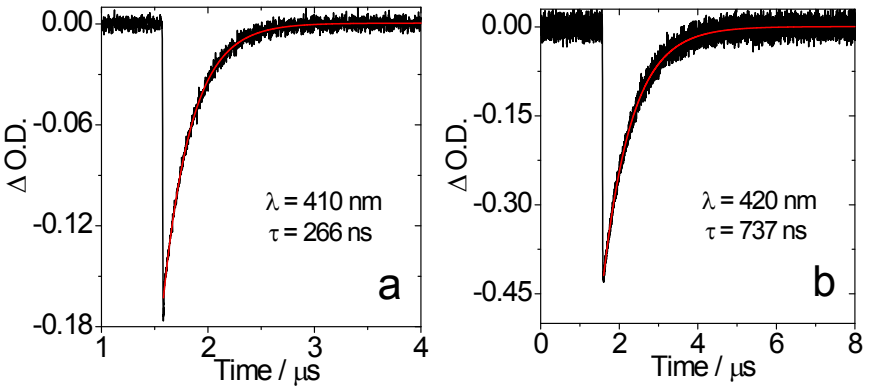


Figure S35. Decay trace of (a) **1PF$_2$** at 410 nm, λ_{ex} = 556 nm; (b) **1PF$_2$-I$_4$**, at 420 nm, λ_{ex} = 589 nm; c = 2.5 × 10^{-6} M in air toluene, 20 °C.

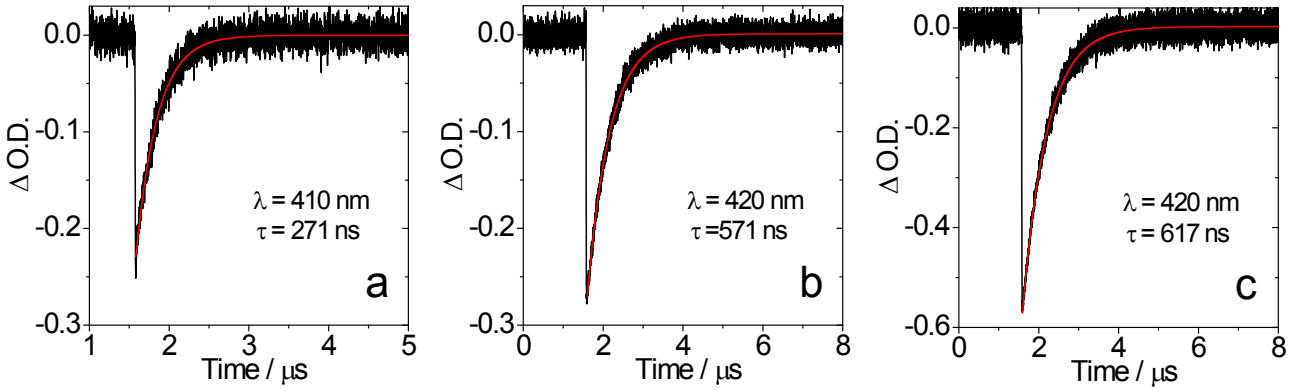


Figure S36. Decay trace of (a) **2PF$_2$** at 410 nm (λ_{ex} = 576 nm); (b) **2PF$_2$-I$_3$** at 420 nm (λ_{ex} = 587 nm); (c) **2PF$_2$-I$_4$** at 420 nm (λ_{ex} = 587 nm); c = 2.5 × 10^{-6} M in air toluene, 20 °C.

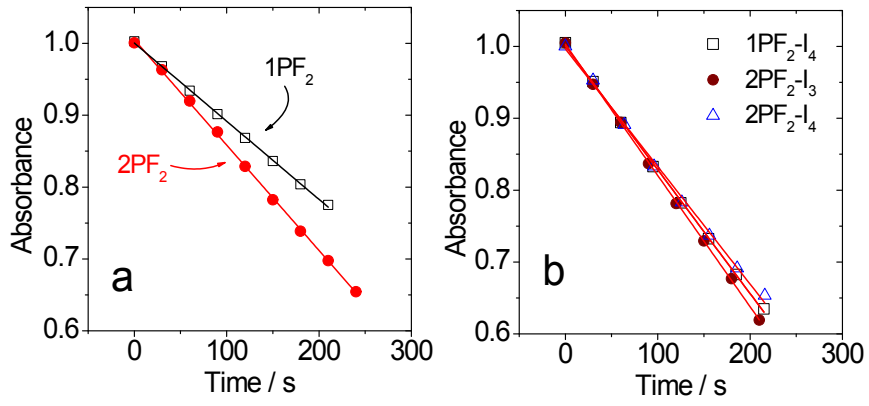


Figure S37. Comparison of the singlet oxygen ($^1O_2$) photosensitizing of (a) **$1PF_2$** and **$2PF_2$**. (b) **$1PF_2$-I_4**, **$2PF_2$-I_3**, and **$2PF_2$-I_4**. The absorption of photosensitizers at 414 nm was used as background. Xenon lamp was used as light source, λ_{ex} = 400 nm, optically matched solutions were used. In toluene. 20 °C.

6. Photoreduction of Corroles Added with Et_3N

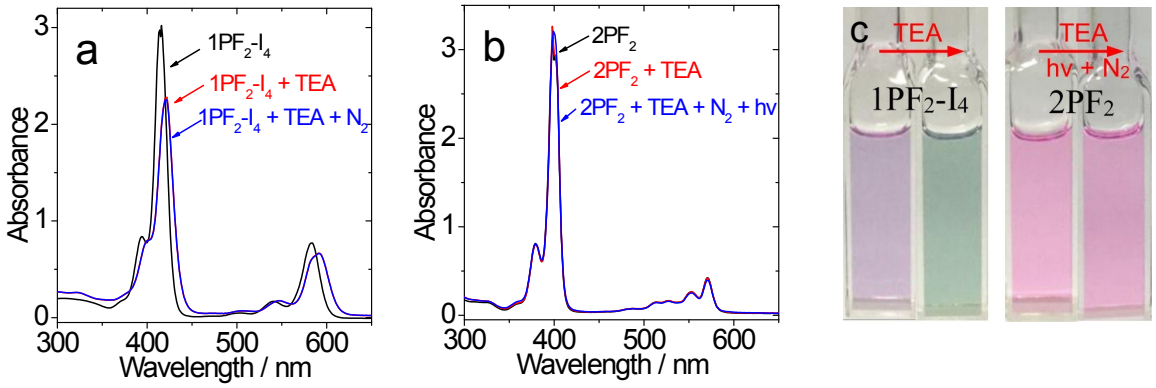


Figure S38. (a) UV–Vis absorption spectra of $\mathbf{1PF_2\text{-}I_4}$ in deaerated MeCN without irradiation; (b) UV-Vis absorption spectra of $\mathbf{2PF_2}$ in the deaerated MeCN upon photoirradiation; (c) Photos showing the color change of the $\mathbf{1PF_2\text{-}I_4}$ and $\mathbf{2PF_2}$. c [$\mathbf{1PF_2\text{-}I_4}$] = 1×10^{-5} M, c [$\mathbf{2PF_2}$] = 1×10^{-5} M, c [Et_3N] = 0.25 M. A xenon lamp was used to photoirradiated $\mathbf{2PF_2}$, photoirradiation power density is 23 mW/cm^2.

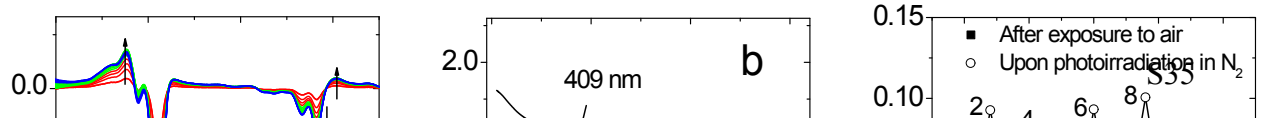
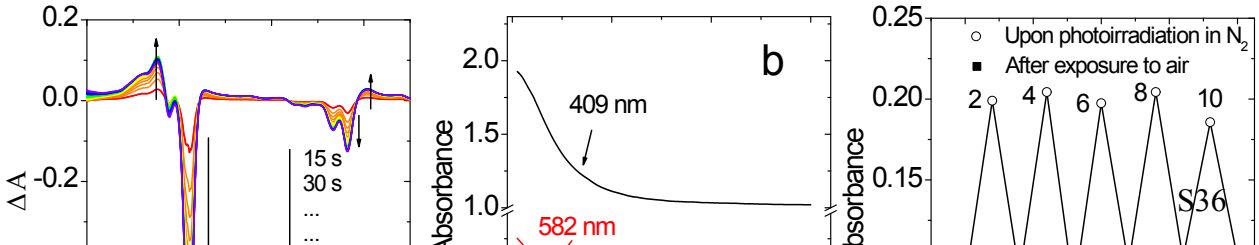


Figure S39. (a) UV–Vis difference absorption spectra of **$2PF_2$-I_3** in the presence of Et_3N in the deaerated MeCN with the photoirradiation by a xenon lamp, photoirradiation power density is 5.2 mW/cm^2. (b) Kinetic absorption plot of **$2PF_2$-I_3** at different wavelengths. (c) Reversibility of the formation of anion monitored at the 605 nm absorption band, Photoirradiation power density is 23 mW/cm^2; (d) The corresponding UV-Vis absorption spectra of (c) for the first 5 points showing the first 2 reversible cycles; (e) Photos showing the color change of the **$2PF_2$-I_3** and TEA mixed solution: 1. Without photoirradiation in the air; 2. Upon 8 seconds photoirradiation in the N_2; 3. Exposure to air without photoirradiation; 4. Upon another 8 seconds photoirradiation in the N_2. c [**$2PF_2$-I_3**] = 1×10^{-5} M, c [Et_3N] = 0.25 M.



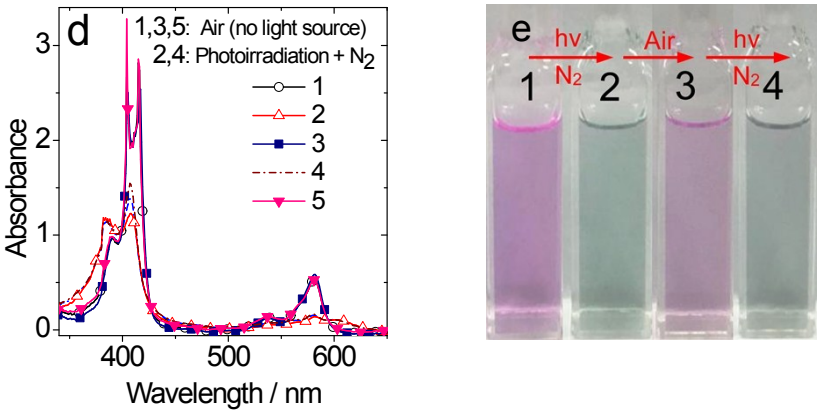


Figure S40. (a) UV-Vis difference absorption spectra of **$2PF_2$-I_4** in the presence of Et_3N in the deaerated MeCN with the photoirradiation by a xenon lamp, photoirradiation power density is 5.2 mW/cm^2. (b) Kinetic absorption plot of **$2PF_2$-I_4** at different wavelengths. (c) Reversibility of the formation of anion monitored at the 605 nm absorption band, Photoirradiation power density is 23 mW/cm^2; (d) The corresponding UV-Vis absorption spectra of (c) for the first 5 points showing the first 2 reversible cycles; (e) Photos showing the color change of the **$2PF_2$-I_4** and TEA mixed solution: 1. Without photoirradiation in the air; 2. Upon 8 seconds photoirradiation in the N_2; 3. Exposure to air without photoirradiation; 4. Upon another 8 seconds photoirradiation in the N_2. c [**$2PF_2$-I_4**] = 1×10^{-5} M, c [Et_3N] = 0.25 M.

7. TTA Upconversion

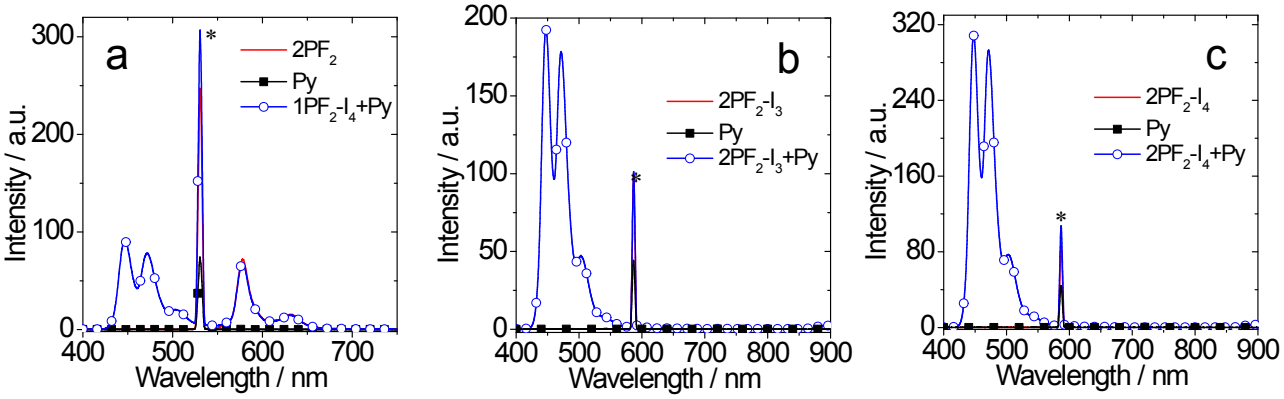


Figure S41. The upconversion fluorescence spectra of (a) **$2PF_2$**, (b) **$2PF_2$-I_3** and (c) **$2PF_2$-I_4** as photosensitizer in toluene. **Py** (perylene) was the acceptor. Excitation was done with a continuous laser of 532 nm for **$2PF_2$** and 589 nm for **$2PF_2$-I_3**, **$2PF_2$-I_4**. The power density is 70.6 mW/cm^2 under deaerated atmosphere. *c* (Sensitizer) = 2.0×10^{-6} M, *c* (**Py**) were 2.4×10^{-5} M, 2.8×10^{-5} M and 3.0×10^{-5} M, respectively, 20 °C.

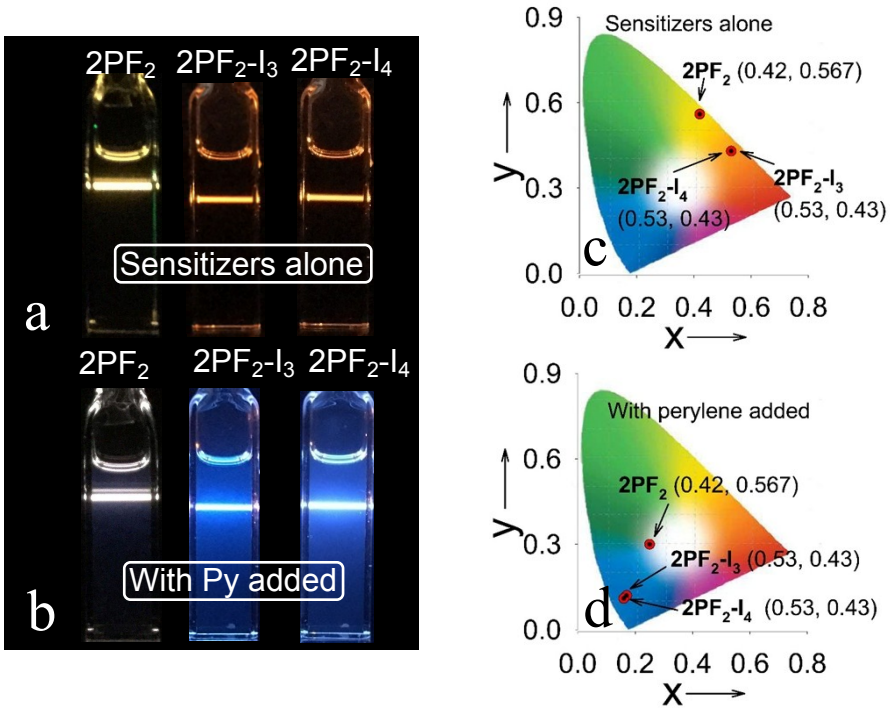


Figure S42. Photographs of (a) the emission of sensitizers alone and (b) the upconversion in toluene. The CIE coordinate changes of triplet sensitizers (**2PF$_2$**, **2PF$_2$-I$_3$**, **2PF$_2$-I$_4$**) (c) before and (d) after adding **Py**. Excitation was done with a continuous laser of 532 nm for **2PF$_2$** and 589 nm for **2PF$_2$-I$_3$**, **2PF$_2$-I$_4$**. The power density both were 4.8 mW under deaerated toluene. *c* (Sensitizers) = 2.0×10^{-6} M. **Py** were added with 2.3×10^{-5} M, 2.8×10^{-5} M and 3.0×10^{-5} M, respectively, 20 °C.

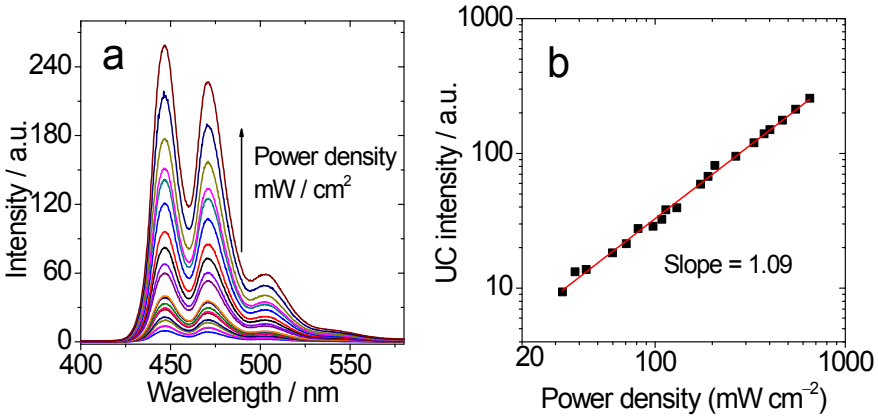


Figure S43. (a) Upconverted luminescence spectra of **$2PF_2$-I_4** and Perylene upon excitation with a CW 589 nm laser at different incident power densities. (b) Upconversion emission intensity data from part (a) plotted as a function of incident power density. All spectra are measured in deaerated toluene. c (**$2PF_2$-I_4**) = 2.0×10^{-6} M, c (perylene) = 3.0×10^{-5} M. 20 °C.

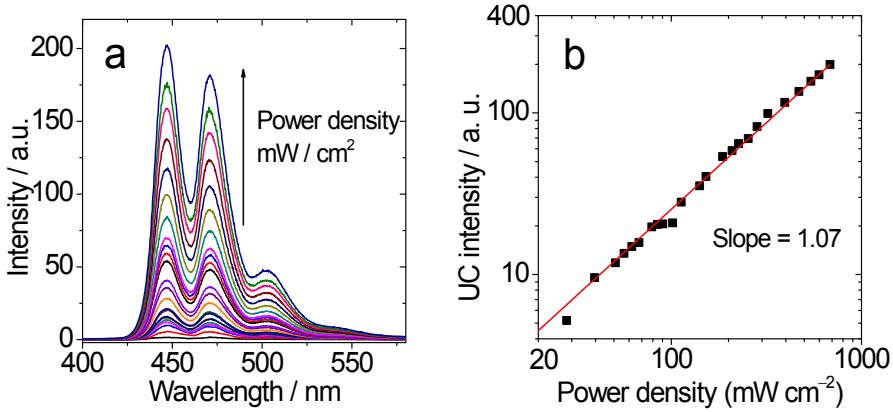


Figure S44. (a) Upconverted luminescence spectra of **$1PF_2$-I_4** and Perylene upon excitation with a CW 589 nm laser at different incident power densities. (b) Upconversion emission intensity data from part (a) plotted as a function of incident power density. All spectra are measured in deaerated toluene. c (**$1PF_2$-I_4**) = 2.0×10^{-6} M, c (perylene) = 2.8×10^{-5} M. 20 °C.

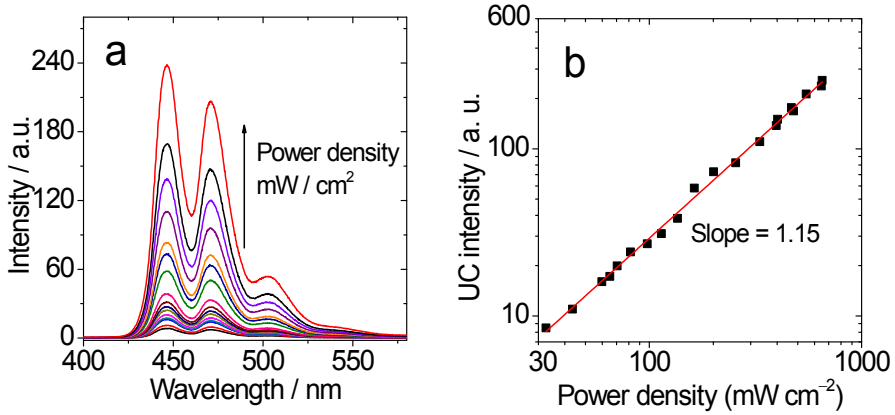


Figure S45. (a) Upconverted luminescence spectra of $\mathbf{2PF_2\text{-}I_3}$ and Perylene upon excitation with a CW 589 nm laser at different incident power densities. (b) Upconversion emission intensity data from part (a) plotted as a function of incident power density. All spectra are measured in deaerated toluene. c ($\mathbf{2PF_2\text{-}I_3}$) = 2.0 × 10^{-6} M, c (perylene) = 2.8 × 10^{-5} M. 20 °C.

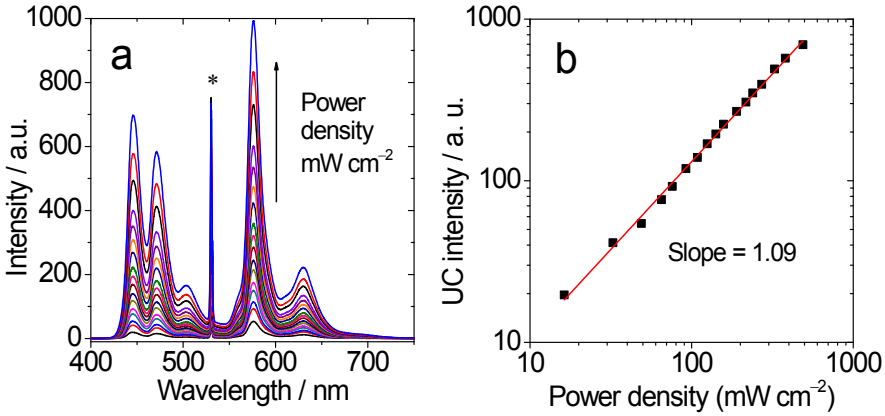


Figure S46. (a) Upconverted luminescence spectra of $\mathbf{1PF_2}$ and Perylene upon excitation with a CW 532 nm laser at different incident power densities. (b) Upconversion emission intensity data from part (a) plotted as a function of incident power density. All spectra are measured in deaerated toluene. c ($\mathbf{1PF_2}$) = 2.0 × 10^{-6} M, c (perylene) = 2.4 × 10^{-5} M. 20 °C.

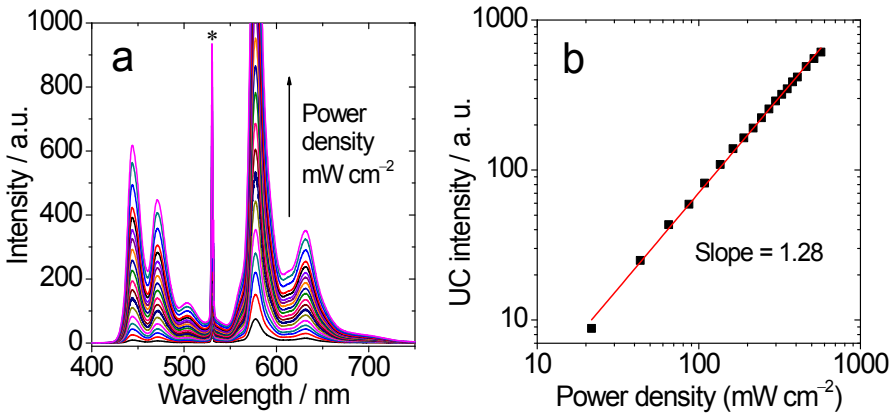


Figure S47. (a) Upconverted luminescence spectra of $\mathbf{2PF_2}$ and Perylene upon excitation with a CW 532 nm laser at different incident power densities. (b) Upconversion emission intensity data from part (a) plotted as a function of incident power density. All spectra are measured in deaerated toluene. c ($\mathbf{2PF_2}$) = 2.0 × 10^{-6} M, c (perylene) = 2.4 × 10^{-5} M. 20 °C.

8. ESR Spectroscopy

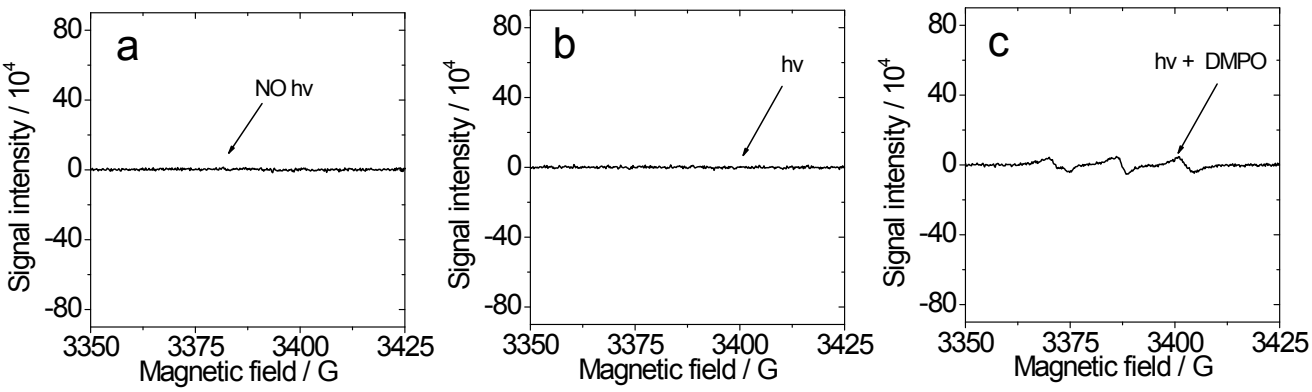


Figure S48. ESR spectrum of the mixtures upon photoirradiation. (a) **$1PF_2$-I_4** (1.0×10^{-5} M) and Et_3N (0.25 M) without Xe lamp; (b) **$1PF_2$-I_4** (1.0×10^{-5} M) and Et_3N (0.25 M) with Xe lamp; (c) **$1PF_2$-I_4** (1.0×10^{-5} M), Et_3N (0.25 M) and DMPO (0.01 M) with Xe lamp. In air-saturated CH_3CN. The samples were photoirradiated with Xe lamp for 60 s (23 mW/cm^2), 20 °C.

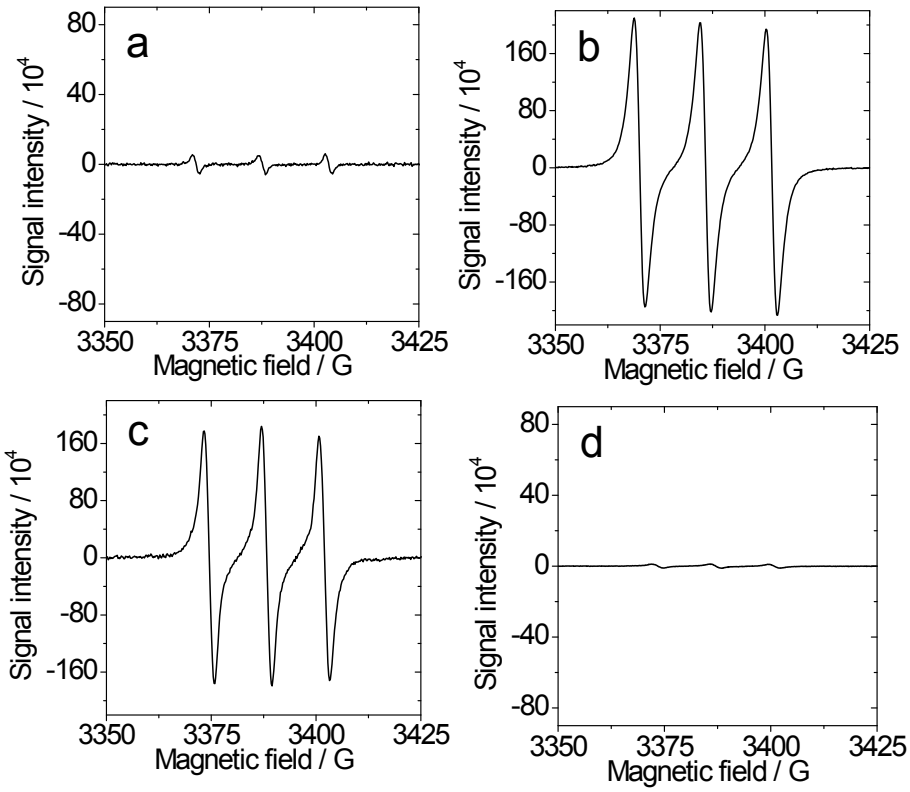


Figure S49. ESR spectrum of the mixtures upon photoirradiation. (a) **$2PF_2$-I_3** (1.0×10^{-5} M), Et_3N (0.25 M) and TEMP (0.1 M); (b) **$2PF_2$-I_3** (1.0×10^{-5} M) and TEMP (0.1 M); (c) **$1PF_2$** (1.0×10^{-5} M), DMPO (0.01 M), Et_3N (0.25 M) (d) **$2PF_2$-I_3** (1.0×10^{-5} M), DMPO (0.01 M). In air-saturated CH_3CN. The samples were photoirradiated with Xe lamp for 60 s (23 mW/cm^2), 20 °C.

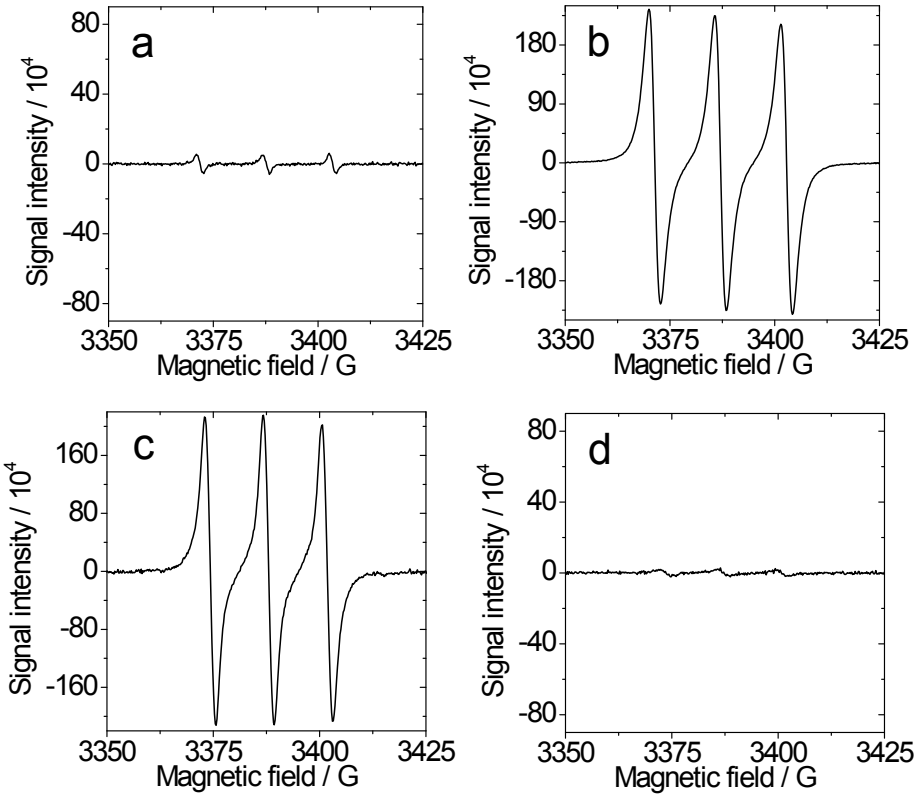


Figure S50. ESR spectrum of the mixtures upon photoirradiation. (a) **$2PF_2$-I_4** (1.0×10^{-5} M), Et_3N (0.25 M) and TEMP (0.1 M); (b) **$2PF_2$-I_4** (1.0×10^{-5} M) and TEMP (0.1 M); (c) **$2PF_2$-I_4** (1.0×10^{-5} M), DMPO (0.01 M), Et_3N (0.25 M) (d) **$2PF_2$-I_4** (1.0×10^{-5} M), DMPO (0.01 M). In air-saturated CH_3CN. The samples were photoirradiated with Xe lamp for 60 s (23 mW/cm^2), 20 °C.

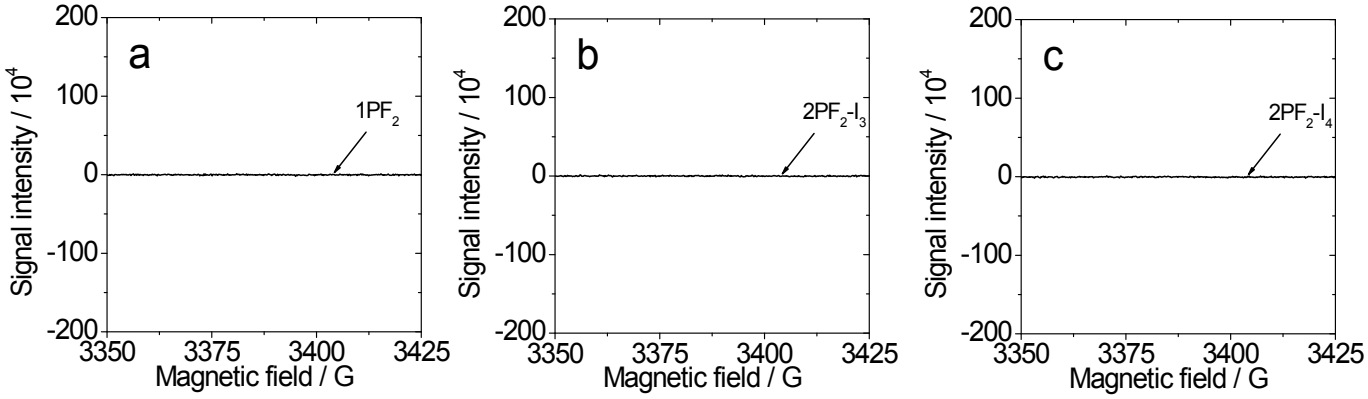


Figure S51. ESR spectrum of the mixtures upon photoirradiation. (a) **$1PF_2$**; (b) **$2PF2\text{-}I_3$**; (c) **$2PF_2\text{-}I_4$**. c = 1.0 × 10^{-5} M in Nitrogen-saturated CH_3CN. The samples were photoirradiated with Xe lamp for 60 s (23 mW/cm2), 20 °C.

9. NMR spectra for Products of Photocatalytic Organic Reactions

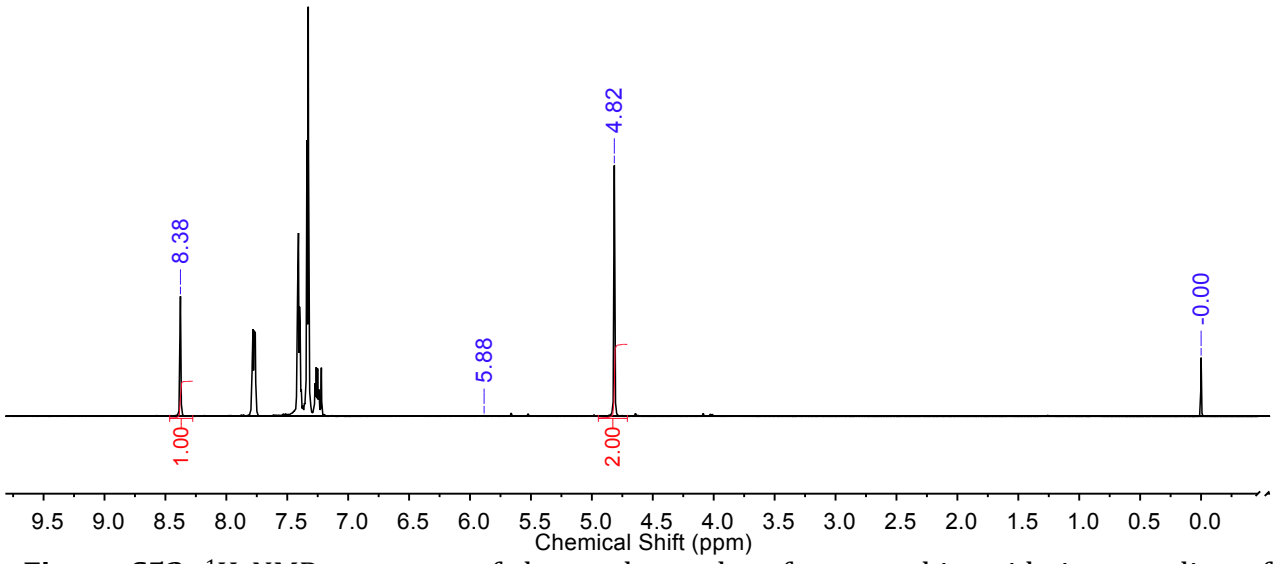


Figure S52. ^{1}H NMR spectrum of the crude product from aerobic oxidative coupling of benzylamine with **Ru(bpy)$_3$[PF$_6$]$_2$** as the photocatalyst (400 MHz, $CDCl_3$). The conversion of the reaction was calculated by integrating the singlet peak of the featured proton in the products (at about 4.82 ppm for -CH=N-*CH$_2$*-) and that of the corresponding proton in the starting materials (at about 3.86 ppm as singlet for H_2N-*CH$_2$*-).

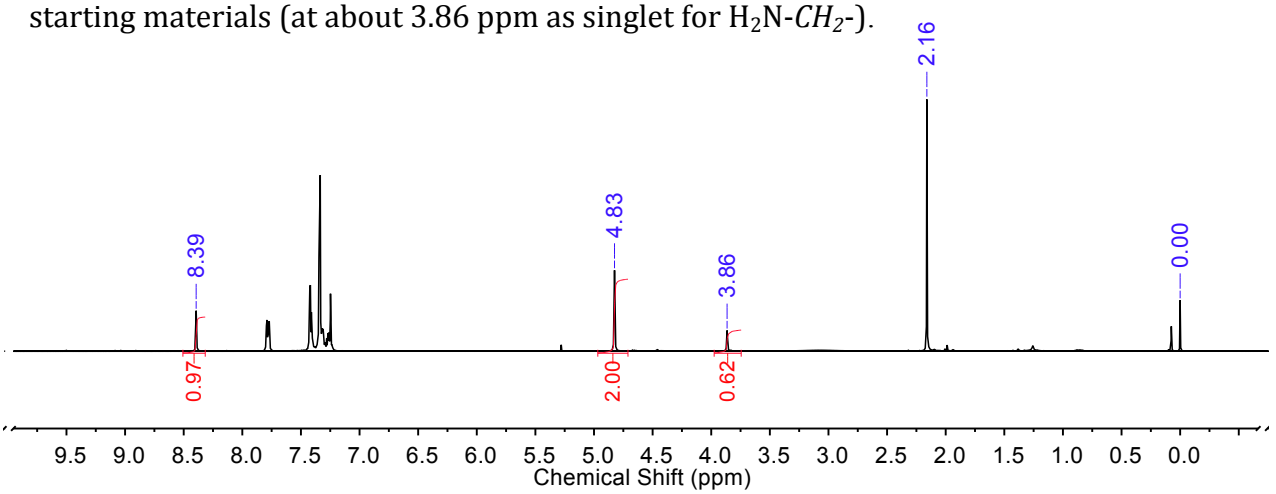


Figure S53. ^{1}H-NMR spectrum of the crude product from aerobic oxidative coupling of benzylamine with **1PF$_2$** as the triplet photosensitizer (400 MHz, $CDCl_3$).

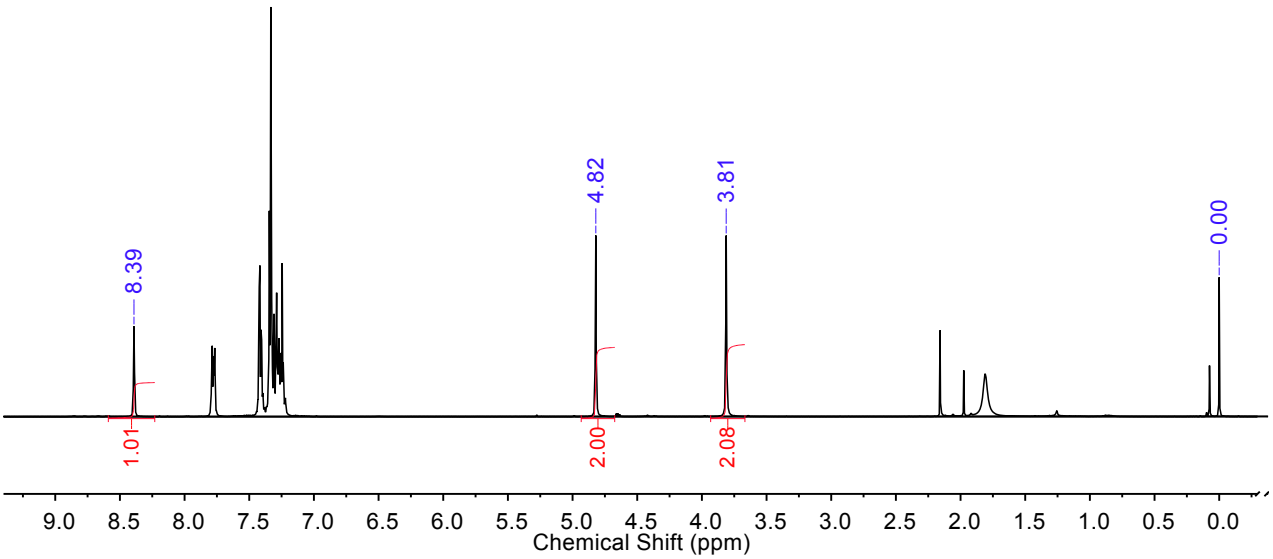


Figure S54. ^{1}H-NMR spectrum of the crude product from aerobic oxidative coupling of benzylamine with **1PF$_2$-I$_4$** as the triplet photosensitizer (400 MHz, $CDCl_3$).

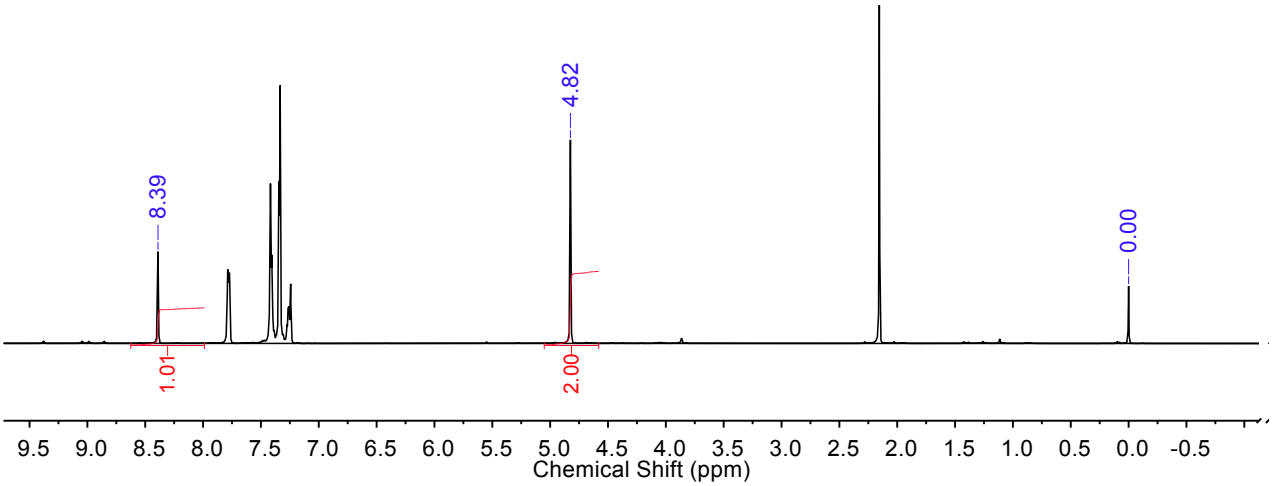


Figure S55. ^{1}H-NMR spectrum of the crude product from aerobic oxidative coupling of benzylamine with **2PF$_2$** as the triplet photosensitizer (400 MHz, $CDCl_3$).

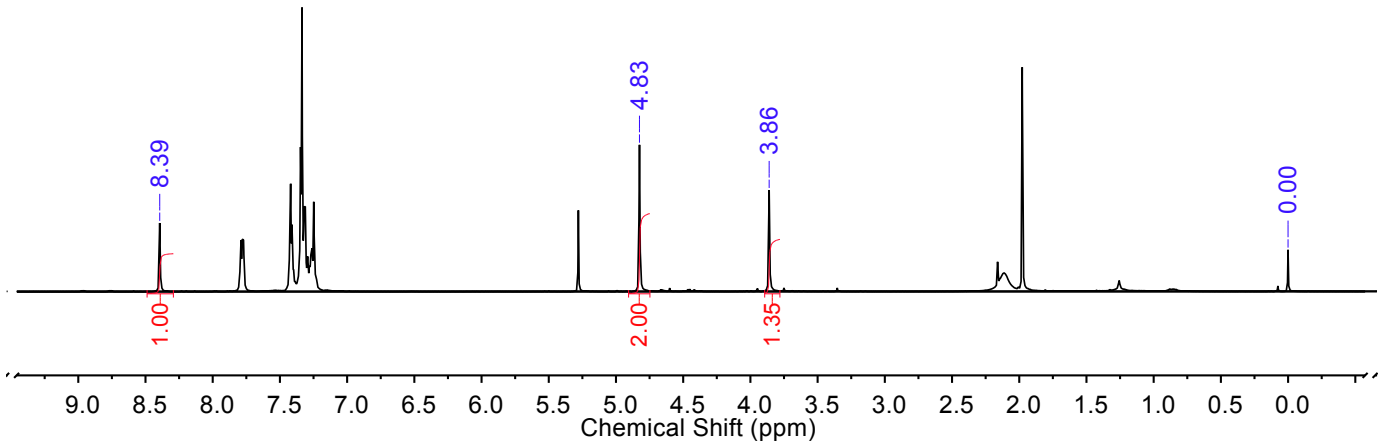


Figure S56. ^{1}H-NMR spectrum of the crude product from aerobic oxidative coupling of benzylamine with **2PF$_2$-I$_3$** as the triplet photosensitizer (400 MHz, $CDCl_3$).

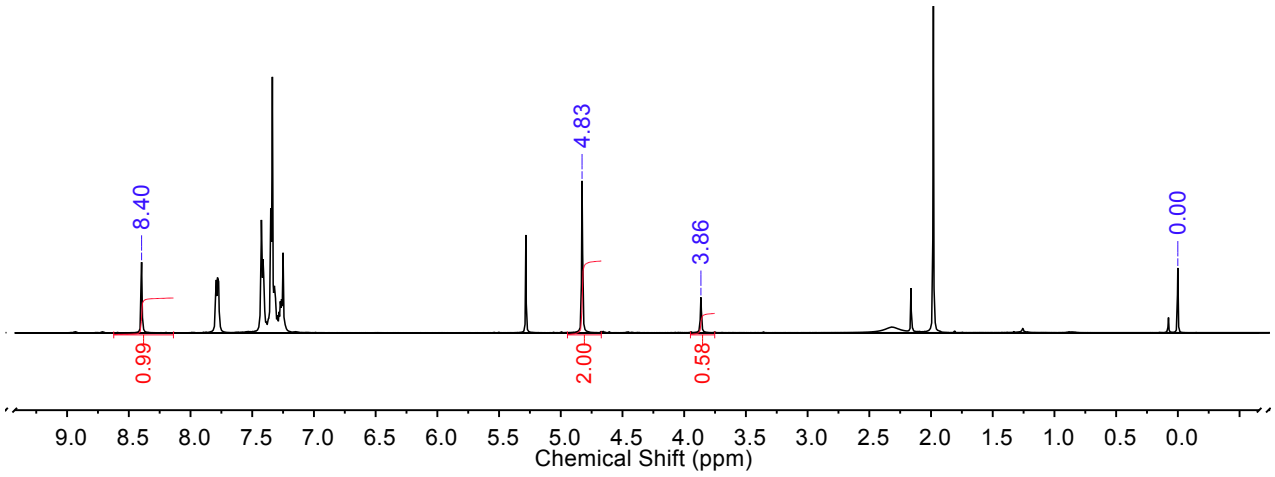


Figure S57. ^{1}H-NMR spectrum of the crude product from aerobic oxidative coupling of benzylamine with **2PF$_2$-I$_4$** as the triplet photosensitizer (400 MHz, $CDCl_3$).

10. Triplet Lifetimes by Similar Extrapolation to Indefinite Diluted Concentration

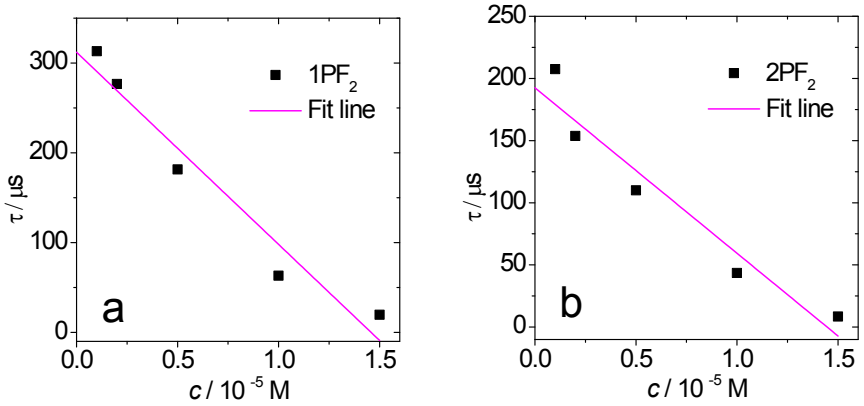


Figure S58. Triplet lifetimes of (a) **$1PF_2$** and (b) **$2PF_2$** in different concentrations. The intercept is 312 μs and 192 μs, respectively.

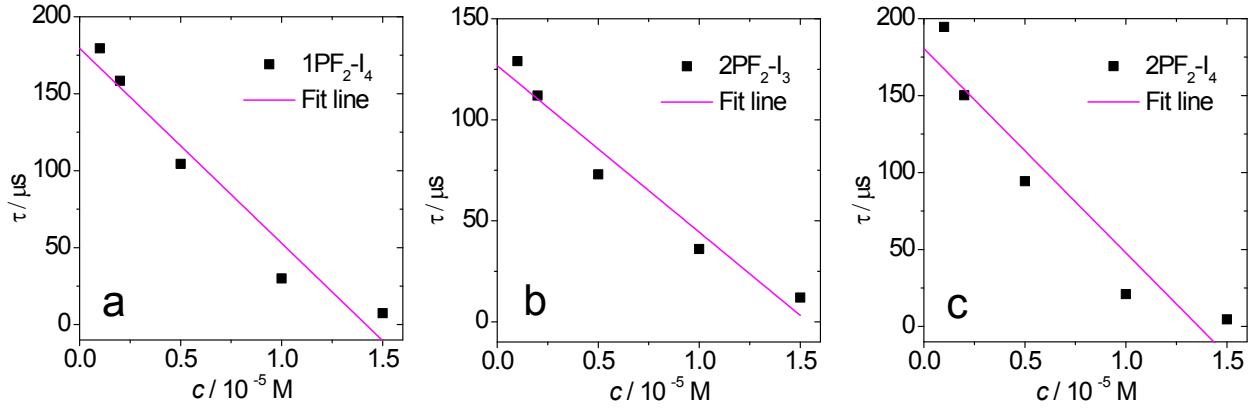


Figure S59. Triplet lifetimes of (a) **$1PF_2$-I_4** and (b) **$2PF_2$-I_3**, (c) **$2PF_2$-I_4** in different concentrations. The intercept is 179 μs 127 μs and 181 μs, respectively.

11. DFT/TDDFT Calculations

Density Functional Theory (DFT) and Time-dependent Density Functional Theory (TD-DFT) were used for geometry optimization and energy calculation of all the compounds in vacuum. All the calculations were performed with Gaussian 16 program. The geometry optimization of the ground state and the excited state was conducted at B3LYP/6-31G(d) level for non-iodo-substituted compounds and B3LYP/GENECP level for iodo-substituted compounds and frequency calculations guarantee the optimal structures are valid. Vertical excitation energies of singlet and triplet states were calculated at B3LYP/6-31G(d) level for non-iodo-substituted compounds and B3LYP/GENECP level for iodo-substituted compounds.

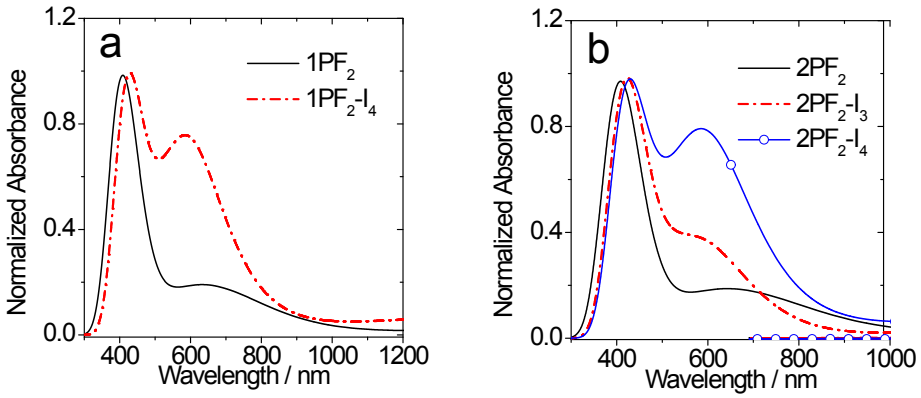


Figure S60. UV–Vis absorption spectra of (a) **$1PF_2$** anion and **$1PF_2$-I_4** anion; (b) **$2PF_2$** anion, **$2PF_2$-I_3** anion and **$2PF_2$-I_4** anion in toluene; Calculated at B3LYP/6-31G(d) level with Gaussian 09W for noniodo-substituted compounds and calculated at B3LYP/GENECP level with Gaussian 09W for iodo-substituted compounds.

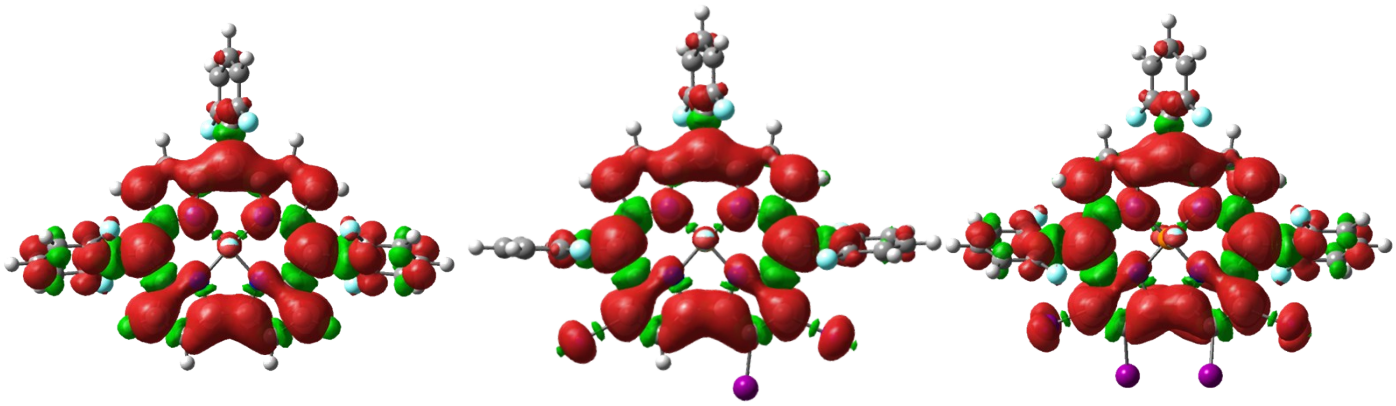


Figure S61. Spin density surfaces of (a) **2PF$_2$** anion at the optimized triplet state geometry, calculated at B3LYP/6-31G(d) level with Gaussian 09W; (b) **2PF$_2$-I$_3$** anion and (c) **2PF$_2$-I$_4$** anion at the optimized triplet state geometry, calculated at B3LYP/GENECP level with Gaussian 09W.

Table S2. Triplet transition from T_1 state of the compounds [a]

	Electronic transition [a]	Energy [b]	f [c]	ESA [d]
1PF$_2$	$T_1 \rightarrow T_{24}$	2.93 eV/424 nm	0.078	437
	$T_1 \rightarrow T_{26}$	3.42 eV/362 nm	0.810	360
1PF$_2$-I$_4$	$T_1 \rightarrow T_{24}$	2.67 eV/464 nm	0.240	462
	$T_1 \rightarrow T_{26}$	3.34 eV/372 nm	0.438	462
2PF$_2$	$T_1 \rightarrow T_{22}$	2.88 eV/431 nm	0.008	433
	$T_1 \rightarrow T_{26}$	3.42 eV/362 nm	0.746	360
2PF$_2$-I$_3$	$T_1 \rightarrow T_{25}$	2.76 eV/449 nm	0.173	445
	$T_1 \rightarrow T_{35}$	3.42 eV/363 nm	0.143	367
2PF$_2$-I$_4$	$T_1 \rightarrow T_{24}$	2.72 eV/455 nm	0.122	451
	$T_1 \rightarrow T_{40}$	3.36 eV/363 nm	0.392	369

[a] TDDFT// B3LYP/GENECP or 6-31G(d), based on the DFT//B3LYP/GENECP or 6-31G(d)-optimized ground state geometries. [b] Only the selected t low lying excited states are presented. [c] Oscillator strengths. [d] Excited absorption wavelength (nm) in ns TA spectra.

$1PF_2$.gjf

Redundant internal coordinates taken from checkpoint file:

$1PF_2$.chk

Charge = 0 Multiplicity = 1

C,0,4.8643423742,0.8912403502,0.7578987318

C,0,4.8358446192,0.7528811548,-0.6351759482

C,0,4.021259266,1.3149416022,1.8083394061

C,0,3.9499866636,0.9670521099,-1.7138252353

C,0,4.76373977,1.2265190657,2.9722361104

H,0,2.9971654502,1.64532044,1.7038709163

C,0,6.0615195353,0.7435663469,2.6337076338

C,0,4.6472441732,0.6542343474,-2.8670214064

H,0,2.9288717697,1.3133959201,-1.6349034502

C,0,5.9604161371,0.2447684323,-2.4926791099

H,0,4.4389702184,1.4771015946,3.9721327503

C,0,7.1846902598,0.4769897712,3.4200453141

N,0,8.5217943667,-0.4947152231,-1.2568367707

H,0,4.2833261341,0.7088831073,-3.8832602559

C,0,7.0582223953,-0.1551511007,-3.2575458937

C,0,8.3566245642,-0.0007370262,2.833158481

C,0,7.1188395219,0.6976590961,4.8887991051

C,0,8.256725971,-0.5077879173,-2.6372639998

C,0,9.8231632336,-0.9502319945,-1.0905587858

C,0,6.9401903387,-0.2001703199,-4.7390718172

C,0,9.5366371904,-0.378947678,3.5401196725

C,0,6.2453015616,-0.0386392254,5.6996359405

C,0,7.9064427875,1.6652912565,5.5259435846

C,0,10.4520371928,-0.8277719208,2.6352205356

C,0,9.4249432631,-0.9769020624,-3.3083089355

C,0,10.3776208957,-1.245568188,-2.3709606628

C,0,7.6788531146,0.6591297883,-5.5626973387
C,0,6.0645190854,-1.0879350159,-5.3767320752
H,0,9.6467262945,-0.3240905812,4.6131779314
C,0,6.1544001113,0.1731127563,7.0730522082
C,0,7.8392154245,1.8870273654,6.899160218
H,0,11.445793287,-1.2013977894,2.8327101501
H,0,9.5038467351,-1.0989452349,-4.3785892684
H,0,11.3807908709,-1.6098479903,-2.5358266445
C,0,7.5640080321,0.6342649461,-6.9502398154
C,0,5.927335854,-1.1244735627,-6.7622182083
C,0,6.9567241112,1.1392199828,7.6749618124
C,0,6.6821443942,-0.2603959936,-7.5517058921
N,0,6.0890543063,0.5459173582,1.2750431036
C,0,9.8646078945,-0.7331618748,1.3391089288
C,0,10.4739853539,-1.0797170657,0.1348691958
C,0,11.8711669809,-1.5973435806,0.15581103
C,0,12.9551755266,-0.7730460193,0.4806586552
C,0,12.1617295955,-2.9317748898,-0.1521337777
C,0,14.2645451447,-1.2475531998,0.5045779914
C,0,13.4637803512,-3.4262734144,-0.1444010428
C,0,14.5188529946,-2.5798492292,0.187893973
N,0,6.0406678991,0.3097224165,-1.1233440847
N,0,8.5763866101,-0.228804302,1.4635636665
P,0,7.3695142153,0.0139735453,0.0903501628
F,0,5.464817122,-0.9842422011,5.1602221652
F,0,5.3105000429,-0.5506732517,7.8161980154
F,0,6.8808849285,1.3474253398,8.9909361763
F,0,8.6065333102,2.819244129,7.4737718299
F,0,8.7586409206,2.4127402913,4.8130084646
F,0,15.2760731826,-0.4315110269,0.8197852944
F,0,15.7699891068,-3.0445424292,0.2028487364

F,0,13.7051047978,-4.7068516253,-0.4450850995
F,0,11.1722415947,-3.7757577339,-0.4714358691
F,0,12.7496666541,0.5145240644,0.7855278971
F,0,8.5287112613,1.5411630312,-5.021196527
F,0,8.2847491308,1.4702107001,-7.7051724032
F,0,6.5607454814,-0.2897576594,-8.8803747113
F,0,5.0842845702,-1.9883945009,-7.3375504658
F,0,5.3271934375,-1.939785508,-4.6522953258
F,0,7.8846932214,1.560922615,-0.0726257767
F,0,6.8986532461,-1.5468622986,0.253534839
Recover connectivity data from disk.

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d)

Charge = 0

Spin = Singlet

E(RB3LYP) = -3672.30918635 a.u.

RMS Gradient Norm = 0.00000454 a.u.

Imaginary Freq = 0

Dipole Moment = 1.8012 Debye

$1PF_2$-I_4.gjf

Redundant internal coordinates taken from checkpoint file:

$1PF_2$-I_4.chk

Charge = 0 Multiplicity = 1

C,0,4.8833039946,1.2501751834,0.7251212317

C,0,4.784012766,0.9423804585,-0.6508278038

C,0,4.1833594162,1.9482078455,1.7409406954

C,0,3.8172681118,0.8784138419,-1.6854093749

C,0,4.9176382934,1.799462659,2.9142313811

C,0,6.0882516457,1.0390892958,2.6168810951

C,0,4.4743122393,0.4286124248,-2.827140375

C,0,5.8411349039,0.1895412556,-2.492861199

C,0,7.1460303413,0.5660276368,3.4069557782

N,0,8.4429886773,-0.4455284265,-1.25079801

C,0,6.9514335526,-0.2174056206,-3.2466468951

C,0,8.2541854903,-0.0308464513,2.8157641582

C,0,7.1249079,0.6347084174,4.8948403822

C,0,8.1675878065,-0.4800394957,-2.6256243536

C,0,9.7646645231,-0.8470897686,-1.0977387292

C,0,6.9119547381,-0.337249455,-4.7312380414

C,0,9.3934037018,-0.513001548,3.5323504264

C,0,6.3574606092,-0.2652604077,5.6406746263

C,0,7.9046010814,1.5552775694,5.6012594313

C,0,10.3199000337,-0.9299376694,2.6265392655

C,0,9.3584537018,-0.8749676519,-3.3110082766

C,0,10.3287347744,-1.0987192316,-2.3829699429

C,0,6.9882313432,0.7979142595,-5.5438492689

C,0,6.8567566825,-1.5813811642,-5.3661928186

H,0,9.47754484,-0.5203842167,4.6084033061

C,0,6.3452685927,-0.2418503464,7.032116016

C,0,7.9080997152,1.5975186425,6.9925977519
H,0,11.2971506739,-1.3448802805,2.8232447846
H,0,9.4397579927,-0.9731022635,-4.3828332043
H,0,11.3479878657,-1.411223594,-2.5540322619
C,0,6.9857220723,0.7078391786,-6.9325497053
C,0,6.8525389865,-1.6959205634,-6.7535019003
C,0,7.1224004101,0.6962061404,7.708678112
C,0,6.9146943148,-0.5454619536,-7.5375887852
N,0,6.0511055206,0.7577384733,1.2659395054
C,0,9.7721708142,-0.732534501,1.3248276798
C,0,10.4122847686,-1.0131410243,0.1220754234
C,0,11.8161790522,-1.5084918511,0.1431300655
C,0,12.8733923493,-0.6872999656,0.554684583
C,0,12.1404165894,-2.8141754017,-0.2453542251
C,0,14.1908132155,-1.1386460543,0.583791268
C,0,13.4516716468,-3.2840142704,-0.2328148243
C,0,14.4799874949,-2.4422322655,0.185937785
N,0,5.9823319657,0.4805996907,-1.1503632535
N,0,8.4938469552,-0.201271313,1.4440456304
P,0,7.3073615943,0.1216904625,0.0782357975
F,0,5.59854848,-1.1104260739,7.7206848949
F,0,8.6569525262,2.4930907679,7.6440432684
F,0,15.1763064843,-0.3286060492,0.9821898228
F,0,13.7268815932,-4.5359501678,-0.6110689867
F,0,7.053754631,1.8095179542,-7.6862018841
F,0,6.7907885932,-2.8970753028,-7.3369216362
F,0,7.899851106,1.6379440257,-0.0824093893
F,0,6.7257225634,-1.3986147306,0.2389973819
I,0,4.390163144,2.6782682919,4.7561642851
I,0,2.5477949713,3.2515091101,1.5341169521
I,0,3.5221740383,0.074059016,-4.6740503634

I,0,1.7322948149,1.0893992829,-1.5327793276

F,0,11.1763473947,-3.6518758073,-0.6471243122

F,0,12.6317955419,0.5722645309,0.9381143543

F,0,15.7384398083,-2.8835492969,0.205916294

F,0,6.9133657849,-0.6454684148,-8.8678387742

F,0,7.0504539567,2.0127622703,-4.9867379272

F,0,6.7930748589,-2.7016924108,-4.6368719954

F,0,5.5969144853,-1.1707437,5.0148829237

F,0,8.6643118299,2.435328886,4.9381715972

F,0,7.1199614949,0.7273885481,9.0422507508

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = GenECP

Charge = 0

Spin = Singlet

E(RB3LYP) = -3715.32679363 a.u.

RMS Gradient Norm = 0.00000256 a.u.

Imaginary Freq = 0

Dipole Moment = 1.6455 Debye

Point Group = C1

$2PF_2$.gjf

Redundant internal coordinates taken from checkpoint file:

$2PF_2$.chk

Charge = 0 Multiplicity = 1

C,0,4.8675386311,0.9052542002,0.7540366707

C,0,4.840667859,0.7680331681,-0.6401068655

C,0,4.0234568197,1.3252719776,1.8043513994

C,0,3.9567660143,0.9816792744,-1.7196716204

C,0,4.763797688,1.2303270313,2.9702516354

H,0,2.999912462,1.6574478093,1.6988633314

C,0,6.0608762457,0.7477907964,2.632562659

C,0,4.6546784115,0.664529538,-2.8724458929

H,0,2.9362234925,1.3303832335,-1.6419671469

C,0,5.9658716182,0.2534953832,-2.496581257

H,0,4.4394535345,1.475660996,3.9715915335

C,0,7.1815722285,0.4776713671,3.4220920697

N,0,8.5234572019,-0.4878801641,-1.2560484148

H,0,4.2937553477,0.7163633249,-3.8899034186

C,0,7.0624951872,-0.1507559081,-3.2618312385

C,0,8.353227743,0.0035017493,2.8330658543

C,0,7.1111849909,0.6899665018,4.8920753317

C,0,8.2585487481,-0.5027480004,-2.6375743037

C,0,9.824667569,-0.9444669568,-1.088079623

C,0,6.9439621247,-0.201430528,-4.7433053135

C,0,9.5336505158,-0.3737159739,3.5400300351

C,0,6.2454498728,-0.0490311755,5.7102779099

C,0,7.8843920278,1.6549653755,5.5520834778

C,0,10.4508375932,-0.8195201717,2.6354264514

C,0,9.4271134071,-0.9742418862,-3.3064800031
C,0,10.3789809796,-1.2424508782,-2.3681476562
C,0,7.6749559336,0.6480411282,-5.5851921536
C,0,6.0727953965,-1.087116999,-5.3918288447
H,0,9.6400239563,-0.3180672263,4.6134675044
C,0,6.1420506093,0.1412699951,7.0832122315
C,0,7.820038908,1.8795691549,6.9222937635
H,0,11.445778309,-1.191502658,2.8301991549
H,0,9.5038210321,-1.0962239658,-4.3769711369
H,0,11.3822540891,-1.6084999892,-2.5286683019
C,0,7.5673738018,0.6284751916,-6.9707800459
C,0,5.9271536451,-1.1421140921,-6.7731228039
C,0,6.9390818725,1.1140426684,7.6861424915
C,0,6.6843736942,-0.2755281894,-7.5611624012
N,0,6.090695418,0.5568338553,1.2723345096
C,0,9.8648204309,-0.7250359785,1.3384438061
C,0,10.4774310131,-1.0732285853,0.1363554284
C,0,11.8741166878,-1.5925124761,0.1588249253
C,0,12.9701222688,-0.7823302378,0.48252082
C,0,12.1795277604,-2.9254385619,-0.1452230229
C,0,14.2809963919,-1.2447564997,0.5098664665
C,0,13.4731565603,-3.4346226877,-0.1371350408
C,0,14.5254903368,-2.5814283588,0.1950601641
N,0,6.0449218004,0.3220639692,-1.1266855852
N,0,8.5754948328,-0.2223282453,1.4623977211
P,0,7.3718511473,0.0227353532,0.0888264085
F,0,7.8890946257,1.5707162593,-0.0733182679
F,0,6.8946808238,-1.5380498108,0.251209729
H,0,6.5855095717,-0.3046305546,-8.642016233
H,0,15.5427963116,-2.9607025086,0.208897935
H,0,6.8736851302,1.2764410408,8.7576832564

H,0,15.079823086,-0.5582120751,0.7678759199
H,0,13.6333796468,-4.4788745895,-0.3818629321
F,0,12.7411921072,0.5090393133,0.786043351
F,0,11.1678123706,-3.7539863721,-0.4649171776
F,0,8.5248621882,1.5279349861,-5.0231825787
F,0,5.3408836867,-1.9297212901,-4.6385298299
F,0,8.7331842613,2.4025556252,4.8220976309
F,0,5.4761793858,-0.9943728519,5.1377758955
H,0,8.4477431664,2.6463798236,7.3627132855
H,0,5.4526217373,-0.4727754218,7.6520897342
H,0,8.1638230436,1.3181844426,-7.5577460552
H,0,5.236388107,-1.8582026854,-7.2044632865

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d)

Charge = 0

Spin = Singlet

E(RB3LYP) = -2779.31269714 a.u.

RMS Gradient Norm = 0.00001335 a.u.

Imaginary Freq = 0

Dipole Moment = 0.9836 Debye

Point Group = C1

$2PF_2$-I_3.gjf

Redundant internal coordinates taken from checkpoint file:

$2PF_2$-I_3.chk

Charge = 0 Multiplicity = 1

C,0,4.8224883651,1.0307058613,0.7432832427

C,0,4.7963211928,0.8949035532,-0.6510329389

C,0,3.9608067093,1.4395646728,1.7761063854

C,0,3.8947913284,1.1086201878,-1.7071810847

C,0,4.6704081603,1.324489584,2.9660594686

C,0,5.9826431399,0.8380456362,2.6526133553

C,0,4.5695428422,0.7649285903,-2.8652028891

C,0,5.8942064361,0.3368368718,-2.5236744683

C,0,7.1089141066,0.5264620417,3.4271705343

N,0,8.4380538415,-0.467853649,-1.2458344406

C,0,6.9904782471,-0.1123915092,-3.2677707856

C,0,8.2638280219,0.036233823,2.8213135768

C,0,7.1408045938,0.6936422477,4.9086857863

C,0,8.1708123276,-0.4813808857,-2.6258080701

C,0,9.736103961,-0.9353916258,-1.0811629459

C,0,6.9584519167,-0.2153815445,-4.7551585934

C,0,9.4457397759,-0.3394044357,3.533627234

C,0,6.8385746261,-0.3580111268,5.7798164611

C,0,7.5374547871,1.8934818474,5.5079099136

C,0,10.3604402783,-0.7979906574,2.6352545108

C,0,9.3373357799,-0.9605077786,-3.2974187631

C,0,10.2873400775,-1.2377823577,-2.3608962026

C,0,7.3280444962,0.8539606763,-5.5774113113

C,0,6.6118432451,-1.4022862442,-5.4086898722

H,0,9.5553113812,-0.2630220882,4.6049235384
C,0,6.9038242493,-0.2390197997,7.1629477022
C,0,7.6182516437,2.062408022,6.8849217196
H,0,11.3540561892,-1.1713607261,2.8330290096
H,0,9.4148650864,-1.0706874306,-4.3687138986
H,0,11.2882760958,-1.6097300046,-2.5214163113
C,0,7.3446775913,0.7725747588,-6.9645721747
C,0,6.612949015,-1.5336579806,-6.7923106466
C,0,7.2944060961,0.9842453286,7.7095633782
C,0,6.9807105561,-0.4325598568,-7.5666557594
N,0,6.0283990954,0.6717922126,1.2817610273
C,0,9.7760811284,-0.7101805558,1.3370462148
C,0,10.3904303909,-1.0689007766,0.1410071516
C,0,11.7803367841,-1.604576158,0.1659164881
C,0,12.885477179,-0.8071287006,0.4909417565
C,0,12.0674147172,-2.9420476574,-0.1376403041
C,0,14.1901851579,-1.2869322222,0.5200053846
C,0,13.3546334442,-3.4674611822,-0.1270896884
C,0,14.4174863744,-2.6272721529,0.2062074501
N,0,5.9862944531,0.4309213287,-1.1465895113
N,0,8.4885007717,-0.1994370836,1.4541611961
P,0,7.3053514886,0.0846717317,0.0844725872
F,0,7.8617597463,1.6166508821,-0.0753481538
F,0,6.7519917681,-1.4481323629,0.2509175983
H,0,6.9860411295,-0.5151089801,-8.6493359375
H,0,15.4296899446,-3.0196762003,0.2217535619
H,0,7.3497895671,1.0972897751,8.7880741897
I,0,3.8621179858,1.7907414213,4.85348829
I,0,1.9825585897,2.0846089082,1.4874228327
I,0,3.6382481558,0.8941743662,-4.7554138217
H,0,2.8819400275,1.4694792066,-1.6214806127

F,0,11.0446282954,-3.7558590119,-0.4583295344
F,0,12.6709712599,0.4868109342,0.7936989069
F,0,7.6764515256,2.0140584282,-4.9924924551
F,0,6.2577339583,-2.4609845205,-4.6582296
F,0,7.8461579618,2.9306140279,4.7092212375
F,0,6.4623258163,-1.5351105215,5.2483120488
H,0,7.635642774,1.6411549618,-7.5448149705
H,0,6.3276552405,-2.4806543723,-7.2368313619
H,0,13.5023614478,-4.5136943352,-0.3709673516
H,0,14.9979229814,-0.6112889082,0.77879655
H,0,6.6495022402,-1.0915916797,7.7828145231
H,0,7.9268977488,3.0214564856,7.2858582872

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = GenECP

Charge = 0

Spin = Singlet

E(RB3LYP) = -2811.58225283 a.u.

RMS Gradient Norm = 0.00000208 a.u.

Imaginary Freq = 0

Dipole Moment = 4.5845 Debye

Point Group = C1

$2PF_2$-I_4.gjf

Redundant internal coordinates taken from checkpoint file:

$2PF_2$-I_4.chk

Charge = 0 Multiplicity = 1

C,0,-0.7062124345,-1.5885207699,-0.035334408

C,0,0.7060998472,-1.5885963474,0.034855892

C,0,-1.7865979636,-2.4795765294,-0.245606516

C,0,1.7863805457,-2.4797892367,0.2450867387

C,0,-2.9545364404,-1.7231572987,-0.1889923241

C,0,-2.5952385499,-0.3595942706,0.0240562125

C,0,2.9543922403,-1.7234598883,0.1887964118

C,0,2.5952452028,-0.3598256468,-0.0240521152

C,0,-3.3500487115,0.8111757916,0.1941465092

N,0,1.3477582627,2.3130254758,-0.1154590603

C,0,3.3501833799,0.8109002927,-0.1938719142

C,0,-2.7190450748,2.0483193097,0.2534873022

C,0,-4.8304270566,0.7991569764,0.364294974

C,0,2.7192908183,2.0480979166,-0.2532731953

C,0,1.2016805843,3.6947697705,-0.152699003

C,0,4.8305964583,0.7987912804,-0.3637189055

C,0,-3.4006008183,3.2950205884,0.4153534032

C,0,-5.4225447937,0.4643182415,1.5869590594

C,0,-5.7061158704,1.182315186,-0.6570018894

C,0,-2.4800335006,4.2951875123,0.3486065927

C,0,3.4009633365,3.2947347521,-0.415143651

C,0,2.4804520228,4.2949728698,-0.3486911123

C,0,5.4229490537,0.4641065355,-1.5863106527

C,0,5.7060927922,1.1817360594,0.6578223812
H,0,-4.466581897,3.3885895059,0.5566795175
C,0,-6.7957167486,0.4884665716,1.7964670328
C,0,-7.0860543943,1.2195738528,-0.4979388093
H,0,-2.6481806414,5.3588457202,0.4277801391
H,0,4.4669750146,3.3882113678,-0.5563014398
H,0,2.6486874477,5.3586093726,-0.4279659977
C,0,6.7961668098,0.4881980526,-1.7955254839
C,0,7.086067926,1.2189249948,0.499057583
C,0,-7.6253031145,0.866355237,0.740007749
C,0,7.6255543753,0.8658638478,-0.7388298877
N,0,-1.2153116248,-0.3131126781,0.076577866
C,0,-1.2013336349,3.694871164,0.1524934723
C,0,0.0001929885,4.378331753,-0.0001775583
C,0,0.0002318359,5.8675736654,-0.0002936833
C,0,-0.5684984419,6.614100362,-1.040892447
C,0,0.5689837961,6.6142490162,1.0401856919
C,0,-0.5828481672,8.004171132,-1.06267149
C,0,0.5833827191,8.0043228334,1.0617389067
C,0,0.0002797333,8.6959799808,-0.000522593
N,0,1.2153280315,-0.3132150696,-0.0767740863
N,0,-1.3475131254,2.3131342493,0.115439074
P,0,0.0000702519,1.0714344912,-0.0000468168
F,0,-0.1310548911,1.0758712719,-1.6318338491
F,0,0.1311952745,1.075747024,1.6317397703
H,0,8.7016613871,0.8881064348,-0.8818529825
H,0,0.0002987237,9.7816835812,-0.000610597
H,0,-8.7013782934,0.8886468573,0.8832621213
I,0,-4.8879691131,-2.5118775977,-0.4786696625
I,0,-1.7145379641,-4.4884531326,-0.8629682565
I,0,4.8877123156,-2.5124040943,0.4786138263

I,0,1.7140672338,-4.4888104978,0.8619444985
H,0,7.7094734318,1.5159780385,1.335081161
H,0,7.1908076007,0.2127677065,-2.7671995612
H,0,1.0395855359,8.5170014574,1.9013464421
H,0,-1.0390351329,8.516729406,-1.9023611049
H,0,-7.1901695857,0.2129086877,2.7681812338
H,0,-7.7096166119,1.5167964764,-1.3337851944
F,0,5.1829673831,1.5210104217,1.8499812111
F,0,4.6200002554,0.0958374195,-2.6004190447
F,0,1.1309360567,5.9503786739,2.0671581556
F,0,-1.1304801558,5.9500824885,-2.0677521802
F,0,-4.6194083245,0.0958342393,2.6008404005
F,0,-5.183222076,1.5217336539,-1.8492218866
Recover connectivity data from disk.

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = GenECP

Charge = 0

Spin = Singlet

E(RB3LYP) = -2822.33696036 a.u.

RMS Gradient Norm = 0.00000273 a.u.

Imaginary Freq = 0

Dipole Moment = 5.5483 Debye

Point Group = C1