Electronic Supplementary Material (ESI) for RSC Advances

Supporting information

for

Chlorophyll tailored 20-trifluoroacetamide and its azacrown derivative as pH sensitive colorimetric sensor probe with response to AcO^-, F^- and CN^- ions

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'Naked eye' detection of selected anions with sensor probe **4** ($8{,}6*10^{-5}$ M, 40 equiv. added potassium salt in DMF:H_2O 7:3).

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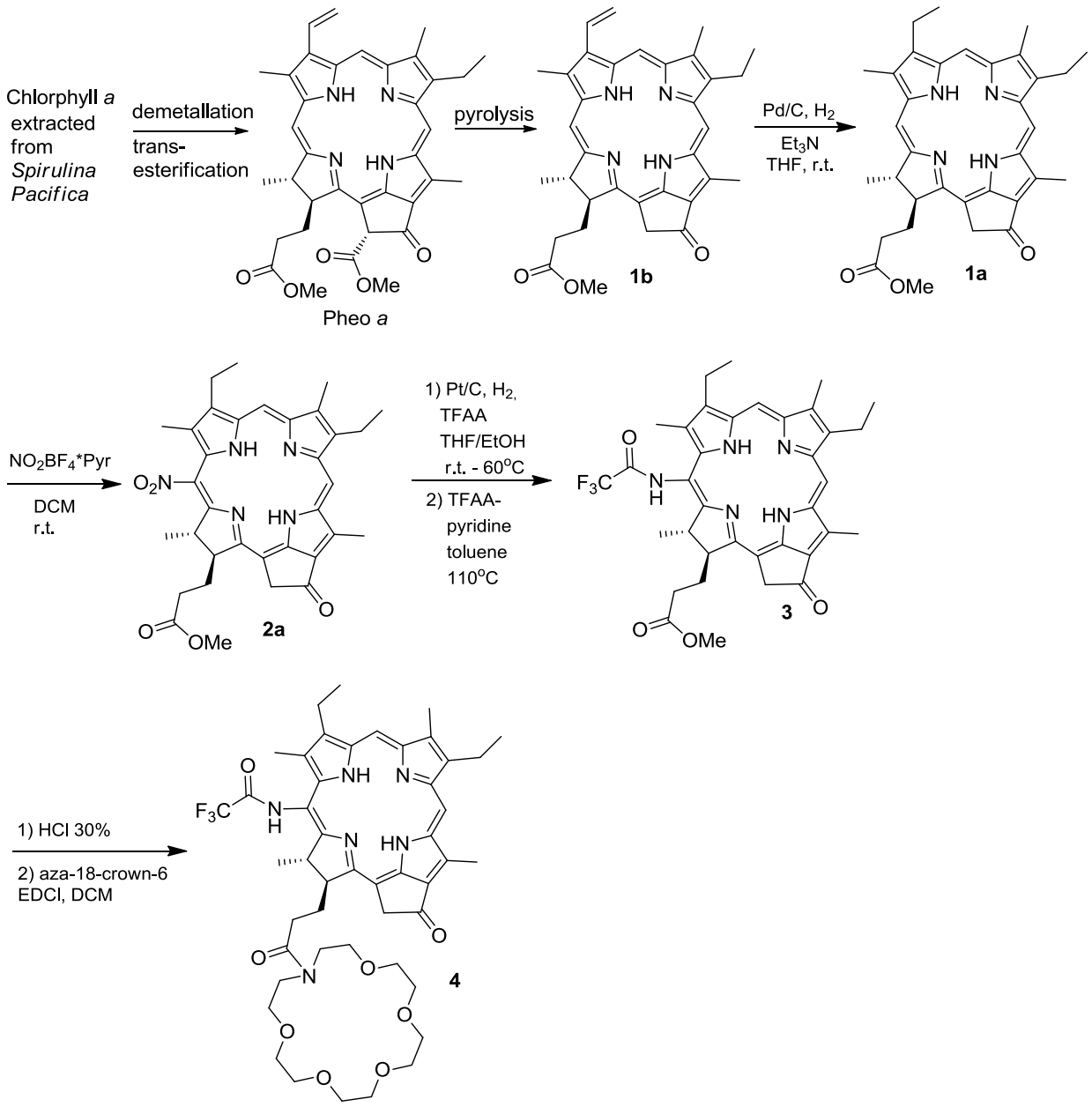
Synthesis and characterization data



Methyl *pyro*pheophorbide *a* (**1b**).

600 mg (1.0 mmol) of pure methyl pheophorbide *a* (Pheo *a*) was dissolved in 125 ml of pyridine and 0.18 ml (10.0 mmol) of dist. water was added. Argon was bubbled carefully through for 15 min and reaction mixture was then refluxed under argon atmosphere overnight. After reaction mixture was cooled, solvent was removed *in vacuo*. Flash column chromatography (eluent hexane/ethyl acetate, grad. 3:1 – 1:1) afforded 450 mg (84%) of

methyl pyropheophoride *a*; ^{1}H NMR (300 MHz, $CDCl_3$, 27^{o}C) δ 9.48 (1H, s), 9.37 (1H, s), 8.54 (1H, s), 7.99 (1H, dd, $^{3}J_{trans}$=17.8 Hz, $^{3}J_{cis}$=11.6 Hz), 6.28 (1H, dd, $^{3}J_{trans}$=17.8 Hz), 6.16 (1H, dd, $^{3}J_{cis}$=11.6 Hz), 5.26 (1H, d, *J*=19.5 Hz), 5.10 (1H, d, *J*=19.5 Hz), 4.46 (1H, m), 4.29 (1H, m), 3.66 (3H, s), 3.63 (2H, q, *J*=7.6 Hz), 3.61 (3H, s), 3.40 (3H, s), 3.22 (3H, s), 2.63 (2H, m), 2.30 (2H, m), 1.81 (3H, d, *J*=7.4 Hz), 1.69 (3H, t, *J*=7.6 Hz), 0.83 (1H, s), -0.69 (1H, s); was found to match literature values.[6b]

Methyl meso*pyro*pheophorbide *a* (1a).

287.4 mg (0.525 mmol) of **1b** was dissolved in 125 ml of THF. Et_3N (30 μl, 0.409 mmol) and 28.8 mg (10%$_{mass}$) of 5% Pd/C were added to the solution. Resulting mixture was stirred at r.t. under H_2 atmosphere for 24 h. After that solvent was evaporated and solid residue was purified with flash-column chromatography (silica, EtOAc:Hex 1:1) to obtain 259.5 mg (89.9 %) of **1a**; ^{1}H NMR (300 MHz, $CDCl_3$, 27^{o}C) δ 9.44 (1H, s), 9.19 (1H, s), 8.45 (1H, s), 5.24 (1H, d, *J*=20.0 Hz), 5.08 (1H, d, *J*=20.0 Hz), 4.45 (1H, m), 4.27 (1H, m), 3.82 (2H, q, *J*=7.6 Hz), 3.65 (3H, s), 3.63 (2H, q, *J*=7.6 Hz), 3.62 (3H, s), 3.29 (3H, s), 3.24 (3H, s), 2.58 (2H, m), 2.29 (2H, m), 1.81 (3H, d, *J*=7.3 Hz), 1.73 (3H, t, J=7.6 Hz), 1.69 (3H, t, *J*=7.6 Hz), 0.64 (1H, s), -1.60 (1H, s); was found to match literature values.[6b]

20-nitro-meso*pyro*pheophorbide *a* methyl ester (2a).

184.3 mg (0.335 mmol) of **1a** was dissolved in 50 ml of DCM and argon was bubbled through the reaction mixture over 20 min. Subsequently 71.1 mg (0.335 mmol) of NO_2BF_4*pyridine complex was added and the mixture was stirred for 4.5 h at r.t. under argon atmosphere. After TLC monitoring indicated that starting material was consumed the mixture was transferred to separating funnel and washed with water and brine. Organic layer was then separated, solvent was evaporated and flash column chromatography (silica, EtOAc/Hex 1:1) was done to obtain 150.9 mg (75.6 %) of pure product; mp 134-137 ^{o}C (lit.,[6b] 145-146 ^{o}C); λ_{max}(DCM)/nm 408 (ε/dm^3·mol^{-1}·cm^{-1} 62317), 507 (4876), 541 (6483), 615 (4166), 671 (25952); ν_{max}/cm^{-1} 2964, 2930 and 2872 (C-H), 1735 (C=O), 1694 (C=O) and 1350 (N=O); ^{1}H NMR (300 MHz, $CDCl_3$, 27^{o}C) δ 9.41 (1H, s), 9.39 (1H, s), 5.18 (1H, d, *J*= 20.1 Hz), 5.11 (1H, d, *J*=20.1 Hz), 4.74 (1H, m), 4.23 (1H, m), 3.80 (2H, q, *J*=15.9, 7.5 Hz), 3.60 (3H, s), 3.58 (2H, q, *J*=15.9, 7.5 Hz), 3.56 (3H, s), 3.18 (3H, s), 3.09 (3H, s), 2.55 (2H, m), 2.17 (2H, m), 1.70 (3H, t, *J*=7.5 Hz), 1.65 (3H, t, *J*=7.5 Hz), 1.53 (2H, d, *J*=7.1 Hz), 0.82 (1H, s), -1.88 (1H, s); was found to match literature values[6b]; ^{13}C NMR (300 MHz, $CDCl_3$, 27^{o}C) δ 195.6, 173.4, 163.8, 161.8, 154.0, 151.7, 149.2, 145.2, 144.9, 139.2, 136.8, 135.0, 134.2, 131.8,

130.8, 128.1, 126.9, 107.2, 105.8, 100.8, 52.7, 51.9, 48.3, 48.0, 30.9, 30.0, 21.9, 19.5, 19.4, 17.5, 17.1, 12.1, 11.3, 11.2; ESI-MS (M^+) 596.2860 (calc. for $C_{34}H_{38}N_5O_5$ 596.2867).

Methyl 20-trifluoroacetamidemeso*pyro*pheophorbide *a* (3):

In 2-neck flask, equipped with septum, to the solution of 30 mg (0.05mmol) of **2a** in 20ml of dry THF/EtOH (1:1) were added 3 mg of Pt/C. Air was removed from the reaction mixture by argon bubbling over 20 min then the mixture was set under H_2-atmosphere and stirred for 1h. After TLC monitoring indicated that the starting material was consumed, the atmosphere was changed back to argon, 8.5 µl (6 mmol) of TFA were injected into reaction vessel, temperature raised to 60^{o}C, followed by additional 19 µl (12 mmol) of TFA after 10 min. After the reaction mixture was heated over 1h the solvents were removed in vacuo on cold bath, 15ml of dry toluene added to dissolve solid residue. Thereafter 12µl (0.15 mmol) of pyridine and 8.5 µl (6 mmol) of TFAA were added into reaction mixture, temperature was raised to 110 ^{o}C, followed by addition of 12.5 µl of TFAA (15 mmol) after 15 min. After 1h heating the reaction mixture was cooled to ambient temperature, evaporated to dryness and purified by column chromatography (eluent DCM/MeOH 20:1), yielding 17 mg (52%) of **3**; mp 233-235 ^{o}C; λ_{max}(CH_3CN:H_2O 95:5)/nm 407 (ε/dm^3·mol^{-1}·cm^{-1} 45200), 504 (4745), 536 (5255), 606 (4303), 662 (20028); ν_{max}/cm^{-1} 2964, 2930 and 2871 (C-H), 1690 (C=O), 1673 (C=O), and 1161 (C-F); ^{1}H NMR (500MHz, $CDCl_3$, 27^{o}C) δ 9.54 (1H, s, 10-H), 9.39 (1H, s, 5-H), 9.09 (1H, s, CF_3CONH, br), 5.14 (1H, d, $^2J_{gem}$=21.1 Hz, 13^2-H), 5.10 (1H, d, $^2J_{gem}$=18.7 Hz, 13^2-H), 4.54-4.12 (2H, m, 18-H and 17-H), 3.82 (2H, q, *J*=6.9 Hz, 3^1-H), 3.71 (2H, q, *J*=7.5 Hz, 8^1-H), 3.67 (3H, s, 12^1-H), 3.48 (3H, br s, 17^5-H), 3.27 (6H, br s, 2^1-H and 7^1-H), 2.10-2.64 (4H, m, 17^1-H and 17^2-H), 1.63-1.76 (6H, m, 8^2-H and 3^2-H), 1.54 (3H, br s, 18^1-H), 0.93 (1H, br s, NH), -1.79 (1H, br s, NH); ^{13}C NMR (300MHz, $CDCl_3$, 27^{o}C) δ 196.1, 173.7, 170.9, 160.6, 154.1, 151.4, 148.8, 145.3, 144.5, 139.4, 139.0, 136.6, 134.9, 131.4, 129.8, 129.0, 122.6, 118.8 and 114.9 (CF_3), 106.6, 105.0, 101.9, 98.4, 51.7 (17^5-C, 17-C, 18-C), 48.2 and 47.8 (13^2-C), 29.9 and 29.7 (17^1-C, 17^2-C), 21.0 (18^1-C), 19.7 and 19.3 (8^1-C, 3^1-C), 17.6 (8^2-C), 17.1 (3^2-C), 14.2 (2^1-C), 12.3 (12^1-C), 11,4 (7^1-C); HRMS: 661.2889 (calc. for $C_{36}H_{38}F_3N_5O_4$ 661.2876).

20-(trifluoroacetamide)-mesopyropheophorbide *a* aza-18-crown-6-amide (4).

34.9 mg (0.053 mmol) of **3** was dissolved in 30% HCl (10 ml) and mixture was stirred for 3 h under argon in darkness. Afterward the reaction mixture was transferred to separating funnel

and DCM was added for extraction. pH of the mixture was adjusted to 5 by treatment with NaOH and $NaHCO_3$. Thereafter organic layer was washed with brine and then separated, solvent was evaporated and column chromatography (silica, CH_2Cl_2/MeOH 10:1) was done to obtain 34.0 mg of dark solid compound (hydrolyzed methyl ester). Thus obtained acid was freshly without characterization dissolved with 18-aza-crown-6 (13.8 mg, 0.053 mmol) in 35 ml of dry DCM. After that EDC (11.2 mg, 0.058 mmol) was added and RM was stirred under Ar atmosphere at RT for 3 h. After full conversion of starting product (TLC control) mixture was additionally diluted by DCM, transferred into separating funnel and washed with water. Organic phase was separated, solvent was evaporated and column chromatography (silica, DCM/MeOH 10:1) was done to obtain 40.2 mg (72.8 %) of pure product; mp 143-145 ^oC λ_{max}(DMF:H_2O 92:8)/nm 410 (ε/$dm^3 \cdot mol^{-1} \cdot cm^{-1}$ 111802), 507 (9814), 538 (11977), 609 (9256), 665 (49477); ν_{max}/cm^{-1} 2963, 2930 and 2869 (C-H), 1734 (C=O), 1696 (C=O), 1614 (C=O) and 1125 (C-F); ^{1}H NMR (500 MHz, DMF-d_7, 27 ^oC) δ 12.66 (1H, $CF_3CO\underline{N}H$), 9.91 (1H, s), 9.64 (1H, s), 5.38 (1H, d, *J*=19.6 Hz), 5,28 (1H, d, *J*=19.6 Hz), 4.50 (1H, m), 4.42 (1H, m), 4.03 (2H, q, *J*=7.5 Hz), 3.75 (2H, q, *J*=7.5 Hz), 3.68 (3H, s), 3.43 (3H, s), 3.38-2.33 (29H, m), 1.99 (2H, m), 1.74 (3H, t, *J*=7.5 Hz), 1.70-1.62 (6H, m), 0.92 (1H, N-$\underline{H}$), -1.83 (1H, N-$\underline{H}$); ^{13}C NMR (500 MHz, DMF-d_7, 27^oC) δ 195.6, 172.7, 171.9, 161.9, 158.7 ($CF_3\underline{C}O$, *J*=36.8 Hz), 154.0, 151.6, 148.3, 145.5, 144.6, 139.3, 138.9, 136.9, 134.9, 131.5, 130.3, 129.5, 117.6 ($\underline{C}F_3$), 107.6, 105.3, 105.3, 104.1, 98.2, 70.2 (7C), 69.3, 69.0, 68.6, 51.9, 48.7, 48.5, 48.2, 46.5, 30.3, 28.2, 20.9, 19.1, 19.0, 17.4, 17.1, 13.8, 10.7; ESI-MS (M^+) 893.4402 (calc. for $C_{47}H_{60}F_3N_6O_8$ 893.4419).

UV-vis spectra

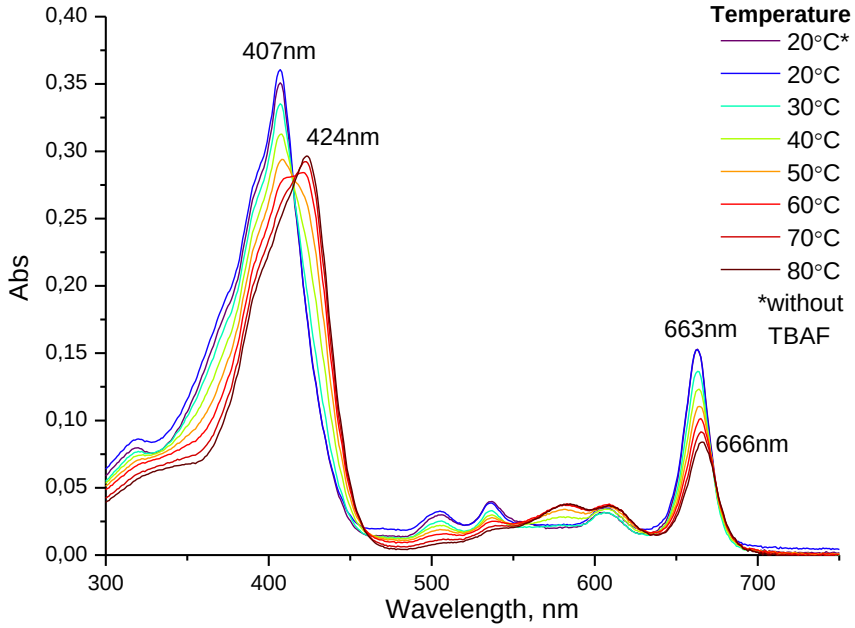


Fig. S1. Variable temperature measurements of **3** in MeCN:H_2O (95:5) with 150 eq. of TBAF ($1.45 \cdot 10^{-5}$ M).

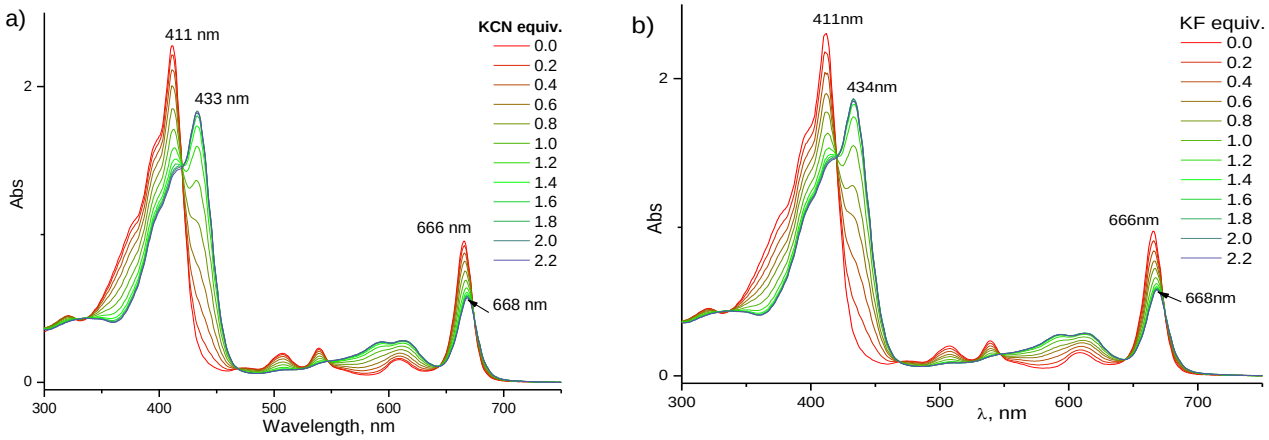
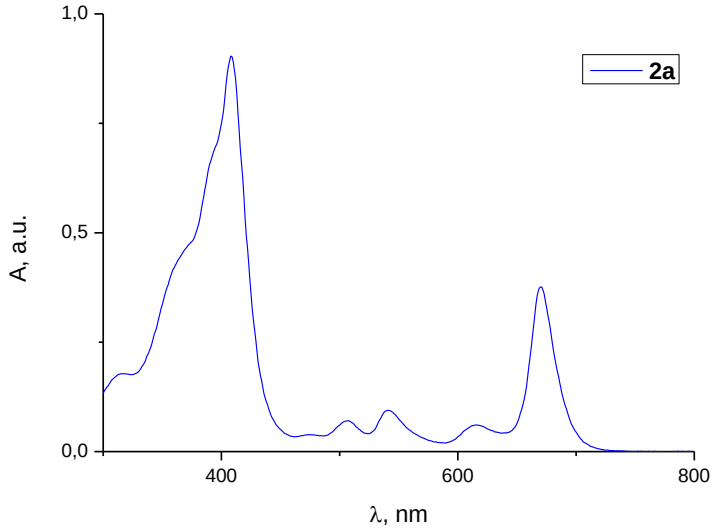
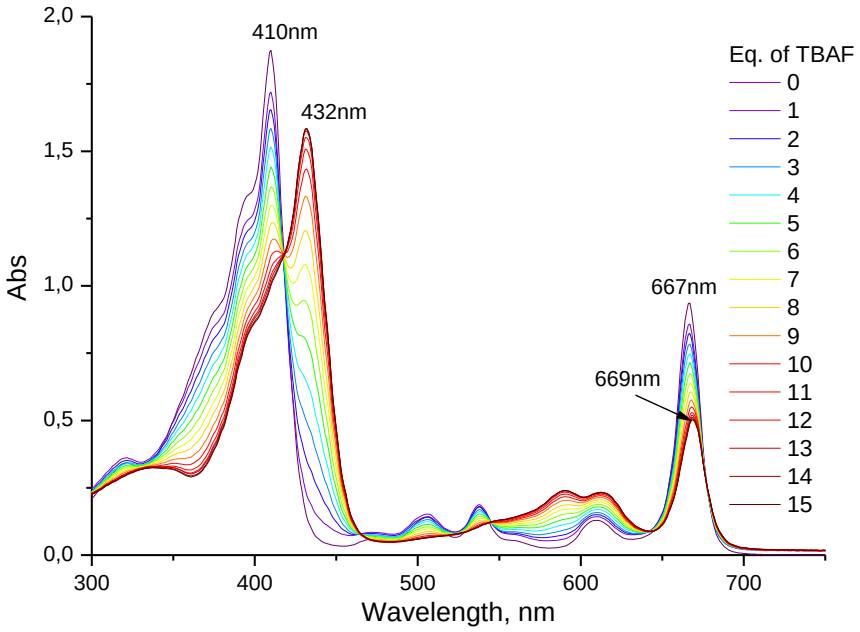


Fig. S2. The titration of **4** a) with KCN and b) with KF in DMSO:H_2O (95:5) ($2.466 \cdot 10^{-5}$ M).

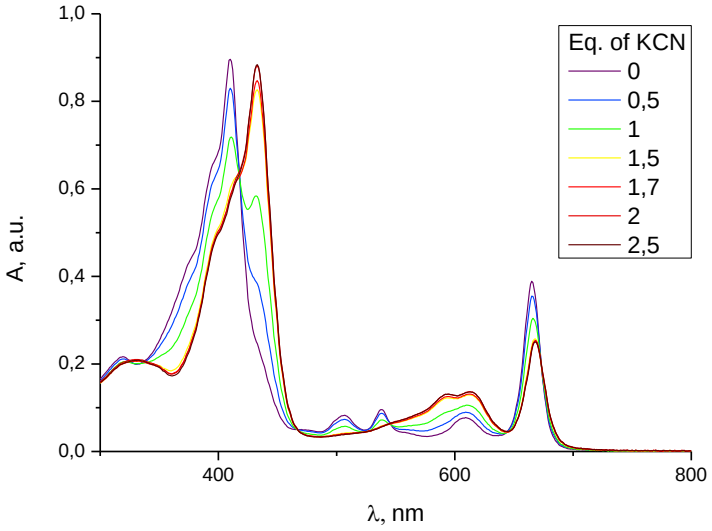


UV-vis characterization of **2a** in DCM ($1.208 \cdot 10^{-5}$ M)

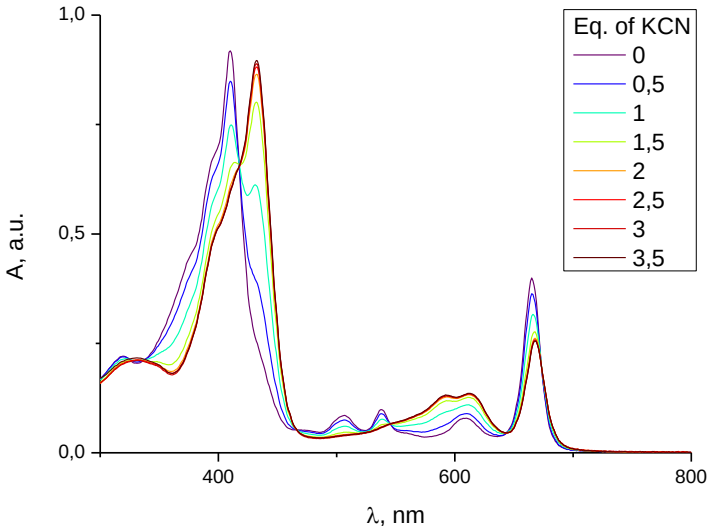


Titration of **3** by TBAF in $CHCl_3$ ($1.45 \cdot 10^{-5}$ M)

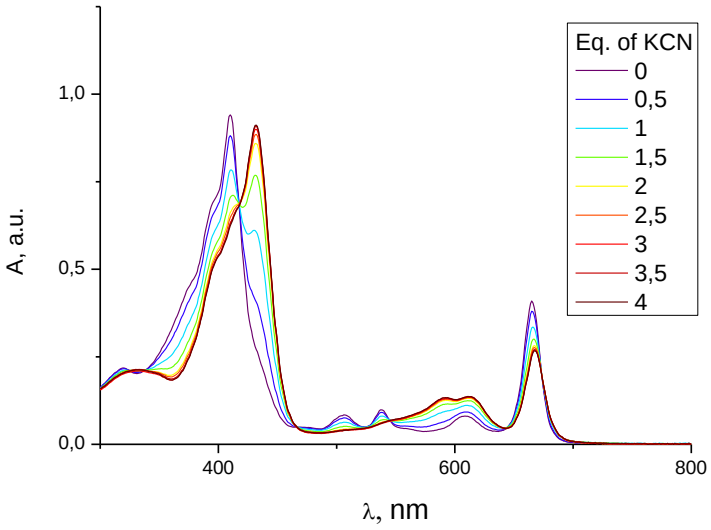
The following 18 spectra related to Fig. 4a in the main body text:



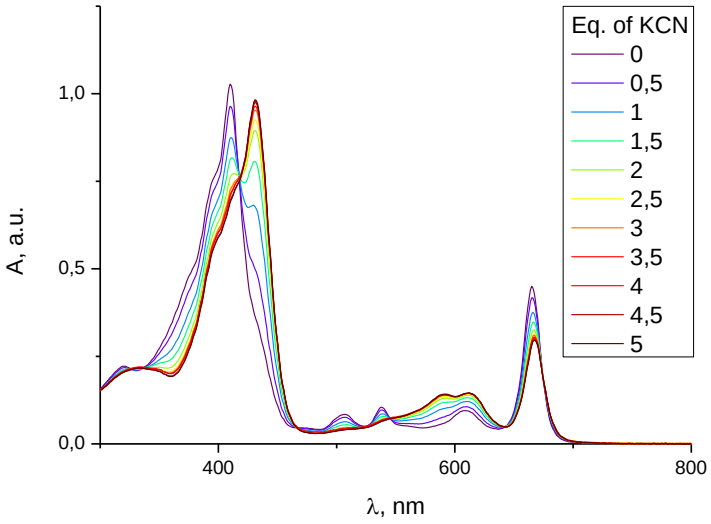
Titration of **4** by KCN in DMF:H_2O 99:1 system ($8.6 \cdot 10^{-6}$ M)



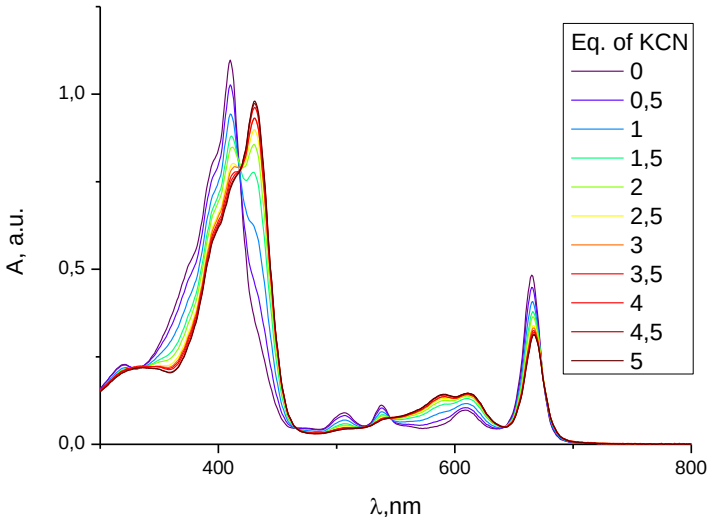
Titration of **4** by KCN in DMF:H_2O 98:2 system ($8.6 \cdot 10^{-6}$ M)



Titration of **4** by KCN in DMF:H_2O 97:3 system ($8.6 \cdot 10^{-6}$ M)



Titration of **4** by KCN in DMF:H_2O 96:4 system ($8.6 \cdot 10^{-6}$ M)



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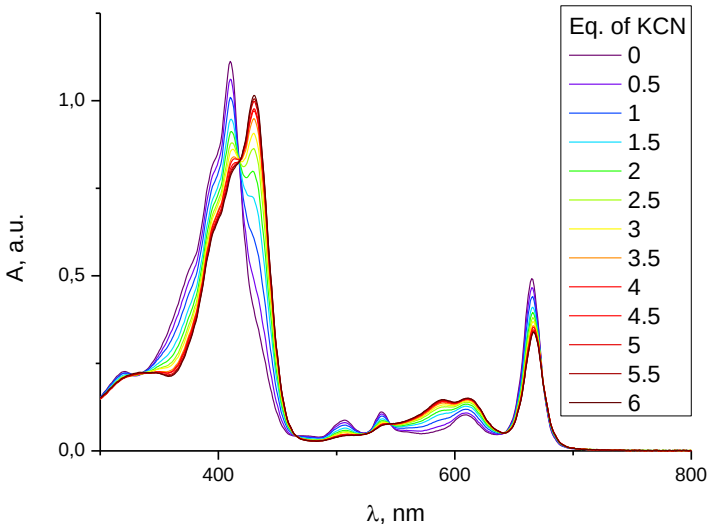
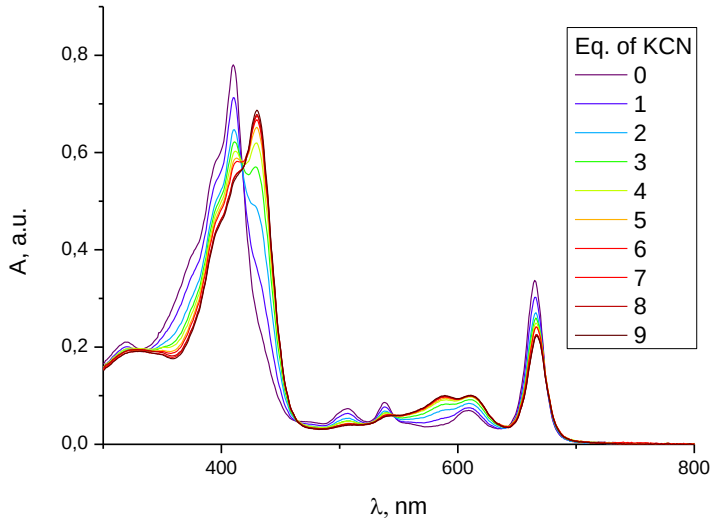
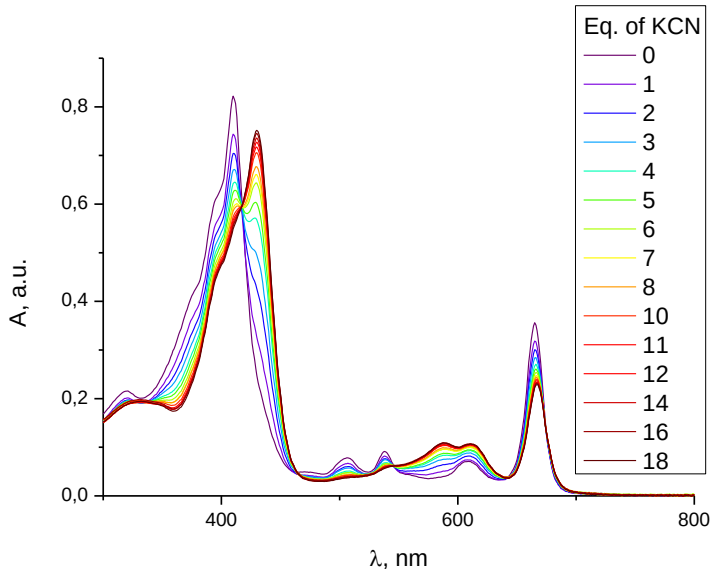


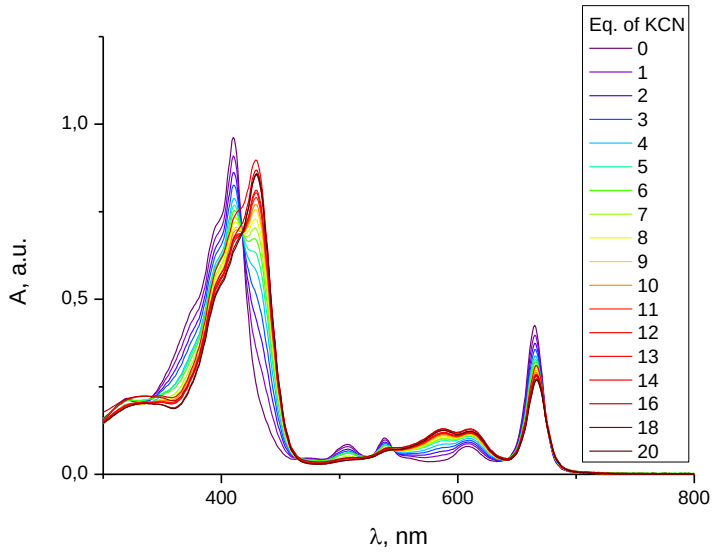
Titration of **4** by KCN in DMF:H_2O 94:6 system ($8.6 \cdot 10^{-6}$ M)



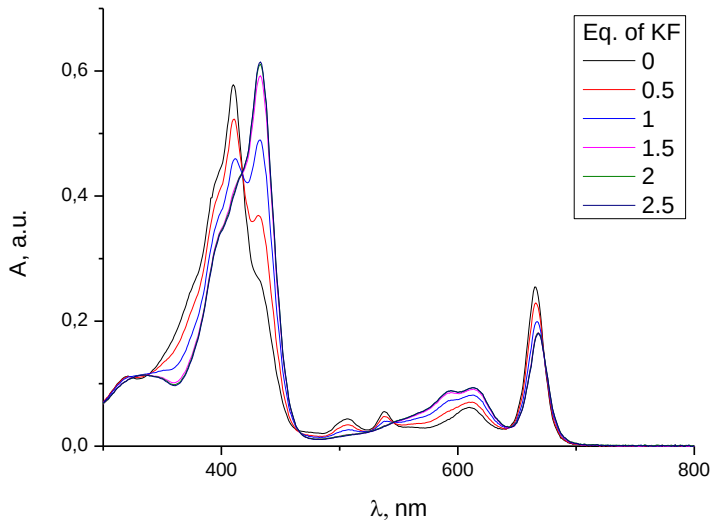
Titration of **4** by KCN in DMF:H_2O 93:7 system ($8.6 \cdot 10^{-6}$ M)



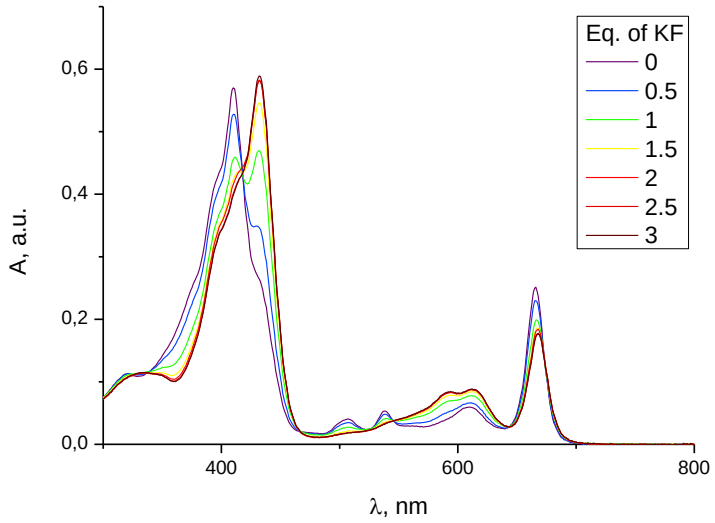
Titration of **4** by KCN in DMF:H_2O 92:8 system ($8.6 \cdot 10^{-6}$ M)



Titration of **4** by KCN in DMF:H_2O 91:9 system ($8.6 \cdot 10^{-6}$ M)



Titration of **4** by KF in DMF:H_2O 99:1 system ($8.6 \cdot 10^{-6}$ M)



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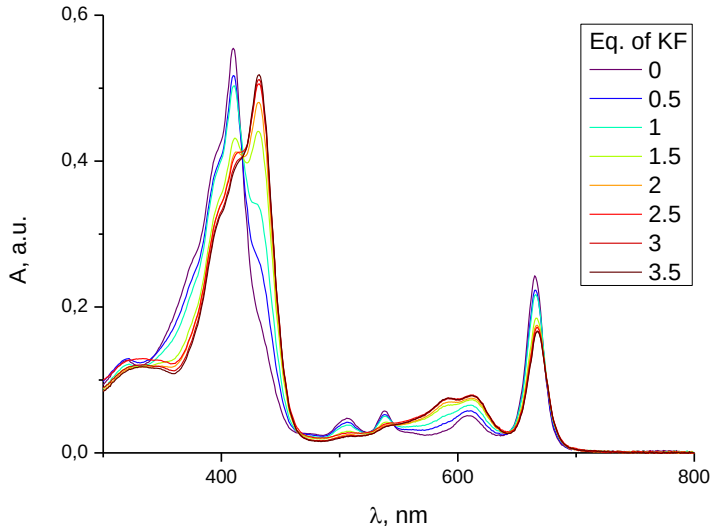
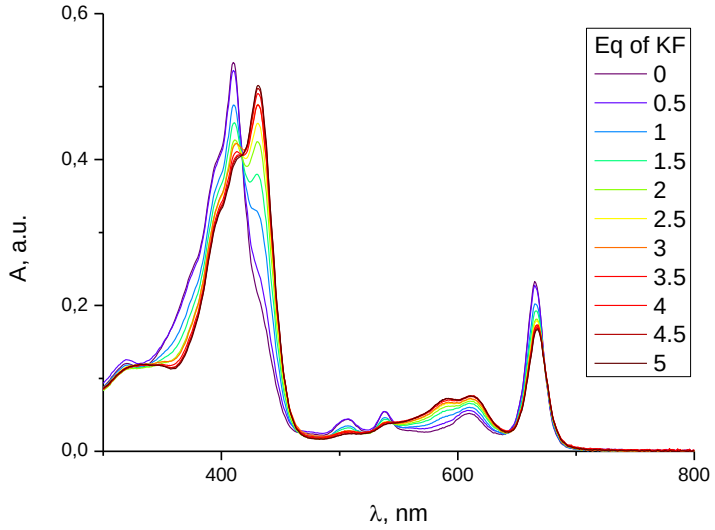
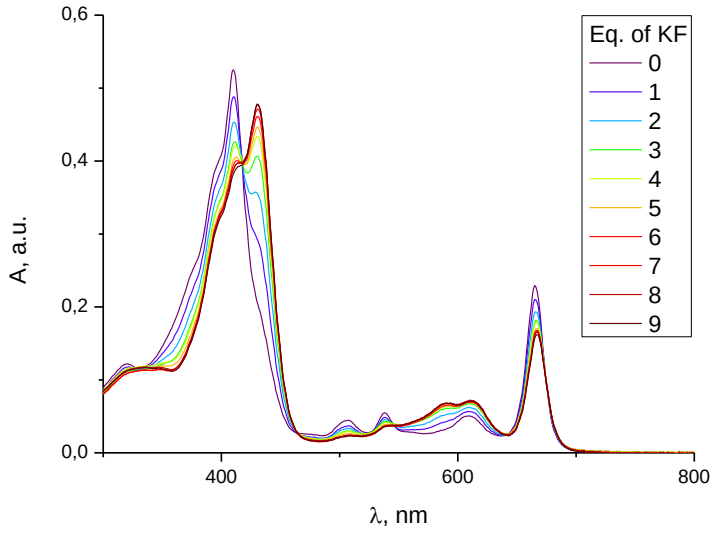


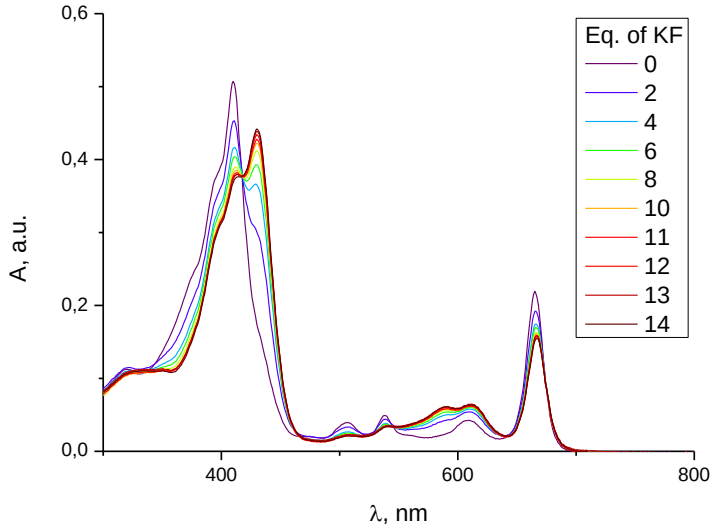
Titration of **4** by KF in DMF:H_2O 97:3 system ($8.6 \cdot 10^{-6}$ M)



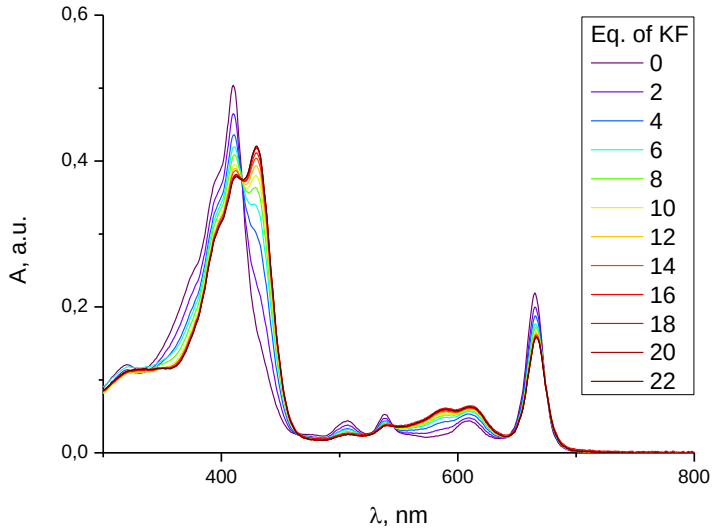
Titration of **4** by KF in DMF:H_2O 96:4 system ($8.6 \cdot 10^{-6}$ M)



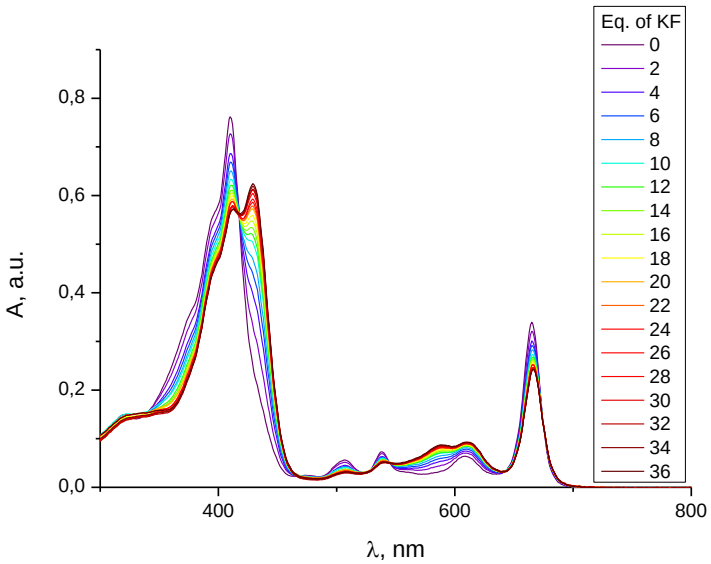
Titration of **4** by KF in DMF:H_2O 95:5 system ($8.6 \cdot 10^{-6}$ M)



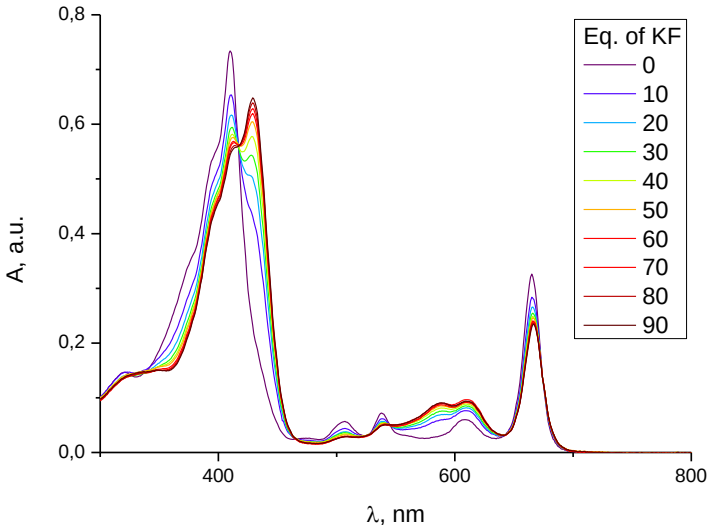
Titration of **4** by KF in DMF:H_2O 94:6 system ($8.6 \cdot 10^{-6}$ M)



Titration of **4** by KF in DMF:H_2O 93:7 system ($8.6 \cdot 10^{-6}$ M)

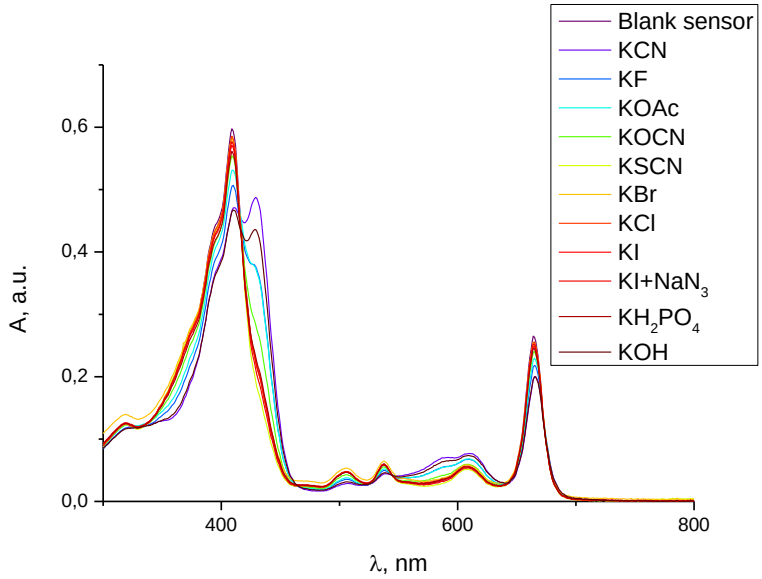


Titration of **4** by KF in DMF:H_2O 92:8 system ($8.6 \cdot 10^{-6}$ M)

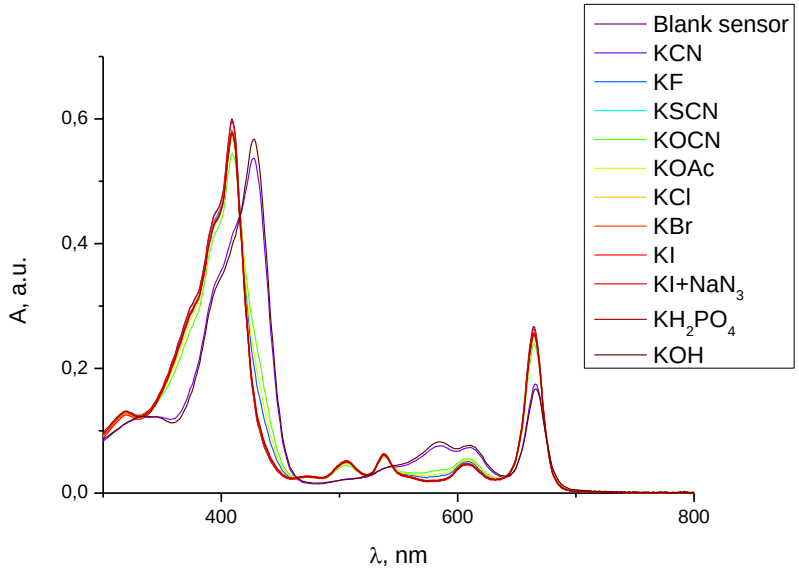


Titration of **4** by KF in DMF:H_2O 91:9 system ($8.6 \cdot 10^{-6}$ M)

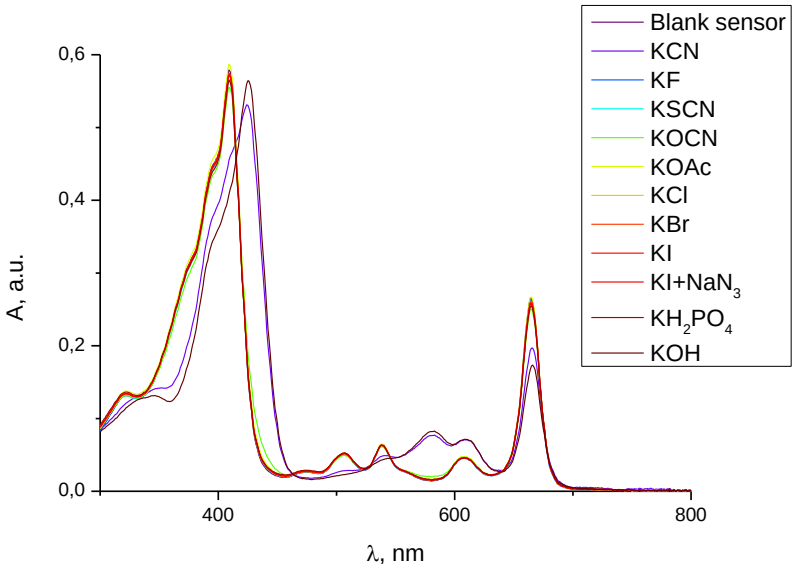
*The following spectra related to Fig. **4b** in main body:*



Titration of **4** by 2.5 eq. excess of various anions in DMF:H_2O 94:6 system ($8.6 \cdot 10^{-6}$ M)



Titration of **4** by 25 eq. excess of various anions in DMF:H_2O 75:15 system ($8.6 \cdot 10^{-6}$ M)

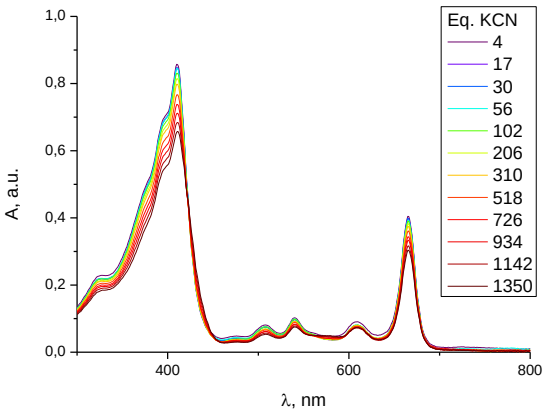


Titration of **4** by 40 eq. excess of various anions in DMF:H_2O 70:30 system ($8.6 \cdot 10^{-6}$ M)

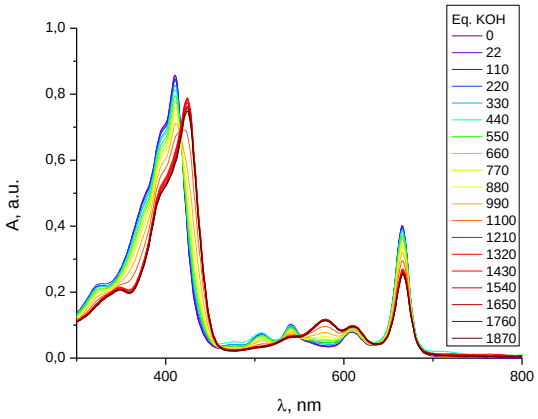
Buffer titrations

DMF/H_2O 1:1 system (with an excess of water)

C(sensor) = $8.6*10^{-6}$ M; 1000 eq. of KH_2PO_4, 1000 eq. of K_2HPO_4.



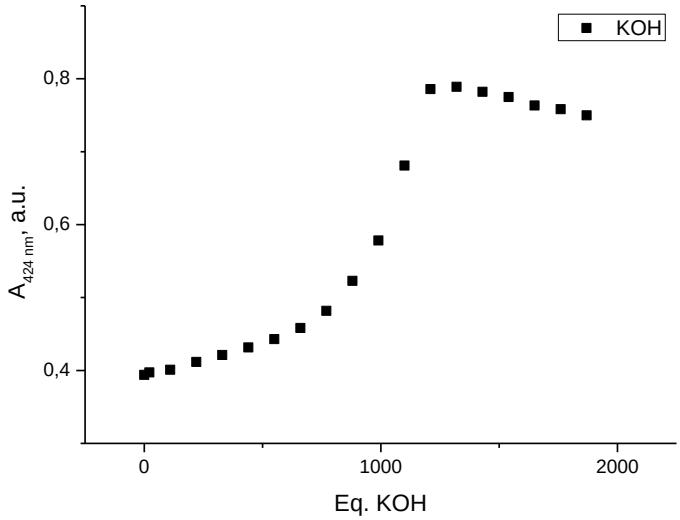
Titration with KCN



Titration with KOH.

Response from KCN was very weak due to strong due to the *buffer* influence. Complete change with KOH takes 1200 equiv (buffer capacity), while addition of same amount of KCN causes only dilution effect.

Monitoring KOH titration absorbance at λ_{max}=424 nm below reveals buffering capacity and dilution effect.

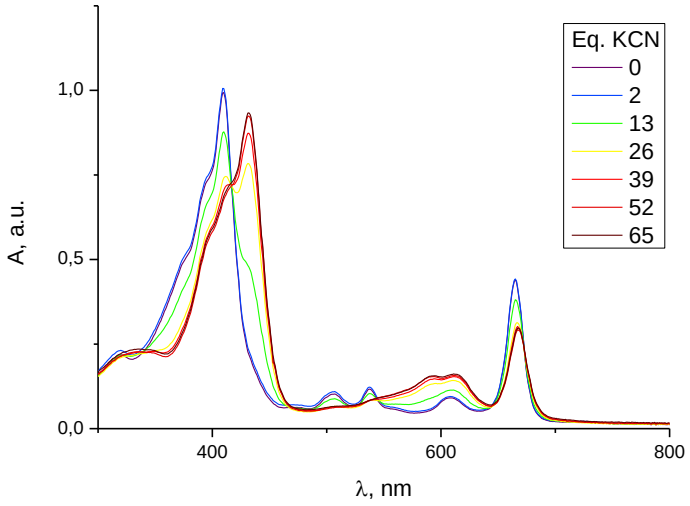


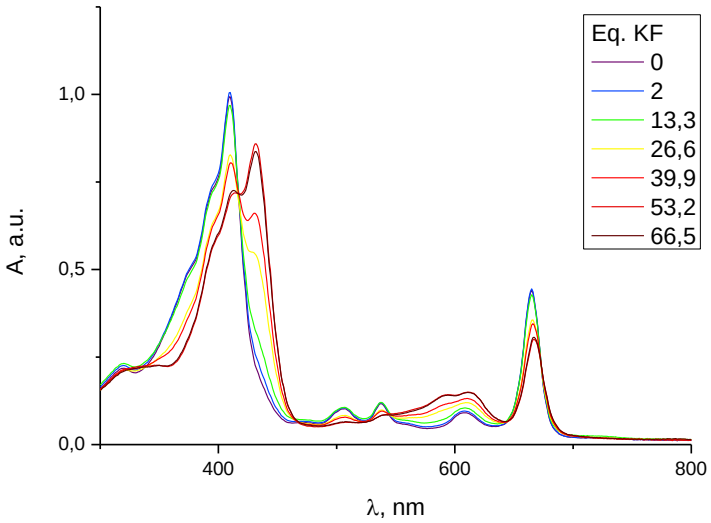
BUFFER TITRATIONS WITH CONSTANT H_2O AMOUNT.

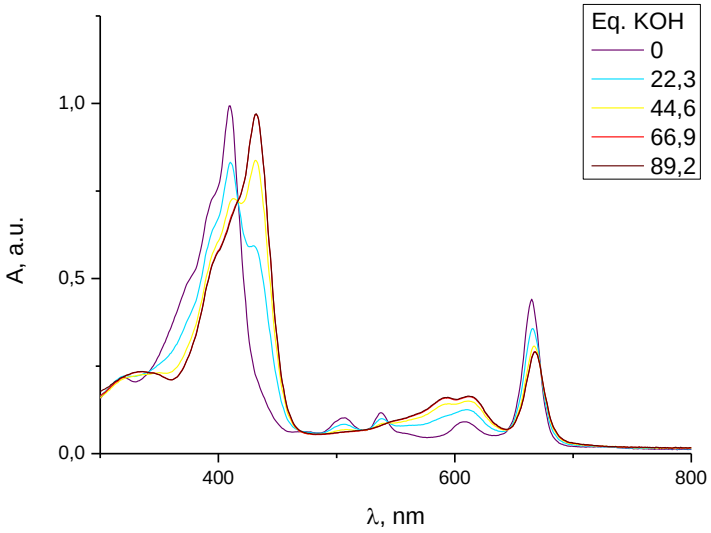
Following three titrations below were performed with constant amount of H_2O (2%).

DMF:H_2O 98:2

100 eq. Na_2HPO_4, 100 eq. NaH_2PO_4; C(sensor)=8.96*10^{-6} M

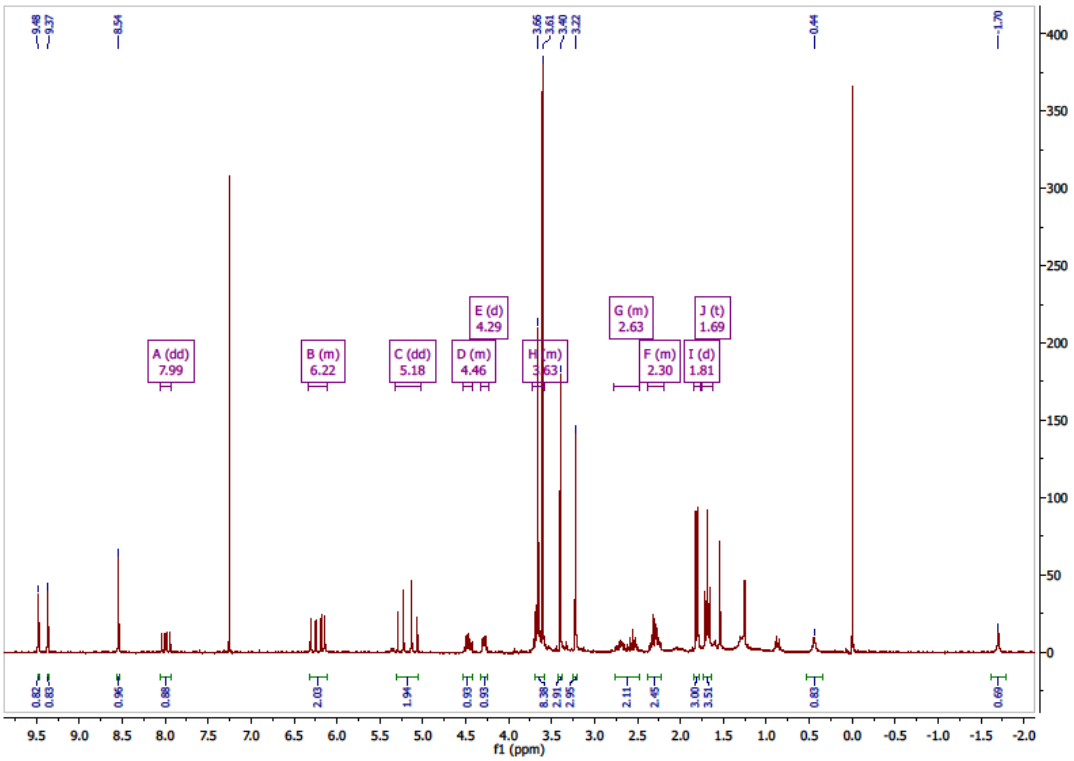




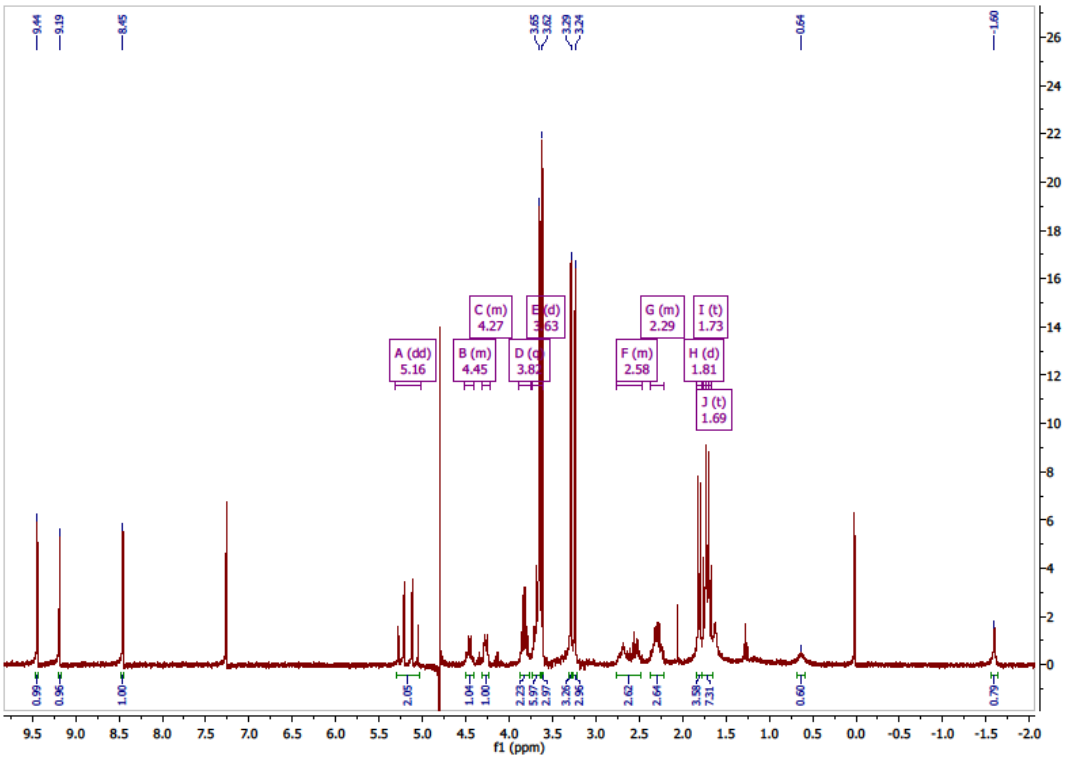


A comparison of the three titrations indicates that for an addition of ~20 equiv. of KCN causes such spectral chances for which twice as much i.e. ~40 equiv. of KF and KOH are needed.

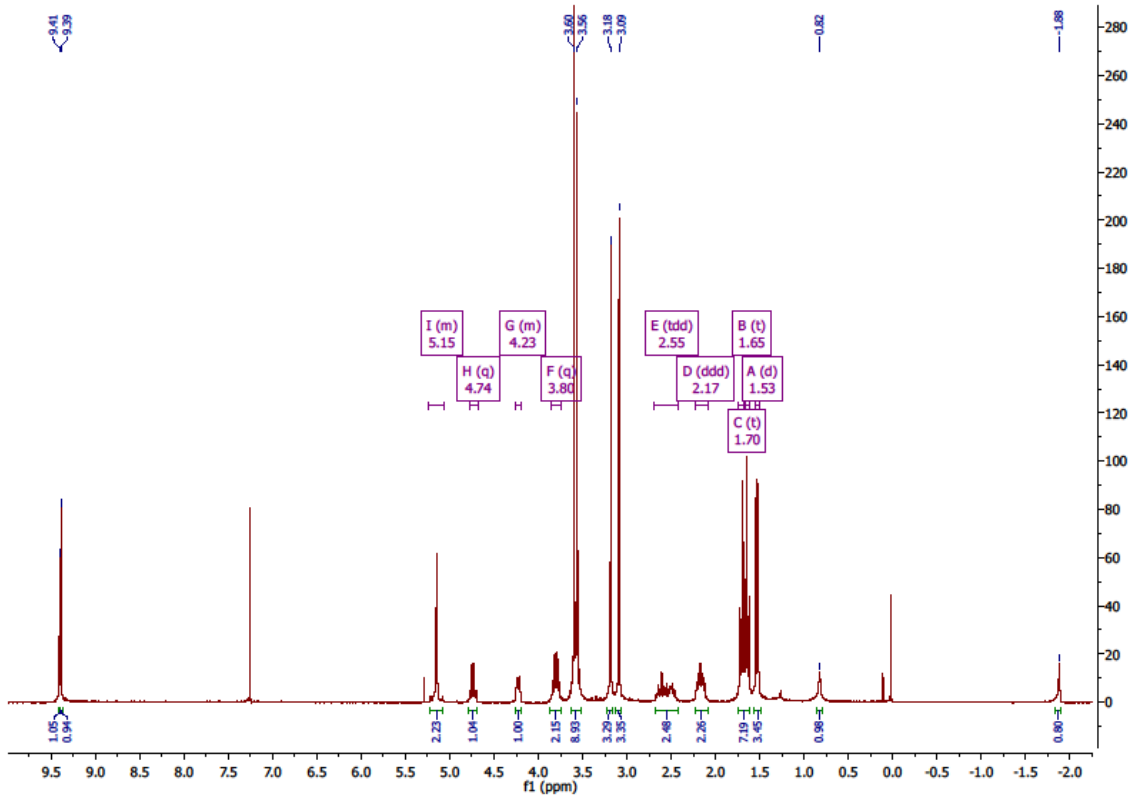
NMR spectra



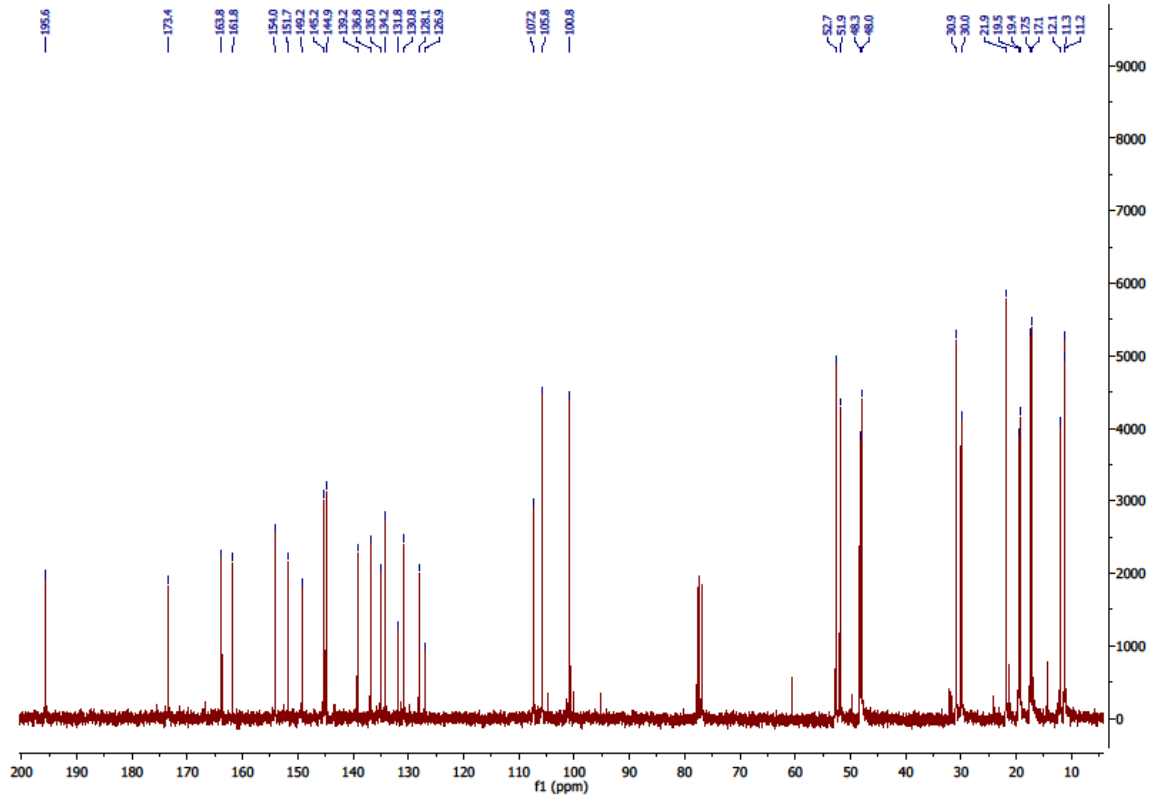
*Pyro*pheophorbide *a* methyl ester (**1b**) ^{1}H NMR



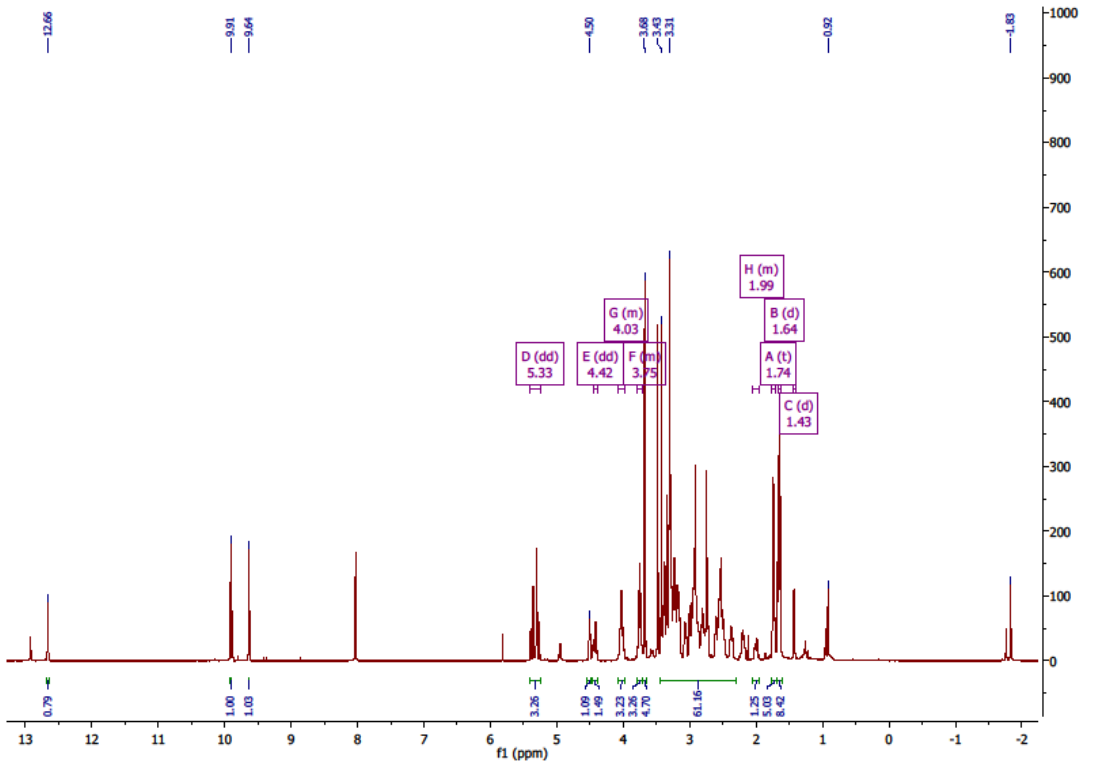
Meso*pyro*pheophorbide *a* methyl ester (**1a**) ^{1}H NMR



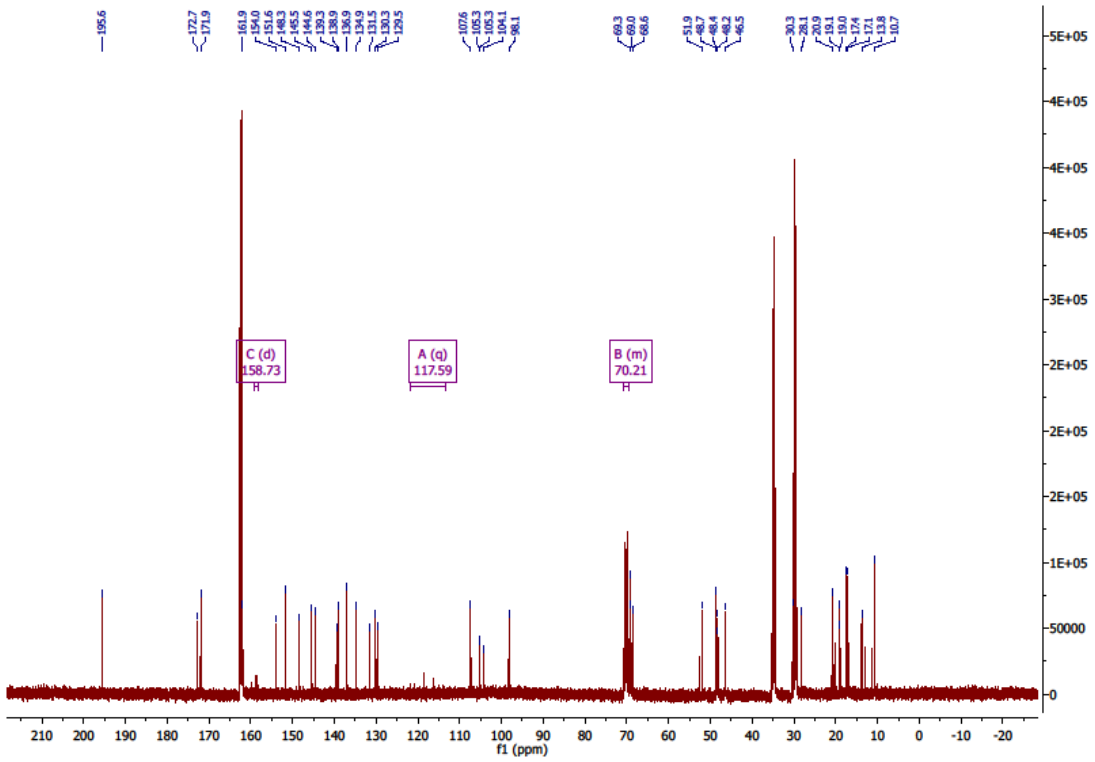
20-nitro-meso*pyro*pheophorbide *a* methyl ester (**2a**) ^{1}H NMR



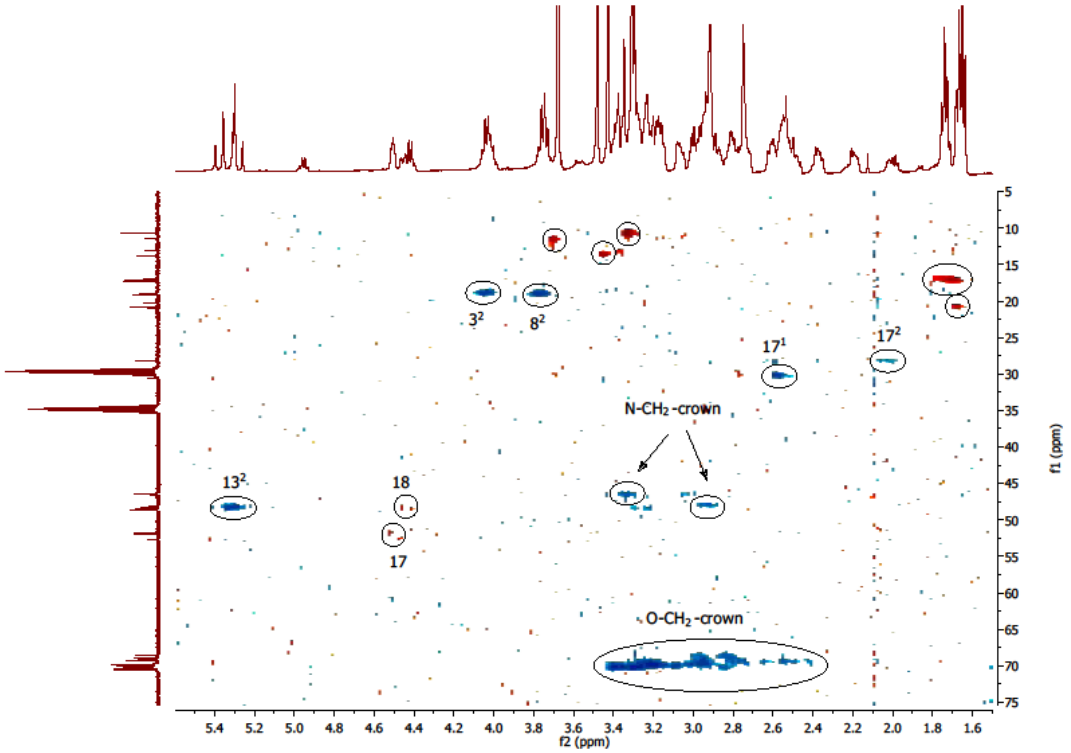
20-nitro-meso*pyro*pheophorbide *a* methyl ester (**2a**) ^{13}C NMR



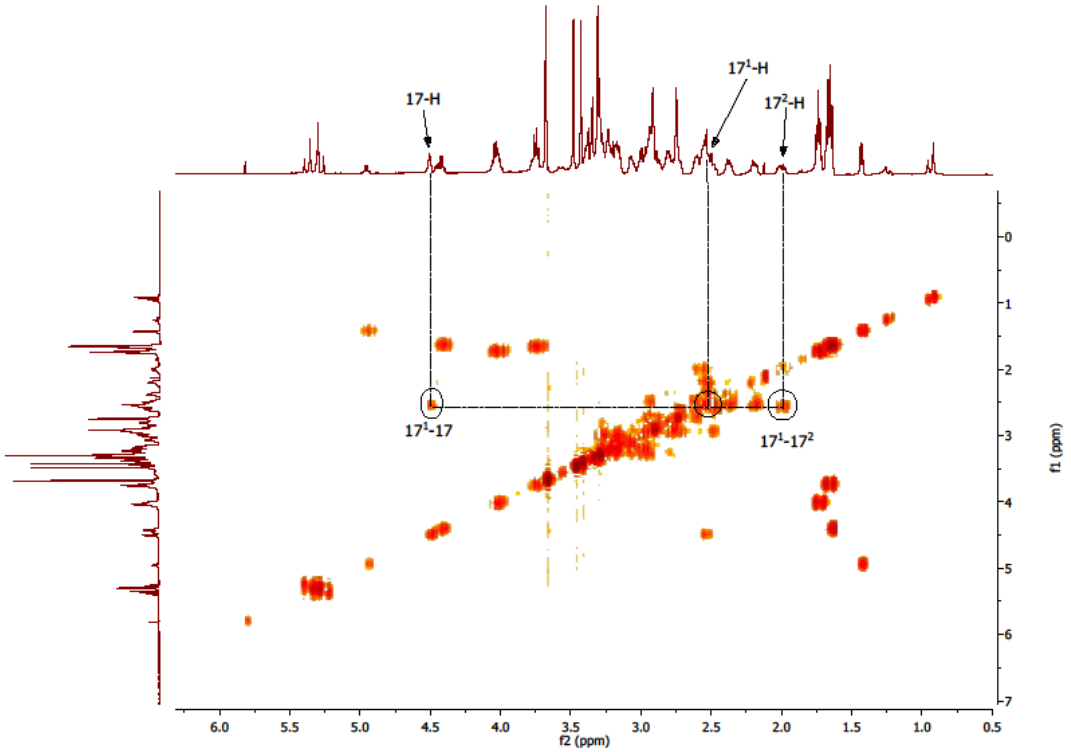
20-(trifluoroacetamide)-mesopyropheophorbide *a* aza-18-crown-6-amide (**4**) ^{1}H NMR



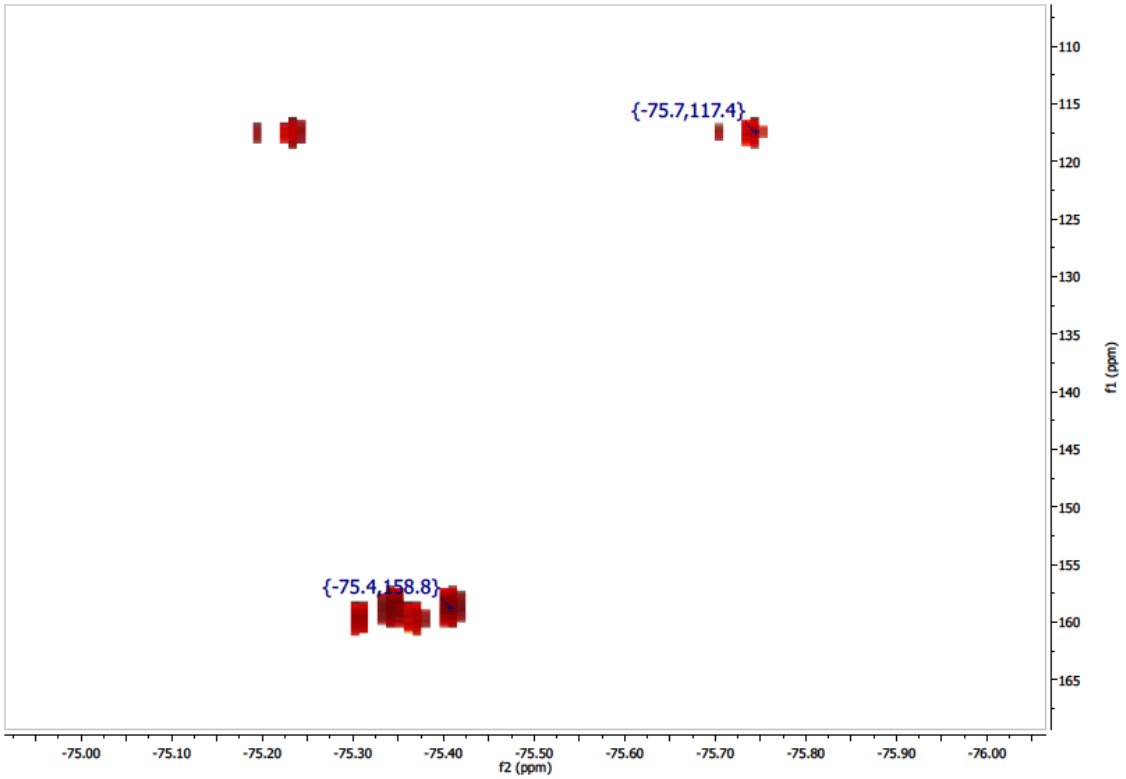
20-(trifluoroacetamide)-meso*pyro*pheophorbide *a* aza-18-crown-6-amide (**4**) ^{13}C NMR



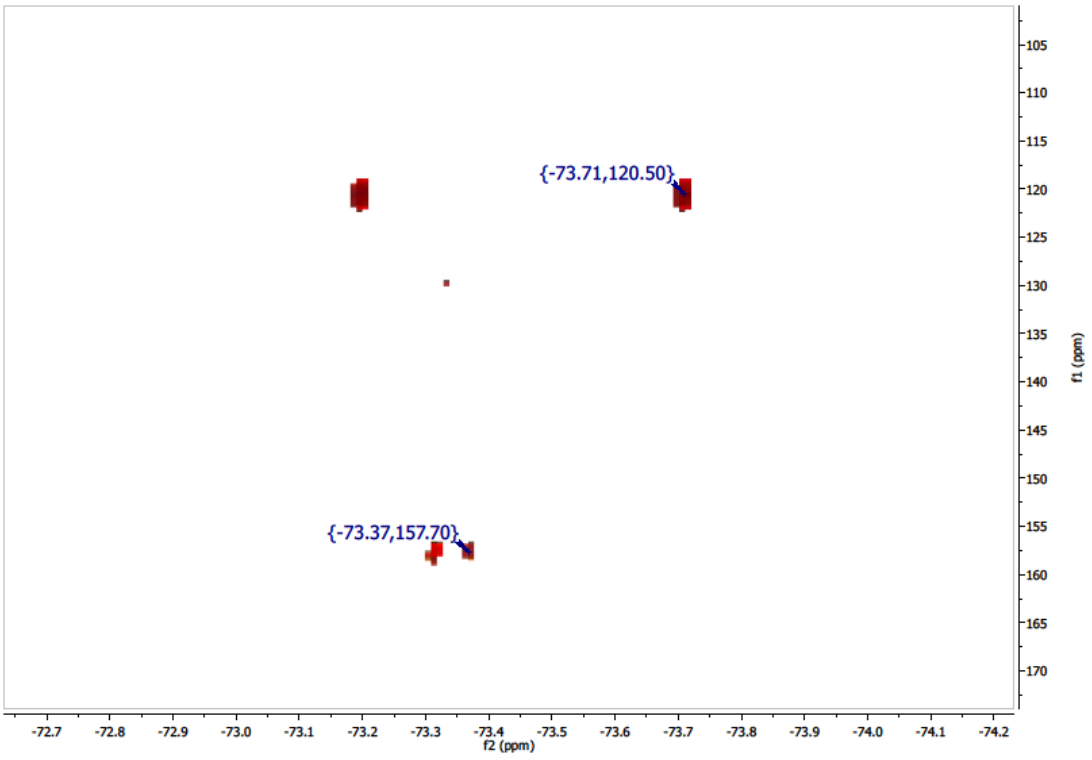
20-(trifluoroacetamide)-meso*pyro*pheophorbide *a* aza-18-crown-6-amide (**4**) ^{1}H -^{13}C HSQC (Multiplicity edit: blue contours – CH_2, red contours – CH and CH_3)



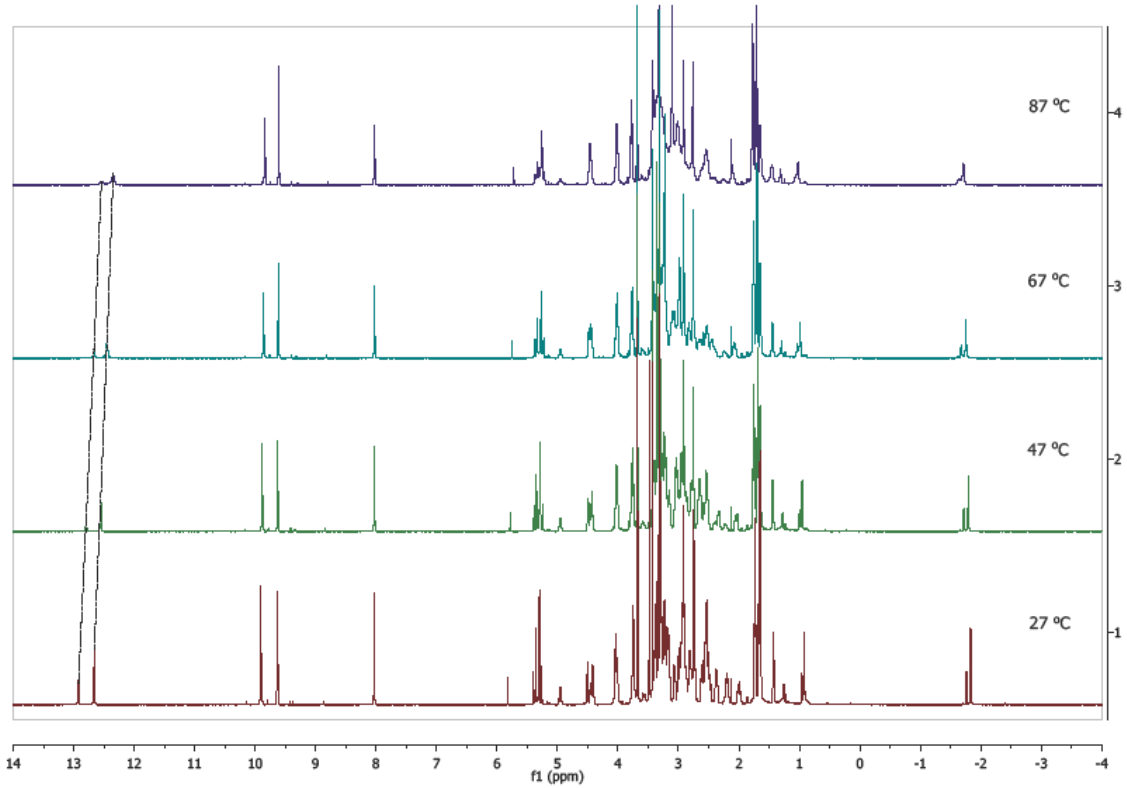
20-(trifluoroacetamide)-meso*pyro*pheophorbide *a* aza-18-crown-6-amide (**4**) ^{1}H-^{1}H COSY



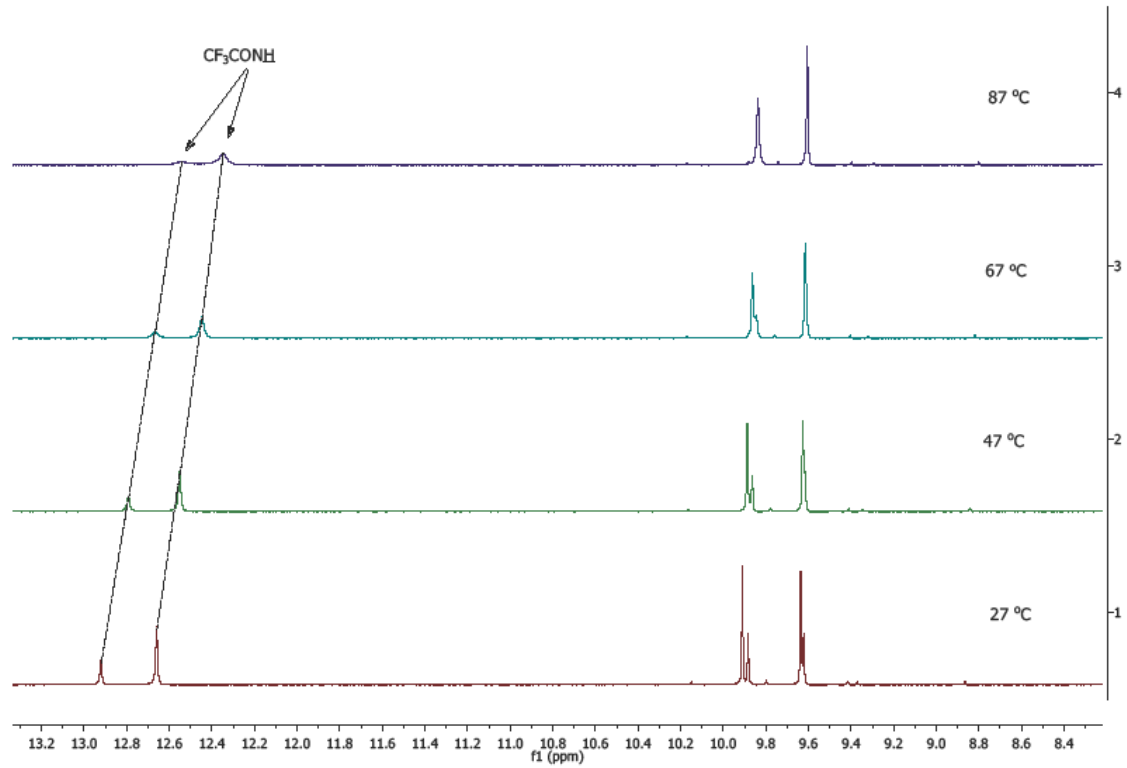
^{19}F-^{13}C HMBC of **4**



^{19}F-^{13}C HMBC of **4** with 3 equiv. of added KF

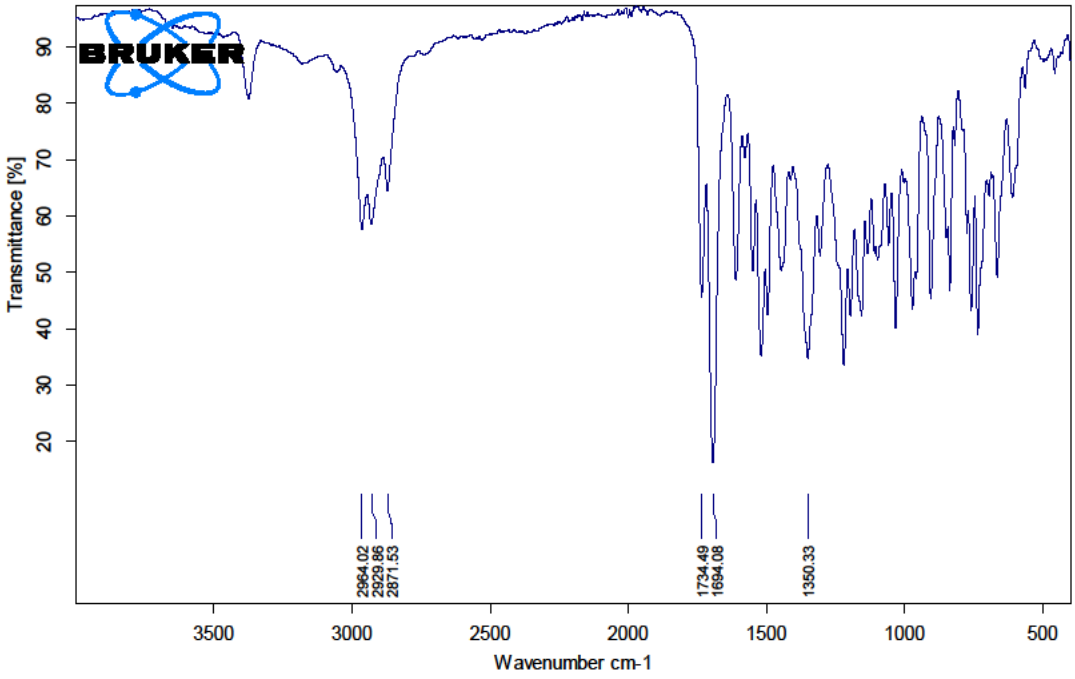


Variable temperature of ^{1}H NMR spectra of **4**

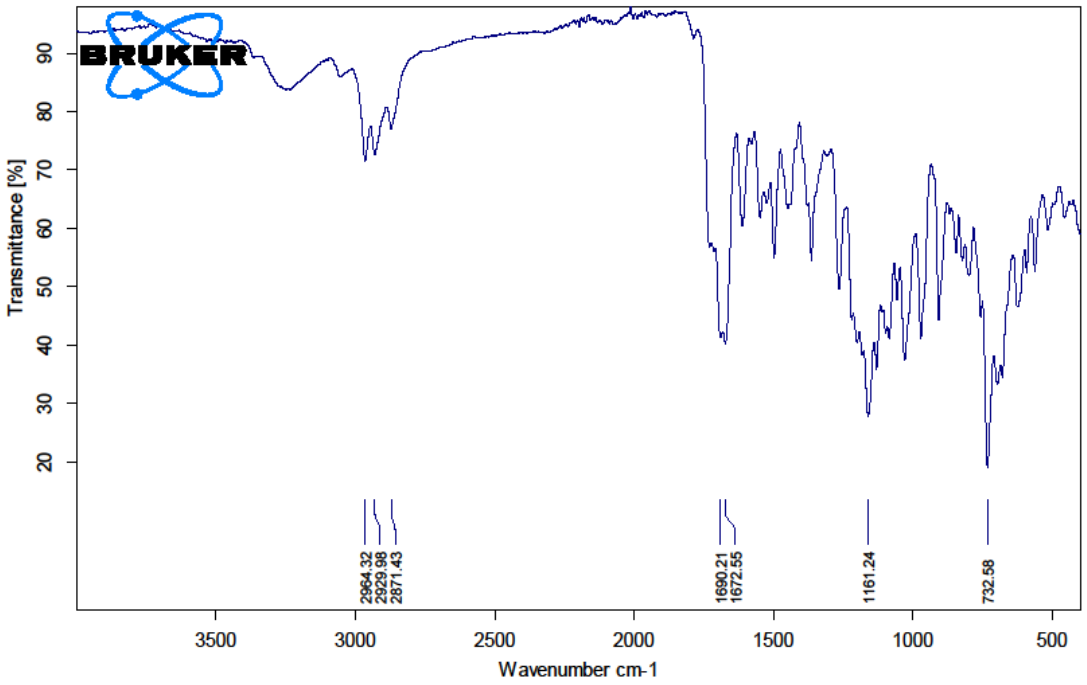


Expanded low field region of the variable temperature ^{1}H NMR spectra of **4**.

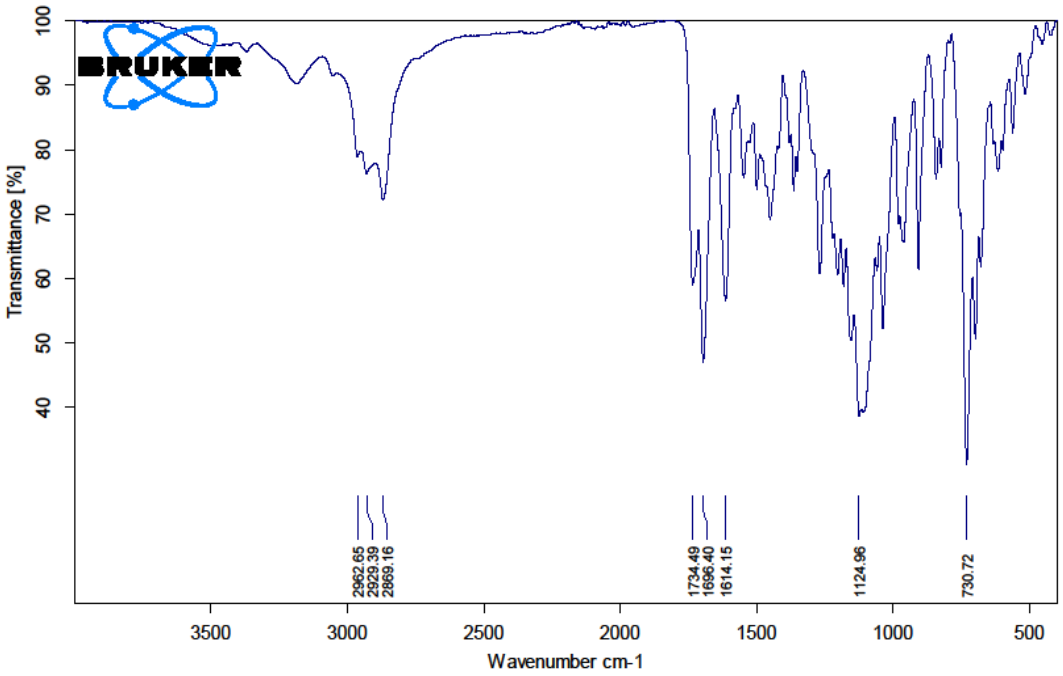
IR spectra



IR spectrum of 20-nitro-meso*pyro*pheophorbide *a* methyl ester (**2a**)



IR spectrum of 20-trifluoroacetamidemeso*pyro*pheophorbide *a* methyl ester (**3**)



IR spectrum of 20-(trifluoroacetamide)-meso*pyro*pheophorbide *a* aza-18-crown-6-amide **(4)**

Computational methods

All computations were performed using Turbomole 6.4 program package.[1] Solvation effects (chloroform) were taken into account using COSMO solvation model (ε = 4.81).[2] The MARI-J approximation was used with suitable auxiliary basis set.[3,4] The structures were first optimized using double ζ quality basis set, def2-SVP,[5] and TPSS-D3 functional.[6-7] Vibrational frequencies were calculated numerically for those structures to obtain the chemical potential in solution at 298.15 K (chem. pot.) and to confirm the nature of the stationary point (minima). The Gibbs free energies were then calculated: G = E(0) + chem. pot.

All structures were then reoptimized with a triple ζ quality basis set, def2-TZVP.[5] Two functionals, TPSS-D3 and PBE-D3[7,8], were both employed and nature of the result was the same in both cases. Structures were only slightly changed with upgrading the basis set, and therefore, due to computational cost, no vibrational frequencies were calculated for def2-TZVP structures. Figures on the structures were made with CylView.[9]

The structures with KCN adduct were also optimized with B3LYP/6-31* in gas phase using Gaussian09.[10]

Results

Table X. The energy difference between **4'** and **4''** with KCN adduct with various methods. The Gibbs free energies were calculated at 298.15 K and only for TPSS-D3/def2-SVP values. Energies are in kcal/mol.

Method	ΔE (**4' – 4''**)	ΔG (**4' – 4''**)
TPSS-D3/def2-SVP	11.5	17.5
TPSS-D3/def2-TZVP	14.3	
PBE-D3/def2-TZVP	11.7	
B3LYP/6-31G*	15.5	

Table X. The energy difference between **4'** and **4''** with KF adduct with various methods. The Gibbs free energies were calculated at 298.15 K and only for TPSS-D3/def2-SVP values. Energies are in kcal/mol.

Method	ΔE (**4' – 4''**)	ΔG (**4' – 4''**)
TPSS-D3/def2-SVP	6.5	9.4
TPSS-D3/def2-TZVP	11.4	
PBE-D3/def2-TZVP	11.9	

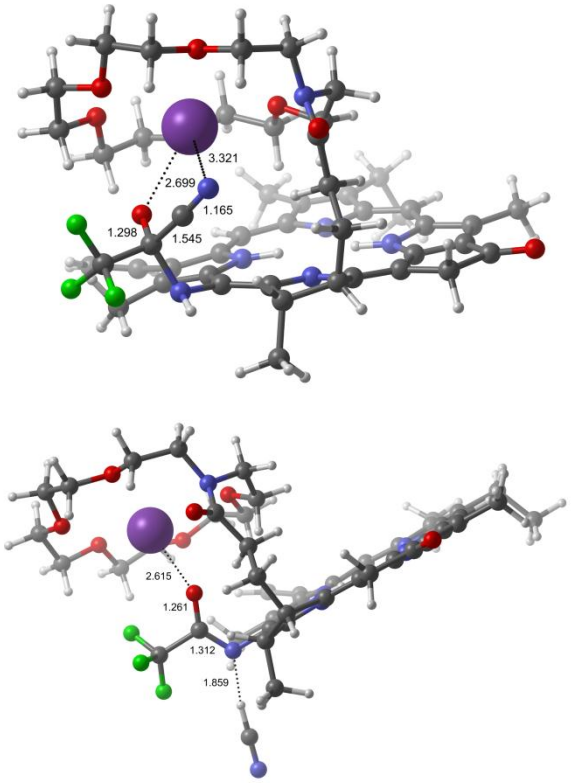


Figure S3. TPSS-D3/def2-TZVP optimized structures of **4'** and **4''** with KCN.

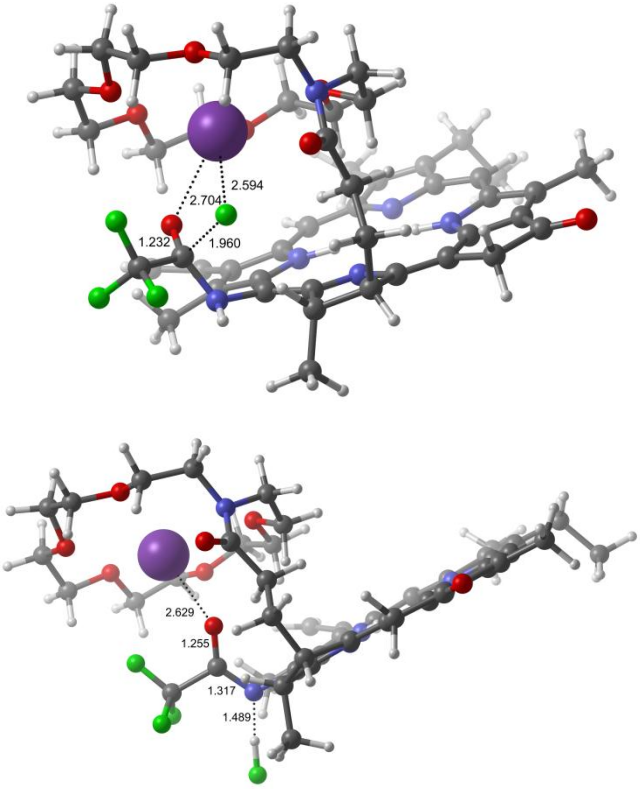


Figure S4. TPSS-D3/def2-TZVP optimized structures of **4'** and **4''** with KF.

Computational References

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10. Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

XYZ coordinates and absolute energies

Energies are in Hartrees unless otherwise noted.

4' with KCN	**4''** with KCN
TPSS-D3/def2-SVP E(0): -3746.3659 chem. pot (298.15 K).: 2312.84 kJ/mol	TPSS-D3/def2-SVP E(0): -3746.384251 chem.pot. (298.15 K): 2287.83 kJ/mol
C -0.173374 -1.116349 2.519740 C 0.261001 -2.444806 3.146025 C -0.695936 -3.442427 2.450778 C -1.809111 -2.505106 1.985185 N -1.403107 -1.199662 1.964087 C 0.618575 0.061470 2.594000 C -3.026623 -2.933349 1.462301 C -3.946874 -2.166208 0.715276 C -5.024041 -2.931351 0.175953 C -5.801367 -2.099765 -0.647264 C -5.163108 -0.810319 -0.590961 N -4.054588 -0.899918 0.257241 C -5.464012 0.395613 -1.249526 C -4.700564 1.569618 -1.112701 C -4.978895 2.847713 -1.776247 C -4.002618 3.720120 -1.339614	C -0.685480 -0.503556 2.221183 C -0.026471 -1.583038 3.082145 C -0.724708 -2.859722 2.552060 C -1.969618 -2.269406 1.897492 N -1.835442 -0.930644 1.655554 C -0.131931 0.795703 2.076035 C -3.084679 -3.004017 1.500793 C -4.192591 -2.529462 0.766408 C -5.180576 -3.525812 0.507828 C -6.207893 -2.953589 -0.260193 C -5.808419 -1.583626 -0.462301 N -4.588347 -1.377074 0.185924 C -6.416624 -0.540936 -1.184324 C -5.855926 0.743562 -1.320721 C -6.440182 1.844448 -2.096360 C -5.555332 2.895938 -1.983132

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C -2.013555 3.492741 0.213263	C -3.339237 3.207088 -0.798279
C -1.048714 2.893106 1.030603	C -2.226179 2.930180 0.007493
C 0.032918 3.590228 1.701381	C -1.126823 3.844264 0.269387
C 0.791990 2.641878 2.399987	C -0.211027 3.191753 1.108596
C 0.207398 1.346814 2.131819	C -0.728192 1.862357 1.349915
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C -4.874804 -4.320111 0.619904	C -4.736867 -4.784311 1.115010
C -3.567443 -4.362026 1.464677	C -3.356065 -4.482964 1.770535
C 0.204725 5.040266 1.642323	C -1.070495 5.196413 -0.286143
C 1.344379 5.743747 1.834469	C 0.028266 5.932331 -0.570400
C -0.041186 -4.177597 1.237519	C 0.147935 -3.628295 1.521329
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C -0.015345 -3.313102 -0.027537	C 0.444221 -2.785994 0.277932
C 1.905962 2.952989 3.350041	C 1.057833 3.779998 1.652472
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H -0.466450 -2.621874 -0.175034	H -0.466450 -2.621874 -0.175034
H 2.006057 3.404710 1.170788	H 2.006057 3.404710 1.170788
H 1.071992 4.773408 1.801019	H 1.071992 4.773408 1.801019
H 1.326161 3.317331 2.790669	H 1.326161 3.317331 2.790669
H -6.340182 4.410705 -3.196971	H -6.340182 4.410705 -3.196971
H -5.573340 5.065658 -1.743869	H -5.573340 5.065658 -1.743869
H -4.577763 4.561583 -3.112667	H -4.577763 4.561583 -3.112667
H -7.572687 2.632212 -3.628176	H -7.572687 2.632212 -3.628176
H -7.731816 0.910428 -3.322204	H -7.731816 0.910428 -3.322204
H -8.280108 -3.239044 -0.230585	H -8.280108 -3.239044 -0.230585
H -7.630366 -3.159028 -1.871816	H -7.630366 -3.159028 -1.871816
H -7.343017 -4.598910 -0.866080	H -7.343017 -4.598910 -0.866080
H -9.732800 2.130837 -2.466429	H -9.732800 2.130837 -2.466429
H -8.849199 1.409855 -1.104383	H -8.849199 1.409855 -1.104383
H -8.698384 3.142909 -1.434484	H -8.698384 3.142909 -1.434484
H -2.636798 -5.179228 1.295945	H -2.636798 -5.179228 1.295945

H 0.137251 6.840708 -0.826751	H 0.137251 6.840708 -0.826751
H 1.193197 5.417069 -0.302980	H 1.193197 5.417069 -0.302980
H -1.871763 5.620229 -0.364149	H -1.871763 5.620229 -0.364149
O -5.329012 -5.858724 1.046627	O -5.329012 -5.858724 1.046627
H -3.450012 -4.762646 2.803344	H -3.450012 -4.762646 2.803344
H -7.243664 -0.676322 -1.726072	H -7.243664 -0.676322 -1.726072
H -4.057341 -0.459922 0.142723	H -4.057341 -0.459922 0.142723
H -2.420007 0.872516 0.711012	H -2.420007 0.872516 0.711012
N 1.117244 0.937150 2.828458	N 1.117244 0.937150 2.828458
C 2.189755 0.437682 2.260876	C 2.189755 0.437682 2.260876
O 2.325844 -0.226262 1.197599	O 2.325844 -0.226262 1.197599
C 3.506068 0.700729 3.027391	C 3.506068 0.700729 3.027391
F 3.414370 1.600942 4.036154	F 3.414370 1.600942 4.036154
F 3.999517 -0.450315 3.565205	F 3.999517 -0.450315 3.565205
F 4.469797 1.169945 2.172987	F 4.469797 1.169945 2.172987
H 0.891348 1.786847 4.466023	H 0.891348 1.786847 4.466023
K 3.798945 -0.120085 -0.960322	K 3.798945 -0.120085 -0.960322
O 2.925122 2.602991 -1.390964	O 2.925122 2.602991 -1.390964
C 3.902316 3.636953 -1.558937	C 3.902316 3.636953 -1.558937
C 5.071041 3.343609 -0.645703	C 5.071041 3.343609 -0.645703
O 5.699735 2.143847 -1.117931	O 5.699735 2.143847 -1.117931
C 6.877929 1.787991 -0.381824	C 6.877929 1.787991 -0.381824
C 7.521183 0.616261 -1.087211	C 7.521183 0.616261 -1.087211
O 6.646709 -0.520278 -1.003065	O 6.646709 -0.520278 -1.003065
C 7.078668 -1.585200 -1.861448	C 7.078668 -1.585200 -1.861448
C 6.179488 -2.784379 -1.678372	C 6.179488 -2.784379 -1.678372
O 4.852108 -2.496531 -2.154404	O 4.852108 -2.496531 -2.154404
C 1.842732 2.711749 -2.326864	C 1.842732 2.711749 -2.326864
C 0.803521 1.672447 -1.987975	C 0.803521 1.672447 -1.987975
O 1.286422 0.351210 -2.301371	O 1.286422 0.351210 -2.301371
C 4.086864 -3.718493 -2.215448	C 4.086864 -3.718493 -2.215448
C 2.663486 -3.462620 -2.691078	C 2.663486 -3.462620 -2.691078
N 1.751374 -2.776454 -1.741394	N 1.751374 -2.776454 -1.741394
C 0.655667 -2.005224 -2.397502	C 0.655667 -2.005224 -2.397502
C 0.314257 -0.617293 -1.867468	C 0.314257 -0.617293 -1.867468
H 3.467644 4.615152 -1.302424	H 3.467644 4.615152 -1.302424
H 4.243112 3.668962 -2.604693	H 4.243112 3.668962 -2.604693
H 4.730306 3.213082 0.391647	H 4.730306 3.213082 0.391647
H 5.781390 4.183159 -0.679905	H 5.781390 4.183159 -0.679905
H 6.618325 1.529350 0.655060	H 6.618325 1.529350 0.655060
H 7.586111 2.630043 -0.365385	H 7.586111 2.630043 -0.365385
H 8.487604 0.381911 -0.616330	H 8.487604 0.381911 -0.616330
H 7.695684 0.872149 -2.142756	H 7.695684 0.872149 -2.142756
H 8.108279 -1.879816 -1.606468	H 8.108279 -1.879816 -1.606468
H 7.061016 -1.248310 -2.909046	H 7.061016 -1.248310 -2.909046
H 6.138967 -3.078813 -0.619010	H 6.138967 -3.078813 -0.619010
H 6.603116 -3.621365 -2.253764	H 6.603116 -3.621365 -2.253764
H 2.217298 2.577141 -3.352972	H 2.217298 2.577141 -3.352972
H 1.377447 3.705718 -2.251124	H 1.377447 3.705718 -2.251124
H -0.111875 1.873045 -2.564541	H -0.111875 1.873045 -2.564541
H 0.562163 1.730227 -0.919317	H 0.562163 1.730227 -0.919317
H 4.097725 -4.210001 -1.239433	H 4.097725 -4.210001 -1.239433
H 4.557704 -4.389814 -2.950582	H 4.557704 -4.389814 -2.950582
H 2.240188 -4.439584 -2.963118	H 2.240188 -4.439584 -2.963118
H 2.704458 -2.847783 -3.593689	H 2.704458 -2.847783 -3.593689
H -0.265450 -2.601489 -2.378649	H -0.265450 -2.601489 -2.378649
H 0.937364 -1.894176 -3.447046	H 0.937364 -1.894176 -3.447046
H 0.233623 -0.577805 -0.775821	H 0.233623 -0.577805 -0.775821
H -0.667525 -0.350006 -2.288857	H -0.667525 -0.350006 -2.288857
C 0.629180 2.308761 5.411056	C 0.629180 2.308761 5.411056
N 0.353730 2.855514 6.393076	N 0.353730 2.855514 6.393076

B3LYP/6-31*	B3LYP/6-31*
E(0): -3747.93134422	E(0): -3747.95605008
C -0.2355 -1.1416 2.3344	C 0.7713 0.4204 1.9438
C 0.2486 -2.4910 2.8806	C 0.0508 1.4896 2.7681
C -0.7095 -3.4767 2.1723	C 0.7124 2.7836 2.2396
C -1.8557 -2.5464 1.7911	C 1.9887 2.2319 1.6153
N -1.4721 -1.2352 1.8120	N 1.9093 0.8858 1.4009
C 0.5232 0.0526 2.4496	C 0.2731 -0.8980 1.8052
C -3.1024 -2.9673 1.3636	C 3.0939 2.9889 1.2666
C -4.1102 -2.1707 0.7869	C 4.2699 2.5237 0.6488
C -5.2474 -2.8958 0.3504	C 5.2512 3.5234 0.4317
C -6.1201 -2.0177 -0.2939	C 6.3525 2.9422 -0.1983
C -5.4801 -0.7362 -0.2419	C 6.0120 1.5592 -0.3638
N -4.2729 -0.8827 0.4382	N 4.7427 1.3597 0.1718
C -5.8570 0.5024 -0.7752	C 6.7156 0.5015 -0.9530
C -5.0848 1.6650 -0.6929	C 6.2269 -0.8034 -1.0703
C -5.4678 2.9783 -1.2135	C 6.9327 -1.9184 -1.7068
C -4.4455 3.8258 -0.8808	C 6.0861 -2.9900 -1.6295
C -3.4571 3.0106 -0.1669	C 4.8825 -2.5092 -0.9396
N -3.8557 1.7214 -0.0809	N 4.9934 -1.2001 -0.6176
C -2.2762 3.5352 0.3888	C 3.7739 -3.3250 -0.6608
C -1.2617 2.9155 1.1108	C 2.5917 -3.0408 0.0178
C -0.1640 3.5922 1.7653	C 1.5181 -3.9794 0.2577
C 0.6269 2.6384 2.3917	C 0.5179 -3.3281 0.9694
C 0.0614 1.3421 2.0853	C 0.9484 -1.9594 1.1609
N -1.0811 1.5702 1.3464	N 2.1943 -1.8495 0.5762
C -5.0502 -4.3095 0.6807	C 4.7346 4.7957 0.9414
C -3.6453 -4.3972 1.3535	C 3.3110 4.4845 1.5003
C -0.0231 5.0469 1.7777	C 1.5777 -5.3786 -0.1691
C 1.1173 5.7491 1.8679	C 0.5626 -6.1248 -0.6270
C -0.0805 -4.1737 0.9289	C -0.1770 3.5547 1.2316
C 0.0952 -2.5589 4.4156	C 0.2902 1.2844 4.2759
C 0.0194 -3.2558 -0.2961	C -0.5393 2.7456 -0.0190
C 1.7538 2.9375 3.3298	C -0.7184 -3.9764 1.5205
C -4.3228 5.2949 -1.1568	C 6.3031 -4.3905 -2.1201
C -6.7573 3.2977 -1.9177	C 8.3231 -1.8598 -2.2754
C -7.4381 -2.3407 -0.9280	C 7.6243 3.6122 -0.6195
C -7.9296 3.5762 -0.9564	C 9.4266 -2.0007 -1.2084
C 0.9732 -3.7476 -1.3718	C -1.5742 3.4455 -0.8874
O 1.6118 -4.7823 -1.2592	O -2.0652 4.5203 -0.5614
H 1.2871 -2.6971 2.6090	H -1.0266 1.4891 2.5816
H -1.0382 -4.2610 2.8641	H 0.9446 3.4716 3.0617
H -2.1451 4.6050 0.2659	H 3.8438 -4.3440 -1.0260
H -0.6691 -5.0603 0.6669	H 0.3172 4.4861 0.9338
H 0.9170 -4.5385 1.1918	H -1.0979 3.8545 1.7446
H -0.9508 -2.4052 4.7046	H 1.3622 1.2930 4.5052
H 0.4119 -3.5401 4.7870	H -0.1860 2.0885 4.8496
H 0.6908 -1.7975 4.9317	H -0.1233 0.3325 4.6187
H 0.3777 -2.2652 0.0005	H -0.9531 1.7681 0.2577
H -0.9798 -3.1023 -0.7193	H 0.3669 2.5356 -0.6011
H 2.7156 2.9427 2.8112	H -1.6260 -3.6829 0.9799
H 1.5996 3.9189 3.7904	H -0.6255 -5.0638 1.4583
H 1.8288 2.1764 4.1064	H -0.8792 -3.7010 2.5642
H -5.1471 5.6551 -1.7799	H 7.2389 -4.4779 -2.6809
H -4.3329 5.8859 -0.2310	H 6.3518 -5.1100 -1.2916
H -3.3872 5.5362 -1.6782	H 5.4919 -4.7208 -2.7822
H -6.6149 4.1703 -2.5673	H 8.4485 -2.6515 -3.0244
H -7.0305 2.4705 -2.5862	H 8.4656 -0.9141 -2.8154
H -8.2644 -1.8170 -0.4302	H 8.4952 3.1865 -0.1048
H -7.4623 -2.0494 -1.9857	H 7.8021 3.5039 -1.6971

H -7.6298 -3.4146 -0.8631	H 7.5791 4.6787 -0.3855
H -8.8487 3.7938 -1.5132	H 10.4221 -1.9425 -1.6644
H -8.1201 2.7155 -0.3062	H 9.3495 -1.2098 -0.4544
H -7.7095 4.4341 -0.3118	H 9.3443 -2.9611 -0.6880
H -3.0249 -5.0996 0.7830	H 2.5822 5.1222 0.9843
H 1.0999 6.8352 1.8812	H 0.7149 -7.1637 -0.9054
H 2.0924 5.2768 1.9281	H -0.4412 -5.7295 -0.7518
H -0.9527 5.6097 1.7002	H 2.5610 -5.8454 -0.1122
O -5.7880 -5.2597 0.4814	O 5.2589 5.8969 0.9474
H -3.7519 -4.8247 2.3593	H 3.2721 4.7658 2.5611
H -6.8132 0.5530 -1.2863	H 7.7004 0.7213 -1.3525
H -3.6691 -0.0719 0.5815	H 4.3202 0.4307 0.1410
H -1.7143 0.8265 1.0764	H 2.7122 -0.9784 0.5585
N 1.8412 -0.0243 2.9733	N -0.9979 -1.1732 2.3747
C 2.9948 0.0445 1.9903	C -2.0382 -0.7968 1.6782
O 2.8964 0.9502 1.0619	O -2.1262 -0.2171 0.5572
C 4.2791 0.1617 2.8772	C -3.3926 -1.1967 2.3037
F 4.3564 1.3339 3.5241	F -3.8122 -2.3935 1.8016
F 4.3373 -0.8256 3.8118	F -3.3967 -1.3002 3.6387
F 5.3872 0.0498 2.1106	F -4.3670 -0.2964 1.9722
H 1.9641 -0.8205 3.5898	H -1.0200 -1.9651 4.2255
K 2.7772 0.0759 -1.4588	K -4.1340 0.3061 -1.0174
O 1.4200 2.4870 -1.9240	O -3.8749 -2.3146 -2.0126
C 2.1171 3.7220 -1.8188	C -4.9938 -3.1774 -2.1289
C 3.3178 3.5249 -0.9182	C -5.8945 -2.9460 -0.9333
O 4.2311 2.6626 -1.5885	O -6.3949 -1.6175 -1.0108
C 5.3862 2.3558 -0.8176	C -7.1835 -1.2326 0.1078
C 6.2350 1.3942 -1.6227	C -7.8172 0.1037 -0.2160
O 5.5435 0.1577 -1.7316	O -6.7977 1.0841 -0.3650
C 6.1730 -0.7761 -2.5904	C -7.2675 2.2696 -0.9872
C 5.5088 -2.1279 -2.4388	C -6.1667 3.3065 -1.0342
O 4.1662 -2.0849 -2.9088	O -5.0793 2.8535 -1.8357
C 0.3706 2.4987 -2.8733	C -2.8959 -2.4880 -3.0262
C -0.5261 1.3049 -2.6327	C -1.6751 -1.6661 -2.6738
O 0.1858 0.0863 -2.8538	O -1.9612 -0.2751 -2.8060
C 3.5984 -3.3989 -2.9049	C -4.2721 3.9577 -2.2610
C 2.1709 -3.3808 -3.4385	C -2.9668 3.4998 -2.9002
N 1.1523 -2.8952 -2.4830	N -2.0046 2.7745 -2.0429
C -0.0617 -2.3291 -3.1196	C -1.0178 1.9655 -2.8017
C -0.6518 -1.0312 -2.5751	C -0.8301 0.5048 -2.4079
H 1.4579 4.4920 -1.3897	H -4.6694 -4.2301 -2.1414
H 2.4492 4.0578 -2.8140	H -5.5439 -2.9759 -3.0619
H 3.0096 3.0782 0.0356	H -5.3246 -3.0884 -0.0054
H 3.7860 4.5048 -0.7265	H -6.7238 -3.6713 -0.9514
H 5.0957 1.9012 0.1387	H -6.5609 -1.1614 1.0108
H 5.9706 3.2695 -0.6177	H -7.9819 -1.9685 0.2934
H 7.2043 1.2439 -1.1213	H -8.5122 0.3934 0.5877
H 6.4244 1.8140 -2.6233	H -8.3898 0.0120 -1.1515
H 7.2372 -0.8848 -2.3251	H -8.1151 2.6905 -0.4225
H 6.1157 -0.4344 -3.6367	H -7.6155 2.0454 -2.0081
H 5.5304 -2.4369 -1.3834	H -5.8155 3.5405 -0.0179
H 6.0869 -2.8625 -3.0236	H -6.5962 4.2250 -1.4627
H 0.7772 2.4832 -3.8979	H -3.2964 -2.1848 -4.0067
H -0.2434 3.4061 -2.7626	H -2.5992 -3.5469 -3.0899
H -1.3870 1.3612 -3.3175	H -0.8527 -1.9427 -3.3528
H -0.9099 1.3392 -1.6041	H -1.3650 -1.8904 -1.6440
H 3.6354 -3.8226 -1.8980	H -4.0656 4.6183 -1.4182
H 4.1942 -4.0437 -3.5716	H -4.8239 4.5256 -3.0281
H 1.9268 -4.4013 -3.7646	H -2.4982 4.4039 -3.3189
H 2.1451 -2.7259 -4.3138	H -3.2099 2.8352 -3.7345
H -0.8722 -3.0728 -3.1193	H -0.0321 2.4462 -2.7616

H 0.1848 -2.1456 -4.1686	H -1.3240 1.9835 -3.8512
H -0.8623 -1.0775 -1.5003	H -0.6592 0.3701 -1.3358
H -1.6191 -0.8965 -3.0864	H 0.0621 0.1449 -2.9456
C 3.1301 -1.3510 1.3035	C -0.9665 -2.4181 5.2186
N 3.1554 -2.2625 0.5771	N -0.9165 -2.9017 6.2704

4' with KF	**4''** with KF
TPSS-D3/def2-SVP	TPSS-D3/def2-SVP
E(0): -3753.380169	E(0): -3753.390597
Chem.pot. (298.15 K): 2295.88 kJ/mol	Chem.pot. (298.15 K): 2283.89 kJ/mol
C -0.250416 -1.025333 2.558842	C -0.655465 -0.493981 2.275528
C 0.250164 -2.347083 3.141588	C 0.005027 -1.556956 3.152680
C -0.742494 -3.363397 2.524890	C -0.704398 -2.839831 2.653968
C -1.856566 -2.441541 2.023692	C -1.950944 -2.255894 1.994830
N -1.478951 -1.126998 2.013694	N -1.810709 -0.923178 1.724179
C 0.528573 0.157987 2.611204	C -0.104201 0.801356 2.121515
C -3.059591 -2.873418 1.469950	C -3.066134 -2.989514 1.597018
C -3.962792 -2.094120 0.712591	C -4.146932 -2.518972 0.820405
C -5.032973 -2.848931 0.146465	C -5.128249 -3.515541 0.538560
C -5.793999 -2.005714 -0.680293	C -6.117601 -2.954046 -0.284878
C -5.154067 -0.718965 -0.598880	C -5.702828 -1.589880 -0.495904
N -4.059563 -0.821832 0.266194	N -4.511694 -1.375787 0.202000
C -5.447312 0.492963 -1.249412	C -6.274841 -0.561889 -1.266033
C -4.696445 1.672257 -1.094232	C -5.710885 0.720861 -1.405050
C -4.978969 2.947799 -1.761470	C -6.273385 1.806391 -2.217379
C -4.018354 3.830039 -1.311132	C -5.405333 2.868877 -2.078854
C -3.164431 3.066489 -0.389549	C -4.331412 2.403308 -1.185966
N -3.588019 1.775177 -0.277761	N -4.536735 1.113066 -0.796888
C -2.051113 3.627291 0.271210	C -3.249504 3.220910 -0.797544
C -1.102980 3.025013 1.103704	C -2.172432 2.955223 0.056962
C 0.012329 3.693272 1.752312	C -1.107569 3.884890 0.397151
C 0.760072 2.723502 2.432587	C -0.219228 3.229216 1.261687
C 0.124372 1.448301 2.183594	C -0.710418 1.878518 1.426629
N -1.001594 1.687766 1.423263	N -1.889278 1.775441 0.711734
C -4.898442 -4.242360 0.579605	C -4.713743 -4.766547 1.181661
C -3.608513 -4.298644 1.449960	C -3.356541 -4.461352 1.883225
C 0.228466 5.136623 1.676118	C -1.052852 5.254911 -0.112805
C 1.398614 5.799505 1.822048	C 0.052592 6.003222 -0.329114
C -0.091195 -4.166893 1.362202	C 0.153657 -3.622966 1.618826
C 0.217470 -2.345138 4.684891	C -0.240553 -1.245102 4.644527
C 0.094721 -3.286742 0.124156	C 0.417629 -2.796268 0.357295
C 1.924652 2.978521 3.342281	C 0.970207 3.832982 1.950447
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PBE-D3/def2-TZVP E(0): -3752.411778 C -0.259572 -0.988594 2.508357 C 0.241273 -2.309285 3.079131 C -0.745746 -3.325420 2.463948 C -1.847280 -2.410731 1.943301 N -1.478522 -1.094585 1.949053 C 0.500533 0.201663 2.582658 C -3.042610 -2.842402 1.388006 C -3.956154 -2.063320 0.653295 C -5.025710 -2.812327 0.087049 C -5.796924 -1.957723 -0.714395 C -5.165803 -0.673988 -0.616108 N -4.065444 -0.787939 0.233887 C -5.468962 0.545317 -1.235121 C -4.731671 1.722594 -1.060989 C -5.038820 3.007457 -1.687242 C -4.089287 3.888518 -1.228413 C -3.216578 3.119522 -0.337914 N -3.616742 1.821065 -0.255237 C -2.114845 3.677971 0.331474 C -1.164040 3.072989 1.148512 C -0.060104 3.738512 1.806354 C 0.694087 2.770148 2.470060 C 0.080889 1.493487 2.195748 N -1.045875 1.734583 1.442217 C -4.873373 -4.204662 0.495999 C -3.578190 -4.266132 1.347482 C 0.138881 5.178584 1.760587 C 1.305395 5.839161 1.885994 C -0.086896 -4.168057 1.340835 C 0.202275 -2.322167 4.617383 C 0.106997 -3.348234 0.068961 C 1.829142 3.030759 3.403544 C -3.941705 5.341642 -1.544515 C -6.200144 3.282379 -2.592603 C -7.017128 -2.284515 -1.506661 C -7.493153 3.612479 -1.826126 C 1.155239 -3.857180 -0.892080 O 1.939242 -4.760450 -0.593494	PBE-D3/def2-TZVP E(0): -3752.430787 C -0.677176 -0.529668 2.256592 C -0.039131 -1.617028 3.112528 C -0.740881 -2.882244 2.574693 C -1.966124 -2.282972 1.904911 N -1.820739 -0.945349 1.673684 C -0.117251 0.760434 2.126243 C -3.080609 -3.001009 1.497048 C -4.175276 -2.510762 0.763702 C -5.171457 -3.489385 0.487594 C -6.179725 -2.895447 -0.284380 C -5.761412 -1.534975 -0.471309 N -4.549426 -1.351509 0.192311 C -6.341104 -0.485203 -1.194665 C -5.766755 0.786463 -1.322282 C -6.328151 1.891987 -2.097790 C -5.437101 2.930284 -1.975387 C -4.350613 2.436869 -1.122779 N -4.570407 1.149146 -0.741642 C -3.242038 3.219168 -0.762783 C -2.153678 2.929004 0.058993 C -1.064473 3.833074 0.361624 C -0.173908 3.172692 1.211436 C -0.690182 1.838983 1.413284 N -1.879580 1.753071 0.717016 C -4.743443 -4.751812 1.083504 C -3.368217 -4.474239 1.747110 C -0.998637 5.192108 -0.157060 C 0.107744 5.907526 -0.432449 C 0.135475 -3.670721 1.570162 C -0.314270 -1.370058 4.604973 C 0.451381 -2.860241 0.316063 C 1.039594 3.775262 1.840130 C -5.527646 4.302986 -2.559141 C -7.639779 1.872751 -2.820784 C -7.432510 -3.512417 -0.807600 C -8.833830 2.193017 -1.904367 C 1.477346 -3.495426 -0.596151 O 2.062427 -4.538918 -0.290591

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