Electronic Supplementary Material (ESI) for Dalton Transactions.

Photophysicochemical, sonochemical, and biological properties of novel hexadeca-substituted phthalocyanines bearing fluorinated groups

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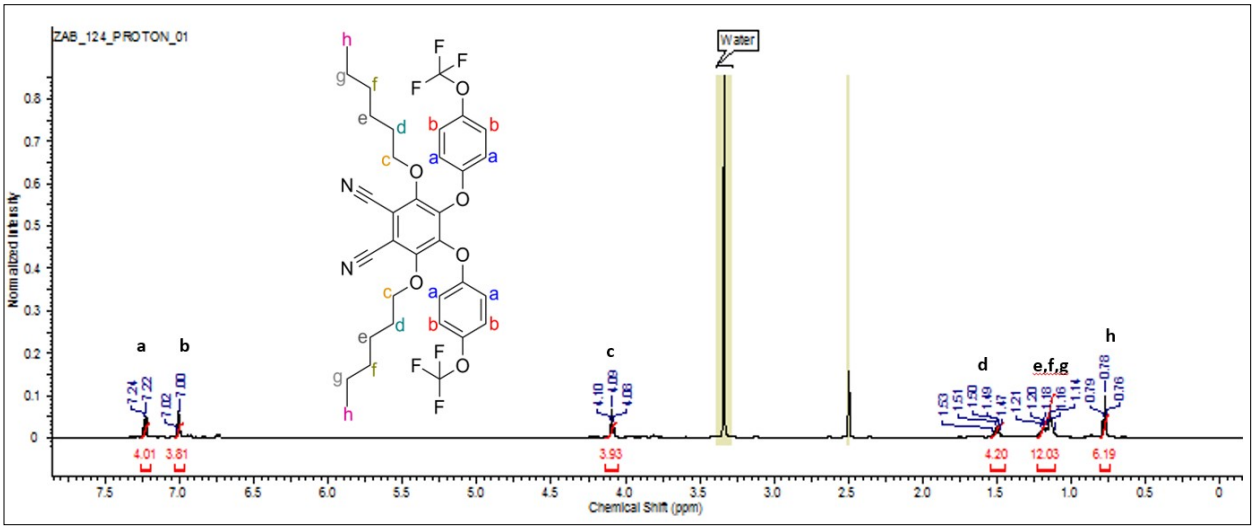
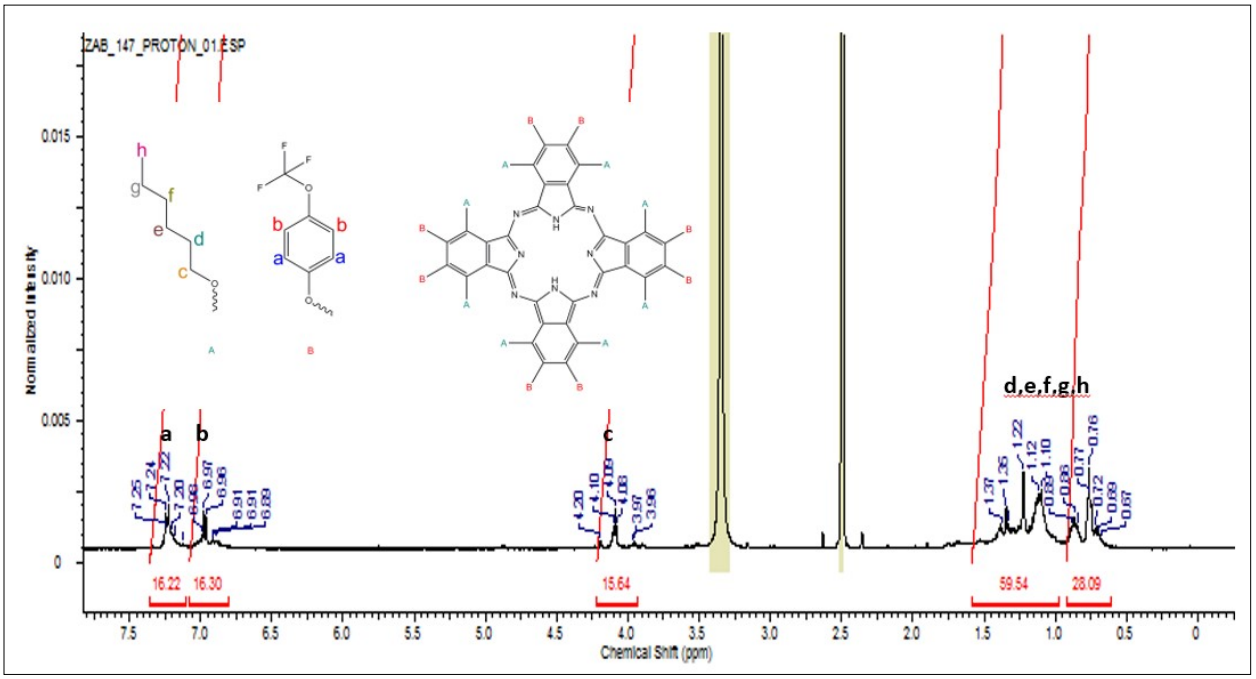
Equipment

IR spectra were recorded on a Perkin-Elmer Spectrum One spectrometer in a 4000-400 cm^{-1} range at room temperature. ^{1}H NMR spectra were recorded on an Agilent VNMRS 500 MHz spectrometer and chemical shifts (δ) are given in ppm. Electronic absorption spectra were obtained using a Scinco Lab Pro Plus UV/Vis spectrophotometer. Mass spectra were obtained using a Bruker Microflex MALDI–TOF mass spectrometer. Elemental analyses were performed with a Thermo Finnigan Flash EA 1112 apparatus at 950 – 1000 °C. Fluorescence spectra were recorded on a Varian Eclipse spectrofluorometer using 1cm path length cuvettes at room temperature. Photo-irradiations were measured using a General Electric quartz line lamp (300W). A 600 nm glass cut off filter (Schott) and a water filter were used to filter off ultraviolet and infrared radiations respectively. An interference filter (Intor, 700 nm with a bandwidth of 40 nm) was additionally placed in the light path before the sample. Light intensities were measured with a POWER MAX5100 (Mol electron detector incorporated) power meter. Bandelin Ultrasonic RK 100 H was used for ultrasound irradiation. High-Purity materials consumed in this study were purchased from commercial suppliers.

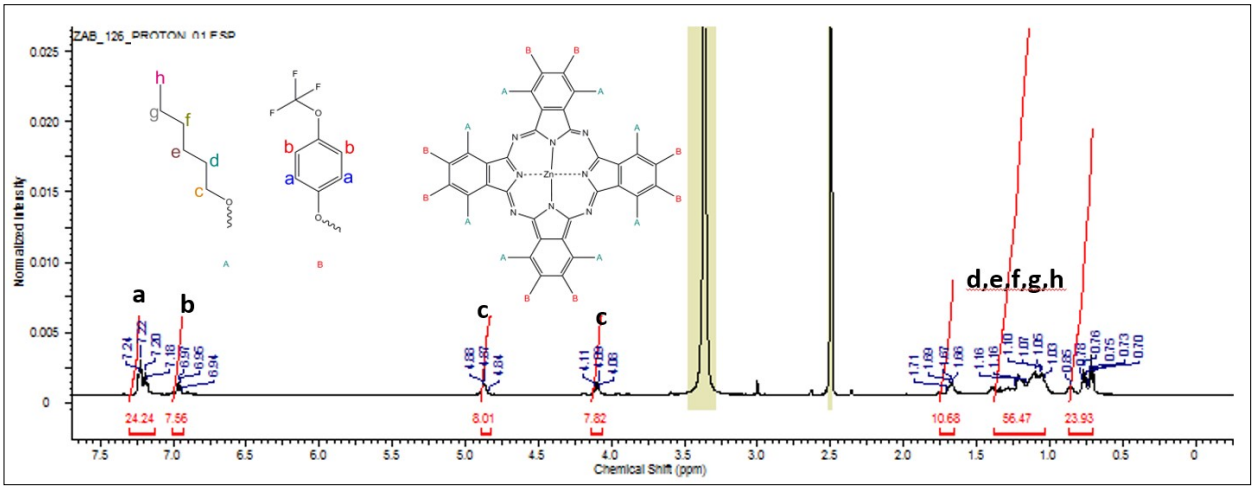
^{1}H NMR spectrum of compound **1**



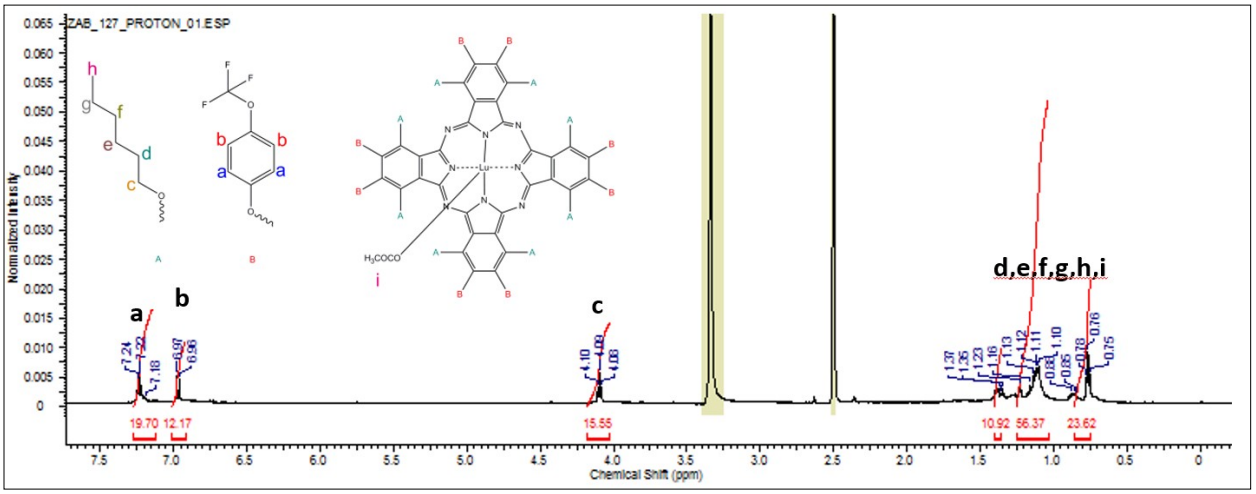
^{1}H NMR spectrum of compound **2**



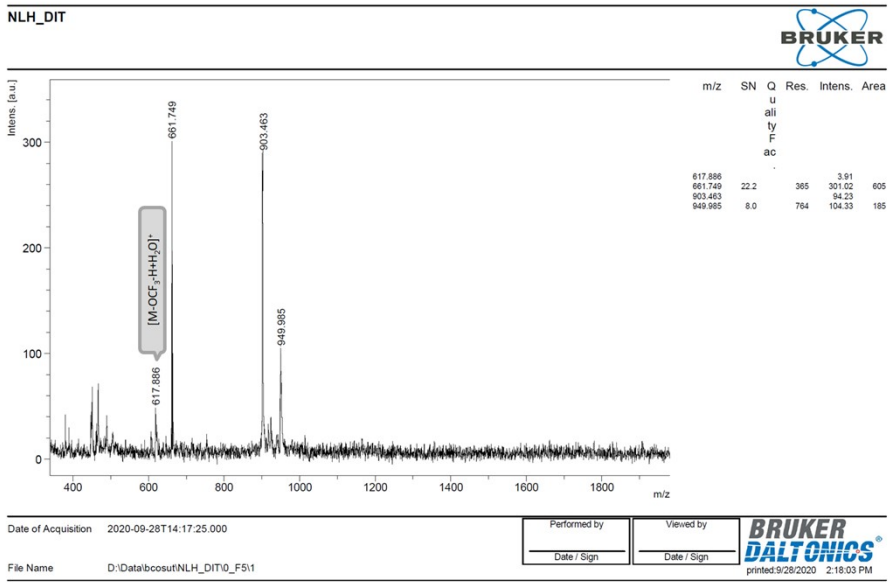
^{1}H NMR spectrum of compound **3**



^{1}H NMR spectrum of compound **6**



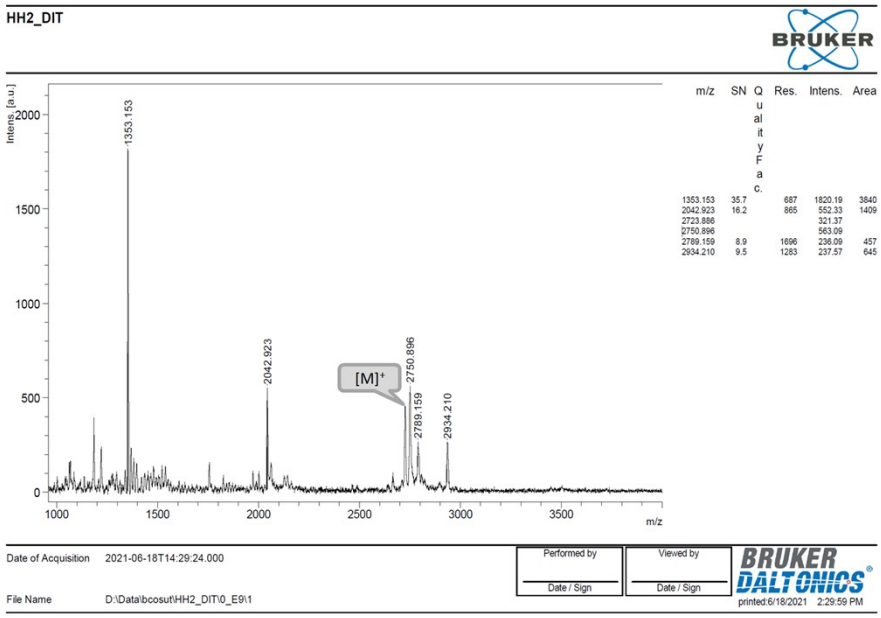
Mass spectrum of compound **1**



m/z	SN	Quality Fac.	Res.	Intens.	Area
617.886				3.91	
661.749	22.2		365	301.02	605
903.463				94.23	
949.985	8.0		764	104.33	185

661.749 m/z: $[2M\text{-}OCF_3+2H+2Na]^{2+}$; 903.463 m/z: $[3M\text{-}3OCF_3\text{-}2H+Na]^{2+}$; 903.463 m/z: $[3M\text{-}2OCF_3+5H+Na]^{2+}$

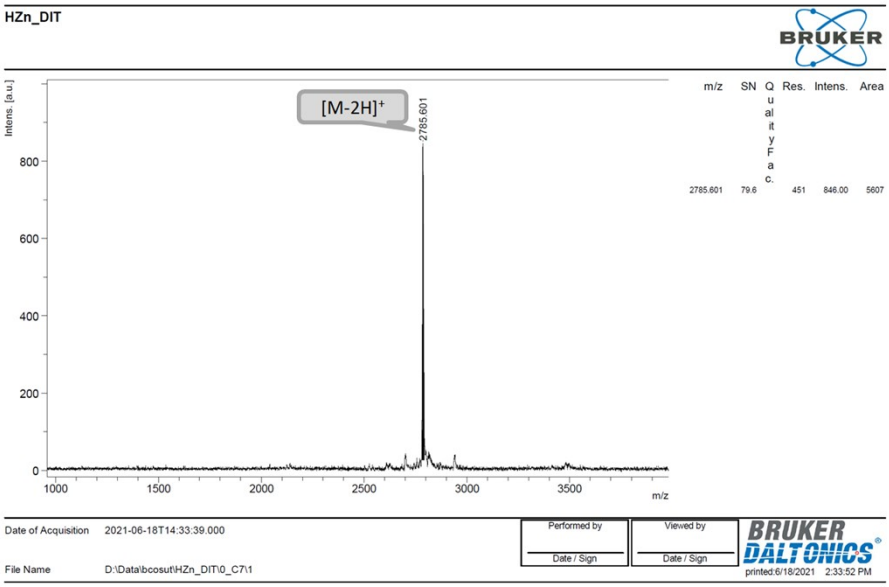
Mass spectrum of compound **2**



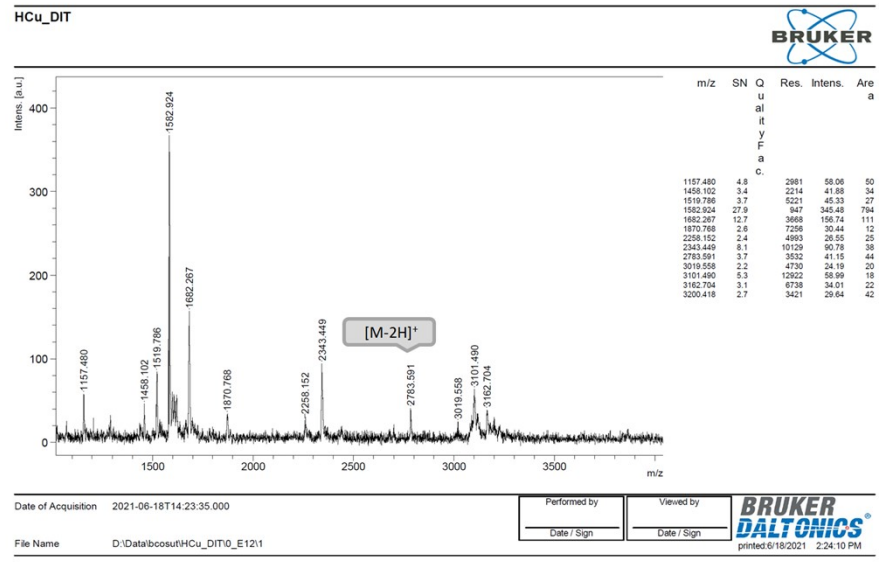
m/z	SN	Quality Fac.	Res.	Intens.	Area
1353.153	35.7		687	1820.19	3840
2042.923	16.2		865	552.33	1409
2723.886				321.37	
2750.896				563.09	
2789.159	8.9		1696	236.09	457
2934.210	9.5		1283	237.57	645

1353.153 m/z: $[M\text{-}OCF_3+2H+H_2O+2Na]^{2+}$; 2042.923 m/z: $[2M\text{-}2OCF_3+2H\text{-}H_2O+2DIT]^{3+}$; 2750.896 m/z: $[M+3H+Na]^{+}$ 2789.159 m/z: $[M+H_2O+2Na]^{+}$; 2934.210 $[M\text{-}3OCF_3\text{-}4H+2H_2O+DIT]^{+}$

Mass spectrum of compound **3**

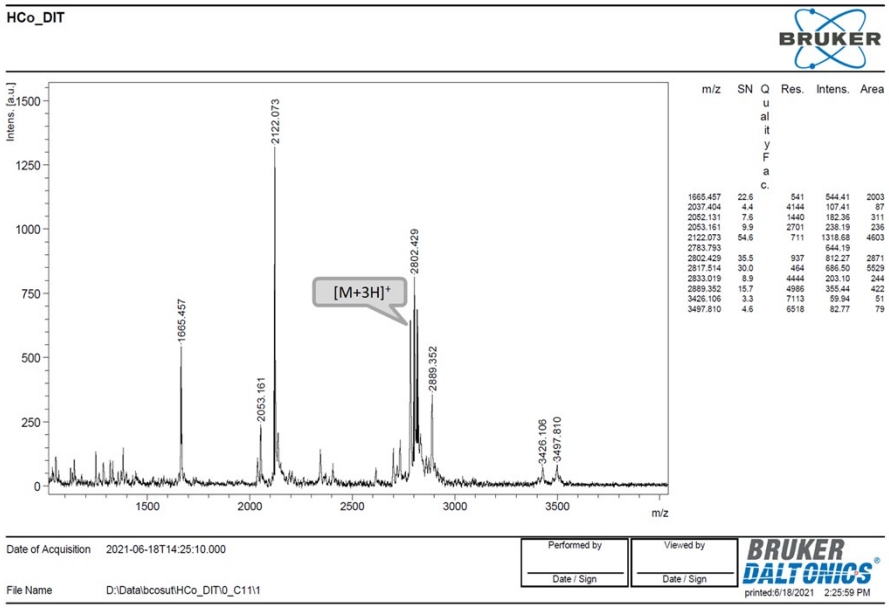


Mass spectrum of compound **4**



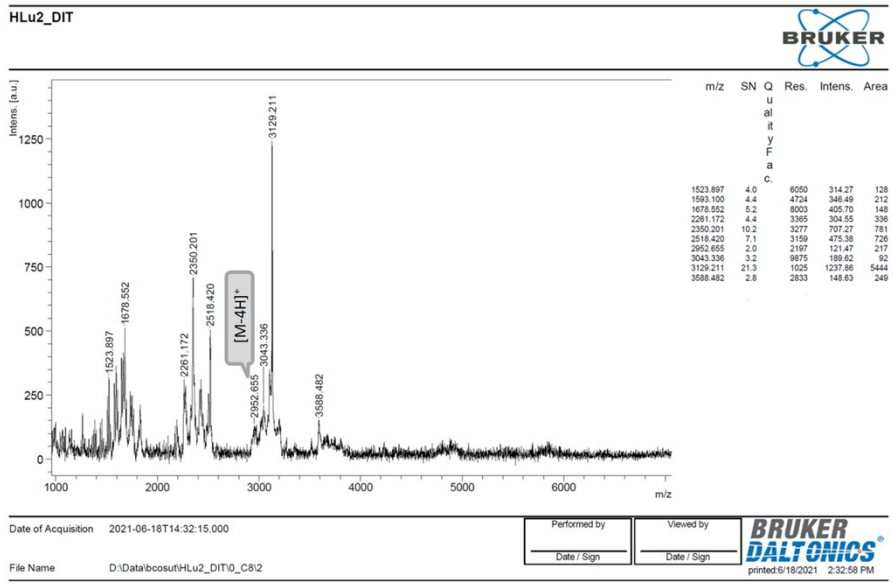
1157.480 m/z: $[M\text{-}6OCF_3\text{+}2H\text{+}2H_2O]^{2+}$; 1458.102 m/z: $[M\text{-}4OCF_3\text{+}2H_2O\text{+}DIT]^{2+}$; 1519.786 m/z: $[M\text{-}2OCF_3\text{-}H_2O\text{+}DIT]^{2+}$; 1582.924 m/z: $[M\text{-}2OCF_3\text{-}H_2O\text{+}DIT]^{2+}$; 1682.267 m/z: : $[2M\text{-}7OCF_3\text{-}3H\text{+}4H_2O]^{3+}$; 1870.768 $[2M\text{-}+H_2O\text{+}Na]^{3+}$; 2258.152 $[2M\text{-}13OCF_3\text{+}H\text{+}3H_2O]^{2+}$; 2343.449 m/z: $[2M\text{-}11OCF_3\text{+}H\text{+}3H_2O]^{2+}$; 3019.558 m/z: : $[2M\text{+}2H_2O\text{+}DIT]^{2+}$; 3101.490 m/z: $[M\text{-}2OCF_3\text{+}4H\text{+}3H_2O\text{+}DIT]^{+}$; 3162.704 m/z: $[M\text{-}OCF_3\text{+}6H\text{+}Na\text{+}DIT]^{+}$

Mass spectrum of compound **5**



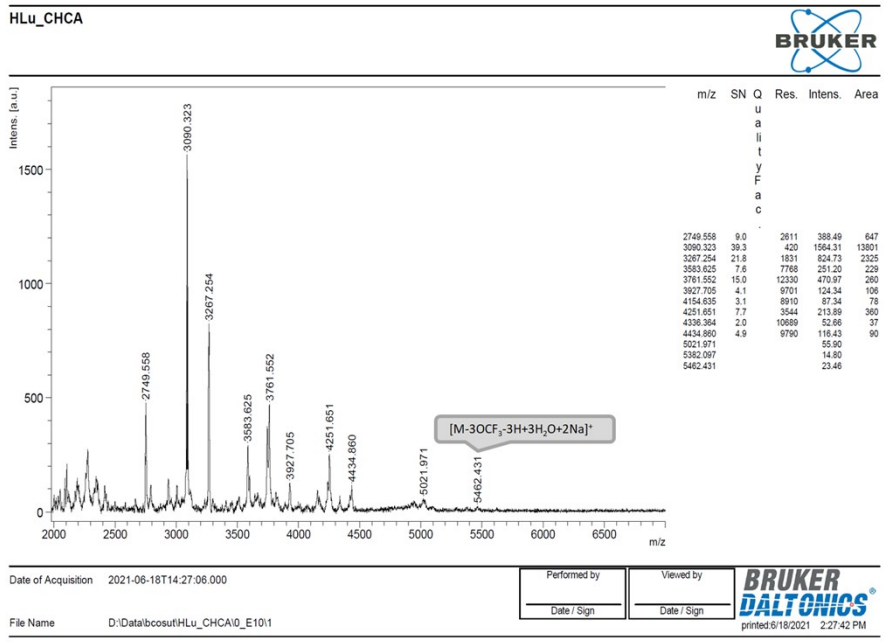
1665.457 m/z: $[M\text{-}4OCF_3+Na+2DIT]^{2+}$; 2053.161 m/z: $[2M\text{-}4OCF_3+4H_2O+2DIT]^{3+}$; 2122.073 m/z: $[M\text{-}8OCF_3\text{-}2H+Na]^{+}$; 2802.429 m/z: $[M\text{-}2H+Na]^{+}$; 2889.352 m/z: $[M\text{-}4OCF_3\text{-}3H+H_2O+DIT]^{+}$; 3426.106 $[M\text{-}3OCF_3\text{-}2H+2H_2O+2DIT]^{+}$; 3497.810 $[M\text{-}2OCF_3+2H+H_2O+2DIT]^{+}$

Mass spectrum of compound **6**



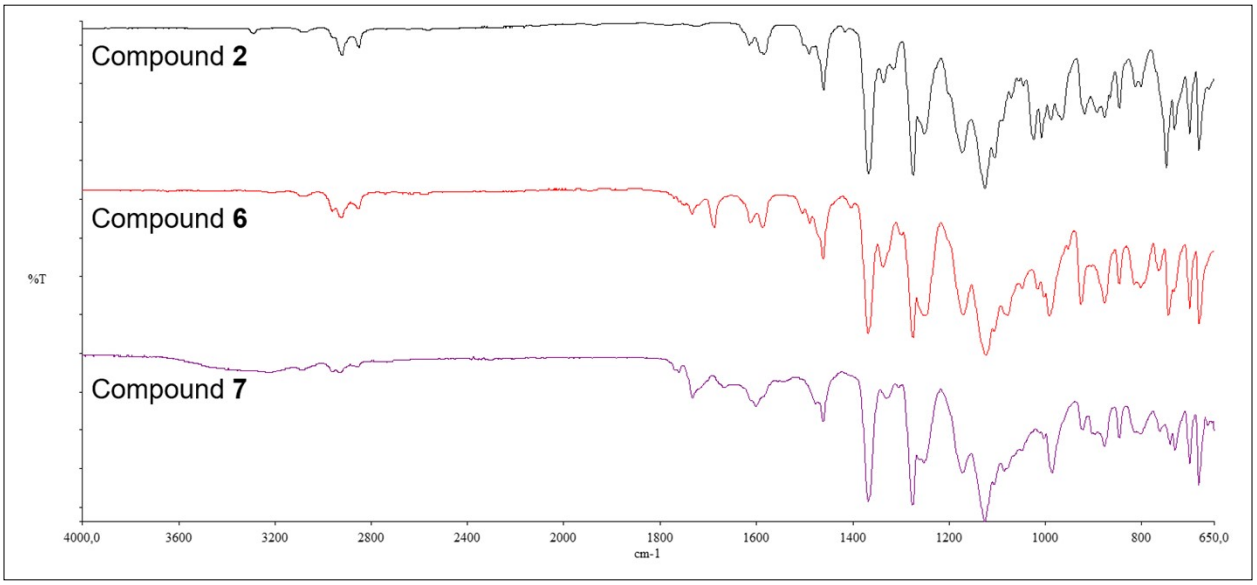
1523.897 m/z: $[M\text{-}4OCF_3\text{-}2H+DIT]^{2+}$; 1678.552 m/z: $[M\text{-}OCF_3\text{-}H+3H_2O+DIT]^{2+}$; 2261.172 m/z: $[2M+3H+2DIT]^{3+}$; 2350.201 m/z: $[M\text{-}7OCF_3\text{-}C_2H_3O_2\text{-}7H+3H_2O]^{+}$; 2518.420 m/z: $[M\text{-}6OCF_3+3H_2O+Na]^{+}$; 3043.336 $[M+H+4H_2O+Na]^{+}$; 3129.211 $[2M\text{-}OCF_3\text{-}2H+DIT]^{2+}$; 3588.482 $[M\text{-}3OCF_3+2H+H_2O+2DIT]^{+}$

Mass spectrum of compound **7**



2749.558 m/z: $[M-2OCF_3-4H+3H_2O]^{2+}$; 3090.323 m/z: $[M-4OCF_3-2H+2H_2O+2DIT]^{2+}$; 3267.254 m/z: $[M-6H+3H_2O+2DIT]^{2+}$; 3583.625 m/z: $[2M-6OCF_3+7H]^{3+}$; 3761.552 m/z: $[2M+2H+H_2O+Na]^{3+}$; 3927.705 $[2M+3H+6H_2O+DIT]^{3+}$; 4251.651 $[M-16OCF_3-8H]^{+}$; 4434.860 $[M-14OCF_3+5H]^{+}$; 5021.971 $[M-7OCF_3-3H]^{+}$

FT-IR spectrum of compound **2**, **6**, and **7**



FT-IR spectrum of compound **3**-**5**