Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Specific labeling of mitochondria of *Chlamydomonas* with cationic helicene fluorophores

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Supporting information

1. General remarks and analysis conditions

Reagents. Fluorophores **1**,[1] **2**,[2] **4**,[3] **5**,[4] **6**, [4] **7**,[3] **8**,[5] **11**[5] and **12**[5] were synthesized according to previously reported procedures. Column chromatography was performed using Silicaflash P60 silicagel (40-63 µm, 60 Å) and Acros Brockmann I basic alumina (40-200 µm, 60 Å). Optical properties were recorded in analytical grade acetonitrile and Milli-Q water.

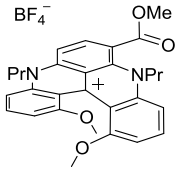
Analytical methods and apparatus. NMR spectra were recorded on Brucker Avance II+ AMX-500 spectrometers at room temperature. NMR chemical shifts are given in ppm (δ) relative to Me_4Si with solvent resonances used as internal standards (CD_2Cl_2: 5.32 ppm for ^1H and 53.8 for ^{13}C). IR spectra were recorded on a Perkin-Elmer 1650 FT-IR spectrometer using a diamond ATR Golden Gate sampling. Melting points (M.P.) were measured in open capillary tubes with a Buchi B-550 melting points apparatus and are uncorrected. UV-vis-NIR absorption spectra were recorded on a JASCO V-650 spectrophotometer at 20°C. Electrospray mass spectra were obtained on a Finnigan SSQ 7000 spectrometer QSTAR pulsar *i* (AB / MDS Sciex), ESI (TIS)/nanoESI/APCI-QqTof by the Department of Mass Spectroscopy of the University of Geneva.

Luminescence. Fluorescence quantum yields in MeCN of cationic dyes were previously reported in literature. [3,4,6,7]

2. Synthetic protocols and characterization

Fluorophores **1**,[1] **2**,[2] **4**,[3] **5**,[4] **6**, [4] **7**,[3] **8**,[5] **11**[5] and **12**[5] were synthesized according to previously reported procedures.

1,13-dimethoxy-6-(methoxycarbonyl)-5,9-dipropyl-5,9-dihydro-13bH-quinolino[2,3,4-kl]acridin-13b-ylium tetrafluoroborate (3)

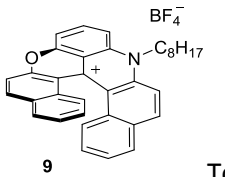


3

6-carboxy-1,13-dimethoxy-5,9-dipropyl-5,9-dihydro-13bH-quinolino[2,3,4-kl]acridin-13b-ylium tetrafluoroborate[3] (100 mg, 0.18 mmol, 1 eq.) was dissolved in 2 mL of anhydrous dichloromethane. To this solution was added $SOCl_2$ (40 µL, 0.56 mmol, 6 eq.) and the reaction was stirred for 10 minutes at room temperature. Then methanol (100 µL, 2.46 mmol, 14 eq.) was added and after 10 min of stirring at room temperature the mixture was concentrated under reduced pressure. The residue was diluted in DCM. The organic phase was washed with a diluted aqueous solution of HBF_4, dried over Na_2SO_4, filtered and finally evaporated. Purification by silica gel column chromatography using DCM/methanol (95/5, R_f = 0.65) afforded the pure product as a dark green solid (98 mg, 98%).

M. P.: 124-126°C. **^{1}H NMR (CD_2Cl_2, 500 MHz):** δ 8.63 (d, ^3J = 9.1 Hz, 1H, CH_{Ar}), 8.03 (dd, ^3J = 8.9 Hz, ^3J = 8.1 Hz, 1H, CH_{Ar}), 7.92 (t, ^3J = 8.1 Hz, 1H, CH_{Ar}), 7.52 (t, ^3J = 9.0 Hz, 2H, CH_{Ar}), 7.46 (dd, ^3J = 8.8 Hz, ^4J = 0.7 Hz, 1H, CH_{Ar}), 7.00 (d, ^3J = 8.1 Hz, 1H, CH_{Ar}), 6.92 (dd, ^{3}J = 8.2 Hz, ^4J = 0.7 Hz, 1H, CH_{Ar}), 4.94 - 4.89 (m, 1H, CH_2), 4.76 – 4.70 (m, 1H, CH_2), 4.56-4.51(m, 1H, CH_2), 4.04 (s, 3H, CO_2CH_3), 3.85-3.79 (m, 1H, CH_2), 3.81 (s, 3H, OCH_3), 3.77 (s, 3H, OCH_3), 2.23 – 2.19 (m, 2H, CH_2), 1.77 – 1.72 (m, 2H, CH_2), 1.28 (t, ^3J = 7.4 Hz, 3H, CH_3), 0.40 (t, ^3J = 7 Hz, 3H, CH_3). **^{13}C{^{1}H} NMR (CD_2Cl_2, 126 MHz):** δ 166.3 (C_{quat}), 160.2 (C_{quat}), 159.5 (C_{quat}), 142.2 (C_{quat}), 141.9 (C_{quat}), 141.6 (C_{quat}), 141.3 (C_{quat}), 140.5 (C_{quat}), 139.8 (CH), 138.6 (CH), 137.3 (CH), 120.6 (C_{quat}), 116.6 (C_{quat}), 114.1 (C_{quat}), 112.5 (C_{quat}), 110.5 (CH), 107.9 (CH), 106.1 (CH), 104.8 (CH), 104.3 (CH), 59.3 (CH_2), 56.5 (OCH_3), 56. 3 (OCH_3), 53.4 (OCH_3), 53.1 (CH_2), 22.7 (CH_2), 21.0 (CH_2), 11.4 (CH_3), 10.8 (CH_3). **^{19}F NMR (CD_2Cl_2, 282 MHz):** δ -153.3. **UV-vis:** λ_{max} (CH_3CN) = 591 nm (ε = 11,400 L.mol^{-1}.cm^{-1}). **IR (neat, cm^{-1}):** 2961, 1642, 1586, 1469, 1267, 840, 760. **HRMS (ESI+)** calculated for [M+]: 471.2278 ($C_{29}H_{31}N_2O_4^+$), Found 471.2278.

11-octylbenzo[a]benzo[5,6]chromeno[2,3,4-kl]acridin-17c(11H)-ylium tetrafluoroborate (9)



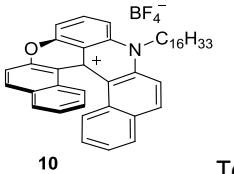
9

To a solution of 11-methoxy-12-(2-methoxynaphthalen-1-yl)-12H-benzo[a]xanthen-12-ylium tetrafluoroborate (prepared following reported procedures)[5] (50 mg, 0.1 mmol) in acetonitrile (10 mL) was added octylamine (0.3 mmol, 3 equiv). The reaction mixture was refluxed until completion of the reaction as monitored by ESI-MS (4 h). Then, the reaction mixture was evaporated. The residue was dissolved in a minimum amount of dichloromethane and the product was precipitated by addition of diethyl ether. The precipitate was separated from the mother liquor

by centrifugation, dissolved in dichloromethane and washed once with 1 M aq. $NaBF_4$ solution and once with 1 M aq. HBF_4 solution. The organic layer was dried over Na_2SO_4, filtered and evaporated. The material was next columned (CombiFlash, 4 g SiO_2, CH_2Cl_2/MeOH, 100:00 to 95:05). The product was finally dissolved in a minimum amount of dichloromethane and precipitated by addition of diethyl ether. The precipitate was separated from the mother liquor by centrifugation. 19 mg were obtained as a dark red solid (33% yield).

R*f* (CH_2Cl_2/MeOH, 95:5): 0.12. **^{1}H NMR (500 MHz, CD_2Cl_2) δ** 8.58 (d, *J* = 9.5 Hz, 1H), 8.37 (d, *J* = 9.0 Hz, 1H), 8.33 (t, *J* = 8.4 Hz, 2H), 8.10 (d, *J* = 9.5 Hz, 1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.82 (d, *J* = 9.0 Hz, 1H), 7.53 (t, *J* = 8.0 Hz, 1H), 7.44 (t, *J* = 8.0 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.02 – 6.89 (m, 3H), 5.16 – 5.04 (m, 1H), 4.99 – 4.83 (m, 1H), 2.29 – 2.15 (m, 2H), 1.80 – 1.69 (m, 2H), 1.45 – 1.31 (m, 5H), 0.90 (t, *J* = 7.2 Hz, 2H). **^{13}C NMR (126 MHz, CD_2Cl_2) δ** 157.1 (C^+), 150.6 (C), 145.26 (C), 142.8 (CH), 142.7 (C), 140.1 (CH), 137.5 (C), 136.4 (CH), 131.2 (C), 129.8 (C), 129.7 (CH), 129.6 (C), 129.6 (CH), 129.5 (CH), 129.0 (CH), 128.6 (CH), 127.8 (C), 127.6 (CH), 125.3 (CH), 124.1 (CH), 119.2 (C), 118.6 (C), 117.9 (CH), 115.3 (CH), 114.8 (C), 111.0 (CH), 110.3 (CH), 32.1 (CH_2), 30.1 (CH_2), 29.6 (CH_2), 29.6 (CH_2), 28.4 (CH_2), 27.2 (CH_2), 23.0 (CH_2), 14.2 (CH_3). **^{19}F NMR (282 MHz, CD_2Cl_2) δ** -152.42, -152.37. **UV/VIS (CH_3CN, 2.10^{-5} M, λ_{max} (nm), (Log ε))** 338 (4.03), 409 (3.84), 561 (3.97). **IR (neat, cm^{-1}) υ** 2928, 2856, 1624, 1597, 1571, 1548, 1529, 1510, 1487, 1459, 1438, 1381, 1348, 1263, 1244, 1208, 1162, 1141 1048, 871, 820, 786, 753, 729, 698, 594, 542. **HRMS** (**ESI**) (M^+) calculated for ($C_{35}H_{32}NO$): 482.2478. Found: 482.2490.

11-hexadecylbenzo[a]benzo[5,6]chromeno[2,3,4-kl]acridin-17c(11H)-ylium tetrafluoroborate (10)



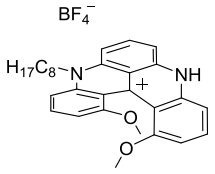
10

To a solution of 11-methoxy-12-(2-methoxynaphthalen-1-yl)-12H-benzo[a]xanthen-12-ylium tetrafluoroborate (prepared following reported procedures)[5] (25 mg, 0.05 mmol) in acetonitrile (5 mL) was added hexadecylamine (0.15 mmol, 3 equiv). The reaction mixture was heated at 70 °C until completion of the reaction as monitored by MS (16 h). Then, the reaction mixture was evaporated. The residue was dissolved in a minimum amount of dichloromethane and the product was precipitated by addition of diethyl ether. The precipitate was separated from the mother liquor by centrifugation, dissolved in dichloromethane and washed once with 1 M aq. $NaBF_4$ solution and once with 1 M aq. HBF_4 solution. The organic layer was dried over Na_2SO_4, filtered and evaporated. The material was next columned (CombiFlash, 4 g SiO_2, CH_2Cl_2/MeOH, 100:00 to 95:05). The product was finally dissolved in a minimum amount of dichloromethane and precipitated by addition of diethyl ether. The precipitate was separated from the mother liquor by centrifugation. 6 mg were obtained as a dark red solid (14% yield).

R*f* (CH_2Cl_2/MeOH, 95:5): 0.13. **^{1}H NMR (500 MHz, CD_2Cl_2) δ** 8.58 (d, *J* = 9.5 Hz, 1H), 8.37 (d, *J* = 9.0 Hz, 1H), 8.34 (dd, *J* = 8.8, 8.1 Hz, 1H), 8.10 (d, *J* = 9.6 Hz, 1H), 8.03 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.99 (d, *J* = 8.7 Hz, 1H), 7.97 – 7.95 (m, 1H), 7.86 (dd, *J* = 8.1, 0.6 Hz, 1H), 7.82 (d, *J* = 9.0 Hz, 1H), 7.53 (ddd, *J* = 8.0, 7.1, 1.1 Hz, 1H), 7.44 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 1H), 7.41 (dd, *J* = 8.3, 0.9 Hz, 1H), 7.00 (dd, *J* = 8.5, 1.0 Hz, 1H), 6.98 – 6.91 (m, 2H), 5.18 – 5.02 (m, 1H), 4.98 – 4.83 (m, 1H), 2.29 - 2.17 (m, 2H), 1.88 – 1.63 (m, 2H), 1.55-1.49 (m, 4H, superimposed with H_2O), 1.44 – 1.38 (m, 2H), 1.28 (brs, 20H), 0.88 (t, *J* = 6.9 Hz, 3H).. **^{13}C NMR (126 MHz, CD_2Cl_2) δ** 157.1 (C), 150.6 (C), 145.3 (C), 142.8 (CH), 142.8 (C), 140.2 (CH), 137.5 (C), 136.4 (CH), 131.3 (C), 129.9 (C), 129.7 (CH), 129.6 (CH), 129.5 (C), 129.1 (CH), 128.6

(CH), 127.8 (C), 127.6 (CH), 125.4 (CH), 124.1 (CH), 119.3 (C), 118.6 (C), 117.9 (CH), 115.3 (CH), 114.8 (C), 111.0 (CH), 110.4 (CH), 32.3 (3 CH_2), 30.1 (CH_2), 30.1 (CH_2), 30.1 (CH_2), 30.0 (CH_2), 30.0 (CH_2), 29.8 (CH_2), 29.7 (CH_2), 28.4 (2 CH_2), 27.2 (2 CH_2), 23.1 (CH_2), 14.3 (CH_3). **^{19}F NMR (282 MHz, CD_2Cl_2) δ** -153.18, -153.24. **UV/VIS (CH_3CN, 1.55.10^{-5} M, λ_{max} (nm), (Log ε))** 339 (4.14), 410 (3.96), 562 (4.08). **IR (neat, cm^{-1}) υ** 2924, 2853, 1624, 1599, 1572, 1548, 1530, 1488, 1465, 1440, 1350, 1264, 1247, 1212, 1160, 1057, 821, 792, 757. **HRMS** (**ESI**) (M^+) calculated for ($C_{43}H_{48}NO$): 594.3730. Found: 594.3736.

1,13-dimethoxy-5-octyl-5,9-dihydro-13bH-quinolino[2,3,4-kl]acridin-13b-ylium tetrafluoroborate (15)

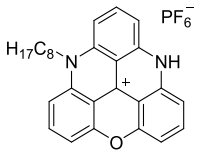


15

10-amino-9-(2,6-dimethoxyphenyl)-1,8-dimethoxy-9,10-dihydroacridin-9-ylium tetrafluoroborate (304 mg, 0.64 mmol) (prepared following reported procedures)[6] was degassed in a red-tinted flask. DMF (3 mL, 0.2 M) was then added and the solution was allowed to stir under N_2 atmosphere at 90 °C for 5 min. Finally, *n*-octylamine (2.63 mL, 15.89 mmol, 25 equiv) was added, the lights were switched off and the reaction mixture was allowed to stir under N_2 atmosphere at 90 °C for 16 h. After complete consumption of the starting material (followed by ESI-MS) the crude reaction mixture was allowed to cool down to RT. 25 mL of a solution of HBF_4 1 M were added and the product was extracted with 25 mL of CH_2Cl_2. The organic layer was washed consecutively with aqueous solutions of LiCl 10% (w/w) (x3), brine, and HBF_4 1 M again, dried over Na_2SO_4 and concentrated. Selective precipitations with Et_2O afforded the quinacridinium tetrafluoroborate salt **15** as a dark green solid (209 mg, 0.40 mmol, 62%).

R_f (basic alumina, CH_2Cl_2/MeOH, 97/3): 0.54. **^{1}H NMR (CD_2Cl_2, 400 MHz)**: δ 11.72 (s, 1H, NH), 8.04 (t, *J* = 8.3 Hz, 1H, CH), 7.82 (dd, *J* = 8.9, 8.0 Hz, 1H, CH), 7.77 (t, *J* = 8.2 Hz, 1H, CH), 7.67 (d, *J* = 8.3 Hz, 1H, CH), 7.50 (dd, *J* = 8.6, 1.0 Hz, 1H, CH), 7.26 – 7.19 (m, 2H, 2xCH), 6.78 (d, *J* = 8.0 Hz, 1H, CH), 6.74 (d, *J* = 8.0 Hz, 1H, CH), 4.58 – 4.47 (m, 1H, CH_2), 4.34 – 4.23 (m, 1H, CH_2), 3.75 (d, *J* = 4.7 Hz, 6H, 2xOCH_3), 2.11 – 1.96 (m, 2H, CH_2), 1.65 – 1.59 (m, 2H, CH_2), 1.53 – 1.45 (m, 2H, CH_2), 1.42 – 1.31 (m, 6H, 3xCH_2), 0.94 – 0.89 (m, 3H, CH_3) ppm. **^{13}C NMR (CD_2Cl_2, 101 MHz):** δ 160.9 (C), 159.4 (C), 144.5 (C), 143.5 (C), 142.6 (C), 138.9 (C), 138.7 (C), 137.3 (CH), 137.1 (CH), 136.7 (CH), 119.3 (C), 113.5 (C), 113.0 (C), 110.6 (CH), 107.3 (CH), 103.8 (CH), 103.1 (CH), 102.9 (CH), 56.0 (2xOCH_3), 50.2 (CH_2), 32.3 (CH_2), 29.8 (2xCH_2), 27.4 (CH_2), 26.5 (CH_2), 23.2 (CH_2), 14.4 (CH_3) ppm. **^{19}F NMR (CD_2Cl_2, 282 MHz):** δ -149.8 (26%), -149.9 (74%) ppm. **UV-vis**: λ_{max} (CH_3CN): 567 nm (ε = 4800 L.mol^{-1}.cm^{-1}). **IR (neat):** 3300, 2928, 2861, 1639, 1589, 1502, 1483, 1346, 1259, 1162, 1118, 1068, 816, 766, 580, 525 cm^{-1}. **HRMS (ESI+)** calculated for [$C_{29}H_{33}N_2O_2^+$ (M^+)]: 441.2537; found: 441.2535.

8-octyl-8,12-dihydro-3a2H-benzo[ij]xantheno[1,9,8-cdef][2,7]naphthyridin-3a2-ylium hexafluorophosphate (13)



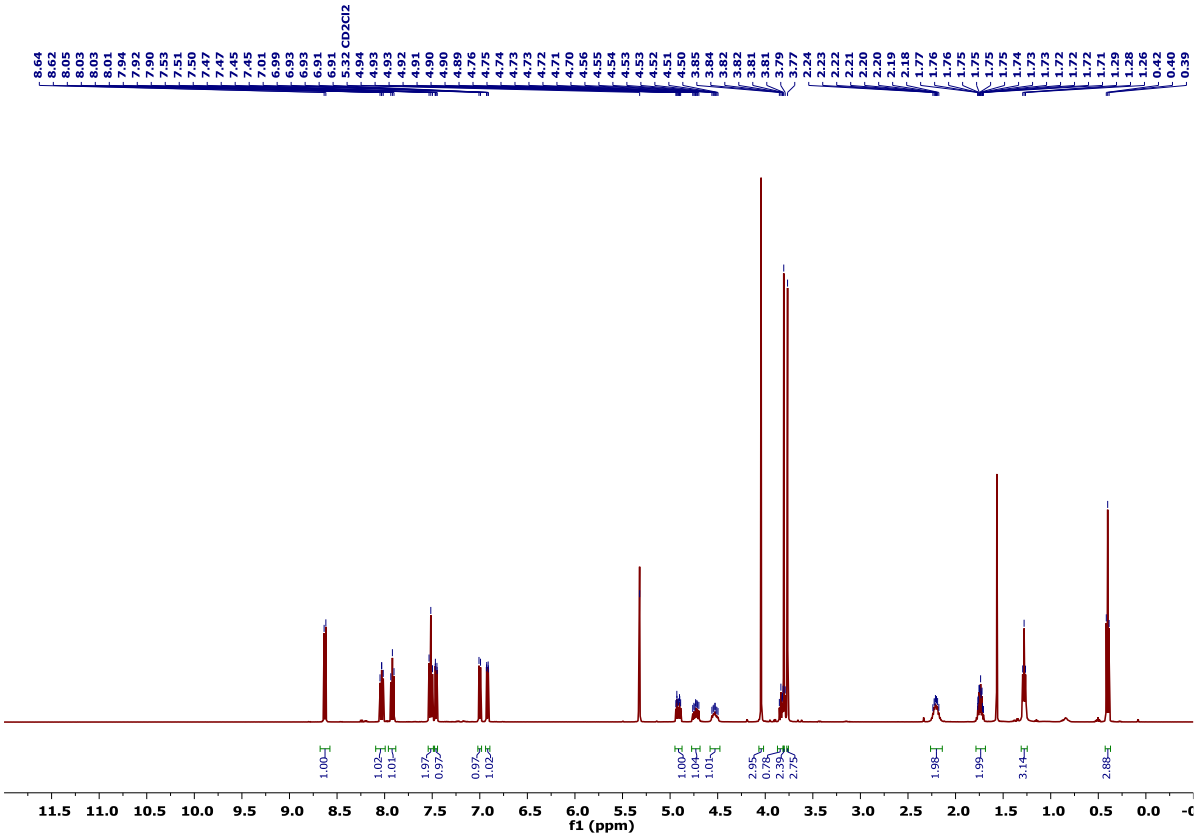
13

Pyridinium chloride (3.10 g, 26.32 mmol, 100 equiv) was melted at 160 °C and let water evaporate for 30 min. Pyridine (0.5 mL) was added in order to avoid crystallization of the pyridinium salt and 1,13-dimethoxy-5-octyl-5,9-dihydro-13bH-quinolino[2,3,4-kl]acridin-13b-ylium tetrafluoroborate **15** (139 mg, 0.26 mmol) was then added. A reflux was set up to the system and the reaction mixture was allowed to stir for 38 h at 160 °C. After complete consumption of the starting material (followed by ESI-MS) the crude reaction mixture was allowed to cool down to room temperature. Ion metathesis was then performed by adding 25 mL of a solution of KPF_6 0.2 M to the crude mixture and extracted it with 25 mL of CH_2Cl_2. The organic phase was dried over Na_2SO_4 and concentrated. Finally, the product was purified by flash chromatography with CH_2Cl_2/MeOH (100/0 to 90/10). Triangulenium hexafluorophosphate salt **13** was obtained as a dark purple solid (122 mg, 0.22 mmol, 85%).

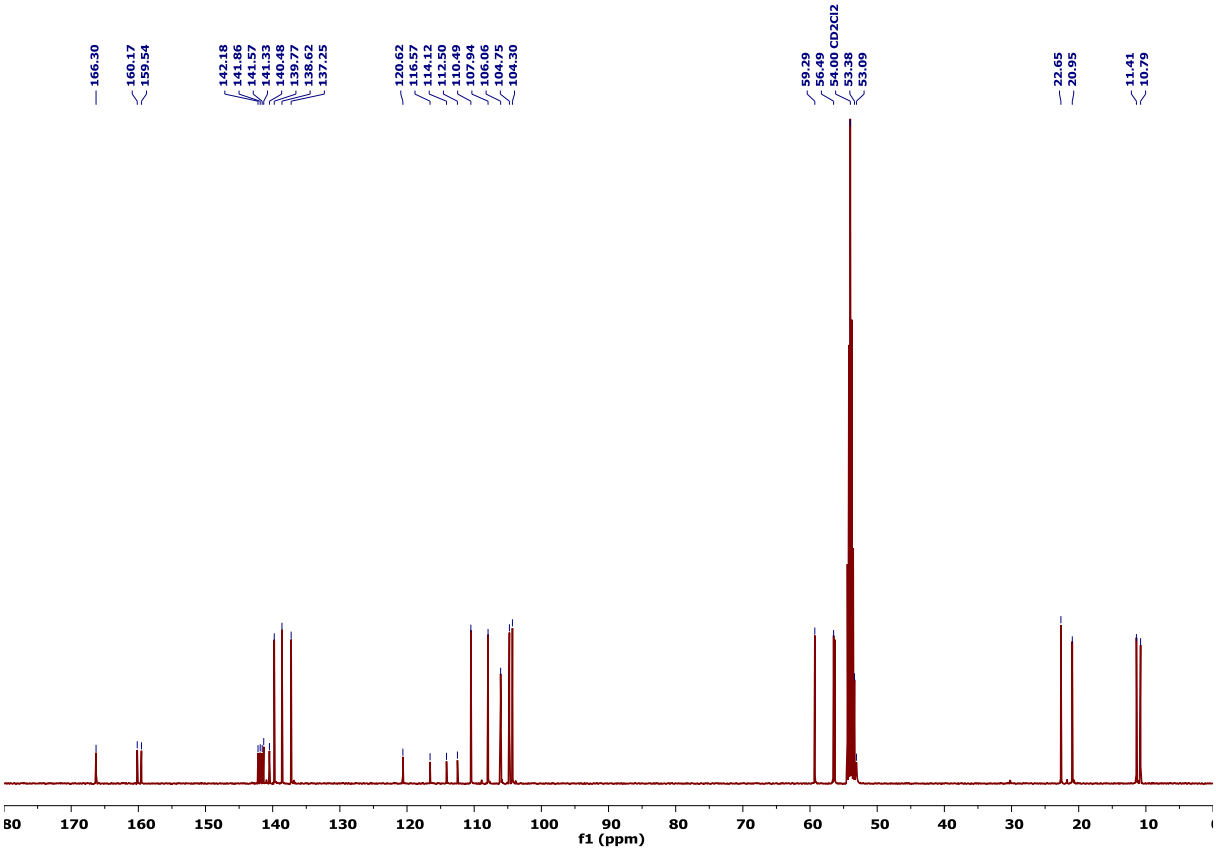
R_f (basic alumina, CH_2Cl_2/MeOH, 97/3): 0.44. **^{1}H NMR (CD_2Cl_2, 500 MHz)**: δ 10.47 (s, 1H, NH), 8.10 (t, *J* = 8.4 Hz, 1H, CH), 8.01 (dd, *J* = 8.8, 8.2 Hz, 1H, CH), 7.94 (t, *J* = 8.3 Hz, 1H, CH), 7.48 (dd, *J* = 8.5, 0.7 Hz, 1H, CH), 7.45 (d, *J* = 8.3 Hz, 1H, CH), 7.34 (d, *J* = 8.8 Hz, 1H, CH), 7.25 (dd, *J* = 8.2, 0.5 Hz, 1H, CH), 7.21 – 7.15 (m, 2H, 2xCH), 4.40 – 4.34 (m, 2H, CH_2), 1.98 – 1.90 (m, 2H, CH_2), 1.63 – 1.56 (m, 2H, CH_2), 1.50 – 1.42 (m, 2H, CH_2), 1.40 – 1.30 (m, 6H, 3xCH_2), 0.92 – 0.88 (m, 3H, CH_3) ppm. **^{13}C NMR (CD_2Cl_2, 126 MHz):** δ 153.8 (C), 152.4 (C), 141.3 (C), 141.0 (C), 140.7 (C), 140.5 (C), 140.2 (CH), 139.4 (C), 139.2 (CH), 139.1 (CH), 111.5 (C), 111.3 (CH), 109.4 (CH), 109.2 (CH), 108.6 (CH), 108.2 (CH), 108.0 (C), 107.5 (C), 105.3 (CH), 48.4 (CH_2), 32.3 (CH_2), 29.8 (2xCH_2), 27.3 (CH_2), 26.1 (CH_2), 23.2 (CH_2), 14.4 (CH_3) ppm. **^{19}F NMR (CD_2Cl_2, 282 MHz):** δ -70.2, -72.7 ppm. **UV-vis**: λ_{max} (CH_3CN): 549 nm (ε = 7800 L.mol^{-1}.cm^{-1}). **IR (neat):** 3315, 2927, 2854, 1649, 1620, 1596, 1523, 1451, 1340, 1258, 1156, 1102, 1075, 1055, 823, 765, 736, 625, 552 cm^{-1}. **HRMS (ESI+)** calculated for [$C_{27}H_{27}N_2O^+$ (M^+)]: 395.2123; found: 395.2122.

3. Structural analyses

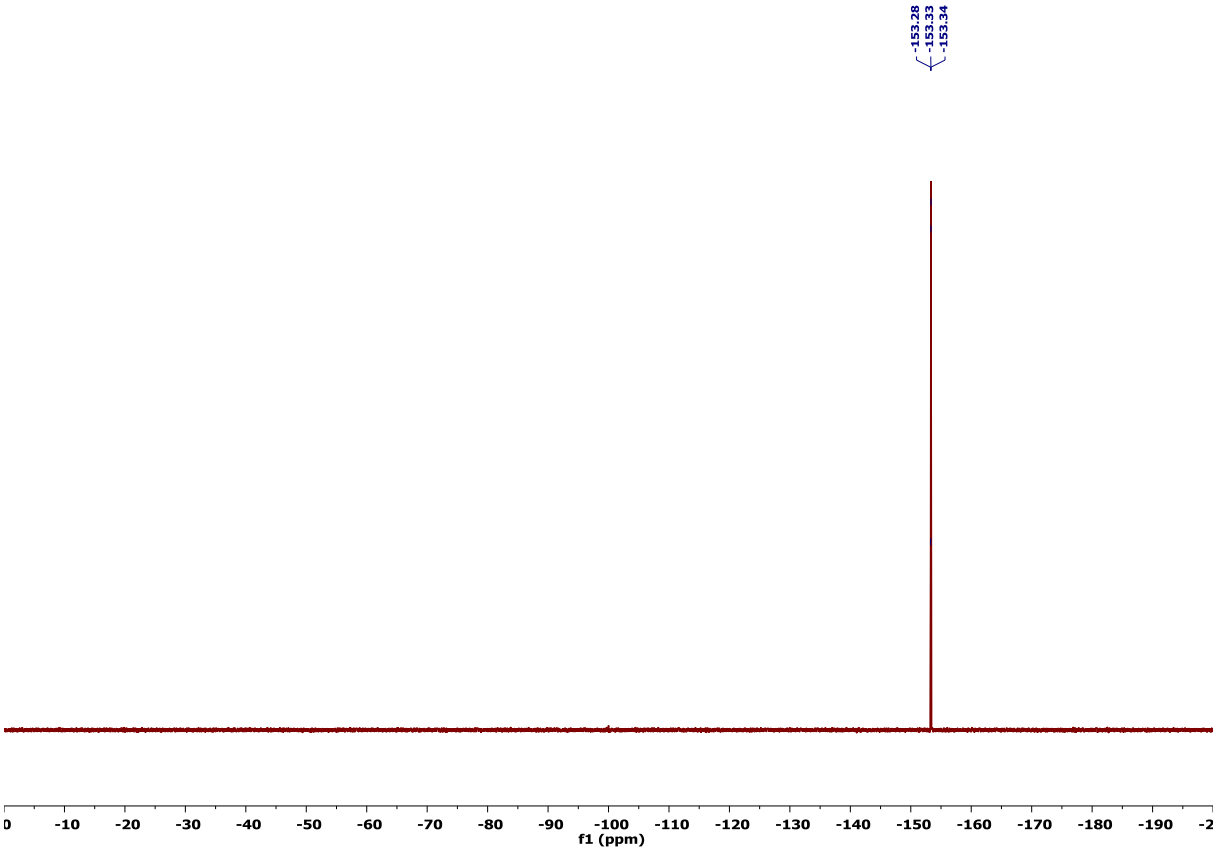
^{1}H NMR (500 MHz, CD_2Cl_2) 3



^{13}C NMR (126 MHz, CD_2Cl_2)



^{19}F NMR (282 MHz, CD_2Cl_2)



HRMS (ESI+)

Mass Spectrometry Core Facility

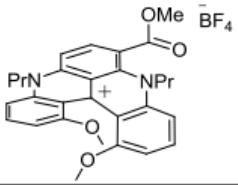
Faculty of Sciences – University of Geneva

UNIVERSITÉ DE GENÈVE
FACULTÉ DES SCIENCES

ESI-HRMS – Certificate of Analysis

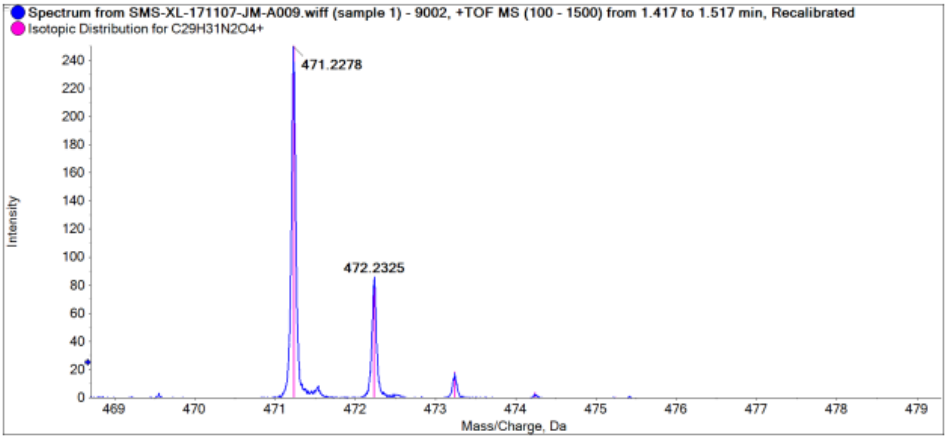
Applicant:	Romain Duwald	Date of reception:	November 7, 2017
Group/Company:	DUR668	Date of certificate:	November 8, 2017
Sample number:	9002	Data filename:	SMSXL-171107-JM-A009
Analyst:	**Julien Meyer**	Instrument:	QSTAR XL (QqTOF)
Contact:	**esi-hrms@unige.ch**	Ionisation mode:	ESI (positive polarity)

Expected Formula	Ion type	Theoretical *m/z*	Observed *m/z*	Accuracy *(ppm)* [a]
$C_{29}H_{31}N_2O_4^+$	$[M]^+$	471.2278	471.2278	-0.2

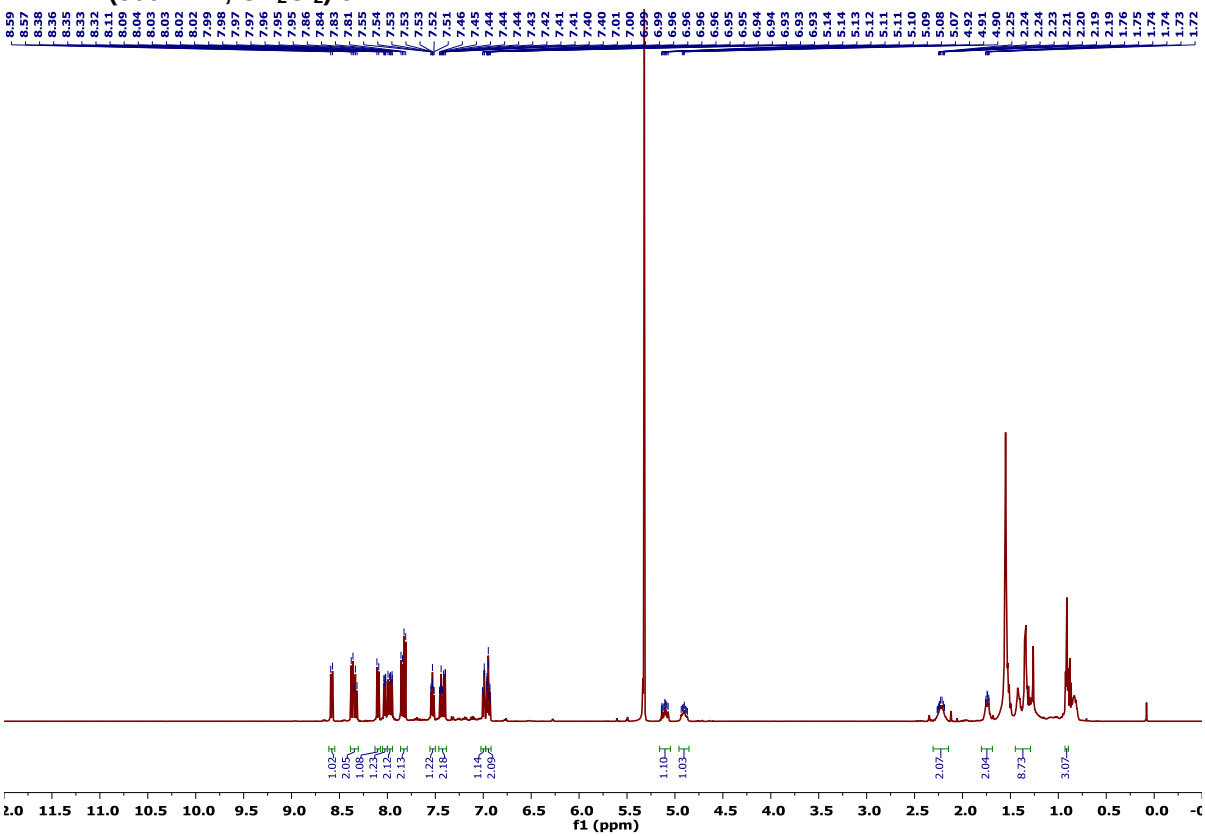


[a] *Mass accuracy is determined after spectrum re-calibration (internal calibration with standards added to the FIA mobile phase).*

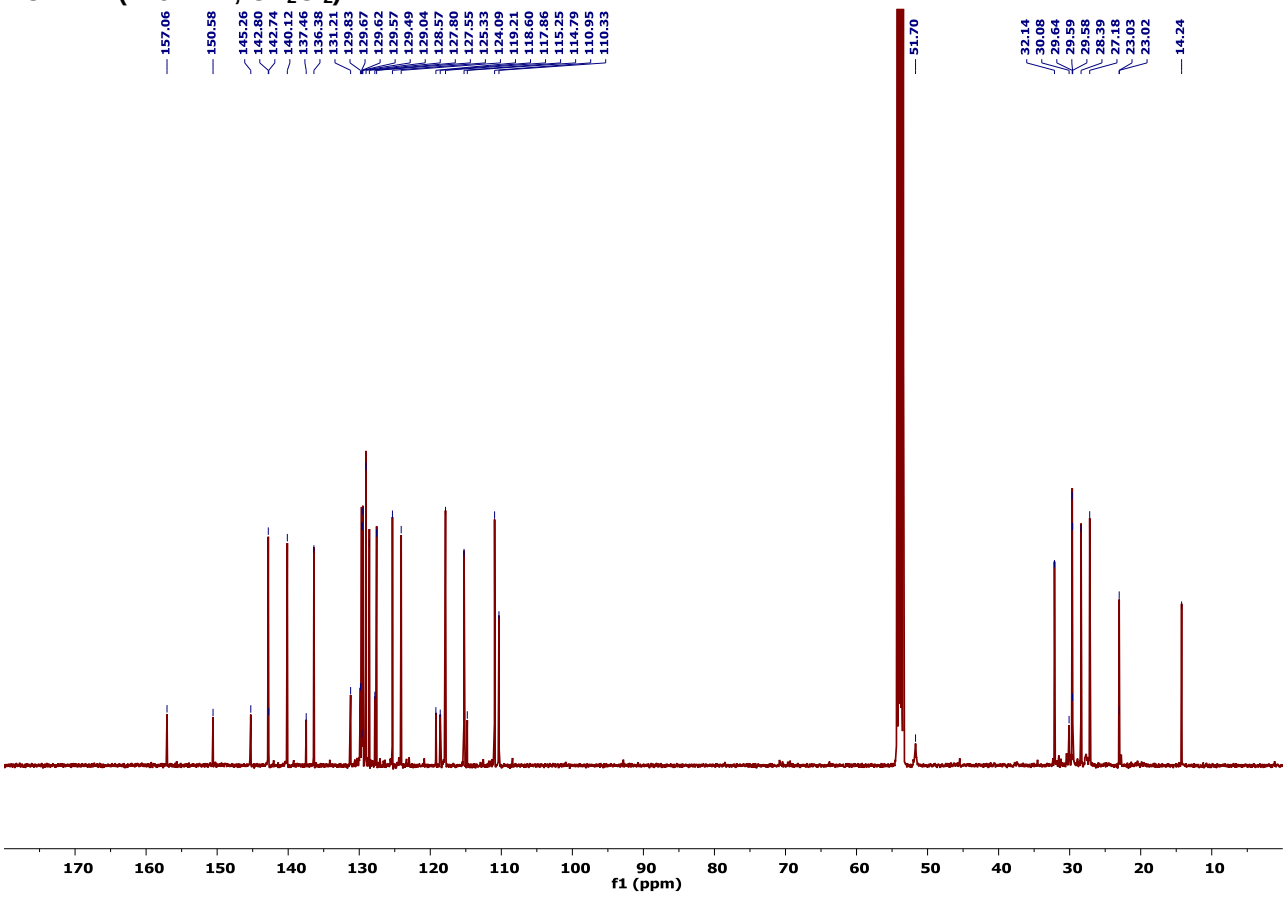
Recalibrated mass spectrum



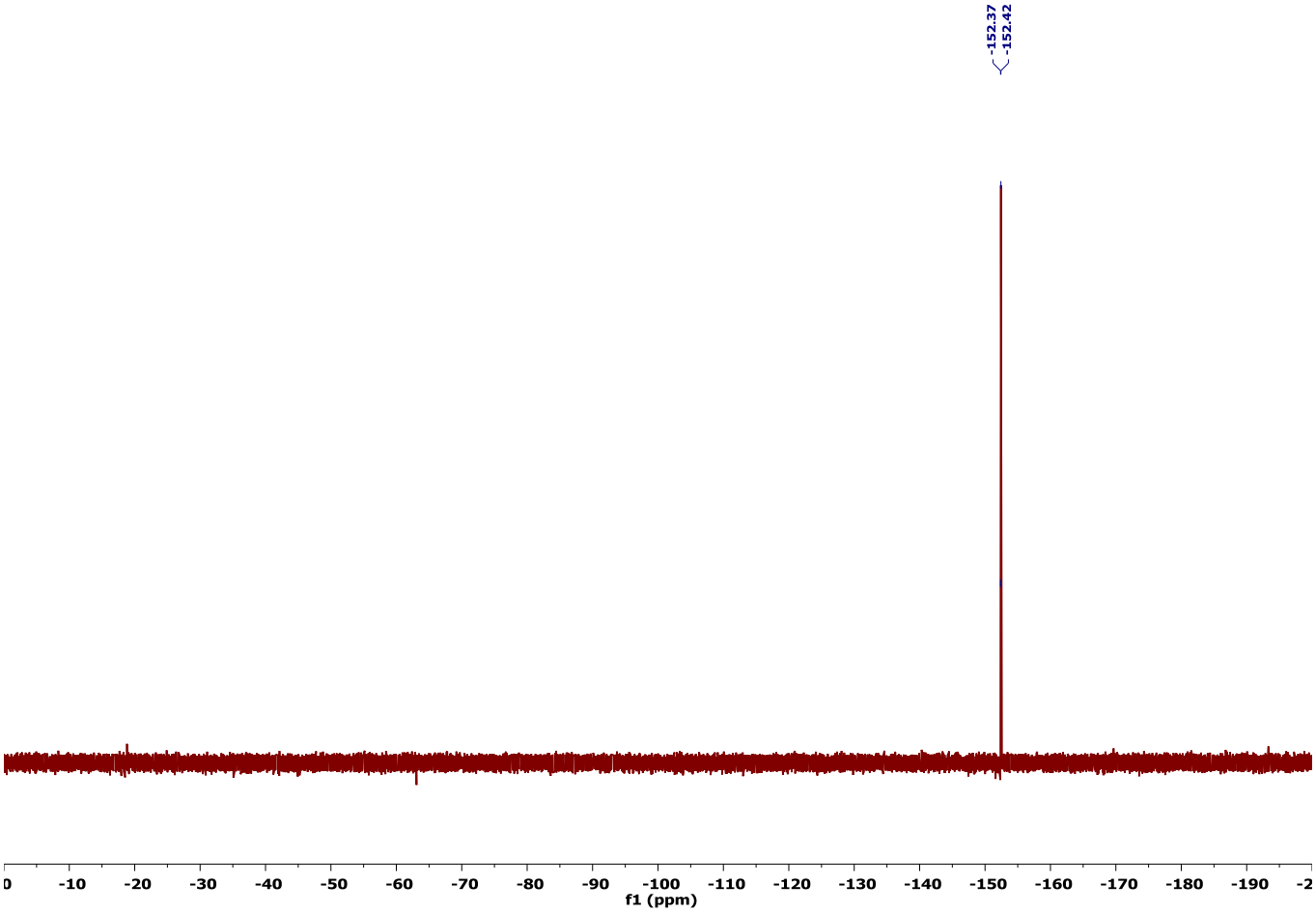
^{1}H NMR (500 MHz, CD_2Cl_2) 9



^{13}C NMR (126 MHz, CD_2Cl_2)



^{19}F NMR (282 MHz, CD_2Cl_2)



HRMS (ESI)

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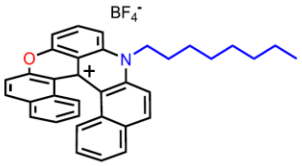
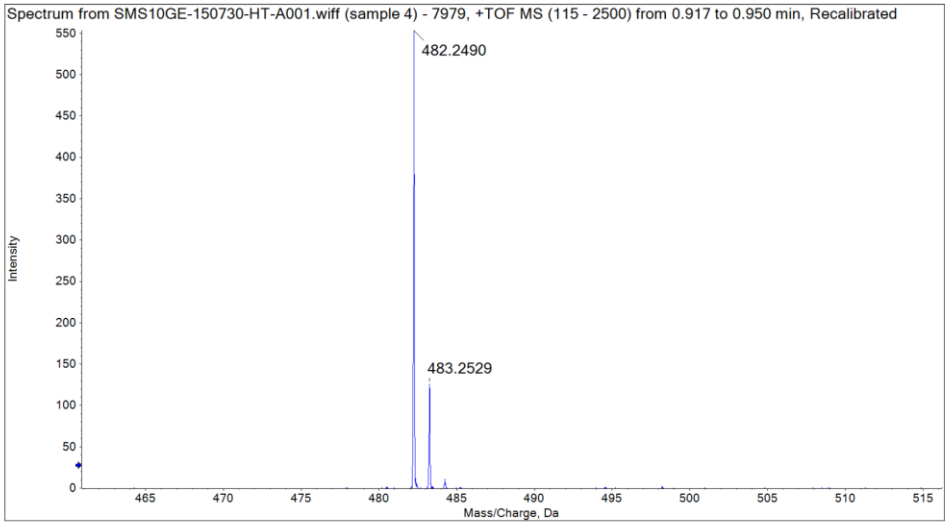
SMS MS

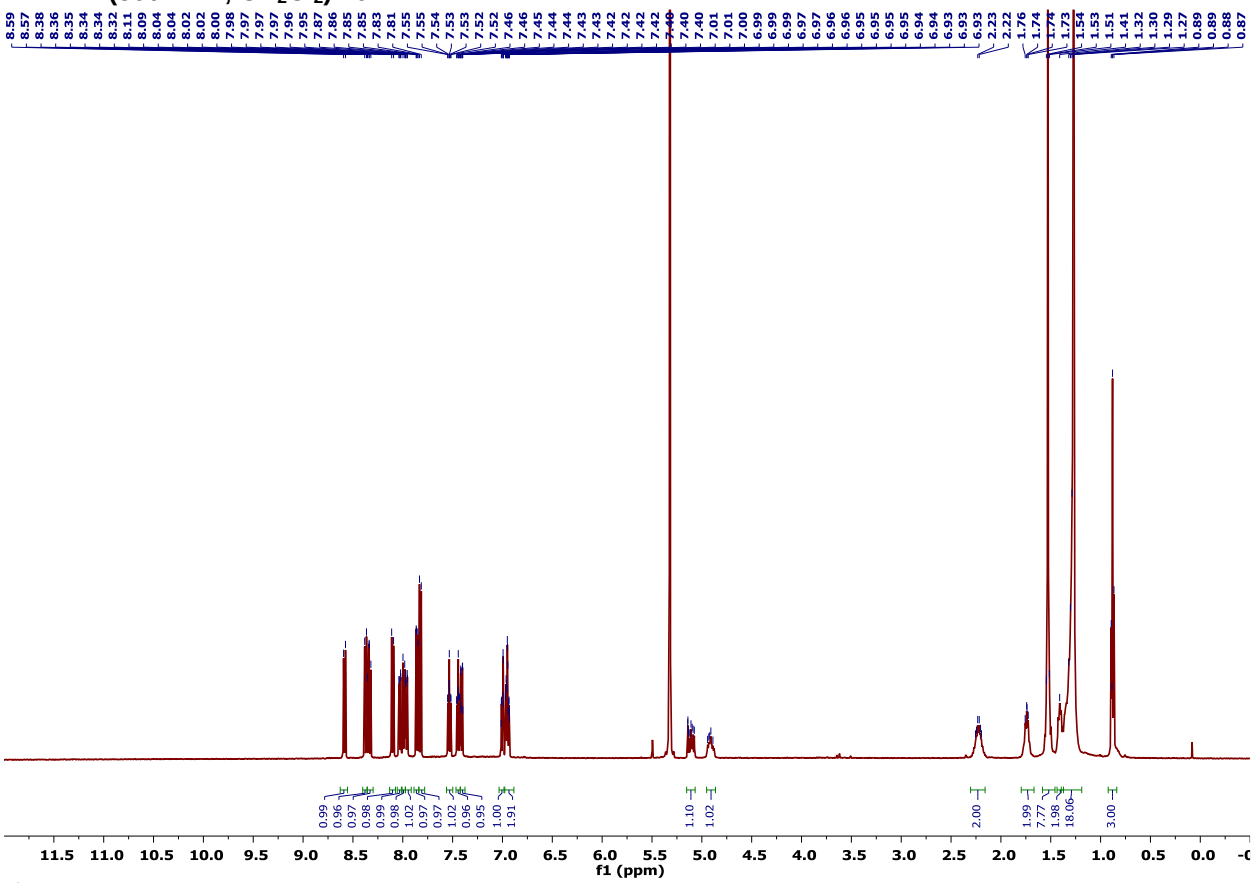
Submitter:	Geraldine Labrador	Date of reception:	29/07/15
Sample name:	GL 443	Date of certificate:	04/08/15
Sample number:	7979	Data filename:	SMS10GE-150730-HT-A001
Operator:	Harry Théraulaz	Instrument:	QSTAR Pulsar (AB/MDS Sciex)
Principal investigator:	Dr. Sophie Michalet	Ionisation mode:	ESI (positive mode)

Expected Formula	Observed *m/z* $[M]^+$	Expected *m/z* (amu)	Accuracy (ppm)
$C_{35}H_{32}NO$	482.2490	482.2478	2.4

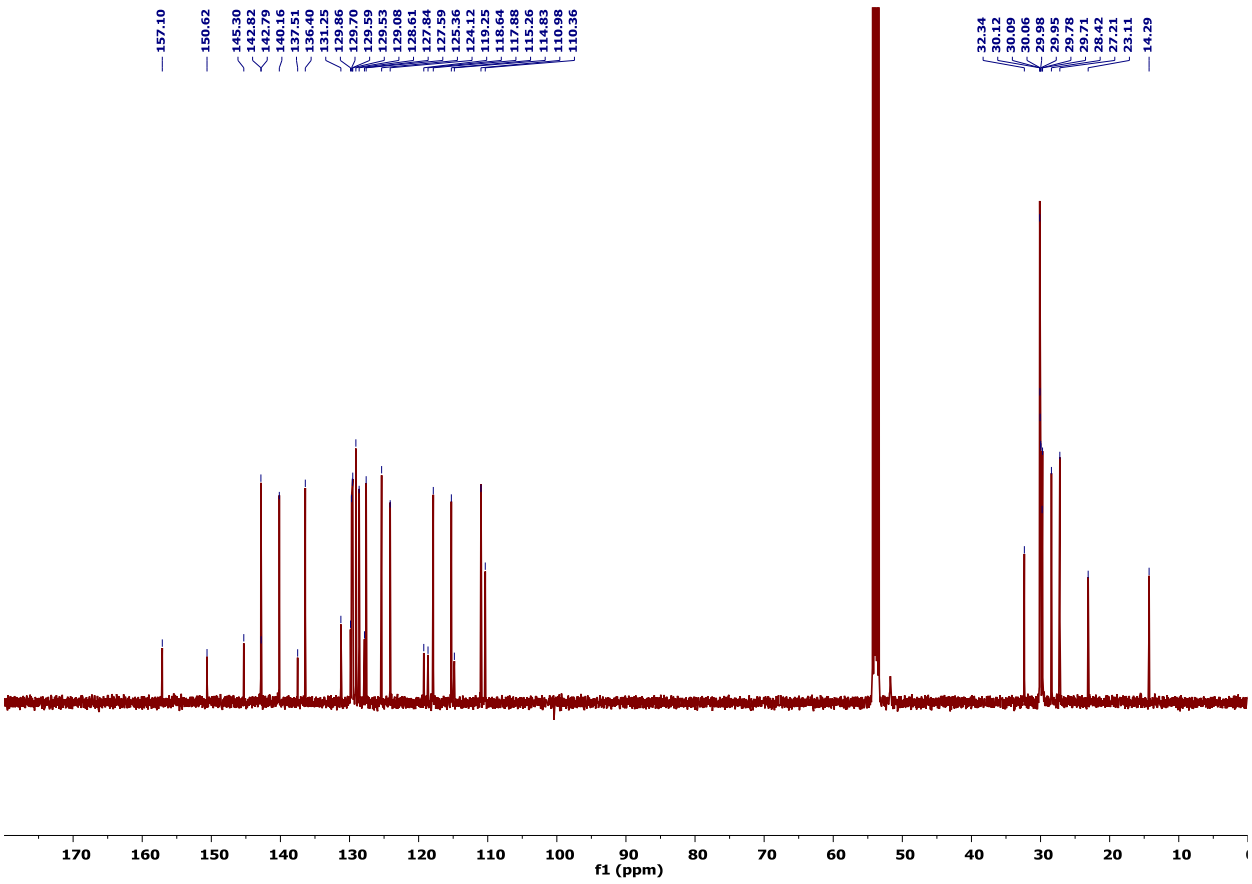




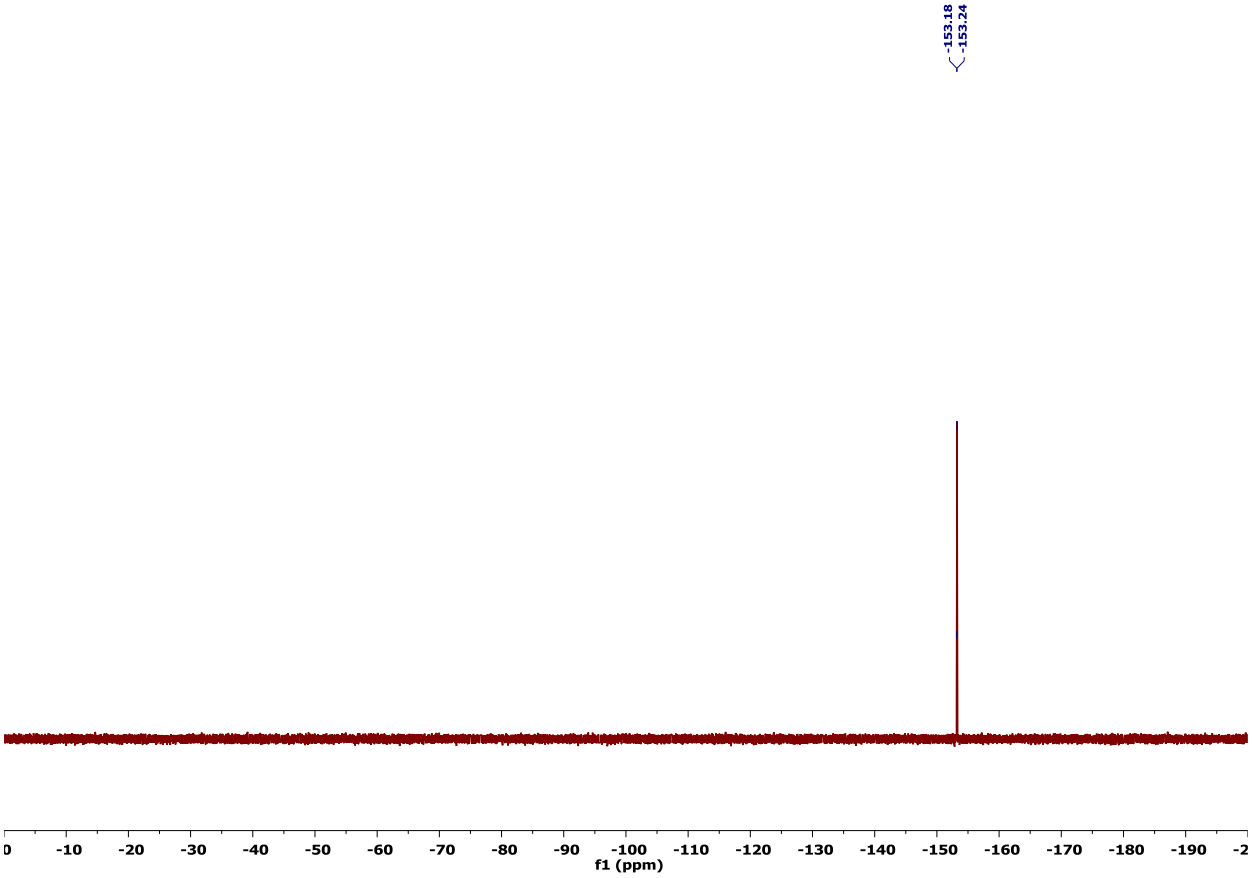
^{1}H NMR (500 MHz, CD_2Cl_2) 10



^{13}C NMR (126 MHz, CD_2Cl_2)



^{19}F NMR (282 MHz, CD_2Cl_2)



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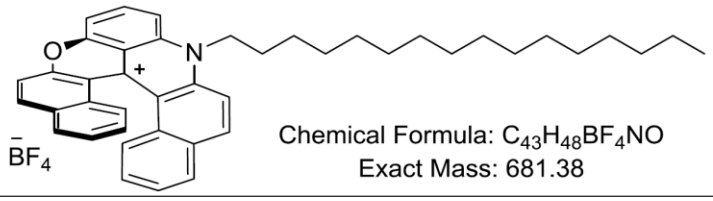
Submitter:	BOSSON	Date of reception:	02/06/16
Sample name:	JB753	Date of certificate:	03/06/16
Sample number:	8424	Data filename:	MS_XL_R3-160602-ES-A001
Operator:	Eliane Sandmeier	Instrument:	XL_R3 (AB/MDS Sciex)
Principal investigator:	Dr. Sophie Michalet	Ionisation mode:	ESI (positive mode)

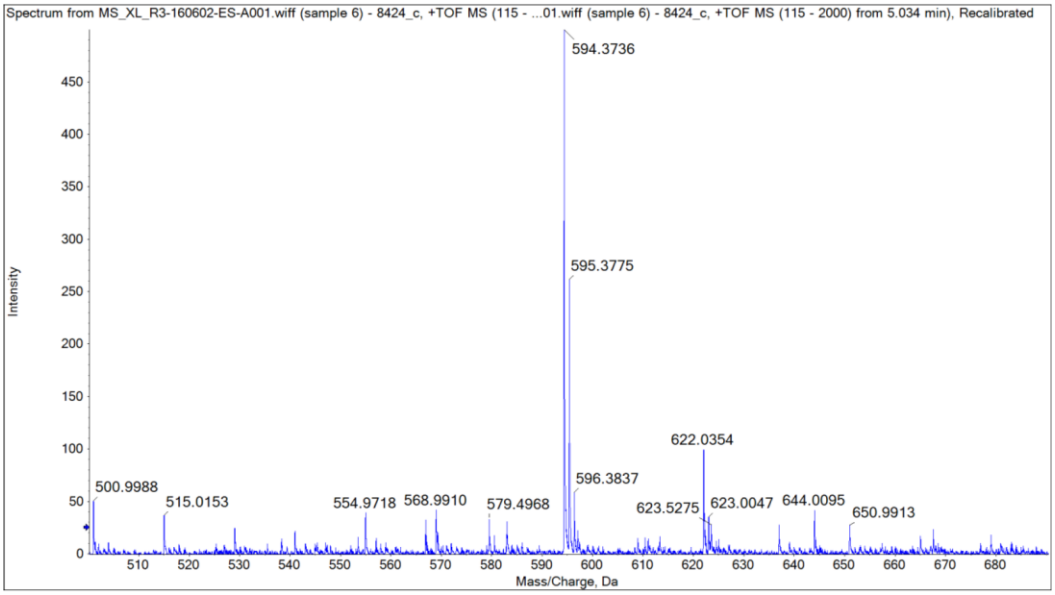
Expected Formula	Observed *m/z*	Expected *m/z* (amu)	Accuracy (ppm)
$C_{43}H_{48}NO$	594.3736 $[M]^+$	594.3730	1.0

JB753



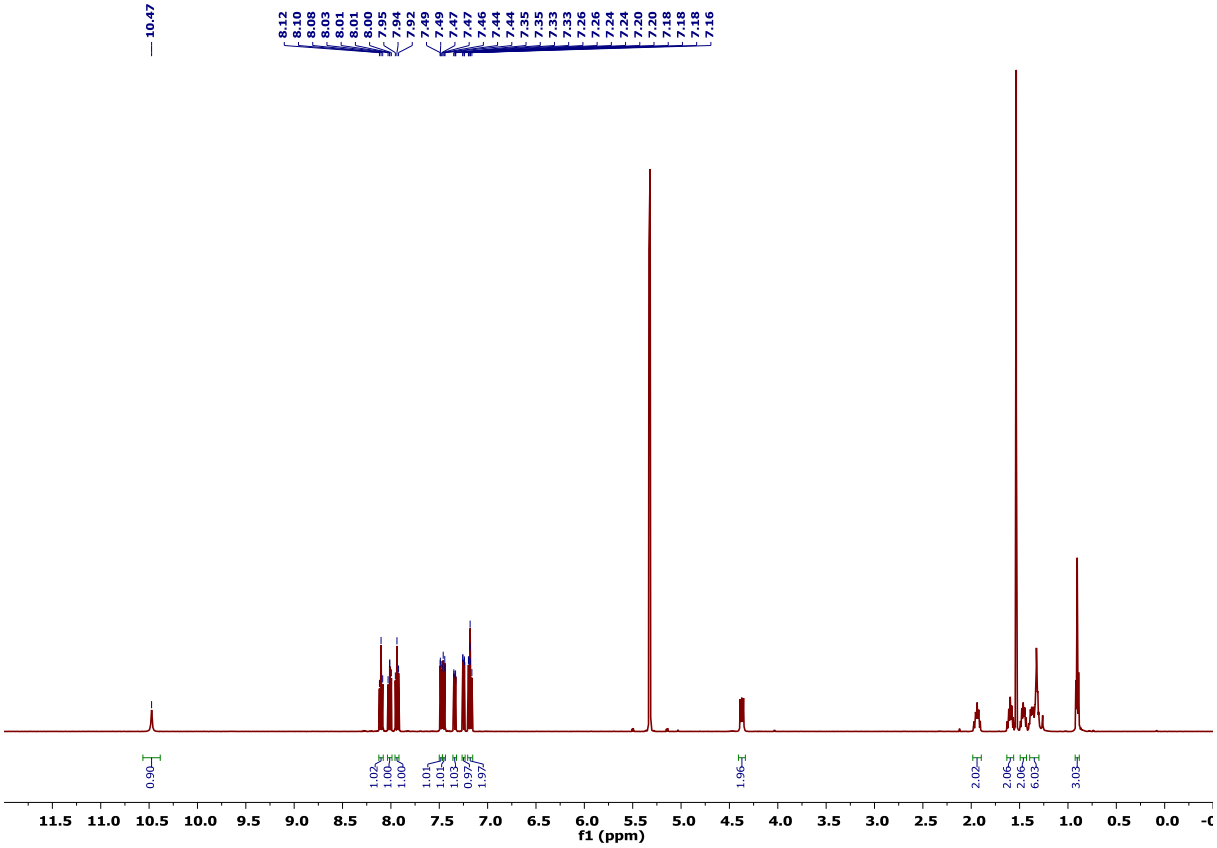
Chemical Formula: $C_{43}H_{48}BF_4NO$

Exact Mass: 681.38

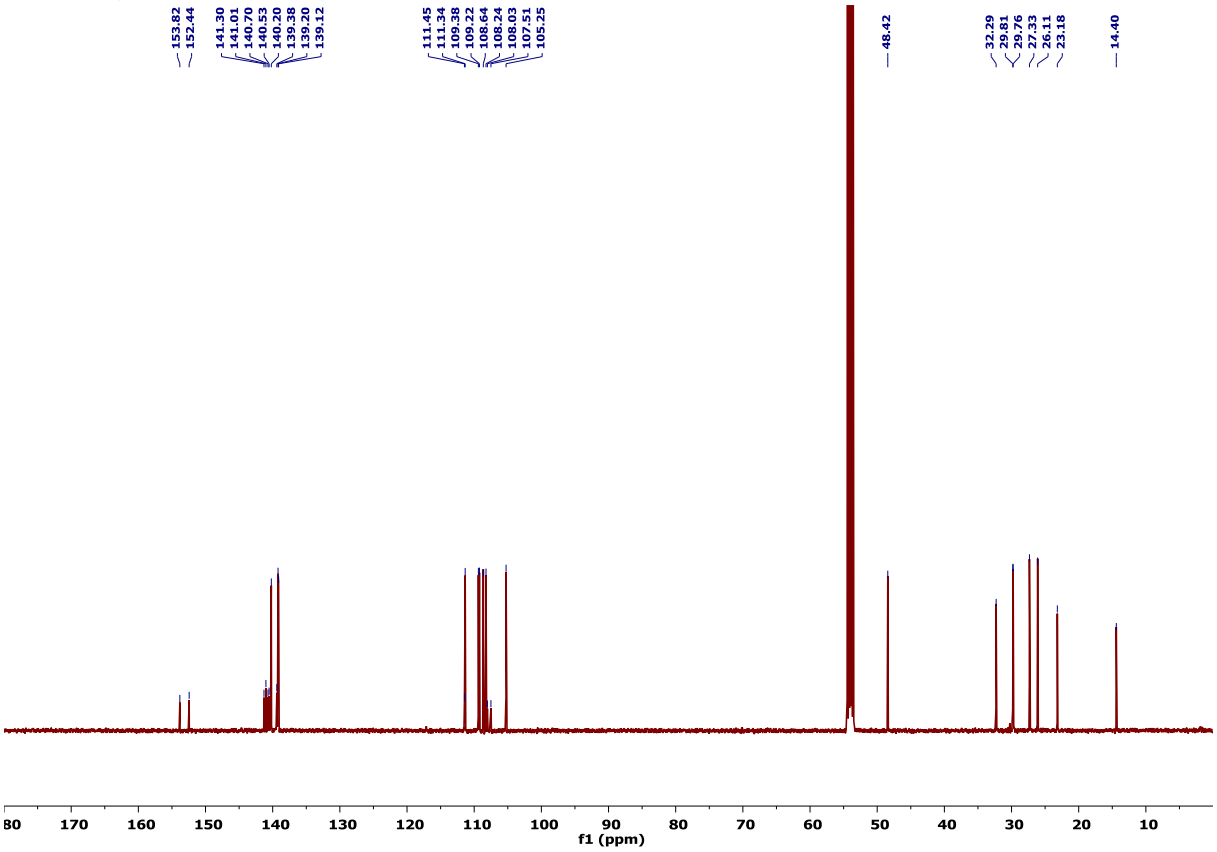


Warning: The analyte signal is mixed with the internal standard at *m/z* 622.0354. It hasn't been used for the calibration.

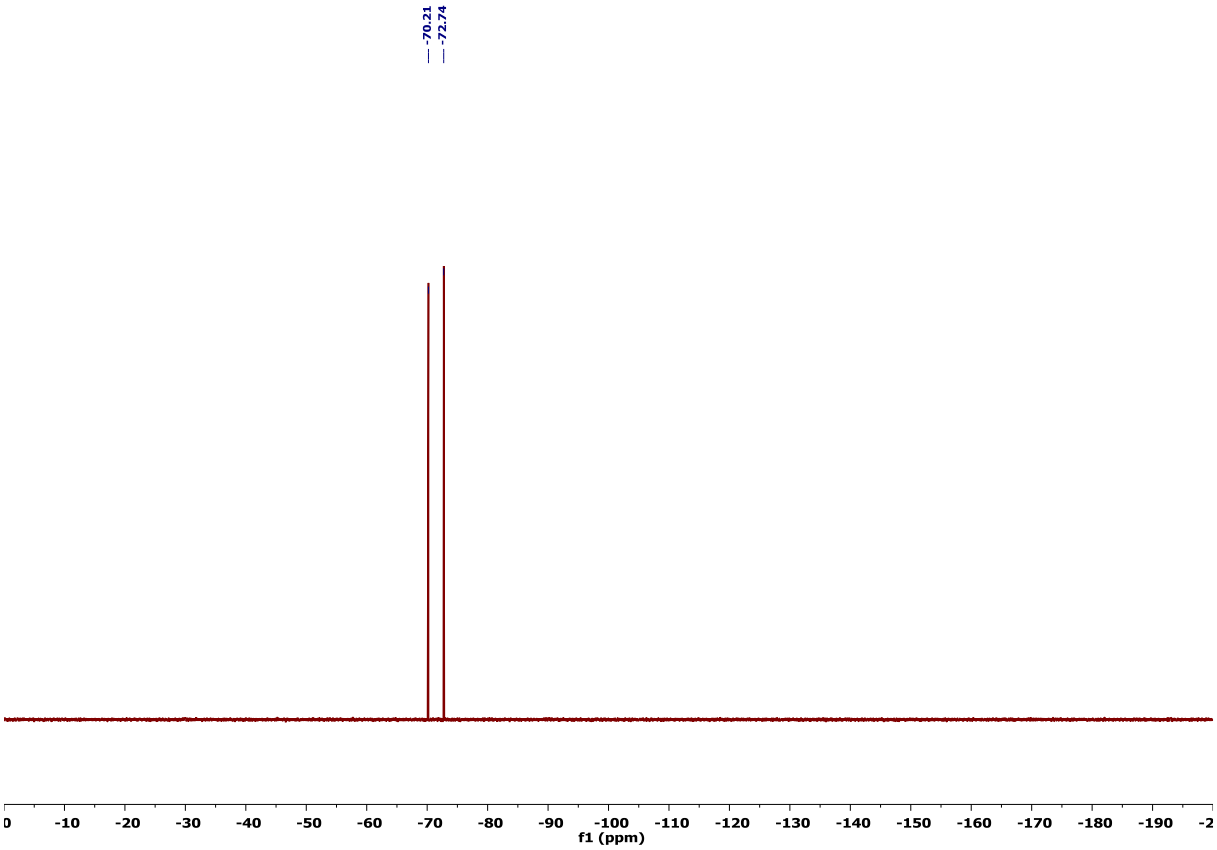
^{1}H NMR (500 MHz, CD_2Cl_2) 13



^{13}C NMR (126 MHz, CD_2Cl_2)



^{19}F NMR (282 MHz, CD_2Cl_2)



HRMS (ESI+)

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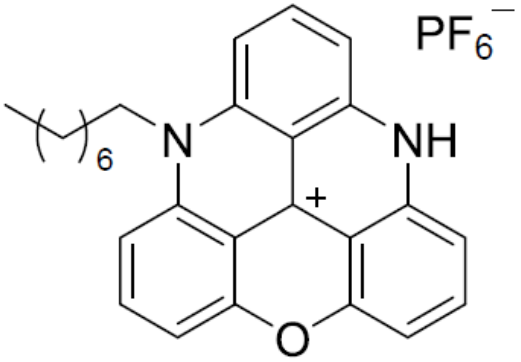
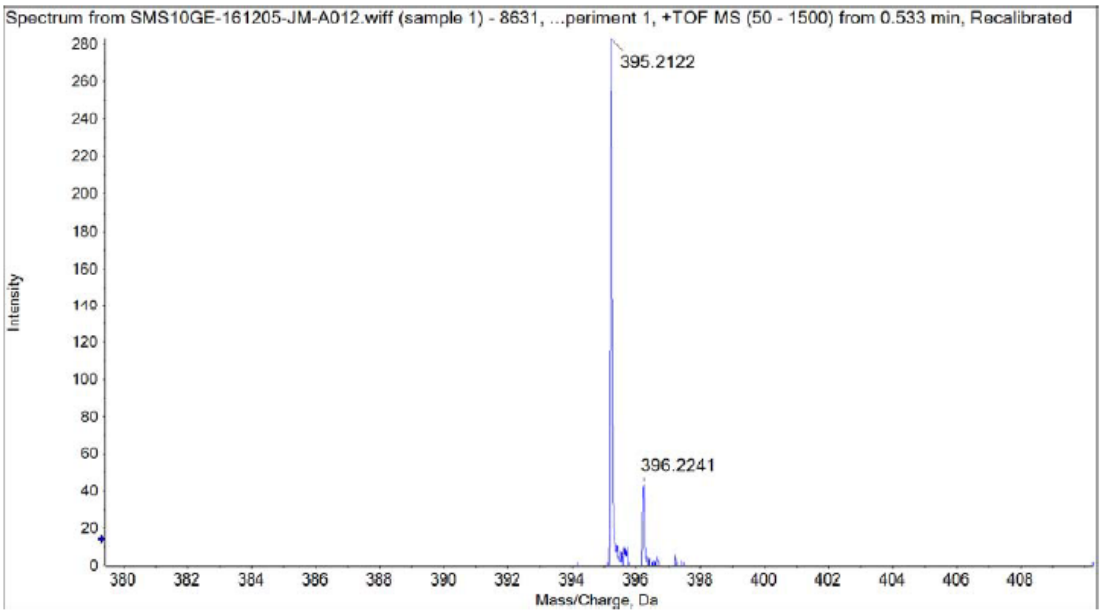
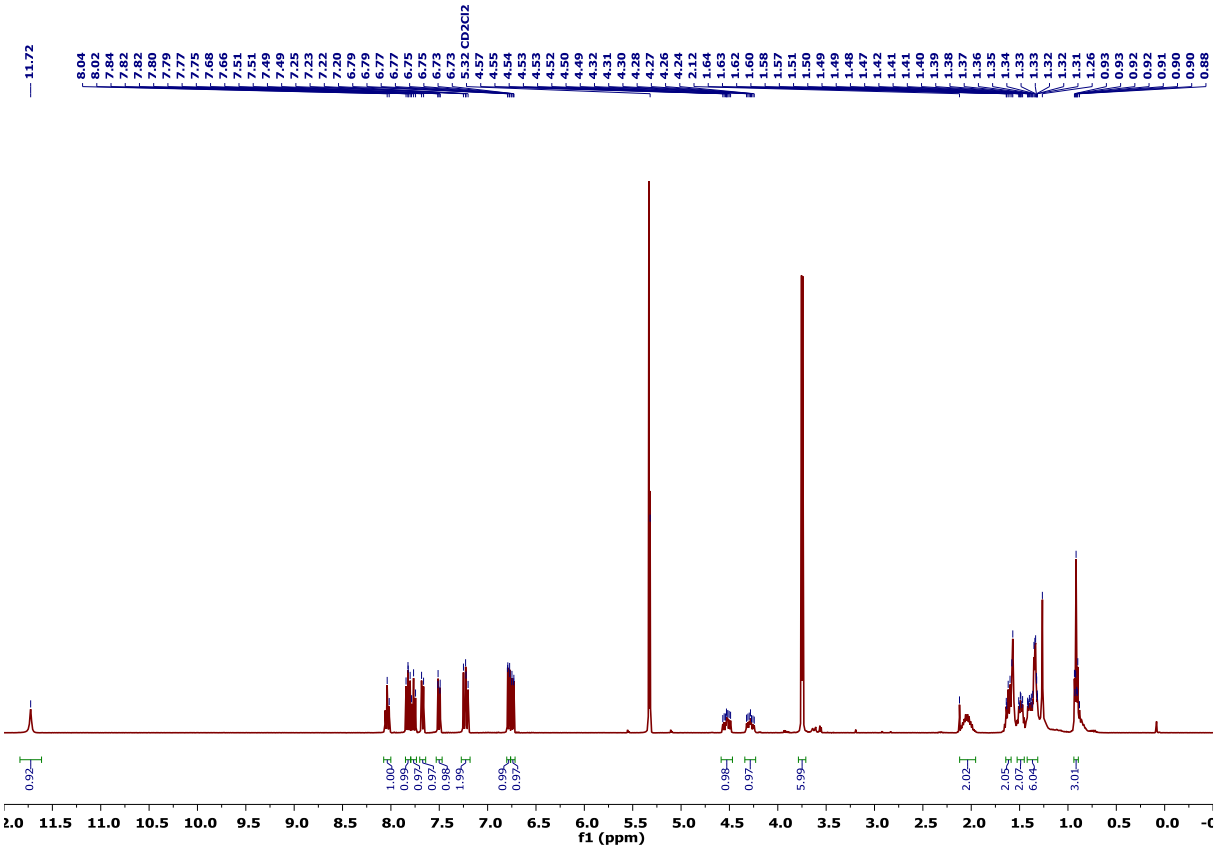
Submitter:	Moneva Lorente Pau	Date of reception:	05/12/2016
Sample name:	PML175	Date of certificate:	05/12/2016
Sample number:	8631	Data filename:	SMS10GE-161205-JM-A012
Operator:	Julien Meyer	Instrument:	QSTAR Pulsar (AB/MDS Sciex)
Principal investigator:	Dr. Sophie Michalet	Ionisation mode:	ESI (positive mode)

Expected Formula	Observed *m/z* $[M]^+$	Expected *m/z* (amu)	Accuracy (ppm)
$C_{27}H_{27}N_2O^+$	395.2122	395.2123	-0.3

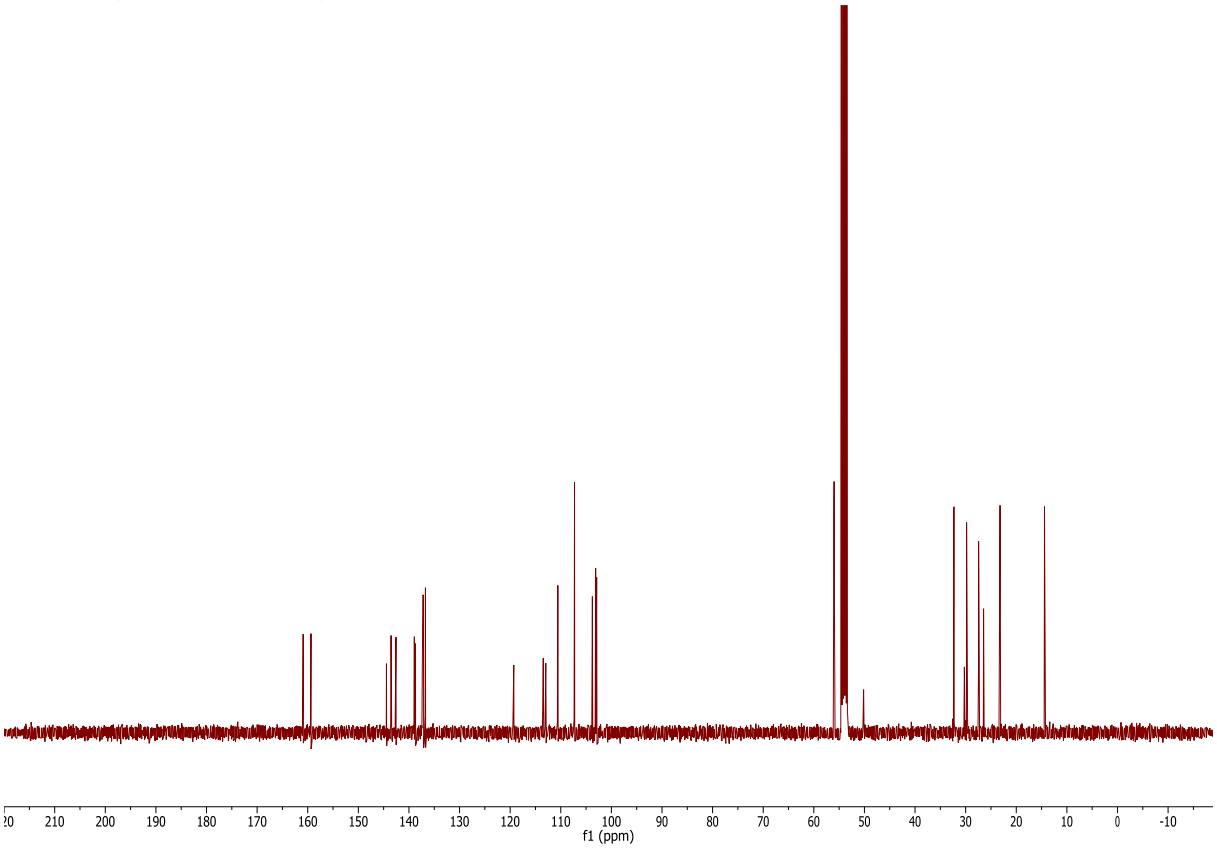




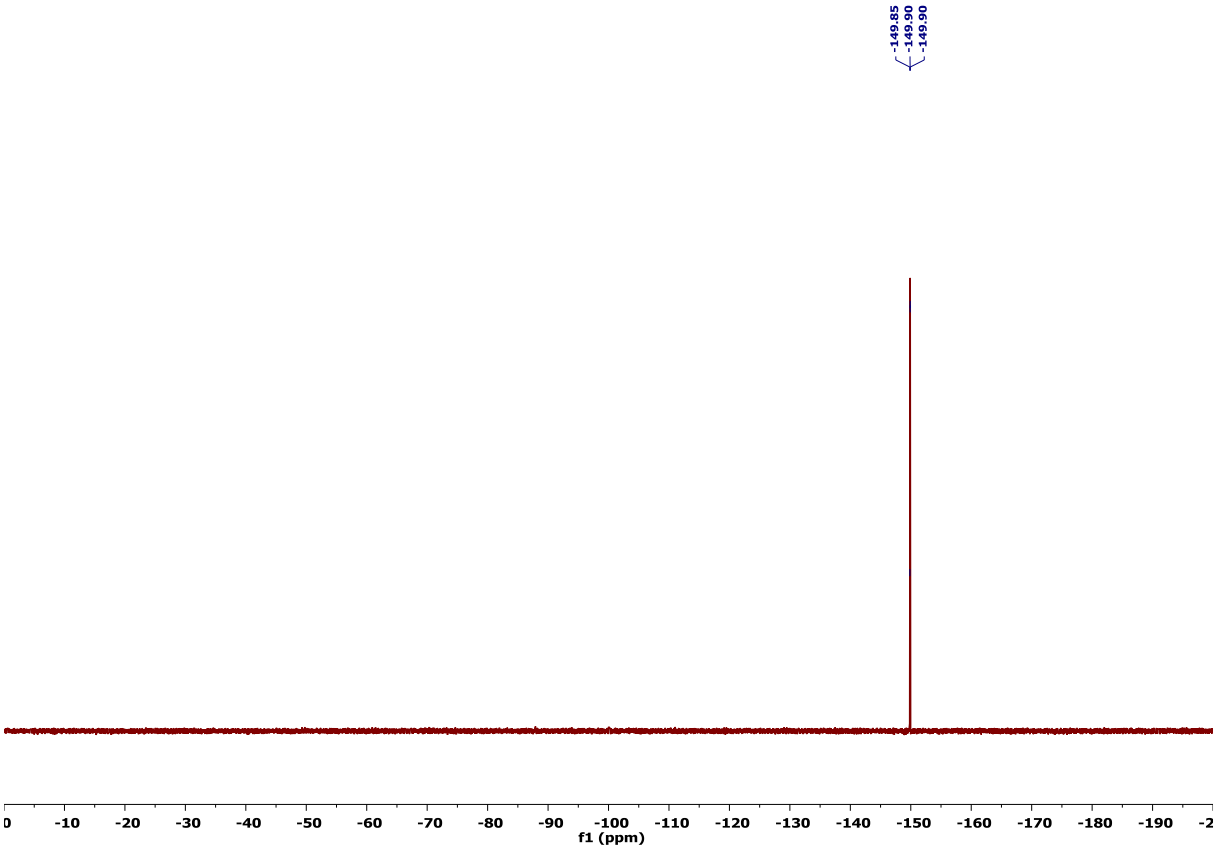
^{1}H NMR (400 MHz, CD_2Cl_2) 15



^{13}C NMR (101 MHz, CD_2Cl_2)



^{19}F NMR (282 MHz, CD_2Cl_2)



HRMS (ESI+)

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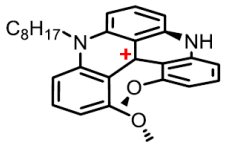
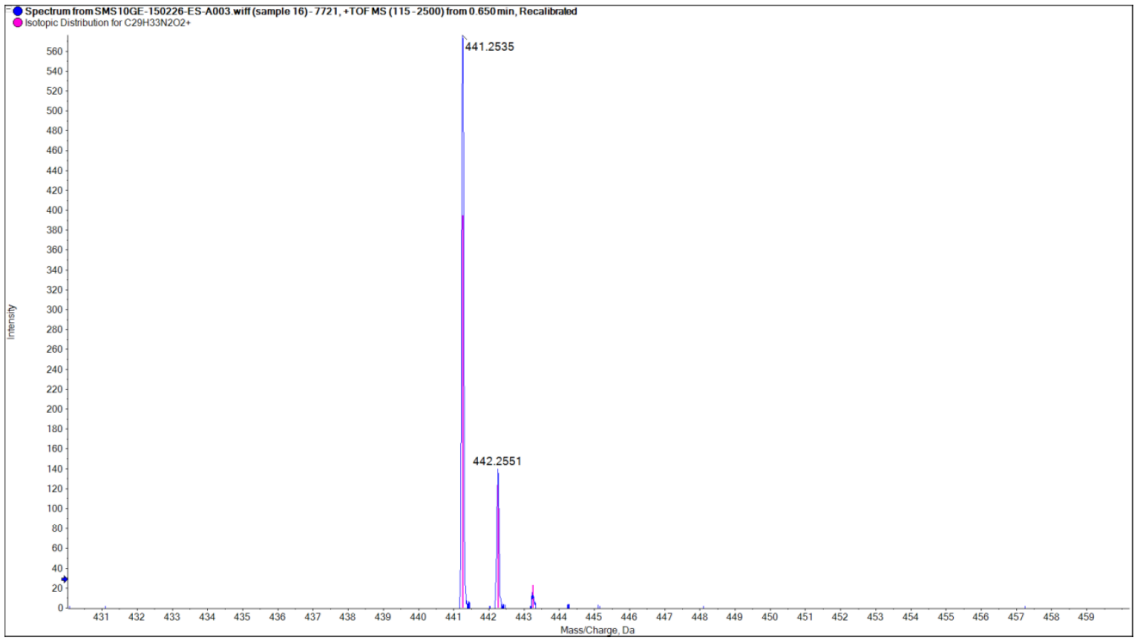
Submitter:	PAU	Date of reception:	26/02/15
Sample name:	PM17	Date of certificate:	02/03/15
Sample number:	7721	Data filename:	SMS10GE-150226-ES-A003
Operator:	Eliane Sandmeier	Instrument:	QSTAR Pulsar (AB/MDS Sciex)
Principal investigator:	Dr. Sophie Michalet	Ionisation mode:	ESI (positive mode)

Expected Formula	Observed *m/z* $[M]^+$	Expected *m/z* (amu)	Accuracy (ppm)
$C_{29}H_{33}N_2O_2$	441.2535	441.2537	-0.3

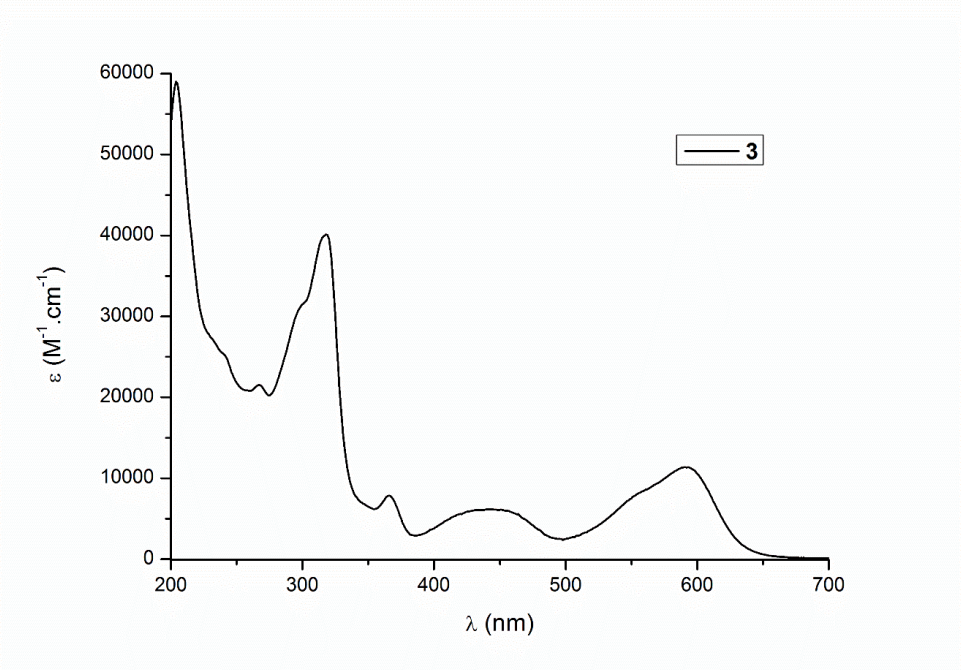


Chemical Formula: $C_{29}H_{33}N_2O_2^+$
Exact Mass: 441.25
Molecular Weight: 441.59

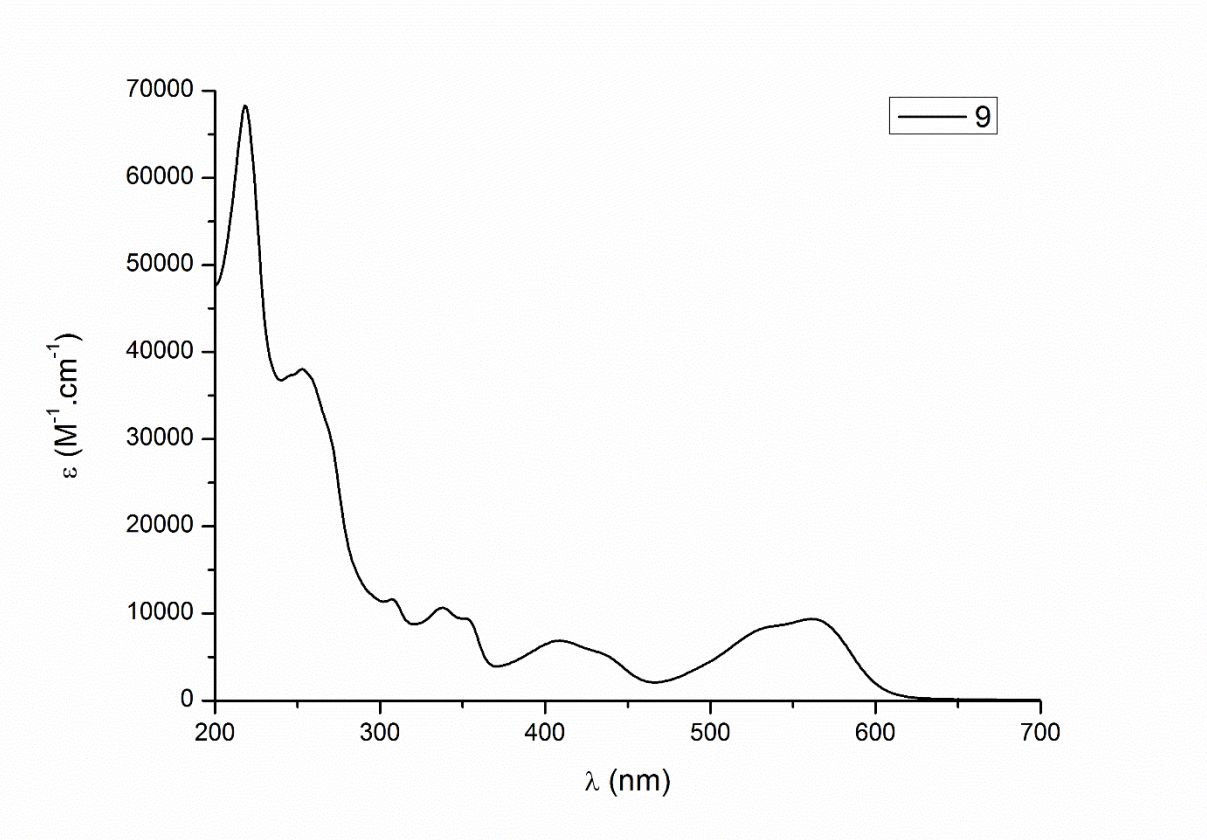


4. Optical properties

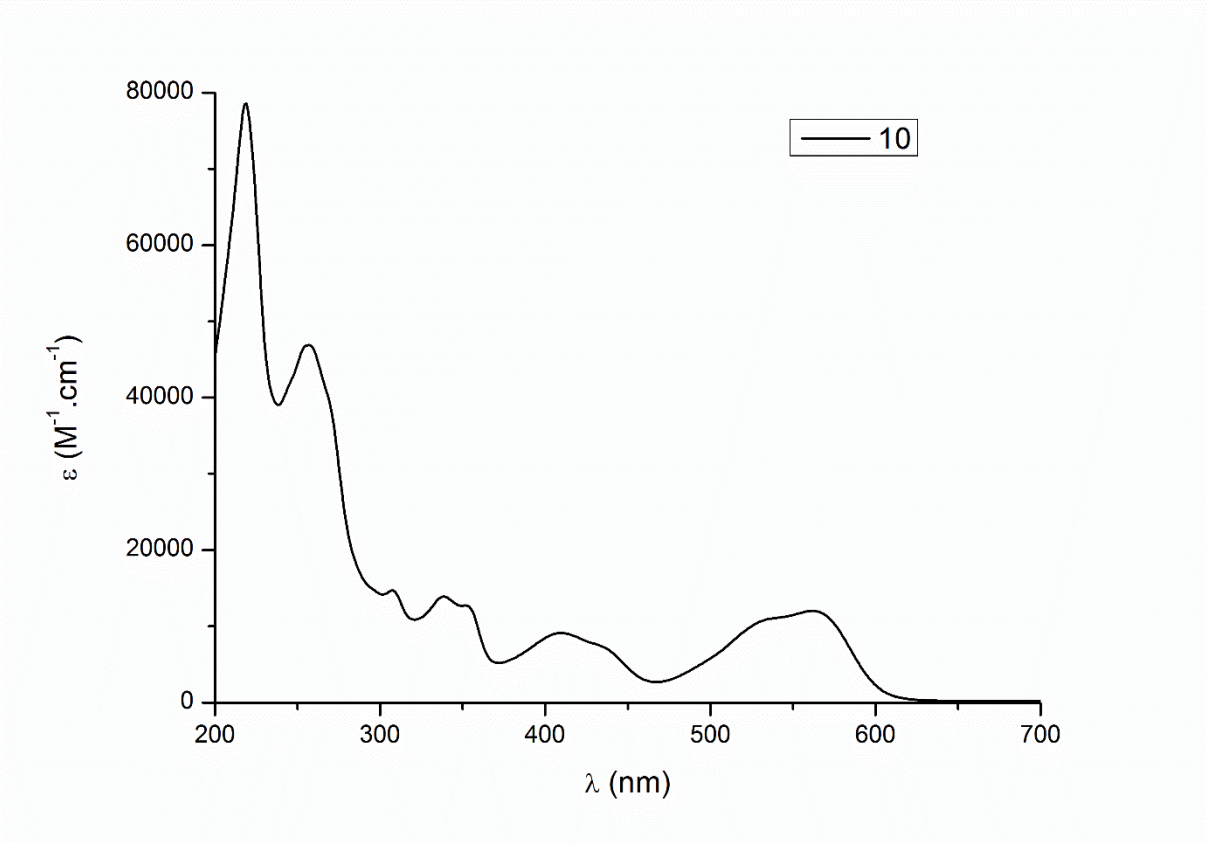
UV-vis (CH_3CN 10^{-5} M) (3)



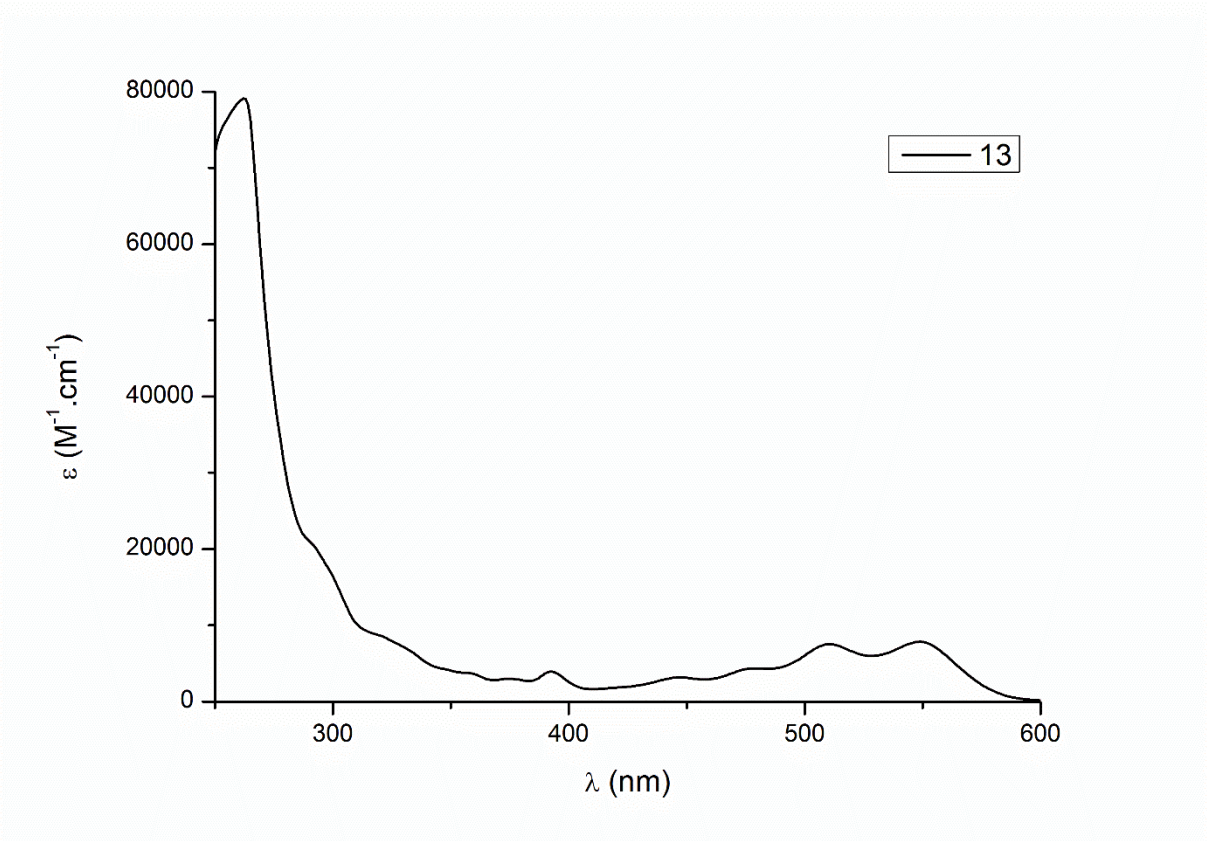
UV-vis (CH_3CN 10^{-5} M) (9)



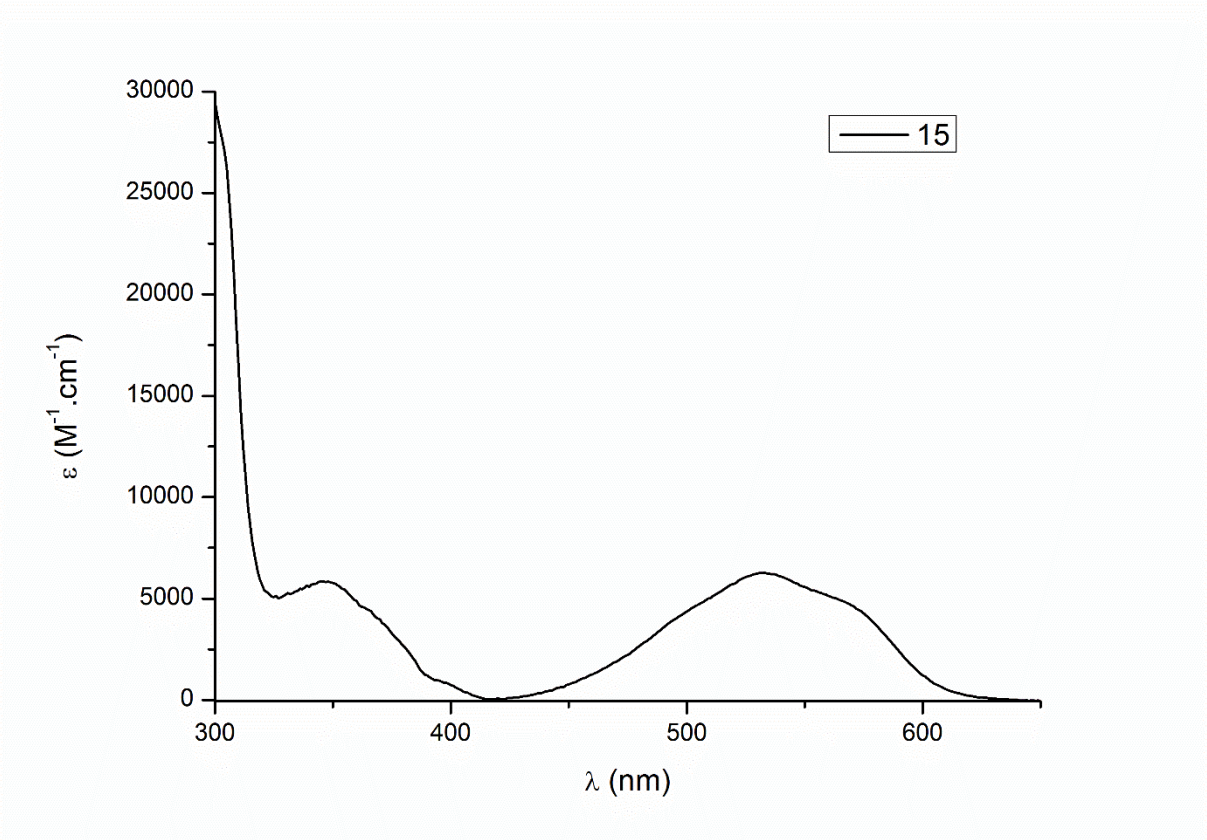
UV-vis (CH_3CN 10^{-5} M) (10)



UV-vis (CH_3CN 10^{-5} M) (13)



UV-vis (CH_3CN 10^{-5} M) (15)



5. References

1 (a) B. W. Laursen and F. C. Krebs, *Angewandte Chemie International Edition*, 2000, **39**, 3432-3434; (b) C. Herse, D. Bas, F. C. Krebs, T. Bürgi, J. Weber, T. Wesolowski, B. W. Laursen and J. Lacour, *Angewandte Chemie International Edition*, 2003, **42**, 3162-3166.

2 B. Laleu, P. Mobian, C. Herse, B. W. Laursen, G. Hopfgartner, G. Bernardinelli and J. Lacour, *Angewandte Chemie International Edition*, 2005, **44**, 1879-1883.

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5 F. Torricelli, J. Bosson, C. Besnard, M. Chekini, T. Bürgi and J. Lacour, *Angew. Chem. Int. Ed.*, 2013, **52**, 1796-1800.

6 A. Wallabregue, P. Sherin, J. Guin, C. Besnard, E. Vauthey and J. Lacour, *European Journal of Organic Chemistry*, 2014, **2014**, 6431-6438.

7 J. Bosson, G. M. Labrador, S. Pascal, F.-A. Miannay, O. Yushchenko, H. Li, L. Bouffier, N. Sojic, R. C. Tovar, G. Muller, D. Jacquemin, A. D. Laurent, B. Le Guennic, E. Vauthey and J. Lacour, *Chem. Eur. J.*, 2016, **22**, 18394-18403.