# Supporting Information

## Excited-state intramolecular proton-transfer solid-state fluorophores with aggregation-induced emission as efficient emitters for electroluminescent devices

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### 1. Single-crystal XRD data

CCDC 2144527 and 2130190 of **PPy-HPI** and **PPy-HPIC**, respectively, contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

**Table S1** Crystal data and structure refinement for **PPy-HPI** and **PPy-HPIC**.

| **Compound** | **PPy-HPI** | **PPy-HPIC** |
|---|---|---|
| CCDC deposition number | 2144527 | 2130190 |
| Empirical formula | $C_{41}H_{31}N_3O$ | $C_{41}H_{29}N_3O$ |
| Formula weight | 581.69 | 579.67 |
| Temperature/K | 100.0 | 100.0 |
| Crystal system | triclinic | monoclinic |
| Space group | P-1 | $P2_1/n$ |
| a/Å | 10.6202(17) | 12.6993(11) |
| b/Å | 11.1341(18) | 16.3312(14) |
| c/Å | 13.581(2) | 14.3395(11) |
| α/° | 106.157(5) | 90 |
| β/° | 97.582(5) | 100.320(3) |

| | | |
|---|---|---|
| γ/° | 98.728(6) | 90 |
| Volume/Å$^3$ | 1498.7(4) | 2925.8(4) |
| Z | 2 | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.289 | 1.316 |
| μ/mm$^{-1}$ | 0.078 | 0.079 |
| F(000) | 612.0 | 1216.0 |
| Crystal size/mm$^3$ | 0.339 × 0.245 × 0.216 | 0.362 × 0.251 × 0.183 |
| Radiation | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 3.886 to 54.204 | 3.948 to 52.744 |
| Index ranges | -13 ≤ h ≤ 13,<br>-14 ≤ k ≤ 14,<br>-17 ≤ l ≤ 17 | -15 ≤ h ≤ 15,<br>-20 ≤ k ≤ 20,<br>-17 ≤ l ≤ 17 |
| Reflections collected | 43101 | 49935 |
| Independent reflections | 6610 [$R_{int}$ = 0.0621,<br>$R_{sigma}$ = 0.0415] | 5972 [$R_{int}$ = 0.0484,<br>$R_{sigma}$ = 0.0288] |
| Data/restraints/parameters | 6610/0/439 | 5972/0/412 |
| Goodness-of-fit on F$^2$ | 1.039 | 1.043 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0462, w$R_2$ = 0.1020 | $R_1$ = 0.0400, w$R_2$ = 0.0945 |
| Final R indexes [all data] | $R_1$ = 0.0688, w$R_2$ = 0.1131 | $R_1$ = 0.0505, w$R_2$ = 0.1005 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.31/-0.33 | 0.34/-0.24 |

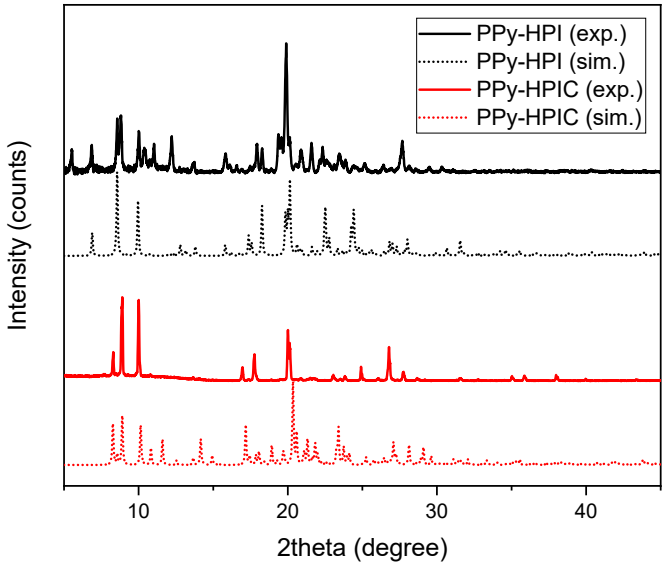



**Fig. S1** Experimental and simulated PXRD data of **PPy-HPI** and **PPy-HPIC**.

## 2. Optical data

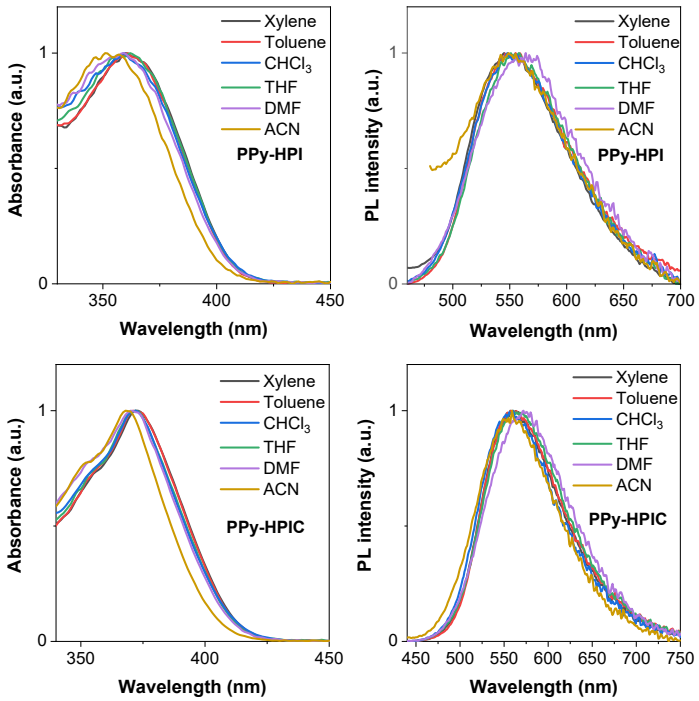



**Fig. S2** UV-vis absorption and PL spectra of **PPy-HPI** and **PPy-HPIC** in various solvents.

## 3. Thermal properties

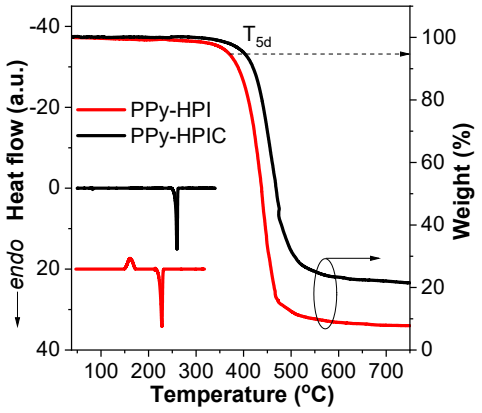



**Fig S3** DSC/TGA thermograms recorded at a heating rate of 10 °C $min^{-1}$ under $N_2$ flow.

## 4. Electrochemical properties

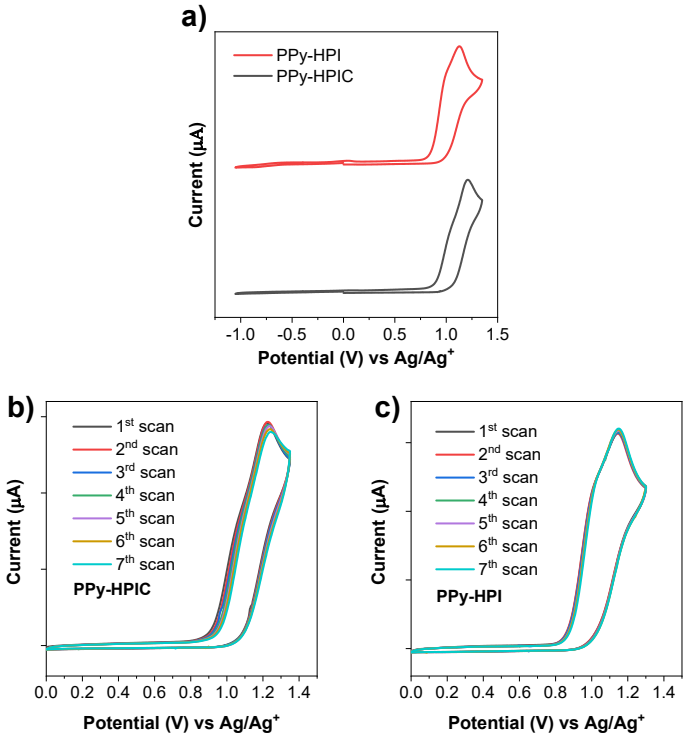



**Fig. S4** (a) CV plots of **PPy-HPIC** and **PPy-HPI** and (b-c) their related multiple scan traces measured in $CH_2Cl_2$ containing *n*-$Bu_4NPF_6$ as a supporting electrolyte at a scan rate of 50 mV $s^{-1}$ under Ar atmosphere.

## 5. Charge transport properties

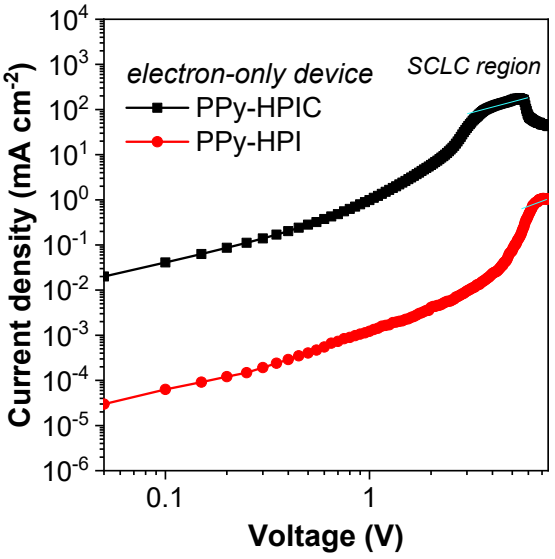



**Fig. S5** Current density-voltage (*J–V*) plots of the electron-only devices of **PPy-HPI** and **PPy-HPIC**.

## 6. Non-doped OLEDs

**Table S2.** Comparison of ESIPT based non-doped fluorescent OLED.

| EML | $V_{on}$ (V) | $\lambda_{EL}$ (nm) | $EQE_{max}$ (%) | $CE_{max}$ (cd $A^{-1}$) | CIE (x, y) | ref |
|---|---|---|---|---|---|---|
| **HOXD** | 7.0 | 451 | - | 0.44 | - | 1 |
| **W1** | 6.7 | - | 0.76 | 0.98 | 0.34, 0.29 | 2 |
| **HBI-Cbz** | 4.8 | 456 | 2.94 | 1.96 | 0.15, 0.11 | 3 |
| **HBT-Py** | - | 582 | 3.00 | 5.32 | - | 4 |
| **HPITPE** | 3.0 | 502 | 3.26 | 3.67 | 0.23, 0.39 | 5 |
| **PTHPI** | 3.3 | 496 | 3.27 | 8.08 | 0.24, 0.38 | 6 |
| ***PPy-HPI** | 3.0 | 553 | 3.61 | 10.56 | 0.41, 0.54 | This work |


1 F. Liang, L. Wang, D. Ma, X. Jing and F. Wang, *Appl Phys Lett*, 2002, **81**, 4–6.

2 S. Park, J. E. Kwon, S. H. Kim, J. Seo, K. Chung, S.-Y. Park, D.-J. Jang, B. M. Medina, J. Gierschner and S. Y. Park, *J Am Chem Soc*, 2009, **131**, 14043–14049.

3 S. Park, J. Seo, S. H. Kim and S. Y. Park, *Adv Funct Mater*, 2008, **18**, 726–731.

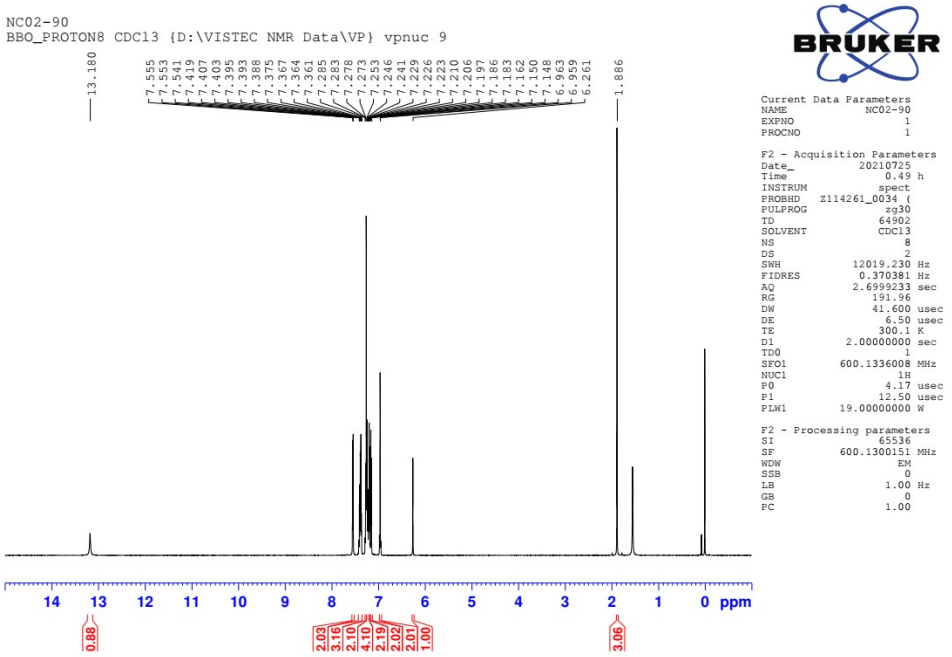
4 Y. Niu, R. Wang, L. Pu and Y. Zhang, *Dyes and Pigments*, 2019, **170**, 107594.

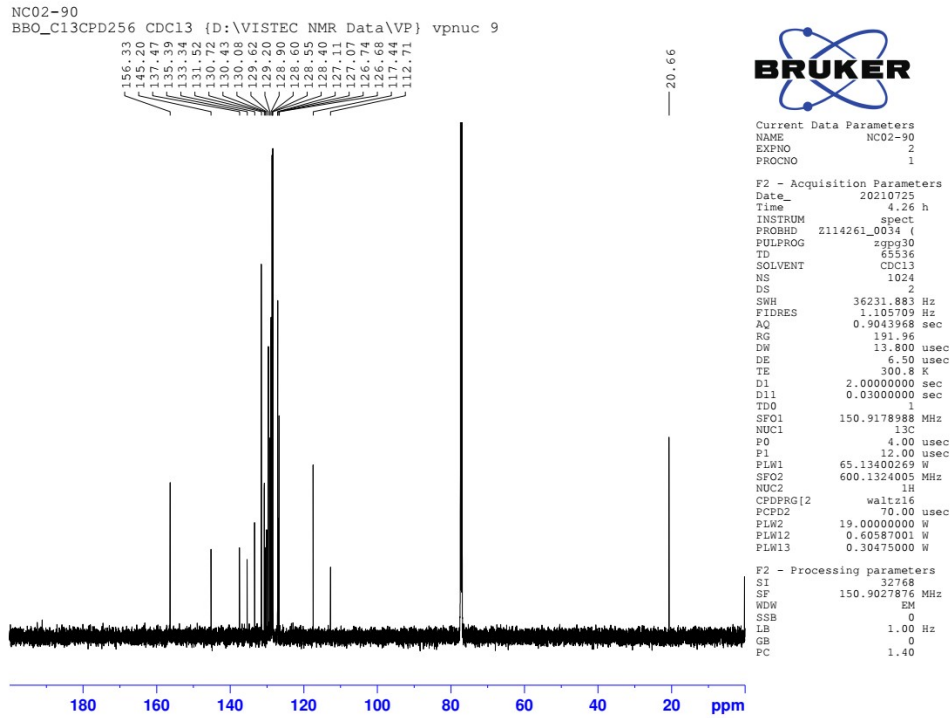
5 S. Petdee, C. Chaiwai, W. Benchaphanthawee, P. Nalaoh, N. Kungwan, S. Namuangruk□, T. Sudyoadsuk and V. Promarak, *Dyes and Pigments*, 2021, **193**, 109488.

6 J. Kumsampao, C. Chaiwai, C. Sukpattanacharoen, P. Nalaoh, T. Chawanpunyawat, P. Chasing, S. Namuangruk, N. Kungwan, T. Sudyoadsuk and V. Promarak, *Adv Photonics Res*, 2022, **3**, 2100141.

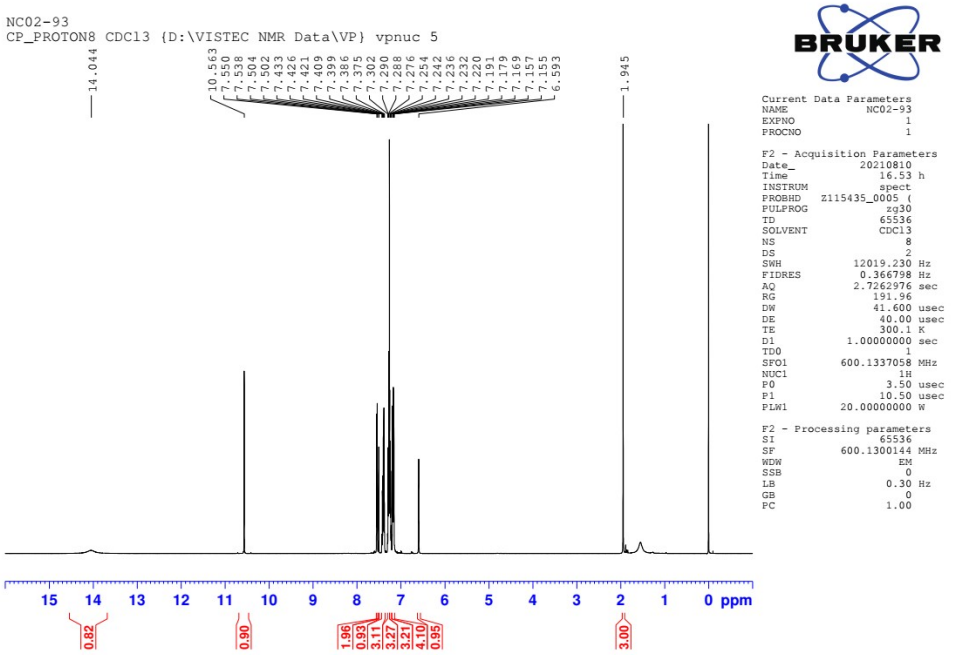
**Fig. S4** Copies of H-NMR, C-NMR and HRMS spectra

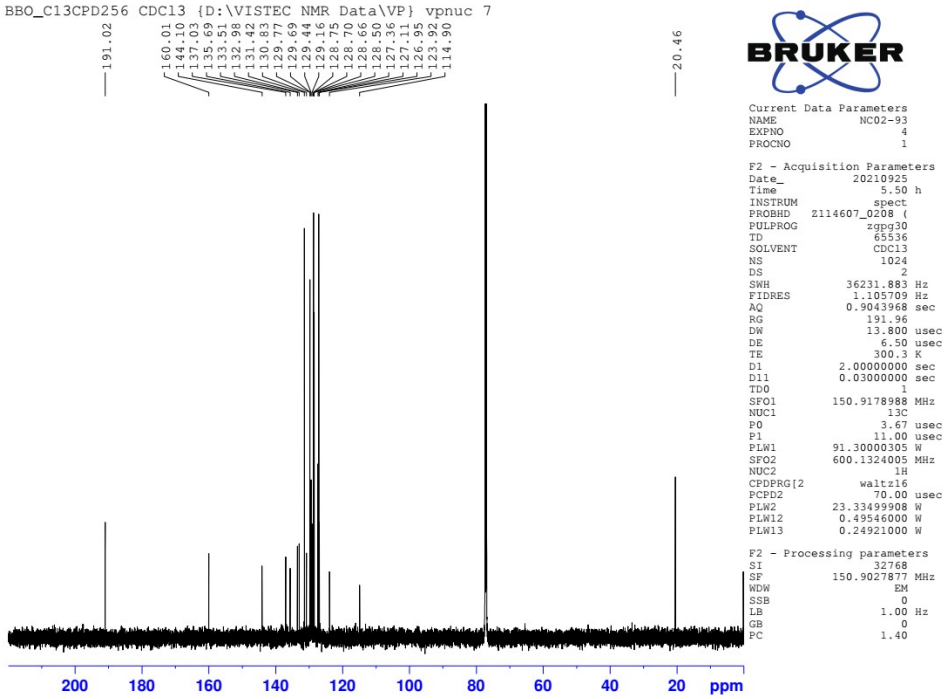
**1H and 13C NMR of compound 2**



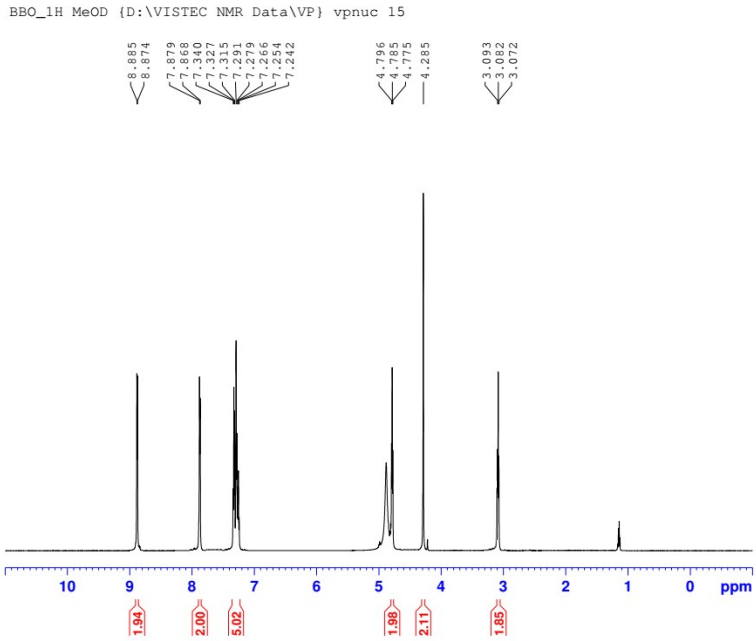



## 1H and 13C NMR of compound 4



## 1H and 13C NMR of compound 7

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PROCNO                      1

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FIDRES                0.366798 Hz
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RG                       31.68
DW                     41.600 usec
DE                     21.24 usec
TE                     294.5 K
D1                1.00000000 sec
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P1                     12.50 usec
PLW1              20.00000000 W

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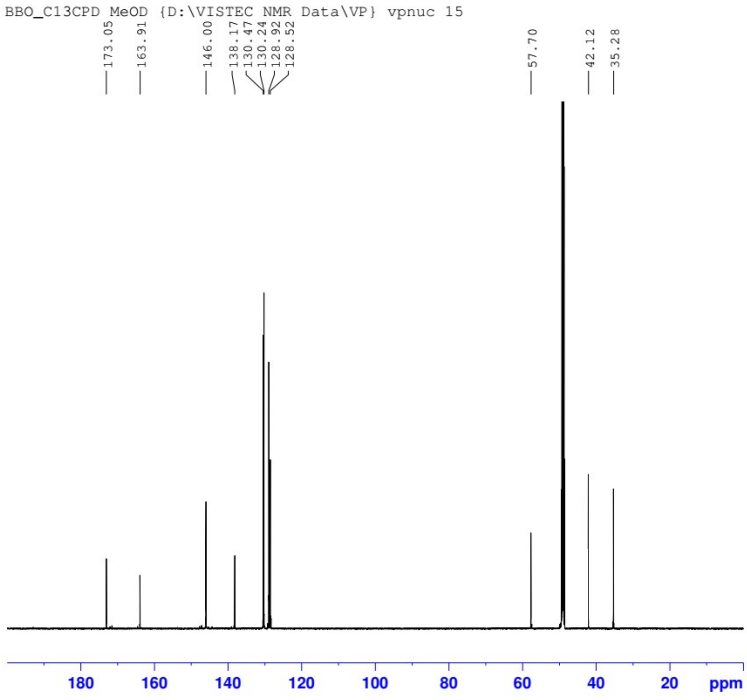


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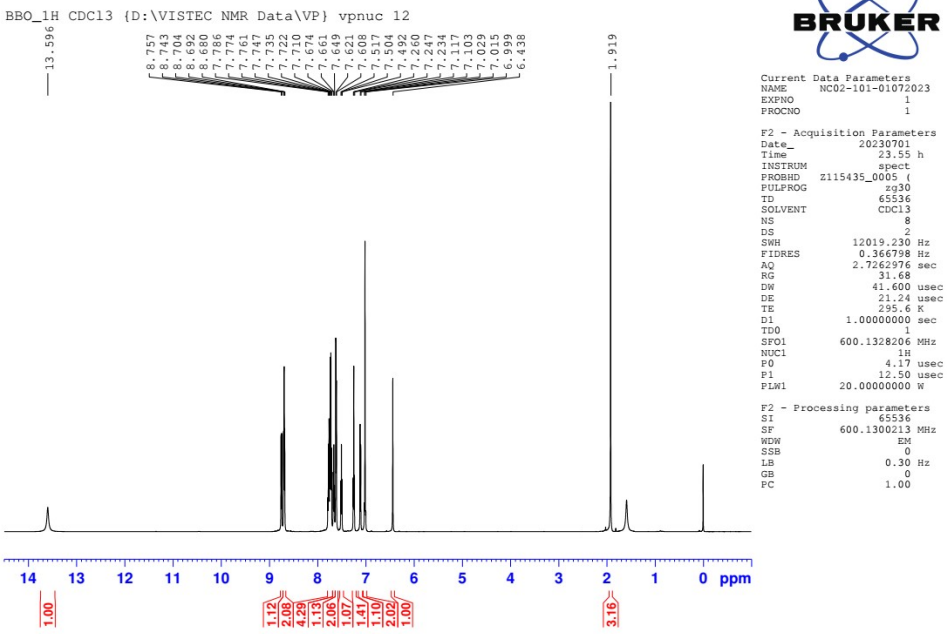
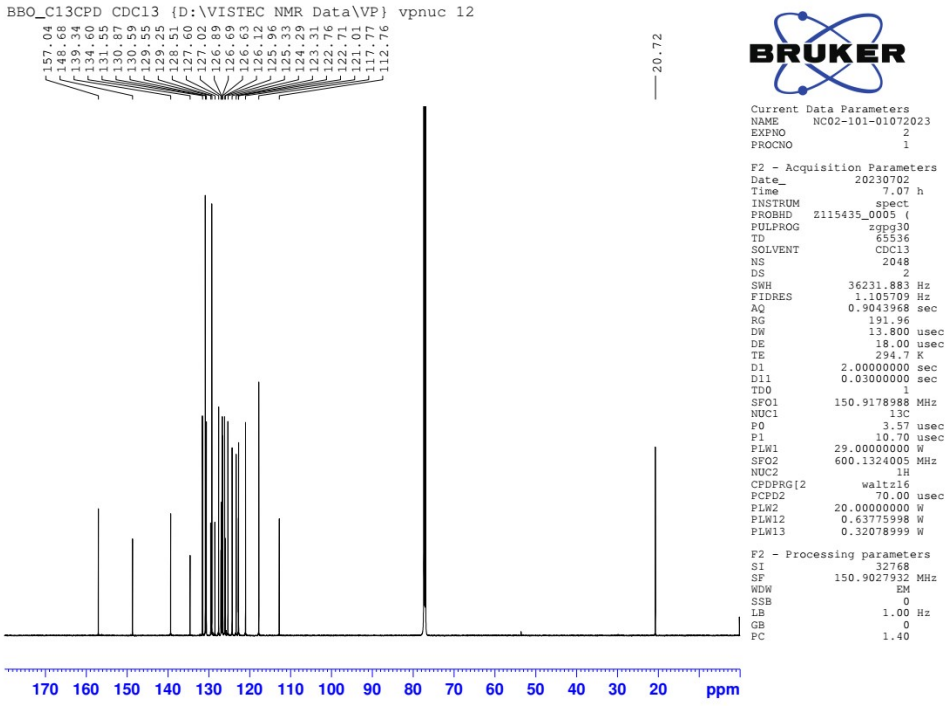
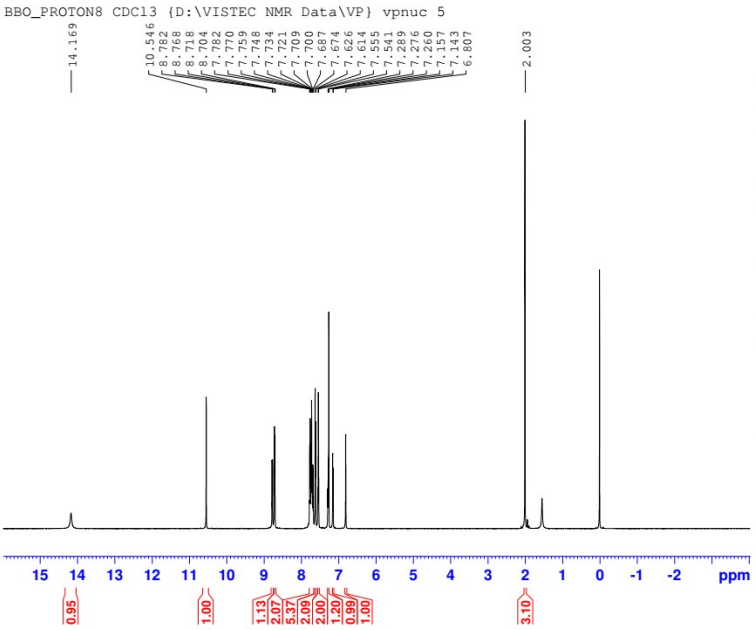
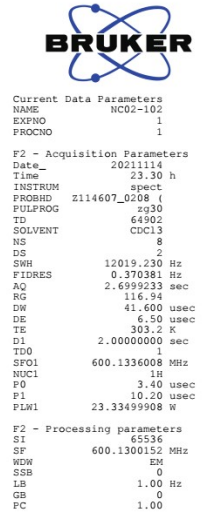
## 1H and 13C NMR of compound 3

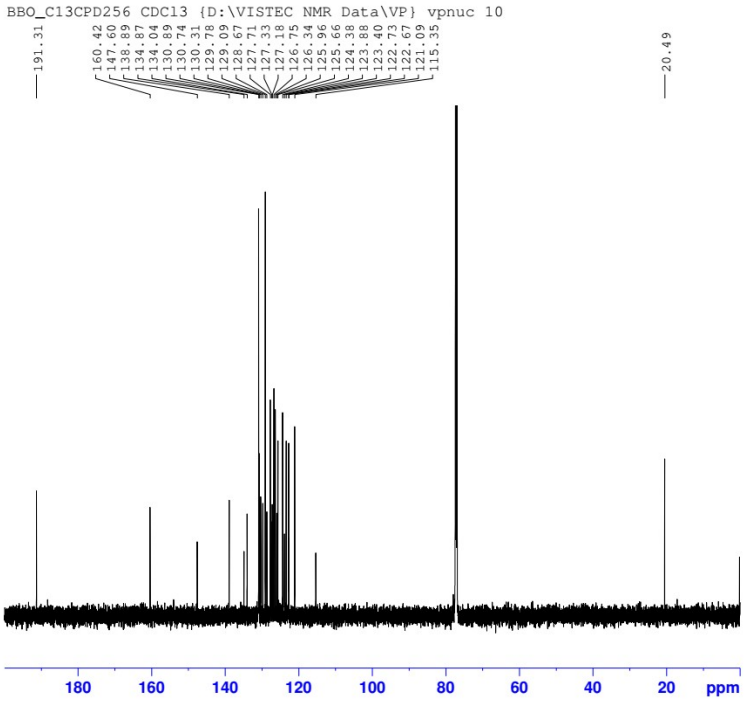


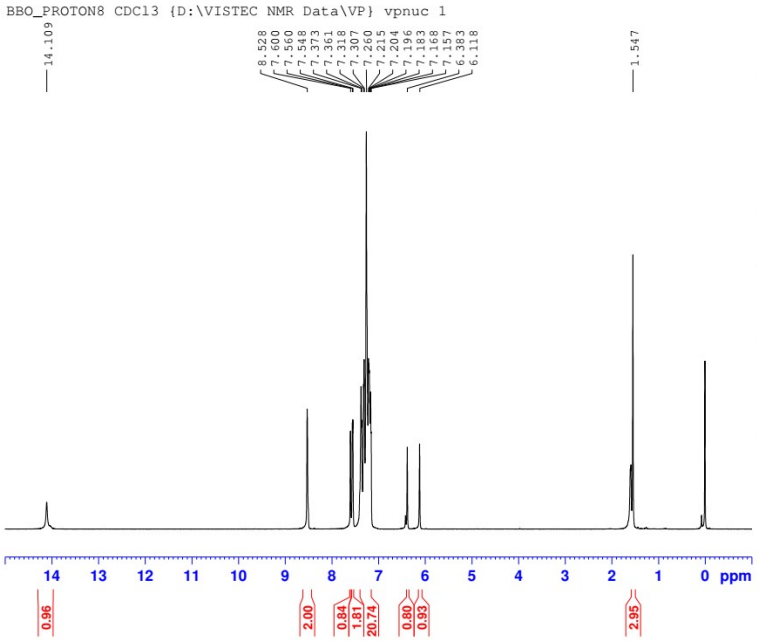
## 1H and 13C NMR of compound 5




## 1H and 13C NMR of compound PPy-HPI

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FIDRES         0.370381 Hz
AQ             2.6999233 sec
RG                 107.65
DW                41.600 usec
DE                 6.50 usec
TE                303.2 K
D1            2.00000000 sec
TD0                    1
SFO1         600.1336008 MHz
NUC1                  1H
P0                 3.40 usec
P1                10.20 usec
PLW1         23.33499908 W

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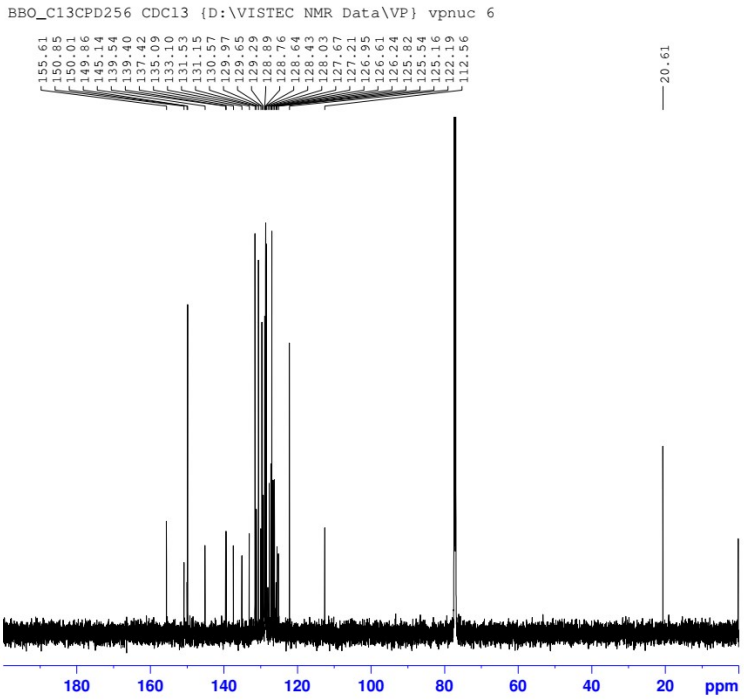


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FIDRES         1.105709 Hz
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RG                 191.96
DW                13.800 usec
DE                 6.50 usec
TE                303.1 K
D1            2.00000000 sec
D11           0.03000000 sec
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NUC1                  13C
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SFO2         600.1324005 MHz
NUC2                  1H
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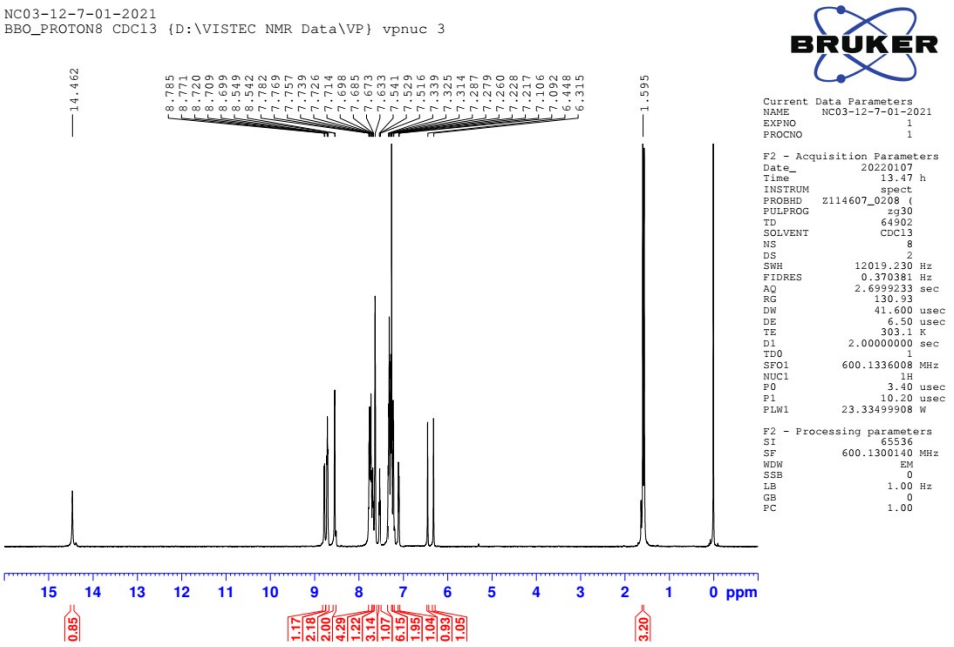
## 1H and 13C NMR of compound PPy-HPIC



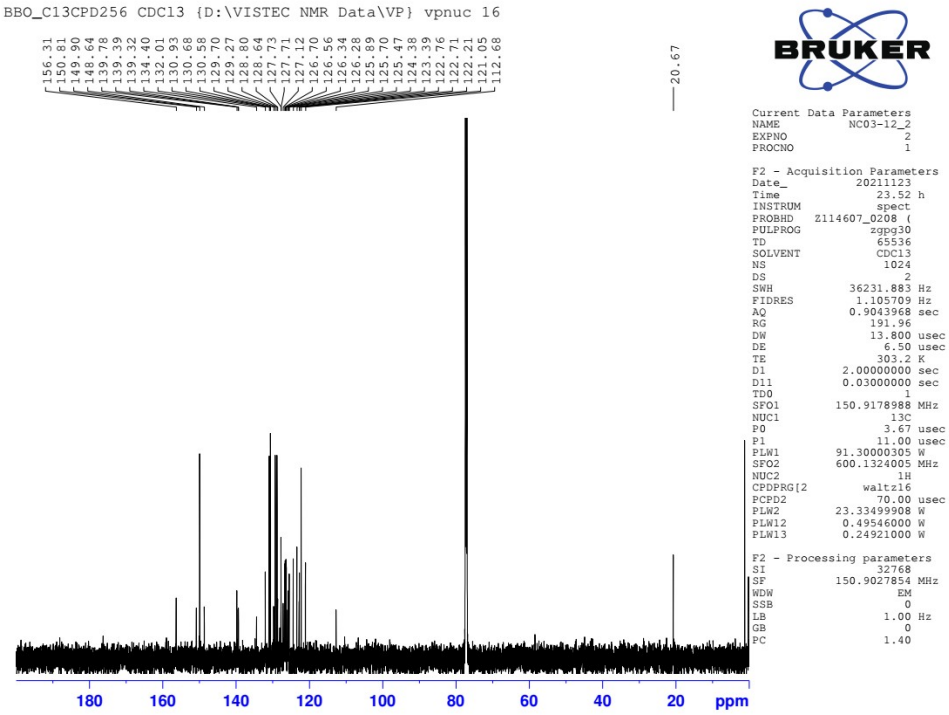
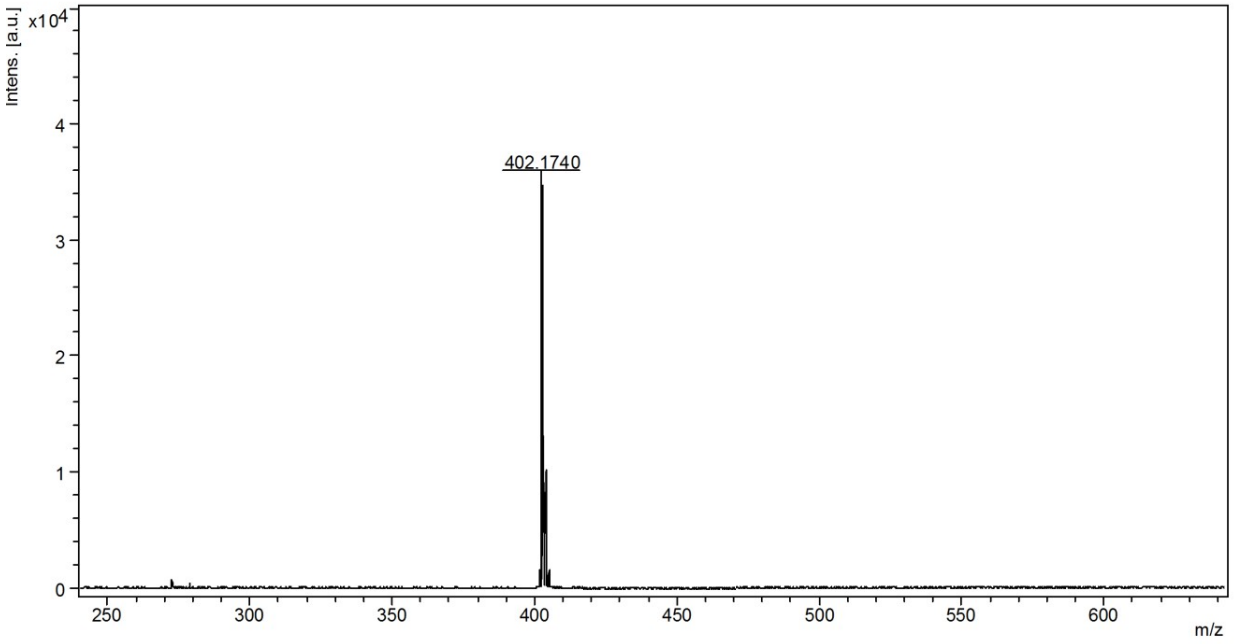
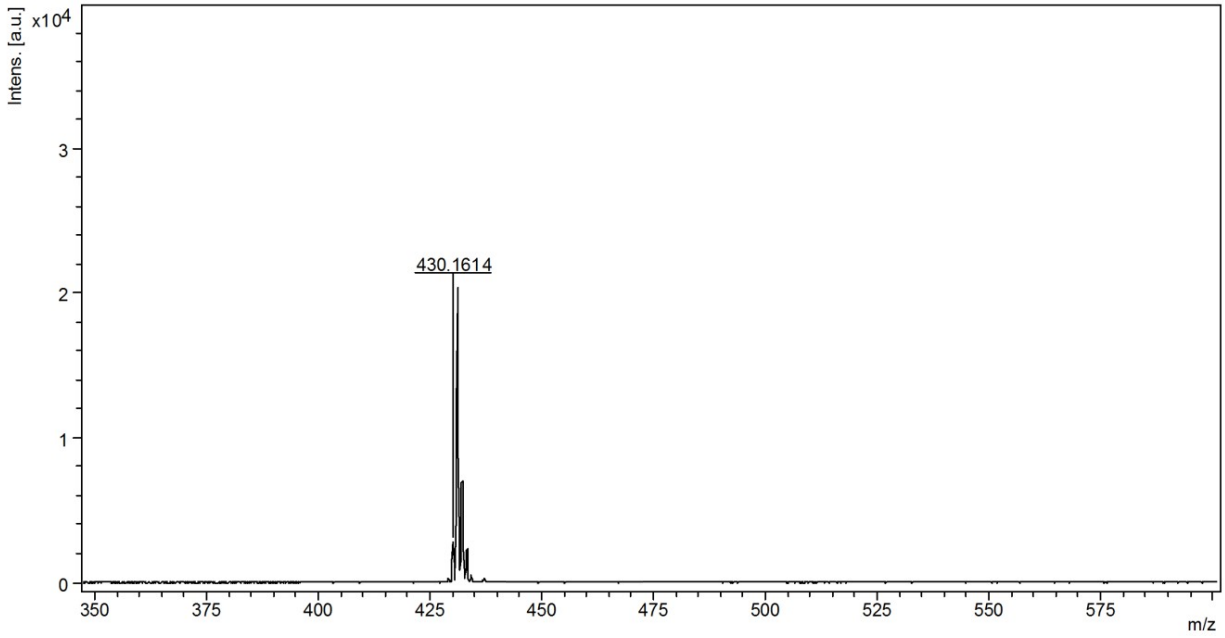



**Fig. S5** Copies of mass spectra

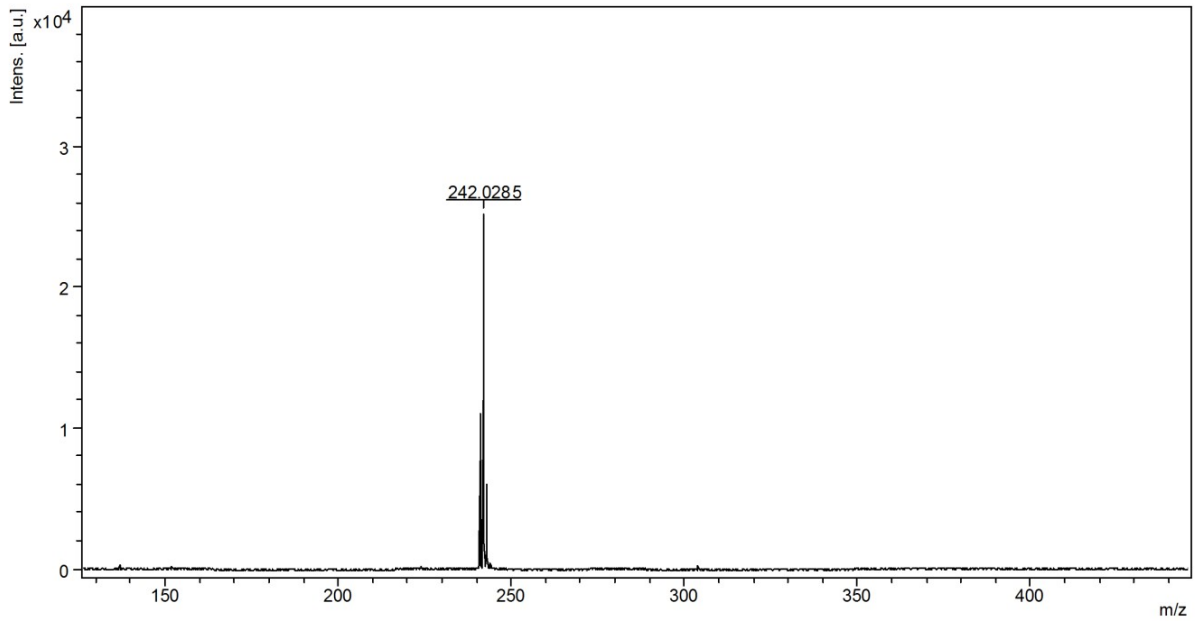
**MALDI-TOF of compound 2**



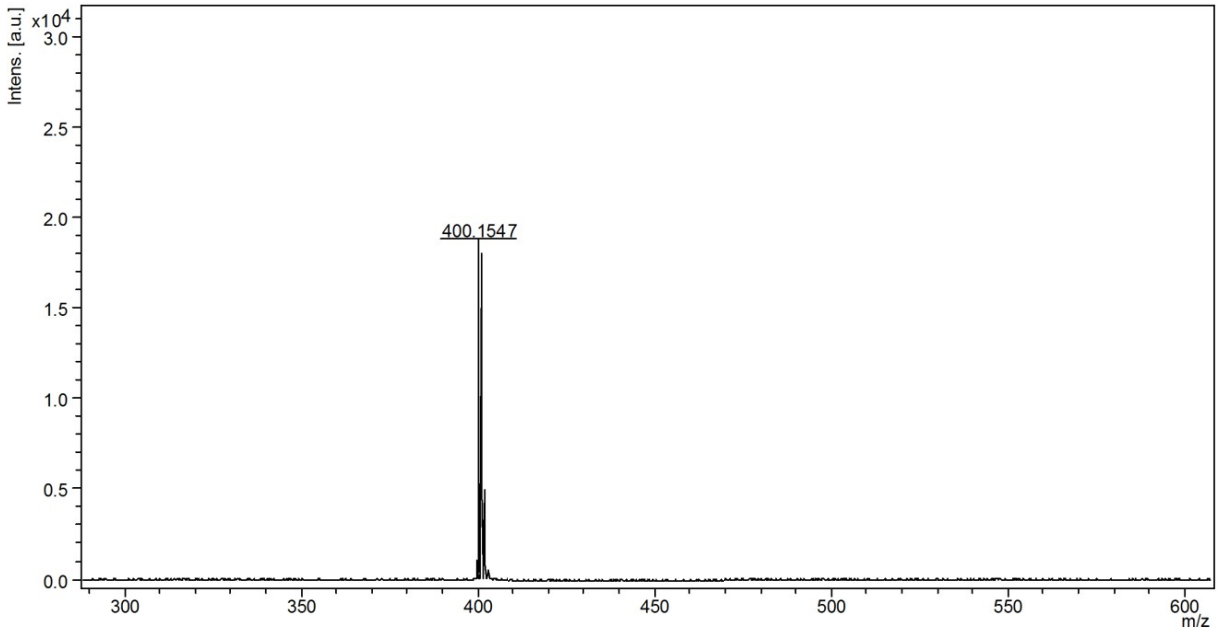

**MALDI-TOF of compound 4**



**MALDI-TOF of compound 7**




**MALDI-TOF of compound 3**



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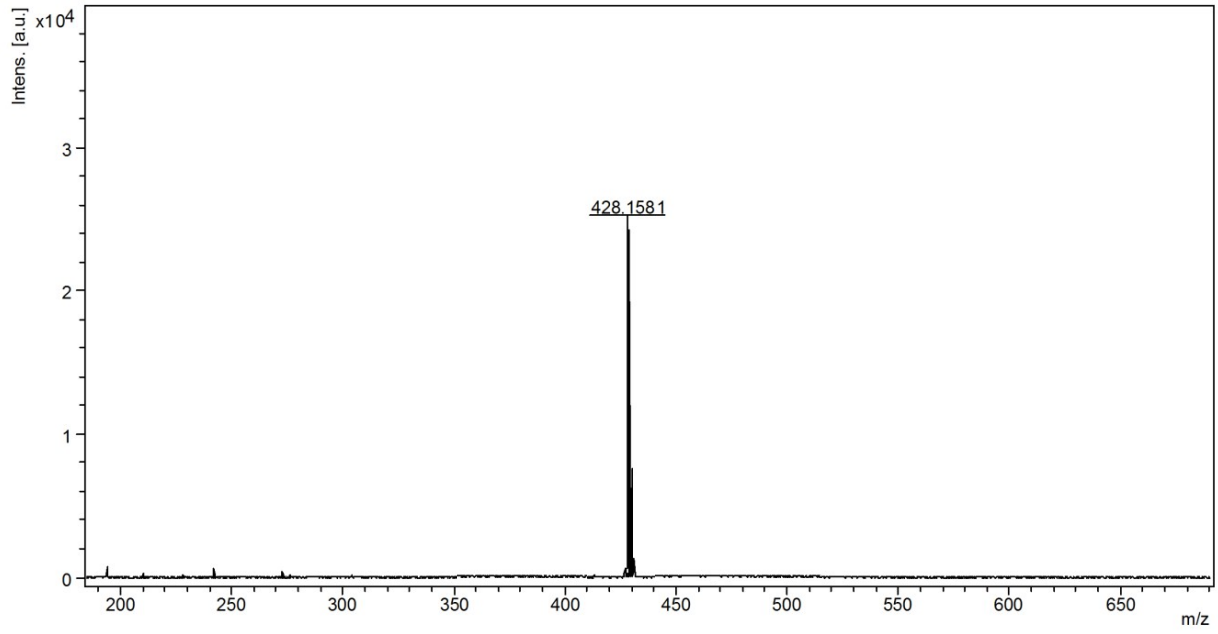
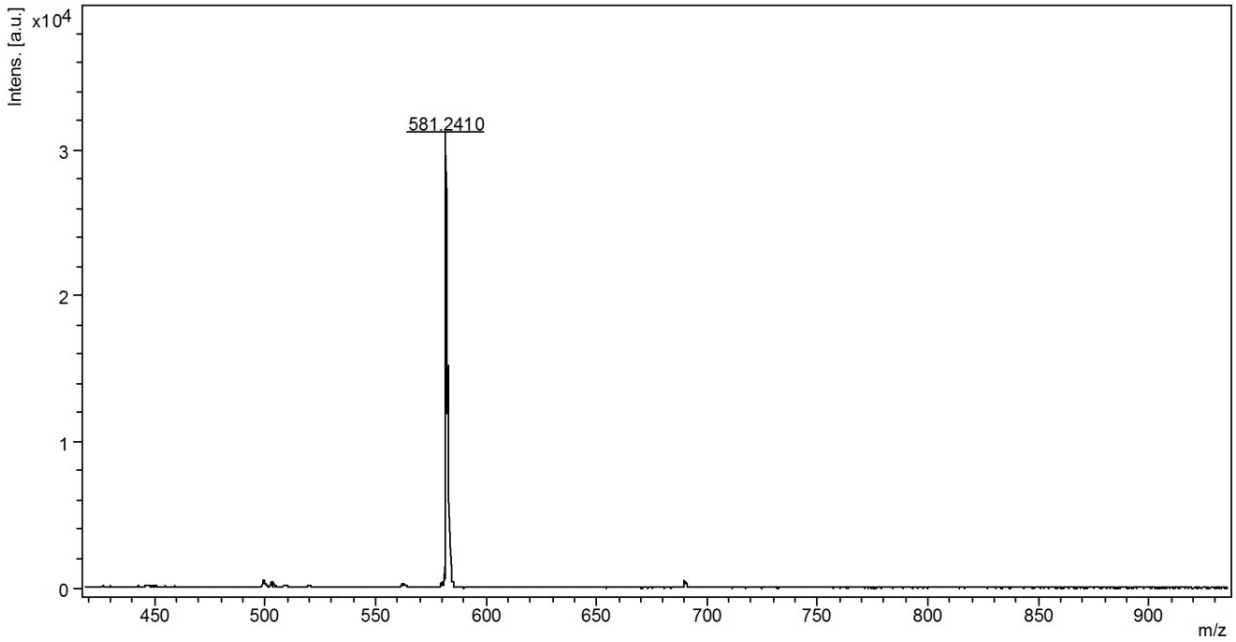



**MALDI-TOF of compound PPy-HPI**



**MALDI-TOF of compound PPy-HPIC**