Synthesis of new water-soluble derivatives of imidazole-4,5-dicarboxylic acid, their self-assembly and application in catalysis

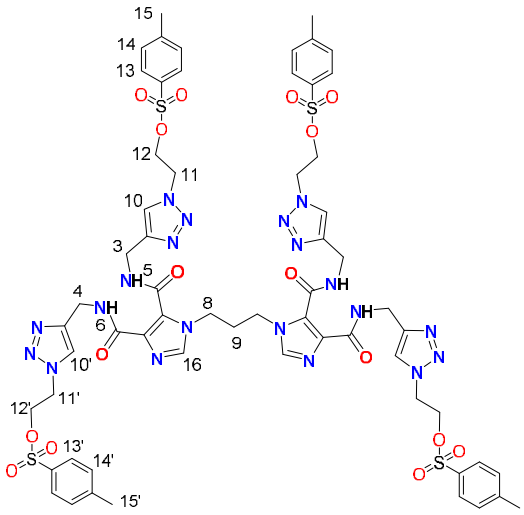
E.D. Sultanova [a], ***V.A. Burilov*** [a], ***E.A. Pushkareva*** [a], ***A.A. Fedoseeva*** [a], ***A.M. Gazalieva*** [a], ***D.D. Radaev*** [a], ***S.E. Solovieva*** [b], ***I.S. Antipin*** [a]

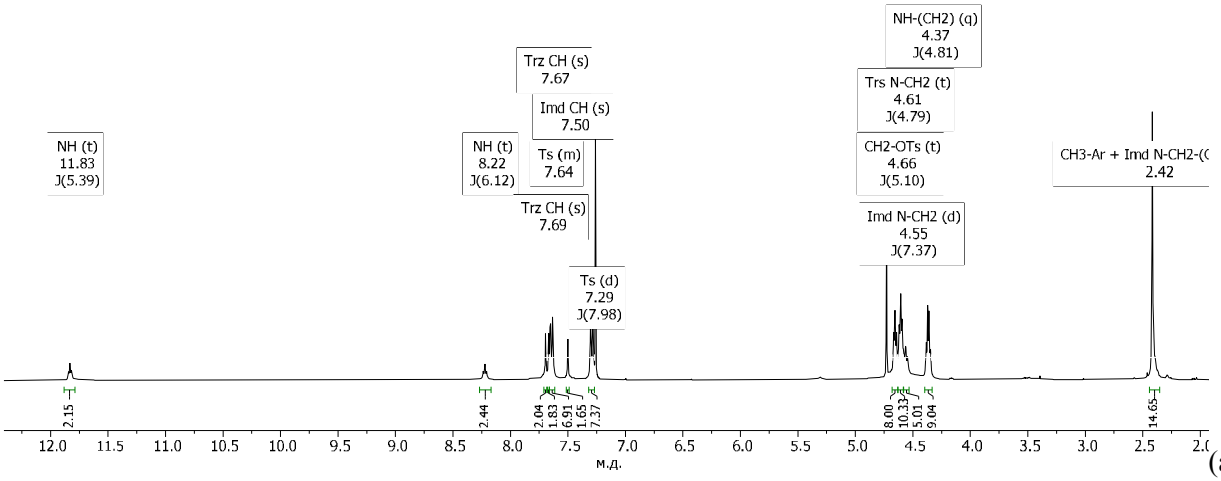
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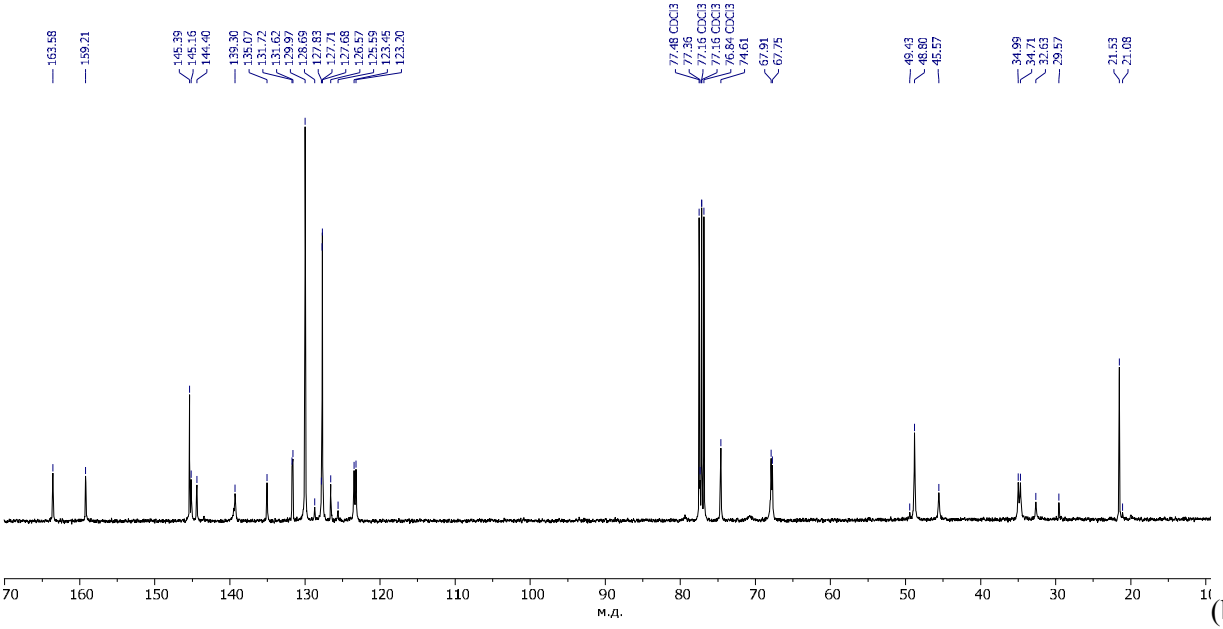
[b] *Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russian Academy of Sciences, 8 Arbuzov str., Kazan, 420088, Russian Federation.*

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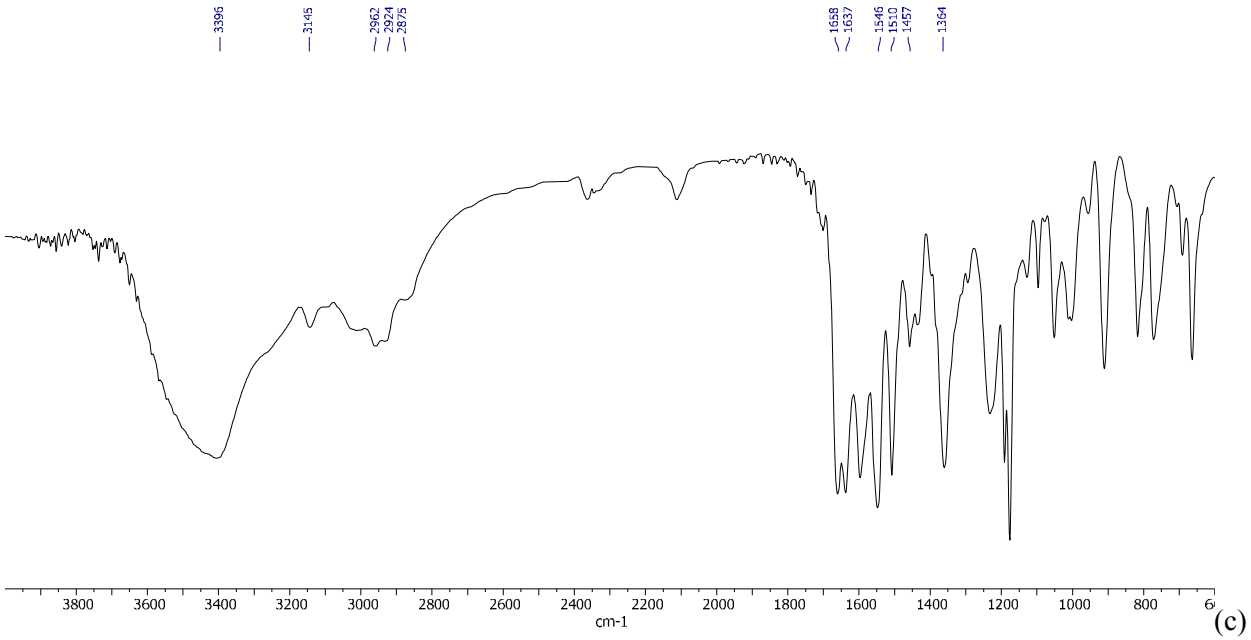

15
14
13
12
11
10
3
4
5
6
8
9
16
10'
11'
12'
13'
14'
15'


NH (t)
11.83
J(5.39)
NH (t)
8.22
J(6.12)
Trz CH (s)
7.67
Imd CH (s)
7.50
Ts (m)
7.64
Trz CH (s)
7.69
Ts (d)
7.29
J(7.98)
NH-(CH2) (q)
4.37
J(4.81)
Trs N-CH2 (t)
4.61
J(4.79)
CH2-OTs (t)
4.66
J(5.10)
Imd N-CH2 (d)
4.55
J(7.37)
CH3-Ar + Imd N-CH2-(
2.42
м.д.

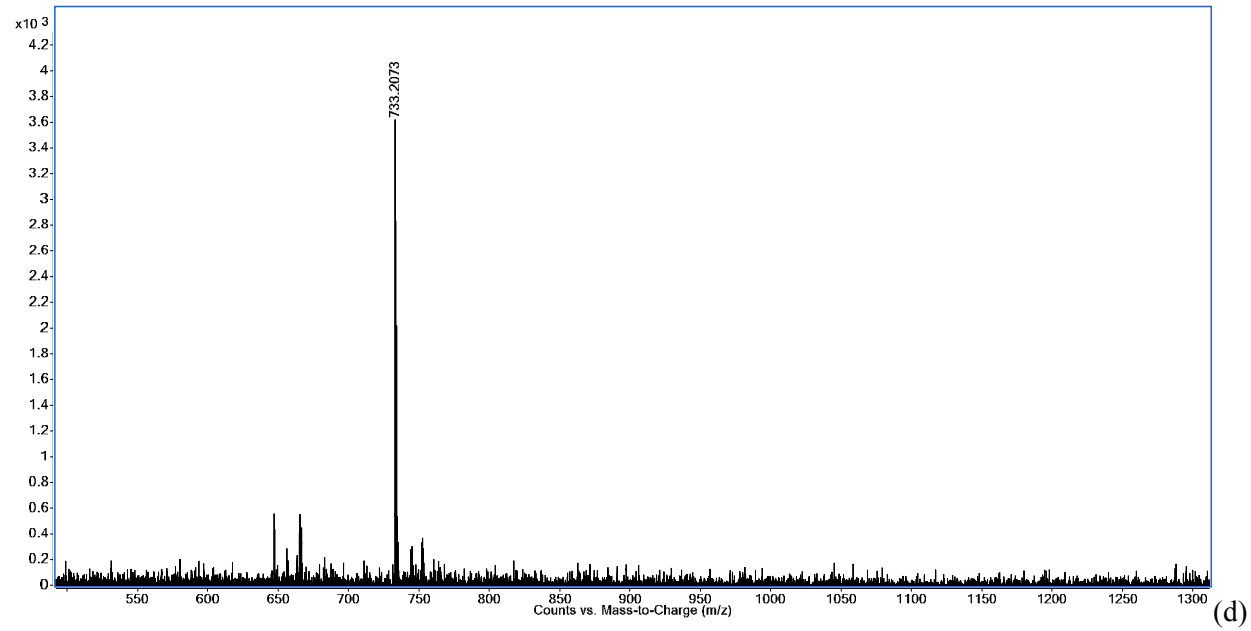
(a)


м.д.

(b)

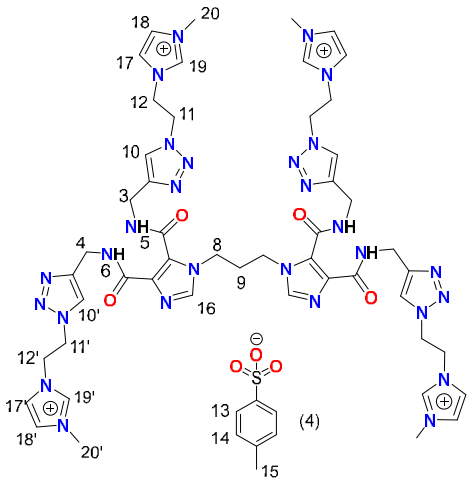


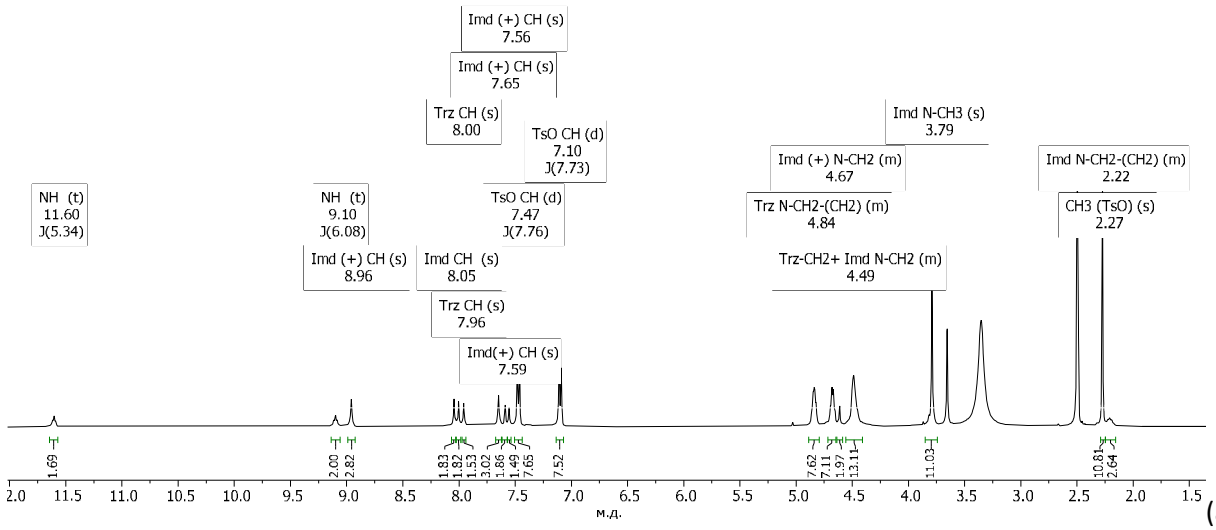
(c)



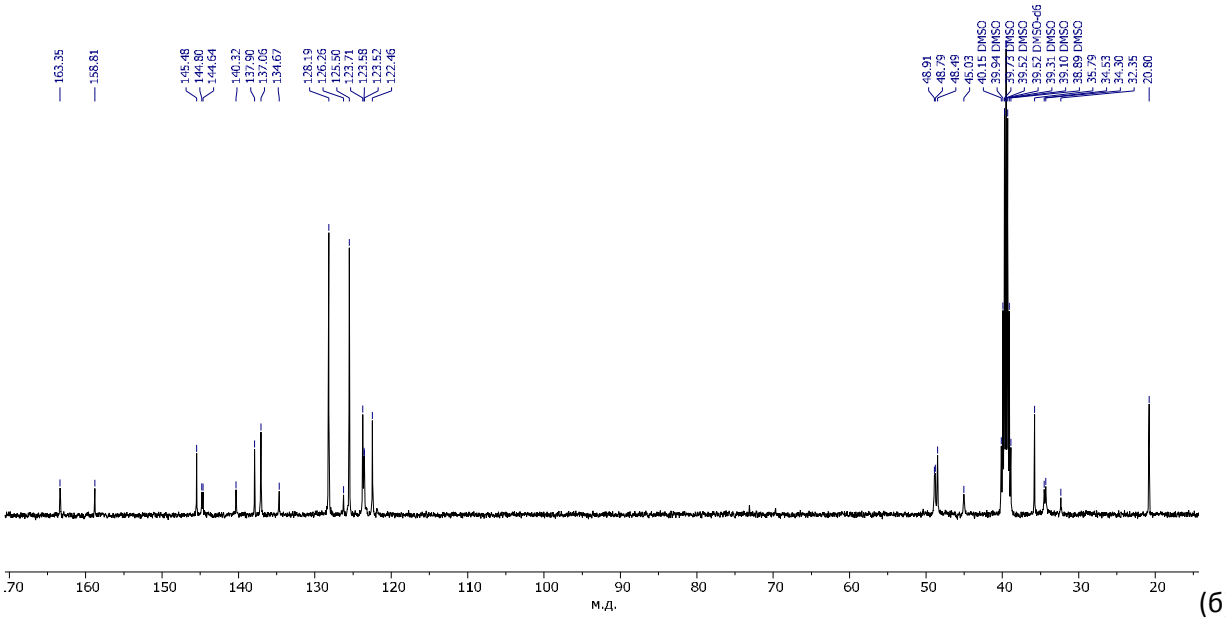
(d)

Fig. S1 ^{1}H NMR (400 MHz) (a), ^{13}C NMR (101 MHz) (b), FT-IR (c) and HRESI MS (d) spectra of 2

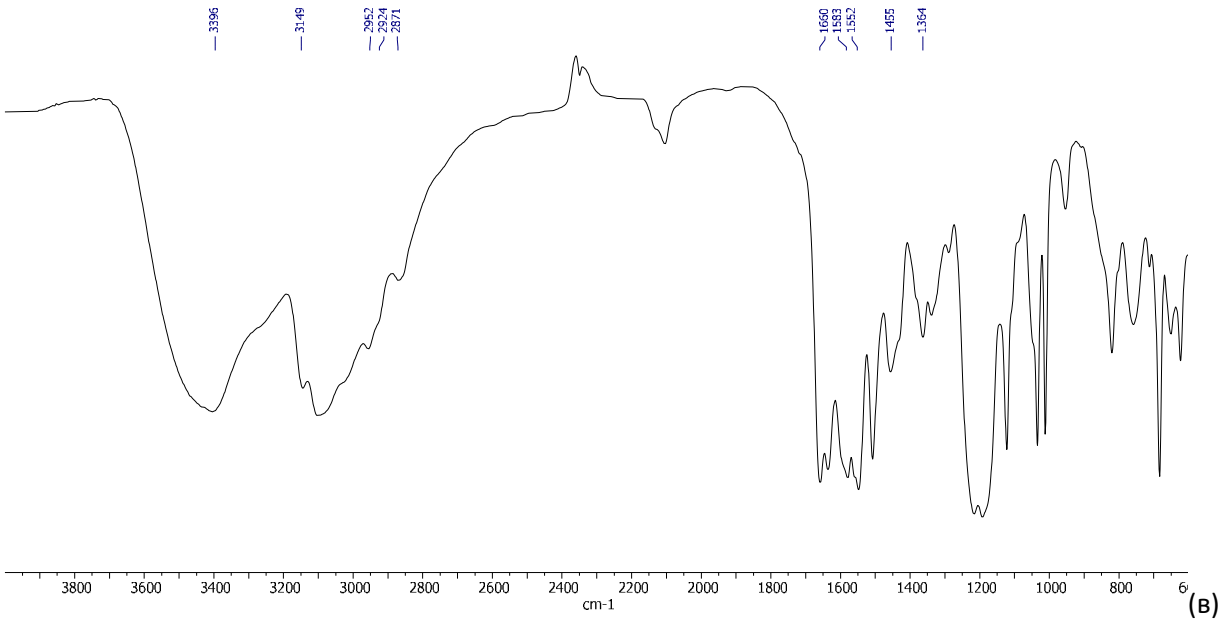

(4)


Imd (+) CH (s)
7.56
Imd (+) CH (s)
7.65
Trz CH (s)
8.00
TsO CH (d)
7.10
J(7.73)
Imd N-CH3 (s)
3.79
Imd (+) N-CH2 (m)
4.67
Imd N-CH2-(CH2) (m)
2.22
NH (t)
11.60
J(5.34)
NH (t)
9.10
J(6.08)
TsO CH (d)
7.47
J(7.76)
Trz N-CH2-(CH2) (m)
4.84
CH3 (TsO) (s)
2.27
Imd (+) CH (s)
8.96
Imd CH (s)
8.05
Trz-CH2+ Imd N-CH2 (m)
4.49
Trz CH (s)
7.96
Imd(+) CH (s)
7.59
м.д.

(а)


м.д.

(б)



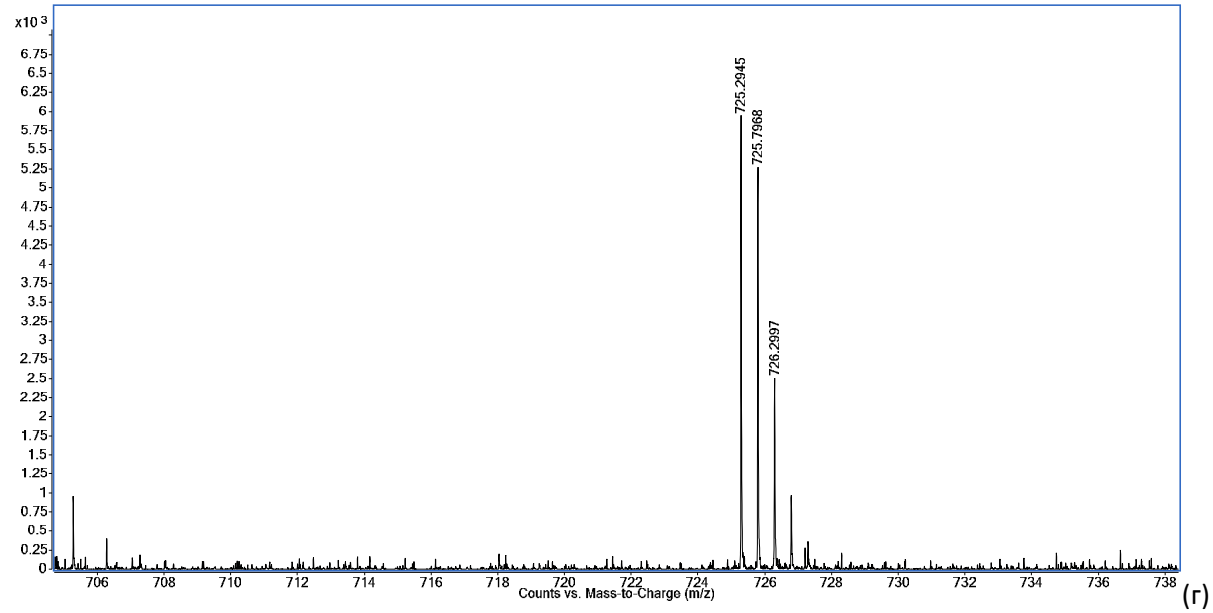
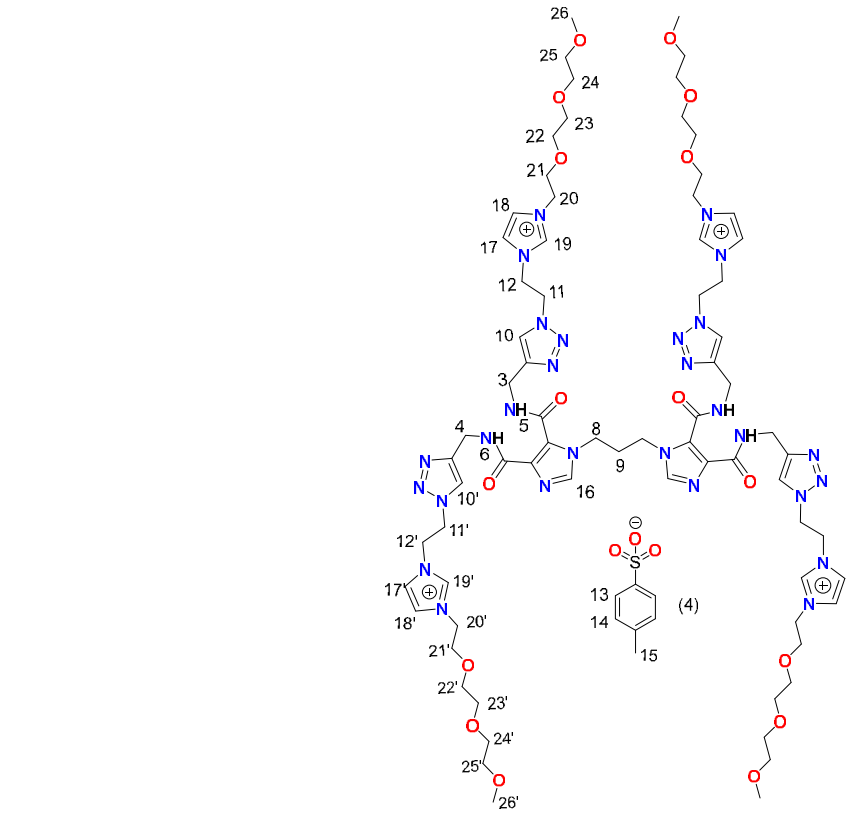
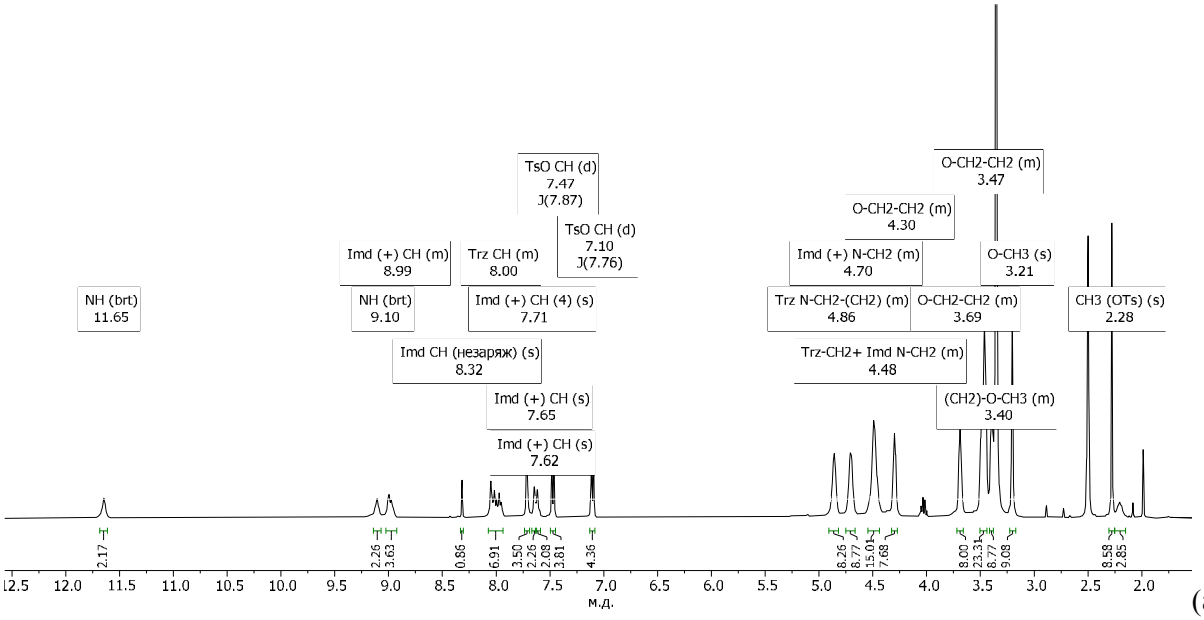


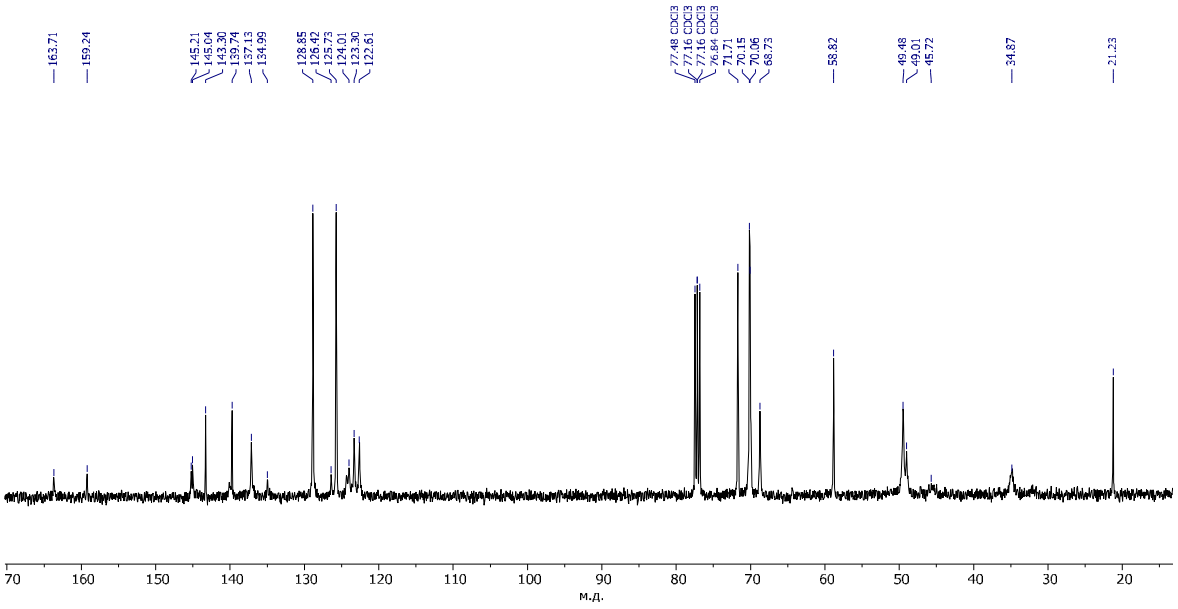
Fig. S2 ^{1}H NMR (400 MHz) (a), ^{13}C NMR (101 MHz) (b), FT-IR (c) and HRESI MS (d) spectra of 3a



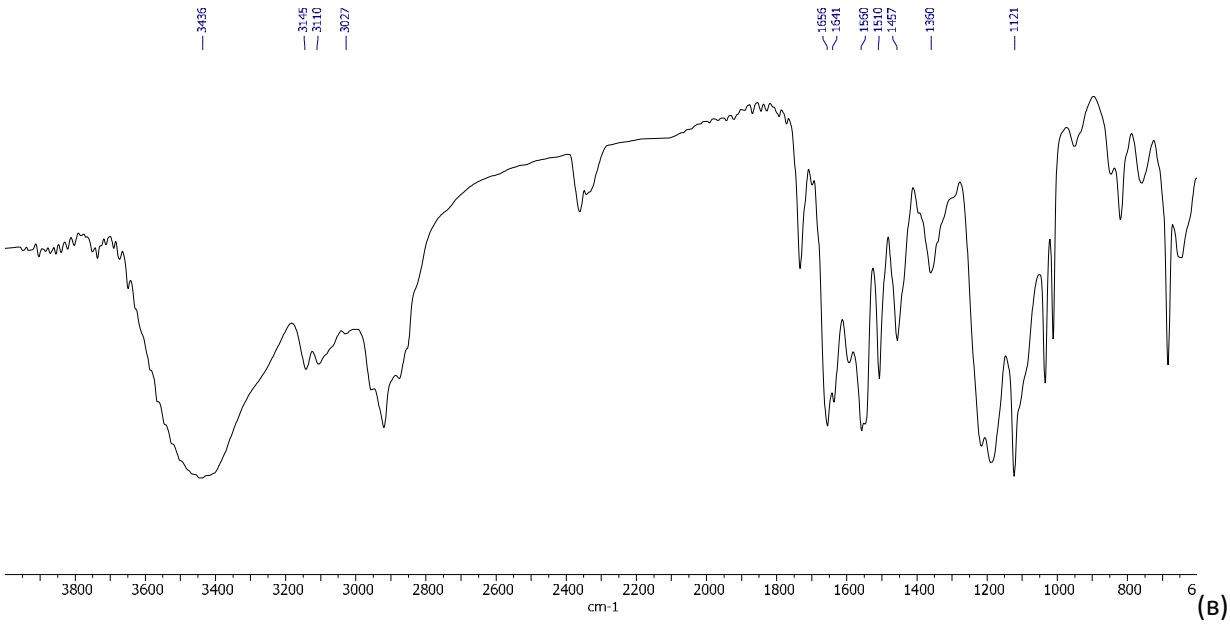
(4)


NH (brt)
11.65
Imd (+) CH (m)
8.99
NH (brt)
9.10
Trz CH (m)
8.00
Imd (+) CH (4) (s)
7.71
TsO CH (d)
7.47
J(7.87)
TsO CH (d)
7.10
J(7.76)
Imd CH (незаряж) (s)
8.32
Imd (+) CH (s)
7.65
Imd (+) CH (s)
7.62
O-CH2-CH2 (m)
4.30
Imd (+) N-CH2 (m)
4.70
Trz N-CH2-(CH2) (m)
4.86
Trz-CH2+ Imd N-CH2 (m)
4.48
O-CH2-CH2 (m)
3.47
O-CH3 (s)
3.21
O-CH2-CH2 (m)
3.69
(CH2)-O-CH3 (m)
3.40
CH3 (OTs) (s)
2.28
м.д.

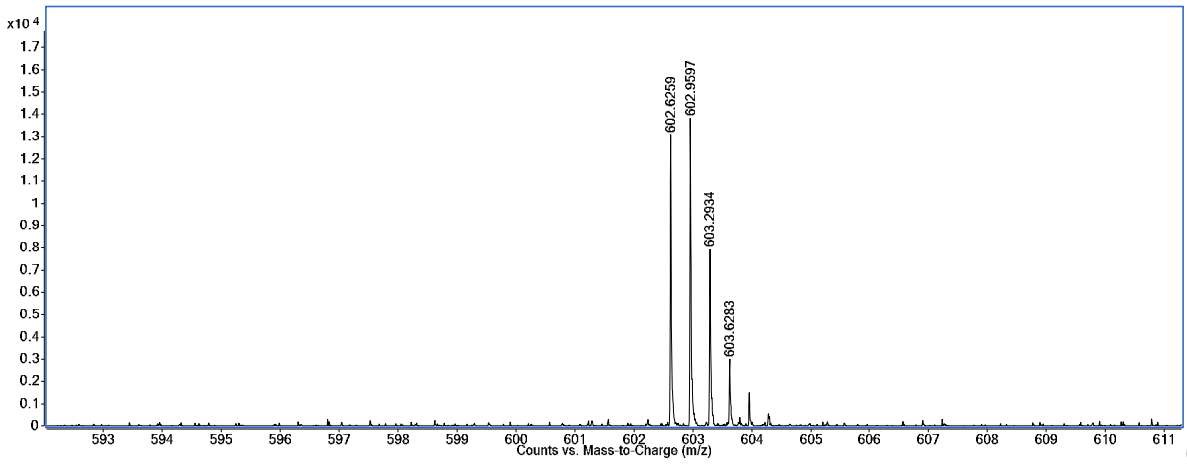
(a)



(б)

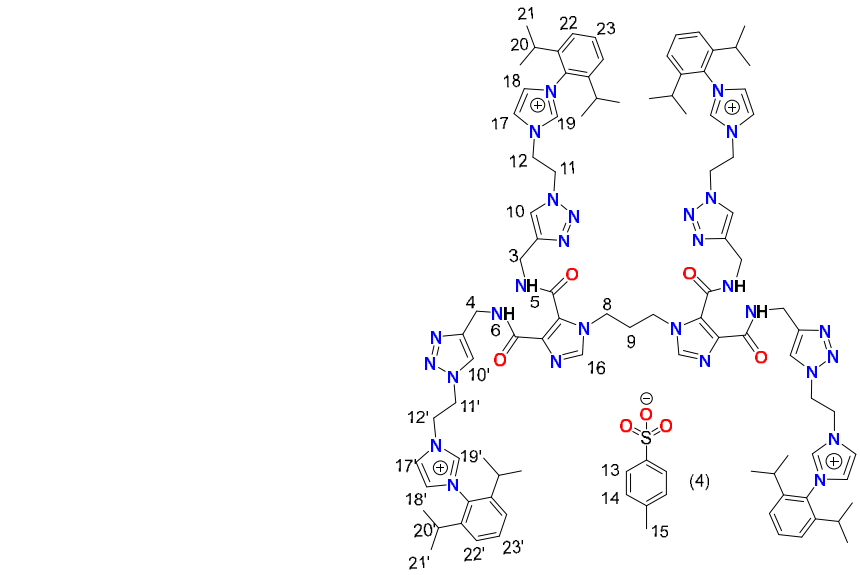


(в)

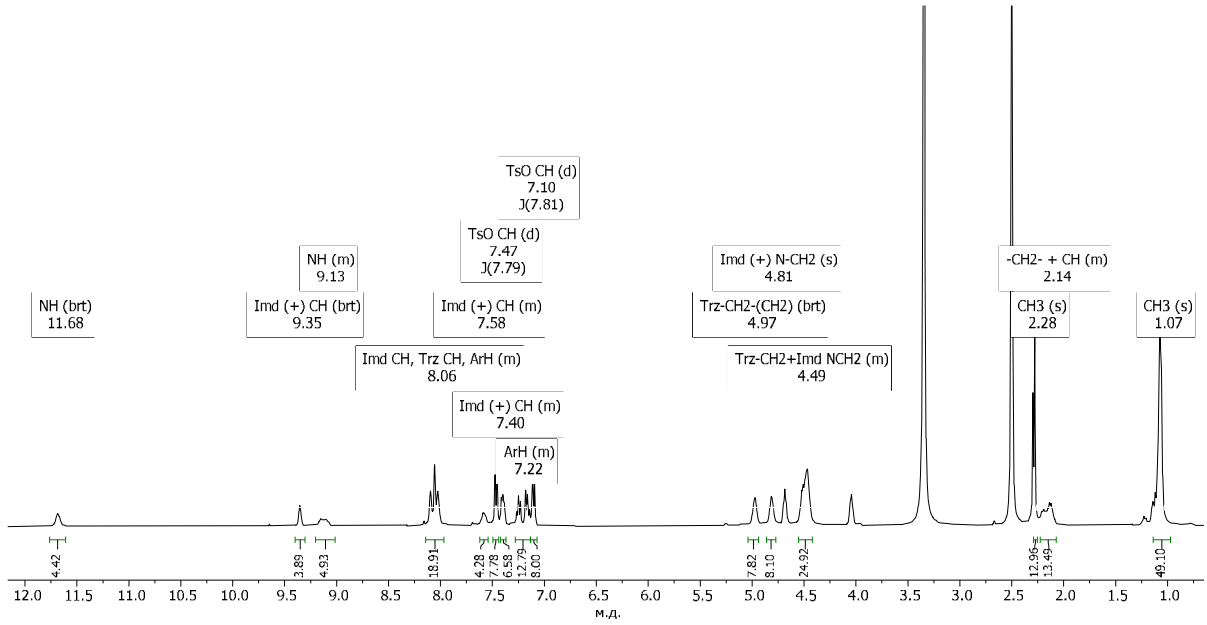


(г)

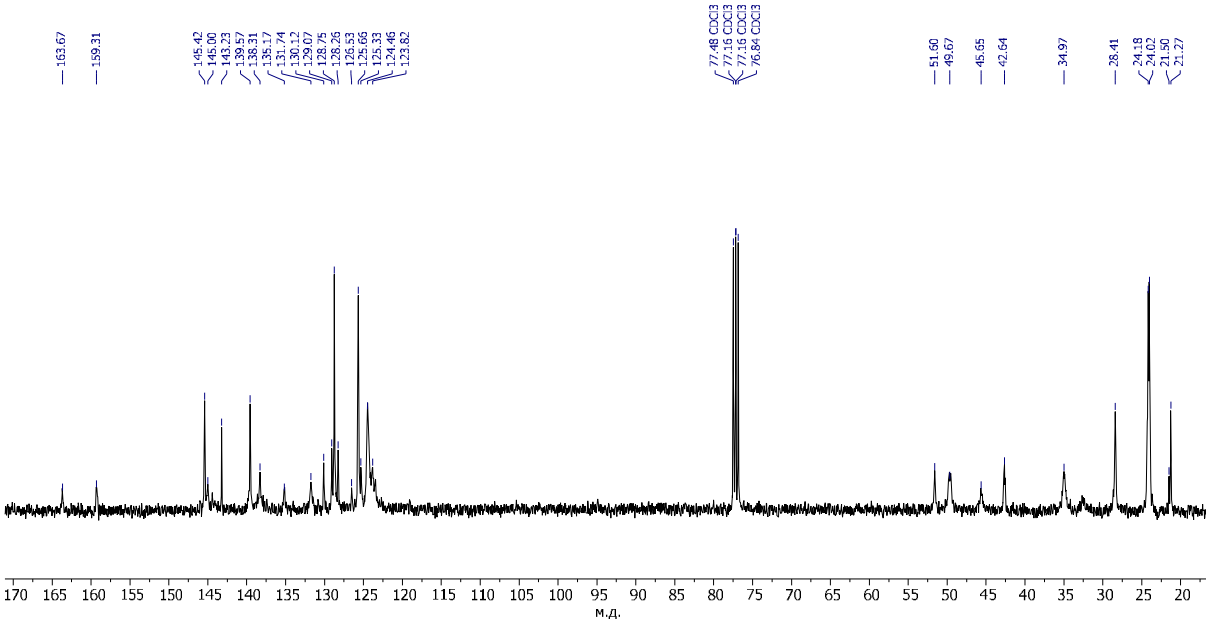
Fig. S3 ^{1}H NMR (400 MHz) (a), ^{13}C NMR (101 MHz) (b), FT-IR (c) and HRESI MS (d) spectra of 3b



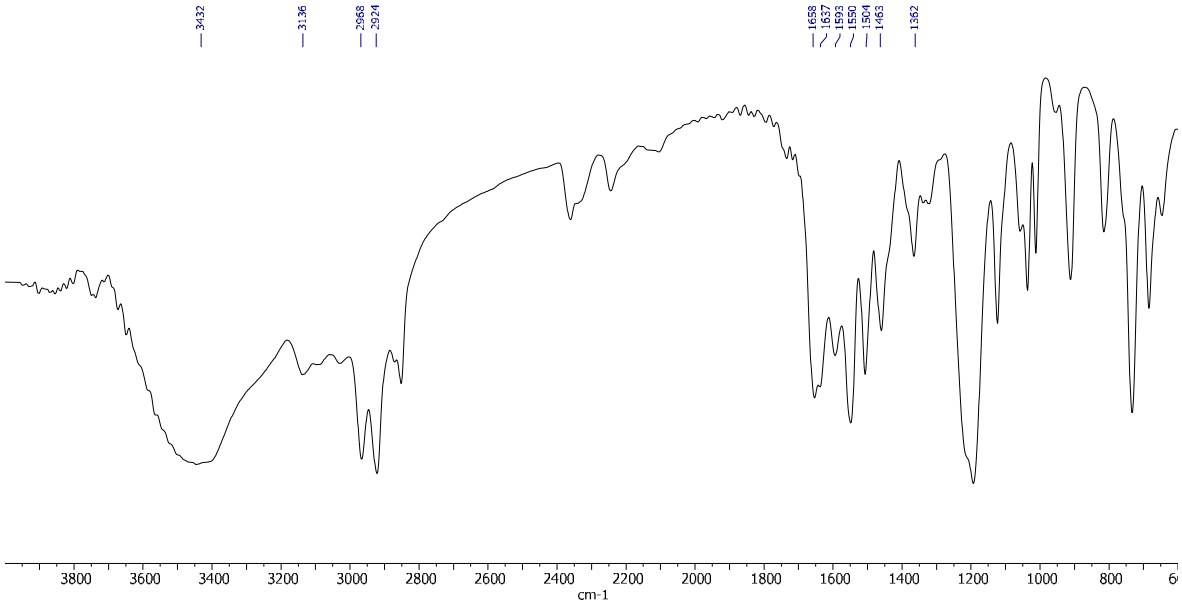
(4)


NH (brt)
11.68
Imd (+) CH (brt)
9.35
NH (m)
9.13
Imd CH, Trz CH, ArH (m)
8.06
TsO CH (d)
7.47
J(7.79)
Imd (+) CH (m)
7.58
TsO CH (d)
7.10
J(7.81)
Imd (+) CH (m)
7.40
ArH (m)
7.22
Trz-CH2-(CH2) (brt)
4.97
Imd (+) N-CH2 (s)
4.81
Trz-CH2+Imd NCH2 (m)
4.49
-CH2- + CH (m)
2.14
CH3 (s)
2.28
CH3 (s)
1.07
м.д.

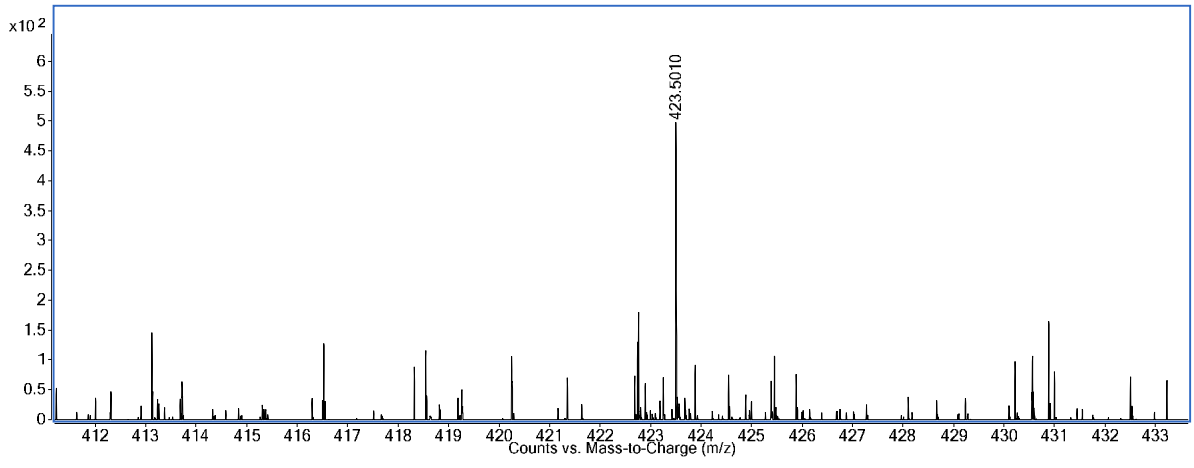
(а)


м.д.

(б)

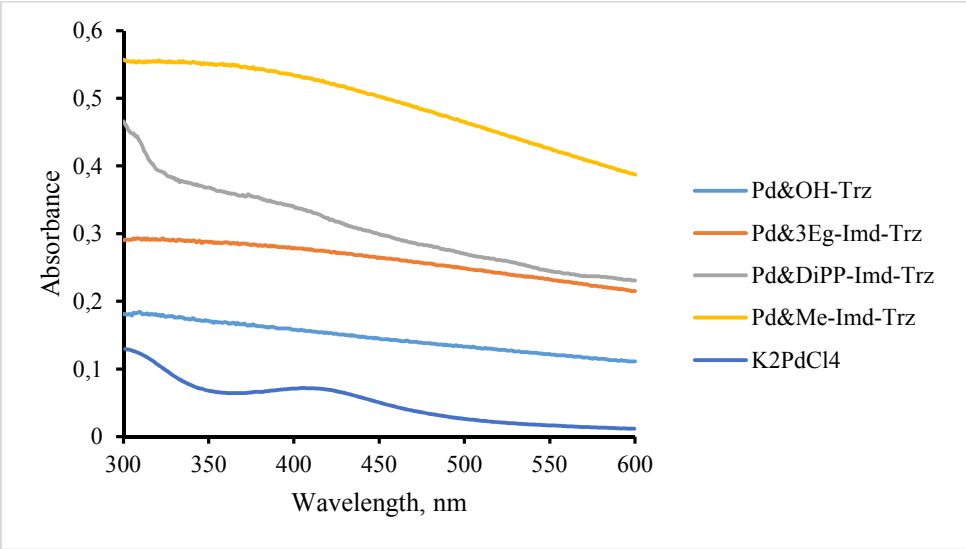


(в)

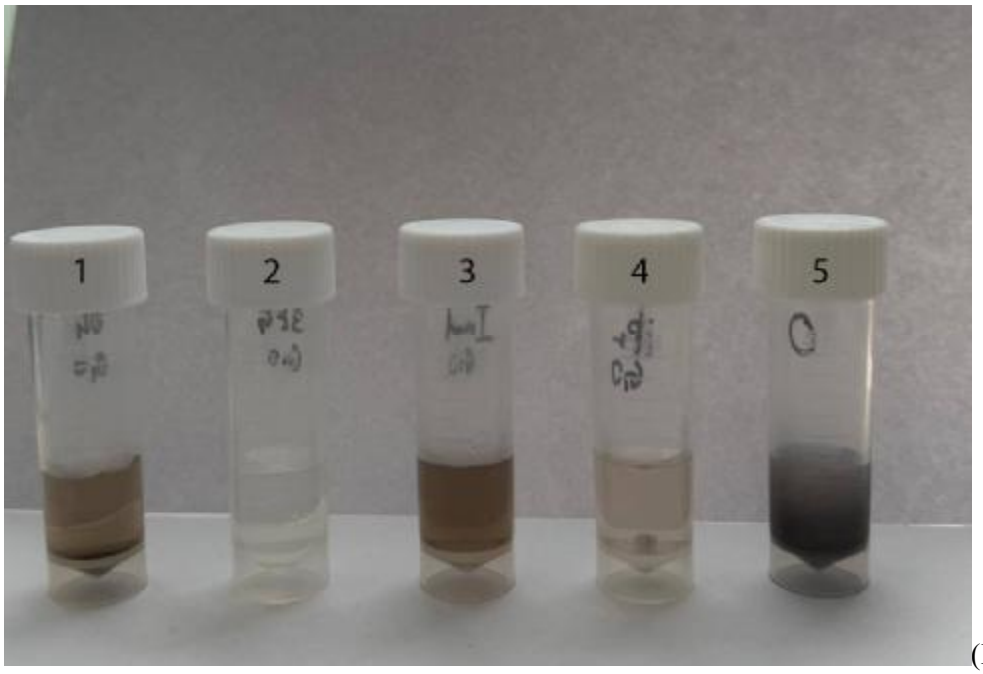


(г)

Fig. S4 ^{1}H NMR (400 MHz) (a), ^{13}C NMR (101 MHz) (b), FT-IR (c) and HRESI MS (d) spectra of 3c



(A)



(Б)

Fig. S5 UV-vis spectra of $K_2[PdCl_4]$ and systems Pd&R-Trz, where R – OH, Me-Imd, 3Eg-Imd, DiPP-Imd obtained after addition of $K_2[PdCl_4]$ with ascorbic acid in the presence of stabilizing agents, [dendrimer] 0.05 мМ, [K□PdCl□] 1 мМ, [ascorbic acid] 10 мМ (A); Photographs of vials containing Pd&R-Trz, where R – OH (1), 3Eg-Imd(2), Me-Imd(3), DiPP-Imd(4) and Pd(0) without stabiliser (5) (B).