GALLIUM(III) AND INDIUM(III) COMPLEXES WITH *MESO*-MONOPHOSPHORYLATED PORPHYRINS: SYNTHESIS AND STRUCTURE. A FIRST EXAMPLE OF DIMERS FORMED BY SELF-ASSEMBLING OF *MESO*-PORPHYRINYL-PHOSPHONIC ACID MONOESTER

Yu.Yu. Enakieva,[a] M.V. Volostnykh,[a,b] S.E. Nefedov,[c] G.A. Kirakosyan,[a,c] Yu.G. Gorbunova,*[,a,c] A.Yu. Tsivadze[a,c] , A.G. Bessmertnykh-Lemeune,[b] C. Stern,[b] and R. Guilard*[,b]

[a] A.N. Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Leninsky pr. 31-4, Moscow, 119071, Russia

[b] Université de Bourgogne Franche-Comté, ICMUB (UMR CNRS 6302), 9 Avenue Alain Savary, BP 47870, 21078 Dijon Cedex, France

[c] N.S. Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Leninsky pr. 31, Moscow, 119991, Russia

Table of contents

1. NMR spectra of gallium(III) and indium(III) complexes with 10-(diethoxyphosphoryl)-5,15- di(aryl)porphyrin (Ga-1a-c, In-1a-c)

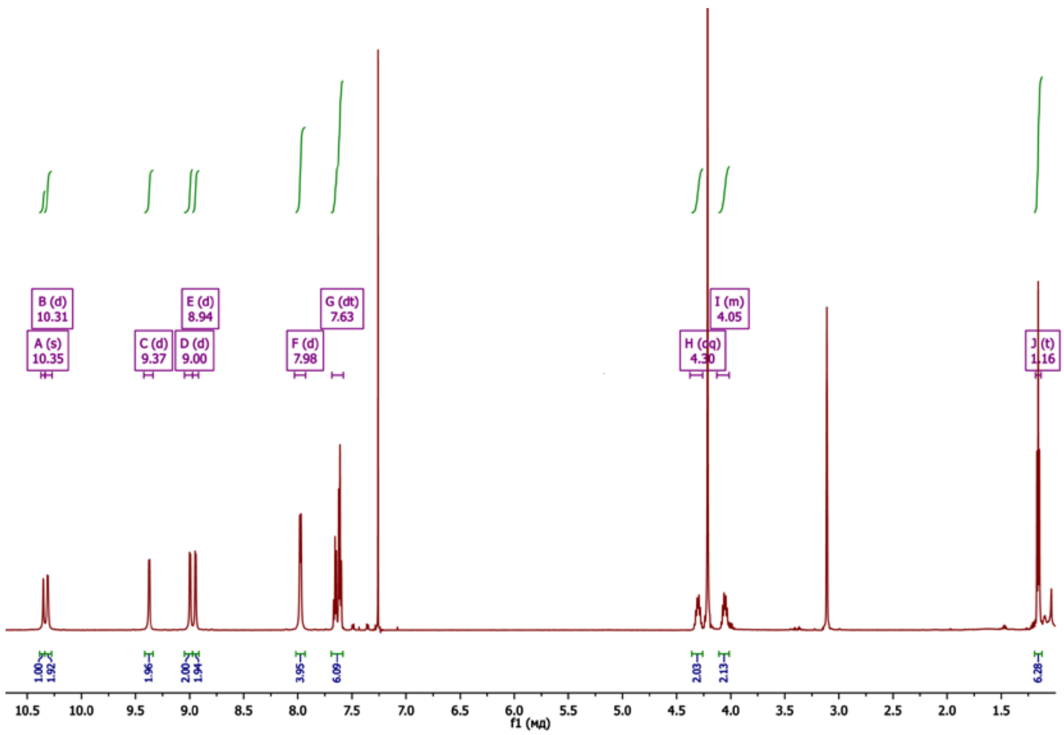


*Figure S1. ^{1}H NMR spectra of **Ga-1a** in the mixture of $CDCl_3$:CD_3OD (2:1 v/v).*

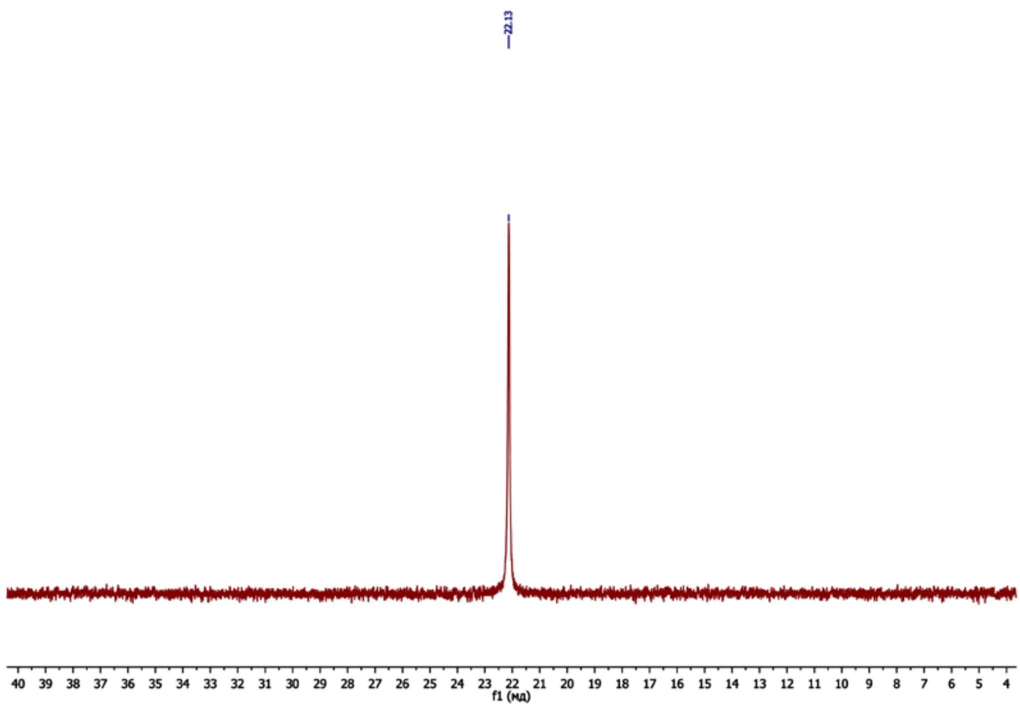


*Figure S2. ^{31}P NMR spectrum of **Ga-1a** in the mixture of $CDCl_3$:CD_3OD (2:1 v/v).*

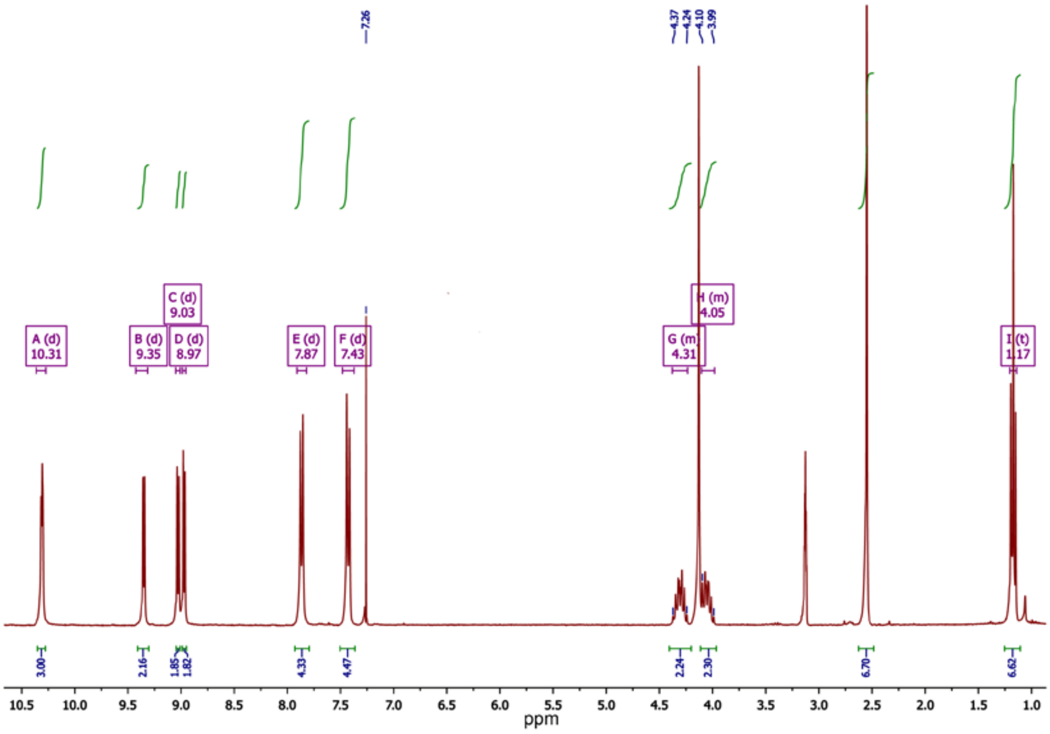


Figure S3. [1]H NMR spectrum of ***Ga-1b*** *in the mixture of $CDCl_3$:CD_3OD (2:1 v/v).*

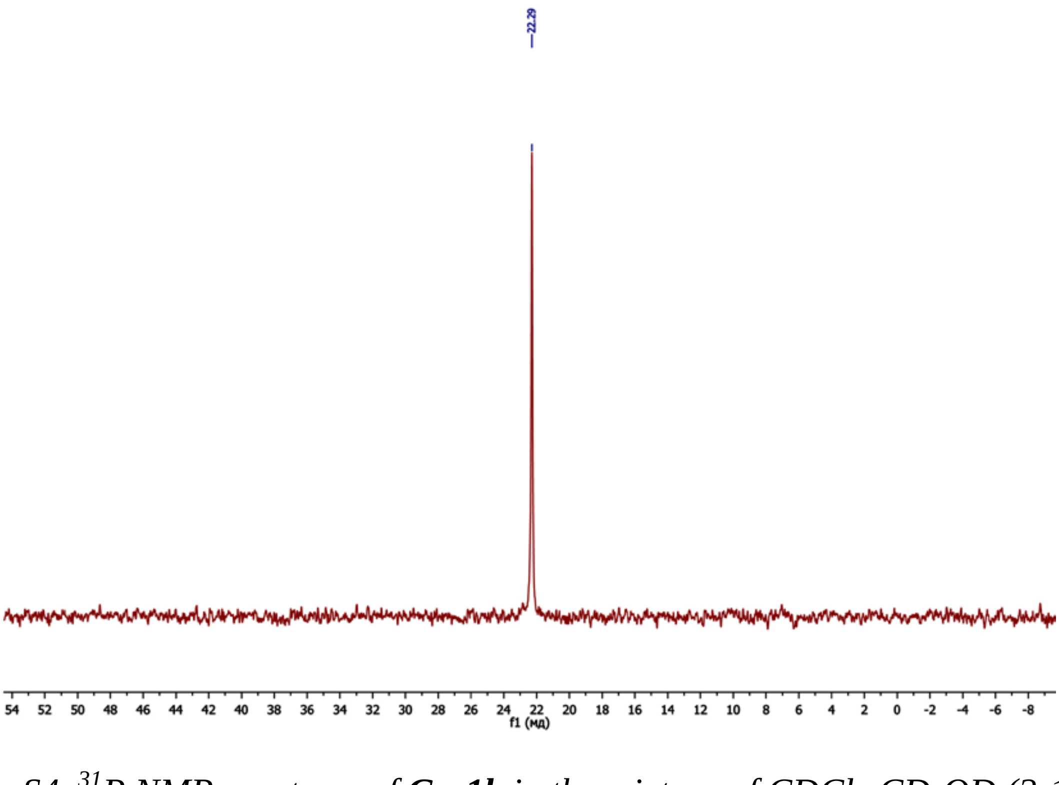


Figure S4. [31]P NMR spectrum of ***Ga-1b*** *in the mixture of $CDCl_3$:CD_3OD (2:1 v/v).*

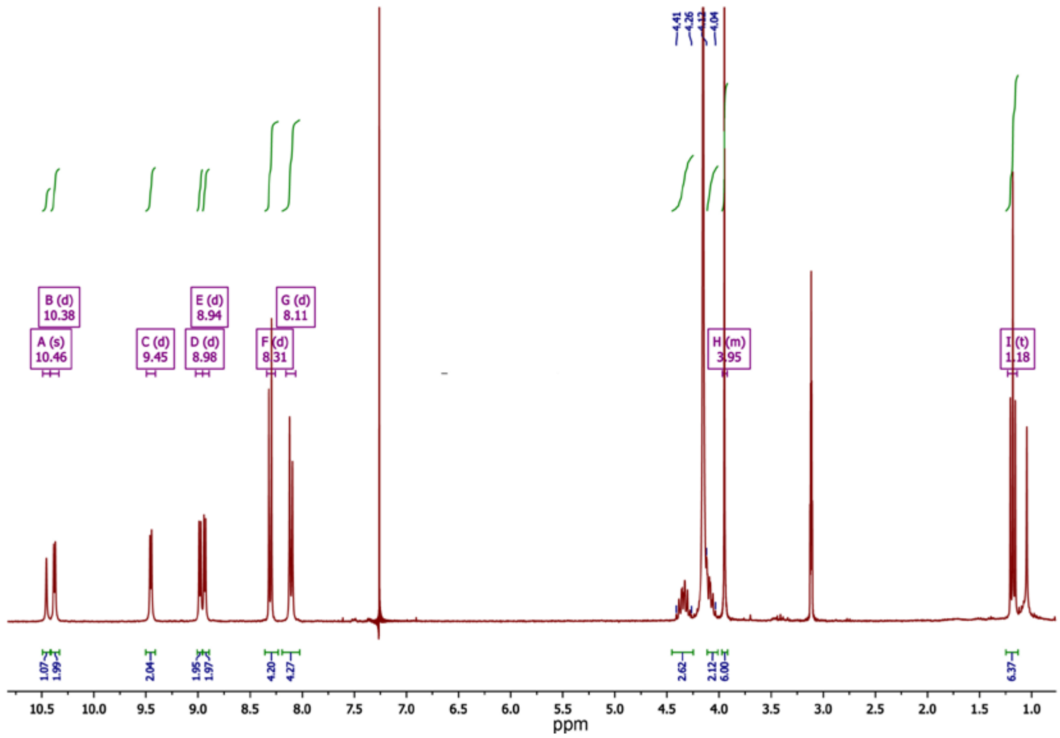


*Figure S5. [1]H NMR spectrum of **Ga-1c** in the mixture of $CDCl_3$:CD_3OD (2:1 v/v).*

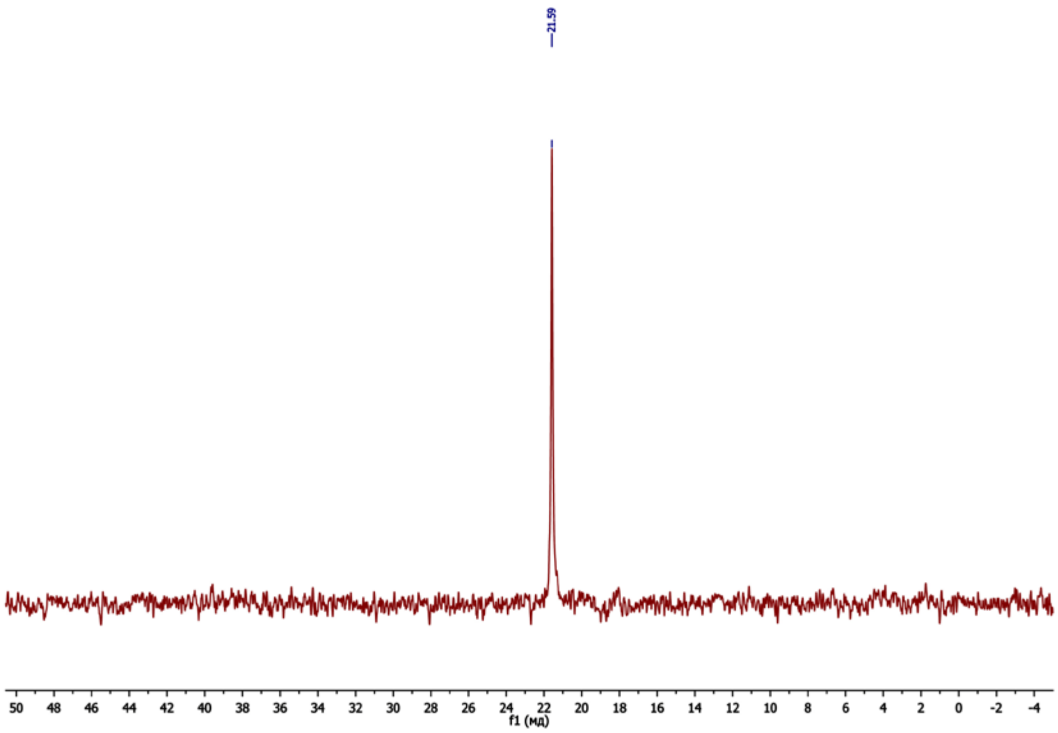


*Figure S6. [31]P NMR spectrum of **Ga-1c** in the mixture of $CDCl_3$:CD_3OD (2:1 v/v).*

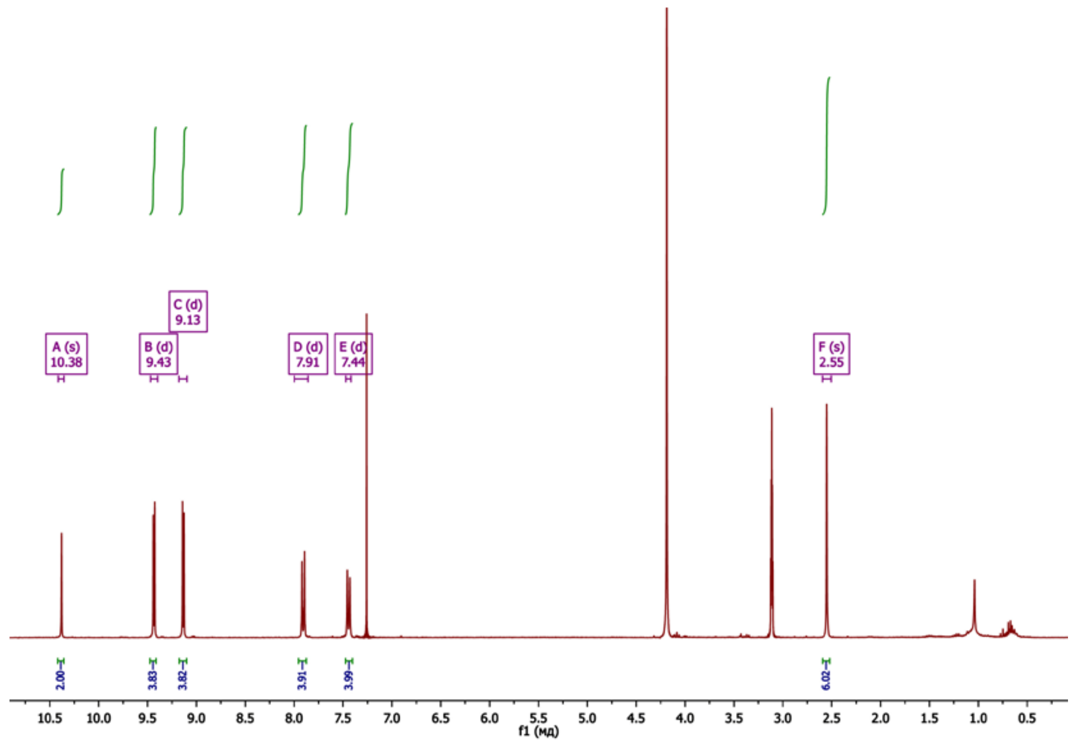


*Figure S7. [1]H NMR spectrum of **Ga-5b** in the mixture of $CDCl_3$:CD_3OD (2:1 v/v).*

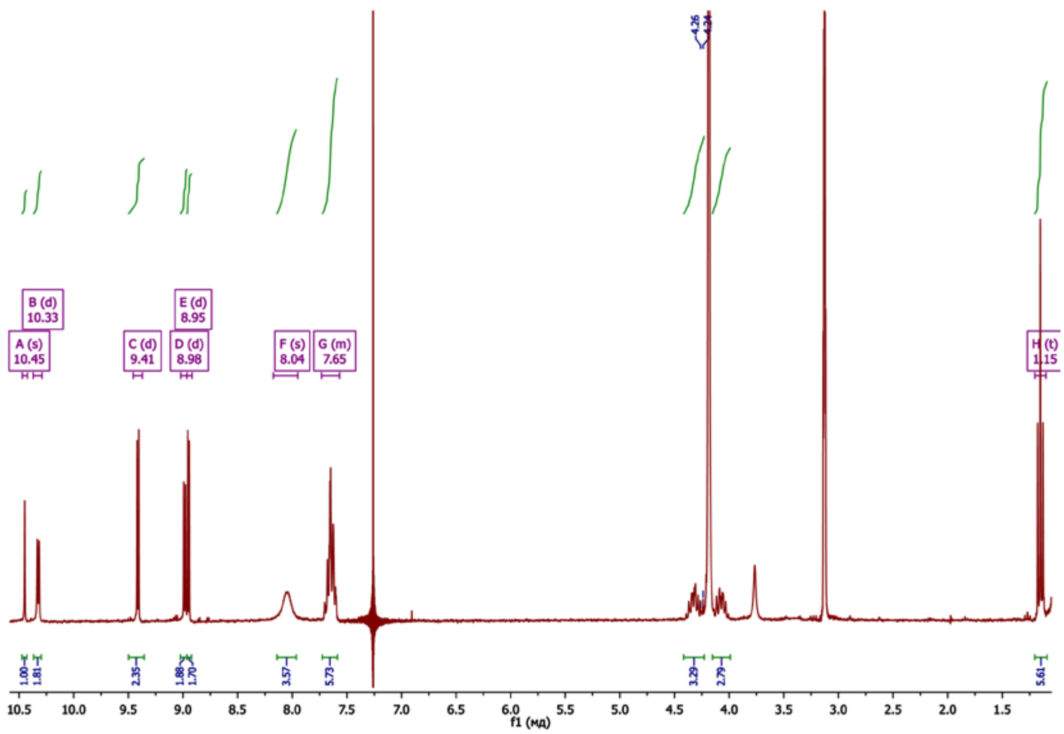


*Figure S8. [1]H NMR spectrum of **In-1a** in the mixture of $CDCl_3$:CD_3OD (2:1 v/v).*

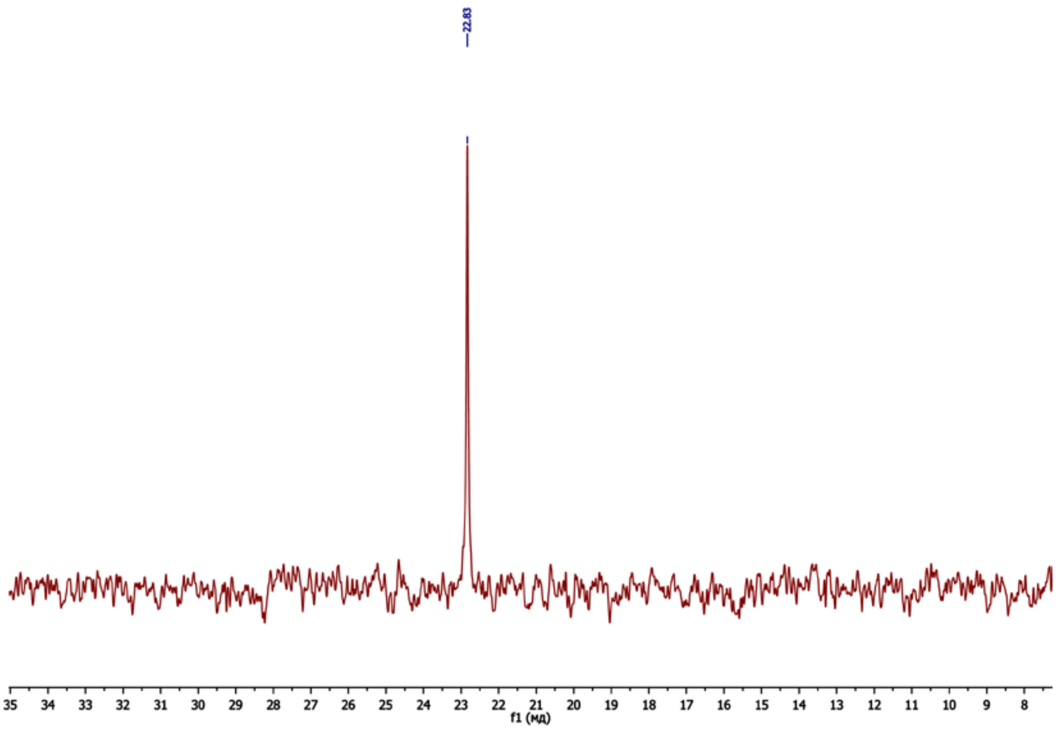


*Figure S9. [31]P NMR spectrum of **In-1a** in the mixture of $CDCl_3$:CD_3OD (2:1 v/v).*

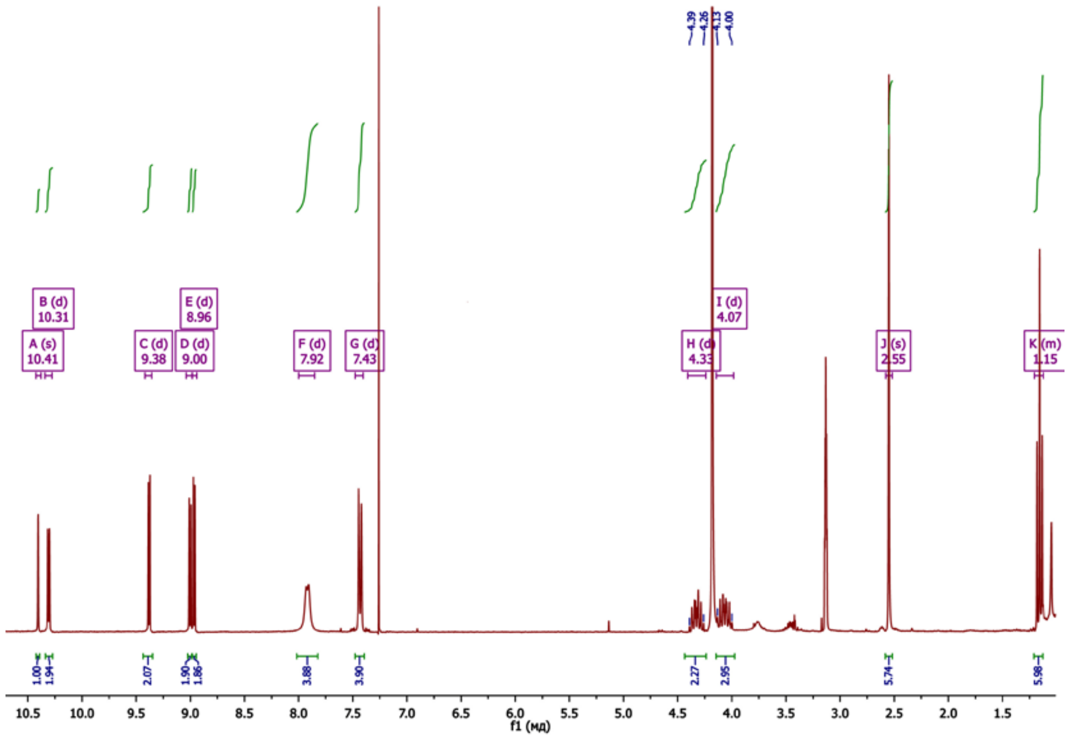


*Figure S10. [1]H NMR spectrum of **In-1b** in the mixture of $CDCl_3$:CD_3OD (2:1 v/v).*

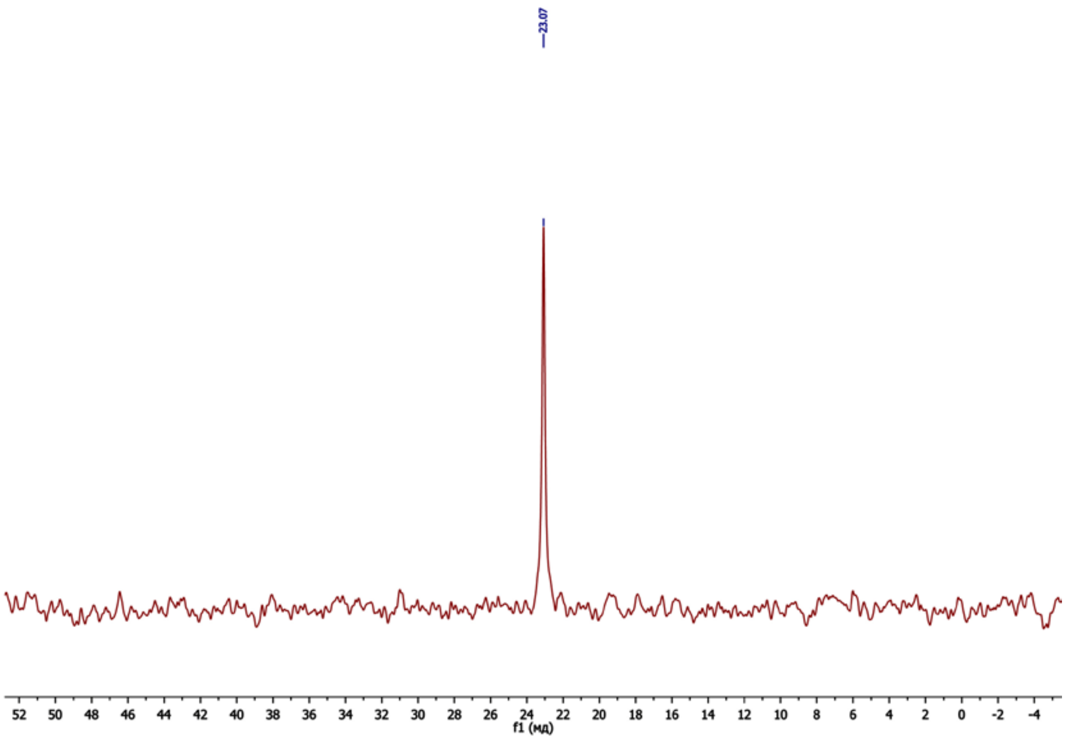


*Figure S11. ^{31}P NMR spectrum of **In-1b** in the mixture of $CDCl_3$:CD_3OD (2:1 v/v).*

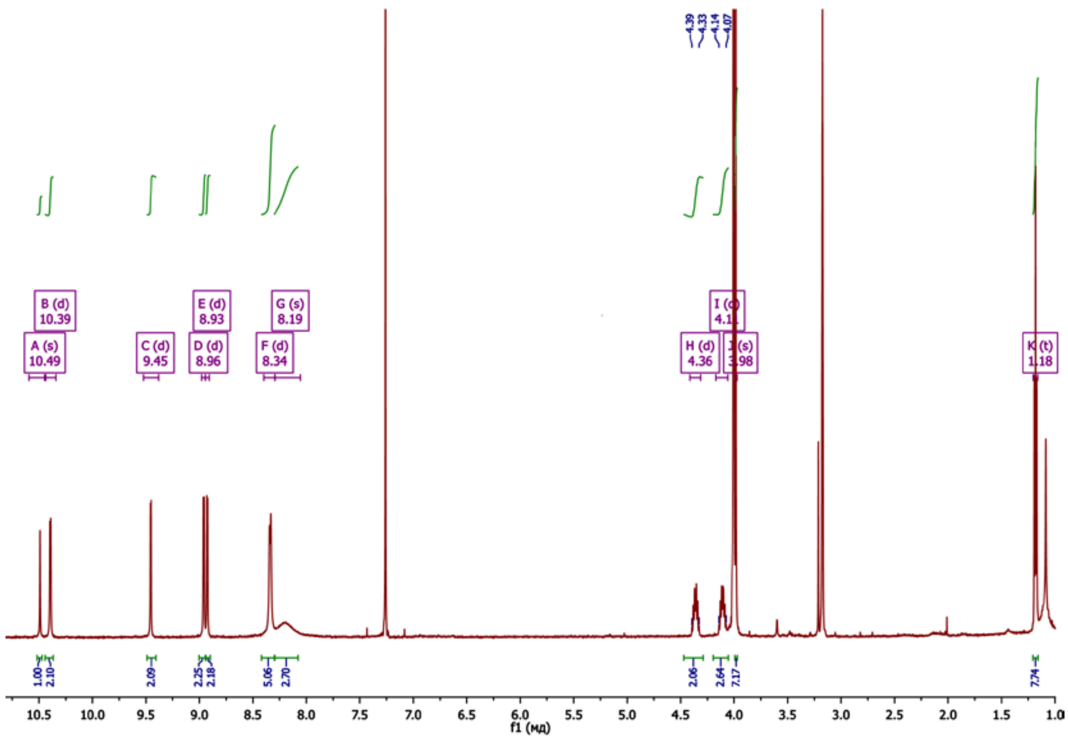


*Figure S12. ^{1}H NMR spectrum of **In-1c** in the mixture of $CDCl_3$:CD_3OD (2:1 v/v).*

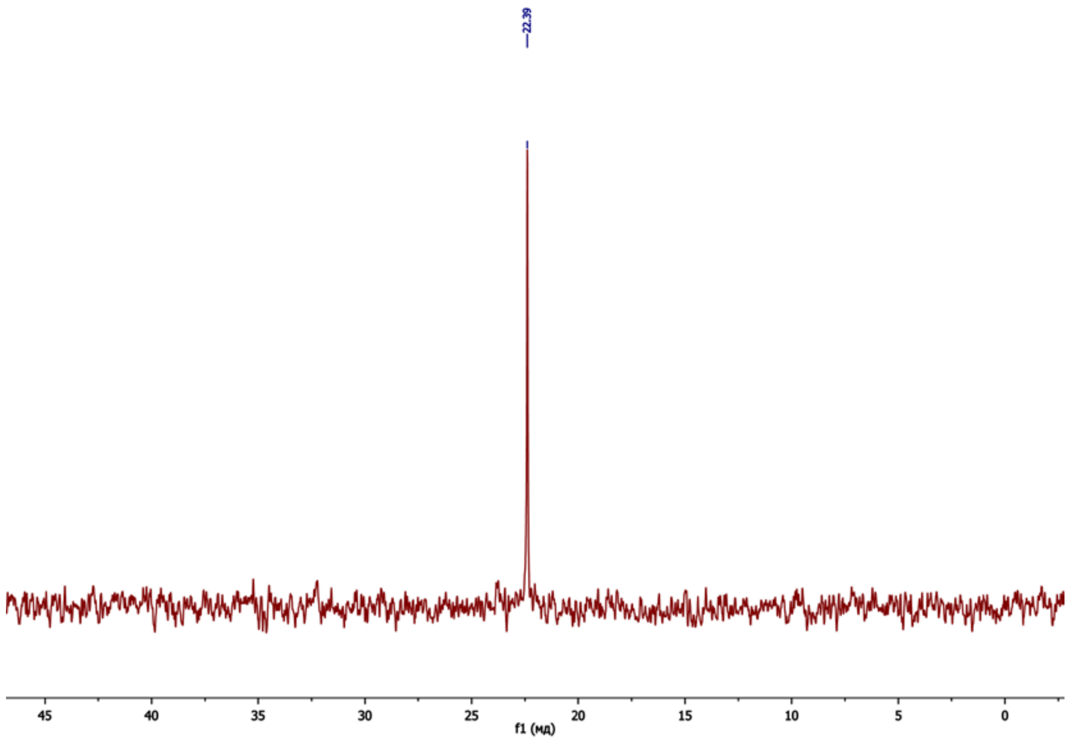


Figure S13. ^{31}*P NMR spectrum of* ***In-1c*** *in the mixture of* $CDCl_3$:CD_3OD *(2:1 v/v).*

2. NMR spectra of Ga-1a-c and In-1a in different solvents

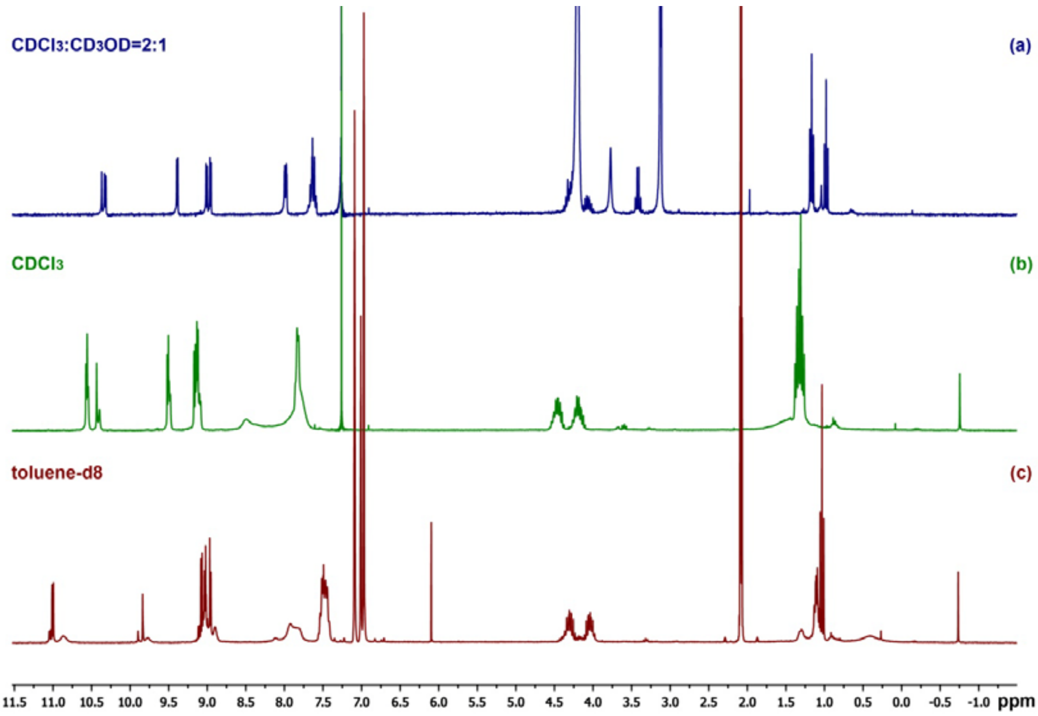


Figure S14. ^{1}*H NMR spectra of* ***Ga-1a***.

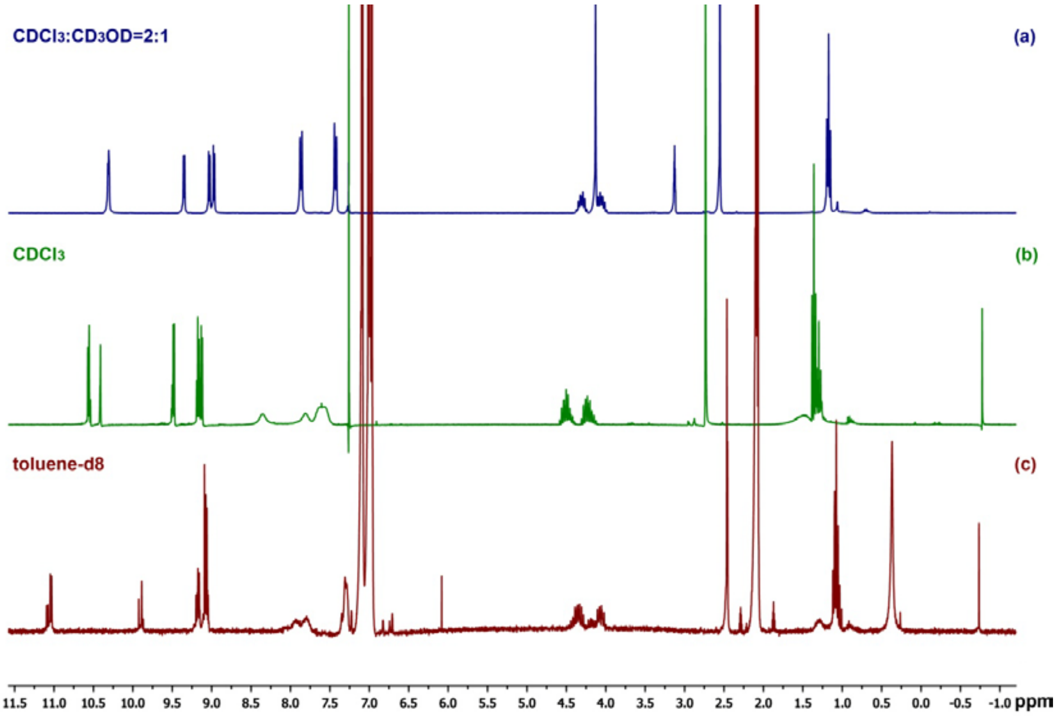


Figure S15. ^{1}H NMR spectra of ***Ga-1b.***

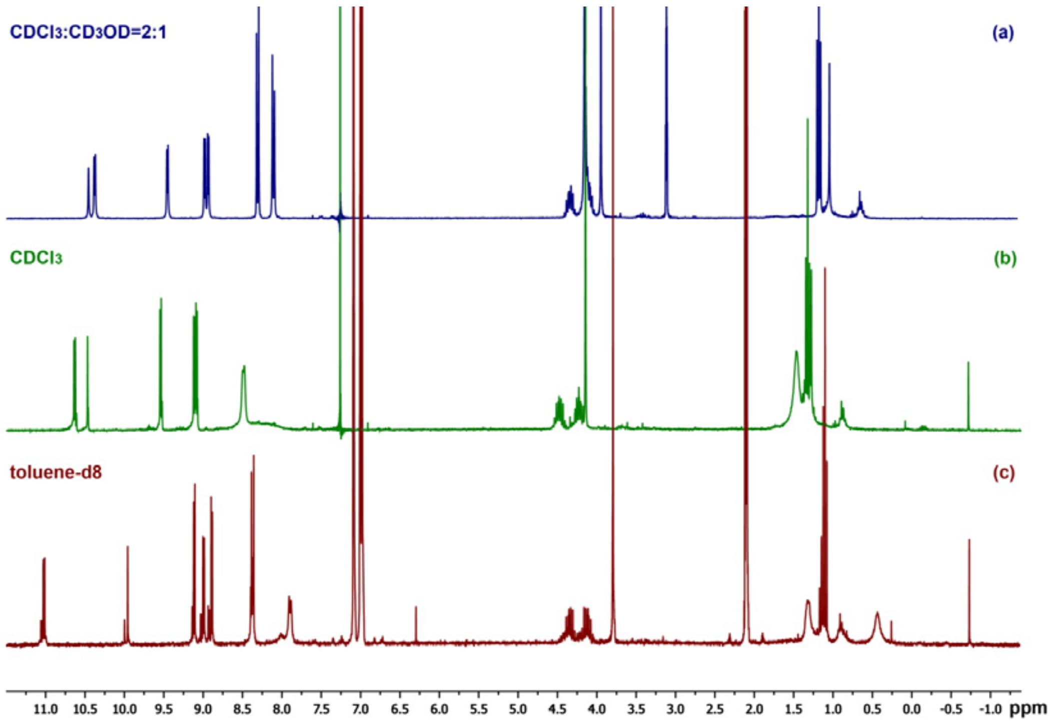


Figure S16. ^{1}H NMR spectra of ***Ga-1c***.

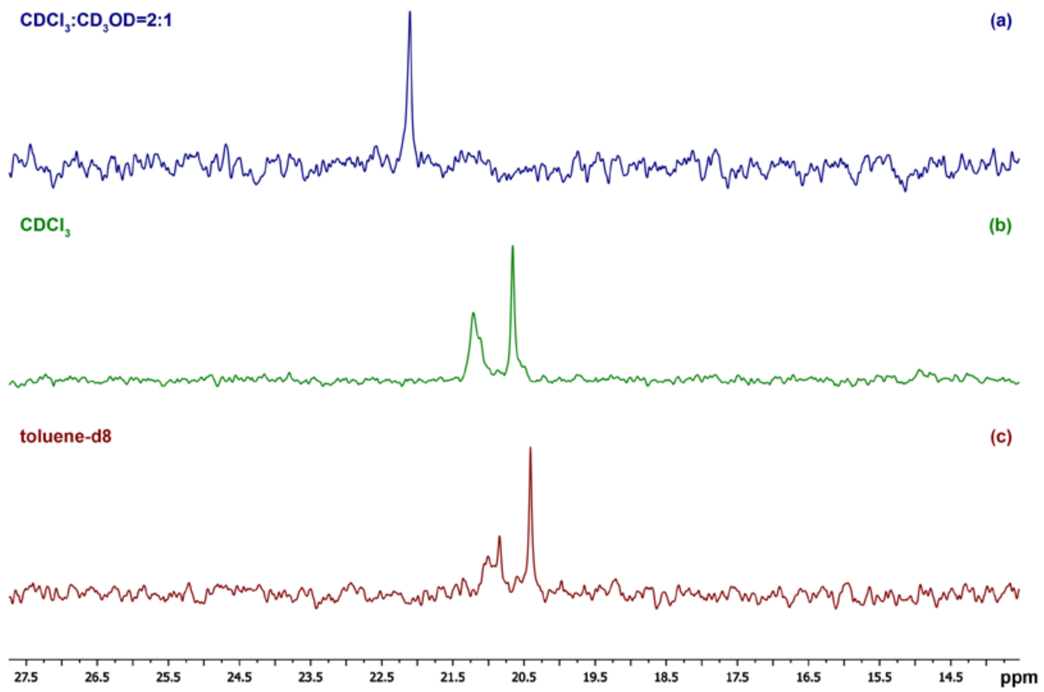


Figure S17. ^{31}P NMR spectra of ***Ga-1a****.*

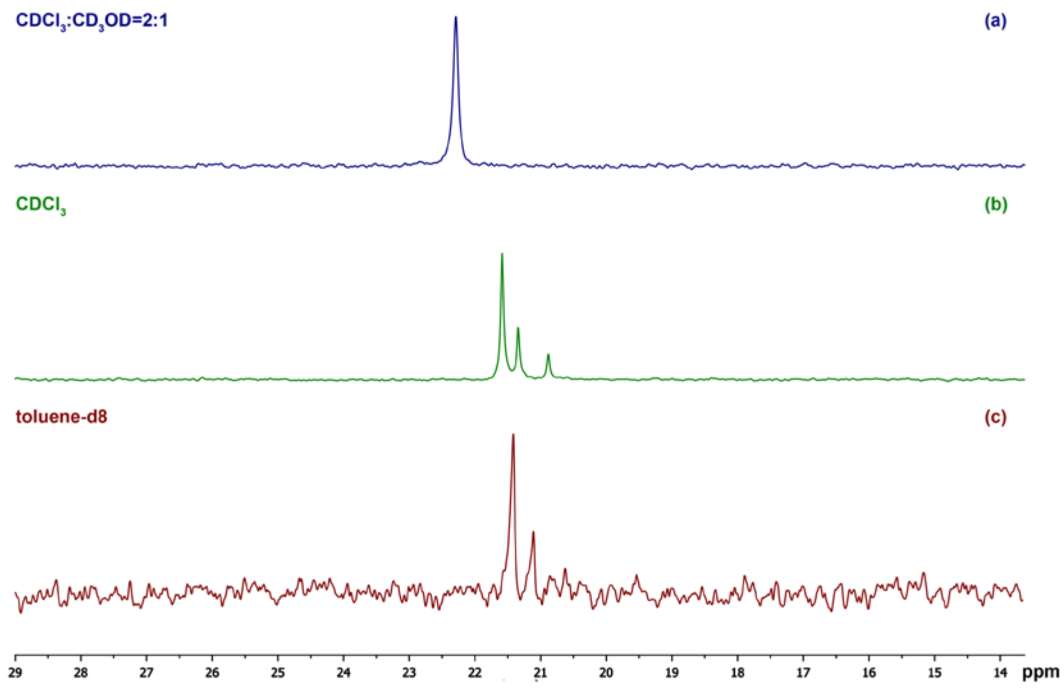


Figure S18. ^{31}P NMR spectra of ***Ga-1b****.*

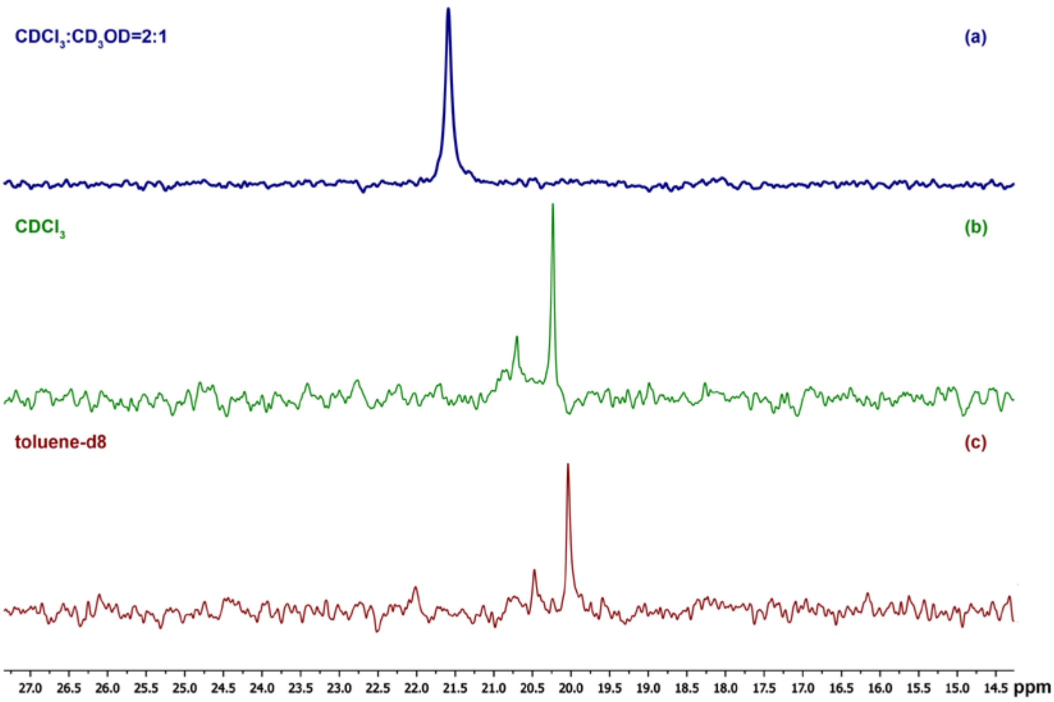


Figure S19. ^{31}*P NMR spectra of* ***Ga-1c***.

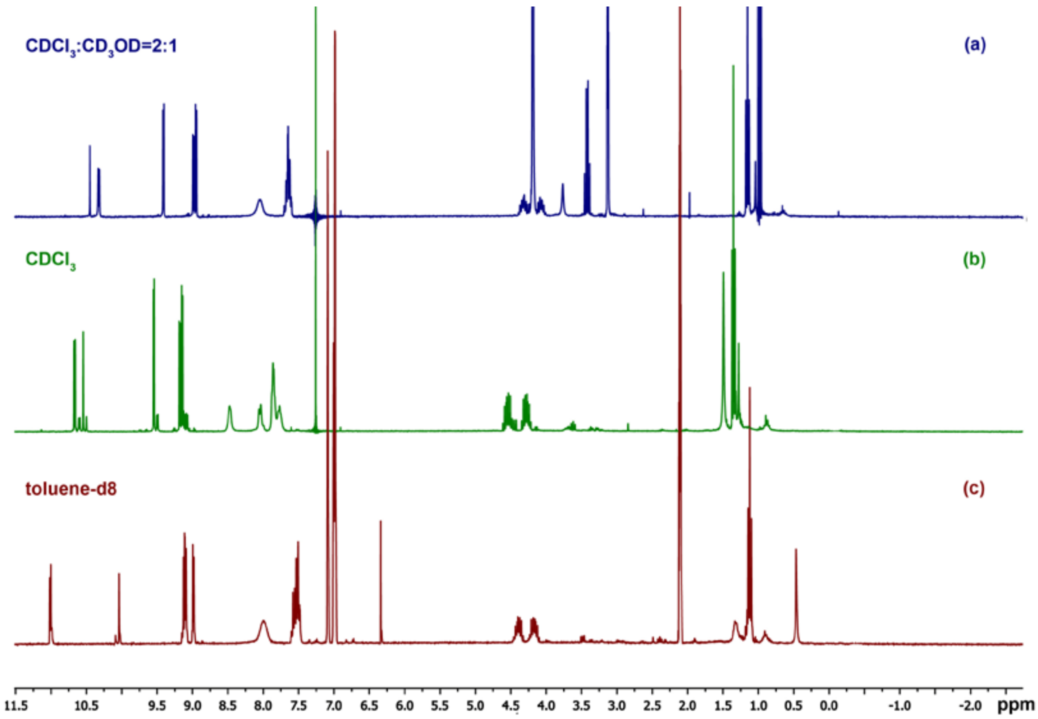


Figure S20. ^{1}*H NMR spectra of* ***In-1a***.

3. NMR spectra of gallium(III) and indium(III) complexes with monoester of *meso*-porphyrinyl phosphonic acids (Ga-2a,b,3c and In-2a,b,3c)

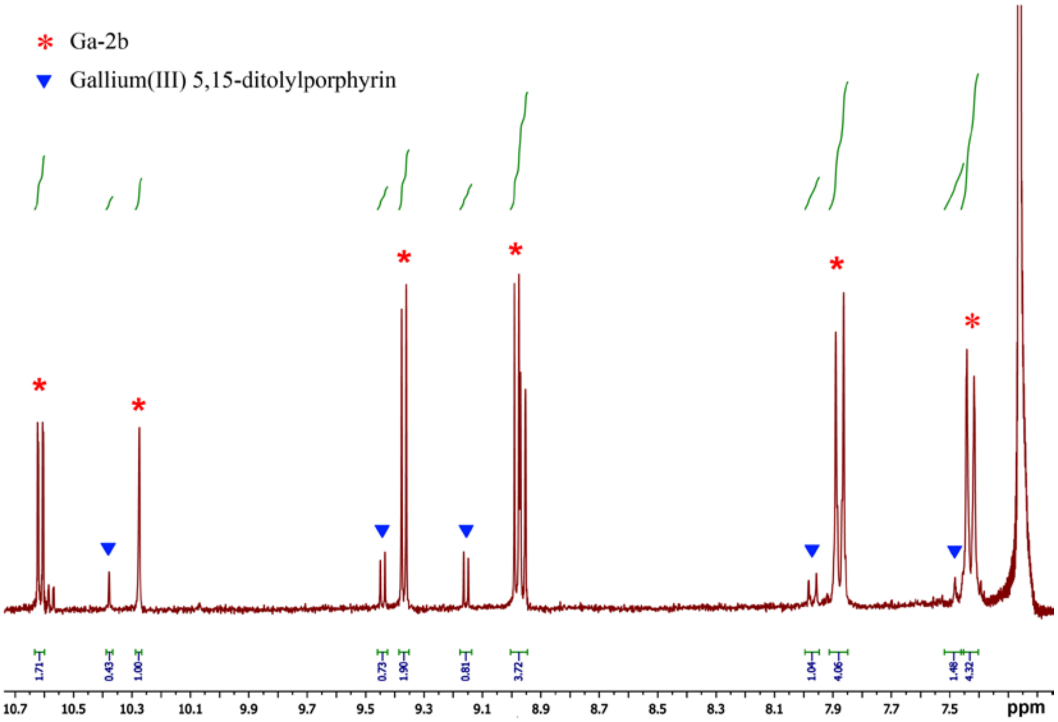


*Figure S21. [1]H NMR spectrum of the reaction mixture of **Ga-2b** and gallium(III) 5,15-ditolylporphyrin in the mixture of $CDCl_3$:CD_3OD (2:1 v/v).*

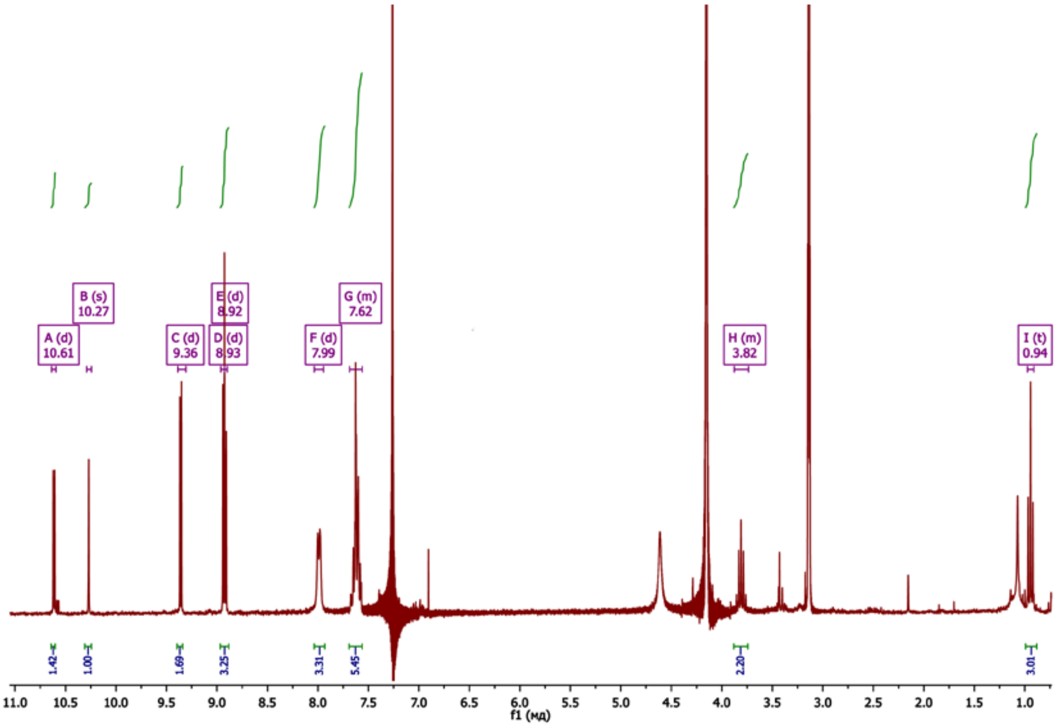


*Figure S22. [1]H NMR spectrum of **Ga-2a** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

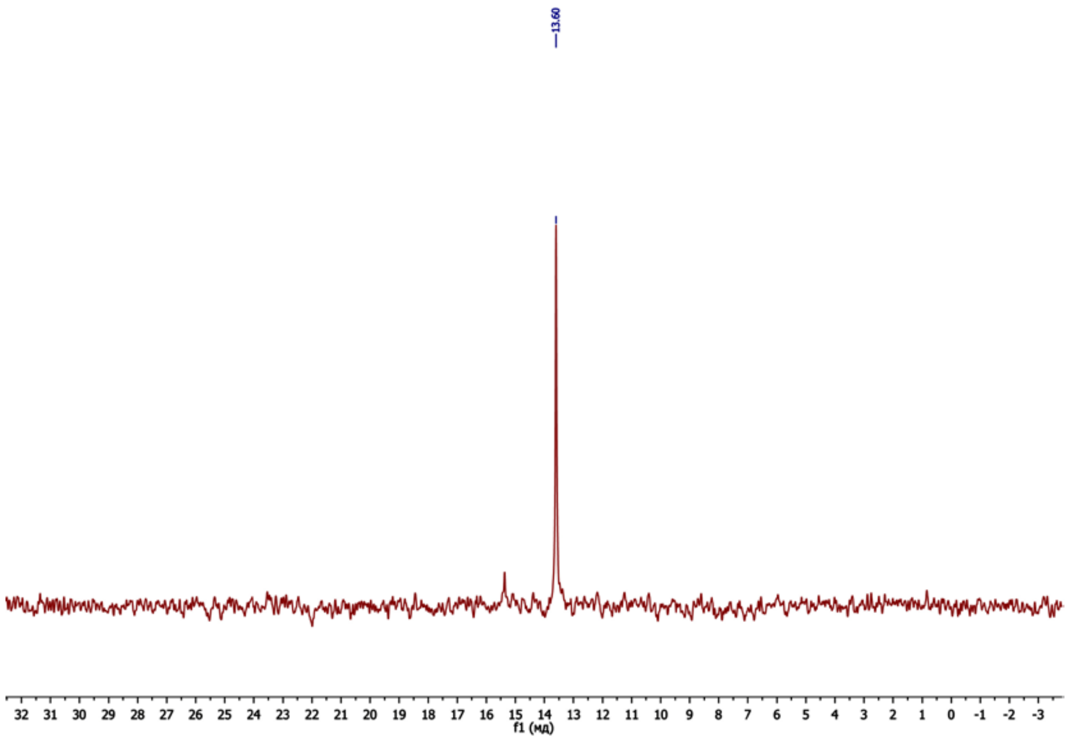


*Figure S23. [31]P NMR spectrum of **Ga-2a** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

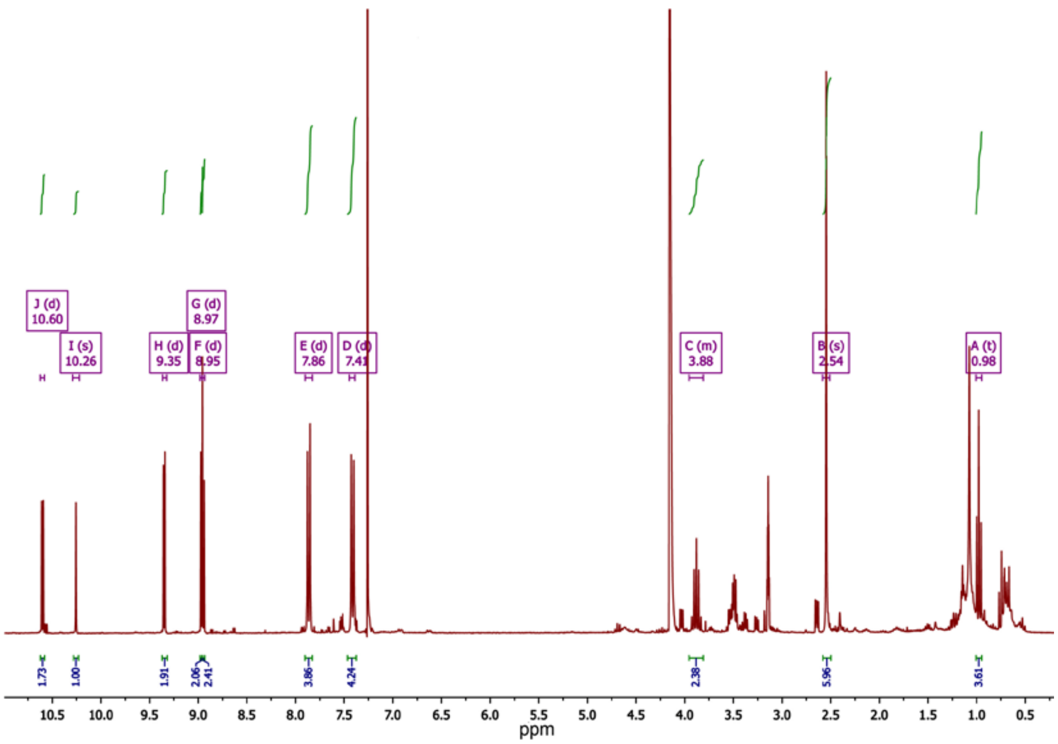


*Figure S24. [1]H NMR spectrum of **Ga-2b** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

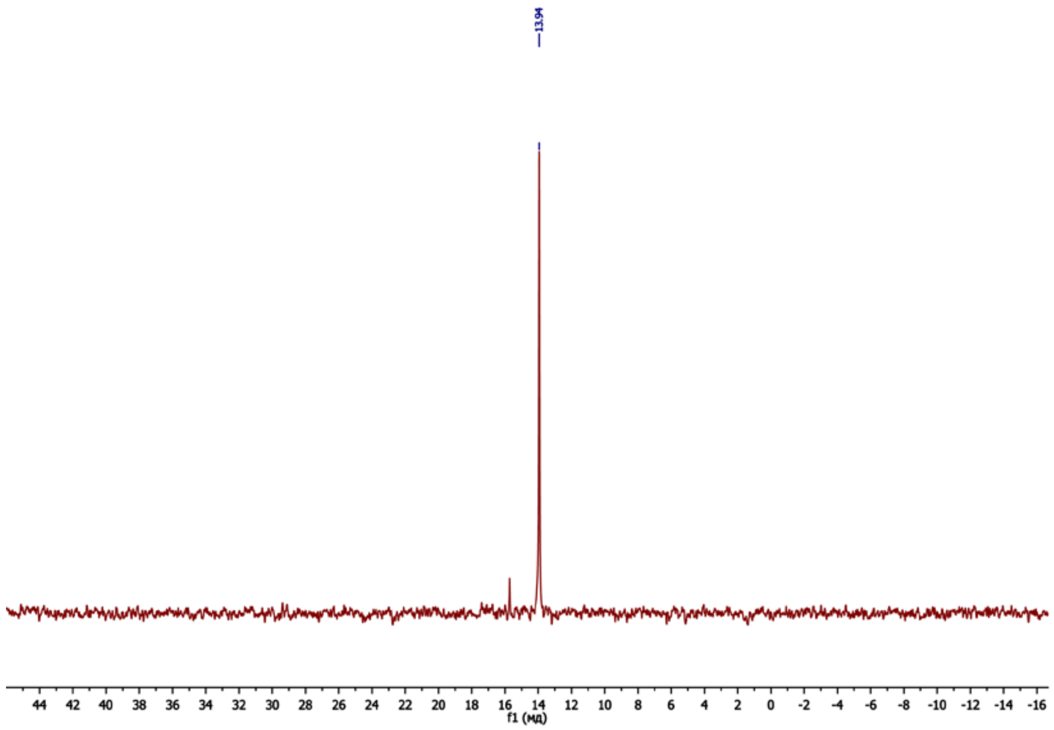


Figure S25. [31]*P NMR spectrum of* ***Ga-2b*** *($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

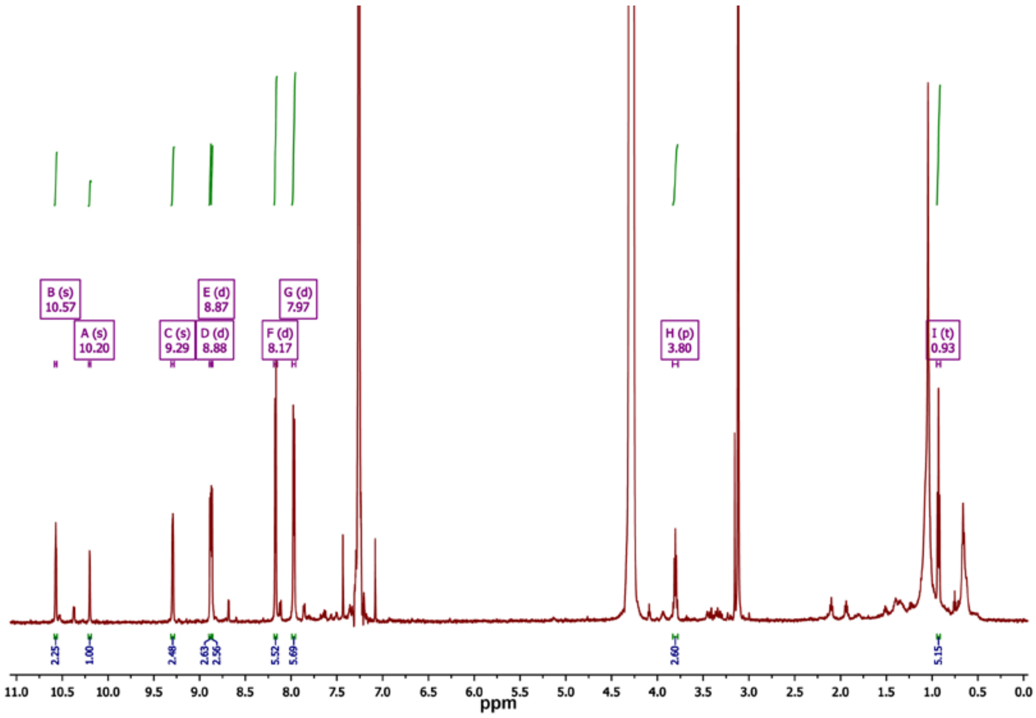


Figure S26. [1]*H NMR spectrum of* ***Ga-3c*** *($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

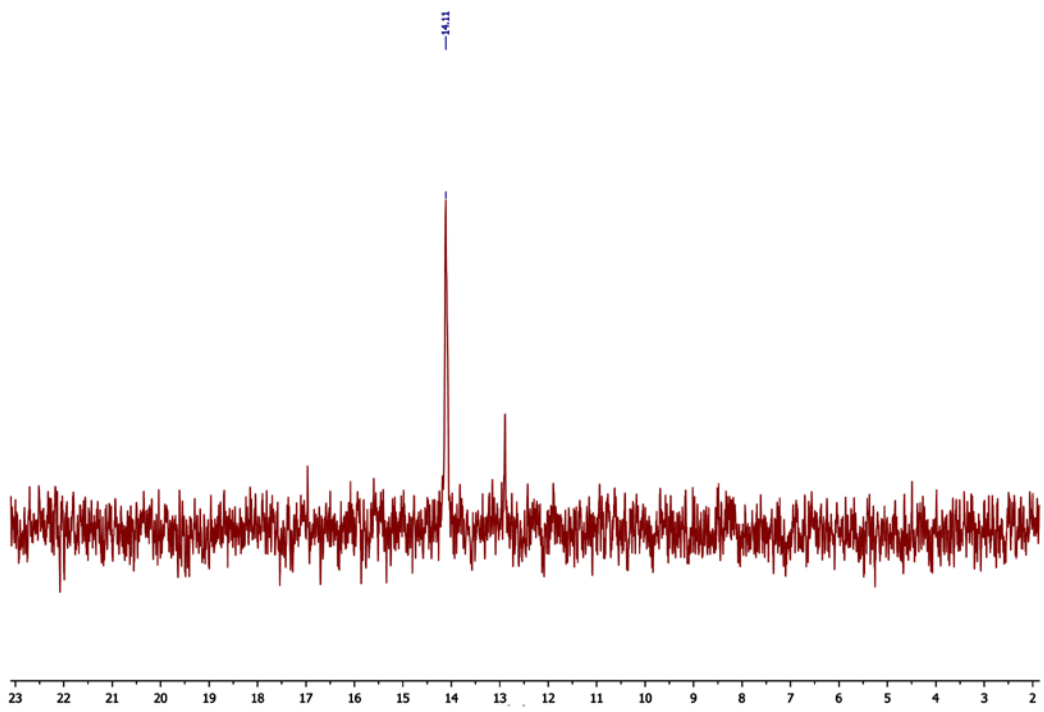


Figure S27. [31]P NMR spectrum of ***Ga-3c*** *($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

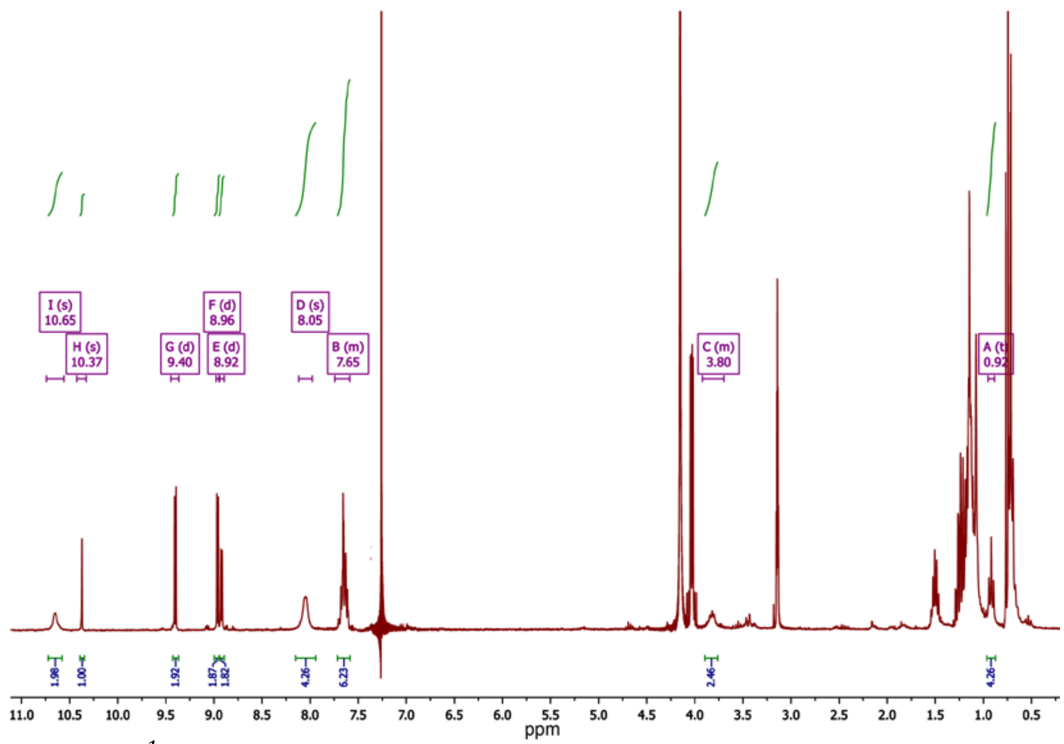


Figure S28. [1]H NMR spectrum of ***In-2a*** *($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

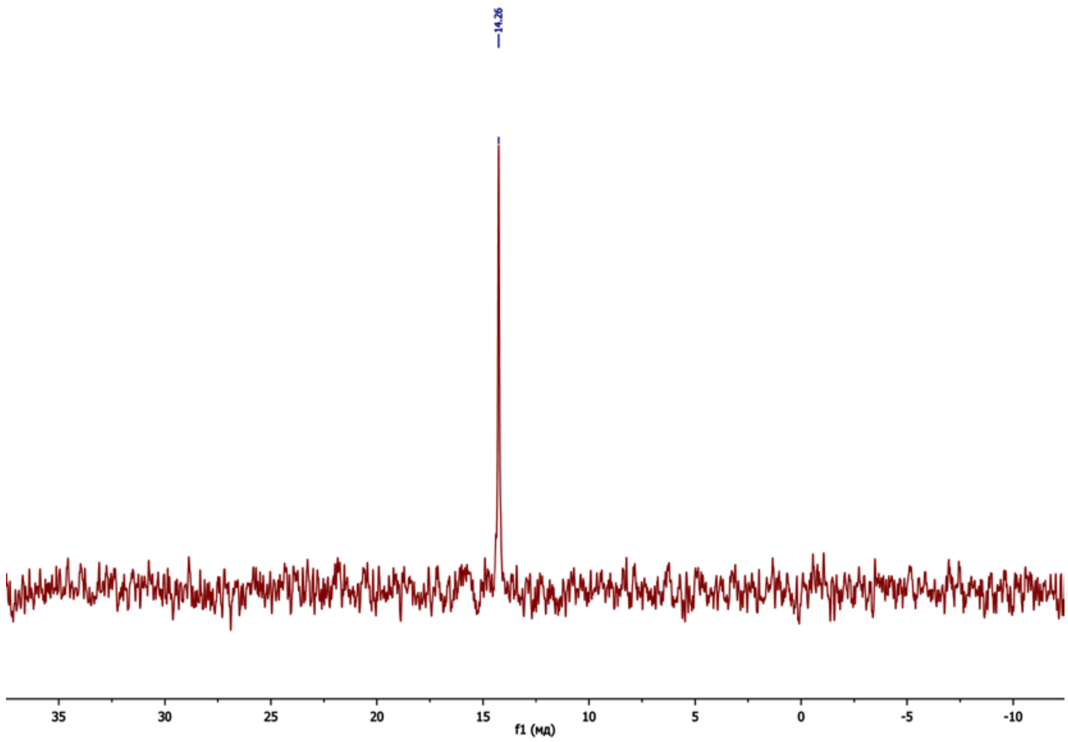


*Figure S29. ^{31}P NMR spectrum of **In-2a** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

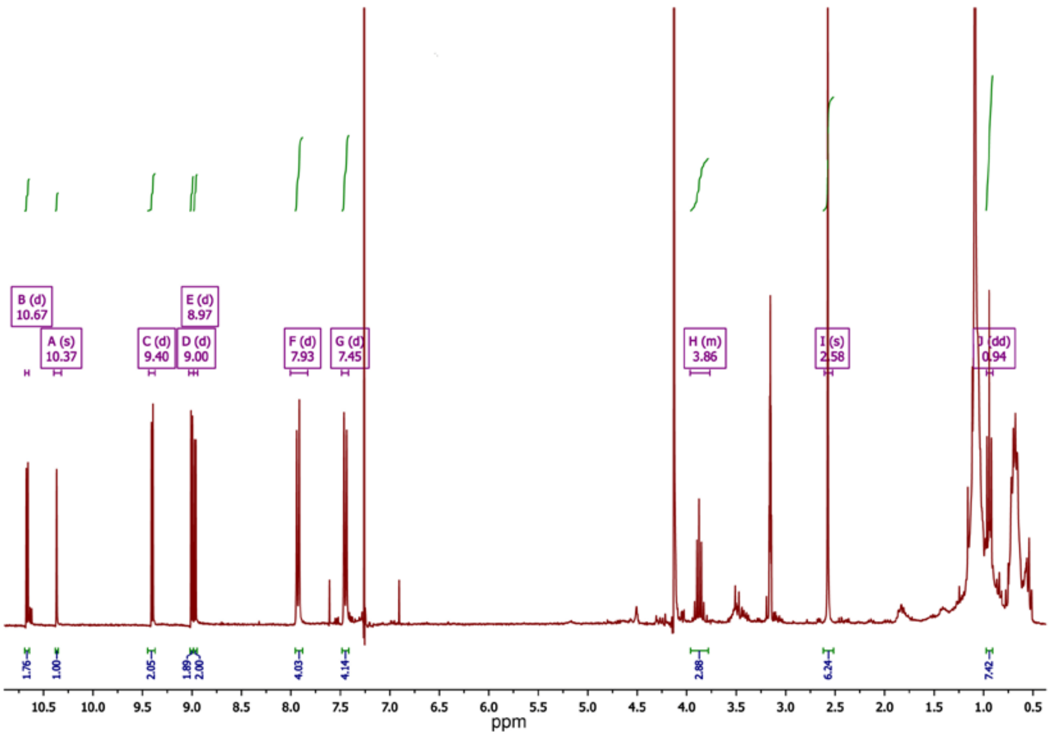


*Figure S30. ^{1}H NMR spectrum of **In-2b** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

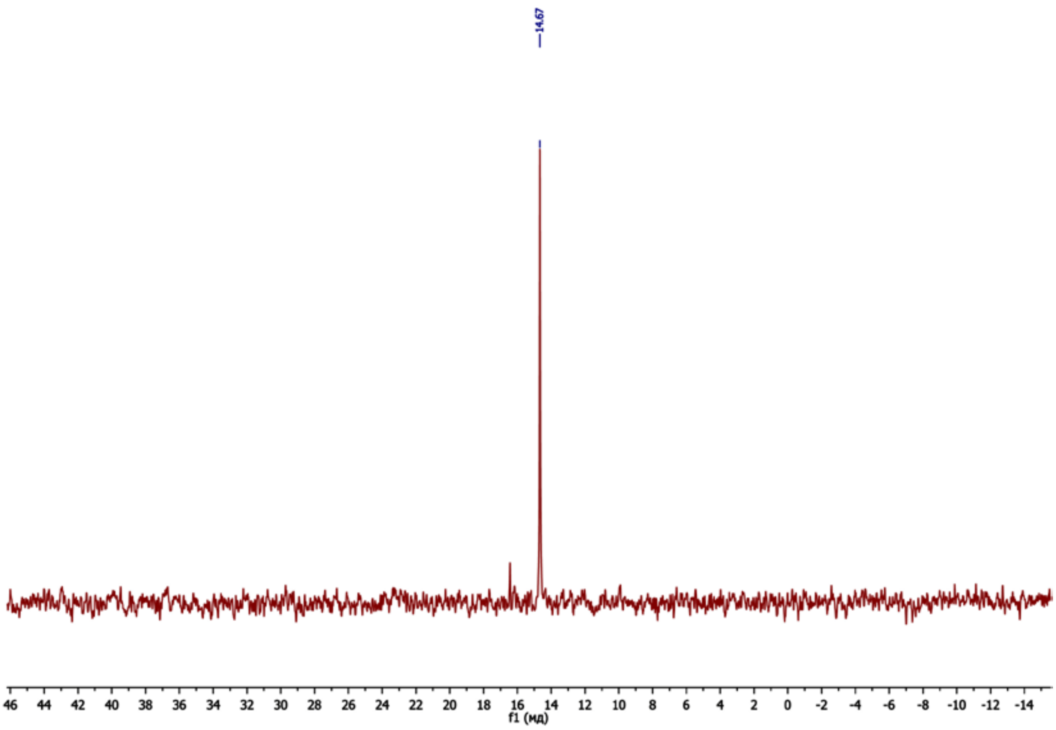


*Figure S31. ^{31}P NMR spectrum of **In-2b** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

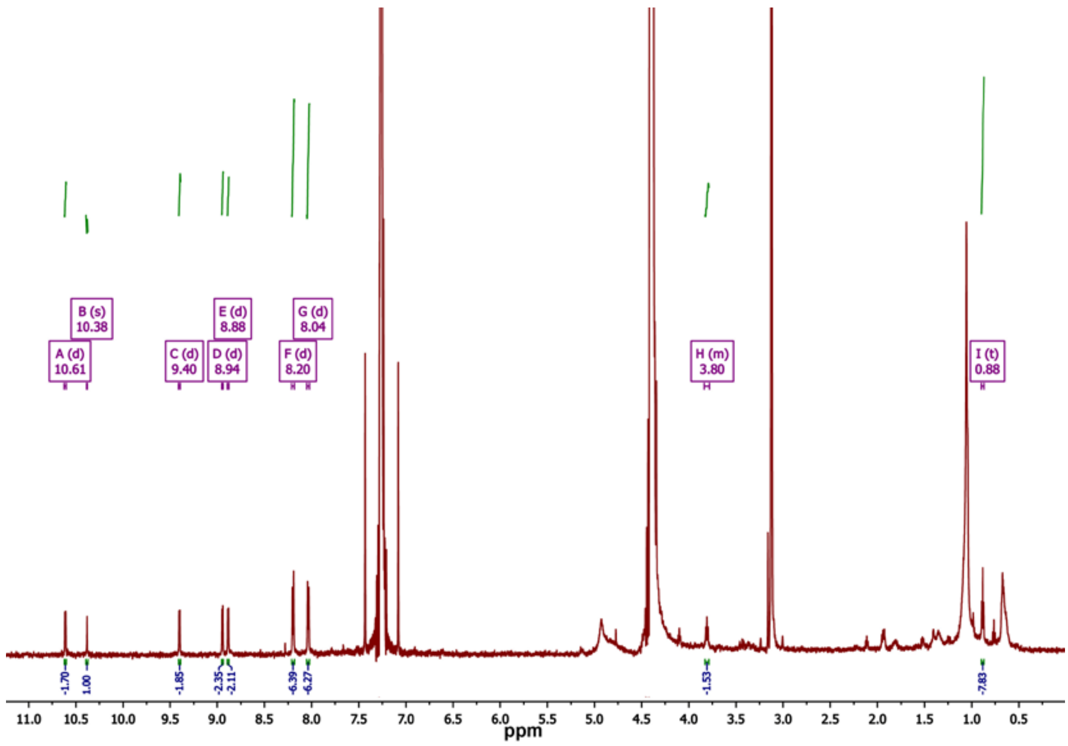


*Figure S32. ^{1}H NMR spectrum of **In-3c** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

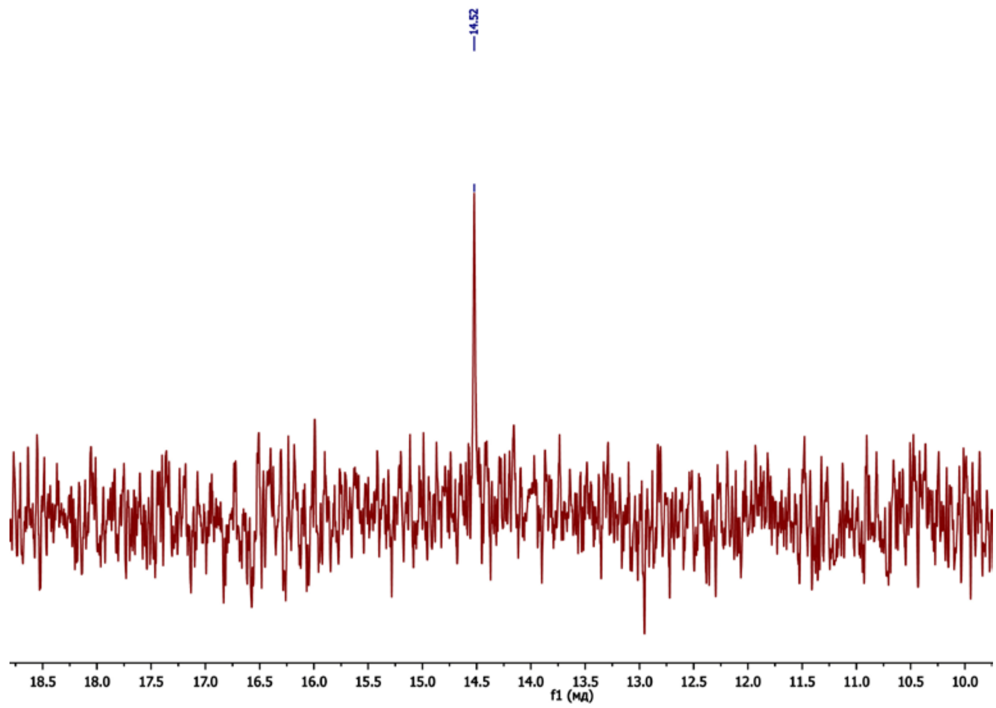


*Figure S33. ^{31}P NMR spectrum of **In-3c** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

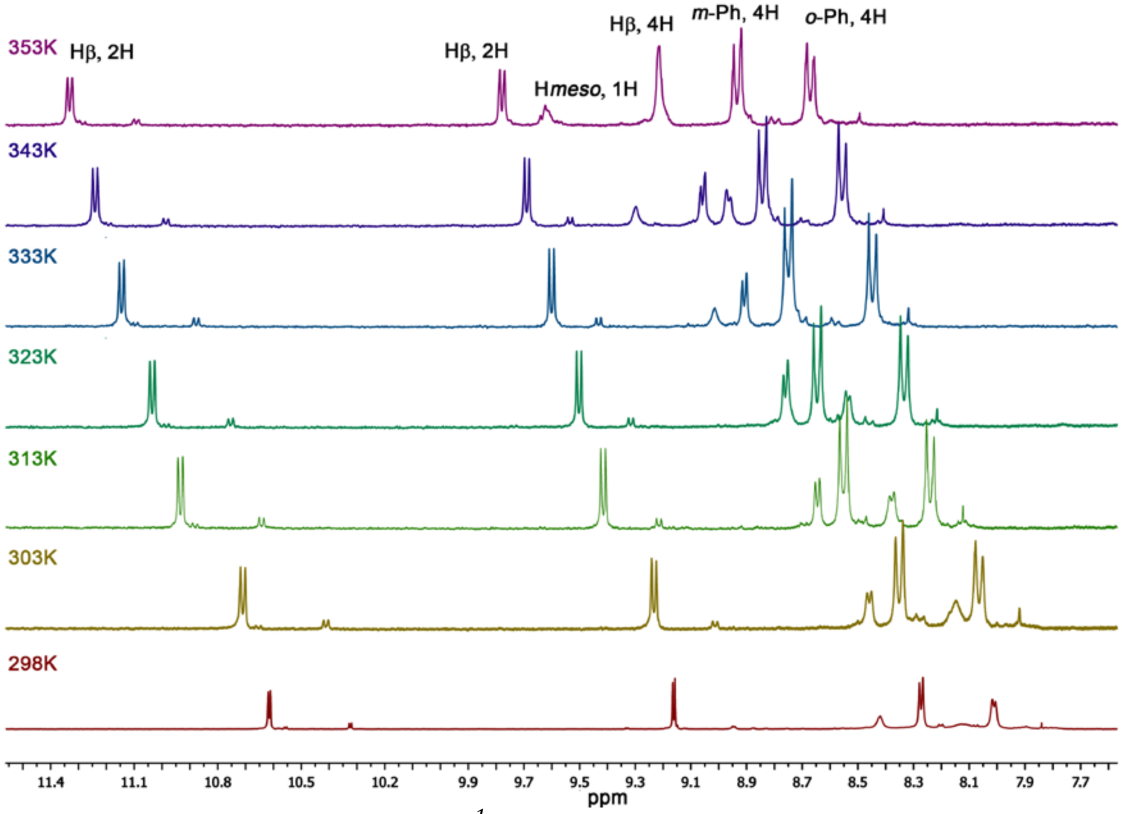


*Figure S34. Variable-temperature ^{1}H NMR spectra of **Ga-3c** (aromatic region) in D_2O in the presence of one drop of saturated solution of NaOH in D_2O.*

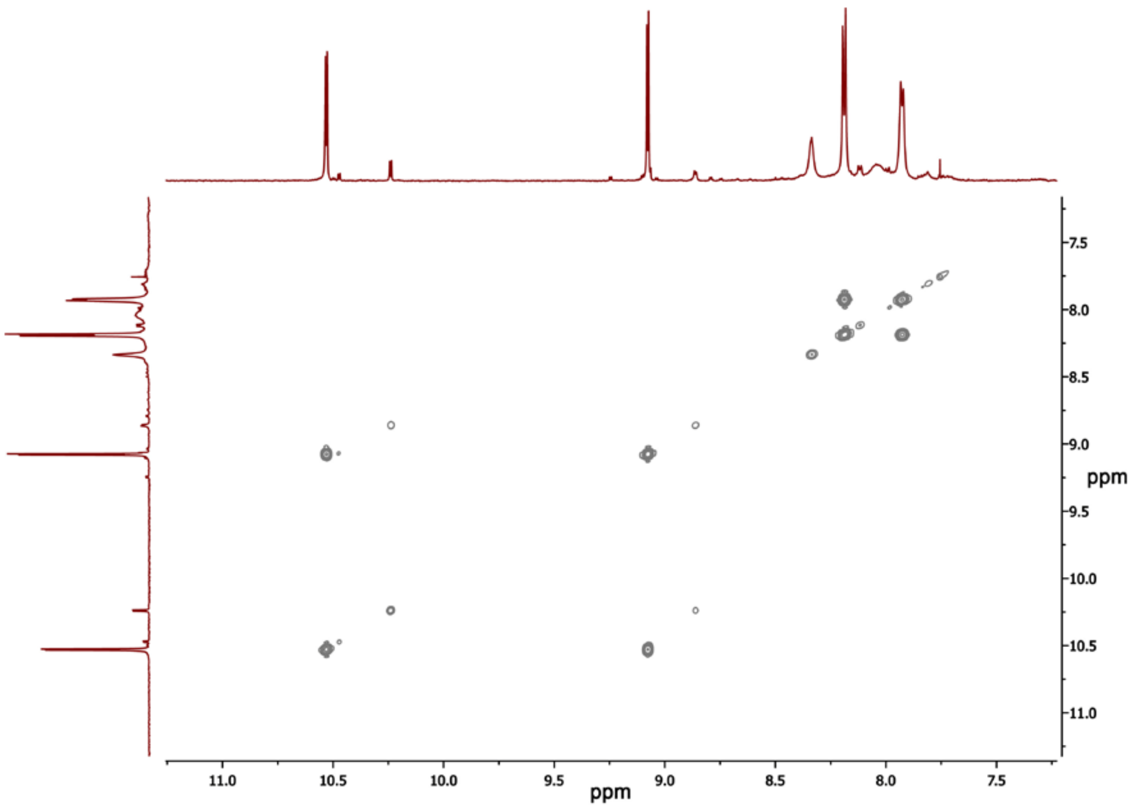


Figure S35. [1]*H,*[1]*H-COSY spectrum of* ***Ga-3c*** *(aromatic region) in* D_2O *in the presence of one drop of saturated solution of NaOH in* D_2O *at 298K.*

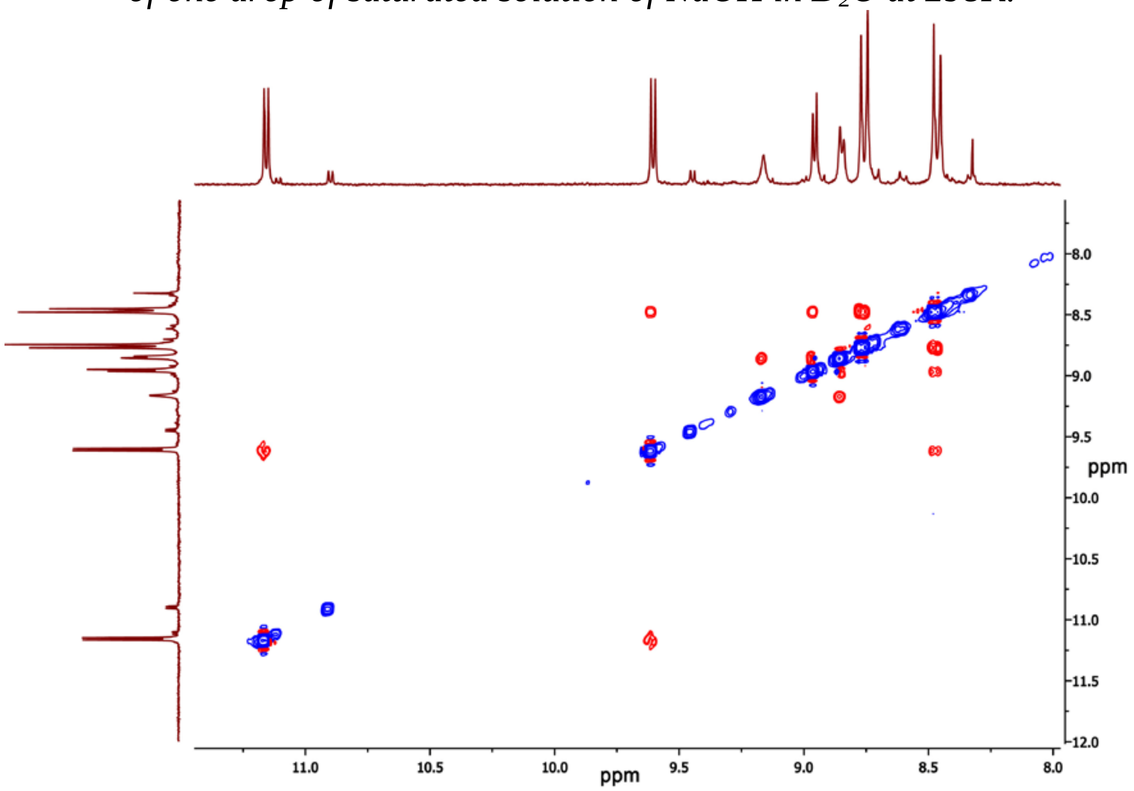


Figure S36 . [1]*H,*[1]*H-NOESY spectrum of* ***Ga-3c*** *(aromatic region) in* D_2O *in the presence of one drop of saturated solution of NaOH in* D_2O *at 353K.*

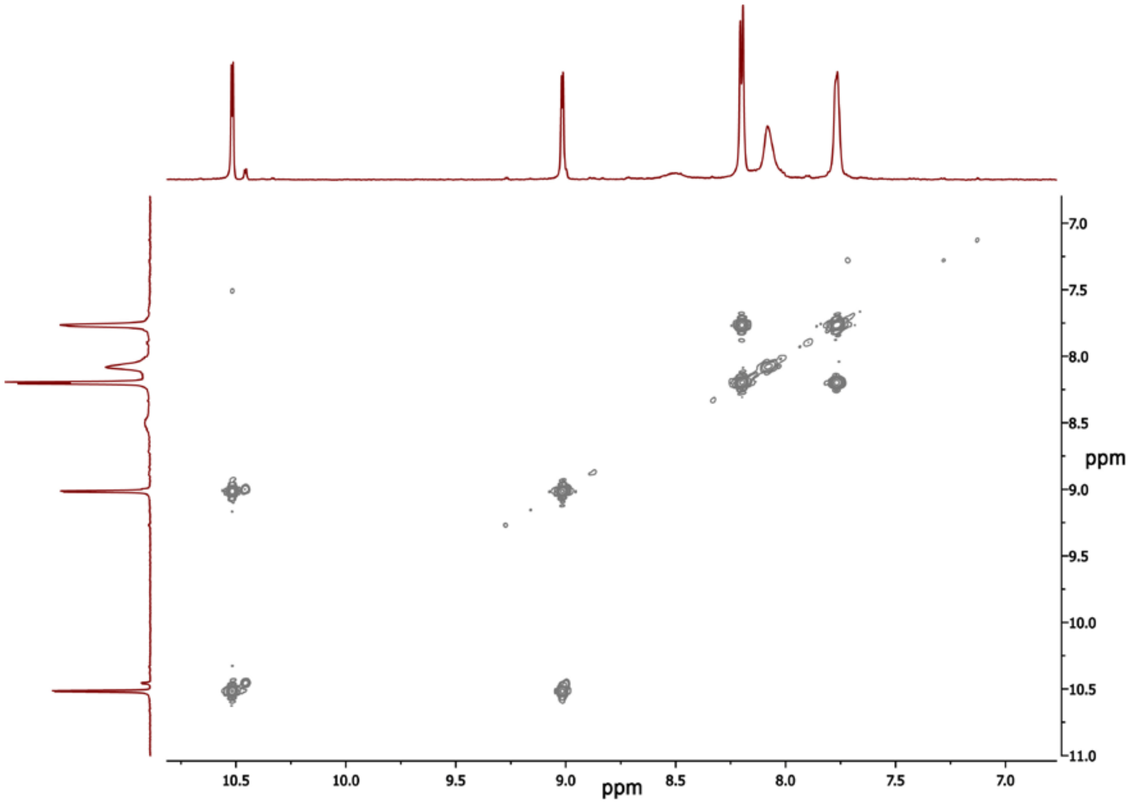


Figure S37. [1]*H,*[1]*H-COSY spectrum of* ***In-3c*** *(aromatic region) in* D_2O *in the presence of one drop of saturated solution of NaOH in* D_2O *at 298 K.*

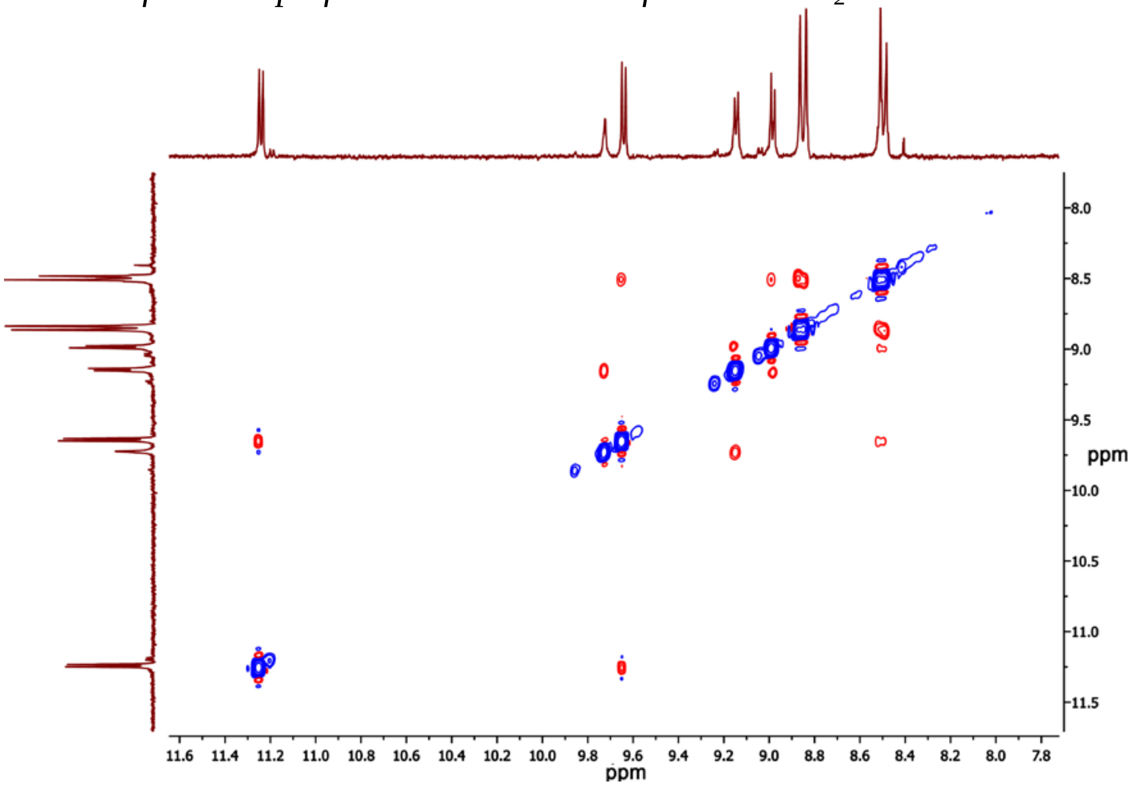


Figure S38. [1]*H,*[1]*H-NOESY spectrum of* ***In-3c*** *(aromatic region) in* D_2O *in the presence of one drop of saturated solution of NaOH in* D_2O *at 363K.*

4. NMR spectra of monoesters of *meso*-porphyrinyl phosphonic acids (2H-2a,b,3c)

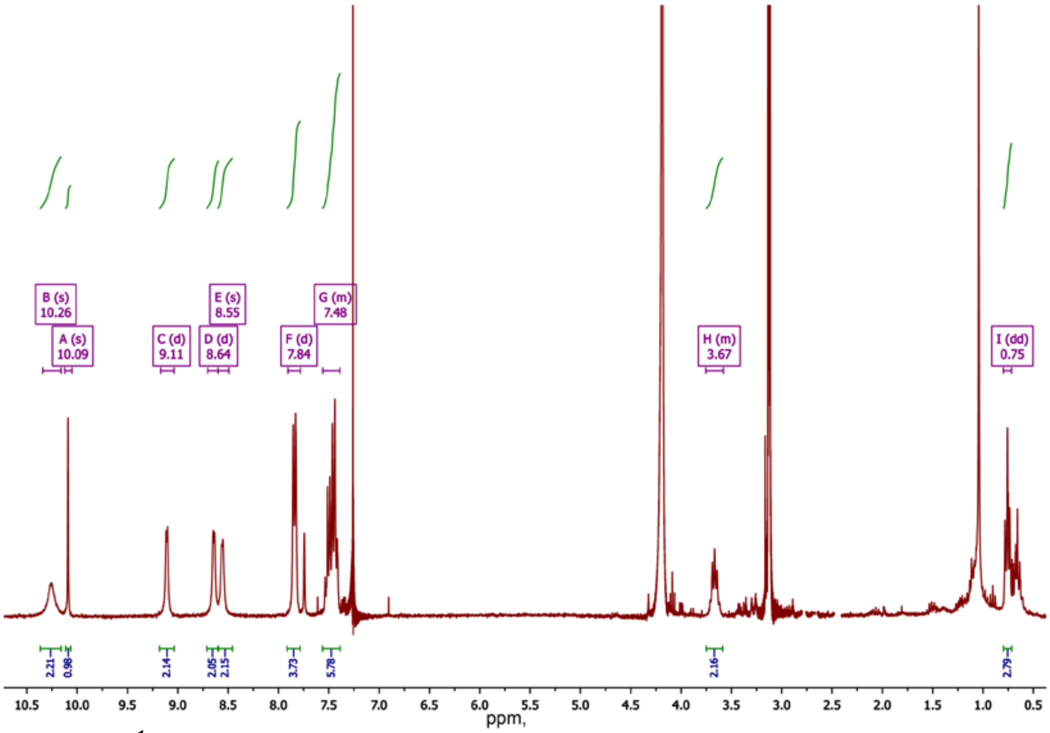


Figure S39. ^{1}*H NMR spectrum of* ***2H-2a*** *(CDCl*$_3$*:CD*$_3$*OD (2:1 v/v)+1 drop of saturated solution of NaOH in D*$_2$*O).*

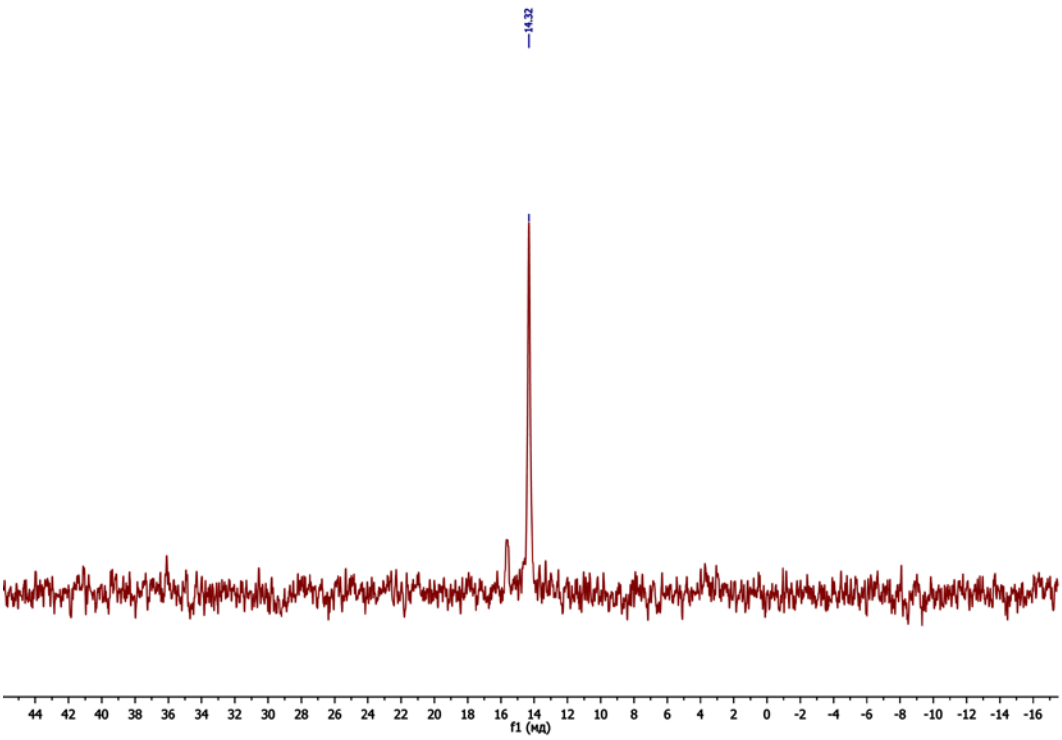


Figure S40. ^{31}*P NMR spectrum of* ***2H-2a*** *(CDCl*$_3$*:CD*$_3$*OD (2:1 v/v)+1 drop of saturated solution of NaOH in D*$_2$*O).*

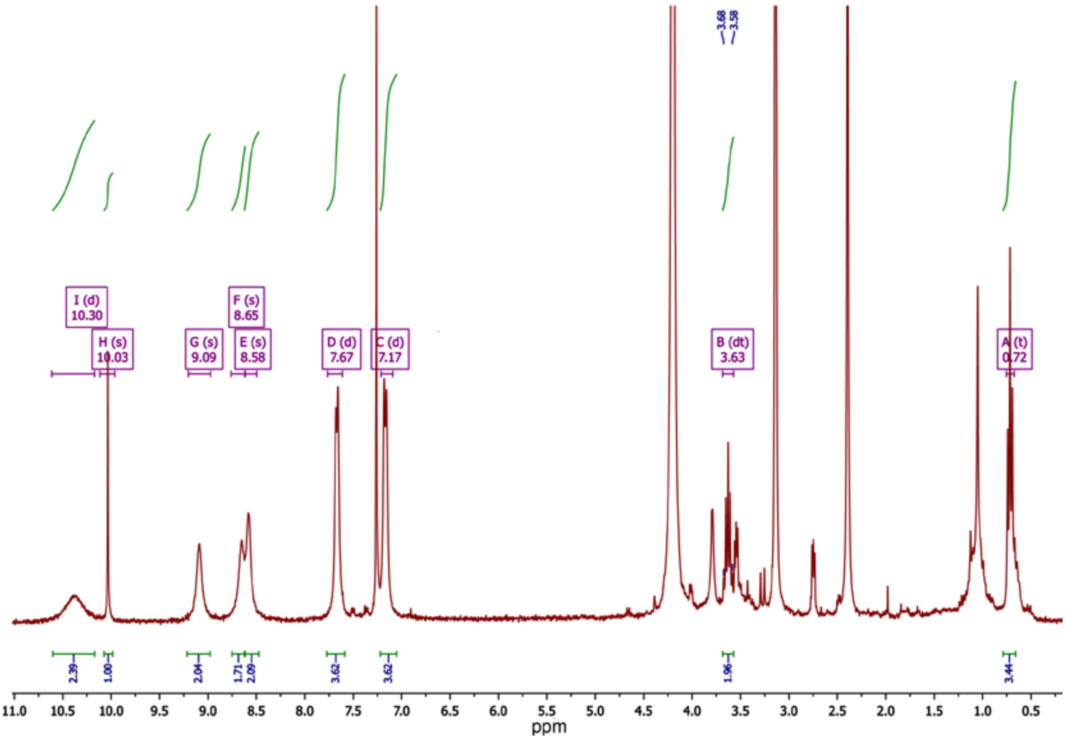


Figure S41. [1]H NMR spectrum of ***2H-2b*** *($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

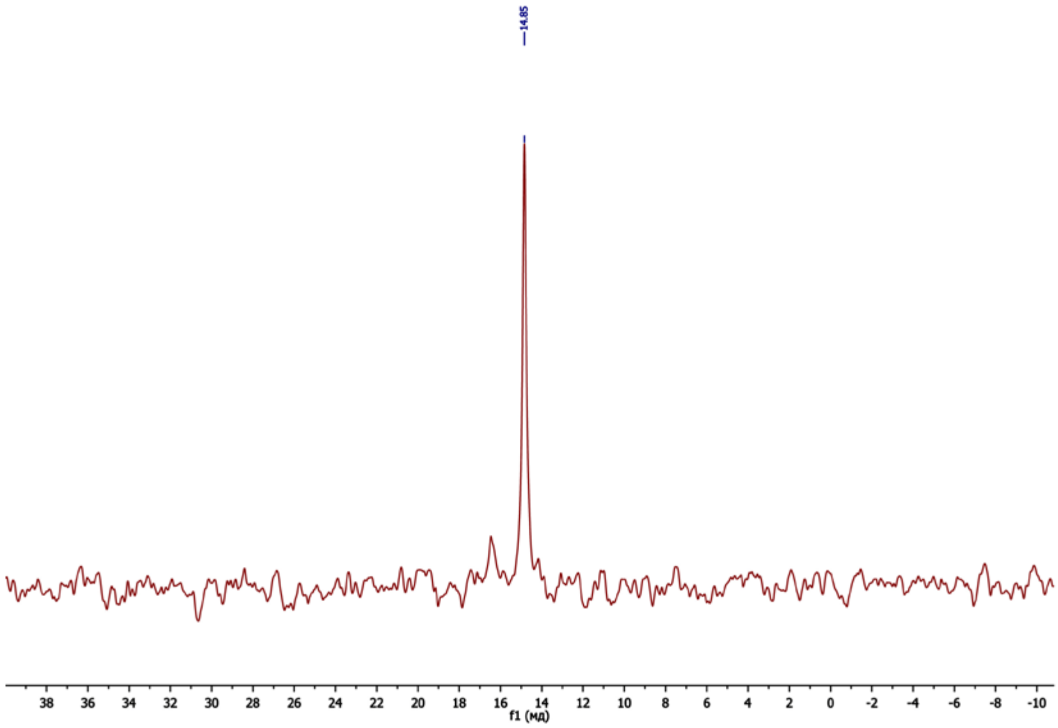


Figure S42. [31]P NMR spectrum of ***2H-2b*** *($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

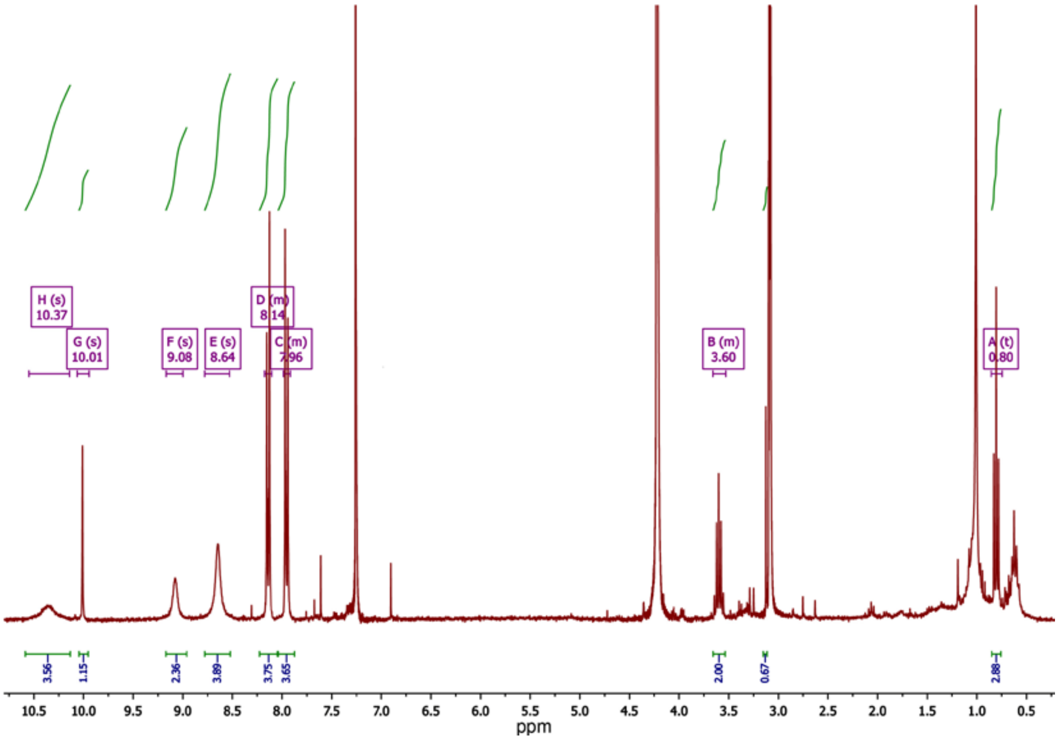


Figure S43. [1]*H NMR spectrum of* ***2H-3c*** *($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

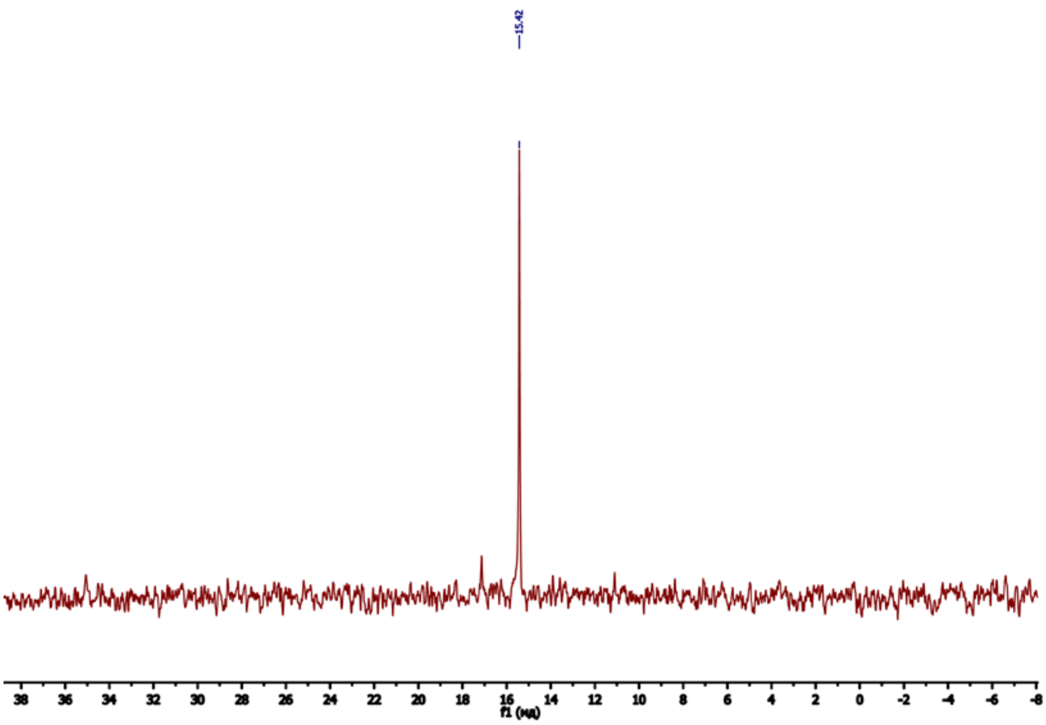


Figure S44. [31]*P NMR spectrum of* ***2H-3c*** *($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

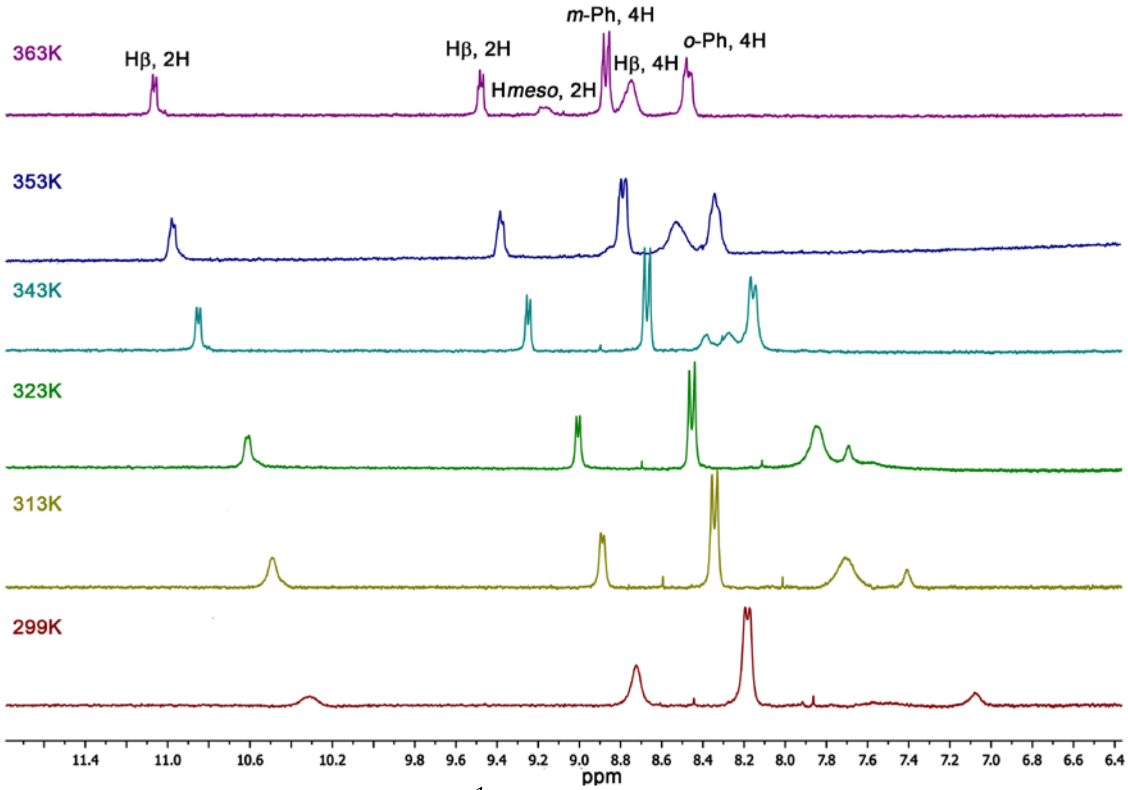


Figure S45. Variable-temperature [1]H NMR spectra of ***2H-3c*** *(aromatic region) in D_2O in the presence of one drop of saturated solution of NaOH in D_2O.*

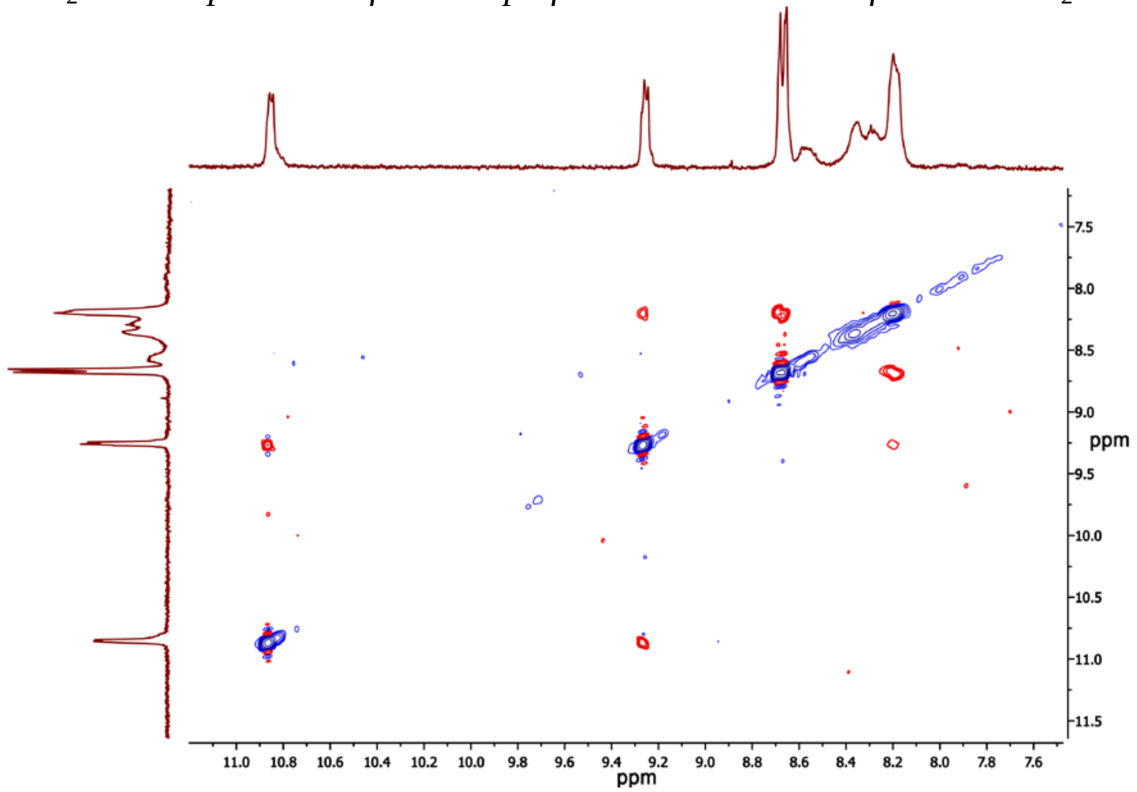


Figure S46. [1]H,[1]H-NOESY spectrum of ***2H-3c*** *(aromatic region) in D_2O in the presence of one drop of saturated solution of NaOH in D_2O at 348K.*

5. NMR spectra of gallium(III) and indium(III) complexes with *meso*-porphyrinyl phosphonic acids (Ga-4a-c and In-4a-c)

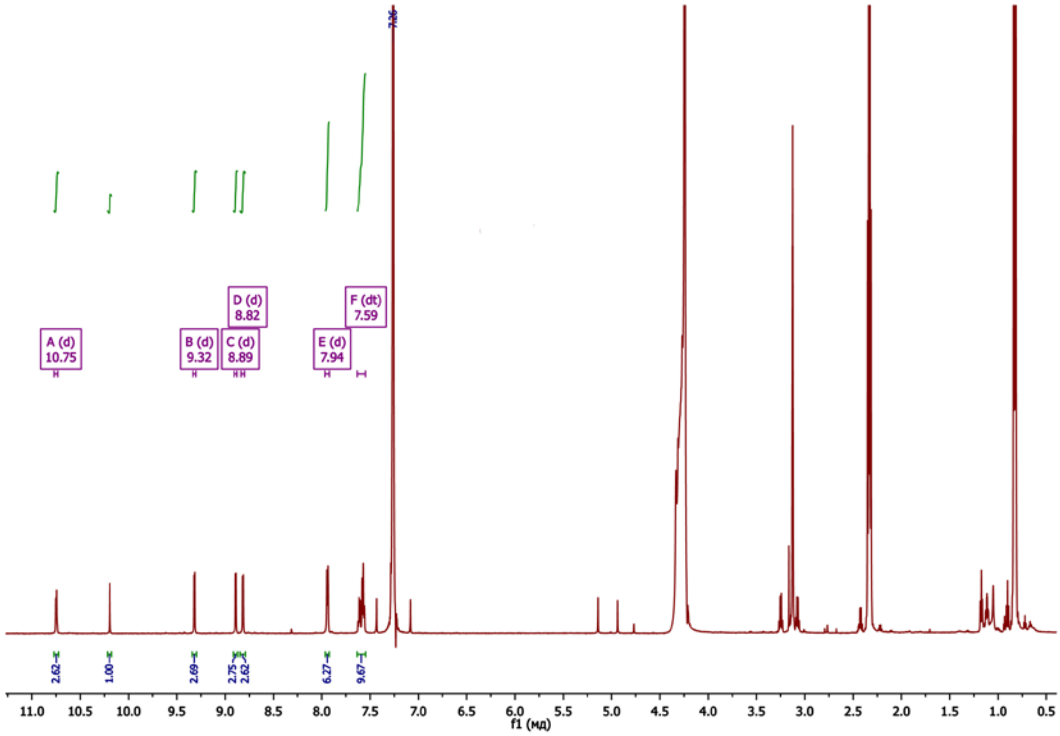


*Figure S47. ^{1}H NMR spectrum of **Ga-4a** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

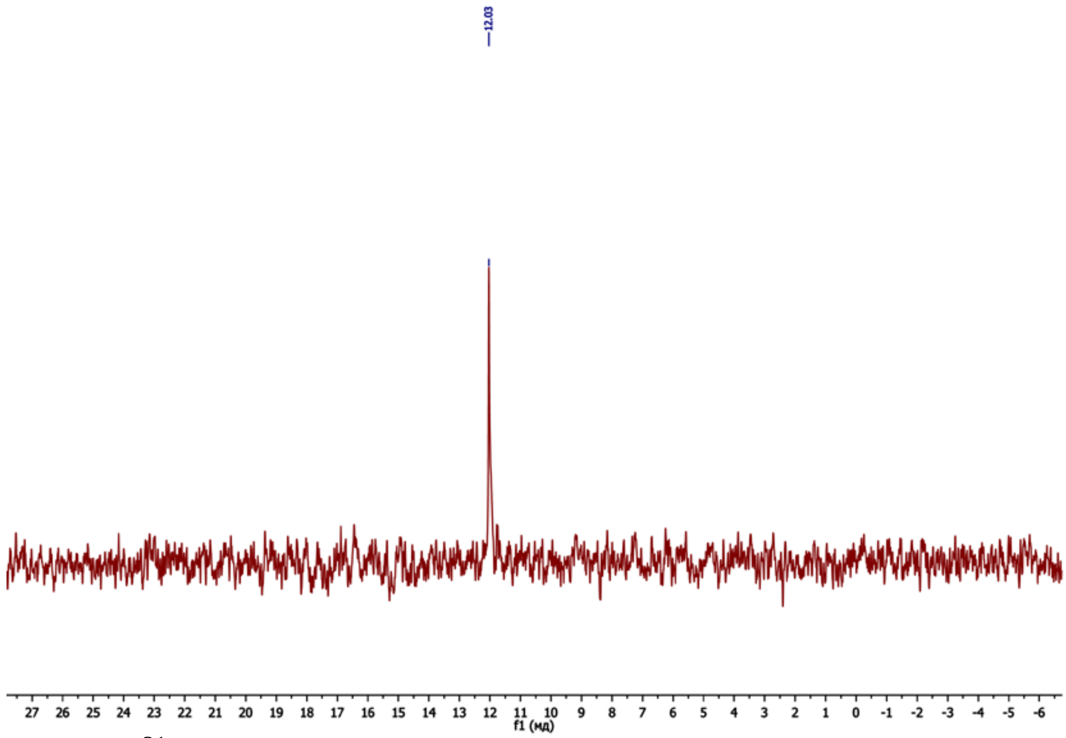


*Figure S48. ^{31}P NMR spectrum of **Ga-4a** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

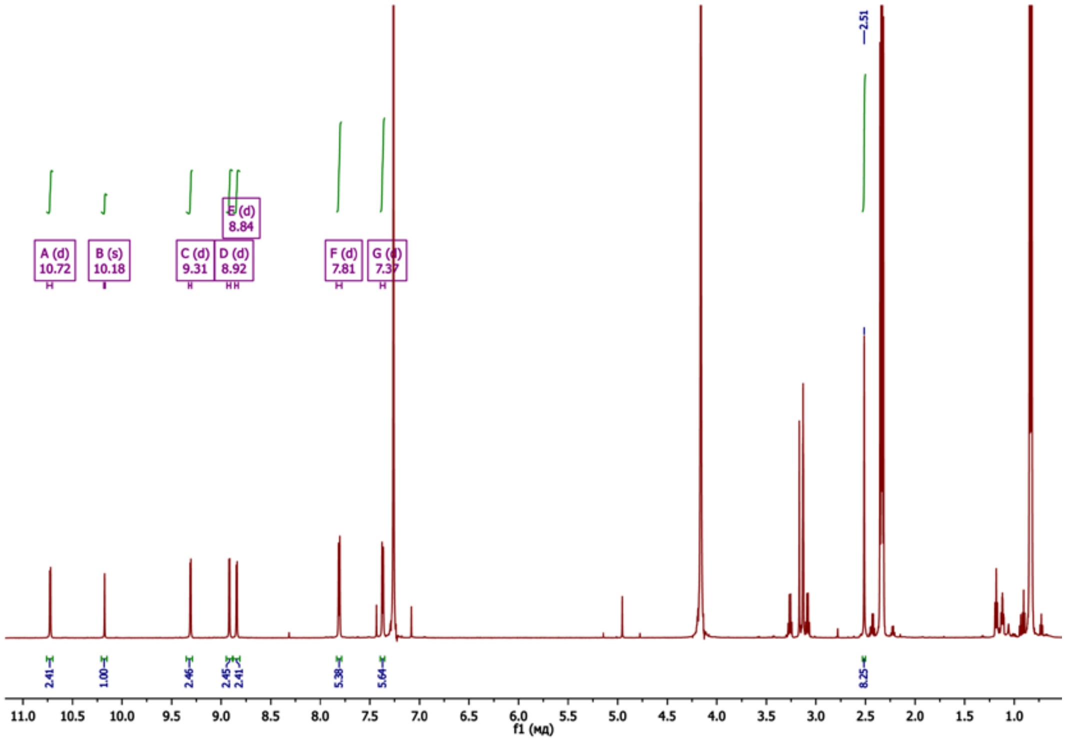


Figure S49. ^{1}H NMR spectrum of **Ga-4b** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).

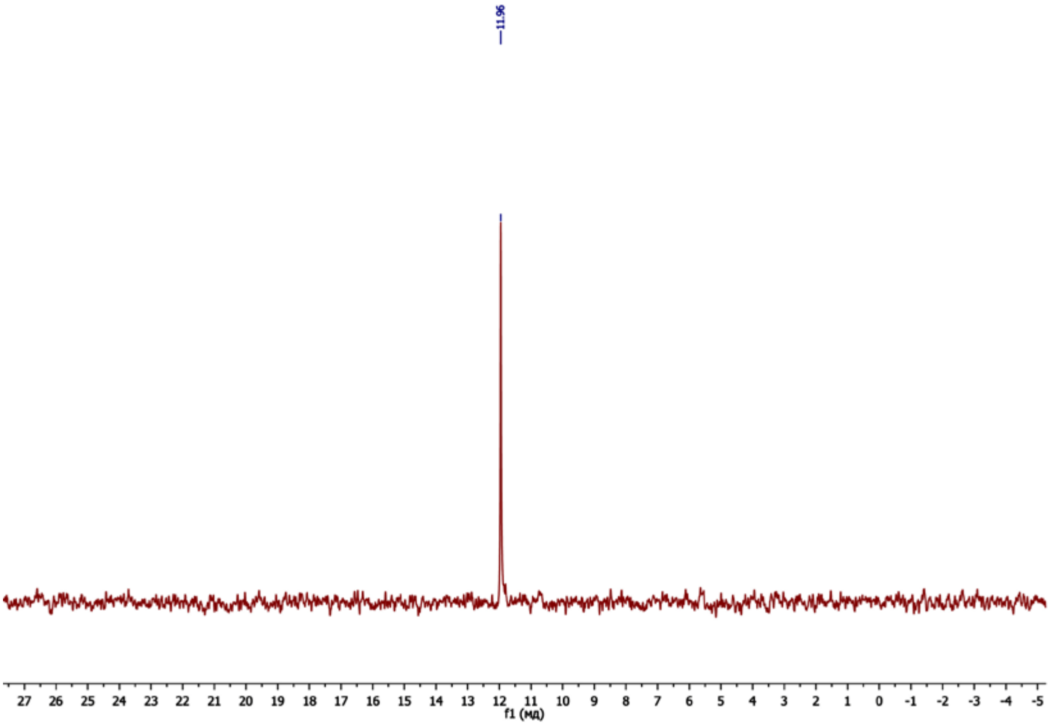


Figure S50. ^{31}P NMR spectrum of **Ga-4b** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).

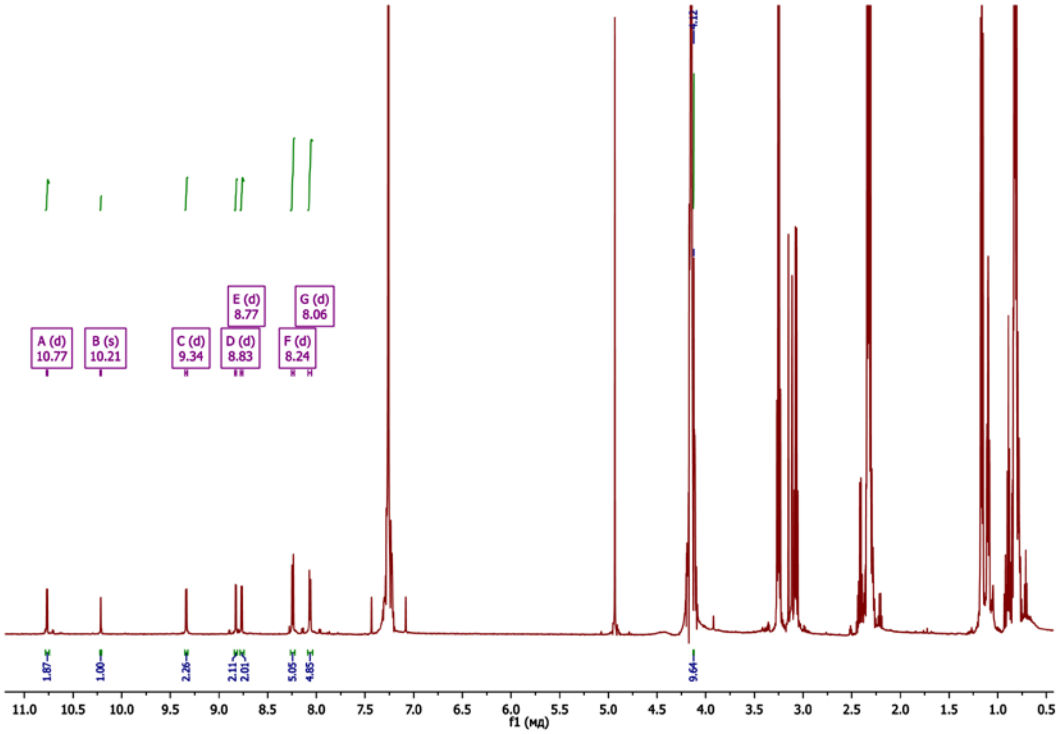


*Figure S51. ¹H NMR spectrum of **Ga-4c** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

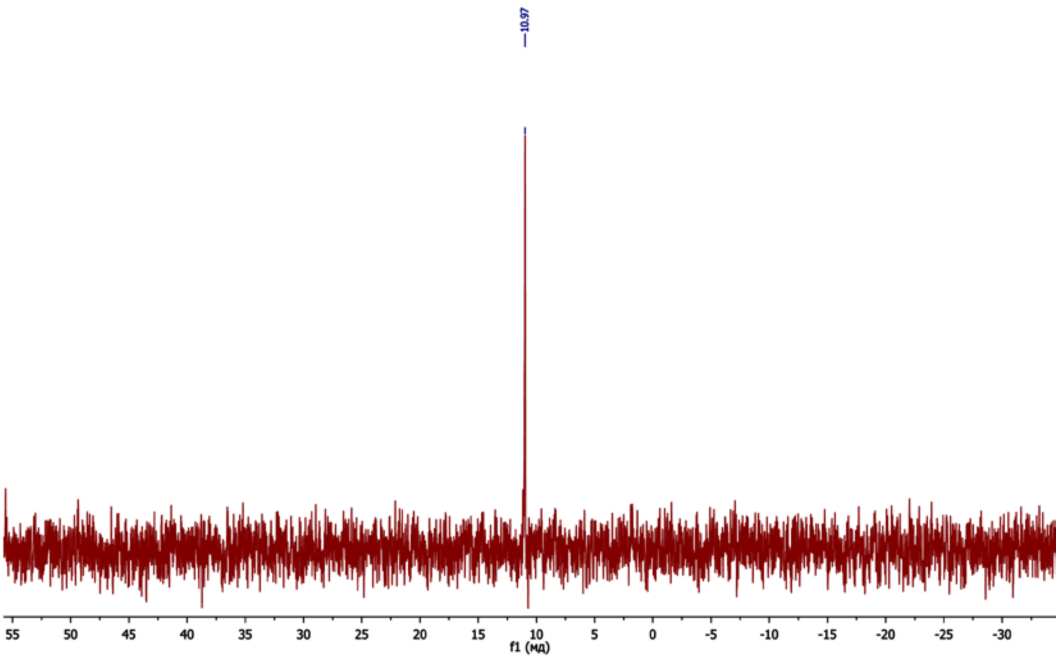


*Figure S52. ³¹P NMR spectrum of **Ga-4c** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

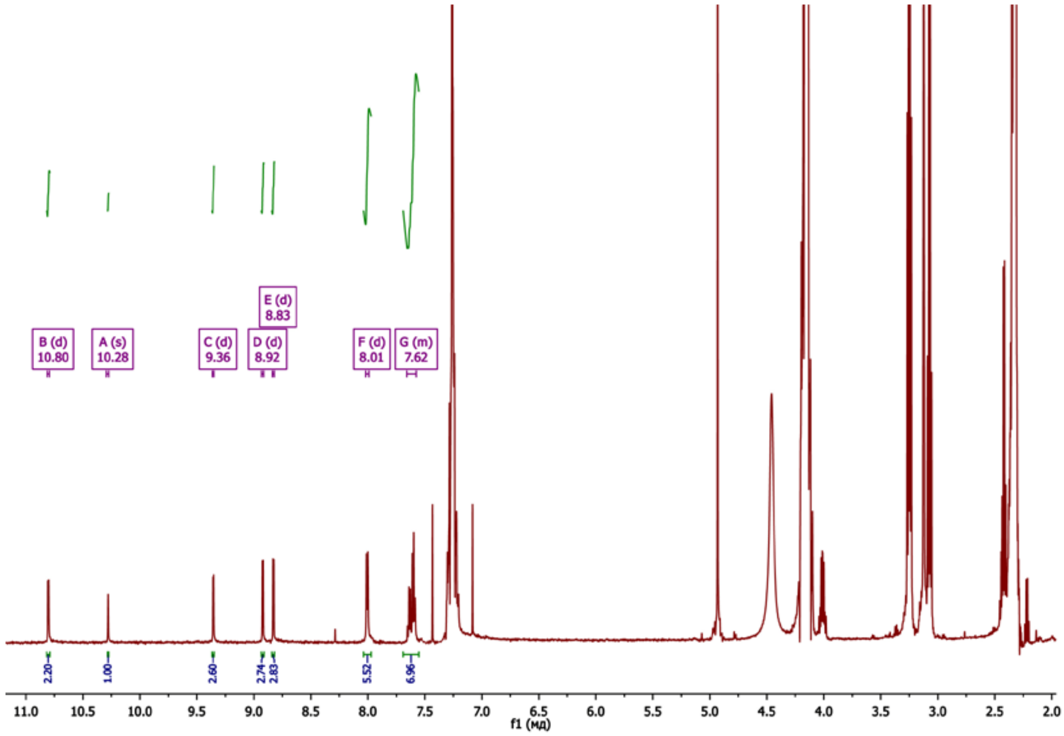


*Figure S53. ^{1}H NMR spectrum of **In-4a** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

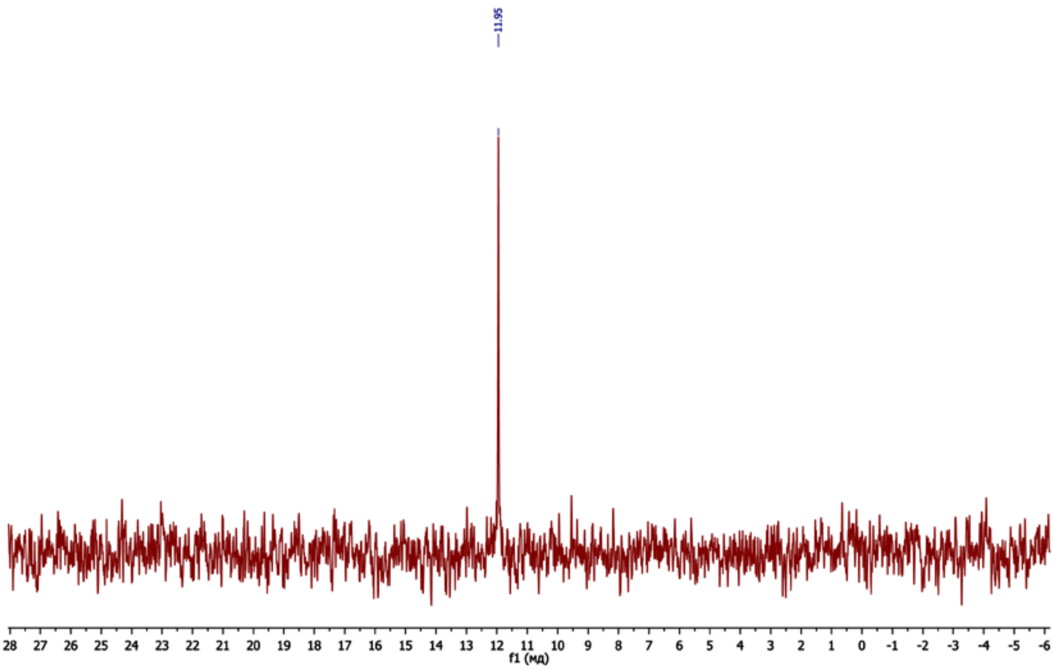


*Figure S54. ^{31}P NMR spectrum of **In-4a** ($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

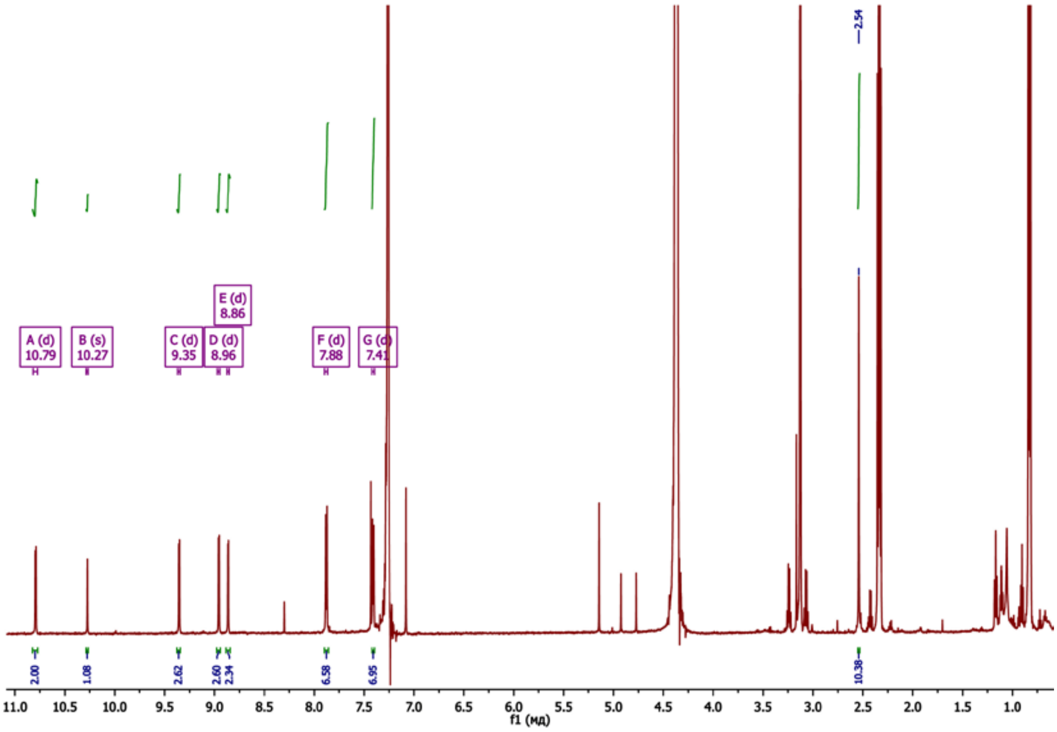


Figure S55. ^{1}H *NMR spectrum of* ***In-4b*** *($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

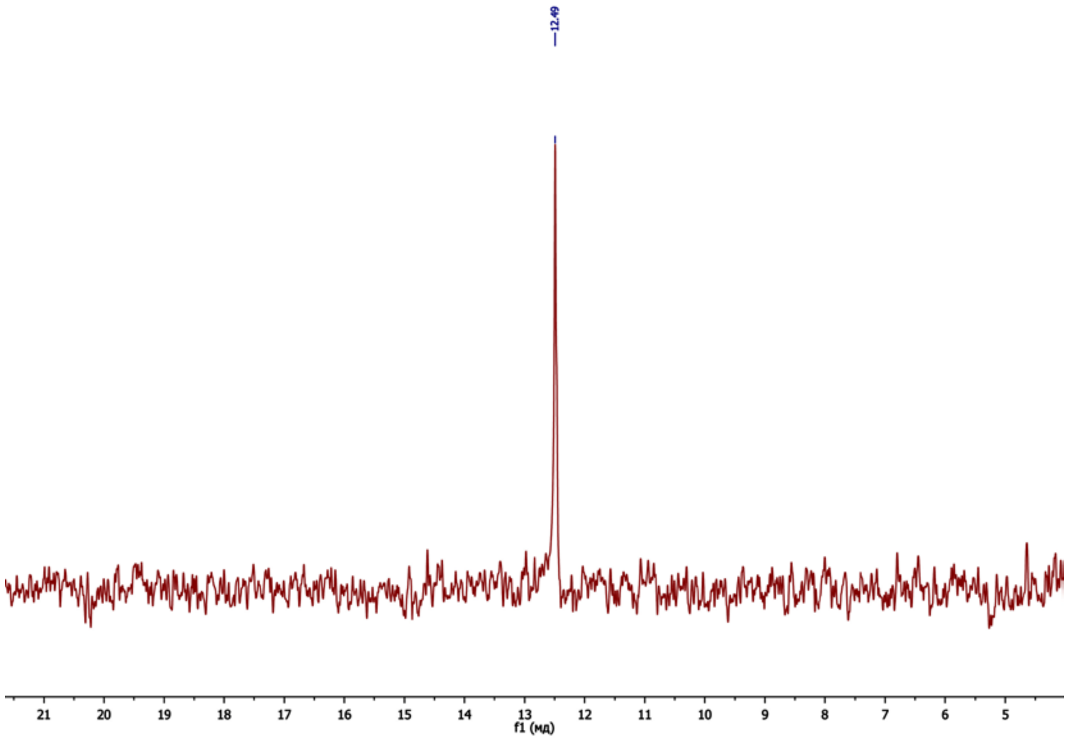


Figure S56. ^{31}P *NMR spectrum of* ***In-4b*** *($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

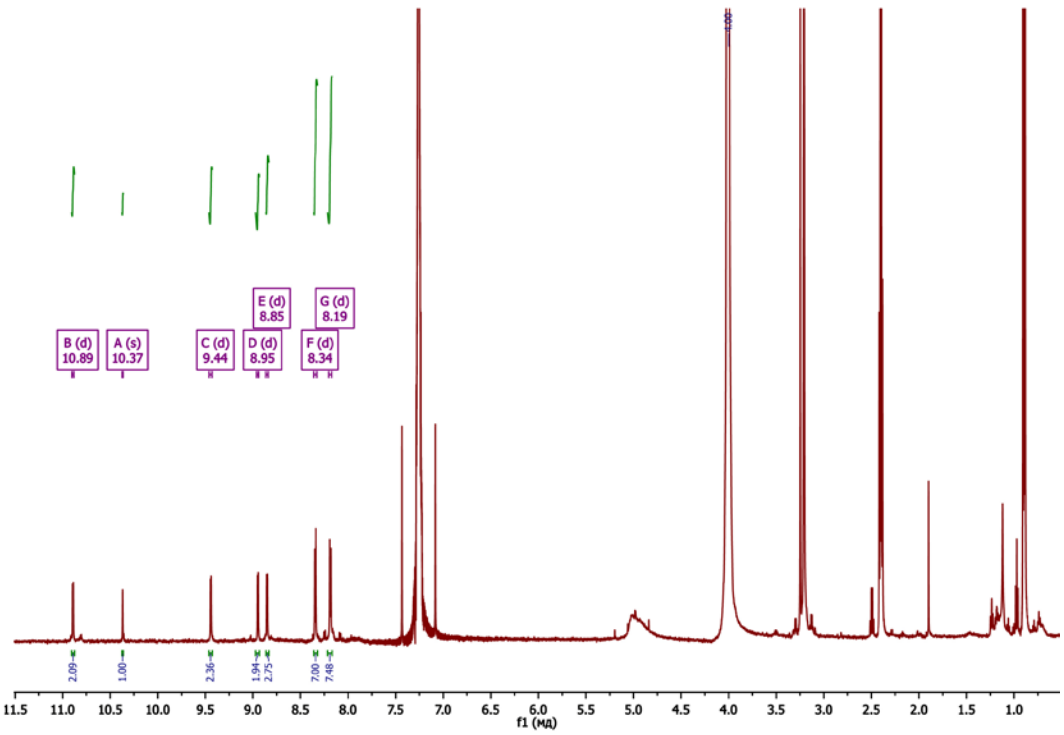


Figure S57. ^{1}*H NMR spectrum of* ***In-4c*** *($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

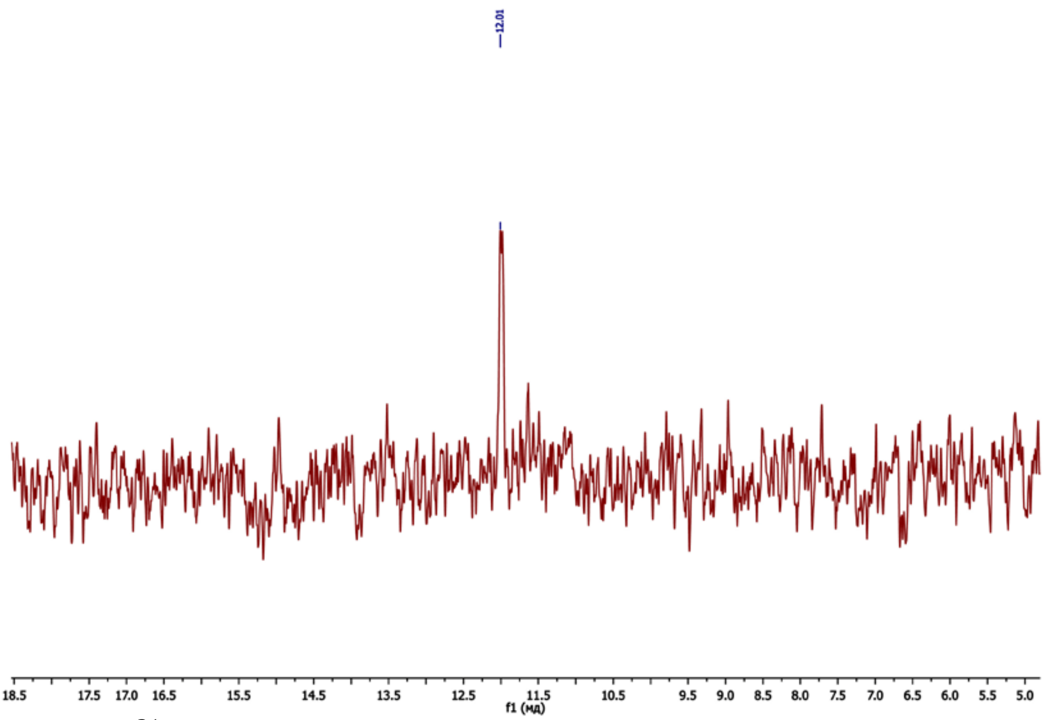


Figure S58. ^{31}*P NMR spectrum of* ***In-4c*** *($CDCl_3$:CD_3OD (2:1 v/v)+1 drop of saturated solution of NaOH in D_2O).*

6. MALDI TOF mass spectra of compounds Ga-1a-c, In-1a-c, Ga-4a-c and In-4a-c

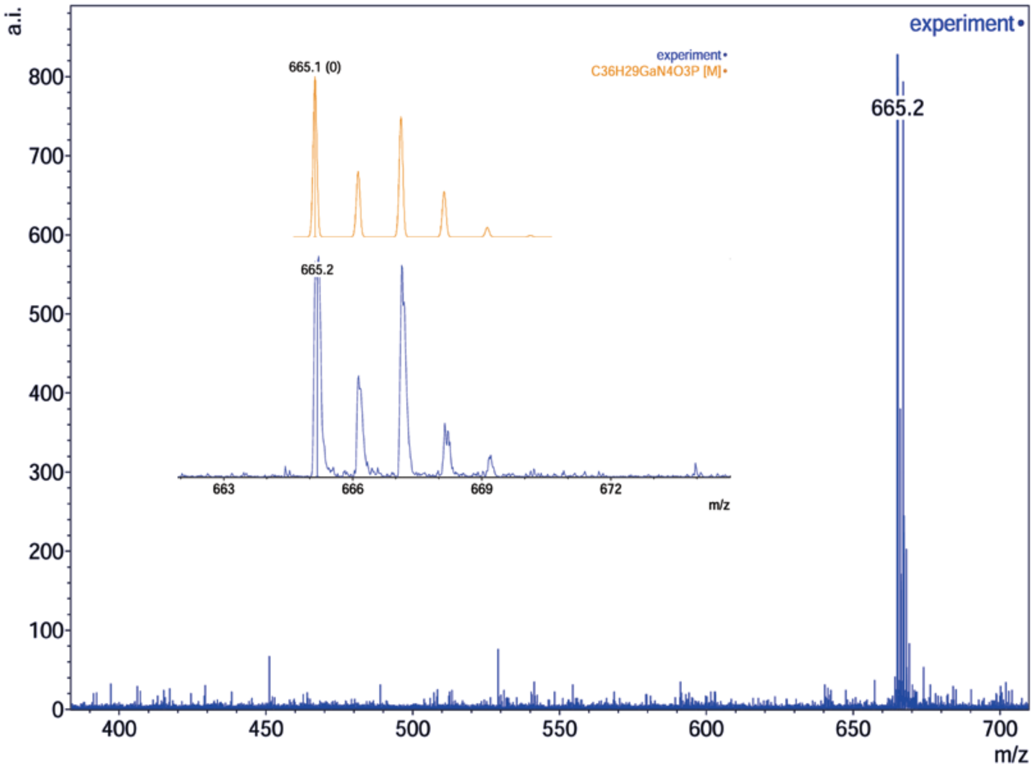


Figure S59. MALDI TOF mass spectrum of ***Ga-1a****.*

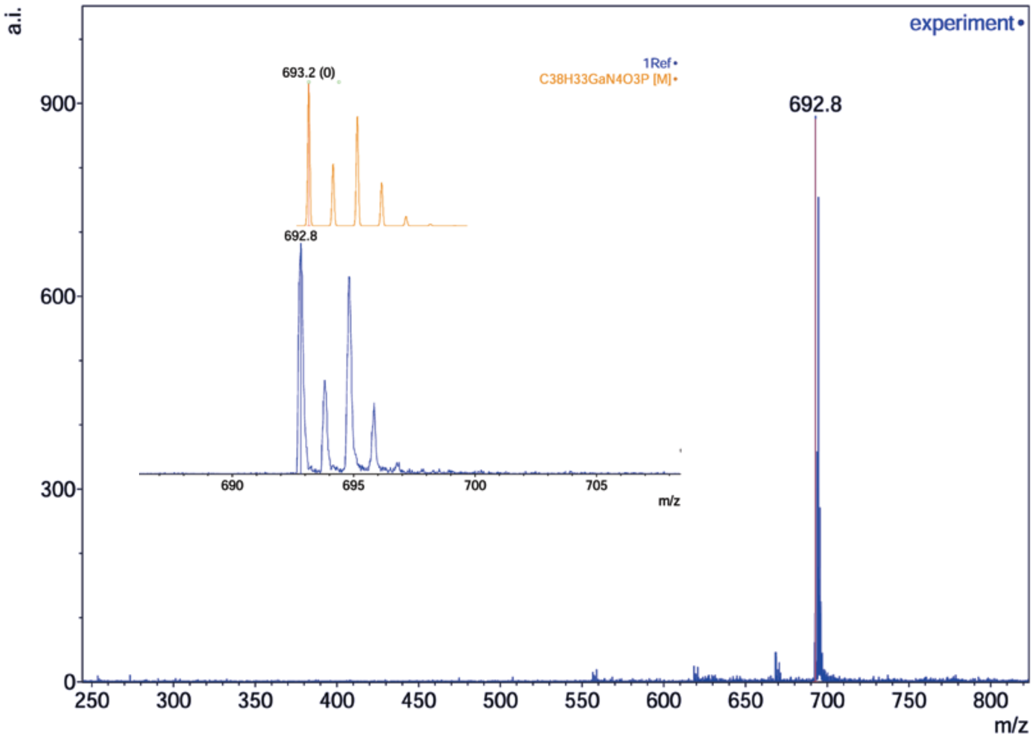


Figure S60. MALDI TOF mass spectrum of ***Ga-1b****.*

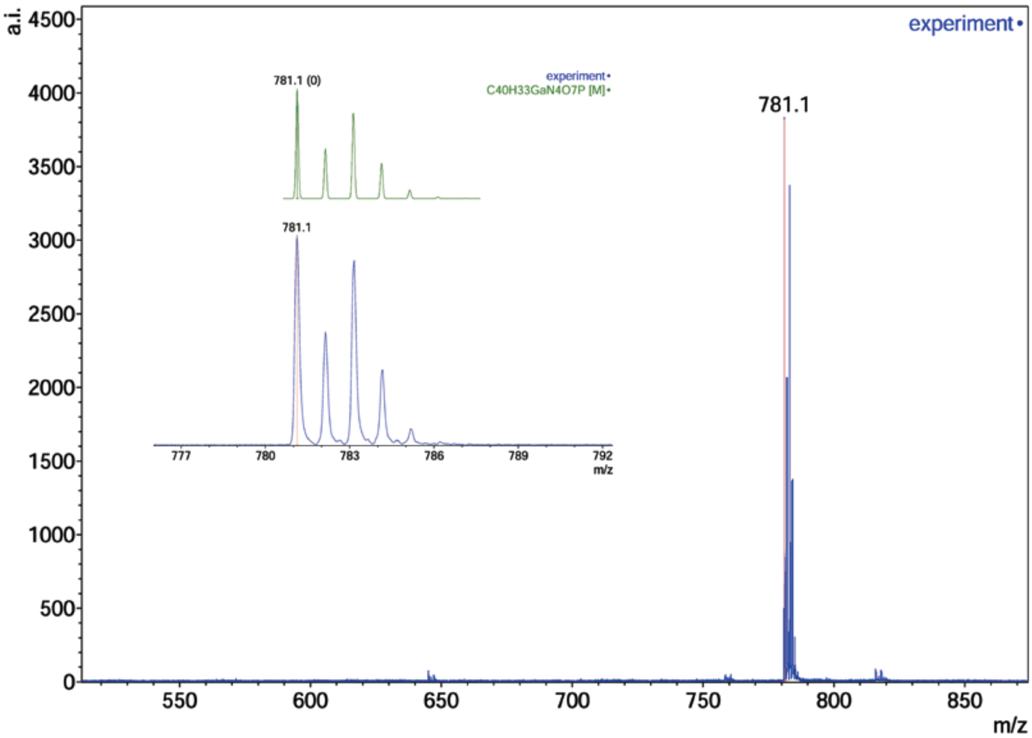


*Figure S61. MALDI TOF mass spectrum of **Ga-1c**.*

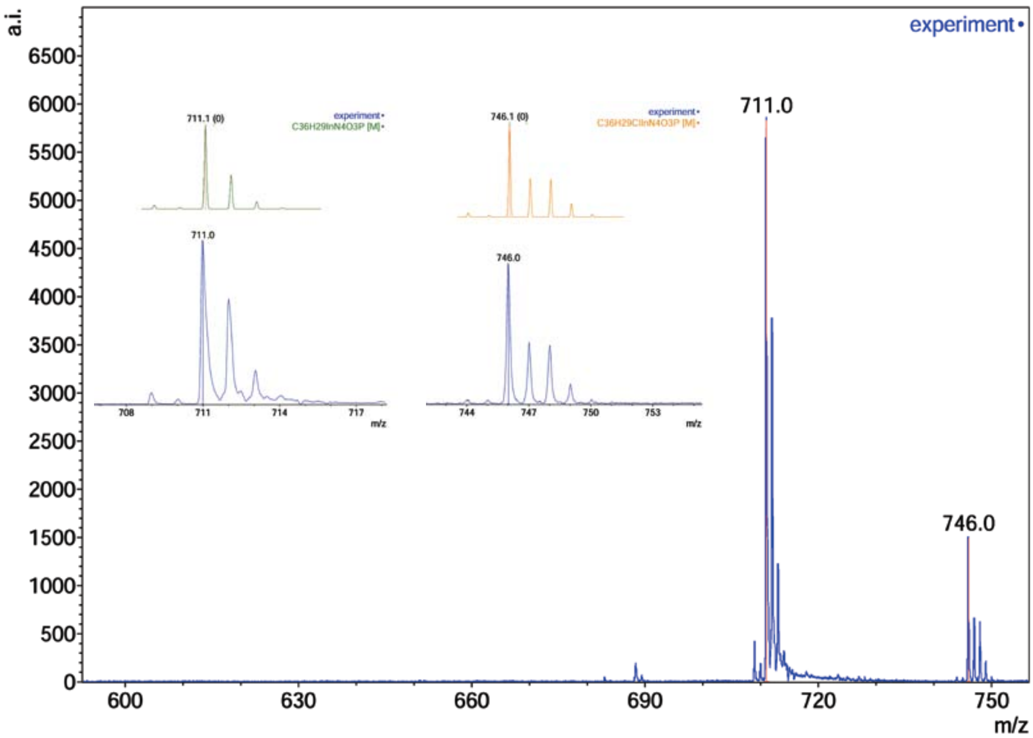


*Figure S62. MALDI TOF mass spectrum of **In-1a**.*

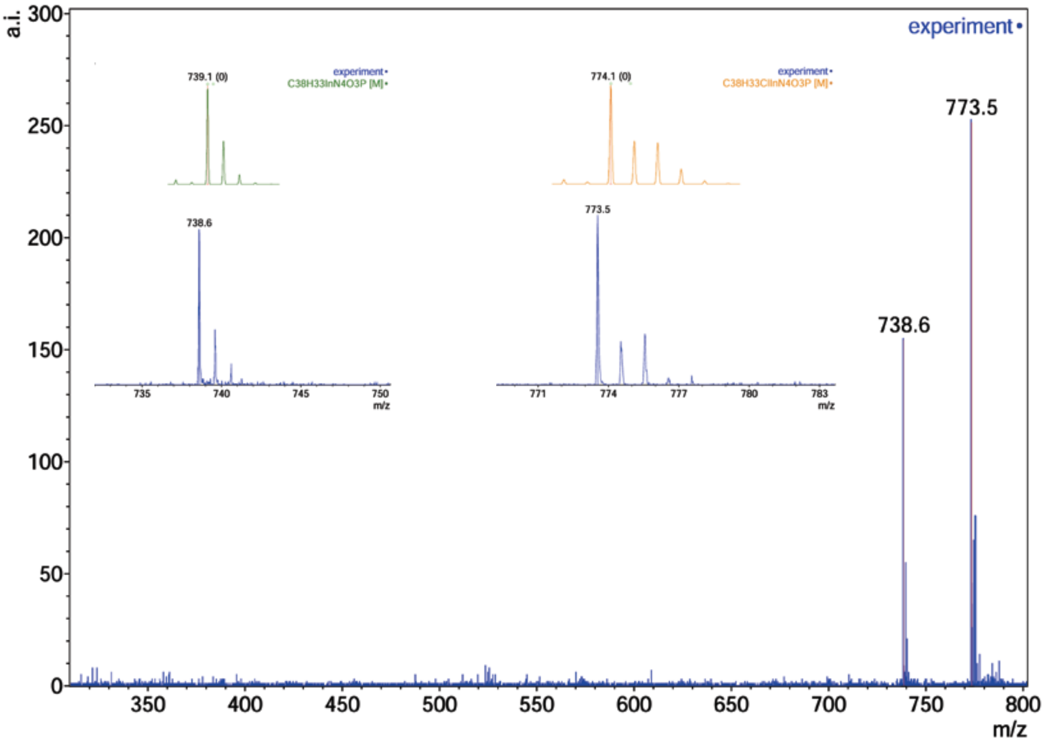


*Figure S63. MALDI TOF mass spectrum of **In-1b**.*

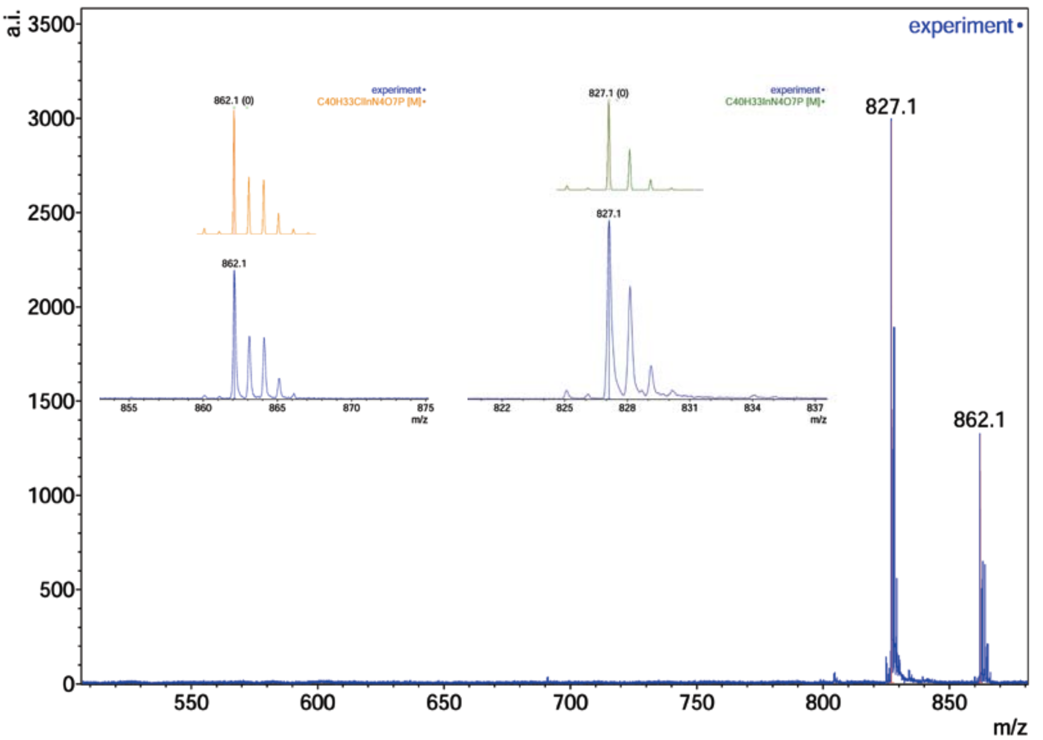


*Figure S64. MALDI TOF mass spectrum of **In-1c**.*

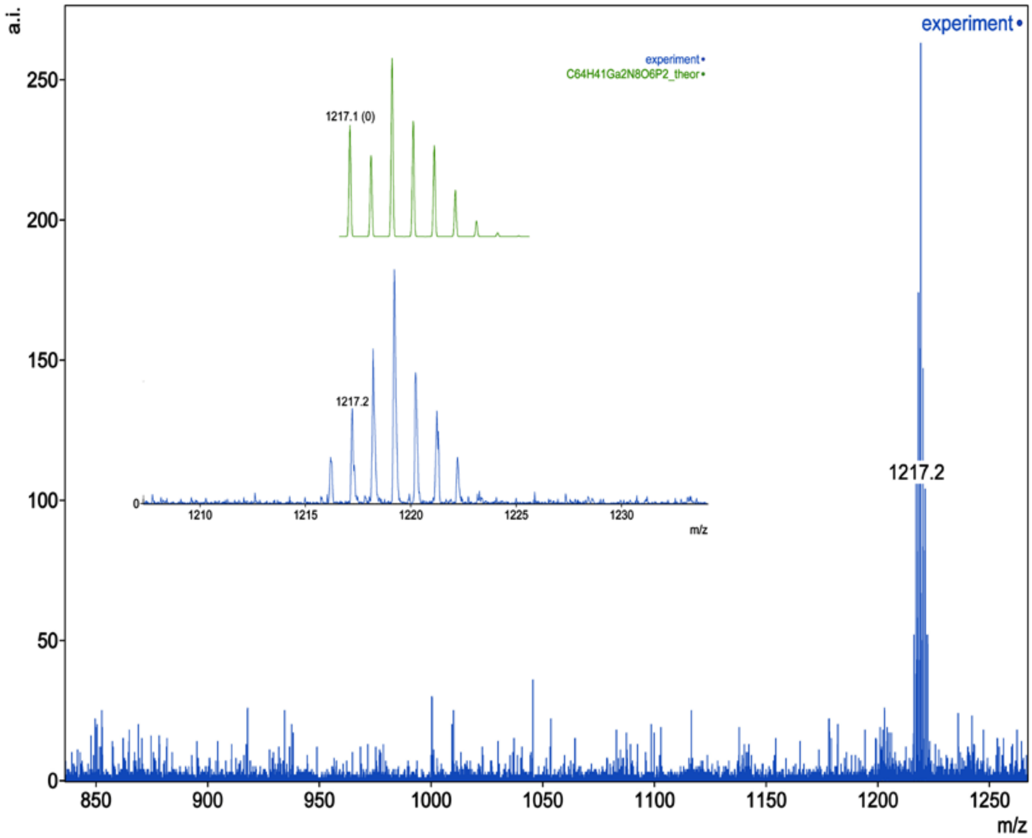


Figure S65. MALDI TOF mass spectrum of ***Ga-4a****.*

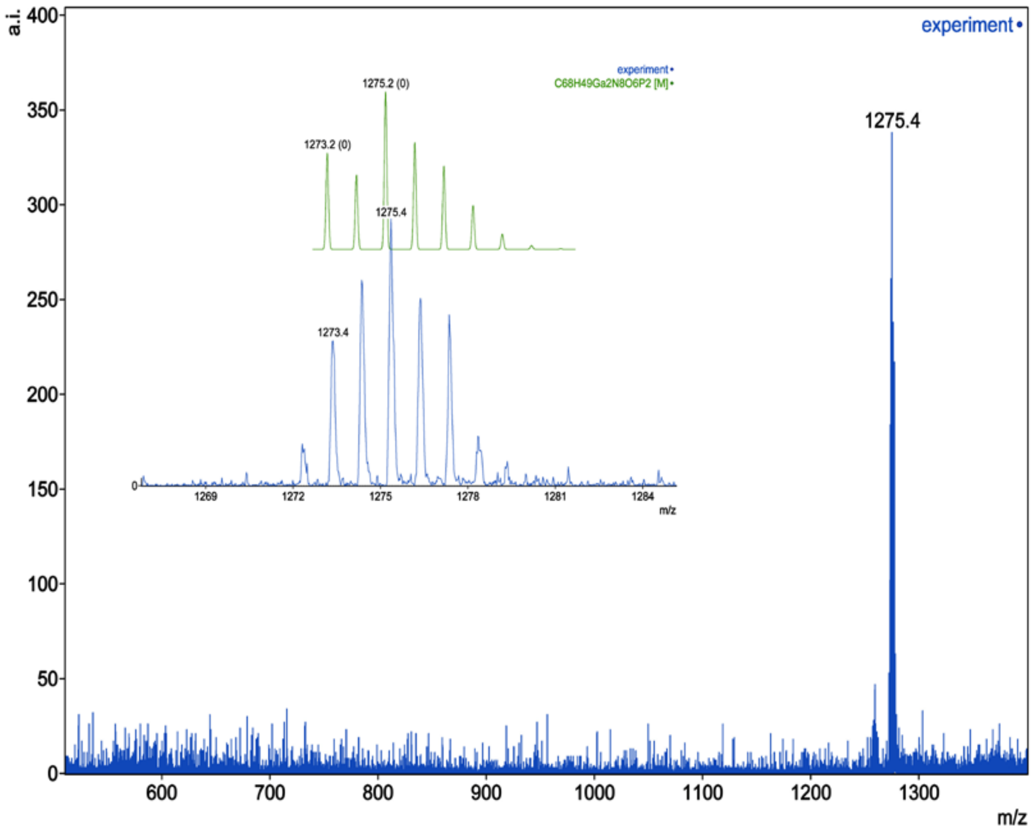


Figure S66. MALDI TOF mass spectrum of ***Ga-4b****.*

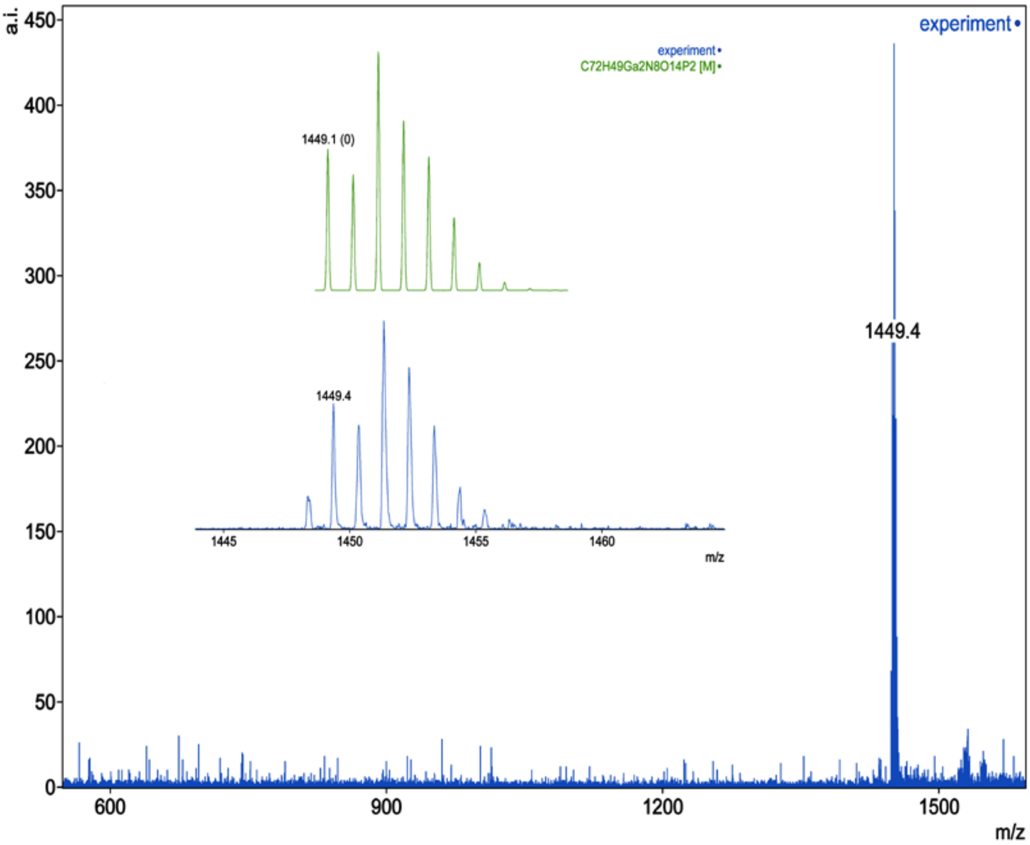


Figure S67. MALDI TOF mass spectrum of ***Ga-4c***.

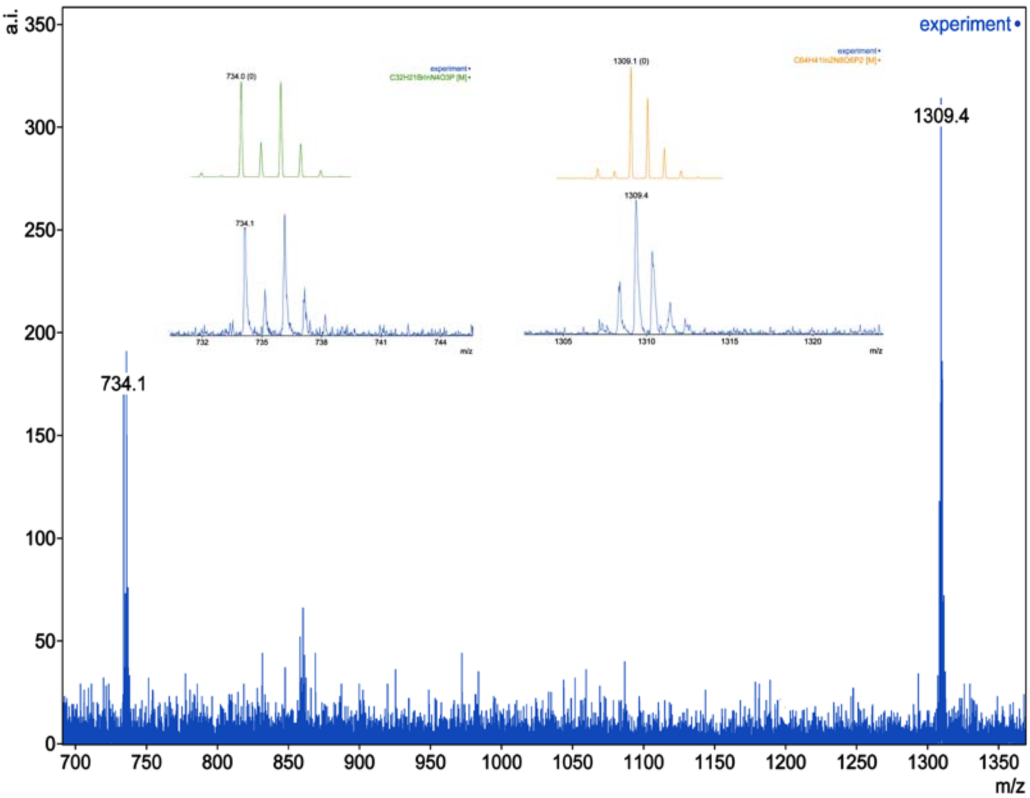


Figure S68. MALDI TOF mass spectrum of ***In-4a***.

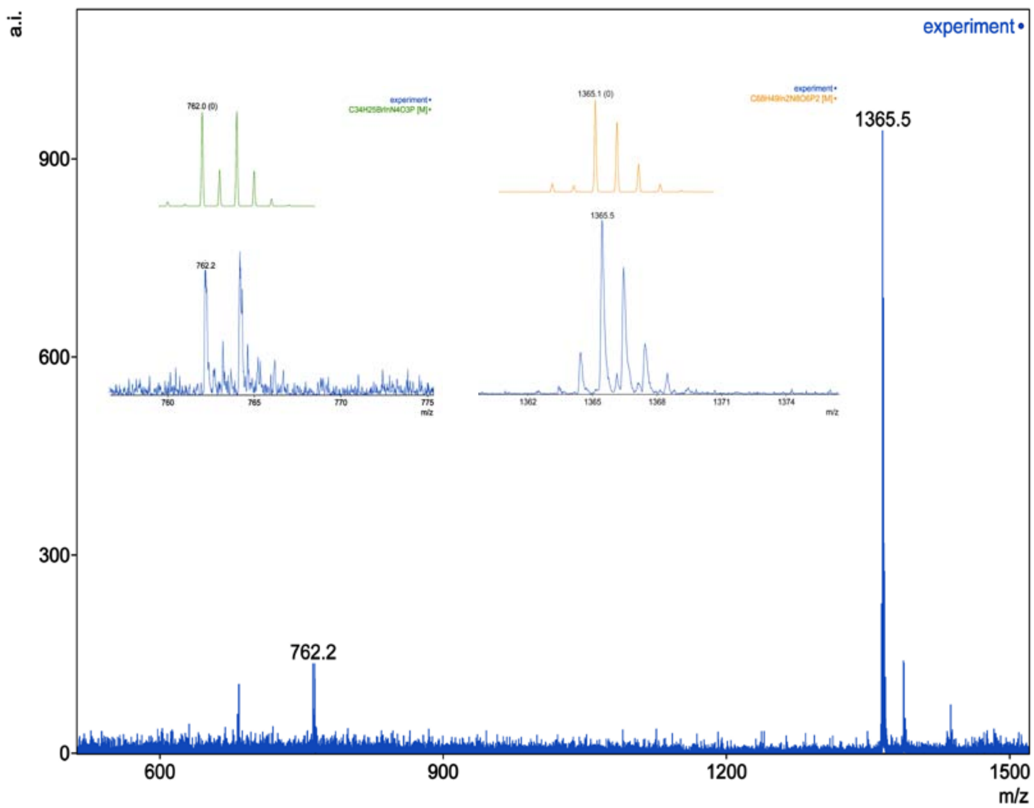


*Figure S69. MALDI TOF mass spectrum of **In-4b**.*

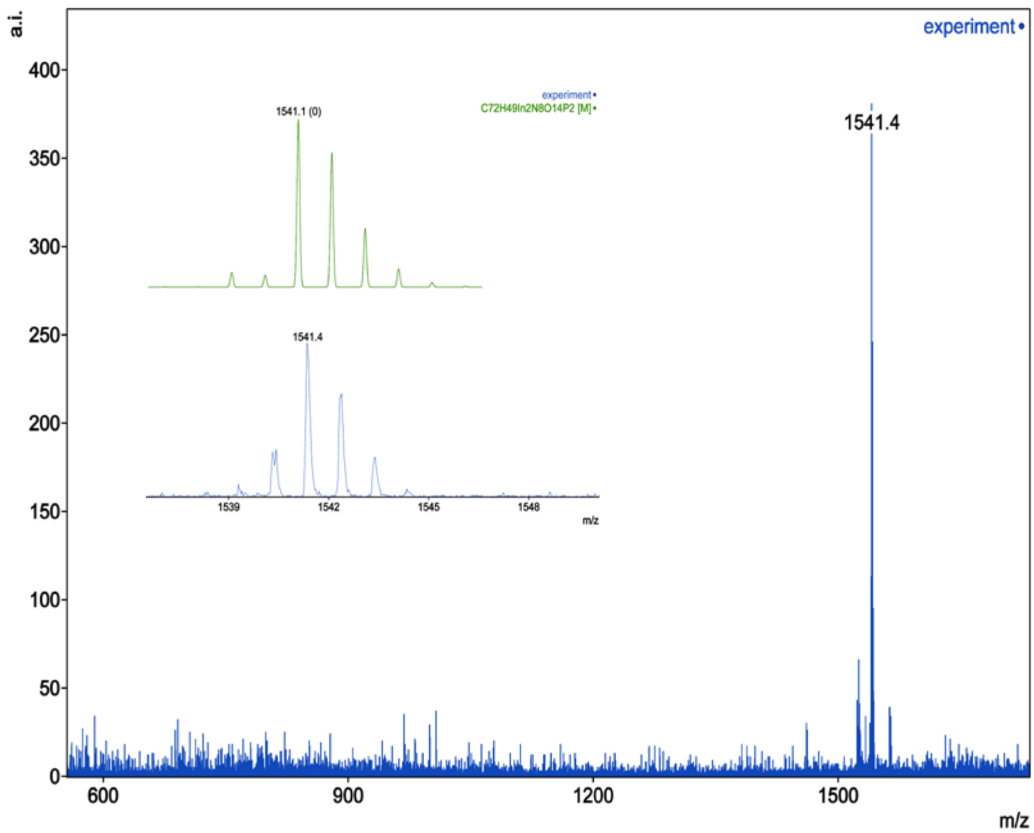
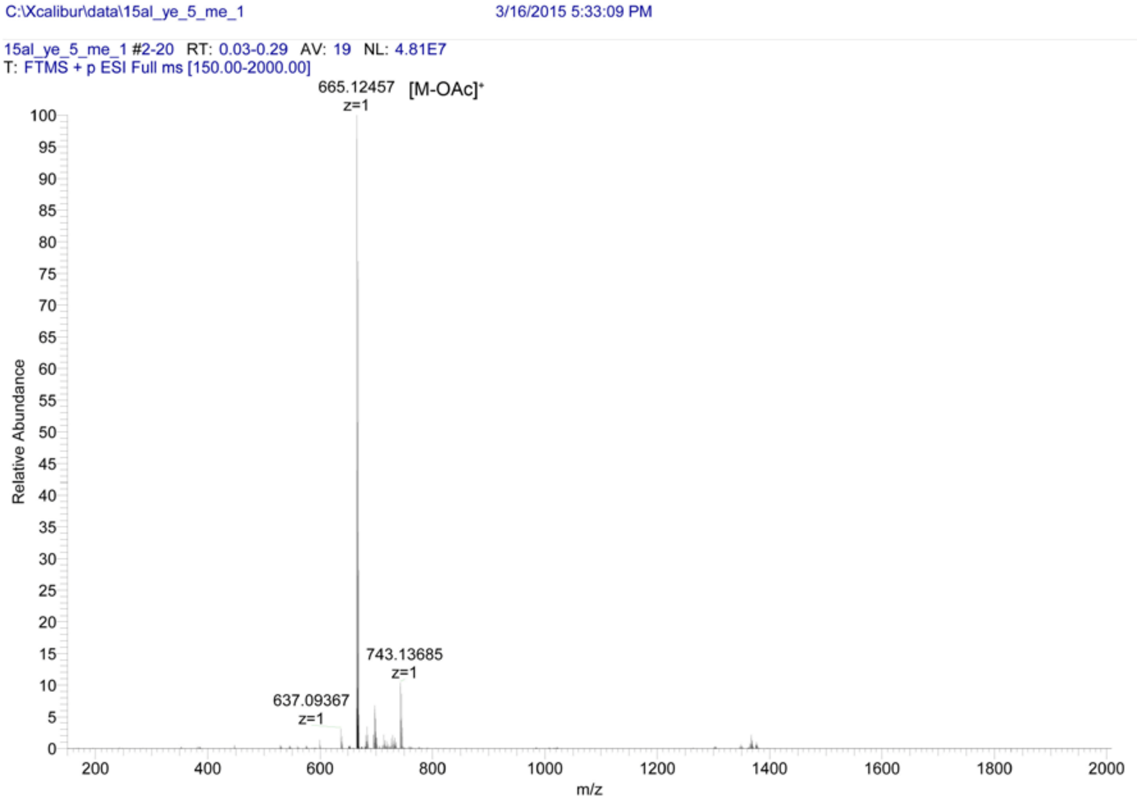


*Figure S70. MALDI TOF mass spectrum of **In-4c**.*

7. ESI-HR mass spectra of compounds Ga-1a-c, In-1a-c, Ga-2a,b, In-2a,b, 2H-2a,b.



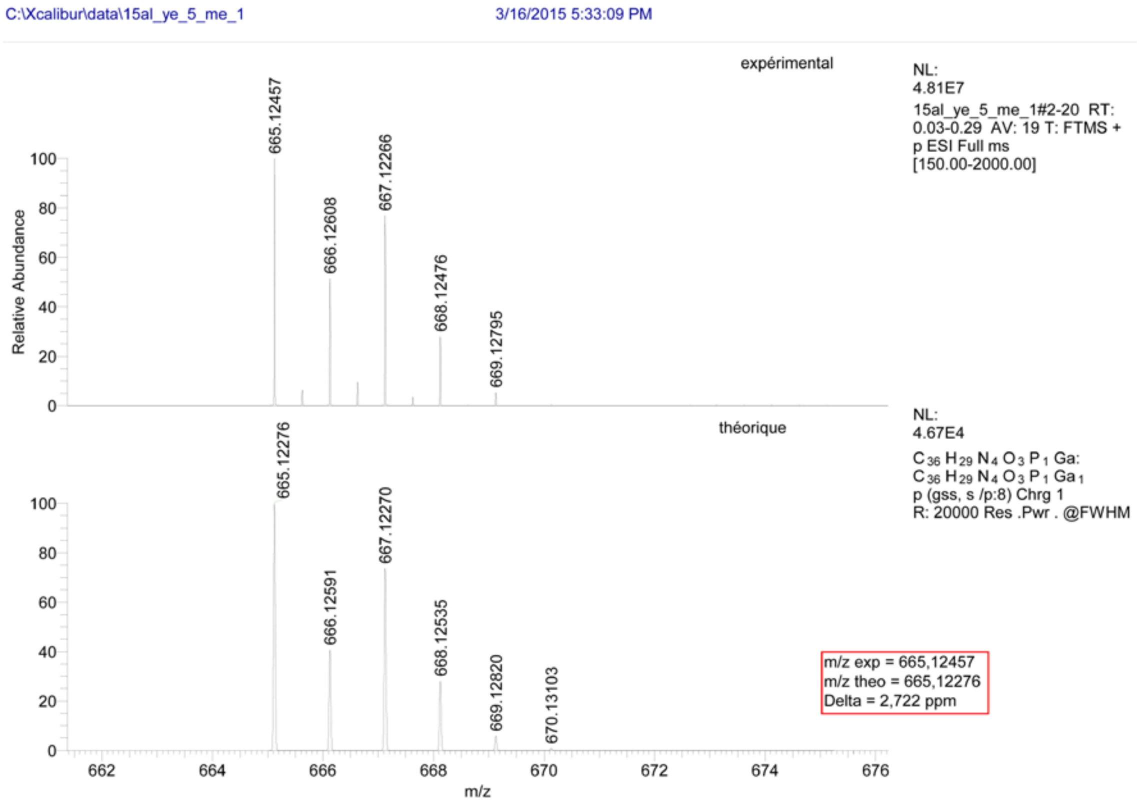


Figure S71. ESI-HR mass spectrum of ***Ga-1a****.*

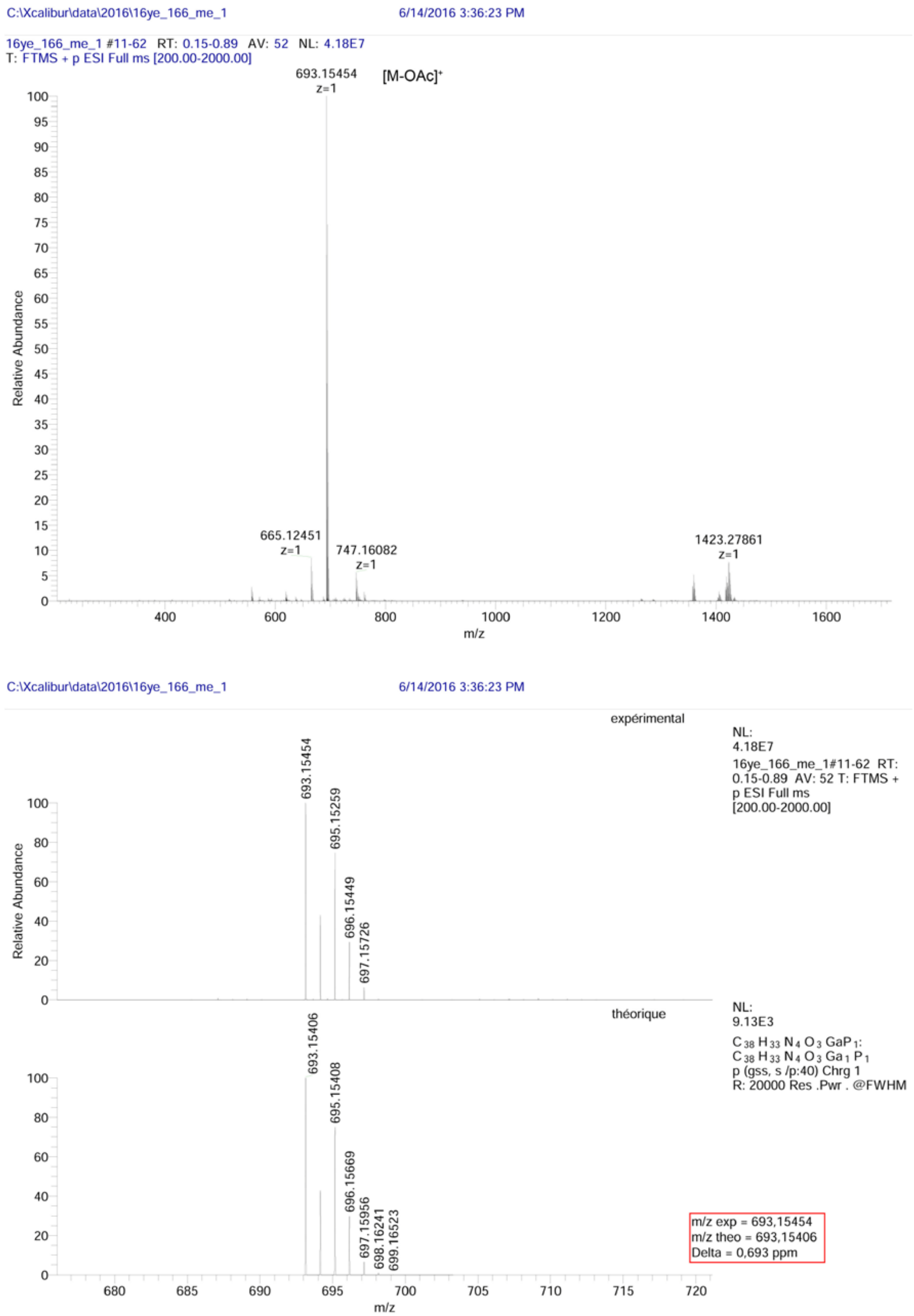
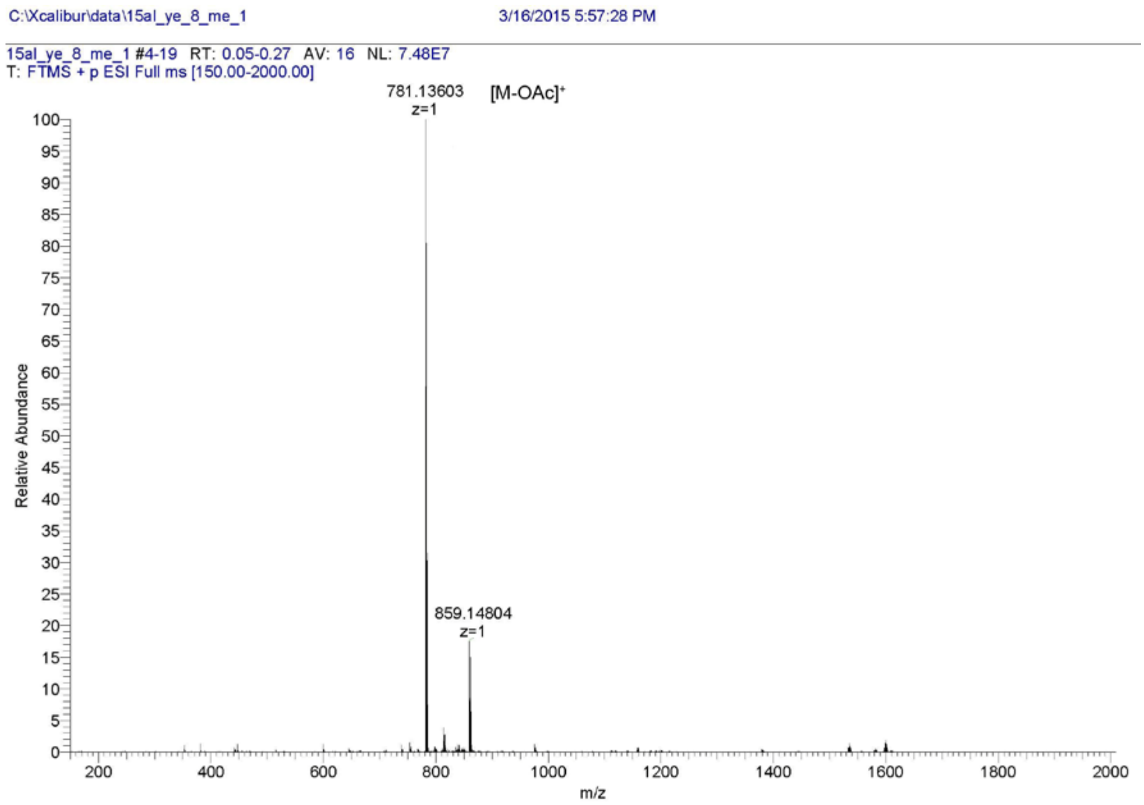


*Figure S72. ESI-HR mass spectrum of **Ga-1b**.*



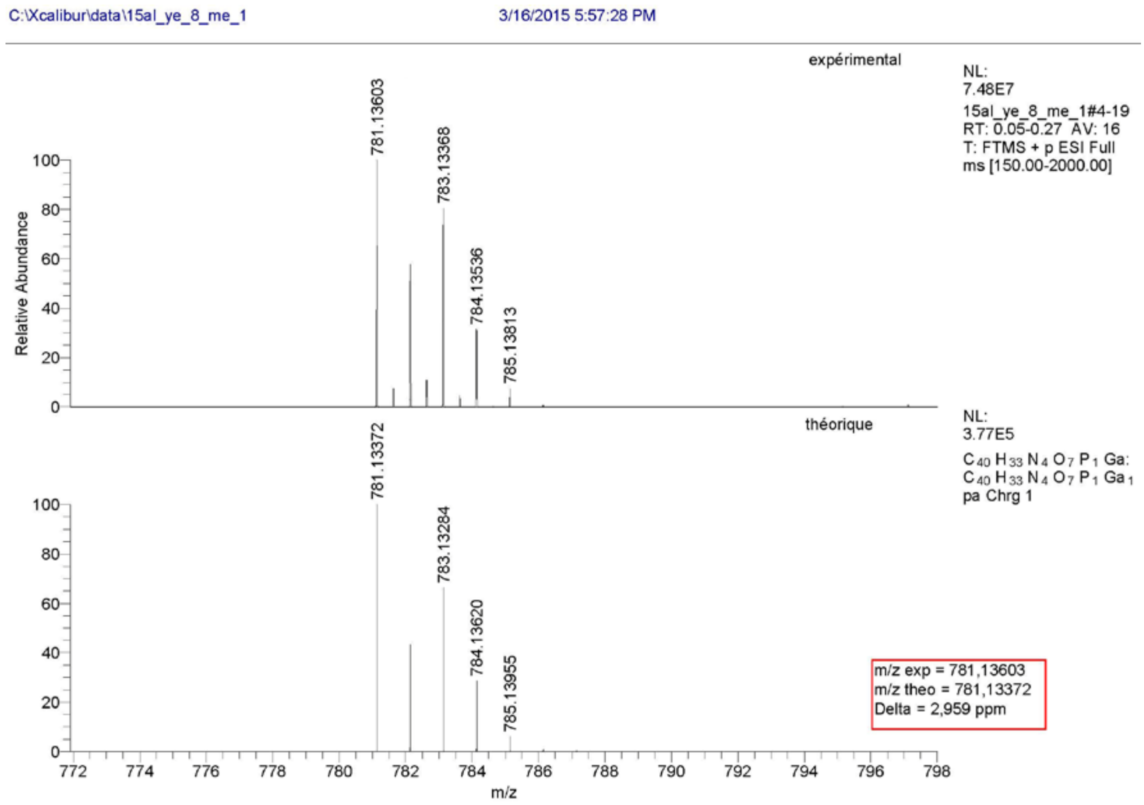
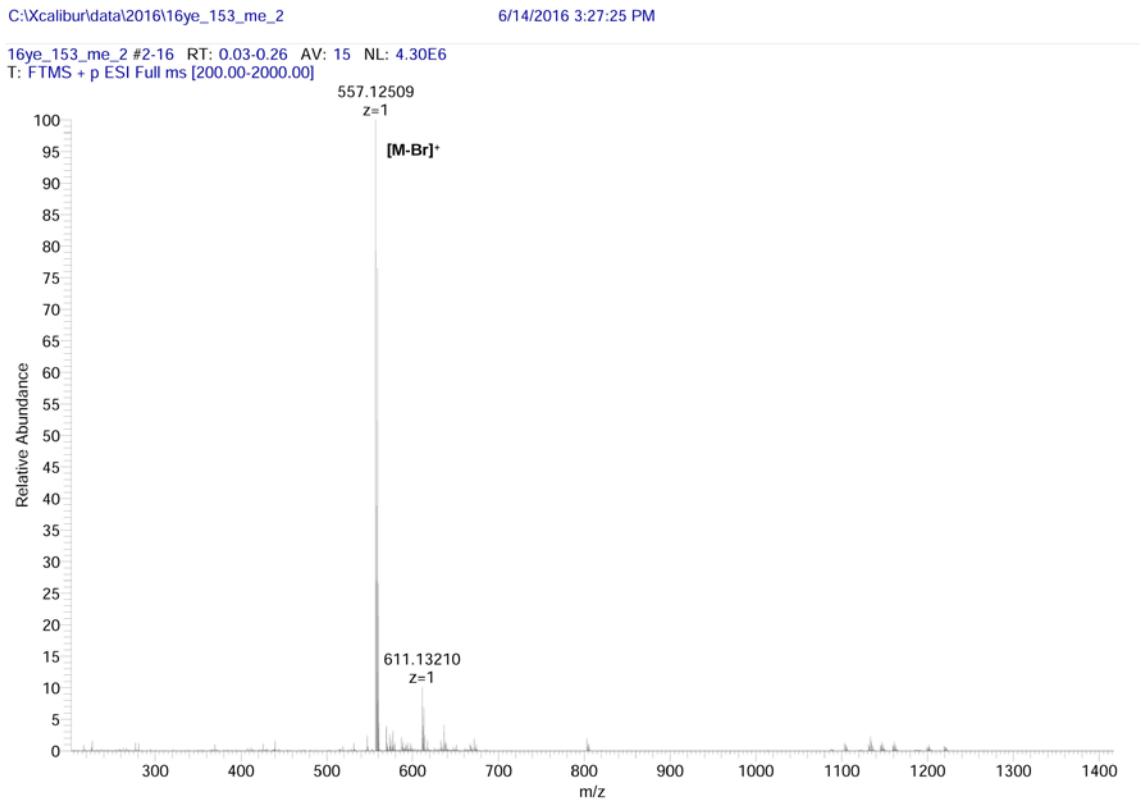


Figure S73. ESI-HR mass spectrum of ***Ga-1c****.*



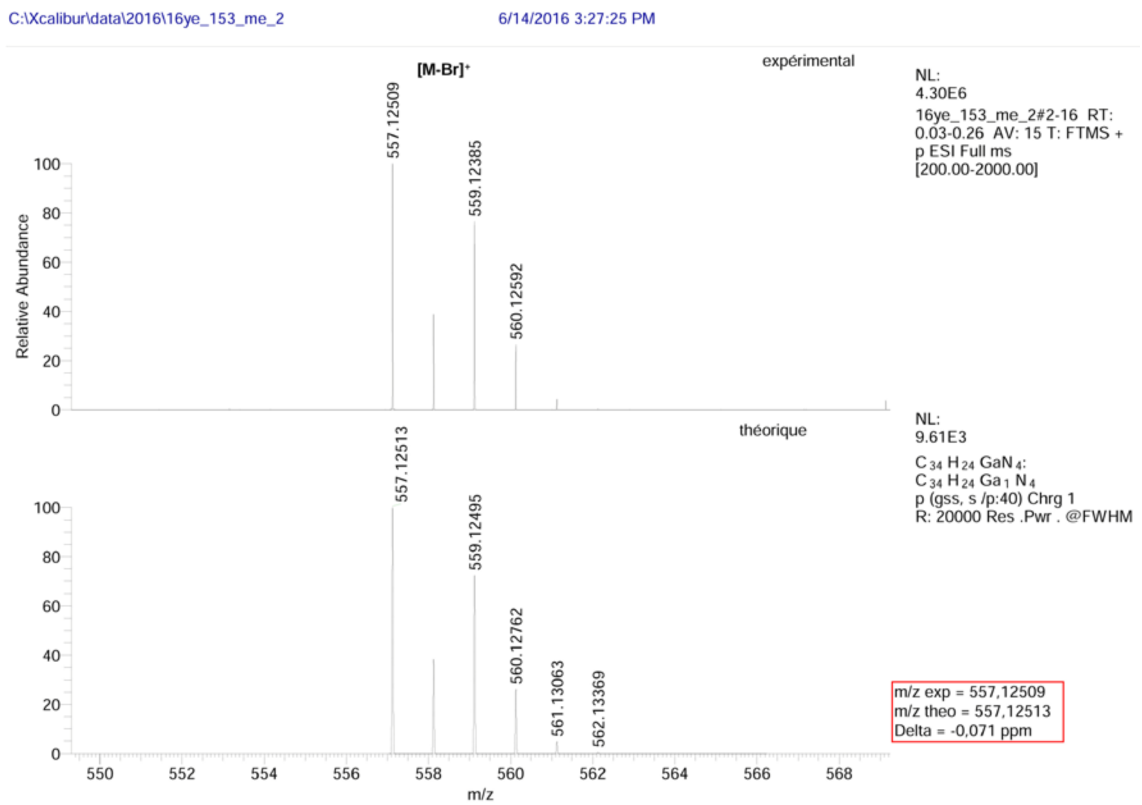
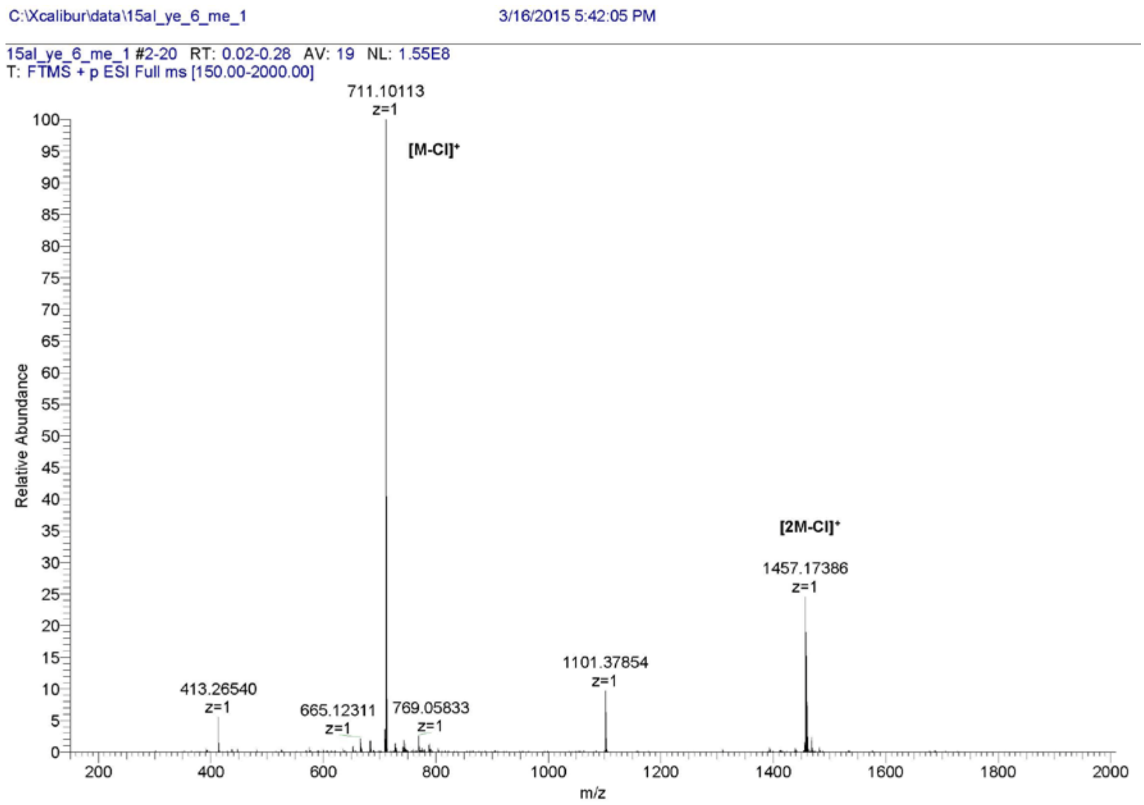


*Figure S74. ESI-HR mass spectrum of **Ga-5b**.*



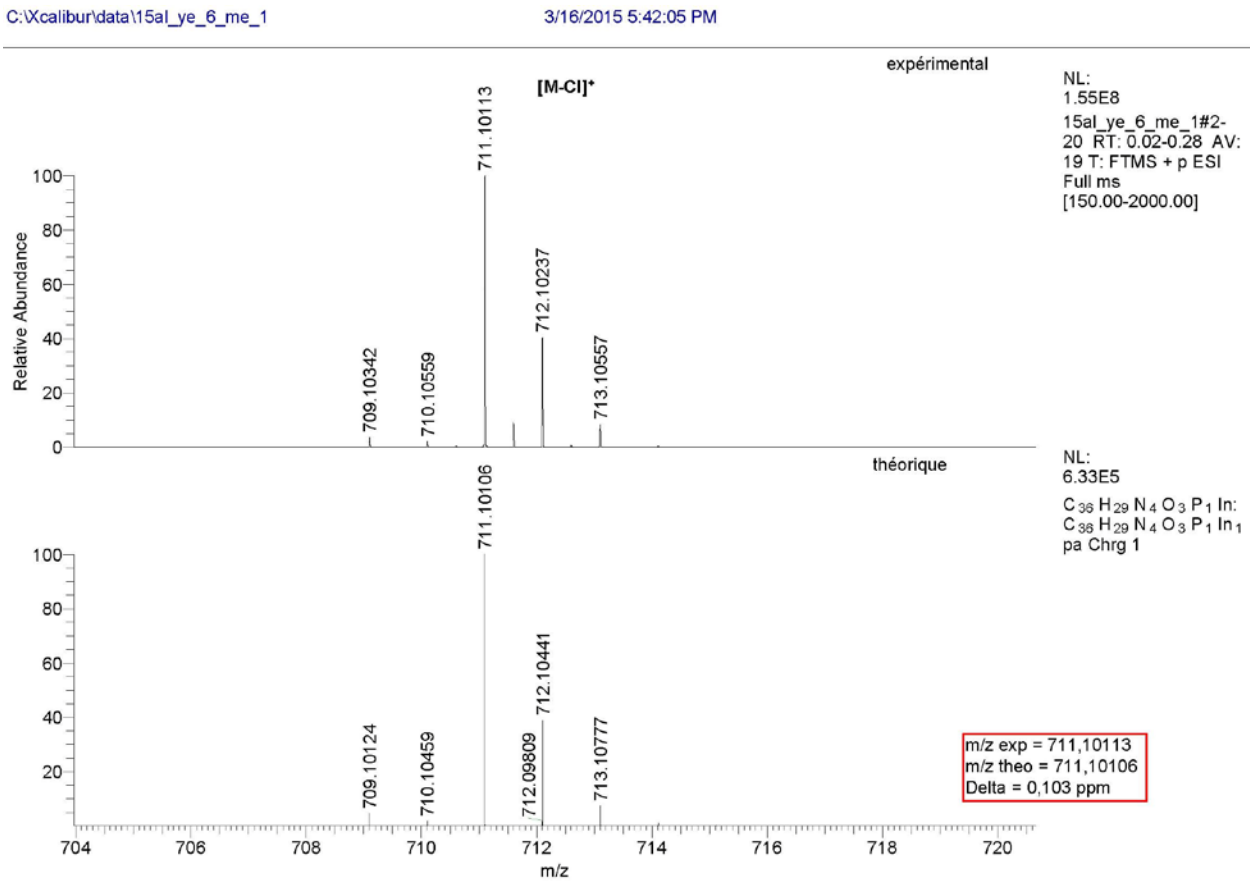
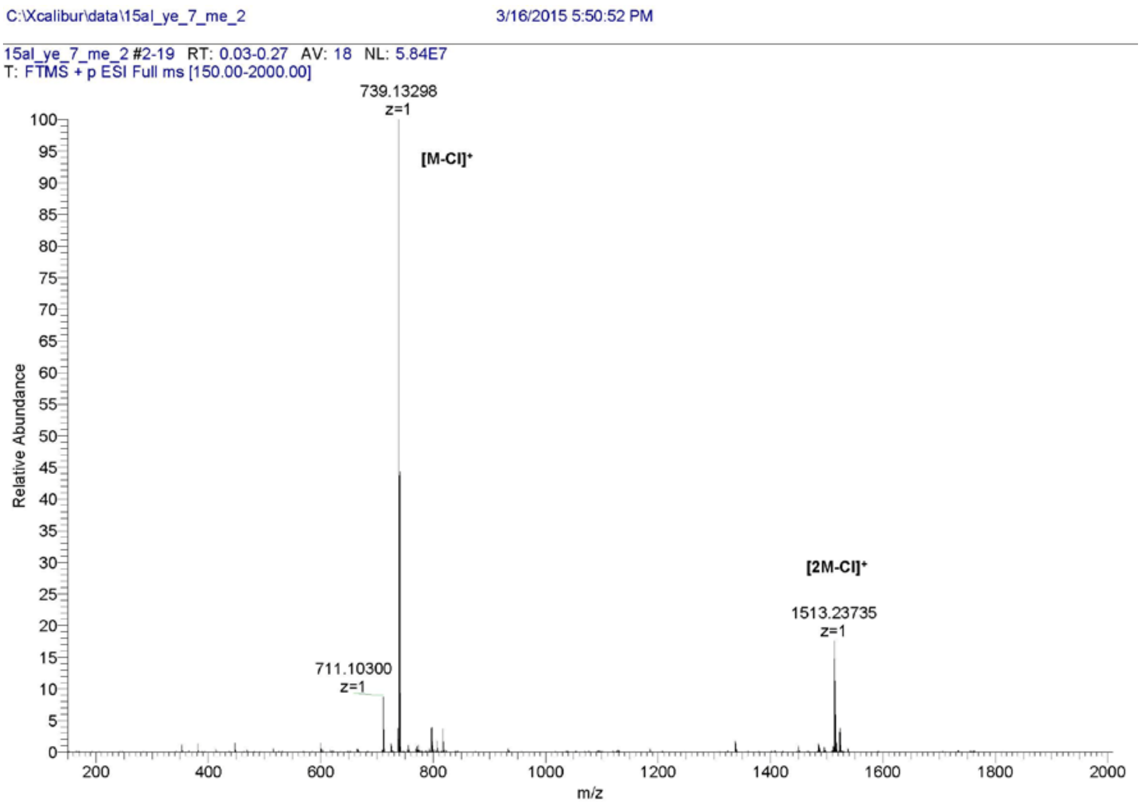


*Figure S75. ESI-HR mass spectrum of **In-1a**.*



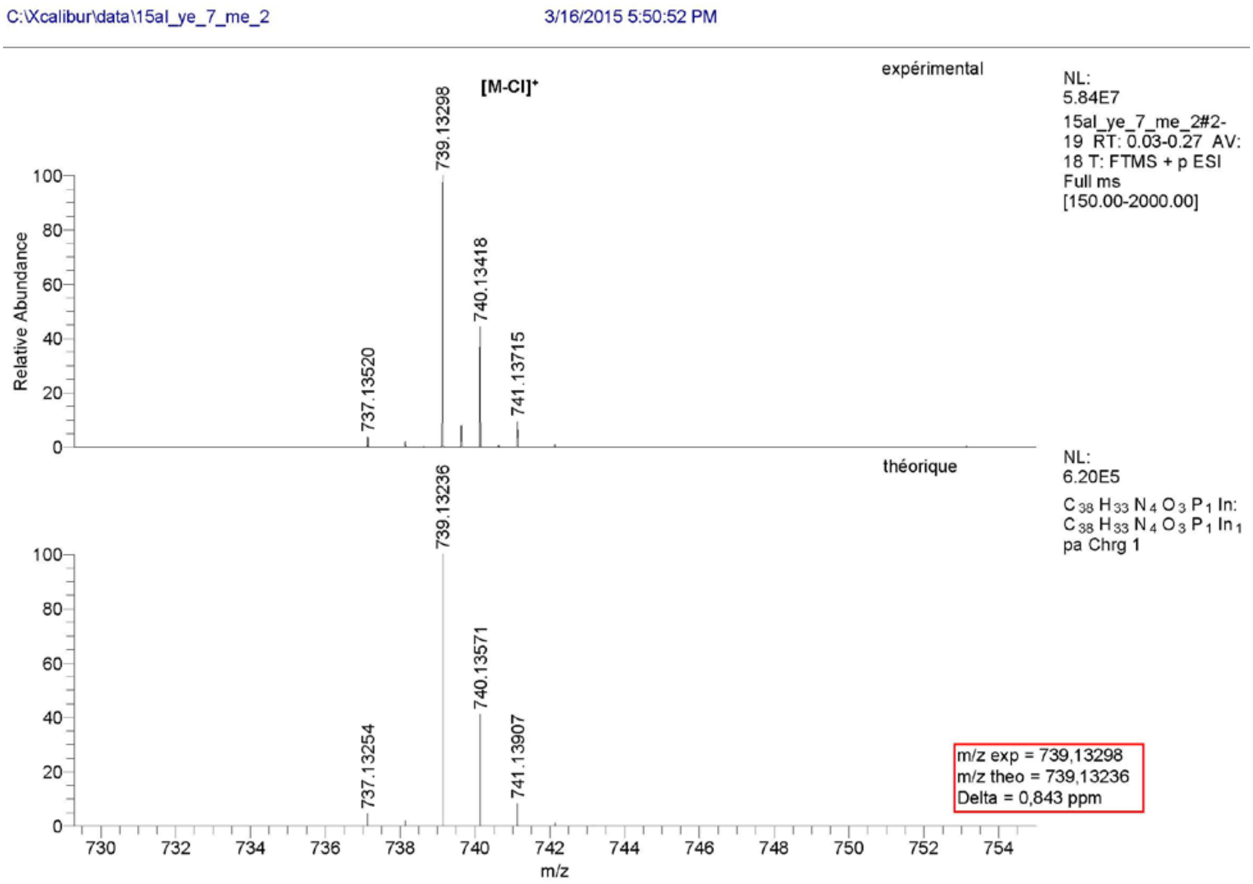
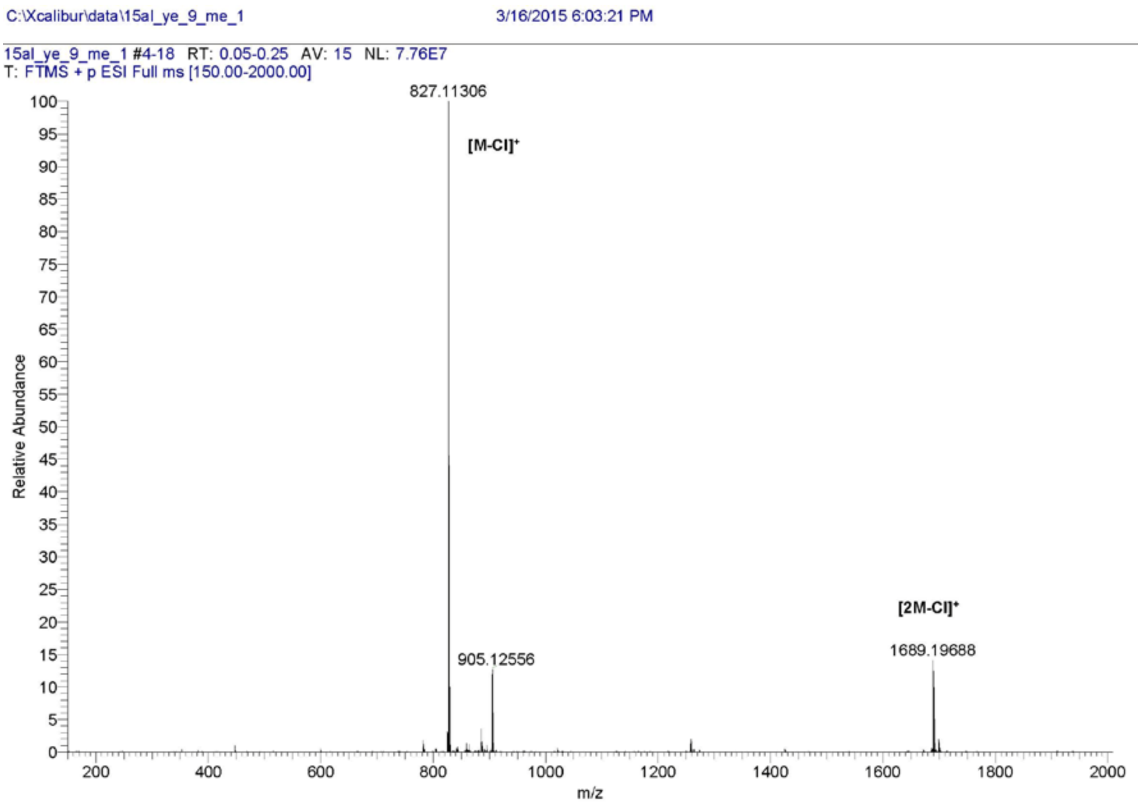


Figure S76. ESI-HR mass spectrum of ***In-1b****.*



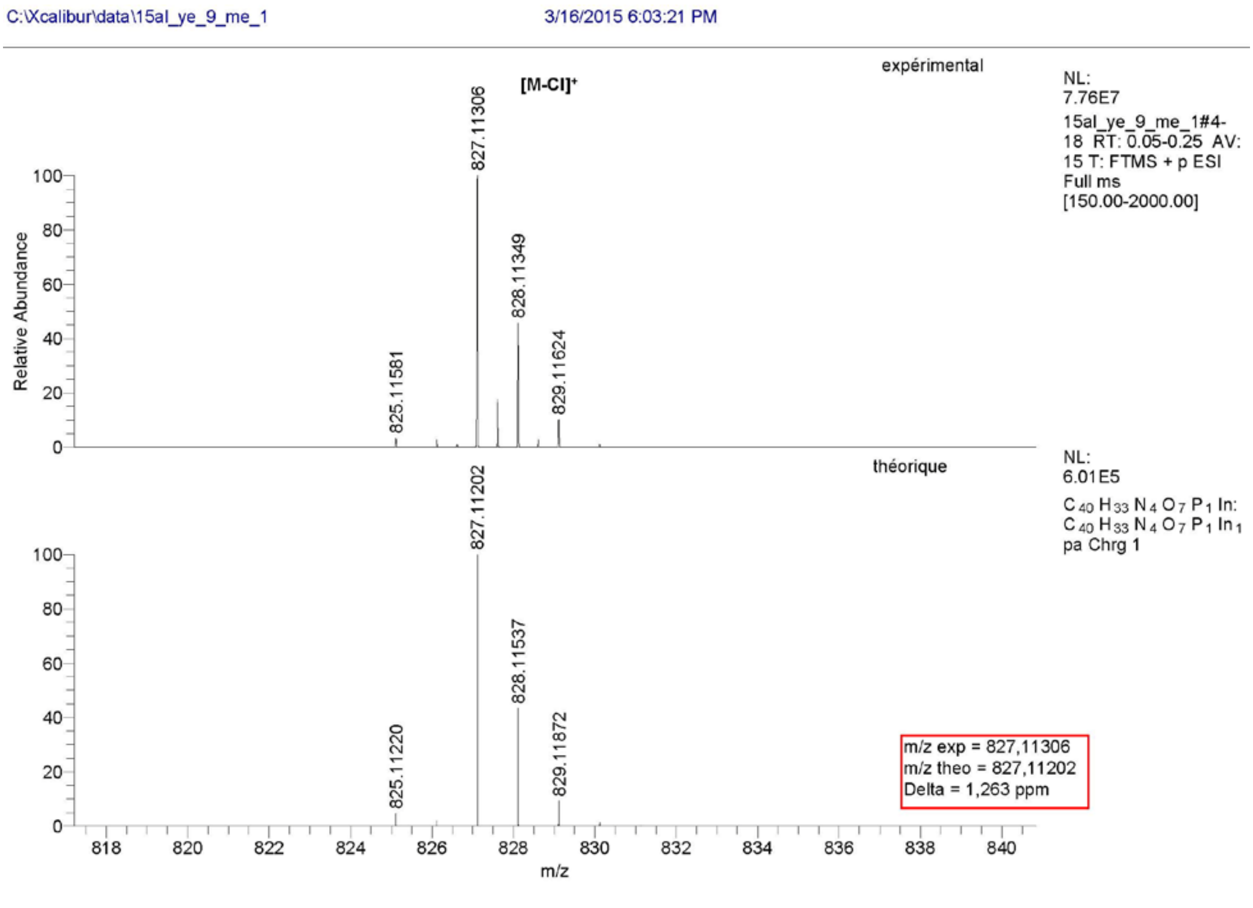
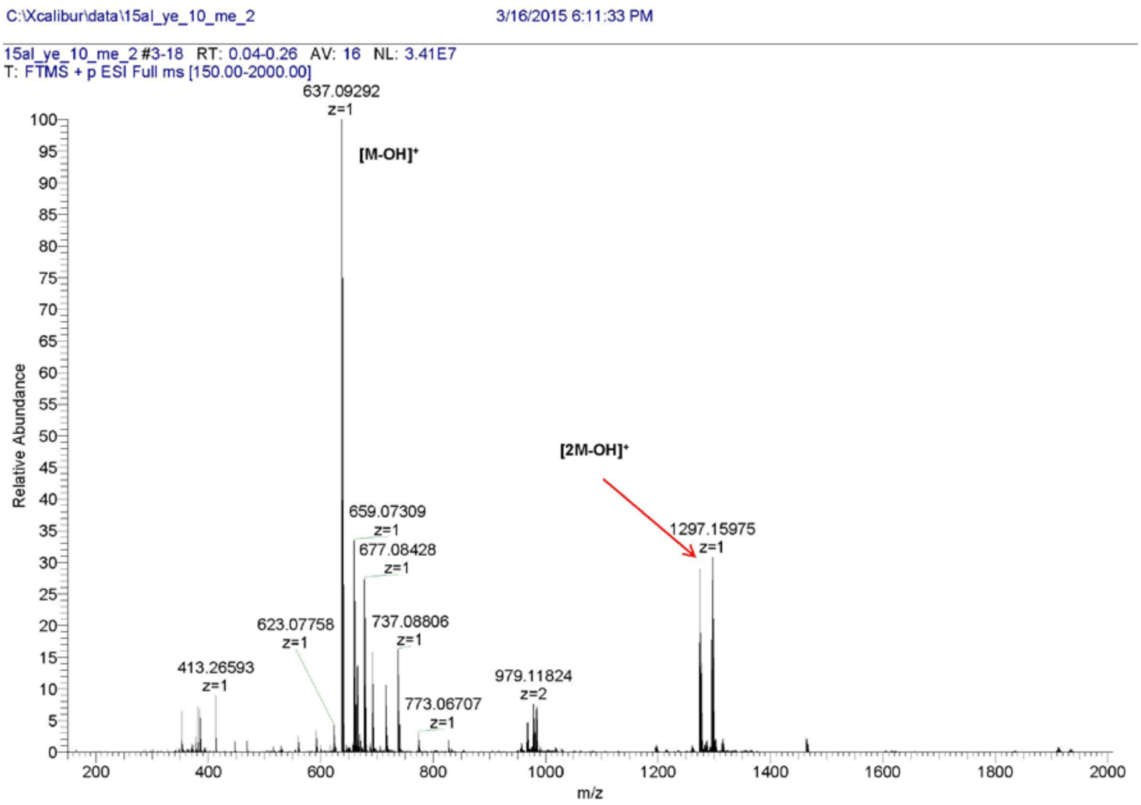


*Figure S77. ESI-HR mass spectrum of **In-1c**.*



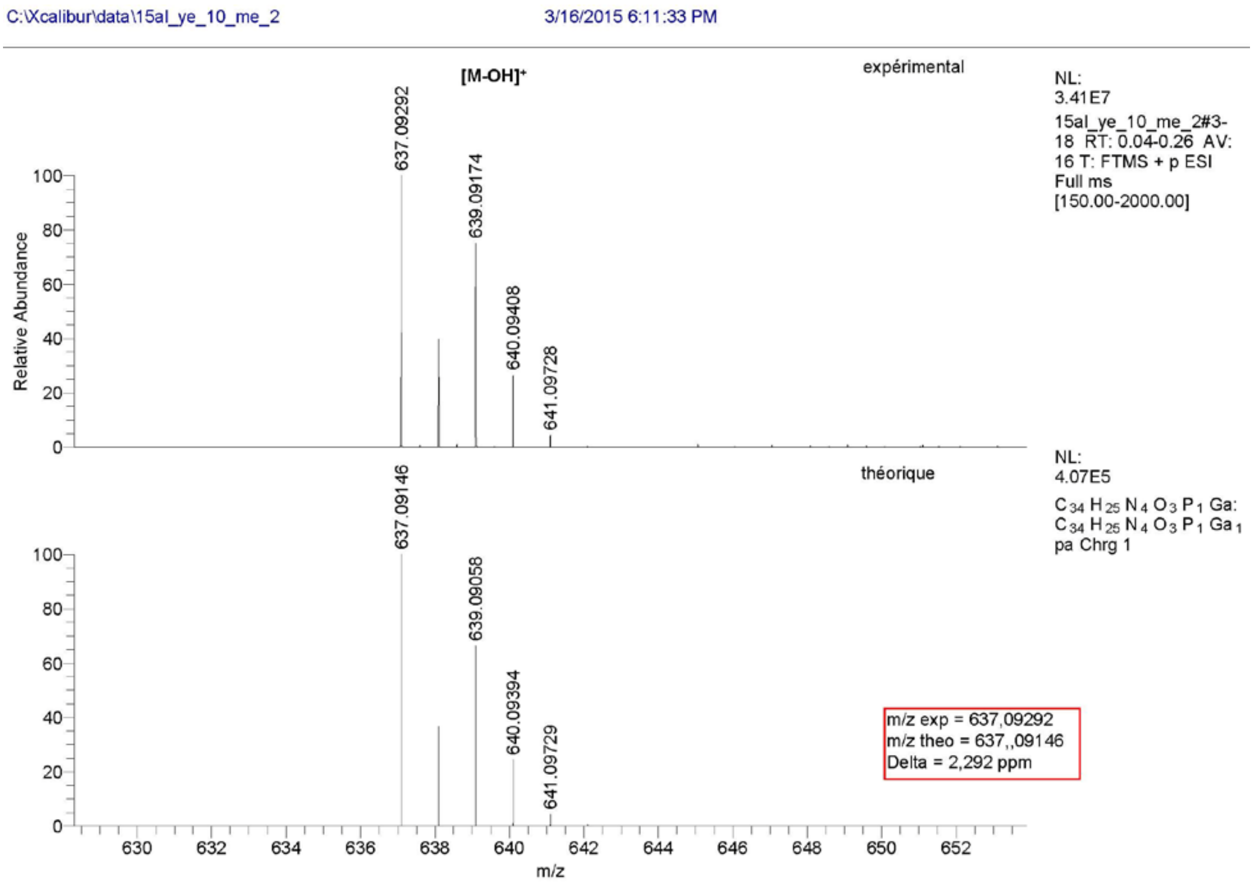


*Figure S78. ESI-HR mass spectrum of **Ga-2a**.*

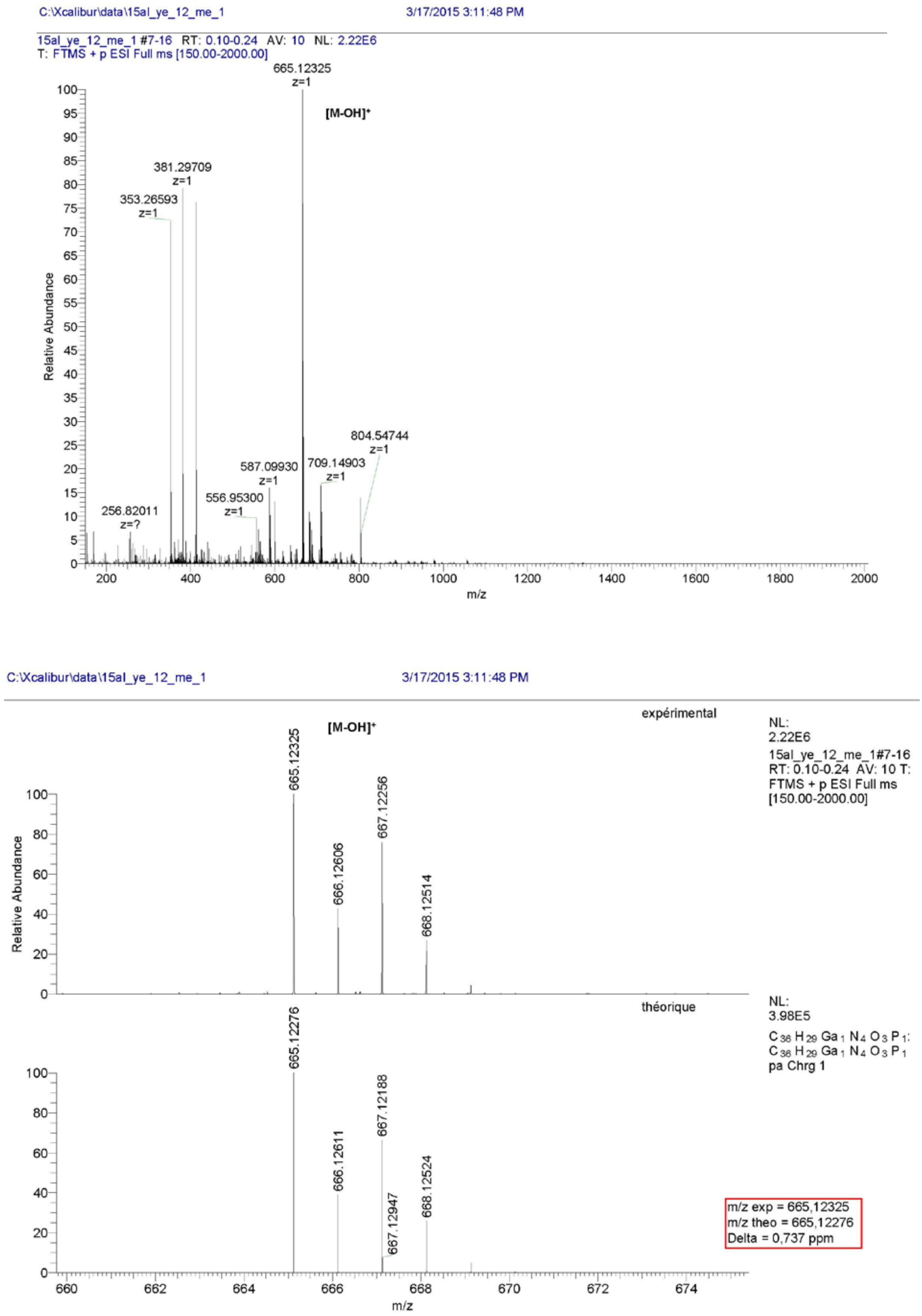


*Figure S79. ESI-HR mass spectrum of **Ga-2b**.*

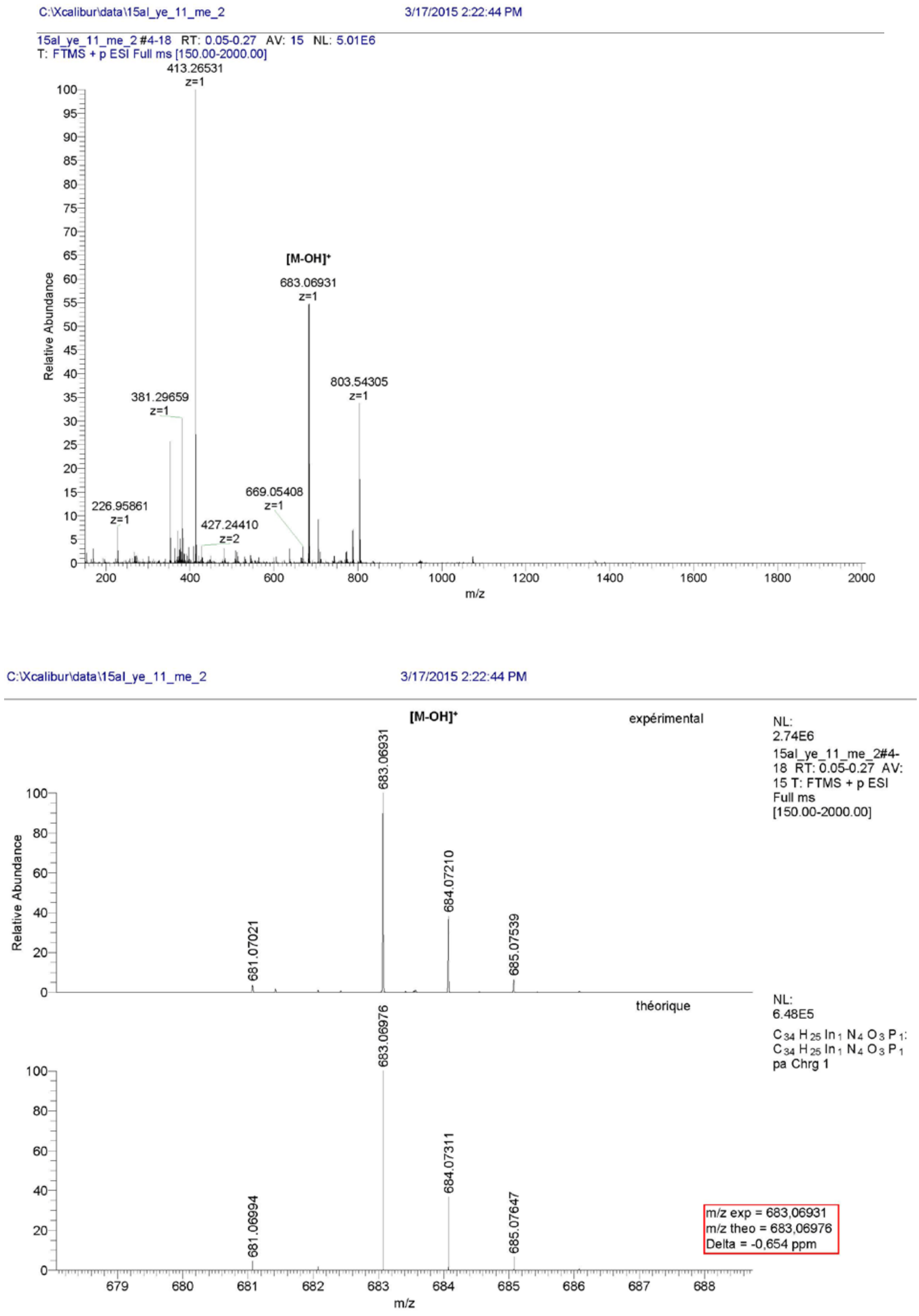
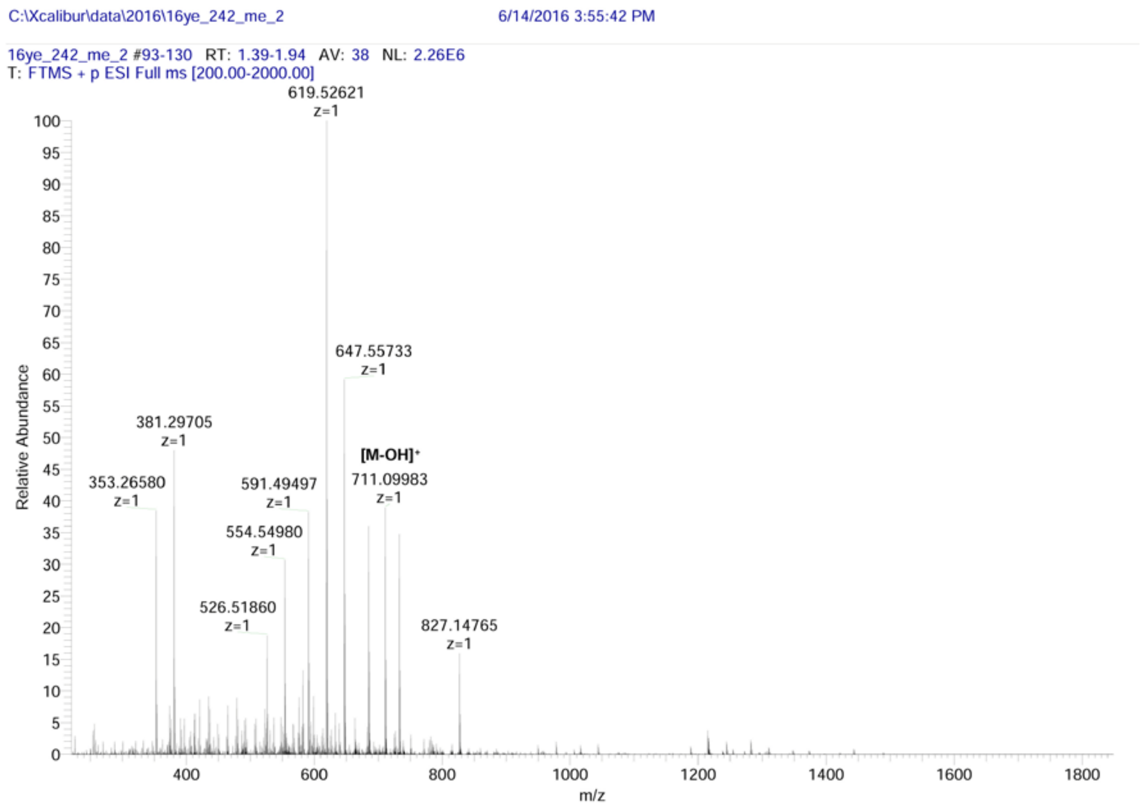


*Figure S80. ESI-HR mass spectrum of **In-2a**.*



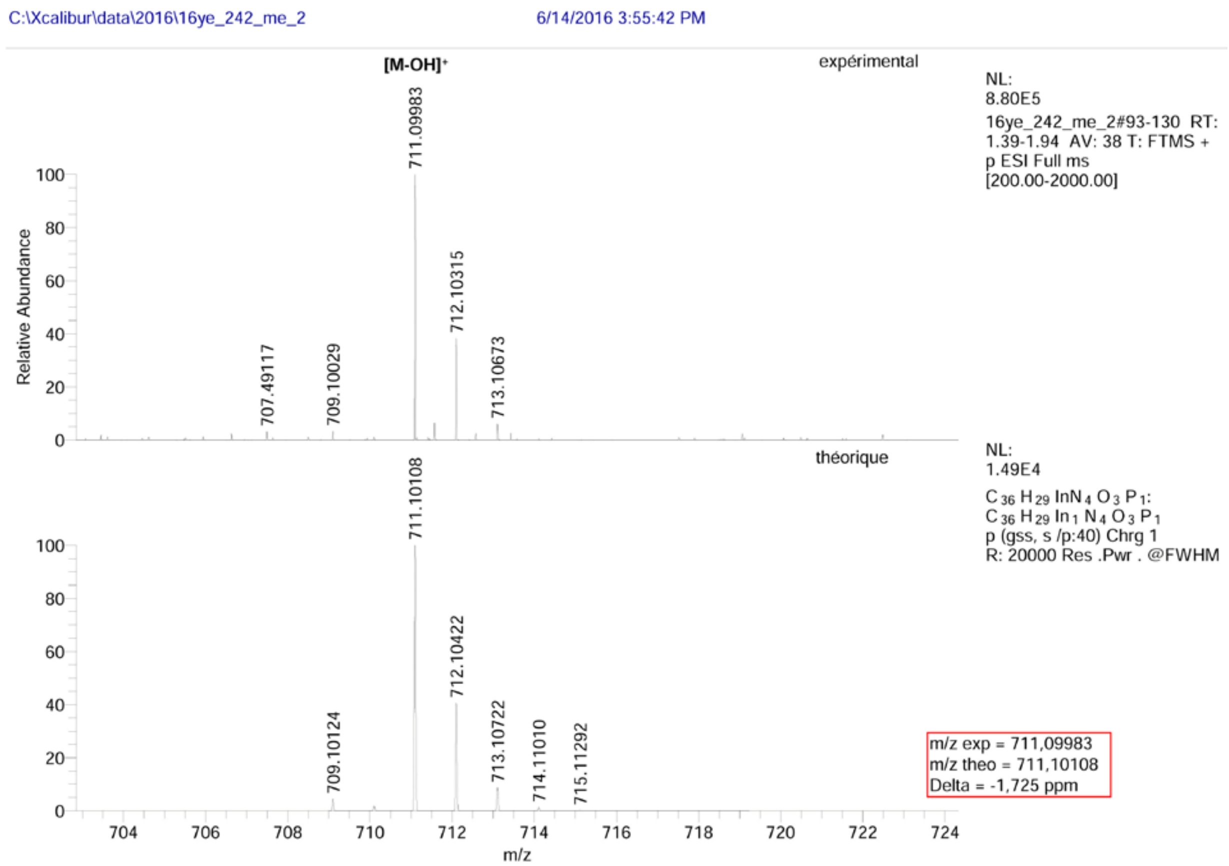
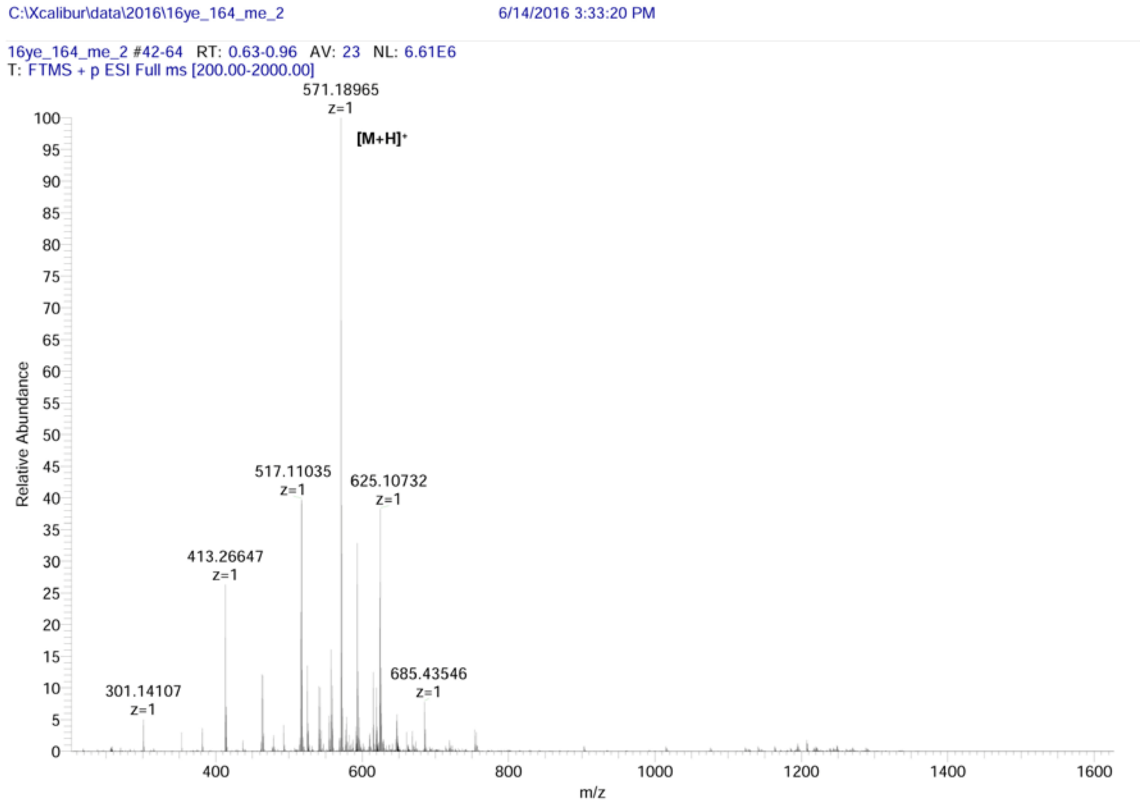


Figure S81. ESI-HR mass spectrum of ***In-2b****.*



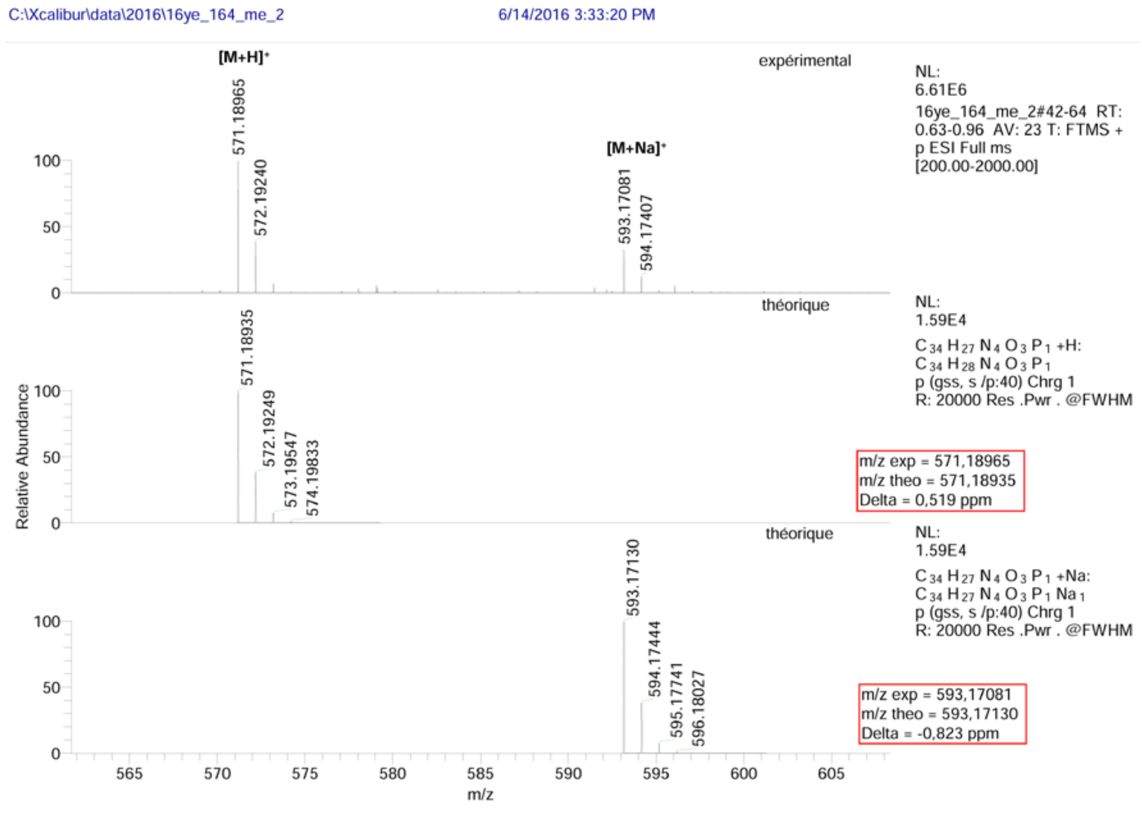
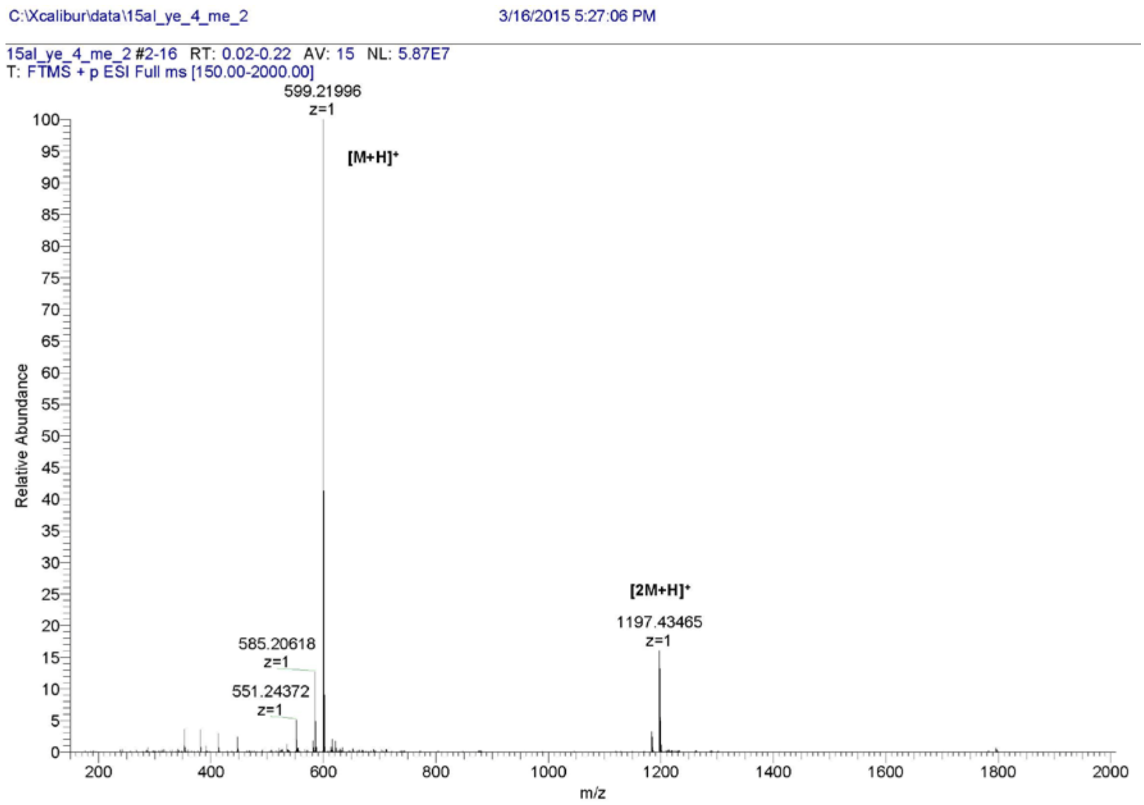


*Figure S82. ESI-HR mass spectrum of **2H-2a**.*



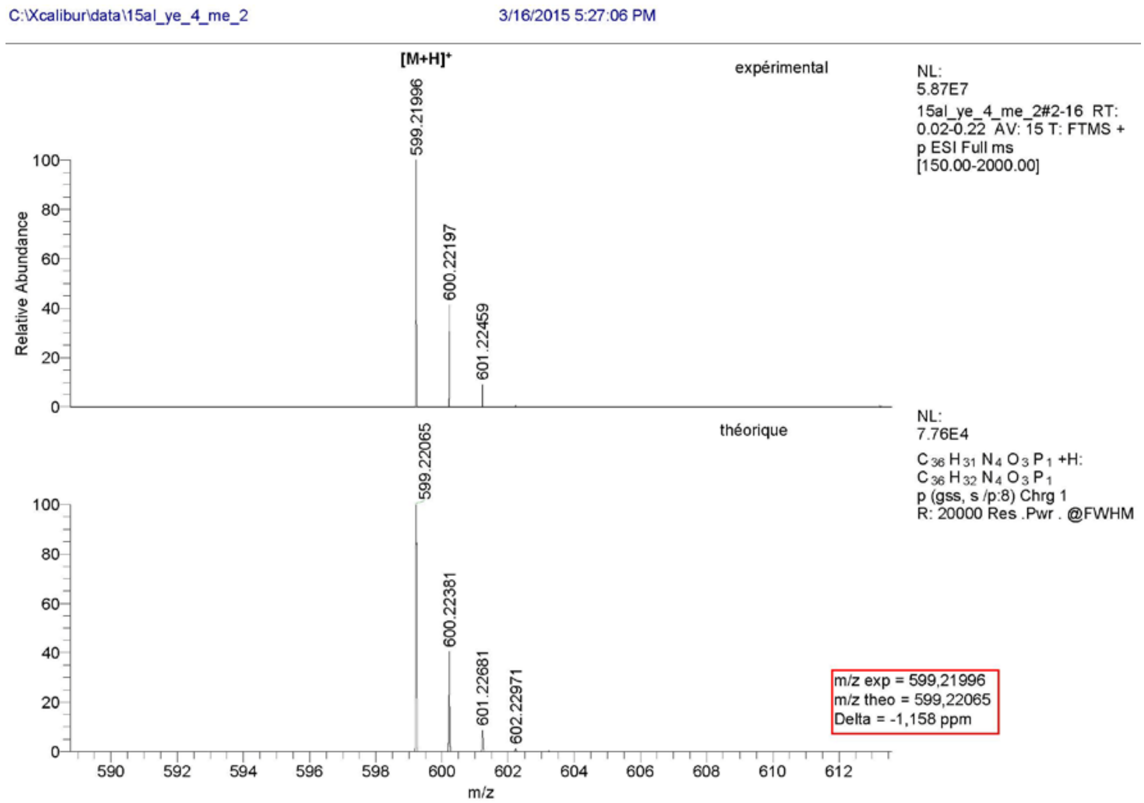
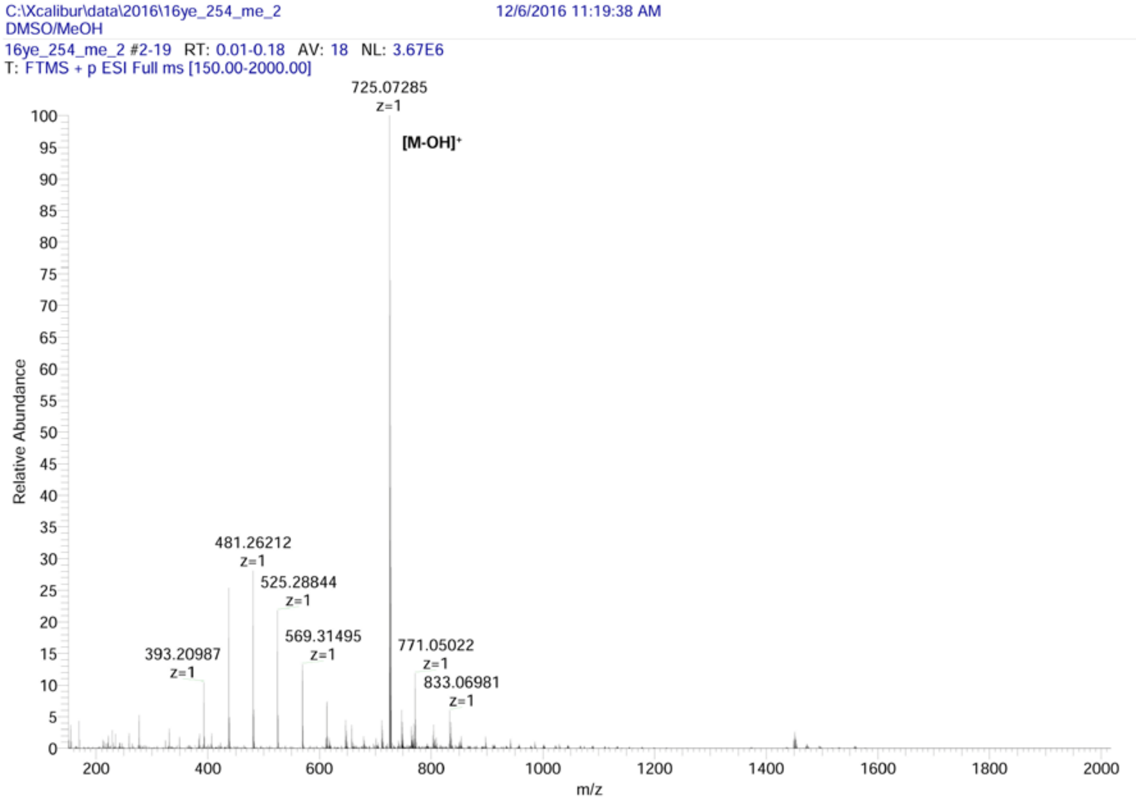


*Figure S83. ESI-HR mass spectrum of **2H-2b**.*



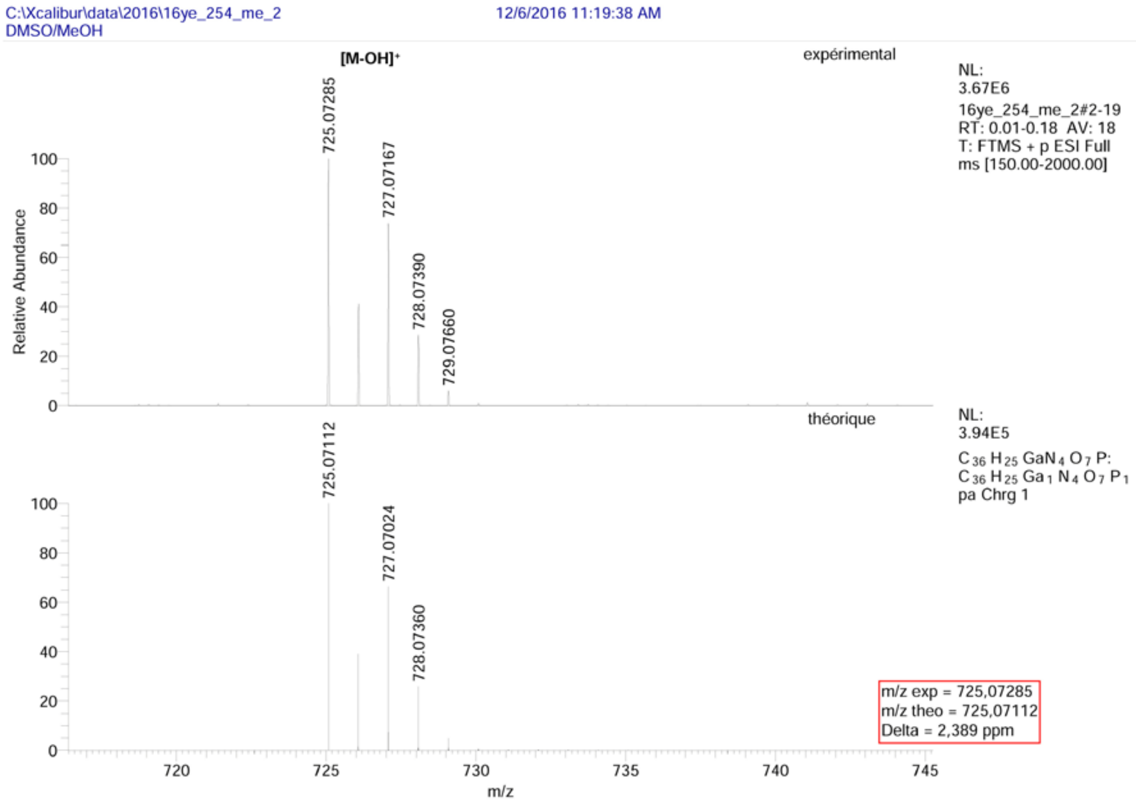
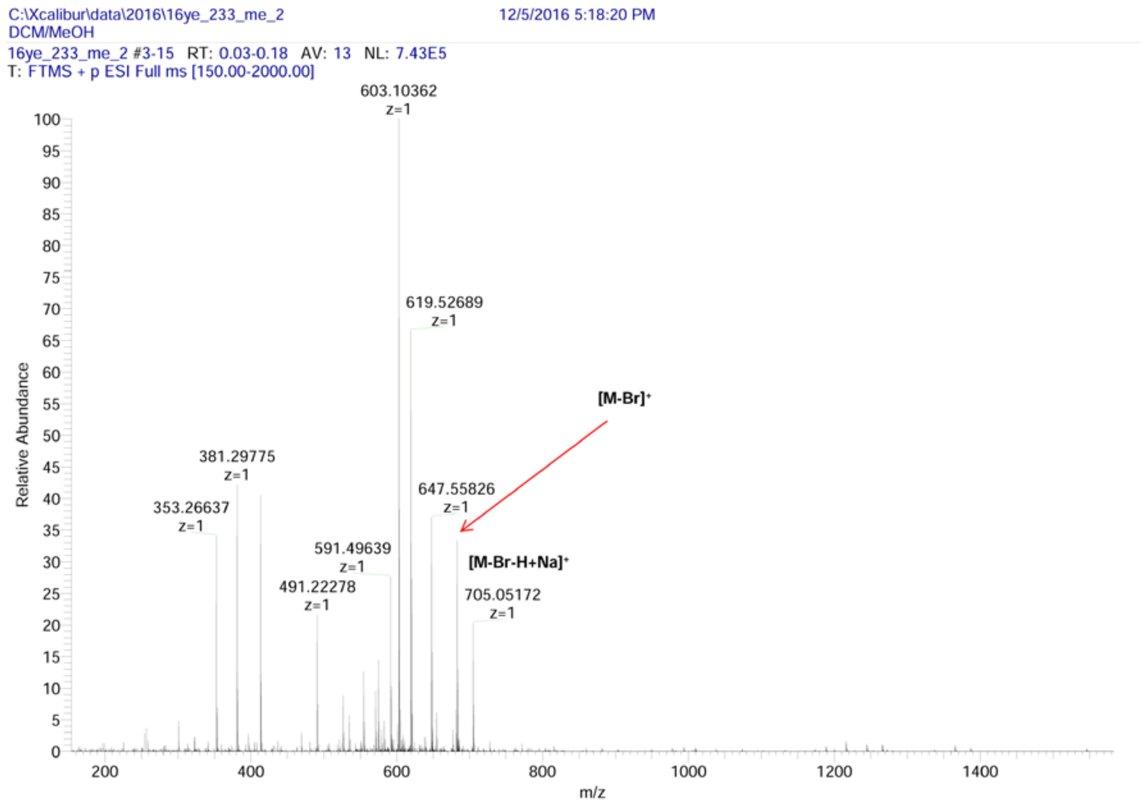


*Figure S84. ESI-HR mass spectrum of **Ga-3c**.*



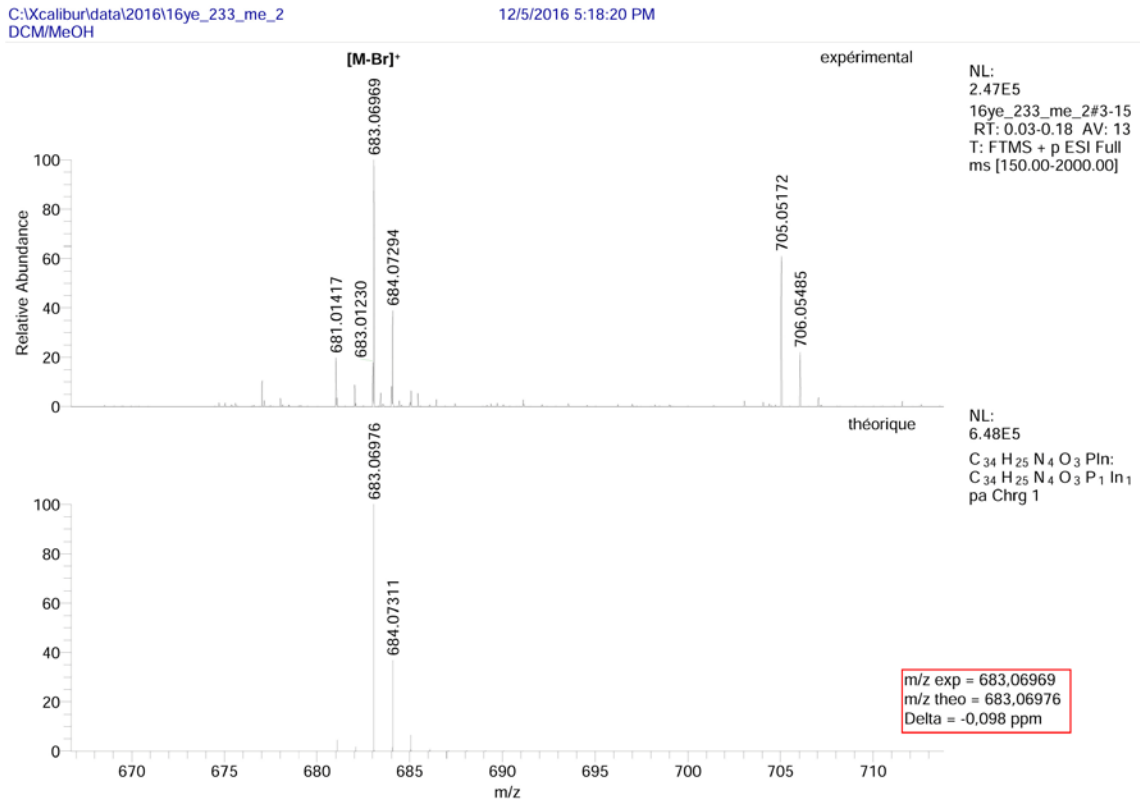
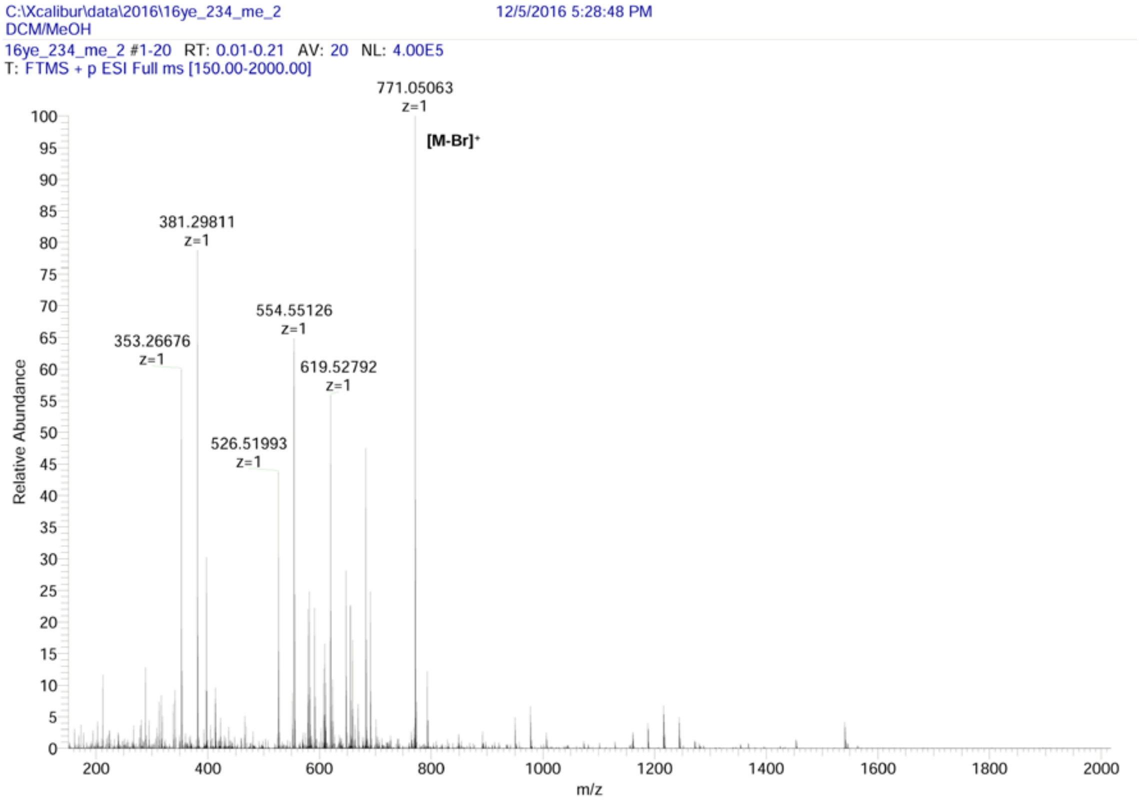


Figure S85. ESI-HR mass spectrum of ***In-4b****.*



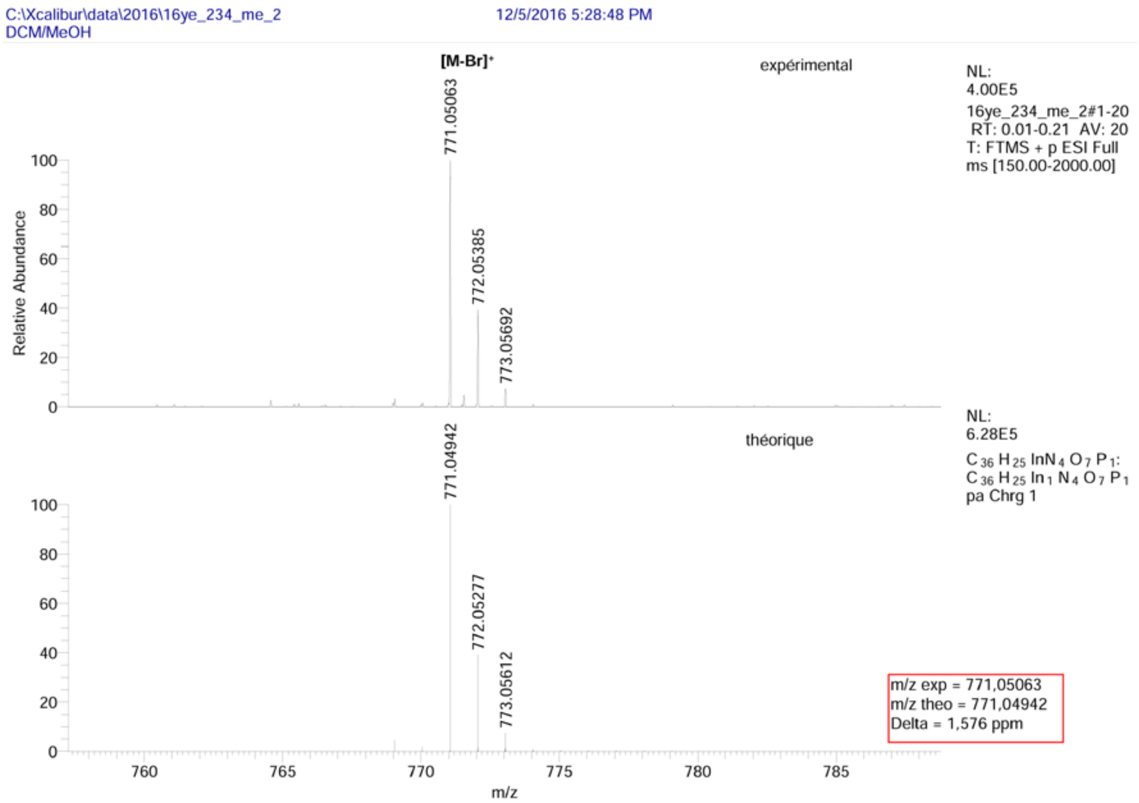


Figure S86. ESI-HR mass spectrum of ***In-4c****.*

8. X-ray crystal data and refinement parameters for In-1b, In-1c, Ga-2b, Ga-5b

Table S1. X-ray crystal data and refinement parameters for ***In-1b, In-1c, Ga-2b, Ga-5b***

Crystal parameters	**In-1b**	**In-1c**	**Ga-2b**	**Ga-5b**
CCDC				
Empirical Formula	$C_{38}H_{33}ClInN_4O_3P$	$C_{82}H_{70}Cl_8In_2N_8O_{14}P_2$	$C_{82}H_{66}Ga_2N_{10}O_6P_2$	$C_{34}H_{24}BrGaN_4$
Formula weight (g.mol^{-1})	774.92	1966.64	1488.82	638.20
Color	Red	Red	Red	Red
Temperature (K)	150(2)	150(2)	150(2)	150(2)
Crystal system	triclinic	triclinic	monoclinic	monoclinic
Space group	P-1	P-1	P 21/c	I 2/a
a(Å)	12.995(3)	12.878(5)	13.1515(8)	23.741(4)
b(Å)	16.152(4)	12.999(5)	16.1484(10)	8.2881(12)
c(Å)	16.714(4)	14.300(6)	19.9763(12)	37.026(5)

α(°)	86.087(4)	98.088(7)	90	90
β(°)	78.858(4)	114.435(6)	96.1430(10)	93.187(4)
γ(°)	88.057(4)	90.425(7)	90	90
Cell volume (Å^3)	3433.4(15)	2152.1(16)	4218.1(4)	7274.1(19)
Z	4	1	2	8
ρ_{calcd}(mg.m^{-3})	1.499	1.517	1.172	1.166
μ (mm^{-1})	0.856	0.888	0.730	1.879
F(000)	1576	994	1536	2576
Crystal size (mm)	0.24 x 0.22 x 0.20	0.14 x 0.12 x 0.10	0.24 x 0.22 x 0.20	0.24 x 0.22 x 0.20
θ range for data collection (deg).	1.827 to 26.000	2.269 to 27.998	2.051 to 30.000	2.603 to 27.000
index ranges	-16<=h<=16, -19<=k<=19, -20<=l<=20	-17<=h<=17, -17<=k<=17, -18<=l<=18	-18<=h<=18, -22<=k<=19, -28<=l<=27	-30<=h<=30, -10<=k<=10, -47<=l<=47

reflns collected	29610	22212	32619	33310
independentreflns	13429[R(int) = 0.0742]	10341 [R(int) = 0.1529]	12263[R(int) = 0.0376]	7919[R(int) = 0.1469]
data / restraints / params	13429 / 1 / 853	10341 / 0 / 526	12263 / 0 / 463	7919 / 1 / 344
goodness-of-fit on F^2	1.014	0.950	1.029	1.003
[a]final R indices [I>2sigma(I)]	R1 = 0.0727, wR2 = 0.1798	R1 = 0.0797, wR2 = 0.1570	R1 = 0.0428, wR2 = 0.1023	R1 = 0.0664, wR2 = 0.1610
[a]R indices (all data)	R1 = 0.1407, wR2 = 0.2206	R1 = 0.2159, wR2 = 0.2147	R1 = 0.0731, wR2 = 0.1139	R1 = 0.1417, wR2 = 0.1922
[b]largest diff. peak and hole(e.A^{-3})	2.179and -1.633	0.927 and -1.278	0.742 and -0.317	1.138and -0.968

[a]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma w(F_o^2)^2\}^{1/2}$

[b]In all structures the largest diff. peak is observed in the vicinity of heavy atom.

*Table S2. Bond lengths [Å] and angles [°] for **In-1b***

In1 N3 2.155(6)	In1 N2 2.156(6)
In1 N1 2.160(6)	In1 N4 2.171(6)
In1 Cl1 2.372(2)	In2 N6 2.140(8)
In2 N7 2.153(8)	In2 N8 2.161(8)
In2 N5 2.167(8)	In2 Cl2 2.386(2)
P1 O1 1.448(6)	P1 O3 1.526(8)
P1 O2 1.581(8)	P1 C5 1.839(8)
P2 O5 1.44(3)	P2 O5A 1.46(3)
P2 O6 1.474(19)	P2 O4A 1.49(3)
P2 O6A 1.70(2)	P2 O4 1.74(3)
P2 C43 1.814(10)	O2 C6 1.521(18)
O3 C8 1.508(18)	O4 C44 1.30(3)
C44 C45 1.55(4)	O4A C44A 1.74(3)
O4A O6A 1.82(3)	C44A C45A 1.4501(11)
O6 C46 1.68(2)	O6A C46 1.40(2)
C46 C47 1.456(18)	N1 C1 1.381(9)
N1 C4 1.382(10)	N2 C10 1.378(9)
N2 C13 1.386(9)	N3 C25 1.378(10)
N3 C22 1.389(10)	N4 C30 1.370(10)
N4 C27 1.383(10)	N5 C39 1.349(11)
N5 C42 1.364(12)	N6 C51 1.360(12)
N6 C48 1.386(13)	N7 C63 1.376(12)
N7 C60 1.374(12)	N8 C65 1.367(11)
N8 C68 1.397(12)	C1 C31 1.405(11)

C1 C2 1.427(11)	C2 C3 1.332(12)
C3 C4 1.434(11)	C4 C5 1.420(11)
C5 C10 1.390(11)	C6 C7 1.48(2)
C8 C9 1.43(2)	C10 C11 1.449(10)
C11 C12 1.335(11)	C12 C13 1.437(10)
C13 C14 1.399(10)	C14 C22 1.407(10)
C14 C15 1.507(10)	C15 C21 1.360(12)
C15 C16 1.379(12)	C16 C17 1.389(12)
C17 C18 1.358(14)	C18 C20 1.379(14)
C18 C19 1.514(12)	C20 C21 1.381(13)
C22 C23 1.441(11)	C23 C24 1.335(11)
C24 C25 1.443(11)	C25 C26 1.383(11)
C26 C27 1.379(11)	C27 C28 1.429(11)
C28 C29 1.348(12)	C29 C30 1.422(10)
C30 C31 1.401(11)	C31 C32 1.510(10)
C32 C33 1.374(12)	C32 C38 1.375(12)
C33 C34 1.382(13)	C34 C35 1.386(13)
C35 C37 1.371(13)	C35 C36 1.505(12)
C37 C38 1.371(12)	C39 C69 1.434(13)
C39 C40 1.434(13)	C40 C41 1.341(14)
C41 C42 1.439(14)	C42 C43 1.420(14)
C43 C48 1.422(15)	C48 C49 1.462(14)
C49 C50 1.325(16)	C50 C51 1.441(14)
C51 C52 1.409(15)	C52 C60 1.386(14)
C52 C53 1.508(14)	C53 C54 1.371(13)
C53 C59 1.385(15)	C54 C55 1.385(14)

C55 C56 1.333(16)	C56 C58 1.366(19)
C56 C57 1.492(17)	C58 C59 1.403(19)
C60 C61 1.447(14)	C61 C62 1.336(14)
C62 C63 1.431(14)	C63 C64 1.365(13)
C64 C65 1.388(13)	C65 C66 1.422(13)
C66 C67 1.361(13)	C67 C68 1.402(12)
C68 C69 1.385(12)	C69 C70 1.518(13)
C70 C76 1.362(14)	C70 C71 1.375(13)
C71 C72 1.380(14)	C72 C73 1.368(15)
C73 C75 1.358(14)	C73 C74 1.505(14)
C75 C76 1.371(15)	
N3 In1 N2 86.1(2) .	N3 In1 N1 147.5(2) .
N2 In1 N1 85.0(2) .	N3 In1 N4 85.8(2) .
N2 In1 N4 147.2(2) .	N1 In1 N4 85.0(2) .
N3 In1 Cl1 106.89(19) .	N2 In1 Cl1 105.75(18) .
N1 In1 Cl1 105.60(18) .	N4 In1 Cl1 107.02(18) .
N6 In2 N7 86.7(3) .	N6 In2 N8 150.9(3) .
N7 In2 N8 85.2(3) .	N6 In2 N5 85.7(3) .
N7 In2 N5 147.3(3) .	N8 In2 N5 86.2(3) .
N6 In2 Cl2 102.8(2) .	N7 In2 Cl2 107.0(2) .
N8 In2 Cl2 106.3(2) .	N5 In2 Cl2 105.7(2) .
O1 P1 O3 118.5(4) .	O1 P1 O2 110.9(4) .
O3 P1 O2 98.1(5) .	O1 P1 C5 113.3(4) .
O3 P1 C5 108.0(4) .	O2 P1 C5 106.5(4) .
O5 P2 O6 131.6(11) .	O5A P2 O4A 116.7(15) .
O5A P2 O6A 138.0(11) .	O4A P2 O6A 69.1(10) .

O5 P2 O4 92.6(13) .	O6 P2 O4 103.4(12) .
O5 P2 C43 109.5(11) .	O5A P2 C43 110.2(11) .
O6 P2 C43 111.7(8) .	O4A P2 C43 115.5(11) .
O6A P2 C43 102.0(7) .	O4 P2 C43 101.0(9) .
C6 O2 P1 120.7(8) .	C8 O3 P1 116.5(8) .
C44 O4 P2 121(2) .	O4 C44 C45 103(3) .
P2 O4A C44A 104.9(14) .	P2 O4A O6A 60.9(11) .
C44A O4A O6A 165.6(18) .	C45A C44A O4A 119(2) .
P2 O6 C46 113.9(14) .	C46 O6A P2 116.6(15) .
C46 O6A O4A 166.4(19) .	P2 O6A O4A 50.0(9) .
O6A C46 C47 152.4(17) .	C47 C46 O6 100.6(13) .
C1 N1 C4 107.5(6) .	C1 N1 In1 125.6(5) .
C4 N1 In1 125.3(5) .	C10 N2 C13 107.7(6) .
C10 N2 In1 125.8(5) .	C13 N2 In1 125.2(5) .
C25 N3 C22 106.9(6) .	C25 N3 In1 125.5(5) .
C22 N3 In1 126.6(5) .	C30 N4 C27 108.0(6) .
C30 N4 In1 126.6(5) .	C27 N4 In1 124.7(5) .
C39 N5 C42 108.5(8) .	C39 N5 In2 125.8(6) .
C42 N5 In2 125.0(6) .	C51 N6 C48 108.0(8) .
C51 N6 In2 124.5(7) .	C48 N6 In2 125.9(7) .
C63 N7 C60 107.3(8) .	C63 N7 In2 125.3(7) .
C60 N7 In2 125.6(7) .	C65 N8 C68 107.3(8) .
C65 N8 In2 124.9(6) .	C68 N8 In2 126.7(6) .
N1 C1 C31 126.3(7) .	N1 C1 C2 107.8(7) .
C31 C1 C2 125.8(7) .	C3 C2 C1 108.8(7) .
C2 C3 C4 107.7(8) .	N1 C4 C5 124.8(7) .

N1 C4 C3 108.1(7) .	C5 C4 C3 127.1(8) .
C10 C5 C4 126.8(7) .	C10 C5 P1 117.4(6) .
C4 C5 P1 115.7(6) .	C7 C6 O2 113.1(12) .
C9 C8 O3 111.1(16) .	N2 C10 C5 124.8(7) .
N2 C10 C11 108.0(6) .	C5 C10 C11 127.0(7) .
C12 C11 C10 107.9(7) .	C11 C12 C13 108.2(7) .
N2 C13 C14 126.6(7) .	N2 C13 C12 108.1(6) .
C14 C13 C12 125.3(7) .	C13 C14 C22 127.0(7) .
C13 C14 C15 116.5(6) .	C22 C14 C15 116.4(7) .
C21 C15 C16 117.8(8) .	C21 C15 C14 121.7(8) .
C16 C15 C14 120.5(8) .	C15 C16 C17 119.8(9) .
C18 C17 C16 122.7(9) .	C17 C18 C20 116.9(8) .
C17 C18 C19 122.1(10) .	C20 C18 C19 121.0(10) .
C18 C20 C21 120.9(10) .	C15 C21 C20 121.9(10) .
N3 C22 C14 124.3(7) .	N3 C22 C23 108.7(7) .
C14 C22 C23 126.8(7) .	C24 C23 C22 107.5(7) .
C23 C24 C25 108.4(7) .	C26 C25 N3 124.3(7) .
C26 C25 C24 127.0(8) .	N3 C25 C24 108.4(7) .
C27 C26 C25 129.1(8) .	C26 C27 N4 125.2(7) .
C26 C27 C28 127.1(8) .	N4 C27 C28 107.6(7) .
C29 C28 C27 108.1(7) .	C28 C29 C30 107.8(7) .
N4 C30 C31 125.7(7) .	N4 C30 C29 108.5(7) .
C31 C30 C29 125.7(7) .	C30 C31 C1 125.8(7) .
C30 C31 C32 116.8(7) .	C1 C31 C32 117.3(7) .
C33 C32 C38 118.0(8) .	C33 C32 C31 121.0(8) .
C38 C32 C31 120.9(7) .	C32 C33 C34 120.3(9) .

C33 C34 C35 122.0(9) .	C37 C35 C34 116.3(8) .
C37 C35 C36 121.9(9) .	C34 C35 C36 121.8(9) .
C35 C37 C38 122.3(9) .	C37 C38 C32 120.9(9) .
N5 C39 C69 126.8(8) .	N5 C39 C40 109.2(8) .
C69 C39 C40 123.9(9) .	C41 C40 C39 106.5(10) .
C40 C41 C42 108.3(9) .	N5 C42 C43 125.9(10) .
N5 C42 C41 107.4(9) .	C43 C42 C41 126.6(9) .
C42 C43 C48 125.9(9) .	C42 C43 P2 116.3(8) .
C48 C43 P2 117.8(8) .	N6 C48 C43 124.2(9) .
N6 C48 C49 108.0(10) .	C43 C48 C49 127.6(10) .
C50 C49 C48 106.4(11) .	C49 C50 C51 109.6(10) .
N6 C51 C52 126.3(9) .	N6 C51 C50 107.9(9) .
C52 C51 C50 125.9(10) .	C60 C52 C51 127.6(10) .
C60 C52 C53 116.2(10) .	C51 C52 C53 116.2(10) .
C54 C53 C59 118.3(10) .	C54 C53 C52 120.2(9) .
C59 C53 C52 121.3(10) .	C53 C54 C55 120.8(10) .
C56 C55 C54 122.3(11) .	C55 C56 C58 117.3(12) .
C55 C56 C57 123.6(14) .	C58 C56 C57 119.1(14) .
C56 C58 C59 122.8(12) .	C53 C59 C58 118.3(12) .
N7 C60 C52 124.4(10) .	N7 C60 C61 108.2(9) .
C52 C60 C61 127.4(10) .	C62 C61 C60 107.8(9) .
C61 C62 C63 107.8(9) .	C64 C63 N7 124.9(9) .
C64 C63 C62 126.2(10) .	N7 C63 C62 108.9(9) .
C63 C64 C65 128.7(10) .	N8 C65 C64 124.8(9) .
N8 C65 C66 108.7(9) .	C64 C65 C66 126.3(9) .
C67 C66 C65 107.4(9) .	C66 C67 C68 108.2(9) .

C69 C68 N8 123.6(9) .	C69 C68 C67 127.8(9) .
N8 C68 C67 108.3(8) .	C68 C69 C39 127.4(9) .
C68 C69 C70 115.8(8) .	C39 C69 C70 116.7(8) .
C76 C70 C71 117.5(9) .	C76 C70 C69 122.3(8) .
C71 C70 C69 120.2(9) .	C70 C71 C72 121.4(10) .
C73 C72 C71 121.1(10) .	C75 C73 C72 116.5(10) .
C75 C73 C74 122.6(10) .	C72 C73 C74 120.8(10) .
C73 C75 C76 123.3(10) .	C70 C76 C75 120.2(10) .

Table S3. Bond lengths [Å] and angles [°] for ***In-1c***

In1 N3 2.115(7)	In1 N4 2.128(7)
In1 N1 2.136(7)	In1 N2 2.148(7)
In1 O1 2.423(6)	In1 Cl1 2.500(3)
P1 O1 1.475(6)	P1 O2 1.572(6)
P1 O3 1.575(6)	P1 C36 1.823(9)
Cl2 C1S 1.752(10)	Cl3 C1S 1.781(11)
Cl4 C1S 1.773(10)	O2 C37 1.460(11)
O3 C39 1.452(10)	O4 C10 1.322(12)
O4 C11 1.482(11)	O5 C10 1.208(11)
O7 C28 1.193(13)	O8 C28 1.369(13)
O8 C29 1.444(12)	N1 C4 1.368(10)
N1 C1 1.386(10)	N2 C17 1.359(11)
N2 C14 1.377(11)	N3 C22 1.361(10)
N3 C19 1.375(10)	N4 C35 1.390(10)
N4 C32 1.401(10)	C1 C2 1.438(11)
C1 C36 1.439(11)	C2 C3 1.358(11)

C3 C4 1.464(11)	C4 C5 1.401(11)
C5 C14 1.411(12)	C5 C6 1.517(11)
C6 C13 1.385(13)	C6 C7 1.403(12)
C7 C8 1.396(12)	C8 C9 1.369(12)
C9 C12 1.370(13)	C9 C10 1.499(12)
C12 C13 1.395(13)	C14 C15 1.468(11)
C15 C16 1.364(12)	C16 C17 1.441(12)
C17 C18 1.399(12)	C18 C19 1.402(12)
C19 C20 1.460(12)	C20 C21 1.354(13)
C21 C22 1.461(11)	C22 C23 1.439(12)
C23 C32 1.411(11)	C23 C24 1.492(12)
C24 C25 1.382(13)	C24 C31 1.420(13)
C25 C26 1.398(13)	C26 C27 1.377(14)
C27 C30 1.416(14)	C27 C28 1.502(14)
C30 C31 1.382(12)	C32 C33 1.440(12)
C33 C34 1.346(11)	C34 C35 1.445(11)
C35 C36 1.416(11)	C36 P1 1.823(9)
C37 C38 1.485(13)	C39 C40 1.502(13)
N3 In1 N4 90.4(3) .	N3 In1 N1 166.4(3) .
N4 In1 N1 88.2(3) .	N3 In1 N2 89.7(3) .
N4 In1 N2 165.5(3) .	N1 In1 N2 88.4(3) .
N3 In1 O1 78.4(2) .	N4 In1 O1 83.6(2) .
N1 In1 O1 88.0(2) .	N2 In1 O1 82.2(2) .
N3 In1 Cl1 92.9(2) .	N4 In1 Cl1 95.6(2) .
N1 In1 Cl1 100.7(2) .	N2 In1 Cl1 98.9(2) .
O1 In1 Cl1 171.31(15) .	O1 P1 O2 107.3(4) .

O1 P1 O3 114.5(4) .	O2 P1 O3 106.5(3) .
O1 P1 C36 112.9(4)	O2 P1 C36 109.2(4)
O3 P1 C36 106.2(3)	P1 O1 In1 145.7(4) .
C37 O2 P1 123.0(5) .	C39 O3 P1 120.9(6) .
C10 O4 C11 116.0(8) .	C28 O8 C29 116.0(9) .
C4 N1 C1 108.8(7) .	C4 N1 In1 125.6(6) .
C1 N1 In1 125.4(5) .	C17 N2 C14 110.0(7) .
C17 N2 In1 124.4(6) .	C14 N2 In1 125.6(6) .
C22 N3 C19 107.5(7) .	C22 N3 In1 126.9(6) .
C19 N3 In1 125.5(6) .	C35 N4 C32 108.4(7) .
C35 N4 In1 127.1(6) .	C32 N4 In1 122.4(6) .
N1 C1 C2 107.8(7) .	N1 C1 C36 125.9(7) .
C2 C1 C36 126.2(8) .	Cl2 C1S Cl4 110.6(6) .
Cl2 C1S Cl3 111.3(6) .	Cl4 C1S Cl3 109.7(6) .
C3 C2 C1 108.4(7) .	C2 C3 C4 106.9(7) .
N1 C4 C5 126.7(8) .	N1 C4 C3 108.0(7) .
C5 C4 C3 125.3(7) .	C4 C5 C14 127.2(8) .
C4 C5 C6 116.8(8) .	C14 C5 C6 116.0(8) .
C13 C6 C7 118.7(8) .	C13 C6 C5 120.6(8) .
C7 C6 C5 120.5(8) .	C8 C7 C6 119.6(9) .
C9 C8 C7 121.6(9) .	C8 C9 C12 118.3(9) .
C8 C9 C10 117.8(9) .	C12 C9 C10 123.9(9) .
O5 C10 O4 123.5(9) .	O5 C10 C9 125.0(10) .
O4 C10 C9 111.4(9) .	C9 C12 C13 122.0(10) .
C6 C13 C12 119.7(9) .	N2 C14 C5 125.7(8) .
N2 C14 C15 106.7(7) .	C5 C14 C15 127.3(8) .

C16 C15 C14 107.3(8) .	C15 C16 C17 107.8(8) .
N2 C17 C18 125.6(8) .	N2 C17 C16 108.2(8) .
C18 C17 C16 126.2(9) .	C17 C18 C19 129.5(9) .
N3 C19 C18 124.7(8) .	N3 C19 C20 109.0(8) .
C18 C19 C20 126.4(8) .	C21 C20 C19 107.1(8) .
C20 C21 C22 106.9(8) .	N3 C22 C23 124.0(8) .
N3 C22 C21 109.5(8) .	C23 C22 C21 126.4(8) .
C32 C23 C22 127.5(8) .	C32 C23 C24 114.5(8) .
C22 C23 C24 118.0(7) .	C25 C24 C31 117.7(9) .
C25 C24 C23 123.4(9) .	C31 C24 C23 118.9(8) .
C24 C25 C26 121.6(10) .	C27 C26 C25 120.1(10) .
C26 C27 C30 119.9(10) .	C26 C27 C28 118.8(10) .
C30 C27 C28 121.3(12) .	O7 C28 O8 124.5(11) .
O7 C28 C27 123.9(12) .	O8 C28 C27 111.4(10) .
C31 C30 C27 119.2(11) .	C30 C31 C24 121.4(9) .
N4 C32 C23 126.9(8) .	N4 C32 C33 107.4(7) .
C23 C32 C33 125.7(8) .	C34 C33 C32 108.3(8) .
C33 C34 C35 108.8(8) .	N4 C35 C36 123.2(7) .
N4 C35 C34 107.1(7) .	C36 C35 C34 129.6(8) .
C35 C36 C1 127.5(8) .	C35 C36 P1 121.2(6)
C1 C36 P1 111.3(6)	O2 C37 C38 108.8(8) .
O3 C39 C40 107.9(7) .	

Table S4. Bond lengths [Å] and angles [°] for ***Ga-2b***

Ga1 O1 1.9705(17)	Ga1 N3 2.026(2)
Ga1 N4 2.028(2)	Ga1 N1 2.034(2)

Ga1 N2 2.036(2)	Ga1 N5 2.207(2)
P1 O2 1.4706(19)	P1 O1 1.5097(17)
P1 O3 1.6032(19)	P1 C22 1.839(2)
O3 C35 1.447(3)	N1 C1 1.372(3)
N1 C4 1.379(3)	N2 C9 1.370(3)
N2 C6 1.377(3)	N3 C21 1.383(3)
N3 C18 1.387(3)	N4 C26 1.381(3)
N4 C23 1.386(3)	N5 C41 1.328(4)
N5 C37 1.334(3)	C1 C27 1.392(4)
C1 C2 1.440(4)	C2 C3 1.340(4)
C3 C4 1.430(4)	C4 C5 1.390(4)
C5 C6 1.380(4)	C6 C7 1.425(4)
C7 C8 1.339(4)	C8 C9 1.444(4)
C9 C10 1.396(4)	C10 C18 1.397(3)
C10 C11 1.486(4)	C11 C17 1.382(4)
C11 C12 1.390(4)	C12 C13 1.393(4)
C13 C14 1.370(5)	C14 C16 1.373(5)
C14 C15 1.527(5)	C16 C17 1.383(4)
C18 C19 1.435(3)	C19 C20 1.336(4)
C20 C21 1.449(3)	C21 C22 1.409(3)
C22 C23 1.401(3)	C22 P1 1.839(2)
C23 C24 1.441(3)	C24 C25 1.339(3)
C25 C26 1.431(3)	C26 C27 1.398(3)
C27 C28 1.500(4)	C28 C34 1.385(4)
C28 C29 1.399(4)	C29 C30 1.386(4)
C30 C31 1.382(4)	C31 C33 1.378(5)

C31 C32 1.501(5)	C33 C34 1.392(4)
C35 C36 1.483(5)	C37 C38 1.377(4)
C38 C39 1.360(4)	C39 C40 1.375(4)
C40 C41 1.381(4)	
O1 Ga1 N3 94.72(8) .	O1 Ga1 N4 92.74(8) .
N3 Ga1 N4 89.88(8) .	O1 Ga1 N1 88.82(8) .
N3 Ga1 N1 176.42(8) .	N4 Ga1 N1 89.42(8) .
O1 Ga1 N2 91.98(8) .	N3 Ga1 N2 89.51(8) .
N4 Ga1 N2 175.27(8) .	N1 Ga1 N2 90.91(9) .
O1 Ga1 N5 175.89(7) .	N3 Ga1 N5 88.97(8) .
N4 Ga1 N5 89.06(8) .	N1 Ga1 N5 87.51(8) .
N2 Ga1 N5 86.24(8) .	O2 P1 O1 118.14(11) .
O2 P1 O3 110.87(11) .	O1 P1 O3 102.46(10) .
O2 P1 C22 112.77(11)	O1 P1 C22 107.53(10)
O3 P1 C22 103.66(10)	P1 O1 Ga1 137.37(11) .
C35 O3 P1 117.83(18) .	C1 N1 C4 106.5(2) .
C1 N1 Ga1 127.62(17) .	C4 N1 Ga1 125.60(19) .
C9 N2 C6 106.6(2) .	C9 N2 Ga1 127.72(17) .
C6 N2 Ga1 125.72(18) .	C21 N3 C18 106.6(2) .
C21 N3 Ga1 127.05(17) .	C18 N3 Ga1 125.99(16) .
C26 N4 C23 106.8(2) .	C26 N4 Ga1 126.26(16) .
C23 N4 Ga1 126.97(17) .	C41 N5 C37 117.1(2) .
C41 N5 Ga1 121.10(19) .	C37 N5 Ga1 121.78(19) .
N1 C1 C27 124.8(2) .	N1 C1 C2 109.2(2) .
C27 C1 C2 125.9(3) .	C3 C2 C1 107.2(3) .
C2 C3 C4 107.8(2) .	N1 C4 C5 125.2(3) .

N1 C4 C3 109.2(2) .	C5 C4 C3 125.6(3) .
C6 C5 C4 126.9(3) .	N2 C6 C5 125.3(3) .
N2 C6 C7 109.4(3) .	C5 C6 C7 125.2(3) .
C8 C7 C6 107.7(3) .	C7 C8 C9 107.3(3) .
N2 C9 C10 125.2(2) .	N2 C9 C8 109.0(2) .
C10 C9 C8 125.7(3) .	C9 C10 C18 124.4(2) .
C9 C10 C11 118.6(2) .	C18 C10 C11 117.0(2) .
C17 C11 C12 117.7(3) .	C17 C11 C10 122.1(3) .
C12 C11 C10 120.1(3) .	C13 C12 C11 120.4(3) .
C14 C13 C12 120.9(3) .	C13 C14 C16 119.0(3) .
C13 C14 C15 120.6(4) .	C16 C14 C15 120.4(4) .
C14 C16 C17 120.5(3) .	C11 C17 C16 121.5(3) .
N3 C18 C10 126.6(2) .	N3 C18 C19 109.0(2) .
C10 C18 C19 124.4(2) .	C20 C19 C18 108.0(2) .
C19 C20 C21 107.8(2) .	N3 C21 C22 125.9(2) .
N3 C21 C20 108.6(2) .	C22 C21 C20 125.5(2) .
C23 C22 C21 123.9(2) .	C23 C22 P1 120.49(18)
C21 C22 P1 115.51(17)	N4 C23 C22 126.0(2) .
N4 C23 C24 108.4(2) .	C22 C23 C24 125.6(2) .
C25 C24 C23 108.0(2) .	C24 C25 C26 107.8(2) .
N4 C26 C27 126.4(2) .	N4 C26 C25 109.1(2) .
C27 C26 C25 124.6(2) .	C1 C27 C26 124.7(2) .
C1 C27 C28 118.7(2) .	C26 C27 C28 116.5(2) .
C34 C28 C29 117.7(3) .	C34 C28 C27 121.9(3) .
C29 C28 C27 120.3(2) .	C30 C29 C28 120.6(3) .
C31 C30 C29 121.4(3) .	C33 C31 C30 118.1(3) .

C33 C31 C32 121.9(3) .	C30 C31 C32 120.0(3) .
C31 C33 C34 121.1(3) .	C28 C34 C33 121.0(3) .
O3 C35 C36 109.4(3) .	N5 C37 C38 123.3(3) .
C39 C38 C37 118.9(3) .	C38 C39 C40 119.0(3) .
C39 C40 C41 118.5(3) .	N5 C41 C40 123.2(3) .

Table S5. Bond lengths [Å] and angles [°] for ***Ga-5b***

Ga1 N4 2.010(5)	Ga1 N3 2.019(5)
Ga1 N1 2.025(5)	Ga1 N2 2.026(5)
Ga1 Br1 2.3956(10)	N1 C1 1.378(8)
N1 C4 1.390(8)	N2 C16 1.363(8)
N2 C13 1.373(8)	N3 C18 1.382(8)
N3 C21 1.385(8)	N4 C33 1.385(8)
N4 C30 1.395(9)	C1 C34 1.379(10)
C1 C2 1.431(10)	C2 C3 1.315(10)
C3 C4 1.447(9)	C4 C5 1.387(9)
C5 C13 1.395(9)	C5 C6 1.520(9)
C6 C12 1.382(9)	C6 C7 1.388(9)
C7 C8 1.375(10)	C8 C9 1.398(12)
C9 C11 1.320(11)	C9 C10 1.531(11)
C11 C12 1.391(10)	C13 C14 1.420(9)
C14 C15 1.347(9)	C15 C16 1.440(9)
C16 C17 1.369(8)	C17 C18 1.383(8)
C18 C19 1.426(8)	C19 C20 1.314(9)
C20 C21 1.432(9)	C21 C22 1.415(10)
C22 C30 1.362(10)	C22 C23 1.511(11)

C23 C29 1.338(13)	C23 C24 1.35(2)
C23 C24A 1.50(2)	C24 C25 1.33(2)
C25 C26 1.58(2)	C24A C25A 1.42(2)
C25A C26 1.45(2)	C26 C28 1.286(13)
C26 C27 1.4506(10)	C28 C29 1.404(12)
C30 C31 1.453(10)	C31 C32 1.317(11)
C32 C33 1.427(10)	C33 C34 1.378(10)
N4 Ga1 N3 86.9(2) .	N4 Ga1 N1 88.6(2) .
N3 Ga1 N1 157.9(2) .	N4 Ga1 N2 157.8(2) .
N3 Ga1 N2 89.2(2) .	N1 Ga1 N2 86.9(2) .
N4 Ga1 Br1 103.04(16) .	N3 Ga1 Br1 99.01(15) .
N1 Ga1 Br1 103.14(15) .	N2 Ga1 Br1 99.13(15) .
C1 N1 C4 105.2(5) .	C1 N1 Ga1 127.6(5) .
C4 N1 Ga1 126.4(4) .	C16 N2 C13 106.4(5) .
C16 N2 Ga1 126.6(4) .	C13 N2 Ga1 126.4(4) .
C18 N3 C21 104.8(5) .	C18 N3 Ga1 127.2(4) .
C21 N3 Ga1 126.5(4) .	C33 N4 C30 105.0(6) .
C33 N4 Ga1 128.6(5) .	C30 N4 Ga1 126.1(4) .
C34 C1 N1 124.4(6) .	C34 C1 C2 125.9(7) .
N1 C1 C2 109.7(7) .	C3 C2 C1 108.5(7) .
C2 C3 C4 107.2(7) .	C5 C4 N1 123.9(6) .
C5 C4 C3 126.7(7) .	N1 C4 C3 109.3(6) .
C4 C5 C13 124.4(6) .	C4 C5 C6 119.4(6) .
C13 C5 C6 115.6(6) .	C12 C6 C7 117.5(7) .
C12 C6 C5 120.4(6) .	C7 C6 C5 122.1(6) .
C8 C7 C6 122.0(7) .	C7 C8 C9 119.3(8) .

C11 C9 C8 118.5(7) .	C11 C9 C10 119.3(9) .
C8 C9 C10 122.0(9) .	C9 C11 C12 123.5(8) .
C6 C12 C11 119.2(7) .	N2 C13 C5 124.6(6) .
N2 C13 C14 109.6(6) .	C5 C13 C14 125.5(6) .
C15 C14 C13 107.9(6) .	C14 C15 C16 106.5(6) .
N2 C16 C17 126.0(6) .	N2 C16 C15 109.7(5) .
C17 C16 C15 124.2(6) .	C16 C17 C18 126.1(6) .
N3 C18 C17 124.0(6) .	N3 C18 C19 110.2(6) .
C17 C18 C19 125.8(6) .	C20 C19 C18 107.3(6) .
C19 C20 C21 108.4(6) .	N3 C21 C22 123.4(6) .
N3 C21 C20 109.2(6) .	C22 C21 C20 127.0(6) .
C30 C22 C21 123.6(7) .	C30 C22 C23 118.7(8) .
C21 C22 C23 117.6(8) .	C29 C23 C24 115.0(13) .
C29 C23 C24A 113.3(12) .	C29 C23 C22 122.7(10) .
C24 C23 C22 117.9(13) .	C24A C23 C22 116.0(11) .
C25 C24 C23 120(2) .	C24 C25 C26 121(2) .
C25A C24A C23 116.4(19) .	C24A C25A C26 120.3(19) .
C28 C26 C27 125.5(10) .	C28 C26 C25A 111.4(10) .
C27 C26 C25A 117.7(12) .	C28 C26 C25 103.5(10) .
C27 C26 C25 122.9(12) .	C26 C28 C29 126.4(10) .
C23 C29 C28 119.6(11) .	C22 C30 N4 125.9(6) .
C22 C30 C31 125.5(7) .	N4 C30 C31 108.3(7) .
C32 C31 C30 108.7(7) .	C31 C32 C33 107.3(7) .
C34 C33 N4 123.8(7) .	C34 C33 C32 125.4(7) .
N4 C33 C32 110.8(7) .	C1 C34 C33 126.4(6) .

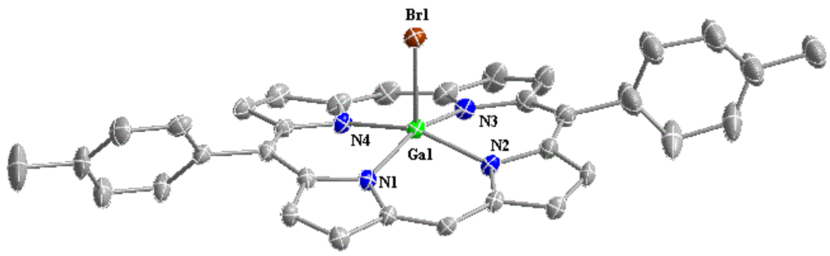


*Figure S87. Molecular structure of the complex **Ga-5b**. Displacement ellipsoids are drawn at 30 % probability level, hydrogen atoms are omitted for clarity.*