Supplementary data for:

**The coordination chemistry and anticancer activity of organo-ruthenium(II), -iridium(III) and -rhodium(III) complexes with sulfonyl-substituted thiourea ligands.**

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Crystallographic information:

Table 1: Selected bond lengths in the molecular structure of complexes **aL1**, **aL2**, **1aL1**, **1bL1**, **2aL1**, **2cL1**, **2dL1** and **$a_2$L1**. Arene = cymene or benzene centroid, Cp* = Cp* centroid.

Table 2: Crystallographic details of complexes **aL1**, **aL2**, **2dL1**, **2aL1**, **1aL1**, **1bL3** and **$a_2$L1**.

Cartesian coordinates:

aL1 – Proximal

aL1 – Distal

aL2 – Proximal

aL2 – Distal

1aL1 – Proximal

1aL1 – Distal

1aL3 – Proximal

1aL3 – Distal

2aL1 – Proximal

2aL1 – Distal

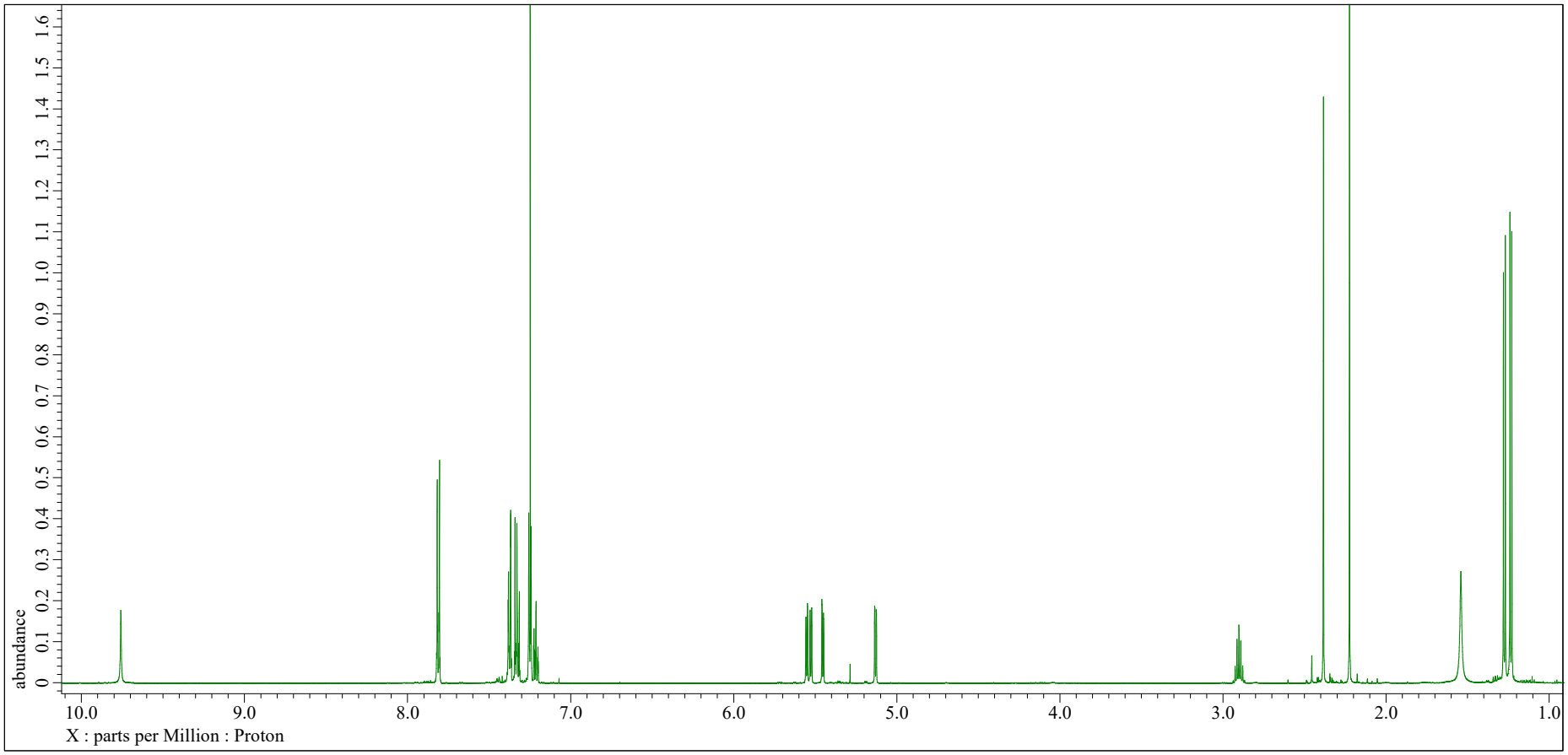


Figure S1: $^{1}H$ NMR spectrum of complex **aL1**

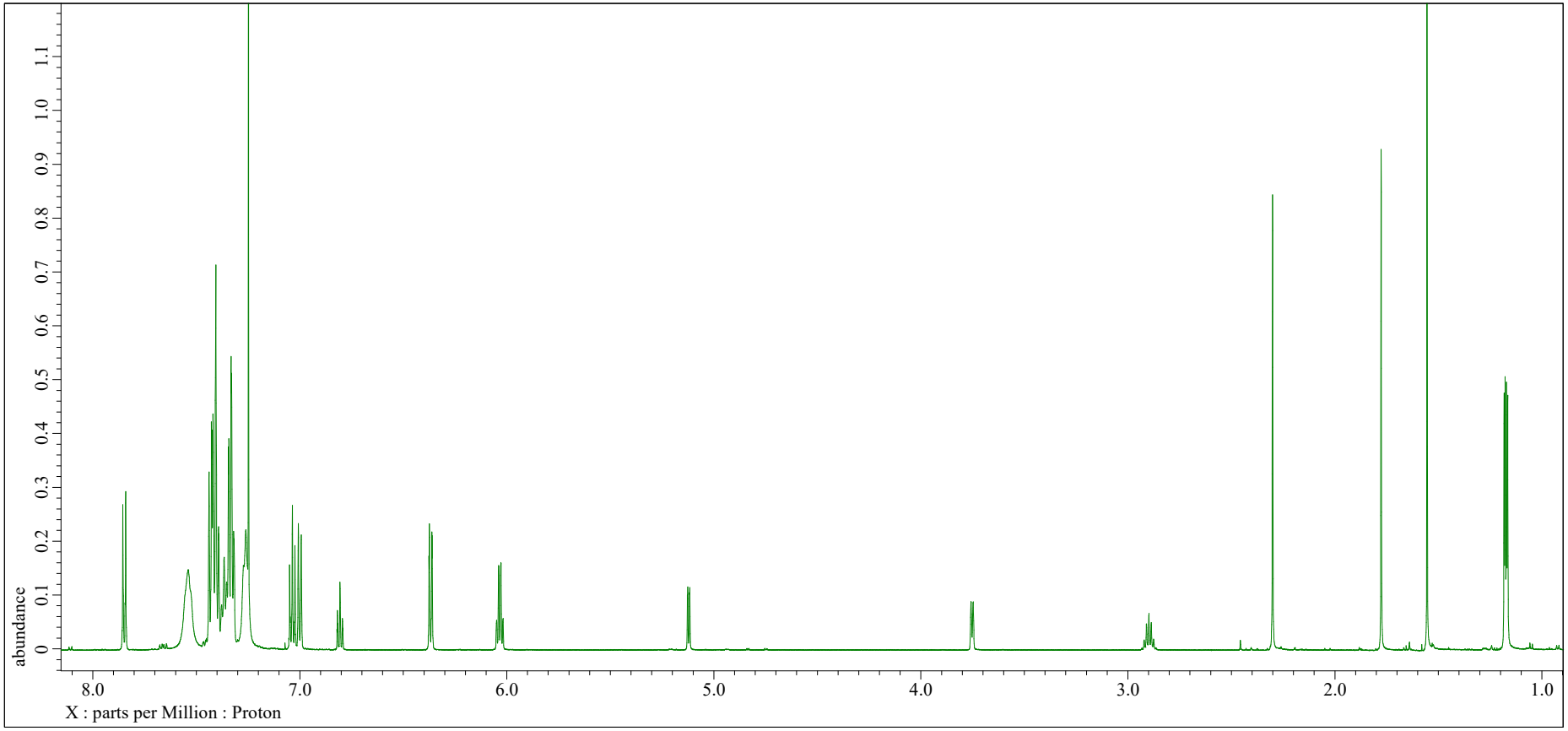


Figure S2: $^{1}H$ NMR spectrum of complex **aL1** + $Ag_2O/PPh_3$

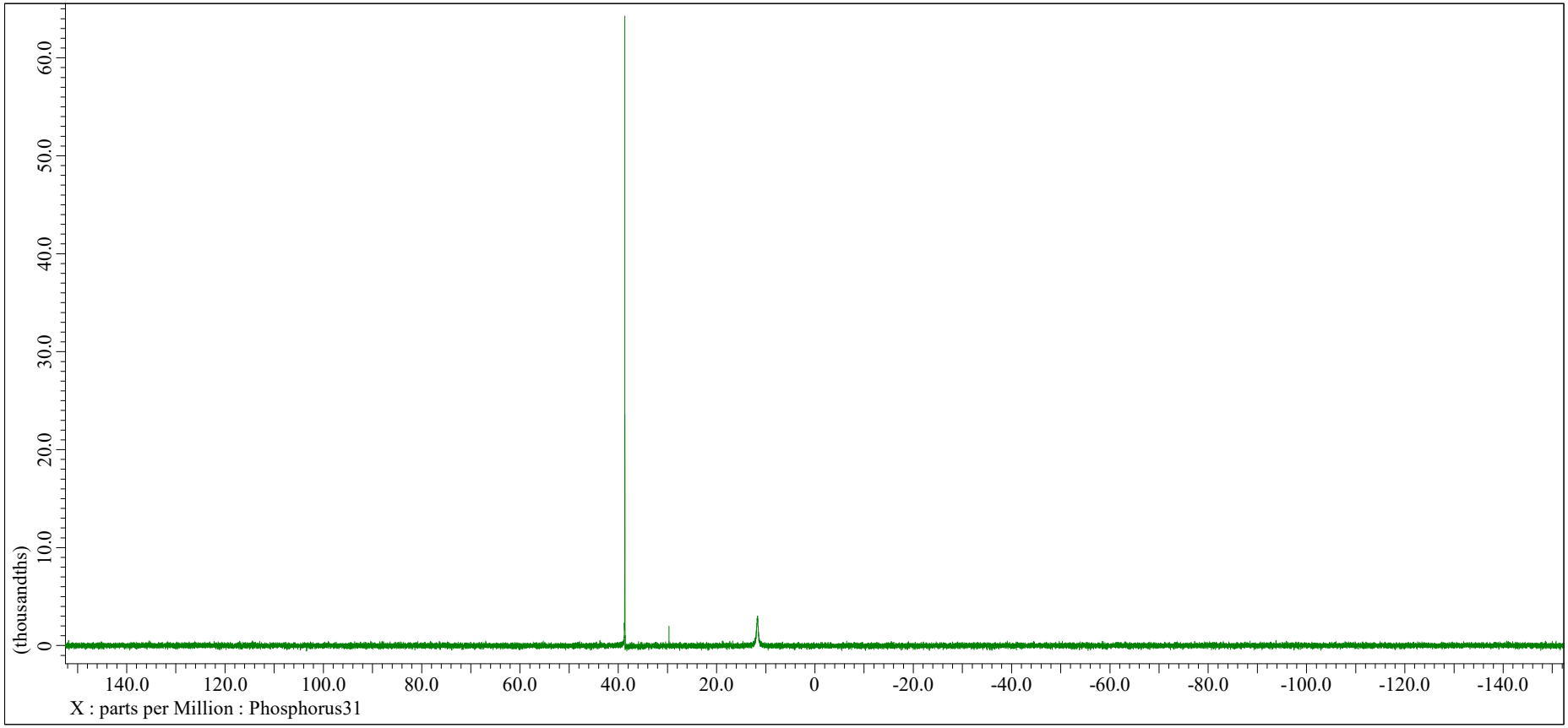


Figure S3: $^{31}P\{^{1}H\}$ NMR spectrum of complex **aL1** + $Ag_2O/PPh_3$

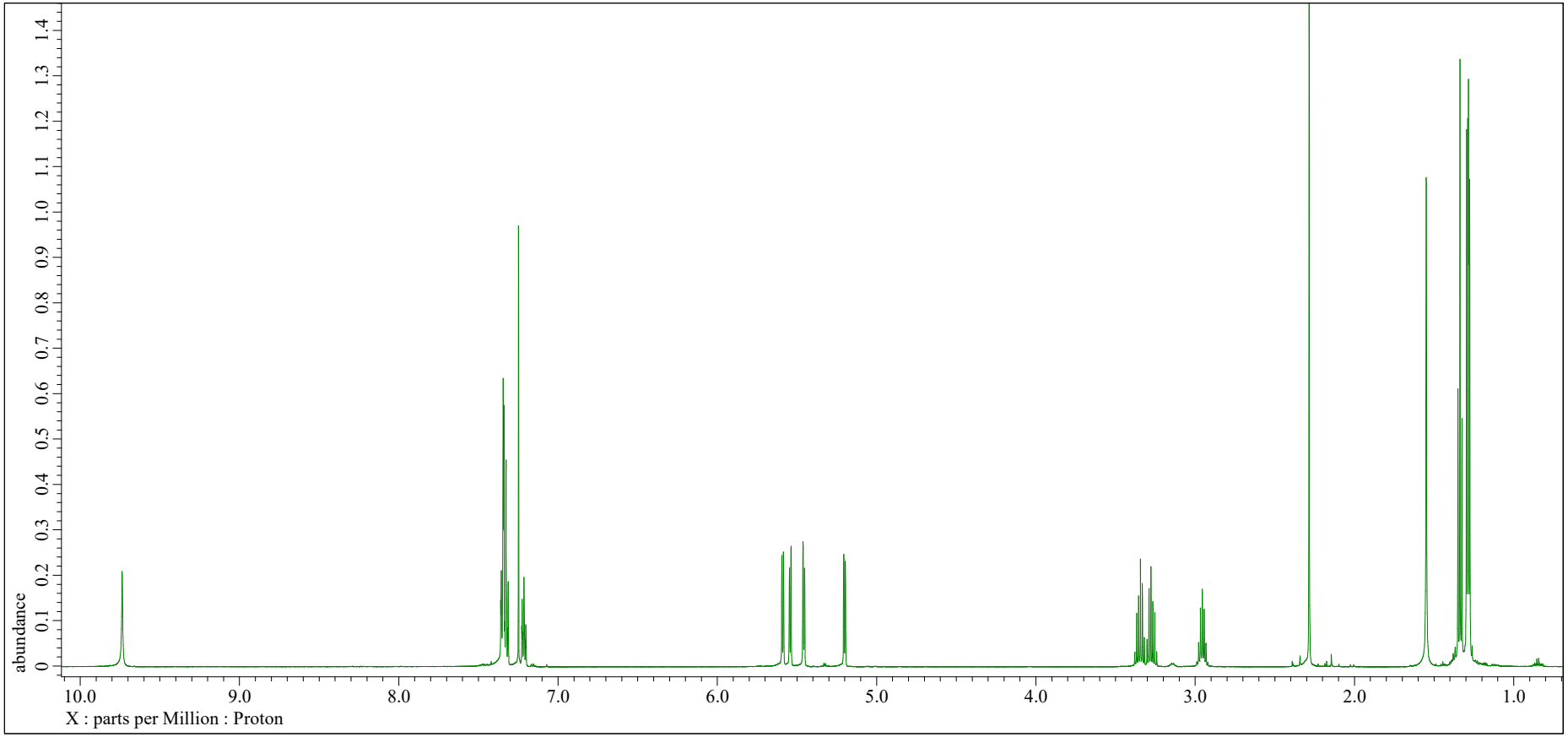


Figure S4: $^{1}H$ NMR spectrum of complex **aL2**

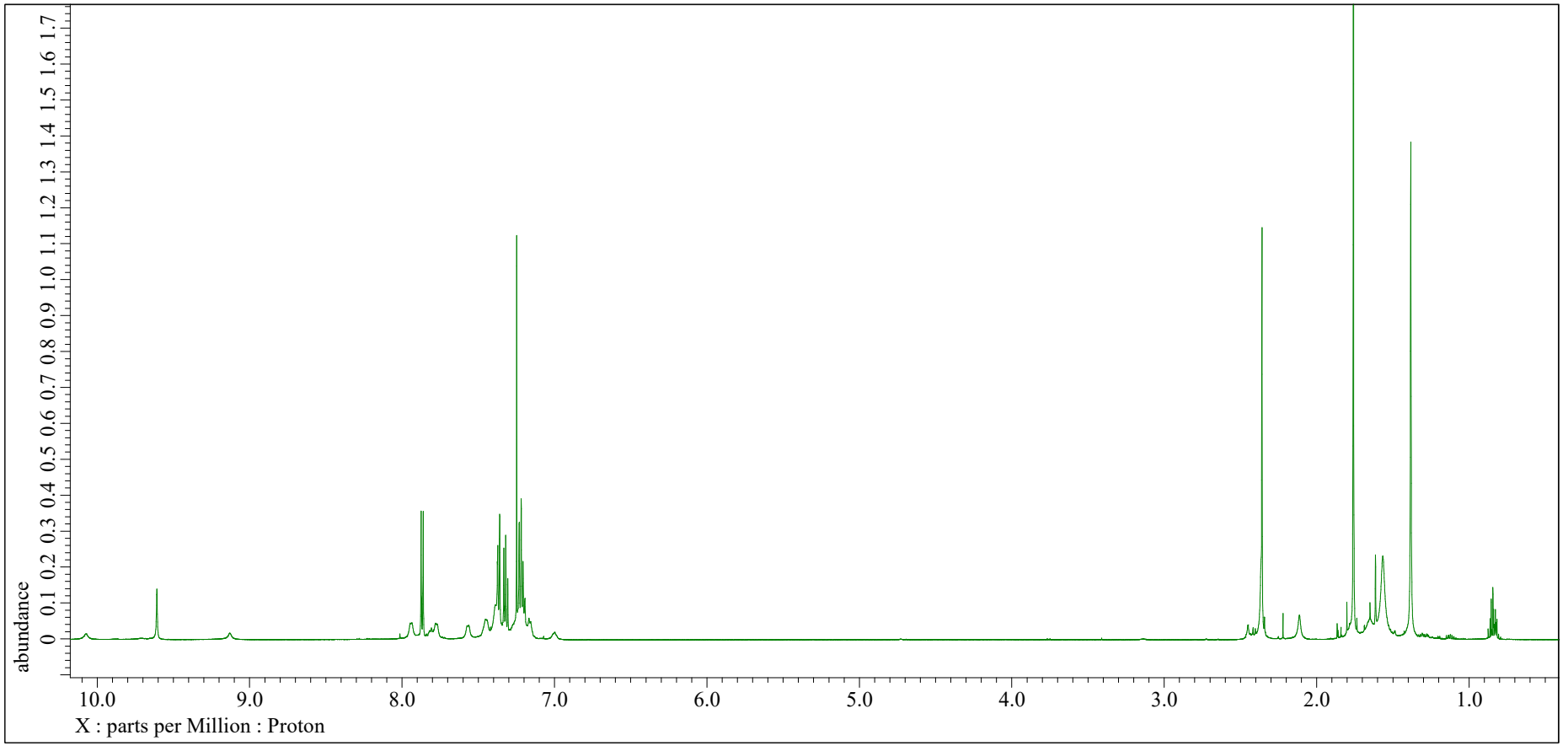


Figure S5: $^{1}$H NMR spectrum of complex **cL1**

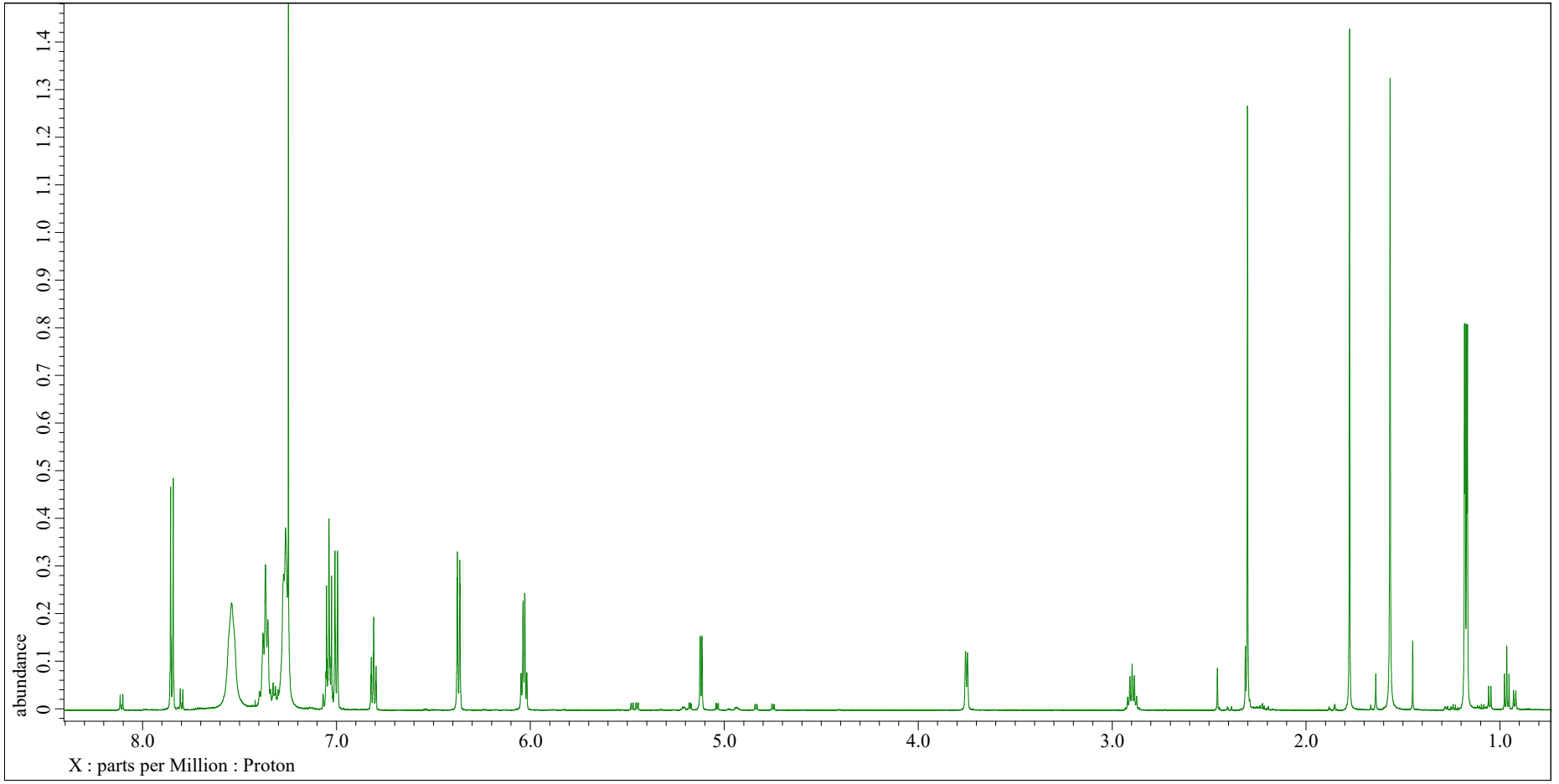


Figure S6: $^{1}$H NMR spectrum of complex **1aL1**, freshly made, proximal to distal ratio 93:7

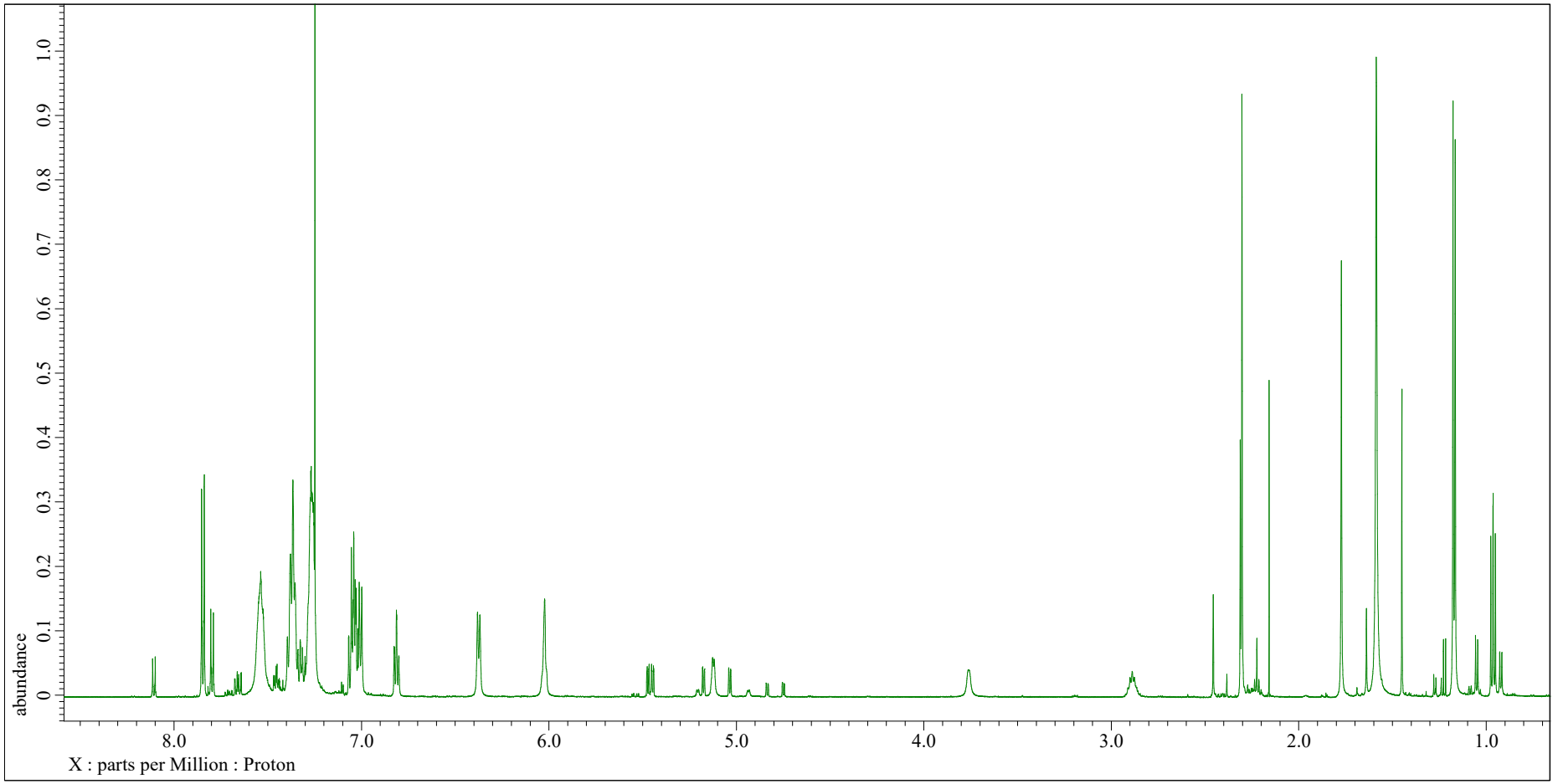


Figure S6a: $^{1}$H NMR spectrum of complex **1aL1**, approximately 2 weeks in solution, proximal to distal ratio 71:29

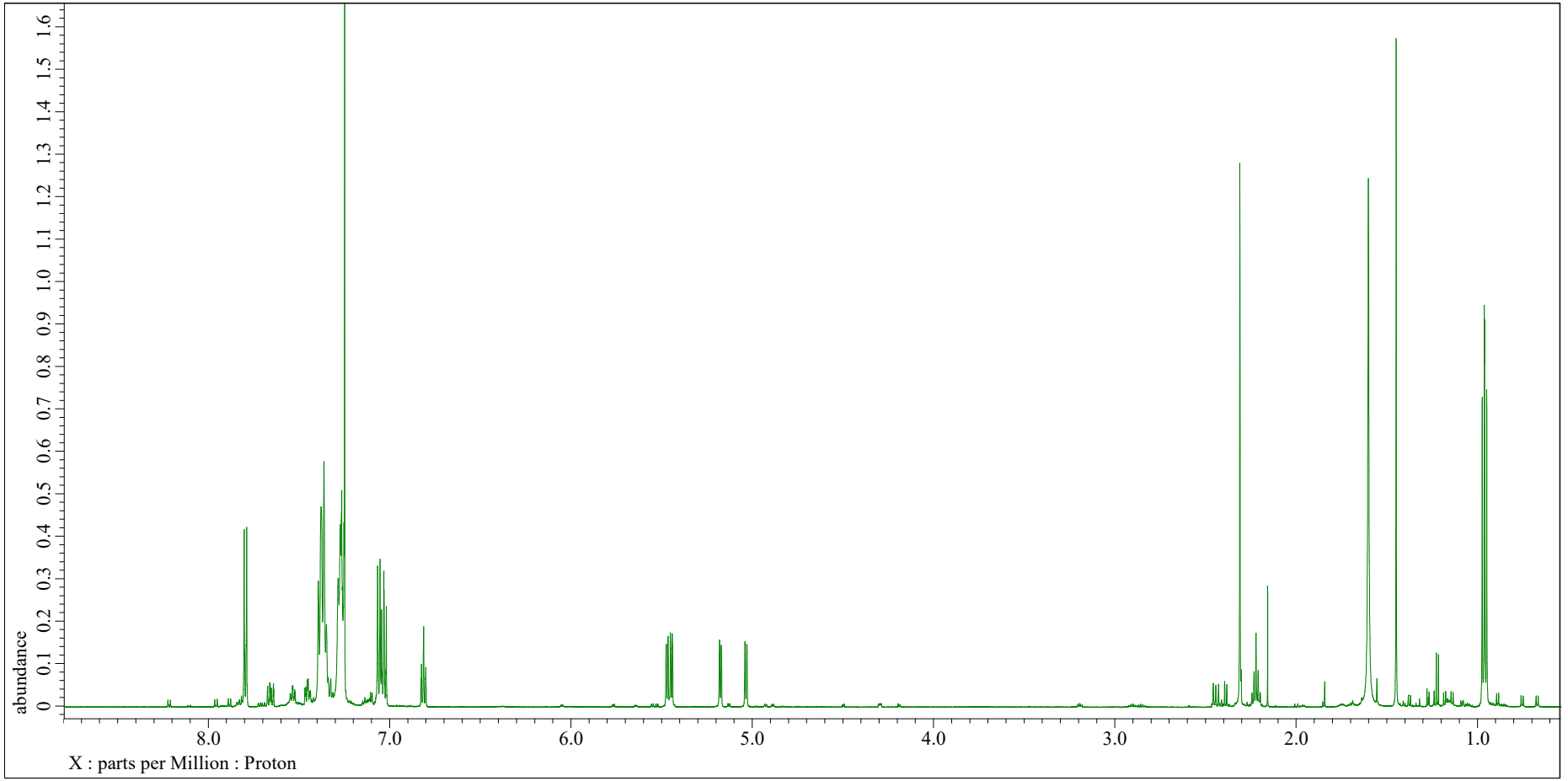


Figure S6b: $^{1}$H NMR spectrum of complex **1aL1**, approximately 7 weeks in solution, proximal to distal ratio 4:96

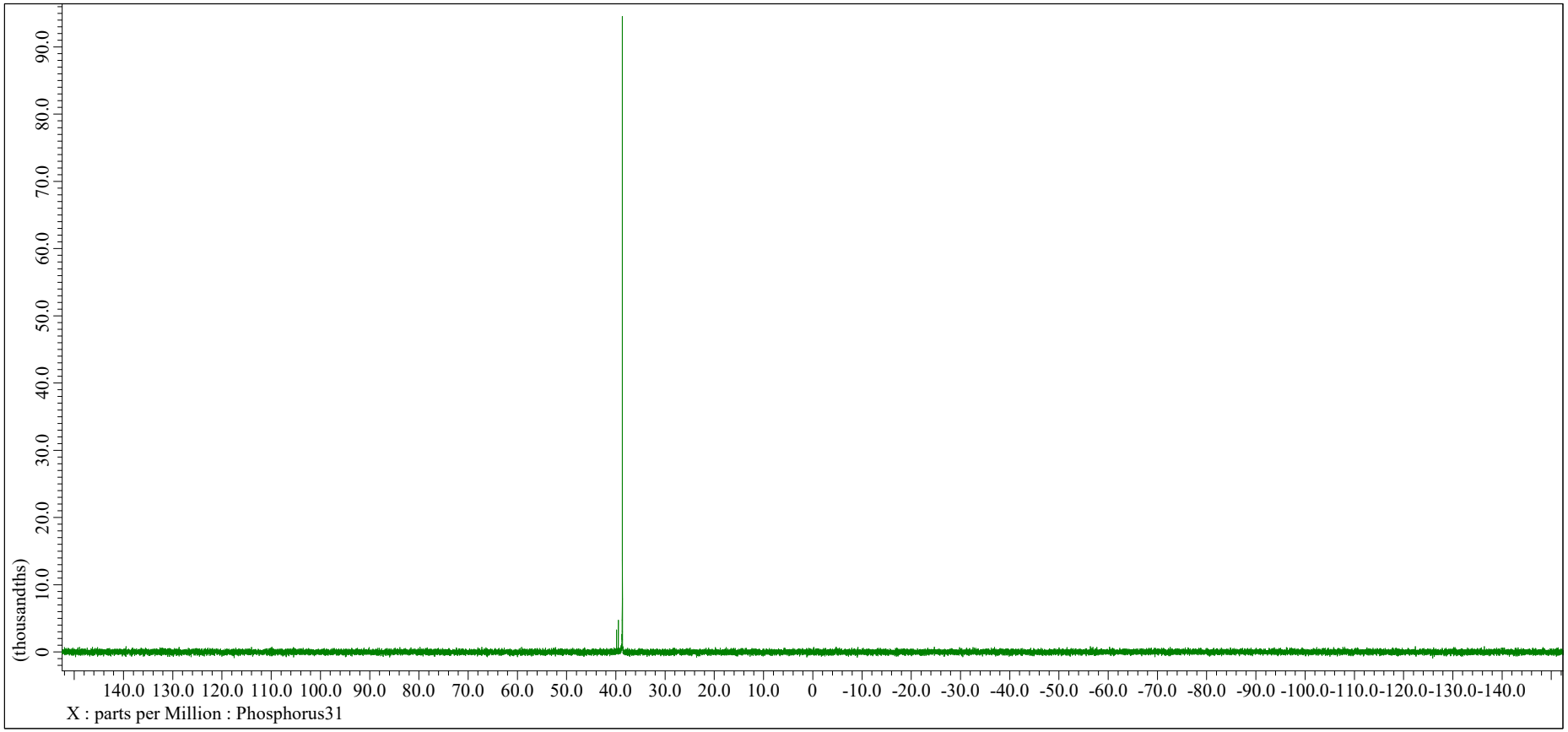


Figure S7: $^{31}$P NMR spectrum of complex **1aL1**, proximal isomer.

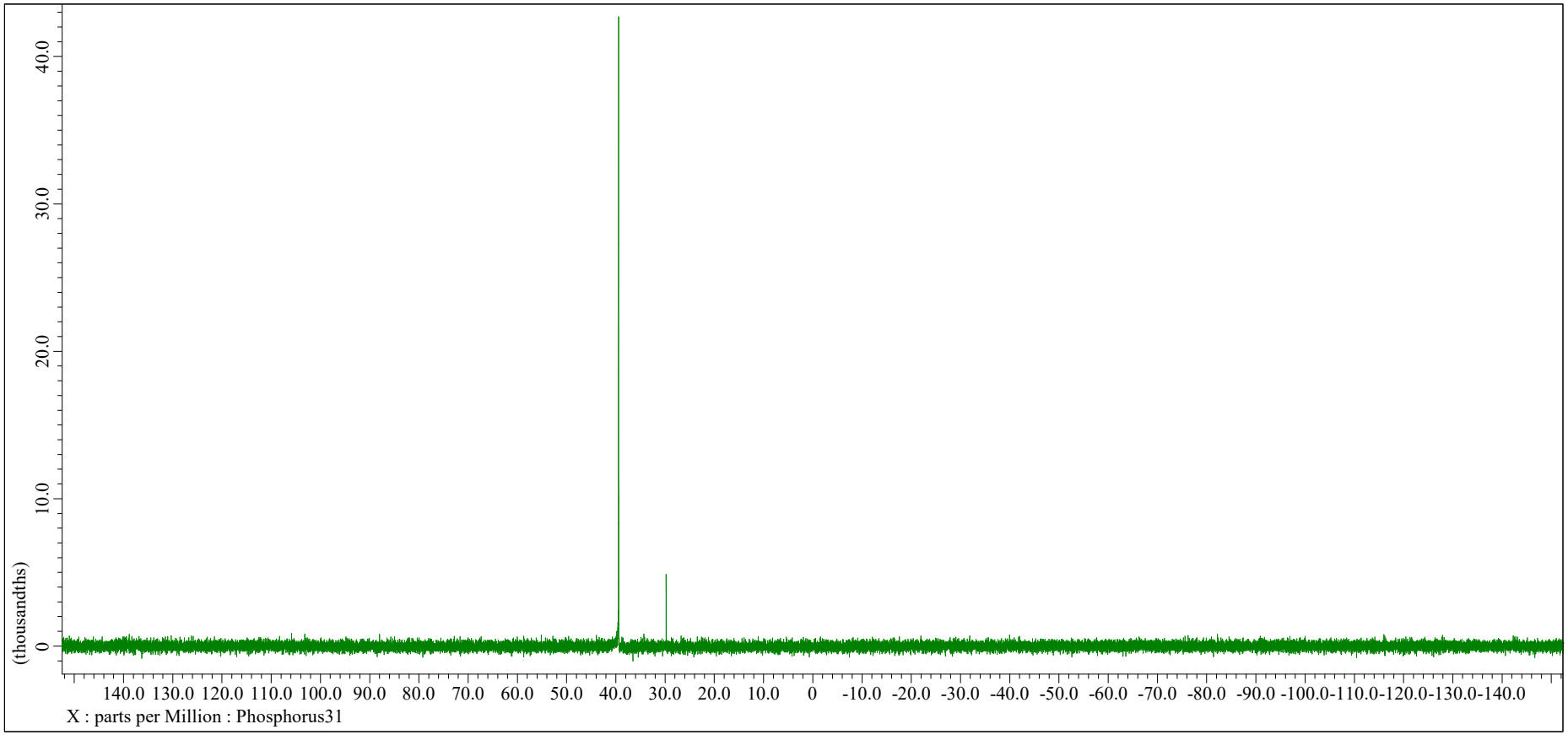


Figure S7a: $^{31}$P NMR spectrum of complex **1aL1**, distal isomer.

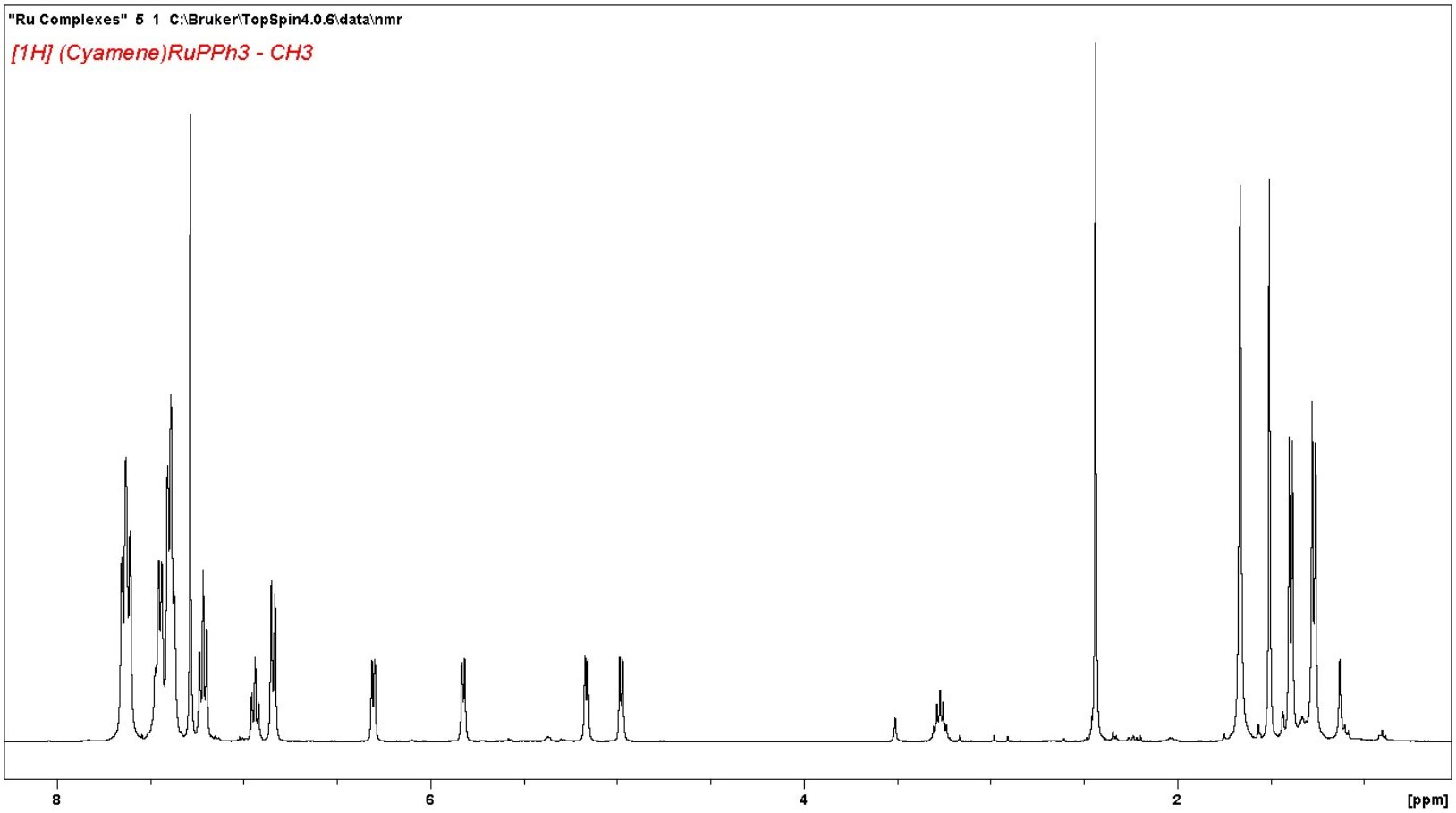


Figure S8: $^{1}$H NMR spectrum of complex **1aL3**

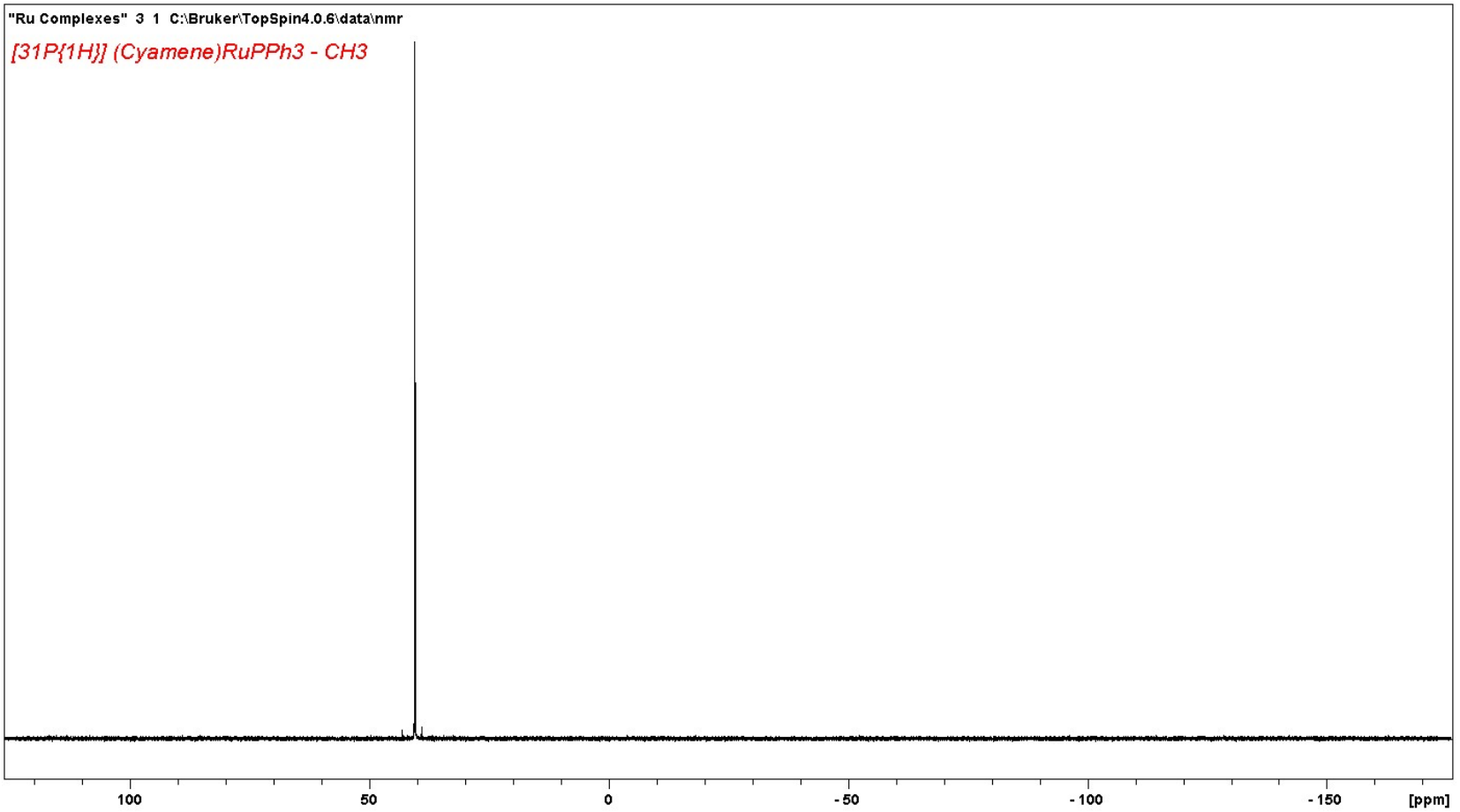


Figure S9: $^{31}$P NMR spectrum of complex **1aL3**

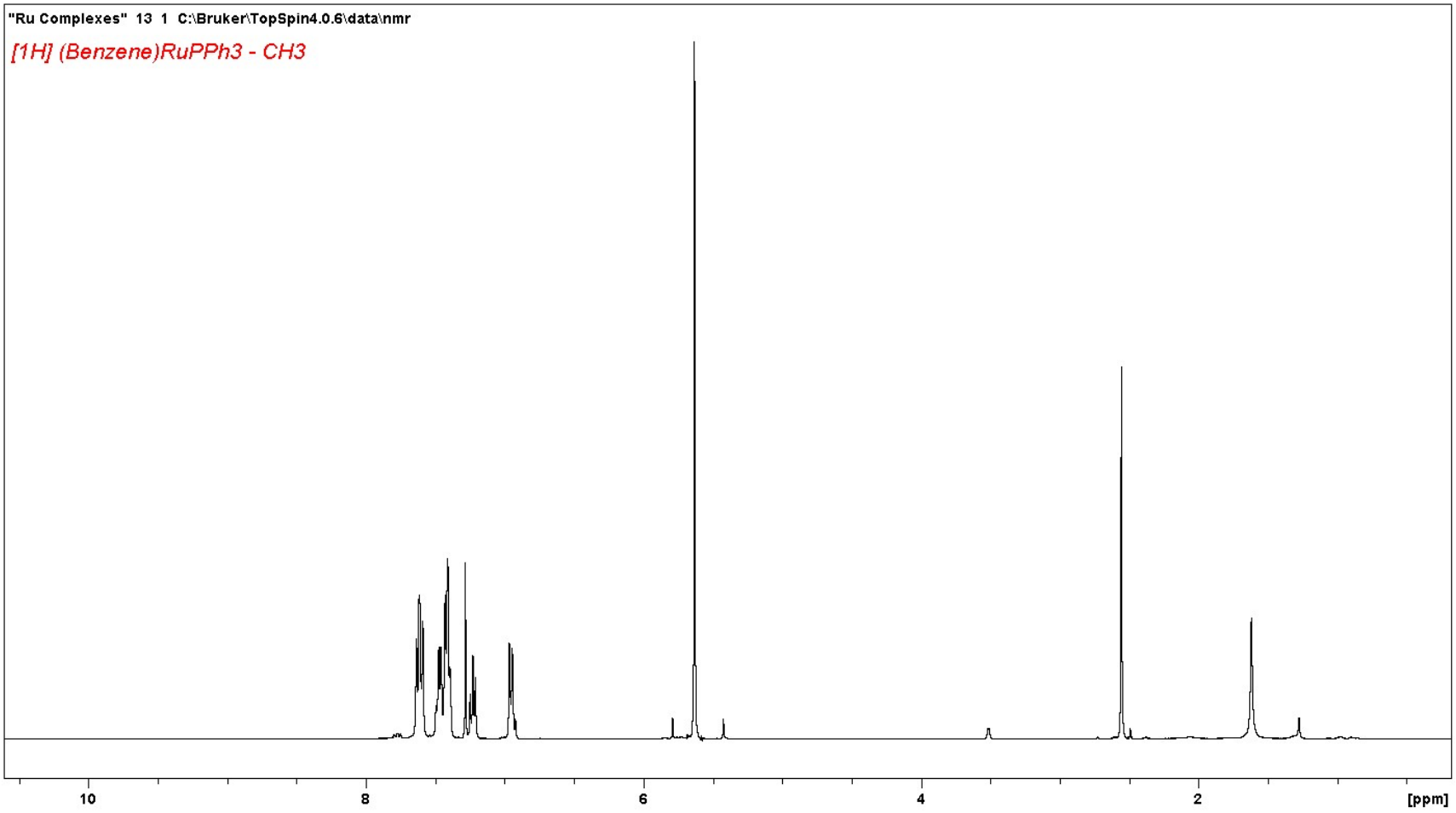


Figure S10: $^{1}$H NMR spectrum of complex **1bL3**

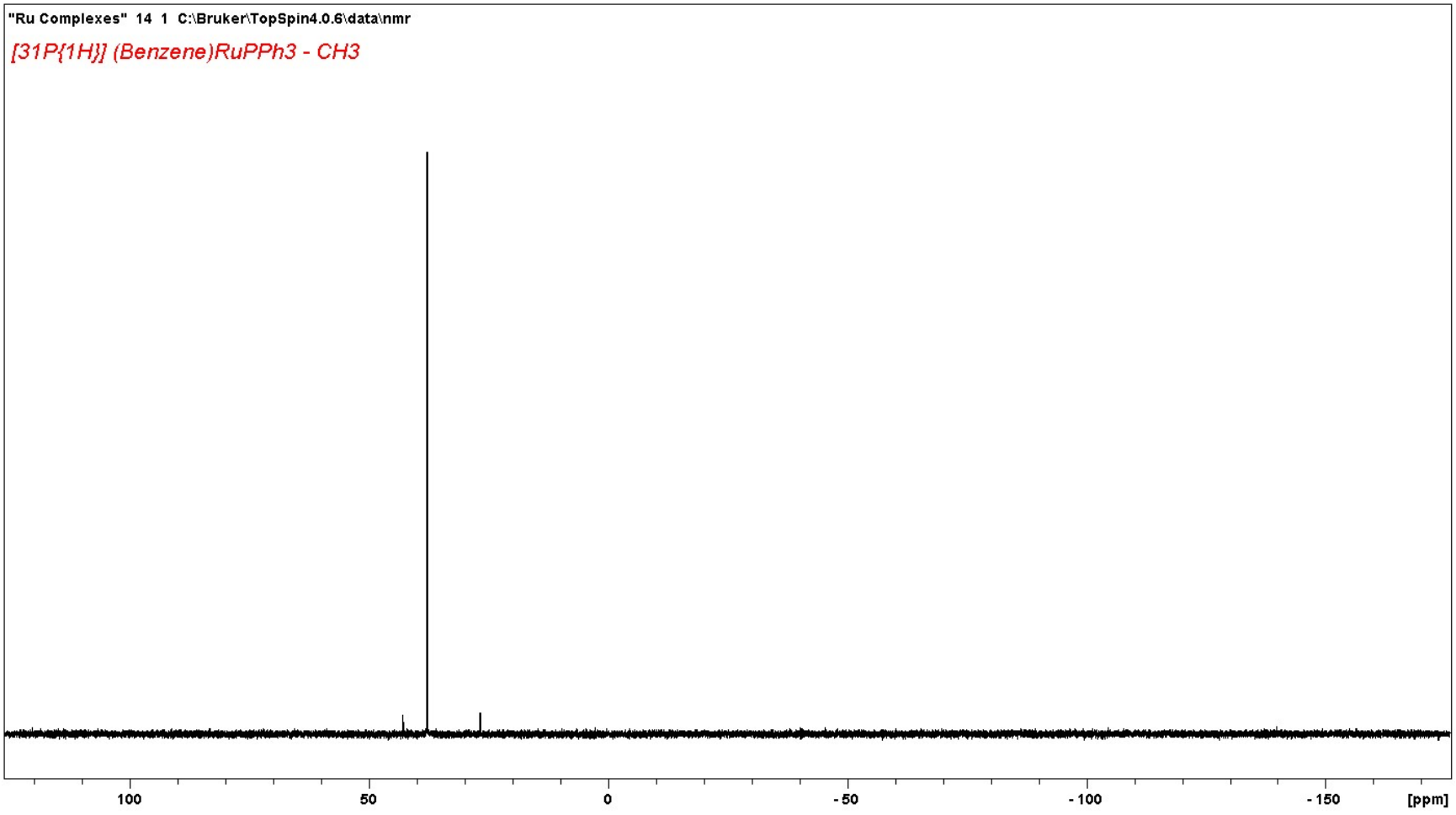


Figure S11: $^{31}P$ NMR spectrum of complex **1bL3**

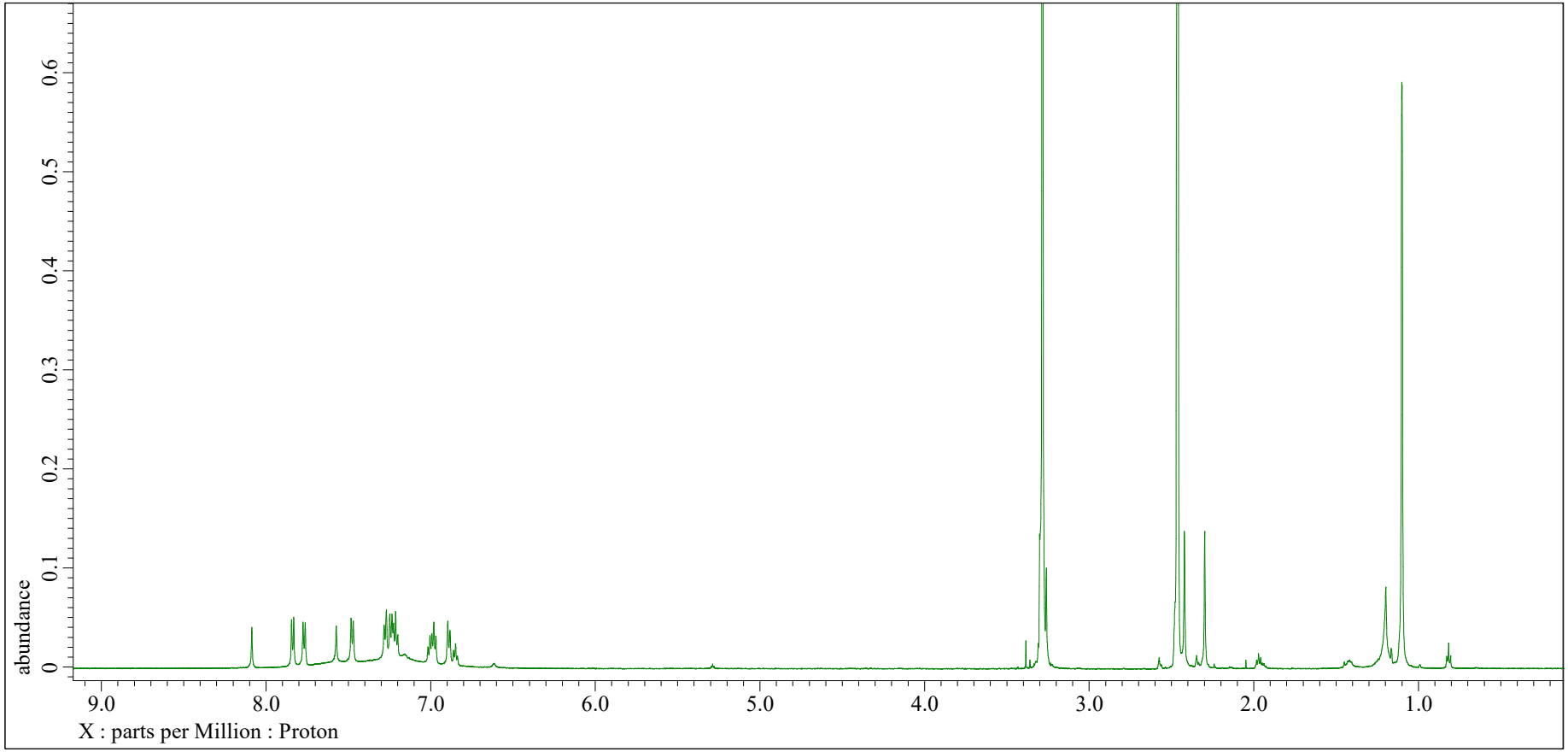


Figure S12: $^{1}$H NMR spectrum of complex **1cL**

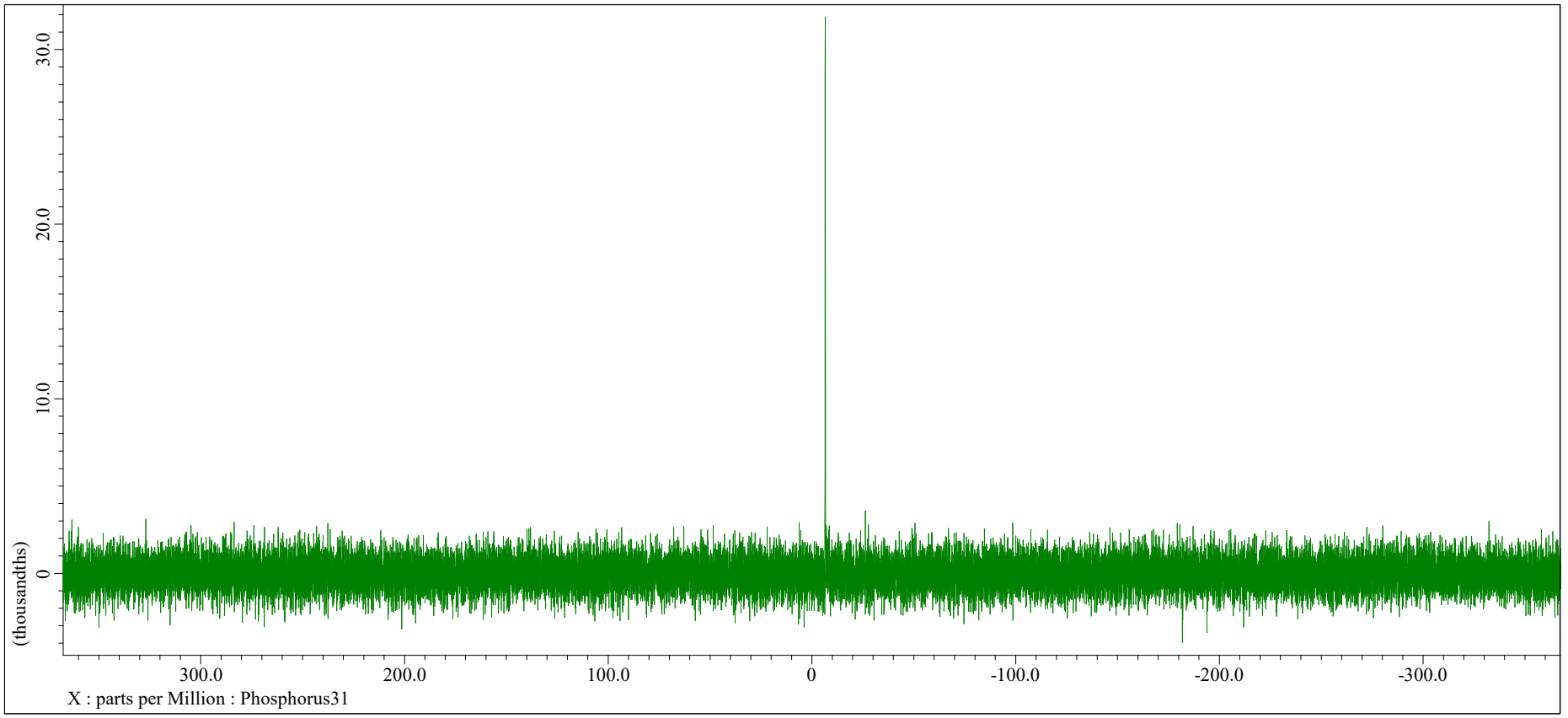


Figure S13: $^{31}$P NMR spectrum of complex **1cL1**

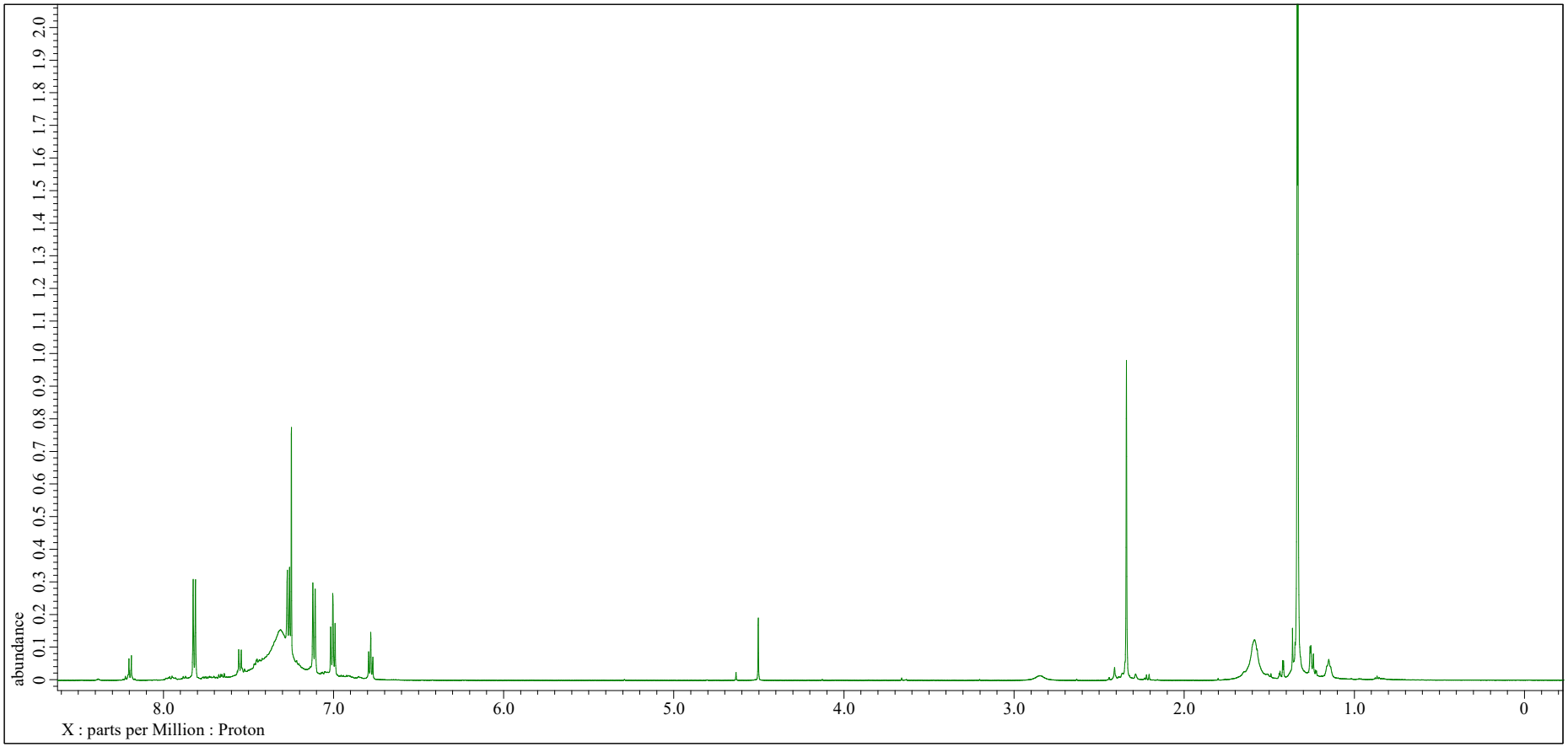


Figure S14: $^{1}$H NMR spectrum of complex **1dL1**

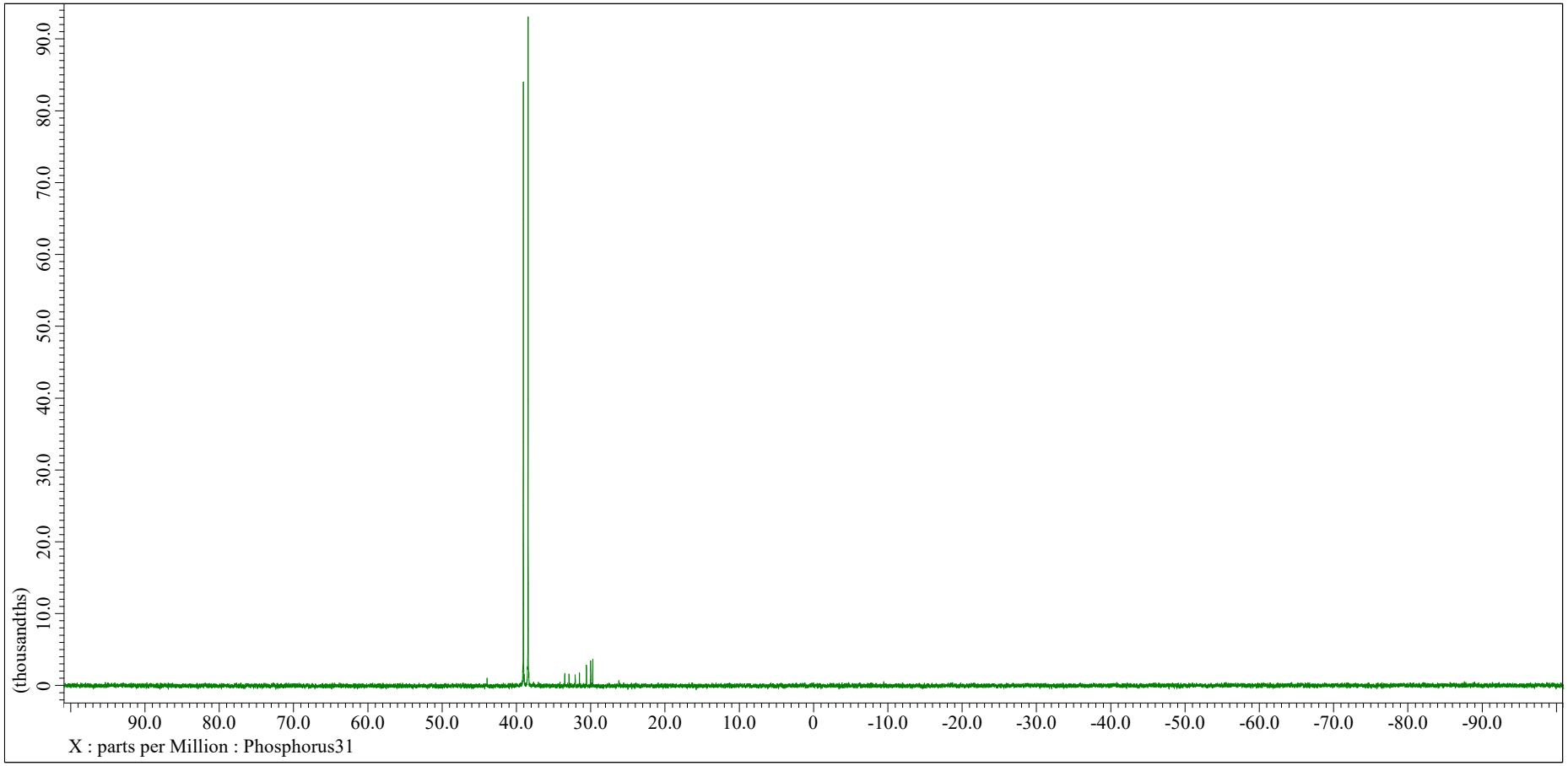


Figure S15: $^{31}$P NMR spectrum of complex **1dL1**

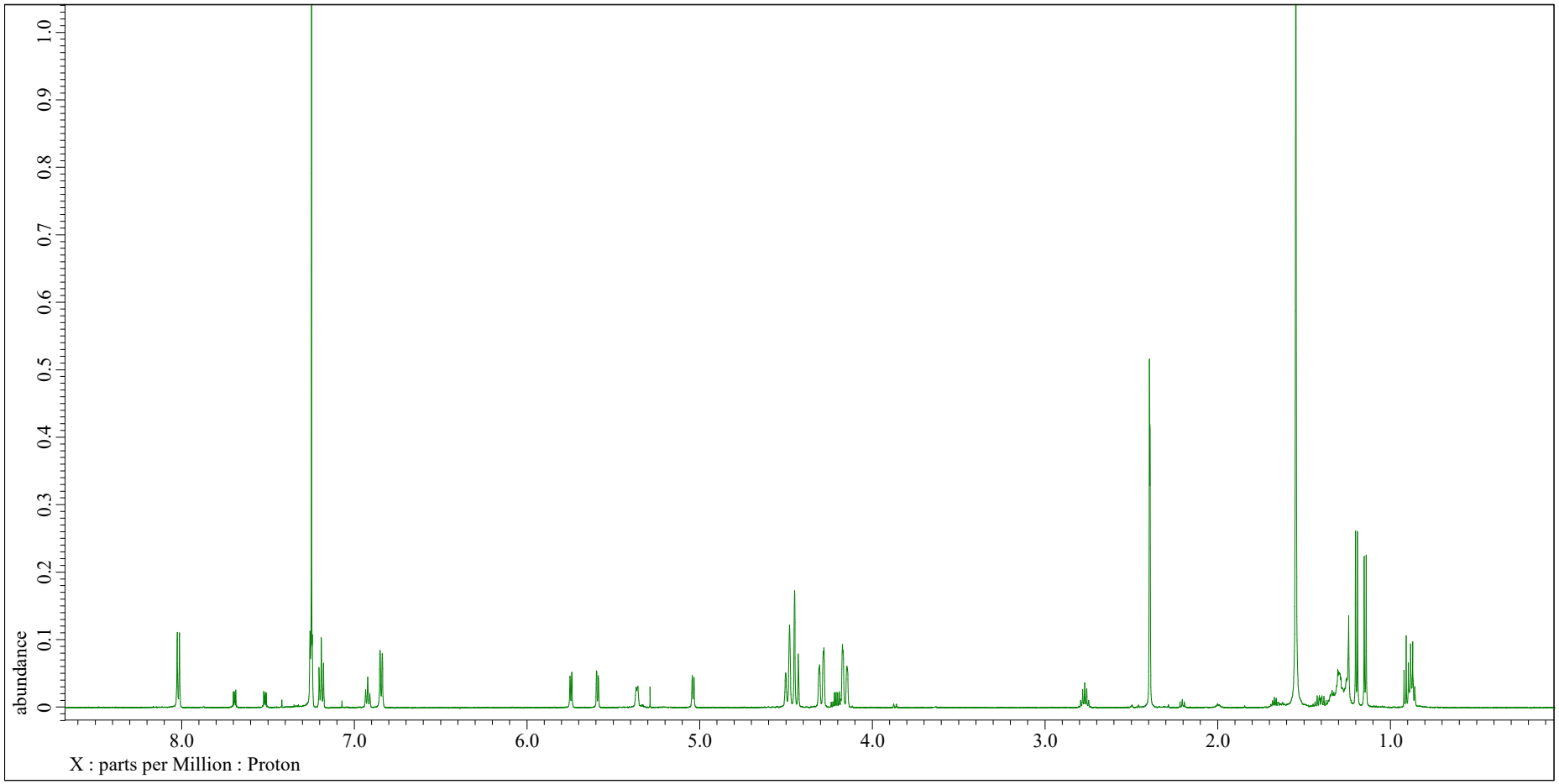


Figure S16: $^{1}$H NMR spectrum of complex **2aL1**

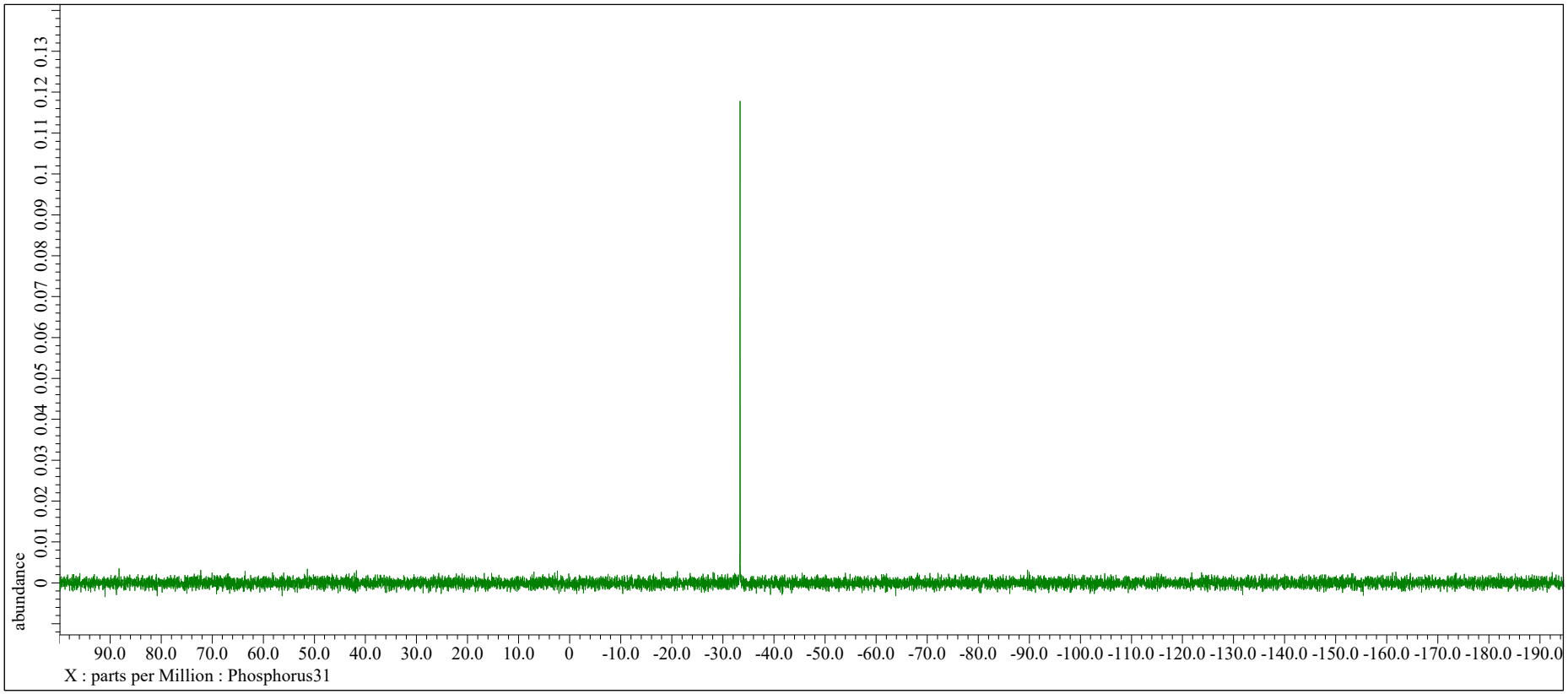


Figure S17: $^{31}$P NMR spectrum of complex **2aL1**

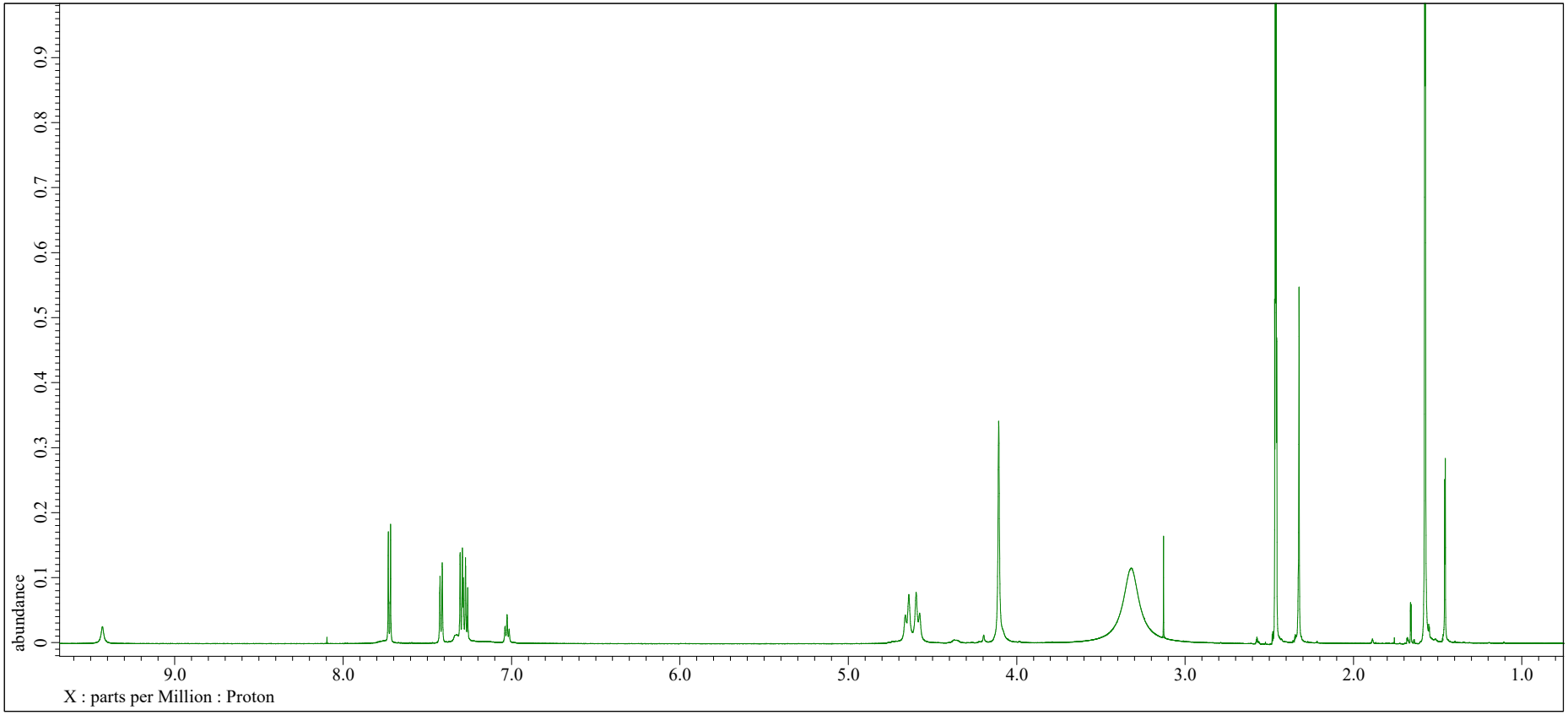


Figure S18: $^{1}$H NMR spectrum of complex **2cL1**

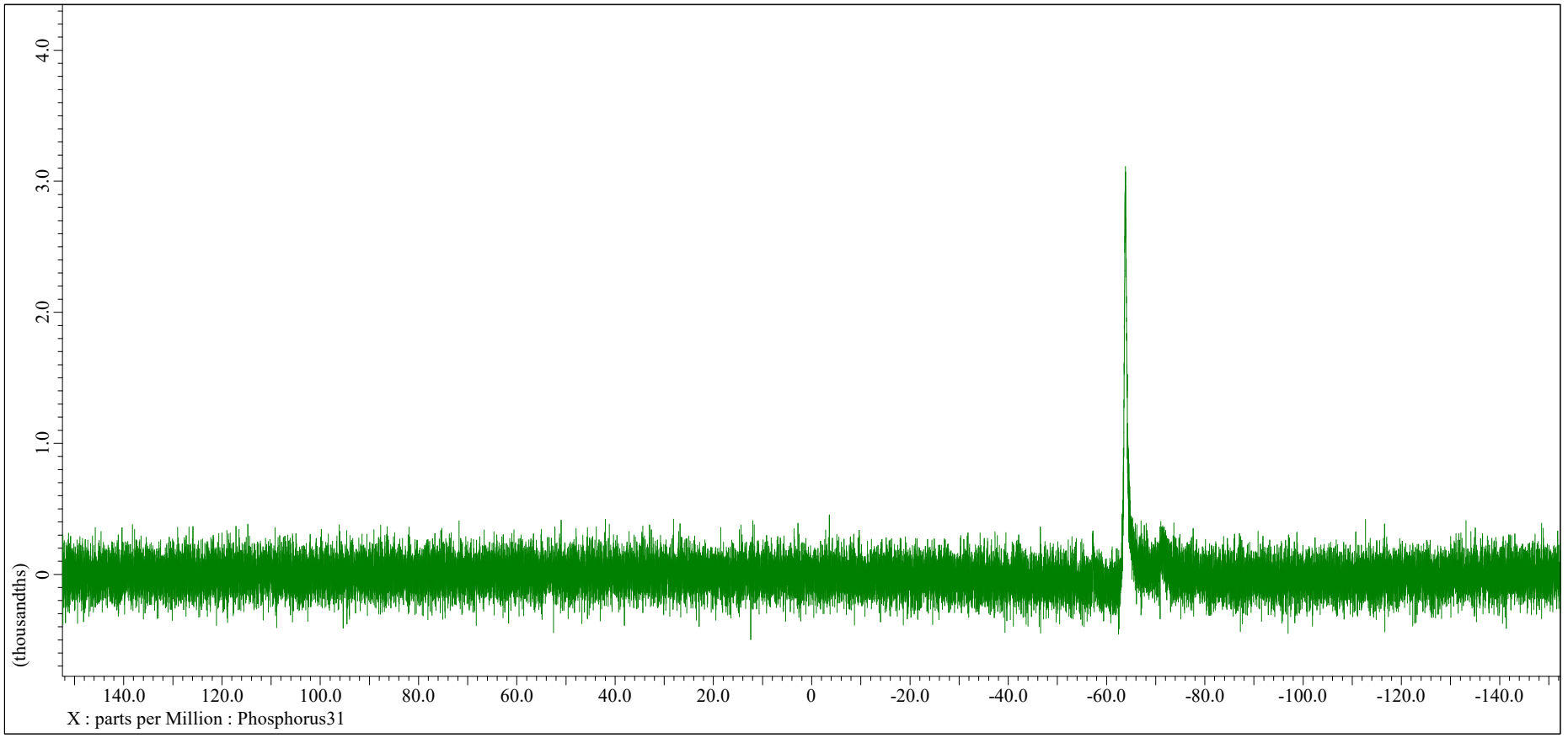


Figure S19: $^{31}P$ NMR spectrum of complex **2cL1**

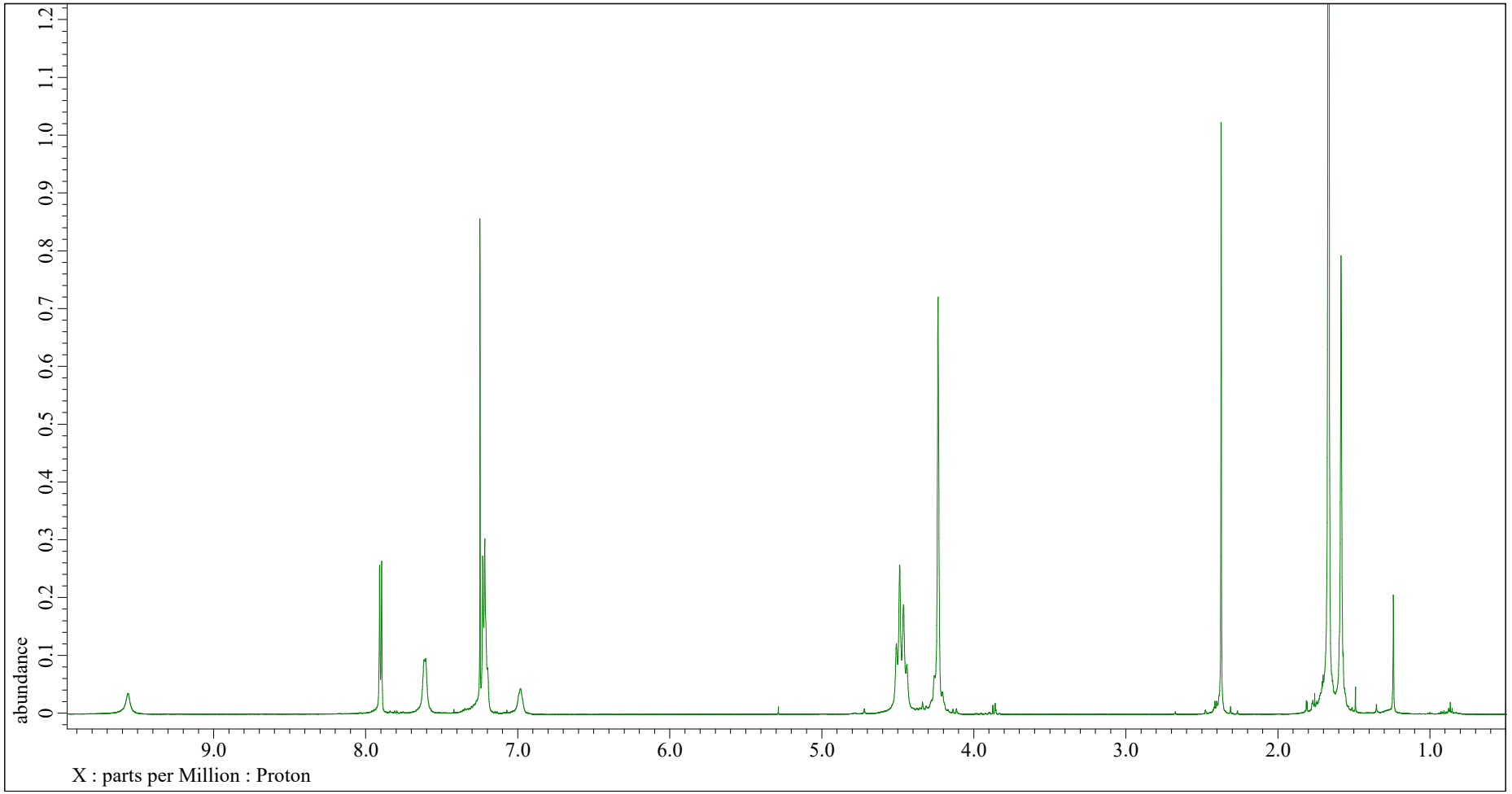


Figure S20: $^{1}$H NMR spectrum of complex **2dL**

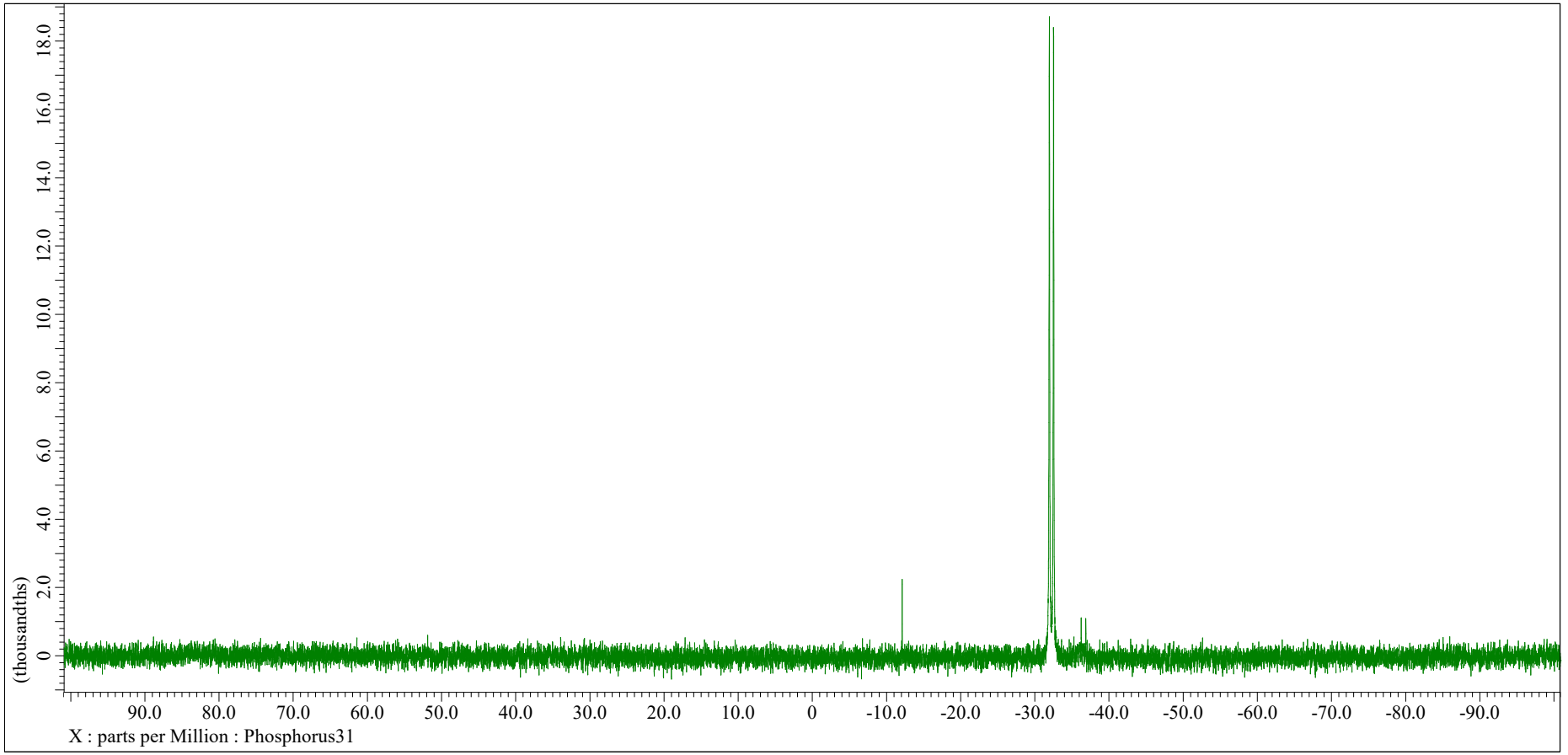


Figure S21: $^{31}P$ NMR spectrum of complex **2dL1**

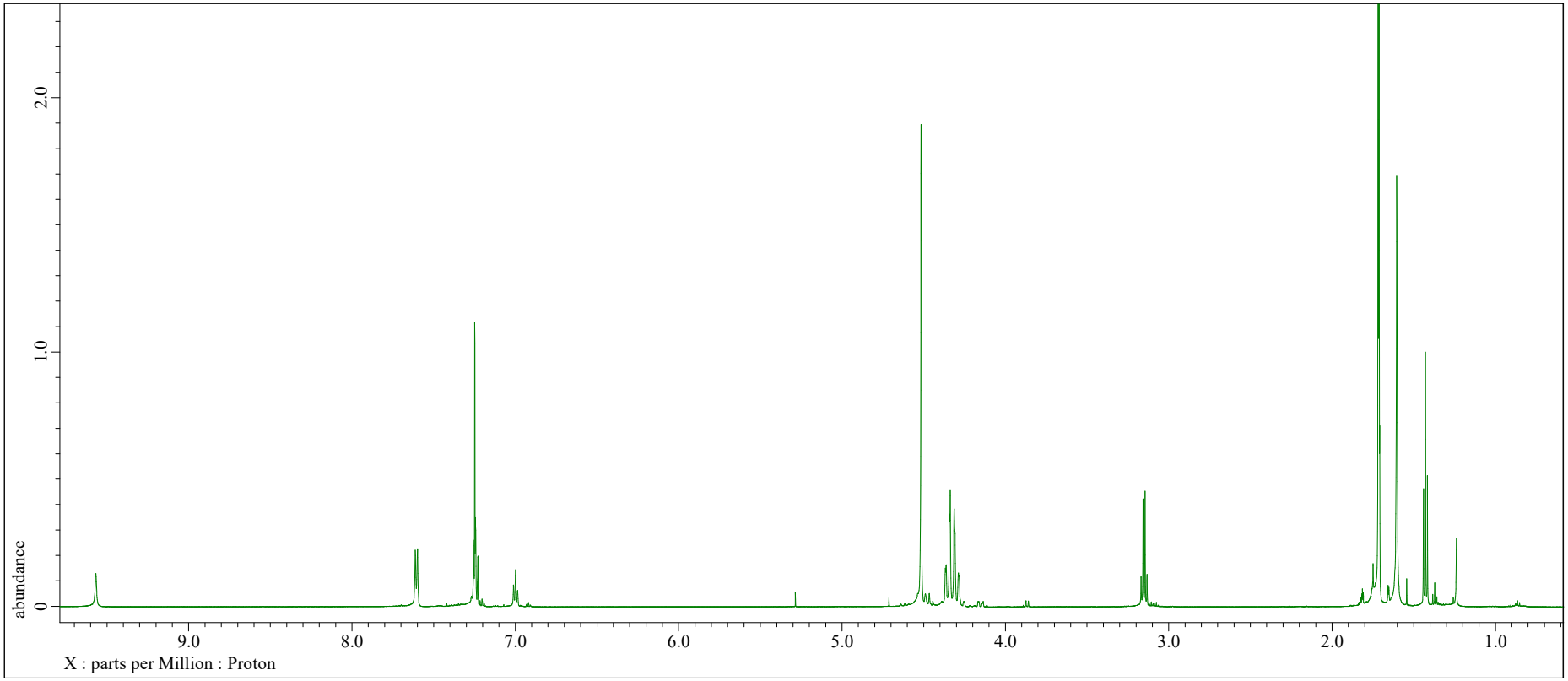


Figure S22: $^{1}$H NMR spectrum of complex **2dL2**

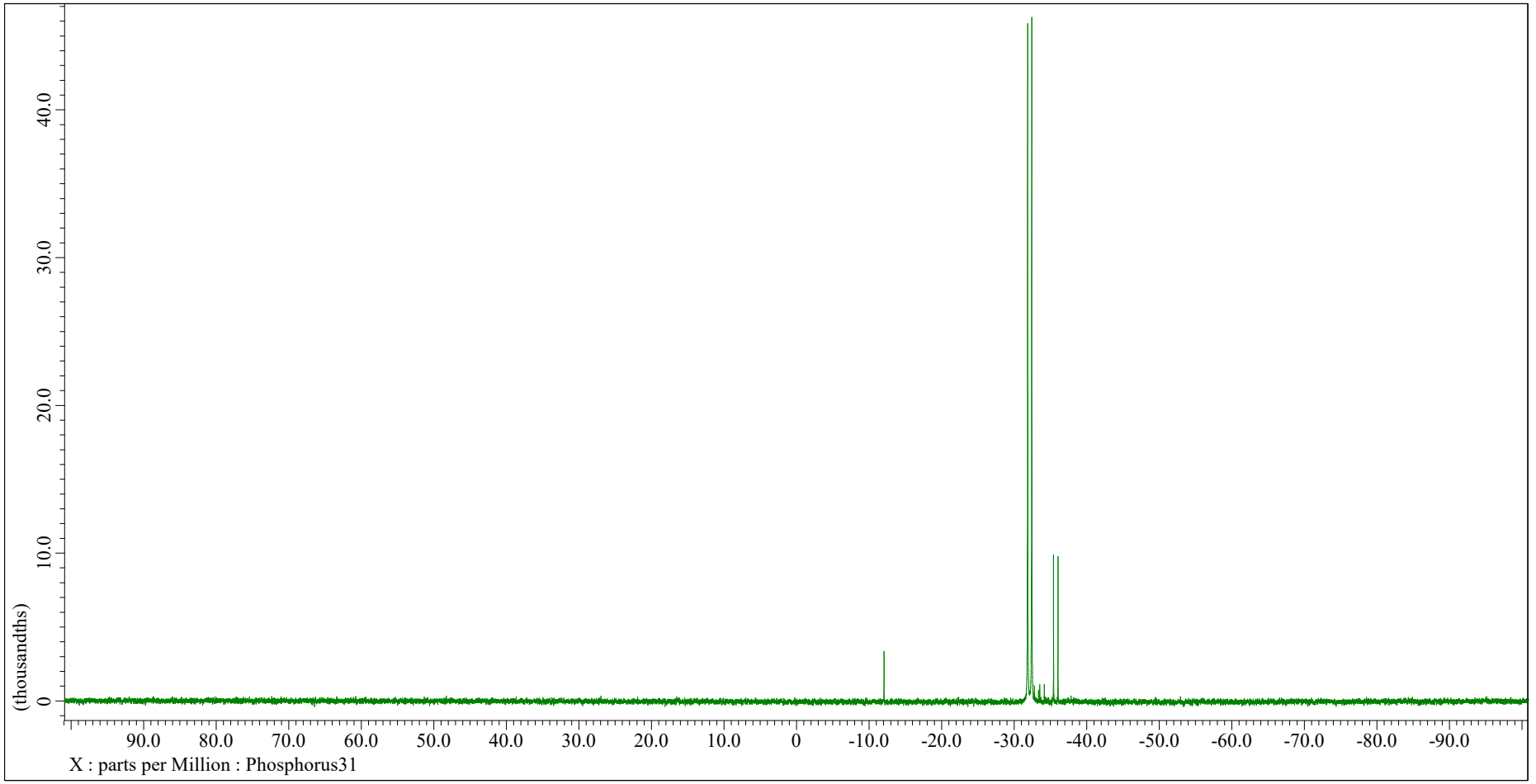


Figure S23: $^{31}$P NMR spectrum of complex **2dL2**

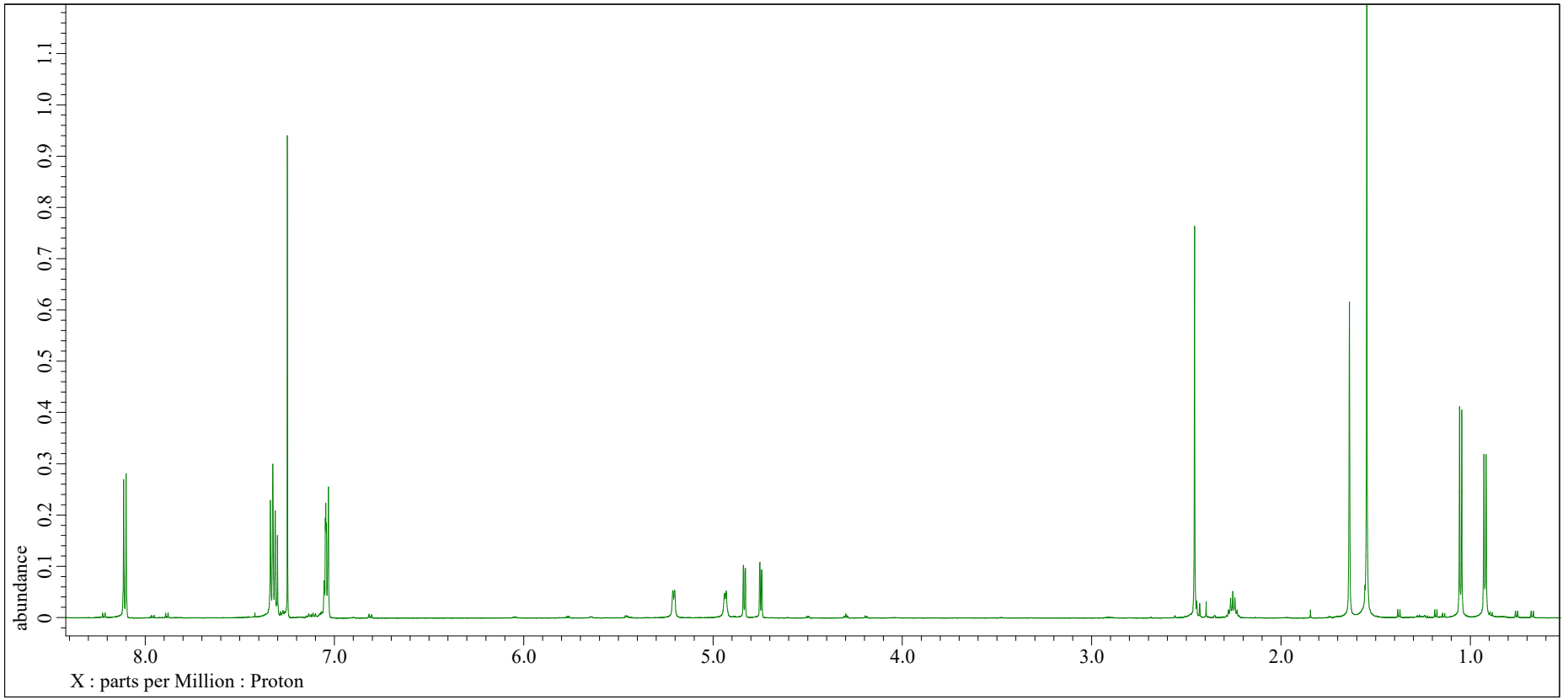


Figure S24: $^{1}$H NMR spectrum of complex **$a_2$L1**

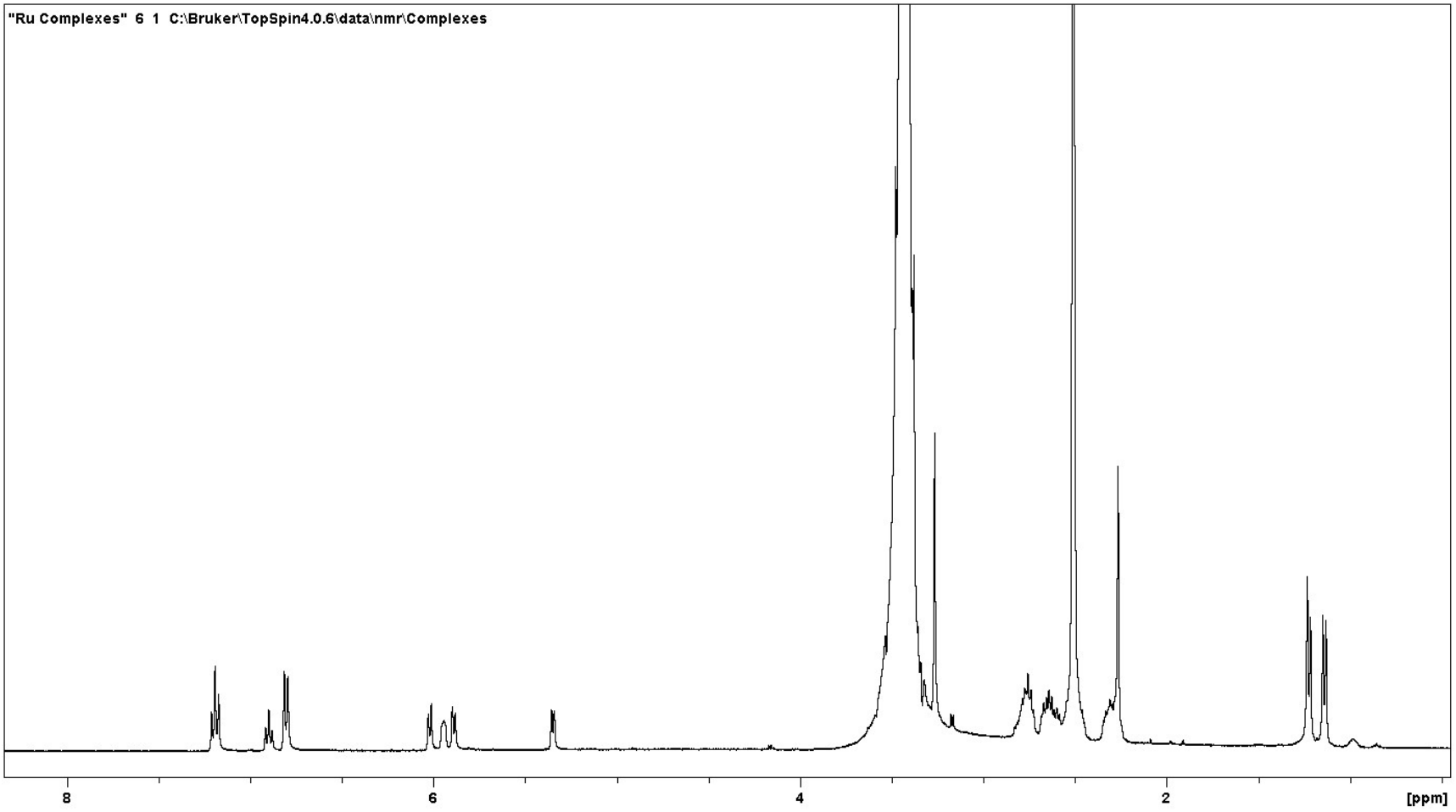


Figure S25: $^{1}$H NMR spectrum of complex **3aL3**

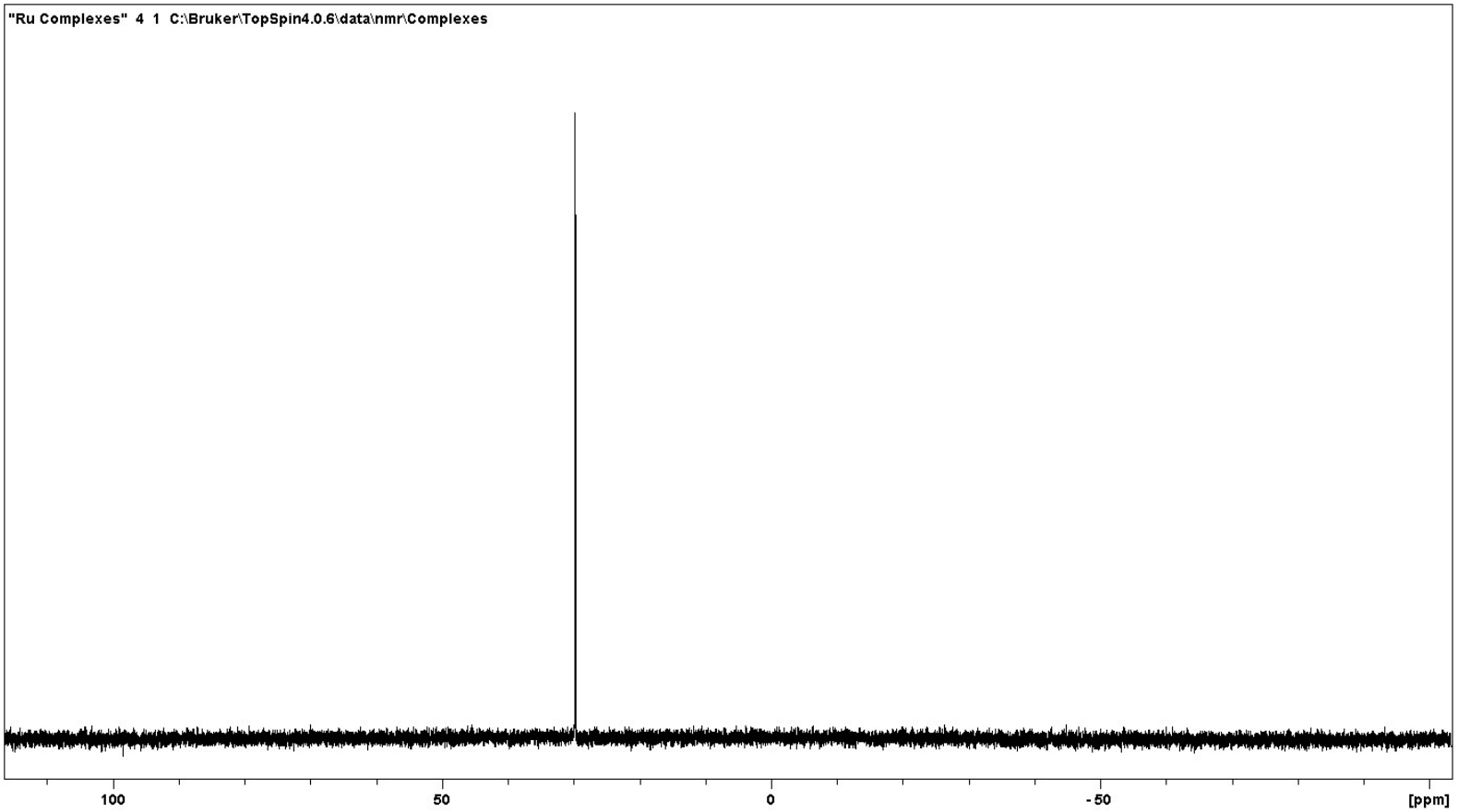


Figure S26: $^{31}P$ NMR spectrum of complex **3aL3**

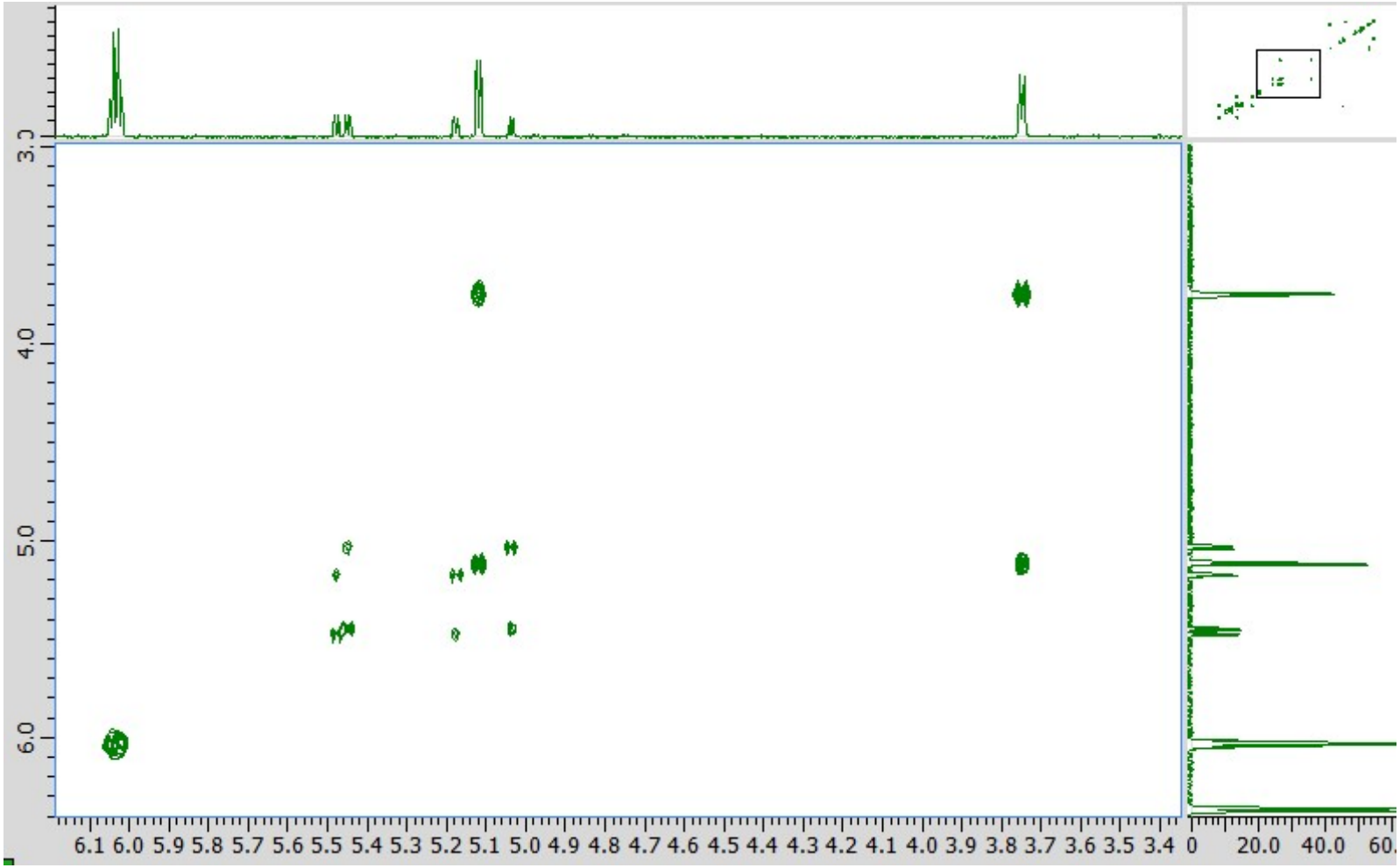


Figure S27: 1H-1H COSY NMR spectrum of complex 1aL1, freshly prepared.

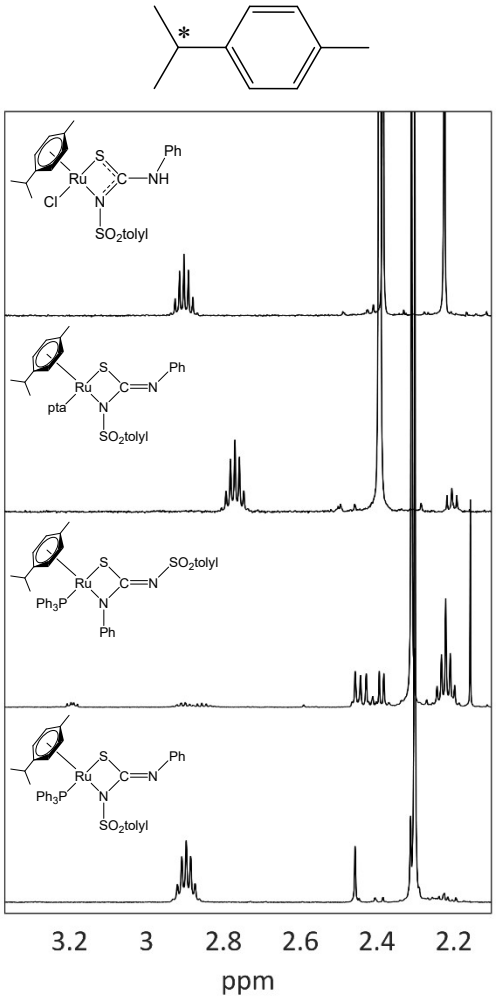


Figure S28: Comparison of the isopropyl CH resonances of complexes **1aL1** proximal/distal, **1L1** and **2aL1.**

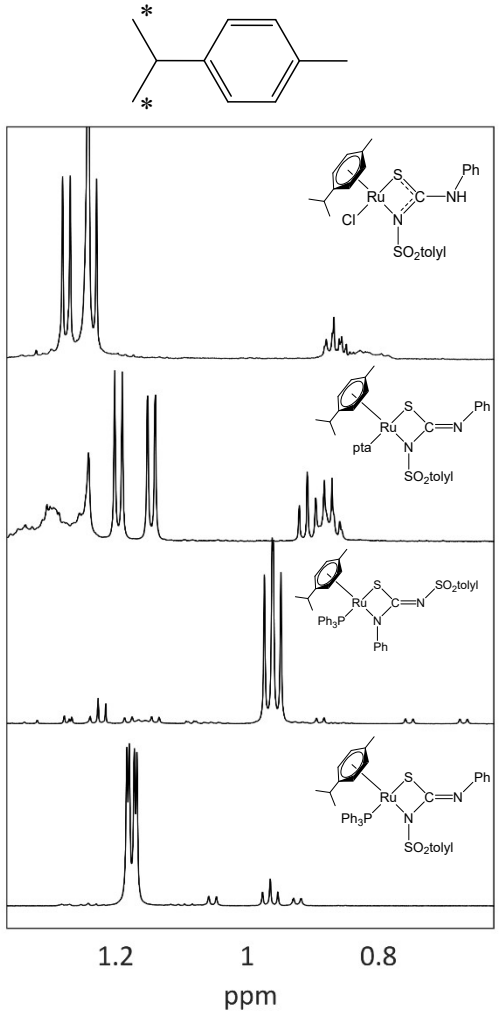


Figure S29: Comparison of the two isopropyl $CH_3$ resonances of complexes **1aL1** proximal/distal, **1L1** and **2aL1.**

# Crystallographic information:

Table 1: Selected bond lengths in the molecular structure of complexes **aL1**, **aL2**, **1aL1**, **1bL1**, **2aL1**, **2cL1**, **2dL1** and **$a_2$L1**. Arene = cymene or benzene centroid, Cp* = Cp* centroid.

| **Bond** | **Bond length (Å)** | | | | | |
|---|---|---|---|---|---|---|
| | **aL1** | **aL2** | **2aL1** | **1aL1** | **1bL3** | **$a_2$L1** |
| **Arene - Ru** | 1.671(2) | 1.666(2) | 1.723(2) | 1.737(3) | 1.727(3) | 1.687(5) |
| **Ru - P** | - | - | 2.300(6) | 2.349(5) | 2.331(7) | - |
| **Ru - Cl** | 2.412(5) | 2.415(5) | - | - | - | - |
| **Ru - S1** | 2.421(5) | 2.429(6) | 2.389(5) | 2.379(7) | 2.393(8) | 2.413(1) |
| **Ru - S1a** | - | - | - | - | - | 2.404(8) |
| **Ru - N1** | - | - | - | 2.099(2) | - | - |
| **Ru - N2** | 2.131(2) | 2.144(2) | 2.113(2) | - | 2.117(2) | 2.126(4) |
| **S1- C1** | 1.715(2) | 1.712(2) | 1.766(2) | 1.767(2) | 1.776(3) | 1.829(4) |
| **C1 - N1** | 1.337(2) | 1.336(3) | 1.278(3) | 1.328(3) | 1.284(4) | 1.270(5) |
| **C1 - N2** | 1.351(3) | 1.348(3) | 1.393(3) | 1.337(4) | 1.378(4) | 1.371(4) |

| | **2dL1** | | **2cL1** | | | |
|---|---|---|---|---|---|---|
| **Cp* - Rh** | 1.834(3) | | **Cp* - Ir** | 1.870(8) | | |
| **Rh - S** | 2.398(6) | | **Ir - P** | 2.276(2) | | |
| **Rh - P** | 2.276(8) | | **Ir - S1** | 2.362(2) | **Ir - S1a** | 2.380(2) |
| **Rh - Cl** | 2.420(1) | | **S1 - C1** | 1.735(7) | **S1a - C1a** | 1.760(8) |
| **S1 - C1** | 1.755(3) | | **C1 - N1** | 1.352(9) | **C1a - N1a** | 1.343(9) |
| **C1 - N1** | 1.360(3) | | **C1 - N2** | 1.315(9) | **C1a - N2a** | 1.322(9) |
| **C1 - N2** | 1.313(3) | | | | | |

Table 2: Crystallographic details for complexes **aL1**, **aL2**, **2dL1**, **2cL1**, **2aL1**, **1aL1**, **1bL3** and **a2L1**.

| Identification code | Complex **aL1** (MCR26_1) | Complex **aL2** (MCR_16) | Complex **2dL1** (MCR_14) | Complex **2cL1** (MCR_12) |
|---|---|---|---|---|
| Empirical formula | $C_{24}H_{27}ClN_2O_2RuS_2$ | $C_{19}H_{25}ClN_2O_2RuS_2$ | $C_{30}H_{41}ClN_5O_{2.5}PRhS_2$ | $C_{46}H_{67}IrN_7O_9PS_4$ |
| Formula weight | 576.14 | 514.07 | 745.156 | 1213.541 |
| Temperature/K | 120.0(4) | 99.9(6) | 99.9(5) | 99.9(5) |
| Crystal system | monoclinic | triclinic | monoclinic | monoclinic |
| Space group | $P2_1/c$ | P-1 | $P2_1/c$ | $P2_1/c$ |
| a/Å | 11.77638(10) | 7.10950(10) | 23.0707(3) | 11.9061(2) |
| b/Å | 18.18345(16) | 10.2048(2) | 8.9830(1) | 16.4040(2) |
| c/Å | 11.48870(11) | 14.9475(3) | 33.0254(3) | 26.5797(3) |
| α/° | 90 | 103.603(2) | 90 | 90 |
| β/° | 100.8584(9) | 92.669(2) | 108.467(1) | 91.392(1) |
| γ/° | 90 | 100.473(2) | 90 | 90 |
| Volume/Å$^3$ | 2416.09(4) | 1031.94(4) | 6491.88(13) | 5189.69(12) |
| Z | 4 | 2 | 8 | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.5838 | 1.6543 | 1.525 | 1.553 |
| μ/mm$^{-1}$ | 8.082 | 9.373 | 6.988 | 7.268 |
| F(000) | 1183.0 | 527.3 | 3100.2 | 2476.8 |
| Crystal size/mm$^3$ | 0.35 × 0.04 × 0.04 | 0.14 × 0.1 × 0.08 | 0.14 × 0.1 × 0.05 | 0.18 × 0.1 × 0.1 |
| Radiation | Cu Kα (λ = 1.54184) | Cu Kα (λ = 1.54184) | Cu Kα (λ = 1.54184) | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 7.64 to 144.94 | 6.12 to 148.12 | 5.64 to 148.7 | 6.34 to 148.6 |
| Index ranges | $-14 \le h \le 14$, $-22 \le k \le 22$, $-14 \le l \le 13$ | $-8 \le h \le 8$, $-12 \le k \le 12$, $-17 \le l \le 18$ | $-28 \le h \le 28$, $-11 \le k \le 10$, $-31 \le l \le 40$ | $-14 \le h \le 14$, $-20 \le k \le 20$, $-32 \le l \le 24$ |
| Reflections collected | 73393 | 29157 | 102852 | 77729 |
| Independent reflections | 4697 [$R_{int}$ = 0.0659, $R_{sigma}$ = 0.0207] | 4084 [$R_{int}$ = 0.0547, $R_{sigma}$ = 0.0309] | 13075 [$R_{int}$ = 0.0661, $R_{sigma}$ = 0.0383] | 10450 [$R_{int}$ = 0.0699, $R_{sigma}$ = 0.0386] |
| Data/restraints/parameters | 4697/0/294 | 4084/0/249 | 13075/3/787 | 10450/0/558 |
| Goodness-of-fit on F$^2$ | 1.035 | 1.027 | 1.015 | 0.707 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0246, $wR_2$ = 0.0662 | $R_1$ = 0.0226, $wR_2$ = 0.0521 | $R_1$ = 0.0295, $wR_2$ = 0.0641 | $R_1$ = 0.0437, $wR_2$ = 0.1209 |
| Final R indexes [all data] | $R_1$ = 0.0258, $wR_2$ = 0.0669 | $R_1$ = 0.0248, $wR_2$ = 0.0531 | $R_1$ = 0.0375, $wR_2$ = 0.0674 | $R_1$ = 0.0476, $wR_2$ = 0.1249 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.45/-0.78 | 0.38/-0.57 | 1.28/-0.78 | 1.61/-1.30 |

| Identification code | Complex **2aL1** (MCR22_01) | Complex **1aL1** (MCR_10) | Complex **1bL3** (Crystal 319) | Complex **$a_2$L1** (MCR25_2) |
|---|---|---|---|---|
| Empirical formula | $C_{31}H_{44}N_5O_4PRuS_2$ | $C_{42}H_{41}N_2O_2PRuS_2$ | $C_{33}H_{31}Cl_2N_2O_2PRuS_2$ | $C_{48}H_{52}N_4O_4Ru_2S_4$ |

| | | | | |
|---|---|---|---|---|
| Formula weight | 746.897 | 801.977 | 754.702 | 1079.367 |
| Temperature/K | 120.00(10) | 100.1(6) | 99.9(5) | 120.0(4) |
| Crystal system | monoclinic | triclinic | monoclinic | monoclinic |
| Space group | C2/c | P-1 | $P2_1/c$ | C2/c |
| a/Å | 38.4923(2) | 9.2306(1) | 8.34223(8) | 23.1894(6) |
| b/Å | 9.48930(5) | 9.8609(1) | 20.4172(3) | 9.2198(2) |
| c/Å | 18.13669(10) | 23.0693(2) | 18.7826(2) | 23.8717(5) |
| α/° | 90 | 78.126(1) | 90 | 90 |
| β/° | 97.5287(5) | 89.588(1) | 98.1698(11) | 112.177(3) |
| γ/° | 90 | 64.356(1) | 90 | 90 |
| Volume/Å$^3$ | 6567.58(6) | 1844.49(4) | 3166.68(6) | 4726.2(2) |
| Z | 8 | 2 | 4 | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.511 | 1.444 | 1.583 | 1.517 |
| μ/mm$^{-1}$ | 5.874 | 5.214 | 7.547 | 7.206 |
| F(000) | 3121.3 | 832.3 | 1547.1 | 2220.1 |
| Crystal size/mm$^3$ | 0.05 × 0.05 × 0.05 | 0.18 × 0.18 × 0.12 | 0.079 × 0.054 × 0.018 | 0.04 × 0.03 × 0.03 |
| Radiation | Cu Kα (λ = 1.54184) | Cu Kα (λ = 1.54184) | Cu Kα (λ = 1.54184) | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 9.28 to 144.92 | 7.86 to 148.52 | 8.66 to 147.76 | 8 to 144.24 |
| Index ranges | -46 ≤ h ≤ 47, -11 ≤ k ≤ 11, -22 ≤ l ≤ 21 | -11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -28 ≤ l ≤ 28 | -10 ≤ h ≤ 10, -23 ≤ k ≤ 25, -23 ≤ l ≤ 23 | -28 ≤ h ≤ 28, -11 ≤ k ≤ 11, -24 ≤ l ≤ 29 |
| Reflections collected | 95269 | 58161 | 29462 | 28202 |
| Independent reflections | 6377 [$R_{int}$ = 0.0385, $R_{sigma}$ = 0.0138] | 7326 [$R_{int}$ = 0.0449, $R_{sigma}$ = 0.0232] | 6346 [$R_{int}$ = 0.0604, $R_{sigma}$ = 0.0409] | 4603 [$R_{int}$ = 0.0796, $R_{sigma}$ = 0.0393] |
| Data/restraints/parameters | 6377/0/467 | 7326/0/456 | 6346/2/395 | 4603/0/285 |
| Goodness-of-fit on $F^2$ | 1.065 | 1.038 | 1.054 | 1.103 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0234, $wR_2$ = 0.0627 | $R_1$ = 0.0315, $wR_2$ = 0.0811 | $R_1$ = 0.0365, $wR_2$ = 0.0858 | $R_1$ = 0.0494, $wR_2$ = 0.1290 |
| Final R indexes [all data] | $R_1$ = 0.0244, $wR_2$ = 0.0631 | $R_1$ = 0.0324, $wR_2$ = 0.0817 | $R_1$ = 0.0449, $wR_2$ = 0.0905 | $R_1$ = 0.0551, $wR_2$ = 0.1338 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.67/-0.55 | 1.72/-0.86 | 0.86/-0.98 | 1.23/-1.35 |

# Cartesian coordinates:

**aL1 – Proximal**

Ru -1.0021030 1.0224776 0.1848485
S 0.5974214 -1.3207405 2.0576034
Cl -0.5944941 -0.5256321 -1.6191089
S 1.1638425 1.9158351 -0.4300805
O 1.9571126 -1.6103547 2.4731495
N 0.6085234 0.0548745 1.1742490
C 1.6634678 0.5665085 0.5021983
O -0.4368807 -1.1623627 3.0474717
N 2.9095330 0.0783380 0.5585800
H 3.0750715 -0.6394941 1.2625133
C -2.6005236 0.6894316 1.6823793
H -2.5924940 -0.1062731 2.4283210
C -1.8430152 2.8902126 0.9623868
H -1.2711201 3.8018485 1.1397984
C 3.8739018 0.4862243 -1.6497724
H 2.9528912 0.1098190 -2.0987401
C -1.2683511 -2.9136089 0.8741085
H -1.9726187 -2.4590349 1.5709230
C -3.0284105 1.4313486 -0.6424100
C -2.4019765 2.6567686 -0.3375300
H -2.2462705 3.3965256 -1.1209771
C -3.5491974 1.0873540 -2.0211611
H -3.2974146 0.0250541 -2.1717344
C -1.2872063 2.1320183 3.3300244
H -0.8475060 1.1927037 3.6909252
H -0.4957893 2.8904913 3.2661828
H -2.0361395 2.4712515 4.0622065
C -1.9293281 1.9229807 1.9886028
C 4.9380711 0.9235697 -2.4343109

H 4.8532633 0.8889707 -3.5216291
C -5.0729417 1.2551015 -2.0380618
H -5.5591876 0.6511504 -1.2567325
H -5.3542555 2.3077872 -1.8730644
H -5.4824149 0.9428183 -3.0098250
C -1.2501284 -5.3711117 -2.0315061
H -1.5690743 -4.8111672 -2.9248270
H -0.4517533 -6.0598303 -2.3389978
H -2.1081447 -5.9656544 -1.6883498
C -2.8750178 1.8779464 -3.1378076
H -3.1388632 2.9478823 -3.1015342
H -1.7821353 1.7667619 -3.0835767
H -3.2079430 1.4954936 -4.1134599
C 6.2165073 1.4267994 -0.4474642
H 7.1300705 1.7917435 0.0242620
C 3.9849107 0.5404466 -0.2592129
C -3.1327841 0.4477894 0.4042574
H -3.5329218 -0.5376416 0.1626124
C 5.1500682 1.0073027 0.3468291
H 5.2106181 1.0444289 1.4361688
C 0.0811837 -2.5725052 0.9448990
C 1.0107570 -3.1557335 0.0841142
H 2.0659588 -2.8903133 0.1575009
C 0.5751492 -4.0755183 -0.8617685
H 1.2991905 -4.5331005 -1.5389139
C 6.1091283 1.3923231 -1.8367974
H 6.9411165 1.7293751 -2.4570783
C -1.6877365 -3.8380182 -0.0753132
H -2.7437530 -4.1122513 -0.1318263
C -0.7778479 -4.4184427 -0.9656460

**aL1 – Distal**

Ru 1.3871712 -0.7349250 -0.6249240
Cl 2.3933079 0.7632211 -2.2057320
S -0.5868121 -0.8216356 -2.0744365
N 0.0664665 0.8376473 -0.3057385
N -1.9029754 1.5291479 -1.4190354
C 3.2737815 -1.8790763 -0.5112264
C 1.0870963 -2.7574821 0.2162039
C 1.0892437 -1.8130150 1.2697393
C 3.2761633 -0.8949380 0.5396480
C 2.2242032 -2.7990892 -0.6635037
C -0.8525504 0.6306430 -1.2070776
C 2.1754421 -0.8919547 1.4239608
C 4.4033923 0.1124402 0.6142504
C -0.0817745 -3.6751731 0.0027394
C 5.5783843 -0.4930347 1.3903691
C 3.9708310 1.4578708 1.1910152
H 4.0530963 -1.8313884 -1.2727996
H 2.2193384 -3.4761368 -1.5179106
H 0.2142478 -1.7331497 1.9173231
H 2.0948952 -0.1086006 2.1783090
H -1.8239410 2.3881300 -0.8749272
H 4.7123559 0.2874829 -0.4289554
H -1.0069734 -3.2112914 0.3689867
H -0.2136687 -3.8987152 -1.0645114
H 0.0798104 -4.6239259 0.5384610
H 5.2947125 -0.6916750 2.4368503
H 5.9138474 -1.4427400 0.9461058
H 6.4333500 0.1987915 1.3961348
H 3.1214945 1.8693573 0.6261484
H 3.6941052 1.3849132 2.2559533
H 4.8023433 2.1743078 1.1230179

C 0.1999069 2.0269258 0.4536203
C 0.6888512 3.1922584 -0.1455105
H 0.9585174 3.1652010 -1.2032128
C 0.8609198 4.3399780 0.6292979
H 1.2440127 5.2492865 0.1634595
C 0.5609058 4.3251152 1.9913512
H 0.7033053 5.2242376 2.5928814
C 0.0789837 3.1572720 2.5850908
H -0.1600869 3.1433552 3.6502281
C -0.1027656 2.0071745 1.8191123
H -0.4866708 1.0851055 2.2620719
S -3.4865027 0.9763050 -1.4189795
O -4.2462638 2.1649249 -1.1549949
O -3.6828556 0.1600308 -2.5745808
C -3.5392344 -0.0709750 -0.0003571
C -3.5749819 -1.4541679 -0.1607266
H -3.6067257 -1.8763011 -1.1649943
C -3.5680321 -2.2683562 0.9713972
H -3.6103148 -3.3535199 0.8502246
C -3.4648537 -0.3254134 2.3911769
H -3.4262246 0.1193327 3.3884236
C -3.4877849 0.5011862 1.2742505
H -3.4709444 1.5873139 1.3851704
C -3.5078224 -1.7216034 2.2570574
C -3.5209016 -2.6065992 3.4762208
H -3.2236597 -3.6348917 3.2297027
H -2.8440604 -2.2264198 4.2544918
H -4.5308010 -2.6479555 3.9135474

**aL2 – Proximal**

Ru -1.0914783 0.6718173 -0.0570668
Cl -0.9192600 -0.4922687 -2.1598388
S 0.2690040 -2.1488964 1.2532781
S 1.1613232 1.4748507 -0.4880072
O -0.8980645 -2.1514411 2.0980697
O 1.5519678 -2.5481282 1.8093103
N 0.4102600 -0.6422472 0.6388002
N 2.7697506 -0.5556401 0.3785562
C 3.9729897 0.0526778 -0.0853563
C -2.8628267 1.8852206 -0.5886462
C -1.6096661 2.1211222 1.5414763
C -2.0623517 0.8283608 1.8931818
C -3.3337117 0.5818551 -0.2062838
C 5.0152790 0.2560341 0.8189564
C -2.0269498 2.6306659 0.2660551
C 1.5432462 -0.0368503 0.2298314
C 6.2150976 0.8081954 0.3744839
C -0.0703991 -3.1733614 -0.1473464
C 6.3652030 1.1694097 -0.9637900
C 5.3170943 0.9636611 -1.8610891
C -2.9342456 0.0713811 1.0454929
C 4.1209214 0.3943541 -1.4302717
C 1.0940951 -3.2482769 -1.1236955
C -4.1885055 -0.1954753 -1.1830410
C -0.6685108 2.8990568 2.4159240
C -5.6208988 0.3507906 -1.1330717
C -4.1512400 -1.7025634 -0.9571821
H -3.0843414 2.2601887 -1.5879719
H -1.6170903 3.5790666 -0.0863066
H -1.6757796 0.3496791 2.7940063
H -3.1839448 -0.9461818 1.3396857

H 3.3008502 0.2123152 -2.1258755
H 5.4334872 1.2364574 -2.9111230
H 7.3018887 1.6090657 -1.3098128
H 7.0315241 0.9643060 1.0810748
H 4.8764541 -0.0174778 1.8667869
H 2.8208414 -1.4018106 0.9456146
H -0.3286427 -4.1512956 0.2869954
H -0.9595722 -2.7374537 -0.6249077
H 1.9999294 -3.6350372 -0.6368204
H 0.8308040 -3.9171553 -1.9538594
H 1.2936143 -2.2574059 -1.5549176
H -3.7601515 0.0052046 -2.1782785
H -0.1718541 2.2366231 3.1371585
H 0.1074388 3.3860868 1.8096048
H -1.2148803 3.6728232 2.9768594
H -6.0701952 0.1826233 -0.1411640
H -5.6545405 1.4311152 -1.3407764
H -6.2482995 -0.1564738 -1.8802016
H -3.1140983 -2.0659621 -0.9650598
H -4.6292364 -1.9893493 -0.0066380
H -4.6959973 -2.2123949 -1.7645125

**aL2 – Distal**

Ru -1.0676461 0.8661797 -0.1695081
Cl -1.0193758 -0.1435579 -2.3469628
S 1.1708589 1.7003827 -0.6468619
N 0.4335643 -0.5160091 0.2815713
N 2.7234665 -0.5757107 -0.2201474
C -3.0810196 1.6631483 -0.5948547
C -1.6177019 2.5150723 1.1998948
C -1.7786305 1.2815639 1.8723580
C -3.2309446 0.3941612 0.0689158
C -2.3119993 2.7019355 -0.0461327
C 1.5092926 0.0893267 -0.1557338
C -2.5773313 0.2336579 1.3087264
C -4.0070070 -0.7147490 -0.6089143
C -0.7255051 3.5944011 1.7414355
C -5.4965176 -0.5766825 -0.2754108
C -3.4720819 -2.1065090 -0.2808932
H -3.4849510 1.7768852 -1.6016900
H -2.1542317 3.6155403 -0.6196216
H -1.2181133 1.0974349 2.7896114
H -2.5930538 -0.7379292 1.8032888
H 2.7044528 -1.5730932 -0.0211068
H -3.8633707 -0.5553640 -1.6898963
H -0.0105948 3.1853614 2.4669687
H -0.1525122 4.0641126 0.9307136
H -1.3277370 4.3699016 2.2394829
H -5.6728892 -0.7257926 0.8024199
H -5.8835011 0.4178253 -0.5456859
H -6.0845099 -1.3286116 -0.8217143
H -2.3992330 -2.1748878 -0.5153801
H -3.6294280 -2.3740393 0.7772426
H -4.0010841 -2.8581111 -0.8846935

C 0.3477506 -1.9129144 0.5108464
C 0.4283238 -2.8105954 -0.5607828
H 0.5662509 -2.4144914 -1.5687894
C 0.2835674 -4.1774493 -0.3234527
H 0.3434540 -4.8762742 -1.1594099
C 0.0471176 -4.6497703 0.9677615
H -0.0730000 -5.7196758 1.1458674
C -0.0386755 -3.7510314 2.0318154
H -0.2212278 -4.1168036 3.0439217
C 0.1130088 -2.3839477 1.8064079
H 0.0535002 -1.6657694 2.6275502
S 4.2423410 0.0235270 -0.5544852
O 4.9979044 -1.1448549 -0.9078382
O 4.1021905 1.1562123 -1.4152811
C 4.8414933 0.5847336 1.0178615
C 4.0391821 1.7326958 1.6130758
H 5.8816213 0.8766074 0.8056543
H 4.8679583 -0.3014457 1.6678752
H 3.9897384 2.5798789 0.9162831
H 4.5142853 2.0681004 2.5452066
H 3.0088901 1.4255593 1.8416228

**1aL1 - Proximal**

Ru 0.2677304 0.1508702 1.2419589
S 2.0182211 -1.1544230 0.2880631
P -1.1085203 -1.2979629 0.0394223
N 3.1999989 0.7635273 -1.3436251
N 0.9493050 0.9725902 -0.5861902
C -1.2057016 -1.2427623 -1.7882432
C -0.0347255 -1.2423420 -2.5614223
C -2.8634423 -1.0766115 0.5065338
C -0.1530506 -3.4831128 1.5100966
C -3.6918825 -2.1047035 0.9672899
C -3.3782558 0.2264426 0.4171299
C -2.4452314 -1.2559883 -2.4444597
C 0.0266698 -4.8353527 1.7945369
C -1.1237350 -5.4099265 -0.2468457
C 2.1822373 0.3269593 -0.7096082
C -1.3033138 -4.0569284 -0.5299343
C -4.6955050 0.4948493 0.7784713
C 0.1848992 2.1472656 2.2722810
C -0.8243517 -3.0773613 0.3514382
C -5.0097386 -1.8318830 1.3432547
C 0.2548443 -0.3875797 3.4524098
C -0.4611589 -5.8018412 0.9161043
C 1.4647419 0.3000040 3.1632816
C -1.3427682 -1.2073677 -4.5945919
C -2.5125657 -1.2433827 -3.8379007
C -0.1041185 -1.2123830 -3.9518157
C -1.0287074 1.4966029 2.5826138
C -5.5134410 -0.5359512 1.2500869
C -1.0046793 0.2026328 3.1810066
C 1.4640443 1.5834685 2.5814381
C -2.2649978 -0.4938708 3.6100387

C 2.7308824 2.3446349 2.2391683
C 2.8557244 3.5650524 3.1594112
C 3.9864172 1.4788503 2.2915668
H 0.1701235 3.0999538 1.7423081
H 2.4092405 -0.2179350 3.3268760
H 0.2940916 -1.3777221 3.9079229
H -1.9818495 1.9622120 2.3292729
H -3.3719453 -1.2638153 -1.8687570
H -3.4867906 -1.2552442 -4.3310479
H -1.3947159 -1.1809922 -5.6847409
H 0.8188698 -1.1866837 -4.5331290
H 0.9347605 -1.2717582 -2.0688558
H -2.7306990 1.0333256 0.0665032
H -5.0803018 1.5138057 0.6988009
H -6.5433509 -0.3262934 1.5455472
H -5.6442164 -2.6399304 1.7120775
H -3.3072264 -3.1234201 1.0469457
H -1.8145731 -3.7612911 -1.4485576
H -1.4980191 -6.1616695 -0.9439018
H -0.3140753 -6.8616585 1.1320264
H 0.5636892 -5.1337644 2.6966972
H 0.2523296 -2.7205347 2.1764810
H -3.1431302 -0.1238558 3.0677460
H -2.1908153 -1.5798941 3.4593675
H -2.4196039 -0.3082032 4.6848112
H 2.6019136 2.7106078 1.2087014
H 1.9768218 4.2233059 3.0865363
H 2.9665826 3.2554488 4.2119001
H 3.7387277 4.1593802 2.8833947
H 4.2156675 1.1504453 3.3197631
H 3.8944592 0.5901274 1.6489642
H 4.8484540 2.0620319 1.9377725
S 0.7288464 2.4470478 -1.2497271

O 1.1457104 3.5050922 -0.3458048
O 1.1994274 2.4540586 -2.6084857
C -1.0426627 2.5787923 -1.3342266
C -1.7331488 3.4293891 -0.4722562
C -1.7186815 1.9418288 -2.3785680
C -3.8046867 2.9661369 -1.6566120
C -3.1079074 3.6131484 -0.6311797
C -3.0880688 2.1325119 -2.5263189
C -5.2878662 3.1583972 -1.8398970
H -1.1609304 1.3166475 -3.0769890
H -3.6123158 1.6263272 -3.3405953
H -3.6425370 4.2892835 0.0407817
H -1.1818090 3.9765190 0.2928282
H -5.8195651 2.1959008 -1.7810626
H -5.7052168 3.8274930 -1.0750357
H -5.5097466 3.5927926 -2.8262355
C 4.3480817 -0.0471226 -1.4249818
C 5.5724789 0.4583170 -0.9690118
H 5.5933164 1.4641535 -0.5460435
C 6.7307407 -0.3088435 -1.0623400
H 7.6760602 0.0973934 -0.6961904
C 6.6918283 -1.5839709 -1.6288358
H 7.6020736 -2.1808342 -1.7076950
C 5.4803272 -2.0812596 -2.1075571
H 5.4381445 -3.0704190 -2.5686237
C 4.3164028 -1.3205576 -2.0104871
H 3.3708986 -1.7031957 -2.4008242

**1aL1 - Distal**

Ru 0.4780760 -1.2826129 -0.1925375
S -3.1140499 2.2862962 0.8898424
S -0.9286650 -0.1138535 1.3112886
P 2.0895750 0.2150714 0.5694078
O -2.4396783 2.2828431 2.1723367
O -3.7603158 3.4898715 0.4325483
N -2.1529717 1.7994515 -0.3106231
N -0.4400820 0.3742313 -1.0957961
C 1.8752258 1.9550768 0.0665791
C 0.9053790 2.7345010 0.7194917
C 3.7888388 -0.2271639 0.0337330
C 1.8322816 -0.7195004 3.1972587
C 4.8480157 -0.3865876 0.9367198
C 4.0279236 -0.4863415 -1.3261618
C -4.3515309 1.0156253 0.9469979
C 0.8570450 0.4694407 -3.1184715
C 2.5832575 2.5107048 -1.0077421
C 2.0285657 -0.6768421 4.5759978
C 3.0858143 1.4817082 4.3525592
C -1.2785424 0.8315611 -0.1456272
C 2.8953718 1.4343452 2.9727910
C 5.2855460 -0.8862656 -1.7707415
C -4.3552490 0.0748709 1.9738682
C 0.4055795 -2.6888837 -1.9736690
C 2.2687822 0.3289871 2.3805574
C 6.1057406 -0.8002581 0.4934689
C 0.4491053 -3.3247487 0.7562042
C 0.6854741 2.2726803 -4.7153304
C -0.7454637 2.2262205 -2.7434290
C 2.6563387 0.4252662 5.1554202
C -0.3197954 2.8289264 -3.9259564

C -0.7984218 -3.1298527 0.0830493
C -0.1474089 1.0273633 -2.3079212
C 1.3432663 4.5723212 -0.7870421
C -5.2902989 0.9372494 -0.0859141
C 2.3193275 3.8133214 -1.4286215
C 0.6389819 4.0313682 0.2886178
C 1.2702485 1.0778159 -4.2999784
C 1.6348365 -2.9153168 -1.3343955
C 6.3285386 -1.0523913 -0.8578164
C 1.6775533 -3.2157008 0.0662774
C -6.2291532 -1.0655288 0.9224355
C -0.8471941 -2.7945130 -1.2798818
C -5.2946957 -0.9576148 1.9553049
C 2.9896373 -3.4808894 0.7516655
C -6.2190944 -0.0962635 -0.0917118
C -2.1294157 -2.4737812 -2.0221703
C -2.5064121 -3.6470257 -2.9341709
C -7.2174278 -2.2028327 0.8823359
C -3.2811351 -2.0878145 -1.0980240
H 0.3929020 -2.3957968 -3.0249918
H -1.7155843 -3.1392096 0.6713060
H 0.4495127 -3.5453629 1.8247183
H 2.5692570 -2.8172471 -1.8886644
H 3.3497827 1.9353655 -1.5272602
H 2.8764108 4.2288295 -2.2700578
H 1.1269313 5.5868505 -1.1273210
H -0.1355136 4.6102696 0.7944728
H 0.3367602 2.3247031 1.5573309
H 3.2160401 -0.3647289 -2.0450735
H 5.4511569 -1.0716316 -2.8339496
H 7.3125146 -1.3759261 -1.2019534
H 6.9149438 -0.9264407 1.2149636
H 4.6918851 -0.2005108 2.0000234

H 3.2297138 2.2671898 2.3501537
H 3.5676194 2.3514814 4.8021573
H 2.8014750 0.4664063 6.2364888
H 1.6751885 -1.4983467 5.2017409
H 1.3110403 -1.5633420 2.7405640
H -1.5272005 2.6859957 -2.1477879
H -0.7958811 3.7634812 -4.2310727
H 1.0042540 2.7589658 -5.6386393
H 2.0609472 0.6134152 -4.8946753
H 1.3327831 -0.4496327 -2.7804188
H -5.2837174 1.6924867 -0.8732824
H -6.9566327 -0.1533214 -0.8964596
H -5.3013793 -1.6914352 2.7652813
H -3.6267622 0.1646523 2.7795707
H 3.8135751 -2.9606909 0.2459593
H 2.9670494 -3.1555083 1.8009096
H 3.2028509 -4.5611614 0.7325745
H -1.8951871 -1.5992713 -2.6547556
H -1.6927487 -3.9067593 -3.6286554
H -2.7399170 -4.5426691 -2.3361414
H -3.3942298 -3.3970065 -3.5328896
H -6.8920124 -2.9785222 0.1702696
H -7.3234432 -2.6787996 1.8667146
H -8.2099535 -1.8586281 0.5580502
H -3.6296045 -2.9476537 -0.5014077
H -2.9954887 -1.2810609 -0.4060134
H -4.1361548 -1.7365328 -1.6928247

**1bL3 - Proximal**

Ru 0.3895525 -0.9762966 -1.1657467
S -0.8846321 -2.5120222 1.4329221
P 1.3435952 0.7007024 0.1075184
S -1.5374904 0.4344952 -1.3276557
O 0.5152330 -2.8059496 1.6983435
O -1.6962873 -3.5815711 0.8922894
N -0.8811795 -1.2026221 0.4754911
N -3.1549697 -0.5632926 0.7011505
C 1.8607553 3.4615890 0.0758501
H 2.0457888 3.3599332 1.1485049
C 1.2276180 2.4895162 -2.0421358
H 0.9007576 1.6224348 -2.6199497
C 1.1241386 0.7385135 2.9393161
H 2.0602501 0.1821711 2.9768106
C 1.4863050 2.3374168 -0.6763540
C -4.2278117 0.1814188 0.1653096
C 1.7356820 4.8452154 -1.8998187
H 1.8267691 5.8235389 -2.3752082
C 0.2365271 -3.1699578 -1.7720821
H -0.4051861 -3.8989689 -1.2744173
C 4.1712956 1.0340968 0.2032270
H 4.0343578 1.9921546 -0.3010973
C 5.6570079 -0.6294644 1.1395816
H 6.6671135 -0.9720355 1.3717702
C -6.4225206 1.6217419 -0.8280578
H -7.2768417 2.1807160 -1.2134367
C 5.4635386 0.5900225 0.4964105
H 6.3207834 1.2061061 0.2189278
C 1.8390154 -1.1117315 -2.8984651
H 2.4461225 -0.3061894 -3.3113234
C -1.2609301 2.1785612 2.9013215

H -2.1910236 2.7493641 2.8778543
C -4.8729740 -0.2286196 -1.0087274
H -4.5088955 -1.1200146 -1.5229105
C -0.6318245 1.8473312 1.7048833
H -1.0753950 2.1520286 0.7547599
C 4.5540345 -1.4163249 1.4828486
H 4.6977073 -2.3746681 1.9854531
C 3.2656003 -0.9881335 1.1760108
H 2.4045177 -1.6208681 1.4161383
C 2.3446829 -1.9161965 -1.8316435
H 3.3316166 -1.7041444 -1.4194545
C -2.0321352 -0.5226385 0.0919803
C -5.7879003 2.0269115 0.3460083
H -6.1451635 2.9074205 0.8842606
C 0.5662682 1.1138430 1.7112319
C 0.5248549 -1.3315087 -3.3619320
H 0.0993357 -0.6754146 -4.1221897
C 1.3539140 3.7369435 -2.6529534
H 1.1380808 3.8449122 -3.7173437
C 3.0619434 0.2521866 0.5419792
C -4.7009946 1.3102879 0.8440048
H -4.2030743 1.6105205 1.7680769
C -0.2707676 -2.3941884 -2.8250944
H -1.2981968 -2.5268438 -3.1614422
C -5.9609582 0.4889661 -1.4995974
H -6.4558387 0.1568138 -2.4146366
C -0.7047220 1.7909737 4.1215960
H -1.2000472 2.0535771 5.0581748
C 0.4898659 1.0749831 4.1369552
H 0.9403528 0.7749201 5.0849366
C 1.9878803 4.7069818 -0.5336846
H 2.2775741 5.5746583 0.0614488
C 1.5511576 -2.9287700 -1.2600007

H 1.9052019 -3.4922915 -0.3983233
C -1.6158519 -1.9751402 2.9426114
H -1.5486856 -2.8243843 3.6349368
H -1.0467903 -1.1165767 3.3203226
H -2.6561604 -1.6993140 2.7401457

**1bL3 - Distal**

Ru 0.5531636 0.1454774 1.6360185
P 1.1485276 -0.4794051 -0.5142853
S -1.2272637 -1.4130286 1.4431379
N -1.1482815 0.9991218 0.7719475
N -3.2789868 0.0982812 0.3104863
C 1.9918747 -2.6903732 -2.0121164
H 1.9232447 -2.0241691 -2.8762530
C 1.7112417 -3.0895744 0.3532812
H 1.4068127 -2.7311592 1.3379020
C 0.2607778 0.6564528 -2.9577979
H 1.1417342 1.2975143 -2.9355382
C 1.6642804 -2.2112861 -0.7335696
C 2.4443597 -4.8775485 -1.0928824
H 2.7438750 -5.9175725 -1.2345833
C 0.6464615 1.5832491 3.4177884
H -0.0762447 2.3698072 3.6384262
C 3.8747225 -0.0394145 -1.2190230
H 4.0016858 -1.1235450 -1.2394104
C 4.8348659 2.1736656 -1.4117554
H 5.6983330 2.8186812 -1.5837913
C 4.9801963 0.7896446 -1.4347233
H 5.9587200 0.3443953 -1.6237773
C 2.4360935 -0.5027580 2.7206542
H 3.1104220 -1.3072750 2.4281914

C -2.0061683 -0.9679459 -3.0724470
H -2.8966187 -1.5965238 -3.0833689
C -1.1210598 -1.0836327 -2.0033723
H -1.3270884 -1.8162500 -1.2211399
C 3.5777578 2.7353027 -1.1666708
H 3.4534490 3.8199668 -1.1502649
C 2.4794782 1.9138071 -0.9362744
H 1.5040914 2.3627172 -0.7199984
C 2.6486457 0.8200347 2.2286356
H 3.4806238 1.0174003 1.5515772
C -2.0529141 0.0001399 0.7664542
C 0.0135671 -0.2590965 -1.9252033
C 1.3097739 -0.7663428 3.5275992
H 1.0952898 -1.7863638 3.8486801
C 2.1010707 -4.4172648 0.1760526
H 2.1205248 -5.0962281 1.0301181
C 2.6157088 0.5127602 -0.9670652
C 0.4256654 0.2907102 3.9132832
H -0.4637009 0.0695168 4.5015467
C -1.7555340 -0.0471311 -4.0905185
H -2.4477542 0.0409012 -4.9303374
C -0.6189146 0.7573058 -4.0350694
H -0.4124064 1.4758837 -4.8304477
C 2.3867832 -4.0132251 -2.1882496
H 2.6389888 -4.3759027 -3.1861433
C 1.7615475 1.8586501 2.5648618
H 1.9180423 2.8558661 2.1548798
C -1.3119799 2.2110134 0.0682654
C -0.7085546 3.3741784 0.5664937
H -0.1865871 3.3260561 1.5210900
C -0.7776283 4.5789229 -0.1316262
H -0.3024358 5.4699852 0.2847122
C -1.4582262 4.6479287 -1.3457310

H -1.5166900 5.5883838 -1.8961095
C -2.0675477 3.4955255 -1.8442553
H -2.6024060 3.5281926 -2.7960284
C -2.0003185 2.2889746 -1.1534891
H -2.4710199 1.3954554 -1.5583845
S -4.2616303 -1.1854452 0.3130115
O -4.1122770 -1.9425693 -0.9164915
O -4.2222125 -1.9189167 1.5623293
C -5.8186267 -0.3581006 0.2243488
H -5.8398063 0.2631275 -0.6780967
H -5.9461312 0.2565559 1.1223552
H -6.5893566 -1.1371293 0.1762585

**2aL1 - Proximal**

Ru -1.6648890 0.5122066 -0.2631098
S 0.5841517 0.1001157 -2.7838250
P 0.0096740 0.9743818 1.2420188
S -1.1795089 -1.7238108 0.4602293
O 0.7397657 -0.9772749 -3.7195586
O -0.0733426 1.3255504 -3.1905474
N 1.0315208 -2.3952040 -1.0854653
N 2.4596952 0.5499593 2.3977486
C 1.1655538 -3.5680354 -0.3156265
N -0.1925383 -0.3954135 -1.4510221
N 0.6249964 1.1507922 3.9225987
N 1.6223605 2.8616928 2.4509140
C 1.6218763 0.0790342 1.2820319
H 1.4308889 -0.9976153 1.3941797
H 2.1533887 0.2260532 0.3317291
C -3.9036301 0.1942866 -0.1446966
C 2.1981804 0.5744730 -2.2329820

C 3.1934380 -0.3923152 -2.0623258
H 2.9808664 -1.4261765 -2.3312584
C 0.2314702 -4.6096316 -0.3839494
H -0.6301943 -4.5023536 -1.0455435
C 4.6860238 1.3170746 -1.1758418
C 2.4478913 1.9105275 -1.9170420
H 1.6707497 2.6547920 -2.0988054
C 0.0513031 -1.6153190 -0.8334110
C 2.2937798 -3.7145145 0.5028309
C -3.5406394 1.2627933 0.7204922
H -3.7836470 1.2181234 1.7807721
C -0.4618139 0.7717691 3.0082018
H -1.3523114 1.3856956 3.2246874
H -0.7398247 -0.2814812 3.1714083
C 1.8138092 0.3198901 3.6907779
H 1.5315180 -0.7394626 3.7685871
H 2.5431995 0.5493045 4.4813528
C -3.5456686 0.2867040 -1.5184262
H -3.7641242 -0.5447869 -2.1890241
C -2.4328770 2.4777114 -1.1497605
C -2.8050711 1.3955682 -1.9954414
H -2.4423427 1.3933648 -3.0233216
C 0.6663802 2.6965393 1.3449723
H 1.1625860 2.9491759 0.3948217
H -0.1675916 3.4057554 1.4765201
C -2.7996052 2.3680824 0.2202256
H -2.4954373 3.1542047 0.9149847
C -1.6813262 3.6666040 -1.6789272
H -1.1157121 4.1616391 -0.8766885
H -0.9820729 3.3487757 -2.4624702
H -2.3790191 4.4035600 -2.1060190
C 4.4227053 -0.0135061 -1.5291304
H 5.1990092 -0.7691692 -1.3865712

C 2.4674355 -4.8703595 1.2614959
C -4.6428373 -1.0335958 0.3490353
H -4.1935391 -1.8886244 -0.1823333
C 2.7783846 1.9726432 2.2748630
H 3.5157027 2.2254453 3.0511232
H 3.2235578 2.1543137 1.2876027
C 3.6887194 2.2747187 -1.3952881
H 3.8887477 3.3237130 -1.1598006
C 0.9993622 2.5568281 3.7427275
H 0.1051152 3.1854753 3.8684530
H 1.7193623 2.8178277 4.5318138
C 6.0067339 1.6991863 -0.5595512
H 6.0309885 1.4201720 0.5064271
H 6.8413982 1.1800122 -1.0511021
H 6.1855476 2.7809666 -0.6274925
C 1.5269808 -5.8995008 1.2045776
C -4.4899286 -1.2787053 1.8480023
H -3.4316832 -1.2878103 2.1496548
H -5.0189847 -0.5158284 2.4419022
H -4.9242941 -2.2532539 2.1121336
C 0.4136184 -5.7646119 0.3746543
H -0.3216001 -6.5696114 0.3121857
C -6.1204242 -0.9233455 -0.0477720
H -6.5938114 -0.0599992 0.4469118
H -6.2424977 -0.7993835 -1.1338638
H -6.6660919 -1.8285763 0.2554910
H 3.0308153 -2.9081281 0.5285335
H 3.3479279 -4.9689280 1.9000308
H 1.6665576 -6.8058314 1.7962004

**2aL1 - Distal**

Ru 1.9317580 -0.7396128 0.2623272
P 1.5937967 1.3809118 -0.5625499
S 0.2268441 -1.2244726 -1.3272660
N -2.1101909 -0.5496507 0.0295576
N -0.0145075 3.5405094 -1.0255962
N 0.0150951 -0.5222940 1.0654937
N 1.7199353 3.0930327 -2.7085750
N 2.3401484 4.0405611 -0.5165308
C -0.0572541 2.1904171 -0.4421628
H -0.8067340 1.5917083 -0.9800070
H -0.3702792 2.2480989 0.6119144
C 3.0254964 -2.6806346 -0.2122200
C -0.8127952 -0.7514711 0.0261622
C 3.8605144 -1.5741779 -0.5473049
H 4.2369249 -1.4555559 -1.5613200
C 1.9334410 1.6854674 -2.3456025
H 2.9722300 1.3946180 -2.5774097
H 1.2679207 1.0413394 -2.9394478
C 0.3287522 3.4953898 -2.4476273
H -0.3521798 2.8001141 -2.9565501
H 0.1875658 4.5023588 -2.8667348
C 2.5095826 -2.7590668 1.1060870
H 1.8121322 -3.5558371 1.3658143
C 3.6772207 -0.6675106 1.7647445
C 2.8106540 -1.7494263 2.0615683
H 2.3322644 -1.7884400 3.0427092
C 2.6233073 2.7503148 0.1285551
H 2.4349973 2.8378942 1.2113436
H 3.6922996 2.5090365 0.0022408
C 4.1549146 -0.5832565 0.4224261
H 4.7729932 0.2697473 0.1335388

C 4.0924839 0.3305331 2.8095490
H 4.2212996 1.3323593 2.3760560
H 3.3500863 0.3912670 3.6162136
H 5.0529894 0.0320635 3.2577890
C 2.6470964 -3.7481783 -1.2199713
H 1.5710584 -3.9356619 -1.0679657
C 0.9293537 4.4116969 -0.3315213
H 0.8006552 5.4334797 -0.7176615
H 0.6967905 4.4116250 0.7432533
C 2.6110612 3.9791935 -1.9580503
H 3.6522262 3.6586939 -2.1138609
H 2.4964484 4.9954531 -2.3621801
C 2.8496883 -3.3256641 -2.6727072
H 2.3321036 -2.3820087 -2.9009481
H 3.9181219 -3.2116967 -2.9185455
H 2.4425164 -4.0967339 -3.3414768
C 3.4260369 -5.0322084 -0.9060059
H 4.5101041 -4.8679591 -1.0169953
H 3.2401022 -5.3822234 0.1199495
H 3.1317759 -5.8347976 -1.5974582
S -2.9046720 -0.5525048 -1.3808823
O -2.6790295 0.7062133 -2.0683291
O -2.7153182 -1.7856096 -2.1147668
C -4.5700255 -0.5338930 -0.7895406
C -5.1832649 0.6793794 -0.4779264
H -4.6308390 1.6093659 -0.6178560
C -7.1986636 -0.5165112 0.1674485
C -5.2558643 -1.7363979 -0.6346667
H -4.7587551 -2.6709659 -0.8969526
C -6.4897924 0.6798360 0.0003205
H -6.9729157 1.6285131 0.2463827
C -6.5636231 -1.7205825 -0.1551076
H -7.1042770 -2.6621516 -0.0329022

C -8.6258528 -0.5003934 0.6518033
H -8.7918081 0.3043576 1.3816885
H -9.3201828 -0.3315401 -0.1867385
H -8.9016324 -1.4541985 1.1221734
C -0.3845584 0.0613304 2.2802118
C -1.6428153 -0.1595412 2.8657797
H -2.3656983 -0.7965747 2.3622141
C -1.9595017 0.4453428 4.0804508
H -2.9430480 0.2631887 4.5184366
C -1.0491658 1.2723868 4.7393105
H -1.3129032 1.7410974 5.6885688
C 0.2026109 1.4890318 4.1655243
H 0.9319648 2.1339230 4.6615065
C 0.5297106 0.8886305 2.9512479
H 1.5035583 1.0568084 2.4871174