Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers

Supporting Information Material

Molecular Recognition: Preparation and Characterization of Two Tripodal Anion Receptors

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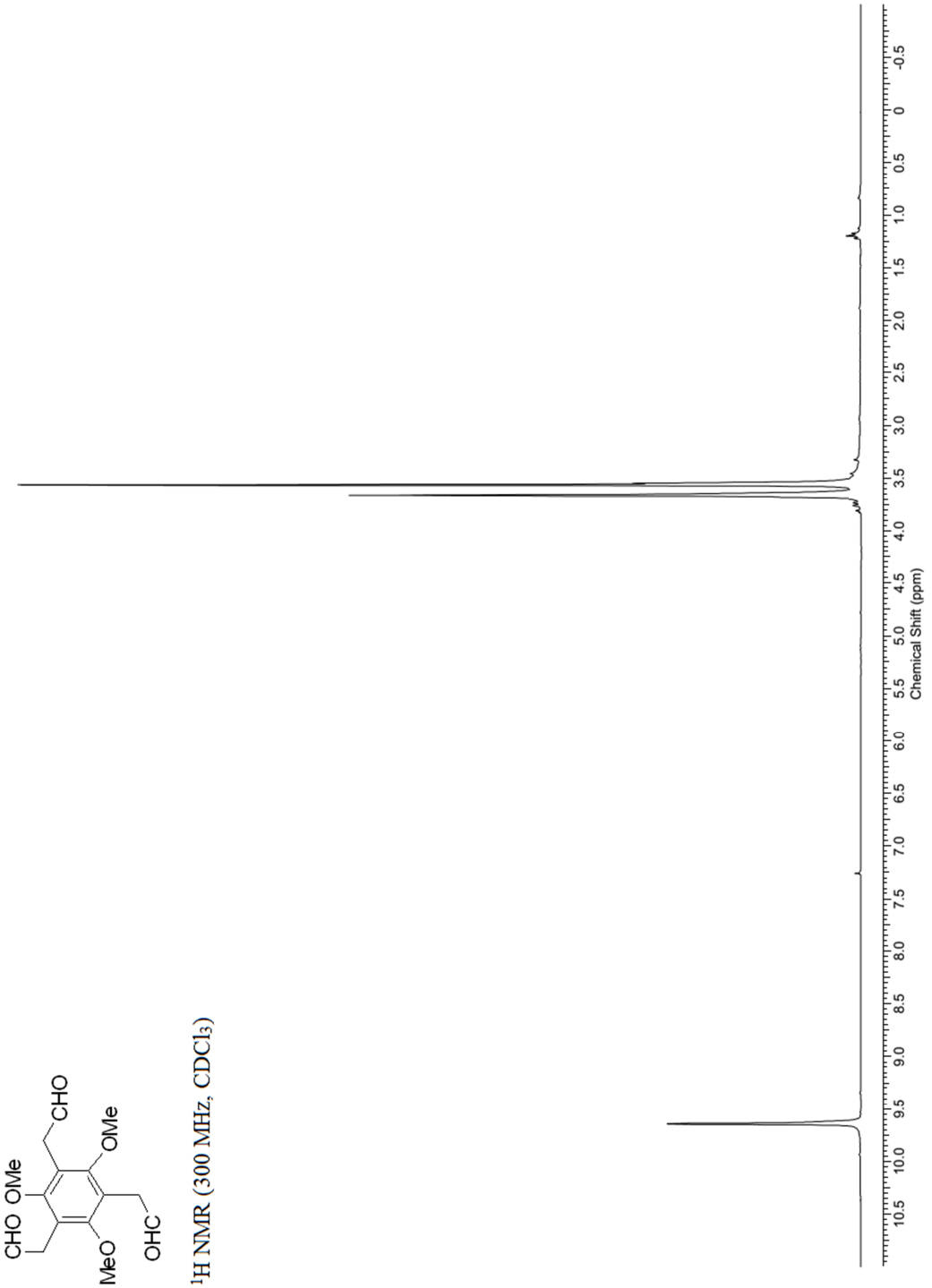
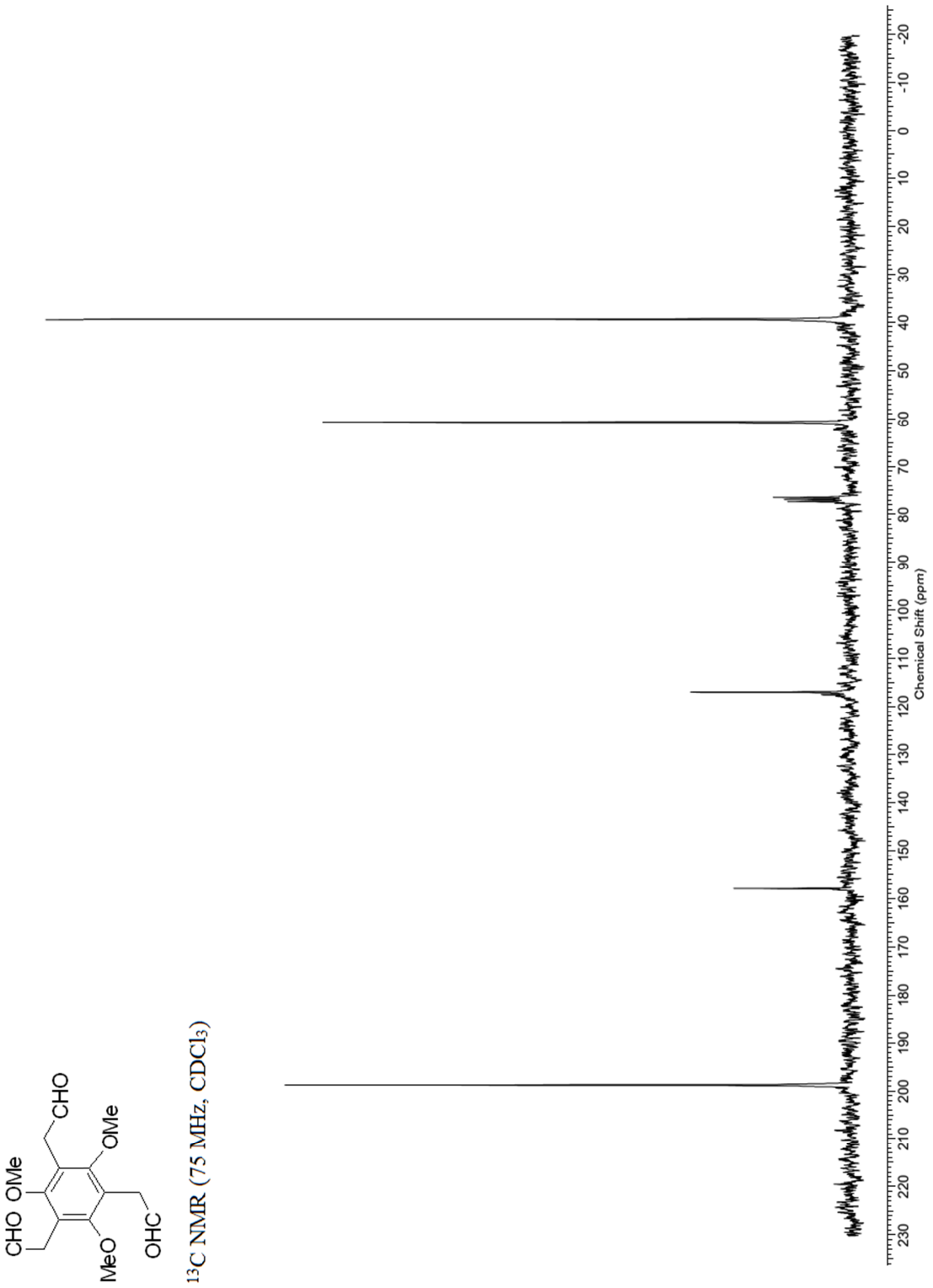
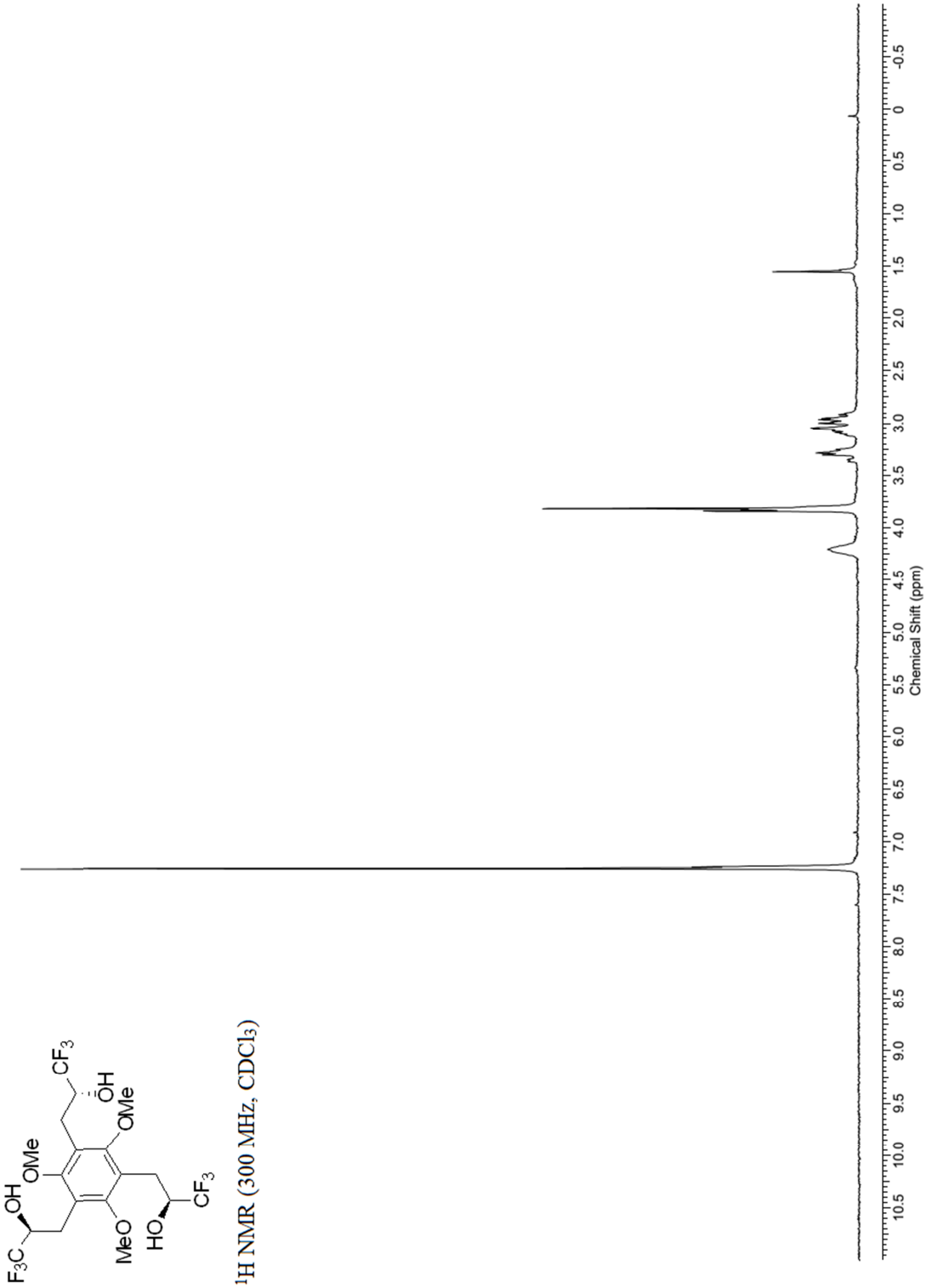
^{1}H and ^{13}C NMR Spectra



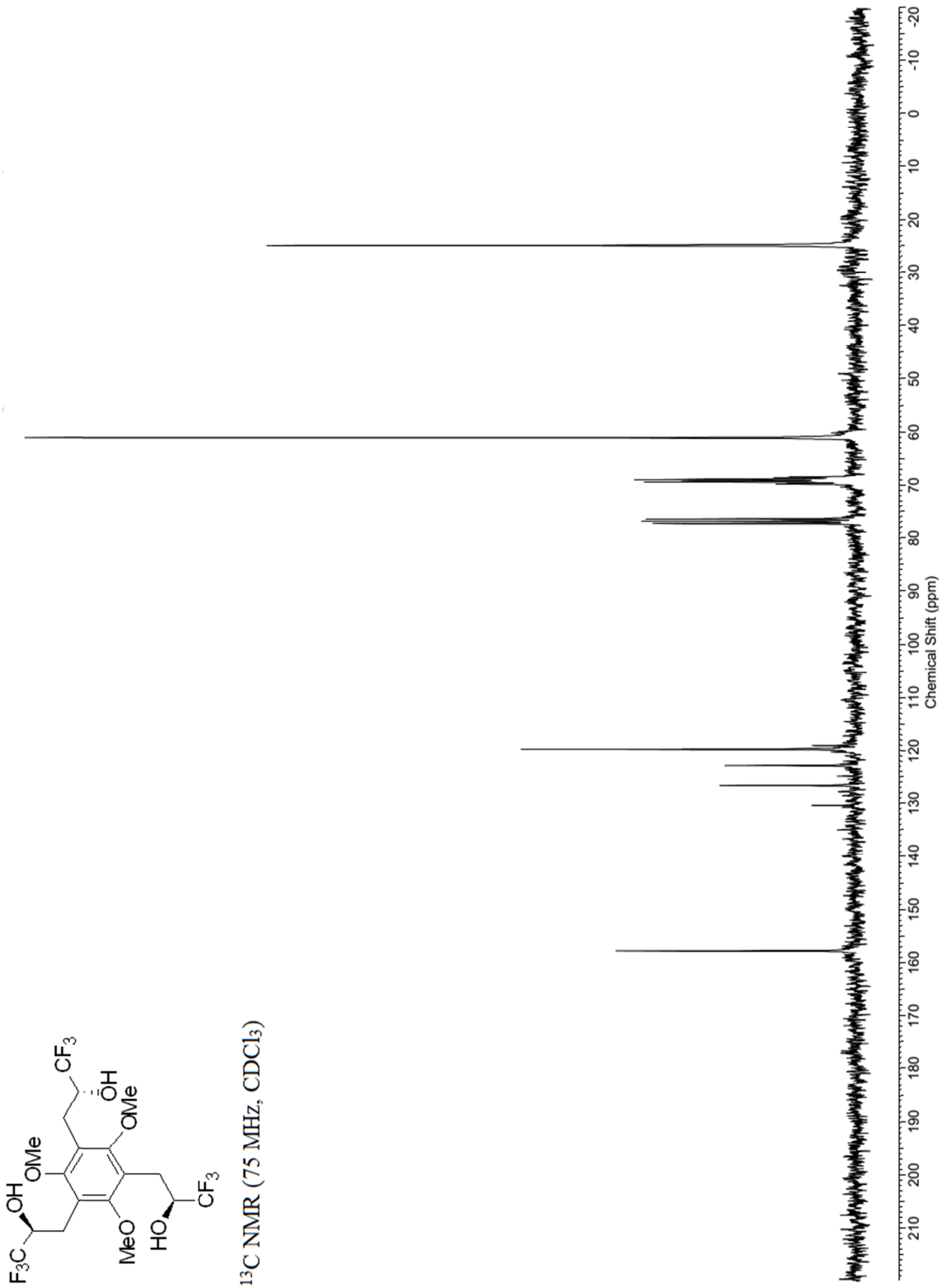
^{1}H NMR (300 MHz, $CDCl_3$)

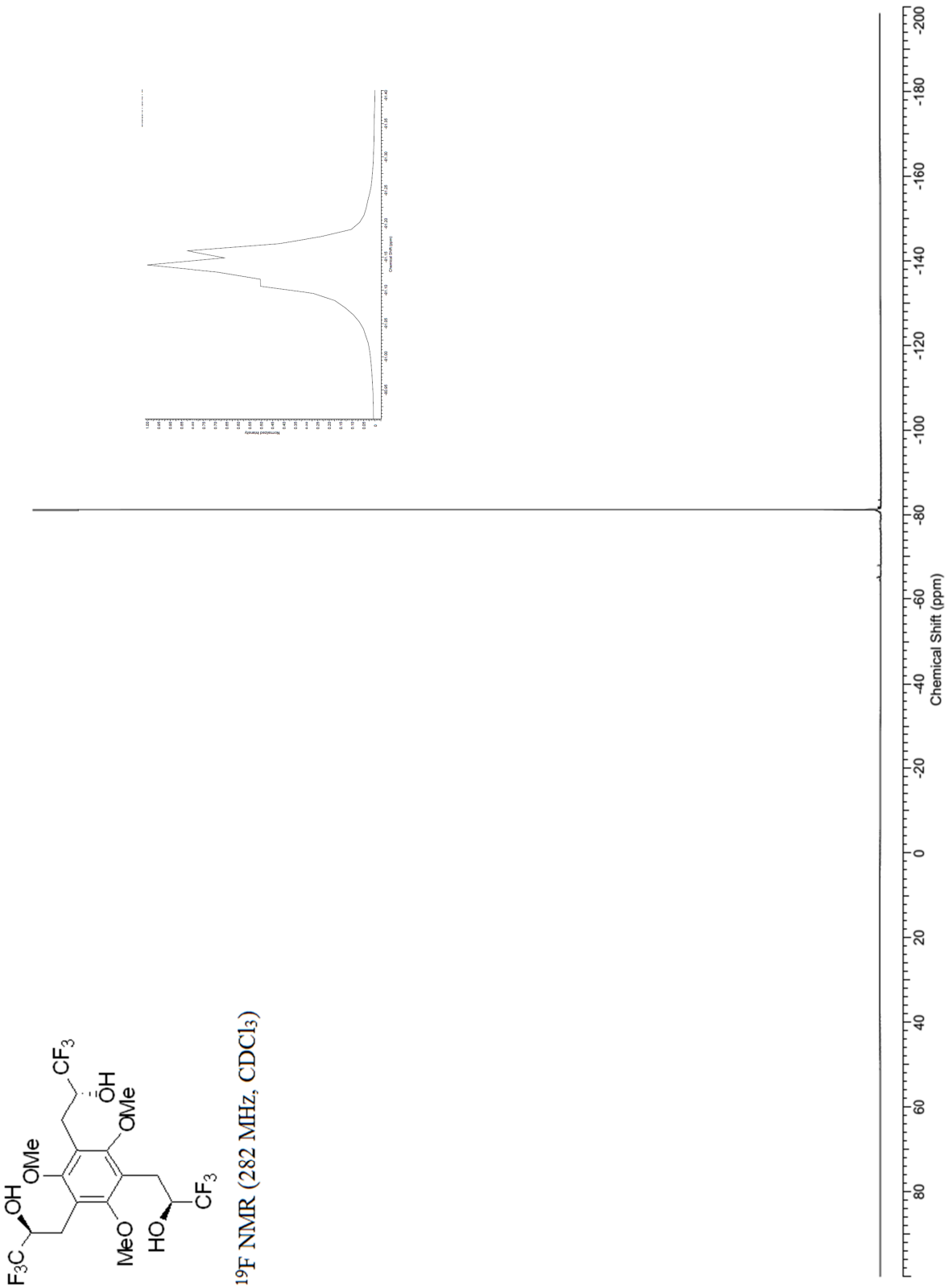


^{13}C NMR (75 MHz, $CDCl_3$)

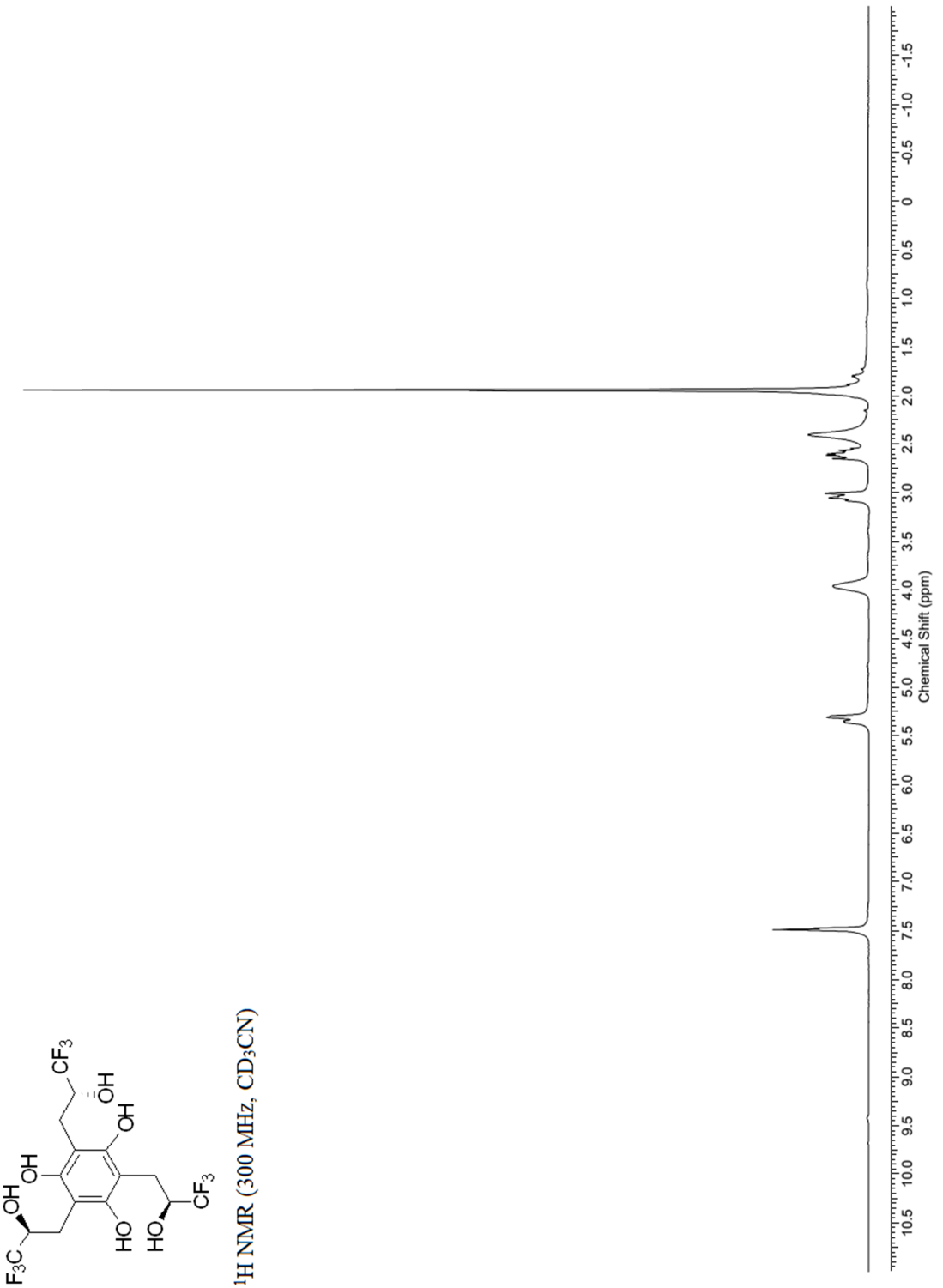


^{1}H NMR (300 MHz, $CDCl_3$)

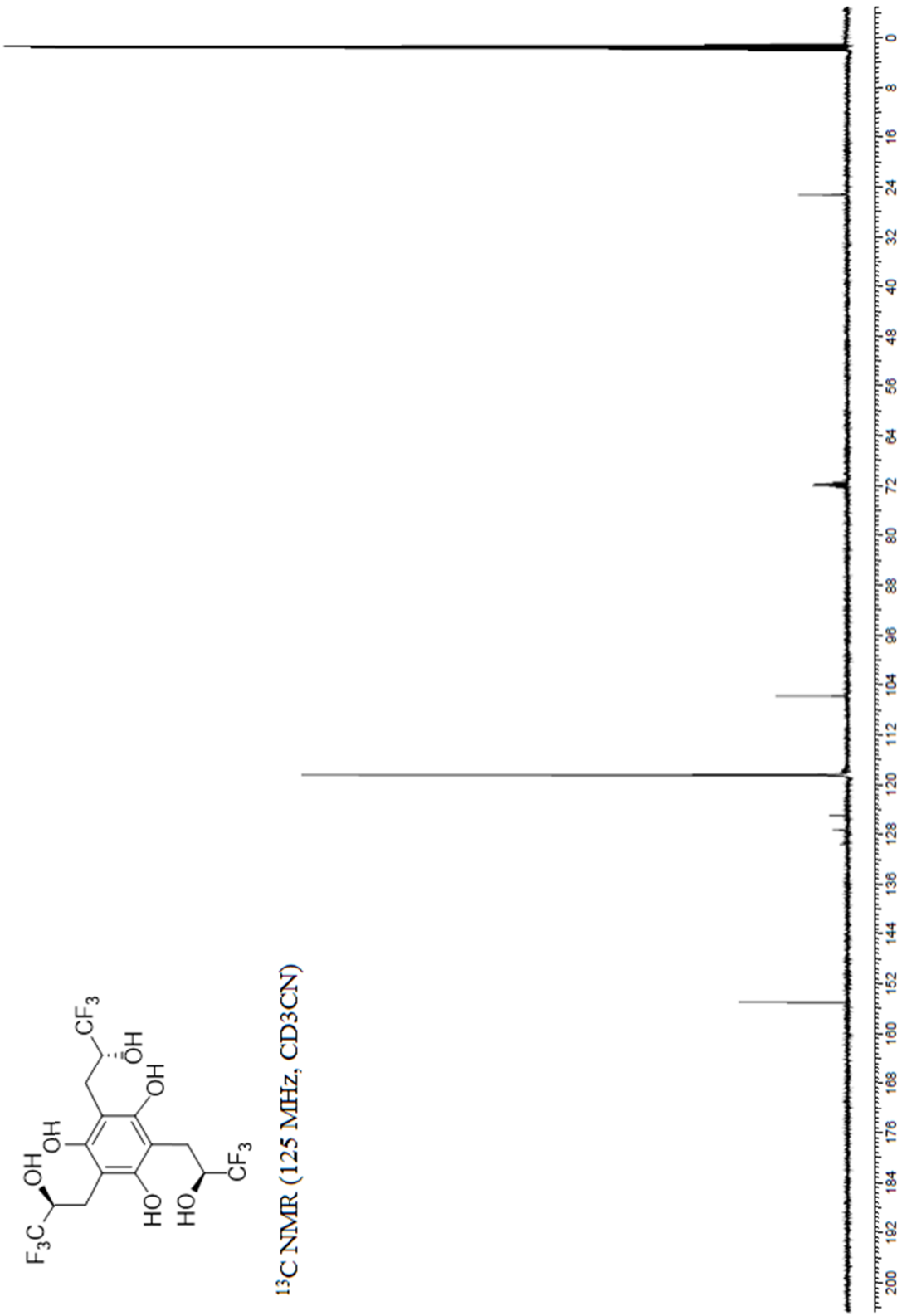

OH
OMe
F3C
CF3
OH
OMe
MeO
HO
CF3
13C NMR (75 MHz, CDCl3)
Chemical Shift (ppm)

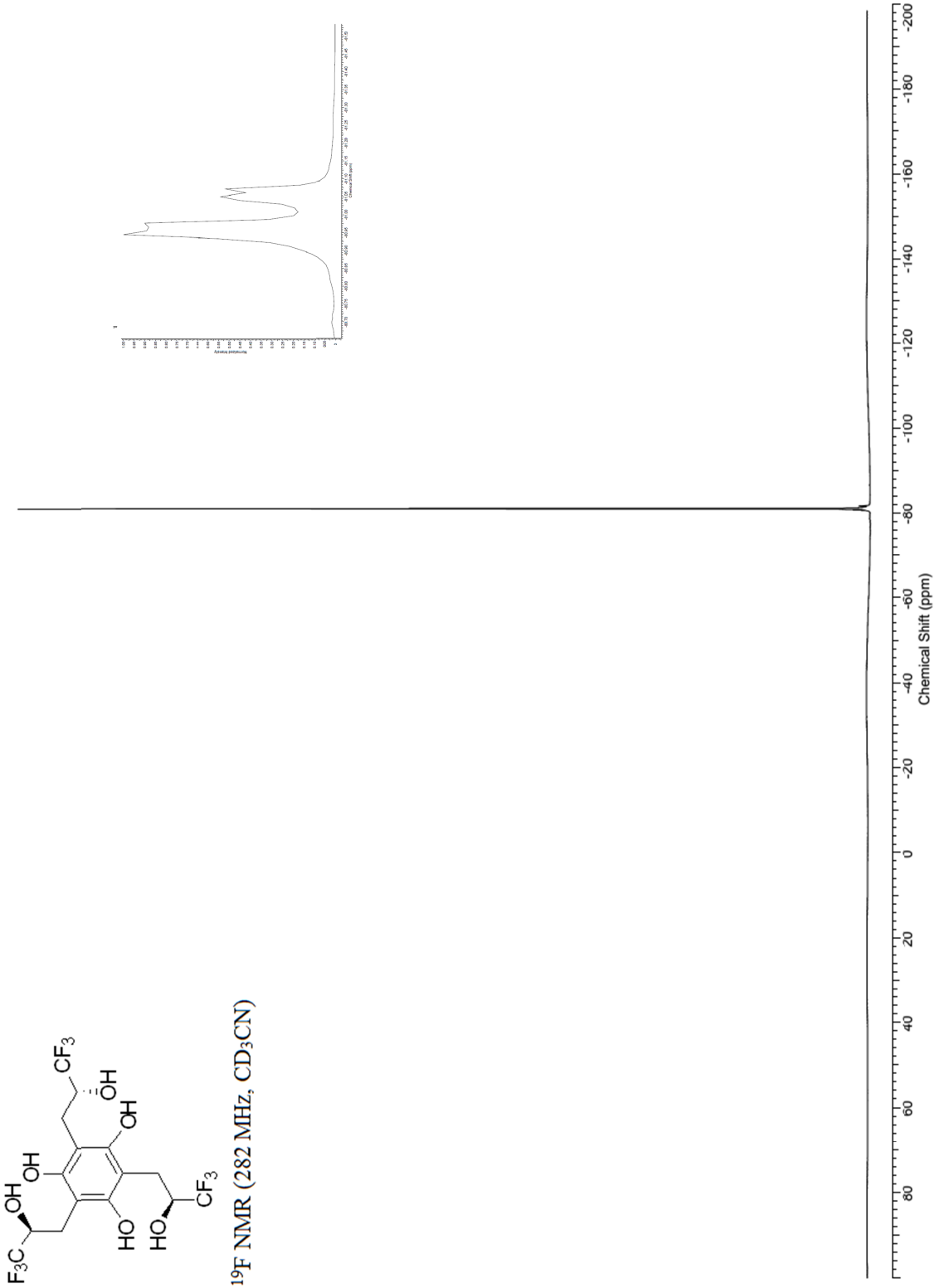


^{19}F NMR (282 MHz, $CDCl_3$)



^{1}H NMR (300 MHz, CD_3CN)


^{13}C NMR (125 MHz, CD3CN)
F_3C
OH
OH
CF_3
OH
OH
HO
HO
CF_3



^{19}F NMR (282 MHz, CD_3CN)

1 (Hexaol)

B3LYP/ aug-cc-pVDZ = -1930.874134, ZPE = 0.311664, thermal correction to the enthalpy = 0.336652

C	0.57158800	1.26938900	-0.39088700
C	-0.67030800	-1.23674100	-0.08889000
C	-0.79138000	1.16725200	-0.05810200
C	1.29712400	0.07276200	-0.54144300
C	0.68854600	-1.19218500	-0.44953800
C	-1.42806700	-0.07251300	0.13445700
C	1.17920100	2.62387700	-0.69205800
H	0.36707300	3.32690700	-0.90285400
H	1.81485700	2.56718600	-1.58765300
C	-2.84568900	-0.17818800	0.65697000
H	-3.01990800	0.57223400	1.44154300
H	-2.97807500	-1.16842200	1.10446800
C	-3.92448800	0.00923000	-0.41280900
H	-3.72043200	-0.63785900	-1.27859400
C	1.47608500	-2.43777700	-0.80362500
H	2.33753800	-2.14771600	-1.41304700
H	0.85825100	-3.11912500	-1.40580000
C	1.98973400	-3.22162600	0.40672000
C	2.02758800	3.20184200	0.44308100
H	1.47303600	3.16523500	1.39247000
O	3.22944800	2.43332600	0.52692300
O	-3.92764400	1.38584300	-0.79663500
H	-4.47426200	1.51733400	-1.58118900
O	0.86810800	-3.84607300	1.03417000
H	1.12301700	-4.22420400	1.88488400
H	3.73253400	2.67655600	1.31397900
C	2.39289400	4.67157600	0.21543000
C	-5.32178800	-0.36891100	0.08716900
C	3.00746100	-4.29976700	0.02301000
F	4.14984400	-3.74892800	-0.44779700
F	2.54670400	-5.15658900	-0.91257800
F	3.34127000	-5.04437500	1.11728100
F	-5.67785900	0.28595600	1.21310400
F	-6.25884900	-0.07396600	-0.85971700
F	-5.41013000	-1.69569600	0.33642700
F	3.00268200	4.89027100	-0.96900700
F	1.29692800	5.46243100	0.26792000
F	3.24692900	5.10173800	1.18957800
O	-1.32376000	-2.43131100	0.06314900
H	-0.69053000	-3.11193500	0.35351200
O	-1.47370500	2.34401500	0.10383800
H	-2.41110600	2.20590700	-0.12250400
O	2.63020600	0.08730000	-0.85508900
H	3.03363400	0.90373600	-0.51113700
H	2.50447300	-2.54752700	1.10726100

1a (Hexaol anion)

B3LYP/ aug-cc-pVDZ = -1930.361405, ZPE = 0.297738, thermal correction to the enthalpy = 0.322021, M06-2X/maug-cc-pVT(+d)Z = -1930.225304

C	1.42739400	-0.06562000	-1.12282800
C	-1.24452700	0.15577500	-0.14050800
C	0.82487600	1.21815200	-0.95685700
C	0.63404900	-1.23791300	-0.92773900
C	-0.65561400	-1.08853000	-0.41545000
C	-0.47626300	1.29426000	-0.44590200
C	1.18467900	-2.56723000	-1.40319300
H	1.62330200	-2.41396100	-2.40133600
H	0.37453200	-3.29808400	-1.53635600
C	2.31456100	-3.22925900	-0.58384900
H	2.50976600	-4.22434400	-1.02576300
C	1.58034000	2.43402100	-1.45706200
H	0.89614600	3.28200100	-1.60187400
H	1.98357600	2.19524600	-2.45353200
C	2.80696300	2.92495500	-0.65573200
C	-2.60131500	0.26640100	0.51784700
H	-2.66865900	1.23251600	1.02998700
H	-2.71861800	-0.52610800	1.27024500
C	-3.78003700	0.16824000	-0.46894900
H	-3.68905800	0.96502500	-1.22490100
O	2.68173300	-0.17040300	-1.48573600
O	-1.08914400	2.51423800	-0.20533900
O	-1.46251100	-2.19764800	-0.15039200
C	-5.11870300	0.42321500	0.22969800
C	1.89855700	-3.54692400	0.86025700
O	-3.87964700	-1.08098500	-1.12998000
H	-3.16721200	-1.65943000	-0.81066300
F	0.68107200	-4.21121100	0.88357400
F	2.78033600	-4.38449500	1.46564500
F	1.76221400	-2.47347700	1.65677800
F	-5.37297100	-0.45202600	1.23654900
F	-6.16666900	0.34146500	-0.63200900
F	-5.16632300	1.67362200	0.77378700
H	-0.41191000	3.18821400	-0.07015900
H	-0.91257900	-2.97421100	0.01200600
O	3.50536800	-2.49597900	-0.57411400
H	3.29789000	-1.57140700	-0.90813800
H	3.15277700	3.86740500	-1.12036300
C	2.46039200	3.33526400	0.78300700
O	3.86845700	2.01420100	-0.63645100
H	3.51507800	1.12694700	-0.94753400
F	2.15149900	2.31470800	1.60139500
F	3.47698200	4.02190600	1.36803800
F	1.37484200	4.19550200	0.79824800

1$^{\bullet}$ (Hexaol Radical)

B3LYP/ aug-cc-pVDZ = -1930.225801, ZPE = 0.298749, thermal correction to the enthalpy = 0.323314, M06-2X/maug-cc-pVT(+d)Z = -1930.082474

C	-1.41662200	0.05365100	-1.16462200
C	1.17755700	-0.11021300	-0.07163200
C	-0.80195500	-1.25305100	-0.97668600
C	-0.65170000	1.27571200	-0.94807900
C	0.59982200	1.15765600	-0.37293300
C	0.45523200	-1.29638100	-0.40176600
C	-1.22675600	2.58958100	-1.42672200
H	-1.68208900	2.42577900	-2.41284900
H	-0.41440400	3.31131400	-1.58081500
C	-2.33094300	3.26782100	-0.57928600
H	-2.49473100	4.27287400	-1.00033400
C	-1.53005800	-2.48004300	-1.47826600
H	-0.81041900	-3.29139700	-1.64837400
H	-1.96227200	-2.24511300	-2.46049700
C	-2.70709000	-3.03799600	-0.64137900
C	2.52940700	-0.19968300	0.57625900
H	2.57205700	-1.09134300	1.21017600
H	2.69308300	0.68620200	1.20041700
C	3.66660600	-0.29297800	-0.46917900
H	3.58484400	-1.23308900	-1.02892300
O	-2.62960100	0.13110500	-1.51813700
O	1.11303000	-2.45654900	-0.11545000
O	1.38472900	2.23590400	-0.06321500
C	5.03564500	-0.32437000	0.22447800
C	-1.89685400	3.51968200	0.87196800
O	3.63838000	0.74229000	-1.42833400
H	3.47653400	1.58614700	-0.98319100
F	-0.66308700	4.15082200	0.89504100
F	-2.74966100	4.32973000	1.52014900
F	-1.76320400	2.39306100	1.60030900
F	5.28326000	0.83043900	0.89693900
F	6.03787000	-0.49651700	-0.66124500
F	5.11041800	-1.33933800	1.12384800
H	0.49209400	-3.19368500	-0.03128000
H	0.84279000	3.02493200	0.08036200
O	-3.55747400	2.58790800	-0.58296400
H	-3.40979200	1.67269400	-0.89311800
H	-2.99044300	-4.00737200	-1.08220600
C	-2.30558700	-3.37015700	0.80295200
O	-3.84347500	-2.21595900	-0.62847200
H	-3.58778500	-1.31951100	-0.92216400
F	-2.03223400	-2.28265600	1.55218000
F	-3.25379000	-4.07873400	1.43854700
F	-1.16228000	-4.15029800	0.80920400

1 • Cl^-

B3LYP/ aug-cc-pVDZ = -2391.239338, ZPE = 0.312803, thermal correction to the enthalpy = 0.338147, M06-2X/maug-cc-pVT(+d)Z = -2391.095834

C	1.55375300	0.01718800	-1.44348900
C	-1.23881600	0.29321200	-1.54814500
C	0.95028000	1.27939700	-1.47855100
C	0.71145900	-1.10700400	-1.42850800
C	-0.68239400	-0.99563100	-1.50580500
C	-0.44321100	1.44715000	-1.54368100
C	3.04200600	-0.12320000	-1.22470000
H	3.56836200	0.73647700	-1.65147800
H	3.41325400	-1.03403300	-1.71329700
C	-1.05090200	2.82940000	-1.51350100
H	-2.08081600	2.78733600	-1.88078900
H	-0.48142400	3.47639100	-2.19473400
C	-1.03147700	3.52708100	-0.11539700
H	-0.90707200	4.60764800	-0.27505700
C	-1.56206900	-2.20976500	-1.32658000
H	-1.05877800	-3.10392900	-1.70791900
H	-2.50455400	-2.08019700	-1.87436000
C	-1.87031700	-2.40485400	0.17609100
H	-0.94669800	-2.67898500	0.70519100
C	3.34629200	-0.20237800	0.28822500
H	3.09671600	0.75726200	0.76282900
O	2.63047500	-1.25635200	0.91302100
O	0.04998700	3.14176300	0.71138300
H	-0.04947400	2.21375200	1.04641800
O	-2.43829800	-1.23934900	0.75184800
H	-1.71833300	-0.75042900	1.22224100
Cl	0.09701200	0.19102800	2.00943900
H	1.82899800	-0.86181400	1.34702400
C	4.83033400	-0.43736800	0.55966000
C	-2.36055600	3.42966000	0.64348000
C	-2.85077100	-3.55125600	0.41149000
F	-2.38188700	-4.71642100	-0.12353700
F	-4.06764300	-3.32734300	-0.15157300
F	-3.06533600	-3.78848900	1.72784400
F	-2.70132200	2.17860300	1.00367300
F	-2.33201500	4.17845100	1.77794200
F	-3.38140500	3.92815400	-0.11736400
F	5.27507100	-1.62238100	0.06387600
F	5.59507000	0.53725100	-0.01391900
F	5.12285000	-0.43082600	1.88224600
O	-2.60926400	0.45273200	-1.52574100
H	-2.93266500	-0.07825200	-0.77249900
O	1.77339500	2.38768500	-1.36976300
H	1.40690100	2.92282800	-0.63940600
O	1.24288700	-2.36813000	-1.25063100
H	1.89083000	-2.29111700	-0.52178100

1 • $Cl^{\bullet}$

B3LYP/ aug-cc-pVDZ = -2391.071480 , ZPE = 0.313350, thermal correction to the enthalpy = 0.338914, M06-2X/maug-cc-pVT(+d)Z = -2390.911790

C	0.02665600	1.43973900	-1.39055800
C	-0.04111300	-1.34957500	-1.26573500
C	-1.22030900	0.70813400	-1.34605200
C	1.24070200	0.71687400	-1.35931200
C	1.24089400	-0.67102500	-1.31614900
C	-1.27606400	-0.67928900	-1.37866400
C	0.02446000	2.92662400	-1.23412800
H	-0.90174900	3.35831600	-1.62353100
H	0.87956400	3.35853300	-1.76902100
C	-2.57822000	-1.43201300	-1.23981300
H	-2.47893800	-2.43822600	-1.65880100
H	-3.36454300	-0.91192800	-1.80305300
C	-2.99475700	-1.52650600	0.24454000
C	2.52303700	-1.44675300	-1.20087300
H	3.34758000	-0.84839300	-1.59825800
H	2.45966200	-2.37894300	-1.77829700
C	2.81827300	-1.79740100	0.27985000
H	3.01097500	-0.88129200	0.85245000
C	0.15014800	3.27833700	0.28066500
H	-0.77402100	2.99745200	0.80232400
O	1.26994500	2.64202300	0.86902900
O	-3.00254800	-0.23463200	0.84365900
H	-2.16429100	-0.13351600	1.35222100
O	1.73449500	-2.51606700	0.85750500
H	1.19658200	-1.87475600	1.38795400
Cl	0.01854200	-0.11181600	1.91487400
H	0.95801200	1.83948500	1.35069300
C	0.31969300	4.78834300	0.46880100
C	4.06918100	-2.67098000	0.40062100
F	5.13906000	-2.04247600	-0.15029400
F	3.92192400	-3.85610500	-0.23926700
F	4.36733700	-2.93380400	1.68661800
F	1.46094800	5.24469400	-0.10011900
F	-0.71451200	5.45701100	-0.10503000
F	0.34845000	5.12403900	1.77209800
O	-0.07714600	-2.65177900	-1.02219800
H	0.69084500	-2.88943500	-0.42369400
O	-2.31160900	1.46008000	-1.13682000
H	-2.90835200	0.95778500	-0.52793100
O	2.43427800	1.36900300	-1.29402600
H	2.35671200	2.03935400	-0.58169500
C	-4.39606000	-2.11781700	0.39982900
F	-4.45784900	-3.34462500	-0.18265300
F	-4.73823500	-2.26510200	1.69418200
F	-5.34151500	-1.34493100	-0.18879700
H	-2.31218300	-2.19104600	0.78981100

1 • OAc^-

B3LYP/ aug-cc-pVDZ = -2159.886483, ZPE = 0.363353, thermal correction to the enthalpy = 0.391139, M06-2X/maug-cc-pVT(+d)Z = -2159.360753

C	-0.51818200	1.27581500	-1.47976400
C	0.58146400	-1.30499200	-1.52888800
C	-1.33113600	0.13928400	-1.50280700
C	0.87131700	1.07912200	-1.46753600
C	1.43990300	-0.19648900	-1.52348500
C	-0.81314200	-1.16271600	-1.50868700
C	-1.11296300	2.65990800	-1.36717500
H	-2.13449400	2.65752900	-1.74785700
H	-0.53177100	3.37177600	-1.96104900
C	-1.71201000	-2.36445200	-1.33073800
H	-2.58101800	-2.31479900	-2.00052600
C	-2.19090100	-2.51607200	0.14150600
H	-2.52947700	-1.54096200	0.51836000
C	2.93431400	-0.37033300	-1.38917700
H	3.44544800	0.52093800	-1.75153800
H	3.27455200	-1.22644900	-1.97868900
C	3.29873100	-0.60677300	0.09267800
C	-1.11589800	3.13943300	0.10058300
H	-1.72028900	2.45277100	0.70341500
O	0.19497100	3.23893200	0.61921900
O	-1.22798800	-3.07972900	0.98378700
H	-0.63534100	-2.38261600	1.35449900
O	2.68444200	-1.78139800	0.58817600
H	1.90950300	-1.51890200	1.16404800
H	0.37382100	2.47095000	1.22890000
C	-1.77673200	4.51006100	0.24993900
C	-3.43047700	-3.40840500	0.22003200
C	4.80523200	-0.75253900	0.28927800
F	5.46804200	0.35078600	-0.15212200
F	5.32435600	-1.80841700	-0.38425200
F	5.14313100	-0.91258300	1.58658000
F	-3.22520700	-4.65402100	-0.25562100
F	-3.90030300	-3.53299500	1.47712500
F	-4.45198300	-2.87338200	-0.51909500
F	-1.13388700	5.47990500	-0.43856400
F	-3.05755000	4.48797900	-0.20796900
F	-1.83461800	4.91114100	1.53821400
O	1.09324200	-2.57519000	-1.50825600
H	1.79311800	-2.58878800	-0.82289000
O	-2.69526700	0.36134100	-1.46324400
H	-3.16167000	-0.46738900	-1.61184900
O	1.72311200	2.15065700	-1.39279000
H	1.35019700	2.77921600	-0.74303300
H	2.98838600	0.25989900	0.68635200
O	0.48173000	-1.17394300	1.94746100
C	0.15669000	0.01002900	2.27654500
O	0.79464800	1.04189100	1.96082400
H	-1.16589300	-3.27006500	-1.59166100
C	-1.07856900	0.15724500	3.16716900
H	-1.80055200	-0.64110400	2.98854200
H	-1.54751100	1.13409000	3.03892300
H	-0.75180400	0.07895100	4.20913900

1 • OAc$^{\bullet}$

B3LYP/ aug-cc-pVDZ = -2159.713432, ZPE = 0.362310, thermal correction to the enthalpy = 0.390054, M06-2X/maug-cc-pVT(+d)Z = -2159.180609

C	-1.02699400	0.98964500	-1.33927400
C	1.00234400	-0.95895400	-1.45161100
C	-1.37369600	-0.35268200	-1.42272100
C	0.38324900	1.33121300	-1.30139500
C	1.39608800	0.37476700	-1.43614100
C	-0.39088300	-1.35808600	-1.45540000
C	-2.07633000	2.06277100	-1.26922500
H	-3.02553900	1.66810500	-1.62825600
H	-1.79442300	2.90489600	-1.90858700
C	-0.75128700	-2.79980000	-1.32396800
H	-1.60902400	-3.04347500	-1.96076800
C	-1.09232700	-3.16738500	0.17189300
H	-1.72487300	-2.38176500	0.60520400
C	2.85038000	0.77534000	-1.34969100
H	2.96897300	1.81145000	-1.66360400
H	3.44922700	0.15315500	-2.02140300
C	3.36640900	0.59829300	0.09203700
C	-2.25496500	2.59480700	0.17612200
H	-2.59594500	1.78566200	0.82874200
O	-1.05252100	3.15404400	0.66383300
O	0.03794600	-3.40240700	0.93692900
H	0.34234200	-2.56443200	1.36154200
O	3.20543100	-0.75090400	0.50540600
H	2.39963800	-0.80702000	1.08998000
H	-0.61421300	2.48681900	1.26367500
C	-3.33768800	3.67693700	0.23110500
C	-1.95994400	-4.43182100	0.19569200
C	4.84692900	0.95625700	0.21304100
F	5.05457100	2.23855800	-0.17519800
F	5.62584300	0.17314400	-0.56390300
F	5.28669200	0.84160100	1.47659200
F	-1.35914200	-5.48843500	-0.37423100
F	-2.31030800	-4.77077700	1.44235500
F	-3.11687000	-4.20499400	-0.49769400
F	-3.02637900	4.74273600	-0.53242200
F	-4.51670300	3.18565500	-0.21987400
F	-3.53354900	4.11112500	1.48537700
O	1.87258000	-1.95853400	-1.38556100
H	2.64136600	-1.66713300	-0.81847300
O	-2.70488800	-0.64492300	-1.41202300
H	-2.86419300	-1.58494500	-1.55458000
O	0.74114500	2.59402200	-1.14988100
H	0.06889100	3.07446400	-0.58743300
H	2.82189100	1.26529700	0.76633700
O	0.87204500	-0.97976100	1.79346000
C	0.16728300	0.00753200	2.18289700
O	0.25661700	1.15685000	1.68104400
H	0.07829200	-3.43477200	-1.62797800
C	-0.79456300	-0.23210500	3.33547900
H	-1.19737500	-1.24570200	3.31335300
H	-1.60084100	0.50181400	3.34594400
H	-0.23246400	-0.12741800	4.26858700

1 • $H_2PO_4^-$

B3LYP/ aug-cc-pVDZ = -2575.035205, ZPE = 0.353598, thermal correction to the enthalpy = , M06-2X/maug-cc-pVT(+d)Z = 0.382507

C	0.32475000	1.38100100	-1.60697800
C	-0.43760700	-1.29936800	-1.40356200
C	1.27788700	0.35519900	-1.62228000
C	-1.02949100	1.01800000	-1.59275800
C	-1.43303600	-0.32432600	-1.52158700
C	0.91980500	-0.99778700	-1.54053900
C	0.73756300	2.82447200	-1.43696400
H	-0.15485400	3.44882900	-1.46877300
H	1.40198800	3.14248800	-2.24521900
C	1.95890000	-2.09615500	-1.51449200
H	1.50070400	-3.02838700	-1.84583700
C	2.55403900	-2.29995500	-0.10850400
H	1.77109700	-2.64589900	0.57390500
C	-2.89294700	-0.72122800	-1.50962200
H	-2.98207200	-1.74741700	-1.86806900
H	-3.45838300	-0.07374300	-2.18728000
C	-3.51891300	-0.62806100	-0.10807300
C	1.48227500	3.05879300	-0.09880900
O	0.81985300	2.51581800	1.03045000
O	3.14013700	-1.10651400	0.38128800
H	2.50101600	-0.71510600	1.03113600
O	-3.46239200	0.70467700	0.38744900
H	-2.75221200	0.73303900	1.06112900
C	3.63246600	-3.38094600	-0.09778200
C	-4.98519000	-1.05187600	-0.10417800
F	-5.75984100	-0.27071300	-0.89295400
F	-5.52367900	-1.01521300	1.13457200
F	-5.12686500	-2.32537800	-0.55423500
F	3.14214400	-4.56567200	-0.54922000
F	4.69010600	-3.07262800	-0.88525400
F	4.11792100	-3.60850100	1.14090200
O	-0.80456100	-2.59453400	-1.08701900
H	-0.86133600	-2.58672900	-0.10604600
O	2.60299900	0.72491400	-1.63596600
H	3.08212400	0.11283400	-1.04218800
O	-1.96467900	2.02400300	-1.59416700
H	-2.69725100	1.75414900	-1.00967400
H	-2.99700800	-1.30600000	0.57394100
H	2.77193900	-1.85179200	-2.20546200
P	-0.17229800	-0.54365800	2.21671600
H	1.23593500	1.66538900	1.29342100
O	1.21924000	-0.04039200	1.87511200
O	-0.76360600	-1.77698000	1.58361600
O	-1.20038000	0.72568800	1.95256500
H	-0.71918100	1.51973500	1.64735500
O	-0.23465800	-0.72419700	3.83938300
H	-0.88371900	-1.39896800	4.06637000
H	2.48926300	2.64382600	-0.17802600
C	1.66979900	4.54981200	0.17237400
F	2.30549400	5.15678400	-0.86672800
F	2.42442600	4.77726200	1.27052500
F	0.50351600	5.20664700	0.35343700

1 • $H_2PO_4^{\bullet}$

B3LYP/ aug-cc-pVDZ = -2574.860015, ZPE = 0.352295, thermal correction to the enthalpy = 0.381211, M06-2X/maug-cc-pVT(+d)Z = -2574.343551

C	0.16891500	1.41210300	-1.61906200
C	-0.13277300	-1.42777300	-1.28643500
C	1.26989600	0.56693400	-1.54834700
C	-1.09202700	0.80546500	-1.52749700
C	-1.26542200	-0.63619600	-1.43478300
C	1.14479100	-0.87729200	-1.44962100
C	0.31982800	2.90869200	-1.49421300
H	-0.64876900	3.37550900	-1.66618500
H	1.01454100	3.28812300	-2.24624900
C	2.35653400	-1.75857600	-1.45894800
H	2.06276800	-2.76504300	-1.75562400
C	3.02784700	-1.82371300	-0.06068700
H	2.36785100	-2.34106900	0.64036100
C	-2.63328100	-1.25931200	-1.47413900
H	-2.53112900	-2.30141100	-1.77786500
H	-3.25274000	-0.74271000	-2.21363500
C	-3.35300800	-1.20553300	-0.10830200
C	0.84746800	3.30985200	-0.08570600
O	0.23317800	2.59373000	0.96393800
O	3.33669000	-0.52806100	0.41390700
H	2.61528600	-0.27636700	1.04929200
O	-3.48481900	0.14573600	0.31956400
H	-2.90061800	0.27280800	1.09585600
C	4.32776200	-2.63036100	-0.11808300
C	-4.75500500	-1.81203000	-0.19711400
F	-5.53825000	-1.15357600	-1.07638900
F	-5.37198300	-1.79244000	0.99497800
F	-4.68483600	-3.10040900	-0.60277000
F	4.08739500	-3.87768000	-0.58444500
F	5.23688500	-2.06163200	-0.93690900
F	4.88491700	-2.74906500	1.09546200
O	-0.25129400	-2.74355000	-0.96550800
H	-0.42149500	-2.73825500	0.01300200
O	2.48024400	1.11581700	-1.47719300
H	3.06864100	0.55005300	-0.90656500
O	-2.15658600	1.58484300	-1.45034000
H	-2.87270700	1.13899300	-0.91959100
H	-2.79268800	-1.78215300	0.63108300
H	3.08828900	-1.37678100	-2.17666100
P	-0.12495400	-0.65964400	2.19589300
H	0.75523400	1.79160700	1.17376200
O	1.08235600	0.08142600	1.64375000
O	-0.61831700	-1.93369400	1.55941400
O	-1.40100700	0.39718600	2.13218900
H	-1.12097300	1.32660900	2.15849300
O	0.14427400	-0.87777000	3.77389400
H	-0.42380900	-1.55813000	4.15487700
H	1.93253900	3.17901300	-0.05538400
C	0.60503600	4.79640600	0.17491700
F	1.15261600	5.54191900	-0.81733600
F	1.16202800	5.19687200	1.33095800
F	-0.70688700	5.10229500	0.22776600

2 (Triol)

B3LYP/ aug-cc-pVDZ = -2048.745852, ZPE = 0.393657, thermal correction to the enthalpy = 0.422290

C	-0.83720200	-1.10701600	-0.03088200
C	0.65968200	1.20886300	0.50311600
C	0.49213600	-1.24487100	0.40227900
C	-1.46369900	0.14855700	-0.14596300
C	-0.68788600	1.28749900	0.11289200
C	1.20717100	-0.06884400	0.68725400
C	-2.91206800	0.25730000	-0.57420100
H	-3.07060400	-0.29629700	-1.50739300
H	-3.15602200	1.30464600	-0.77590200
C	-3.89869200	-0.29149300	0.46454800
H	-3.64112600	-1.33058000	0.71140200
C	1.12961300	-2.60707300	0.58144100
H	0.36871300	-3.38278500	0.45219800
H	1.52080200	-2.70377400	1.60213400
C	2.28790700	-2.88322900	-0.38663400
H	3.03696700	-2.08330600	-0.31240200
C	1.49983400	2.45831000	0.65743700
H	2.35243800	2.26026700	1.31161600
H	0.91385200	3.26424900	1.11337900
C	2.05385900	2.95935500	-0.69290400
H	2.75189600	2.21456800	-1.10374900
O	-1.59715900	-2.23824000	-0.27681600
O	2.52967000	-0.18272900	1.09756900
O	-1.22743500	2.55123200	-0.11590600
C	-1.86492900	3.17177800	1.02114300
H	-2.70580400	2.56205300	1.36953300
H	-2.21884400	4.14702900	0.67194300
H	-1.14707000	3.31207100	1.84206600
C	2.71398500	-0.18513500	2.52074700
H	2.36050400	0.75497600	2.96895100
H	3.78998700	-0.29210000	2.69256400
H	2.18102300	-1.02542900	2.98907100
C	-1.56292100	-2.72685800	-1.63314500
H	-1.90736200	-1.95574900	-2.33720800
H	-2.25000200	-3.57875500	-1.66119800
H	-0.55050400	-3.04431500	-1.90732300
C	3.01882800	-4.17981700	-0.02207800
C	2.88235200	4.23541900	-0.49039300
C	-5.32677800	-0.32936700	-0.08892100
O	1.77330100	-2.98606600	-1.70610100
H	2.50624300	-2.99623600	-2.33415700
O	1.06750800	3.20655500	-1.67038900
H	0.20271000	3.29402700	-1.23683400
F	-5.43404000	-1.20804600	-1.11712700
F	-6.19878800	-0.73672700	0.87633100
F	-5.76131300	0.87035900	-0.53269000
F	2.14612700	5.25312300	0.02492000
F	3.41847100	4.67408300	-1.64852700
F	3.91682800	4.01612000	0.37057000
F	2.20576000	-5.25755000	0.02794400
F	3.98841500	-4.45329500	-0.93856700
F	3.63208400	-4.07631300	1.18530900
O	-3.86180600	0.53626500	1.61935500
H	-4.37947300	0.12324800	2.32173700

2 • Cl^-

B3LYP/ aug-cc-pVDZ = -2509.108688, ZPE = 0.392721, thermal correction to the enthalpy = 0.422134, M06-2X/maug-cc-pVT(+d)Z = -2508.935269

C	1.20529100	0.28387200	1.19379300
C	-1.45437300	-0.57714900	1.13776600
C	0.94856800	-1.09293400	1.14322800
C	0.19087500	1.25238700	1.18879400
C	-1.13180500	0.78840100	1.19498100
C	-0.39654500	-1.50014600	1.14524300
C	2.07719100	-2.07659900	0.93658400
H	2.90834100	-1.86684100	1.62074600
H	1.72508800	-3.09665700	1.11507500
C	0.52248200	2.71561900	1.01128500
H	-0.34980600	3.33342400	1.24336600
H	1.34812700	3.01331100	1.66834900
C	-2.88493100	-1.00883100	0.91383100
H	-2.98748400	-2.08417600	1.08523000
H	-3.56379600	-0.47598400	1.59047500
O	-0.68593300	-2.85470800	1.09172500
O	2.53049700	0.71445700	1.13820000
O	-2.17550400	1.70643700	1.16964800
C	-0.83060100	-3.46553000	2.36959100
H	-1.65598200	-3.01070100	2.94192100
H	0.09670300	-3.38534900	2.96088500
H	-1.05461600	-4.52279700	2.18578500
C	-2.61309900	2.12324200	2.46006100
H	-2.95862900	1.26783500	3.06293600
H	-3.44727800	2.81572200	2.29852400
H	-1.80875200	2.64056100	3.00763300
C	3.14207400	0.89265400	2.41450600
H	3.16172400	-0.04993500	2.98361200
H	2.61334600	1.65460700	3.00853400
H	4.16901100	1.22563900	2.22579900
C	-3.30661400	-0.72343800	-0.55321900
C	0.92034400	2.99988500	-0.46199100
H	1.76569900	2.35327000	-0.74004000
C	2.59630100	-2.00841300	-0.52484800
H	2.89325600	-0.97491700	-0.75635300
O	1.66665100	-2.50017600	-1.45015400
O	-0.15617500	2.85111900	-1.34618600
H	-0.13426500	1.94289300	-1.73572400
H	-3.15602000	0.34384400	-0.77280900
O	-2.63996700	-1.54372200	-1.47358600
H	-1.83627800	-1.08055300	-1.81084900
C	1.43484300	4.43268100	-0.60827200
C	3.86928200	-2.84220700	-0.67706700
C	-4.80498600	-0.97110000	-0.73309600
F	4.38692800	-2.77477800	-1.92478400

F	4.85269400	-2.40574200	0.17249800
F	3.68115600	-4.15866300	-0.39661700
F	-5.54335600	-0.18441500	0.11186000
F	-5.23060900	-0.68929800	-1.98551800
F	-5.16781100	-2.25500900	-0.47121900
F	2.51415100	4.65816900	0.20574800
F	1.84213800	4.71108500	-1.86738000
F	0.50590500	5.36810200	-0.27626100
Cl	-0.03809900	-0.06105000	-2.46130400
H	1.12616500	-1.75202600	-1.80004600

2 • $Cl^{\bullet}$

B3LYP/ aug-cc-pVDZ = -2508.932582, ZPE = 0.393950, thermal correction to the enthalpy = 0.423476, M06-2X/maug-cc-pVT(+d)Z = -2508.748768

C	1.28541200	-0.01666800	1.19442200
C	-1.50017500	-0.32021800	1.02512700
C	0.71994400	-1.32463800	1.13297400
C	0.54447300	1.15825900	1.10098500
C	-0.87917300	0.99533400	1.01550400
C	-0.68447100	-1.44421900	1.12546200
C	1.59909500	-2.50999300	0.86850600
H	2.49441100	-2.49517100	1.49841600
H	1.05026700	-3.43913800	1.03720200
C	1.30293200	2.46565800	1.02260900
H	0.74206300	3.30125100	1.43875600
H	2.22045800	2.37142100	1.60869600
C	-2.99269800	-0.43914900	0.92582500
H	-3.28995000	-1.46128200	1.17147900
H	-3.46258000	0.25796600	1.63033700
O	-1.25592000	-2.68919500	1.09698600
O	2.65626100	0.08245100	1.20100600
O	-1.80430500	1.94417900	1.02128900
C	-1.41183100	-3.31383100	2.38046800
H	-2.08618800	-2.72663600	3.02182400
H	-0.44232600	-3.43420100	2.88667400
H	-1.85016100	-4.29711700	2.18611600
C	-1.63253700	3.38128700	0.96942400
H	-2.65074400	3.75857100	0.84498900
H	-1.00351900	3.65751600	0.11847400
H	-1.22319500	3.73913700	1.92098900
C	3.28709700	-0.04280200	2.48983800
H	3.00321100	-0.98190300	2.98370300
H	3.01383000	0.80377100	3.13592400
H	4.36431900	-0.03356800	2.30145000
C	-3.53671000	-0.13334600	-0.50264700
C	1.70402100	2.80558400	-0.43880000
H	2.32201200	1.99124800	-0.84316500
C	2.05265300	-2.49584100	-0.62807400

H	2.59717000	-1.56367200	-0.83551300
O	0.98516800	-2.69156700	-1.51211100
O	0.59234700	3.06453700	-1.26058100
H	0.30009300	2.22269800	-1.67529900
H	-3.18907600	0.85712500	-0.82827000
O	-3.19380400	-1.12568700	-1.42741400
H	-2.34461100	-0.86922800	-1.83644500
C	2.58321300	4.05874400	-0.46539800
C	3.05848900	-3.62616100	-0.87116400
C	-5.06551800	-0.05030200	-0.46534000
F	3.52003300	-3.61896800	-2.13590300
F	4.13939300	-3.48643300	-0.04822300
F	2.53367100	-4.84905500	-0.63003500
F	-5.46966400	0.93469600	0.39118800
F	-5.57995000	0.24407800	-1.67473700
F	-5.64032300	-1.20025600	-0.04258900
F	3.69373500	3.88475300	0.30505400
F	3.00189300	4.35533000	-1.70900400
F	1.93316500	5.14776900	0.01940900
Cl	-0.39987200	0.22939300	-2.02989900
H	0.60150300	-1.82962200	-1.76621900

2 • OAc^-

B3LYP/ aug-cc-pVDZ = -2277.383435, ZPE =0.442481 , thermal correction to the enthalpy = 0.474212, M06-2X/maug-cc-pVT(+d)Z = -2277.192331

C	-1.13486100	0.40392800	-1.39107700
C	1.45112400	-0.65591600	-1.33838200
C	-0.04999600	1.29387900	-1.37112500
C	-0.98176200	-0.99034200	-1.38336800
C	0.32846500	-1.49661700	-1.38546100
C	1.23388600	0.73094300	-1.37793400
C	-0.26419500	2.77982000	-1.20322900
H	-1.10118700	3.12438000	-1.82074300
H	0.63518700	3.32857400	-1.49806900
C	2.83596600	-1.19715600	-1.07148500
H	3.58216600	-0.70152400	-1.70353500
H	2.86799500	-2.27373800	-1.26129100
C	-2.17883000	-1.89933700	-1.22495300
H	-1.91000500	-2.92669200	-1.48721900
H	-3.00190100	-1.57419400	-1.87206700
O	-2.42470900	0.92874100	-1.31969900
O	0.51478000	-2.87099200	-1.36630600
O	2.34421700	1.56534900	-1.34084600
C	2.83738000	1.92964700	-2.62660600
H	3.12954400	1.04304900	-3.21279800
H	3.71765300	2.56013800	-2.45622600
H	2.08531000	2.49852300	-3.19701900
C	0.66932100	-3.44998600	-2.65756300

H	1.54849800	-3.03945400	-3.18104500
H	-0.22417100	-3.28289100	-3.28197500
H	0.80819400	-4.52624500	-2.50205300
C	-3.02549900	1.18768200	-2.58720700
H	-2.44236600	1.92243400	-3.16410100
H	-4.02292100	1.59359800	-2.38376000
H	-3.11975400	0.26514400	-3.18143300
C	-2.66927700	-1.90451200	0.24819500
H	-2.89278300	-0.86932200	0.55133500
C	-0.55004300	3.12728900	0.28081400
H	-1.40271600	2.52906600	0.63659300
C	3.20384800	-0.96640500	0.42020300
H	3.14519300	0.11027500	0.64190800
O	2.42171900	-1.72762500	1.29891900
H	1.56511100	-1.27207600	1.48691800
C	4.65906800	-1.35791100	0.67667100
C	-3.99768500	-2.65288400	0.36436700
C	-1.00427200	4.58768600	0.39799200
O	0.58068800	2.94015400	1.07435900
O	-1.77272800	-2.52551500	1.12325300
H	-1.09030500	-1.86504400	1.43206300
F	-4.95908600	-2.08812200	-0.43160600
F	-4.49145400	-2.63651700	1.62548900
F	-3.91133300	-3.95633700	-0.00878000
F	-0.07707600	5.47198800	-0.06005100
F	-1.28646100	4.93956700	1.67311200
F	-2.14542900	4.82204200	-0.32781100
F	5.04138300	-1.12647900	1.95381400
F	4.91238200	-2.66865100	0.42020900
F	5.51193500	-0.63949400	-0.11814900
C	-0.29069700	0.05263100	2.91890700
O	-0.02670100	-0.66531900	1.89212500
O	-0.08005900	1.28577100	3.01376100
H	0.37576900	2.27672700	1.79673800
C	-0.89933000	-0.66490200	4.12294400
H	-1.26176500	0.05526000	4.86469300
H	-0.12556800	-1.29842000	4.58097400
H	-1.71224900	-1.32927200	3.80131800

2 • $OAc^{\bullet}$

B3LYP/ aug-cc-pVDZ = -2277.209273, ZPE = 0.443365, thermal correction to the enthalpy = 0.474990, M06-2X/maug-cc-pVT(+d)Z = -2277.009141

C	-1.30797400	0.25696900	-1.43082700
C	1.38396600	-0.56086100	-1.38696300
C	-0.36168000	1.27268300	-1.40314900
C	-0.98263600	-1.13978700	-1.39548300
C	0.38224600	-1.51566300	-1.44996500
C	1.01119800	0.84626600	-1.40399000

C	-0.84515500	2.69667200	-1.25163400
H	-1.84920100	2.78017300	-1.67281400
H	-0.21398500	3.40983300	-1.78129900
C	2.82112600	-0.94653500	-1.20931000
H	3.46708600	-0.33101600	-1.84444800
H	2.95249200	-2.00149900	-1.46036400
C	-2.04173600	-2.14690900	-1.10828000
H	-1.69642300	-3.15402300	-1.35080100
H	-2.96169500	-1.92048200	-1.65624000
O	-2.63495200	0.58986400	-1.35245200
O	0.70819200	-2.84410800	-1.43214800
O	2.08980700	1.60384100	-1.47446200
C	2.19085100	3.04795700	-1.56155000
H	3.26821200	3.22729300	-1.59359200
H	1.73809300	3.49611700	-0.67299500
H	1.72902600	3.39423900	-2.49244600
C	0.75172000	-3.47365400	-2.72264900
H	1.52825400	-3.01629600	-3.35371600
H	-0.22048900	-3.40400600	-3.23346200
H	0.99616300	-4.52352500	-2.53718800
C	-3.34798200	0.63789600	-2.60404400
H	-2.95768000	1.44700700	-3.23745800
H	-4.39240100	0.83597800	-2.34799100
H	-3.27054500	-0.31650900	-3.14270400
C	-2.39306500	-2.13657100	0.43036800
H	-2.71879400	-1.12302300	0.70937800
C	-0.90424200	3.08447400	0.25106900
H	-1.64328300	2.44628400	0.75891000
C	3.25598900	-0.76322700	0.28128900
H	3.11669600	0.28826200	0.57661000
O	2.59466600	-1.63948600	1.14083300
H	1.71792500	-1.25565300	1.38511300
C	4.75791000	-1.03222900	0.41400700
C	-3.60657300	-3.04530000	0.66274400
C	-1.42290900	4.52172200	0.39186300
O	0.35262600	2.98099800	0.84593600
O	-1.35666300	-2.60280000	1.22333800
H	-0.74191800	-1.84857000	1.44847000
F	-4.67404700	-2.62163500	-0.07630500
F	-3.99085100	-3.03489900	1.95346400
F	-3.36929500	-4.32976500	0.31283100
F	-0.61093900	5.42067900	-0.22736400
F	-1.53104900	4.89538000	1.67916500
F	-2.65830100	4.65559700	-0.17433500
F	5.19006600	-0.84438700	1.67581700
F	5.09719400	-2.28941300	0.04629500
F	5.46778600	-0.17943000	-0.38323500
C	0.06465800	0.16201300	2.76872200
O	0.18880400	-0.48093800	1.65694500
O	0.10276300	1.41040700	2.86074100
H	0.29644000	2.35074600	1.64126100

C	-0.12453000	-0.65752700	4.03378000
H	-0.33007000	-0.00680000	4.88882600
H	0.79151200	-1.23467200	4.22437800
H	-0.93952600	-1.38157500	3.90173400

2 • $H_2PO_4^-$

B3LYP/ aug-cc-pVDZ = -2692.49481202, ZPE = 0.430847, thermal correction to the enthalpy = 0.472980, M06-2X/maug-cc-pVT(+d)Z = -2692.344694

C	-1.11341400	0.24781600	-1.52691100
C	1.59656800	-0.43982700	-1.44018400
C	-0.16317900	1.28181000	-1.48920300
C	-0.76615600	-1.11147400	-1.52705600
C	0.60301900	-1.42834700	-1.51691200
C	1.18772400	0.90442500	-1.46675000
C	-0.59595200	2.72689500	-1.38096900
H	-1.44663700	2.91771300	-2.04443300
H	0.22264700	3.39315700	-1.66837600
C	3.04620600	-0.78948800	-1.19456800
H	3.70610200	-0.16412300	-1.80676900
H	3.23135100	-1.84013100	-1.43514000
C	-1.82583700	-2.18444000	-1.41926300
H	-1.42370600	-3.14682200	-1.74906400
H	-2.69175300	-1.93382000	-2.04202700
O	-2.46337100	0.58934100	-1.47949100
O	0.98039300	-2.76222500	-1.52275600
O	2.16832800	1.88546400	-1.39836800
C	2.63845800	2.33134800	-2.66746200
H	1.82907100	2.79567400	-3.25358500
H	3.06798200	1.50226400	-3.25292300
H	3.41604000	3.07710700	-2.46693600
C	1.22359400	-3.28826500	-2.82328300
H	2.04121500	-2.74957900	-3.32998900
H	0.32051500	-3.23452000	-3.45370600
H	1.50931900	-4.33757800	-2.68601200
C	-3.07947600	0.75079200	-2.75619700
H	-3.04133300	-0.18163000	-3.34078300
H	-2.59602600	1.55191700	-3.33680000
H	-4.12460500	1.01959600	-2.56624100
C	-2.29896500	-2.35693400	0.04887800
H	-2.64448000	-1.38882600	0.44181200
C	-0.98765000	3.10047000	0.07035500
H	-1.65841100	2.32973500	0.47905100
C	3.40449100	-0.58357700	0.30255800
H	3.14752300	0.44537900	0.59818600
O	2.81094100	-1.53622100	1.14140300
C	4.91569400	-0.70092900	0.50678900
C	-3.51620100	-3.28035200	0.10637400
C	-1.80657200	4.39714500	0.08041300

O	0.14423800	3.28295900	0.86796500
O	-1.31710300	-2.92587900	0.87068800
H	-0.74604500	-2.20795600	1.23808100
F	-3.26443600	-4.52507800	-0.38151600
F	-4.55320400	-2.78066200	-0.63634000
F	-3.98915400	-3.44018700	1.36306100
F	-1.13463100	5.45298700	-0.45182000
F	-2.18058900	4.75773400	1.33072300
F	-2.96220700	4.27297900	-0.64588000
F	5.28313300	-0.48989500	1.79106600
F	5.40695700	-1.91772200	0.14975900
F	5.59113100	0.22161600	-0.24588200
H	0.12295800	2.64506800	1.62959900
P	-0.32887500	0.08207000	2.86120400
H	1.90225200	-1.25140300	1.40202500
O	-1.98289500	-0.06654200	2.68590000
H	-2.40604500	0.69725100	3.09945600
O	-0.05364100	-0.48634800	4.39678700
H	0.04440400	-1.44708400	4.35541400
O	0.03764700	1.56001700	2.87414800
O	0.25092100	-0.93441600	1.86033700

2 • $H_2PO_4^{\bullet}$

B3LYP/ aug-cc-pVDZ = -2692.320330, ZPE = 0.431897, thermal correction to the enthalpy = 0.465122, M06-2X/maug-cc-pVT(+d)Z = -2692.163271

C	-1.40047600	-0.01460100	-1.36824400
C	1.46410700	0.20562200	-1.47063200
C	-0.79185600	1.26234500	-1.33235800
C	-0.65190300	-1.17863700	-1.43921500
C	0.79786300	-1.06222000	-1.54951500
C	0.64085700	1.32837000	-1.40625200
C	-1.62450900	2.48392600	-1.12785600
H	-2.52024700	2.42018100	-1.75525800
H	-1.07163300	3.39229200	-1.37068300
C	2.95813300	0.42053500	-1.35590100
H	3.19479200	1.42189000	-1.72135100
H	3.53464100	-0.28729200	-1.95070100
C	-1.30474100	-2.52635500	-1.35565300
H	-0.75275700	-3.26604200	-1.94121200
H	-2.32840300	-2.45732300	-1.73127900
O	-2.76433400	-0.09205000	-1.21264200
O	1.33731100	-2.24269000	-1.77847300
O	1.22002400	2.55914800	-1.31594900
C	1.35215100	3.29361500	-2.54774500
H	0.37902000	3.42525800	-3.04074800
H	2.04048400	2.77689500	-3.23223400
H	1.76292200	4.26840900	-2.27120800
C	2.73186200	-2.59408300	-1.94945700

H	3.11590600	-2.13341300	-2.86680300
H	2.71011500	-3.68088600	-2.05768900
H	3.29806000	-2.29399700	-1.06282900
C	-3.53334000	-0.08729800	-2.42935900
H	-3.29586900	-0.96401400	-3.04828600
H	-3.35039100	0.82687500	-3.01157300
H	-4.58211900	-0.12338800	-2.12197700
C	-1.37029800	-3.04831800	0.11877300
H	-1.84976100	-2.28760800	0.75229700
C	-2.10155000	2.65031200	0.36622400
H	-2.42281900	1.66988200	0.74824800
C	3.41762700	0.32440900	0.12586500
H	2.83839800	1.03596800	0.73227500
O	3.31385100	-0.98527400	0.62398100
C	4.88493400	0.74516600	0.24179800
C	-2.28127400	-4.28056000	0.17362000
C	-3.34854200	3.54218000	0.39346900
O	-1.14282200	3.25323700	1.16433700
O	-0.12033600	-3.42373400	0.61143000
H	0.25743000	-2.67737700	1.13883200
F	-1.82591000	-5.29497200	-0.60160600
F	-3.53665100	-3.97782900	-0.26766600
F	-2.40649600	-4.75211700	1.42907900
F	-3.11569100	4.77406900	-0.11660000
F	-3.81748900	3.69812900	1.64689400
F	-4.35773400	2.99232200	-0.34380700
F	5.32009700	0.71516100	1.51480400
F	5.70527100	-0.05715200	-0.48848800
F	5.06615900	2.01489300	-0.21844300
H	-0.51006700	2.55833800	1.49440100
P	0.27915700	-0.06509300	2.47633800
H	2.47304500	-1.08158600	1.14087200
O	-1.32679900	-0.47515600	2.58161700
H	-1.80704200	0.15047200	3.14165400
O	0.75773000	0.04804400	4.04661500
H	0.93479800	-0.82949400	4.41338700
O	0.46491400	1.30949300	1.84422200
O	0.94119400	-1.28684500	1.80534800

Fig. S1. Non-linear plot for the binding of **1** with chloride ion.

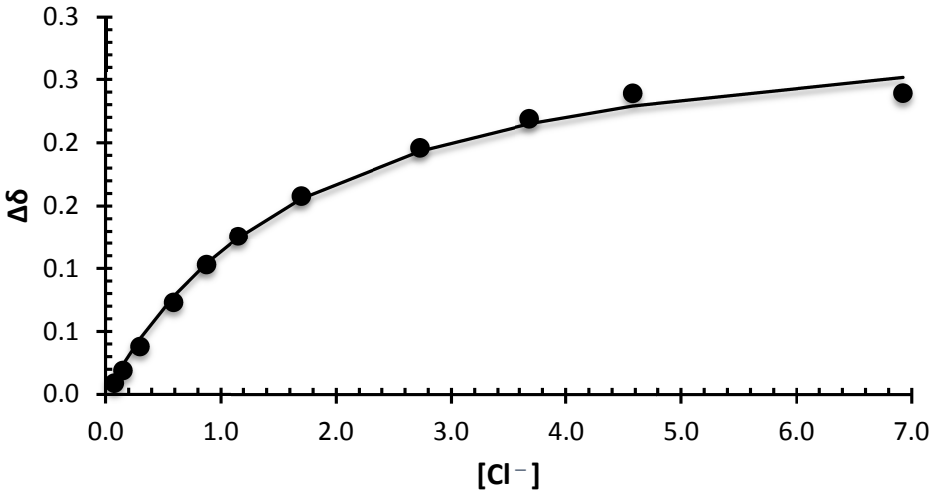


Table S1. Titration data for chloride binding to **1**.[a]

μL (Cl^-added)	[Cl^-]	[**1**]	δ (C-H)	Δδ	%bound
0	0.00	0.32	3.804	0.000	0.0
3	0.07	0.32	3.813	0.009	3.8
5	0.15	0.32	3.823	0.019	7.9
10	0.30	0.32	3.842	0.038	15.9
20	0.59	0.32	3.877	0.073	30.5
30	0.87	0.32	3.907	0.103	43.1
40	1.15	0.32	3.930	0.126	52.7
60	1.70	0.32	3.962	0.158	66.1
100	2.73	0.32	4.000	0.196	82.0
140	3.68	0.32	4.023	0.219	91.6
180	4.58	0.32	4.0430	0.239	100.0
300	6.92	0.32	4.0431	0.239	100.0

[a] Chemical shifts and concentrations are given in ppm and mM, respectively.

Fig. S2. Non-linear plot for the binding of **2** with chloride ion.

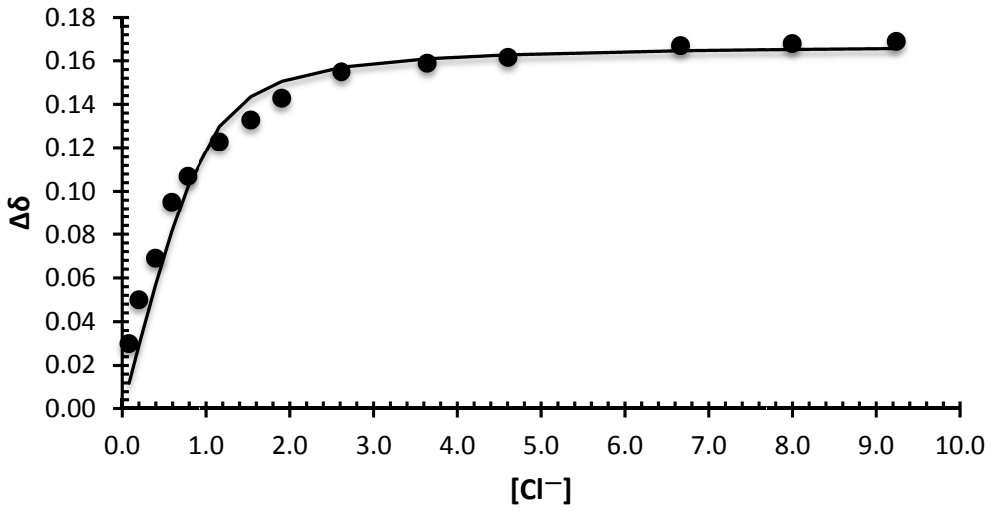


Table S2. Titration data for chloride binding to **2**.[a]

µL (Cl^- added)	[Cl^-]	[**2**]	δ (C-H)	Δδ	%bound
0	0.00	1.00	4.396	0.000	0.0
2	0.08	1.00	4.426	0.030	17.8
5	0.20	0.99	4.446	0.050	29.6
10	0.40	0.99	4.465	0.069	40.8
15	0.59	0.99	4.491	0.095	56.2
20	0.78	0.98	4.503	0.107	63.3
30	1.17	0.97	4.519	0.123	72.8
40	1.54	0.96	4.529	0.133	78.7
50	1.91	0.95	4.539	0.143	84.6
70	2.62	0.93	4.551	0.155	91.7
100	3.64	0.91	4.555	0.159	94.1
130	4.60	0.89	4.558	0.162	95.6
200	6.67	0.83	4.563	0.167	98.8
250	8.00	0.80	4.564	0.168	99.4
300	9.23	0.77	4.565	0.169	100.0

[a] Chemical shifts and concentrations are given in ppm and mM, respectively.

Fig. S2. Non-linear plot for the binding of **2** with chloride ion.

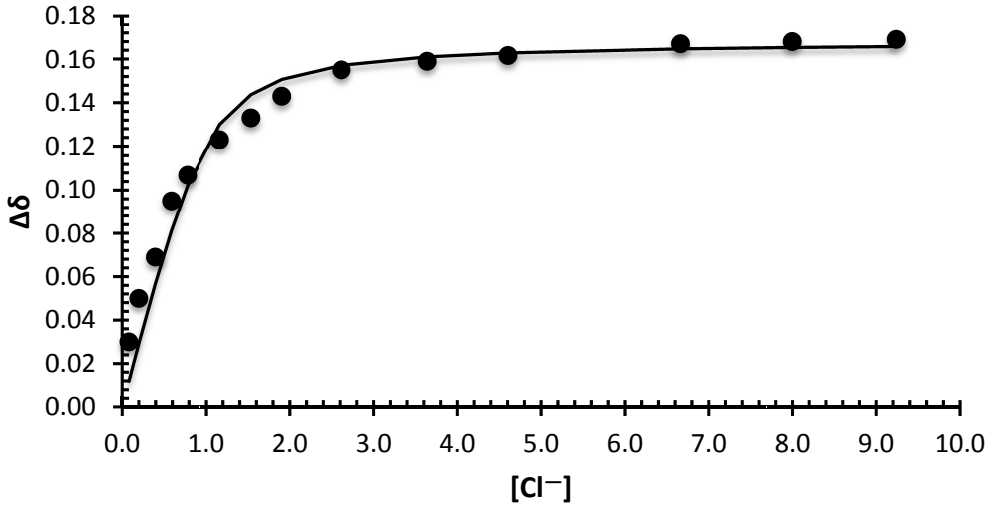


Table S2. Titration data for chloride binding to **2**.[a]

μL (Cl^- added)	[Cl^-]	[**2**]	δ (C-H)	Δδ	%bound
0	0.00	1.00	4.396	0.000	0.0
2	0.08	1.00	4.426	0.030	17.8
5	0.20	0.99	4.446	0.050	29.6
10	0.40	0.99	4.465	0.069	40.8
15	0.59	0.99	4.491	0.095	56.2
20	0.78	0.98	4.503	0.107	63.3
30	1.17	0.97	4.519	0.123	72.8
40	1.54	0.96	4.529	0.133	78.7
50	1.91	0.95	4.539	0.143	84.6
70	2.62	0.93	4.551	0.155	91.7
100	3.64	0.91	4.555	0.159	94.1
130	4.60	0.89	4.558	0.162	95.6
200	6.67	0.83	4.563	0.167	98.8
250	8.00	0.80	4.564	0.168	99.4
300	9.23	0.77	4.565	0.169	100.0

[a] Chemical shifts and concentrations are given in ppm and mM, respectively.