Electronic Supplementary Information

Sequential nucleophilic aromatic substitutions on cyanuric chloride: synthesis of BODIPY derivatives and mechanistic insights.

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CONTENTS:

1. NMR SPECTRUM OF ALL ISOLATED COMPOUNDS

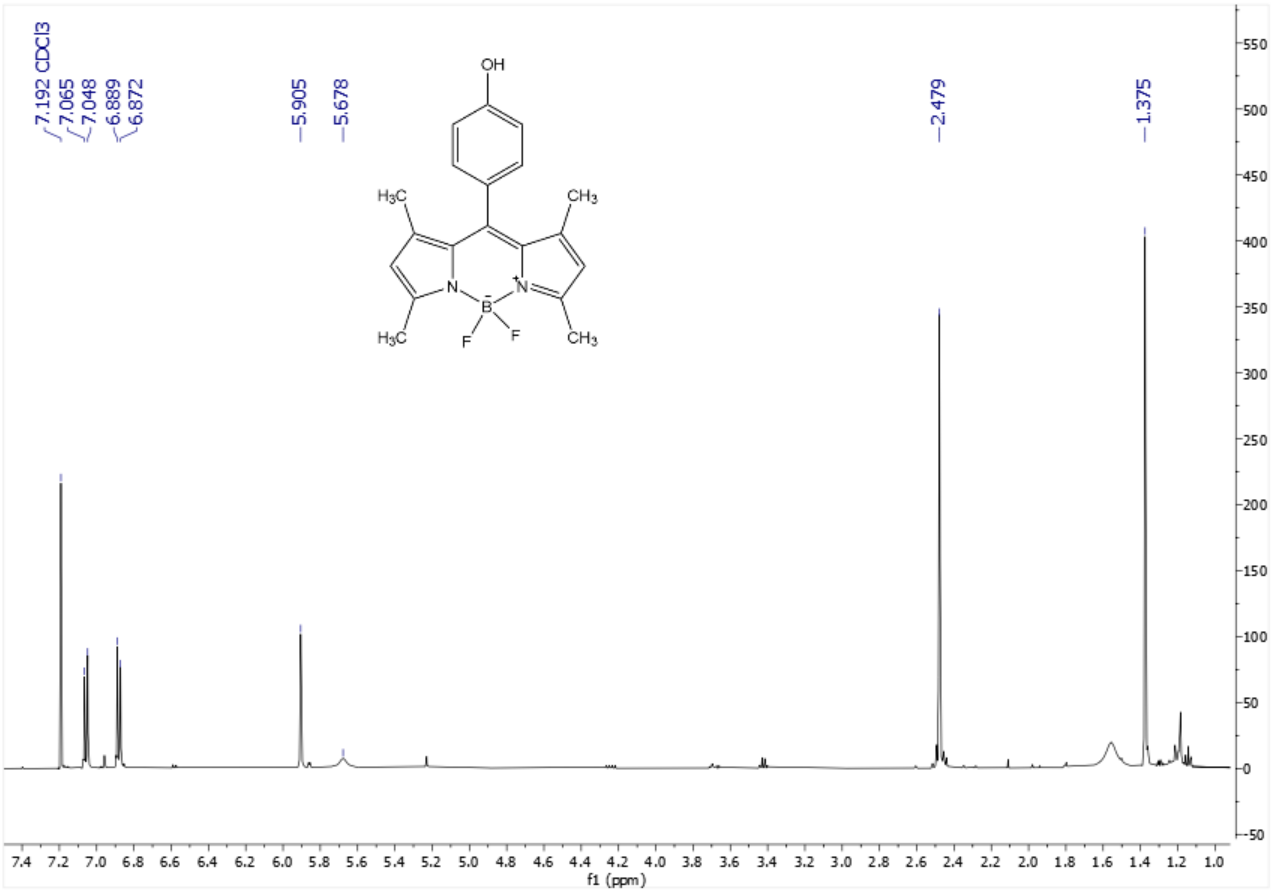

Figure S1 – ^{1}H NMR spectrum (500 MHz) of **(I)** in $CDCl_3$**.**

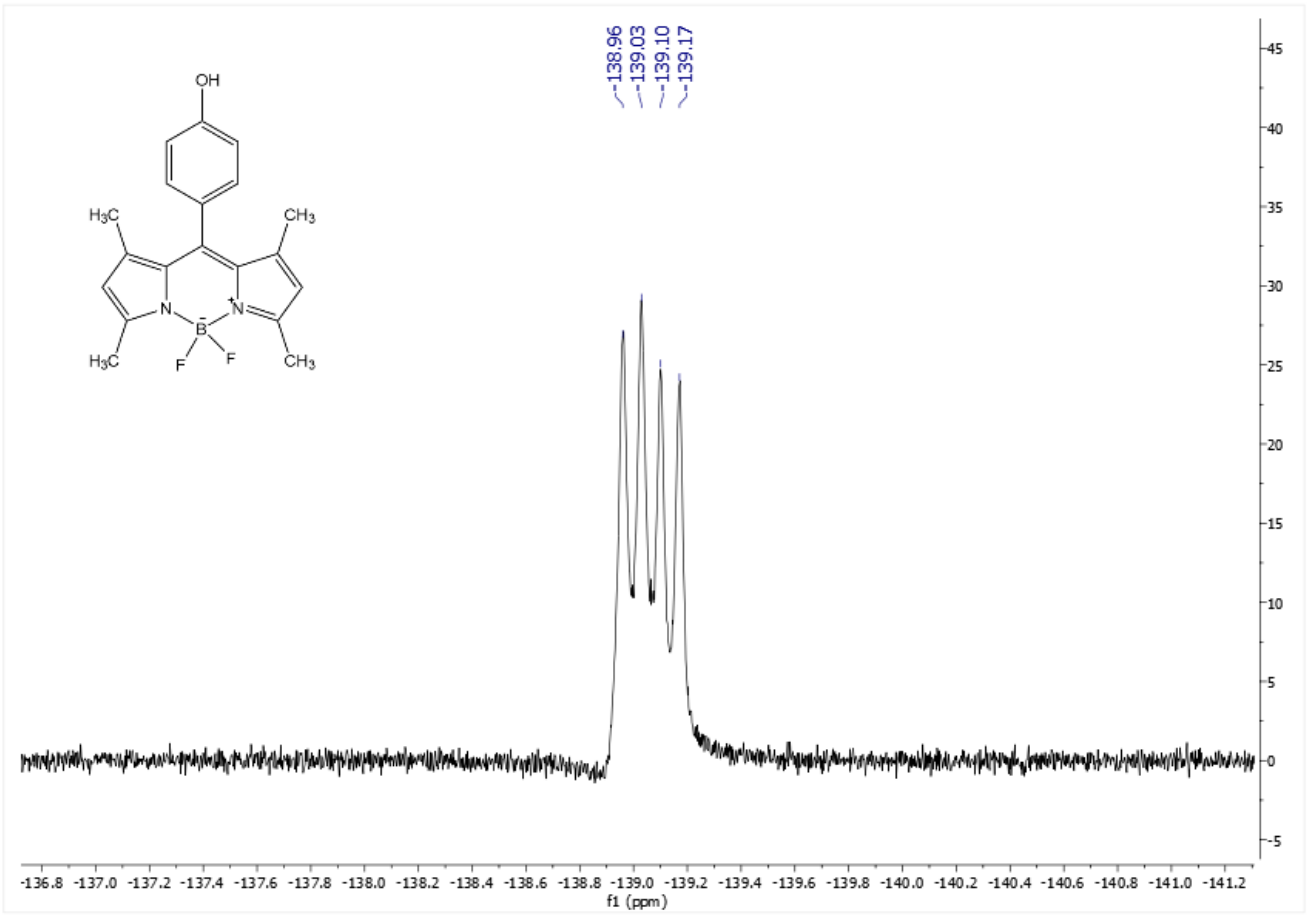

Figure S2 – ^{19}F NMR spectrum (470 MHz) of **(I)** in $CDCl_3$.

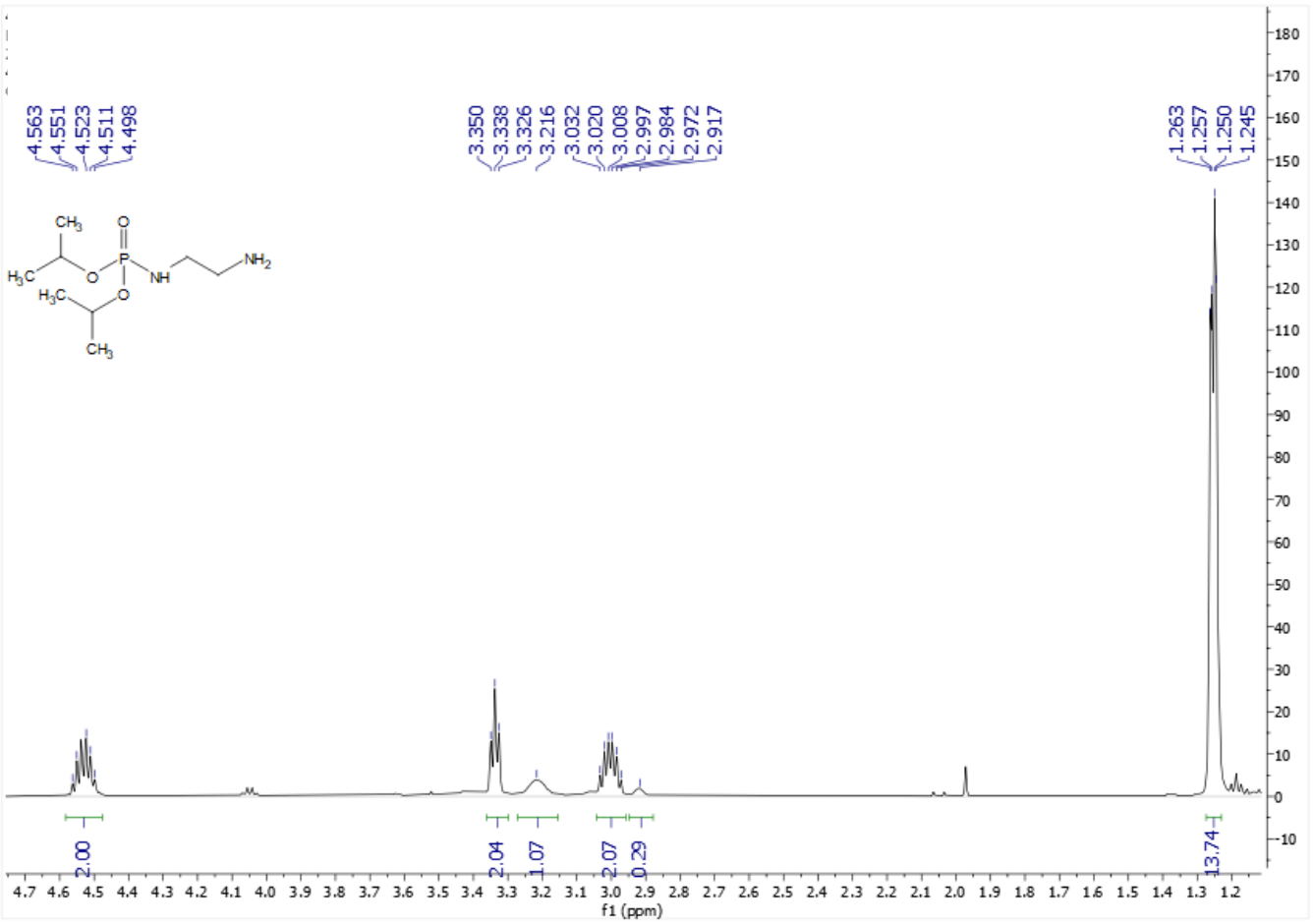

Figure S3 – ^{1}H NMR spectrum (500 MHz) of **IIa** in $CDCl_3$.

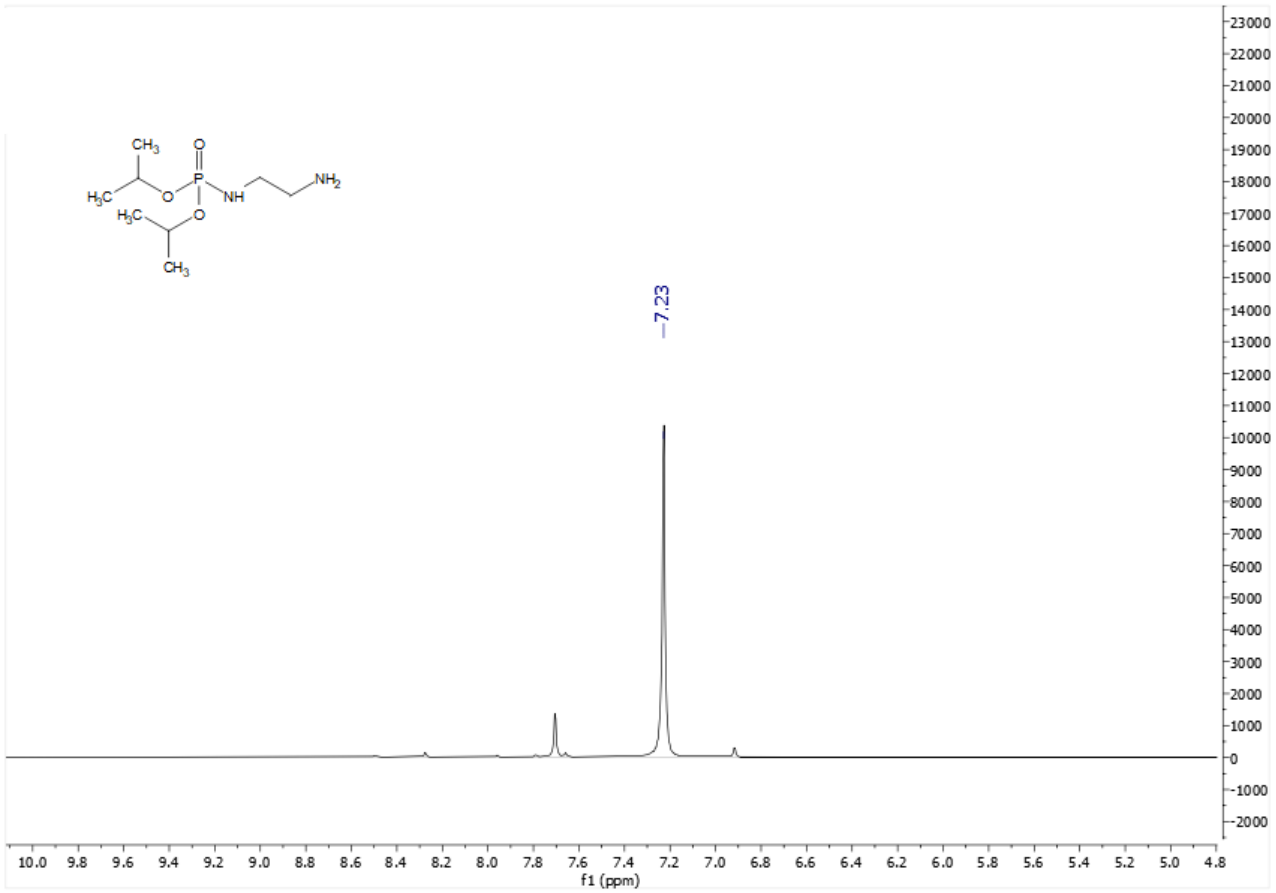

Figure S4 – ^{31}P NMR spectrum (202 MHz) of **IIa** in $CDCl_3$.

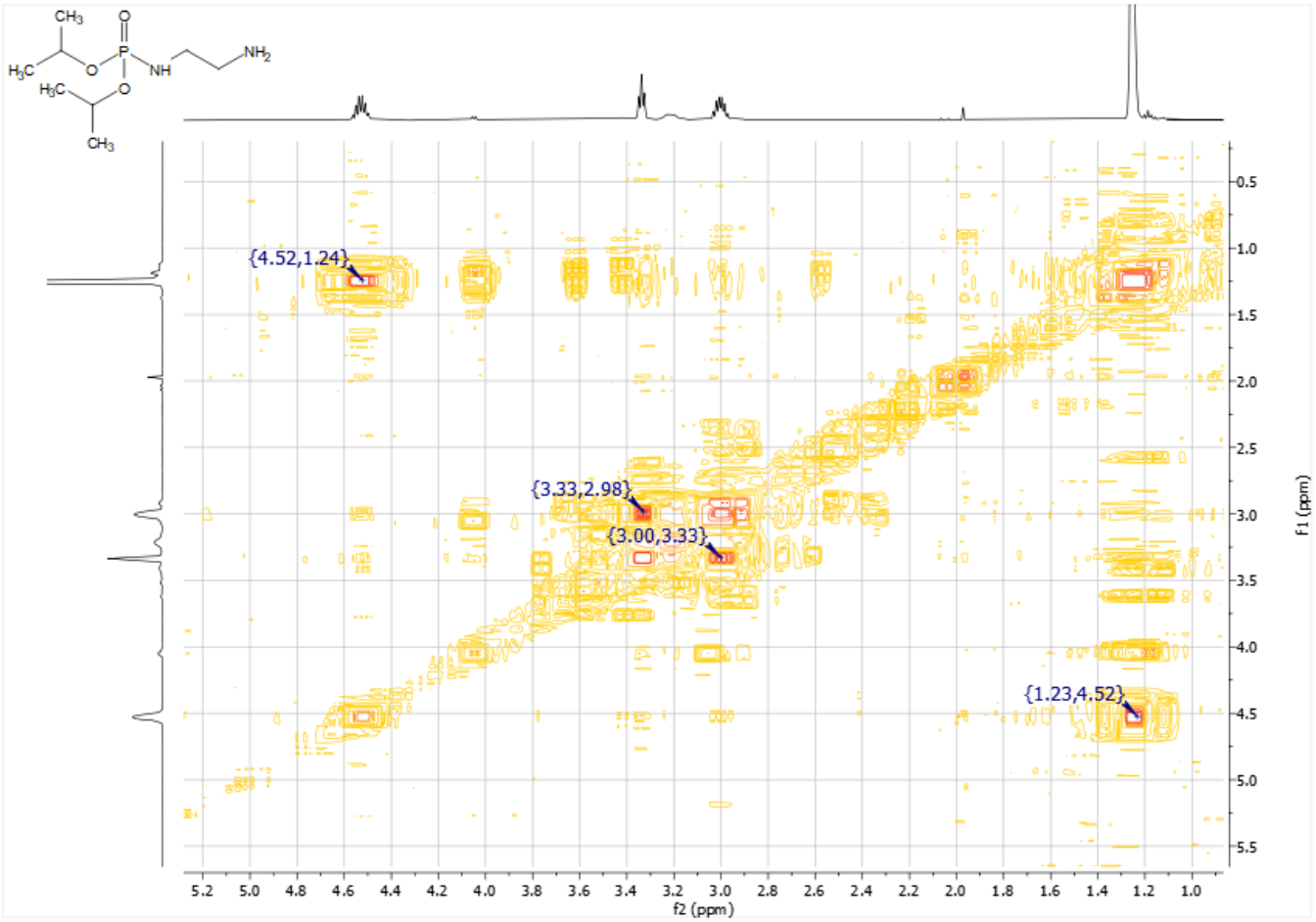

Figure S5 – ^{1}Hx^{1}H-COSY spectrum of **IIa**.

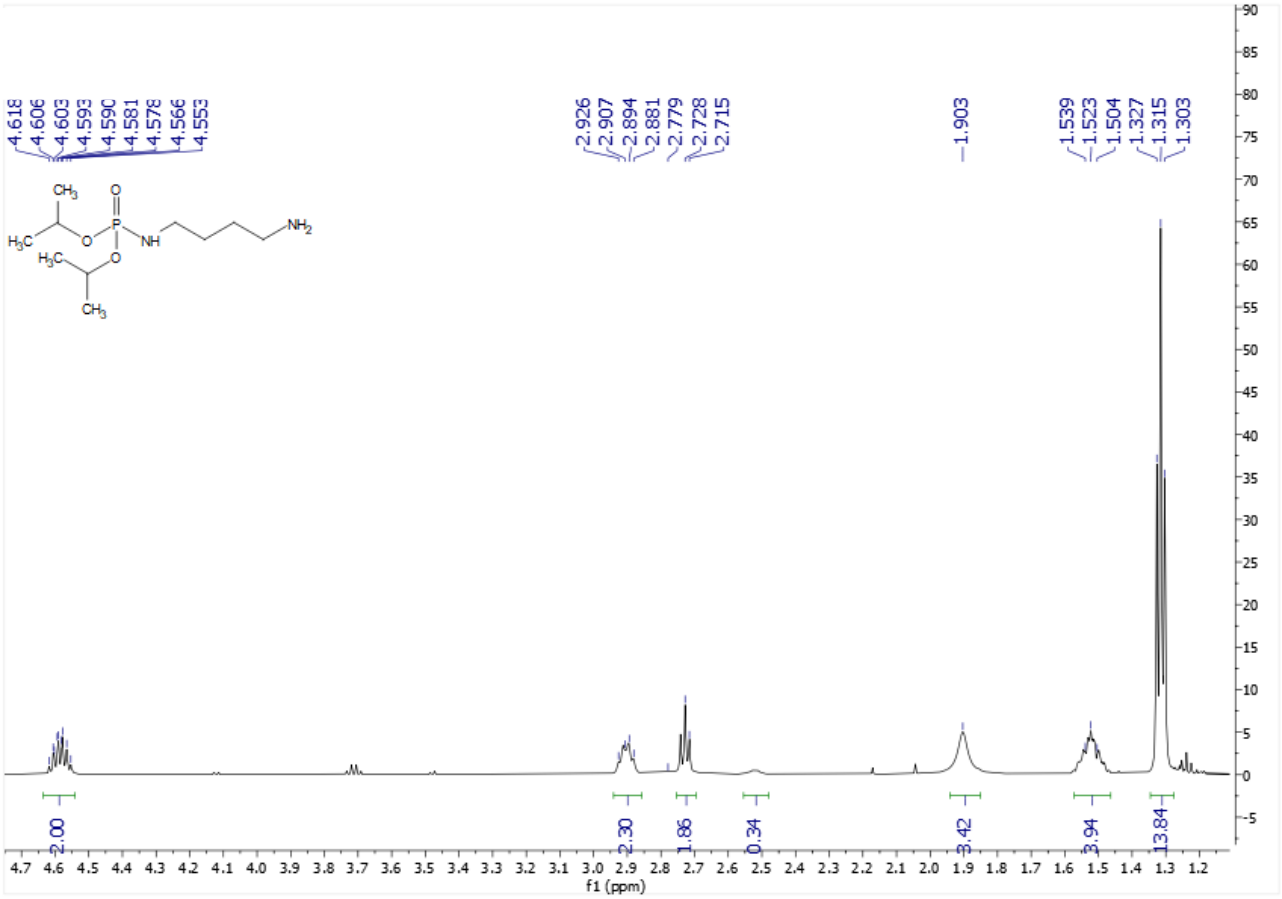

Figure S6 – ^{1}H NMR spectrum (500 MHz) of **IIb** in $CDCl_3$.

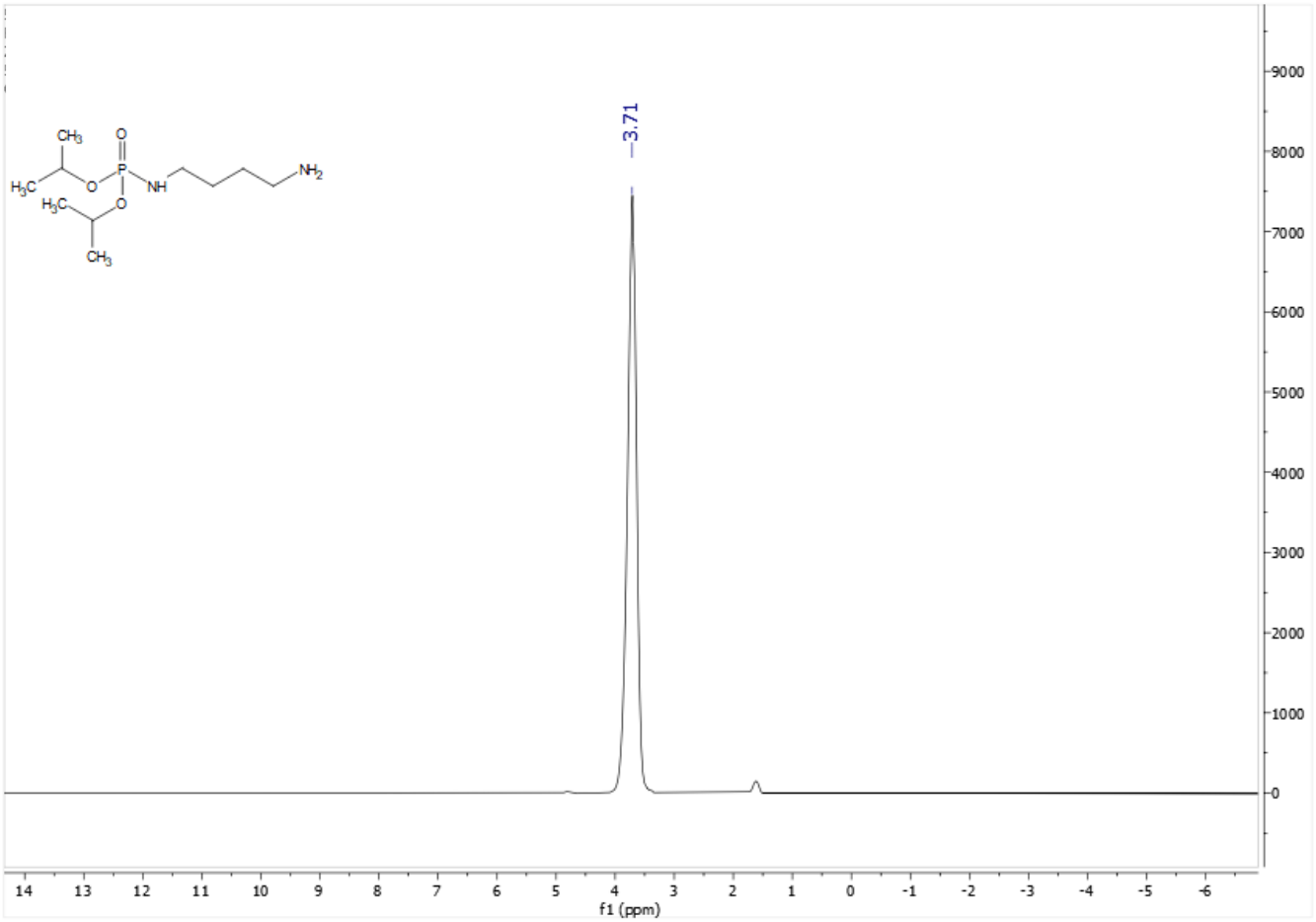

Figure S7 – ^{31}P NMR spectrum (202 MHz) of **IIb** in $CDCl_3$.

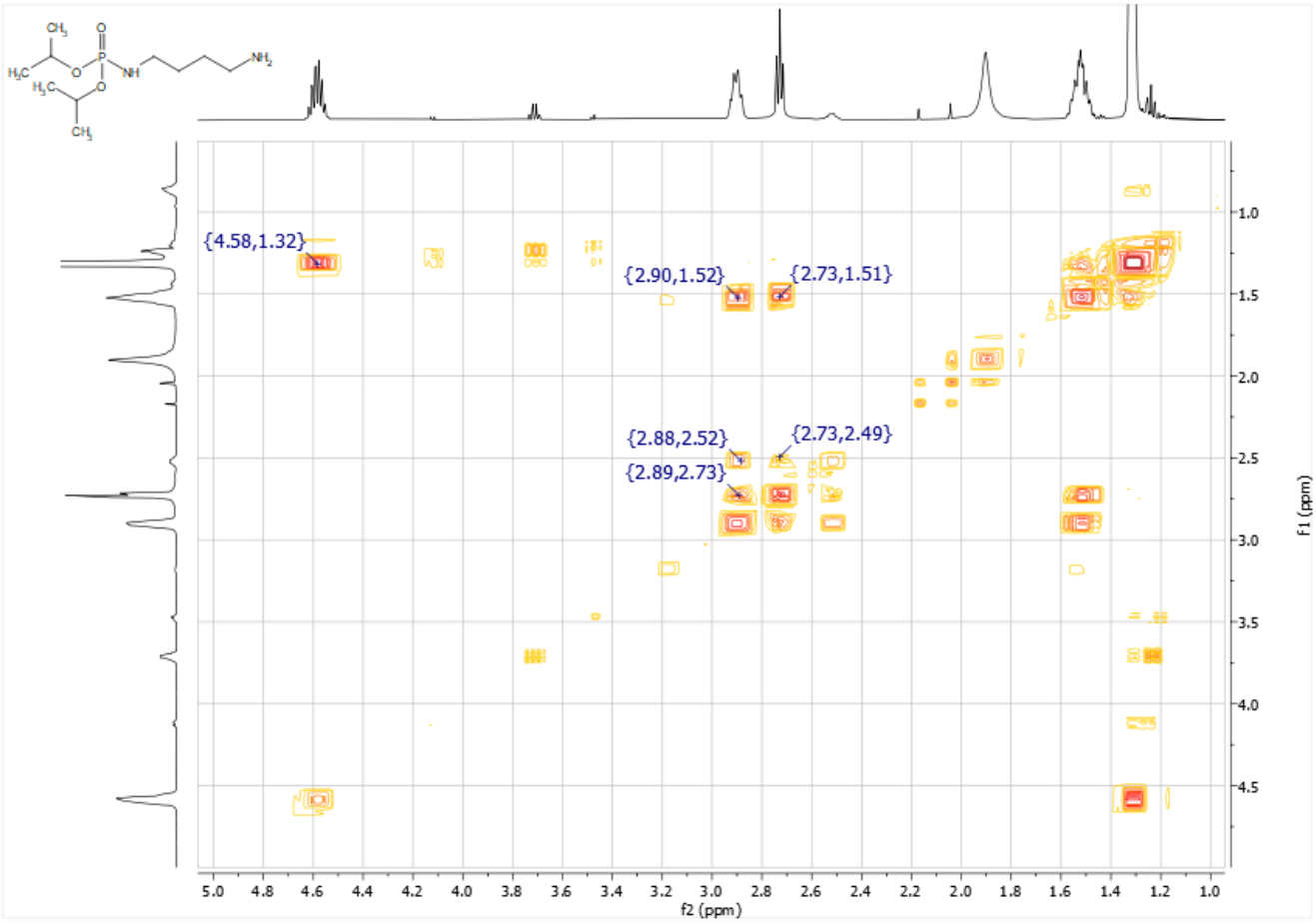

Figure S8 – ^{1}Hx^{1}H-COSY spectrum of **IIb**.

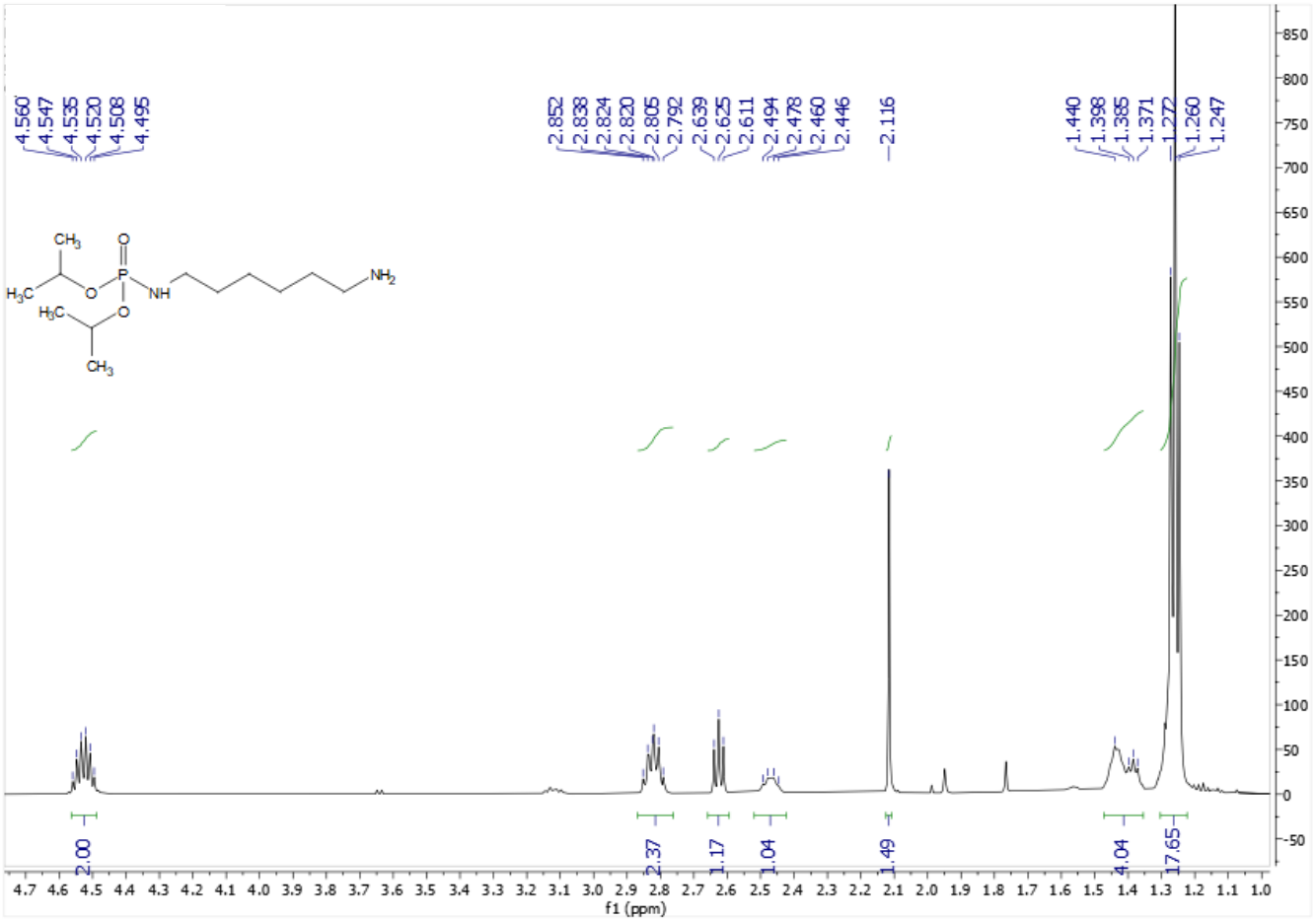

Figure S9 – ^{1}H NMR spectrum (500 MHz) of **IIc** in $CDCl_3$.

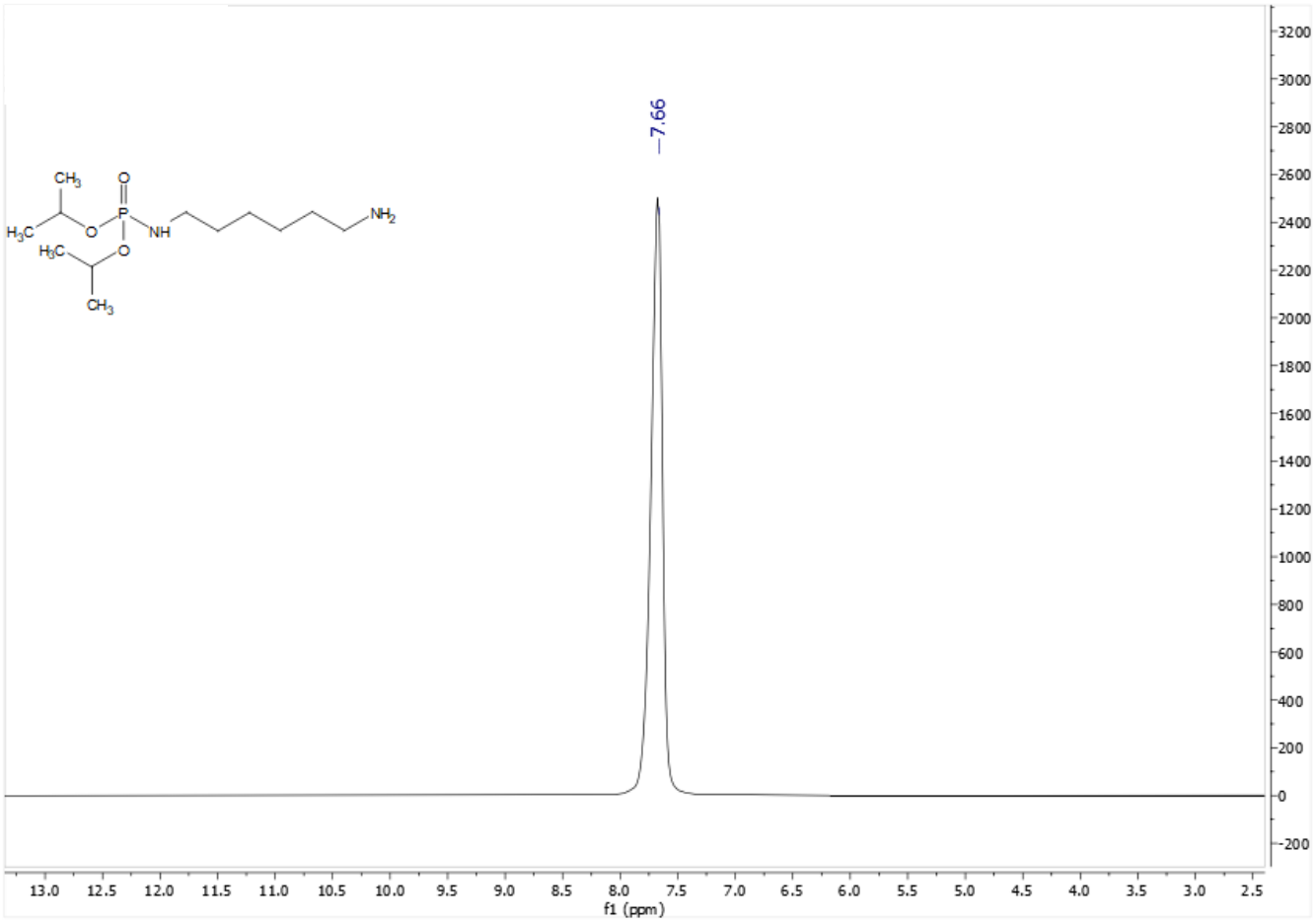

Figure S10 – ^{31}P NMR spectrum (202 MHz) of **IIc** in $CDCl_3$.

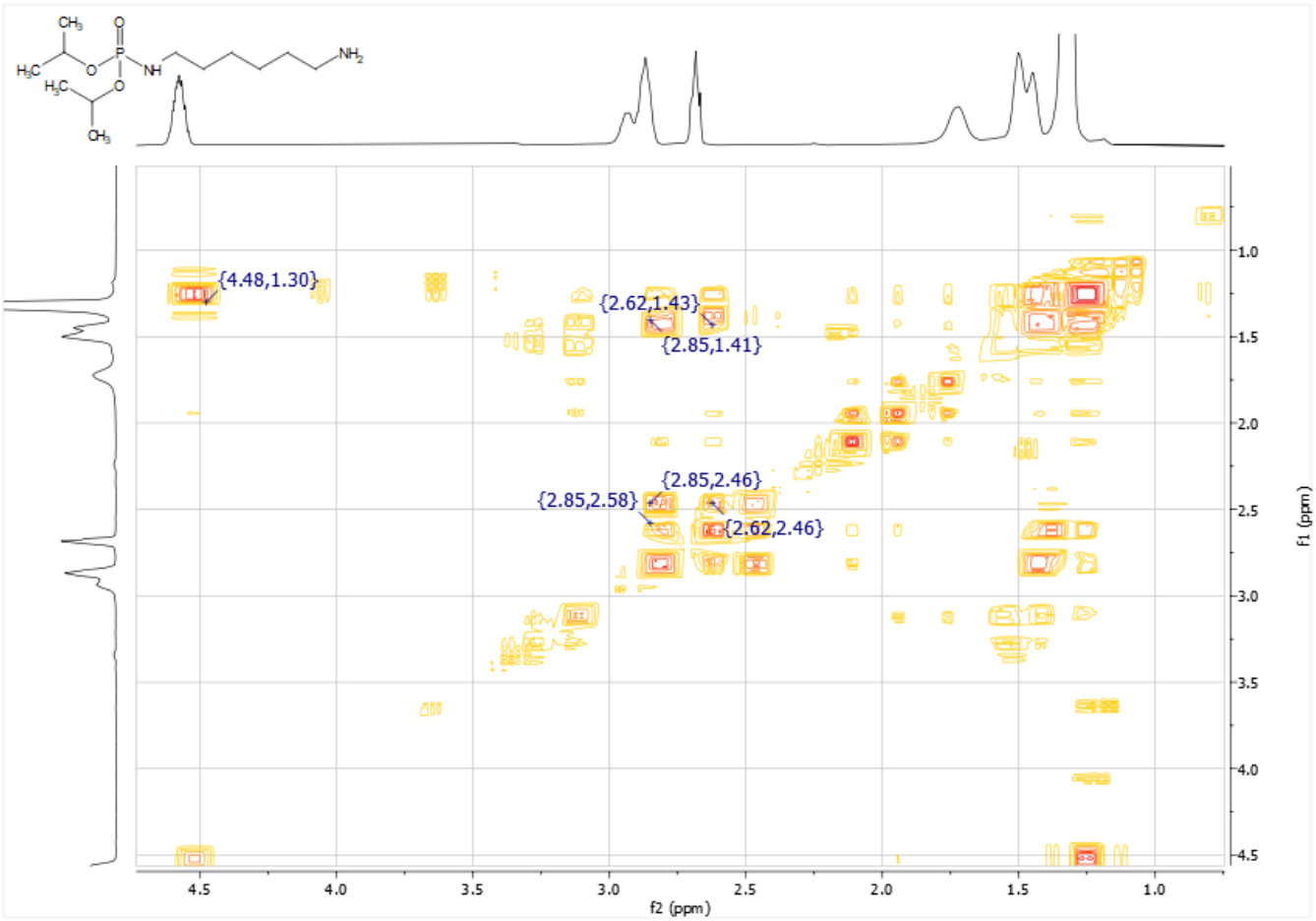

Figure S11 – ^{1}Hx^{1}H-COSY spectrum of **IIc**.

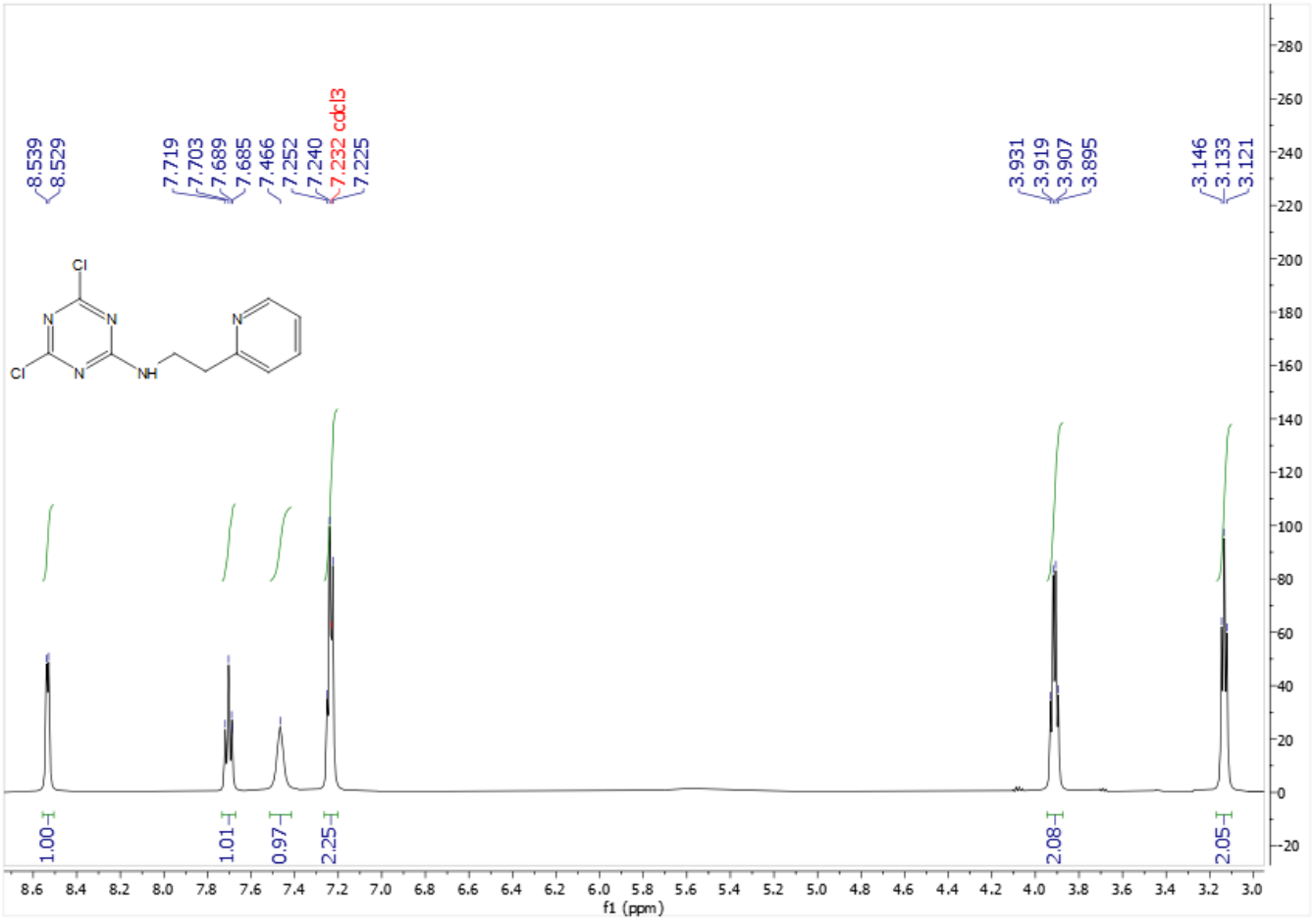

Figure S12 – ^{1}H NMR spectrum (500 MHz) of **1** in $CDCl_3$.

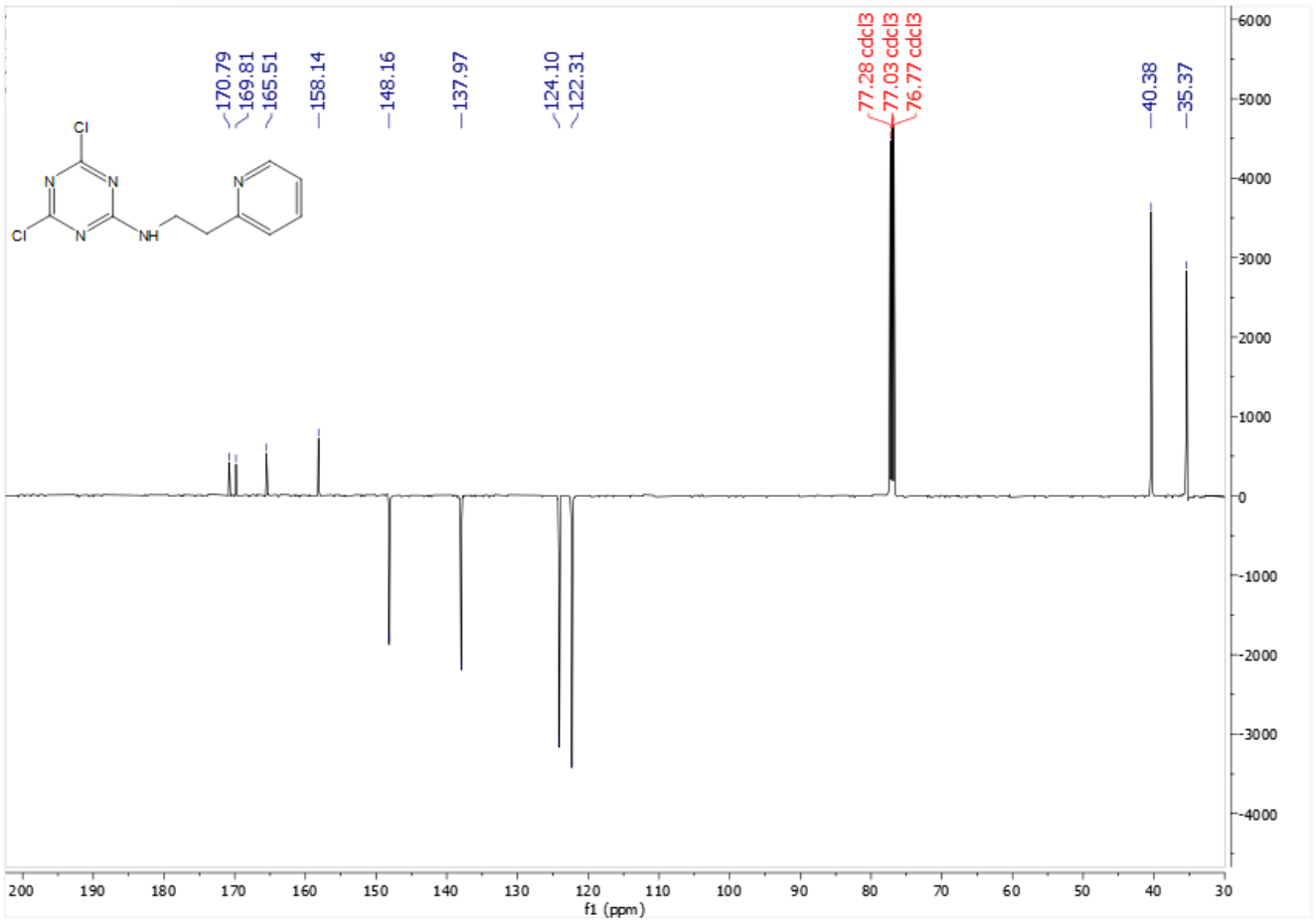

Figure S13 – ^{13}C-APT NMR spectrum (125 MHz) of **1** in $CDCl_3$.

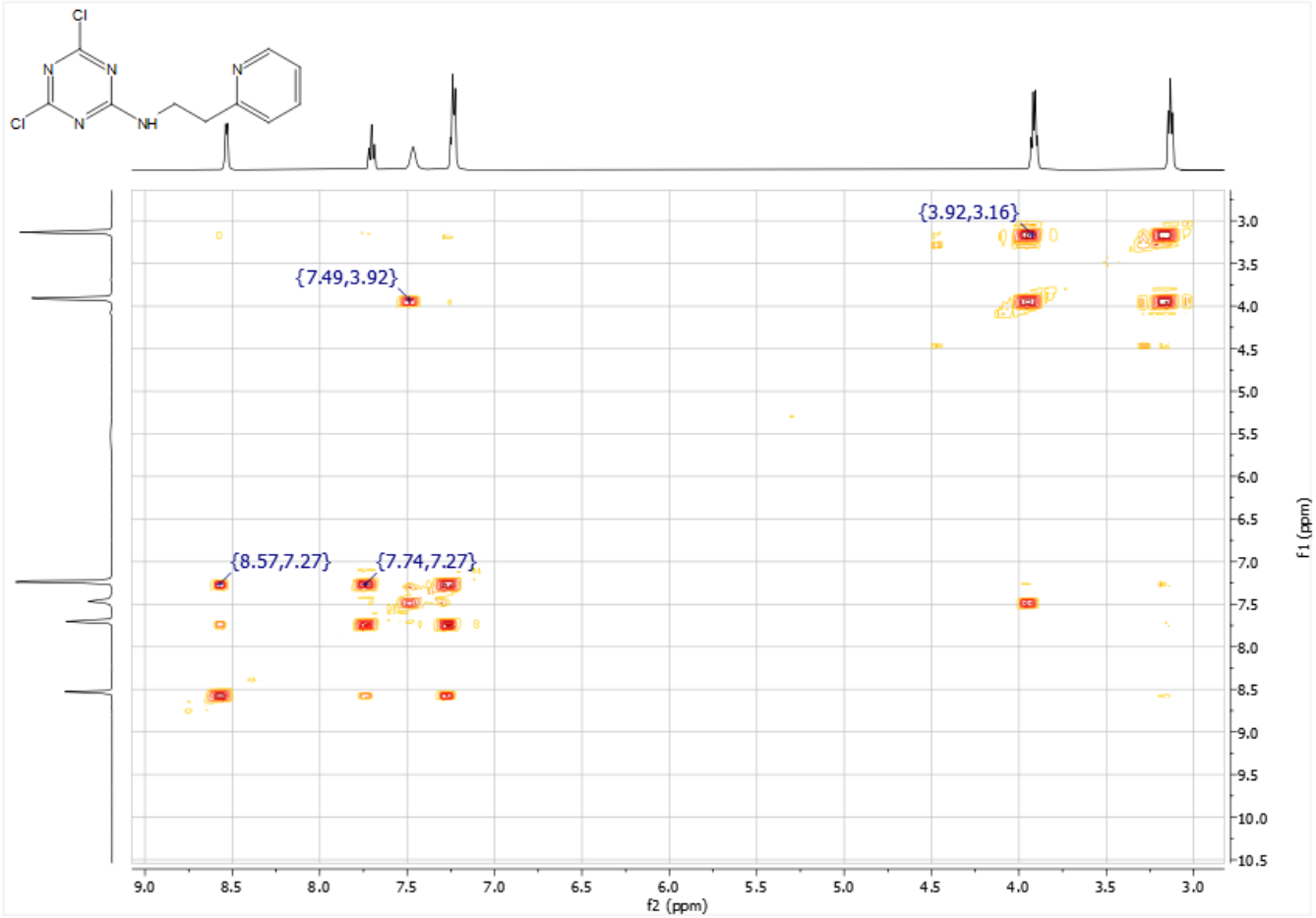

Figure S14 – ^{1}Hx^{1}H-COSY spectrum of **1**.

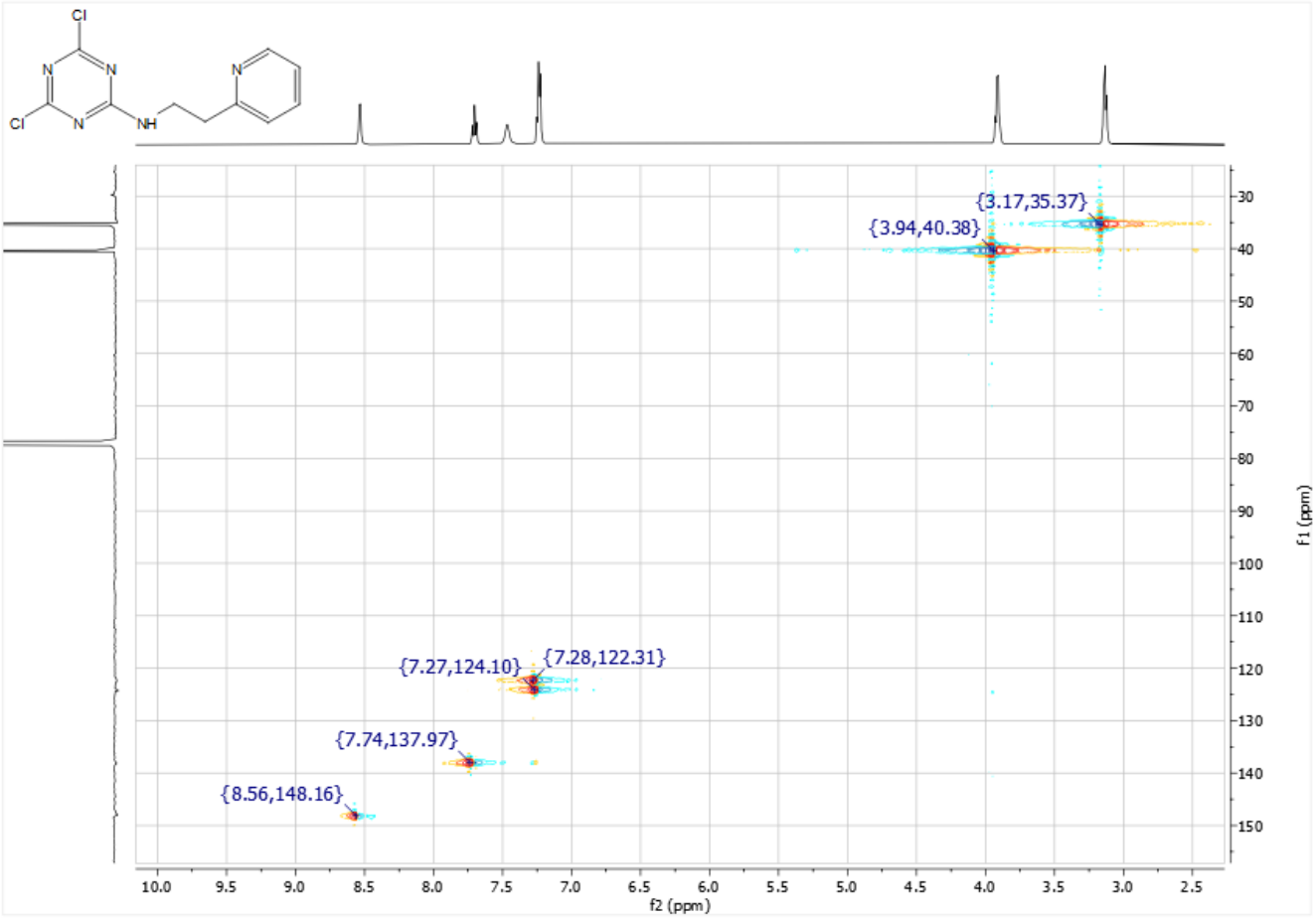

Figure S15 – $^{1}Hx^{13}C$ – HSQC spectrum of **1**.

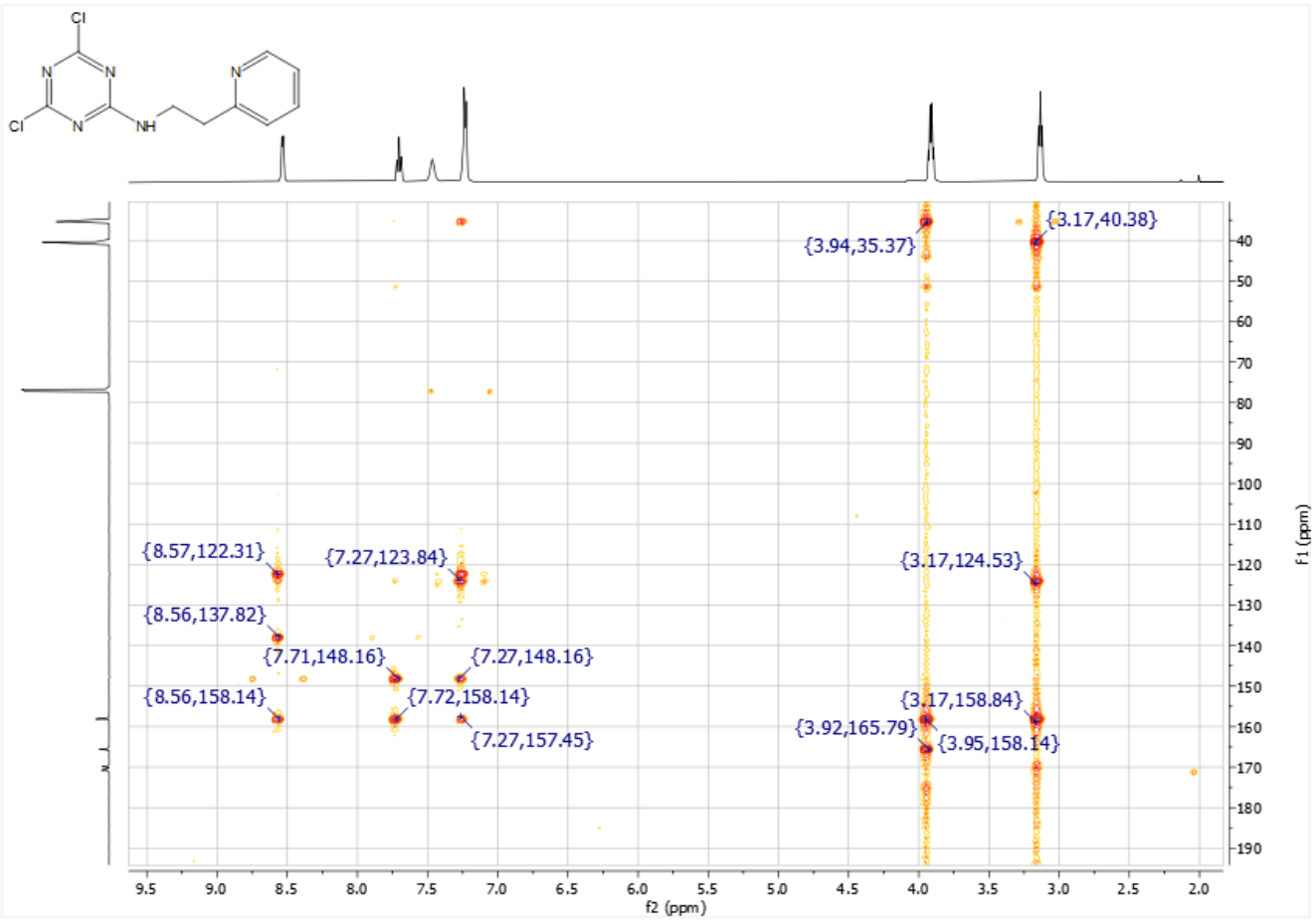

Figure S16 – $^{1}Hx^{13}C$ – HMBC spectrum of **1**.

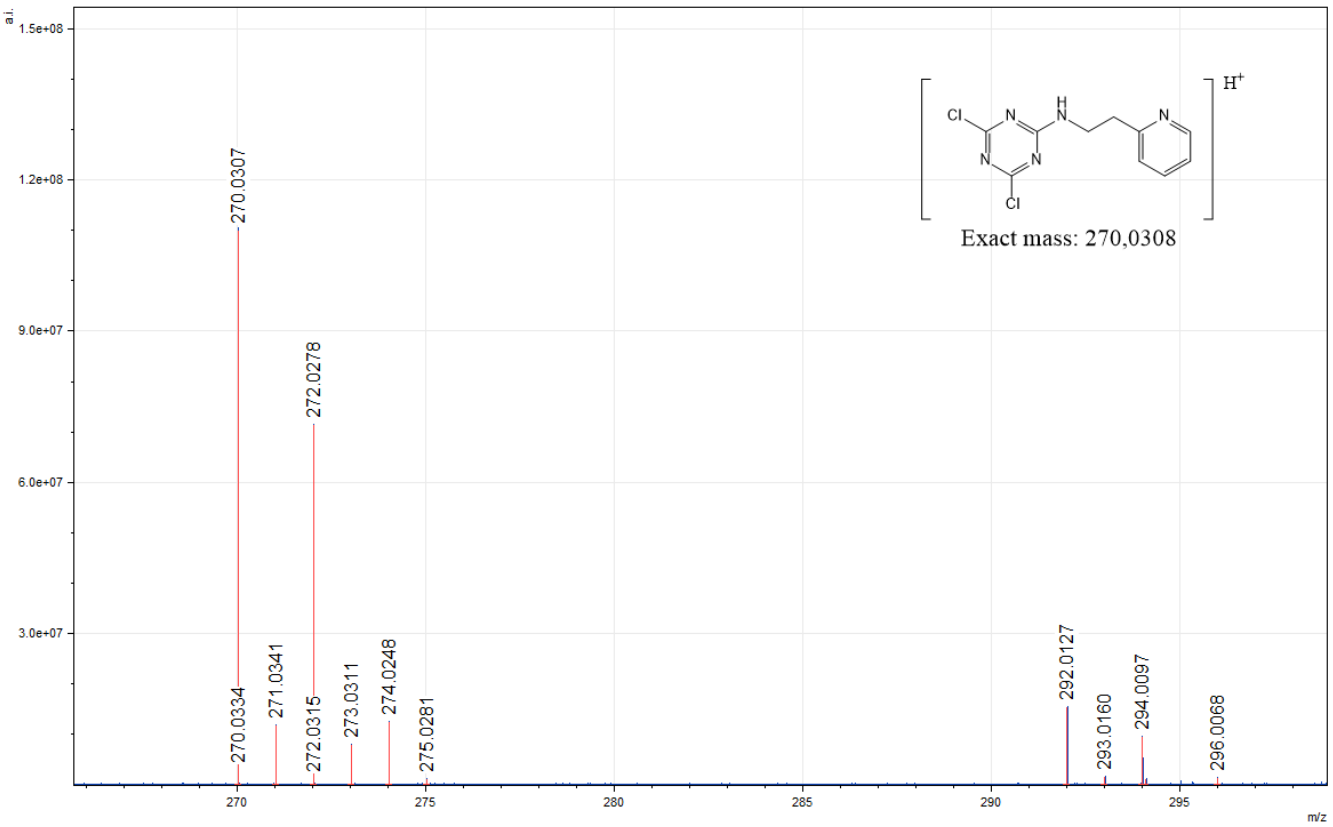

Figure S17 – HRMS spectrum of **1**.

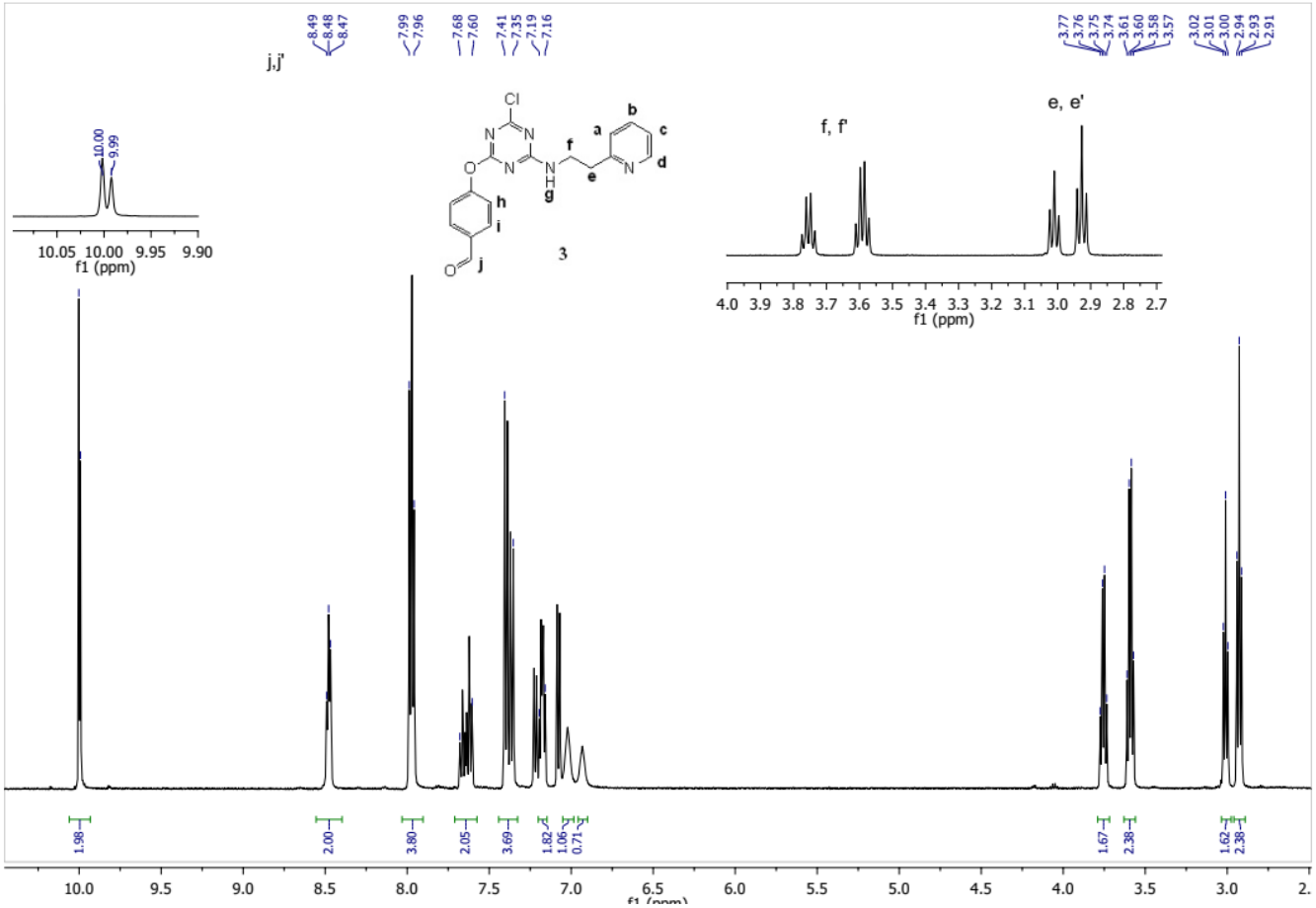

Figure S18 – ^{1}H NMR spectrum (500 MHz) of **3** in CD_3CN.

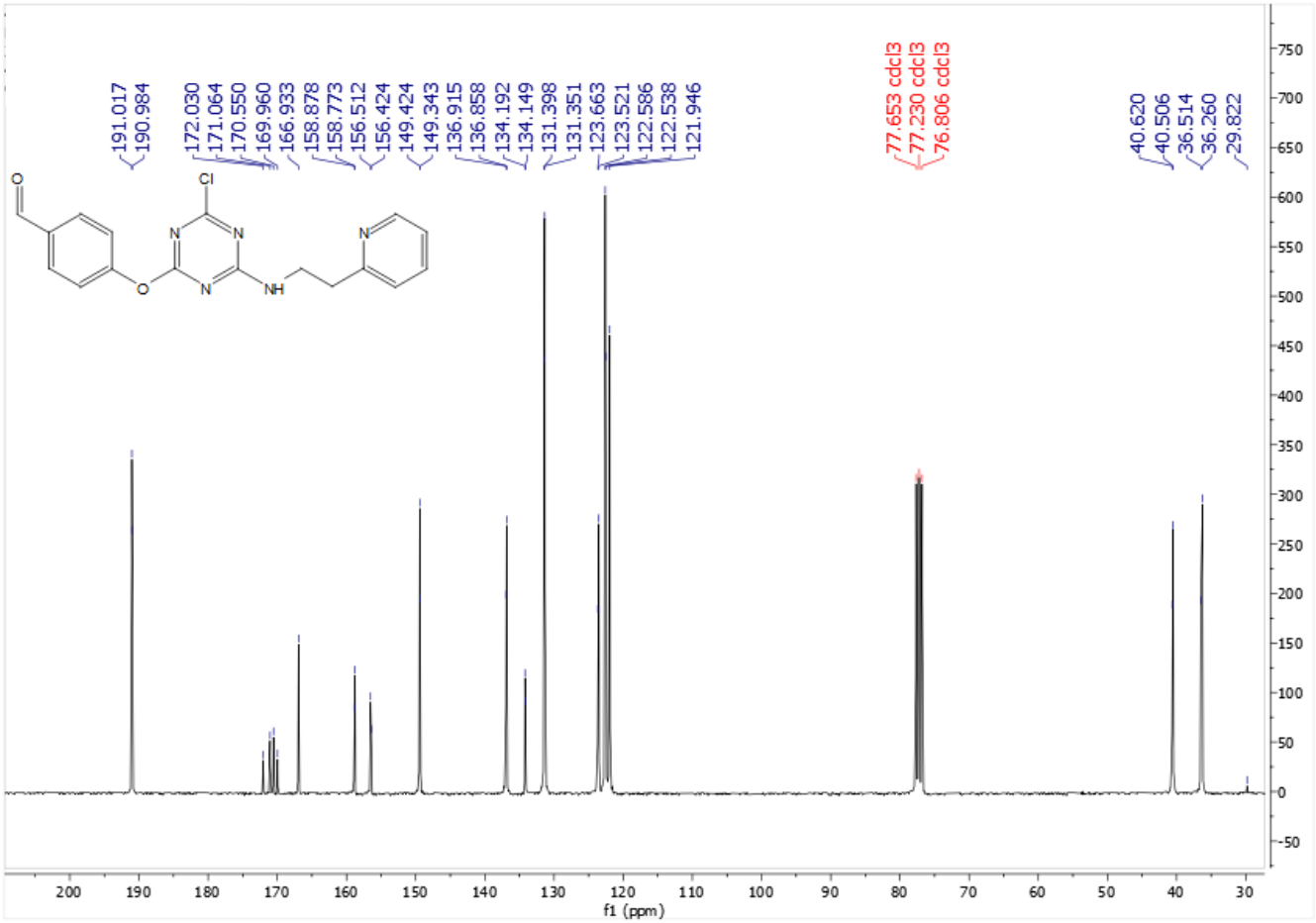

Figure S19 – ^{13}C NMR spectrum (75 MHz) of **3** in $CDCl_3$.

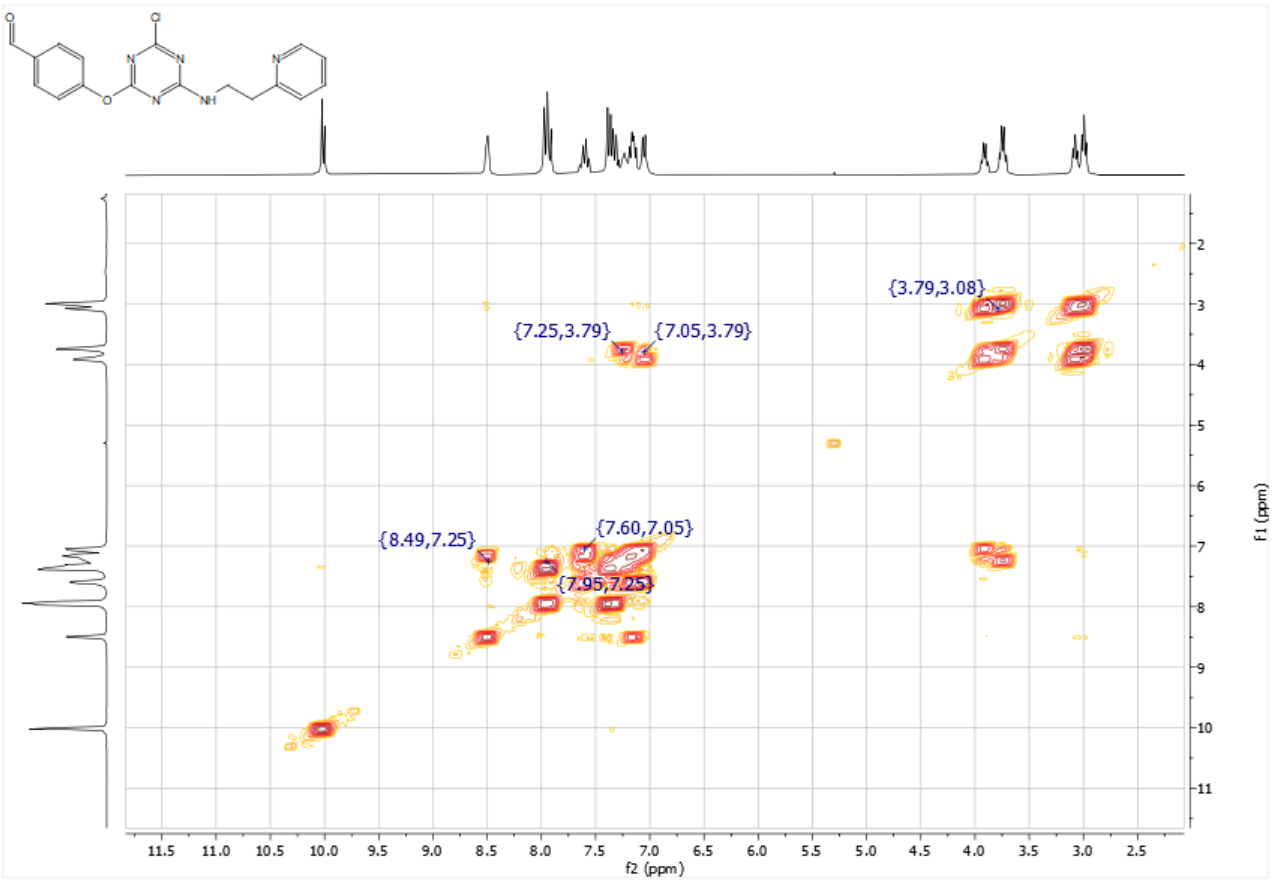

Figure S20 – ^{1}Hx^{1}H-COSY spectrum of **3**.

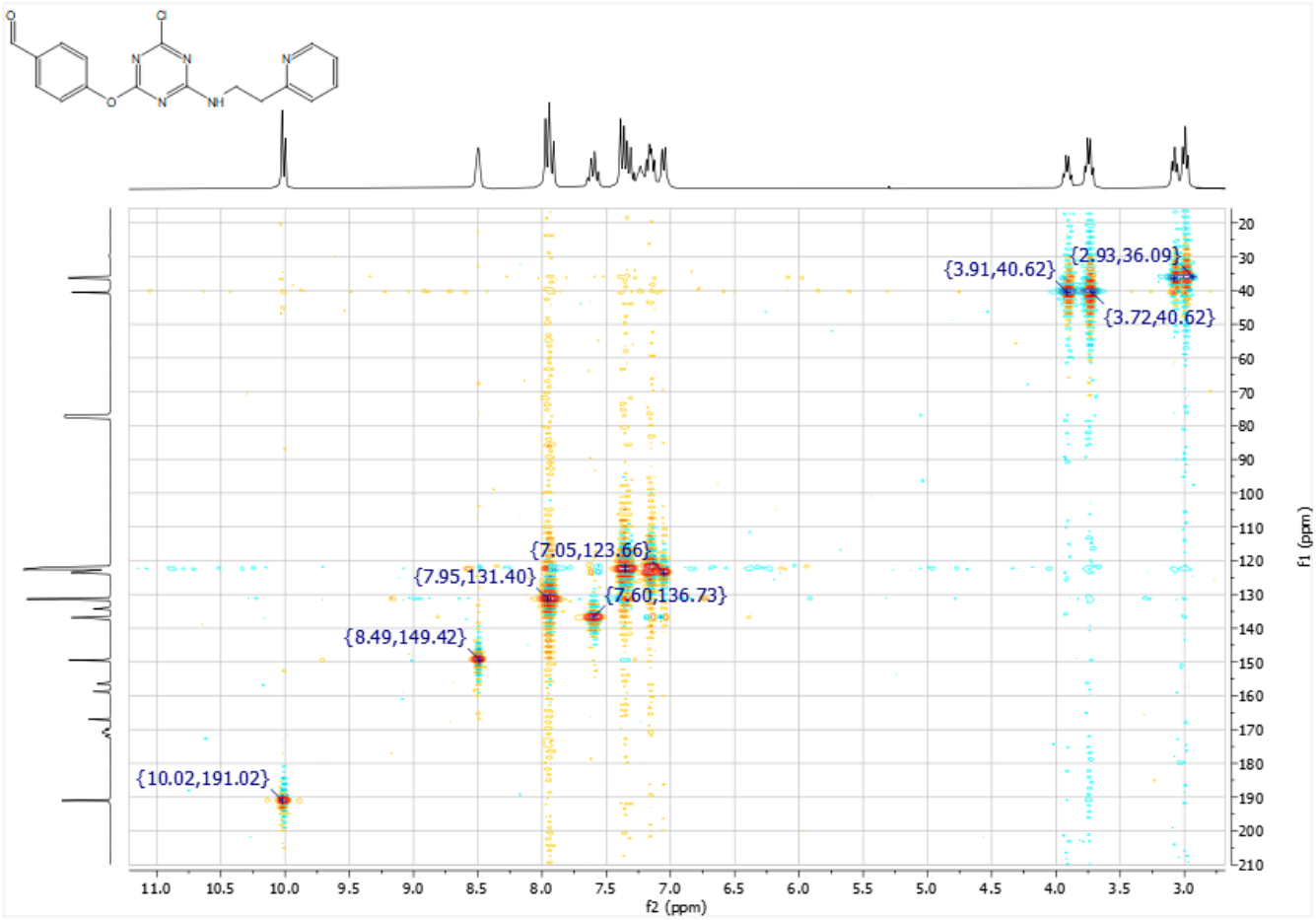

Figure S21 – $^{1}Hx^{13}C$ - HSQC spectrum of **3**.

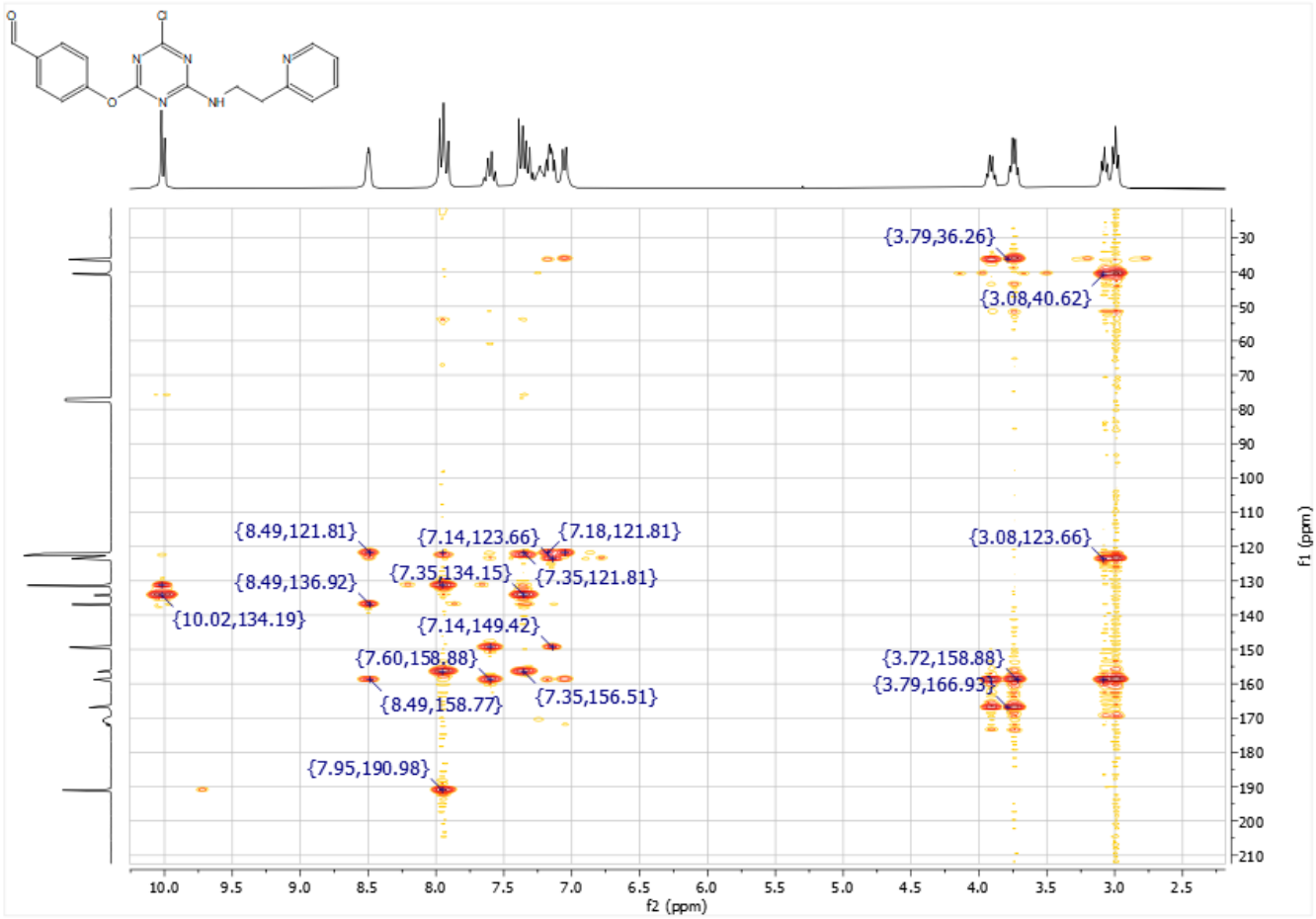

Figure S22 –$^{1}Hx^{13}C$ – HMBC spectrum of **3**.

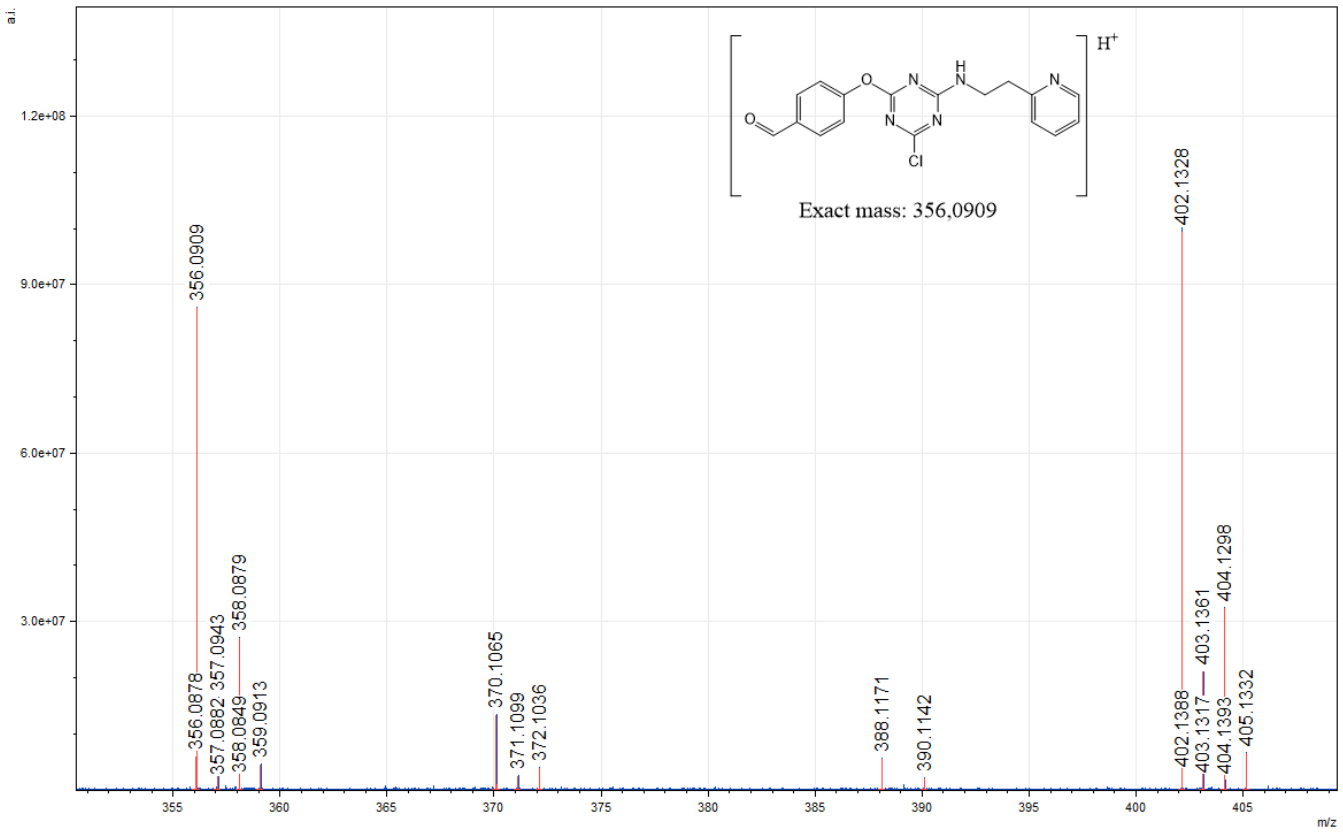

Figure S23 – HRMS spectrum of **3**.

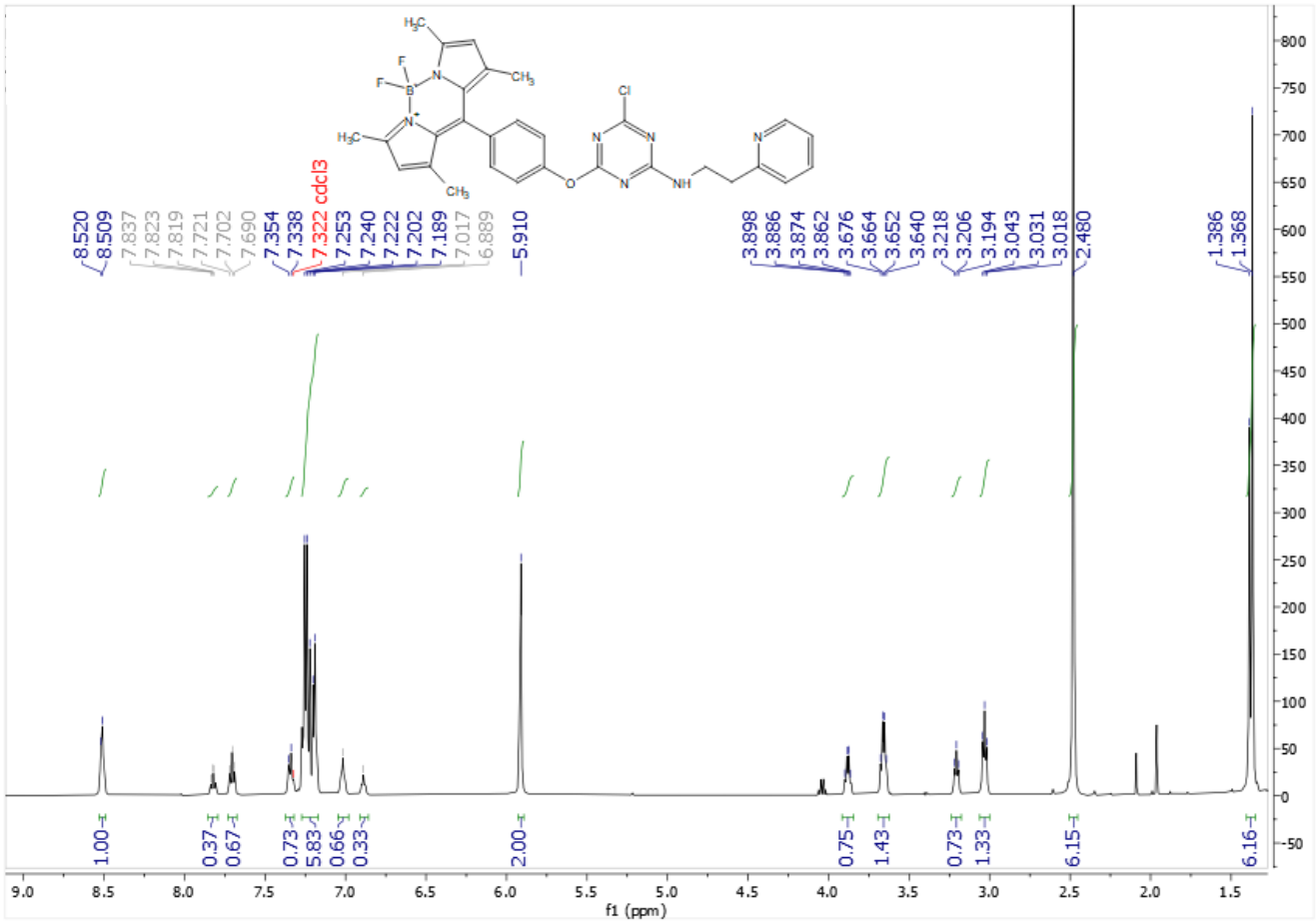

Figure S24 – ^{1}H NMR spectrum (500 MHz) of **4** in $CDCl_3$.

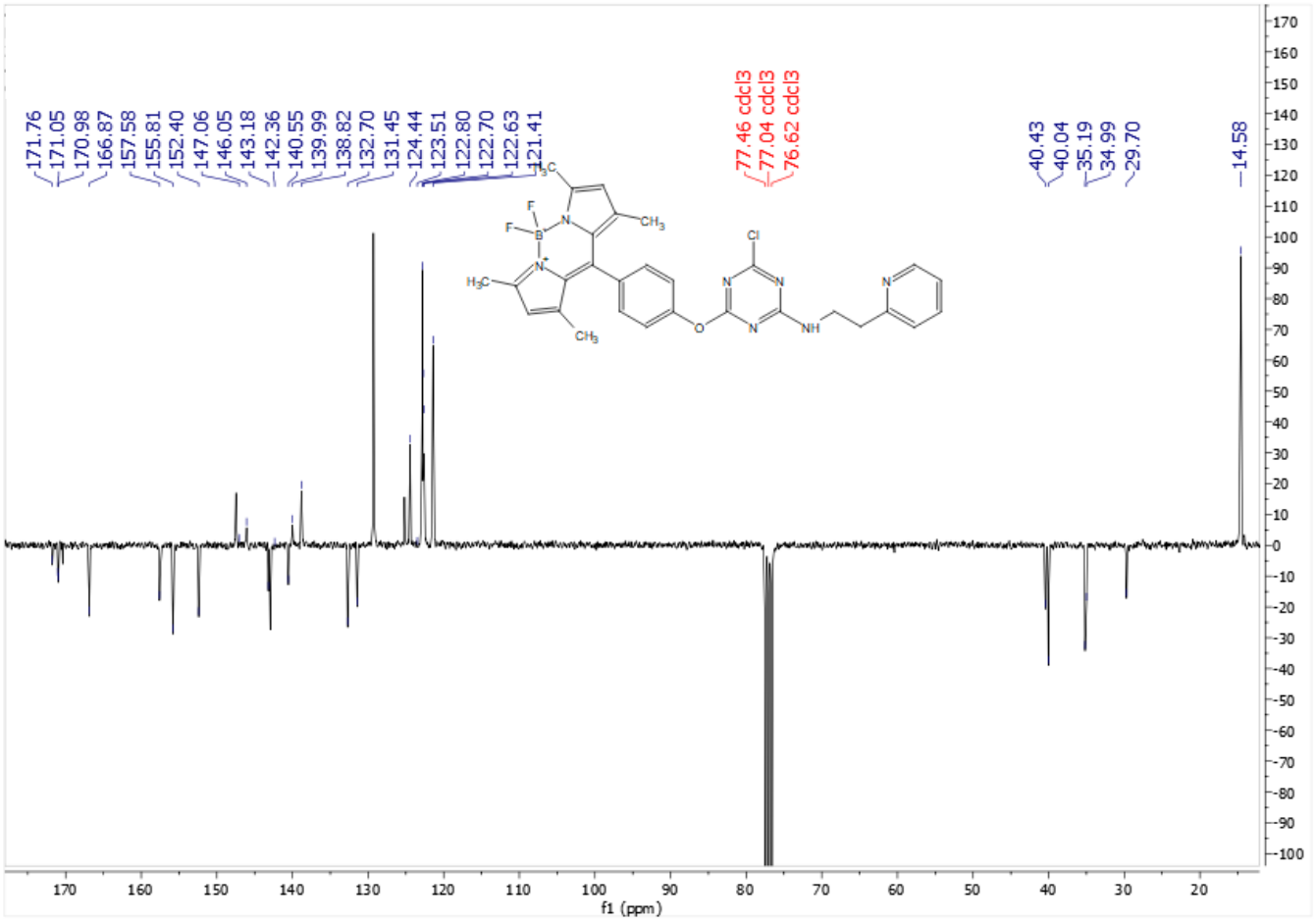

Figure S25 – ^{13}C-APT NMR spectrum (125 MHz) of **4** in $CDCl_3$**.**

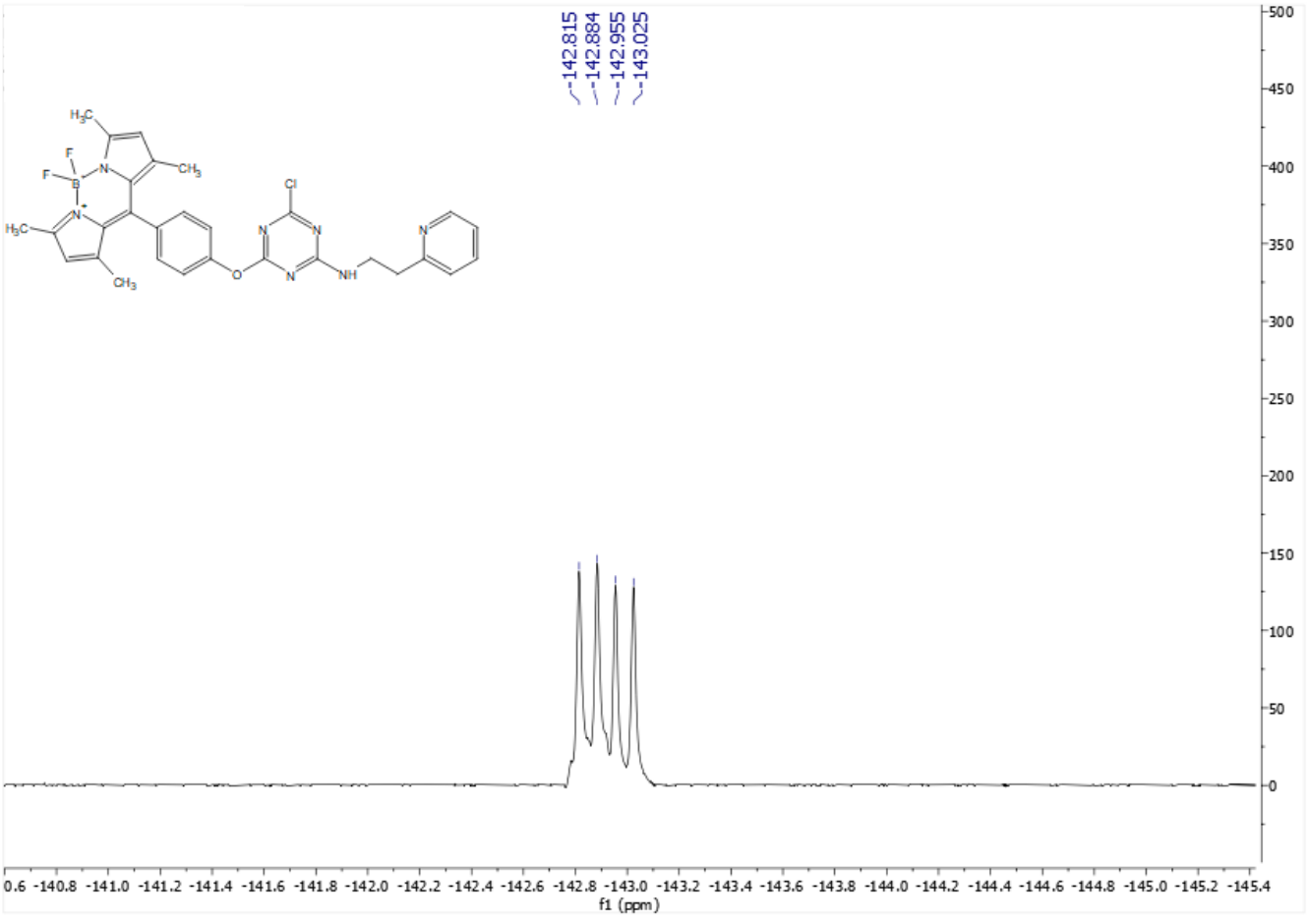

Figure S26 – ^{19}F NMR spectrum (470 MHz) of **4** in $CDCl_3$.

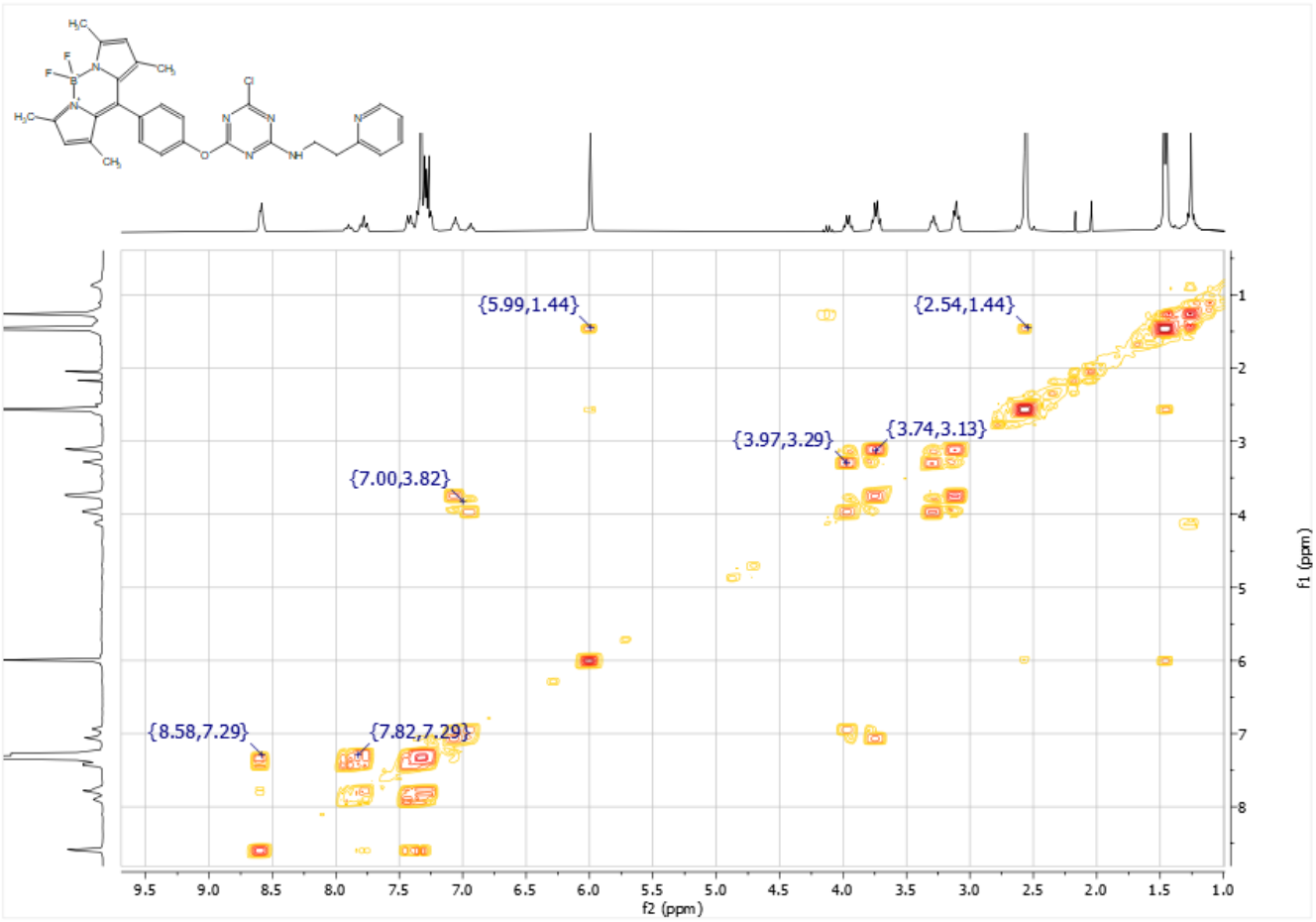

Figure S27 – ^{1}Hx^{1}H-COSY spectrum of **4**.

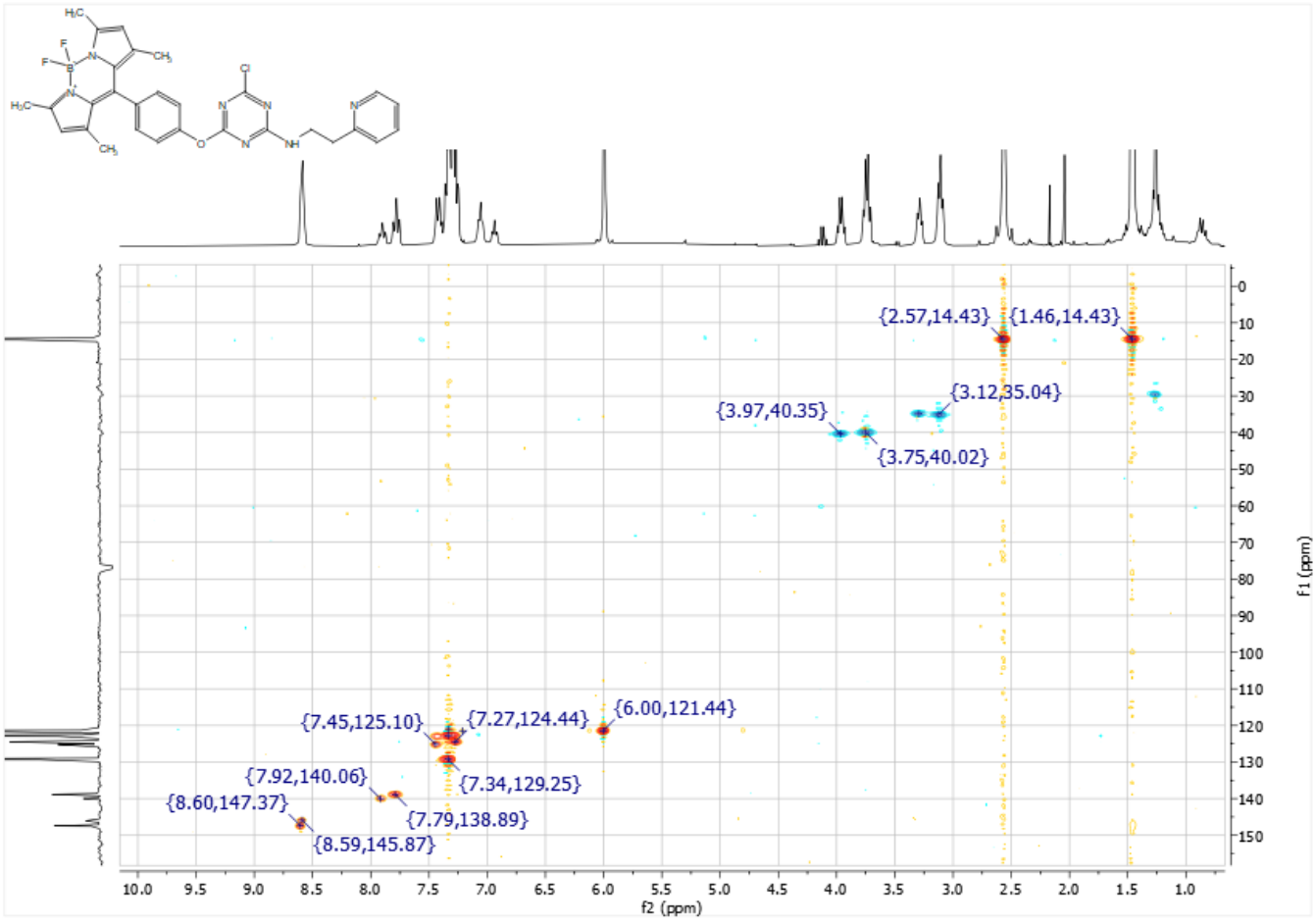

Figure S28 –^{1}Hx^{13}C – HSQC spectrum of **4**.

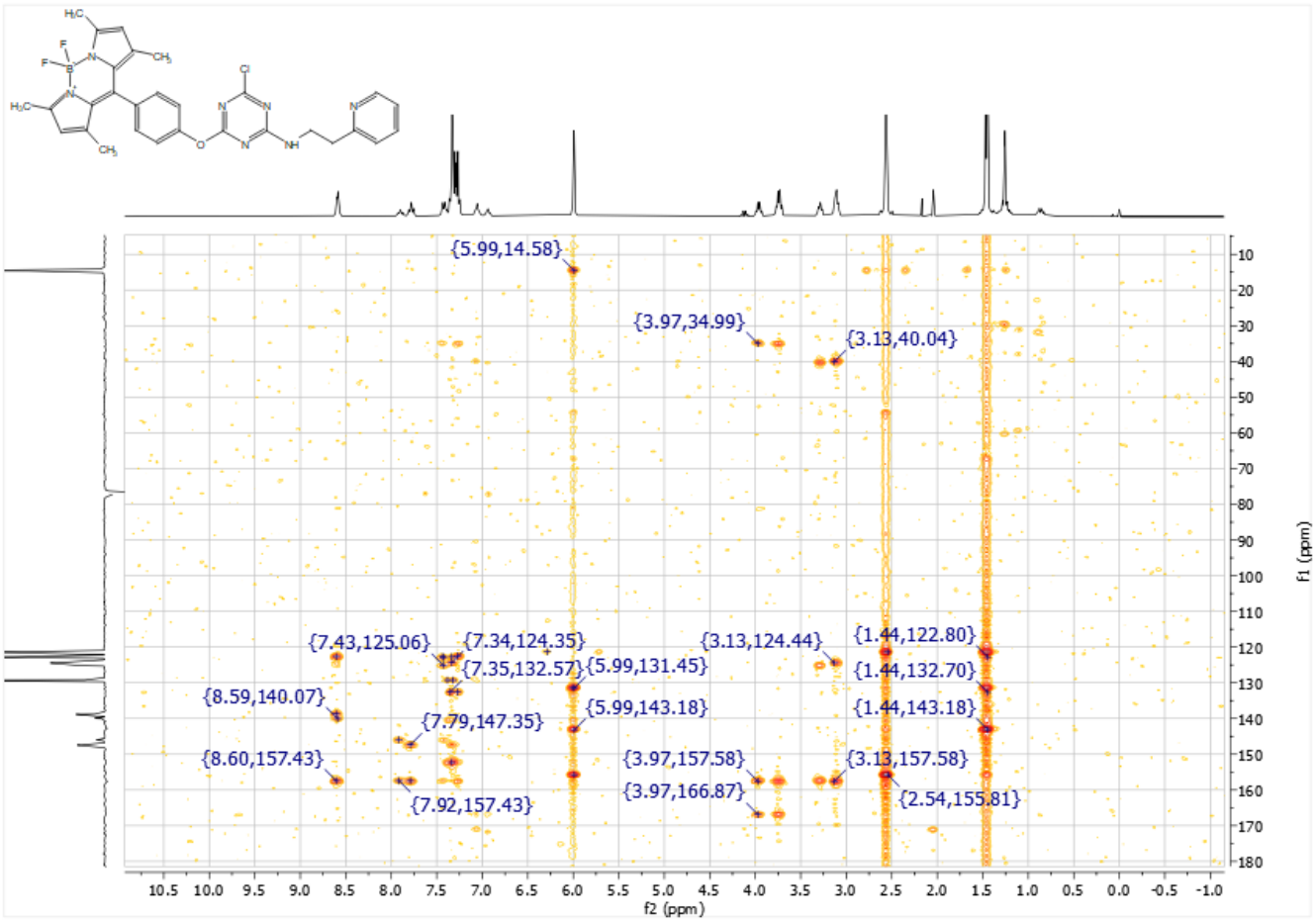

Figure S29 – $^{1}Hx^{13}C$ – HMBC spectrum of **4**.

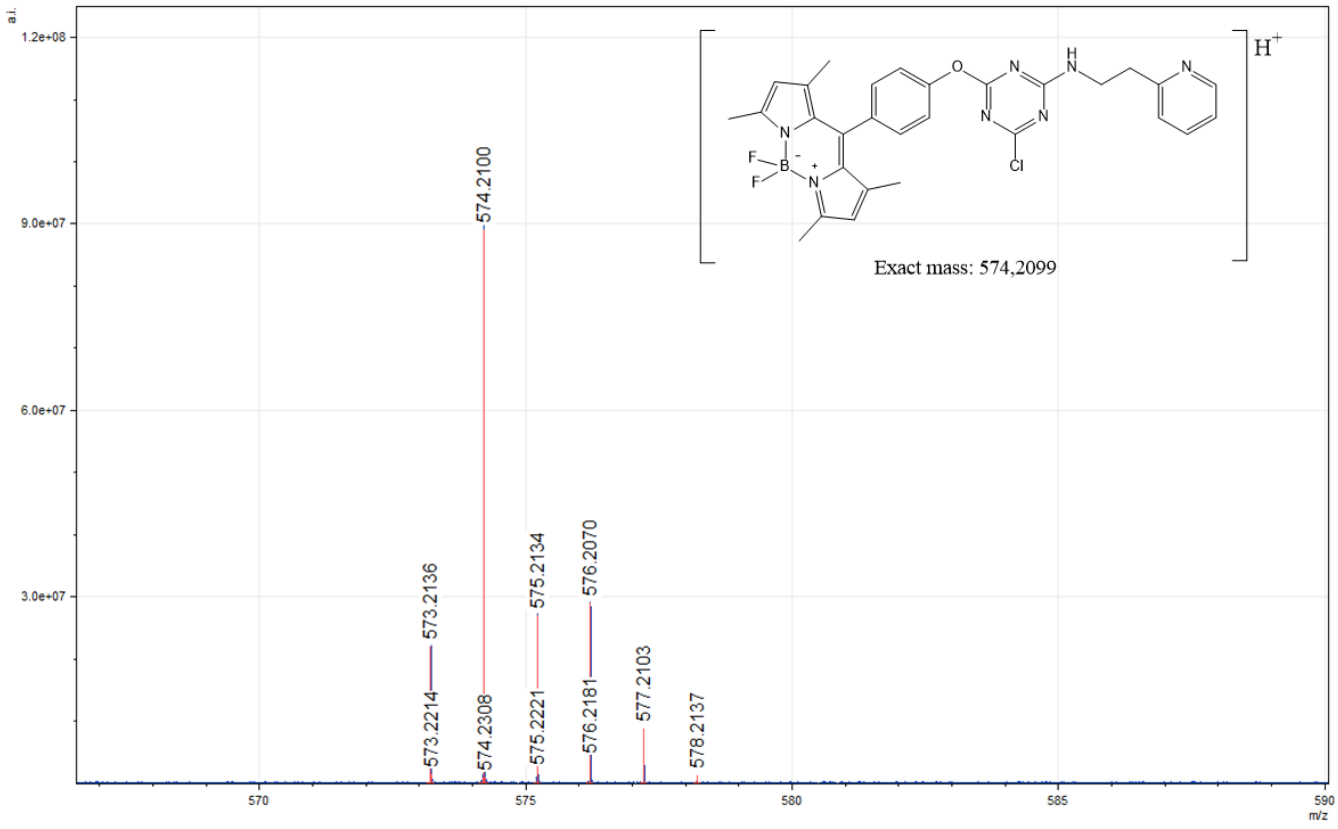

Figure S30– HRMS spectrum of **4**.

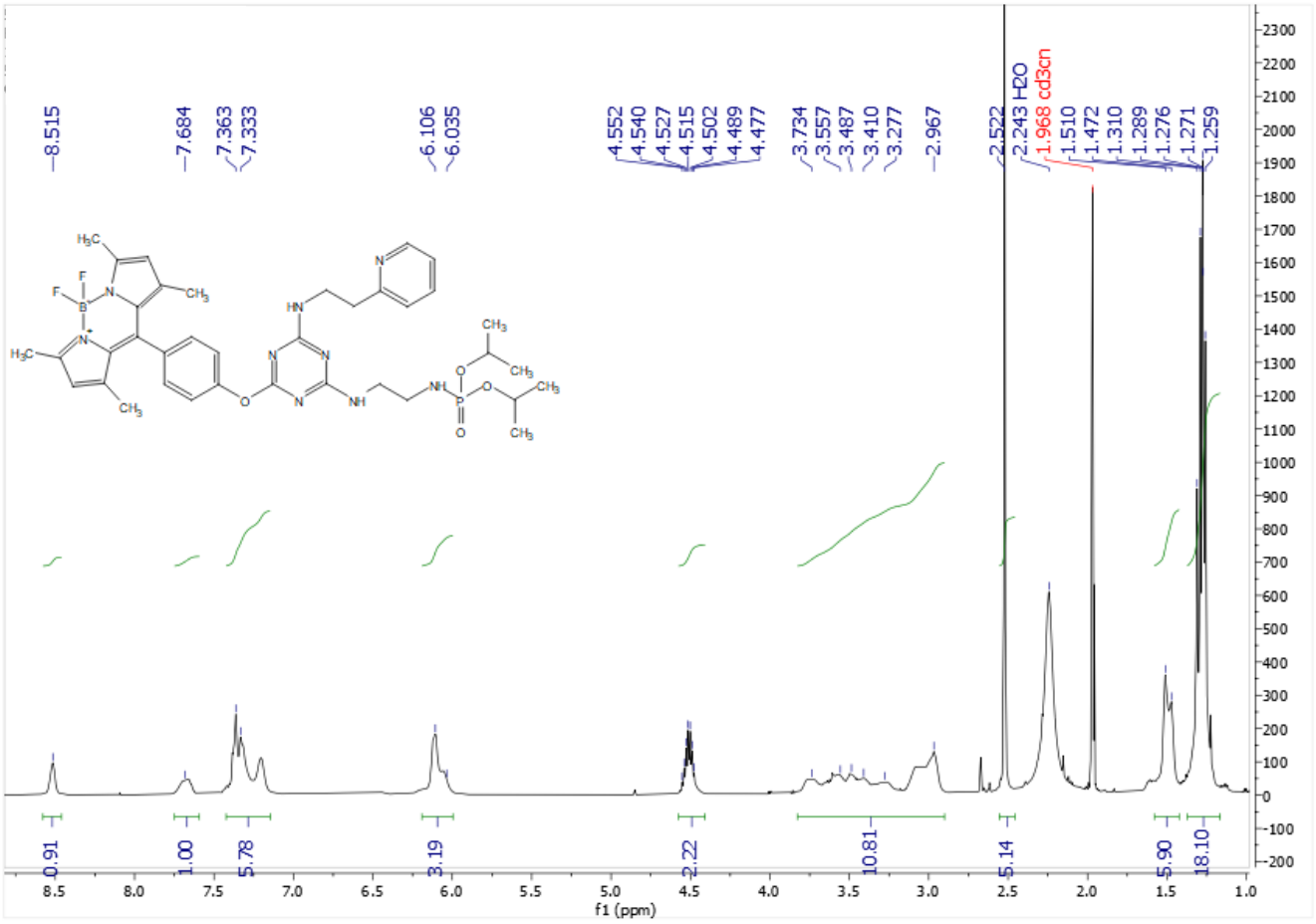

Figure S31 – ^{1}H NMR spectrum (500 MHz) of **5a** in CD_3CN.

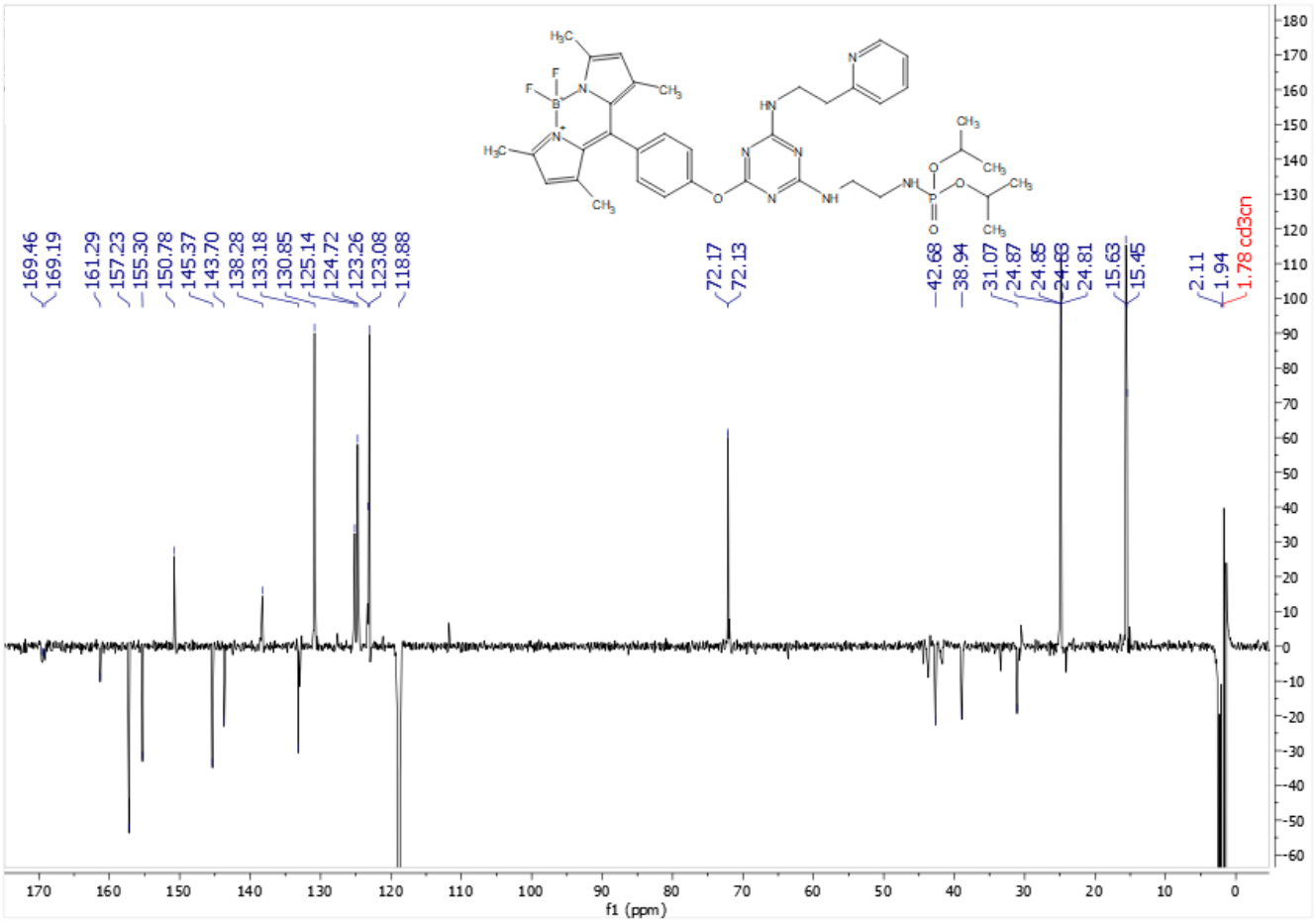

Figure S32 – ^{13}C-APT NMR spectrum (125 MHz) of **5a** in CD_3CN.

Figure S33 – ^{31}P NMR spectrum (202 MHz) of **5a** in CD_3CN.

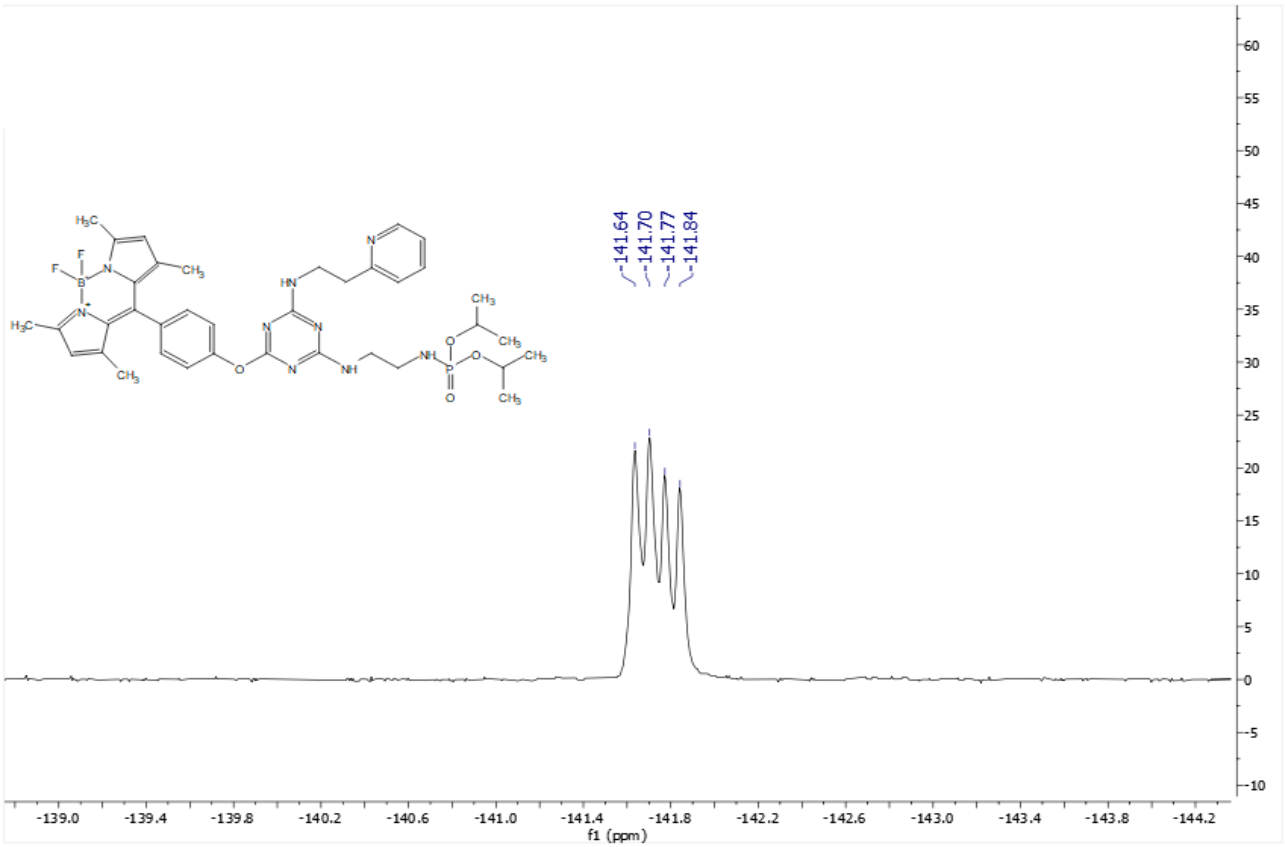

Figure S34 – ^{19}F NMR spectrum (470 MHz) of **5a** in CD_3CN.

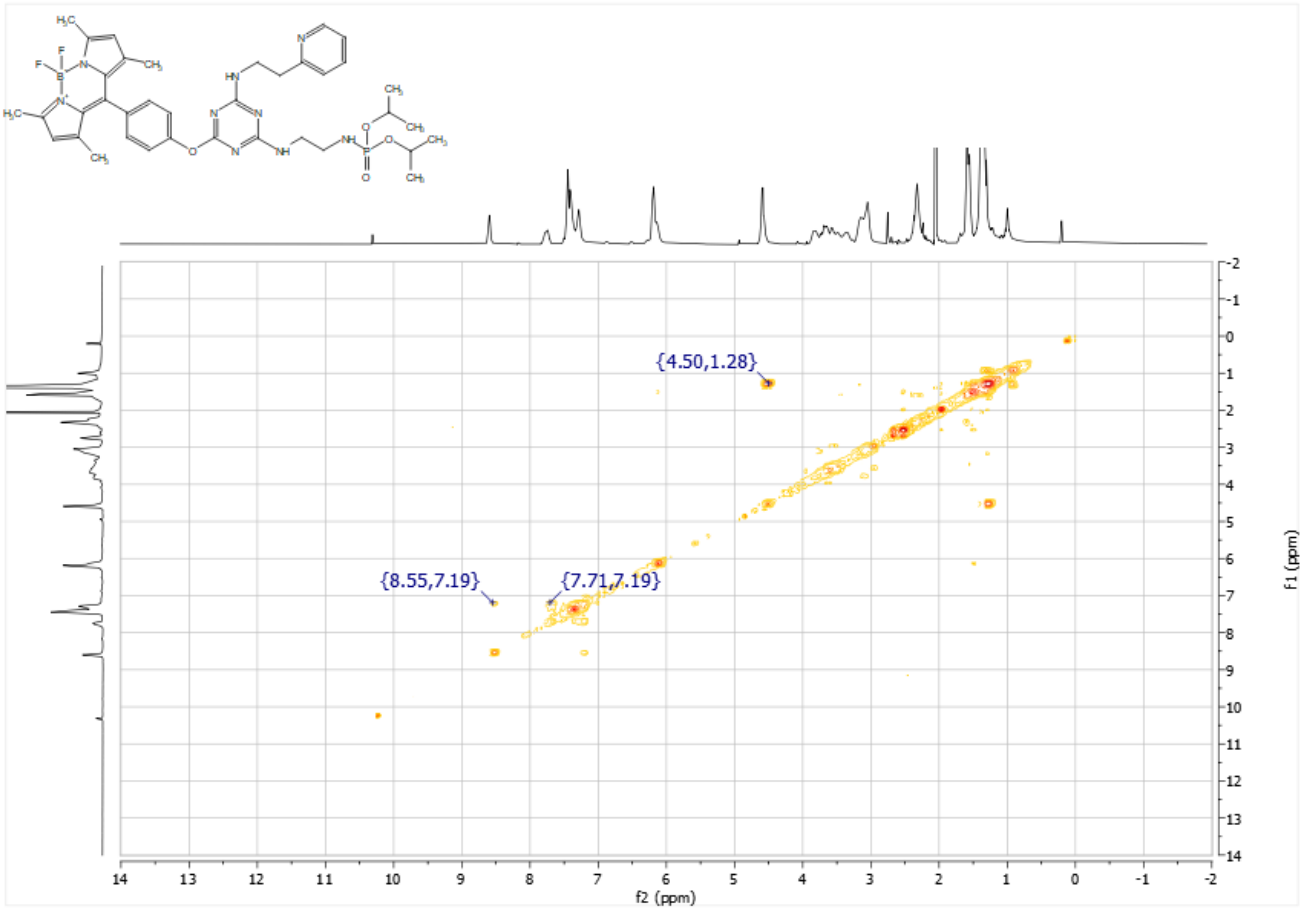

Figure S35 – ^{1}Hx^{1}H-COSY spectrum of **5a**.

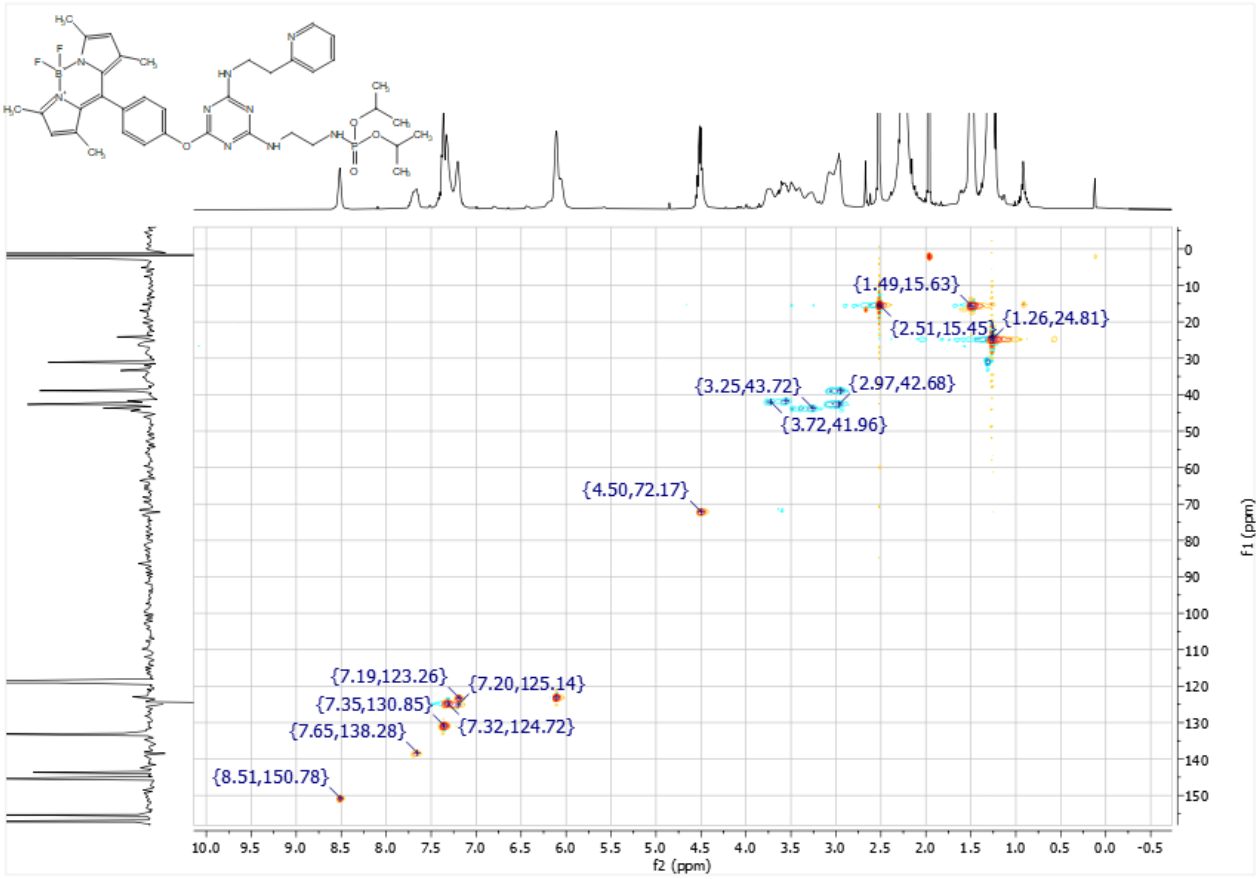

Figure S36 – ^{1}Hx^{13}C – HSQC spectrum of **5a**.

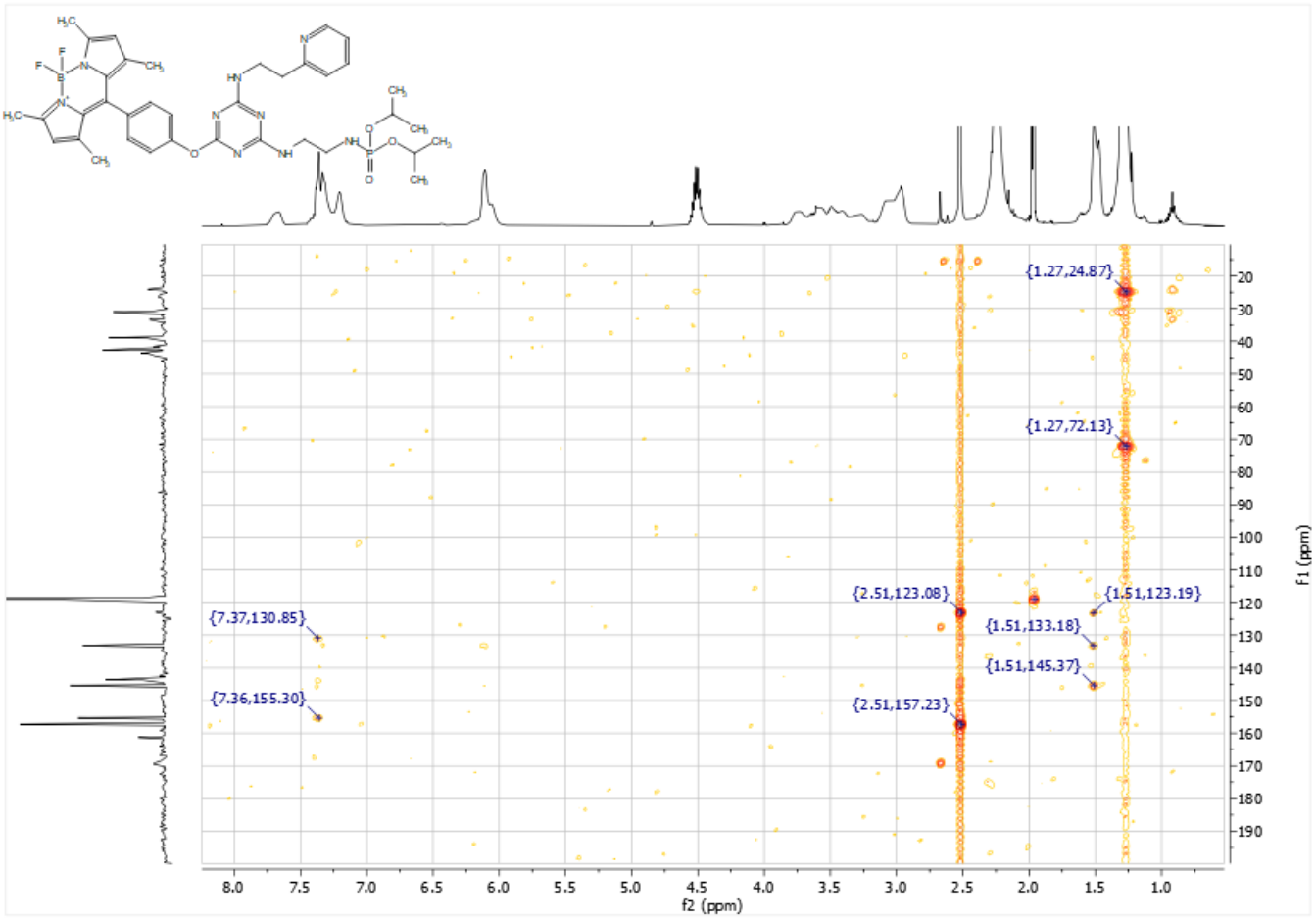

Figure S37 – $^{1}Hx^{13}C$ – HMBC spectrum of **5a**.

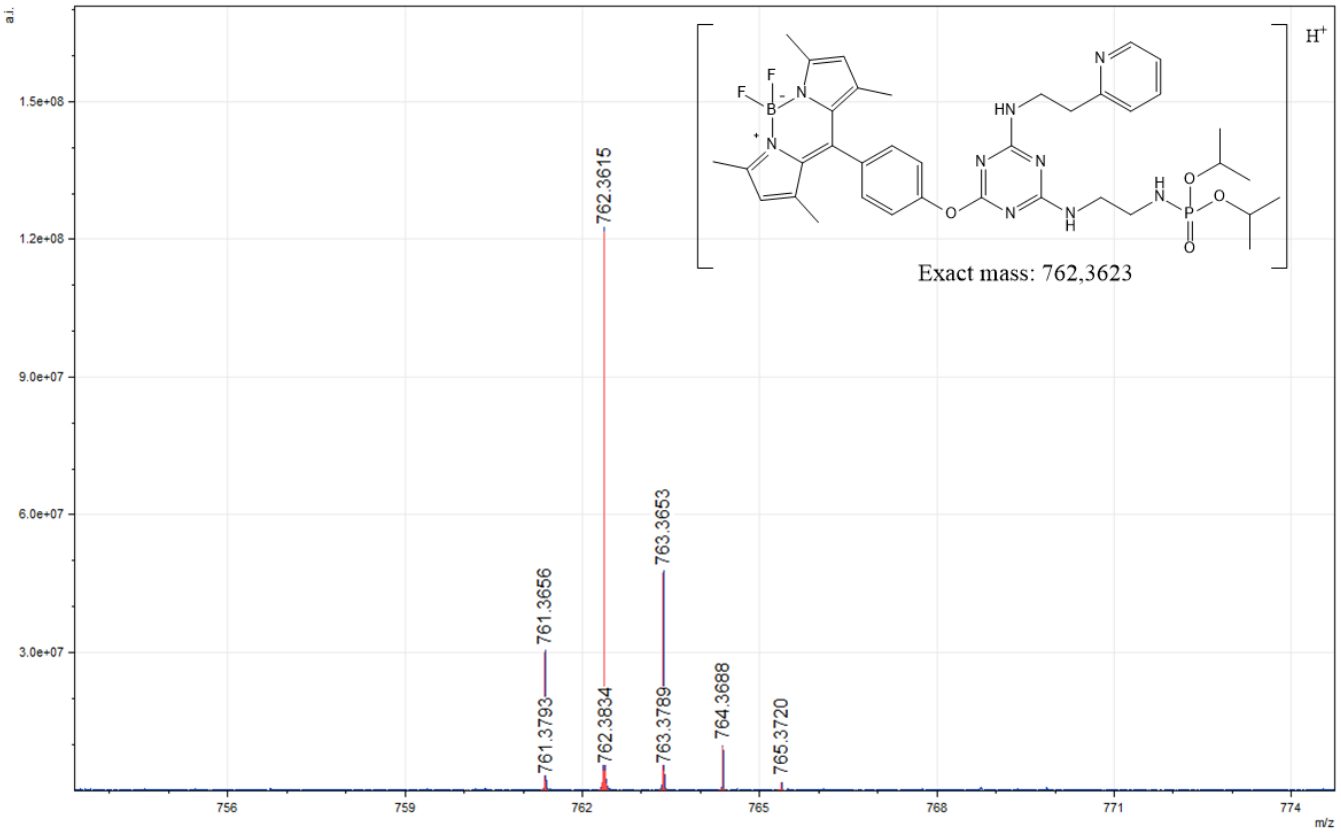

Figure S38 – HRMS spectrum of **5a**.

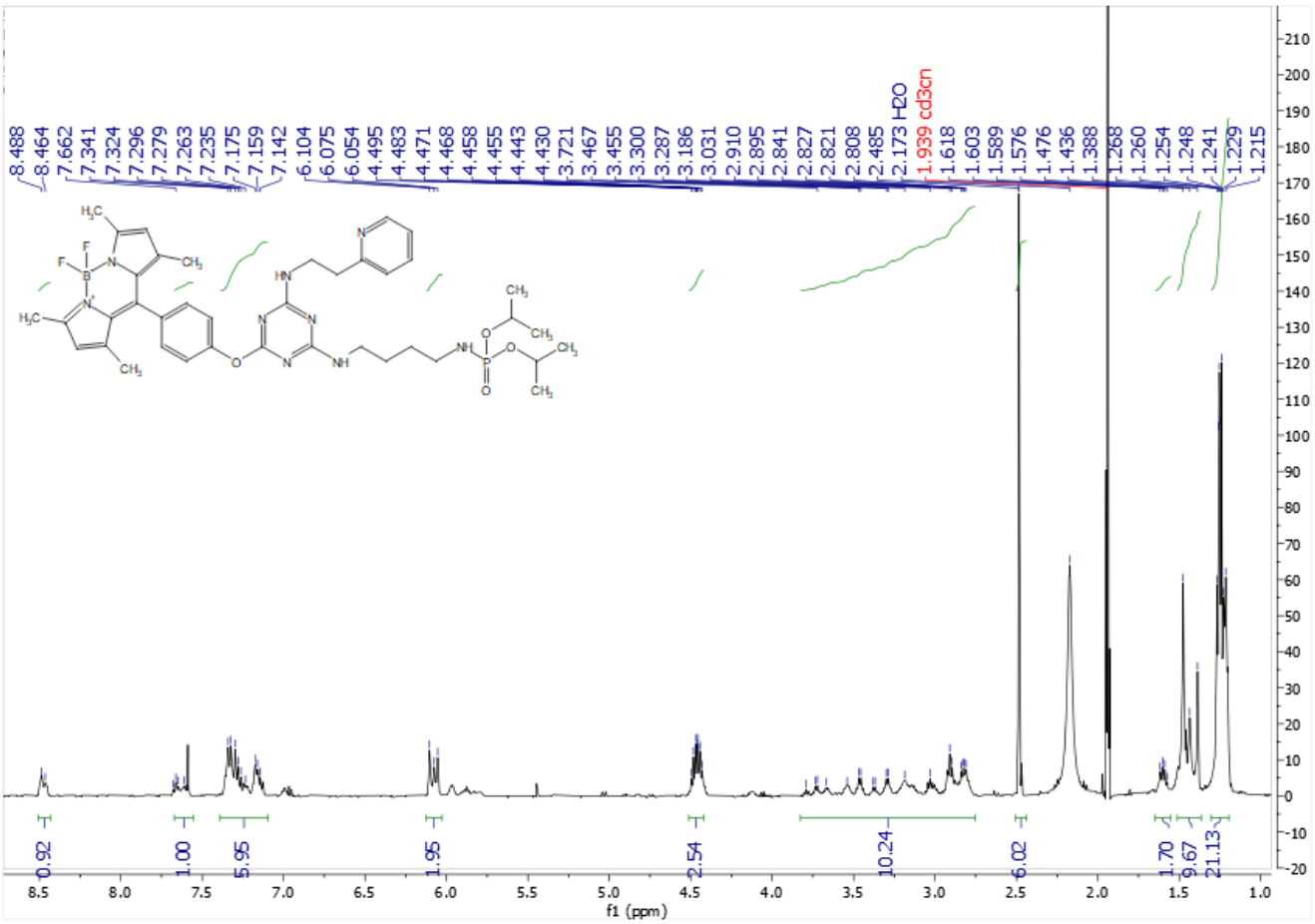

Figure S39 – ^{1}H NMR spectrum (500 MHz) of **5b** in CD_3CN.

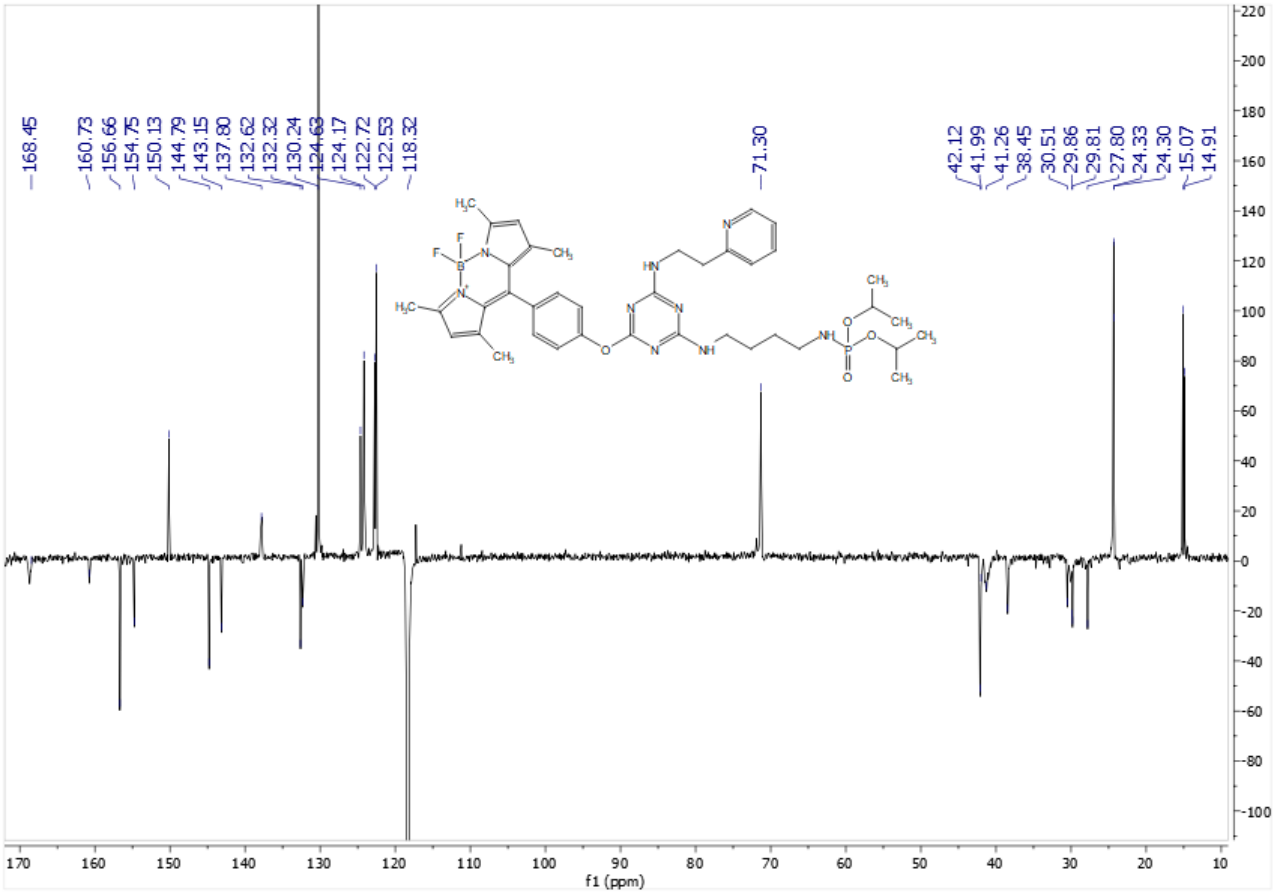

Figure S40 – ^{13}C-APT NMR spectrum (125 MHz) of **5b** in CD_3CN.

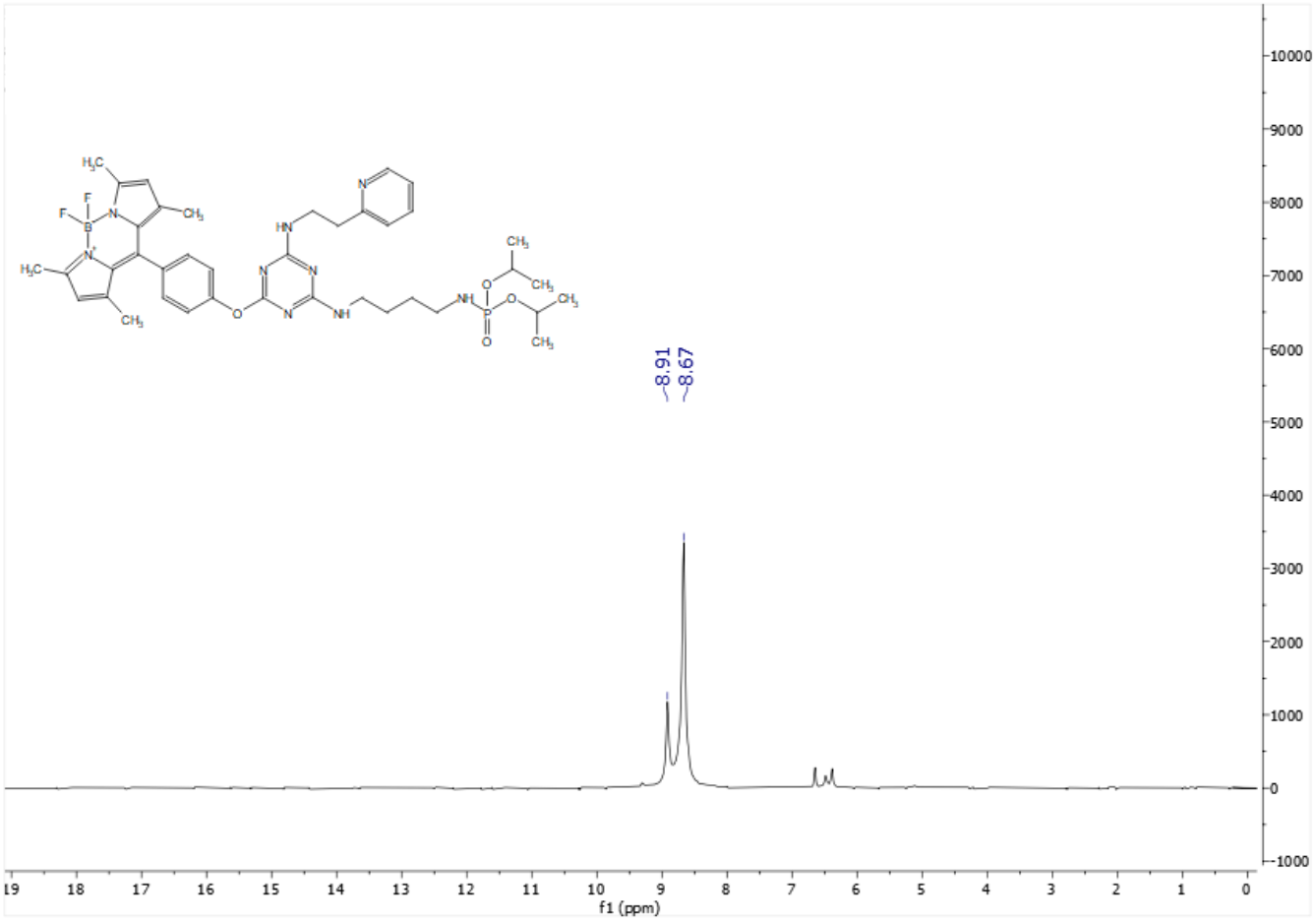

Figure S41 – ^{31}P NMR spectrum (202 MHz) of **5b** in CD_3CN.

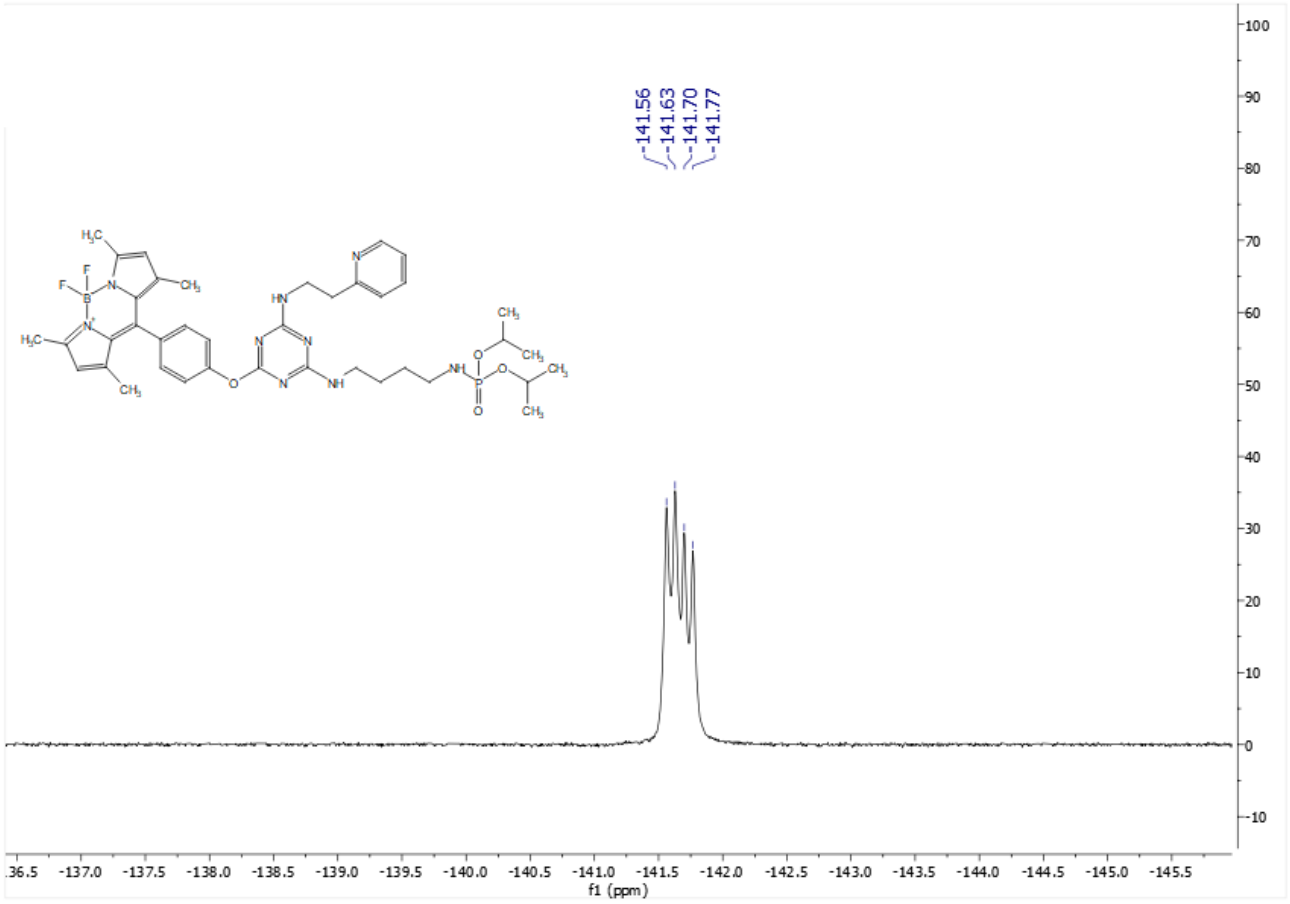

Figure S42 – ^{19}F NMR spectrum (470 MHz) of **5b** in CD_3CN.

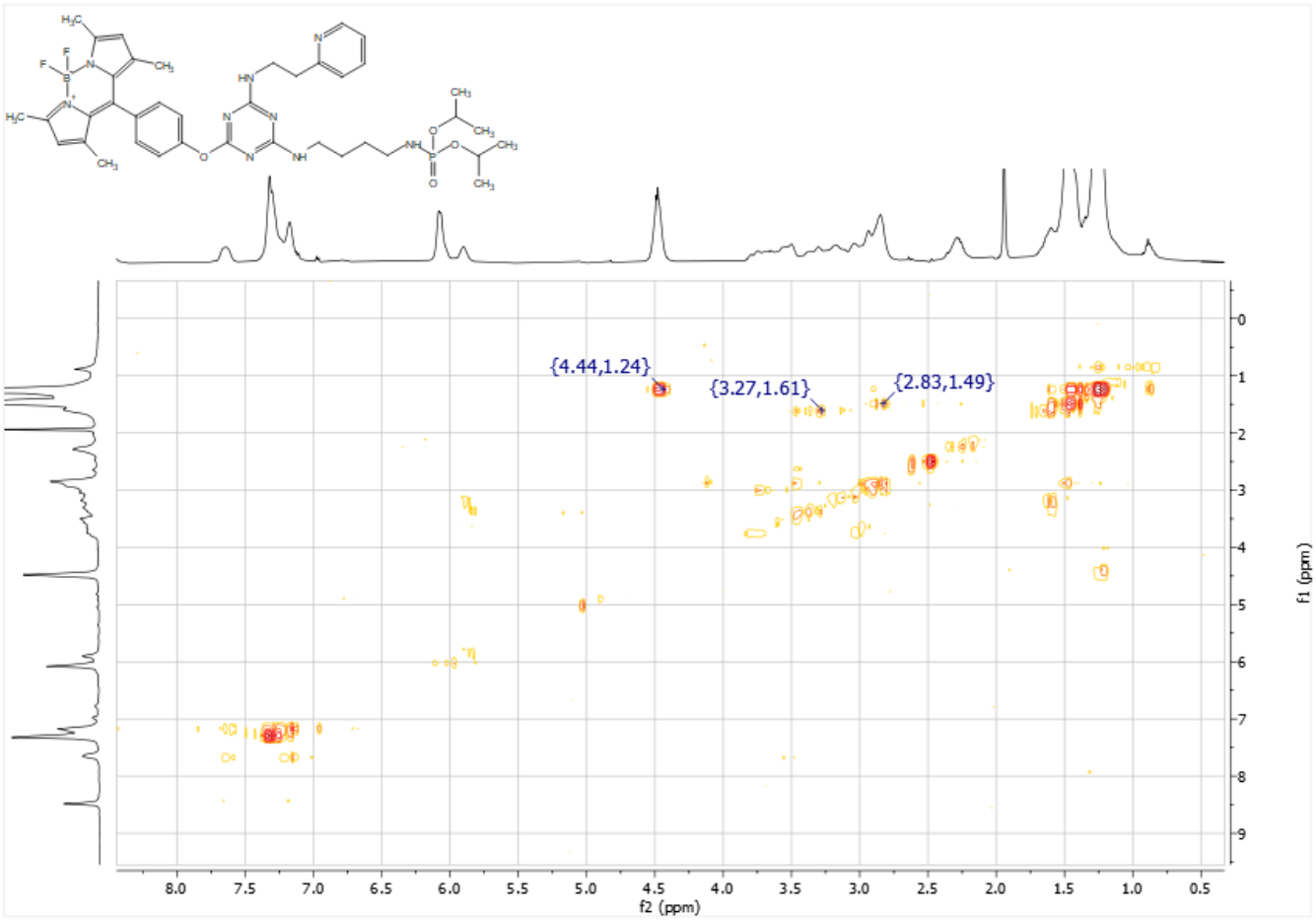

Figure S43 – ^{1}Hx^{1}H-COSY of **5b**.

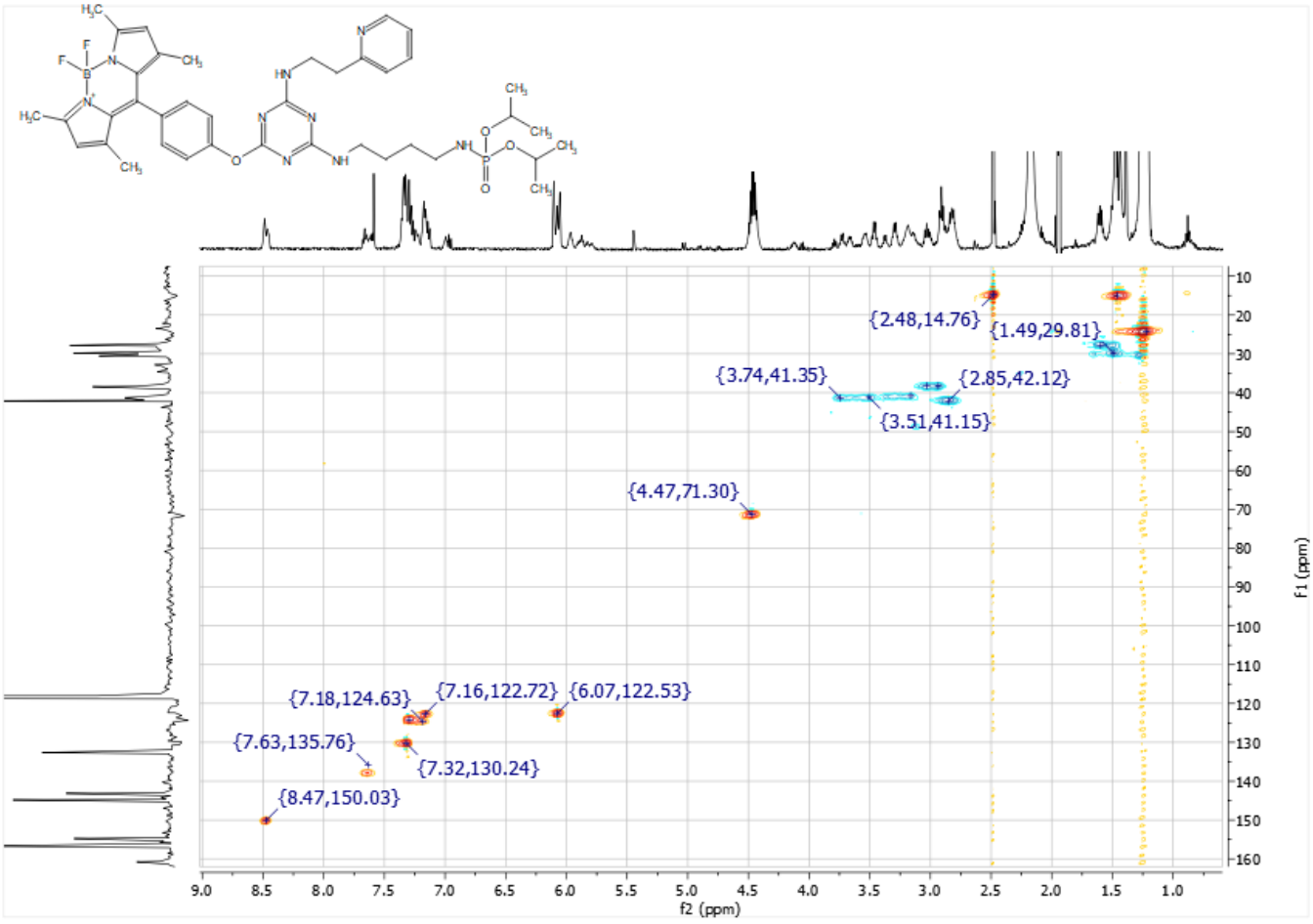

Figure S44 – ^{1}Hx^{13}C - HSQC spectrum of **5b**.

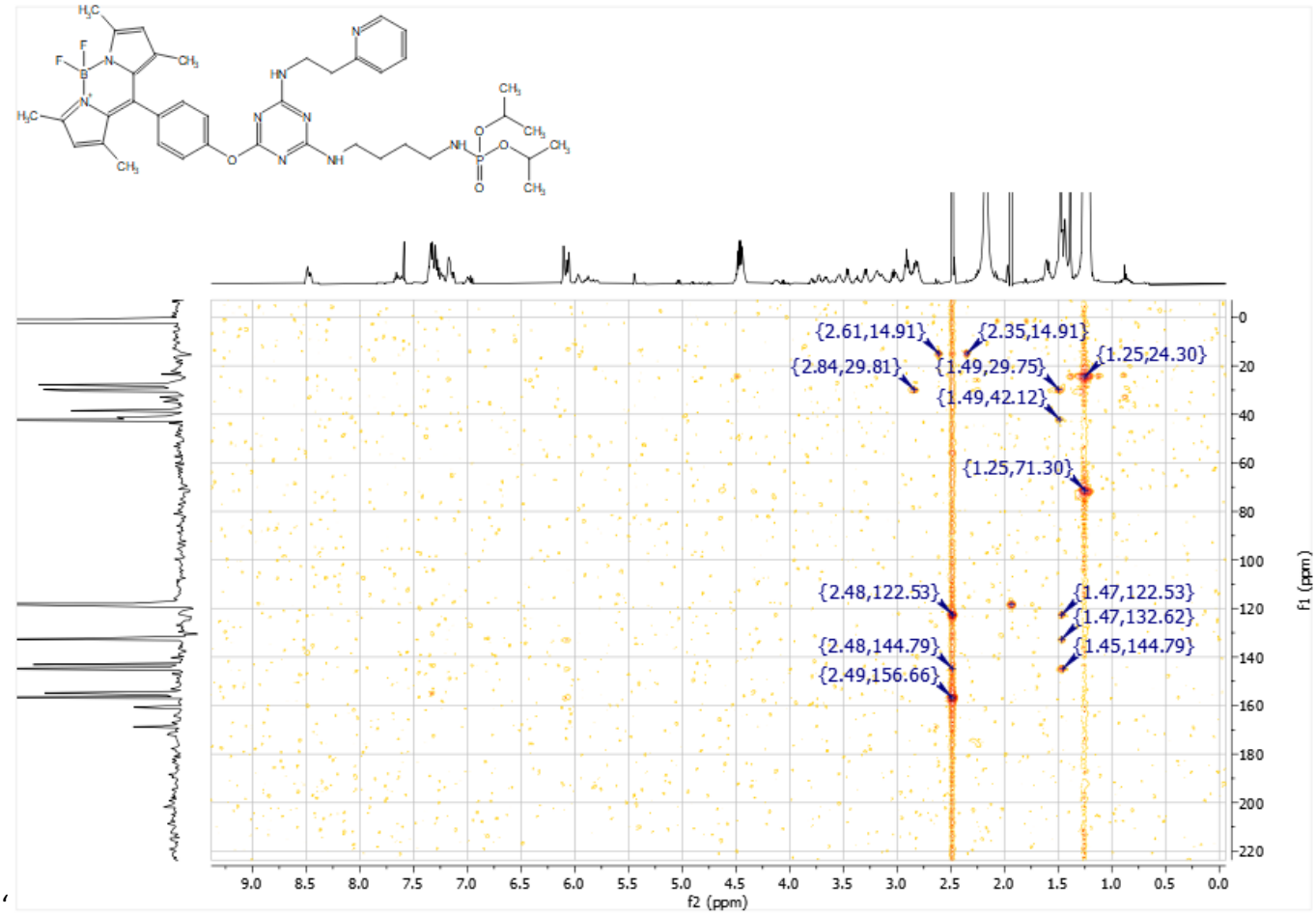

Figure S45 – $^{1}Hx^{13}C$ – HMBC spectrum of **5b**.

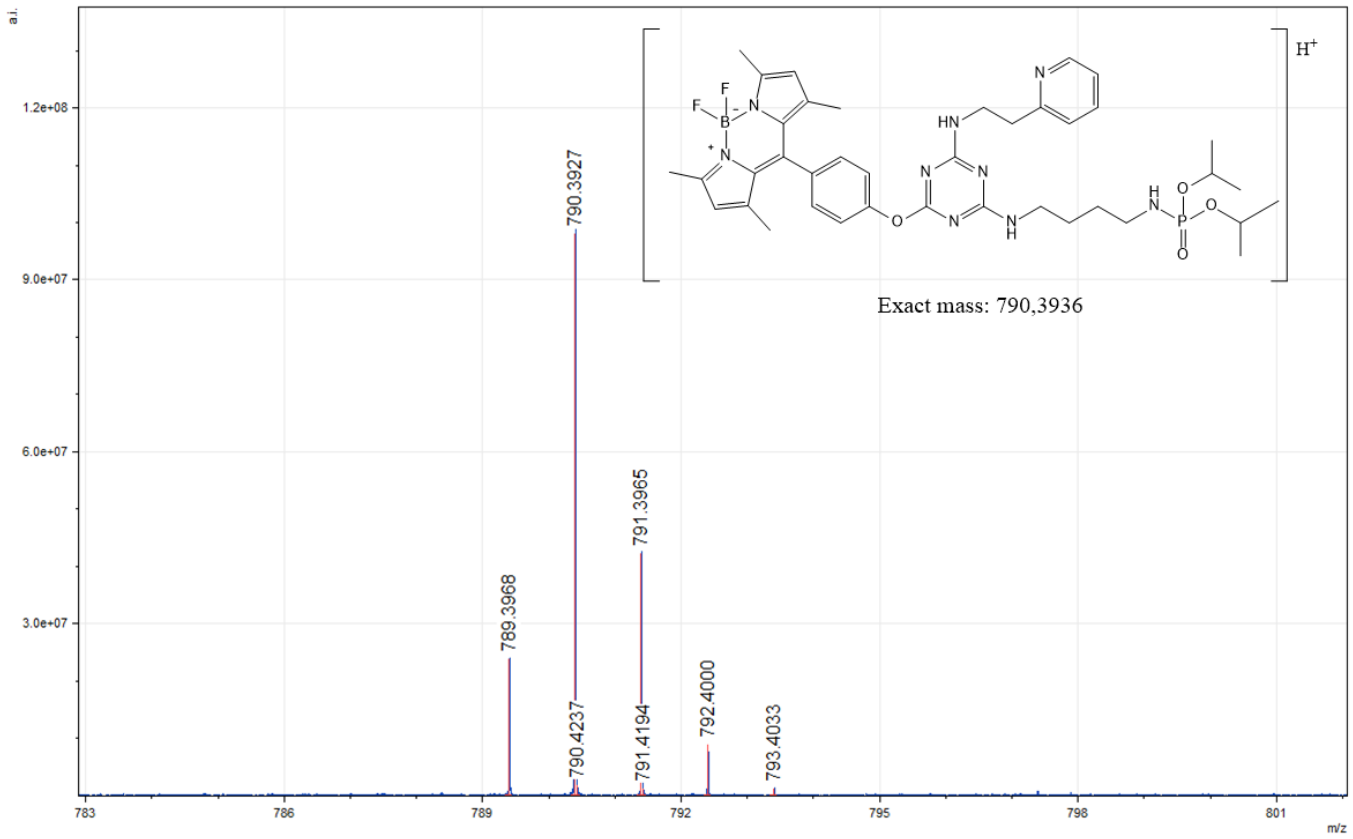

Figure S46 – HRMS spectrum of **5b**.

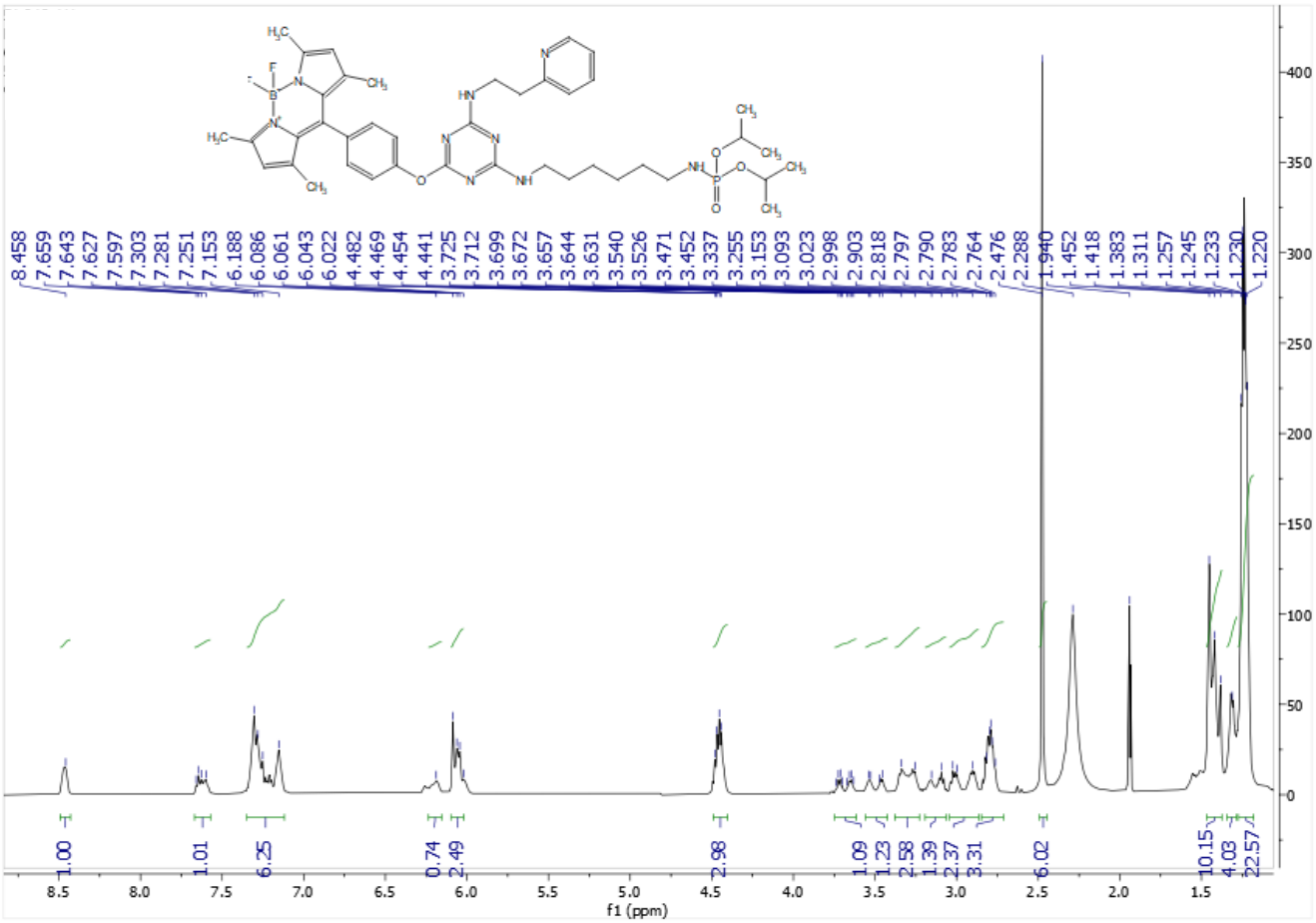

Figure S47 – ^{1}H NMR spectrum (500 MHz) of **5c** in CD_3CN.

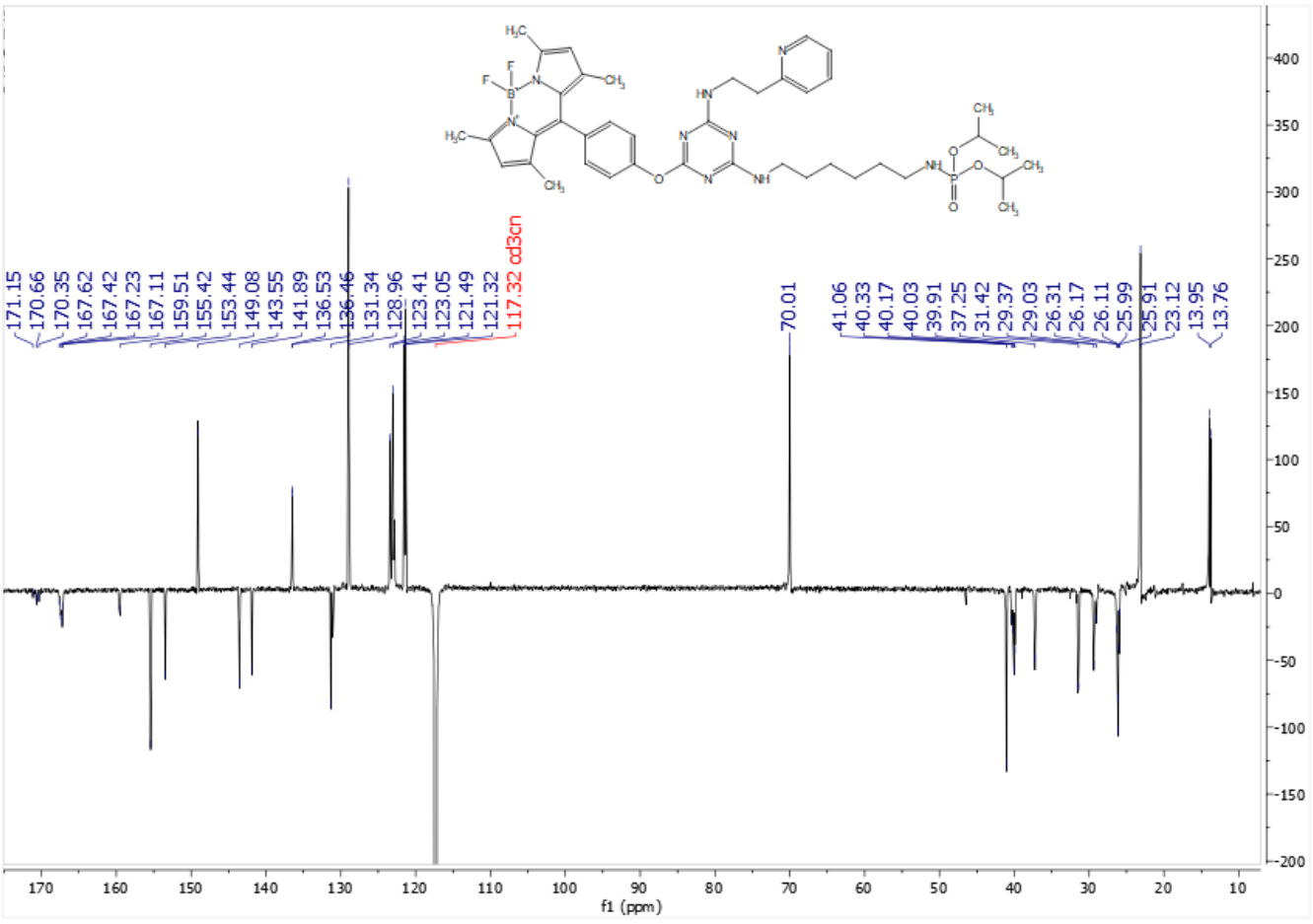

Figure S48 – ^{13}C-APT NMR spectrum (125 MHz) of **5c** in CD_3CN.

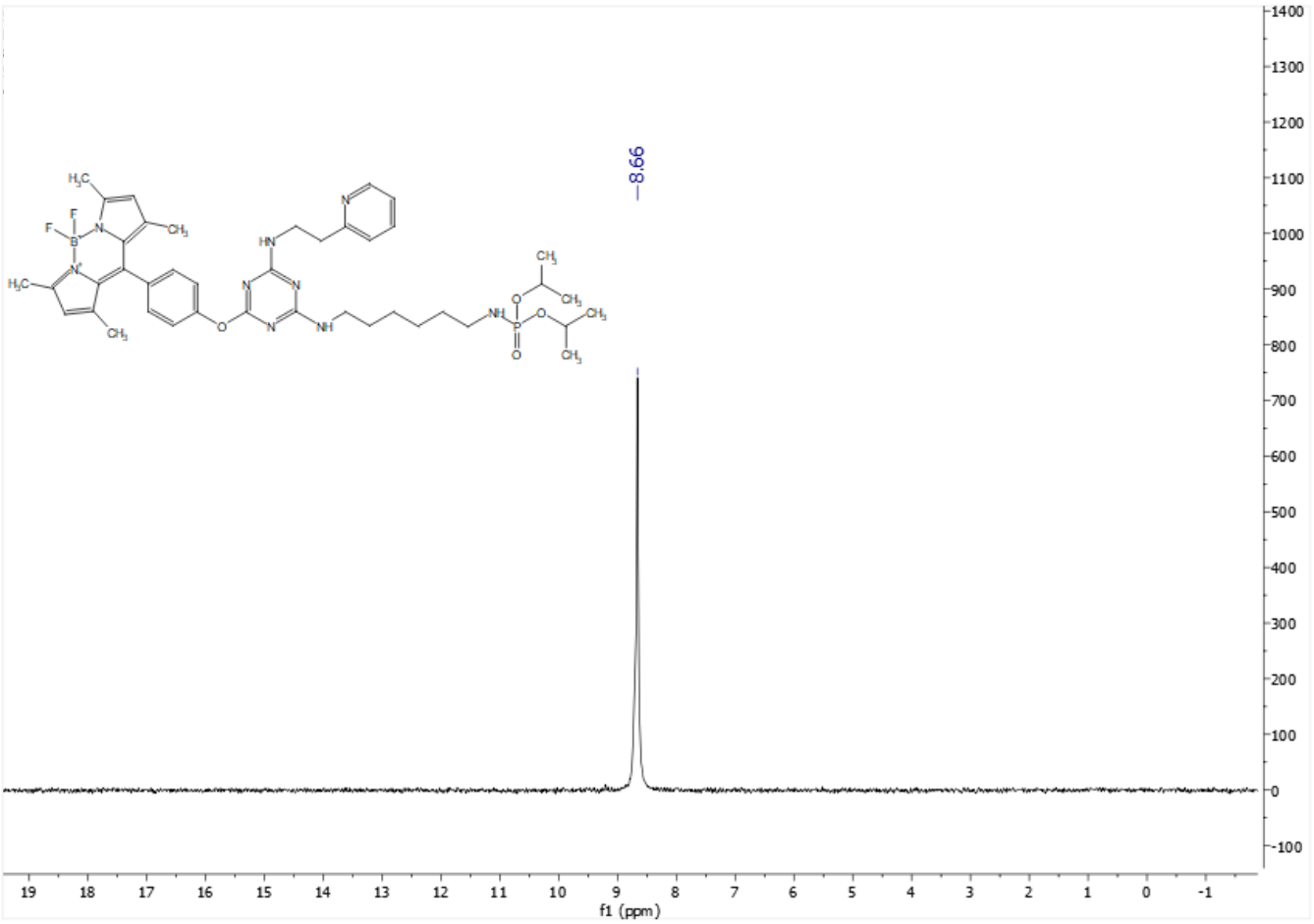

Figure S49 – ^{31}P NMR spectrum (202 MHz) of **5c** in CD_3CN.

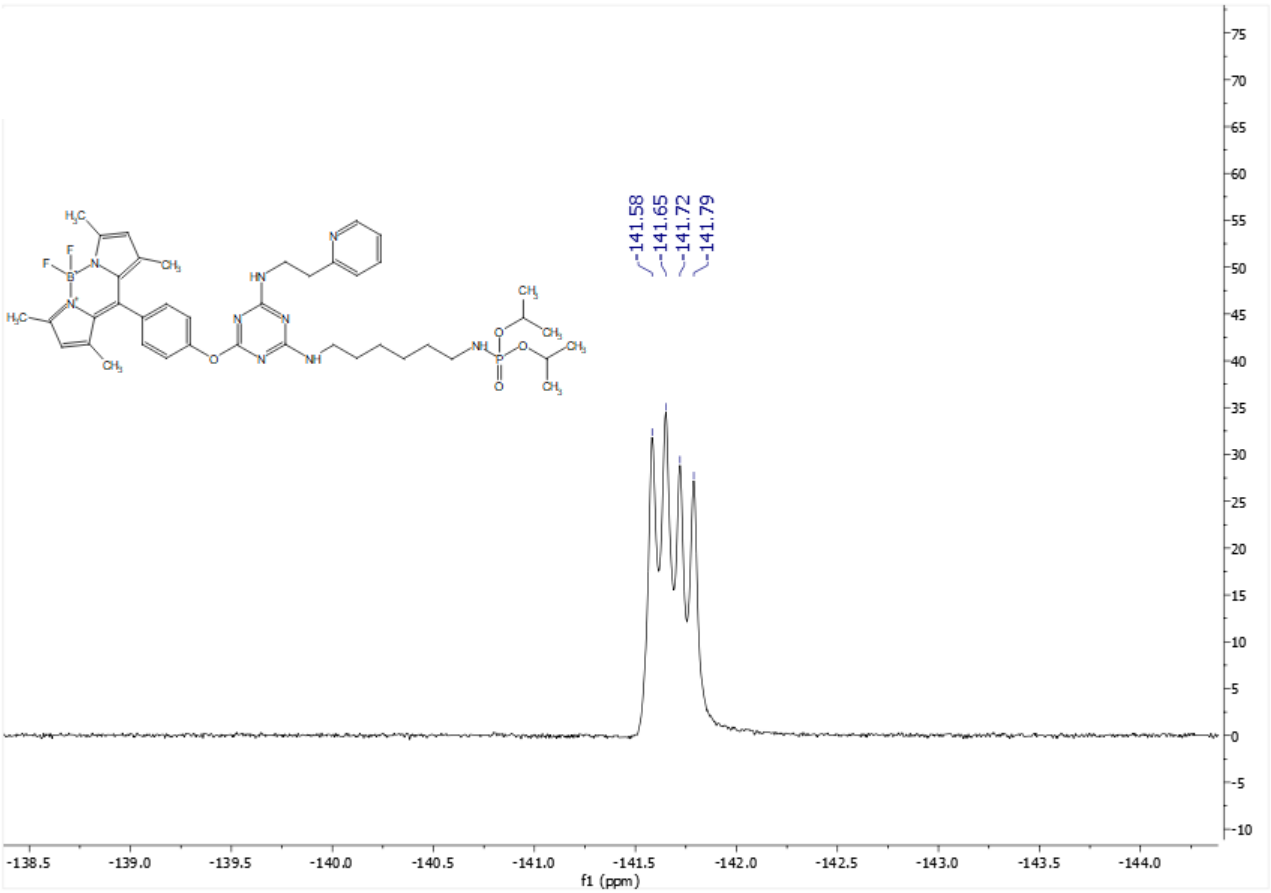

Figure S50 – ^{19}F NMR spectrum (470 MHz) of **5c** in CD_3CN.

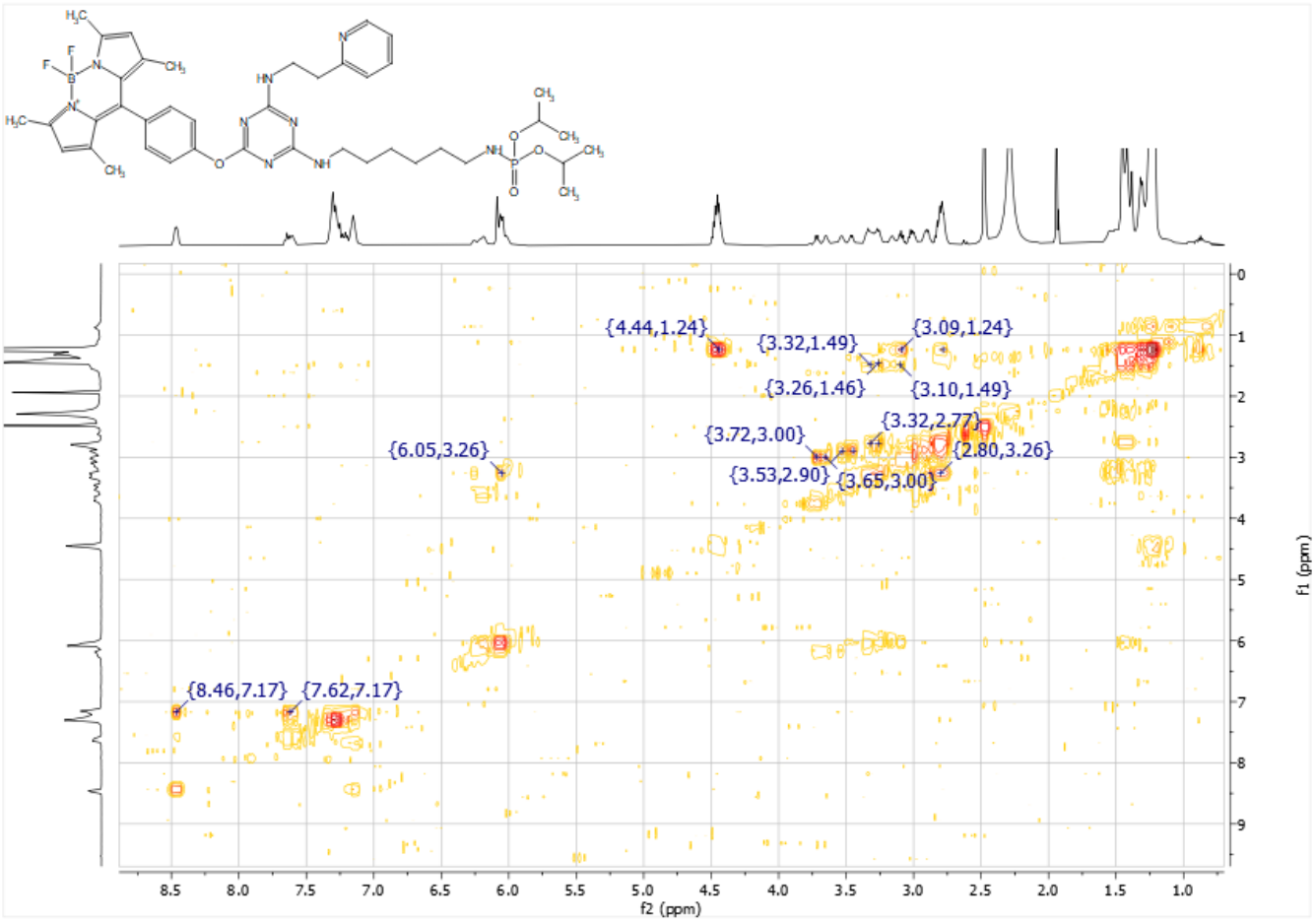

Figure S51 – ^{1}Hx^{1}H-COSY spectrum of **5c**.

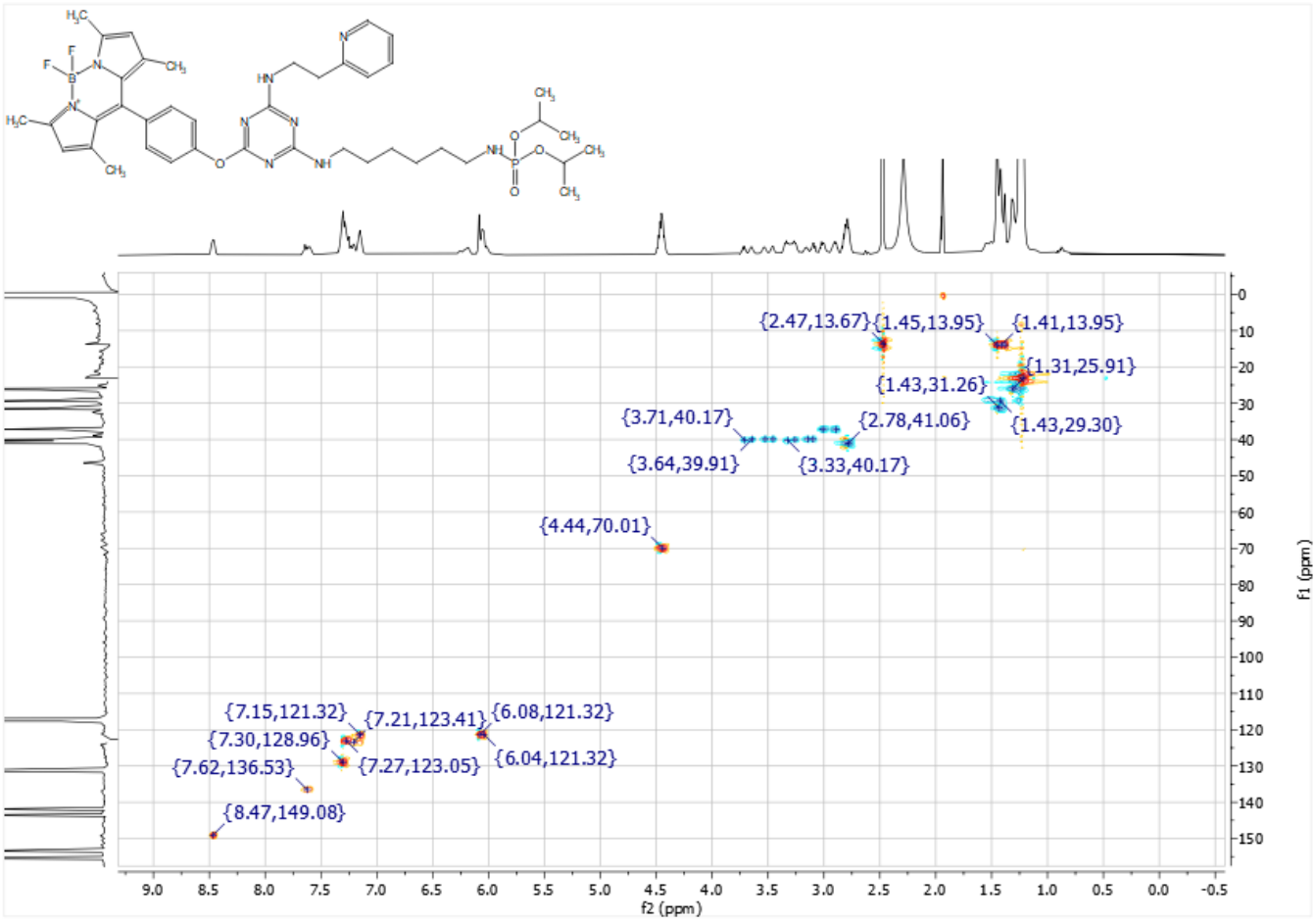

Figure S52 – ^{1}Hx^{13}C - HSQC spectrum of **5c**.

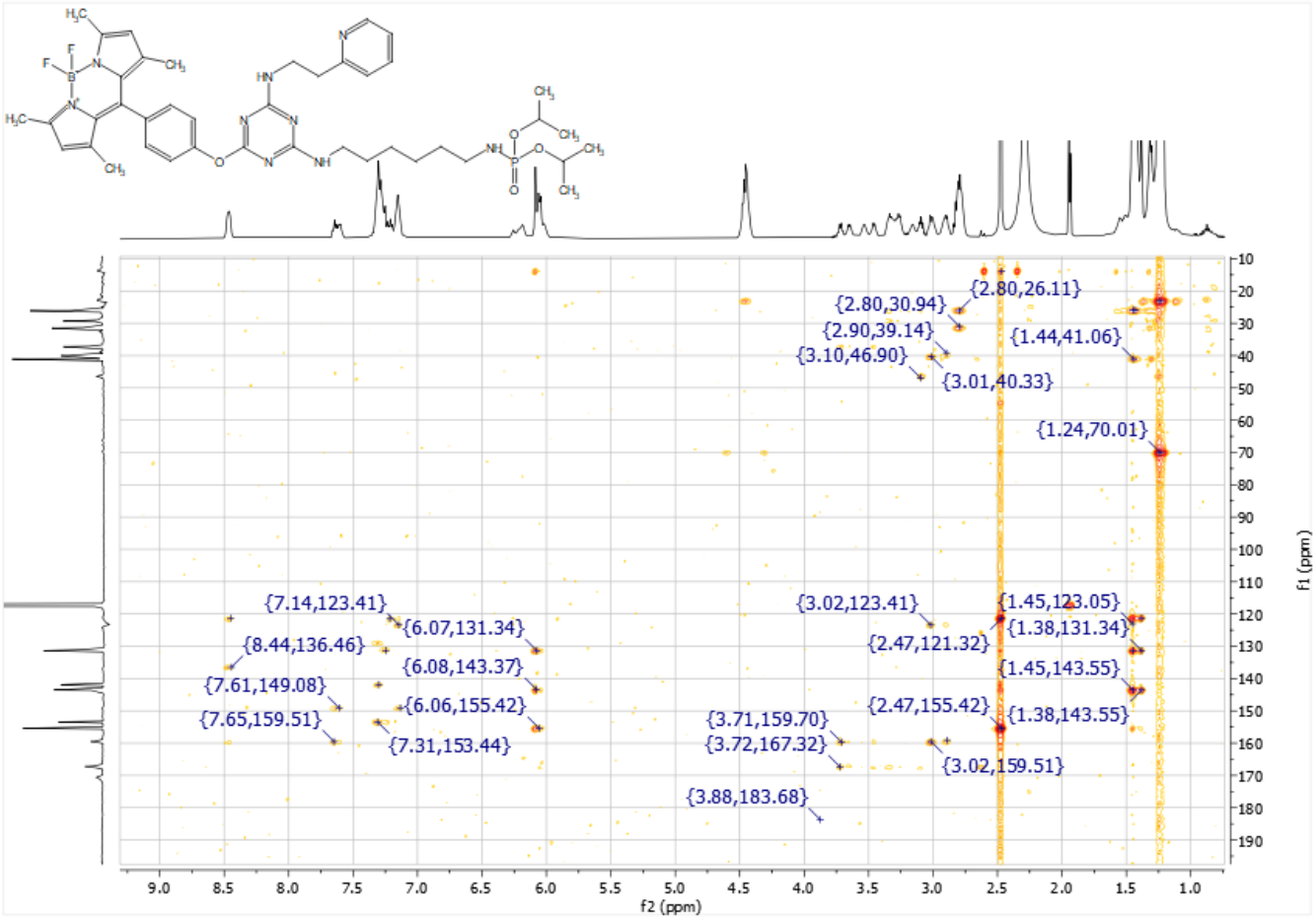

Figure S53 – $^{1}Hx^{13}C$ – HMBC spectrum of **5c**.

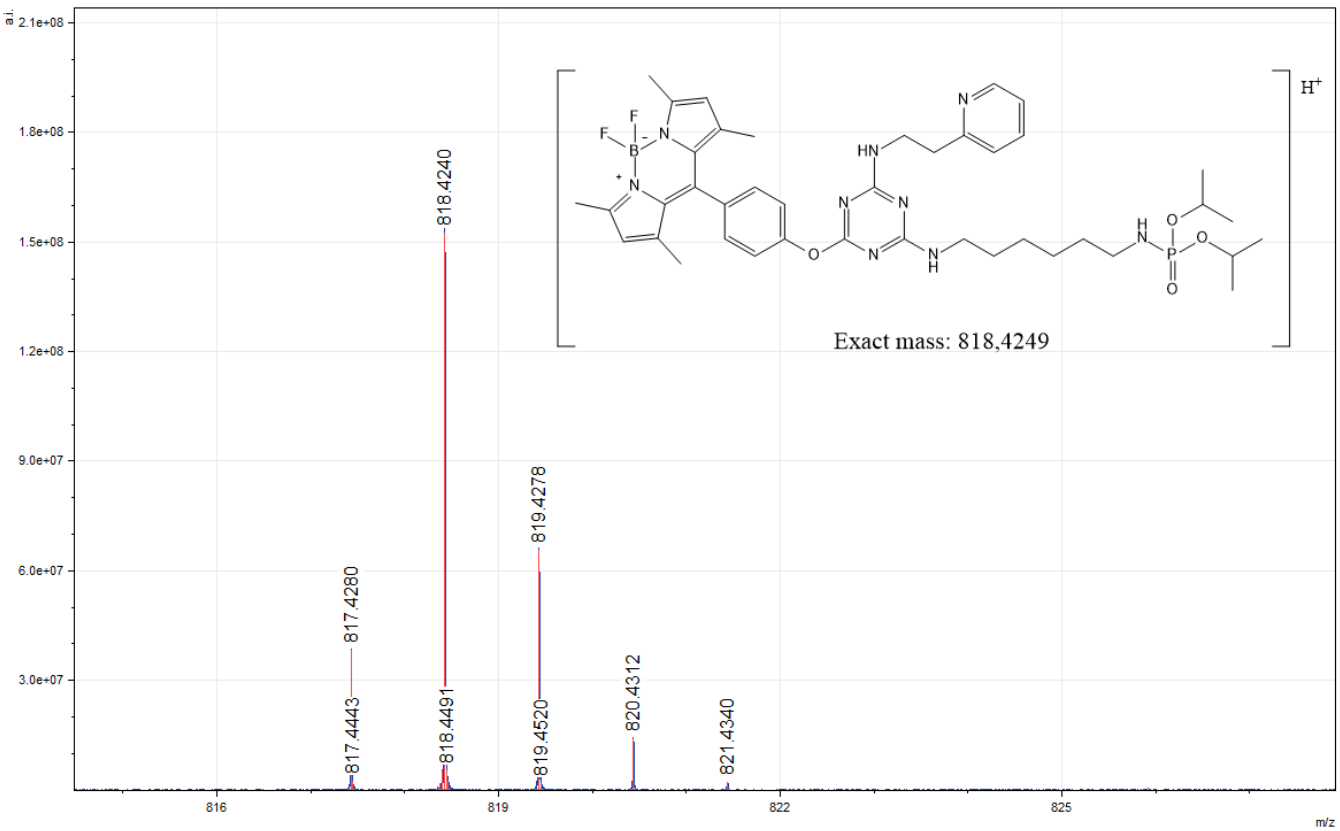

Figure S54 – HRMS spectrum of **5c**.

2. THEORETICAL EVALUATIONS

2.1 Rotational isomerism

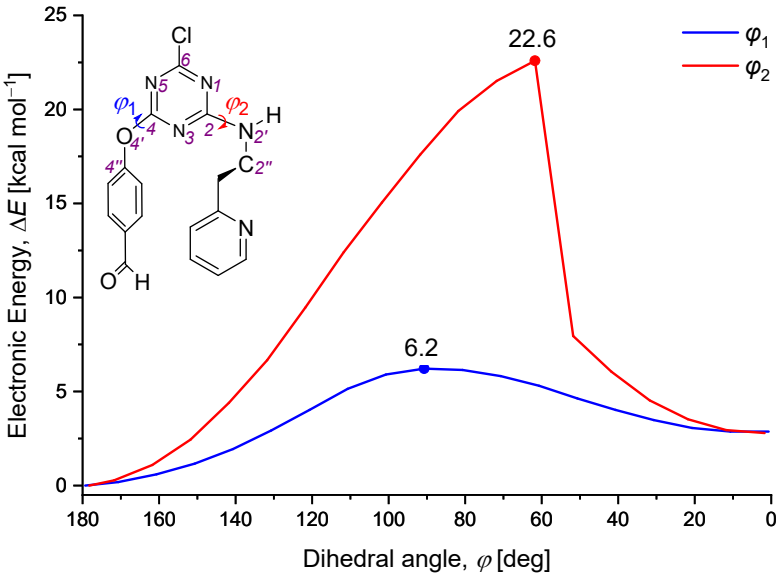

Figure S55: Evaluated dihedral angles for the bond rotations C_4–$O_{4'}$ (φ_1 = N_5–C_4–$O_{4'}$–$C_{4'}$) and C_2–$N_{2'}$ (φ_2 = N_1–C_2–$O_{2'}$–$C_{2''}$) of compound **3**. Energy profile (in kcal mol^{-1}) obtained from the relaxed scan of φ_1 and φ_2, ranging from 180° to 0°, at B3LYP-D3/def2-TZVP/IEFPCM=dichloromethane level.

2.2 Conformational analysis

Due to the high flexibility of the nucleophiles, particularly the nitrogenates, a conformational search was conducted at the molecular mechanics level using the Monte Carlo method in SPARTAN'10 software, employing the MMFF force field. This approach facilitated the identification of the lowest energy conformations constituting the conformational distribution of the system. The most stable conformers identified were subsequently subjected to full optimization using the DFT B3LYP-D3/def2-TZVP level. Notably, only a single conformation was identified for the nucleophiles BODIPY-OH (I) and p-hydroxybenzaldehyde (IV). In the case of 2-(pyridin-2-yl)ethanamine (III), the most stable conformation (***ii***, ΔH = –1.5 kcal mol^{-1}) featured a six-membered pseudo-ring with hydrogen bond (HB) donation from the -NH_2 unit (nucleophile site) to the pyridinic nitrogen — figure S56, (III). This suggests that the equilibrium is delocalized towards the most reactive conformation, characterized by the most nucleophilic -**N**H_2. For aminoalkyl phosphoramidates (II), only the IIa (n=2) and IIc (n=6) were evaluated. Regarding IIa, the less reactive form was more populated (***iii***, ΔH = –1.0 kcal mol^{-1}), wherein the nucleophile site exhibited an acceptor HB character. The most reactive form (***i***) was 0.7 kcal mol^{-1} less stable, being less populated in the conformational equilibrium (figure S56, (IIa)). In the case of IIc, evaluated in the final substitution step, all conformers presented a linear chair conformation, with no intramolecular HB capable of stabilizing the system.

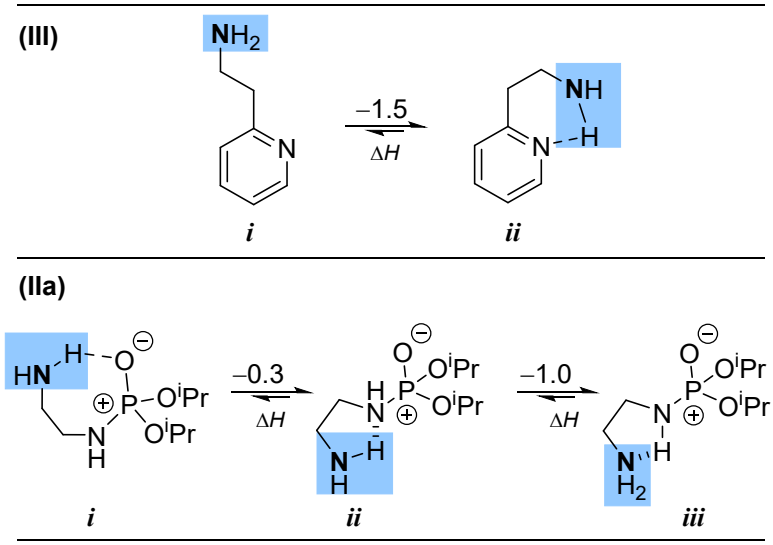

Figure S56: Bidimensional representation of the most stable conformer for the nitrogen nucleophiles depicting the intramolecular interactions obtained by DFT. Optimized structures at the B3LYP-D3/def2-TZVP/IEFPCM=dichloromethane level and nucleophilic site is highlighted in blue.

Table S1: Energies relative to isolated reactants (substrate + nucleophile) in kcal mol^{-1} for the stationary points of nucleophilic aromatic substitution reactions, calculated at the B3LYP-D3/def2-TZVP/IEFPCM level of theory.

Entry	Pre-reactive complex	Transition state	Final complex
		First substitution	
I	ΔE = –97.1; ΔH = –96.0; ΔG = –84.3	$\Delta E^{\ddagger}$ = –94.4; $\Delta H^{\ddagger}$ = –94.3; $\Delta G^{\ddagger}$ = –82.1	ΔE = –128.0; ΔH = –125.4; ΔG = –115.1
IIa	ΔE = –97.0; ΔH = –96.0; ΔG = –85.6	$\Delta E^{\ddagger}$ = –88.2; $\Delta H^{\ddagger}$ = –87.6; $\Delta G^{\ddagger}$ = –73.4	ΔE = –105.7; ΔH = –103.3; ΔG = –90.5
III	ΔE = –98.9; ΔH = –98.0; ΔG = –87.7	$\Delta E^{\ddagger}$ = –92.1; $\Delta H^{\ddagger}$ = –91.5; $\Delta G^{\ddagger}$ = –78.2	ΔE = –123.5; ΔH = –123.6; ΔG = –112.6
IV	ΔE = –96.4; ΔH = –95.5; ΔG = –84.3	$\Delta E^{\ddagger}$ = –89.3; $\Delta H^{\ddagger}$ = –89.3; $\Delta G^{\ddagger}$ = –76.9	ΔE = –120.4; ΔH = –118.1; ΔG = –108.1
		Second substitution	
Via (IV)	ΔE = –7.4; ΔH = –6.1; ΔG = 5.7	$\Delta E^{\ddagger}$ = 9.2; $\Delta H^{\ddagger}$ = 9.4; $\Delta G^{\ddagger}$ = 21.0	ΔE = –28.7; ΔH = –25.9; ΔG = –14.4
Via (III)	ΔE = –12.2; ΔH = –10.8; ΔG = 1.3	$\Delta E^{\ddagger}$ = –2.7; $\Delta H^{\ddagger}$ = –1.6; $\Delta G^{\ddagger}$ = 12.7	ΔE = –34.5; ΔH = –34.3; ΔG = –22.8
		Third substitution	
IIc	ΔE = –12.6; ΔH = –10.7; ΔG = 2.9	$\Delta E^{\ddagger}$ =4.5; $\Delta H^{\ddagger}$ = 5.9; $\Delta G^{\ddagger}$ = 21.9	ΔE = –30.5; ΔH = –28.3; ΔG = –14.6

2.3 Nucleophilic substitutions at cyanuric chloride

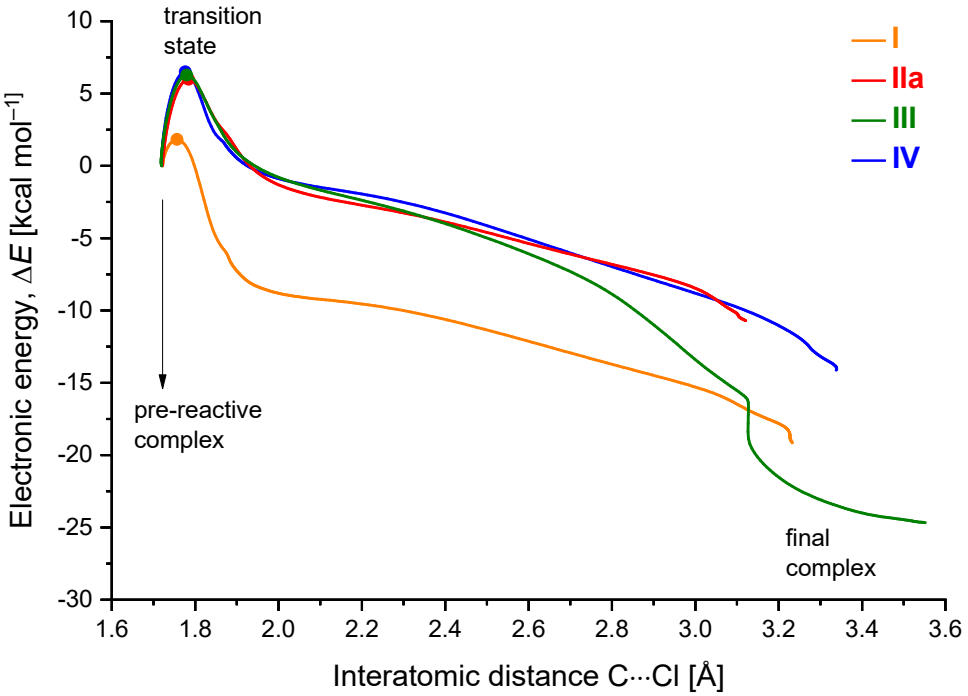

Figure S57: Minimum energy path along the interatomic distance carbon—nucleofuge (Cl) obtained from the intrinsic reaction coordinate calculations (at B3LYP-D3/def2-TZVP/IEFPCM=dichloromethane) for the first chlorine substitution.

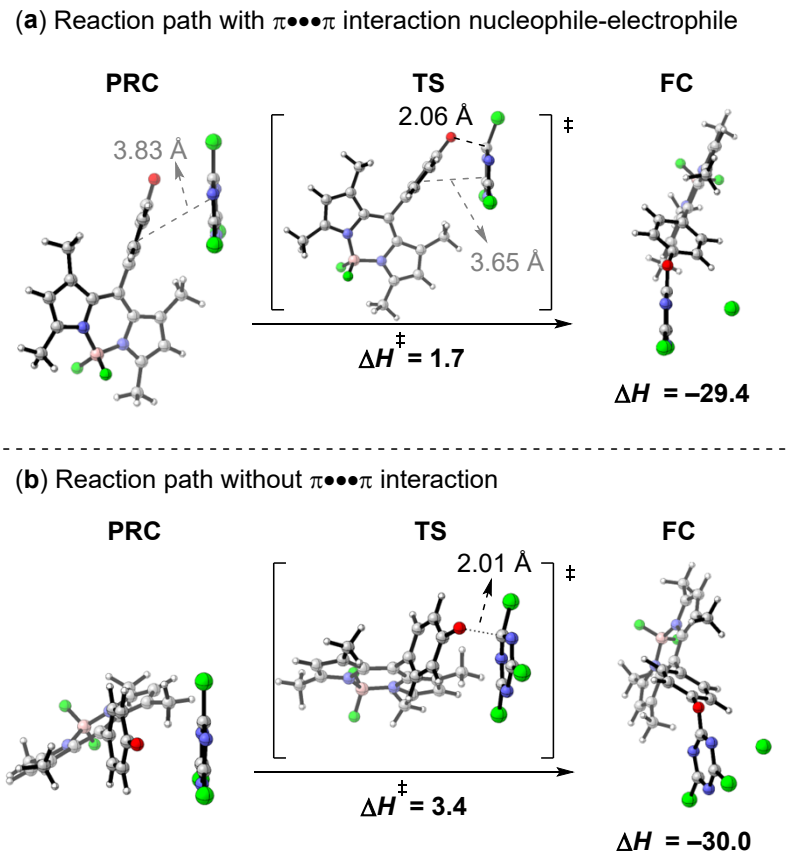

Figure S58: Optimized structures of the stationary points for the substitution with BODIPY (**I**) calculated (**a**) with and (**b**) without π_{I}•••$\pi_{electrophile}$ interactions (in gray). Energy profile in terms of relative enthalpy (kcal mol^{-1}) calculated at B3LYP-D3/def2-TZVP/IEFPCM=dichloromethane. PRC: Pre-reactive complex, TS: Transition state structure, FC: Final complex.

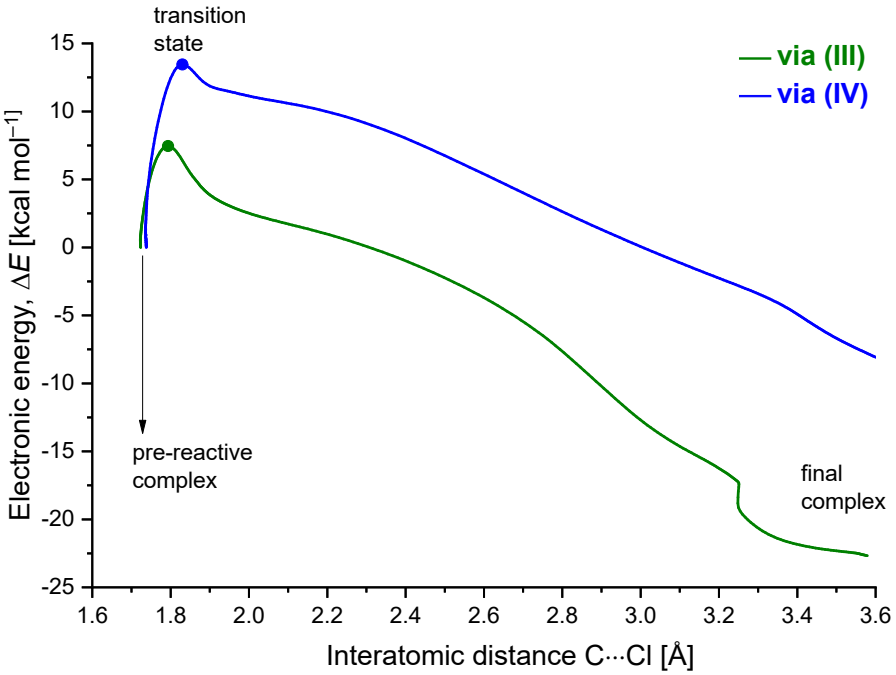

Figure S59: Minimum energy path along the interatomic distance carbon—nucleofuge (Cl) obtained from the intrinsic reaction coordinate calculations (at B3LYP-D3/def2-TZVP/IEFPCM=dichloromethane) for the second chlorine substitution.

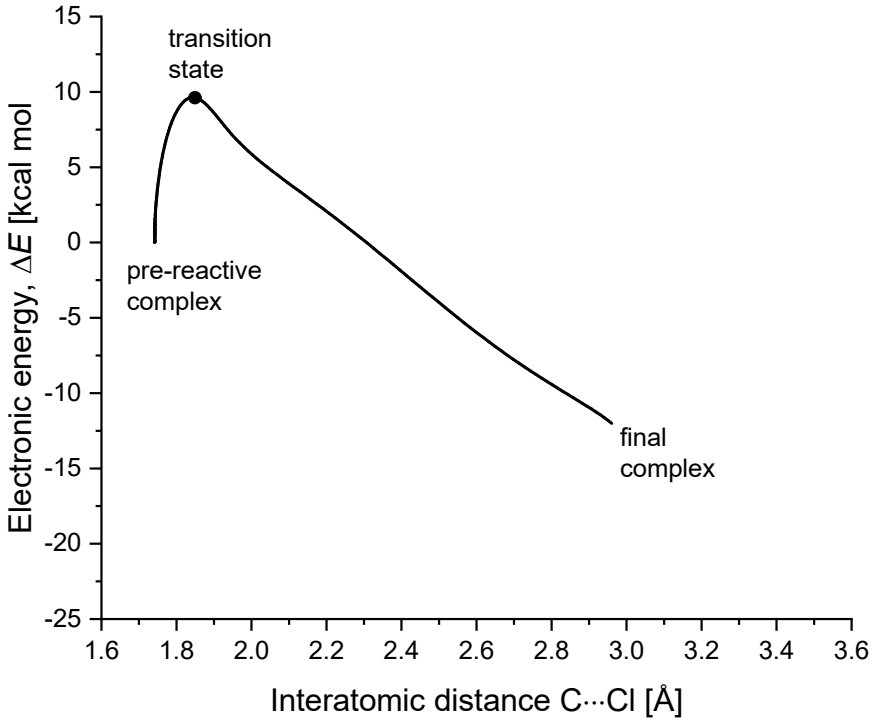

Figure S60: Minimum energy path along the interatomic distance carbon—nucleofuge (Cl) obtained from the intrinsic reaction coordinate (at B3LYP-D3/def2-TZVP/IEFPCM=tetrahydrofuran,) for the third chlorine substitution.

2.4 Cartesian coordinate matrices of relevant stationary points

Rotational isomerism:

Rotamer ***a***

N	-3.708275000	1.003115000	-0.203691000	C	2.304609000	2.597090000	0.276113000
C	-2.383145000	0.986383000	-0.042962000	C	1.483218000	2.533745000	1.404381000
N	-1.628995000	-0.060892000	0.209832000	C	0.112206000	2.381092000	1.266917000
C	-2.297779000	-1.223993000	0.318071000	C	3.762029000	2.708515000	0.451151000
N	-3.641460000	-1.338628000	0.170780000	H	4.097416000	2.804961000	1.501475000
C	-4.243669000	-0.202576000	-0.080938000	O	4.572279000	2.684527000	-0.453113000
Cl	-5.975688000	-0.280052000	-0.281488000	H	-2.131894000	-3.192453000	0.617819000
O	-1.802065000	2.191710000	-0.172802000	H	0.149680000	-1.501613000	1.322770000
N	-1.607009000	-2.332715000	0.591582000	H	0.095072000	-3.262907000	1.305084000
C	-0.159381000	-2.368348000	0.739089000	H	0.339323000	-3.293998000	-1.145728000
C	0.574986000	-2.371594000	-0.611783000	H	0.214496000	-1.530944000	-1.204863000
C	2.062843000	-2.263521000	-0.416251000	H	2.163159000	-0.169634000	-0.888427000
C	2.721101000	-1.045190000	-0.586701000	H	4.617233000	-0.038053000	-0.495784000
C	4.088988000	-0.973755000	-0.363628000	H	5.826140000	-2.122680000	0.212009000
C	4.760129000	-2.125176000	0.028464000	H	4.515551000	-4.213358000	0.483848000
C	4.024539000	-3.294821000	0.179445000	H	-0.090204000	2.309971000	-2.123854000
N	2.709111000	-3.373155000	-0.034043000	H	2.384921000	2.579475000	-1.867224000
C	-0.421129000	2.292063000	-0.009472000	H	1.921757000	2.596060000	2.392897000
C	0.371430000	2.374204000	-1.148183000	H	-0.539269000	2.320221000	2.127378000
C	1.738690000	2.526195000	-1.001383000				

E = – 1541.1542052 a. u.
H = – 1540.839169 a. u.
G = – 1540.915144 a. u.

Transition state

N	-0.654715000	2.998480000	-0.577890000	C	-4.573468000	-1.862773000	-0.265525000
C	-1.240833000	1.856203000	-0.222584000	C	-3.420360000	-1.862834000	-1.054846000
N	-0.749653000	0.952204000	0.617102000	C	-2.682806000	-0.701000000	-1.220242000
C	0.442496000	1.246339000	1.126694000	C	-5.339210000	-3.111748000	-0.104366000
N	1.126998000	2.362047000	0.839823000	H	-4.919279000	-3.985195000	-0.639360000
C	0.518742000	3.177186000	-0.003844000	O	-6.353729000	-3.222718000	0.552180000
Cl	1.355877000	4.644866000	-0.403715000	H	1.108249000	0.733148000	2.926037000
O	-2.434128000	1.654928000	-0.787625000	H	3.036137000	0.610741000	1.369418000
N	1.013378000	0.302255000	2.011192000	H	2.733180000	-0.792463000	2.401047000
C	2.332377000	-0.204066000	1.576385000	H	1.501470000	-1.906663000	0.565271000
C	2.196102000	-1.095648000	0.339335000	H	1.776335000	-0.519625000	-0.488676000
C	3.528558000	-1.669163000	-0.064384000	H	3.838719000	-0.339514000	-1.726480000
C	4.248600000	-1.153561000	-1.142737000	H	6.062280000	-1.313013000	-2.287185000
C	5.487981000	-1.696630000	-1.453447000	H	6.933038000	-3.196977000	-0.879946000
C	5.974103000	-2.739810000	-0.676351000	H	5.536333000	-4.004387000	1.008021000
C	5.190744000	-3.189810000	0.379891000	H	-4.555998000	1.407099000	0.676779000
N	3.999201000	-2.674341000	0.686344000	H	-5.883861000	-0.695243000	0.967029000
C	-3.112072000	0.450930000	-0.580030000	H	-3.100709000	-2.776217000	-1.541699000
C	-4.257599000	0.481778000	0.203758000	H	-1.788059000	-0.681364000	-1.826278000
C	-4.988581000	-0.682937000	0.360082000				

E = – 1541.1179898 a. u.
H = – 1540.805072 a. u.
G = – 1540.881297 a. u.
f = 72.2226i

Rotamer ***b***

N	0.846805000	2.788729000	0.048663000	C	5.458674000	-1.433531000	0.210937000
C	1.522935000	1.632333000	0.043023000	C	4.998526000	-0.914801000	1.422898000
N	1.028720000	0.428629000	-0.131679000	C	4.101944000	0.144385000	1.438066000
C	-0.307734000	0.393118000	-0.329544000	C	6.408890000	-2.558994000	0.221991000
N	-1.097367000	1.490931000	-0.342370000	H	6.692800000	-2.915342000	1.231116000
C	-0.446382000	2.614447000	-0.150091000	O	6.871066000	-3.087196000	-0.768344000
Cl	-1.414619000	4.067057000	-0.154834000	H	-0.250151000	-1.594530000	-0.463354000
O	2.841180000	1.785923000	0.251458000	H	-2.695393000	-0.246200000	-1.349255000
N	-0.868258000	-0.801391000	-0.529589000	H	-2.416196000	-1.981434000	-1.215109000
C	-2.294547000	-1.027438000	-0.704374000	H	-2.654005000	-1.844046000	1.256885000
C	-3.059809000	-1.048800000	0.628502000	H	-2.904260000	-0.097673000	1.138424000
C	-4.527548000	-1.289845000	0.400480000	H	-5.123213000	0.753639000	0.707923000
C	-5.452941000	-0.247501000	0.462605000	H	-7.526865000	0.280080000	0.253299000
C	-6.791394000	-0.513031000	0.207326000	H	-8.197755000	-2.069135000	-0.310905000
C	-7.167133000	-1.812757000	-0.105779000	H	-6.433776000	-3.815394000	-0.388712000
C	-6.178182000	-2.788480000	-0.148699000	H	3.770236000	0.622651000	-1.909985000
N	-4.889672000	-2.543684000	0.095564000	H	5.383554000	-1.286924000	-1.928538000
C	3.675415000	0.670109000	0.229746000	H	5.343500000	-1.341688000	2.356905000
C	4.124243000	0.176776000	-0.990801000	H	3.733676000	0.563085000	2.364299000
C	5.016177000	-0.879222000	-0.996259000				

E = – 1541.1497637 a. u.
H = – 1540.834915 a. u.
G = – 1540.913115 a. u.

First substitution: **nucleophile BODIPY-OH (I)**

Pre-reactive complex with π-π interaction (I):

B	-4.637338000	-0.429475000	0.206852000	H	-0.891367000	3.892808000	-0.120785000
F	-5.675268000	-0.572522000	-0.740835000	C	-6.241810000	2.149855000	0.540040000
F	-5.174687000	-0.699920000	1.485141000	H	-6.432201000	1.642393000	1.487259000
Cl	2.474244000	-0.286453000	2.969520000	H	-6.822621000	1.627928000	-0.222742000
C	3.984772000	-1.415895000	-0.336143000	H	-6.595936000	3.177132000	0.610703000
N	4.420540000	0.504220000	1.425203000	C	-2.143833000	-1.048578000	-0.284137000
C	5.144021000	0.350519000	0.324635000	C	-1.382083000	-2.250946000	-0.279451000
O	3.517346000	1.996907000	-1.212217000	C	-2.298010000	-3.294019000	-0.141303000
C	2.330036000	1.595151000	-1.010644000	H	-2.063075000	-4.346310000	-0.099325000
C	1.585023000	1.950478000	0.166861000	C	-3.577764000	-2.749080000	-0.030635000
H	2.083069000	2.564997000	0.907366000	C	0.096528000	-2.452579000	-0.332888000
C	0.289391000	1.536623000	0.361952000	H	0.347995000	-3.433909000	0.072108000
H	-0.242289000	1.843528000	1.255516000	H	0.634215000	-1.697117000	0.235502000
C	-0.370557000	0.699041000	-0.557947000	H	0.487860000	-2.407998000	-1.350374000
C	0.351073000	0.300525000	-1.700068000	C	-4.865377000	-3.467305000	0.180061000
C	1.634564000	0.736105000	-1.932732000	H	-5.296378000	-3.211747000	1.149963000
H	2.158667000	0.445065000	-2.835736000	H	-4.704670000	-4.543415000	0.138263000
C	-1.762469000	0.310877000	-0.346564000	H	-5.599244000	-3.186879000	-0.577205000
C	-2.742719000	1.319088000	-0.187157000	N	-4.059785000	0.995989000	0.156104000
C	-2.690332000	2.725477000	-0.399125000	N	-3.487815000	-1.404340000	-0.110397000
C	-3.970179000	3.209630000	-0.124593000	N	3.191533000	-1.389915000	0.724996000
H	-4.289495000	4.238332000	-0.188602000	C	3.461150000	-0.396150000	1.556856000
C	-4.790315000	2.130934000	0.207195000	N	4.988151000	-0.596734000	-0.591486000
C	-1.576826000	3.582656000	-0.911421000	H	-0.139175000	-0.335310000	-2.428418000
H	-1.992156000	4.484555000	-1.364041000	Cl	3.689008000	-2.669542000	-1.488962000
H	-0.976168000	3.060766000	-1.655348000	Cl	6.476537000	1.421307000	0.116085000

E = – 2804.3248 a. u.
H = – 2803.9215 a. u.
G = – 2804.0196 a. u.

Transition state with π-π interaction (I):

B	-4.688945000	0.481184000	-0.038442000	H	-0.993232000	-3.692287000	-0.692028000
F	-5.536655000	0.696462000	1.066541000	C	-6.406294000	-2.051272000	-0.121252000
F	-5.420509000	0.734825000	-1.215360000	H	-6.734083000	-1.551638000	-1.034834000
Cl	3.192341000	1.284988000	-2.894747000	H	-6.827259000	-1.491263000	0.715577000
C	3.856031000	1.226178000	0.858025000	H	-6.804681000	-3.064078000	-0.108223000
N	4.487529000	-0.252819000	-1.233227000	C	-2.125568000	0.988066000	0.078159000
C	4.835544000	-0.594505000	0.026930000	C	-1.301844000	2.152860000	0.059519000
O	3.533773000	-2.146466000	0.381189000	C	-2.168682000	3.238144000	0.022941000
C	2.299879000	-1.725331000	0.312071000	H	-1.888372000	4.279484000	-0.001519000
C	1.590597000	-1.699196000	-0.914889000	C	-3.485474000	2.756164000	0.009606000
H	2.101577000	-2.044388000	-1.804558000	C	0.186672000	2.251799000	0.050750000
C	0.279377000	-1.259587000	-0.981496000	H	0.492709000	3.282919000	-0.123887000
H	-0.243860000	-1.270480000	-1.930724000	H	0.632245000	1.626160000	-0.720693000
C	-0.384829000	-0.802848000	0.159109000	H	0.625090000	1.926705000	0.994220000
C	0.306216000	-0.791683000	1.373635000	C	-4.746481000	3.544641000	-0.039063000
C	1.612382000	-1.244177000	1.454782000	H	-5.314971000	3.309090000	-0.940716000
H	2.136917000	-1.246248000	2.401838000	H	-4.523934000	4.610022000	-0.028520000
C	-1.803648000	-0.373722000	0.091511000	H	-5.386108000	3.305233000	0.812294000
C	-2.815682000	-1.343090000	0.045735000	N	-4.162264000	-0.969815000	-0.036052000
C	-2.765322000	-2.767007000	0.104400000	N	-3.459889000	1.411038000	0.039596000
C	-4.084109000	-3.203447000	0.042697000	N	3.394688000	1.641359000	-0.318512000
H	-4.419965000	-4.228321000	0.065617000	C	3.751545000	0.824684000	-1.305292000
C	-4.920560000	-2.082186000	-0.041884000	N	4.598952000	0.181415000	1.108645000
C	-1.580892000	-3.669849000	0.227152000	H	-0.196061000	-0.435379000	2.265704000
H	-1.912535000	-4.685758000	0.443265000	Cl	3.445954000	2.237118000	2.222849000
H	-0.903559000	-3.346605000	1.017509000	Cl	6.253638000	-1.623577000	0.151293000

E = –2804.3206 a. u.
H = –2803.9188 a. u.
G = –2804.0161 a. u.
f = 192.2337i

Final complex with π-π interaction (I):

B	5.271376000	0.423683000	-0.166759000	C	-1.280109000	-0.922062000	-0.491191000
F	5.918087000	0.641004000	-1.396408000	H	-1.970664000	-0.979966000	-1.325564000
F	6.214934000	0.563887000	0.868195000	C	2.365432000	-0.231095000	0.222612000
Cl	-7.859954000	-0.889519000	0.437319000	C	3.286788000	-1.267627000	0.053867000
C	-4.817414000	1.358478000	0.023953000	C	3.124287000	-2.685285000	0.019817000
N	-5.288209000	-1.133195000	0.756288000	C	4.391807000	-3.212694000	-0.185148000
C	-4.061101000	-0.614784000	0.687373000	H	4.644067000	-4.258193000	-0.265899000
O	-3.088325000	-1.457990000	1.016707000	C	5.306785000	-2.151876000	-0.275027000
C	-1.748600000	-1.105348000	0.799832000	C	1.875867000	-3.494089000	0.162336000
C	-0.918141000	-1.035015000	1.903459000	H	2.109774000	-4.554688000	0.073787000
H	-1.322512000	-1.191892000	2.894072000	H	1.140303000	-3.240004000	-0.601868000
C	0.429451000	-0.755895000	1.709097000	H	1.393507000	-3.328369000	1.126675000
H	1.093942000	-0.691651000	2.560754000	C	6.775977000	-2.227839000	-0.494660000
C	0.927476000	-0.551936000	0.424800000	H	7.314549000	-1.734378000	0.316240000
C	0.066681000	-0.641249000	-0.669035000	H	7.054000000	-1.716556000	-1.418209000

H	7.094763000	-3.266667000	-0.554139000	H	6.244363000	3.175331000	0.647687000
C	2.771504000	1.105350000	0.204021000	H	5.395991000	4.554856000	-0.079830000
C	2.038155000	2.322981000	0.343224000	H	5.992750000	3.220404000	-1.087727000
C	2.970286000	3.346068000	0.238037000	N	4.644927000	-0.989532000	-0.132226000
H	2.767582000	4.403889000	0.294336000	N	4.118003000	1.436986000	0.019779000
C	4.238003000	2.776488000	0.040004000	N	-6.081760000	0.964806000	0.001769000
C	0.572267000	2.524336000	0.553723000	C	-6.231909000	-0.294297000	0.393993000
H	0.354959000	3.588078000	0.646326000	N	-3.769825000	0.644082000	0.372090000
H	0.218346000	2.021012000	1.454064000	H	0.452033000	-0.485583000	-1.668348000
H	-0.014726000	2.127098000	-0.275323000	Cl	-4.515485000	3.000630000	-0.440343000
C	5.539099000	3.477181000	-0.128870000	Cl	-4.207385000	-0.918288000	-2.680751000

E = – 2804.3741 a. u.
H = – 2803.9684 a. u.
G = – 2804.0686 a. u.

First substitution: **nucleophile aminoalkyl phosphoramidate (IIa)**

Pre-reactive complex (IIa):

P	1.962202000	-0.216671000	0.378014000	H	2.131174000	4.032273000	-1.217511000
O	1.598627000	-0.935695000	1.617279000	H	0.849974000	2.864080000	-0.867134000
O	2.320335000	1.288913000	0.723128000	H	1.561118000	3.815510000	0.446916000
O	3.189140000	-0.855180000	-0.406815000	H	4.570945000	3.479908000	-0.462073000
N	0.858294000	-0.108209000	-0.843616000	H	4.856500000	1.971084000	0.419794000
C	0.409721000	-1.273163000	-1.620561000	H	3.982439000	3.299871000	1.200063000
C	-0.158202000	-2.431006000	-0.795163000	H	4.297172000	-1.218819000	1.315400000
N	-1.161666000	-1.960631000	0.166838000	H	4.700413000	-3.629375000	0.780585000
C	2.829837000	2.231533000	-0.273179000	H	2.973175000	-3.237807000	0.810706000
C	1.775325000	3.299925000	-0.490867000	H	3.814874000	-3.425345000	-0.741382000
C	4.142101000	2.777779000	0.254778000	H	5.733446000	-0.186781000	-0.425255000
C	4.250620000	-1.584146000	0.287223000	H	5.487366000	-1.592421000	-1.475688000
C	3.910570000	-3.062847000	0.284163000	H	6.378125000	-1.767031000	0.046151000
C	5.541782000	-1.259873000	-0.437309000	N	-3.229494000	0.232210000	1.424122000
H	0.113806000	0.550966000	-0.654708000	C	-2.235494000	0.941968000	0.917131000
H	-0.351413000	-0.907787000	-2.309542000	N	-2.004688000	1.163431000	-0.369872000
H	1.246260000	-1.636884000	-2.220169000	C	-2.883259000	0.583799000	-1.173918000
H	-0.631433000	-3.131878000	-1.486786000	N	-3.914147000	-0.157561000	-0.806773000
H	0.667064000	-2.966056000	-0.309519000	C	-4.020155000	-0.301507000	0.505652000
H	-0.677637000	-1.590645000	0.979842000	Cl	-5.317832000	-1.280737000	1.074816000
H	-1.714005000	-2.742127000	0.499996000	Cl	-1.116808000	1.631435000	2.025631000
H	3.001615000	1.682747000	-1.201254000	Cl	-2.653830000	0.818880000	-2.865740000

E = – 2653.8664 a. u.
H = – 2653.4959 a. u.
G = – 2653.5869 a. u.

Transition state (IIa):

P	-2.640440000	-0.488553000	0.704486000	N	0.738030000	-1.520281000	-0.611898000
O	-3.373148000	-0.110292000	1.930169000	C	-4.866950000	0.101740000	-0.667045000
O	-3.542826000	-0.519836000	-0.600317000	C	-4.721088000	1.526316000	-1.169772000
O	-1.397305000	0.477346000	0.422136000	C	-5.705847000	-0.774735000	-1.574894000
N	-1.912914000	-1.954122000	0.593291000	C	-1.348546000	1.853491000	0.930239000
C	-0.681816000	-2.315918000	1.281565000	C	-0.390712000	1.892612000	2.103946000
C	0.458846000	-2.629964000	0.316316000	C	-0.930867000	2.735961000	-0.228045000

H	-2.424387000	-2.692883000	0.137983000	H	-0.346097000	2.902510000	2.514800000
H	-0.388355000	-1.485762000	1.925347000	H	-0.720873000	1.213703000	2.890163000
H	-0.840604000	-3.178071000	1.932818000	H	0.613394000	1.610617000	1.786101000
H	1.364548000	-2.823683000	0.896409000	H	-1.635589000	2.647697000	-1.055039000
H	0.237525000	-3.523126000	-0.266044000	H	0.061600000	2.456811000	-0.582965000
H	0.302413000	-0.651468000	-0.304803000	H	-0.897727000	3.778366000	0.092219000
H	0.411954000	-1.704243000	-1.554094000	N	2.900240000	1.428727000	0.185649000
H	-5.277900000	0.102210000	0.343387000	C	3.084273000	0.326899000	0.909607000
				N	3.045327000	-0.915923000	0.507763000
H	-5.704413000	1.990388000	-1.260859000	C	2.659169000	-1.057067000	-0.788363000
H	-4.126626000	2.126806000	-0.480388000	N	2.606428000	-0.019537000	-1.668917000
H	-4.238632000	1.536907000	-2.148817000	C	2.699673000	1.152439000	-1.103368000
H	-6.717325000	-0.372311000	-1.647744000	Cl	2.571543000	2.535960000	-2.153795000
H	-5.764482000	-1.789929000	-1.181448000	Cl	3.444119000	0.588258000	2.593226000
H	-5.274367000	-0.811115000	-2.577035000	Cl	3.199283000	-2.589047000	-1.522560000
H	-2.351872000	2.116549000	1.267667000				

E = –2653.8525 a. u.
H = –2653.4825 a. u.
G = –2653.5675 a. u.
f = 227.917i

Final complex (IIa):

P	-2.181834000	-0.017177000	-0.375097000	H	-3.581058000	4.041644000	1.044718000
O	-1.541159000	-0.664266000	-1.562322000	H	-2.032689000	3.200400000	0.914891000
O	-2.861315000	1.326062000	-0.817718000	H	-2.750622000	3.962110000	-0.518452000
O	-3.230841000	-0.938411000	0.356085000	H	-5.698161000	2.937254000	-0.013767000
N	-1.151676000	0.359590000	0.855153000	H	-5.507172000	1.402881000	-0.875156000
C	-0.395289000	-0.658860000	1.598356000	H	-4.859489000	2.896912000	-1.574375000
C	0.151729000	-1.844383000	0.801661000	H	-4.235890000	-1.463780000	-1.394320000
N	0.767758000	-1.464746000	-0.542347000	H	-4.140115000	-3.929053000	-0.925601000
C	-3.712878000	2.131720000	0.078683000	H	-2.534535000	-3.190612000	-0.966241000
C	-2.968531000	3.411657000	0.398106000	H	-3.293934000	-3.585900000	0.592377000
C	-5.025641000	2.352758000	-0.643278000	H	-5.860575000	-0.814818000	0.363592000
C	-4.121637000	-1.853219000	-0.380445000	H	-5.334036000	-2.177628000	1.367558000
C	-3.477294000	-3.224537000	-0.421096000	H	-6.162366000	-2.475404000	-0.170138000
C	-5.451849000	-1.824921000	0.341574000	N	4.018340000	0.993622000	-0.474152000
H	-0.570863000	1.156103000	0.625000000	C	2.810252000	1.399203000	-0.120607000
H	0.435774000	-0.159742000	2.089948000	N	1.705738000	0.664589000	-0.138459000
H	-1.026500000	-1.089741000	2.377151000	C	1.916687000	-0.577196000	-0.521391000
H	0.924674000	-2.336419000	1.386829000	N	3.047080000	-1.107639000	-0.939776000
H	-0.633455000	-2.548010000	0.533978000	C	4.071480000	-0.265532000	-0.880076000
H	-0.047388000	-1.061003000	-1.118466000	Cl	5.600024000	-0.863419000	-1.381469000
H	1.069474000	-2.325312000	-1.002506000	Cl	2.645683000	3.026798000	0.402079000
H	-3.876849000	1.551959000	0.988781000	Cl	3.049408000	-1.099809000	2.465299000

E = –2653.50752 a. u.
H = –2653.59475 a. u.
G = –2653.880272 a. u.

First substitution: **nucleophile 2-(pyridin-2-yl)ethanamine (III)**

Pre-reactive complex (III):

N	-1.273818000	-1.505252000	0.412692000	C	-0.759565000	-0.517704000	1.129741000

N	-1.266751000	0.696075000	1.275599000	C	2.168535000	1.795852000	-1.645844000
C	-2.382411000	0.886342000	0.589050000	C	0.662271000	1.859137000	-1.307074000
N	-3.014114000	-0.008311000	-0.153902000	N	-0.131011000	0.705931000	-1.738709000
C	-2.401185000	-1.179771000	-0.200734000	H	4.833918000	0.226460000	1.858608000
Cl	-3.141067000	-2.405413000	-1.162192000	H	4.505632000	-2.136615000	1.085396000
Cl	0.728265000	-0.838120000	1.936329000	H	3.111812000	-2.534308000	-0.930768000
Cl	-3.083590000	2.458860000	0.674552000	H	3.753821000	2.060507000	0.570780000
C	4.237906000	0.005665000	0.982107000	H	2.619011000	2.766124000	-1.425248000
C	4.058556000	-1.304980000	0.557775000	H	2.283588000	1.607481000	-2.715953000
C	3.281487000	-1.524762000	-0.571406000	H	0.553872000	1.973315000	-0.224790000
N	2.705635000	-0.546460000	-1.273735000	H	0.234011000	2.755913000	-1.759005000
C	2.877545000	0.721311000	-0.866918000	H	-0.281540000	0.751421000	-2.740679000
C	3.637570000	1.029127000	0.264065000	H	0.400692000	-0.146059000	-1.584258000

E = – 2041.802344 a. u.
H = – 2041.584272 a. u.
G = – 2041.653118 a. u.

Transition state (III):

N	-0.963320000	1.698589000	-0.411498000	C	3.580820000	-0.688078000	0.006975000
C	-0.527813000	0.758333000	-1.244844000	C	1.933877000	-2.324484000	1.032943000
N	-0.897394000	-0.494663000	-1.307957000	C	0.542159000	-2.562028000	0.424176000
C	-1.742375000	-0.863133000	-0.310675000	N	-0.493548000	-1.700405000	1.014527000
N	-2.392609000	0.030904000	0.484284000	H	4.874068000	0.827701000	-0.798094000
C	-1.920553000	1.244580000	0.398106000	H	3.540646000	2.690845000	0.215780000
Cl	-2.636500000	2.435900000	1.449562000	H	1.519639000	2.110367000	1.542465000
Cl	0.658420000	1.274515000	-2.409389000	H	4.127045000	-1.516535000	-0.424083000
Cl	-2.694498000	-2.318031000	-0.691732000	H	2.622450000	-3.054623000	0.606370000
C	3.994817000	0.620753000	-0.201570000	H	1.891395000	-2.505018000	2.110260000
C	3.259494000	1.656593000	0.358411000	H	0.576825000	-2.344965000	-0.646543000
C	2.134657000	1.332847000	1.104769000	H	0.249174000	-3.603251000	0.544225000
N	1.738179000	0.077533000	1.319602000	H	-1.060084000	-2.171528000	1.710815000
C	2.446953000	-0.928015000	0.780672000	H	-0.058688000	-0.871449000	1.428817000

E = – 2041.7915 a. u.
H = – 2041.5740 a. u.
G = – 2041.6380 a. u.
f = 235.2425i

Final complex (III):

N	-0.376915000	-2.256233000	0.557987000	C	2.805917000	1.712250000	0.276972000
C	-0.009453000	-1.162969000	1.215367000	C	0.974138000	2.845908000	-1.046495000
N	-0.219924000	0.084742000	0.868623000	C	-0.371538000	2.665980000	-0.319507000
C	-0.863713000	0.231885000	-0.300589000	N	-1.117911000	1.481909000	-0.758252000
N	-1.322254000	-0.793379000	-1.045626000	H	4.265202000	0.571409000	1.365739000
C	-1.043779000	-1.977939000	-0.558350000	H	4.028023000	-1.413234000	-0.146945000
Cl	-1.593780000	-3.345953000	-1.473205000	H	2.442851000	-1.264010000	-2.053183000
Cl	0.850066000	-1.419606000	2.700359000	H	2.868848000	2.583058000	0.916628000
Cl	-3.948567000	2.130490000	0.783793000	H	1.408516000	3.783530000	-0.694523000
C	3.580004000	0.590162000	0.528055000	H	0.793069000	2.941466000	-2.118301000
C	3.452670000	-0.511968000	-0.309123000	H	-0.220944000	2.586499000	0.754382000
C	2.563808000	-0.428281000	-1.372189000	H	-1.004993000	3.532214000	-0.507324000
N	1.813317000	0.647955000	-1.621942000	H	-2.857200000	1.833938000	0.134432000
C	1.920439000	1.701079000	-0.801613000	H	-1.439746000	1.489715000	-1.717708000

E = – 2041.8415 a. u.

H = – 2041.6252 a. u.
G = – 2041.6927 a. u.

First substitution: **nucleophile p-hydroxybenzaldehyde (IV)**

Pre-reactive complex with π-π interaction (IV):

N	0.130996000	0.088191000	-1.554380000	C	-1.936299000	1.408006000	1.028833000
C	0.856483000	1.107967000	-1.118594000	H	-0.162301000	2.234434000	1.898554000
N	1.958848000	1.040259000	-0.390714000	C	-2.139130000	-1.003123000	1.091863000
C	2.314785000	-0.198443000	-0.079679000	H	-0.520352000	-2.057868000	2.007421000
N	1.671715000	-1.305853000	-0.422545000	C	-2.674438000	0.248335000	0.706489000
C	0.589133000	-1.087705000	-1.151984000	H	-2.335851000	2.375455000	0.738585000
Cl	-0.293722000	-2.477648000	-1.668046000	H	-2.702604000	-1.896694000	0.849278000
Cl	0.333179000	2.684241000	-1.591555000	C	-3.921183000	0.360486000	0.002231000
O	1.003478000	-0.013357000	2.571246000	O	-4.662033000	-0.562032000	-0.342490000
C	-0.141336000	0.074331000	2.045867000	H	-4.212338000	1.404714000	-0.240646000
C	-0.729089000	1.338109000	1.675237000	Cl	3.794015000	-0.391159000	0.782001000
C	-0.935270000	-1.094211000	1.734644000				

E = – 2079.882511 a. u.
H = – 2079.7277 a. u.
G = – 2079.7918 a. u.

Transition state with π-π interaction (IV):

N	0.700592000	0.078843000	1.731996000	C	-2.326502000	-1.446563000	-0.757883000
C	1.180535000	-1.016236000	1.144930000	H	-0.468329000	-2.290558000	-1.437659000
N	1.868505000	-1.109784000	0.042486000	C	-2.490410000	0.965272000	-0.872083000
C	2.011881000	0.070966000	-0.621959000	H	-0.757713000	1.977270000	-1.637070000
N	1.694682000	1.272051000	-0.062190000	C	-3.066070000	-0.273907000	-0.541866000
C	1.021893000	1.177020000	1.049514000	H	-2.768224000	-2.404883000	-0.506127000
Cl	0.497553000	2.682783000	1.772183000	H	-3.066118000	1.866998000	-0.704340000
Cl	0.870748000	-2.514025000	1.997778000	C	-4.410327000	-0.365653000	0.011246000
O	0.777341000	-0.084487000	-2.045529000	O	-5.160384000	0.572934000	0.231802000
C	-0.455640000	-0.149881000	-1.599484000	H	-4.742478000	-1.399204000	0.238175000
C	-1.049159000	-1.392370000	-1.277357000	Cl	3.444826000	0.129351000	-1.670092000
C	-1.216603000	1.029213000	-1.389556000				

E = – 2079.8713 a. u.
H = – 2079.7178 a. u.
G = – 2079.7799 a. u.
f = 308.5013*i*

Final complex with π-π interaction (IV):

N	-3.052618000	-0.707904000	-0.526793000	C	1.821361000	0.221535000	0.882250000
C	-1.839484000	-1.227326000	-0.633043000	C	2.474888000	1.261387000	-1.221679000
N	-0.695716000	-0.576327000	-0.636001000	C	3.122254000	-0.229899000	1.041383000
C	-0.828128000	0.735879000	-0.473003000	H	1.041483000	0.016245000	1.608150000
N	-1.981776000	1.398585000	-0.403479000	C	3.769427000	0.805388000	-1.047874000
C	-3.037127000	0.615624000	-0.428002000	H	2.189593000	1.844794000	-2.086313000
Cl	-4.583424000	1.390865000	-0.327114000	C	4.101822000	0.054362000	0.084561000
Cl	-1.751465000	-2.948671000	-0.803023000	H	3.382963000	-0.807765000	1.920174000
O	0.254023000	1.510322000	-0.425990000	H	4.534484000	1.021296000	-1.781526000
C	1.523597000	0.956700000	-0.255885000	C	5.472483000	-0.439881000	0.286657000

O	6.400250000	-0.255616000	-0.475983000	Cl	-1.275729000	-0.113746000	2.770635000
H	5.621997000	-1.018935000	1.218565000				

E = – 2079.9209 a. u.
H = – 2079.7639 a. u.
G = – 2079.8297 a. u.

Second substitution — reaction in (1): **nucleophile aminoalkyl phosphoramidate (IIa)**

Pre-reactive complex (IIa in 1):

N	-0.801848000	-0.235247000	-0.759152000	C	2.312552000	-2.144032000	-0.653818000
C	-1.457926000	-0.177886000	0.396682000	C	2.011096000	-3.001609000	0.574671000
N	-2.588907000	-0.753137000	0.698912000	N	0.684543000	-2.691222000	1.120597000
C	-3.135118000	-1.476383000	-0.304335000	C	2.843669000	2.271158000	-1.035794000
N	-2.533828000	-1.662086000	-1.507244000	C	1.445860000	2.682723000	-1.457490000
C	-1.405008000	-1.023304000	-1.646792000	C	3.814027000	3.432844000	-0.943020000
Cl	-0.573130000	-1.206719000	-3.162852000	C	5.786175000	-0.116815000	0.762527000
Cl	-0.695888000	0.769293000	1.636733000	C	6.079348000	-1.539593000	1.202442000
C	-4.221347000	2.614663000	1.374059000	C	6.882749000	0.485151000	-0.093846000
C	-3.809855000	2.881212000	0.073490000	H	1.223885000	-0.361562000	-0.525587000
C	-4.241338000	2.032646000	-0.936706000	H	1.625749000	-2.407807000	-1.459162000
N	-5.013798000	0.964085000	-0.722936000	H	3.325864000	-2.355562000	-1.001360000
C	-5.387856000	0.692924000	0.534204000	H	2.024258000	-4.049890000	0.265598000
C	-5.022823000	1.508478000	1.606754000	H	2.813480000	-2.868130000	1.311557000
C	-6.149454000	-0.587072000	0.753190000	H	0.721913000	-1.789922000	1.586090000
C	-5.212296000	-1.787654000	1.001649000	H	0.440784000	-3.363713000	1.838796000
N	-4.321420000	-2.052861000	-0.119293000	H	3.231749000	1.517260000	-1.723734000
H	-3.914816000	3.253546000	2.192307000	H	1.476218000	3.143886000	-2.446391000
H	-3.174311000	3.725862000	-0.155419000	H	0.779999000	1.821094000	-1.496093000
H	-3.951591000	2.214518000	-1.966279000	H	1.036731000	3.406098000	-0.749396000
H	-5.349123000	1.261980000	2.608887000	H	3.920841000	3.911574000	-1.918005000
H	-6.805913000	-0.499449000	1.621232000	H	4.795382000	3.088573000	-0.616688000
H	-6.769621000	-0.792025000	-0.120630000	H	3.449815000	4.174369000	-0.229486000
H	-4.604323000	-1.615627000	1.886814000	H	5.607636000	0.509808000	1.638510000
H	-5.807206000	-2.685096000	1.168415000	H	6.992207000	-1.567907000	1.800154000
H	-4.703643000	-2.513414000	-0.931563000	H	5.257655000	-1.927870000	1.803566000
P	3.134257000	0.156045000	0.584350000	H	6.214841000	-2.182794000	0.330399000
O	3.074938000	-0.103633000	2.038045000	H	6.626703000	1.501466000	-0.393684000
O	2.753043000	1.669275000	0.293978000	H	7.034979000	-0.115021000	-0.993059000
O	4.572059000	-0.119182000	-0.048624000	H	7.819074000	0.515114000	0.465683000
N	2.178854000	-0.699556000	-0.443327000				

E = – 2575.50362 a. u.
H = – 2574.972396 a. u.
G = – 2575.079732 a. u.

Transition state (IIa in 1):

N	0.805767000	-0.276752000	0.911065000	C	4.904227000	2.375770000	0.727145000
C	1.345131000	0.551494000	0.050093000	C	4.689133000	1.509081000	1.792352000
N	2.142061000	0.305236000	-0.960608000	C	4.828198000	0.146736000	1.565993000
C	2.456644000	-1.010308000	-1.075873000	N	5.140160000	-0.375426000	0.377173000
N	1.967773000	-1.980087000	-0.301488000	C	5.315381000	0.457871000	-0.656041000
C	1.084277000	-1.591284000	0.631769000	C	5.221804000	1.843435000	-0.511801000
Cl	1.214840000	-2.592858000	2.169777000	C	5.532635000	-0.170740000	-2.005620000
Cl	0.935885000	2.246463000	0.298424000	C	4.204120000	-0.444295000	-2.743770000

N	3.327868000	-1.367280000	-2.041250000	C	-6.719592000	-0.306971000	-0.506307000
H	4.813517000	3.446436000	0.858931000	H	-1.229048000	0.312327000	1.097133000
H	4.423826000	1.876560000	2.774450000	H	-1.409537000	-1.327231000	2.569239000
H	4.676916000	-0.561439000	2.373863000	H	-3.093629000	-1.641952000	2.171658000
H	5.375792000	2.487184000	-1.368296000	H	-1.464421000	-3.453545000	1.498613000
H	6.134779000	0.483656000	-2.640076000	H	-2.543540000	-2.898534000	0.217635000
H	6.073055000	-1.110732000	-1.881690000	H	-0.830140000	-1.666580000	-0.740529000
H	3.663384000	0.486771000	-2.897535000	H	-0.208011000	-3.165178000	-0.446922000
H	4.422347000	-0.871655000	-3.723187000	H	-4.140537000	1.980217000	1.156513000
H	3.609217000	-2.335050000	-2.004654000	H	-3.004479000	4.112676000	1.802727000
P	-2.932398000	0.132519000	-0.348236000	H	-1.846375000	2.785422000	1.620858000
O	-2.350706000	-0.506578000	-1.553328000	H	-1.999279000	4.004141000	0.346213000
O	-2.980045000	1.699334000	-0.547823000	H	-5.153067000	4.106690000	0.322726000
O	-4.391125000	-0.372789000	0.019826000	H	-5.375753000	2.787154000	-0.836392000
N	-2.156551000	-0.107129000	1.090162000	H	-4.132031000	4.015795000	-1.123069000
C	-2.114603000	-1.420003000	1.745868000	H	-5.109043000	-0.182181000	-1.923863000
C	-1.710861000	-2.605662000	0.861571000	H	-5.985647000	-2.525857000	-2.034997000
N	-0.545385000	-2.316617000	-0.001071000	H	-4.259156000	-2.479781000	-1.644964000
C	-3.627290000	2.596951000	0.416104000	H	-5.453084000	-2.787761000	-0.365187000
C	-2.549917000	3.424030000	1.088573000	H	-6.738569000	0.765563000	-0.312424000
C	-4.635239000	3.426030000	-0.354866000	H	-6.960534000	-0.832736000	0.419496000
C	-5.360043000	-0.737970000	-1.017466000	H	-7.485826000	-0.539596000	-1.247251000
C	-5.254725000	-2.228033000	-1.281420000				

$E = -2575.4796$ a. u.
$H = -2574.9490$ a. u.
$G = -2575.0501$ a. u.
$f = 273.3656i$

Final complex (IIa in 1):

N	0.630319000	0.742249000	-0.449019000	P	-3.283583000	0.215747000	-0.411515000
C	1.746268000	1.473614000	-0.440958000	O	-2.840125000	-0.109991000	-1.801042000
N	2.859086000	1.222817000	-1.073007000	O	-3.935298000	1.645461000	-0.397966000
C	2.868183000	0.074347000	-1.788618000	O	-4.284896000	-0.835112000	0.203222000
N	1.783177000	-0.741335000	-1.891122000	N	-2.087360000	0.234949000	0.724636000
C	0.750280000	-0.337089000	-1.207729000	C	-1.327930000	-0.973307000	1.082098000
Cl	1.155542000	-3.478245000	2.219061000	C	-0.909257000	-1.901170000	-0.061549000
Cl	1.689484000	2.915123000	0.518309000	N	-0.434812000	-1.181092000	-1.317608000
C	4.976724000	1.080879000	2.181391000	C	-4.609057000	2.207591000	0.786475000
C	4.053682000	0.094973000	2.507655000	C	-3.741785000	3.323419000	1.331926000
C	3.899198000	-0.980865000	1.641312000	C	-5.980239000	2.665601000	0.334780000
N	4.586445000	-1.103231000	0.500835000	C	-5.336039000	-1.480832000	-0.601672000
C	5.459350000	-0.141365000	0.175130000	C	-4.811370000	-2.812162000	-1.101102000
C	5.690422000	0.961086000	0.998177000	C	-6.548384000	-1.599398000	0.297391000
C	6.122717000	-0.264812000	-1.170915000	H	-1.461262000	1.019863000	0.582335000
C	5.272090000	0.353131000	-2.298406000	H	-0.446985000	-0.647566000	1.627653000
N	3.968271000	-0.284428000	-2.438041000	H	-1.914252000	-1.587223000	1.765442000
H	5.133015000	1.931145000	2.833241000	H	-0.113448000	-2.557412000	0.292983000
H	3.466838000	0.149521000	3.414817000	H	-1.748359000	-2.499633000	-0.410912000
H	3.189352000	-1.772183000	1.864171000	H	-1.280574000	-0.631929000	-1.667636000
H	6.407905000	1.716316000	0.703637000	H	-0.220388000	-1.889549000	-2.021027000
H	7.087322000	0.246496000	-1.173987000	H	-4.704491000	1.408535000	1.524000000
H	6.298869000	-1.318733000	-1.391629000	H	-4.224895000	3.773893000	2.200364000
H	5.113174000	1.413231000	-2.115504000	H	-2.768015000	2.944131000	1.640754000
H	5.791112000	0.246181000	-3.250426000	H	-3.597256000	4.095998000	0.574876000
H	3.927697000	-1.188353000	-2.885170000	H	-6.527544000	3.082128000	1.181587000

H	-6.553687000	1.832580000	-0.071928000	H	-4.528077000	-3.446753000	-0.259531000
H	-5.889490000	3.435156000	-0.433681000	H	-6.871025000	-0.618267000	0.645967000
H	-5.559135000	-0.826206000	-1.447116000	H	-6.317902000	-2.220641000	1.164523000
H	-5.586273000	-3.322594000	-1.675029000	H	-7.370543000	-2.060240000	-0.251741000
H	-3.945830000	-2.665244000	-1.746357000				

E = – 2575.5179 a. u.
H = – 2574.9841 a. u.
G = – 2575.0884 a. u.

Second substitution — reaction in (1): **nucleophile p-hydroxybenzaldehyde (IV)**

Pre-reactive complex (IV in 1):

N	0.827862000	2.098561000	0.842943000	H	-3.590908000	-1.996864000	0.654520000
C	0.137564000	0.990060000	1.089238000	H	-3.279666000	-2.351925000	-1.796081000
N	-0.343045000	0.132981000	0.230032000	H	-3.056910000	-0.960575000	-2.862551000
C	-0.070984000	0.425677000	-1.059479000	H	-0.996192000	-2.032135000	-0.857692000
N	0.625990000	1.524287000	-1.446319000	H	-0.980741000	-2.311198000	-2.587744000
C	1.022851000	2.283223000	-0.460442000	H	-0.306158000	-0.091404000	-2.961234000
Cl	1.895025000	3.728802000	-0.893257000	O	4.169203000	0.703768000	-0.196486000
Cl	-0.187979000	0.662781000	2.770566000	C	3.438799000	-0.305798000	-0.002029000
C	-3.978337000	-0.038557000	1.455022000	C	3.027175000	-0.727922000	1.316149000
C	-3.987981000	1.320212000	1.161430000	C	2.940699000	-1.118848000	-1.092277000
C	-3.659588000	1.713023000	-0.128606000	C	2.203489000	-1.805784000	1.503689000
N	-3.321503000	0.858372000	-1.097941000	H	3.374555000	-0.139995000	2.157853000
C	-3.290015000	-0.448143000	-0.807859000	C	2.117757000	-2.189996000	-0.884262000
C	-3.626843000	-0.933124000	0.457641000	H	3.231558000	-0.826217000	-2.094793000
C	-2.799410000	-1.375182000	-1.886567000	C	1.711279000	-2.566877000	0.418807000
C	-1.277126000	-1.602202000	-1.815157000	H	1.893604000	-2.076338000	2.508895000
N	-0.504226000	-0.388329000	-2.019064000	H	1.742962000	-2.765073000	-1.723331000
H	-4.231430000	-0.391722000	2.446603000	C	0.795412000	-3.641272000	0.654506000
H	-4.245552000	2.057848000	1.909515000	O	0.242765000	-4.349931000	-0.193987000
H	-3.666722000	2.763939000	-0.398910000	H	0.572058000	-3.817996000	1.728100000

E = – 2001.5180 a. u.
H = – 2001.2024 a. u.
G = – 2001.2828 a. u.

Transition state (IV in 1):

N	0.167051000	-1.790254000	0.839654000	N	0.568766000	1.246281000	-1.792745000
C	0.358297000	-0.546396000	1.168988000	H	4.333177000	1.361673000	2.613710000
N	0.467079000	0.524997000	0.411393000	H	4.810774000	-0.942966000	1.747776000
C	0.411011000	0.227264000	-0.910299000	H	4.333195000	-1.428964000	-0.640402000
N	0.212345000	-0.986715000	-1.414065000	H	3.354683000	3.037076000	1.054870000
C	-0.040229000	-1.956936000	-0.512362000	H	2.950829000	3.654043000	-1.341682000
Cl	0.553633000	-3.594829000	-1.073368000	H	2.961271000	2.391783000	-2.578056000
Cl	0.526112000	-0.241376000	2.910377000	H	0.794583000	2.799697000	-0.451061000
C	4.135446000	1.103797000	1.581010000	H	0.682693000	3.281314000	-2.141070000
C	4.402854000	-0.174586000	1.104943000	H	0.636197000	0.947146000	-2.752911000
C	4.133052000	-0.445002000	-0.229417000	O	-1.759108000	-2.365036000	-0.639758000
N	3.621317000	0.452442000	-1.075876000	C	-2.525687000	-1.327049000	-0.343510000
C	3.337402000	1.674789000	-0.610126000	C	-2.979704000	-1.118423000	0.974409000
C	3.595141000	2.038389000	0.713257000	C	-2.884519000	-0.386917000	-1.337490000
C	2.654958000	2.624082000	-1.556493000	C	-3.746196000	-0.011752000	1.283811000
C	1.115648000	2.547218000	-1.459132000	H	-2.697992000	-1.837275000	1.731201000

C	-3.649444000	0.714483000	-1.021785000	H	-3.918777000	1.438516000	-1.780670000
H	-2.529161000	-0.554230000	-2.344996000	C	-4.888487000	2.086617000	0.657280000
C	-4.087984000	0.923414000	0.296249000	O	-5.256385000	2.967446000	-0.104388000
H	-4.083786000	0.145672000	2.302617000	H	-5.164673000	2.137519000	1.730176000

E = – 2001.4916 a. u.
H = – 2001.1777 a. u.
G = – 2001.2584 a. u.
f = 343.371i

Final complex (IV in 1):

N	0.856649000	-1.730808000	-1.640574000	H	5.078670000	0.940557000	1.374006000
C	2.006919000	-1.747701000	-0.994509000	H	3.802314000	0.898025000	3.517069000
N	2.231293000	-1.529313000	0.278349000	H	2.095236000	1.352365000	3.520235000
C	1.118413000	-1.240884000	0.988301000	H	3.266345000	-1.289020000	2.501804000
N	-0.122656000	-1.214297000	0.459180000	H	2.387132000	-1.052211000	4.011156000
C	-0.175308000	-1.454716000	-0.831301000	H	0.377672000	-0.671922000	2.736587000
Cl	-1.270495000	3.327911000	-1.979873000	O	-1.359739000	-1.443254000	-1.460943000
Cl	3.417052000	-2.103819000	-1.965650000	C	-2.501552000	-1.044239000	-0.763899000
C	4.212978000	1.715938000	-0.438595000	C	-3.343080000	-2.023774000	-0.260692000
C	3.034082000	2.155168000	-1.027926000	C	-2.796981000	0.311121000	-0.676582000
C	1.878282000	2.185152000	-0.256131000	C	-4.517813000	-1.631701000	0.364263000
N	1.844873000	1.791990000	1.021466000	H	-3.073257000	-3.066251000	-0.358875000
C	2.975341000	1.342665000	1.581748000	C	-3.972058000	0.689111000	-0.051964000
C	4.183830000	1.305620000	0.885965000	H	-2.127843000	1.054821000	-1.097793000
C	2.858404000	0.791985000	2.977971000	C	-4.838540000	-0.276191000	0.475895000
C	2.484656000	-0.705340000	2.982041000	H	-5.190081000	-2.379145000	0.768608000
N	1.231228000	-0.980751000	2.296453000	H	-4.231005000	1.736368000	0.031117000
H	5.136556000	1.685037000	-1.003040000	C	-6.088919000	0.110194000	1.147298000
H	3.003620000	2.473505000	-2.061340000	O	-6.473575000	1.250933000	1.308559000
H	0.941866000	2.534742000	-0.682000000	H	-6.693830000	-0.740080000	1.519997000

E = – 2001.5519 a. u.
H = – 2001.2340 a. u.
G = – 2001.3148 a. u.

Second substitution — reaction in (2): **nucleophile 2-(pyridin-2-yl)ethanamine (III)**

Pre-reactive complex (III in 2):

N	1.032464000	-1.254984000	0.438165000	C	0.409538000	3.470267000	-0.514936000
C	1.263981000	-1.011315000	-0.846538000	C	1.606716000	2.622281000	-0.965827000
N	2.462188000	-0.818702000	-1.396053000	N	2.515146000	2.171464000	0.091986000
C	3.451997000	-0.843130000	-0.528886000	H	-3.928360000	2.889350000	1.124577000
N	3.363120000	-1.062345000	0.778994000	H	-3.247423000	0.776052000	2.290461000
C	2.119737000	-1.259874000	1.183752000	H	-0.891397000	0.007556000	2.050349000
Cl	1.889058000	-1.542513000	2.875791000	H	-2.221841000	4.126282000	-0.194769000
Cl	5.040248000	-0.579621000	-1.153881000	H	-0.060208000	3.930291000	-1.389450000
C	-2.910003000	2.526139000	1.066203000	H	0.775779000	4.300508000	0.100835000
C	-2.537508000	1.353919000	1.714635000	H	1.238524000	1.741873000	-1.497645000
C	-1.223951000	0.929379000	1.587270000	H	2.188233000	3.197196000	-1.689847000
N	-0.302490000	1.594534000	0.886330000	H	2.988129000	2.967916000	0.505639000
C	-0.652408000	2.725267000	0.263805000	H	1.955388000	1.748376000	0.825168000
C	-1.960045000	3.216460000	0.330380000	O	0.254711000	-0.920354000	-1.711763000

C	-1.080277000	-1.031398000	-1.324619000	C	-3.767618000	-1.176300000	-0.731752000
C	-1.907773000	0.012010000	-1.705821000	H	-3.916301000	0.751012000	-1.675205000
C	-1.564952000	-2.162826000	-0.676033000	H	-3.321651000	-3.087187000	0.134519000
C	-3.257490000	-0.064025000	-1.402799000	C	-5.200384000	-1.222138000	-0.398366000
H	-1.487266000	0.869324000	-2.211013000	O	-5.748130000	-2.129707000	0.193460000
C	-2.913139000	-2.226169000	-0.377170000	H	-5.780066000	-0.338694000	-0.729239000
H	-0.893903000	-2.964141000	-0.406149000				

E = – 2001.96121 a. u.
H = – 2001.632861 a. u.
G = – 2001.715927 a. u.

Transition state (III in 2):

N	-0.041493000	-1.286834000	-0.489594000	H	-3.437066000	3.449557000	0.908900000
C	-0.332402000	-0.808201000	0.720842000	H	-3.958334000	2.808541000	-0.643241000
N	-1.485774000	-0.883639000	1.347953000	H	-2.781377000	1.136363000	1.633713000
C	-2.483460000	-1.400442000	0.597402000	H	-4.506761000	1.299207000	1.304289000
N	-2.269923000	-2.090856000	-0.565922000	H	-4.316280000	-0.128027000	-0.451879000
C	-1.062849000	-1.939873000	-1.033978000	H	-2.807480000	0.439390000	-0.873045000
Cl	-0.722935000	-2.704842000	-2.569636000	O	0.627371000	-0.164013000	1.414217000
Cl	-3.824904000	-2.071270000	1.580719000	C	1.957913000	-0.195539000	1.028225000
C	0.313610000	3.840513000	-0.429827000	C	2.604765000	1.028063000	0.944249000
C	0.698190000	2.906385000	-1.382420000	C	2.637401000	-1.397970000	0.839823000
C	-0.225885000	1.944721000	-1.767661000	C	3.959278000	1.052675000	0.648384000
N	-1.464781000	1.888068000	-1.277121000	H	2.041498000	1.935725000	1.104372000
C	-1.841993000	2.788217000	-0.355052000	C	3.986039000	-1.362346000	0.543154000
C	-0.969666000	3.777231000	0.096381000	H	2.107901000	-2.335812000	0.921481000
C	-3.249385000	2.663552000	0.176760000	C	4.658654000	-0.137907000	0.441133000
C	-3.519725000	1.306397000	0.846057000	H	4.477133000	2.001531000	0.574785000
N	-3.418661000	0.178737000	-0.093341000	H	4.538533000	-2.279753000	0.390021000
H	1.004727000	4.603595000	-0.095042000	C	6.094162000	-0.086944000	0.124739000
H	1.690688000	2.911857000	-1.811089000	O	6.799427000	-1.056012000	-0.071983000
H	0.037651000	1.183313000	-2.492245000	H	6.519836000	0.934129000	0.072518000
H	-1.295242000	4.484963000	0.847091000				

E = – 2001.94612 a. u.
H = – 2001.61823 a. u.
G = – 2001.69775 a. u.
f = 238.2188i

Final complex (III in 2):

N	-0.502563000	-0.921479000	0.805399000	C	1.934188000	3.122584000	-0.928322000
C	-0.066172000	-0.416774000	-0.348349000	C	4.070613000	1.826218000	-0.526762000
N	1.193270000	-0.283500000	-0.723662000	C	3.924230000	0.395886000	-1.079180000
C	2.083596000	-0.684672000	0.184425000	N	3.411129000	-0.562577000	-0.093886000
N	1.770702000	-1.251269000	1.370044000	H	0.028668000	4.092476000	-1.140317000
C	0.481527000	-1.328035000	1.593621000	H	-0.652769000	3.545212000	1.211112000
Cl	-0.003449000	-2.033900000	3.108030000	H	0.943299000	2.294086000	2.643085000
Cl	4.013162000	-3.326928000	-1.678372000	H	2.259088000	3.328644000	-1.939867000
C	0.690808000	3.543646000	-0.482965000	H	4.500185000	2.438898000	-1.321730000
C	0.308146000	3.240760000	0.818590000	H	4.774370000	1.817519000	0.307366000
C	1.201602000	2.541863000	1.619039000	H	3.254621000	0.381064000	-1.935513000
N	2.401709000	2.134151000	1.199348000	H	4.898138000	0.033236000	-1.406880000
C	2.761131000	2.406053000	-0.061840000	H	3.761464000	-2.239447000	-0.992948000

H	3.989326000	-0.699366000	0.725418000	H	-2.576650000	-1.993135000	-1.703289000
O	-0.960226000	0.015006000	-1.246998000	C	-5.036131000	0.011439000	-0.472811000
C	-2.320362000	-0.010190000	-0.936933000	H	-4.731233000	2.003287000	0.280597000
C	-2.894009000	1.123707000	-0.385852000	H	-5.042556000	-1.976187000	-1.280176000
C	-3.068091000	-1.132727000	-1.270508000	C	-6.486791000	0.042043000	-0.215876000
C	-4.261308000	1.128411000	-0.152226000	O	-7.253927000	-0.866147000	-0.459668000
H	-2.272796000	1.975571000	-0.148160000	H	-6.857440000	0.983615000	0.233495000
C	-4.430866000	-1.118470000	-1.034676000				

E = – 2001.9968 a. u.
H = – 2001.6703 a. u.
G = – 2001.7543 a. u.

Third substitution — reaction in (4): **nucleophile aminoalkyl phosphoramidate (IIc)**

Pre-reactive complex (IIc in 4):

N	2.306403000	3.672794000	0.020234000	C	-4.917798000	-0.740777000	-0.595009000
C	1.304299000	2.789725000	0.061807000	C	-3.923394000	-1.744034000	-0.799105000
N	1.304718000	1.622421000	0.665544000	C	-4.602912000	-2.951462000	-0.868363000
C	2.434212000	1.332087000	1.346489000	H	-4.161548000	-3.925270000	-1.008562000
N	3.491325000	2.182325000	1.431964000	C	-5.973962000	-2.701768000	-0.702092000
C	3.350959000	3.275531000	0.733900000	C	-2.442824000	-1.594761000	-0.911181000
Cl	4.717216000	4.369521000	0.740363000	H	-1.973618000	-2.577130000	-0.935065000
O	0.216753000	3.191251000	-0.623237000	H	-2.025503000	-1.038900000	-0.071500000
N	2.527176000	0.162502000	1.971569000	H	-2.161001000	-1.059022000	-1.818776000
C	1.508759000	-0.872633000	1.877616000	C	-7.087626000	-3.687500000	-0.694277000
C	0.353809000	-0.637962000	2.855120000	H	-7.783149000	-3.489298000	-1.511914000
C	-0.809655000	-1.573558000	2.641356000	H	-7.659463000	-3.619214000	0.232771000
C	-2.117281000	-1.148657000	2.889729000	H	-6.696678000	-4.697739000	-0.798862000
C	-3.169993000	-2.026366000	2.685264000	C	-5.966233000	1.430261000	-0.265337000
C	-2.889506000	-3.312248000	2.240206000	C	-6.139907000	2.842601000	-0.144280000
C	-1.562483000	-3.652606000	2.020969000	C	-7.502714000	3.049899000	0.015887000
N	-0.541868000	-2.812280000	2.212829000	H	-7.995344000	4.001953000	0.134601000
C	-0.992370000	2.508011000	-0.538422000	C	-8.149388000	1.803886000	-0.008512000
C	-1.593859000	2.225975000	0.680867000	C	-5.113835000	3.928644000	-0.186545000
C	-2.840173000	1.619724000	0.690794000	H	-5.605370000	4.901175000	-0.182048000
C	-3.490348000	1.300062000	-0.500108000	H	-4.488156000	3.862424000	-1.077108000
C	-2.879071000	1.610088000	-1.711609000	H	-4.441713000	3.883831000	0.671892000
C	-1.629961000	2.218010000	-1.734199000	C	-9.604665000	1.527013000	0.124267000
C	-4.825129000	0.646566000	-0.458300000	H	-9.992285000	1.058143000	-0.782060000
H	3.444080000	-0.066333000	2.354826000	H	-10.148770000	2.451827000	0.305875000
H	1.122940000	-0.910799000	0.859250000	H	-9.792895000	0.833809000	0.945929000
H	1.989888000	-1.825341000	2.077850000	N	-6.161312000	-1.379522000	-0.538305000
H	0.724357000	-0.747338000	3.879665000	N	-7.230194000	0.837430000	-0.180873000
H	0.007639000	0.391240000	2.754634000	N	5.530638000	0.085096000	2.365998000
H	-2.297184000	-0.138330000	3.232047000	C	6.870816000	-0.499886000	2.466661000
H	-4.191416000	-1.710458000	2.854385000	N	5.936339000	-1.133337000	-2.491820000
H	-3.678040000	-4.027065000	2.051204000	P	4.524238000	-1.121872000	-1.653294000
H	-1.303527000	-4.645323000	1.667517000	O	4.504143000	-0.185917000	-0.512087000
H	-1.093675000	2.472930000	1.605232000	C	8.030183000	0.437433000	2.076906000
H	-3.319465000	1.397675000	1.634095000	C	7.841343000	1.170206000	0.743771000
H	-3.379674000	1.377685000	-2.642314000	C	7.723433000	0.251637000	-0.474820000
H	-1.150904000	2.475825000	-2.668355000	C	7.101024000	0.953593000	-1.681011000
B	-7.514755000	-0.680152000	-0.273932000	C	6.768560000	0.029417000	-2.852849000
F	-8.073287000	-1.143824000	0.931616000	O	3.351313000	-0.873784000	-2.696429000
F	-8.413683000	-0.944617000	-1.320162000	C	2.003943000	-0.526227000	-2.235547000

C	1.397246000	0.361392000	-3.301474000	H	6.294863000	0.613805000	-3.648940000
C	1.205544000	-1.791299000	-1.980744000	H	7.693187000	-0.382262000	-3.262619000
O	4.301870000	-2.656540000	-1.291371000	H	2.113005000	0.036802000	-1.307955000
C	5.135967000	-3.317379000	-0.287944000	H	1.991292000	1.265701000	-3.435578000
C	4.457041000	-3.218617000	1.064907000	H	1.341605000	-0.168801000	-4.254251000
C	5.338427000	-4.741454000	-0.765291000	H	0.388335000	0.649335000	-3.005573000
H	5.512252000	1.008361000	2.787082000	H	1.105722000	-2.372984000	-2.899311000
H	7.032885000	-0.845796000	3.491496000	H	0.209796000	-1.527281000	-1.626426000
H	6.881814000	-1.394611000	1.840285000	H	1.686252000	-2.412284000	-1.226284000
H	6.036907000	-1.918147000	-3.118535000	H	6.099732000	-2.801799000	-0.259925000
H	8.150795000	1.184655000	2.868953000	H	4.348914000	-2.176726000	1.359354000
H	8.957895000	-0.146005000	2.059459000	H	5.055451000	-3.730313000	1.820752000
H	8.668385000	1.872374000	0.599939000	H	3.471432000	-3.686327000	1.026395000
H	6.938863000	1.785048000	0.808725000	H	4.378135000	-5.255197000	-0.839565000
H	8.706867000	-0.154553000	-0.736999000	H	5.969659000	-5.285833000	-0.061180000
H	7.098021000	-0.601842000	-0.219985000	H	5.818108000	-4.754841000	-1.744538000
H	6.192064000	1.462505000	-1.357133000	H	5.294071000	0.224868000	1.386247000
H	7.776352000	1.726667000	-2.061248000				

E = – 3417.44668 a. u.
H = – 3416.43602 a. u.
G = – 3416.60144 a. u.

Transition state (IIc in 4):

N	2.618806000	2.965823000	1.028165000	H	-2.494188000	-4.989078000	2.356031000
C	1.602436000	2.202422000	0.692651000	H	-1.016531000	2.363732000	1.912447000
N	1.392428000	0.936552000	1.009161000	H	-3.337035000	1.537806000	1.640504000
C	2.357564000	0.409569000	1.789839000	H	-2.755035000	1.284072000	-2.589327000
N	3.443705000	1.060031000	2.217262000	H	-0.437467000	2.139214000	-2.312777000
C	3.570962000	2.307963000	1.744414000	B	-7.387104000	-0.242724000	-0.790934000
Cl	4.399914000	3.430855000	2.949110000	F	-8.154276000	-0.625804000	0.324977000
O	0.671192000	2.829876000	-0.078027000	F	-8.150852000	-0.441913000	-1.953658000
N	2.204530000	-0.878424000	2.173213000	C	-4.788196000	-0.557759000	-0.756517000
C	0.959703000	-1.612740000	2.040296000	C	-3.880593000	-1.658674000	-0.800185000
C	-0.016247000	-1.345974000	3.197864000	C	-4.661710000	-2.797378000	-0.936213000
C	-1.354505000	-1.995084000	2.964728000	H	-4.304676000	-3.813471000	-0.988460000
C	-2.527757000	-1.240374000	2.929626000	C	-6.010251000	-2.412862000	-0.962157000
C	-3.736314000	-1.868628000	2.668256000	C	-2.390814000	-1.664410000	-0.708889000
C	-3.741044000	-3.240198000	2.454368000	H	-2.040231000	-2.682689000	-0.544418000
C	-2.529418000	-3.916295000	2.516174000	H	-2.028149000	-1.042566000	0.107708000
N	-1.361246000	-3.319721000	2.762897000	H	-1.932483000	-1.291432000	-1.626062000
C	-0.601260000	2.289005000	-0.188784000	C	-7.208239000	-3.287515000	-1.071535000
C	-1.406294000	2.129022000	0.931988000	H	-7.796745000	-3.030278000	-1.953974000
C	-2.699666000	1.658381000	0.774950000	H	-7.860593000	-3.157212000	-0.206195000
C	-3.195435000	1.342066000	-0.489961000	H	-6.907277000	-4.331364000	-1.136448000
C	-2.379008000	1.521903000	-1.602833000	C	-5.656306000	1.710650000	-0.596391000
C	-1.081858000	2.000171000	-1.455815000	C	-5.707554000	3.136013000	-0.520170000
C	-4.580194000	0.818994000	-0.626571000	C	-7.053286000	3.474359000	-0.542356000
H	2.893335000	-1.218098000	2.824108000	H	-7.462592000	4.471472000	-0.504294000
H	0.492714000	-1.321055000	1.102811000	C	-7.808515000	2.294412000	-0.633219000
H	1.189447000	-2.675364000	1.983177000	C	-4.584914000	4.119715000	-0.444491000
H	0.420132000	-1.724349000	4.126776000	H	-4.973303000	5.132549000	-0.549134000
H	-0.141424000	-0.268012000	3.308142000	H	-3.842740000	3.951240000	-1.225154000
H	-2.483053000	-0.173329000	3.095357000	H	-4.056186000	4.056196000	0.508032000
H	-4.654267000	-1.297318000	2.616884000	C	-9.288568000	2.157765000	-0.687086000
H	-4.655582000	-3.772694000	2.233415000	H	-9.597219000	1.670784000	-1.613785000

H	-9.760052000	3.136607000	-0.624862000	H	7.504465000	3.603406000	0.156563000
H	-9.649089000	1.535396000	0.134000000	H	8.427403000	2.113886000	0.214737000
N	-6.085282000	-1.073525000	-0.854753000	H	7.982820000	2.973765000	-2.118662000
N	-6.972206000	1.241849000	-0.669721000	H	6.273375000	2.791957000	-1.851188000
N	5.015328000	2.294213000	0.445500000	H	8.335289000	0.640724000	-2.329476000
C	6.382449000	1.892957000	0.807235000	H	6.994908000	0.246755000	-1.281564000
N	5.809628000	-1.683575000	-2.588127000	H	5.405534000	1.081510000	-3.063093000
P	4.582724000	-1.458275000	-1.520972000	H	6.765591000	1.206886000	-4.161618000
O	4.460160000	-0.072278000	-1.022059000	H	5.547106000	-0.866793000	-4.531410000
C	7.460744000	2.535099000	-0.078347000	H	7.202069000	-1.183309000	-4.023016000
C	7.245997000	2.366134000	-1.587032000	H	2.211791000	-1.428103000	-0.479264000
C	7.304383000	0.913855000	-2.082975000	H	1.795372000	0.205895000	-2.269809000
C	6.391384000	0.669367000	-3.284799000	H	0.980411000	-1.039505000	-3.242425000
C	6.238374000	-0.796381000	-3.685089000	H	0.279344000	-0.493708000	-1.705376000
O	3.252859000	-2.006352000	-2.185855000	H	1.064536000	-3.501237000	-2.409065000
C	1.979137000	-1.783876000	-1.483347000	H	0.324221000	-3.009969000	-0.877422000
C	1.210525000	-0.712316000	-2.226315000	H	1.882746000	-3.846573000	-0.872755000
C	1.270606000	-3.119846000	-1.407195000	H	6.699295000	-1.711855000	0.049839000
O	4.855303000	-2.559973000	-0.407543000	H	5.049762000	-0.982030000	1.752107000
C	6.010780000	-2.440632000	0.485204000	H	6.387126000	-1.855063000	2.515730000
C	5.536510000	-1.952168000	1.838611000	H	4.833454000	-2.668281000	2.269253000
C	6.676579000	-3.801658000	0.527135000	H	5.981608000	-4.549693000	0.913185000
H	4.965442000	3.249658000	0.107165000	H	7.550725000	-3.770720000	1.179436000
H	6.557041000	2.172642000	1.846750000	H	6.998873000	-4.106615000	-0.468977000
H	6.414677000	0.807172000	0.750388000	H	4.641793000	1.652622000	-0.257241000
H	6.038723000	-2.654588000	-2.742466000				

E = – 3417.4194 a. u.
H = – 3416.4096 a. u.
G = – 3416.5711 a. u.
f = 237.1554i

Final complex (IIc in 4):

N	2.896002000	2.482576000	0.143931000	C	-4.579599000	0.800959000	-0.722558000
C	1.693113000	1.903094000	0.128991000	H	2.756879000	-1.179112000	2.840009000
N	1.344259000	0.816326000	0.782358000	H	0.318075000	-1.419993000	1.212856000
C	2.297787000	0.294071000	1.574296000	H	0.905661000	-2.565361000	2.411104000
N	3.526026000	0.841926000	1.737668000	H	0.170495000	-1.090925000	4.246363000
C	3.736598000	1.873180000	0.965505000	H	-0.283445000	0.162613000	3.097928000
Cl	5.383366000	4.122657000	3.403902000	H	-2.627157000	0.376308000	3.054353000
O	0.800481000	2.523325000	-0.659898000	H	-4.879685000	-0.667810000	2.841623000
N	2.033131000	-0.840861000	2.226475000	H	-5.037604000	-3.167487000	2.827563000
C	0.740460000	-1.509049000	2.212234000	H	-2.942762000	-4.485785000	3.028007000
C	-0.230102000	-0.916793000	3.243391000	H	-0.864304000	2.584209000	1.408387000
C	-1.610683000	-1.512438000	3.141930000	H	-3.240581000	1.877026000	1.338688000
C	-2.739644000	-0.698646000	3.047392000	H	-2.828566000	0.883491000	-2.801192000
C	-3.993205000	-1.281751000	2.935166000	H	-0.454732000	1.619392000	-2.733176000
C	-4.084768000	-2.666643000	2.927566000	B	-7.400648000	-0.225676000	-0.603498000
C	-2.910724000	-3.401153000	3.032557000	F	-8.117292000	-0.430750000	0.589797000
N	-1.700040000	-2.848612000	3.136037000	F	-8.219518000	-0.577911000	-1.689514000
C	-0.533550000	2.110727000	-0.655780000	C	-4.805913000	-0.576769000	-0.636389000
C	-1.303785000	2.213944000	0.493178000	C	-3.913001000	-1.688367000	-0.556580000
C	-2.628343000	1.809512000	0.450166000	C	-4.711337000	-2.820714000	-0.493523000
C	-3.181560000	1.305651000	-0.727025000	H	-4.368644000	-3.839600000	-0.410180000
C	-2.402933000	1.258374000	-1.879844000	C	-6.055480000	-2.420729000	-0.516825000
C	-1.074995000	1.666755000	-1.849465000	C	-2.420115000	-1.706308000	-0.522164000

H	-2.070008000	-2.690832000	-0.213318000
H	-2.019260000	-0.967276000	0.169480000
H	-1.996765000	-1.490465000	-1.504167000
C	-7.266681000	-3.280524000	-0.443071000
H	-7.908154000	-3.120623000	-1.311151000
H	-7.860082000	-3.034191000	0.439630000
H	-6.981459000	-4.329781000	-0.397880000
C	-5.642901000	1.705441000	-0.778456000
C	-5.675014000	3.126357000	-0.919355000
C	-7.016235000	3.481431000	-0.931161000
H	-7.412669000	4.479898000	-1.026293000
C	-7.787599000	2.314581000	-0.806473000
C	-4.538236000	4.087892000	-1.049535000
H	-4.918437000	5.077536000	-1.301614000
H	-3.832790000	3.781204000	-1.822174000
H	-3.970636000	4.170034000	-0.121144000
C	-9.269823000	2.197000000	-0.779003000
H	-9.626319000	1.632243000	-1.642642000
H	-9.726700000	3.184648000	-0.789135000
H	-9.599219000	1.658178000	0.110852000
N	-6.111229000	-1.079057000	-0.603152000
N	-6.965284000	1.254041000	-0.719714000
N	5.054837000	2.471768000	1.010094000
C	6.227312000	1.525095000	1.071570000
N	5.788007000	-1.589745000	-2.684795000
P	4.556268000	-1.574838000	-1.599333000
O	4.368761000	-0.274262000	-0.927082000
C	7.444978000	2.150865000	0.400455000
C	7.315711000	2.272733000	-1.124899000
C	7.302753000	0.916294000	-1.854956000
C	6.305044000	0.861446000	-3.011041000
C	6.138710000	-0.521818000	-3.641072000
O	3.253939000	-2.108170000	-2.335705000
C	1.973603000	-2.040593000	-1.621261000
C	1.135421000	-0.959551000	-2.268182000
C	1.346663000	-3.418724000	-1.667284000
O	4.877368000	-2.803298000	-0.639328000
C	5.962825000	-2.725483000	0.338169000
C	5.382776000	-2.350172000	1.688567000
C	6.657197000	-4.072594000	0.327178000
H	5.126278000	3.132871000	1.900655000
H	6.404957000	1.329363000	2.125664000
H	5.917506000	0.607911000	0.582063000
H	6.067762000	-2.512431000	-2.983498000
H	7.640939000	3.128123000	0.849789000
H	8.304606000	1.521534000	0.644117000
H	8.130776000	2.896460000	-1.496974000
H	6.402730000	2.825632000	-1.375503000
H	8.308248000	0.680243000	-2.215976000
H	7.044966000	0.127415000	-1.149985000
H	5.335623000	1.210088000	-2.653260000
H	6.612866000	1.544413000	-3.808933000
H	5.397703000	-0.461735000	-4.445023000
H	7.082718000	-0.827503000	-4.096455000
H	2.180851000	-1.765013000	-0.584757000
H	1.664607000	-0.007844000	-2.242515000
H	0.915977000	-1.214756000	-3.306790000
H	0.196896000	-0.842270000	-1.729225000
H	1.162247000	-3.719696000	-2.700232000
H	0.394796000	-3.411435000	-1.133321000
H	2.001960000	-4.153233000	-1.198867000
H	6.661781000	-1.953023000	0.006482000
H	4.905008000	-1.373185000	1.640800000
H	6.175861000	-2.312599000	2.437531000
H	4.647229000	-3.094810000	2.000193000
H	5.957528000	-4.860072000	0.613564000
H	7.487337000	-4.071765000	1.035186000
H	7.047684000	-4.297597000	-0.665731000
H	5.122019000	3.082290000	0.196185000

$E = -3417.475255$ a. u.
$H = -3416.464085$ a. u.
$G = -3416.629391$ a. u.