Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Belonging to the manuscript

Playing with Pearson's concept: Orthogonally functionalized 1,4-diaza-1,3-butadienes leading to heterobinuclear complexes

by

J. P. Neu, P. Di Martino-Fumo, B. Oelkers, Y. Sun, A. Neuba, M. Gerhards, and W. R. Thiel*

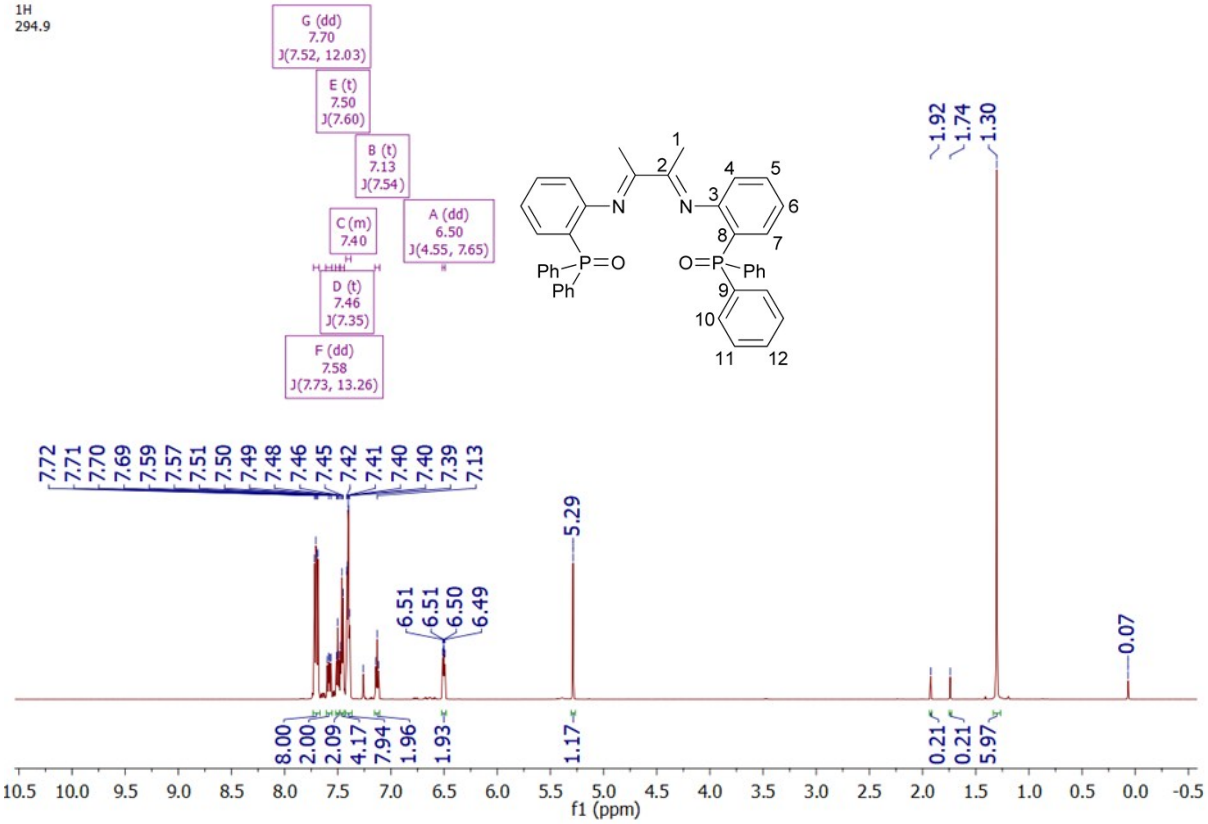
Fachbereich Chemie, Technische Universität Kaiserslautern,
Erwin-Schrödinger Straße 52-54
67663 Kaiserslautern, Germany

Email: thiel@chemie.uni-kl.de

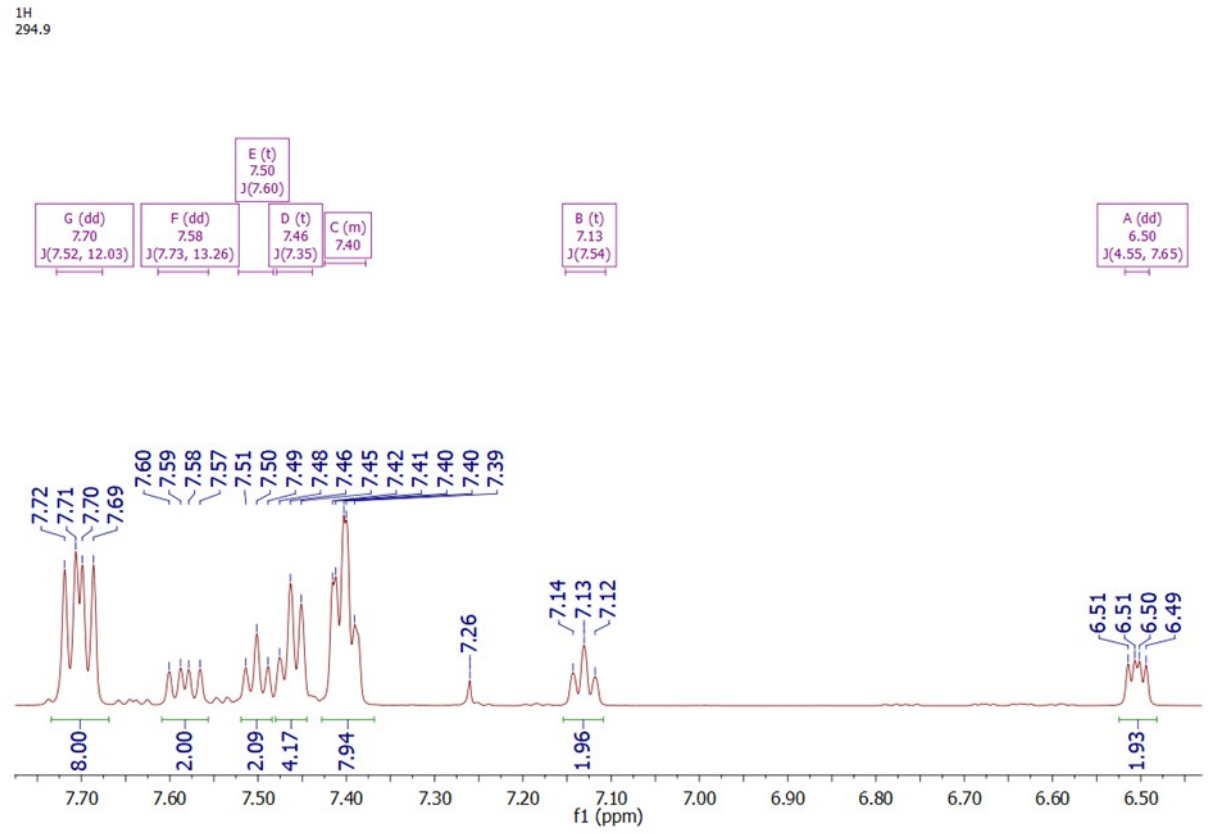
1. Spectroscopic data

1,4-Bis(2-diphenylphosphorylphenyl)-1,4-diaza-2,3-dimethyl-1,3-butadiene (3a)

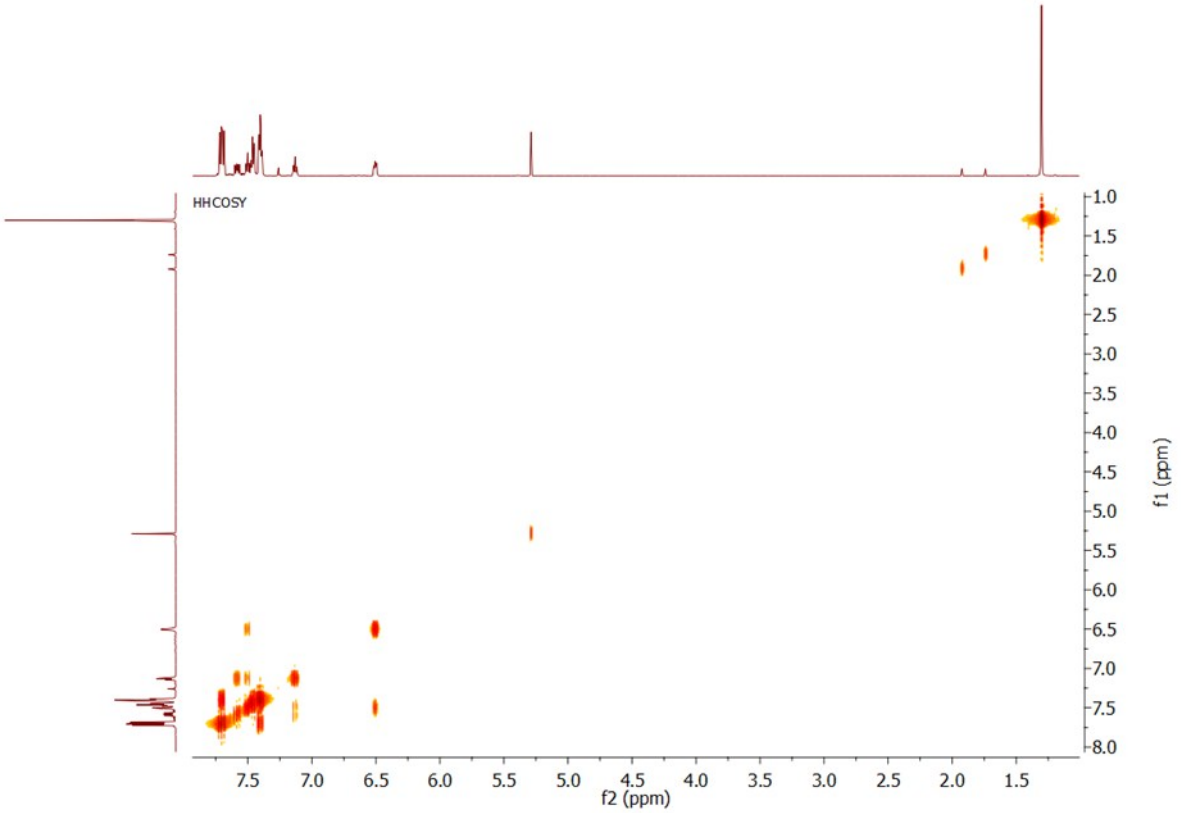
^{1}H NMR spectrum



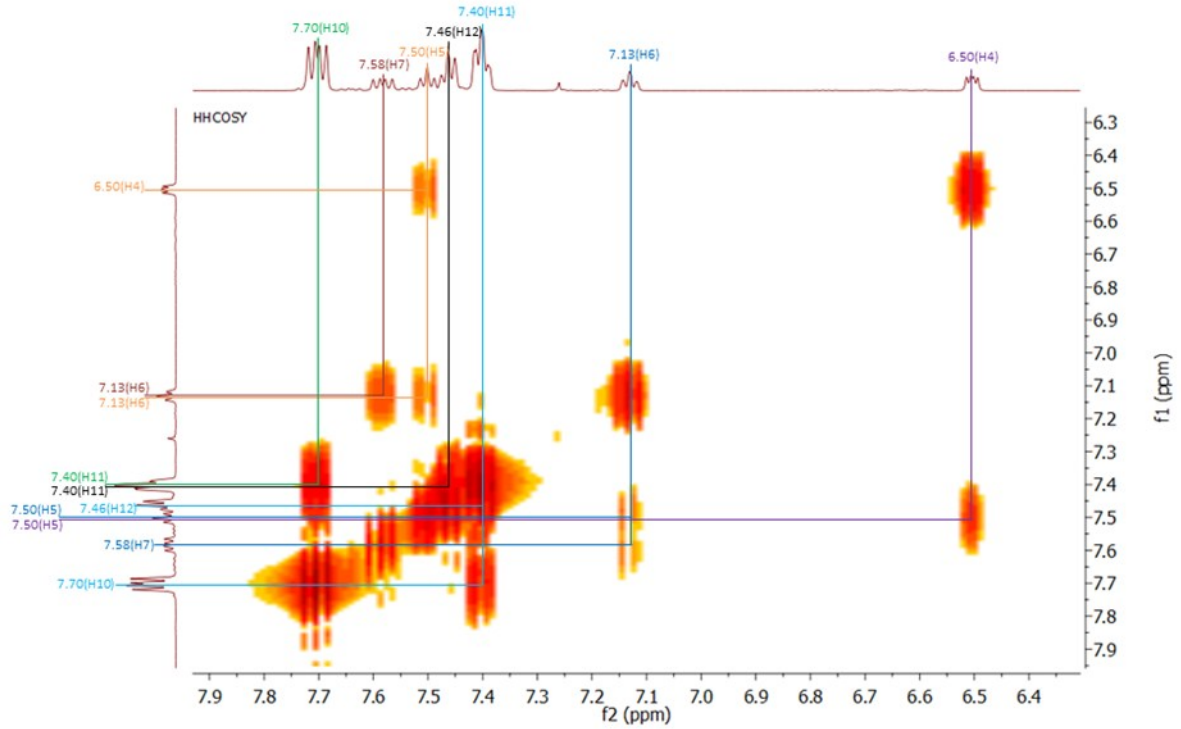
^{1}H NMR spectrum (aromatic region)



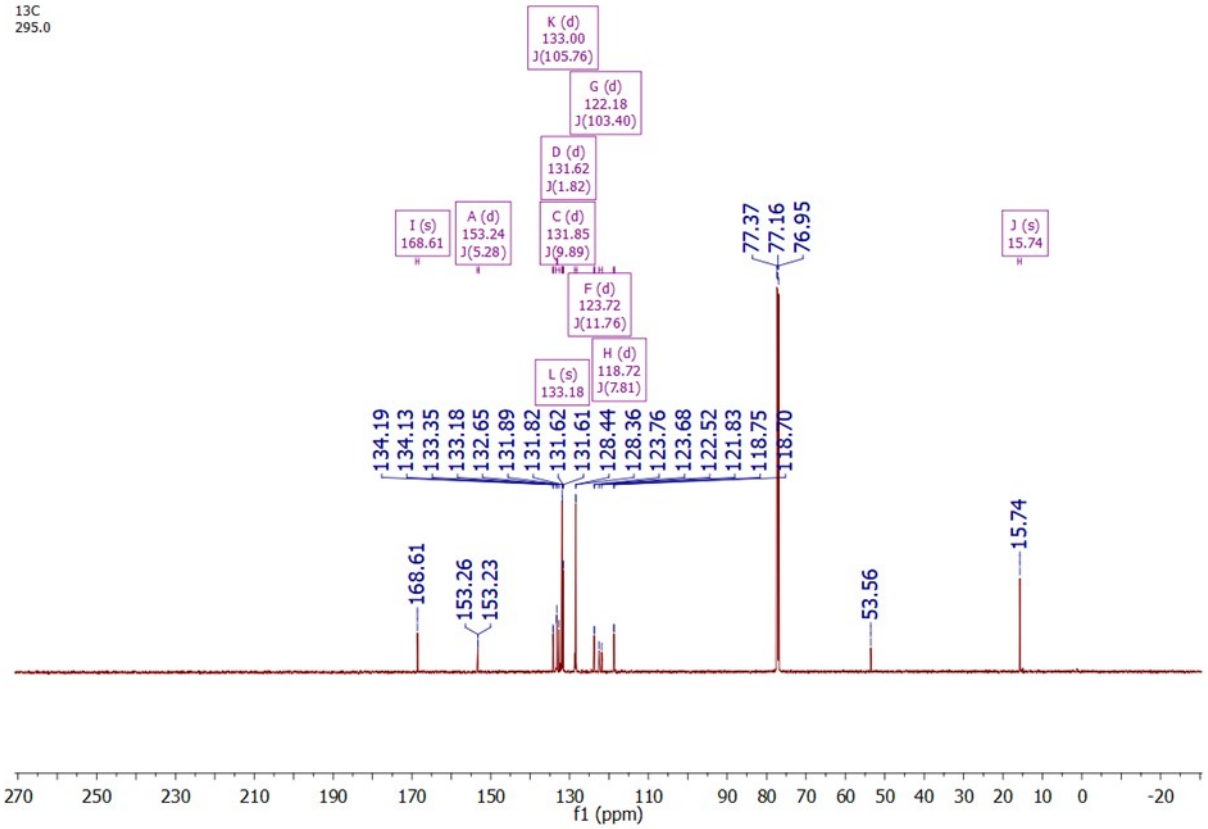
HH-COSY



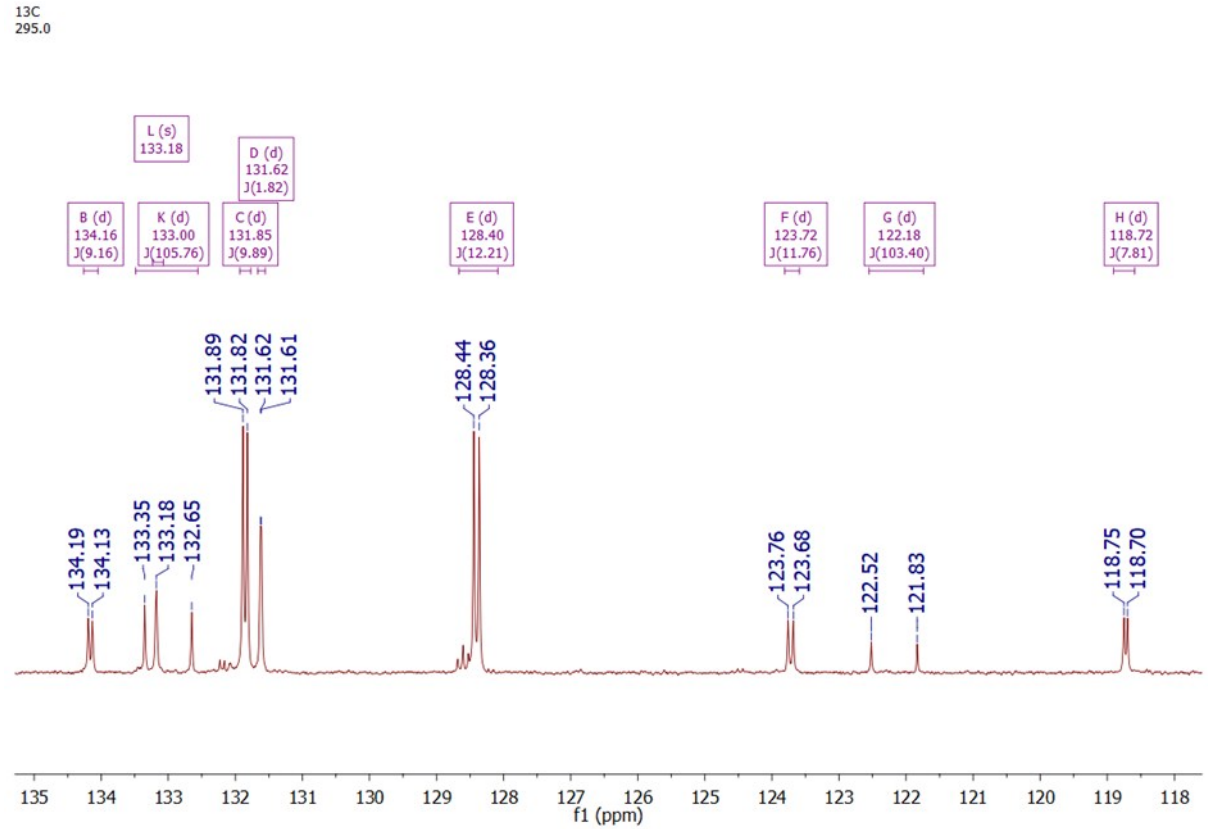
HH-COSY (aromatic region)



$^{13}C\{^{1}H\}$ NMR spectrum



$^{13}C\{^{1}H\}$ NMR spectrum (aromatic region)



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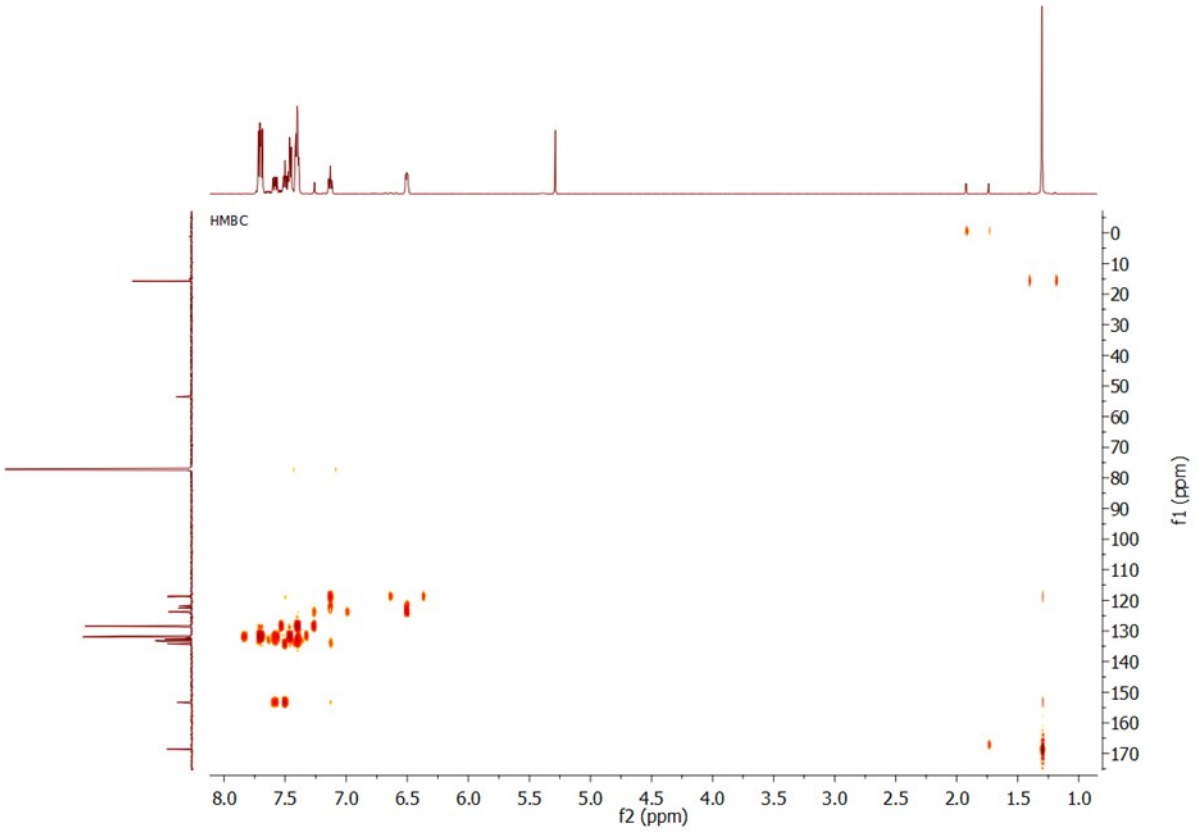

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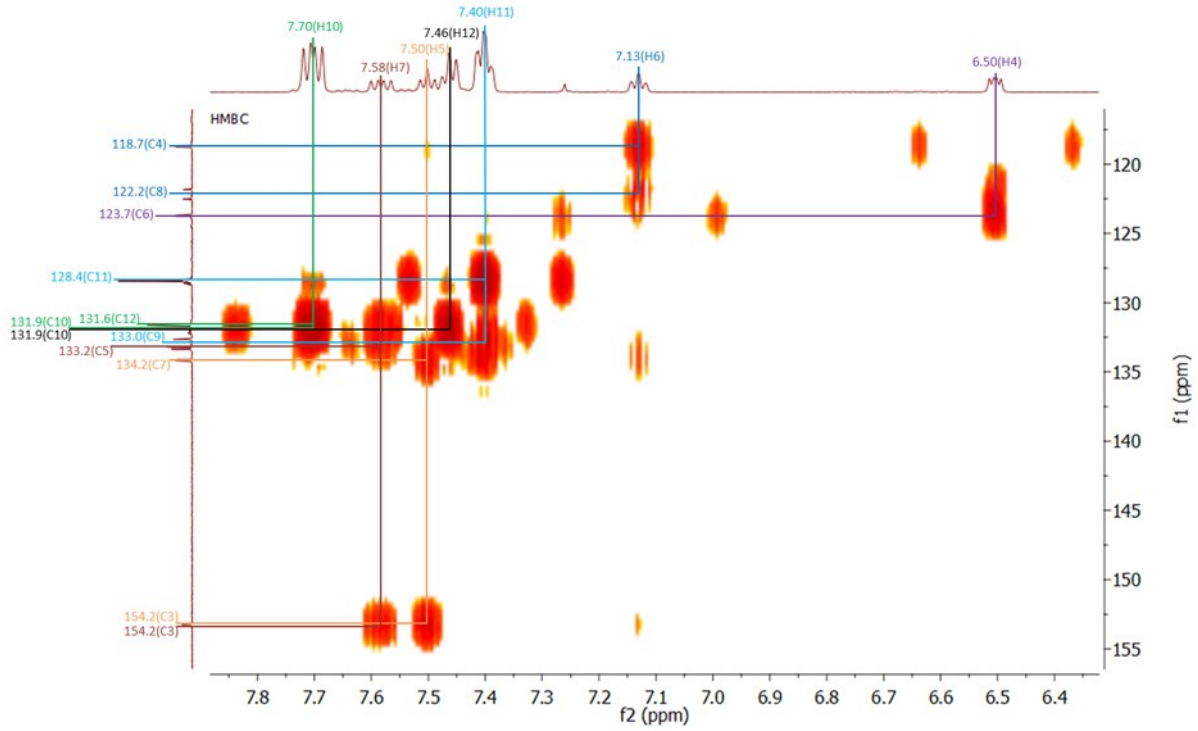

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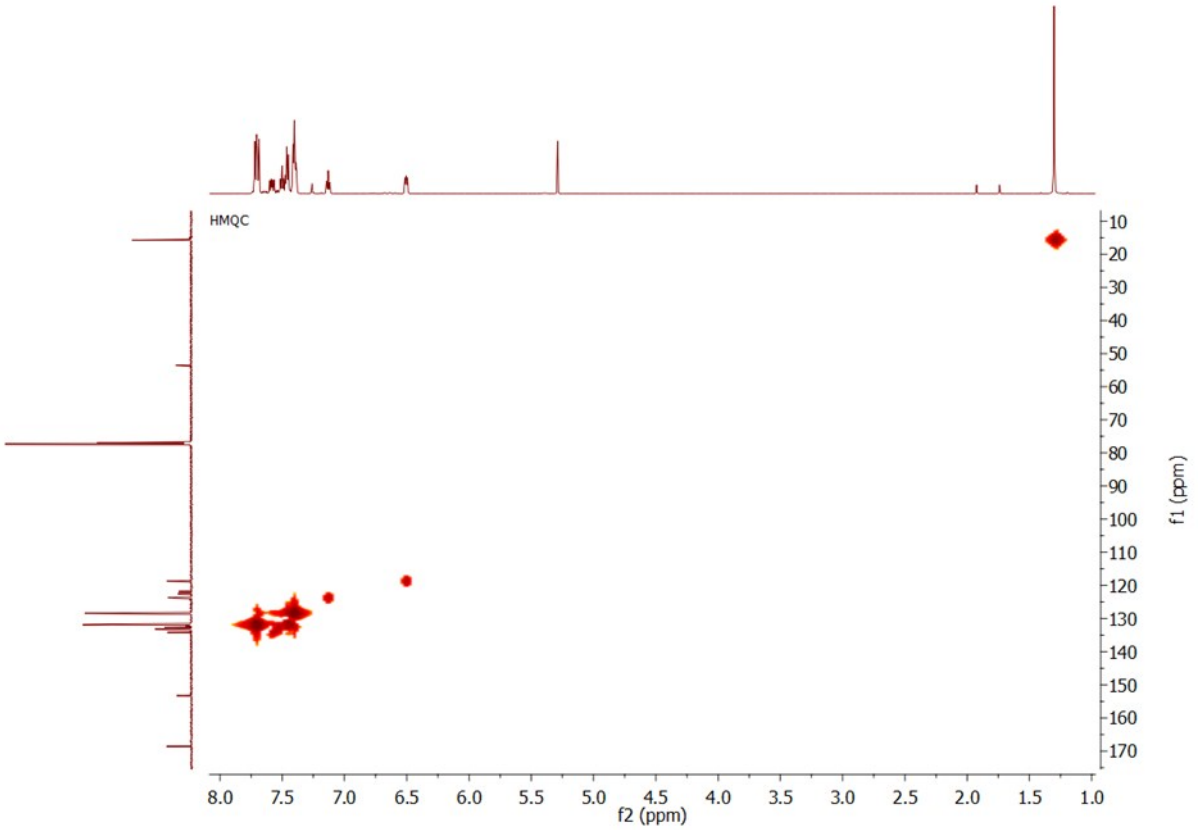
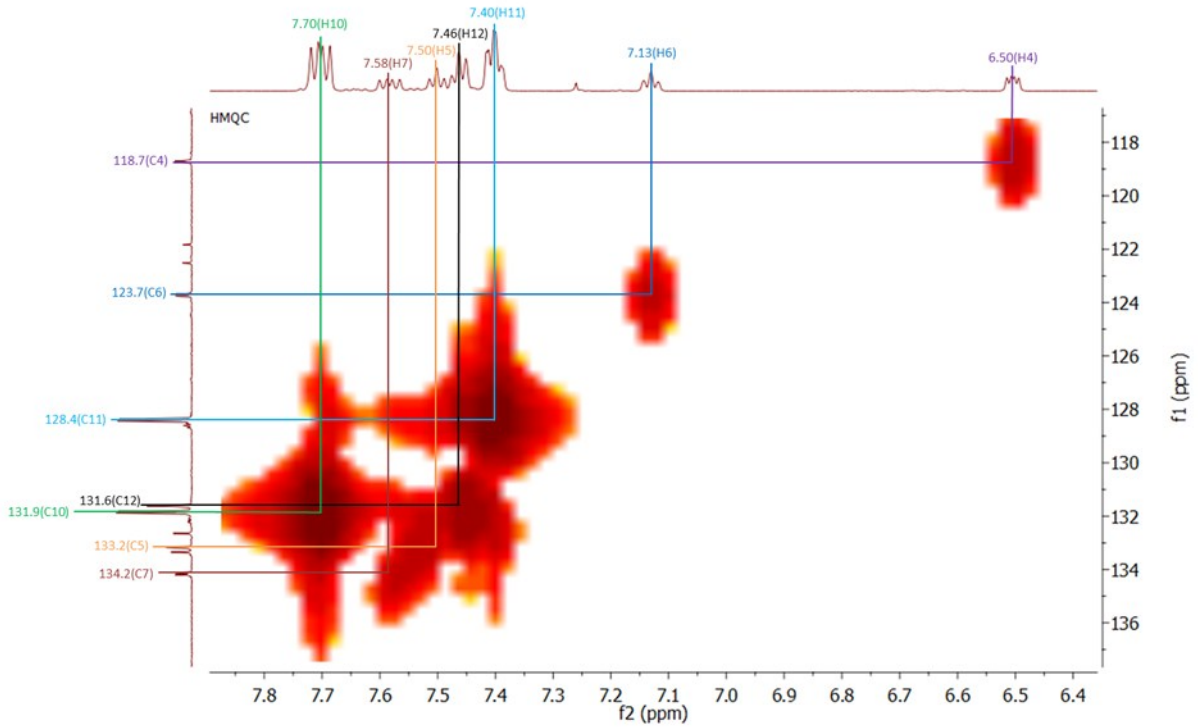
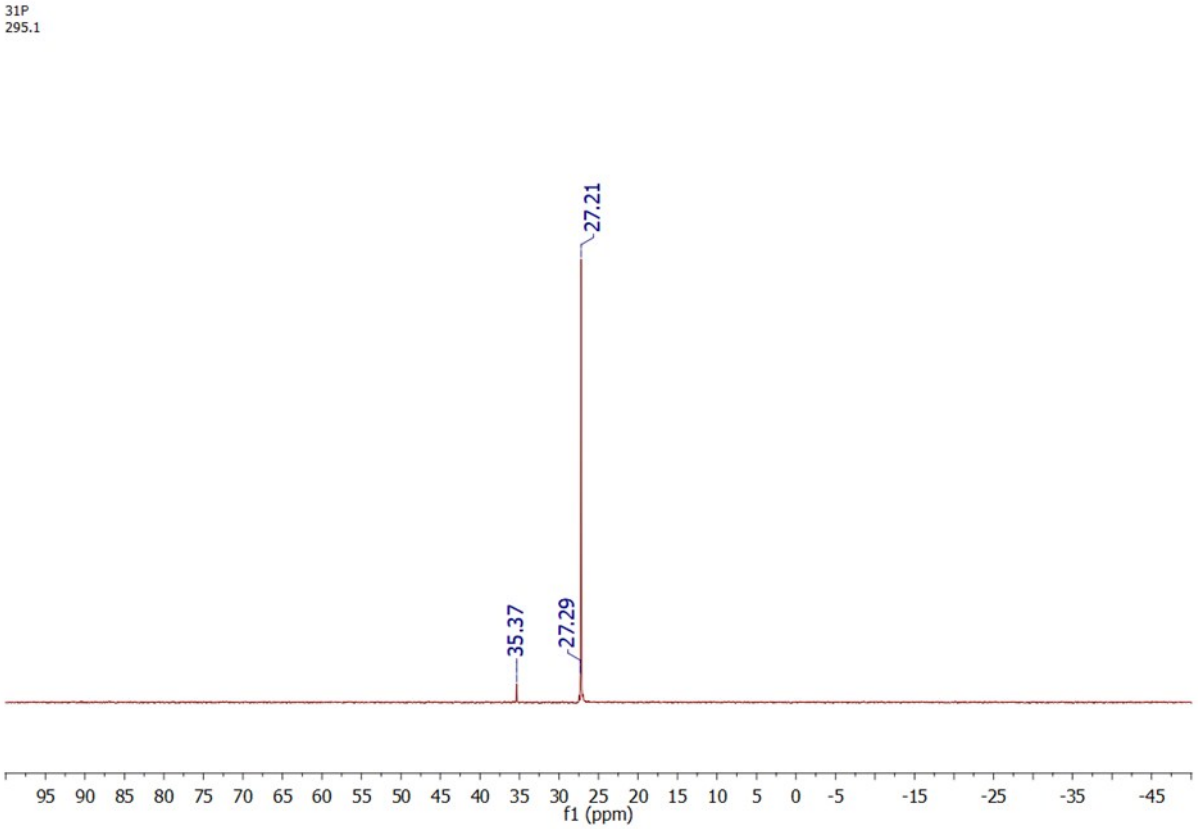


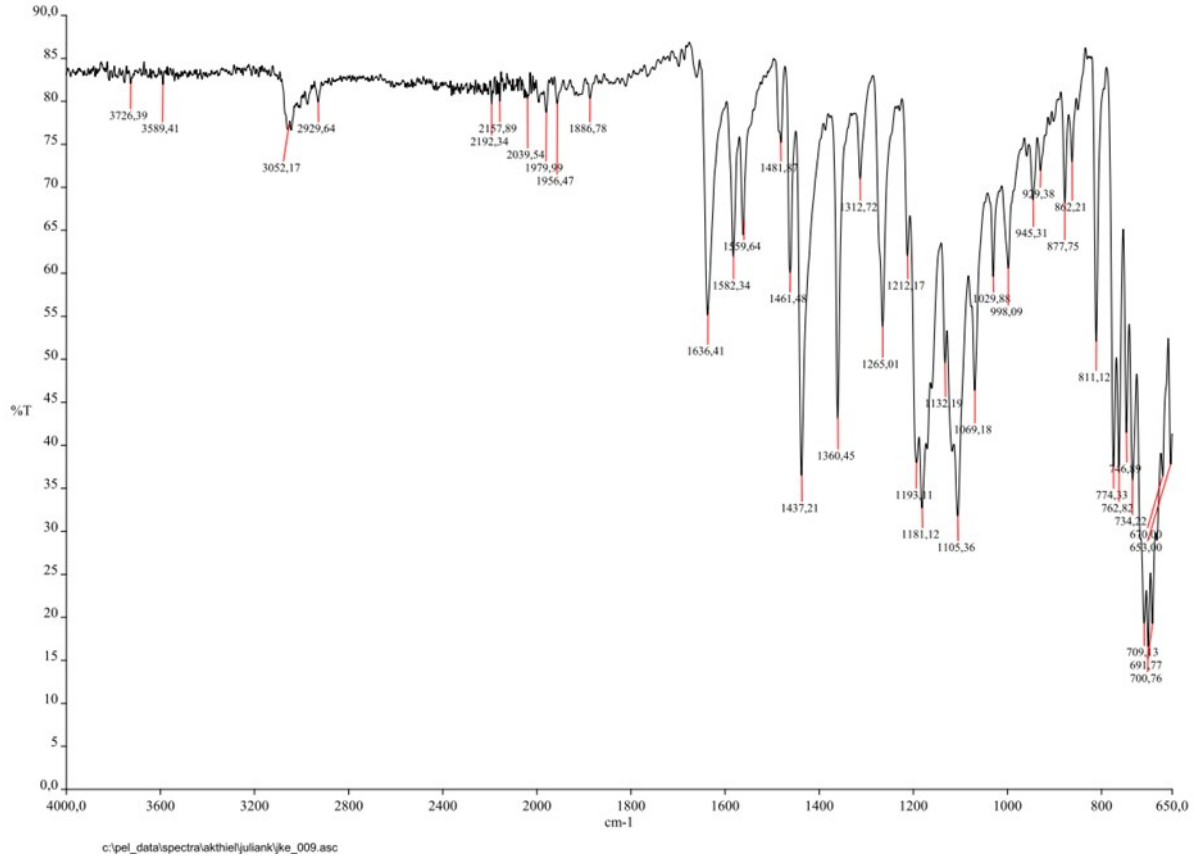
HMQC (aromatic region)



$^{31}P\{^{1}H\}$ NMR spectrum

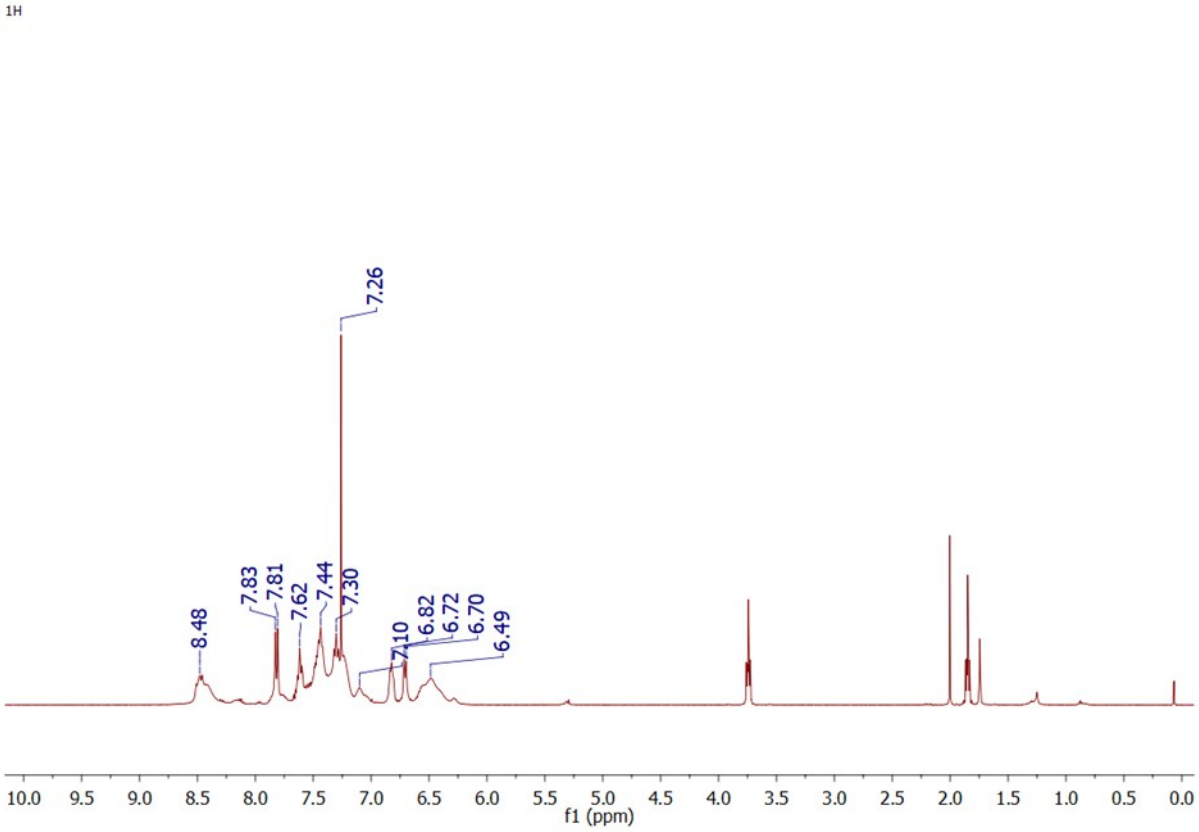


IR spectrum

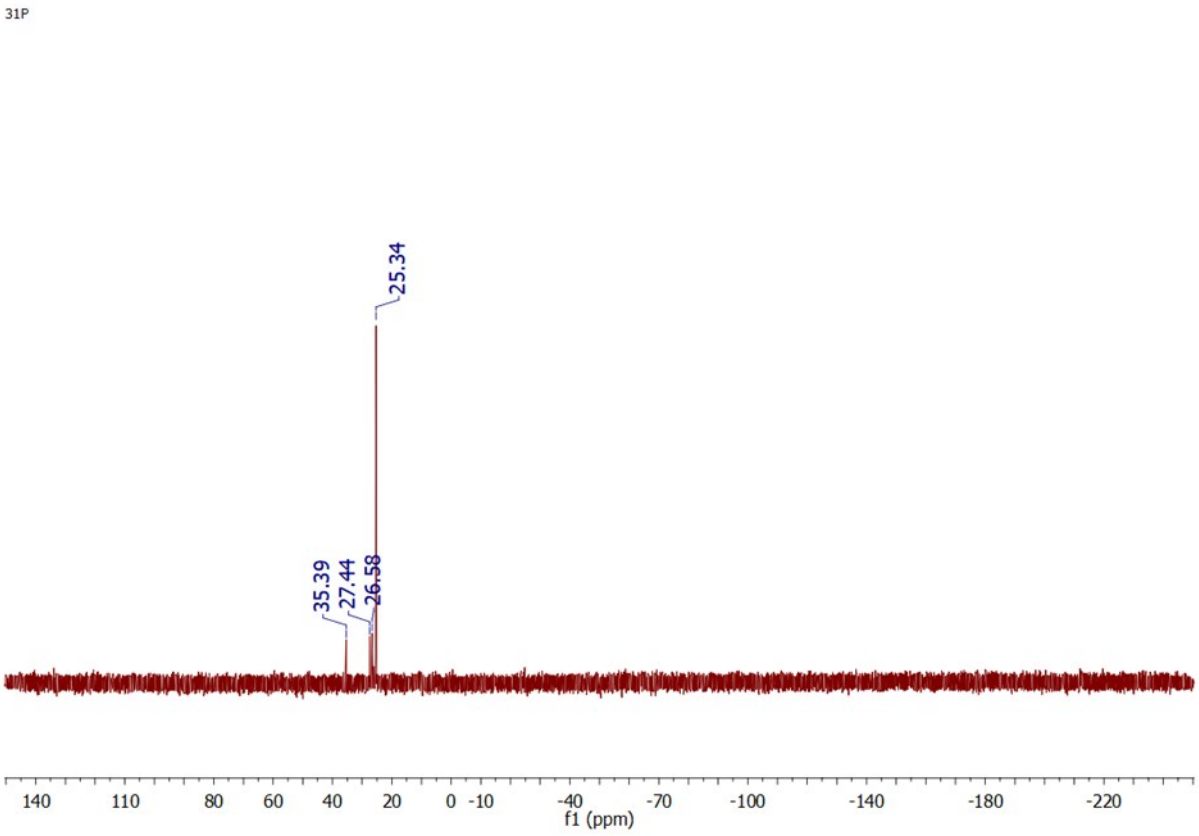


N,*N*'-1,2-Acenaphthylenediylidene(2-diphenylphosphorylphenyl)amine (3b)

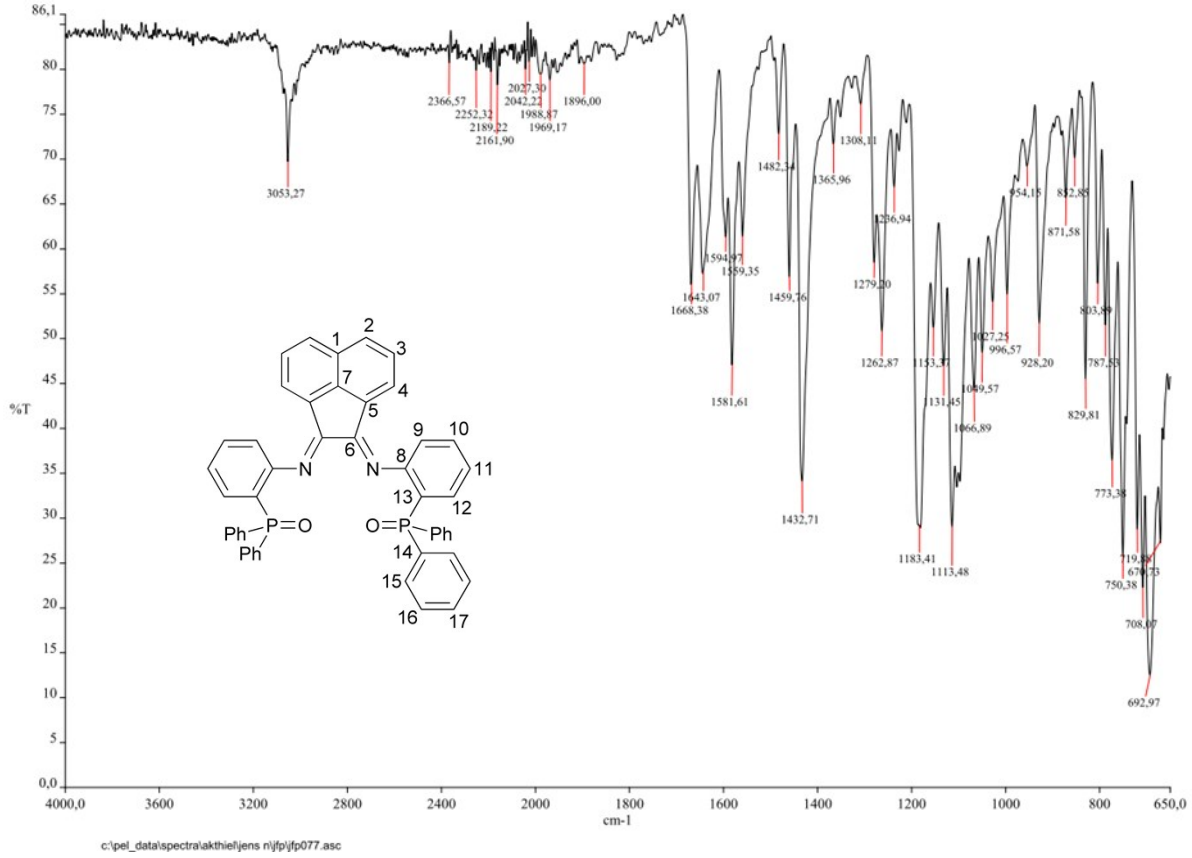
^{1}H NMR spectrum



^{31}P{^{1}H} NMR spectrum



IR spectrum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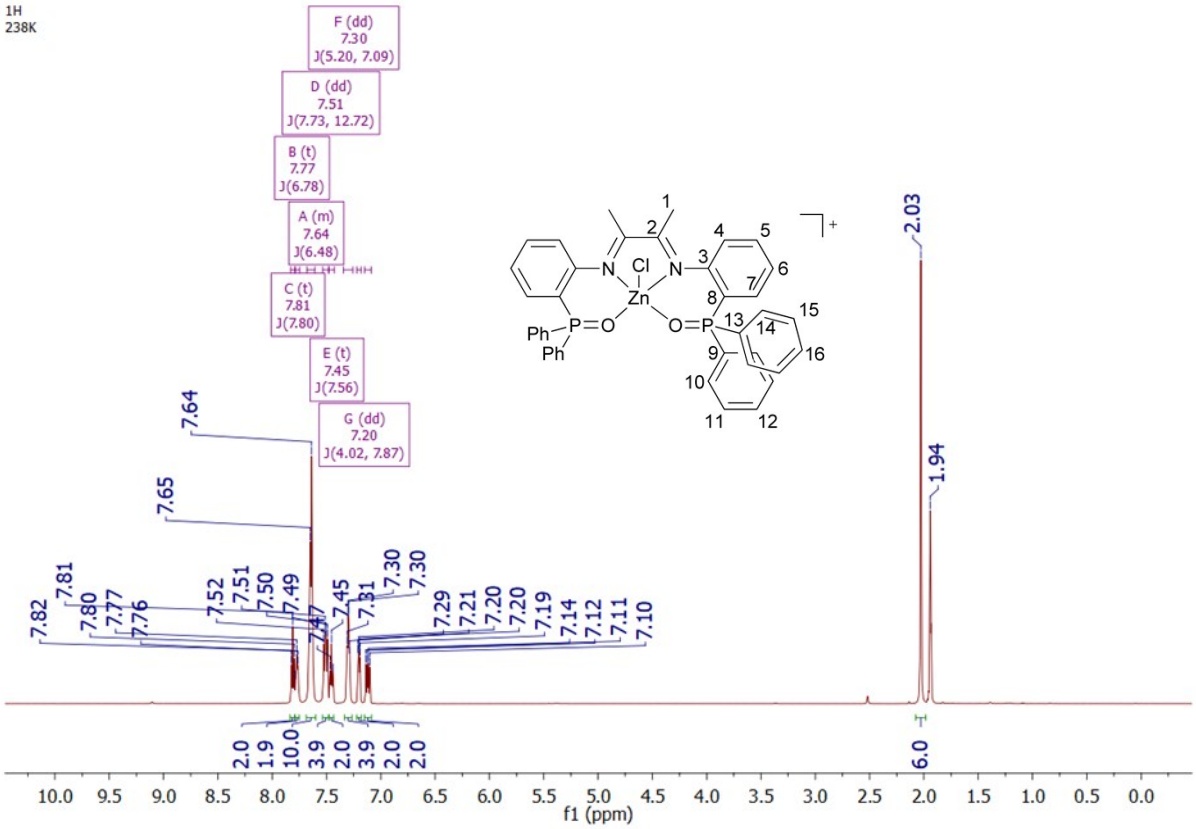
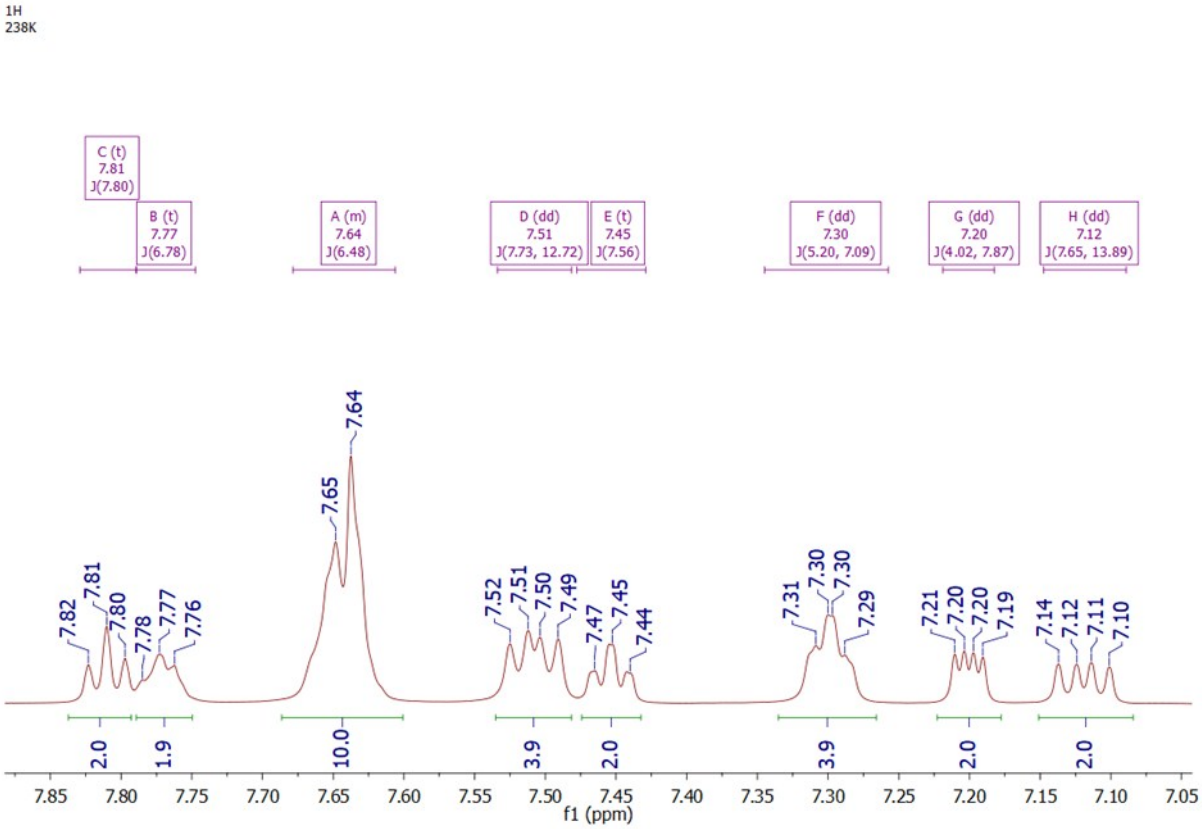
Bis[(1,4-bis(2-diphenylphosphorylphenyl)-1,4-diaza-2,3-dimethyl-1,3-butadiene-κ^2N,κ^2O)chloridozinc] hexachloridodizincate (4a)

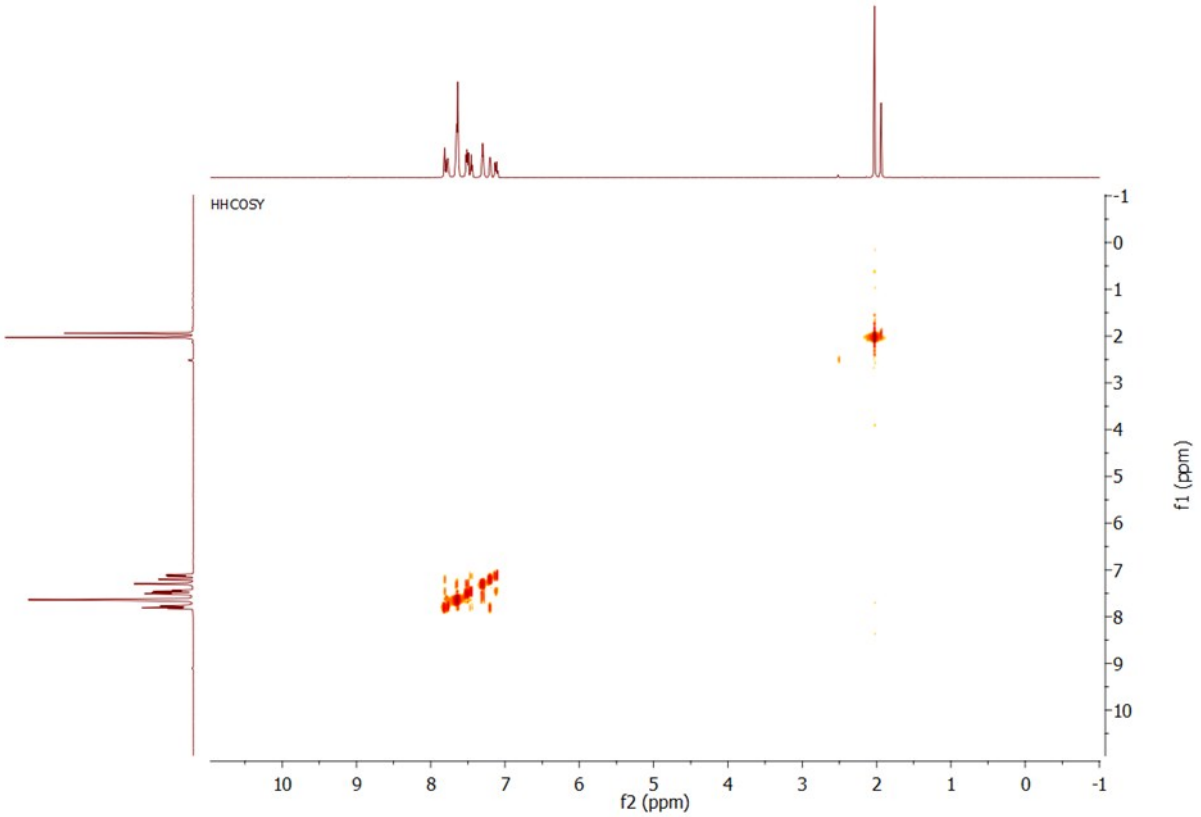
^{1}H NMR spectrum



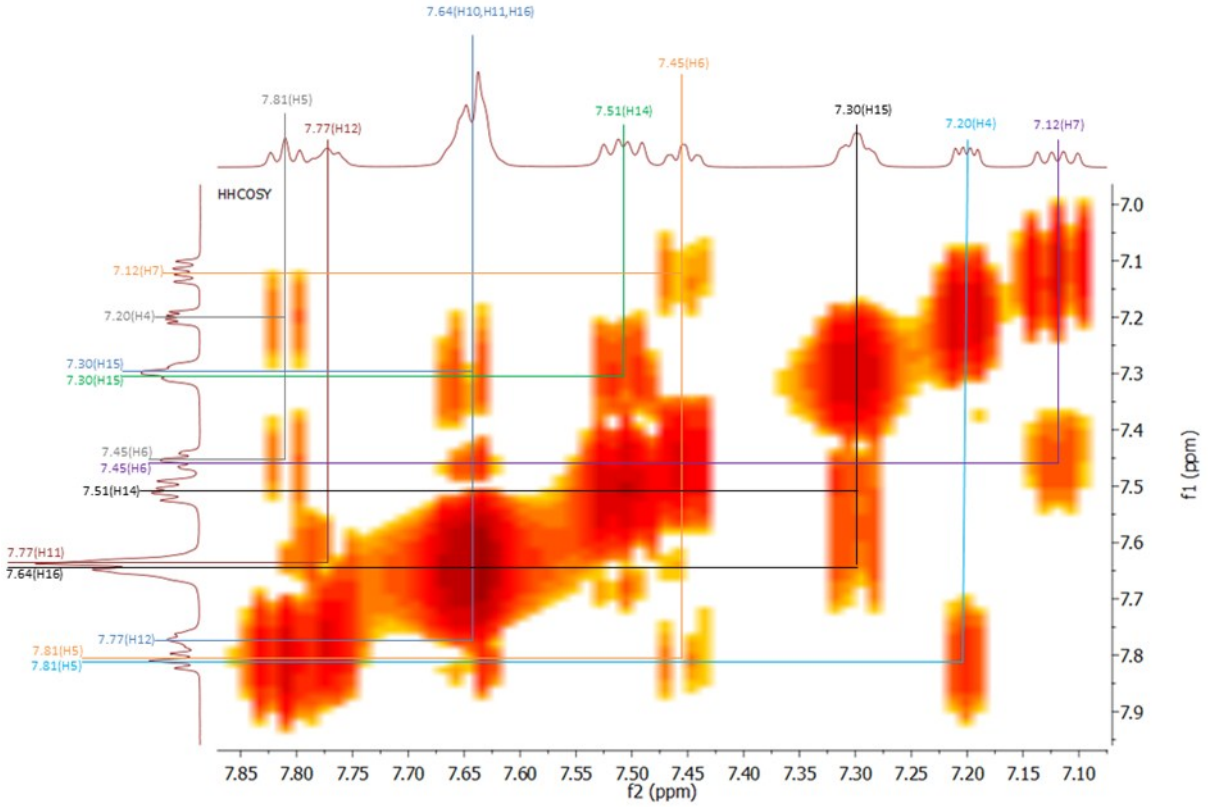
^{1}H NMR spectrum (aromatic region)



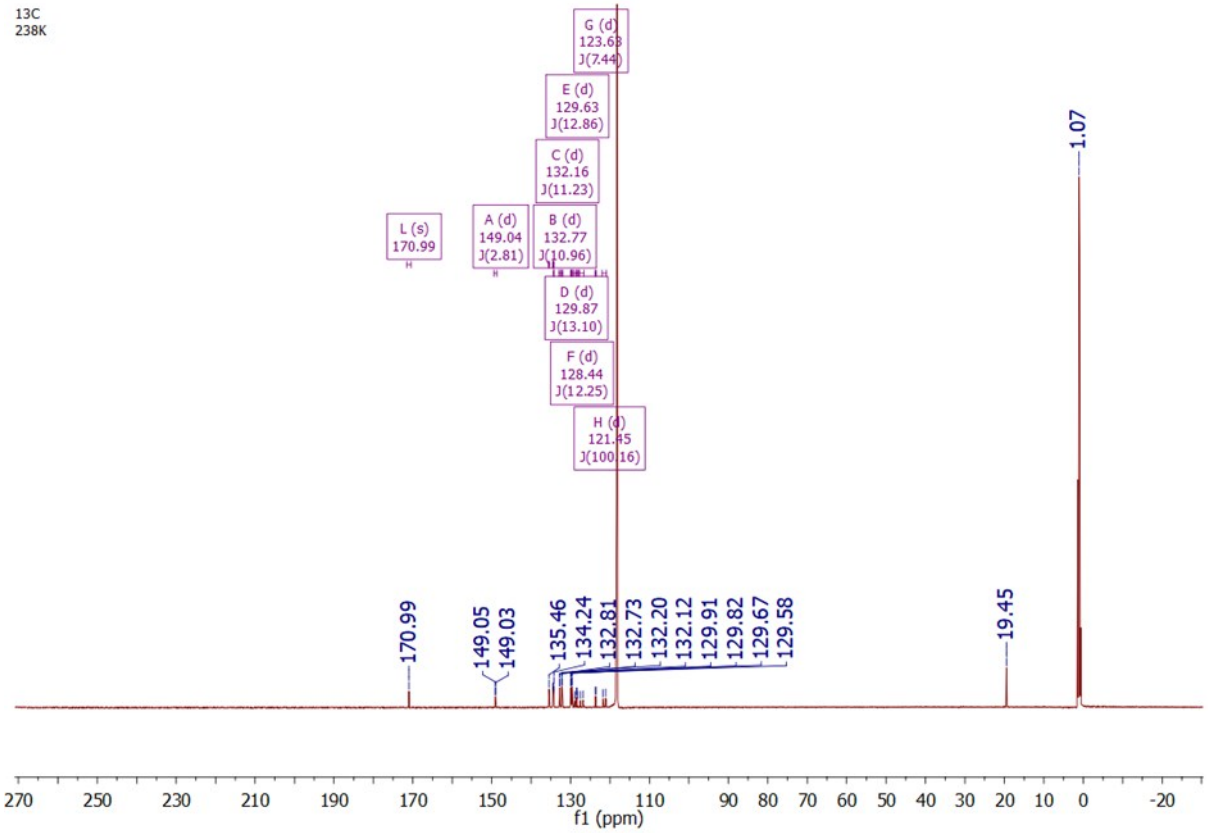
HH-COSY



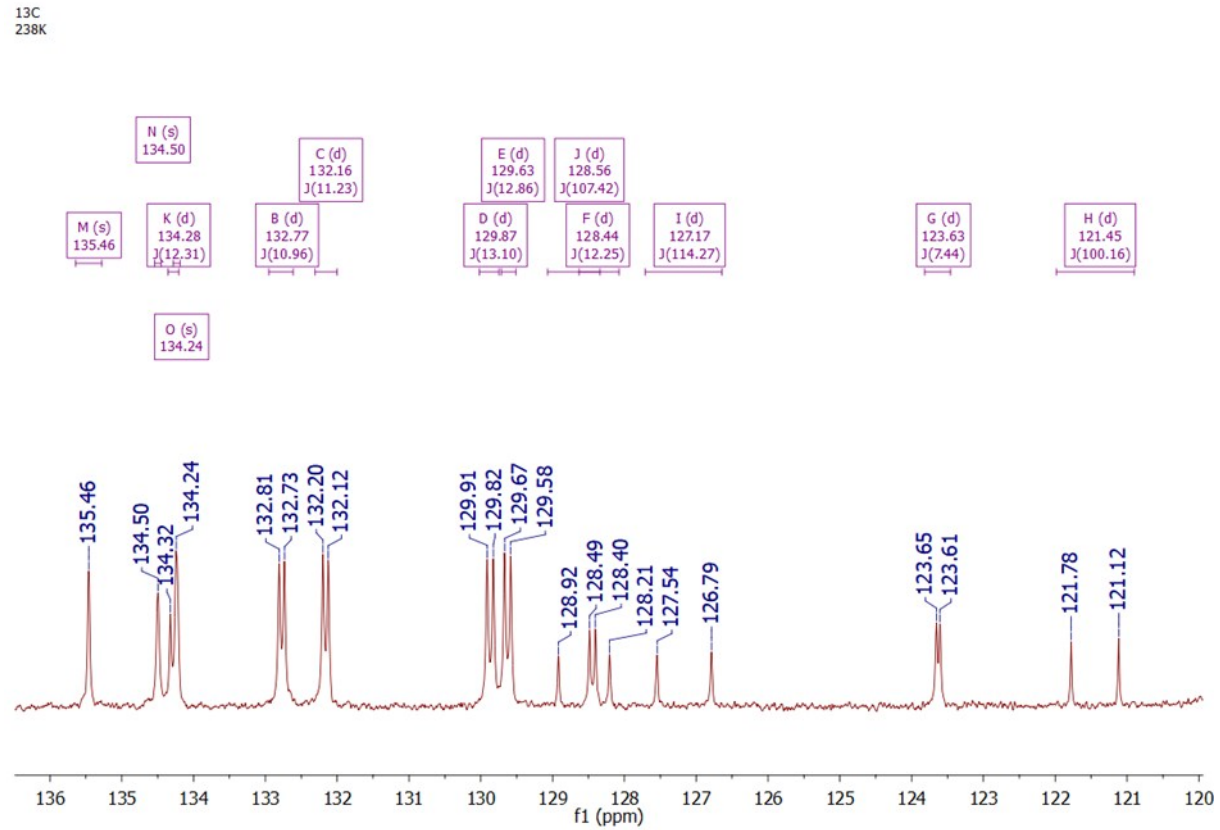
HH-COSY (aromatic region)



$^{13}C\{^{1}H\}$ NMR spectrum



$^{13}C\{^{1}H\}$ NMR spectrum (aromatic region)



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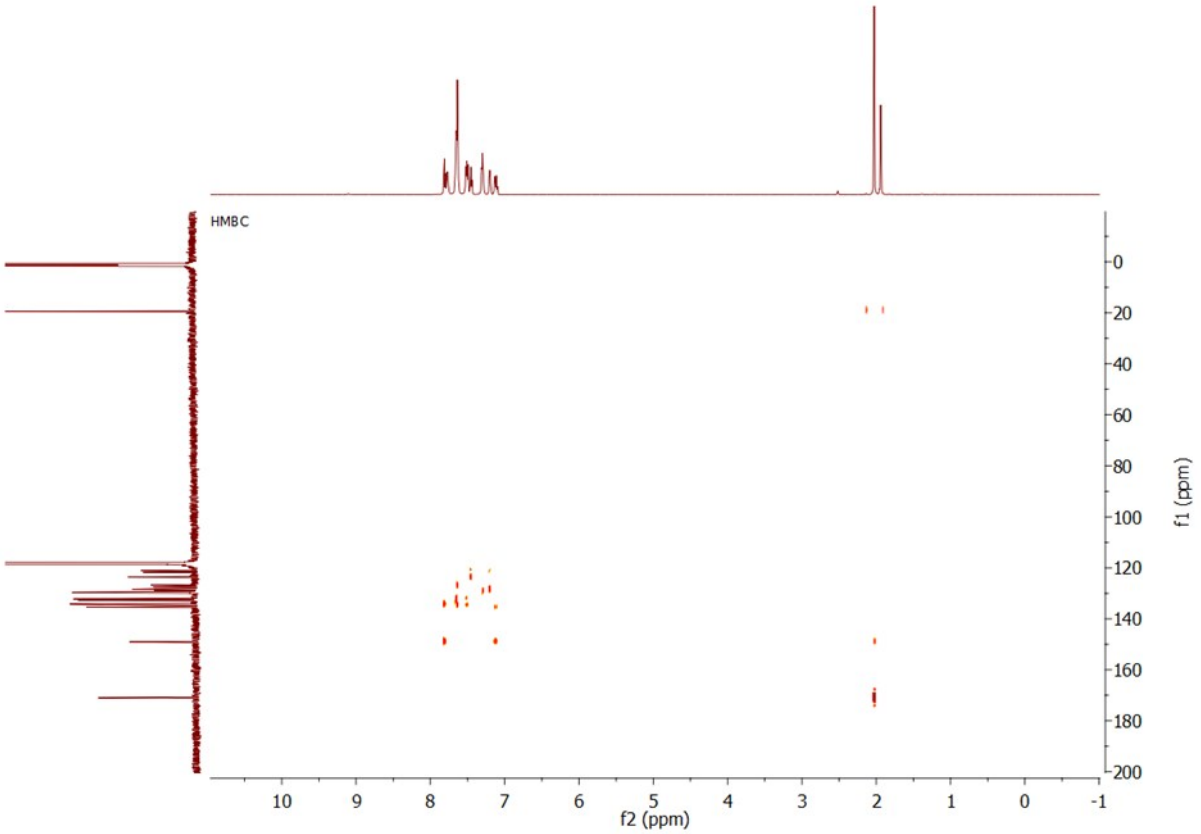

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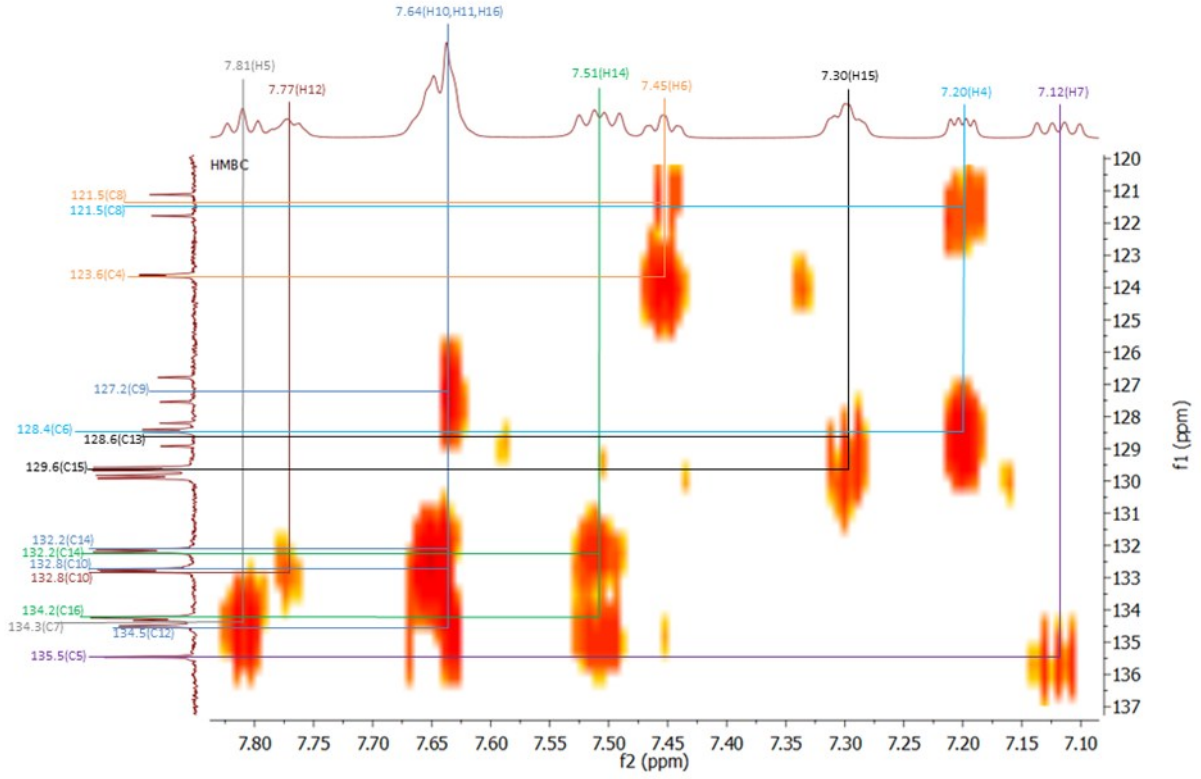

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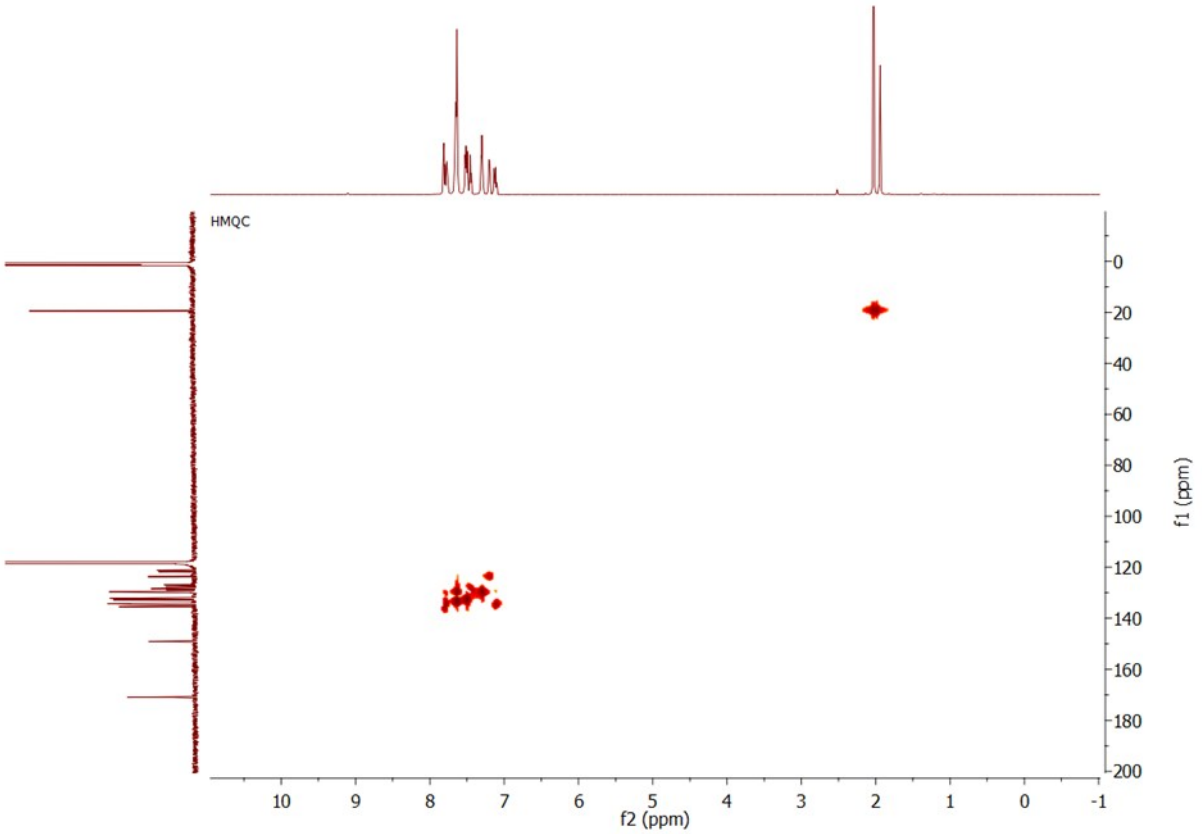
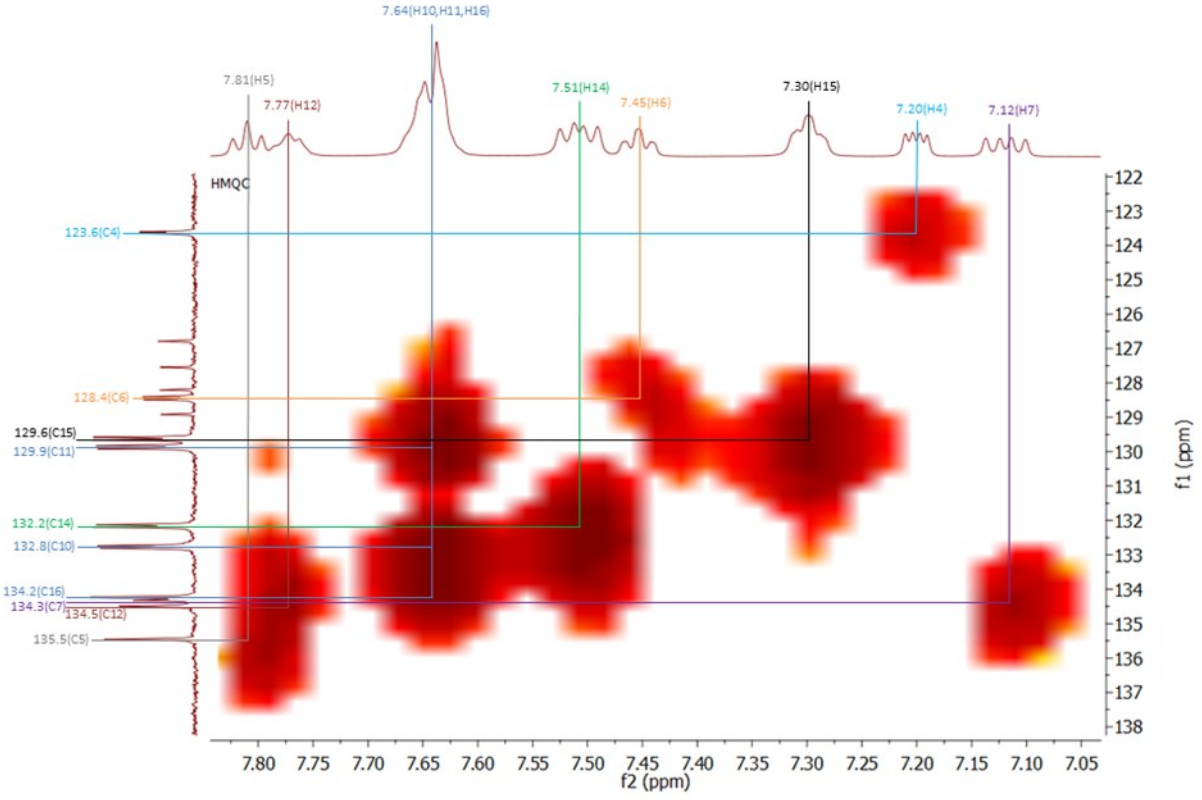
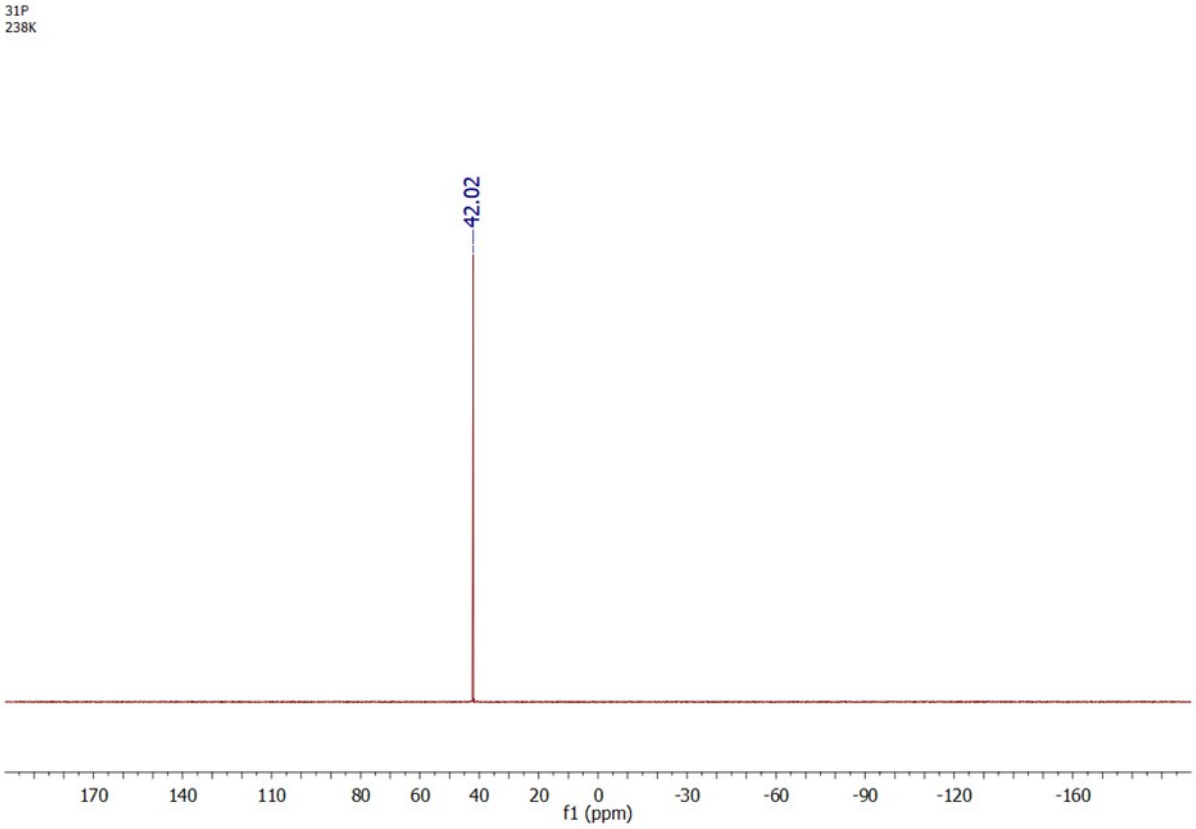


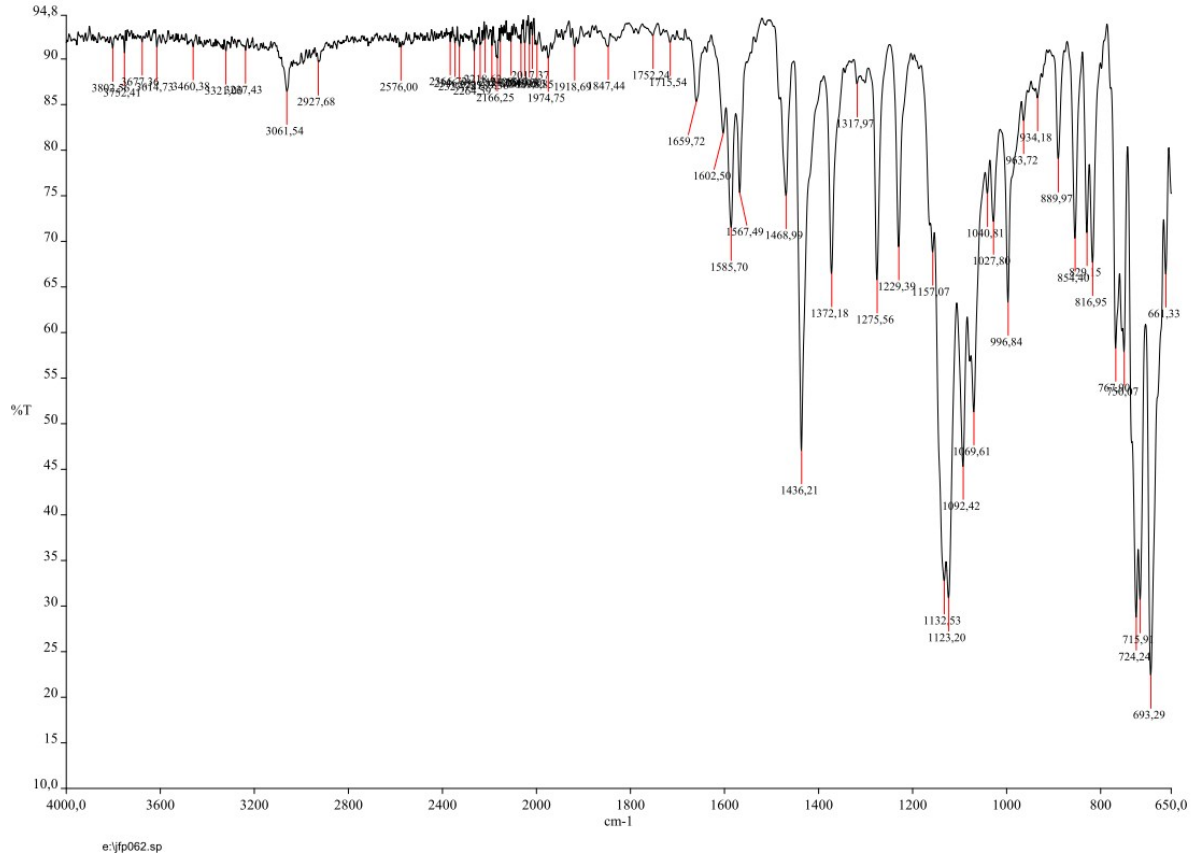
HMQC (aromatic region)



$^{31}P\{^{1}H\}$ NMR spectrum

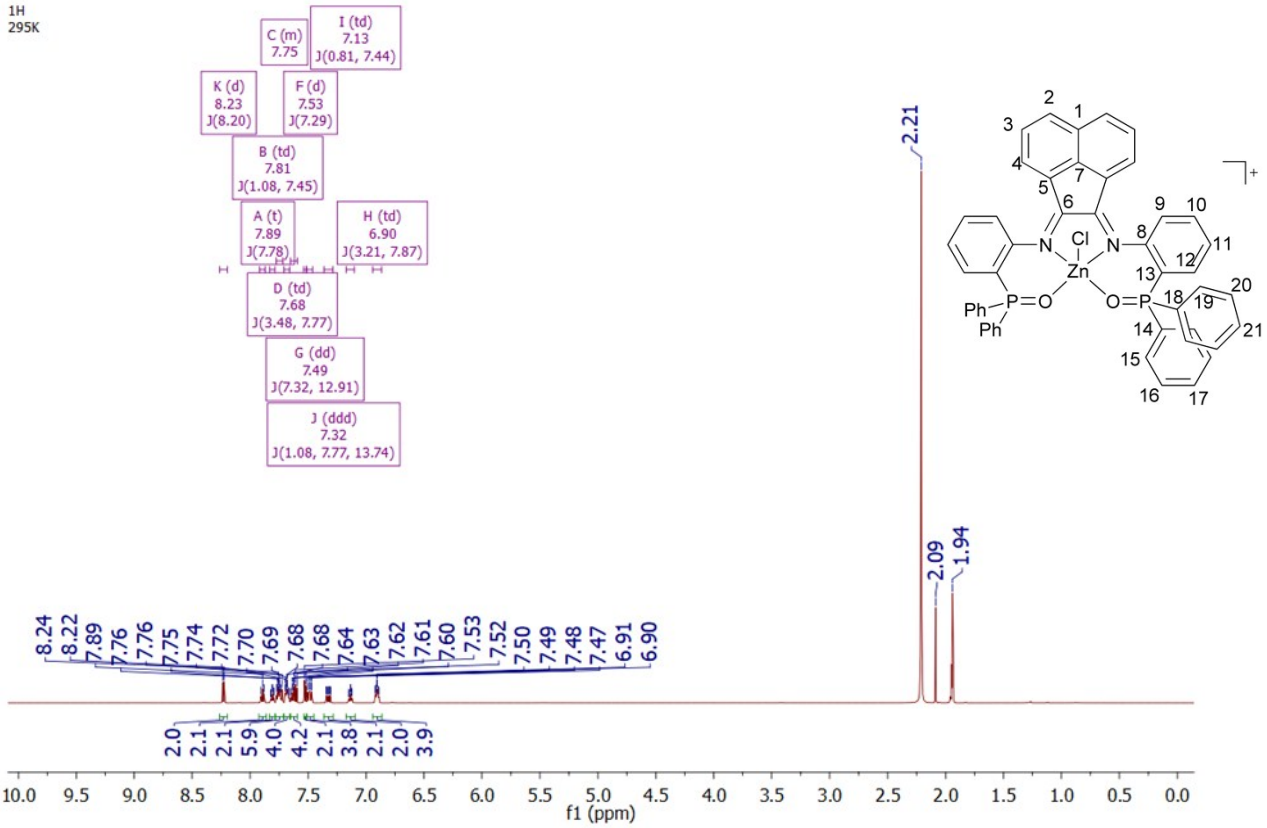


IR spectrum

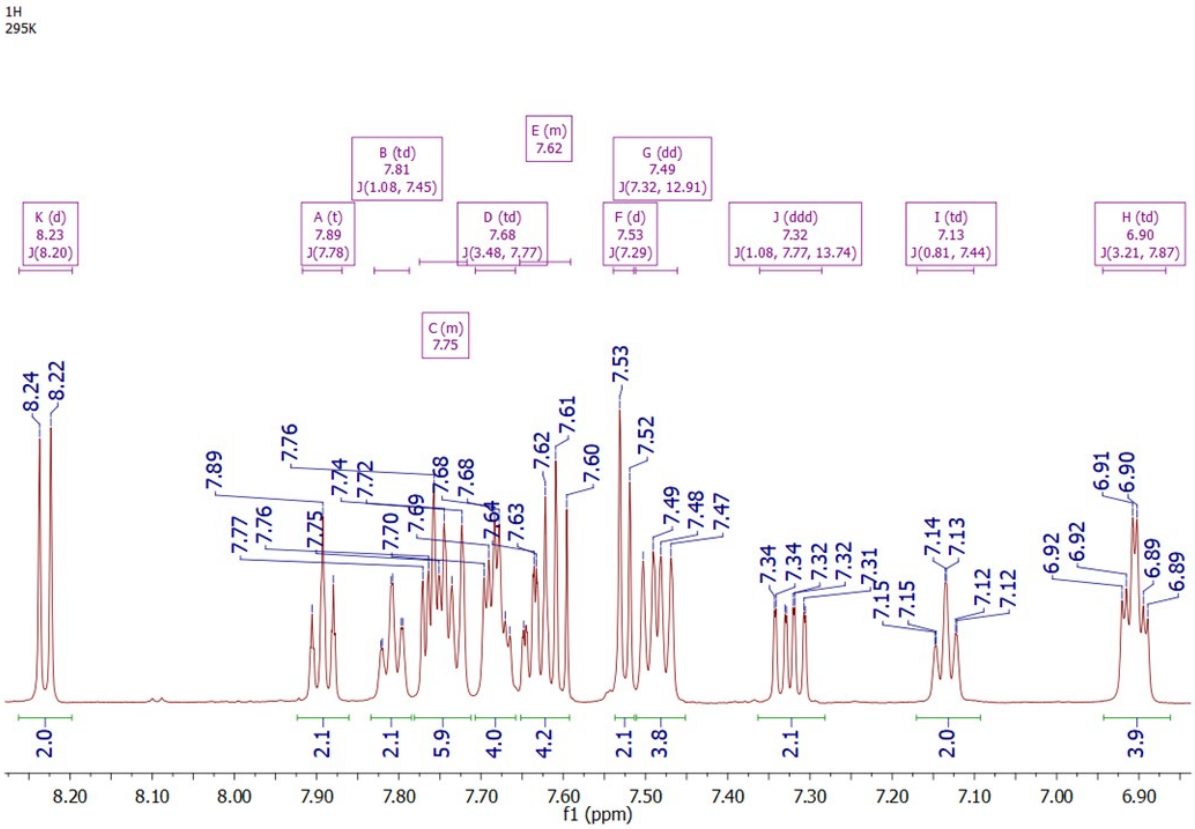


Bis[(*N*,*N*'-1,2-acenaphthylenediylidene(2-diphenylphosphoryl-phenyl)amine-κ^2N,κ^2O)-chloridozinc] hexachloridodizincate (4b)

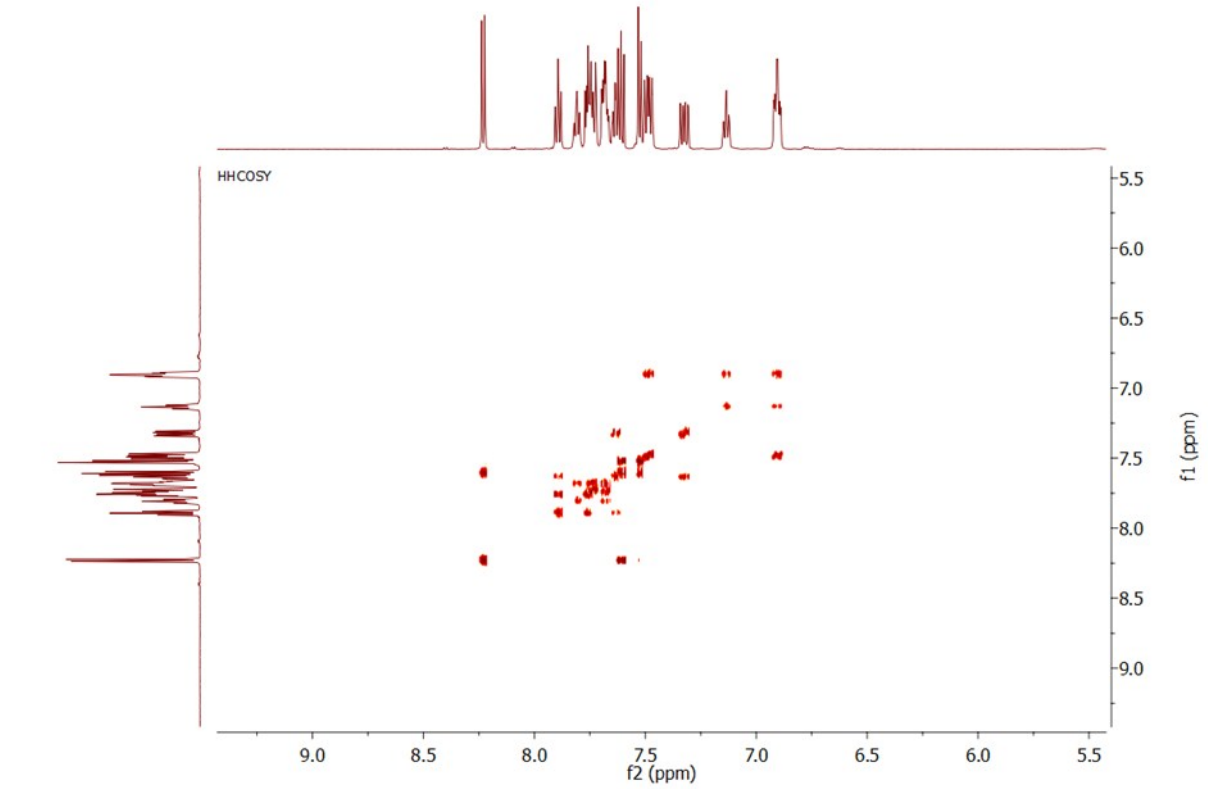
^{1}H NMR spectrum



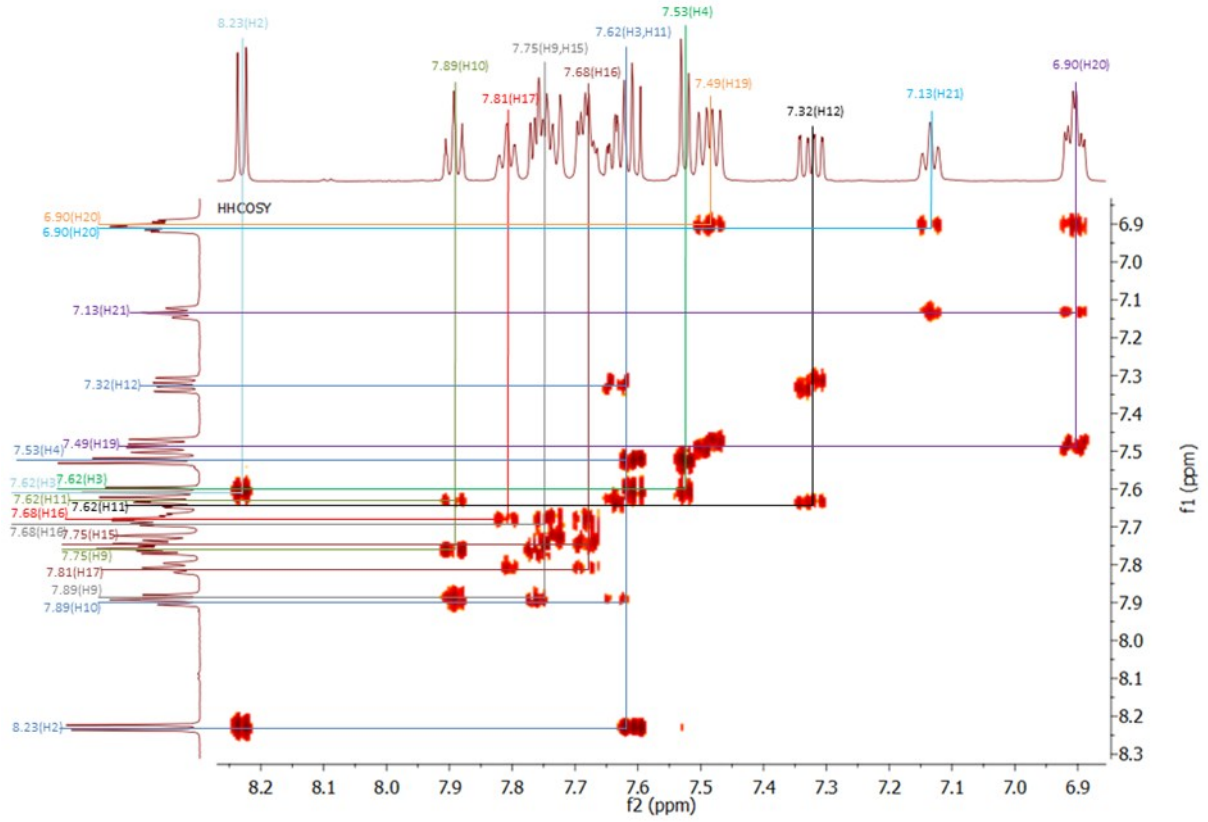
^{1}H NMR spectrum (aromatic region)



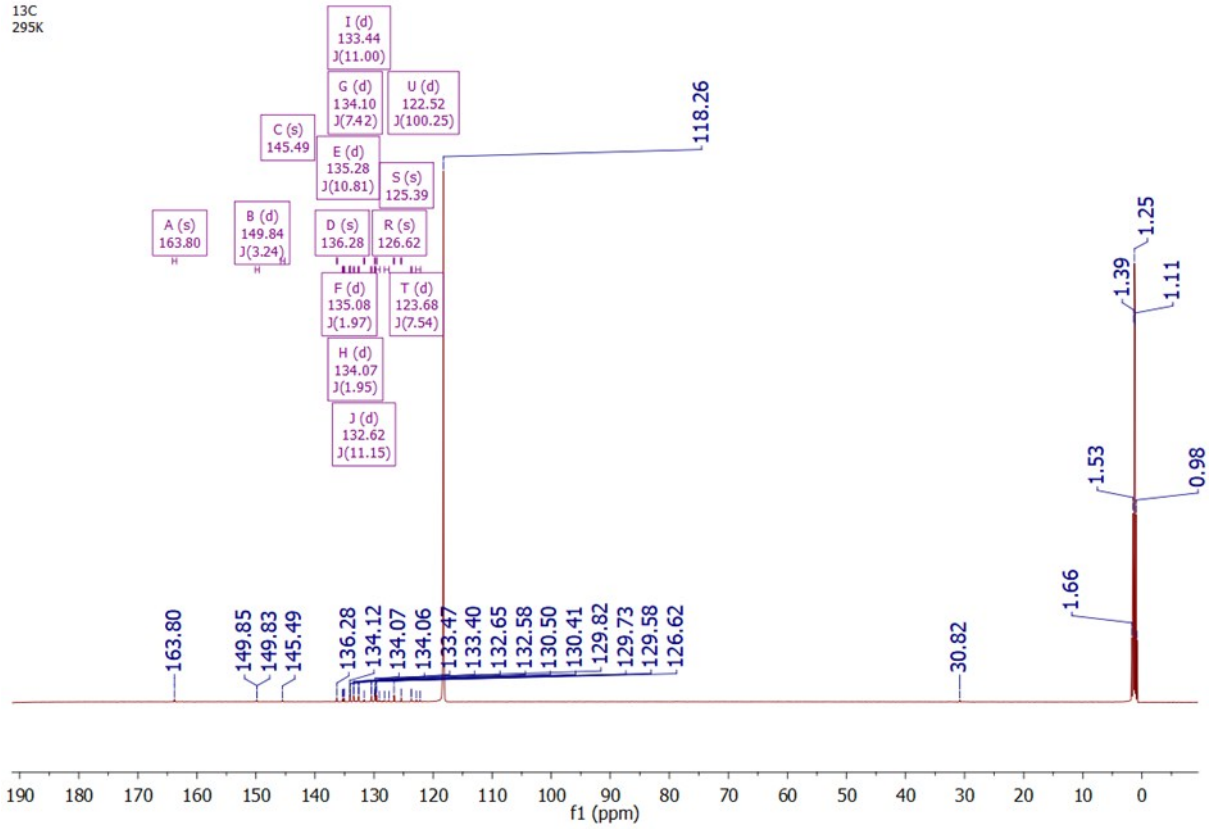
HH-COSY



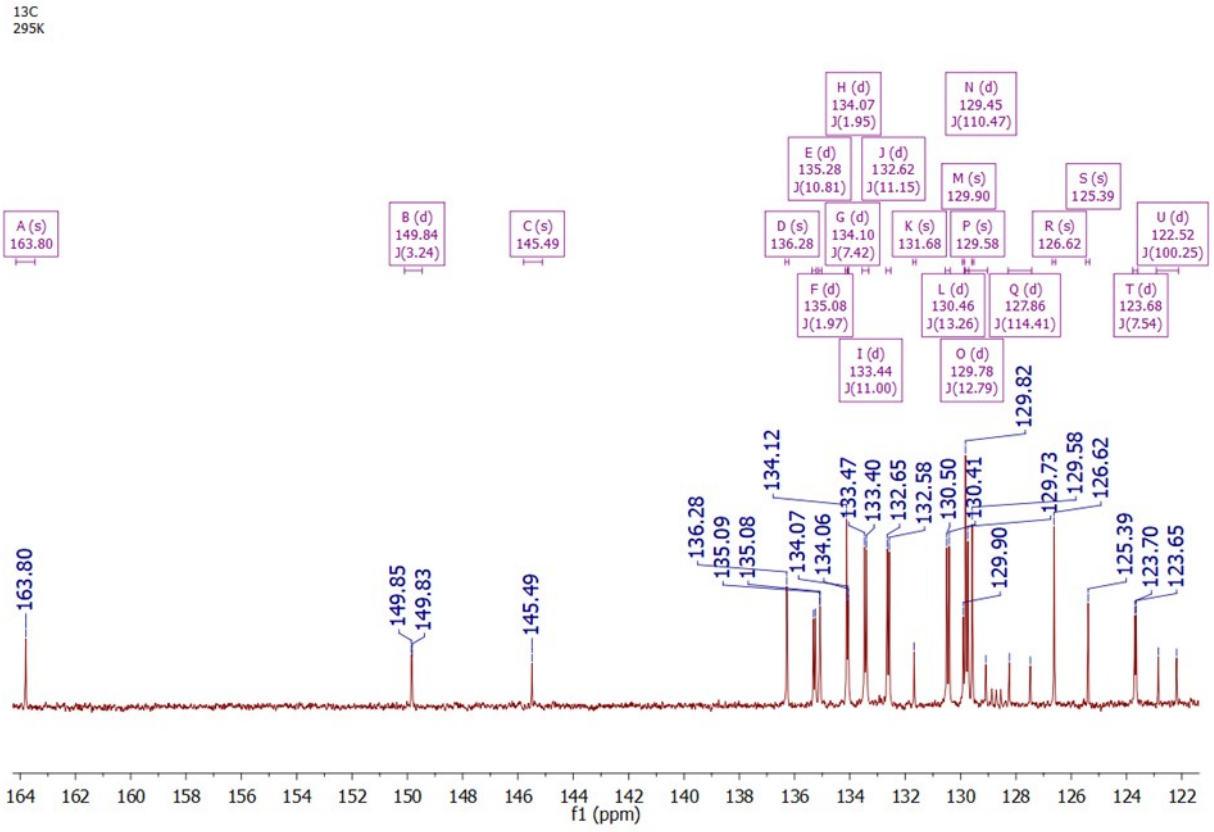
HH-COSY (aromatic region)



$^{13}C\{^{1}H\}$ NMR spectrum



$^{13}C\{^{1}H\}$ NMR spectrum (aromatic region)



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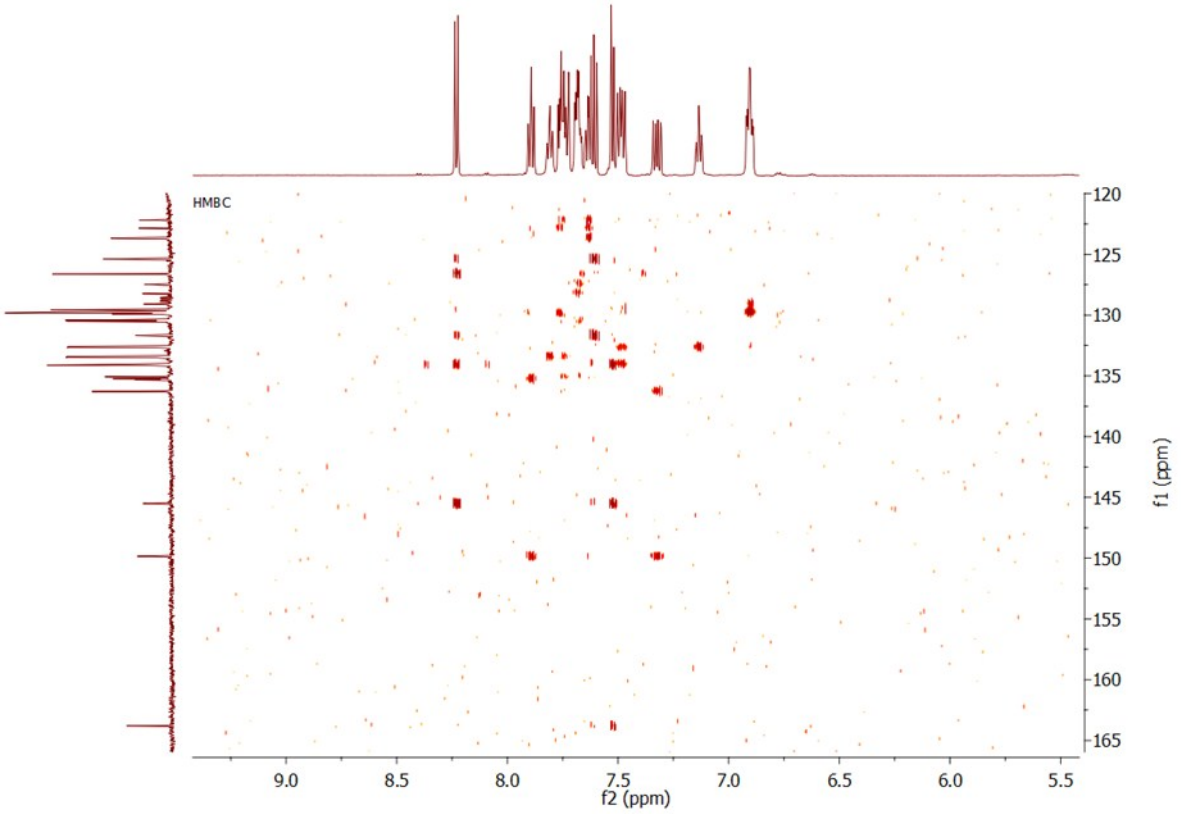

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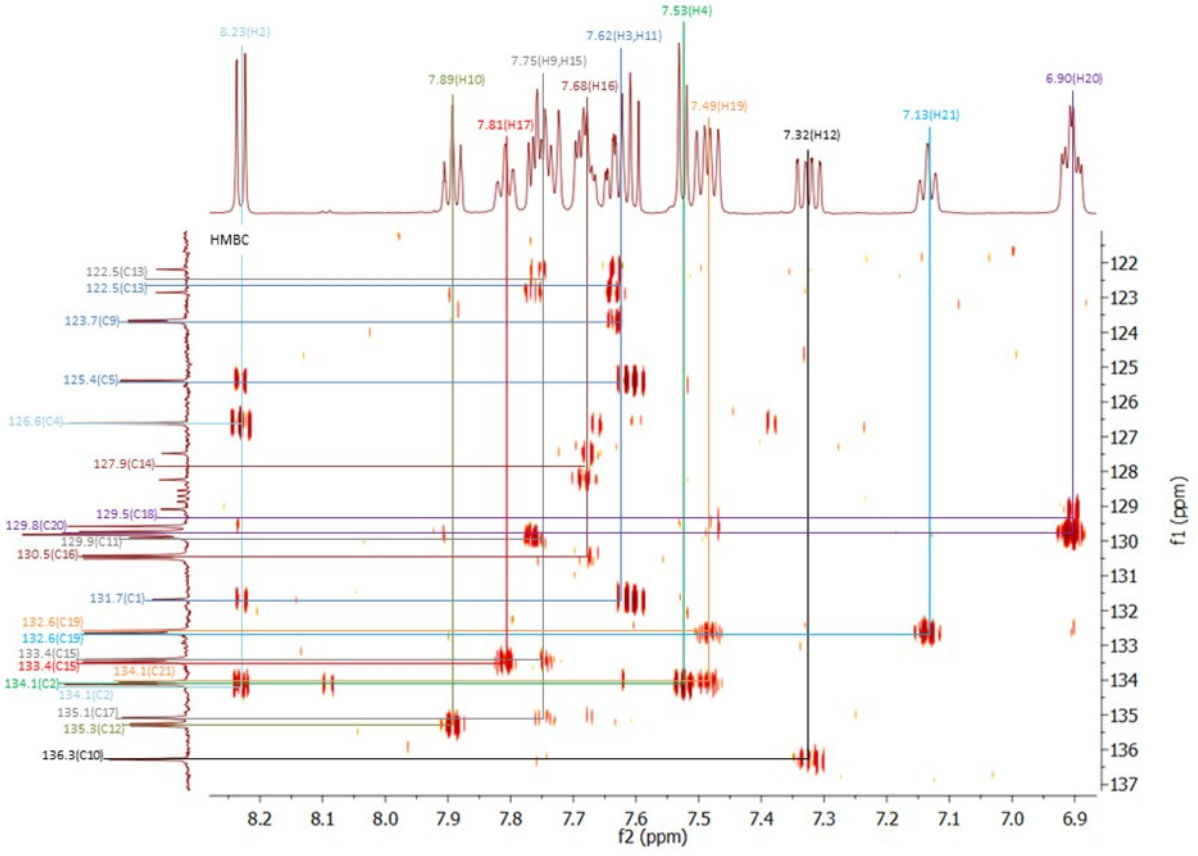

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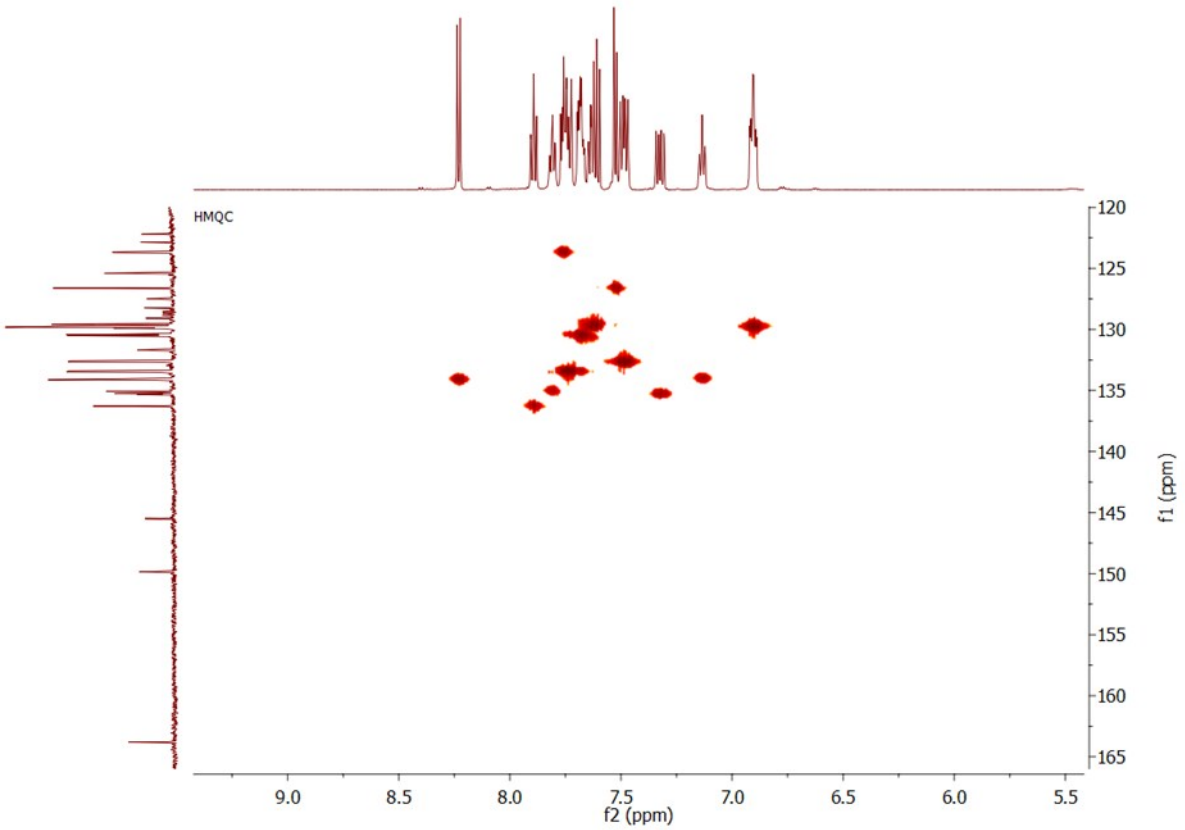

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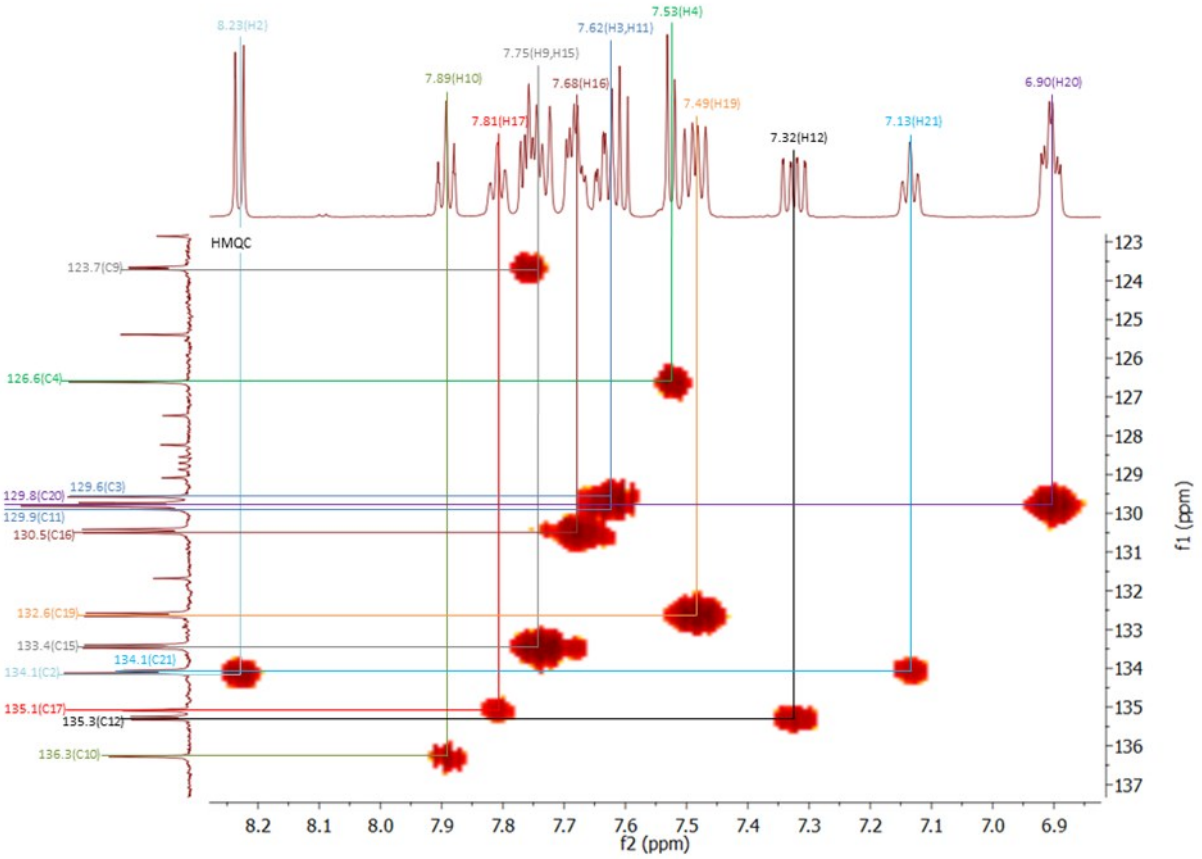
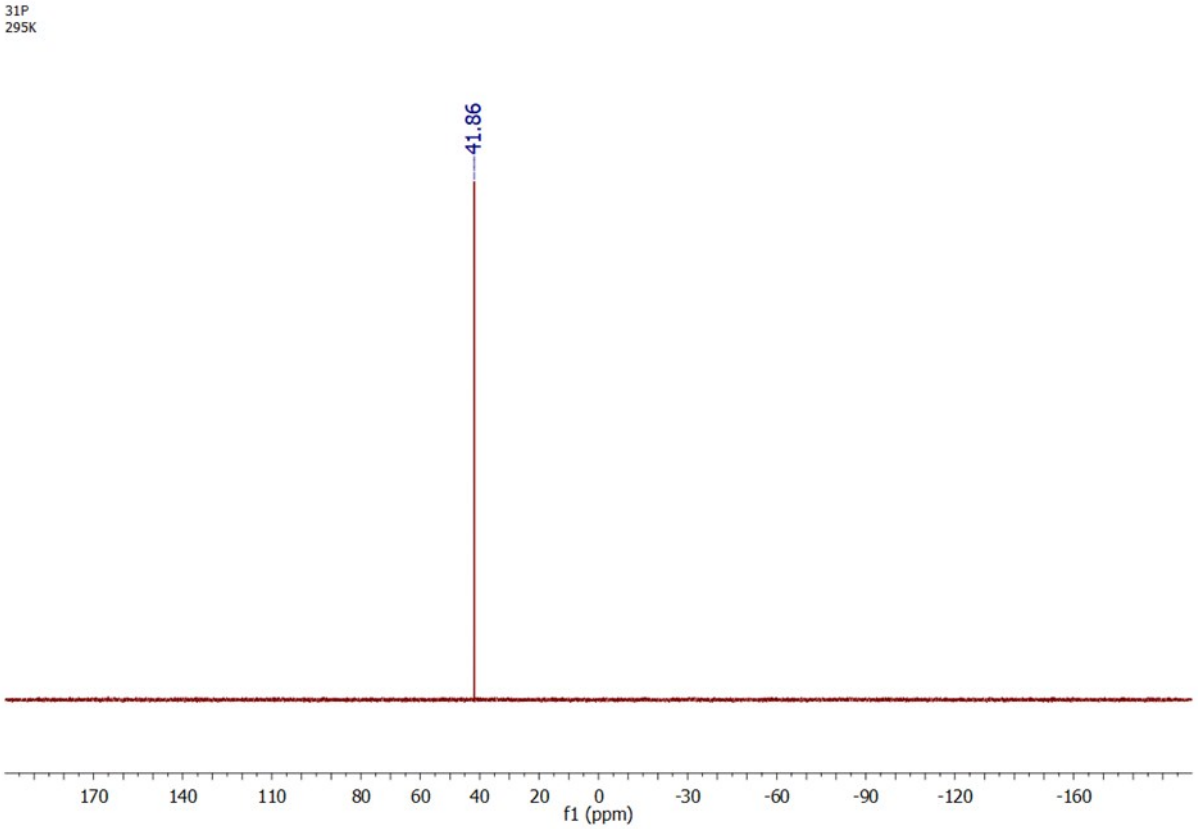
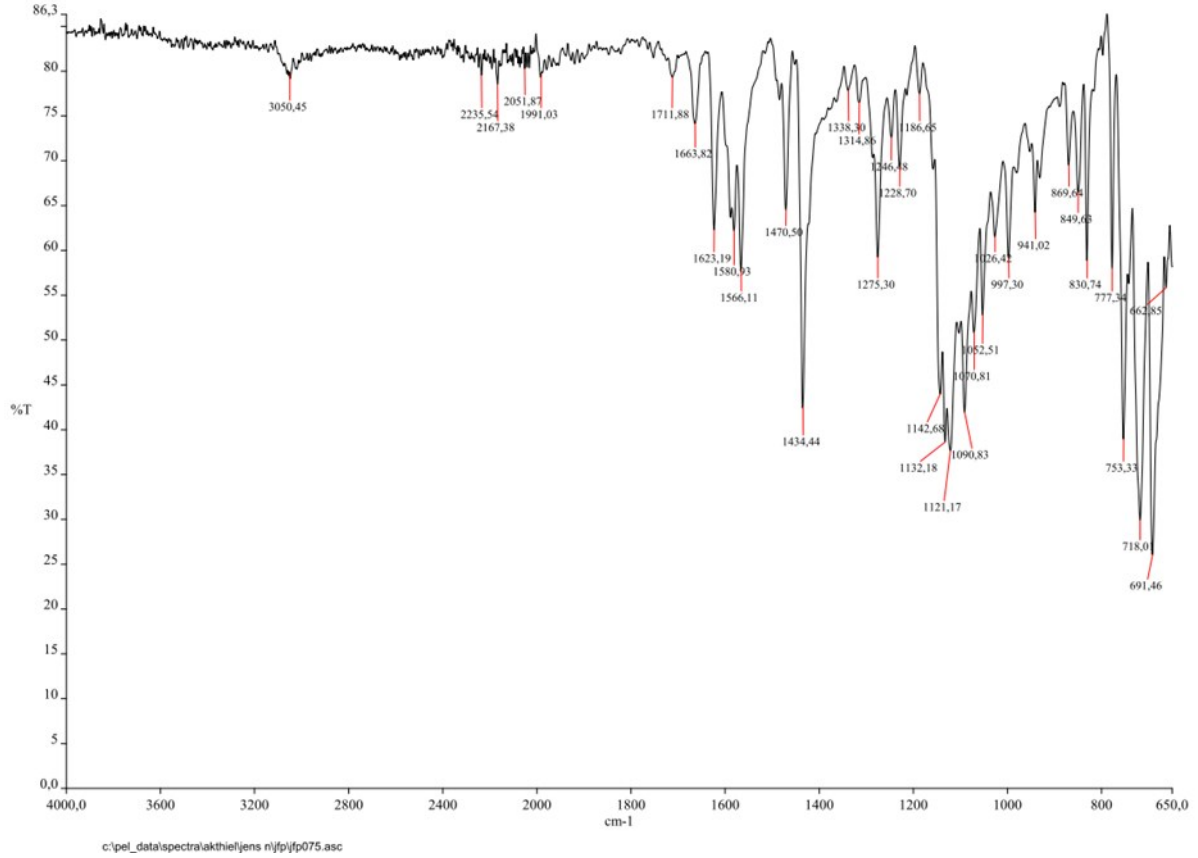


$^{31}P\{^{1}H\}$ NMR spectrum

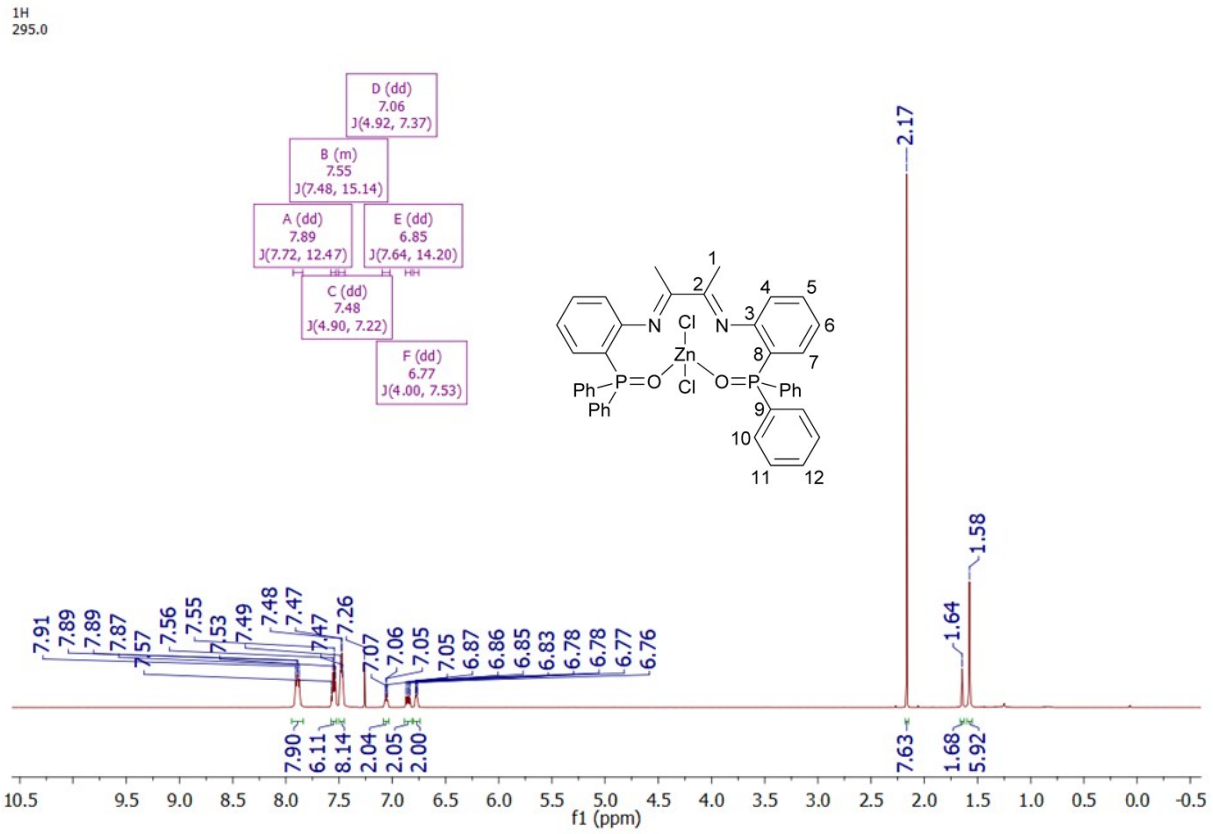


IR spectrum

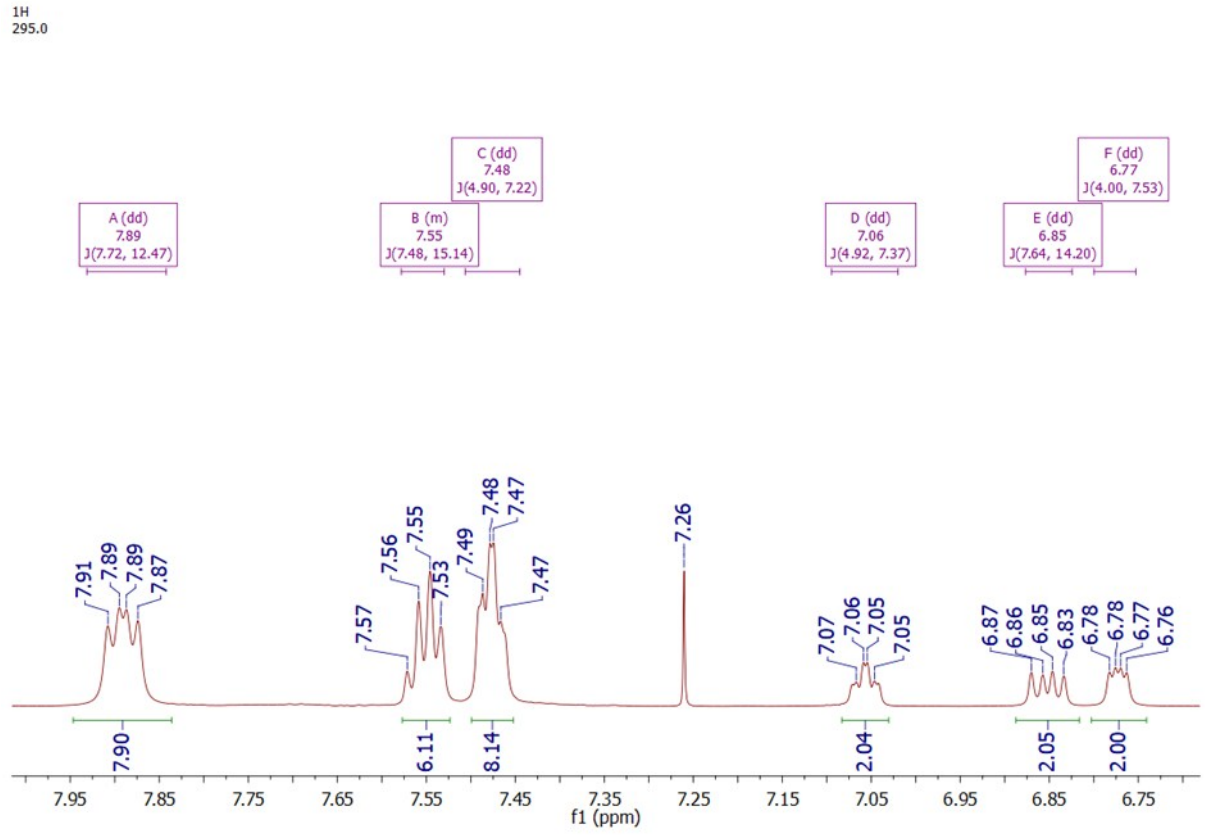


(1,4-Bis(2-diphenylphosphorylphenyl)-1,4-diaza-2,3-dimethyl-1,3-butadiene-κ²*O*)dichloridozinc (5a)

^{1}H NMR spectrum



^{1}H NMR spectrum (aromatic region)



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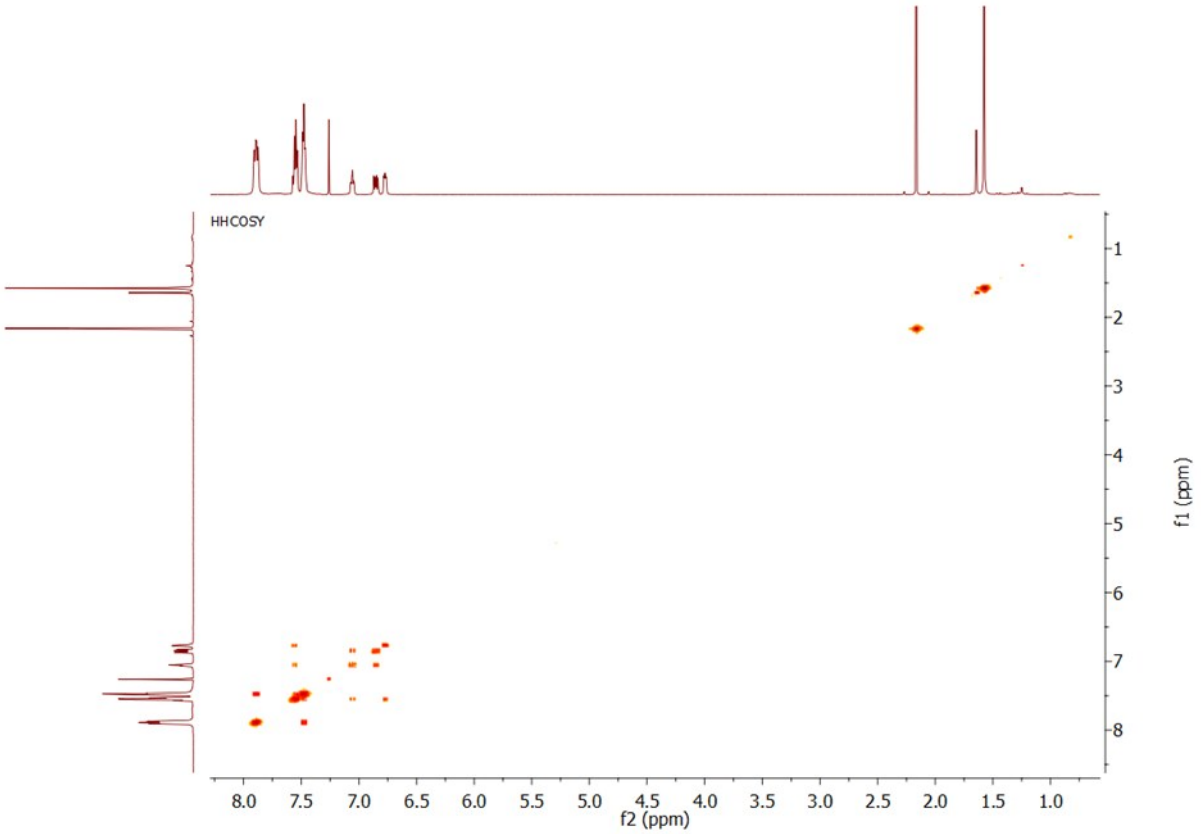
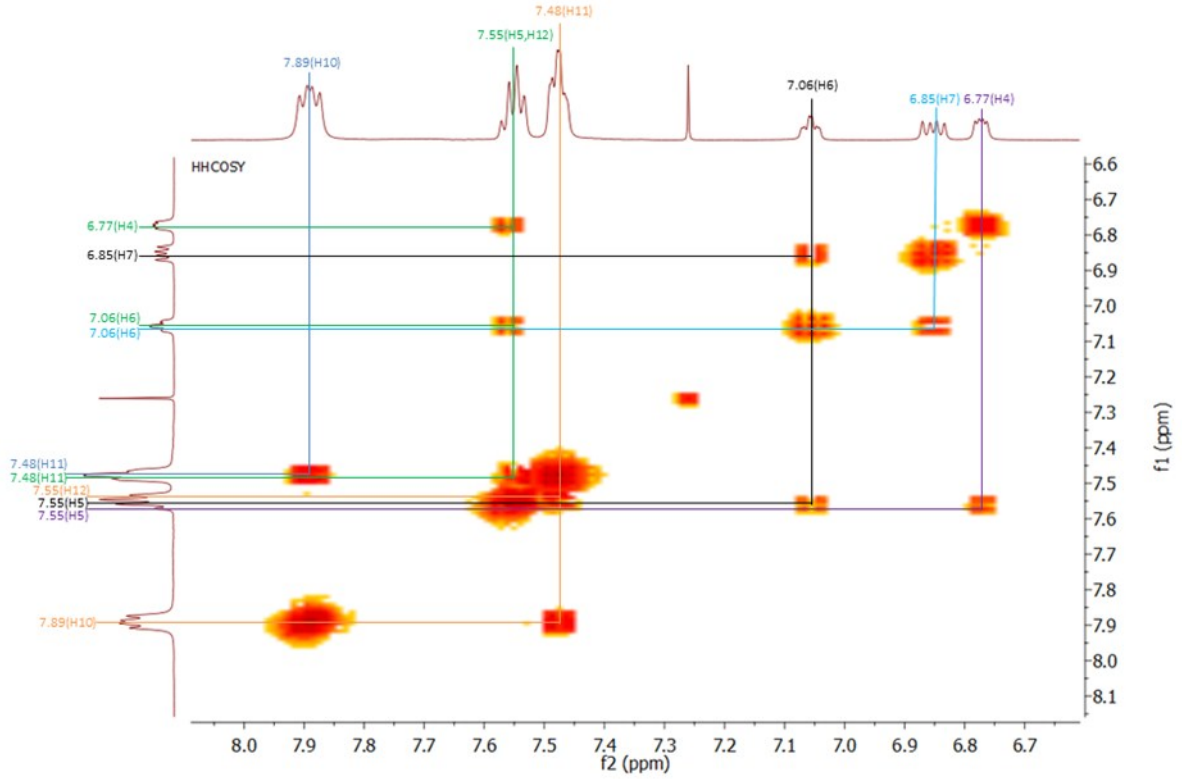
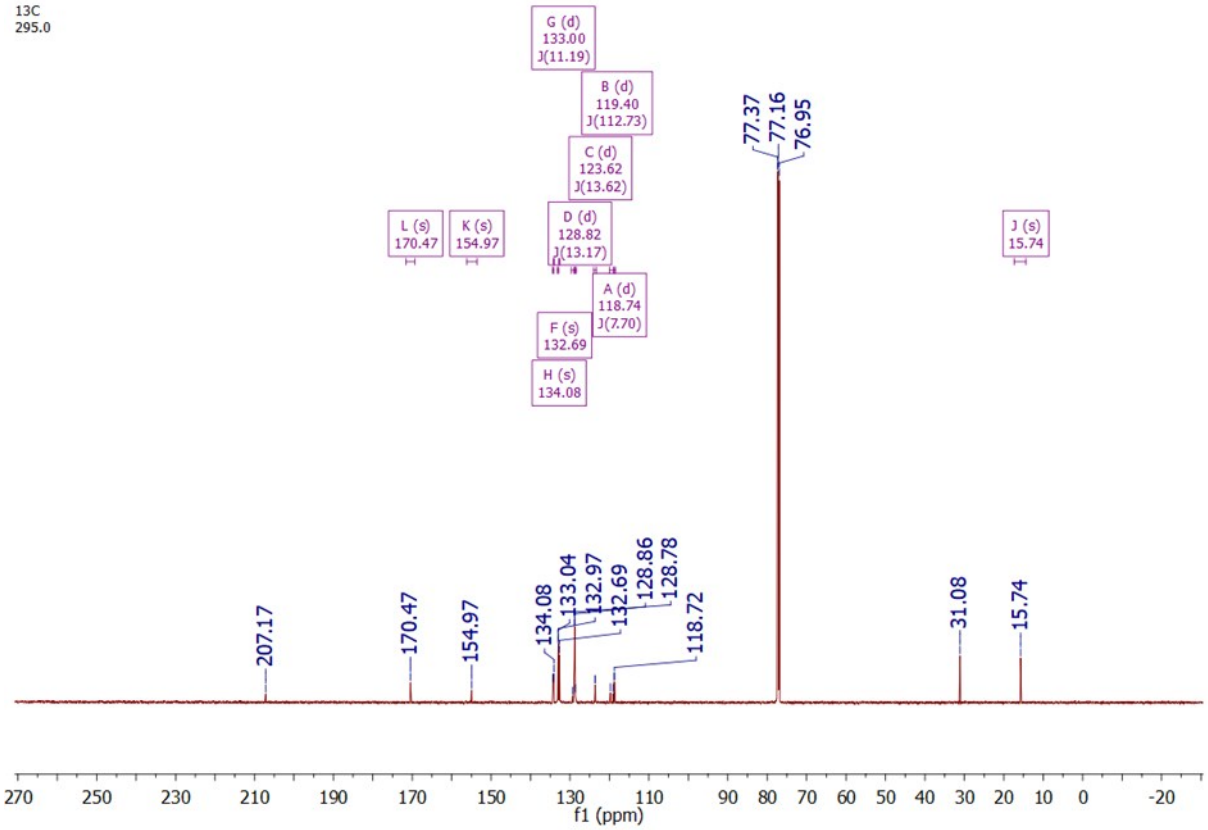


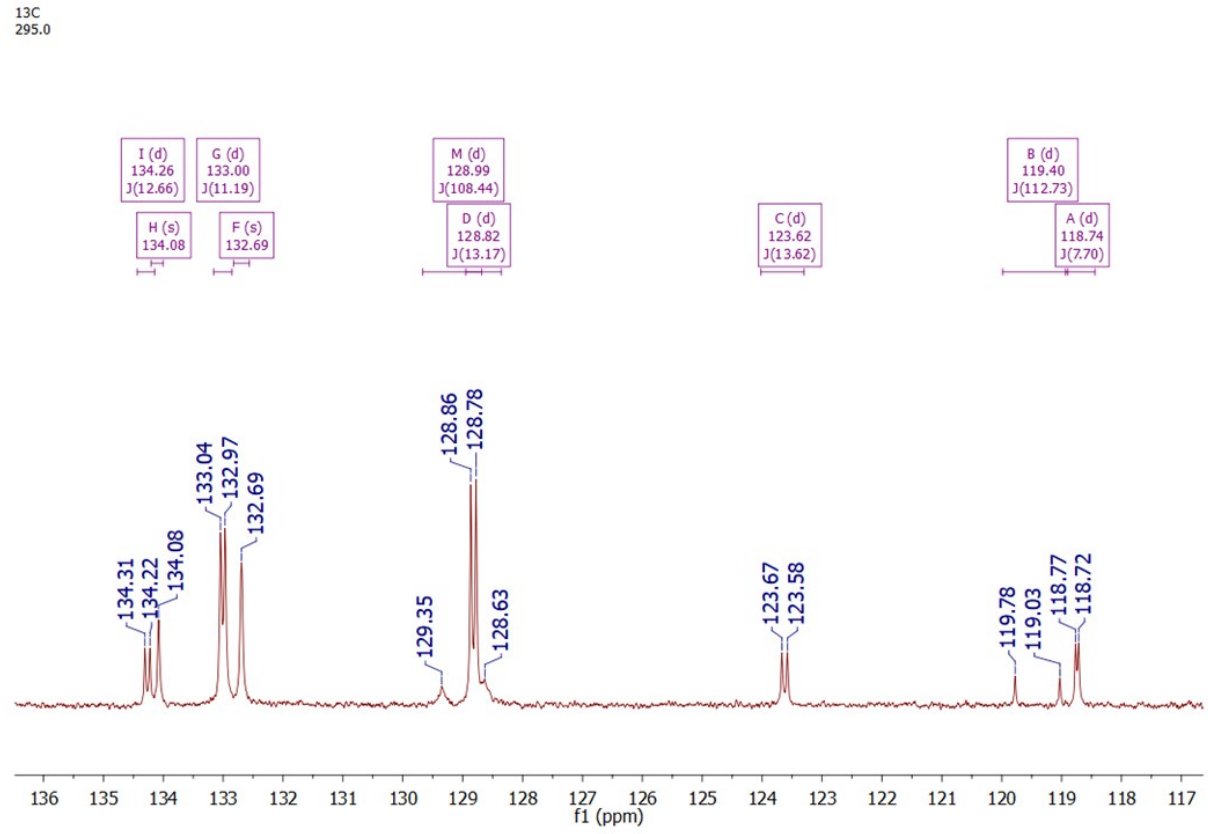
HH-COSY (aromatic region)



$^{13}C\{^{1}H\}$ NMR spectrum



$^{13}C\{^{1}H\}$ NMR spectrum (aromatic region)



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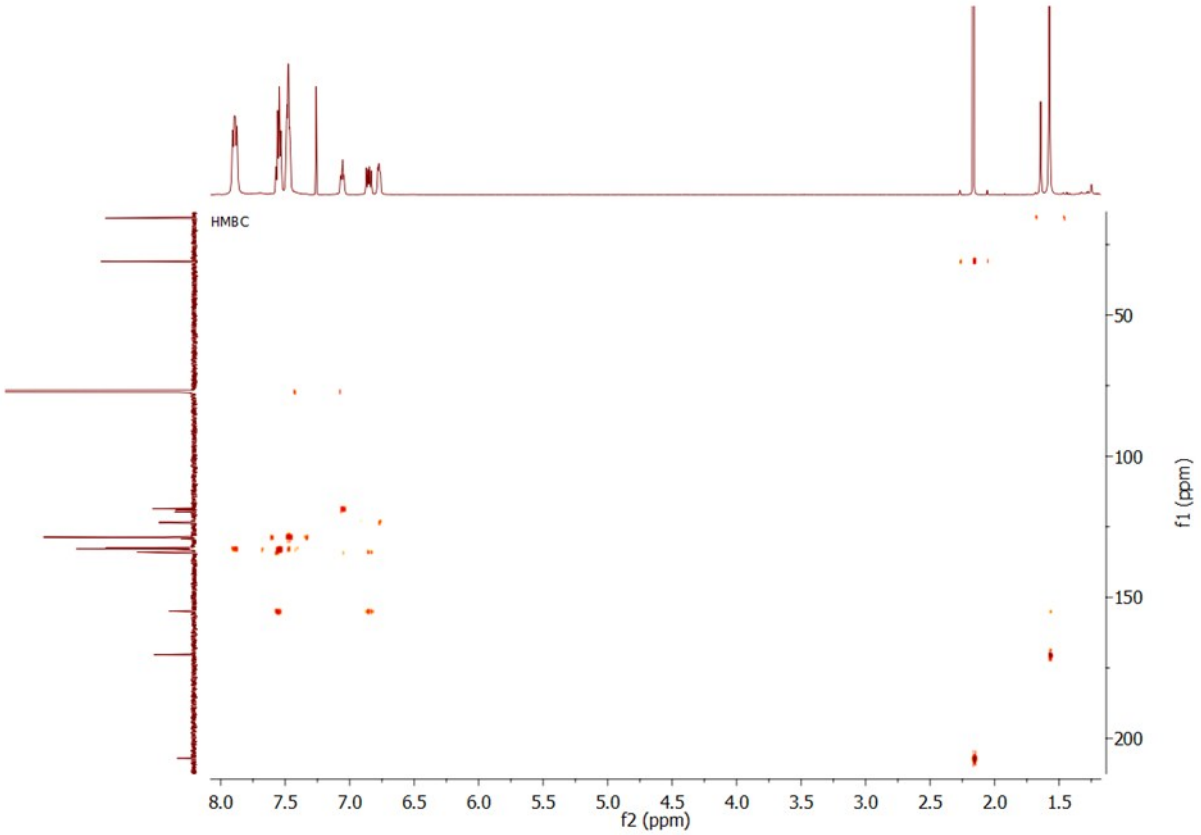
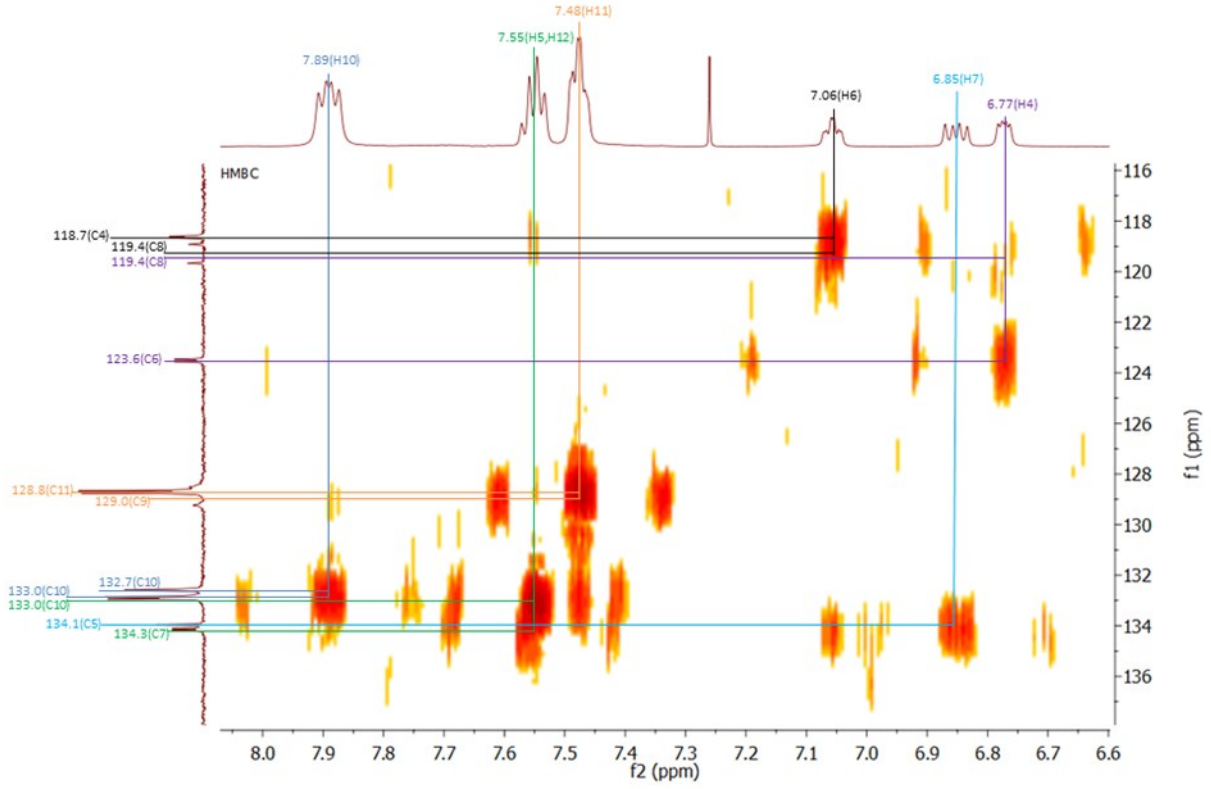
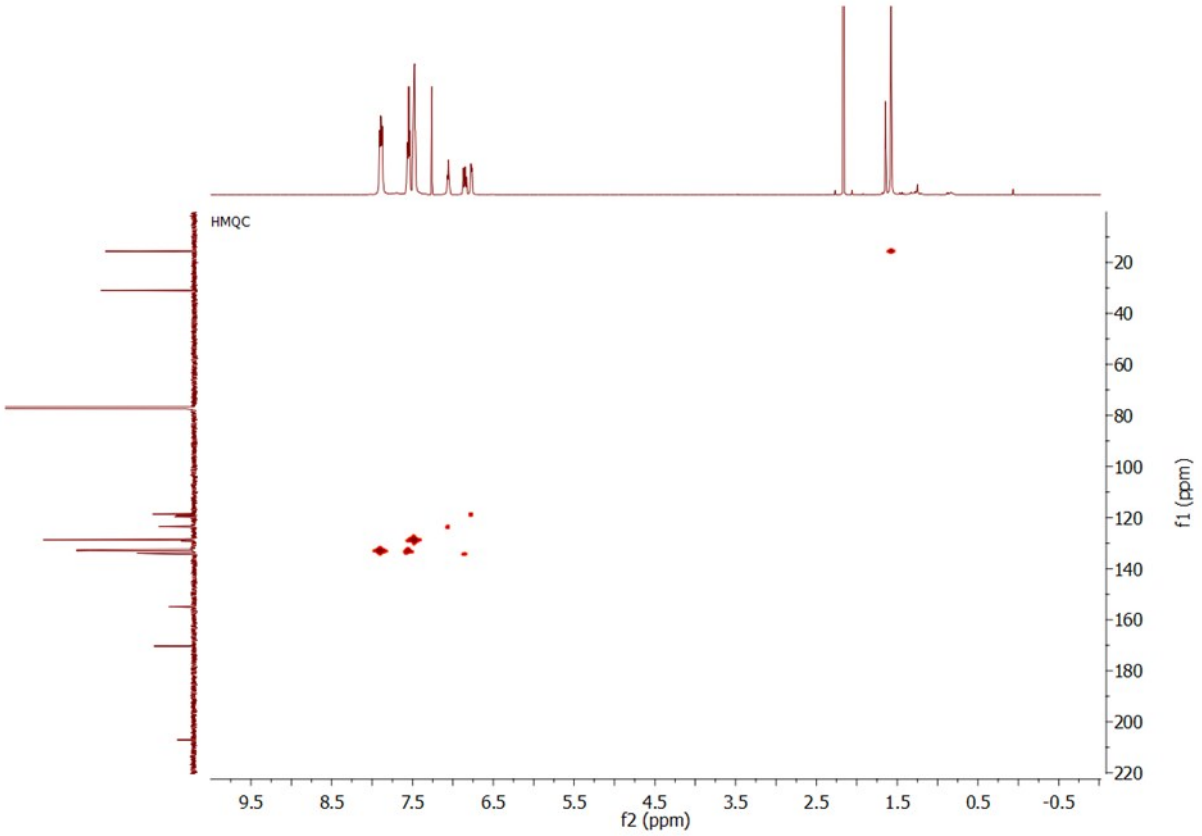


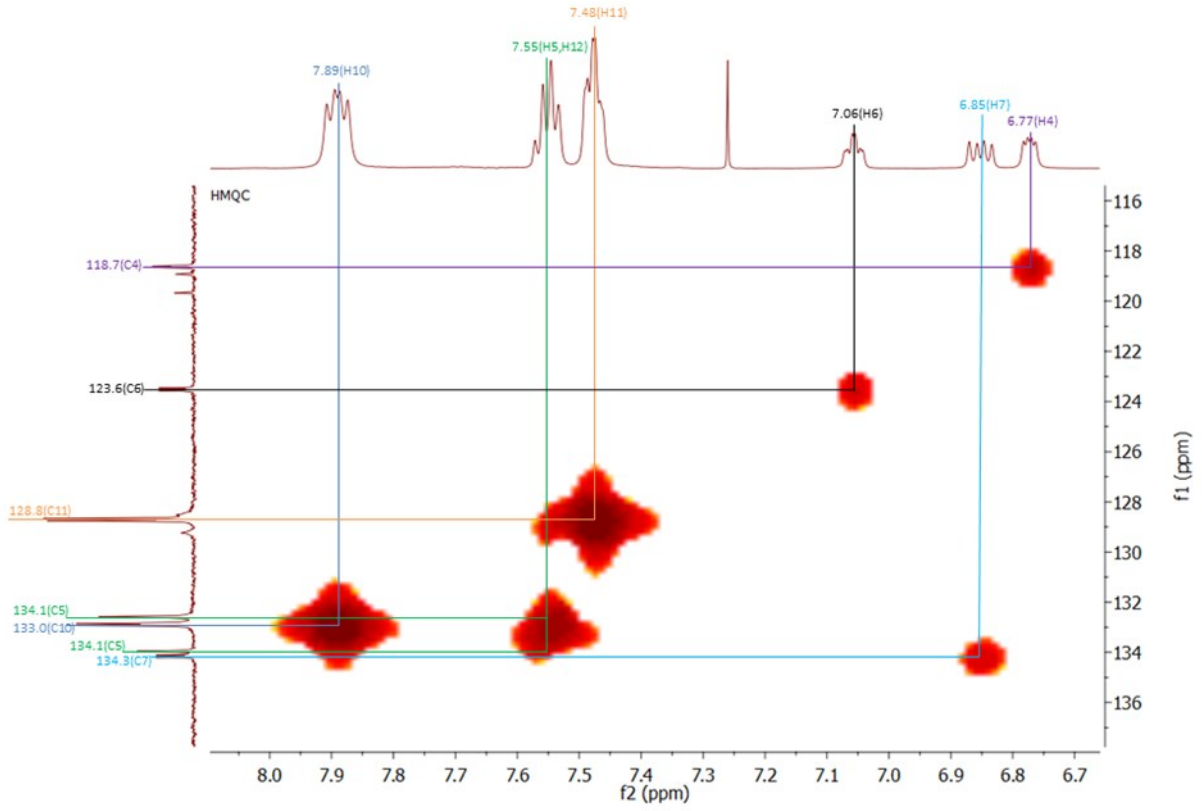
HMBC (aromatic region)



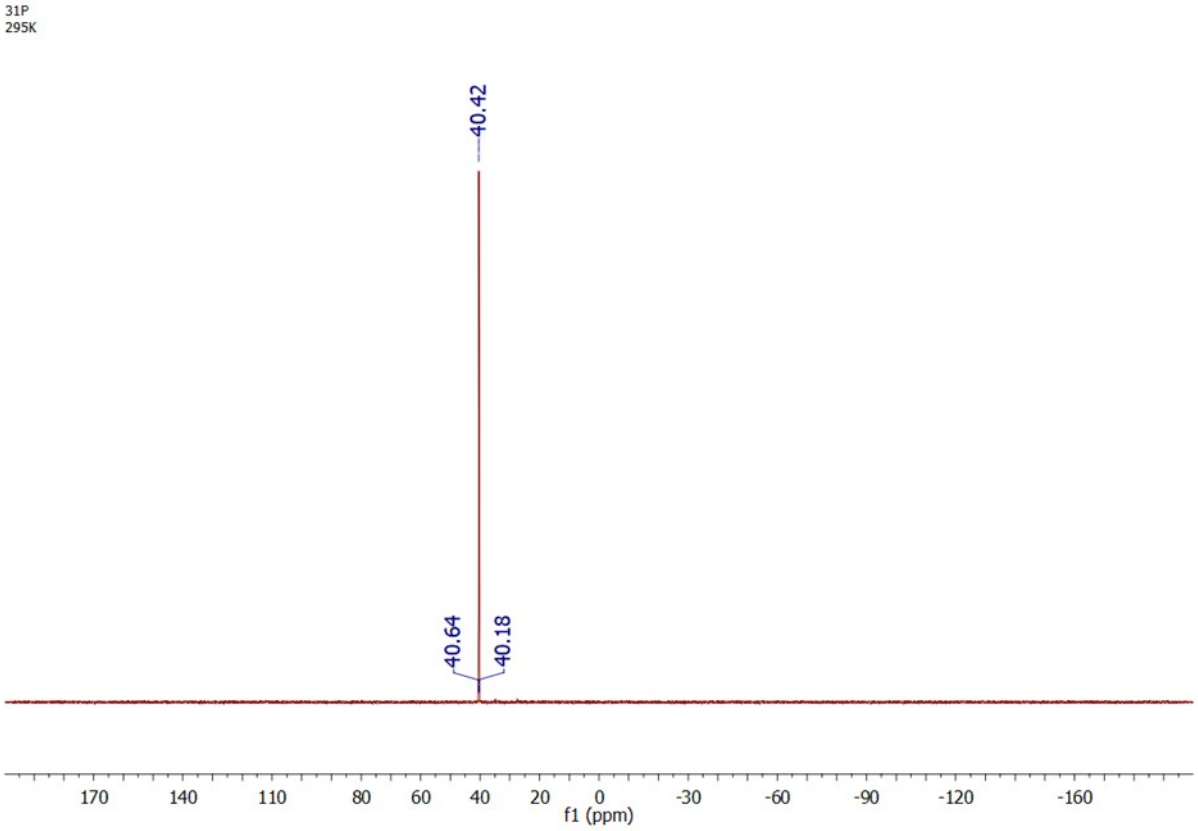
HMQC



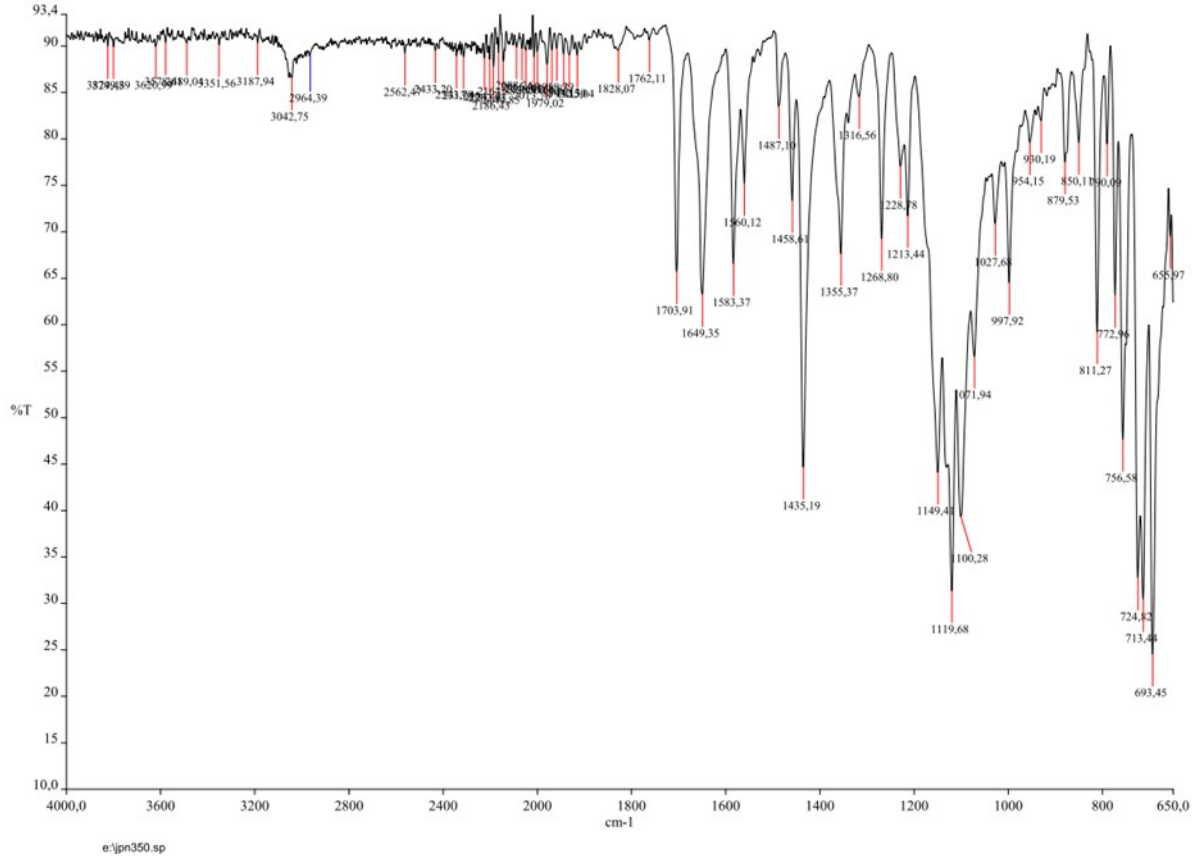
HMQC (aromatic region)



$^{31}P\{^{1}H\}$ NMR spectrum

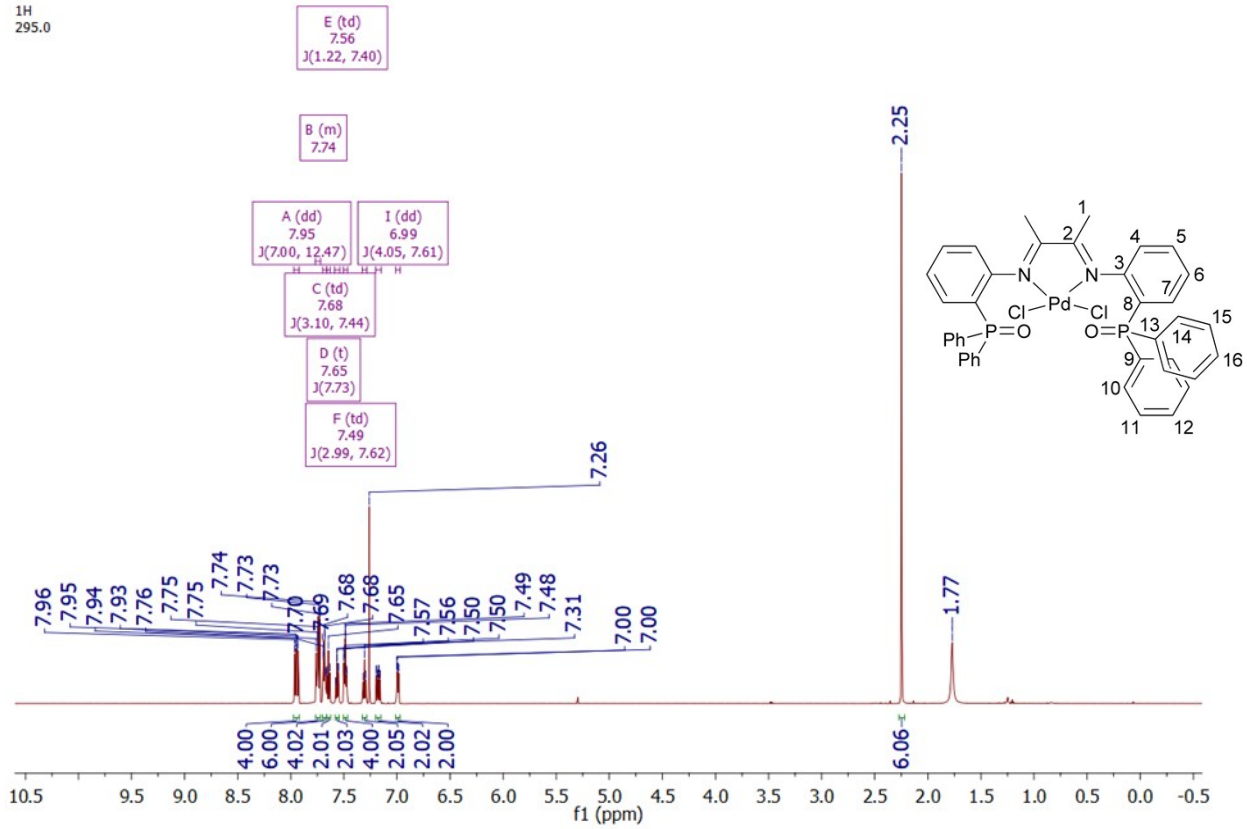


IR spectrum

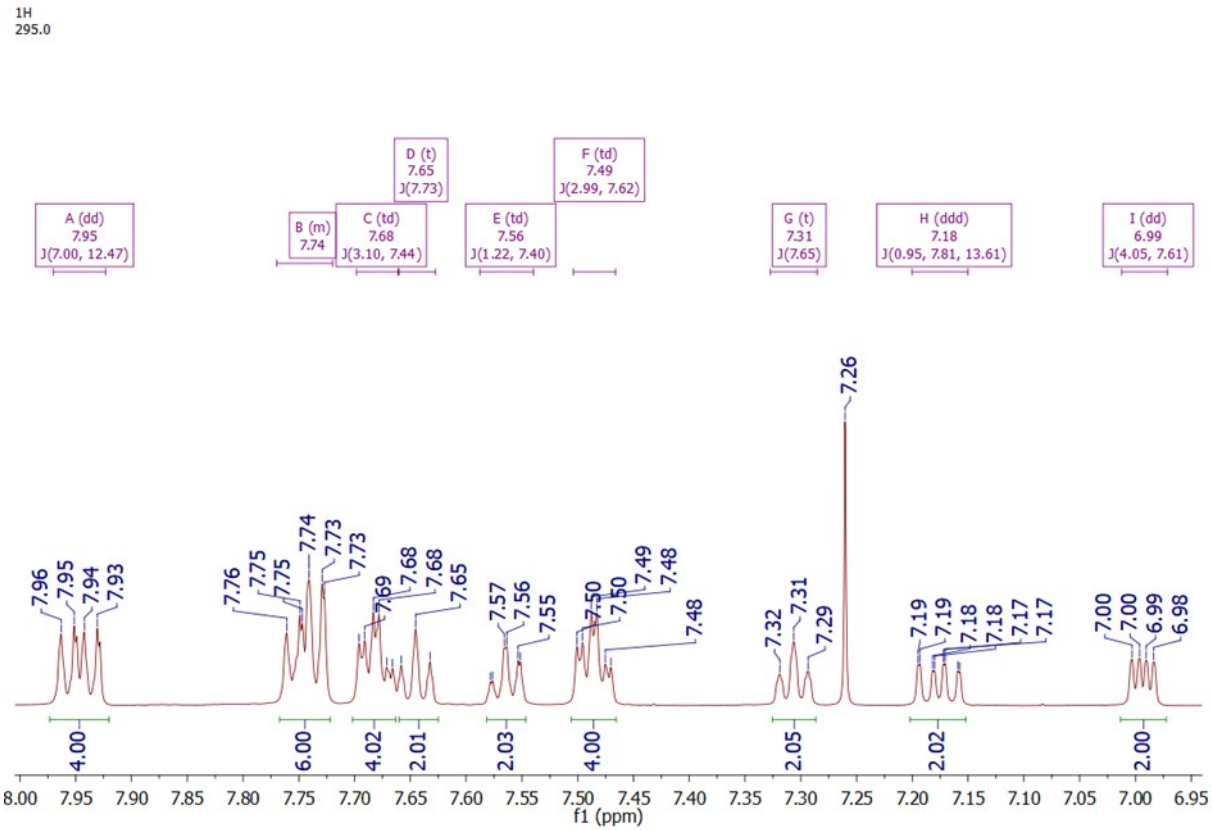


(1,4-Bis(2-diphenylphosphorylphenyl)-1,4-diaza-2,3-dimethyl-1,3-butadiene-κ²*N*)(dichloridopalladium) (6a)

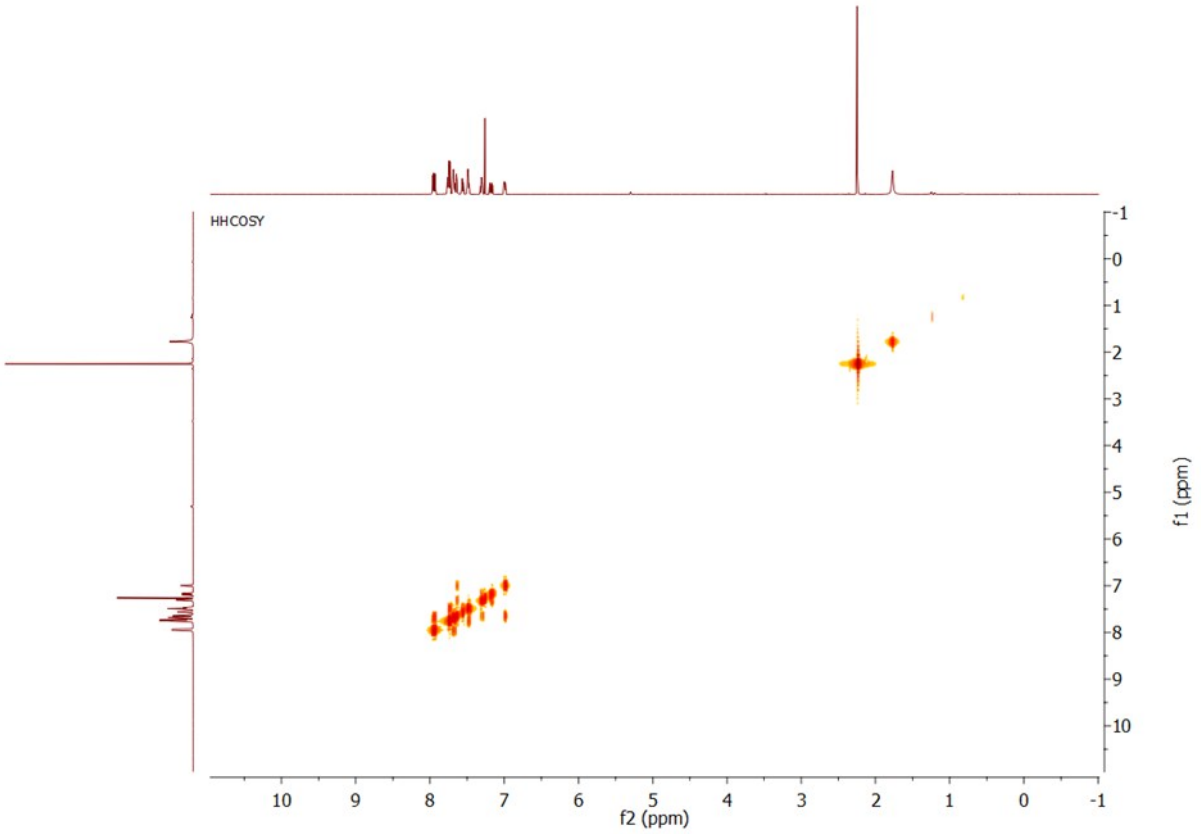
^{1}H NMR spectrum



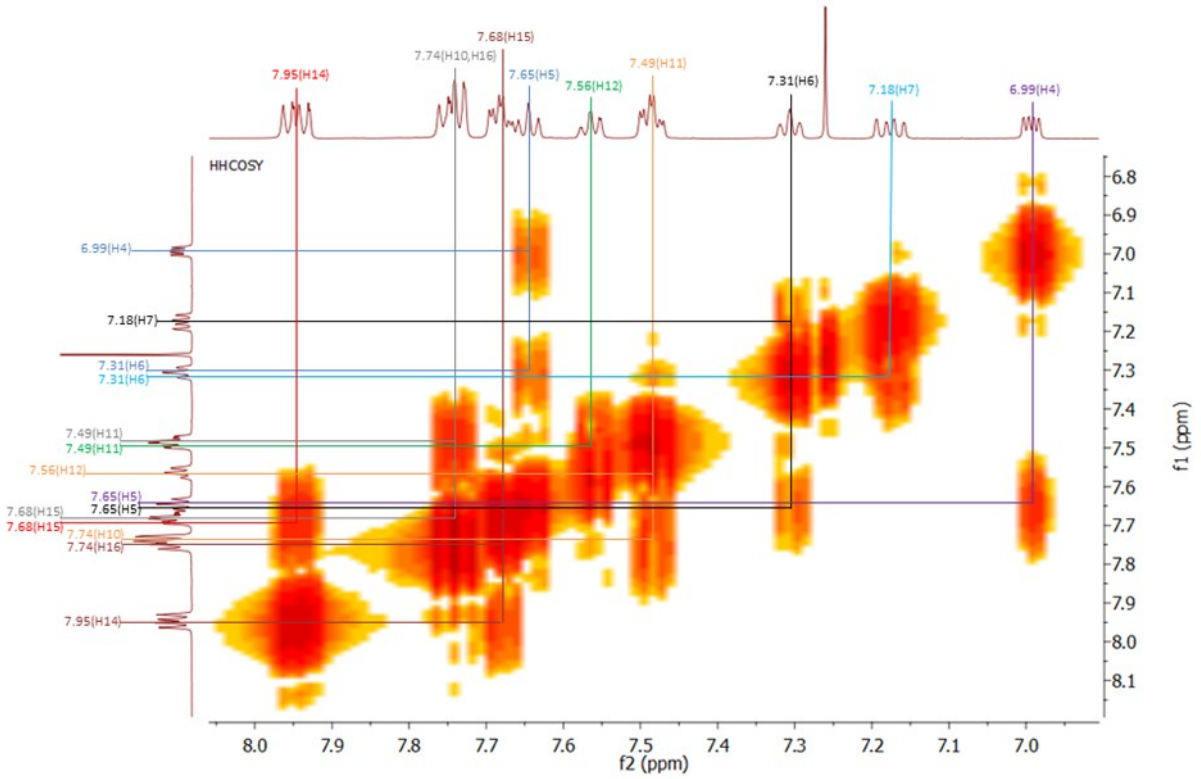
^{1}H NMR spectrum (aromatic region)



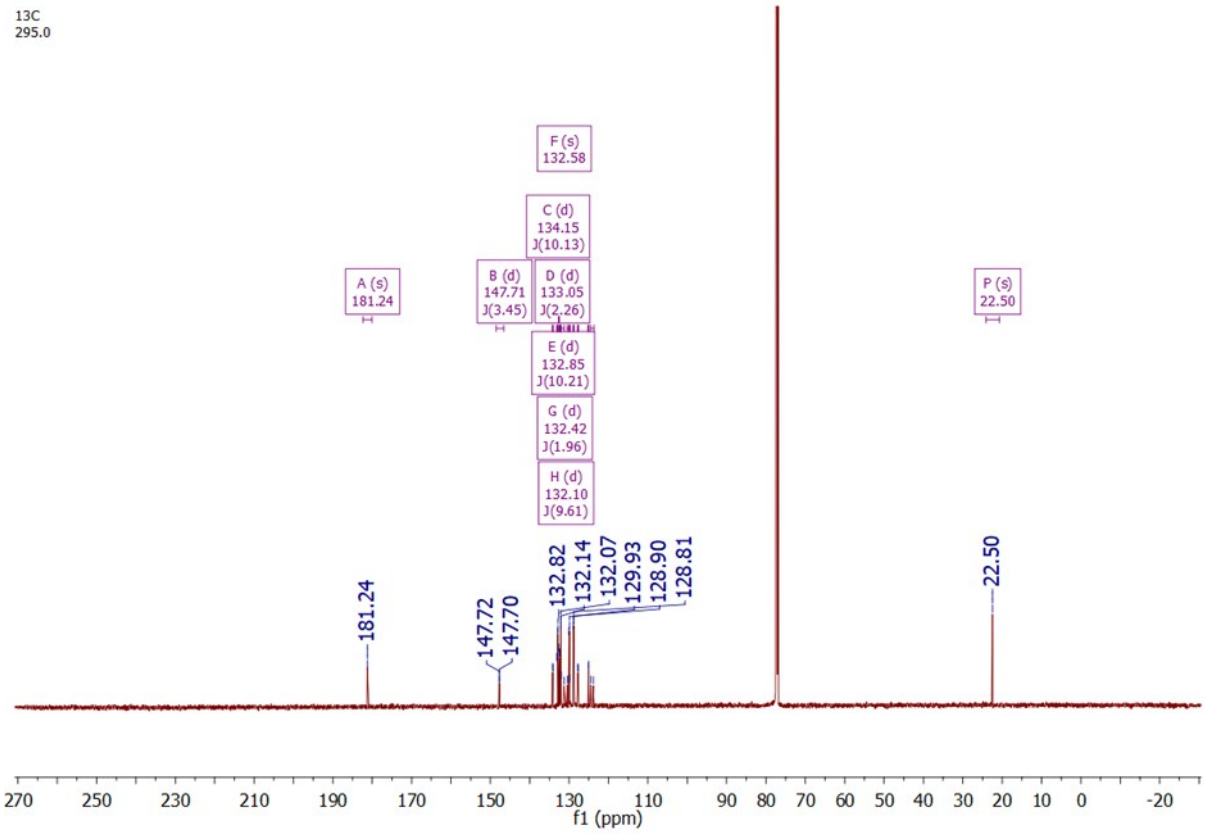
HH-COSY



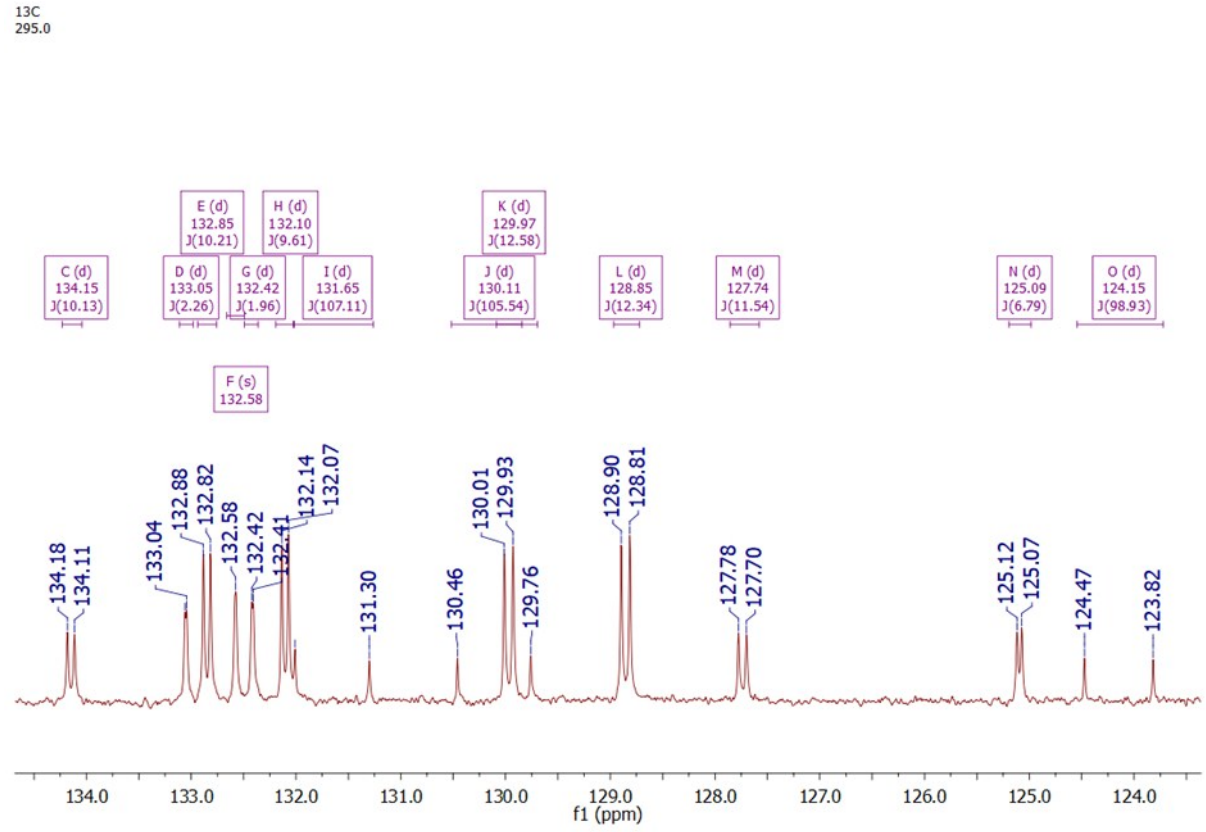
HH-COSY (aromatic region)



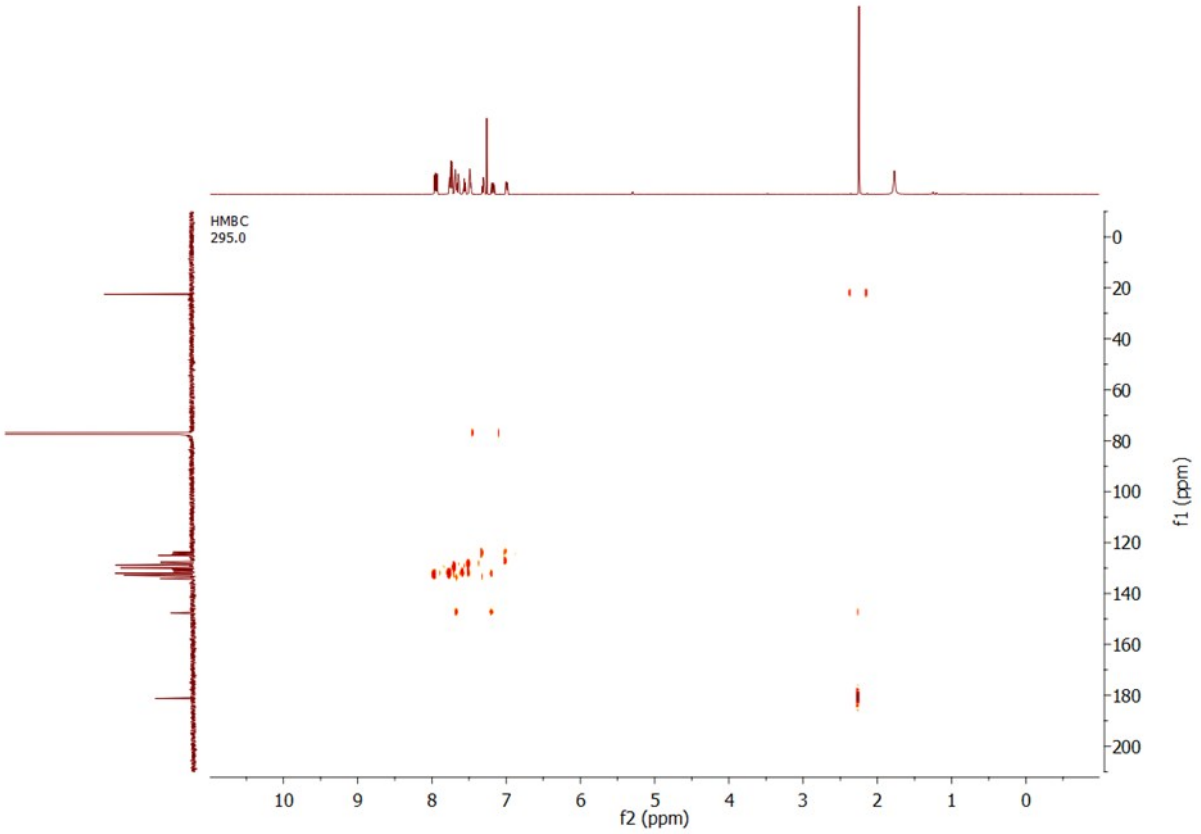
$^{13}C\{^{1}H\}$ NMR spectrum



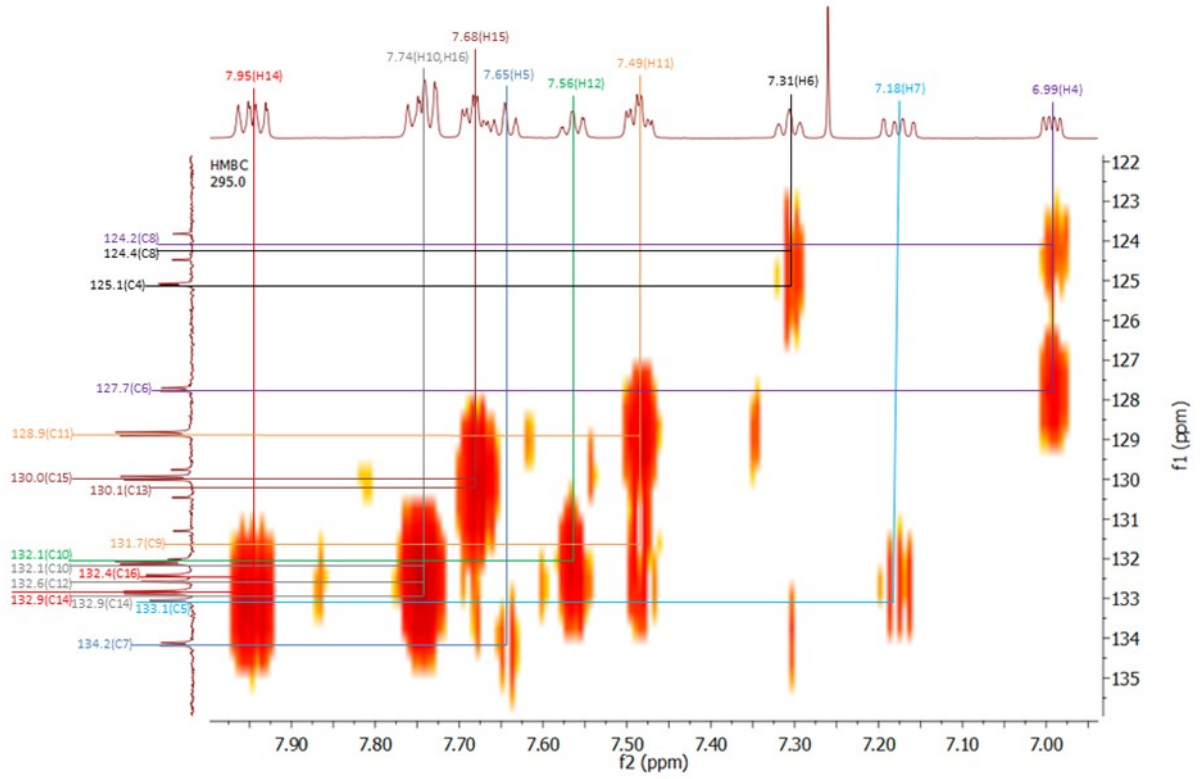
$^{13}C\{^{1}H\}$ NMR spectrum (aromatic region)



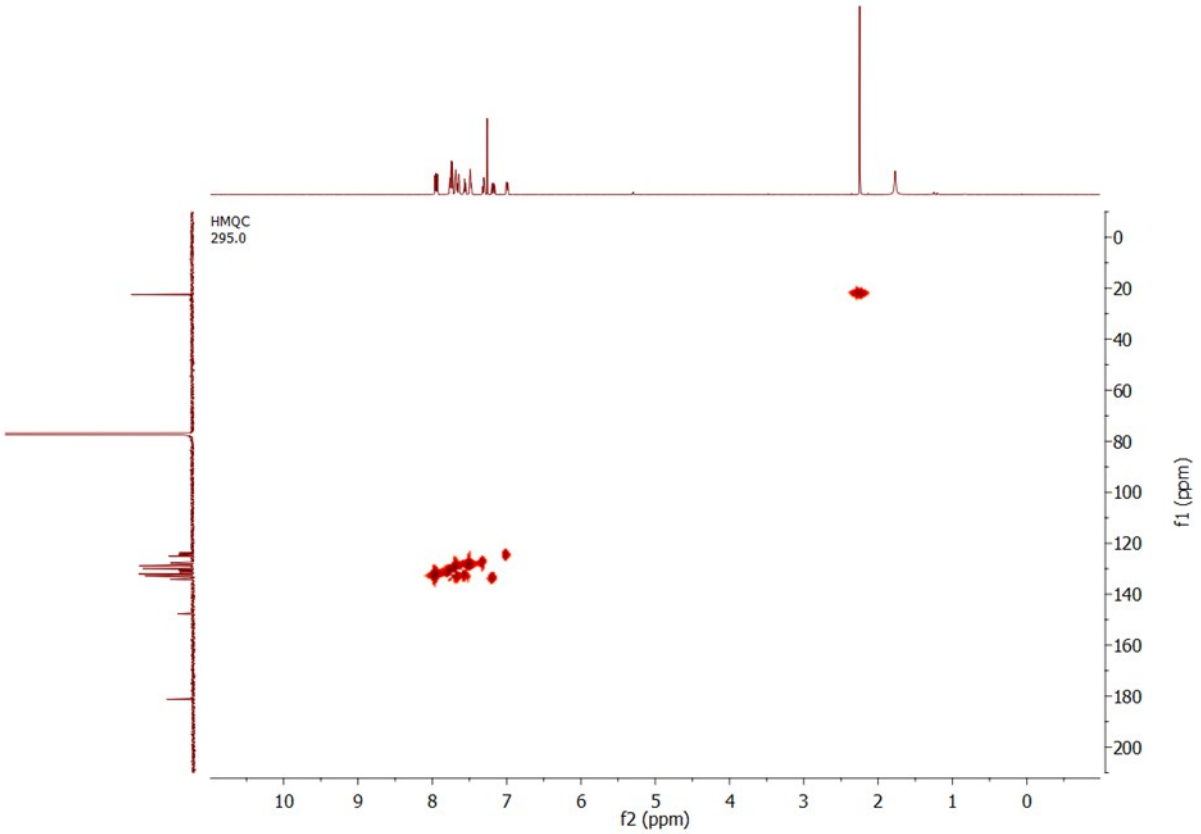
HMBC



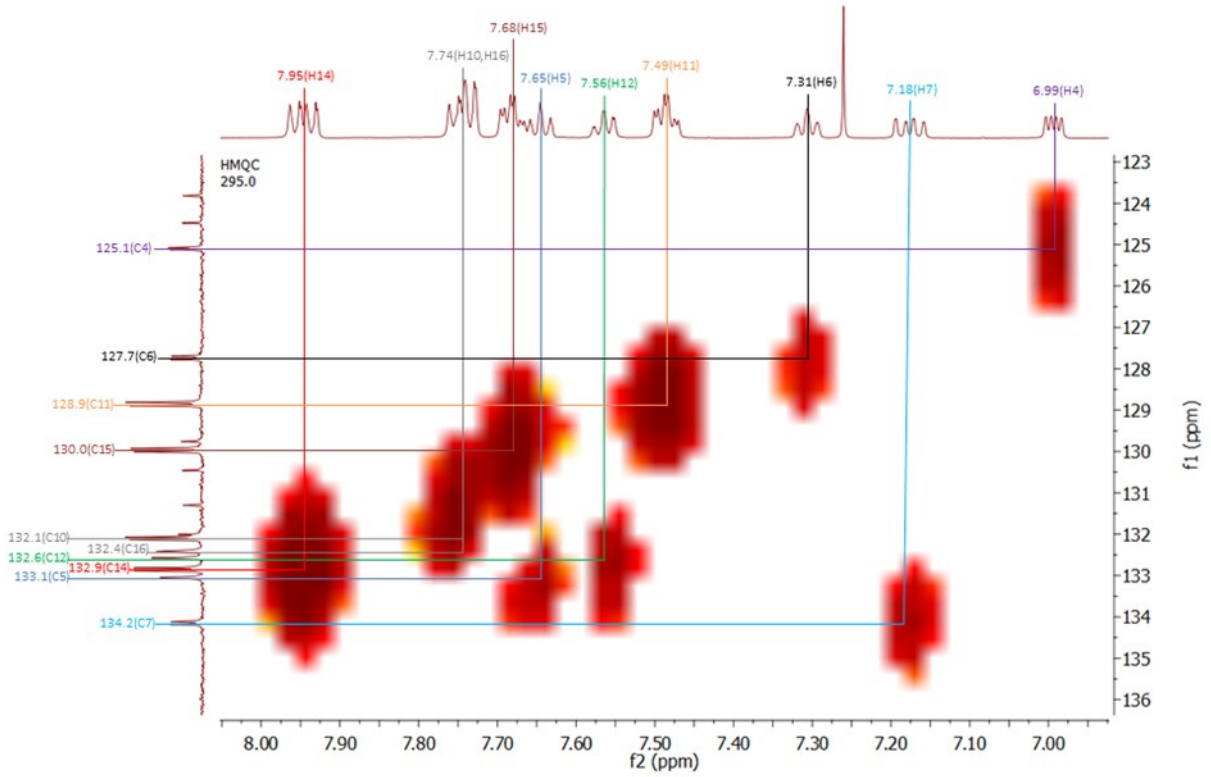
HMBC (aromatic region)



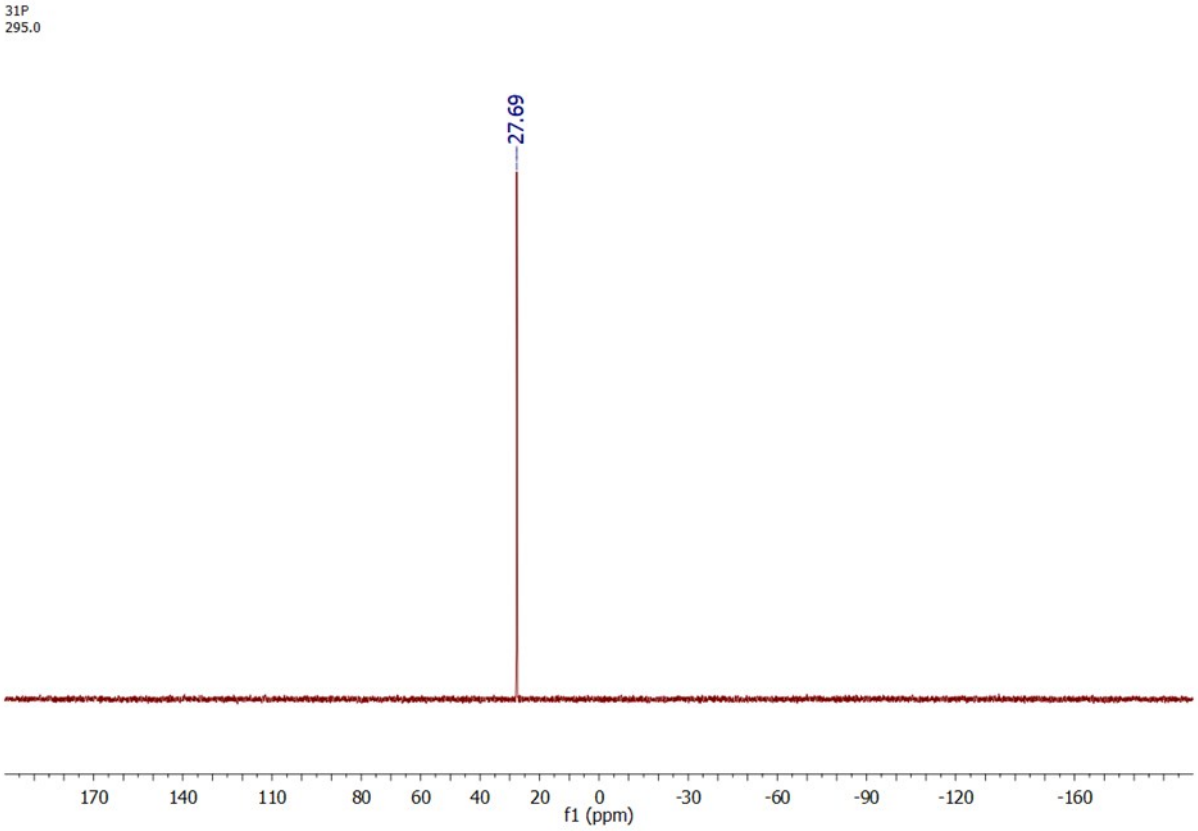
HMQC



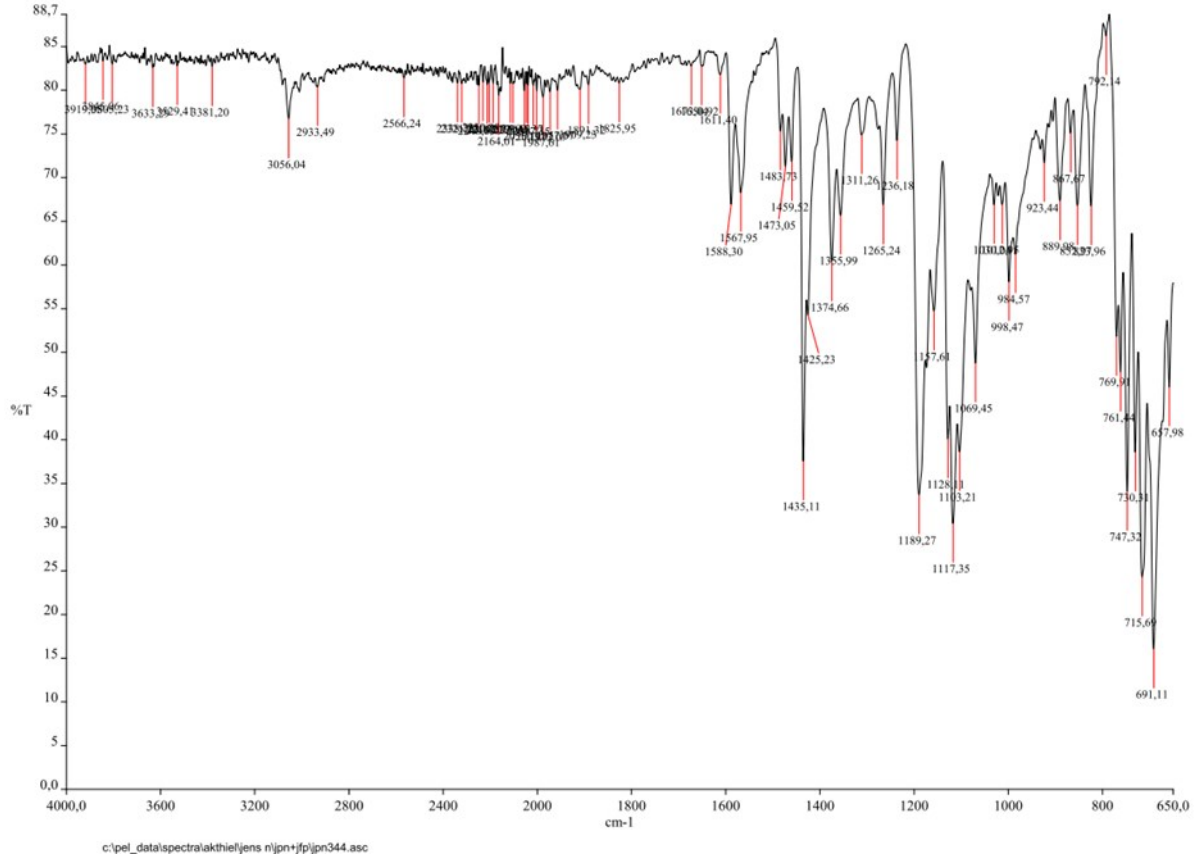
HMQC (aromatic region)



$^{31}P\{^{1}H\}$ NMR spectrum



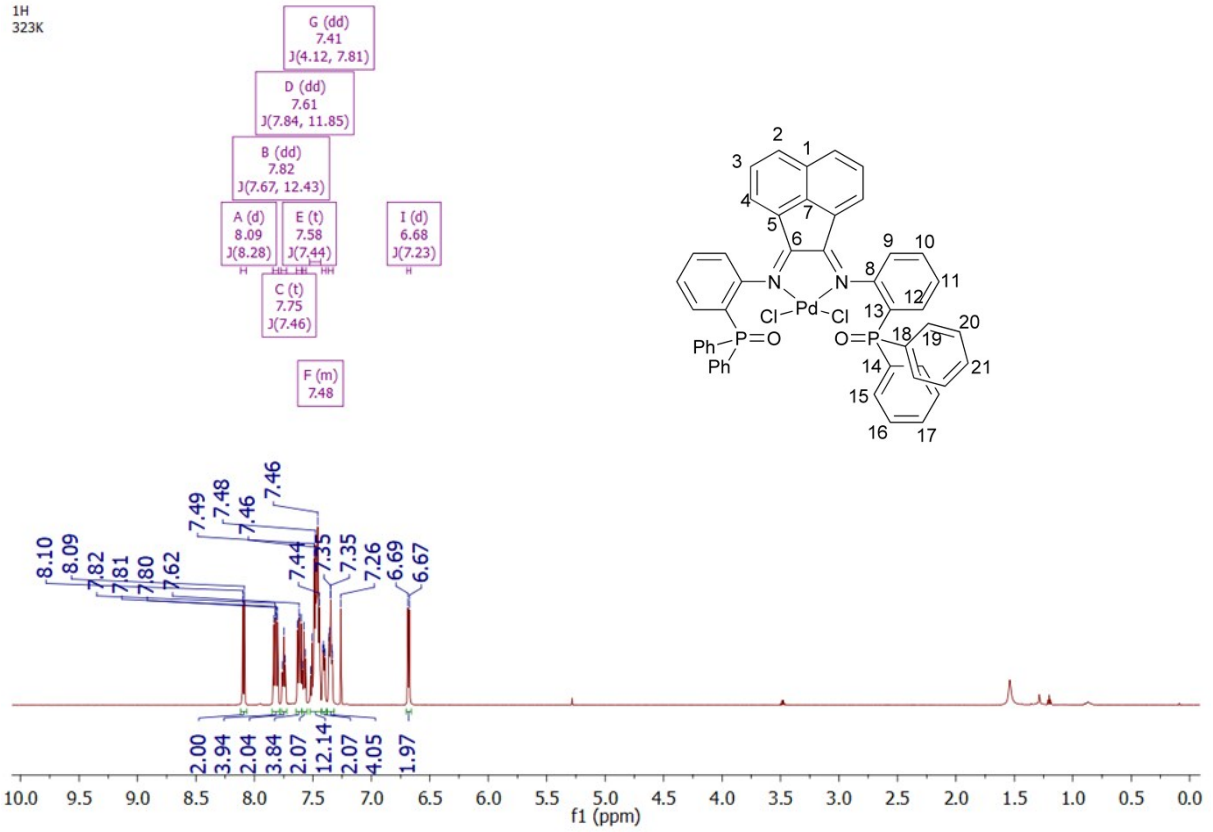
IR spectrum



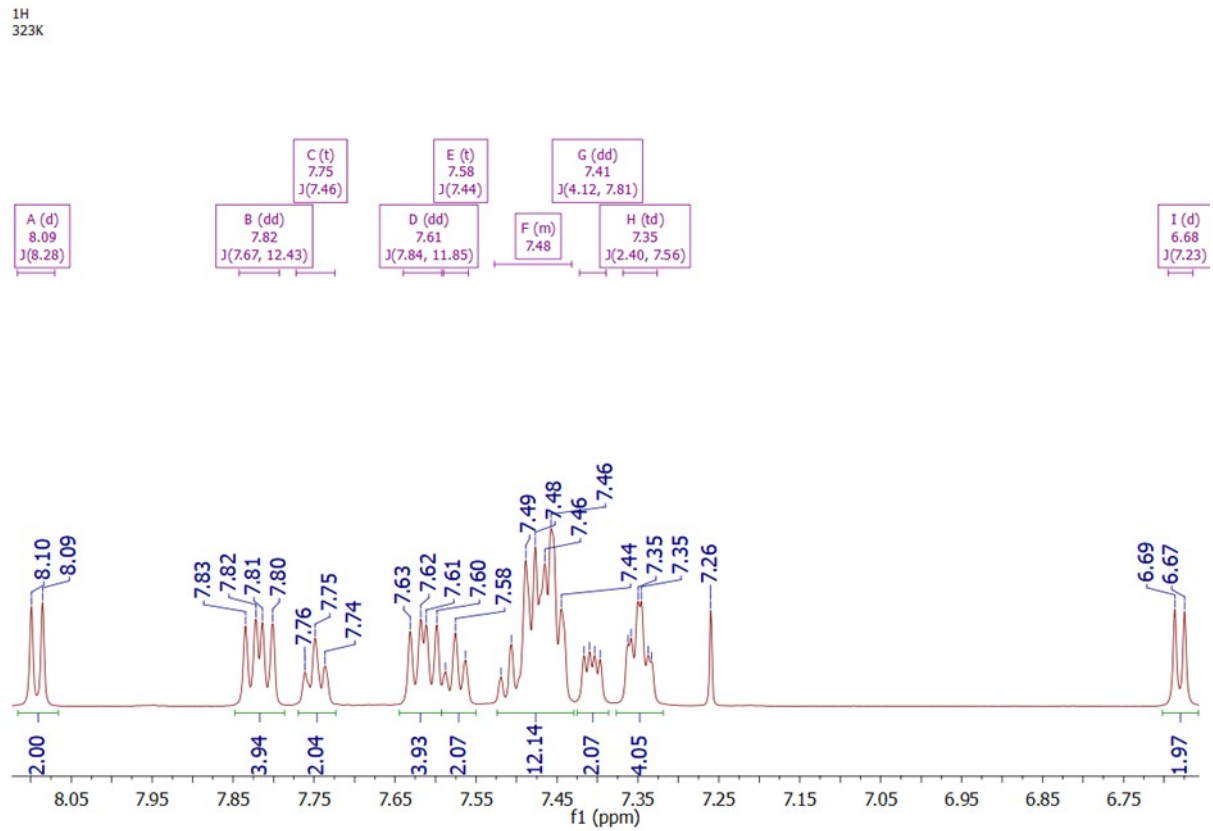
c:\pel_data\spectra\akthiel\jens n\jpn+jfp\jpn344.asc

[*N*,*N*'-1,2-Acenaphthylenediylidene(2-diphenylphosphorylphenyl)amine-κ²*N*](dichloridopalladium) (6b)

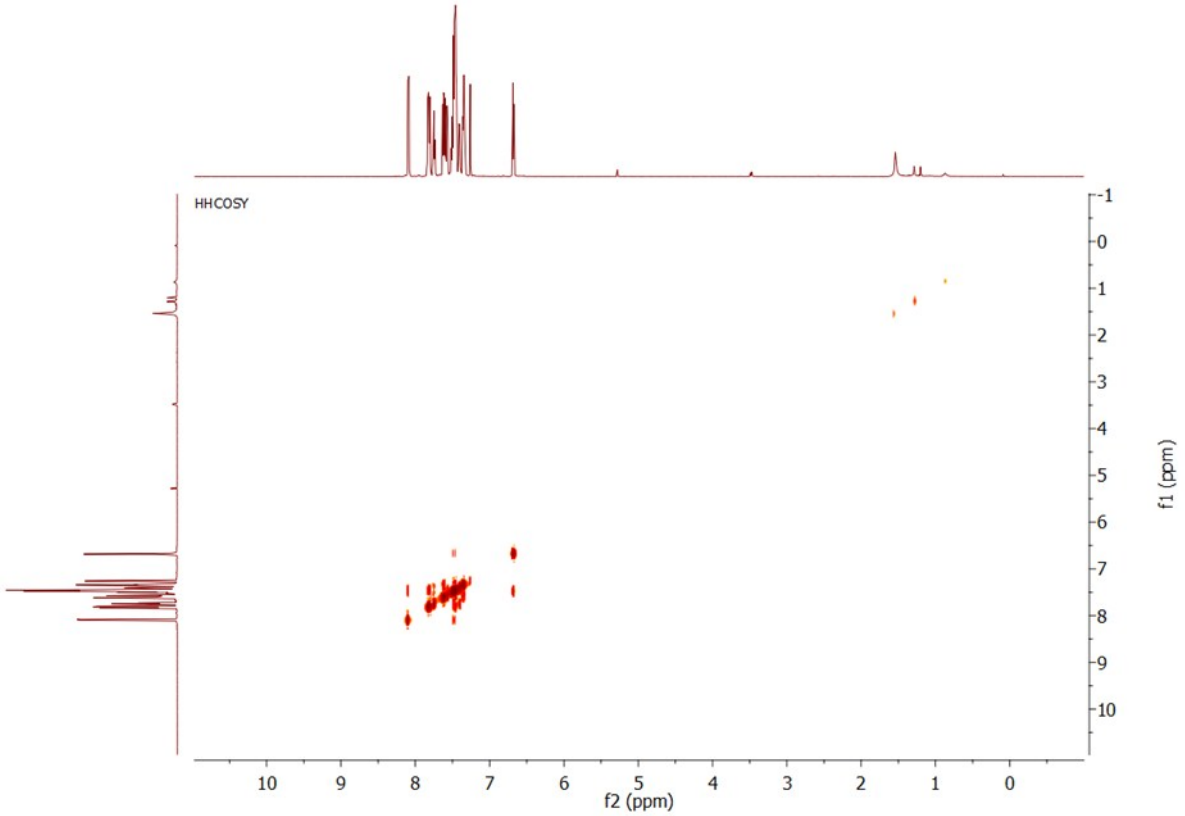
^{1}H NMR spectrum



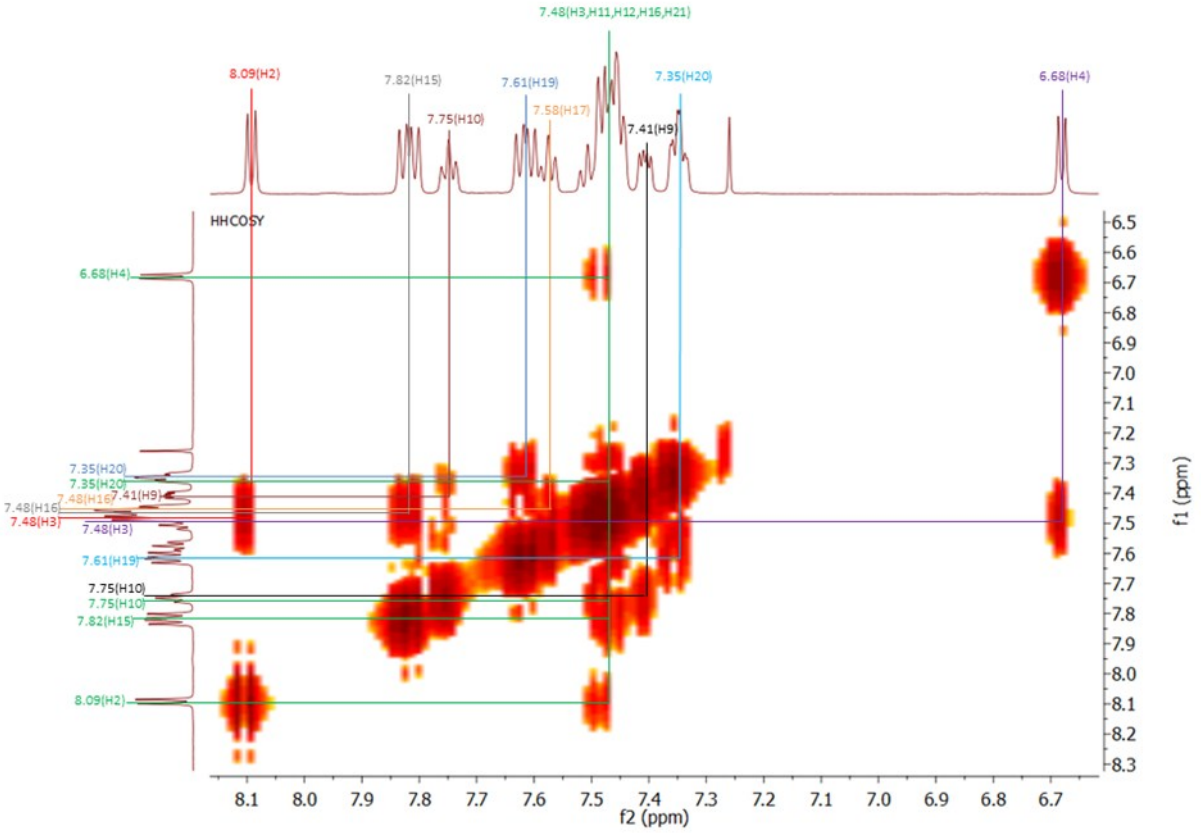
^{1}H NMR spectrum (aromatic region)



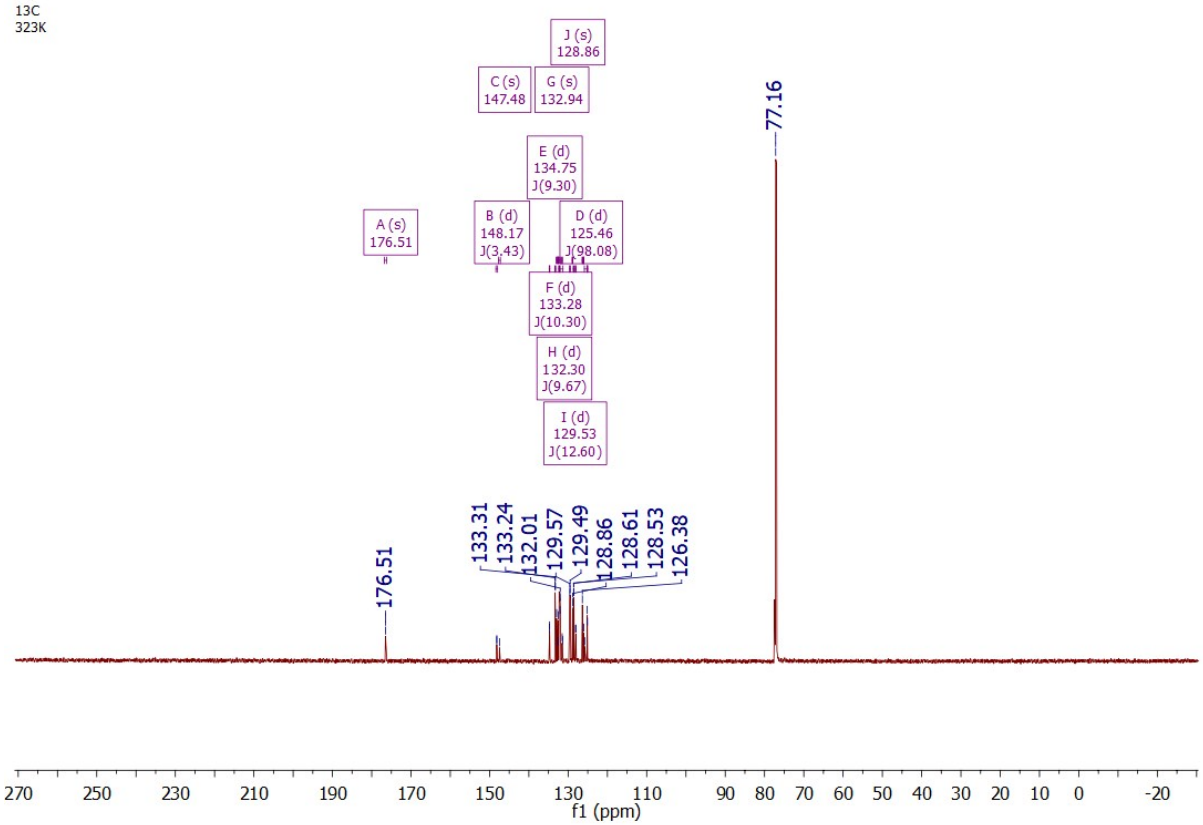
HH-COSY



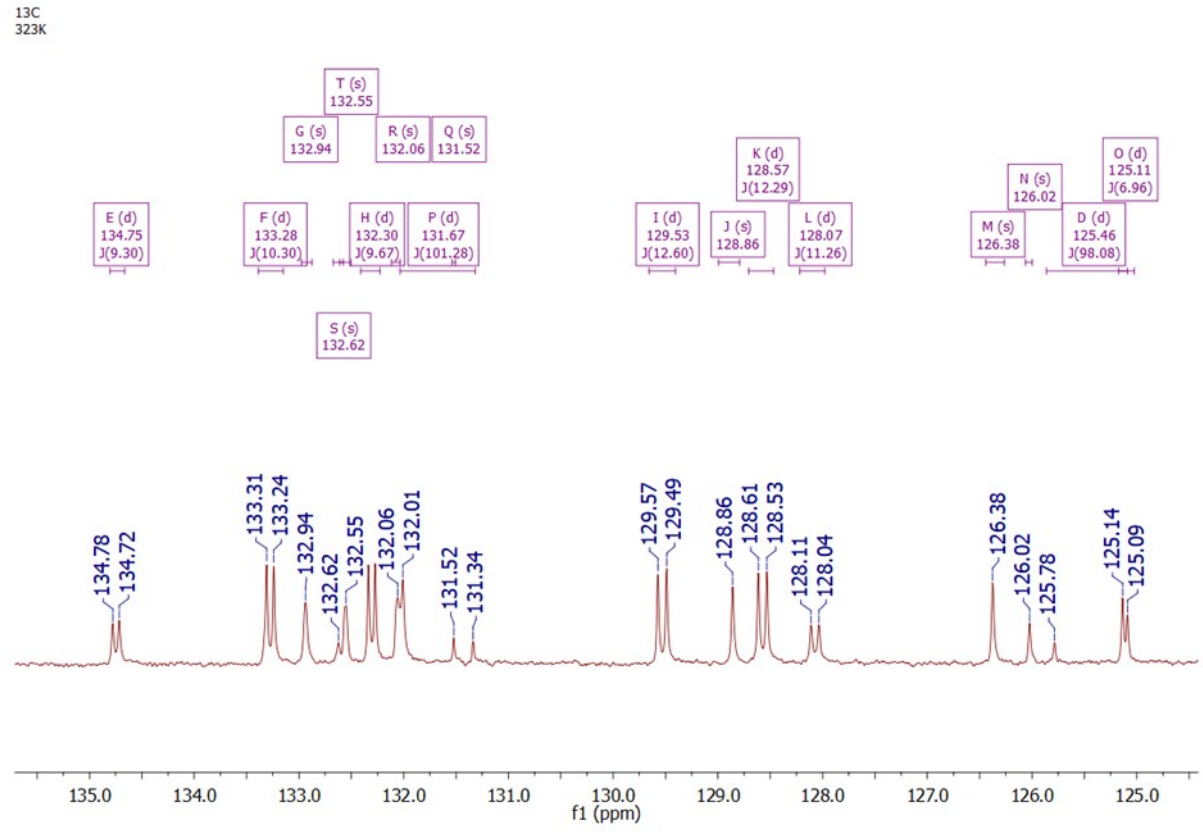
HH-COSY (aromatic region)



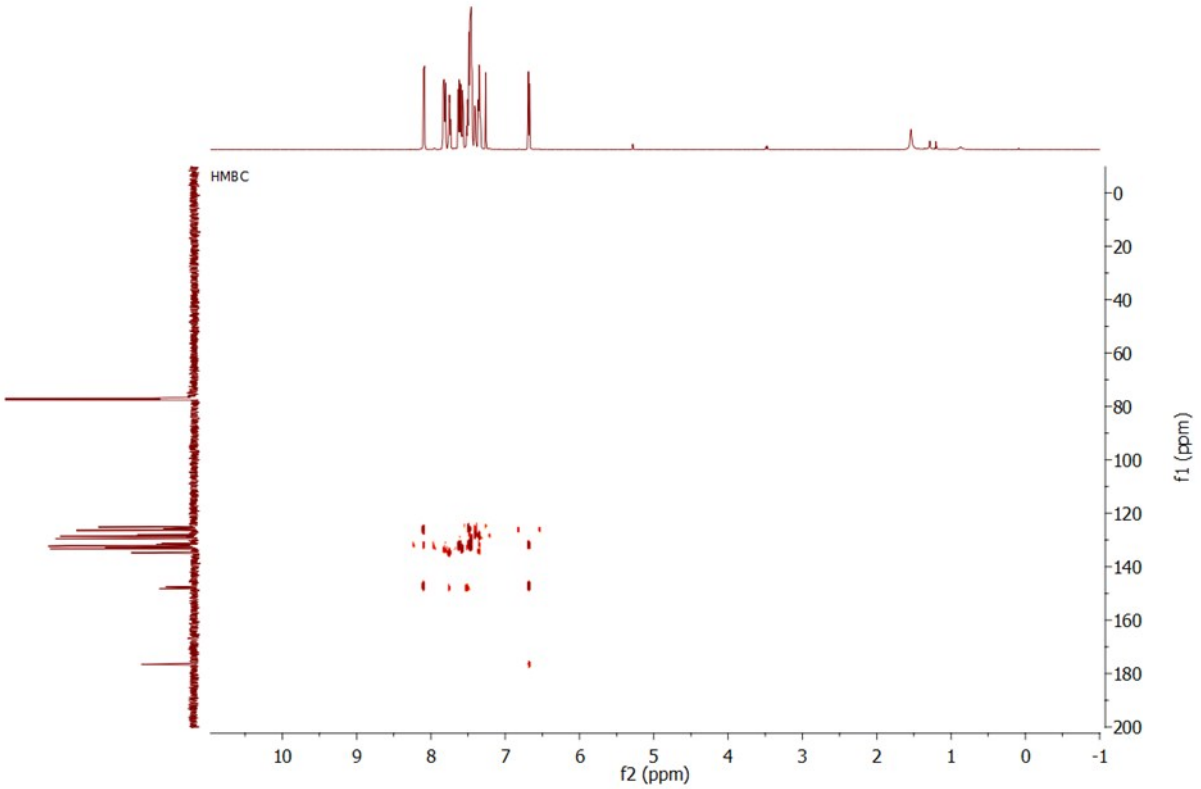
$^{13}C\{^{1}H\}$ NMR spectrum



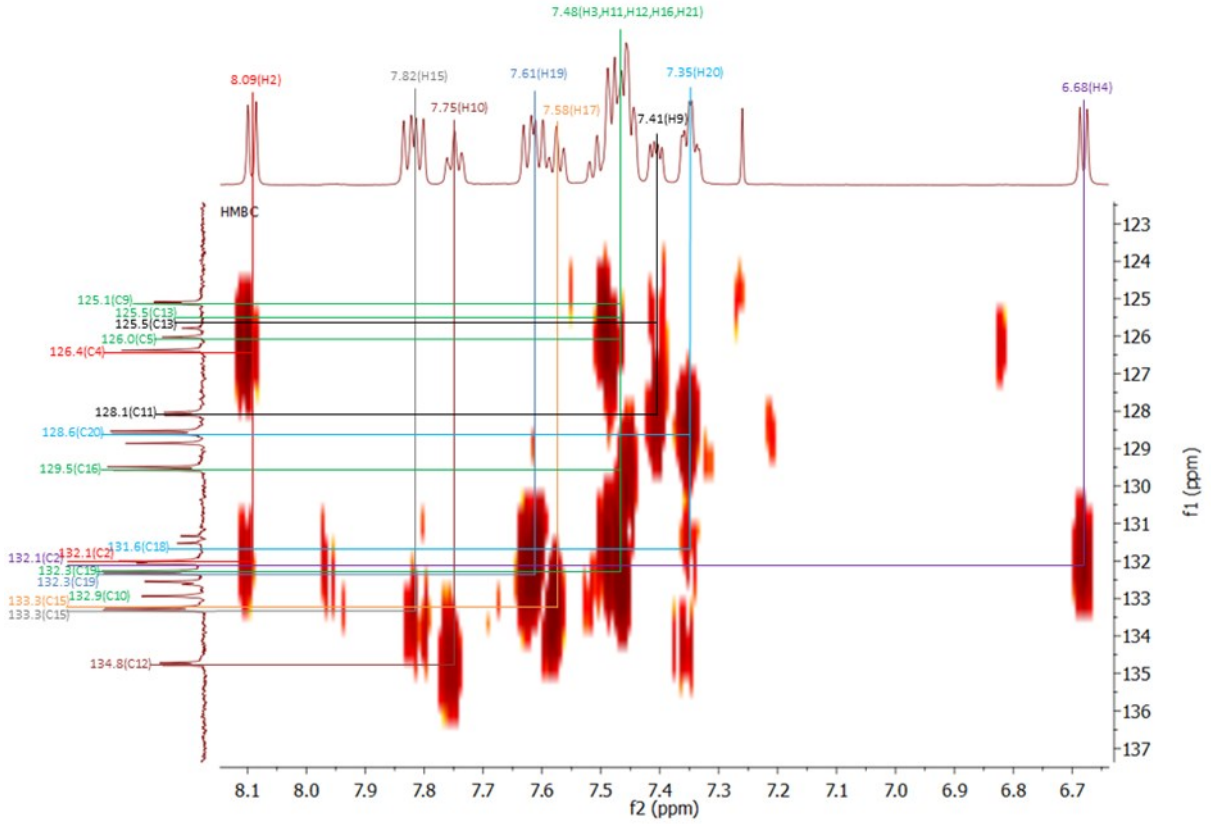
$^{13}C\{^{1}H\}$ NMR spectrum (aromatic region)



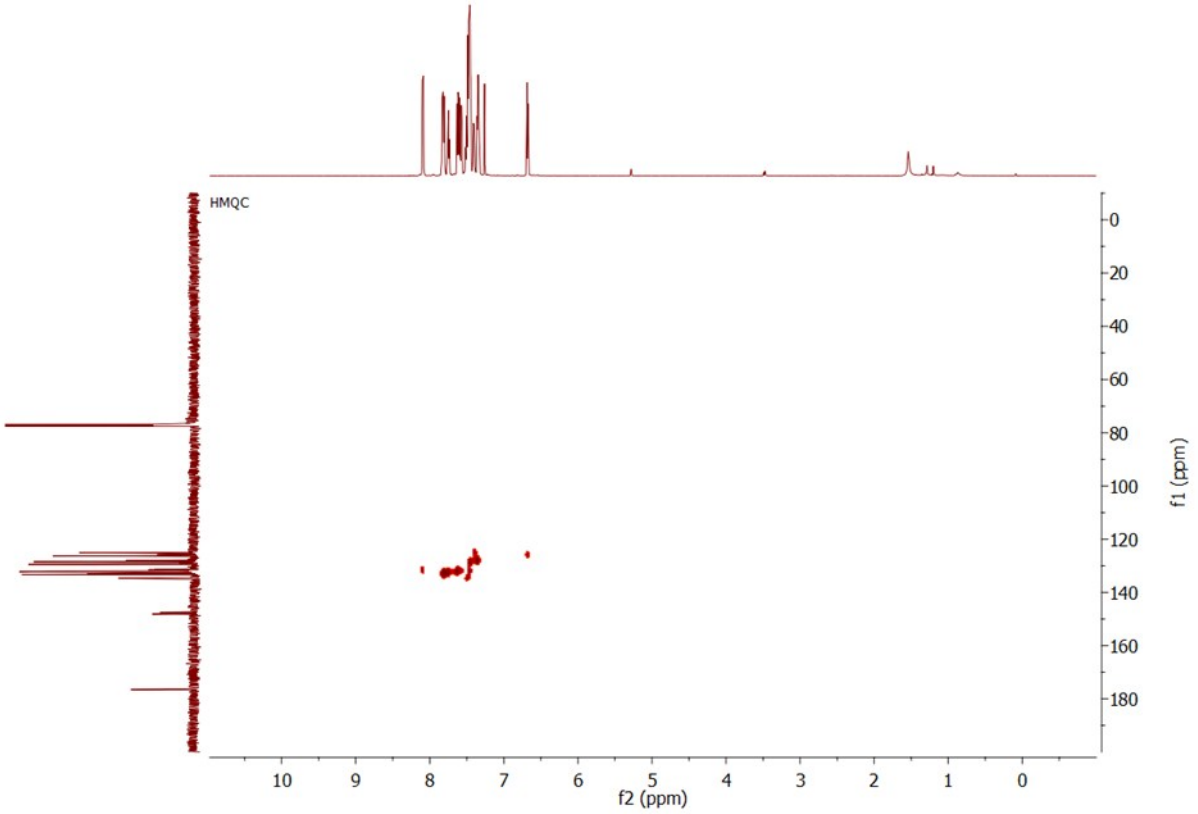
HMBC



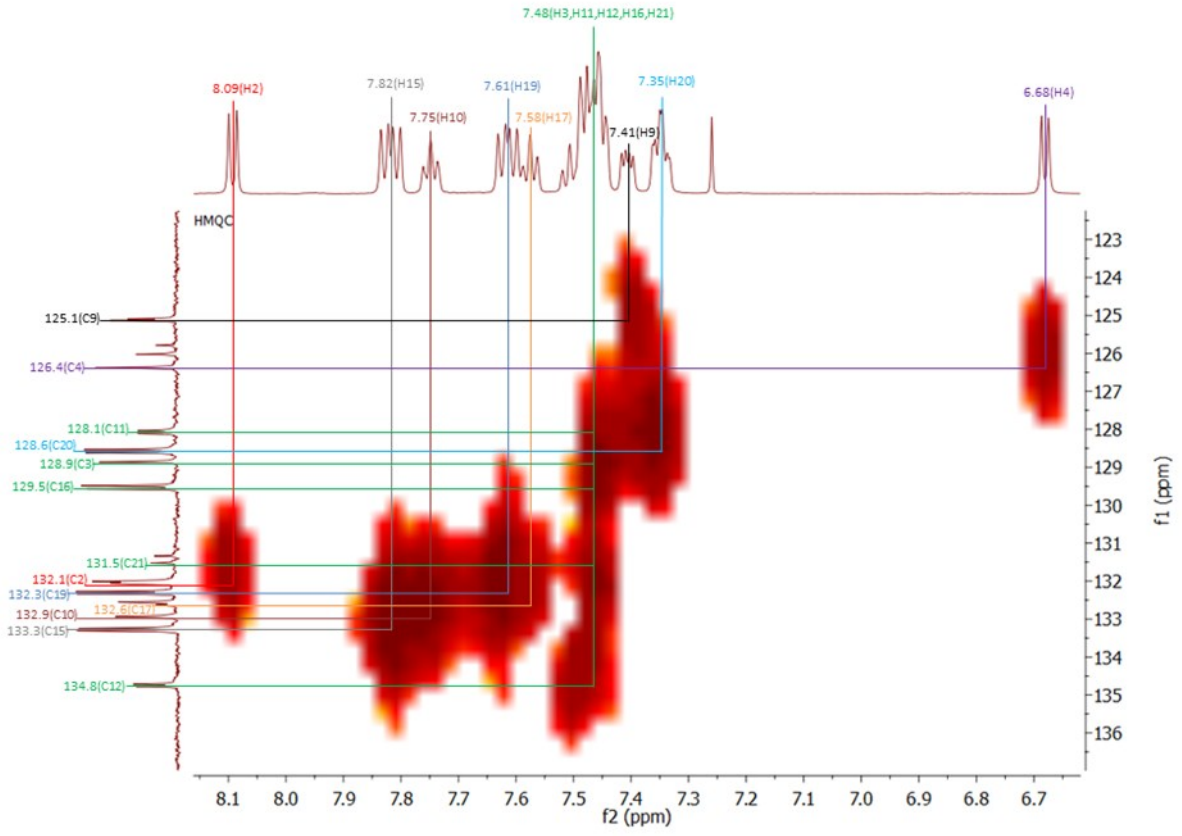
HMBC (aromatic region)



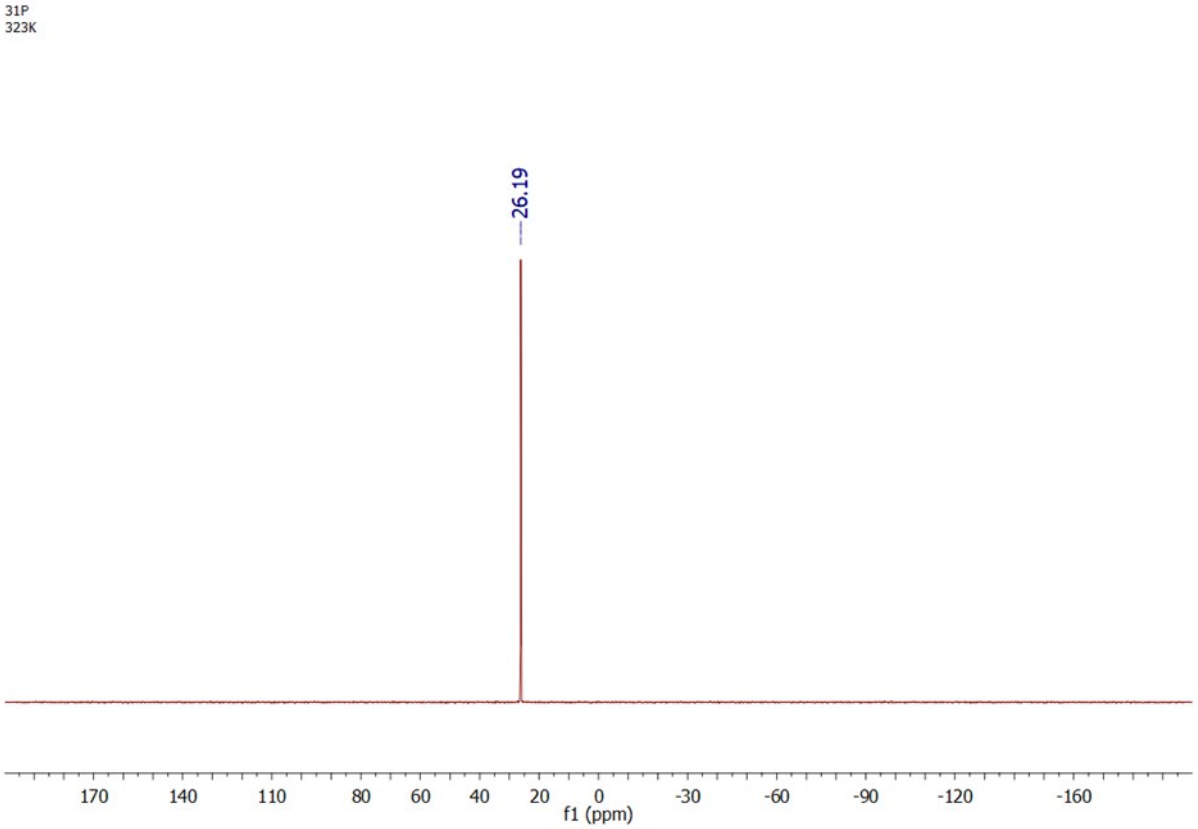
HMQC



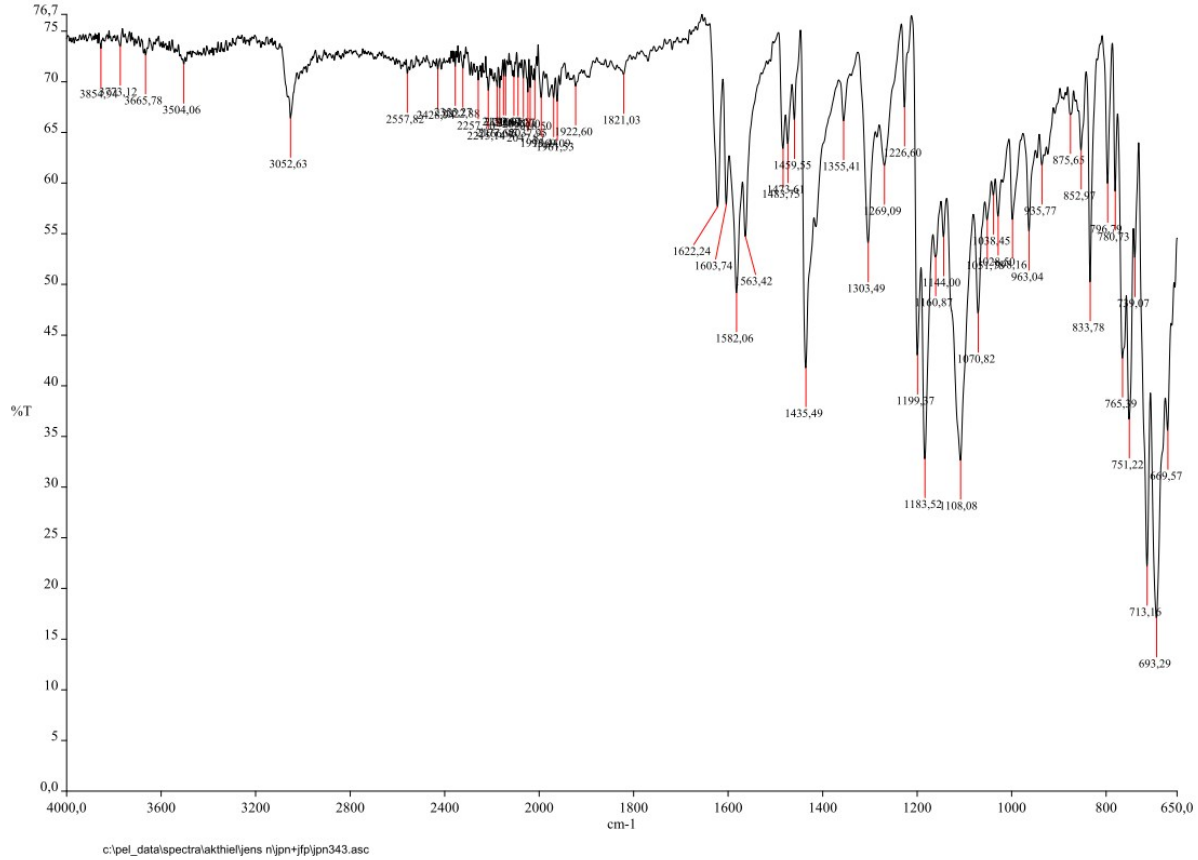
HMQC (aromatic region)



$^{31}P\{^{1}H\}$ NMR spectrum

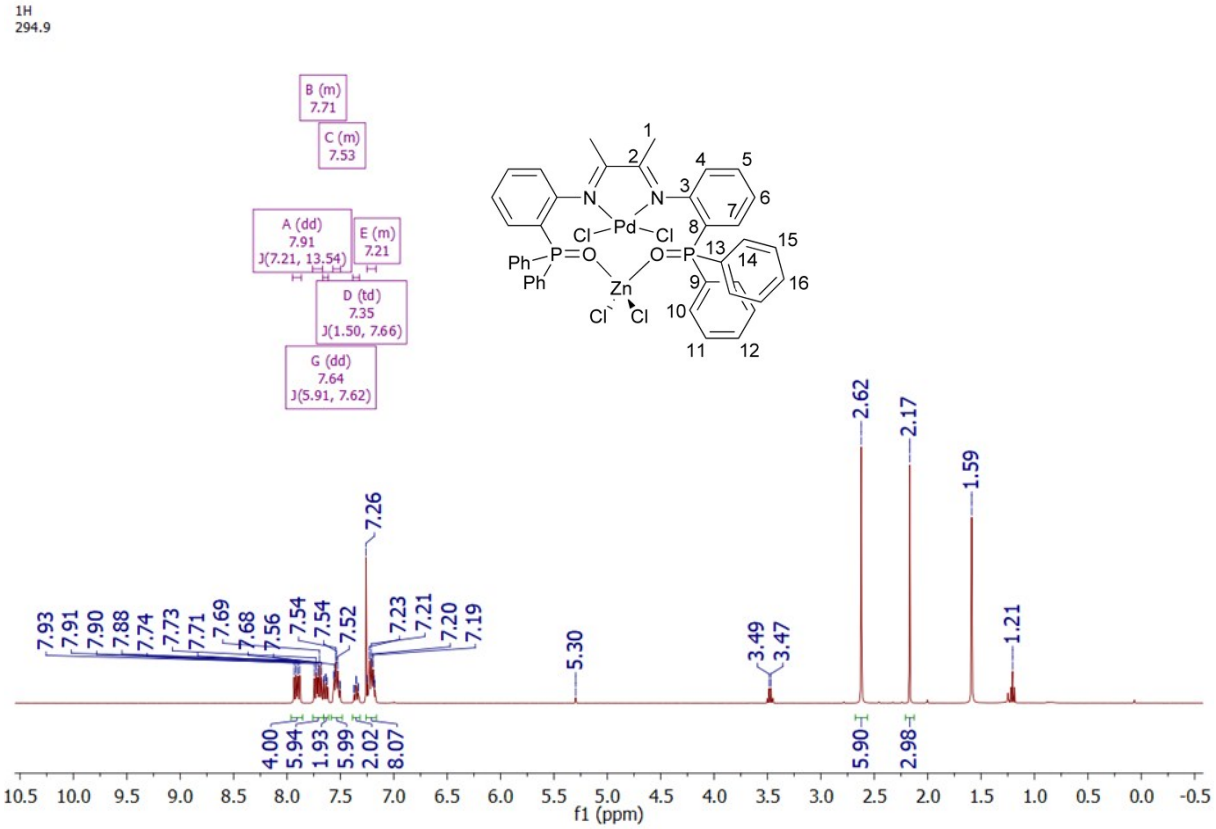


IR spectrum

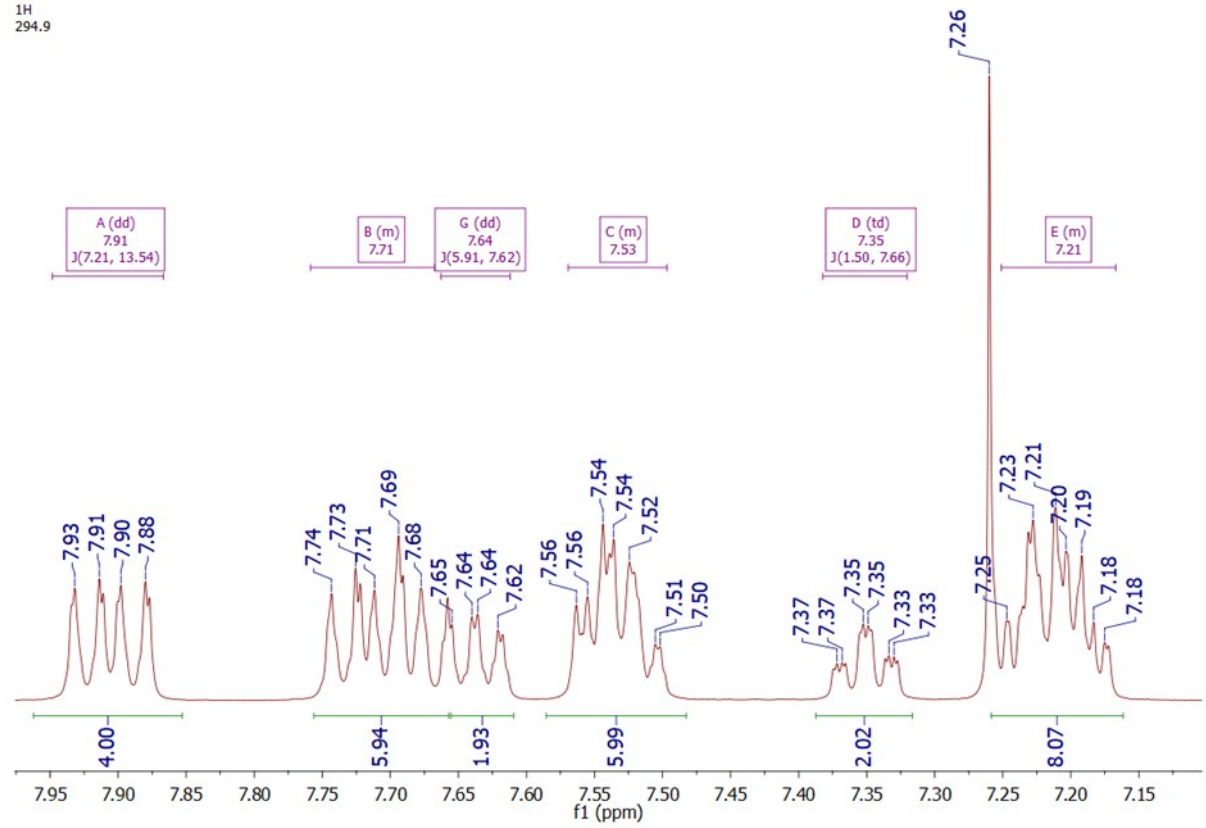


(1,4-Bis(2-diphenylphosphorylphenyl)-1,4-diaza-2,3-dimethyl-1,3-butadiene-1κ²N,2κ²O)-(dichloridopalladium)(dichloridozinc) (7a)

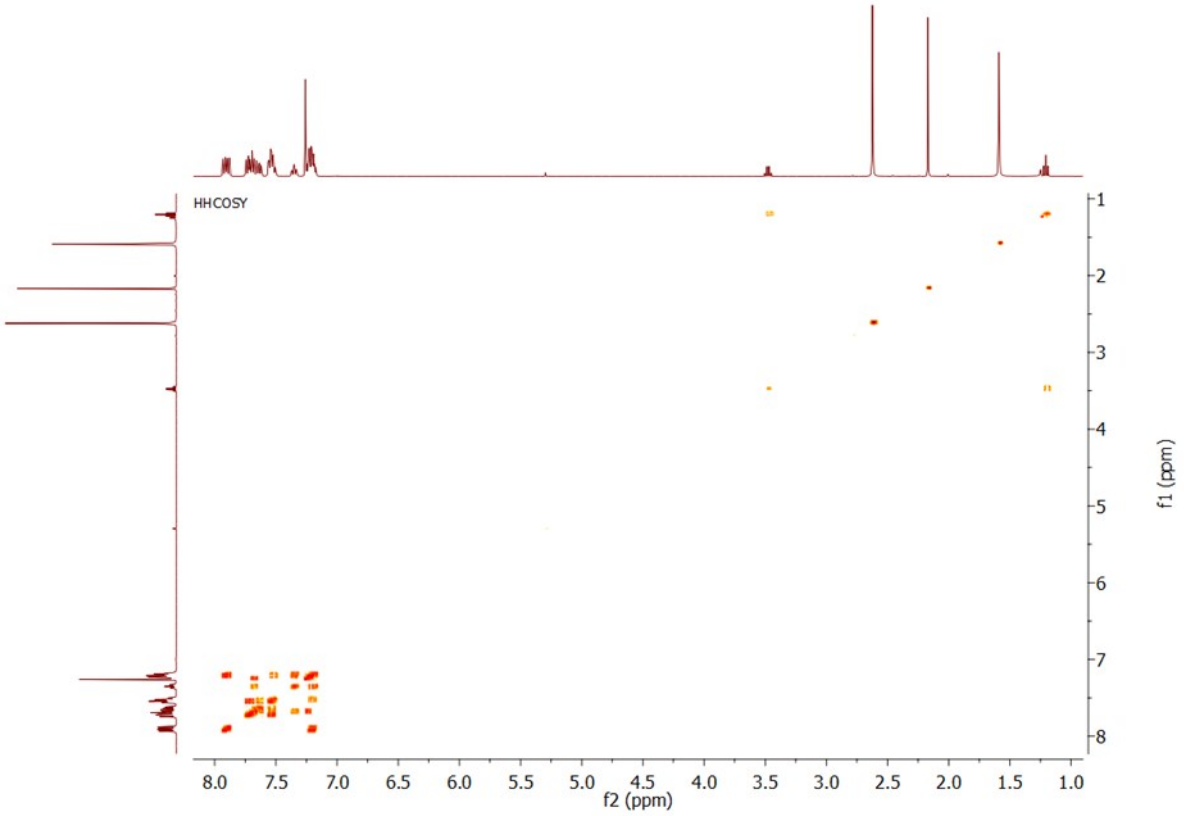
^{1}H NMR spectrum



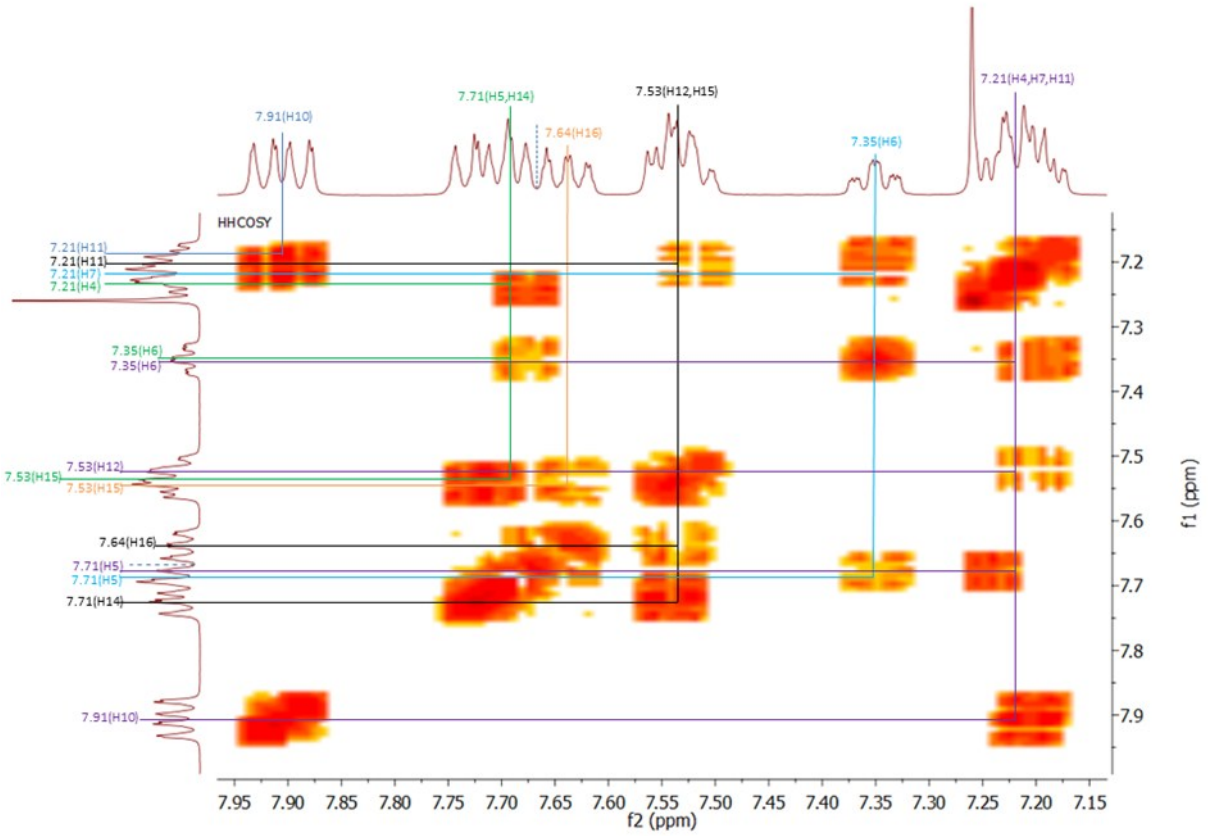
^{1}H NMR spectrum (aromatic region)



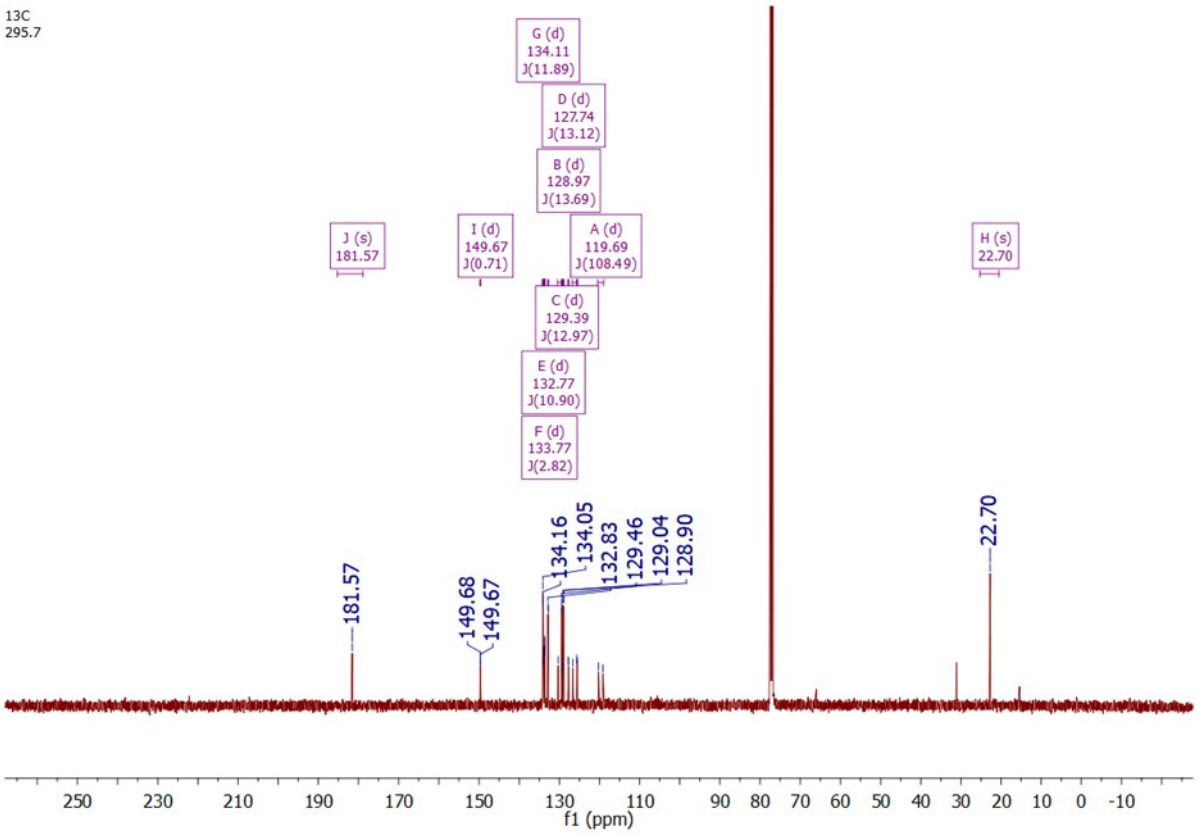
HH-COSY



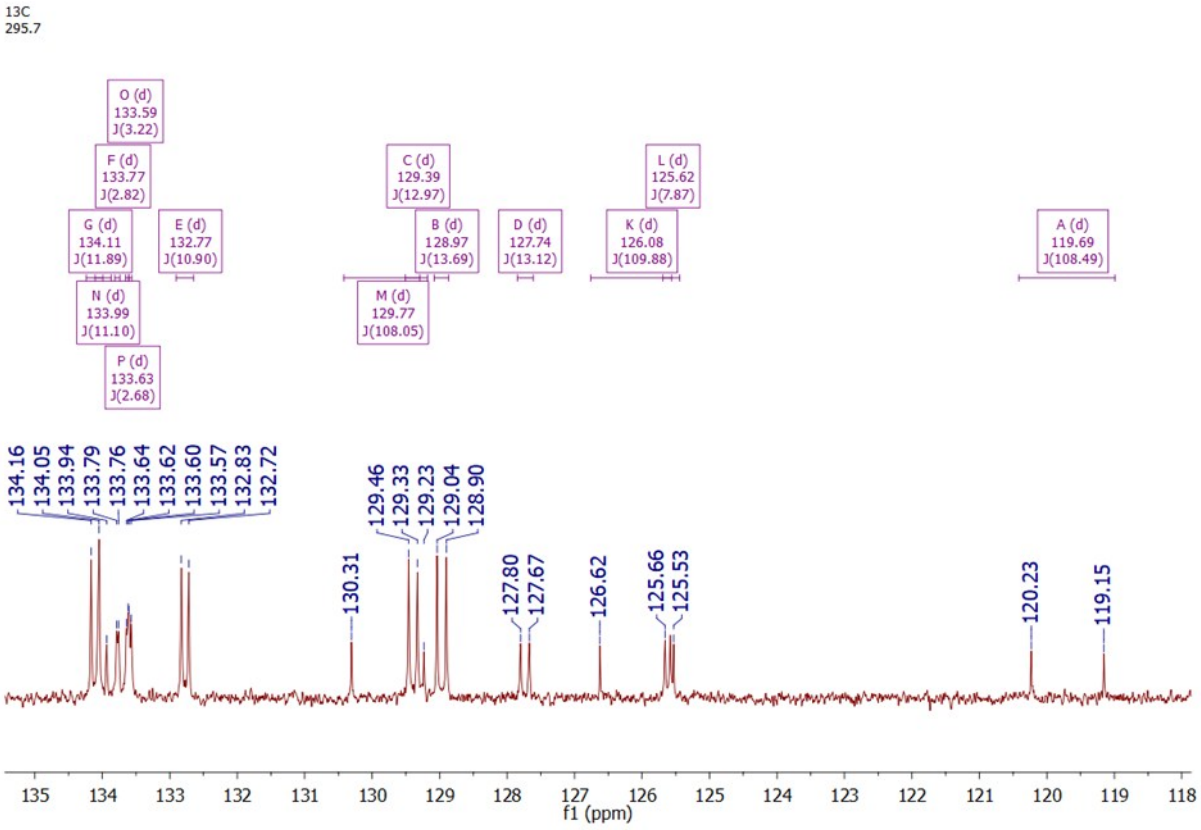
HH-COSY (aromatic region)



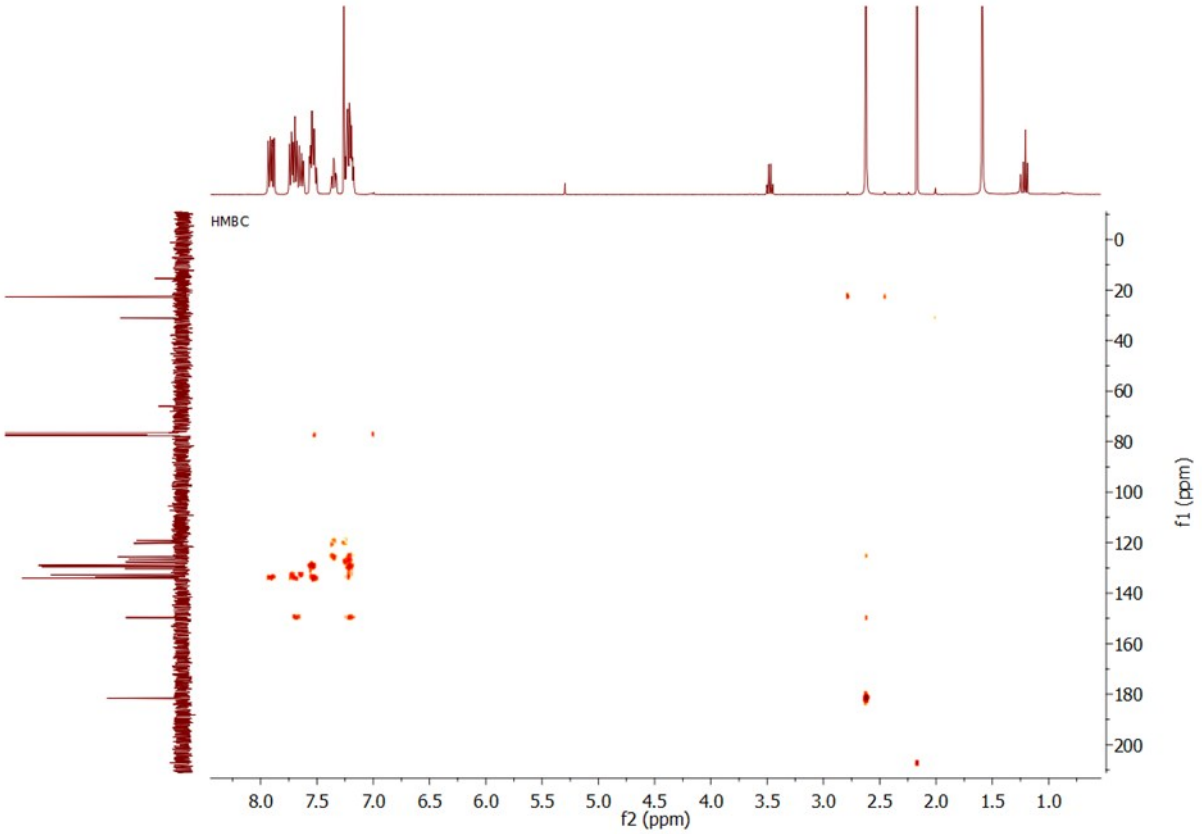
$^{13}C\{^{1}H\}$ NMR spectrum



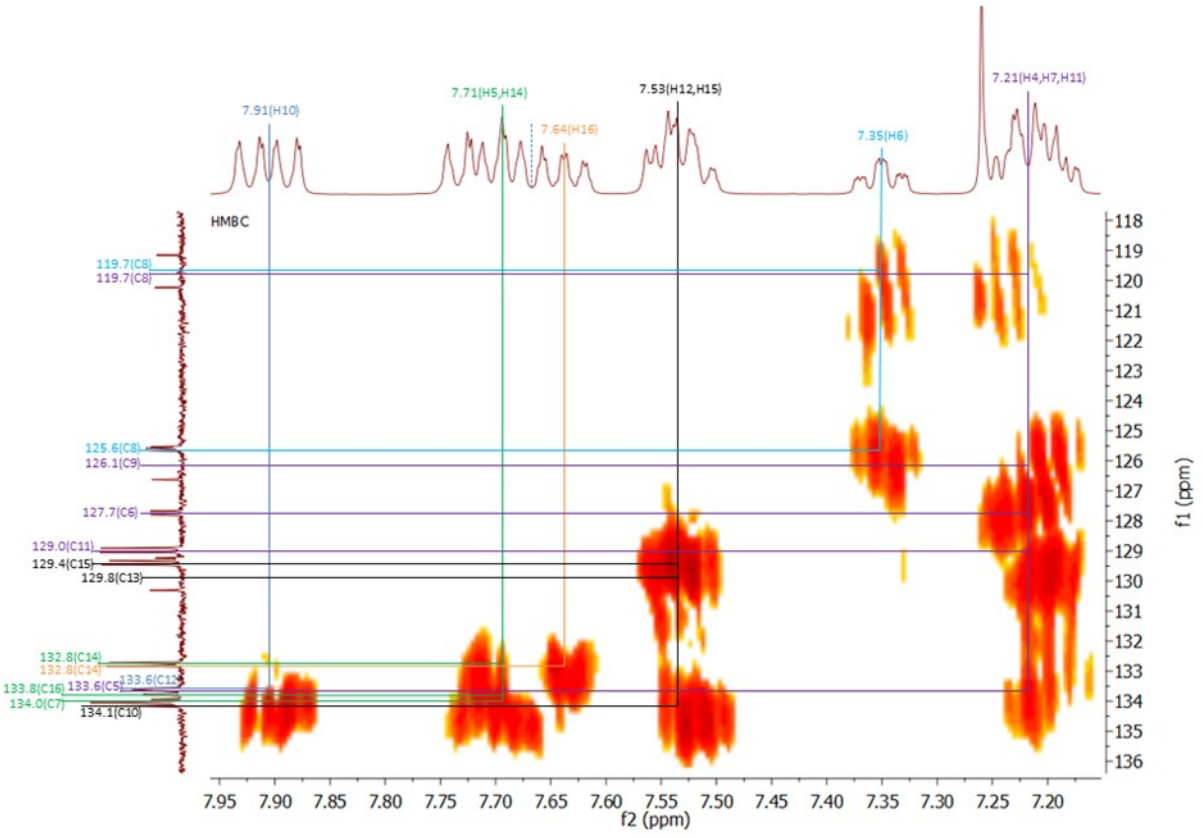
$^{13}C\{^{1}H\}$ NMR spectrum (aromatic region)



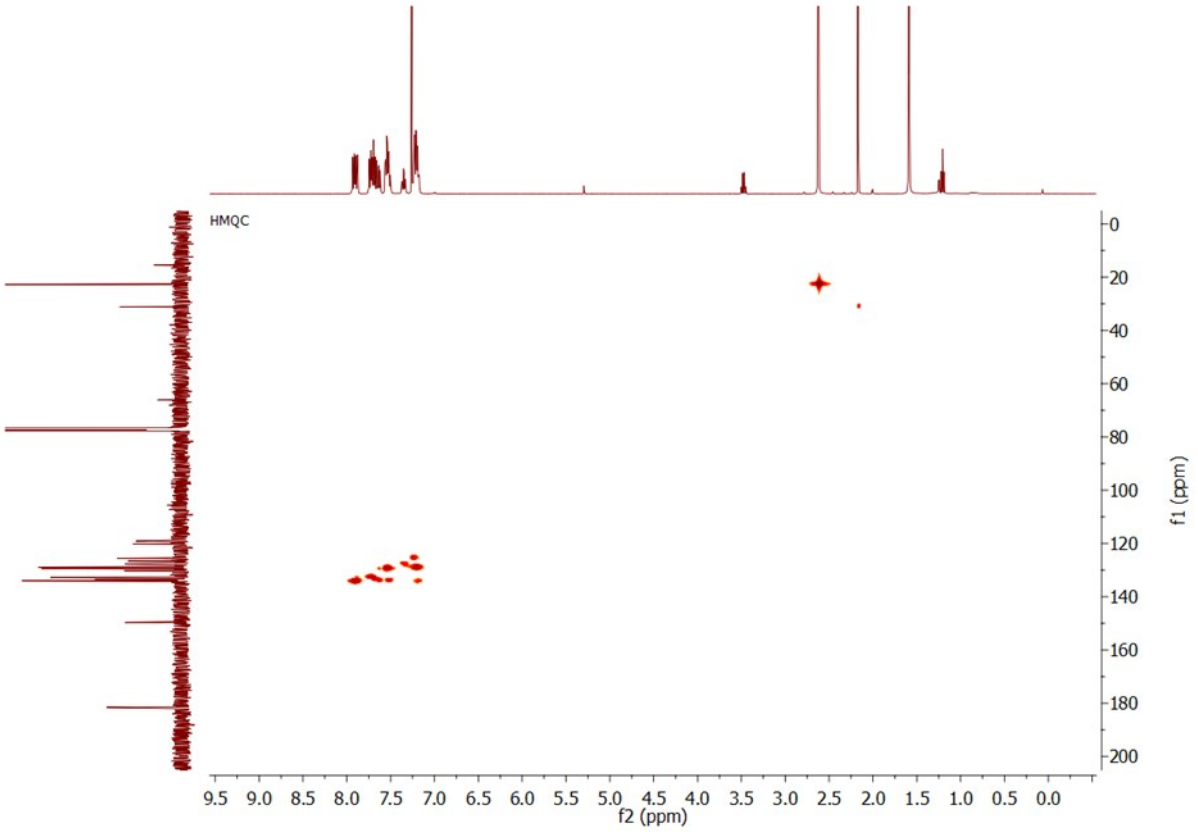
HMBC



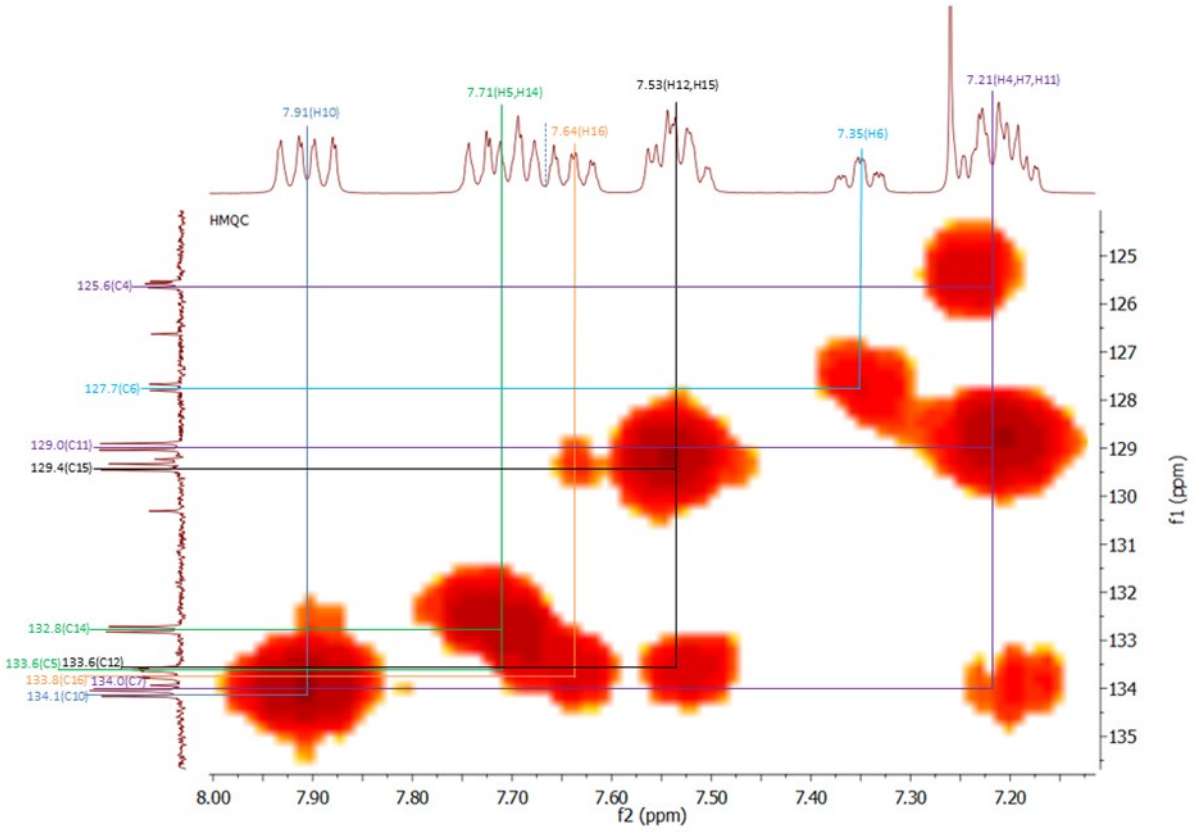
HMBC (aromatic region)



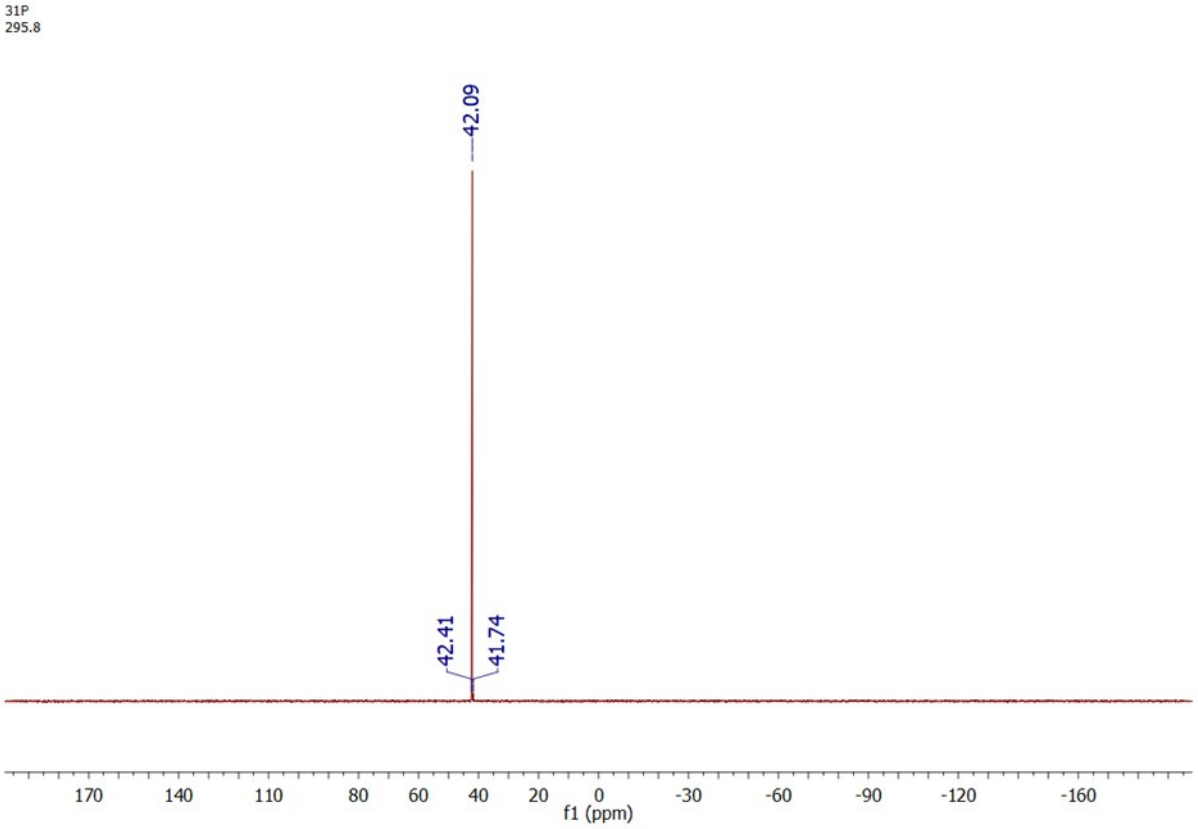
HMQC



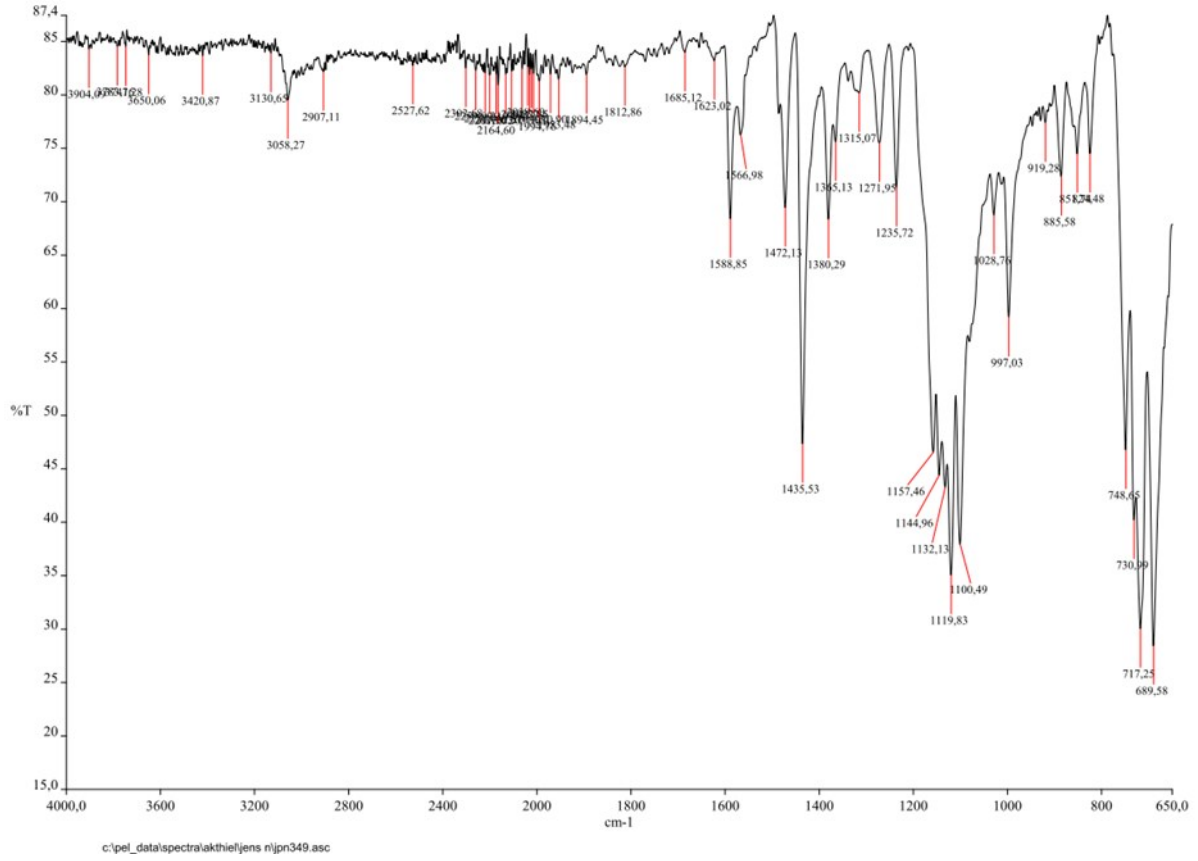
HMQC (aromatic region)



$^{31}P\{^{1}H\}$ NMR spectrum

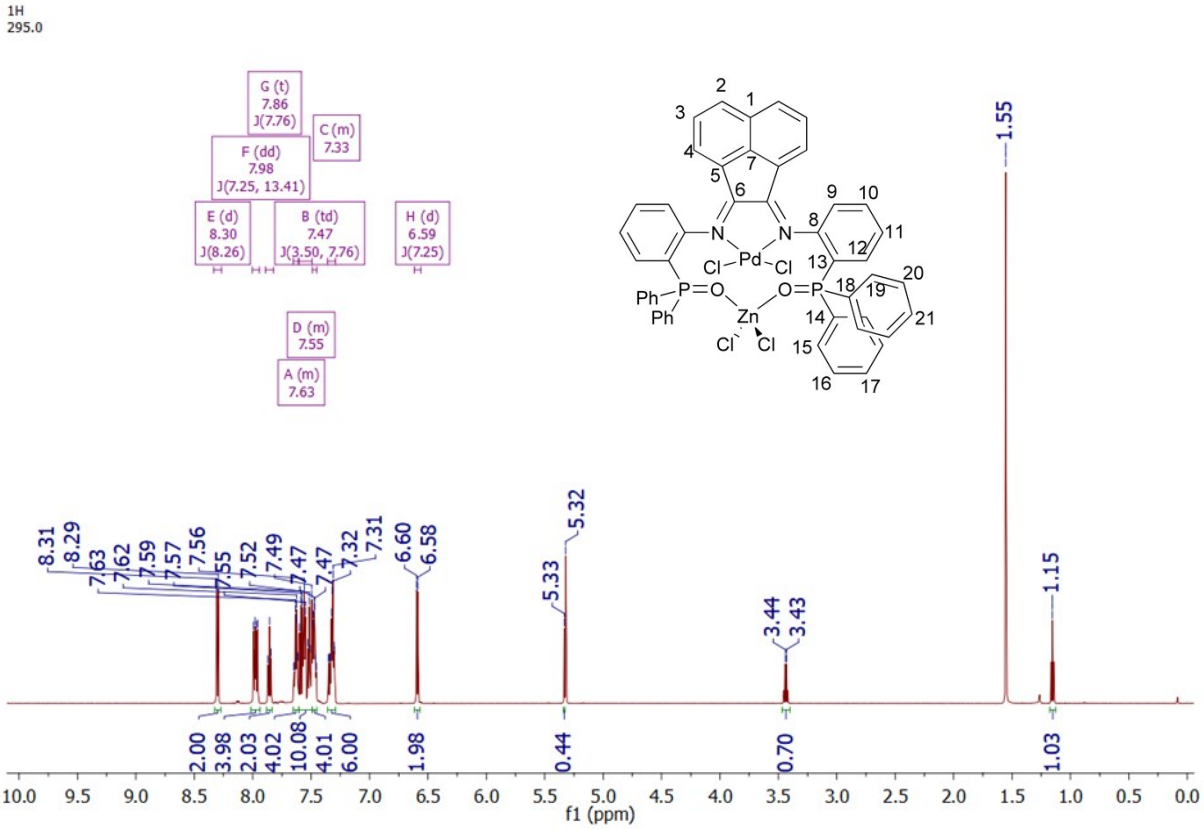


IR spectrum

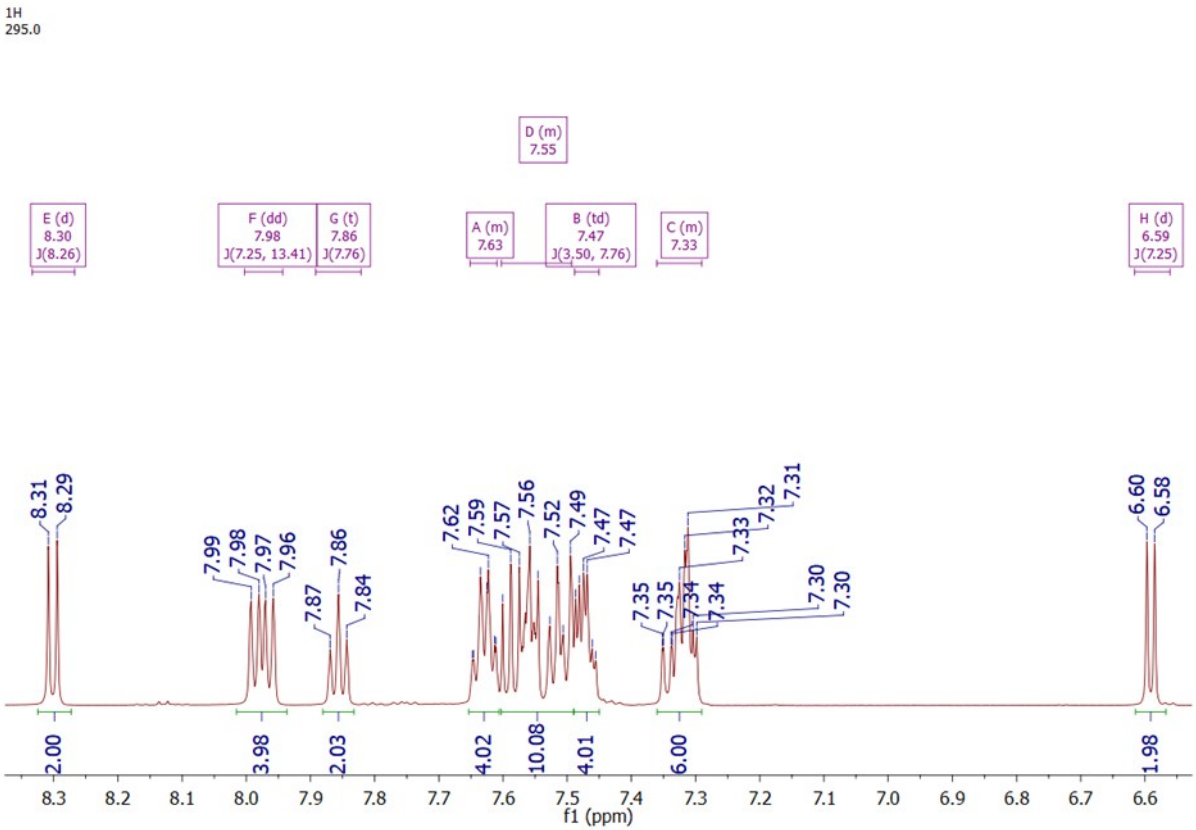


**[*N*,*N*'-1,2-Acenaphthylenediylidene(2-diphenylphosphoryl-phenyl)amine-1κ^2*N*,2κ^2*O*](dichloridopalladium)(dichloridozinc) (7b)

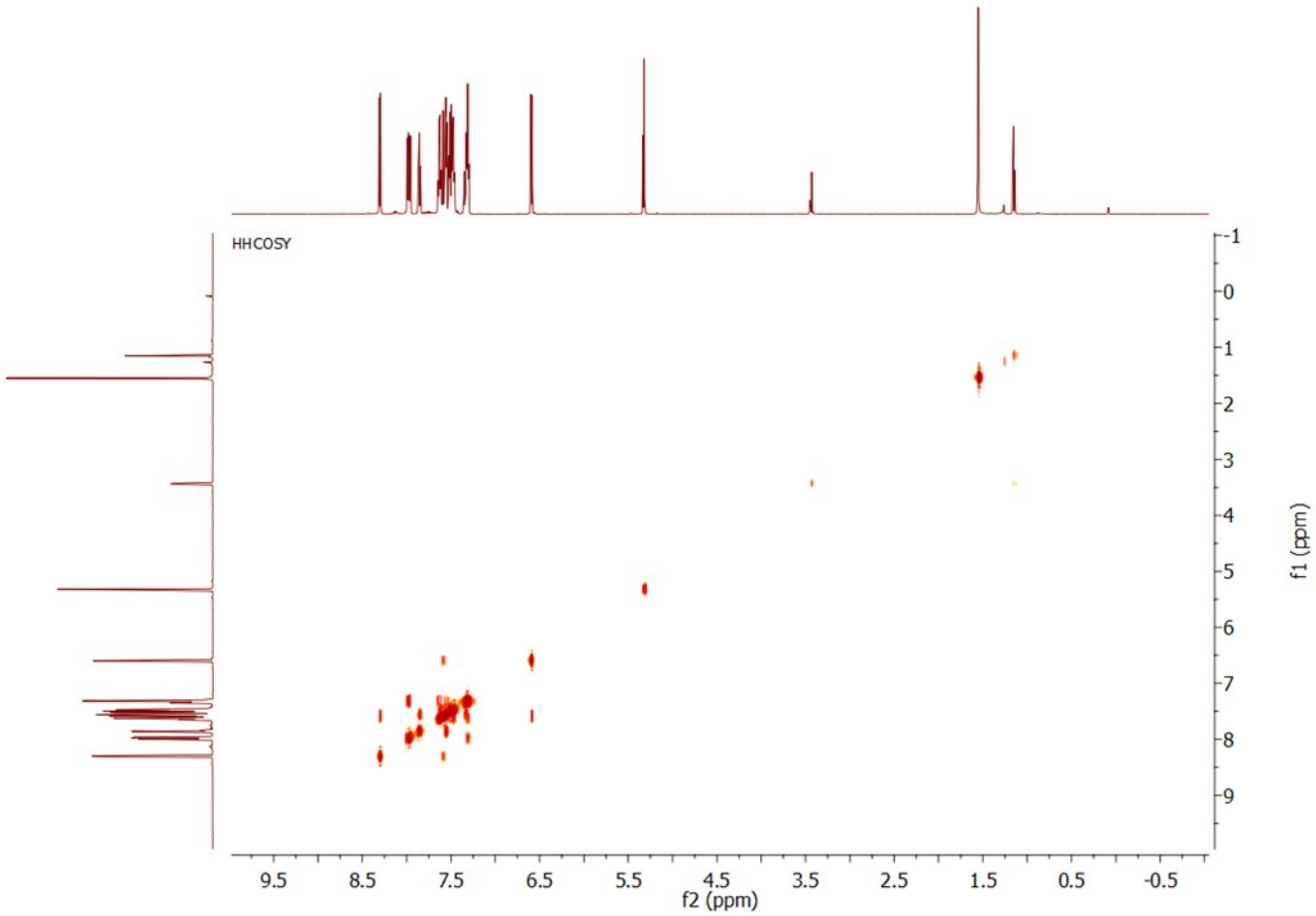
^{1}H NMR spectrum



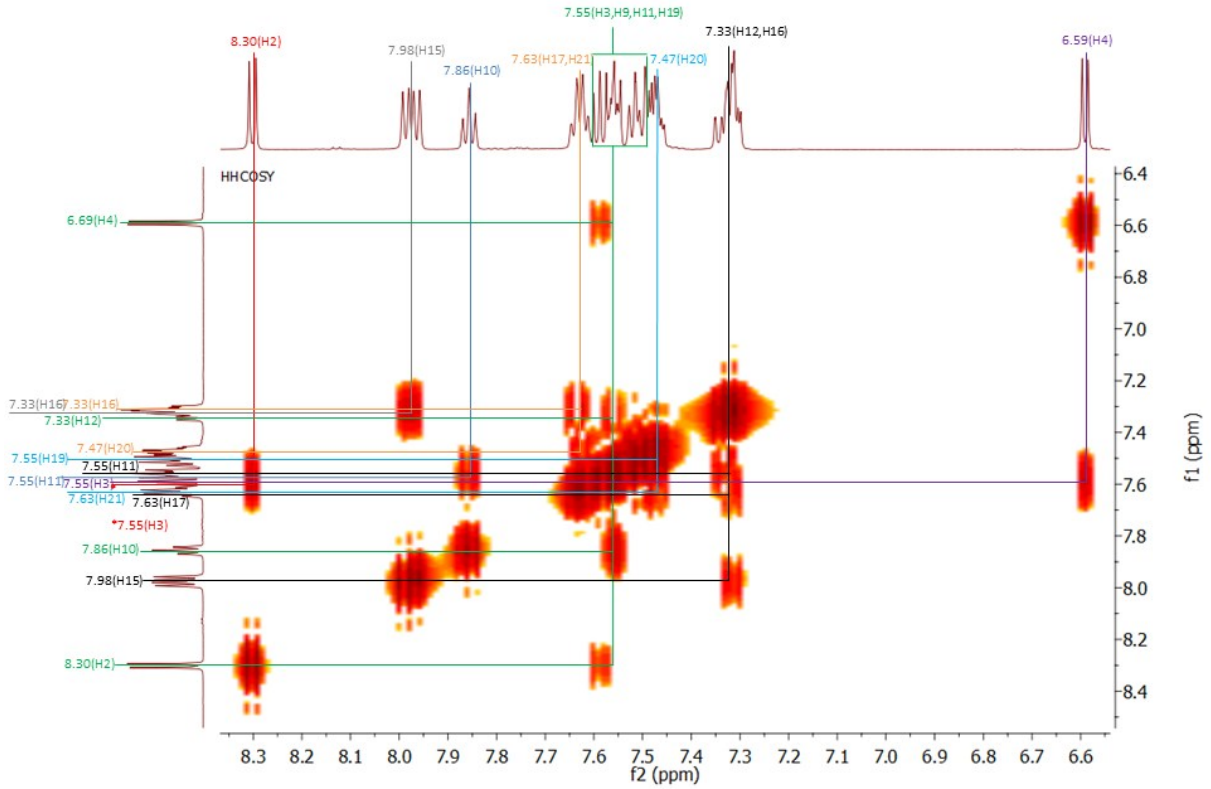
^{1}H NMR spectrum (aromatic region)



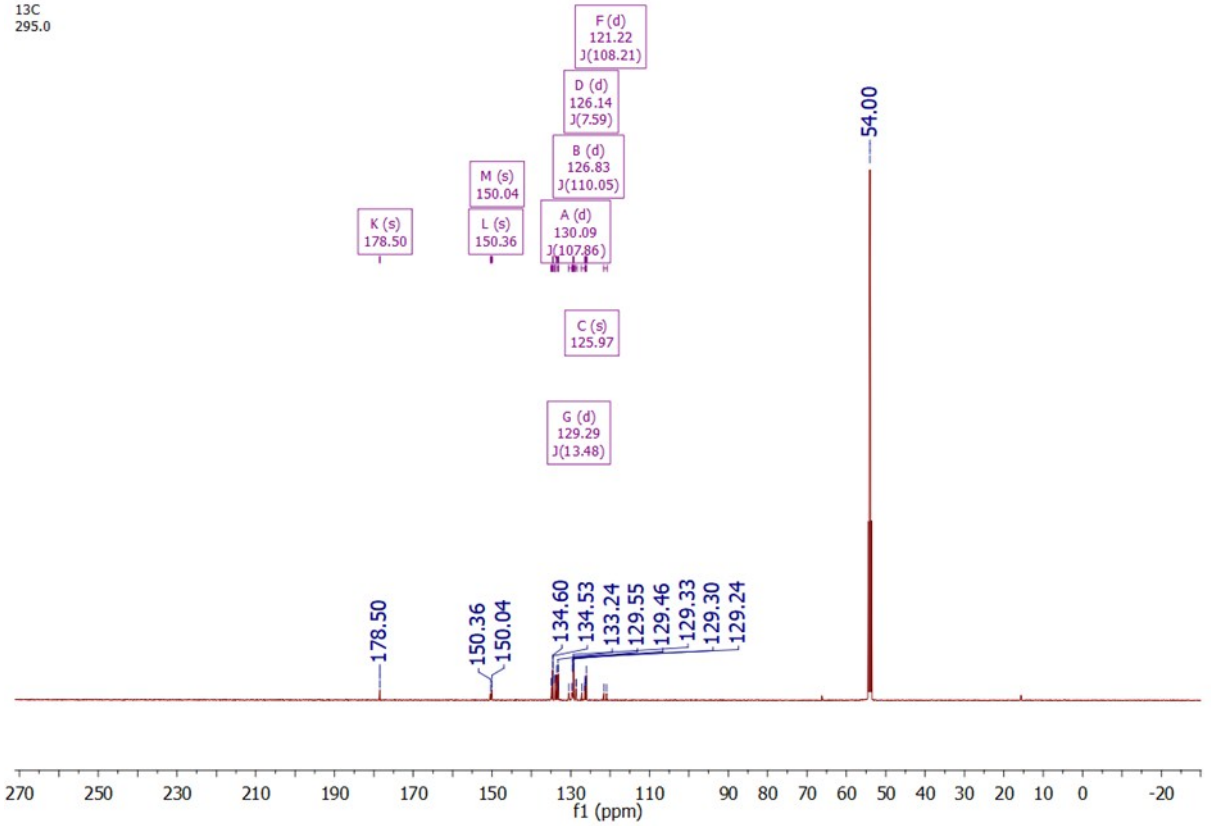
HH-COSY



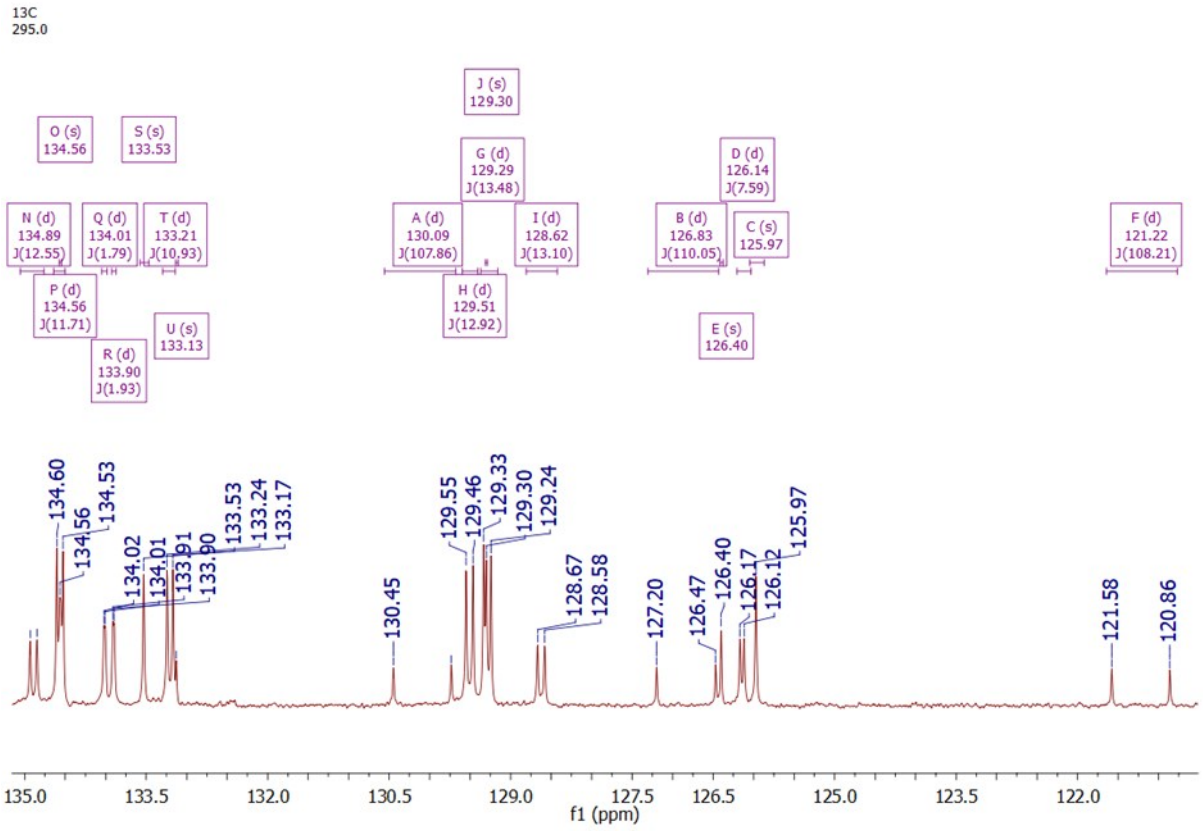
HH-COSY (aromatic region)



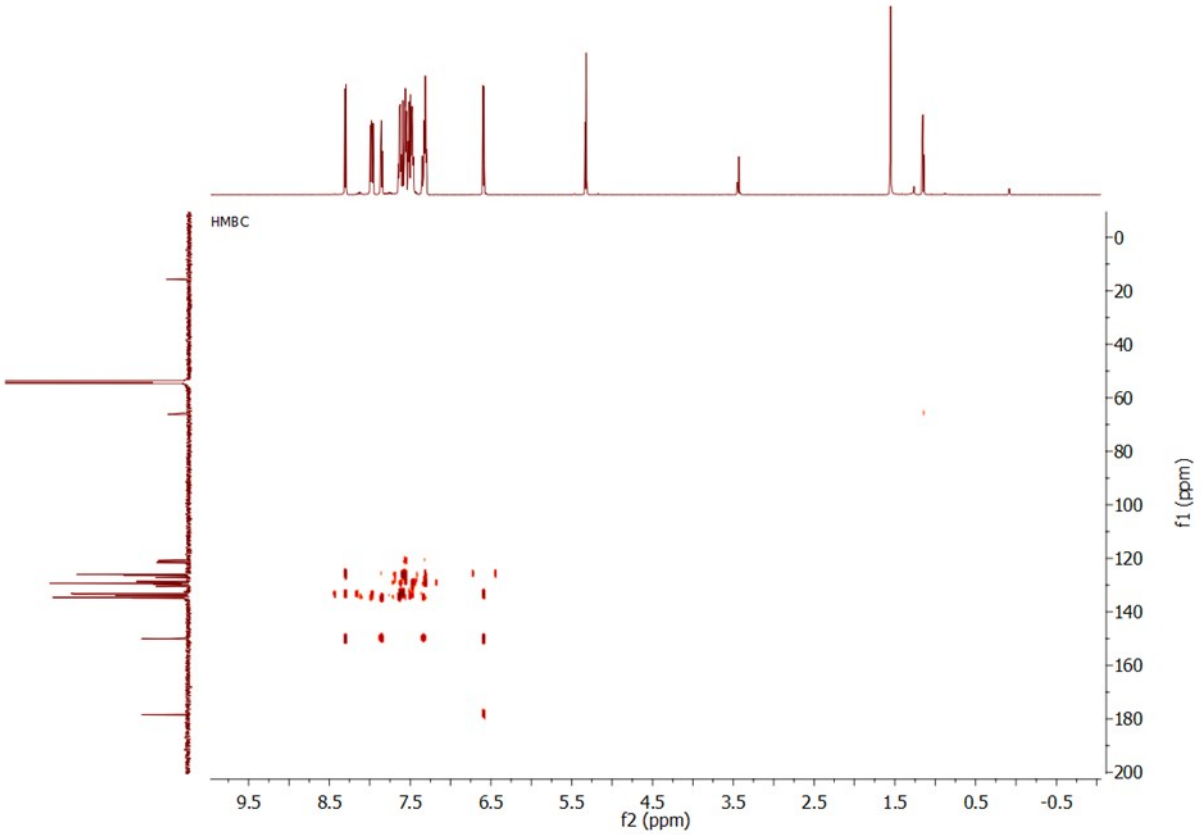
$^{13}C\{^{1}H\}$ NMR spectrum



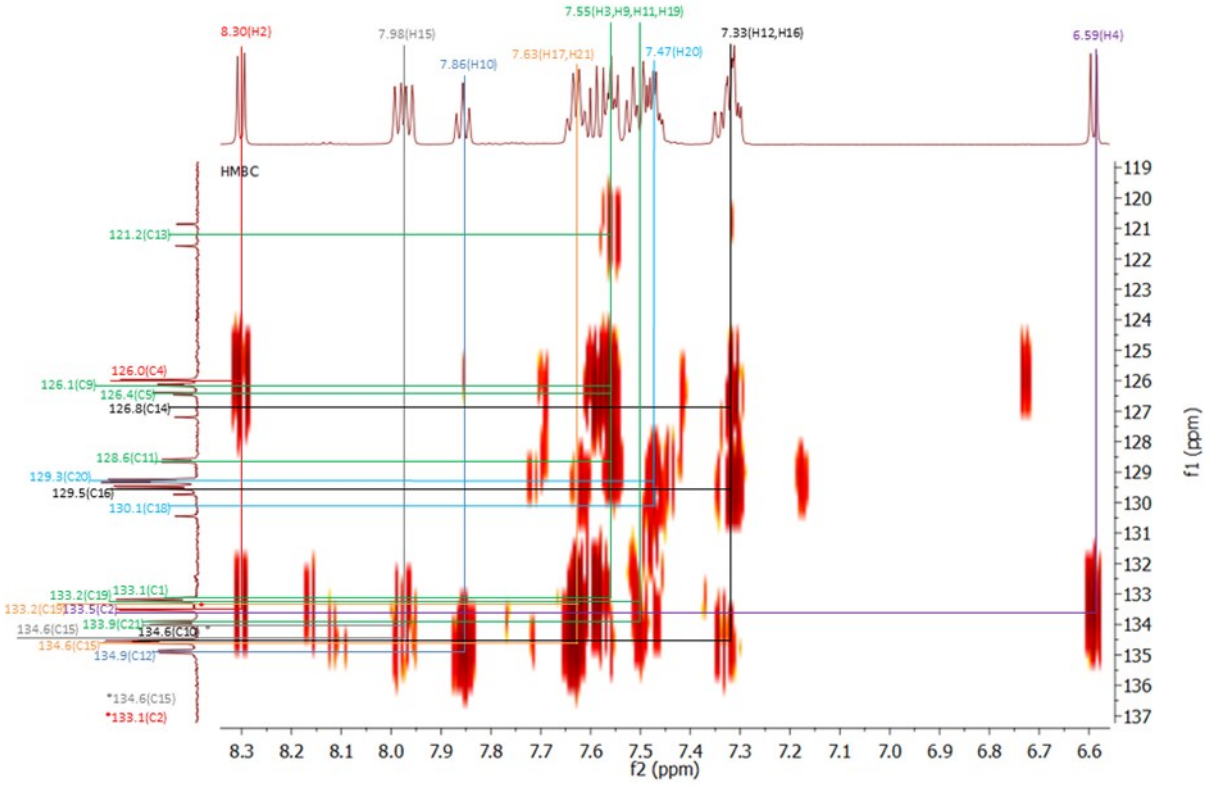
$^{13}C\{^{1}H\}$ NMR spectrum (aromatic region)


13C
295.0
J (s)
129.30
O (s)
134.56
S (s)
133.53
G (d)
129.29
J(13.48)
D (d)
126.14
J(7.59)
N (d)
134.89
J(12.55)
Q (d)
134.01
J(1.79)
T (d)
133.21
J(10.93)
A (d)
130.09
J(107.86)
I (d)
128.62
J(13.10)
B (d)
126.83
J(110.05)
C (s)
125.97
F (d)
121.22
J(108.21)
P (d)
134.56
J(11.71)
H (d)
129.51
J(12.92)
U (s)
133.13
R (d)
133.90
J(1.93)
E (s)
126.40
134.60
134.56
134.53
134.02
134.01
133.91
133.90
133.53
133.24
133.17
130.45
129.55
129.46
129.33
129.30
129.24
128.67
128.58
127.20
126.47
126.40
126.17
126.12
125.97
121.58
120.86
135.0
133.5
132.0
130.5
129.0
127.5
126.5
125.0
123.5
122.0
f1 (ppm)

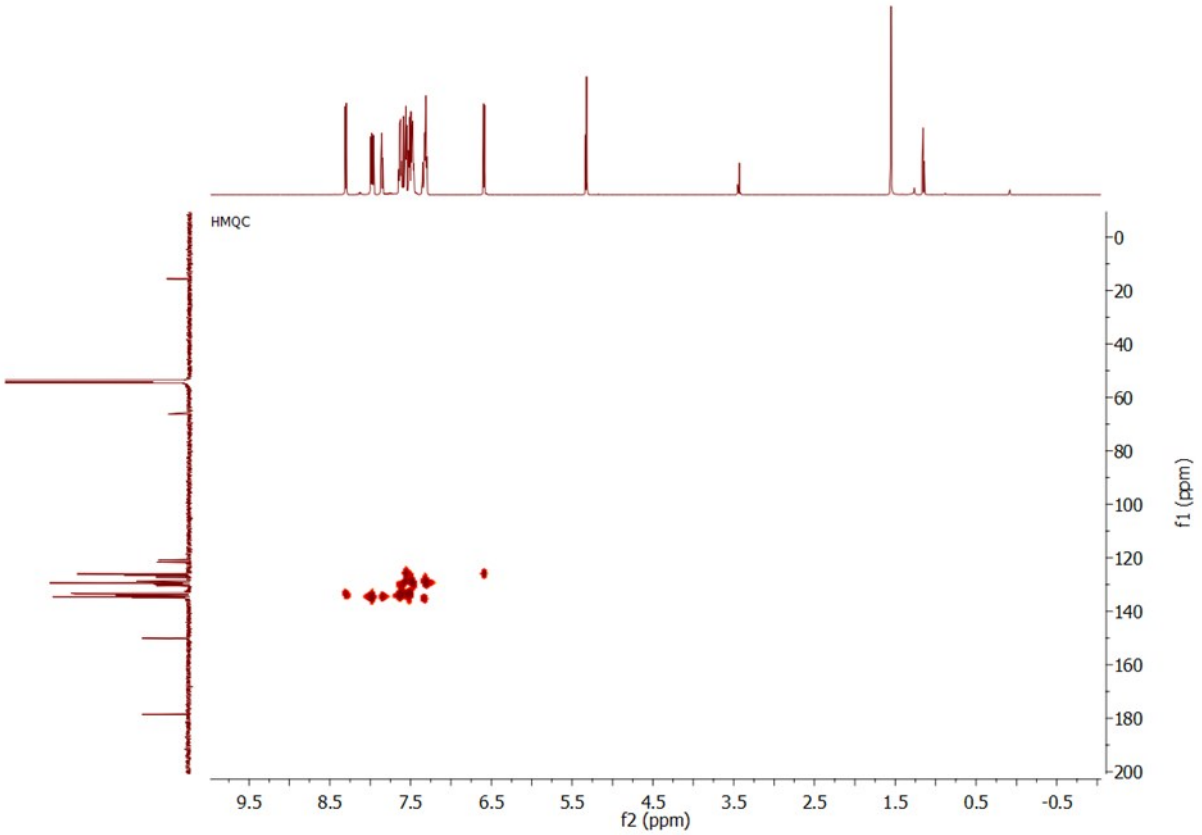
HMBC



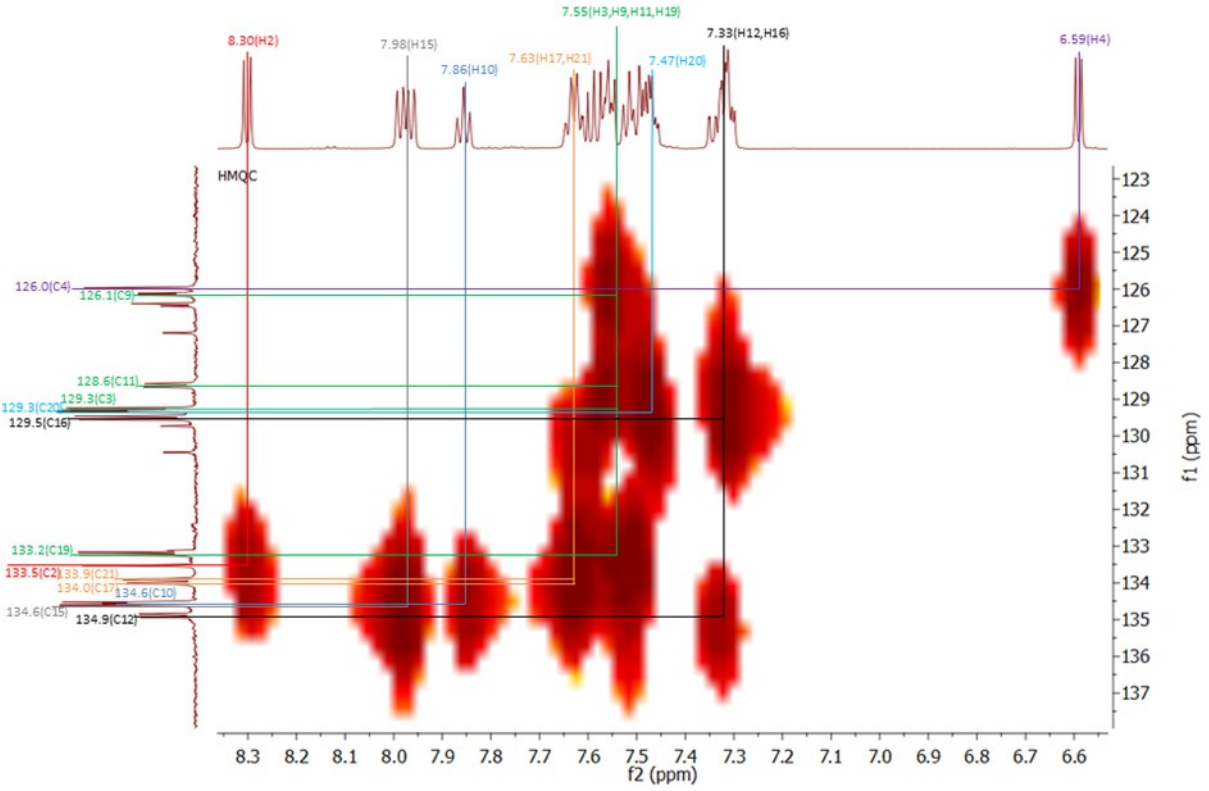
HMBC (aromatic region)



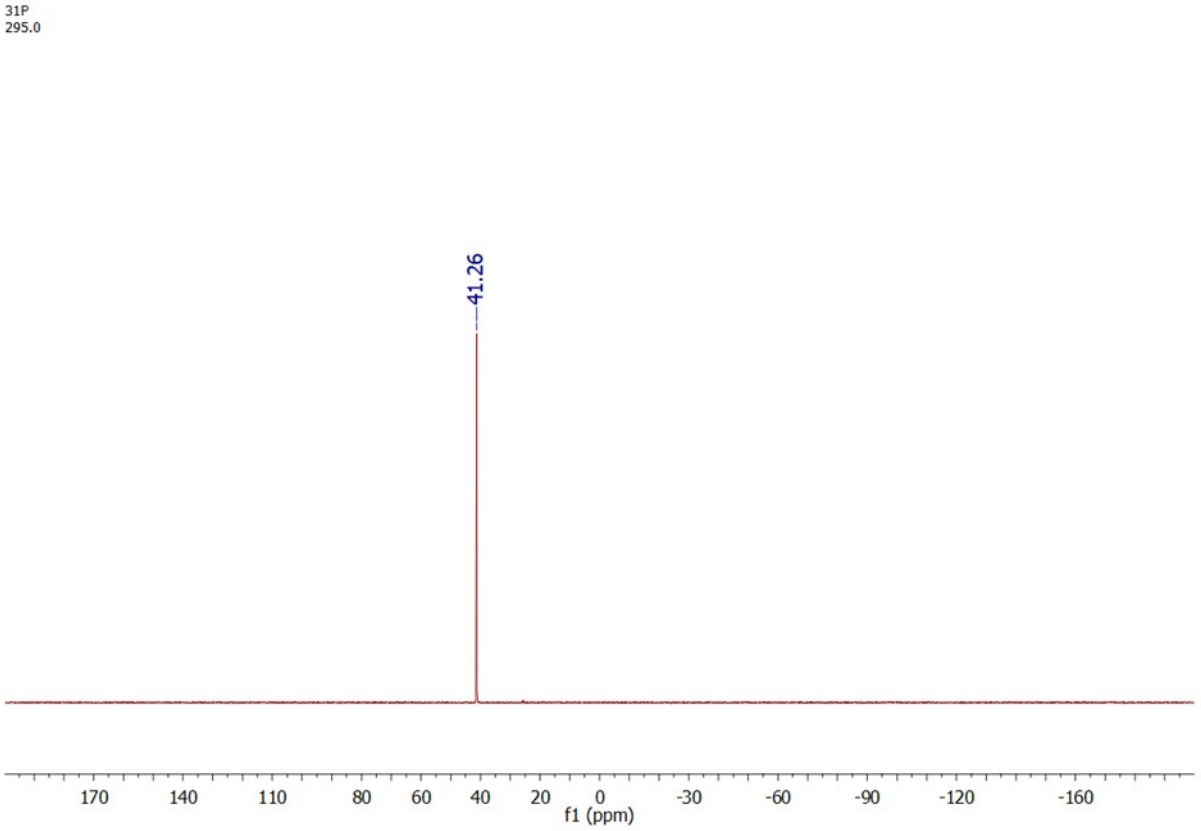
HMQC



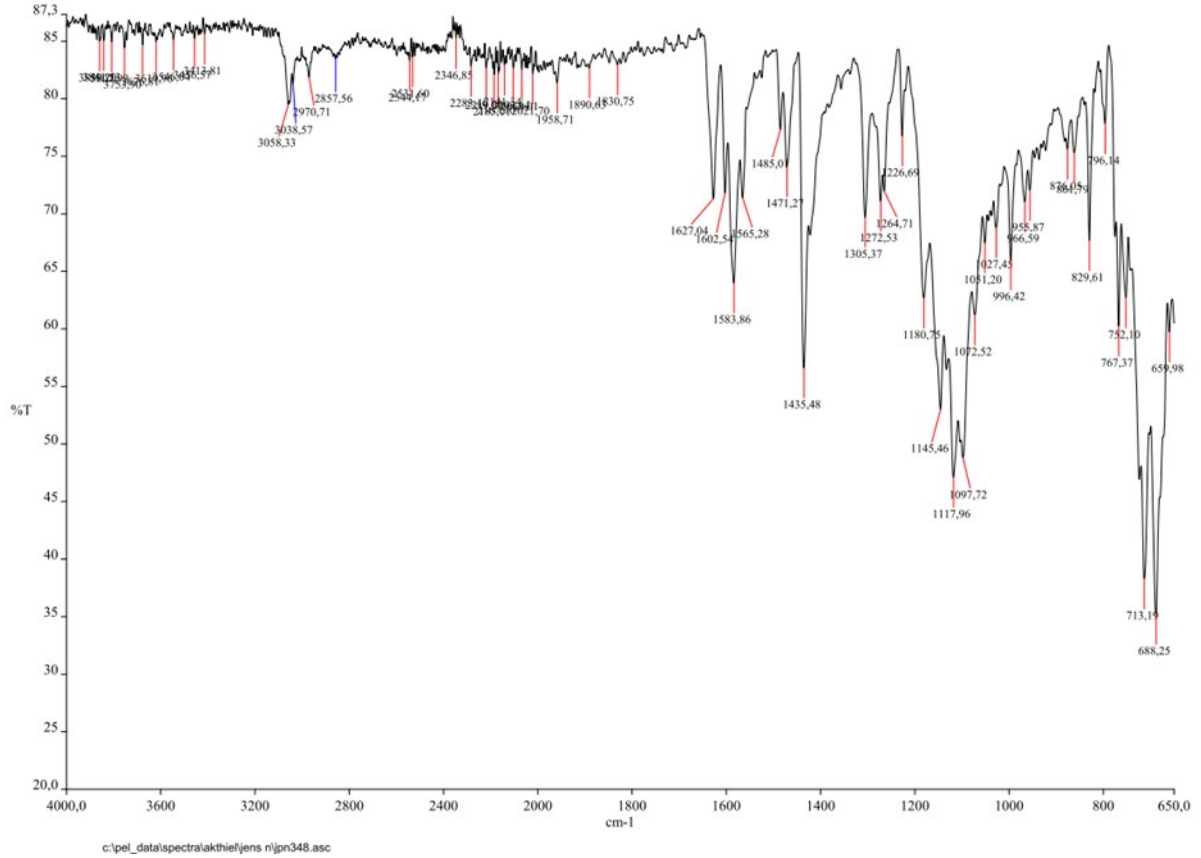
HMQC (aromatic region)



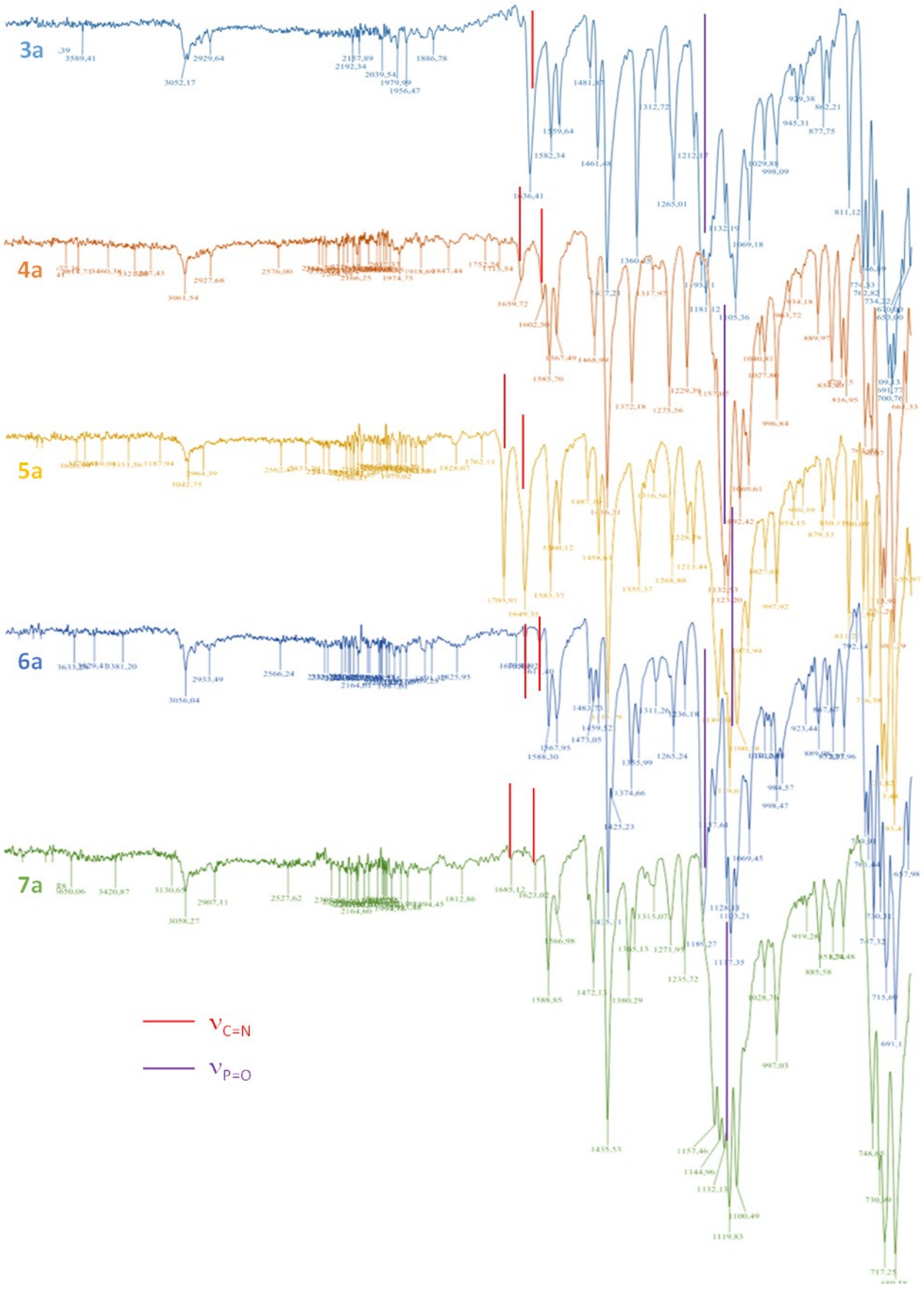
$^{31}P\{^{1}H\}$ NMR spectrum



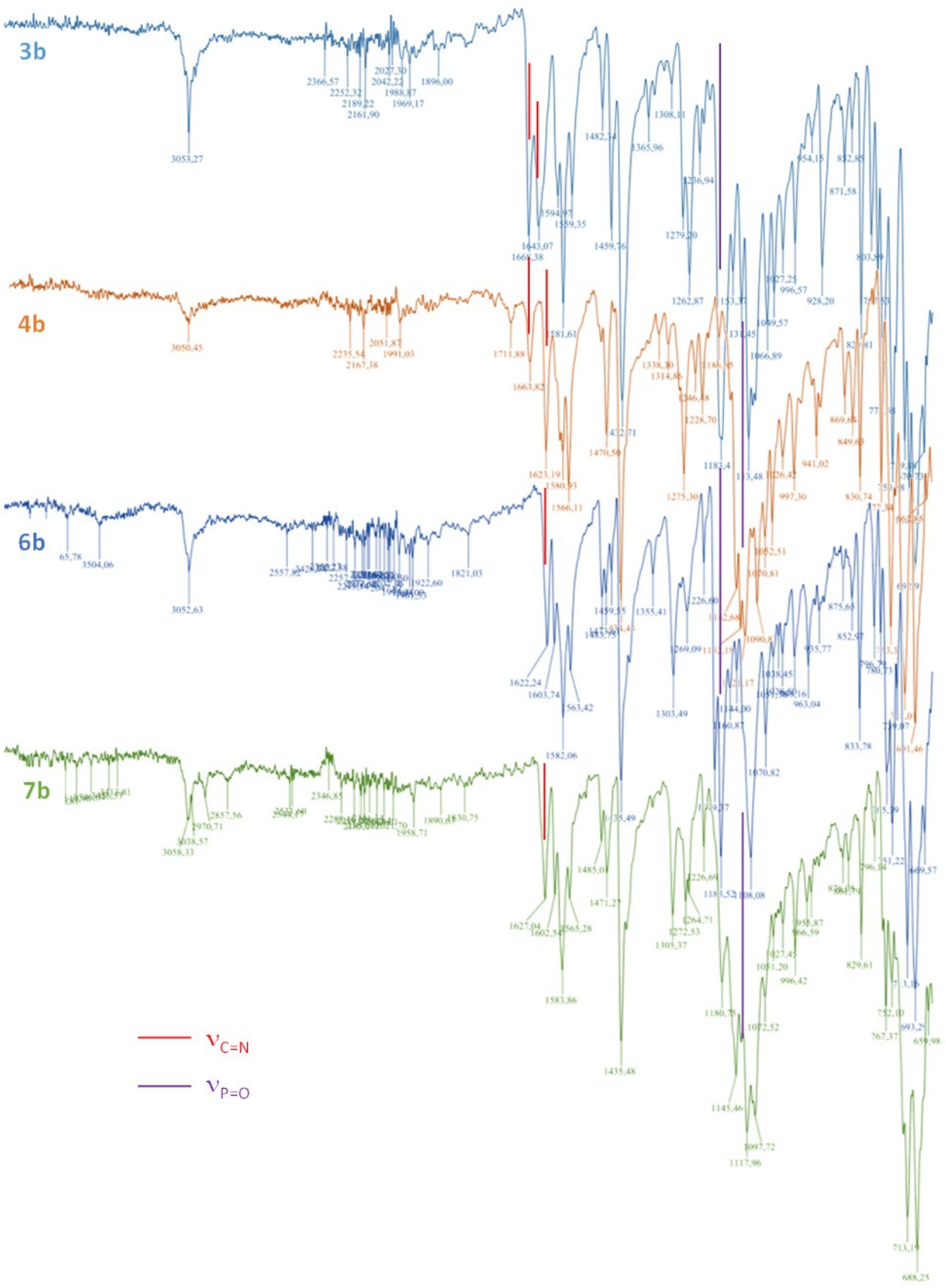
IR spectrum



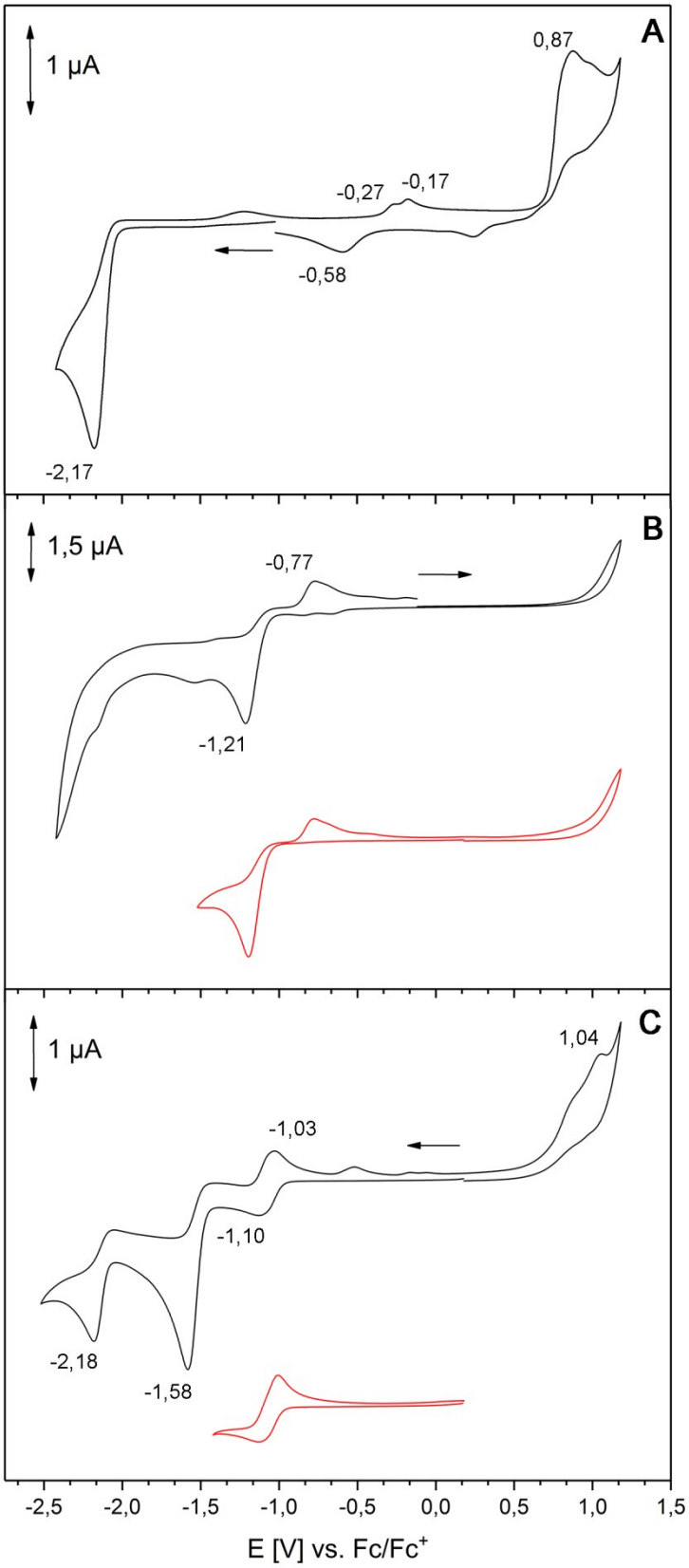
yComparison of the IR data (**3a**, **4a**, **5a**, **6a**, **7a**)



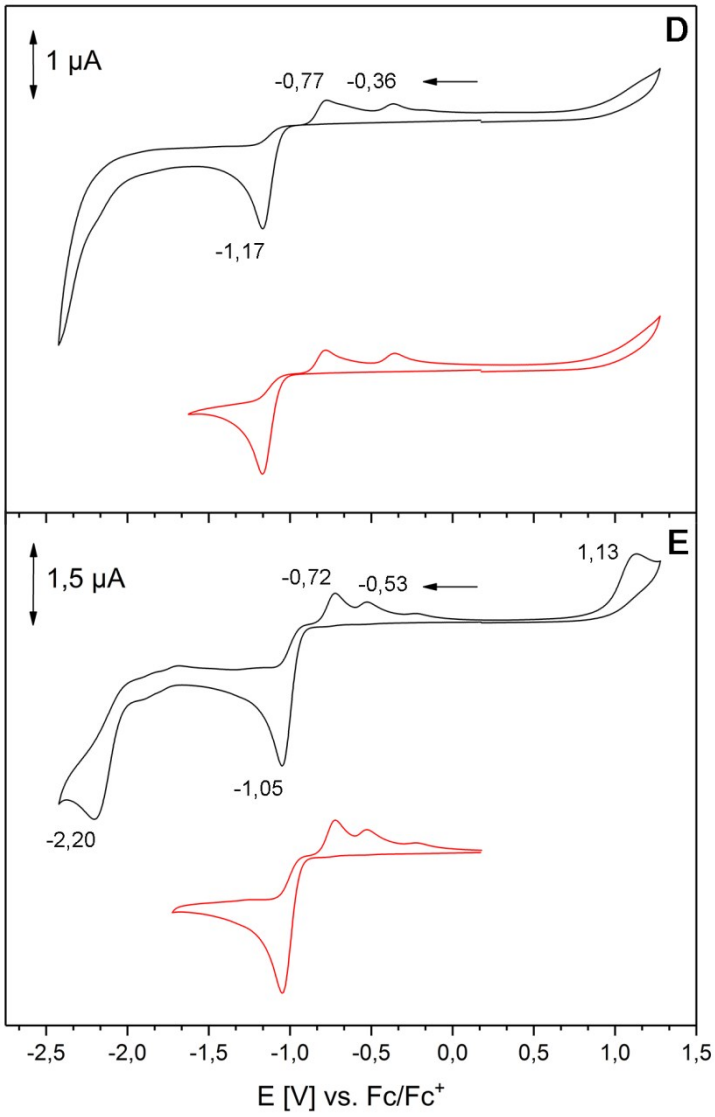
Comparison of the IR data (**3b**, **4b**, **6b**, **7b**)



2. Electrochemistry



Cyclic voltammograms of **3a** (A), **6a** (B) and **5a** (C) in dichloromethane at room temperature with a scan rate of 100 mV/s.



Cyclic voltammograms of **7a** (D), **6b** (E) in in dichloromethane at room temperature with a scan rate of 100 mV/s.

3. Quantum chemical calculations (optimized structures)

3.1 woelfling calculations on the trans-cis isomerization of compound **5a**

difference angle / °	ΔE / kJ·mol^{-1}
147.2	19.4304223
141.1	20.9961235
135.0	22.2458615
129.5	25.2126765
123.6	28.5286830
117.7	31.8525660
110.7	35.7356805
103.5	41.3096170
95.8	49.3121410
89.7	49.6245755
84.6	44.5468585
79.0	40.2436640
72.2	32.1387455
64.8	22.2668655
56.9	13.5239505
48.6	10.0714180
38.2	5.6185700
26.0	1.9717505
13.2	0.6800045
0.0	0.0000000

		dist	rms(g)	rms(g^S)	energy	rms(step)
structure	1	0.000	0.361E-02	0.000E+00	-5179.432703	0.000E+00
structure	2	2.257	0.644E-04	0.644E-04	-5179.436266	0.794E-03
structure	3	2.257	0.818E-04	0.786E-04	-5179.435548	0.949E-03
structure	4	2.257	0.949E-04	0.900E-04	-5179.434625	0.103E-02
structure	5	2.257	0.112E-03	0.106E-03	-5179.433494	0.123E-02
structure	6	2.257	0.122E-03	0.115E-03	-5179.432159	0.137E-02
structure	7	2.257	0.128E-03	0.118E-03	-5179.430623	0.145E-02
structure	8	2.257	0.159E-03	0.134E-03	-5179.428637	0.160E-02
structure	9	2.257	0.160E-03	0.125E-03	-5179.425542	0.150E-02
structure	10	2.257	0.192E-03	0.173E-03	-5179.425291	0.193E-02
structure	11	2.257	0.162E-03	0.138E-03	-5179.428398	0.157E-02
structure	12	2.257	0.140E-03	0.108E-03	-5179.430681	0.112E-02
structure	13	2.257	0.178E-03	0.124E-03	-5179.434437	0.145E-02
structure	14	2.257	0.178E-03	0.121E-03	-5179.438946	0.144E-02
structure	15	2.257	0.183E-03	0.158E-03	-5179.442655	0.170E-02
structure	16	2.257	0.143E-03	0.129E-03	-5179.444244	0.139E-02
structure	17	2.257	0.121E-03	0.885E-04	-5179.446795	0.999E-03
structure	18	2.257	0.838E-04	0.701E-04	-5179.448825	0.773E-03
structure	19	2.257	0.599E-04	0.594E-04	-5179.449863	0.670E-03
structure	20	2.257	0.365E-02	0.000E+00	-5179.446490	0.000E+00

3.2 DFT freq calculation of the optimized geometry of exo-**7a**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.968390	-1.016699	-2.402921
2	6	0	-0.499277	-1.237791	-2.327769
3	6	0	1.521626	-0.145397	-3.475313
4	1	0	2.603525	-0.078666	-3.421163
5	1	0	1.236687	-0.537745	-4.454762
6	1	0	1.096341	0.857830	-3.387720
7	6	0	-1.380600	-0.638232	-3.367481
8	1	0	-2.424074	-0.891291	-3.207965
9	1	0	-1.079280	-0.983354	-4.359359
10	1	0	-1.266743	0.449822	-3.355310
11	6	0	3.074330	-1.425451	-1.397407
12	6	0	3.892416	-2.408300	-1.940620
13	1	0	3.432065	-3.272342	-2.398553
14	6	0	5.271918	-2.288595	-1.864957
15	1	0	5.899556	-3.060173	-2.291920
16	6	0	5.840132	-1.191407	-1.230544
17	1	0	6.915869	-1.092292	-1.165576
18	6	0	5.023204	-0.221444	-0.666391
19	1	0	5.473946	0.626743	-0.170130
20	6	0	3.629579	-0.318212	-0.732290
21	6	0	2.042311	0.259118	1.641774
22	6	0	1.074429	0.972513	2.360350
23	1	0	0.660101	1.894306	1.970031
24	6	0	0.637036	0.485033	3.580582
25	1	0	-0.114621	1.031733	4.130963
26	6	0	1.139404	-0.714242	4.080514
27	1	0	0.768408	-1.102482	5.021060
28	6	0	2.097211	-1.422177	3.368093
29	1	0	2.465651	-2.372988	3.728672
30	6	0	2.561660	-0.929360	2.154553
31	1	0	3.288675	-1.502053	1.598981
32	6	0	3.632300	2.368066	0.453916
33	6	0	4.429050	2.422047	1.600077
34	1	0	4.432367	1.593999	2.298312
35	6	0	5.200267	3.548501	1.854544
36	1	0	5.813427	3.591586	2.745876
37	6	0	5.169673	4.626195	0.973820
38	1	0	5.763581	5.508120	1.179812
39	6	0	4.365755	4.580519	-0.160439
40	1	0	4.326694	5.426411	-0.834821
41	6	0	3.597354	3.453652	-0.423901
42	1	0	2.951711	3.420962	-1.292118
43	6	0	-2.285849	-2.219097	-1.119058
44	6	0	-2.728833	-3.479684	-1.512814
45	1	0	-2.012960	-4.169190	-1.938342
46	6	0	-4.049208	-3.849836	-1.327392
47	1	0	-4.378278	-4.833127	-1.637731
48	6	0	-4.939406	-2.965780	-0.726931
49	1	0	-5.972308	-3.248151	-0.570524
50	6	0	-4.495566	-1.718717	-0.321195
51	1	0	-5.196279	-1.038115	0.142780
52	6	0	-3.166378	-1.317239	-0.506632

53	6	0	-4.003823	1.474394	-0.384823
54	6	0	-3.829201	2.203194	-1.564097
55	1	0	-2.915267	2.111124	-2.136075
56	6	0	-4.814180	3.086811	-1.987038
57	1	0	-4.660003	3.660670	-2.891777
58	6	0	-5.978105	3.243412	-1.242918
59	1	0	-6.742634	3.936348	-1.571948
60	6	0	-6.154717	2.523162	-0.064826
61	1	0	-7.053020	2.656212	0.524919
62	6	0	-5.170292	1.644548	0.367186
63	1	0	-5.301215	1.112069	1.300539
64	6	0	-2.684420	0.254073	1.891769
65	6	0	-2.594005	-0.966935	2.563775
66	1	0	-2.480905	-1.894673	2.018031
67	6	0	-2.624798	-0.992703	3.953287
68	1	0	-2.545274	-1.941522	4.468044
69	6	0	-2.752653	0.190624	4.670938
70	1	0	-2.790091	0.165524	5.753371
71	6	0	-2.810698	1.412159	4.003047
72	1	0	-2.881247	2.337082	4.561537
73	6	0	-2.766042	1.449904	2.617131
74	1	0	-2.780937	2.401686	2.101320
75	7	0	1.662397	-1.610228	-1.490703
76	7	0	-0.901582	-1.933753	-1.320253
77	8	0	1.475151	1.369176	-0.842715
78	8	0	-1.376975	0.755237	-0.527204
79	15	0	2.592996	0.941689	0.077413
80	15	0	-2.683389	0.334065	0.091888
81	30	0	-0.254552	2.415337	-0.898017
82	17	0	-0.580455	3.844209	0.777782
83	17	0	-0.503321	2.918508	-3.080268
84	46	0	0.590170	-2.794746	-0.185528
85	17	0	2.417783	-3.916845	0.655382
86	17	0	-0.830470	-3.926659	1.222826

Recovered energy= -6235.24917834 dipole= -0.352907635858
0.015205213029 -0.648182394393
Low frequencies --- -0.0160 -0.0135 -0.0113 -0.0069 0.0105 0.0165
Low frequencies --- 7.8905 23.6793 25.8575
Zero-point correction= 0.645389 (Hartree/Particle)
Thermal correction to Energy= 0.696151
Thermal correction to Enthalpy= 0.697095
Thermal correction to Gibbs Free Energy= 0.557315
Sum of electronic and zero-point Energies= -6234.603789
Sum of electronic and thermal Energies= -6234.553028
Sum of electronic and thermal Enthalpies= -6234.552083
Sum of electronic and thermal Free Energies= -6234.691863

3.3 DFT freq calculation of the optimized geometry of endo-**7a**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.741238	-0.948740	-2.405059
2	6	0	-0.741083	-0.948551	-2.405042
3	6	0	1.489202	-0.101638	-3.381568
4	1	0	2.558157	-0.288529	-3.336925
5	1	0	1.141698	-0.271952	-4.401500
6	1	0	1.316783	0.951477	-3.142643
7	6	0	-1.488736	-0.100920	-3.381323
8	1	0	-2.557777	-0.287365	-3.336730
9	1	0	-1.141295	-0.271044	-4.401284
10	1	0	-1.315883	0.952046	-3.142027
11	6	0	2.697142	-1.896567	-1.410983
12	6	0	3.193511	-3.098033	-1.909031
13	1	0	2.506042	-3.790840	-2.375337
14	6	0	4.533638	-3.416783	-1.762231
15	1	0	4.905618	-4.355895	-2.151276
16	6	0	5.383323	-2.553452	-1.079340
17	1	0	6.422996	-2.812970	-0.928321
18	6	0	4.883138	-1.368881	-0.562844
19	1	0	5.535012	-0.718050	0.006510
20	6	0	3.541914	-1.009490	-0.734746
21	6	0	3.761145	0.756990	1.539863
22	6	0	4.716613	1.741976	1.801240
23	1	0	5.025250	2.425794	1.021003
24	6	0	5.260880	1.850623	3.074674
25	1	0	5.997075	2.616974	3.282273
26	6	0	4.846973	0.984858	4.082614
27	1	0	5.265261	1.078573	5.077423
28	6	0	3.890018	0.008525	3.822971
29	1	0	3.551170	-0.651363	4.610666
30	6	0	3.344564	-0.114203	2.553545
31	1	0	2.590054	-0.866451	2.359854
32	6	0	3.581536	1.872882	-1.170002
33	6	0	2.843642	3.060810	-1.203152
34	1	0	1.957166	3.170823	-0.588417
35	6	0	3.248335	4.102460	-2.029754
36	1	0	2.674211	5.020469	-2.045729
37	6	0	4.380519	3.967204	-2.826582
38	1	0	4.691684	4.780650	-3.470637
39	6	0	5.113849	2.784697	-2.797971
40	1	0	5.993452	2.674348	-3.420018
41	6	0	4.717576	1.739532	-1.972247
42	1	0	5.289517	0.821286	-1.966783
43	6	0	-2.697276	-1.896232	-1.411461
44	6	0	-3.193766	-3.097608	-1.909631
45	1	0	-2.506307	-3.790541	-2.375761
46	6	0	-4.533998	-3.416075	-1.763214
47	1	0	-4.906084	-4.355096	-2.152375
48	6	0	-5.383660	-2.552598	-1.080474
49	1	0	-6.423421	-2.811909	-0.929709
50	6	0	-4.883349	-1.368169	-0.563794
51	1	0	-5.535195	-0.717316	0.005562
52	6	0	-3.542020	-1.008996	-0.735419
53	6	0	-3.581452	1.873626	-1.169635

54	6	0	-2.842371	3.060796	-1.203711
55	1	0	-1.955083	3.169924	-0.589999
56	6	0	-3.247035	4.102859	-2.029810
57	1	0	-2.672023	5.020300	-2.046462
58	6	0	-4.380350	3.968759	-2.825218
59	1	0	-4.691497	4.782527	-3.468871
60	6	0	-5.114844	2.786993	-2.795707
61	1	0	-5.995322	2.677534	-3.416671
62	6	0	-4.718606	1.741423	-1.970489
63	1	0	-5.291485	0.823761	-1.964334
64	6	0	-3.761091	0.756594	1.539760
65	6	0	-3.344077	-0.114678	2.553186
66	1	0	-2.589199	-0.866498	2.359295
67	6	0	-3.889621	0.007351	3.822640
68	1	0	-3.550430	-0.652619	4.610117
69	6	0	-4.847121	0.983070	4.082566
70	1	0	-5.265486	1.076252	5.077392
71	6	0	-5.261485	1.848906	3.074870
72	1	0	-5.998121	2.614778	3.282677
73	6	0	-4.717115	1.740966	1.801419
74	1	0	-5.026165	2.424829	1.021387
75	7	0	1.288913	-1.699146	-1.513418
76	7	0	-1.288942	-1.699150	-1.513662
77	8	0	1.470390	0.629789	0.008652
78	8	0	-1.470366	0.629858	0.008342
79	15	0	2.971990	0.575486	-0.060381
80	15	0	-2.971960	0.575737	-0.060587
81	30	0	0.000117	1.299182	1.263805
82	17	0	0.000163	0.245912	3.202804
83	17	0	0.000496	3.546980	1.000325
84	46	0	-0.000112	-2.507674	-0.128215
85	17	0	1.651941	-3.282510	1.258619
86	17	0	-1.652447	-3.283061	1.258018

Recovered energy= -6235.22641058 dipole= 0.000242232818
0.912407693541 -5.211824412720
Low frequencies --- -0.0204 -0.0179 -0.0045 0.0066 0.0100 0.0175
Low frequencies --- 11.3921 15.3531 19.3344
Zero-point correction= 0.643630 (Hartree/Particle)
Thermal correction to Energy= 0.695273
Thermal correction to Enthalpy= 0.696217
Thermal correction to Gibbs Free Energy= 0.551431
Sum of electronic and zero-point Energies= -6234.582781
Sum of electronic and thermal Energies= -6234.531138
Sum of electronic and thermal Enthalpies= -6234.530194
Sum of electronic and thermal Free Energies= -6234.674980