

First—Stepwise Synthesis of 2,6-difunctionalized Ethyl Pyrazolo[1,5-*a*]pyrimidine-3-carboxylate *via* site-selective cross-coupling reactions: Experimental and Computational Studies.

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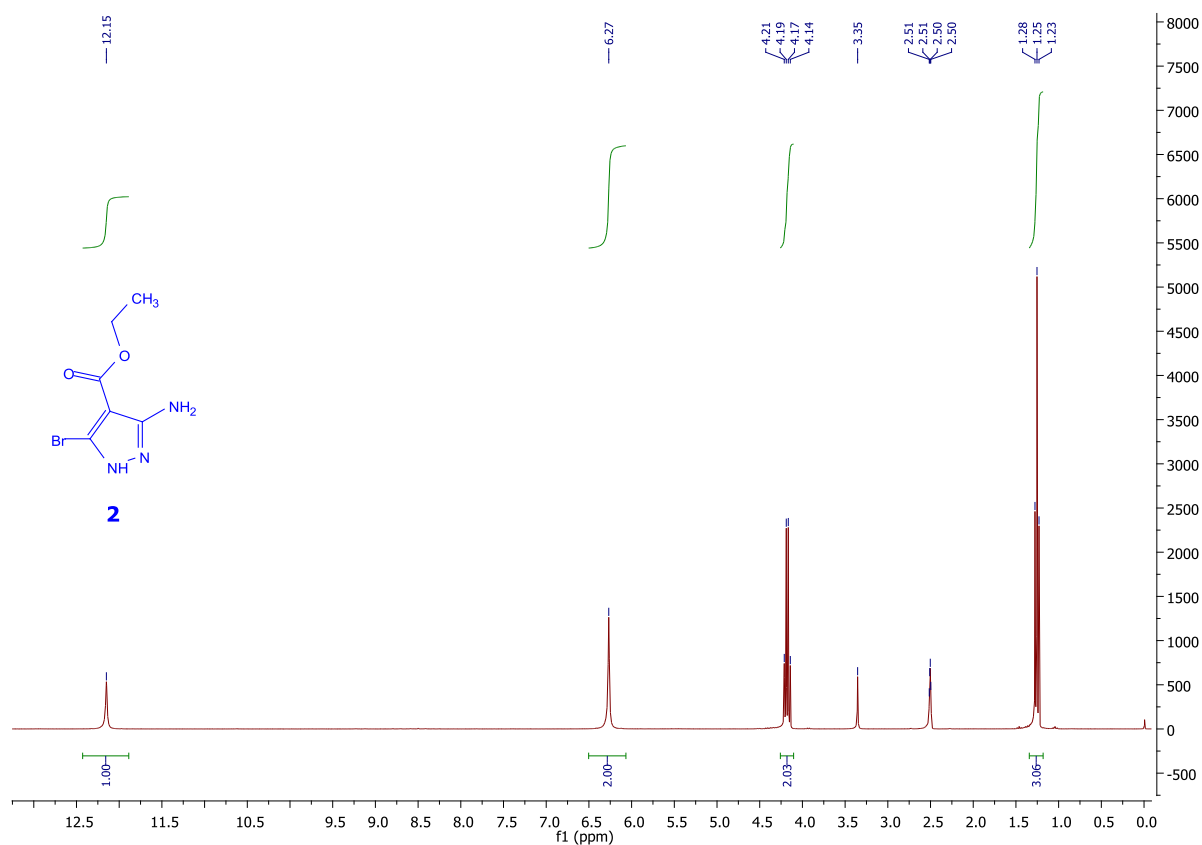
^c Materials Science and Nano-Engineering (MSN) Department, Mohammed VI Polytechnic University (UM6P), Lot 660–Hay Moulay Rachid, Benguerir 43150, Morocco.

^d Faculté de Pharmacie, Université de Tours, EA 7502 SIMBA, 31 Avenue Monge, 37200 Tours, France.

1. ¹ H, ¹³ C and ¹⁹ F NMR and IR spectra of products 2–3 , 4a–j , 5a–i , 6a–f , 7a–c , 8a–b and 9a–b .	S2–S53
2. Details of DFT calculations	S54–S82
3. References	S83

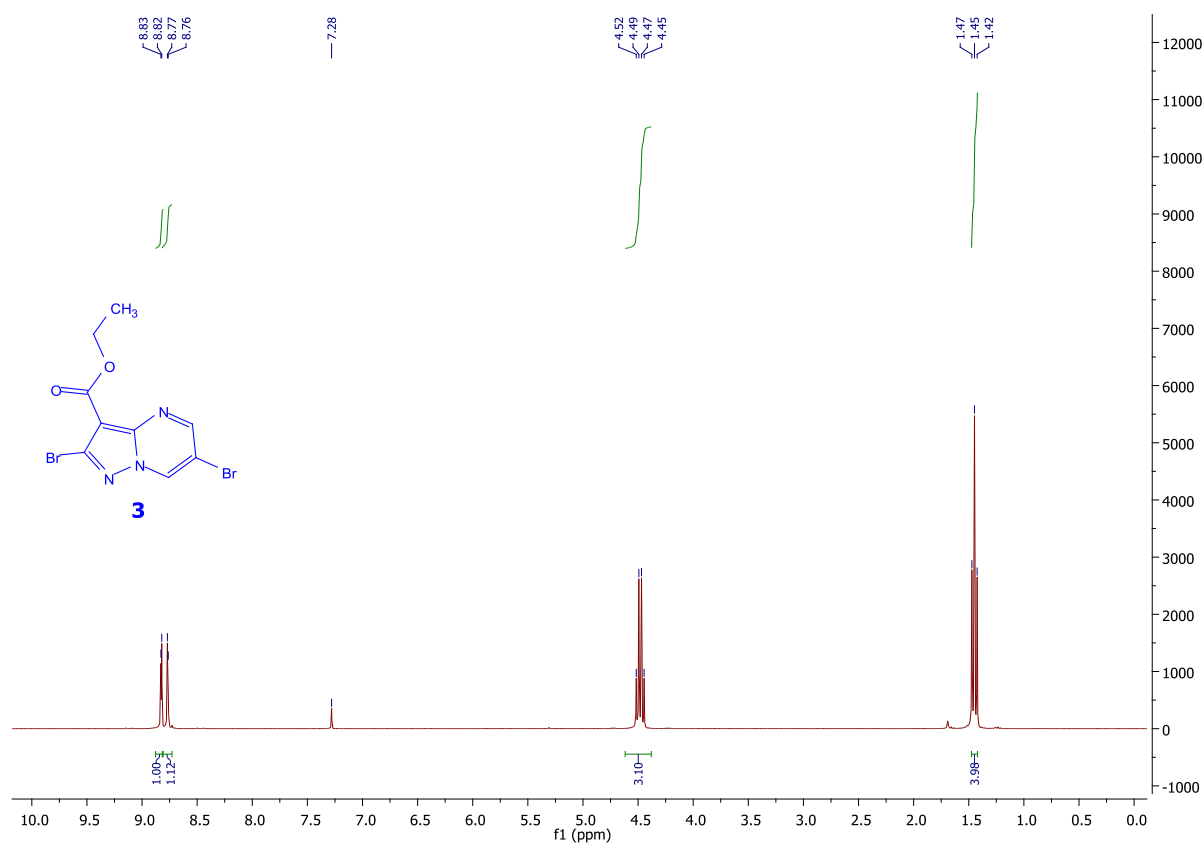
Ethyl 3-amino-5-bromo-1H-pyrazole-4-carboxylate (2)

^1H NMR (300 MHz, CDCl_3)

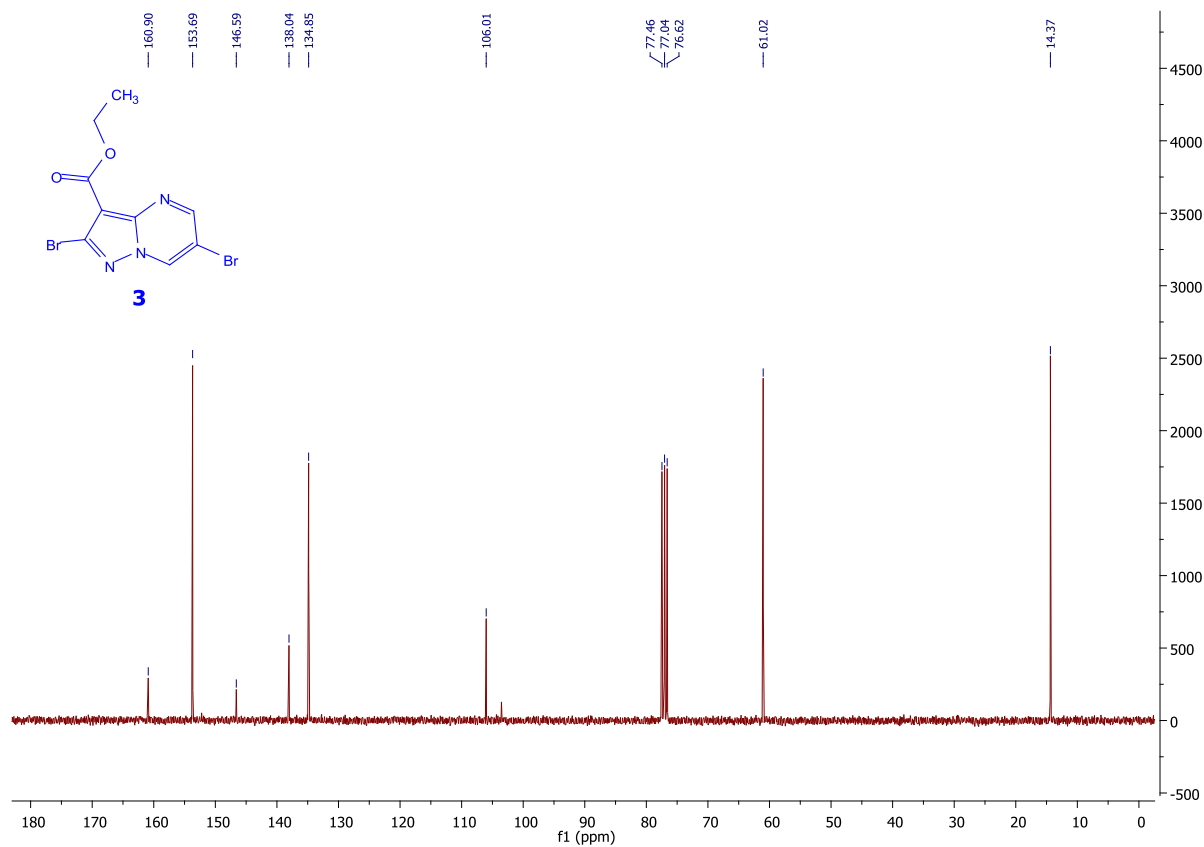


Ethyl 2,6-dibromopyrazolo[1,5- σ]pyrimidine-3-carboxylate (3)

^1H NMR (300 MHz, CDCl_3)

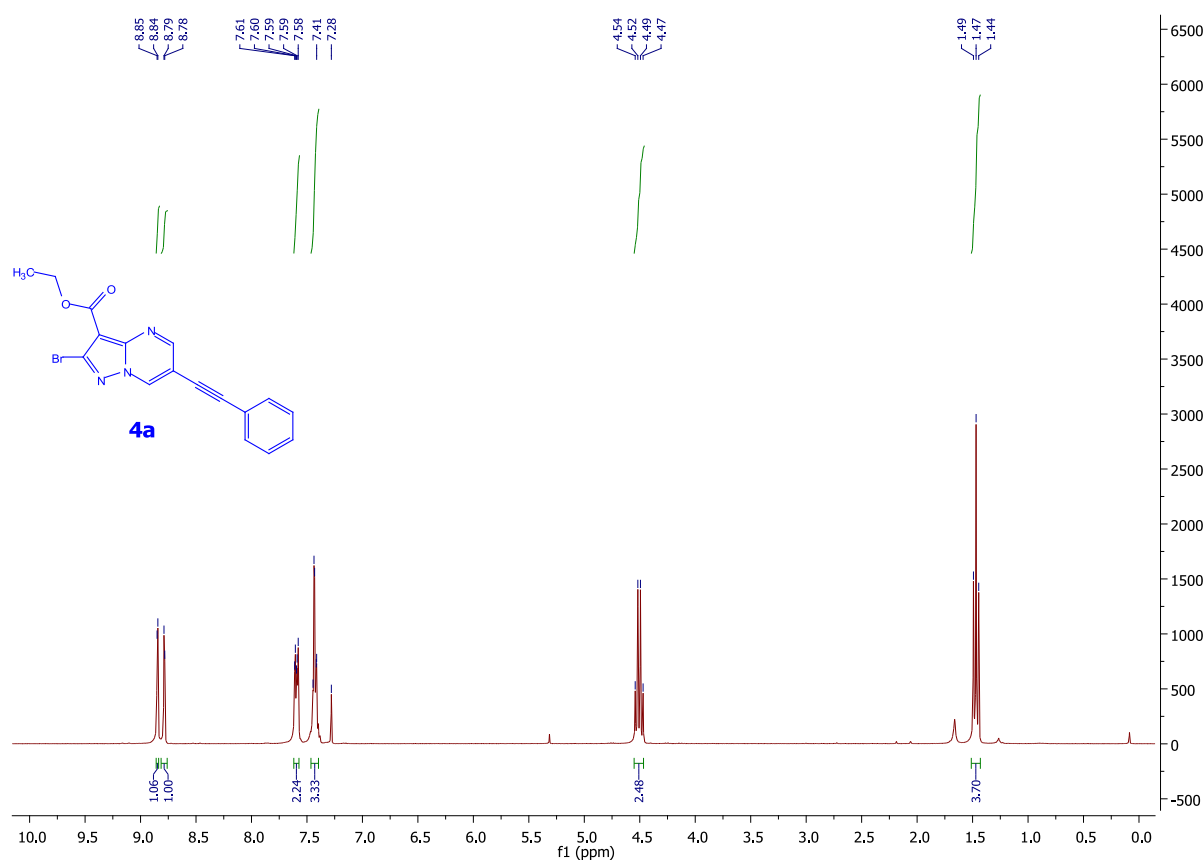


^{13}C NMR (75 MHz, CDCl_3)

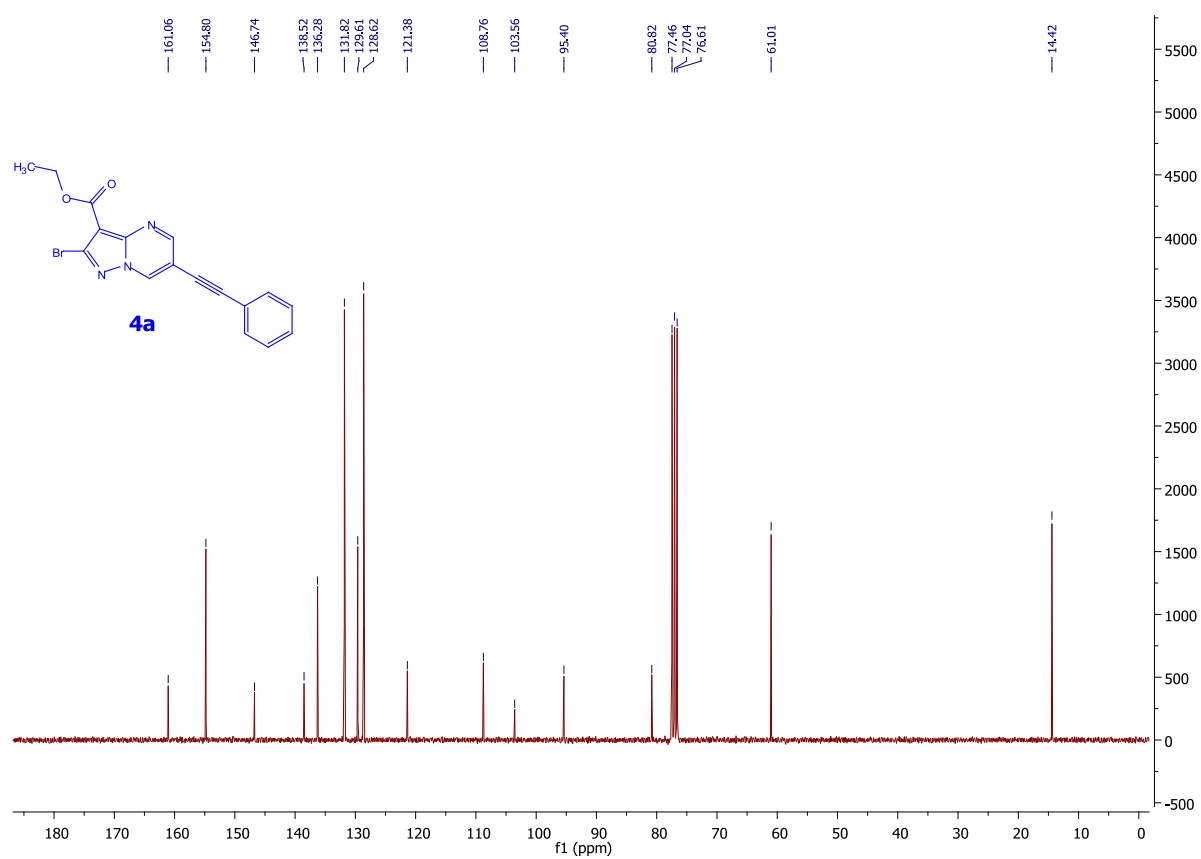


Ethyl 2-bromo-6-(phenylethynyl)pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (**4a**)

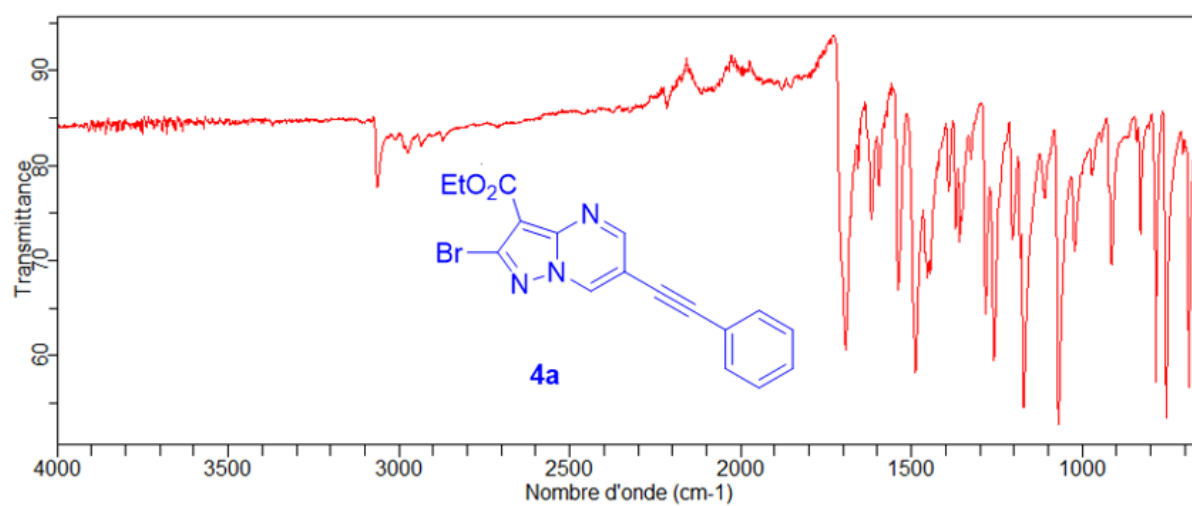
^1H NMR (300 MHz, CDCl_3)



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

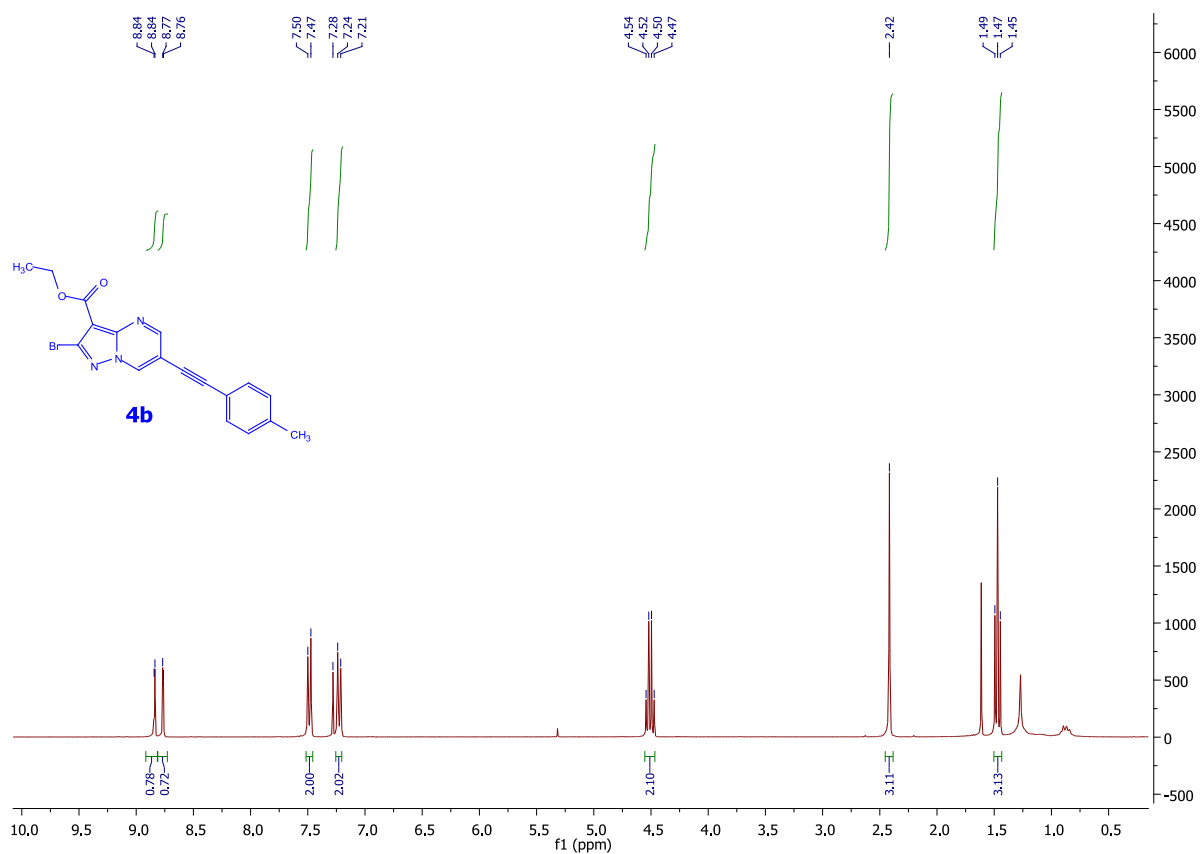


IR

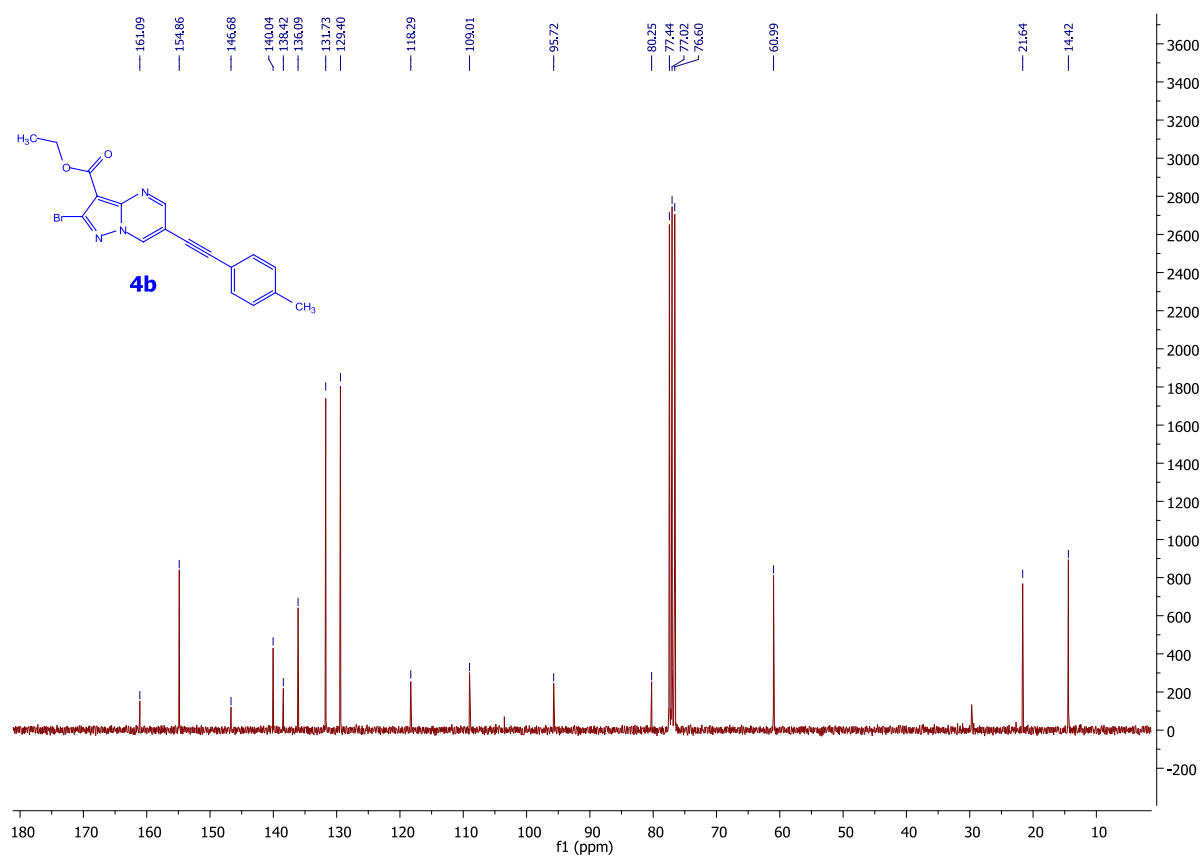


Ethyl 2-bromo-6-(*p*-tolylethynyl)pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4b**)**

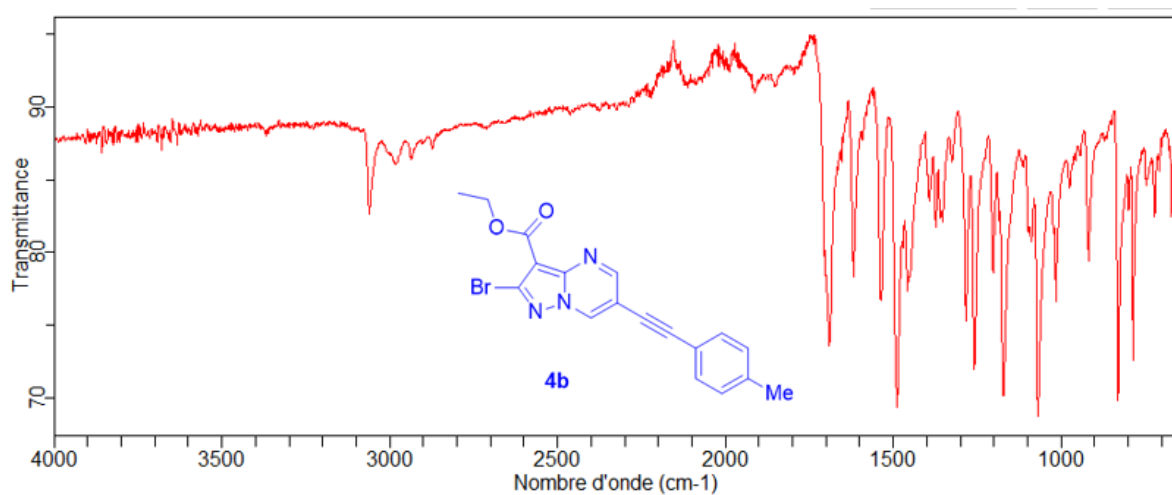
^1H NMR (300 MHz, CDCl_3)



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

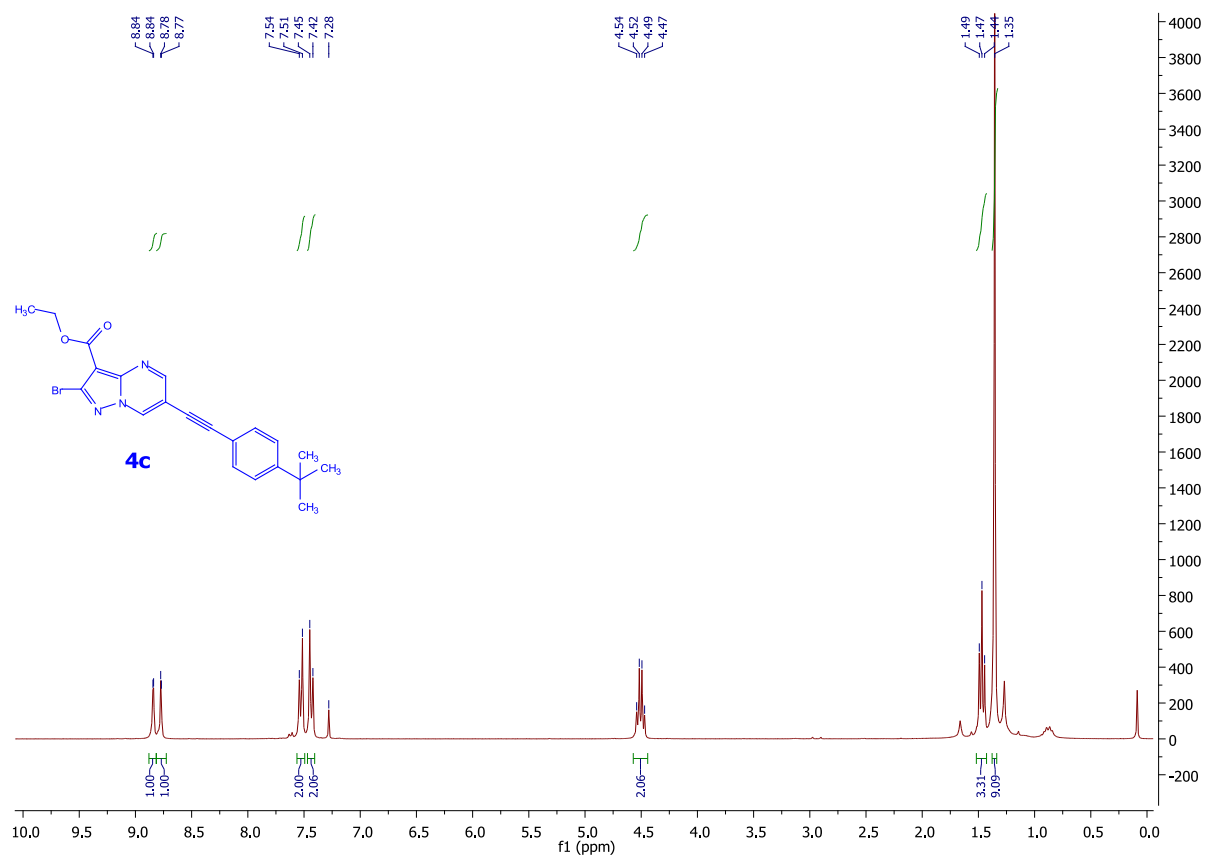


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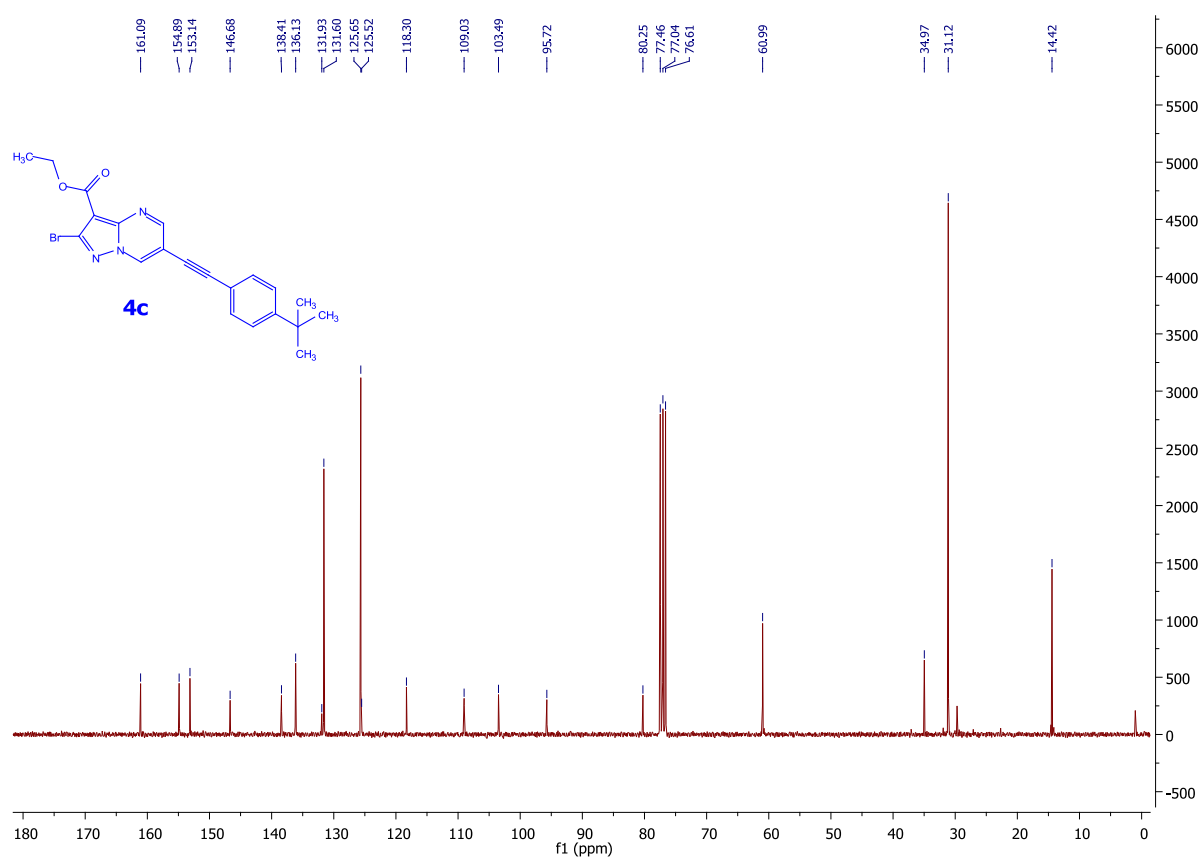


Ethyl 2-bromo-6-[(4-(*tert*-butyl)phenyl)ethynyl]pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4c**)**

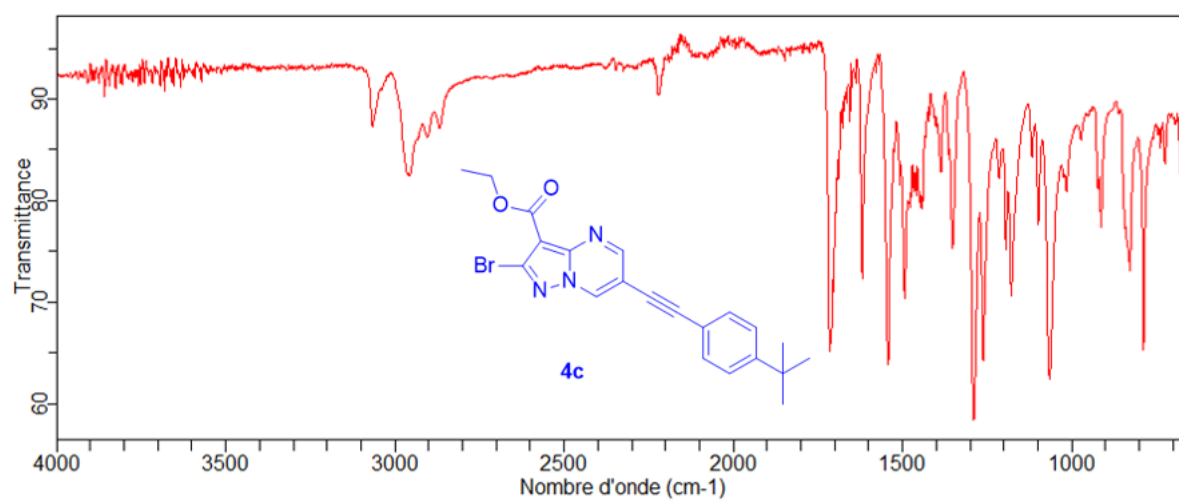
¹H NMR (300 MHz, CDCl₃)



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

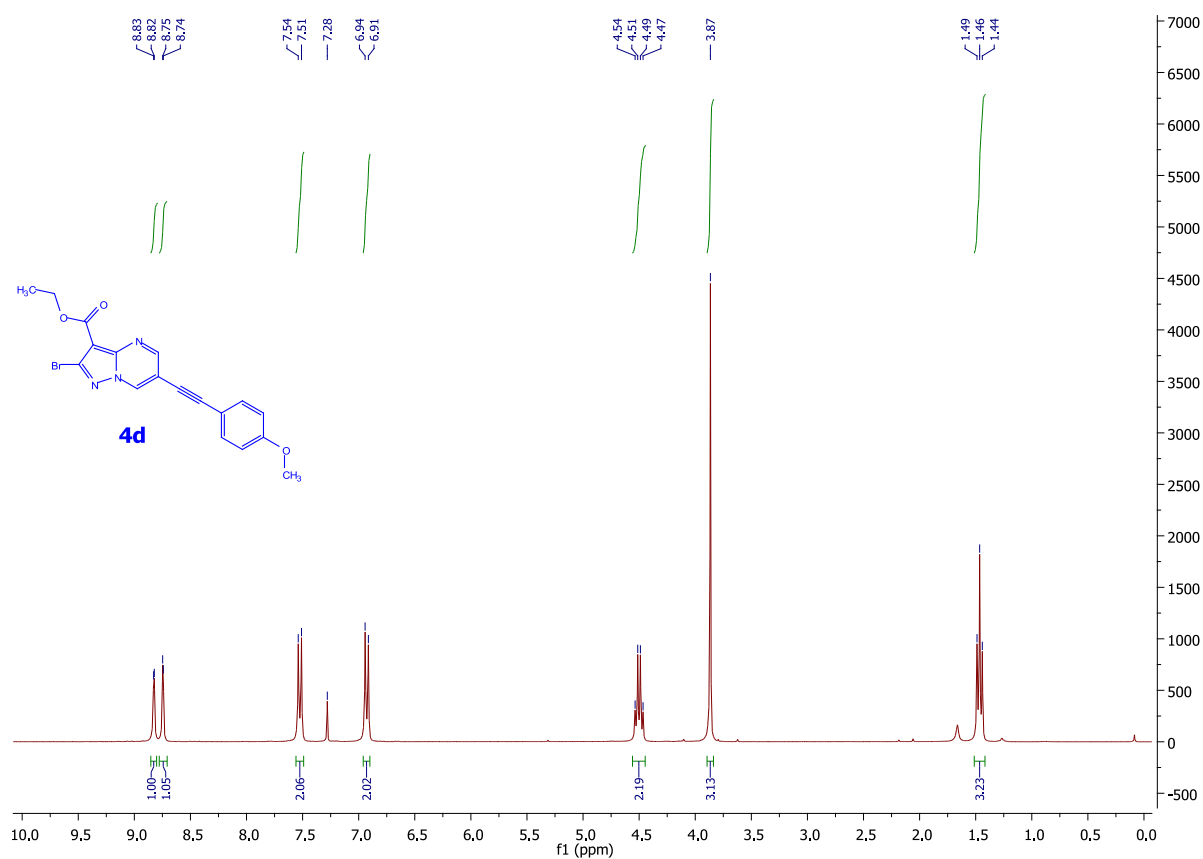


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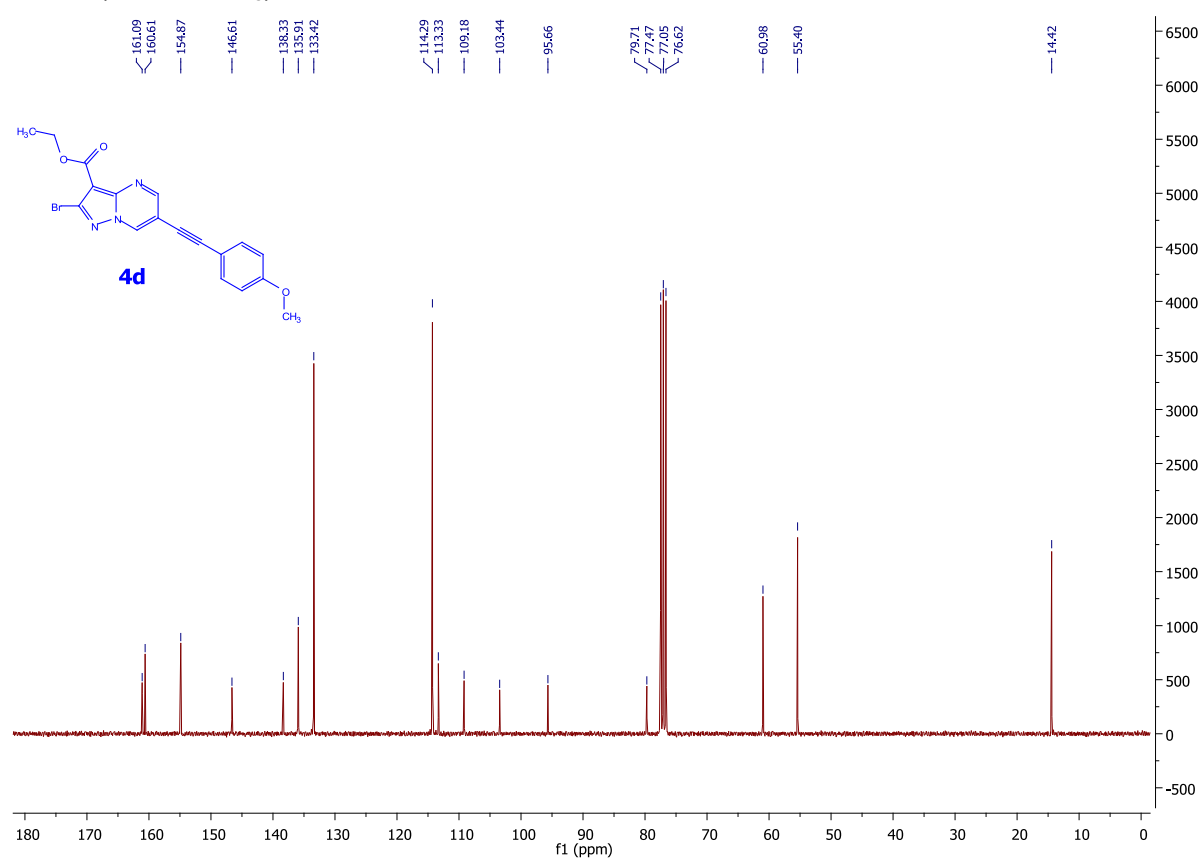


Ethyl 2-bromo-6-[(4-methoxyphenyl)ethynyl]pyrazolo[1,5-a]pyrimidine-3-carboxylate (4d**)**

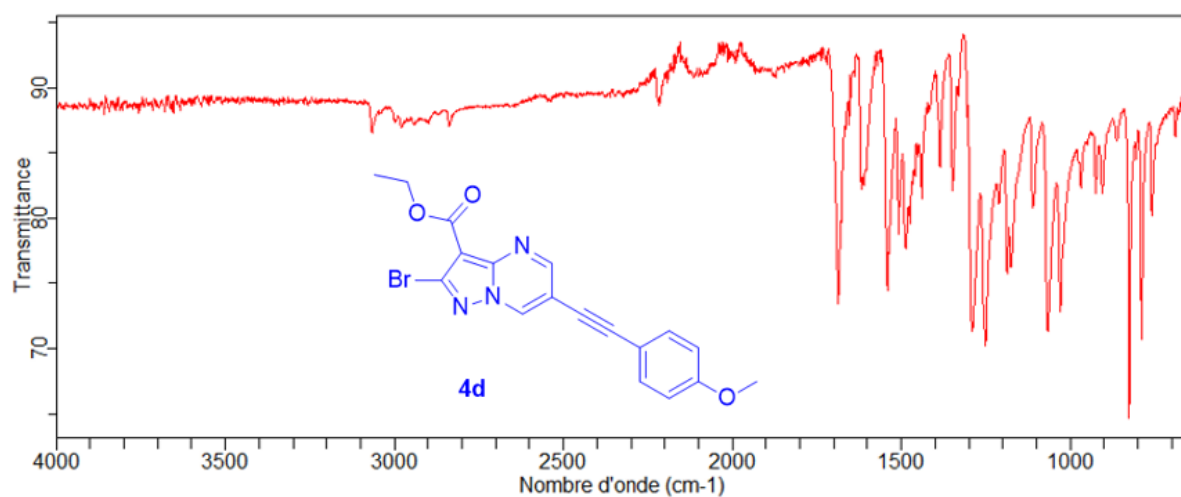
^1H NMR (300 MHz, CDCl_3)



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

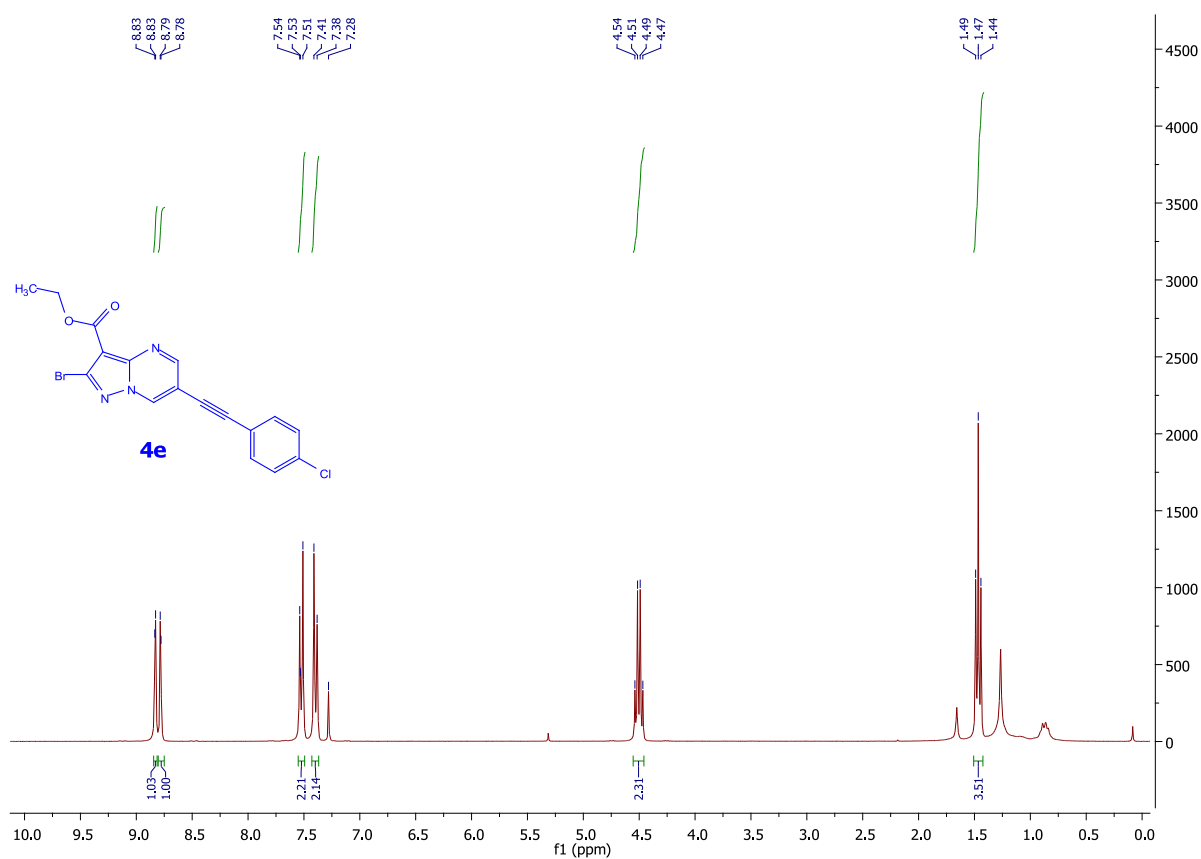


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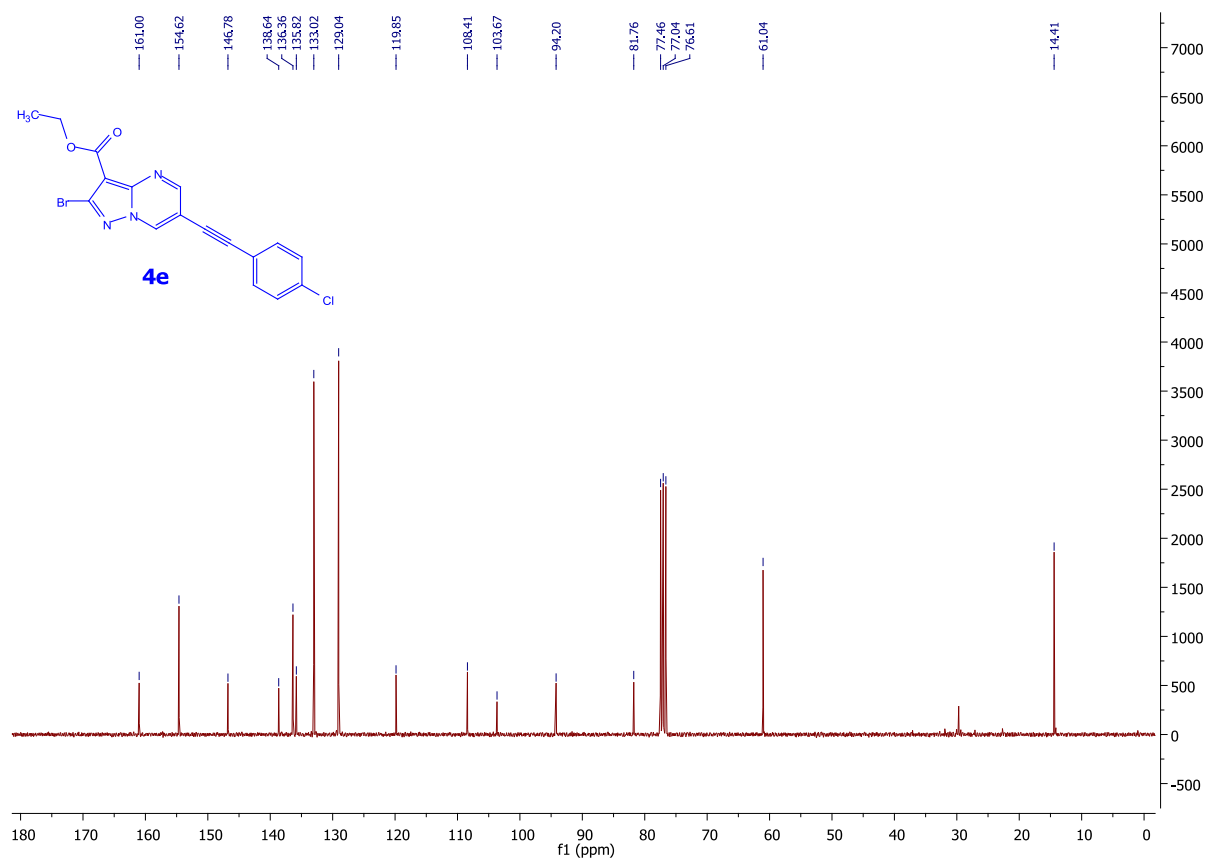


Ethyl 2-bromo-6-[(4-chlorophenyl)ethynyl]pyrazolo[1,5-a]pyrimidine-3-carboxylate (4e**)**

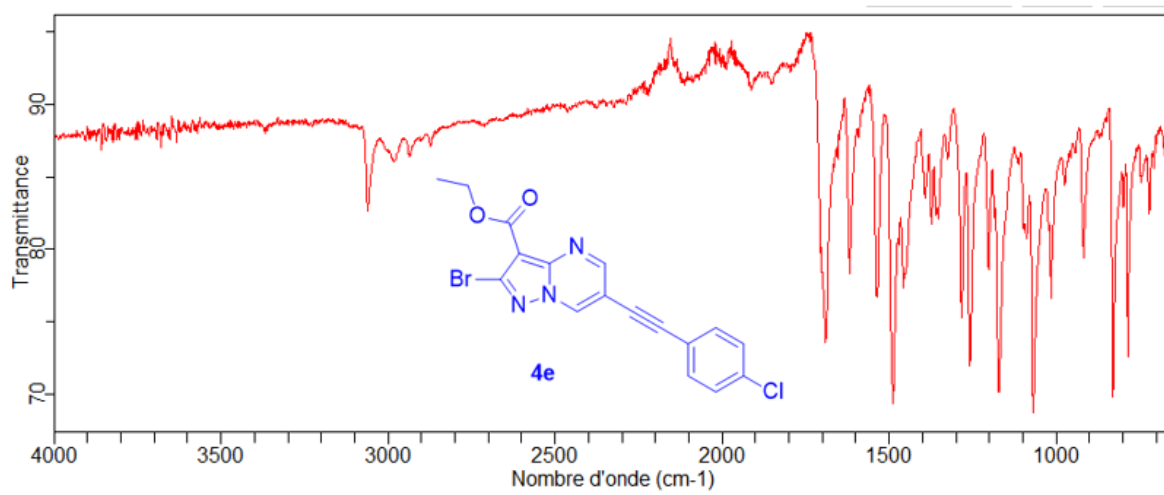
¹H NMR (300 MHz, CDCl₃)



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

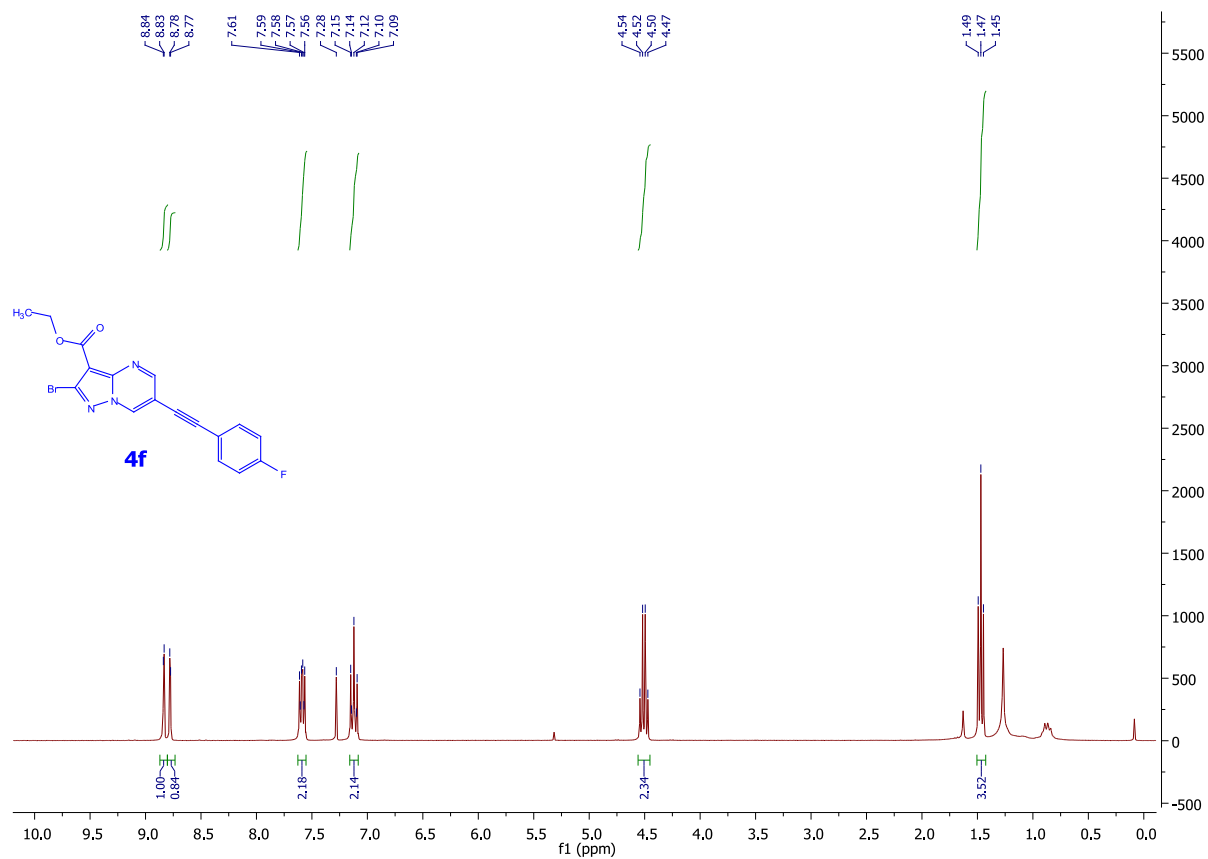


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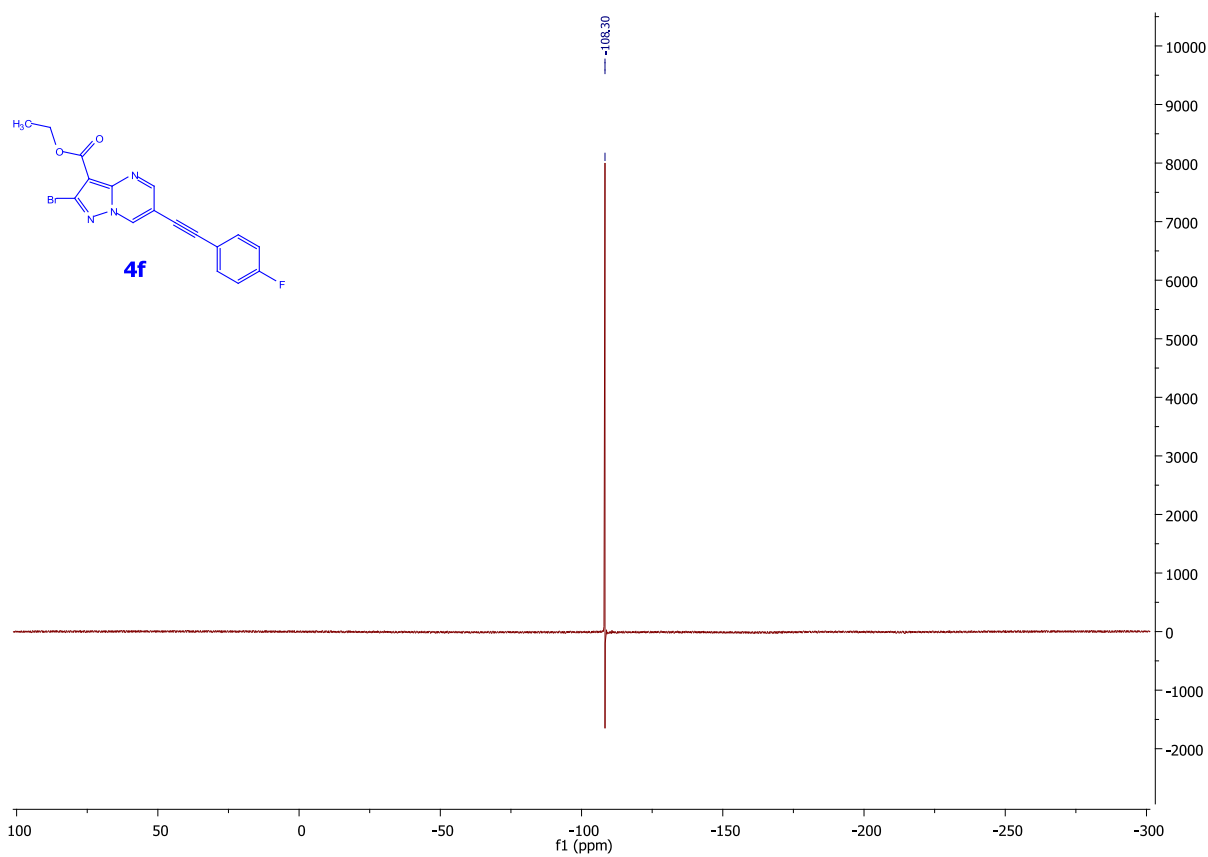


Ethyl 2-bromo-6-[(4-fluorophenyl)ethynyl]pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4f**)**

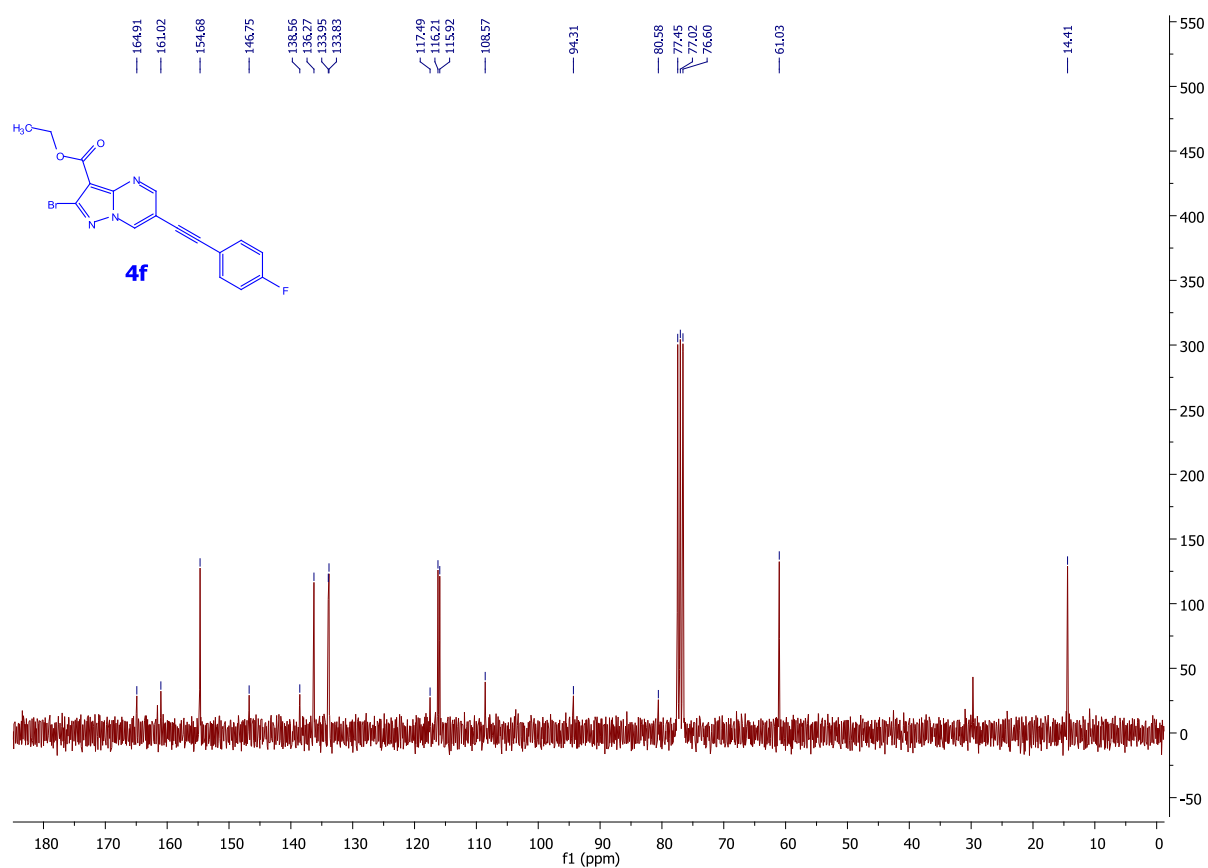
^1H NMR (300 MHz, CDCl_3)



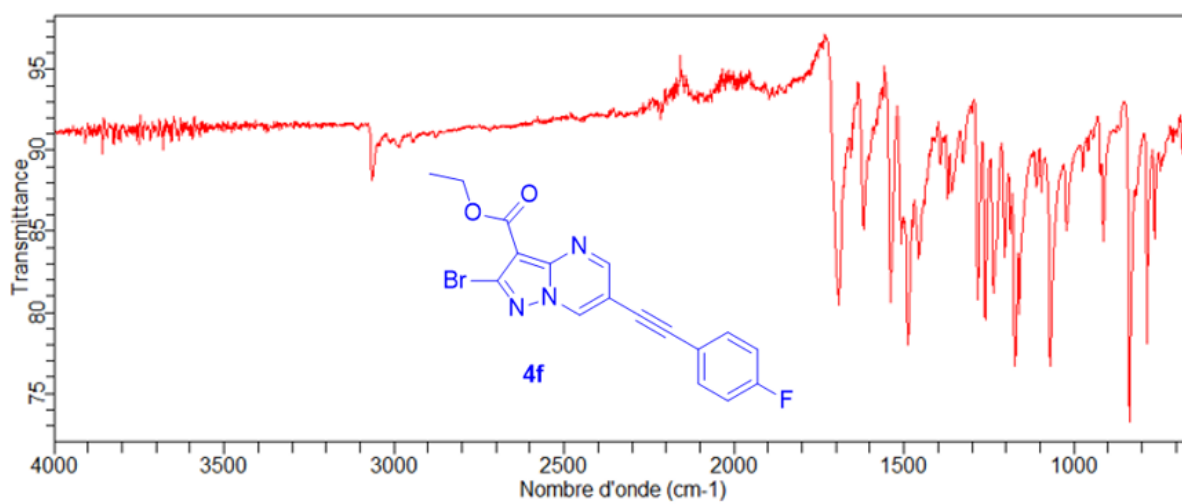
^{19}F NMR (282 MHz, CDCl_3)



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

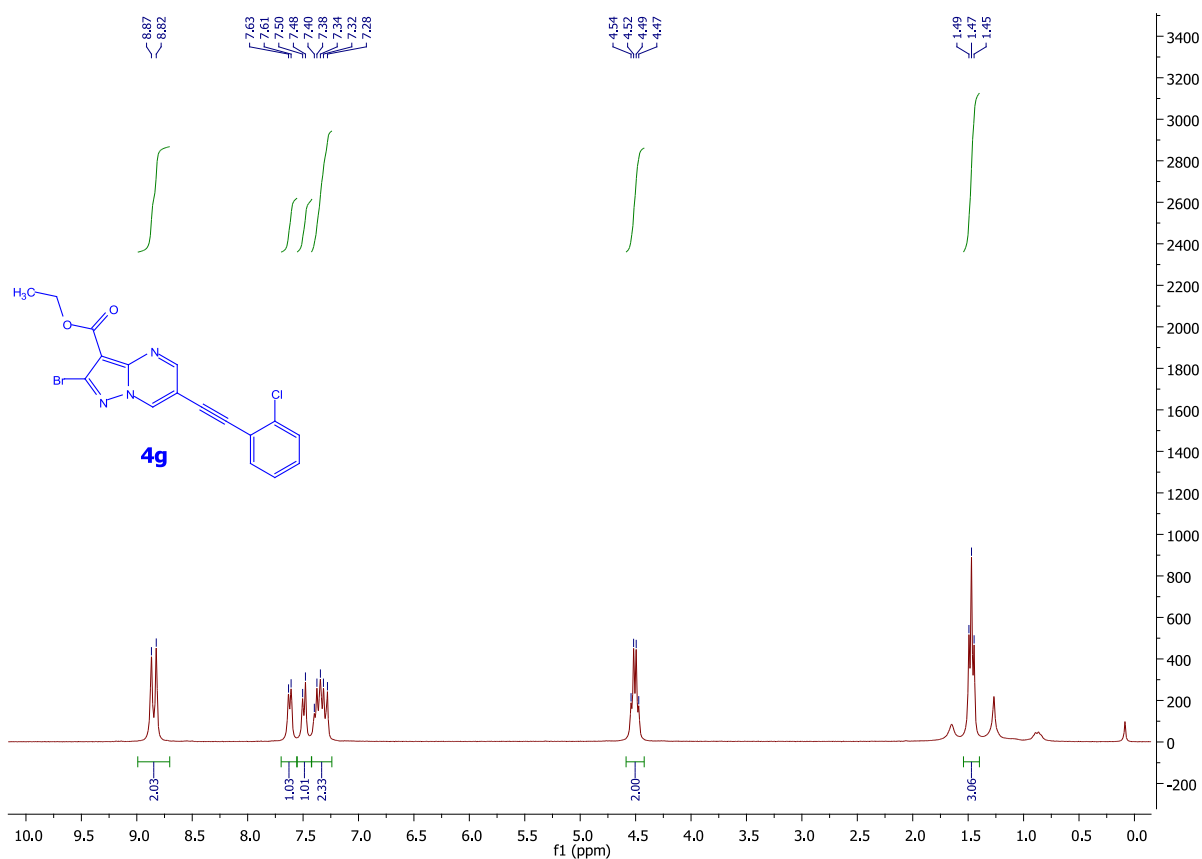


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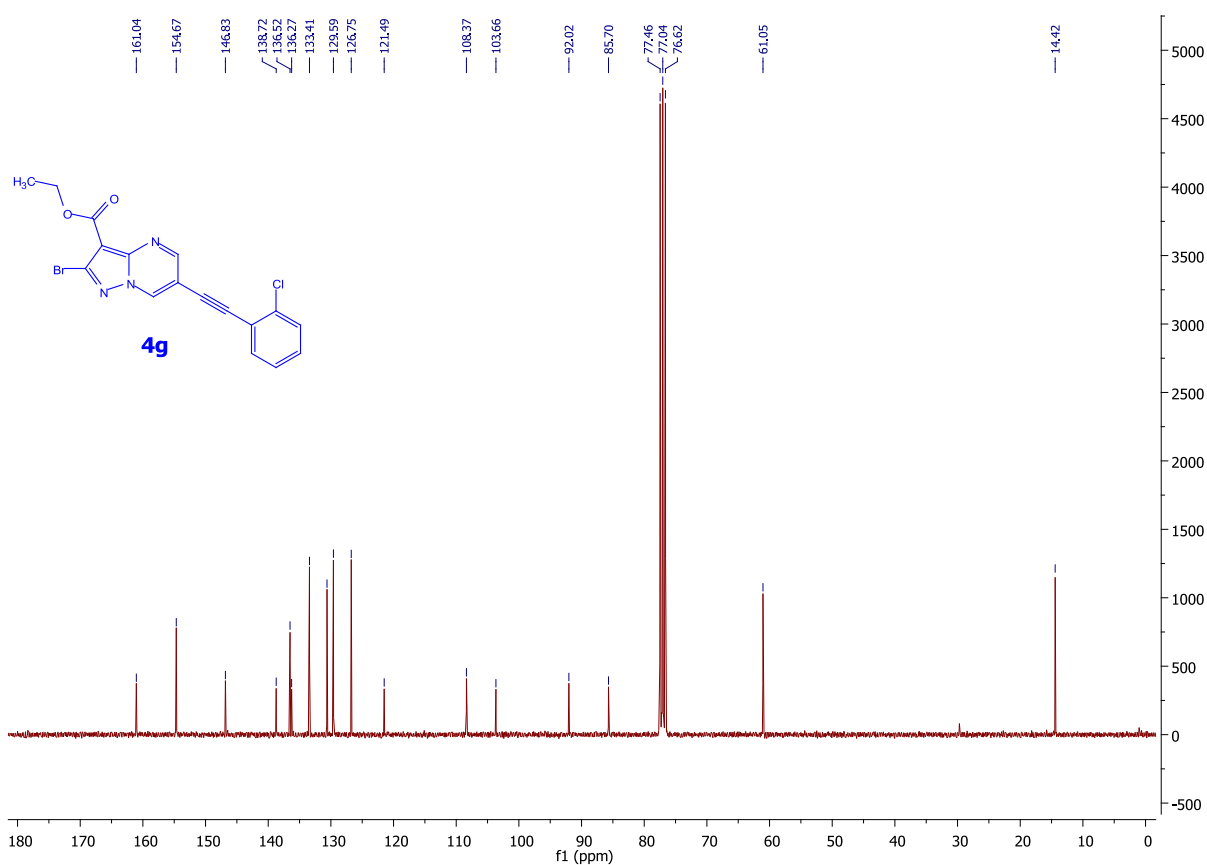


Ethyl 2-bromo-6-[(2-chlorophenyl)ethynyl]pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4g**)**

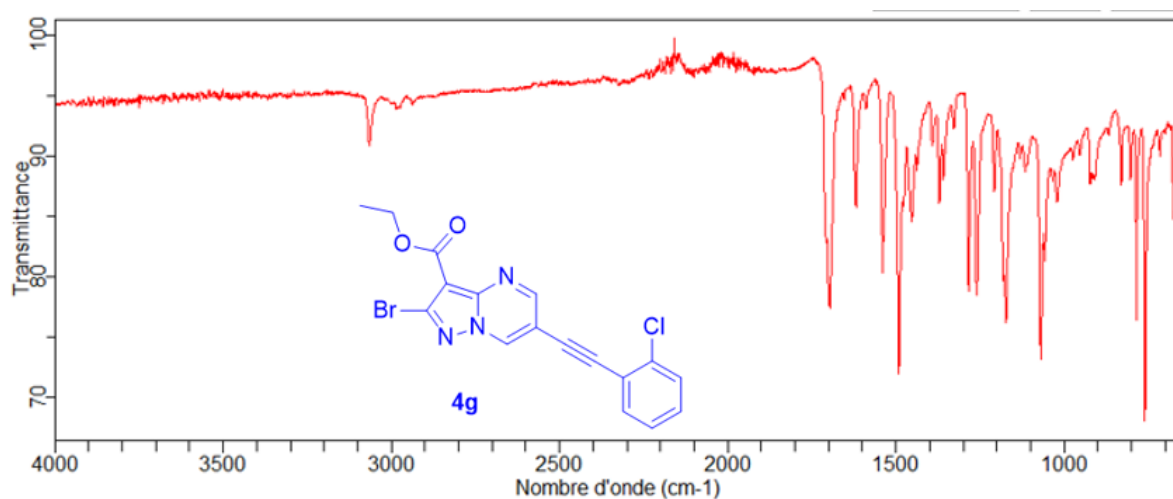
^1H NMR (300 MHz, CDCl_3)



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

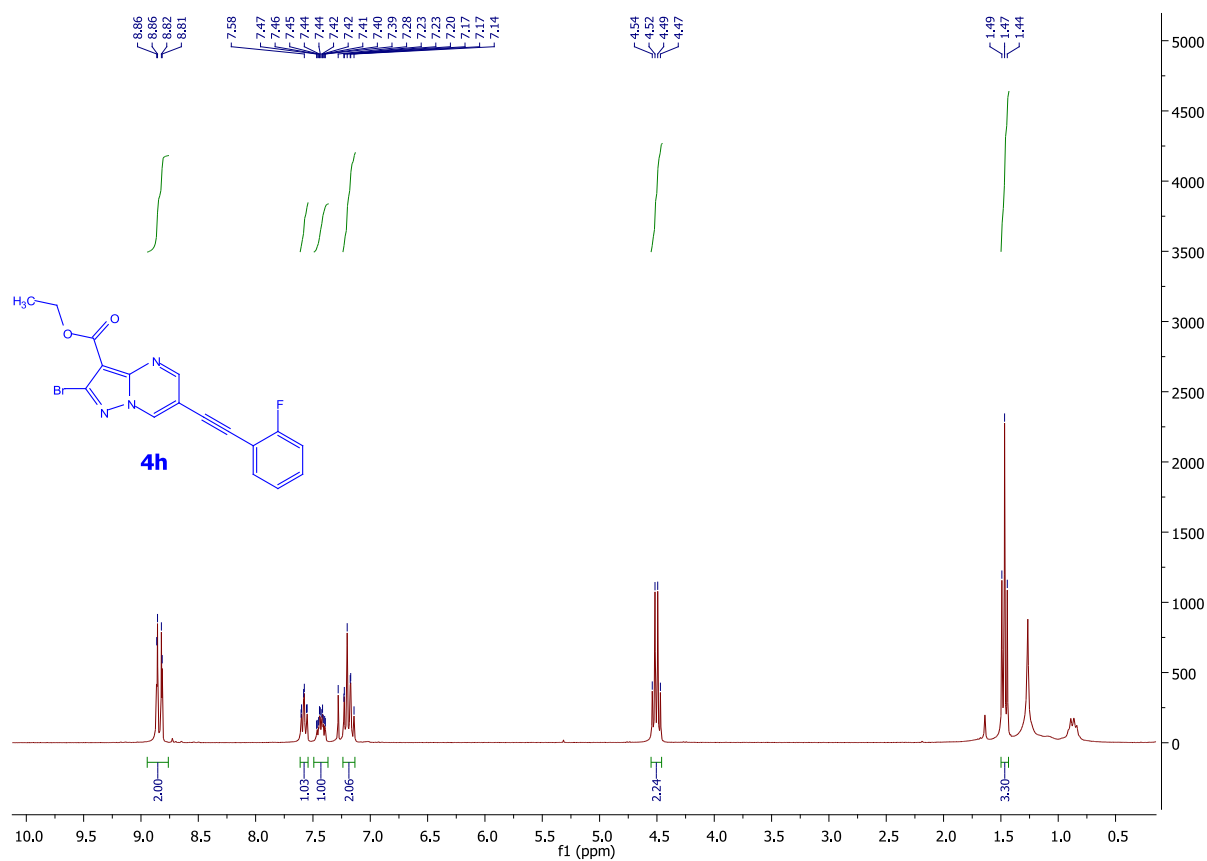


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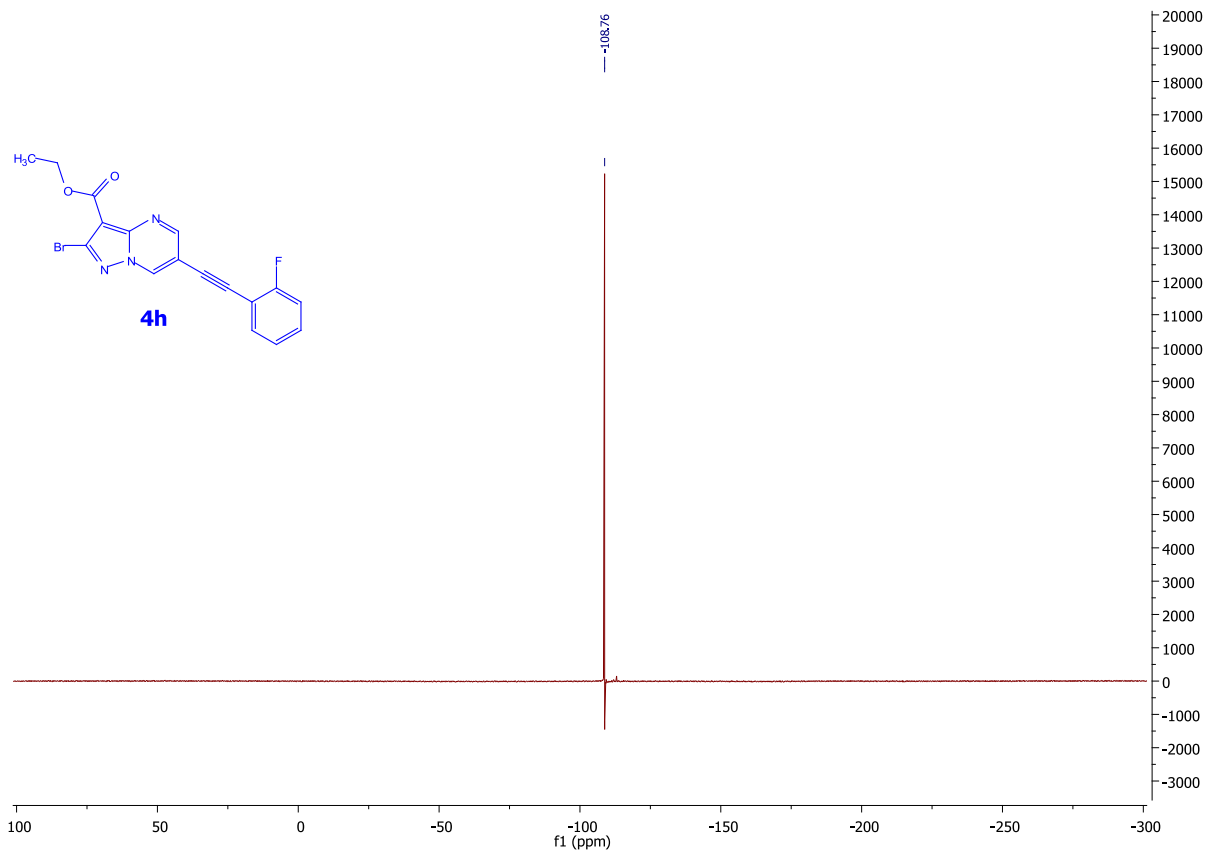


Ethyl 2-bromo-6-[(2-fluorophenyl)ethynyl]pyrazolo[1,5-a]pyrimidine-3-carboxylate (4h**)**

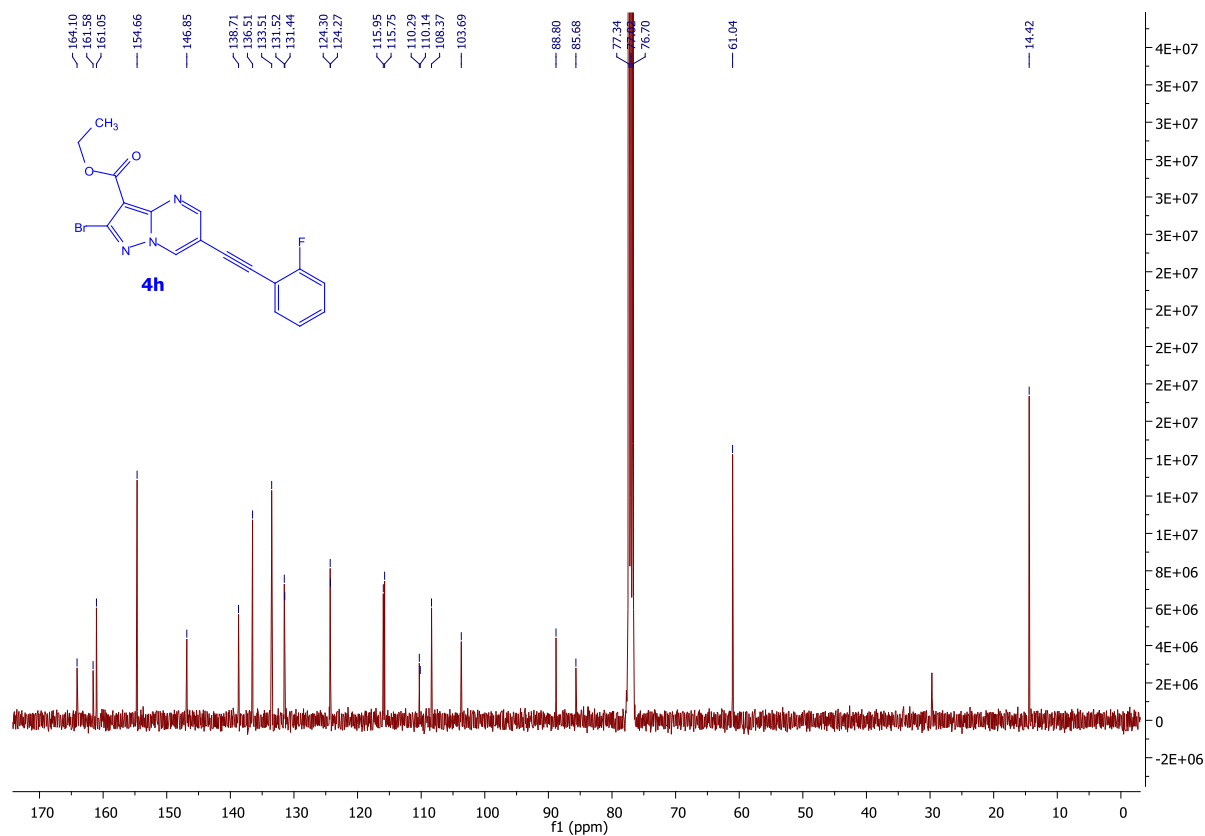
¹H NMR (300 MHz, CDCl₃)



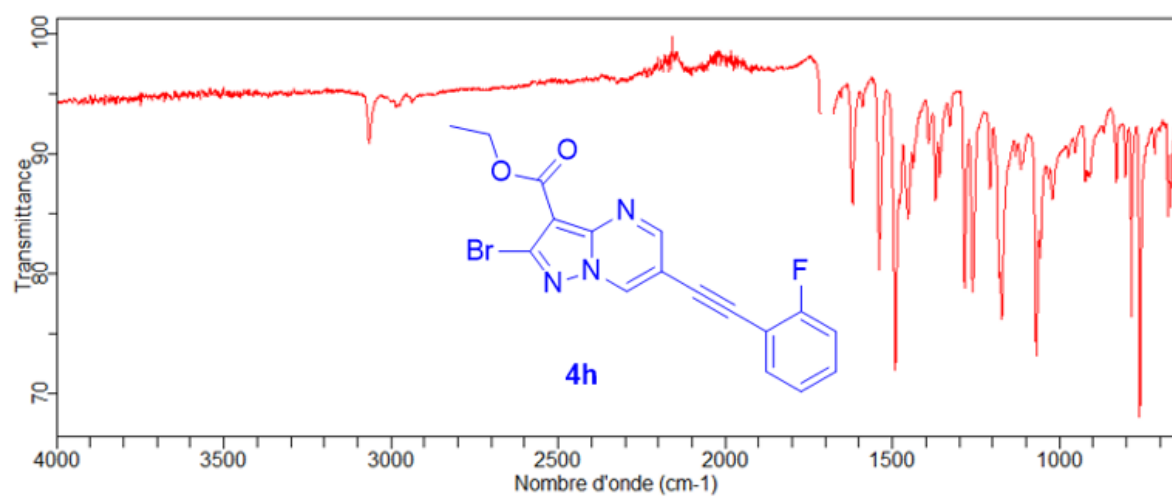
¹⁹F NMR (282 MHz, CDCl₃)



¹³C NMR (75 MHz, CDCl₃)

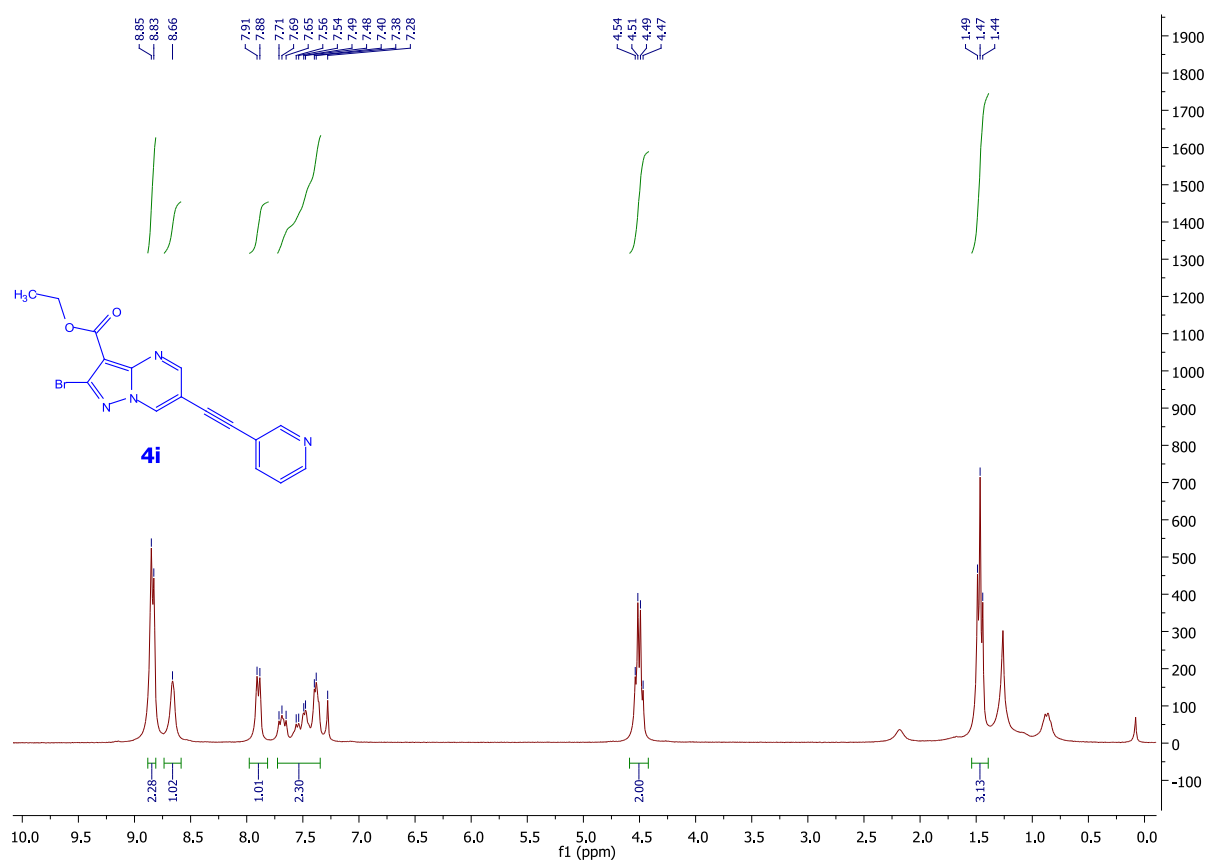


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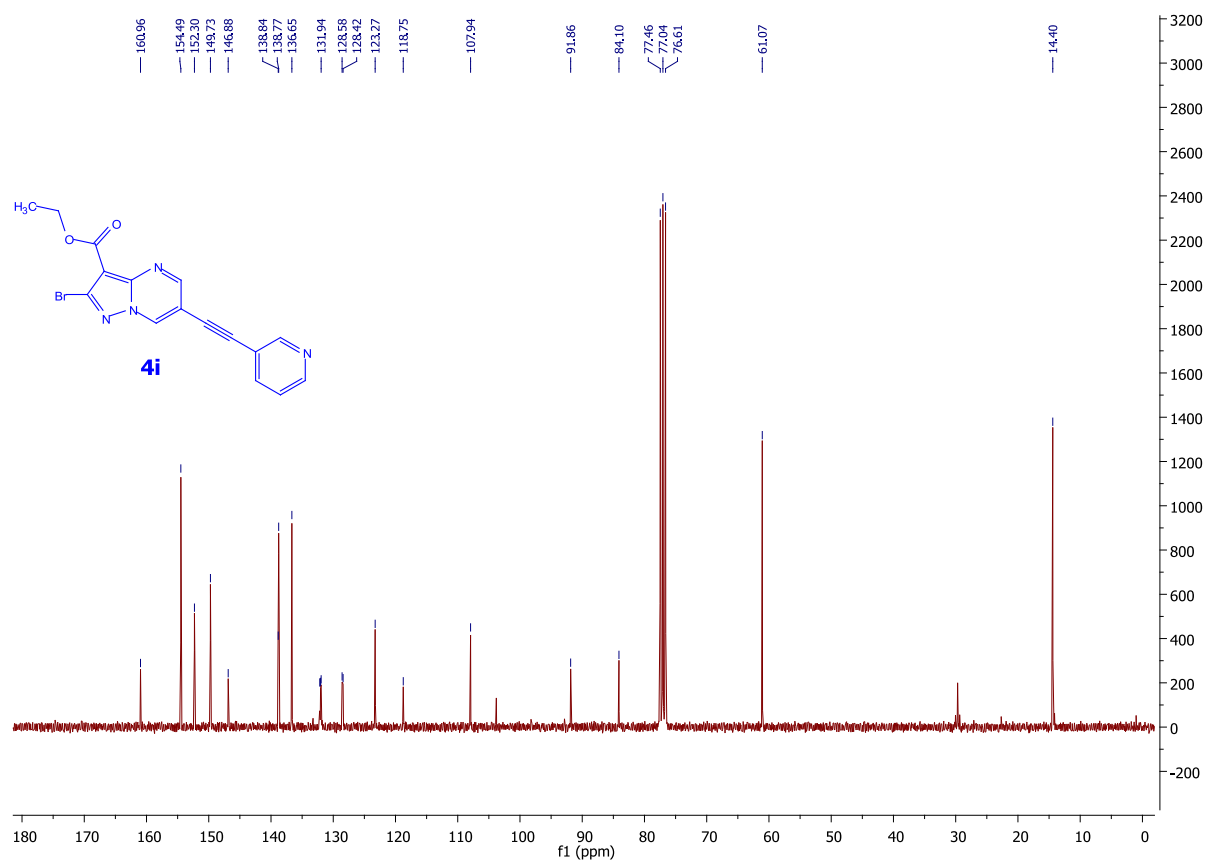


Ethyl 2-bromo-6-(pyridine-3-ethynyl)pyrazolo[1,5-a]pyrimidine-3-carboxylate (4i**)**

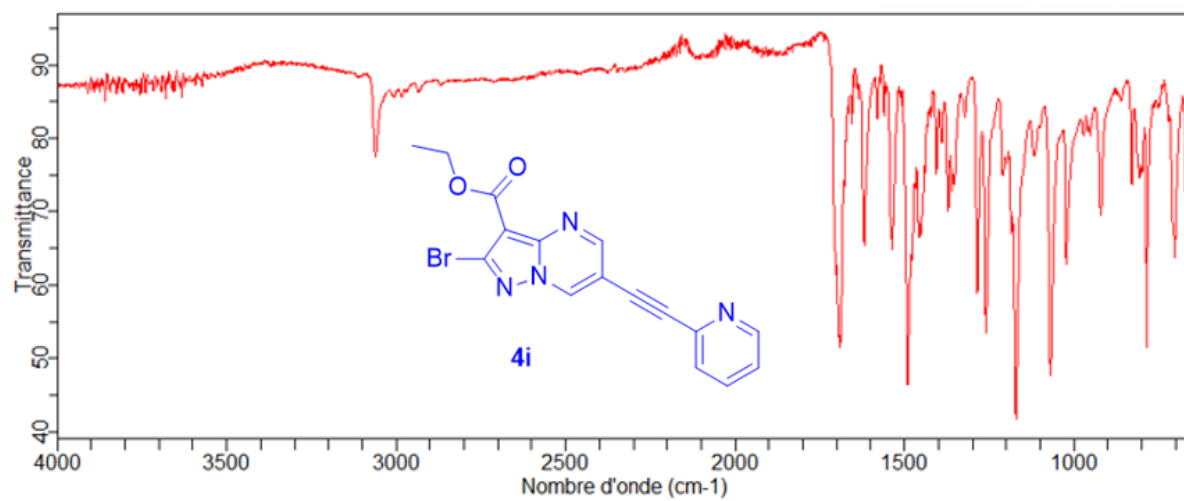
^1H NMR (300 MHz, CDCl_3)



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

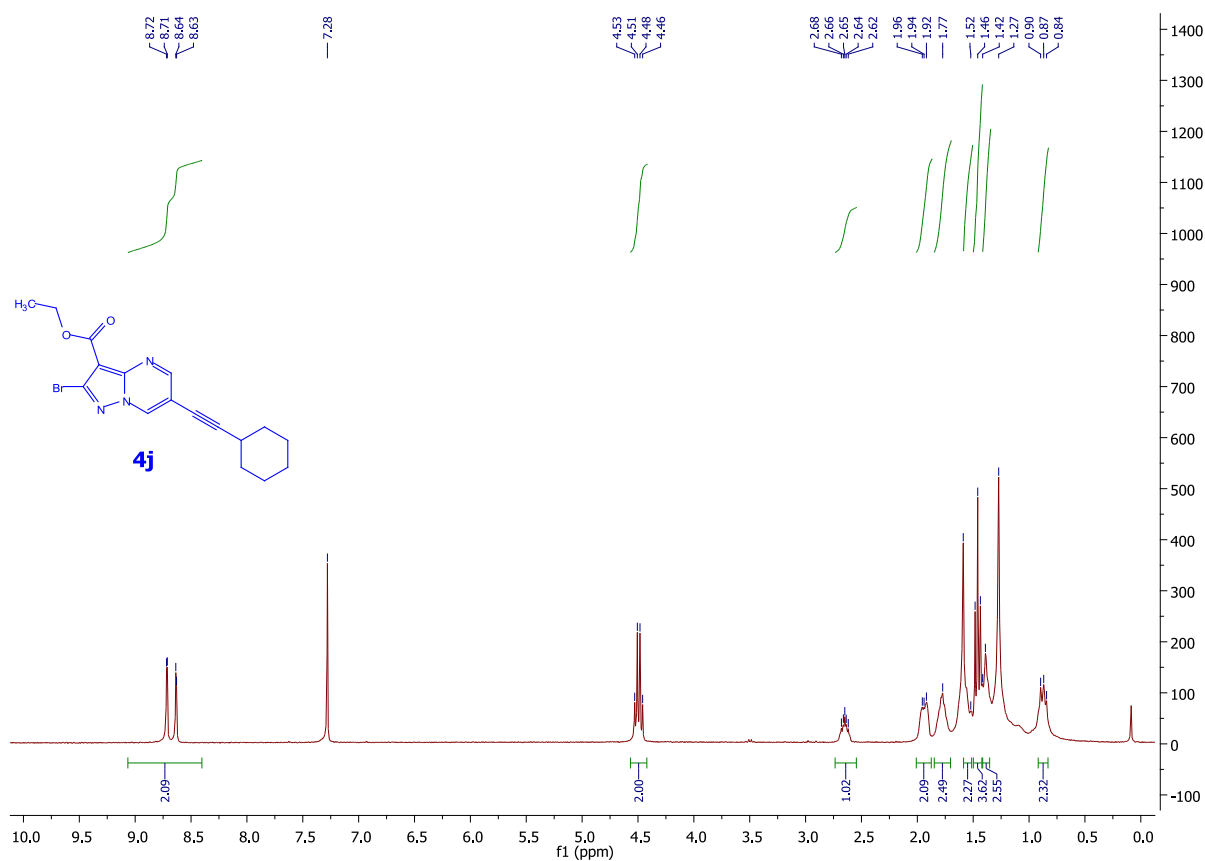


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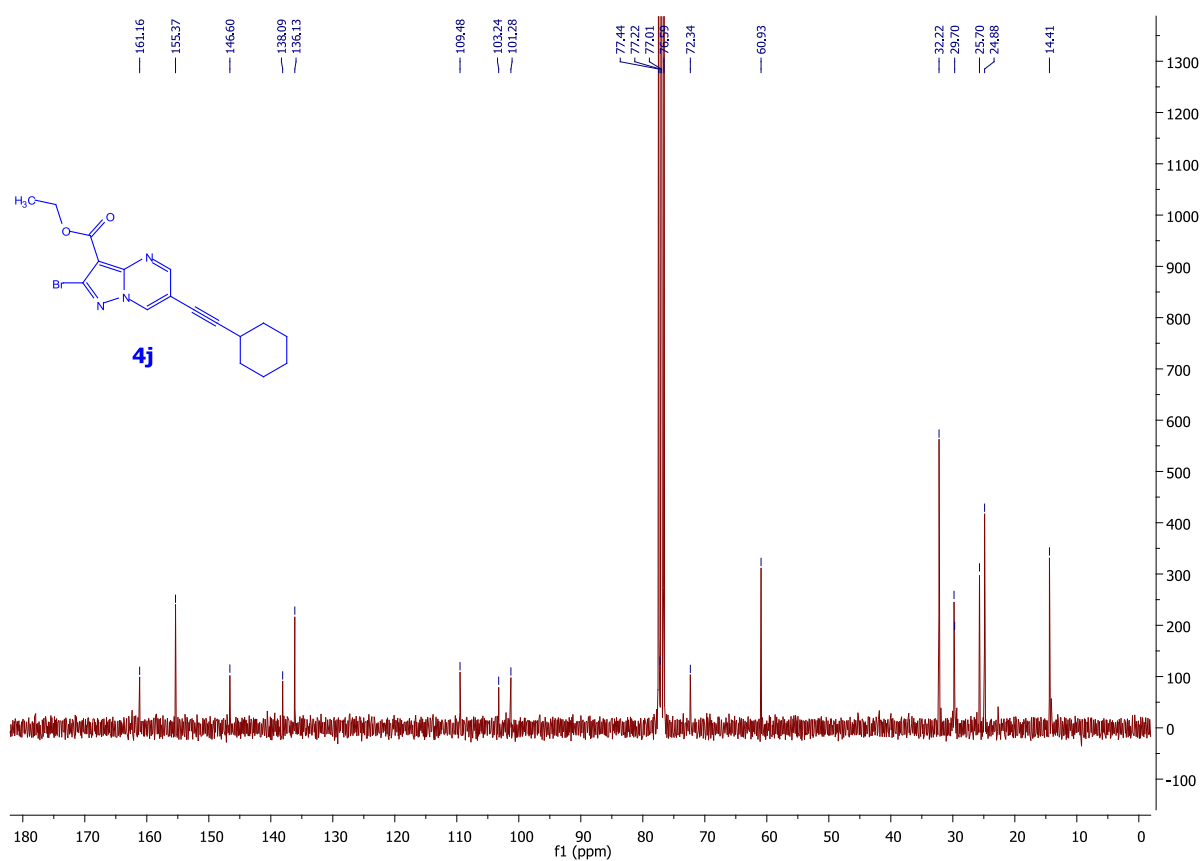


Ethyl 2-bromo-6-(cyclohexylethynyl)pyrazolo[1,5-a]pyrimidine-3-carboxylate (4j**)**

^1H NMR (300 MHz, CDCl_3)

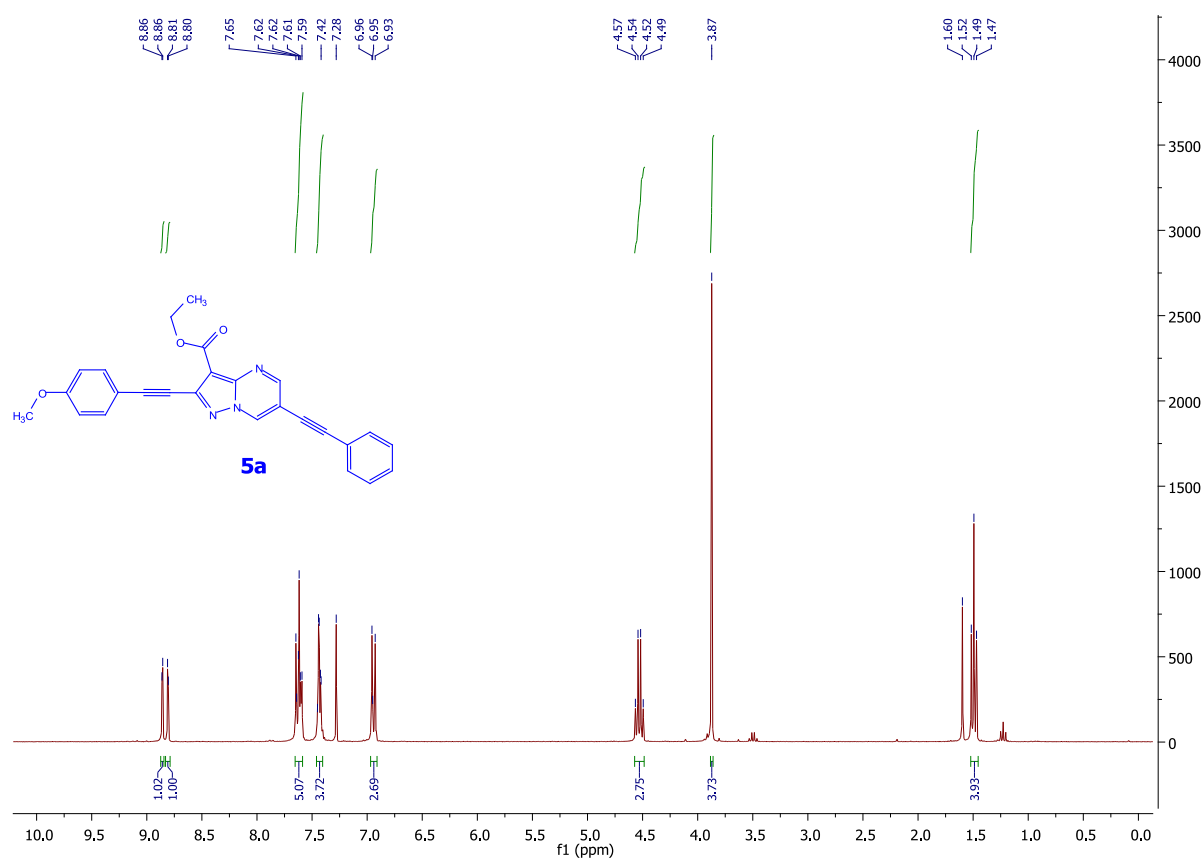


^{13}C NMR (75 MHz, CDCl_3)

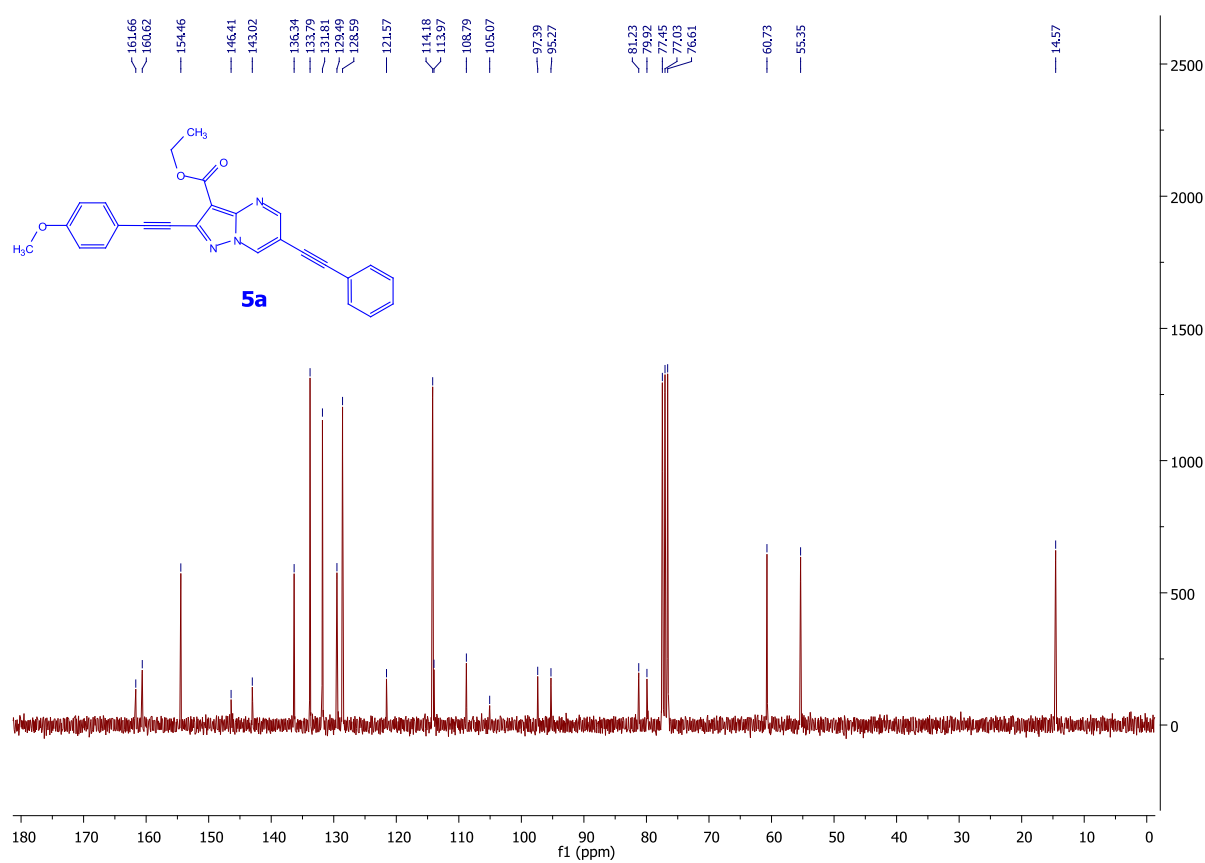


Ethyl 2-[(4-methoxyphenyl)ethynyl]pyrazolo[1,5-a]pyrimidine-3-carboxylate (5a**)**

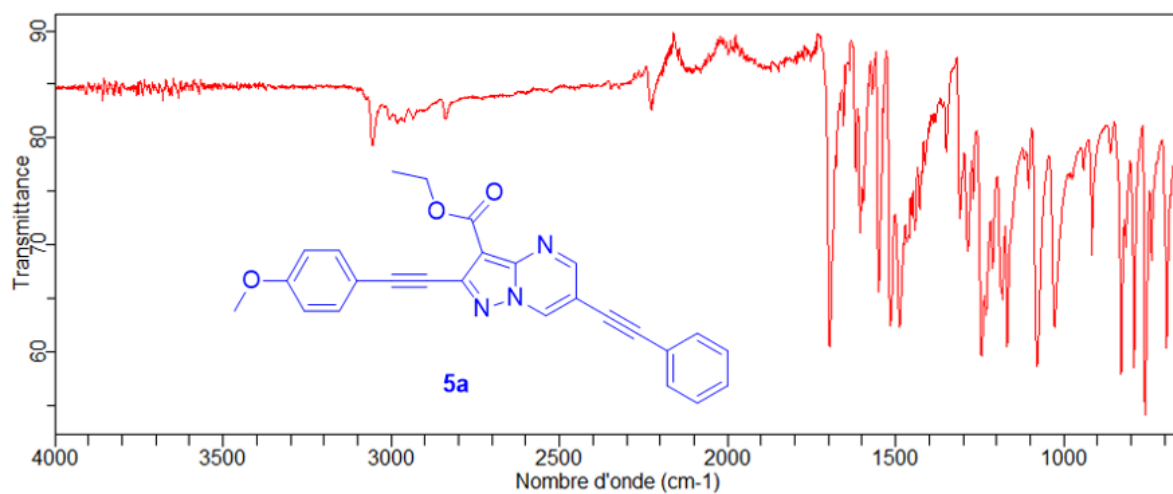
^1H NMR (300 MHz, CDCl_3)



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

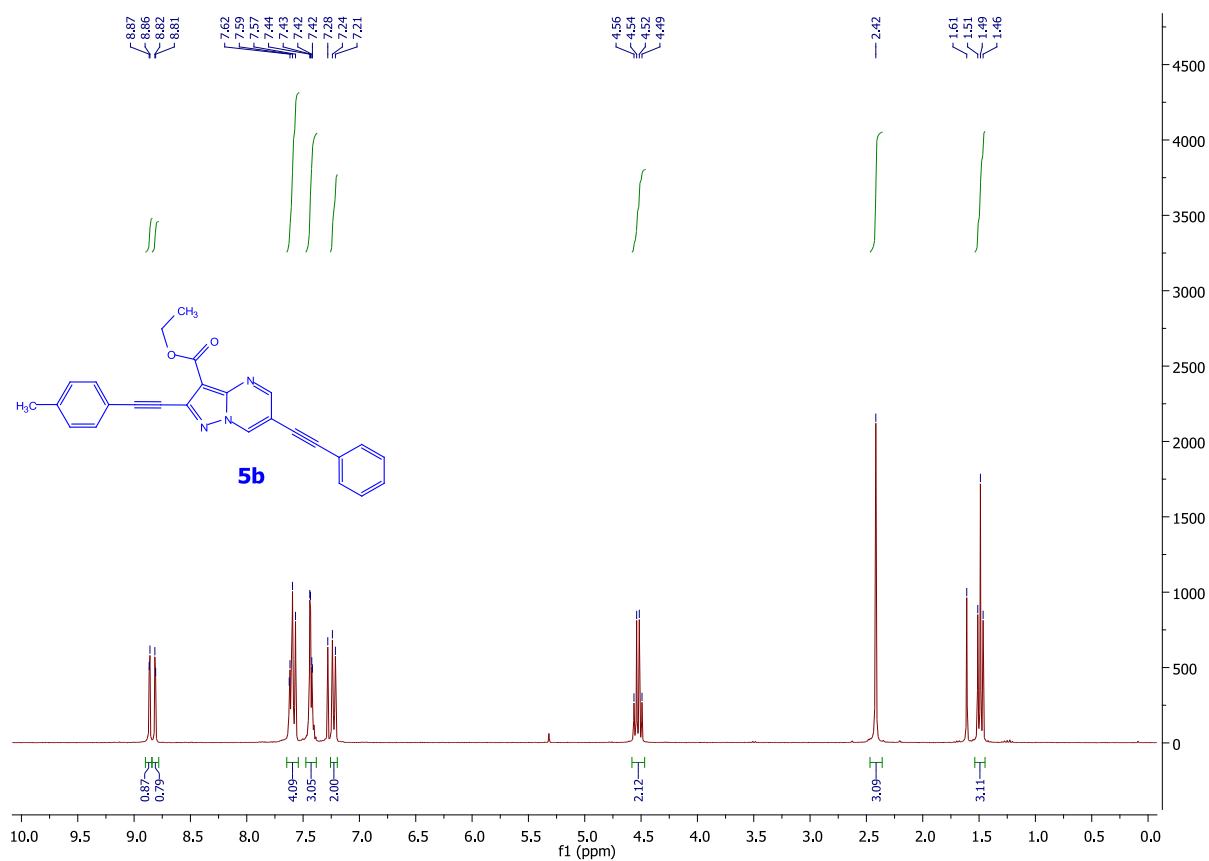


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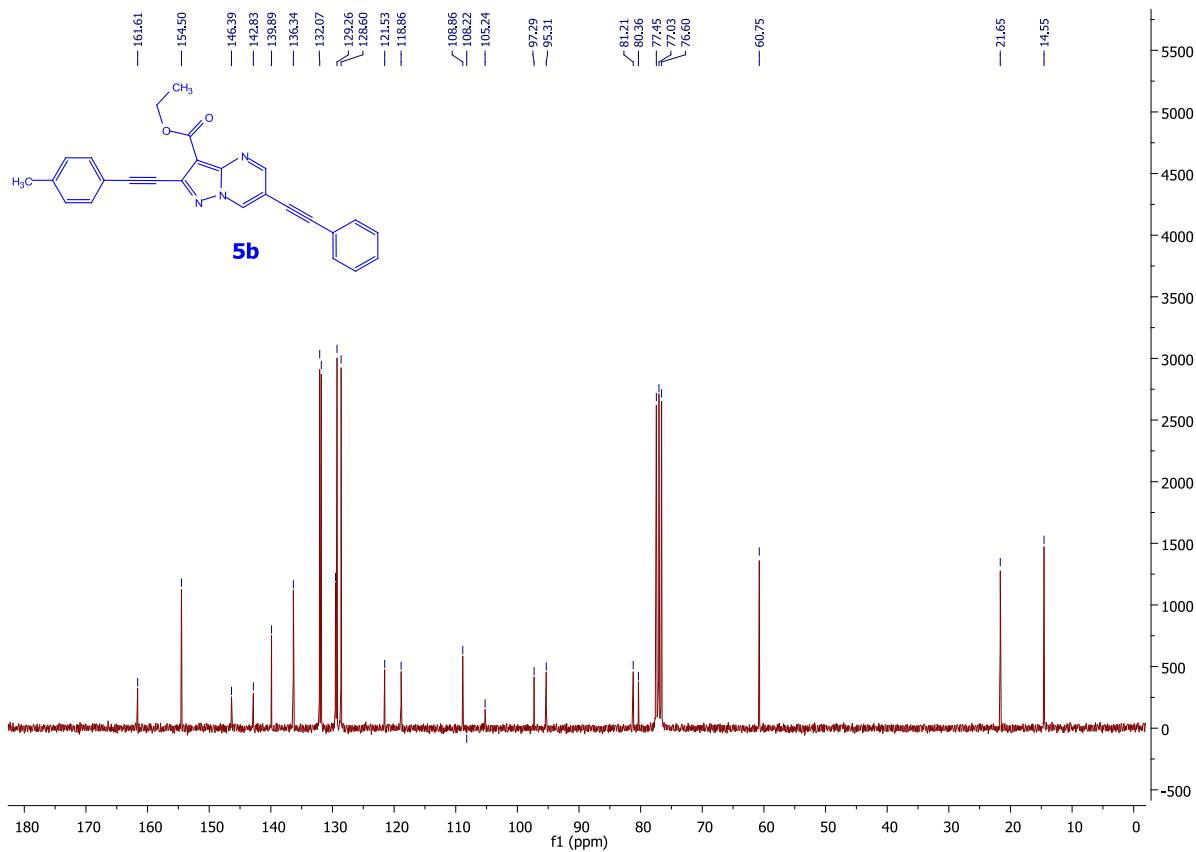


Ethyl 6-(phenylethynyl)-2-(p-tolyethynyl)pyrazolo[1,5-a]pyrimidine-3-carboxylate (5b**)**

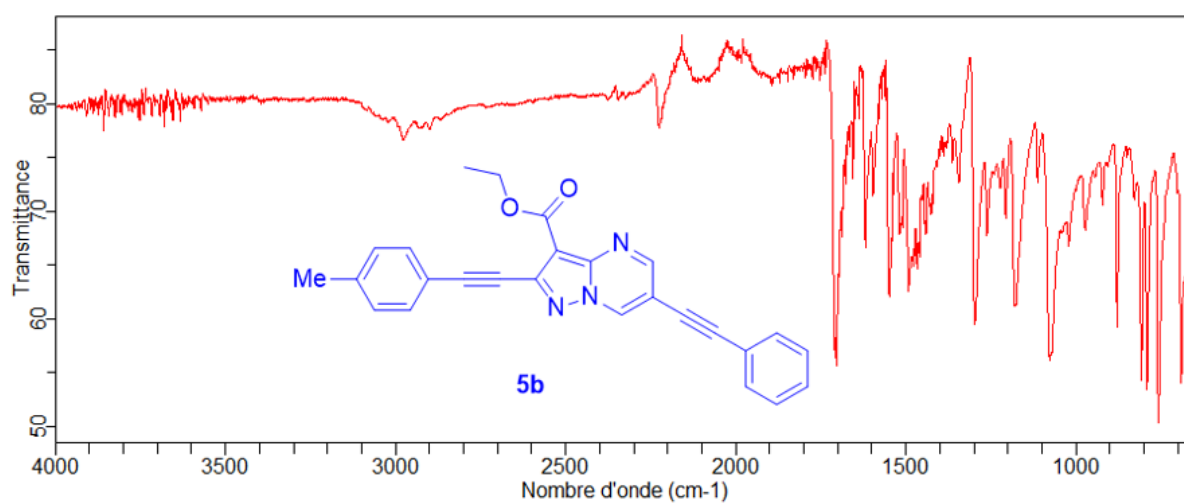
^1H NMR (300 MHz, CDCl_3)



¹³C NMR (75 MHz, CDCl₃)

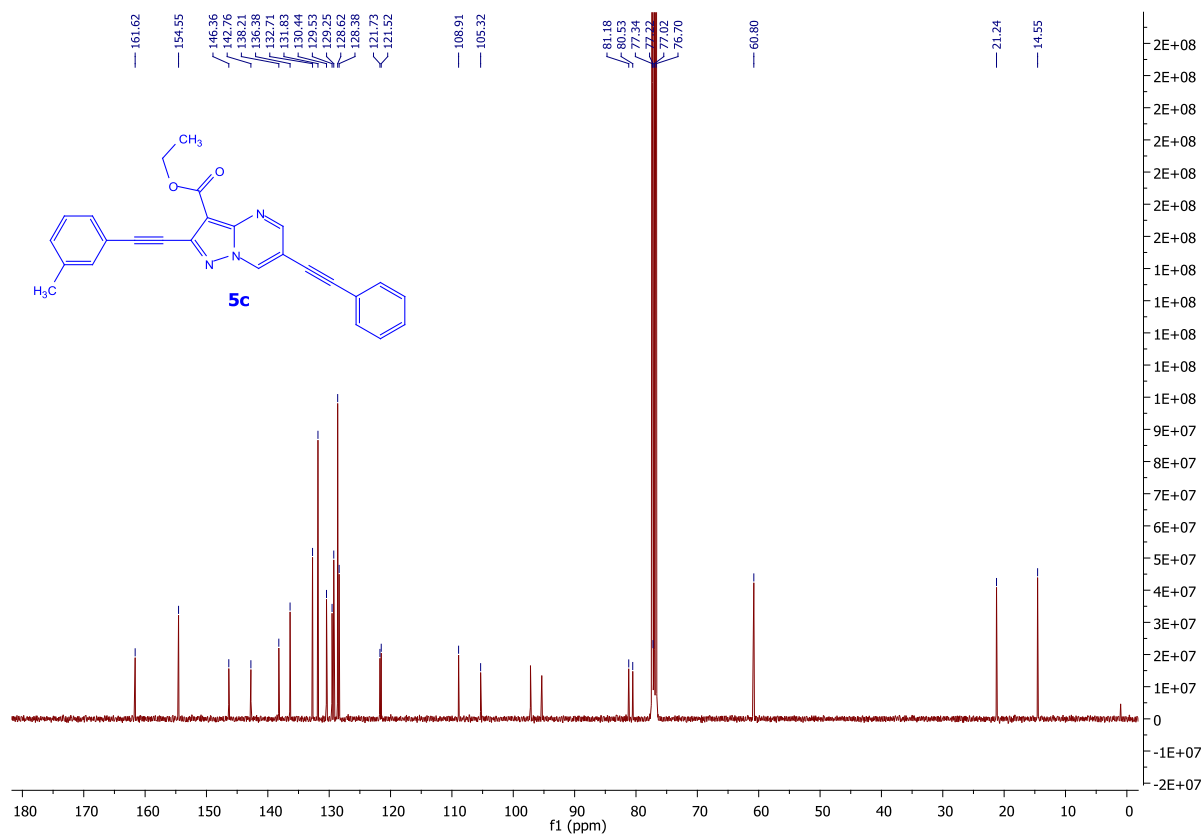
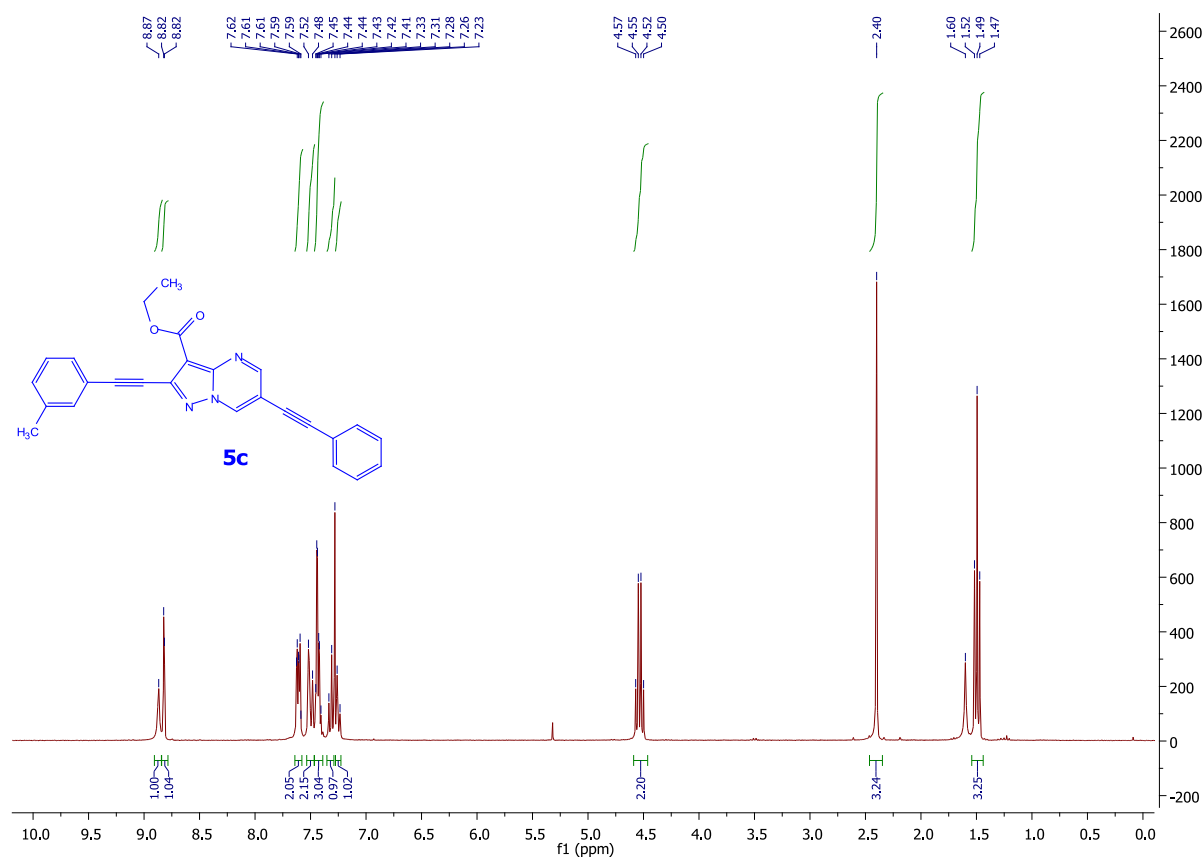


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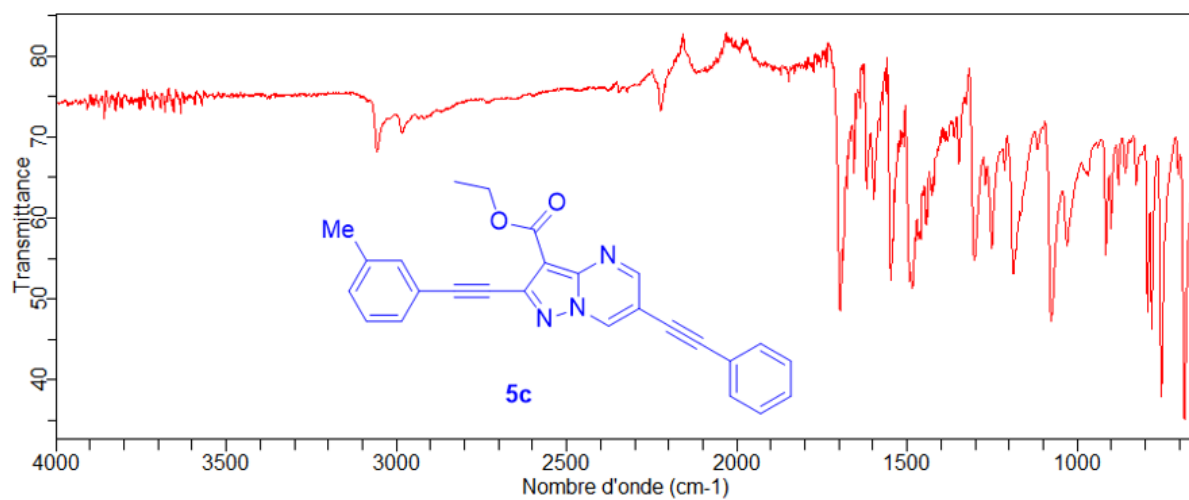
Ethyl 6-(phenylethynyl)-2-(*m*-tolylethynyl)pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (5c**)**

¹H NMR (300 MHz, CDCl₃)



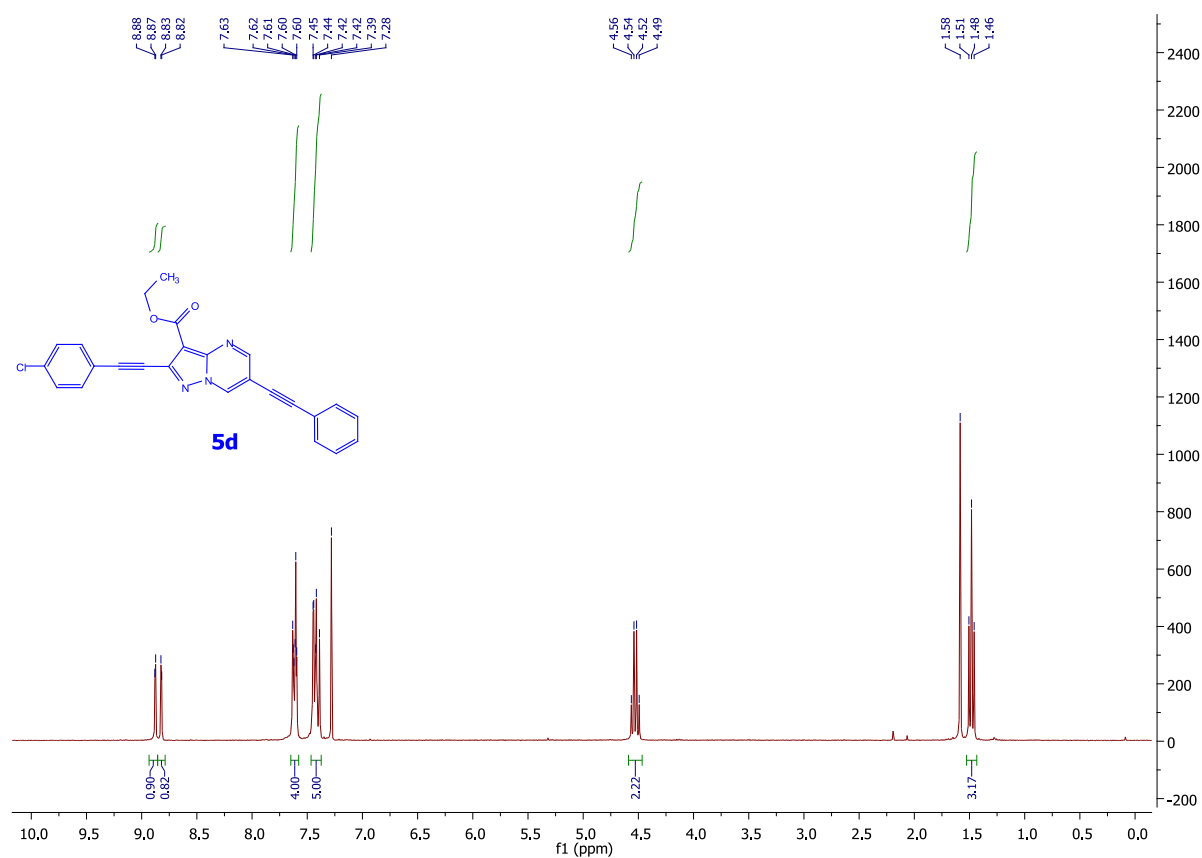
¹³C NMR (75 MHz, CDCl₃)

IR

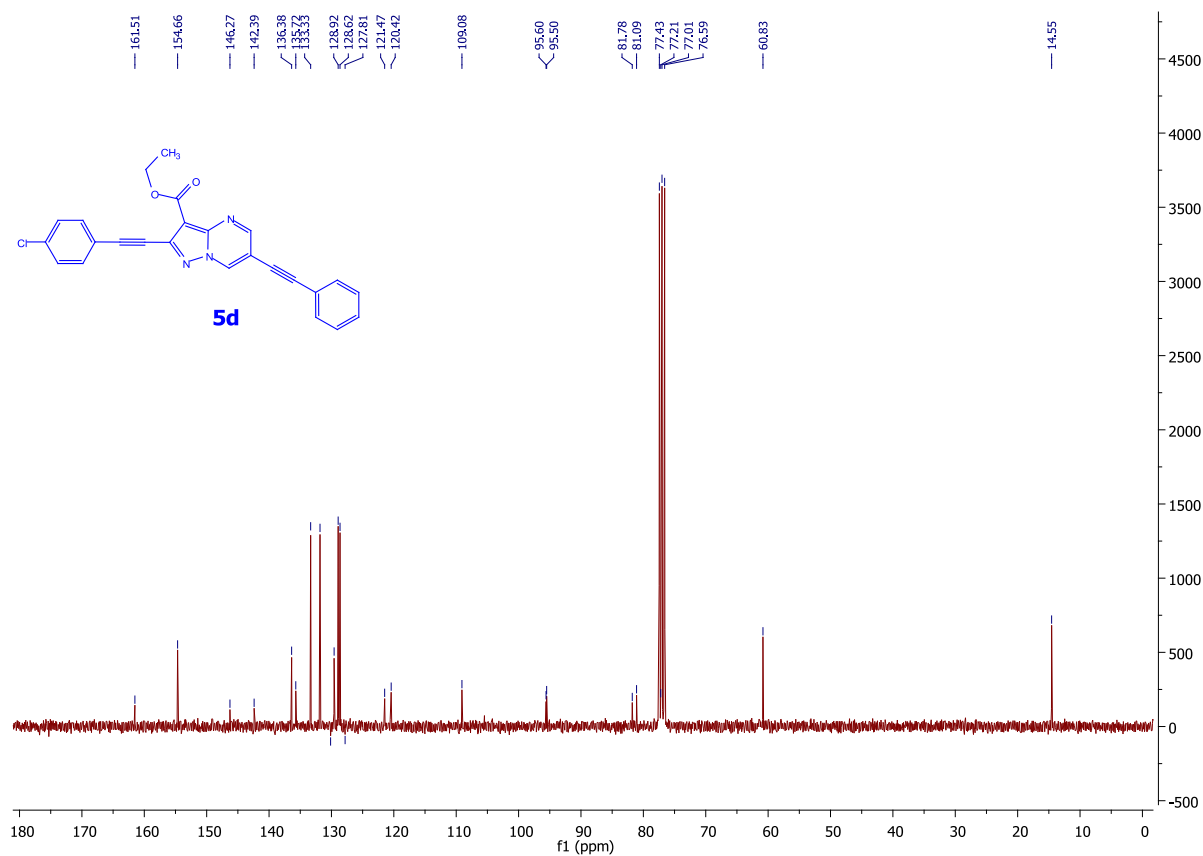


Ethyl 2-[(4-chlorophenyl)ethynyl]-6-(phenylethynyl)pyrazolo[1,5-a]pyrimidine-3-carboxylate (5d)

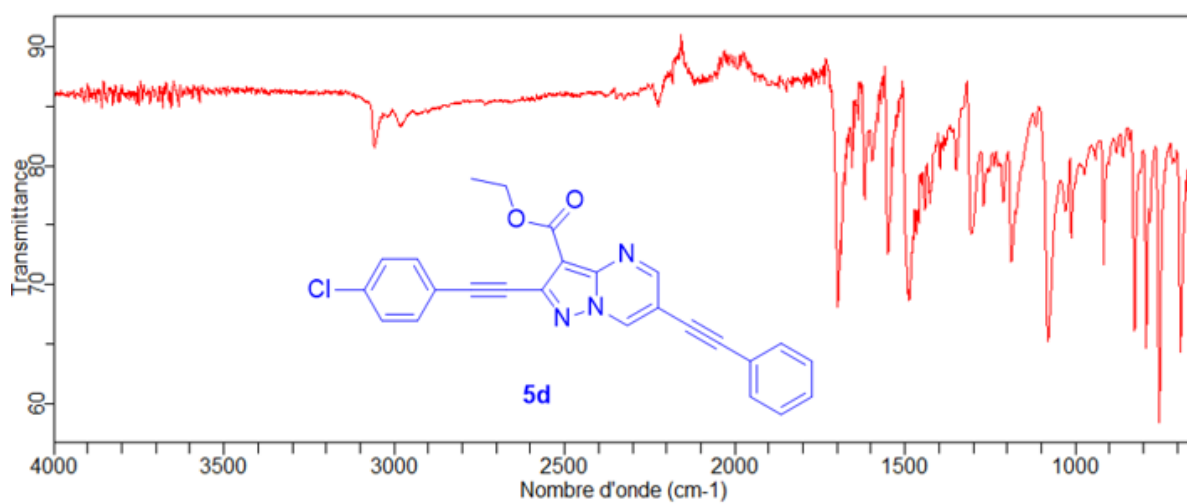
^1H NMR (300 MHz, CDCl_3)



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

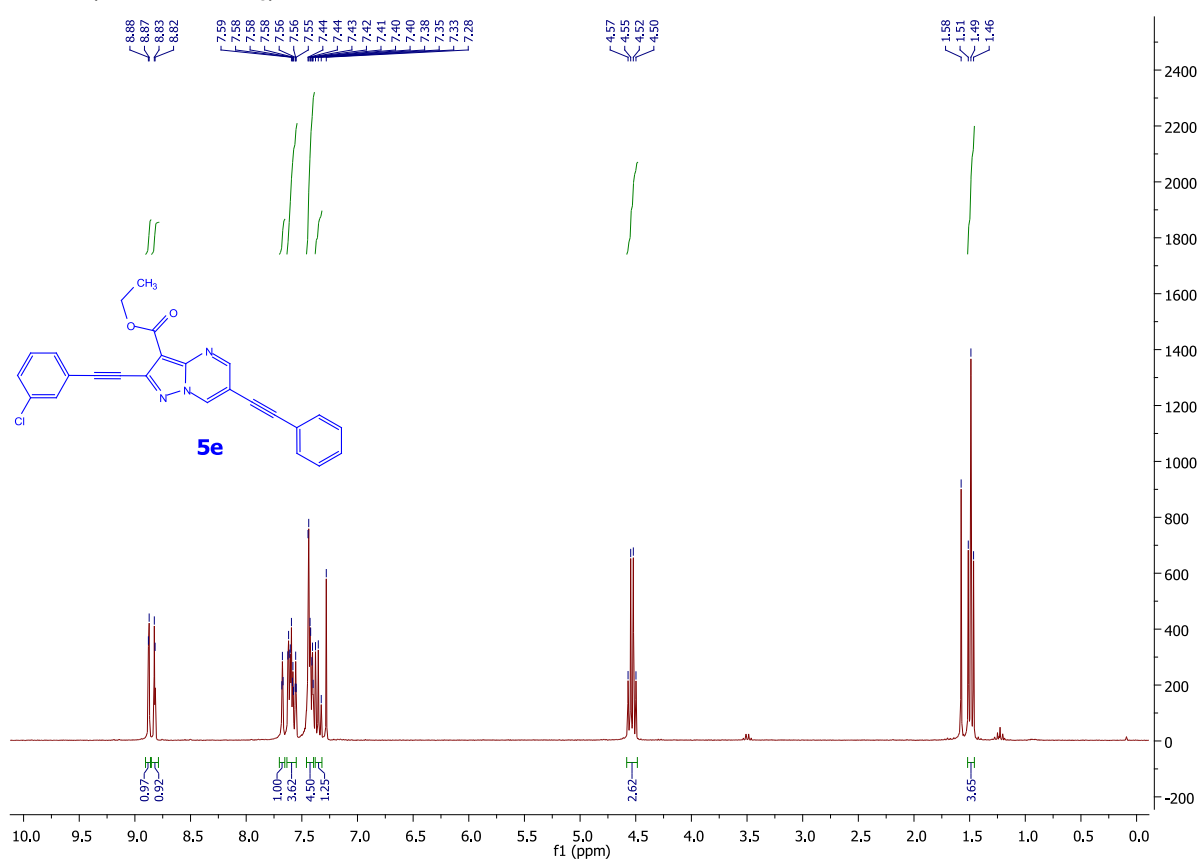


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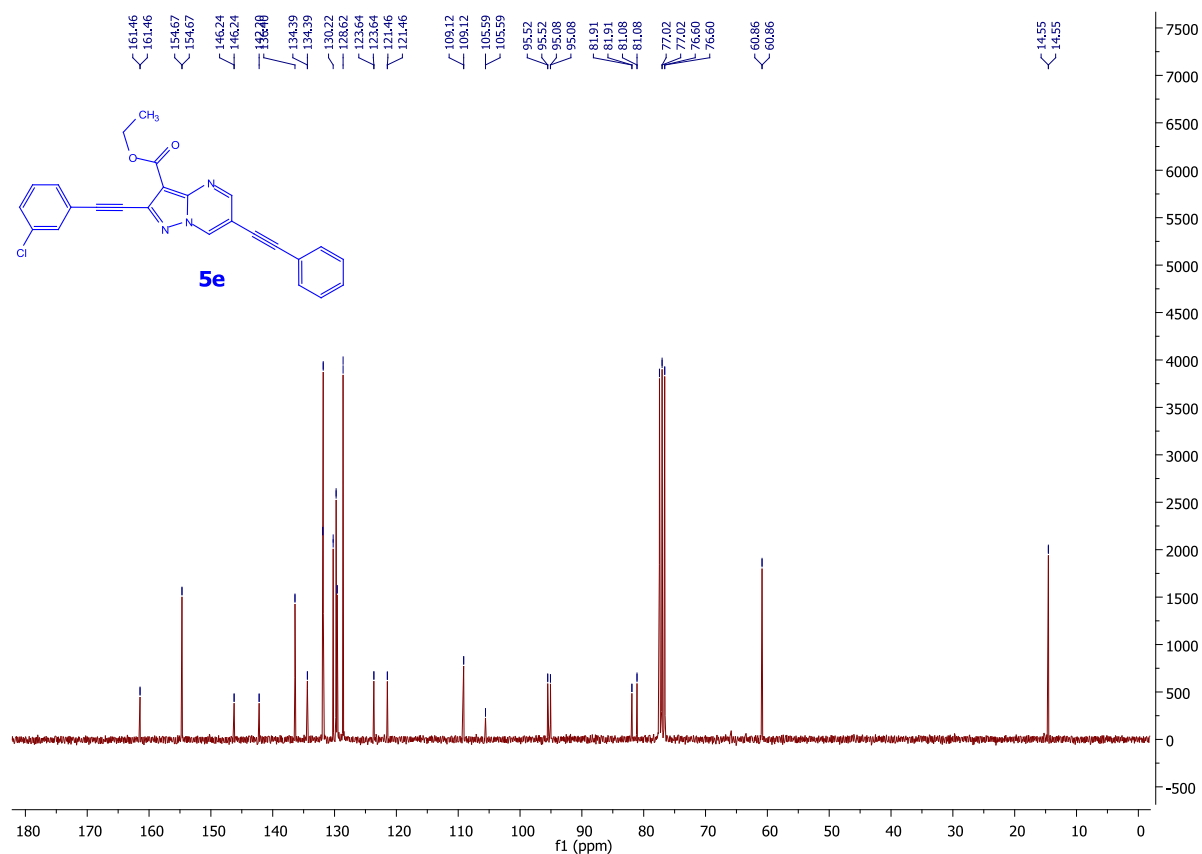


Ethyl 2-[(3-chlorophenyl)ethynyl]-6-(phenylethynyl)pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (5e**)**

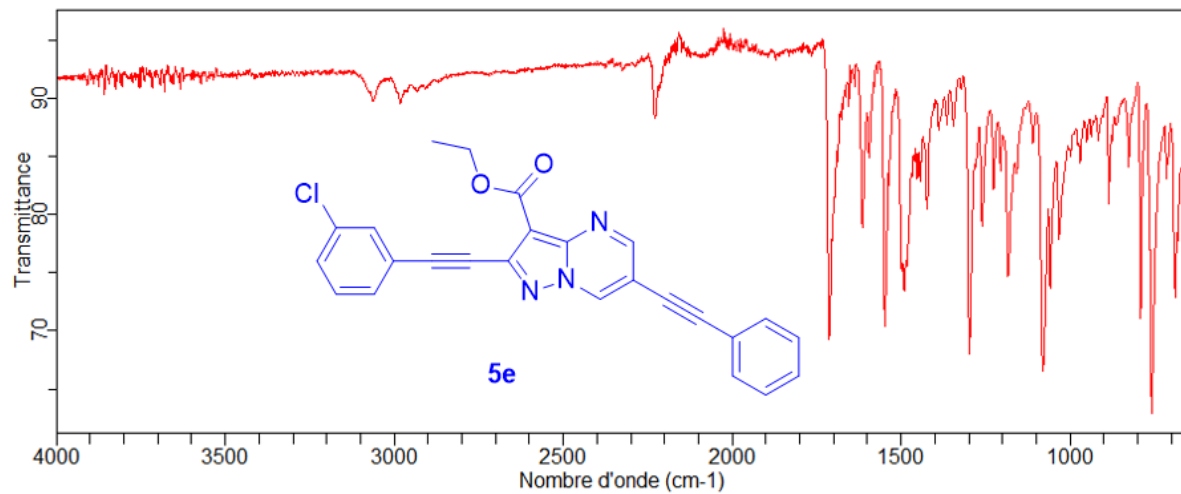
¹H NMR (300 MHz, CDCl₃)



¹³C NMR (75 MHz, CDCl₃)

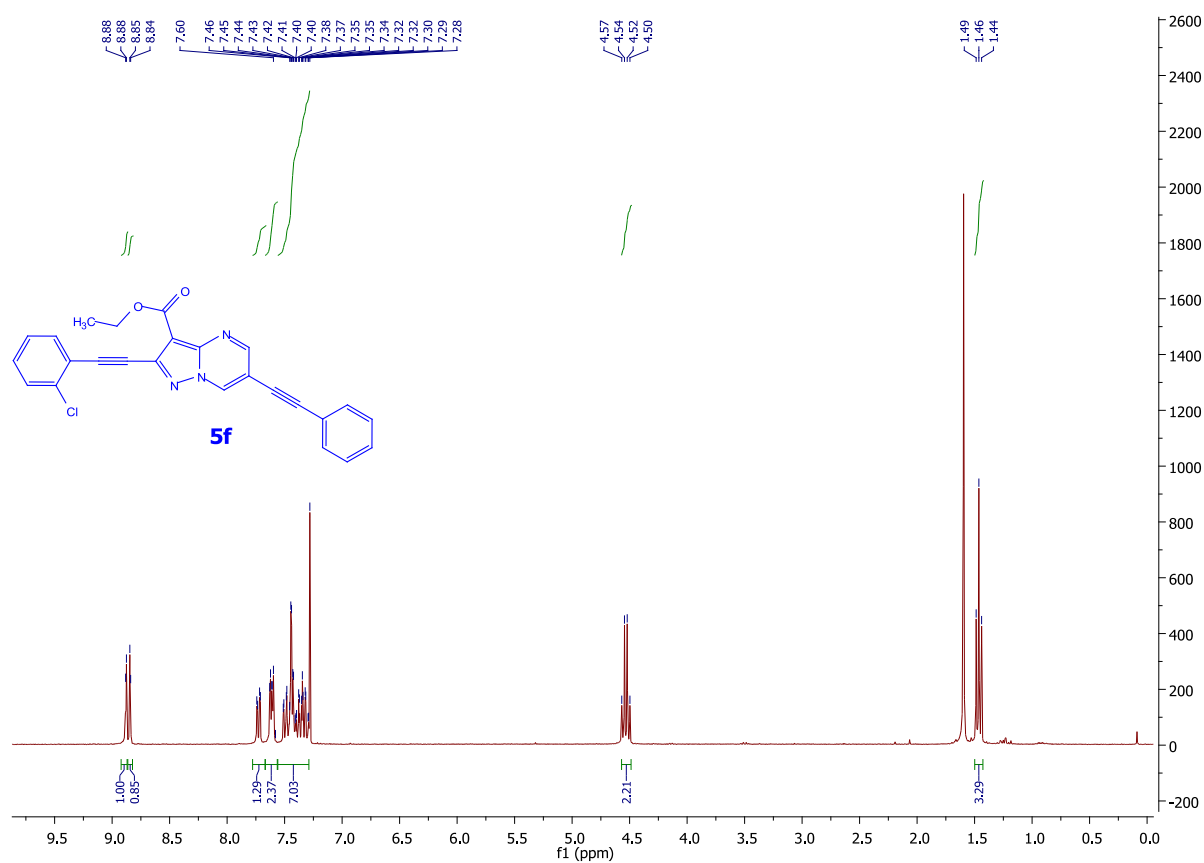


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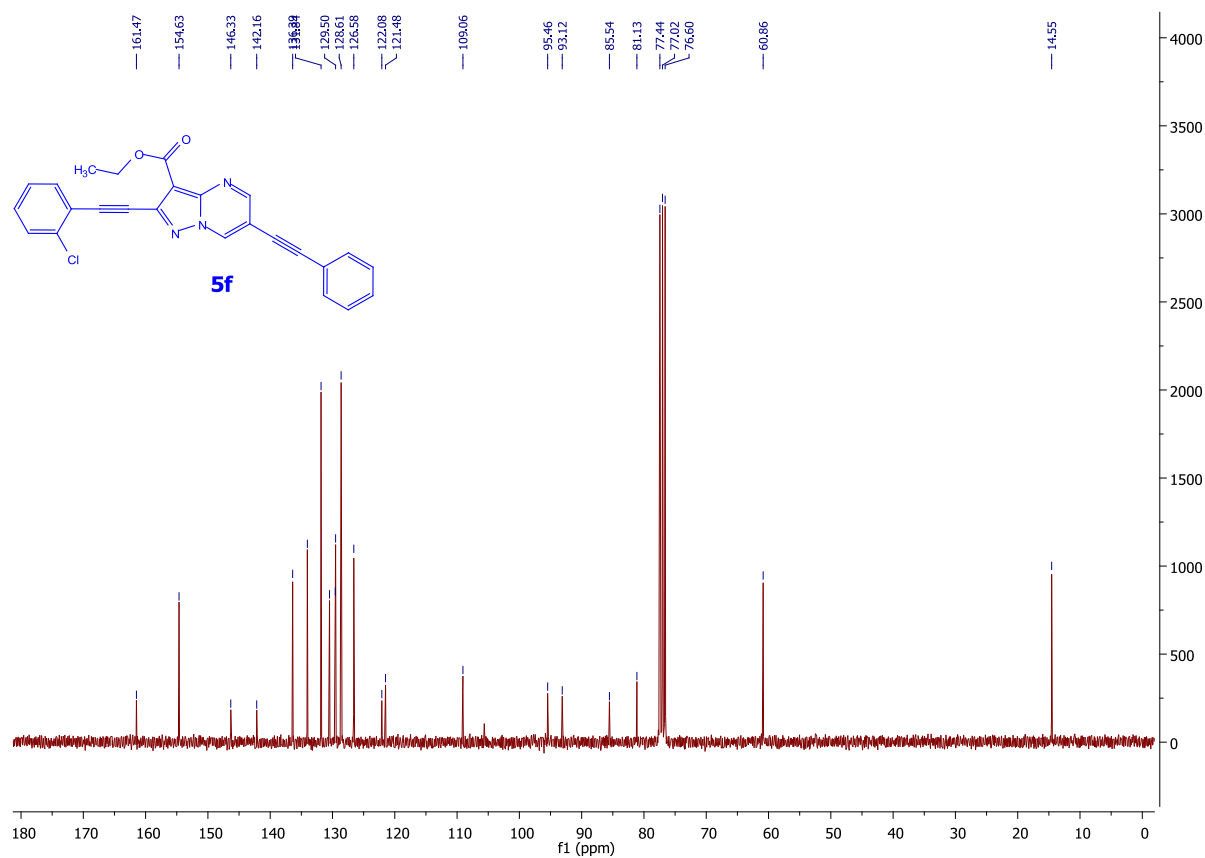


Ethyl 2-[(2-chlorophenyl)ethynyl]-6-(phenylethynyl)pyrazolo[1,5-a]pyrimidine-3-carboxylate (5f**)**

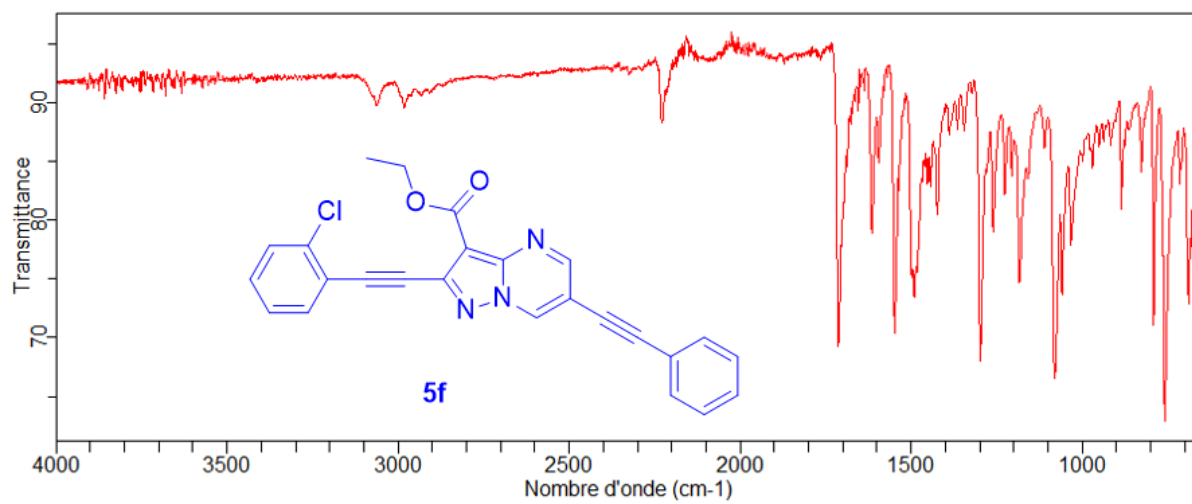
¹H NMR (300 MHz, CDCl₃)



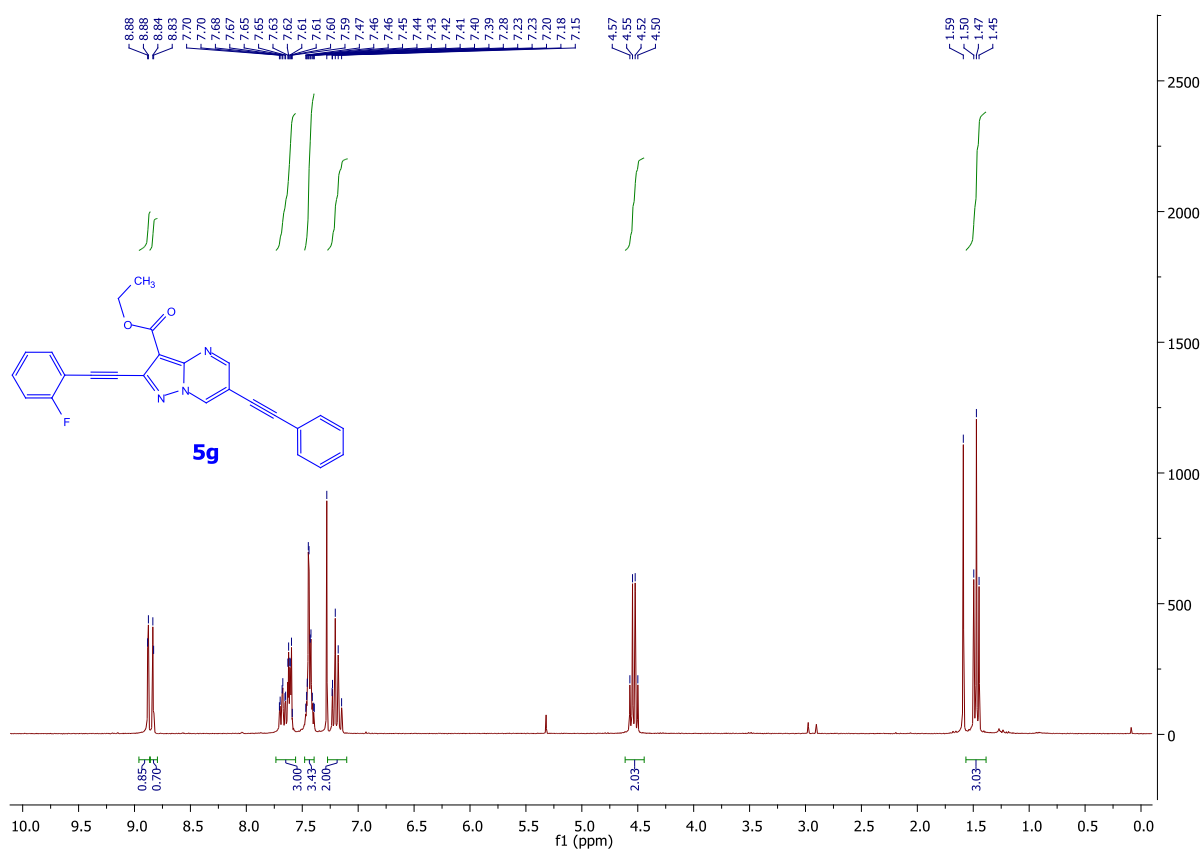
¹³C NMR (75 MHz, CDCl₃)



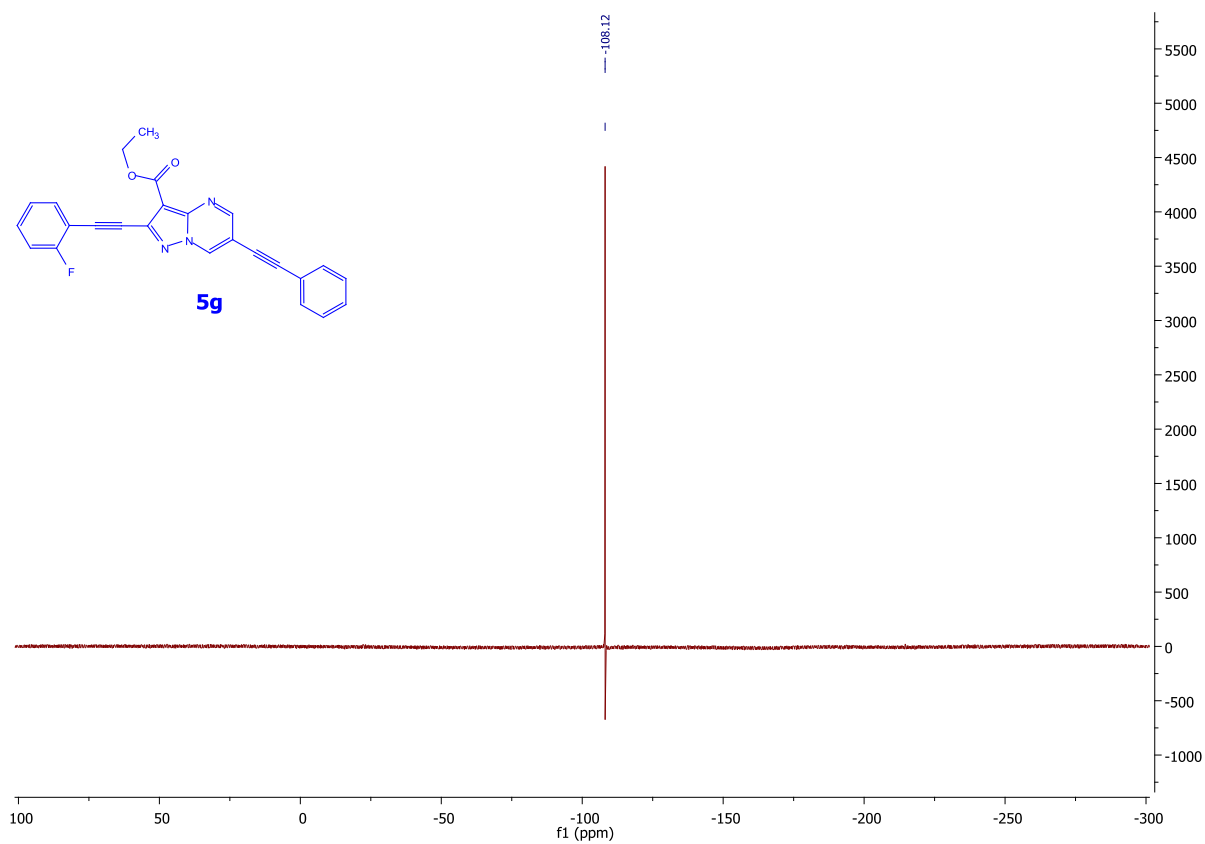
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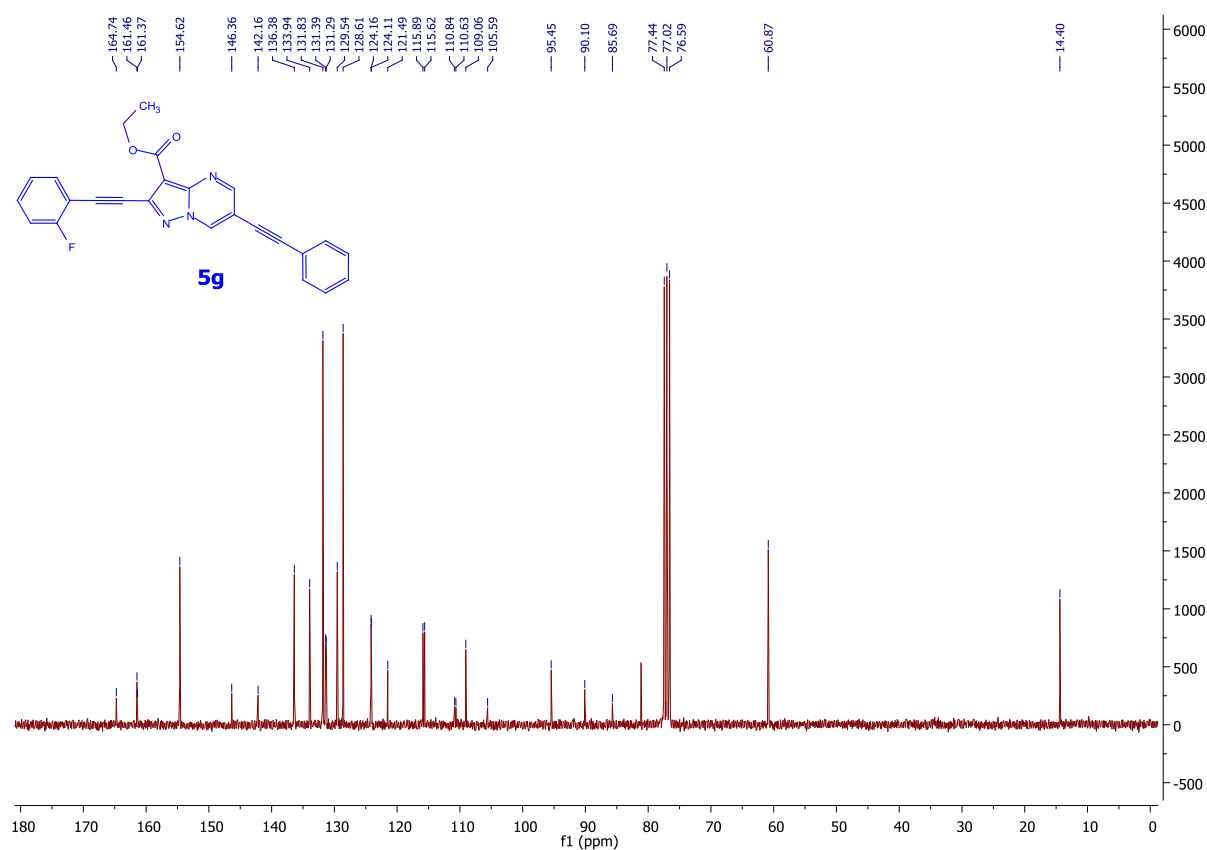
Ethyl 2-[(2-fluorophenyl)ethynyl]-6-(phenylethynyl)pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (5g**)**
¹H NMR (300 MHz, CDCl₃)



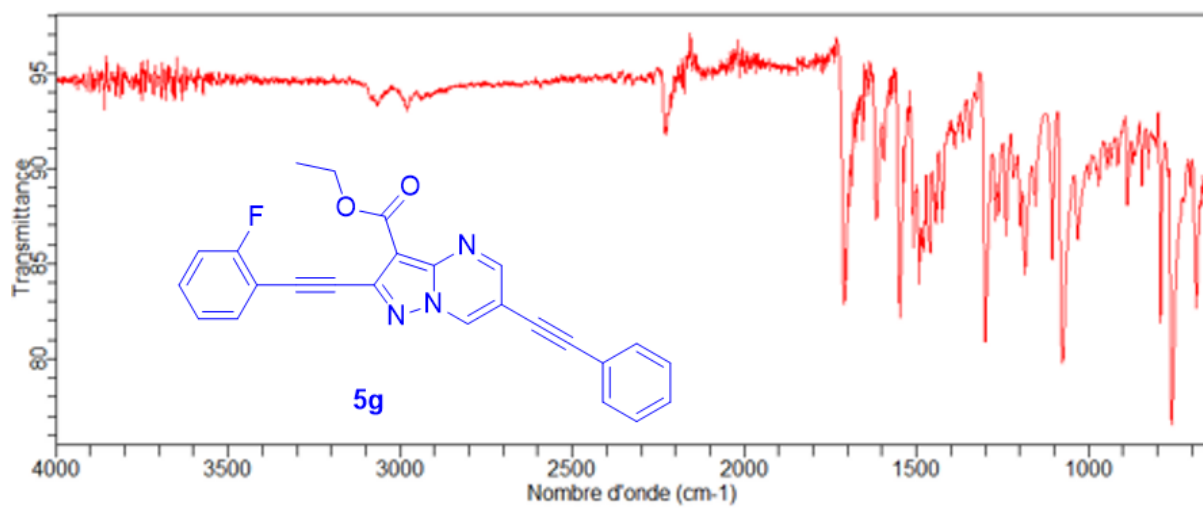
¹⁹F NMR (282 MHz, CDCl₃)



¹³C NMR (75 MHz, CDCl₃)

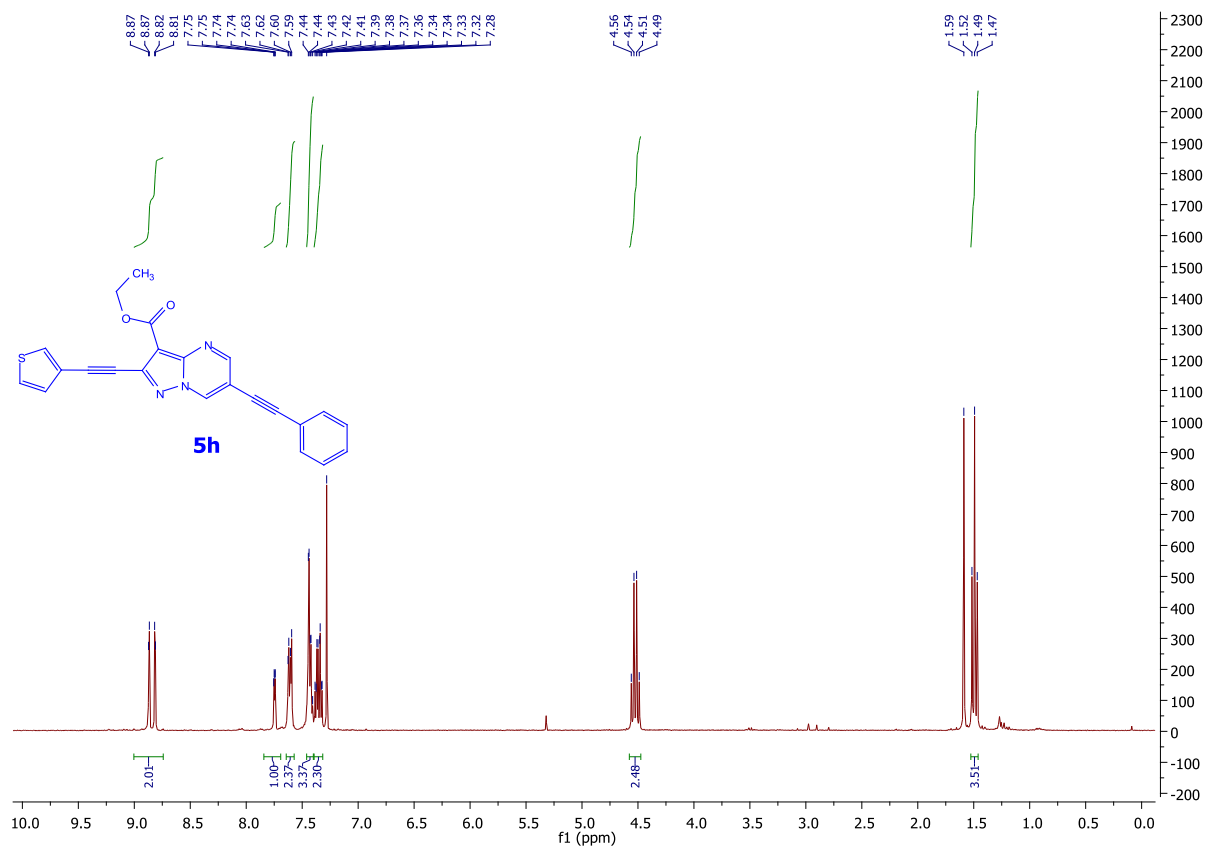


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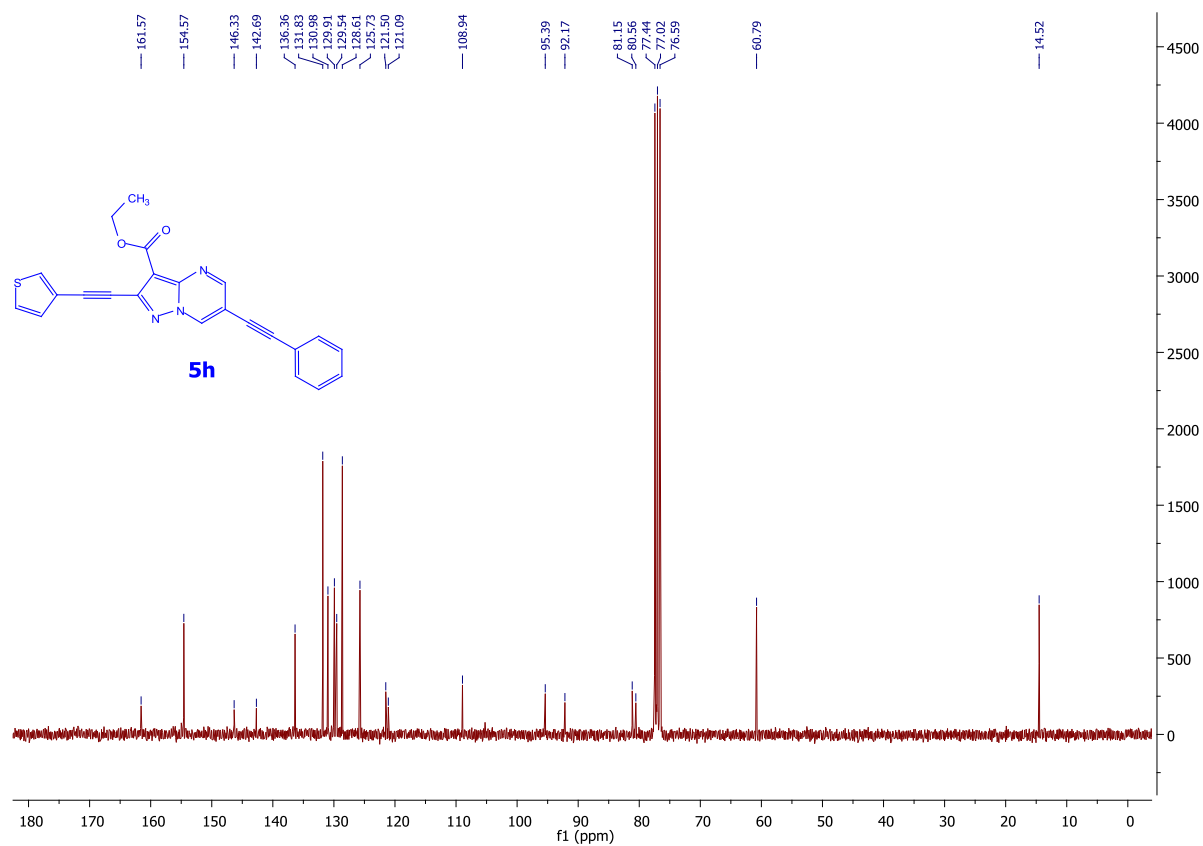


Ethyl 6-(phenylethynyl)-2-(thiophen-3-ethynyl)pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (5h**)**

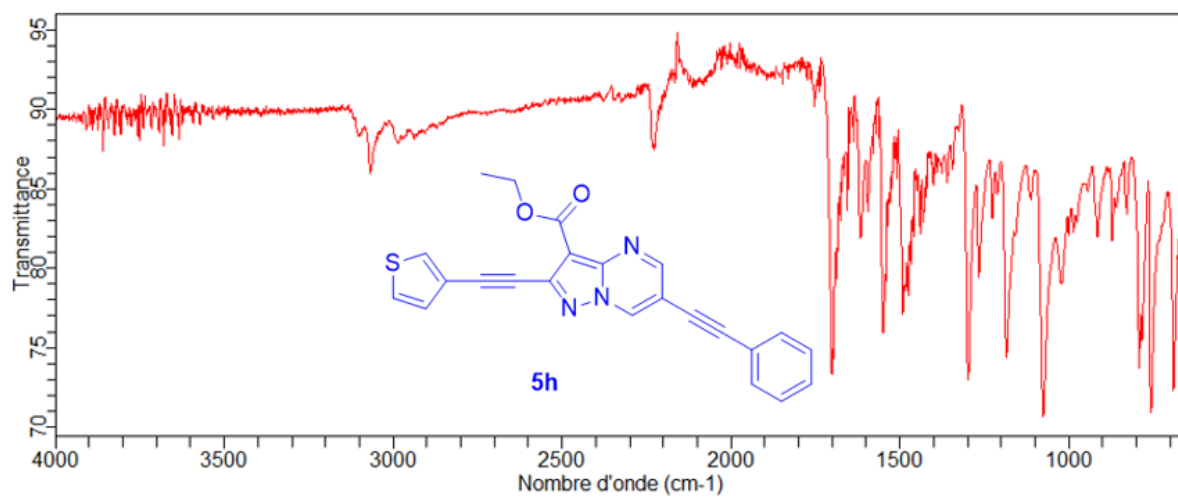
¹H NMR (300 MHz, CDCl₃)



¹³C NMR (75 MHz, CDCl₃)

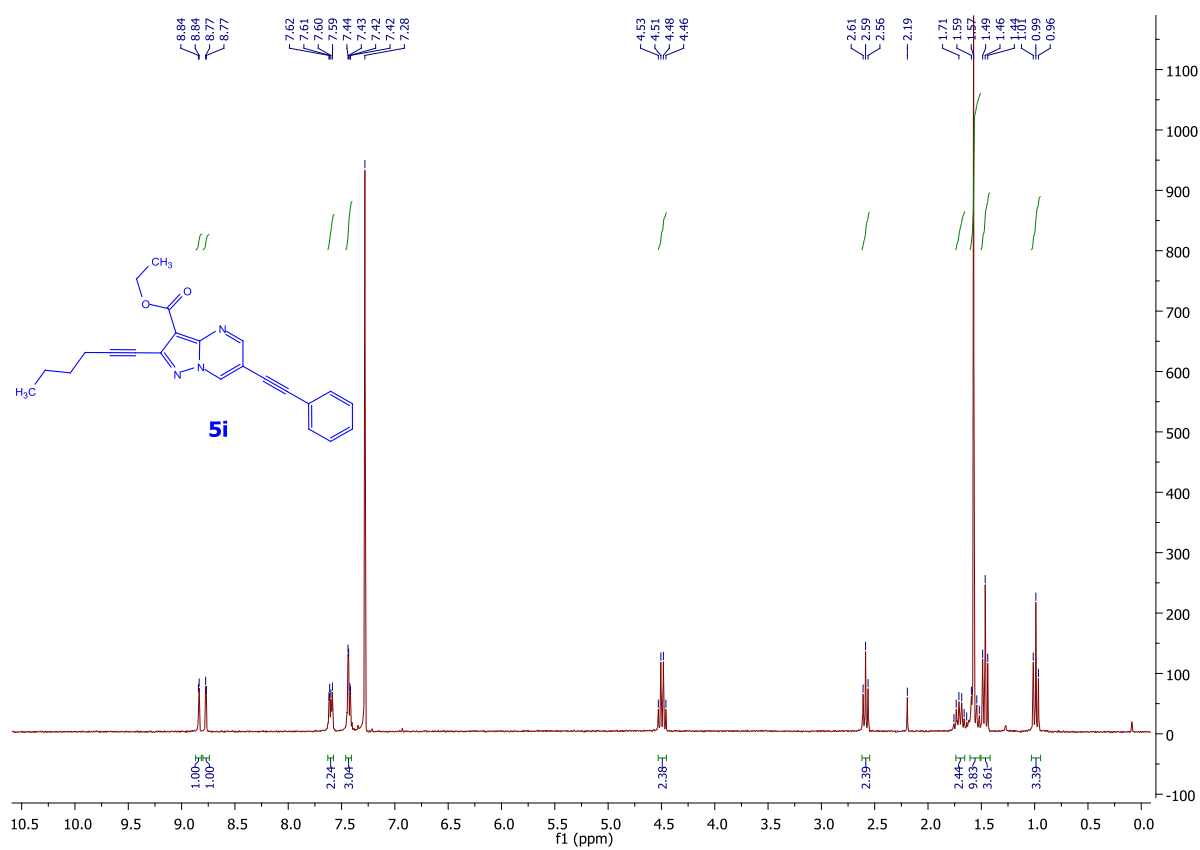


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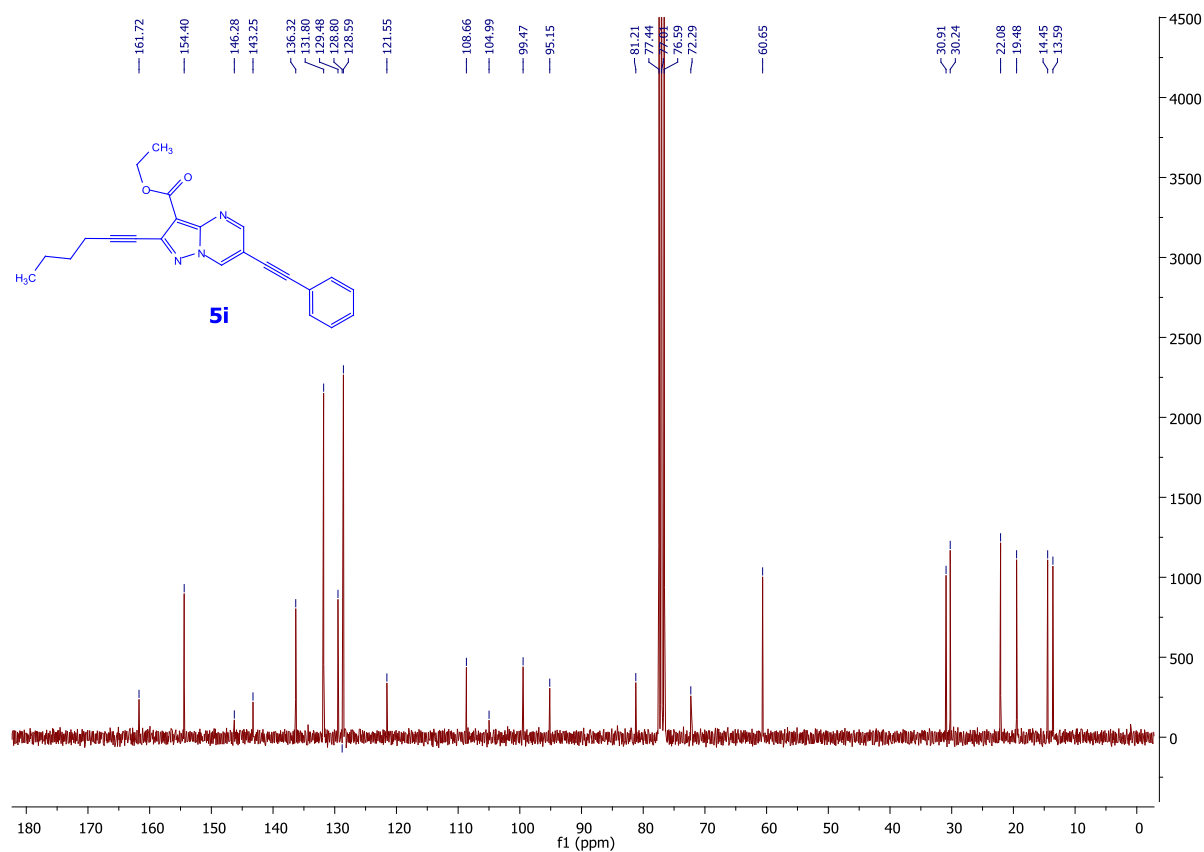


Ethyl 2-(hex-1-yn-1-yl)-6-(phenylethynyl)pyrazolo[1,5-a]pyrimidine-3-carboxylate (5i**)**

^1H NMR (300 MHz, CDCl_3)

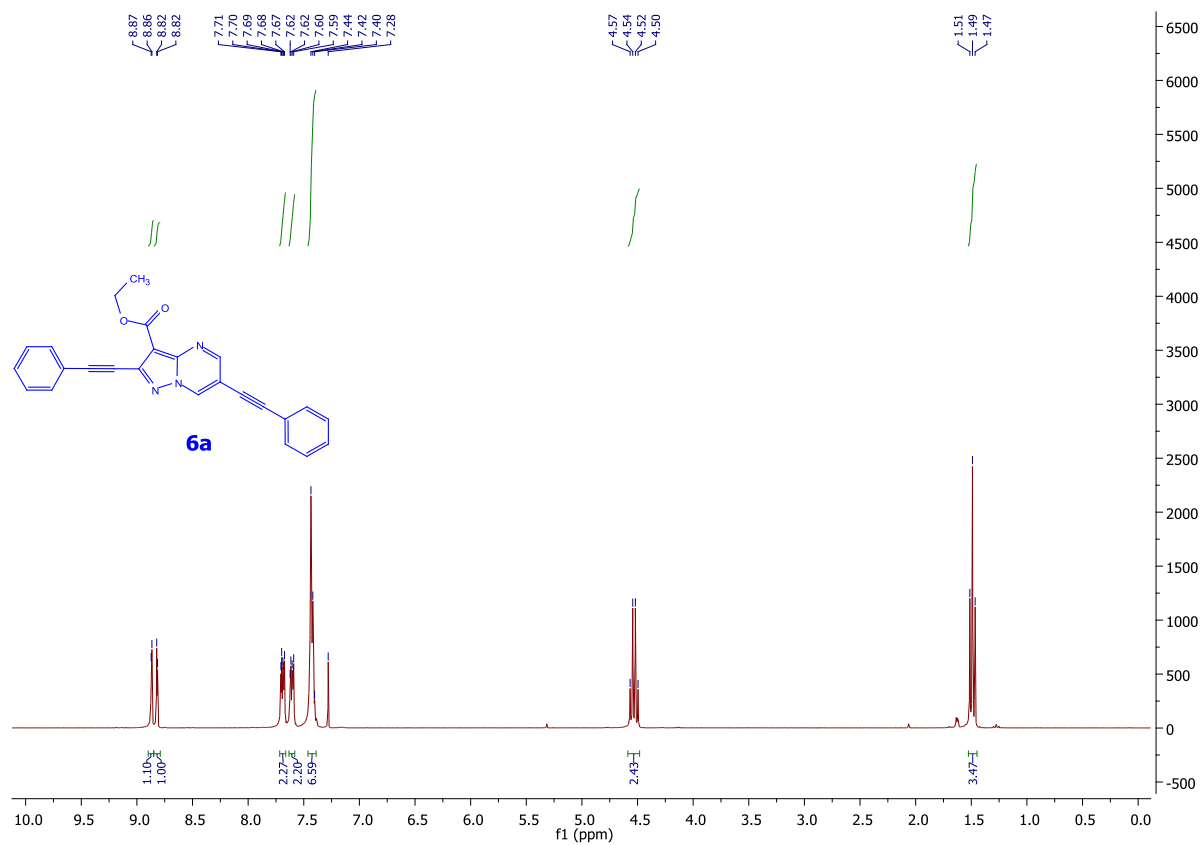


^{13}C NMR (75 MHz, CDCl_3)

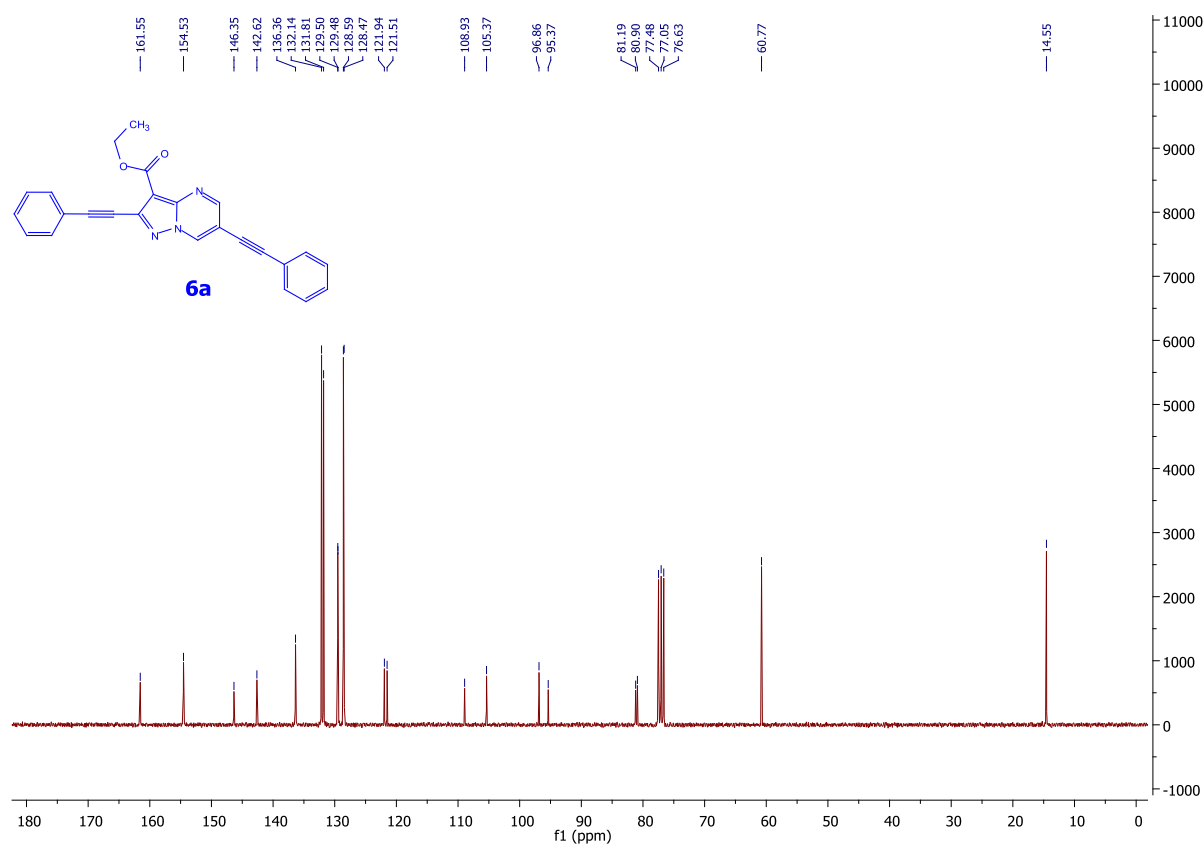


Ethyl 2,6-bis(phenylethynyl)pyrazolo[1,5-a]pyrimidine-3-carboxylate (6a)

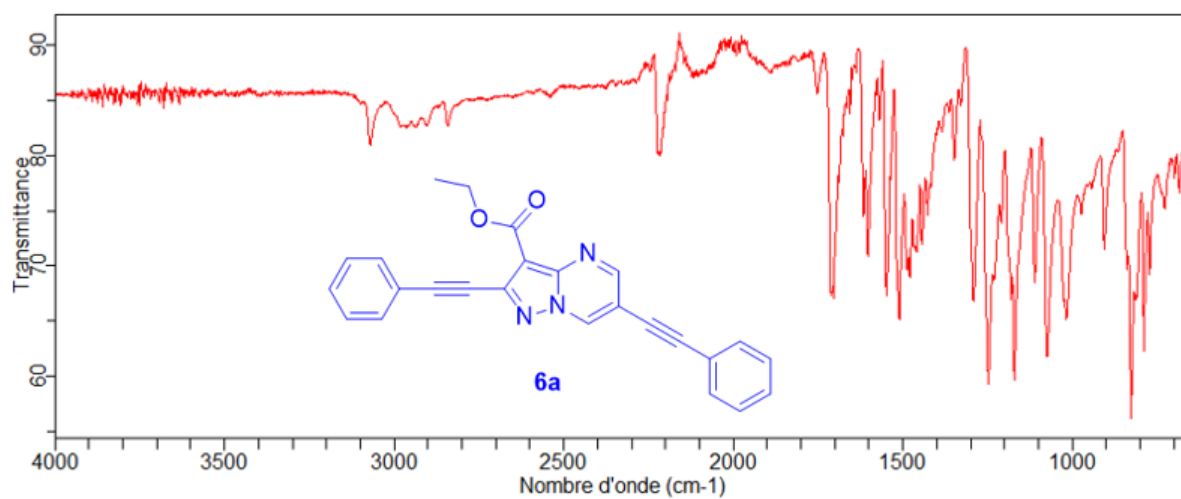
¹H NMR (300 MHz, CDCl₃)



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

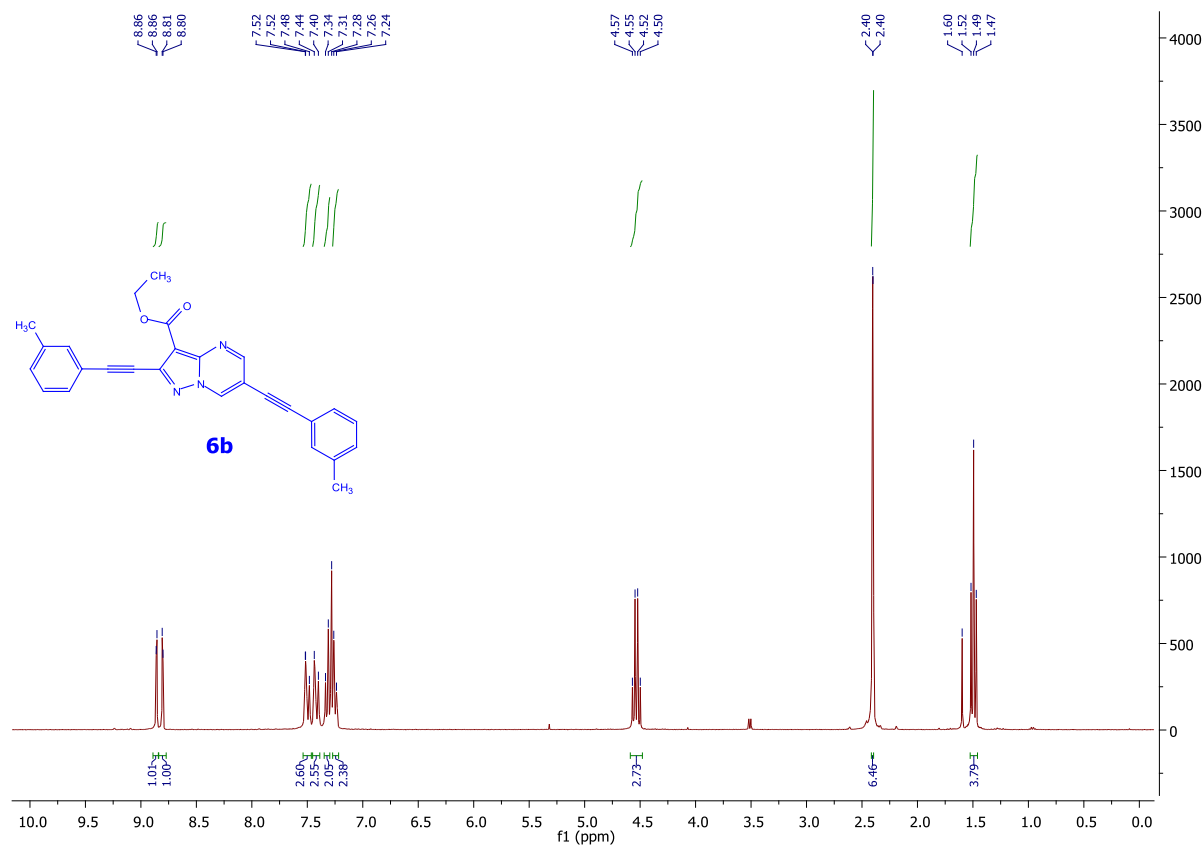


IR

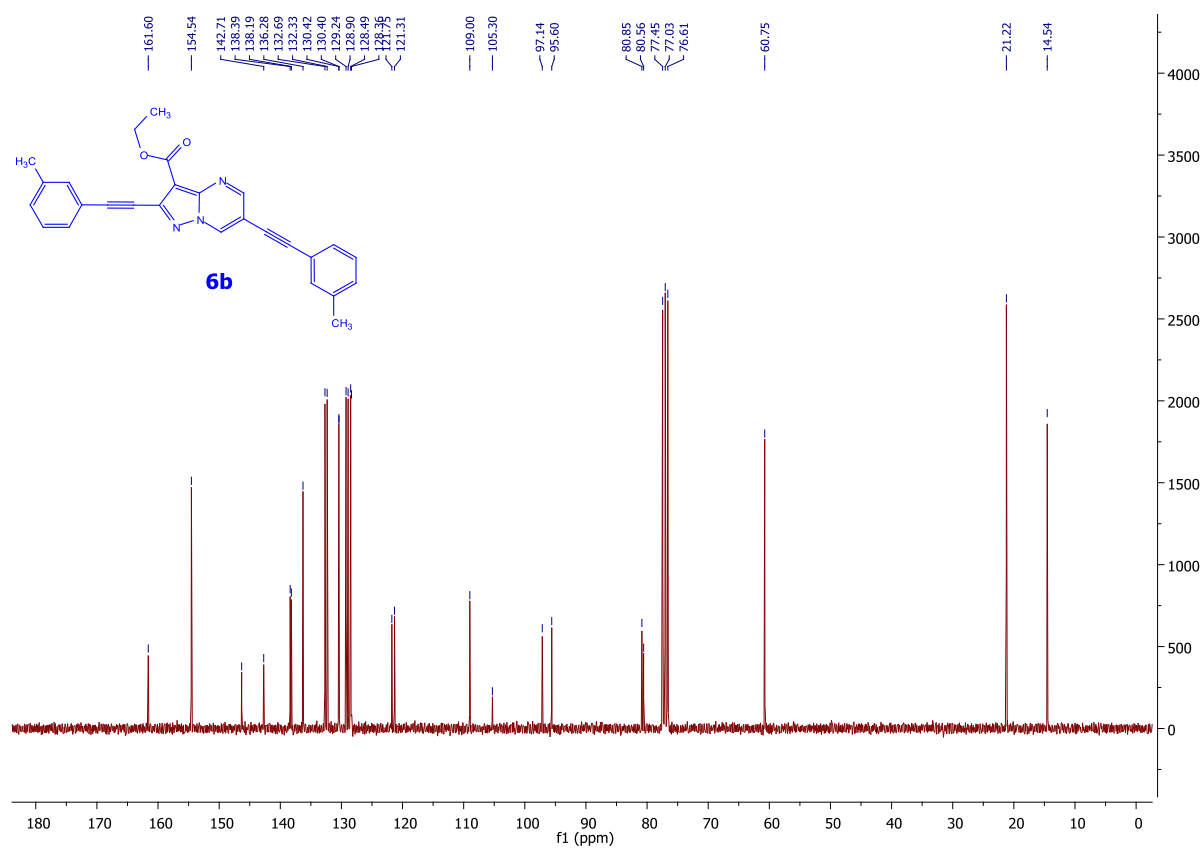


Ethyl 2,6-bis(*m*-tolylethynyl)pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (6b**)**

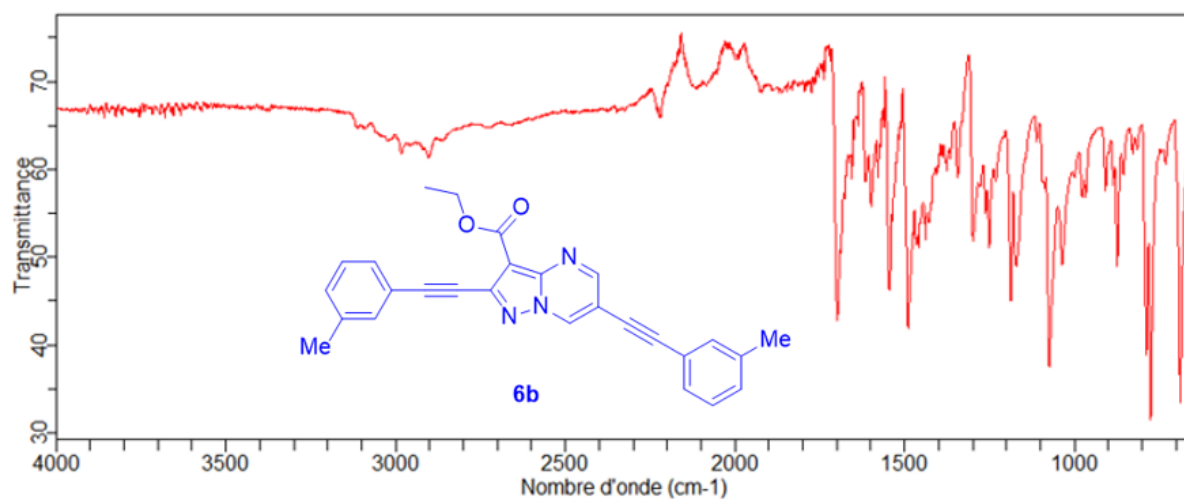
^1H NMR (300 MHz, CDCl_3)



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

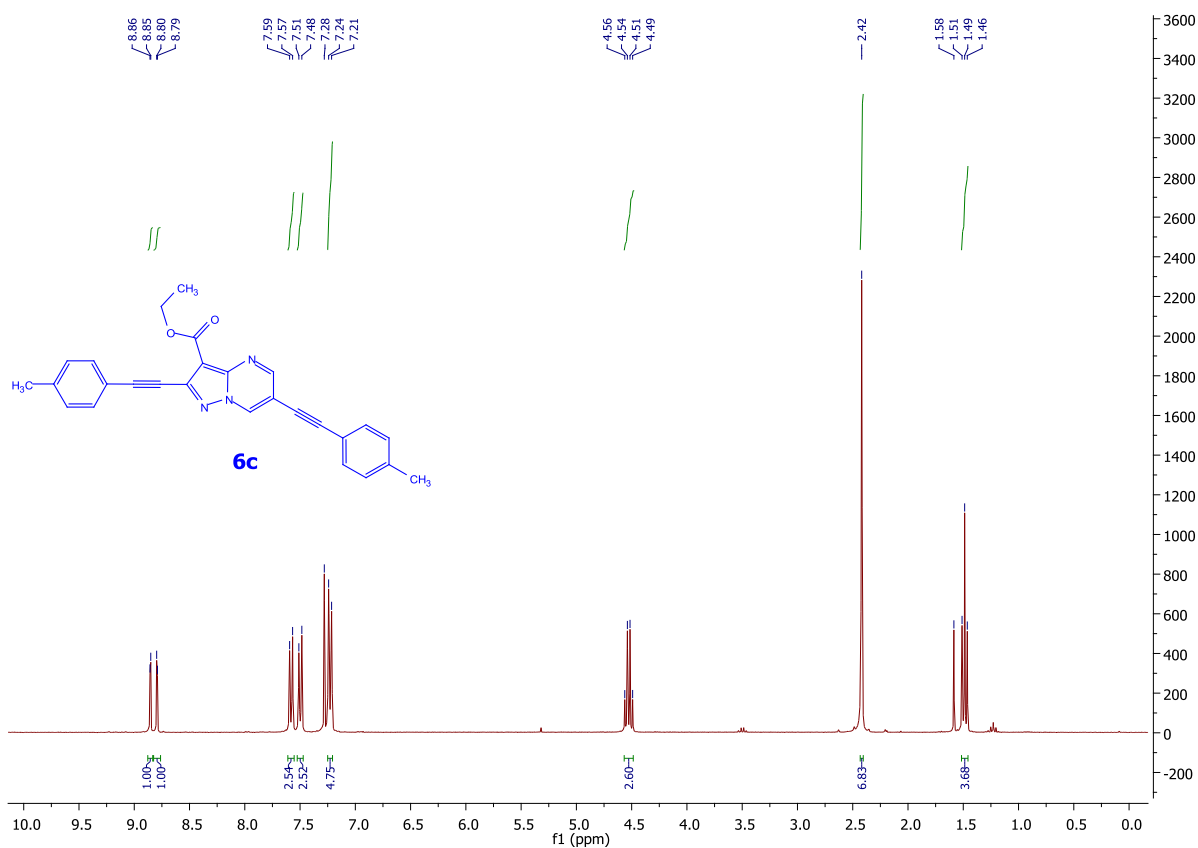


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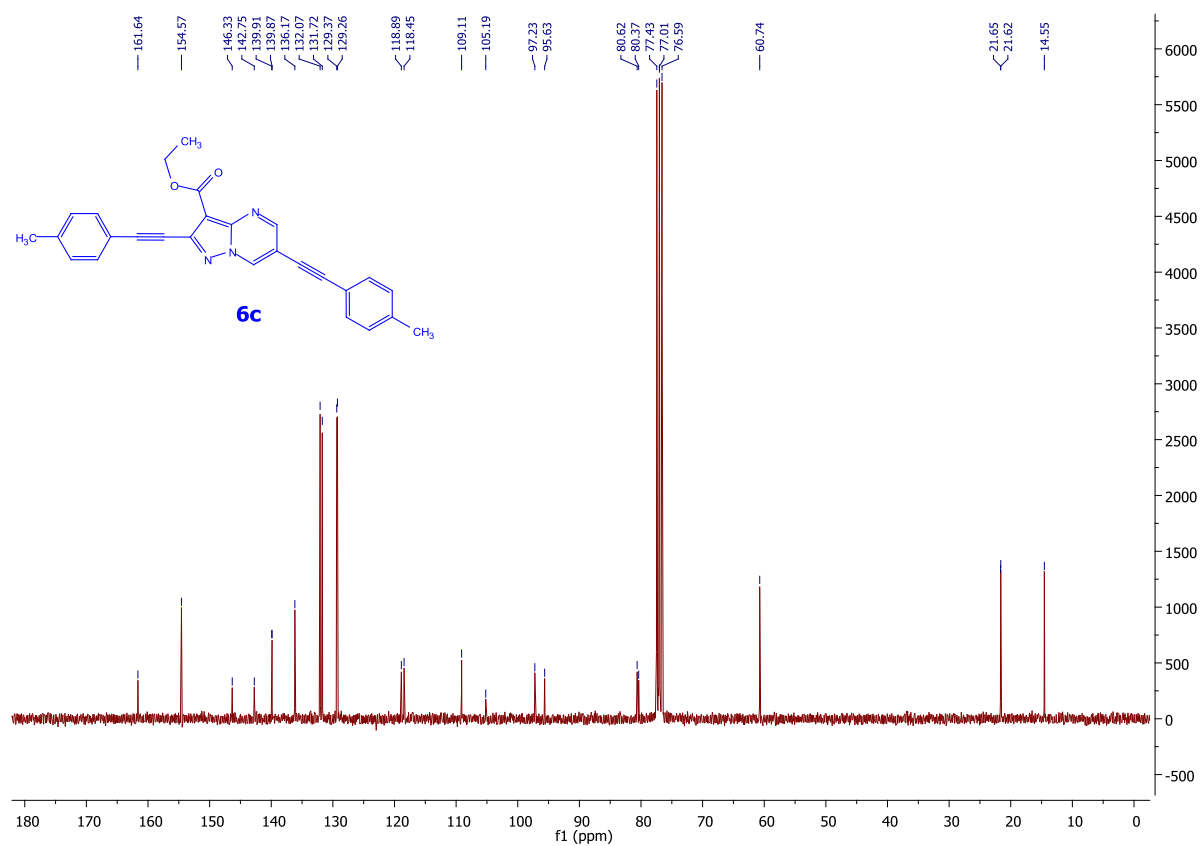


Ethyl 2,6-bis(*p*-tolylethynyl)pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (**6c**)

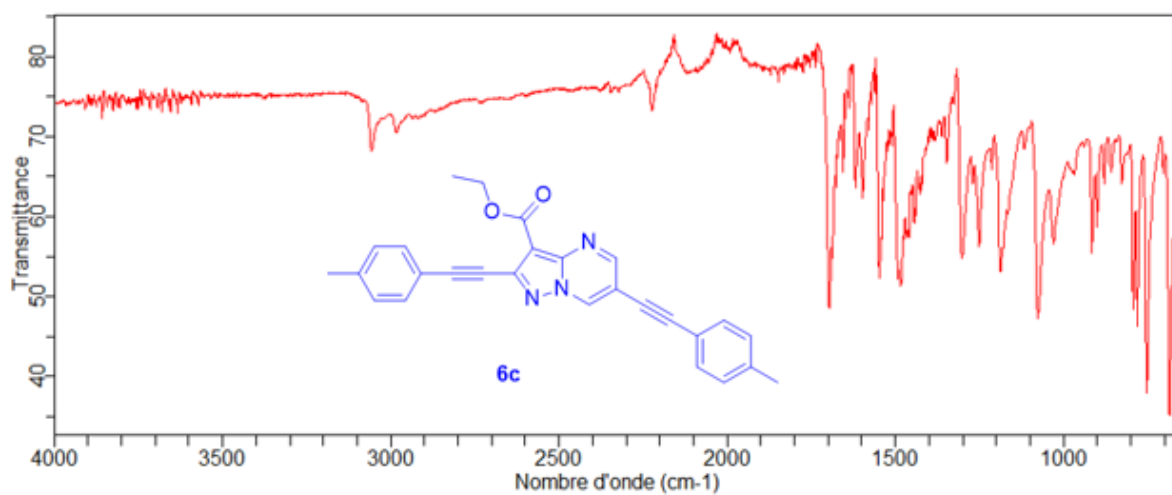
¹H NMR (300 MHz, CDCl₃)



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

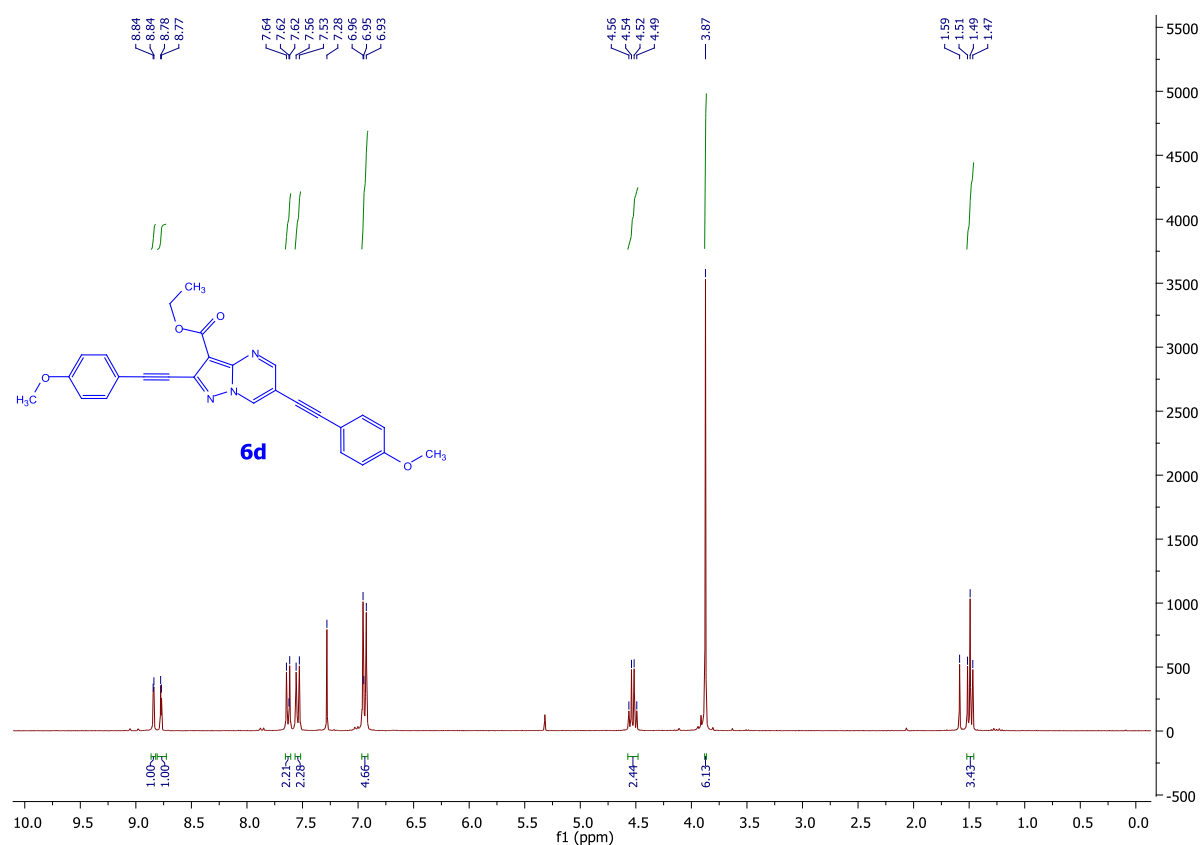


IR

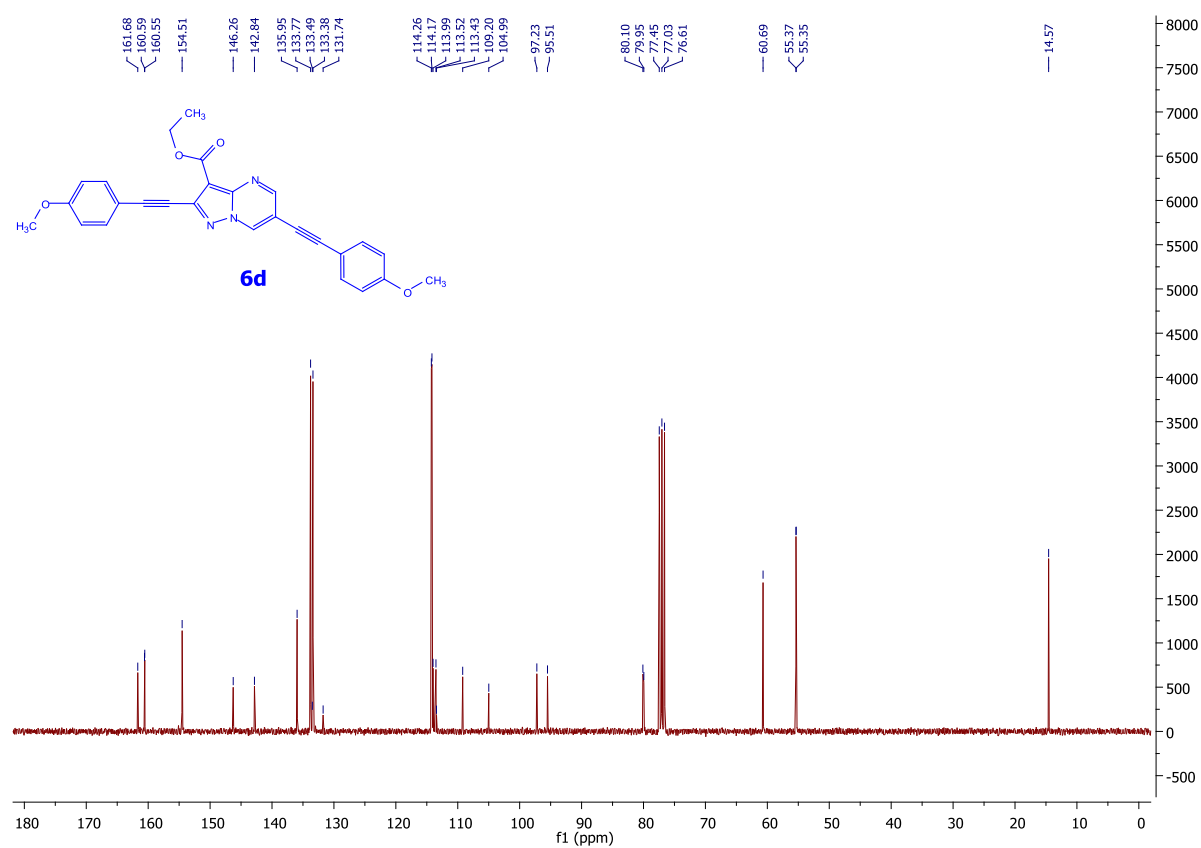


Ethyl 2,6-bis(4-methoxyphenyl)ethynylpyrazolo[1,5-*a*]pyrimidine-3-carboxylate (6d**)**

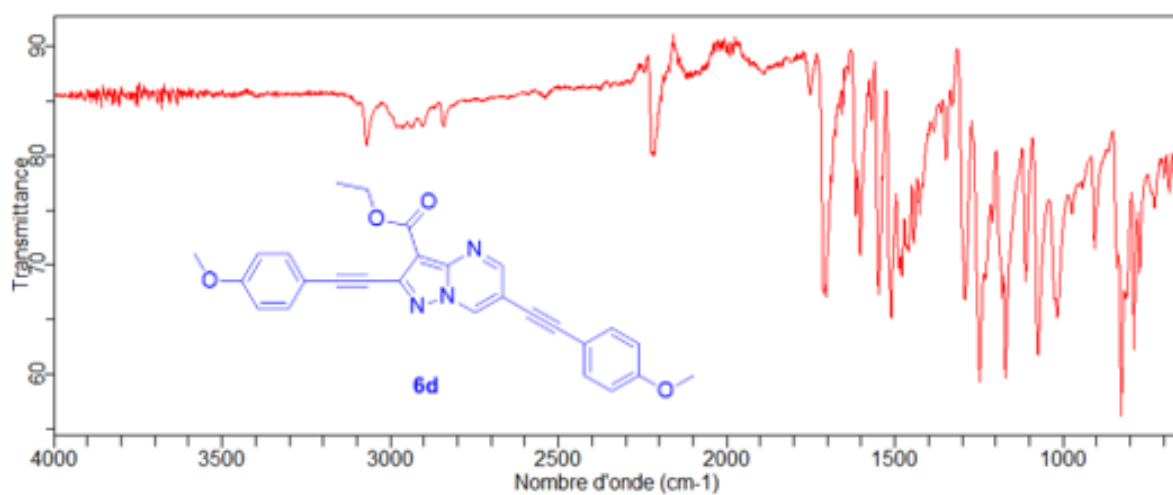
^1H NMR (300 MHz, CDCl_3)



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

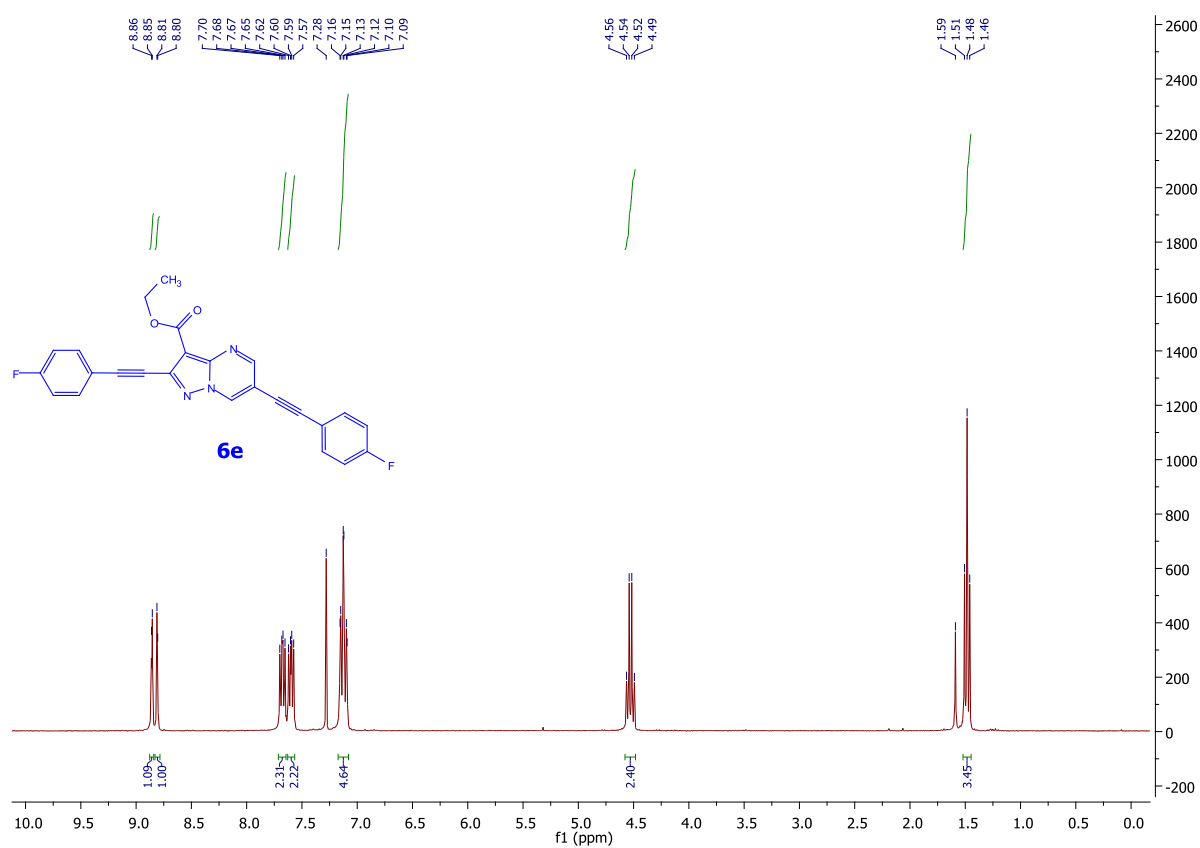


IR

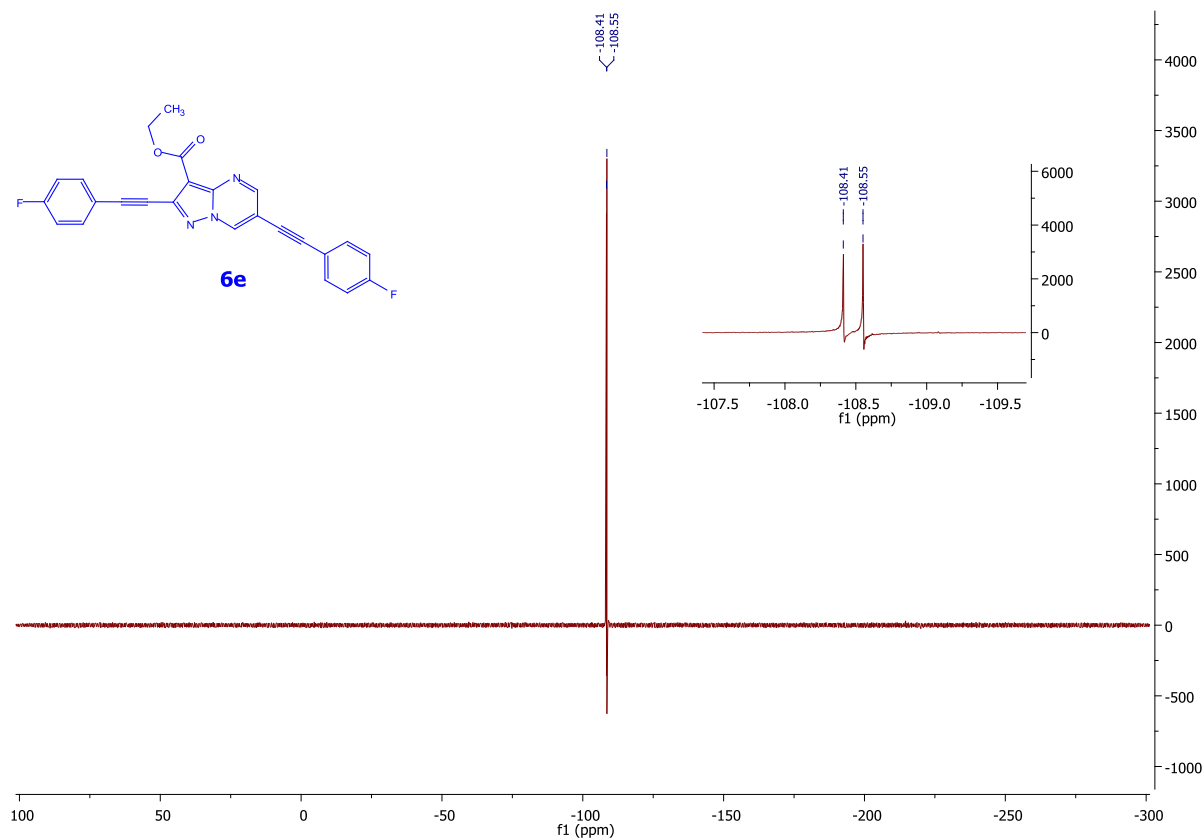


Ethyl 2,6-bis(4-fluorophenyl)ethynylpyrazolo[1,5-*a*]pyrimidine-3-carboxylate (**6e**)

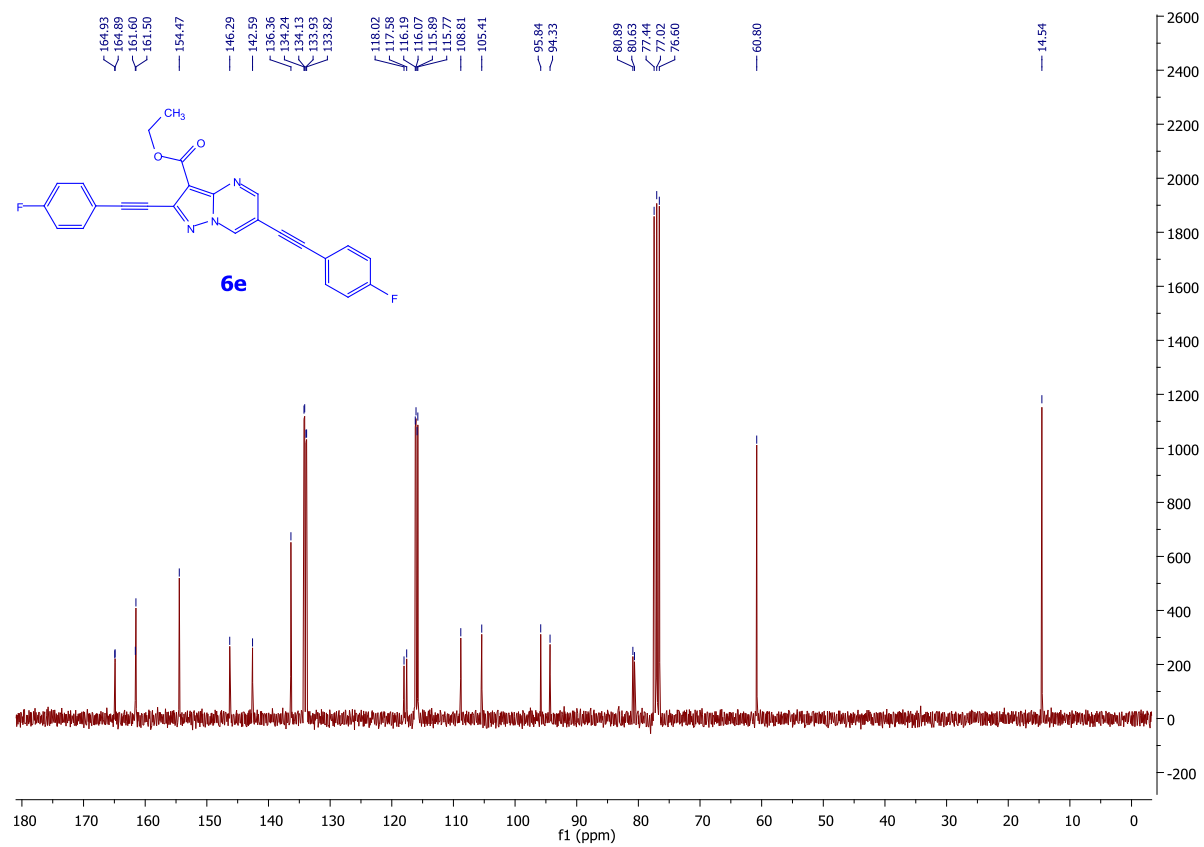
¹H NMR (300 MHz, CDCl₃)



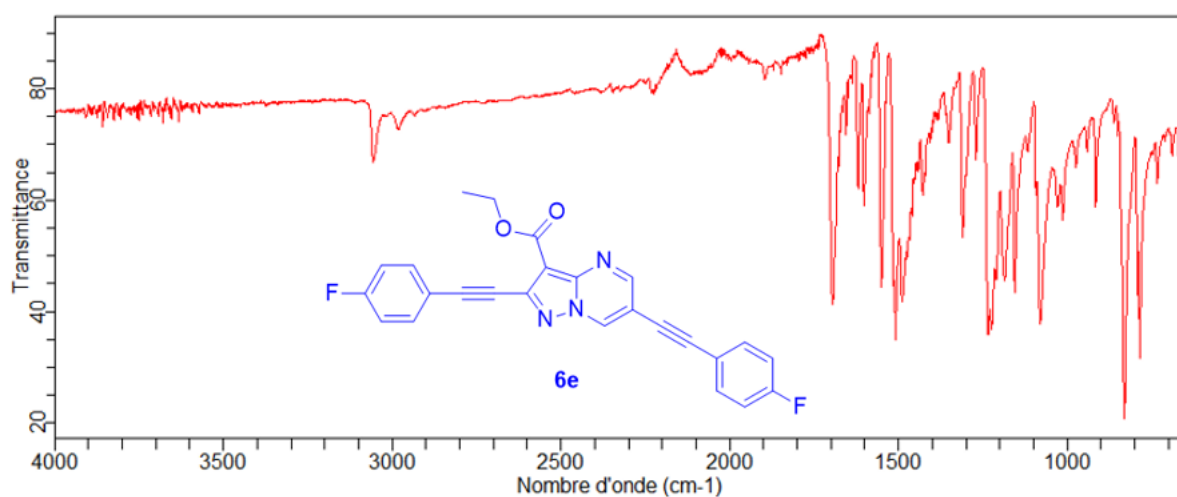
^{19}F NMR (282 MHz, CDCl_3)



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

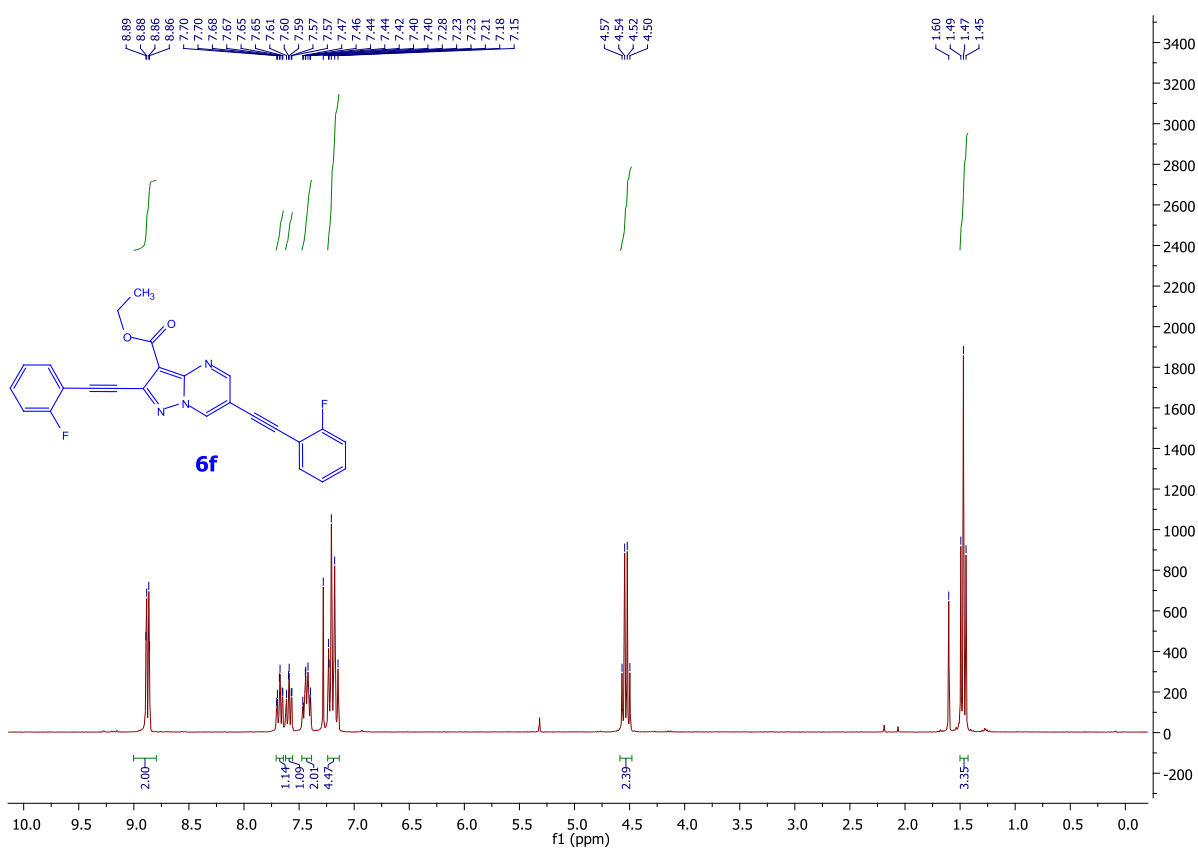


IR

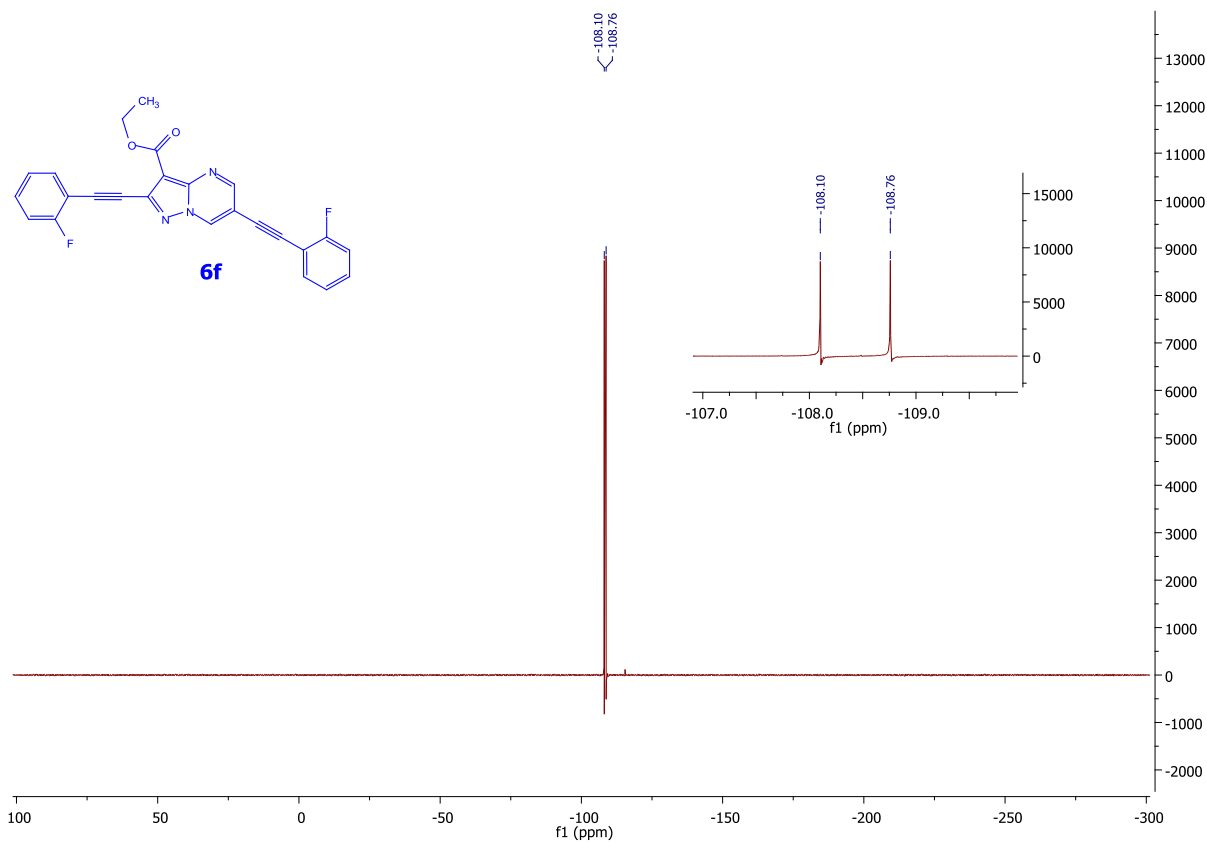


Ethyl 2,6-bis(2-fluorophenyl)ethynylpyrazolo[1,5-a]pyrimidine-3-carboxylate (6f**)**

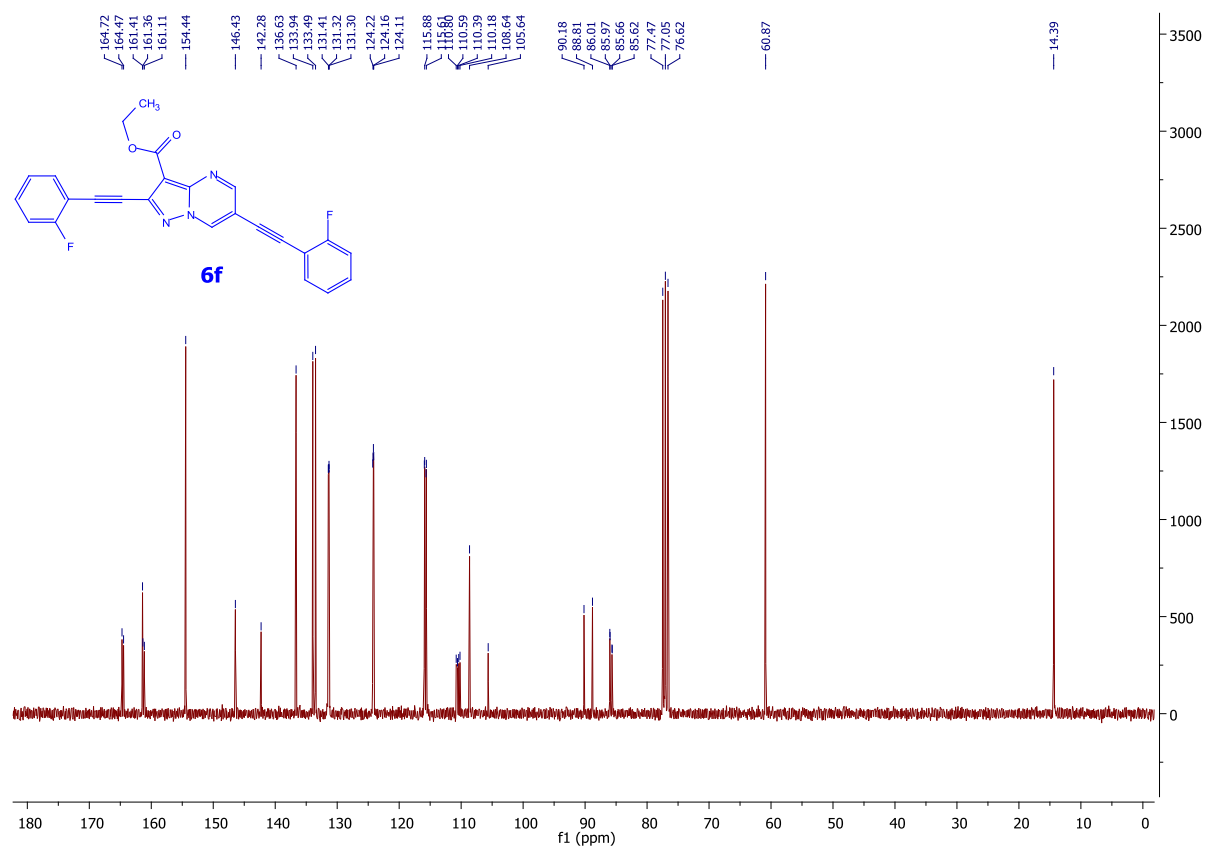
^1H NMR (300 MHz, CDCl_3)

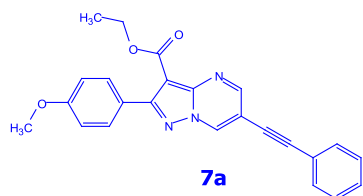


^{19}F NMR (282 MHz, CDCl_3)

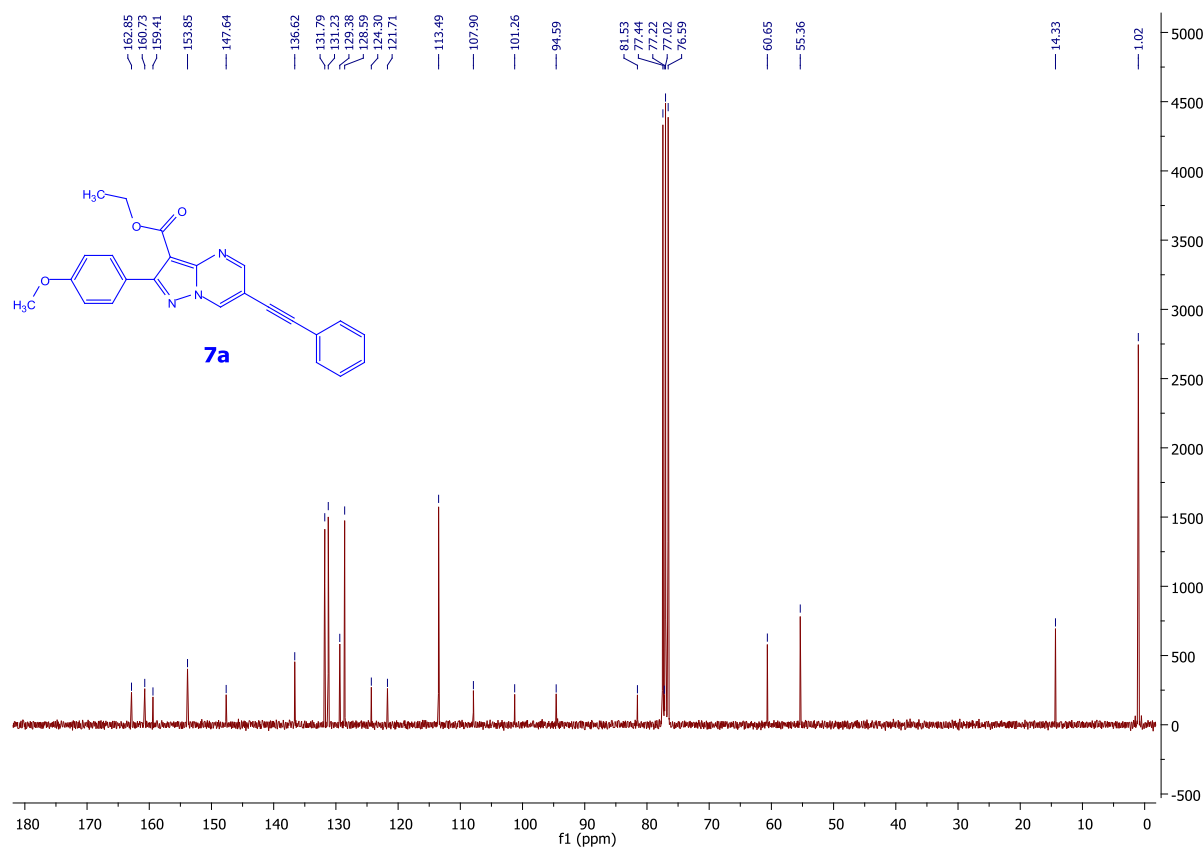


^{13}C NMR (75 MHz, CDCl_3)

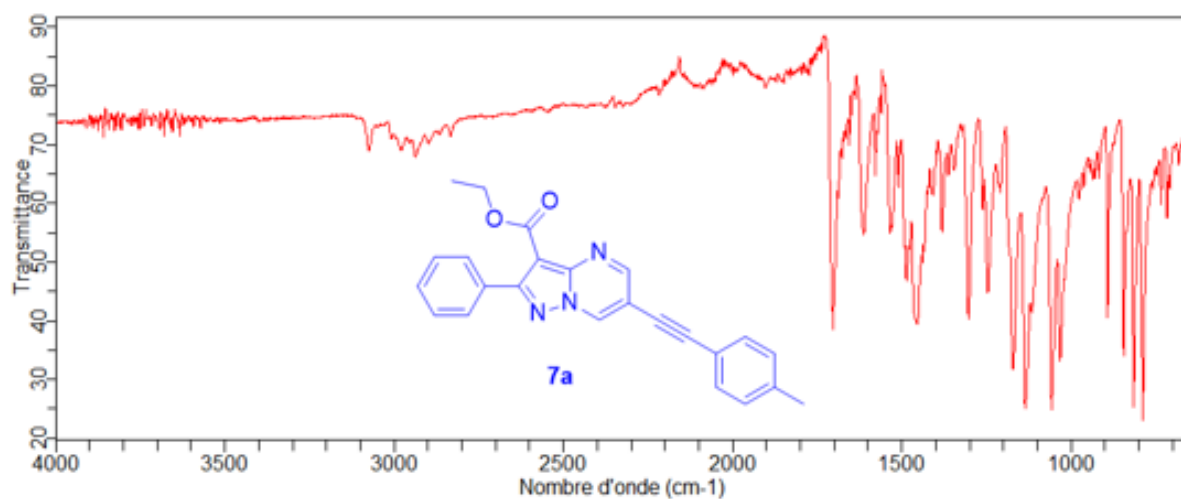


¹H NMR (300 MHz, CDCl₃)

2.85
0.73
9.41
3.85
7.64

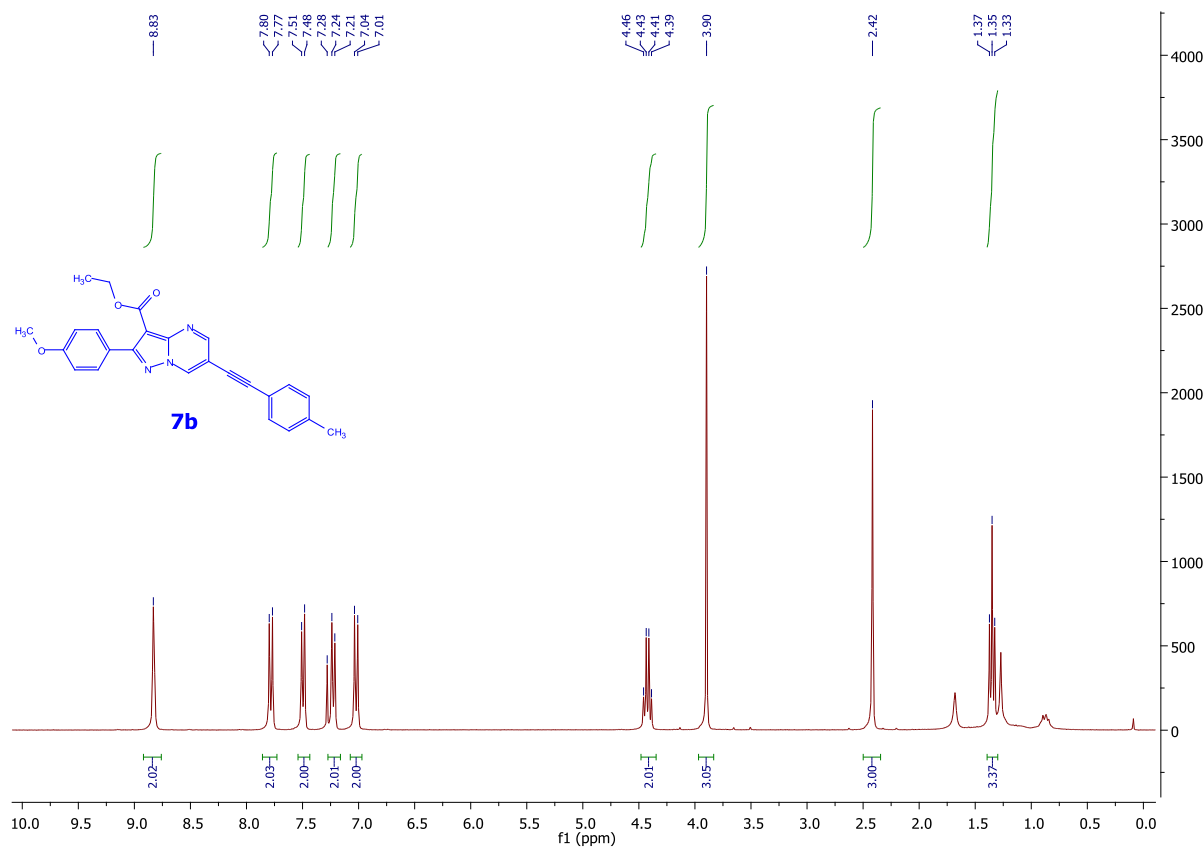


IR

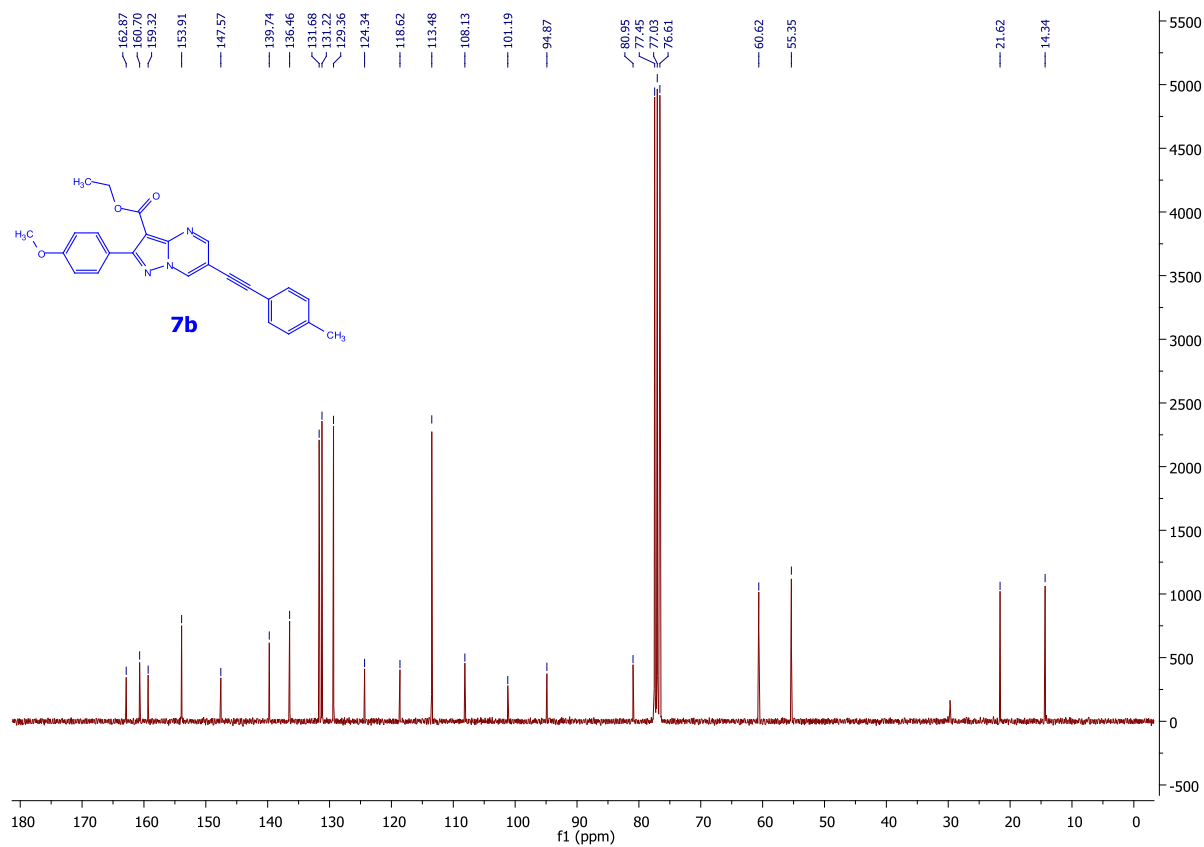


Ethyl 2-(4-methoxyphenyl)-6-(*p*-tolylethynyl)pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (7b**)**

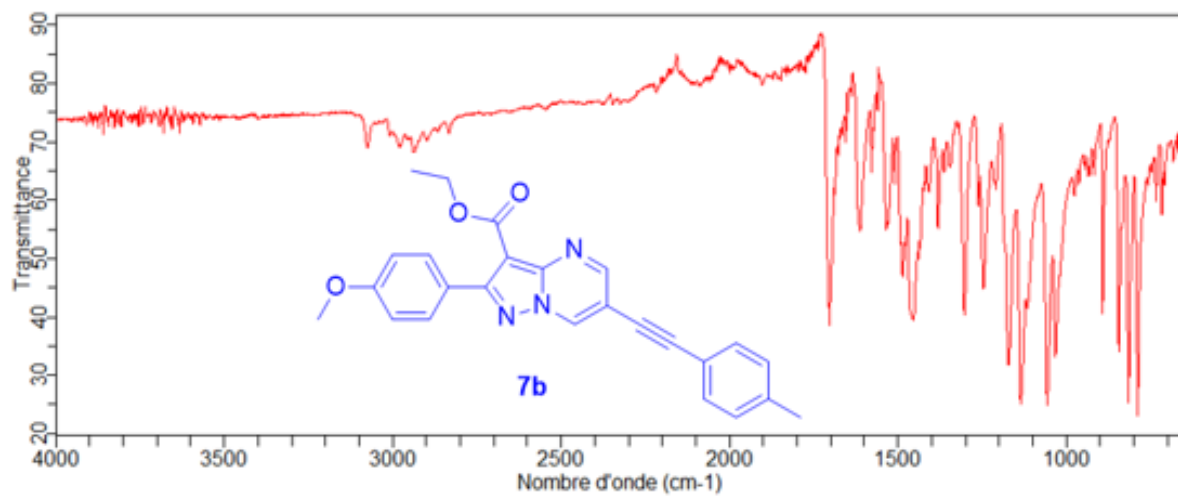
¹H NMR (300 MHz, CDCl₃)



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

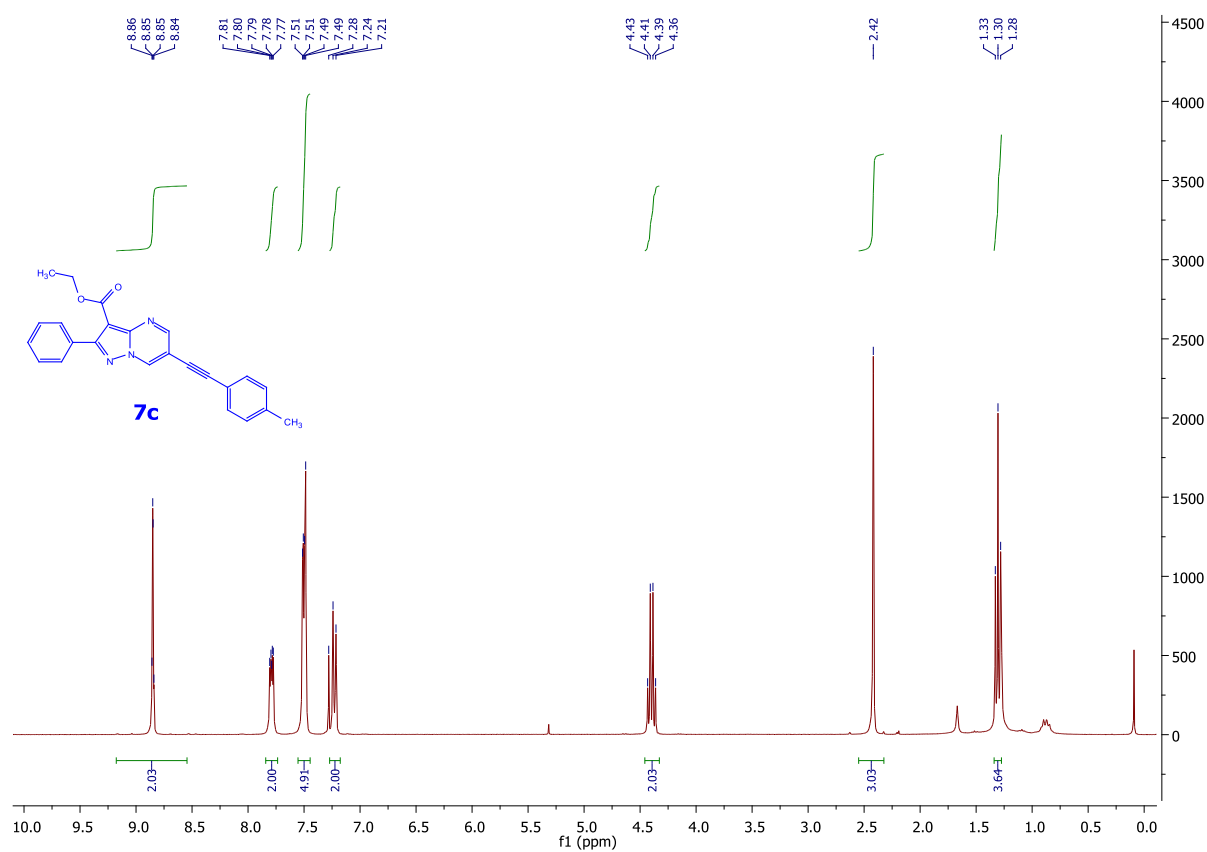


IR

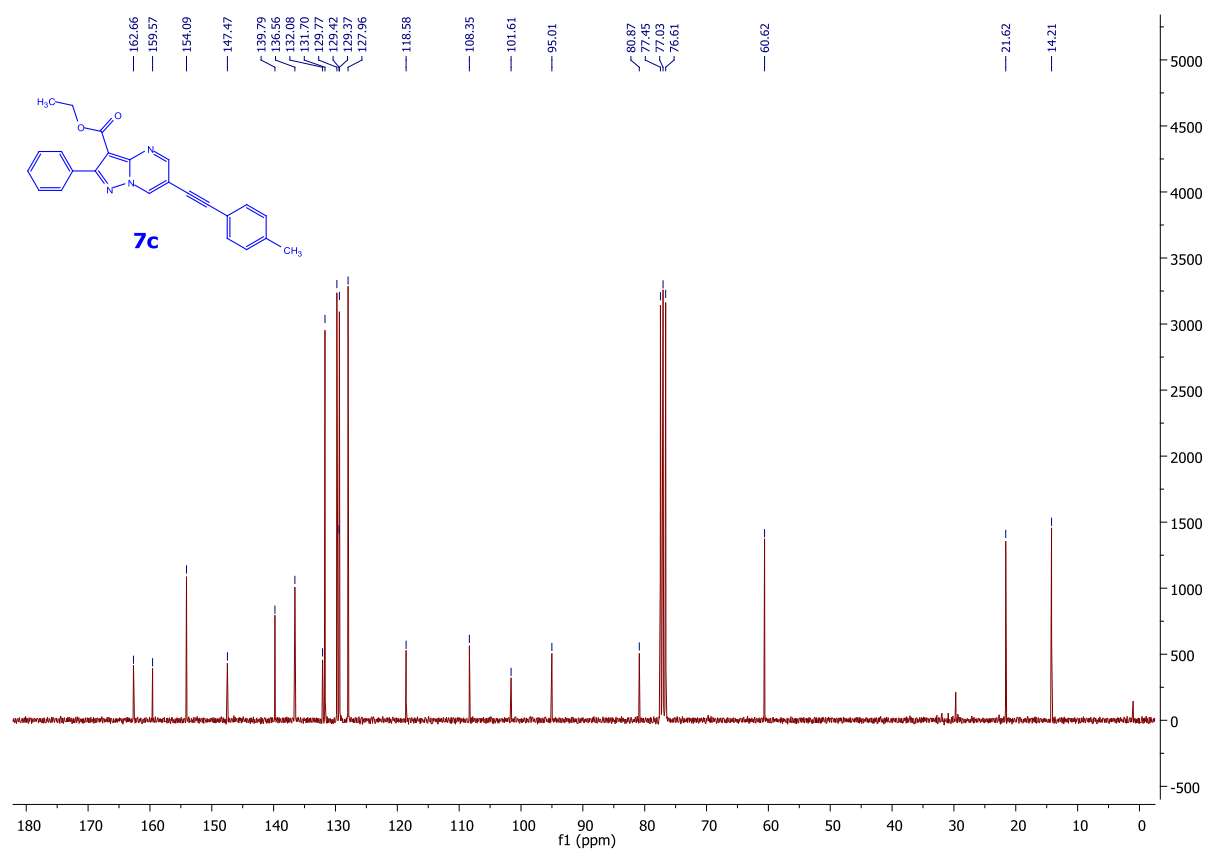


Ethyl 2-phenyl-6-(*p*-tolylethynyl)pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (7c**)**

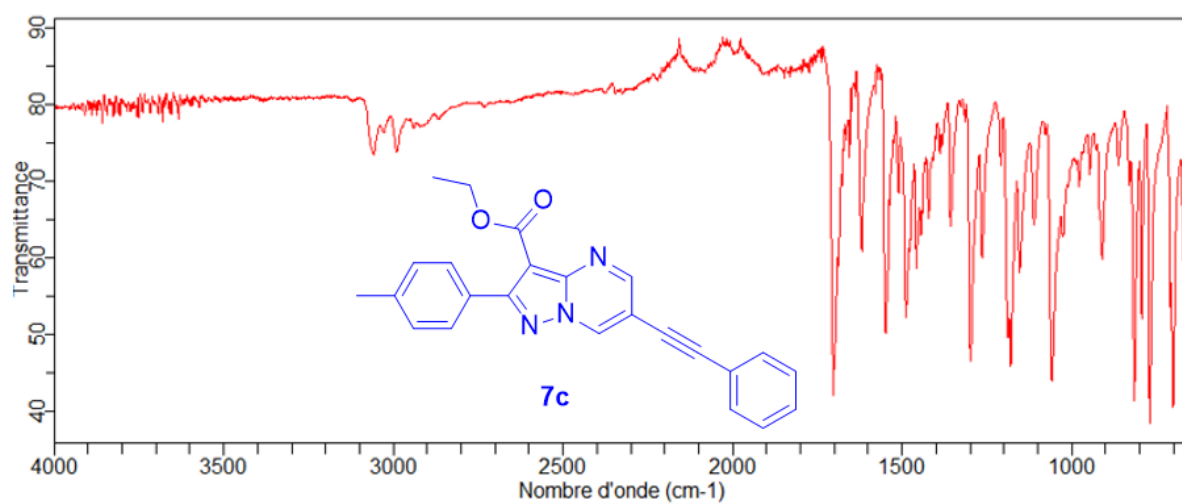
^1H NMR (300 MHz, CDCl_3)



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

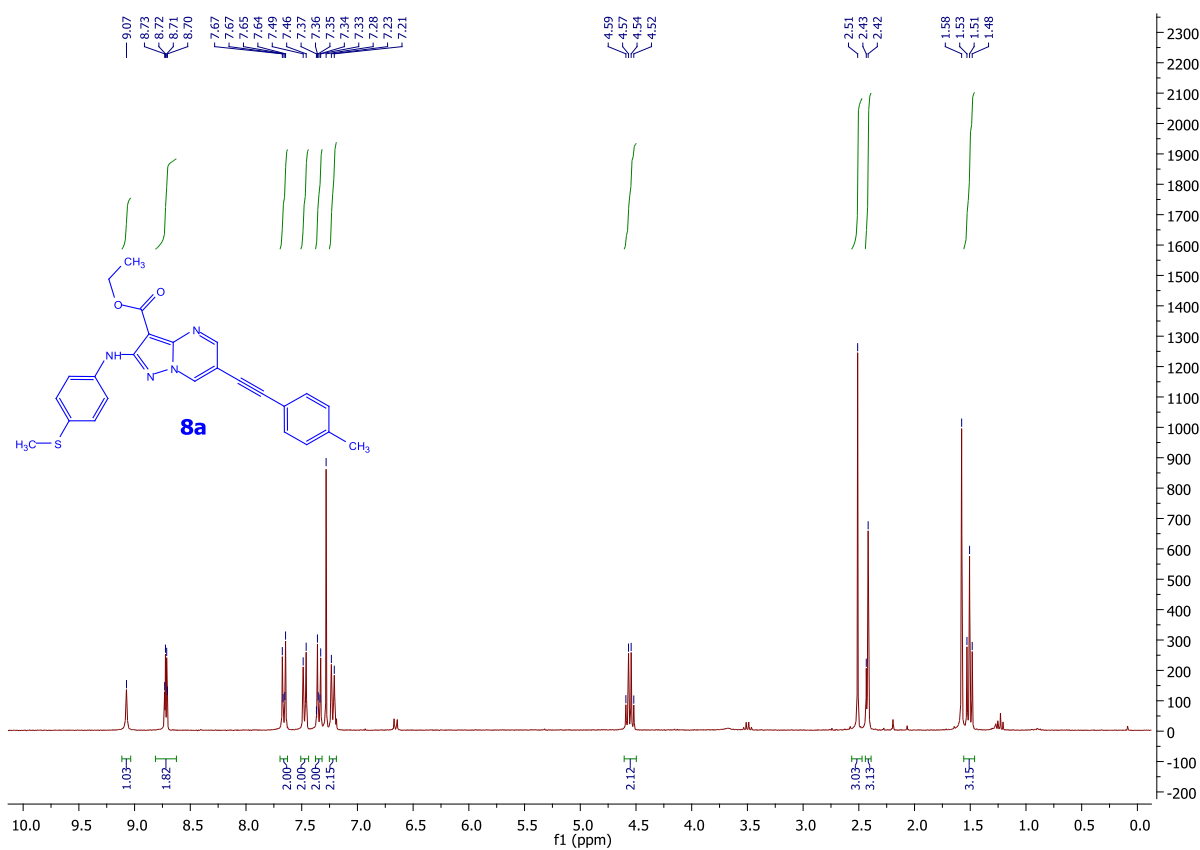


IR

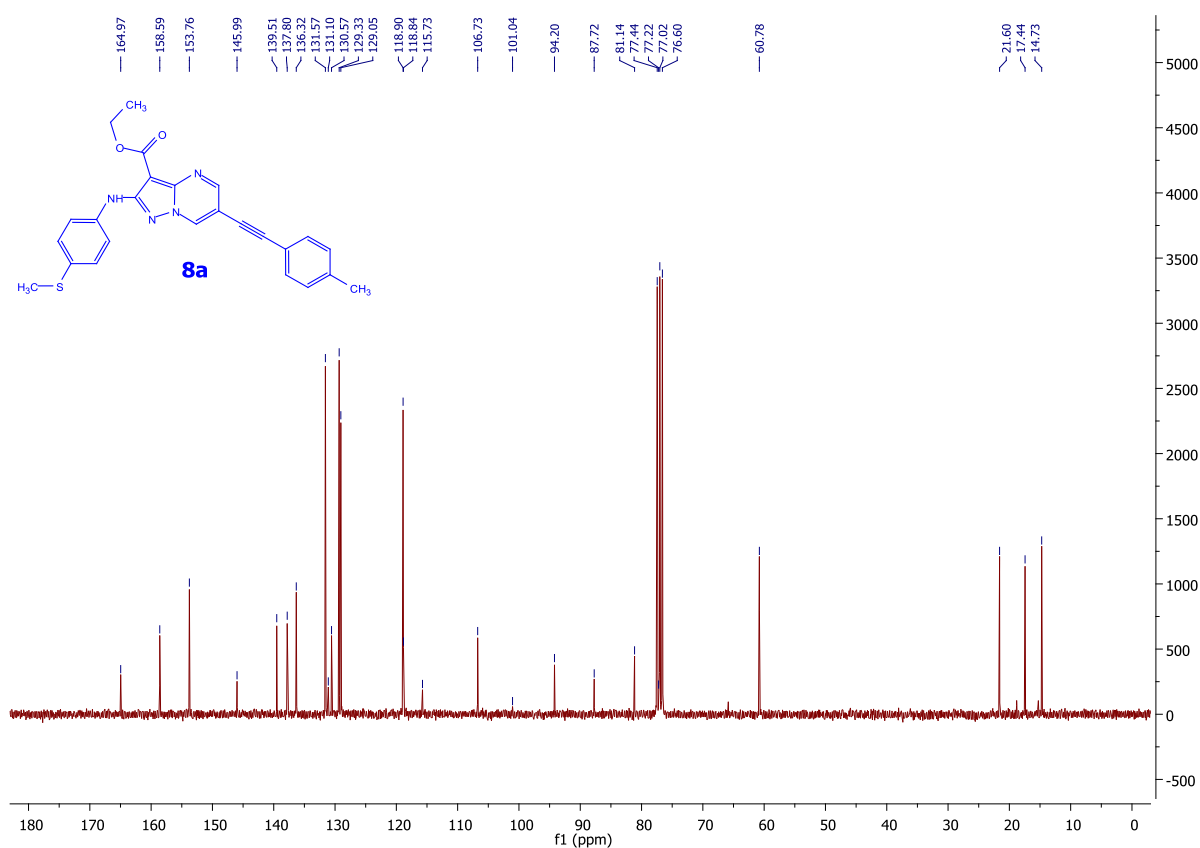


Ethyl 2-[(4-(methylthio)phenyl)amino]-6-(*p*-tolylethynyl)pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (8a**)**

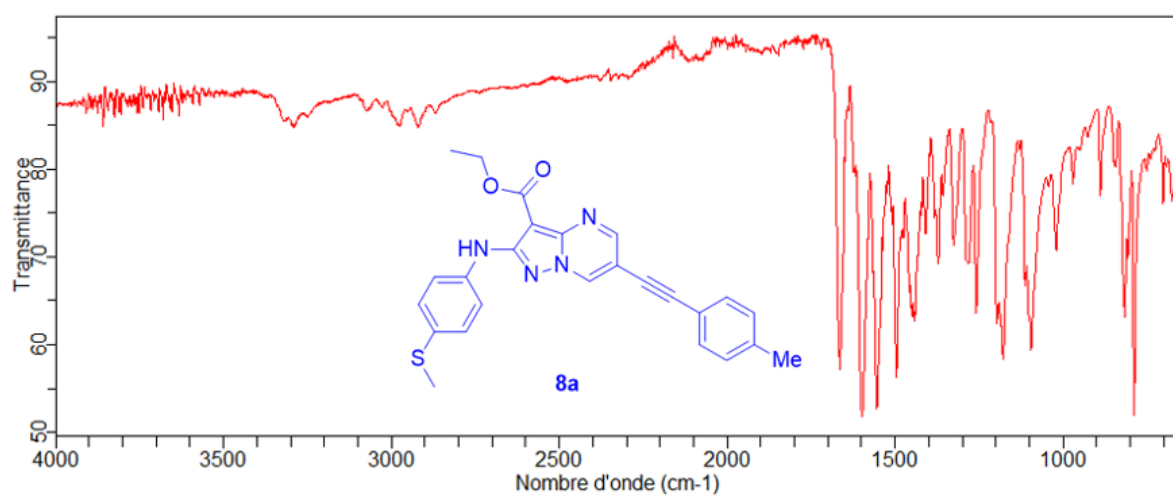
^1H NMR (300 MHz, CDCl_3)



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

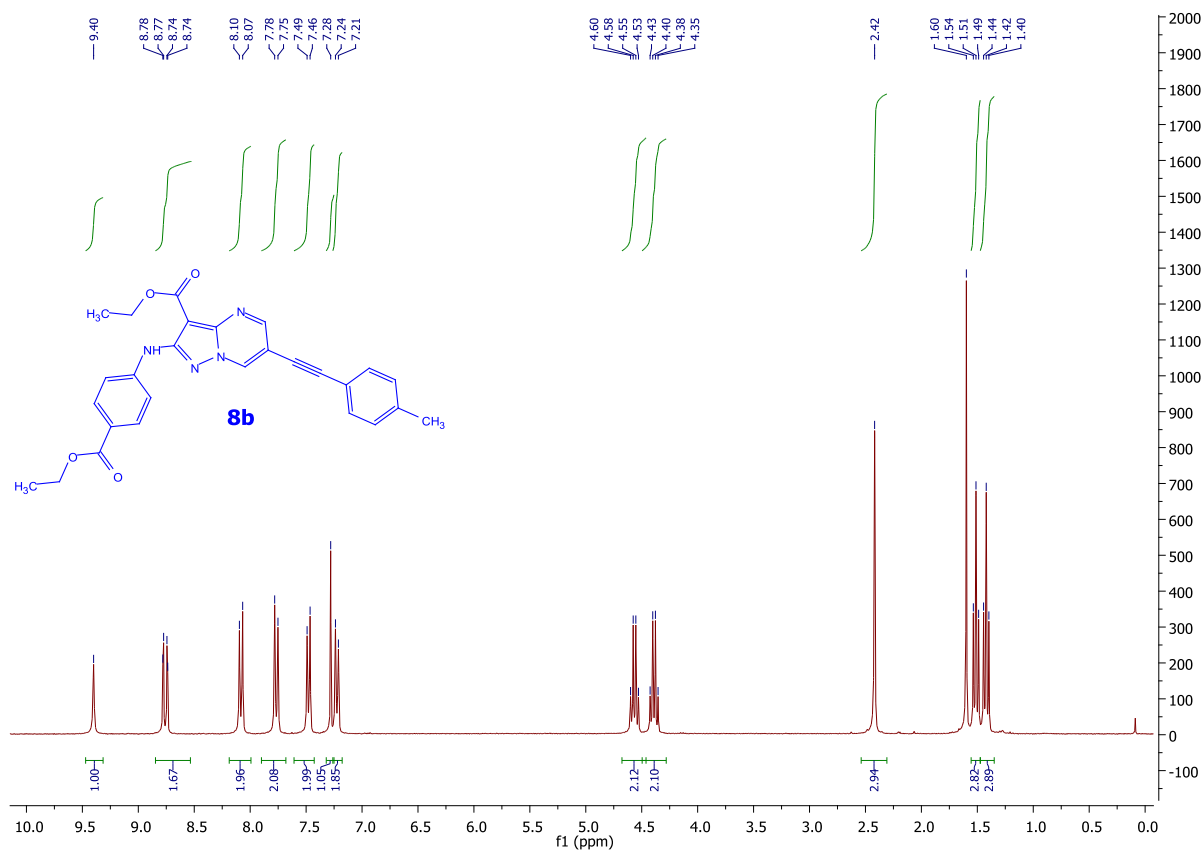


IR

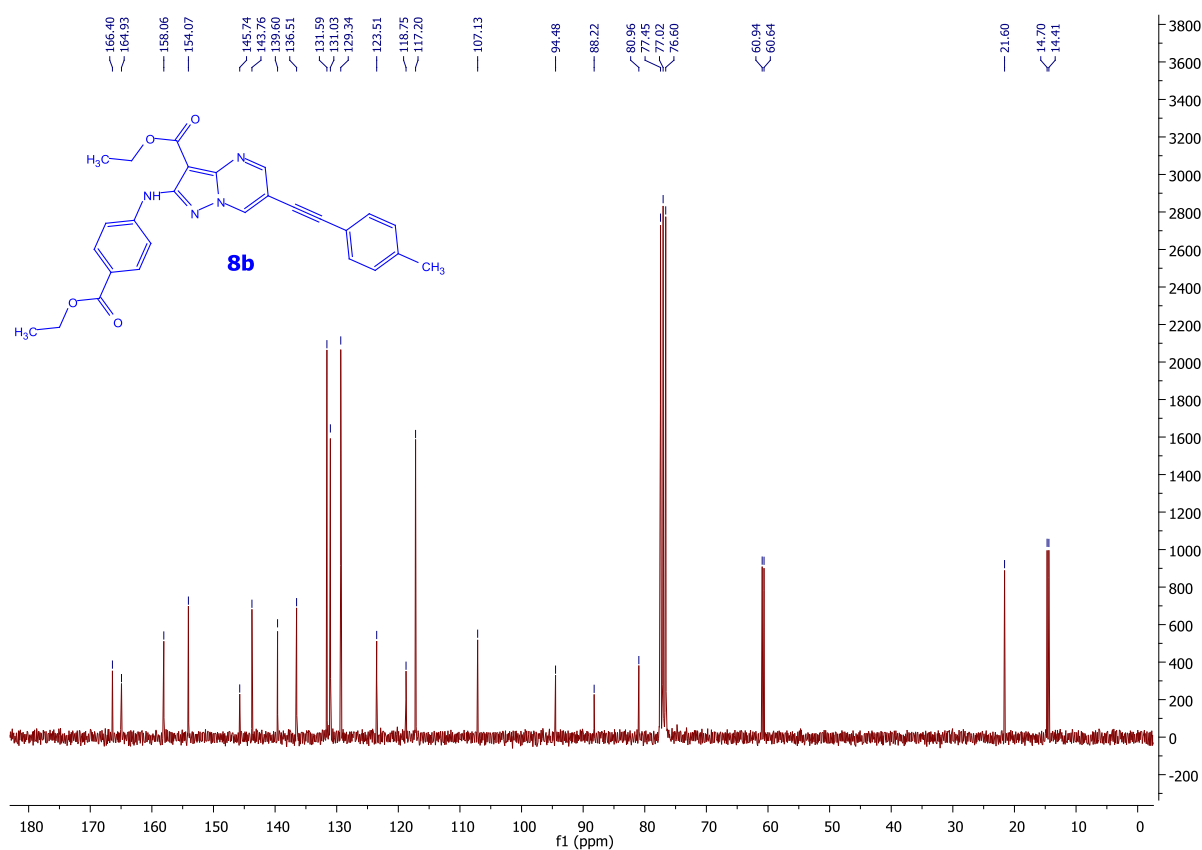


Ethyl 2-[(4-(ethoxycarbonyl)phenyl)amino]-6-(*p*-tolylethynyl)pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (8b**)**

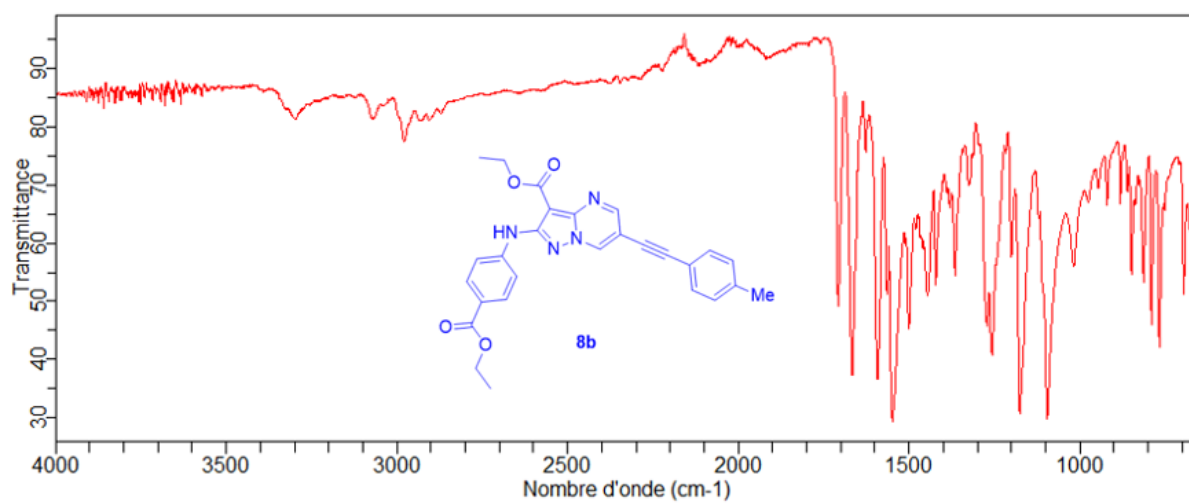
^1H NMR (300 MHz, CDCl_3)



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

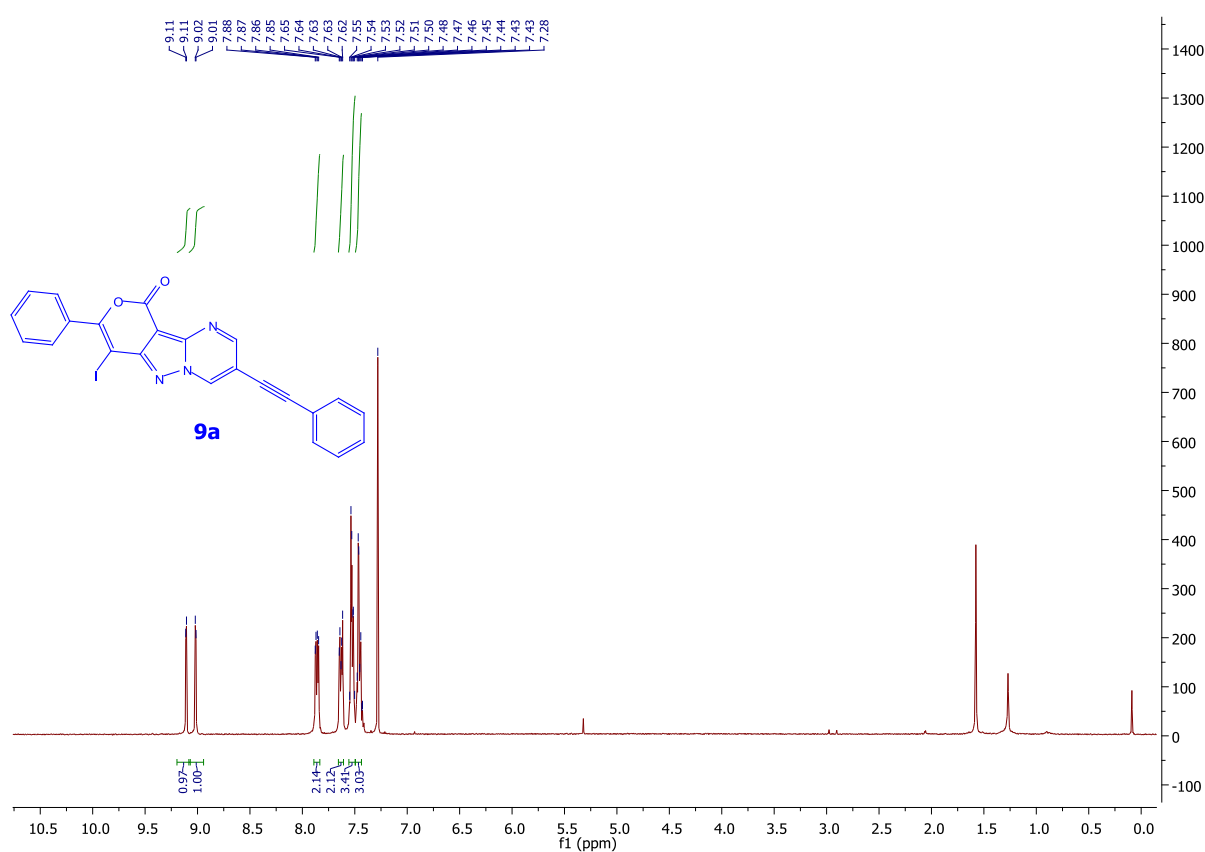


IR

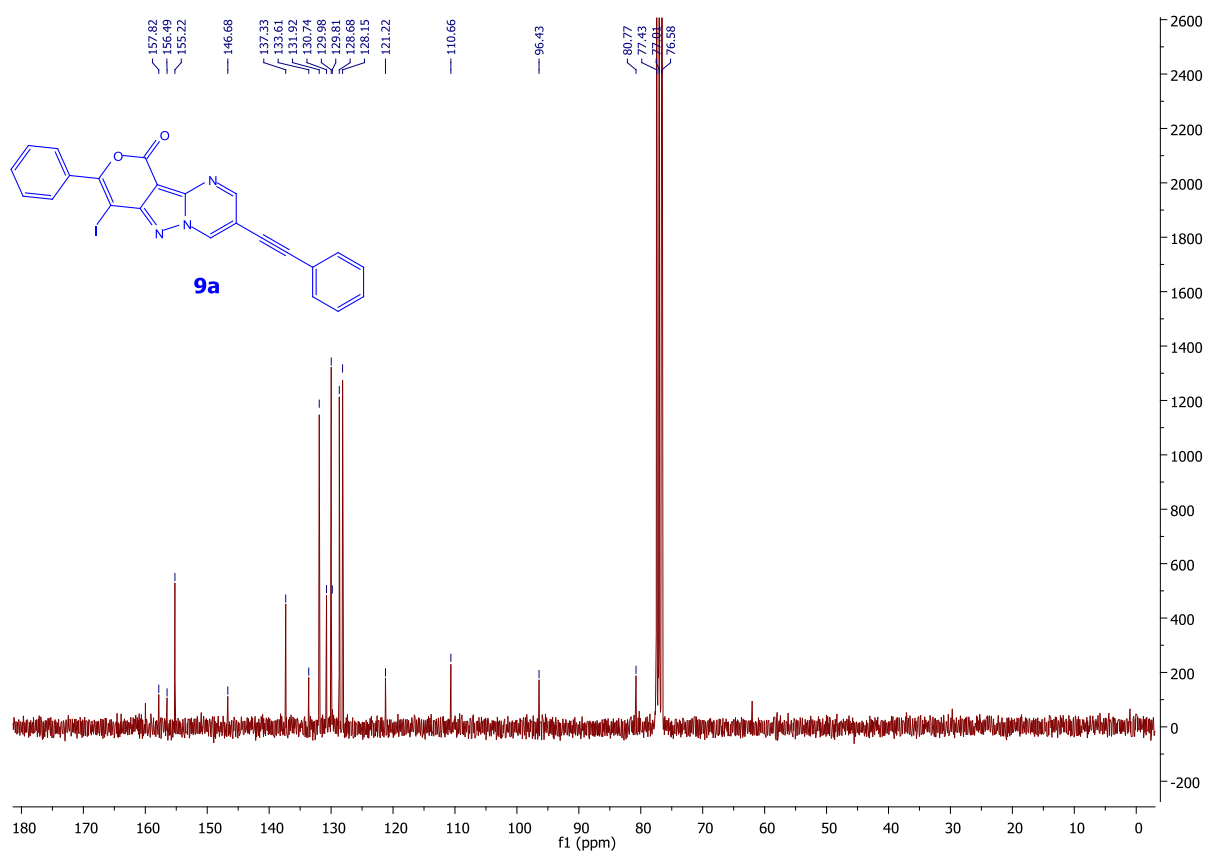


7-Iodo-8-phenyl-3-(phenylethynyl)-10H-pyrano[4',3':3,4]pyrazolo[1,5-a]pyrimidin-10-one (9a)

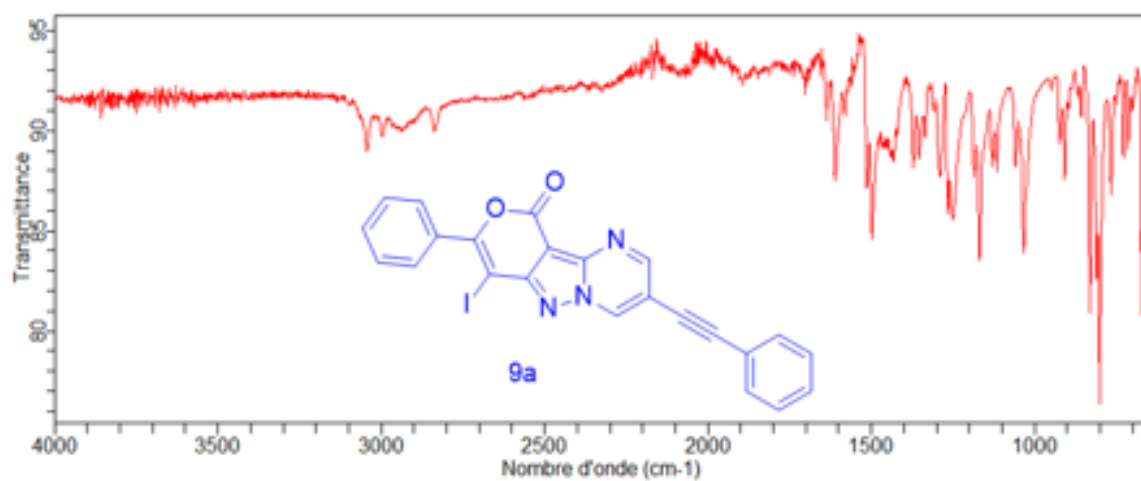
¹H NMR (300 MHz, CDCl₃)



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

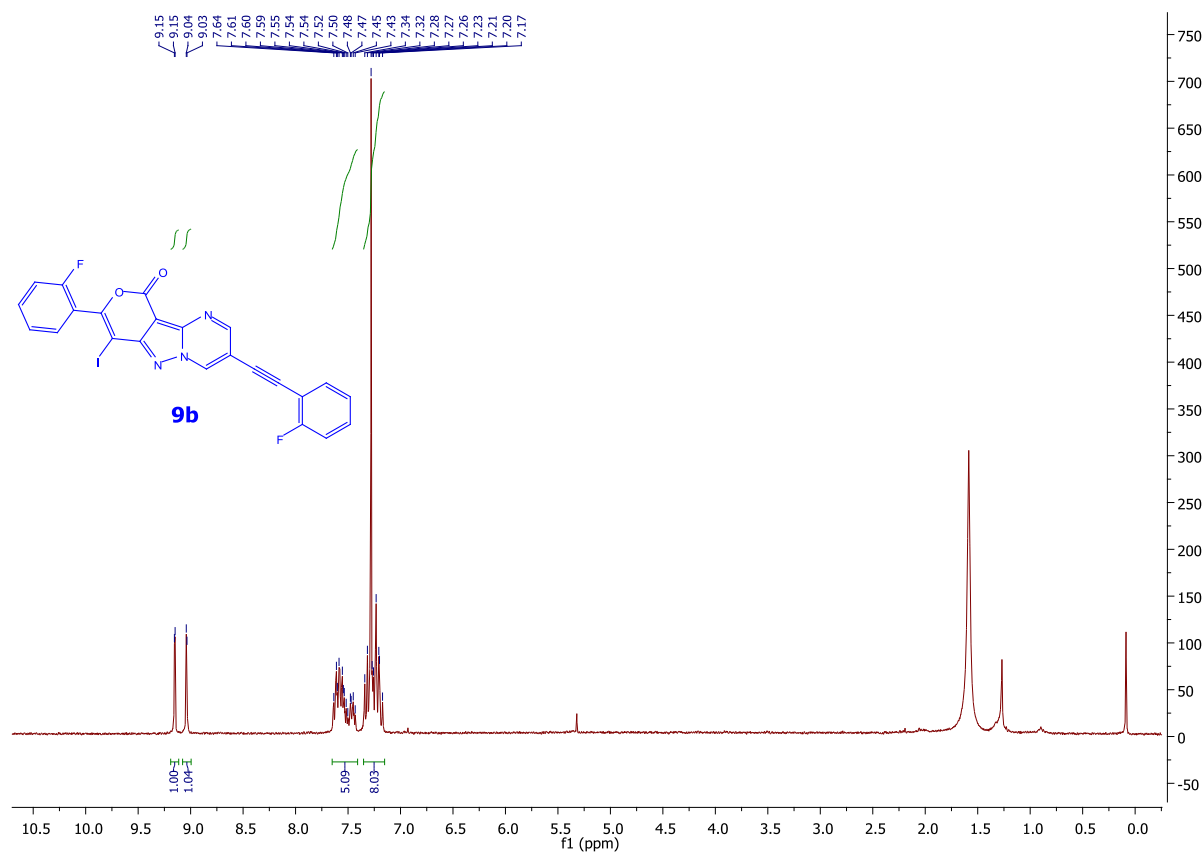


IR

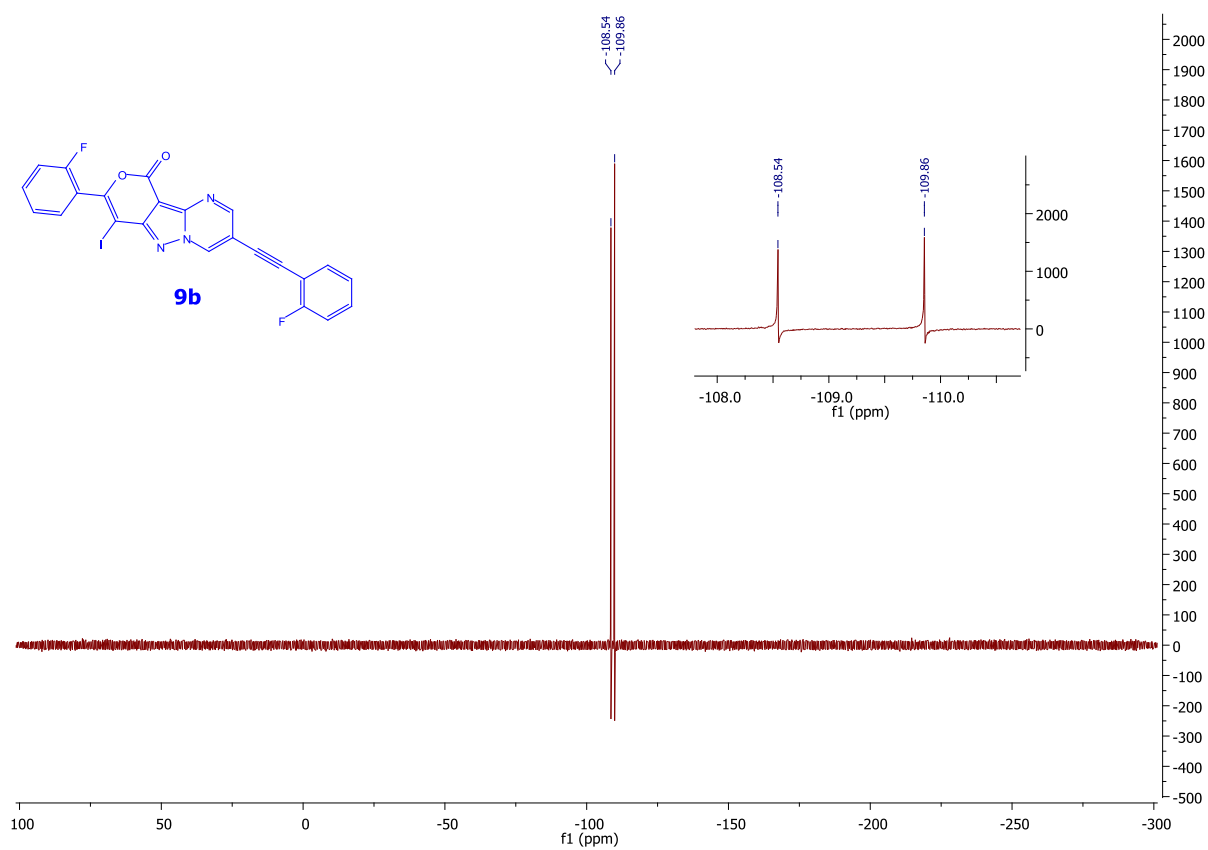


8-(2-Fluorophenyl)-3-[(2-fluorophenyl)ethynyl]-7-iodo-10H-pyrano[4',3':3,4]pyrazolo[1,5-a]pyrimidin-10-one
(9b)

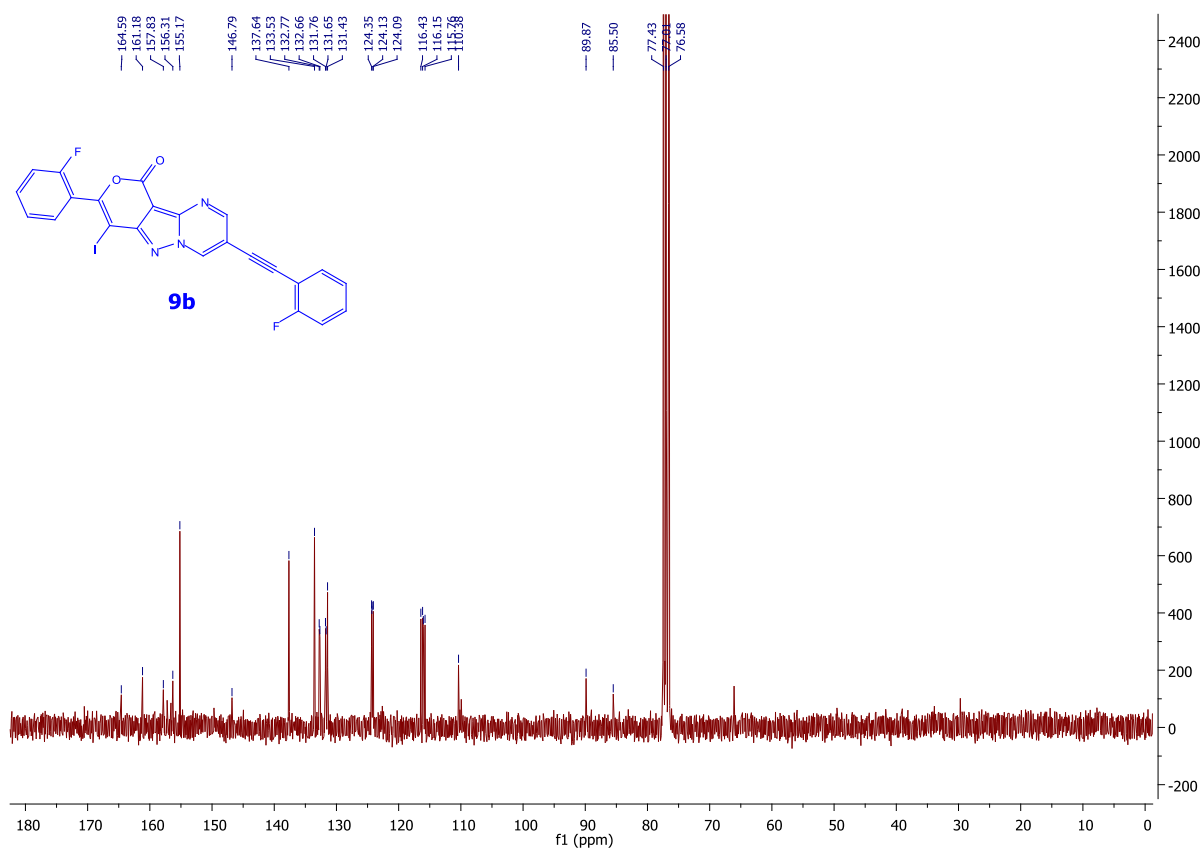
^1H NMR (300 MHz, CDCl_3)



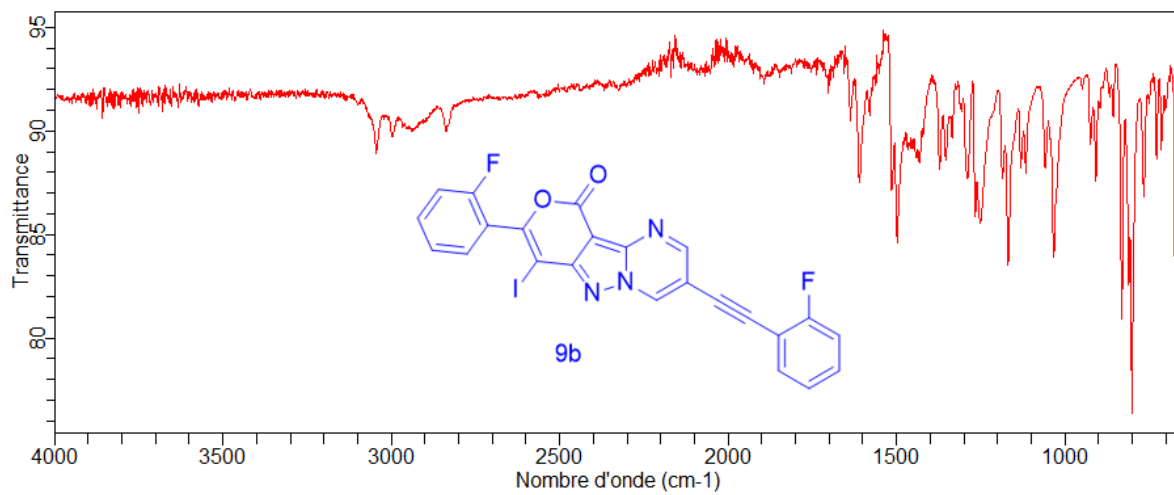
^{19}F NMR (282 MHz, CDCl_3)



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



IR



2. Details of DFT calculations

The structure of each studied species was optimized by using the Turbomole 7.4 program package.^{S1} Before their visualization using TmoleX (version 4.5.3), the structure of each individual species was optimized in the gas phase, with a convergence criterion of 10^{-8} Hartree, using the hybrid functional B3LYP and the triplet- ζ basis set 6-311+G*,^{S2} to collect its more stable 3D conformer. The stability of each structure was then investigated during further DFT calculations. During this step, the energy of each cluster was then minimized again using DFT calculations combining the Resolution of Identity (RI) approximation,^{S3-S4} within the Turbomole 7.4 program package using the B3LYP function with the def2-TZVP basis set.^{S5-S7} All minimum energy structures were obtained with full optimization, without constraints. Corrections for long range non-bonding interactions were given using the Grimme D3 dispersion model.^{S8} An implicit solvent model was additionally undertaken, using the COSMO Model implemented in Turbomole to determine thermodynamic properties in the liquid phase. Analytical frequencies were then run on each structure at 1 atm and 298.15 K to calculate finally each energy.

2.1. Cartesian coordinates of ethyl 2,6-dibromopyrazolo[1,5-a]pyrimidine-3-carboxylate, 3

	x	y	z
C	-2.112306	1.822941	0.000000
C	-3.430011	1.265065	0.000000
C	-3.577653	-0.112726	0.000000
N	-2.437676	-0.862852	0.000000
C	-1.151438	-0.259062	0.000000
N	-1.016347	1.078907	0.000000
C	-0.238649	-1.345300	0.000000
C	-1.084401	-2.493506	0.000000
N	-2.398255	-2.209935	0.000000
Br	-0.570395	-4.293799	0.000000
C	1.240765	-1.326918	0.000000
O	1.946299	-2.322659	0.000000
O	1.722823	-0.059712	0.000000
C	3.162200	0.063991	0.000000
C	3.500656	1.545597	0.000000
Br	-4.954286	2.391912	0.000000
H	-1.984314	2.920677	0.000000
H	-4.529500	-0.663174	0.000000
H	3.568749	-0.458931	-0.894103
H	3.568749	-0.458931	0.894103
H	4.604090	1.681668	0.000000
H	3.085449	2.048374	0.899767
H	3.085449	2.048374	-0.899767

2.2. Cartesian coordinates of 2,6-dibromopyrazolo[1,5-a]pyrimidine, 3'

	x	y	z
C	-0.421129	-0.779369	0.000000
N	-0.305694	0.643064	0.000000
N	-1.494260	1.271616	0.000000
C	-2.383332	0.256454	0.000000
C	-1.803271	-1.029870	0.000000
C	0.917617	1.250558	0.000000
C	2.032966	0.429496	0.000000
C	1.860633	-0.993551	0.000000
N	0.669745	-1.571111	0.000000
H	-2.297989	-2.005673	0.000000
H	0.924078	2.350076	0.000000
H	2.749586	-1.649846	0.000000
Br	-4.223063	0.644922	0.000000
Br	3.774113	1.183235	0.000000

2.3. Cartesian coordinates of Pd(PPh₃)₂, Cat.

	x	y	z
Pd	-1.916934	0.592737	-0.044865
P	-2.955247	-1.445739	-0.214830
C	-3.427862	-2.212518	1.409963
C	-4.009041	-3.322870	3.944805
C	-2.531894	-2.044482	2.490328
C	-4.623607	-2.932667	1.617751
C	-4.912317	-3.481269	2.880539
C	-2.816140	-2.604153	3.745888
H	-1.611024	-1.454124	2.338226
H	-5.340773	-3.061775	0.790451
H	-5.853578	-4.036256	3.031442
H	-2.106603	-2.466609	4.579011
H	-4.238168	-3.752987	4.934145
C	-1.961930	-2.783181	-1.036488
C	-0.393284	-4.711134	-2.384148
C	-1.952116	-4.126357	-0.603378
C	-1.167938	-2.414340	-2.146174
C	-0.396625	-3.373723	-2.820718
C	-1.168564	-5.083348	-1.273251
H	-2.555172	-4.428716	0.268719
H	-1.150447	-1.358318	-2.468518
H	0.217041	-3.072366	-3.686167
H	-1.164802	-6.128564	-0.920851

H	0.221918	-5.462656	-2.906707
C	-4.547529	-1.461737	-1.170713
C	-7.002914	-1.349357	-2.567792
C	-5.368450	-0.314154	-1.088380
C	-4.965261	-2.547696	-1.970054
C	-6.186136	-2.488960	-2.665976
C	-6.591939	-0.261920	-1.775604
H	-5.027079	0.547295	-0.487517
H	-4.330017	-3.444304	-2.057084
H	-6.499392	-3.341643	-3.291610
H	-7.222672	0.639582	-1.701891
H	-7.958457	-1.304863	-3.116668
P	-0.874034	2.622218	0.186112
C	-1.720073	4.054621	-0.640114
C	0.853053	2.714139	-0.492452
C	-0.669736	3.203633	1.938470
C	-2.277256	3.828911	-1.919585
C	-1.845680	5.332259	-0.054557
C	1.658622	1.558075	-0.381508
C	1.386594	3.864569	-1.112314
C	-1.703391	2.893889	2.851355
C	0.457209	3.919615	2.396185
C	-2.926885	4.865828	-2.607022
H	-2.207155	2.822386	-2.368354
C	-2.509148	6.366105	-0.740011
H	-1.428948	5.522643	0.948130
C	2.977637	1.559483	-0.862729
H	1.231486	0.648286	0.076071
C	2.704360	3.859872	-1.604029
H	0.767018	4.770038	-1.219868
C	-1.620416	3.309304	4.190013
H	-2.570963	2.307368	2.500794
C	0.543757	4.324345	3.740429
H	1.278600	4.157827	1.700796
C	-3.047000	6.137587	-2.017420
H	-3.354233	4.675840	-3.605864
H	-2.606092	7.358403	-0.267974
C	3.503205	2.710598	-1.477289
H	3.595355	0.650824	-0.768606
H	3.107973	4.763024	-2.092011
C	-0.494766	4.024216	4.638405
H	-2.434794	3.061866	4.891244
H	1.432478	4.877783	4.087499

H	-3.568060	6.949143	-2.552327
H	4.535405	2.709014	-1.865690
H	-0.423467	4.340659	5.692538

2.4. Cartesian coordinates of TS1

	x	y	z
C	-2.417245	2.064914	0.618161
C	-3.154937	-0.061076	-0.292902
N	-1.914599	-0.528045	0.032276
C	-0.943517	0.308391	0.645747
N	-1.218044	1.594471	0.926893
C	0.193085	-0.522042	0.823551
C	-0.223529	-1.778240	0.292443
N	-1.481427	-1.786224	-0.181116
Br	0.767640	-3.363309	0.190465
C	1.509735	-0.195587	1.414201
O	2.434390	-0.984256	1.525084
O	1.566180	1.096478	1.821107
C	2.815938	1.513580	2.413765
C	2.680717	2.977196	2.800097
H	-2.627149	3.123662	0.855641
H	-3.842948	-0.777483	-0.764506
H	3.635773	1.347685	1.679938
H	3.031684	0.866182	3.292673
H	3.626605	3.335719	3.261444
H	1.857183	3.120817	3.532168
H	2.465098	3.605371	1.909217
Pd	-5.089651	1.587836	1.368723
P	-5.978744	-0.201655	2.643138
C	-4.908350	-1.352758	3.590436
C	-3.186421	-3.119673	4.923183
C	-3.566685	-1.467705	3.196566
C	-5.376800	-2.126888	4.662781
C	-4.518766	-3.004704	5.325143
C	-2.713611	-2.351733	3.857661
H	-3.196728	-0.868757	2.370815
H	-6.408226	-2.033714	4.986732
H	-4.891136	-3.598215	6.155712
H	-1.677271	-2.434623	3.542608
H	-2.518897	-3.802664	5.441391
C	-6.834466	-1.260176	1.413497
C	-8.246267	-2.770494	-0.473245

C	-7.247282	-2.565405	1.718777
C	-7.123668	-0.719849	0.153072
C	-7.833025	-1.474793	-0.782801
C	-7.948081	-3.317363	0.778133
H	-7.015863	-2.994680	2.688566
H	-6.776169	0.273089	-0.111237
H	-8.046148	-1.048497	-1.758814
H	-8.259904	-4.329815	1.019727
H	-8.791368	-3.358935	-1.206349
C	-7.328238	0.184643	3.830755
C	-9.349711	0.927898	5.634038
C	-7.005436	0.680098	5.103605
C	-8.677168	0.075921	3.469816
C	-9.678955	0.442347	4.368817
C	-8.007000	1.050515	5.997945
H	-5.967661	0.767041	5.402545
H	-8.945984	-0.289353	2.485474
H	-10.720007	0.356364	4.071619
H	-7.735556	1.434236	6.977453
H	-10.132777	1.215272	6.330199
P	-5.154823	3.498803	2.769026
C	-6.910269	4.011421	2.671175
C	-4.247750	4.996256	2.201536
C	-4.686009	3.461393	4.539124
C	-7.509295	3.915354	1.401666
C	-7.671045	4.455199	3.756958
C	-2.847410	4.981758	2.300408
C	-4.878906	6.120002	1.656725
C	-4.189959	2.259618	5.060590
C	-4.747946	4.593032	5.366352
C	-8.841784	4.283661	1.226526
H	-6.933283	3.556168	0.552413
C	-9.006526	4.817898	3.575554
H	-7.236184	4.493006	4.748698
C	-2.094513	6.069315	1.865928
H	-2.348461	4.114374	2.724352
C	-4.122062	7.209908	1.219269
H	-5.960327	6.147763	1.576491
C	-3.799372	2.175946	6.398080
H	-4.109374	1.395961	4.405491
C	-4.367122	4.507320	6.704324
H	-5.083186	5.541558	4.957289
C	-9.592918	4.739278	2.312848

H	-9.293310	4.206024	0.241553
H	-9.591360	5.149281	4.428839
C	-2.731309	7.188971	1.322566
H	-1.011703	6.044308	1.950449
H	-4.623942	8.077235	0.799101
C	-3.898278	3.296896	7.223293
H	-3.415673	1.238907	6.791669
H	-4.425702	5.385903	7.340697
H	-10.633684	5.020162	2.176688
H	-2.145538	8.038555	0.983167
H	-3.596810	3.233934	8.265069
C	-3.527587	1.289060	-0.115419
Br	-5.387619	1.722978	-0.613081

2.5. Cartesian coordinates of TS2

	x	y	z
C	0.617723	1.880116	-0.497502
C	0.105124	1.665251	-1.816079
C	-0.460495	0.439035	-2.126852
N	-0.493333	-0.501794	-1.138925
C	0.029912	-0.237919	0.155506
N	0.577316	0.954711	0.449442
C	-0.184005	-1.435081	0.886354
C	-0.818296	-2.295161	-0.057897
N	-1.004918	-1.741824	-1.268522
C	0.156605	-1.749507	2.291388
O	-0.069069	-2.817555	2.836939
O	0.754886	-0.699236	2.905542
C	1.127162	-0.908437	4.285668
C	1.775908	0.369942	4.790236
Br	0.196883	3.036435	-3.121695
H	1.070708	2.854767	-0.240075
H	-0.887748	0.149047	-3.097607
H	1.816432	-1.779969	4.344769
H	0.217109	-1.174829	4.867898
H	2.077231	0.247260	5.853360
H	1.071837	1.226916	4.722086
H	2.681292	0.617944	4.195644
Pd	-3.037847	-2.356353	0.659916
P	-3.696349	-1.552752	2.790015
C	-3.279426	0.138423	3.367993
C	-2.508579	2.702328	4.202122

C	-2.191317	0.784116	2.761743
C	-3.981468	0.792862	4.391476
C	-3.597203	2.068385	4.804661
C	-1.806382	2.057318	3.182546
H	-1.646607	0.285528	1.966615
H	-4.834989	0.309843	4.855783
H	-4.148883	2.567264	5.596819
H	-0.960640	2.546783	2.707970
H	-2.211683	3.696727	4.523995
C	-2.865976	-2.674252	3.980583
C	-1.726336	-4.462996	5.806903
C	-2.306510	-2.202137	5.176938
C	-2.841403	-4.047068	3.699421
C	-2.276889	-4.936147	4.615884
C	-1.737310	-3.093111	6.084527
H	-2.311019	-1.138842	5.395441
H	-3.234313	-4.422121	2.760582
H	-2.257461	-5.997280	4.384928
H	-1.300900	-2.719524	7.006765
H	-1.280515	-5.156312	6.514958
C	-5.465705	-1.728404	3.258564
C	-8.202161	-2.021294	3.821157
C	-6.393093	-0.770213	2.820885
C	-5.928884	-2.840443	3.973249
C	-7.287996	-2.981296	4.254374
C	-7.750432	-0.915330	3.097911
H	-6.053216	0.099021	2.270765
H	-5.230061	-3.599169	4.305705
H	-7.631368	-3.851812	4.805452
H	-8.452154	-0.163350	2.747749
H	-9.260342	-2.136224	4.039295
P	-4.868438	-1.965778	-0.793833
C	-6.008991	-3.339080	-0.384822
C	-4.578817	-2.183559	-2.598295
C	-5.842623	-0.414868	-0.785305
C	-5.407850	-4.590408	-0.155785
C	-7.396341	-3.212559	-0.267184
C	-3.849034	-1.184999	-3.262470
C	-5.020842	-3.296927	-3.321448
C	-5.428008	0.614984	0.068979
C	-6.938507	-0.200339	-1.634888
C	-6.193254	-5.697115	0.160822
H	-4.328406	-4.698531	-0.228044

C	-8.176702	-4.323977	0.055007
H	-7.869138	-2.246446	-0.397724
C	-3.569457	-1.296463	-4.621777
H	-3.503669	-0.315455	-2.709588
C	-4.738002	-3.408506	-4.685081
H	-5.588668	-4.075425	-2.823304
C	-6.120269	1.826567	0.105392
H	-4.555918	0.456820	0.698185
C	-7.635770	1.005608	-1.591885
H	-7.235701	-0.974307	-2.336515
C	-7.580458	-5.567233	0.263617
H	-5.718037	-6.658271	0.334799
H	-9.252315	-4.211174	0.156087
C	-4.014045	-2.411360	-5.338550
H	-3.005060	-0.514841	-5.122523
H	-5.087665	-4.277297	-5.236008
C	-7.231200	2.018170	-0.717102
H	-5.789499	2.618481	0.771410
H	-8.488405	1.161081	-2.247033
H	-8.191619	-6.429236	0.516849
H	-3.797022	-2.499991	-6.399314
H	-7.772889	2.959457	-0.689285
Br	-1.364805	-4.140472	0.209336

2.6. Cartesian coordinates of TS3

	x	y	z
C	-2.417245	2.064914	0.618161
C	-3.154937	-0.061076	-0.292902
N	-1.914599	-0.528045	0.032276
C	-0.943517	0.308391	0.645747
N	-1.218044	1.594471	0.926893
C	0.193085	-0.522042	0.823551
C	-0.223529	-1.778240	0.292443
N	-1.481427	-1.786224	-0.181116
Br	0.767640	-3.363309	0.190465
H	-2.627149	3.123662	0.855641
H	-3.842948	-0.777483	-0.764506
Pd	-5.089651	1.587836	1.368723
P	-5.978744	-0.201655	2.643138
C	-4.908350	-1.352758	3.590436
C	-3.186421	-3.119673	4.923183
C	-3.566685	-1.467705	3.196566

C	-5.376800	-2.126888	4.662781
C	-4.518766	-3.004704	5.325143
C	-2.713611	-2.351733	3.857661
H	-3.196728	-0.868757	2.370815
H	-6.408226	-2.033714	4.986732
H	-4.891136	-3.598215	6.155712
H	-1.677271	-2.434623	3.542608
H	-2.518897	-3.802664	5.441391
C	-6.834466	-1.260176	1.413497
C	-8.246267	-2.770494	-0.473245
C	-7.247282	-2.565405	1.718777
C	-7.123668	-0.719849	0.153072
C	-7.833025	-1.474793	-0.782801
C	-7.948081	-3.317363	0.778133
H	-7.015863	-2.994680	2.688566
H	-6.776169	0.273089	-0.111237
H	-8.046148	-1.048497	-1.758814
H	-8.259904	-4.329815	1.019727
H	-8.791368	-3.358935	-1.206349
C	-7.328238	0.184643	3.830755
C	-9.349711	0.927898	5.634038
C	-7.005436	0.680098	5.103605
C	-8.677168	0.075921	3.469816
C	-9.678955	0.442347	4.368817
C	-8.007000	1.050515	5.997945
H	-5.967661	0.767041	5.402545
H	-8.945984	-0.289353	2.485474
H	-10.720007	0.356364	4.071619
H	-7.735556	1.434236	6.977453
H	-10.132777	1.215272	6.330199
P	-5.154823	3.498803	2.769026
C	-6.910269	4.011421	2.671175
C	-4.247750	4.996256	2.201536
C	-4.686009	3.461393	4.539124
C	-7.509295	3.915354	1.401666
C	-7.671045	4.455199	3.756958
C	-2.847410	4.981758	2.300408
C	-4.878906	6.120002	1.656725
C	-4.189959	2.259618	5.060590
C	-4.747946	4.593032	5.366352
C	-8.841784	4.283661	1.226526
H	-6.933283	3.556168	0.552413
C	-9.006526	4.817898	3.575554

H	-7.236184	4.493006	4.748698
C	-2.094513	6.069315	1.865928
H	-2.348461	4.114374	2.724352
C	-4.122062	7.209908	1.219269
H	-5.960327	6.147763	1.576491
C	-3.799372	2.175946	6.398080
H	-4.109374	1.395961	4.405491
C	-4.367122	4.507320	6.704324
H	-5.083186	5.541558	4.957289
C	-9.592918	4.739278	2.312848
H	-9.293310	4.206024	0.241553
H	-9.591360	5.149281	4.428839
C	-2.731309	7.188971	1.322566
H	-1.011703	6.044308	1.950449
H	-4.623942	8.077235	0.799101
C	-3.898278	3.296896	7.223293
H	-3.415673	1.238907	6.791669
H	-4.425702	5.385903	7.340697
H	-10.633684	5.020162	2.176688
H	-2.145538	8.038555	0.983167
H	-3.596810	3.233934	8.265069
C	-3.527587	1.289060	-0.115419
Br	-5.387619	1.722978	-0.613081
H	1.158254	-0.259398	1.256641

2.7. Cartesian coordinates of TS4

	x	y	z
C	-0.235507	-0.178153	0.042210
N	-0.643776	0.357716	-1.215885
N	-1.934768	0.732659	-1.238840
C	-2.366137	0.440125	0.005888
C	-1.383708	-0.120750	0.849308
C	0.233701	0.455732	-2.257982
C	1.528347	0.014685	-2.039994
C	1.885860	-0.515080	-0.756913
N	1.026663	-0.605162	0.245812
H	-1.475919	-0.442050	1.891038
H	-0.156040	0.879175	-3.194882
H	2.918397	-0.867333	-0.581564
Br	2.817165	0.111405	-3.428991
Pd	-3.482651	-1.544605	-0.013427
P	-3.661671	-2.932312	-1.926265

C	-2.186581	-3.590078	-2.797704
C	0.126280	-4.464127	-4.120689
C	-0.971792	-2.909232	-2.626894
C	-2.229359	-4.717003	-3.632500
C	-1.077905	-5.150842	-4.289215
C	0.176079	-3.342800	-3.290748
H	-0.930601	-2.039486	-1.979303
H	-3.159604	-5.261177	-3.758609
H	-1.121397	-6.025923	-4.931935
H	1.110690	-2.806424	-3.153340
H	1.022748	-4.804516	-4.631627
C	-4.516944	-1.890761	-3.170617
C	-5.943367	-0.386746	-5.051331
C	-4.023871	-1.738820	-4.474823
C	-5.723751	-1.275552	-2.810874
C	-6.434618	-0.530934	-3.753875
C	-4.733502	-0.987986	-5.409817
H	-3.083616	-2.202284	-4.756746
H	-6.096953	-1.351219	-1.795267
H	-7.365500	-0.053148	-3.462499
H	-4.342610	-0.870114	-6.416720
H	-6.494681	0.199891	-5.781190
C	-4.768248	-4.396772	-1.817365
C	-6.456170	-6.618537	-1.493057
C	-4.288827	-5.581401	-1.237233
C	-6.107365	-4.336777	-2.223697
C	-6.942247	-5.443019	-2.064779
C	-5.125416	-6.683126	-1.074465
H	-3.254784	-5.648326	-0.921021
H	-6.500220	-3.425354	-2.659036
H	-7.979272	-5.378501	-2.380696
H	-4.735097	-7.589908	-0.620703
H	-7.110442	-7.476926	-1.368004
P	-3.650305	-2.977864	1.866644
C	-5.452682	-3.280819	1.983940
C	-3.235723	-2.267563	3.513152
C	-2.807581	-4.600771	1.968728
C	-6.280515	-2.170959	1.733834
C	-6.033917	-4.518668	2.274604
C	-1.878713	-2.057259	3.804922
C	-4.198781	-1.905555	4.461514
C	-1.961373	-4.967459	0.914321
C	-2.929486	-5.452743	3.076907

C	-7.666271	-2.301856	1.800478
H	-5.841357	-1.206552	1.490580
C	-7.422678	-4.644019	2.335003
H	-5.410706	-5.391873	2.426494
C	-1.492979	-1.499006	5.020598
H	-1.123455	-2.337521	3.075471
C	-3.810493	-1.343687	5.680319
H	-5.251178	-2.064698	4.252314
C	-1.278016	-6.184238	0.945242
H	-1.841813	-4.286815	0.075340
C	-2.254933	-6.672001	3.103758
H	-3.543391	-5.153481	3.921415
C	-8.240814	-3.538420	2.104753
H	-8.295250	-1.437827	1.606165
H	-7.863436	-5.613403	2.549276
C	-2.460171	-1.139575	5.963873
H	-0.438911	-1.343829	5.232924
H	-4.567654	-1.067763	6.409121
C	-1.433291	-7.041961	2.035003
H	-0.623979	-6.458115	0.122234
H	-2.360913	-7.330009	3.961762
H	-9.321584	-3.641203	2.150212
H	-2.161089	-0.704018	6.913091
H	-0.904099	-7.990391	2.060635
Br	-4.210941	0.806291	0.481521

2.8. Cartesian coordinates of 1-cis

	x	y	z
C	-1.809812	1.524985	0.122537
C	-1.906048	-0.084126	1.895892
N	-0.861628	-0.713347	1.268048
C	-0.313569	-0.207563	0.071612
N	-0.802451	0.909839	-0.493708
C	0.737283	-1.111787	-0.264719
C	0.695121	-2.069664	0.789076
N	-0.254901	-1.840610	1.707528
Br	1.801573	-3.572276	1.019468
C	1.664205	-1.087830	-1.408766
O	2.552239	-1.903221	-1.613219
O	1.420376	-0.031561	-2.233281
C	2.277463	0.070654	-3.384727
C	1.850394	1.300166	-4.171590

H	-2.186367	2.437759	-0.375243
H	-2.263412	-0.584593	2.808462
H	2.191963	-0.860551	-3.988454
H	3.336819	0.137775	-3.048313
H	2.490012	1.416259	-5.073821
H	1.942954	2.218899	-3.552935
H	0.791922	1.212938	-4.498990
Pd	-4.007229	2.031089	2.202997
P	-6.134451	2.814725	3.150078
C	-6.879818	1.566922	4.310428
C	-8.001089	-0.369417	6.043906
C	-6.448071	0.222852	4.260556
C	-7.882596	1.928383	5.241394
C	-8.439438	0.965117	6.099078
C	-7.005510	-0.736442	5.123504
H	-5.689733	-0.077062	3.518443
H	-8.228896	2.972102	5.307139
H	-9.222139	1.262434	6.816915
H	-6.658295	-1.781347	5.068032
H	-8.437906	-1.123906	6.719222
C	-7.406987	3.090816	1.831986
C	-9.272455	3.627665	-0.218853
C	-8.773060	2.798495	2.018294
C	-6.981865	3.641938	0.603855
C	-7.910669	3.917802	-0.411956
C	-9.699405	3.063746	0.995004
H	-9.121152	2.344335	2.959354
H	-5.909792	3.834752	0.435574
H	-7.563871	4.342333	-1.368424
H	-10.763727	2.819202	1.148026
H	-10.000656	3.829991	-1.021723
C	-6.274847	4.378451	4.154830
C	-6.476830	6.733036	5.720151
C	-5.819850	4.398203	5.493693
C	-6.816397	5.561627	3.608095
C	-6.914319	6.728812	4.385719
C	-5.925803	5.562831	6.270579
H	-5.398366	3.488317	5.949312
H	-7.183143	5.572250	2.570073
H	-7.349653	7.639768	3.942421
H	-5.579405	5.550113	7.317398
H	-6.568158	7.645588	6.332333
P	-2.524645	3.477231	3.250986

C	-3.038756	5.240624	3.027027
C	-0.762107	3.488340	2.666145
C	-2.298151	3.161548	5.059052
C	-3.457844	5.617157	1.729852
C	-2.995191	6.215757	4.043393
C	0.087973	2.430497	3.065170
C	-0.257573	4.482563	1.802525
C	-3.065035	2.156450	5.685591
C	-1.317596	3.849415	5.811809
C	-3.791037	6.951469	1.447062
H	-3.518260	4.855484	0.932824
C	-3.343916	7.547537	3.760288
H	-2.699386	5.939937	5.067344
C	1.412175	2.370503	2.606282
H	-0.283156	1.645493	3.743542
C	1.070389	4.417380	1.343941
H	-0.896600	5.321039	1.485241
C	-2.876646	1.861015	7.047385
H	-3.804822	1.590907	5.093679
C	-1.138774	3.559616	7.173969
H	-0.672593	4.600281	5.326777
C	-3.731400	7.921105	2.463004
H	-4.105473	7.232378	0.428374
H	-3.312210	8.299008	4.566191
C	1.906611	3.362609	1.740740
H	2.060350	1.537036	2.922778
H	1.449305	5.201744	0.668201
C	-1.919670	2.567445	7.794673
H	-3.477501	1.067908	7.521560
H	-0.373235	4.103537	7.751621
H	-3.997859	8.968481	2.244561
H	2.944833	3.309168	1.374387
H	-1.768928	2.334228	8.861767
C	-2.415142	1.079430	1.342150
Br	-5.361174	0.434090	0.835153

2.9. Cartesian coordinates of 1-trans

	x	y	z
C	-2.021914	1.680254	0.281177
C	-3.321039	1.184990	-0.076401
C	-3.379099	-0.148745	-0.455832
N	-2.226706	-0.891902	-0.459280

C	-0.984627	-0.320869	-0.113959
N	-0.896321	0.968533	0.254866
C	-0.039151	-1.380601	-0.248300
C	-0.840956	-2.484001	-0.659494
N	-2.145698	-2.201735	-0.789567
Br	-0.274690	-4.237799	-1.031594
C	1.415268	-1.373269	-0.016457
O	2.146606	-2.349910	-0.095040
O	1.868315	-0.128164	0.299568
C	3.280792	-0.025949	0.558061
C	3.587697	1.427075	0.886168
H	-1.908784	2.732395	0.604182
H	-4.278724	-0.698694	-0.772319
H	3.843358	-0.379948	-0.335059
H	3.549263	-0.707980	1.396140
H	4.672190	1.548675	1.099898
H	3.013317	1.762354	1.776598
H	3.320808	2.091411	0.036012
Pd	-4.967341	2.369819	-0.045209
P	-4.806909	2.716284	-2.390643
C	-6.421874	2.467797	-3.254393
C	-3.652501	1.597872	-3.310910
C	-4.227733	4.407919	-2.875191
C	-7.289980	1.461374	-2.778471
C	-6.790200	3.219521	-4.388404
C	-2.257128	1.768235	-3.151805
C	-4.125109	0.526119	-4.097159
C	-4.470372	5.502186	-2.016270
C	-3.564286	4.629605	-4.104580
C	-8.498247	1.196154	-3.441768
H	-7.022520	0.892304	-1.871962
C	-8.007232	2.960267	-5.041539
H	-6.132087	4.021054	-4.760262
C	-1.357406	0.886531	-3.769402
H	-1.865839	2.597513	-2.540244
C	-3.219626	-0.358991	-4.710003
H	-5.207538	0.376675	-4.236629
C	-4.054602	6.793424	-2.382151
H	-5.010774	5.339428	-1.068274
C	-3.151408	5.923605	-4.463965
H	-3.359866	3.787623	-4.785057
C	-8.860235	1.946874	-4.573752
H	-9.168533	0.407508	-3.061881

H	-8.290684	3.560672	-5.921953
C	-1.836573	-0.182952	-4.547907
H	-0.273407	1.031366	-3.632213
H	-3.604162	-1.194056	-5.318466
C	-3.393342	7.007875	-3.603181
H	-4.251924	7.638866	-1.702442
H	-2.633816	6.082075	-5.424695
H	-9.815122	1.747033	-5.087757
H	-1.128987	-0.881455	-5.023688
H	-3.064421	8.021868	-3.885457
Br	-7.014440	3.879394	-0.007827
P	-5.176034	2.060724	2.302185
C	-6.623088	1.027506	2.825062
C	-8.865774	-0.496511	3.620538
C	-7.781053	0.987010	2.017557
C	-6.599936	0.297003	4.036242
C	-7.716850	-0.459500	4.429354
C	-8.894478	0.229043	2.417431
H	-7.812894	1.574625	1.084784
H	-5.702817	0.310685	4.675321
H	-7.684996	-1.025731	5.375004
H	-9.793078	0.207822	1.779073
H	-9.739961	-1.093510	3.929505
C	-5.352104	3.666187	3.202396
C	-5.474599	6.129461	4.572897
C	-6.115562	3.785943	4.381808
C	-4.659543	4.792894	2.708257
C	-4.713380	6.015568	3.396250
C	-6.177814	5.015081	5.060644
H	-6.674610	2.919856	4.770851
H	-4.085504	4.712325	1.769901
H	-4.168793	6.889161	3.001610
H	-6.785321	5.100621	5.976726
H	-5.526544	7.093053	5.106366
C	-3.751053	1.246721	3.161547
C	-1.514239	-0.027777	4.332322
C	-3.523630	-0.135158	2.960609
C	-2.844137	1.979950	3.955132
C	-1.731621	1.343779	4.534923
C	-2.416690	-0.767288	3.546261
H	-4.222173	-0.727583	2.347599
H	-3.004559	3.055807	4.128097
H	-1.030690	1.931242	5.150670

H	-2.254155	-1.844948	3.380955
H	-0.639590	-0.523988	4.783795

2.10. Cartesian coordinates of 2-cis

	x	y	z
C	-0.951273	2.389675	-0.322684
C	-2.200860	2.674375	0.306823
C	-3.007162	1.620362	0.713083
N	-2.551363	0.359283	0.487959
C	-1.295981	0.126532	-0.139912
N	-0.521624	1.152957	-0.536318
C	-1.187585	-1.283986	-0.194619
N	-3.198521	-0.786429	0.817806
C	-0.100468	-2.109502	-0.727291
O	-0.153401	-3.329426	-0.891408
O	1.003978	-1.385875	-1.032988
C	2.123313	-2.118101	-1.566609
C	3.261628	-1.132393	-1.779788
Br	-2.759418	4.470025	0.586448
H	-0.302265	3.221257	-0.652979
H	-3.983801	1.710422	1.210203
H	1.816471	-2.611063	-2.516885
H	2.400817	-2.927140	-0.855010
H	4.147198	-1.658197	-2.199014
H	3.557929	-0.656871	-0.820032
H	2.962914	-0.327824	-2.485511
Pd	-2.808047	-3.707249	0.841871
P	-3.062441	-5.983014	1.694264
C	-4.087219	-6.120091	3.240368
C	-5.645446	-6.286745	5.597203
C	-4.379502	-4.959682	3.989747
C	-4.592693	-7.365355	3.683405
C	-5.362053	-7.446938	4.855844
C	-5.154687	-5.045672	5.159228
H	-3.973026	-3.987187	3.666418
H	-4.400228	-8.281409	3.102142
H	-5.745636	-8.425989	5.188584
H	-5.371166	-4.129348	5.733060
H	-6.252096	-6.351431	6.516098
C	-1.393257	-6.674402	2.108318
C	1.173993	-7.751794	2.572187
C	-1.200569	-7.650411	3.108000

C	-0.286590	-6.227989	1.352744
C	0.987806	-6.774281	1.579882
C	0.078656	-8.183436	3.339884
H	-2.047291	-7.990228	3.725071
H	-0.413029	-5.429404	0.602682
H	1.844318	-6.414938	0.986061
H	0.219344	-8.938261	4.131490
H	2.177741	-8.169791	2.757171
C	-3.801887	-7.349544	0.664161
C	-4.972002	-9.421500	-0.873656
C	-5.204977	-7.427645	0.506046
C	-2.993796	-8.311972	0.021992
C	-3.576517	-9.338939	-0.741098
C	-5.784513	-8.457951	-0.250979
H	-5.859190	-6.689860	0.997186
H	-1.898484	-8.270957	0.128203
H	-2.928309	-10.085787	-1.228766
H	-6.881780	-8.508592	-0.349472
H	-5.427231	-10.235721	-1.461960
P	-4.004780	-3.845520	-1.136984
C	-3.499837	-5.276158	-2.197307
C	-3.902916	-2.403380	-2.305582
C	-5.833849	-3.952717	-0.872592
C	-2.110598	-5.463694	-2.390073
C	-4.410579	-6.146198	-2.830771
C	-4.645951	-1.238612	-2.003649
C	-3.086977	-2.416839	-3.455399
C	-6.334614	-4.015481	0.444257
C	-6.744711	-3.897461	-1.953311
C	-1.650267	-6.484321	-3.238940
H	-1.388395	-4.799661	-1.882195
C	-3.940322	-7.171469	-3.669074
H	-5.493366	-6.039291	-2.665008
C	-4.575352	-0.115289	-2.842056
H	-5.281656	-1.207529	-1.105106
C	-3.016937	-1.287128	-4.289672
H	-2.502660	-3.313715	-3.711938
C	-7.720470	-4.051769	0.679258
H	-5.626800	-4.015245	1.291293
C	-8.128054	-3.942691	-1.716798
H	-6.373464	-3.798208	-2.986444
C	-2.562190	-7.336998	-3.884255
H	-0.565721	-6.614242	-3.390060

H	-4.662391	-7.848074	-4.155451
C	-3.759403	-0.134728	-3.987165
H	-5.164607	0.784041	-2.596940
H	-2.375522	-1.313700	-5.186240
C	-8.618445	-4.023847	-0.400555
H	-8.096302	-4.093975	1.714754
H	-8.828866	-3.903018	-2.567216
H	-2.198270	-8.139391	-4.547711
H	-3.704299	0.749631	-4.643437
H	-9.705602	-4.050467	-0.217236
C	-2.383571	-1.781685	0.419207
Br	-1.484662	-3.210069	2.922008

2.11. Cartesian coordinates of 2-trans

	x	y	z
C	-2.195752	2.016594	0.259377
C	-3.433104	1.439235	0.676723
C	-3.532933	0.058461	0.775549
N	-2.431198	-0.674100	0.461360
C	-1.221254	-0.052602	0.047550
N	-1.129603	1.286982	-0.043240
C	-0.332963	-1.131448	-0.181131
C	-1.080721	-2.320288	0.119771
N	-2.343567	-2.027733	0.502902
C	1.064846	-1.101270	-0.624841
O	1.757838	-2.095992	-0.831982
O	1.539989	0.161615	-0.777362
C	2.905568	0.278859	-1.221236
C	3.245642	1.759738	-1.285299
Br	-4.924114	2.540509	1.097465
H	-2.103283	3.115278	0.179645
H	-4.424786	-0.501940	1.091290
H	3.008812	-0.214576	-2.213725
H	3.567497	-0.271874	-0.516314
H	4.293954	1.894982	-1.630402
H	3.141560	2.234940	-0.286039
H	2.571473	2.291774	-1.990560
Pd	-0.455693	-4.220209	0.077883
P	-0.061086	-4.184481	2.406222
C	-0.984599	-5.557789	3.227953
C	-0.589349	-2.675039	3.350300
C	1.708540	-4.344566	2.922570

C	-2.322699	-5.774896	2.828373
C	-0.415169	-6.384430	4.216445
C	0.149302	-1.482270	3.172852
C	-1.712270	-2.662624	4.202942
C	2.681397	-4.769416	1.993335
C	2.103328	-4.026758	4.243901
C	-3.085259	-6.787911	3.430512
H	-2.762182	-5.152619	2.030006
C	-1.178589	-7.407119	4.806222
H	0.634363	-6.243516	4.518913
C	-0.226096	-0.306063	3.840166
H	1.033682	-1.474701	2.515422
C	-2.086948	-1.481318	4.868852
H	-2.298529	-3.581749	4.358438
C	4.027154	-4.880178	2.383998
H	2.375915	-5.027169	0.966762
C	3.448806	-4.144047	4.628813
H	1.357879	-3.675309	4.975947
C	-2.514044	-7.607825	4.420176
H	-4.129001	-6.947842	3.112796
H	-0.719257	-8.056149	5.570259
C	-1.347269	-0.301251	4.689917
H	0.362485	0.614483	3.692280
H	-2.964244	-1.490136	5.537139
C	4.413434	-4.570784	3.698706
H	4.778518	-5.211440	1.648393
H	3.744838	-3.894953	5.661468
H	-3.108813	-8.412489	4.883733
H	-1.641470	0.623159	5.214126
H	5.470697	-4.657553	4.000403
Br	0.312868	-6.648871	0.059771
P	-0.943137	-4.399751	-2.230603
C	-2.424432	-5.444902	-2.612967
C	-4.665232	-7.065975	-3.190506
C	-2.861358	-6.413792	-1.684348
C	-3.120079	-5.296893	-3.835682
C	-4.233307	-6.104603	-4.120993
C	-3.976134	-7.218626	-1.975589
H	-2.306614	-6.548782	-0.740763
H	-2.796359	-4.541712	-4.570192
H	-4.767827	-5.978587	-5.077377
H	-4.306004	-7.972567	-1.241818
H	-5.541900	-7.696885	-3.413753

C	0.455095	-5.135396	-3.187641
C	2.656222	-6.180621	-4.606274
C	0.261108	-6.137467	-4.159998
C	1.760897	-4.666829	-2.916442
C	2.851988	-5.183968	-3.633686
C	1.360644	-6.658154	-4.864232
H	-0.749262	-6.525947	-4.363032
H	1.919363	-3.895998	-2.142942
H	3.867734	-4.812605	-3.418157
H	1.199864	-7.448405	-5.616327
H	3.517604	-6.592747	-5.158156
C	-1.331634	-2.826264	-3.132079
C	-1.967389	-0.378317	-4.396987
C	-2.557205	-2.174650	-2.859715
C	-0.429990	-2.236553	-4.041722
C	-0.747778	-1.017915	-4.668062
C	-2.872444	-0.962555	-3.492147
H	-3.271078	-2.619997	-2.147795
H	0.527248	-2.731400	-4.269271
H	-0.033360	-0.570204	-5.378879
H	-3.834713	-0.468682	-3.276368
H	-2.215808	0.576050	-4.890348

2.12. Cartesian coordinates of 3-cis

	x	y	z
C	-0.563302	0.104744	1.005753
N	-0.275885	1.114056	0.053001
N	-1.375375	1.756851	-0.391082
C	-2.376786	1.152265	0.279259
C	-1.965501	0.128846	1.154936
C	1.016116	1.362876	-0.341270
C	1.666524	-0.374695	1.186294
N	0.417464	-0.634742	1.560673
H	-2.572975	-0.508127	1.804411
H	1.123911	2.140882	-1.111980
H	2.446561	-1.001120	1.658026
Br	-4.154764	1.721121	-0.009959
Pd	3.987576	0.871164	-0.352654
P	6.233004	0.900184	-1.356413
C	6.324958	1.833753	-2.960813
C	6.426294	3.250870	-5.408320
C	5.136298	2.164292	-3.647775

C	7.566654	2.224450	-3.515481
C	7.615011	2.924984	-4.732176
C	5.189380	2.869704	-4.862451
H	4.165072	1.838700	-3.240396
H	8.506734	1.990488	-2.990751
H	8.591109	3.219485	-5.152476
H	4.251335	3.116509	-5.386580
H	6.465581	3.802656	-6.362358
C	6.771007	-0.830589	-1.745140
C	7.601877	-3.493799	-2.186454
C	7.512422	-1.163413	-2.896674
C	6.437081	-1.847431	-0.823943
C	6.858971	-3.169075	-1.038037
C	7.921547	-2.490207	-3.115999
H	7.760208	-0.390237	-3.640997
H	5.820782	-1.603079	0.056834
H	6.586776	-3.953738	-0.312957
H	8.489793	-2.740423	-4.027206
H	7.920784	-4.534458	-2.363253
C	7.724643	1.575877	-0.463142
C	9.978579	2.652036	0.876963
C	7.918540	2.974433	-0.382710
C	8.668941	0.726522	0.152785
C	9.785395	1.262451	0.818299
C	9.038012	3.506707	0.275993
H	7.201540	3.661589	-0.858944
H	8.545326	-0.366369	0.100125
H	10.515675	0.580958	1.285164
H	9.176816	4.600155	0.313337
H	10.862275	3.069597	1.387678
P	4.344942	2.210101	1.508691
C	5.784052	1.625724	2.515792
C	2.991323	2.349127	2.773123
C	4.617742	3.993626	1.096713
C	5.845754	0.238684	2.785706
C	6.775053	2.472738	3.050810
C	1.840089	3.099547	2.438499
C	3.051161	1.711444	4.029344
C	4.659744	4.391828	-0.255913
C	4.701717	4.979796	2.107152
C	6.858485	-0.284499	3.605421
H	5.086707	-0.436197	2.353488
C	7.795435	1.943423	3.859968

H	6.763942	3.550895	2.829652
C	0.772738	3.205892	3.342344
H	1.775238	3.609054	1.463808
C	1.978048	1.820333	4.932556
H	3.938959	1.127190	4.316776
C	4.811304	5.747531	-0.596650
H	4.555958	3.630315	-1.048038
C	4.863346	6.331913	1.764539
H	4.618458	4.694510	3.168649
C	7.834713	0.569261	4.147774
H	6.886835	-1.366257	3.816365
H	8.567591	2.616219	4.267832
C	0.837569	2.563617	4.592067
H	-0.119988	3.788496	3.062464
H	2.039293	1.314947	5.910497
C	4.921443	6.717946	0.412764
H	4.835261	6.042621	-1.658320
H	4.930417	7.092165	2.560397
H	8.633382	0.160280	4.788511
H	-0.005596	2.641662	5.297779
H	5.037559	7.781828	0.147373
C	2.040517	0.626962	0.228843
Br	3.330581	-0.591218	-2.271225

2.13. Cartesian coordinates of 3-trans

	x	y	z
C	-0.879060	1.230874	0.376070
N	-0.188635	1.959819	-0.624080
N	-0.983163	2.804322	-1.312181
C	-2.194405	2.614096	-0.751336
C	-2.218127	1.665947	0.289725
C	1.155908	1.769980	-0.831966
C	1.067078	0.185831	0.970649
N	-0.239055	0.345706	1.166133
H	-3.062242	1.336176	0.902423
H	1.581830	2.367734	-1.652745
H	1.564613	-0.537802	1.644127
Br	-3.672395	3.600074	-1.392788
Pd	3.824670	0.506602	-0.275532
P	4.339807	1.945754	1.542151
C	5.493504	1.149998	2.747641
C	2.924889	2.492313	2.605769

C	5.141135	3.545496	1.058797
C	5.355821	-0.233794	2.992044
C	6.471872	1.882437	3.450483
C	1.989104	3.415974	2.083883
C	2.716358	1.964040	3.896959
C	5.914545	3.608644	-0.121003
C	5.015643	4.701142	1.864632
C	6.170714	-0.869962	3.941843
H	4.613396	-0.817272	2.422203
C	7.295836	1.239137	4.390302
H	6.602318	2.959749	3.258560
C	0.874546	3.804969	2.841260
H	2.133923	3.842241	1.077711
C	1.594046	2.351899	4.650508
H	3.433988	1.245749	4.323685
C	6.549633	4.807610	-0.485861
H	6.036648	2.703073	-0.739068
C	5.652722	5.897032	1.492833
H	4.411511	4.673279	2.785581
C	7.144453	-0.134934	4.640946
H	6.054380	-1.950906	4.125331
H	8.064712	1.818949	4.927267
C	0.671668	3.270590	4.126425
H	0.154473	4.525336	2.419760
H	1.443554	1.928422	5.657394
C	6.419789	5.953689	0.316650
H	7.152611	4.841996	-1.408384
H	5.545219	6.791334	2.128984
H	7.793168	-0.637891	5.377142
H	-0.209851	3.570058	4.716948
H	6.916385	6.894196	0.025194
C	1.841122	0.868703	-0.031235
Br	6.312722	0.041735	-0.582820
P	3.364377	-0.952289	-2.092260
C	3.641180	-2.748888	-1.731500
C	4.113781	-5.481357	-1.185566
C	4.579133	-3.128399	-0.746448
C	2.942749	-3.753070	-2.442098
C	3.180632	-5.110606	-2.168962
C	4.812004	-4.487938	-0.478660
H	5.145013	-2.349808	-0.207323
H	2.201357	-3.476961	-3.208735
H	2.628142	-5.883105	-2.729291

H	5.548686	-4.769552	0.291847
H	4.295563	-6.547463	-0.969977
C	4.398396	-0.568444	-3.575975
C	5.884182	0.125913	-5.872320
C	4.838439	-1.568589	-4.467037
C	4.718877	0.781447	-3.837733
C	5.449141	1.126857	-4.985963
C	5.581590	-1.220451	-5.608122
H	4.612083	-2.628368	-4.267270
H	4.405785	1.564024	-3.126384
H	5.693171	2.184220	-5.180784
H	5.929225	-2.011361	-6.293197
H	6.468778	0.396149	-6.767313
C	1.636419	-0.922977	-2.758175
C	-1.047812	-0.759822	-3.633253
C	0.595004	-1.500008	-1.994376
C	1.316227	-0.264449	-3.963867
C	-0.020107	-0.182907	-4.395632
C	-0.735533	-1.422702	-2.432345
H	0.822237	-2.015395	-1.046997
H	2.111942	0.189529	-4.575231
H	-0.255627	0.339419	-5.337499
H	-1.535434	-1.875054	-1.823763
H	-2.094910	-0.688806	-3.970150

2.14. Cartesian coordinates of 4-cis

	x	y	z
C	-0.233748	-0.275706	0.178359
N	-0.236525	1.133713	-0.065555
N	-1.480692	1.620994	-0.260867
C	-2.299214	0.547709	-0.135366
C	-1.584061	-0.648075	0.128100
C	0.923913	1.845273	-0.082231
C	2.102734	1.151167	0.144476
C	2.053985	-0.259154	0.385056
N	0.919325	-0.941951	0.400106
H	-1.979702	-1.654278	0.297548
H	0.840980	2.926067	-0.267698
H	2.992056	-0.814436	0.568406
Br	3.769975	2.070393	0.137587
Pd	-4.298875	0.811675	-0.254646
P	-4.130462	0.613075	-2.555698

C	-5.355412	-0.618622	-3.198221
C	-2.531766	0.016871	-3.292481
C	-4.364217	2.201035	-3.476300
C	-5.452697	-1.837834	-2.487121
C	-6.153875	-0.429356	-4.344230
C	-1.451893	0.926225	-3.376320
C	-2.350803	-1.306165	-3.745580
C	-4.628543	3.379655	-2.747899
C	-4.199394	2.279908	-4.878967
C	-6.303552	-2.860684	-2.936373
H	-4.850708	-1.984123	-1.573578
C	-7.015451	-1.450216	-4.782948
H	-6.119751	0.522468	-4.895733
C	-0.218360	0.513720	-3.903469
H	-1.573107	1.961209	-3.020752
C	-1.112199	-1.714330	-4.271349
H	-3.179788	-2.028939	-3.698533
C	-4.758631	4.612735	-3.410797
H	-4.713389	3.328815	-1.648739
C	-4.339430	3.510913	-5.539462
H	-3.937635	1.379321	-5.458255
C	-7.085158	-2.669615	-4.089333
H	-6.360790	-3.808914	-2.376827
H	-7.639426	-1.285957	-5.676673
C	-0.043287	-0.808004	-4.350898
H	0.615005	1.233107	-3.964494
H	-0.987485	-2.752023	-4.622708
C	-4.623432	4.678451	-4.807373
H	-4.958421	5.526290	-2.827337
H	-4.212739	3.561066	-6.633716
H	-7.757792	-3.469464	-4.440722
H	0.927779	-1.129827	-4.761998
H	-4.723306	5.645306	-5.328361
Br	-4.183798	0.850479	2.245784
P	-6.708191	1.272219	-0.008896
C	-7.038533	3.011051	0.559553
C	-7.491306	5.659213	1.446500
C	-5.990914	3.762348	1.136999
C	-8.316530	3.604414	0.430320
C	-8.539920	4.918492	0.873732
C	-6.219227	5.077909	1.576122
H	-4.996862	3.302009	1.264627
H	-9.145222	3.042782	-0.030089

H	-9.542309	5.366403	0.767847
H	-5.390785	5.649022	2.026674
H	-7.667870	6.691898	1.791276
C	-7.480364	0.173488	1.269178
C	-8.647979	-1.621284	3.110682
C	-8.491935	0.612275	2.146716
C	-7.048635	-1.169100	1.332932
C	-7.636075	-2.063731	2.241175
C	-9.069286	-0.281871	3.064715
H	-8.824771	1.662119	2.130366
H	-6.229168	-1.508513	0.678214
H	-7.285745	-3.108252	2.283186
H	-9.851937	0.076032	3.754411
H	-9.100538	-2.319453	3.834479
C	-7.914092	1.116988	-1.422887
C	-9.724432	0.923314	-3.595646
C	-7.949829	2.113610	-2.425402
C	-8.787643	0.014385	-1.536081
C	-9.684060	-0.080448	-2.614726
C	-8.850454	2.019883	-3.498101
H	-7.283117	2.988384	-2.361929
H	-8.783140	-0.774269	-0.767339
H	-10.364444	-0.945933	-2.678523
H	-8.870686	2.816244	-4.260970
H	-10.437582	0.853642	-4.434030

2.15. Cartesian coordinates of 4-trans

	x	y	z
C	-0.246063	-0.823043	-0.114568
N	-0.173802	0.570083	0.194932
N	-1.390570	1.154548	0.235997
C	-2.272332	0.158157	-0.042155
C	-1.615235	-1.080515	-0.272799
C	1.023547	1.178645	0.418587
C	2.164255	0.394597	0.336277
C	2.039872	-0.997513	0.028442
N	0.869401	-1.579663	-0.188459
H	-2.059079	-2.048193	-0.528902
H	0.997460	2.251955	0.656245
H	2.946960	-1.626127	-0.033932
Br	3.878309	1.165023	0.637388
Pd	-4.241186	0.534199	-0.034273

P	-4.238076	0.811278	-2.385762
C	-5.551911	-0.198584	-3.205394
C	-2.697126	0.331235	-3.296694
C	-4.512601	2.555084	-2.954040
C	-5.834046	-1.477154	-2.676870
C	-6.251120	0.248180	-4.344646
C	-1.530917	1.111142	-3.116634
C	-2.638865	-0.808285	-4.125020
C	-5.229296	3.454982	-2.135399
C	-4.030042	2.997542	-4.208095
C	-6.786372	-2.304284	-3.292611
H	-5.311960	-1.818082	-1.766773
C	-7.214106	-0.577277	-4.950433
H	-6.054494	1.250721	-4.757453
C	-0.335843	0.758036	-3.760980
H	-1.557089	1.998999	-2.464276
C	-1.435903	-1.162652	-4.762418
H	-3.537585	-1.425742	-4.280701
C	-5.458891	4.772322	-2.567162
H	-5.626369	3.109104	-1.166385
C	-4.262875	4.316425	-4.633273
H	-3.460791	2.312439	-4.856802
C	-7.480553	-1.854587	-4.429590
H	-6.999170	-3.300783	-2.871462
H	-7.763221	-0.213925	-5.835028
C	-0.283431	-0.381792	-4.584011
H	0.564907	1.377393	-3.615989
H	-1.405744	-2.057057	-5.406819
C	-4.976550	5.207349	-3.813176
H	-6.021843	5.463734	-1.918458
H	-3.879916	4.648421	-5.612663
H	-8.238850	-2.498458	-4.905513
H	0.658376	-0.660373	-5.085054
H	-5.155321	6.243362	-4.146273
Br	-6.757226	0.981761	-0.005534
P	-4.260970	0.374587	2.331362
C	-5.188861	-1.060055	3.050331
C	-6.624674	-3.235689	4.140977
C	-6.180125	-1.714446	2.287487
C	-4.922956	-1.507157	4.366027
C	-5.639629	-2.587616	4.906599
C	-6.892188	-2.796078	2.833688
H	-6.408859	-1.353131	1.270813

H	-4.145276	-1.014671	4.971465
H	-5.422368	-2.925845	5.933473
H	-7.665147	-3.297377	2.227922
H	-7.183360	-4.086382	4.565835
C	-5.017434	1.894321	3.061215
C	-6.062763	4.289342	4.124081
C	-5.870448	1.860181	4.182234
C	-4.701136	3.136279	2.467017
C	-5.214182	4.327679	3.003469
C	-6.392409	3.054858	4.707851
H	-6.142388	0.897182	4.643002
H	-4.056694	3.164776	1.571627
H	-4.959701	5.292095	2.533470
H	-7.067345	3.016626	5.579068
H	-6.475757	5.224498	4.537677
C	-2.624749	0.248335	3.195117
C	-0.089330	-0.008838	4.421181
C	-1.901016	-0.962802	3.101288
C	-2.061399	1.328758	3.905071
C	-0.800602	1.198419	4.514765
C	-0.644595	-1.090263	3.713384
H	-2.323648	-1.817999	2.549894
H	-2.609529	2.279944	3.989010
H	-0.375115	2.051205	5.069575
H	-0.093455	-2.041521	3.631188
H	0.899109	-0.108904	4.899485

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