

SUPPLEMENTARY INFORMATION

Experimental and theoretical study of the [3+2] cycloaddition of carbonyl ylides with alkynes

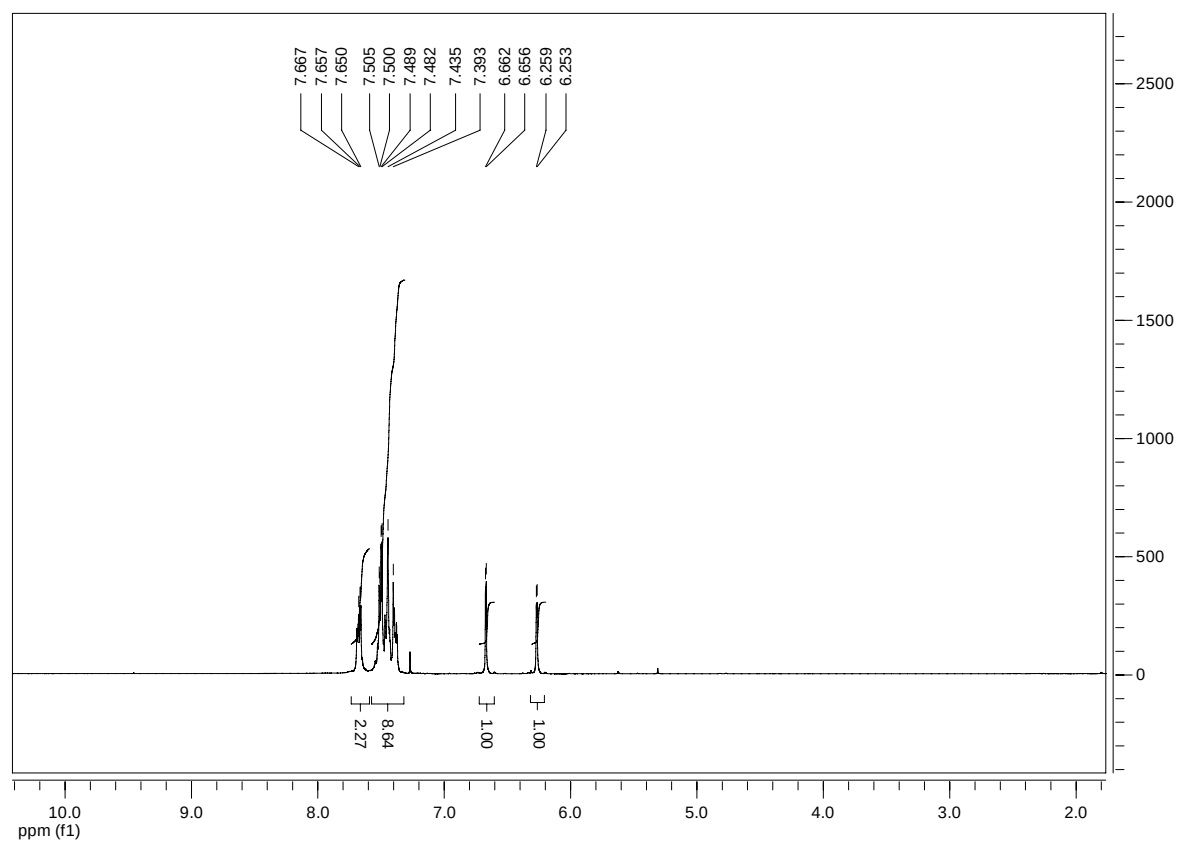
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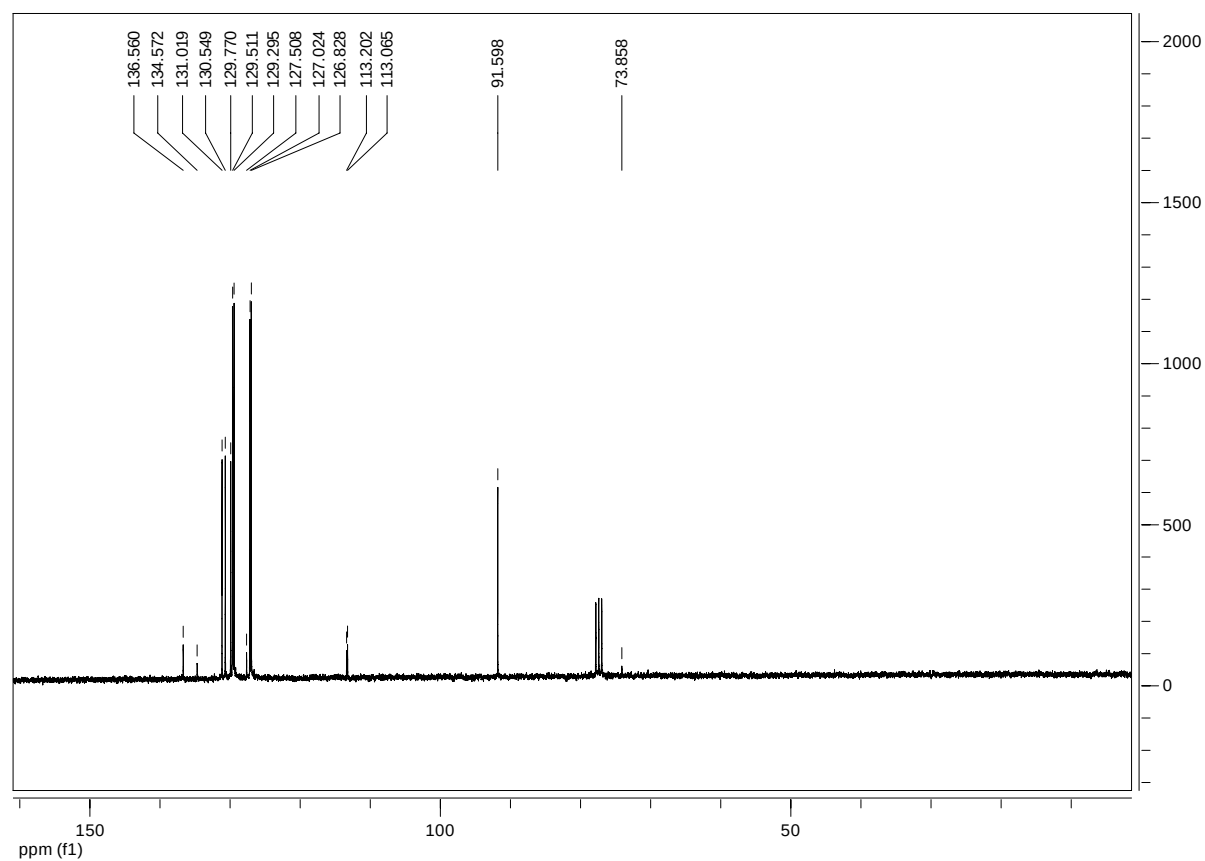
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Compound 3a

^1H NMR (300 MHz, CDCl_3):

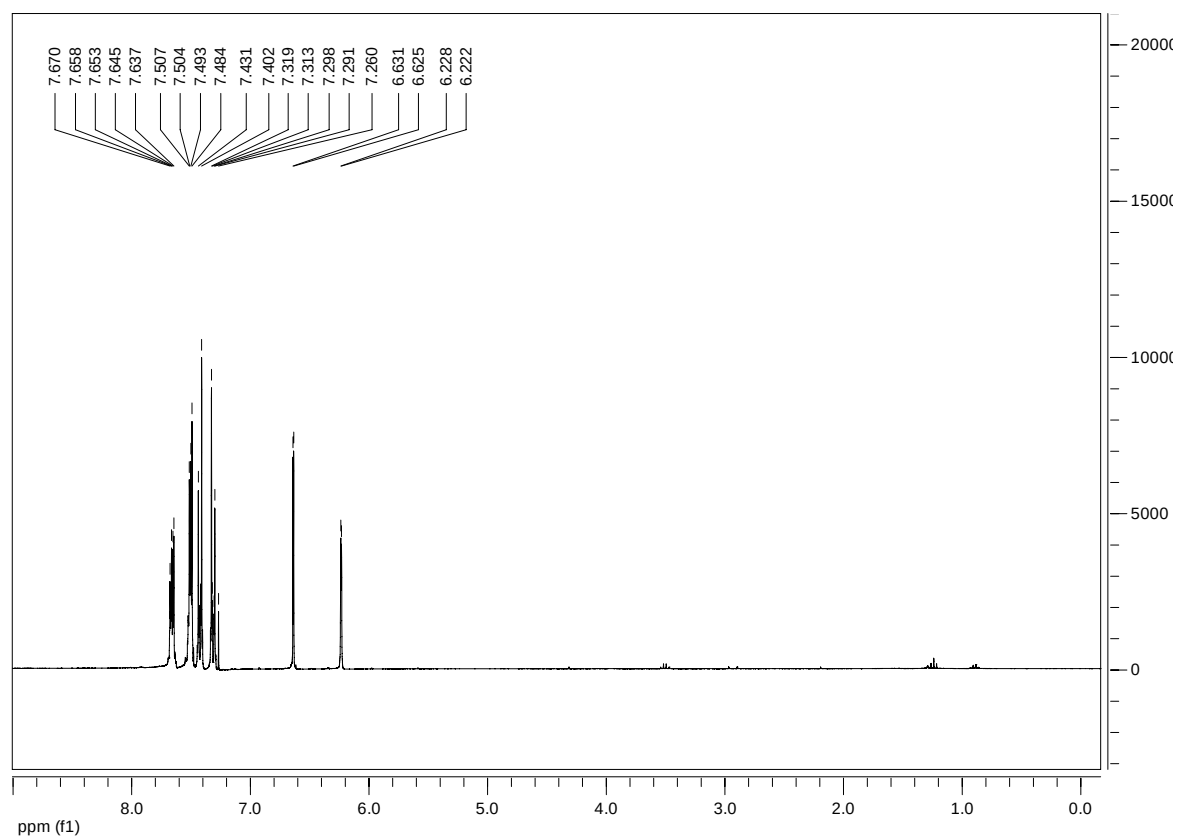


^{13}C NMR (75 MHz, CDCl_3):

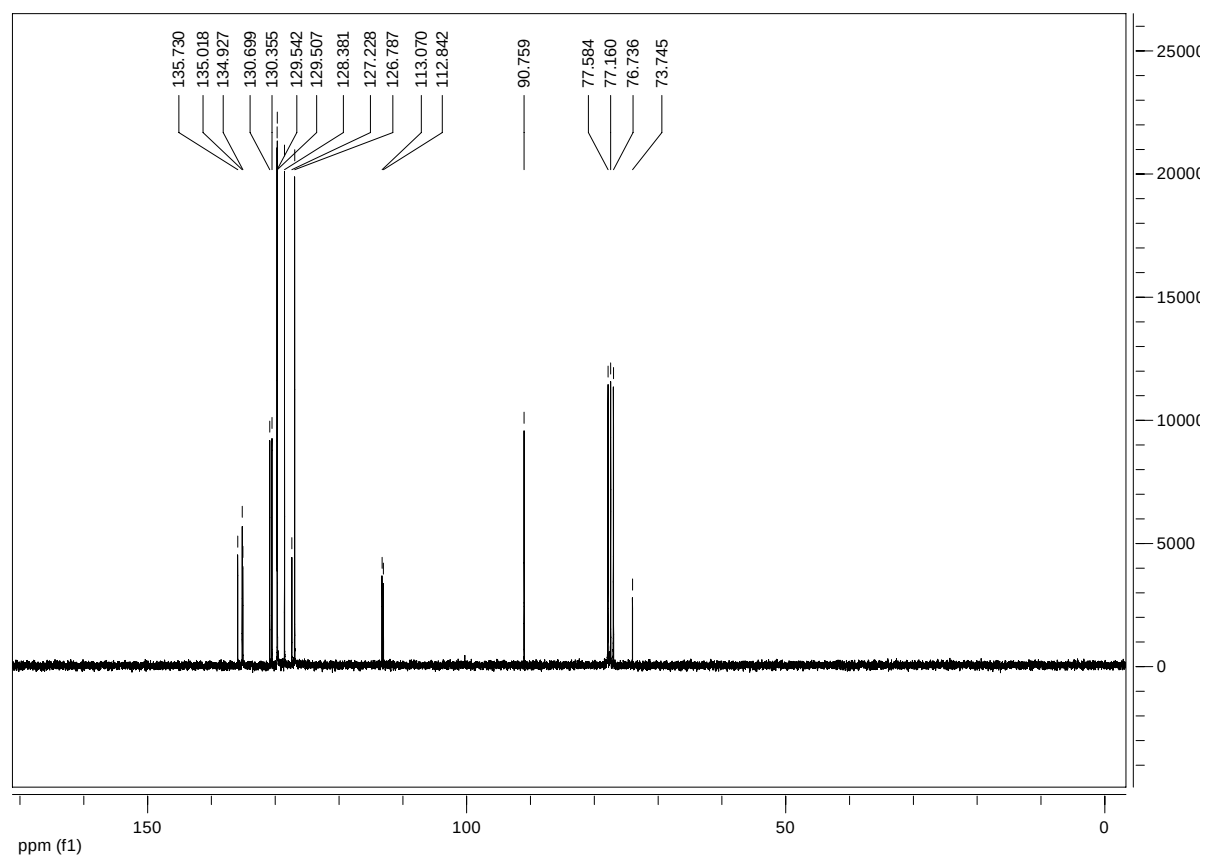


Compound **3b**

^1H NMR (300 MHz, CDCl_3):

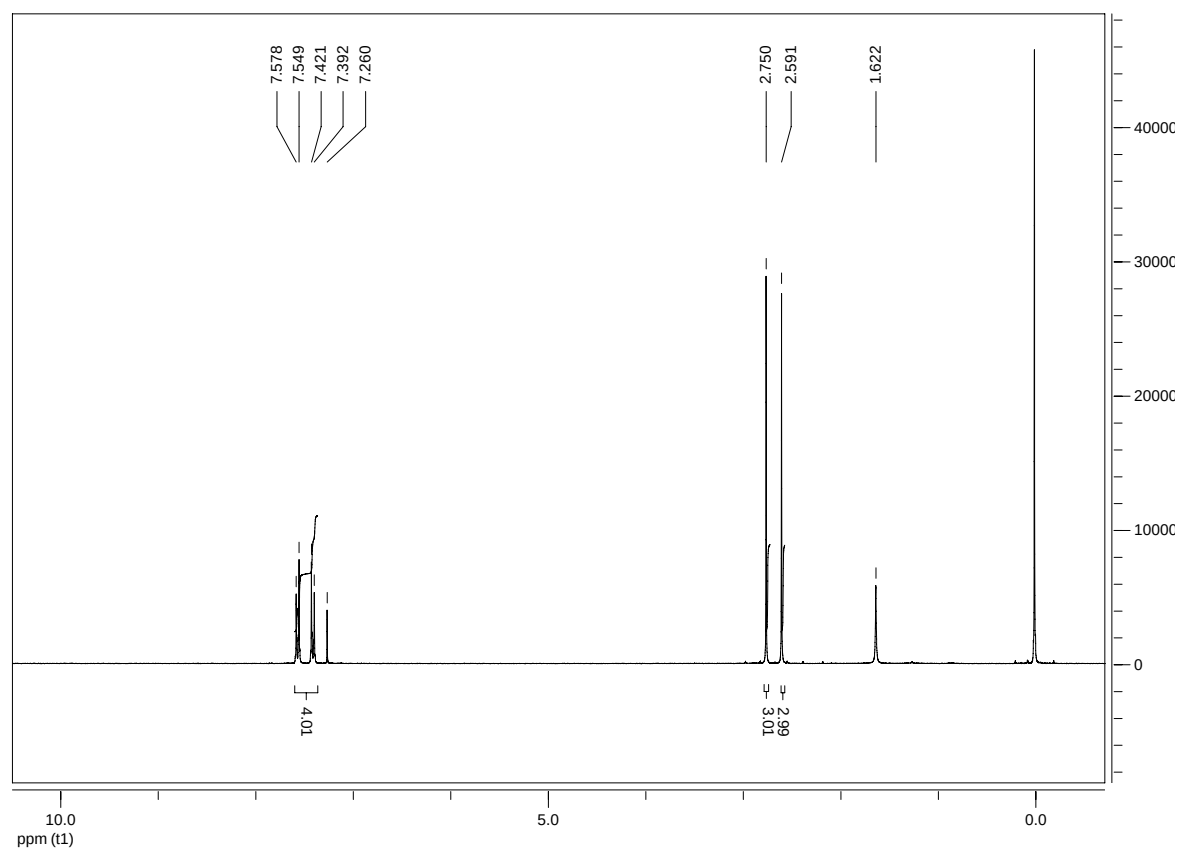


^{13}C NMR (75 MHz, CDCl_3):

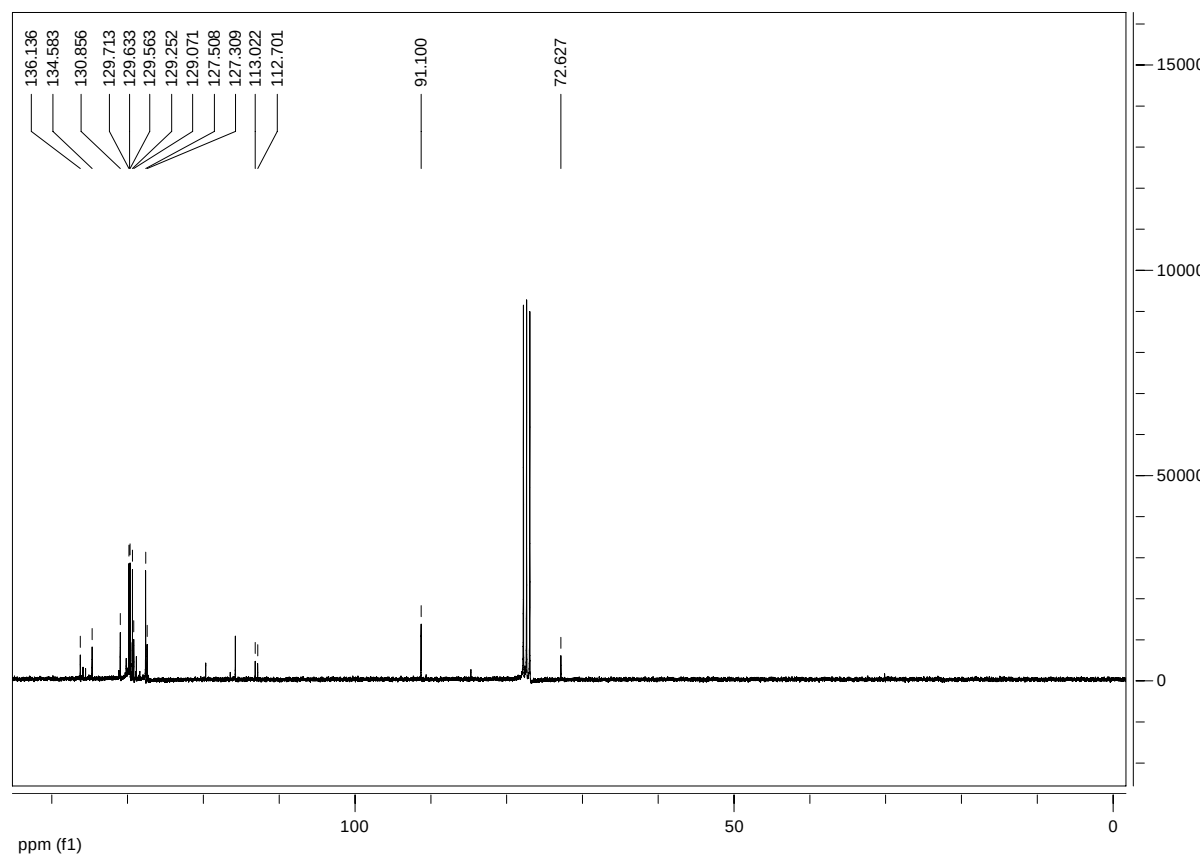


Compound 3'b

^1H NMR (300 MHz, CDCl_3):

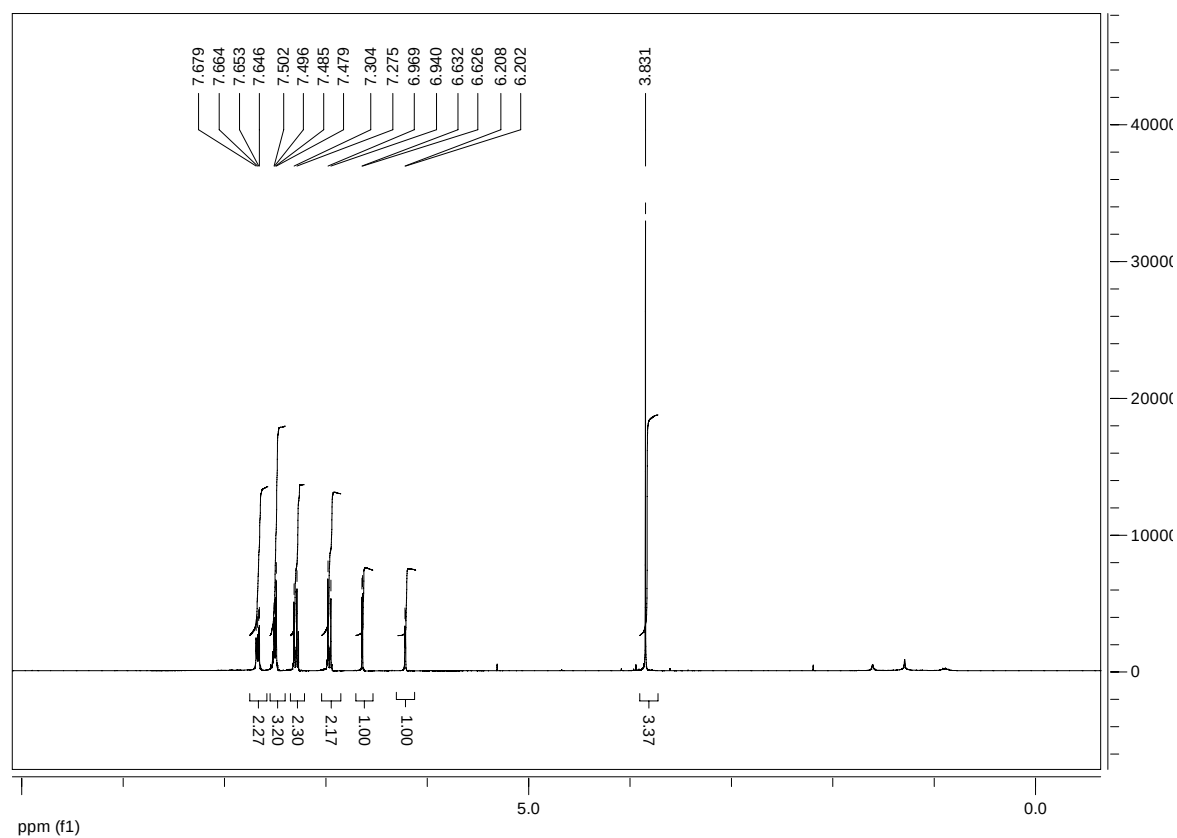


^{13}C NMR (75 MHz, CDCl_3):

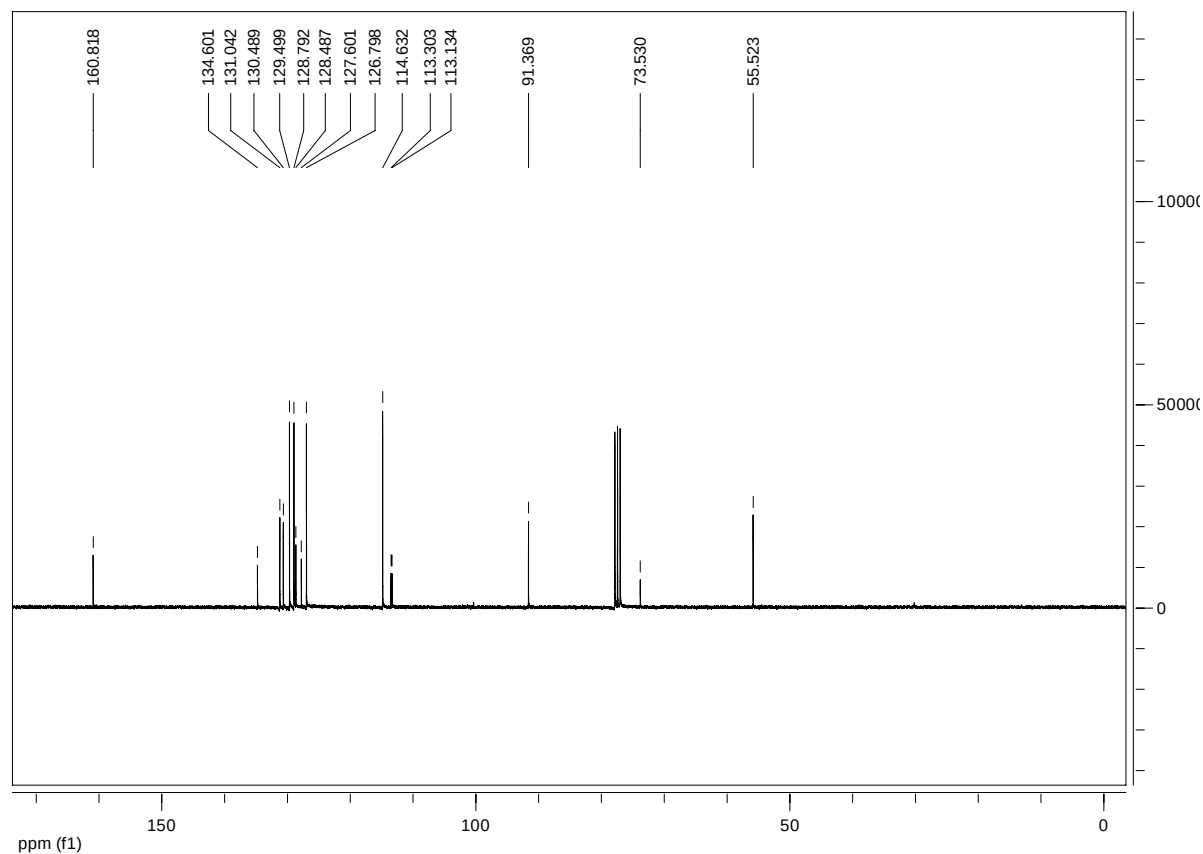


Compound 3c

^1H NMR (300 MHz, CDCl_3):

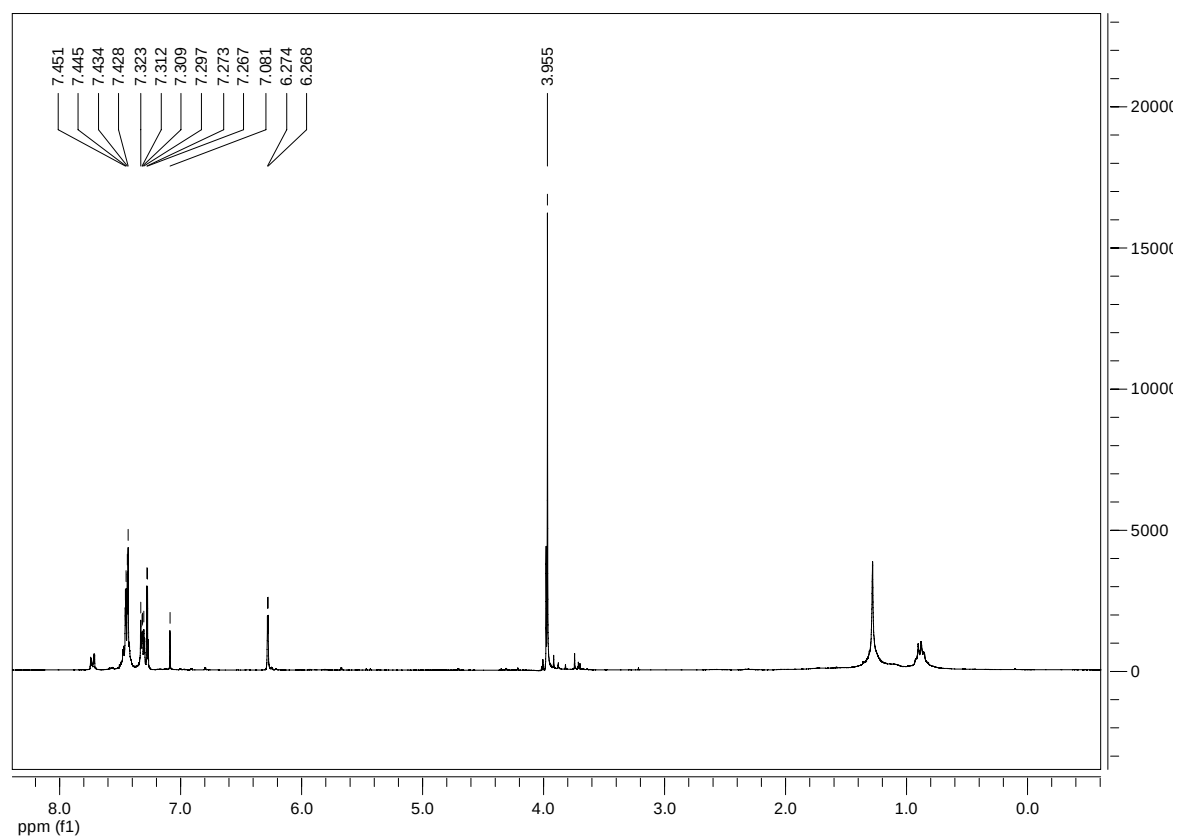


^{13}C NMR (75 MHz, CDCl_3):

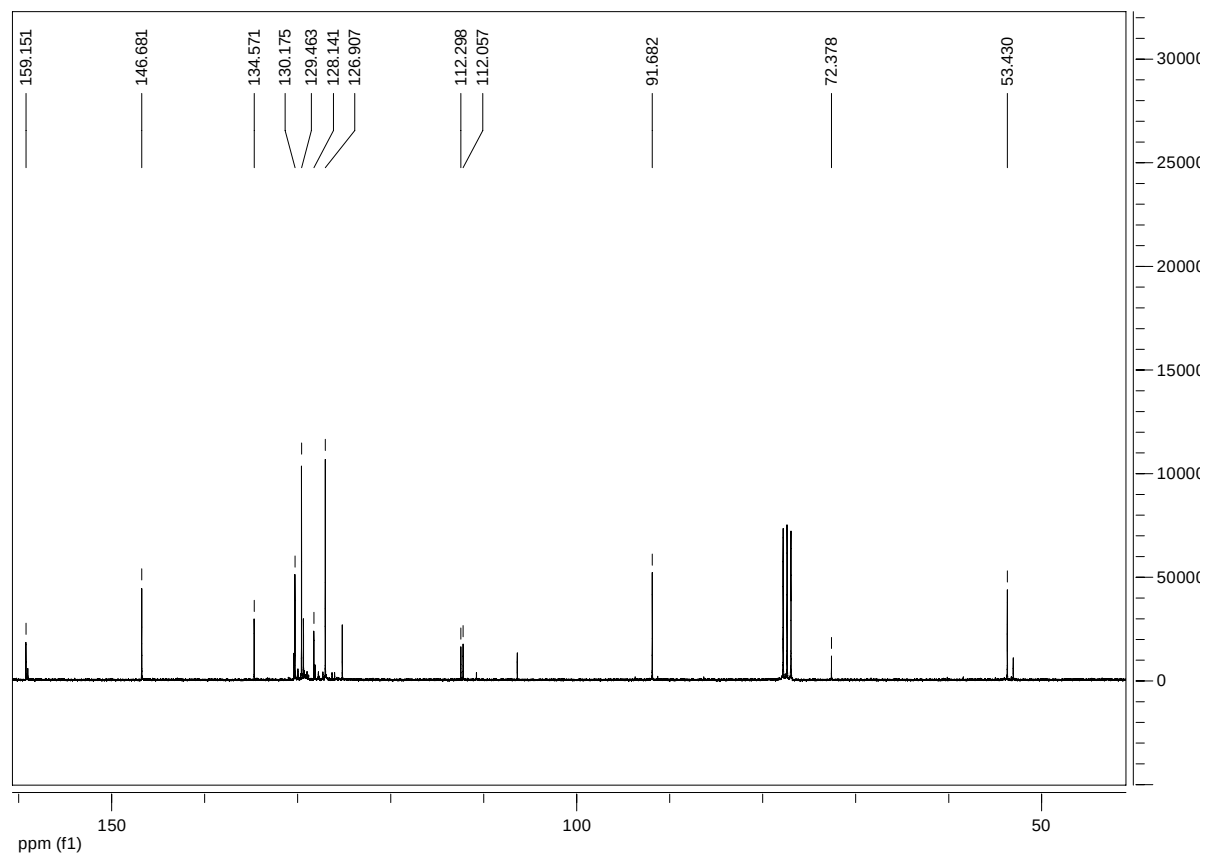


Compound 5a

^1H NMR (300 MHz, CDCl_3):

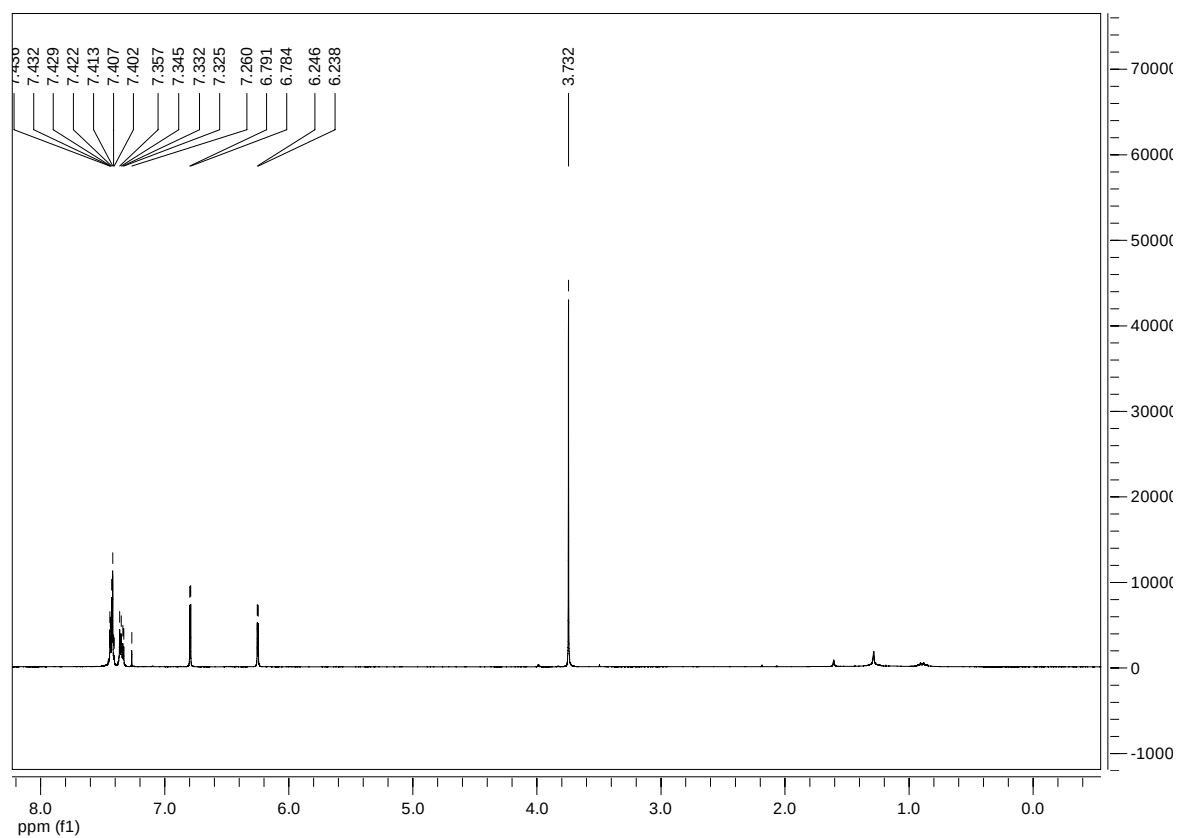


^{13}C NMR (75 MHz, CDCl_3):

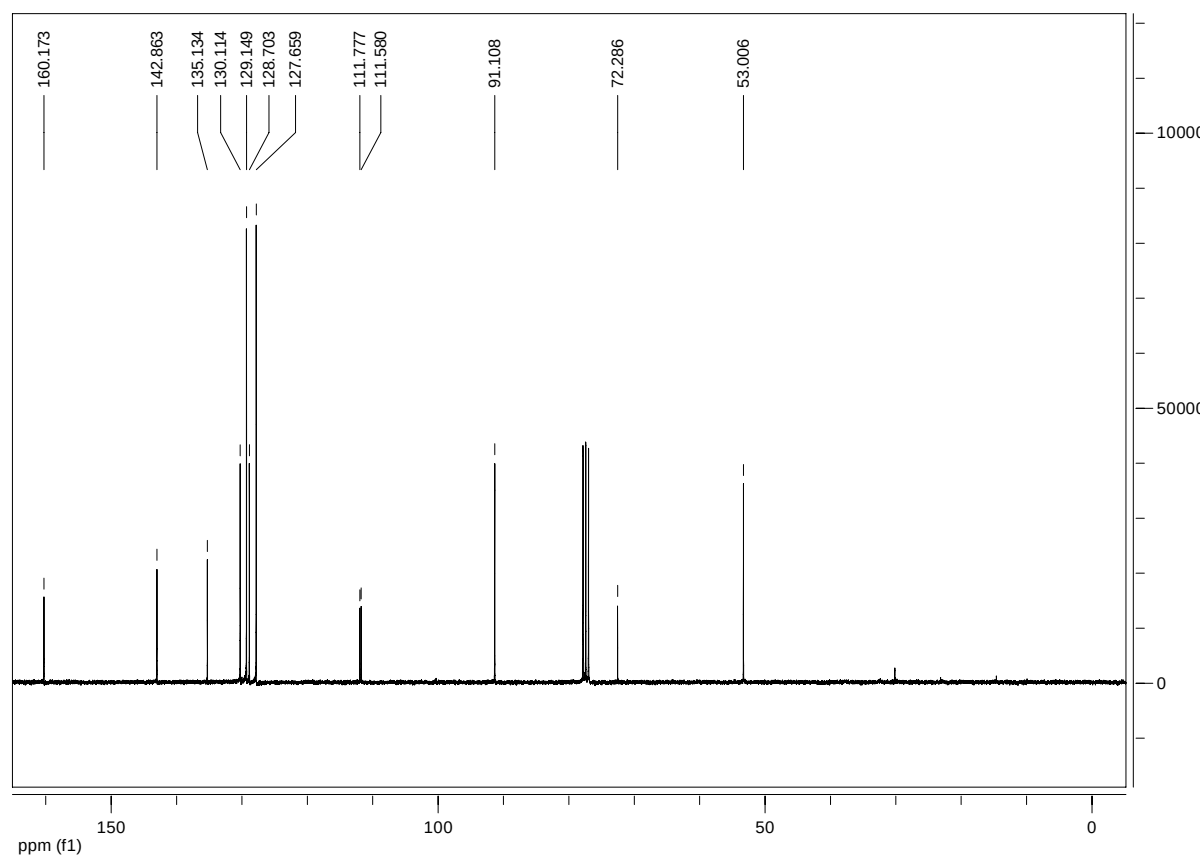


Compound 5'a

^1H NMR (300 MHz, CDCl_3):

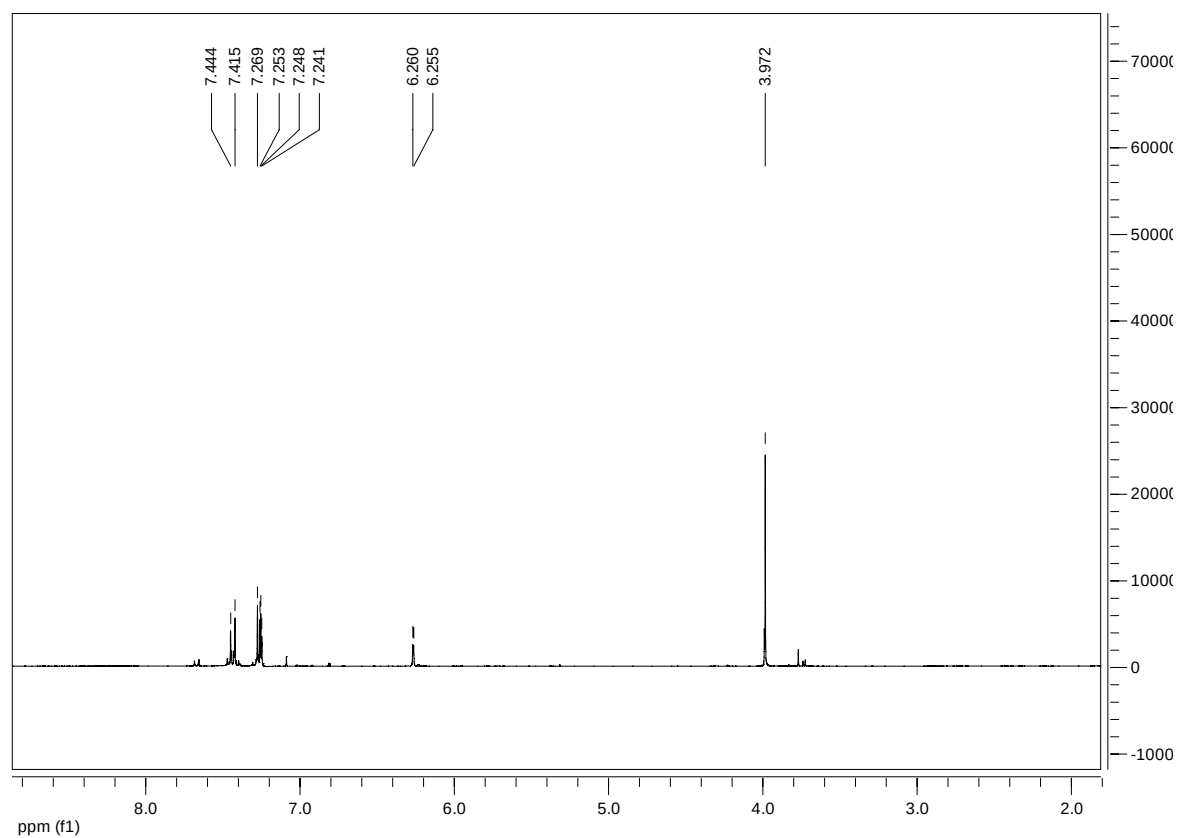


^{13}C NMR (75 MHz, CDCl_3):

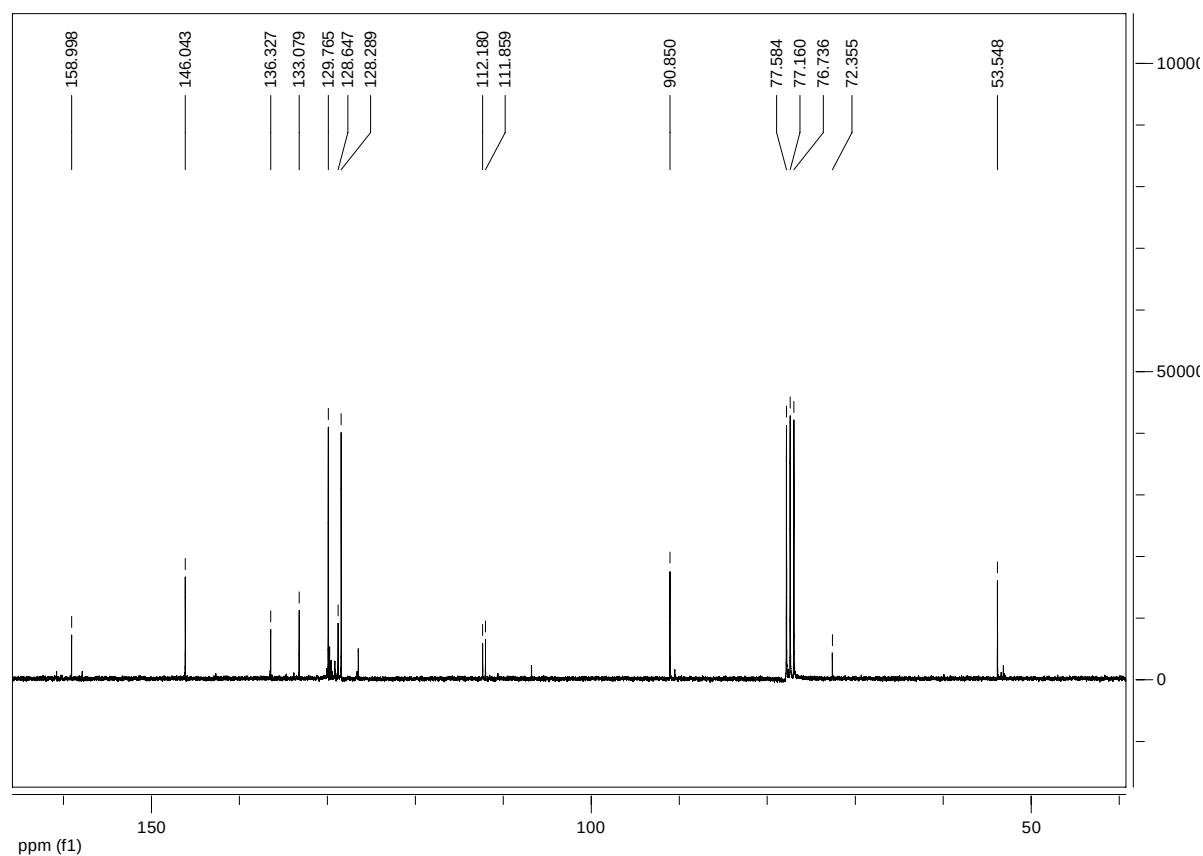


Compound **5b**

^1H NMR (300 MHz, CDCl_3):

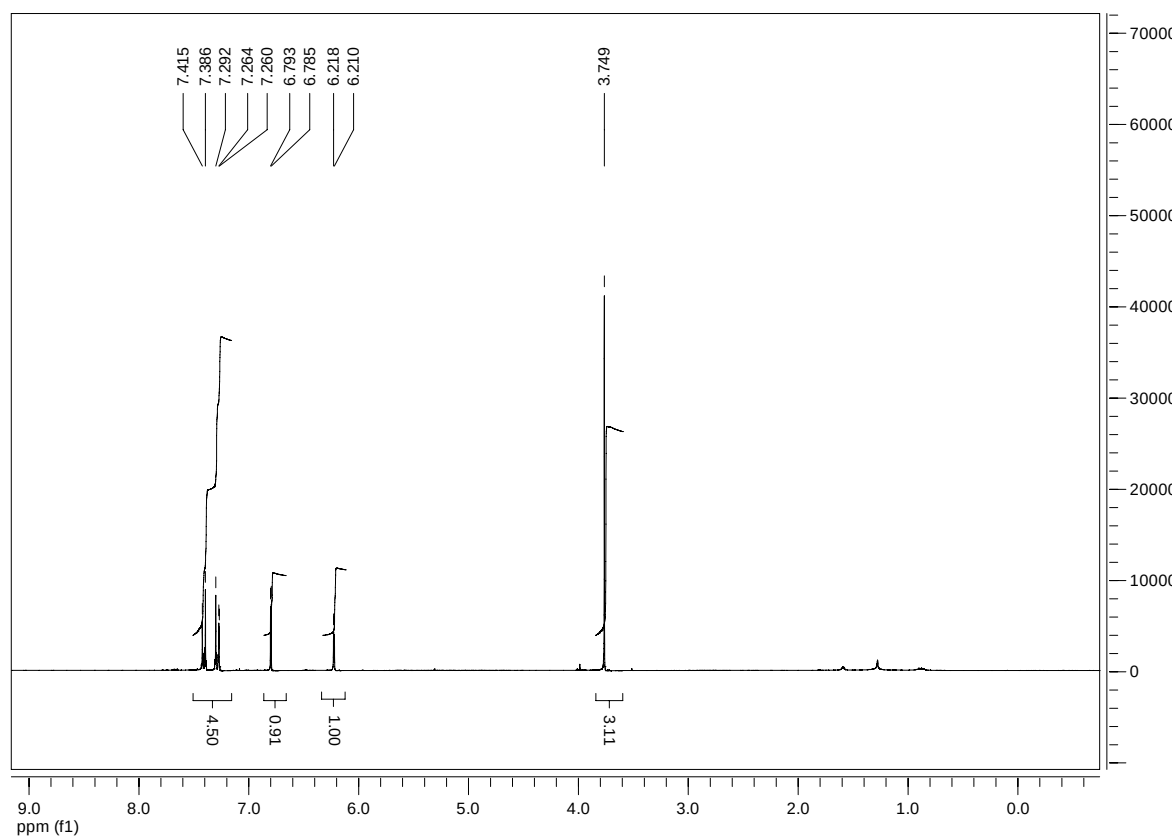


^{13}C NMR (75 MHz, CDCl_3):

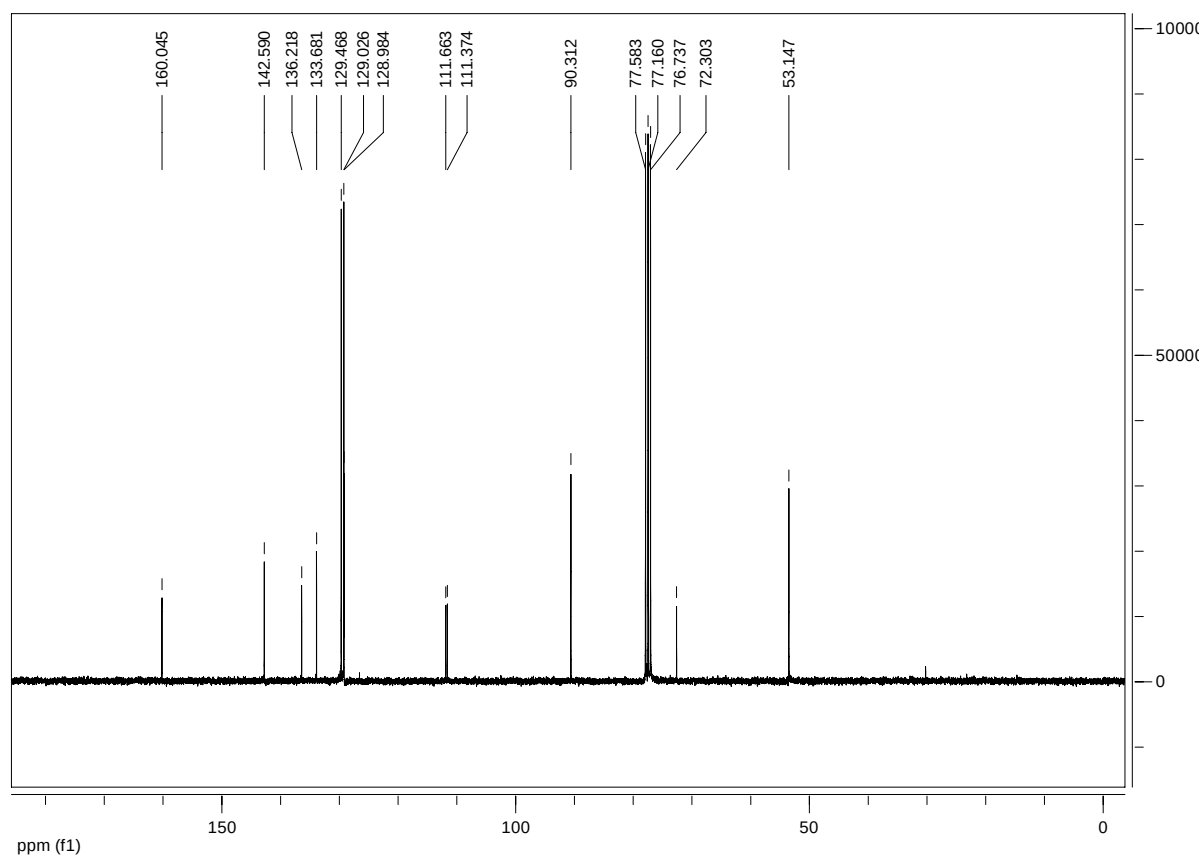


Compound 5'b

¹H NMR (300 MHz, CDCl₃):

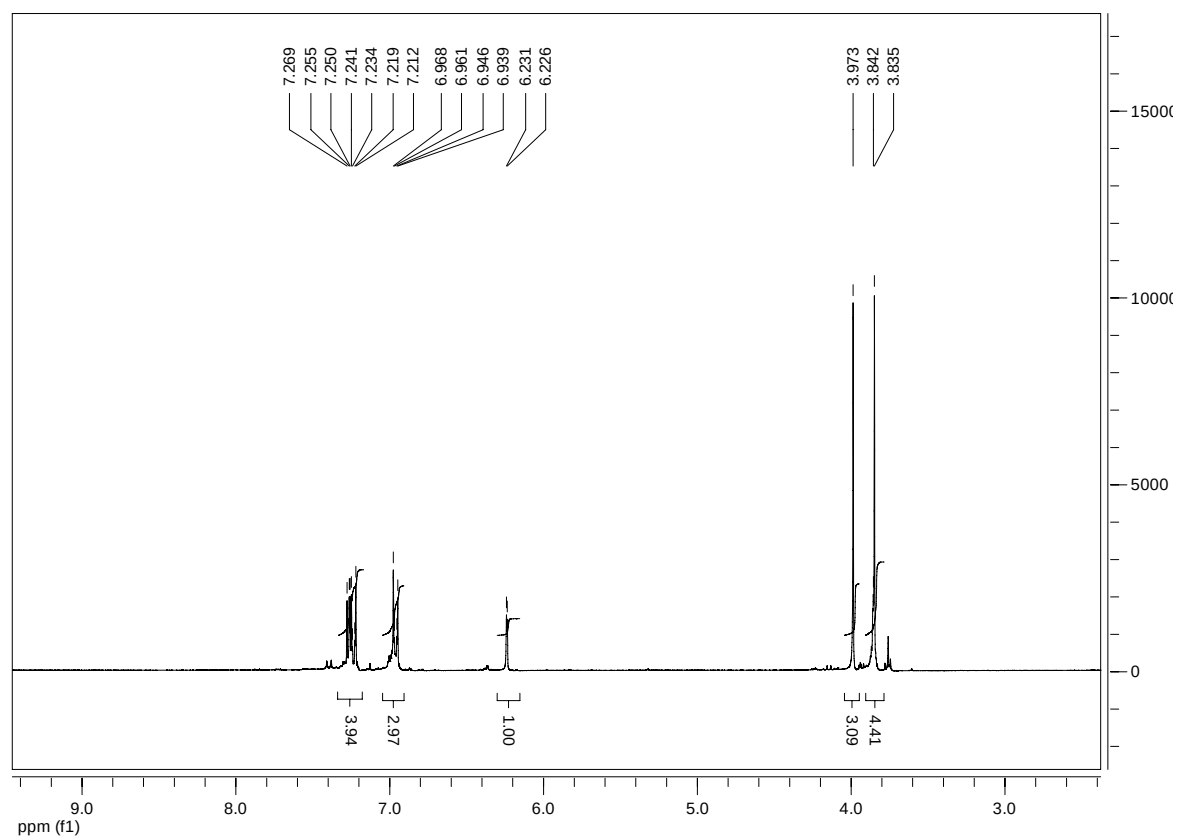


¹³C NMR (75 MHz, CDCl₃):

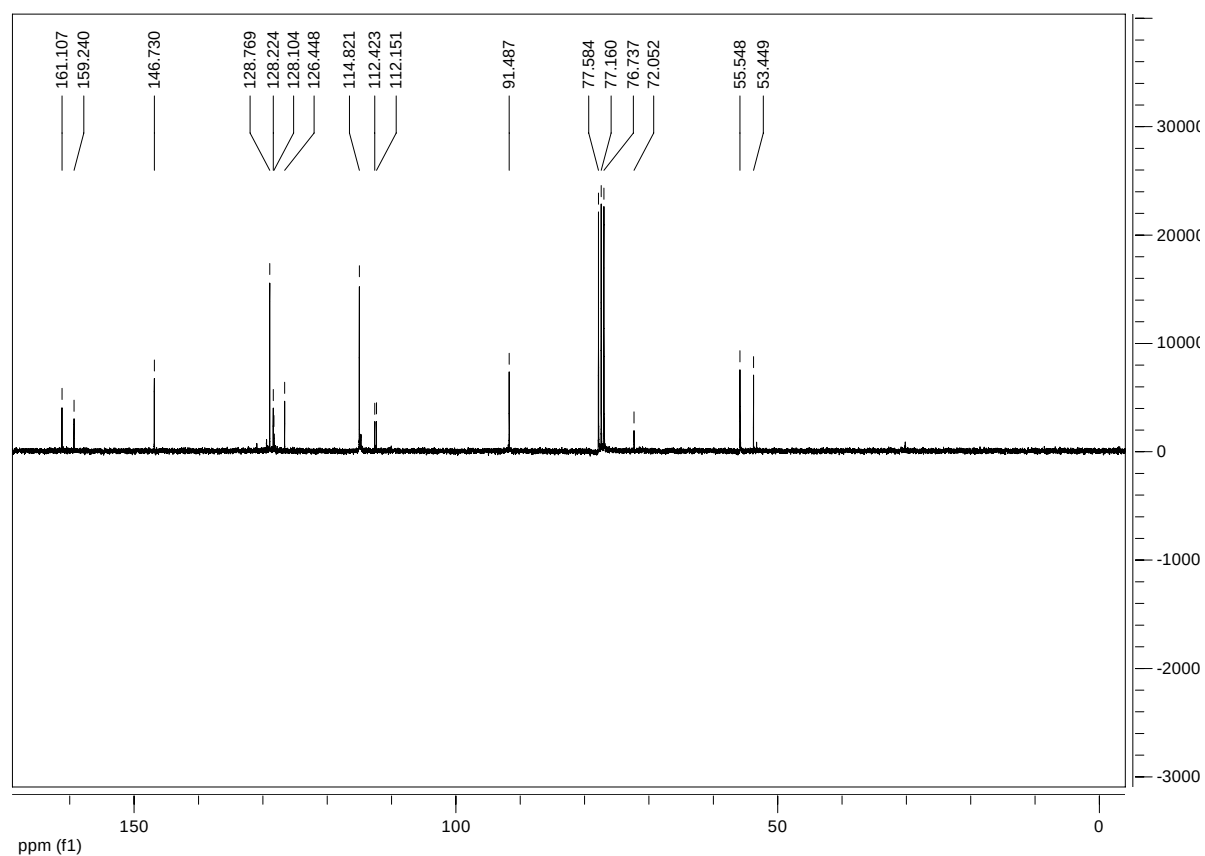


Compound 5c

¹H NMR (300 MHz, CDCl₃):

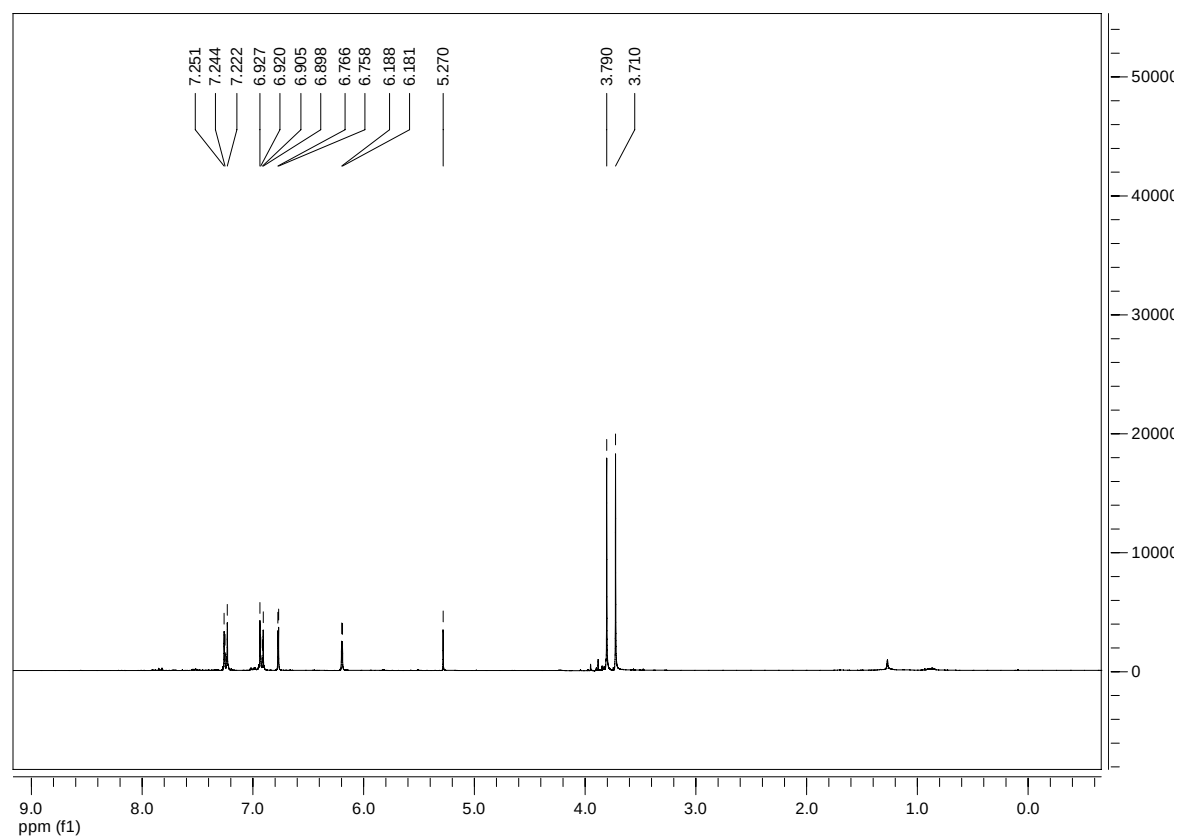


¹³C NMR (75 MHz, CDCl₃):

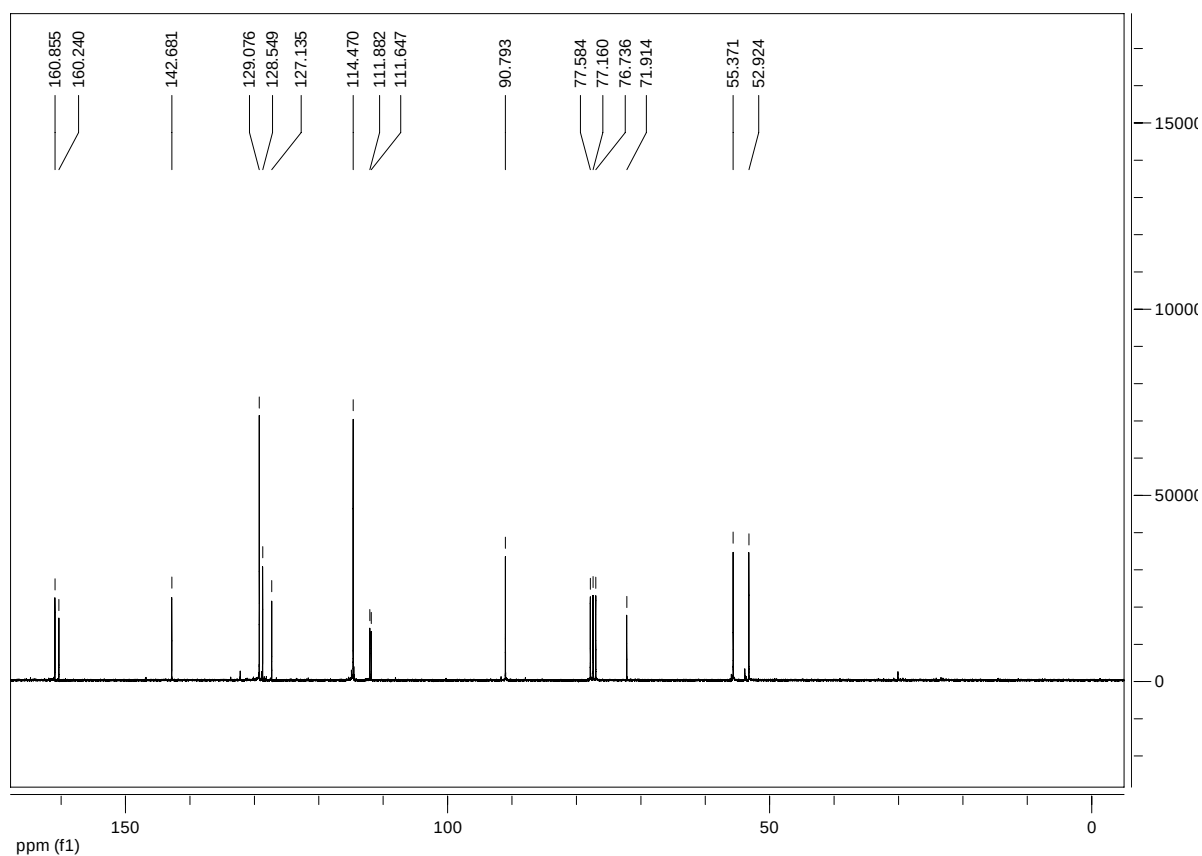


Compound 5'c

^1H NMR (300 MHz, CDCl_3):

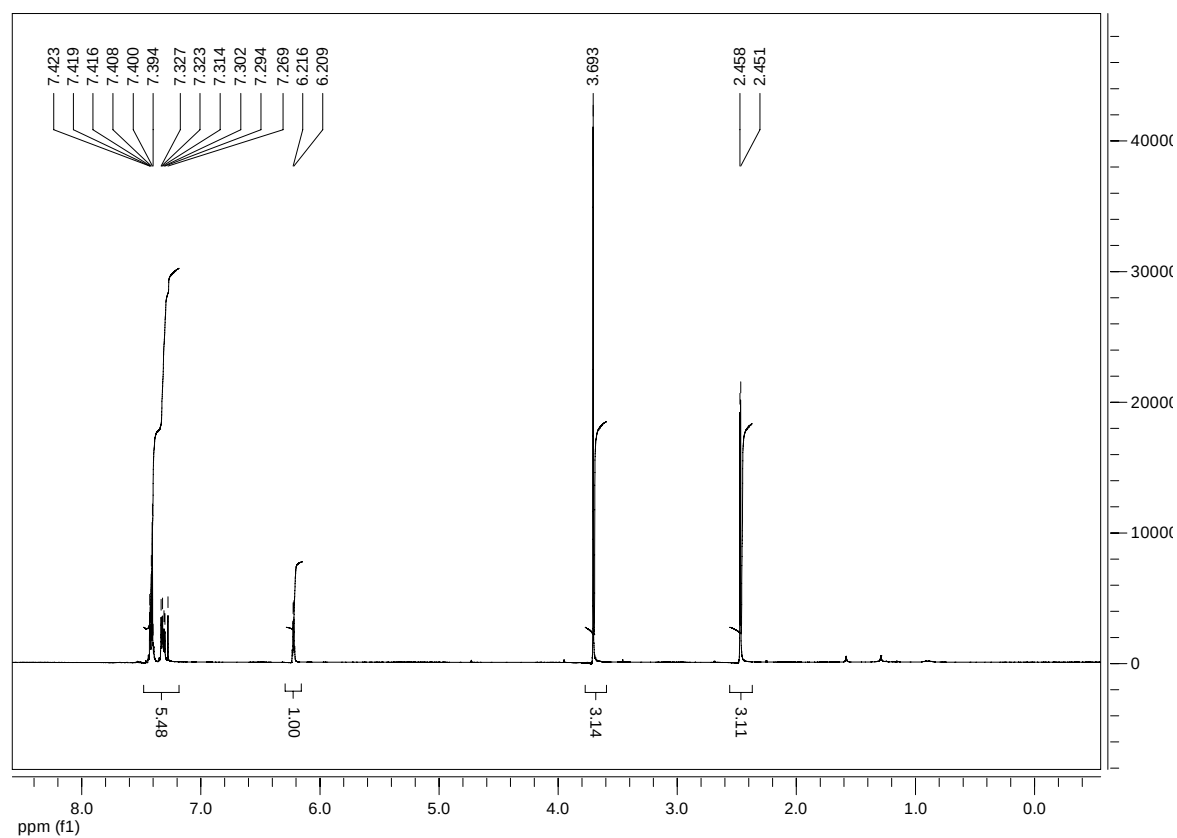


^{13}C NMR (75 MHz, CDCl_3):

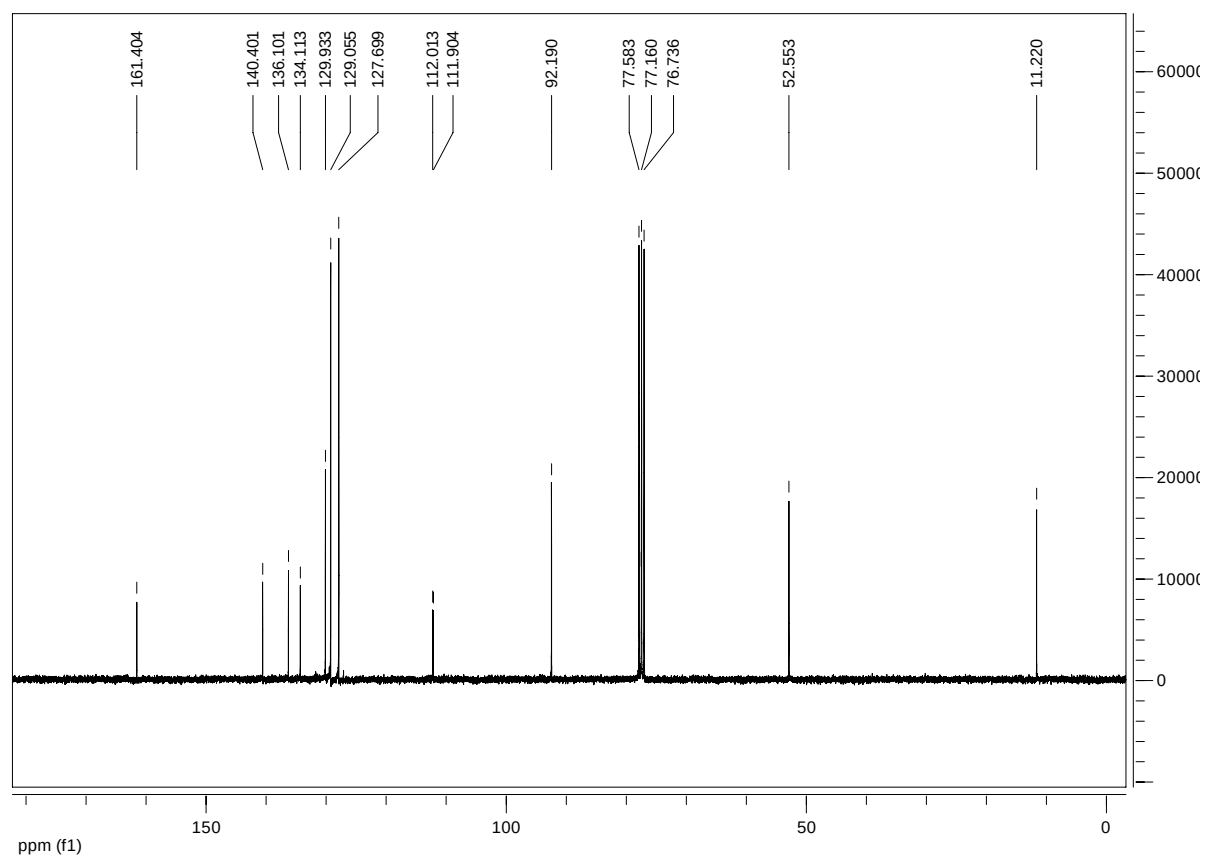


Compound 8a

^1H NMR (300 MHz, CDCl_3):

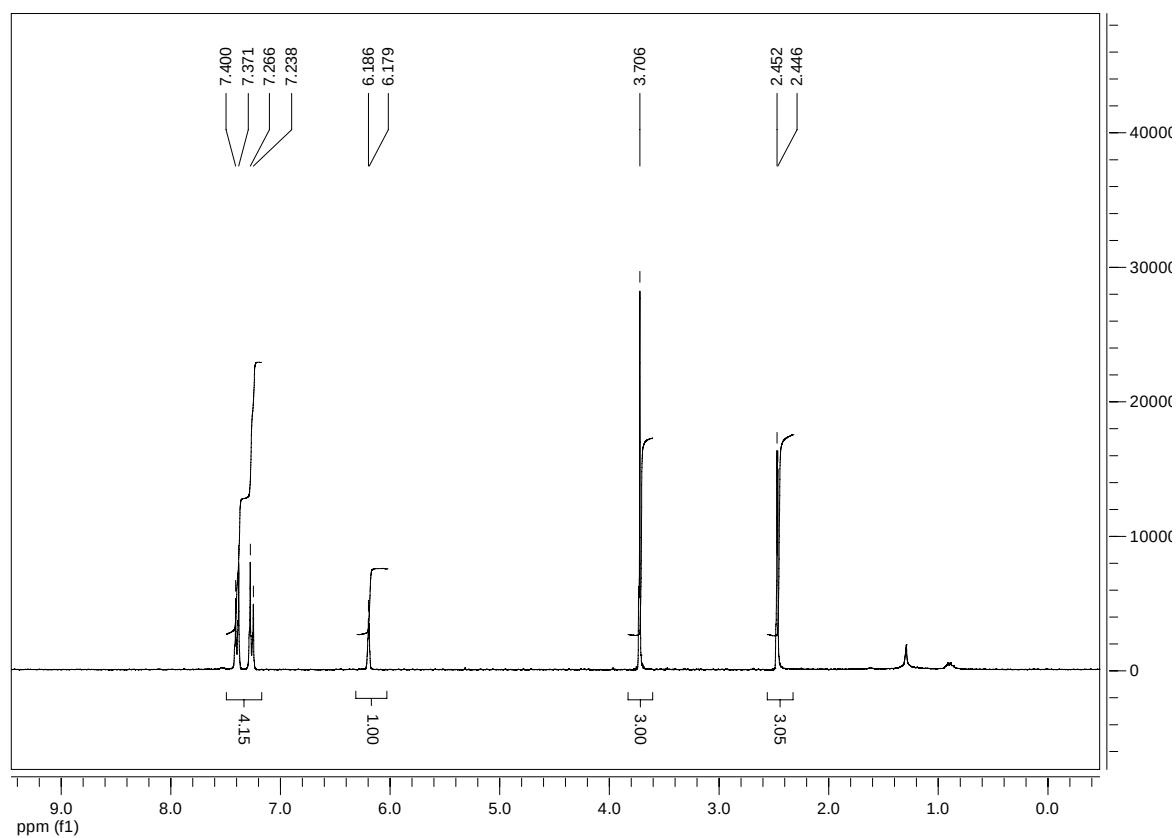


^{13}C NMR (75 MHz, CDCl_3):

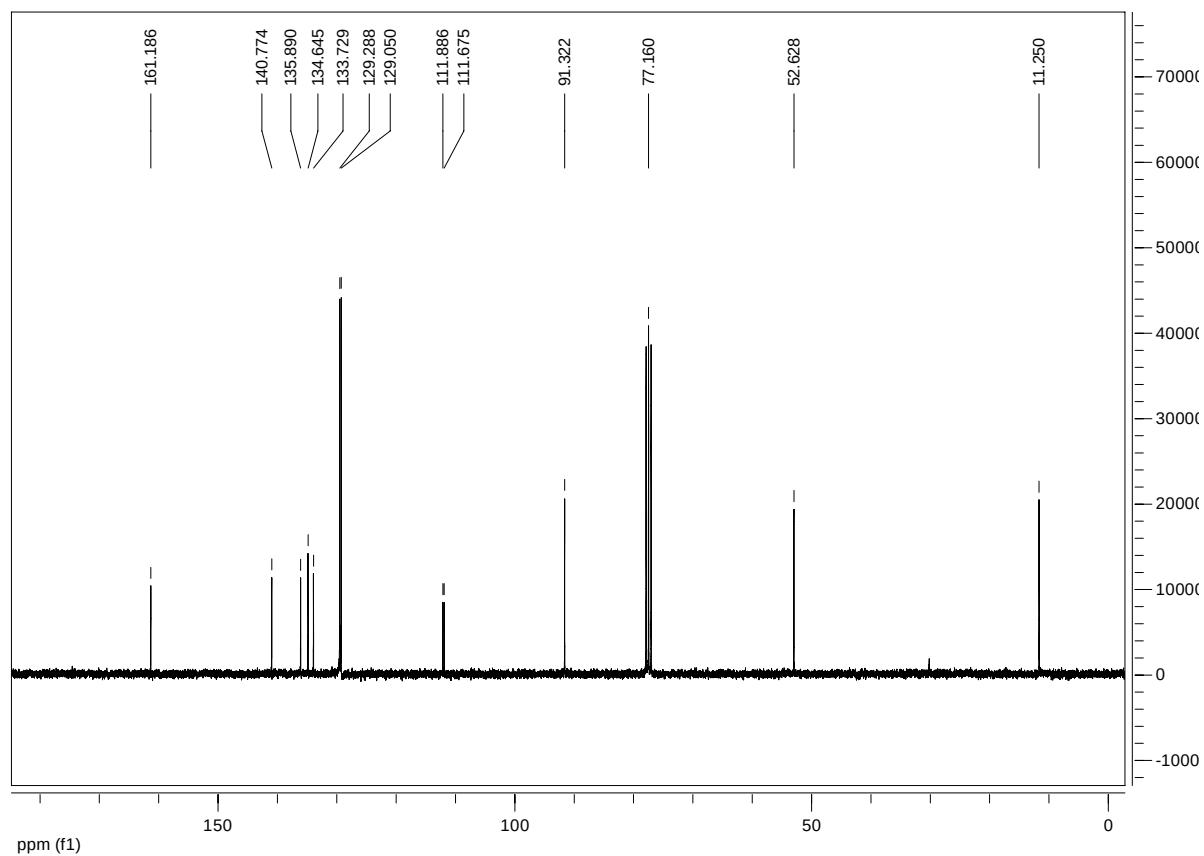


Compound **8b**

^1H NMR (300 MHz, CDCl_3):

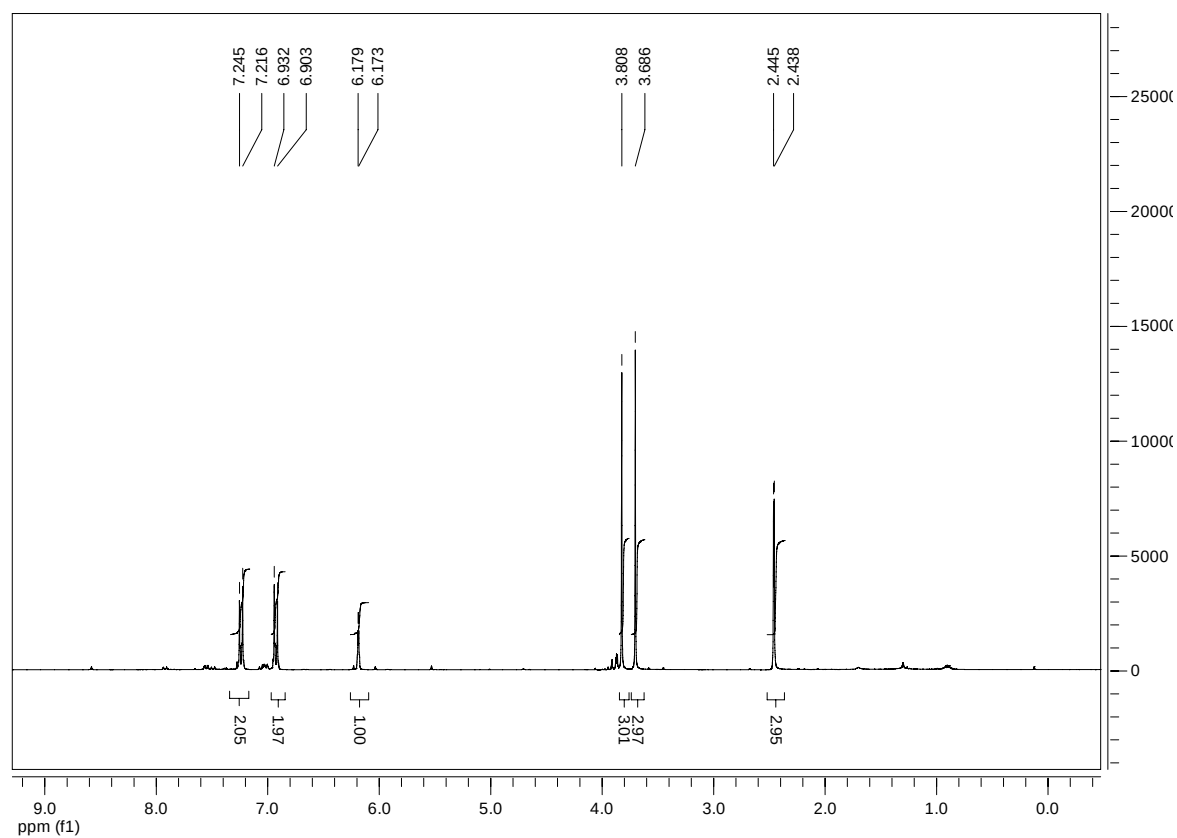


^{13}C NMR (75 MHz, CDCl_3):

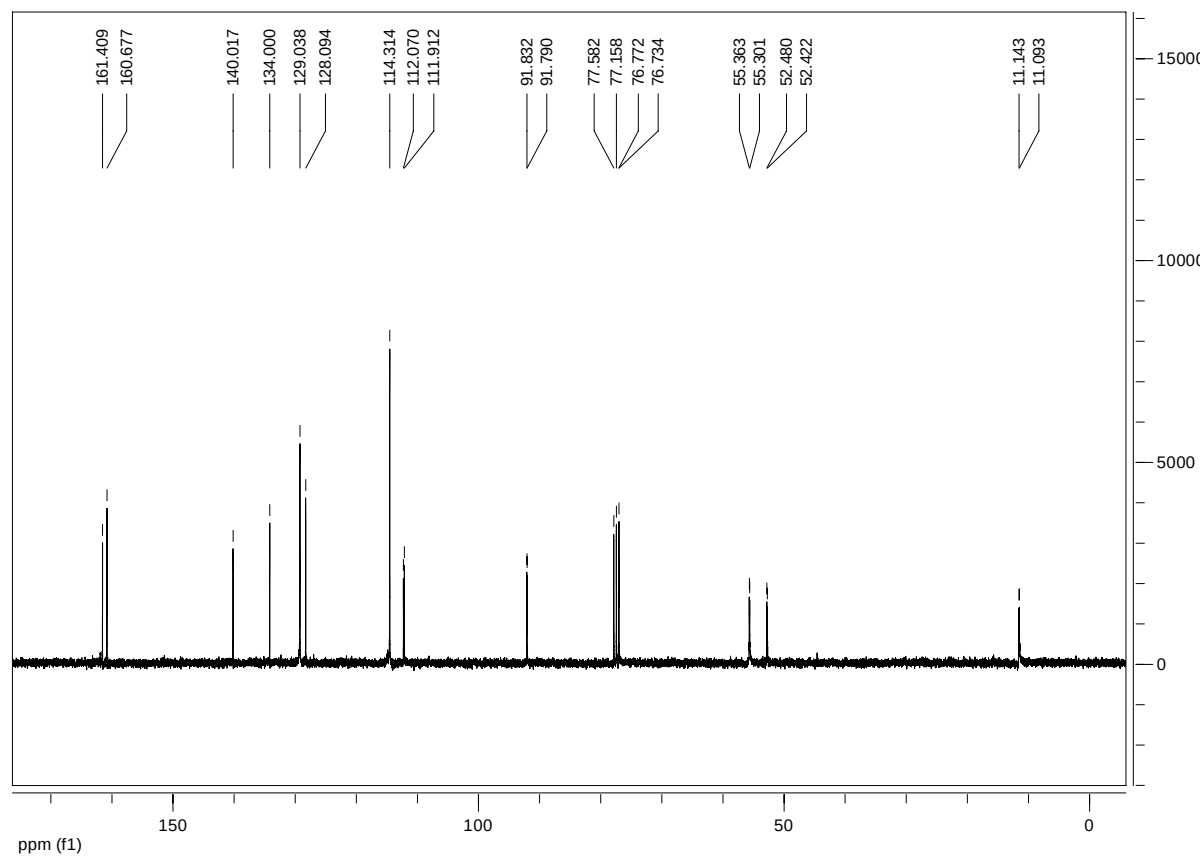


Compound **8c**

^1H NMR (300 MHz, CDCl_3):

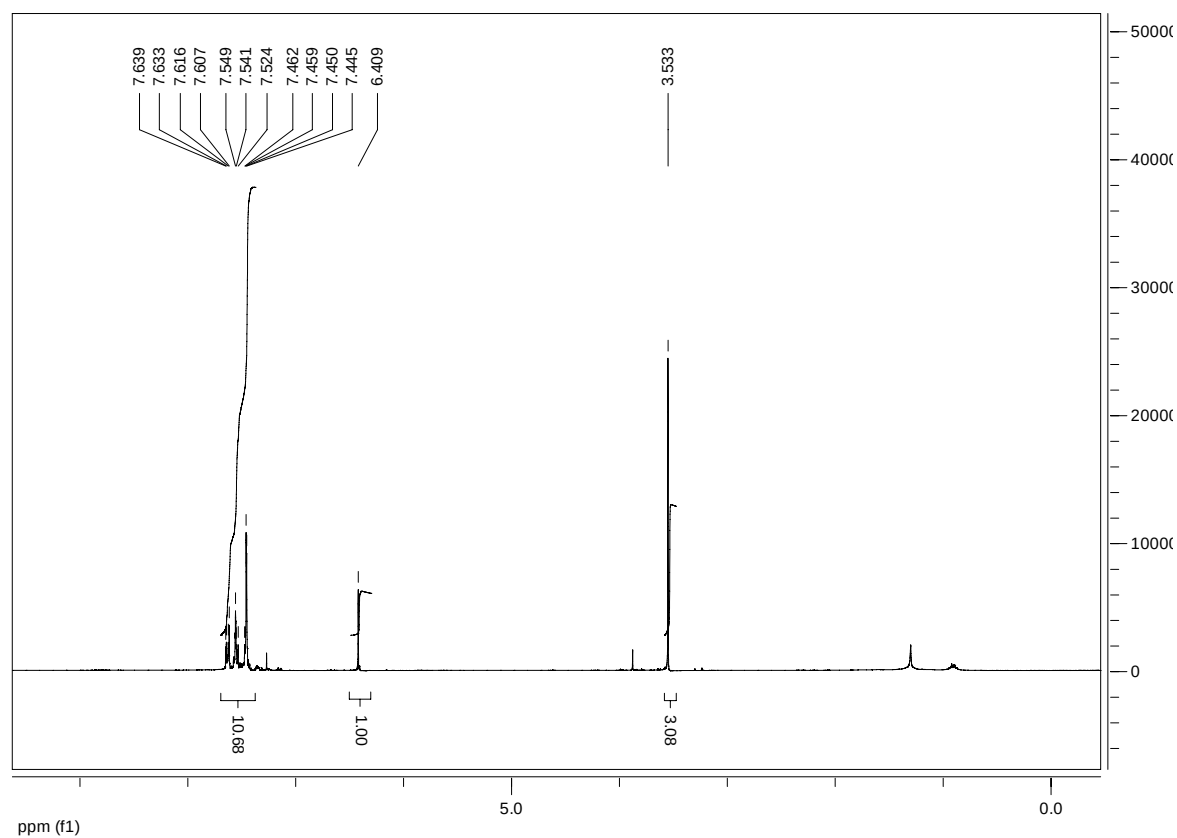


^{13}C NMR (75 MHz, CDCl_3):

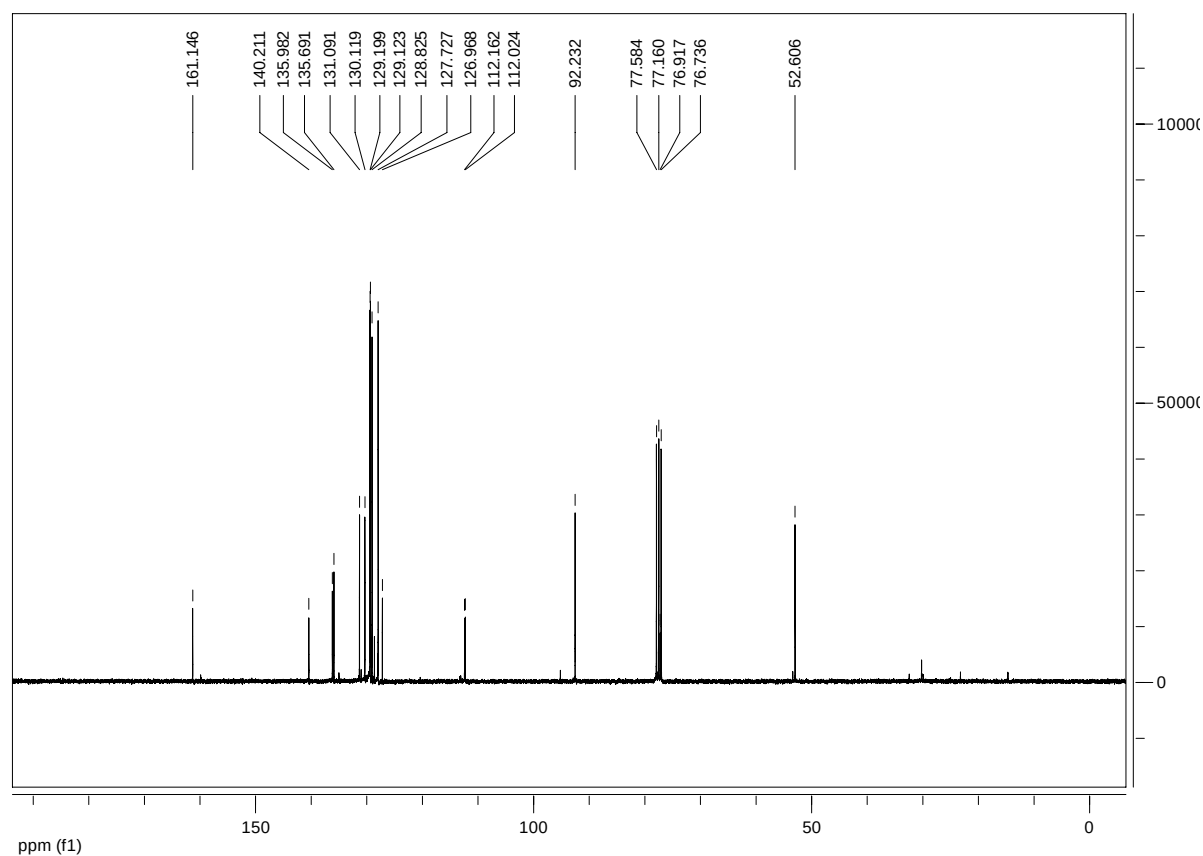


Compound 9a

^1H NMR (300 MHz, CDCl_3):

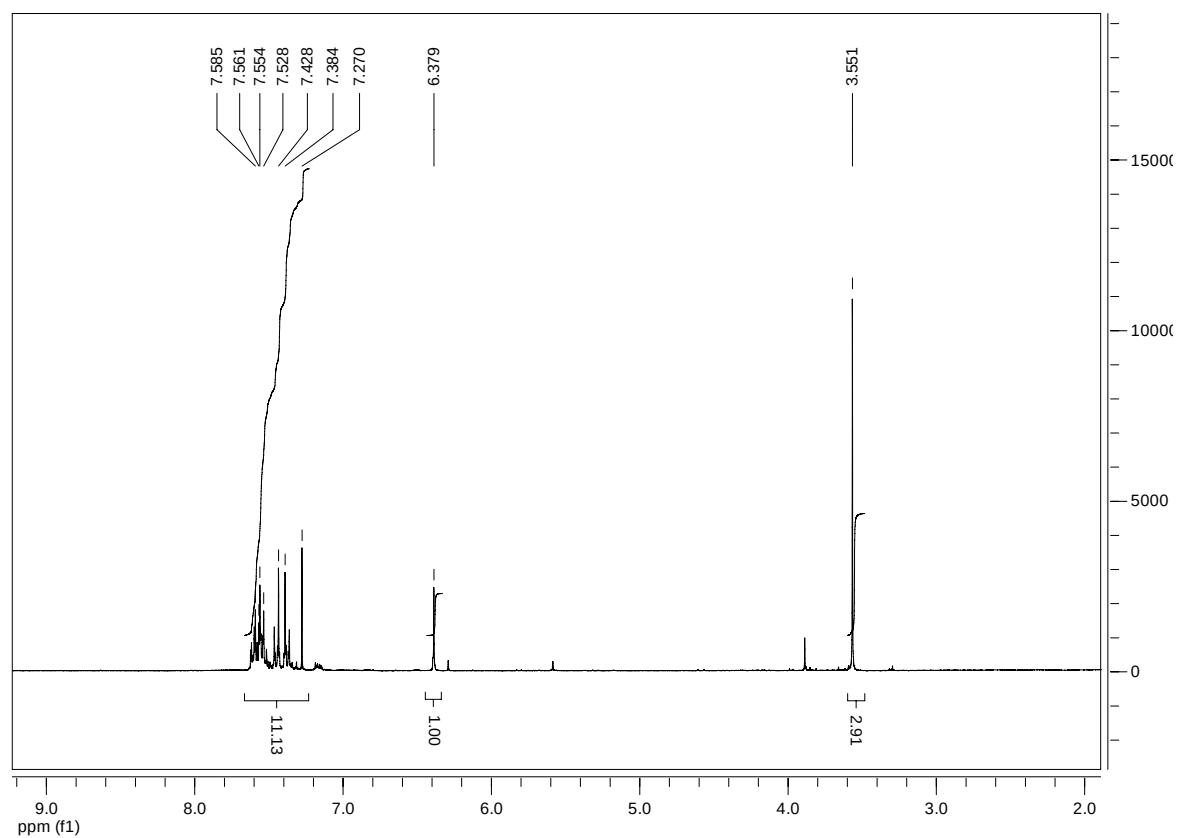


^{13}C NMR (75 MHz, CDCl_3):

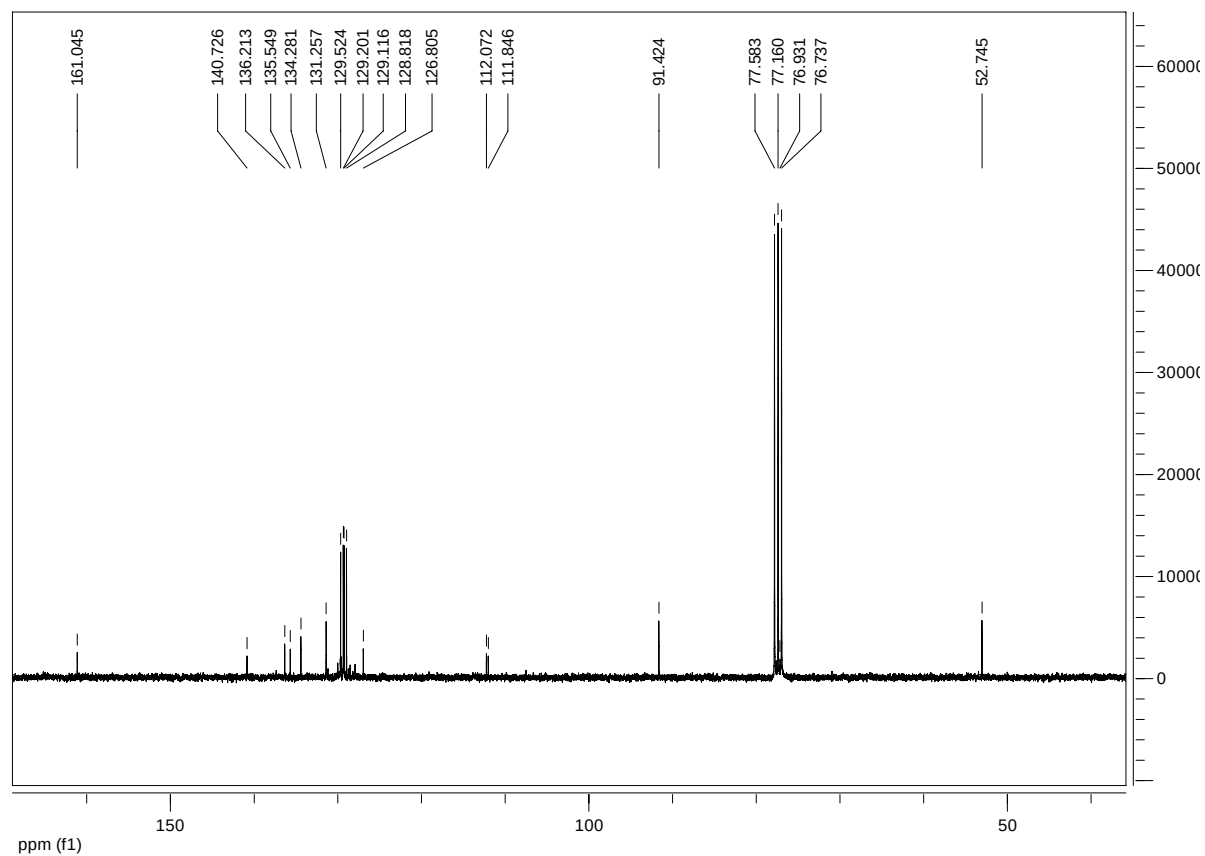


Compound **9b**

^1H NMR (300 MHz, CDCl_3):

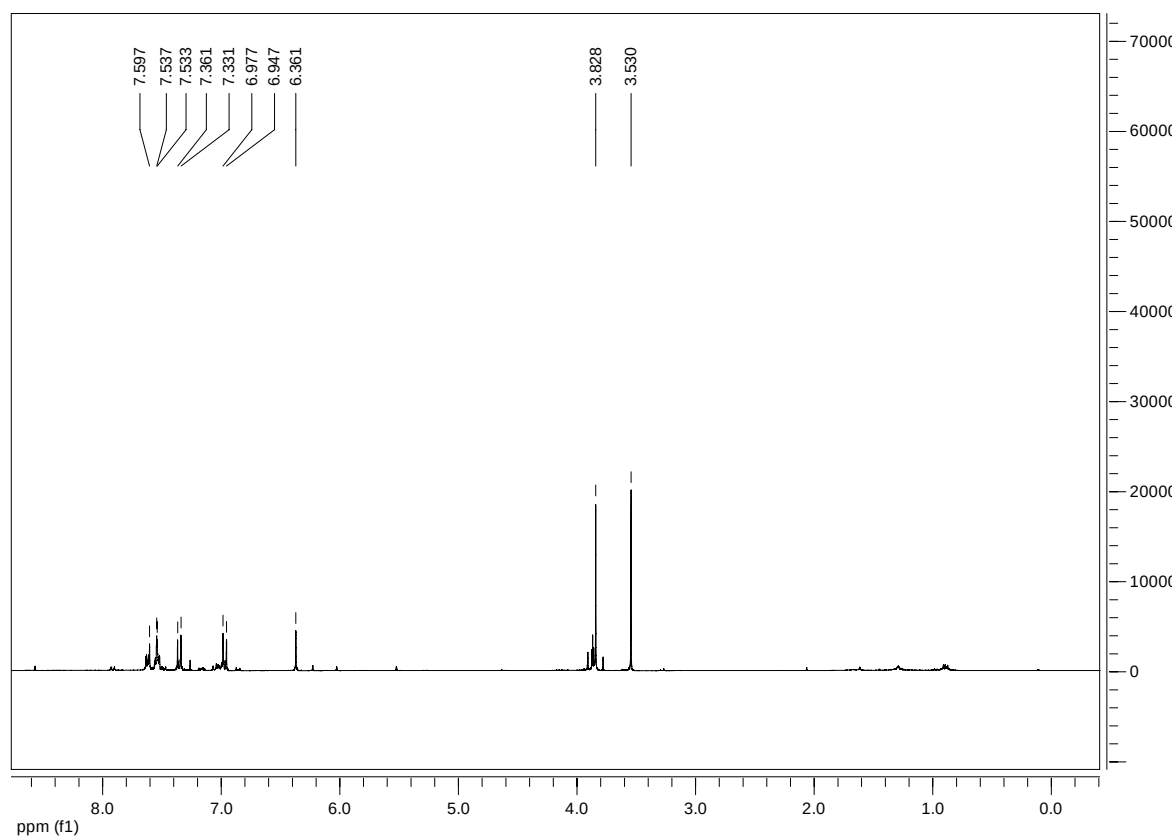


^{13}C NMR (75 MHz, CDCl_3):

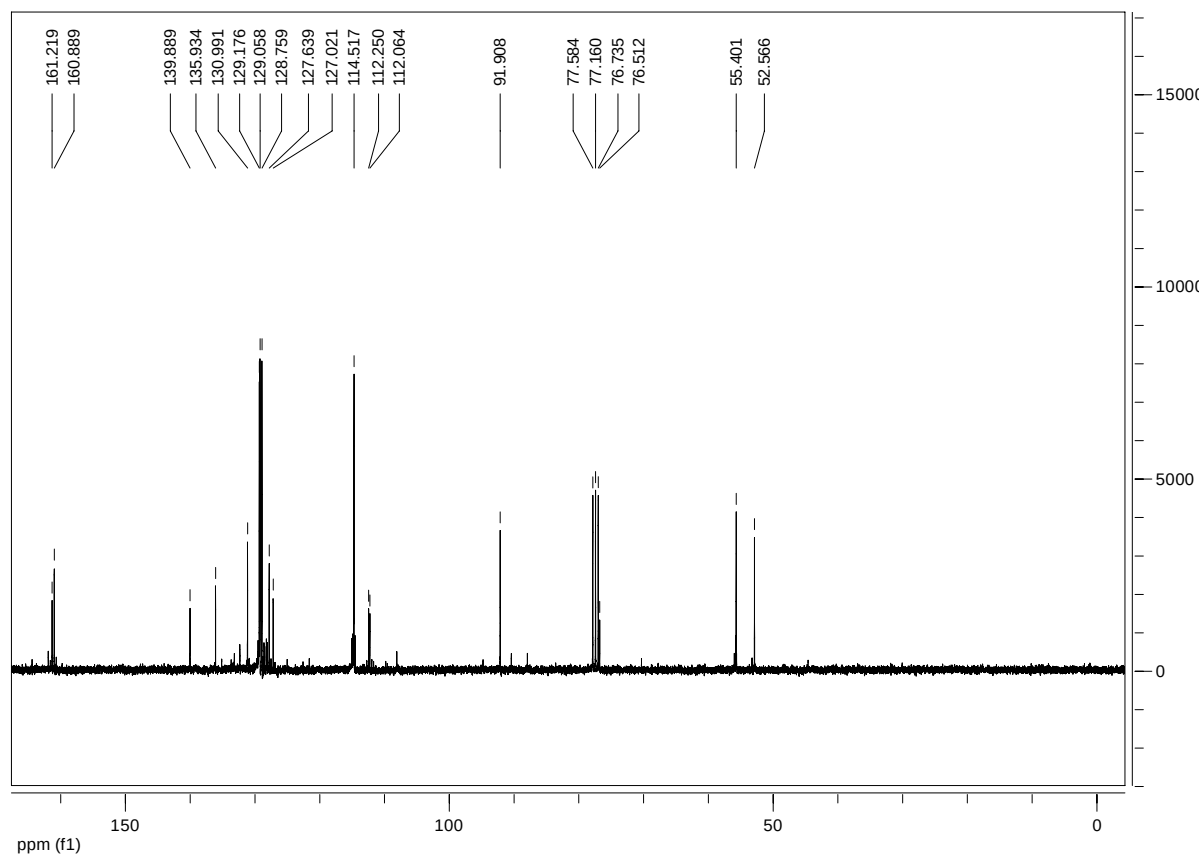


Compound **9c**

^1H NMR (300 MHz, CDCl_3):



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



X-Ray diagrams

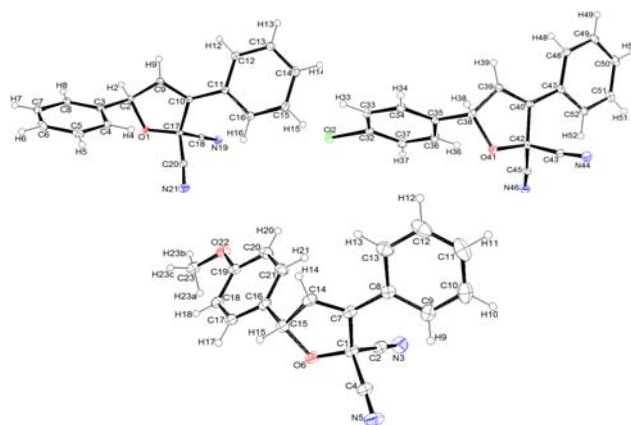


Figure 1 ORTEP diagram (30% probability) of racemic **3a** (top left), **3b** (top right), and **3c** (bottom).

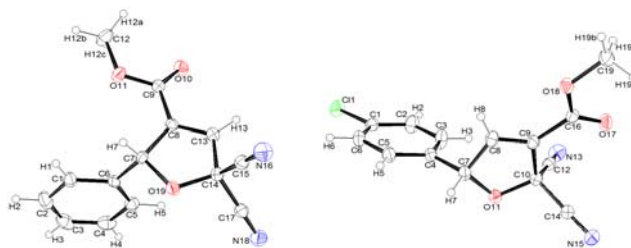


Figure 2 ORTEP diagram (30% probability) of racemic **5'a** (left) and **5b** (right).

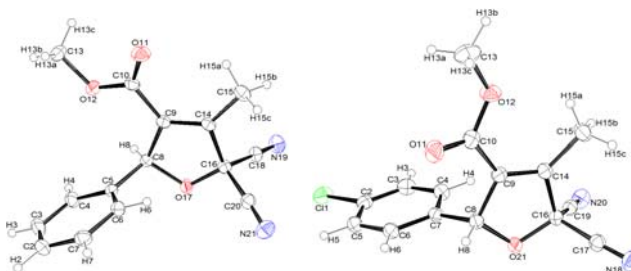


Figure 3 ORTEP diagram (30% probability) of racemic **8a** (left) and **8b** (right).

Table S1. B3LYP/6-31G*, B3LYP/6-311G* and B3LYP/6-311+G* total (E, in au, relative to **1'a+4** and **1'a+6**) and relative (ΔE , in kcal·mol⁻¹) energies of the stationary points involved in the 32CA reactions of CY **1'a** with methyl propiolate (**4**) and methyl but-2-ynoate (**6**).

	B3LYP/6-31G*		B3LYP/6-311G*		B3LYP/6-311+G*	
	E	ΔE	E	ΔE	E	ΔE
1'a	-569.2890344		-569.4217055		-569.4217055	
4	-305.2009399		-305.2825981		-305.2910342	
TS1m	-874.4863567	2.3	-874.6987677	3.5	-874.6987677	8.8
TS1o	-874.4830535	4.3	-874.6953445	5.6	-874.6953445	10.9
CA1m	-874.6044824	-71.9	-874.8118137	-67.5	-874.8274811	-72.0
CA1o	-874.6057291	-72.6	-874.8132229	-68.3	-874.828673	-72.7
6	-344.5302239		-344.6194703		-344.628183	
TS2m	-913.813585	3.6	-914.0332395	5.0	-914.0497172	0.1
TS2o	-913.806748	7.9	-914.026689	9.1	-914.0427307	4.5
CA2m	-913.9281258	-68.3	-914.1425992	-63.6	-914.1425992	-58.2
CA2o	-913.9300348	-69.5	-914.1446201	-64.9	-914.1446201	-59.4

Table S2. Total (E, in au) energies in toluene, and total enthalpies (H, in au), entropies (S, in eu) and free energies (G, in au) at 110 °C in toluene of the stationary points involved in the 32CA reactions of CY **1'a** with methyl propiolate (**4**) and methyl but-2-ynoate (**6**).

	E	H	S	G
1'a	-569.298832	-569.147496	120.1	-569.220966
4	-305.204925	-305.124479	86.0	-305.177108
TS1m	-874.496734	-874.264564	163.8	-874.364774
TS1o	-874.494074	-874.262105	165.2	-874.363148
CA1m	-874.612753	-874.377419	159.1	-874.474749
CA1o	-874.614524	-874.379184	157.8	-874.475720
6	-344.533805	-344.423889	100.1	-344.485118
TS2m	-913.822652	-913.561256	173.1	-913.667148
TS2o	-913.817043	-913.555725	176.1	-913.663413
CA2m	-913.935196	-913.671318	167.6	-913.773854
CA2o	-913.938039	-913.673939	168.8	-913.777191

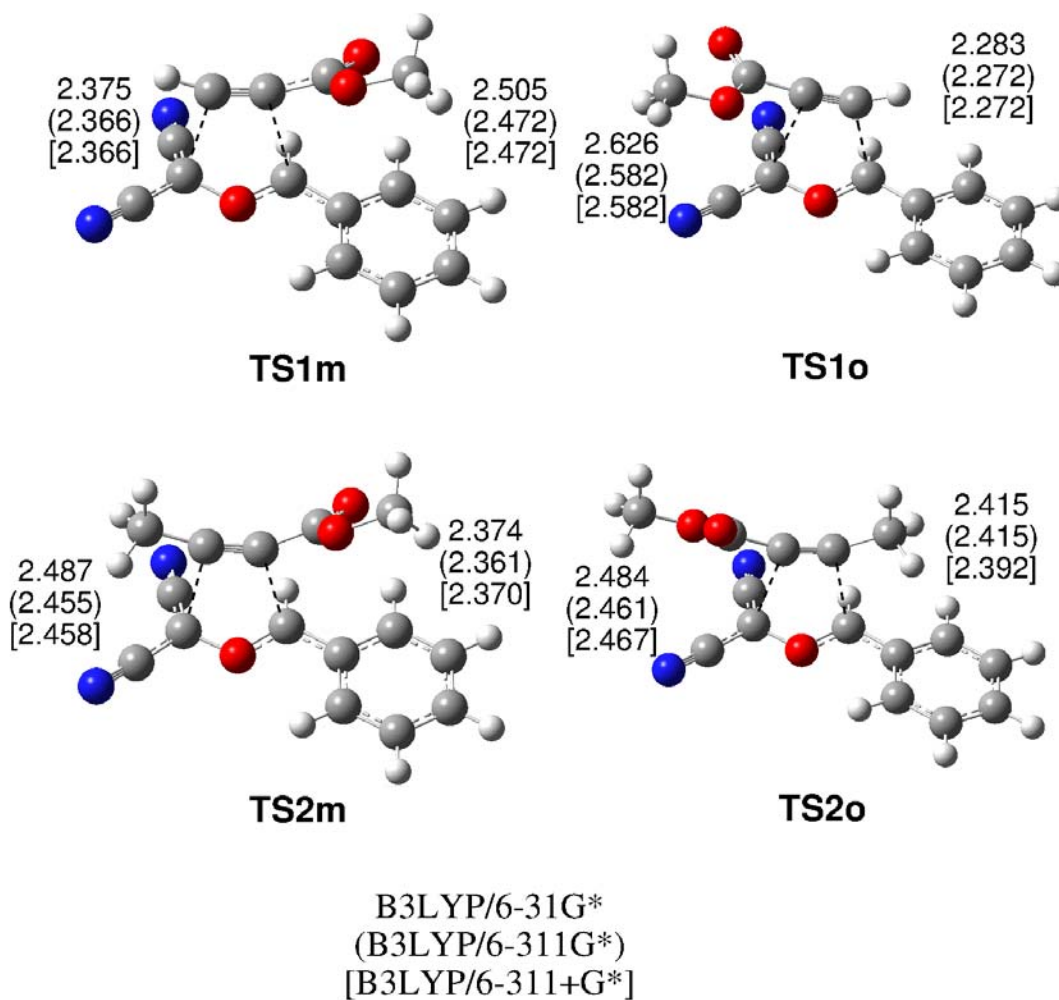


Figure S4. B3LYP/6-31G*, B3LYP/6-311G* and B3LYP/6-311+G* transition structures involved in the reactions between CY **1'a** and methyl propiolate (**4**) and methyl but-2-ynoate (**6**) (distances are given in Å).

B3LYP/6-31G* computed total energies, unique frequency imaginary, and cartesian coordinates of the stationary points involved in the 32CA reactions of CY **1'a** with methyl propiolate (**4**) and methyl but-2-ynoate (**6**).

1'a

$E(RB+HF-LYP) = -569.289034408 \text{ a.u.}$

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.36869473
C	1.03251942	0.00000000	2.14859756
H	2.01763360	-0.00009822	1.68644133
C	1.22441601	-0.00128640	-0.67681378
N	2.29182842	-0.00227515	-1.15807982
C	-1.26793529	-0.00013998	-0.59702795
N	-2.32449988	0.00307034	-1.09682663
C	0.85767362	0.00005438	3.56592089
C	2.01259243	-0.00000311	4.38043106
C	-0.41892468	0.00029386	4.17568120
C	1.89312793	0.00020367	5.76483404
H	2.99541182	-0.00021110	3.91620241
C	-0.52407223	0.00050593	5.55887475
H	-1.30867752	0.00032470	3.55465531
C	0.62710008	0.00046370	6.35782516
H	2.78543936	0.00017080	6.38362077
H	-1.50594300	0.00069927	6.02295608
H	0.53509328	0.00063270	7.44003154

4

$E(RB+HF-LYP) = -305.200939927 \text{ a.u.}$

X	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.11085600
X	1.53187600	0.00000000	0.66468200
H	-0.41536100	0.98312700	1.11297100
C	0.46921300	-1.11213600	1.10816100
C	0.97149000	-2.47192900	1.08813800
O	0.29539800	-3.44616800	0.83585900
O	2.28532200	-2.50462300	1.38660400
C	2.87247800	-3.81888100	1.39093200
H	3.92070100	-3.66463400	1.64647400
H	2.38248600	-4.45406899	2.13337100
H	2.77852800	-4.28303400	0.40577200

TS1m

$E(RB+HF-LYP) = -874.486356677 \text{ a.u.}$

1 imaginary frequency found: -292.14 cm^{-1}

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.37000146
C	1.10620574	0.00000000	2.06752392
C	1.81716860	2.13279376	0.96271355
C	1.24723220	2.01714867	-0.12048901
H	2.02091513	-0.33112519	1.58464327
C	0.96259207	-0.78801260	-0.68186058

N	1.78226618	-1.41988891	-1.22122752
C	-1.27213876	0.24234554	-0.57393698
N	-2.29244197	0.49377167	-1.08014579
C	1.01590544	0.08935360	3.50104989
C	2.18931927	-0.10521454	4.25953574
C	-0.20000849	0.37150431	4.16124721
C	2.14381774	-0.01921730	5.64781040
H	3.12760064	-0.30670700	3.75270437
C	-0.23346583	0.44894204	5.54672519
H	-1.10303532	0.52226830	3.57901880
C	0.93556952	0.25495915	6.29374787
H	3.05009817	-0.17173955	6.22639386
H	-1.17146267	0.66144950	6.05125510
H	0.90151333	0.31619001	7.37784801
H	0.92888658	2.21764702	-1.12182515
C	2.68443041	2.51876764	2.05447104
O	3.72258693	1.95065219	2.33841010
O	2.18357640	3.57375428	2.72529224
C	2.97661621	4.01960704	3.84155424
H	2.43321107	4.86795122	4.25744986
H	3.07400057	3.22227051	4.58256228
H	3.97133128	4.32470292	3.50726857

TS1o

$E(\text{RB}+\text{HF-LYP}) = -874.4830535 \text{ a.u.}$

1 imaginary frequency found: -316.47 cm^{-1}

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.36170786
C	1.11352451	0.00000000	2.05993419
C	1.84913589	2.03468401	1.33090412
C	1.36330727	2.23317558	0.22006652
H	1.99624291	-0.42767527	1.59149641
H	2.43011672	2.25732437	2.20227767
C	1.03250567	-0.67863144	-0.68832651
N	1.91258172	-1.24922705	-1.20116870
C	-1.25652065	0.24667339	-0.59451155
N	-2.27068515	0.48723501	-1.11948379
C	1.01168304	0.06307752	3.50276702
C	2.15495944	-0.23559608	4.26886893
C	-0.17851201	0.44210828	4.15552007
C	2.10871094	-0.15920245	5.65780057
H	3.07415774	-0.53325905	3.76990723
C	-0.21694605	0.50894686	5.54301690
H	-1.05978478	0.67697190	3.56768998
C	0.92356870	0.21136622	6.29797594
H	2.99408285	-0.39462429	6.24103396
H	-1.13806501	0.79669397	6.04140938
H	0.88675530	0.26822140	7.38205878
C	0.92679510	2.63097207	-1.10873134
O	1.54703892	2.39993590	-2.12465770
O	-0.24365120	3.29124065	-1.04307403
C	-0.79050925	3.69334420	-2.31548956
H	-0.98937018	2.81554949	-2.93376013
H	-1.71949133	4.20931720	-2.07535610
H	-0.09703543	4.35941901	-2.83475712

CA1m

$E(\text{RB}+\text{HF-LYP}) = -874.604482443 \text{ a.u.}$

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.41918962
C	1.35643563	0.00000000	1.94349214
C	2.21493727	0.06159528	0.69708346
C	1.46570177	0.08032115	-0.40409190
H	1.51776433	-0.95042084	2.46718872
C	-0.61966818	-1.25176547	-0.51376499
N	-1.07066103	-2.24631694	-0.90486117
C	-0.76899505	1.16837118	-0.50495407
N	-1.32914324	2.10658809	-0.89431457
C	1.55637417	1.14850029	2.91498038
C	2.30071476	0.94340341	4.08099961
C	1.02694353	2.41692199	2.64939535
C	2.52040297	1.99574361	4.97021019
H	2.71967067	-0.03777498	4.28567200
C	1.24117245	3.46594706	3.54258663
H	0.43197362	2.58253181	1.75617339
C	1.98987478	3.25850783	4.70333987
H	3.10025421	1.82587379	5.87317630
H	0.81971768	4.44513482	3.33265879
H	2.15436406	4.07705632	5.39883757
H	1.78928689	0.11479995	-1.43602090
C	3.69664876	0.00222305	0.77122084
O	4.30002557	-0.30230866	1.77925308
O	4.27422658	0.29726099	-0.40707662
C	5.71306814	0.22125213	-0.42381702
H	6.00481668	0.49394539	-1.43762568
H	6.13744377	0.91840353	0.30265281
H	6.04294968	-0.79282436	-0.18474911

CA1o

$E(RB+HF-LYP) = -874.605729071 \text{ a.u.}$

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.42485878
C	1.35493123	0.00000000	1.94543994
C	2.21287405	0.11671318	0.71894878
C	1.47692843	0.12817203	-0.39244527
H	1.52966028	-0.96654429	2.44036280
H	3.29435864	0.18190726	0.74720703
C	-0.59400351	-1.27012623	-0.49571788
N	-1.03928649	-2.28187026	-0.84629747
C	-0.81331294	1.14911140	-0.47535825
N	-1.42633358	2.07711541	-0.80377085
C	1.55579044	1.11552671	2.95401525
C	2.24441993	0.85616094	4.14277512
C	1.09332616	2.41119507	2.69325047
C	2.48033153	1.88152943	5.06001548
H	2.59334368	-0.15186124	4.35652828
C	1.32090105	3.43236363	3.61408604
H	0.54071831	2.61652435	1.78106988
C	2.01831690	3.17128075	4.79650789
H	3.01449614	1.66915379	5.98191042
H	0.95208127	4.43338427	3.40870585
H	2.19427088	3.96963783	5.51214309
C	1.99781111	0.22299642	-1.77702757
O	3.17204034	0.33546669	-2.05582966
O	0.99270664	0.16290864	-2.66881844
C	1.37593443	0.24068816	-4.05562370

H	2.03732901	-0.59094395	-4.30999562
H	0.44371181	0.18082981	-4.61570509
H	1.88851672	1.18538976	-4.25176245

6

$E(RB+HF-LYP) = -344.530223853 \text{ a.u.}$

X	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.70722200
X	1.36592400	0.00000000	1.01628600
C	-0.57039600	1.30614000	2.01107300
C	0.47875500	-1.08291200	1.45655400
C	0.97834200	-2.40148600	1.14142700
O	0.28806600	-3.33834200	0.79584700
O	2.32173900	-2.45918100	1.28153800
C	2.90452700	-3.73989700	0.98651400
H	3.97547200	-3.61349500	1.14700700
H	2.50254800	-4.50795101	1.65270700
H	2.70059600	-4.02590000	-0.04881600
H	-0.46089600	1.53909700	3.07696400
H	-0.06325200	2.09590700	1.44436400
H	-1.63775500	1.34129800	1.76465500

TS2m

$E(RB+HF-LYP) = -913.813585039 \text{ a.u.}$

1 imaginary frequency found: -290.04 cm^{-1}

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.36882638
C	1.11304819	0.00000000	2.06182869
C	1.88994697	2.00003808	1.04656518
C	1.39137258	2.06014677	-0.08266594
H	2.00880911	-0.40526745	1.59970766
C	0.95684374	-0.77848556	-0.69446240
N	1.77339339	-1.39455364	-1.25822194
C	-1.25227188	0.30394182	-0.57984099
N	-2.25084891	0.62030551	-1.09527020
C	1.00781284	0.09555399	3.49958190
C	2.14876220	-0.17687076	4.28088234
C	-0.19805236	0.45961971	4.13543591
C	2.08123905	-0.08810791	5.66849537
H	3.08138189	-0.44052933	3.79298921
C	-0.25518711	0.53954687	5.52053317
H	-1.07661258	0.67151764	3.53513582
C	0.88209037	0.26693898	6.29085533
H	2.96361520	-0.30146657	6.26465173
H	-1.18688085	0.81568925	6.00570192
H	0.83063980	0.33096406	7.37417412
C	1.03938089	2.46241188	-1.44637410
C	2.84140557	2.37140066	2.07864185
O	2.49739388	3.53264215	2.66982398
O	3.81655652	1.71089954	2.38354722
H	-0.03964461	2.61582213	-1.55524355
H	1.54688660	3.40398381	-1.69056166
H	1.35200367	1.70452165	-2.17309530
C	3.38076780	3.96606039	3.72086455
H	2.95447399	4.90023023	4.08669772
H	3.41933681	3.22018581	4.51883267
H	4.38929979	4.12851976	3.33225059

TS2o

$E(\text{RB}+\text{HF-LYP}) = -913.806747963 \text{ a.u.}$

1 imaginary frequency found: -298.86 cm^{-1}

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.36177901
C	1.11969862	0.00000000	2.04934778
C	1.89071422	2.09773216	1.13430855
C	1.26820150	2.13494181	0.06872995
H	1.99935102	-0.42546770	1.57471770
C	2.80134930	2.53868605	2.20105121
C	1.00843439	-0.73003951	-0.67833795
N	1.86882019	-1.34407116	-1.17293401
C	-1.26541267	0.22509052	-0.59024431
N	-2.28567894	0.45300053	-1.10814555
C	1.03173110	0.08856504	3.48796378
C	2.15704054	-0.26765604	4.25798447
C	-0.13468559	0.53982486	4.14137323
C	2.11786715	-0.17578041	5.64618726
H	3.05490248	-0.62693434	3.76125859
C	-0.16563698	0.62379785	5.52773556
H	-1.00277500	0.81810781	3.55277643
C	0.95773953	0.26908750	6.28453830
H	2.98906303	-0.45726168	6.23044743
H	-1.06757198	0.96923870	6.02466336
H	0.92617036	0.33877113	7.36804596
C	0.71497856	2.73190583	-1.14228446
O	0.80250039	1.91602584	-2.20744870
O	0.24601395	3.85060744	-1.16677689
H	3.28064970	3.48153395	1.91342447
H	2.25990616	2.70178148	3.13875588
H	3.58771478	1.80124452	2.39881006
C	0.24063842	2.43600132	-3.42769439
H	0.43638315	1.67217874	-4.17980025
H	-0.83401728	2.59294585	-3.30767890
H	0.72015680	3.37994213	-3.69775943

CA2m

$E(\text{RB}+\text{HF-LYP}) = -913.928125846 \text{ a.u.}$

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.41312876
C	1.36146077	0.00000000	1.92812466
C	2.21562106	0.09419933	0.67933907
C	1.47075942	0.11296142	-0.43542137
H	1.52695963	-0.95719738	2.43783532
C	-0.59571424	-1.26400977	-0.51426382
N	-1.02184386	-2.26965712	-0.90530939
C	-0.79502135	1.15257541	-0.50108637
N	-1.37016150	2.08260528	-0.88839141
C	1.53241662	1.13062594	2.92444024
C	1.99013002	0.86059822	4.21698374
C	1.23396568	2.45103159	2.56521516
C	2.15788329	1.89465286	5.13934215
H	2.21797609	-0.16355575	4.50193960
C	1.39637087	3.48388891	3.48659407
H	0.86118830	2.67228160	1.56881482
C	1.86165326	3.20843265	4.77511629

H	2.51291672	1.67207798	6.14190300
H	1.15705628	4.50406902	3.19959647
H	1.98690614	4.01470398	5.49271203
C	1.84223428	0.18799214	-1.87834124
C	3.70131428	0.10498435	0.71366910
O	4.42957304	0.39321223	-0.21461845
O	4.14917534	-0.27247837	1.92825372
C	5.58029484	-0.29355353	2.08191350
H	5.75599266	-0.59942583	3.11293724
H	6.02721303	-1.00617315	1.38423007
H	5.99597819	0.69970921	1.89629300
H	1.44922741	-0.68150802	-2.42058162
H	1.39925824	1.08053842	-2.33877838
H	2.92471052	0.23230687	-1.99267647

CA2o

$E(RB+HF-LYP) = -913.930034843 \text{ a.u.}$

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.42343546
C	1.35086598	0.00000000	1.93506452
C	2.23299058	0.13137971	0.71043261
C	1.47458697	0.13766858	-0.39820158
H	1.53899203	-0.97313462	2.41391903
C	3.71845480	0.20607985	0.83598739
C	-0.59042200	-1.27544448	-0.48897865
N	-1.02976849	-2.29370353	-0.82825189
C	-0.82662572	1.14407514	-0.46672551
N	-1.44858311	2.07011720	-0.78391514
C	1.53387772	1.09799639	2.96510289
C	2.18507826	0.82107312	4.17100695
C	1.08396054	2.39967384	2.70883574
C	2.39728498	1.83350098	5.10875567
H	2.52117024	-0.19164426	4.38271470
C	1.28939489	3.40821472	3.64833710
H	0.55831654	2.61834254	1.78379682
C	1.94971330	3.12870278	4.84800845
H	2.90146861	1.60648725	6.04398816
H	0.93095475	4.41347736	3.44518326
H	2.10715354	3.91696524	5.57901035
C	1.92517135	0.22347368	-1.80582449
O	3.07623796	0.34656108	-2.17392614
O	0.86962312	0.14450019	-2.63928313
C	1.16806858	0.21517624	-4.04607421
H	1.81353033	-0.61726194	-4.33645723
H	0.20333902	0.15111789	-4.54769063
H	1.66647890	1.15912970	-4.27882560
H	4.19592782	0.24740329	-0.14199394
H	3.99828788	1.09206865	1.41864544
H	4.09185484	-0.66532707	1.39001832