Supporting Information

Regio- and stereoselective (3+2)-cycloaddition reactions of nitrones with cyclic allenes

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Computation details

Table S1. Theoretically calculated Fukui functions *f*(+) and *f*(–), global electrophilicity (ω) and nucleophilicity (*N*) indexes for optimized equilibrium model structures of dipolarophiles **1a**–**1d** in toluene solution (B3LYP/6-311++G** level of theory)[a].[1]

Dipolarophile	Fukui function	=C=	==C	HOMO, eV	LUMO, eV	ω, eV	*N*, eV
1a	*f*(–)	0.34	0.15	-6.60	-0.12	0.87	2.52
	f(+)	–1.07	0.57				
1b	*f*(–)	0.22	0.21	-6.45	-0.29	0.92	2.67
	f(+)	0.08	0.31				
1c	*f*(–)	0.34	0.19	-6.62	-0.14	0.88	2.50
	f(+)	–0.95	0.47				
1d	*f*(–)	0.35	0.23	-6.76	-0.49	1.05	2.36
	f(+)	–0.08	0.19				

[a] The electronic chemical potential μ, chemical hardness η, global electrophilicity ω and nucleophilicity *N* indexes were calculated using the following formulas:

$$\mu \approx \frac{E_{HOMO} + E_{LUMO}}{2},$$

$$\eta \approx E_{LUMO} - E_{HOMO},$$

$$\omega = \frac{\mu^2}{2\eta},$$

$$N = E_{HOMO,\,Nu} - E_{HOMO,\,TCNE},$$

where E_{HOMO} and E_{LUMO} – energies of the frontier molecular orbitales, Nu – nucleophile, TCNE – tetracyanoethylene $C_2(CN)_4$ (a reference in nucleophilicity scale proposed by Domingo et al.;[2] – 2, а не 3 $E_{HOMO,\,TCNE}$ = –9.12 eV at the B3LYP/6-31G(d) level of theory).

Table S2. Theoretically calculated NBO atomic charges for optimized equilibrium model structures of dipolarophiles **1a**–**1d** in toluene solution (B3LYP/6-311++G** level of theory).[3]

Dipolarophile	=C=	==C
1a	0.04	-0.27
1b	0.05	-0.27
1c	0.04	-0.26
1d	0.03	-0.26

Table S3. Calculated total energies, enthalpies, Gibbs free energies (Hartree), and entropies (cal/mol•K) for optimized equilibrium model structures in toluene solution (E, H, G, and S, respectively), B3LYP/6-31G** level of theory.

Model structure	E	H	G	S
1b	-350.128826289	-349.934759	-349.976441	87.728
8a	-800.656723251	-800.405710	-800.464168	123.037
TS_for_9c	-1150.75814736	-1150.311996	-1150.391466	167.258
TS_for_10c	-1150.75352059	-1150.307775	-1150.387403	167.590
TS_for_11c	-1150.75316341	-1150.307154	-1150.386109	166.174
TS_for_12c	-1150.74964344	-1150.303393	-1150.381873	165.177
biradical_intermediate_to_9c	-1150.77005410	-1150.322868	-1150.404570	171.958
biradical_intermediate_to_10c	-1150.77612847	-1150.328575	-1150.410450	172.320
biradical_intermediate_to_11c	-1150.74054271	-1150.293279	-1150.375418	172.876
biradical_intermediate_to_12c	-1150.73679980	-1150.289277	-1150.370102	170.112
TS_for_biradical_to_9c	-1150.71723381	-1150.273124	-1150.355266	172.882
TS_for_biradical_to_10c	-1150.71095375	-1150.267447	-1150.351397	176.686
TS_for_biradical_to_11c	-1150.71318273	-1150.268877	-1150.353481	178.066
TS_for_biradical_to_12c	-1150.70590862	-1150.261839	-1150.345131	175.304

Table S4 Calculated values of total activation energies (E_a), enthalpies of activation ($\Delta H^{\neq}$) and Gibbs free energies of activation ($\Delta G^{\neq}$) for concerted cycloaddition in toluene solution (in kcal/mol), B3LYP/6-31G** level of theory.

Transformation	E_a	$\Delta H^{\neq}$	$\Delta G^{\neq}$
1b + 8a → 9c	17.2	17.9	30.8
1b + 8a → 10c	20.1	20.5	33.4
1b + 8a → 11c	20.3	20.9	34.2
1b + 8a → 12c	22.5	23.3	36.9

Table S5. Calculated values of total activation and reaction energies (E_a and ΔE), enthalpies and Gibbs free energies of activation ($\Delta H^{\neq}$ and $\Delta G^{\neq}$) and reaction (ΔH and ΔG) for the formation of hypothetical biradical intermediates for stepwise cycloaddition in toluene solution (in kcal/mol), B3LYP/6-31G** level of theory.

Transformation	E_a	$\Delta H^{\neq}$	$\Delta G^{\neq}$	ΔE	ΔH	ΔG
1b + 8a → biradical_intermediate_to_9c	42.9	42.3	53.6	9.7	11.0	22.6
1b + 8a → biradical_intermediate_to_10c	46.8	45.8	56.0	5.9	7.5	18.9
1b + 8a → biradical_intermediate_to_11c	45.4	44.9	54.7	28.2	29.6	40.9
1b + 8a → biradical_intermediate_to_12c	50.0	49.3	59.9	30.6	32.1	44.2

Table S6. Cartesian atomic coordinates for optimized equilibrium model structures in toluene solution (B3LYP/6-31G** level of theory). Nuclear charges of elements are shown in the second column.

Model structure	Charge	X	Y	Z
1b				
	6	2.089309	-0.679076	-0.176031
	6	1.852903	0.774600	0.339986
	6	0.990399	-1.607630	0.308122
	6	-0.243104	-1.561131	-0.131361
	6	-1.475077	-1.316445	-0.499400
	6	-2.260613	-0.147202	0.076963
	6	-1.369595	0.950681	0.707666
	6	-0.490471	1.628920	-0.310597
	6	0.837533	1.545361	-0.470940
	1	3.054785	-1.039435	0.194863
	1	2.148660	-0.671007	-1.269718
	1	2.807157	1.314489	0.300875
	1	1.564717	0.725613	1.395920
	1	1.222795	-2.245153	1.162622
	1	-1.959277	-1.919493	-1.267330
	1	-2.979353	-0.505698	0.827404
	1	-2.863554	0.288484	-0.730973
	1	-2.033586	1.695733	1.166118
	1	-0.774091	0.512845	1.514205
	1	-1.035323	2.232796	-1.038782

	1	1.259366	2.082359	-1.321648
8a				
	7	-1.425986	-0.137409	-0.002490
	8	-0.881553	-1.293289	0.150217
	6	-2.884691	-0.130582	0.024150
	6	-0.764947	0.986076	-0.195306
	6	-3.590212	0.932983	0.588701
	6	-4.984134	0.887009	0.594974
	6	-5.655757	-0.207336	0.047494
	6	-4.932082	-1.269322	-0.500394
	6	-3.539758	-1.241609	-0.506879
	6	0.706338	1.166754	-0.204792
	8	1.148475	2.306427	-0.370627
	7	1.446352	0.032622	-0.027115
	6	2.843788	-0.106628	0.013514
	6	3.345318	-1.401647	0.235331
	6	4.716927	-1.626343	0.287568
	6	5.612505	-0.567172	0.120915
	6	5.113879	0.717379	-0.098434
	6	3.741444	0.961163	-0.154042
	1	-1.345827	1.878176	-0.374558
	1	-3.067481	1.767185	1.043158
	1	-5.542089	1.703812	1.041666
	1	-6.740954	-0.237220	0.056528
	1	-5.451281	-2.124019	-0.922366
	1	-2.955305	-2.057514	-0.913602
	1	0.877040	-0.809490	0.086908
	1	2.650825	-2.227536	0.367493
	1	5.085654	-2.633445	0.459825
	1	6.683253	-0.742299	0.161522
	1	5.799713	1.549711	-0.229568
	1	3.356810	1.956693	-0.323287

TS_for_9c				
	8	-0.989942	-0.867133	-1.314908
	6	-0.874503	-0.575736	0.920028
	7	-1.551348	-1.051293	-0.151879
	6	-2.964802	-1.286869	-0.124705
	6	-3.588864	-1.769816	1.032854
	6	-4.964220	-1.992890	1.025346
	6	-5.714598	-1.757338	-0.128611
	6	-5.078081	-1.301157	-1.284741
	6	-3.704529	-1.069165	-1.292147
	6	0.576737	-0.884771	1.176767
	7	1.303228	-1.272675	0.088499
	8	0.998388	-0.787617	2.329446
	6	2.638163	-1.714461	0.034388
	6	3.101412	-2.194580	-1.203019
	6	4.412448	-2.640074	-1.339979
	6	5.282654	-2.619172	-0.247591
	6	4.820553	-2.144854	0.980525
	6	3.509974	-1.692259	1.135207
	1	-1.438640	-0.537026	1.843013
	1	-3.009569	-1.993501	1.922030
	1	-5.446144	-2.368371	1.922921
	1	-6.784645	-1.940623	-0.129741
	1	-5.652204	-1.124677	-2.189472
	1	-3.192664	-0.728728	-2.183026
	1	0.762365	-1.289550	-0.777148
	1	2.424454	-2.219837	-2.053386
	1	4.752445	-3.007226	-2.304131
	1	6.305607	-2.967399	-0.353208
	1	5.487238	-2.123065	1.838143
	1	3.153596	-1.325265	2.087085
	6	-0.714211	1.442146	-1.026394

	6	-0.651408	1.431805	0.341500
	6	0.486293	1.630861	-1.934234
	6	1.575234	2.588652	-1.398284
	6	0.805821	4.322538	1.146388
	6	-0.512827	3.629239	1.609886
	6	-0.512065	2.117133	1.470190
	6	1.116620	4.019849	-1.374085
	6	0.779902	4.745959	-0.301938
	1	-1.688010	1.421285	-1.508081
	1	0.947673	0.654590	-2.126997
	1	0.125011	1.987021	-2.906529
	1	1.889416	2.254429	-0.405194
	1	2.448126	2.496042	-2.057635
	1	0.958902	5.215835	1.762810
	1	1.650423	3.656313	1.351706
	1	-0.678994	3.861809	2.667350
	1	-1.354664	4.061840	1.057707
	1	-0.360940	1.569931	2.398727
	1	1.007300	4.485621	-2.354864
	1	0.408977	5.756100	-0.478833
TS_for_10c				
	8	0.138507	1.091165	-1.256566
	6	0.042706	0.684685	0.970103
	7	0.552199	1.400456	-0.058412
	6	1.775440	2.136906	0.055321
	6	2.100242	2.807174	1.242008
	6	3.293831	3.521614	1.319305
	6	4.152352	3.589533	0.219848
	6	3.804718	2.942887	-0.968054
	6	2.616180	2.221626	-1.060035
	6	-1.437611	0.434258	1.138546

	7	-2.185773	0.542776	0.002937
	8	-1.860584	0.170494	2.262614
	6	-3.578559	0.414901	-0.148774
	6	-4.107783	0.676332	-1.424418
	6	-5.474341	0.557117	-1.658052
	6	-6.336301	0.176063	-0.627108
	6	-5.809486	-0.082467	0.638737
	6	-4.442039	0.032290	0.890567
	1	0.525090	0.839144	1.927067
	1	1.419945	2.796983	2.086487
	1	3.542785	4.042072	2.239094
	1	5.078135	4.152801	0.284922
	1	4.460360	3.000788	-1.831808
	1	2.319655	1.730575	-1.977530
	1	-1.633847	0.790769	-0.821427
	1	-3.440498	0.975909	-2.228749
	1	-5.865156	0.764155	-2.650253
	1	-7.402708	0.083871	-0.809063
	1	-6.468569	-0.379656	1.449801
	1	-4.035201	-0.167048	1.871599
	6	0.429040	-1.358805	-0.918496
	6	0.639154	-1.242551	0.421446
	6	1.458601	-1.691516	-1.973982
	6	2.941523	-1.673660	-1.580491
	6	1.585619	-4.073759	0.353965
	6	1.138556	-3.372929	1.653351
	6	1.001561	-1.867297	1.538173
	6	3.543378	-2.774391	-0.736894
	6	3.020966	-3.751955	0.014943
	1	-0.596011	-1.333206	-1.280880

	1	1.201250	-2.682212	-2.379140
	1	1.318824	-1.000714	-2.813078
	1	3.516575	-1.652295	-2.516652
	1	3.172359	-0.714244	-1.094906
	1	1.488642	-5.156453	0.497402
	1	0.897642	-3.808632	-0.451411
	1	0.177691	-3.792716	1.985980
	1	1.853750	-3.594699	2.455576
	1	1.156424	-1.308530	2.458401
	1	4.634122	-2.732793	-0.752030
	1	3.743890	-4.386111	0.530472
TS_for_11c				
	6	0.587711	-1.054812	0.972922
	8	0.734714	-0.812679	-1.266947
	7	1.230978	-1.339928	-0.177110
	6	2.618020	-1.704814	-0.196846
	6	3.131029	-2.581542	0.766464
	6	4.481453	-2.923862	0.727868
	6	5.312549	-2.412851	-0.271165
	6	4.783850	-1.556259	-1.239359
	6	3.436930	-1.200914	-1.212063
	6	-0.895409	-1.137352	1.151196
	7	-1.641328	-1.122643	0.008837
	8	-1.338129	-1.212120	2.300049
	6	-3.035649	-1.231736	-0.135715
	6	-3.540163	-1.236624	-1.447862
	6	-4.908508	-1.340076	-1.677292
	6	-5.798364	-1.441497	-0.605394
	6	-5.296636	-1.436725	0.696452
	6	-3.927632	-1.332731	0.944792

	1	1.123512	-1.274711	1.888061
	1	2.480533	-3.012643	1.519908
	1	4.878825	-3.605691	1.473551
	1	6.362084	-2.688957	-0.300864
	1	5.422930	-1.159474	-2.022555
	1	3.008744	-0.540581	-1.955072
	1	-1.085515	-1.014226	-0.839549
	1	-2.850371	-1.161278	-2.284810
	1	-5.278863	-1.342573	-2.698469
	1	-6.866258	-1.522933	-0.783695
	1	-5.977537	-1.514216	1.539626
	1	-3.541559	-1.327143	1.953945
	6	0.784898	1.193104	0.681002
	6	0.617653	1.243777	-0.670327
	6	-0.227294	1.856556	1.607143
	6	0.320041	3.181425	2.210511
	6	-0.135511	4.167984	-0.870665
	6	0.220126	3.289994	-2.092381
	6	0.332604	1.798217	-1.830325
	6	1.184325	4.066750	1.333527
	6	1.011446	4.450172	0.062406
	1	1.808427	1.159255	1.056663
	1	-1.150895	2.032637	1.049572
	1	-0.495964	1.200389	2.442056
	1	0.918210	2.924925	3.092375
	1	-0.535747	3.751054	2.599545
	1	-0.487676	5.133549	-1.259912
	1	-0.983114	3.723589	-0.341874
	1	-0.558834	3.421165	-2.854226
	1	1.147136	3.659643	-2.555122

	1	0.134050	1.154065	-2.685928
	1	2.088019	4.429663	1.823096
	1	1.794823	5.073784	-0.372556
TS_for_12c				
	6	-0.004664	-1.086625	0.938893
	8	0.212180	-0.498268	-1.226223
	7	0.574434	-1.304425	-0.260257
	6	1.832506	-1.977605	-0.398626
	6	2.122681	-3.098759	0.388457
	6	3.344984	-3.748807	0.227681
	6	4.265836	-3.300784	-0.721602
	6	3.955344	-2.195924	-1.517420
	6	2.739595	-1.531862	-1.365813
	6	-1.484613	-0.923251	1.132308
	7	-2.201126	-0.589578	0.019908
	8	-1.945940	-1.099225	2.260517
	6	-3.589902	-0.412203	-0.113670
	6	-4.069609	-0.096985	-1.396805
	6	-5.430656	0.093838	-1.613285
	6	-6.337396	-0.028211	-0.557832
	6	-5.860031	-0.342246	0.714983
	6	-4.498514	-0.536034	0.950165
	1	0.465420	-1.565410	1.789267
	1	1.393992	-3.476703	1.097478
	1	3.568562	-4.619574	0.836550
	1	5.212889	-3.816200	-0.848272
	1	4.662717	-1.845053	-2.262877
	1	2.482229	-0.676699	-1.977066
	1	-1.627884	-0.446954	-0.811436
	1	-3.366913	-0.004669	-2.221121
	1	-5.781958	0.337574	-2.611889
	1	-7.399793	0.119392	-0.726370

	1	-6.554289	-0.440240	1.544992
	1	-4.130769	-0.778554	1.936875
	6	0.488823	1.125576	1.040058
	6	0.513258	1.373634	-0.304468
	6	1.706493	1.277261	1.954241
	6	3.097824	1.321603	1.307179
	6	1.543039	4.081042	0.085736
	6	0.805536	3.668639	-1.208496
	6	0.613597	2.167796	-1.348766
	6	3.577989	2.534215	0.539772
	6	2.987655	3.642639	0.072351
	1	-0.455198	1.324002	1.547099
	1	1.556898	2.195756	2.538055
	1	1.706988	0.469208	2.695064
	1	3.826994	1.162375	2.114318
	1	3.223778	0.448030	0.651802
	1	1.507273	5.174135	0.166569
	1	0.999755	3.690617	0.948582
	1	-0.172760	4.169460	-1.248089
	1	1.365016	4.030082	-2.080529
	1	0.566937	1.760754	-2.356336
	1	4.646293	2.458874	0.326419
	1	3.642109	4.326100	-0.471247

Table S7. Cartesian atomic coordinates for optimized equilibrium model structures in toluene solution (B3LYP/6-311++G** level of theory). Nuclear charges of elements are shown in the second column.

Model structure	Charge	X	Y	Z
1a				
	6	2.206712	0.501261	0.067175
	6	1.750705	-0.960208	-0.151375
	6	1.199035	1.503310	-0.471330

	6	0.006870	1.649305	0.043127
	6	-1.196712	1.550741	0.537562
	6	-2.158553	0.451295	0.114477
	6	-1.555569	-0.652942	-0.772450
	6	-0.763235	-1.761968	-0.048830
	6	0.534159	-1.405397	0.706852
	1	3.166672	0.659165	-0.432697
	1	2.378516	0.665800	1.135896
	1	2.603728	-1.609142	0.074140
	1	1.534687	-1.108383	-1.215594
	1	1.457041	2.040485	-1.382640
	1	-1.544979	2.250577	1.295448
	1	-3.005931	0.913804	-0.407758
	1	-2.584391	0.005500	1.023284
	1	-2.382945	-1.147196	-1.293575
	1	-0.942347	-0.194434	-1.554798
	1	-1.441794	-2.242416	0.667848
	1	-0.522898	-2.534322	-0.790677
	1	0.822531	-2.303360	1.264074
	1	0.321635	-0.648461	1.465810
1b				
	6	-1.595604	1.056944	0.584644
	6	-2.116732	-0.388687	0.290416
	6	-0.699222	1.562847	-0.524138
	6	0.595858	1.521240	-0.368044
	6	1.812473	1.178869	-0.035189
	6	2.223610	-0.287448	0.024634
	6	1.108159	-1.201506	0.607429
	6	0.066393	-1.651895	-0.383423

	6	-1.231264	-1.341287	-0.494165
	1	-2.466087	1.705517	0.727009
	1	-1.031809	1.065093	1.519267
	1	-2.391373	-0.838897	1.252403
	1	-3.053449	-0.303718	-0.267563
	1	-1.143382	1.777718	-1.494346
	1	2.529511	1.922614	0.305141
	1	2.533323	-0.657860	-0.959615
	1	3.105510	-0.358181	0.668003
	1	1.594575	-2.104416	0.996495
	1	0.651508	-0.698821	1.463918
	1	0.446852	-2.360461	-1.119505
	1	-1.757214	-1.843060	-1.304190
1c				
	6	-1.991532	1.166931	-0.129921
	6	-2.092426	-0.215510	0.575520
	6	-0.768688	1.956790	0.302158
	6	0.430050	1.779833	-0.184101
	6	1.611558	1.428418	-0.613385
	6	2.407321	0.277866	-0.015384
	6	1.621329	-0.679804	0.900303
	6	0.894213	-1.834558	0.181604
	6	-0.230934	-1.513387	-0.829302
	6	-1.670581	-1.422869	-0.282330
	1	-2.882273	1.758116	0.099367
	1	-1.984216	1.025119	-1.214470
	1	-3.134914	-0.383409	0.867789
	1	-1.521136	-0.191517	1.508952
	1	-0.899951	2.646616	1.135425

	1	2.078712	1.973747	-1.432233
	1	3.249408	0.706884	0.542797
	1	2.862824	-0.288404	-0.837532
	1	2.333695	-1.138092	1.594954
	1	0.927476	-0.104949	1.520136
	1	0.494742	-2.515554	0.943943
	1	1.662972	-2.409630	-0.349206
	1	0.015763	-0.615239	-1.401534
	1	-0.242682	-2.329101	-1.561559
	1	-2.349937	-1.462811	-1.143480
	1	-1.872338	-2.334036	0.295682
1d				
	6	-1.984864	-2.119145	0.270582
	6	-0.680655	-1.520388	0.824777
	6	-2.899095	-1.078335	-0.357748
	6	-2.802389	0.179372	-0.021693
	6	-2.439606	1.367526	0.379040
	6	-1.282135	2.133578	-0.220632
	6	-0.503349	1.421080	-1.334253
	6	0.377336	0.183027	-1.123365
	6	0.294335	-1.103198	-0.263868
	6	1.398174	-0.105228	-0.065561
	17	3.071992	-0.545776	-0.577038
	17	1.456216	0.848302	1.444371
	1	-2.514086	-2.639807	1.077791
	1	-1.757738	-2.883381	-0.481037
	1	-0.174725	-2.278664	1.432098
	1	-0.911460	-0.690601	1.492662
	1	-3.612651	-1.408594	-1.109052

	1	-2.953414	1.837529	1.216540
	1	-1.659652	3.071964	-0.646421
	1	-0.618425	2.433610	0.594441
	1	-1.214798	1.144598	-2.120211
	1	0.160060	2.165559	-1.788982
	1	0.784657	-0.081741	-2.095910
	1	0.626183	-1.963159	-0.840238

biradical_intermediate_to_9c				
	8	0.704477	-1.441016	1.395985
	6	0.738963	-0.135487	-0.614541
	7	1.347323	-1.105977	0.329005
	6	2.649995	-1.623542	0.135411
	6	3.518745	-1.115486	-0.847316
	6	4.784603	-1.676539	-1.001447
	6	5.202413	-2.732069	-0.189223
	6	4.340081	-3.223424	0.795913
	6	3.073689	-2.677635	0.965610
	6	-0.778005	-0.321879	-0.927381
	7	-1.492336	-1.144989	-0.117882
	8	-1.214009	0.285357	-1.899687
	6	-2.855329	-1.498975	-0.202287
	6	-3.348309	-2.352758	0.798590
	6	-4.680524	-2.754304	0.788293
	6	-5.542291	-2.312395	-0.218149
	6	-5.050895	-1.463954	-1.210498
	6	-3.717902	-1.051189	-1.214909
	1	1.194604	-0.334211	-1.585078
	1	3.235063	-0.271524	-1.462702
	1	5.450761	-1.275005	-1.759077

	1	6.190192	-3.163528	-0.317594
	1	4.655332	-4.041903	1.436206
	1	2.397023	-3.050583	1.723285
	1	-0.963277	-1.512793	0.673590
	1	-2.679571	-2.697721	1.583036
	1	-5.044388	-3.414727	1.570144
	1	-6.581963	-2.625206	-0.227225
	1	-5.710884	-1.112259	-1.998620
	1	-3.340822	-0.391535	-1.983061
	6	0.906304	1.809262	1.084789
	6	1.074864	1.314550	-0.239322
	6	-0.310837	1.660532	1.940409
	6	-1.358092	2.737302	1.481060
	6	0.116333	4.307687	-0.894842
	6	1.532060	3.653294	-1.145498
	6	1.477339	2.149362	-1.252382
	6	-0.795368	4.137100	1.506621
	6	-0.145836	4.773365	0.519236
	1	1.503075	2.686689	1.318383
	1	-0.765493	0.670802	1.862982
	1	-0.059949	1.826928	2.995015
	1	-1.690977	2.471368	0.472243
	1	-2.234195	2.673577	2.137597
	1	0.034475	5.180517	-1.553021
	1	-0.652428	3.601583	-1.221460
	1	1.941832	4.049716	-2.079317
	1	2.220068	3.975021	-0.352909
	1	1.613643	1.727516	-2.246595
	1	-0.869389	4.651956	2.465168

	1	0.256620	5.760454	0.751953
biradical_intermediate_to_10c				
	8	0.318355	-1.478670	-1.292512
	6	-0.050862	-0.199665	0.704325
	7	-0.357802	-1.330222	-0.201710
	6	-1.425933	-2.223262	0.051636
	6	-2.399083	-1.964079	1.033479
	6	-3.420506	-2.887247	1.247002
	6	-3.491330	-4.061897	0.496132
	6	-2.529109	-4.306964	-0.488580
	6	-1.503138	-3.398326	-0.717707
	6	1.456570	0.076355	0.973738
	7	2.331794	-0.249560	-0.011281
	8	1.737951	0.611175	2.041219
	6	3.731267	-0.084603	-0.037698
	6	4.407479	-0.595443	-1.158425
	6	5.789199	-0.469896	-1.265099
	6	6.519293	0.165560	-0.258209
	6	5.845939	0.673033	0.853343
	6	4.460859	0.556009	0.976167
	1	-0.416062	-0.496674	1.685213
	1	-2.390191	-1.041415	1.599763
	1	-4.171683	-2.677705	2.002510
	1	-4.289853	-4.775998	0.671363
	1	-2.575194	-5.216110	-1.080623
	1	-0.750936	-3.577250	-1.474814
	1	1.899499	-0.719965	-0.807199
	1	3.842223	-1.091671	-1.943363
	1	6.294809	-0.872071	-2.138334

	1	7.597611	0.262991	-0.339919
	1	6.401904	1.170347	1.643292
	1	3.941447	0.948654	1.838600
	6	-0.702171	1.459827	-1.057765
	6	-0.761146	1.112423	0.290531
	6	-1.384468	2.608302	-1.739712
	6	-2.814814	2.256242	-2.249563
	6	-3.365791	3.373422	0.633431
	6	-1.986322	3.167844	1.379332
	6	-1.352360	1.801894	1.354615
	6	-3.757601	1.678119	-1.215181
	6	-3.984692	2.143269	0.018679
	1	-0.188321	0.765702	-1.717523
	1	-1.431911	3.485617	-1.094905
	1	-0.790076	2.903164	-2.612882
	1	-3.245715	3.164951	-2.695353
	1	-2.720716	1.537339	-3.070719
	1	-4.073500	3.797007	1.353654
	1	-3.233811	4.137347	-0.138866
	1	-1.275729	3.904922	0.985170
	1	-2.126896	3.433689	2.430949
	1	-1.292325	1.310752	2.322205
	1	-4.287789	0.775425	-1.515584
	1	-4.672876	1.583890	0.651815
biradical_intermediate_to_11c				
	6	0.646072	-0.374682	0.681094
	8	0.533514	-1.520731	-1.415186
	7	1.215695	-1.273615	-0.349667
	6	2.503136	-1.849313	-0.224147

	6	3.400571	-1.476357	0.793756
	6	4.655390	-2.078249	0.861141
	6	5.035380	-3.045559	-0.069980
	6	4.143548	-3.407799	-1.084392
	6	2.888717	-2.817659	-1.170059
	6	-0.825490	-0.665212	1.064749
	7	-1.669888	-0.963211	0.044433
	8	-1.140901	-0.543422	2.247141
	6	-3.056194	-1.213401	0.086835
	6	-3.684166	-1.513387	-1.133912
	6	-5.052086	-1.764824	-1.178464
	6	-5.816226	-1.722247	-0.010013
	6	-5.190653	-1.424909	1.200967
	6	-3.820294	-1.169867	1.263723
	1	1.184445	-0.570320	1.605659
	1	3.145797	-0.717549	1.522794
	1	5.340235	-1.780678	1.649478
	1	6.014428	-3.510150	-0.008196
	1	4.427315	-4.159152	-1.815335
	1	2.191100	-3.089706	-1.951112
	1	-1.201136	-1.085615	-0.852526
	1	-3.093586	-1.545657	-2.046141
	1	-5.520995	-1.994224	-2.131096
	1	-6.883507	-1.918866	-0.044450
	1	-5.772706	-1.389128	2.117735
	1	-3.337612	-0.940003	2.202638
	6	0.886328	1.133954	0.298186
	6	0.253664	1.452165	-0.993810
	6	0.491046	2.068868	1.486130

	6	1.481483	3.227645	1.730966
	6	-0.252178	4.515712	-0.648926
	6	-0.666471	3.703225	-1.886549
	6	-0.321166	2.219221	-1.889683
	6	1.959530	4.032297	0.537803
	6	1.237631	4.568619	-0.452602
	1	1.974309	1.209073	0.157672
	1	-0.524894	2.435223	1.325047
	1	0.440235	1.475280	2.404508
	1	2.370019	2.808732	2.218625
	1	1.034520	3.899025	2.478480
	1	-0.621966	5.540798	-0.789895
	1	-0.758288	4.129144	0.238589
	1	-1.750847	3.799296	-2.037390
	1	-0.208610	4.148903	-2.781896
	1	-0.610950	1.732861	-2.830420
	1	3.036054	4.196968	0.502908
	1	1.779654	5.107302	-1.231547
biradical_intermediate_to_12c				
	6	-0.257062	0.199135	1.081615
	8	-0.427118	0.216341	-1.267362
	7	-0.735822	0.814610	-0.168422
	6	-1.391280	2.070361	-0.238347
	6	-1.706273	2.833534	0.901556
	6	-2.360001	4.055414	0.755146
	6	-2.711324	4.532985	-0.508074
	6	-2.397448	3.772010	-1.638141
	6	-1.743874	2.552240	-1.513526
	6	1.287208	0.246588	1.230241

	7	1.993627	0.102303	0.078385
	8	1.756669	0.367609	2.357993
	6	3.391239	0.078456	-0.106960
	6	3.853532	-0.098388	-1.421596
	6	5.218687	-0.131151	-1.688660
	6	6.143789	0.012450	-0.652207
	6	5.682114	0.187401	0.652665
	6	4.316770	0.221360	0.938523
	1	-0.620757	0.794184	1.914585
	1	-1.442654	2.502395	1.897978
	1	-2.592266	4.636468	1.642468
	1	-3.220948	5.485736	-0.611516
	1	-2.663428	4.131383	-2.627824
	1	-1.494764	1.955874	-2.381155
	1	1.421650	-0.028242	-0.754172
	1	3.135933	-0.209825	-2.230622
	1	5.558178	-0.269102	-2.711215
	1	7.209169	-0.012561	-0.860146
	1	6.391390	0.298593	1.468121
	1	3.961506	0.352559	1.950693
	6	-0.766162	-1.264634	1.326424
	6	-0.306210	-2.229095	0.313531
	6	-2.260082	-1.329720	1.775167
	6	-3.369769	-0.785581	0.854009
	6	-2.936578	-3.767626	-0.396753
	6	-1.524132	-4.225097	-0.799818
	6	-0.366329	-3.304109	-0.436026
	6	-3.498515	-1.271436	-0.574728
	6	-3.347564	-2.496895	-1.087690

	1	-0.214755	-1.532805	2.241055
	1	-2.459797	-2.368477	2.049099
	1	-2.322306	-0.763796	2.714480
	1	-4.322392	-0.969522	1.374943
	1	-3.285375	0.305413	0.820705
	1	-3.635027	-4.566149	-0.682579
	1	-3.005765	-3.678519	0.689488
	1	-1.324812	-5.213616	-0.361081
	1	-1.493026	-4.379057	-1.887921
	1	0.572012	-3.618272	-0.911593
	1	-3.793973	-0.490058	-1.274175
	1	-3.503265	-2.601808	-2.162512
TS_for_biradical_to_9c				
	8	0.902672	-1.072432	1.340516
	6	0.633001	-0.573394	-0.936643
	7	1.431552	-1.062225	0.156053
	6	2.762047	-1.510105	0.003853
	6	3.350328	-1.698862	-1.261999
	6	4.668103	-2.141749	-1.347834
	6	5.412427	-2.404506	-0.196457
	6	4.820130	-2.224650	1.058306
	6	3.507331	-1.785208	1.167247
	6	-0.787759	-0.901387	-1.106693
	7	-1.468090	-1.339038	0.002146
	8	-1.306415	-0.713177	-2.219863
	6	-2.818975	-1.697155	0.125619
	6	-3.237941	-2.172975	1.382138
	6	-4.561989	-2.543291	1.592501
	6	-5.494863	-2.449323	0.556804

	6	-5.079149	-1.979717	-0.689657
	6	-3.756032	-1.601525	-0.918078
	1	1.162933	-0.453840	-1.866534
	1	2.792959	-1.526990	-2.174208
	1	5.111205	-2.287475	-2.328388
	1	6.439187	-2.747729	-0.274352
	1	5.386795	-2.430072	1.961731
	1	3.038539	-1.648241	2.132651
	1	-0.899794	-1.386187	0.845034
	1	-2.515022	-2.251277	2.190584
	1	-4.864384	-2.906971	2.570480
	1	-6.528516	-2.739065	0.719696
	1	-5.793732	-1.902368	-1.504611
	1	-3.436862	-1.238598	-1.884316
	6	1.621623	1.919199	0.199328
	6	0.671124	1.804495	-0.751002
	6	1.301376	2.076610	1.661570
	6	0.020144	2.896976	1.941128
	6	-1.326862	4.335895	-0.597624
	6	-0.611008	3.674233	-1.815216
	6	-0.273381	2.211603	-1.569367
	6	0.166017	4.327065	1.494664
	6	-0.377628	4.918030	0.422822
	1	2.666755	1.778282	-0.076131
	1	1.191748	1.068509	2.096954
	1	2.164104	2.535291	2.160449
	1	-0.829312	2.412757	1.450080
	1	-0.171128	2.864013	3.021335
	1	-1.961156	5.146607	-0.975276

	1	-2.000009	3.601867	-0.142449
	1	-1.269222	3.725483	-2.688245
	1	0.290321	4.246311	-2.060412
	1	-0.897974	1.474038	-2.071106
	1	0.849368	4.925287	2.099717
	1	-0.089493	5.952529	0.232237
TS_for_biradical_to_10c				
	8	-0.372858	-2.201632	0.930716
	6	-0.148922	-0.986975	-1.027592
	7	0.305599	-1.825673	-0.109032
	6	1.639919	-2.388583	-0.222220
	6	2.684439	-1.675471	-0.817023
	6	3.942705	-2.271303	-0.903360
	6	4.154096	-3.556389	-0.401151
	6	3.102717	-4.248358	0.205047
	6	1.841913	-3.665676	0.304764
	6	-1.523844	-0.437903	-1.131552
	7	-2.366243	-0.734672	-0.099745
	8	-1.809381	0.224761	-2.134962
	6	-3.710468	-0.366191	0.070580
	6	-4.352133	-0.827755	1.233753
	6	-5.683323	-0.507165	1.478837
	6	-6.398980	0.277799	0.571501
	6	-5.761532	0.735652	-0.582167
	6	-4.427320	0.423719	-0.843980
	1	0.477585	-0.818503	-1.889477
	1	2.536257	-0.660844	-1.168041
	1	4.761470	-1.719863	-1.354975
	1	5.136403	-4.013205	-0.472696

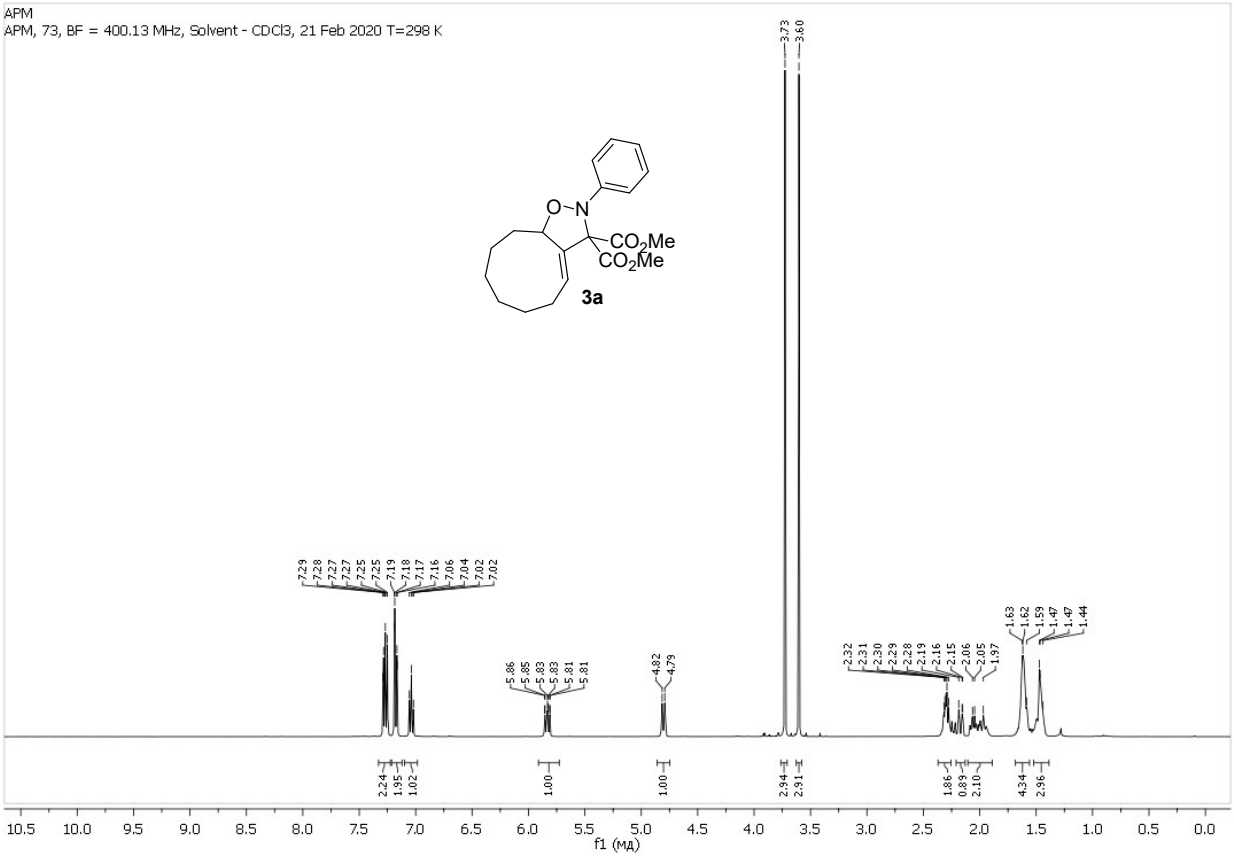
	1	3.262822	-5.245973	0.602257
	1	1.013797	-4.176857	0.779247
	1	-1.933332	-1.327240	0.614508
	1	-3.797378	-1.438557	1.941398
	1	-6.161944	-0.873673	2.382487
	1	-7.438171	0.528088	0.762259
	1	-6.306824	1.346704	-1.296227
	1	-3.935005	0.777553	-1.738397
	6	1.037485	1.110875	1.236396
	6	0.623717	1.450569	-0.015449
	6	1.852352	1.955265	2.197724
	6	3.373020	1.978505	1.908249
	6	2.089902	4.169321	-0.222517
	6	1.021831	3.707919	-1.230351
	6	0.490489	2.299075	-1.067494
	6	3.870309	2.475850	0.569025
	6	3.361441	3.363883	-0.294929
	1	0.756042	0.123008	1.603672
	1	1.458372	2.973994	2.240862
	1	1.722475	1.538051	3.202695
	1	3.857066	2.564030	2.705438
	1	3.752419	0.956906	2.036142
	1	2.331872	5.214424	-0.457668
	1	1.668400	4.177636	0.783123
	1	0.170532	4.405752	-1.197204
	1	1.420508	3.794302	-2.251845
	1	-0.112857	1.943034	-1.905889
	1	4.825991	2.033949	0.283841
	1	3.937043	3.534687	-1.206652

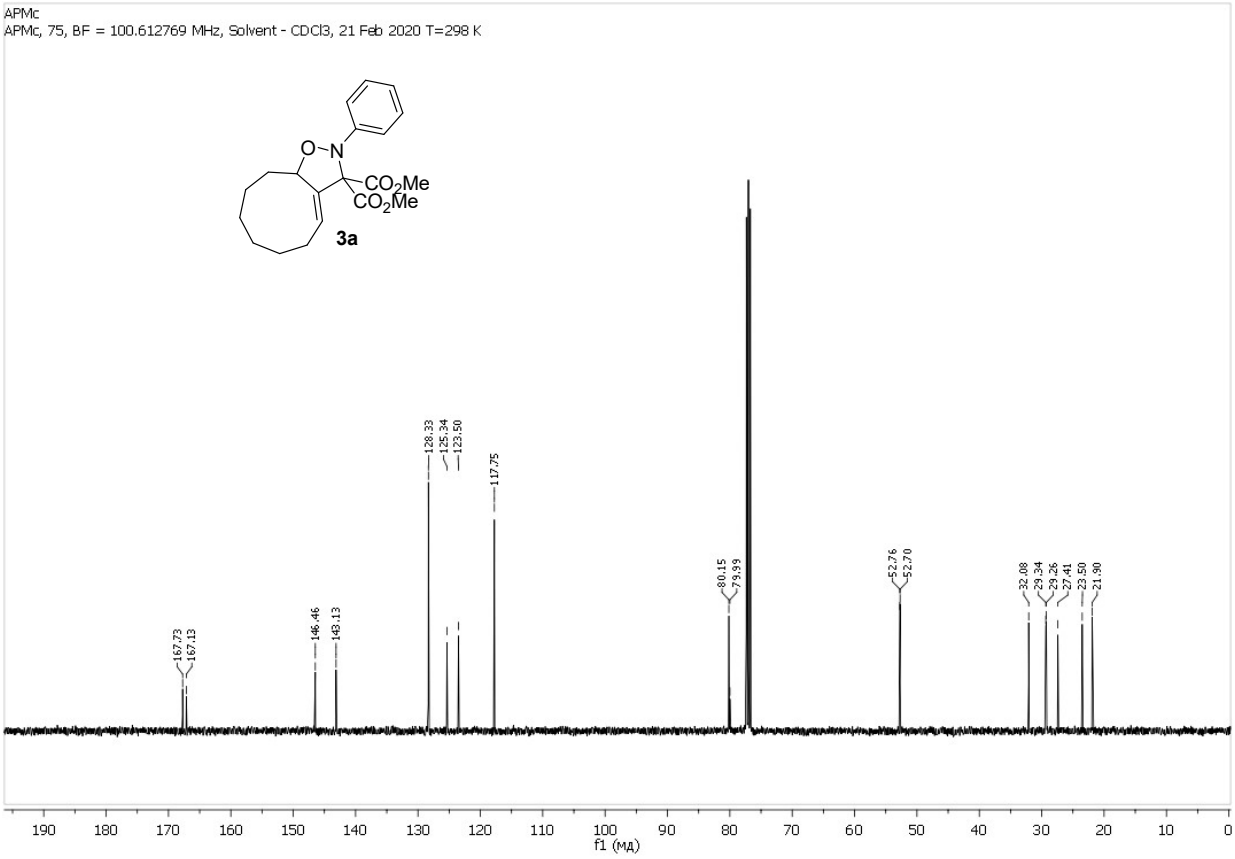
TS_for_biradical_to_11c				
	6	0.093515	0.569121	0.872612
	8	0.098196	0.969789	-1.436691
	7	-0.307263	1.357048	-0.267632
	6	-1.133151	2.496397	-0.175283
	6	-1.400000	3.124673	1.056572
	6	-2.219284	4.250577	1.089141
	6	-2.778529	4.763766	-0.082881
	6	-2.505039	4.138721	-1.304721
	6	-1.687383	3.017615	-1.360866
	6	1.492610	0.165942	1.108392
	7	2.348814	0.261671	0.036186
	8	1.799654	-0.287189	2.218479
	6	3.712996	-0.062269	-0.032378
	6	4.371053	0.196009	-1.248818
	6	5.722267	-0.099500	-1.397129
	6	6.444386	-0.655264	-0.338145
	6	5.791457	-0.910105	0.868491
	6	4.436793	-0.622457	1.034585
	1	-0.436636	0.807603	1.780442
	1	-0.956337	2.763612	1.976273
	1	-2.412689	4.734180	2.041957
	1	-3.417257	5.640635	-0.046347
	1	-2.932707	4.529846	-2.223247
	1	-1.466450	2.526499	-2.299611
	1	1.914353	0.582877	-0.825029
	1	3.813871	0.631432	-2.074703
	1	6.212030	0.106956	-2.344565
	1	7.499236	-0.885520	-0.452881

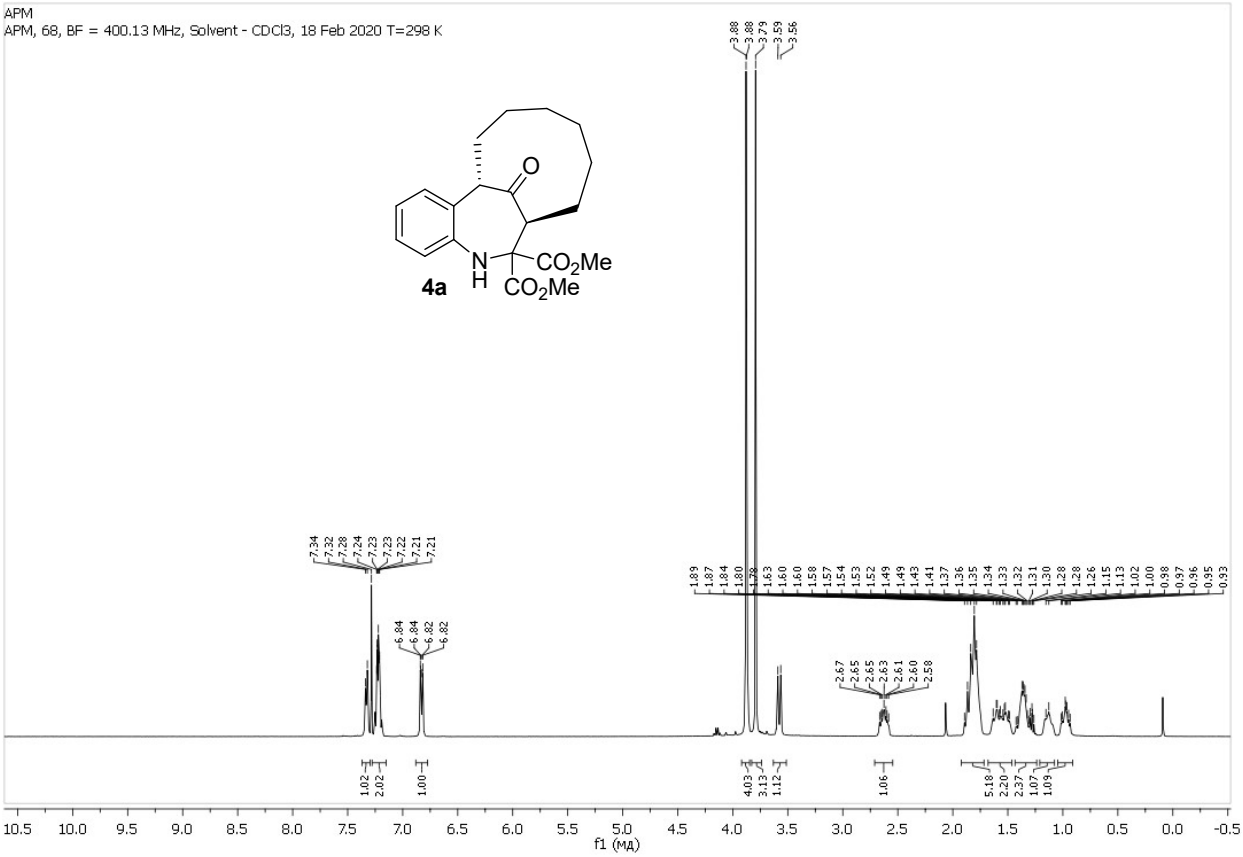
	1	6.340420	-1.342401	1.700628
	1	3.931520	-0.820671	1.968818
	6	-0.965245	-1.415246	0.695768
	6	-2.274350	-1.094226	0.690800
	6	-0.345087	-2.108965	-0.520542
	6	-1.356844	-2.963516	-1.328354
	6	-4.429223	-2.996021	-0.453541
	6	-4.648759	-1.888743	0.611716
	6	-3.549087	-0.829207	0.608515
	6	-2.064989	-3.990665	-0.488063
	6	-3.348405	-3.988135	-0.100126
	1	-0.509891	-1.630621	1.661428
	1	0.086871	-1.364225	-1.195638
	1	0.478555	-2.736429	-0.163375
	1	-0.795269	-3.461738	-2.129854
	1	-2.074231	-2.294399	-1.812645
	1	-5.374566	-3.541611	-0.567314
	1	-4.226851	-2.516337	-1.416516
	1	-5.603092	-1.389104	0.415763
	1	-4.733571	-2.345322	1.605566
	1	-3.870573	0.207483	0.478812
	1	-1.430789	-4.796034	-0.113851
	1	-3.667823	-4.789552	0.567244
TS_for_biradical_to_12c				
	6	0.073985	0.326286	0.610091
	8	0.257540	1.278489	-1.520580
	7	-0.183601	1.407309	-0.310483
	6	-0.901328	2.568094	0.045158
	6	-1.171944	2.886096	1.389293

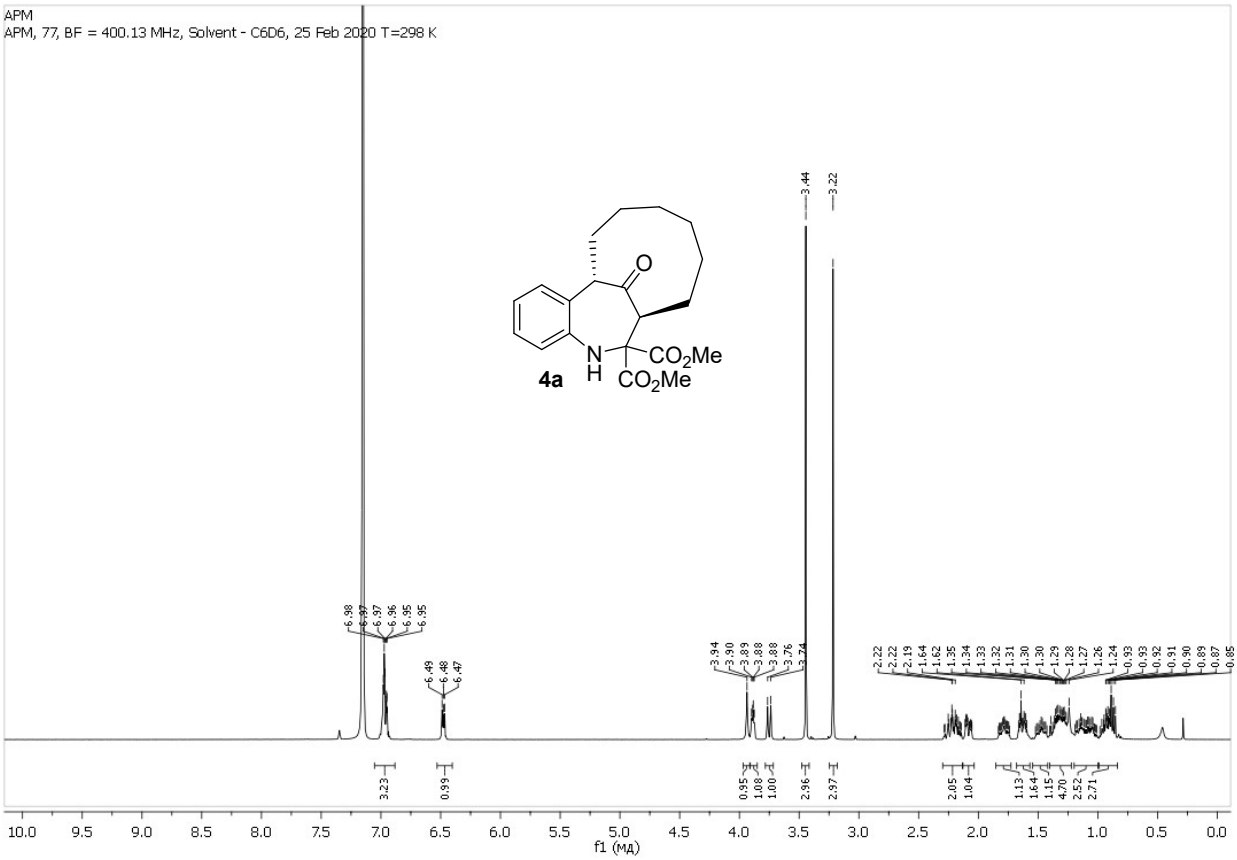
	6	-1.881780	4.046208	1.689286
	6	-2.328236	4.893869	0.673350
	6	-2.050483	4.574743	-0.660564
	6	-1.339947	3.425299	-0.981910
	6	1.438676	-0.166620	0.861613
	7	2.362445	0.085044	-0.125056
	8	1.663314	-0.826382	1.886317
	6	3.718572	-0.275951	-0.176920
	6	4.429288	0.078209	-1.338252
	6	5.777785	-0.238955	-1.465294
	6	6.445112	-0.911842	-0.438864
	6	5.740207	-1.261198	0.713513
	6	4.387341	-0.953405	0.857351
	1	-0.569758	0.301364	1.475663
	1	-0.812478	2.255720	2.193619
	1	-2.080039	4.289828	2.728720
	1	-2.883758	5.794132	0.916676
	1	-2.391654	5.228232	-1.458097
	1	-1.115809	3.166890	-2.008732
	1	1.989036	0.566664	-0.939435
	1	3.914797	0.603409	-2.139355
	1	6.308051	0.042029	-2.370800
	1	7.497669	-1.159551	-0.536958
	1	6.246112	-1.784588	1.520224
	1	3.842933	-1.229315	1.748847
	6	-0.989501	-1.405571	-0.449464
	6	-2.177973	-0.848457	-0.739116
	6	-0.876931	-2.559760	0.537311
	6	-1.988216	-2.705404	1.587733

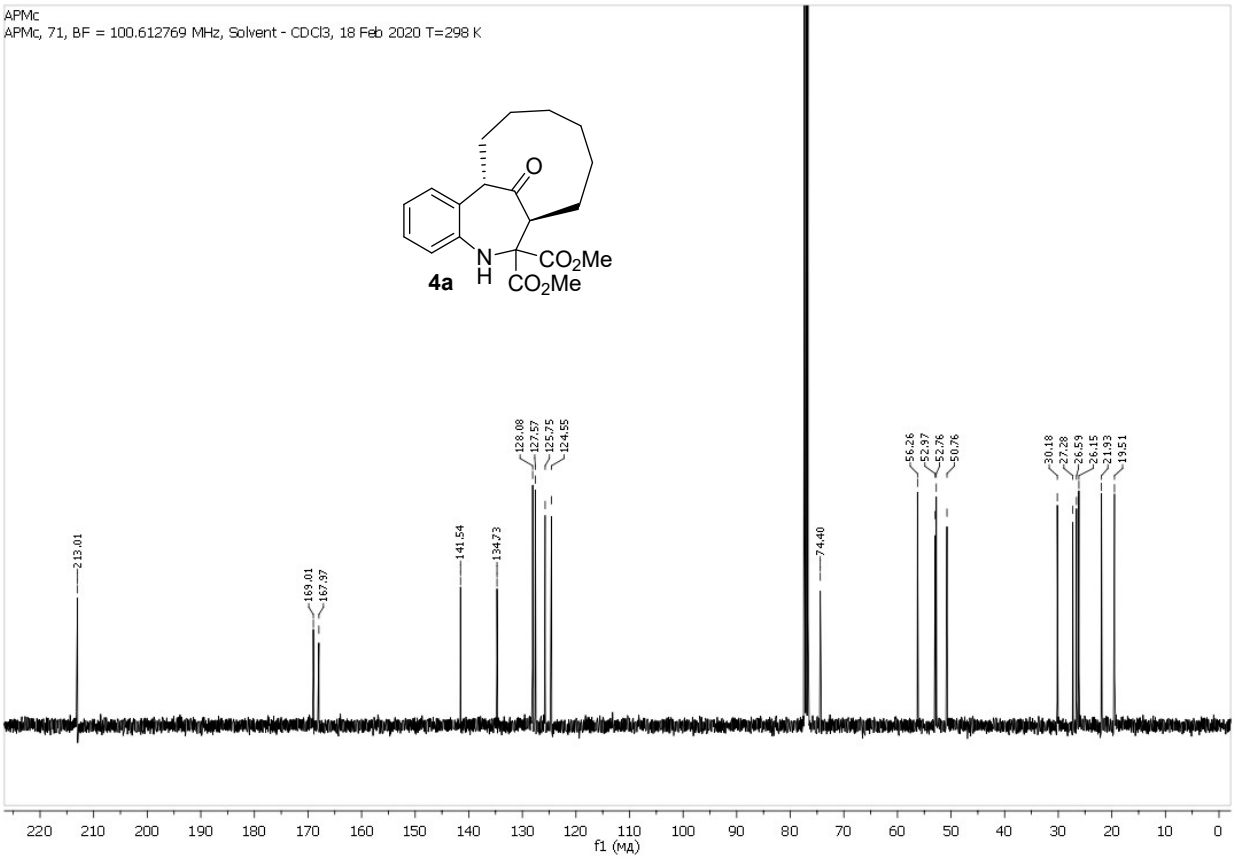
	6	-3.827332	-3.078023	-1.305166
	6	-4.293748	-1.650539	-1.679768
	6	-3.421360	-0.581475	-1.028950
	6	-3.374239	-3.227599	1.260427
	6	-4.101214	-3.399570	0.146092
	1	-0.213249	-1.354906	-1.211607
	1	-0.808273	-3.478825	-0.061191
	1	0.076639	-2.475505	1.068685
	1	-1.591155	-3.372851	2.363877
	1	-2.117514	-1.741652	2.104739
	1	-4.370401	-3.795432	-1.931484
	1	-2.769103	-3.184885	-1.559085
	1	-4.286565	-1.527545	-2.771206
	1	-5.330982	-1.498872	-1.357785
	1	-3.872652	0.381331	-0.786510
	1	-3.893800	-3.507852	2.179163
	1	-5.107187	-3.787758	0.313207

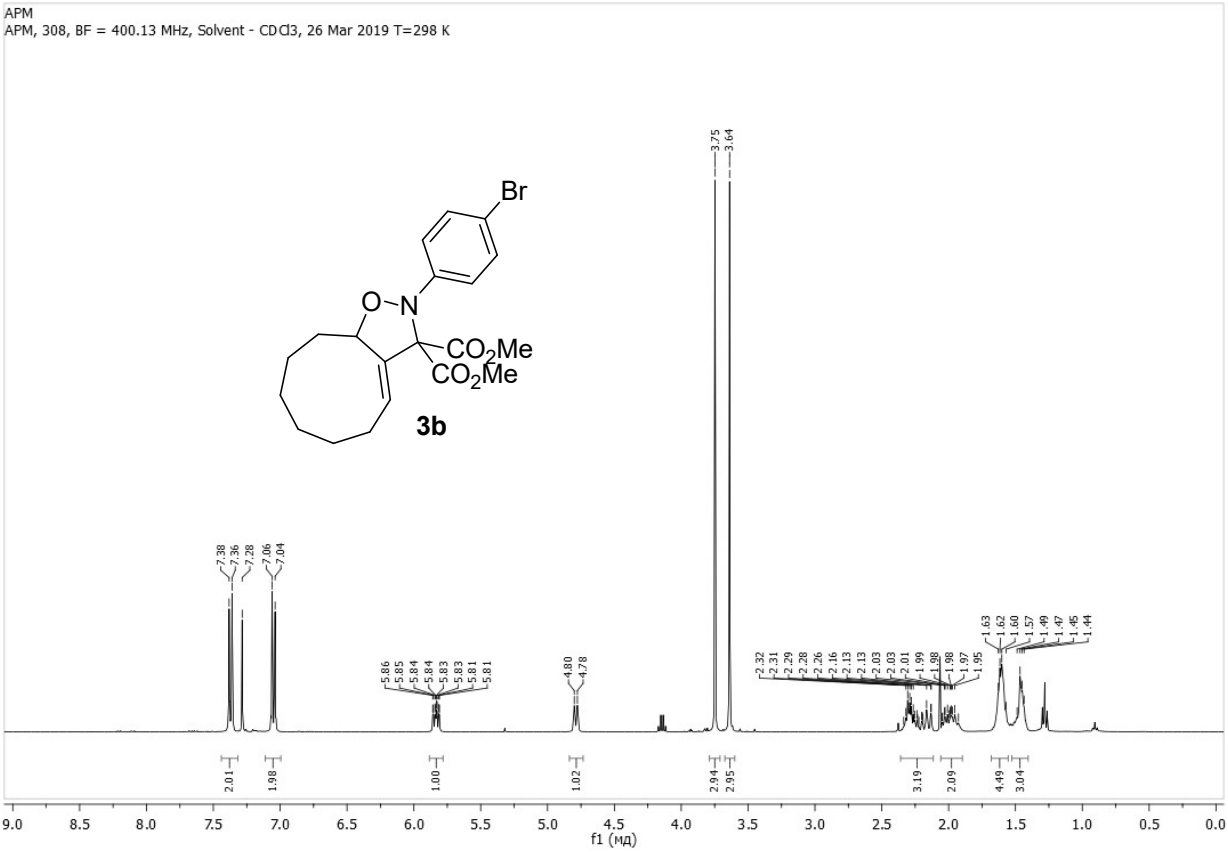

APM
APM, 73, BF = 400.13 MHz, Solvent - CDCl3, 21 Feb 2020 T=298 K
3a
f1 (мд)

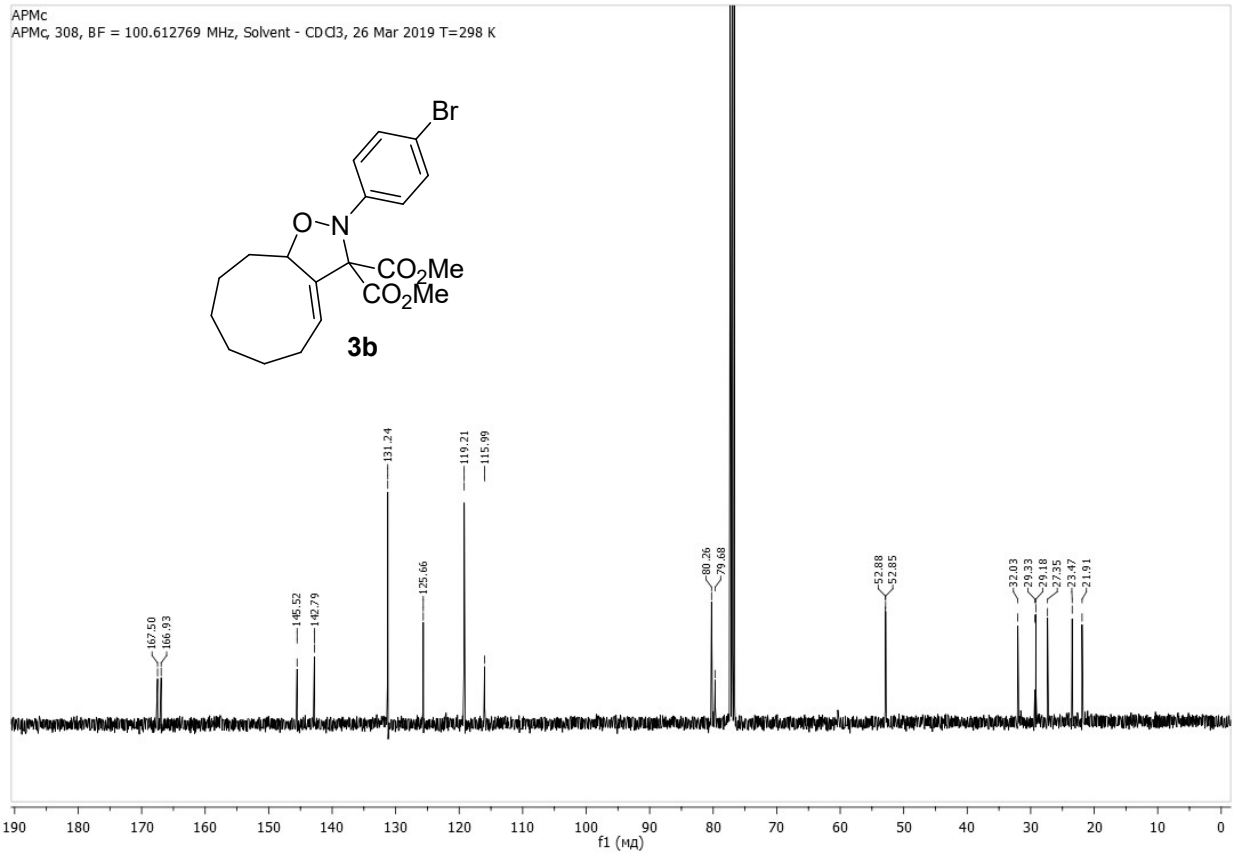

APMc
APMc, 75, BF = 100.612769 MHz, Solvent - CDCl3, 21 Feb 2020 T=298 K
3a
f1 (мд)

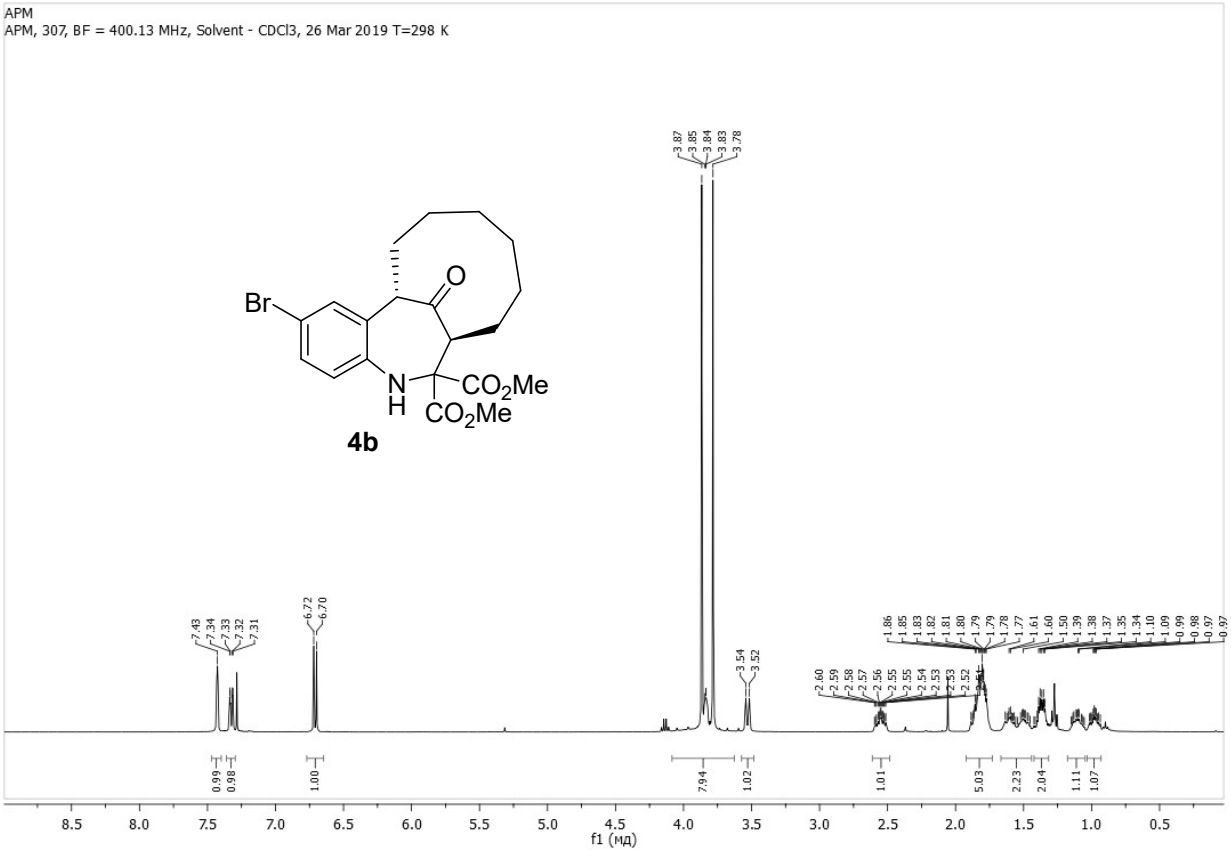

APM
APM, 68, BF = 400.13 MHz, Solvent - CDCl3, 18 Feb 2020 T=298 K
4a
f1 (мд)

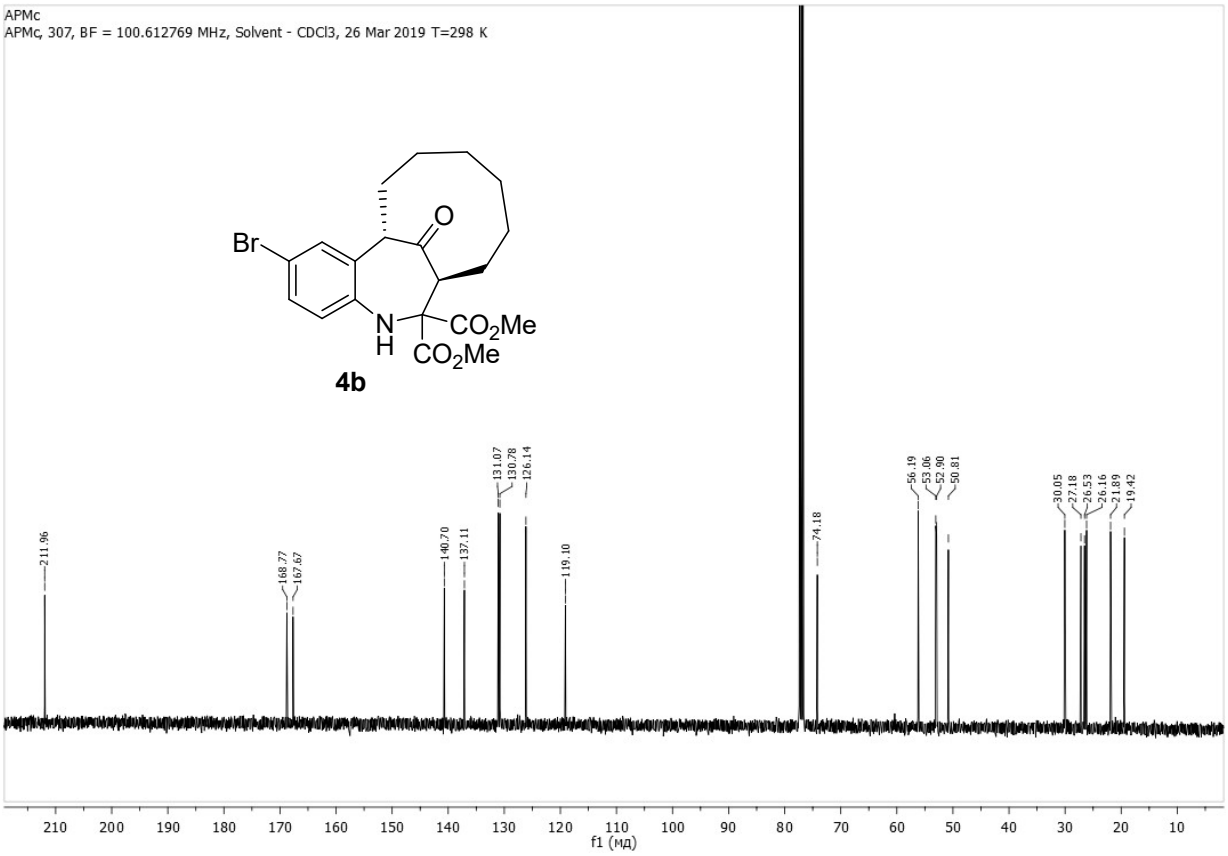

APM
APM, 77, BF = 400.13 MHz, Solvent - C6D6, 25 Feb 2020 T=298 K
4a
f1 (мд)

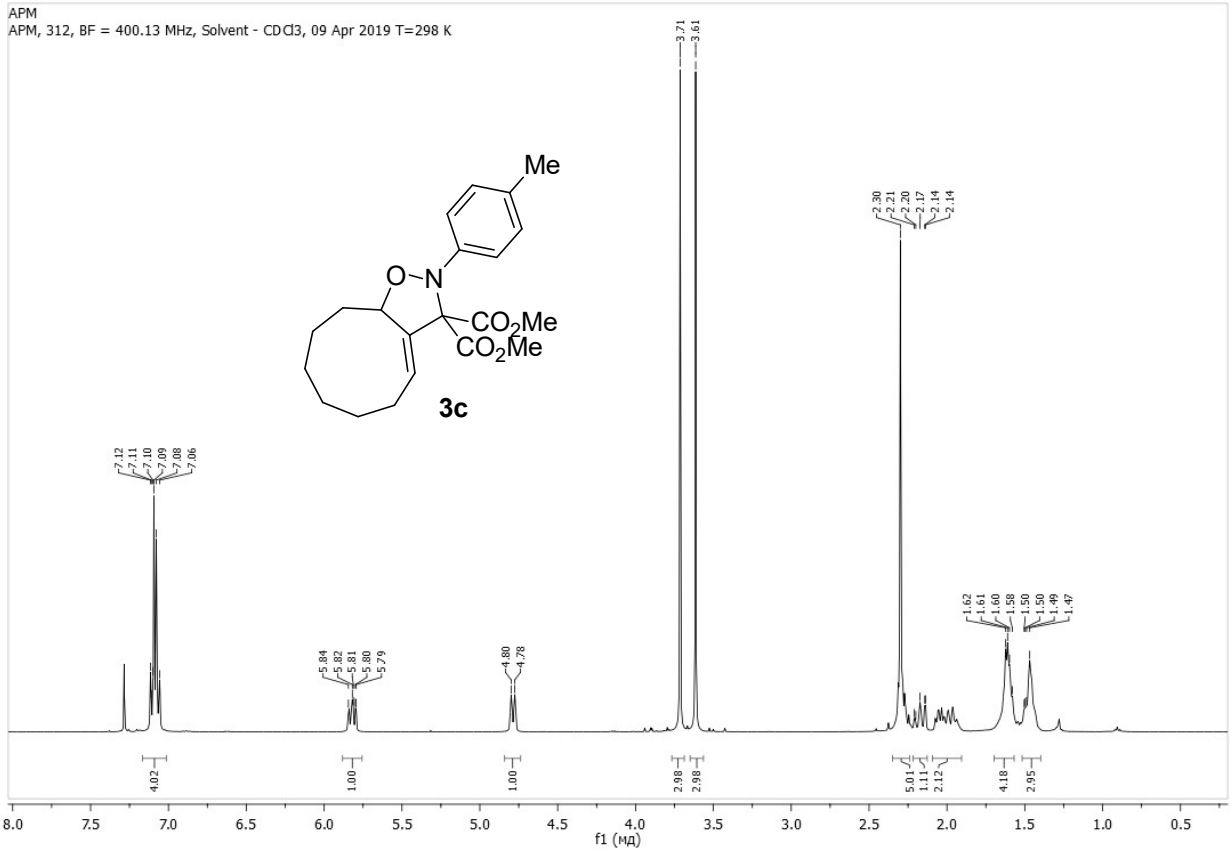

APMc
APMc, 71, BF = 100.612769 MHz, Solvent - CDCl3, 18 Feb 2020 T=298 K
O
N
H
CO2Me
CO2Me
4a
213.01
169.01
167.97
141.54
134.73
128.08
127.57
125.75
124.55
77.40
56.26
52.97
52.76
50.76
30.18
27.28
26.59
26.15
21.93
19.51
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (мд)

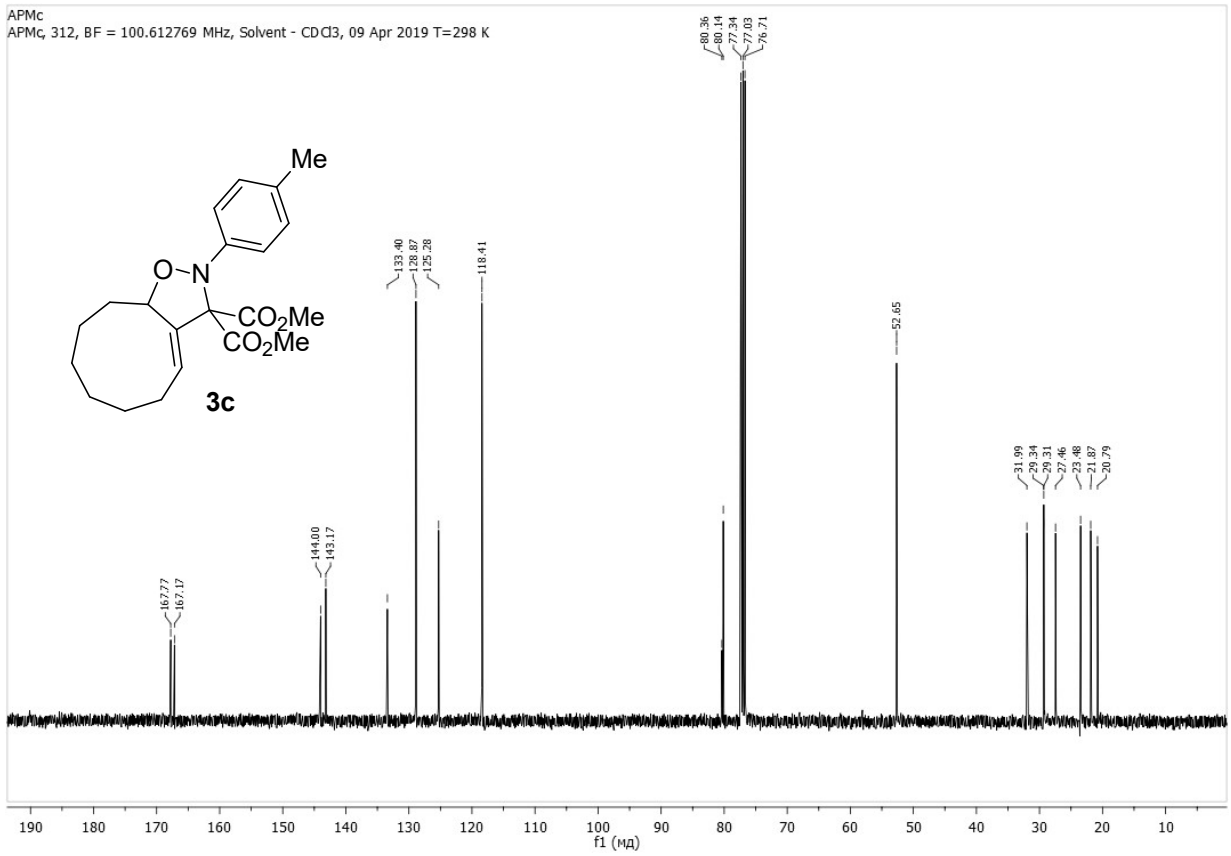

APM
APM, 308, BF = 400.13 MHz, Solvent - CDCl3, 26 Mar 2019 T=298 K
Br
O
N
CO2Me
CO2Me
3b
f1 (мд)

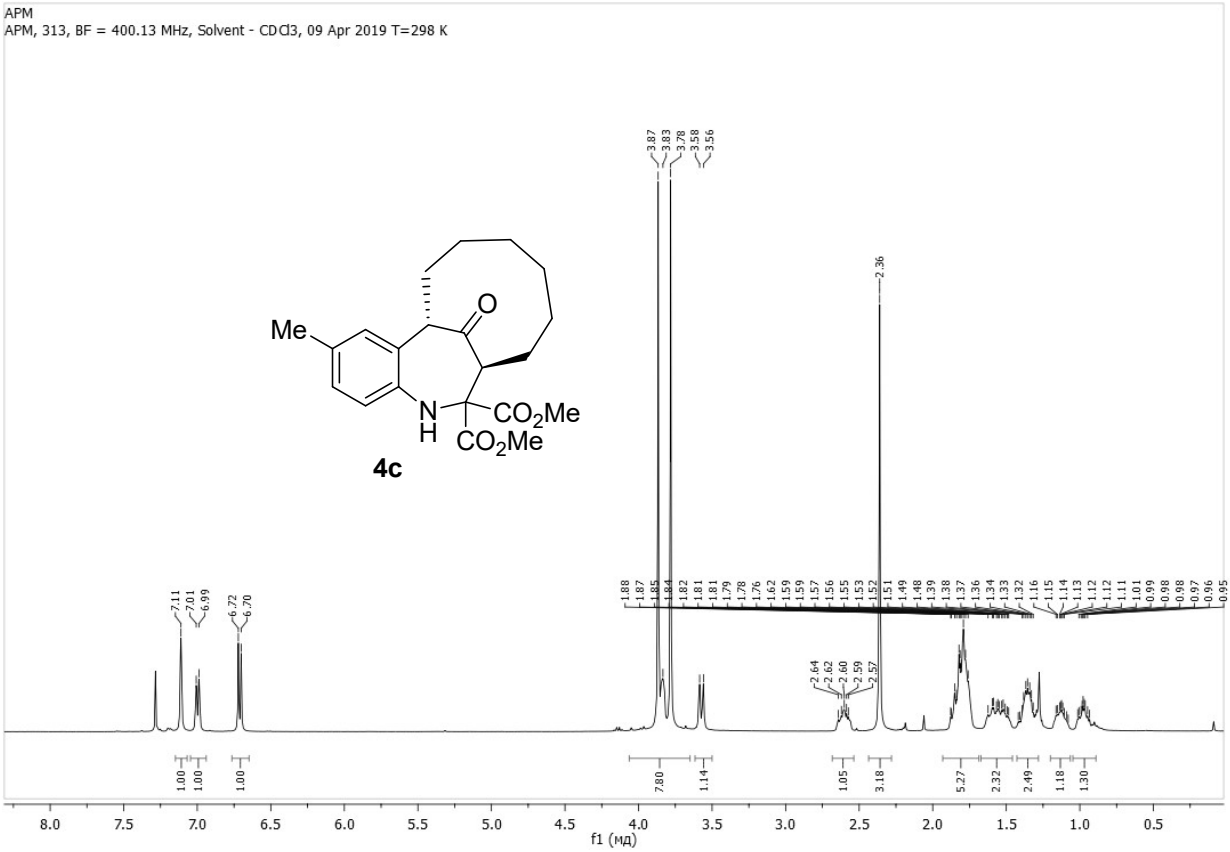

APMc
APMc, 308, BF = 100.612769 MHz, Solvent - CDCl3, 26 Mar 2019 T=298 K
Br
O
N
CO2Me
CO2Me
3b
f1 (мд)

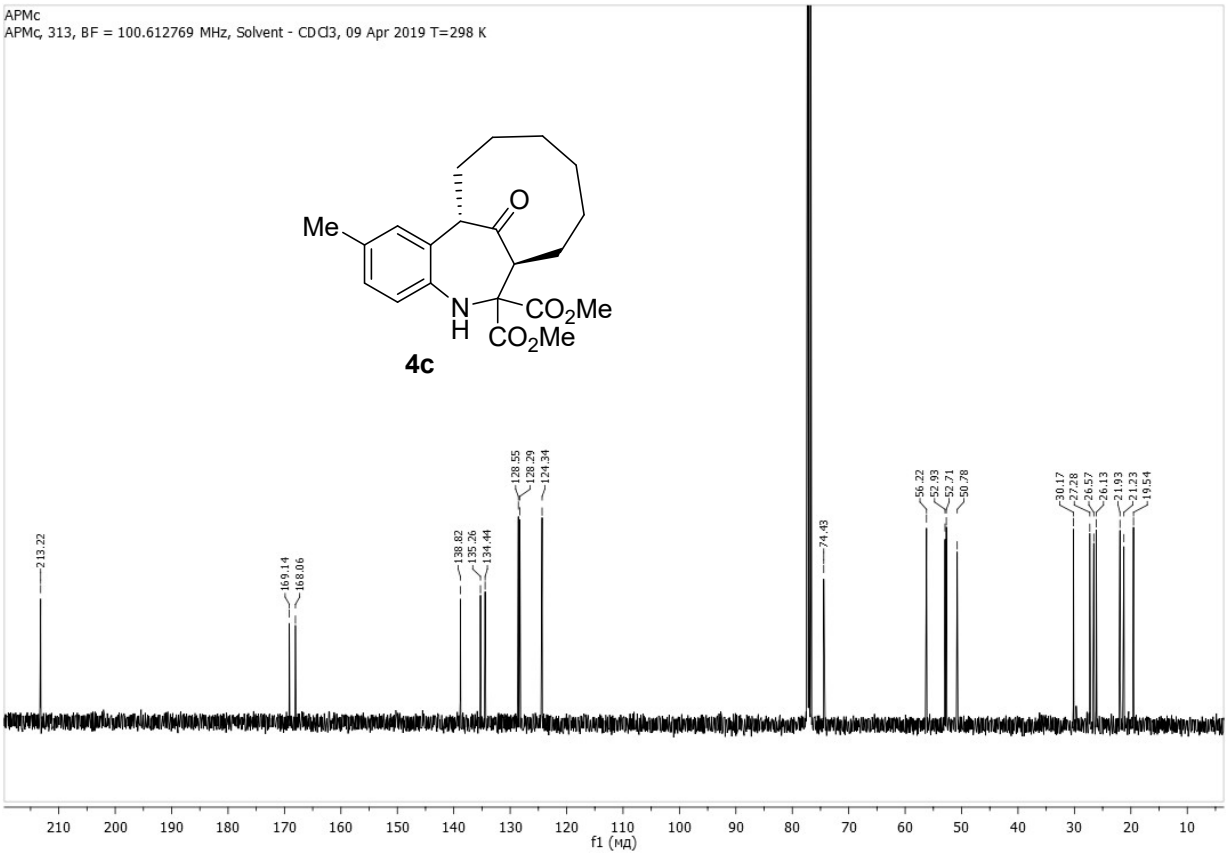

APM
APM, 307, BF = 400.13 MHz, Solvent - CDCl3, 26 Mar 2019 T=298 K
Br
O
N
H
CO2Me
CO2Me
4b
f1 (мд)

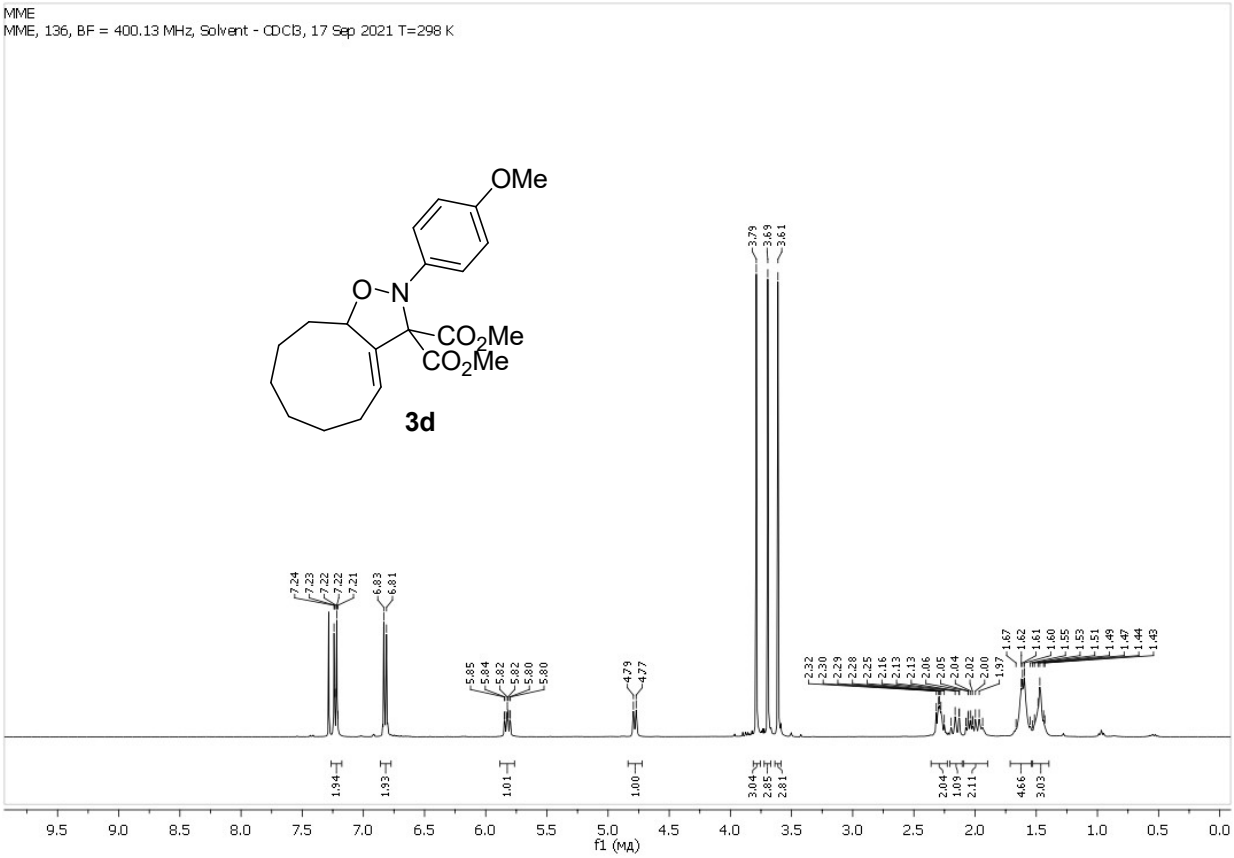

APMc
APMc, 307, BF = 100.612769 MHz, Solvent - CDCl3, 26 Mar 2019 T=298 K
Br
O
N
H
CO2Me
CO2Me
4b
f1 (мд)

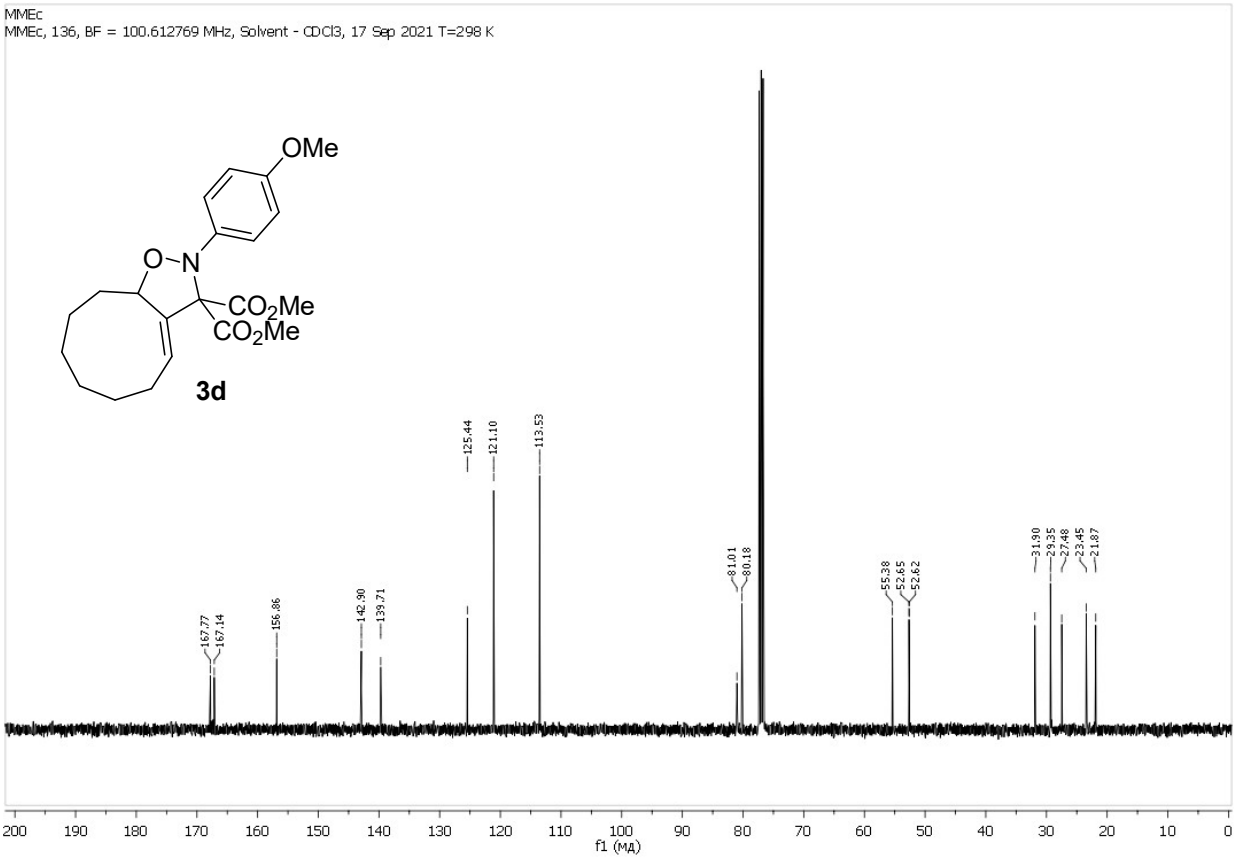

APM
APM, 312, BF = 400.13 MHz, Solvent - CDCl3, 09 Apr 2019 T=298 K
Me
O
N
CO2Me
CO2Me
3c
f1 (мд)

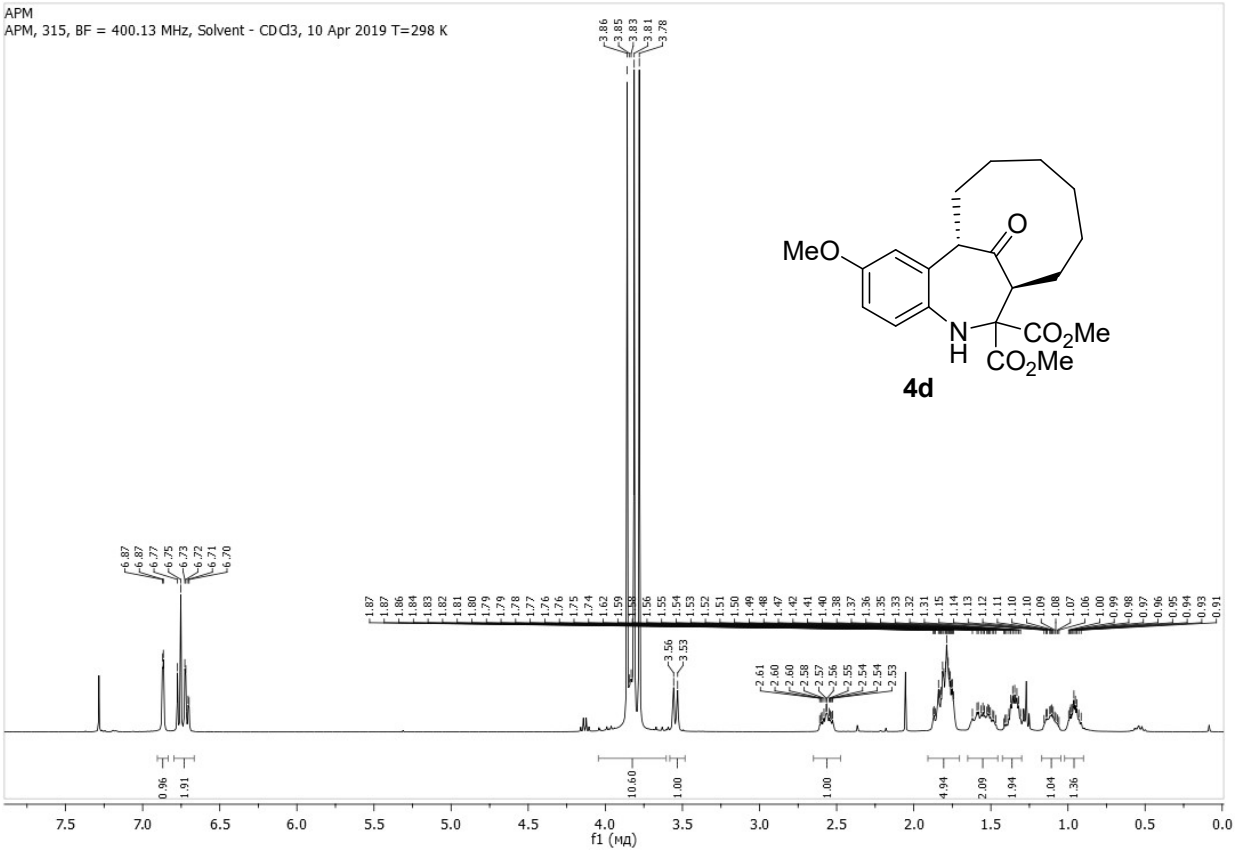

APMc
APMc, 312, BF = 100.612769 MHz, Solvent - CDCl3, 09 Apr 2019 T=298 K
Me
O
N
CO2Me
CO2Me
3c
f1 (мд)

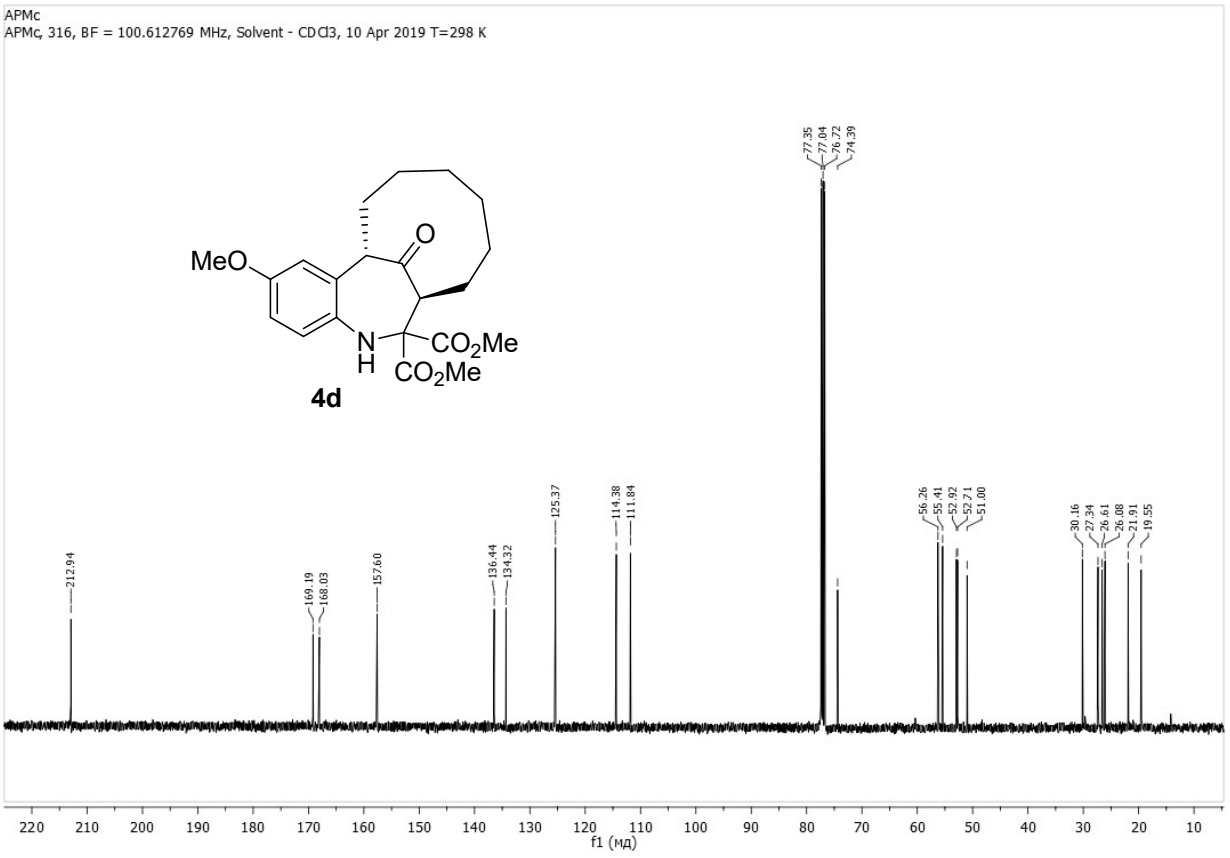

APM
APM, 313, BF = 400.13 MHz, Solvent - CDCl3, 09 Apr 2019 T=298 K
Me
O
N
H
CO2Me
CO2Me
4c
f1 (мд)

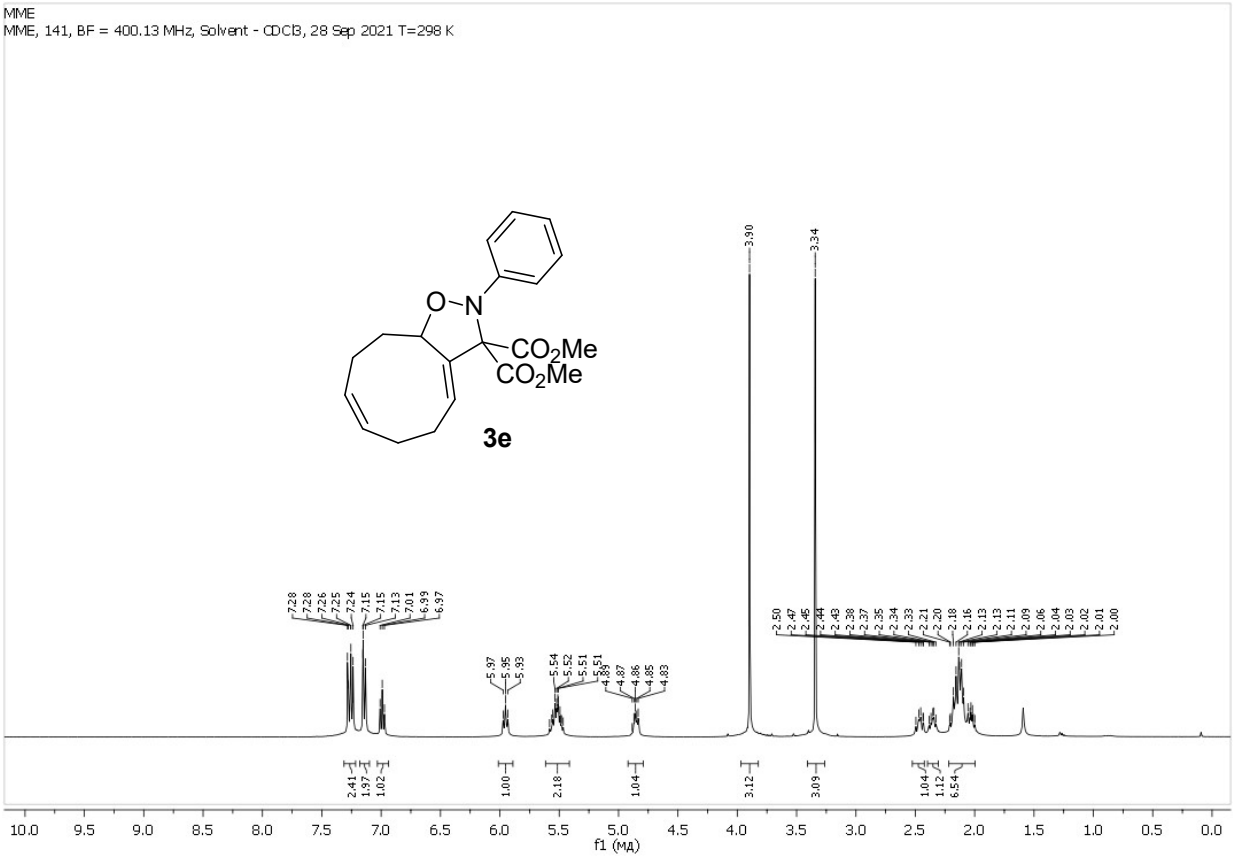

APMc
APMc, 313, BF = 100.612769 MHz, Solvent - CDCl3, 09 Apr 2019 T=298 K
Me
O
N
H
CO2Me
CO2Me
4c
f1 (мд)

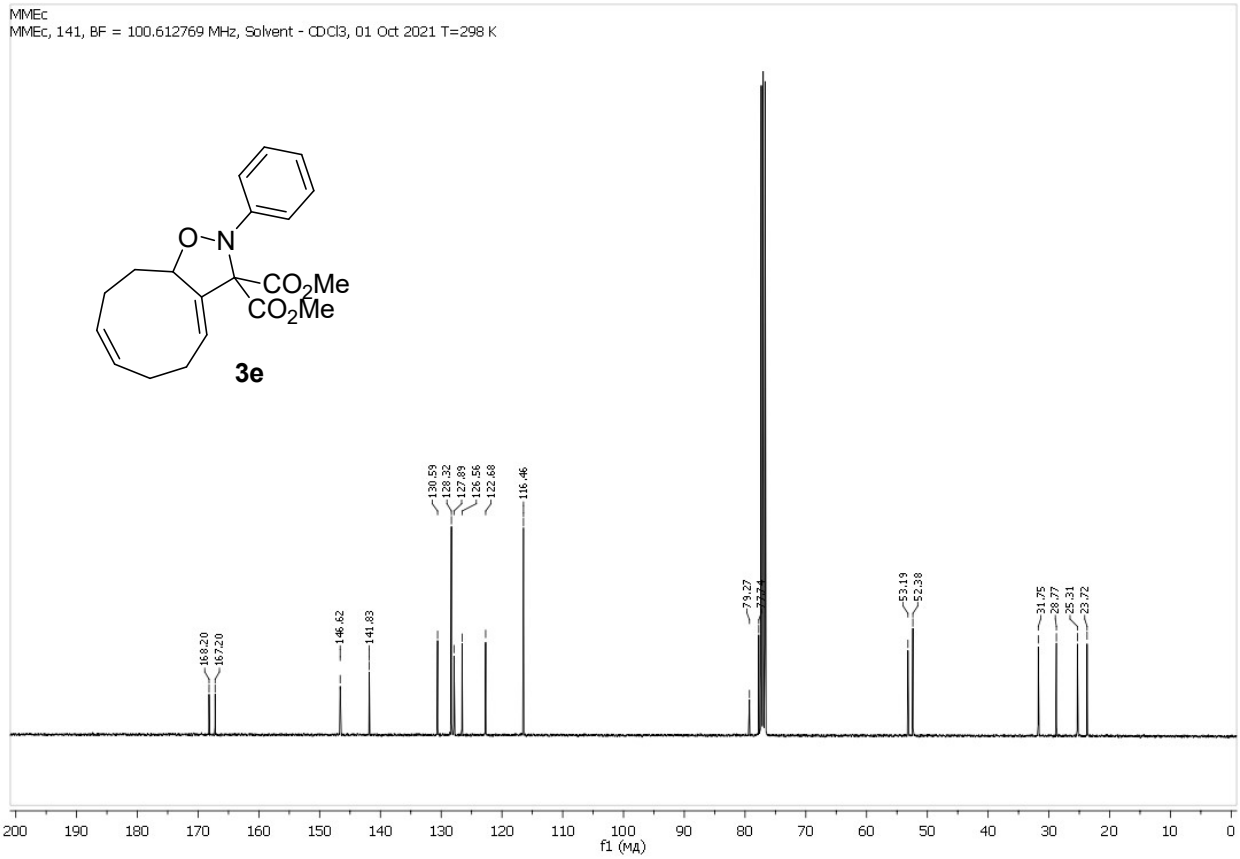

MME
MME, 136, BF = 400.13 MHz, Solvent - CDCl3, 17 Sep 2021 T=298 K
OMe
O
N
CO2Me
CO2Me
3d
f1 (мд)

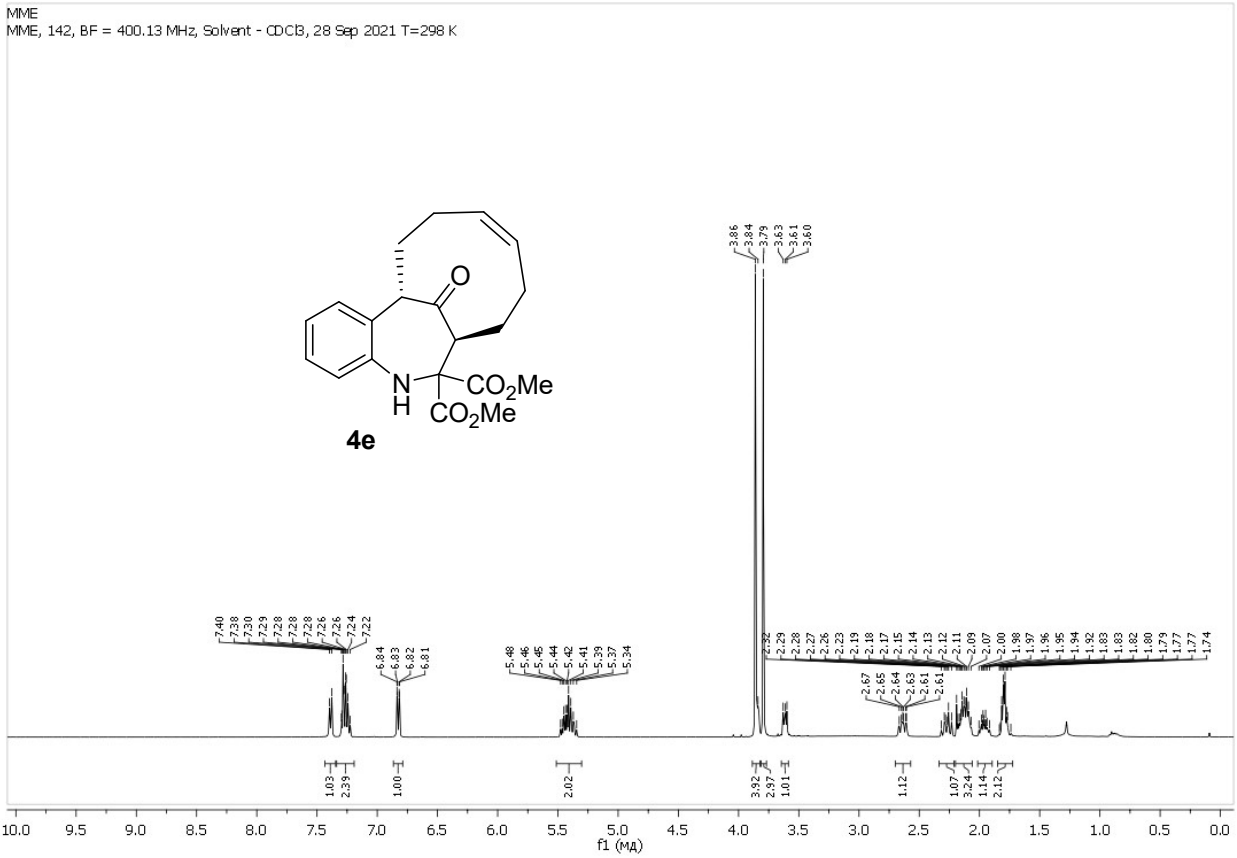

MMEc
MMEc, 136, BF = 100.612769 MHz, Solvent - CDCl3, 17 Sep 2021 T=298 K
OMe
O
N
CO2Me
CO2Me
3d
f1 (мд)

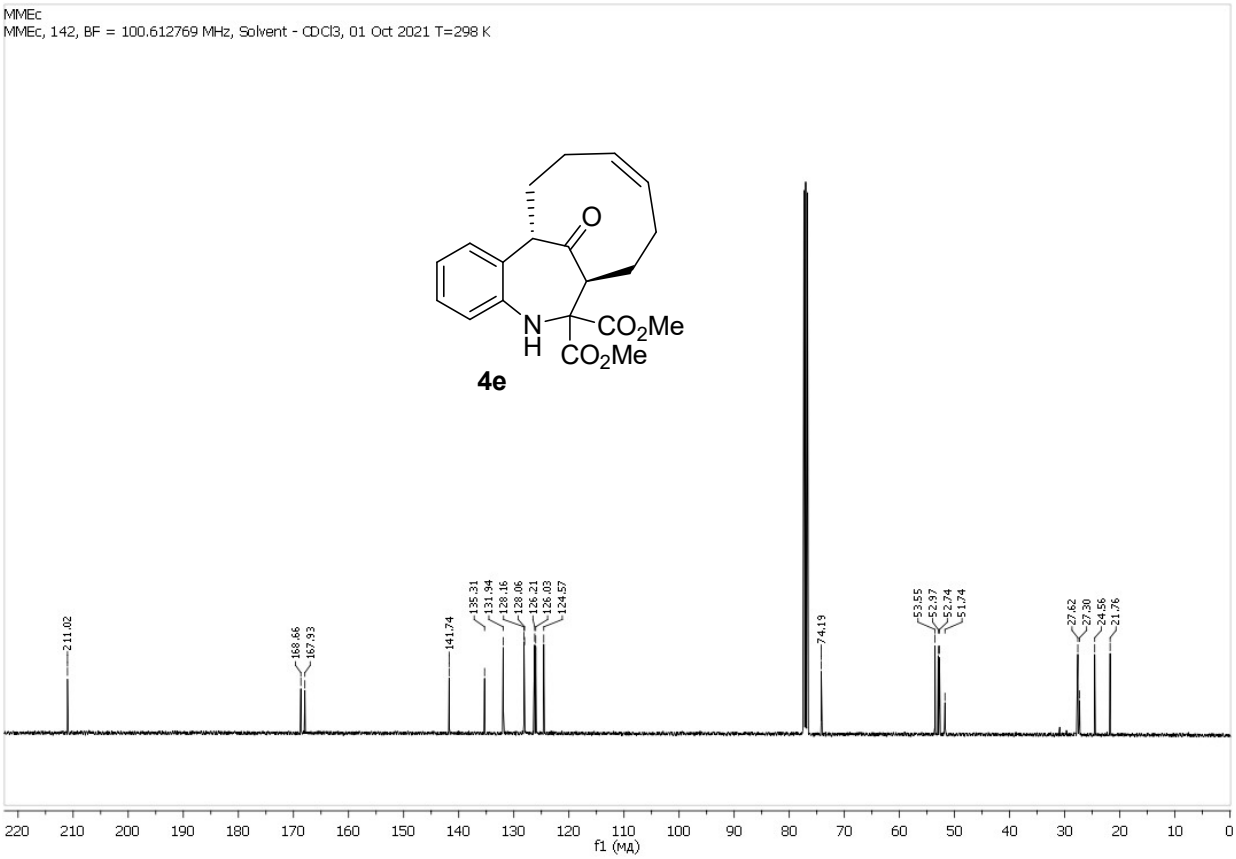

APM
APM, 315, BF = 400.13 MHz, Solvent - CDCl3, 10 Apr 2019 T=298 K
MeO
O
N
H
CO2Me
CO2Me
4d
f1 (мд)

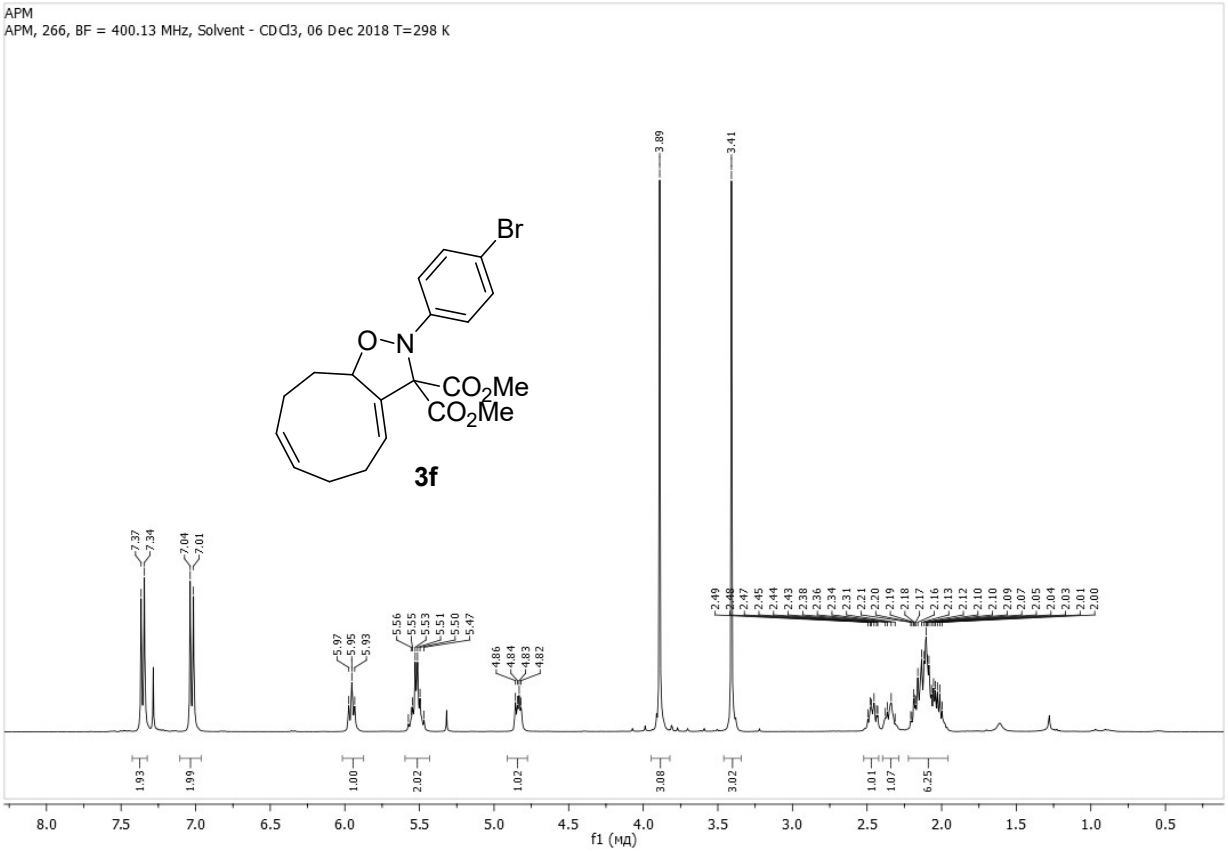

APMc
APMc, 316, BF = 100.612769 MHz, Solvent - CDCl3, 10 Apr 2019 T=298 K
MeO
O
N
H
CO2Me
CO2Me
4d
f1 (мд)

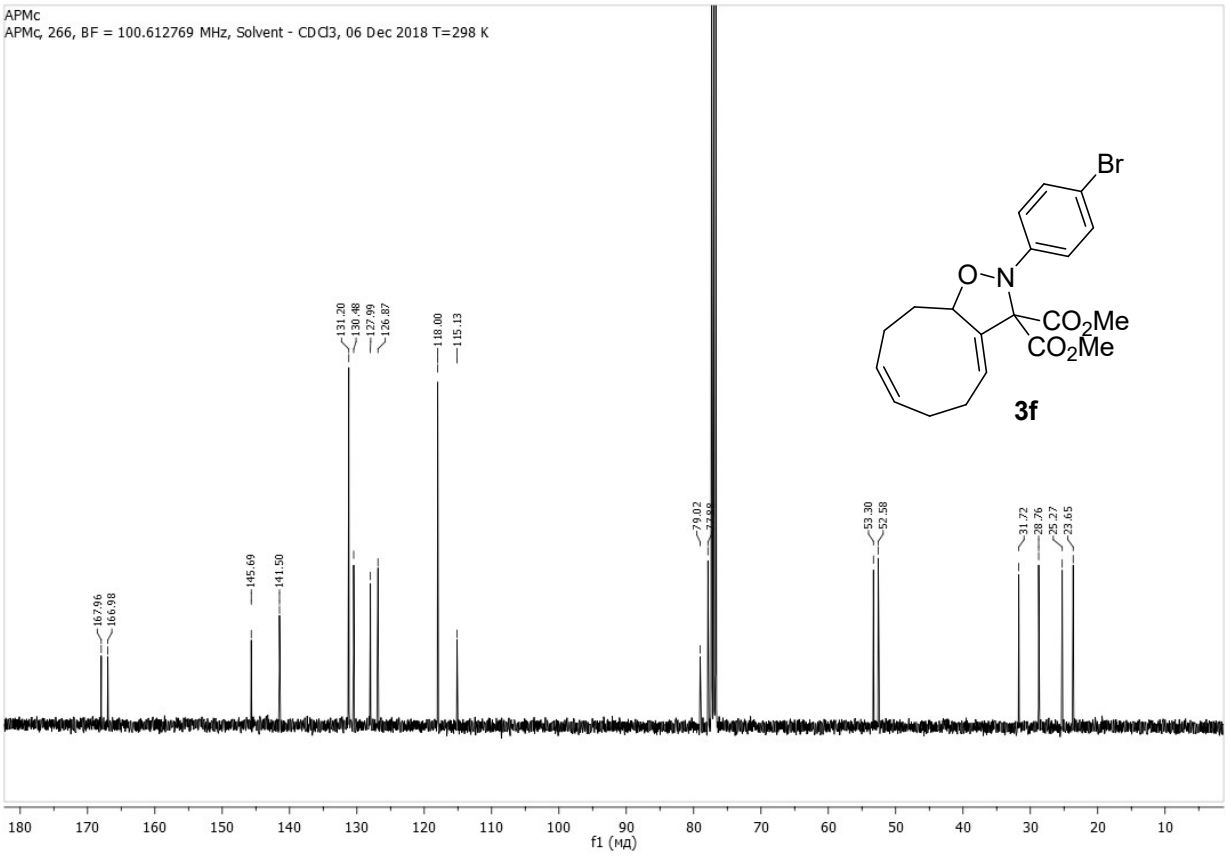

MME
MME, 141, BF = 400.13 MHz, Solvent - CDCl3, 28 Sep 2021 T=298 K
O
N
CO2Me
CO2Me
3e
f1 (мд)

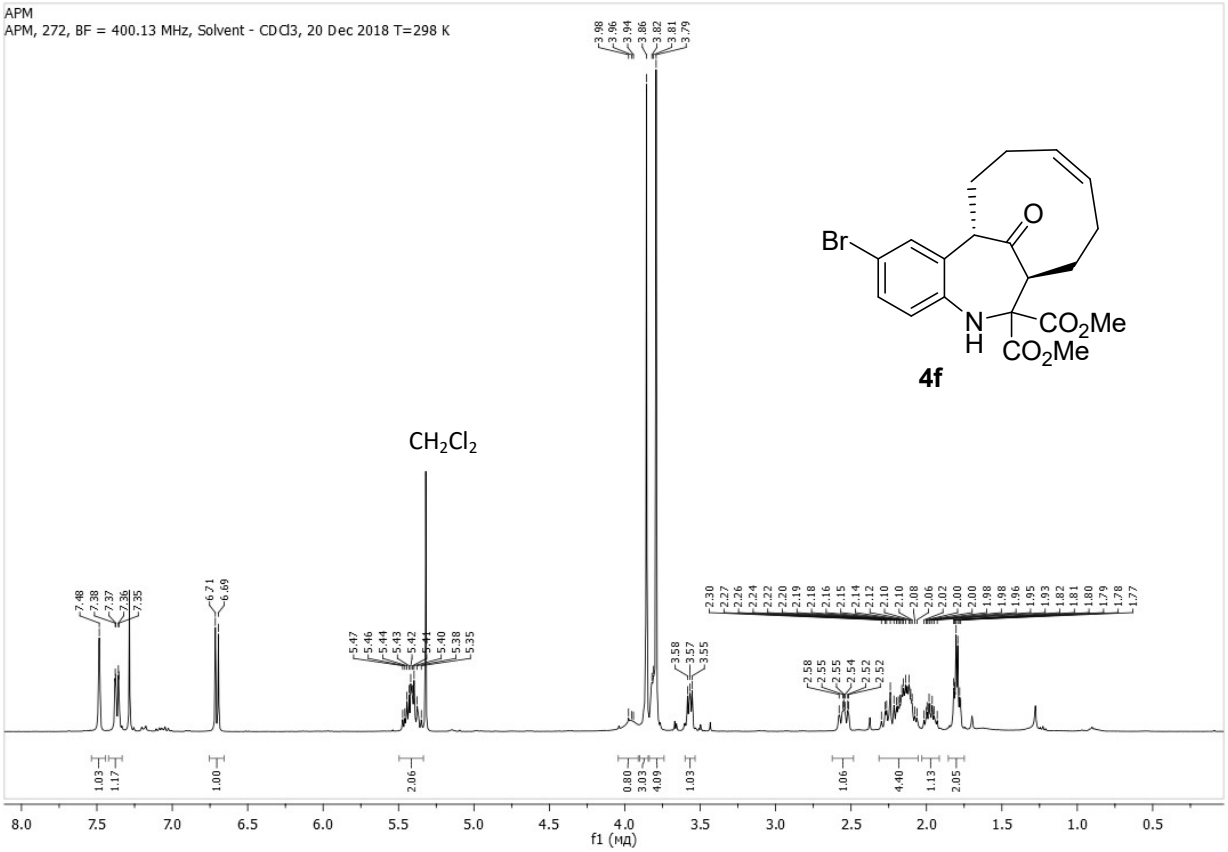

MMEc
MMEc, 141, BF = 100.612769 MHz, Solvent - CDCl3, 01 Oct 2021 T=298 K
O
N
CO2Me
CO2Me
3e
f1 (мд)

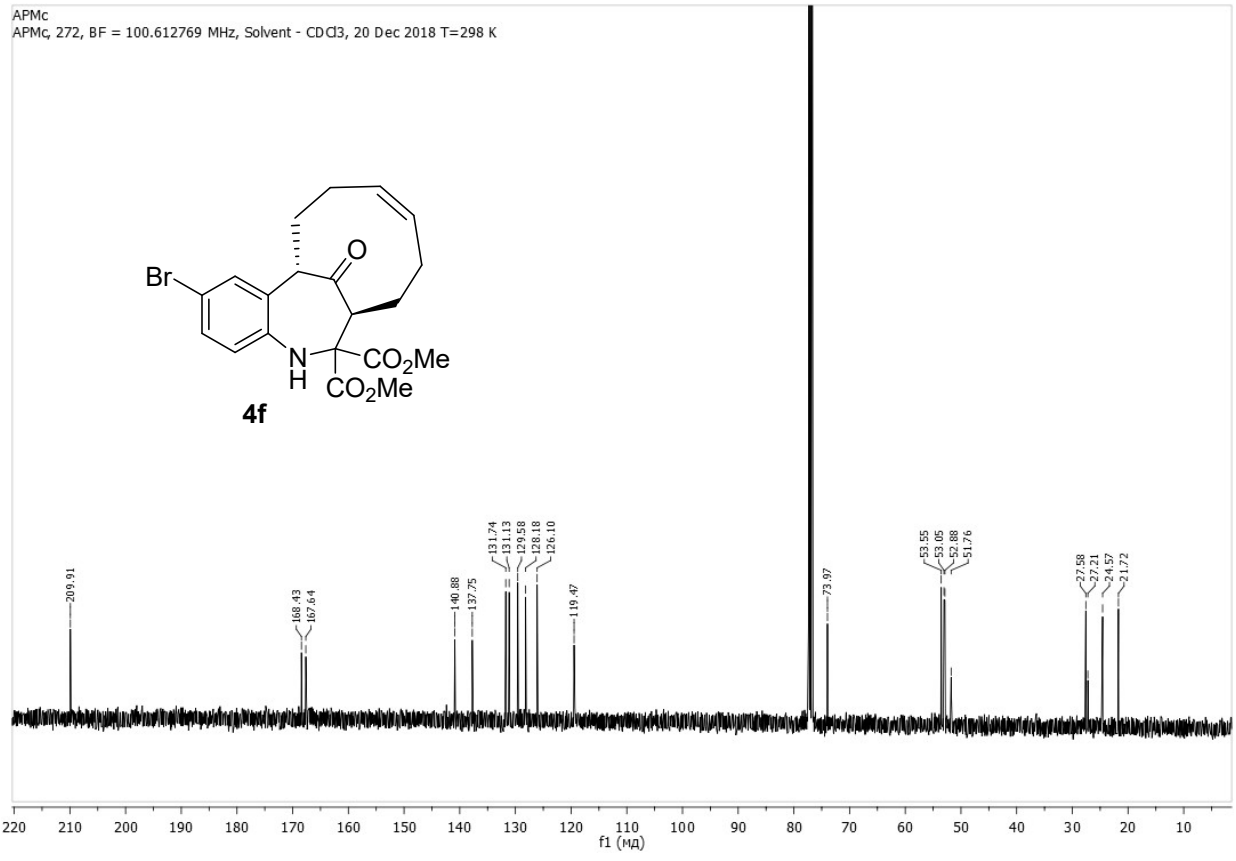

MME
MME, 142, BF = 400.13 MHz, Solvent - CDCl3, 28 Sep 2021 T=298 K
O
N
H
CO2Me
CO2Me
4e
f1 (мд)

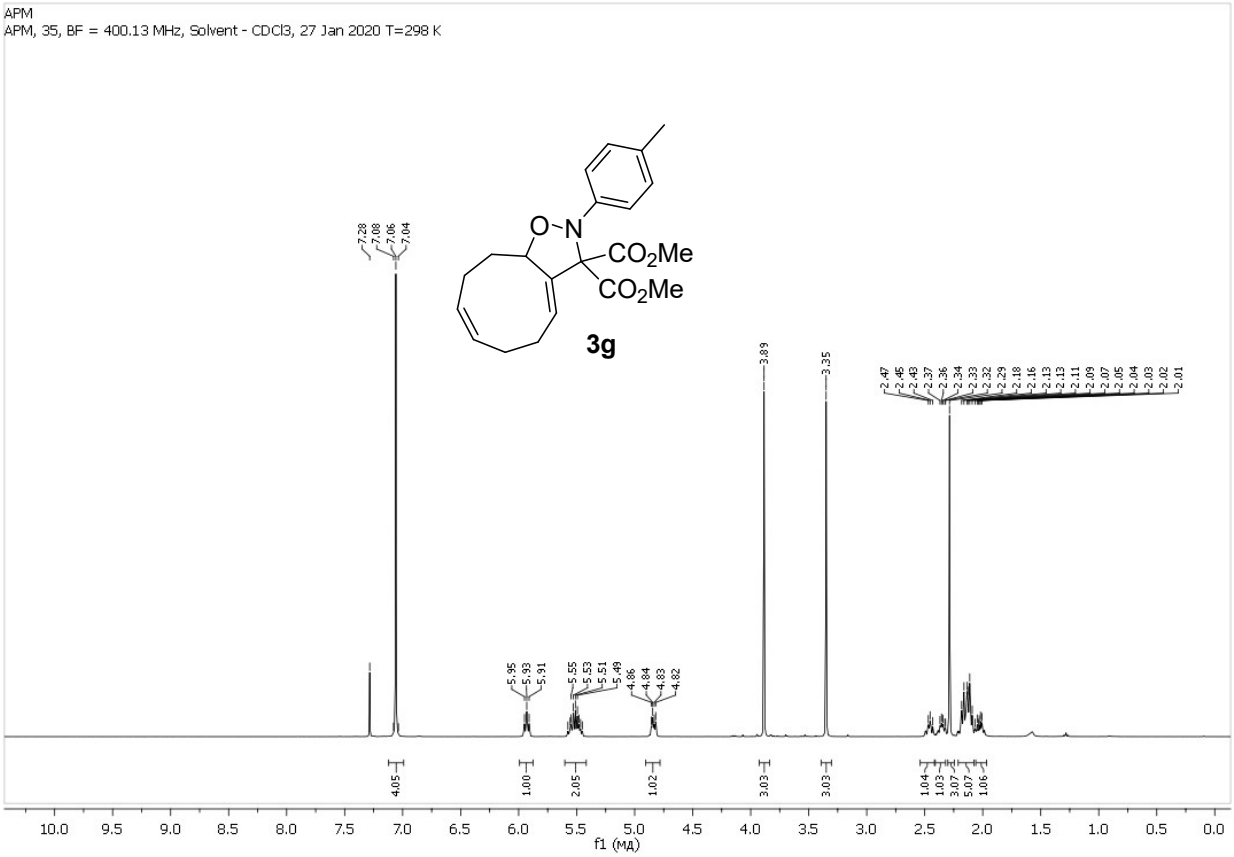

MMEc
MMEc, 142, BF = 100.612769 MHz, Solvent - CDCl3, 01 Oct 2021 T=298 K
O
N
H
CO2Me
CO2Me
4e
f1 (мд)

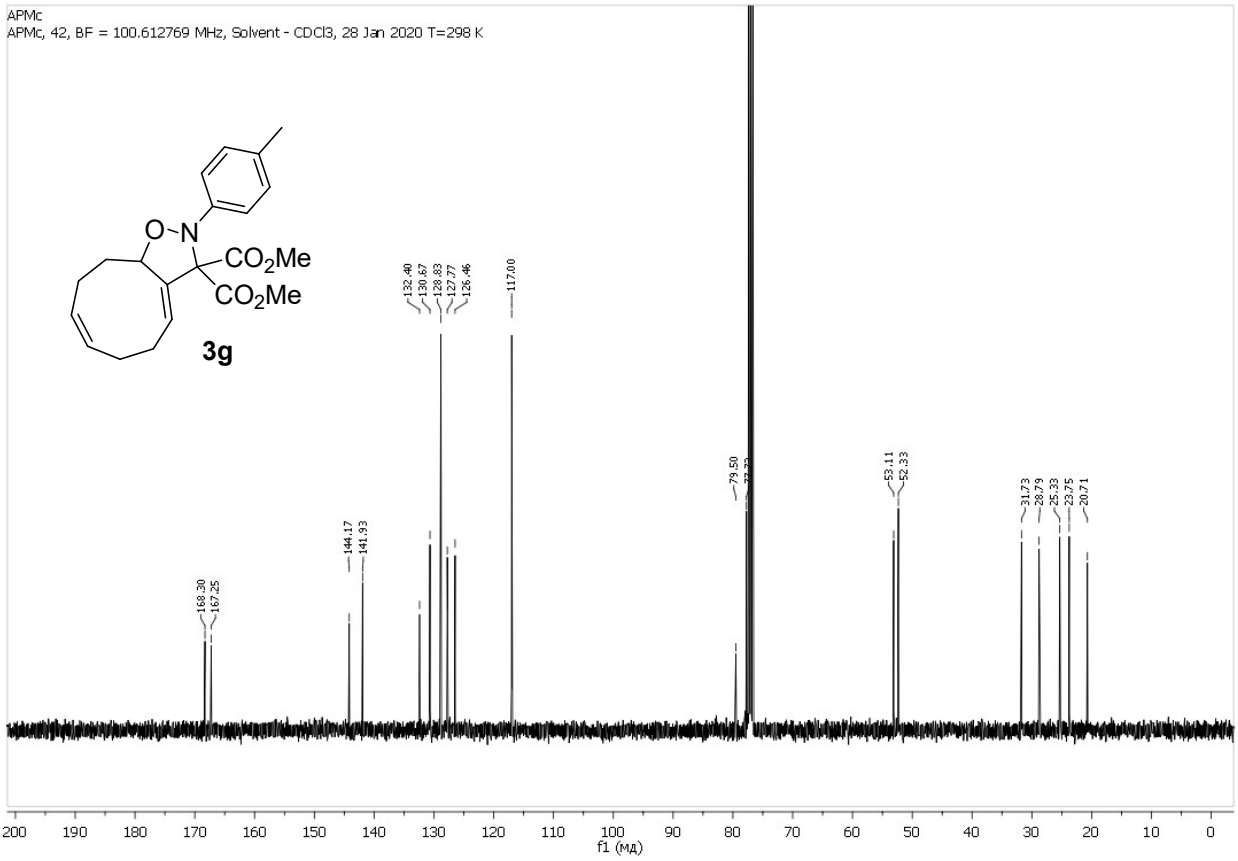

APM
APM, 266, BF = 400.13 MHz, Solvent - CDCl3, 06 Dec 2018 T=298 K
Br
O
N
CO2Me
CO2Me
3f
f1 (мд)

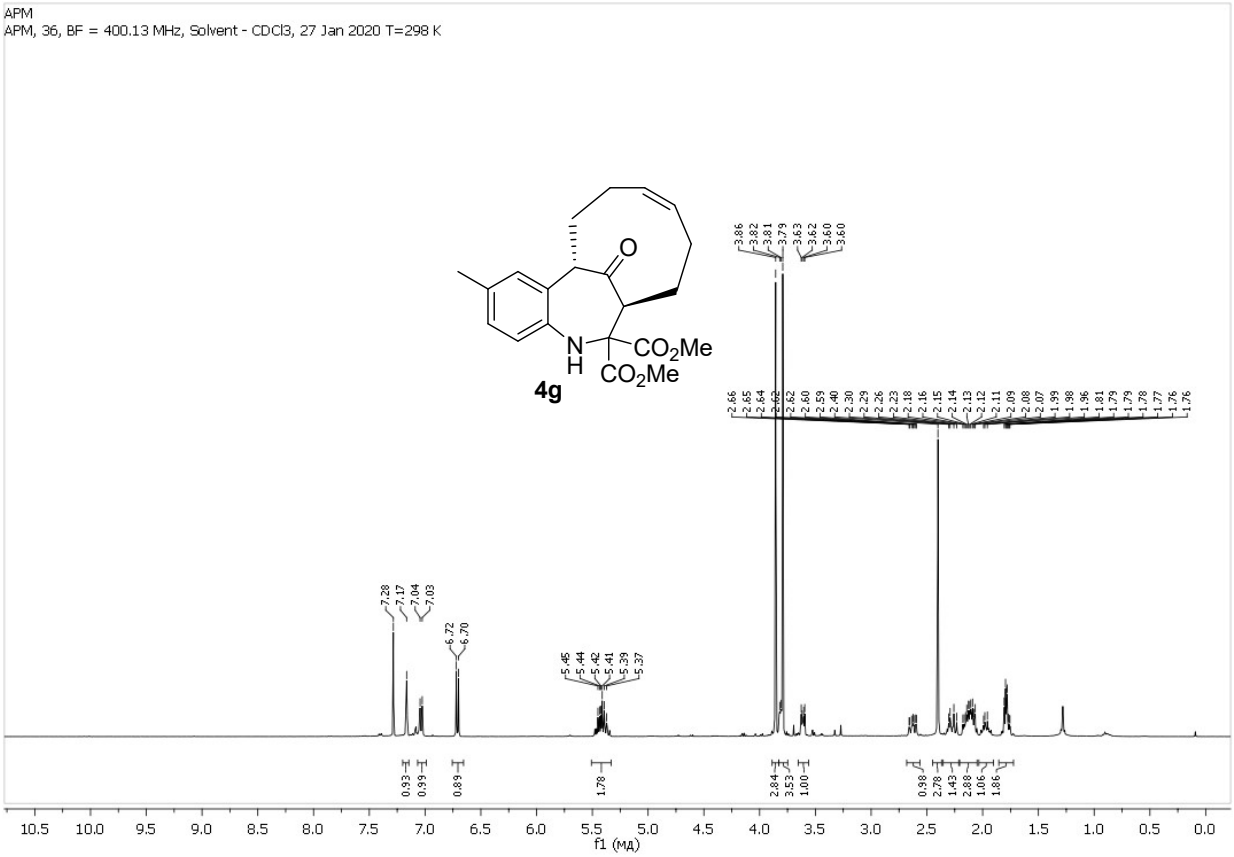

APMc
APMc, 266, BF = 100.612769 MHz, Solvent - CDCl3, 06 Dec 2018 T=298 K
Br
O
N
CO2Me
CO2Me
3f
f1 (мд)

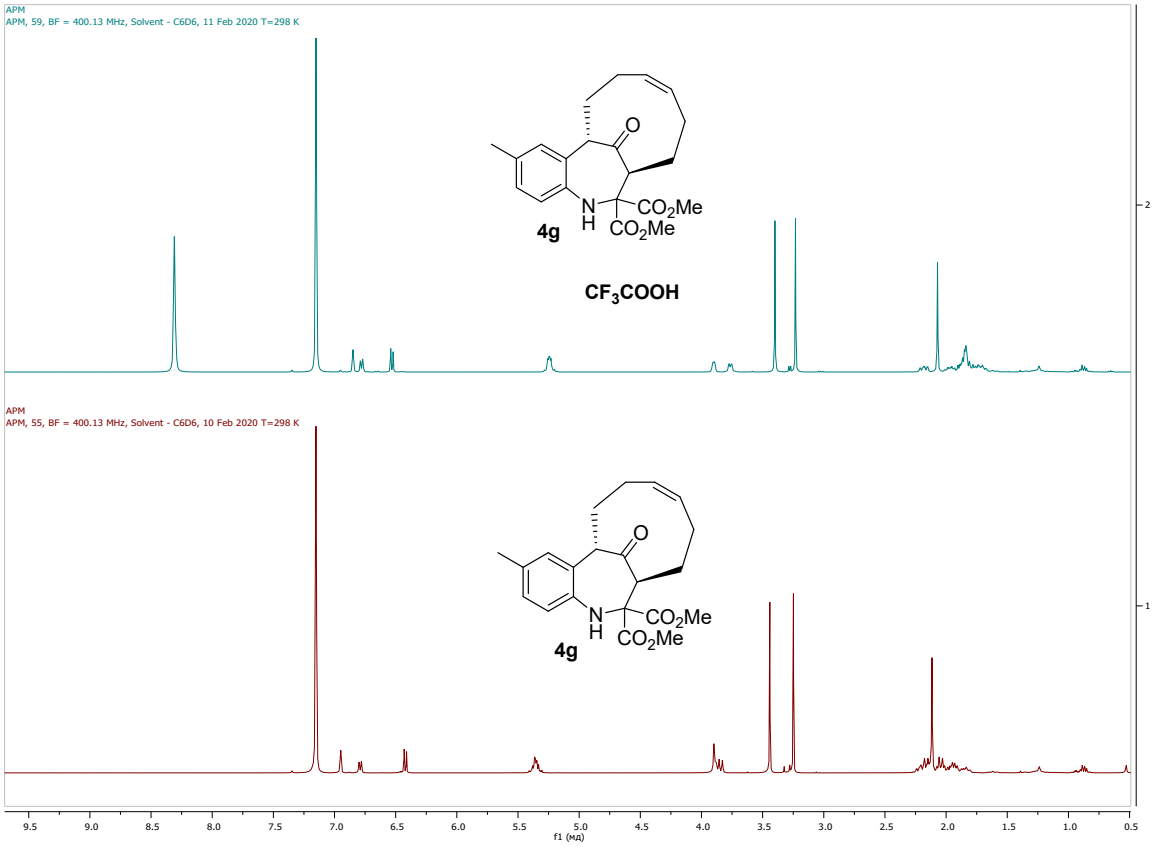

APM
APM, 272, BF = 400.13 MHz, Solvent - CDCl3, 20 Dec 2018 T=298 K
CH2Cl2
Br
O
N
H
CO2Me
CO2Me
4f
f1 (мд)

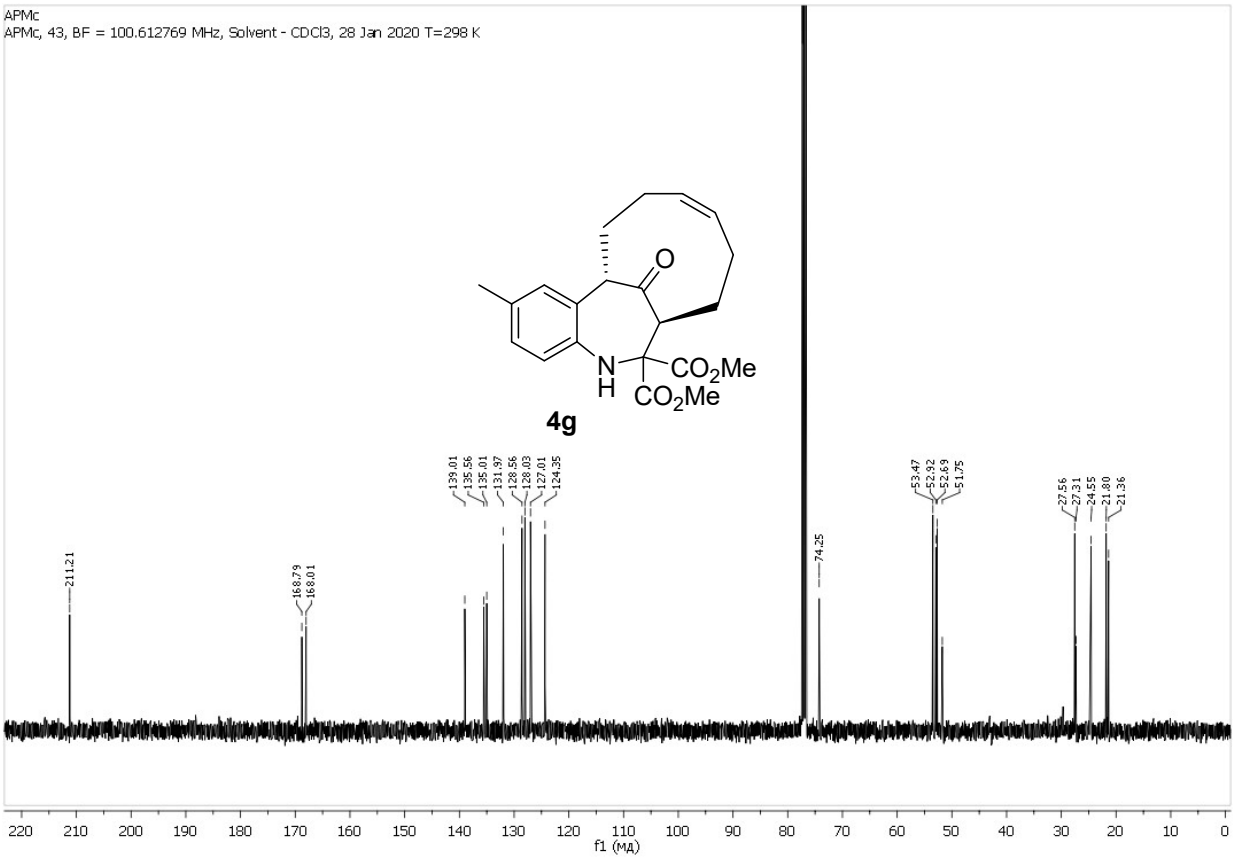

APMc
APMc, 272, BF = 100.612769 MHz, Solvent - CDCl3, 20 Dec 2018 T=298 K
Br
O
N
H
CO2Me
CO2Me
4f
f1 (мд)

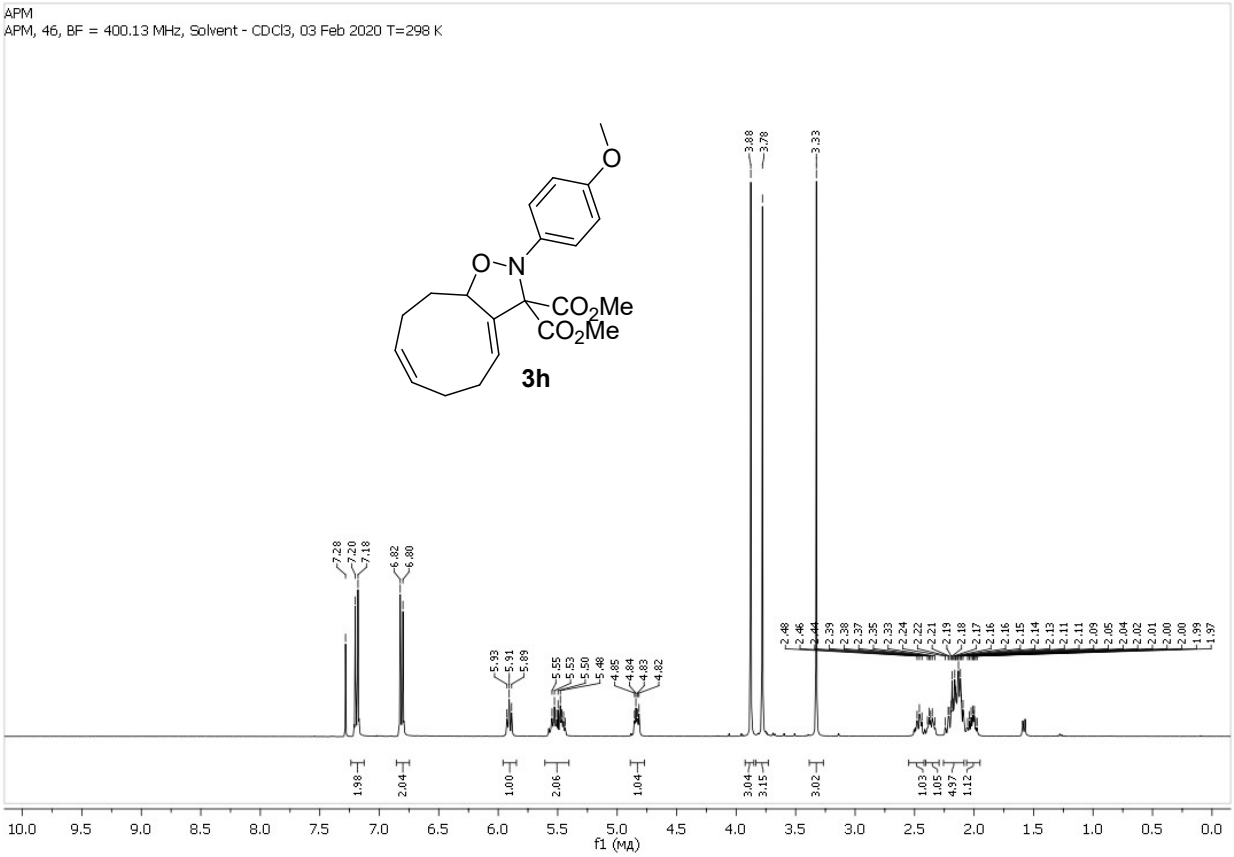

APM
APM, 35, BF = 400.13 MHz, Solvent - CDCl3, 27 Jan 2020 T=298 K
O
N
CO2Me
CO2Me
3g
7.28
7.08
7.06
7.04
5.95
5.93
5.91
5.55
5.53
5.51
5.49
4.86
4.84
4.83
4.82
3.89
3.35
2.47
2.45
2.43
2.37
2.36
2.34
2.33
2.32
2.29
2.18
2.16
2.13
2.13
2.11
2.09
2.07
2.05
2.04
2.03
2.02
2.01
4.05
1.00
2.05
1.02
3.03
3.03
1.04
1.03
3.07
5.07
1.06
f1 (мд)

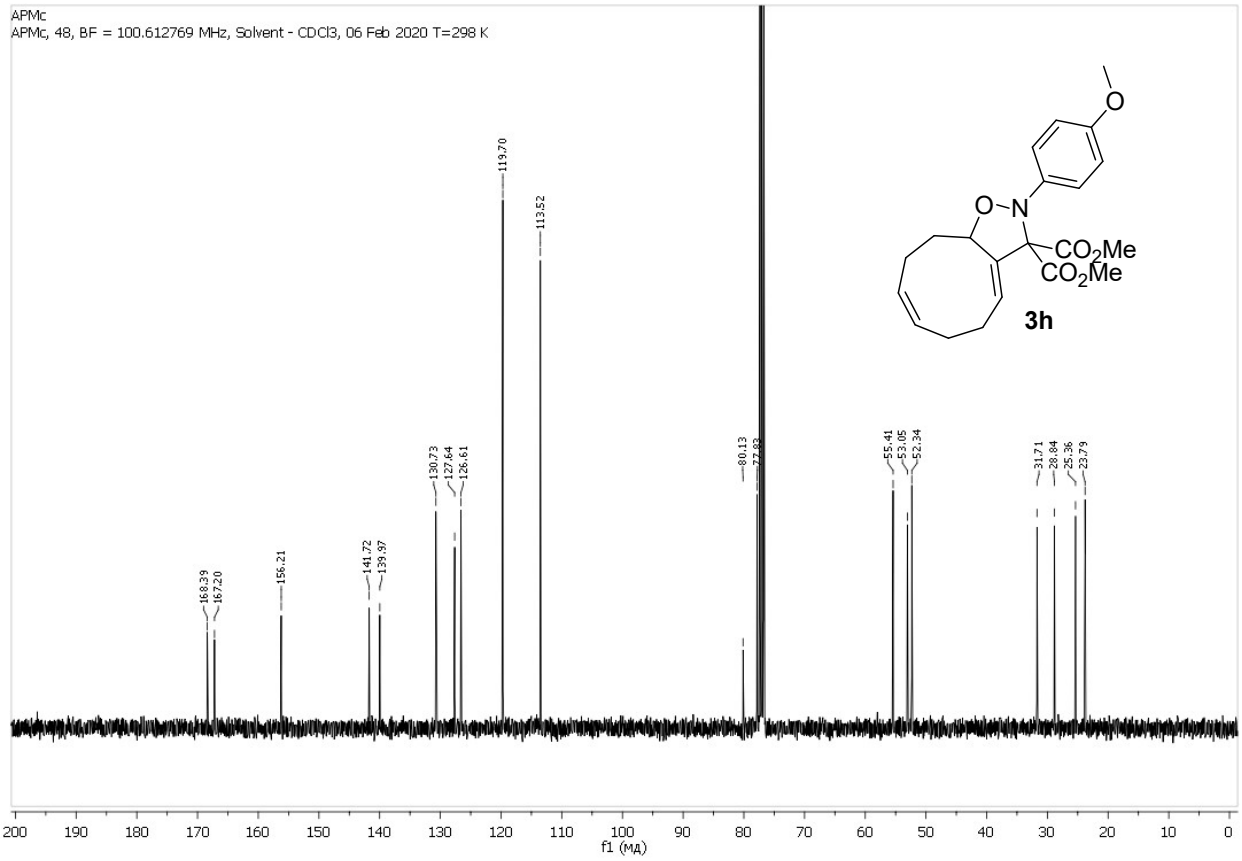

APMc
APMc, 42, BF = 100.612769 MHz, Solvent - CDCl3, 28 Jan 2020 T=298 K
O
N
CO2Me
CO2Me
3g
168.30
167.25
144.17
141.93
132.40
130.67
128.83
127.77
126.46
117.00
79.50
53.11
52.33
31.73
28.79
25.33
23.75
20.71
f1 (мд)

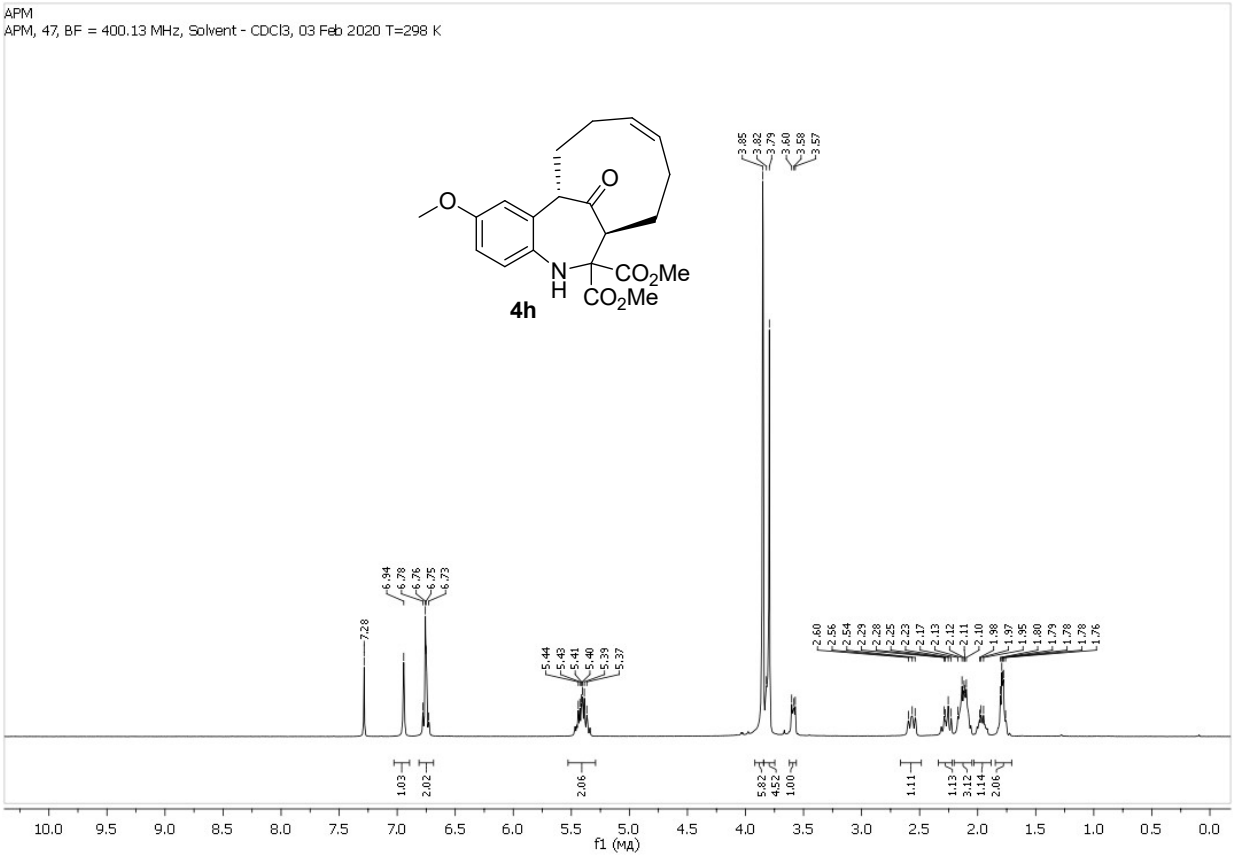

APM
APM, 36, BF = 400.13 MHz, Solvent - CDCl3, 27 Jan 2020 T=298 K
4g
f1 (мд)

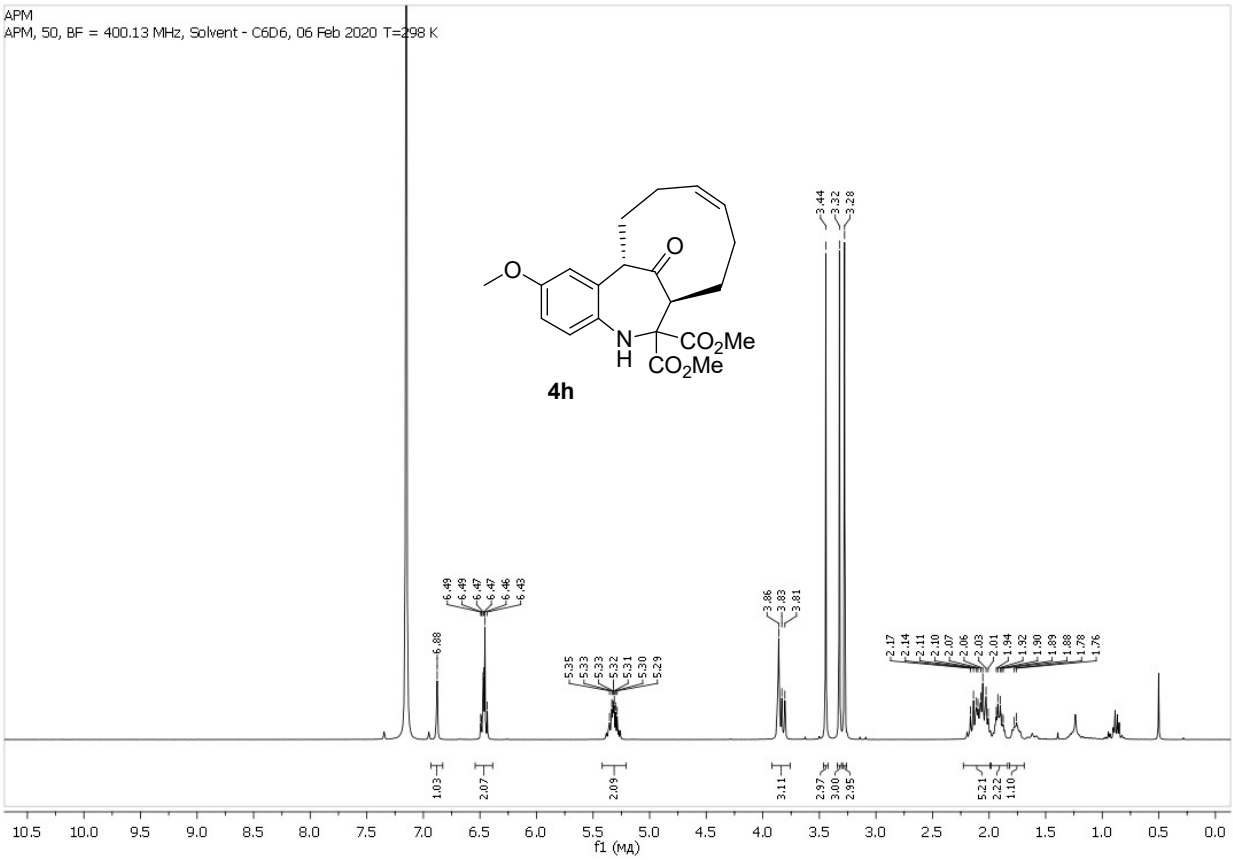

APM
APM, 59, BF = 400.13 MHz, Solvent - C6D6, 11 Feb 2020 T=298 K
4g
CF3COOH
APM
APM, 55, BF = 400.13 MHz, Solvent - C6D6, 10 Feb 2020 T=298 K
4g
f1 (мд)

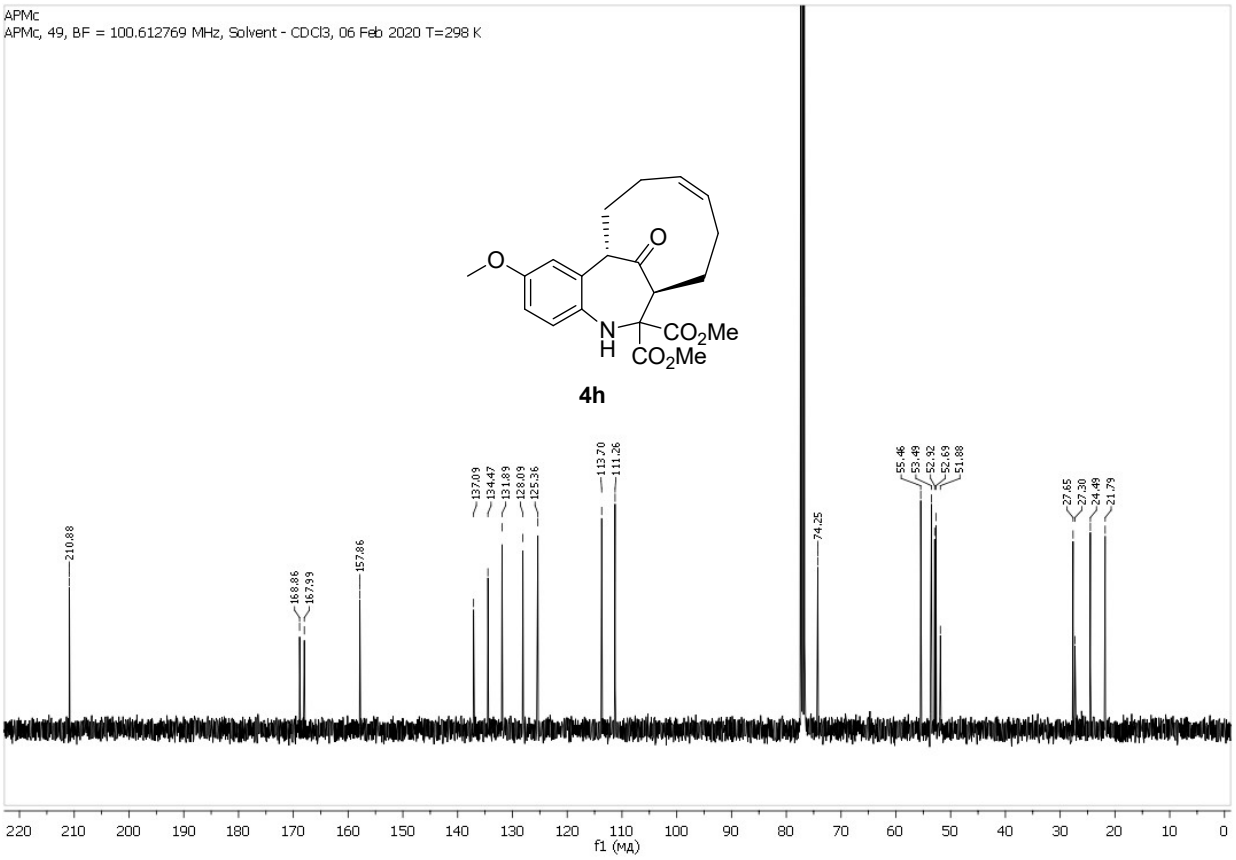

APMc
APMc, 43, BF = 100.612769 MHz, Solvent - CDCl3, 28 Jan 2020 T=298 K
O
N
H
CO2Me
CO2Me
4g
211.21
168.79
168.01
139.01
135.56
135.01
131.97
128.56
128.03
127.01
124.35
74.25
53.47
52.92
52.69
51.75
27.56
27.31
24.55
21.80
21.36
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (мд)

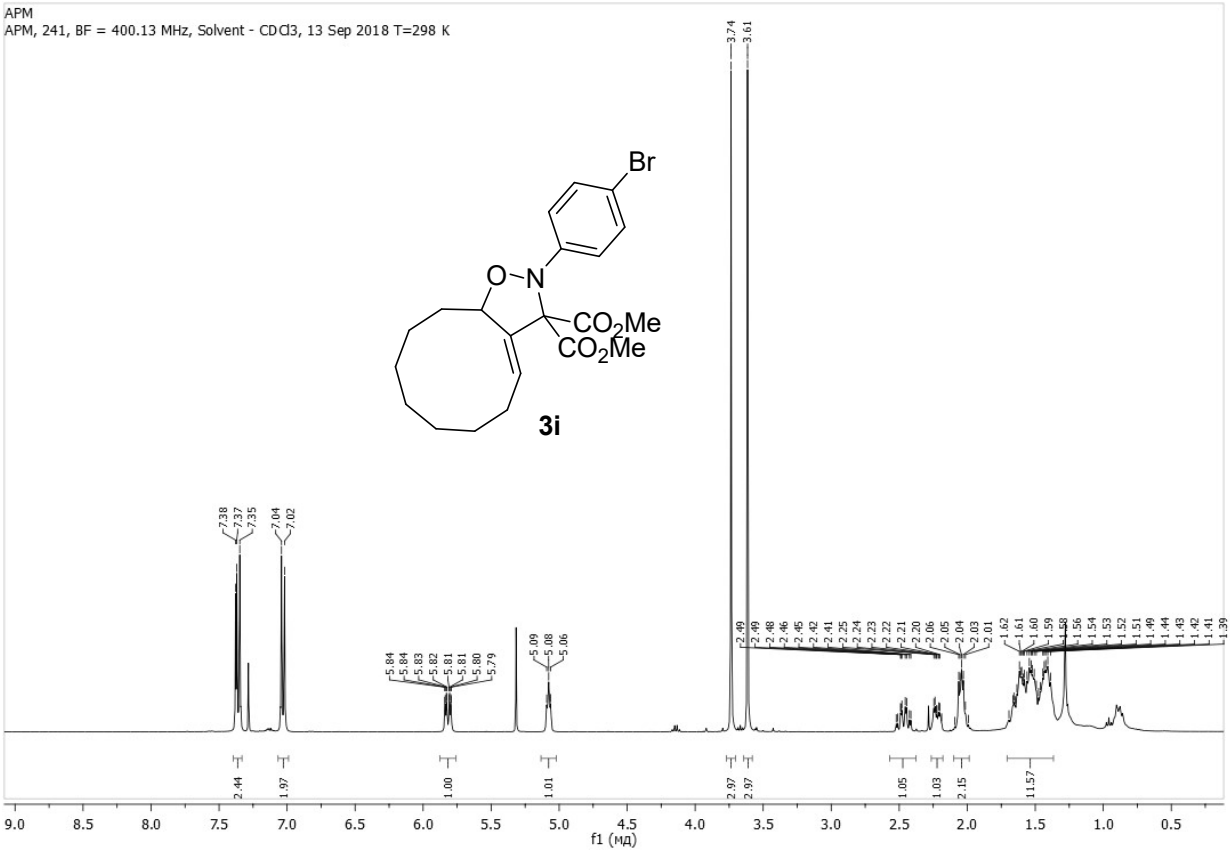

APM
APM, 46, BF = 400.13 MHz, Solvent - CDCl3, 03 Feb 2020 T=298 K
O
O
N
CO2Me
CO2Me
3h
7.28
7.20
7.18
6.82
6.80
5.93
5.91
5.89
5.55
5.53
5.50
5.48
4.85
4.84
4.83
4.82
3.88
3.78
3.33
2.48
2.46
2.44
2.39
2.38
2.37
2.35
2.33
2.24
2.22
2.21
2.19
2.18
2.17
2.16
2.16
2.15
2.14
2.13
2.11
2.11
2.09
2.05
2.04
2.02
2.01
2.00
2.00
1.99
1.97
1.98
2.04
1.00
2.06
1.04
3.04
3.15
3.02
1.03
1.05
4.97
1.12
f1 (мд)

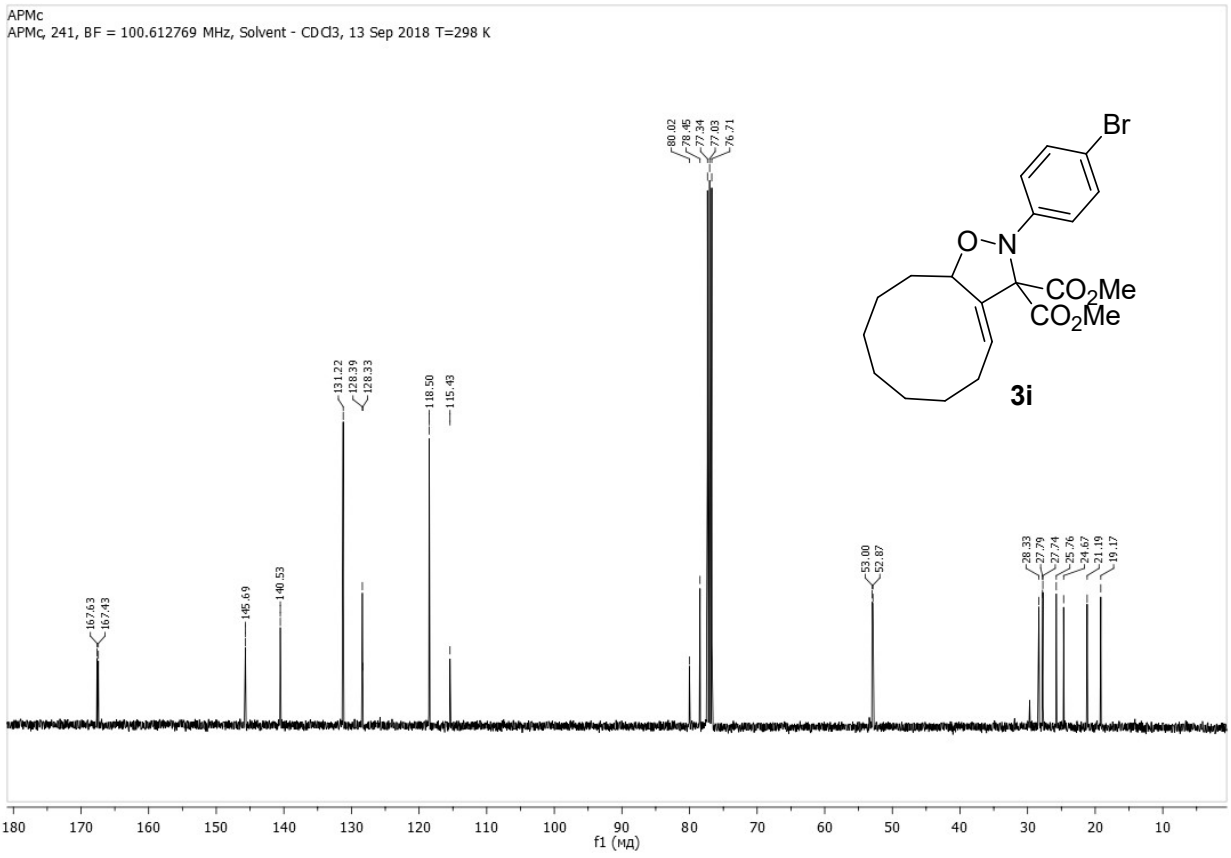

APMc
APMc, 48, BF = 100.612769 MHz, Solvent - CDCl3, 06 Feb 2020 T=298 K
O
O
N
CO2Me
CO2Me
3h
168.39
167.20
156.21
141.72
139.97
130.73
127.64
126.61
119.70
113.52
80.13
77.83
55.41
53.05
52.34
31.71
28.84
25.36
23.79
f1 (мд)

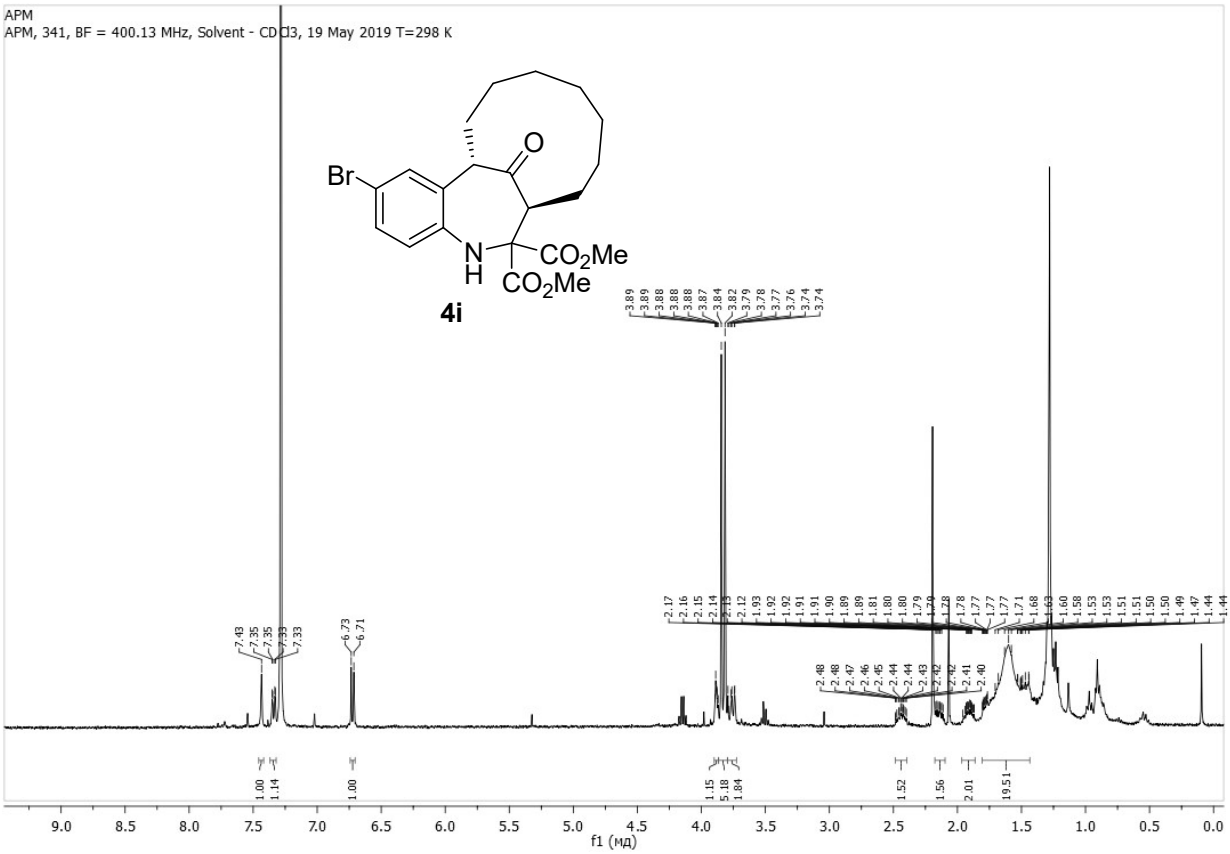

APM
APM, 47, BF = 400.13 MHz, Solvent - CDCl3, 03 Feb 2020 T=298 K
4h
f1 (мд)

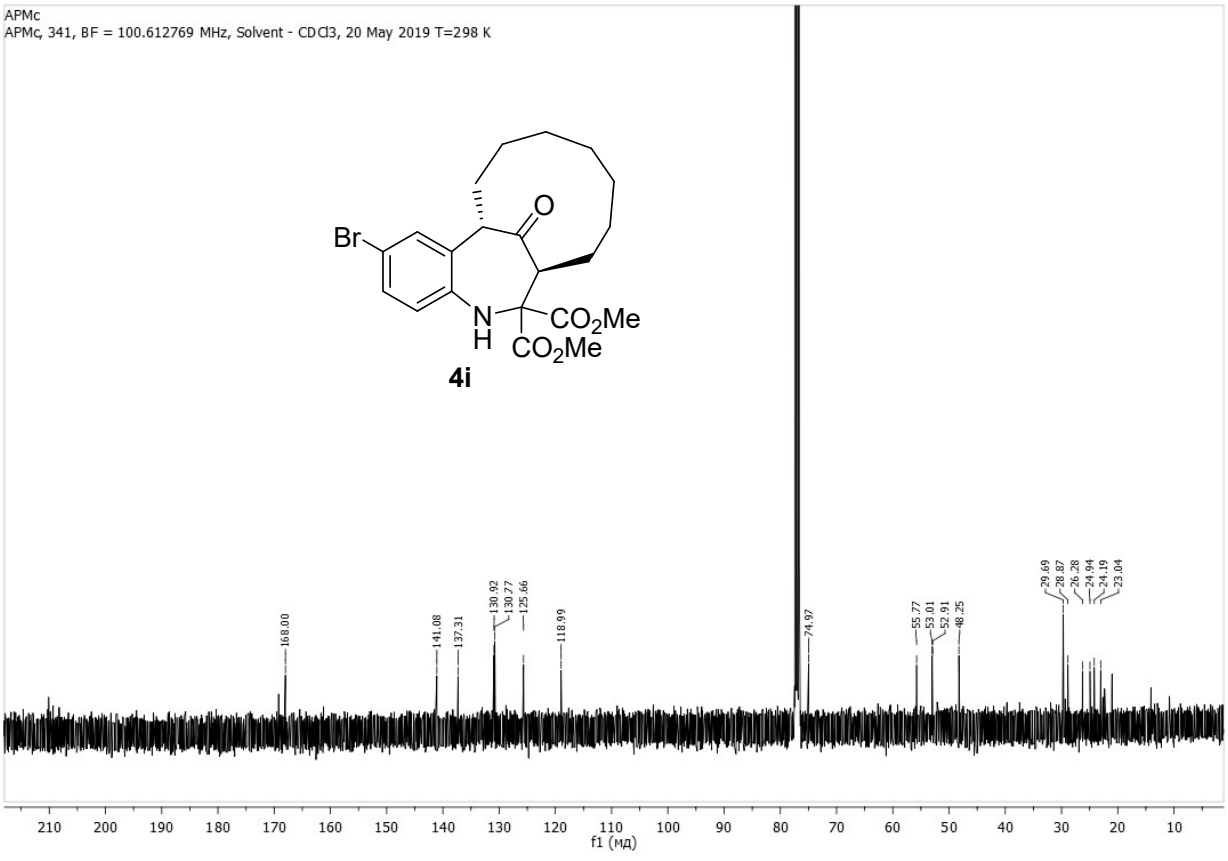

APM
APM, 50, BF = 400.13 MHz, Solvent - C6D6, 06 Feb 2020 T=298 K
4h
f1 (мд)

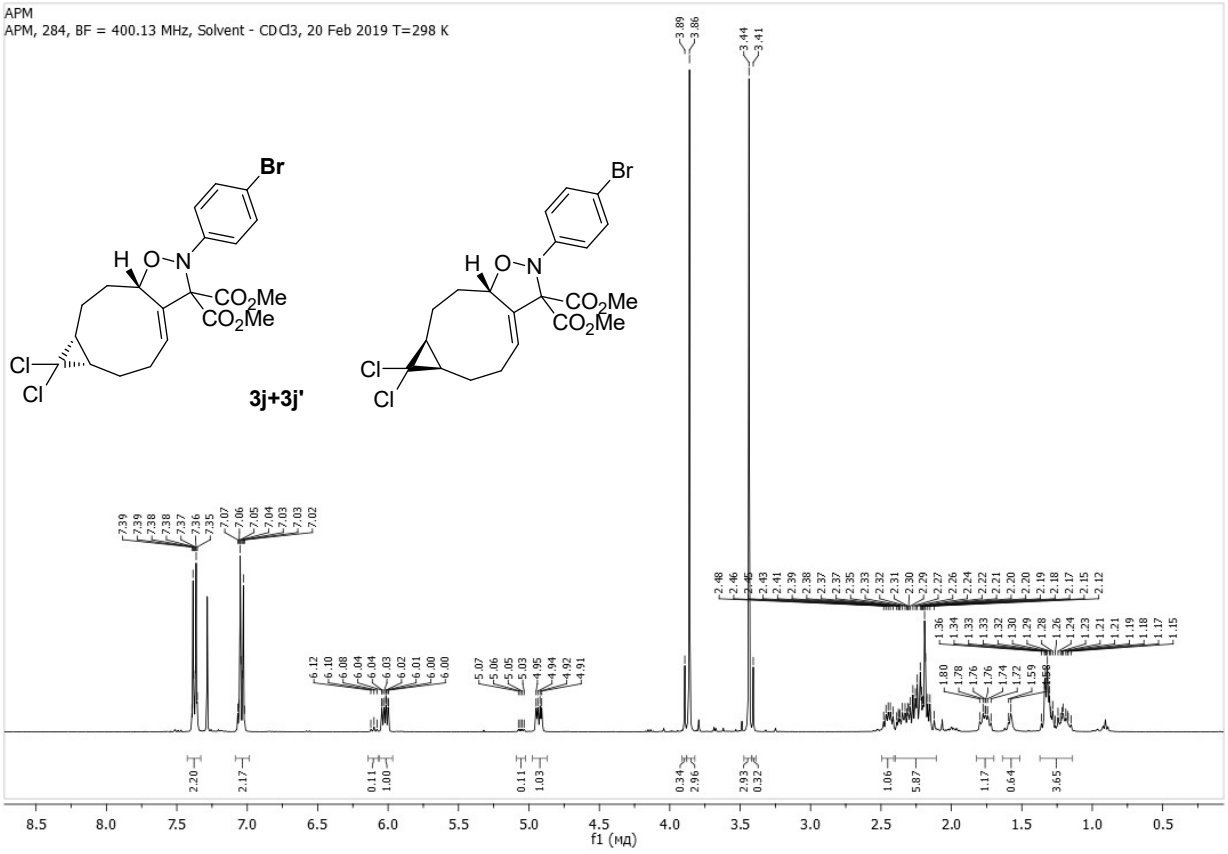

APMc
APMc, 49, BF = 100.612769 MHz, Solvent - CDCl3, 06 Feb 2020 T=298 K
O
O
N
H
CO2Me
CO2Me
4h
210.88
168.86
167.99
157.86
137.09
134.47
131.89
128.09
125.36
113.70
111.26
74.25
55.46
53.49
52.92
52.69
51.88
27.65
27.30
24.49
21.79
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (мд)

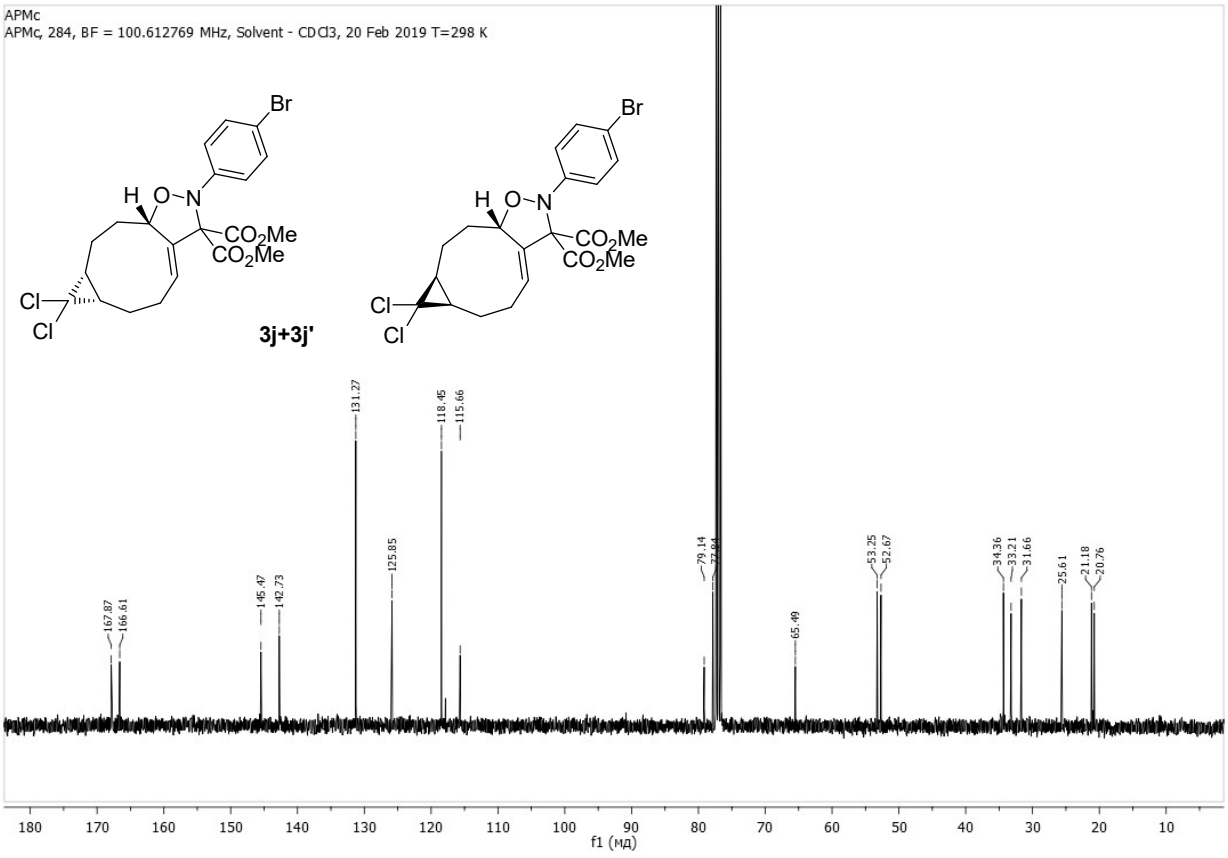

APM
APM, 241, BF = 400.13 MHz, Solvent - CDCl3, 13 Sep 2018 T=298 K
Br
O
N
CO2Me
CO2Me
3i
f1 (мд)

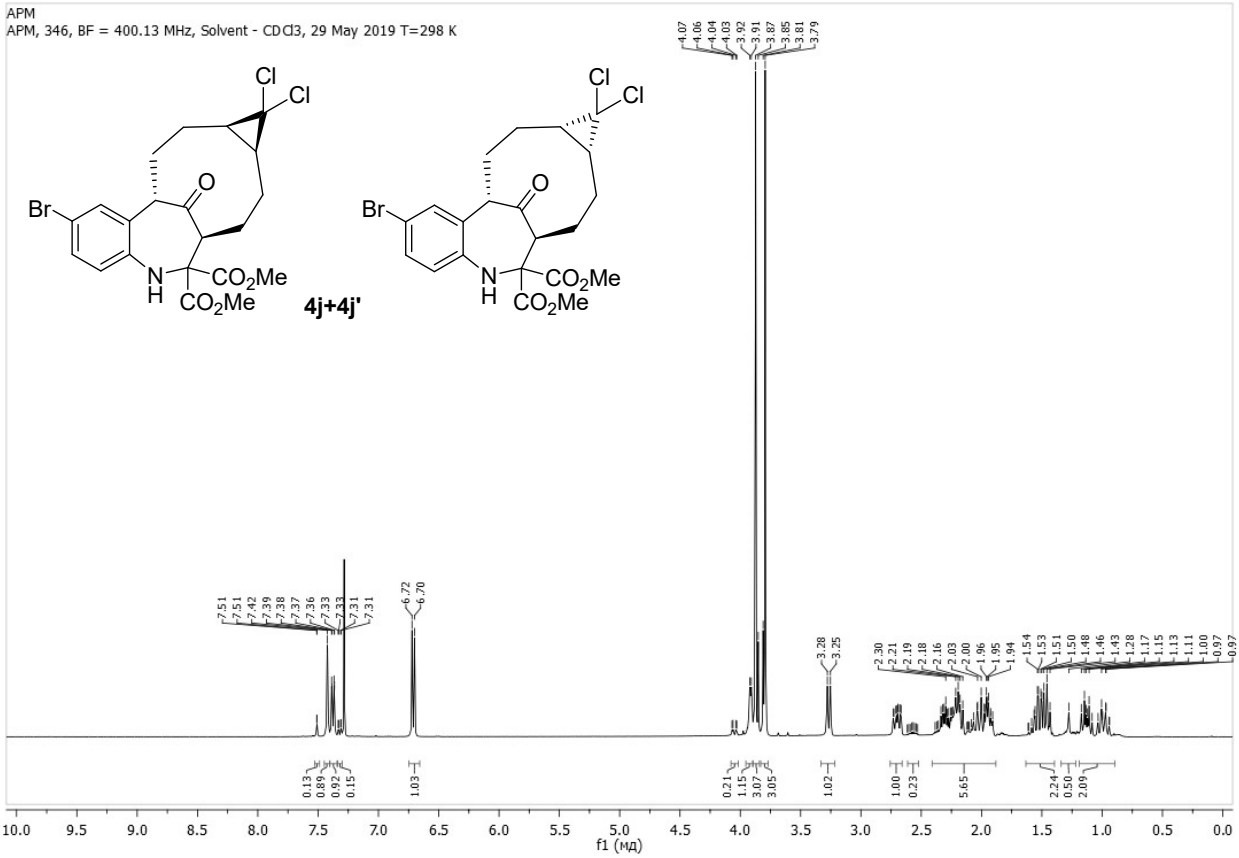

APMc
APMc, 241, BF = 100.612769 MHz, Solvent - CDCl3, 13 Sep 2018 T=298 K
Br
O
N
CO2Me
CO2Me
3i
f1 (мд)

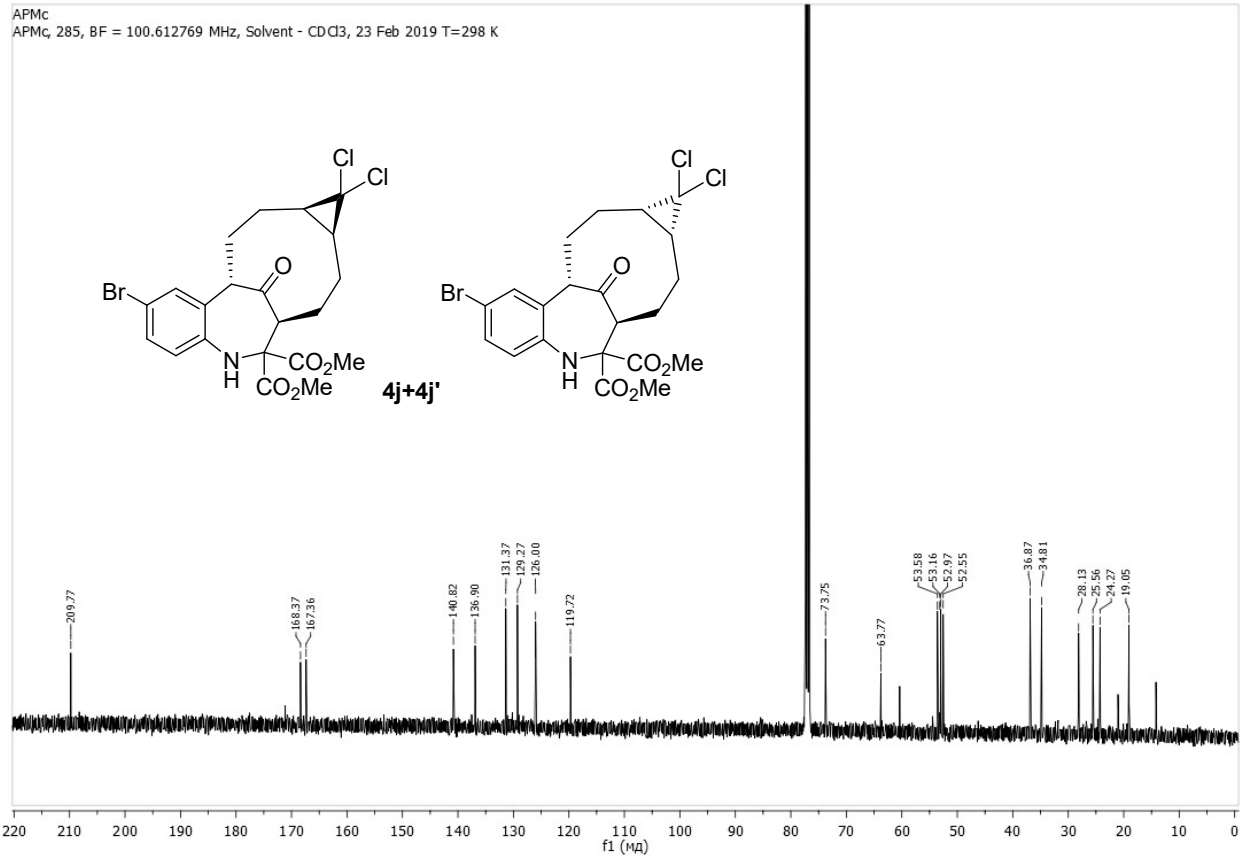

APM
APM, 341, BF = 400.13 MHz, Solvent - CDCl3, 19 May 2019 T=298 K
Br
O
N
H
CO2Me
CO2Me
4i
f1 (мд)

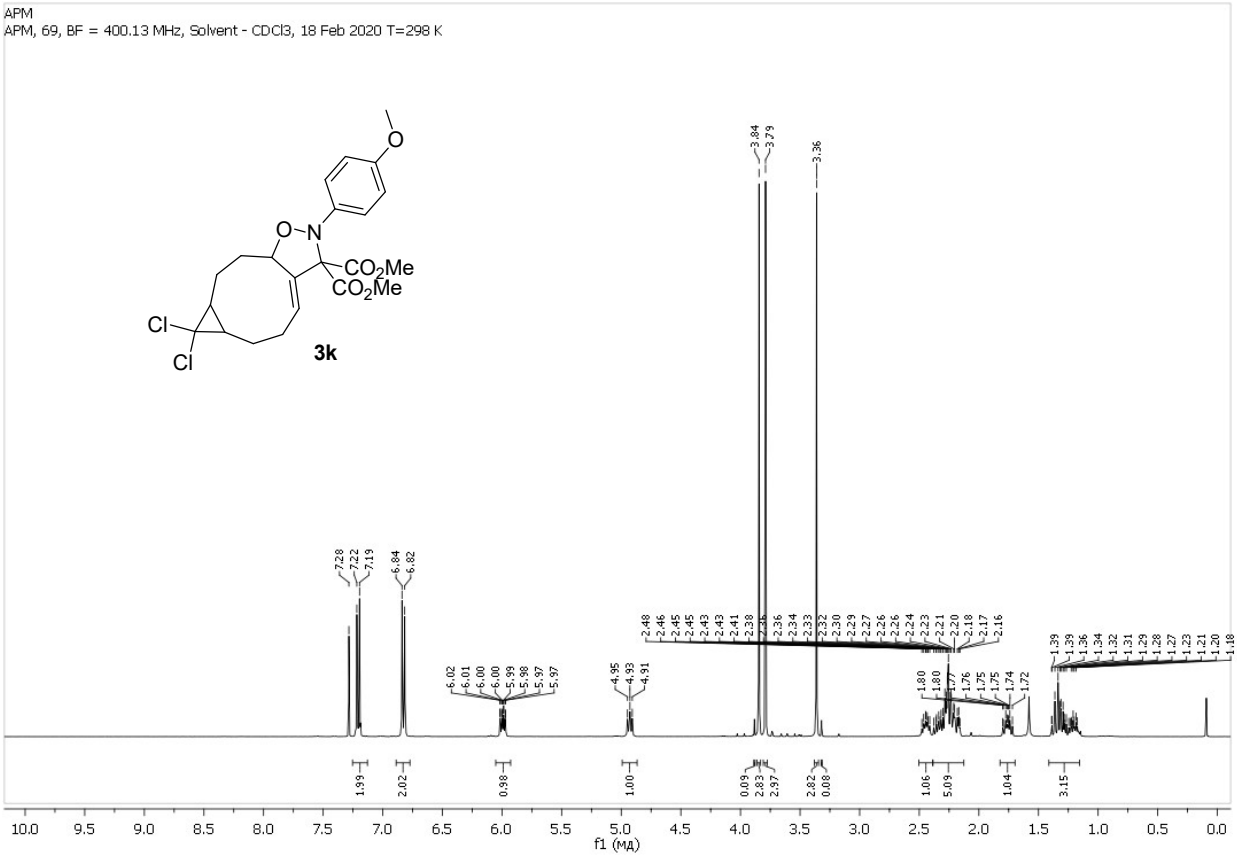

APMc
APMc, 341, BF = 100.612769 MHz, Solvent - CDCl3, 20 May 2019 T=298 K
Br
O
N
H
CO2Me
CO2Me
4i
f1 (мд)

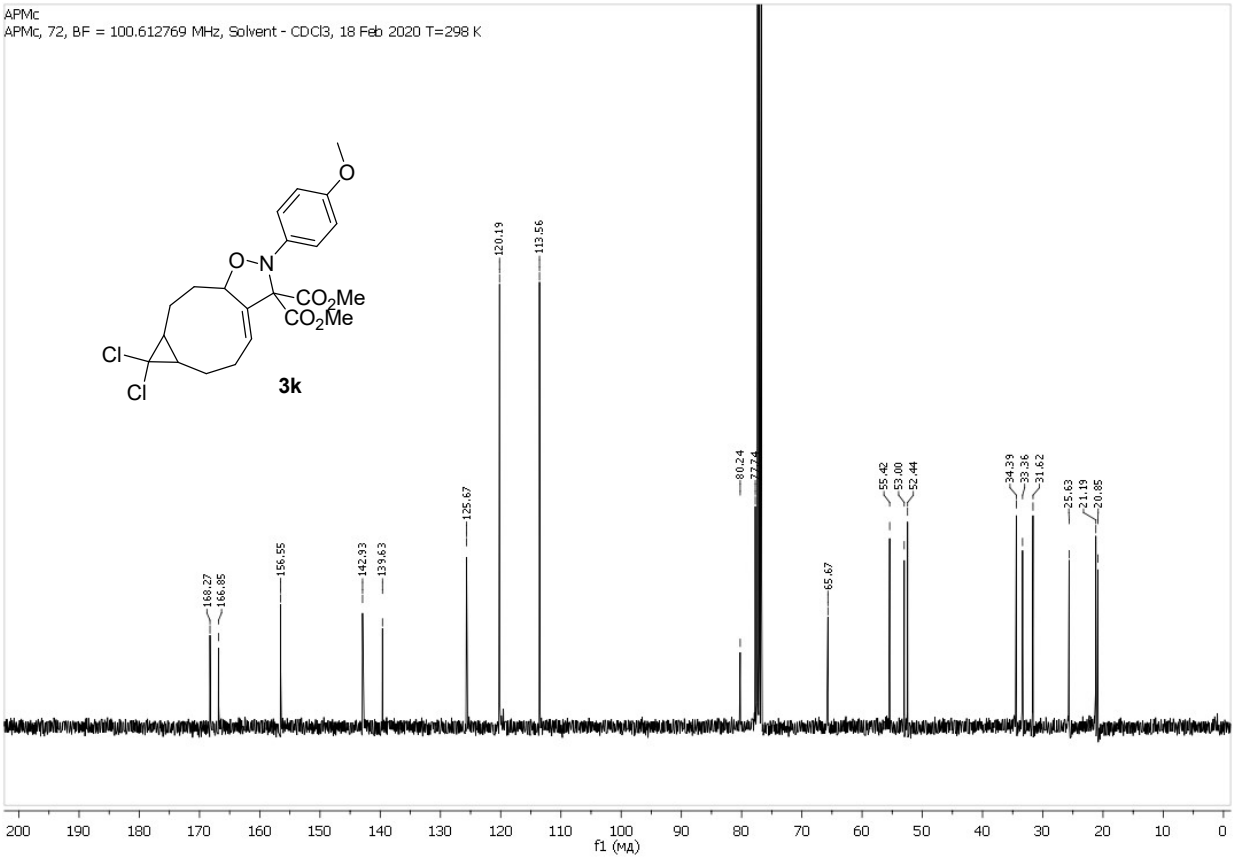

APM
APM, 284, BF = 400.13 MHz, Solvent - CDCl3, 20 Feb 2019 T=298 K
Br
H O N
CO2Me
CO2Me
Cl
Cl
3j+3j'
f1 (мд)

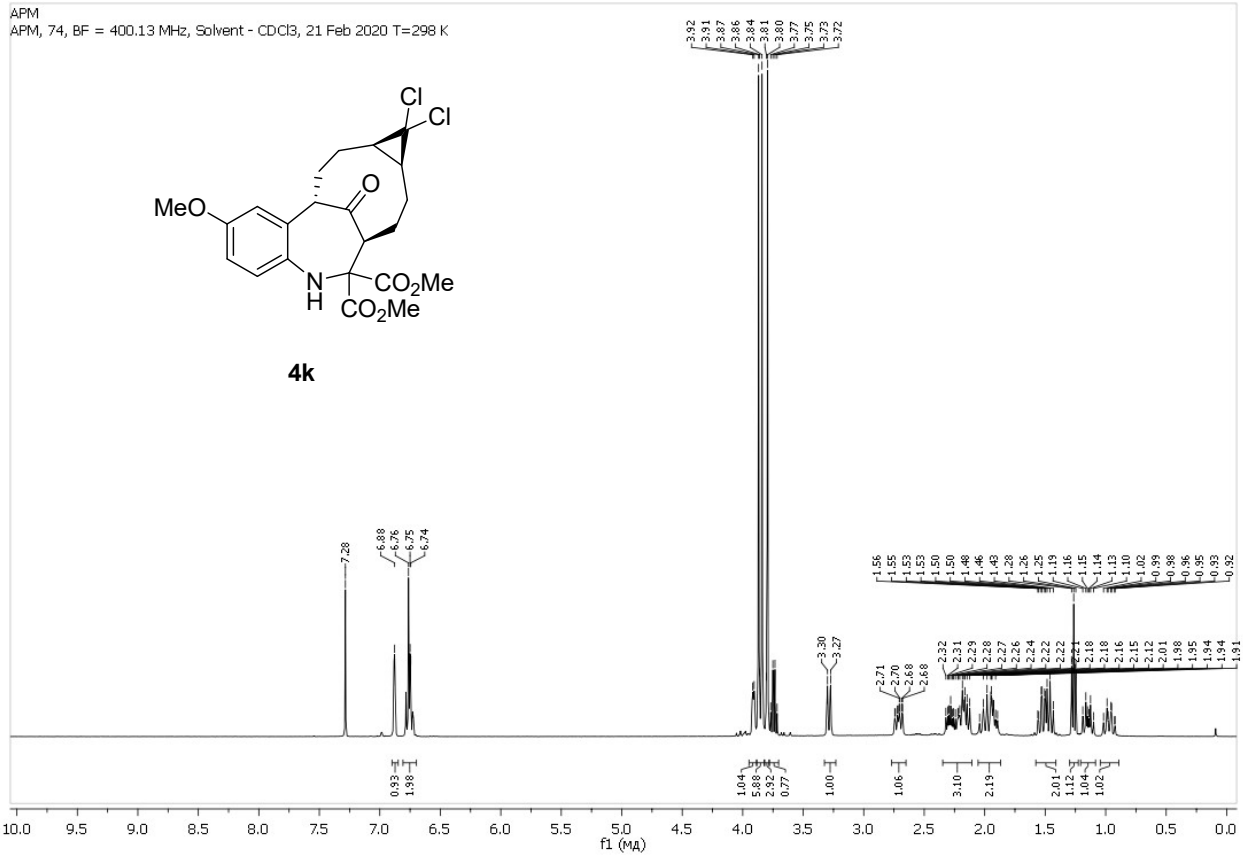

APMc
APMc, 284, BF = 100.612769 MHz, Solvent - CDCl3, 20 Feb 2019 T=298 K
Br
H O N
CO2Me
CO2Me
Cl
Cl
3j+3j'
f1 (мд)


APM
APM, 346, BF = 400.13 MHz, Solvent - CDCl3, 29 May 2019 T=298 K
4j+4j'
f1 (мд)

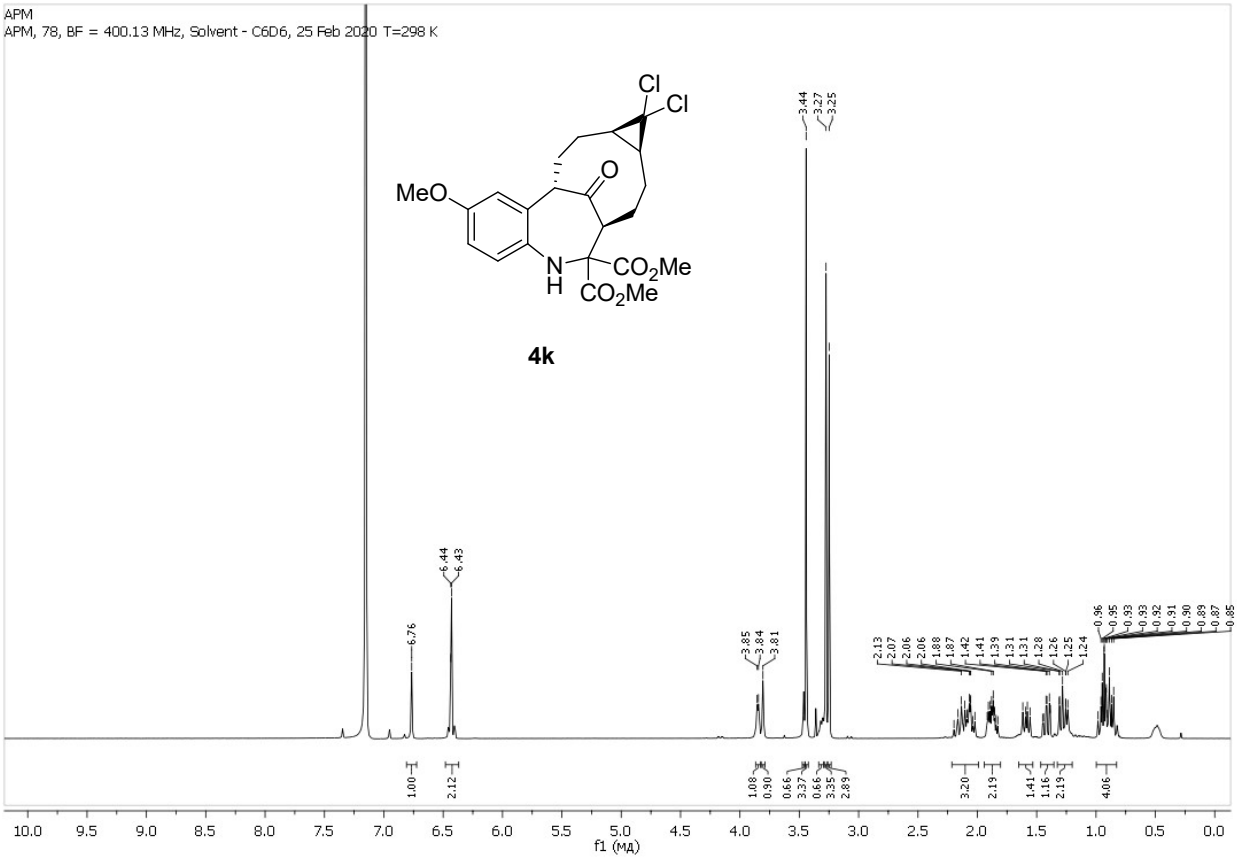

APMc
APMc, 285, BF = 100.612769 MHz, Solvent - CDCl3, 23 Feb 2019 T=298 K
4j+4j'
f1 (мд)


APM
APM, 69, BF = 400.13 MHz, Solvent - CDCl3, 18 Feb 2020 T=298 K
O
O-N
CO2Me
CO2Me
Cl
Cl
3k
7.28
7.22
7.19
6.84
6.82
6.02
6.01
6.00
5.99
5.98
5.97
5.97
4.95
4.93
4.91
3.84
3.79
3.36
2.48
2.46
2.45
2.45
2.43
2.43
2.41
2.38
2.36
2.34
2.33
2.32
2.30
2.29
2.27
2.26
2.26
2.24
2.23
2.21
2.20
2.18
2.17
2.16
1.80
1.80
1.77
1.76
1.75
1.75
1.74
1.72
1.39
1.39
1.36
1.34
1.32
1.31
1.29
1.28
1.27
1.23
1.21
1.20
1.18
1.99
2.02
0.98
1.00
0.09
2.83
2.97
2.82
0.08
1.06
5.09
1.04
3.15
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (мд)

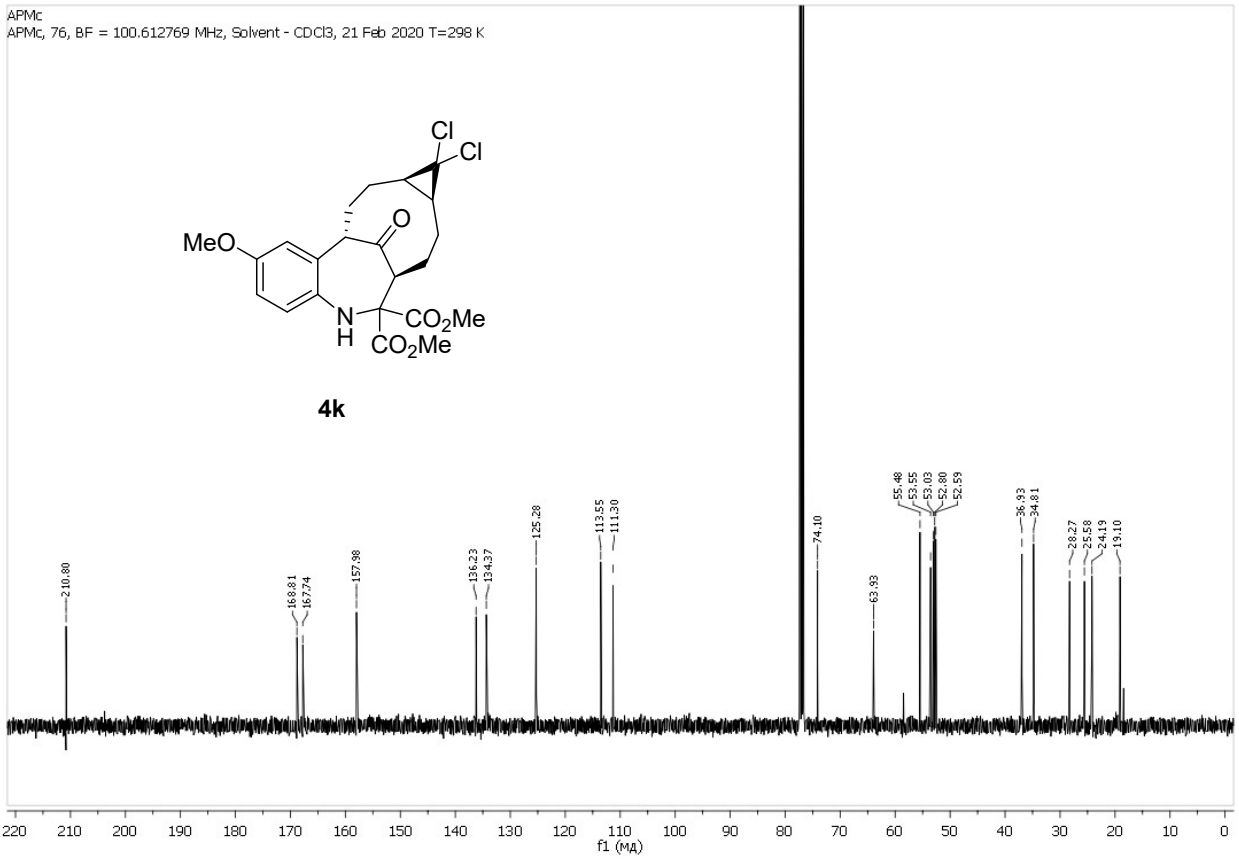

APMc
APMc, 72, BF = 100.612769 MHz, Solvent - CDCl3, 18 Feb 2020 T=298 K
O
O-N
CO2Me
CO2Me
Cl
Cl
3k
168.27
166.85
156.55
142.93
139.63
125.67
120.19
113.56
80.24
77.74
65.67
55.42
53.00
52.44
34.39
33.36
31.62
25.63
21.19
20.85
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (мд)

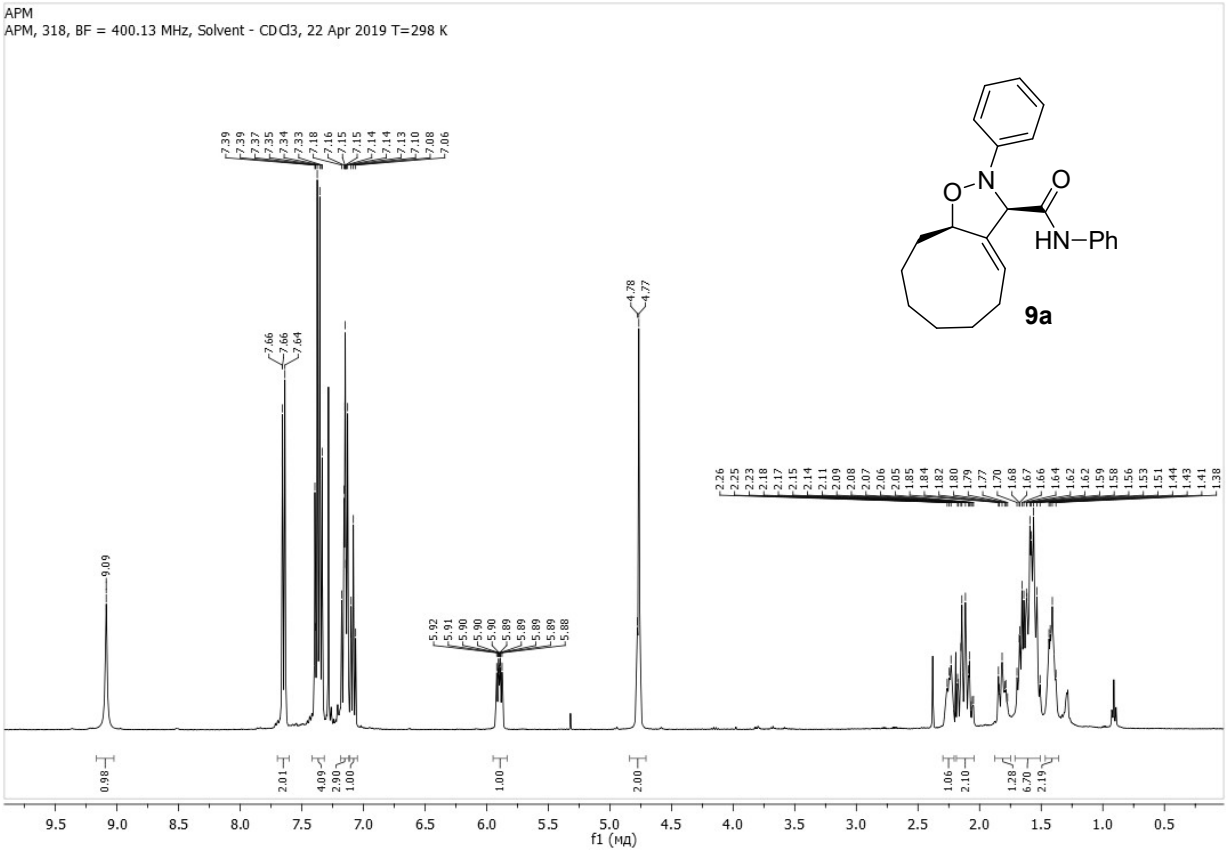

APM
APM, 74, BF = 400.13 MHz, Solvent - CDCl3, 21 Feb 2020 T=298 K
Cl
Cl
O
MeO
N
H
CO2Me
CO2Me
f1 (мд)

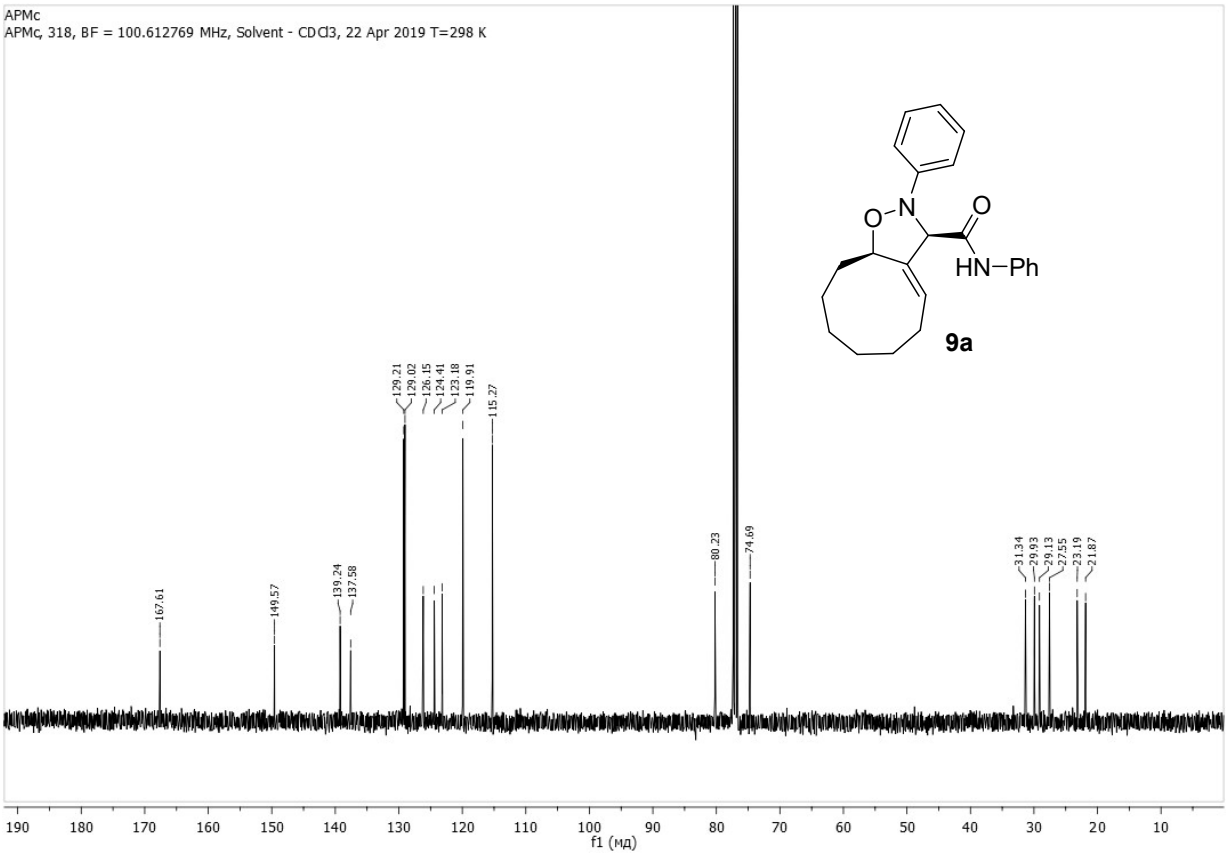
4k

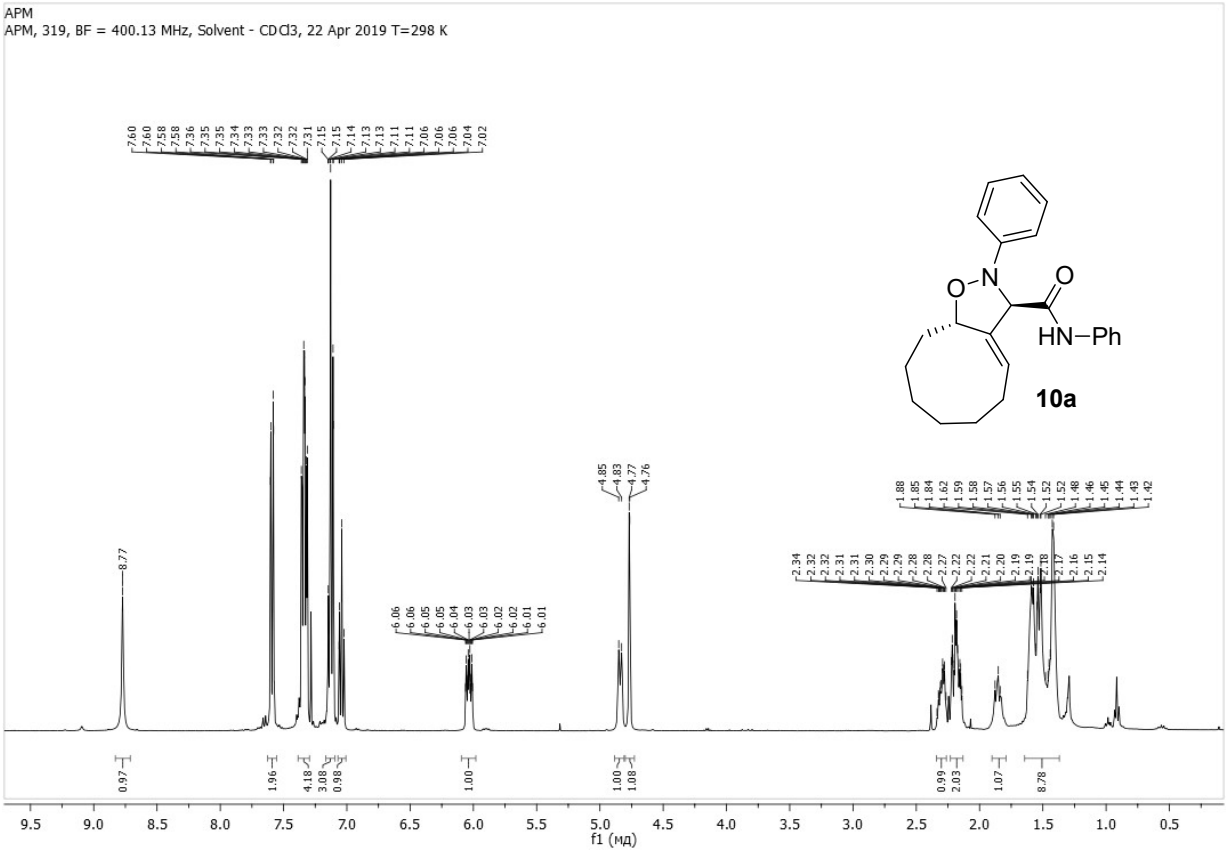

APM
APM, 78, BF = 400.13 MHz, Solvent - C6D6, 25 Feb 2020 T=298 K
Cl
Cl
O
MeO
N
H
CO2Me
CO2Me
f1 (мд)

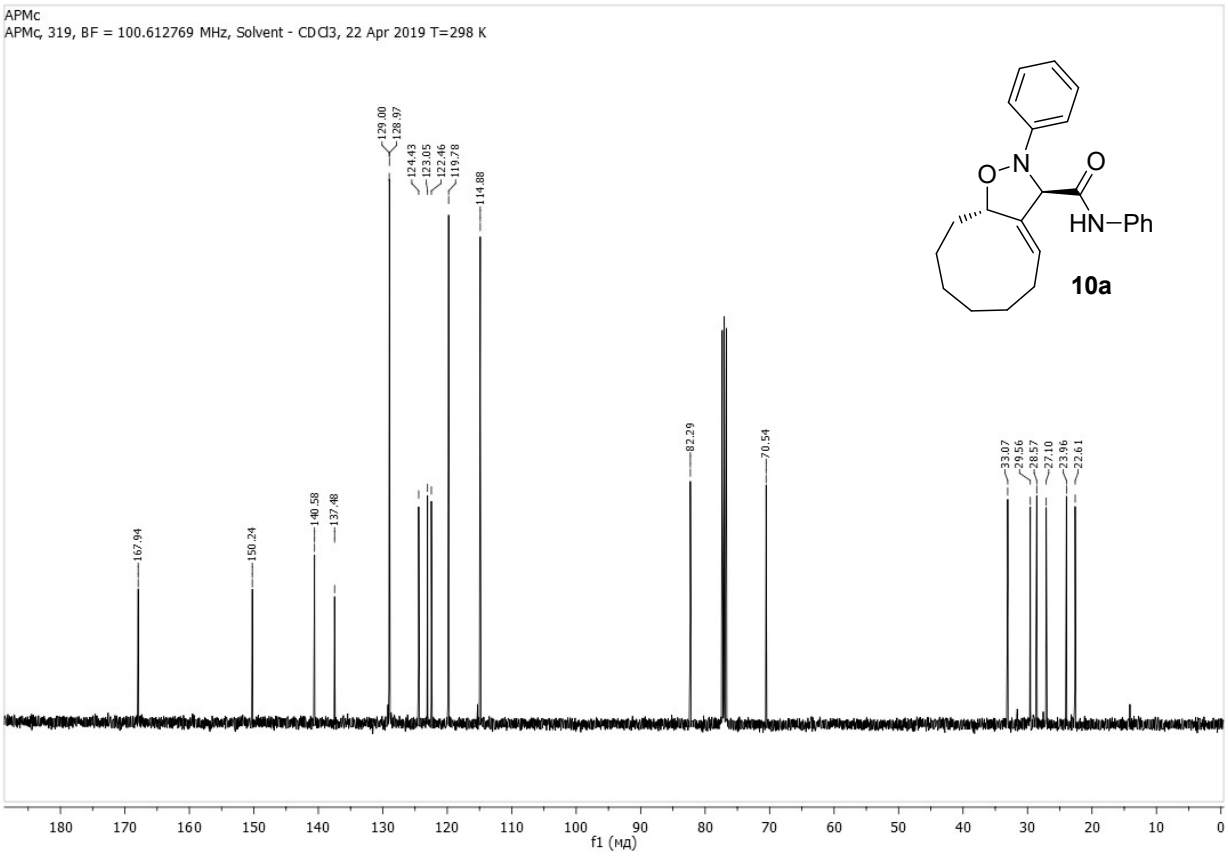
4k

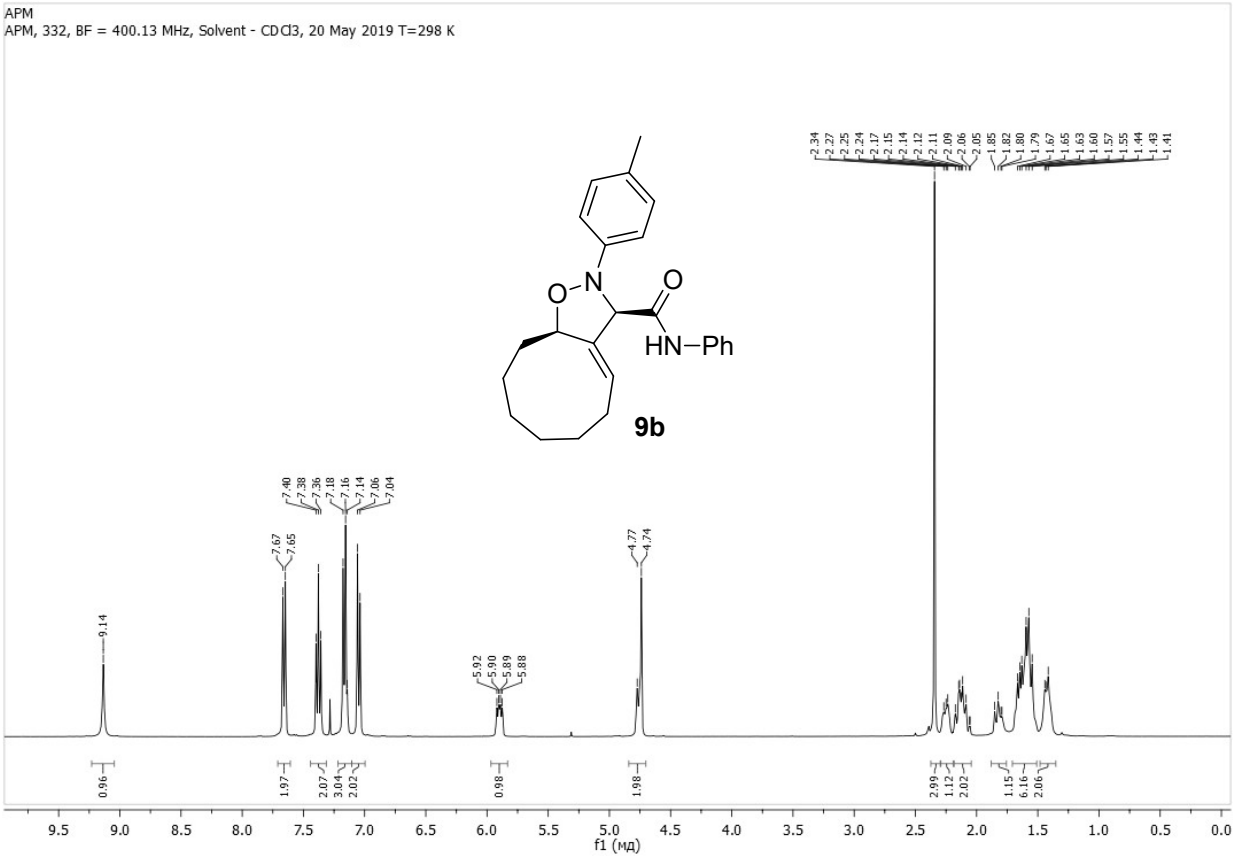

APMc
APMc, 76, BF = 100.612769 MHz, Solvent - CDCl3, 21 Feb 2020 T=298 K
Cl
Cl
O
MeO
N
H
CO2Me
CO2Me
4k
210.80
168.81
167.74
157.98
136.23
134.37
125.28
113.55
111.30
74.10
63.93
55.48
53.55
53.03
52.80
52.59
36.93
34.81
28.27
25.58
24.19
19.10
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (мд)

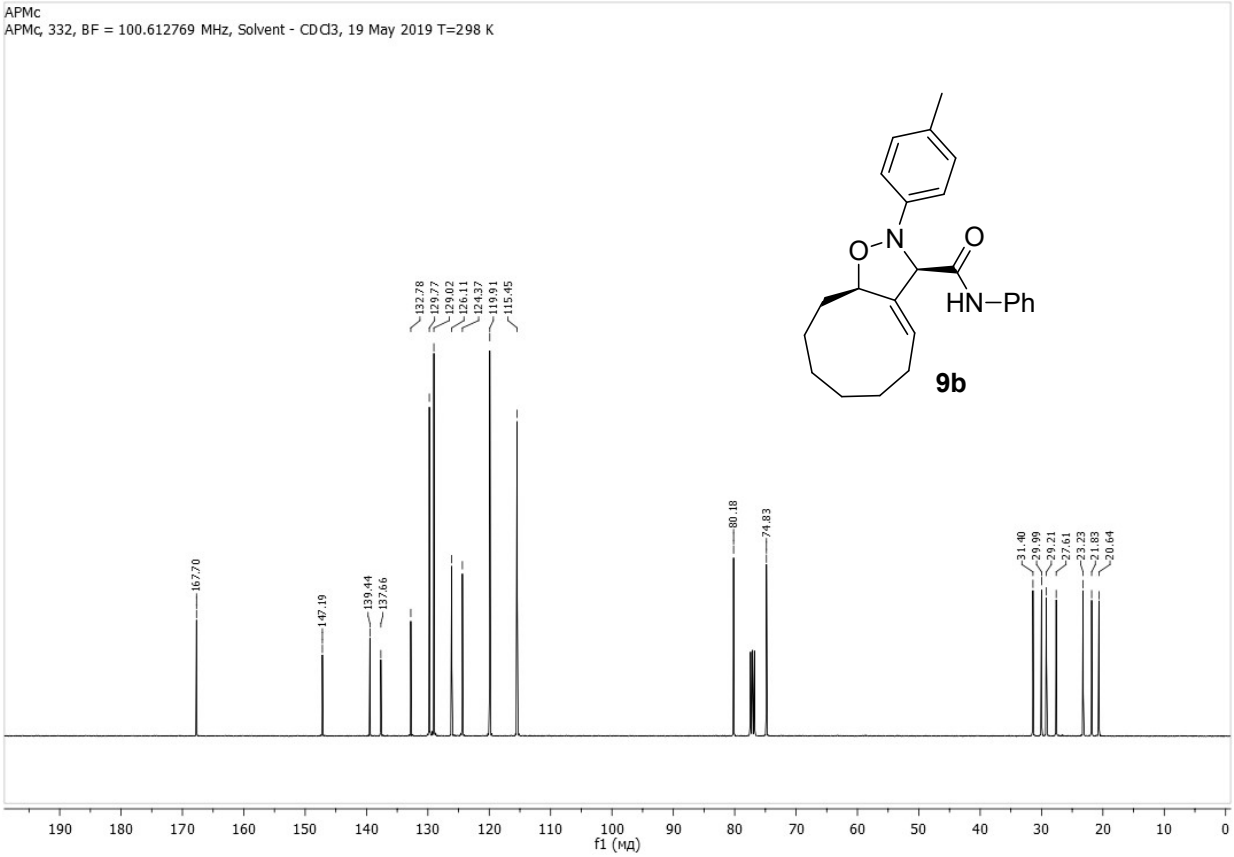

APM
APM, 318, BF = 400.13 MHz, Solvent - CDCl3, 22 Apr 2019 T=298 K
9a
f1 (мд)

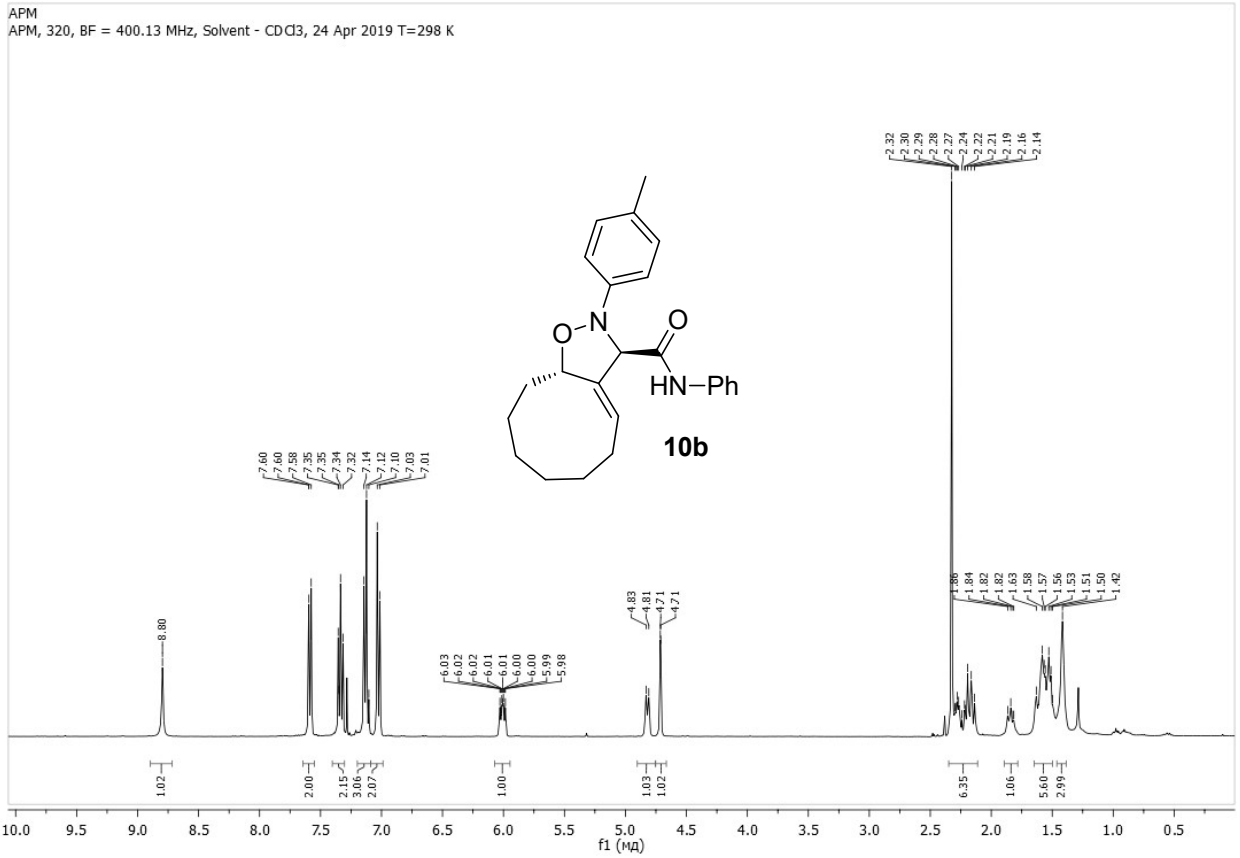

APMc
APMc, 318, BF = 100.612769 MHz, Solvent - CDCl3, 22 Apr 2019 T=298 K
9a
f1 (мд)

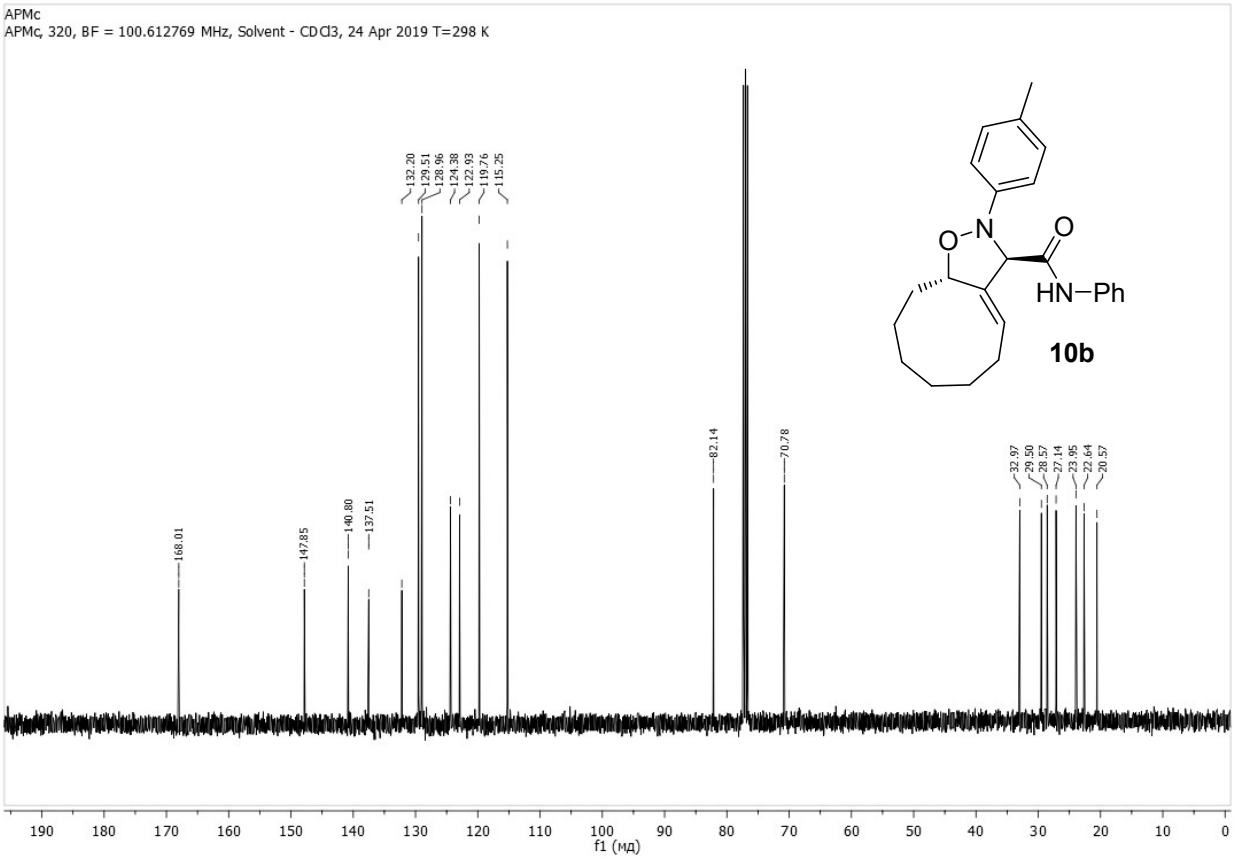

APM
APM, 319, BF = 400.13 MHz, Solvent - CDCl3, 22 Apr 2019 T=298 K
HN−Ph
10a
f1 (мд)


APMc
APMc, 319, BF = 100.612769 MHz, Solvent - CDCl3, 22 Apr 2019 T=298 K
HN−Ph
10a
f1 (мд)

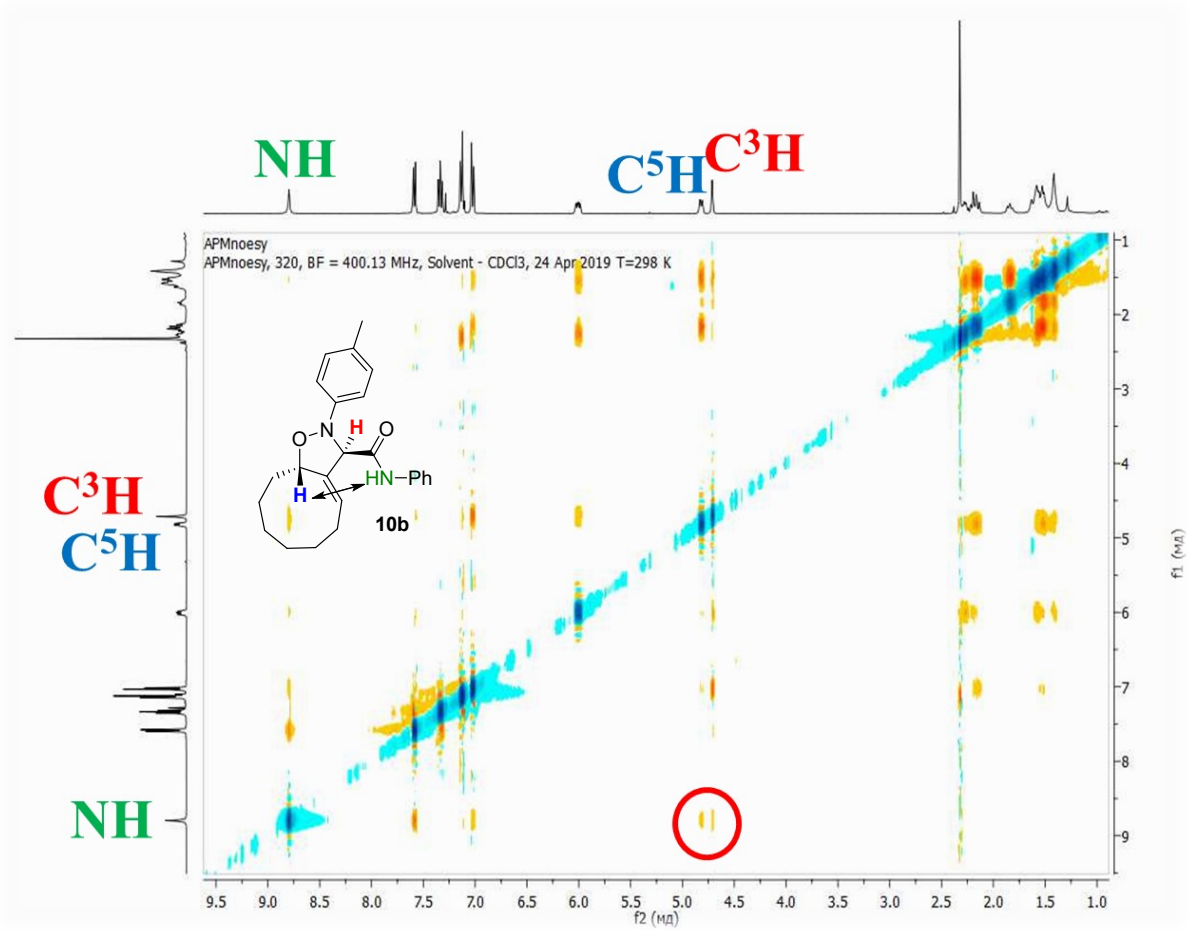

APM
APM, 332, BF = 400.13 MHz, Solvent - CDCl3, 20 May 2019 T=298 K
HN−Ph
9b
f1 (мд)

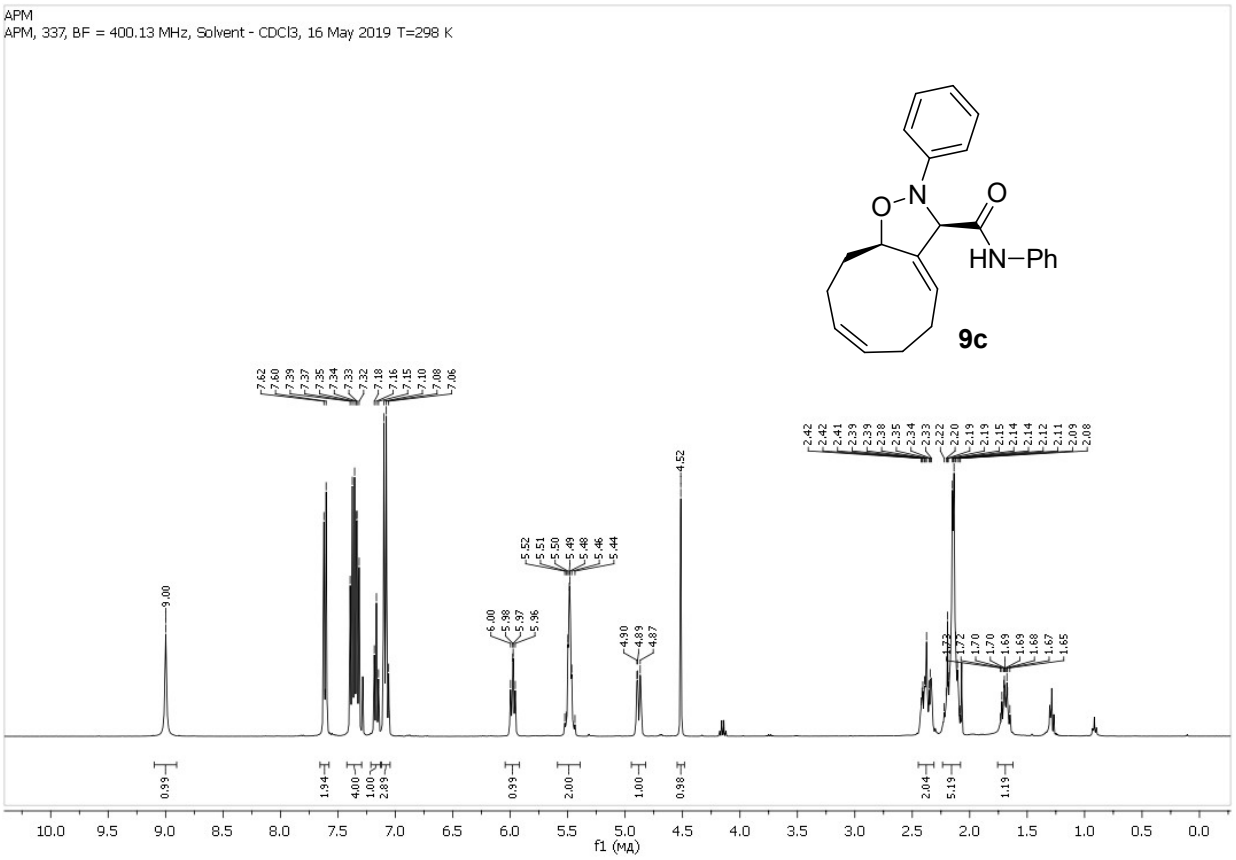

APMc
APMc, 332, BF = 100.612769 MHz, Solvent - CDCl3, 19 May 2019 T=298 K
HN−Ph
9b
f1 (мд)

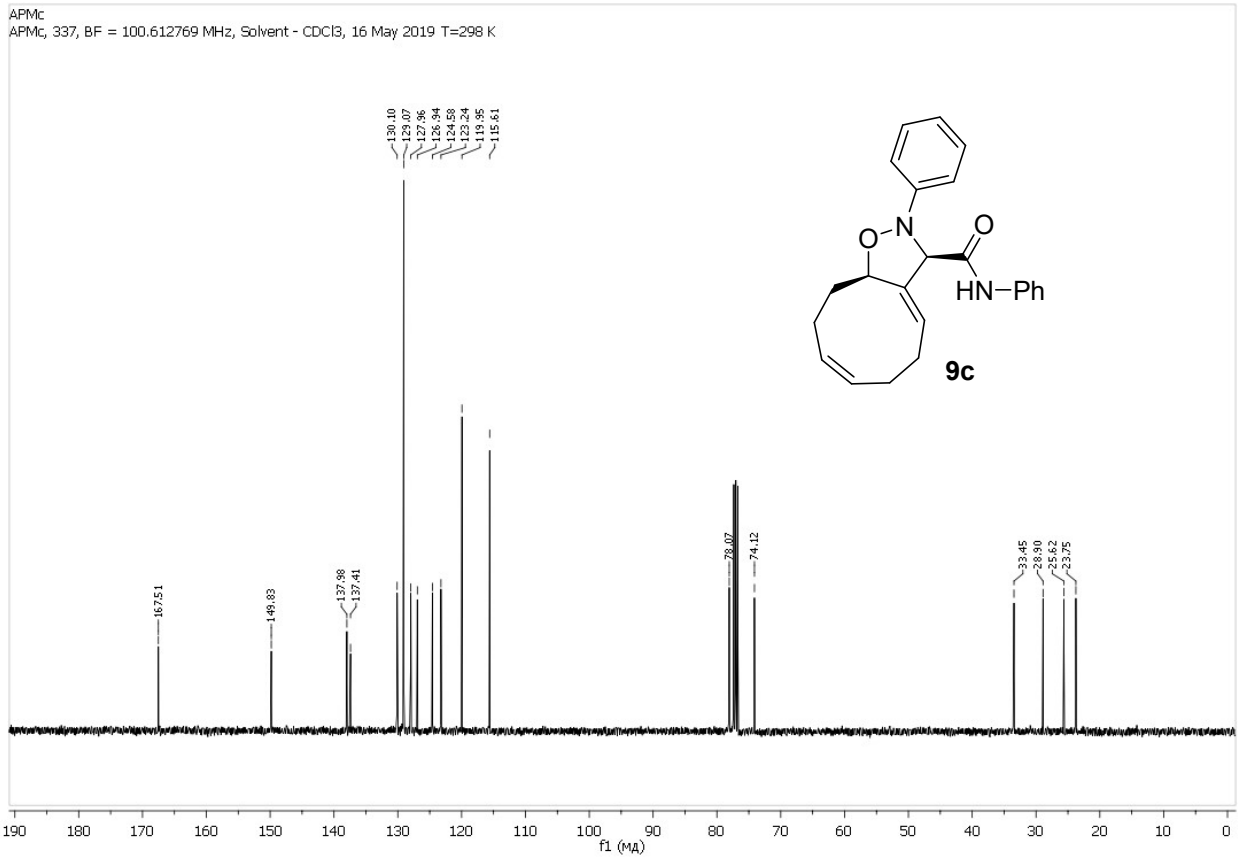

APM
APM, 320, BF = 400.13 MHz, Solvent - CDCl3, 24 Apr 2019 T=298 K
10b
f1 (мд)

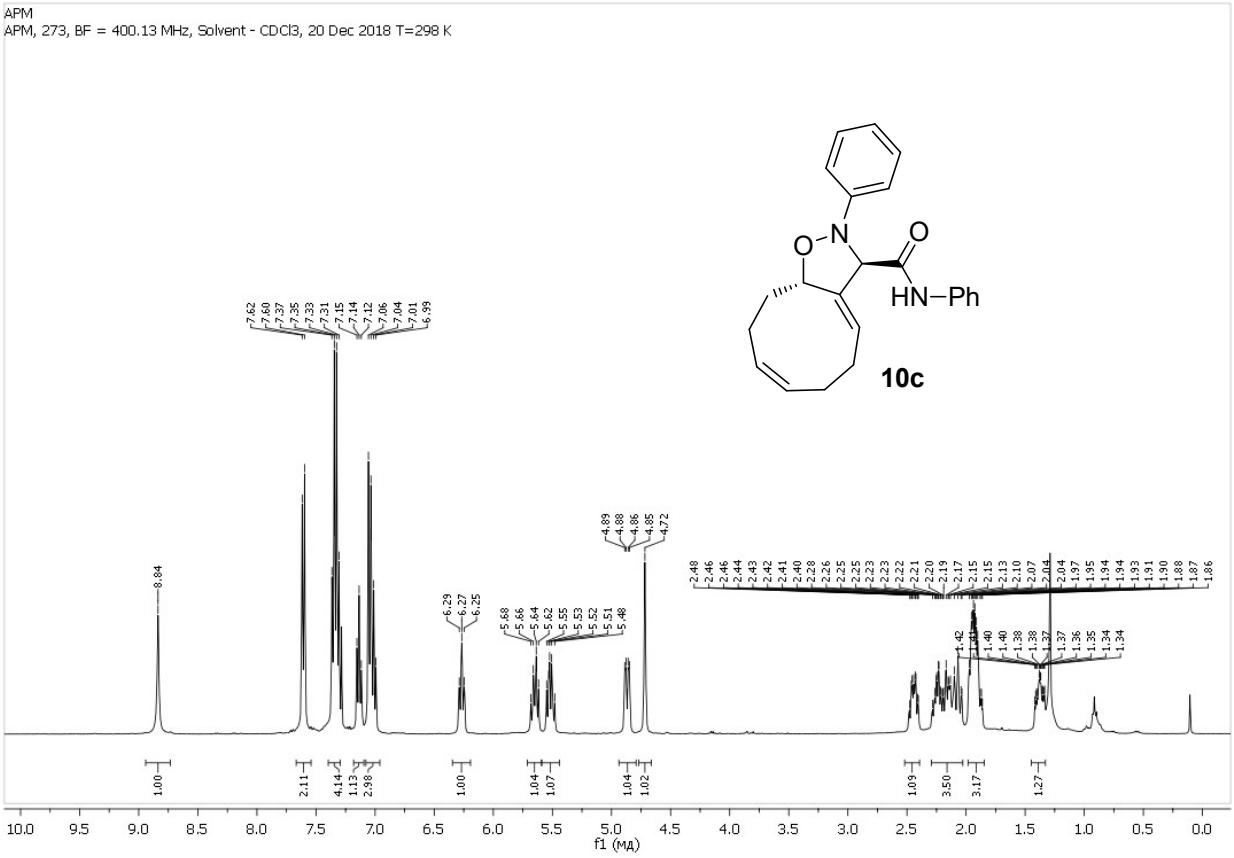

APMc
APMc, 320, BF = 100.612769 MHz, Solvent - CDCl3, 24 Apr 2019 T=298 K
10b
f1 (мд)

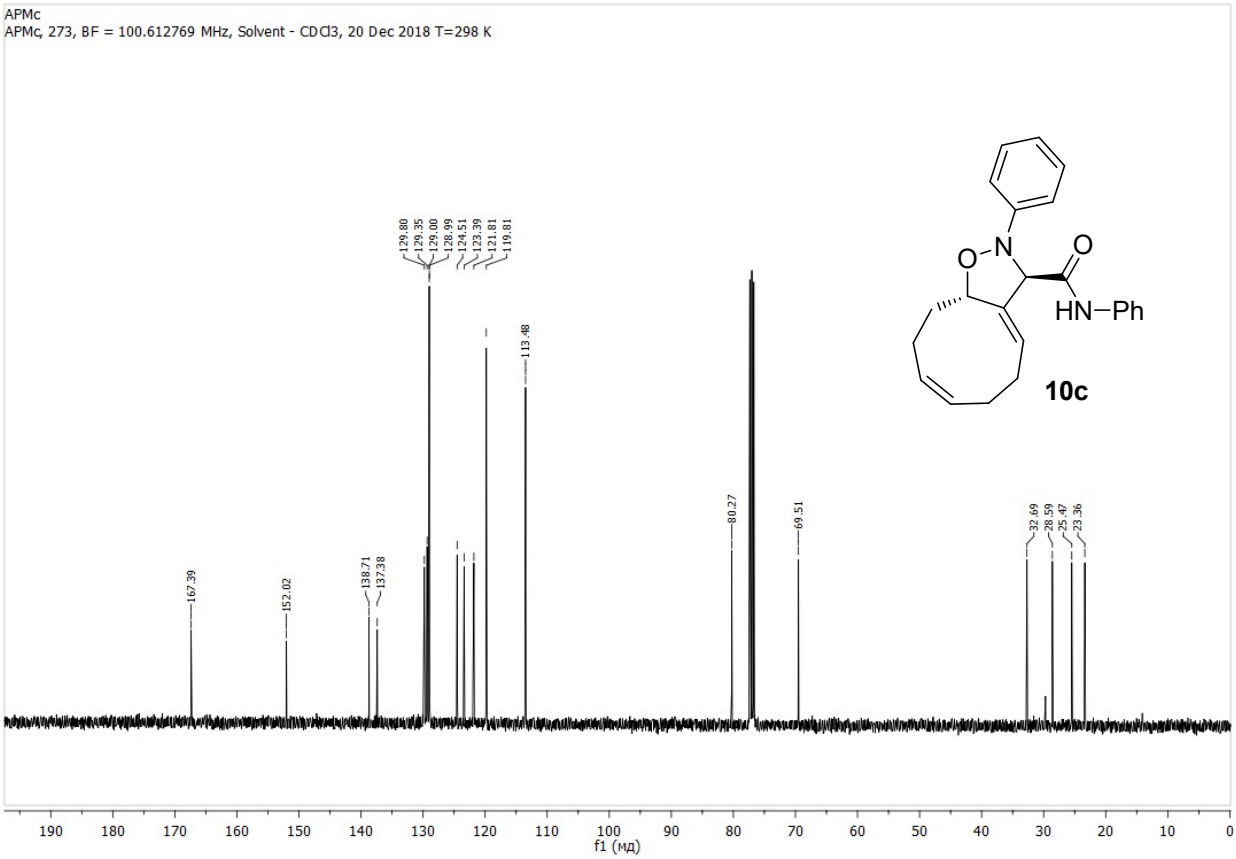
NOESY spectrum for compound **10b**

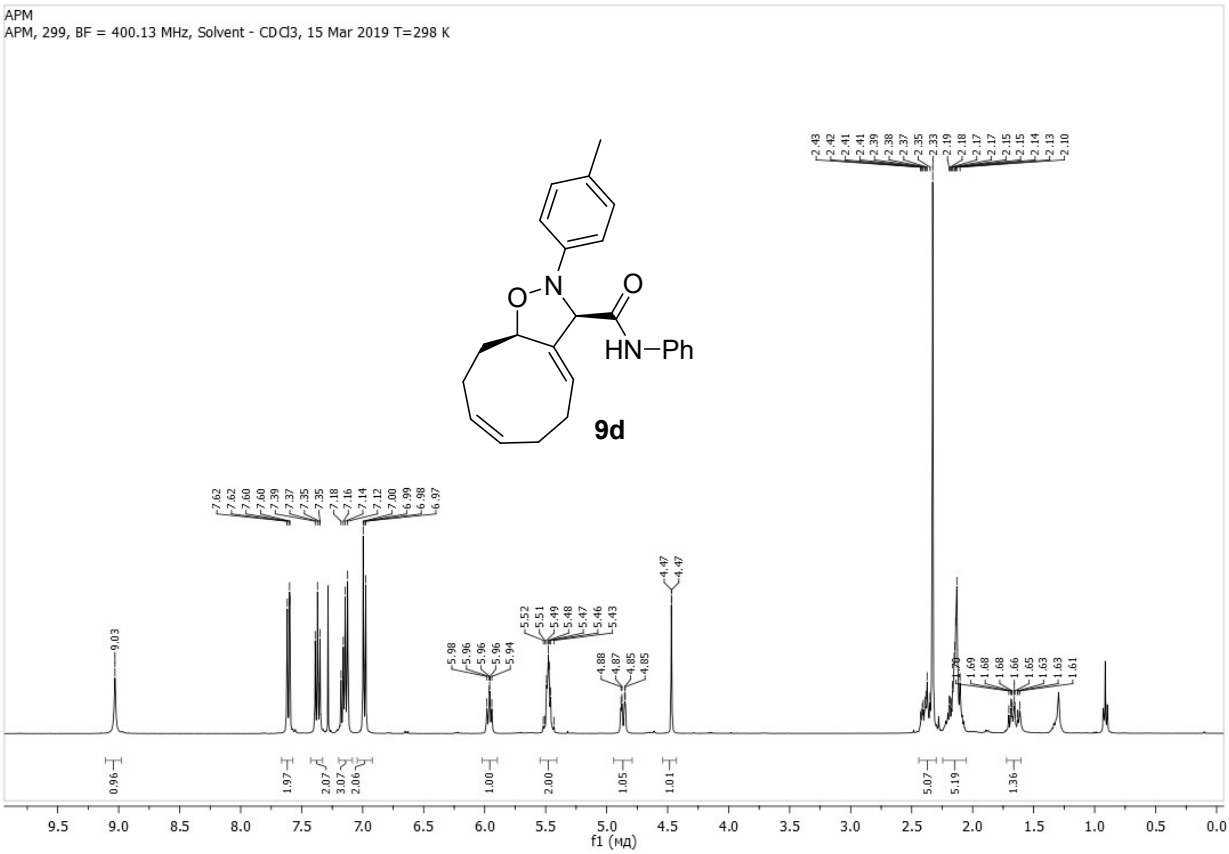


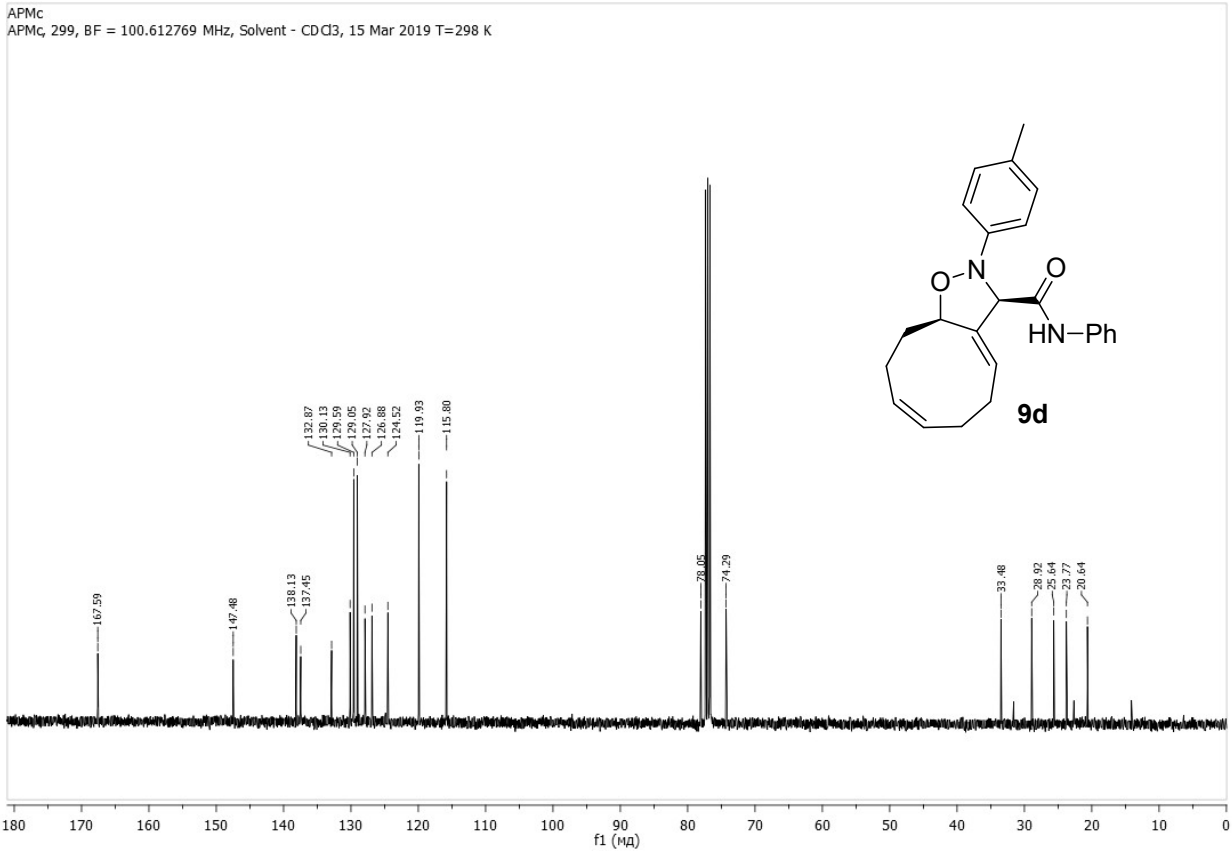

APM
APM, 337, BF = 400.13 MHz, Solvent - CDCl3, 16 May 2019 T=298 K
O
N
O
HN−Ph
9c
f1 (мд)

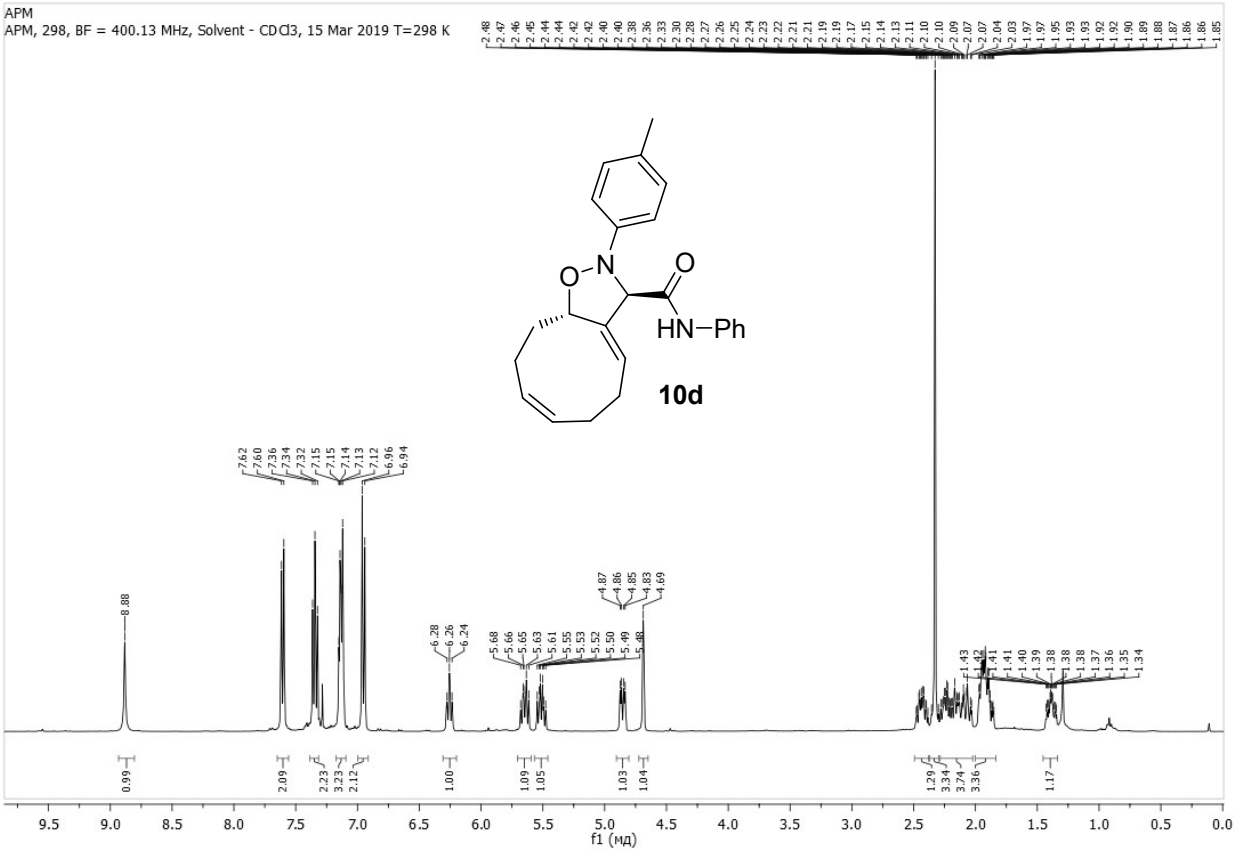

APMc
APMc, 337, BF = 100.612769 MHz, Solvent - CDCl3, 16 May 2019 T=298 K
O
N
O
HN−Ph
9c
f1 (мд)

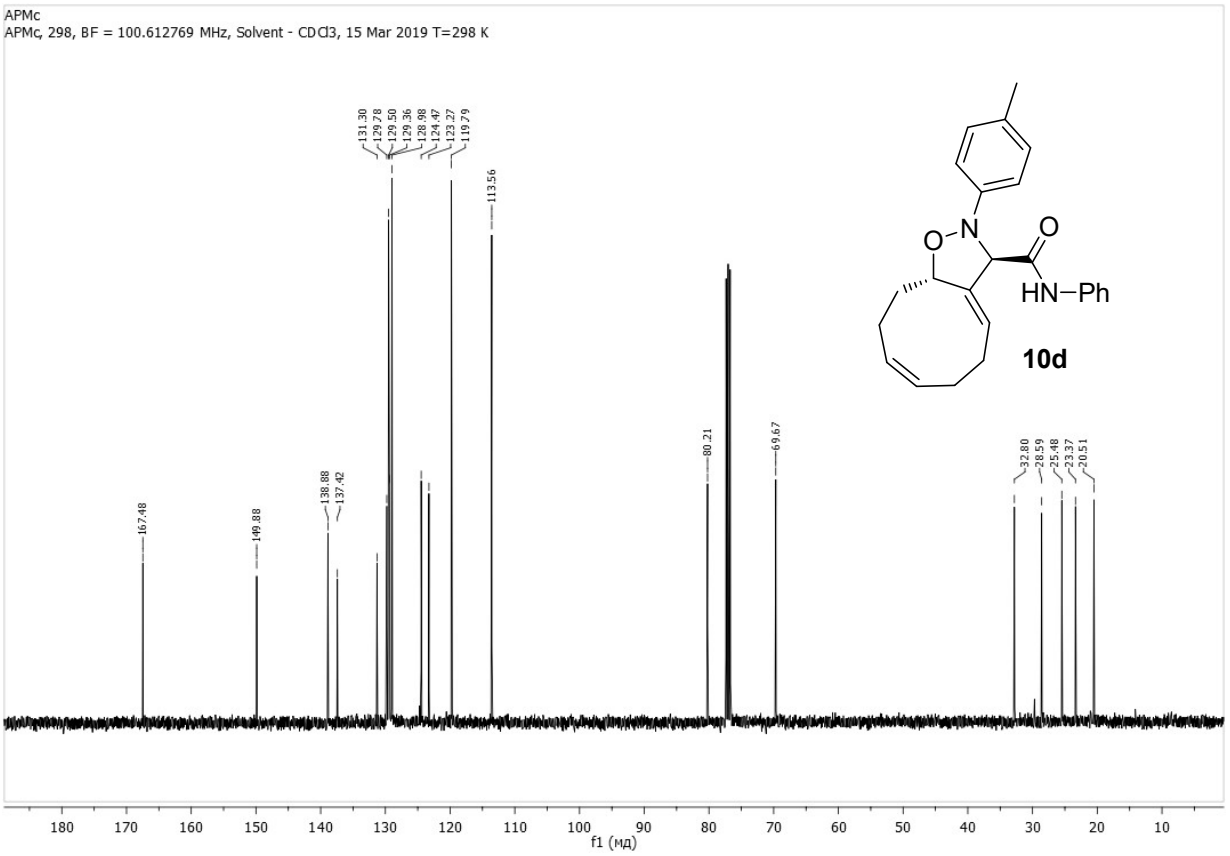

APM
APM, 273, BF = 400.13 MHz, Solvent - CDCl3, 20 Dec 2018 T=298 K
10c
f1 (мд)

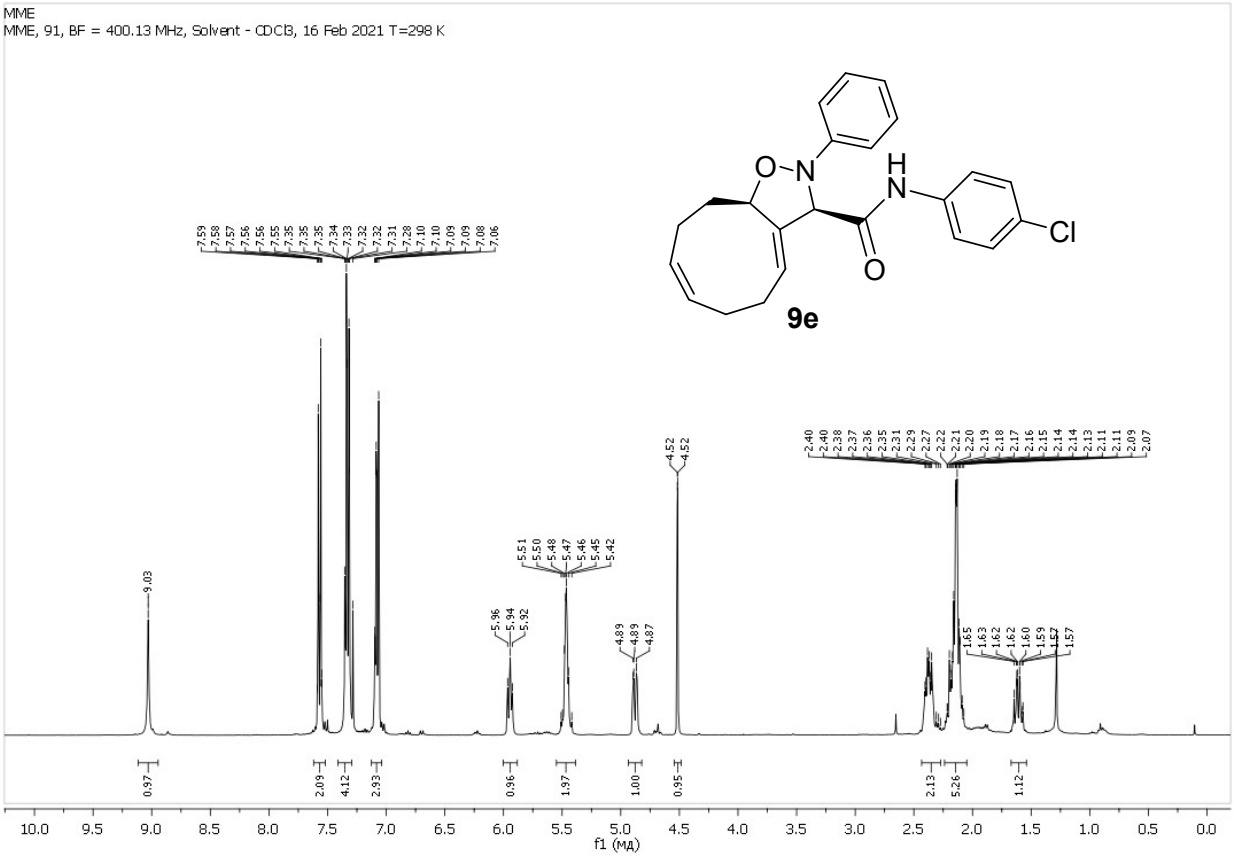

APMc
APMc, 273, BF = 100.612769 MHz, Solvent - CDCl3, 20 Dec 2018 T=298 K
10c
f1 (мд)

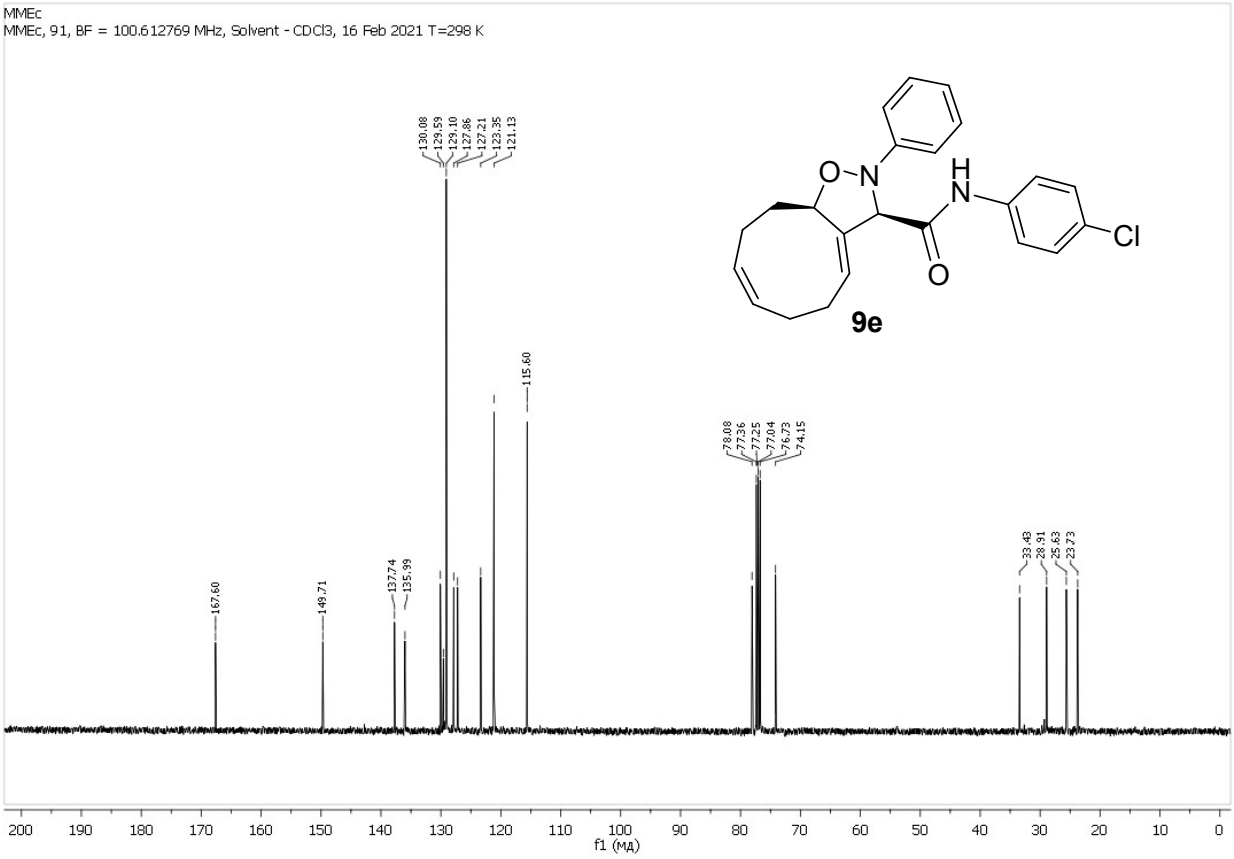

APM
APM, 299, BF = 400.13 MHz, Solvent - CDCl3, 15 Mar 2019 T=298 K
O
N
O
HN−Ph
9d
f1 (мд)

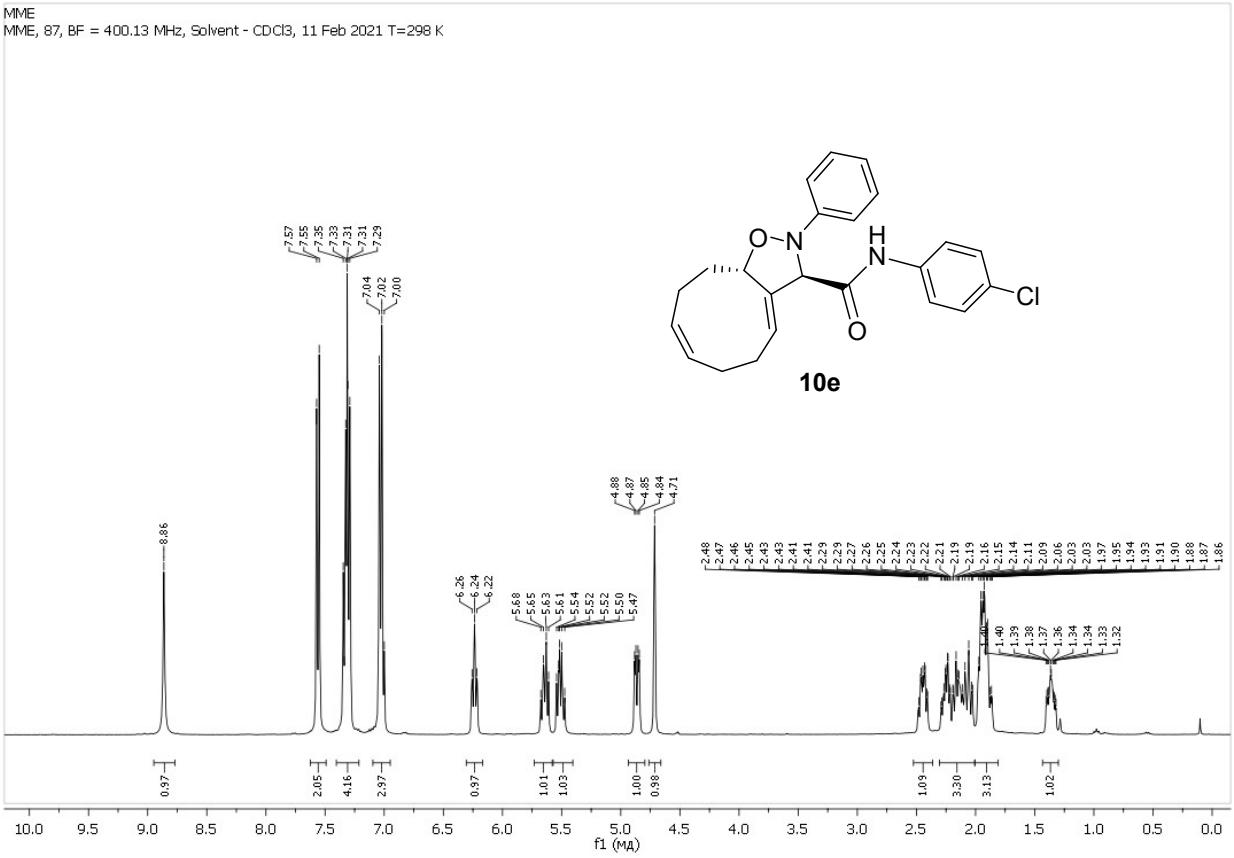

APMc
APMc, 299, BF = 100.612769 MHz, Solvent - CDCl3, 15 Mar 2019 T=298 K
O
N
O
HN−Ph
9d
f1 (мд)

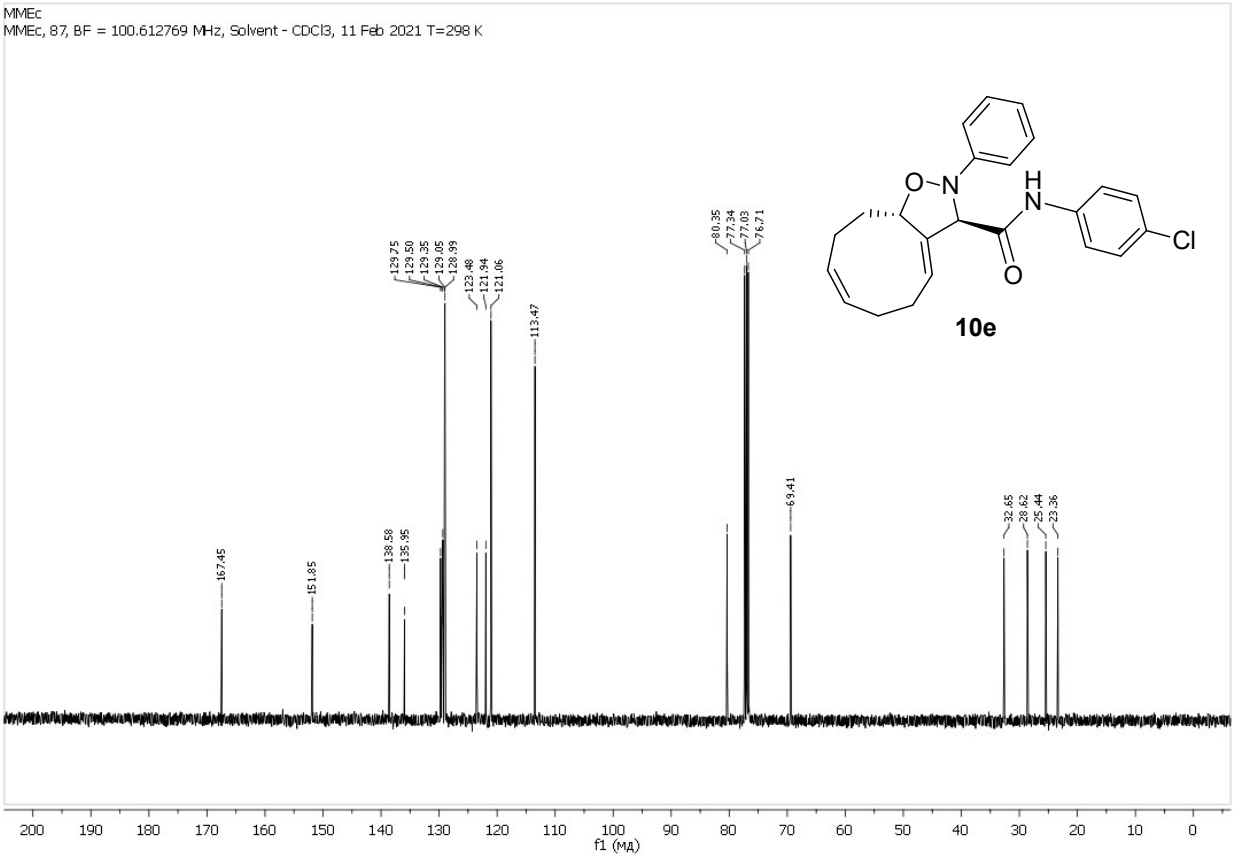

APM
APM, 298, BF = 400.13 MHz, Solvent - CDCl3, 15 Mar 2019 T=298 K
HN−Ph
10d
f1 (мд)

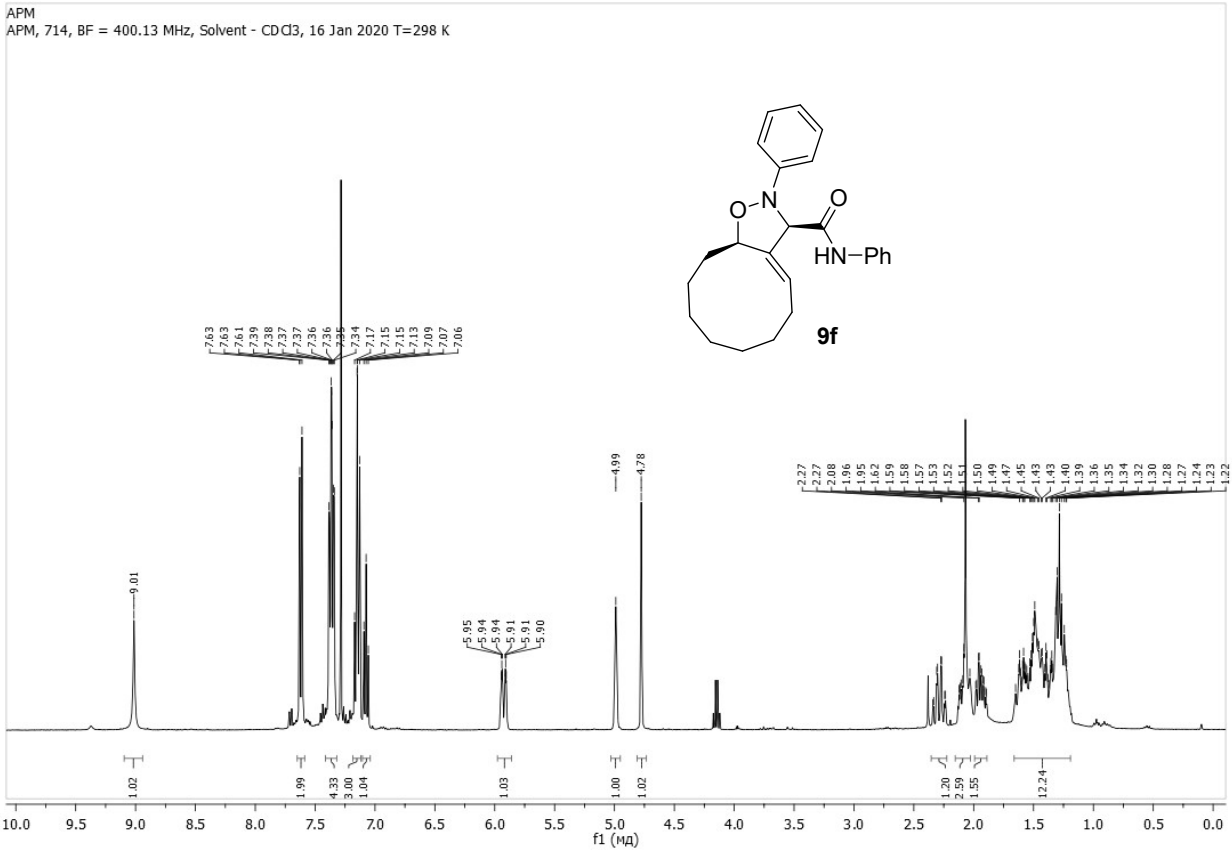

APMc
APMc, 298, BF = 100.612769 MHz, Solvent - CDCl3, 15 Mar 2019 T=298 K
HN−Ph
10d
f1 (мд)

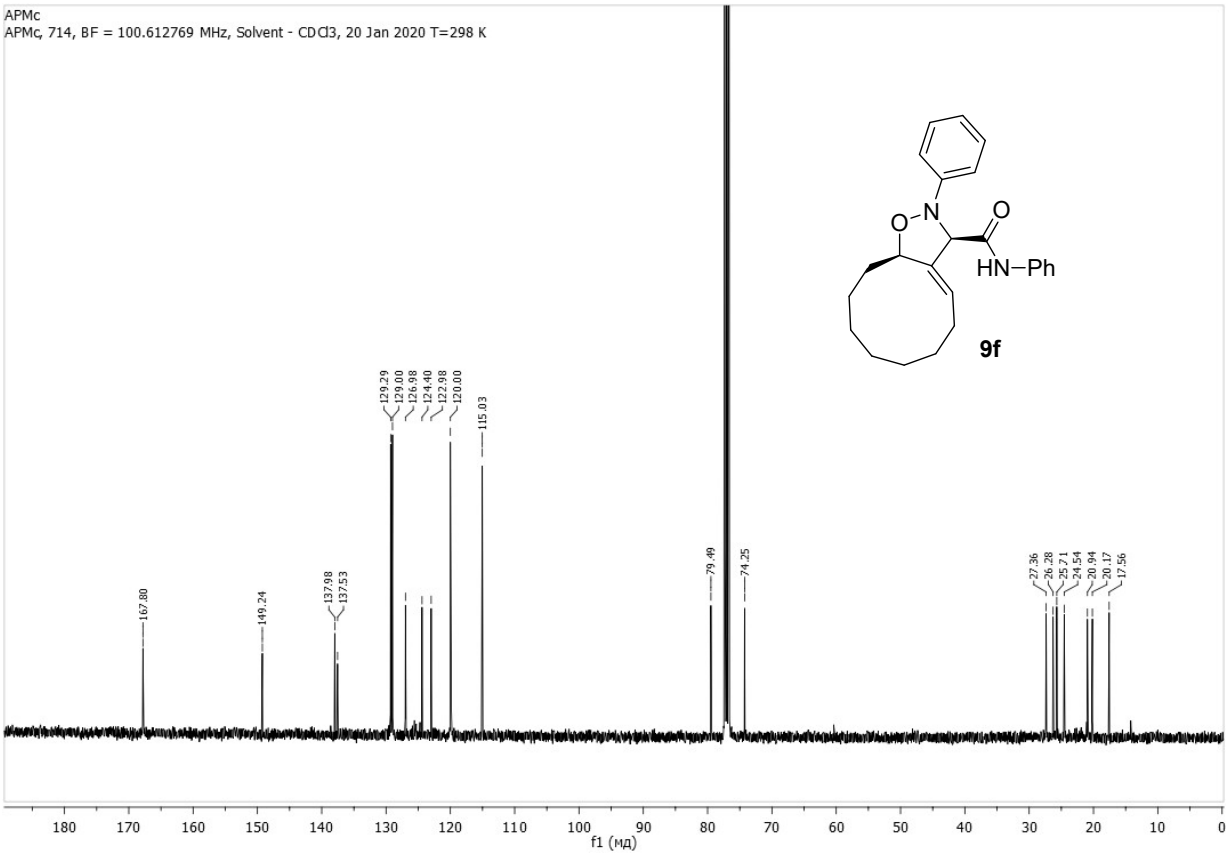

MME
MME, 91, BF = 400.13 MHz, Solvent - CDCl3, 16 Feb 2021 T=298 K
9e
f1 (мд)

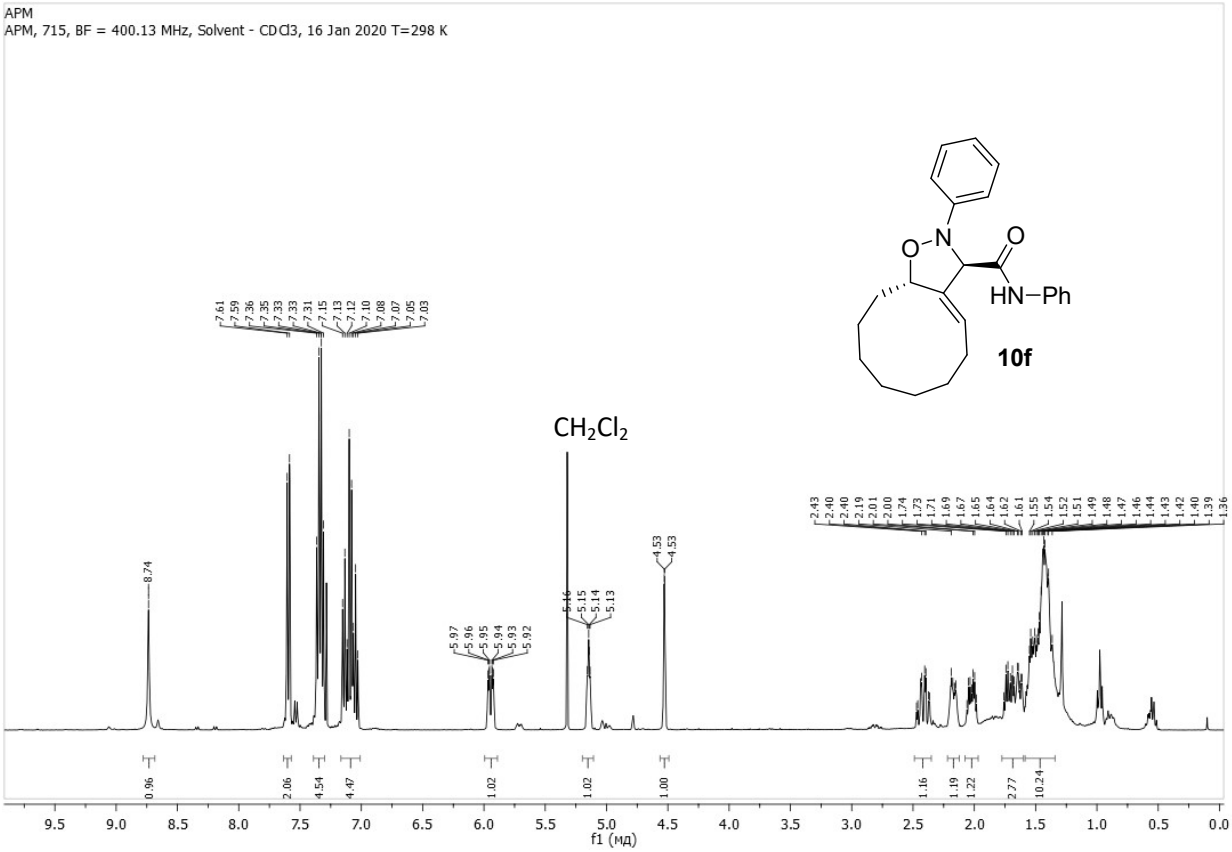

MMEc
MMEc, 91, BF = 100.612769 MHz, Solvent - CDCl3, 16 Feb 2021 T=298 K
9e
f1 (мд)

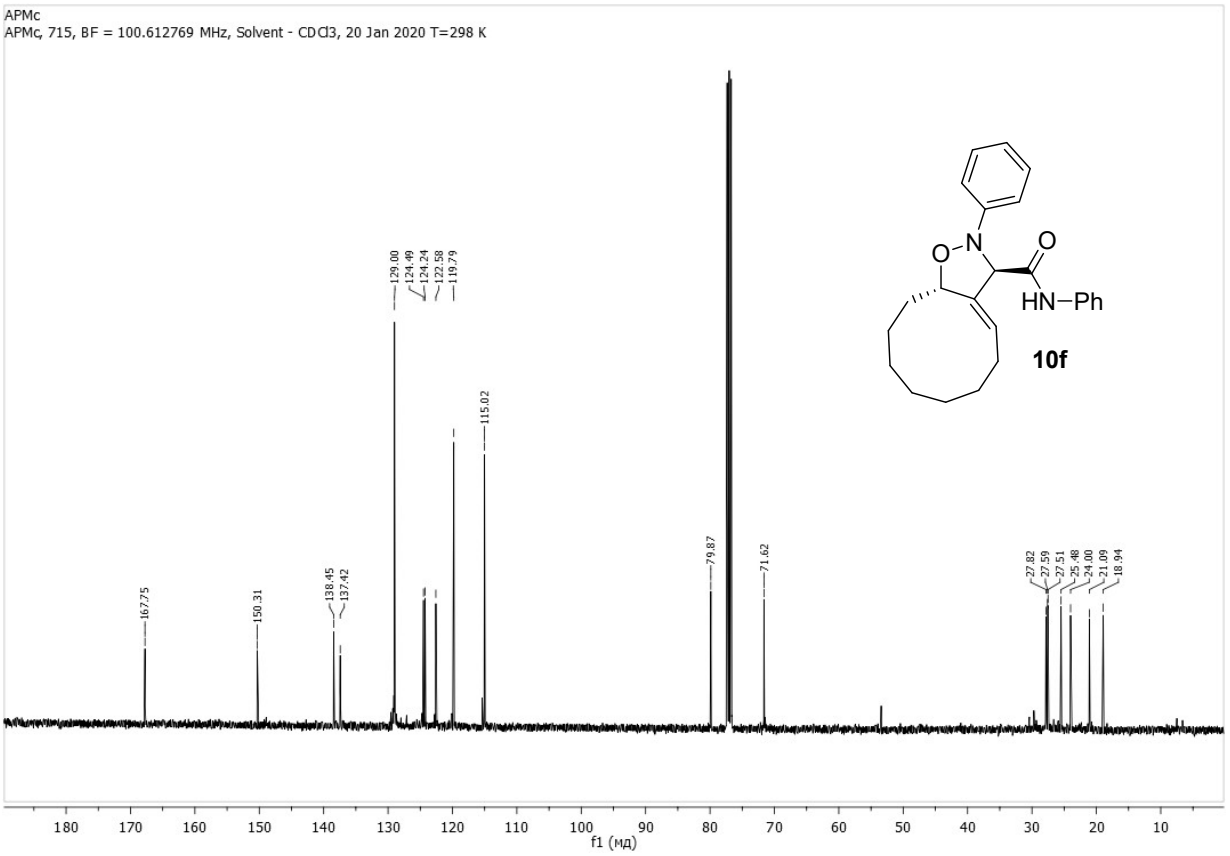

MME
MME, 87, BF = 400.13 MHz, Solvent - CDCl3, 11 Feb 2021 T=298 K
10e
f1 (мд)

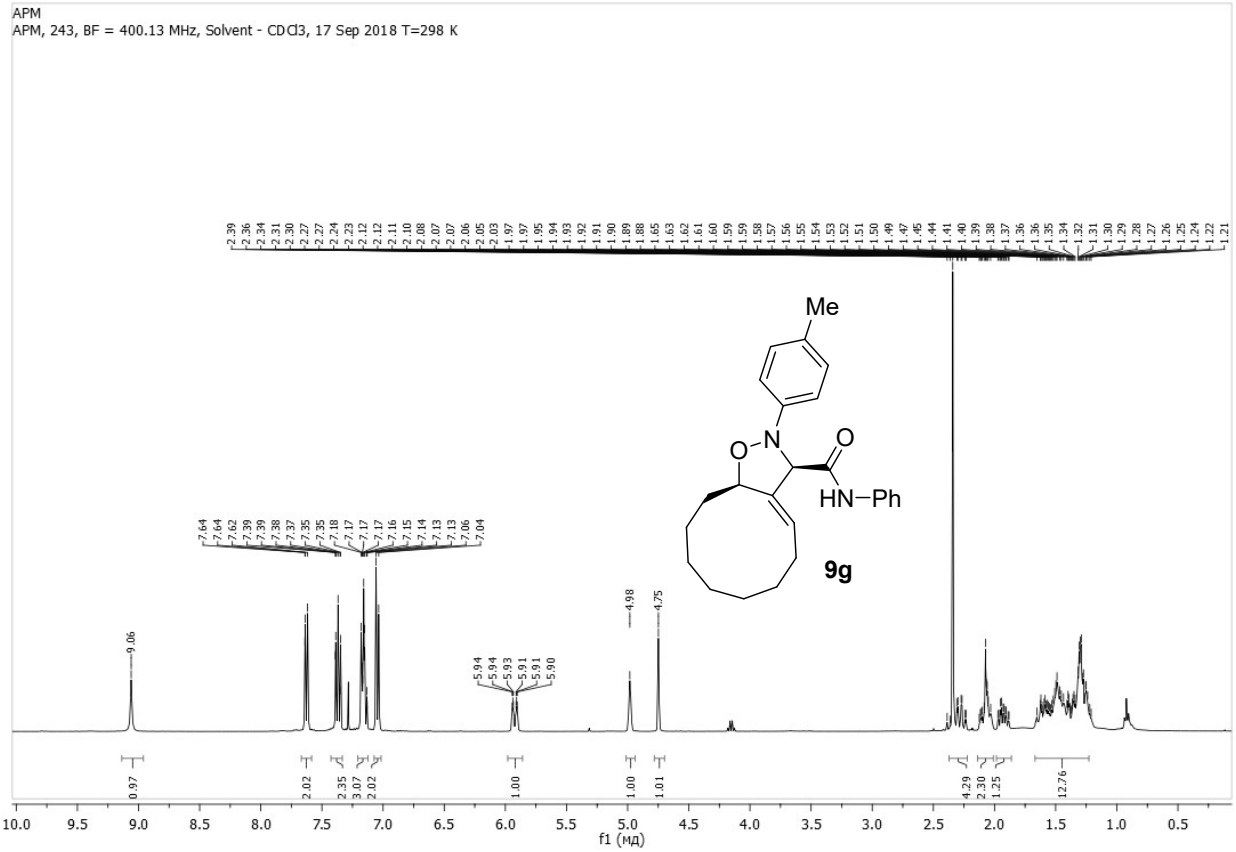

MMEc
MMEc, 87, BF = 100.612769 MHz, Solvent - CDCl3, 11 Feb 2021 T=298 K
10e
f1 (мд)

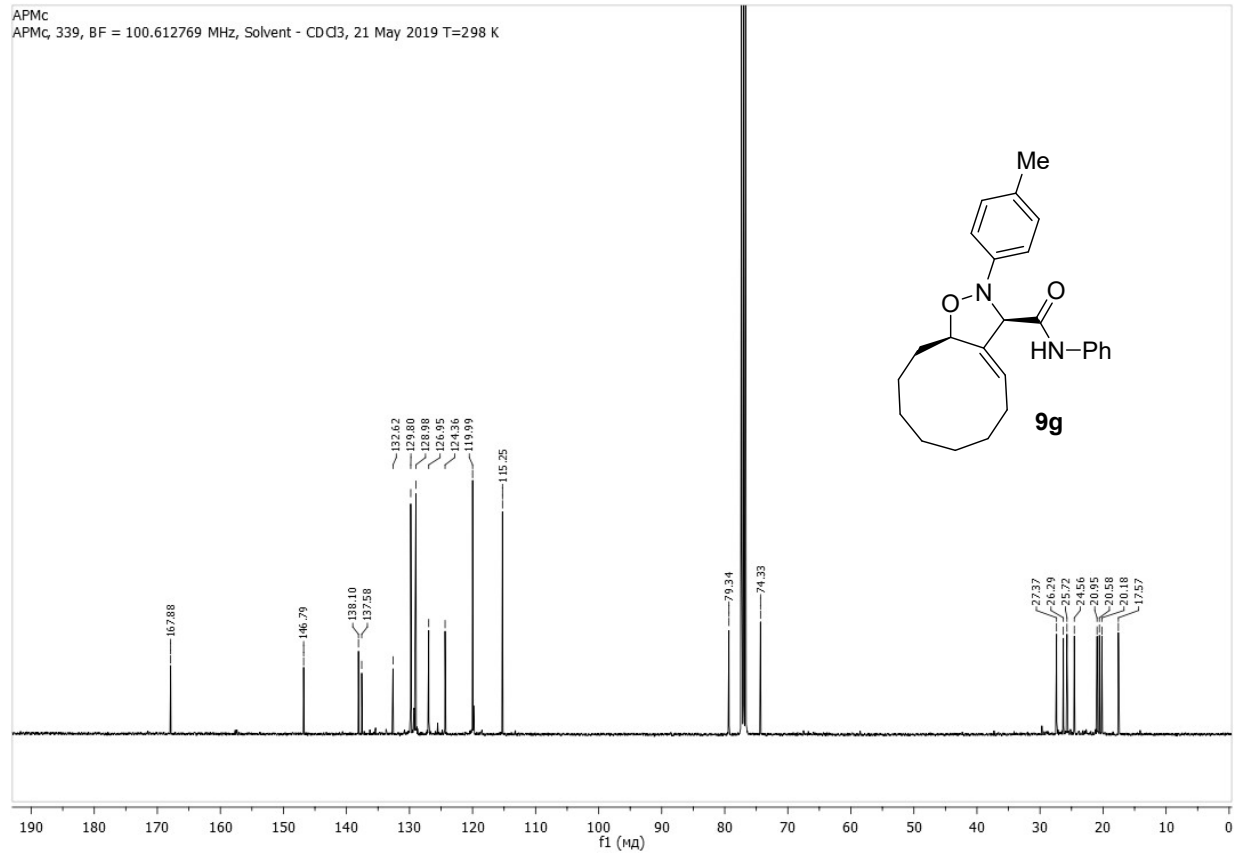

APM
APM, 714, BF = 400.13 MHz, Solvent - CDCl3, 16 Jan 2020 T=298 K
9f
f1 (мд)

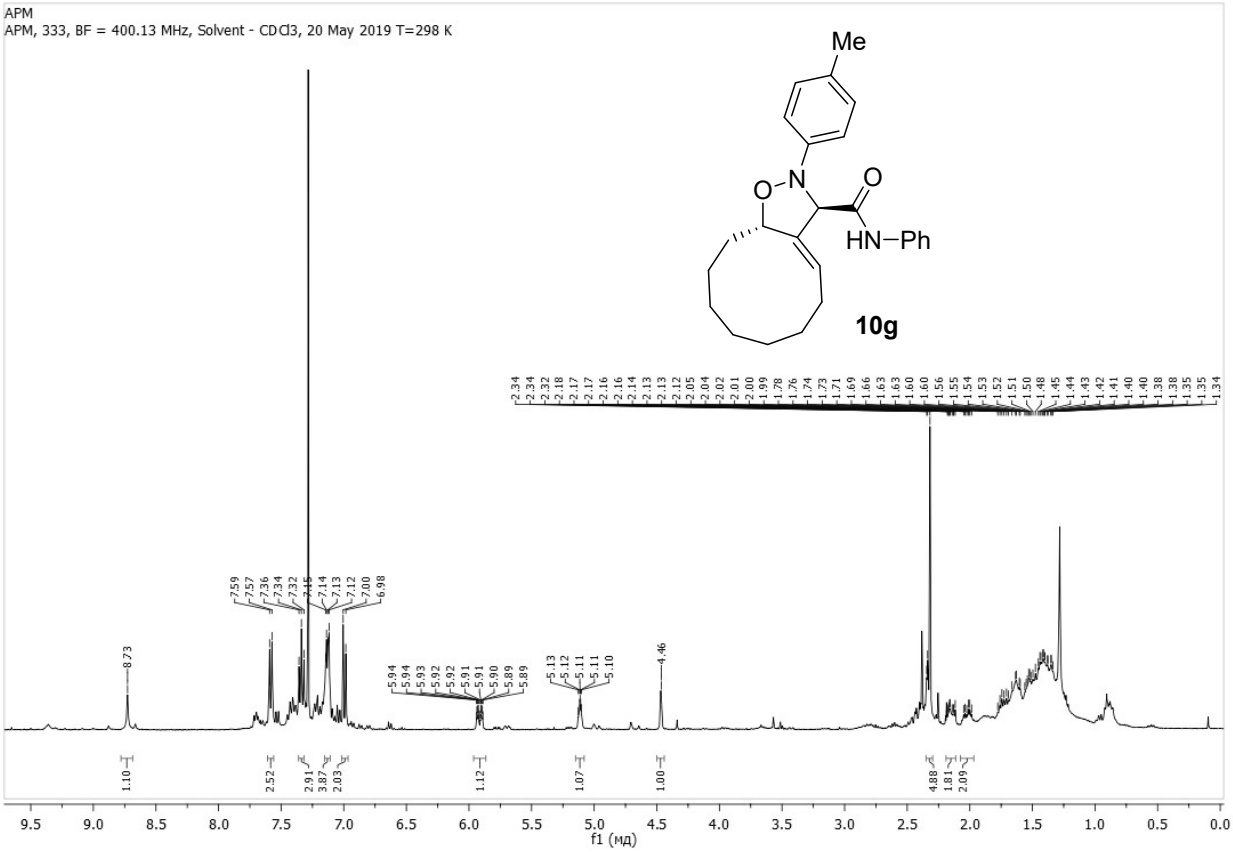

APMc
APMc, 714, BF = 100.612769 MHz, Solvent - CDCl3, 20 Jan 2020 T=298 K
9f
f1 (мд)

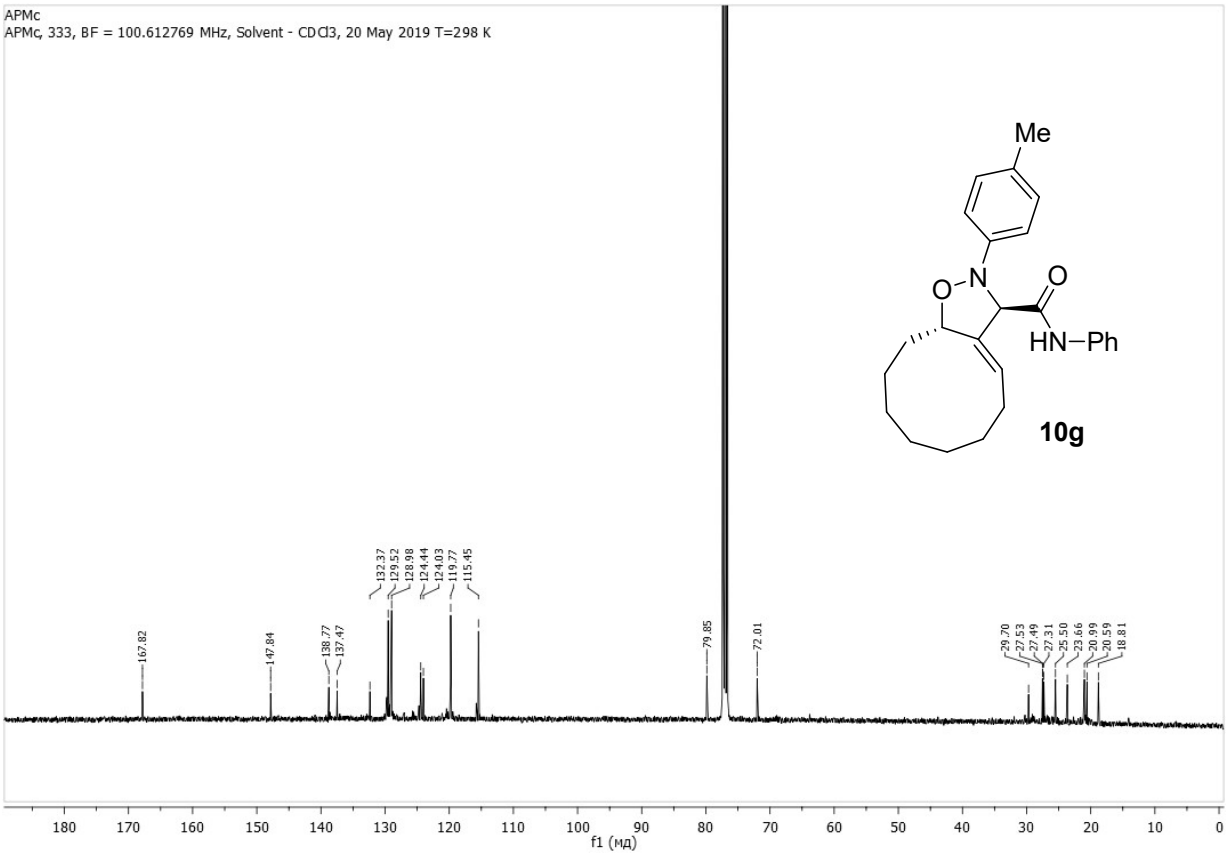

APM
APM, 715, BF = 400.13 MHz, Solvent - CDCl3, 16 Jan 2020 T=298 K
CH2Cl2
HN−Ph
10f
f1 (мд)

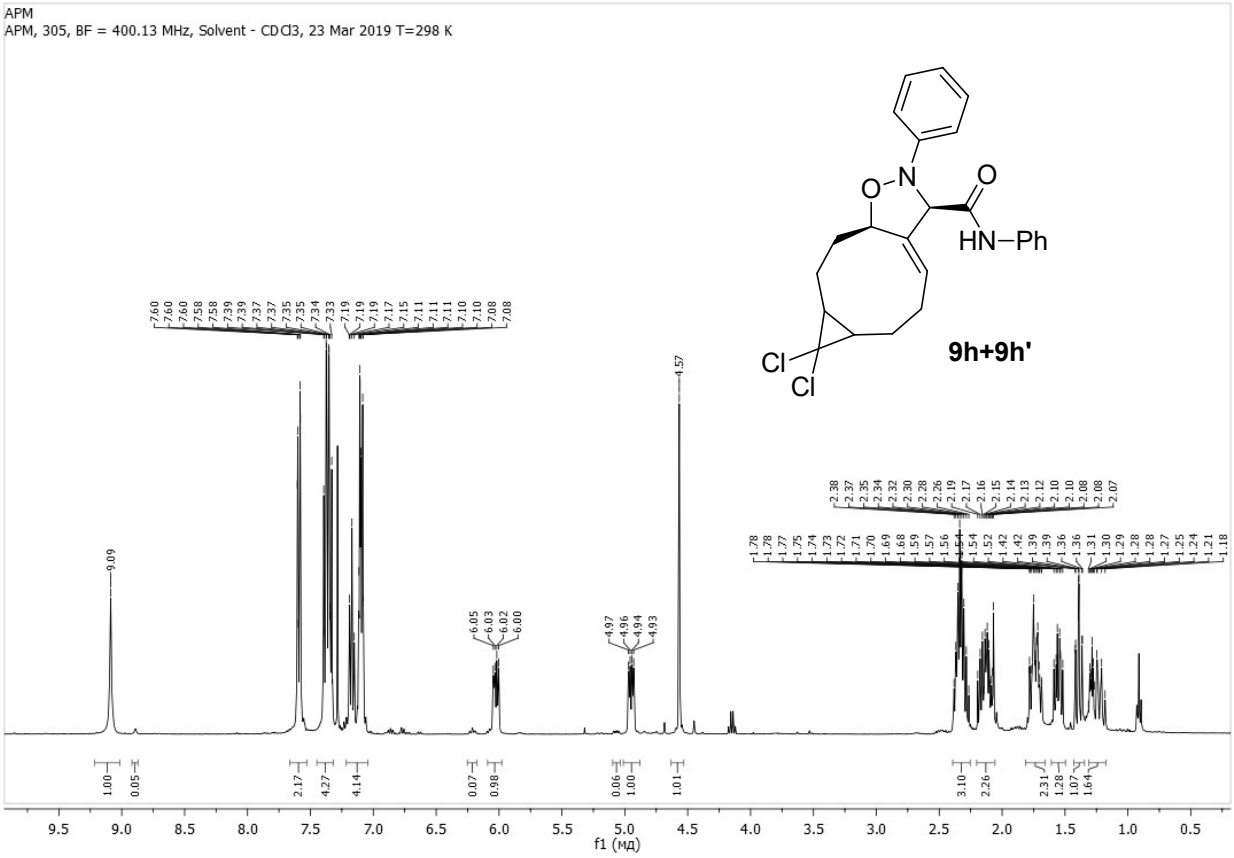

APMc
APMc, 715, BF = 100.612769 MHz, Solvent - CDCl3, 20 Jan 2020 T=298 K
HN−Ph
10f
f1 (мд)

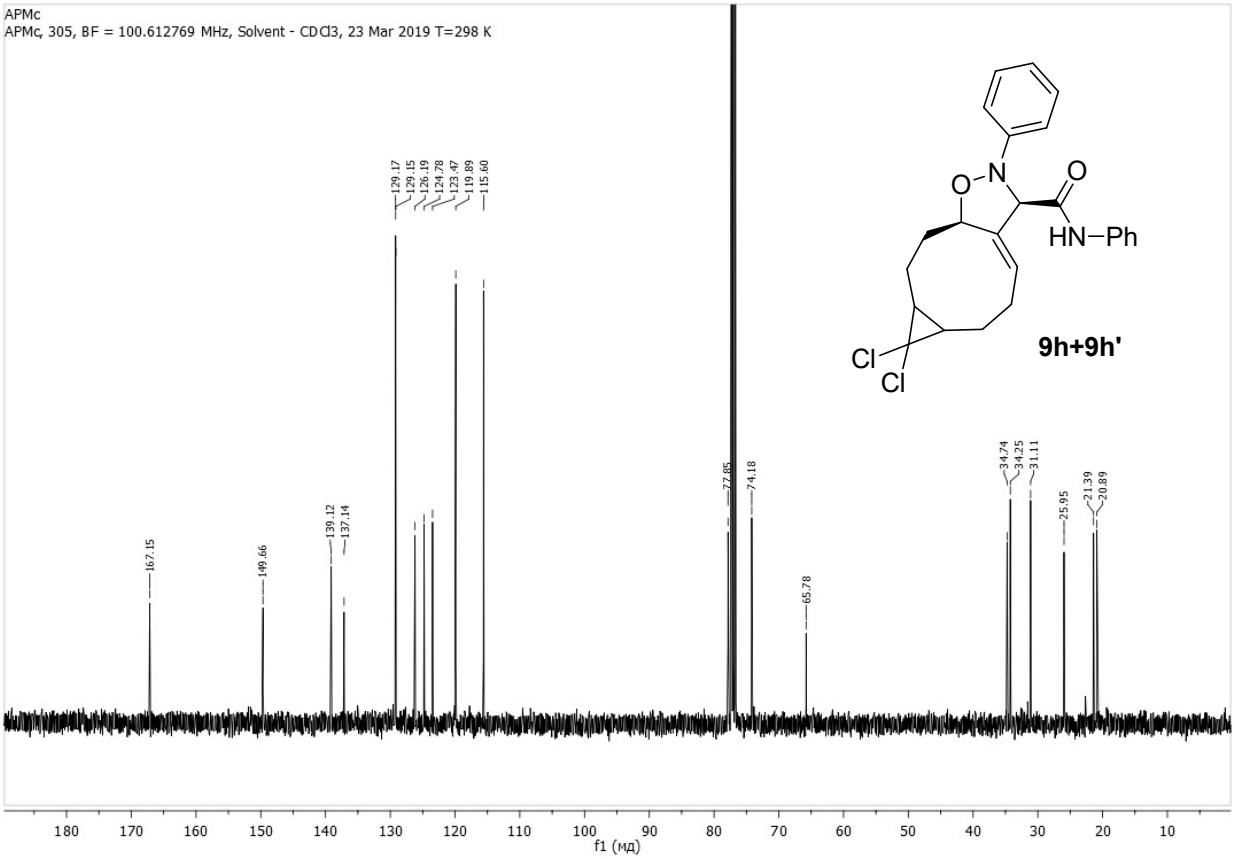

APM
APM, 243, BF = 400.13 MHz, Solvent - CDCl3, 17 Sep 2018 T=298 K
Me
O
N
O
HN−Ph
9g
f1 (мд)

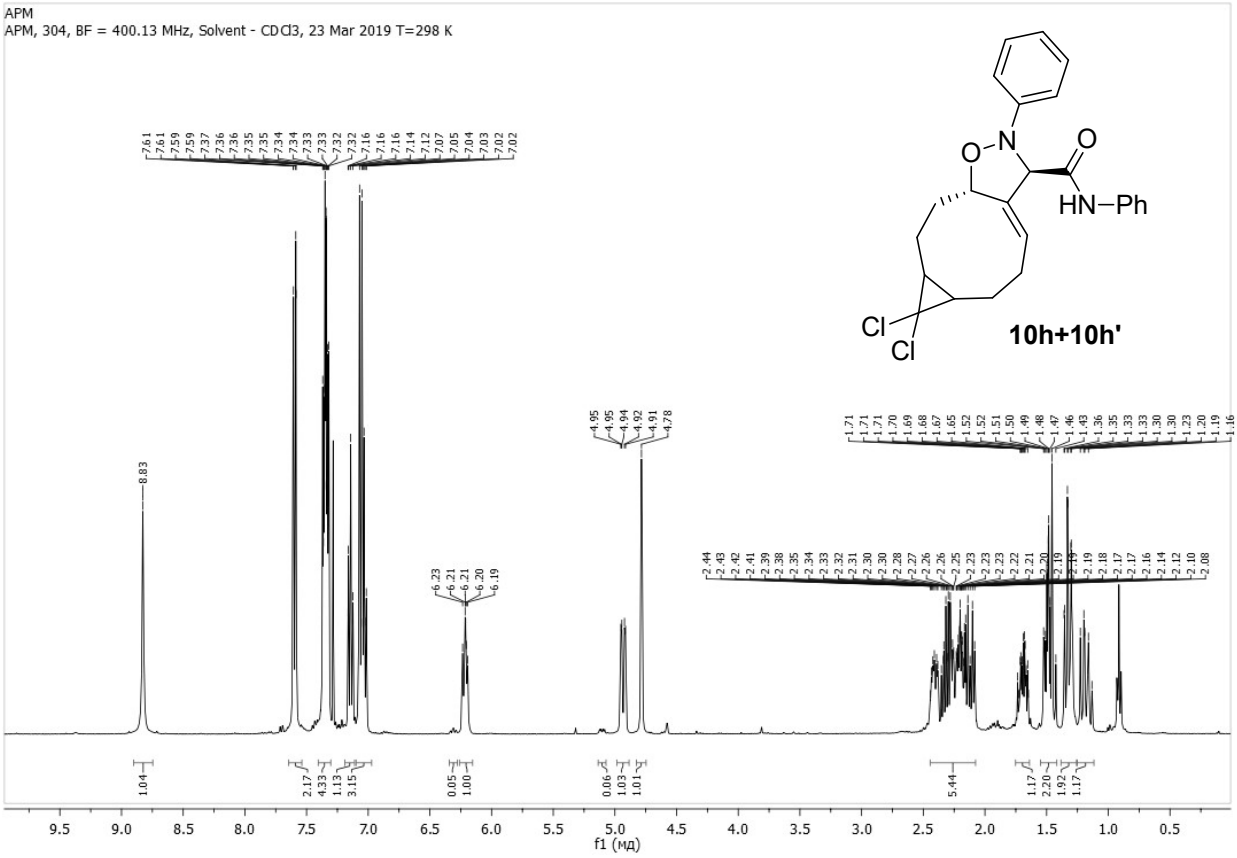

APMc
APMc, 339, BF = 100.612769 MHz, Solvent - CDCl3, 21 May 2019 T=298 K
Me
O
N
O
HN−Ph
9g
f1 (мд)

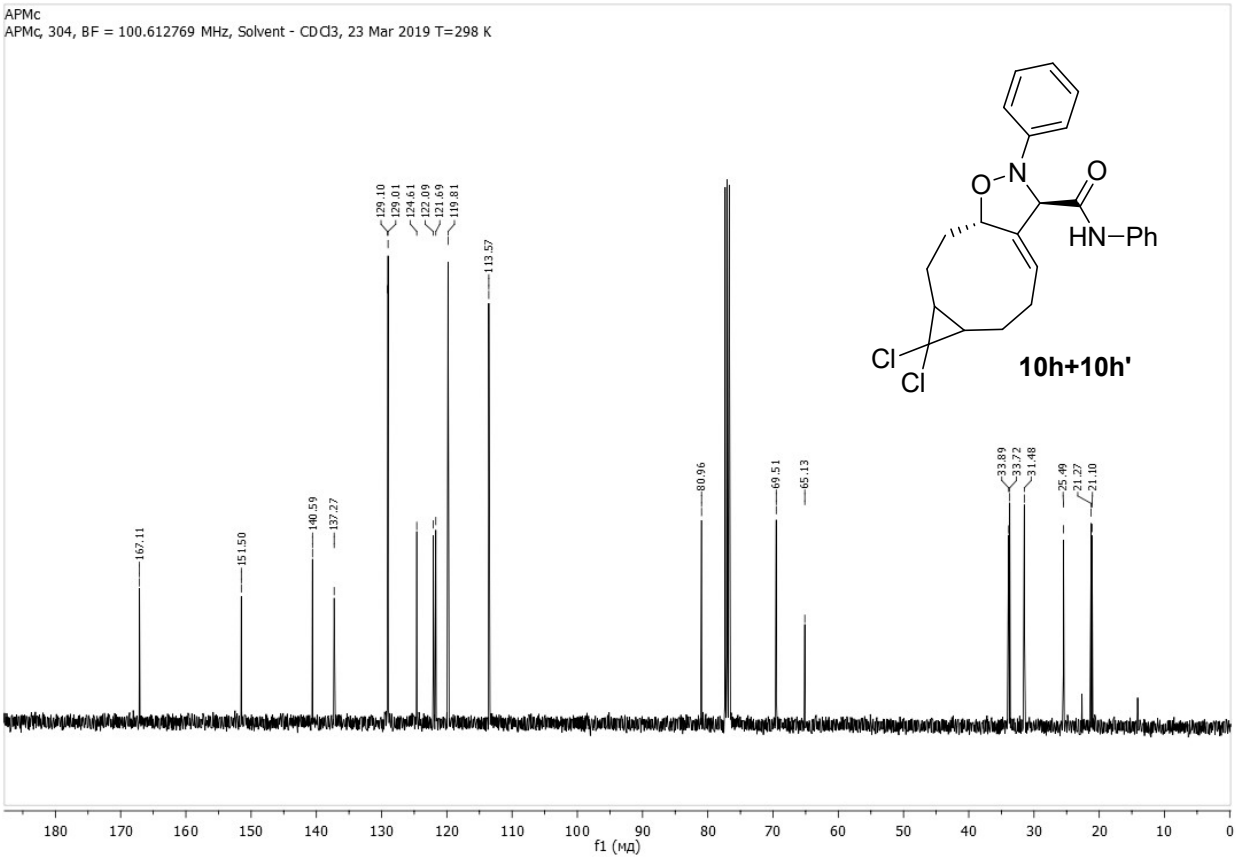

APM
APM, 333, BF = 400.13 MHz, Solvent - CDCl3, 20 May 2019 T=298 K
Me
O
N
O
HN–Ph
10g
f1 (мд)


APMc
APMc, 333, BF = 100.612769 MHz, Solvent - CDCl3, 20 May 2019 T=298 K
Me
O
N
O
HN–Ph
10g
f1 (мд)


APM
APM, 305, BF = 400.13 MHz, Solvent - CDCl3, 23 Mar 2019 T=298 K
9h+9h'
f1 (мд)


APMc
APMc, 305, BF = 100.612769 MHz, Solvent - CDCl3, 23 Mar 2019 T=298 K
9h+9h'
f1 (мд)


APM
APM, 304, BF = 400.13 MHz, Solvent - CDCl3, 23 Mar 2019 T=298 K
HN–Ph
10h+10h'
f1 (мд)


APMc
APMc, 304, BF = 100.612769 MHz, Solvent - CDCl3, 23 Mar 2019 T=298 K
HN–Ph
10h+10h'
f1 (мд)

X-ray diffraction analysis data

Compound 3e

CCDC 2085047

Table S7 Crystal data and structure refinement for **3e**.	
Identification code	13129-MAA-2
Empirical formula	$C_{20}H_{23}NO_5$
Formula weight	357.39
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	8.32060(10)
b/Å	10.38740(10)
c/Å	20.71850(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1790.69(3)
Z	4
ρ_{calc}g/cm^3	1.326
μ/mm^{-1}	0.783
F(000)	760.0
Crystal size/mm^3	0.11 × 0.1 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.524 to 140.812
Index ranges	$-9 \leq h \leq 10$, $-12 \leq k \leq 12$, $-25 \leq l \leq 25$
Reflections collected	37970
Independent reflections	3424 [R_{int} = 0.0934, R_{sigma} = 0.0298]
Data/restraints/parameters	3424/0/238
Goodness-of-fit on F^2	1.028
Final R indexes [I>=2σ (I)]	R_1 = 0.0354, wR_2 = 0.0928
Final R indexes [all data]	R_1 = 0.0357, wR_2 = 0.0932
Largest diff. peak/hole / e Å^{-3}	0.19/-0.29
Flack parameter	0.4(2)

Compound 4a

CCDC 2085045

Table S8 Crystal data and structure refinement for **4a**.	
Identification code	16022_APM-501
Empirical formula	$C_{20}H_{25}NO_5$
Formula weight	359.43
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	13.5595(2)
b/Å	7.54710(10)
c/Å	18.0224(3)
α/°	90
β/°	106.000(2)
γ/°	90
Volume/Å^3	1772.87(5)
Z	4
ρ_{calc}g/cm^3	1.3465
μ/mm^{-1}	0.791
F(000)	770.6
Crystal size/mm^3	0.15 × 0.14 × 0.13
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.78 to 140.68
Index ranges	$-16 \leq h \leq 16$, $-9 \leq k \leq 9$, $-18 \leq l \leq 22$
Reflections collected	10486
Independent reflections	3378 [R_{int} = 0.0324, R_{sigma} = 0.0350]
Data/restraints/parameters	3378/0/237
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0362, wR_2 = 0.0869
Final R indexes [all data]	R_1 = 0.0420, wR_2 = 0.0911
Largest diff. peak/hole / e Å^{-3}	0.25/-0.25

Compound 3k

CCDC 2085048

Table S9 Crystal data and structure refinement for **3k**.	
Identification code	17723_MME-6
Empirical formula	$C_{22}H_{25}Cl_2NO_6$
Formula weight	470.33
Temperature/K	100.0(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.0854(3)
b/Å	7.50448(14)
c/Å	22.3639(5)
α/°	90
β/°	92.532(2)
γ/°	90
Volume/Å^3	2193.97(8)
Z	4
ρ_{calc}g/cm^3	1.424
μ/mm^{-1}	3.003
F(000)	984.0
Crystal size/mm^3	0.12 × 0.11 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.682 to 139.998
Index ranges	$-15 \leq h \leq 15$, $-9 \leq k \leq 8$, $-27 \leq l \leq 23$
Reflections collected	21013
Independent reflections	4140 [R_{int} = 0.0370, R_{sigma} = 0.0256]
Data/restraints/parameters	4140/0/283
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0303, wR_2 = 0.0787
Final R indexes [all data]	R_1 = 0.0330, wR_2 = 0.0805
Largest diff. peak/hole / e Å^{-3}	0.35/-0.28

Compound 4k

CCDC 2085046

Table S10 Crystal data and structure refinement for **4k**.	
Identification code	16022_APM-502
Empirical formula	$C_{22}H_{25}Cl_2NO_6$
Formula weight	470.33
Temperature/K	100.00(11)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.9201(3)
b/Å	27.3837(9)
c/Å	9.5899(3)
α/°	90
β/°	109.369(4)
γ/°	90
Volume/Å^3	2209.90(14)
Z	4
ρ_{calc}g/cm^3	1.414
μ/mm^{-1}	2.981
F(000)	984.0
Crystal size/mm^3	0.16 × 0.13 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.456 to 154.77
Index ranges	$-9 \leq h \leq 11$, $-29 \leq k \leq 32$, $-12 \leq l \leq 11$
Reflections collected	18890
Independent reflections	4524 [R_{int} = 0.0374, R_{sigma} = 0.0321]
Data/restraints/parameters	4524/0/283
Goodness-of-fit on F^2	1.064
Final R indexes [I>=2σ (I)]	R_1 = 0.0314, wR_2 = 0.0827
Final R indexes [all data]	R_1 = 0.0341, wR_2 = 0.0845
Largest diff. peak/hole / e Å^{-3}	0.31/-0.26

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2. (a) L. R. Domingo, J.A. Saéz, R.J. Zaragozá, M. Arnó *J. Org. Chem.* 2008, **73**, 8791;
   (b) L. R. Domingo, M.T. Picher, J.A. Saéz *J. Org. Chem.* 2009, **74**, 2726;
   (c) L. R. Domingo, P. Pérez *Org. Biomol. Chem.* 2013, **11**, 4350.
3. E. D. Glendening, C. R. Landis, F. Weinhold, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2012, **2**, 1.