Highly Enantioselective Synthesis of Naphthoquinones and Pyranonaphthoquinones Catalyzed by Bifunctional Chiral Bis-Squaramides

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Supporting information

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Fig. S1. Molecular structure of **4d** shown with 50% ellipsoidal probability. (CCDC 1030663)

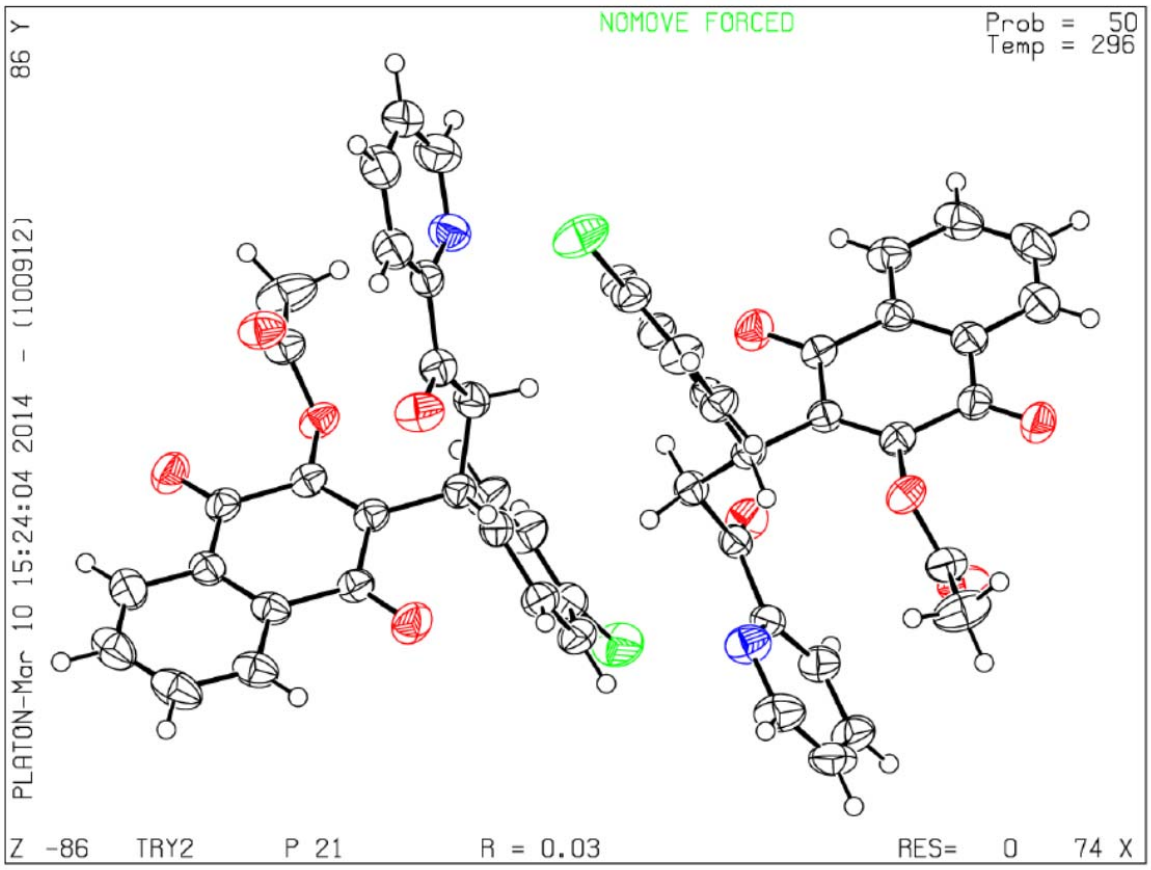
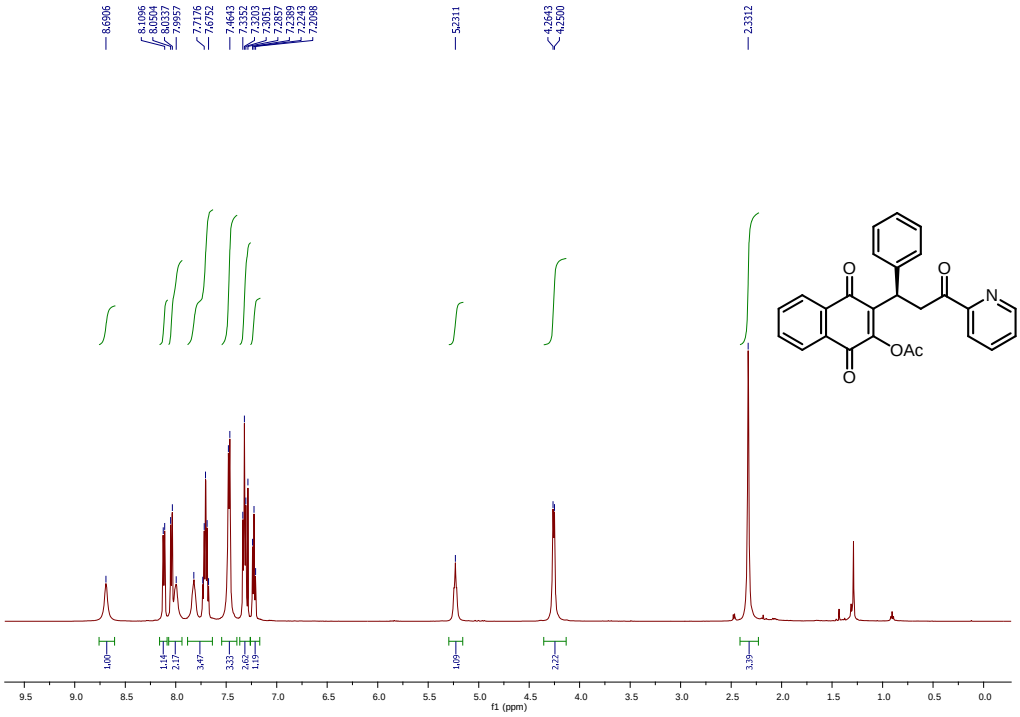


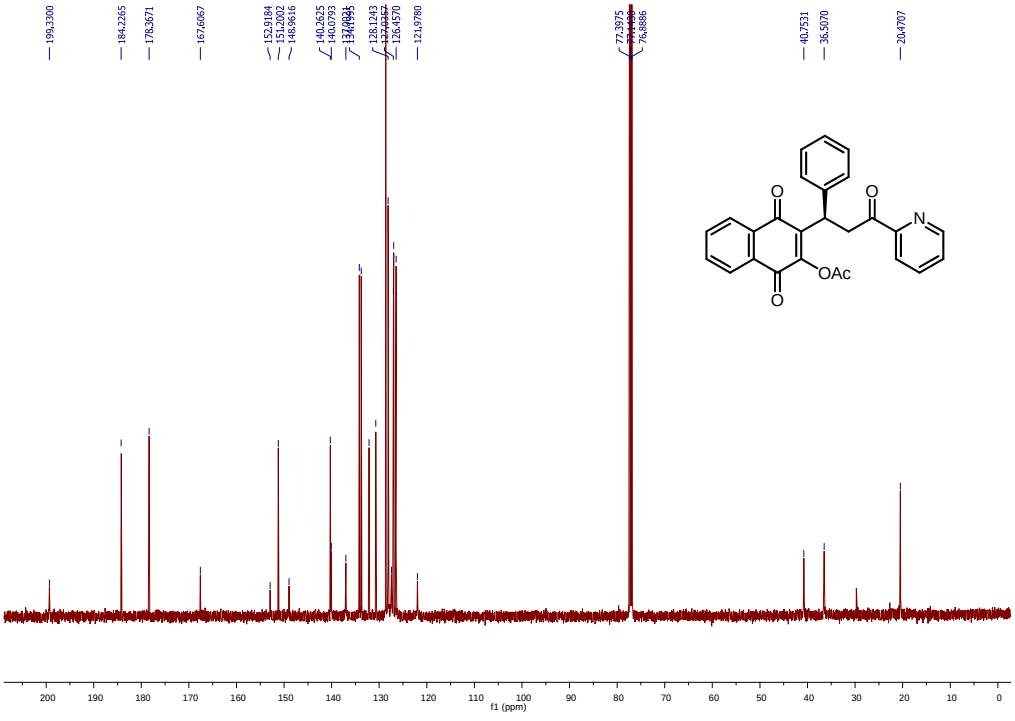
Table S1.Crystal data and structure refinement for 4d.

Empirical formula	C26 H18 Cl N O5	
Formula weight	459.86	
Temperature	296 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 8.5053 (3) Å	α= 90.000°.
	b = 18.3634 (5) Å	β= 106.636(2)°.
	c = 14.5843 (4) Å	γ = 90.000°.
Volume	2182.52 (12) $Å^3$	
Z	4	
Density (calculated)	1.400 Mg/m^3	
Absorption coefficient	0.214 mm^{-1}	

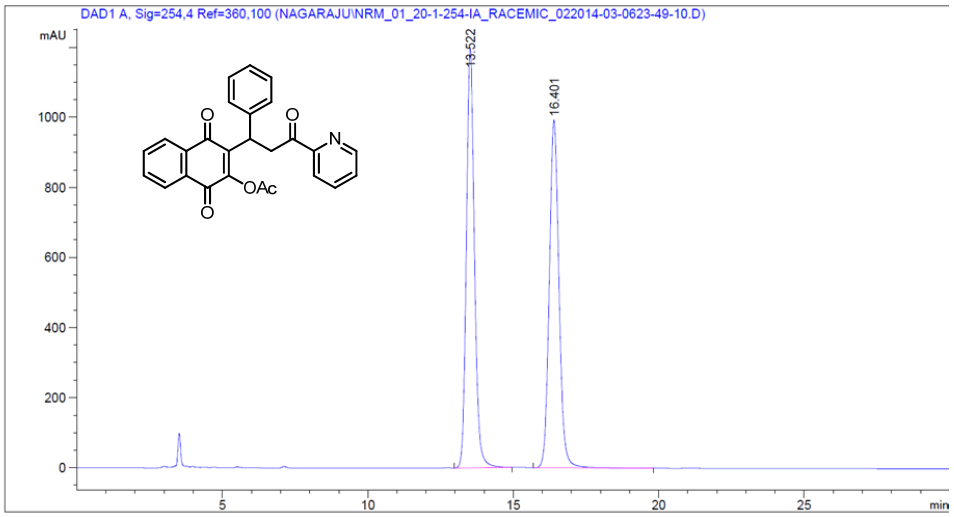
F(000)	952
Crystal size	0.0043 x 0.0032 x 0.0028 mm^3
Theta range for data collection	1.457 to 28.011°.
Index ranges	-11<=h<=11, 0<=k<=24, -19<=l<=19
Reflections collected	10341
Independent reflections	5399 [R(int) = 0.0219]
Completeness to theta = 28.011°	99.0 %
Absorption correction	Multi-scan
Data / restraints / parameters	5399 / 1 / 597
Goodness-of-fit on F^2	1.230
Final R indices [I>2sigma(I)]	R1 = 0.0438, wR2 = 0.1062
R indices (all data)	R1 = 0.0329, wR2 = 0.0939
Absolute structure parameter	0.07(6)



500 MHz ^{1}H NMR spectra of compound **4a** in $CDCl_3$

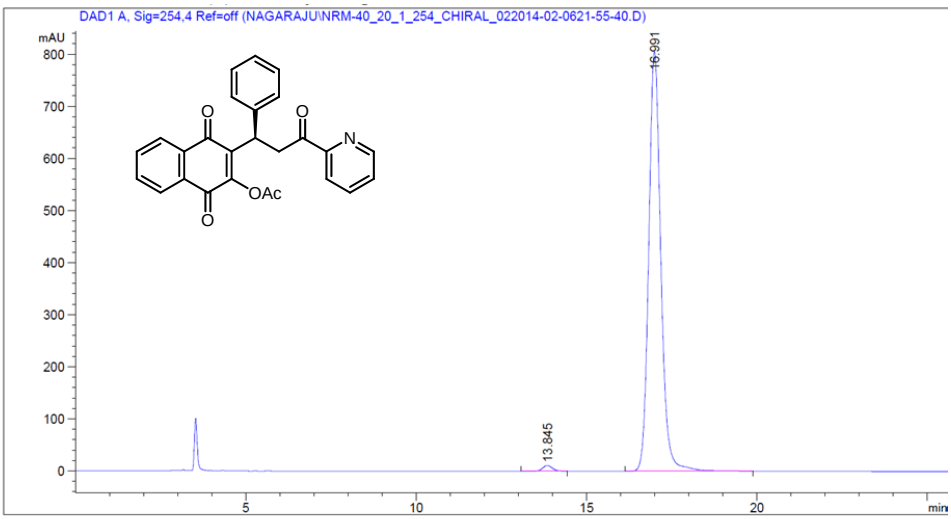


125 MHz ^{13}C NMR spectra of compound **4a** in $CDCl_3$



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.522	BB	0.2953	2.30620e4	1194.43591	50.0665
2	16.401	BB	0.3561	2.30008e4	993.36804	49.9335
Totals :				4.60627e4	2187.80396	

HPLC graph of compound **4a** (racemic)



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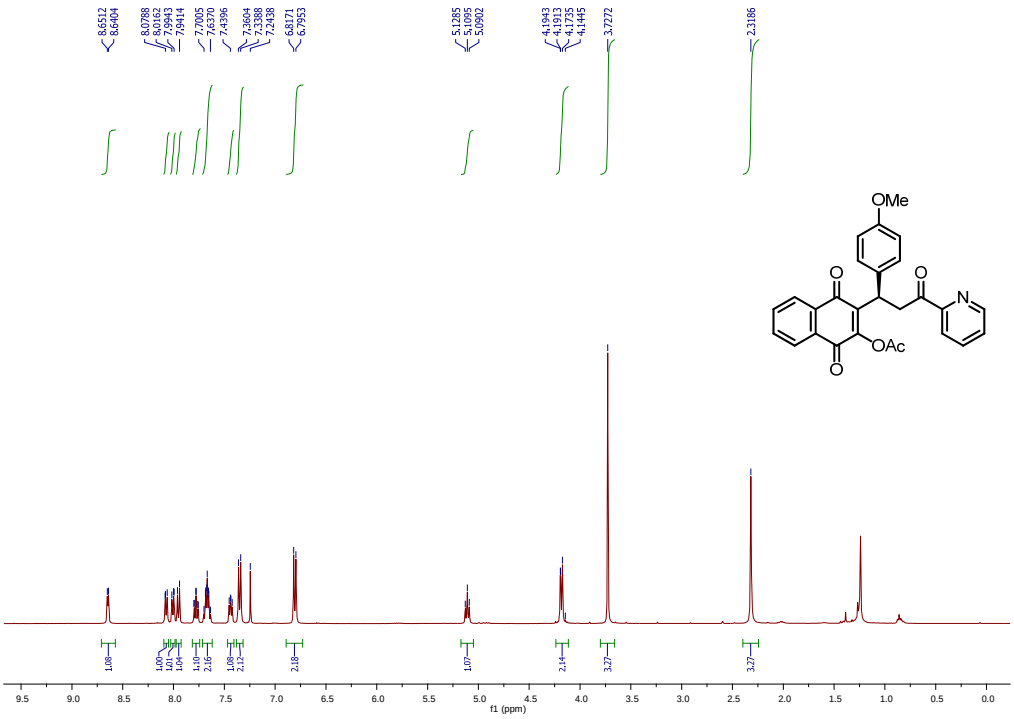
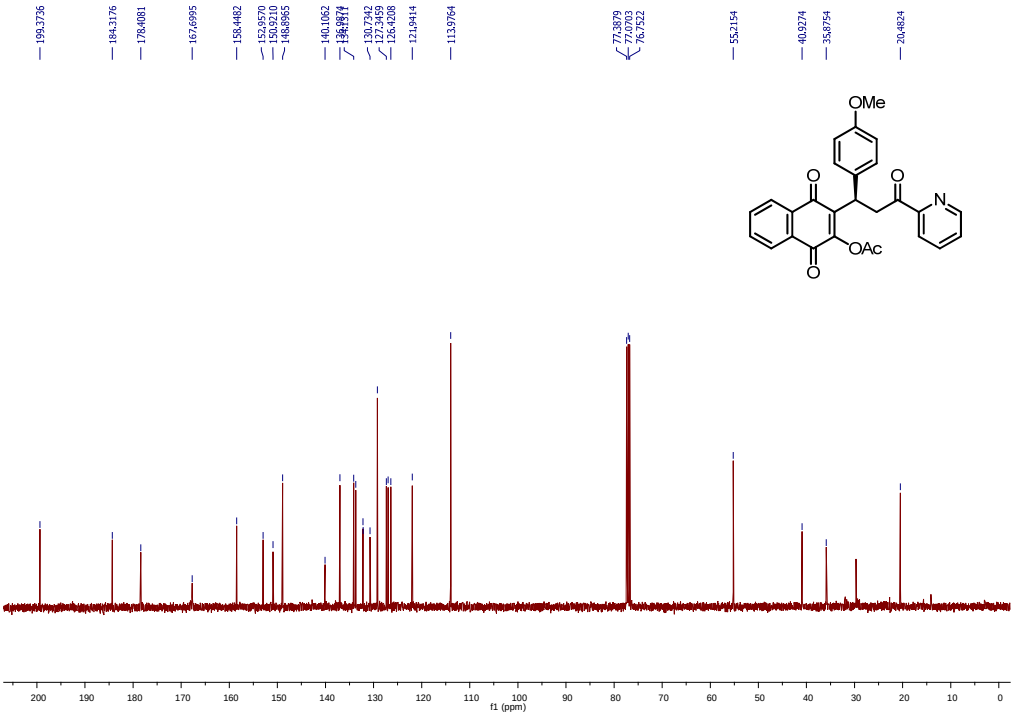
1	13.845	BB	0.3034	218.58113	11.01890	1.0857
2	16.991	BB	0.3783	1.99150e4	805.80005	98.9143
Totals :				2.01336e4	816.81895	

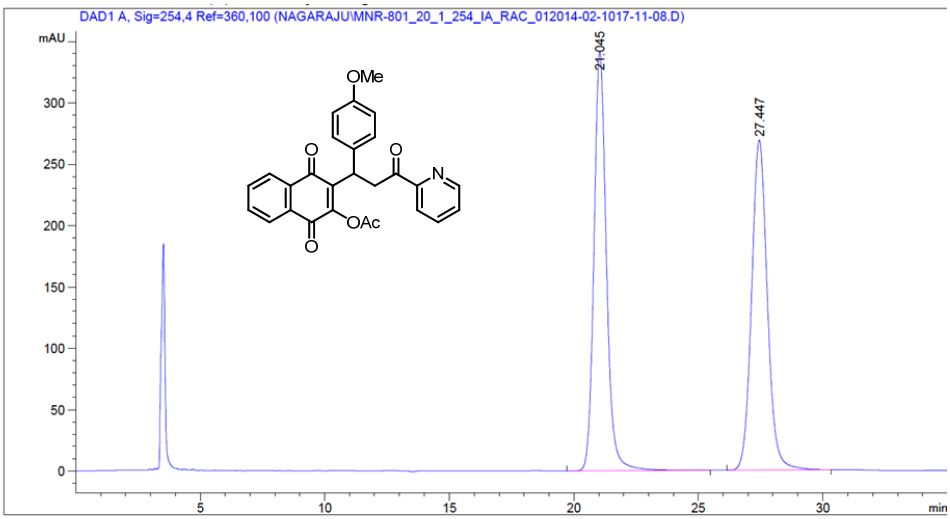
HPLC graph of compound **4a** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **4b** in $CDCl_3$

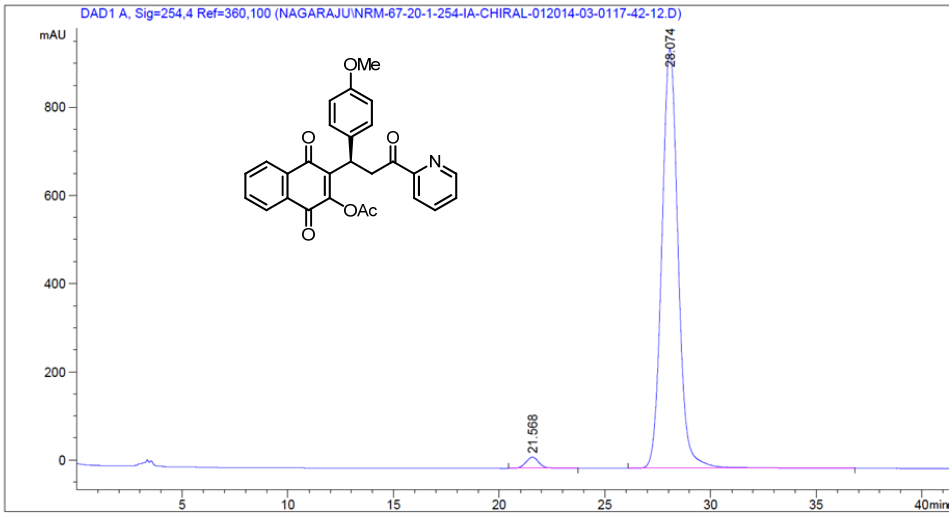


100 MHz ^{13}C NMR spectra of compound **4b** in $CDCl_3$



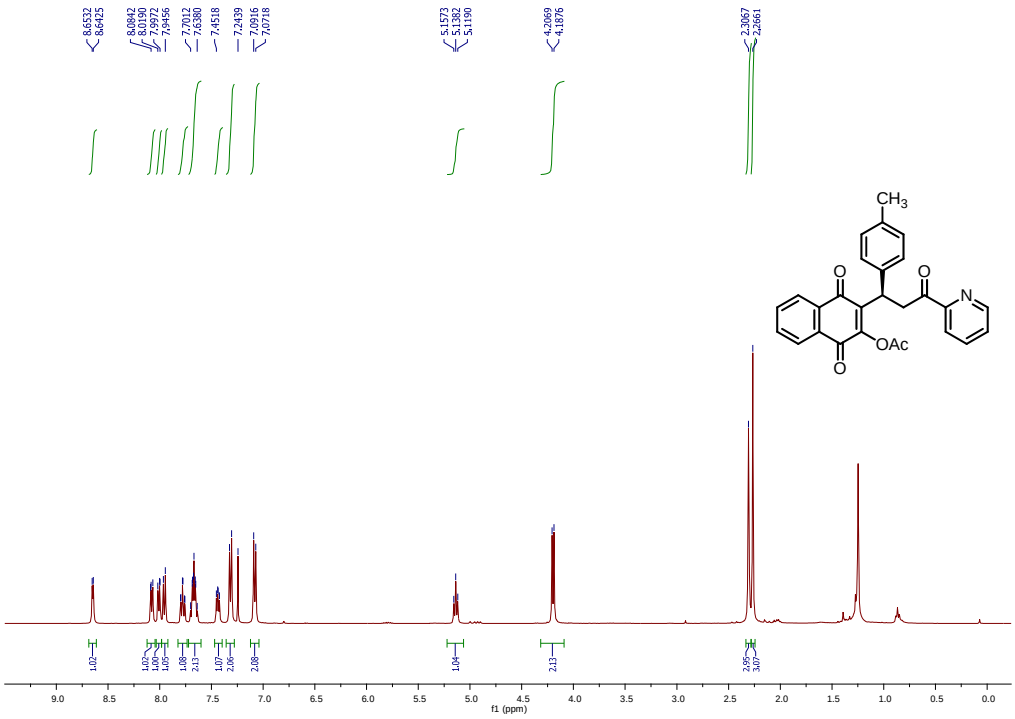
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.045	BB	0.5302	1.18810e4	341.21704	50.0814
2	27.447	BB	0.6779	1.18423e4	268.83881	49.9186
Totals :				2.37233e4	610.05585	

HPLC graph of compound **4b** (racemic)

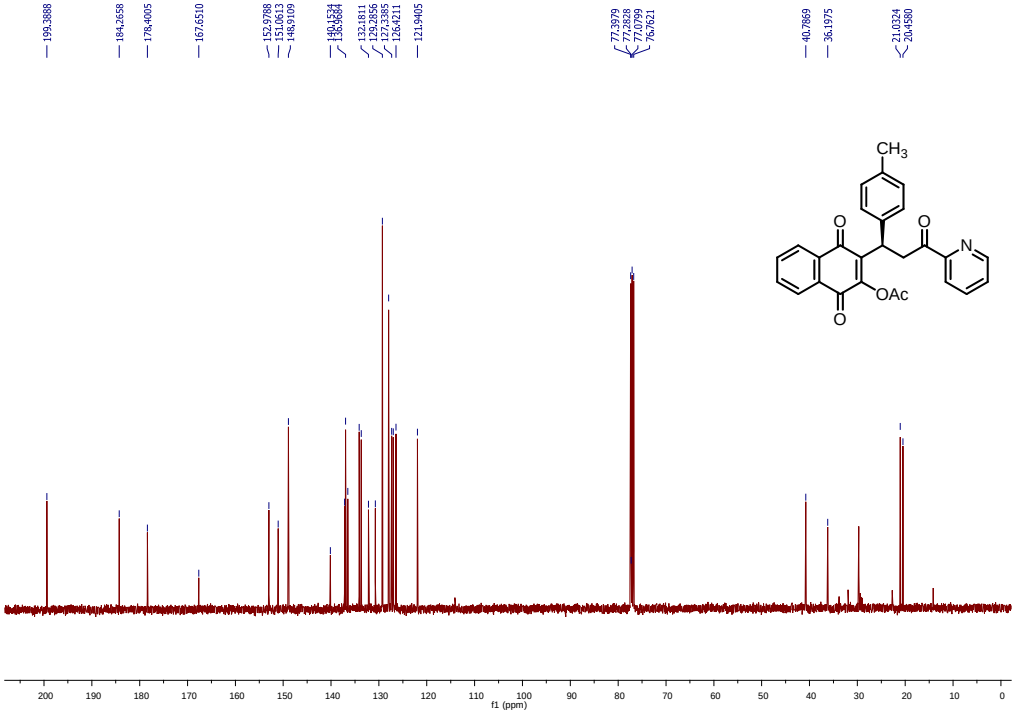


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.568	BB	0.6596	1078.84045	25.19127	2.0769
2	28.074	BB	0.8262	5.08647e4	950.75537	97.9231
Totals :				5.19435e4	975.94665	

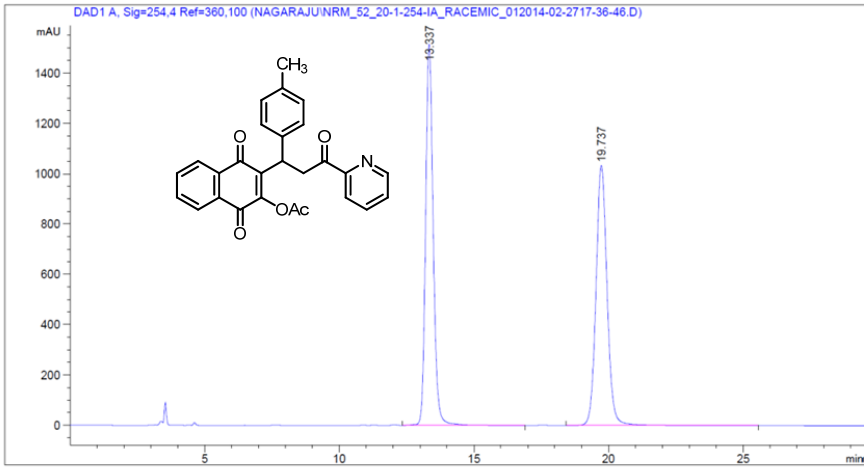
HPLC graph of compound **4b** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **4c** in $CDCl_3$

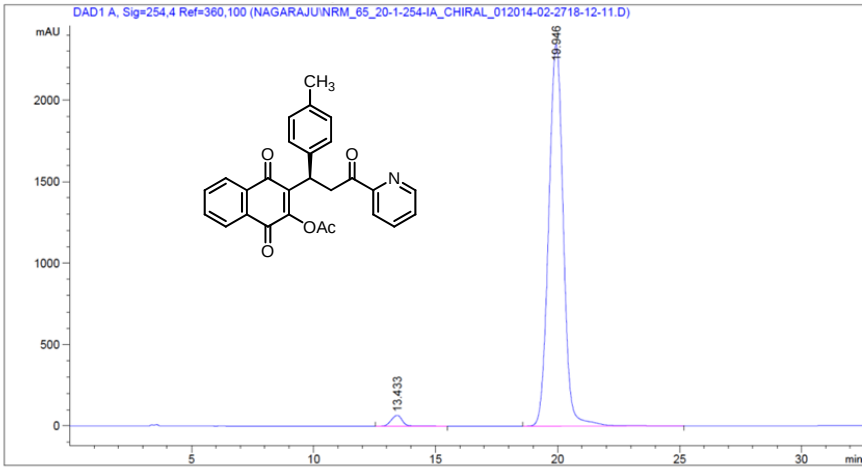


100 MHz ^{13}C NMR spectra of compound **4c** in $CDCl_3$



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.337	BB	0.2972	2.95101e4	1515.30151	49.7667
2	19.737	BB	0.4420	2.97868e4	1034.18274	50.2333
Totals :				5.92969e4	2549.48425	

HPLC graph of compound **4c** (racemic)



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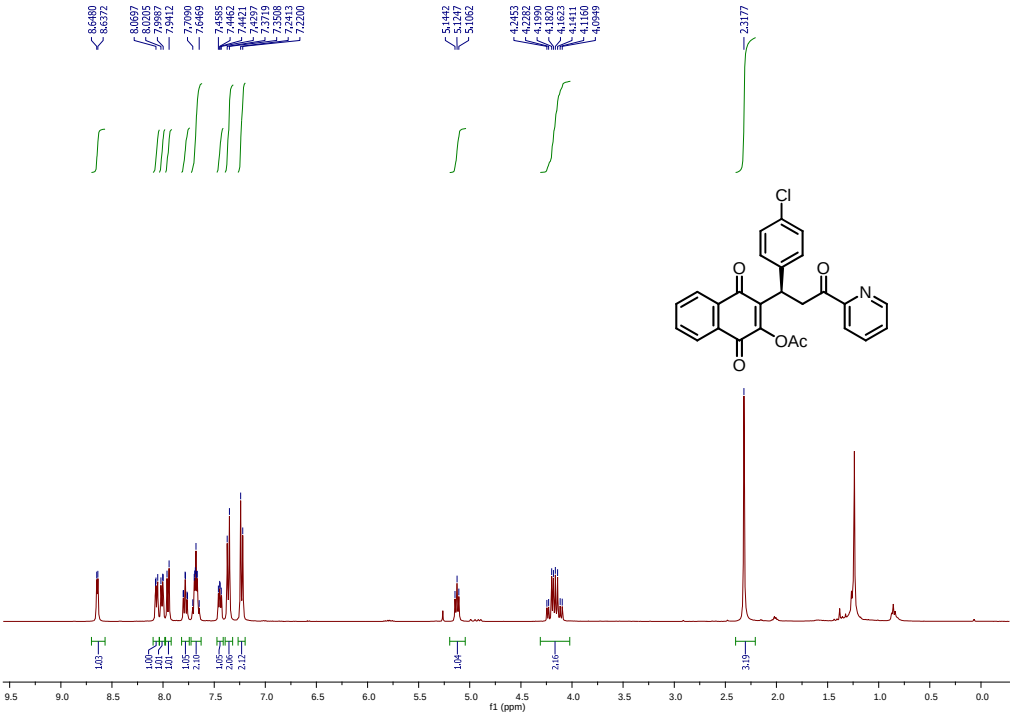
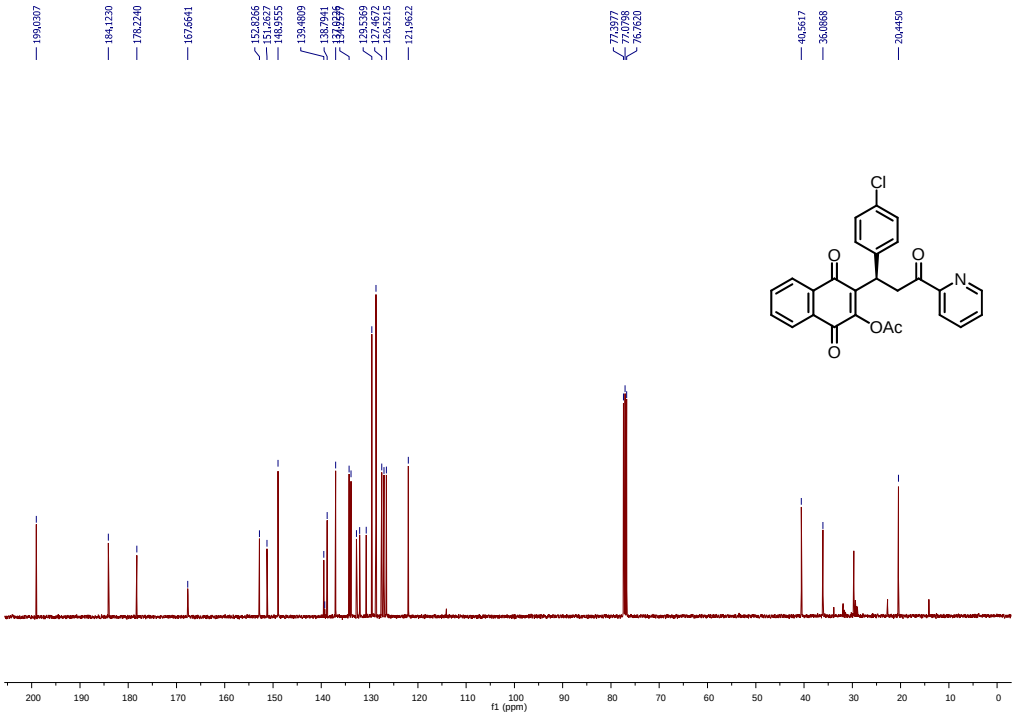
1	13.433	BB	0.4982	2080.84058	66.66316	2.0903
2	19.946	BB	0.6477	9.74659e4	2341.39355	97.9097
Totals :				9.95468e4	2408.05672	

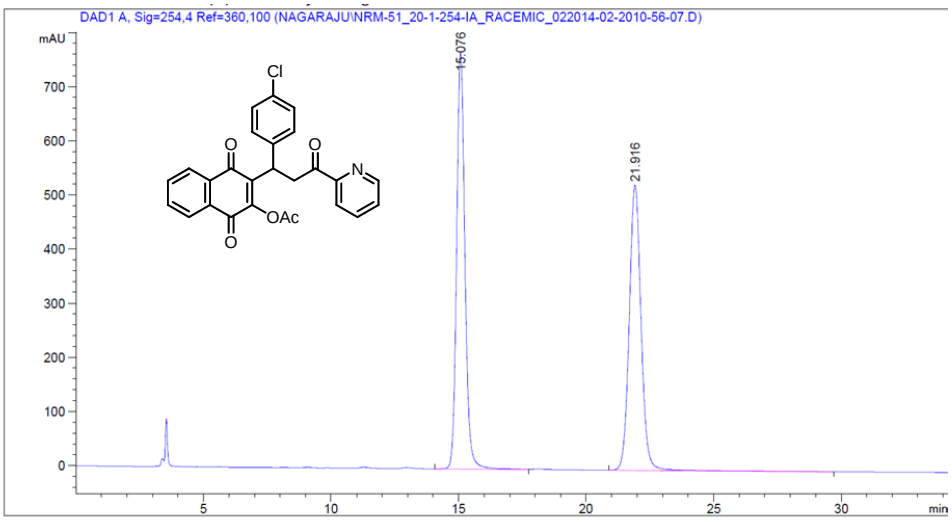
HPLC graph of compound **4c** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **4d** in $CDCl_3$

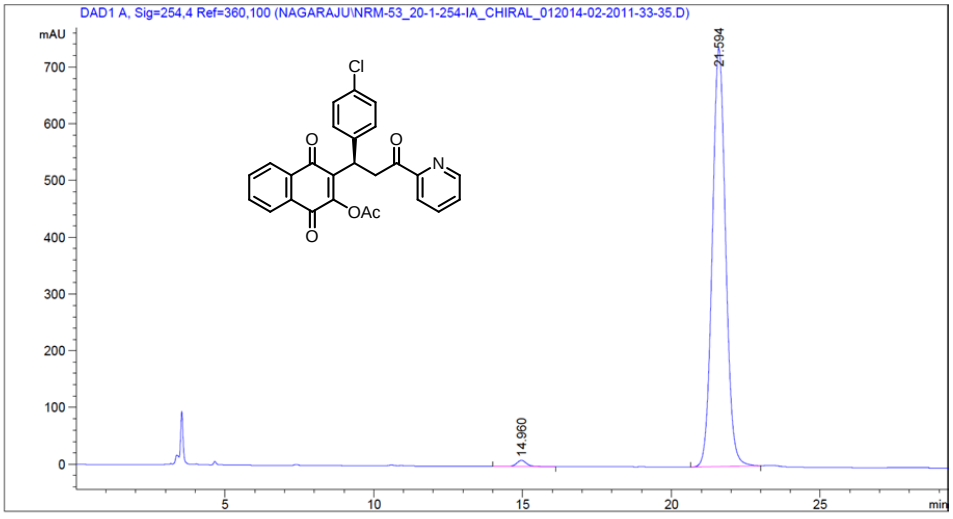


100 MHz ^{13}C NMR spectra of compound **4d** in $CDCl_3$



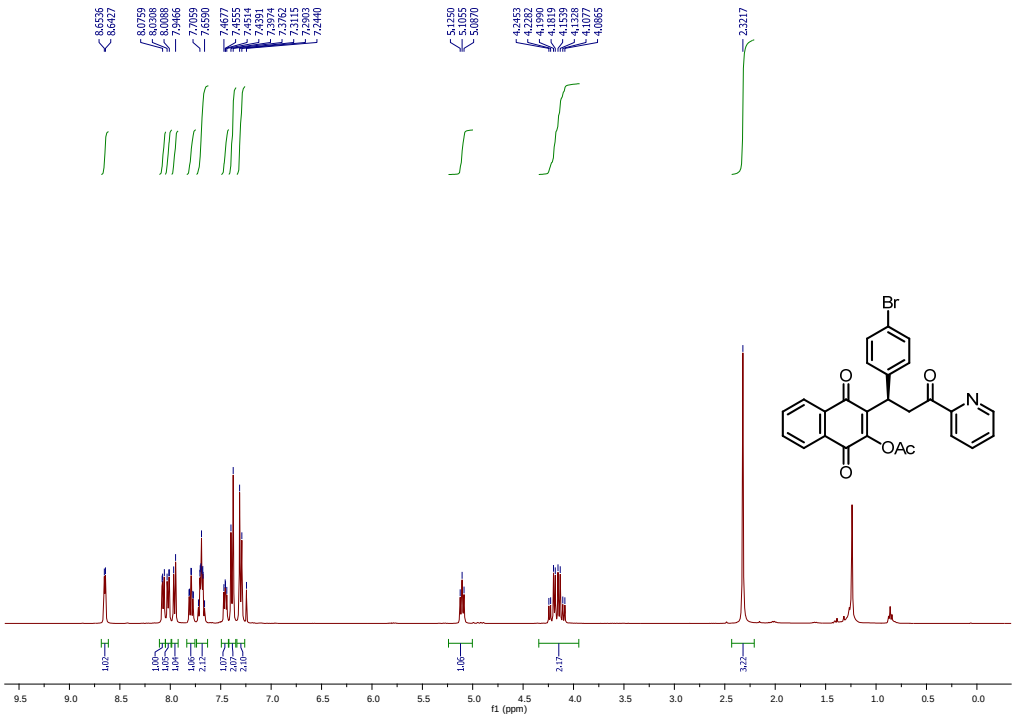
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.076	BB	0.3448	1.73320e4	769.52887	50.5189
2	21.916	BB	0.4959	1.69760e4	526.91565	49.4811
Totals :				3.43080e4	1296.44452	

HPLC graph of compound **4d** (racemic)

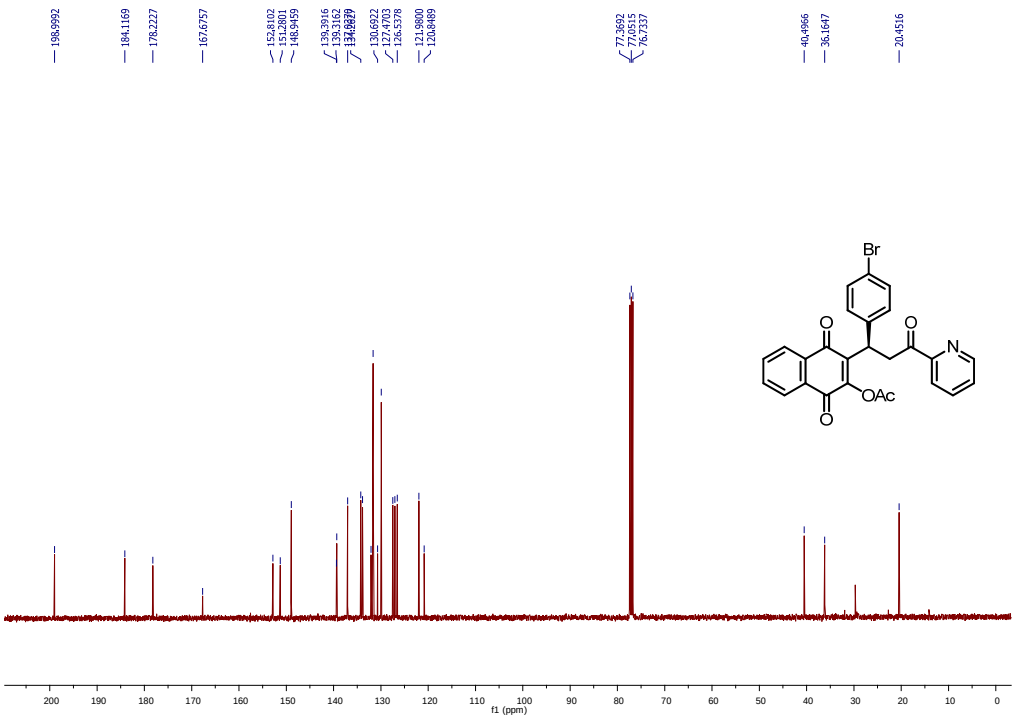


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.960	BB	0.3508	250.65576	10.87778	1.0817
2	21.594	BB	0.4808	2.29215e4	737.09180	98.9183
Totals :				2.31722e4	747.96958	

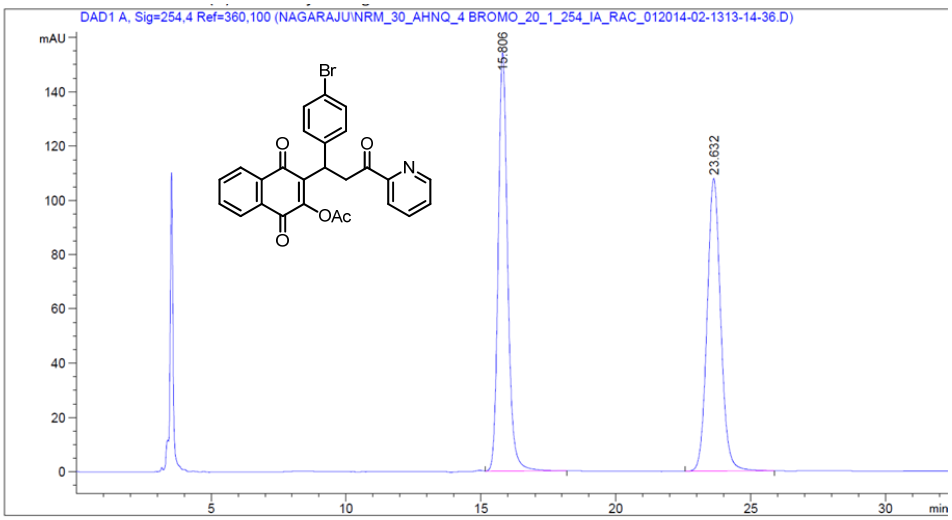
HPLC graph of compound **4d** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **4e** in $CDCl_3$

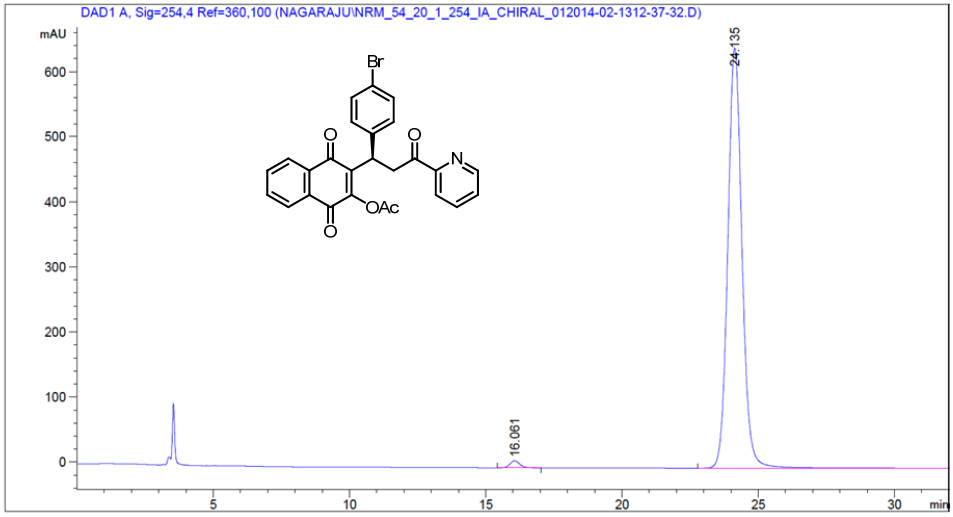


100 MHz ^{13}C NMR spectra of compound **4e** in $CDCl_3$



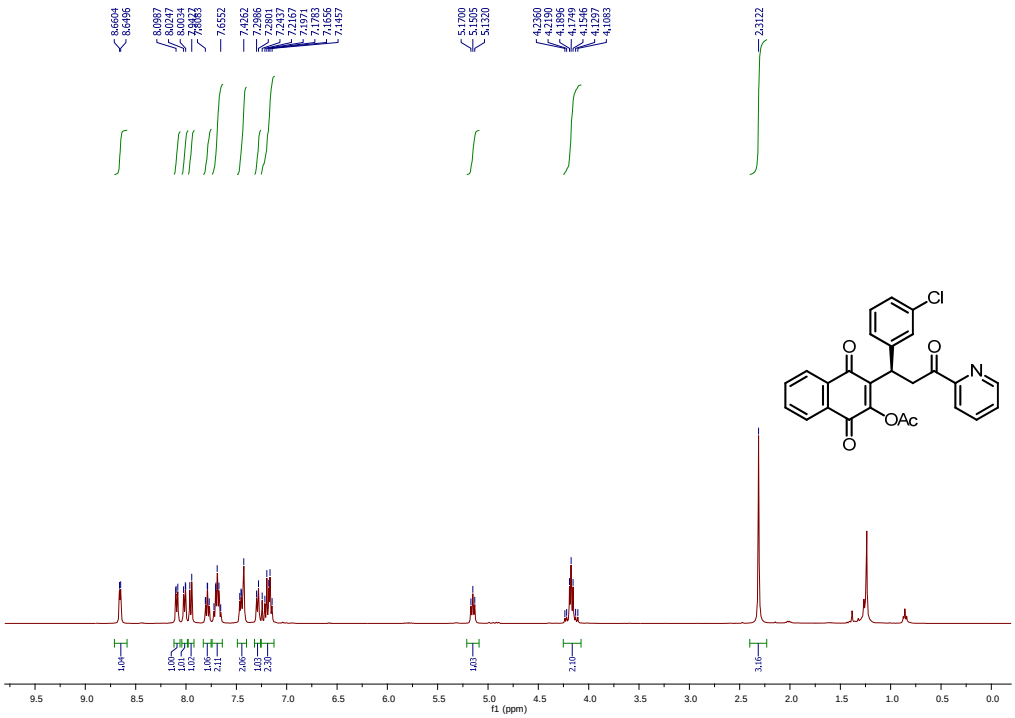
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.806	BB	0.3725	3758.61646	154.15044	49.9052
2	23.632	BB	0.5383	3772.89600	107.80363	50.0948
Totals :				7531.51245	261.95406	

HPLC graph of compound **4e** (racemic)

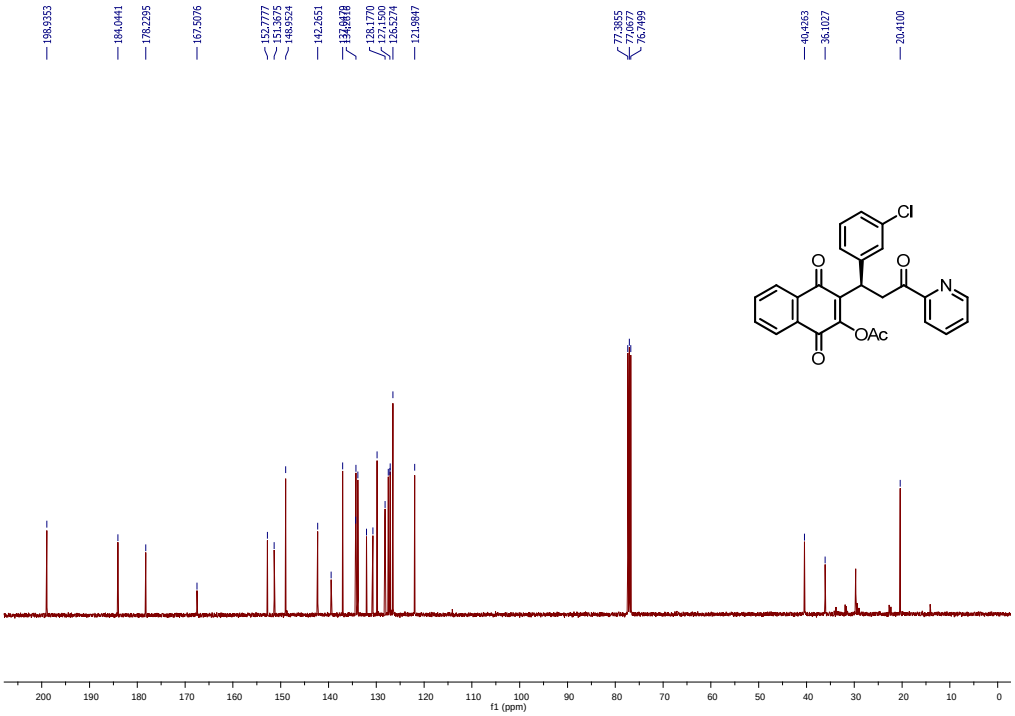


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.061	BB	0.3772	265.67657	10.79063	1.1227
2	24.135	BBA	0.5569	2.33978e4	645.53967	98.8773
Totals :				2.36634e4	656.33031	

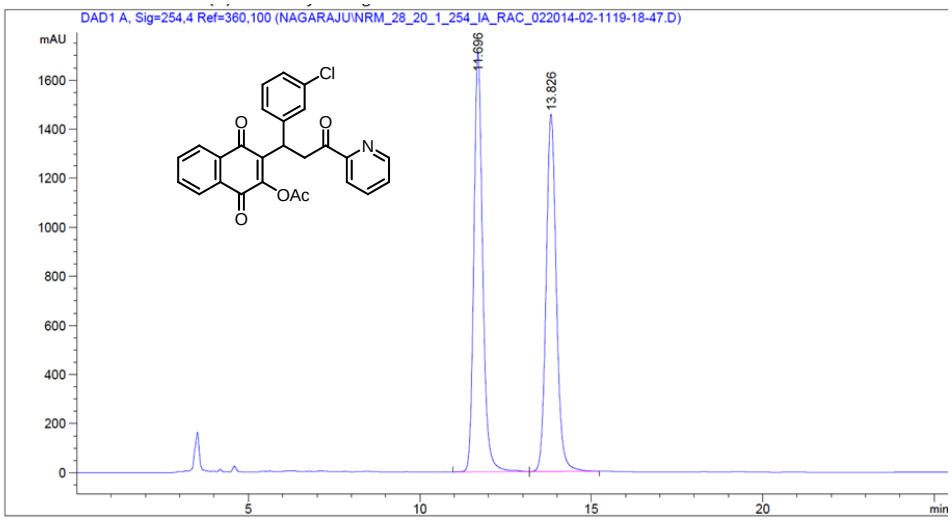
HPLC graph of compound **4e** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **4f** in $CDCl_3$

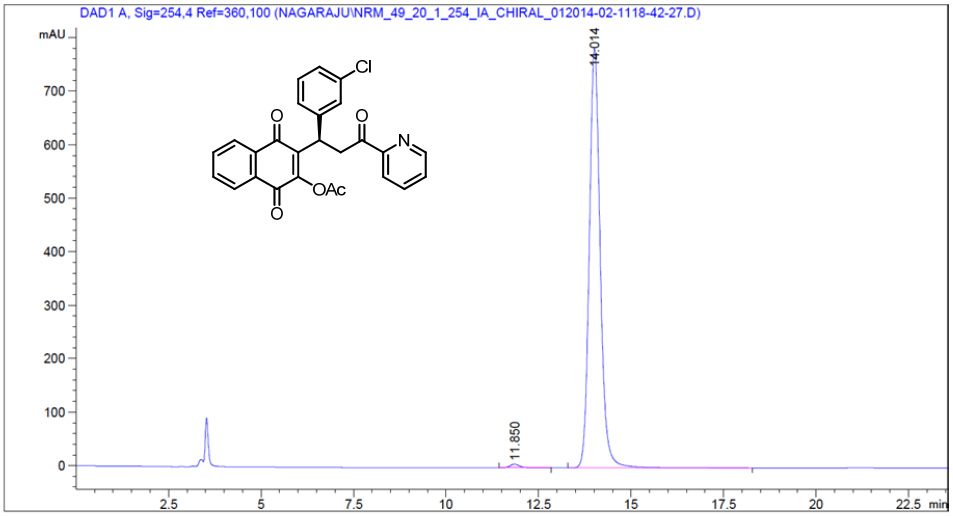


100 MHz ^{13}C NMR spectra of compound **4f** in $CDCl_3$



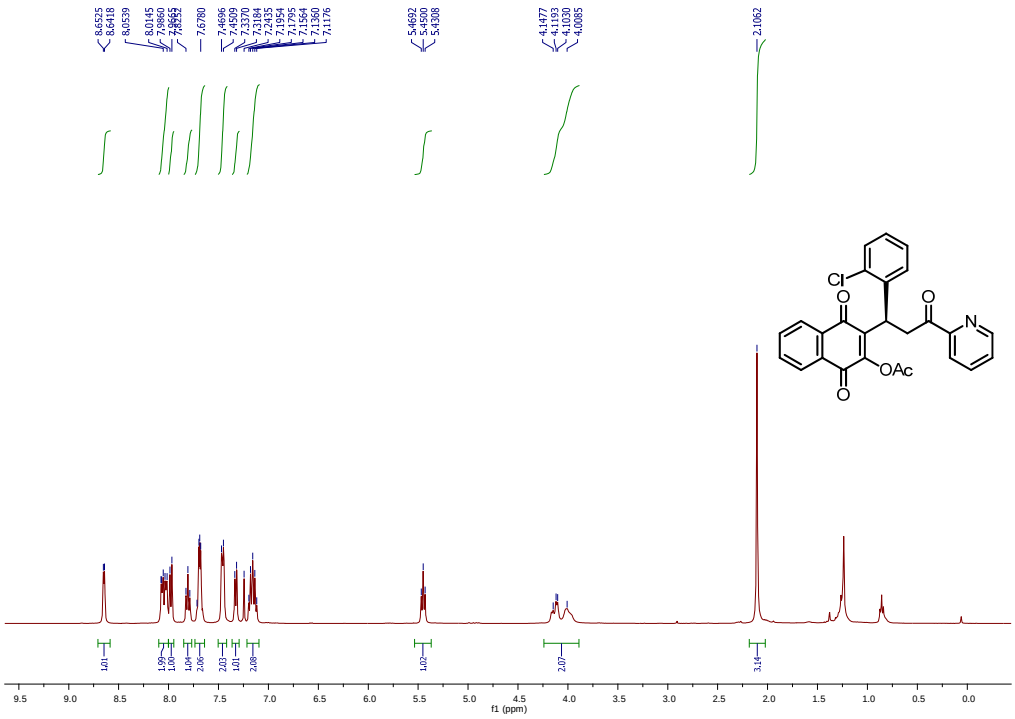
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.696	VB	0.2756	3.06576e4	1706.76807	50.4259
2	13.826	BB	0.3173	3.01397e4	1456.93420	49.5741
Totals :				6.07972e4	3163.70227	

HPLC graph of compound **4f** (racemic)

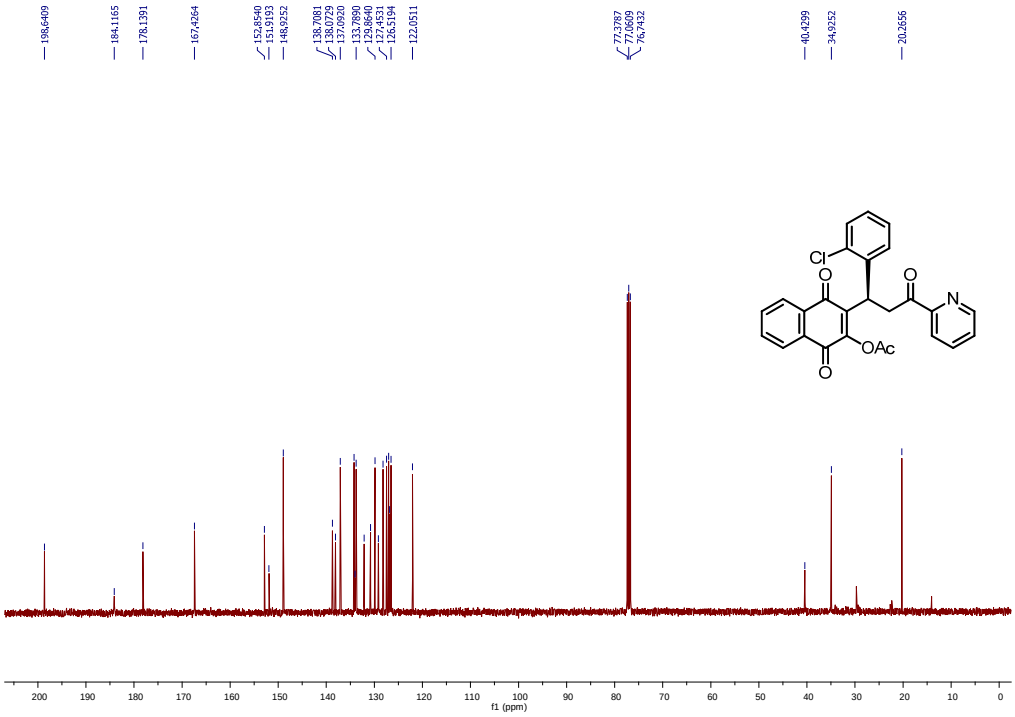


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.850	BB	0.2741	119.51410	6.63739	0.7371
2	14.014	BB	0.3154	1.60939e4	784.40973	99.2629
Totals :				1.62134e4	791.04711	

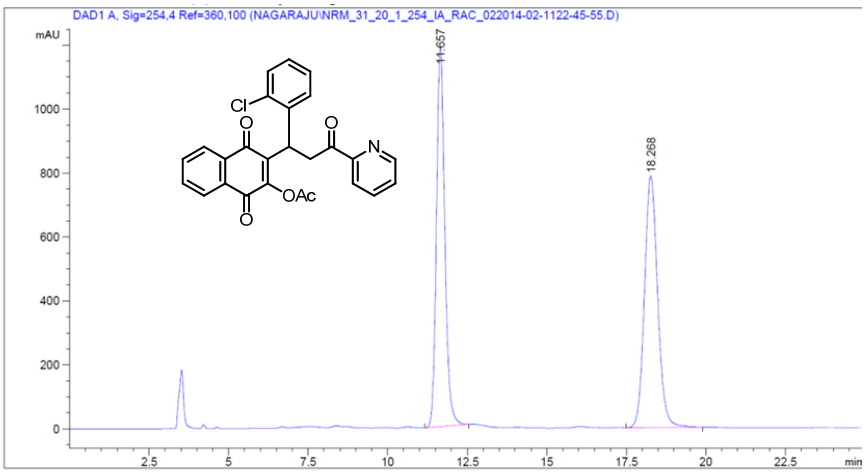
HPLC graph of compound **4f** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **4g** in $CDCl_3$

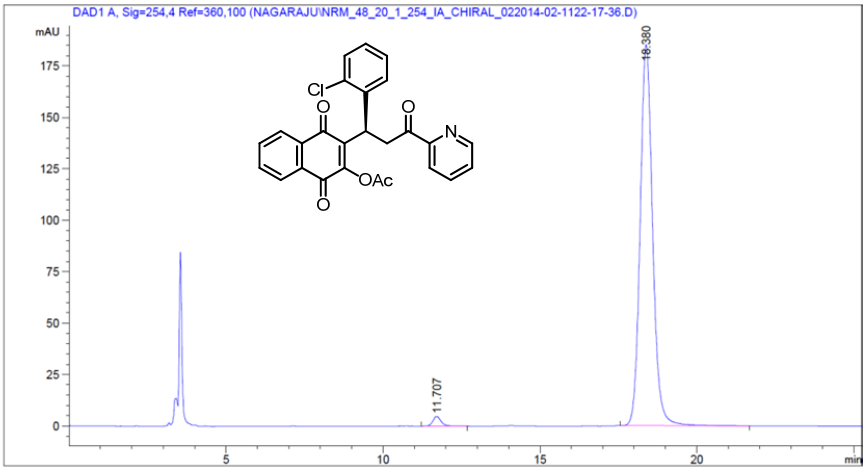


100 MHz ^{13}C NMR spectra of compound **4g** in $CDCl_3$



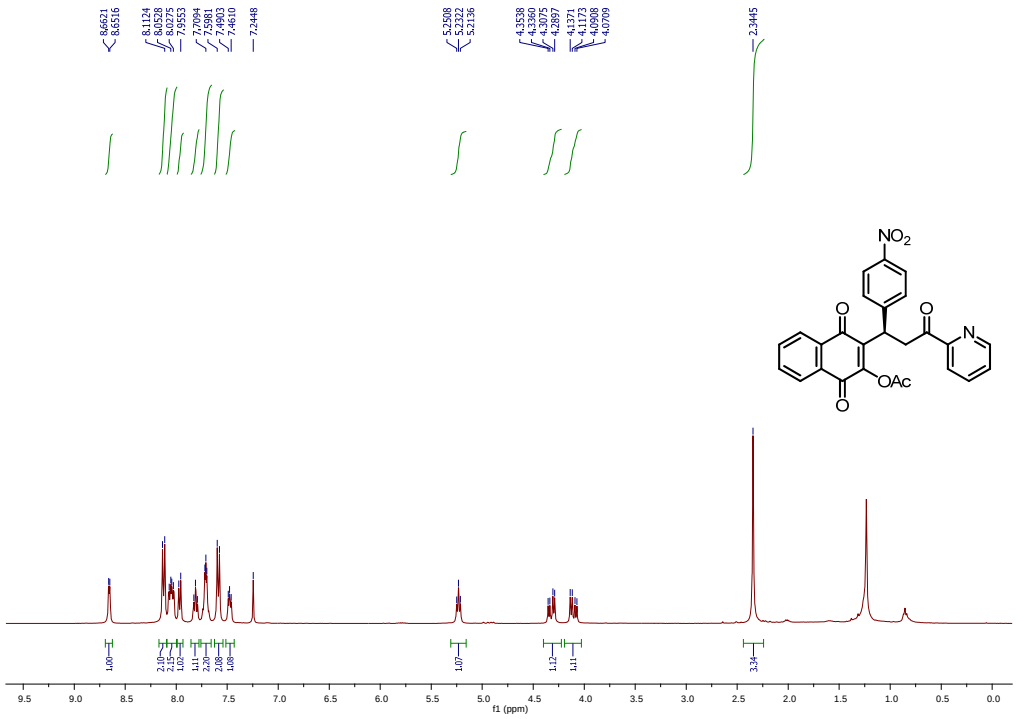
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.657	BB	0.2813	2.16805e4	1186.05835	48.9270
2	18.268	BB	0.4436	2.26315e4	786.79675	51.0730
Totals :				4.43120e4	1972.85510	

HPLC graph of compound **4g** (racemic)

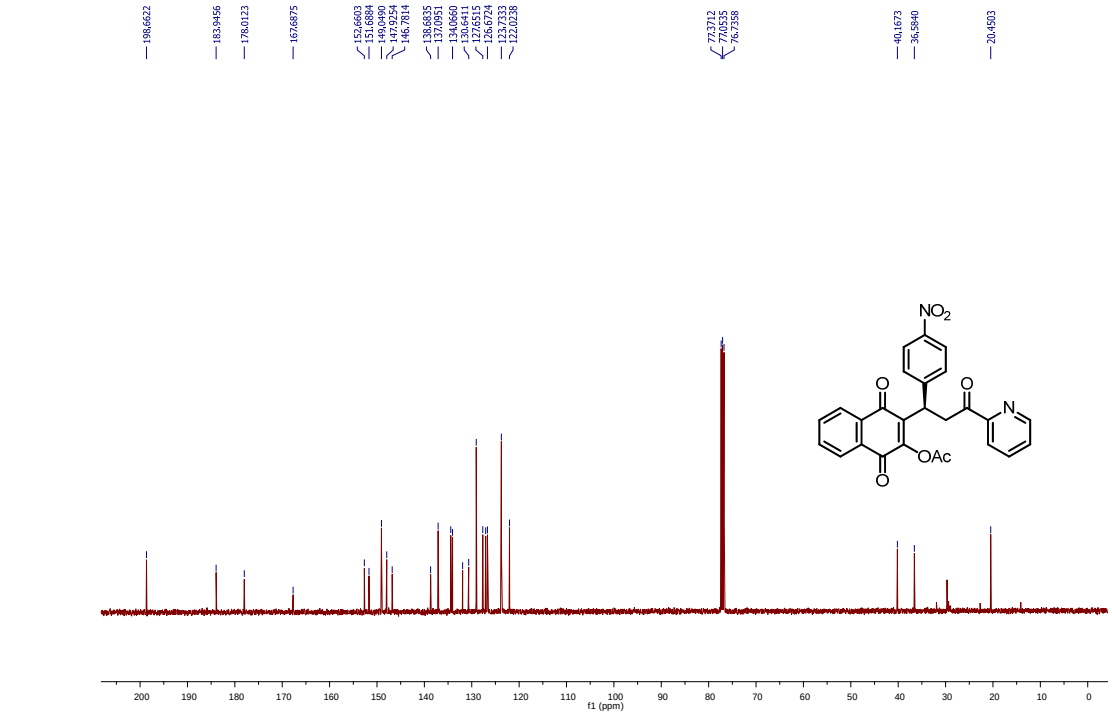


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.707	BB	0.2758	86.02570	4.73875	1.6570
2	18.380	BB	0.4216	5105.67480	185.23135	98.3430
Totals :				5191.70050	189.97010	

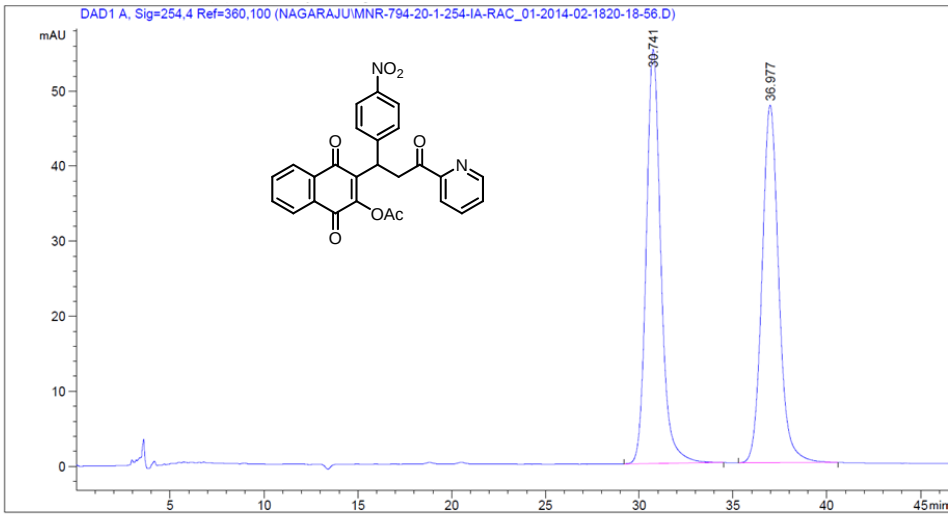
HPLC graph of compound **4g** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **4h** in $CDCl_3$

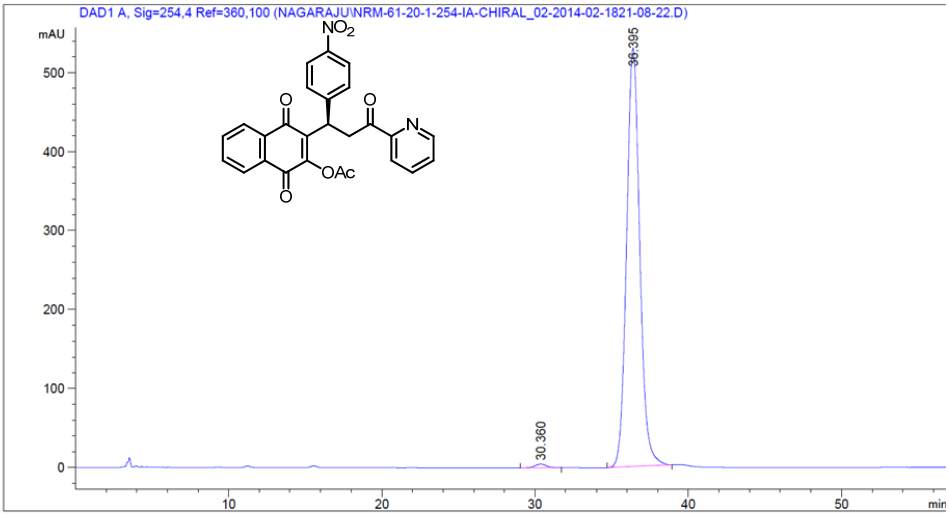


400 MHz ^{13}C NMR spectra of compound **4h** in $CDCl_3$



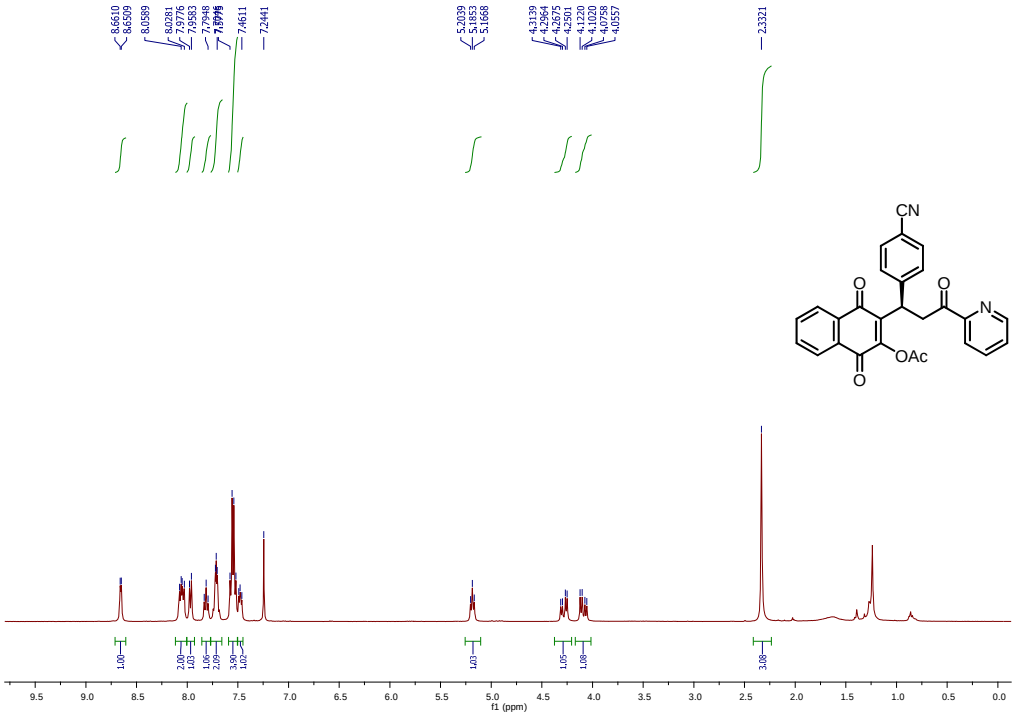
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.741	BB	0.8253	2986.93750	55.19859	50.3022
2	36.977	BB	0.9481	2951.05029	47.67592	49.6978
Totals :				5937.98779	102.87450	

HPLC graph of compound **4h** (racemic)

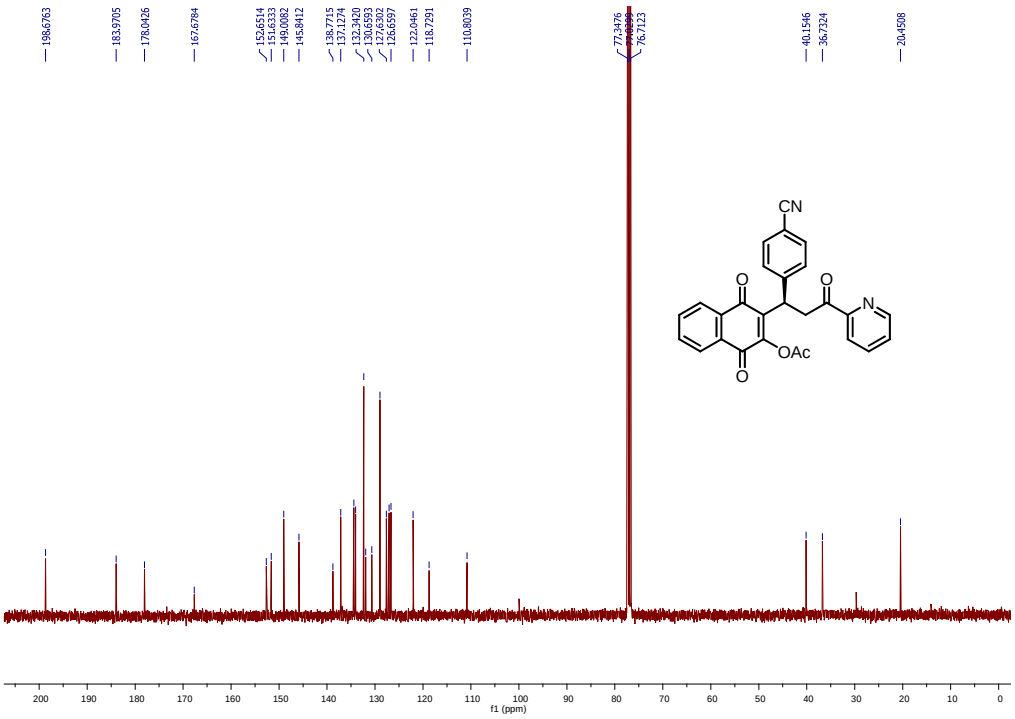


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.360	BB	0.7735	234.26370	4.60493	0.7351
2	36.395	BB	0.9188	3.16332e4	529.62671	99.2649
Totals :				3.18674e4	534.23164	

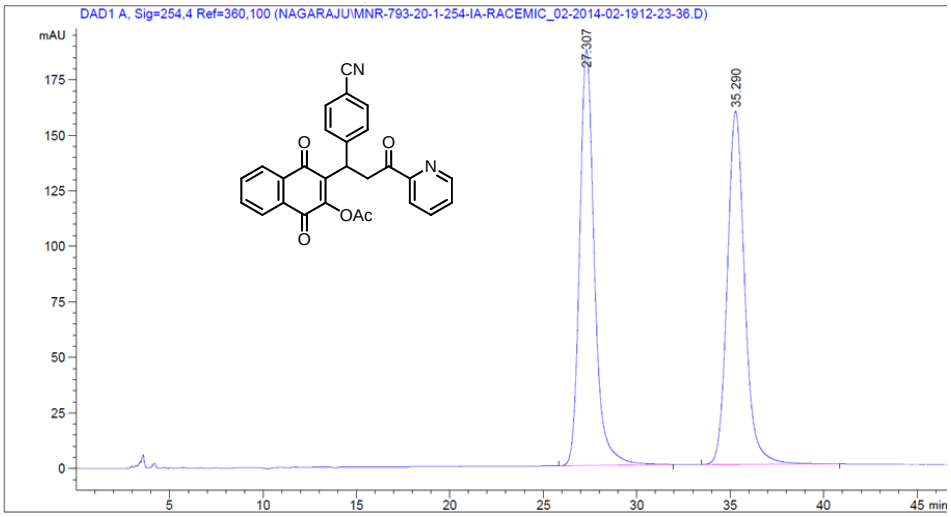
HPLC graph of compound **4h** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **4i** in $CDCl_3$

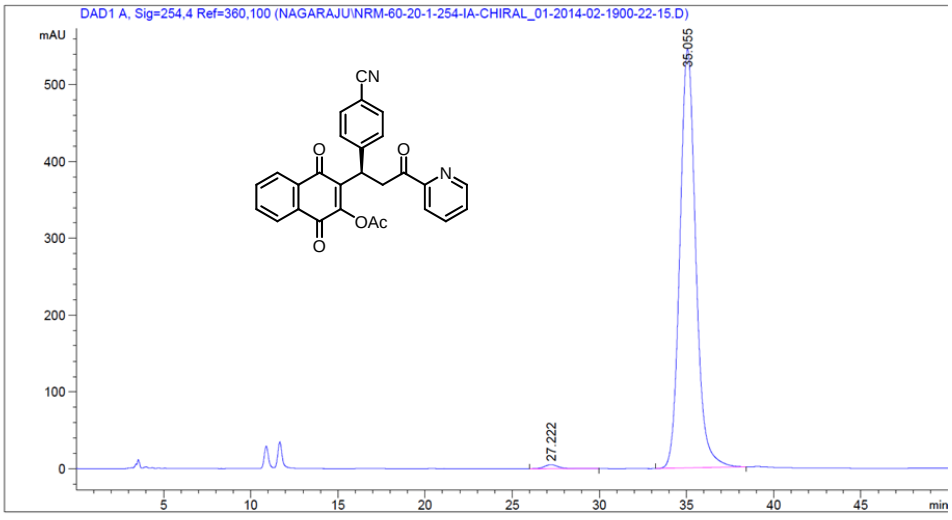


100 MHz ^{13}C NMR spectra of compound **4i** in $CDCl_3$



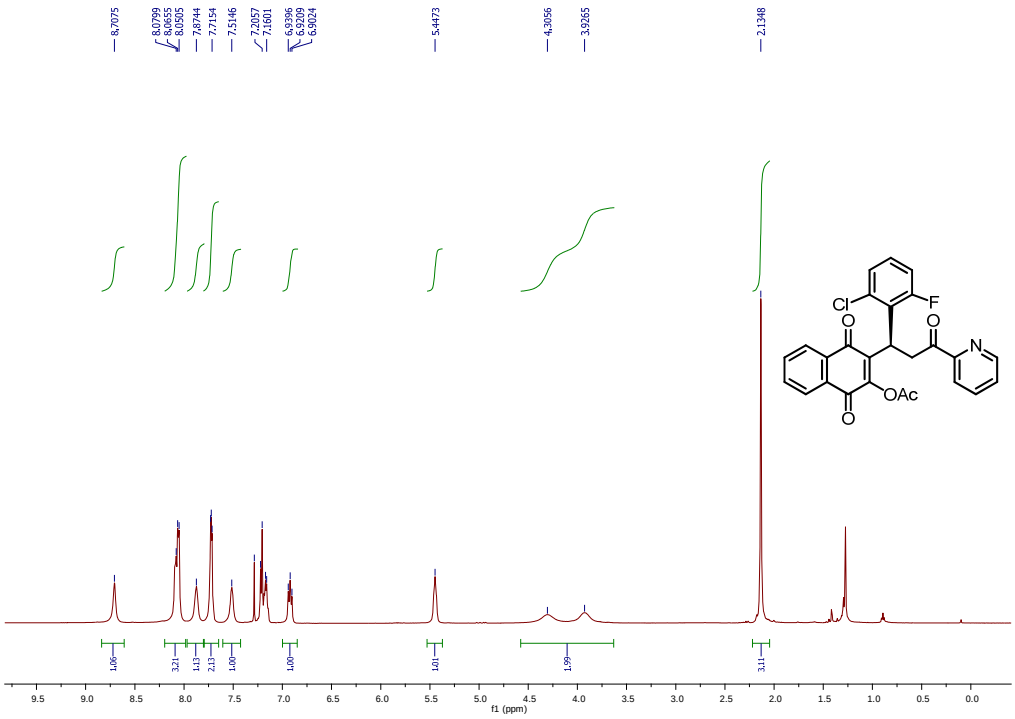
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.307	BB	0.8315	1.02743e4	187.43593	49.9178
2	35.290	BB	0.9900	1.03081e4	159.08565	50.0822
Totals :				2.05824e4	346.52158	

HPLC graph of compound **4i** (racemic)

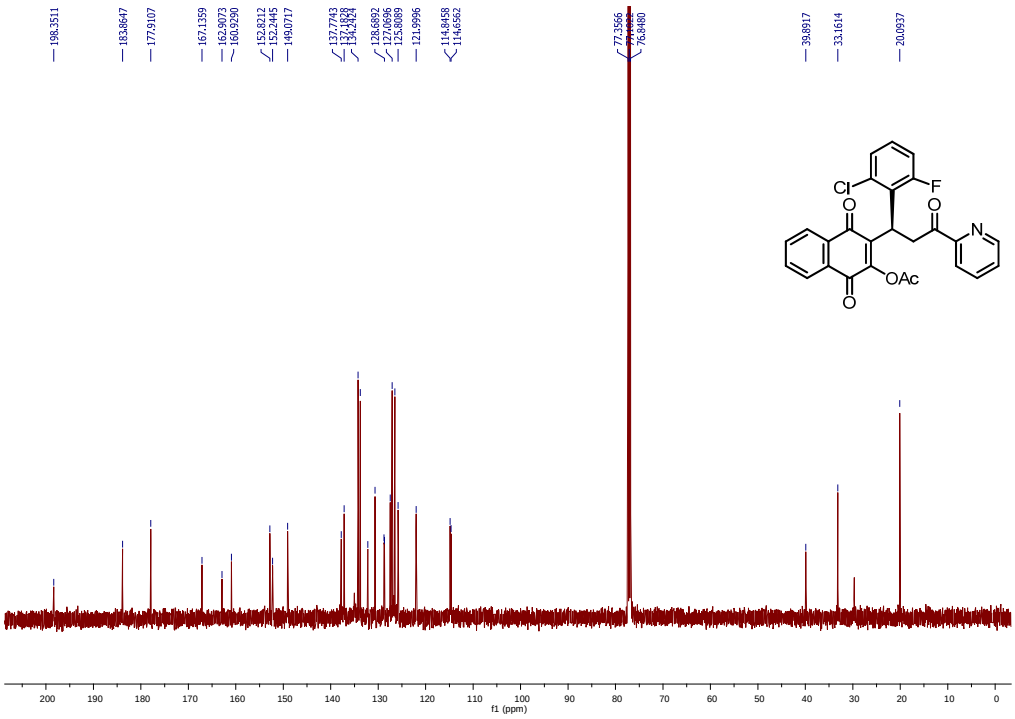


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.222	BB	0.8236	282.18890	5.09926	0.8106
2	35.055	BB	0.9724	3.45317e4	545.60199	99.1894
Totals :				3.48139e4	550.70125	

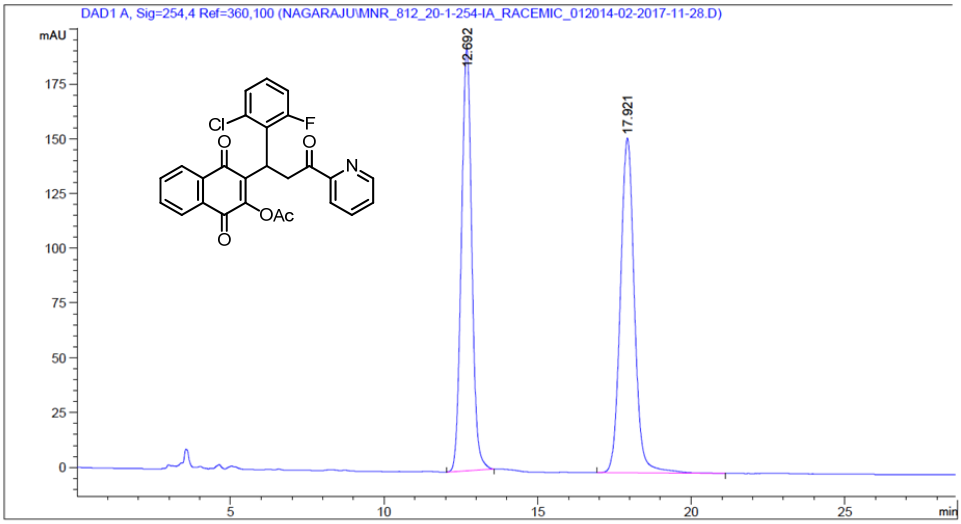
HPLC graph of compound **4i** (enantioenriched)



500 MHz ^{1}H NMR spectra of compound **4j** in $CDCl_3$

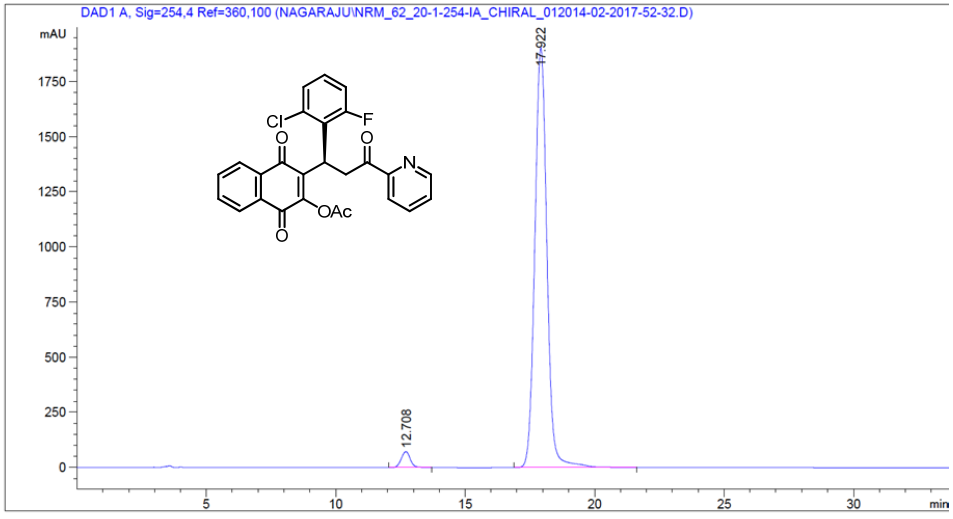


125 MHz ^{13}C NMR spectra of compound **4j** in $CDCl_3$



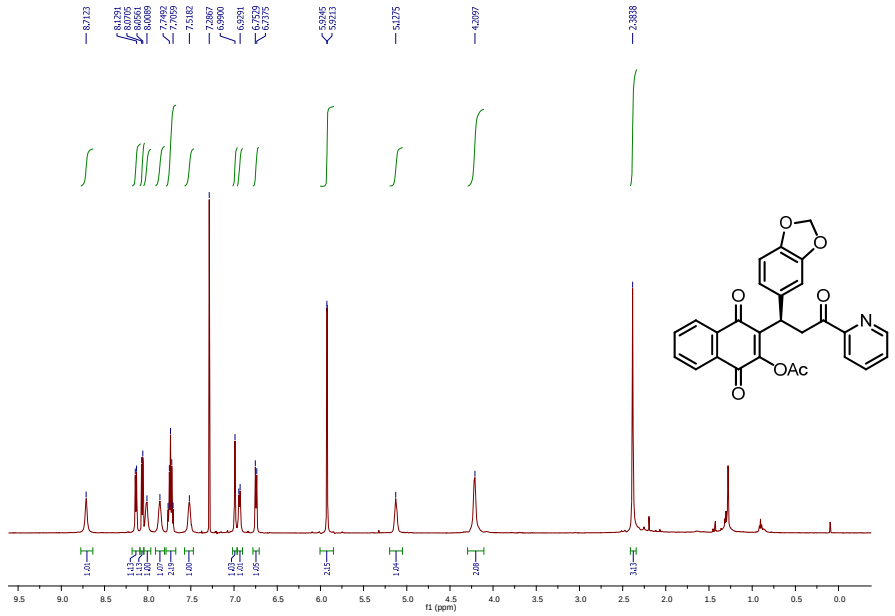
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.692	BB	0.3672	4540.83203	192.48878	48.3626
2	17.921	BB	0.4904	4848.30713	152.71901	51.6374
Totals :				9389.13916	345.20779	

HPLC graph of compound **4j** (racemic)

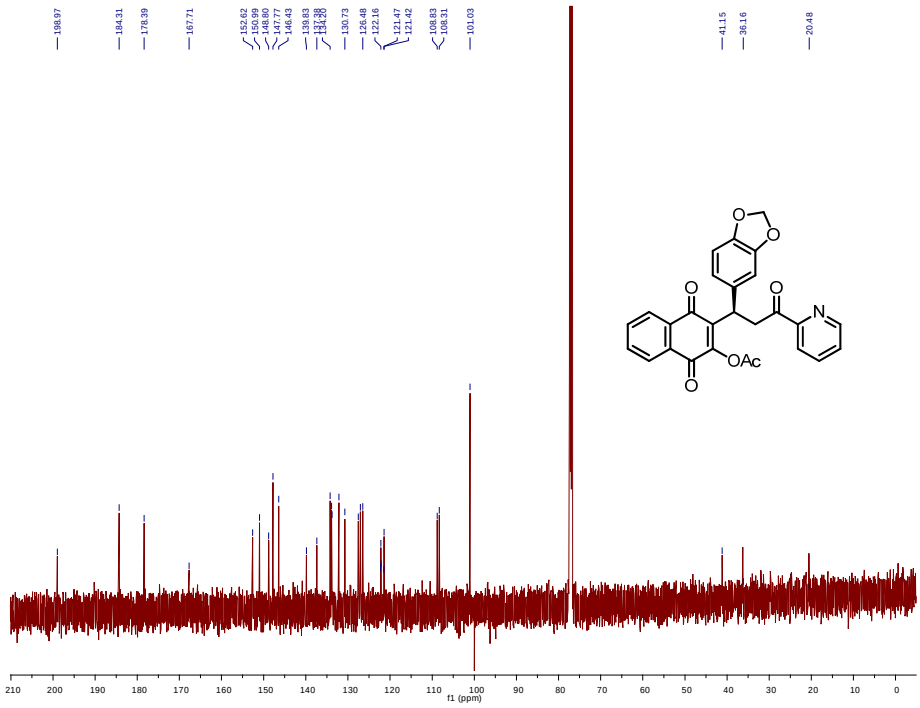


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.708	BB	0.3784	1755.79968	72.53642	2.7569
2	17.922	BB	0.5057	6.19319e4	1903.01941	97.2431
Totals :				6.36877e4	1975.55582	

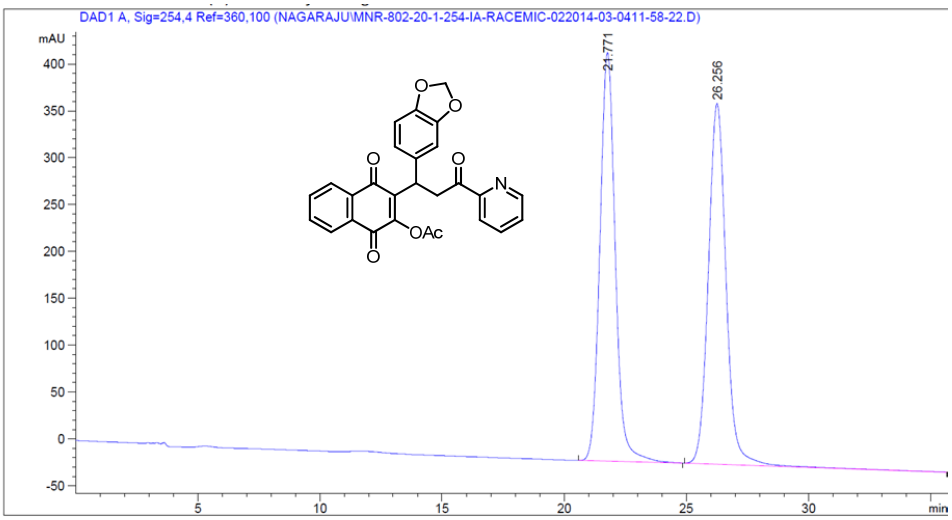
HPLC graph of compound **4j** (enantioenriched)



500 MHz ^{1}H NMR spectra of compound **4k** in $CDCl_3$

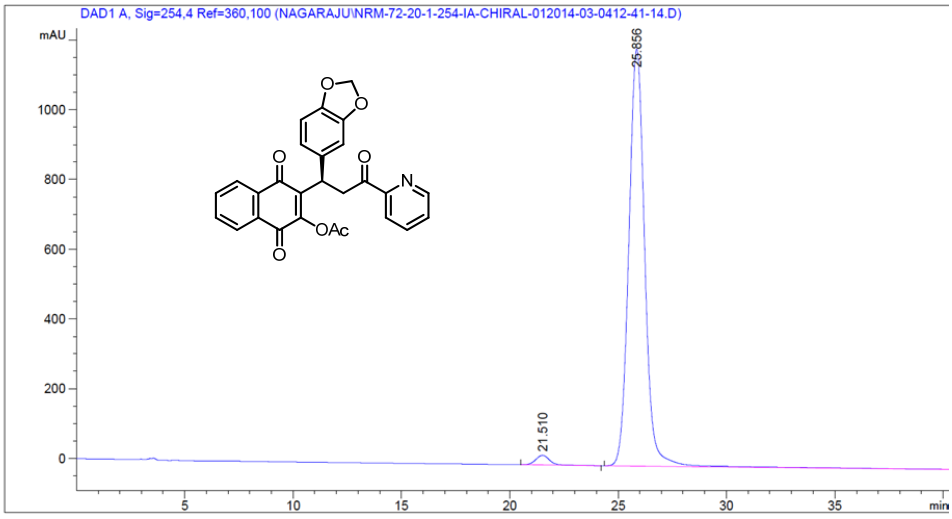


125 MHz ^{13}C NMR spectra of compound **4k** in $CDCl_3$



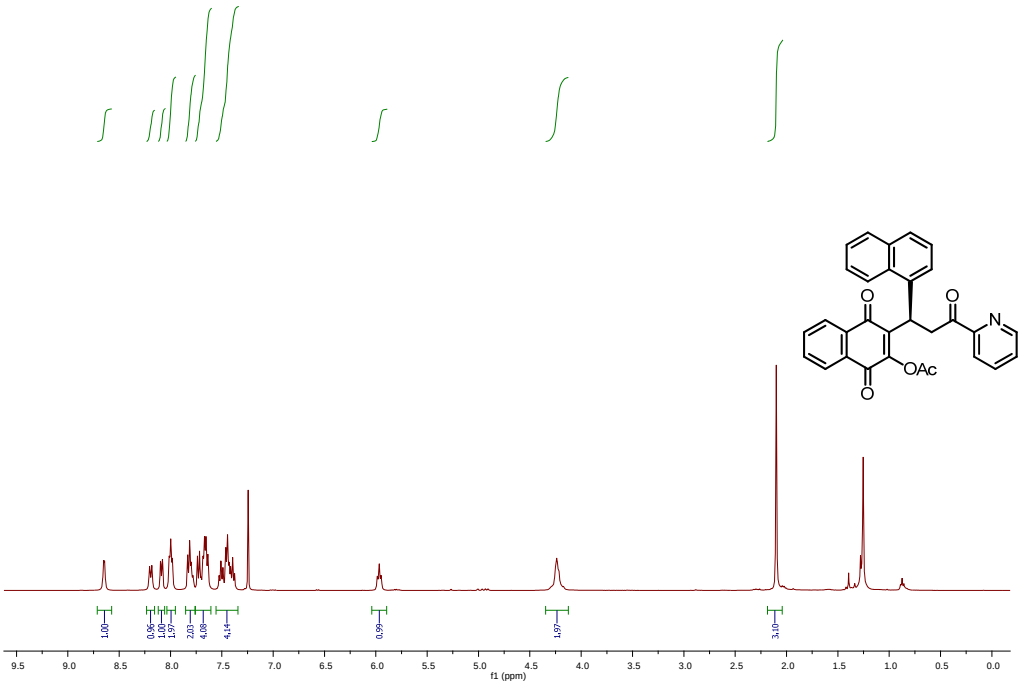
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.771	BB	0.6719	1.90452e4	435.77667	49.6238
2	26.256	BBA	0.7744	1.93339e4	384.68365	50.3762
Totals :				3.83791e4	820.46033	

HPLC graph of compound **4k** (racemic)

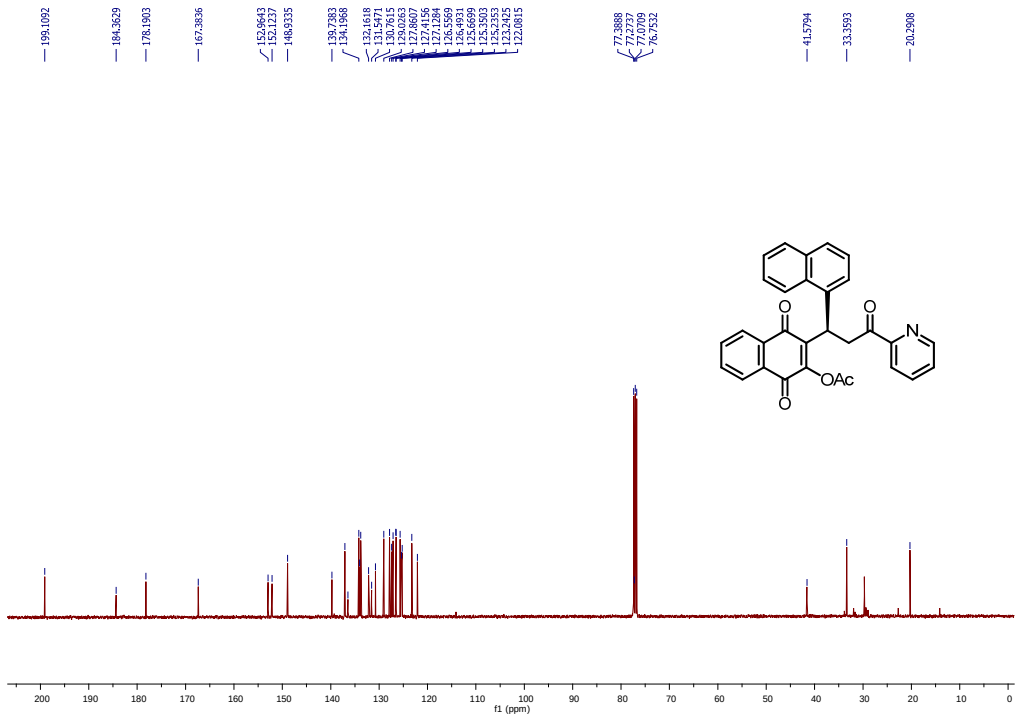


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.510	BB	0.6849	1250.26074	28.00299	2.0043
2	25.856	BBA	0.7882	6.11296e4	1196.11902	97.9957
Totals :				6.23799e4	1224.12201	

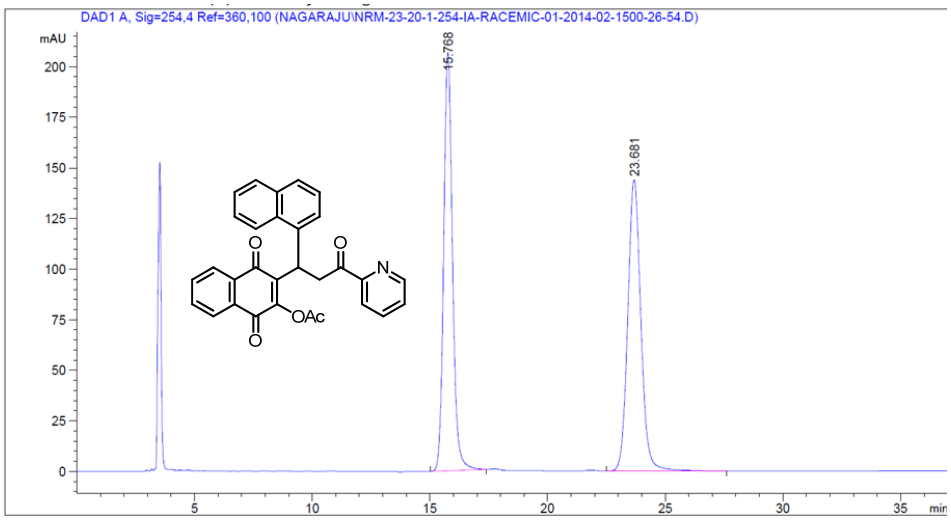
HPLC graph of compound **4k** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **4l** in $CDCl_3$

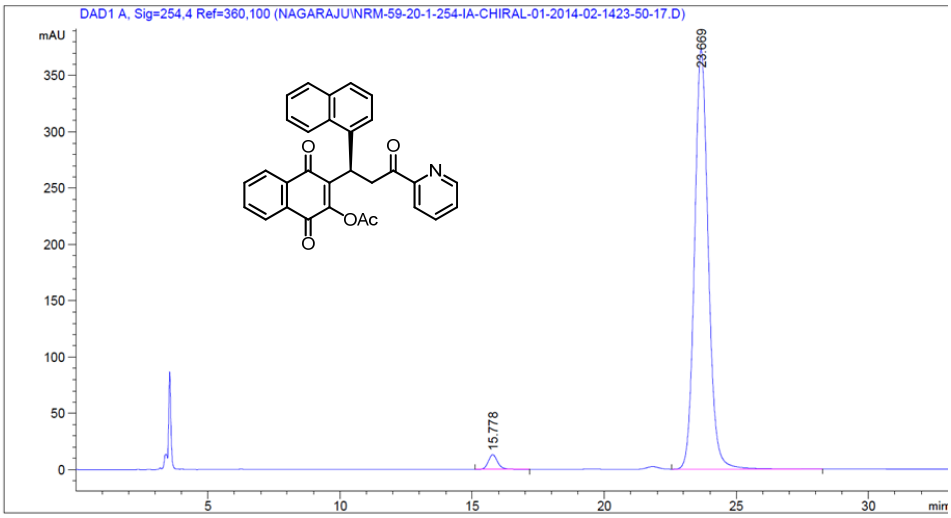


100 MHz ^{13}C NMR spectra of compound **4l** in $CDCl_3$



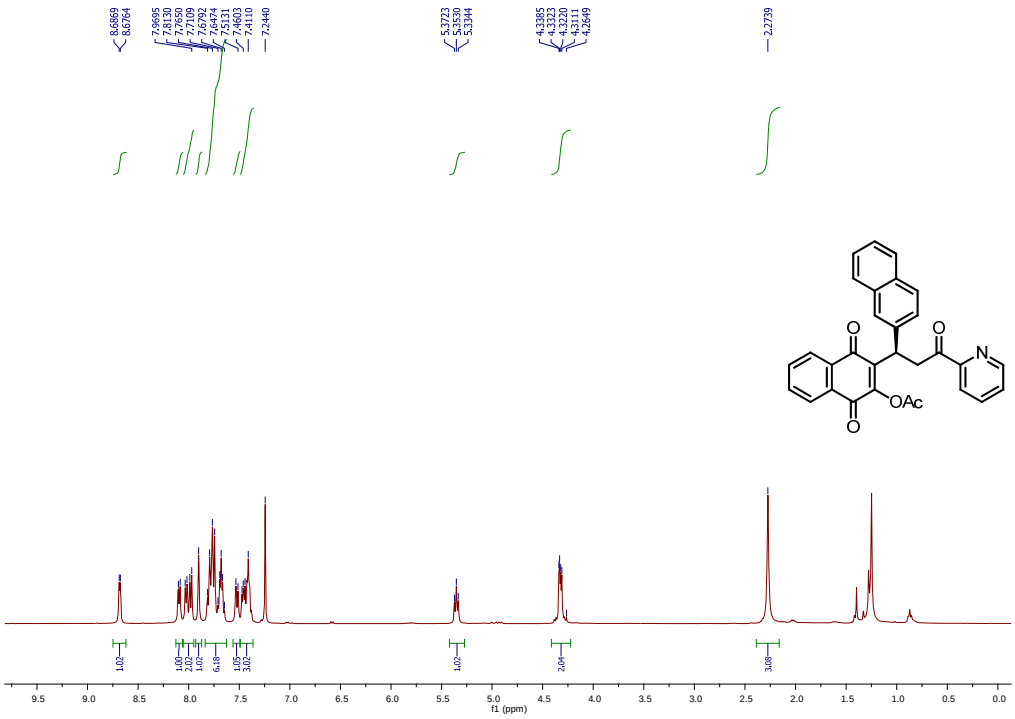
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.768	BB	0.3989	5364.03027	206.59294	49.0511
2	23.681	BB	0.5937	5571.56982	143.89941	50.9489
Totals :				1.09356e4	350.49236	

HPLC graph of compound **4l** (racemic)

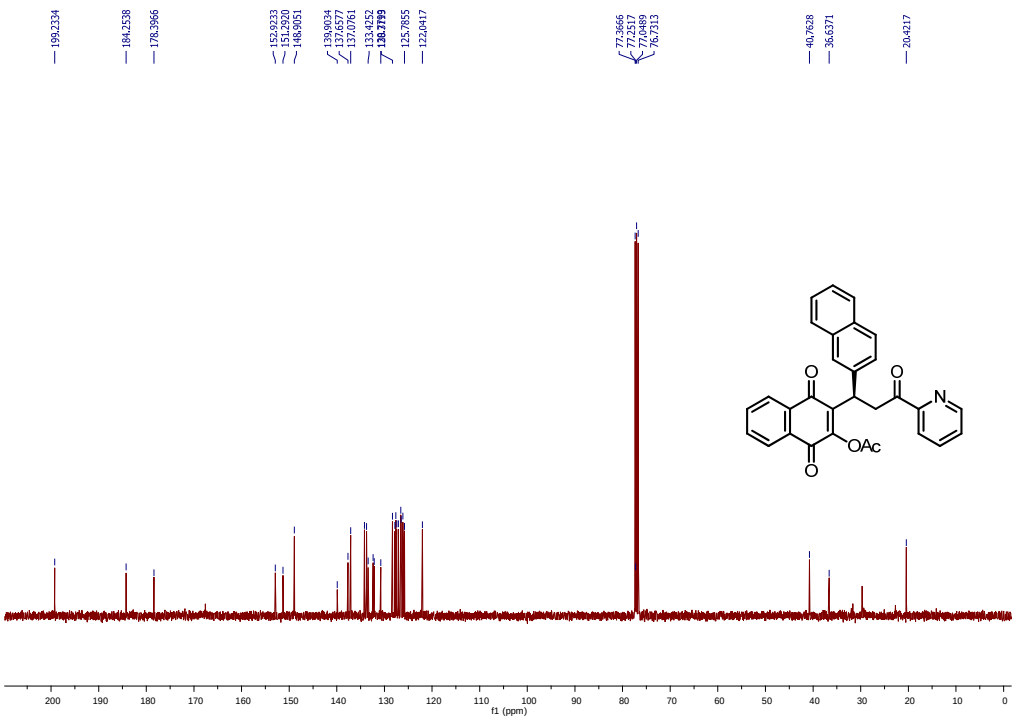


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.778	BB	0.3781	323.75613	13.11046	2.3449
2	23.669	BB	0.5559	1.34832e4	372.84573	97.6551
Totals :				1.38070e4	385.95619	

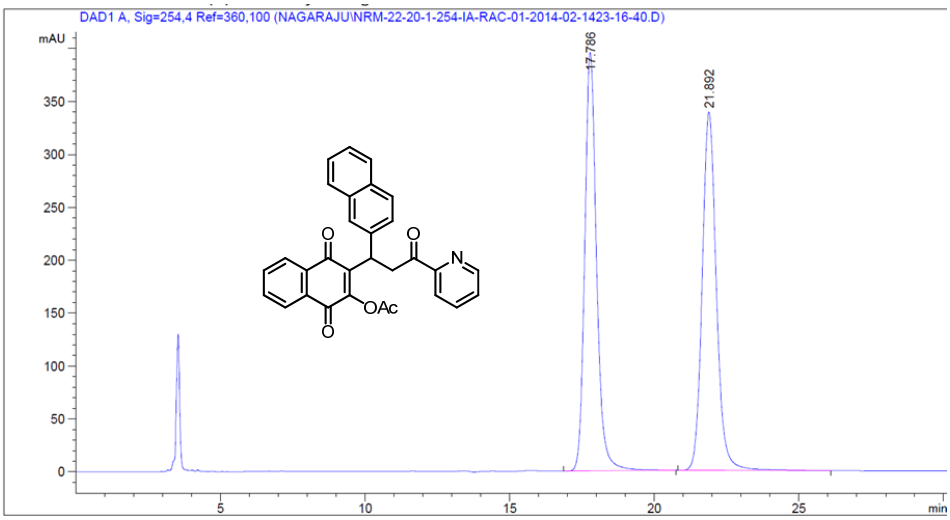
HPLC graph of compound **4l** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **4m** in $CDCl_3$

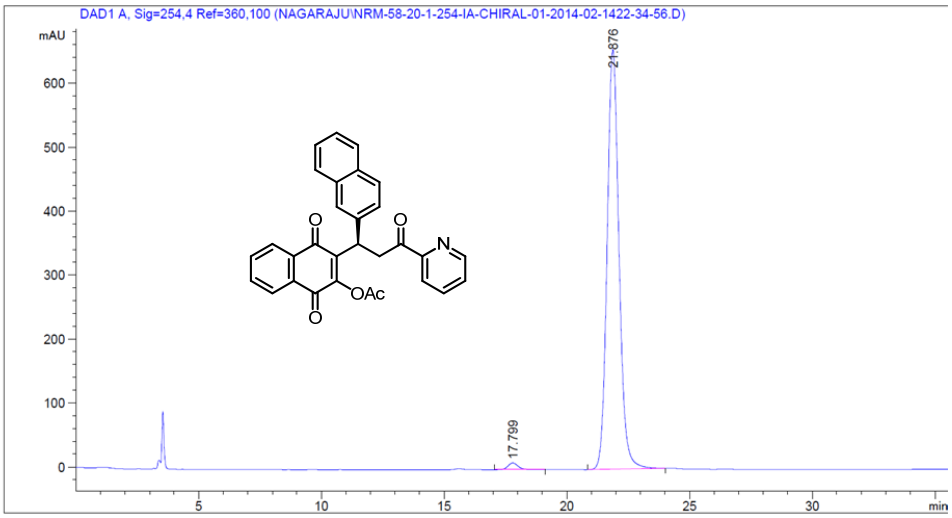


100 MHz ^{13}C NMR spectra of compound **4m** in $CDCl_3$



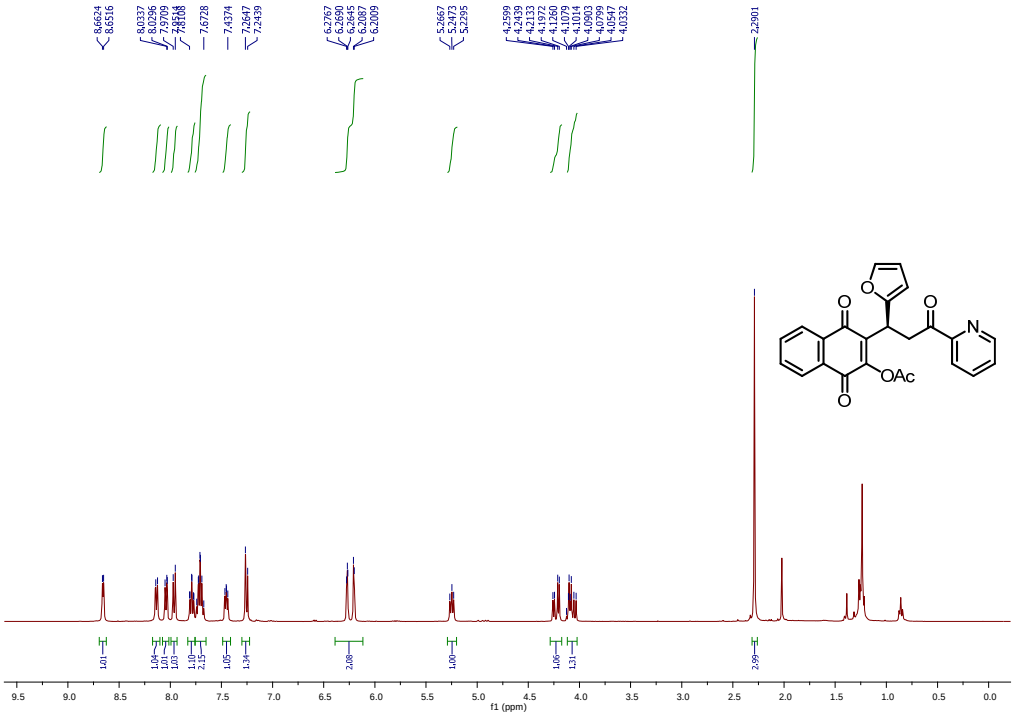
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.786	BB	0.4337	1.12376e4	395.27710	49.3114
2	21.892	BB	0.5219	1.15515e4	338.70789	50.6886
Totals :				2.27891e4	733.98499	

HPLC graph of compound **4m** (racemic)

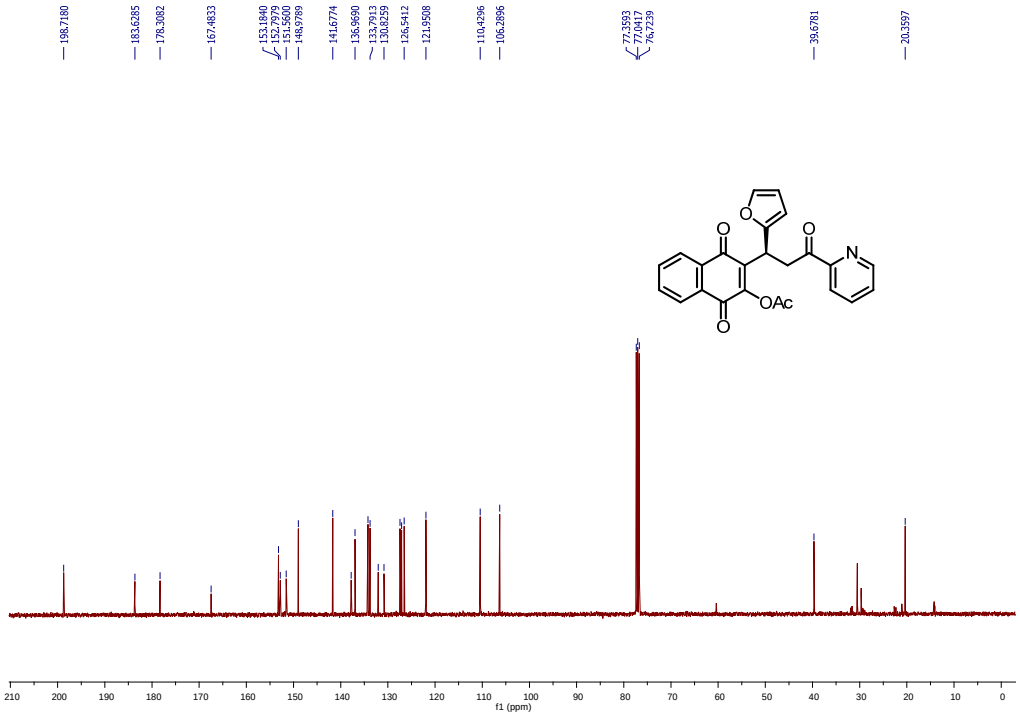


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.799	BB	0.4392	302.64041	10.59669	1.3537
2	21.876	BB	0.5161	2.20532e4	656.21271	98.6463
Totals :				2.23558e4	666.80940	

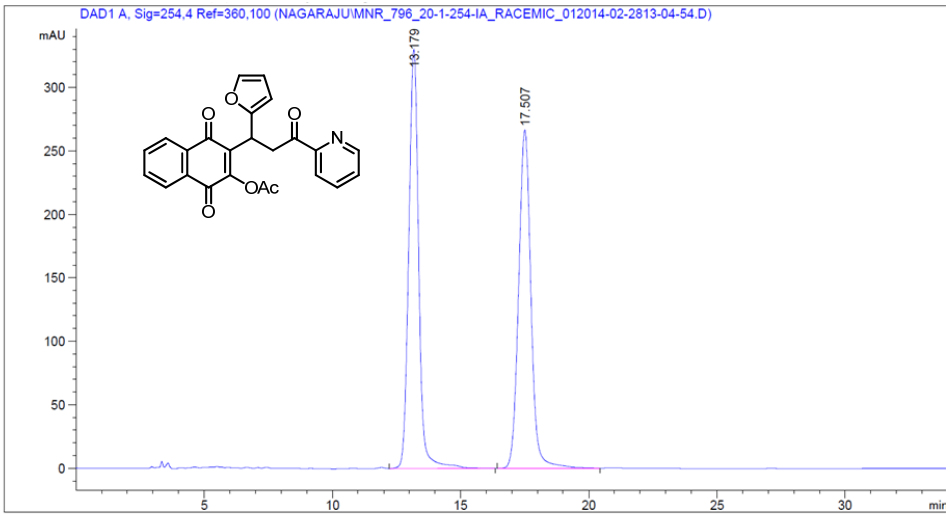
HPLC graph of compound **4m** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **4n** in $CDCl_3$

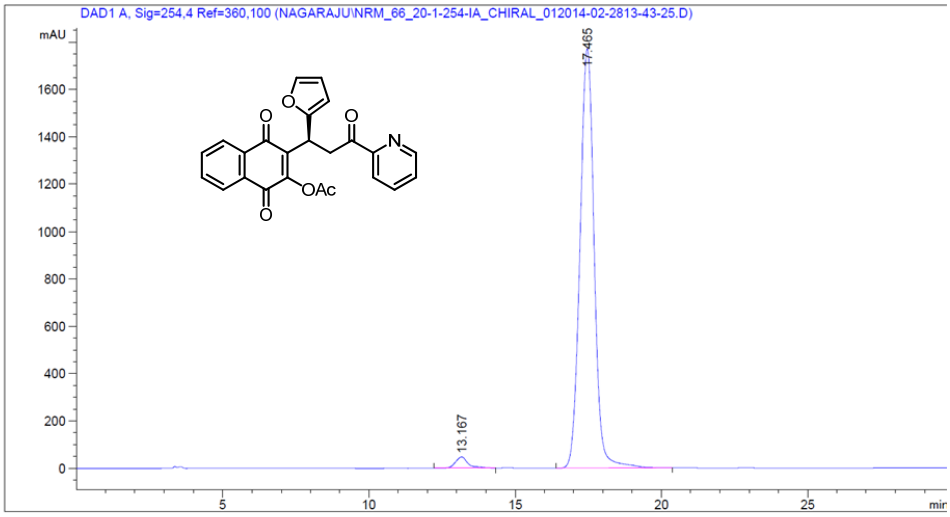


100 MHz ^{13}C NMR spectra of compound **4n** in $CDCl_3$



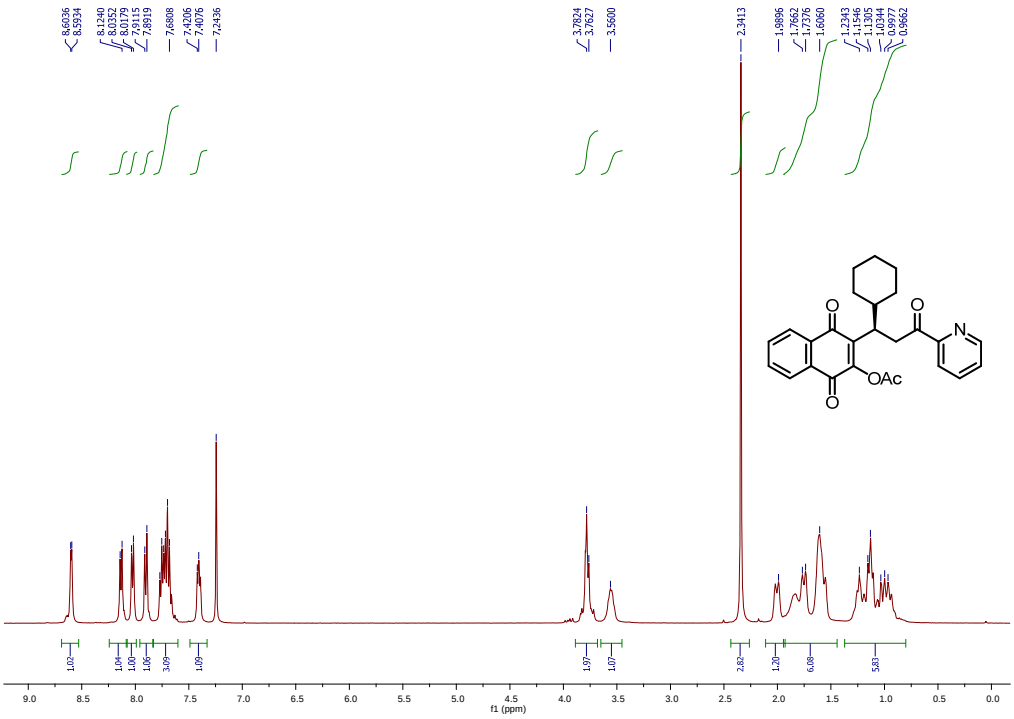
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.179	BB	0.4204	8957.25293	330.30847	50.1589
2	17.507	BB	0.5135	8900.50586	266.56442	49.8411
Totals :				1.78578e4	596.87289	

HPLC graph of compound **4n** (racemic)

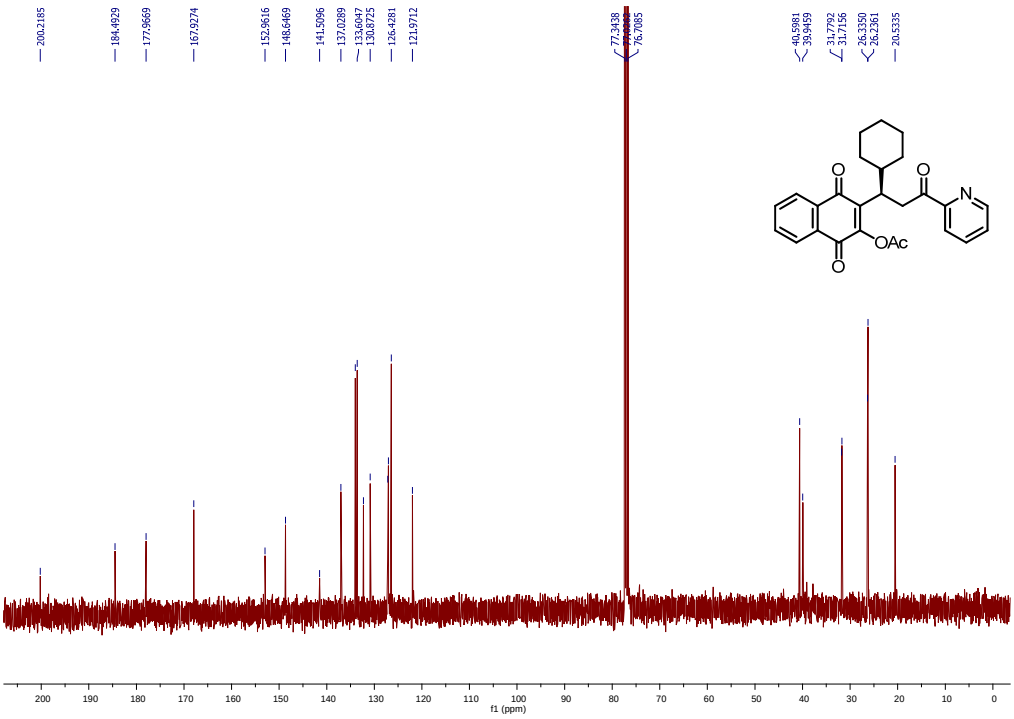


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.167	BB	0.4547	1415.10266	47.07498	2.3157
2	17.465	BB	0.5232	5.96932e4	1771.18921	97.6843
Totals :				6.11083e4	1818.26419	

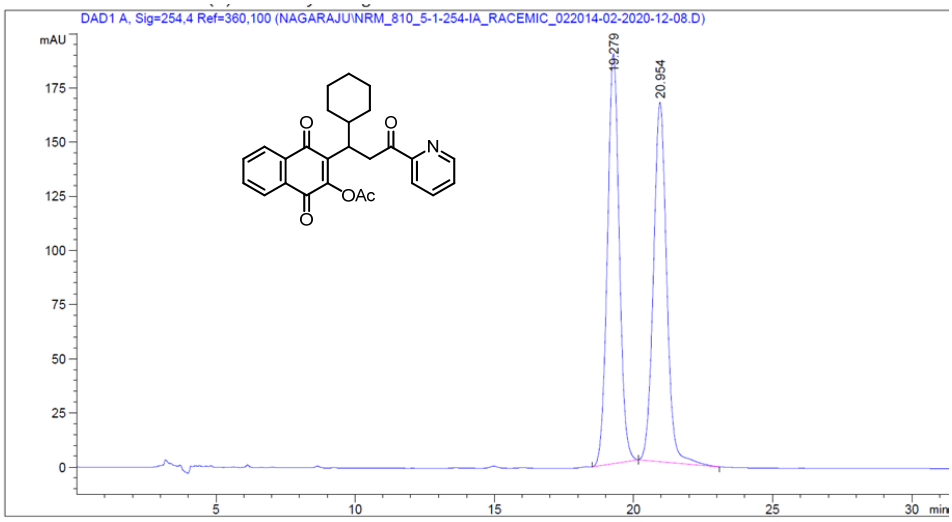
HPLC graph of compound **4n** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **4n** in $CDCl_3$

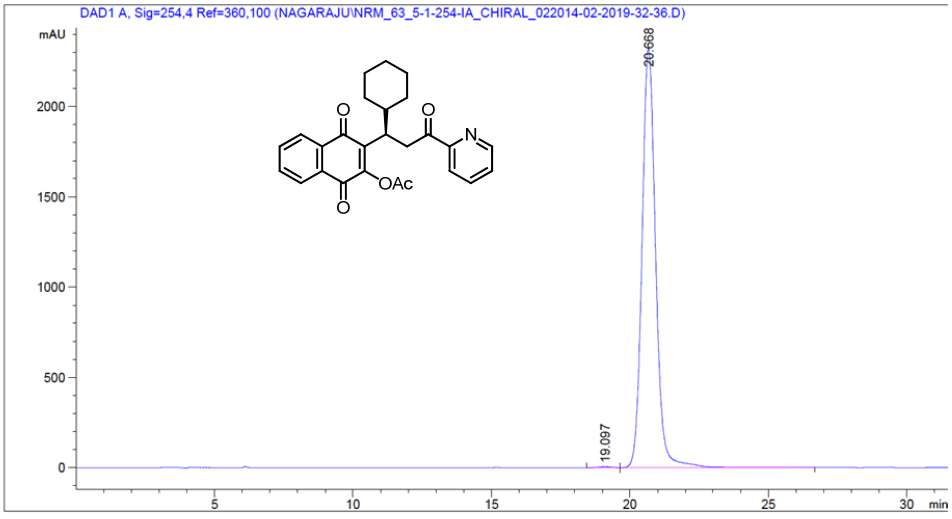


100 MHz ^{13}C NMR spectra of compound **4n** in $CDCl_3$



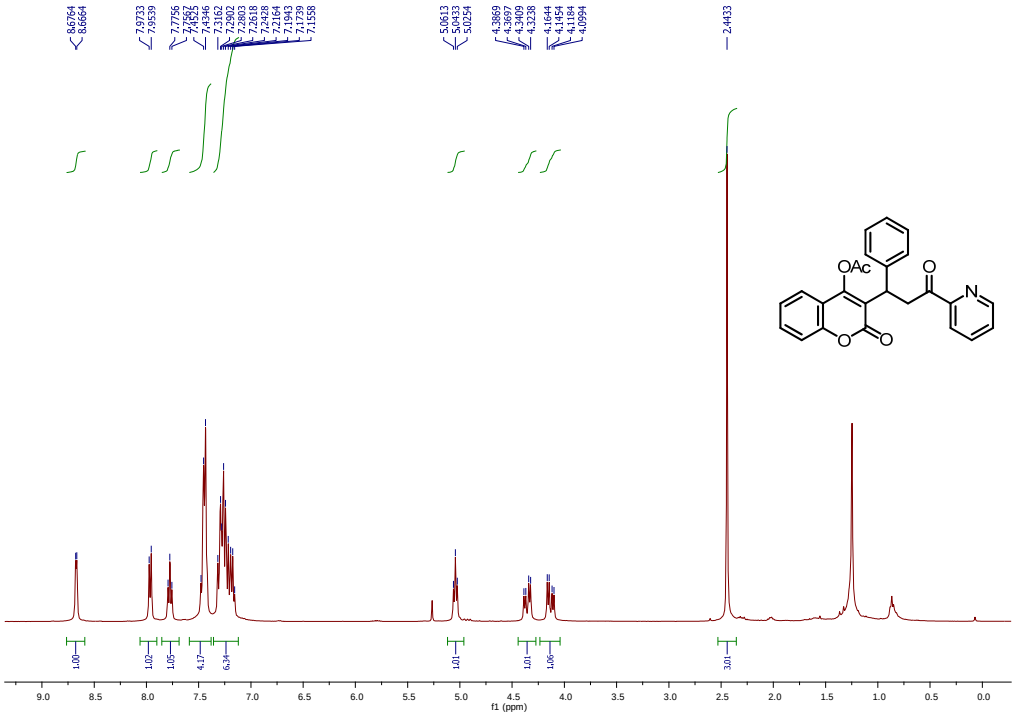
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.279	BB	0.4547	5585.60791	189.06068	50.5643
2	20.954	BB	0.5062	5460.93750	165.83333	49.4357
Totals :				1.10465e4	354.89401	

HPLC graph of compound of **4n** (racemic)

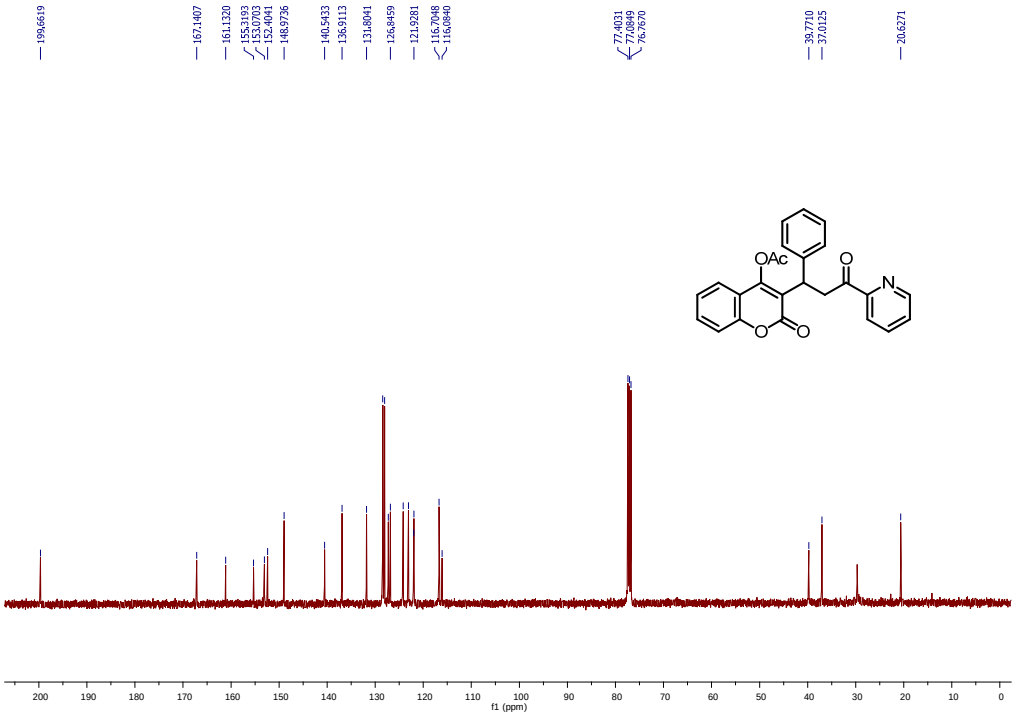


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.097	BB	0.4437	167.25217	5.77759	0.2105
2	20.668	BB	0.5226	7.93054e4	2321.08765	99.7895
Totals :				7.94727e4	2326.86524	

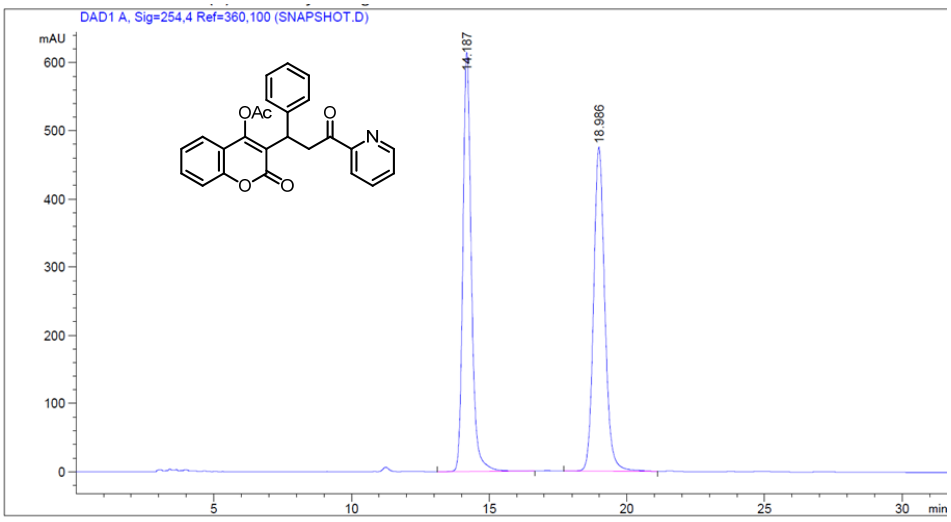
HPLC graph of compound of **4n** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **9a** in $CDCl_3$

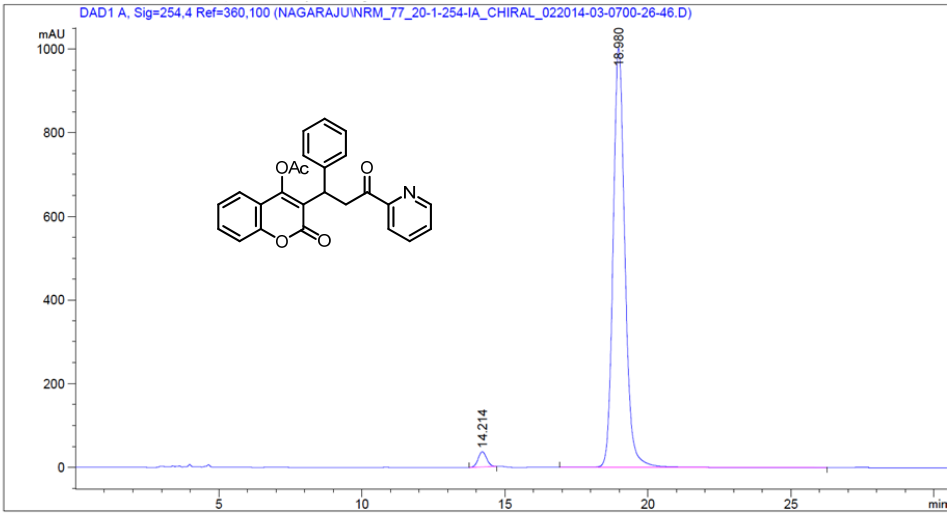


100 MHz ^{13}C NMR spectra of compound **9a** in $CDCl_3$



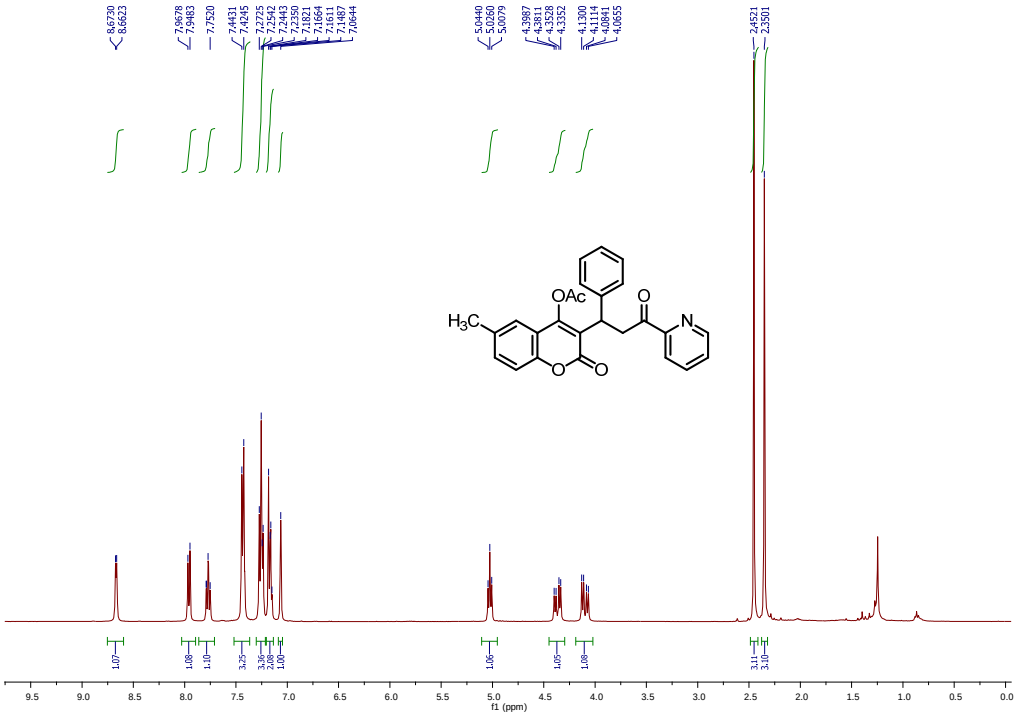
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.187	BB	0.3264	1.31843e4	614.34564	49.5038
2	18.986	BB	0.4340	1.34486e4	475.43228	50.4962
Totals :				2.66329e4	1089.77792	

HPLC graph of compound **9a** (racemic)

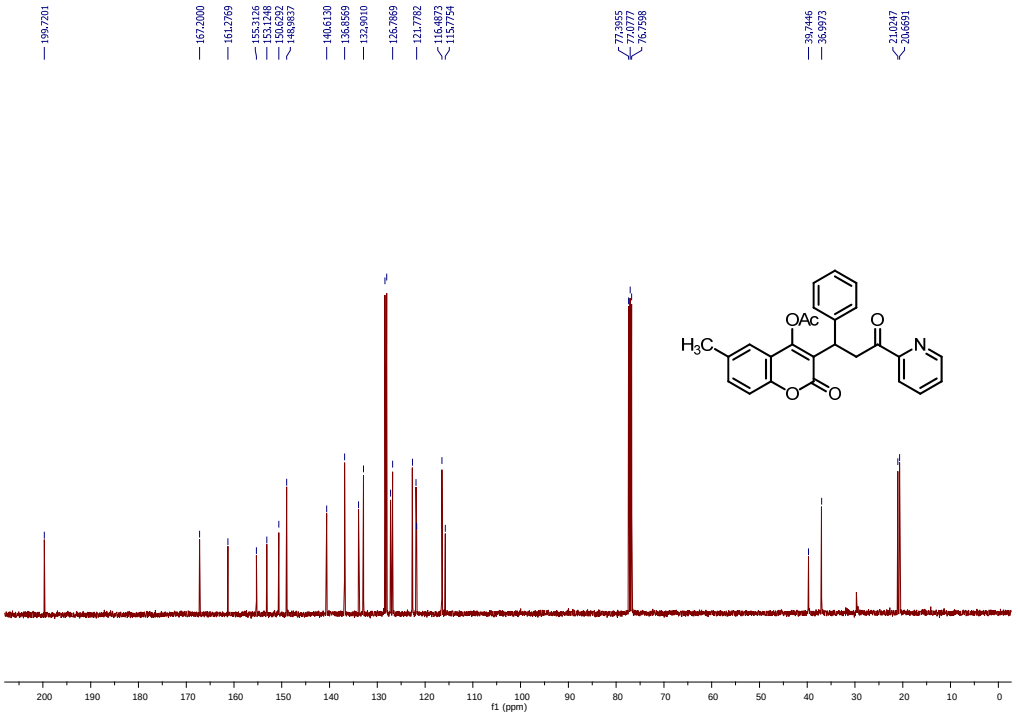


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.214	BB	0.3164	747.55634	36.57778	2.5256
2	18.980	BB	0.4418	2.88513e4	1002.33673	97.4744
Totals :				2.95988e4	1038.91451	

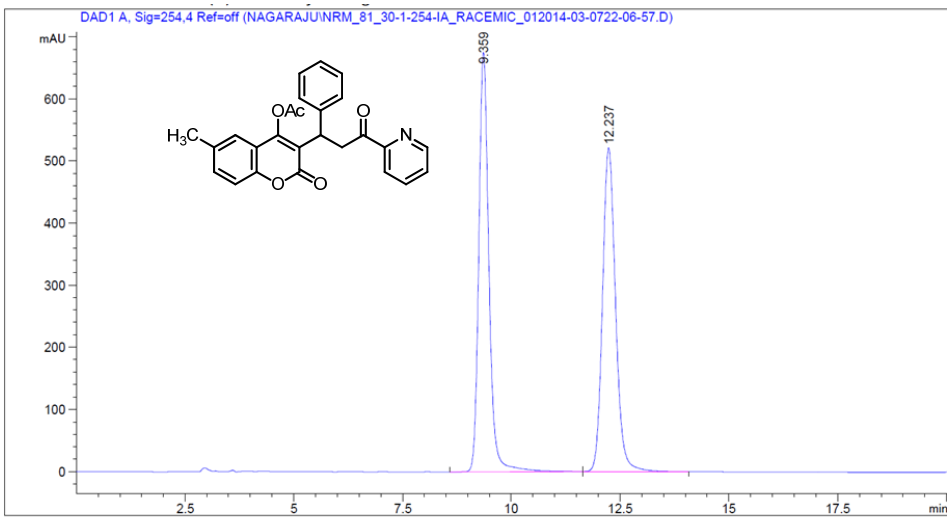
HPLC graph of compound **9a** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **9b** in $CDCl_3$

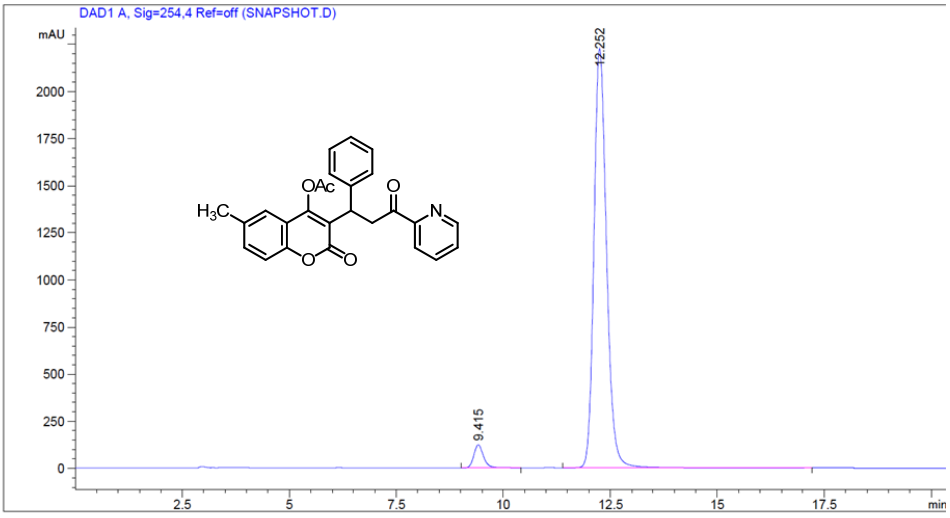


100 MHz ^{13}C NMR spectra of compound **9b** in $CDCl_3$



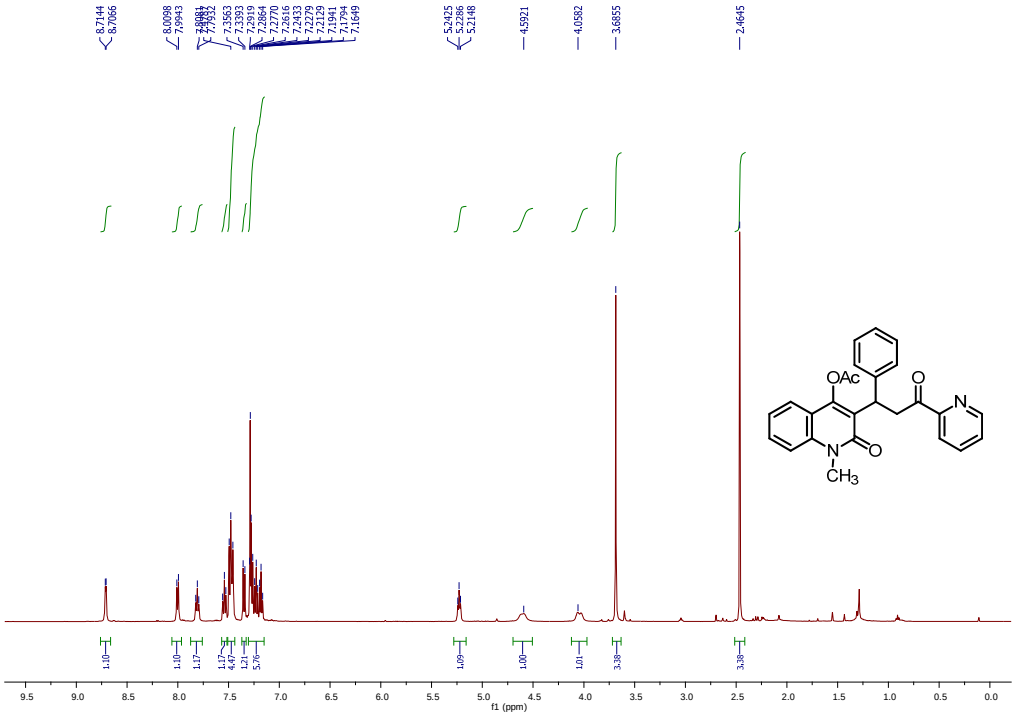
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.359	BB	0.2471	1.09418e4	675.04193	50.2477
2	12.237	BB	0.3184	1.08340e4	521.43561	49.7523
Totals :				2.17758e4	1196.47754	

HPLC graph of compound **9b** (racemic)

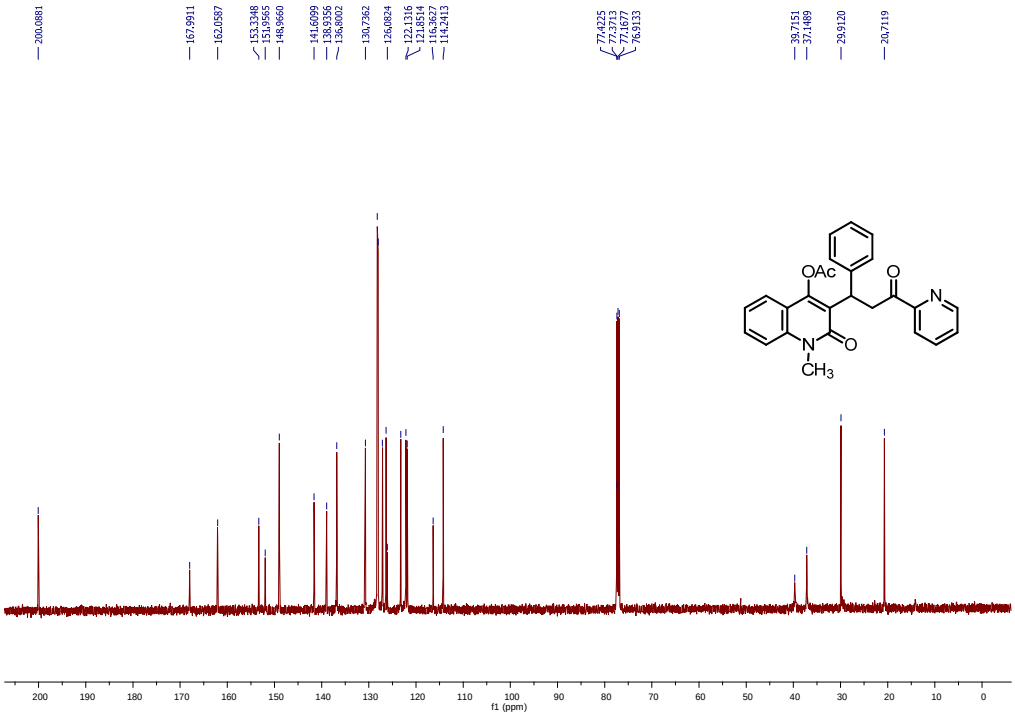


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.415	BB	0.2397	1947.36780	123.65936	4.0926
2	12.252	BB	0.3152	4.56354e4	2226.21118	95.9074
Totals :				4.75828e4	2349.87054	

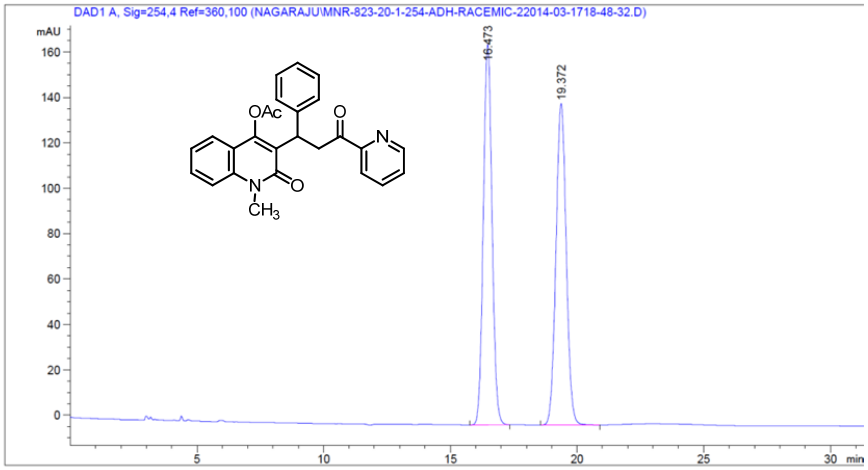
HPLC graph of compound **9b** (enantioenriched)



500 MHz ^{1}H NMR spectra of compound **9c** in $CDCl_3$

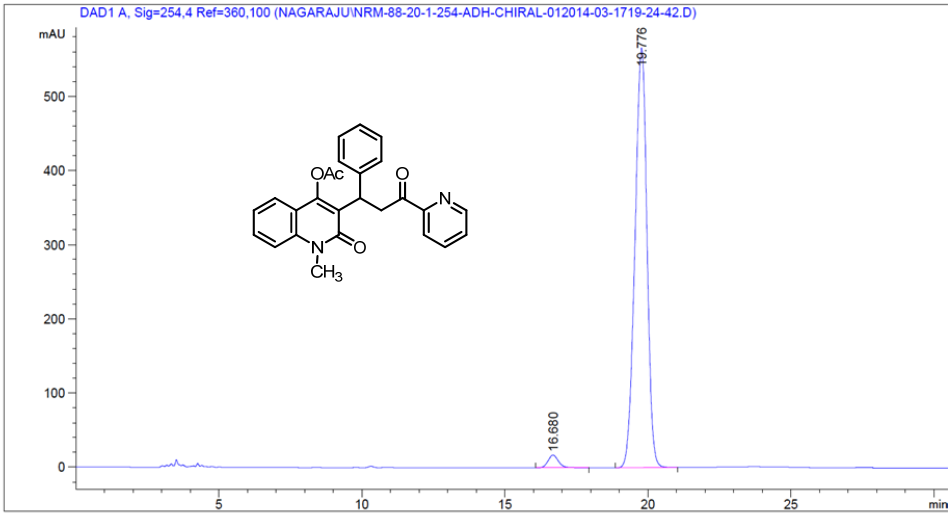


125 MHz ^{13}C NMR spectra of compound **9c** in $CDCl_3$



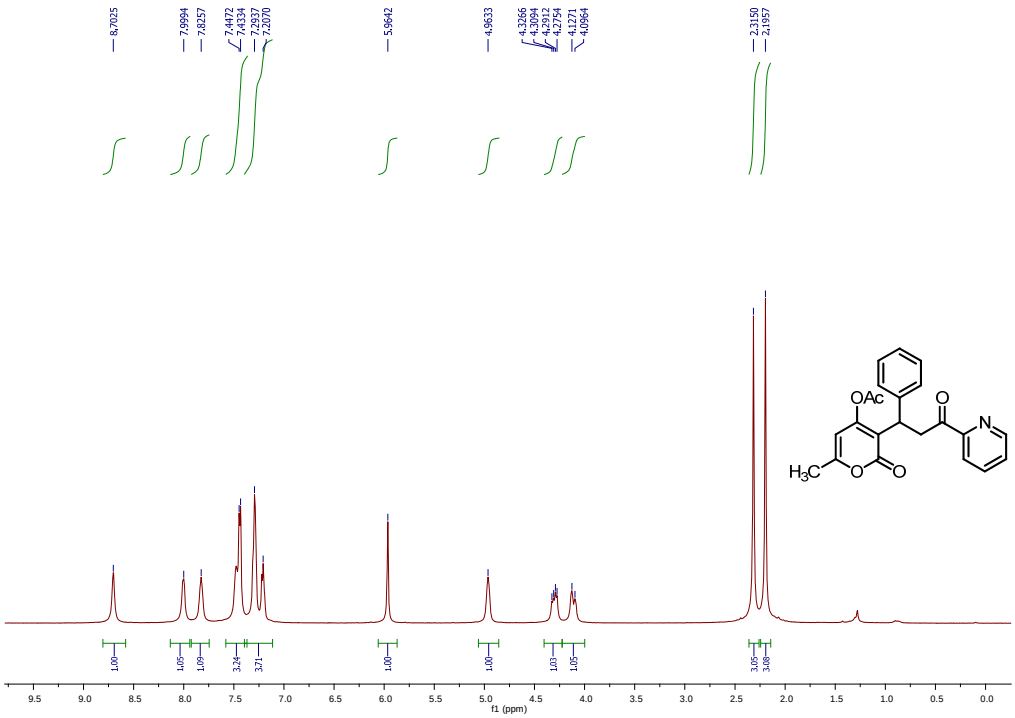
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.473	BB	0.3704	3999.40405	167.57361	50.0013
2	19.372	BB	0.4396	3999.18823	141.57529	49.9987
Totals :				7998.59229	309.14890	

HPLC graph of compound **9c** (racemic)

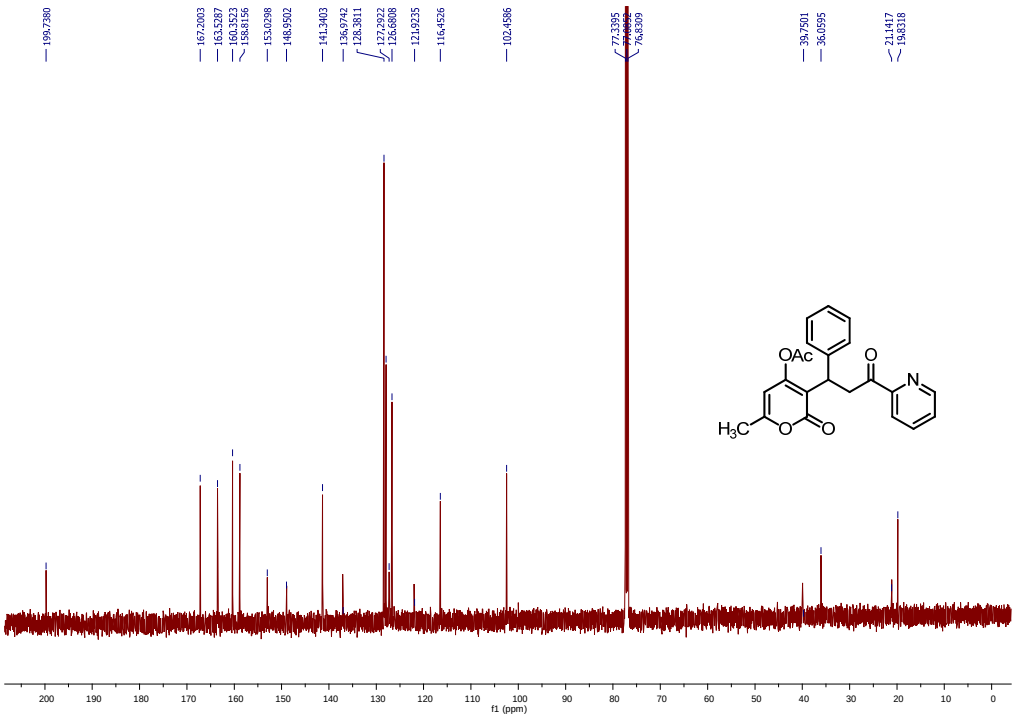


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.680	BB	0.3940	436.62445	17.09608	2.5839
2	19.776	BB	0.4515	1.64612e4	565.70795	97.4161
Totals :				1.68978e4	582.80402	

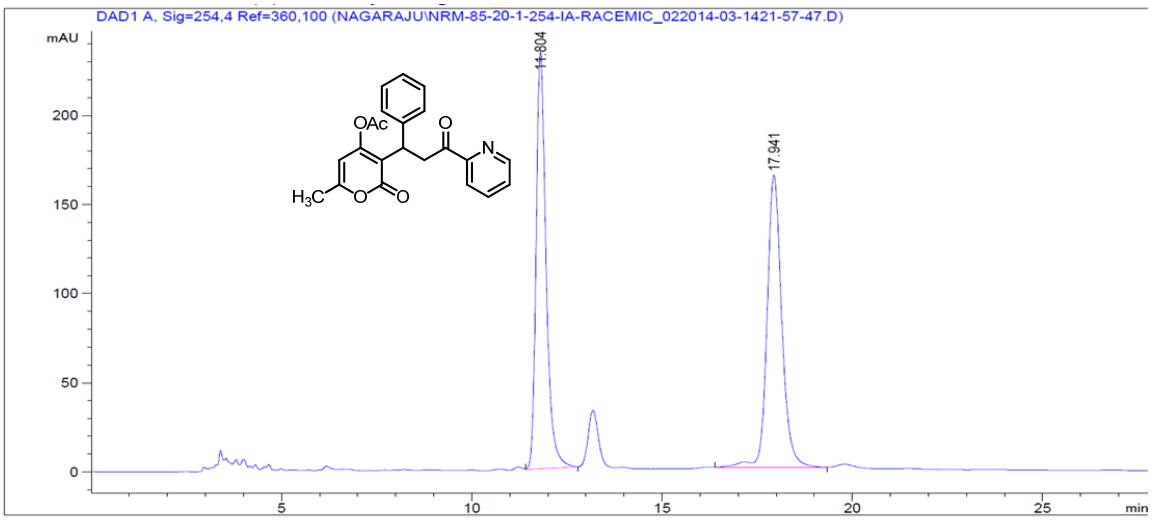
HPLC graph of compound **9c** (enantioenriched)



500 MHz ^{1}H NMR spectra of compound **10a** in $CDCl_3$

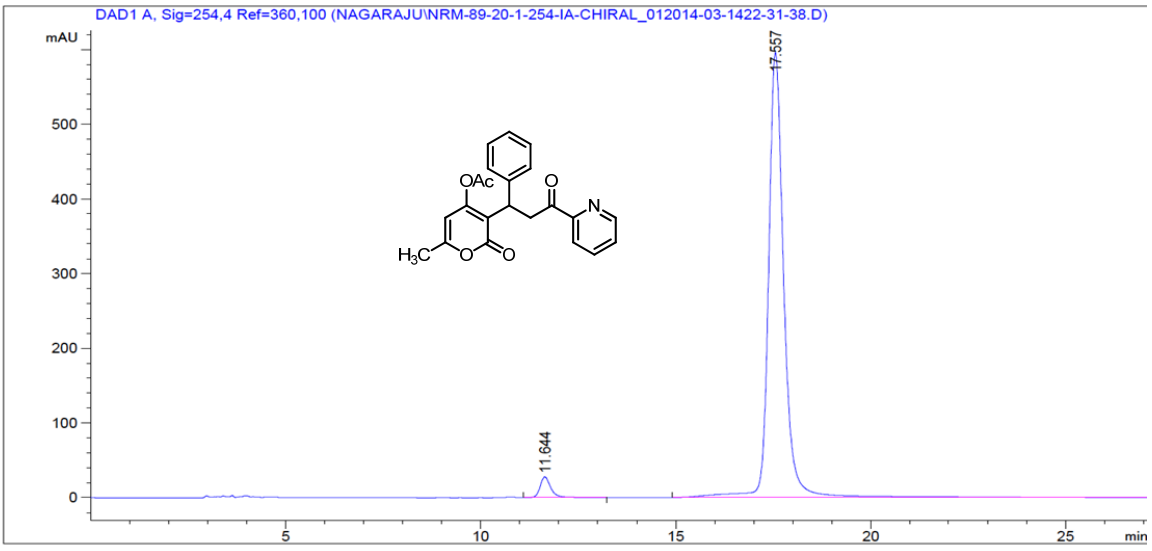


125 MHz ^{13}C NMR spectra of compound **10a** in $CDCl_3$



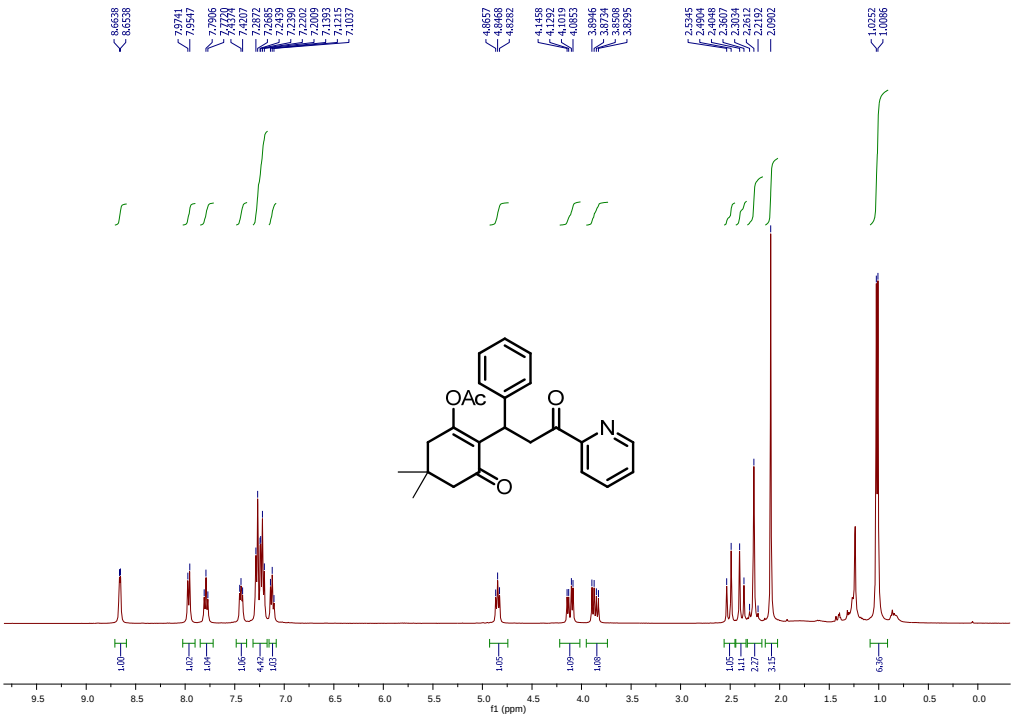
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.804	VB	0.2754	4236.53369	233.81841	48.9158
2	17.941	BB	0.4088	4424.33350	163.99329	51.0842
Totals :				8660.86719	397.81169	

HPLC graph of compound **10a** (racemic)

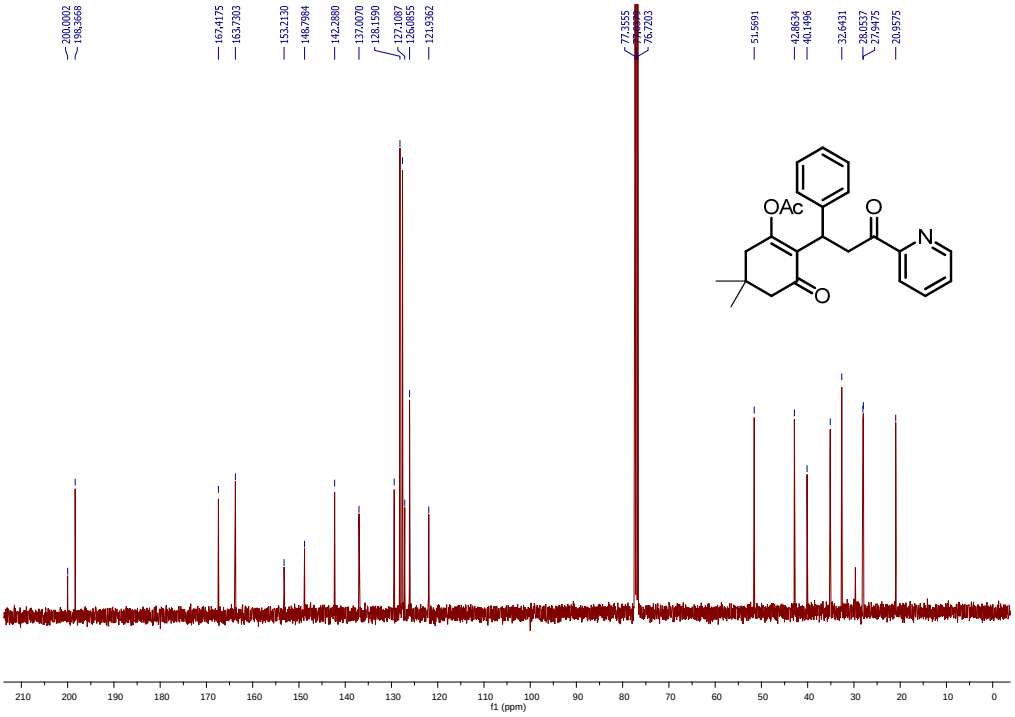


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.644	BB	0.2907	534.35773	27.74753	3.1446
2	17.557	BBA	0.4142	1.64587e4	595.90967	96.8554
Totals :				1.69931e4	623.65720	

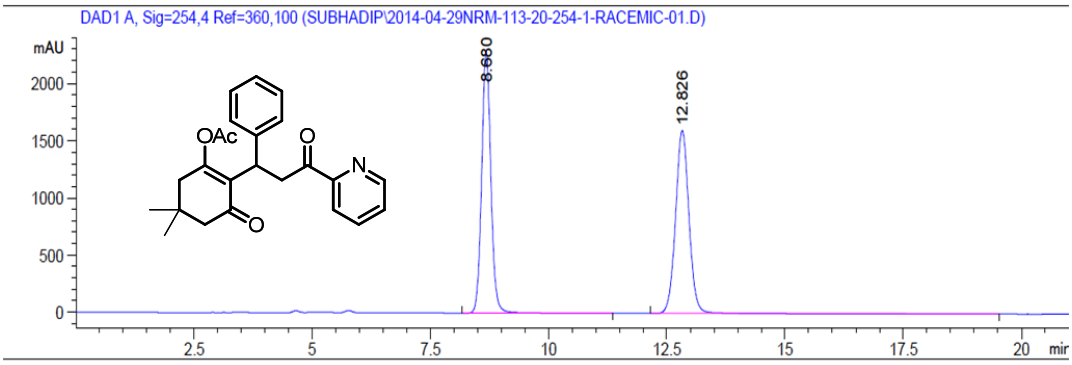
HPLC graph of compound **10a** (enantioenriched)



400 MHz ^{1}H NMR spectra of compound **11a** in $CDCl_3$

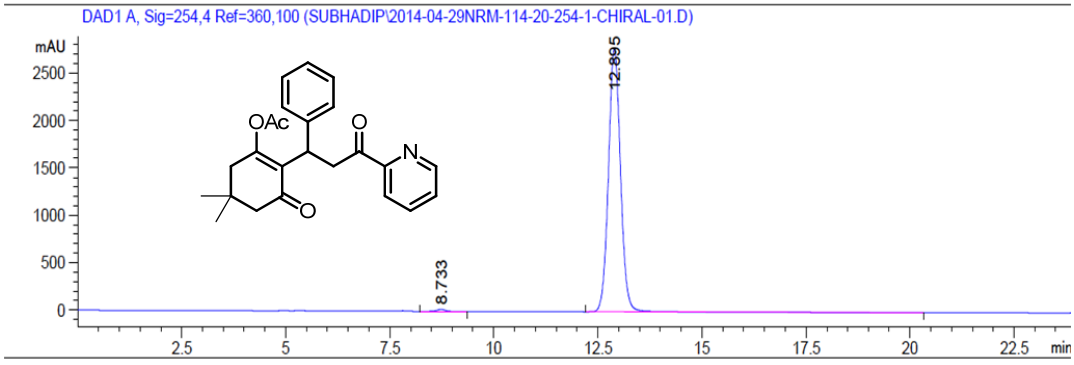


100 MHz ^{13}C NMR spectra of compound **11a** in $CDCl_3$



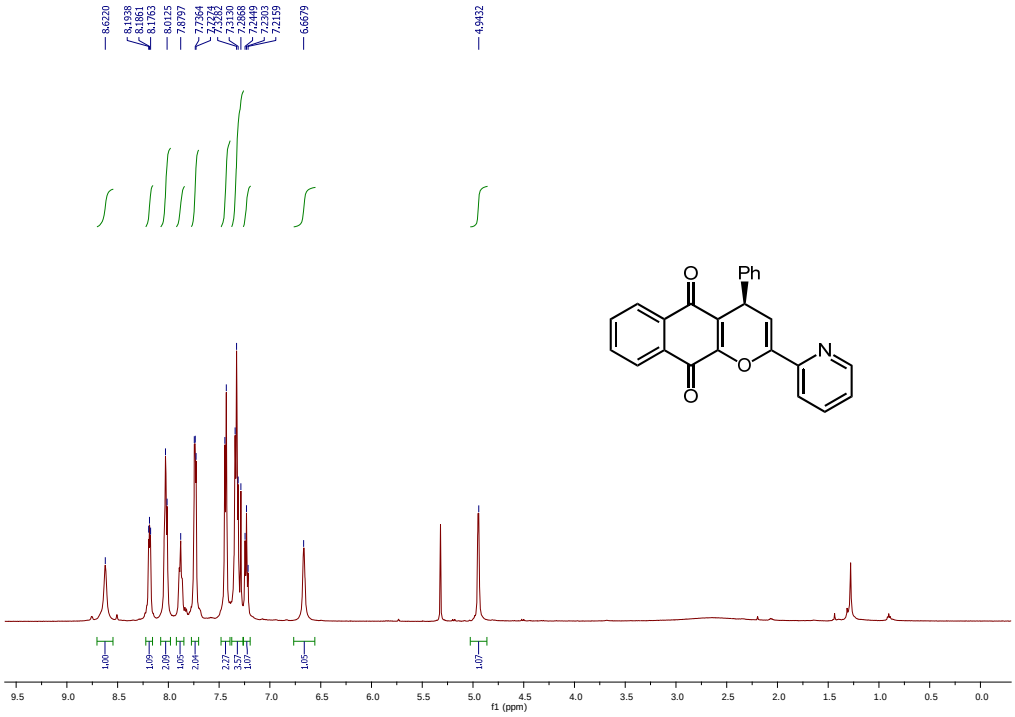
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.680	BB	0.2062	3.11650e4	2297.72656	49.5381
2	12.826	BBA	0.3031	3.17462e4	1602.95081	50.4619
Totals :				6.29112e4	3900.67737	

HPLC graph of compound **11a** (racemic)

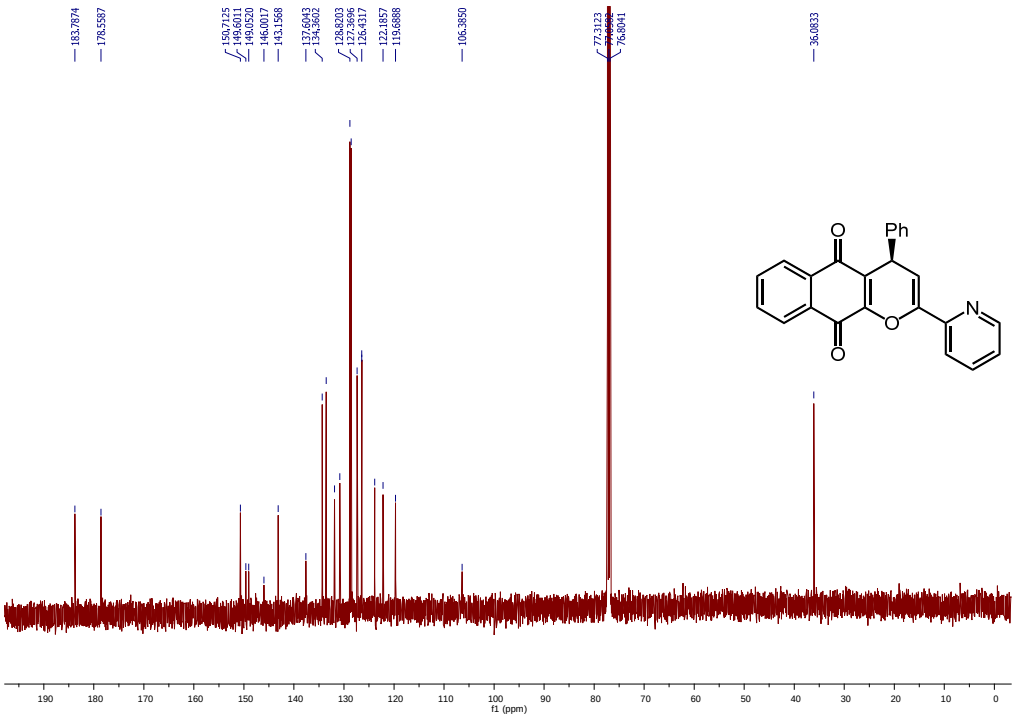


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.733	BB	0.2098	324.65018	23.40358	0.5734
2	12.895	BBA	0.3129	5.62910e4	2772.72925	99.4266
Totals :				5.66157e4	2796.13283	

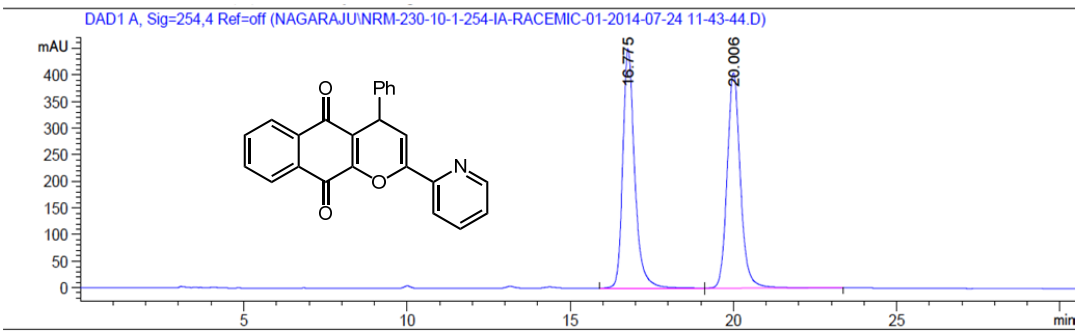
HPLC graph of compound **11a** (enantioenriched)



500 MHz ^{1}H NMR spectra of compound **12a** in $CDCl_3$

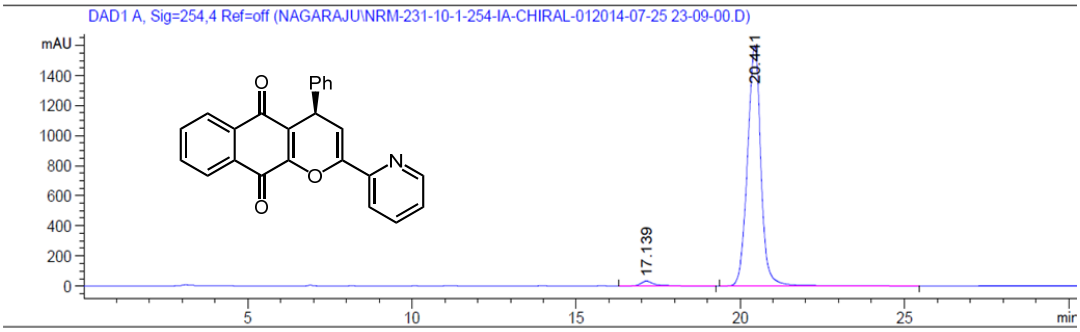


125 MHz ^{13}C NMR spectra of compound **12a** in $CDCl_3$



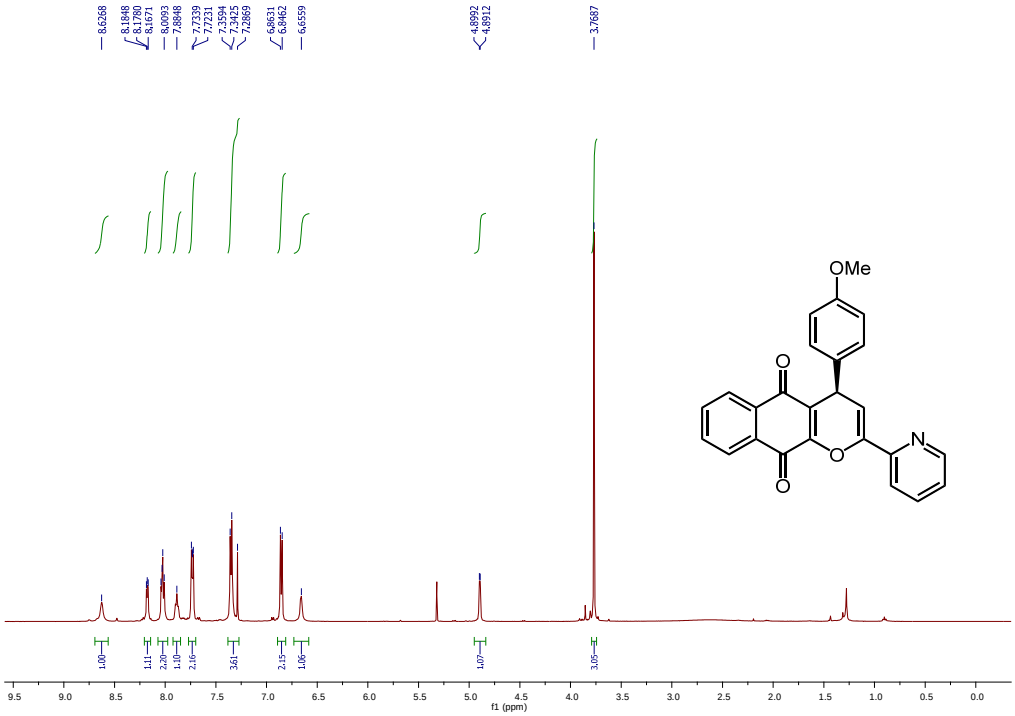
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.775	BB	0.3817	1.13969e4	449.72794	49.9654
2	20.006	BB	0.4311	1.14127e4	404.53232	50.0346
Totals :				2.28095e4	854.26025	

HPLC graph of compound **12a** (racemic)

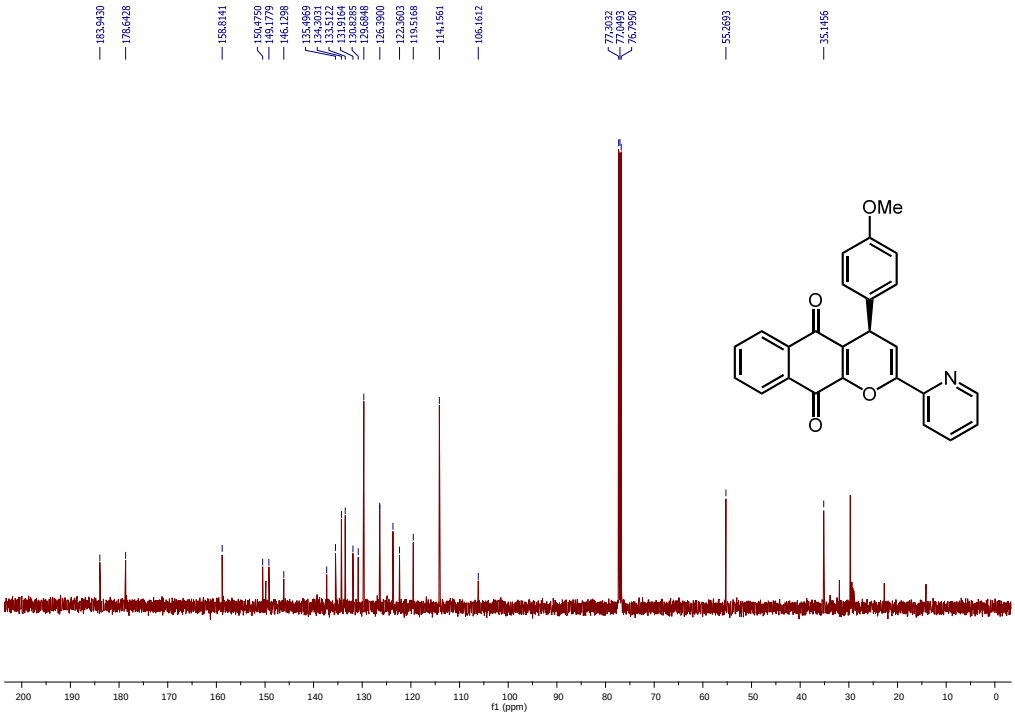


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.139	BB	0.4395	962.10339	32.11730	2.0661
2	20.441	BB	0.4373	4.56031e4	1596.18640	97.9339
Totals :				4.65653e4	1628.30370	

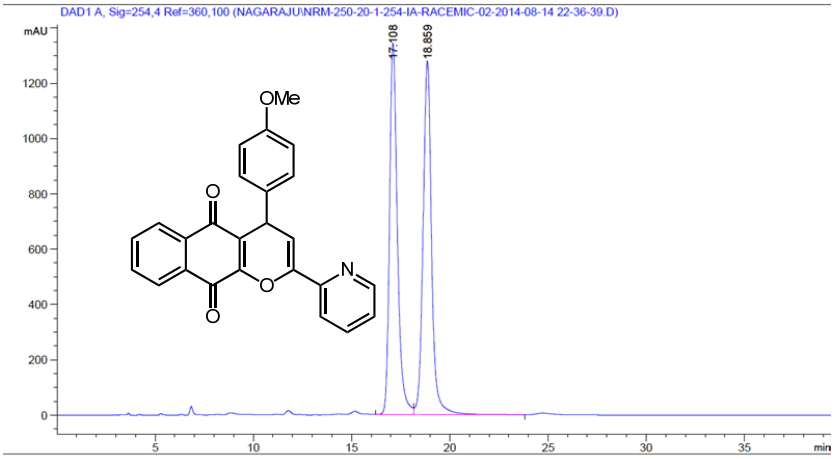
HPLC graph of compound **12a** (enantioenriched)



500 MHz ^{1}H NMR spectra of compound **12b** in $CDCl_3$

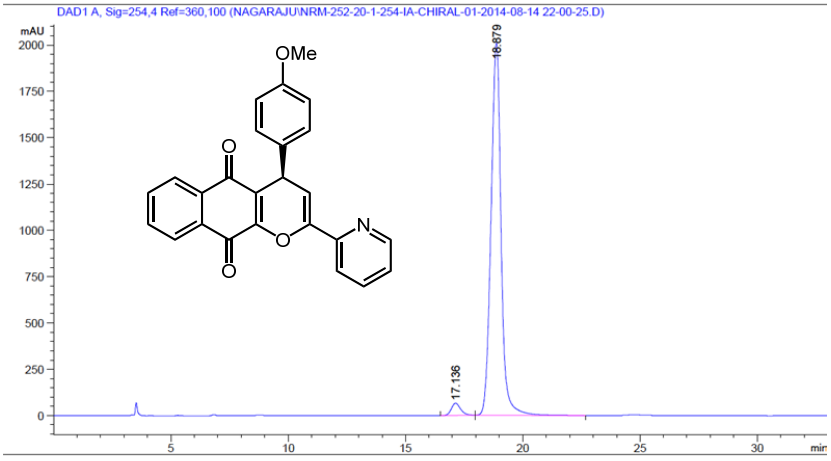


125 MHz ^{13}C NMR spectra of compound **12b** in $CDCl_3$



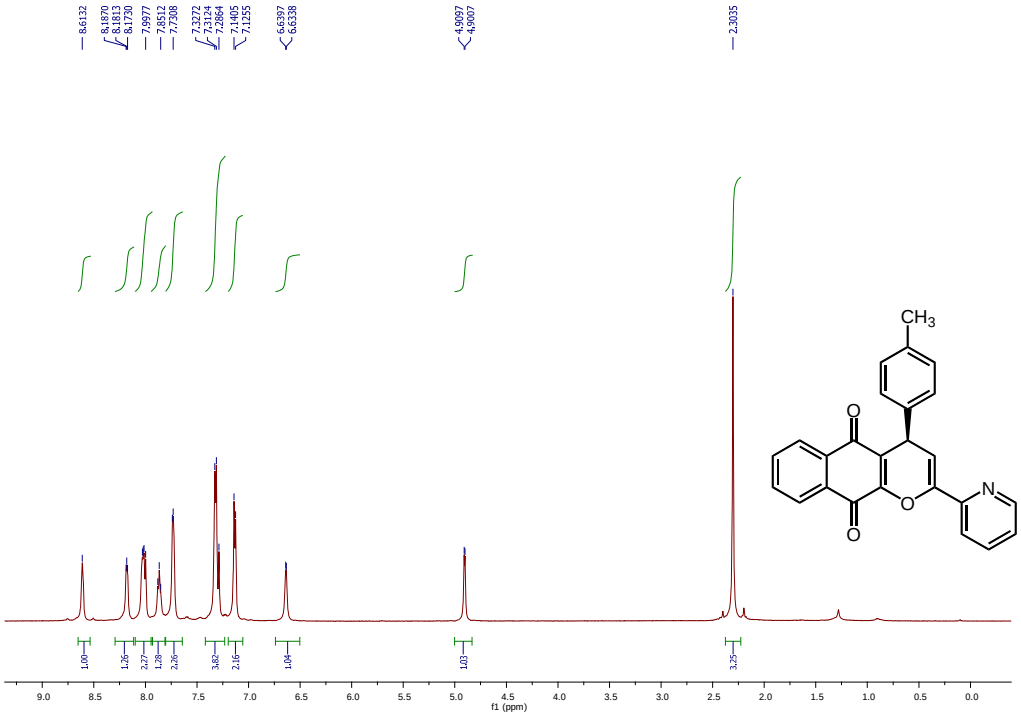
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.108	BV	0.4204	3.73173e4	1342.00049	49.1140
2	18.859	VB	0.4586	3.86637e4	1279.10840	50.8860
Totals :				7.59811e4	2621.10889	

HPLC graph of compound **12b** (racemic)

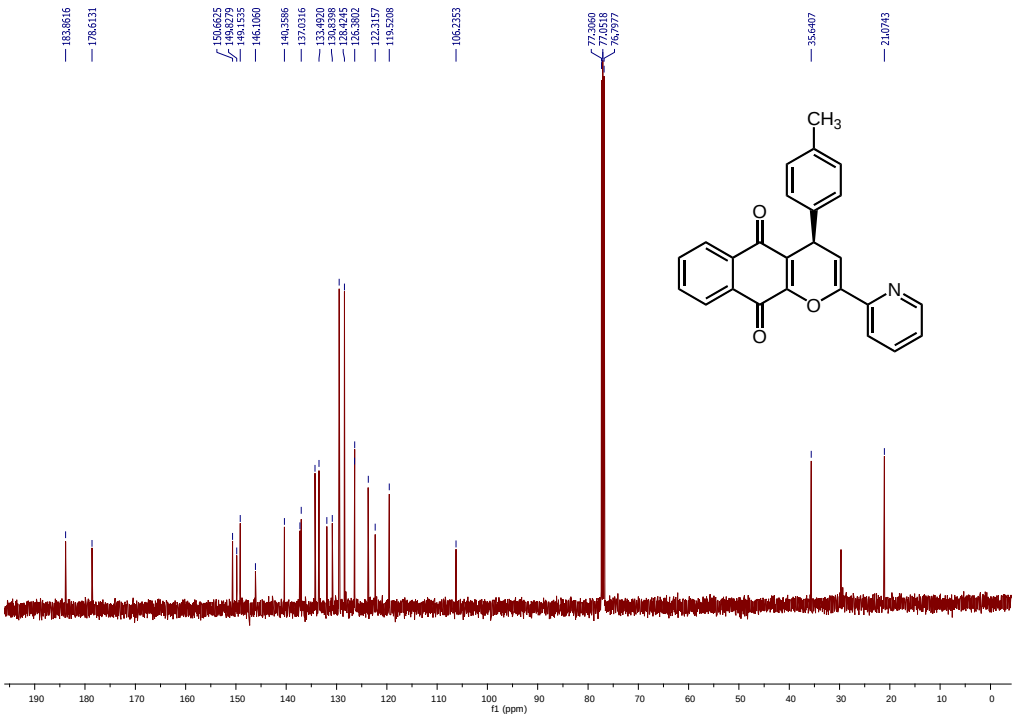


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.136	BB	0.4250	1828.17468	66.03540	2.9737
2	18.879	BB	0.4545	5.96491e4	2008.13208	97.0263
Totals :				6.14773e4	2074.16748	

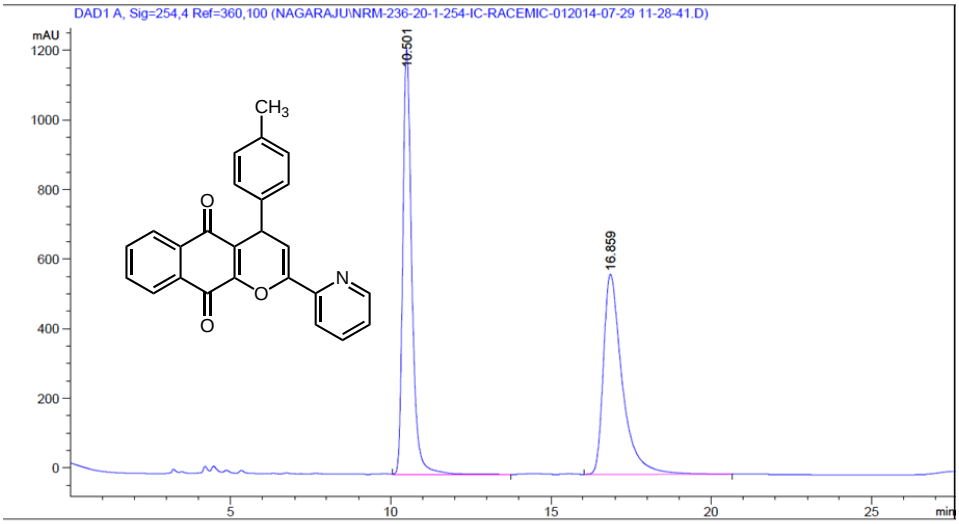
HPLC graph of compound **12b** (enantioenriched)



500 MHz ^{1}H NMR spectra of compound **12c** in $CDCl_3$

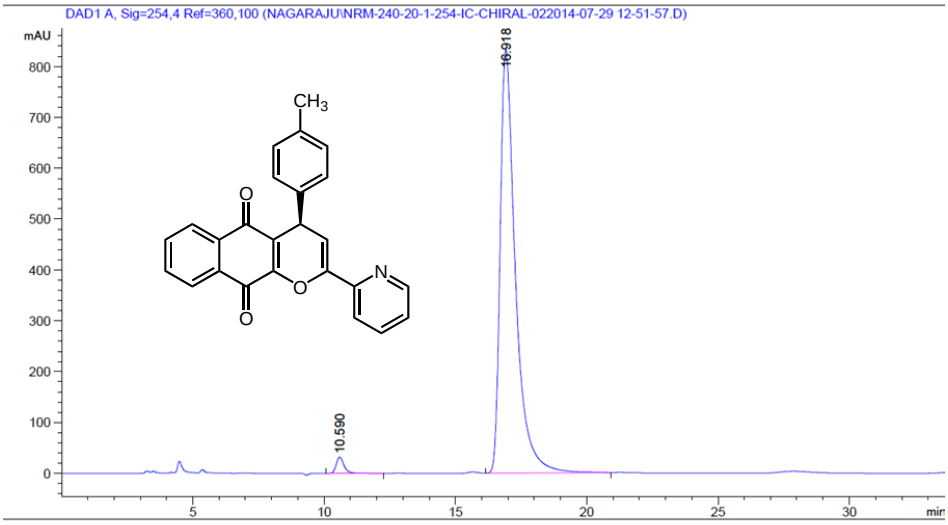


125 MHz ^{13}C NMR spectra of compound **12c** in $CDCl_3$



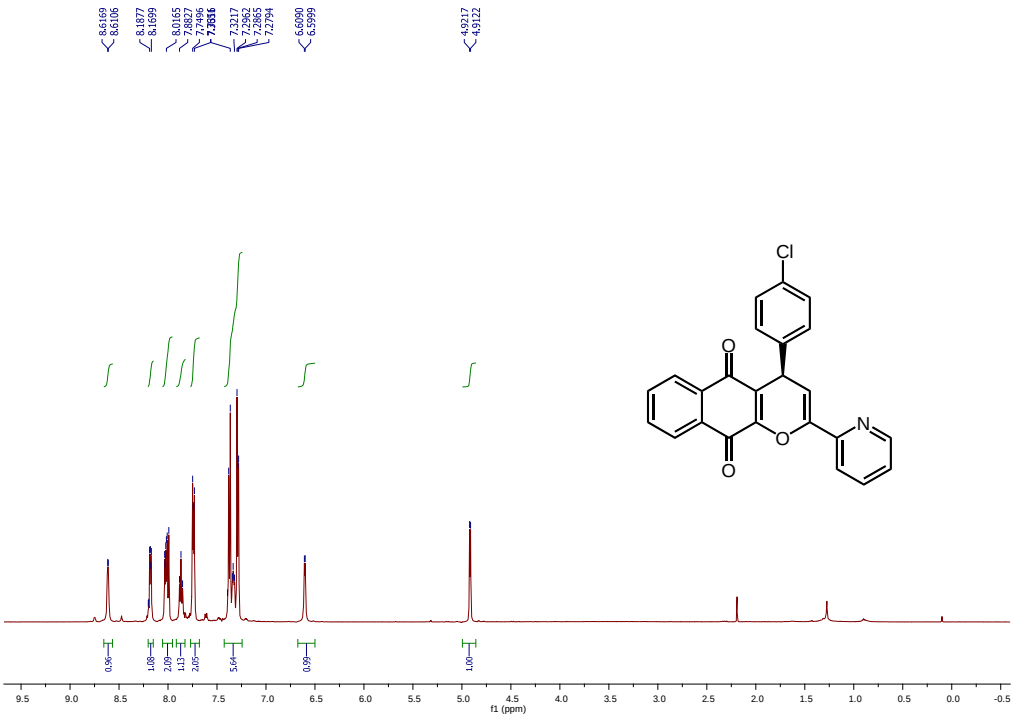
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.501	VB	0.2966	2.39607e4	1222.76404	50.4765
2	16.859	BB	0.6085	2.35083e4	575.57910	49.5235
Totals :				4.74691e4	1798.34314	

HPLC graph of compound **12c** (racemic)

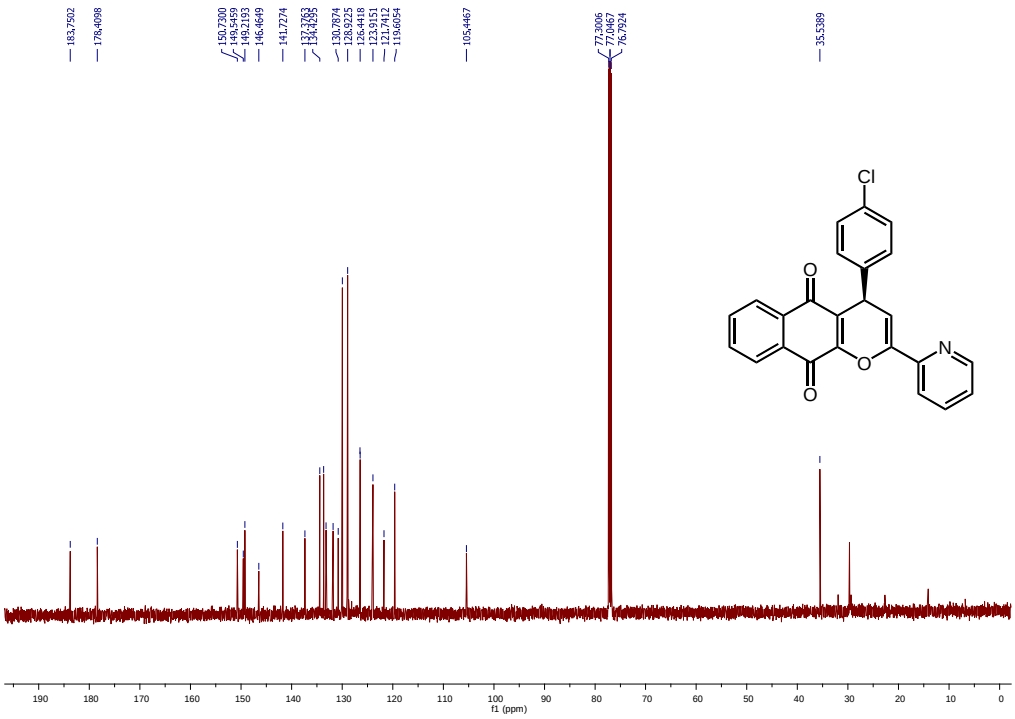


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.590	BB	0.3189	677.65234	32.02551	1.9713
2	16.918	BB	0.6019	3.36980e4	833.16016	98.0287
Totals :				3.43757e4	865.18567	

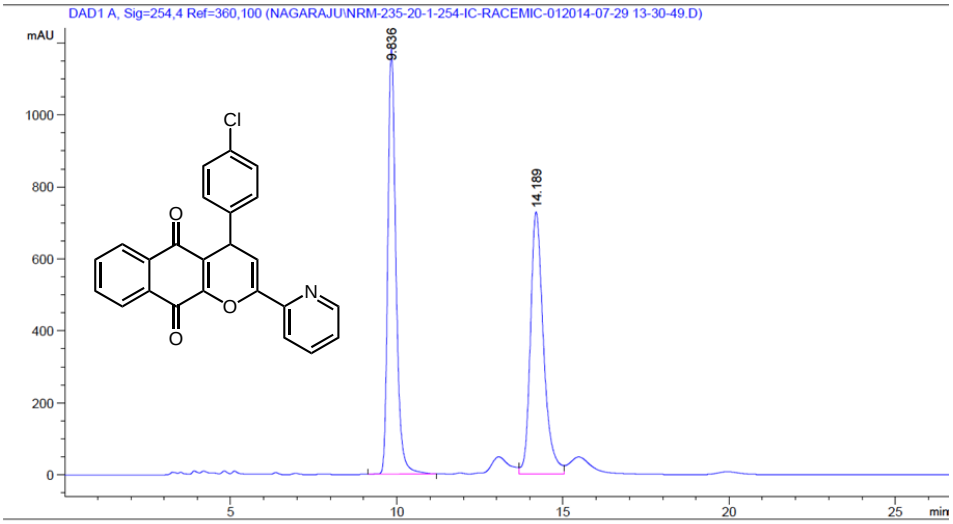
HPLC graph of compound **12c** (enantioenriched)



500 MHz ^{1}H NMR spectra of compound **12d** in $CDCl_3$

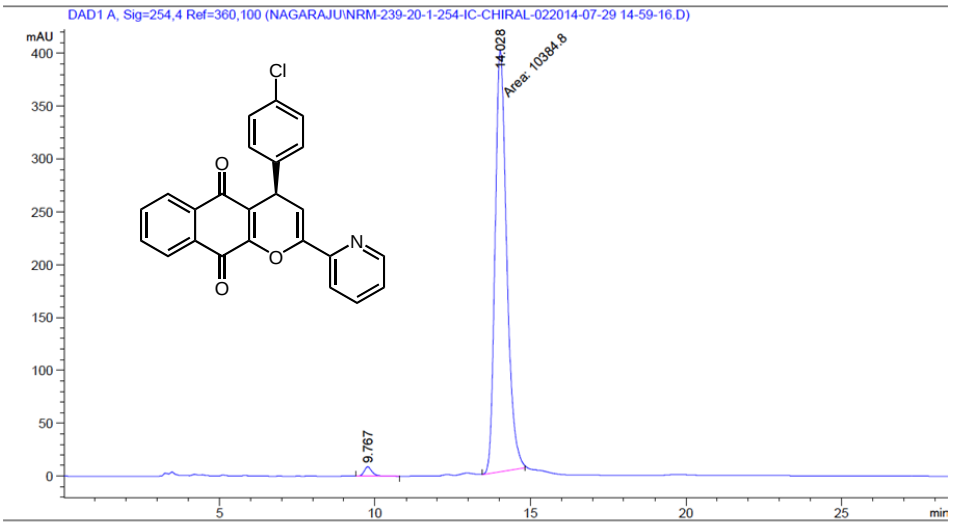


125 MHz ^{13}C NMR spectra of compound **12d** in $CDCl_3$



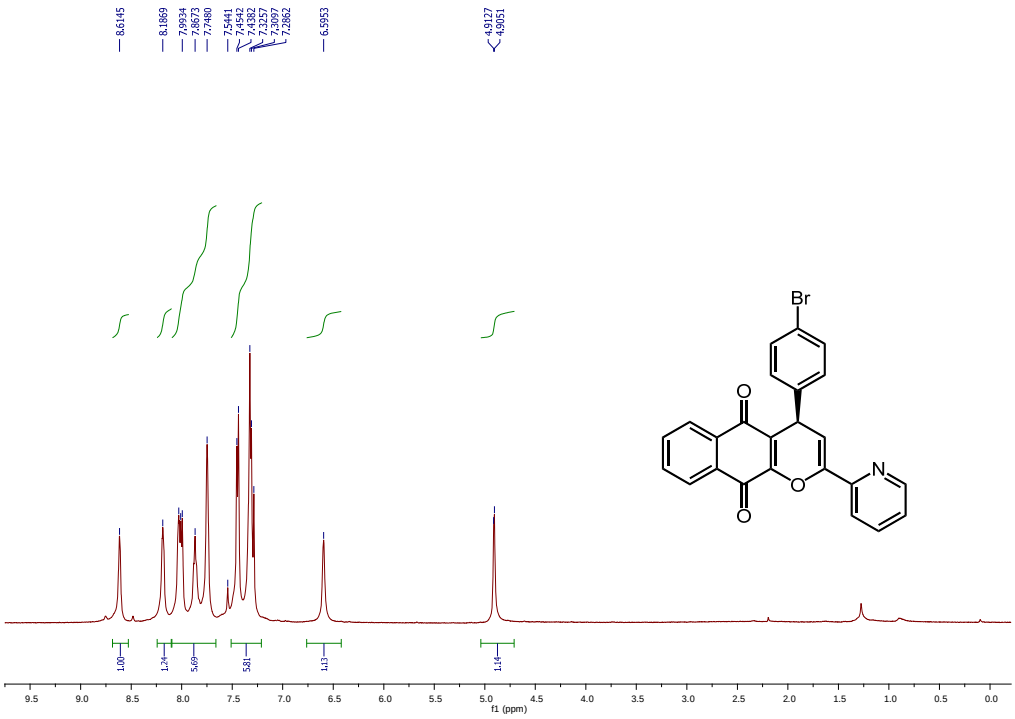
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.836	BB	0.2578	2.00293e4	1181.48499	50.0449
2	14.189	VV	0.4139	1.99934e4	729.10400	49.9551
Totals :				4.00227e4	1910.58899	

HPLC graph of compound **12d** (racemic)

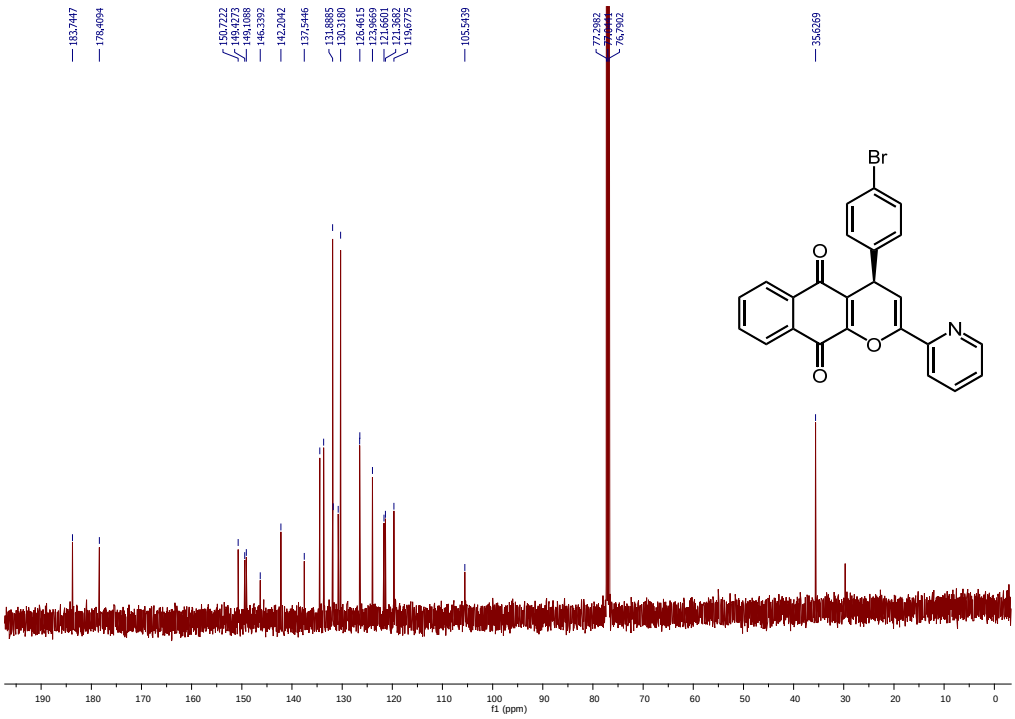


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.767	BB	0.2644	152.39029	8.78471	1.4462
2	14.028	MM	0.4342	1.03848e4	398.64413	98.5538
Totals :				1.05372e4	407.42884	

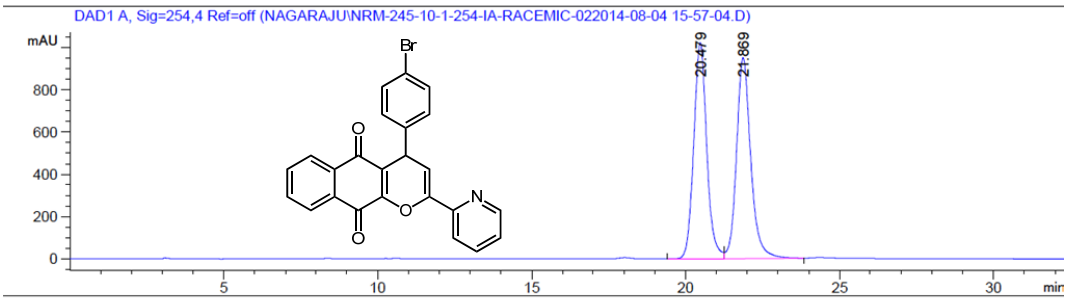
HPLC graph of compound **12d** (enantioenriched)



500 MHz ^{1}H NMR spectra of compound **12e** in $CDCl_3$

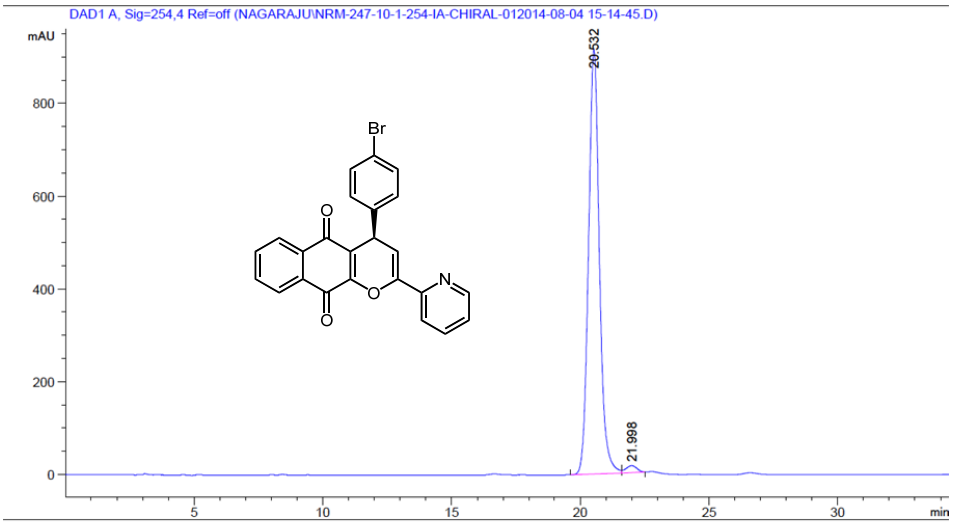


125 MHz ^{13}C NMR spectra of compound **12e** in $CDCl_3$



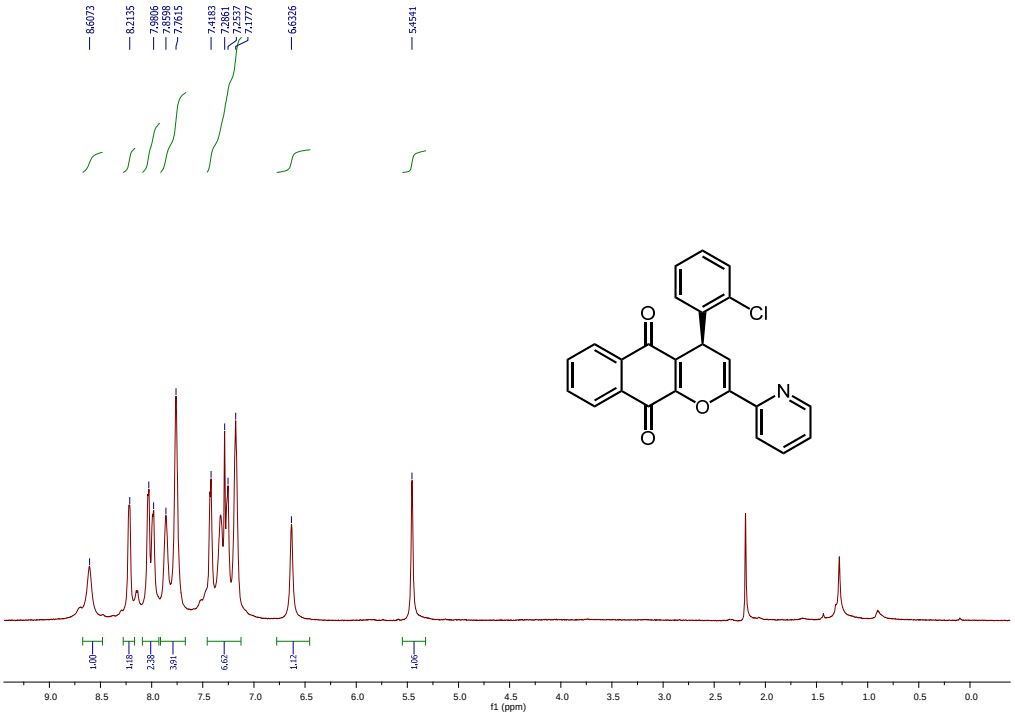
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.479	BV	0.4484	2.99385e4	1020.17767	49.5177
2	21.869	VB	0.4872	3.05216e4	948.96906	50.4823
Totals :				6.04601e4	1969.14673	

HPLC Graph of compound **12e** (racemic)

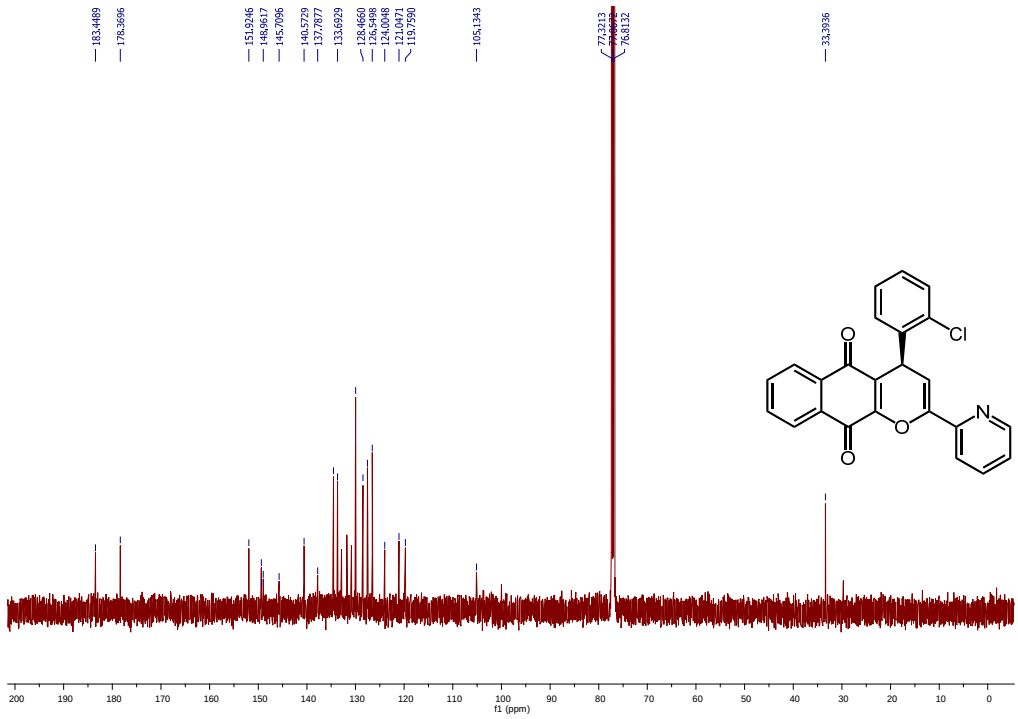


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.532	BV	0.4485	2.68560e4	914.68817	98.3338
2	21.998	VB	0.4660	455.05002	15.08413	1.6662
Totals :				2.73110e4	929.77230	

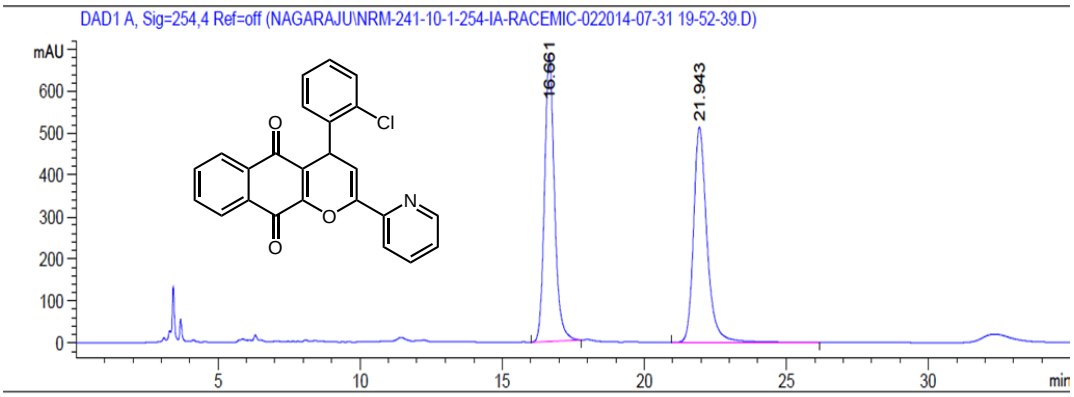
HPLC Graph of compound **12e** (enantioenriched)



500 MHz ^{1}H NMR spectra of compound **12g** in $CDCl_3$

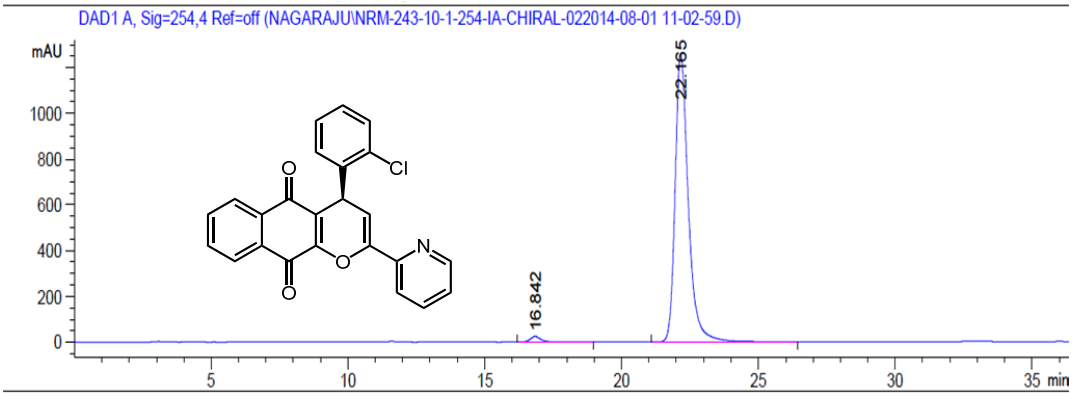


125 MHz ^{13}C NMR spectra of compound **12g** in $CDCl_3$



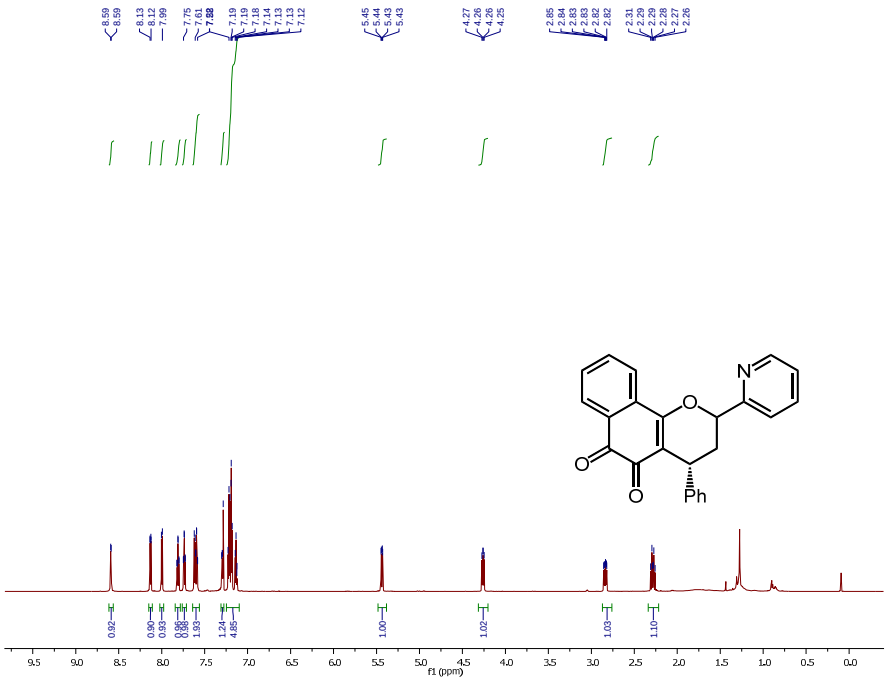
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.661	BB	0.3673	1.65997e4	683.53534	49.5724
2	21.943	BB	0.4952	1.68861e4	514.07507	50.4276
Totals :				3.34858e4	1197.61041	

HPLC graph of compound **12g** (racemic)

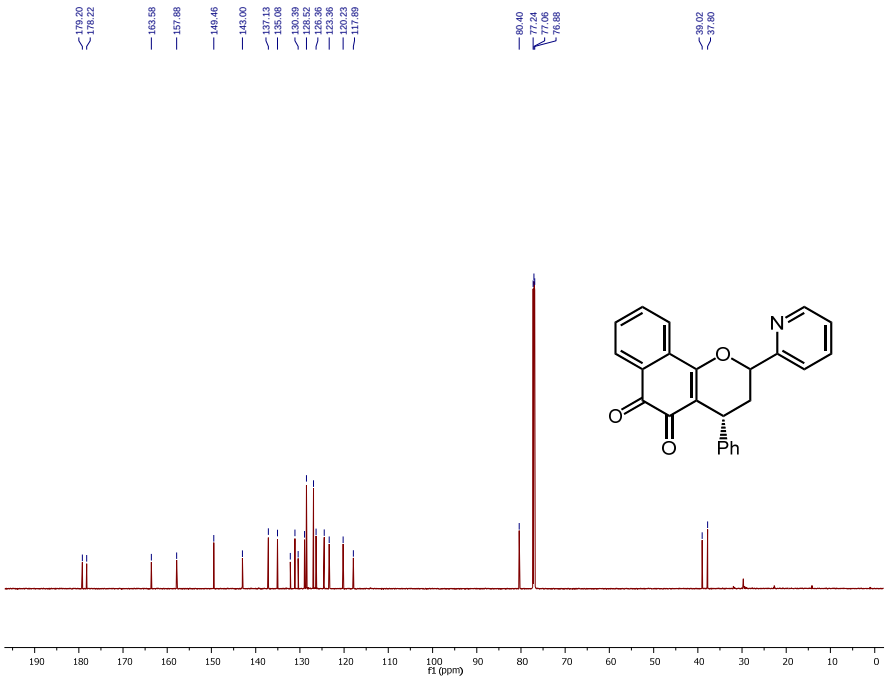


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.842	BB	0.4287	699.95898	24.54583	1.6343
2	22.165	BB	0.5047	4.21280e4	1258.02356	98.3657
Totals :				4.28280e4	1282.56939	

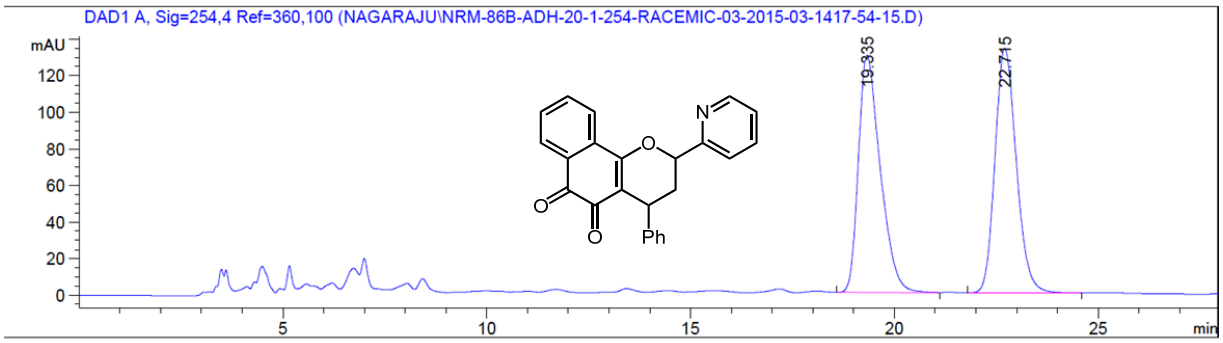
HPLC graph of compound **12g** (enantioenriched)



700 MHz ^{1}H NMR spectra of compound **13a** in $CDCl_3$

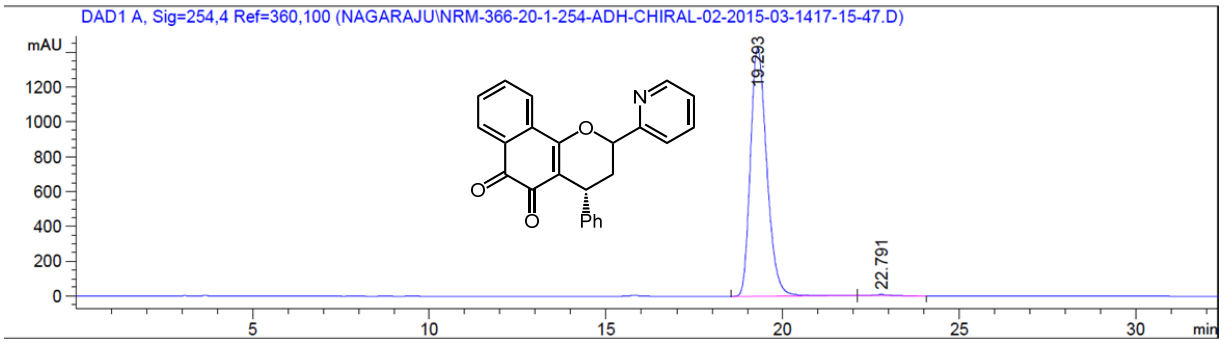


175 MHz ^{13}C NMR spectra of compound **13a** in $CDCl_3$



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.335	BB	0.5547	4833.99316	129.72635	49.7830
2	22.715	BB	0.5674	4876.13916	133.72658	50.2170

HPLC graph of compound **13a** (racemic)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.293	BB	0.4980	4.58966e4	1424.16162	99.4864
2	22.791	BB	0.5648	236.92154	6.50613	0.5136

HPLC graph of compound **13a** (enantioenriched)