SUPPORTING INFORMATION

Organocatalytic Asymmetric Addition of Aromatic *α*-Cyanoketones to *o*-Quinone Methides: Synthesis of 3,4-Dihydrocoumarins and Tetra-Substituted Chromans

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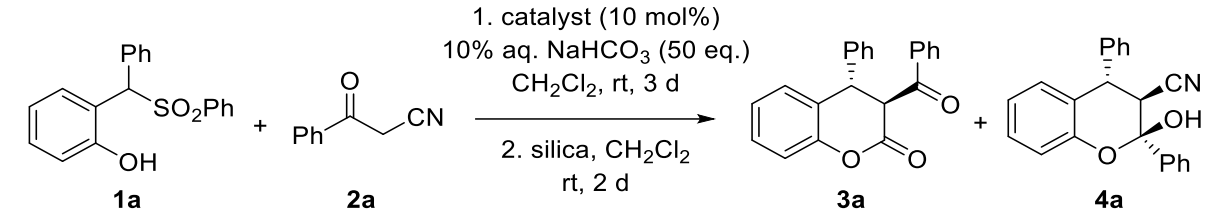
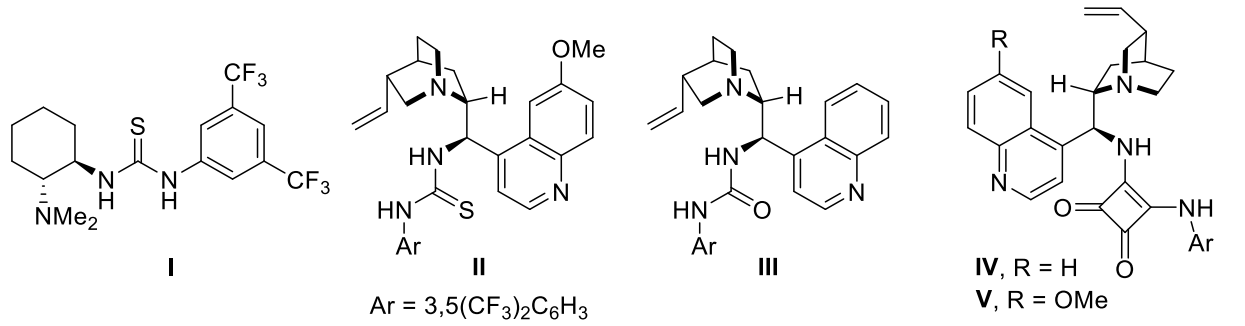
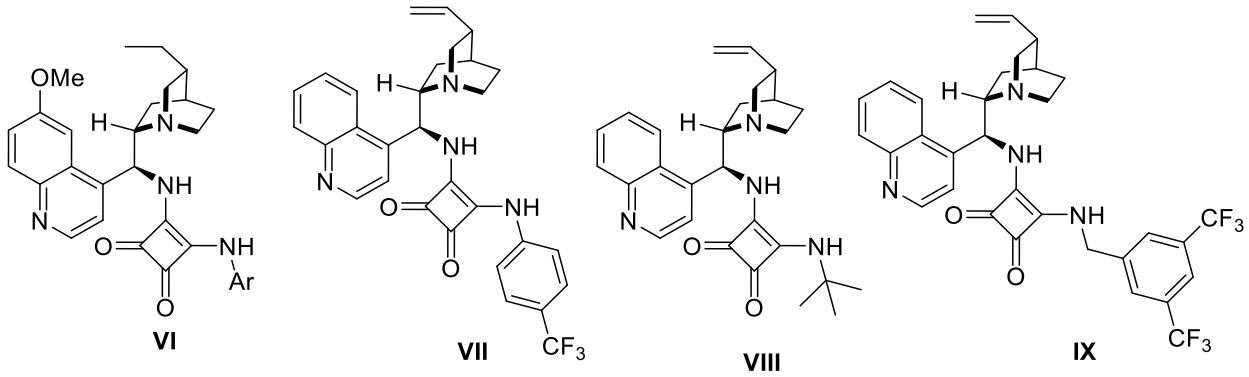
1. Optimization table:

Table 1. Catalyst screening





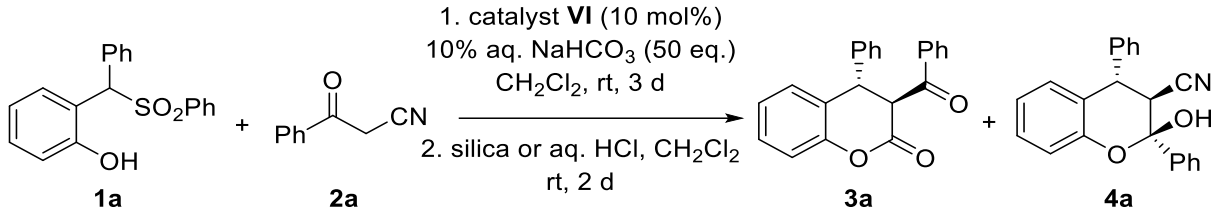


entry[a]	catalyst	**3a/4a**[b]	yield (**3a**)[c]	dr (**3a**)[d]	ee (**3a**)[e]
1	**I**	2.2:1	59	>20:1	72
2	**II**	1.9:1	58	>20:1	76
3	**III**	1.5:1	54	>20:1	74
4	**IV**	1.6:1	52	>20:1	94
5	**V**	1.2:1	48	>20:1	96
6	**VI**	**1.7:1**	**57**	**>20:1**	**96**

7	**VII**	1.2:1	52	>20:1	92
8	**VIII**	0.2:1	12	>20:1	90
9	**IX**	2.1:1	41	>20:1	92

[a]Reaction condition: Unless otherwise mentioned, 0.05 mmol of **1a** and 0.1 mmol of **2a** in 0.6 mL CH_2Cl_2 using 10 mol% catalyst and 10% aq. $NaHCO_3$ at room temperature for 3 days and then work up using 1 N HCl/CH_2Cl_2 and and then 100 mg silica (60-120 mesh) in 1 mL CH_2Cl_2 at room temperature for 2 days. [b]Determined by ^{1}H NMR. [c]Isolated yield of **3a** after silica gel column chromatography. [d]Determined by ^{1}H NMR. [e]Determined by HPLC using stationary phase chiral column.

Table 2. Acidic condition and catalyst loading optimization

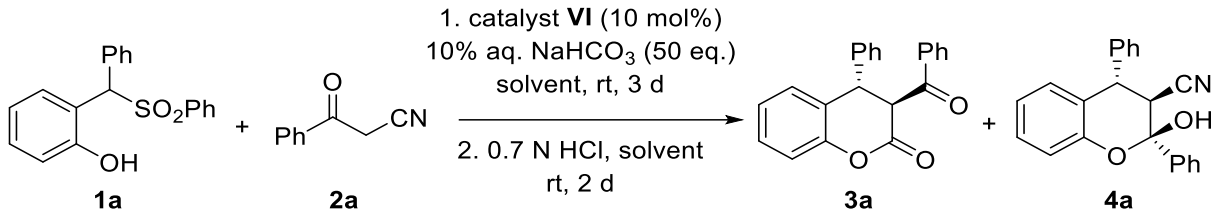


entry[a]	acidic conditions	**3a**/**4a**[b]	yield (**3a**)[c]	dr (**3a**)[d]	ee (**3a**)[e]
1	aq. work up then stirring with 100 mg silica	0.8:1	46	>20:1	92
2	1 N HCl work up then stirring with 100 mg silica	1.7:1	57	>20:1	96
3	1 N HCl work up then stirring with 300 mg silica	0.8:1	25	>20:1	96
4	1 N HCl work up then stirring with 500 mg silica	0.6:1	21	>20:1	97

5	0.3 N HCl work up then stirring with 1 mL 0.3 N HCl	1.3:1	56	>20:1	95
6	0.5 N HCl work up then stirring with 1 mL 0.5 N HCl	2.8:1	70	>20:1	98
7	0.7 N HCl work up then stirring with 1 mL 0.7 N HCl	**3.9:1**	**78**	**>20:1**	**98**
8	1 N HCl work up then stirring with 1 mL 1 N HCl	2.1:1	67	>20:1	97
9	3 N HCl work up then stirring with 1 mL 3 N HCl	2:1	63	>20:1	98
10	6 N HCl work up then stirring with 1 mL 6 N HCl	2:1	63	>20:1	92
11	9 N HCl work up then stirring with 1 mL 9 N HCl	1.9:1	61	>20:1	87
12[f]	0.7 N HCl work up then stirring with 1 mL 0.7 N HCl	2.7:1	69	>20:1	98

[a]Reaction condition: 0.05 mmol of **1a** and 0.1 mmol of **2a** in 0.6 mL CH_2Cl_2 using 10 mol% **VI** catalyst and 10% aq. $NaHCO_3$ at room temperature for 3 days and then work up and then stirring under acidic conditions using 1 mL CH_2Cl_2 at room temperature for 2 days. [b]Determined by ^1H NMR. [c]Isolated yield of **3a**. [d]Determined by ^1H NMR. [e]Determined by HPLC using stationary phase chiral column. [f]5 mol% catalyst **VI** was used instead of 10 mol%.

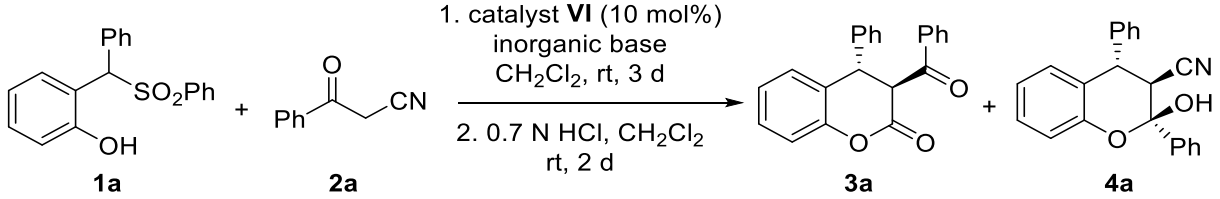
Table 3. Solvent screening



entry[a]	solvent	**3a/4a**[b]	yield (**3a**)[c]	dr (**3a**)[d]	ee (**3a**)[e]
1	**CH_2Cl_2**	**3.9:1**	**78**	**>20:1**	**98**
2	$CHCl_3$	3.3:1	75	>20:1	98
3	$(CH_2Cl)_2$	2.5:1	67	>20:1	86
4	Et_2O	0.2:1	17	>20:1	66
5	toluene	2.3:1	64	>20:1	90
6	$PhCF_3$	4.3:1	80	>20:1	94

[a]Reaction condition: 0.05 mmol of **1a** and 0.1 mmol of **2a** in 0.6 mL solvent using 10 mol% **VI** catalyst and 10% aq. $NaHCO_3$ at room temperature for 3 days and then acidic work up followed by stirring with 0.7 N HCl in 1 mL same solvent at room temperature for 2 days. [b]Determined by ^{1}H NMR. [c]Isolated yield of **3a**. [d]Determined by ^{1}H NMR. [e]Determined by HPLC using stationary phase chiral column.

Table 4. Inorganic base optimization



entry[a]	inorganic base [eq.]	**3a/4a**[b]	yield (**3a**)[c]	dr (**3a**)[d]	ee (**3a**)[e]
1	**10% aq. $NaHCO_3$ [50]**	**3.9:1**	**78**	**>20:1**	**98**
2	10% aq. Na_2CO_3 [50]	4.3:1	80	>20:1	89

3	10% aq. K_2CO_3 [50]	3.3:1	72	>20:1	70
4	10% aq. $NaHCO_3$ [25]	2.8:1	68	>20:1	97
5	10% aq. $NaHCO_3$ [10]	2.9:1	70	>20:1	96
6	10% aq. $NaHCO_3$ [2]	0.9:1	46	>20:1	99

[a]Reaction condition: 0.05 mmol of **1a** and 0.1 mmol of **2a** in 0.6 mL CH_2Cl_2 using 10 mol% **VI** catalyst and 10% aq. inorganic base at room temperature for 3 days and then acidic work up followed by stirring with 0.7 N HCl and 1 mL CH_2Cl_2 at room temperature for 2 days. [b]Determined by ^{1}H NMR. [c]Isolated yield of **3a**. [d]Determined by ^{1}H NMR. [e]Determined by HPLC using stationary phase chiral column.

2. Crystal structure of products (3u) & (4j) for absolute stereochemistry determination:

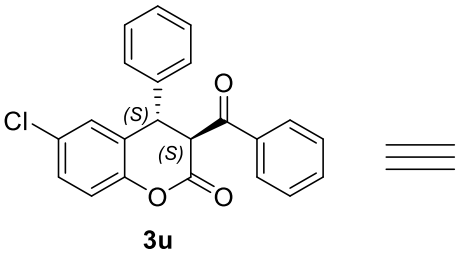
Single-crystal X-ray diffraction data were collected on a Bruker KAPPA APEX II DUO diffractometer using graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å). Data collection was carried out at 100 K. Temperature was controlled by an Oxford Cryostream cooling system (Oxford Cryostat). Cell refinement and data reduction were performed using the program SAINT. The structure was solved by direct methods and refined by full-matrix least-squares methods based on F^2 using SHELXL-2013.

a) Crystal Structure of Product (3u)

Method for crystal growth:

Dissolved 25mg of compound **3u** in 1ml hexane+1ml dicholomethane, kept it for slow evaporation.

Ellipsoid contour % probability levels in the caption for the image of the structure is 50.



3u

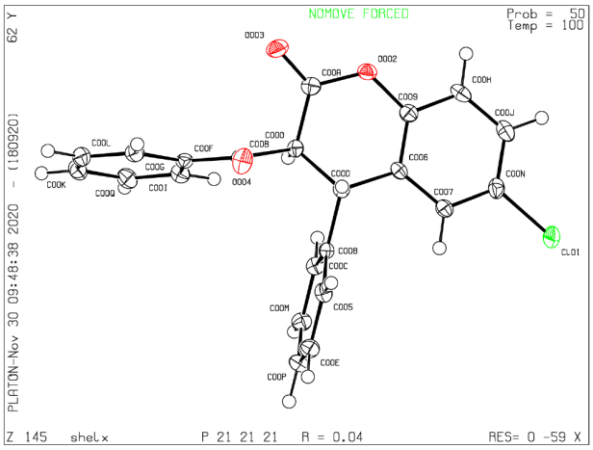


Table 5. Crystal data and structure refinement for compound 3u

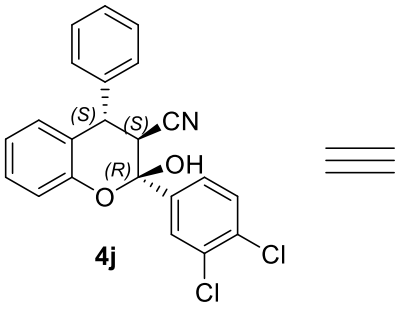
Parameters	3u
Moiety Formula	$C_{22}H_{15}ClO_3$
Sum Formula	C3.14 H2.14 Cl0.14 O0.43
Fw	51.83
Crystal system	orthorhombic
Space group	P 21 21 21
Hall group	P 2ac 2ab
a/Å	5.5812(3)
b/Å	16.1683(11)
c/Å	19.0660(14)
α/°	90
β/°	90
γ/°	90
V/Å^3	1720.5(2)
Z	28

Dx, g cm-3	1.401
Mu (mm-1)	0.241
F000	752.0
h, k, l max	7, 22, 26
T/K	100 K
Theta(max)	30.061
Nref	5032
Parameters refined	235
R (reflections)	0.0366(4394)
wR2 (reflections)	0.0945(5032)
GOF (F^2)	1.043
CCDC No.	**2047120**

b) Crystal Structure of Product (4j)

Method for crystal growth:

Dissolved 15mg of compound 3j in 1ml hexane+1ml dicholomethane, kept it for slow evaporation. Ellipsoid contour % probability levels in the caption for the image of the structure is 50.



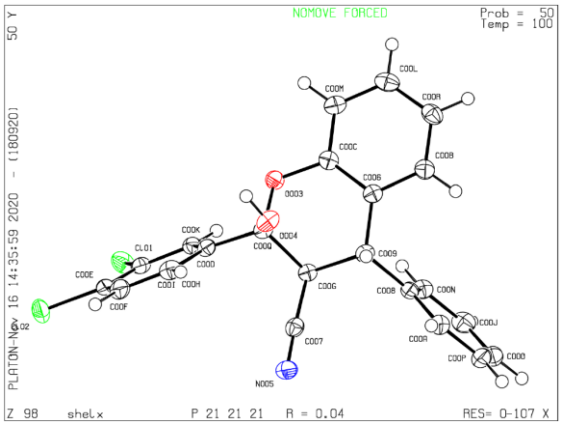


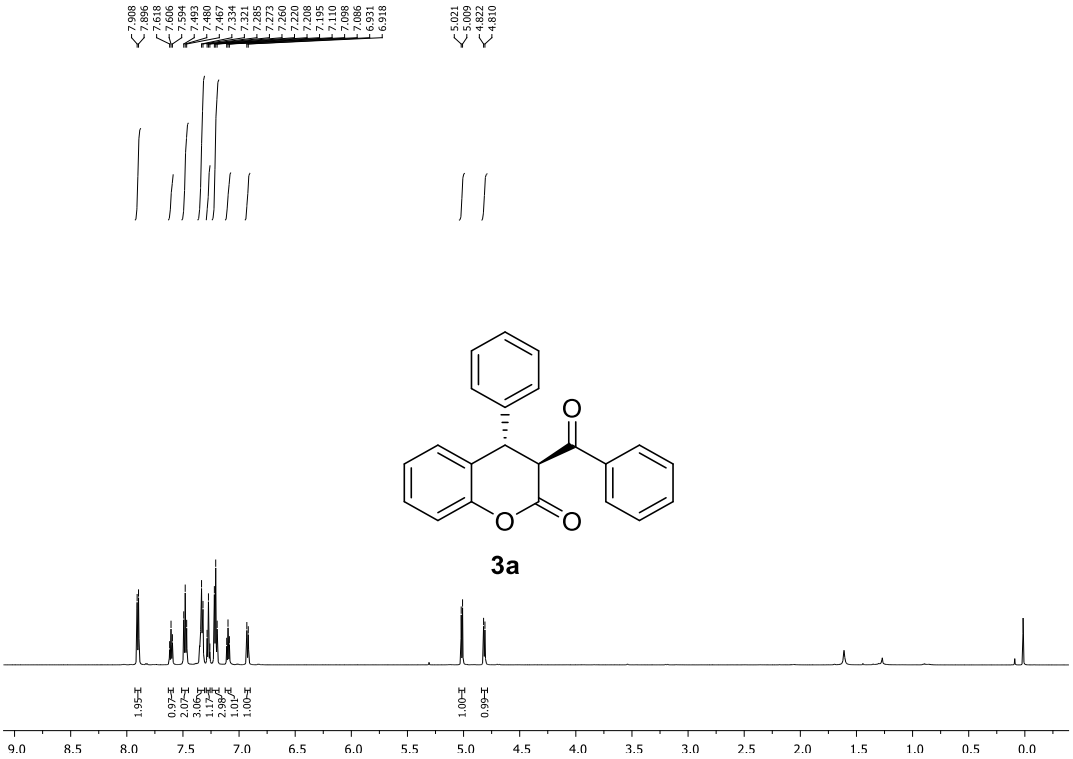
Table 6. Crystal data and structure refinement for compound 4j

Parameters	**4j**
Moiety Formula	$C_{22}H_{15}Cl_2NO_2$
Sum Formula	C3.67 H2.50 Cl0.33 N0.17 O0.33
Fw	66.04
Crystal system	orthorhombic
Space group	P 21 21 21
Hall group	P 2ac 2ab
a/Å	6.2728(4)
b/Å	12.0399(8)
c/Å	24.8487(18)
α/°	90
β/°	90
γ/°	90
V/Å^3	1876.7(2)
Z	24

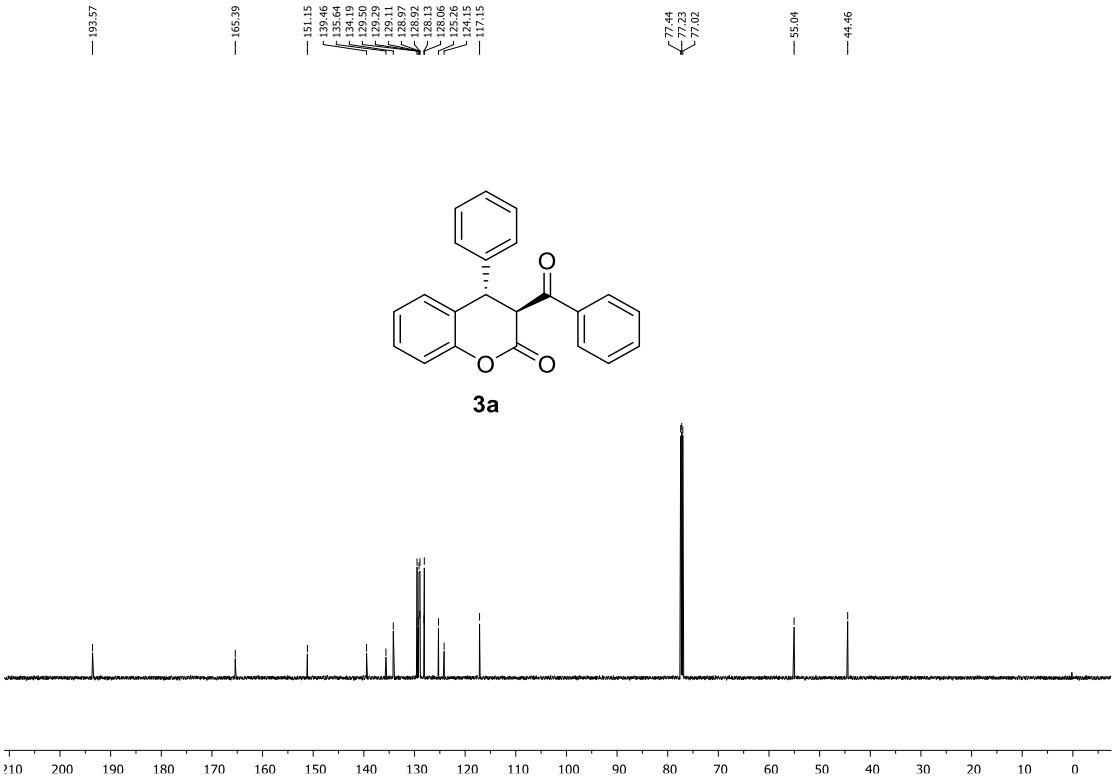
Dx, g cm-3	1.402
Mu (mm-1)	0.363
F000	816.0
h, k, l max	8, 16, 34
T/K	100 K
Theta(max)	30.042
Nref	5475
Parameters refined	245
R (reflections)	0.0385(4086)
wR2 (reflections)	0.0858(5475)
GOF (F^2)	0.939
CCDC No.	**2047123**

3. NMR spectra of the products:

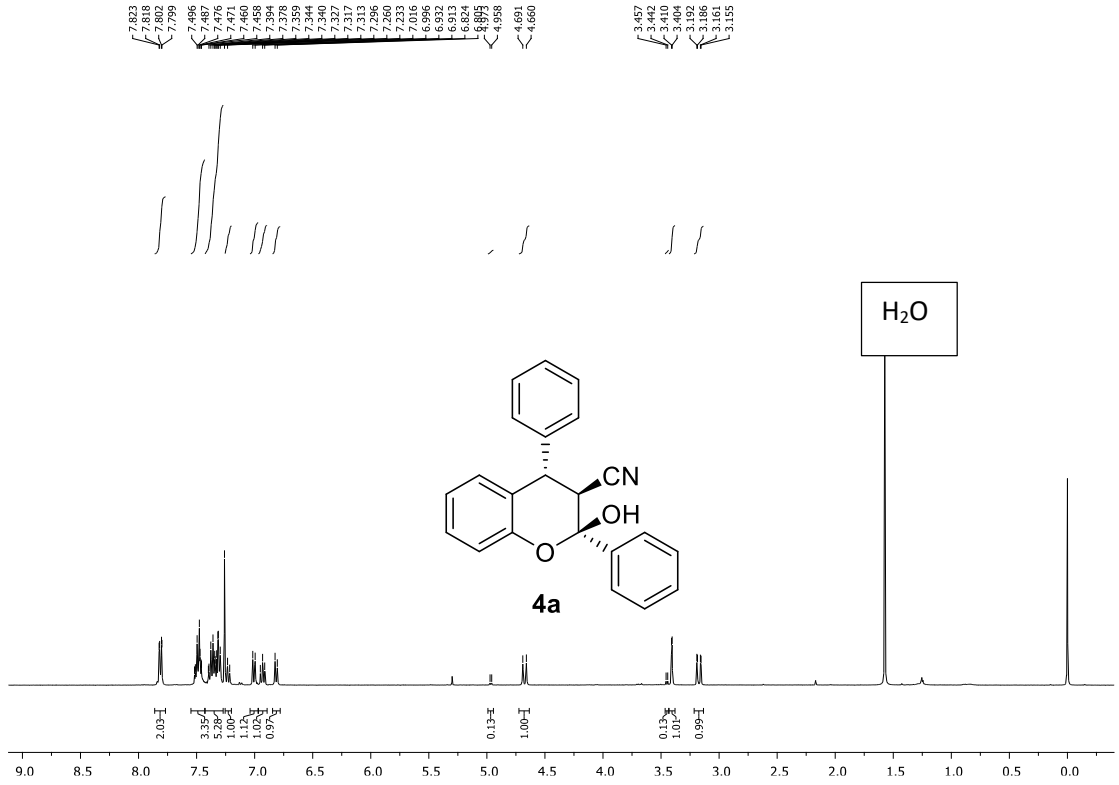
^{1}H NMR of 3a (600 MHz, $CDCl_3$)



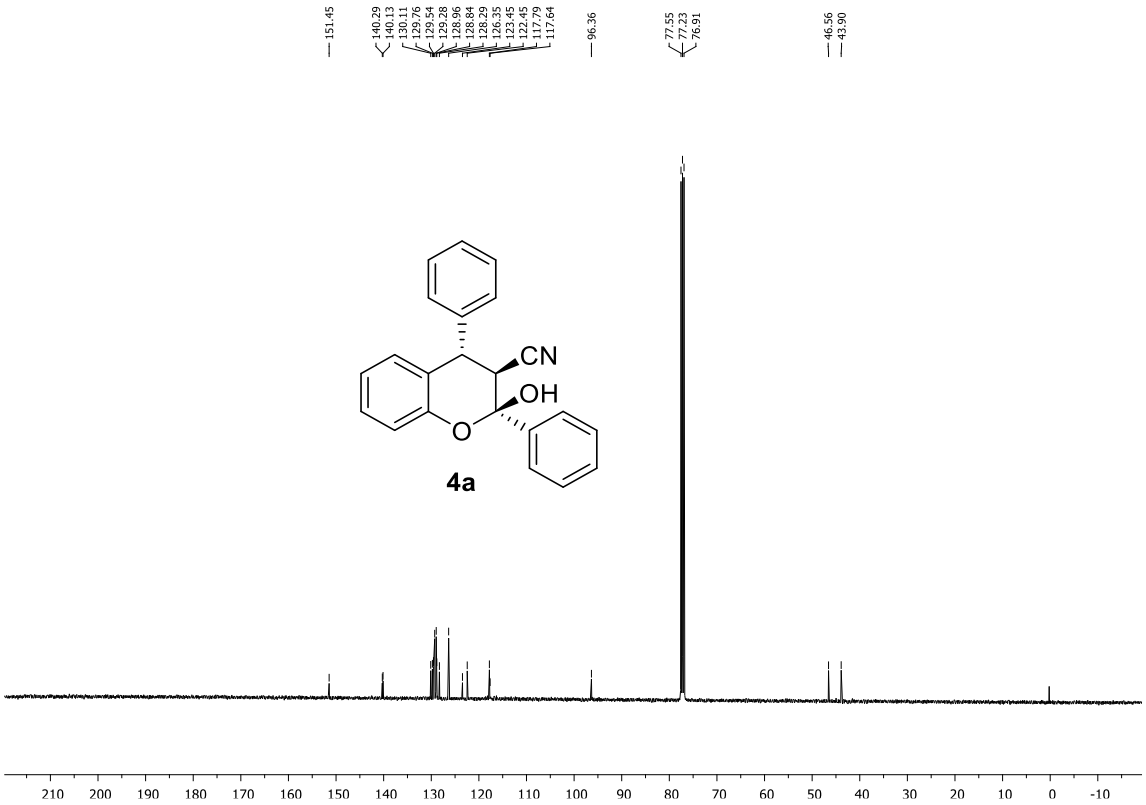
^{13}C{^{1}H} NMR of 3a (150 MHz, $CDCl_3$)



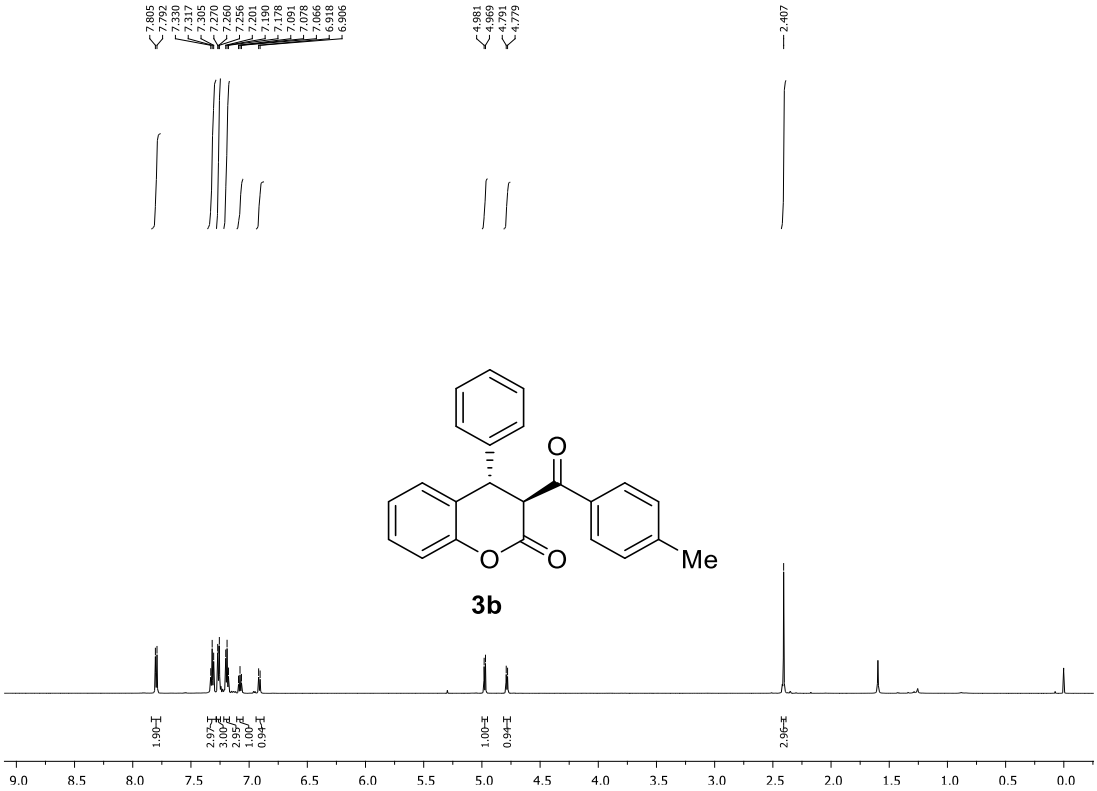
^{1}H NMR of 4a (400 MHz, $CDCl_3$)



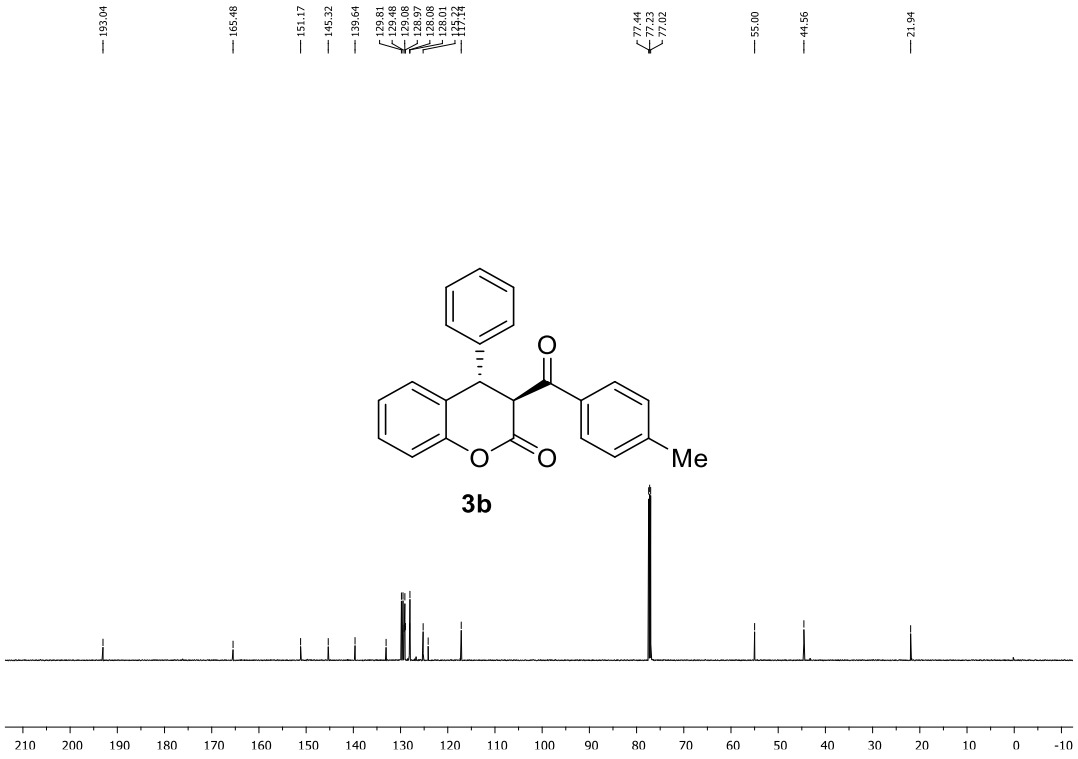
^{13}C{^{1}H} NMR of 4a (100 MHz, $CDCl_3$)



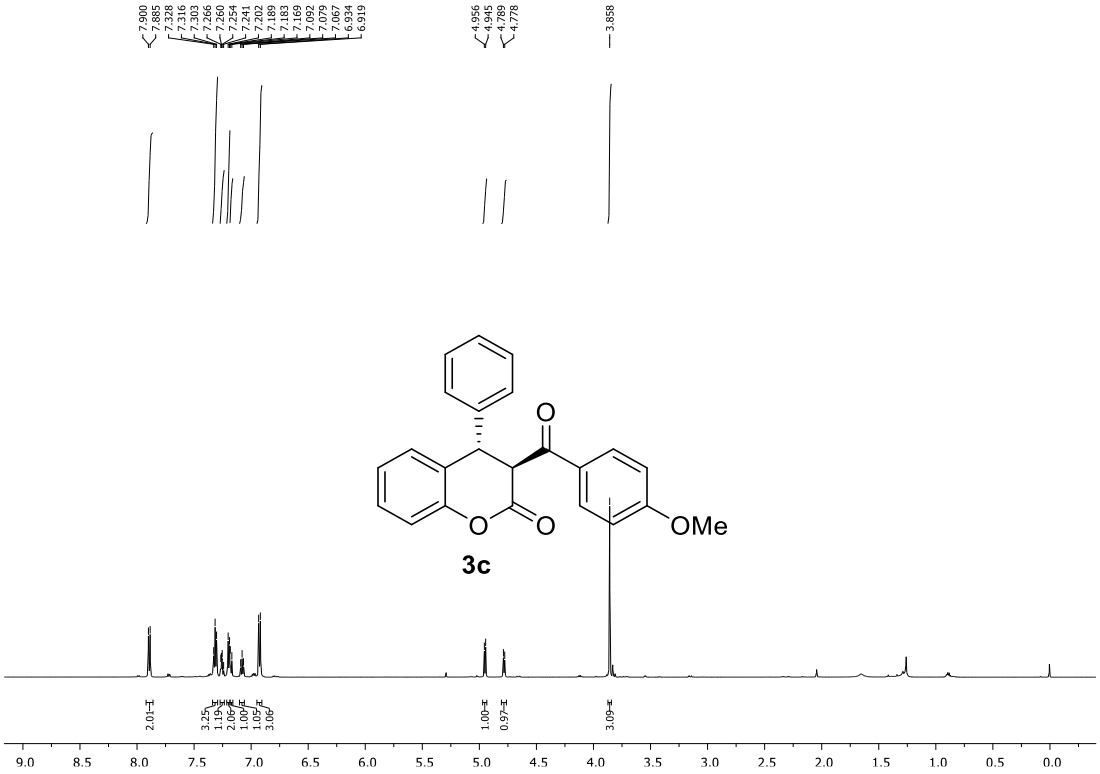
^{1}H NMR of 3b (600 MHz, $CDCl_3$)



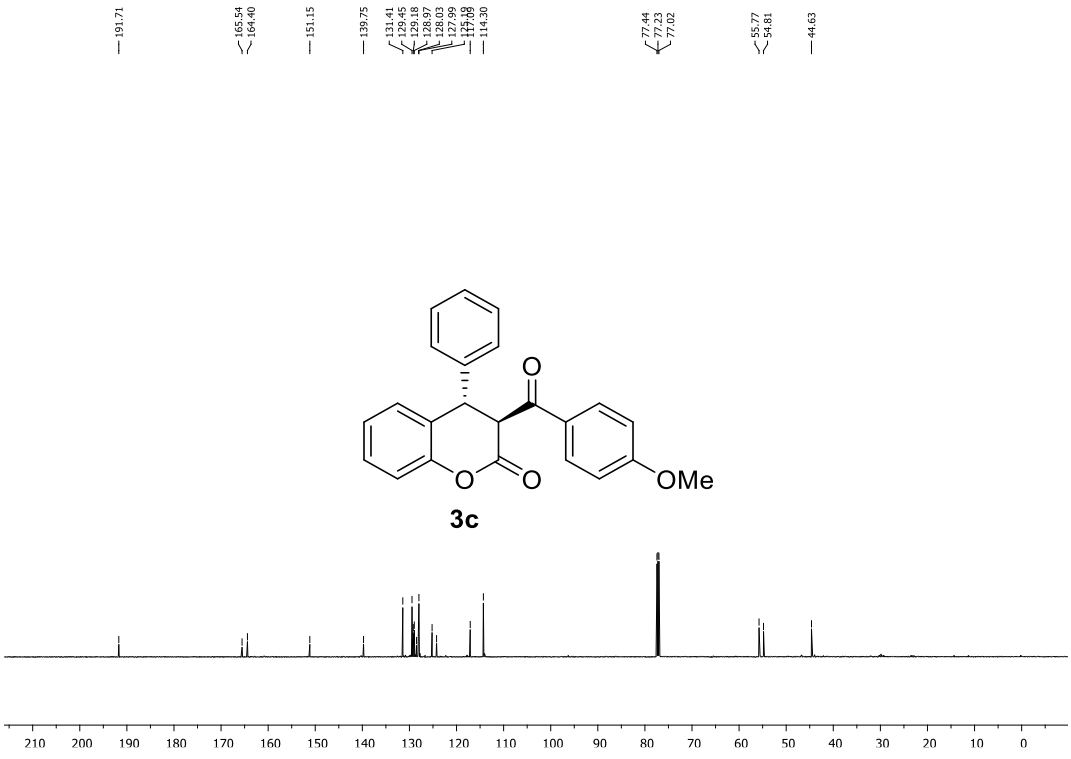
^{13}C{^{1}H} NMR of 3b (150 MHz, $CDCl_3$)



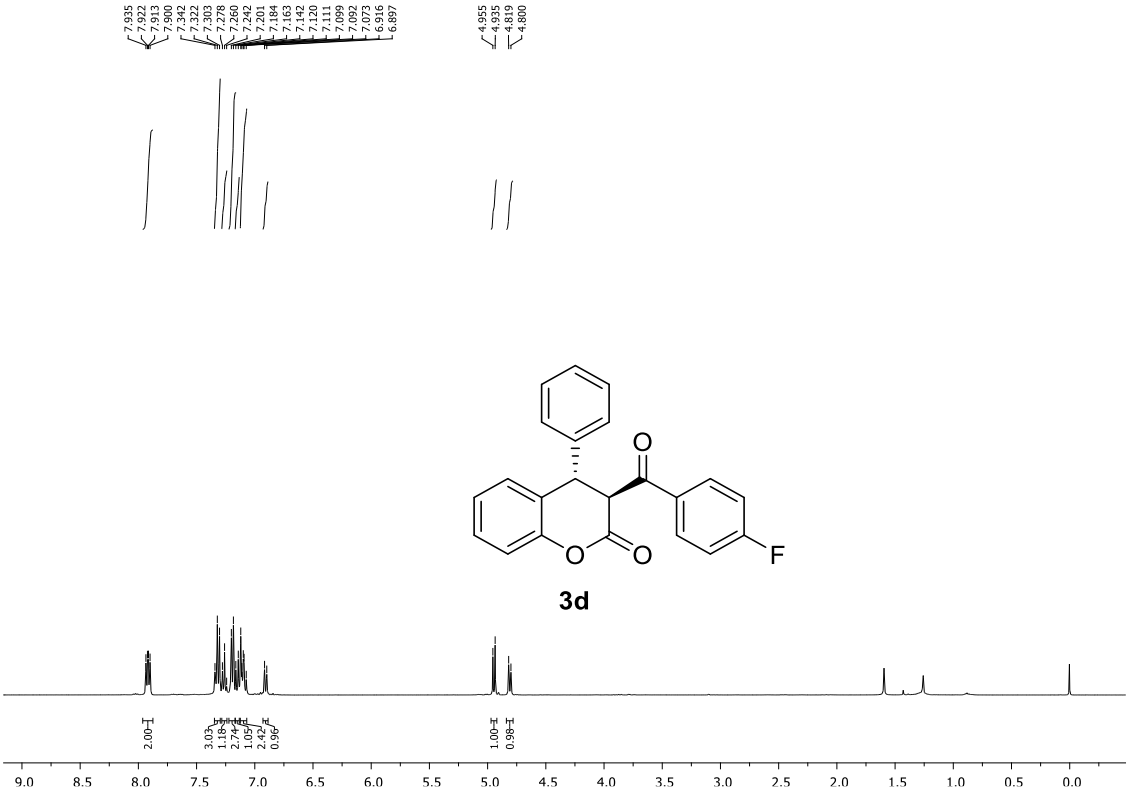
^{1}H NMR of 3c (600 MHz, $CDCl_3$)



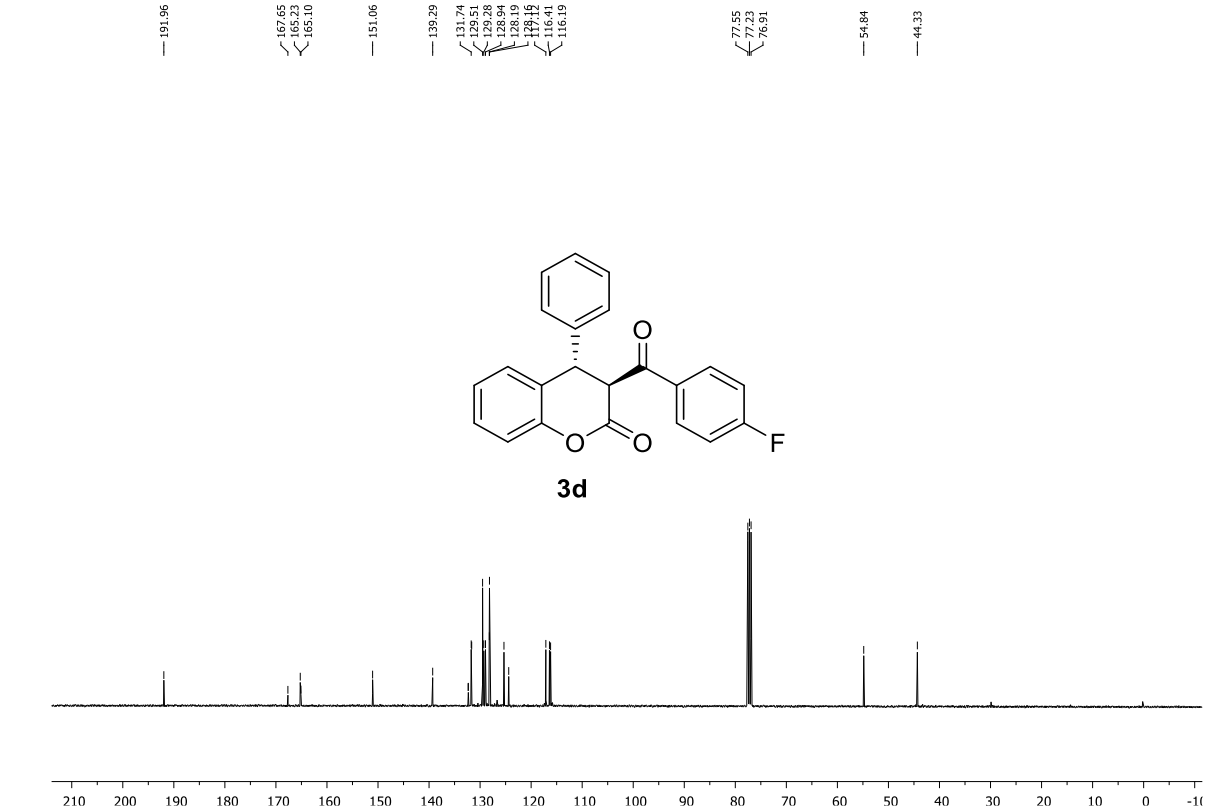
^{13}C{^{1}H} NMR of 3c (150 MHz, $CDCl_3$)



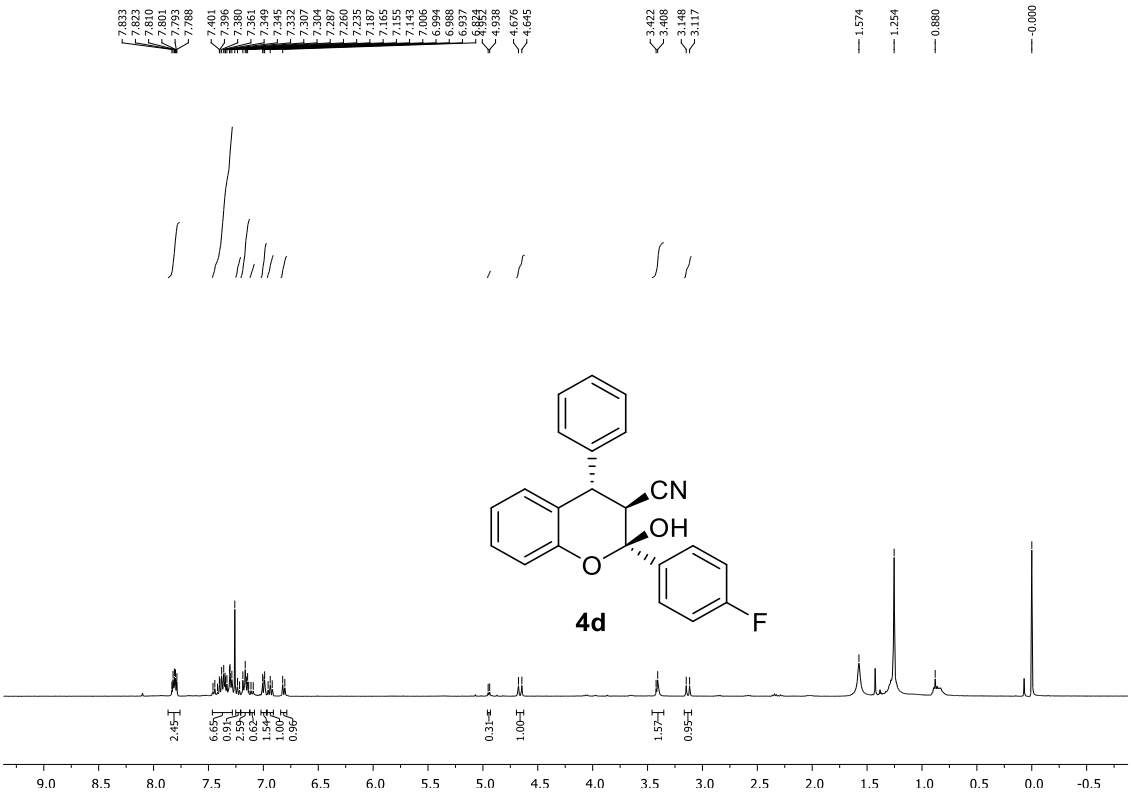
^{1}H NMR of 3d (400 MHz, $CDCl_3$)



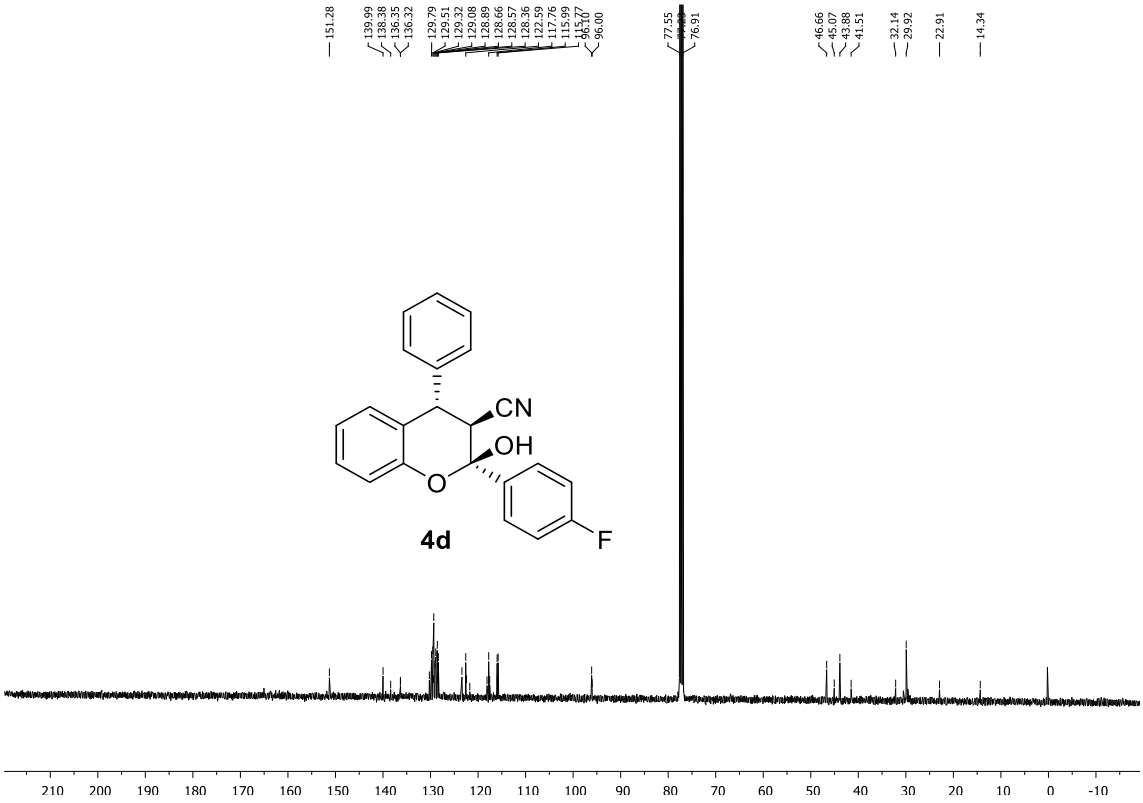
^{13}C{^{1}H} NMR of 3d (100 MHz, $CDCl_3$)



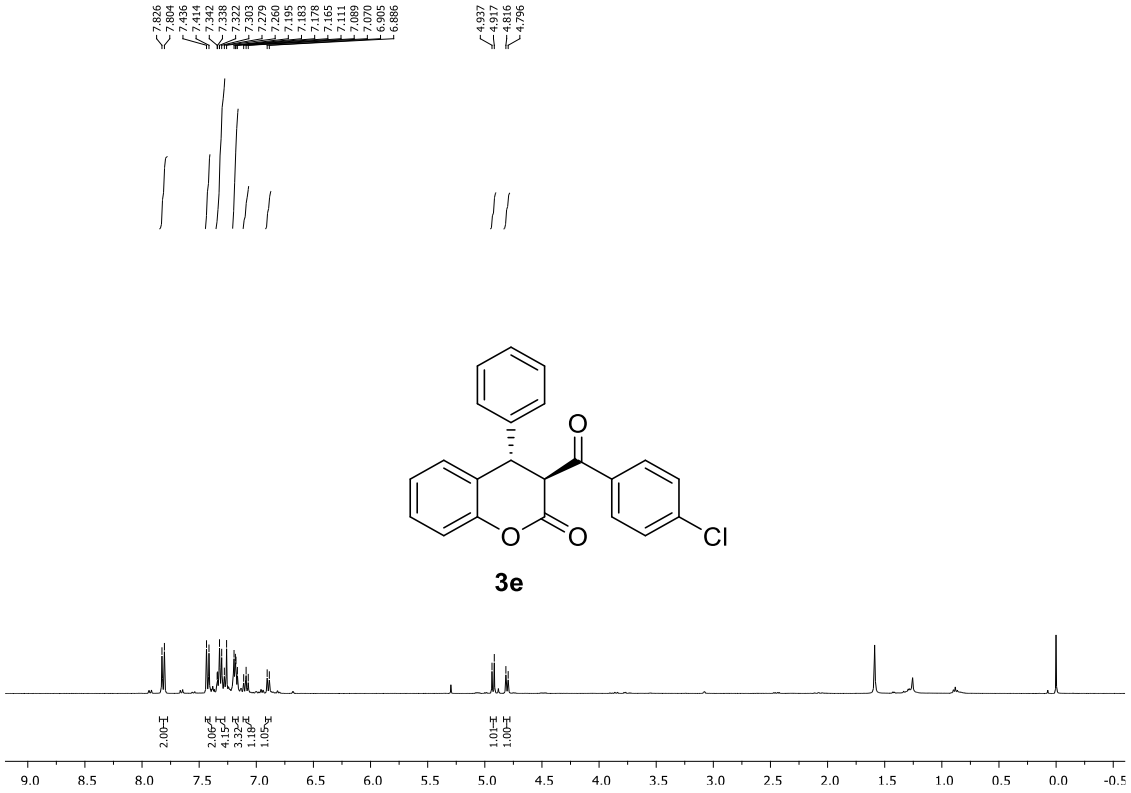
^{1}H NMR of 4d (400 MHz, $CDCl_3$)



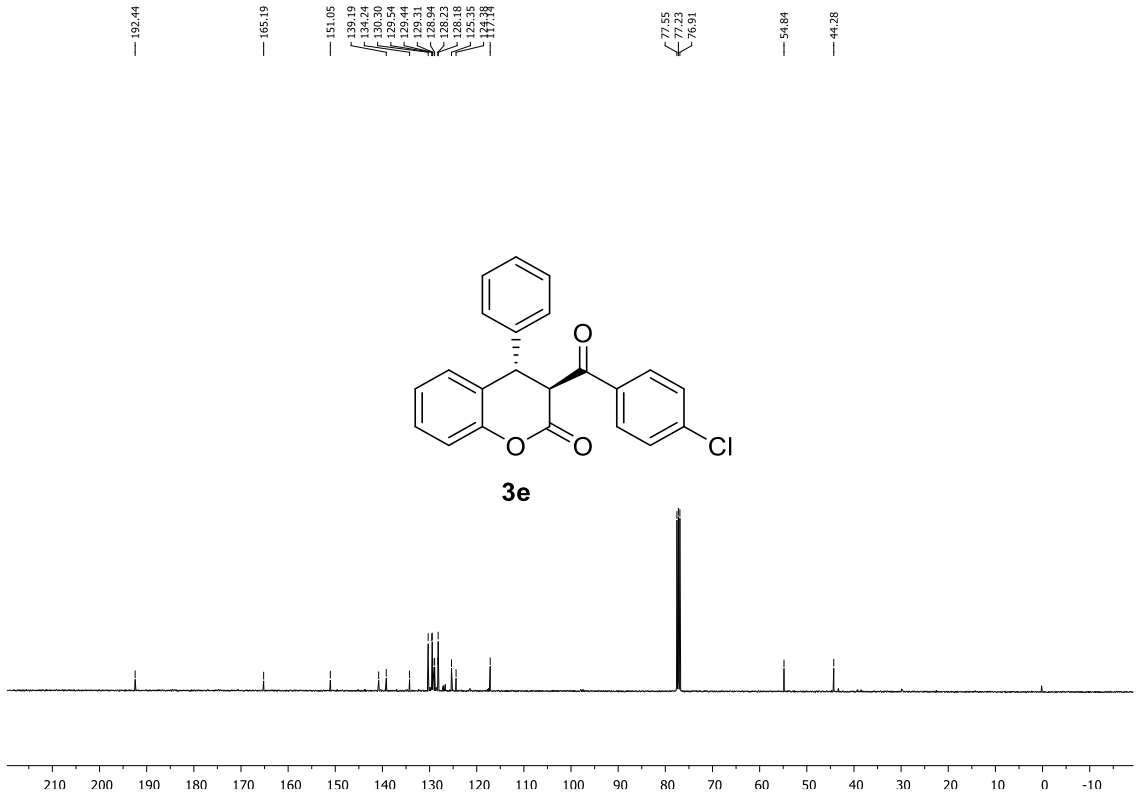
^{13}C{^{1}H} NMR of 4d (100 MHz, $CDCl_3$)



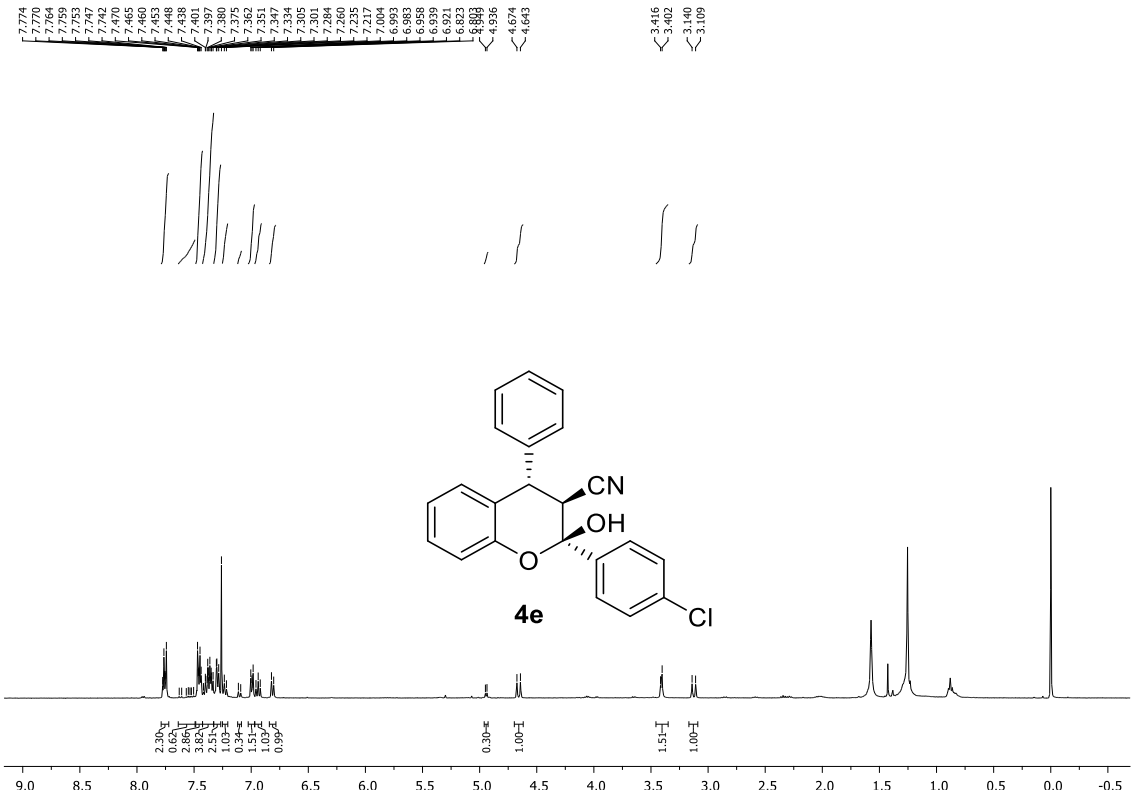
^{1}H NMR of 3e (400 MHz, $CDCl_3$)



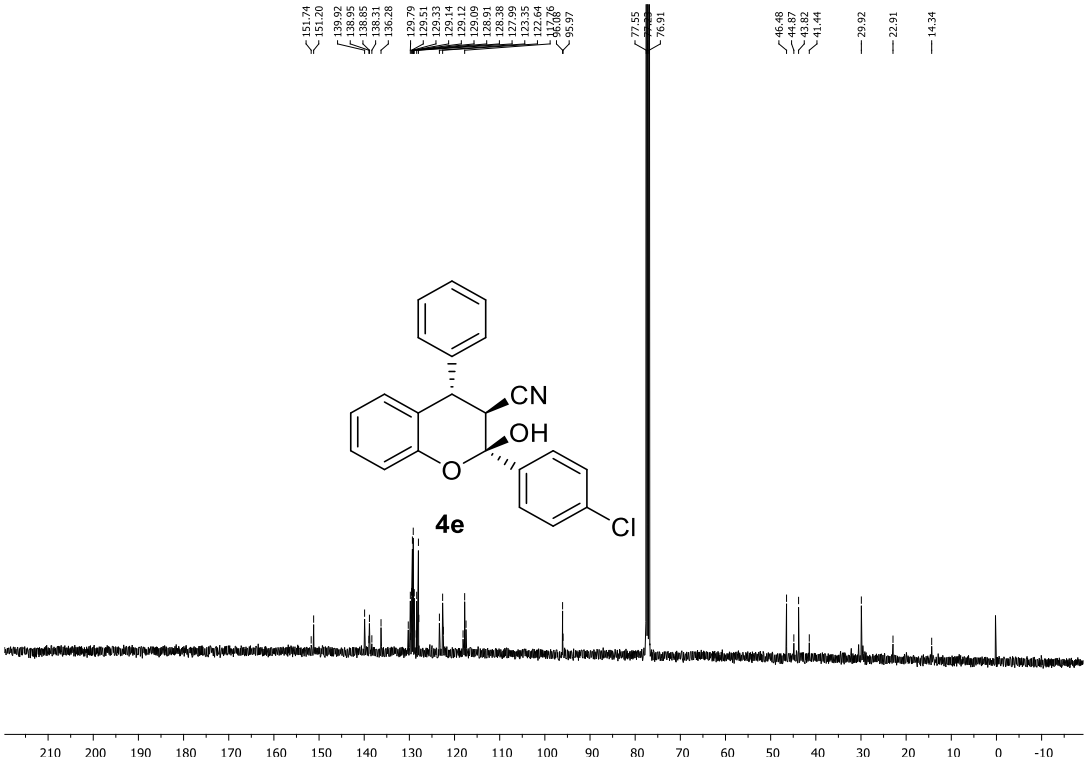
^{13}C{^{1}H} NMR of 3e (100 MHz, $CDCl_3$)



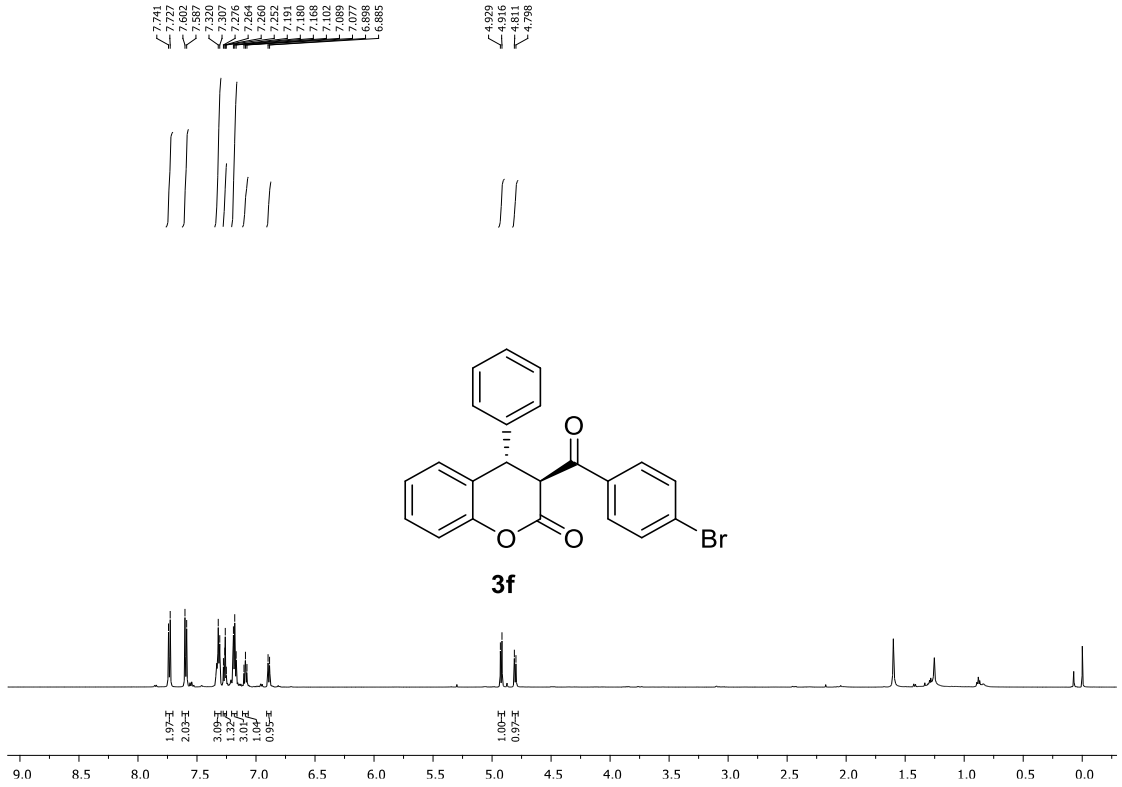
^{1}H NMR of 4e (400 MHz, $CDCl_3$)



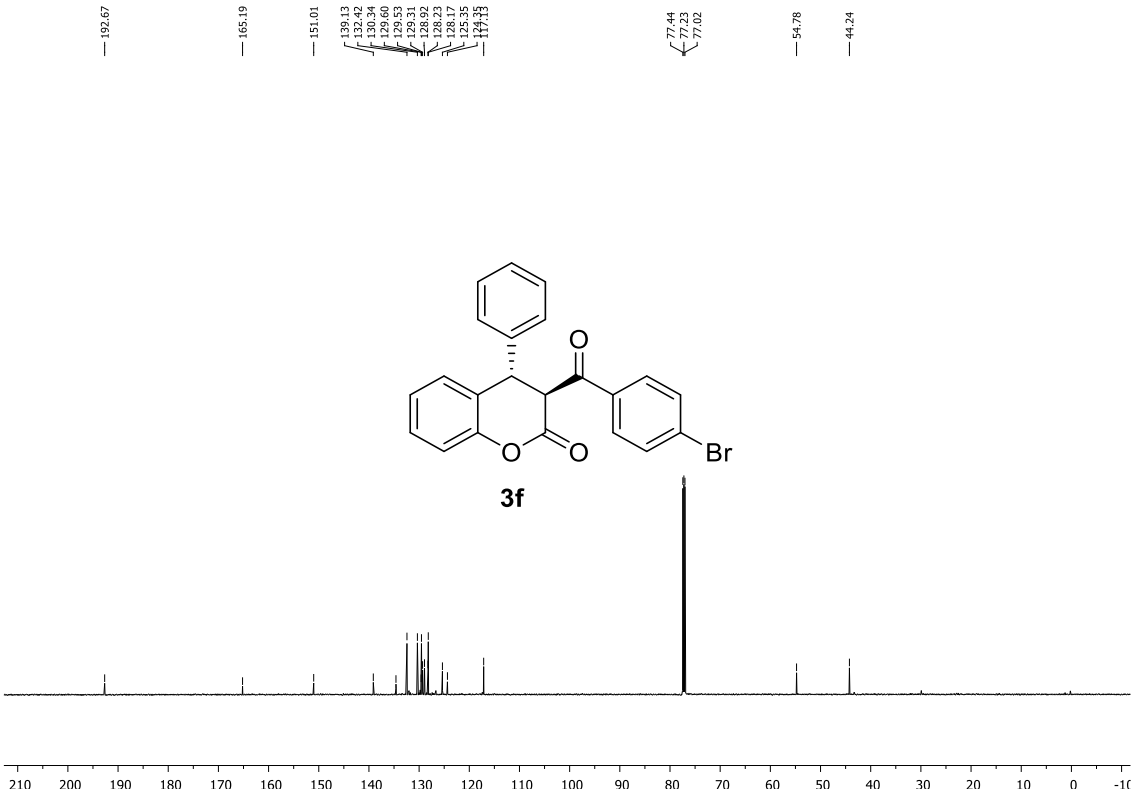
^{13}C{^{1}H} NMR of 4e (100 MHz, $CDCl_3$)



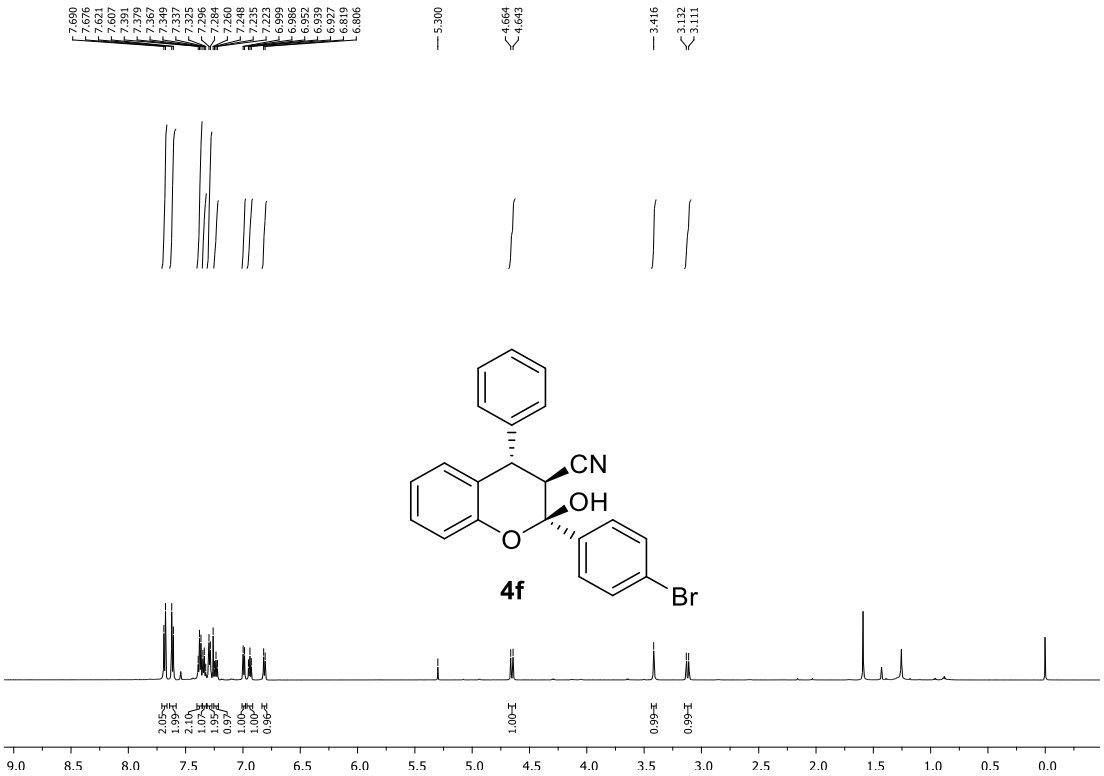
^{1}H NMR of 3f (600 MHz, $CDCl_3$)



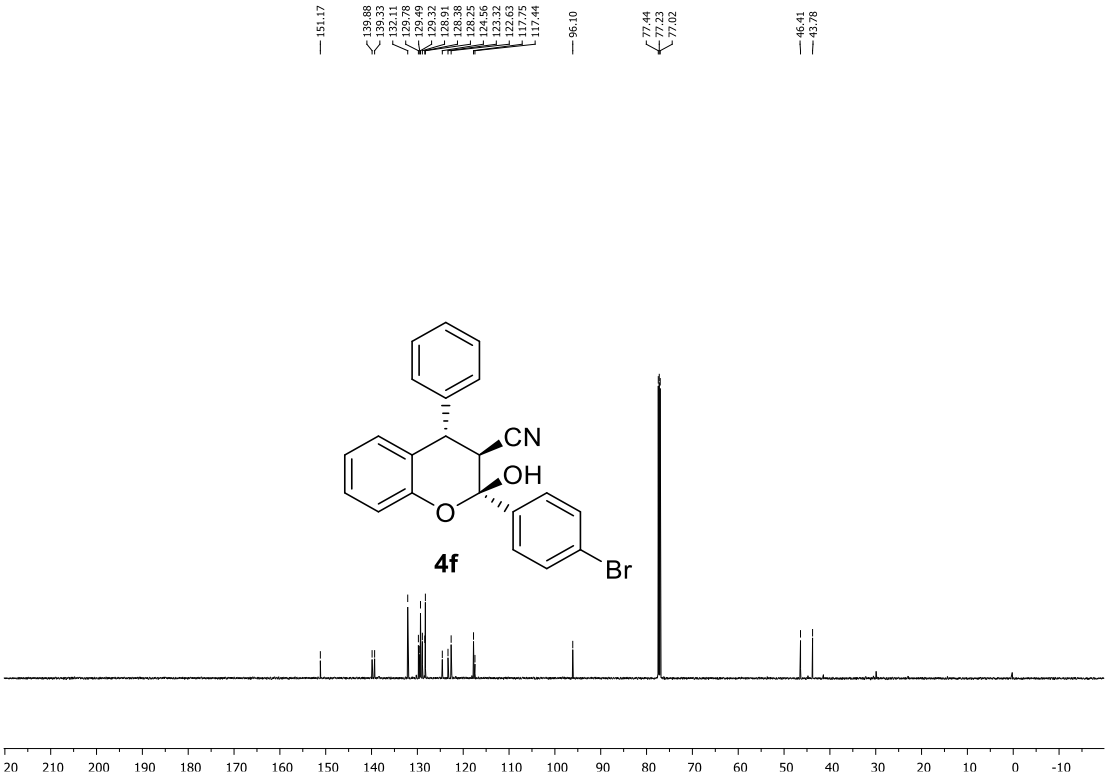
^{13}C{^{1}H} NMR of 3f (150 MHz, $CDCl_3$)



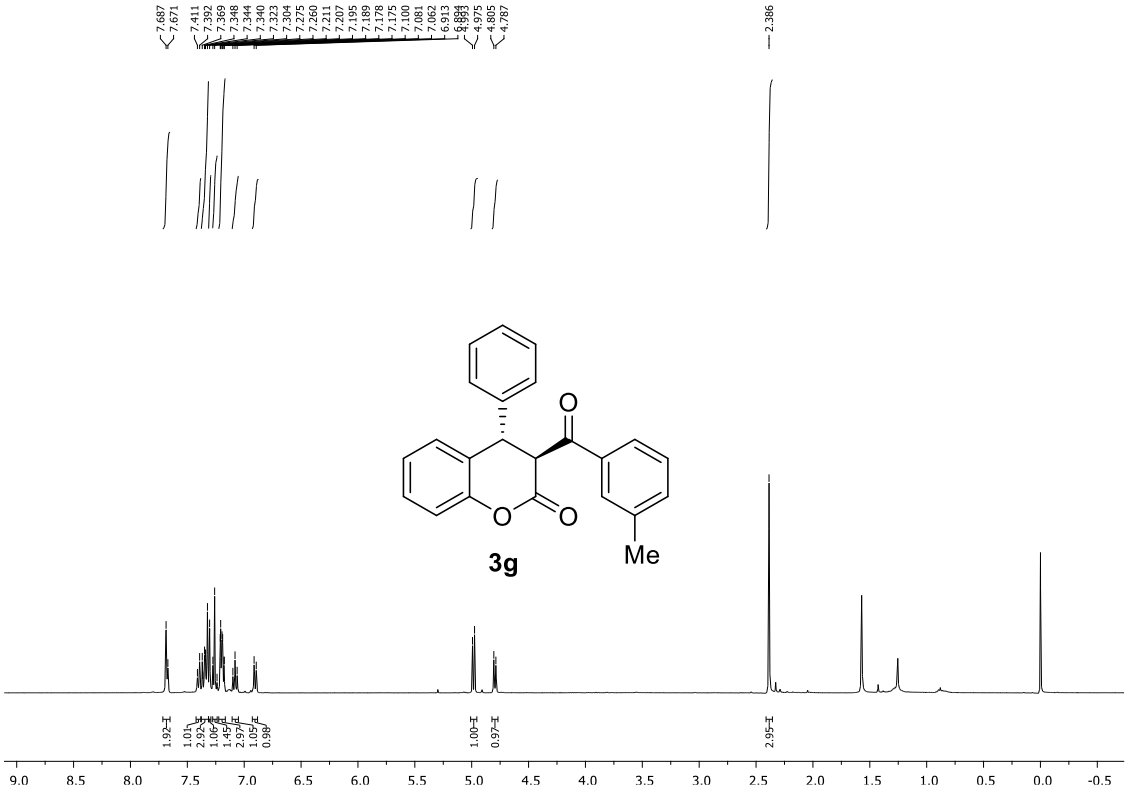
^{1}H NMR of 4f (600 MHz, $CDCl_3$)



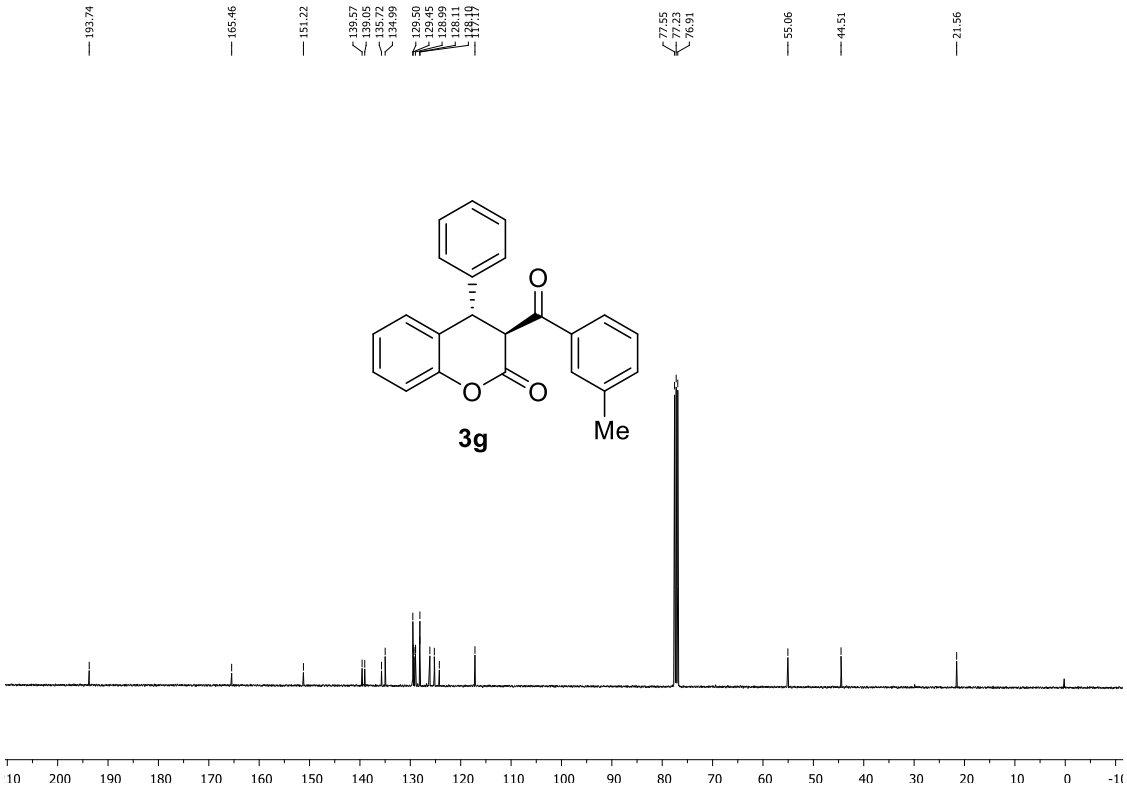
^{13}C{^{1}H} NMR of 4f (150 MHz, $CDCl_3$)



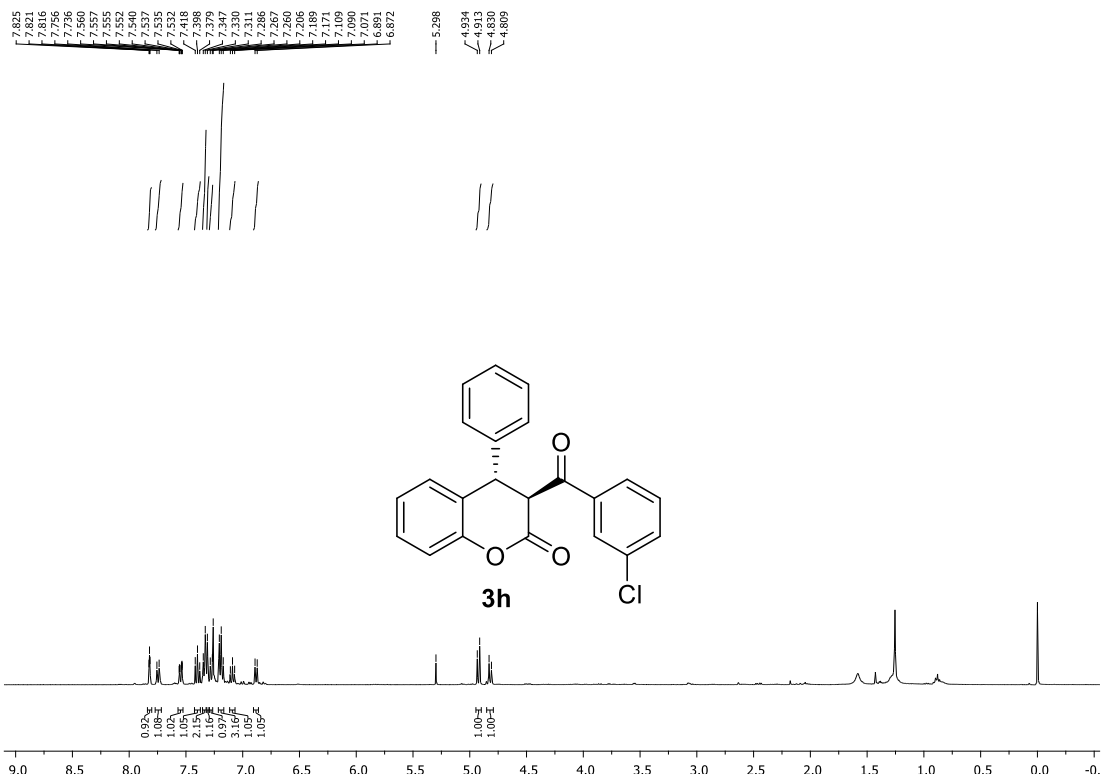
^{1}H NMR of 3g (400 MHz, $CDCl_3$)



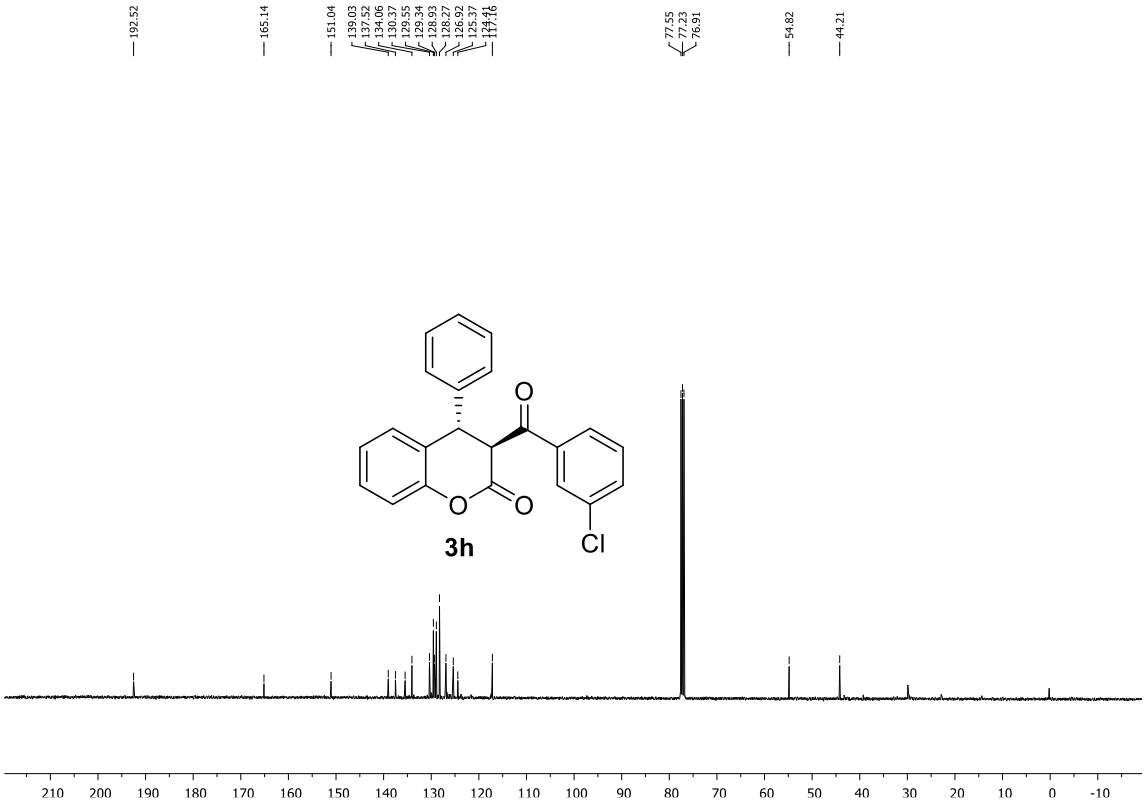
^{13}C{^{1}H} NMR of 3g (150 MHz, $CDCl_3$)



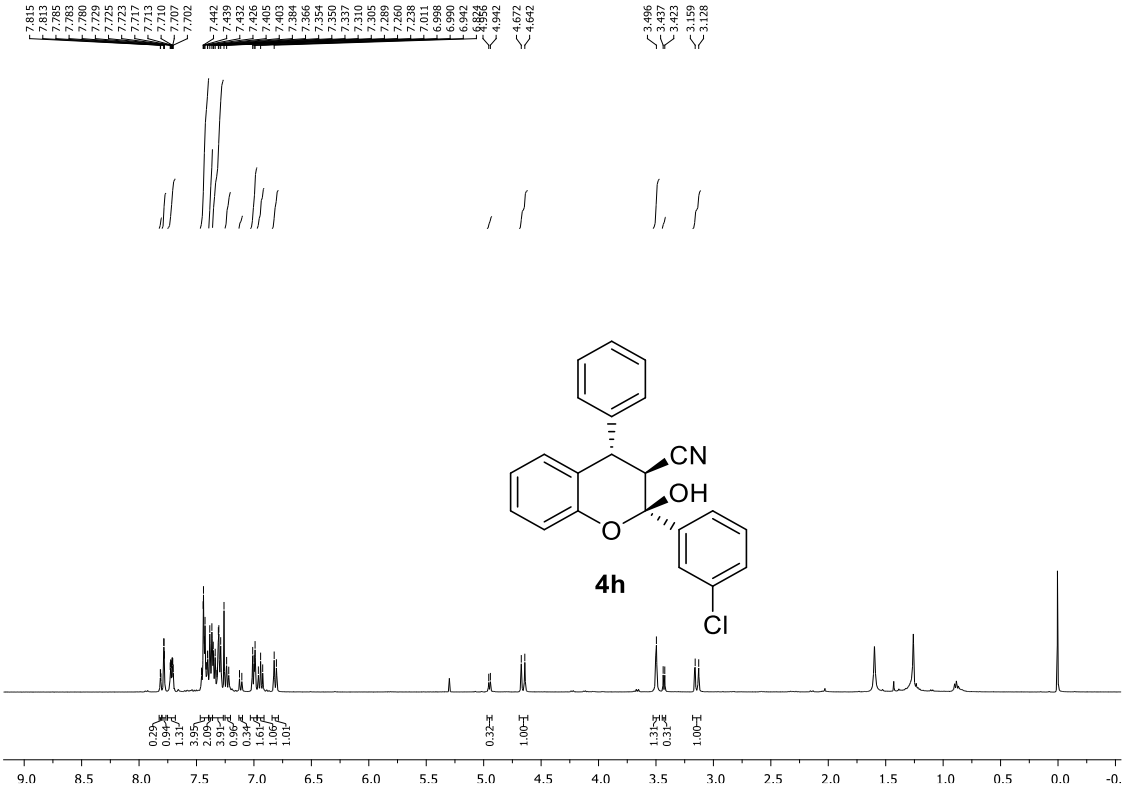
^{1}H NMR of 3h (400 MHz, $CDCl_3$)



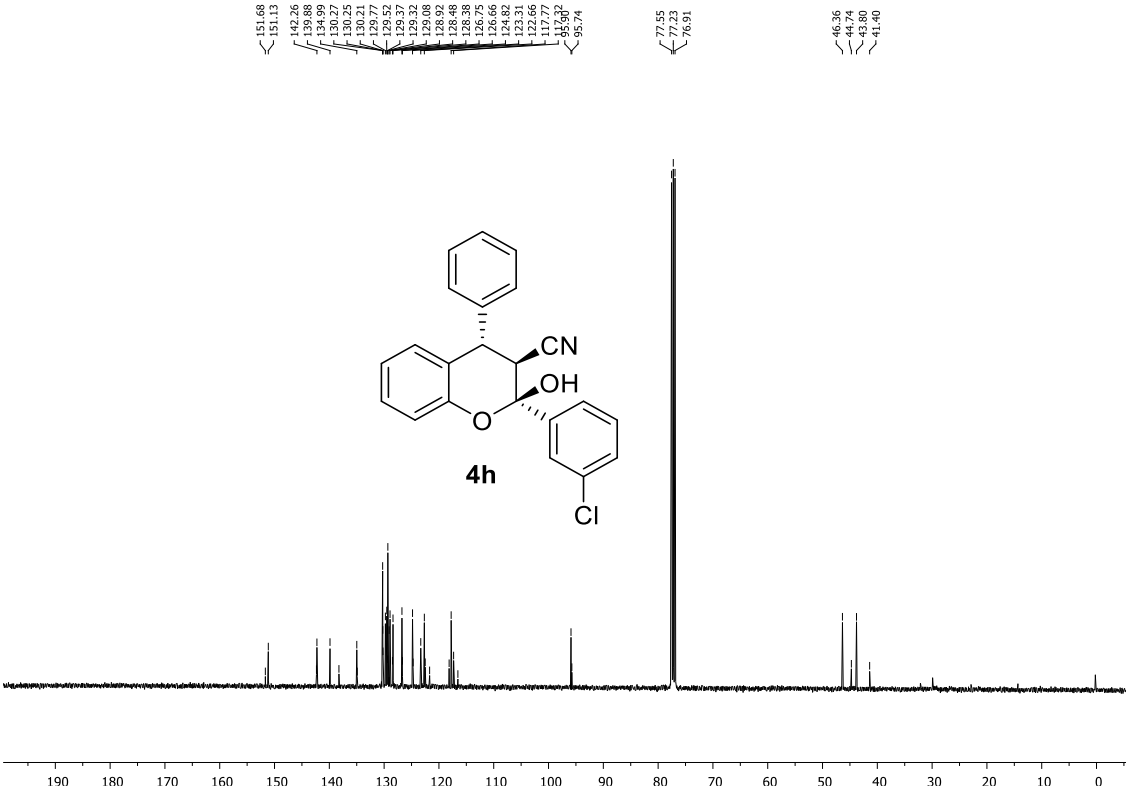
^{13}C{^{1}H} NMR of 3h (100 MHz, $CDCl_3$)



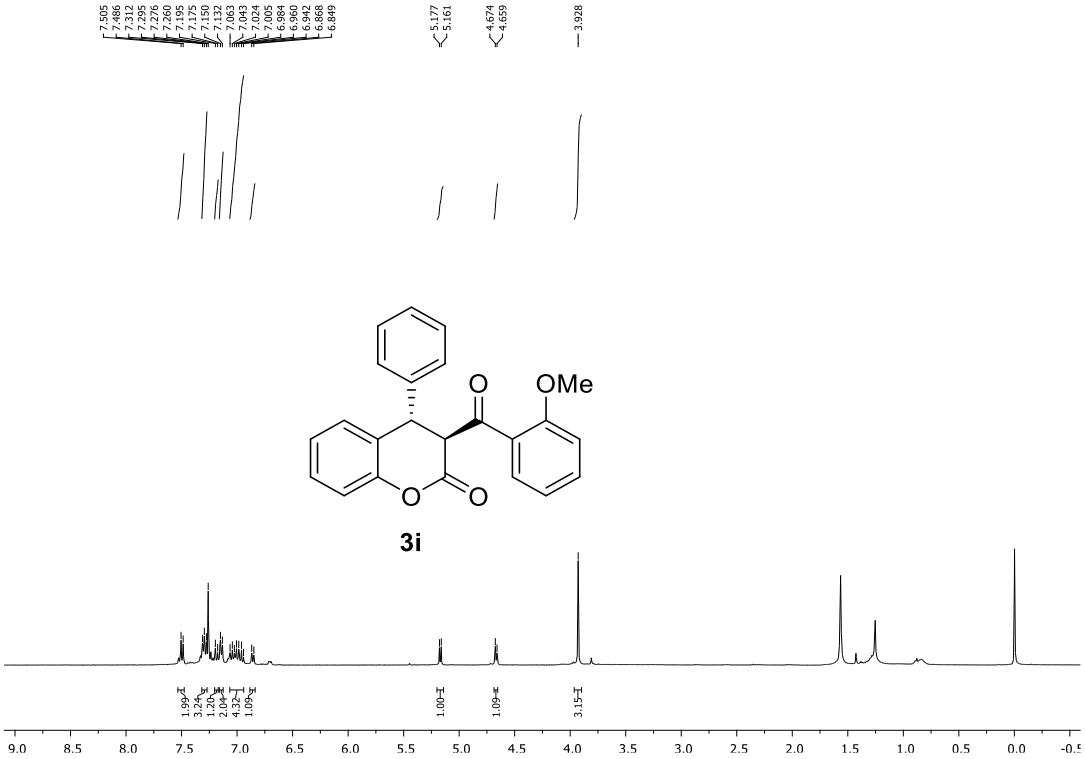
^{1}H NMR of 4h (400 MHz, $CDCl_3$)



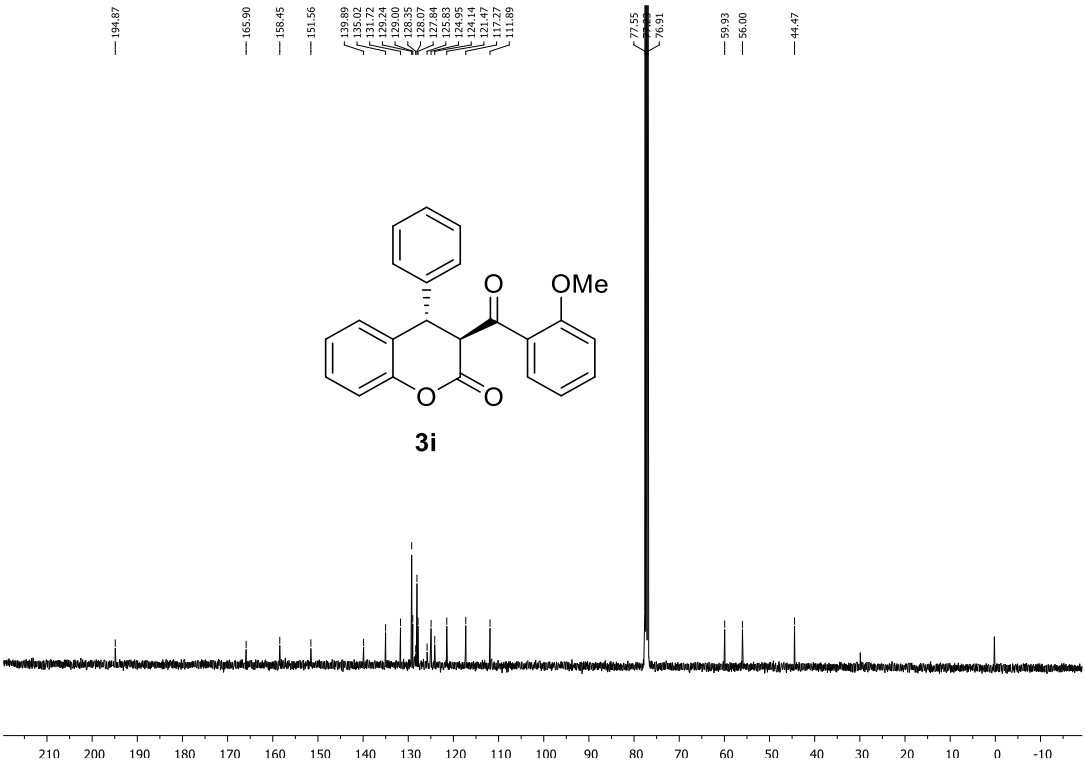
^{13}C{^{1}H} NMR of 4h (100 MHz, $CDCl_3$)



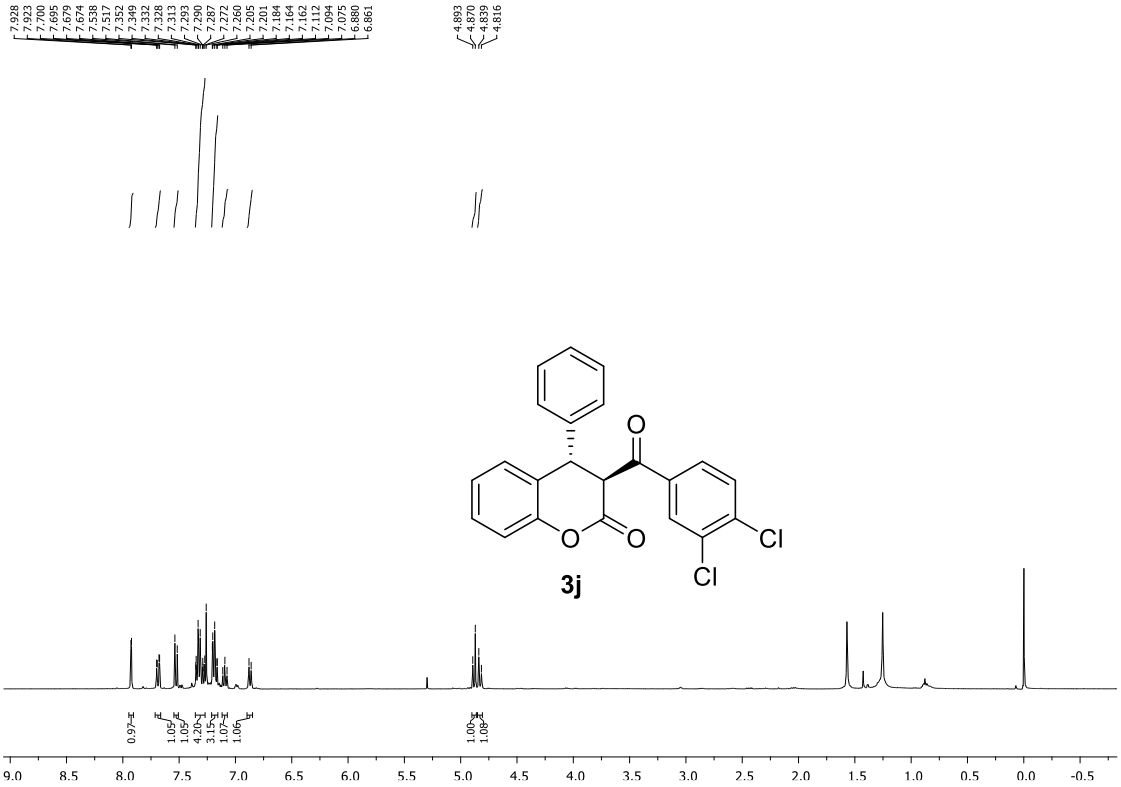
^{1}H NMR of 3i (400 MHz, $CDCl_3$)



^{13}C{^{1}H} NMR of 3i (100 MHz, $CDCl_3$)

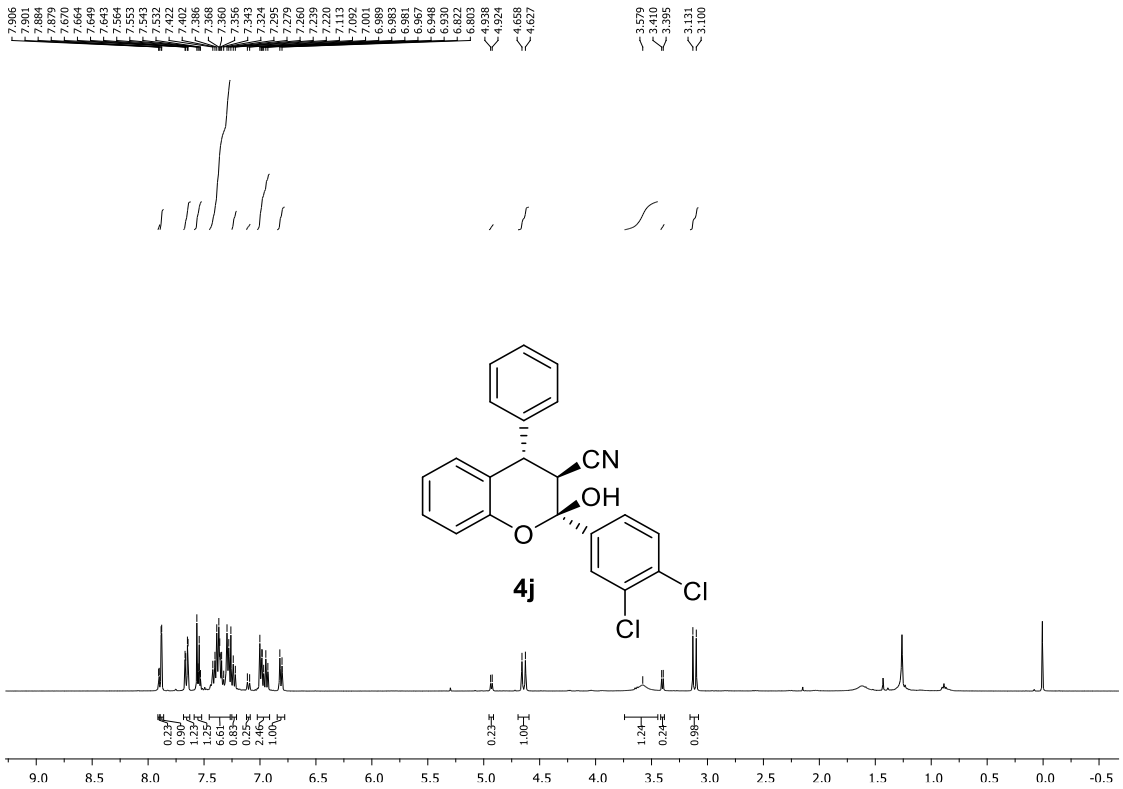


^{1}H NMR of 3j (400 MHz, $CDCl_3$)

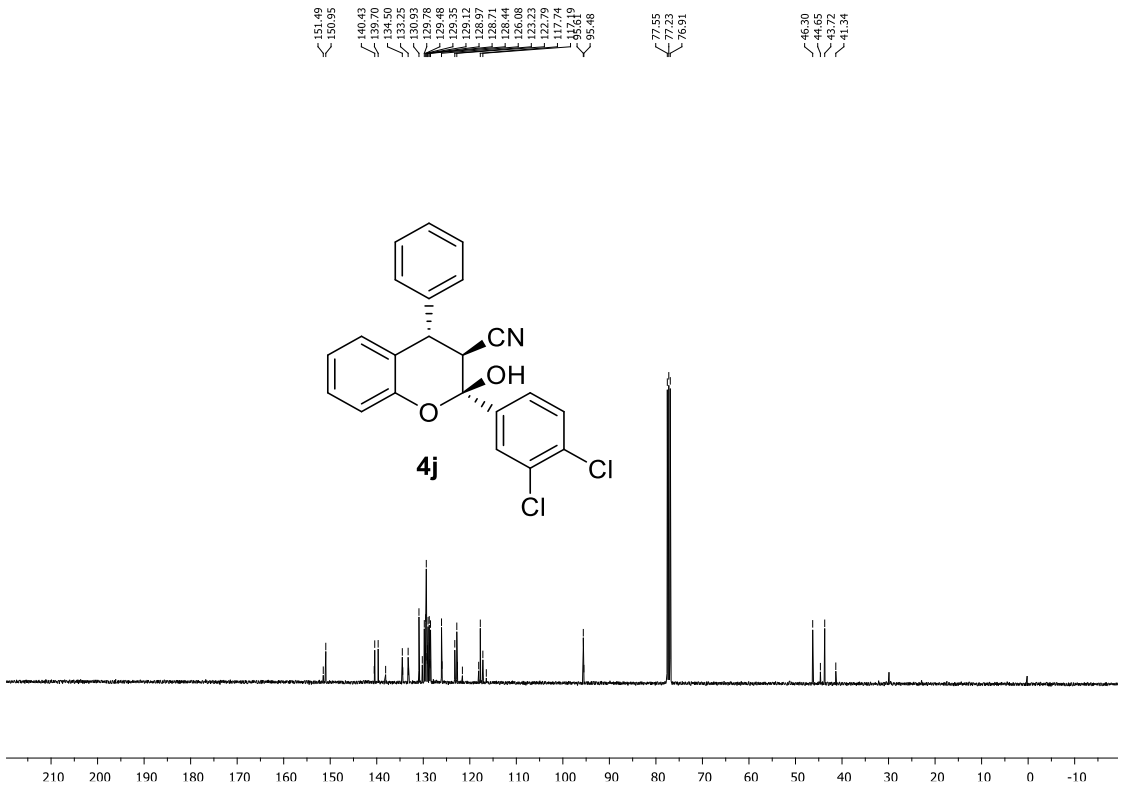


^{13}C{^{1}H} NMR of 3j (100 MHz, $CDCl_3$)

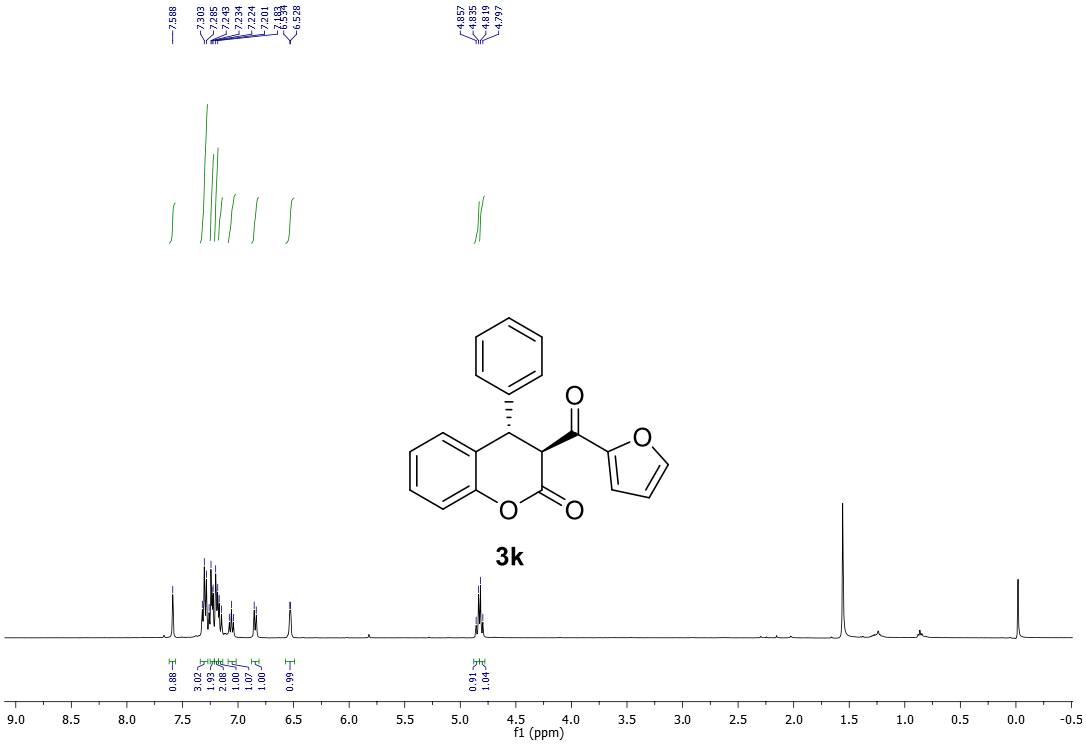
^{1}H NMR of 4j (400 MHz, $CDCl_3$)



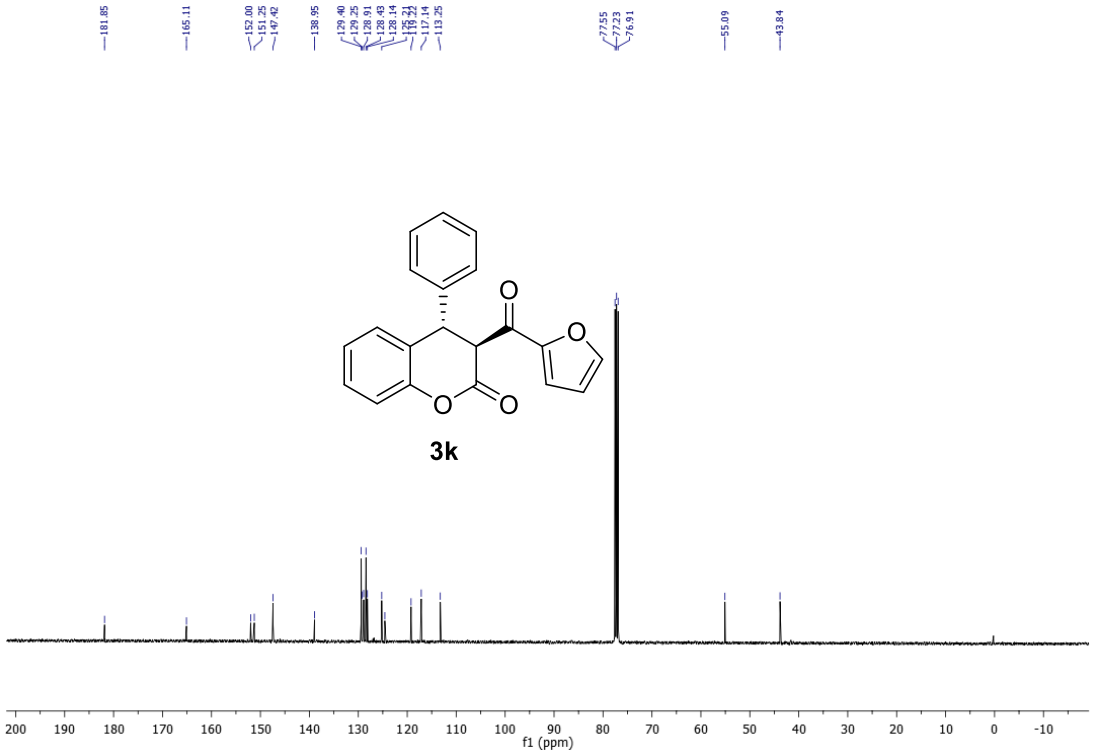
^{13}C{^{1}H} NMR of 4j (100 MHz, $CDCl_3$)



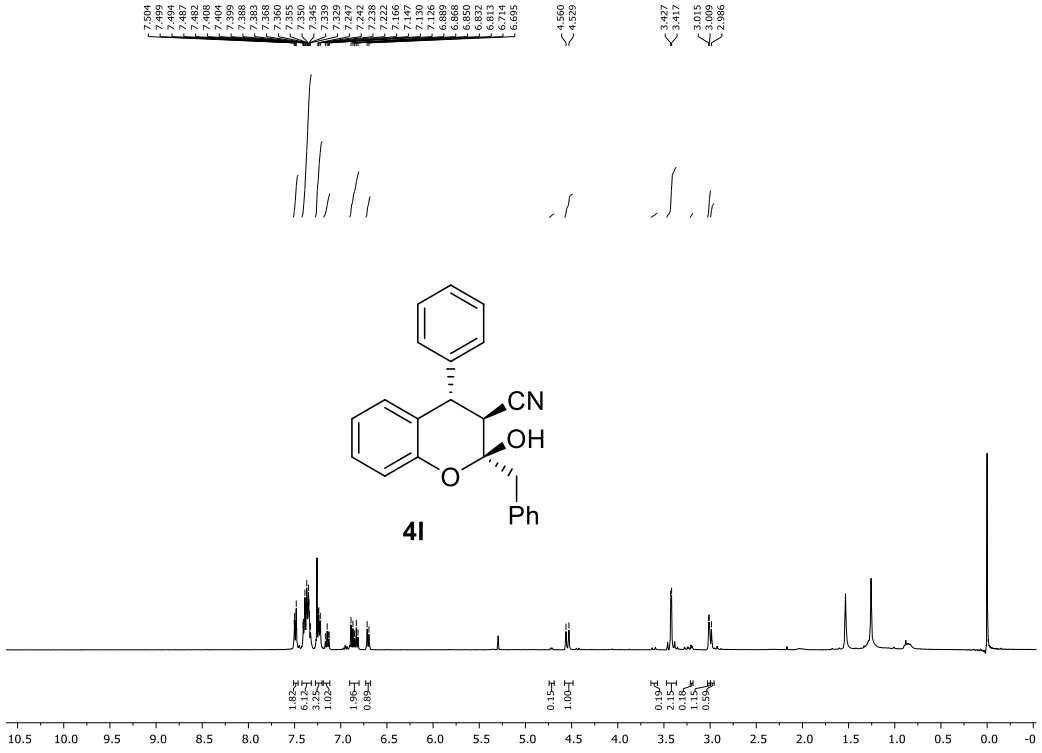
^{1}H NMR of 3k (400 MHz, $CDCl_3$)



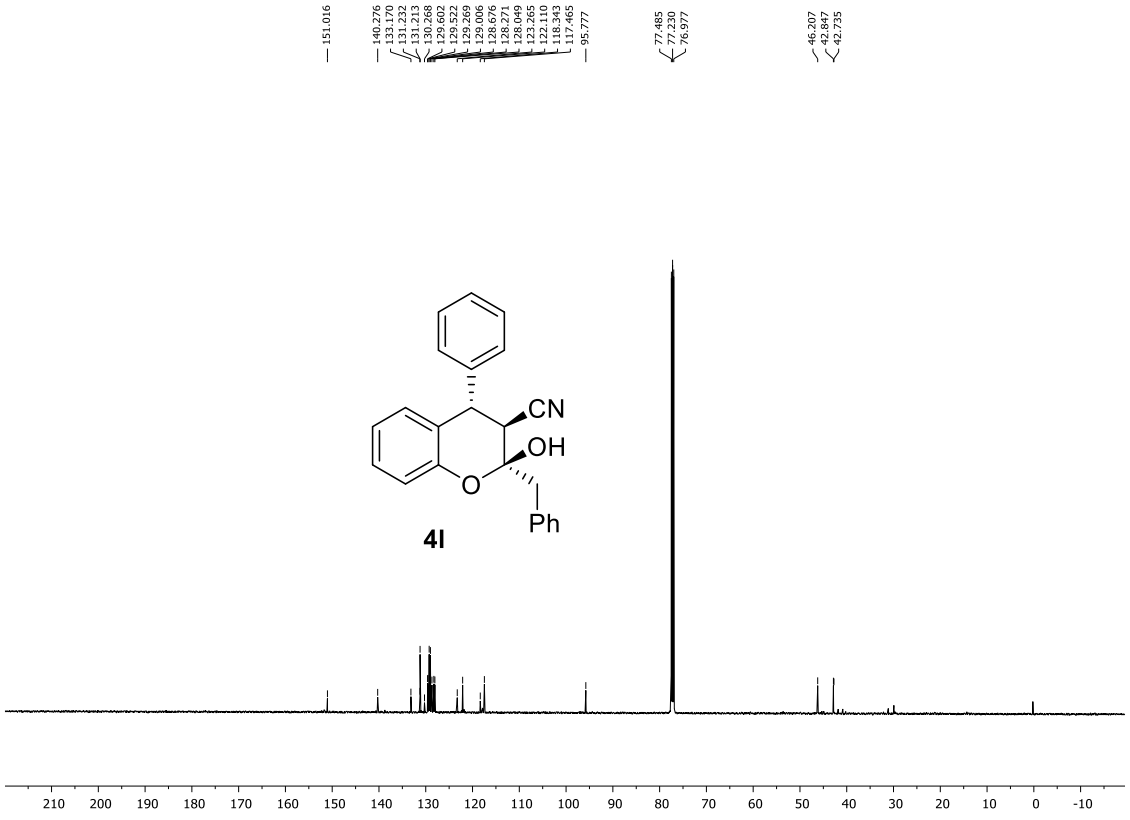
^{13}C{^{1}H} NMR of 3k (100 MHz, $CDCl_3$)



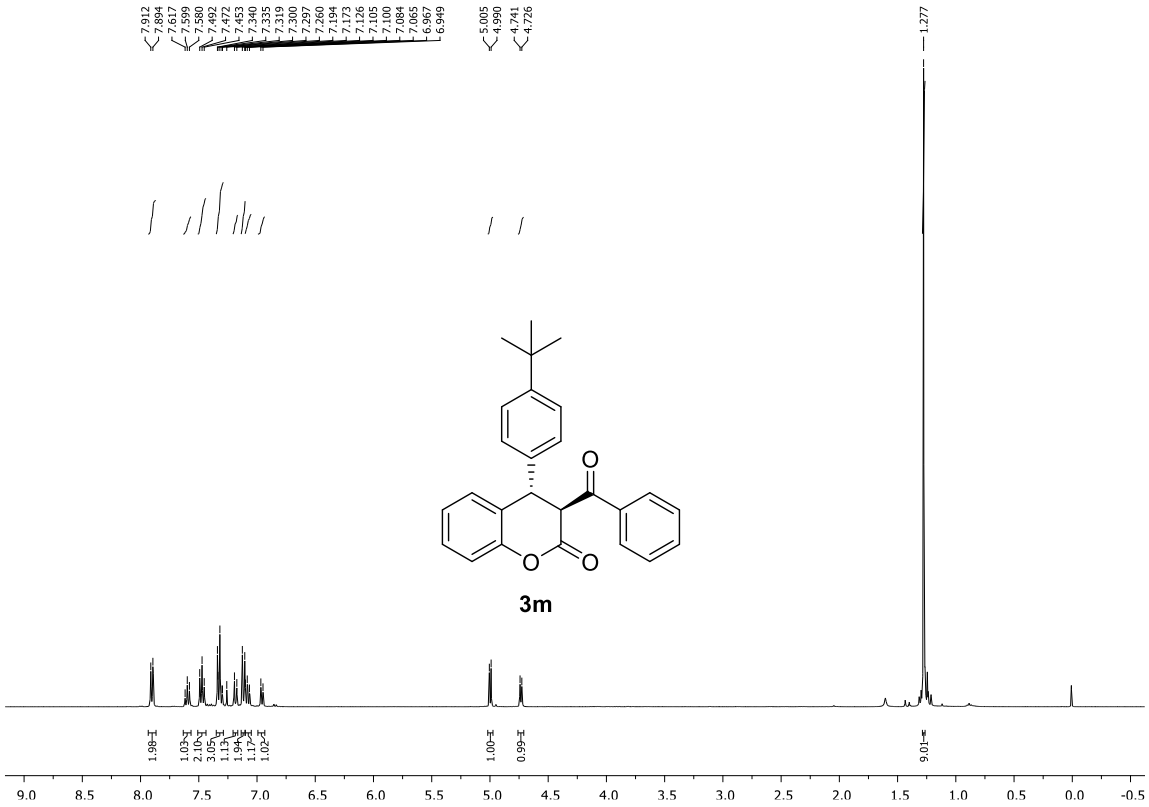
^{1}H NMR of 4l (400 MHz, $CDCl_3$)



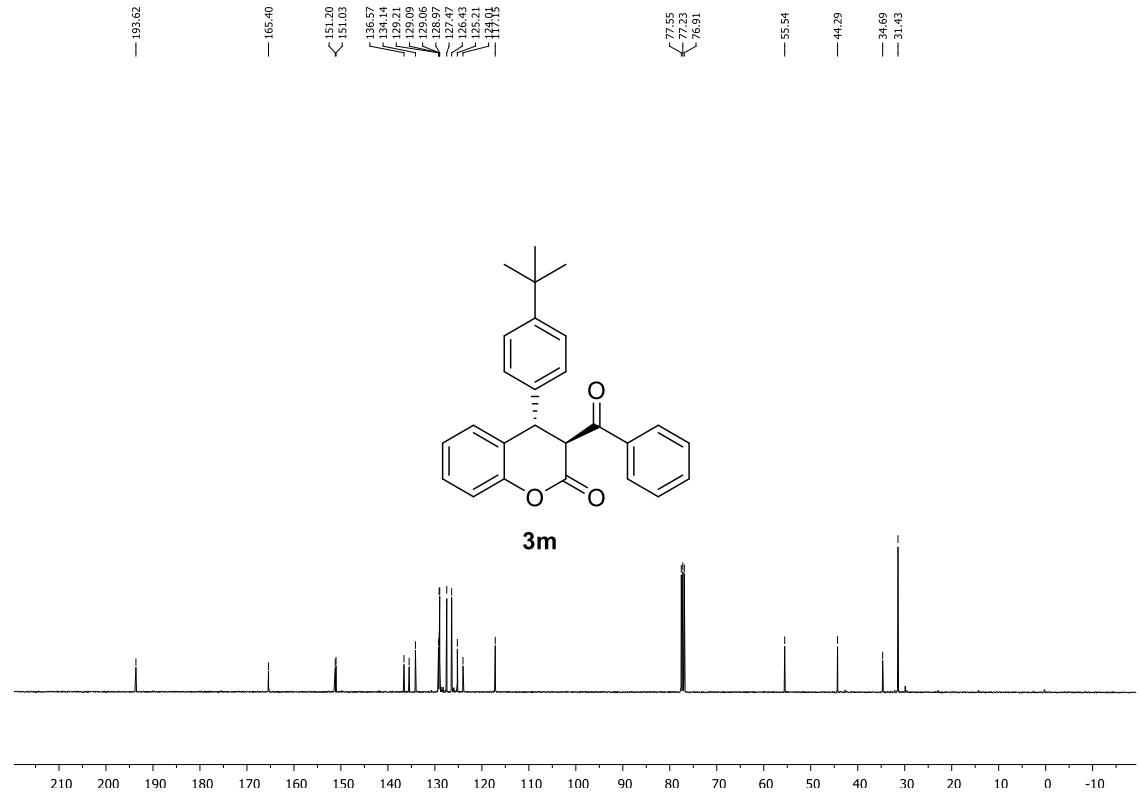
^{13}C{^{1}H} NMR of 4l (125 MHz, $CDCl_3$)



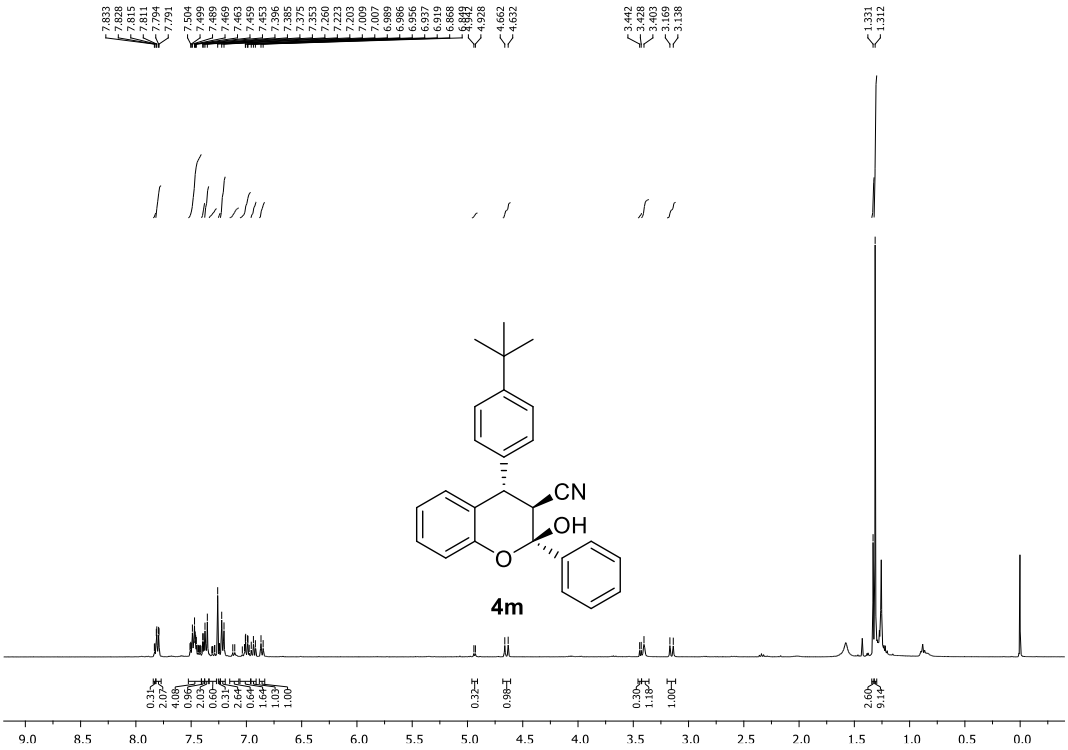
^{1}H NMR of 3m (400 MHz, $CDCl_3$)



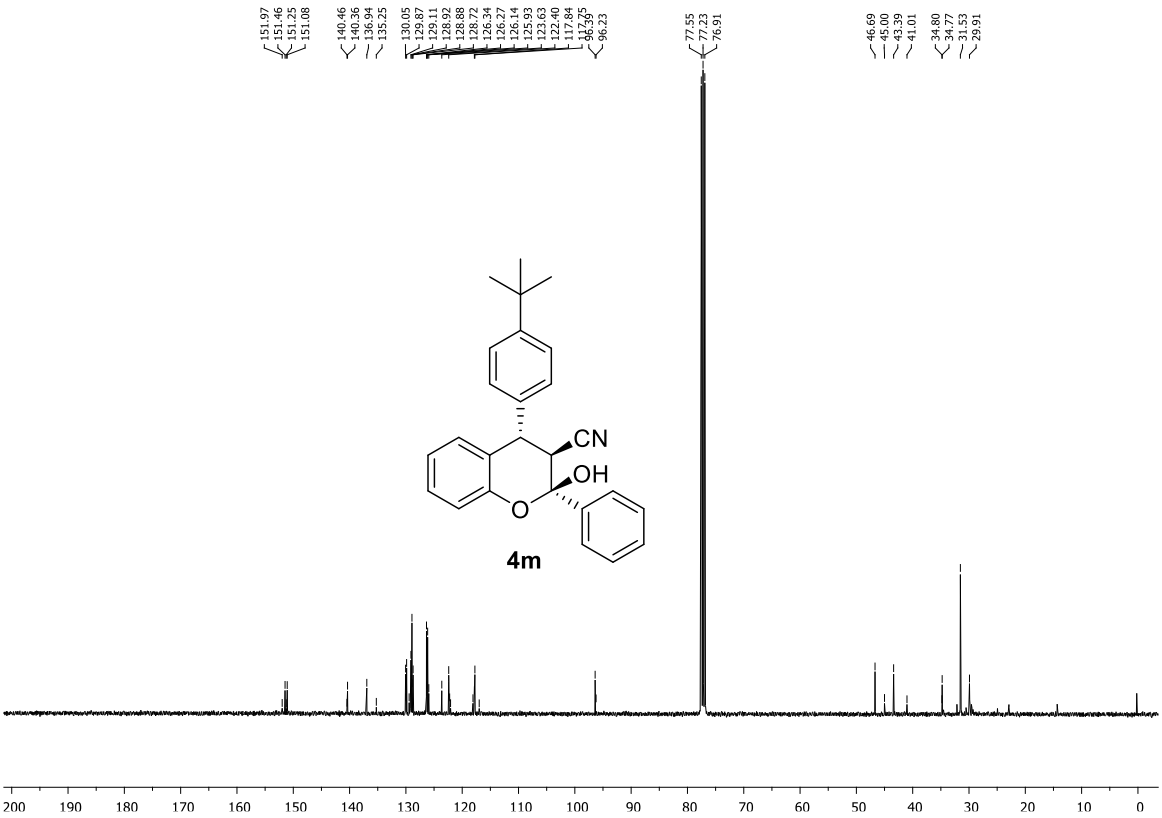
^{13}C{^{1}H} NMR of 3m (100 MHz, $CDCl_3$)



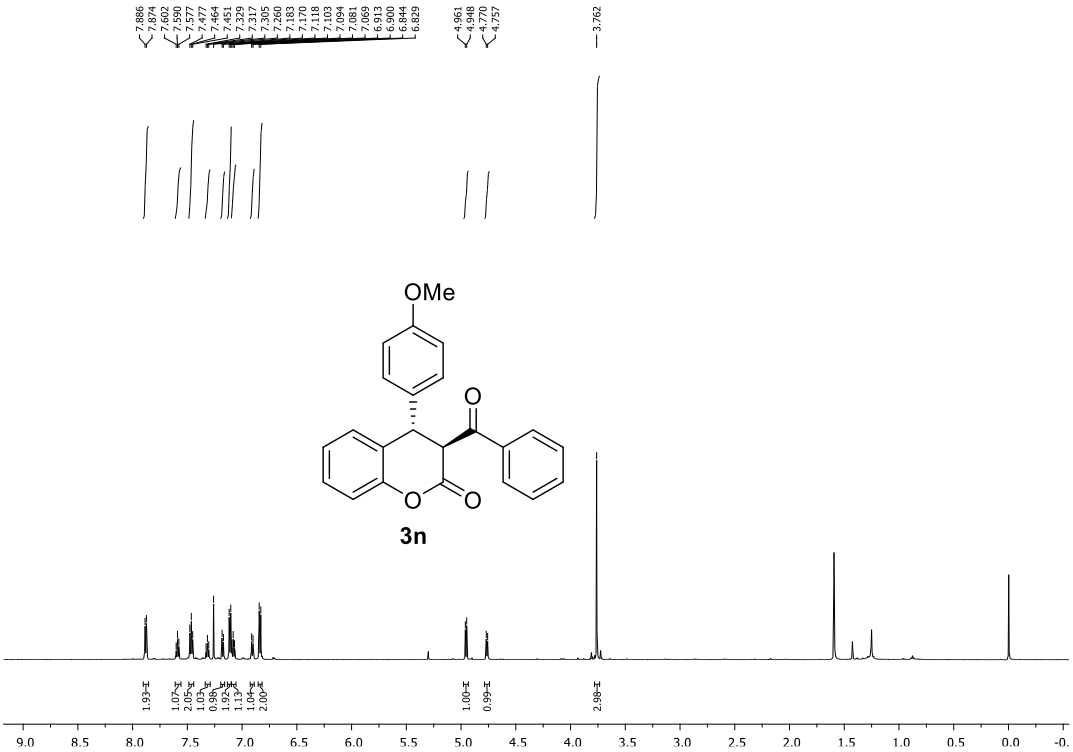
^{1}H NMR of 4m (400 MHz, $CDCl_3$)



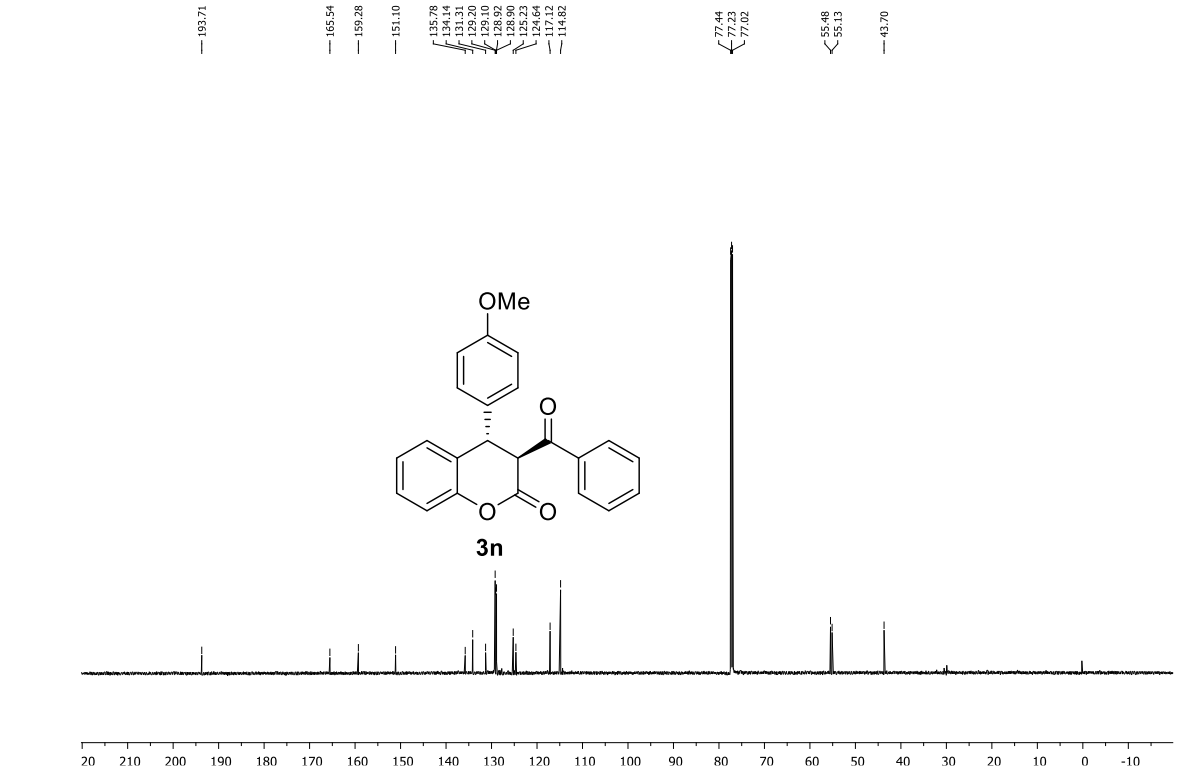
^{13}C{^{1}H} NMR of 4m (100 MHz, $CDCl_3$)



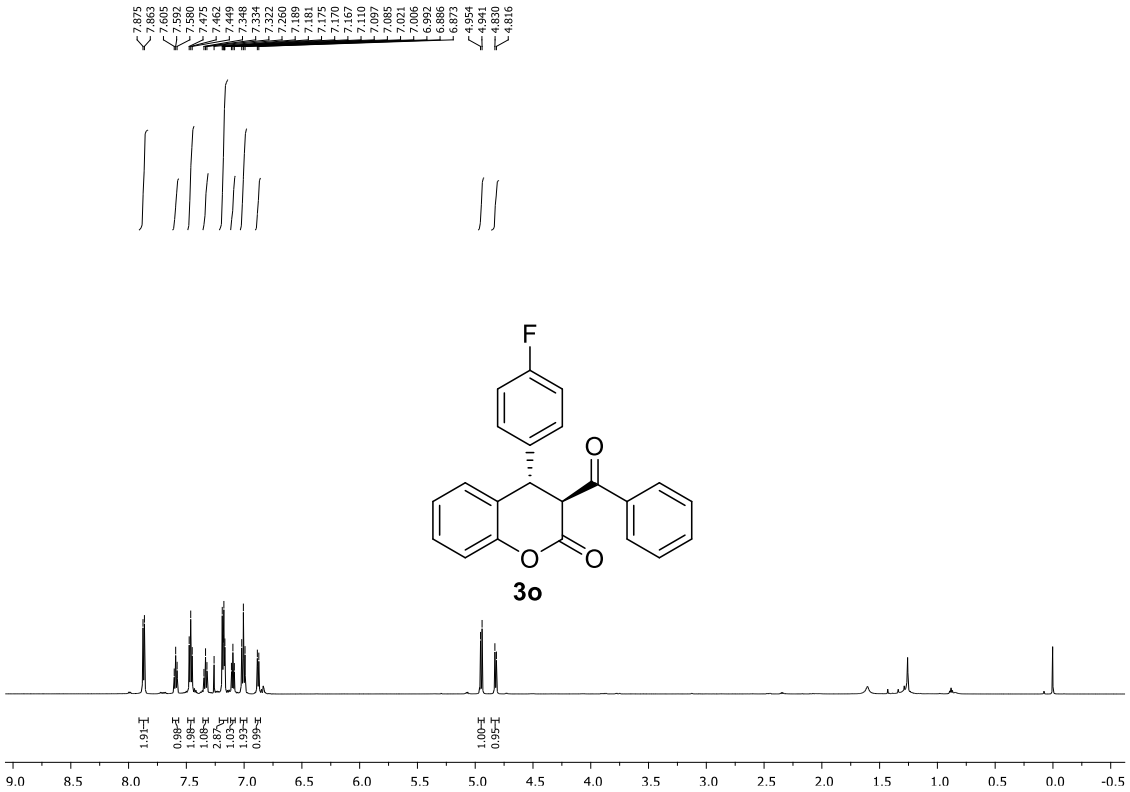
^{1}H NMR of 3n (600 MHz, $CDCl_3$)



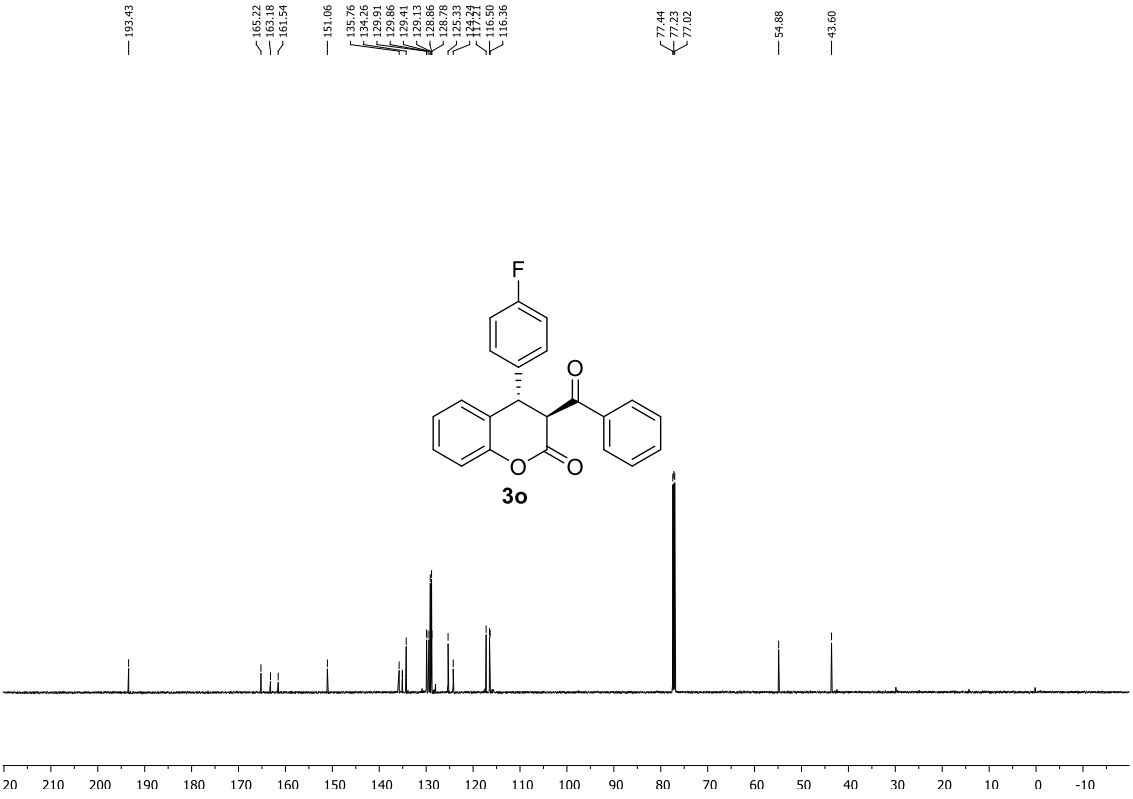
^{13}C{^{1}H} NMR of 3n (150 MHz, $CDCl_3$)



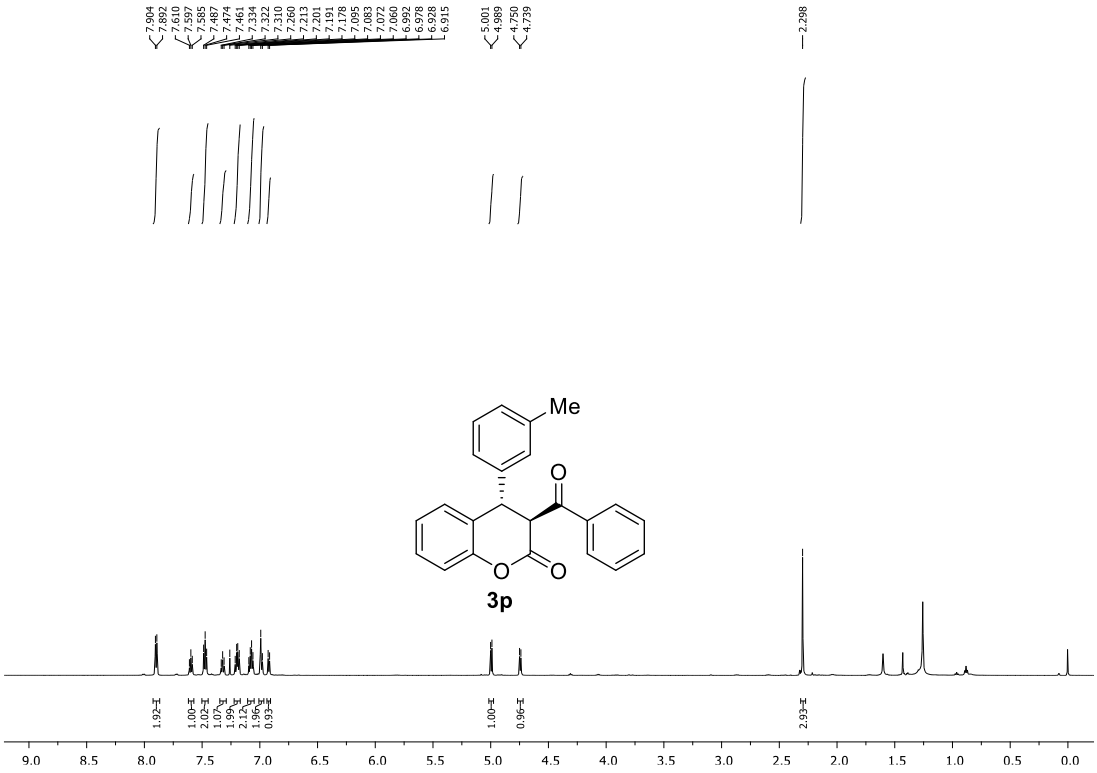
^{1}H NMR of 3o (600 MHz, $CDCl_3$)



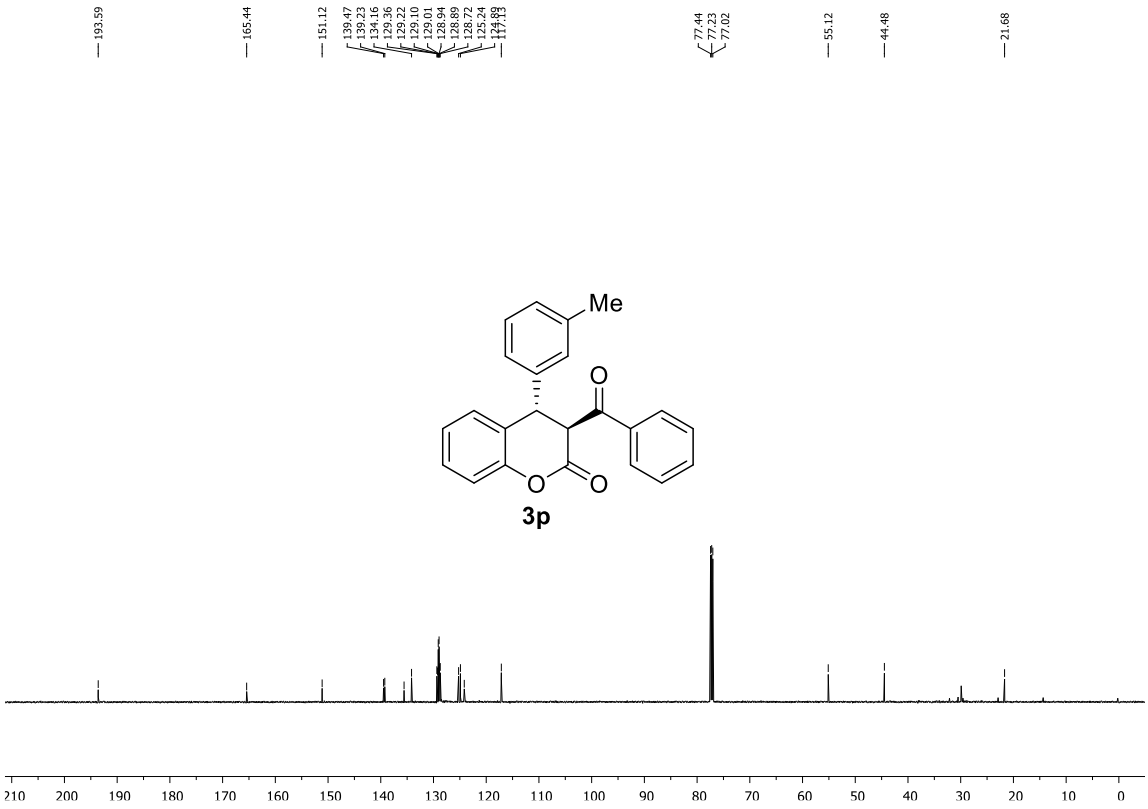
^{13}C{^{1}H} NMR of 3o (150 MHz, $CDCl_3$)



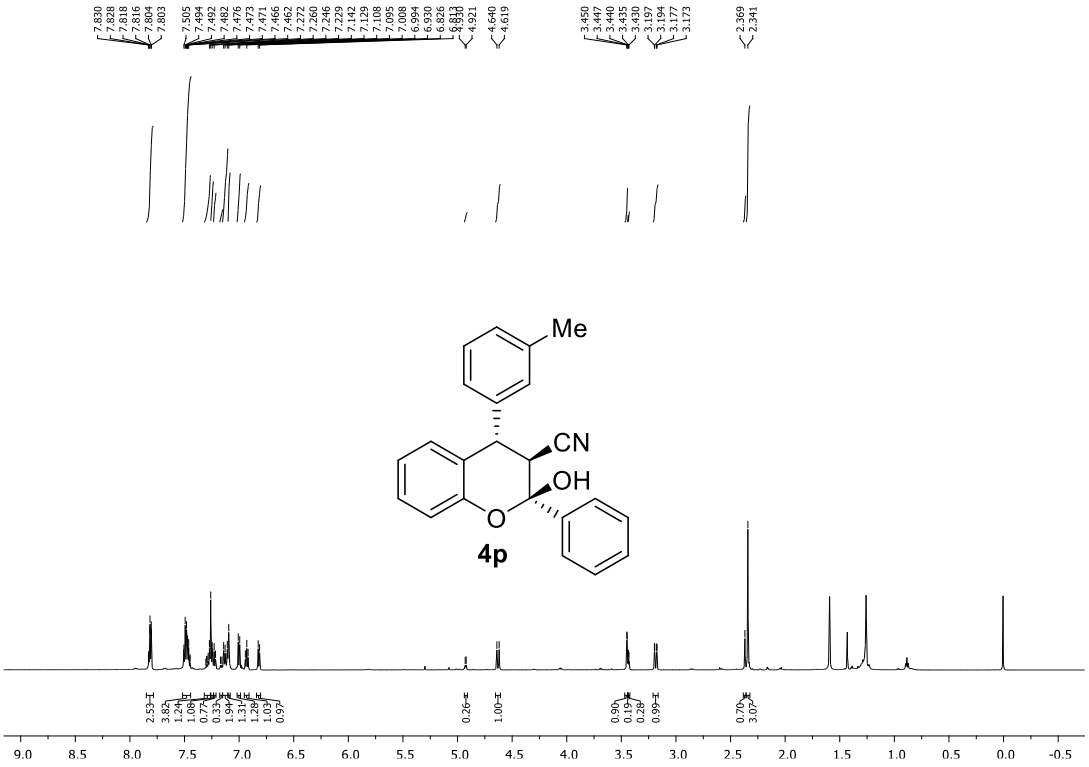
^{1}H NMR of 3p (600 MHz, $CDCl_3$)



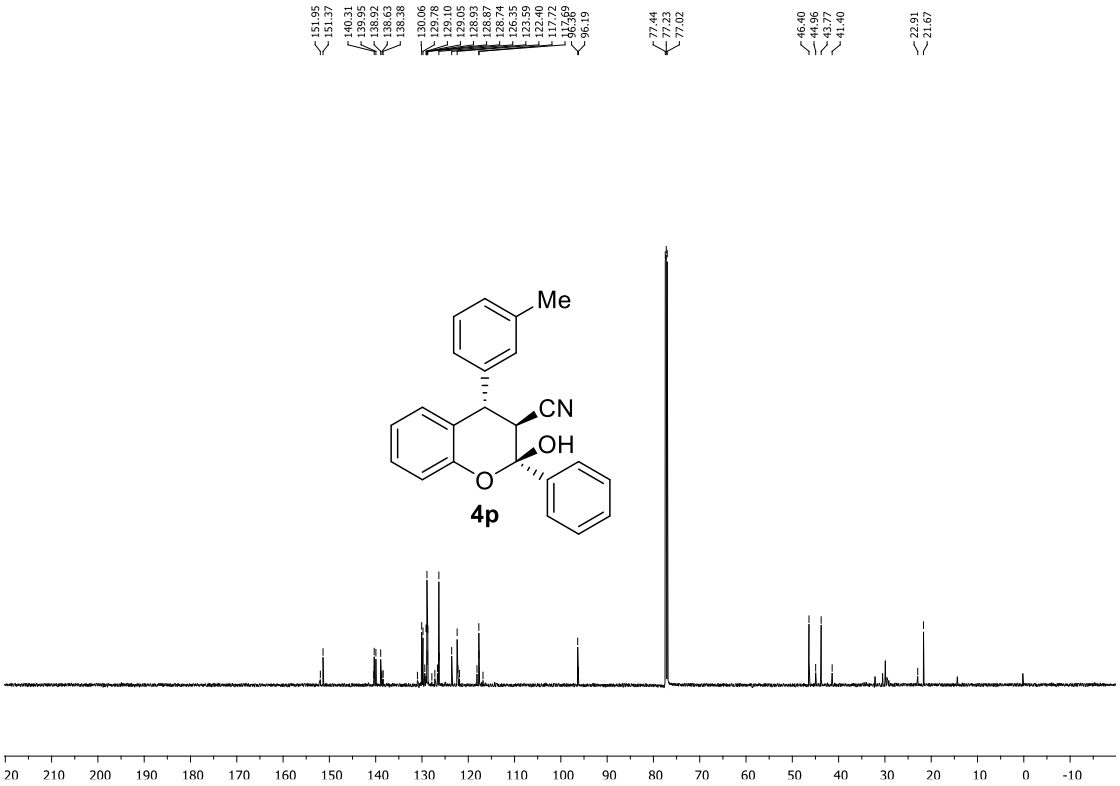
^{13}C{^{1}H} NMR of 3p (150 MHz, $CDCl_3$)



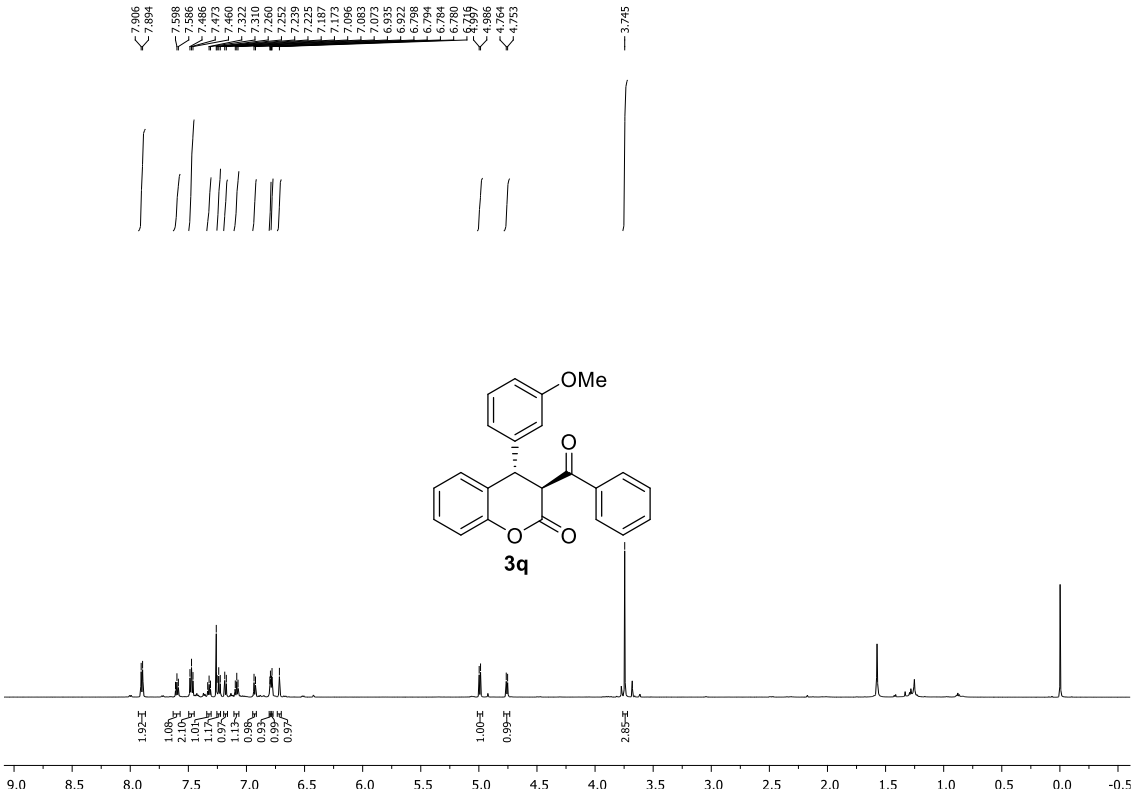
^{1}H NMR of 4p (600 MHz, $CDCl_3$)



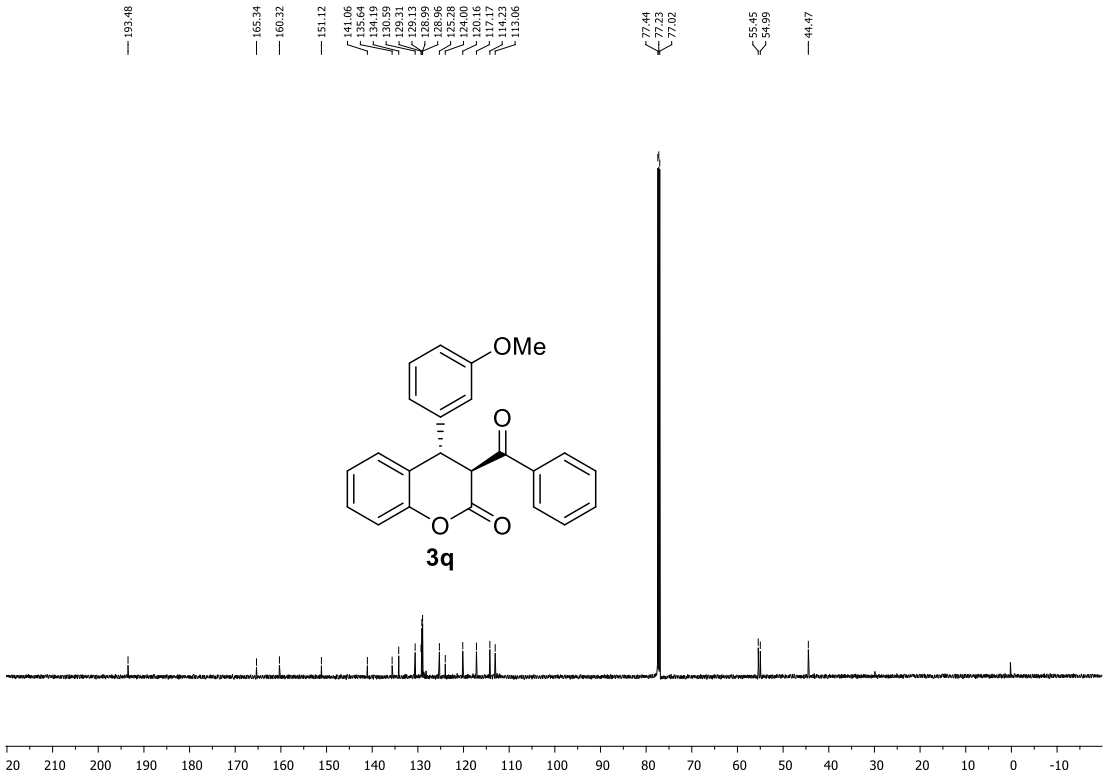
^{13}C{^{1}H} NMR of 4p (150 MHz, $CDCl_3$)



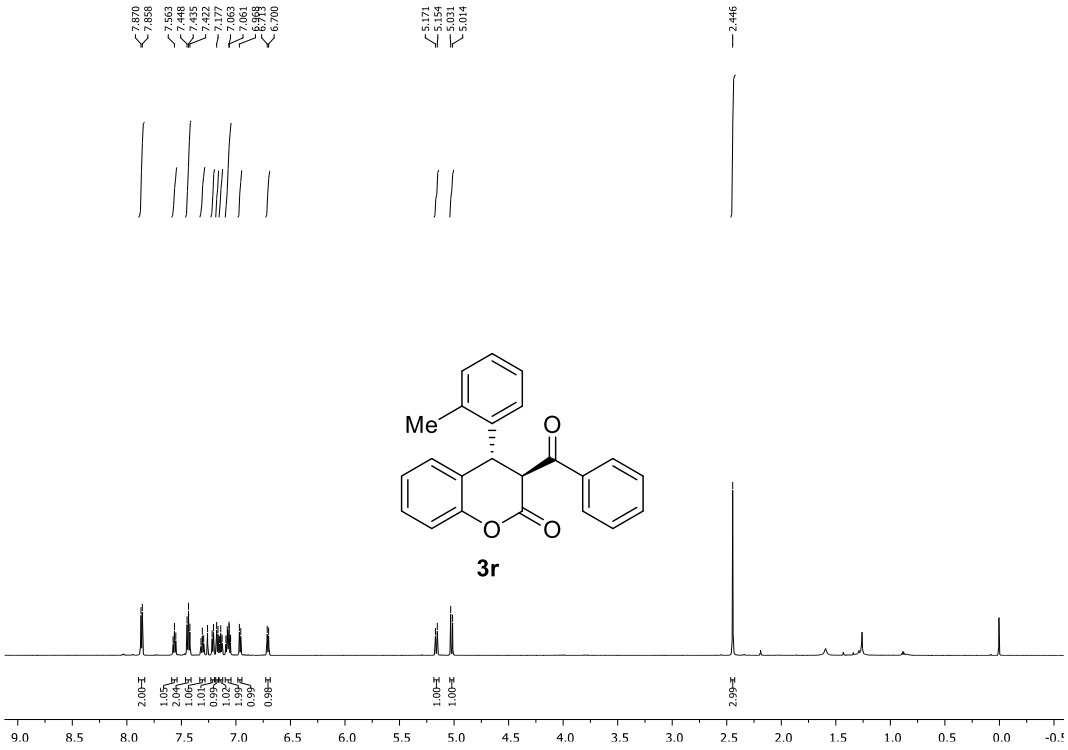
^{1}H NMR of 3q (600 MHz, $CDCl_3$)



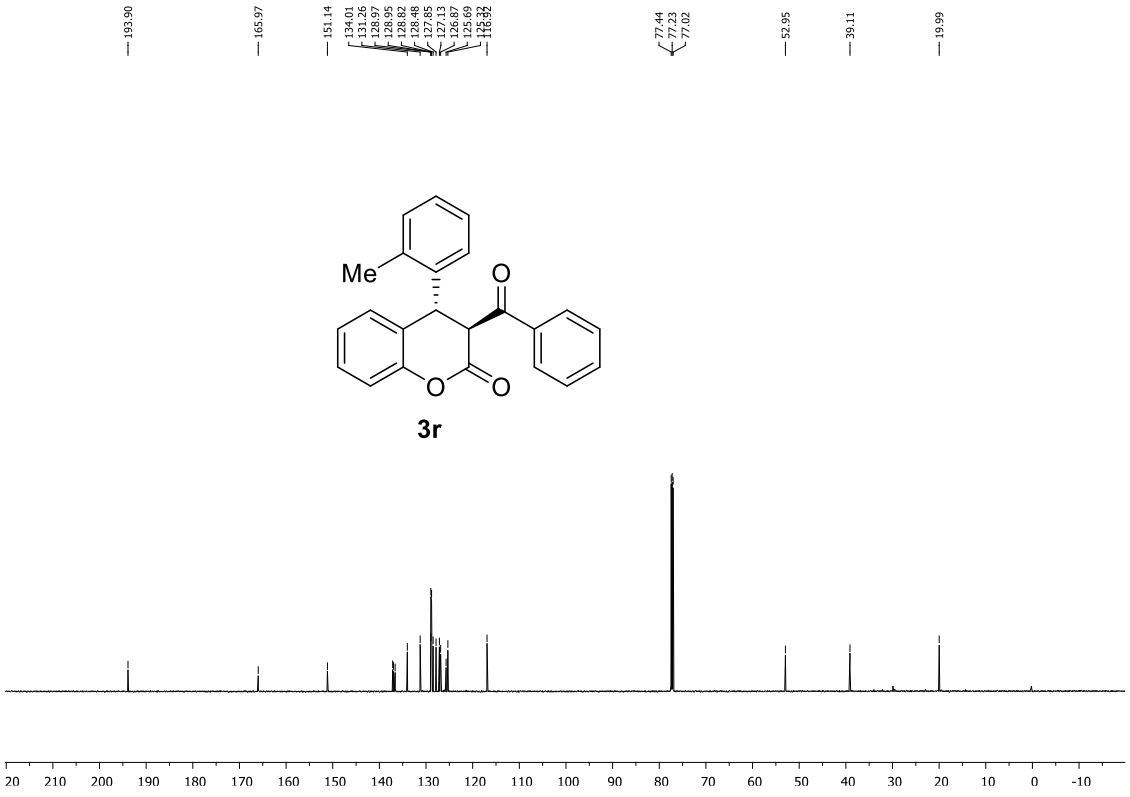
^{13}C{^{1}H} NMR of 3q (150 MHz, $CDCl_3$)



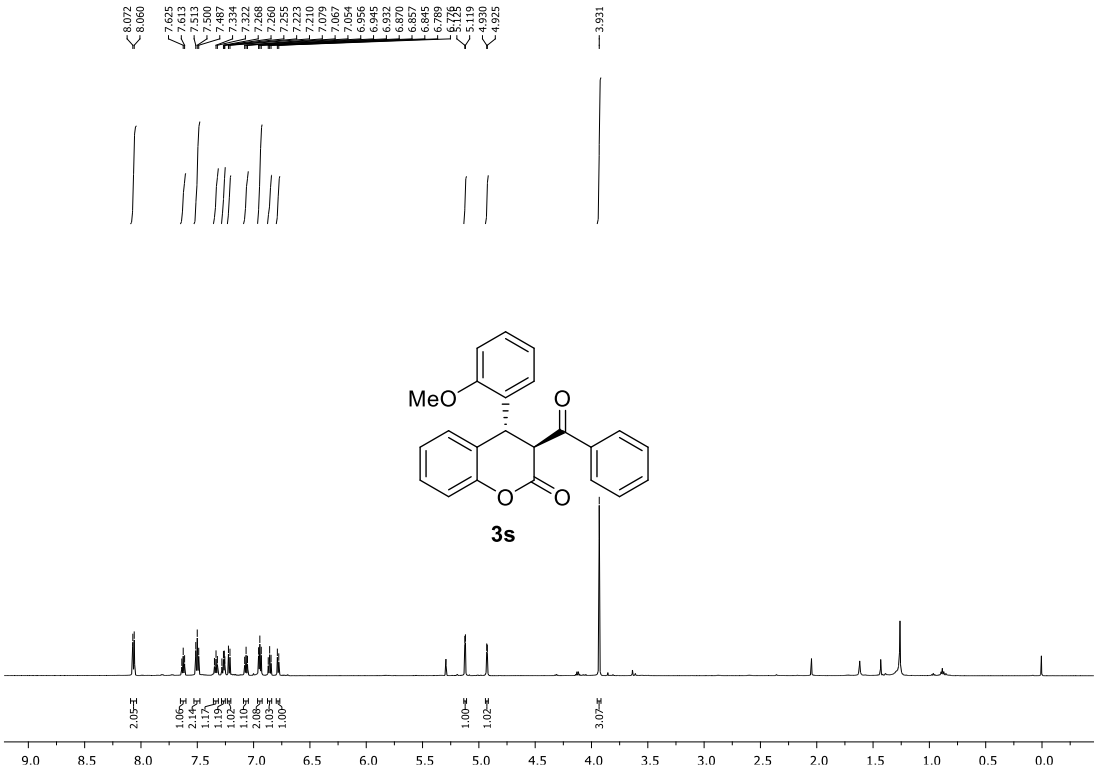
^{1}H NMR of 3r (600 MHz, $CDCl_3$)



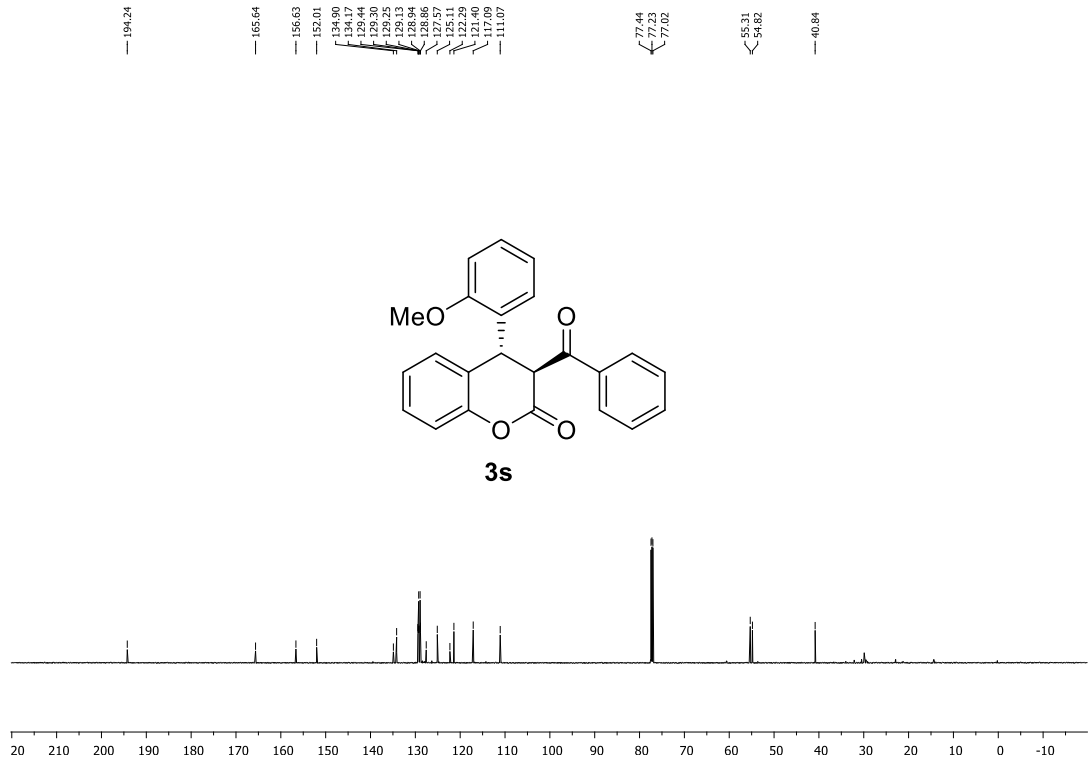
^{13}C{^{1}H} NMR of 3r (150 MHz, $CDCl_3$)



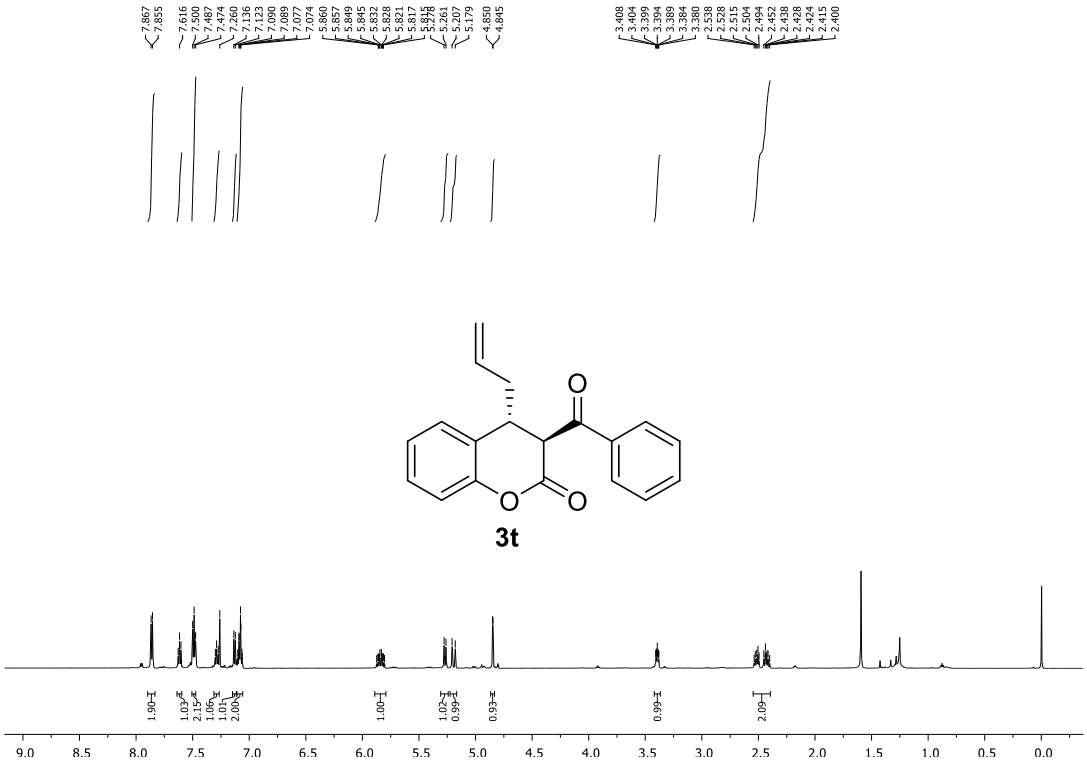
^{1}H NMR of 3s (600 MHz, $CDCl_3$)



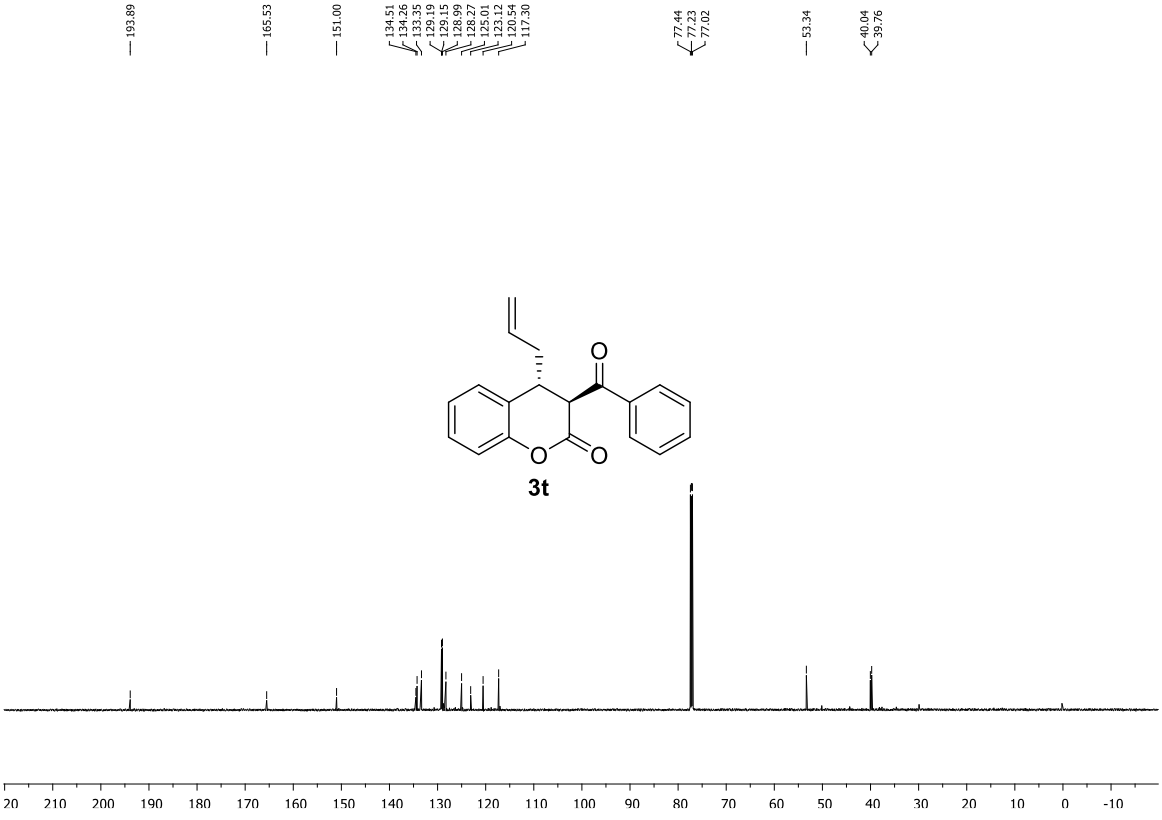
^{13}C{^{1}H} NMR of 3s (150 MHz, $CDCl_3$)



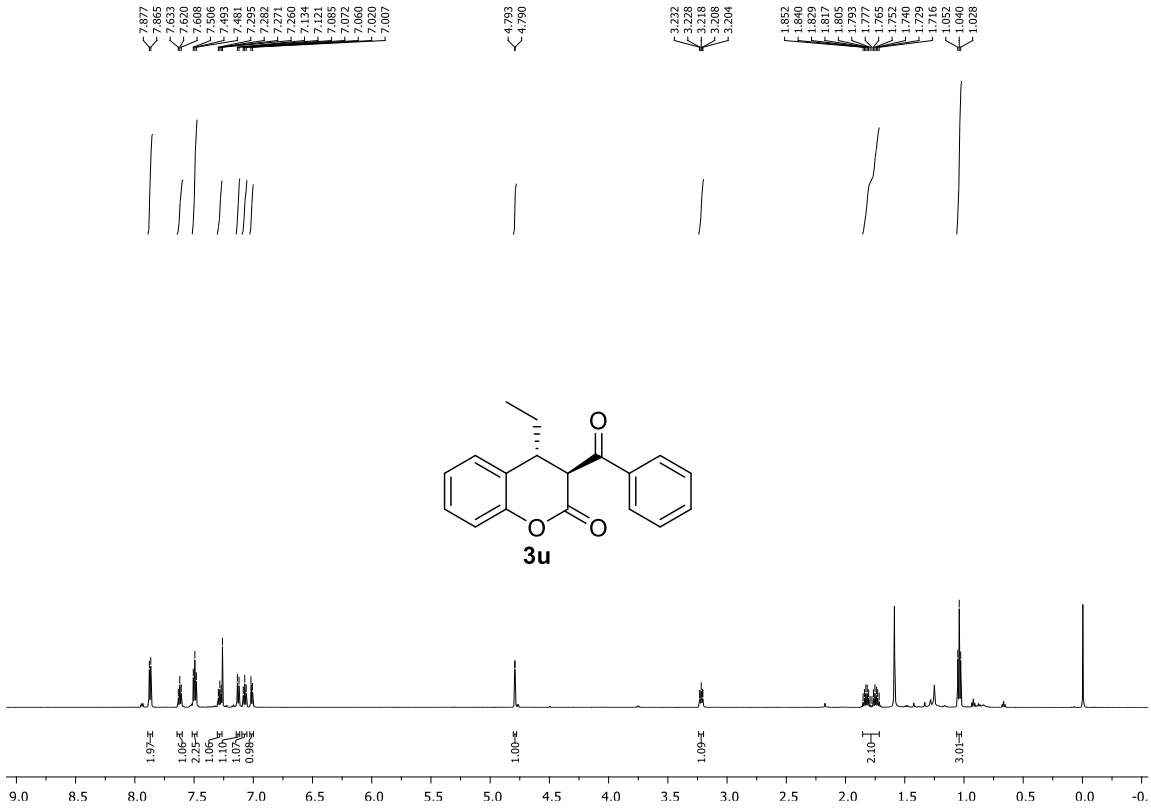
^{1}H NMR of 3t (600 MHz, $CDCl_3$)



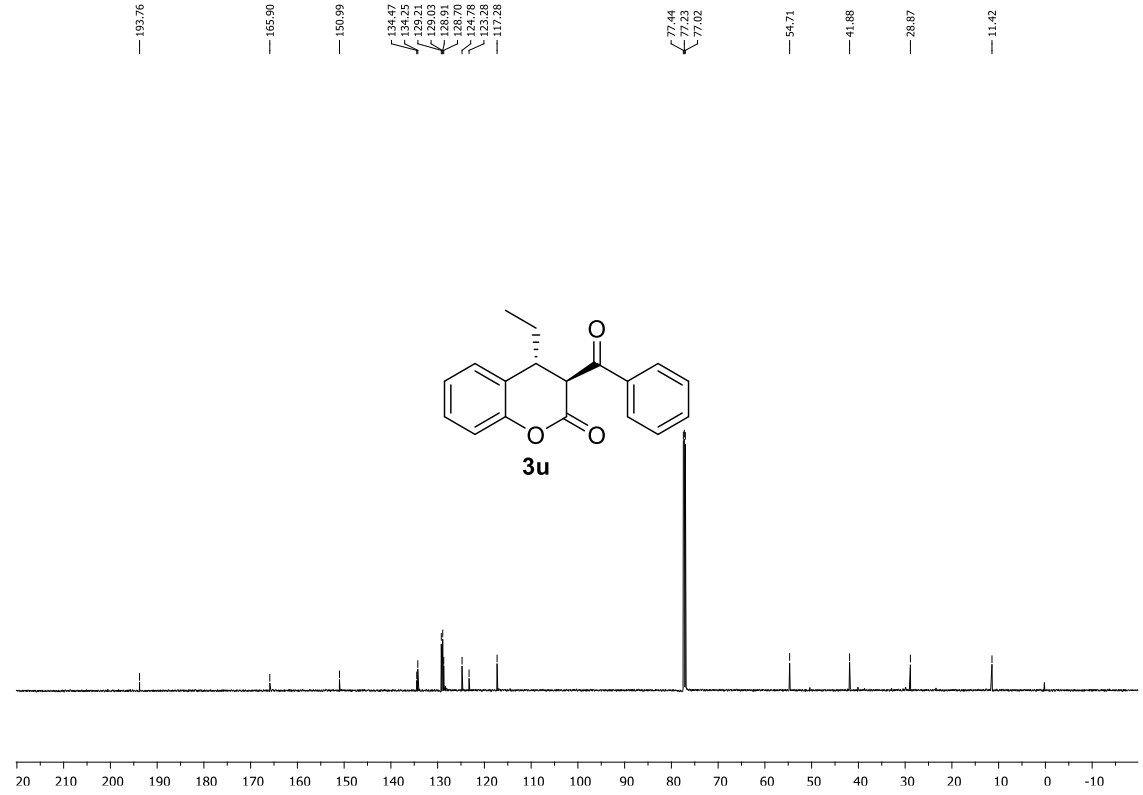
^{13}C{^{1}H} NMR of 3t (150 MHz, $CDCl_3$)



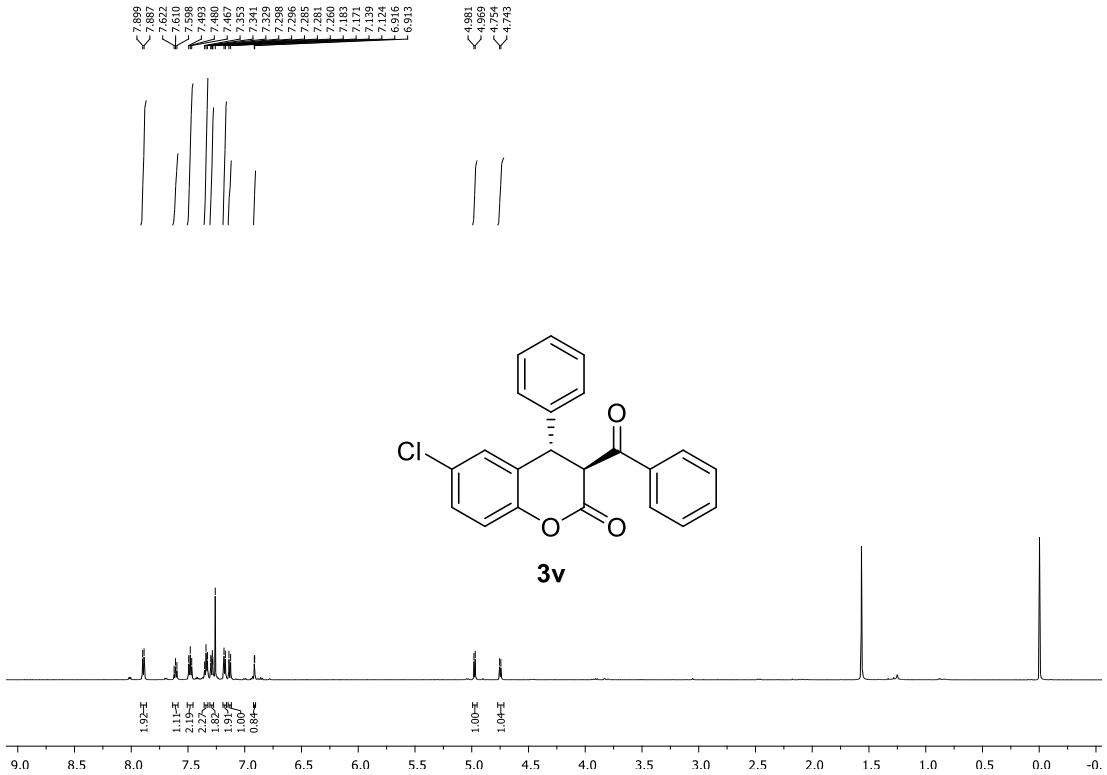
^{1}H NMR of 3u (600 MHz, $CDCl_3$)



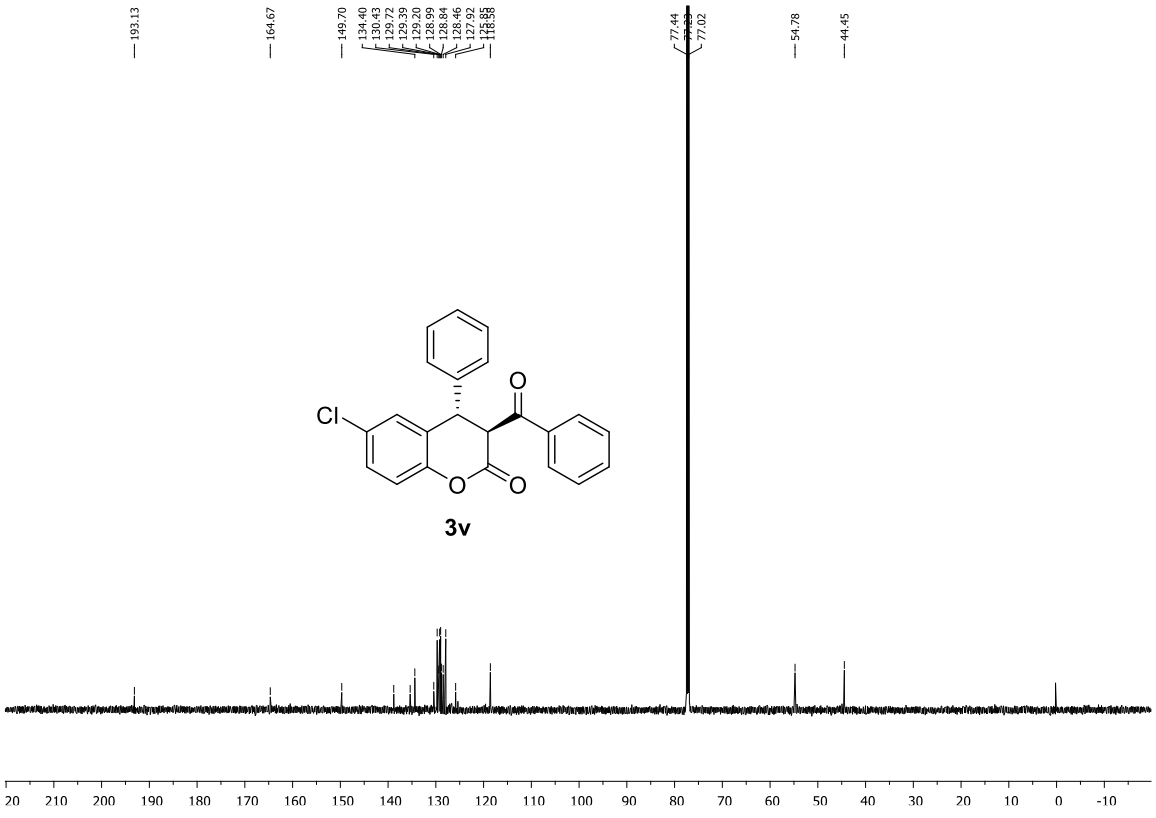
^{13}C{^{1}H} NMR of 3u (150 MHz, $CDCl_3$)



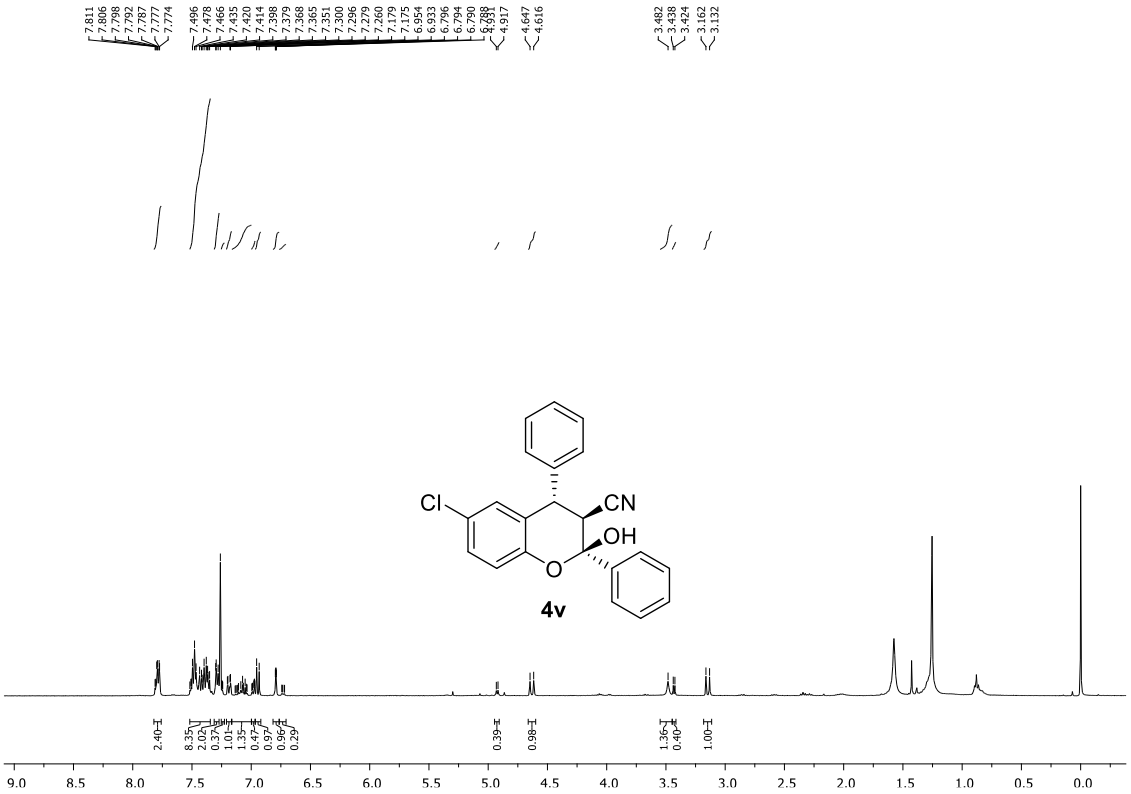
^{1}H NMR of 3v (600 MHz, $CDCl_3$)



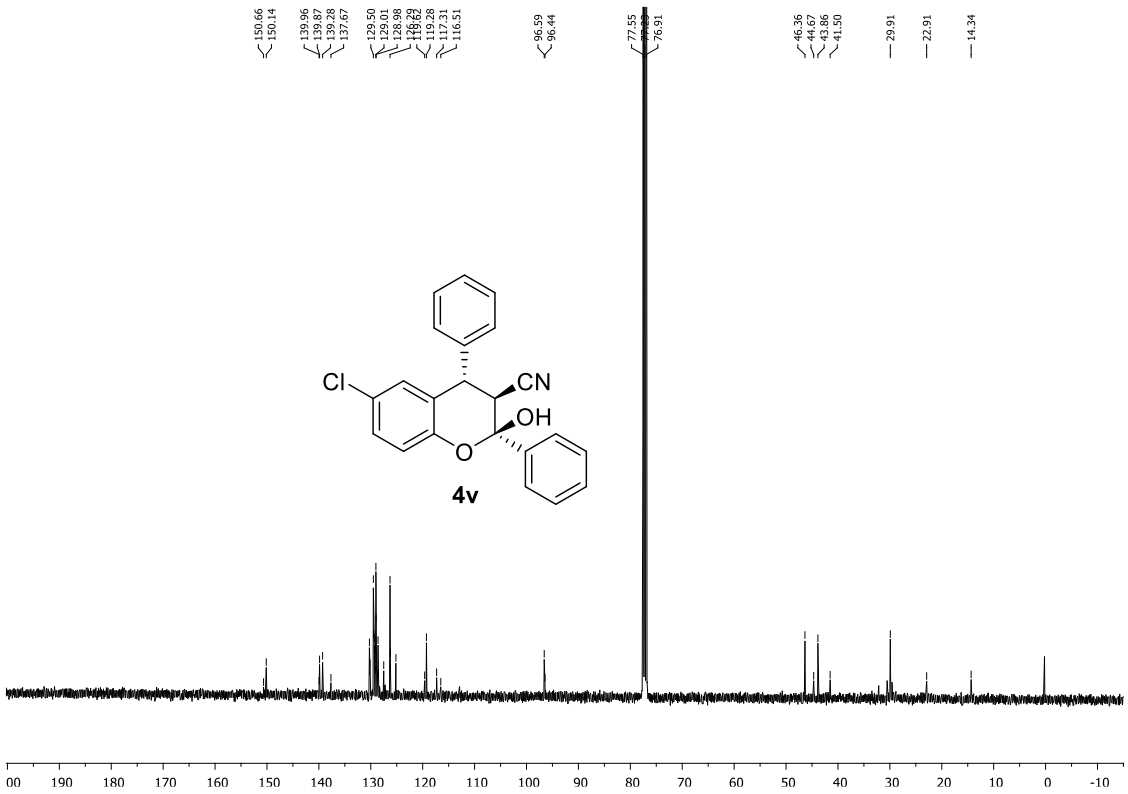
^{13}C{^{1}H} NMR of 3v (150 MHz, $CDCl_3$)



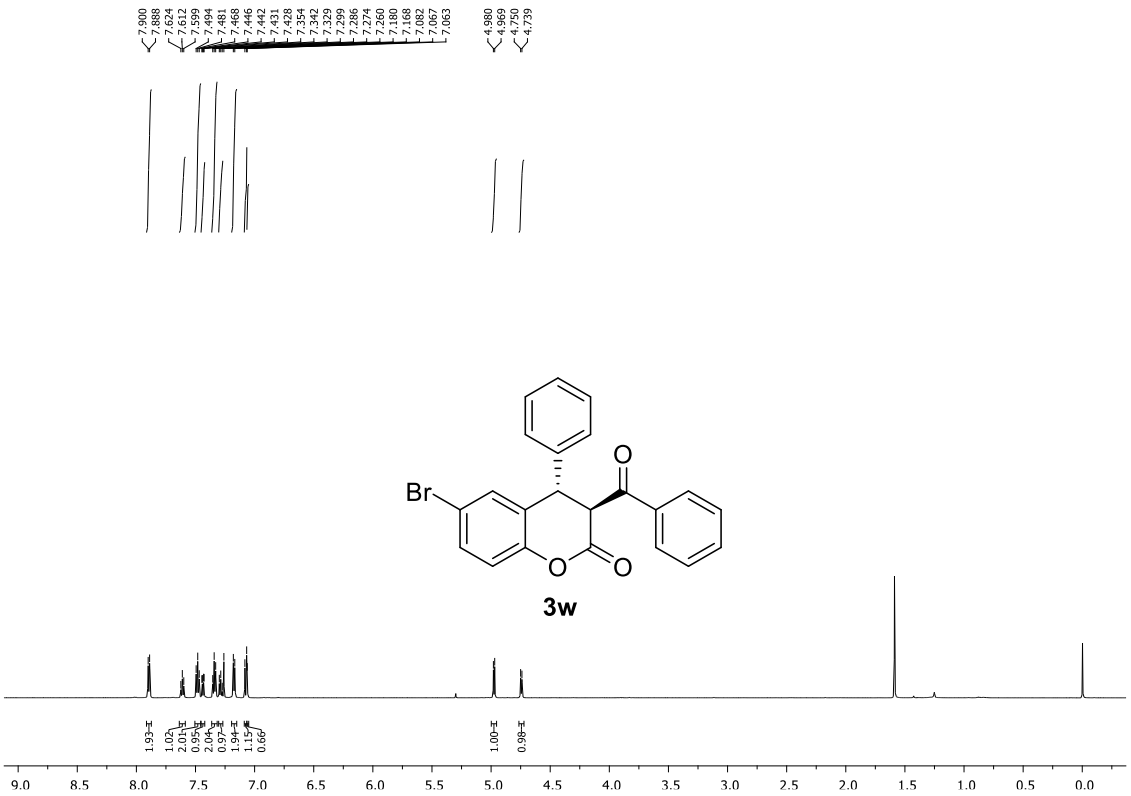
^{1}H NMR of 4v (400 MHz, $CDCl_3$)



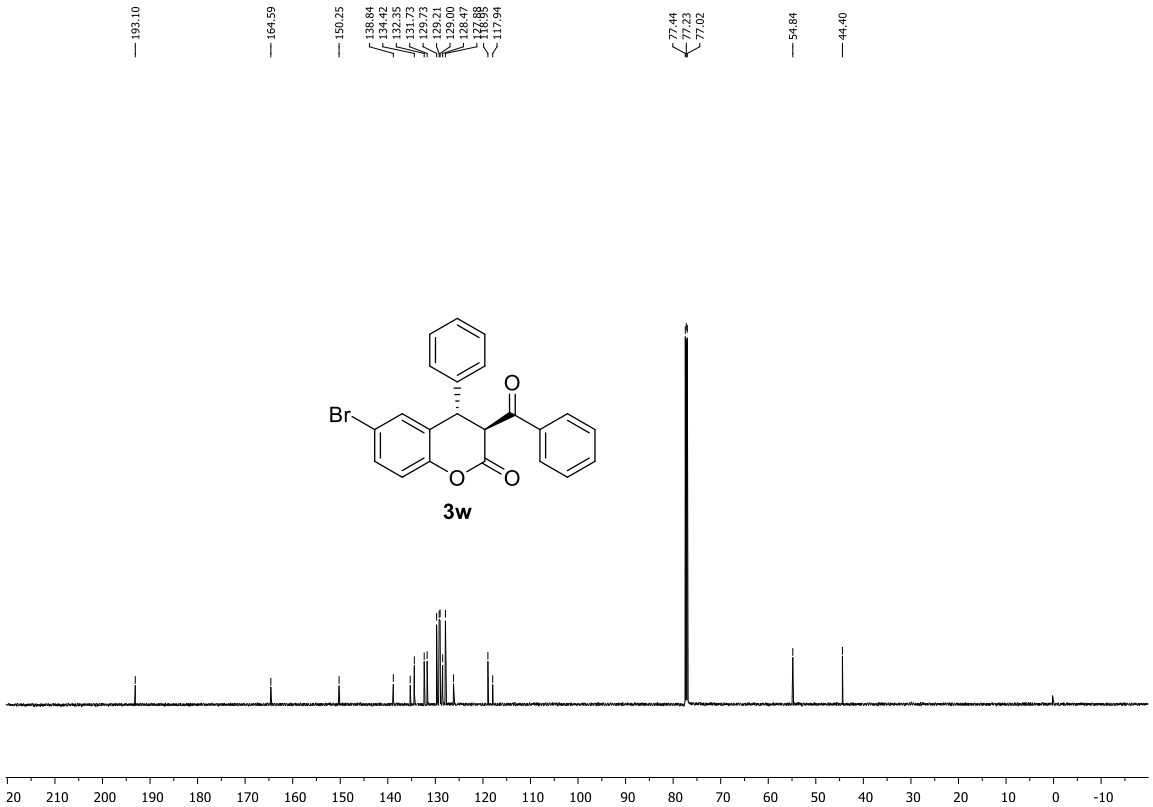
^{13}C{^{1}H} NMR of 4v (100 MHz, $CDCl_3$)



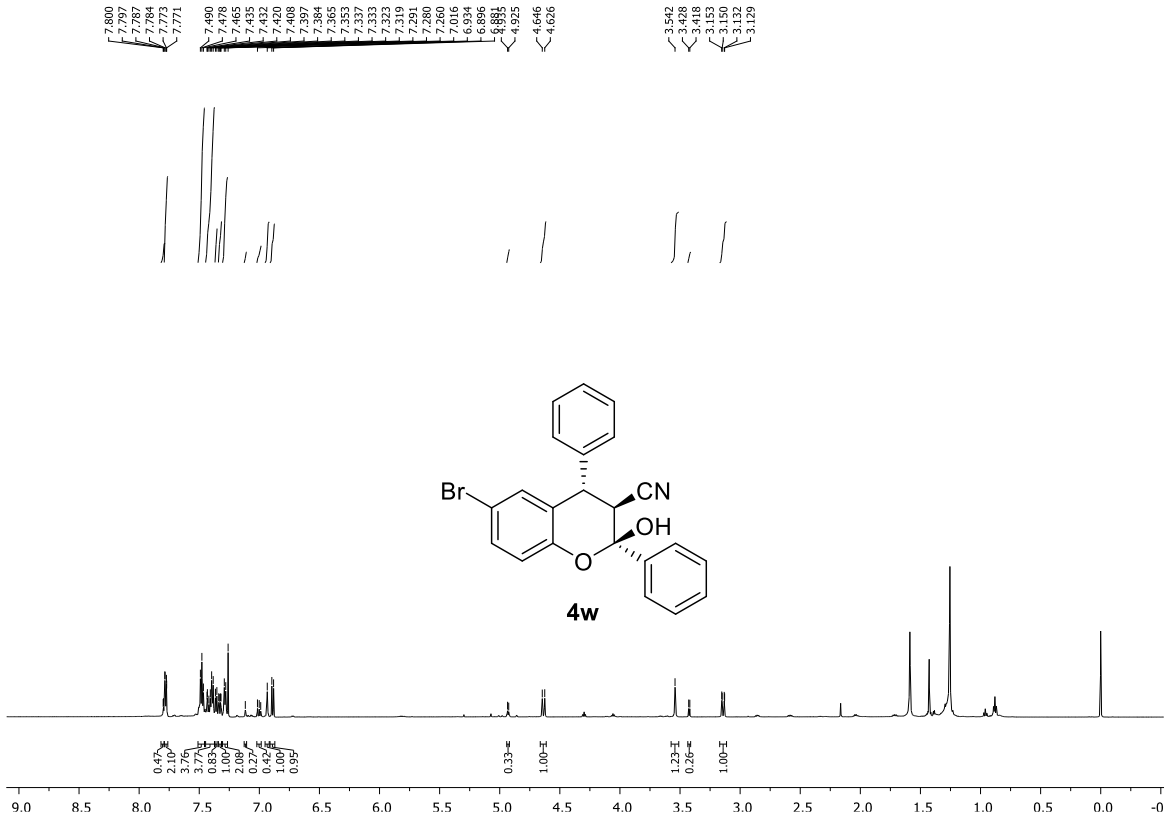
^{1}H NMR of 3w (600 MHz, $CDCl_3$)



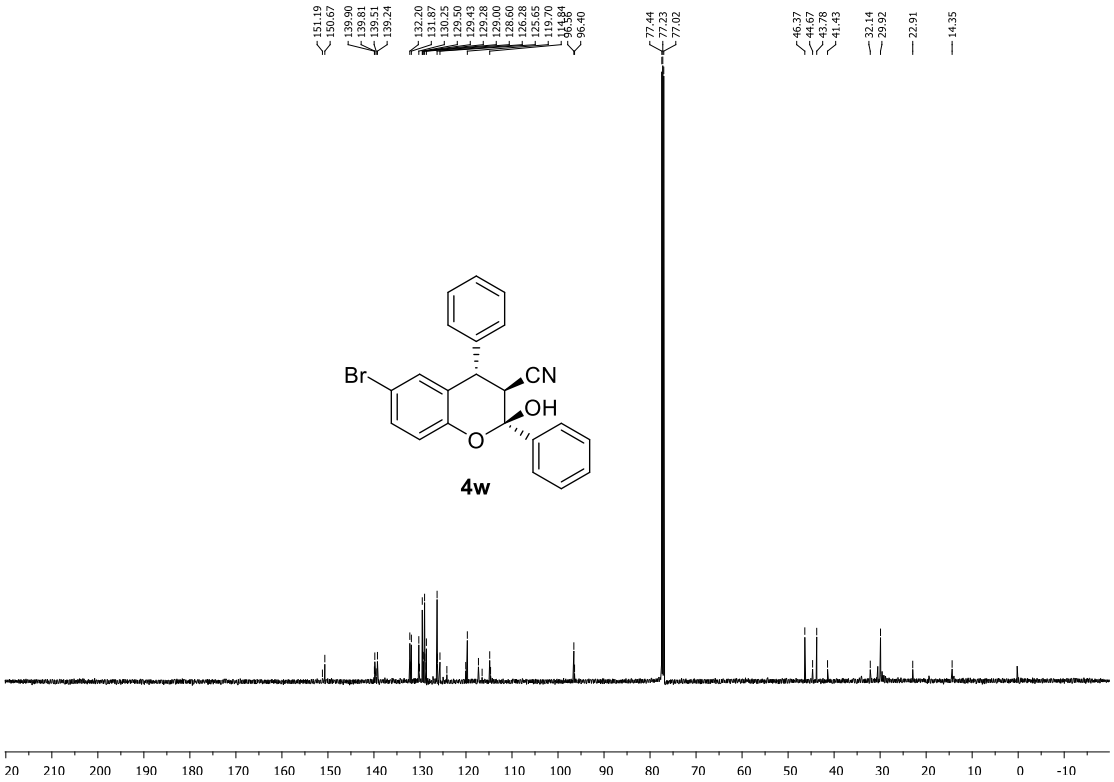
^{13}C{^{1}H} NMR of 3w (150 MHz, $CDCl_3$)



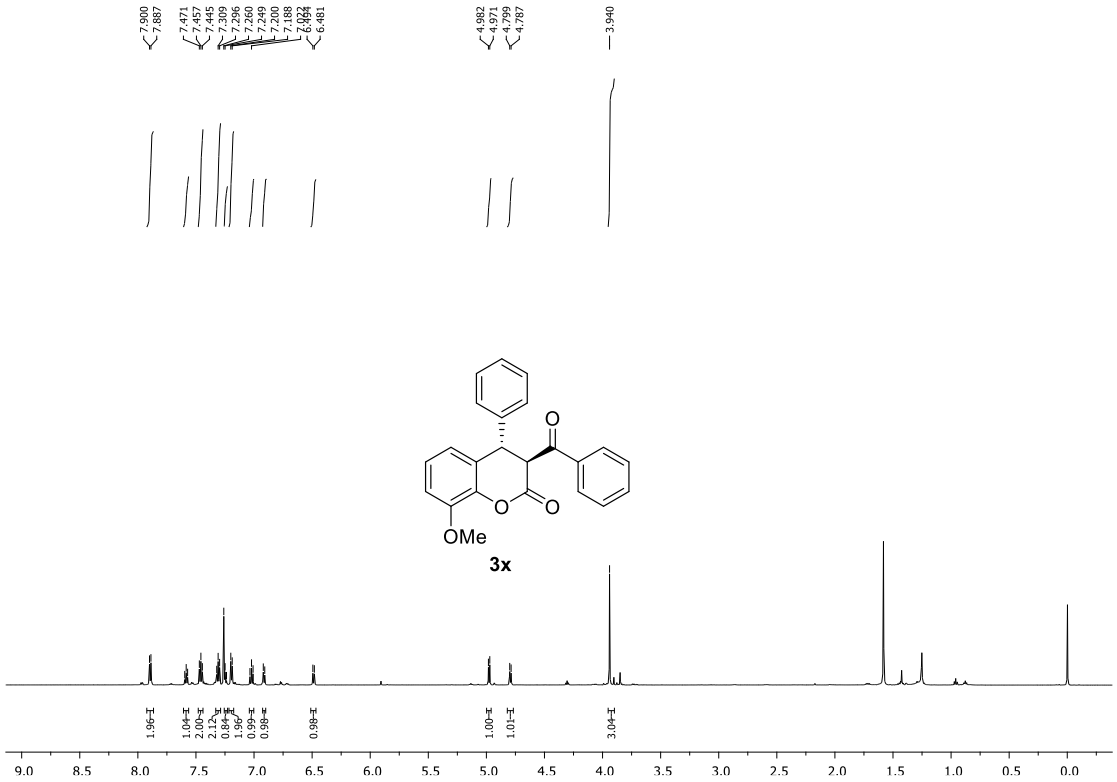
^{1}H NMR of 4w (600 MHz, $CDCl_3$)



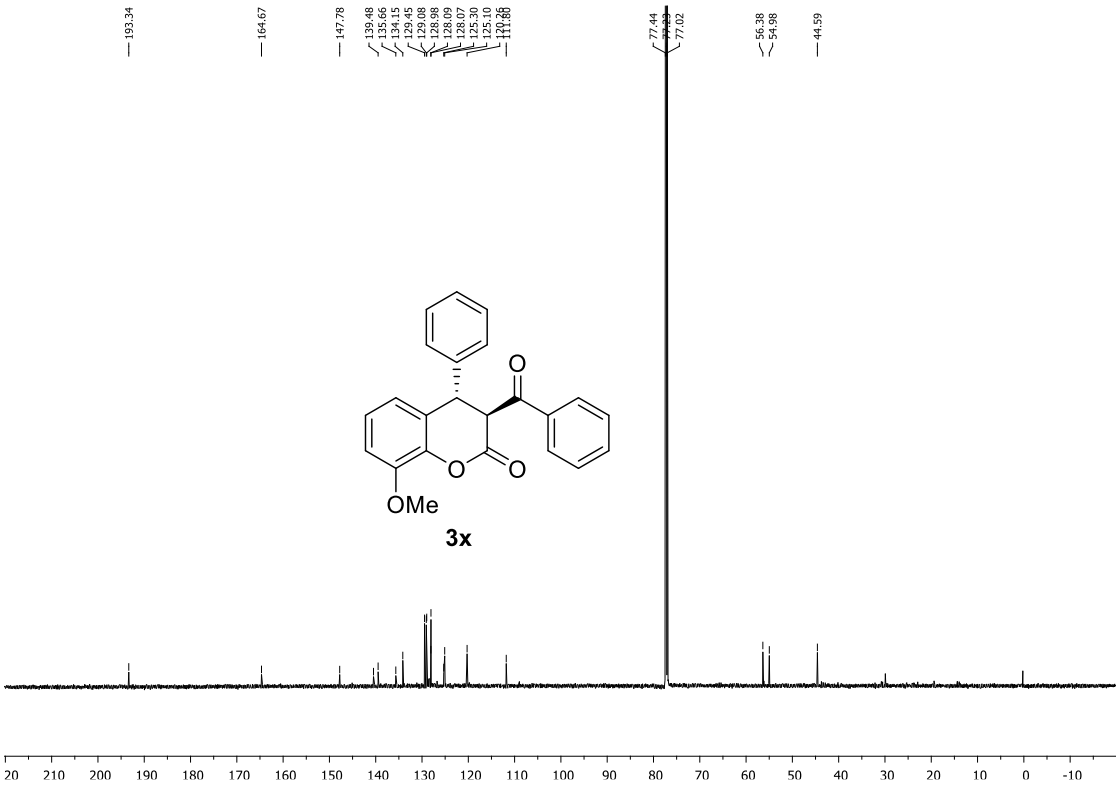
^{13}C{^{1}H} NMR of 4w (150 MHz, $CDCl_3$)



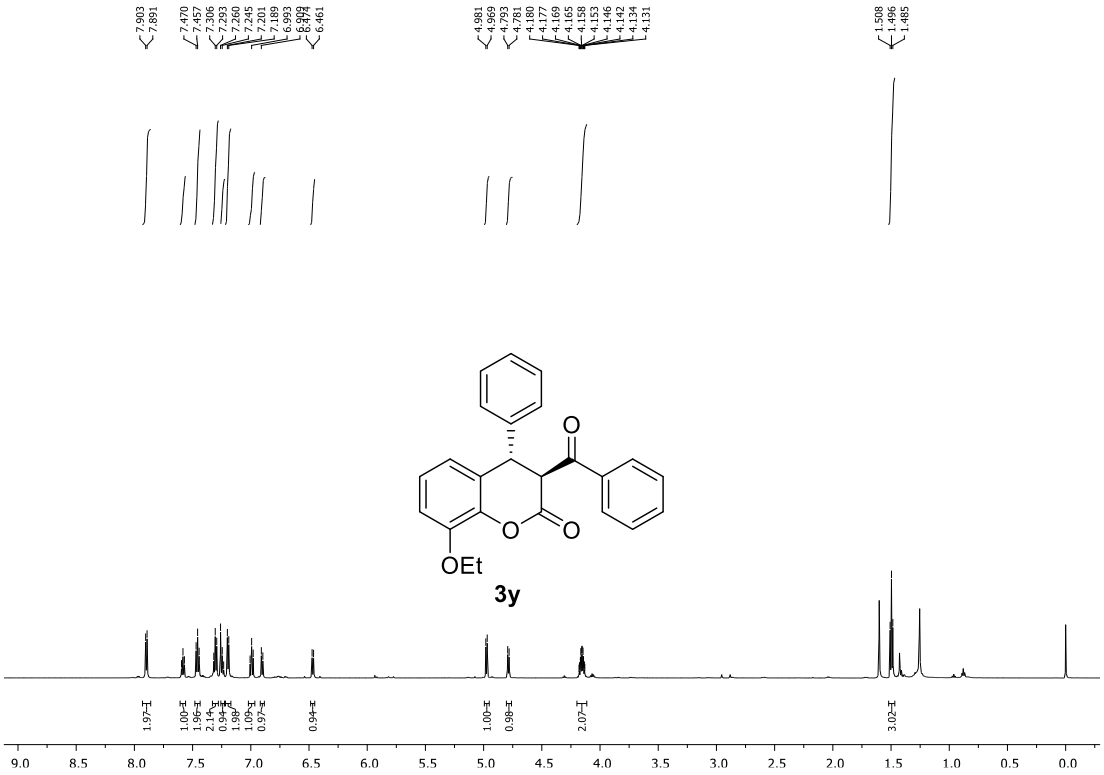
^{1}H NMR of 3x (600 MHz, $CDCl_3$)



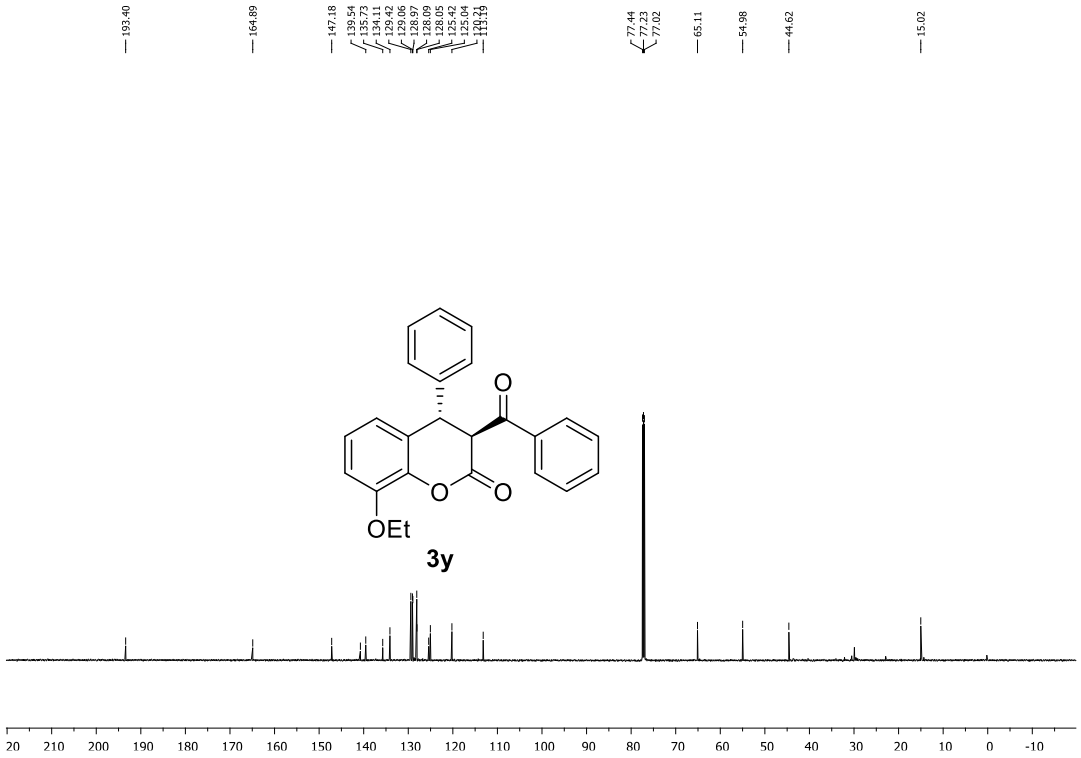
^{13}C{^{1}H} NMR of 3x (150 MHz, $CDCl_3$)



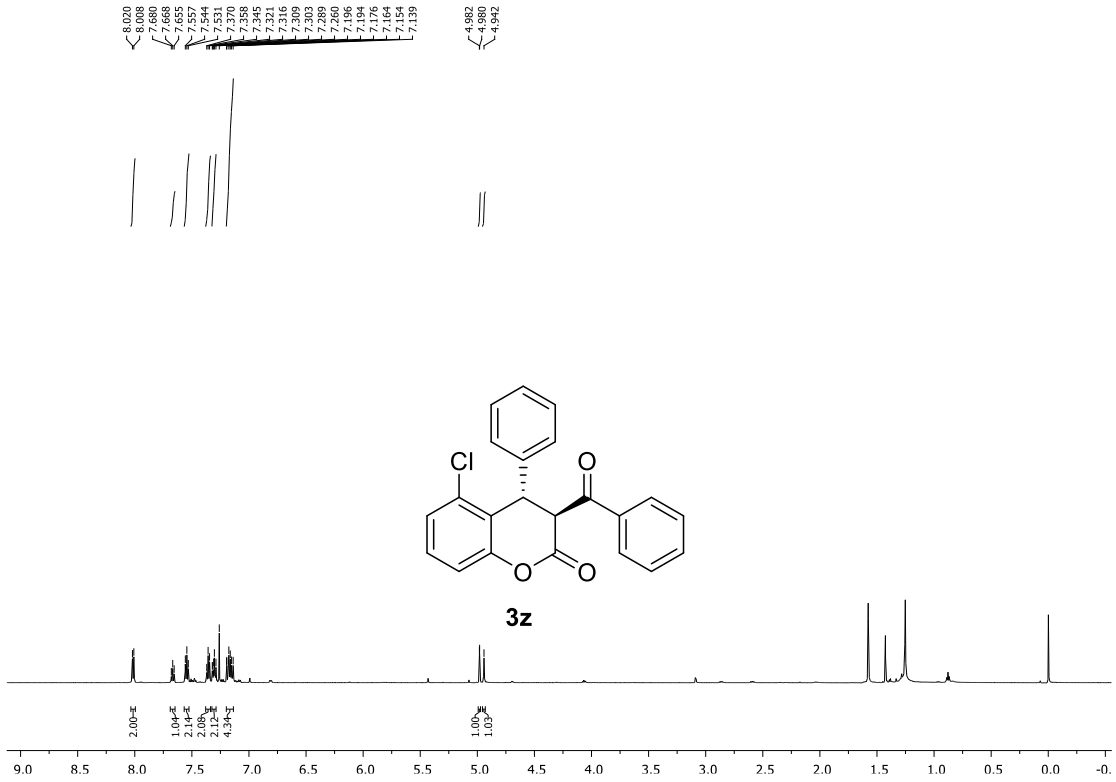
^{1}H NMR of 3y (600 MHz, $CDCl_3$)



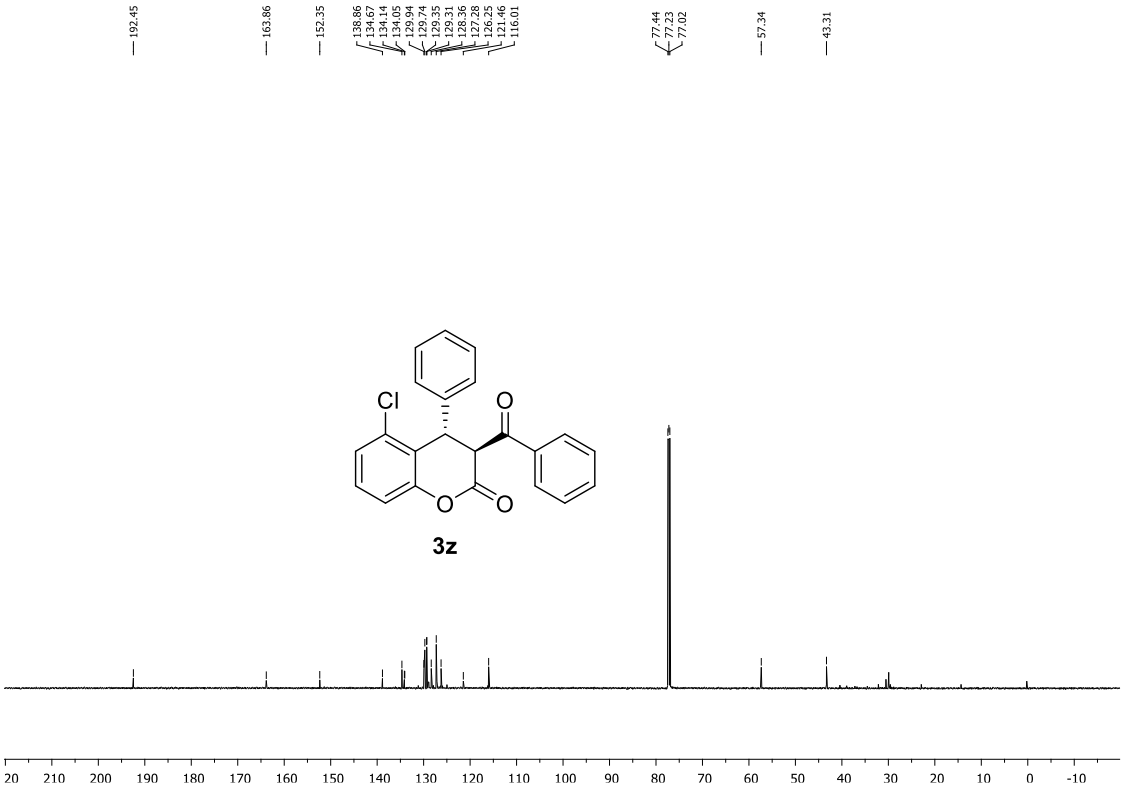
^{13}C{^{1}H} NMR of 3y (150 MHz, $CDCl_3$)



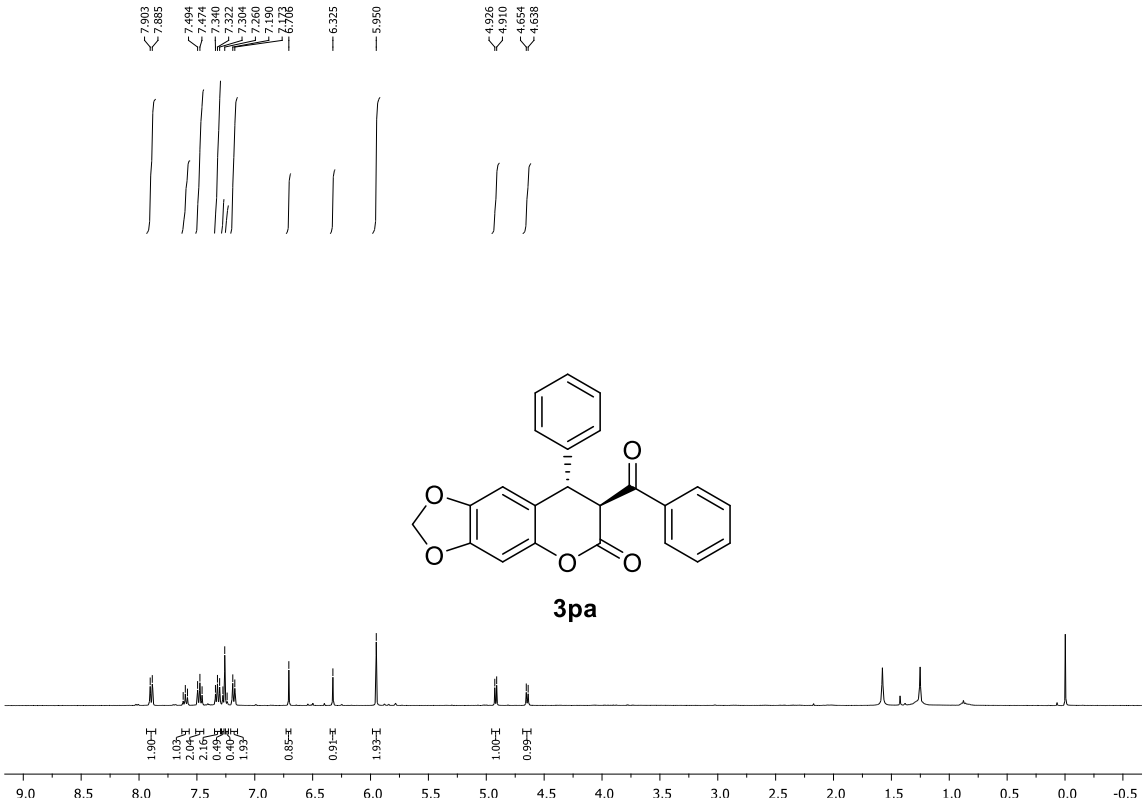
^{1}H NMR of 3z (600 MHz, $CDCl_3$)



^{13}C{^{1}H} NMR of 3z (150 MHz, $CDCl_3$)

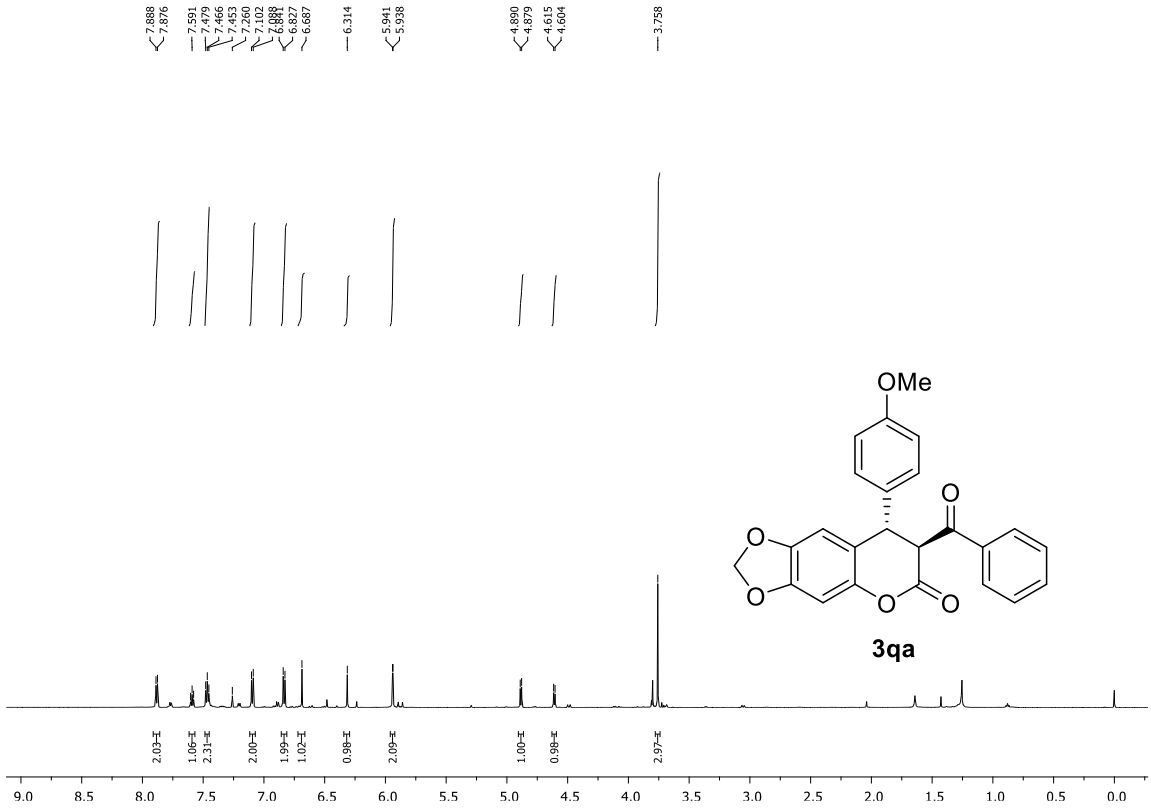


^{1}H NMR of 3pa (400 MHz, $CDCl_3$)

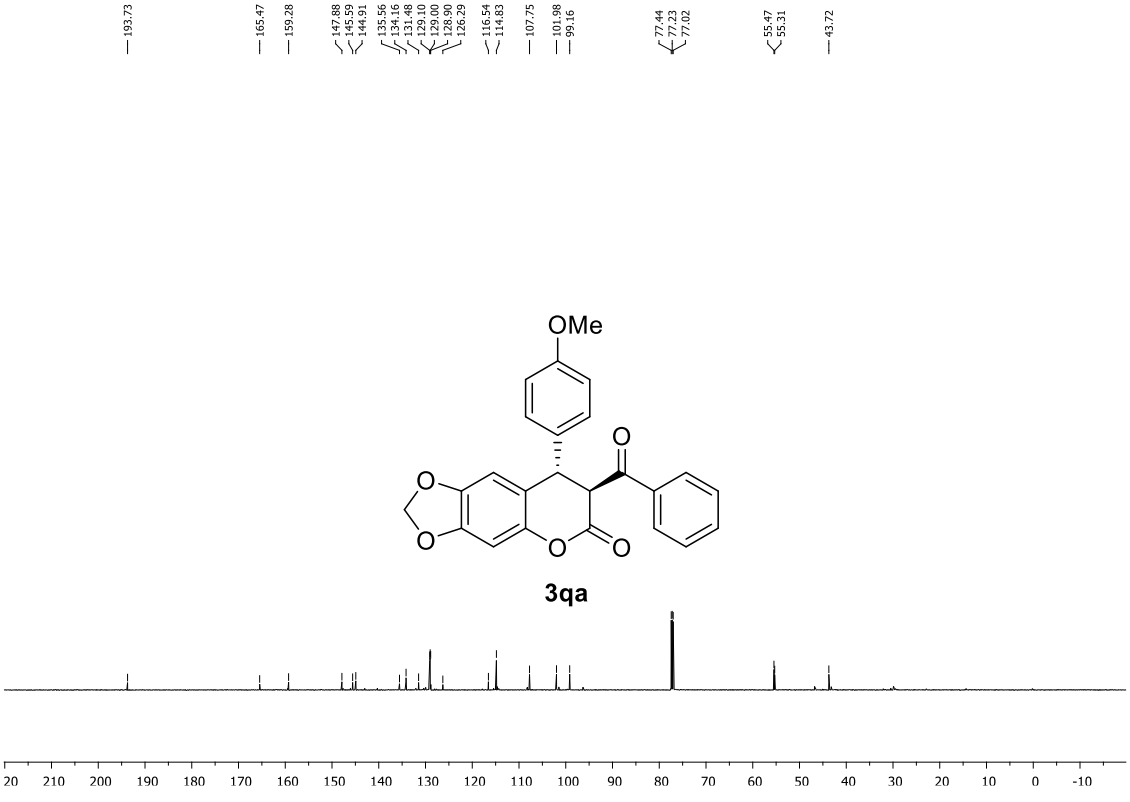


^{13}C{^{1}H} NMR of 3pa (100 MHz, $CDCl_3$)

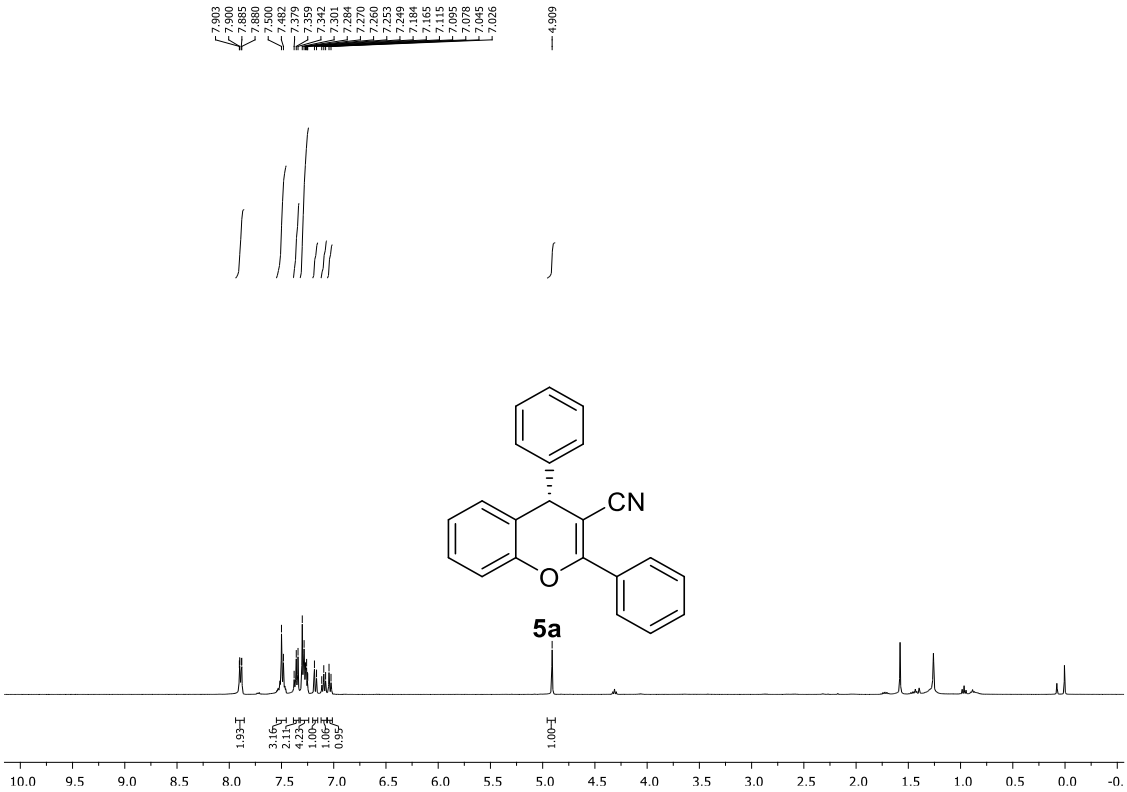
^{1}H NMR of 3qa (600 MHz, $CDCl_3$)



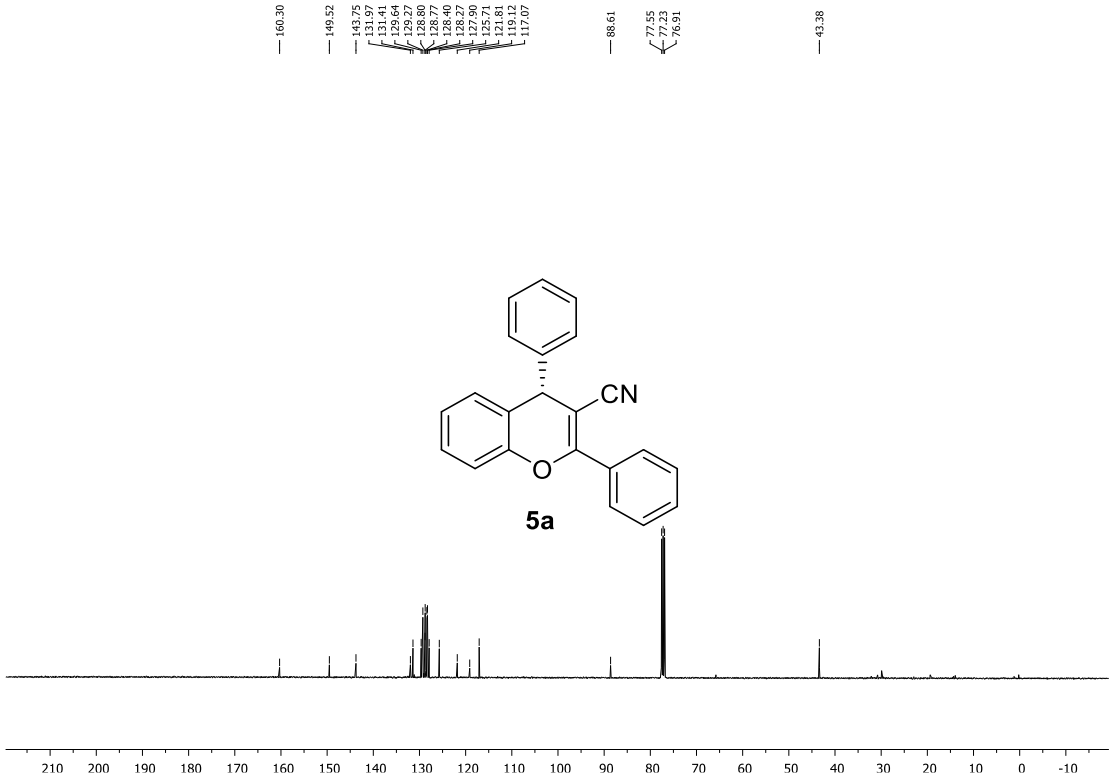
^{13}C{^{1}H} NMR of 3qa (150 MHz, $CDCl_3$)



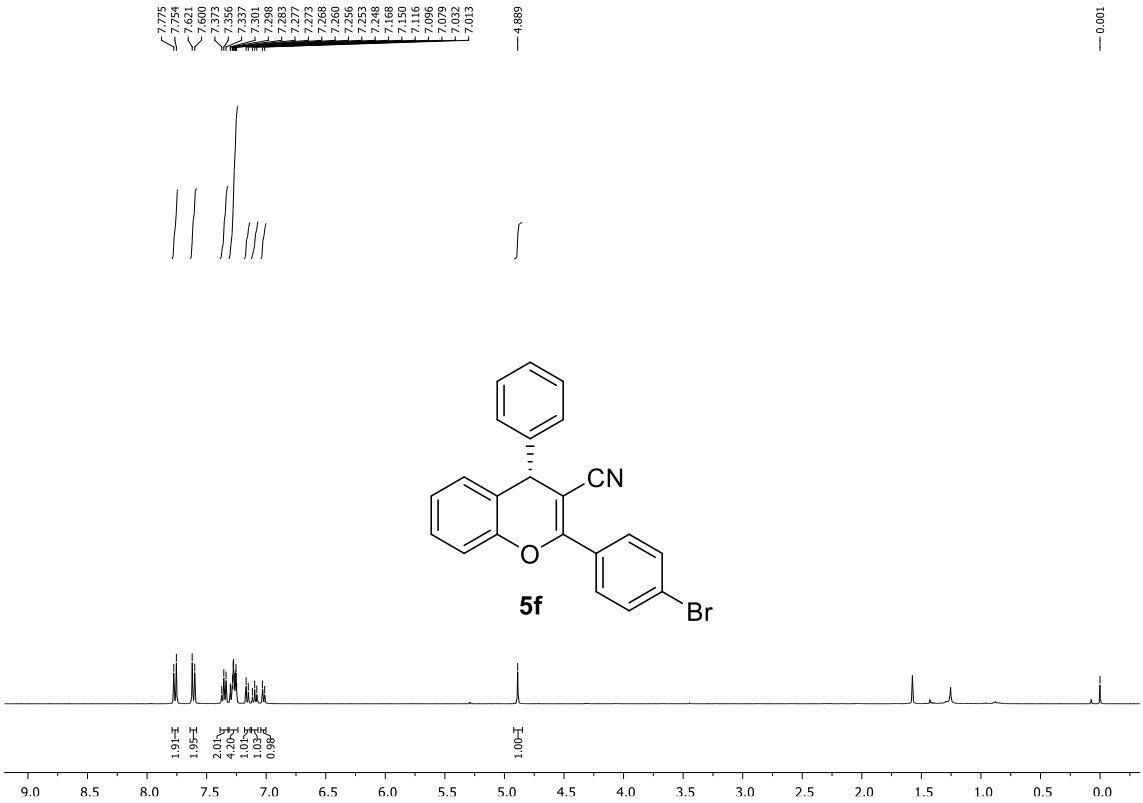
^{1}H NMR of 5a (400 MHz, $CDCl_3$)



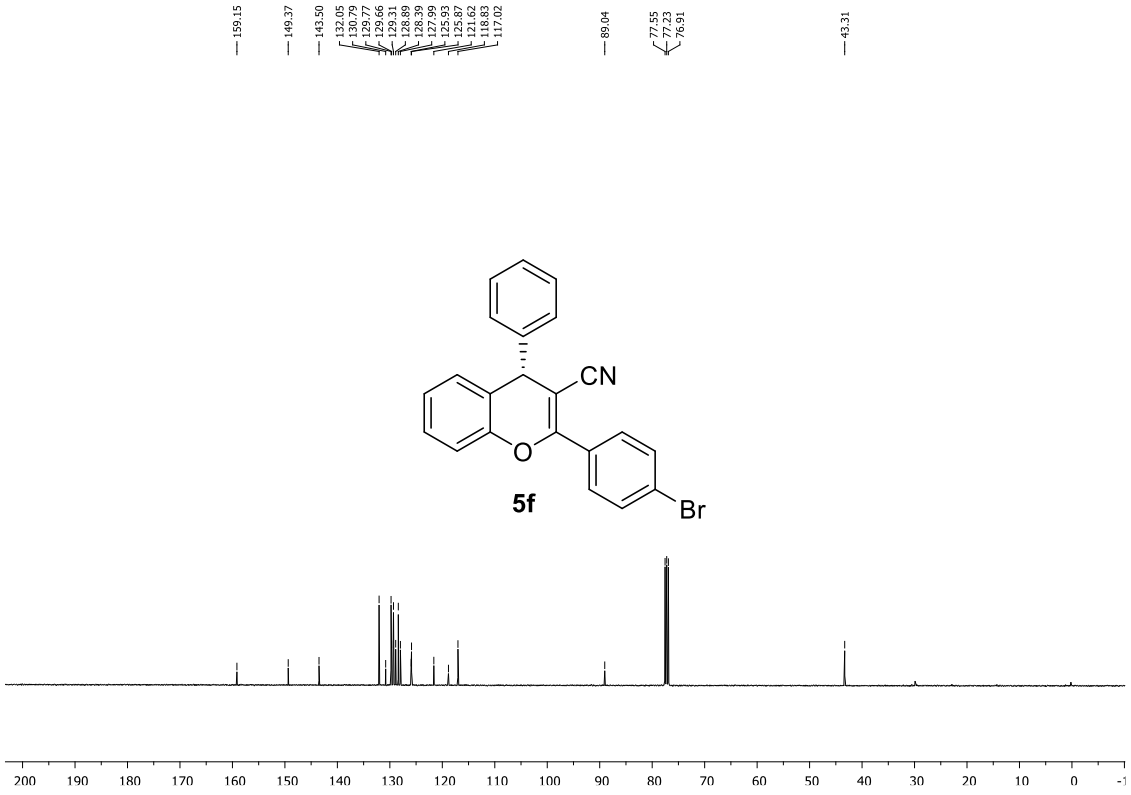
^{13}C{^{1}H} NMR of 5a (100 MHz, $CDCl_3$)



^{1}H NMR of 5f (400 MHz, $CDCl_3$)

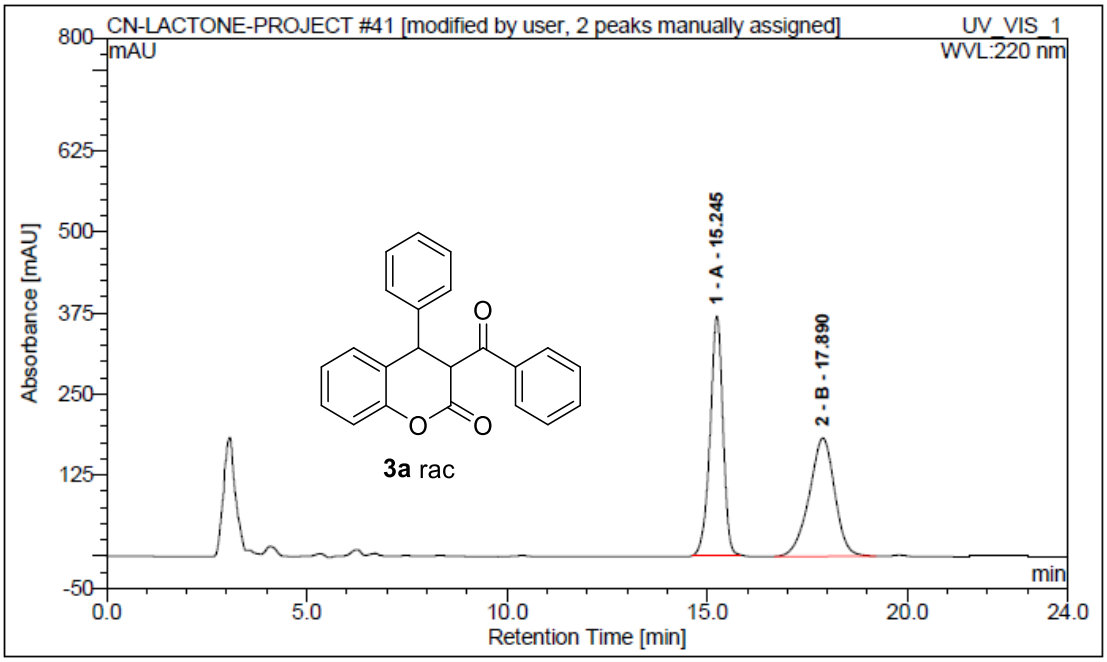


^{13}C{^{1}H} NMR of 5f (100 MHz, $CDCl_3$)

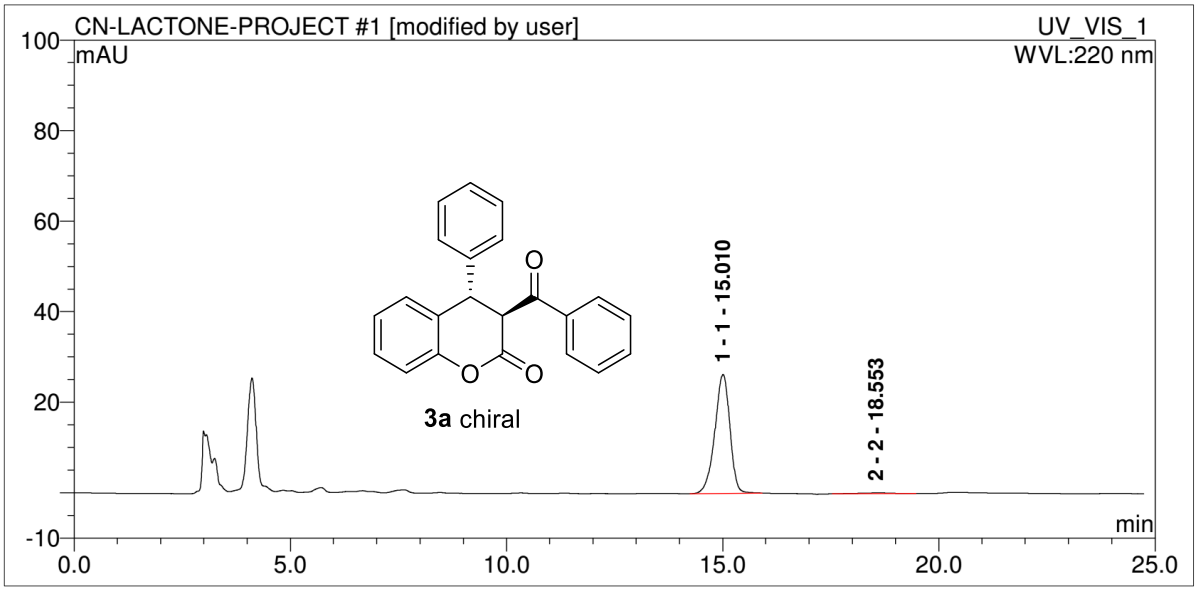


4. HPLC chromatogram of the products:

SAL-CN-LAC-LUX-C4-RAC

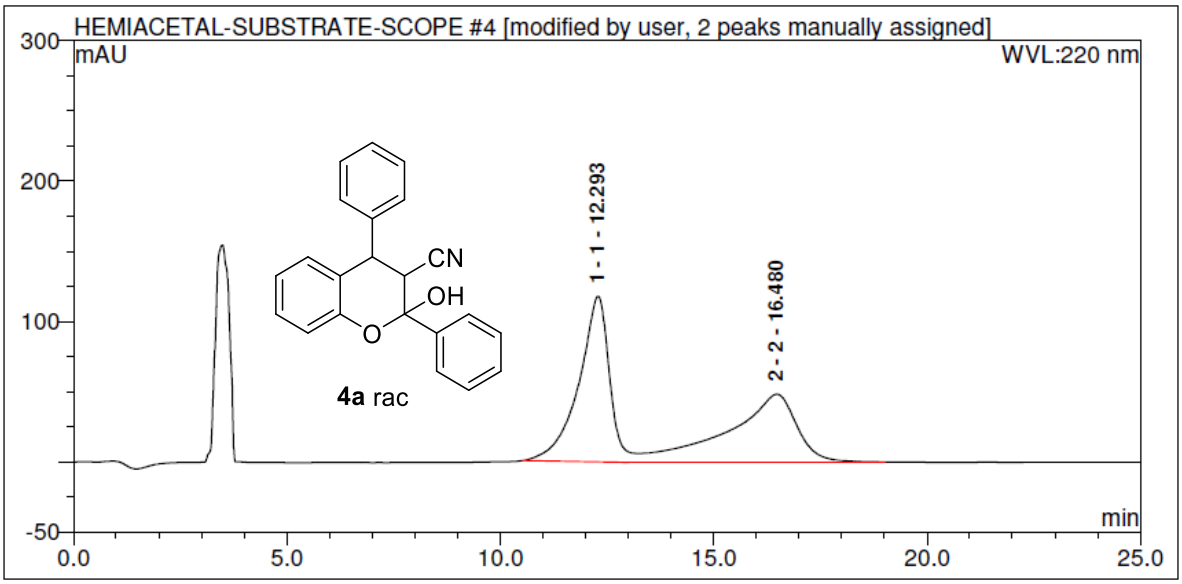


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	15.25	136.4721	50.26780547	368.9556	n.a.
2	B	17.89	135.018	49.73219453	182.886	n.a.

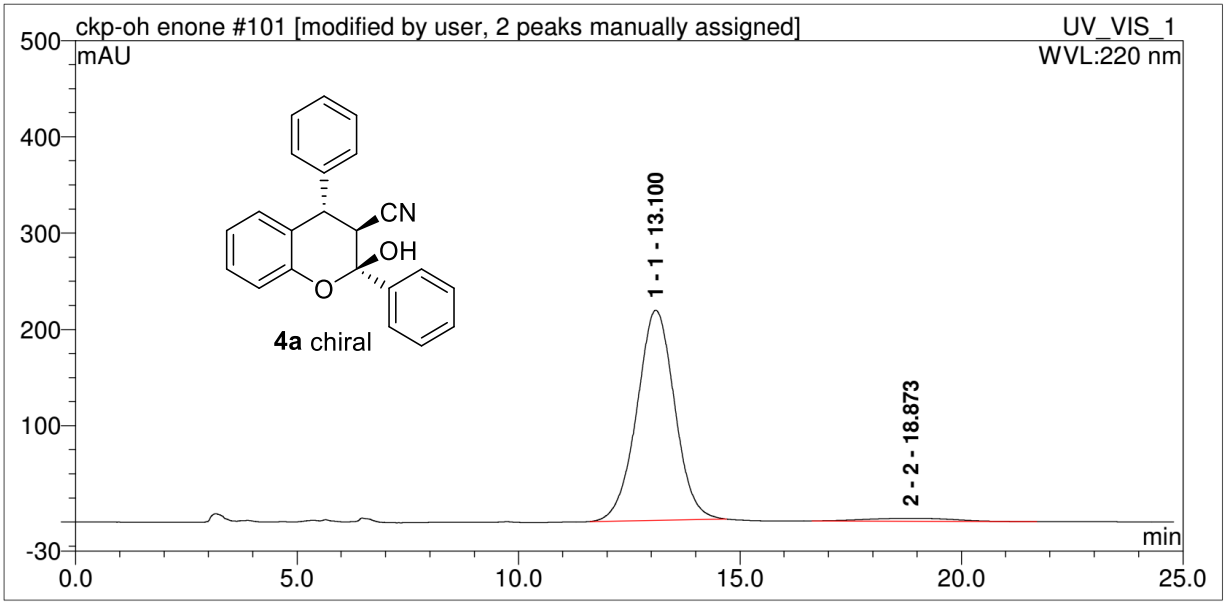


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	15.01	10.6442	98.43194676	26.29118	n.a.
2	2	18.55	0.170	1.568053243	0.183	n.a.

Ph-CN-HEMI-RAC-ID

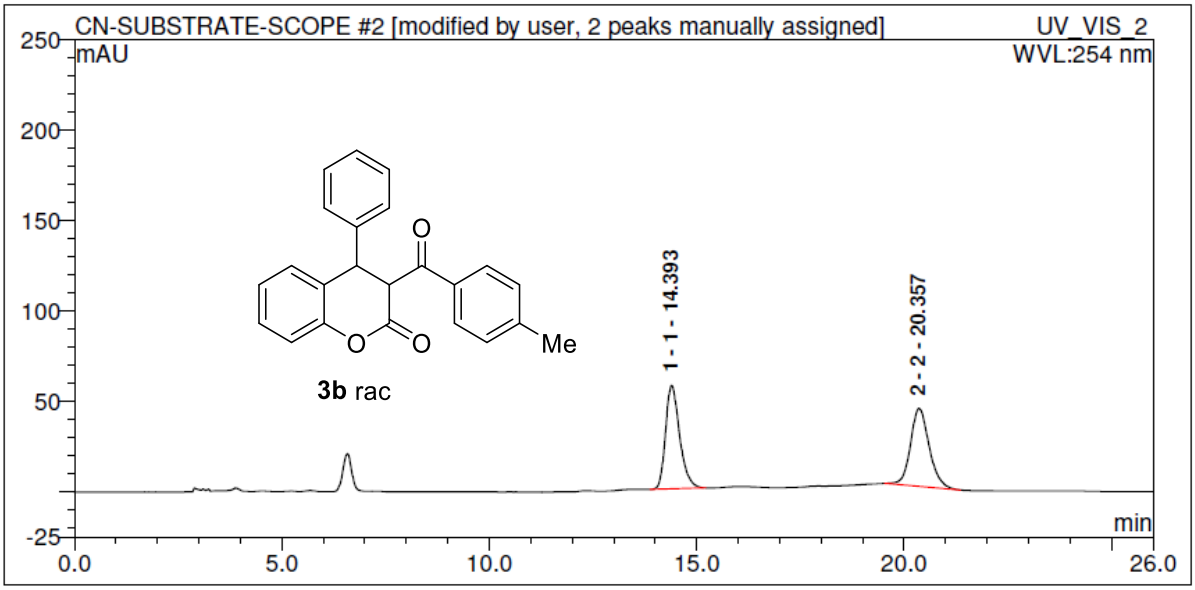


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	12.29	97.24595	51.31021662	117.9519	n.a.
2	2	16.48	92.280	48.68978338	48.304	n.a.



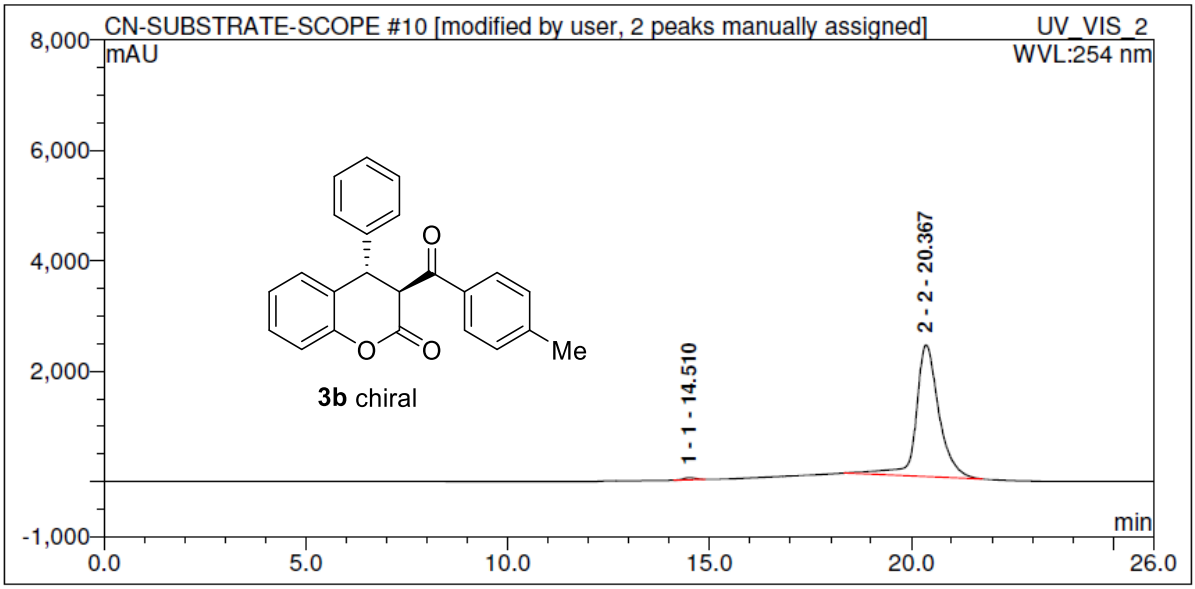
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	13.10	215.8537	96.77278563	218.2557	n.a.
2	2	18.87	7.198	3.227214371	3.161	n.a.

4-Me-CN-RAC-IA



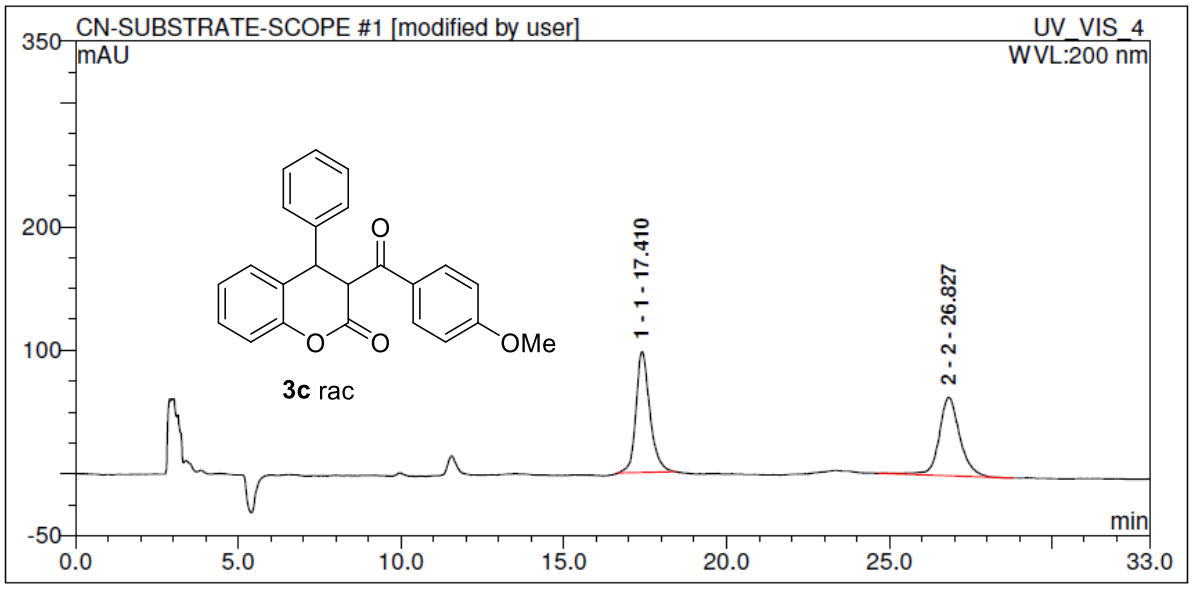
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	14.39	22.55273	50.05065655	57.27174	n.a.
2	2	20.36	22.507	49.94934345	43.092	n.a.

4-Me-CN-CHI-IA



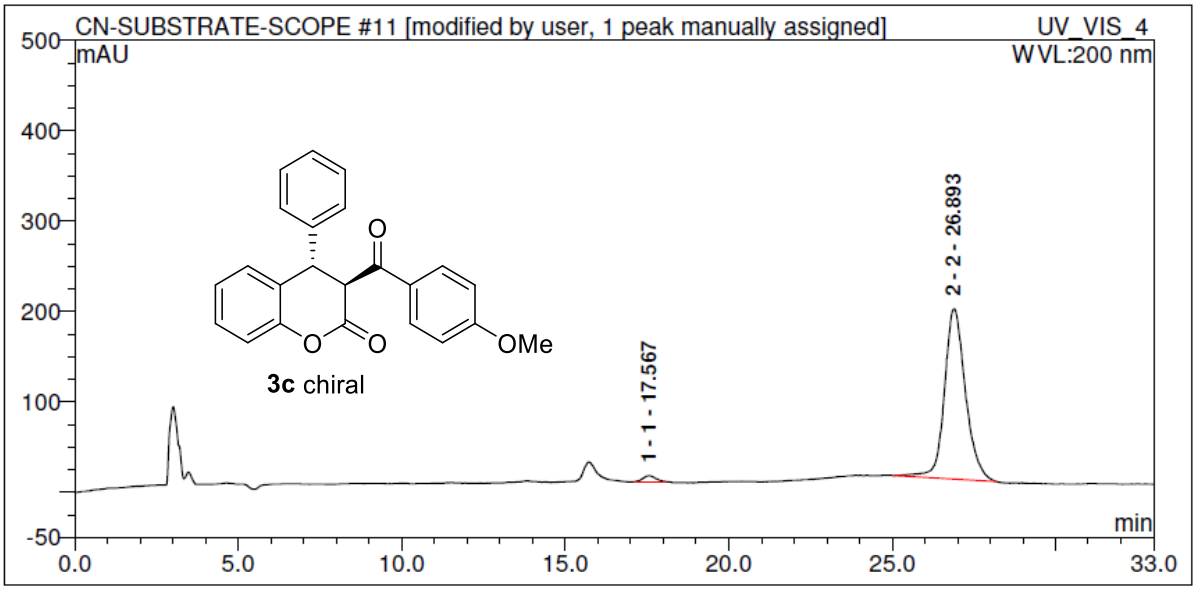
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	14.51	13.53862	0.8545055578	37.68191	n.a.
2	2	20.37	1570.842	99.14549444	2382.895	n.a.

4-OMe-CN-RAC-IA



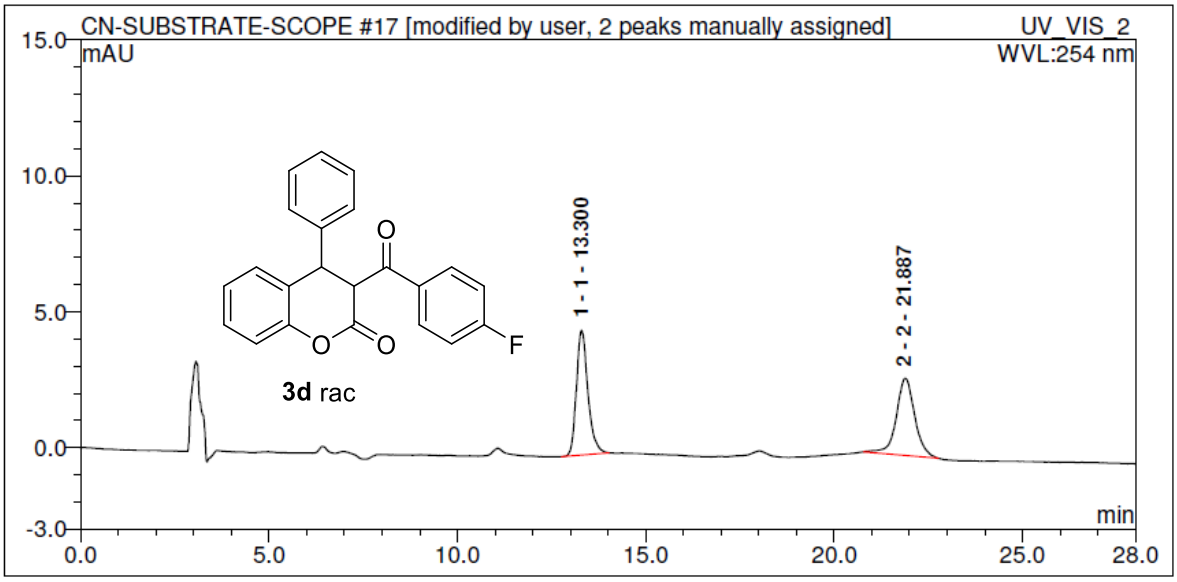
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	17.41	48.48898	50.76832058	97.69576	n.a.
2	2	26.83	47.021	49.23167942	63.434	n.a.

4-OMe-CN-CHI-IA



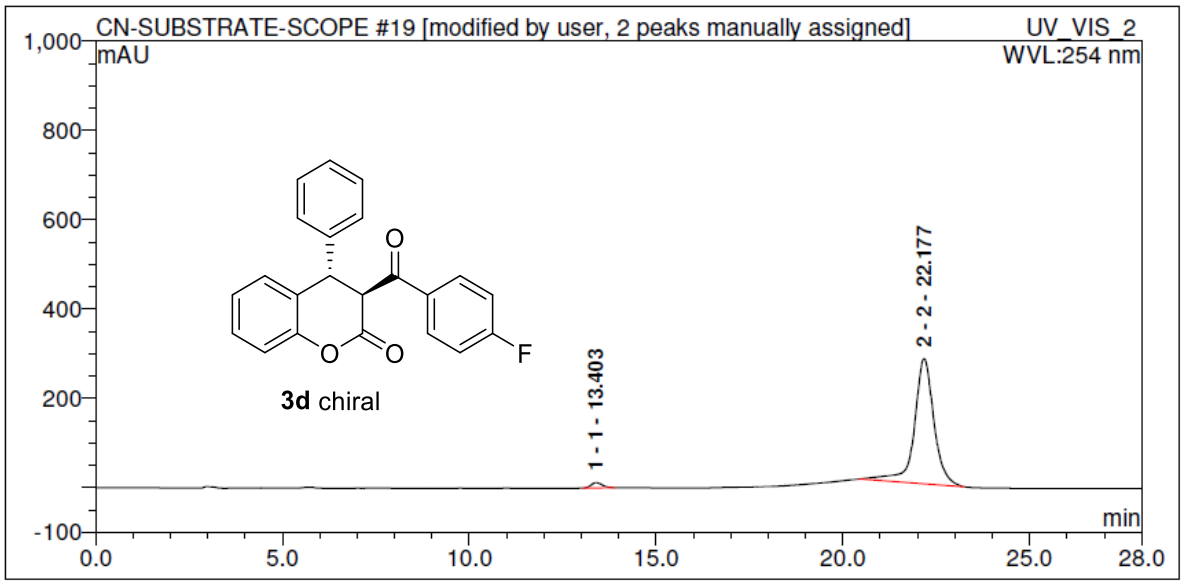
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	17.57	3.112234	2.164409019	6.89078	n.a.
2	2	26.89	140.679	97.83559098	188.281	n.a.

4-F-CN-RAC-IA



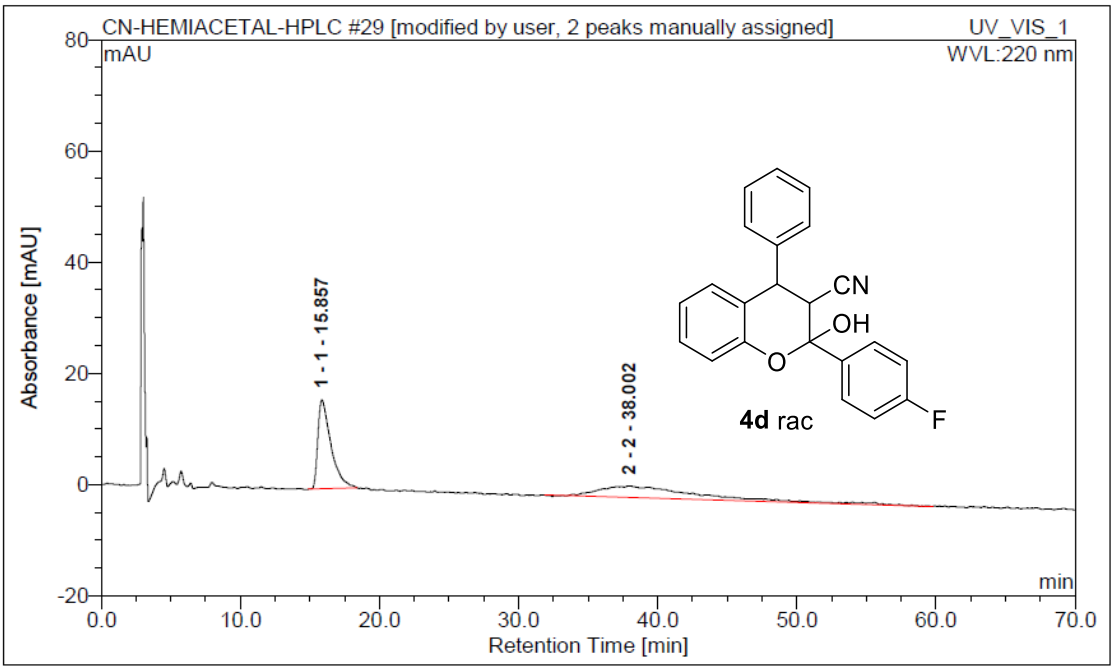
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	13.30	1.6253	50.22419728	4.58619	n.a.
2	2	21.89	1.611	49.77580272	2.836	n.a.

4-F-CN-CHI-IA



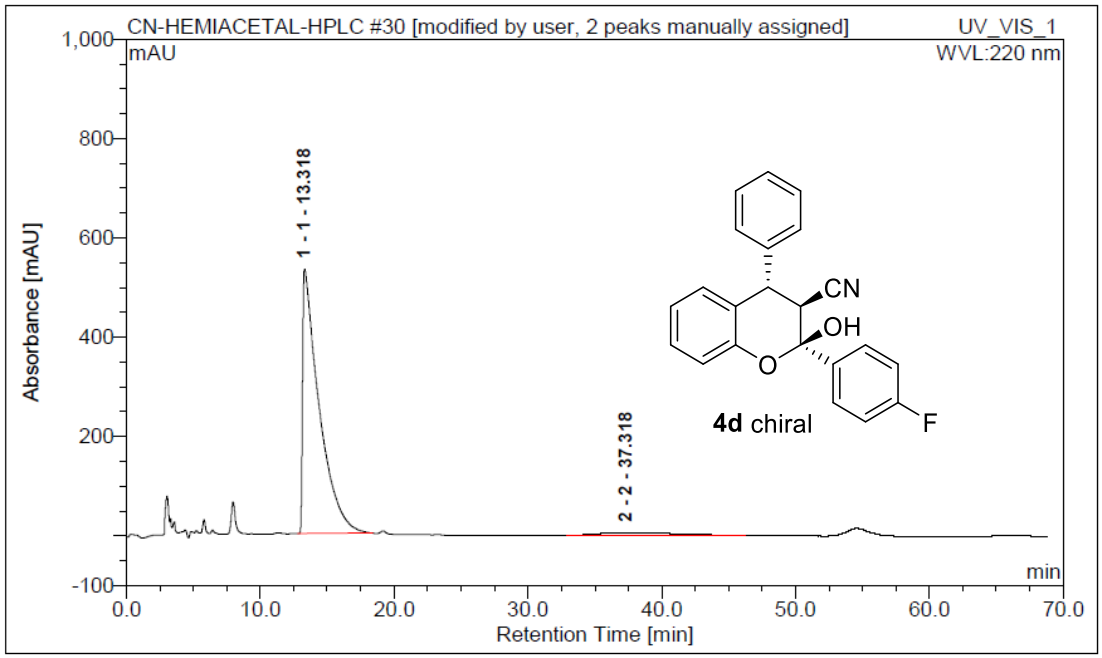
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	13.40	4.029324	2.302847138	11.85236	n.a.
2	2	22.18	170.942	97.69715286	279.955	n.a.

4-F-CN-HEMI-RAC-LUX-AMYLOSE-2



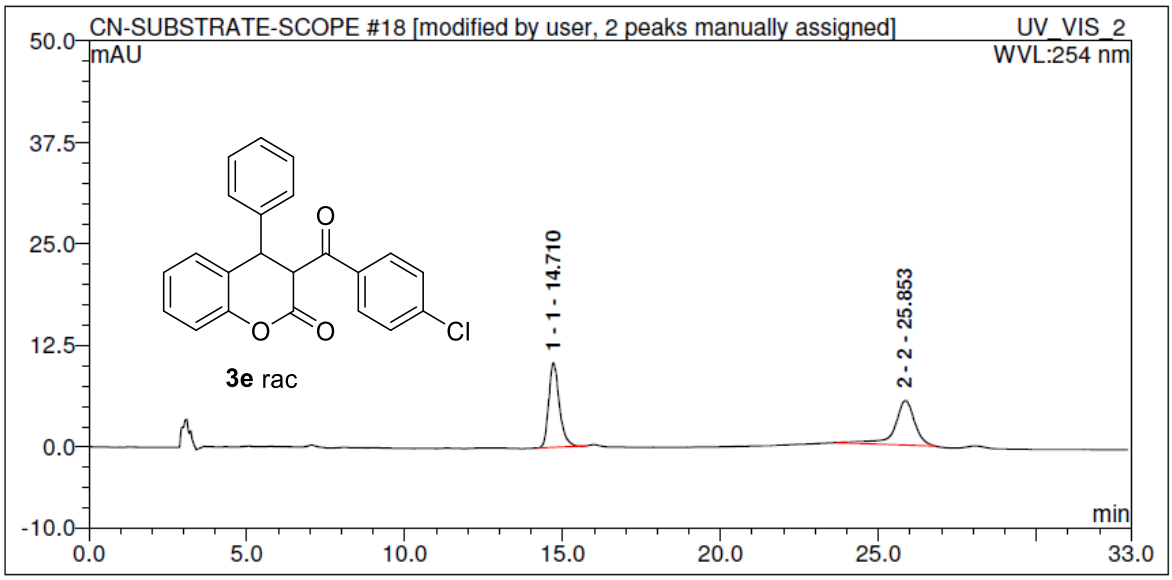
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	15.86	17.41874	50.3109587	15.99927	n.a.
2	2	38.00	17.203	49.6890413	2.081	n.a.

4-F-CN-HEMI-CHI-LUX-AMYLOSE-2



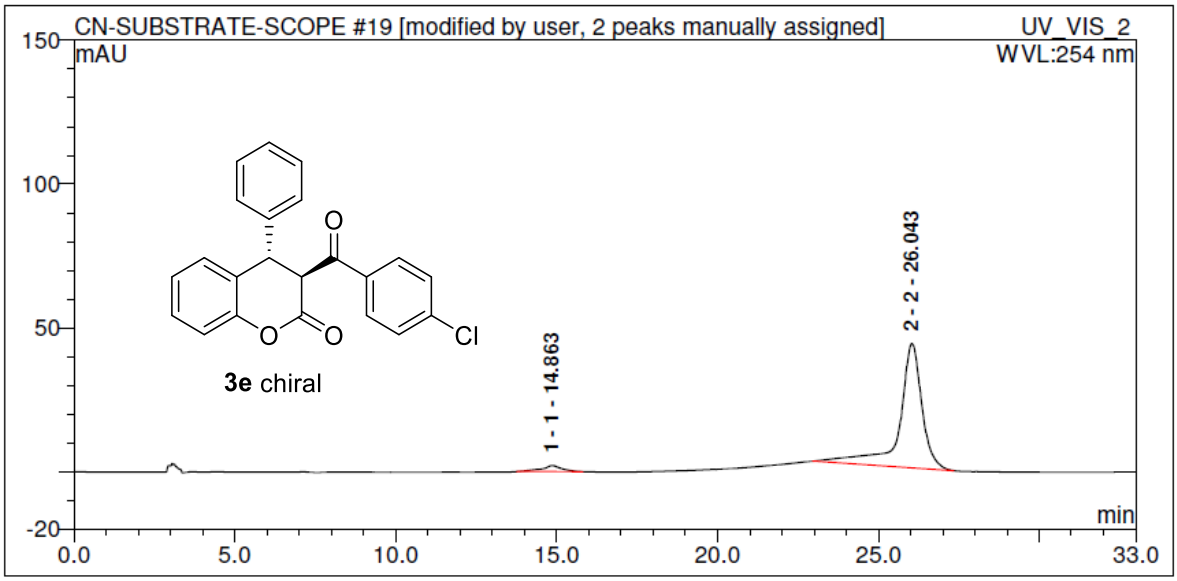
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	13.32	761.417	95.65251956	532.4339	n.a.
2	2	37.32	34.607	4.34748044	5.344	n.a.

4-Cl-CN-RAC-IA



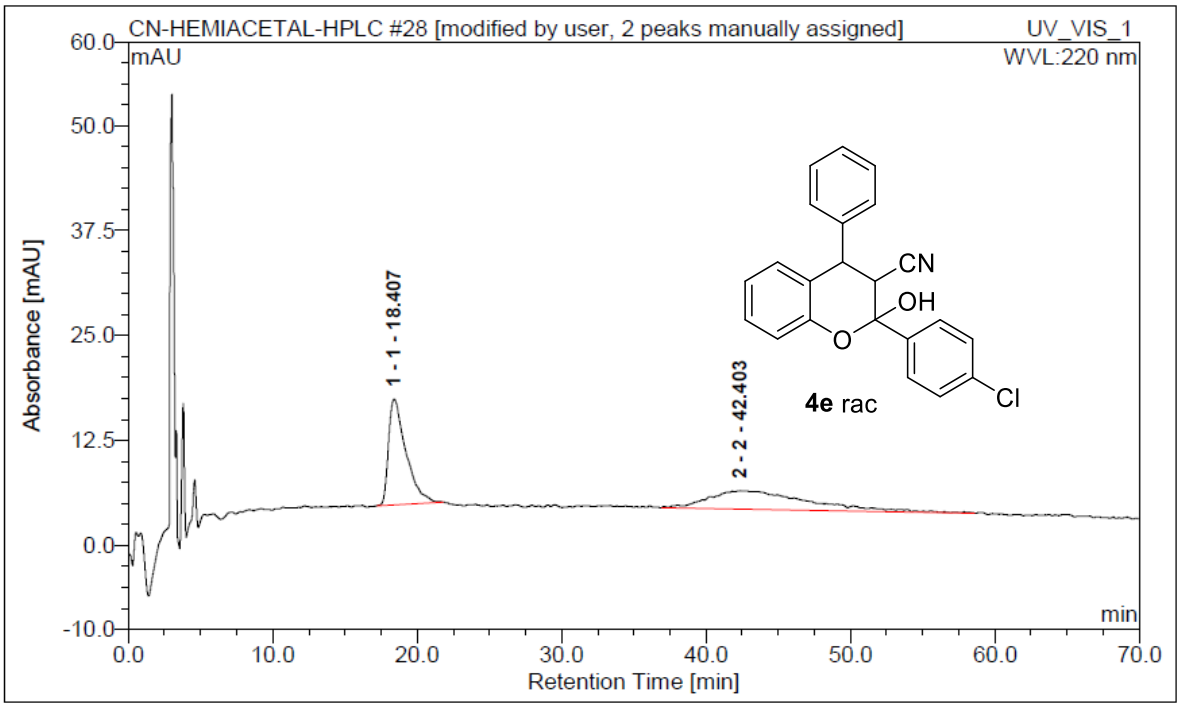
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	14.71	4.074471	50.24900474	10.40881	n.a.
2	2	25.85	4.034	49.75099526	5.492	n.a.

4-Cl-CN-CHI-IA

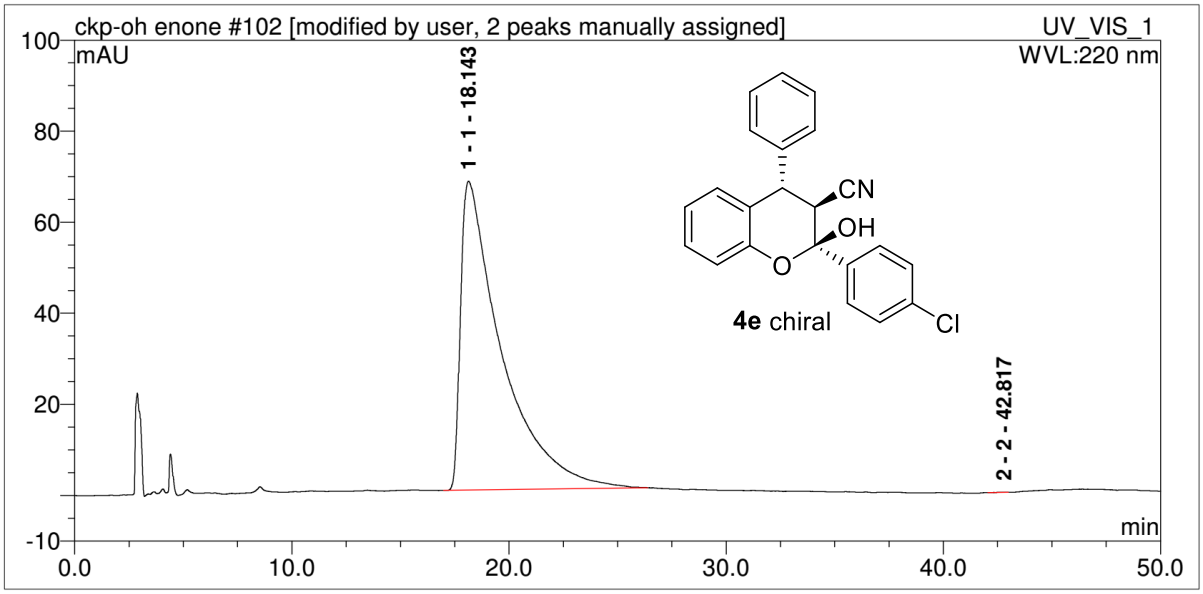


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	14.86	1.514946	4.099077009	2.06983	n.a.
2	2	26.04	35.443	95.90092299	43.206	n.a.

4-Cl-CN-HEMIACETAL-RAC-AMYLOSE-2

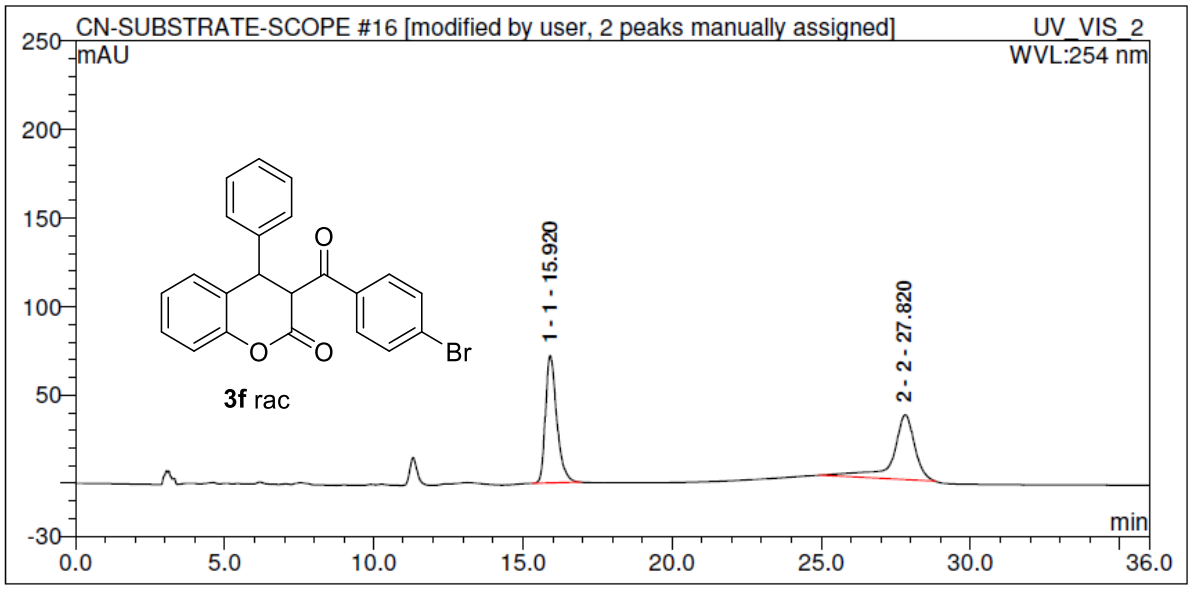


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	18.41	17.58656	50.03398124	12.59358	n.a.
2	2	42.40	17.563	49.96601876	2.168	n.a.



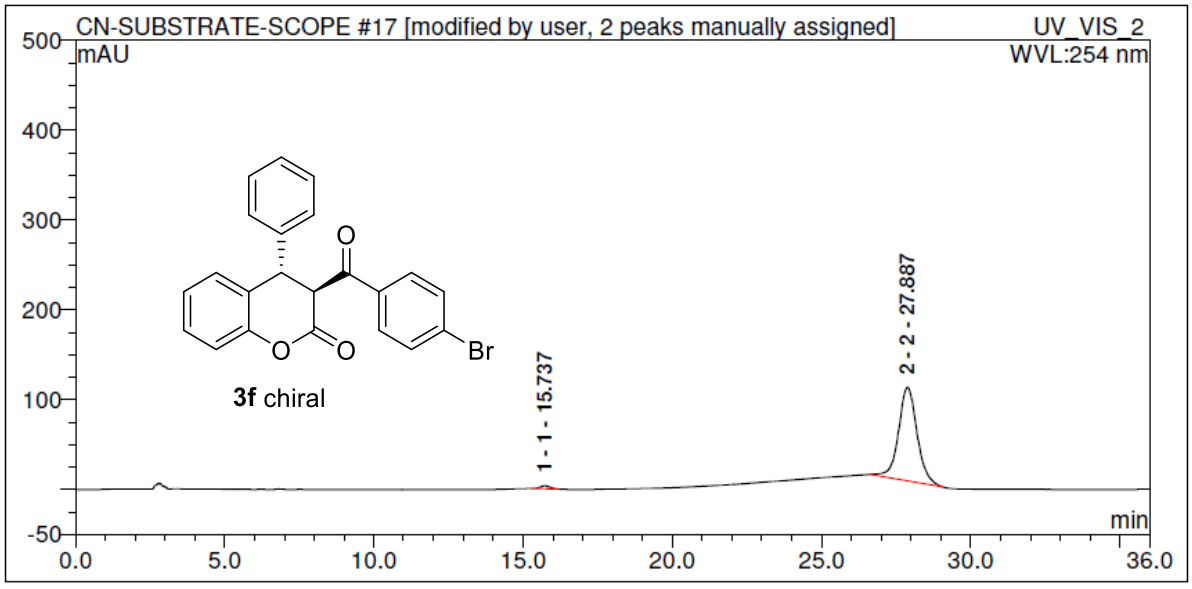
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	18.14	147.3784	99.98483006	67.82454	n.a.
2	2	42.82	0.022	0.01516994416	0.033	n.a.

4-Br-CN-RAC-IA



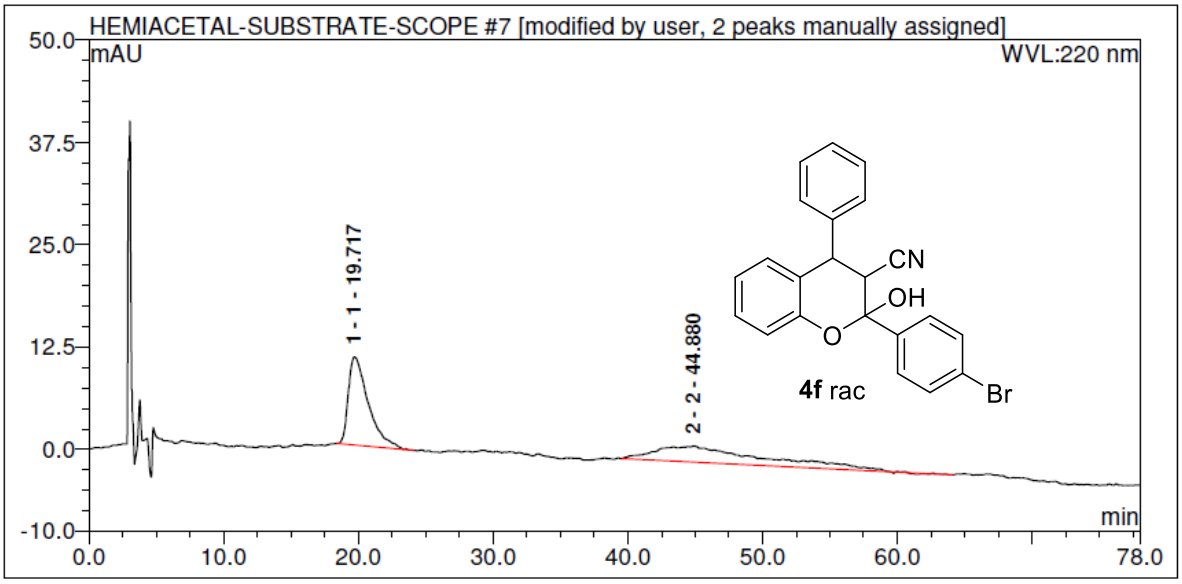
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	15.92	31.62463	50.2794753	71.92021	n.a.
2	2	27.82	31.273	49.7205247	36.582	n.a.

4-Br-CN-CHI-IA

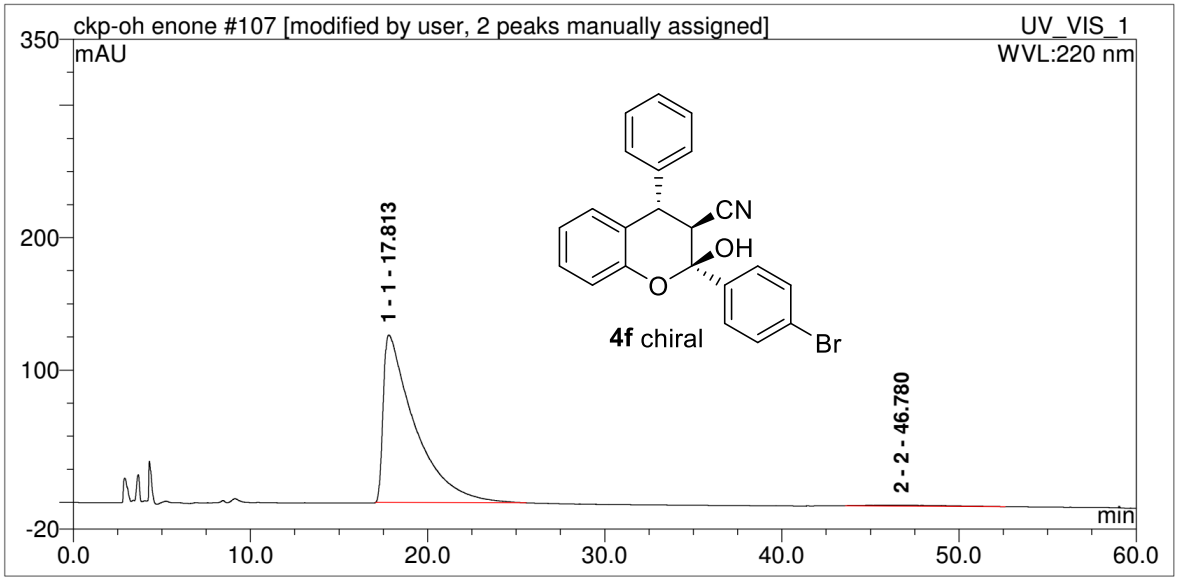


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	15.74	1.236182	1.620315046	3.23087	n.a.
2	2	27.89	75.057	98.37968495	104.212	n.a.

4-Br-CN-HEMIAACETAL-RAC-AMYLOSE-2

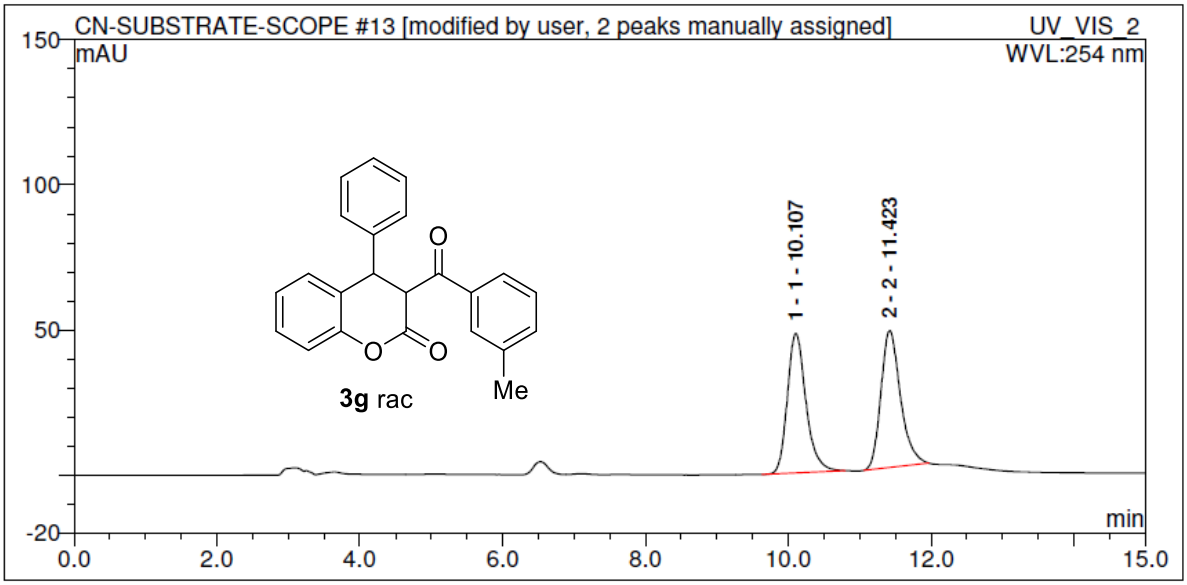


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	19.72	18.42363	50.05588804	10.74858	n.a.
2	2	44.88	18.382	49.94411196	1.950	n.a.



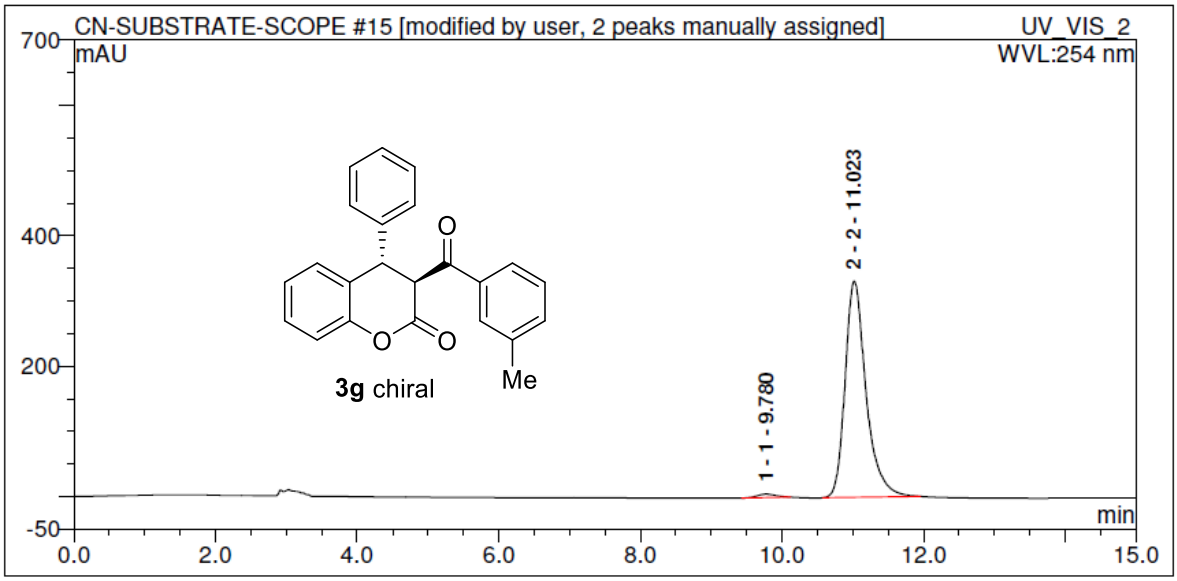
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	17.81	261.0243	98.63746523	126.606	n.a.
2	2	46.78	3.606	1.362534772	0.691	n.a.

3-Me-CN-RAC-IA



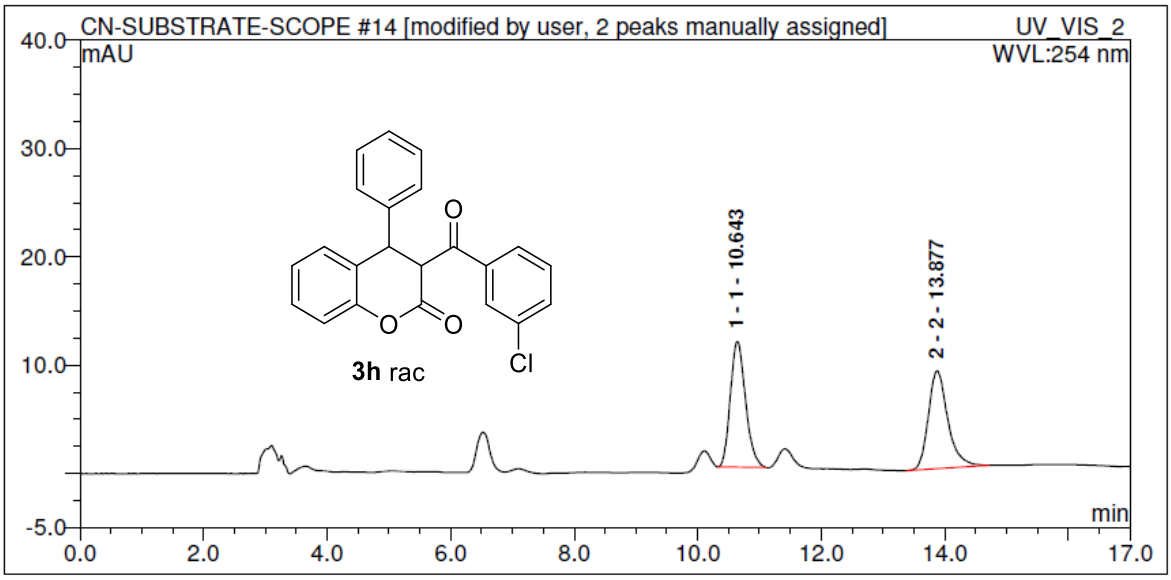
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	10.11	14.49526	49.25737545	48.09379	n.a.
2	2	11.42	14.932	50.74262455	47.081	n.a.

3-Me-CN-CHI-IA



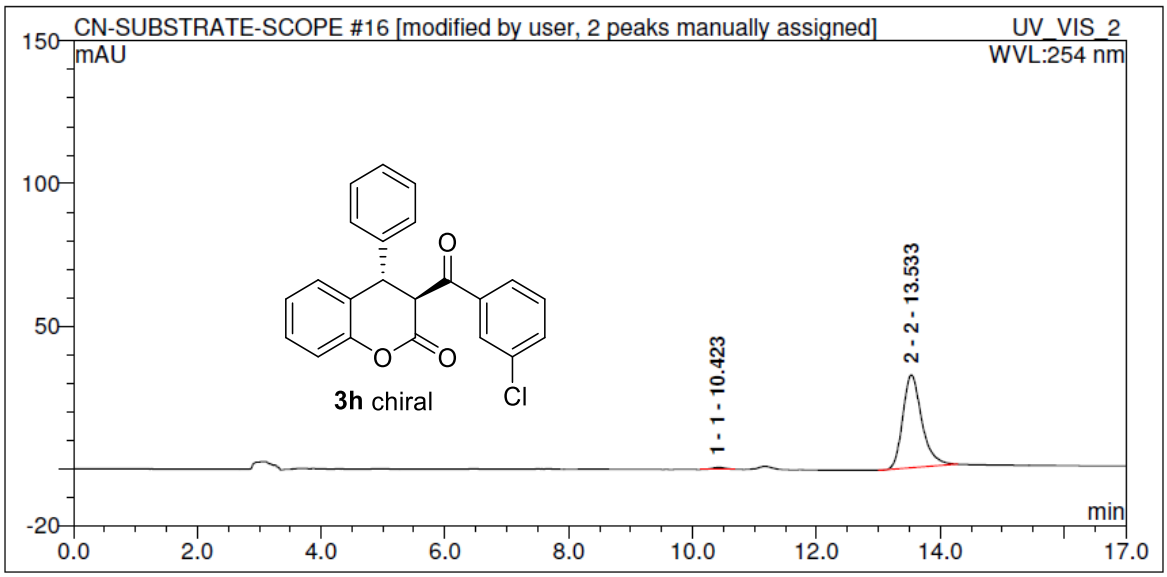
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	9.78	1.599297	1.384731243	5.39538	n.a.
2	2	11.02	113.896	98.61526876	331.553	n.a.

3-Cl-CN-RAC-IA



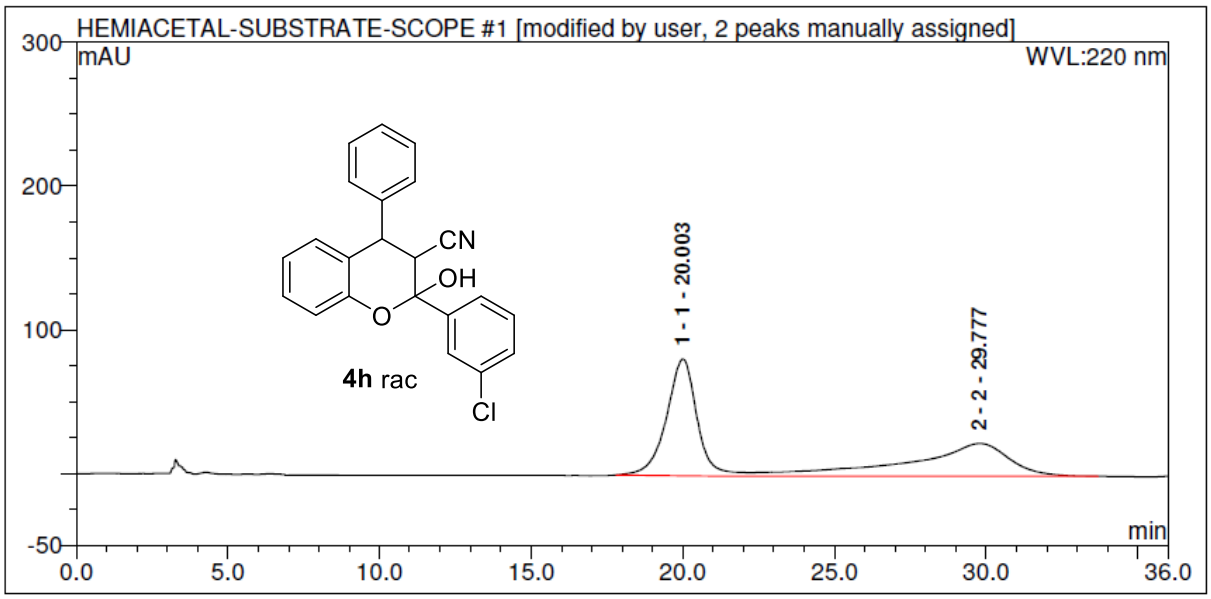
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	10.64	3.305136	50.08737703	11.58018	n.a.
2	2	13.88	3.294	49.91262297	9.028	n.a.

3-Cl-CN-CHI-IA



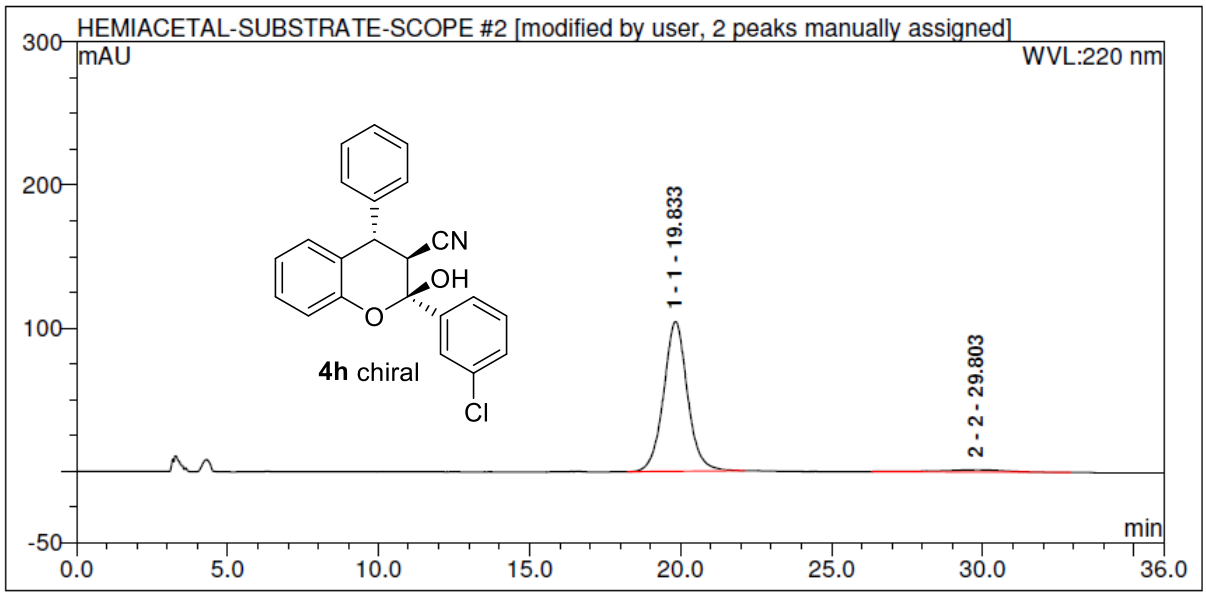
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	10.42	0.173115	1.462934795	0.65534	n.a.
2	2	13.53	11.660	98.5370652	32.541	n.a.

3-Cl-CN-HEMIACETAL-RAC-ID



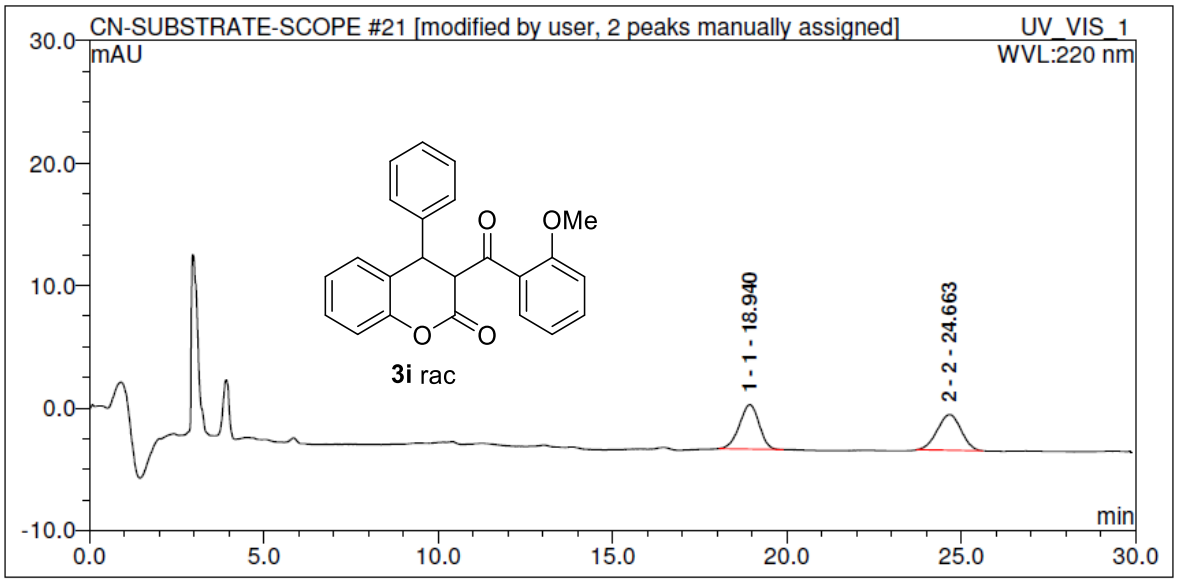
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	20.00	93.99393	50.69430226	81.17246	n.a.
2	2	29.78	91.419	49.30569774	22.902	n.a.

3-Cl-CN-HEMIACETAL-CHI-ID



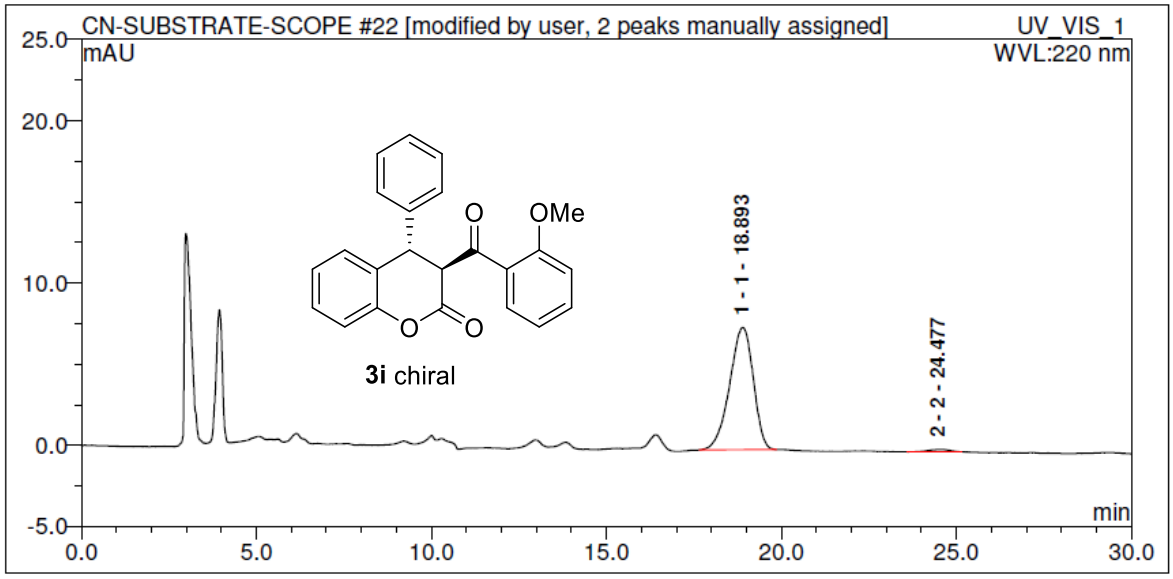
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	19.83	96.03059	96.32625982	104.5742	n.a.
2	2	29.80	3.662	3.673740179	1.481	n.a.

2-OMe-CN-RAC-LUX-C4

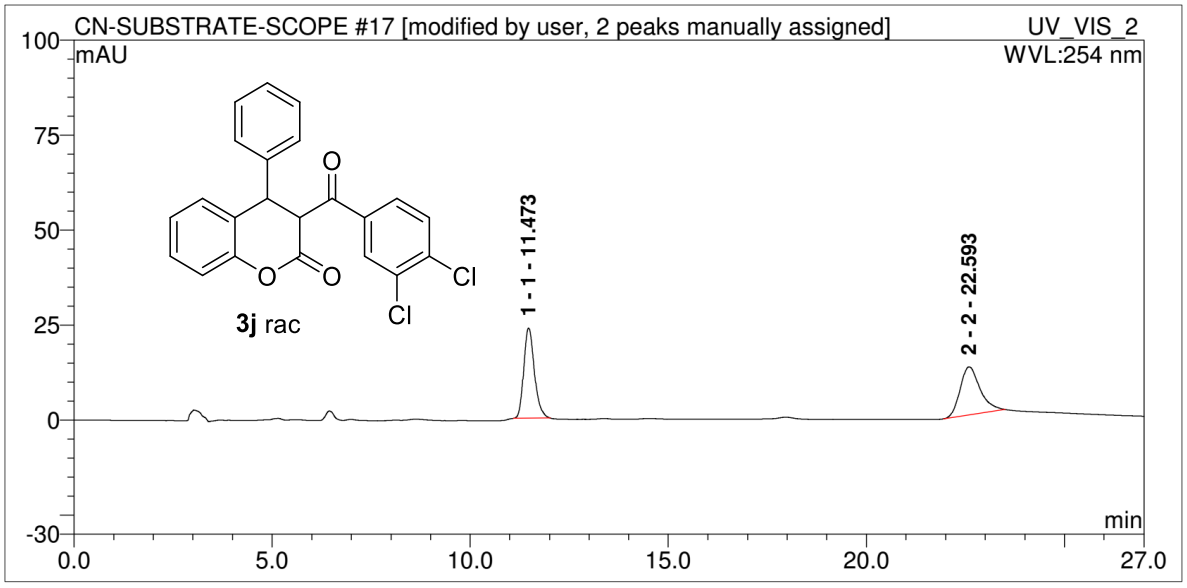


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	18.94	2.359148	50.44210083	3.61541	n.a.
2	2	24.66	2.318	49.55789917	2.913	n.a.

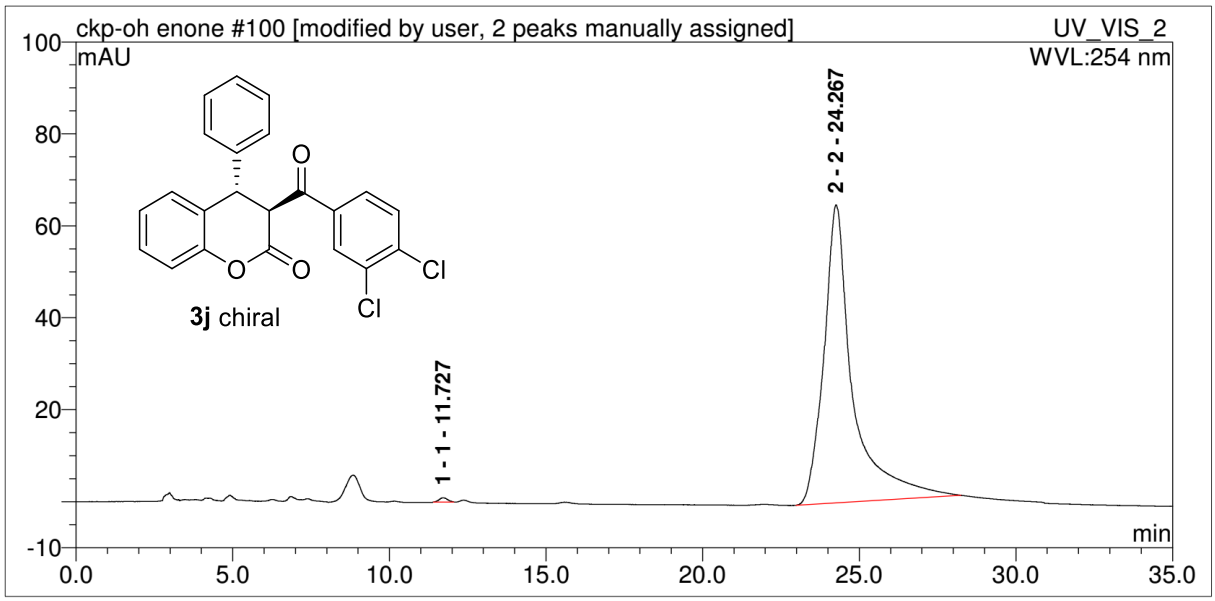
2-OMe-CN-CHI-LUX-C4



No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	18.89	5.894331	98.2467419	7.53288	n.a.
2	2	24.48	0.105	1.753258097	0.143	n.a.

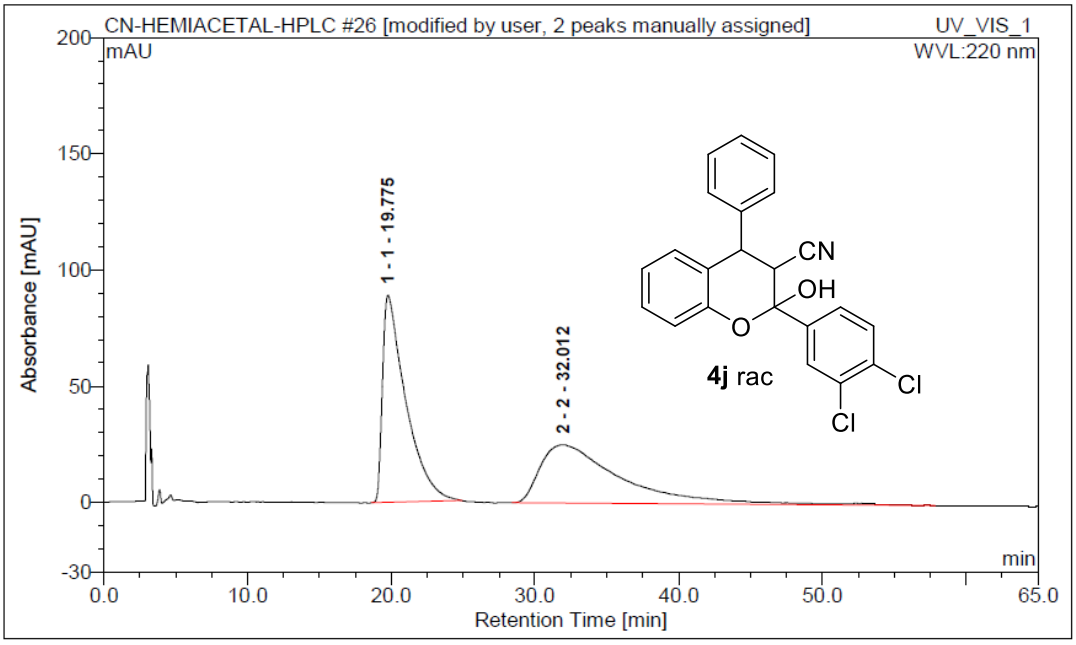


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	11.47	7.405565	49.98428399	23.71285	n.a.
2	2	22.59	7.410	50.01571601	12.673	n.a.



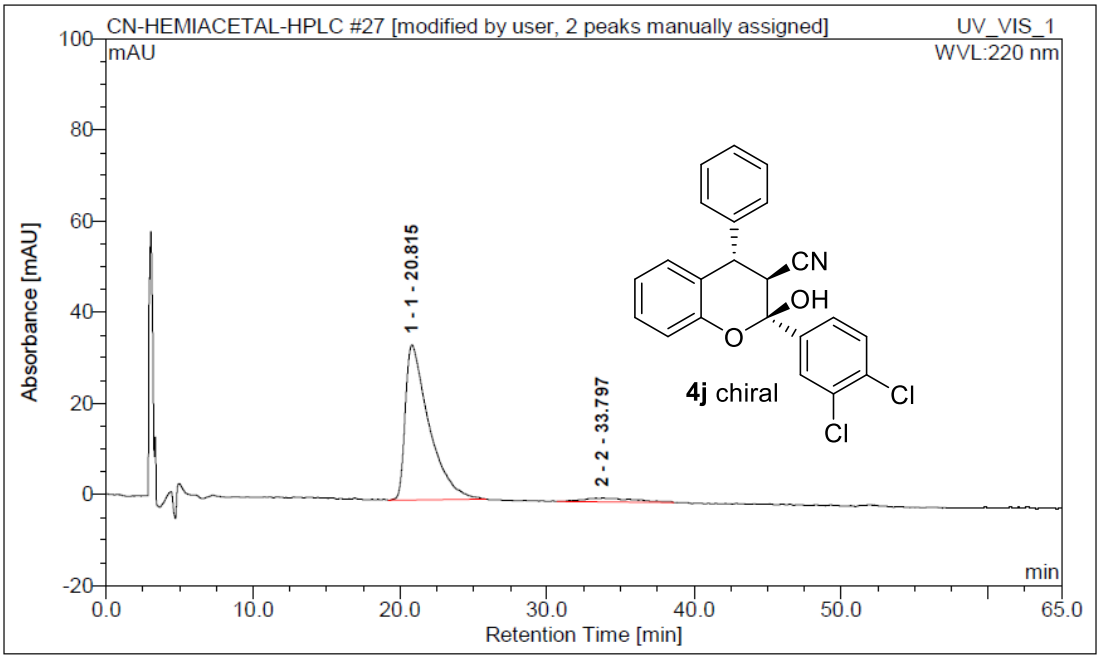
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	11.73	0.283772	0.4072128545	0.92692	n.a.
2	2	24.27	69.403	99.59278715	64.818	n.a.

3,4-DiCl-CN-HEMI-RAC-AMYLOSE-2



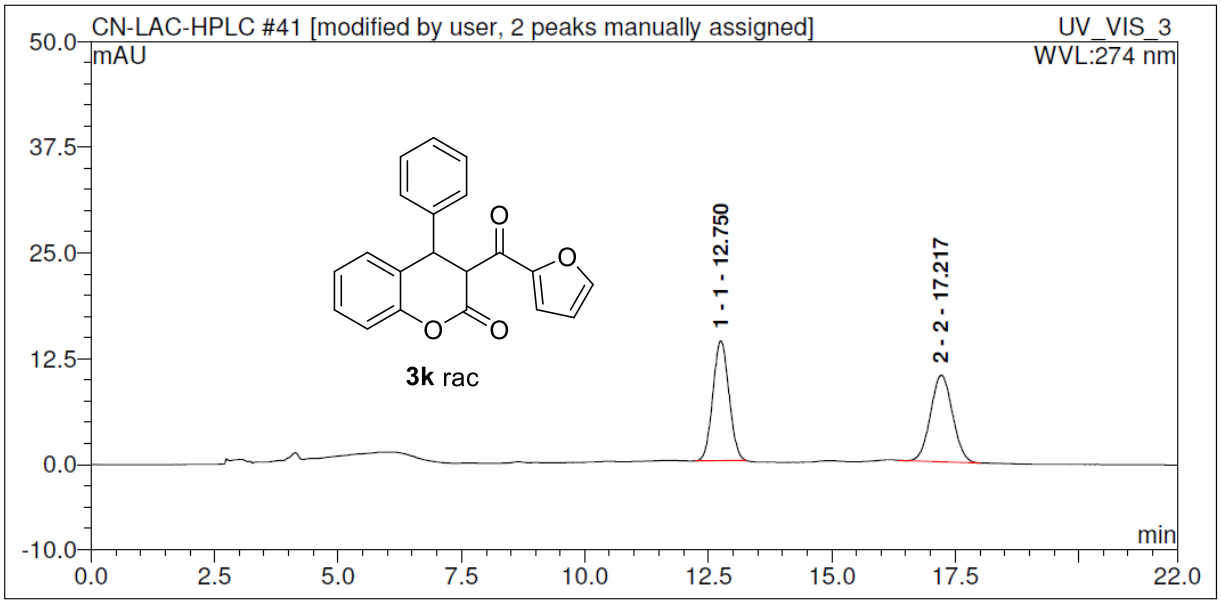
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	19.78	167.0471	50.51010466	89.26506	n.a.
2	2	32.01	163.673	49.48989534	25.186	n.a.

3,4-DiCl-CN-HEMI-CHI-AMYLOSE-2

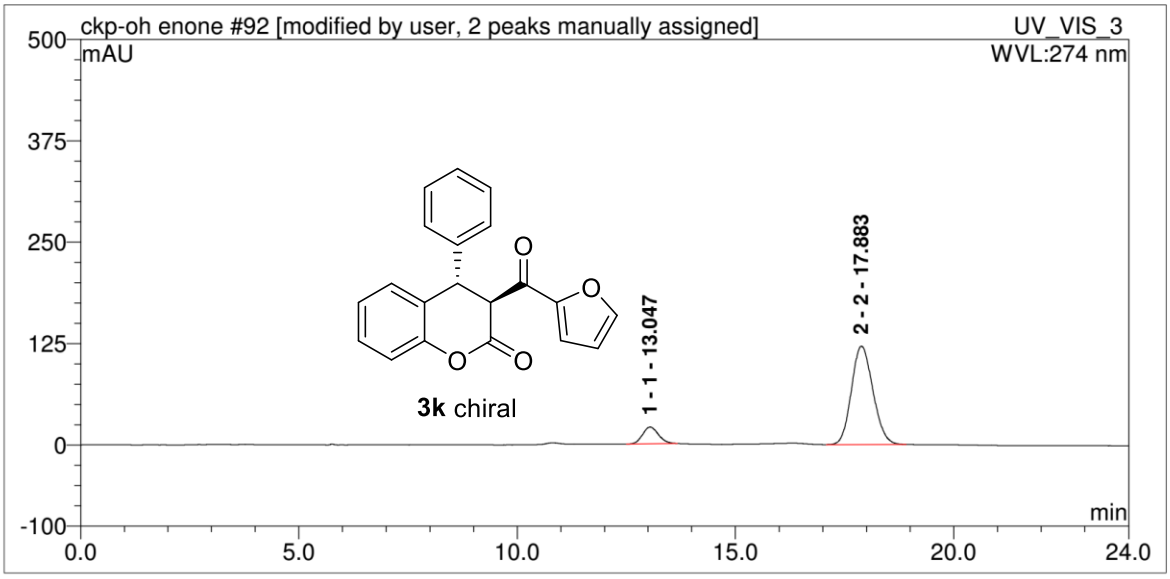


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	20.82	63.71896	94.96840696	34.00319	n.a.
2	2	33.80	3.376	5.031593042	0.864	n.a.

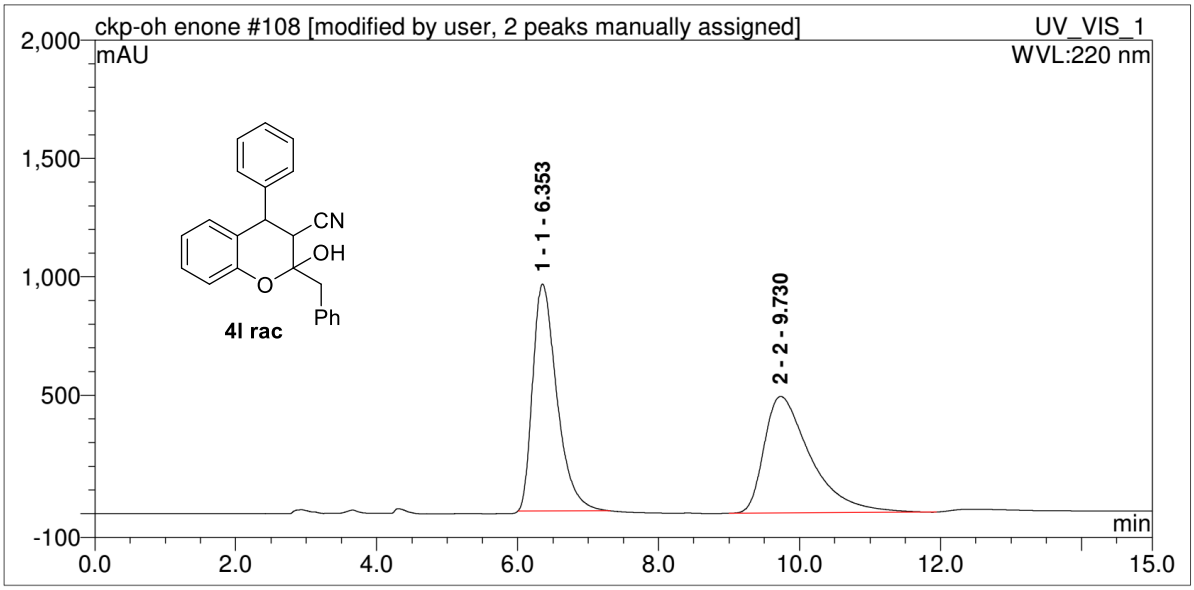
2-FUROYL-CN-LAC-RAC-CHIRAL-ART



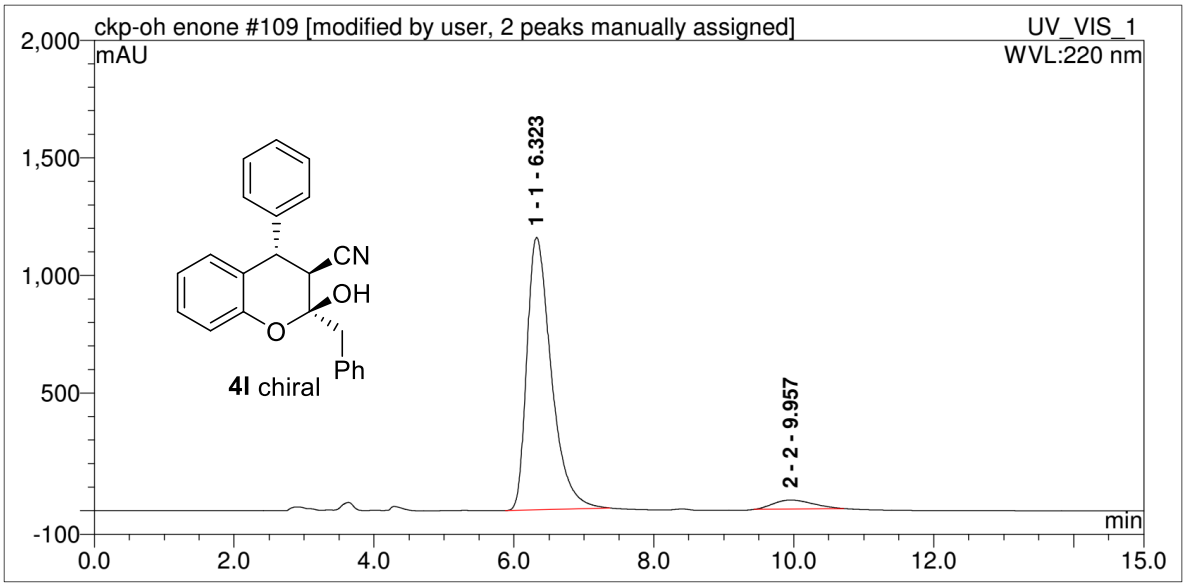
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	12.75	5.343333	50.3346251	14.14163	n.a.
2	2	17.22	5.272	49.6653749	10.225	n.a.



No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	13.05	8.739181	11.19976652	20.67098	n.a.
2	2	17.88	69.291	88.80023348	121.285	n.a.

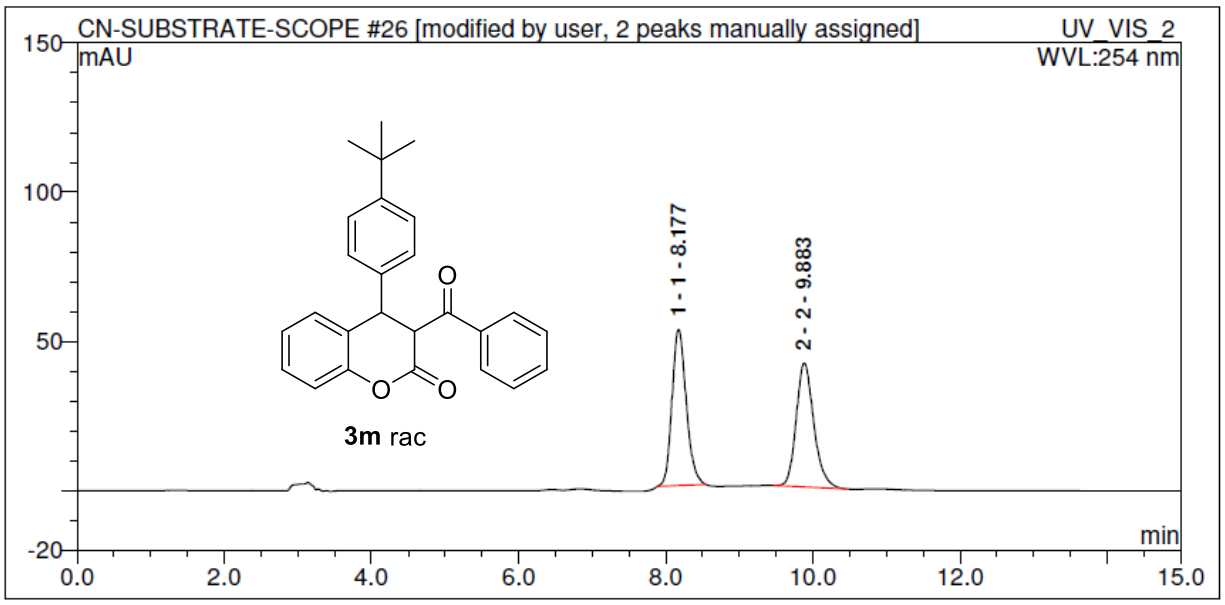


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	6.35	380.7585	50.34134374	958.1523	n.a.
2	2	9.73	375.595	49.65865626	492.287	n.a.



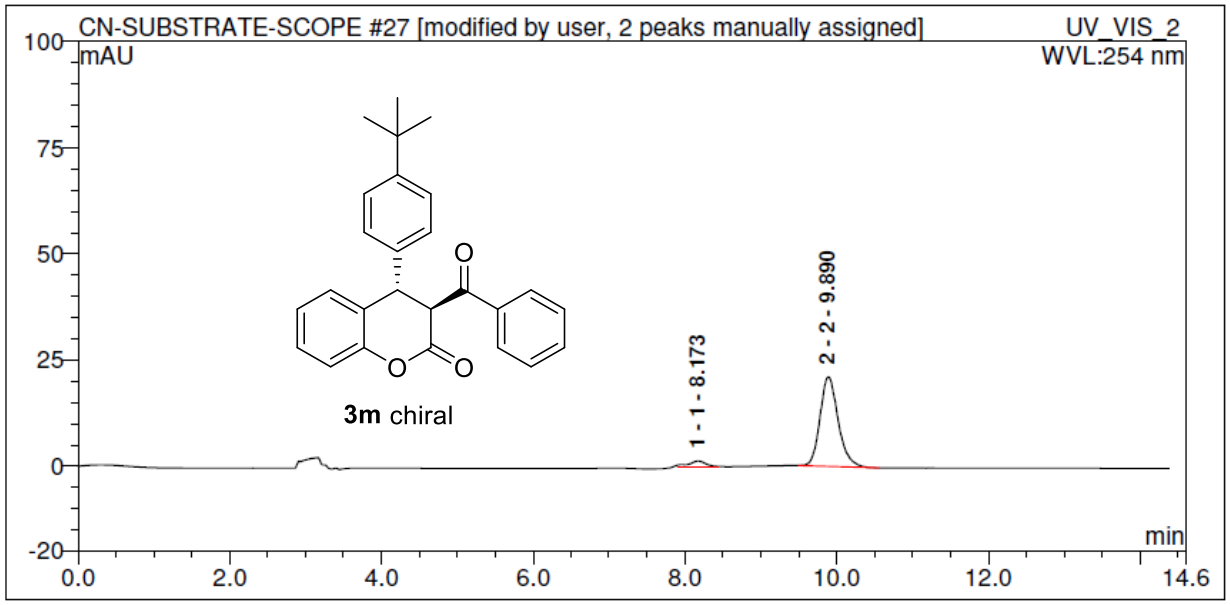
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	6.32	468.1129	94.91393122	1158.157	n.a.
2	2	9.96	25.084	5.08606878	38.449	n.a.

4-tBUT-GR-CN-LAC-RAC-IA



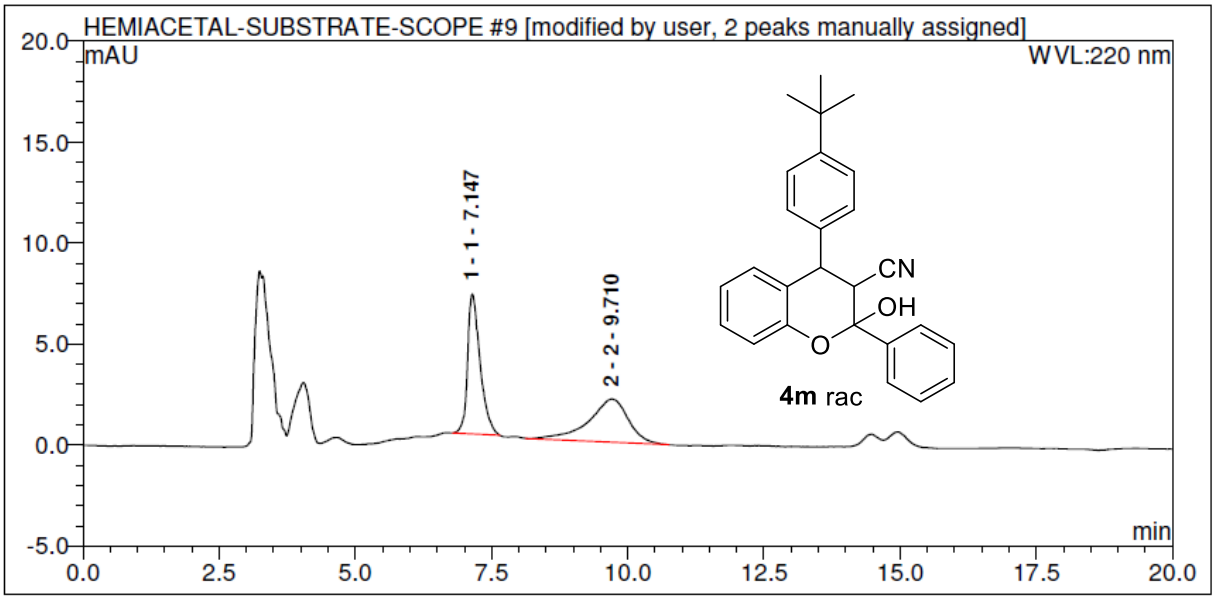
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	8.18	11.73508	50.39577756	52.27256	n.a.
2	2	9.88	11.551	49.60422244	41.475	n.a.

4-tBUT-GR-CN-LAC-CHI-IA



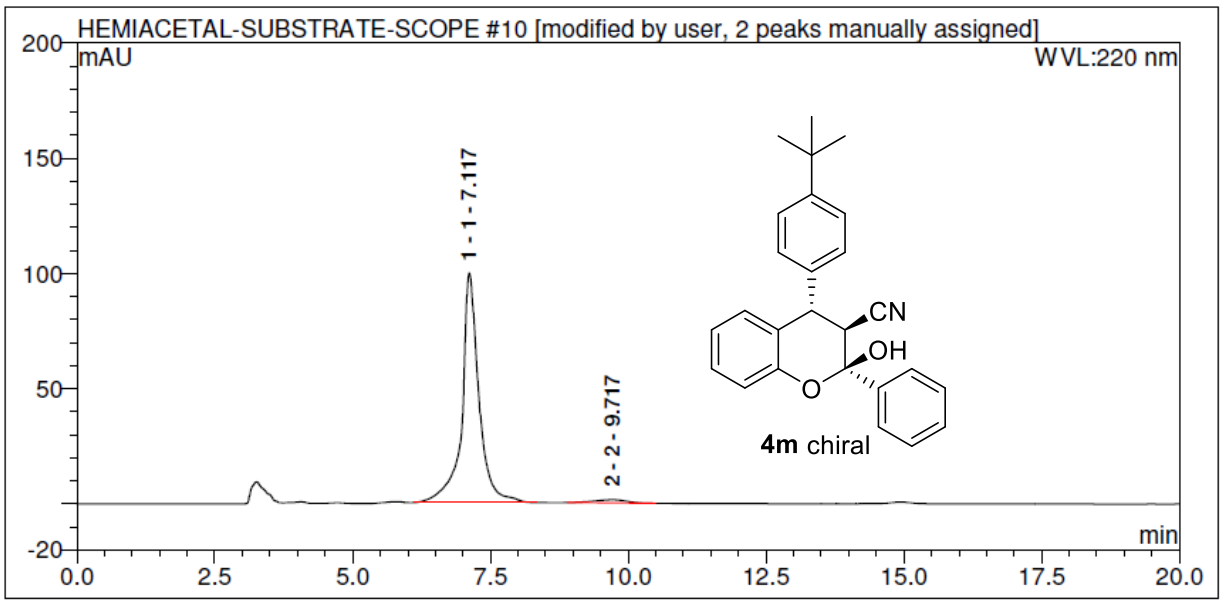
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	8.17	0.314171	5.101574125	1.27551	n.a.
2	2	9.89	5.844	94.89842588	21.055	n.a.

4-tBUT-GR-HEMIACETAL-RAC-ID



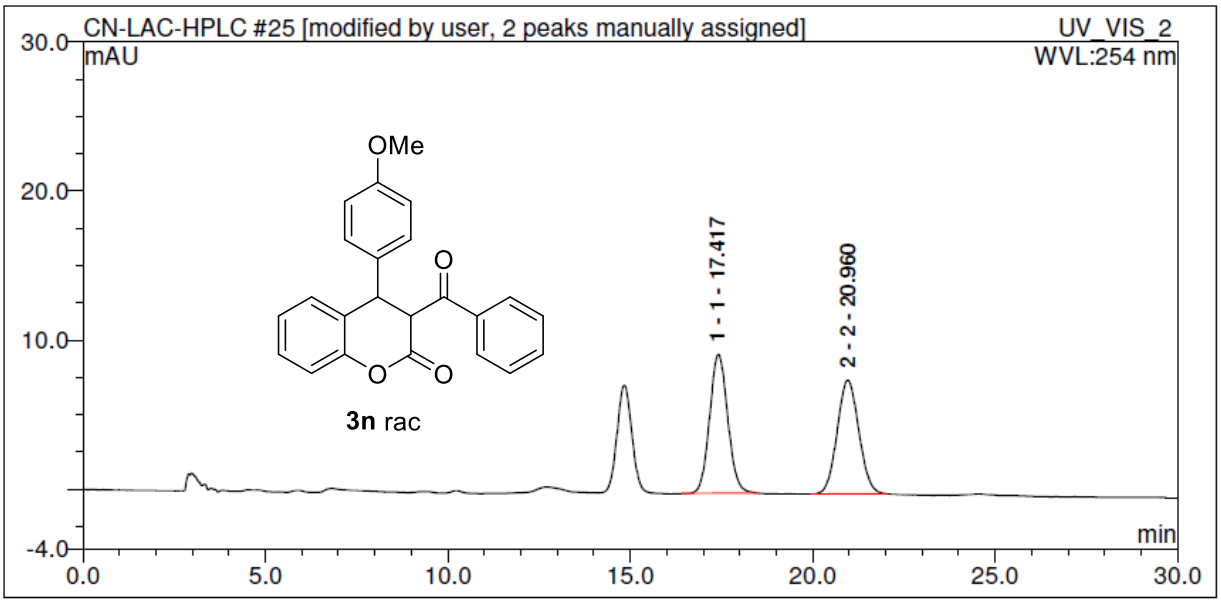
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	7.15	1.849384	50.60998816	6.92625	n.a.
2	2	9.71	1.805	49.39001184	2.138	n.a.

4-tBUT-GR-HEMIACETAL-CHI-ID



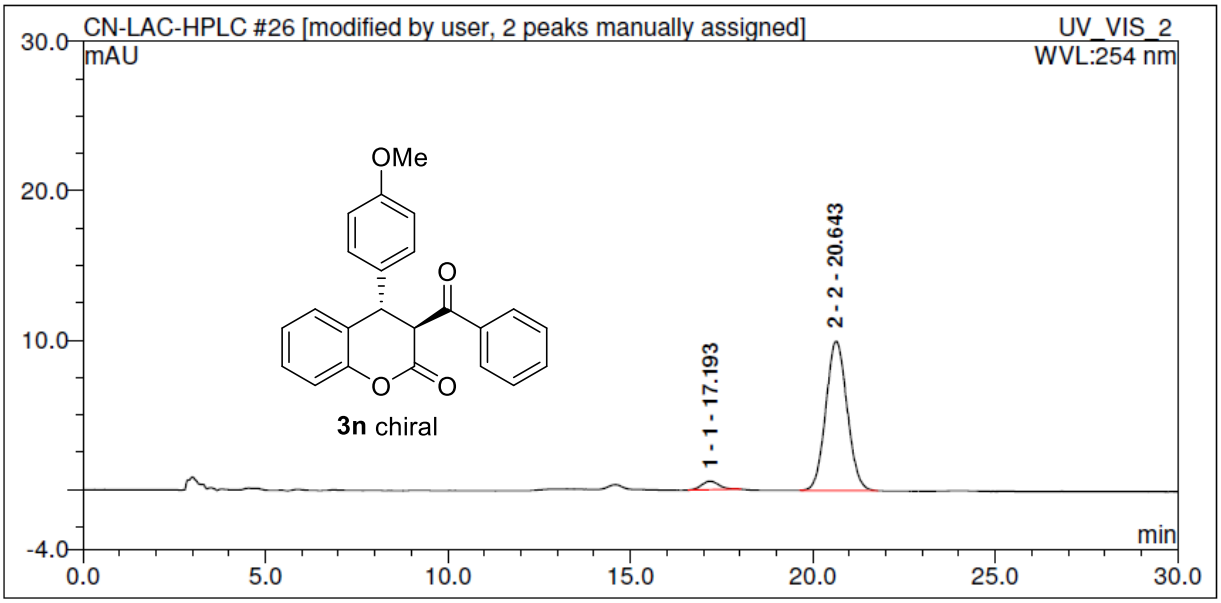
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	7.12	35.68963	97.52228695	99.55876	n.a.
2	2	9.72	0.907	2.477713051	1.337	n.a.

4-OMe-GR-LAC-CN-RAC-AMYLOSE-C



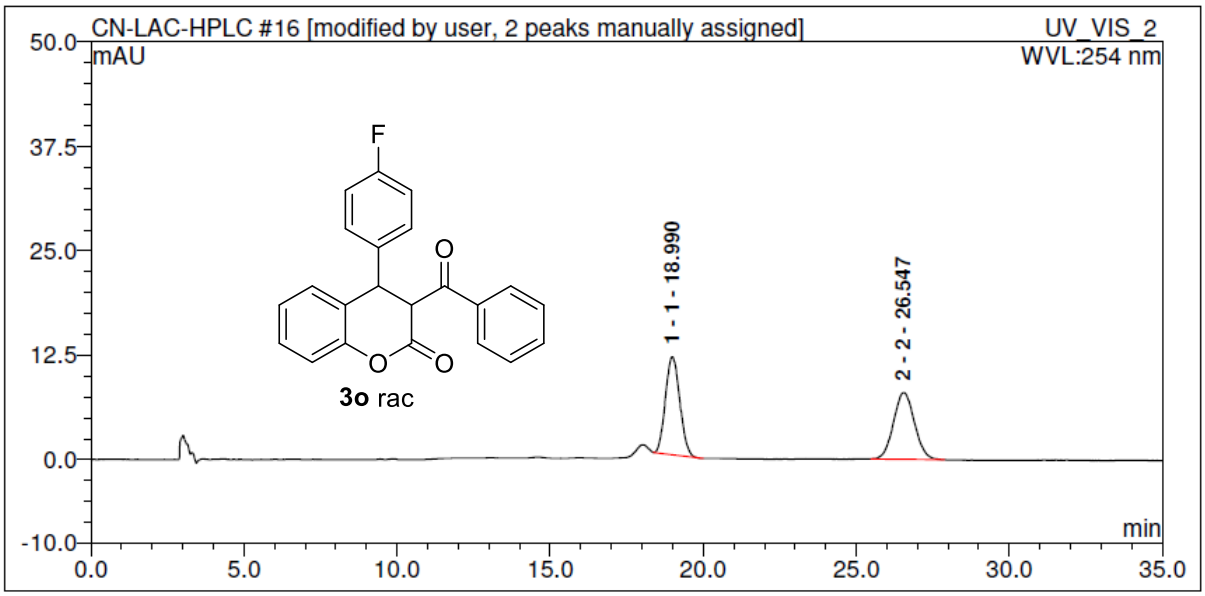
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	17.42	5.37078	50.58797963	9.31782	n.a.
2	2	20.96	5.246	49.41202037	7.618	n.a.

4-OMe-GR-LAC-CN-CHI-AMYLOSE-C



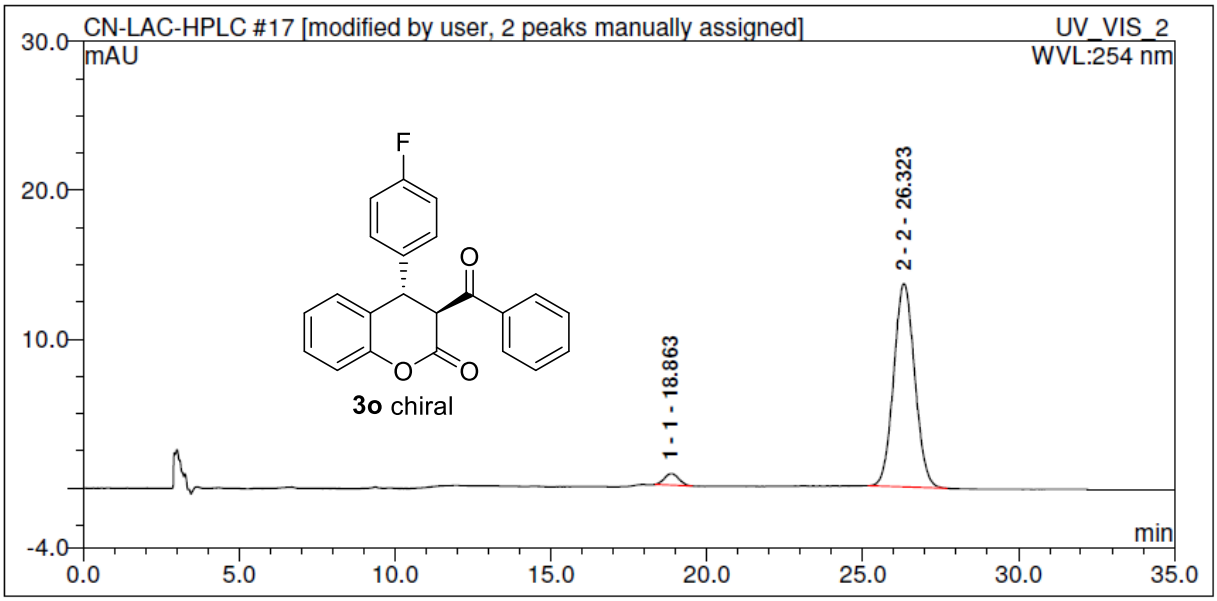
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	17.19	0.312166	4.403582471	0.56917	n.a.
2	2	20.64	6.777	95.59641753	9.989	n.a.

4-F-GR-LAC-RAC-AMYLOSE-C



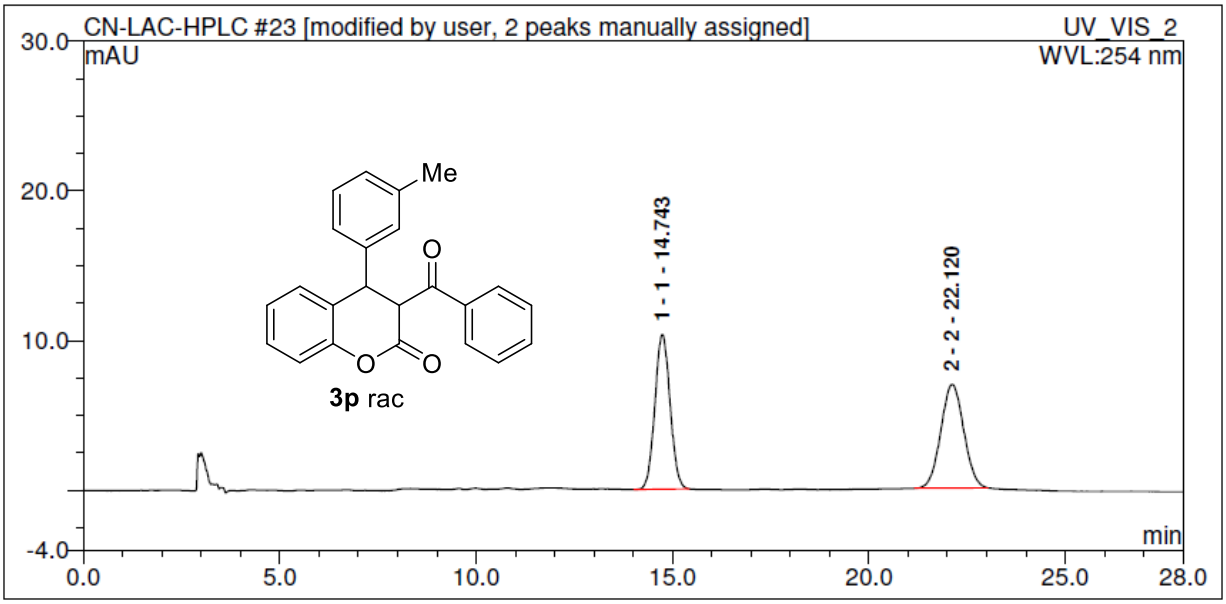
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	18.99	6.382619	50.17717921	11.72745	n.a.
2	2	26.55	6.338	49.82282079	7.986	n.a.

4-F-GR-LAC-CHI-AMYLOSE-C



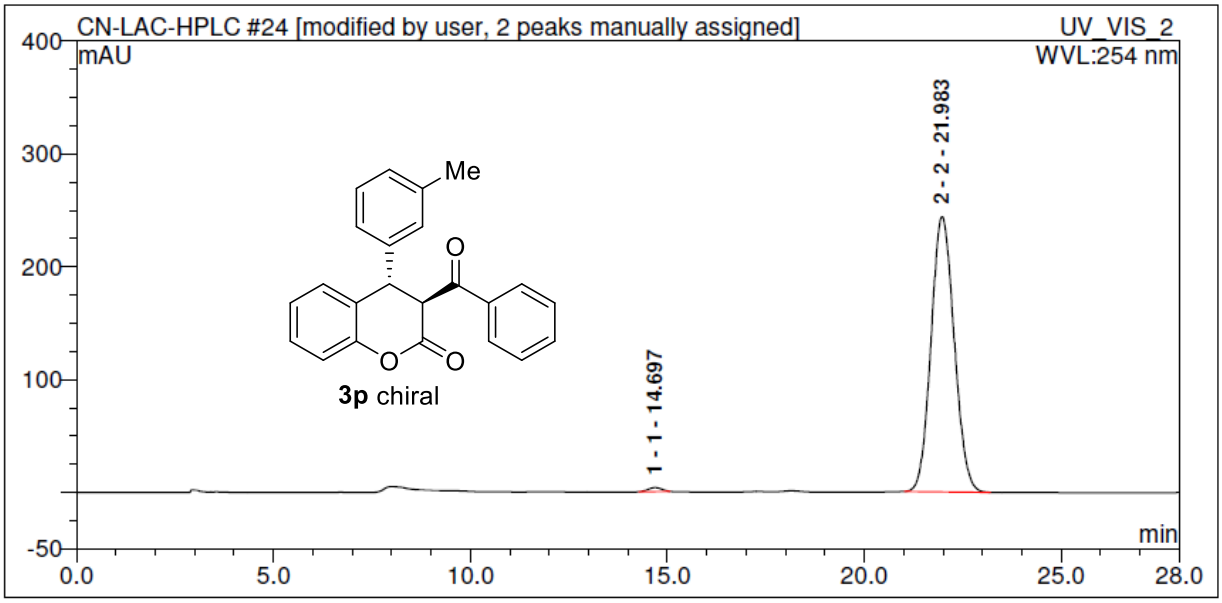
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	18.86	0.409135	3.68972579	0.77244	n.a.
2	2	26.32	10.679	96.31027421	13.644	n.a.

3-Me-GR-LAC-CN-RAC-AMYLOSE-C



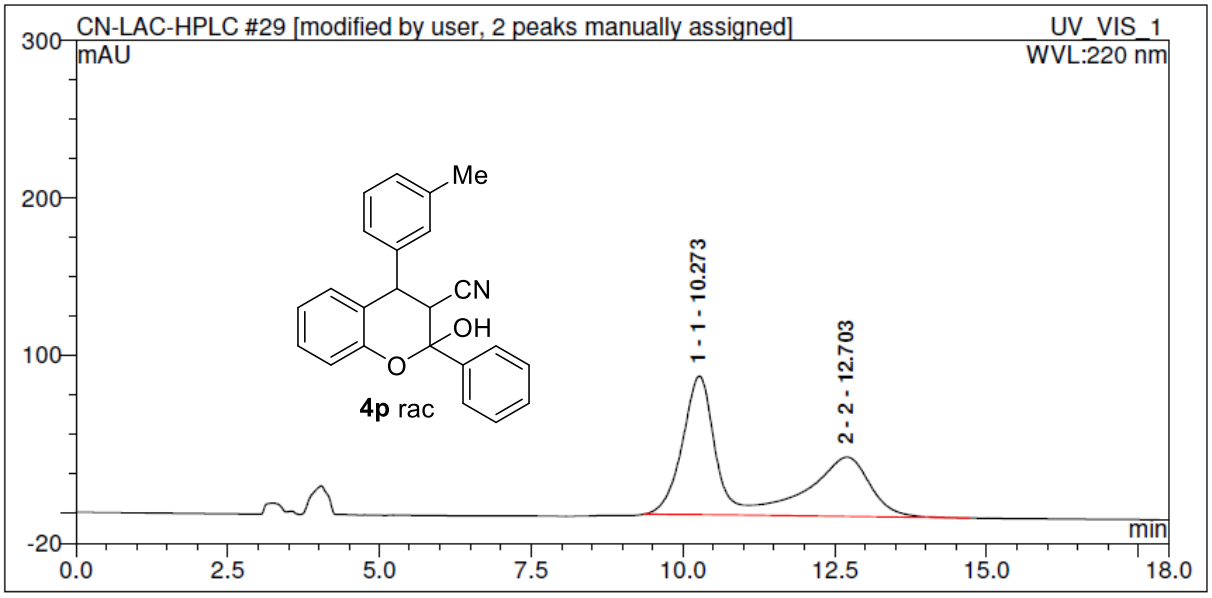
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	14.74	4.641356	49.76616671	10.33713	n.a.
2	2	22.12	4.685	50.23383329	6.923	n.a.

3-Me-GR-LAC-CN-CHI-AMYLOSE-C



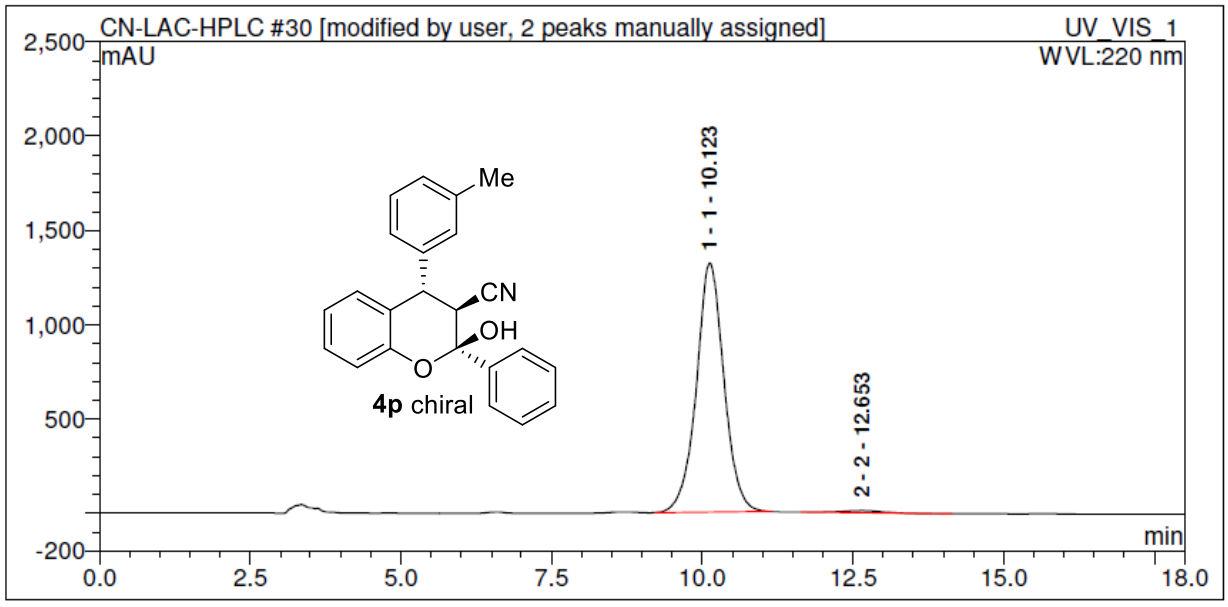
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	14.70	1.411064	0.8421534334	3.50763	n.a.
2	2	21.98	166.143	99.15784657	243.781	n.a.

3-Me-GR-HEMI-CN-RAC-ID



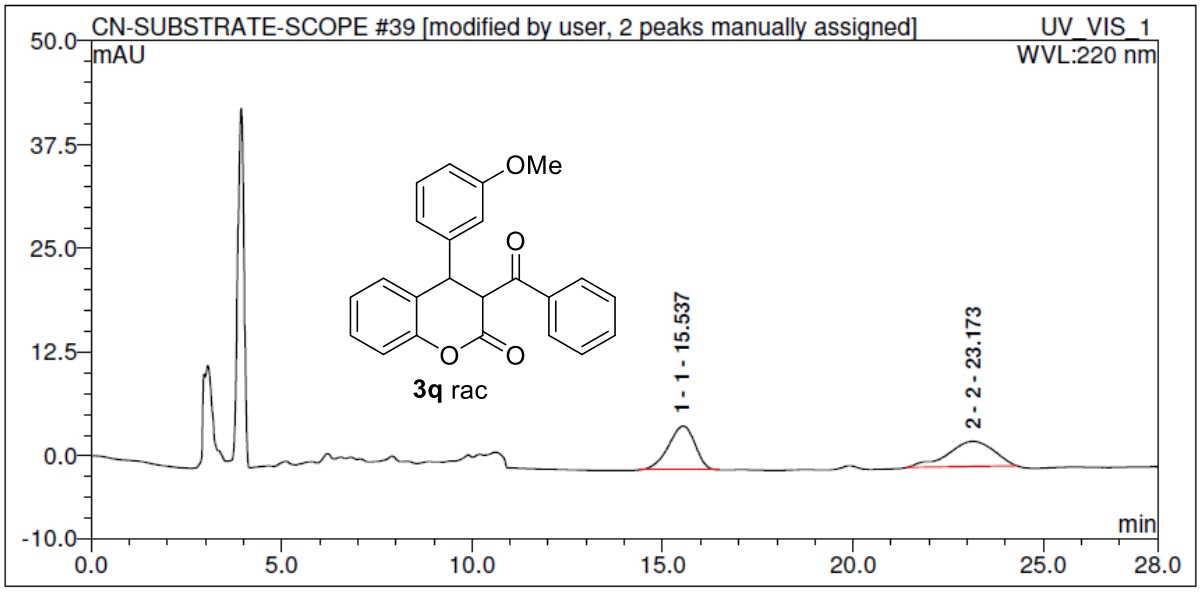
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	10.27	51.02077	51.43021789	88.19643	n.a.
2	2	12.70	48.183	48.56978211	37.768	n.a.

3-Me-GR-HEMI-CN-CHI-ID



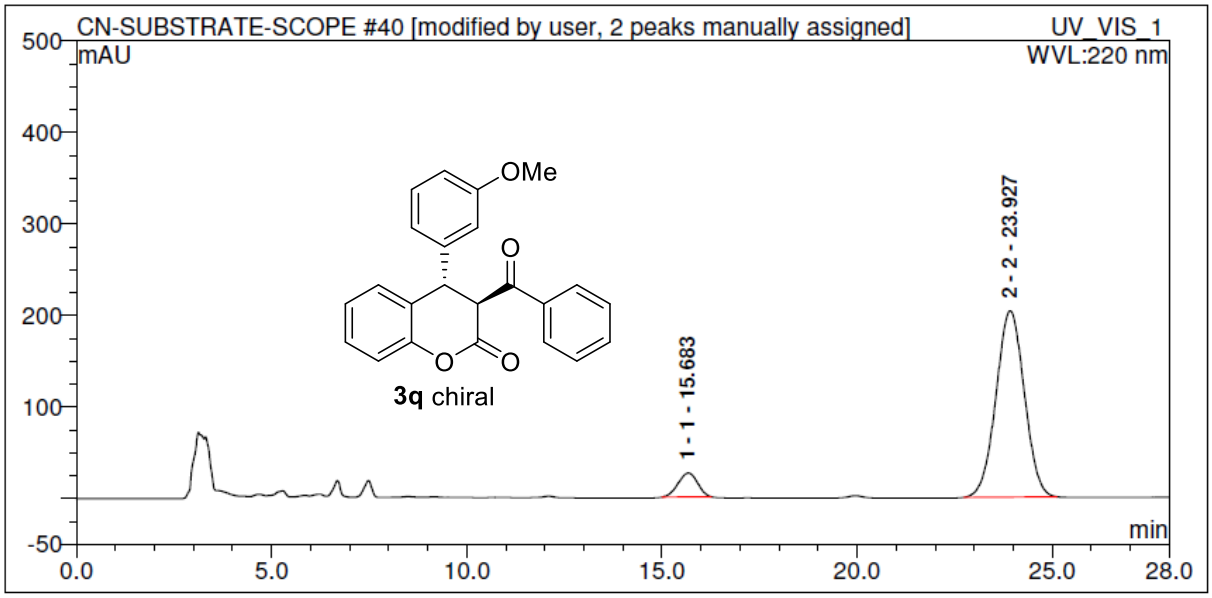
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	10.12	702.7869	98.78523246	1320.731	n.a.
2	2	12.65	8.642	1.214767543	11.639	n.a.

m-OMe-GR-CN-LAC-RAC-LUX-C4



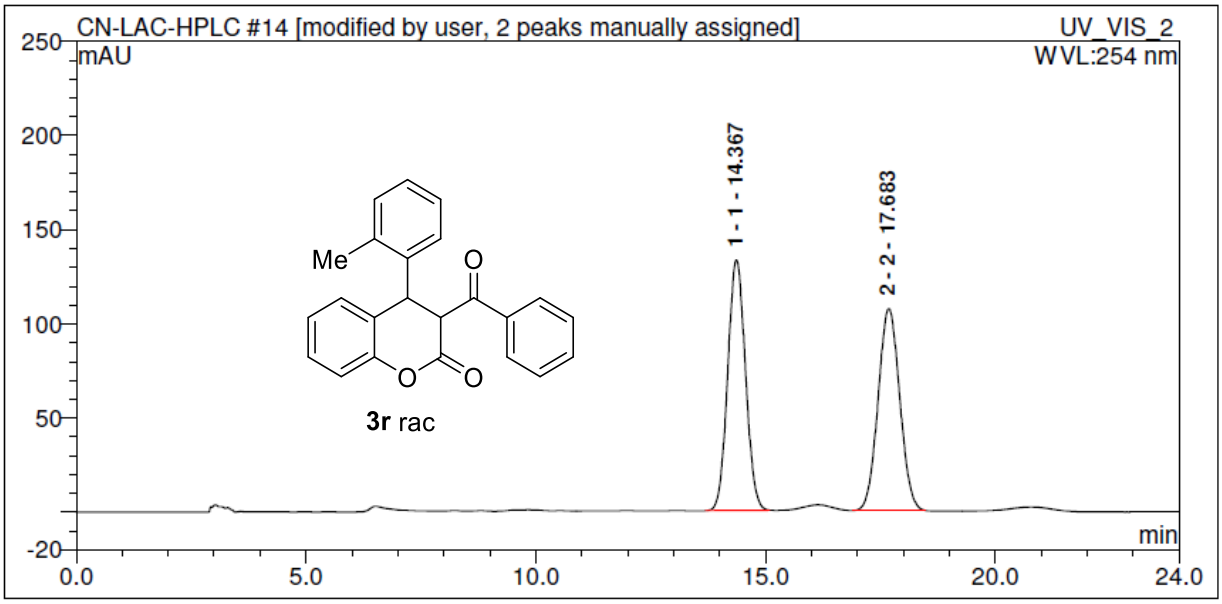
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	15.54	4.314857	50.49188897	5.27763	n.a.
2	2	23.17	4.231	49.50811103	3.013	n.a.

m-OMe-GR-CN-LAC-CHI-LUX-C4



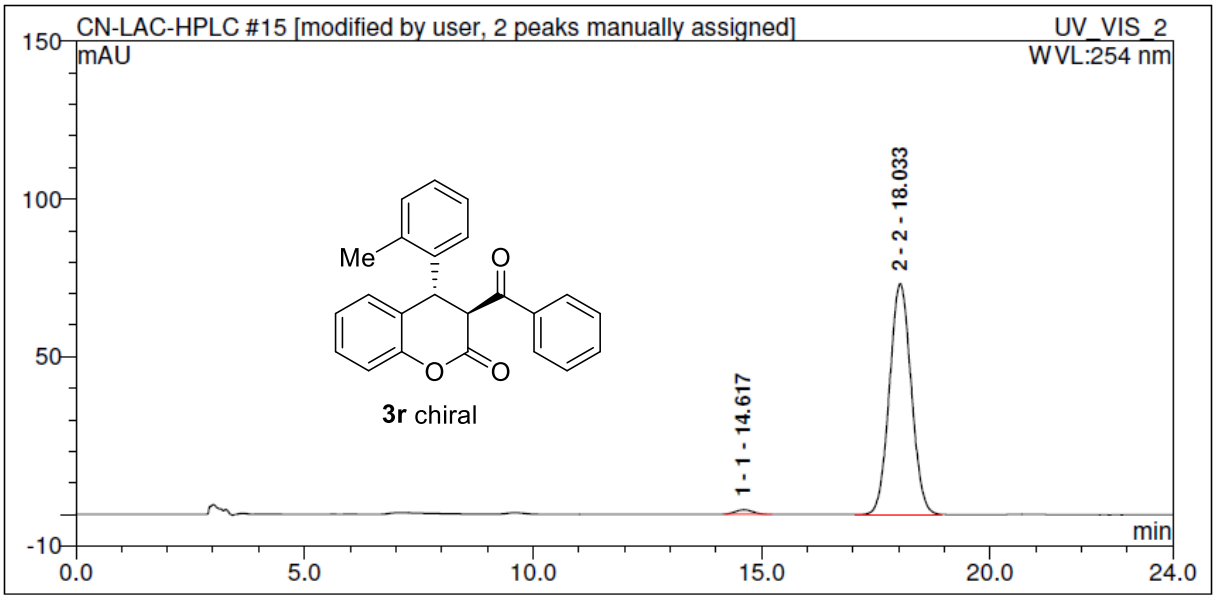
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	15.68	15.01994	8.061222349	26.0494	n.a.
2	2	23.93	171.303	91.93877765	203.427	n.a.

2-Me-GR-LAC-RAC-AMYLOSE-C



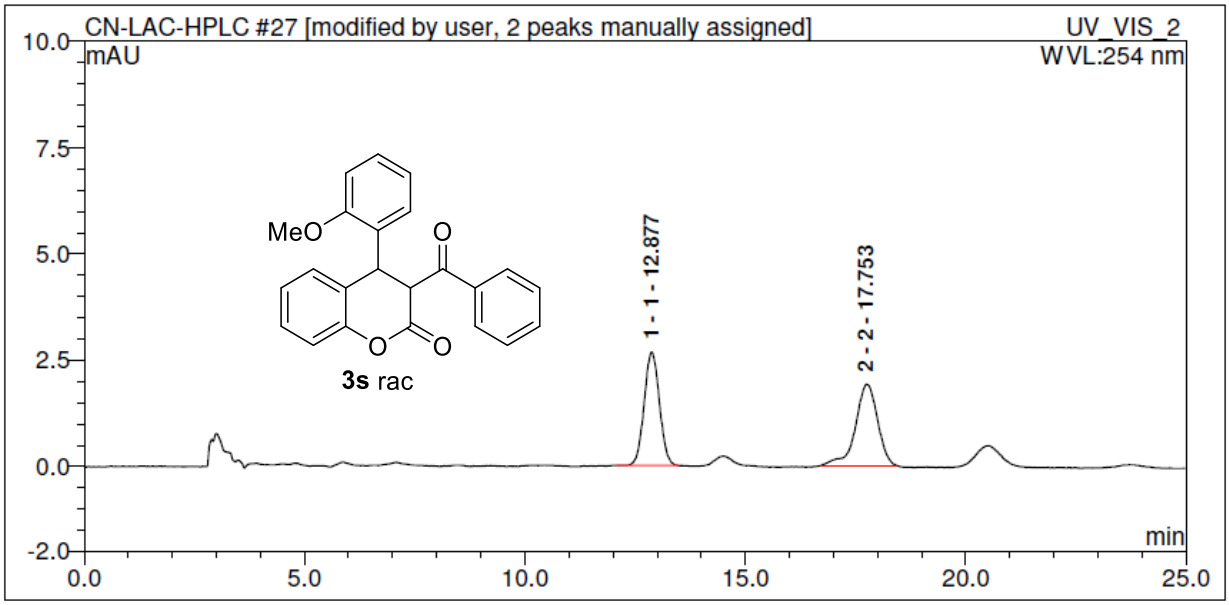
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	14.37	59.56869	50.38152233	132.9801	n.a.
2	2	17.68	58.667	49.61847767	107.197	n.a.

2-Me-GR-LAC-CHI-AMYLOSE-C



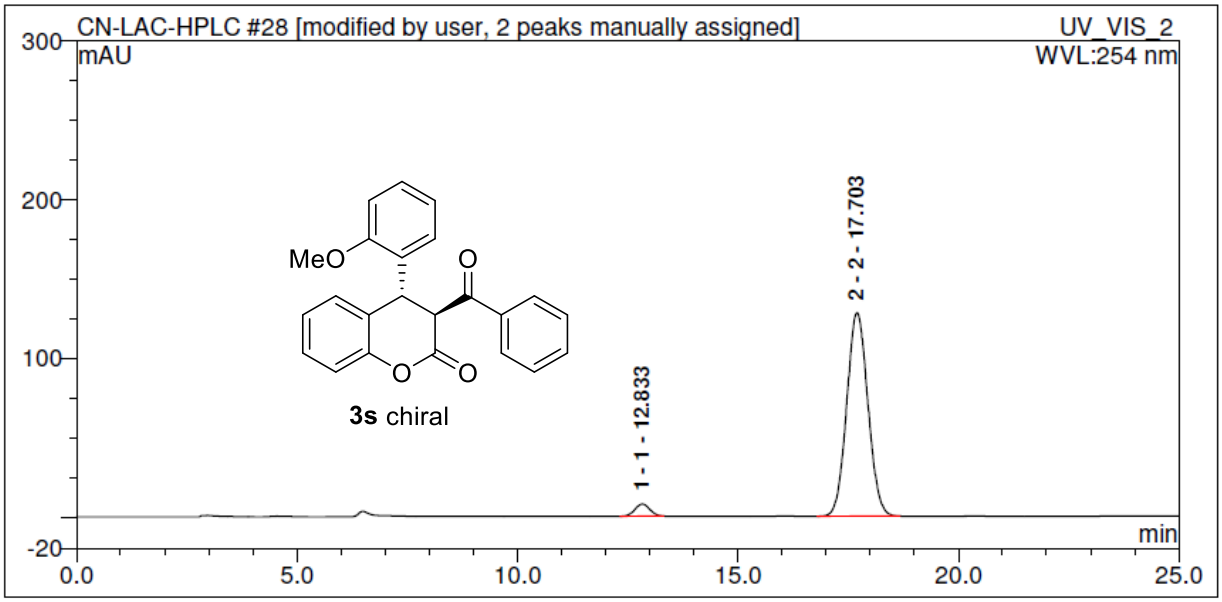
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	14.62	0.60292	1.473648929	1.42279	n.a.
2	2	18.03	40.311	98.52635107	73.173	n.a.

2-OMe-GR-CN-LAC-RAC-AMYLOSE-C



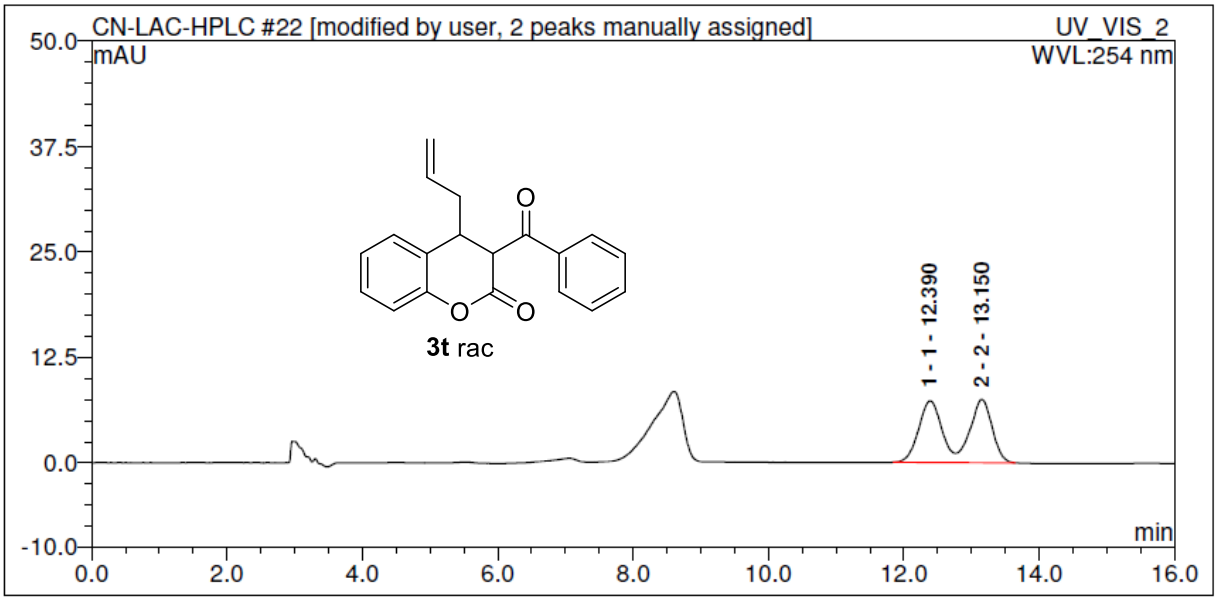
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	12.88	1.071964	49.07464216	2.66871	n.a.
2	2	17.75	1.112	50.92535784	1.913	n.a.

2-OMe-GR-CN-LAC-CHI-AMYLOSE-C



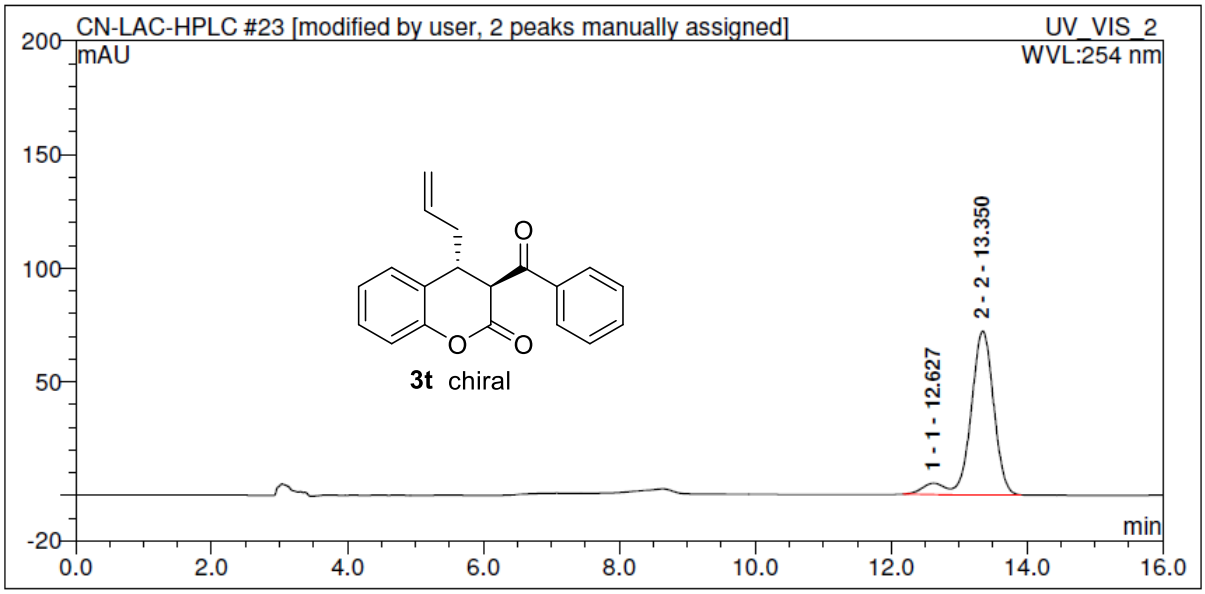
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	12.83	2.980543	4.002150838	7.62035	n.a.
2	2	17.70	71.493	95.99784916	128.266	n.a.

ALLYL-GR-LAC-RAC-AMYLOSE-C



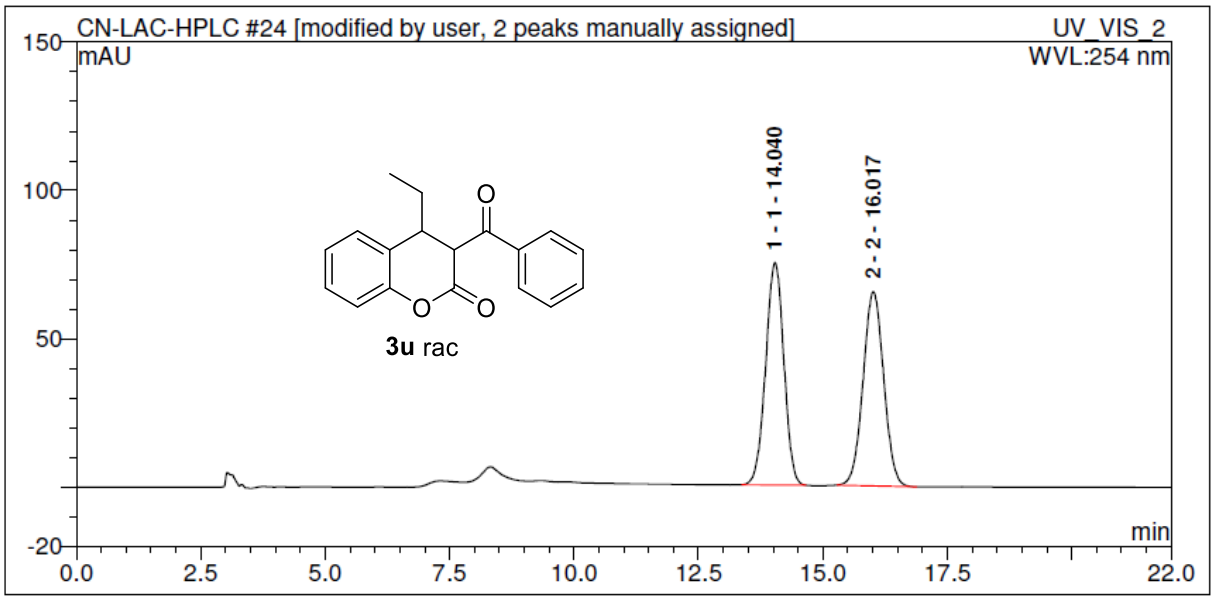
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	12.39	2.867478	50.12746649	7.29741	n.a.
2	2	13.15	2.853	49.87253351	7.515	n.a.

ALLYL-GR-LAC-CHI-AMYLOSE-C



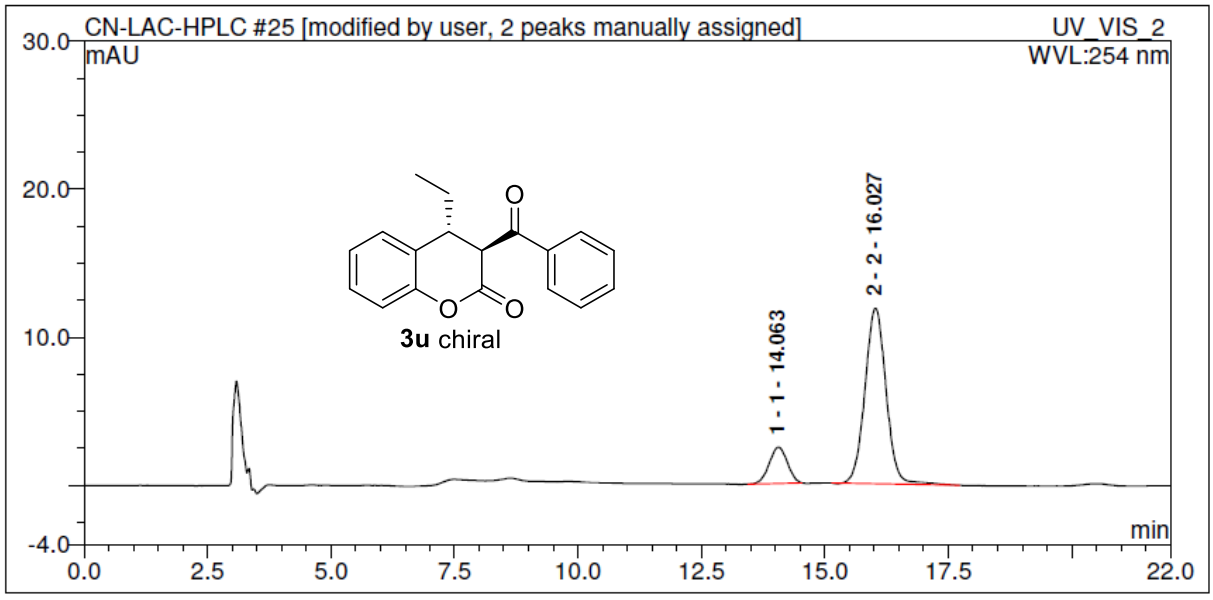
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	12.63	1.999556	6.872492523	4.98881	n.a.
2	2	13.35	27.096	93.12750748	72.018	n.a.

ETHYL-GR-LAC-RAC-AMYLOSE-C

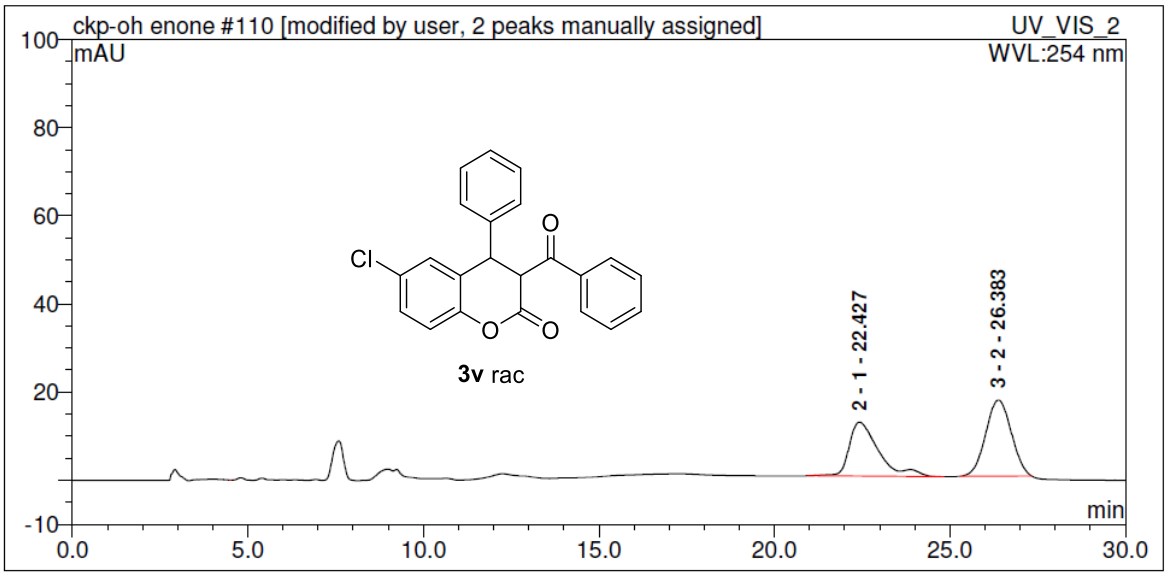


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	14.04	31.75854	50.24126188	74.98356	n.a.
2	2	16.02	31.454	49.75873812	65.406	n.a.

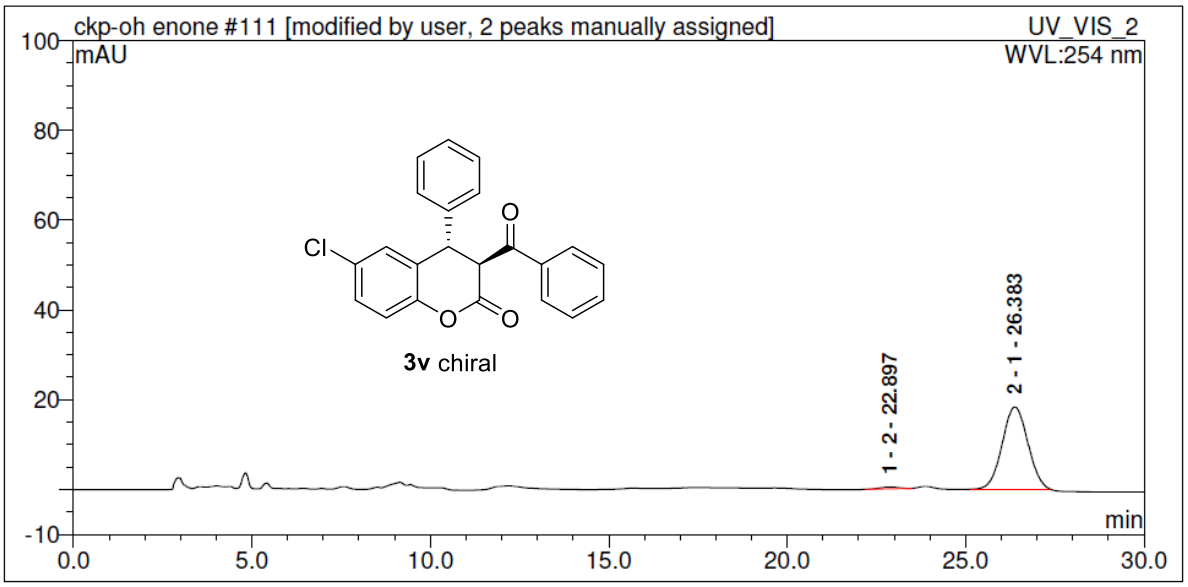
ETHYL-GR-LAC-CHI-AMYLOSE-C



No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	14.06	1.048826	15.09102167	2.44835	n.a.
2	2	16.03	5.901	84.90897833	11.853	n.a.

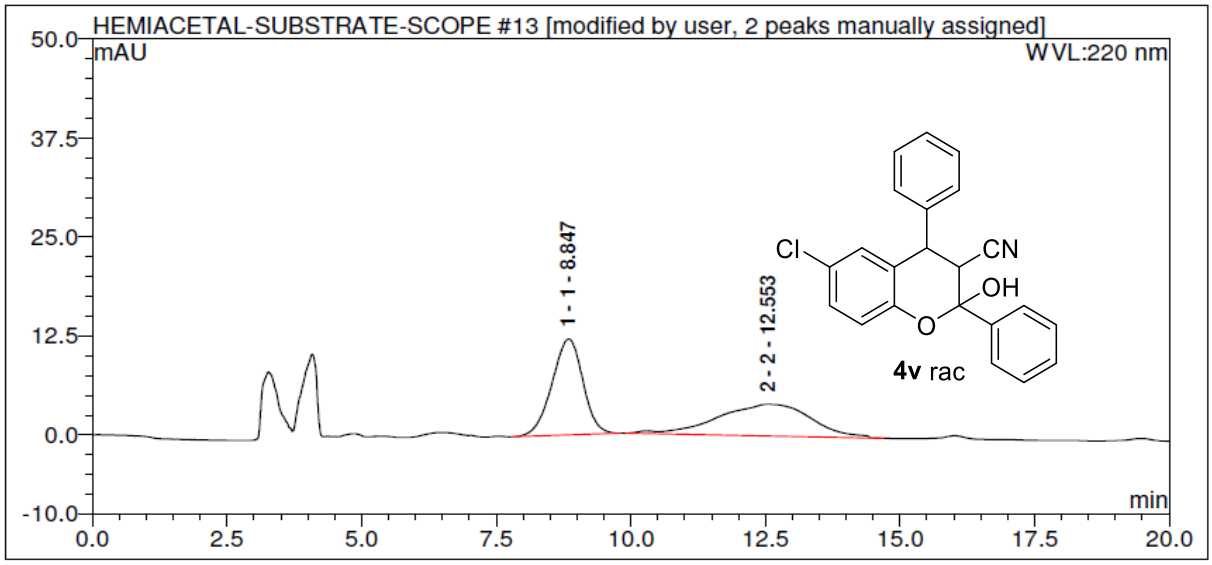


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
2	1	22.43	11.89179	44.9233906	12.24114	n.a.
3	2	26.38	14.579	55.0766094	17.236	n.a.



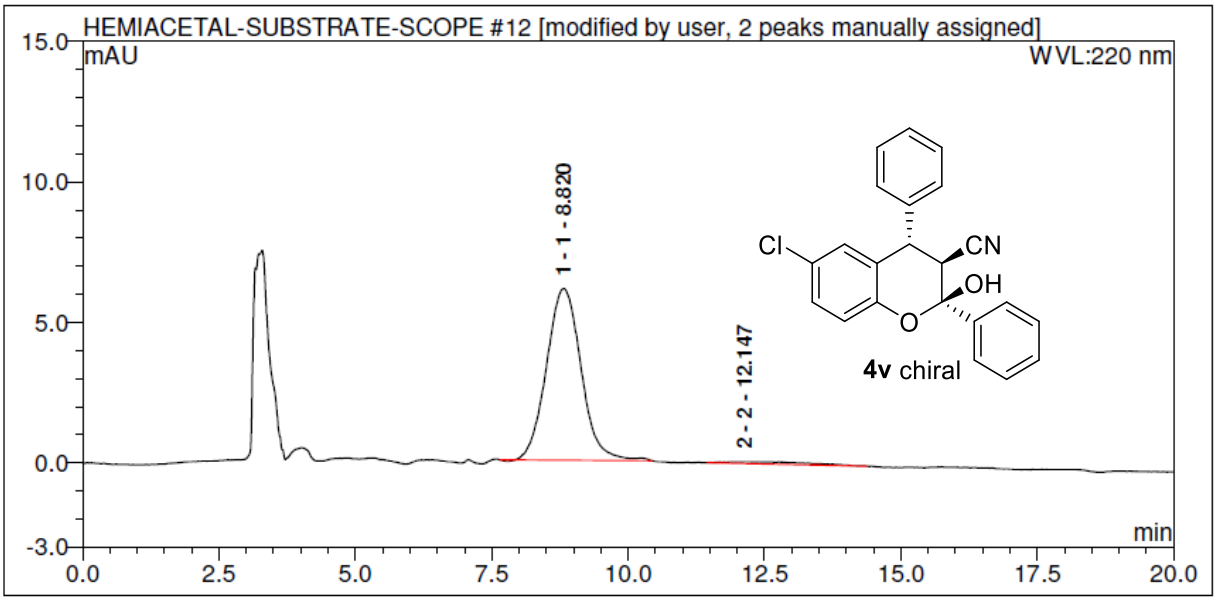
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	2	22.90	0.246631	1.592374767	0.4109	n.a.
2	1	26.38	15.242	98.40762523	18.296	n.a.

5-Cl-SAL-HEMIACETAL-RAC-ID

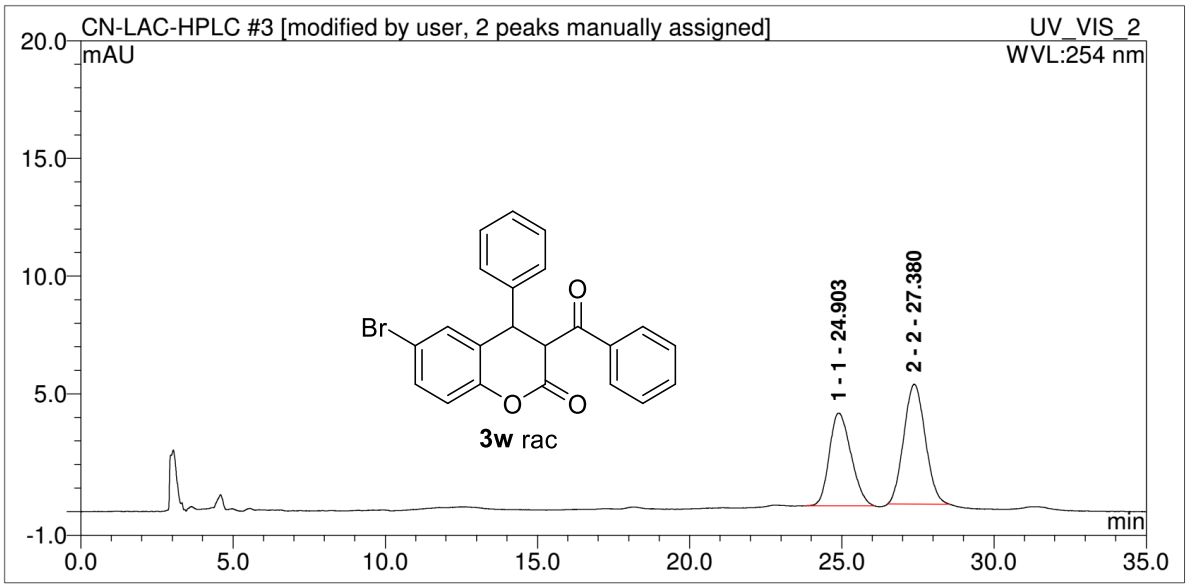


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	8.85	8.093723	50.20283315	12.12266	n.a.
2	2	12.55	8.028	49.79716685	4.020	n.a.

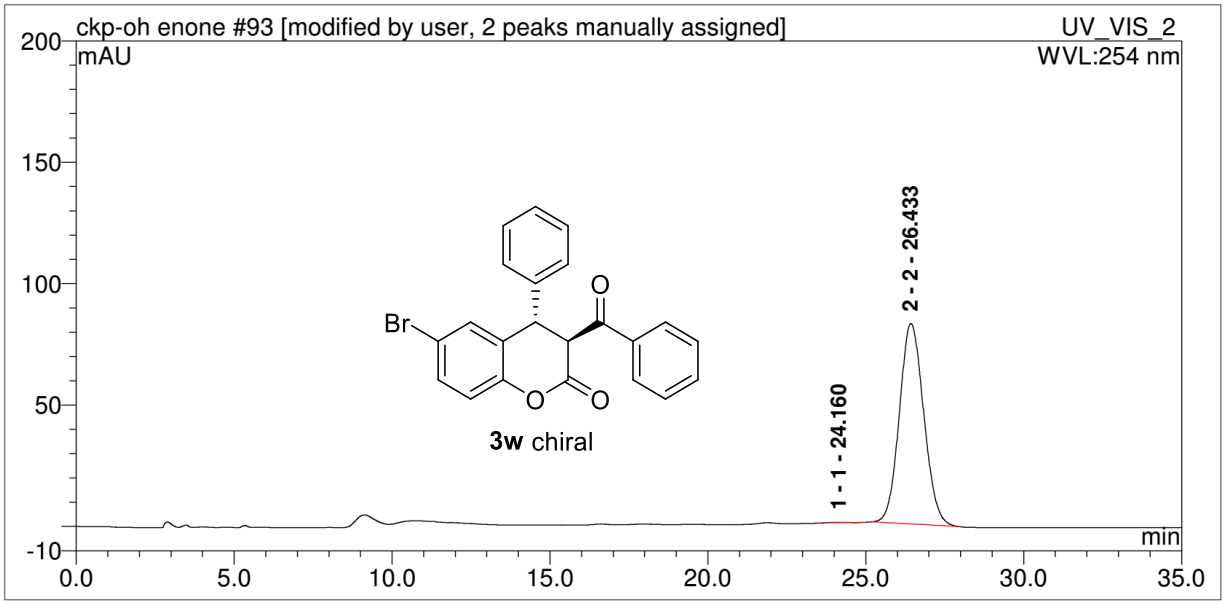
5-Cl-SAL-HEMIACETAL-CHI-ID



No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	8.82	4.506917	97.1805759	6.11552	n.a.
2	2	12.15	0.131	2.819424104	0.065	n.a.

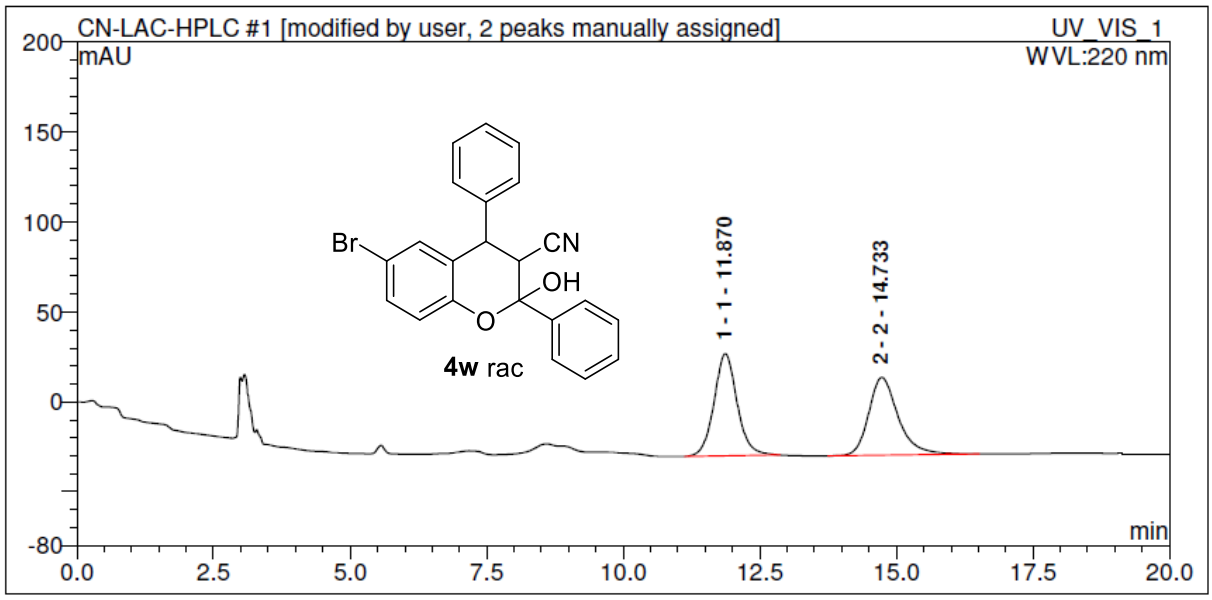


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	24.90	3.263209	43.91263832	3.93659	n.a.
2	2	27.38	4.168	56.08736168	5.088	n.a.



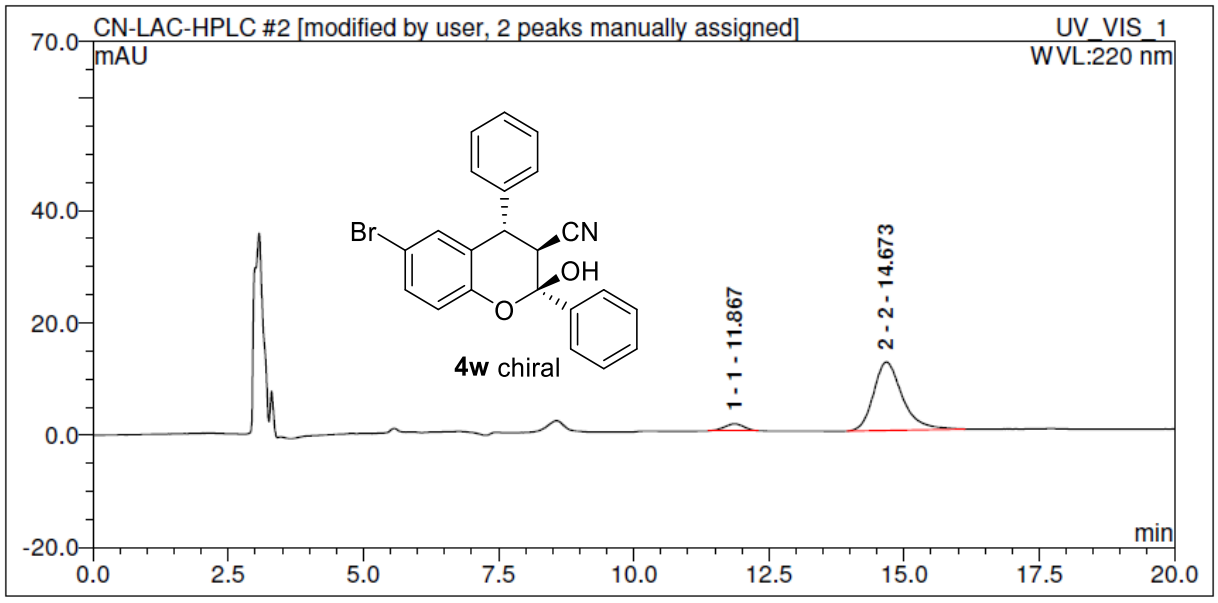
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	24.16	0.033708	0.04545899507	0.12532	n.a.
2	2	26.43	74.117	99.954541	82.561	n.a.

5-Br-SAL-HEMI-RAC-LUX-AMYLOSE-2



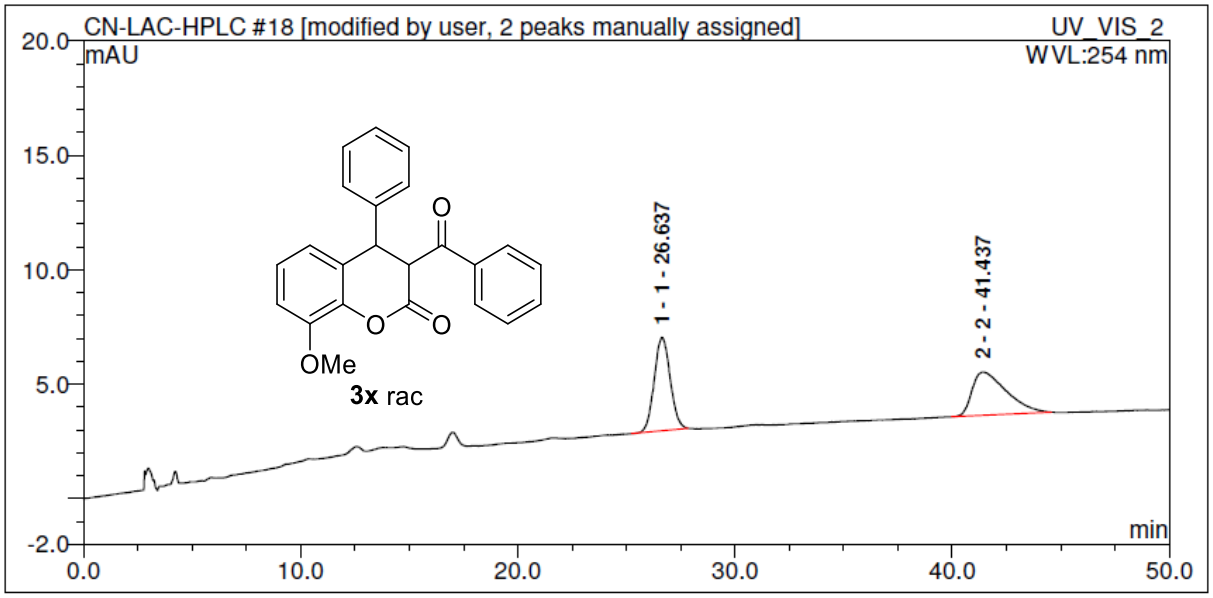
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	11.87	27.85115	50.77153676	56.68509	n.a.
2	2	14.73	27.005	49.22846324	43.151	n.a.

5-Br-SAL-HEMI-CHI-LUX-AMYLOSE-2



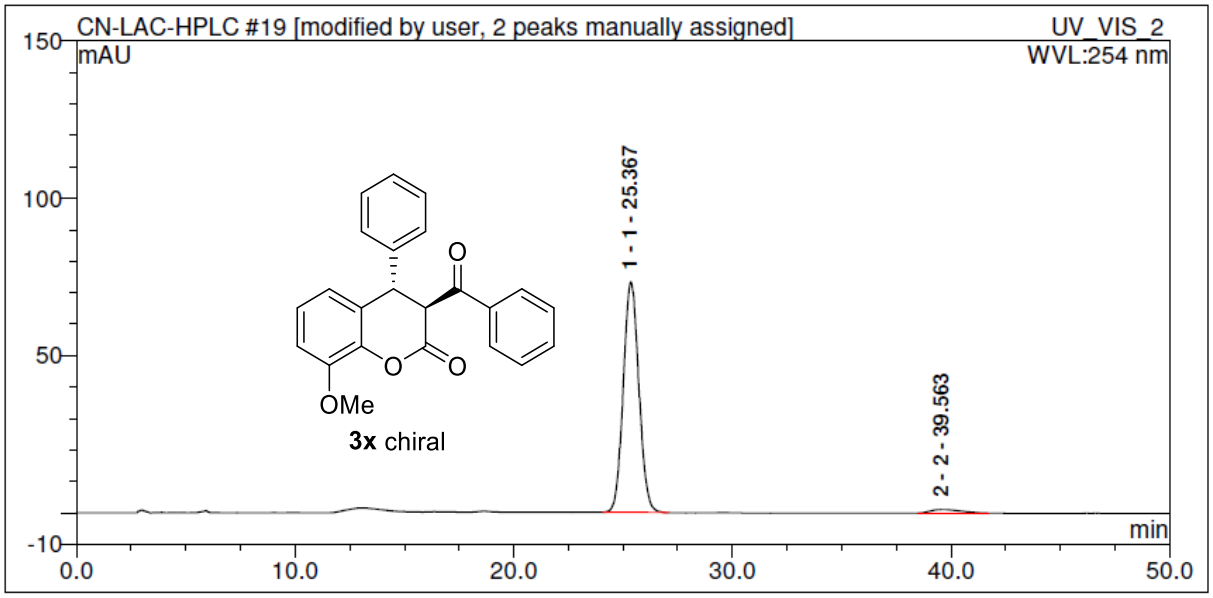
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	11.87	0.517302	6.435097222	1.2399	n.a.
2	2	14.67	7.521	93.56490278	12.158	n.a.

3-OMe-SAL-LAC-RAC-AMYLOSE-C



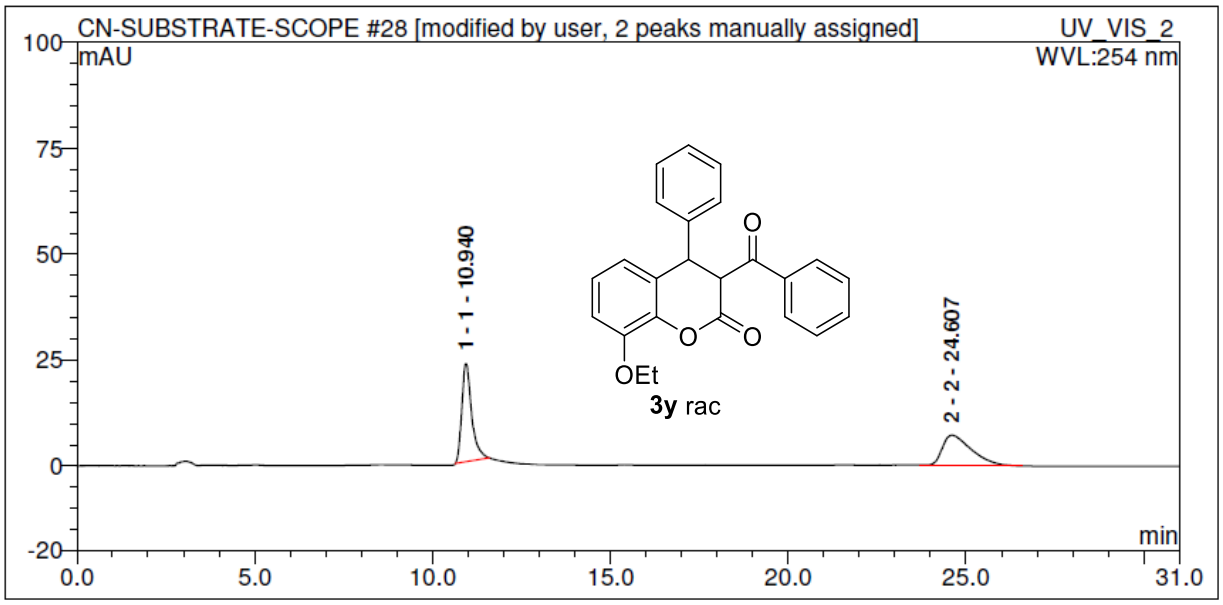
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	26.64	3.488201	50.27271919	4.08045	n.a.
2	2	41.44	3.450	49.72728081	1.890	n.a.

3-OMe-SAL-LAC-CHI-AMYLOSE-C



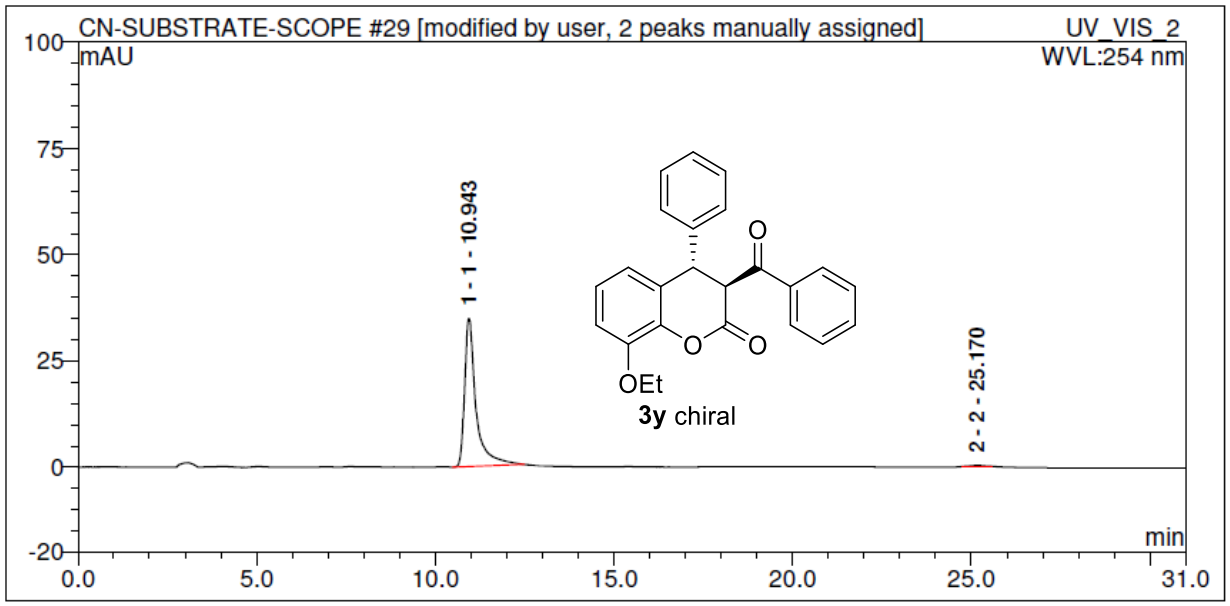
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	25.37	60.56249	97.2137053	73.2387	n.a.
2	2	39.56	1.736	2.786294703	1.113	n.a.

3-OEt-SAL-CN-LAC-RAC-IA



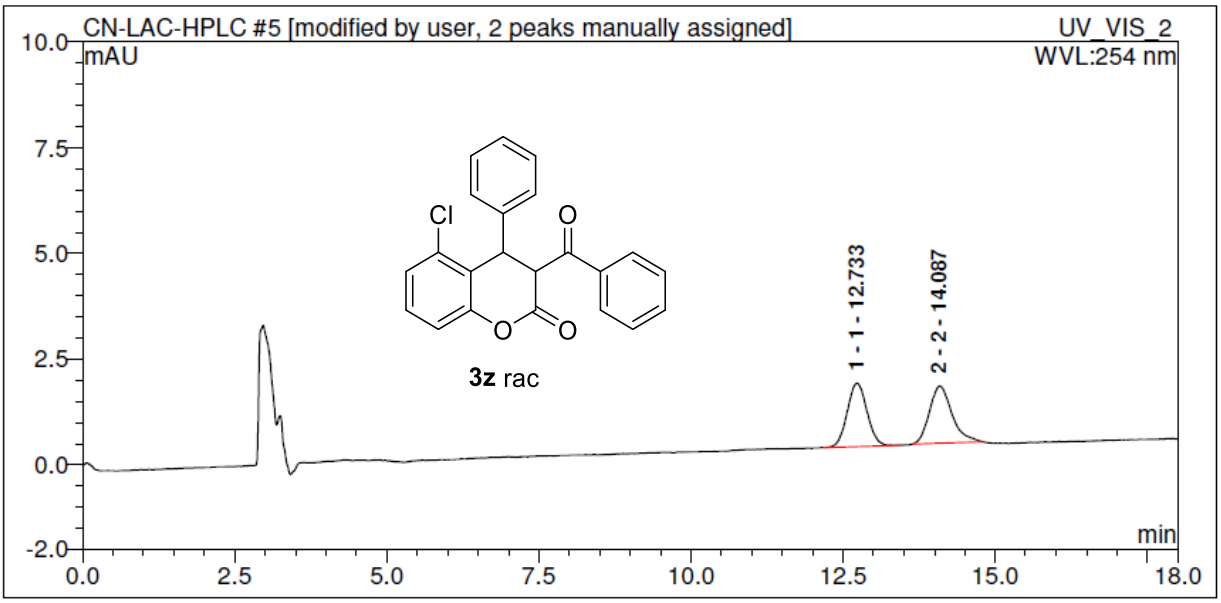
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	10.94	7.450163	51.25209789	23.16992	n.a.
2	2	24.61	7.086	48.74790211	7.286	n.a.

3-OEt-SAL-CN-LAC-CHI-IA



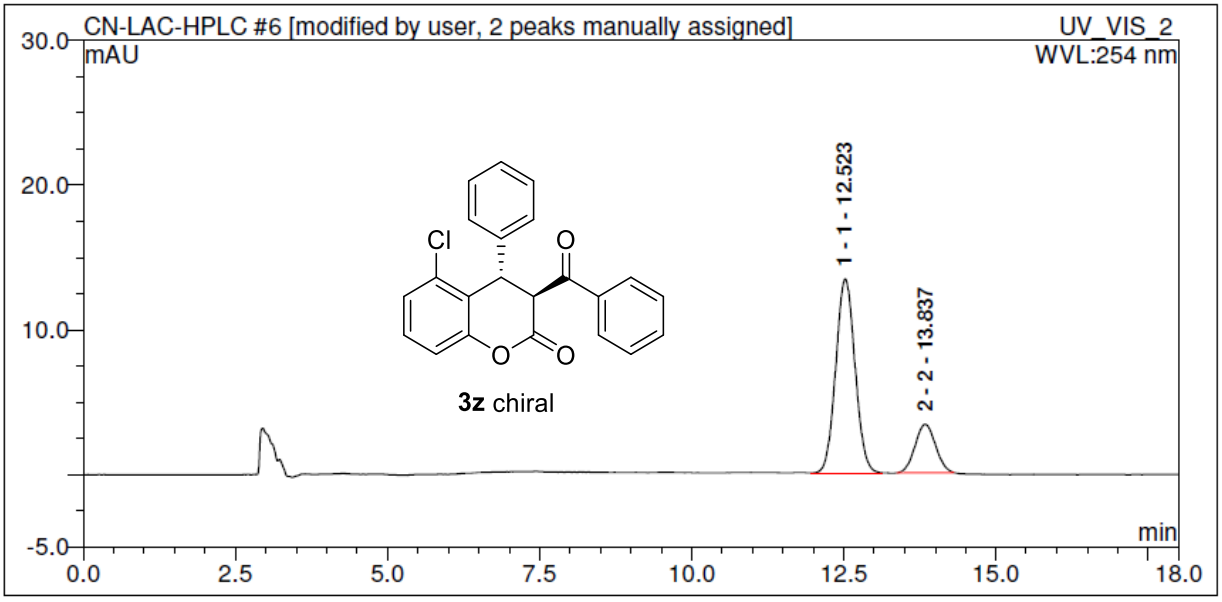
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	10.94	12.90782	98.87624078	34.83891	n.a.
2	2	25.17	0.147	1.123759221	0.286	n.a.

6-Cl-SAL-CN-LAC-RAC-AMYLOSE-C



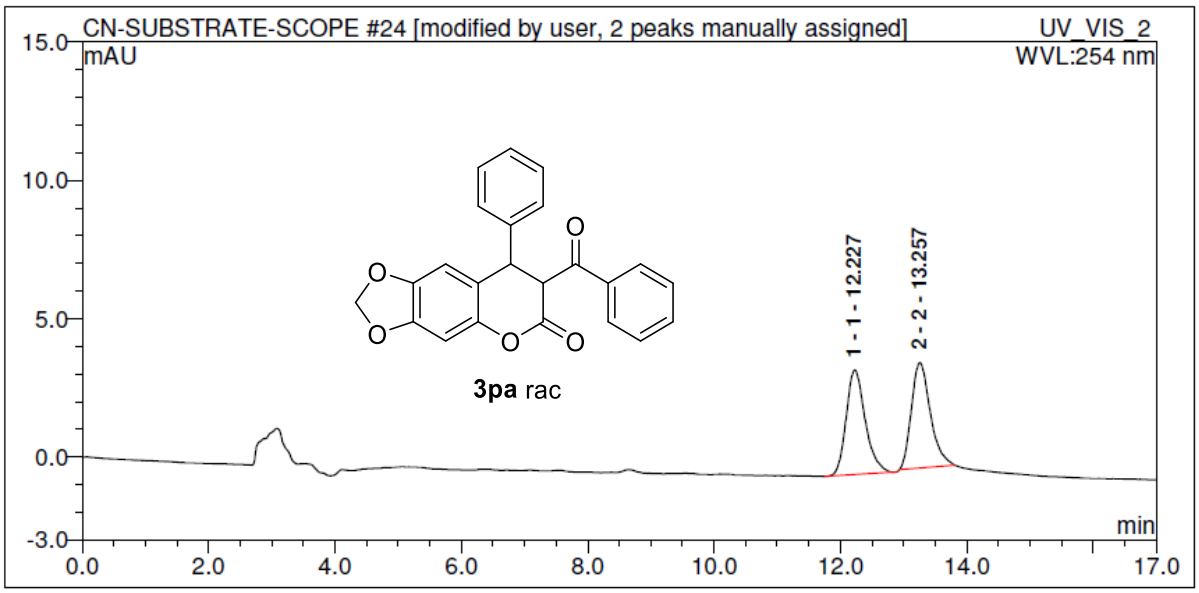
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	12.73	0.563412	49.22237871	1.49902	n.a.
2	2	14.09	0.581	50.77762129	1.351	n.a.

6-Cl-SAL-CN-LAC-CHI-AMYLOSE-C



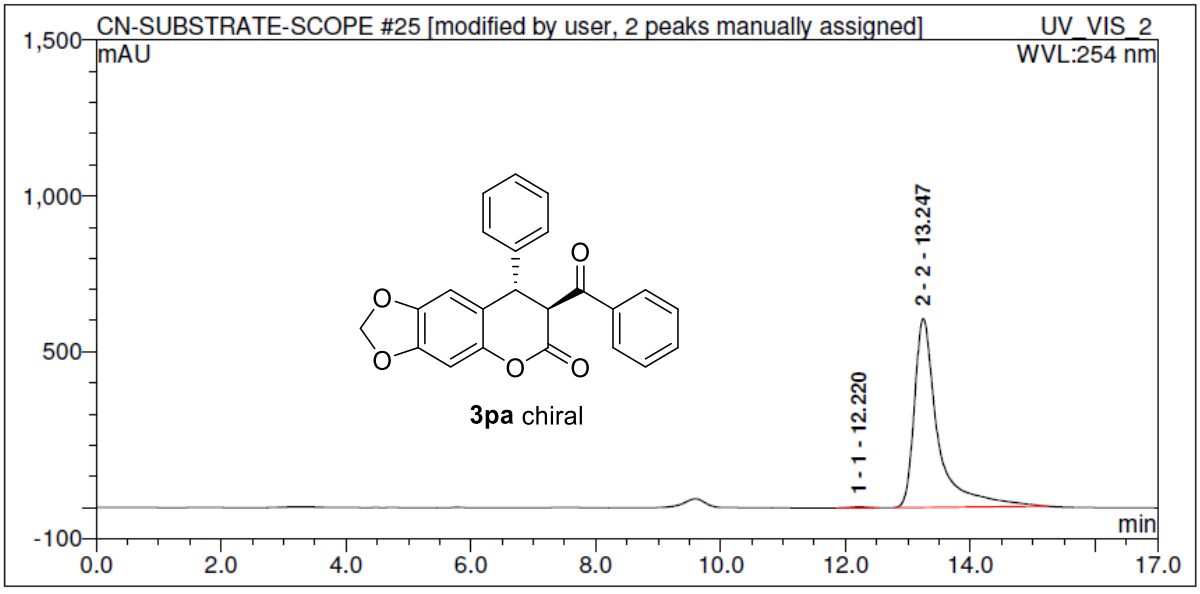
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	12.52	4.914421	79.03703752	13.39699	n.a.
2	2	13.84	1.303	20.96296248	3.342	n.a.

SESAMOL-LAC-RAC-IA



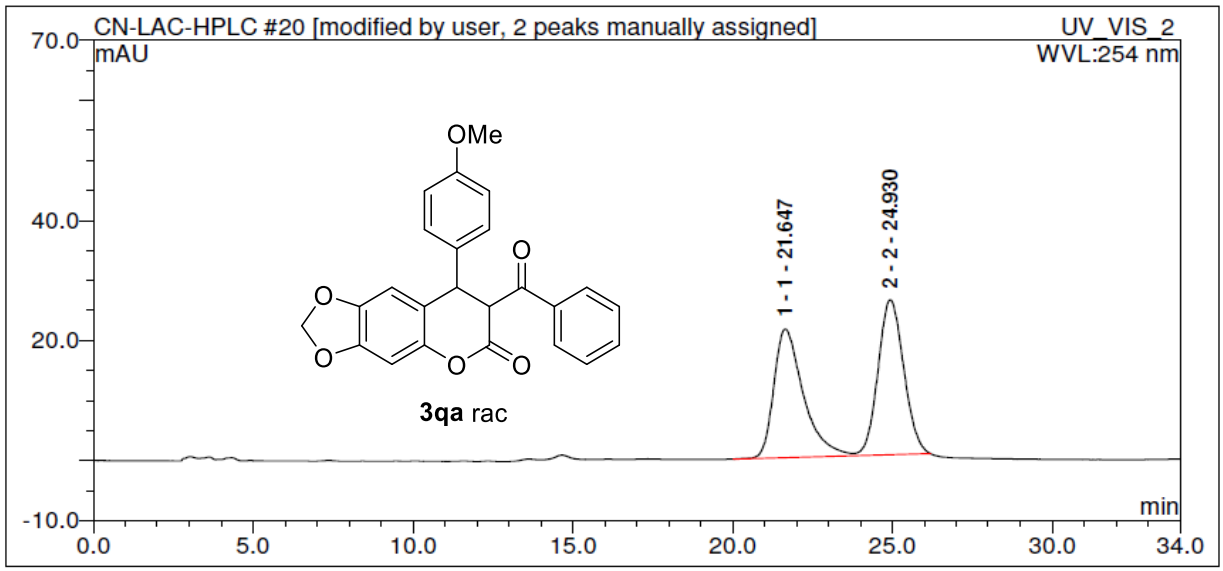
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	12.23	1.322484	49.90033957	3.78161	n.a.
2	2	13.26	1.328	50.09966043	3.817	n.a.

SESAMOL-LAC-CHI-IA



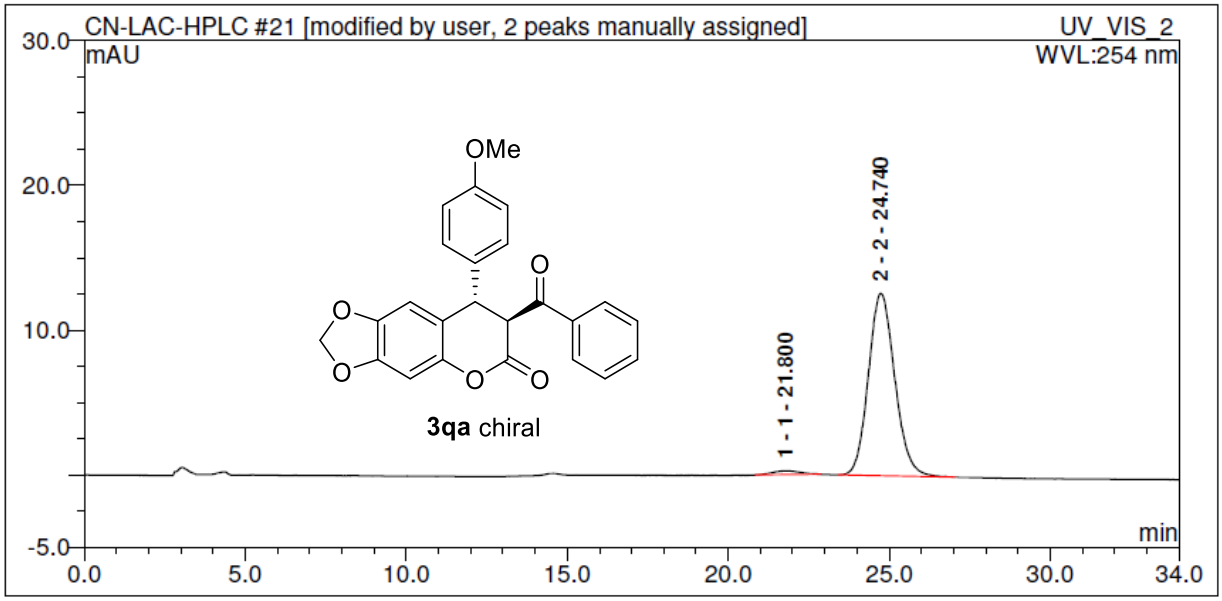
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	12.22	1.053754	0.3933872298	3.36645	n.a.
2	2	13.25	266.813	99.60661277	605.565	n.a.

SES-4-OMe-GR-LAC-RAC-AMYLOSE-C



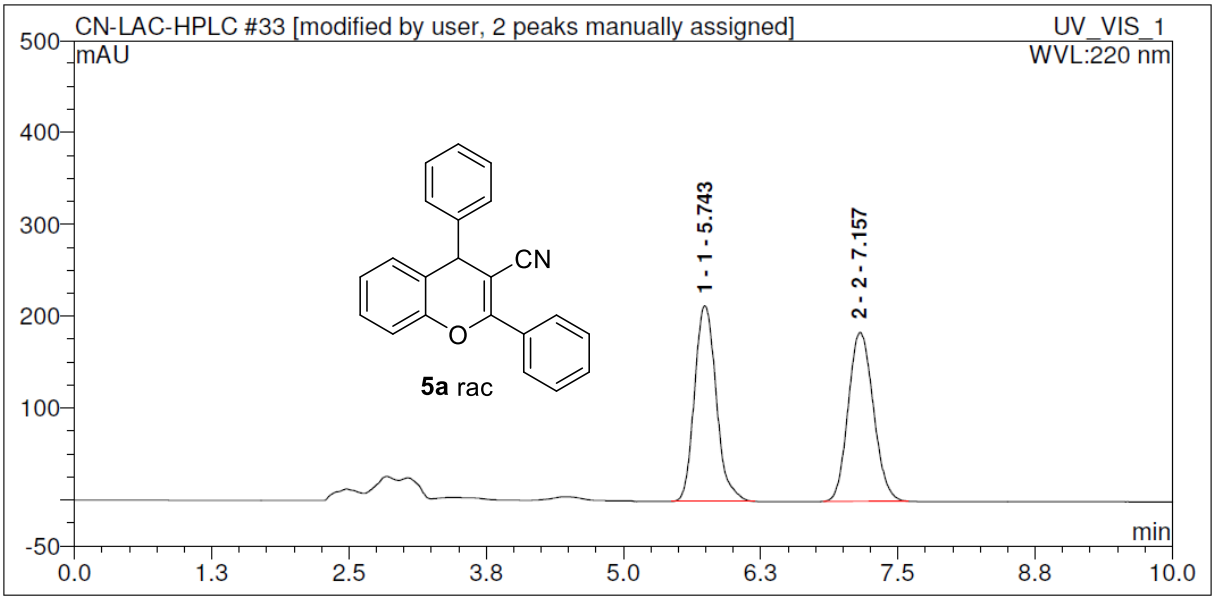
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	21.65	22.98897	48.88588928	21.40385	n.a.
2	2	24.93	24.037	51.11411072	25.790	n.a.

SES-4-OMe-GR-LAC-CHI-AMYLOSE-C



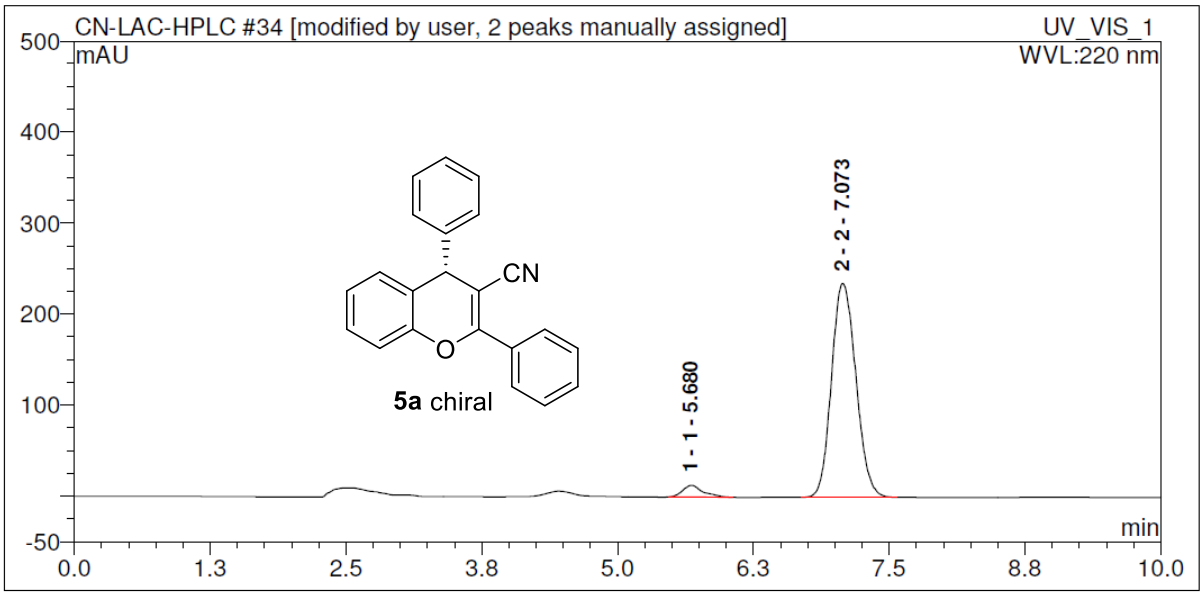
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	21.80	0.264909	2.162875294	0.26179	n.a.
2	2	24.74	11.983	97.83712471	12.593	n.a.

PH-CN-HEMI-PTSA-RAC-AD-H



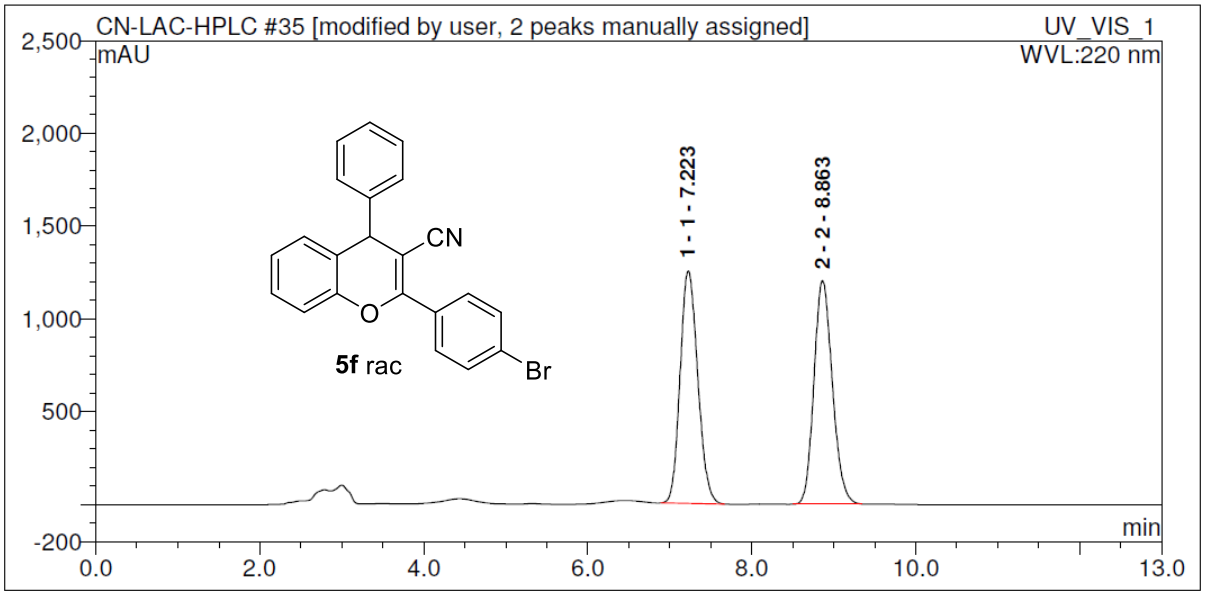
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	5.74	48.9811	50.07746577	212.9774	n.a.
2	2	7.16	48.830	49.92253423	183.816	n.a.

PH-CN-HEMI-PTSA-CHI-AD-H



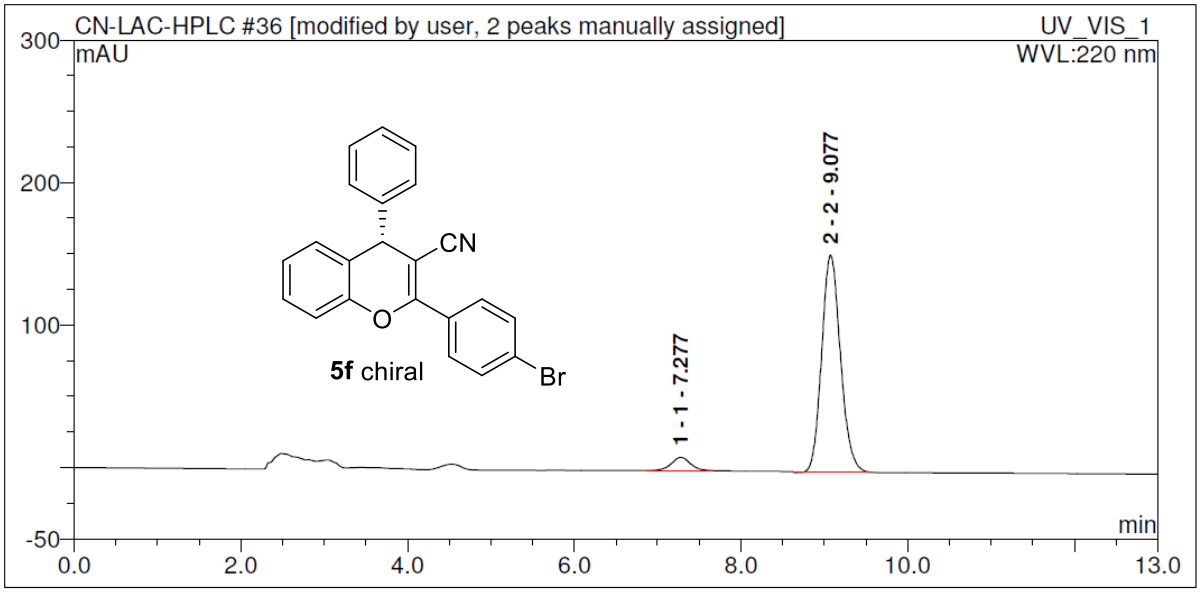
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	5.68	2.769882	4.327212904	12.82446	n.a.
2	2	7.07	61.241	95.6727871	234.946	n.a.

4-Br-CN-HEMI-PTSA-RAC-AD-H



No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	7.22	311.7883	49.8857927	1252.683	n.a.
2	2	8.86	313.216	50.1142073	1203.769	n.a.

4-Br-CN-HEMI-PTSA-CHI-AD-H



No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	1	7.28	2.442942	5.77327232	9.27164	n.a.
2	2	9.08	39.872	94.22672768	152.382	n.a.