

**Organocatalytic asymmetric Michael-hemiacetalization reaction between
2-hydroxyacetophenones and enals: A route to chiral β,γ -disubstituted γ -
butyrolactones**

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1. Solvent optimization:

Preliminary solvent screening with catalyst (**I** and **VII**):

Solvent	Time (days)	Yield ^[c] (%))	ee ^[e]
Toluene	3	57	97
Xylene	5	32	96
Chloroform	5	25	98
Acetonitrile	5	47	86

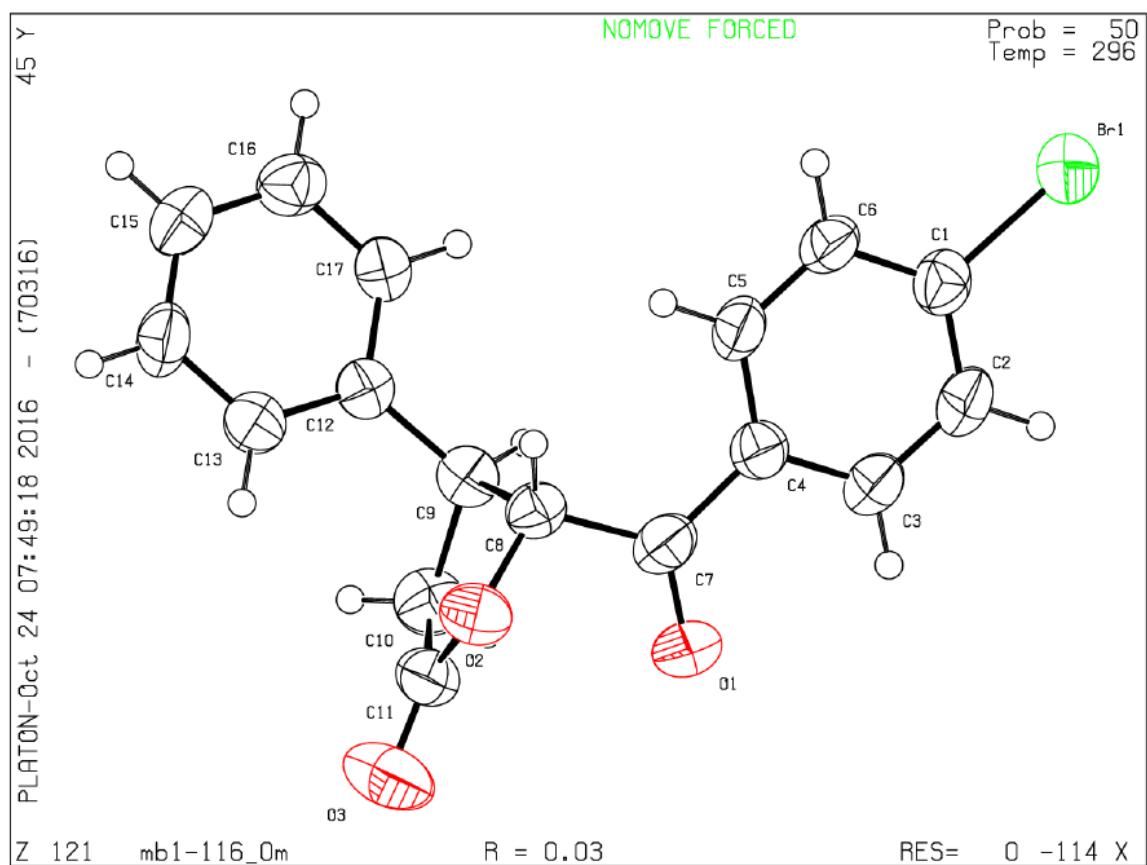
^[c] Isolated combined yield after silica gel column chromatography. ^[d] Determined by ¹H NMR. ^[e] Determined by HPLC using stationary phase chiral column of the major diastereomers.

2. Crystal structure and data:

Crystal structure and data of 4o:

CCDC number assigned to structure 4o is 1511229

Bond precision:	C-C = 0.0058 Å	Wavelength=0.71073	
Cell:	a=5.7218 (8) alpha=90	b=5.9498 (8) beta=90	c=42.706 (6) gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	1453.9 (3)	1453.9 (4)	
Space group	P 21 21 21	P 21 21 21	
Hall group	P 2ac 2ab	P 2ac 2ab	
Moiety formula	C17 H13 Br O3	C17 H13 Br O3	
Sum formula	C17 H13 Br O3	C17 H13 Br O3	
Mr	345.17	345.18	
Dx, g cm ⁻³	1.577	1.577	
Z	4	4	
Mu (mm ⁻¹)	2.834	2.834	
F000	696.0	696.0	
F000'	695.17		
h,k,lmax	6,7,51	6,7,51	
Nref	2618 [1592]	2619	
Tmin, Tmax	0.447, 0.712	0.447, 0.712	
Tmin'	0.400		
Correction method= #	Reported T Limits: Tmin=0.447 Tmax=0.712		
AbsCorr =	MULTI-SCAN		
Data completeness=	1.65/1.00	Theta (max) = 25.230	
R(reflections)=	0.0316 (2110)	wR2 (reflections) = 0.0973 (2619)	
S =	1.067	Npar= 190	



CCDC No.

1511229

Empirical Formula

C₁₇H₁₂BrO₃

Formula weight

345.18

Crystal habit, colour

Needle/colourless

Crystal size, mm³

0.32 x 0.24 x 0.12

Temperature, T

296(2) K

Wavelength, λ (Å)

0.71073

Crystal system

Orthorhombic

Space group

P 21 21 21

Unit cell dimensions	$a = 5.7218(8) \text{ \AA}$
	$b = 5.9498(8) \text{ \AA}$
	$c = 42.706(6) \text{ \AA}$
	$\alpha = 90.00^\circ, \beta = 90.00^\circ, \gamma = 90.00^\circ$
Volume, V (\AA^3)	1453.9(4)
Z	4
Calculated density, Mg/m ³	1.577
Absorption coefficient, μ (mm-1)	2.834
F (000)	696
θ range for data collection	2.86° to 21.81°
Limiting indices	-6 ≤ h ≤ 6, -7 ≤ k ≤ 6, -51 ≤ l ≤ 49
Reflection collected/unique	2619/2110
Completeness to θ	
Max. and Min. transmission	0.712/ 0.447
Refinement method	SHELXL-97 (Sheldrick, 1997)
Data/restraints/parameters	2619/0/190
Goodness-of-fit on F ²	1.067
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0316, wR2 = 0.0762
R indices (all data)	R1 = 0.0494, wR2 = 0.0973

Flack Parameter value 0.008(12)

(Since the value of Flack Parameter is close to zero. So, there is no uncertainty in determining the absolute configuration of compound.)

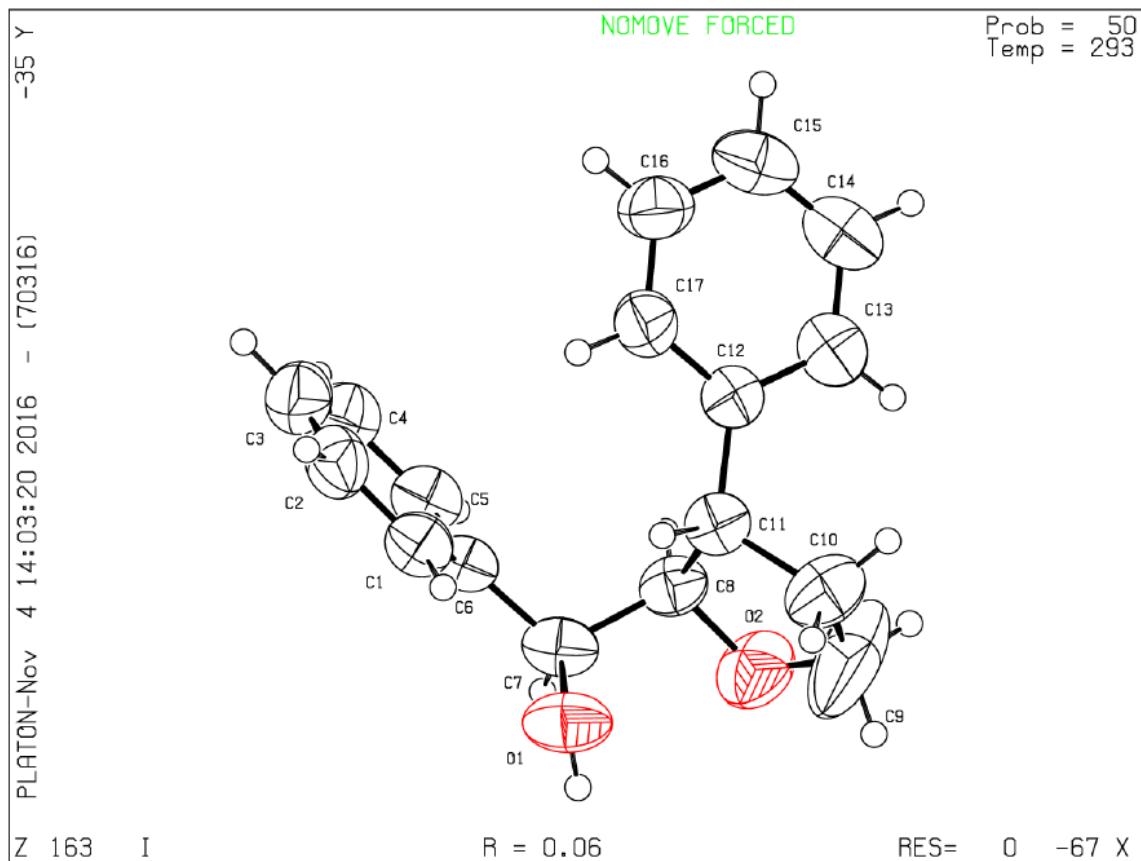
Crystal structure and data of 7:

CCDC number assigned to structure 7 is 1515196.

Bond precision:	C-C = 0.0056 Å	Wavelength=0.71073	
Cell:	a=7.9793 (9) alpha=90	b=5.7456 (9) beta=103.111 (7)	c=15.4757 (16) gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	691.00 (15)	691.00 (15)	
Space group	P 21	P 21	
Hall group	P 2yb	P 2yb	
Moiety formula	C17 H18 O2	C17 H18 O2	
Sum formula	C17 H18 O2	C17 H18 O2	
Mr	254.31	254.31	
Dx, g cm ⁻³	1.222	1.222	
Z	2	2	
Mu (mm ⁻¹)	0.079	0.079	
F000	272.0	272.0	
F000'	272.12		
h, k, lmax	9, 6, 18	9, 6, 18	
Nref	2372 [1318]	2131	
Tmin, Tmax	0.978, 0.991	0.978, 0.991	
Tmin'	0.975		

Correction method= # Reported T Limits: Tmin=0.978 Tmax=0.991
AbsCorr = MULTI-SCAN

Data completeness= 1.62/0.90	Theta (max) = 24.740
R(reflections) = 0.0562 (1360)	wR2(reflections) = 0.1343 (213)
S = 1.083	Npar= 172



CCDC No.

1515196

Empirical Formula

C₁₇H₁₈O₂

Formula weight

254.31

Crystal habit, colour

Needle/colourless

Crystal size, mm³

0.32 x 0.24 x 0.12

Temperature, T

296(2) K

Wavelength, λ (Å)

0.71073

Crystal system

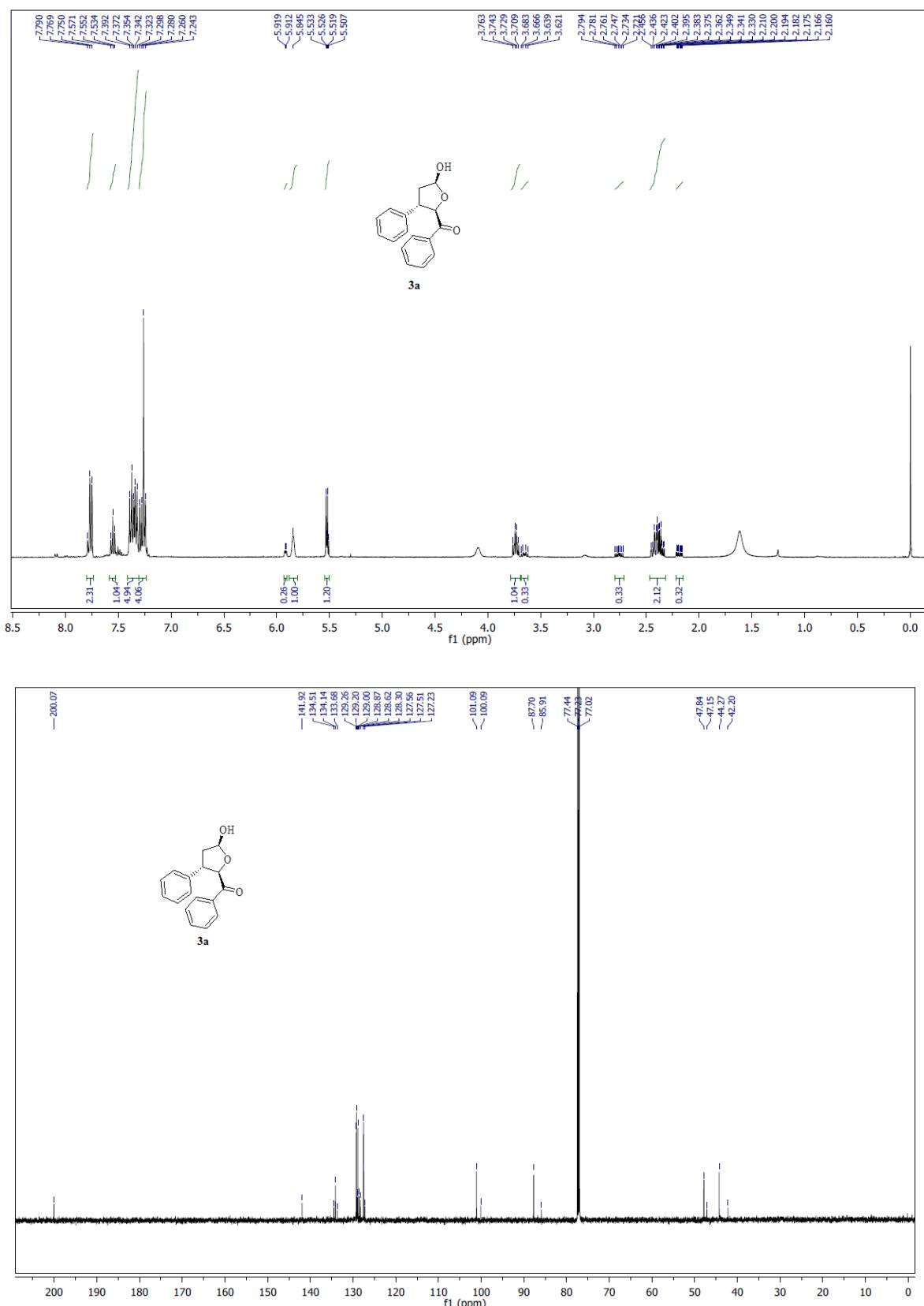
Monoclinic

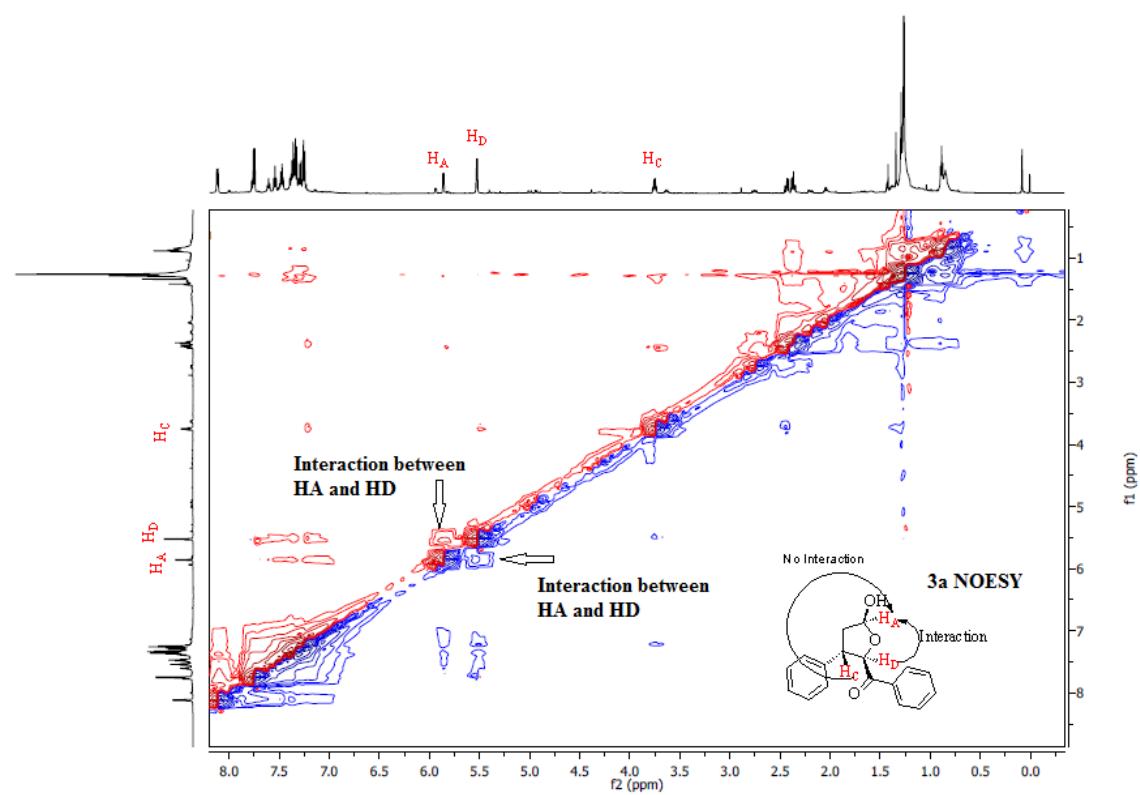
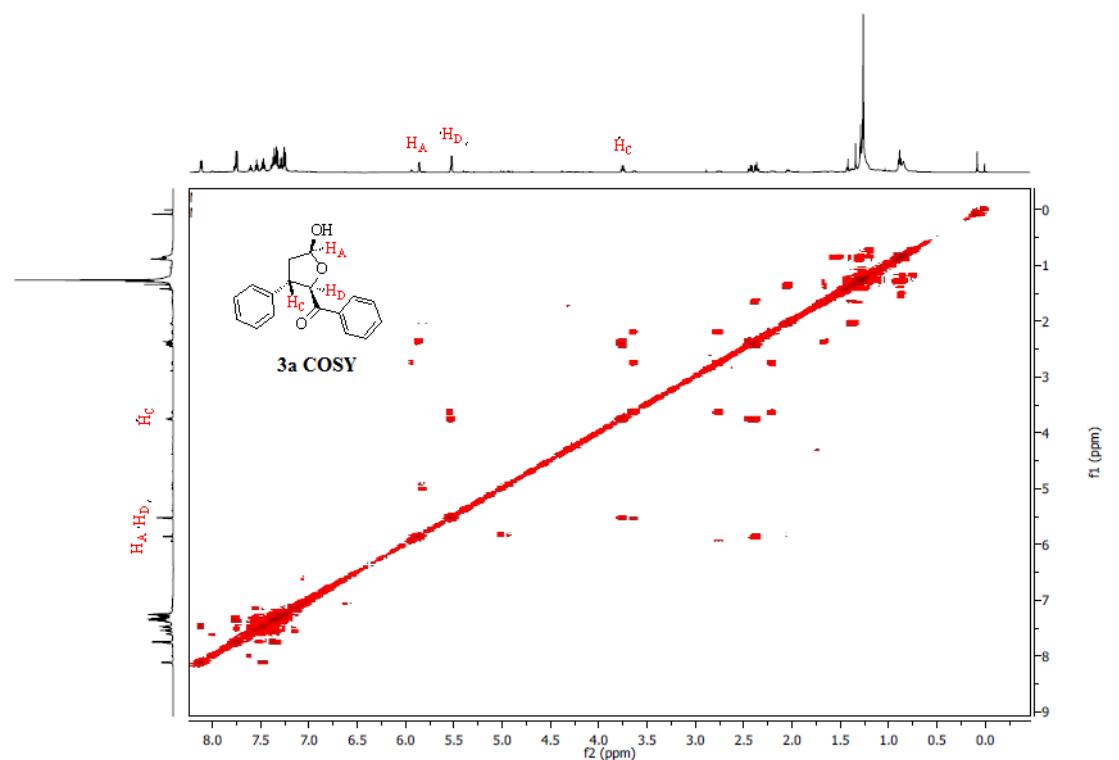
Space group

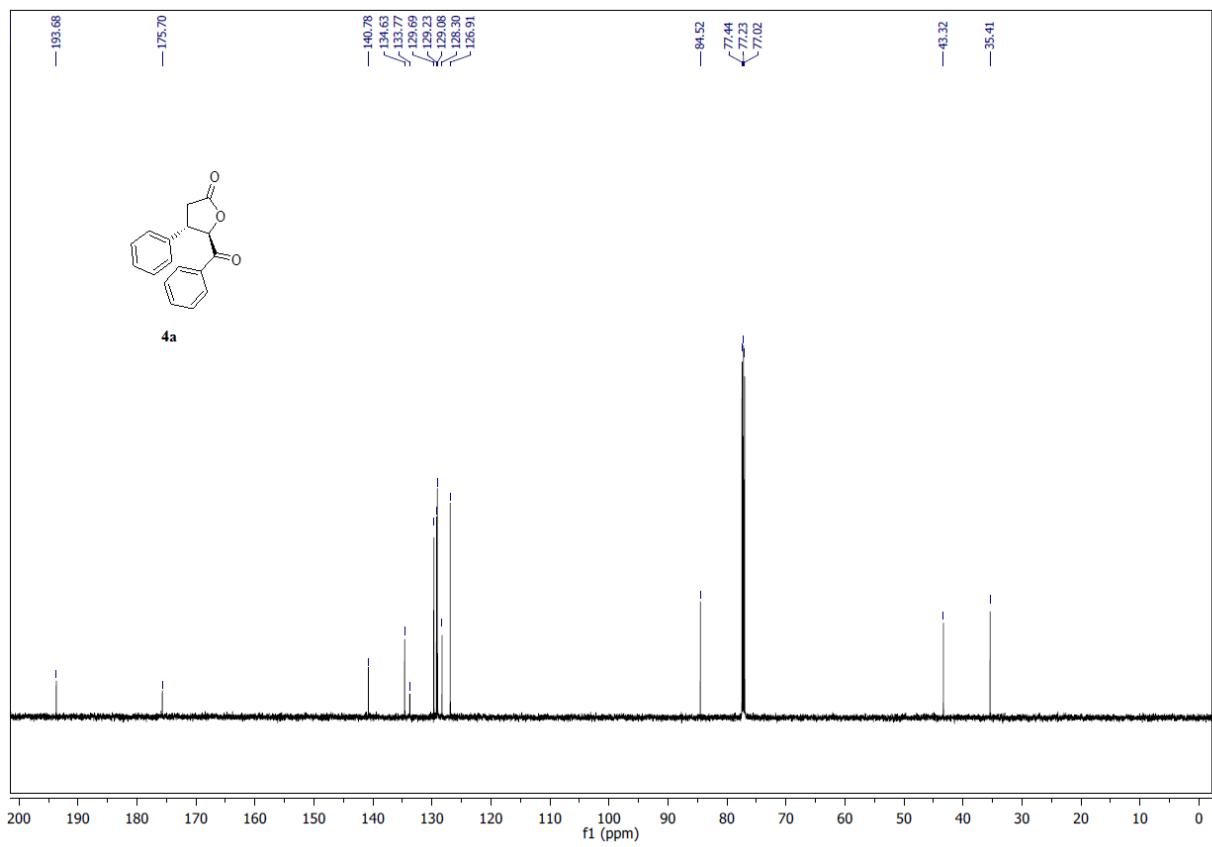
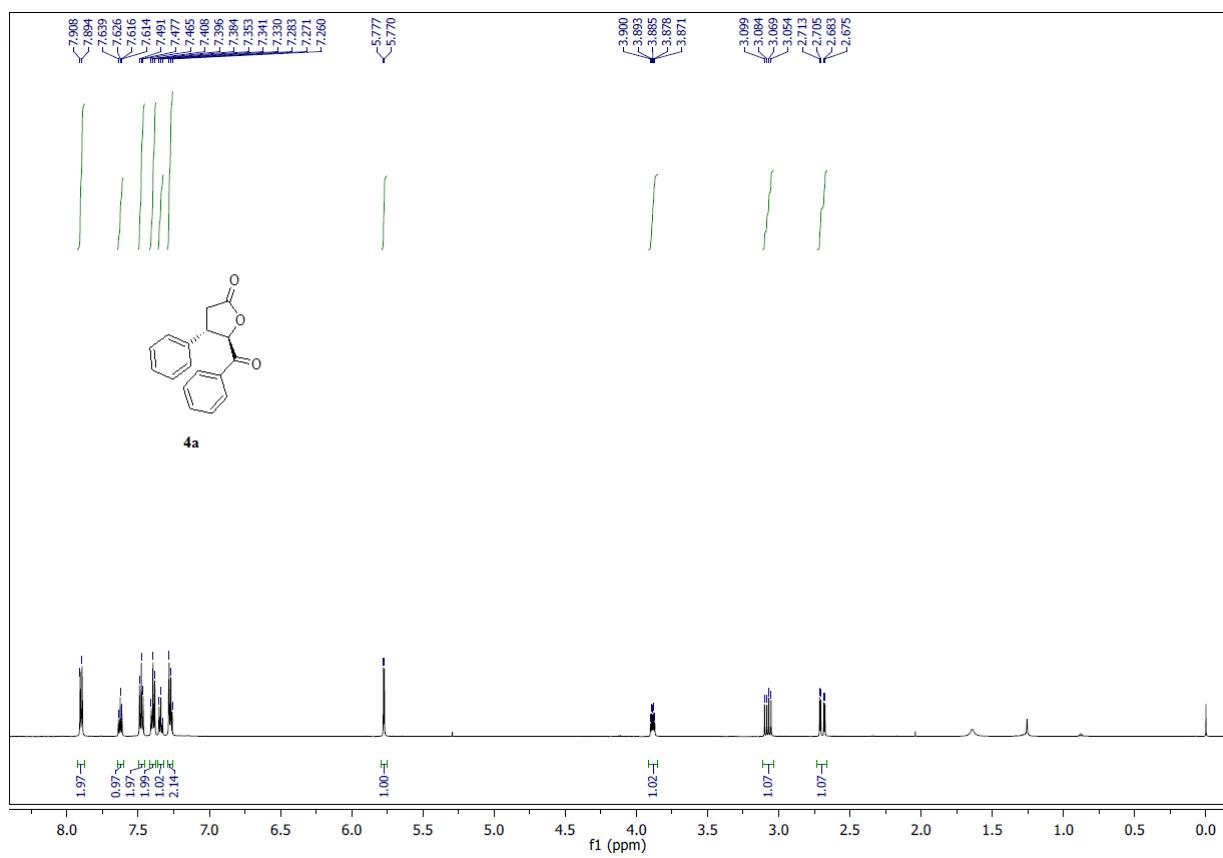
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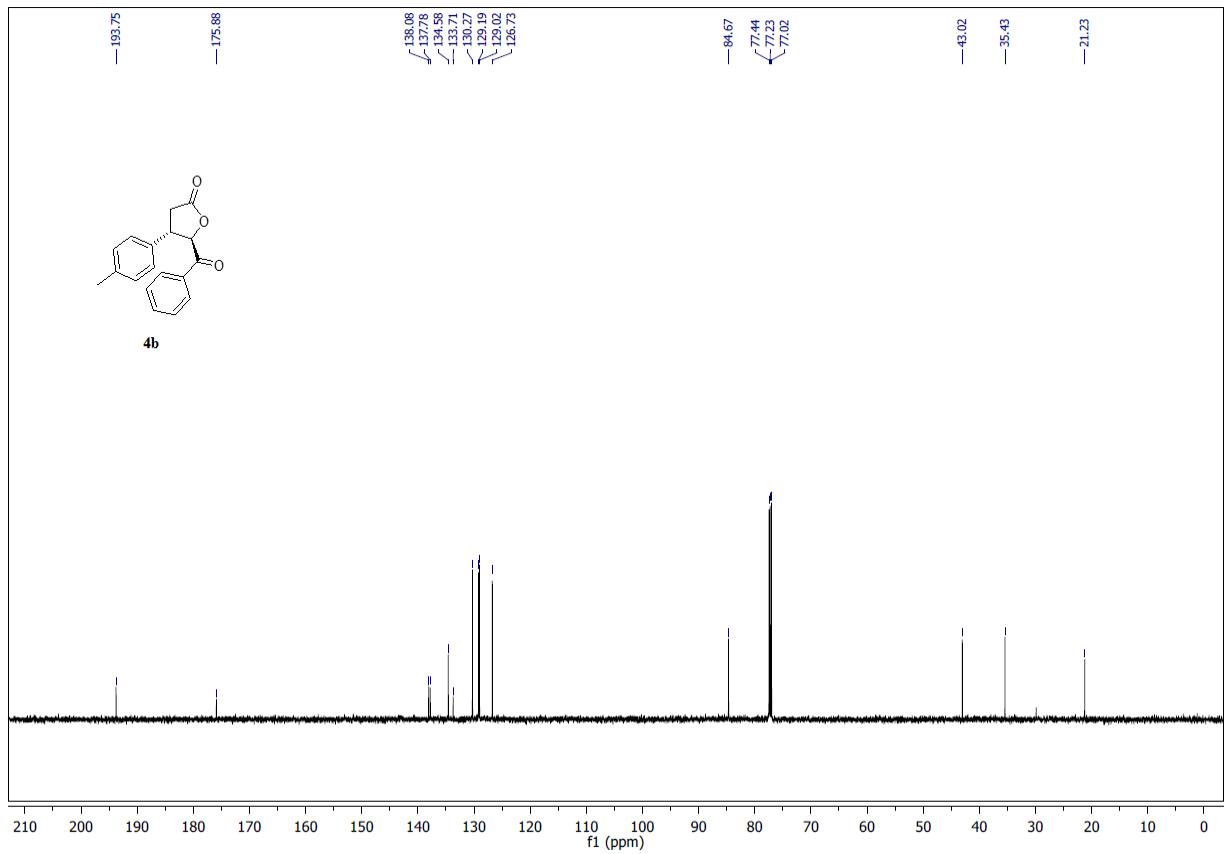
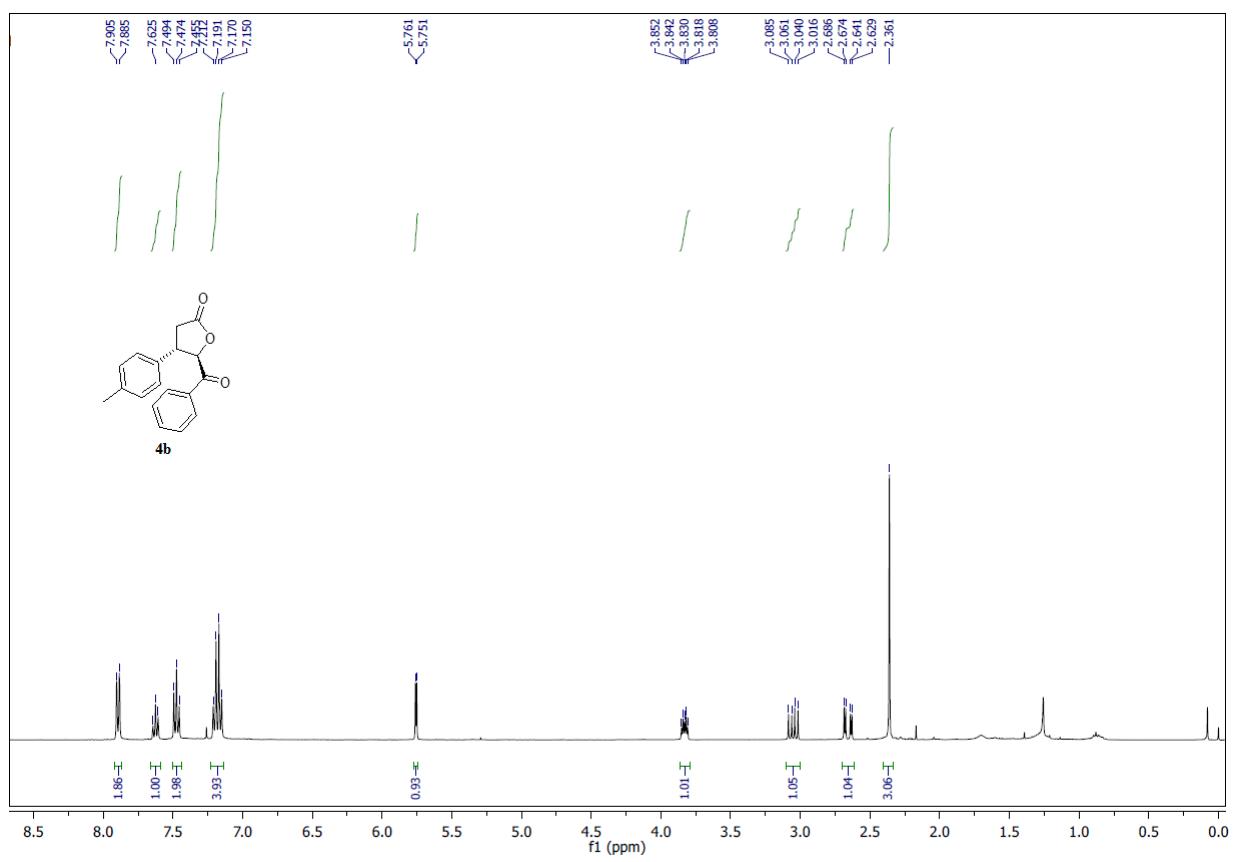
Unit cell dimensions	$a = 7.9793(9) \text{ \AA}$
	$b = 5.7456(9) \text{ \AA}$
	$c = 15.4757(16) \text{ \AA}$
	$\alpha = 90.00^\circ, \beta = 103.111(7)^\circ, \gamma = 90.00^\circ$
Volume, V (\AA^3)	691.00(15)
Z	2
Calculated density, Mg/m ³	1.222
Absorption coefficient, μ (mm-1)	0.079
F (000)	272
θ range for data collection	1.35° to 24.74°
Limiting indices	-8 ≤ h ≤ 9, -6 ≤ k ≤ 6, -18 ≤ l ≤ 18
Reflection collected/unique	2131/1360
Max. and Min. transmission	0.991 / 0.978
Refinement method	SHELXL-97 (Sheldrick, 1997)
Data/restraints/parameters	2131/1/172
Goodness-of-fit on F ²	1.083
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0562, wR2 = 0.1209
R indices (all data)	R1 = 0.0910, wR2 = 0.1343

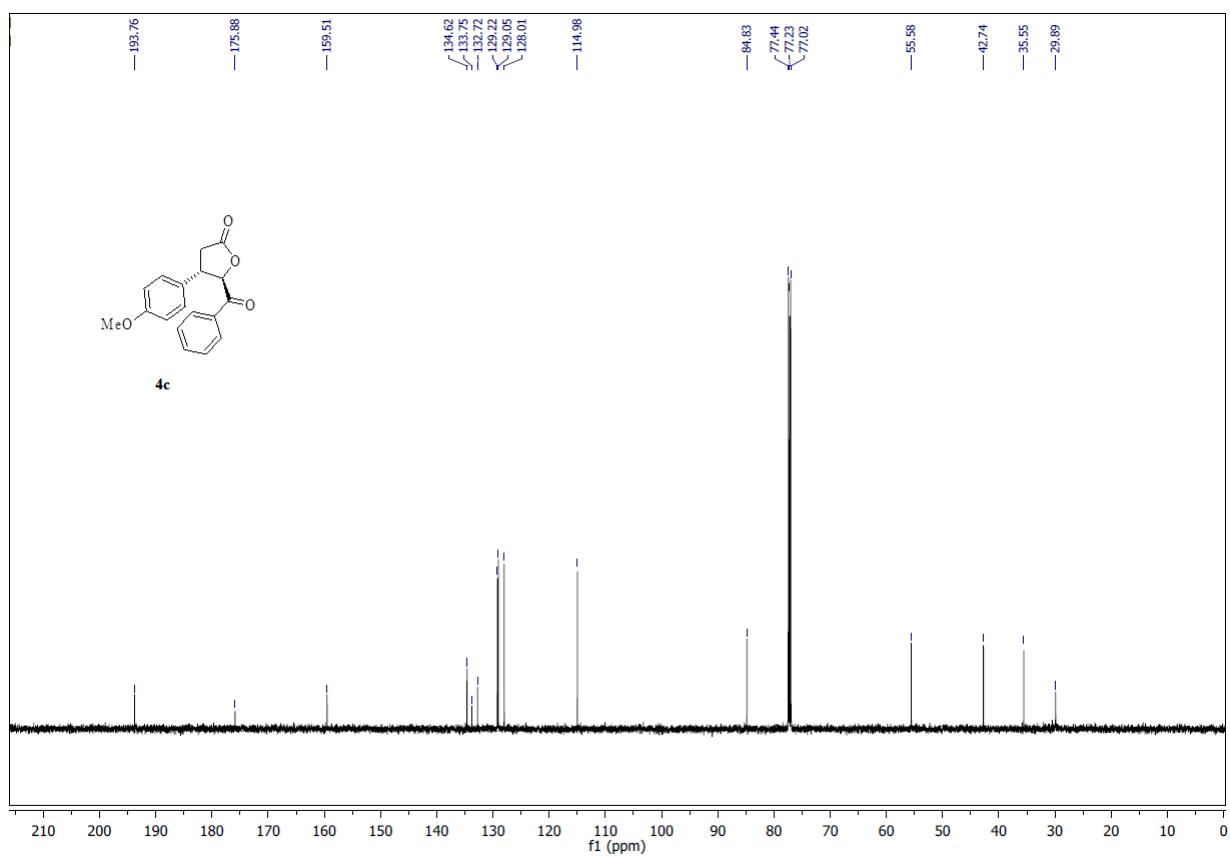
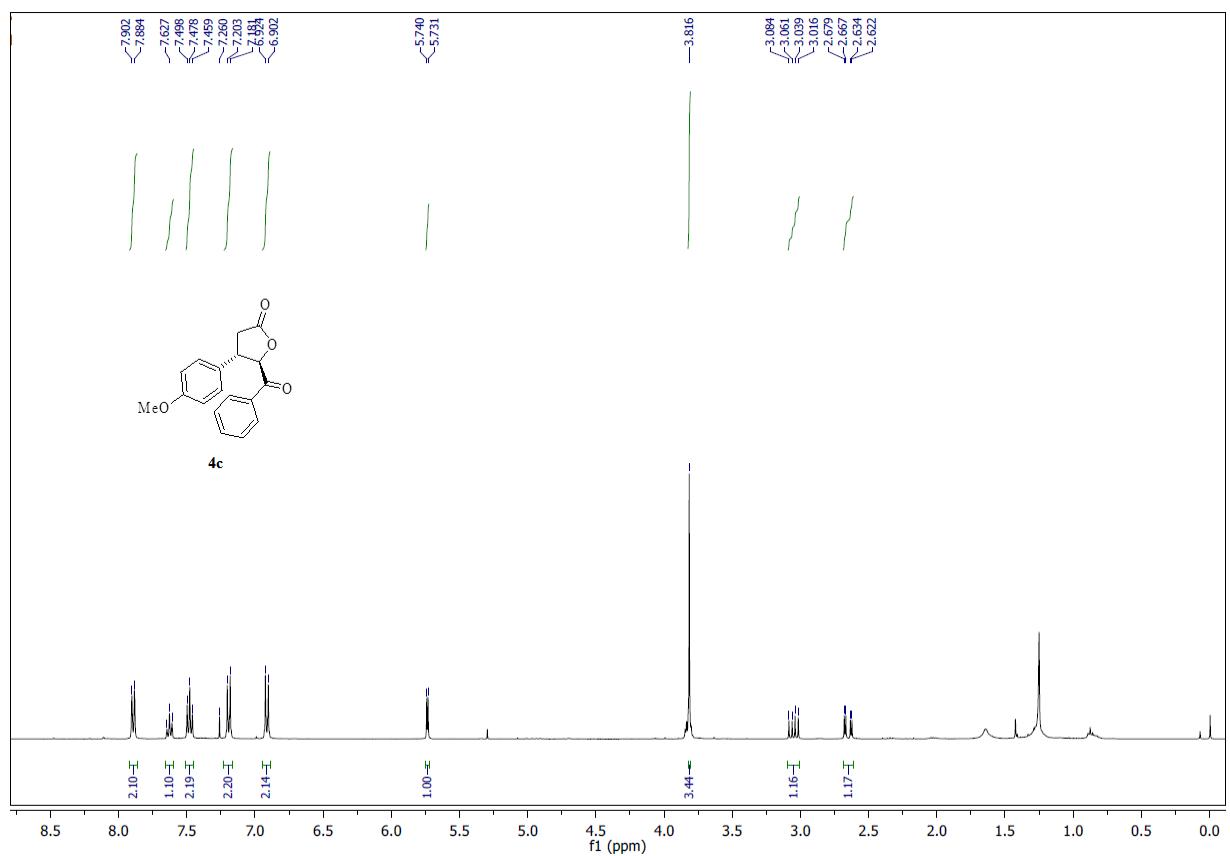
3. NMR spectra of the products:

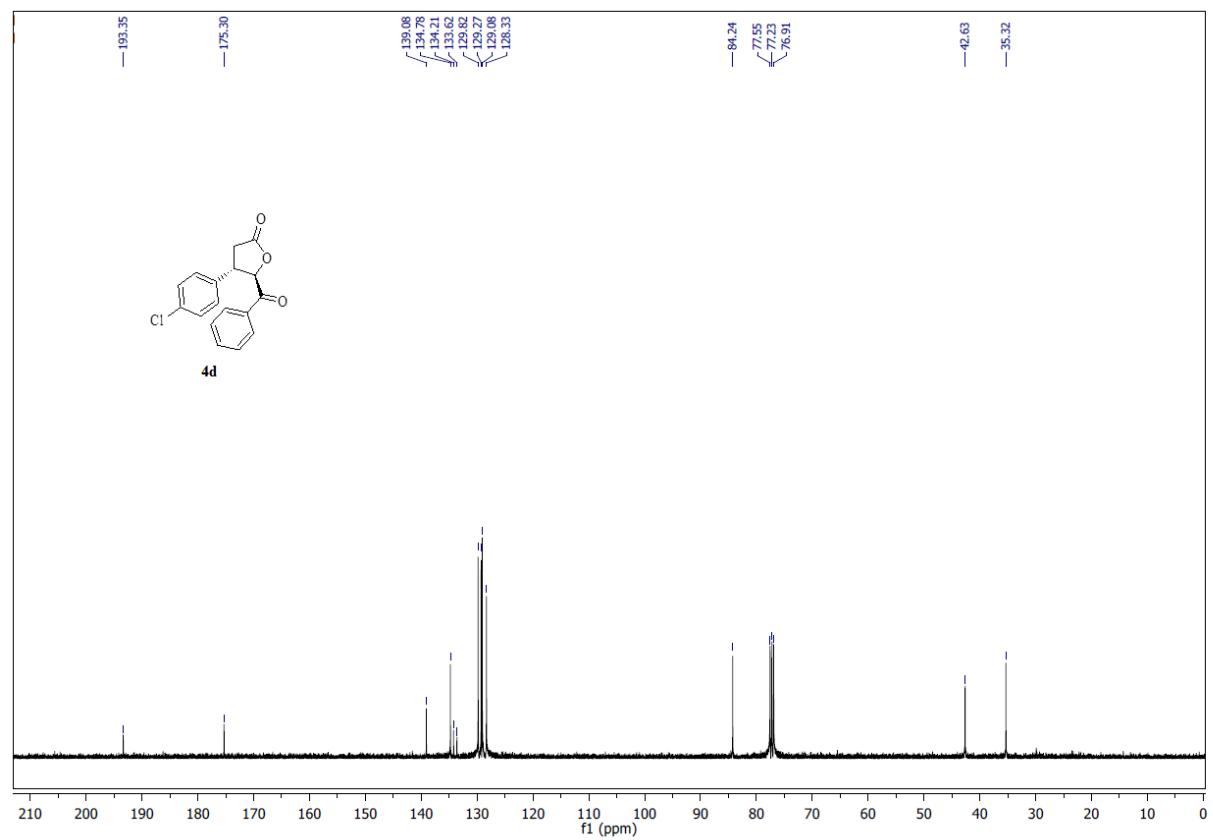
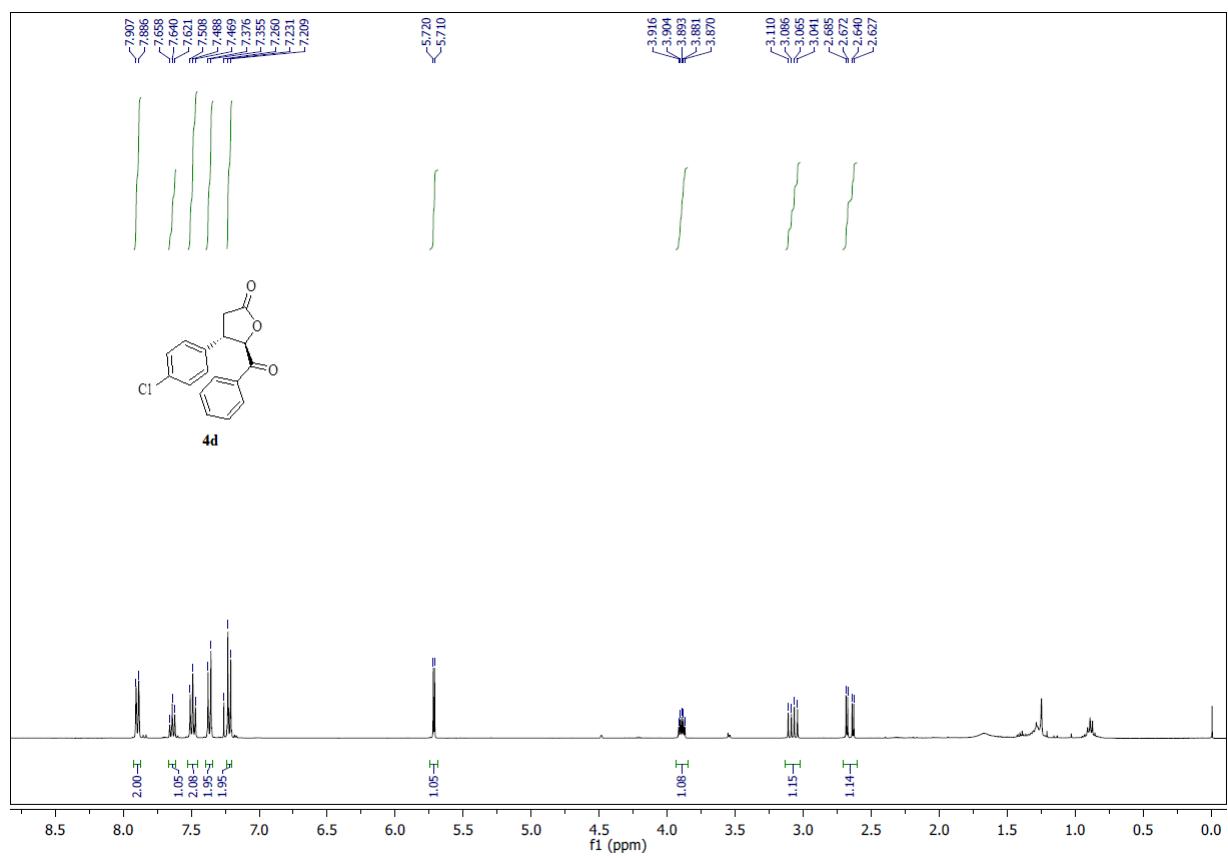


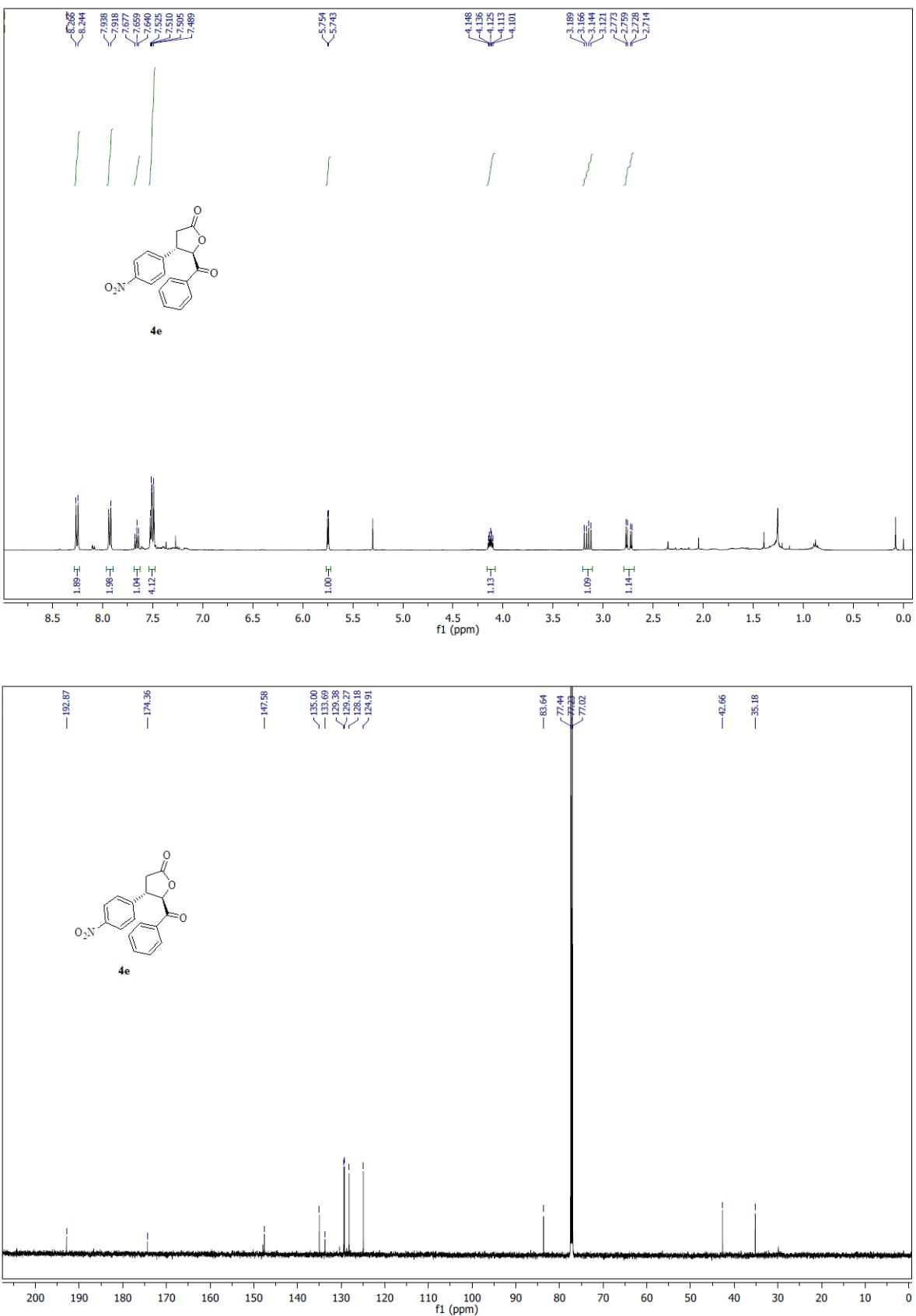


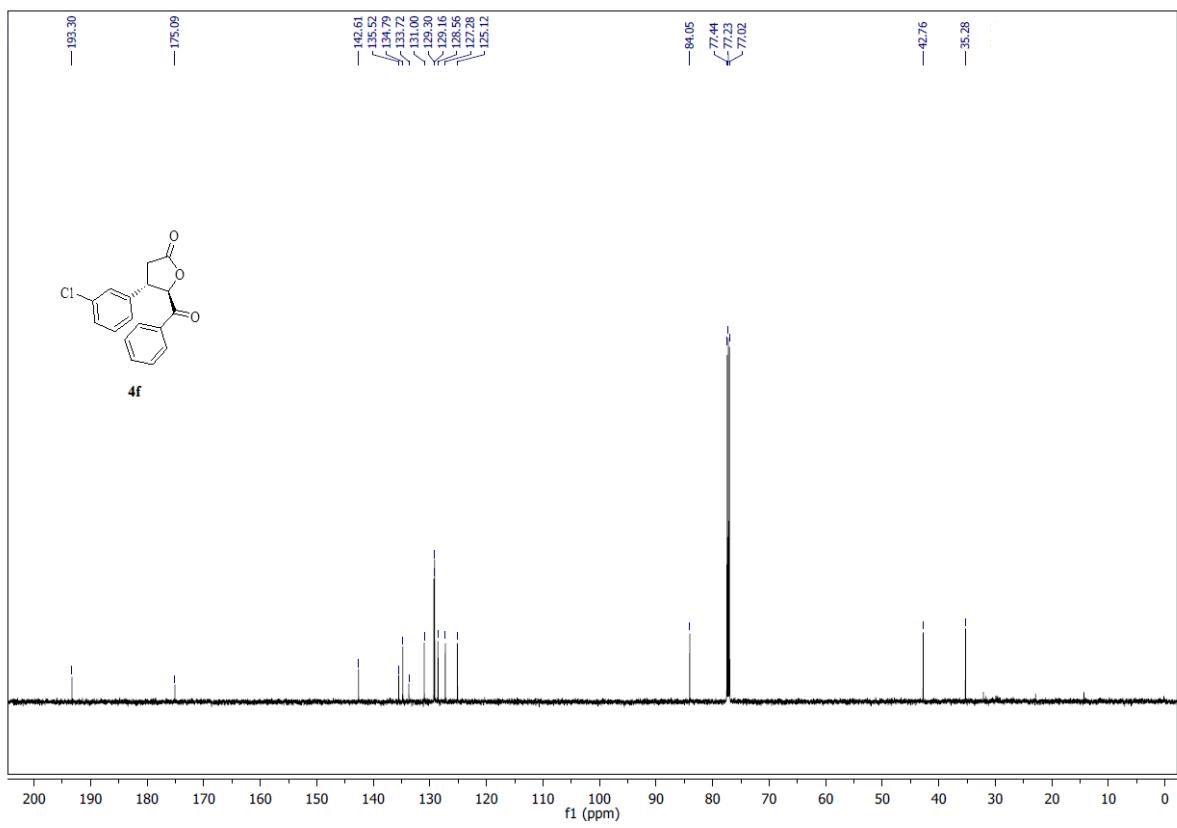
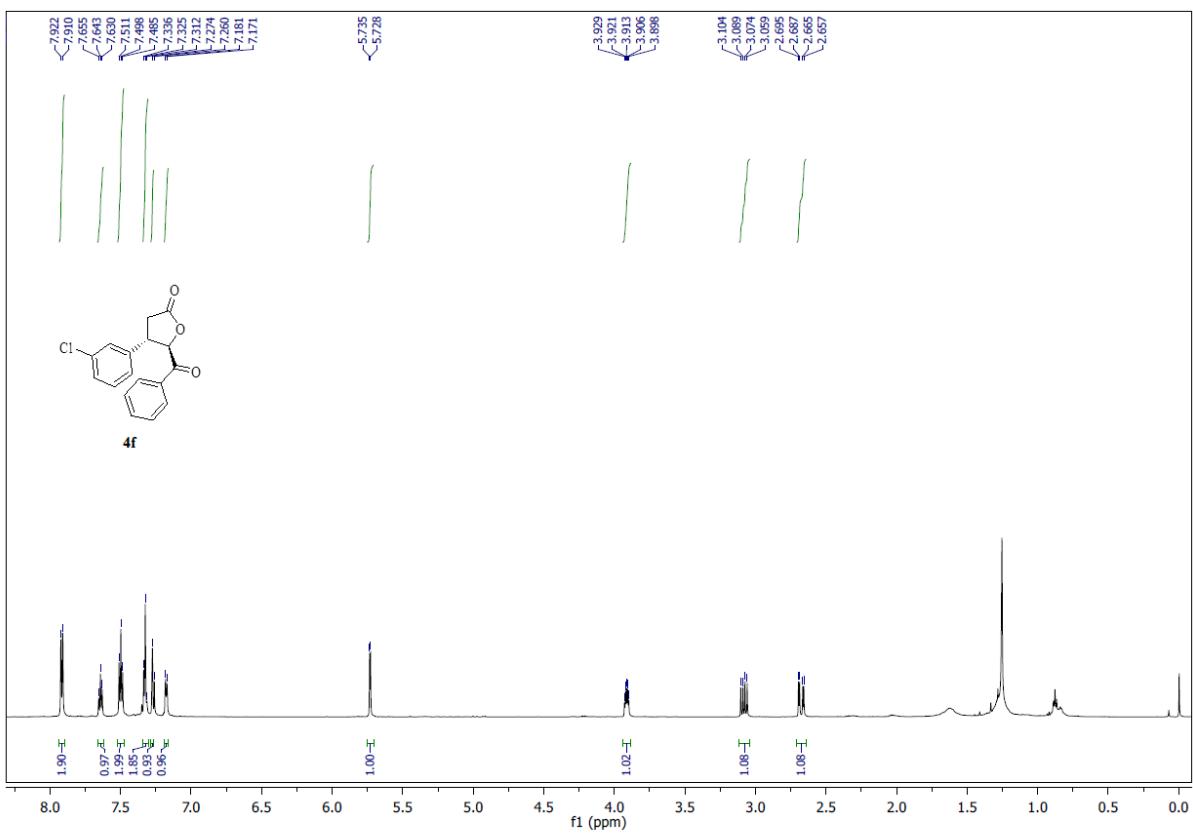


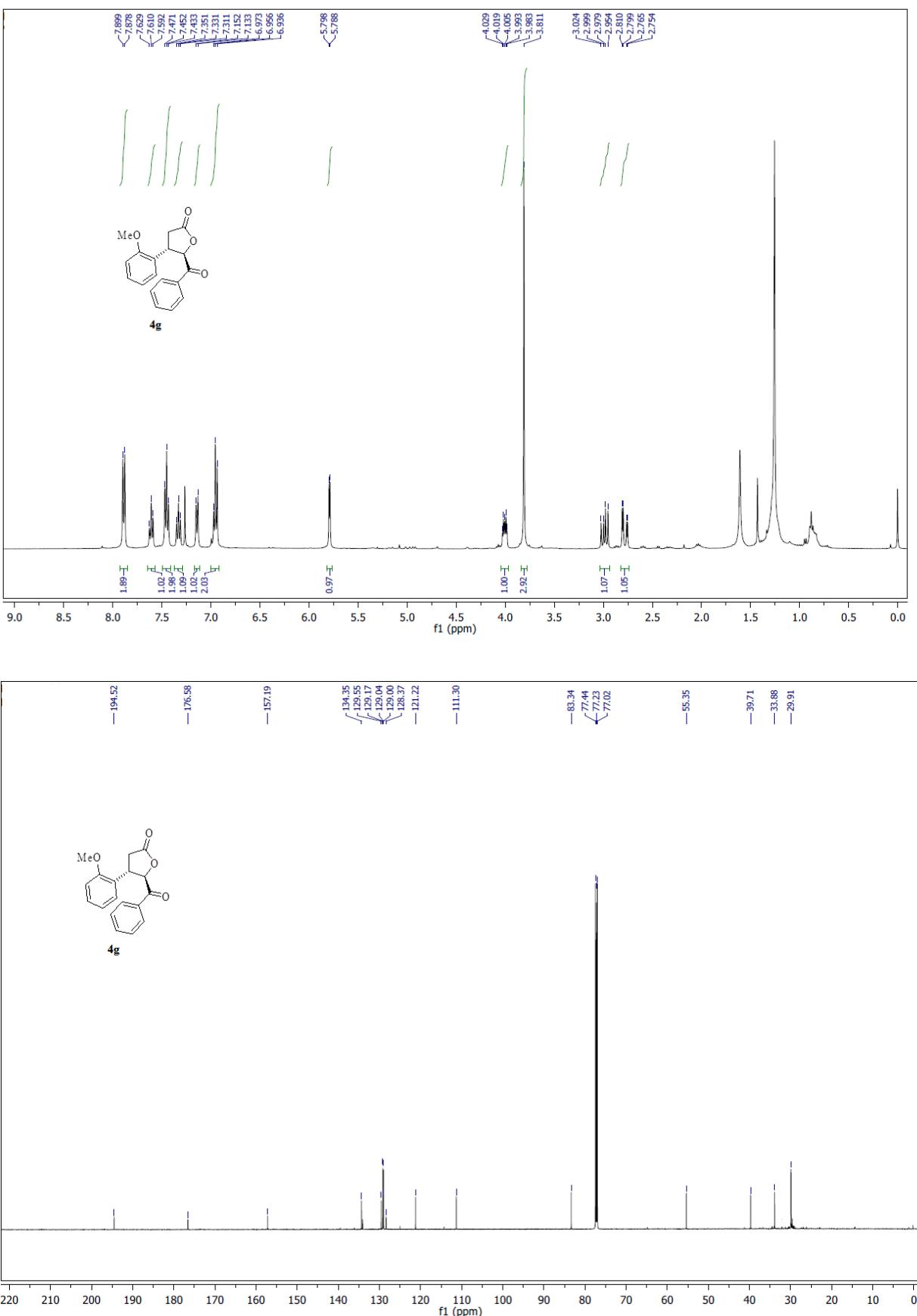


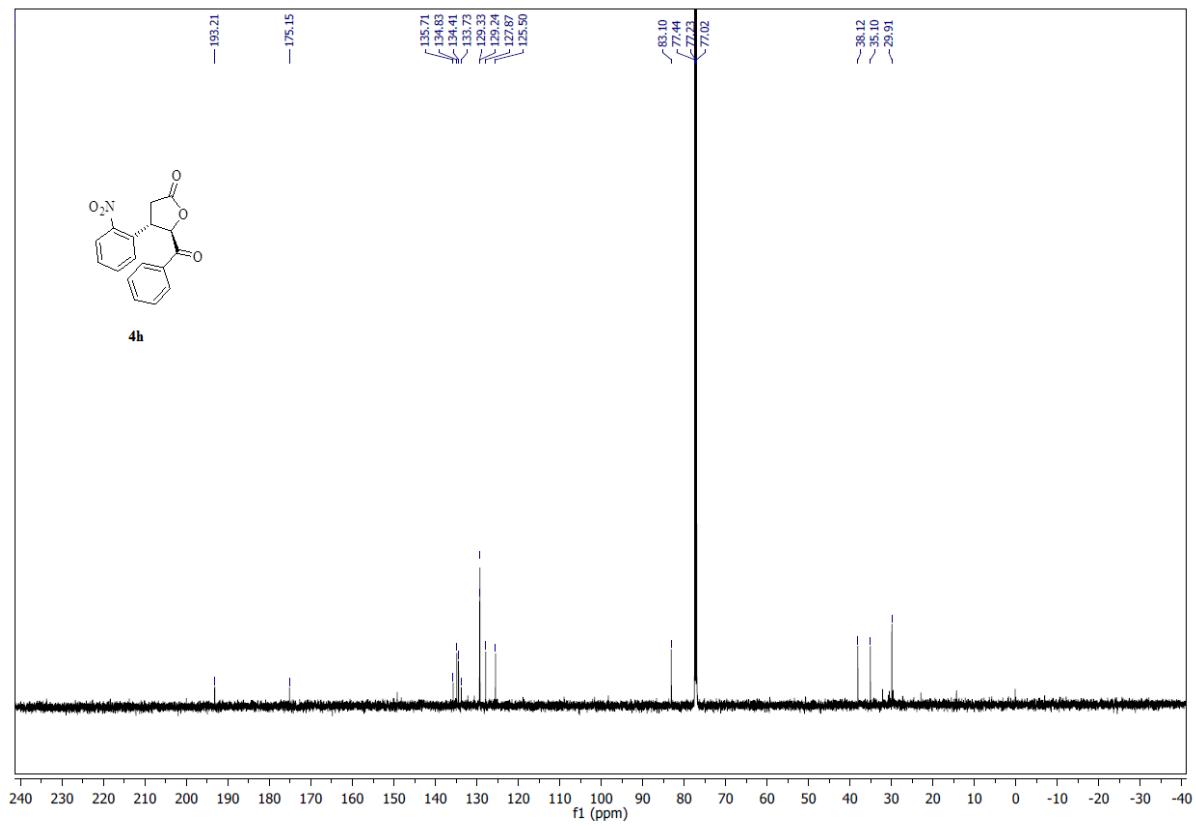
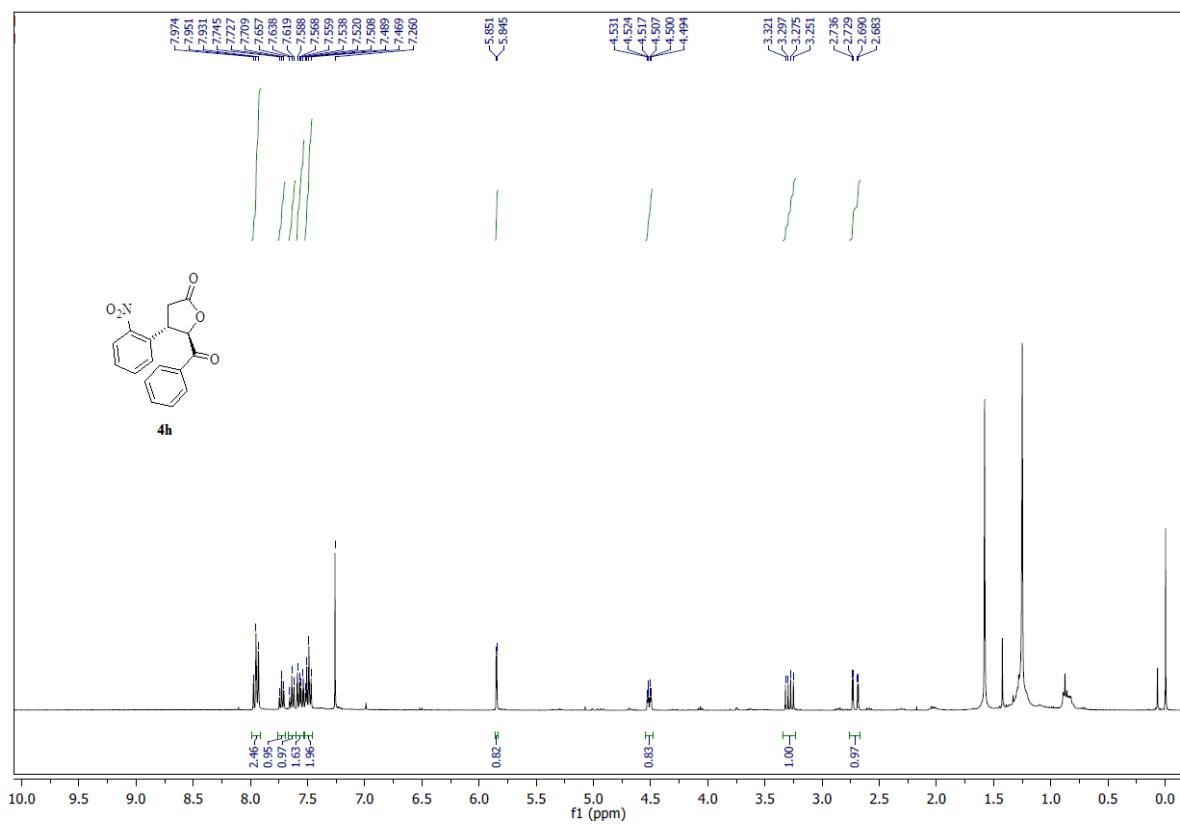


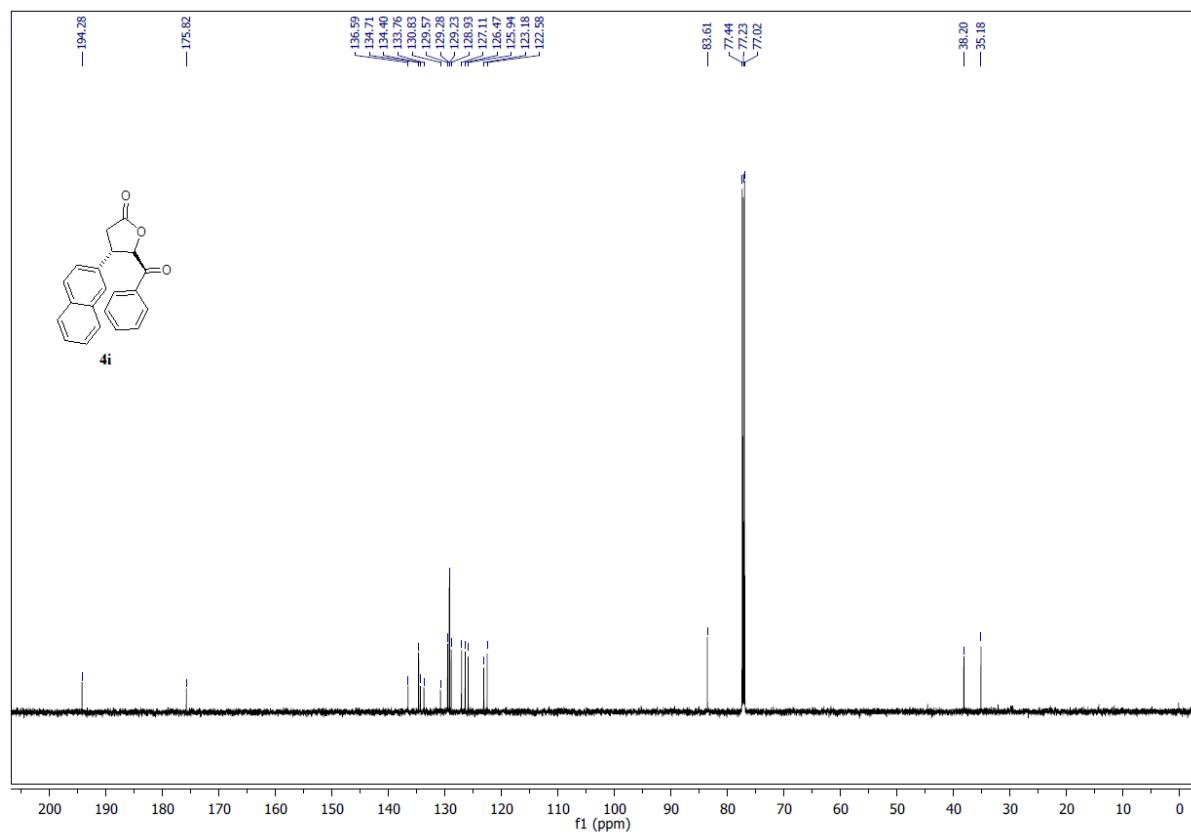
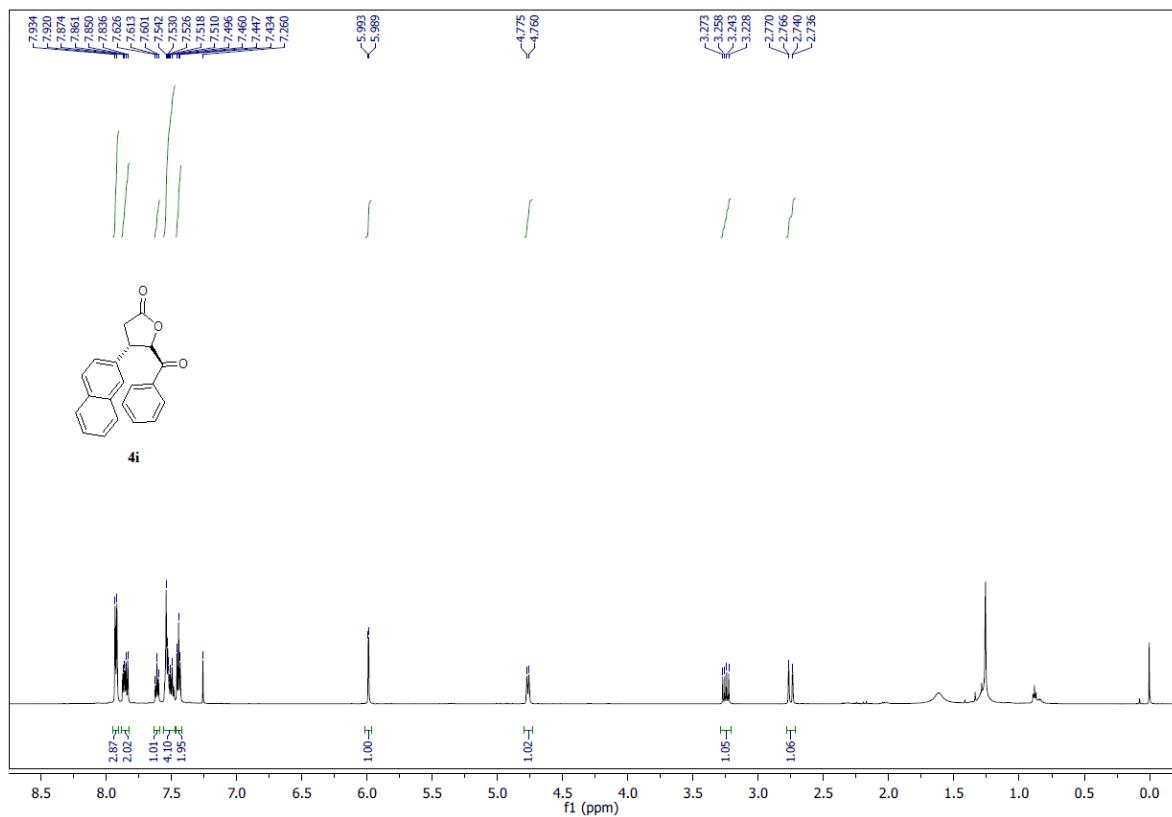


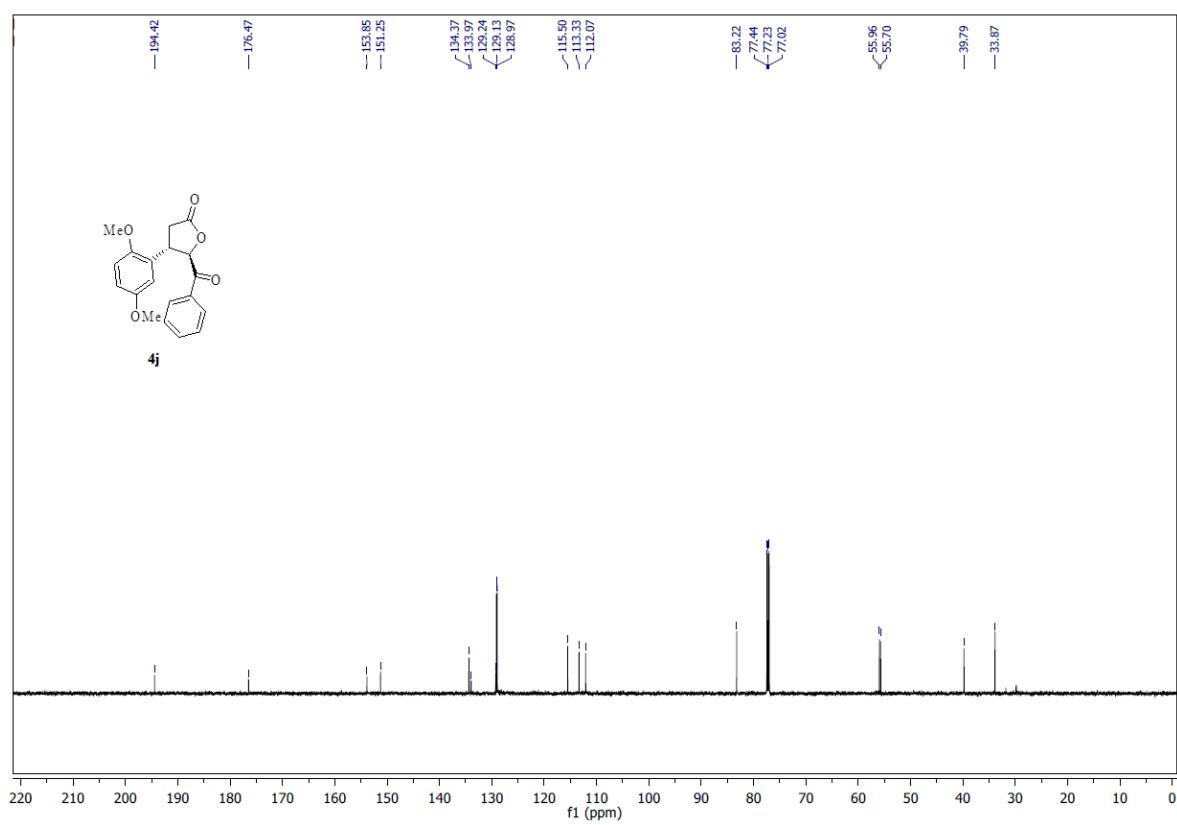
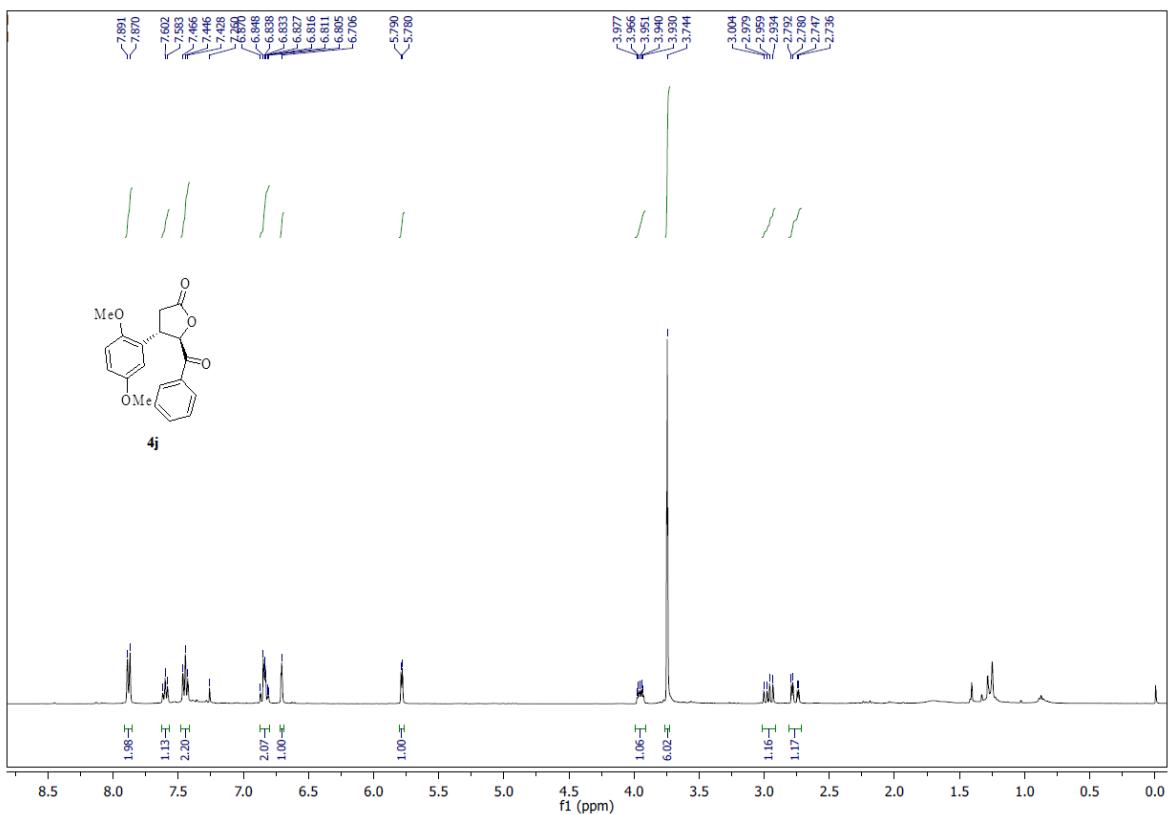


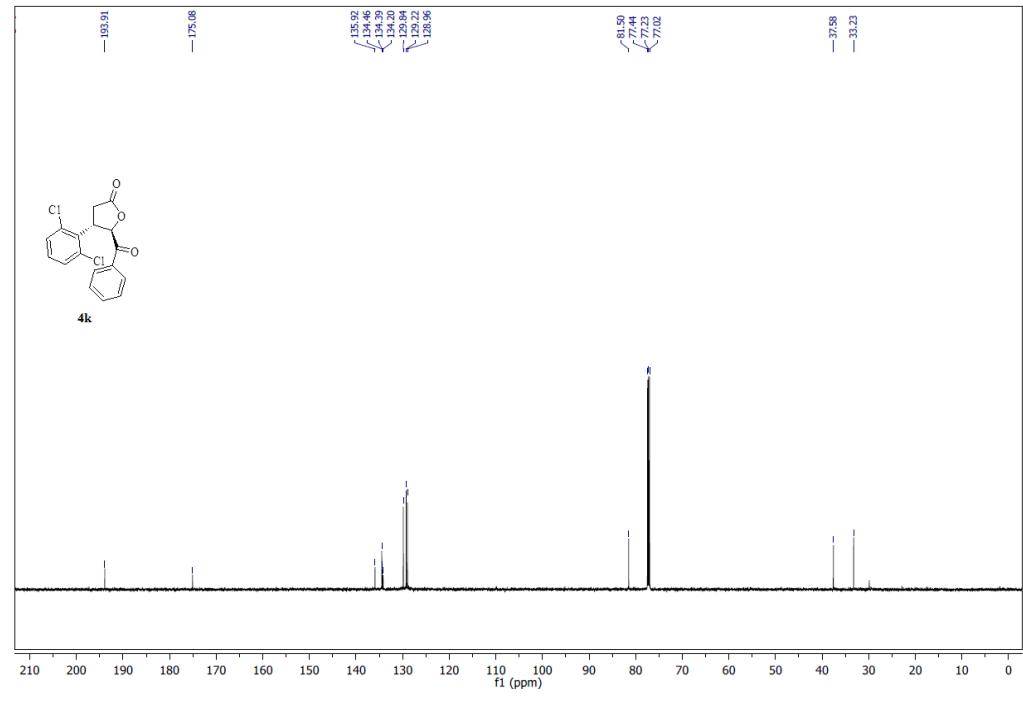
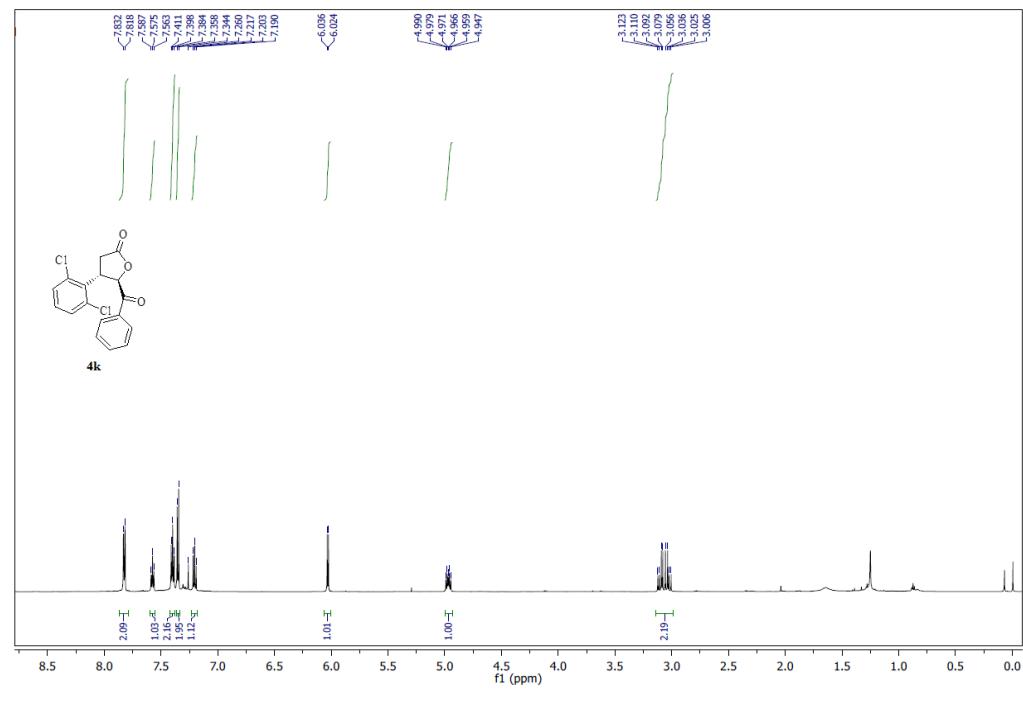


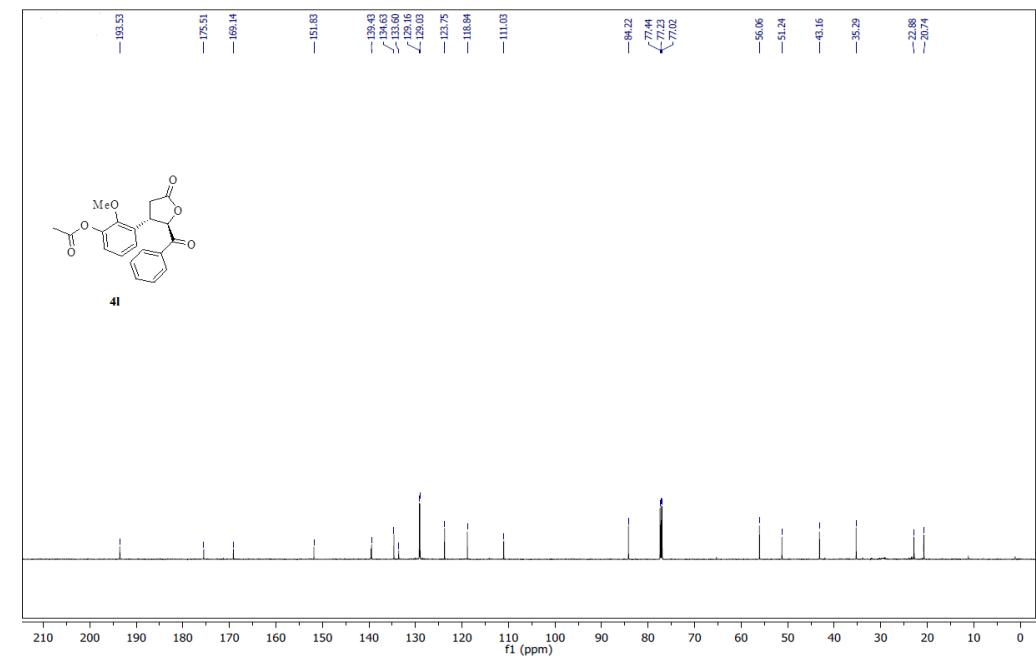
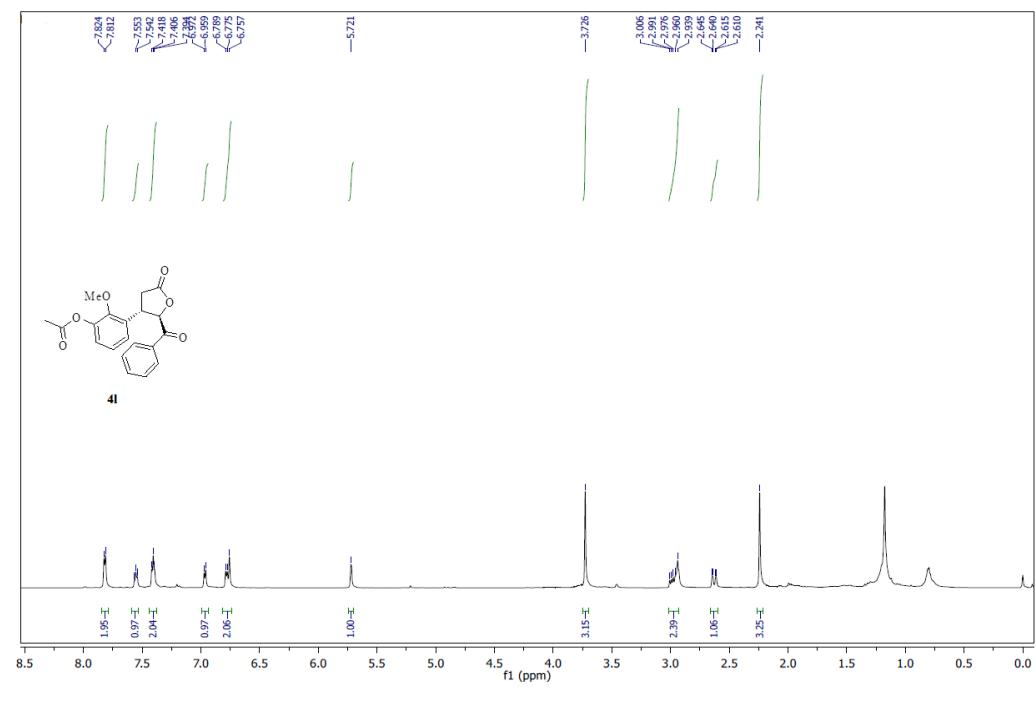


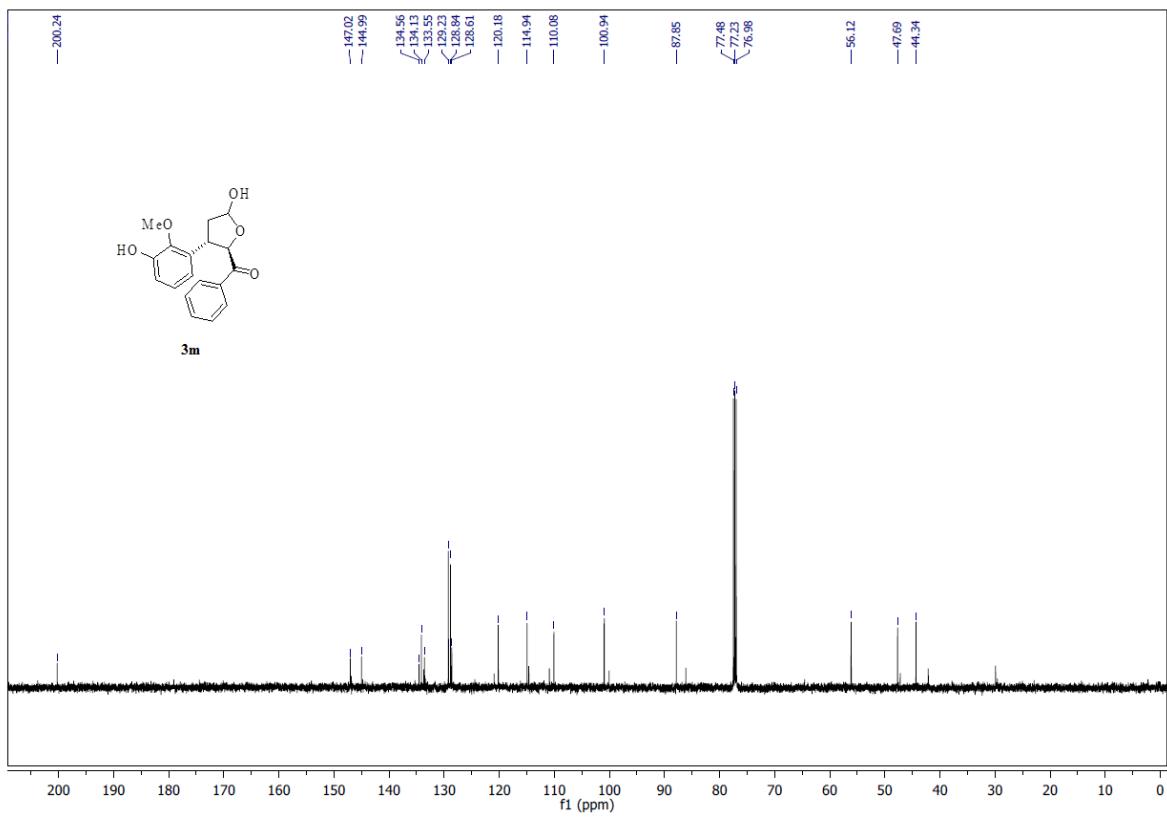
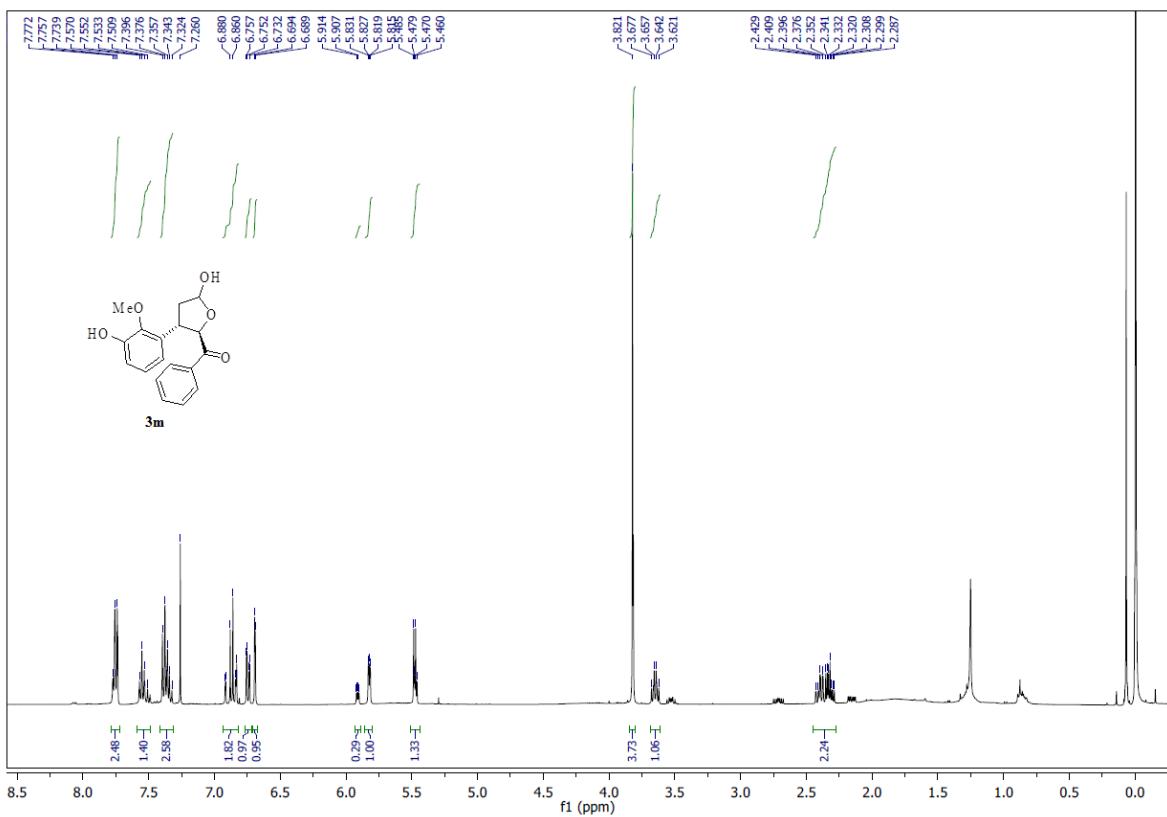


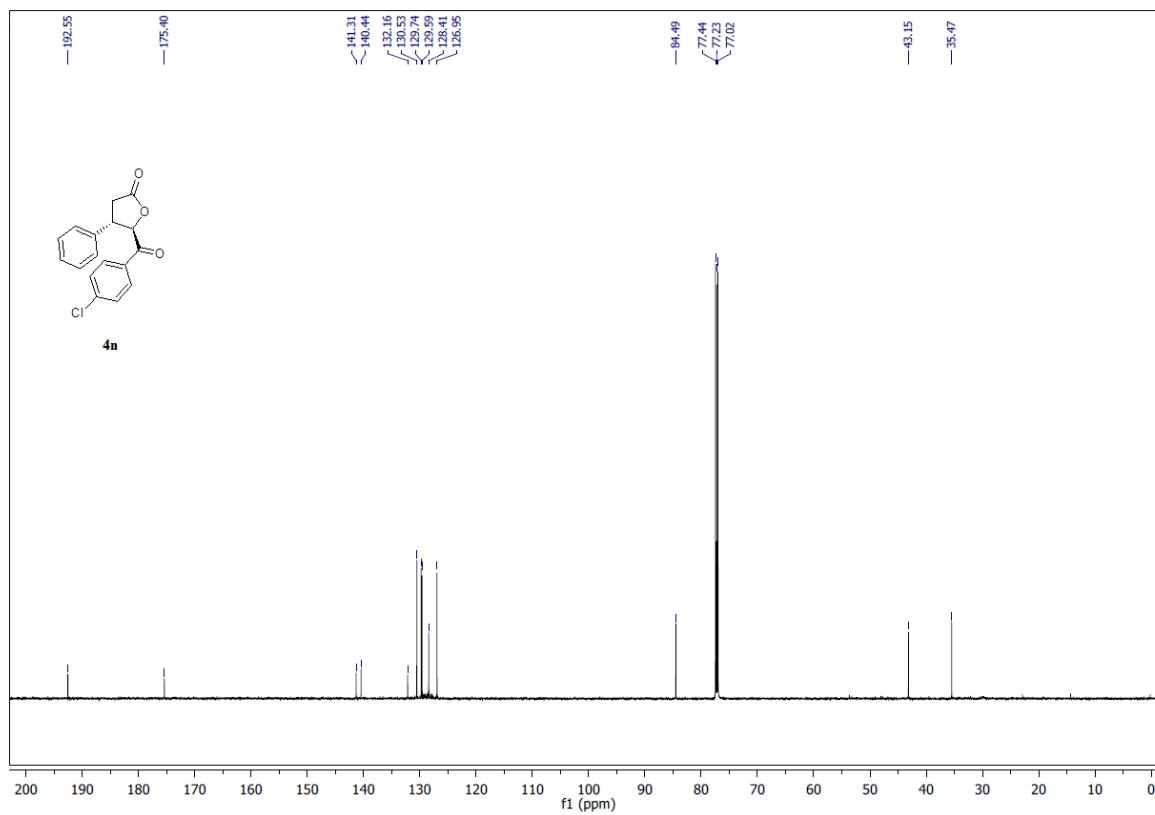
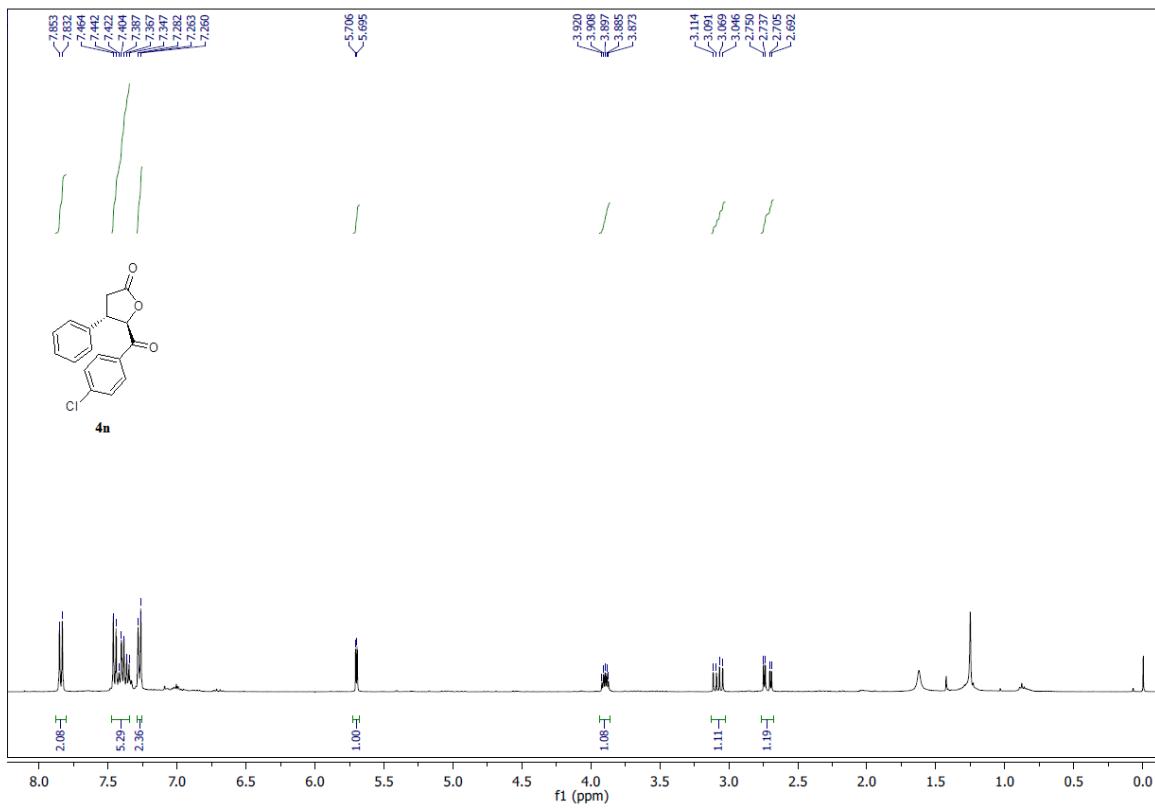


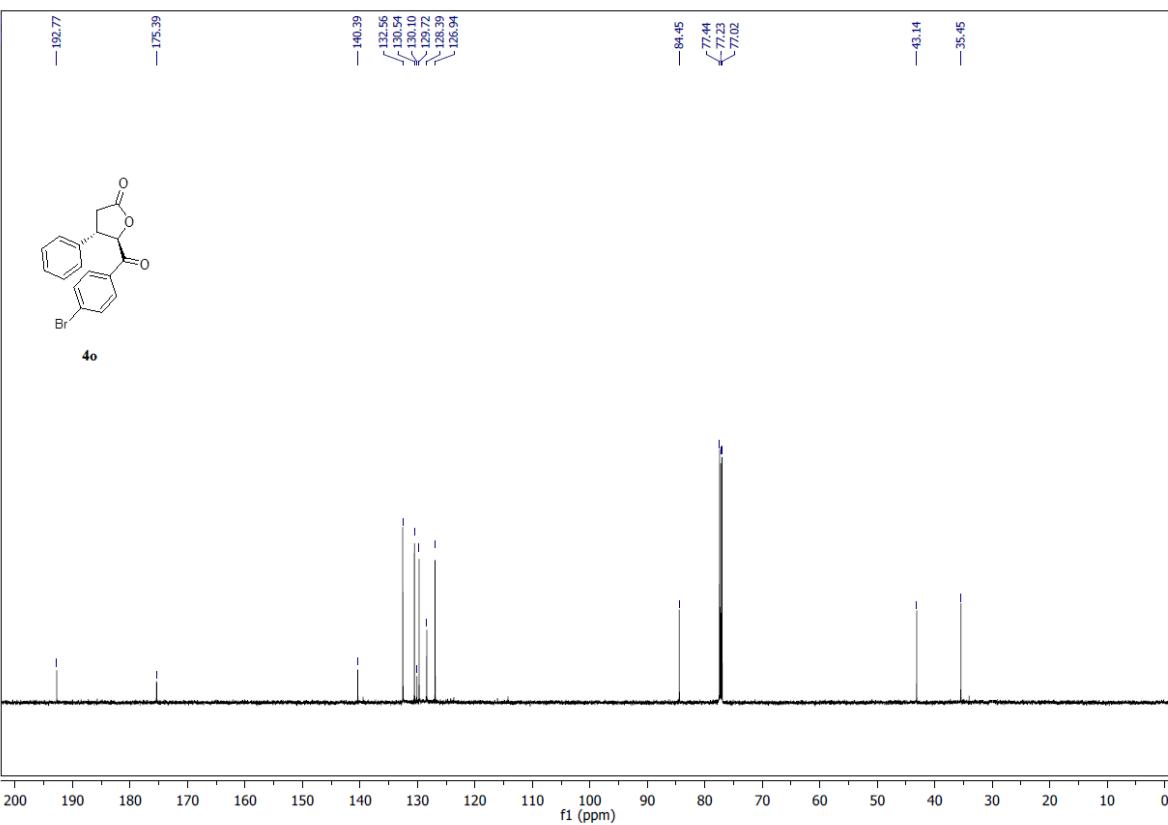
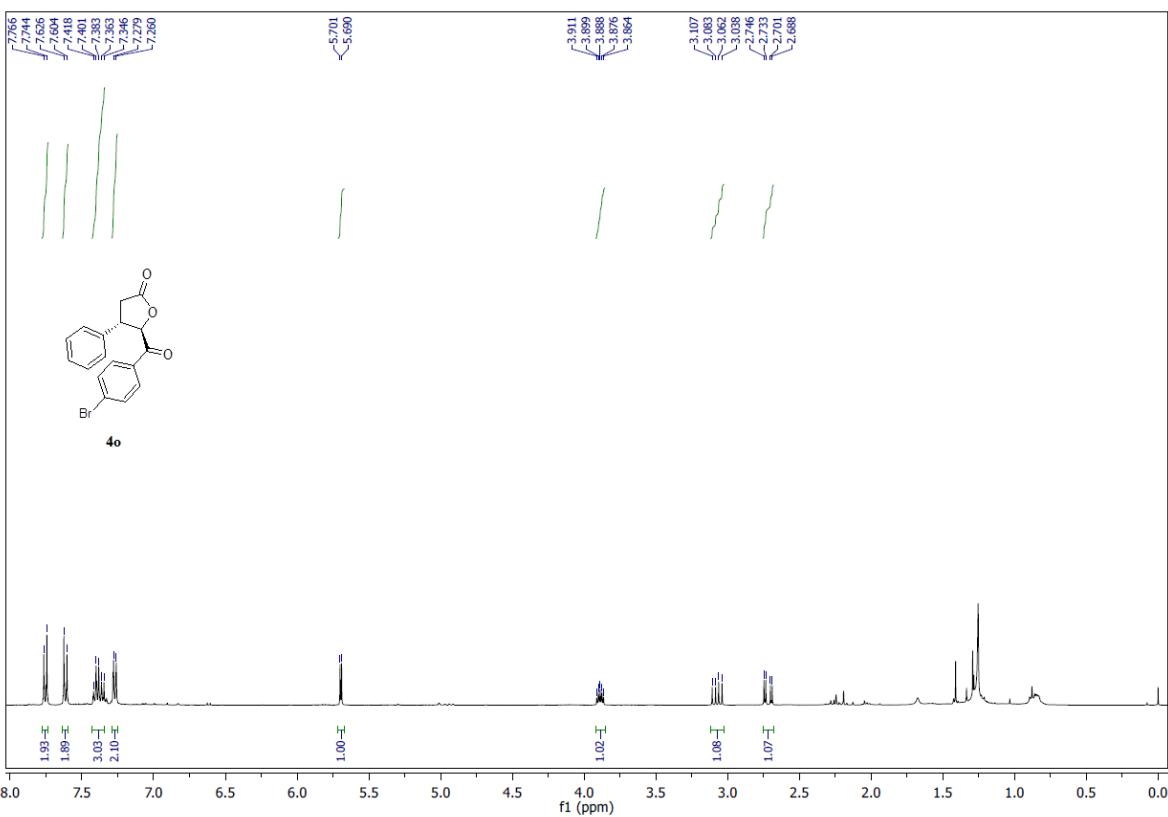


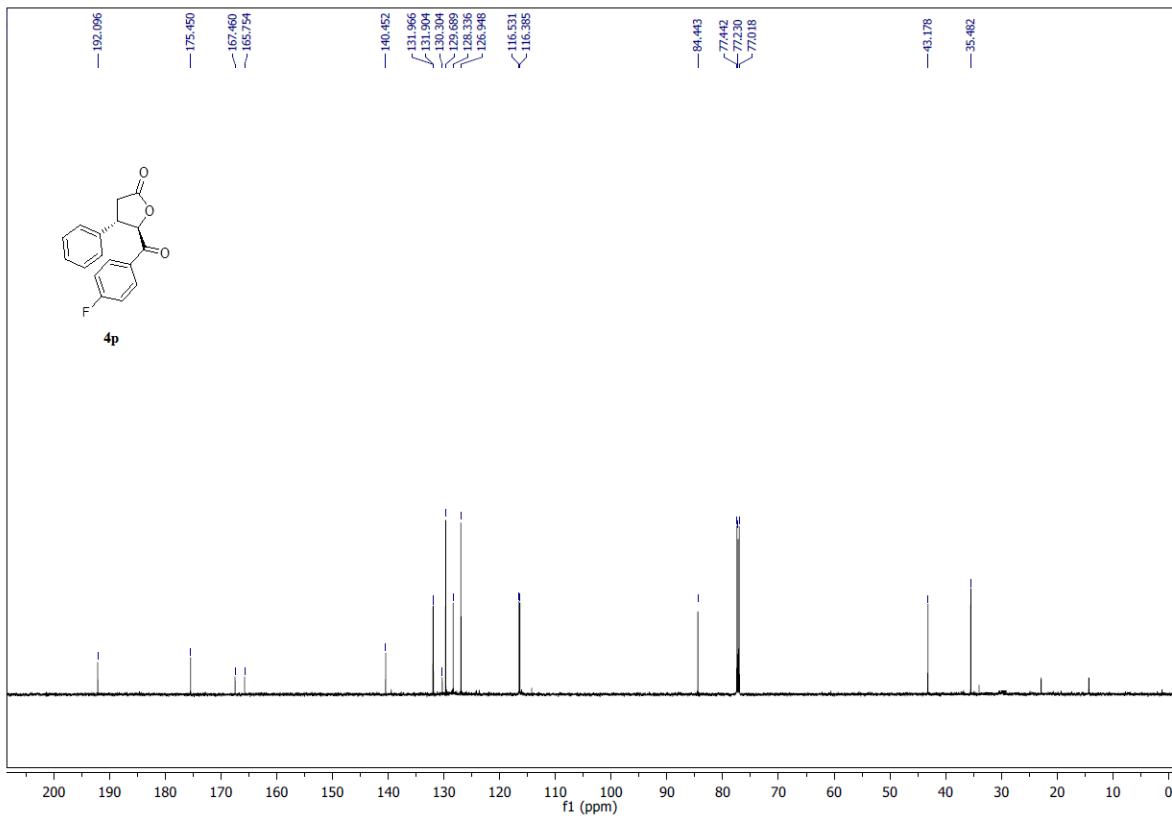
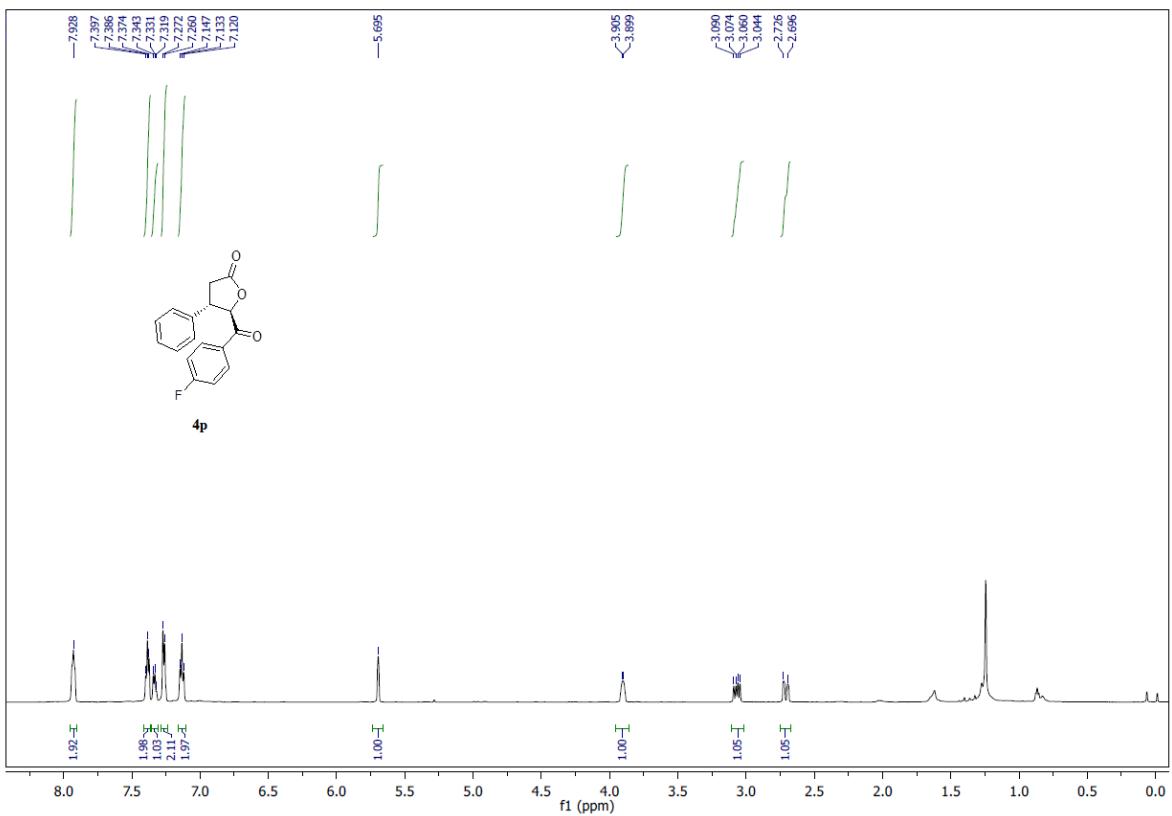


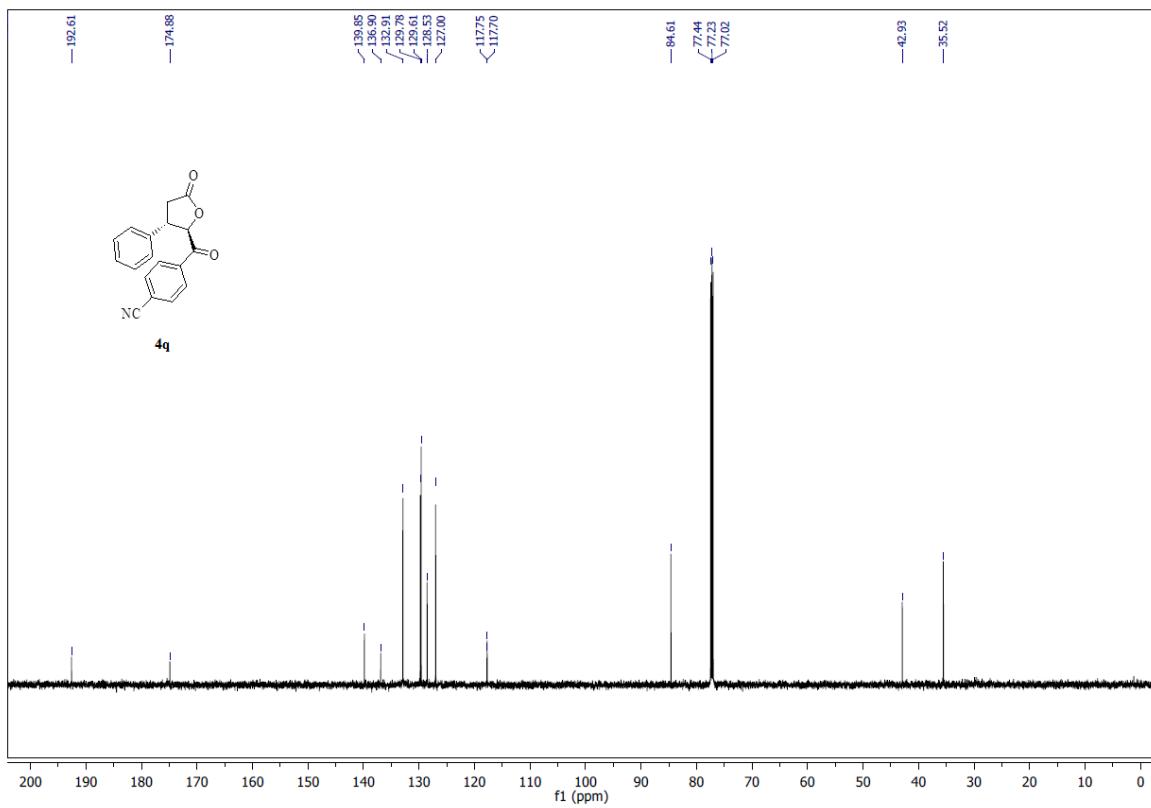
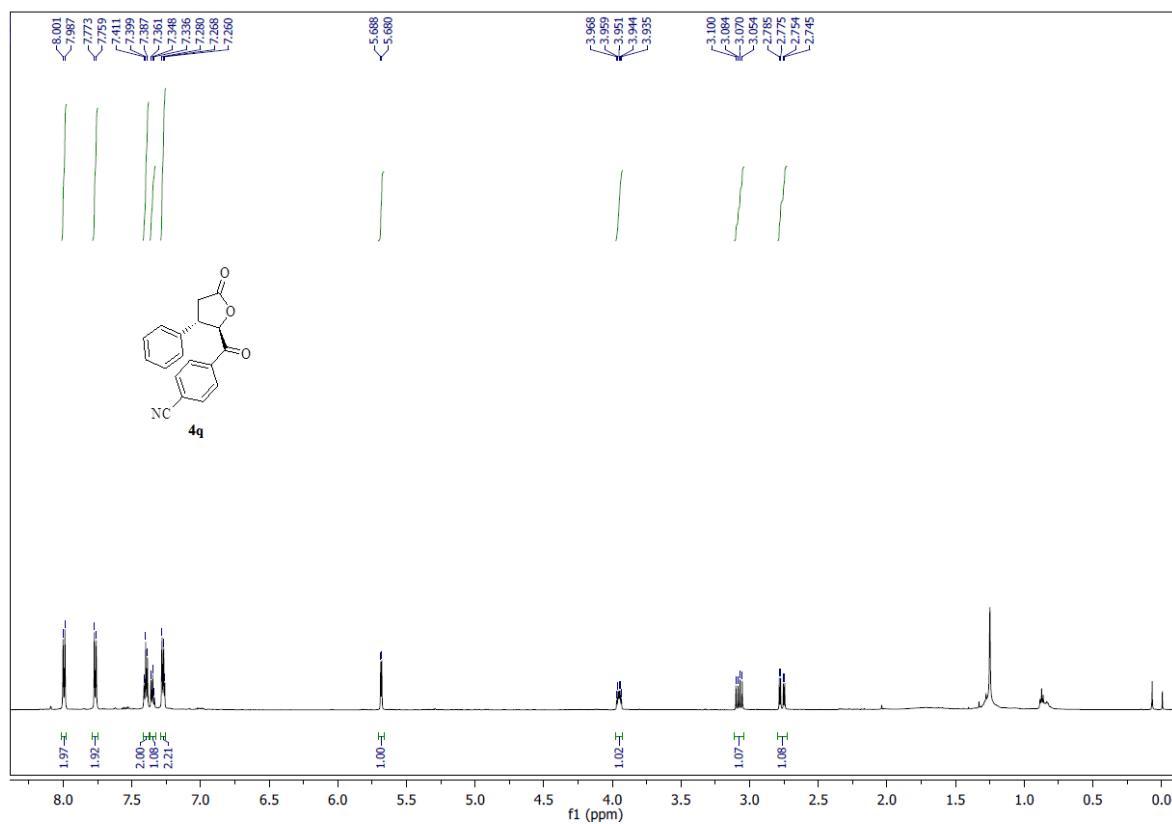


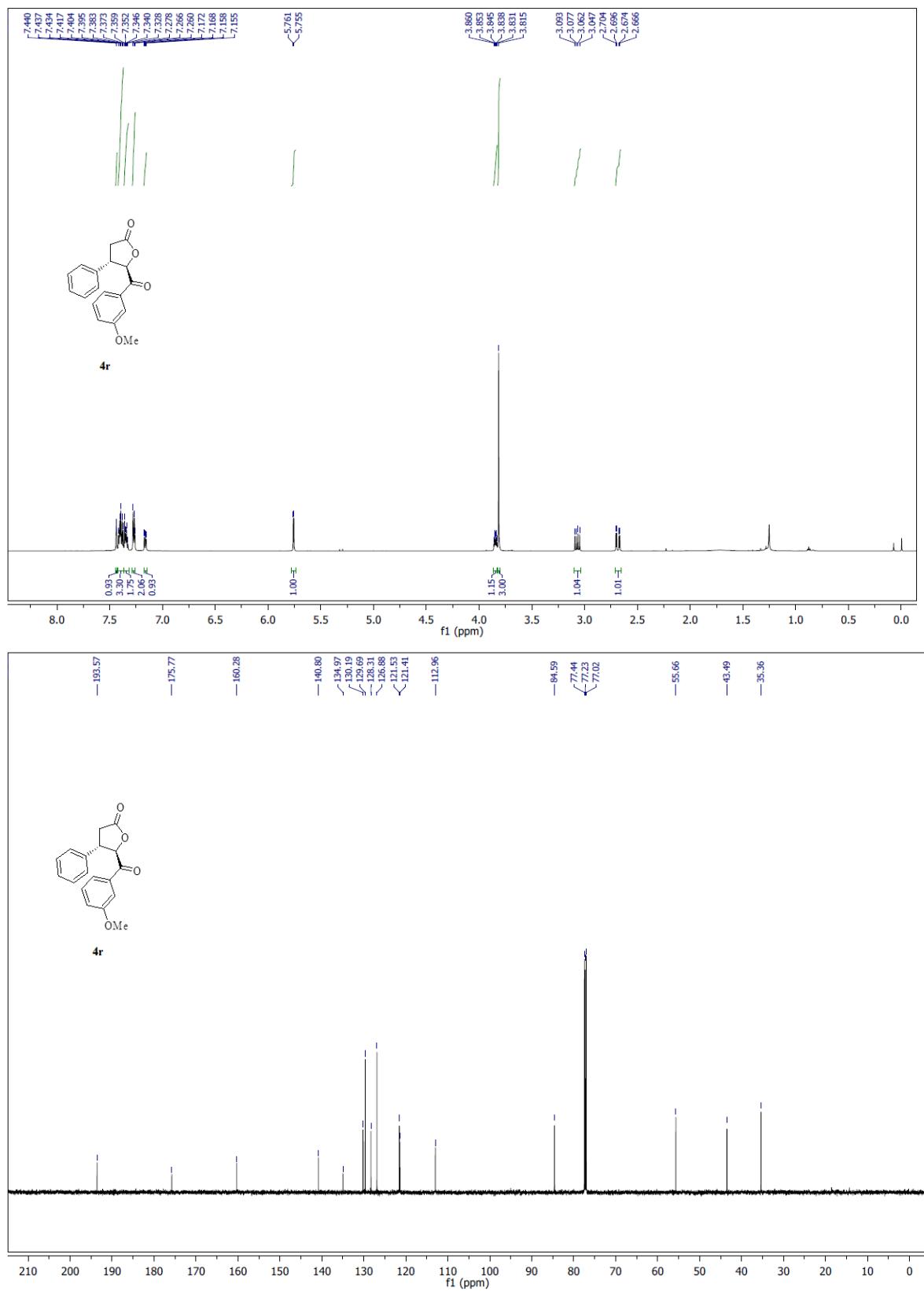


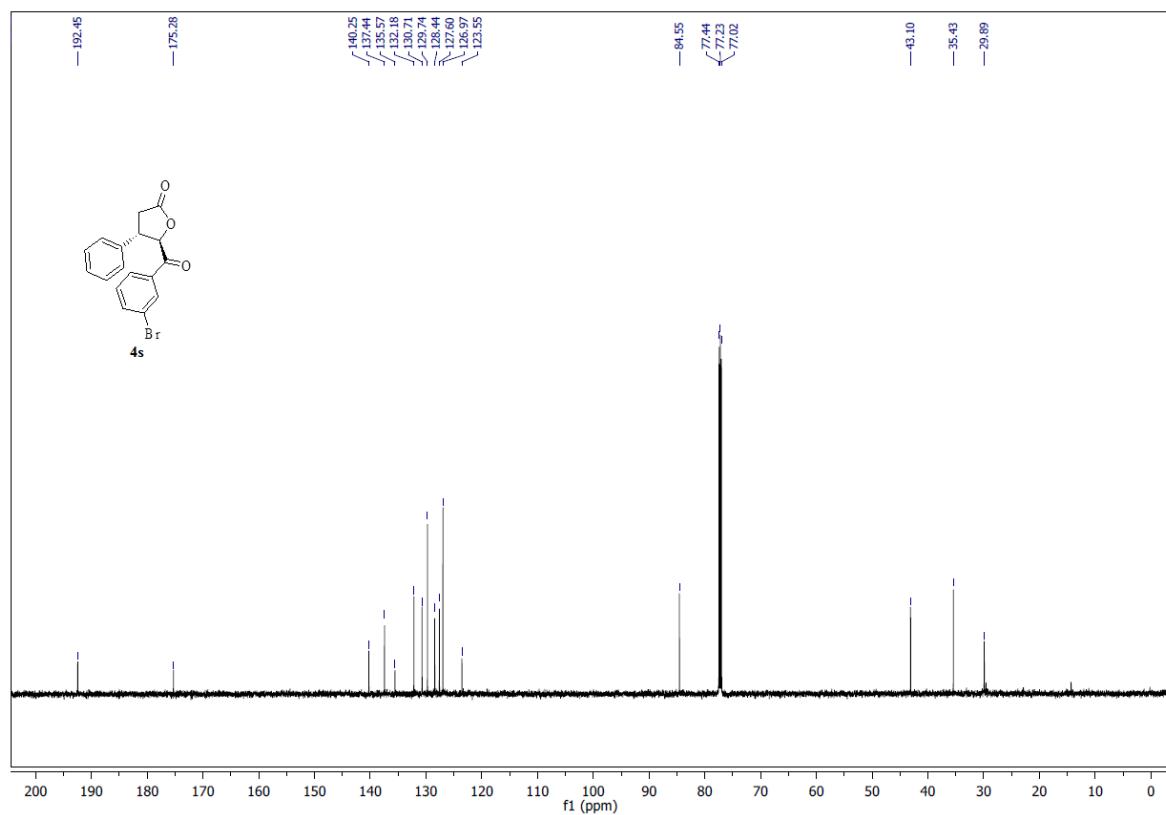
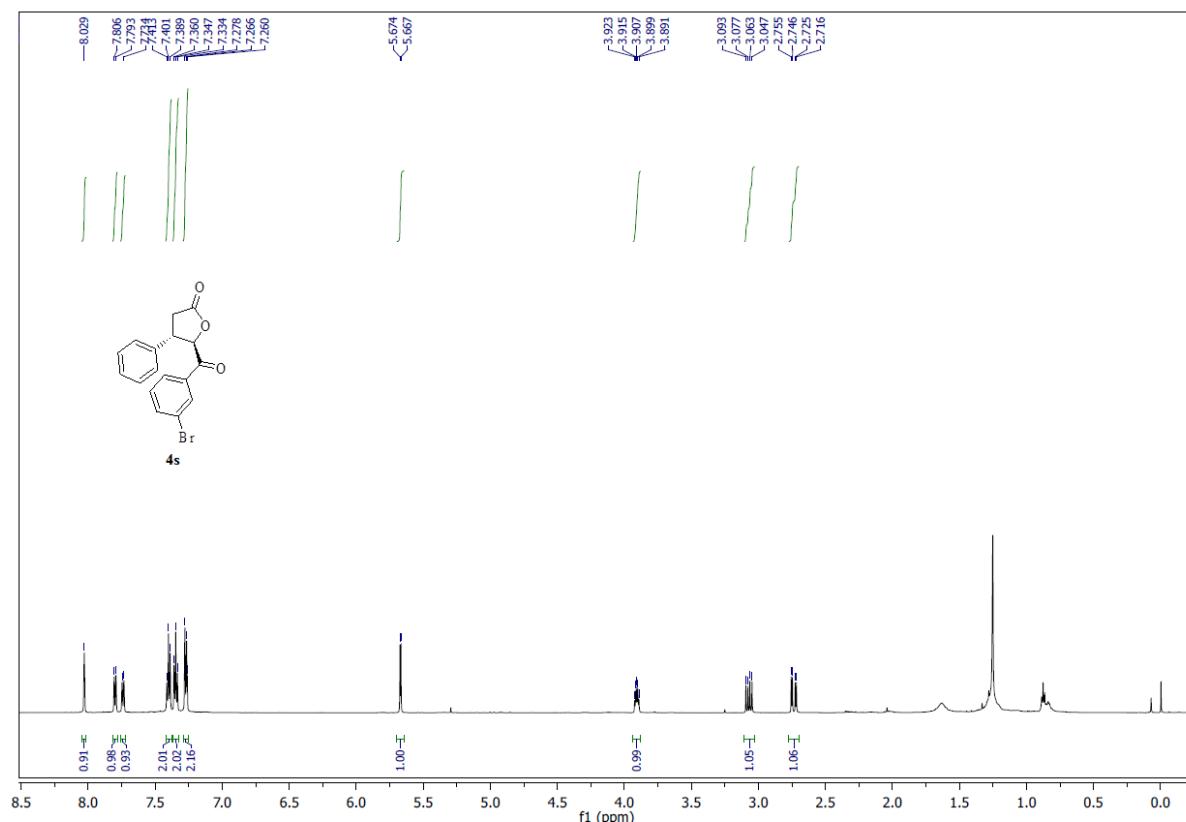


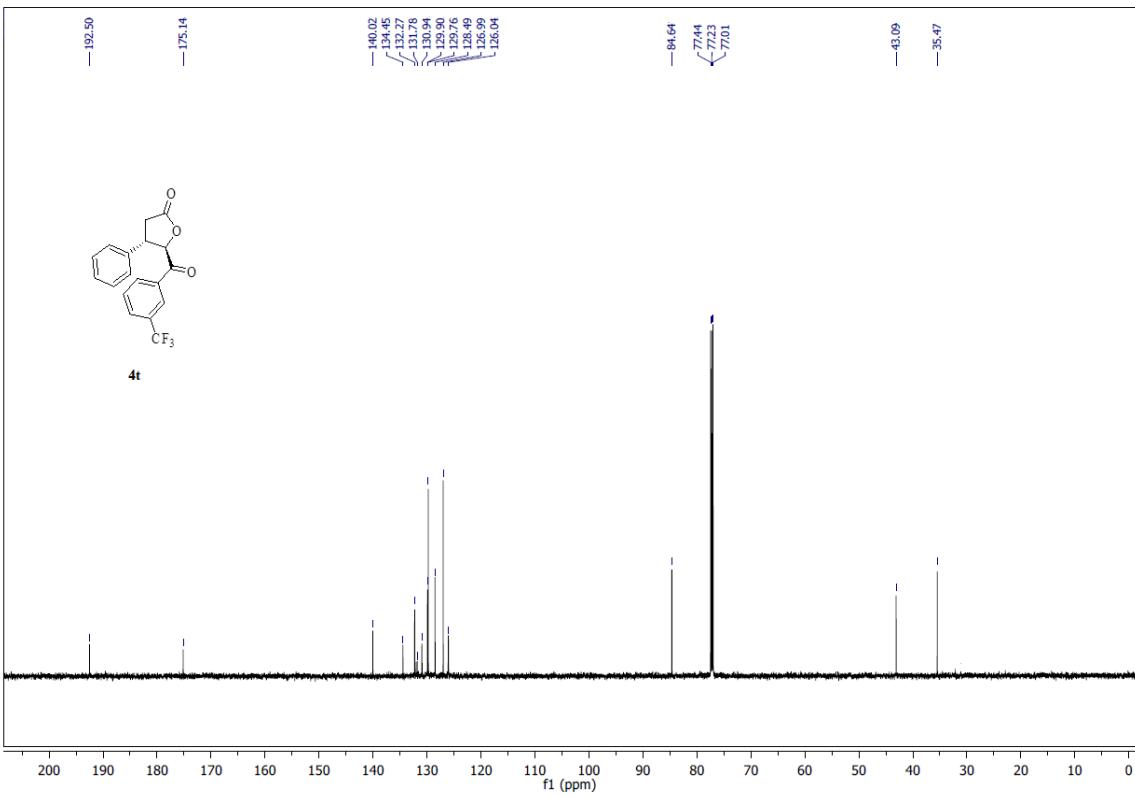
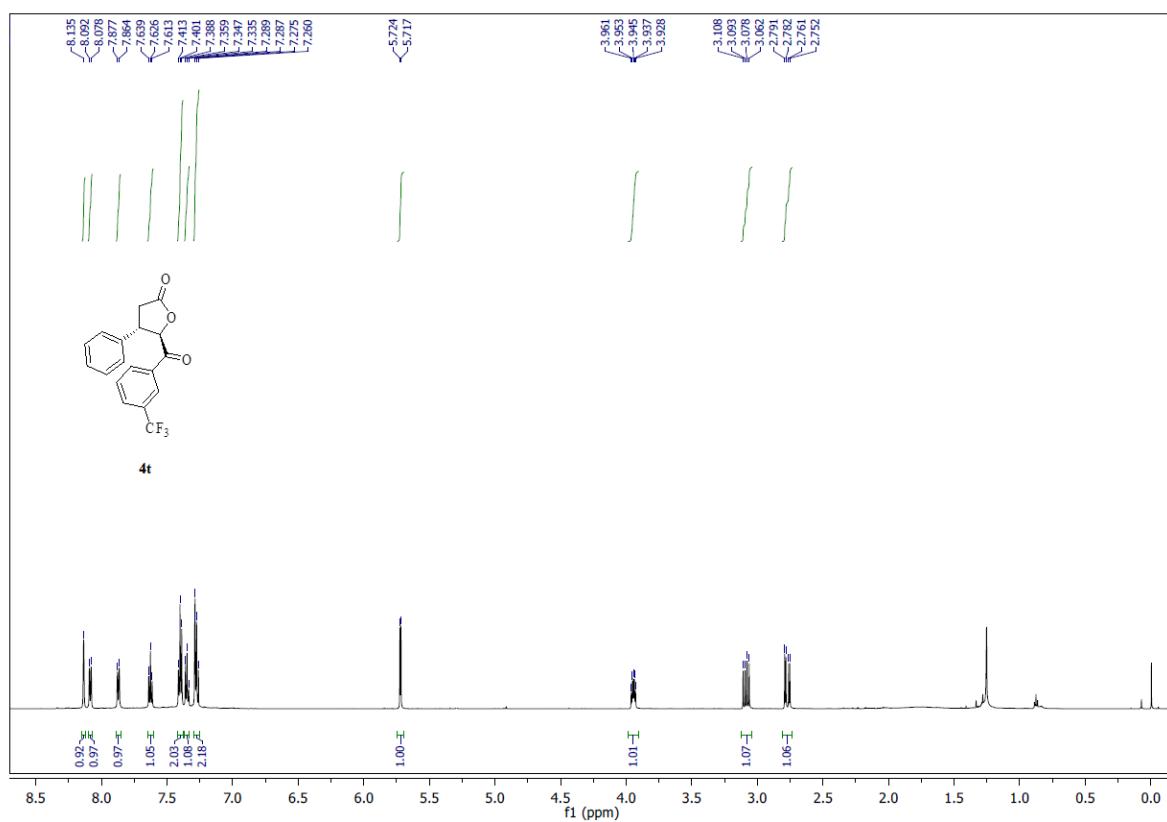


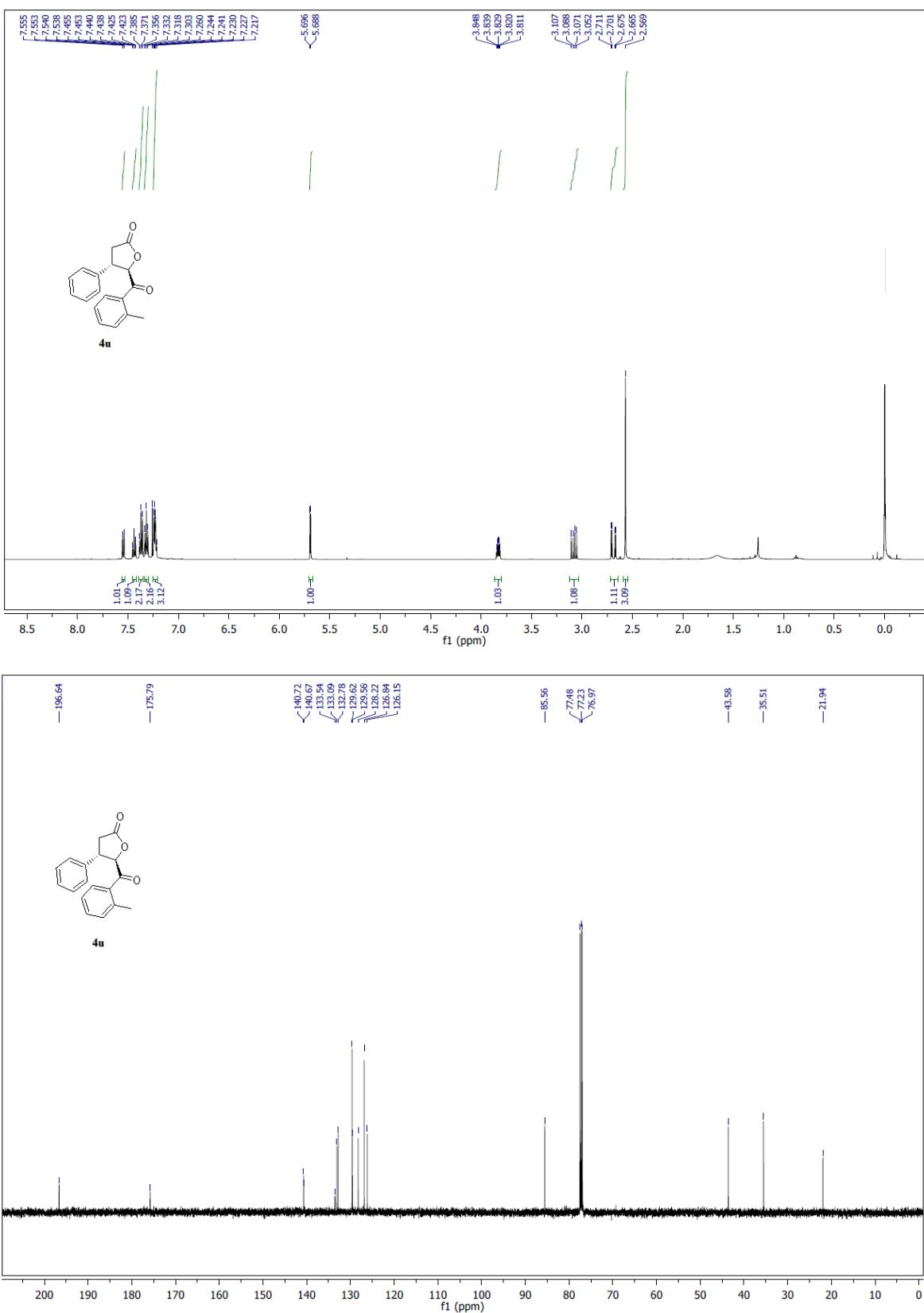


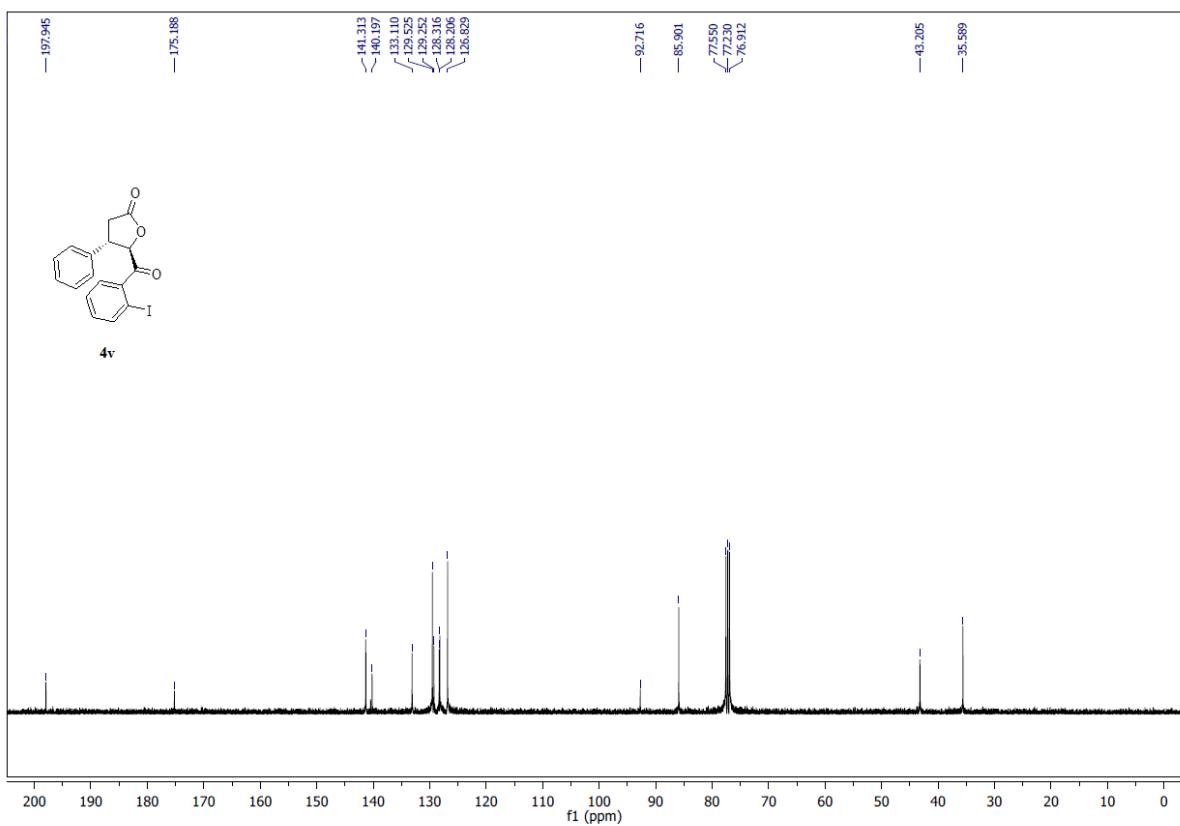
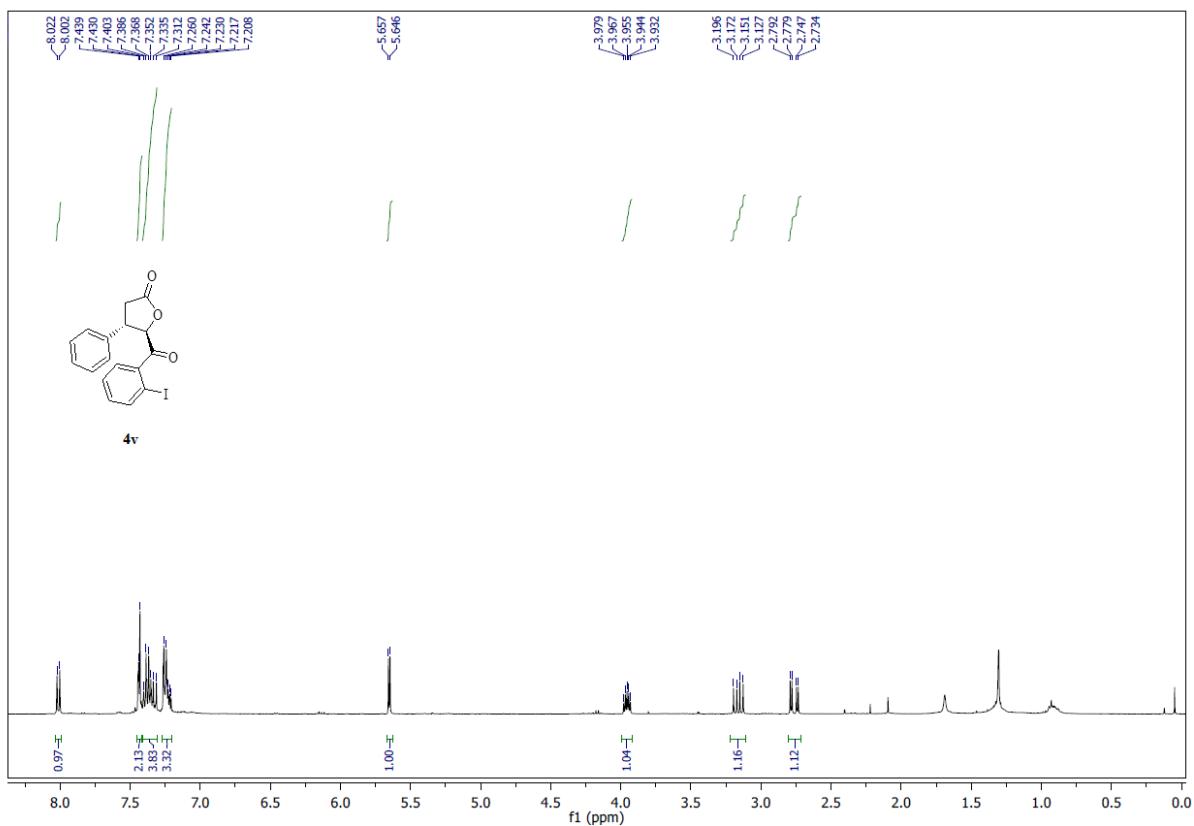


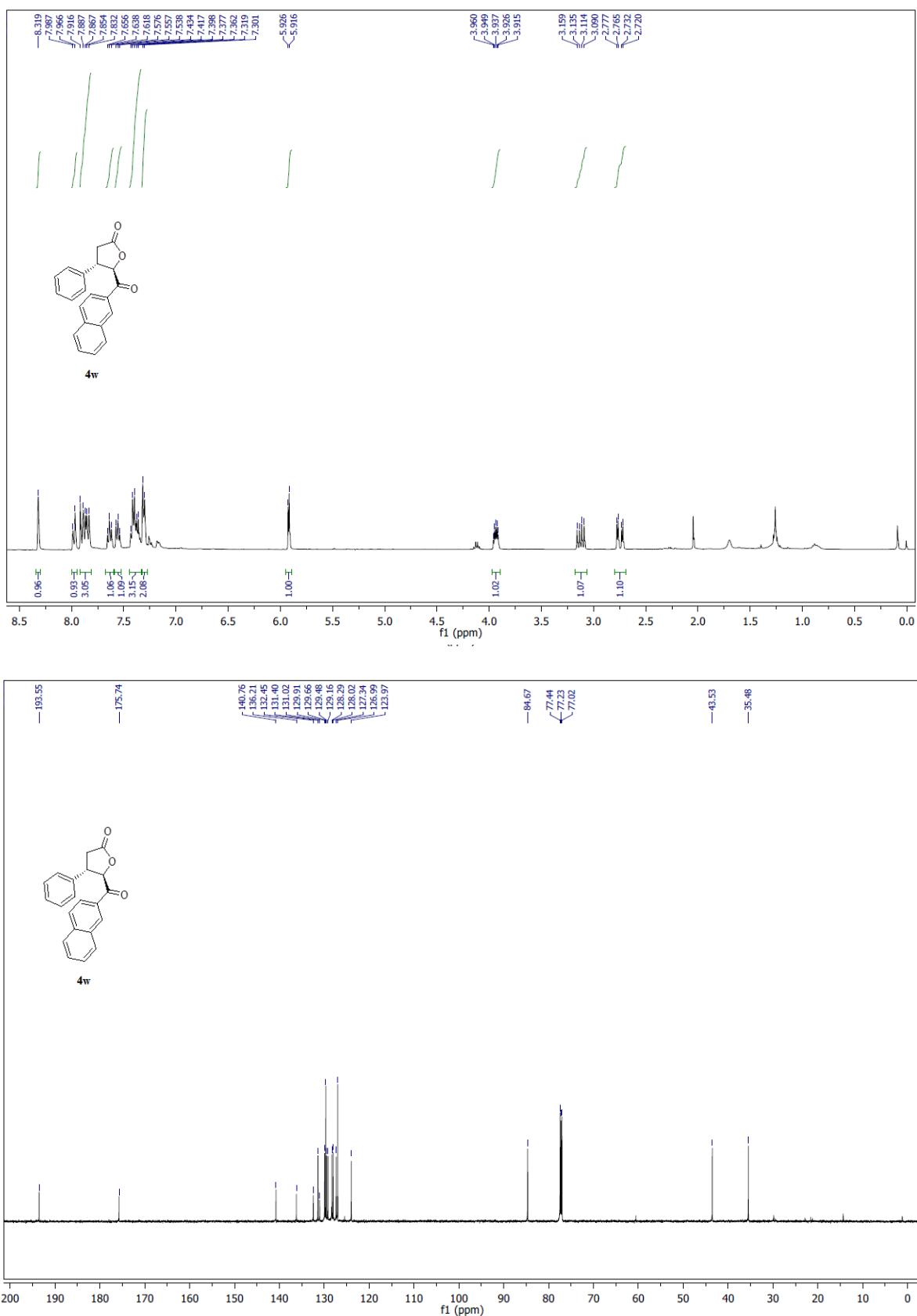


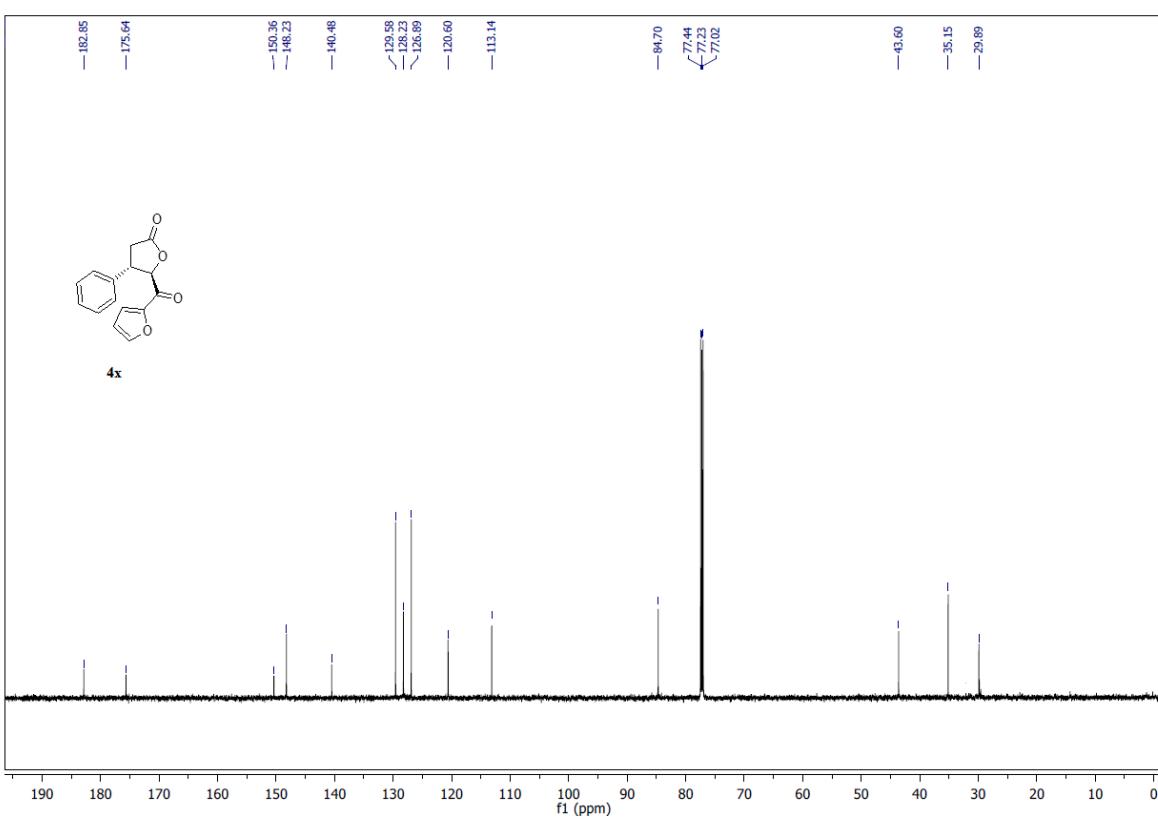
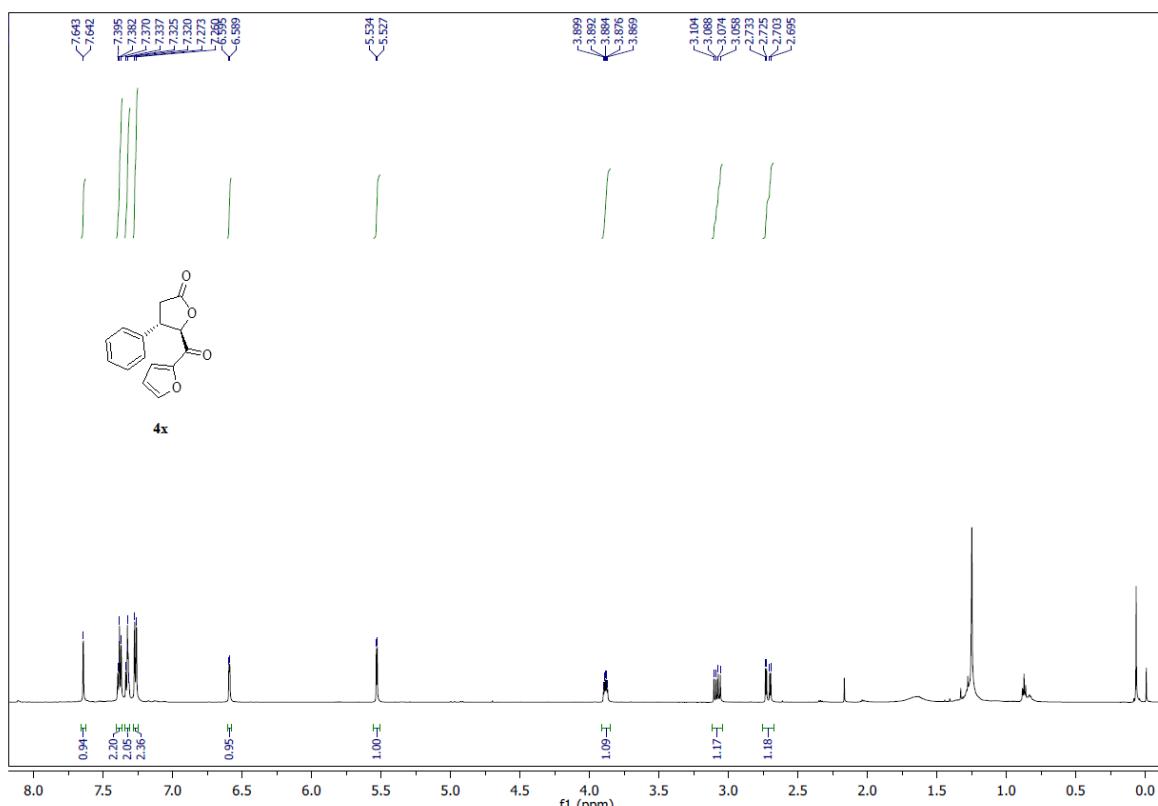


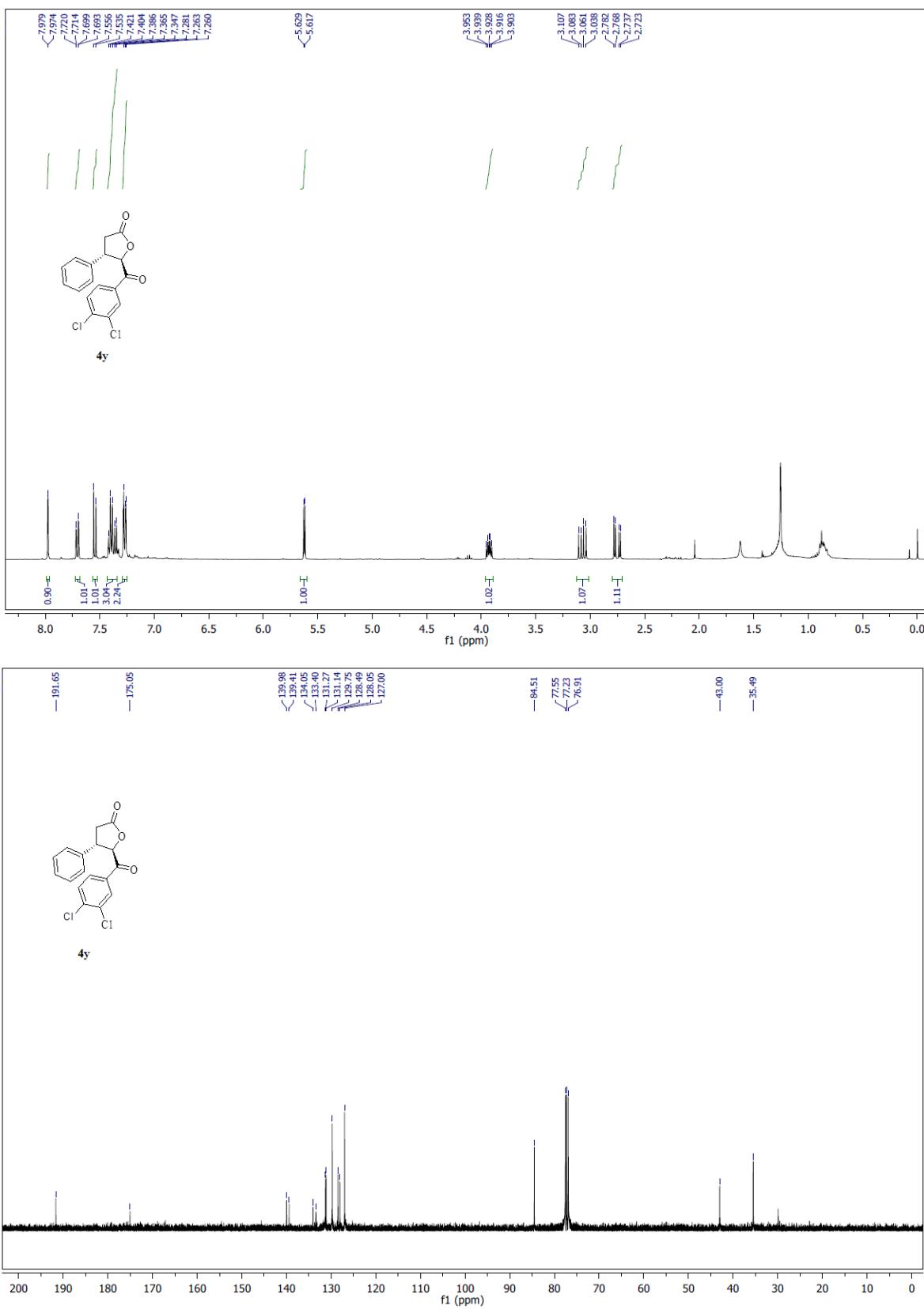


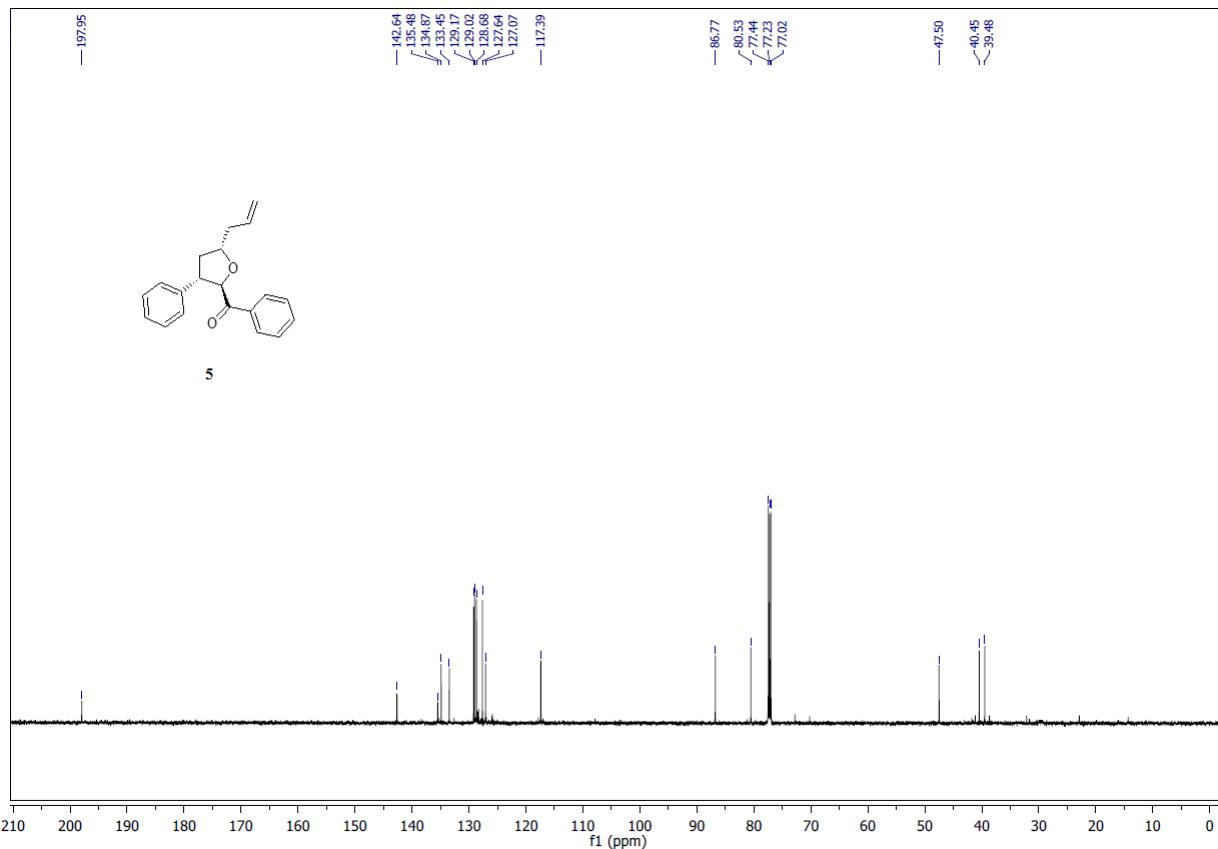
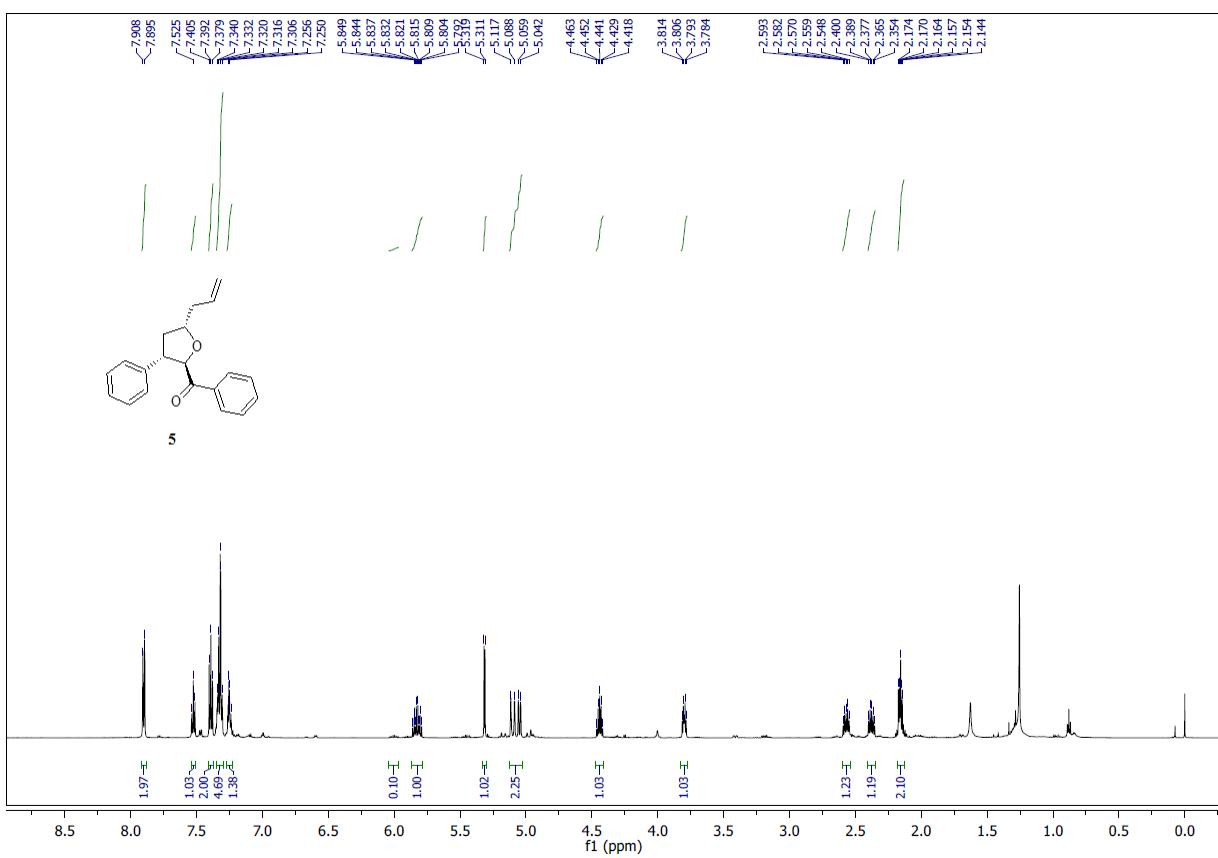


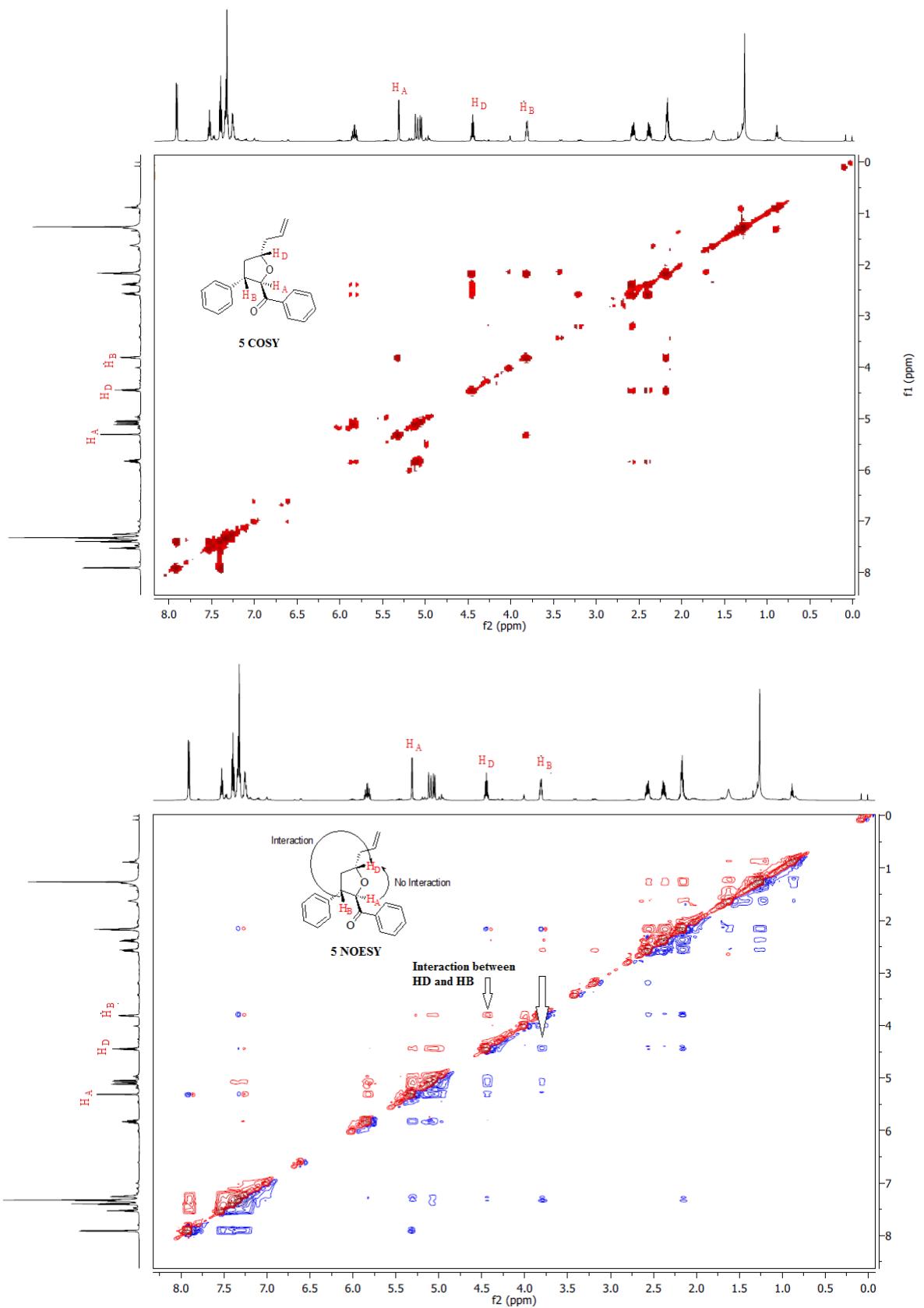


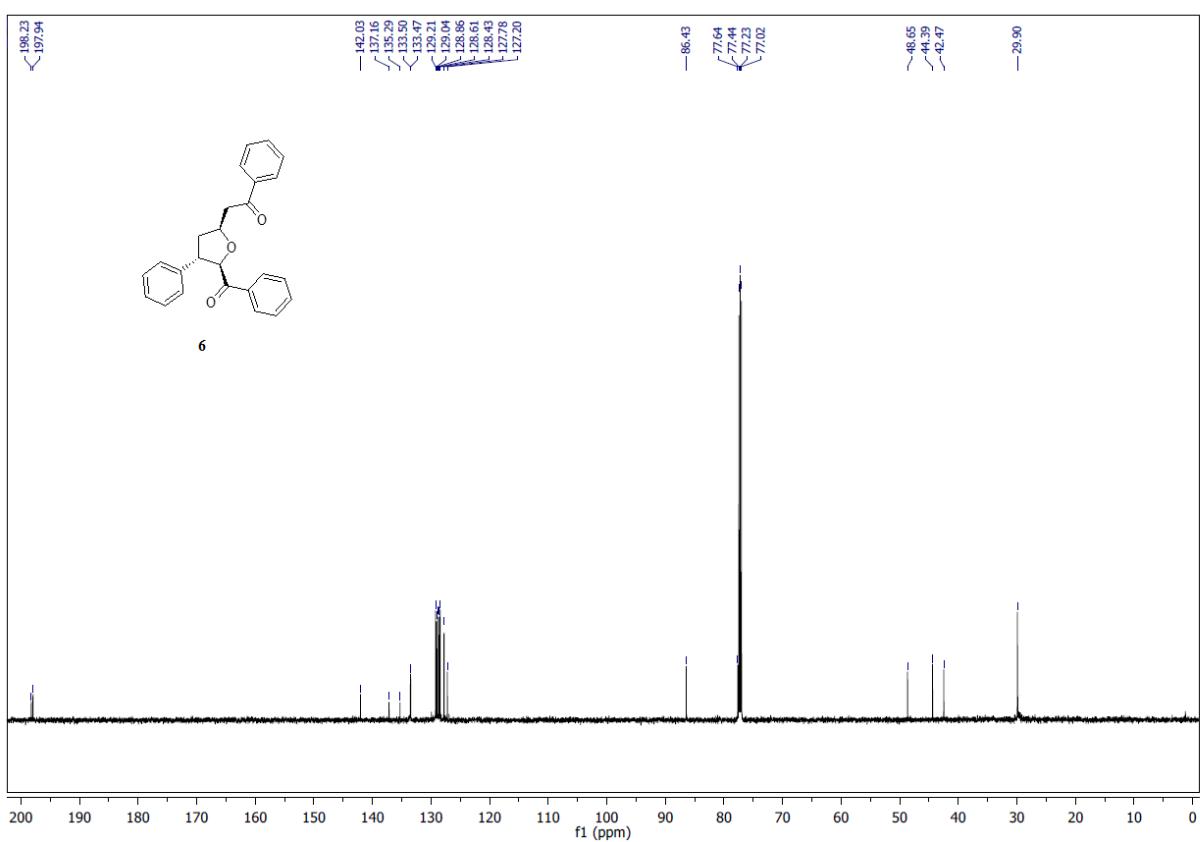
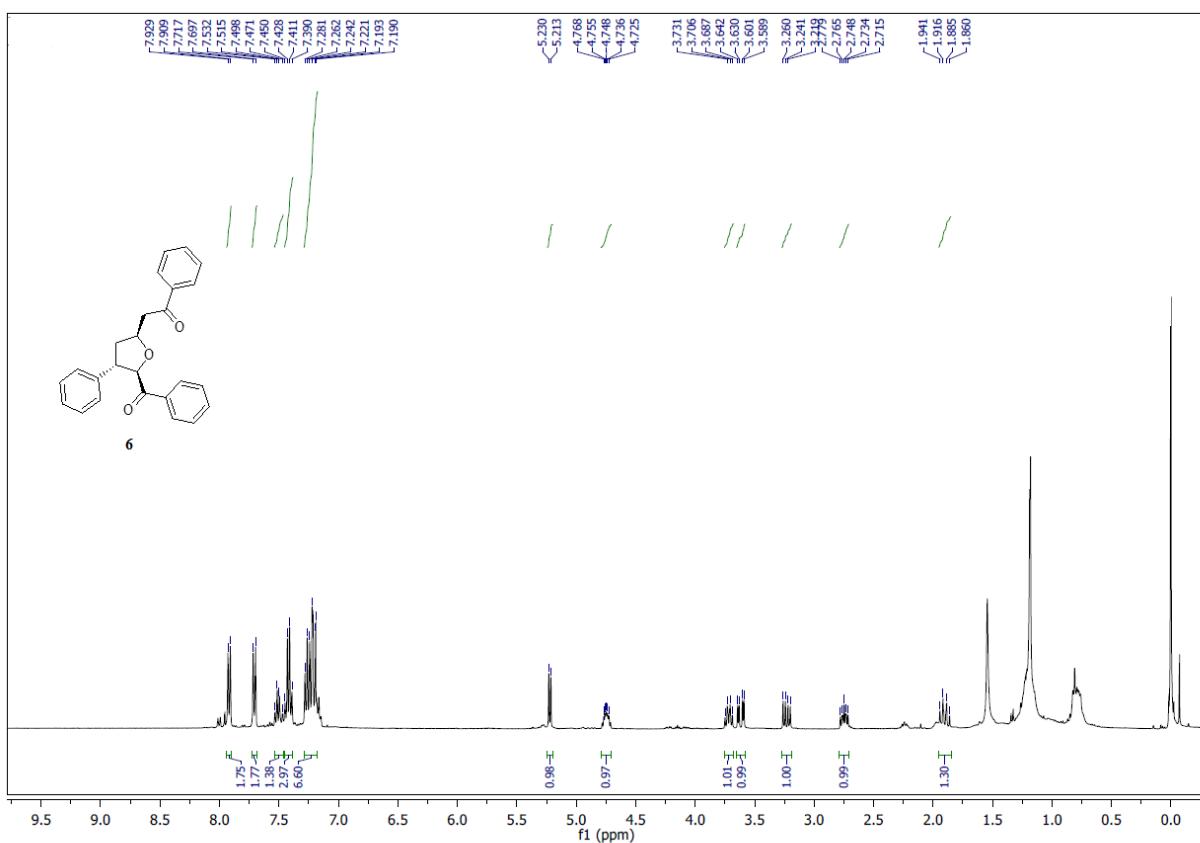


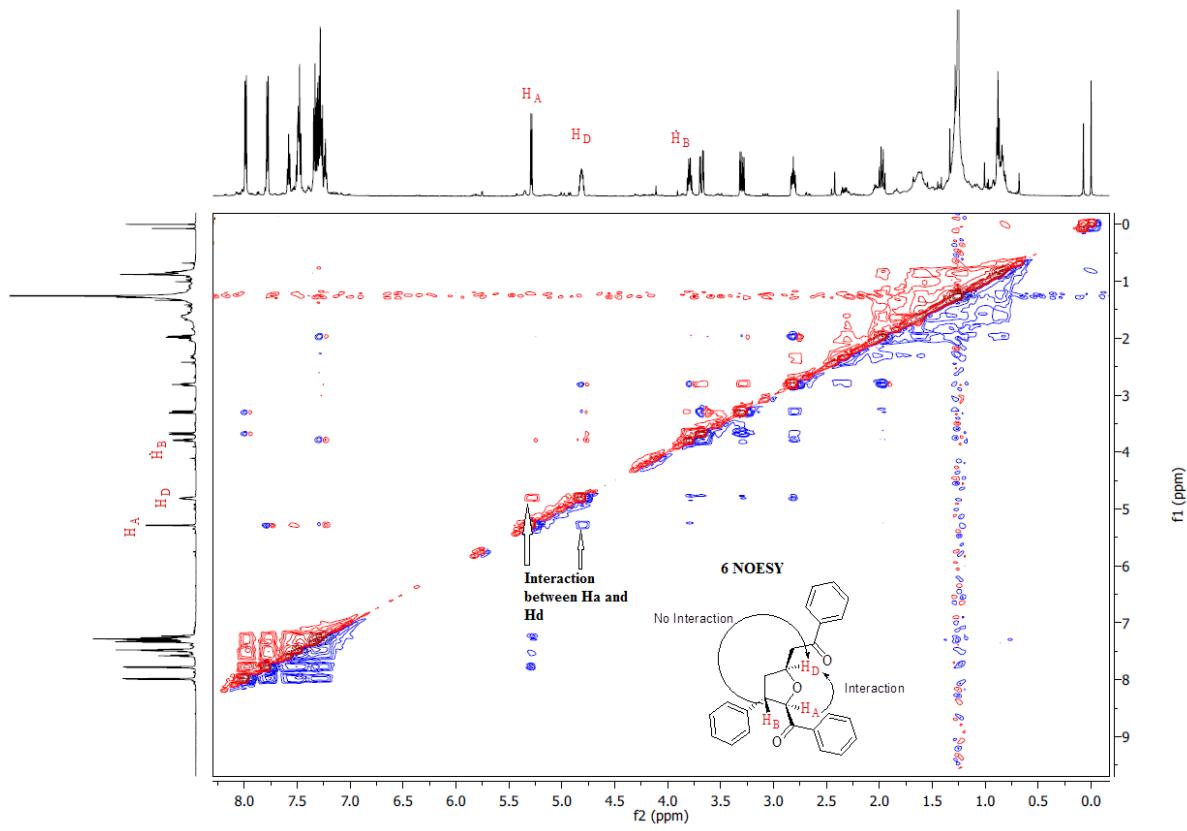
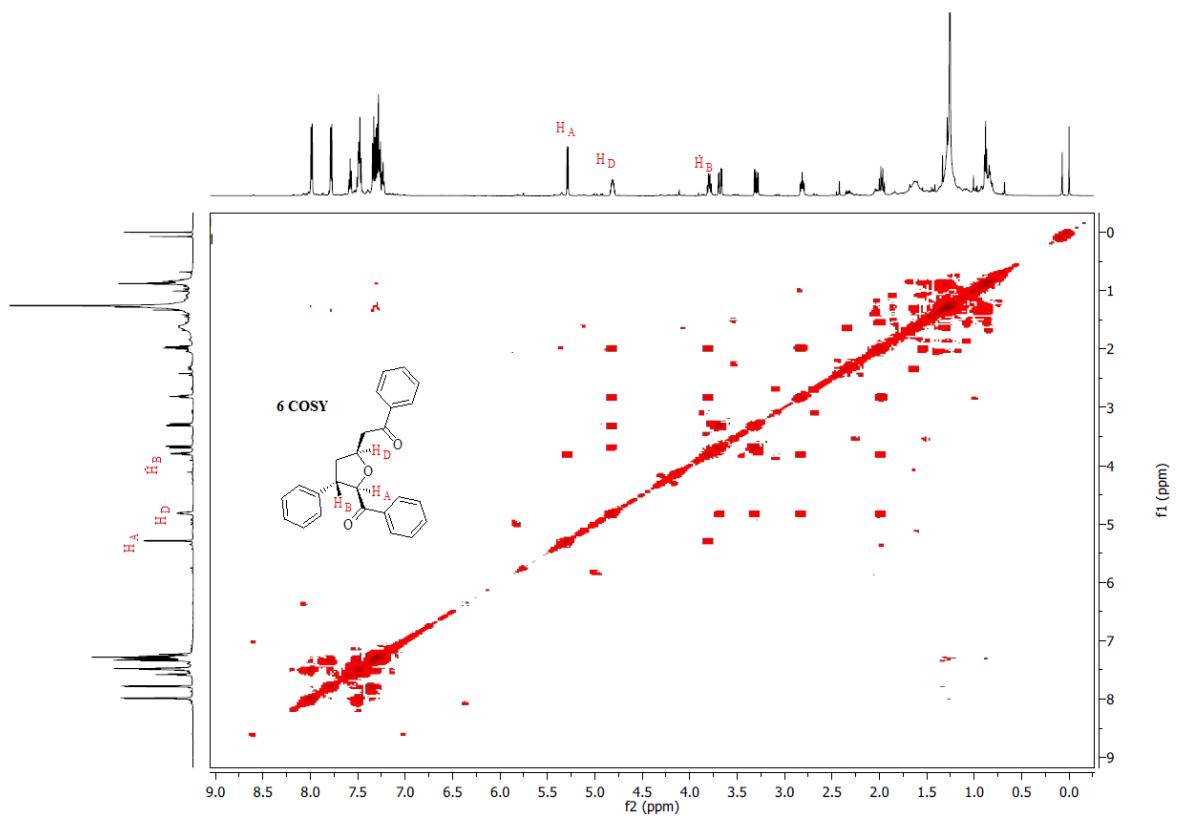


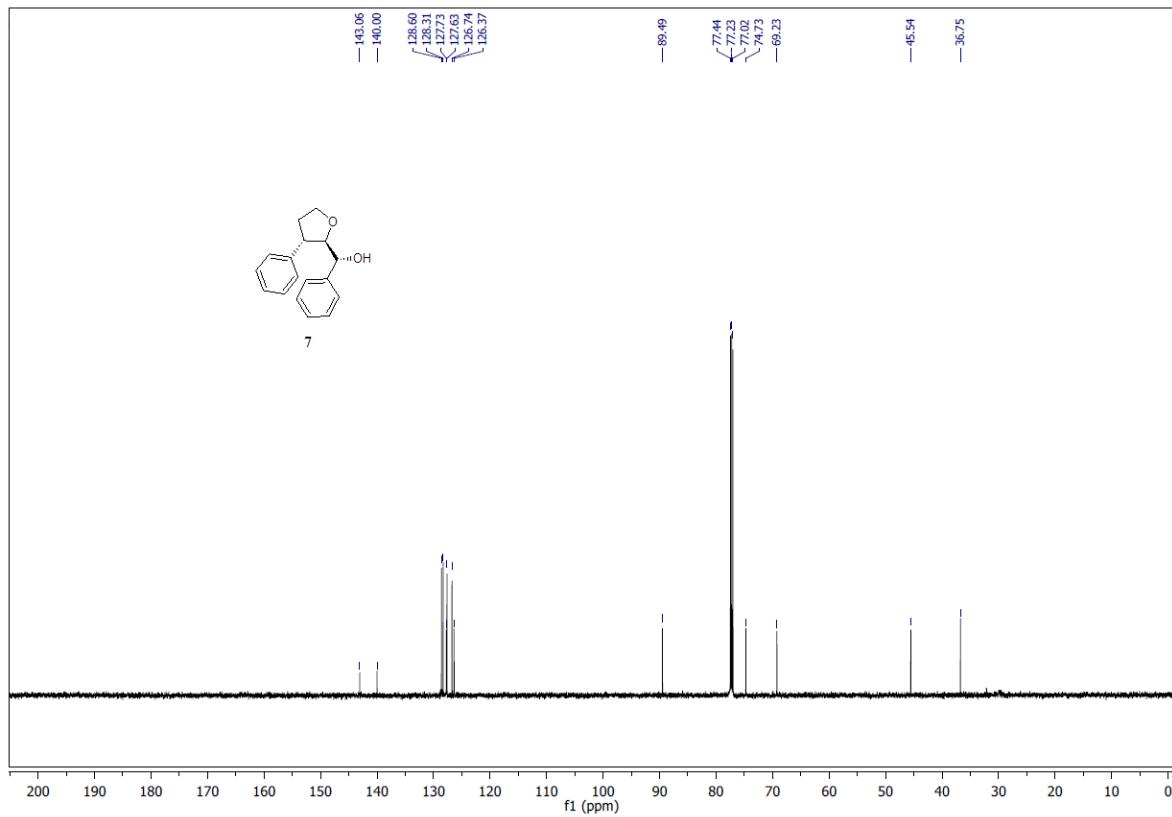
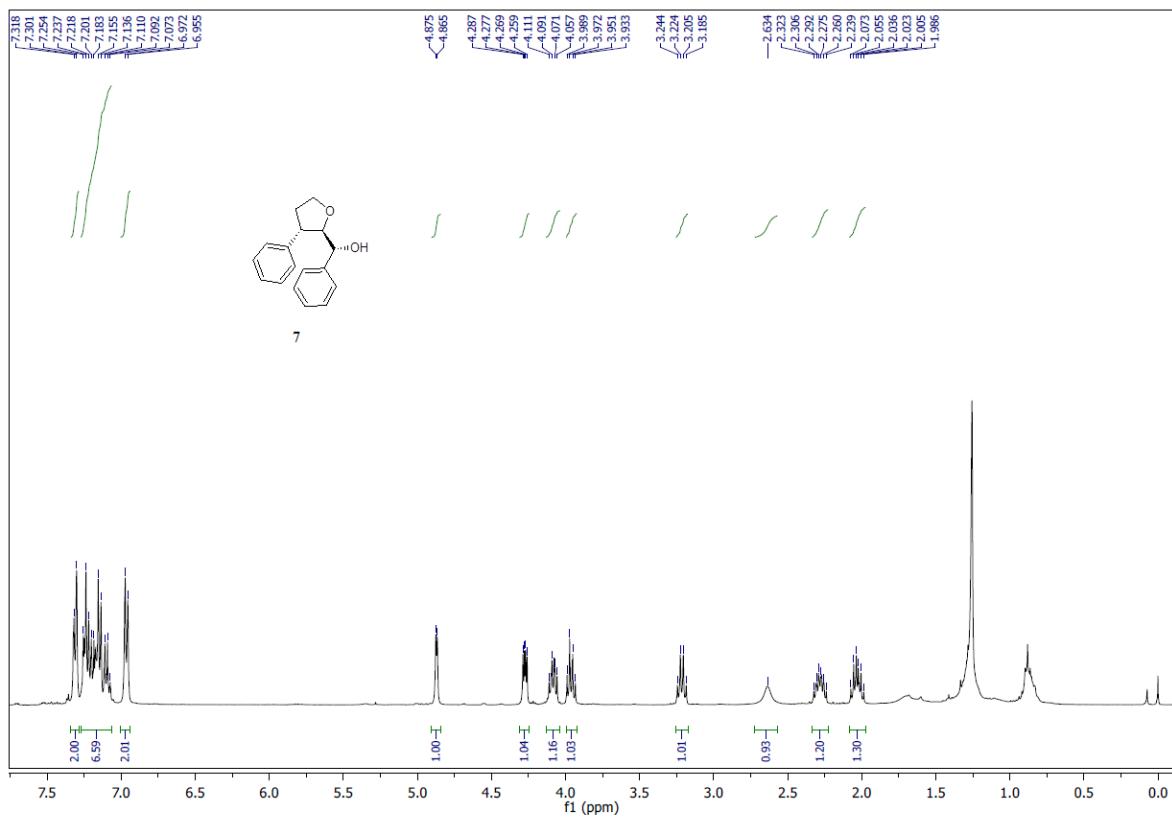


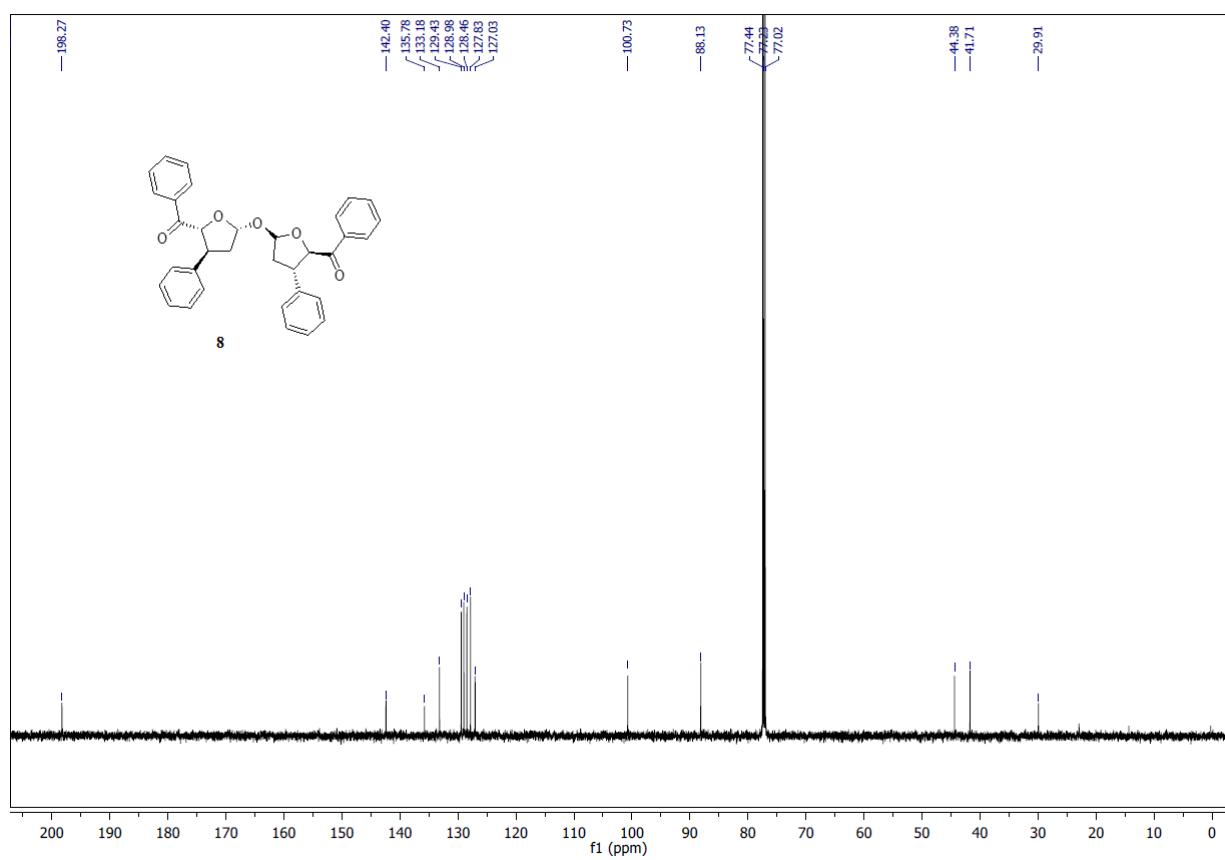
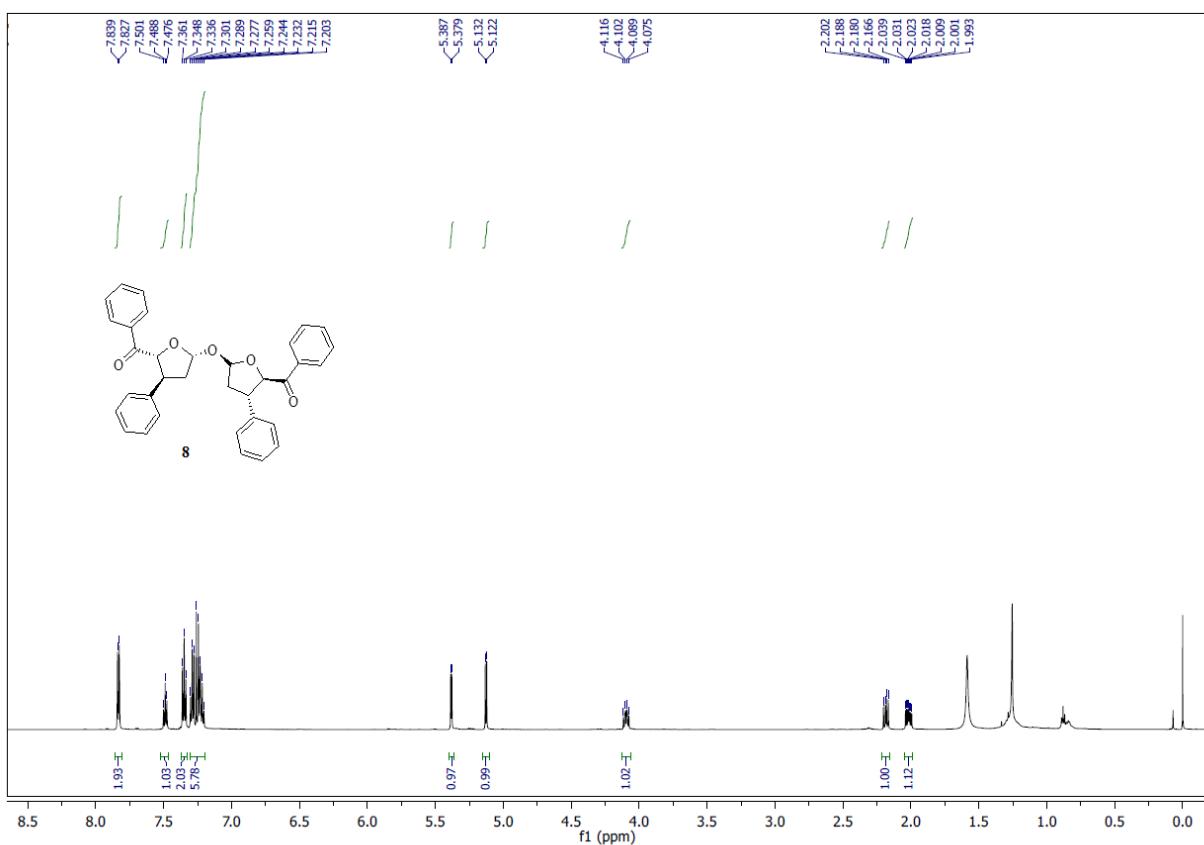


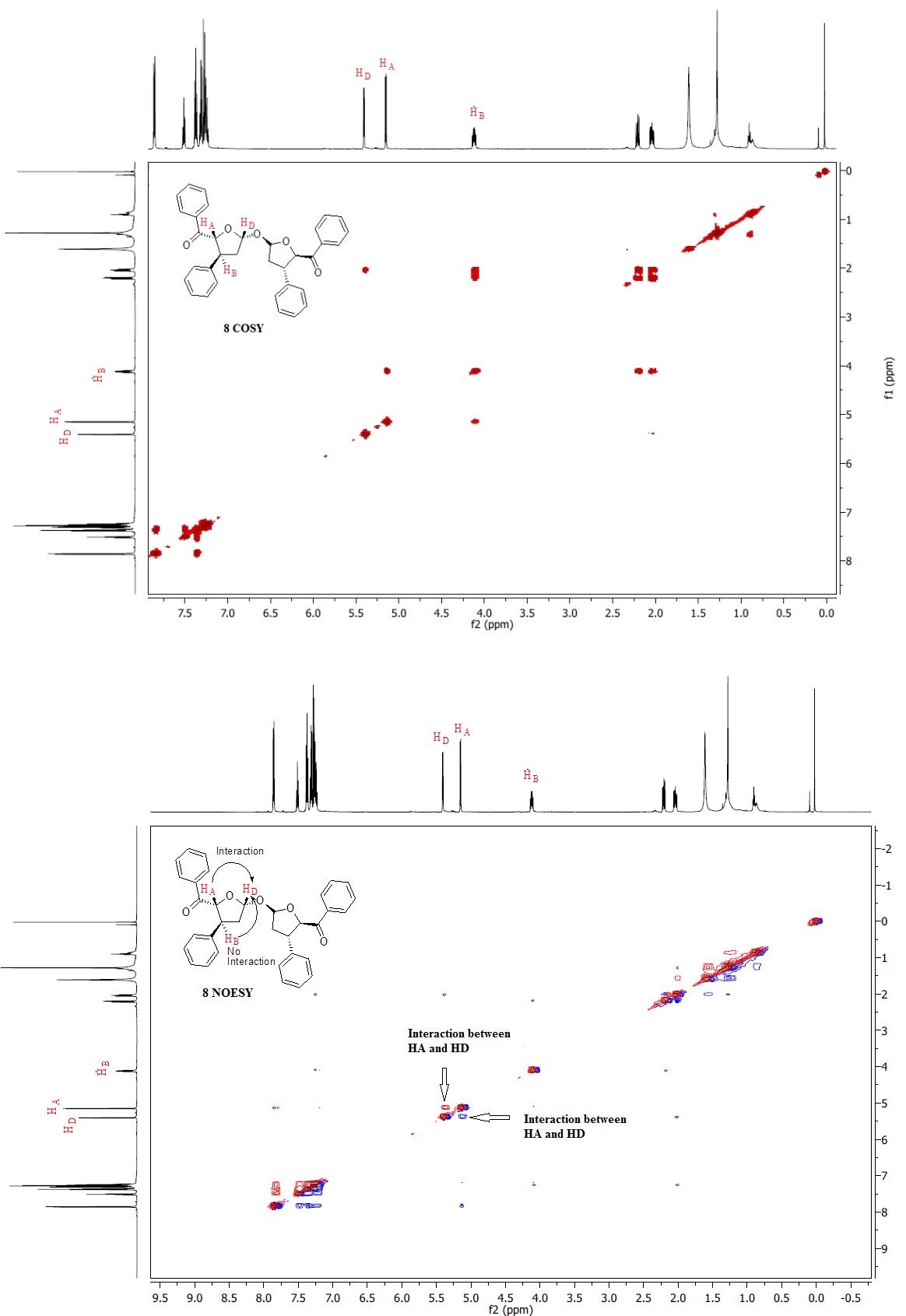


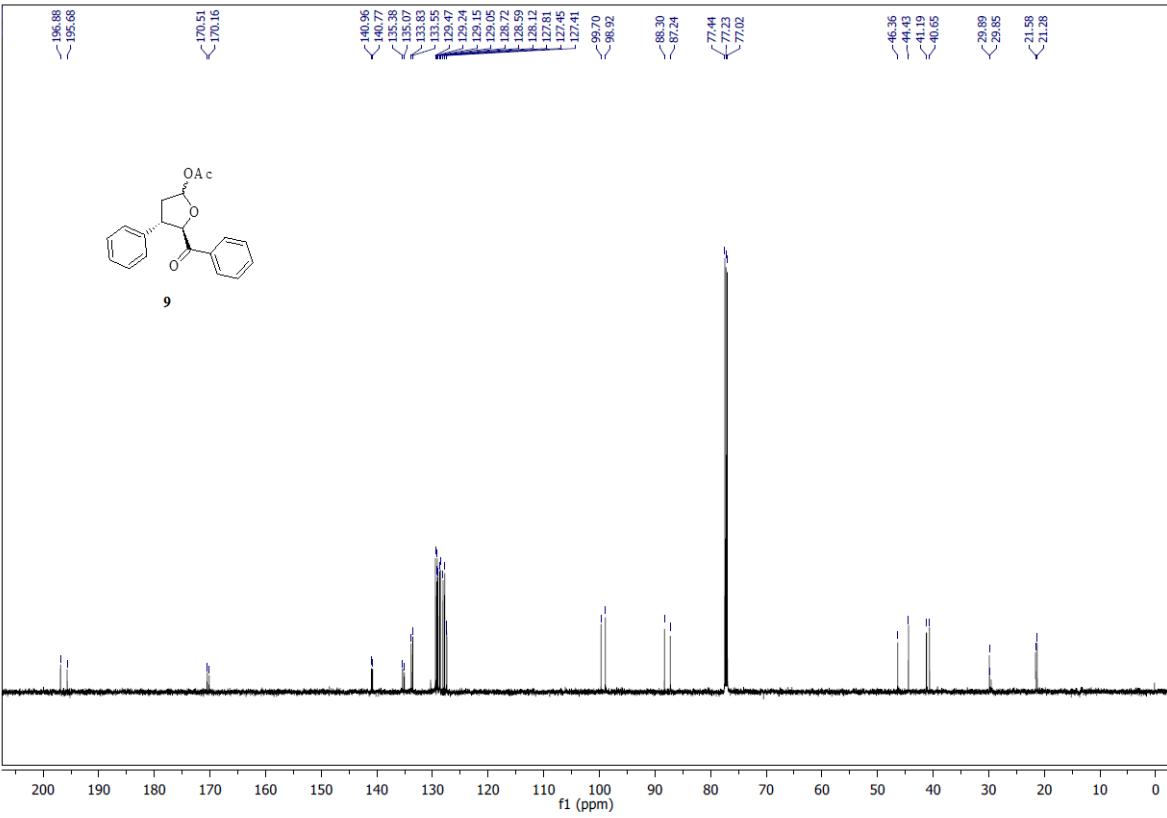
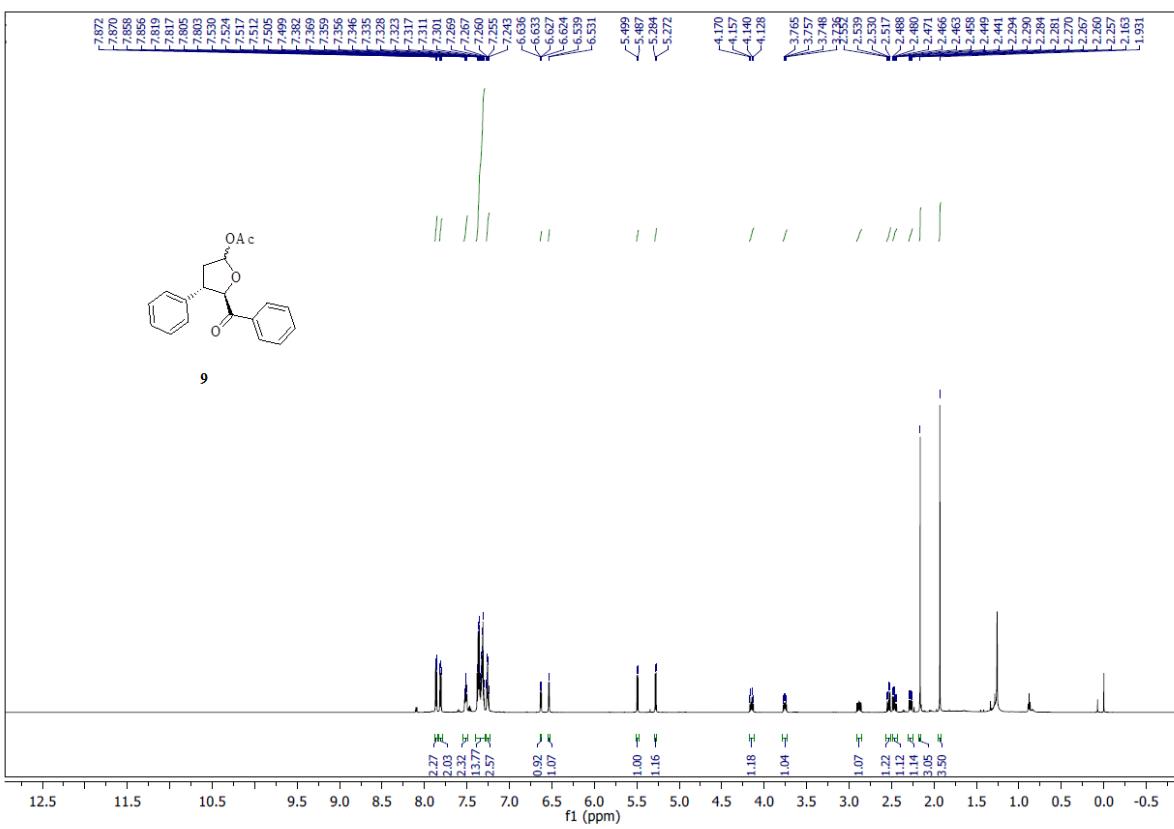




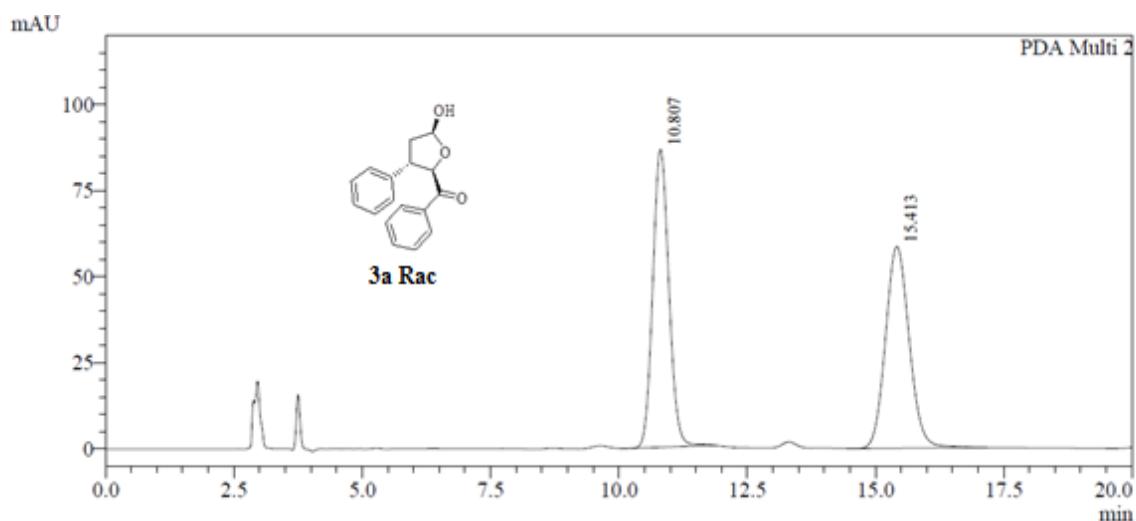








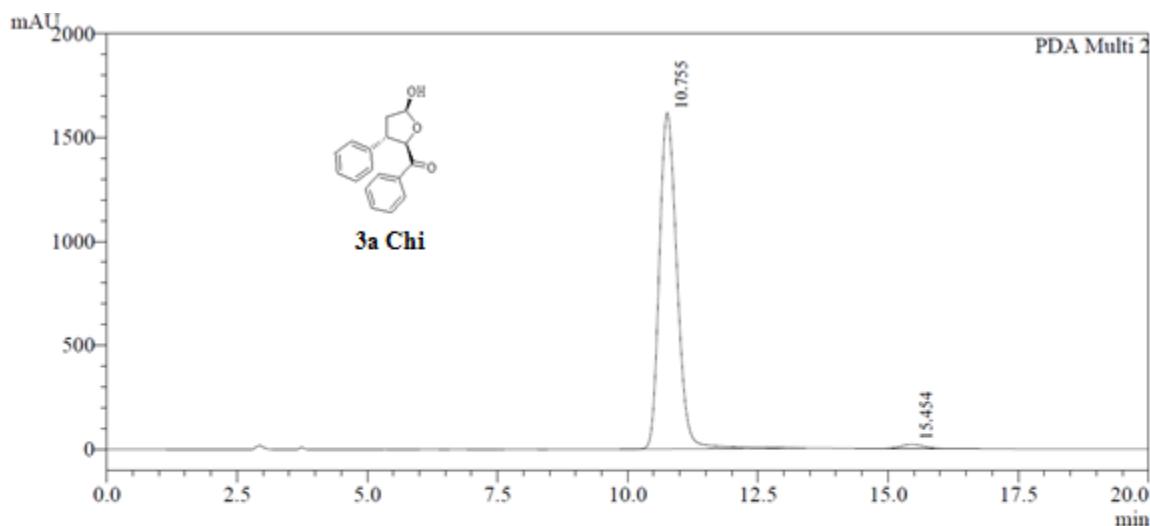
4. HPLC chromatogram of the products:



PeakTable

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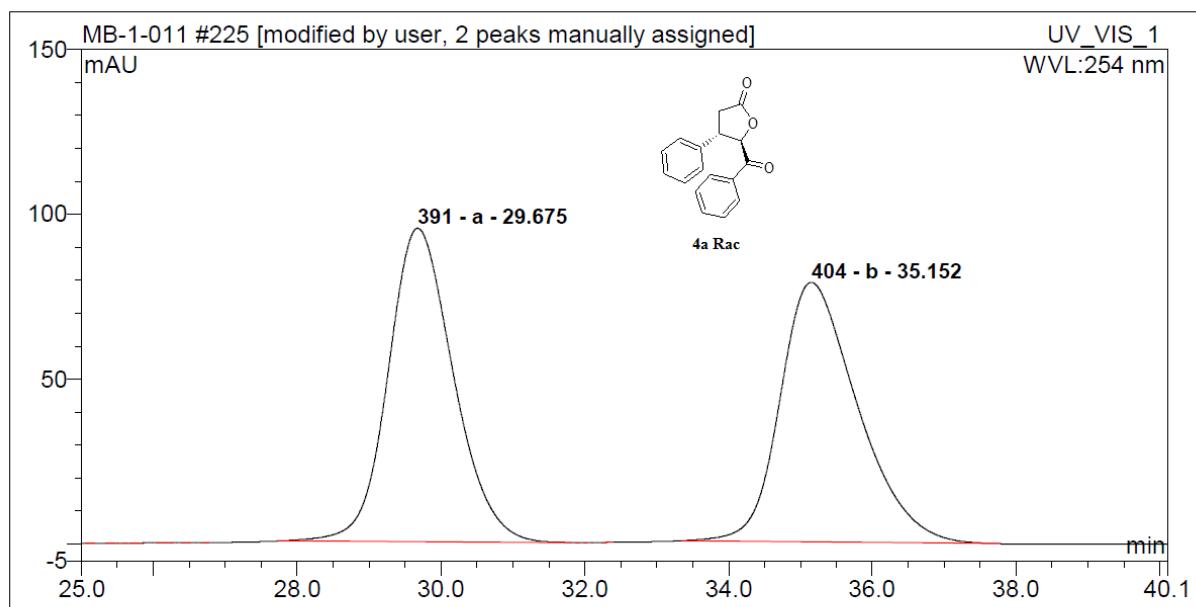
Peak#	Ret. Time	Area	Area %
1	10.807	1893076	50.083
2	15.413	1886805	49.917
Total		3779881	100.000



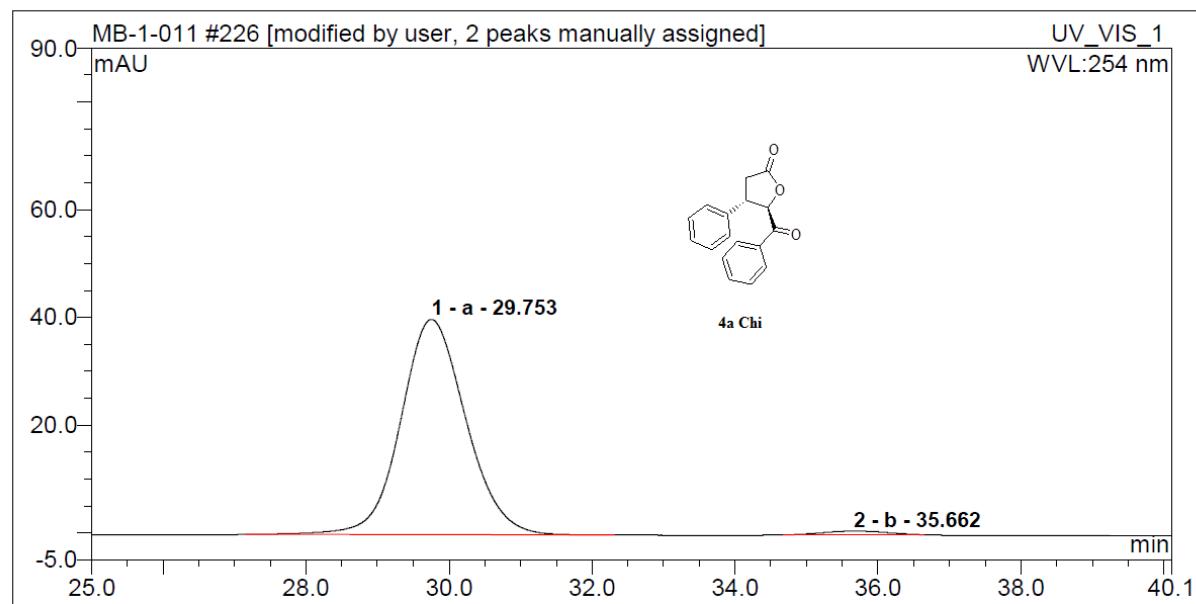
PeakTable

PDA Ch2 210nm 4nm

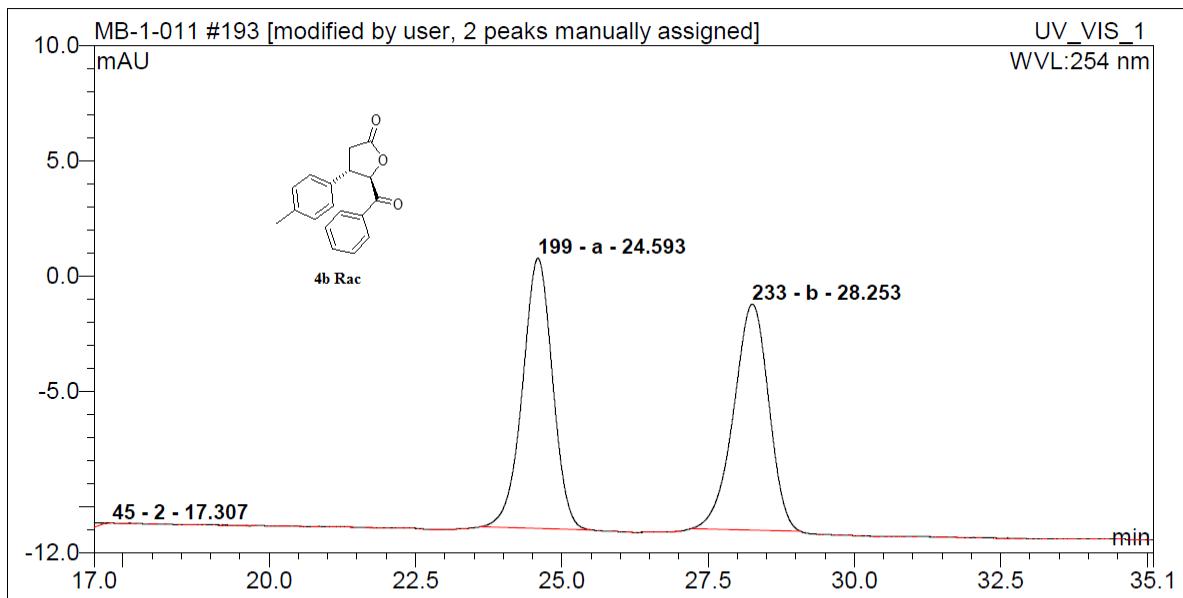
Peak#	Ret. Time	Area	Area %
1	10.755	38229920	98.389
2	15.454	625776	1.611
Total		38855696	100.000



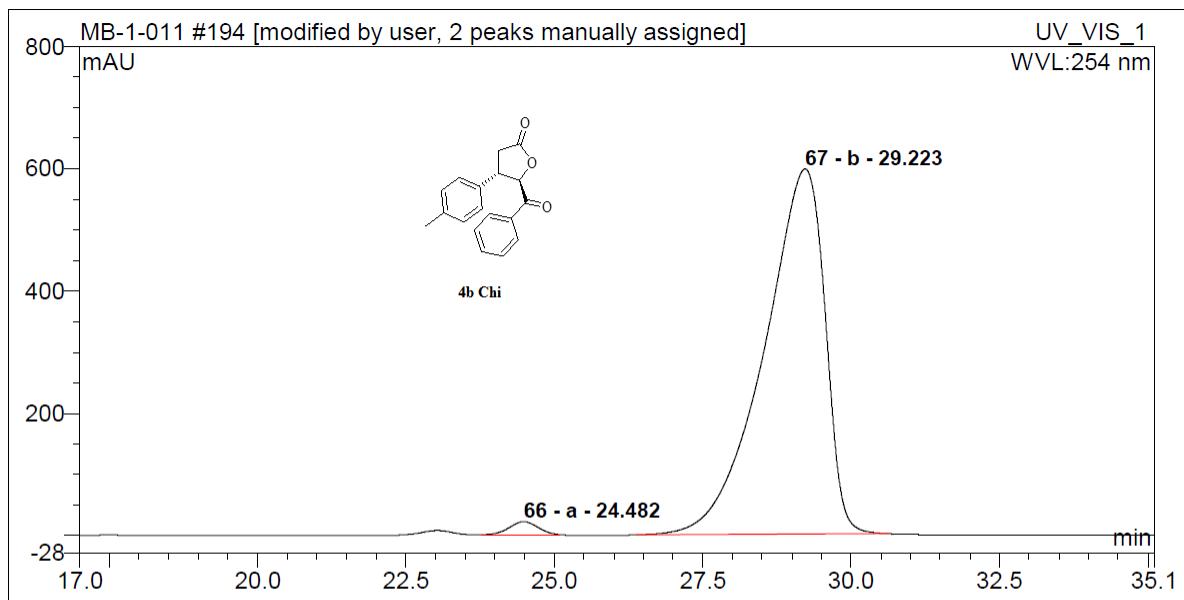
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
	391 a		29.68	99.94931	50.41093327	94.98738 n.a.
	404 b		35.15	98.320	49.58904435	78.648 n.a.



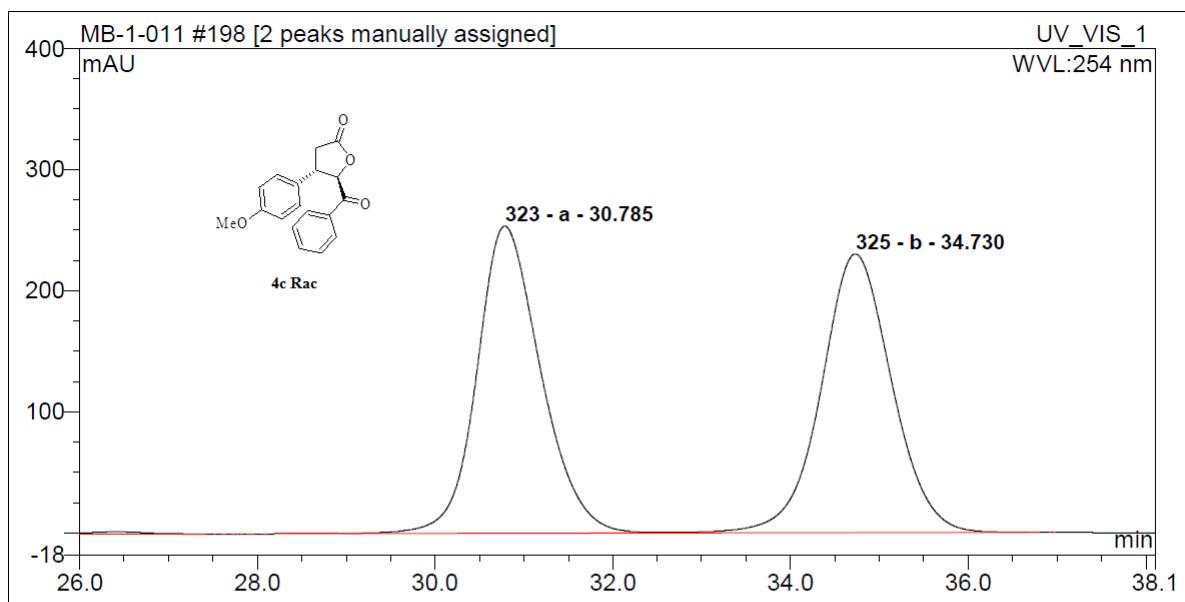
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
	1 a		29.75	42.39513	98.31651009	40.01889 n.a.
	2 b		35.66	0.726	1.683489912	0.706 n.a.



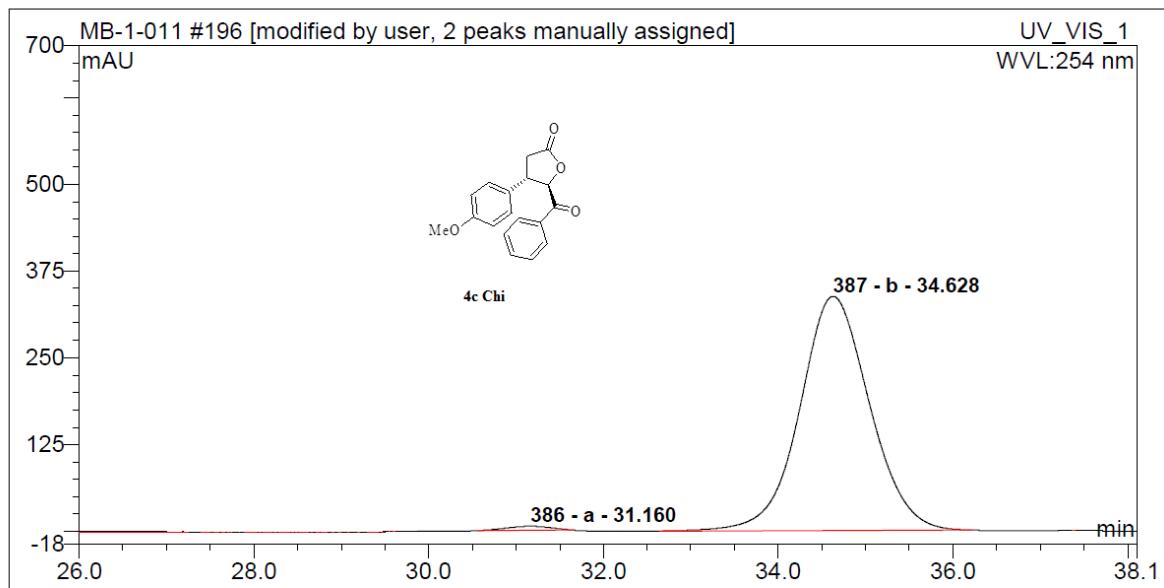
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
	199 a	24.59	7.005816	50.6774752	11.74024	n.a.
	233 b	28.25	6.818	49.32222967	9.812	n.a.



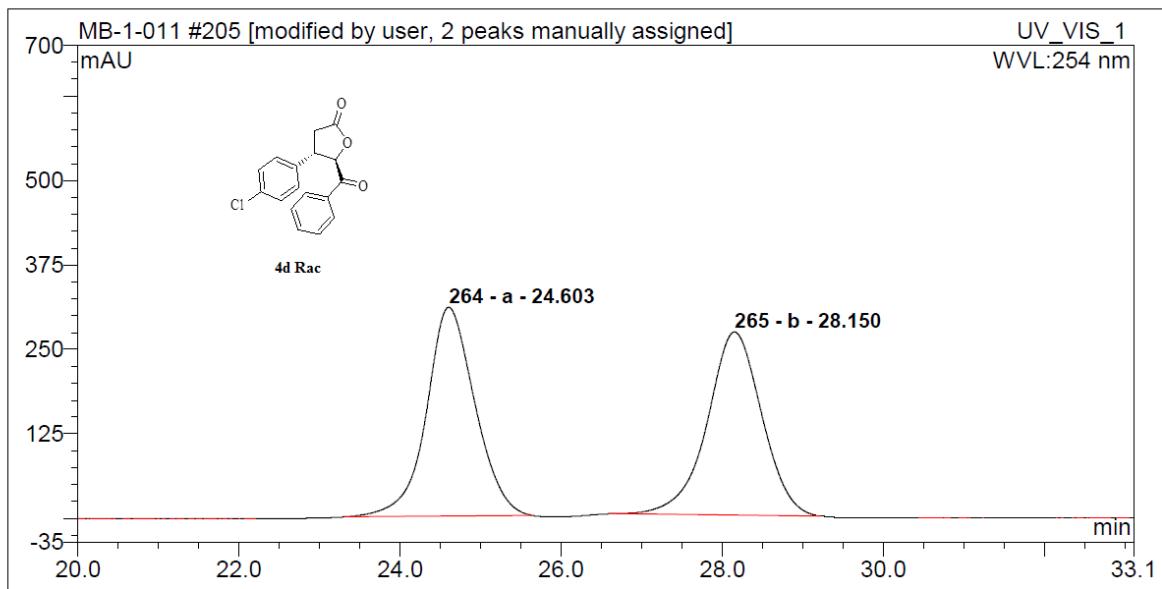
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
	66 a	24.48	11.89446	1.650660849	21.42983	n.a.
	67 b	29.22	708.693	98.34932878	597.511	n.a.



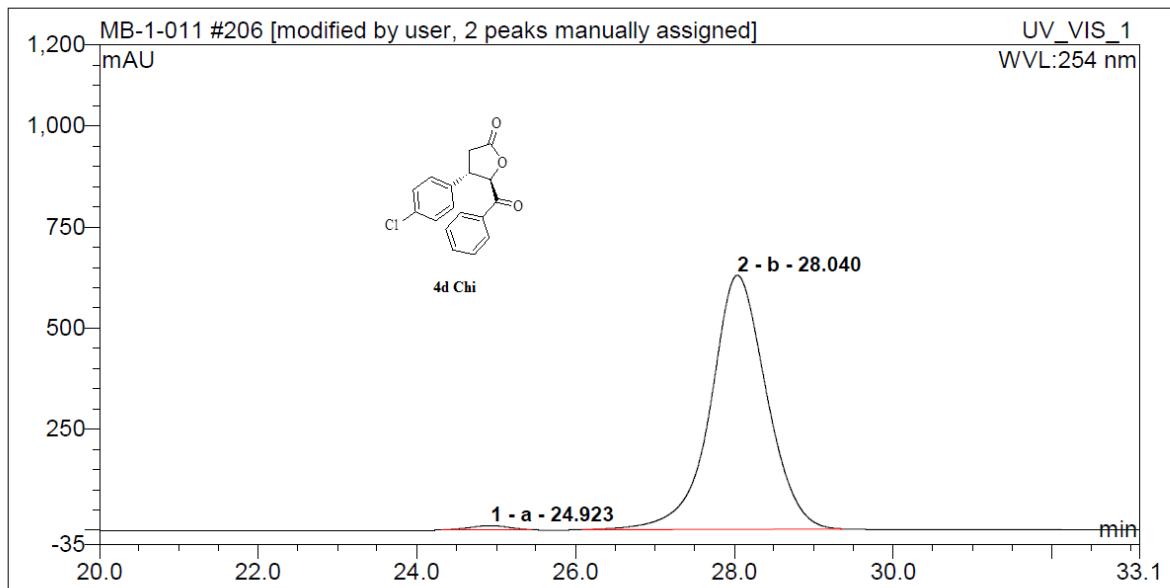
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
	323 a	30.79	211.2738	49.93390297	253.7027	n.a.
	325 b	34.73	211.832	50.06595216	230.141	n.a.



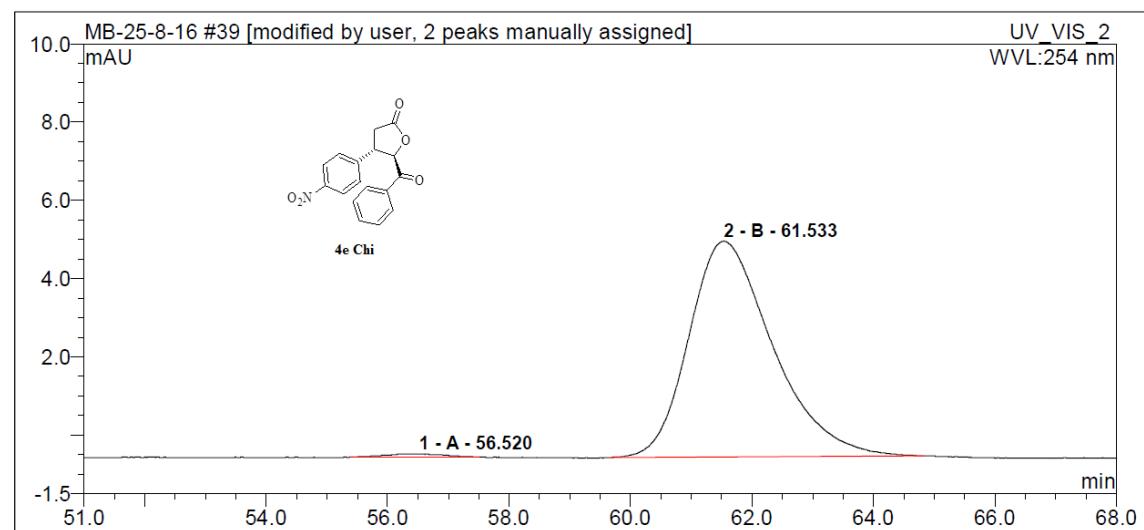
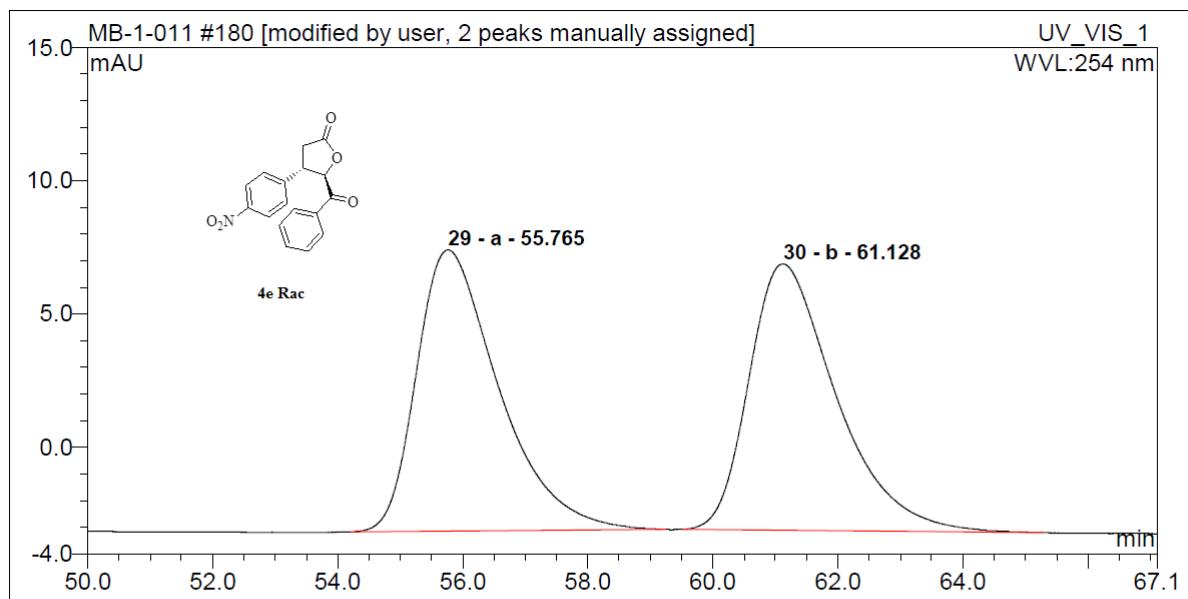
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
	386 a	31.16	3.547923	1.12482513	5.92349	n.a.
	387 b	34.63	311.872	98.87517011	337.632	n.a.



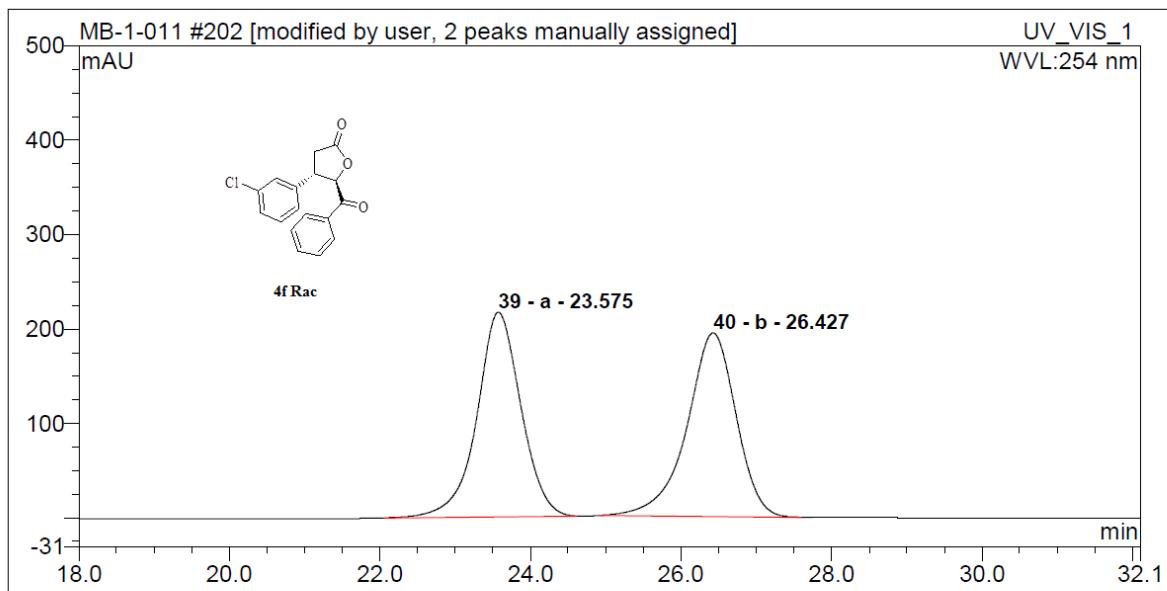
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
	264 a	24.60	215.6855	50.33818059	308.9842	n.a.
	265 b	28.15	212.787	49.6617891	270.969	n.a.



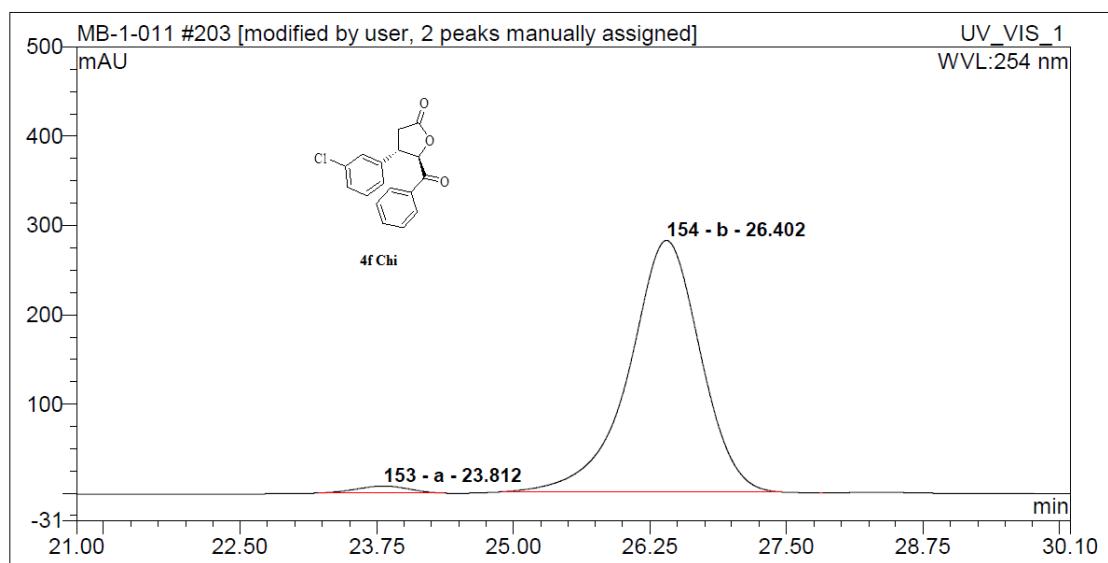
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
	1 a	24.92	5.685287	1.095889504	10.12236	n.a.
	2 b	28.04	513.098	98.9041105	628.026	n.a.



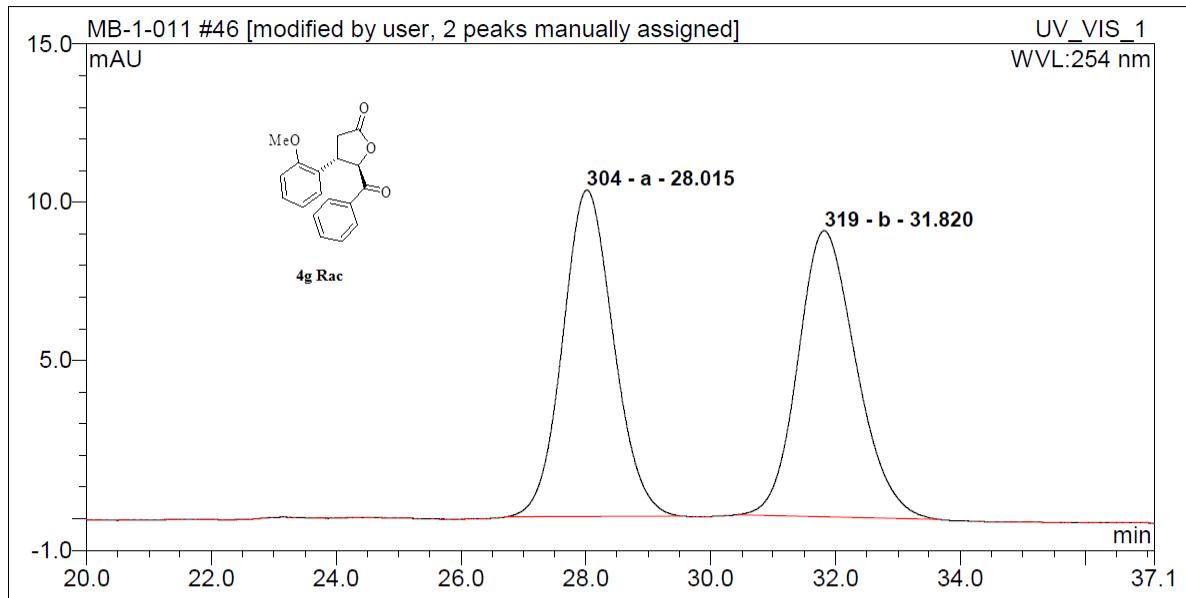
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
1	A	56.52	0.090554	1.017308772	0.08018	n.a.
2	B	61.53	8.811	98.98269123	5.518	n.a.



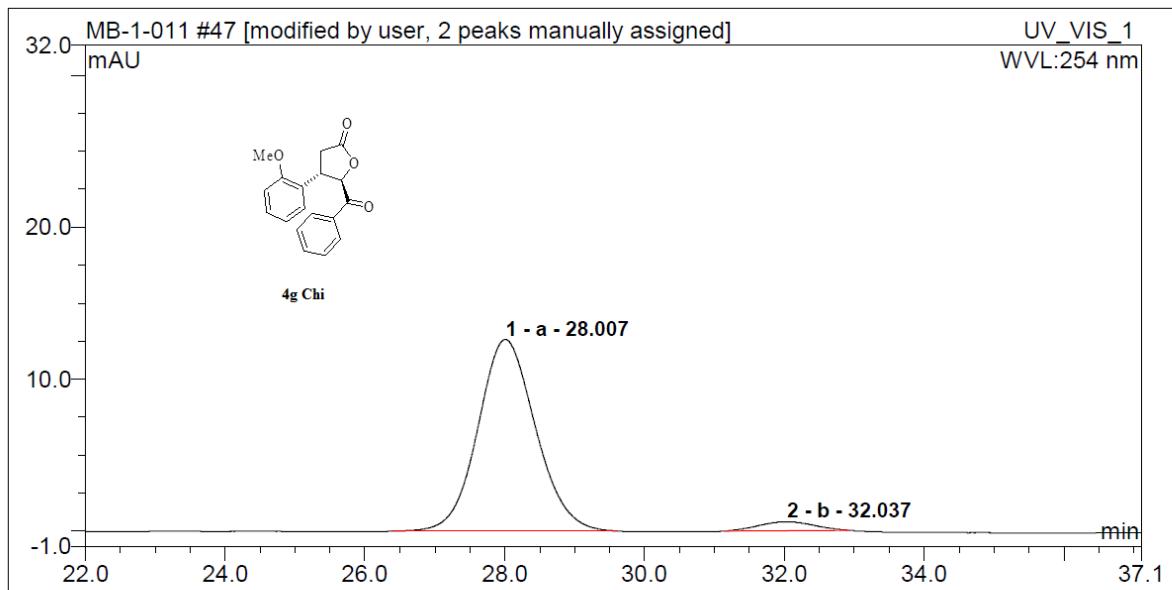
Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
39 a	23.58	146.7169	50.00072774	216.6623	n.a.
40 b	26.43	146.713	49.99927226	194.325	n.a.



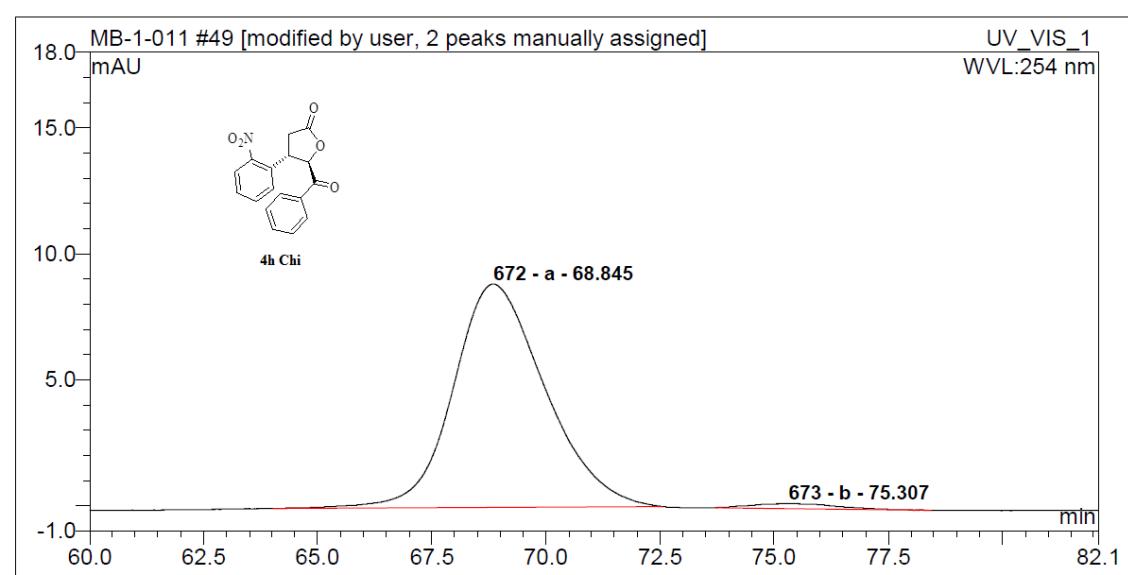
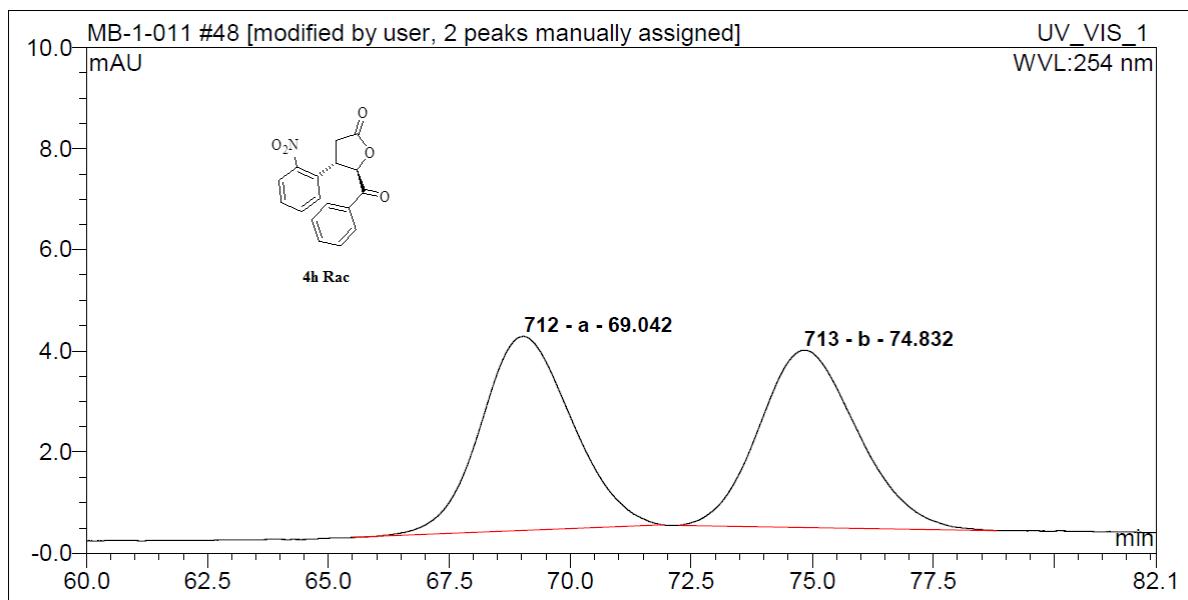
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
153 a		23.81	4.368909	2.007186859	7.85256	n.a.
154 b		26.40	213.294	97.99278616	281.687	n.a.



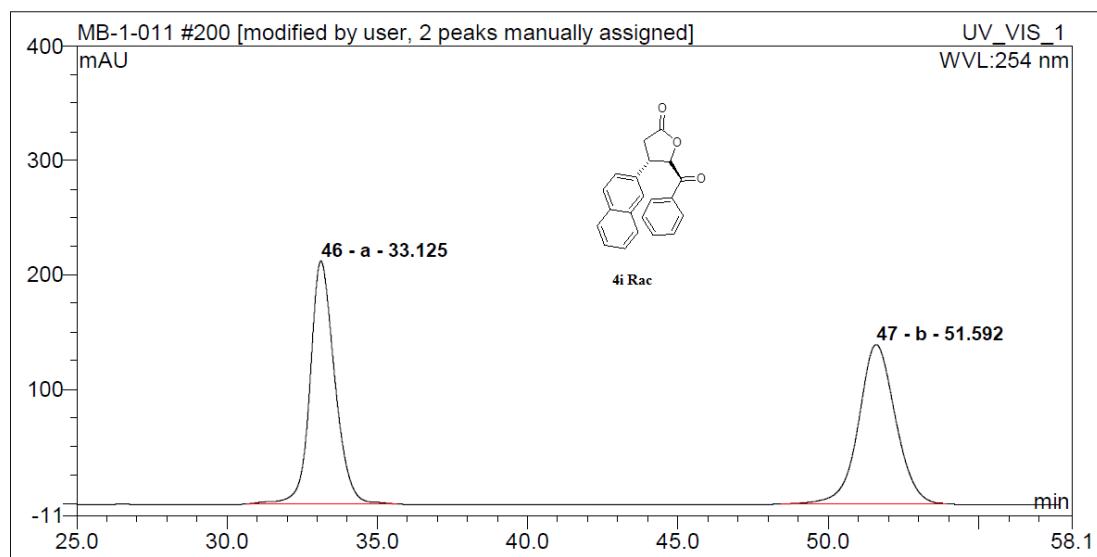
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
	304 a	28.02	9.736786	49.933208	10.31427	n.a.
	319 b	31.82	9.763	50.06652533	9.030	n.a.



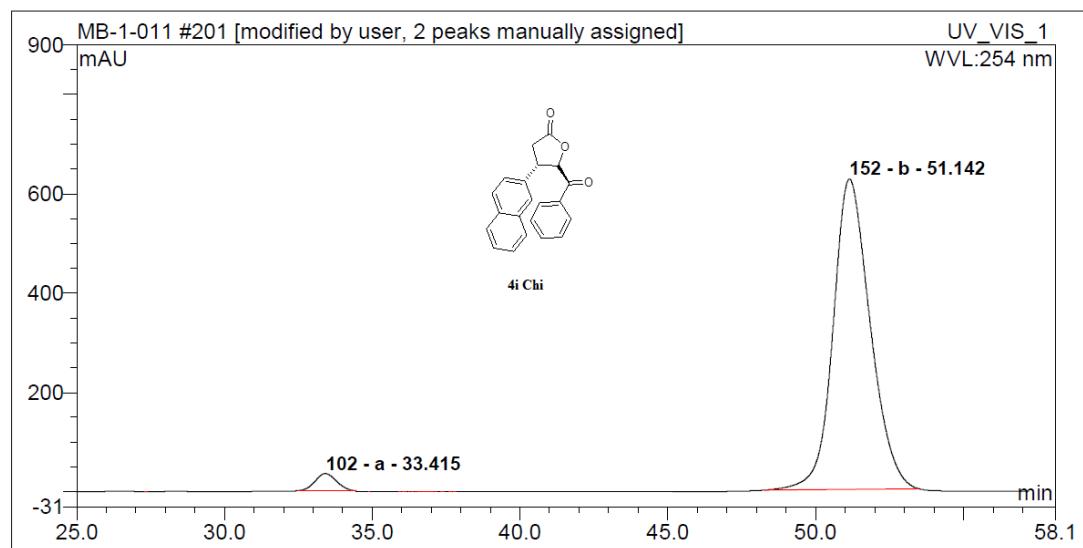
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
	1 a	28.01	12.07241	95.77319143	12.62226	n.a.
	2 b	32.04	0.533	4.22680857	0.580	n.a.



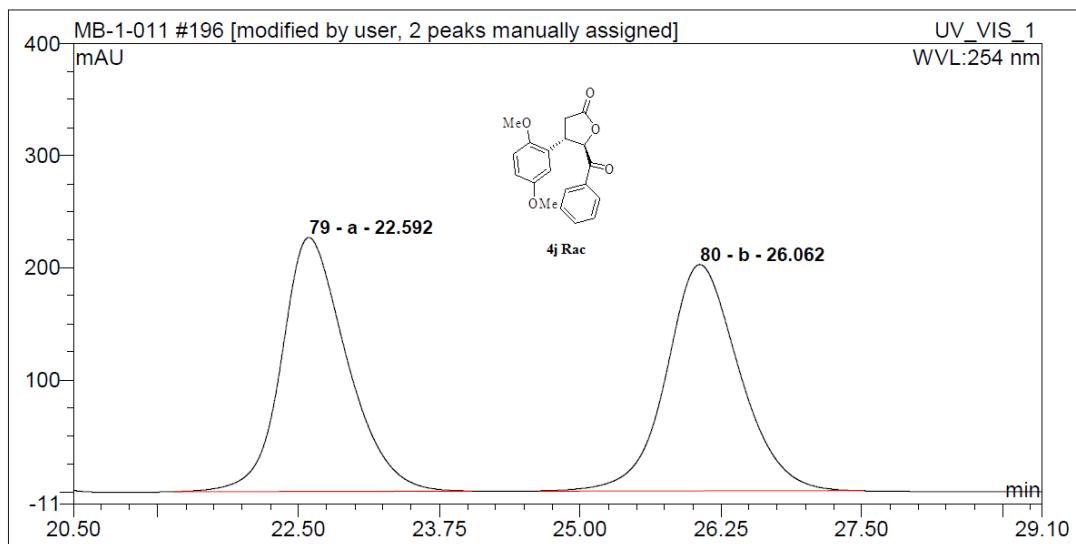
Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
672 a		68.85	20.714	98.05293135	8.86167 n.a.
673 b		75.31	0.411	1.946793857	0.200 n.a.



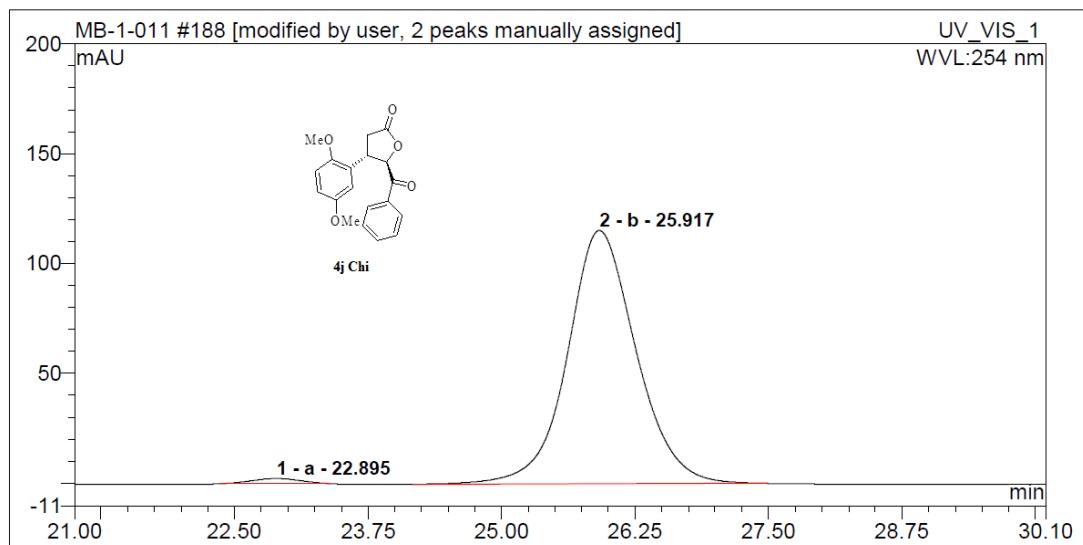
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
46 a		33.13	201.9602	50.42314966	212.419	n.a.
47 b		51.59	198.571	49.57684121	139.407	n.a.



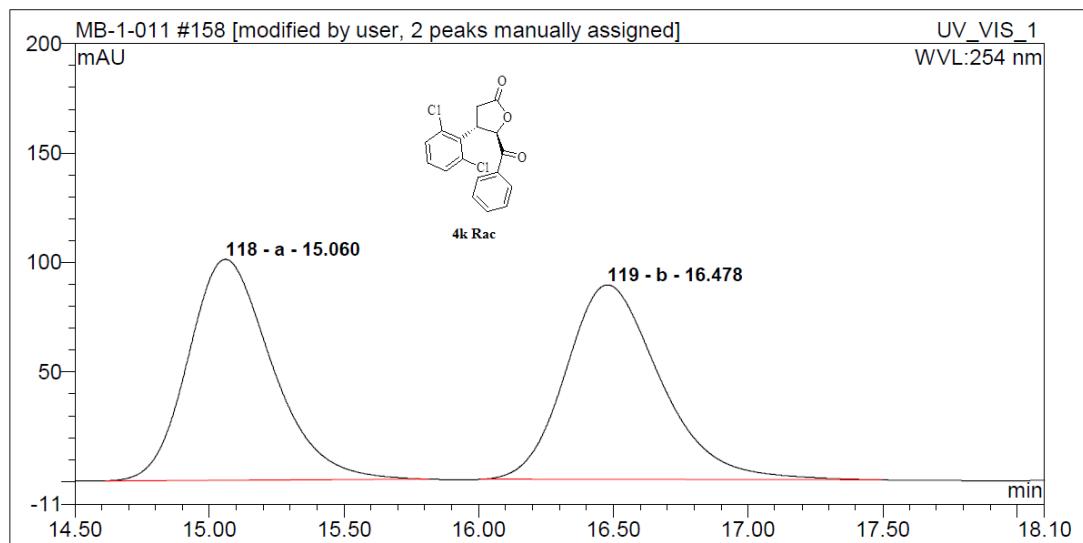
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
102 a		33.42	29.06784	3.104634261	34.59969	n.a.
152 b		51.14	907.205	96.89536063	624.451	n.a.



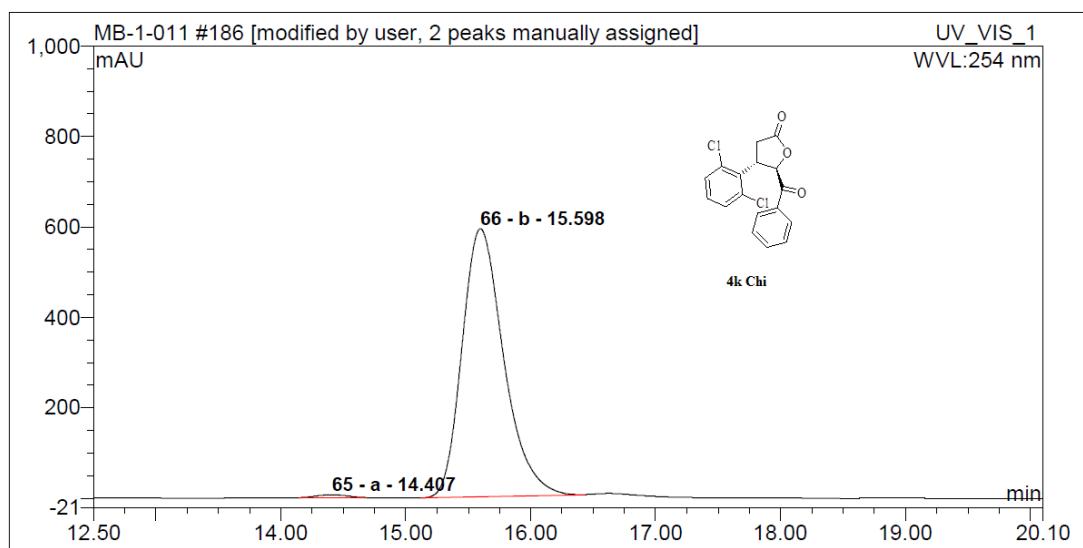
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
	79 a	22.59	152.4777	50.04856682	226.4484	n.a.
	80 b	26.06	152.182	49.95140341	201.817	n.a.



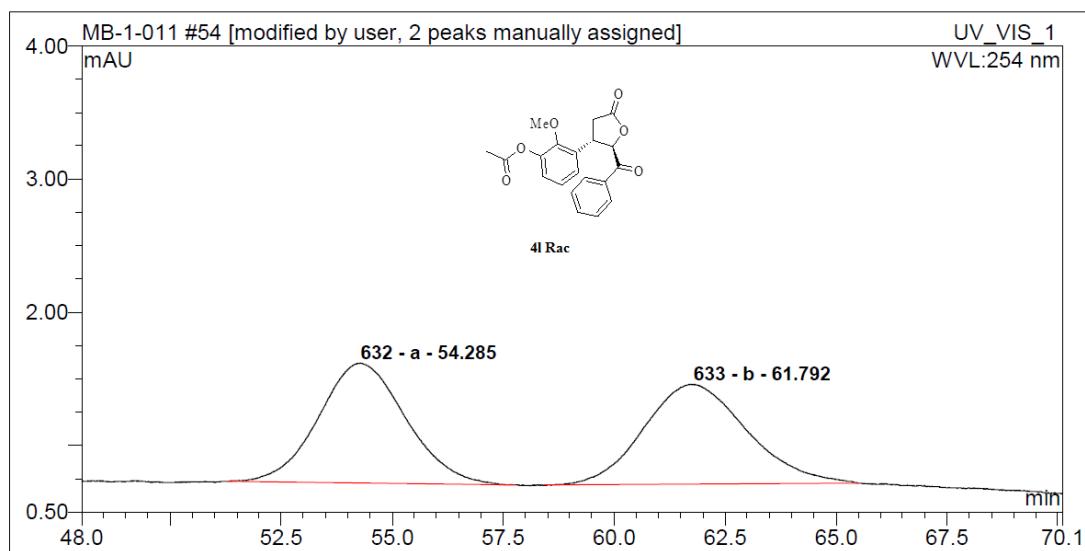
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
	1 a	22.90	1.242828	1.422733338	2.35329	n.a.
	2 b	25.92	86.112	98.57726666	115.347	n.a.



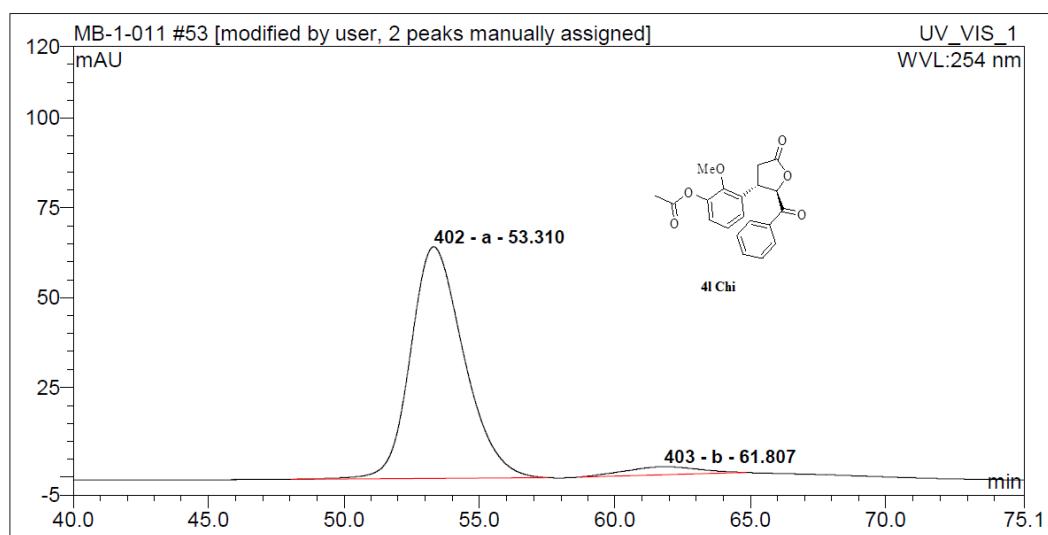
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
118 a		15.06	36.37068	50.05296393	100.886	n.a.
119 b		16.48	36.294	49.94699001	88.903	n.a.



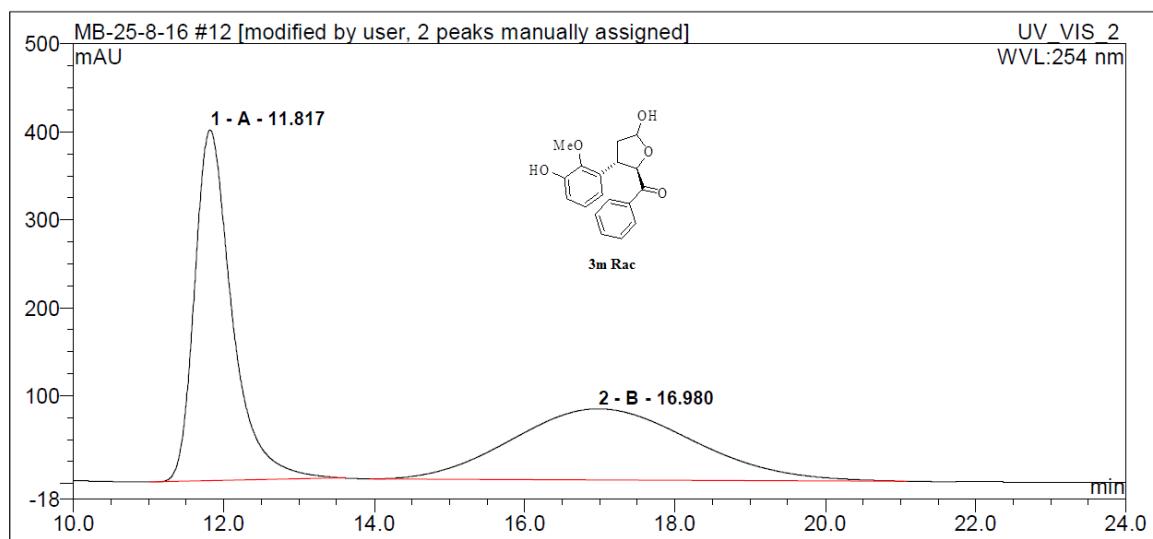
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
65 a		14.41	1.769398	0.7682954691	6.29678	n.a.
66 b		15.60	228.532	99.23168919	592.921	n.a.



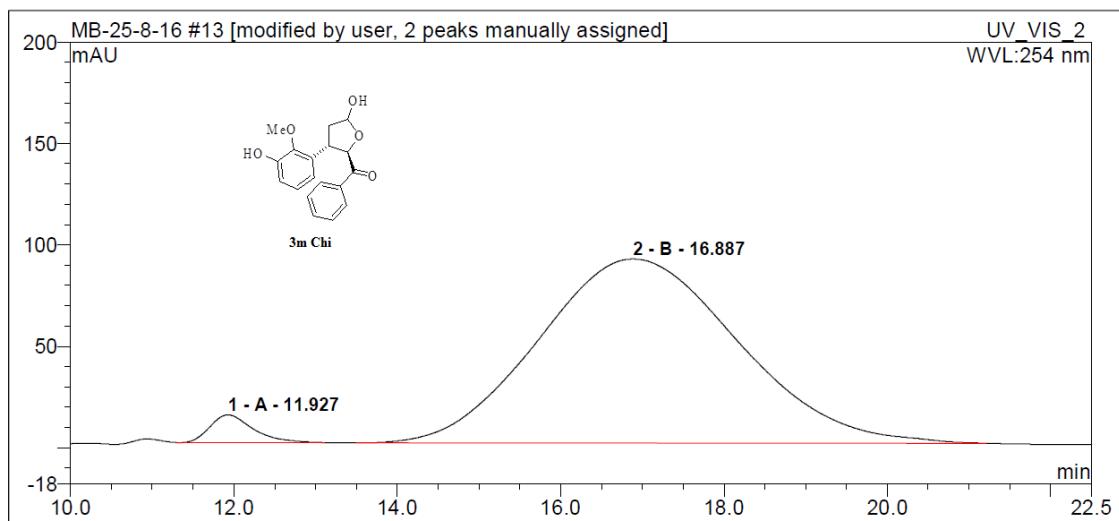
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
632 a		54.29	2.053643	50.4787878	0.90074	n.a.
633 b		61.79	2.015	49.51928532	0.749	n.a.



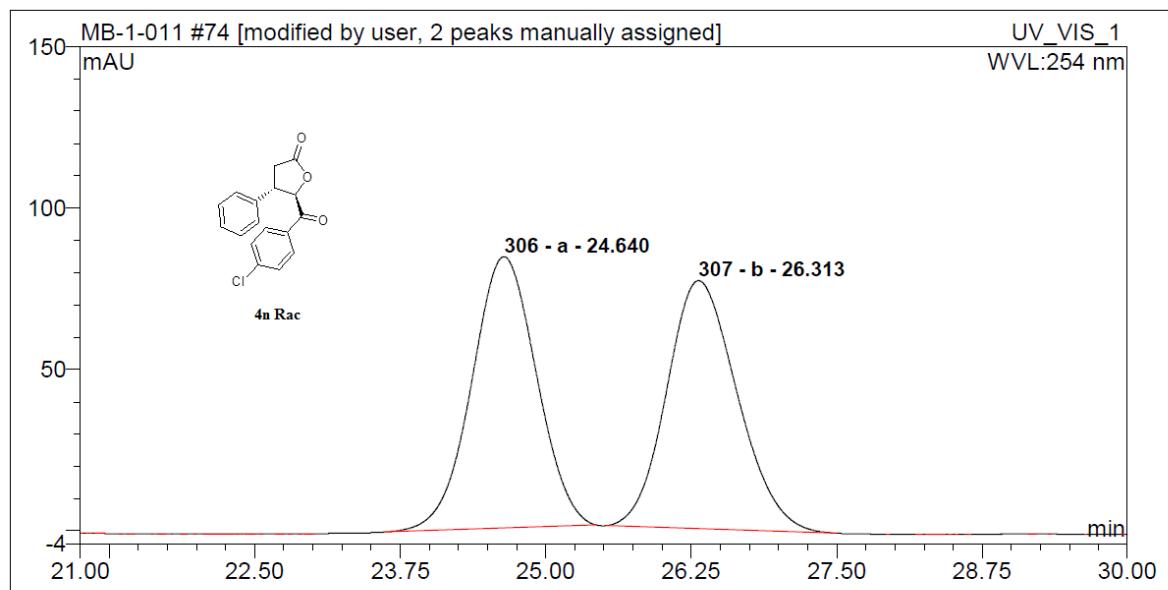
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
402 a		53.31	146.9797	95.43245978	64.47315	n.a.
403 b		61.81	7.035	4.567519027	2.248	n.a.



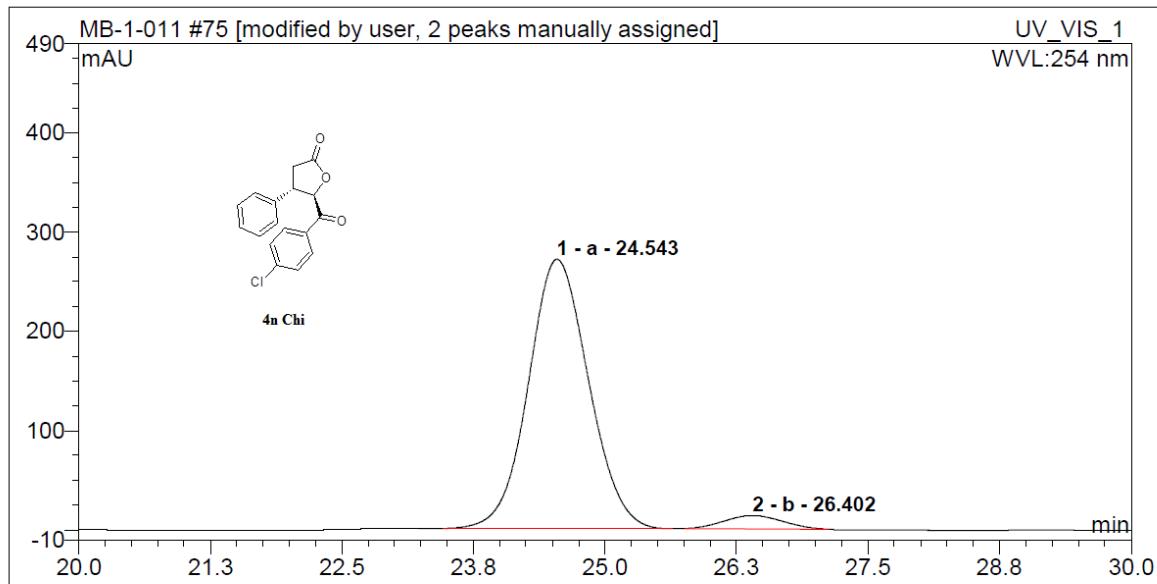
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A		11.82	230.8958	50.70558931	399.3564 n.a.
2	B		16.98	224.470	49.29441069	80.884 n.a.



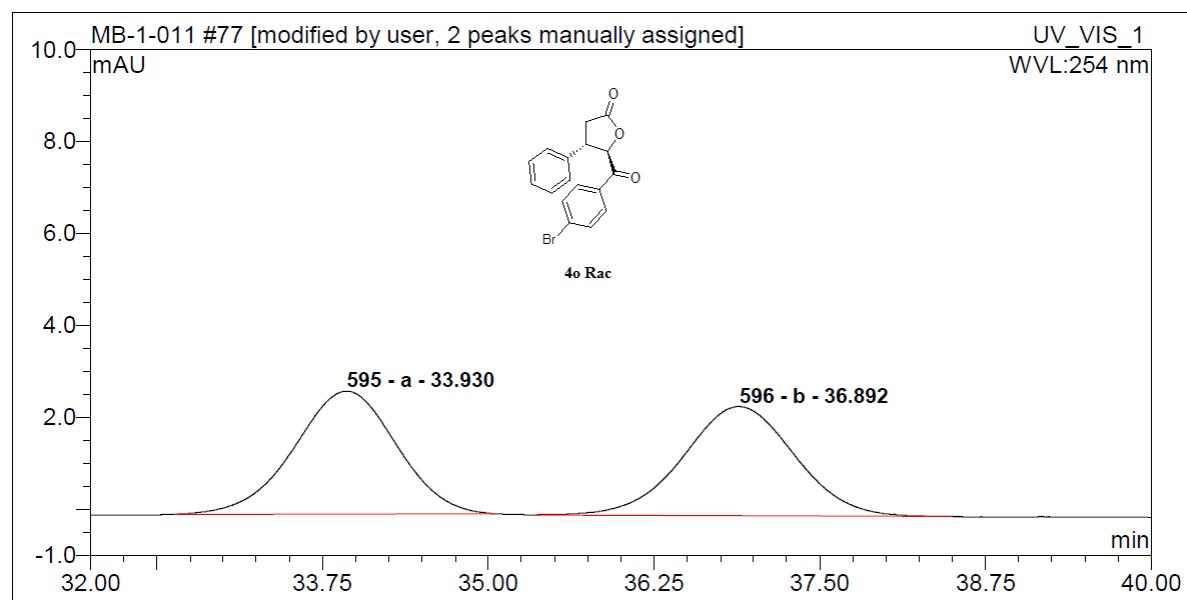
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A		11.93	8.335955	3.146997602	13.64385 n.a.
2	B		16.89	256.550	96.8530024	90.817 n.a.



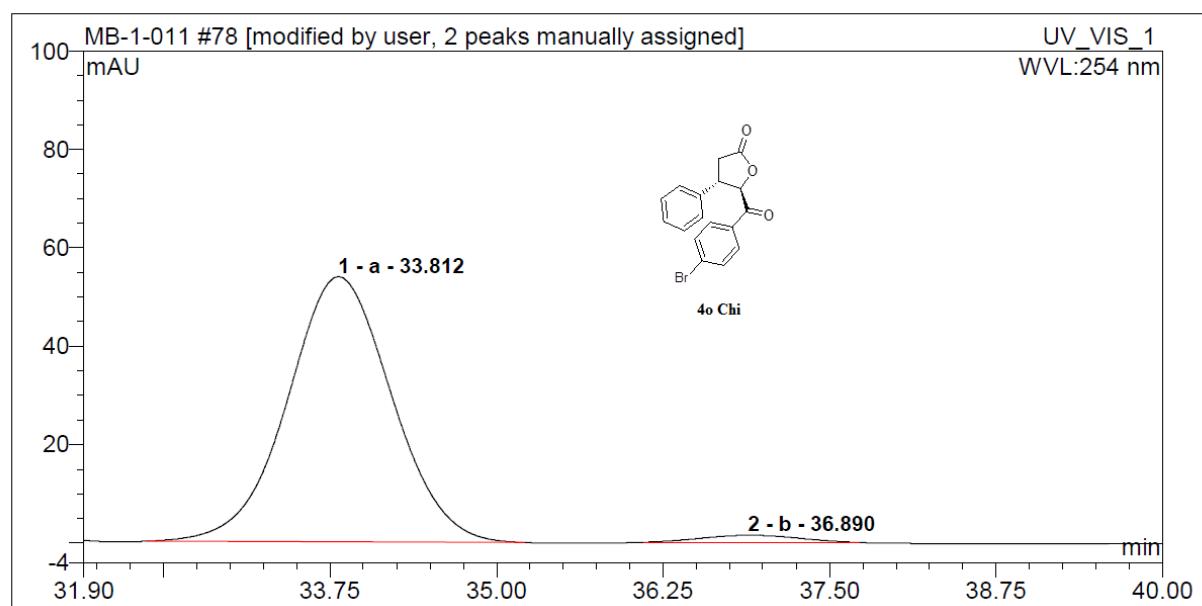
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
306 a		24.64	54.19721	50.08401951	84.13543	n.a.
307 b		26.31	54.015	49.91579996	76.894	n.a.



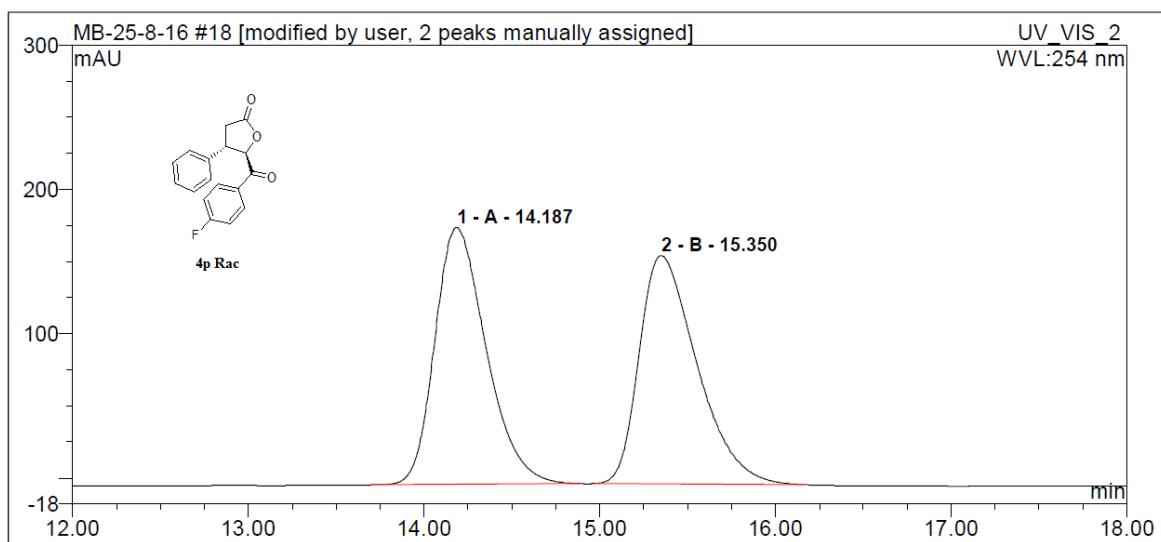
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
1 a		24.54	180.1373	95.40089306	271.4456	n.a.
2 b		26.40	8.684	4.599106943	13.453	n.a.



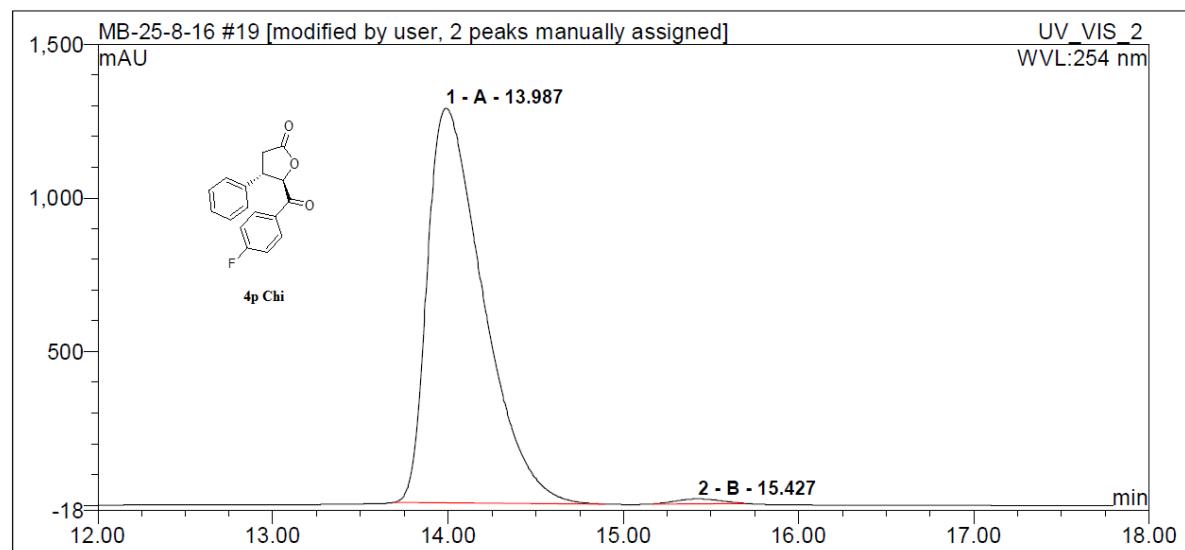
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
	595 a		33.93	2.38791	50.72912066	2.66961 n.a.
	596 b		36.89	2.319	49.26820204	2.374 n.a.



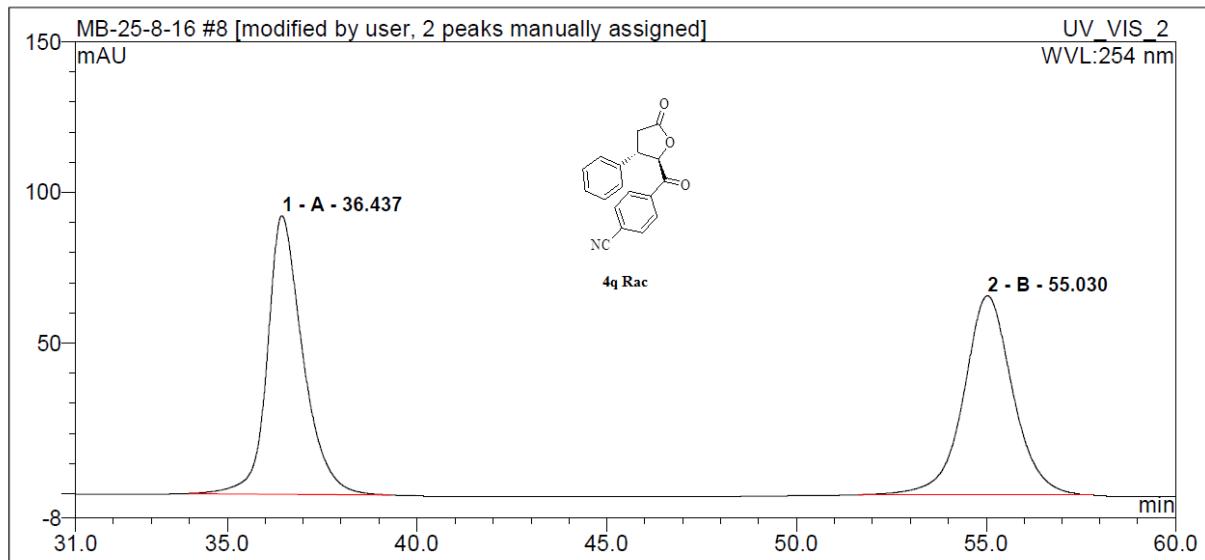
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
	1 a		33.81	48.93304	97.56103327	53.93234 n.a.
	2 b		36.89	1.223	2.438966727	1.461 n.a.



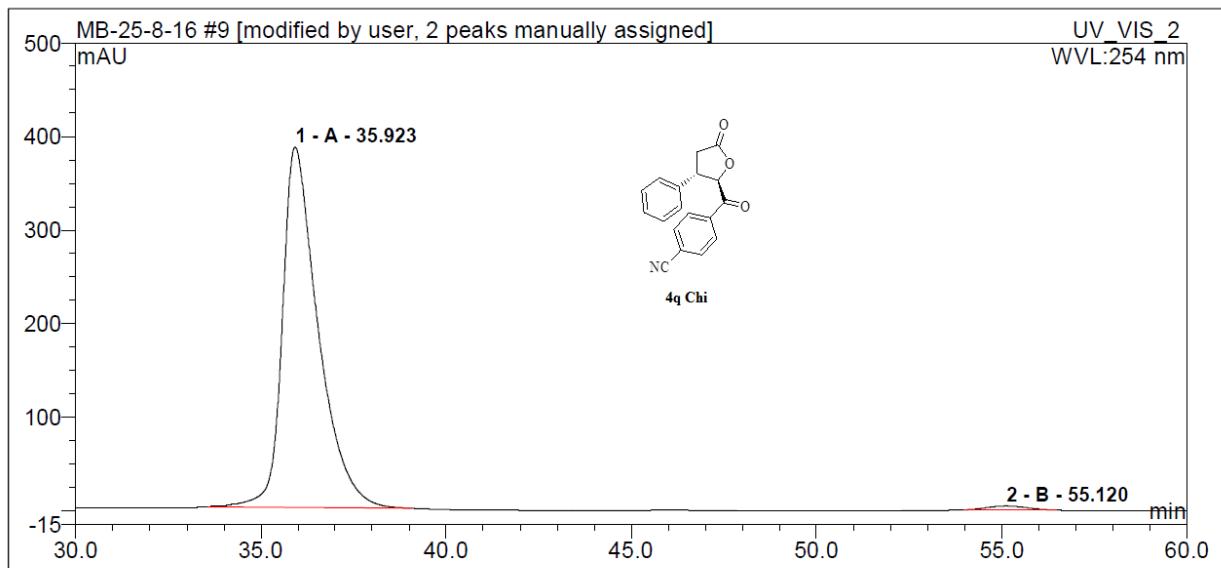
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
1	A	14.19	60.45521	50.16013201	177.8762	n.a.
2	B	15.35	60.069	49.83986799	158.195	n.a.



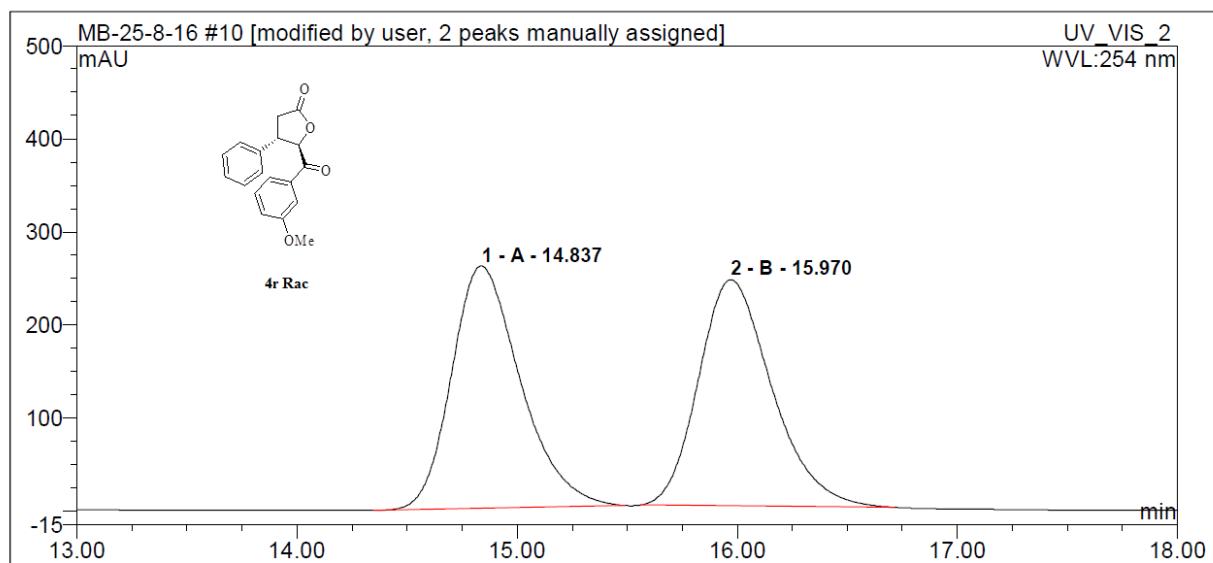
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
1	A	13.99	474.5087	99.07618954	1284.097	n.a.
2	B	15.43	4.424	0.923810462	15.240	n.a.



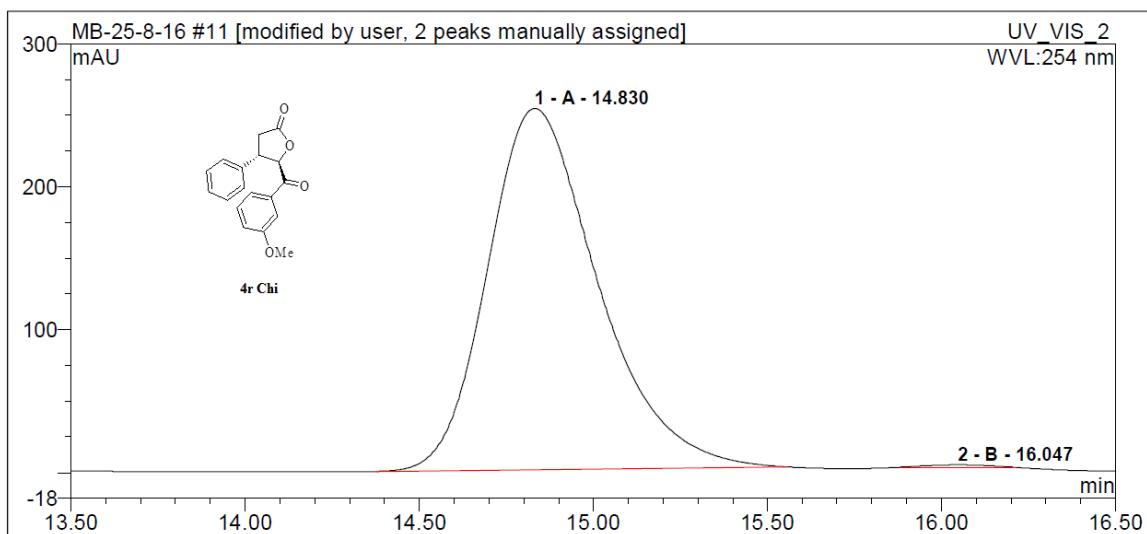
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	36.44	100.3646	50.27015235	92.29022	n.a.
2	B	55.03	99.286	49.72984765	66.031	n.a.



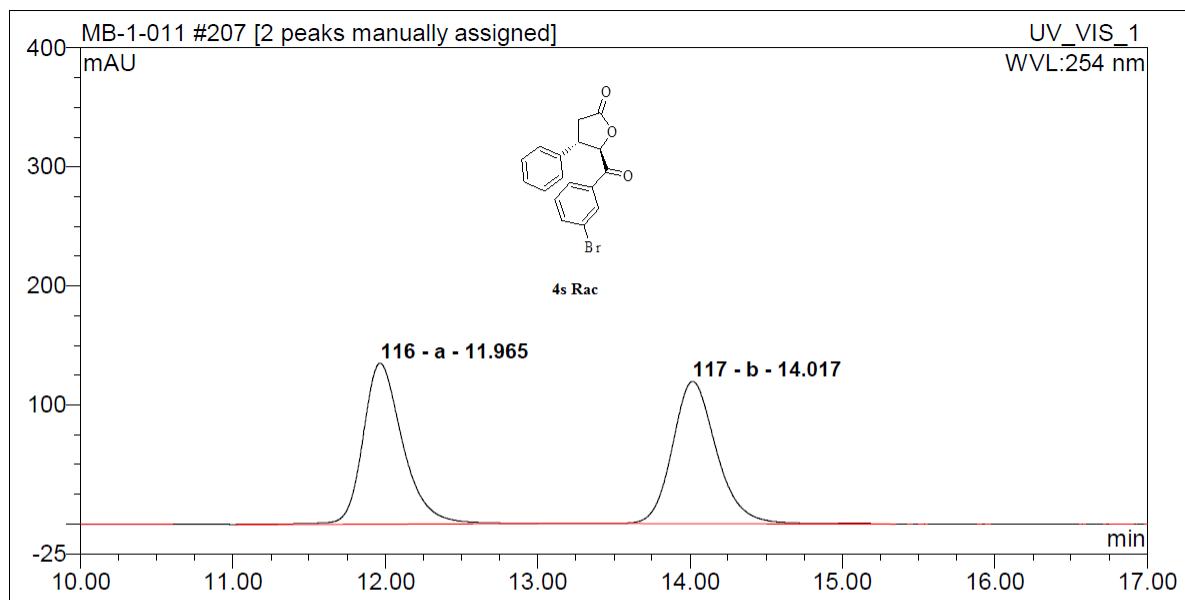
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	35.92	431.8022	98.77404007	385.1076	n.a.
2	B	55.12	5.359	1.225959929	4.323	n.a.



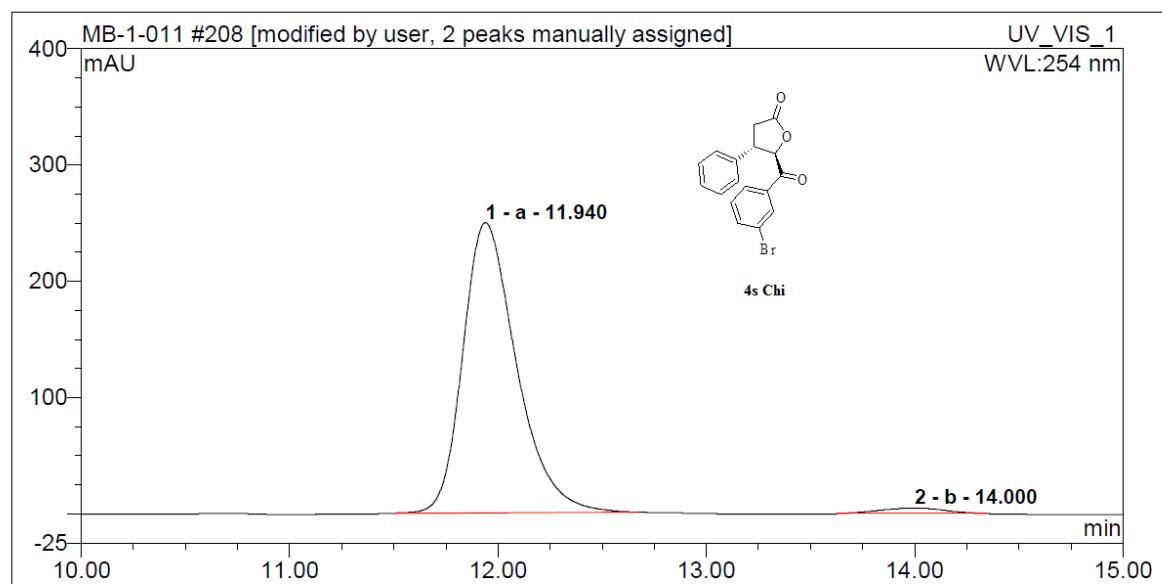
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	14.84	94.56229	50.16407093	260.2805	n.a.
2	B	15.97	93.944	49.83592907	242.996	n.a.



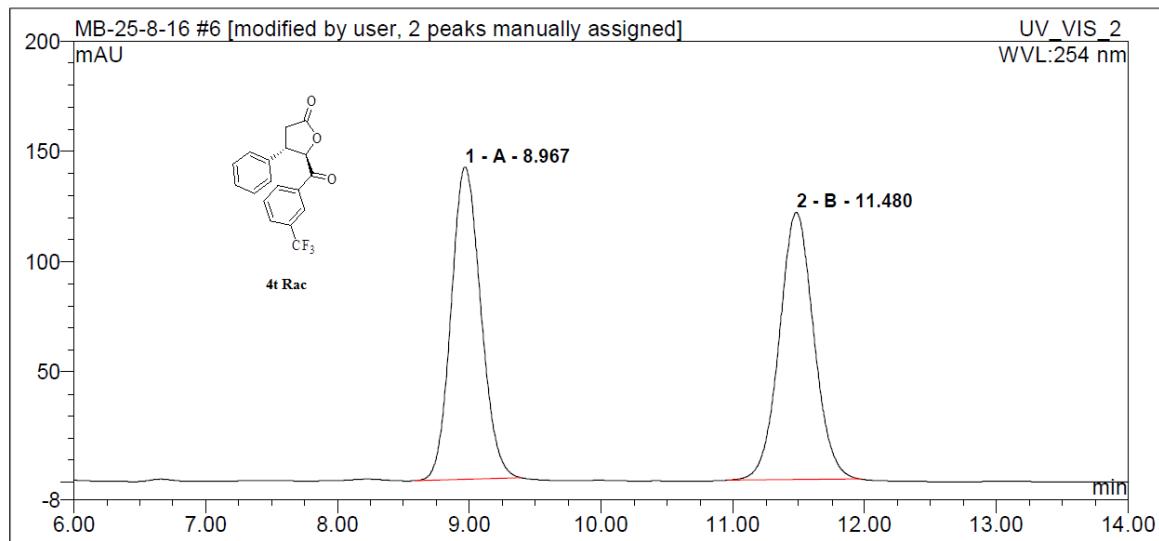
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	14.83	92.78744	99.60979436	252.6538	n.a.
2	B	16.05	0.363	0.3902056434	1.765	n.a.



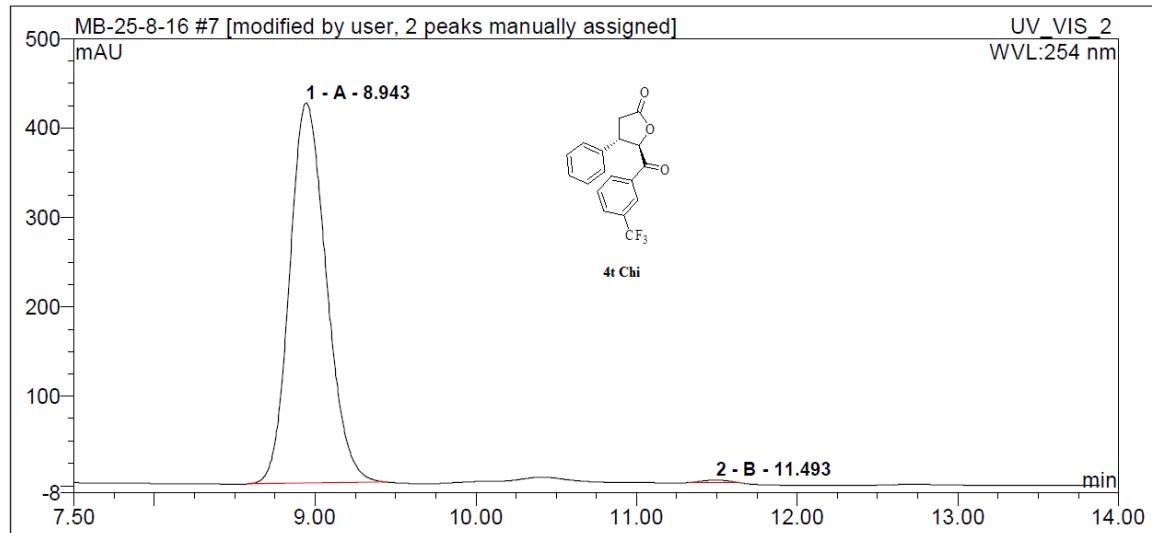
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
116 a		11.97	41.05002	50.50084597	135.1438	n.a.
117 b		14.02	40.236	49.49912071	119.623	n.a.



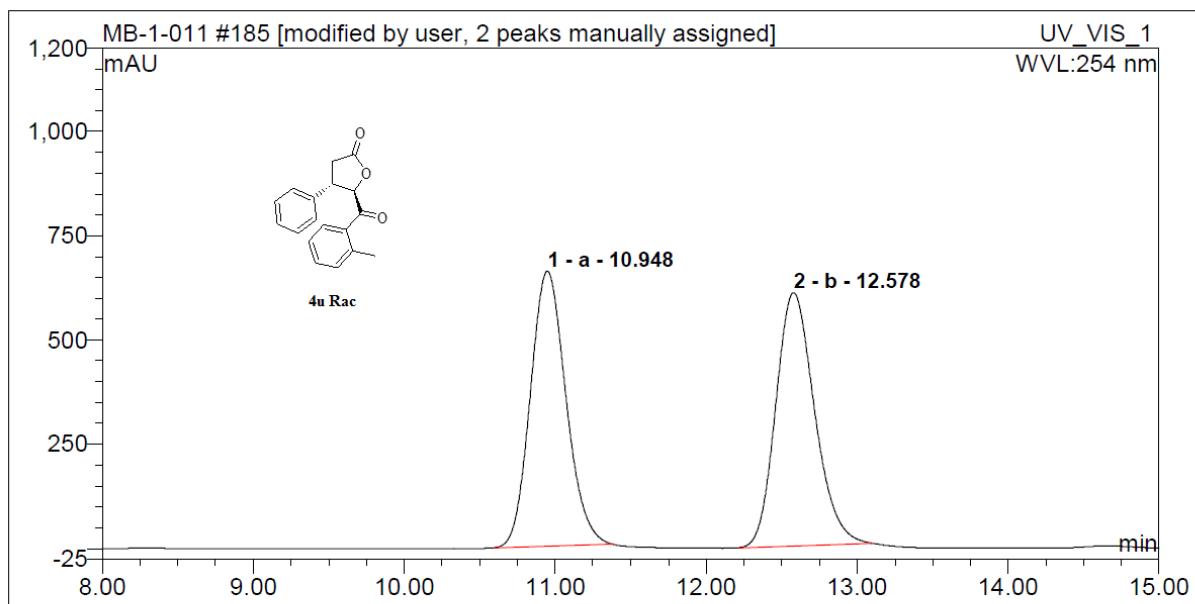
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1 a		11.94	74.4642	97.68224503	249.2906	n.a.
2 b		14.00	1.767	2.317754967	4.833	n.a.



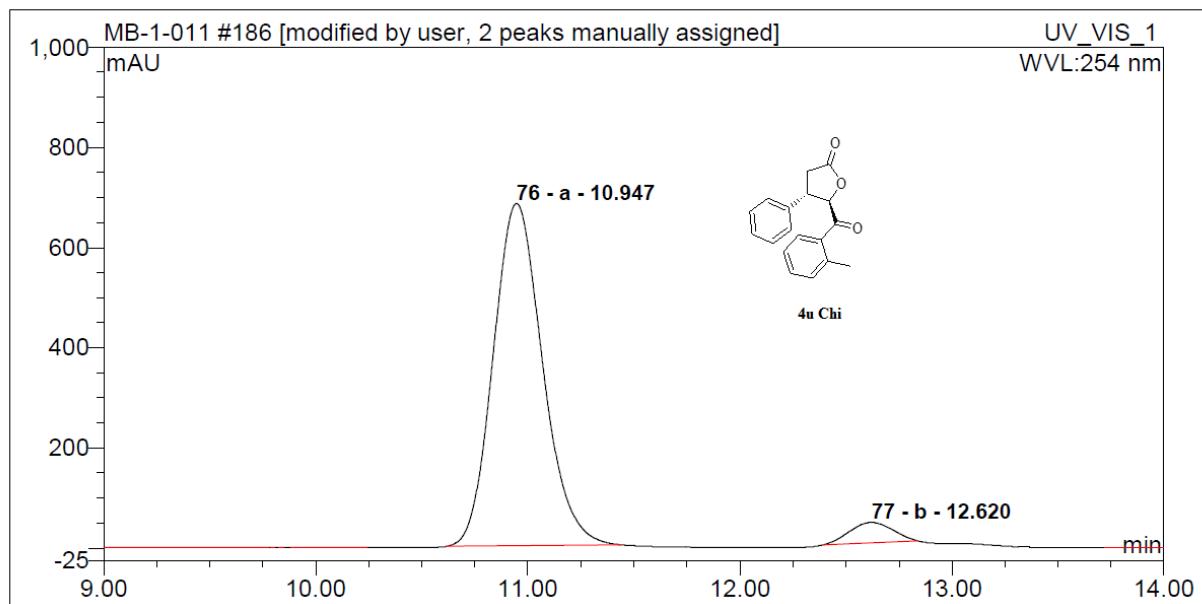
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
1	A	8.97	36.93619	50.12050683	141.447	n.a.
2	B	11.48	36.759	49.87949317	121.152	n.a.



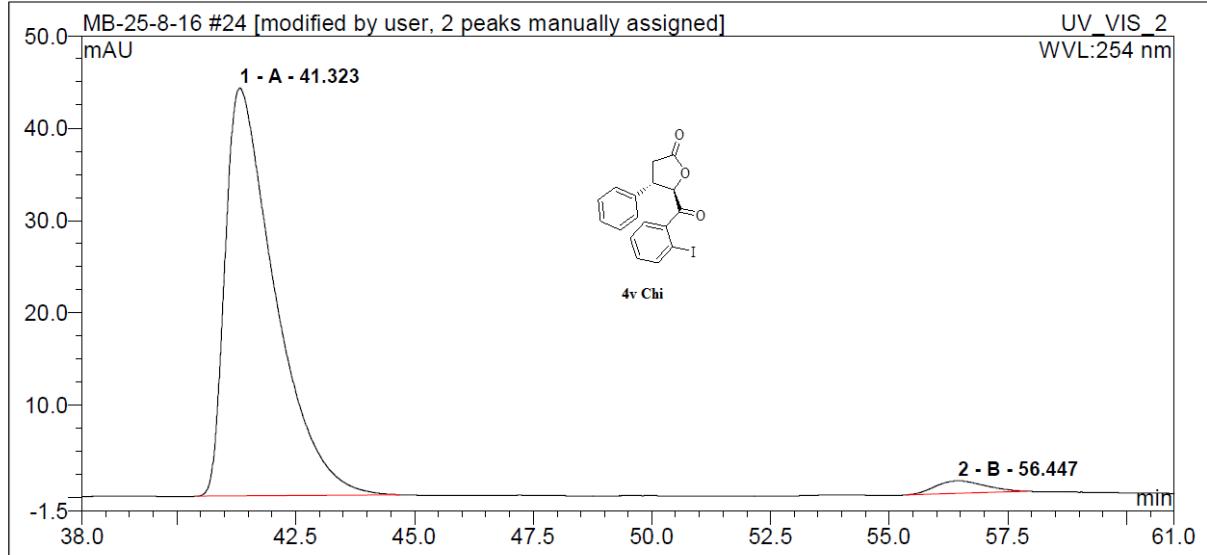
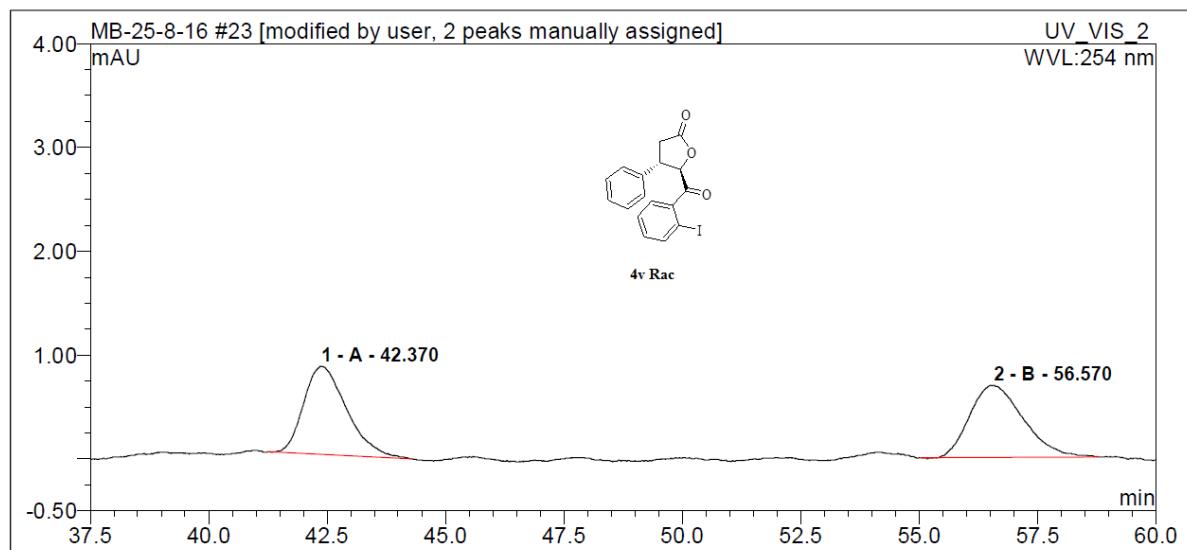
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
1	A	8.94	112.5761	99.50603703	424.8767	n.a.
2	B	11.49	0.559	0.4939629686	2.944	n.a.

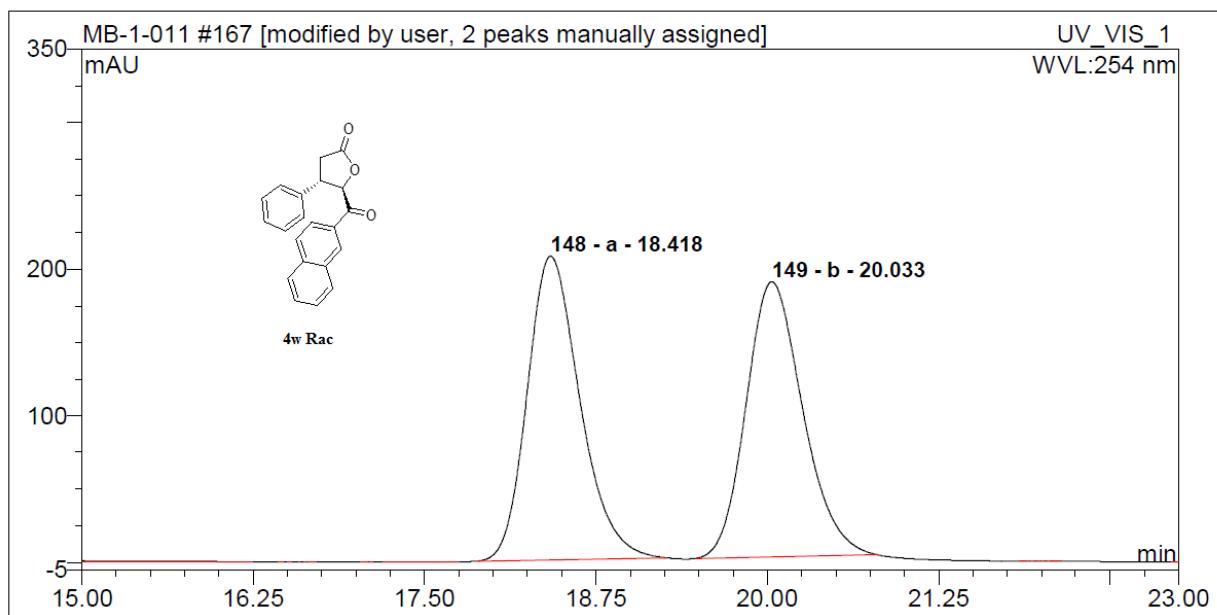


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1 a		10.95	180.0921	49.9087365	659.9301	n.a.
2 b		12.58	180.751	50.0912635	607.361	n.a.

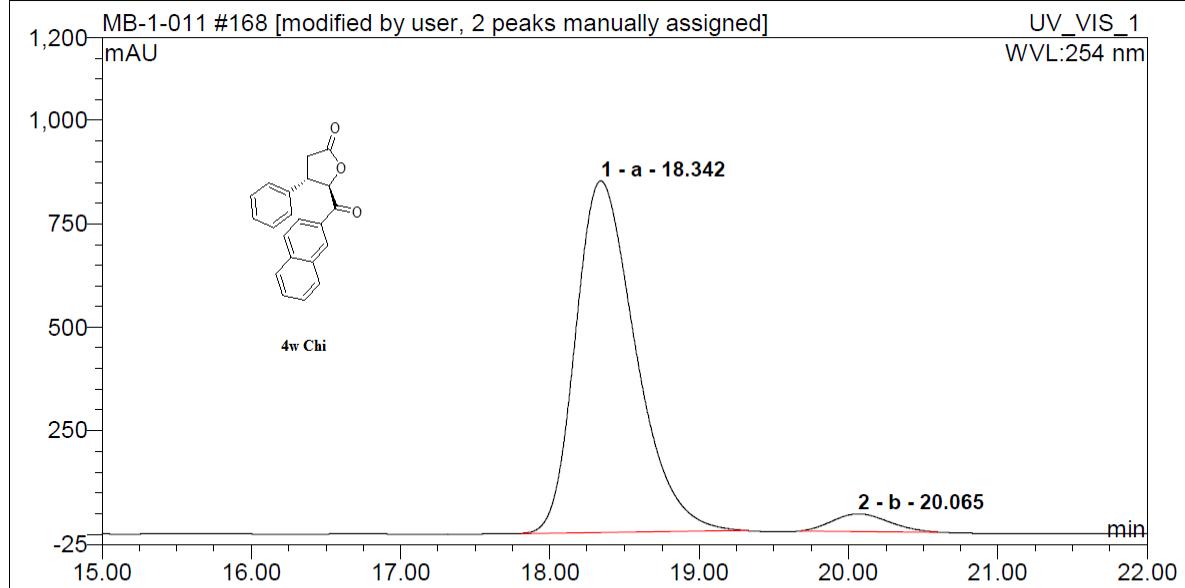


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
76 a		10.95	184.102	95.11297891	683.6687	n.a.
77 b		12.62	9.459	4.886964947	40.344	n.a.

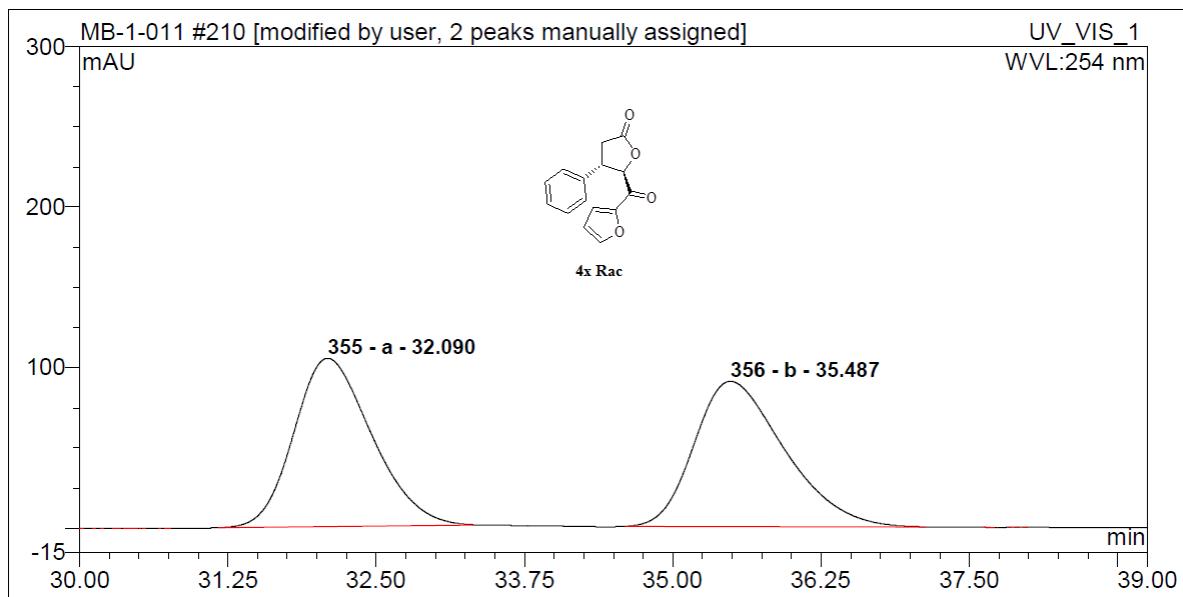




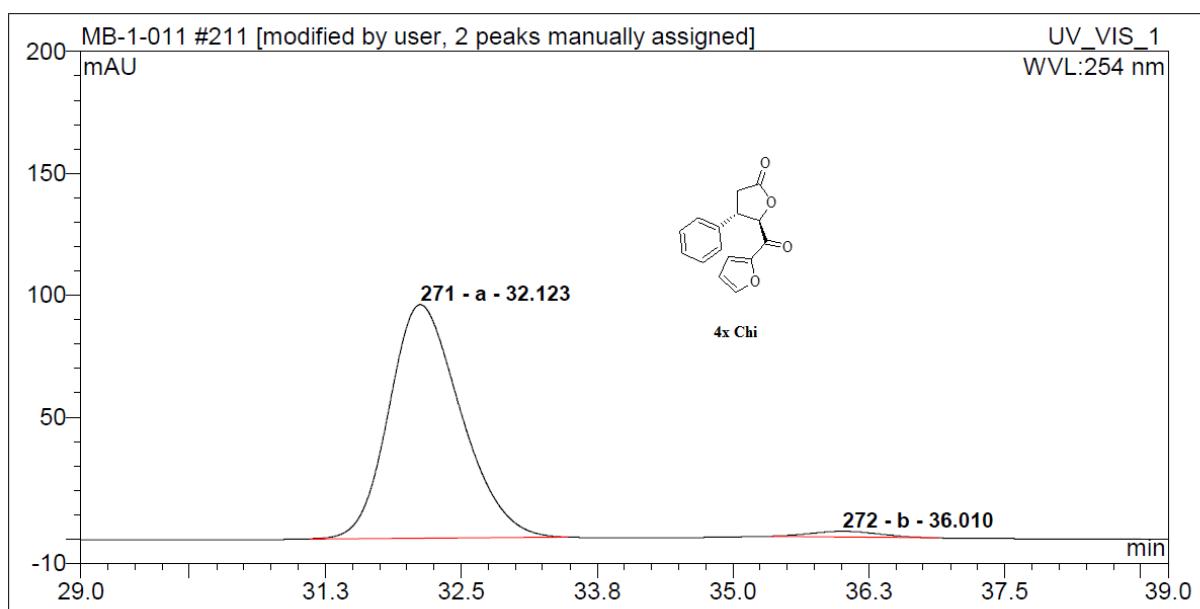
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
	148 a		18.42	92.15637	50.64773479	207.1681 n.a.
	149 b		20.03	89.798	49.35147223	187.699 n.a.



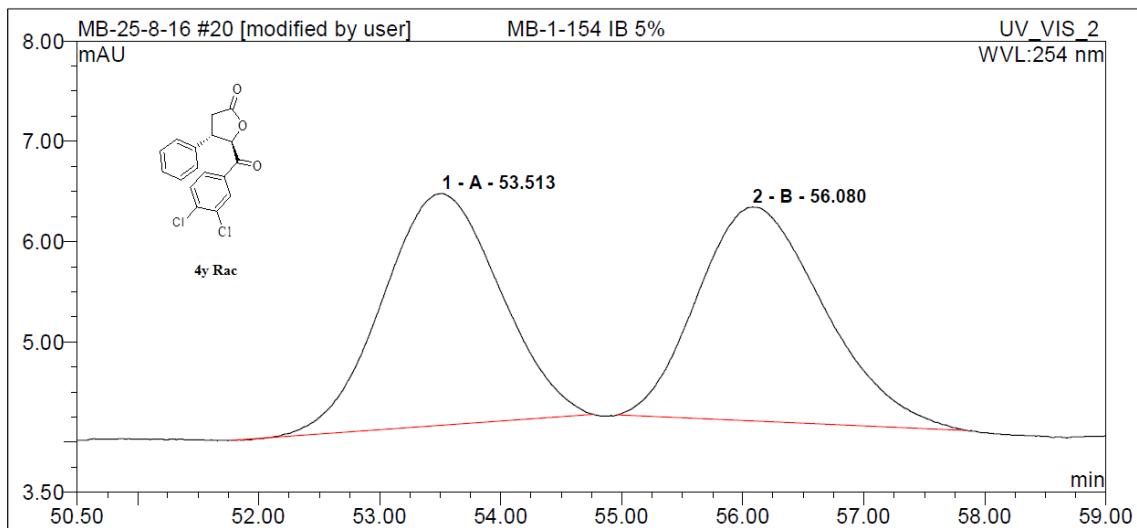
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
	1 a		18.34	395.1686	95.54062656	849.9232 n.a.
	2 b		20.07	18.445	4.459373442	42.431 n.a.



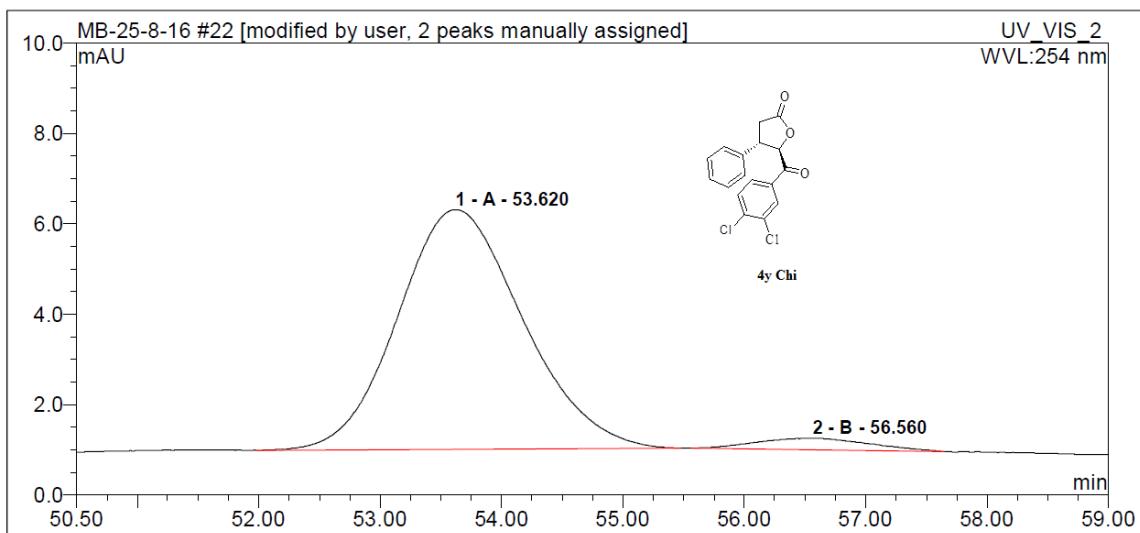
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
	355 a	32.09	79.73833	49.96019634	104.8315	n.a.
	356 b	35.49	79.865	50.03973563	90.502	n.a.



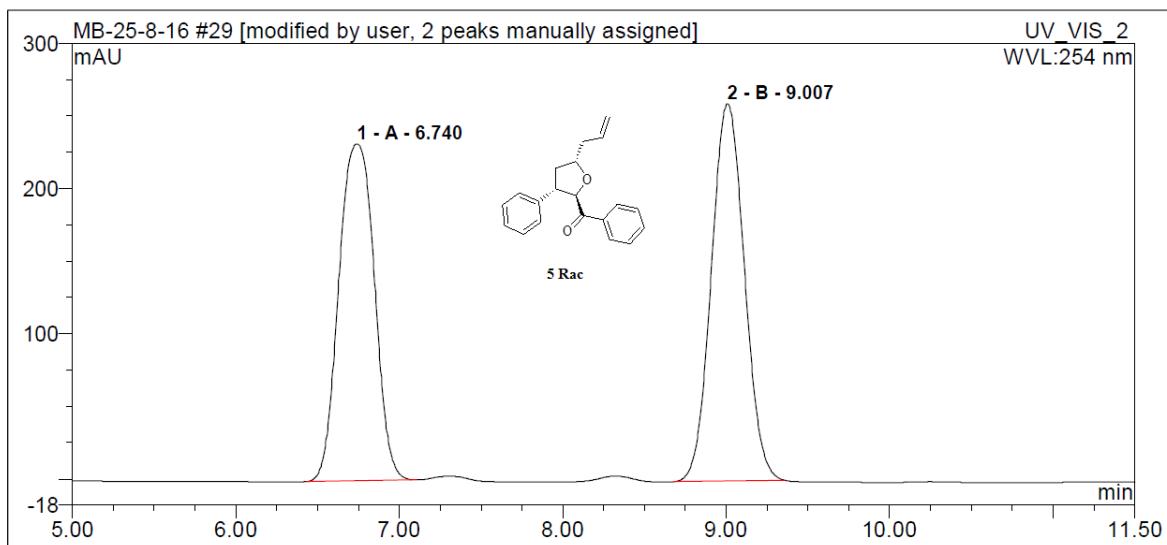
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
	271 a	32.12	73.30616	97.76183648	95.75967	n.a.
	272 b	36.01	1.678	2.238019957	2.298	n.a.



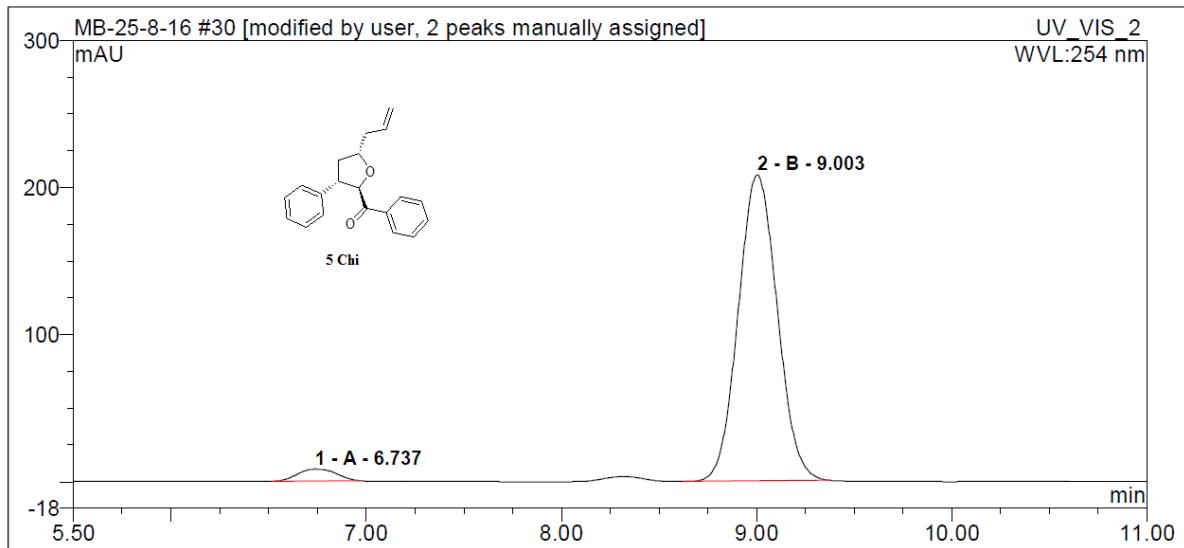
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	53.51	2.59955	50.1582203	2.30984	n.a.
2	B	56.08	2.583	49.8417797	2.132	n.a.



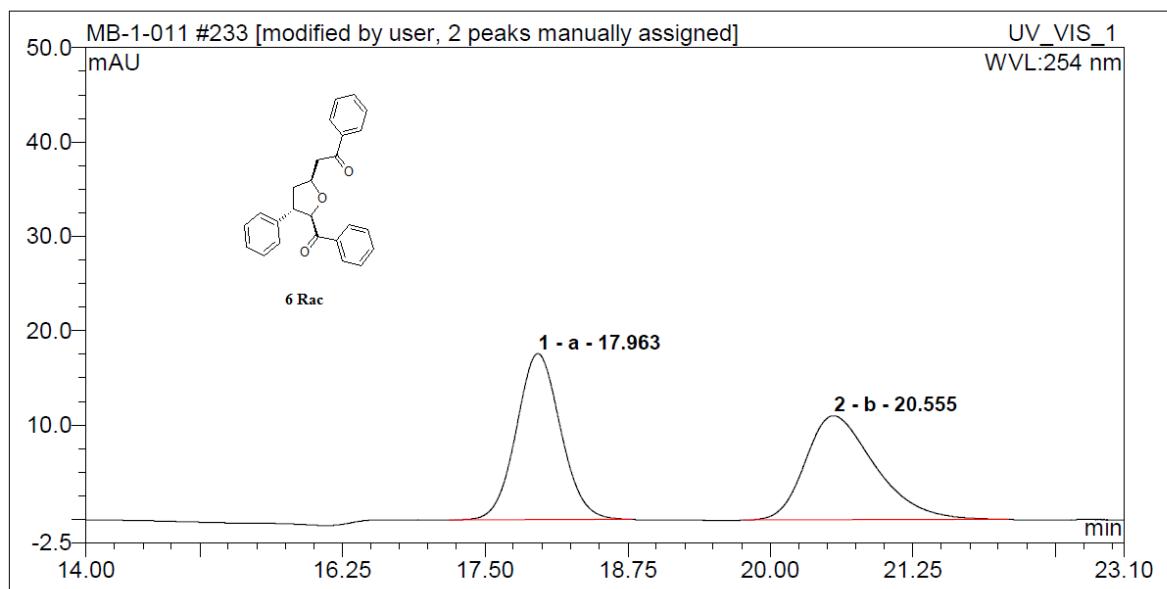
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	A	53.62	6.309404	95.8962818	5.29364	n.a.
2	B	56.56	0.270	4.103718199	0.253	n.a.



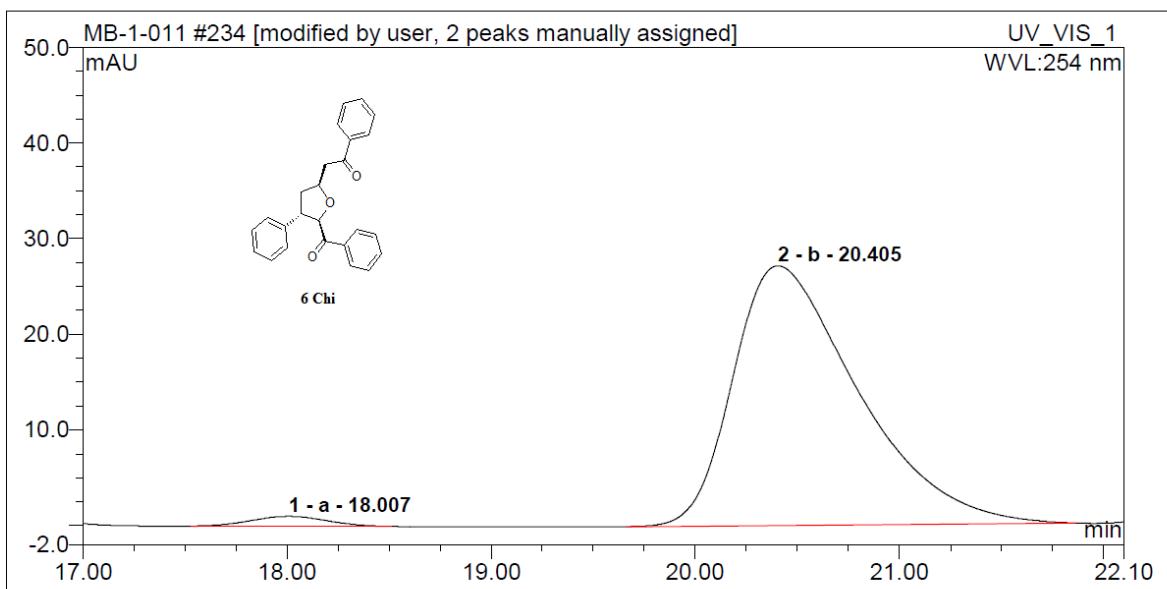
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
1	A	6.74	58.41951	48.99512401	231.9066	n.a.
2	B	9.01	60.816	51.00487599	259.867	n.a.



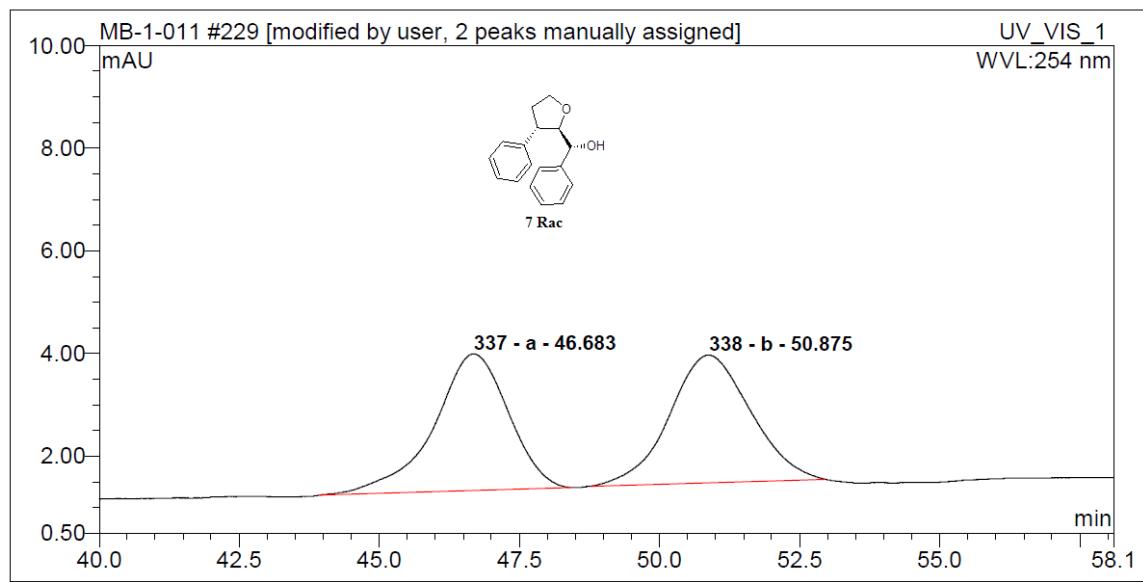
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
1	A	6.74	1.833884	3.662965885	8.13691	n.a.
2	B	9.00	48.232	96.33703411	208.043	n.a.



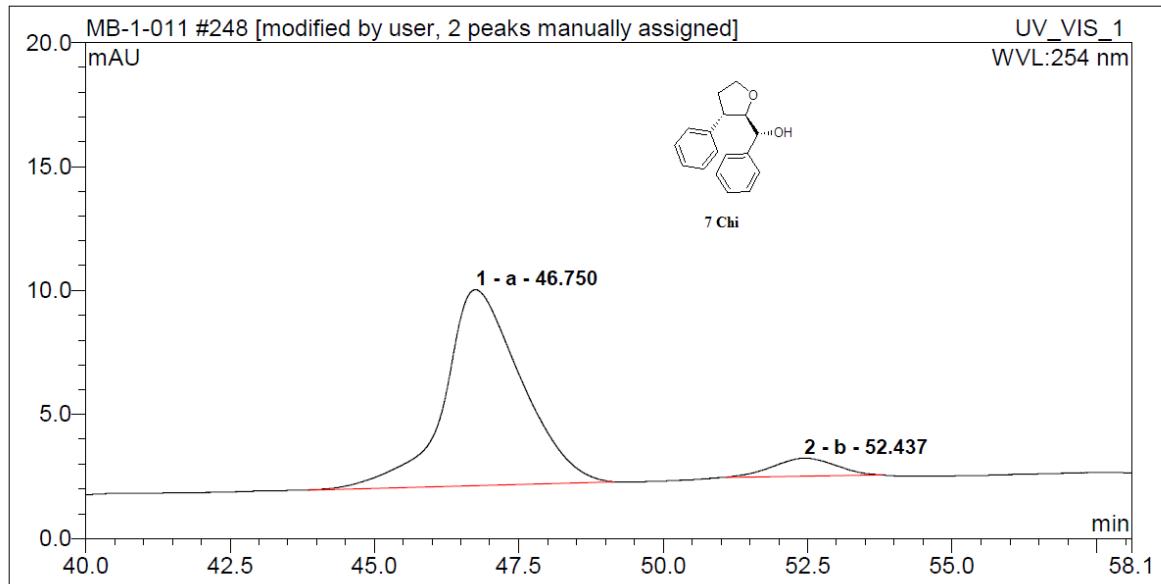
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1 a		17.96	7.942766	50.30993227	17.61185	n.a.
2 b		20.56	7.845	49.69006773	11.050	n.a.



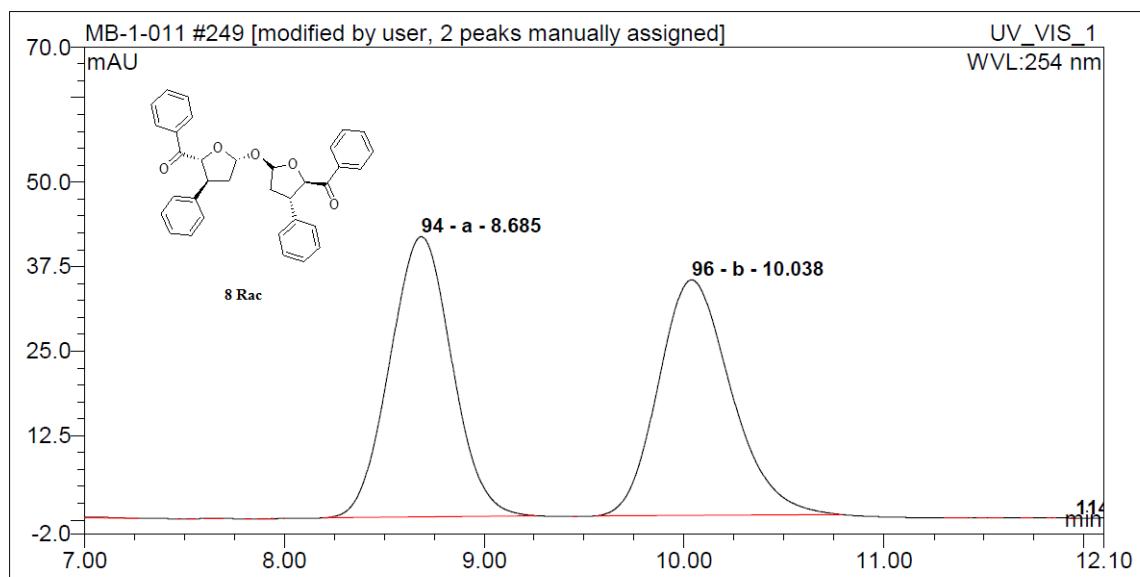
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1 a		18.01	0.445667	2.262511532	1.04063	n.a.
2 b		20.41	19.252	97.73748847	27.170	n.a.



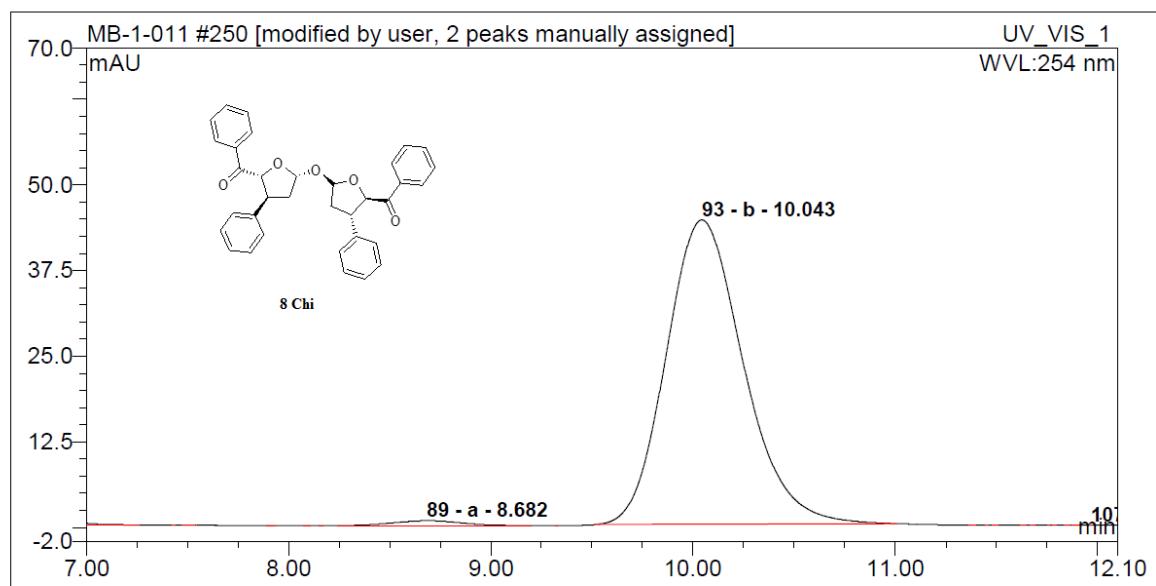
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
	337 a		46.68	4.106298	49.577969	2.66554 n.a.
	338 b		50.88	4.176	50.42176397	2.492 n.a.



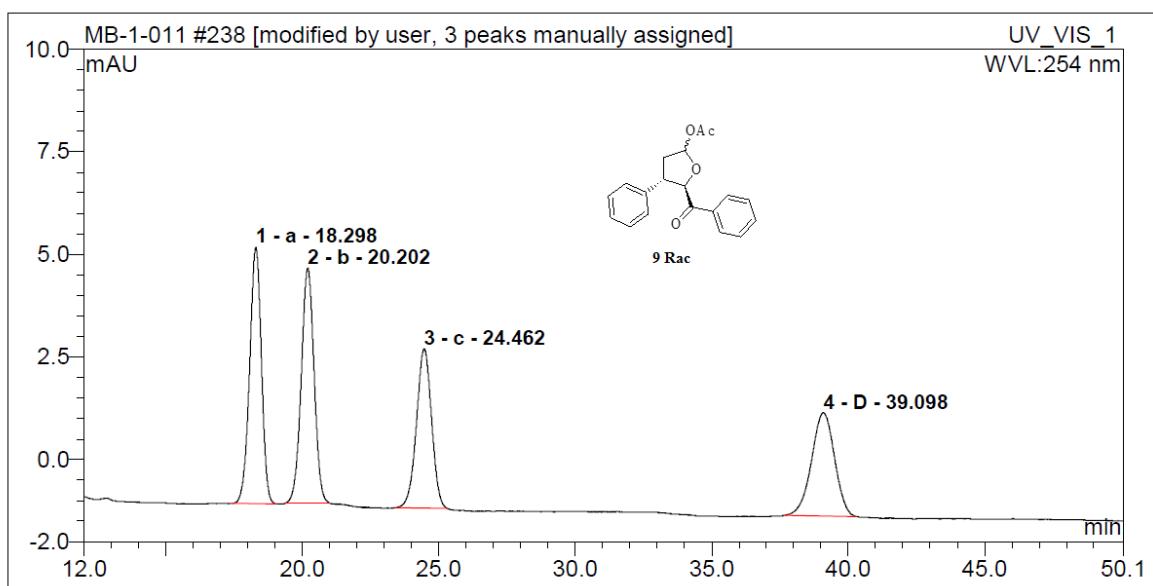
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
	1 a		46.75	12.24679	93.11527463	7.89623 n.a.
	2 b		52.44	0.905	6.884725365	0.727 n.a.



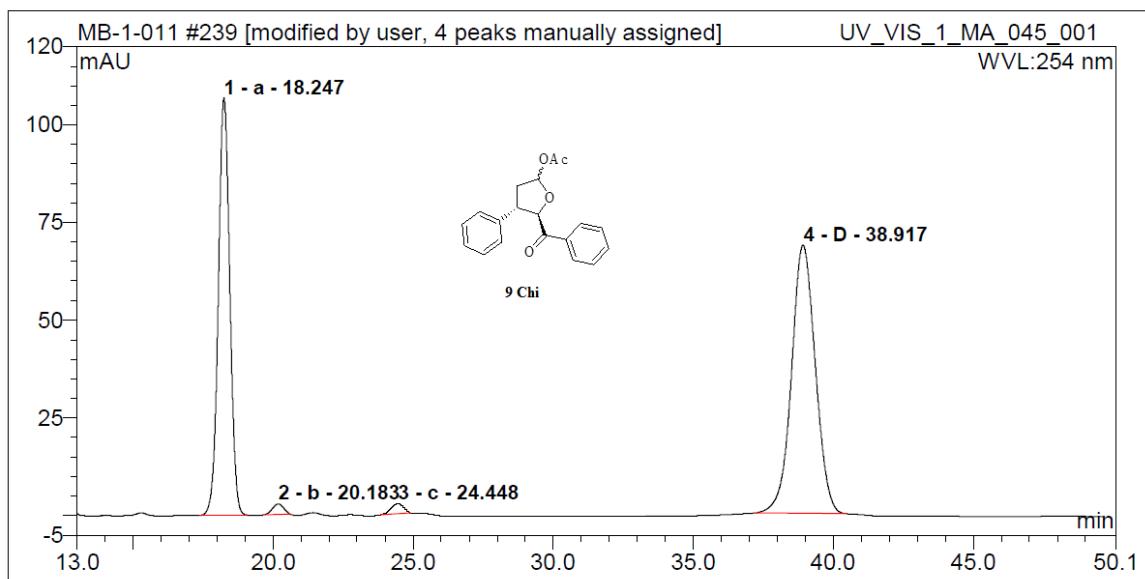
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
94 a			8.69	14.93028	50.33792702	41.46754 n.a.
96 b			10.04	14.730	49.66174201	34.851 n.a.



No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
89 a			8.68	0.27468	1.378520679	0.70978 n.a.
93 b			10.04	19.651	98.6213063	44.447 n.a.



No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
1 a		18.30	3.12949	27.90095192	6.24932	n.a.
2 b		20.20	3.130243	27.90766647	5.73387	n.a.
3 c		24.46	2.493796	22.23342312	3.88216	n.a.
4 D		39.10	2.463	21.95795849	2.516	n.a.



No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount mAU
1 a		18.25	50.53586	41.83101589	106.7652	n.a.
2 b		20.18	1.263556	1.045907166	2.7045	n.a.
3 c		24.45	1.35343	1.120300874	2.53674	n.a.
4 D		38.92	67.657	56.00277607	68.631	n.a.