Access to Chiral Phthalidyl Ester prodrugs via Isothiourea-Catalyzed Dynamic Kinetic Resolution Reaction

[Supporting Information]

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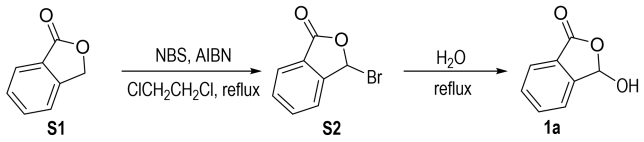
I. General information

Commercially available materials purchased from Energy Chemical and J&K were used directly in the experiment without further purification. ^{1}HNMR, ^{13}C NMR and ^{19}F NMR spectra were recorded either on a JEOL-ECX-500 (500 MHz) or on a Bruker ASCEND 400 (400 MHz) Spectrometer in $CDCl_3$ with trimethylchlorosilane as the internal reference. Chemical shifts (δ) for ^{1}H and ^{13}C NMR spectra are given in ppm relative to TMS. The residual solvent signals were used as references for ^{1}H and ^{13}C NMR spectra and the chemical shifts converted to the TMS scale ($CDCl_3$: δH = 7.26 ppm, δC = 77.16 ppm). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, doublet of doublets (dd), m = multiplet, and etc. High resolution mass spectra (HRMS) were obtained on Thermo Fisher Q Exactive mass spectrometer. HPLC analyses were measured Shimadzu Prominence LC-20A (Shimadzu, Japan) detector, chiralcel brand chiral columns from Daicel Chemical Industries were used with model IA, IB, OD-H in 4.6 × 250 mm size. Melting points were measured on a Beijing Tech Instrument X-4 digital display micro melting point apparatus and are uncorrected. Analytical thin-layer chromatography (TLC) was carried out on pre-coated silica gel plate (0.2 mm thickness). Visualization was performed using a UV lamp. Meanwhile, the reaction process was aslo monitored using Agilent 7890B-5977B gas chromatography-mass spectrometry (GC-MS).

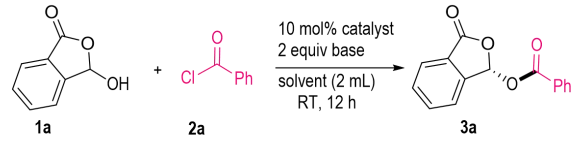
II. Preparation of substrates

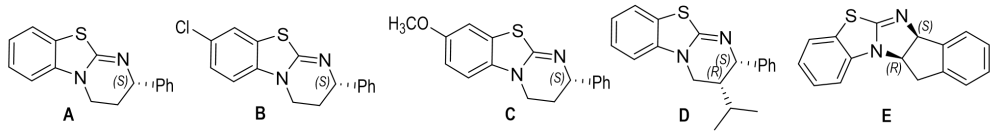


Based on previously reported methods.[1] To a solution of **S1** (2.0 mmol) in $ClCH_2CH_2Cl$ (10 mL), NBS (2.2 mmol, 1.1 eq) and AIBN (0.2 mmol, 0.1 eq) were added at room temperature. The mixture was heated to reflux overnight. After cooling to room temperature, it was concentrated under reduced pressure and purified by chromatography to obtain compound **S2**. Subsequently, **S2** was suspended in H_2O (20 mL) and heated to reflux for 1 hour. The mixture was allowed to cool to room temperature and then extracted with EtOAc. The combined extracts were dried over $MgSO_4$, filtered, and concentrated under reduced pressure to yield the crude product as a solid. Finally, the solid was purified by chromatography to obtain the desired product as a white solid. Compounds **1s-1u** were synthesized using the same method, and the relevant spectra have been reported in previous literature.[2,3] Additionally, compounds **1x-1v** were obtained commercially and did not require further purification.

Simpler acyl chlorides were obtained commercially, while some acyl chlorides were synthesized from the corresponding carboxy acids using oxalyl chloride or $SOCl_2$ as acylating agents.

III. Conditions optimization

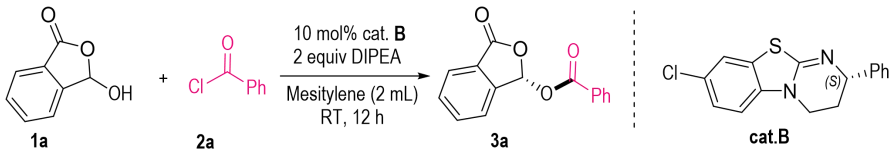




Entry	Cat.	Solvent	Base	Yield (% yield[b])	er[c]
1	A	THF	DIPEA	89	91:9
2	B	THF	DIPEA	91	92:8
3	C	THF	DIPEA	88	90:10
4	D	THF	DIPEA	87	90:10
5	E	THF	DIPEA	83	49:51
6	B	DCM	DIPEA	96	86:14
7	B	Toluene	DIPEA	81	95:5
8	B	Chlorobenzene	DIPEA	85	93:7
9	B	Mesitylene	DIPEA	92	95:5
10	B	Mesitylene	K_2CO_3	86	90:10
11	B	Mesitylene	DBU	97	60:40
12	B	Mesitylene	Et_3N	91	93:7
13	B	Mesitylene	DIPEA	81	95:5[b]
14	B	Mesitylene	DIPEA	76	95:5[c]
15	B	Mesitylene	Without DIPEA	<10% yield	88:12[d]
16	B	Mesitylene	DIPEA	95	93:7[e]

[a] Reaction conditions: **1** (0.10 mmol), **2a** (0.15 mmol), Cat. (0.01 mmol), Base (0.20 mmol), Solvent (2.0 mL), RT., 12 h. [b]Cat. (0.005 mmol). [c] DIPEA (0.15 mmol). [d] Without DIPEA. [e] Mesitylenet (1.0 mL). Yields were isolated yields. Er values were determined via HPLC using a chiral stationary phase.

IV. General Procedure for the Synthesis of 3a



Isothiourea catalyst B (0.01 mmol) and acyl chloride **2a** (0.15 mmol) were added to a 4 mL oven-dried vial equipped with a magnetic stir bar, then 2 mL of mesitylene

was added as solvent. Subsequently, Phthalide **1a** (0.10 mmol) and DIPEA (0.20 mmol) were added to the reaction mixture and the mixture was stirred for 12 hours at room temperature. Notably, the stirring speed should be controlled between 200-300 r/min, as vigorous stirring is not suitable in the early stage of the reaction. The solvent was removed in vacuo and the residual was purified by column chromatography on silica gel (10:1 to 5:1 petroleum ether / EtOAc) directly to give the desired pure products **3a**.

V. Determination of the yield of compound 3a by HPLC

Based on previously reported methods.[4] Compound **1a** was dissolved in CH_3CN to a concentration range of 0.05-0.6 mg/mL. The peak area was detected by HPLC with an injection volume of 5 μL. A standard curve was prepared based on the concentration and peak area (Table S1) .HPLC was used to determine the yield of the target compound **3a**. The procedure involved adding 2 mL of CH_3CN to the reaction mixture after the reaction was complete, stirring for 2.0 min to ensure full dissolution of the compound. Subsequently, 100 μL of the mixture was taken and diluted to 1.0 mL with acetonitrile, resulting in a 20-fold dilution of the reaction system.

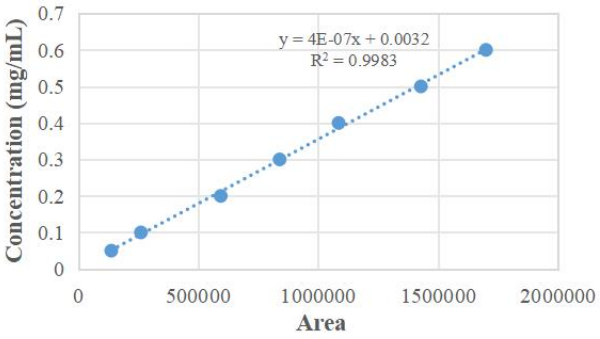
HPLC analysis: IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm, Injection volume = 5 μL, Dilution times = 20.

$$\text{Yield(HPLC)} = \frac{(4\text{E}{-}07\times\text{Area}+ 0.0032)\times 2\times \text{ dilution times}}{\text{theoretical yield}} \times 100\%$$

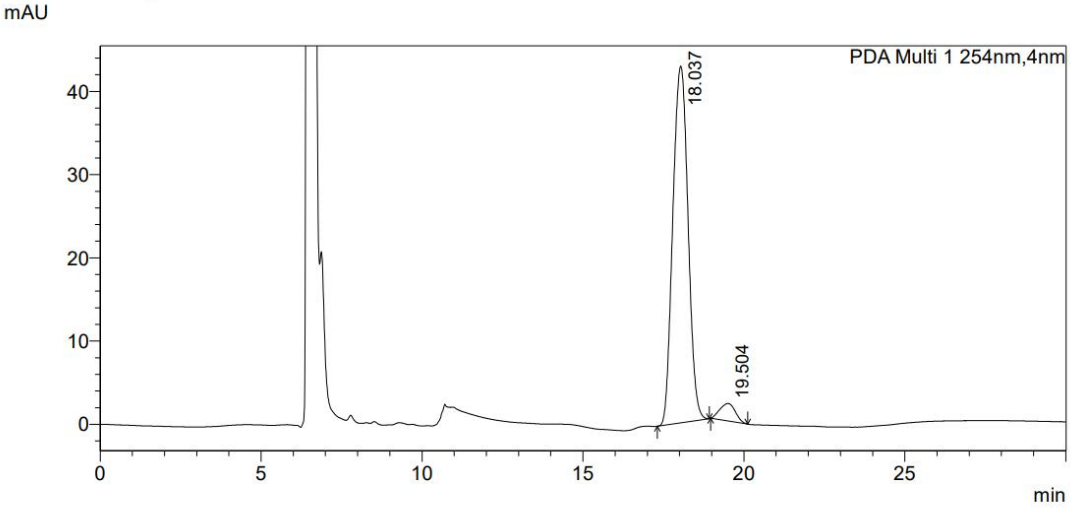
$$\text{Yield(HPLC)} = \frac{(4\text{E}{-}07\times 1476877+ 0.0032)\times 2\times 20}{25} \times 100\% \approx 95$$

Table S1. Stock solutions of varying concentrations **3a**

Sample	Concentration (mg/mL)	Area
1	0.05	137294
2	0.1	260937
3	0.2	593534
4	0.3	839018
5	0.4	1084867
6	0.5	1427828
7	0.6	1699139



<Chromatogram>



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	18.037	1406673	95.246
2	19.504	70204	4.754
Total		1476877	100.000

VI. Scaling-up reaction for the synthesis of compound (*S*)-3a

To investigate the practicality of the reaction, we performed a scale-up experiment with compound **1a** at a 5 mmol scale. Initially, benzoyl chloride **2a** (1.05 g) was added dropwise into the solution of Isothiourea catalyst **B** (0.15 g) in mesitylene (80 mL). Then the reaction mixture was allowed to proceed at room temperature for 20 minutes. Subsequently, **1a** (0.75 g) and a portion of DIPEA (0.32

g) were added into the reaction mixture. After an additional 5 minutes, the remaining DIPEA dissolved in 20 mL mesitylene was gradually added into the reaction system over 30 minutes. The mixture was stirred for 12 hours to obtain 0.99 g of the desired compound (*S*) -**3a**, with a yield of 78% and er value of 93:7.

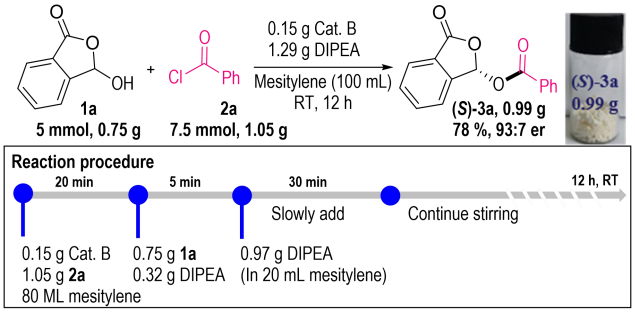


Figure S1. Scaling-up reaction for the synthesis of compound (*S*)-**3a**

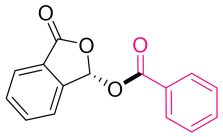
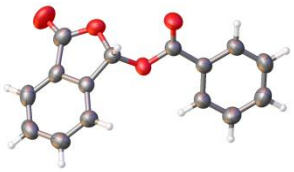
VII. X-ray crystallography of compound *(S)*-3a.

Experimental: Good quality crystal of **(*S*)-3a** (white block crystal) was obtained by vaporization of a isopropyl alcohol / hexane solution of compound (*S*)-**3a**. The crystallographic data for ***(S)*-3a** have been submitted and deposited in the Cambridge Crystallographic Data Centre. http://www.ccdc.cam.ac.uk/data_request/cif.

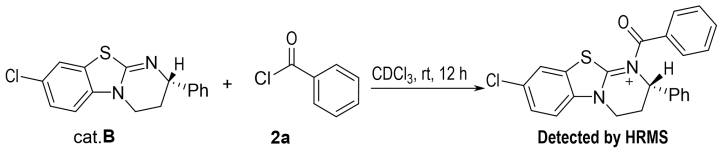
Crystal structure determination of *(S)*-3a

Crystal Data for $C_{15}H_{10}O_4$ (M =254.23 g/mol): triclinic, space group P1 (no. 1), a = 4.0759(2) Å, b = 7.1675(4) Å, c = 10.4870(6) Å, α = 96.968(3)°, β = 93.261(3)°, γ = 91.060(3)°, V = 303.51(3) Å^3, Z = 1, T = 303.00 K, μ(CuKα) = 0.847 mm^{-1}, *Dcalc* = 1.391 g/cm^3, 3426 reflections measured (8.51° ≤ 2Θ ≤ 131.98°), 1708 unique (R_{int} = 0.0295, R_{sigma} = 0.0408) which were used in all calculations. The final R_1 was 0.0333 (I > 2σ(I)) and wR_2 was 0.1180 (all data).

Table 1 Crystal data and structure refinement for (*S*)-**3a**.

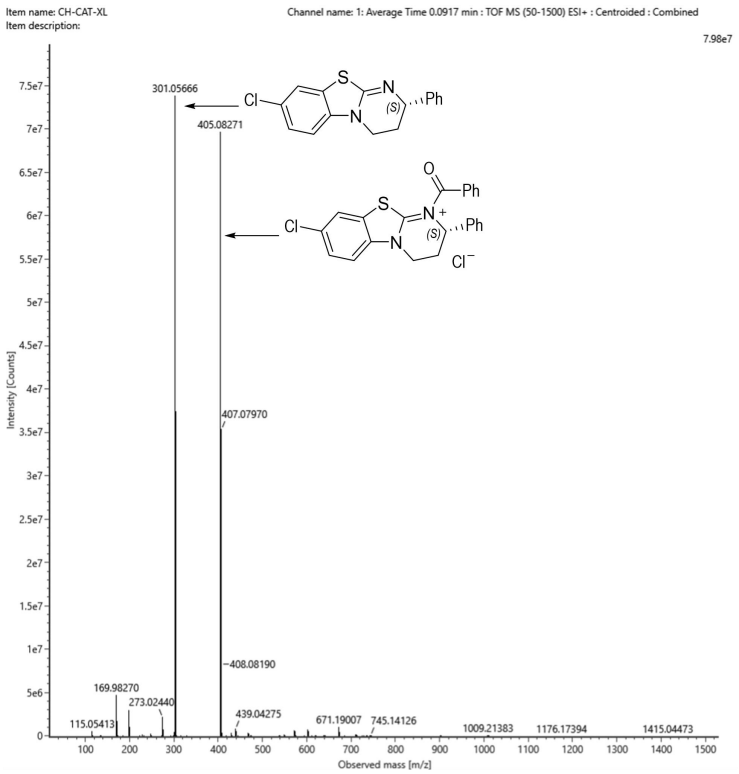
	
CCDC No.	2358966
Empirical formula	$C_{15}H_{10}O_4$
Formula weight	254.23
Temperature/K	303.00
Crystal system	triclinic
Space group	P1
a/Å	4.0759(2)
b/Å	7.1675(4)
c/Å	10.4870(6)
α/°	96.968(3)
β/°	93.261(3)
γ/°	91.060(3)
Volume/Å^3	303.51(3)
Z	1
ρ_{calc}g/cm^3	1.391
μ/mm^{-1}	0.847
F(000)	132.0
Crystal size/mm^3	0.11 × 0.1 × 0.08
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	8.51 to 131.98
Index ranges	-4 ≤ h ≤ 4, -8 ≤ k ≤ 8, -12 ≤ l ≤ 12
Reflections collected	3426
Independent reflections	1708 [R_{int} = 0.0295, R_{sigma} = 0.0408]
Data/restraints/parameters	1708/3/172
Goodness-of-fit on F^2	1.201
Final R indexes [I>=2σ (I)]	R_1 = 0.0333, wR_2 = 0.0979
Final R indexes [all data]	R_1 = 0.0364, wR_2 = 0.1180
Largest diff. peak/hole / e Å^{-3}	0.20/-0.23
Flack parameter	0.00(8)

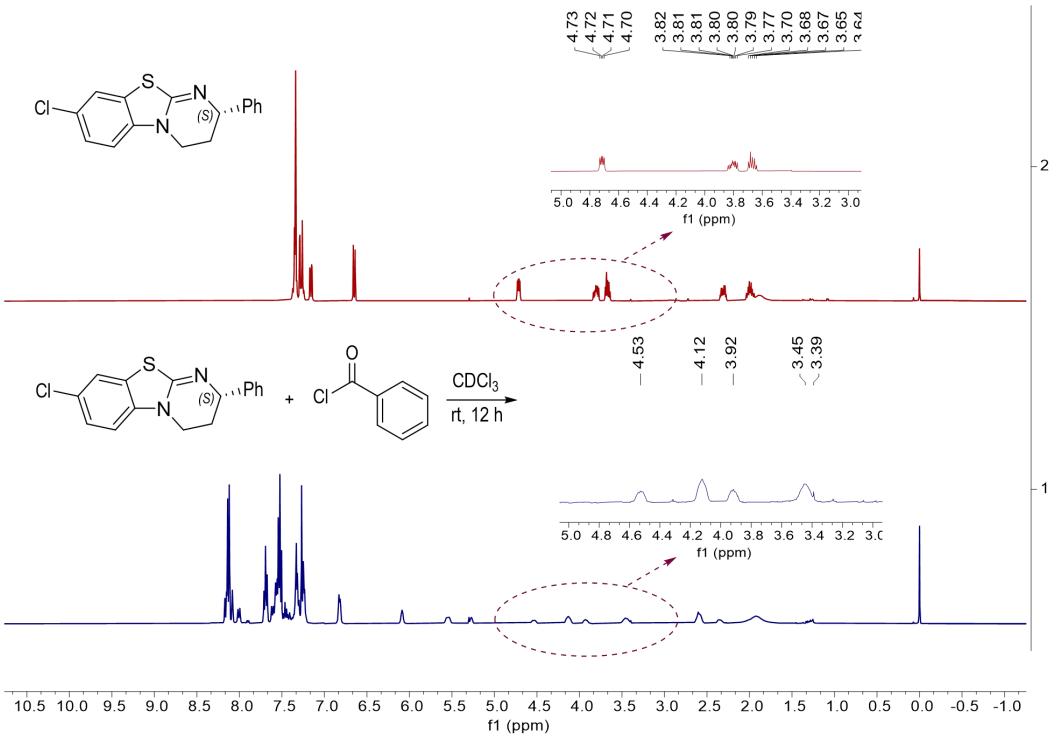
VIII. Controlled experiment



To a 4 mL val containing isothiourea catalyst B (15 mg, 0.050 mmol) in $CDCl_3$ (2 mL) was added benzoyl chloride (11 mg, 0.075 mmol) at room temperature. After stirring for 12 hours, directly take the reaction system for HRMS and ^1H NMR monitoring.

HRMS (ESI, m/z) calcd. for $C_{23}H_{19}ClN_2OS$ $[M+H]^+$: 405.0823, found: 405.0827.





IX. References

The preparation procedures for the same or similar substrates refer to relevant references 1-4, and the characterization data of the known target compound refer to relevant references 5 and 6.

(1) M. Zhou, T. Gridneva, Z. Zhang, E. He, Y. Liu and W. Zhang, *Angew. Chem. Int. Ed.,* 2021, **60**, 1641−1645.

(2) Y.-L. Pan, H.-L. Zheng, J. Wang, C. Yang, X. Li and J.-P. Cheng, *ACS Catal.*, 2020, **10**, 8069-8076.

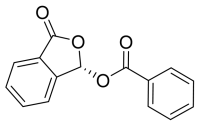
(3) D. E. Beck, K. Agama, C. Marchand, A. Chergui, Y. Pommier and M. Cushman, *J. Med. Chem.*, 2014, **57**, 1495-1512.

(4) Q. Liu, K. Teng, Y. Zhang, Y. Lv, Y. R. Chi and Z. Jin, *Angew. Chem. Int. Ed.*, 2024, e202406386.

(5) Y. Liu, P. K. Majhi, R. Song, C. Mou, L. Hao, H. Chai, Z. Jin and Y. R. Chi, *Angew. Chem. Int. Ed.*, 2020, **59**, 3859-3863.

(6) Y. Liu, Q. Chen, C. Mou, L. Pan, X. Duan, X. Chen, H. Chen, Y. Zhao, Y. Lu, Z. Jin, Y. R. Chi, *Nat. Commun.* 2019, **10**, 1675.

X. Characterization data of products



(**3a**) ***(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl benzoate**.[5]

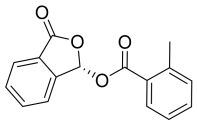
92 % yield, white solid, 23.4 mg, mp 61-62 ℃, $[\alpha]_D^{25}$ = +84.5 (c = 0.50 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.08 – 8.05 (m, 2H), 7.99 – 7.97 (m, 1H), 7.77 (td, *J* = 7.3, 6.9, 1.2 Hz, 1H), 7.71 – 7.67 (m, 3H), 7.64 – 7.59 (m, 1H), 7.48 – 7.44 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 167.96, 165.11, 144.50, 134.94, 134.12, 131.37, 130.20 (2C), 128.65 (2C), 128.41, 126.62, 125.88, 123.79, 93.30.

HRMS (ESI, m/z) calcd. for $C_{15}H_{10}O_4Na$ $[M+Na]^+$: 247.0471, found: 277.0476.

HPLC analysis: 95:5 er (IB column, 25 ºC, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 17.1 min (major), 18.4 min (minor).



(**3b**) ***(R)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 2-methyl- benzoate**.[6]

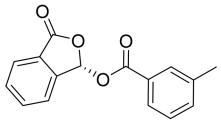
95 % yield, 25.5 mg, white solid, mp 137-138 ℃, $[\alpha]_D^{25}$ = +24.0 (c = 0.33 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.98 – 7.95 (m, 1H), 7.92 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.78 (td, *J* = 7.3, 1.1 Hz, 1H), 7.69 (d, *J* = 1.6 Hz, 1H), 7.68 – 7.64 (m, 2H), 7.45 (td, *J* = 7.5, 1.5 Hz, 1H), 7.28 (d, *J* = 7.8 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 2.65 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 168.04, 165.47, 144.61, 141.62, 134.91, 133.23, 132.02, 131.30, 131.19, 127.32, 126.65, 125.94, 125.86, 123.70, 93.07, 21.94.

HRMS (ESI, m/z) calcd. for $C_{16}H_{12}O_4Na$ $[M+Na]^+$: 291.0628, found: 291.0616.

HPLC analysis: 94:6 er (IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 15.7 min (major), 17.2 min (minor).



(**3c**) ***(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 3-methylbenzoate**.[6]

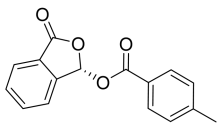
97 % yield, 26.0 mg, white solid, mp 104-105 °C, $[\alpha]_D^{25}$ = +23.8 (c = 0.40 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.99 – 7.97 (m, 1H), 7.87 – 7.84 (m, 2H), 7.78 (td, *J* = 7.4, 1.2 Hz, 1H), 7.71 – 7.67 (m, 3H), 7.42 (ddt, *J* = 7.6, 2.0, 0.9 Hz, 1H), 7.34 (td, *J* = 7.5, 1.1 Hz, 1H), 2.39 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 167.99, 165.29, 144.58, 138.55, 134.90 (2C), 131.33, 130.66, 128.54, 128.32, 127.37, 126.66, 125.87, 123.80, 93.30, 21.22.

HRMS (ESI, m/z) calcd. for $C_{16}H_{12}O_4Na$ $[M+Na]^+$: 291.0628, found: 291.0620.

HPLC analysis: 97:3 er (IB column, 25 °C, hexane/i-propanol = 95/5, flow rate = 0.5 mL/min, λ = 254 nm), Rt = 19.8 min (major), 21.1 min (minor).



(**3d**) ***(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 4-methylbenzoate**.[6]

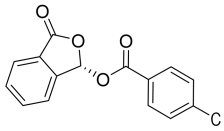
93 % yield, 25.0 mg,white solid, mp 110-111 °C, $[\alpha]_D^{25}$ = +38.3 (c = 0.20 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.01 – 7.98 (m, 1H), 7.96 – 7.93 (m, 2H), 7.79 – 7.75 (m, 1H), 7.70 – 7.66 (m, 3H), 7.28 – 7.24 (m, 2H), 2.41 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 168.04, 165.15, 145.11, 144.63, 134.87, 131.30, 130.25, 129.37, 129.23, 126.67, 126.58, 125.85, 125.64, 123.77, 93.25, 21.78.

HRMS (ESI, m/z) calcd. for $C_{16}H_{12}O_4Na$ $[M+Na]^+$: 291.0628, found: 291.0619.

HPLC analysis: 97:3 er (IB column, 25 °C, hexane/i-propanol = 95/5, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 21.0 min (major), 22.8 min (minor).



(**3e**) ***(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 4-chlorobenzoate**.[5,6]

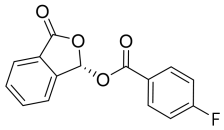
86 % yield, 24.9 mg, white solid, mp 147-148 °C, $[\alpha]_D^{25}$ = +33.3 (c = 0.20 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.99 (ddd, J = 7.3, 4.7, 2.0 Hz, 3H), 7.79 (td, J = 7.5, 1.2 Hz, 1H), 7.71 – 7.67 (m, 3H), 7.43 (d, J = 8.6 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 167.82, 164.29, 144.28, 140.73, 134.99, 131.55 (2C), 131.46, 129.06 (2C), 126.87, 126.57, 125.93, 123.78, 93.34.

HRMS (ESI, m/z) calcd. for $C_{15}H_9ClO_4Na$ $[M+Na]^+$: 311.0082, found: 311.0072.

HPLC analysis: 92:8 er (IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 18.2 min (major), 19.7 min (minor).



(**3f**) ***(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 4-fluorobenzoate**.[6]

89 % yield, 24.2 mg, white solid, mp 137-138 °C, $[\alpha]_D^{25}$ = +29.2 (c = 0.40 in $CHCl_3$).

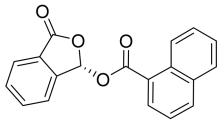
^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.10 – 8.06 (m, 2H), 7.98 (dd, J = 7.3, 1.5 Hz, 1H), 7.79 (td, J = 7.4, 1.2 Hz, 1H), 7.71 – 7.67 (m, 3H), 7.13 (t, J = 8.6 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 167.86, 166.42 (d, J = 256.4 Hz), 164.12, 144.35, 134.97, 132.94, 132.84, 131.43, 126.59, 125.91, 124.68 (d, J = 2.9 Hz), 123.77, 116.04, 115.82, 93.30.

^{19}F NMR (377 MHz, $CDCl_3$) δ: -103.26.

HRMS (ESI, m/z) calcd. for $C_{15}H_9FO_4Na$ $[M+Na]^+$: 295.0377, found: 295.0372.

HPLC analysis: 96:4 er (IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 17.2 min (major), 19.0 min (minor).



(**3g**) ***(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 1-naphthoate**.[6]

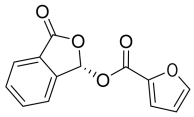
76 % yield, 23.1 mg, white solid, mp 133-134 °C, $[\alpha]_D^{25}$ = +10.6 (c = 0.33 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.02 (d, J = 8.7 Hz, 1H), 8.22 (dd, J = 7.4, 1.4 Hz, 1H), 8.06 (d, J = 8.2 Hz, 1H), 7.97 (d, J = 7.6 Hz, 1H), 7.89 (dd, J = 8.2, 1.5 Hz, 1H), 7.79 – 7.73 (m, 3H), 7.66 (tdd, J = 8.7, 4.9, 1.4 Hz, 2H), 7.56 (ddd, J = 8.1, 6.8, 1.3 Hz, 1H), 7.45 (t, J = 7.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 168.07, 165.44, 144.60, 134.96, 134.92, 133.87, 131.62, 131.53, 131.35, 128.80, 128.48, 126.67, 126.59, 125.89, 125.53, 124.52, 124.43, 123.78, 93.25.

HRMS (ESI, m/z) calcd. for $C_{19}H_{12}O_4Na$ $[M+Na]^+$: 327.0628, found: 327.0619.

HPLC analysis: 92:7 er (IB column, 25 °C, hexane/i-propanol = 95/5, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 21.7 min (major), 25.7 min (minor).



(**3h**) ***(R)*-3-oxo-1,3-dihydroisobenzofuran-1-yl furan-2-carboxylate**.[5]

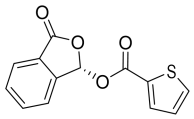
87 % yield, 21.2 mg, white solid, mp 152-153 °C, $[\alpha]_D^{25}$ = +15.6 (c = 0.40 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.97 (dt, J = 7.5, 1.1 Hz, 1H), 7.78 (td, J = 7.4, 1.1 Hz, 1H), 7.70 – 7.64 (m, 4H), 7.28 (dd, J = 3.5, 0.8 Hz, 1H), 6.55 (dd, J = 3.5, 1.7 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ:167.76, 156.82, 147.75, 144.13, 142.98, 134.96, 131.45, 126.60, 125.92, 123.81, 120.41, 112.34, 92.94.

HRMS (ESI, m/z) calcd. for $C_{13}H_8O_5Na$ $[M+Na]^+$: 267.0264, found: 267.0254.

HPLC analysis: 94:6 er (IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 26.4 min (major), 30.7 min (minor).



(**3i**) ***(R)*-3-oxo-1,3-dihydroisobenzofuran-1-yl thiophene-2-carboxylate**.[5]

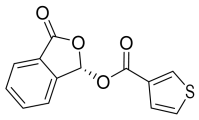
91 % yield, 23.7 mg, light yellow solid, mp 150-151 °C, $[\alpha]_D^{25}$ = +19.3 (c = 0.20 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.97 (dt, J = 7.7, 1.1 Hz, 1H), 7.87 (dd, J = 3.8, 1.3 Hz, 1H), 7.78 (td, J = 7.5, 1.1 Hz, 1H), 7.70 – 7.63 (m, 4H), 7.13 (dd, J = 5.0, 3.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 167.89, 160.58, 144.11, 135.28, 134.96, 134.40, 131.60, 131.41, 128.18, 126.59, 125.88, 123.79, 93.22.

HRMS (ESI, m/z) calcd. for $C_{13}H_8O_4SNa$ $[M+Na]^+$: 283.0036, found: 283.0025.

HPLC analysis: 97:3 er (IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 23.1 min (major), 25.1 min (minor).



(**3j**) ***(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl thiophene-3-carboxylate**.[5]

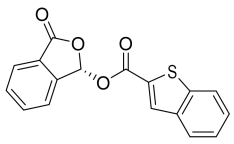
86 % yield, 22.4 mg, white solid, mp 120-121 °C, $[\alpha]_D^{25}$ = +16.8 (c = 0.20 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.19 (dd, J = 3.0, 1.2 Hz, 1H), 7.97 (dd, J = 7.6, 1.0 Hz, 1H), 7.76 (dd, J = 7.5, 1.1 Hz, 1H), 7.70 – 7.64 (m, 3H), 7.56 (dd, J = 5.1, 1.2 Hz, 1H), 7.34 (dd, J = 5.1, 3.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 167.94, 160.88, 144.48, 134.90, 134.80, 131.64, 131.35, 128.04, 126.64 (2C), 125.87, 123.75, 93.08.

HRMS (ESI, m/z) calcd. for $C_{13}H_8O_4SNa$ $[M+Na]^+$: 283.0036, found: 283.0023.

HPLC analysis: 97:3 er (IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 23.7 min (major), 26.3 min (minor).



(**3k**) ***(R)*-3-oxo-1,3-dihydroisobenzofuran-1-yl benzo[b]thiophene-2-carboxylate**.

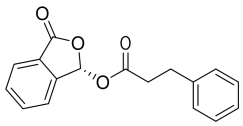
81 % yield, 25.1 mg, white solid, mp 152-153 °C, $[\alpha]_D^{25}$ = 10.0 (c = 0.25 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.13 (d, J = 0.8 Hz, 1H), 8.00 – 7.98 (m, 1H), 7.89 – 7.85 (m, 2H), 7.82 – 7.78 (m, 1H), 7.72 – 7.67 (m, 3H), 7.49 (ddd, J = 8.3, 7.1, 1.3 Hz, 1H), 7.42 (ddd, J = 8.0, 7.1, 1.1 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 167.81, 161.31, 144.16, 142.85, 138.49, 135.00, 132.53, 131.49, 131.35, 127.68, 126.60, 125.95, 125.93, 125.25, 123.82, 122.85, 93.40.

HRMS (ESI, m/z) calcd. for $C_{17}H_{10}O_4SNa$ $[M+Na]^+$: 333.0192, found: 333.0180.

HPLC analysis: 92:8 er (IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 31.8 min (major), 27.4 min (minor).



(**3l**) ***(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 3-phenylpropanoate**.[5]

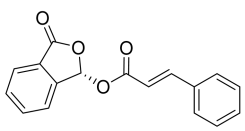
77 % yield, 21.7 mg, light yellow solid, mp 176-177 °C, $[\alpha]_D^{25}$ = -31.7 (c = 0.33 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.92 (d, J = 7.5, 1H), 7.72 (td, J = 7.5, 1.2 Hz, 1H), 7.64 (td, J = 7.5, 1.0 Hz, 1H), 7.47 (dd, J = 7.6, 0.9 Hz, 1H), 7.42 (s, 1H), 7.32 – 7.27 (m, 2H), 7.24 – 7.19 (m, 3H), 3.01 (t, J = 7.7 Hz, 2H), 2.78 – 2.74 (m, 2H)

^{13}C NMR (101 MHz, $CDCl_3$) δ: 171.45, 167.87, 144.29, 139.75, 134.82, 131.27, 128.65 (2C), 128.35 (2C), 126.55, 126.48, 125.80, 123.58, 92.68, 35.63, 30.57.

HRMS (ESI, m/z) calcd. for $C_{17}H_{14}O_4Na$ $[M+Na]^+$: 305.0784, found: 305.0775.

HPLC analysis: 96:4 er (IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), Rt = 22.8 min (major), 25.1 min (minor).



(**3m**) ***(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl cinnamate**.[6]

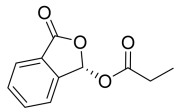
80 % yield, 22.4, brown solid, mp 118-119 °C, $[\alpha]_D^{25}$ = +46.54 (c = 0.40 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.96 (d, J = 7.5, 1H), 7.81 (d, J = 15.9 Hz, 1H), 7.76 (dd, J = 7.5, 1.1 Hz, 1H), 7.67 (td, J = 8.1, 7.5, 1.2 Hz, 2H), 7.59 (s, 1H), 7.56 – 7.50 (m, 2H), 7.45 – 7.36 (m, 3H), 6.46 (d, J = 16.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 167.97, 165.23, 147.74, 144.53, 134.87, 133.82, 131.30, 131.07, 129.06 (2C), 128.43 (2C), 126.61, 125.83, 123.73, 116.04, 92.97.

HRMS (ESI, m/z) calcd. for $C_{17}H_{12}O_4Na$ $[M+Na]^+$: 303.0628, found: 303.0616.

HPLC analysis: 97:3 er (IB column, 25 °C, hexane/i-propanol = 70/30, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 26.8 min (major), 19.3 min (minor).



(**3n**) ***(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl propionate**.[6]

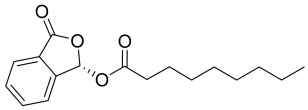
97 % yield, 19.9 mg, Yellow oil, $[\alpha]_D^{25}$ = +27.6 (c = 0.33 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.93 (d, J = 7.6 Hz, 1H), 7.77 (d, J = 1.1 Hz, 1H), 7.67 – 7.67 (m, 1H), 7.61 (d, J = 7.6 Hz, 1H), 7.46 (s, 1H), 2.46 (t, J = 7.5 Hz, 2H), 1.21 (t, J = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 172.97, 167.94, 144.38, 134.86, 131.25, 126.47, 125.73, 123.57, 92.62, 27.39, 8.66.

HRMS (ESI, m/z) calcd. for $C_{11}H_{10}O_4Na$ $[M+Na]^+$: 229.0471, found: 229.0460.

HPLC analysis: 97:3 er (IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 15.2 min (major), 17.5 min (minor).



(**3o**) ***(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl nonanoate**.

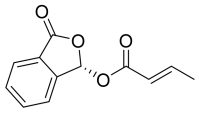
75 % yield, 20.8 mg, colorless oil, $[\alpha]_D^{25}$ = +13.1 (c = 0.33 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.93 (d, J = 7.6 Hz, 1H), 7.76 (td, J = 7.5, 1.1 Hz, 1H), 7.66 (t, J = 7.5 Hz, 1H), 7.60 (d, J = 7.6 Hz, 1H), 7.45 (s, 1H), 2.43 (t, J = 7.5 Hz, 2H), 1.67 (q, J = 7.4 Hz, 2H), 1.29 (dp, J = 8.8, 4.6, 4.0 Hz, 10H), 0.87 (d, J = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 172.32, 167.95, 144.43, 134.83, 131.22, 126.48, 125.74, 123.54, 92.60, 34.00, 31.74, 29.11, 29.04, 28.94, 24.51, 22.60, 14.05.

HRMS (ESI, m/z) calcd. for $C_{17}H_{22}O_4Na$ $[M+Na]^+$: 313.1410, found: 313.1397.

HPLC analysis: 96:4 er (IB column, 25 ºC, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 12.1 min (major), 13.7 min (minor).



(**3p**) ***(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl (E)-but-2-enoate**.[6]

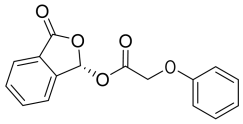
74 % yield, 16.1 mg, white solid, mp 63-64 ºC, $[\alpha]_D^{25}$ = +18.2 (c = 0.25 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.86 (d, J = 7.6, 1H), 7.68 (td, J = 7.5, 1.1 Hz, 1H), 7.60 – 7.52 (m, 2H), 7.43 (s, 1H), 7.07 (dq, J = 15.6, 6.9 Hz, 1H), 5.82 (dq, J = 15.5, 1.7 Hz, 1H), 1.85 (dd, J = 7.0, 1.7 Hz, 3H)

^{13}C NMR (101 MHz, $CDCl_3$) δ: 166.96, 163.55, 147.44, 143.53, 133.76, 130.18, 125.55, 124.74, 122.60, 120.06, 91.72, 17.27.

HRMS (ESI, m/z) calcd. for $C_{12}H_{10}O_4Na$ $[M+Na]^+$: 241.0471, found: 241.0464.

HPLC analysis: 97:3 er (IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 16.8 min (major), 18.7 min (minor).



(**3q**) ***(R)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 2-phenoxyacetate**.

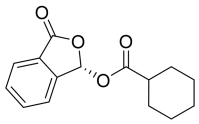
67 % yield, 19.0 mg, white solid, mp 133-134 °C, $[\alpha]_D^{25}$ = +4.4 (c = 0.33 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) *δ*: 7.93 (d, J = 7.8 Hz, 1H), 7.75 (td, J = 7.5, 1.1 Hz, 1H), 7.66 (td, J = 7.5, 1.0 Hz, 1H), 7.54 (dd, J = 7.5, 0.8 Hz, 1H), 7.51 (s, 1H), 7.34 – 7.27 (m, 2H), 7.07 – 6.97 (m, 1H), 6.95 – 6.88 (m, 2H), 4.74 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ*: 167.88, 167.61, 157.50, 143.76, 135.03, 131.57, 129.72 (2C), 126.33, 125.92, 123.70, 122.19, 114.76 (2C), 92.98, 65.06.

HRMS (ESI, m/z) calcd. for $C_{16}H_{12}O_5Na$ $[M+Na]^+$: 307.0577, found: 307.0566.

HPLC analysis: 90:10 er (IA column, 25 °C, hexane/i-propanol = 80/20, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 21.5 min (major), 27.8 min (minor).



(**3r**) ***(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl cyclohexanecarboxylate**.[6]

71 % yield, 18.5 mg, white solid, mp 64-65 °C, $[\alpha]_D^{25}$ = +14.0 (c = 0.40 in $CHCl_3$).

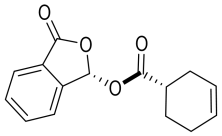
^{1}H NMR (400 MHz, $CDCl_3$) *δ*: 7.86 (d, *J* = 7.6, 1H), 7.67 (td, *J* = 7.5, 1.1 Hz, 1H), 7.58 (td, *J* = 7.5, 1.0 Hz, 1H), 7.51 – 7.49 (m, 1H), 7.37 (s, 1H), 2.33 (tt, *J* = 11.2, 3.7

Hz, 1H), 1.91 – 1.84 (m, 2H), 1.73 – 1.54 (m, 4H), 1.48 – 1.38 (m, 2H), 1.27 – 1.11 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 173.48, 166.98, 143.56, 133.78, 130.17, 125.53, 124.77, 122.42, 91.57, 41.87, 27.66, 27.60, 24.54, 24.19, 24.16.

HRMS (ESI, m/z) calcd. for $C_{15}H_{16}O_4Na$ $[M+Na]^+$: 283.0941, found: 283.0929.

HPLC analysis: 99:1 er (IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 13.0 min (major), 14.0 min (minor).



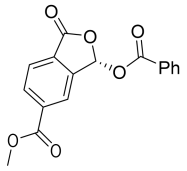
(**3s**) **(*S*)-3-oxo-1,3-dihydroisobenzofuran-1-yl (*S*)-cyclohex-3-ene-1-carboxylate**.

80 % yield, 20.7 mg, white solid, mp 66-67 °C, $[\alpha]_D^{25}$ = -5.2 (c = 0.40 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.94 (d, J = 7.6 Hz, 1H), 7.76 (td, J = 7.6, 1.1 Hz, 1H), 7.66 (td, J = 7.5, 1.0 Hz, 1H), 7.59 (d, J = 7.6 Hz, 1H), 7.47 (s, 1H), 5.76 – 5.61 (m, 2H), 2.72 – 2.64 (m, 1H), 2.35 – 2.27 (m, 2H), 2.16 – 2.00 (m, 3H), 1.80 – 1.68 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 174.29, 167.95, 144.48, 134.85, 131.25, 126.85, 126.54, 125.80, 124.59, 123.49, 92.65, 39.13, 27.04, 24.74, 24.12.

HRMS (ESI, m/z) calcd. for $C_{15}H_{14}O_4Na$ $[M+Na]^+$: 281.0784, found: 281.0787.



(**3t**) **methyl *(S)*-3-(benzoyloxy)-1-oxo-1,3-dihydroisobenzofuran-5-carboxylate**.

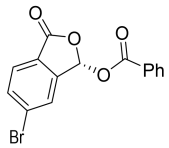
93 % yield, 29.0 mg, white solid, mp 89-90 °C, $[\alpha]_D^{25}$ = +59.6 (c = 0.33 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.36 (dd, J = 7.9, 1.4 Hz, 1H), 8.05 (m, 3H), 7.73 (s, 1H), 7.66 – 7.60 (m, 1H), 7.49 – 7.44 (m, 2H), 3.99 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 166.92, 165.34, 164.92, 144.59, 136.30, 134.26, 132.67, 130.26 (2C), 130.23, 128.69 (2C), 128.16, 125.96, 125.04, 93.05, 52.93.

HRMS (ESI, m/z) calcd. for $C_{17}H_{12}O_6Na$ $[M+Na]^+$: 335.0526, found: 335.0518.

HPLC analysis: 97:3 er (IA column, 25 °C, hexane/i-propanol = 80/20, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 21.6 min (major), 23.1 min (minor).



(3u) *(S)*-6-bromo-3-oxo-1,3-dihydroisobenzofuran-1-yl benzoate.

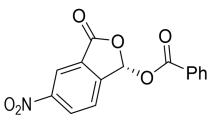
85 % yield, 28.3 mg, white solid, mp 148-149 °C. $[\alpha]_D^{25}$ = +150.5 (c = 0.33 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.07 (d, J = 1.2 Hz, 1H), 8.05 (t, J = 1.7 Hz, 1H), 7.84 (dt, J = 10.8, 1.1 Hz, 3H), 7.65 – 7.61 (m, 2H), 7.49 – 7.45 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 166.94, 164.94, 146.22, 134.97, 134.29, 130.26 (2C), 130.16, 128.71, 128.13 (2C), 127.31, 127.11, 125.55, 92.60.

HRMS (ESI, m/z) calcd. for $C_{15}H_9BrO_4Na$ $[M+Na]^+$: 354.9576, found: 354.9561.

HPLC analysis: 98:2 er (IB column, 25 °C, hexane/i-propanol = 95/5, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 22.9 min (major), 25.0 min (minor).



(3v) *(S)*-5-nitro-3-oxo-1,3-dihydroisobenzofuran-1-yl benzoate.

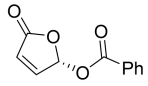
80 % yield, 24.0 mg, white solid, mp 135-136 °C, $[\alpha]_D^{25}$ = +24.9 (c = 0.33 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.79 (d, J = 2.0 Hz, 1H), 8.65 (dd, J = 8.3, 2.0 Hz, 1H), 8.15 – 8.01 (m, 2H), 7.92 (d, J = 8.3 Hz, 1H), 7.77 (s, 1H), 7.67 – 7.63 (m, 1H), 7.48 (t, J = 7.9 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.43, 164.69, 150.48, 149.45, 134.53, 130.27 (2C), 129.84, 128.80 (2C), 128.59, 127.77, 125.37, 121.42, 92.83.

HRMS (ESI, m/z) calcd. for $C_{15}H_9NO_6Na$ $[M+Na]^+$: 322.0322, found: 322.0317.

HPLC analysis: 90:10 er (IB column, 25 °C, hexane/i-propanol = 80/20, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 31.8 min (major), 37.4 min (minor).



(**3w**) ***(R)*-5-oxo-2,5-dihydrofuran-2-yl benzoate**.

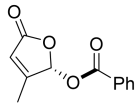
73 % yield, 14.8 mg, light yellow solid, mp 82-83 °C, $[\alpha]_D^{25}$ = +5.3 (c = 0.20 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.07 – 8.04 (m, 2H), 7.65 – 7.61 (m, 1H), 7.50 – 7.46 (m, 3H), 7.26 – 7.25 (m, 1H), 6.39 (dd, J = 5.6, 1.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.68, 164.58, 149.84, 134.21, 130.18 (2C), 128.69 (2C), 128.17, 125.42, 94.49.

HRMS (ESI, m/z) calcd. for $C_{11}H_8O_4Na$ $[M+Na]^+$: 227.0315, found: 227.0304.

HPLC analysis: 91:9 er (IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 11.5 min (major), 12.0 min (minor).



(**3x**) ***(R)*-3-methyl-5-oxo-2,5-dihydrofuran-2-yl benzoate**.

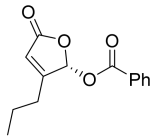
84 % yield, 18.3 mg, light yellow solid, mp 58-59 ℃, $[\alpha]_D^{25}$ = -16.87 (c = 0.50 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.05 – 8.03 (m, 2H), 7.62 – 7.59 (m, 1H), 7.48 – 7.44 (m, 2H), 7.04 – 7.03 (m, 1H), 6.02 (q, J = 1.4 Hz, 1H), 2.14 (d, J = 1.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 170.06, 164.84, 163.12, 134.21, 130.14 (2C), 128.71 (2C), 128.24, 119.67, 94.99, 13.35.

HRMS (ESI, m/z) calcd. for $C_{12}H_{10}O_4Na$ $[M+Na]^+$: 241.0471, found: 241.0472.

HPLC analysis: 91:9 er (IA column, 25 ºC, hexane/i-propanol = 80/20, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 12.2 min (major), 14.0 min (minor).



(**3y**) ***(R)*-5-oxo-2,5-dihydrofuran-2-yl benzoate.**

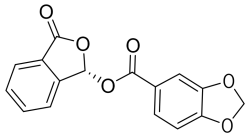
79 % yield, 19.5 mg, Colorless oil, $[\alpha]_D^{25}$ = -40.3 (c = 0.40 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.07 – 8.05 (m, 2H), 7.65 – 7.61 (m, 1H), 7.50 – 7.46 (m, 2H), 7.11 (d, J = 0.9 Hz, 1H), 6.02 (q, J = 0.8 Hz, 1H), 2.47 – 2.35 (m, 2H), 1.75 – 1.64 (m, 2H), 1.03 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 170.11, 167.44, 164.82, 134.19, 130.18 (2C), 128.72 (2C), 128.28, 118.59, 94.47, 29.58, 20.09, 13.74.

HRMS (ESI, m/z) calcd. for $C_{14}H_{14}O_4Na$ $[M+Na]^+$: 269.0784, found: 269.0780.

HPLC analysis: 92:8 er (IA column, 25 °C, hexane/i-propanol = 80/20, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 11.0 min (major), 12.5 min (minor).



(4a) *(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl benzo[d][1,3]dioxole-5-carboxylate.[6]

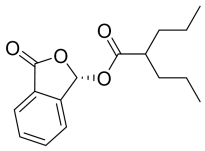
79 % yield, 23.5 mg, white solid, mp 128-129 °C, $[\alpha]_D^{25}$ = +26.2 (c = 0.20 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.97 (dt, J = 7.8, 1.1 Hz, 1H), 7.77 (td, J = 7.5, 1.1 Hz, 1H), 7.70 – 7.65 (m, 4H), 7.46 (d, J = 1.7 Hz, 1H), 6.84 (d, J = 8.2 Hz, 1H), 6.05 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 167.97, 164.39, 152.67, 147.99, 144.56, 134.88, 131.32, 126.65, 126.49, 125.86, 123.74, 122.20, 109.84, 108.23, 102.09, 93.25.

HRMS (ESI, m/z) calcd. for $C_{16}H_{10}O_6Na$ $[M+Na]^+$: 321.0370, found: 321.0551.

HPLC analysis: 90:10 er (IA column, 25 °C, hexane/i-propanol = 70/30, flow rate = 0.5 mL/min, λ = 254 nm), Rt = 19.7 min (major), 25.4 min (minor).



(4b) *(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 2-propylpentanoate.[6]

73 % yield, 20.2 mg, colorless oil, $[\alpha]_D^{25}$ = +18.3 (c = 0.33 in $CHCl_3$).

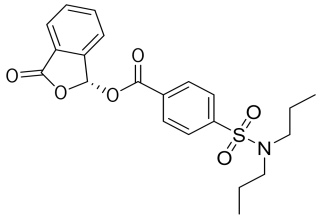
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.94 (dt, J = 7.6, 1.0 Hz, 1H), 7.75 (td, J = 7.5, 1.1 Hz, 1H), 7.65 (td, J = 7.6, 1.0 Hz, 1H), 7.55 (dq, J = 7.6, 0.8 Hz, 1H), 7.47 (s, 1H),

2.47 (m, 1H), 1.65 (m, 2H), 1.47 (m, 2H), 1.38 – 1.32 (m, 4H), 0.91 (td, *J* = 7.3, 2.4 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ*: 175.07, 168.02, 144.63, 134.80, 131.19, 126.63, 125.83, 123.37, 92.57, 45.14, 34.29, 34.25, 20.56, 20.51, 13.97, 13.94.

HRMS (ESI, m/z) calcd. for $C_{16}H_{20}O_4Na$ $[M+Na]^+$: 299.1254, found: 299.1241.

HPLC analysis: 99:1 er (IA column, 25 °C, hexane/i-propanol = 95/5, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 13.2 min (major), 14.8 min (minor).



(4c) *(R)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 4-(N,N-dipropylsulfamoyl) benzoate.

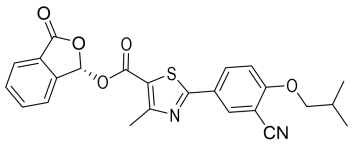
87 % yield, 35.7 mg, light yellow oil, $[\alpha]_D^{25}$ = +31.3 (c = 0.40 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) *δ*: 8.19 – 8.17 (m, 2H), 7.99 (d, *J* = 7.5 Hz, 1H), 7.90 – 7.88 (m, 2H), 7.80 (td, *J* = 7.5, 1.1 Hz, 1H), 7.73 – 7.69 (m, 3H), 3.12 – 3.08 (m, 4H), 1.54 (dd, *J* = 15.2, 7.5 Hz, 4H), 0.86 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ*: 167.70, 163.88, 145.40, 144.04, 135.08, 131.67, 131.60, 130.83, 127.18, 126.51, 126.00, 123.80, 93.47, 49.86, 21.87, 11.13.

HRMS (ESI, m/z) calcd. for $C_{21}H_{24}NO_6S$ $[M+H]^+$: 418.1319, found: 418.1301.

HPLC analysis: 86:14 er (IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 36.3 min (major), 40.1 min (minor).



(**4d**) ***(R)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 2-(3-cyano-4-isobutoxyphenyl)-4-methylthiazole-5-carboxylate**.

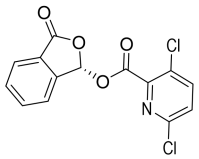
80 % yield, 35.8 mg, white solid, mp 160-161 °C, $[\alpha]_D^{25}$ = +40.6 (c = 0.50 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.16 (d, J = 2.3 Hz, 1H), 8.06 (dd, J = 8.9, 2.3 Hz, 1H), 7.98 (dt, J = 7.5, 1.0 Hz, 1H), 7.79 (td, J = 7.5, 1.1 Hz, 1H), 7.72 – 7.66 (m, 2H), 7.60 (s, 1H), 7.00 (d, J = 9.0 Hz, 1H), 3.89 (d, J = 6.5 Hz, 2H), 2.79 (s, 3H), 2.23 – 2.16 (m, 1H), 1.08 (d, J = 6.8 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 167.77, 166.67, 162.84, 161.78, 159.31, 142.99, 134.00, 131.67, 131.25, 130.49, 125.53, 124.97, 124.59, 122.62, 118.46, 114.22, 111.67, 102.09, 92.06, 74.74, 27.12, 18.01 (2C), 16.79.

HRMS (ESI, m/z) calcd. for $C_{24}H_{21}N_2O_5S$ $[M+H]^+$: 449.1166, found: 449.1158.

HPLC analysis: 94:6 er (IB column, 25 °C, hexane/i-propanol = 80/20, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 34.6 min (major), 41.3 min (minor).



(**4e**) ***(R)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 3,6-dichloropicolinate**.

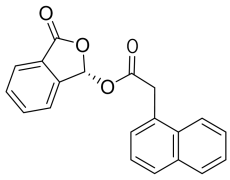
72 % yield, 23.3 mg, white solid, mp 149-150 °C, $[\alpha]_D^{25}$ = +13.8 (c = 0.33 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.96 – 7.94 (m, 1H), 7.79 – 7.76 (m, 2H), 7.74 – 7.66 (m, 2H), 7.65 (s, 1H), 7.44 (d, J = 8.5 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 166.55, 160.71, 148.23, 144.52, 142.61, 140.38, 134.03, 130.59, 129.62, 127.22, 125.47, 124.91, 122.99, 92.85.

HRMS (ESI, m/z) calcd. for $C_{14}H_7Cl_2NO_4Na$ $[M+Na]^+$: 345.9644, found: 345.9639.

HPLC analysis: 97:3 er (OD-H column, 25 °C, hexane/i-propanol = 80/20, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 20.6 min (major), 23.0 min (minor).



(4f) *(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 2-(naphthalen-1-yl)acetate:

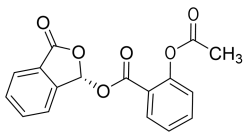
88 % yield, 28.0 mg, colorless oil, $[\alpha]_D^{25}$ = +11.5 (c = 0.33 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.97 – 7.87 (m, 3H), 7.82 (dd, J = 6.3, 3.3 Hz, 1H), 7.65 (m, 2H), 7.57 – 7.49 (m, 2H), 7.43 (m, 3H), 4.18 (d, J = 2.1 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 170.20, 167.85, 144.20, 134.82, 133.89, 131.95, 131.30, 129.17, 128.91, 128.58, 128.28, 126.62, 126.47, 125.98, 125.81, 125.53, 123.54, 123.52, 93.06, 38.75.

HRMS (ESI, m/z) calcd. for $C_{20}H_{14}O_4Na$ $[M+Na]^+$: 341.0784, found: 341.0773.

HPLC analysis: 95:5 er (IB column, 25 °C, hexane/i-propanol = 95/5, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 24.4 min (major), 38.8 min (minor).



(**4g**) ***(R)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 2-acetoxybenzoate**.

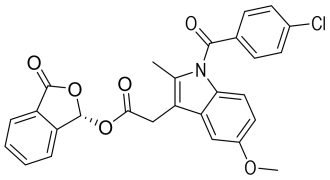
97 % yield, 26.2 mg, light brown oil, $[\alpha]_D^{25}$ = +135.4 (c = 0.50 in $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.00 (dd, J = 7.9, 1.7 Hz, 1H), 7.95 – 7.92 (m, 1H), 7.78 – 7.74 (m, 1H), 7.68 – 7.64 (m, 2H), 7.61 (d, J = 2.0 Hz, 1H), 7.60 – 7.57 (m, 1H), 7.29 (td, J = 7.7, 1.2 Hz, 1H), 7.12 (dd, J = 8.1, 1.2 Hz, 1H), 2.19 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.57, 167.82, 162.88, 151.20, 144.25, 135.12, 135.04, 132.20, 131.48, 126.43, 126.22, 125.84, 124.17, 123.94, 121.57, 93.19, 20.81.

HRMS (ESI, m/z) calcd. for $C_{17}H_{12}O_6Na$ $[M+Na]^+$: 335.0526, found: 335.0518.

HPLC analysis: 93:7 er (IB column, 25 °C, hexane/i-propanol = 90/10, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 23.1 min (major), 25.7 min (minor).



(4h) *(S)*-3-oxo-1,3-dihydroisobenzofuran-1-yl 2-(1-(4-chlorobenzoyl)- 5-methoxy-2- methyl-1H-indol-3-yl)acetate.[6]

81 % yield, 39.6 mg, white solid, mp 160-161 °C, $[\alpha]_D^{25}$ = +11.5 (c = 0.23 in $CHCl_3$).

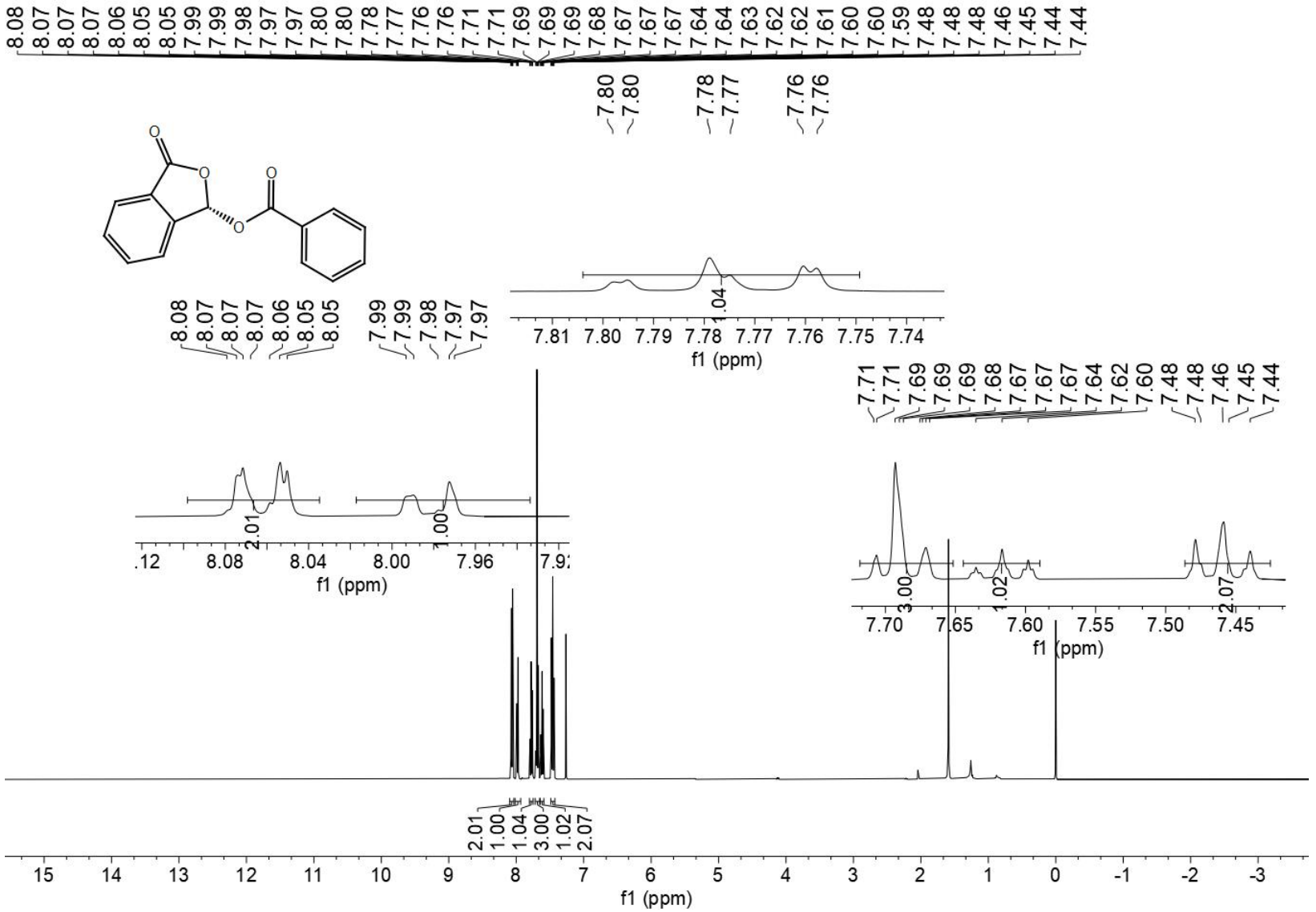
^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.94 (dt, J = 7.3, 1.1 Hz, 1H), 7.72 (td, J = 7.5, 1.2 Hz, 1H), 7.69 – 7.57 (m, 3H), 7.53 – 7.44 (m, 3H), 7.43 (s, 1H), 6.91 (d, J = 2.5 Hz, 1H), 6.89 (d, J = 9.0 Hz, 1H), 6.69 (dd, J = 9.0, 2.5 Hz, 1H), 3.78 (d, J = 4.5 Hz, 5H), 2.37 (s, 3H).

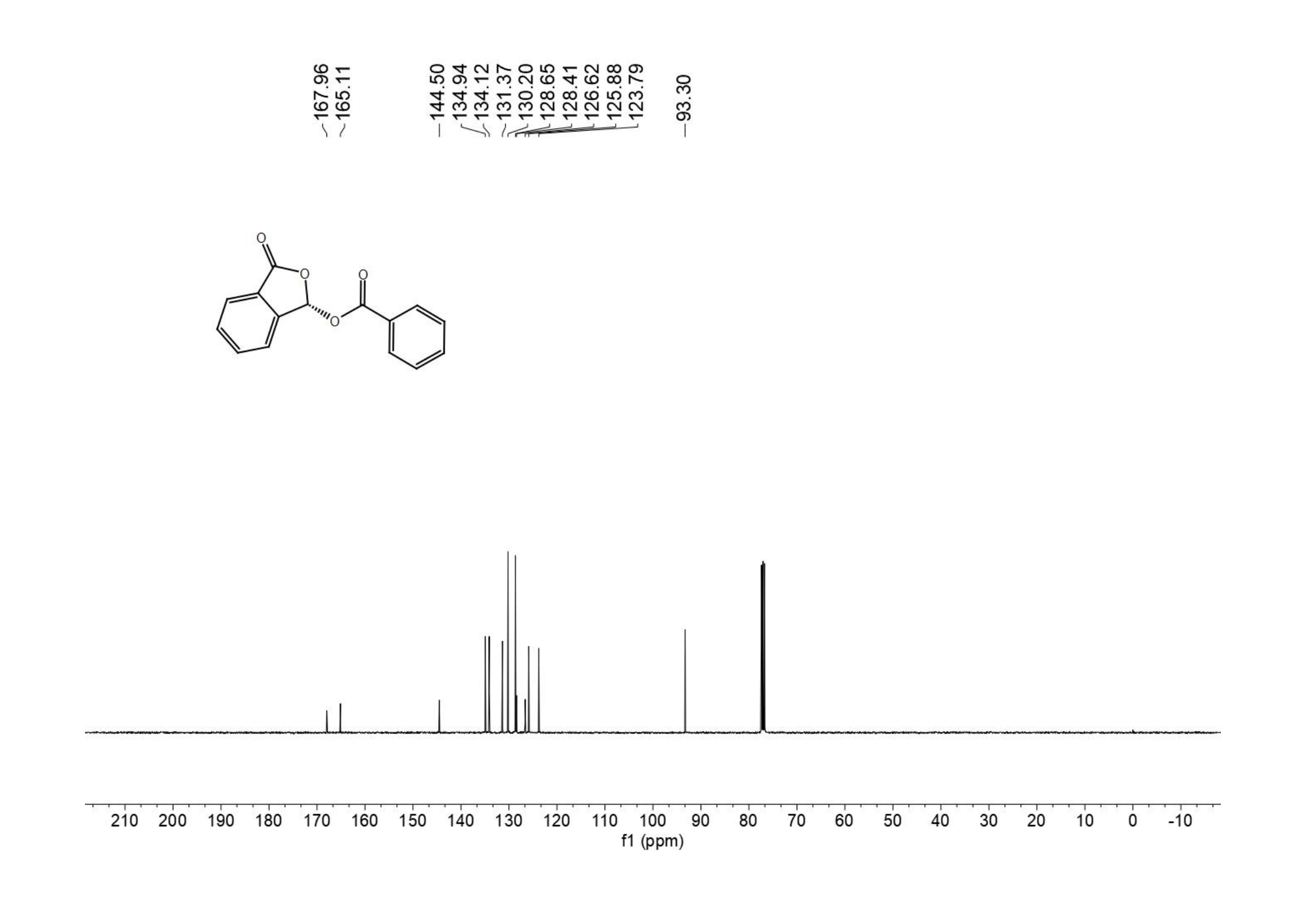
^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.39, 168.31, 156.12, 144.16, 139.48, 136.34, 134.88, 133.73, 131.39, 131.24 (2C), 130.82, 130.23, 129.21 (2C), 126.48, 125.91, 123.55, 115.05, 112.01, 111.22, 101.09, 93.07, 55.70, 30.21, 13.43.

HRMS (ESI, m/z) calcd. For $C_{27}H_{21}ClNO_6$ $[M+H]^+$: 490.1052, found: 490.1046.

HPLC analysis: 90:10 er (IB column, 25 °C, hexane/i-propanol = 80/20, flow rate = 0.5 mL/min, λ = 254 nm), R_t = 36.0 min (major), 40.2 min (minor)

XI. ^{1}H NMR, ^{13}C NMR, ^{19}F NMR, and HPLC spectra




167.96
165.11
144.50
134.94
134.12
131.37
130.20
128.65
128.41
126.62
125.88
123.79
93.30
O
O
O
O
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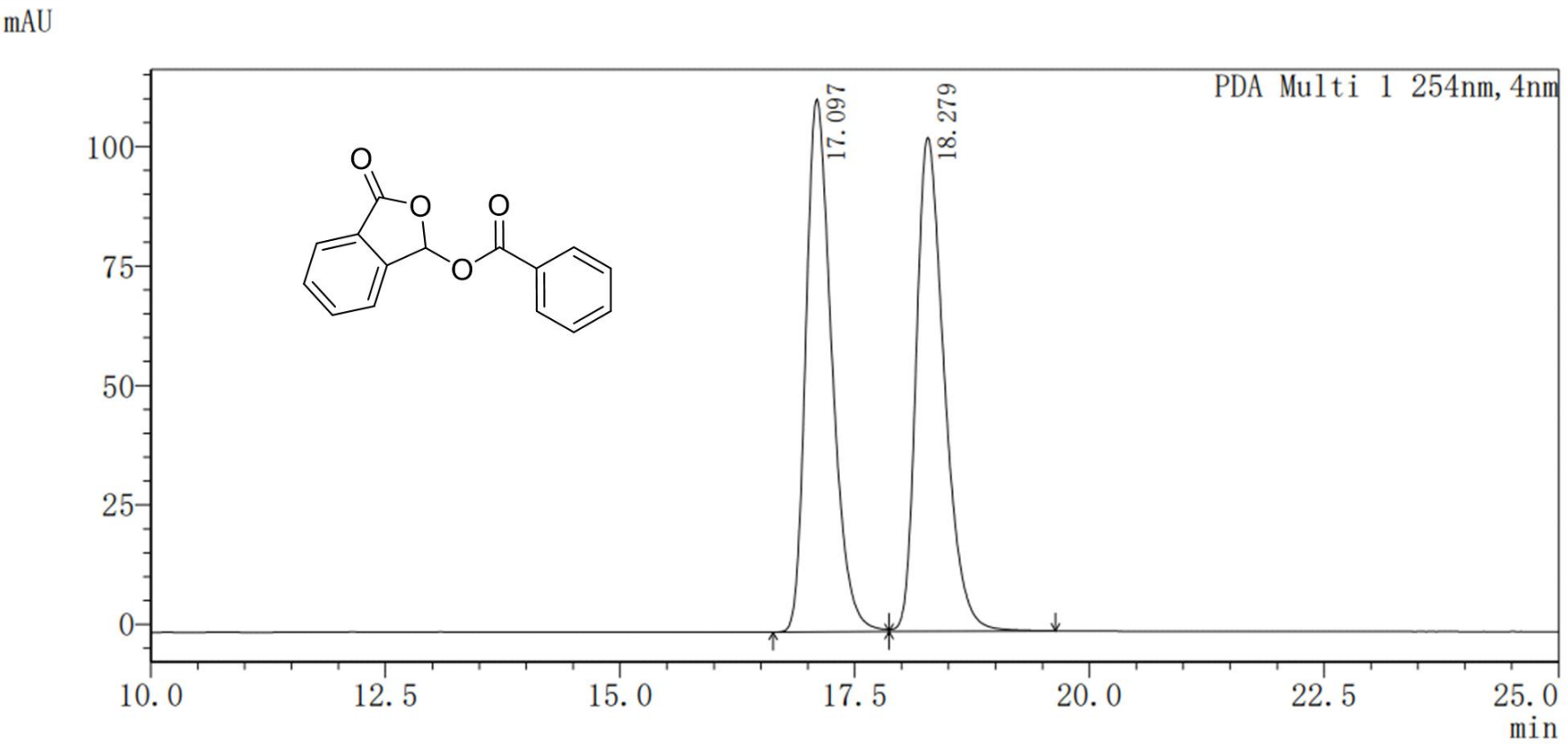
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

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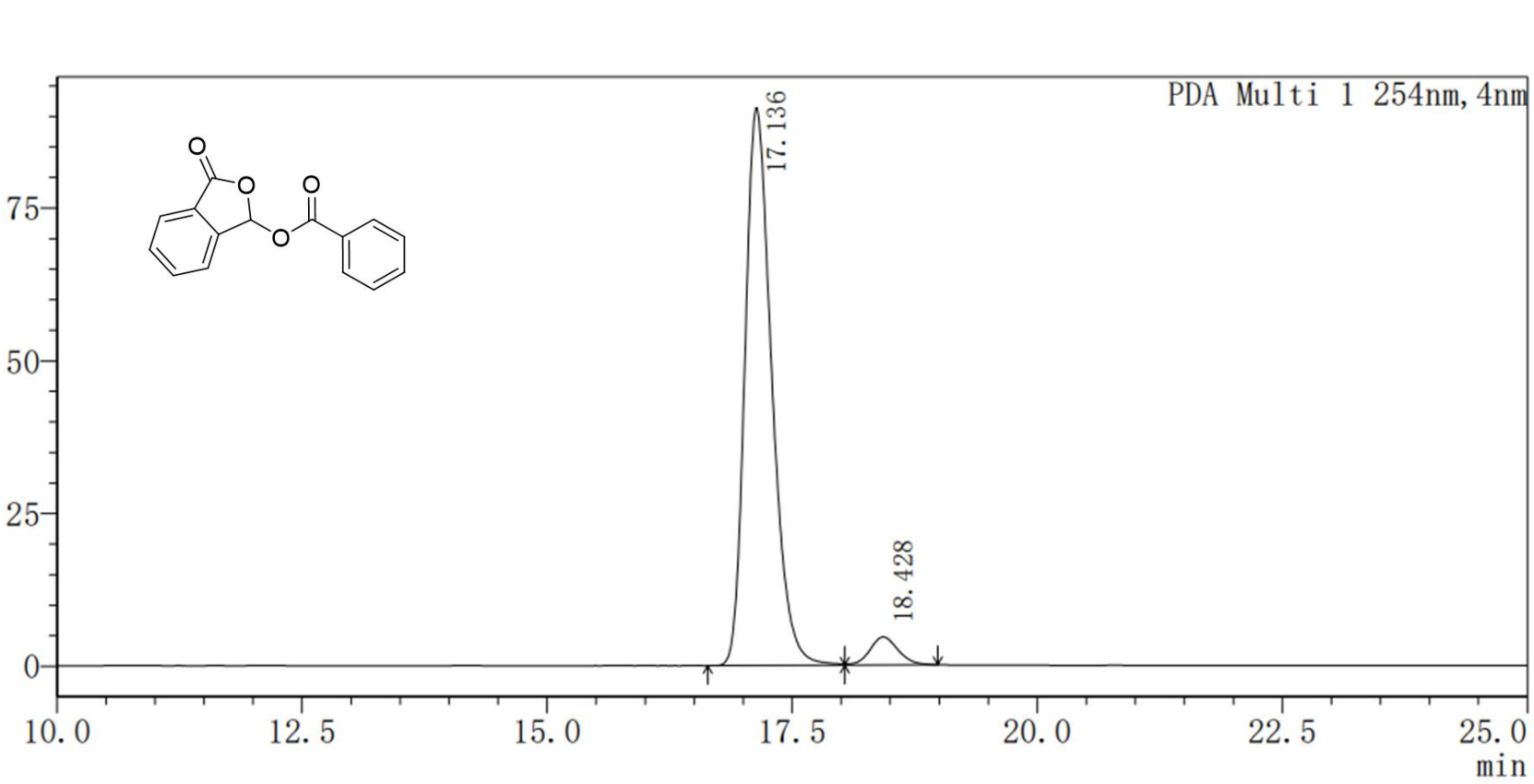

<Peak Table>

PDA Ch1 254nm

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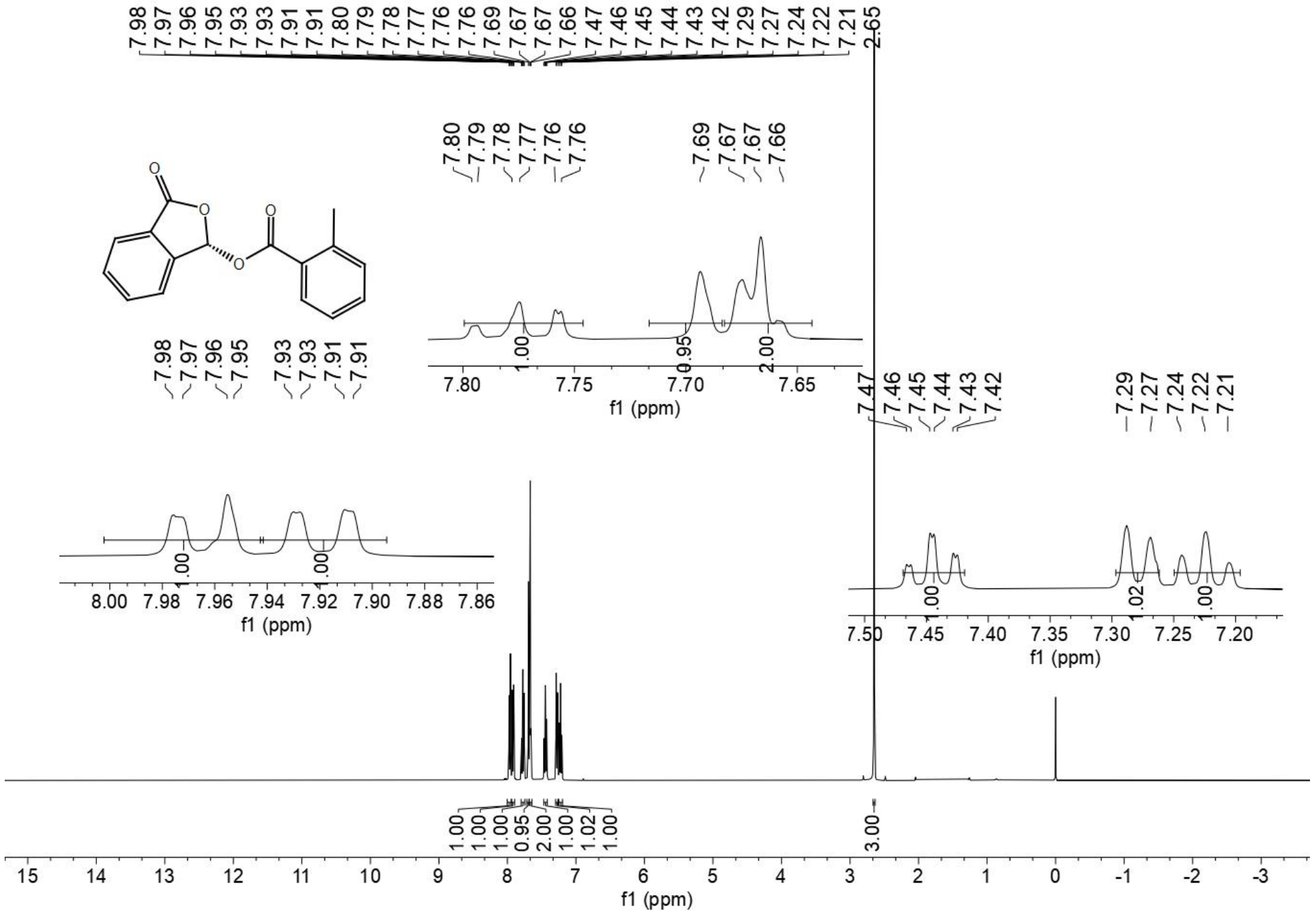
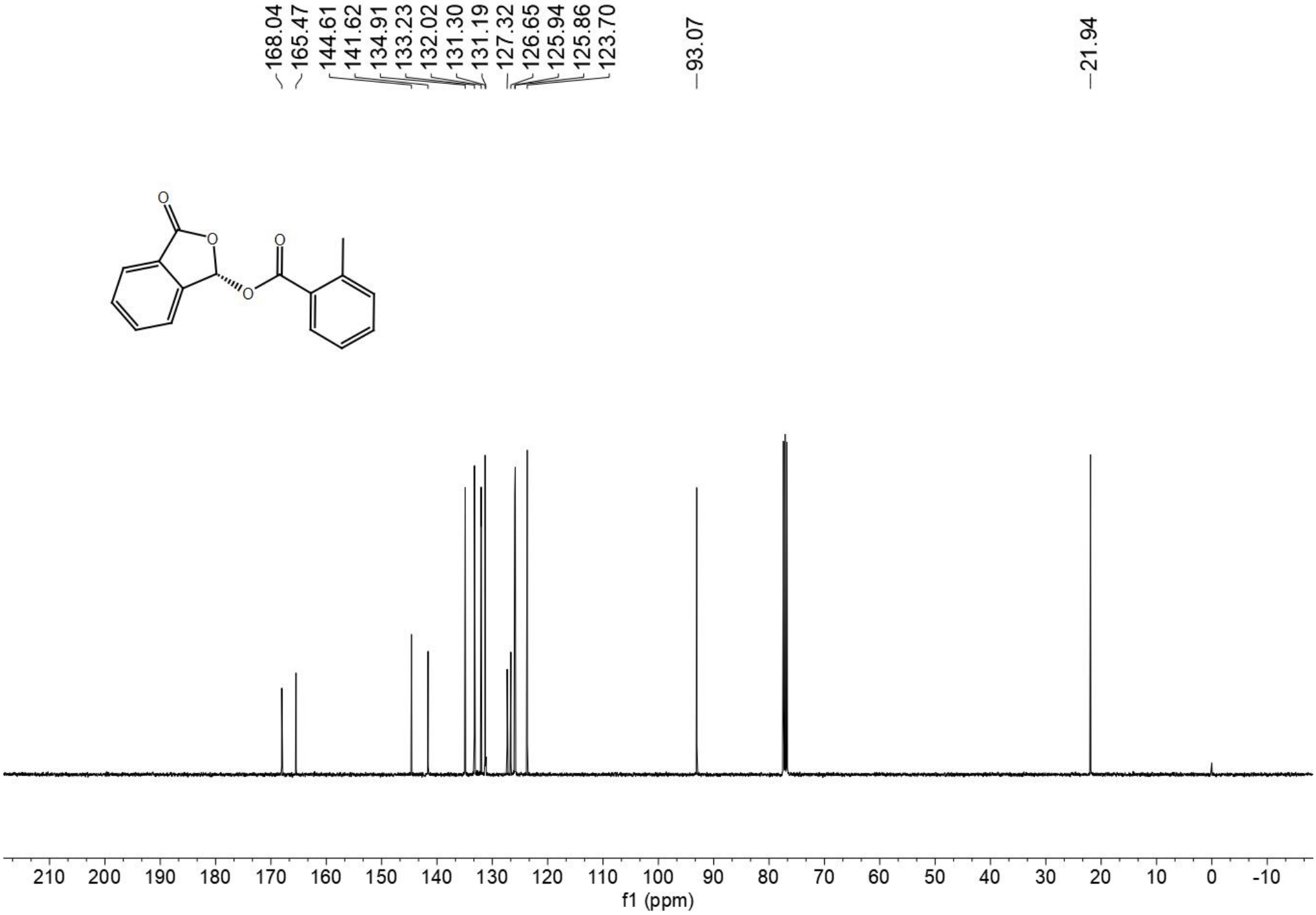
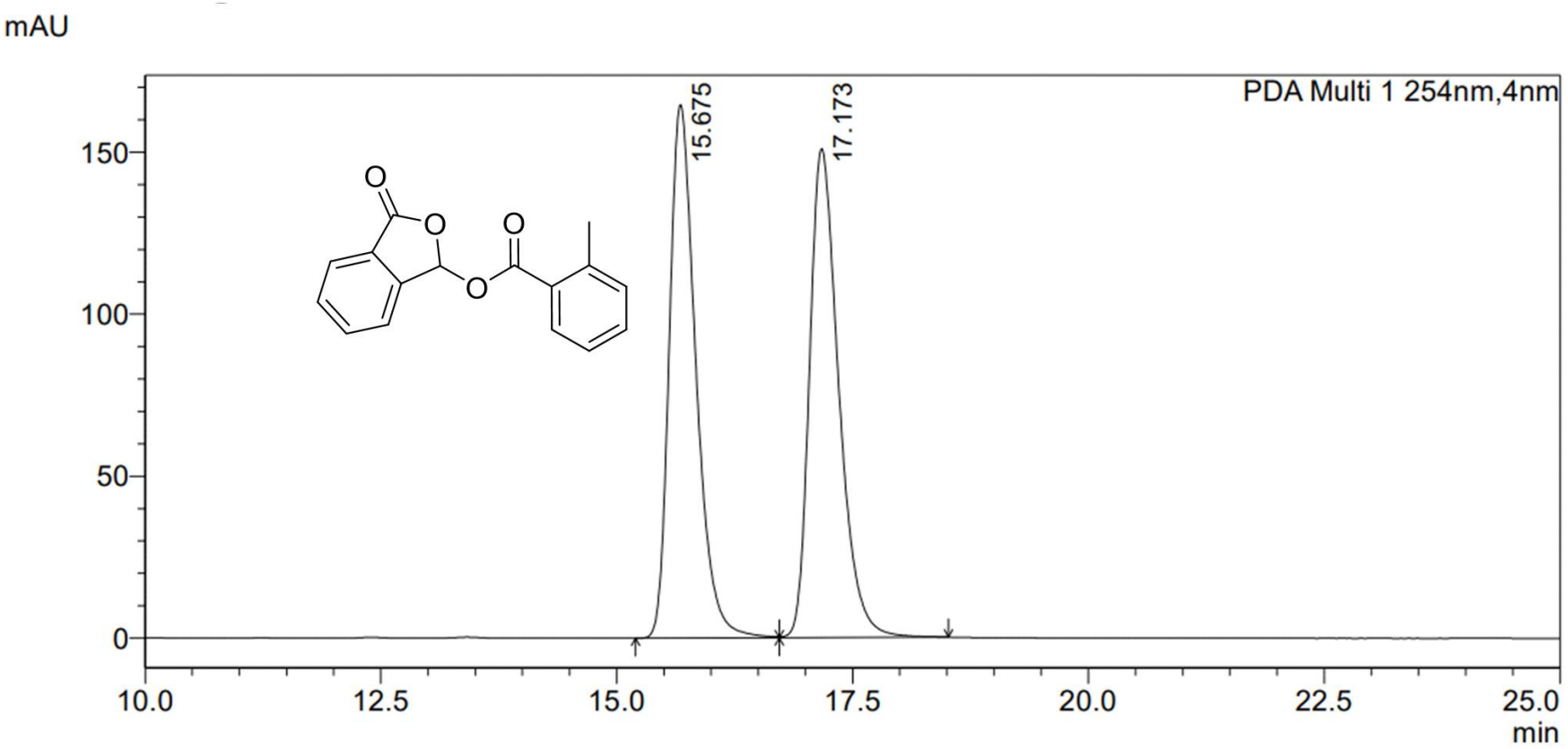

7.98 7.97 7.96 7.95 7.93 7.93 7.91 7.91 7.80 7.79 7.78 7.77 7.76 7.76 7.69 7.67 7.67 7.66 7.47 7.46 7.45 7.44 7.43 7.42 7.29 7.27 7.24 7.22 7.21 2.65
O
O
O
O
7.80 7.79 7.78 7.77 7.76 7.76
7.69 7.67 7.67 7.66
1.00 0.95 2.00
7.80 7.75 7.70 7.65
f1 (ppm)
7.98 7.97 7.96 7.95 7.93 7.93 7.91 7.91
1.00 1.00
8.00 7.98 7.96 7.94 7.92 7.90 7.88 7.86
f1 (ppm)
7.47 7.46 7.45 7.44 7.43 7.42
7.29 7.27 7.24 7.22 7.21
1.00 1.02 1.00
7.50 7.45 7.40 7.35 7.30 7.25 7.20
f1 (ppm)
1.00 1.00 1.00 0.95 2.00 1.00 1.02 1.00
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

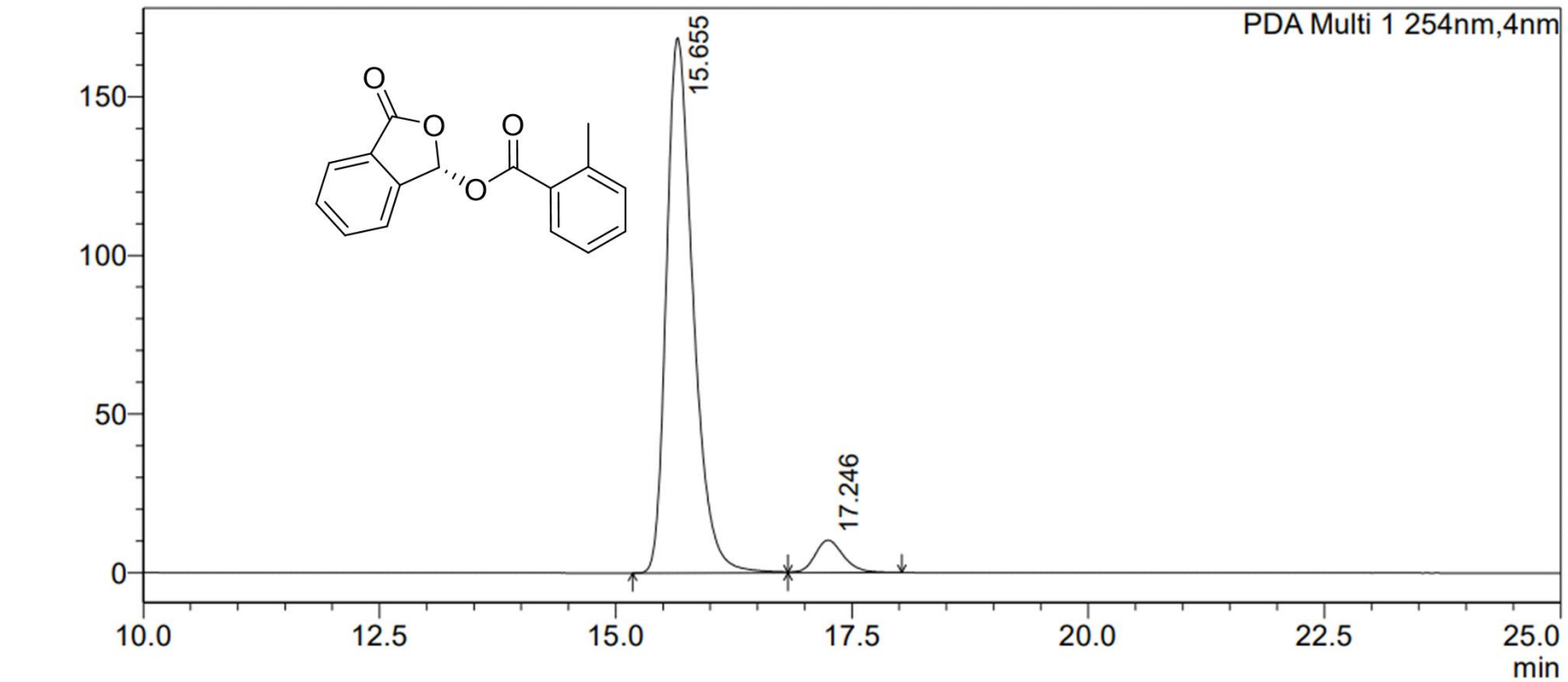

168.04
165.47
144.61
141.62
134.91
133.23
132.02
131.30
131.19
127.32
126.65
125.94
125.86
123.70
93.07
21.94
O
O
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

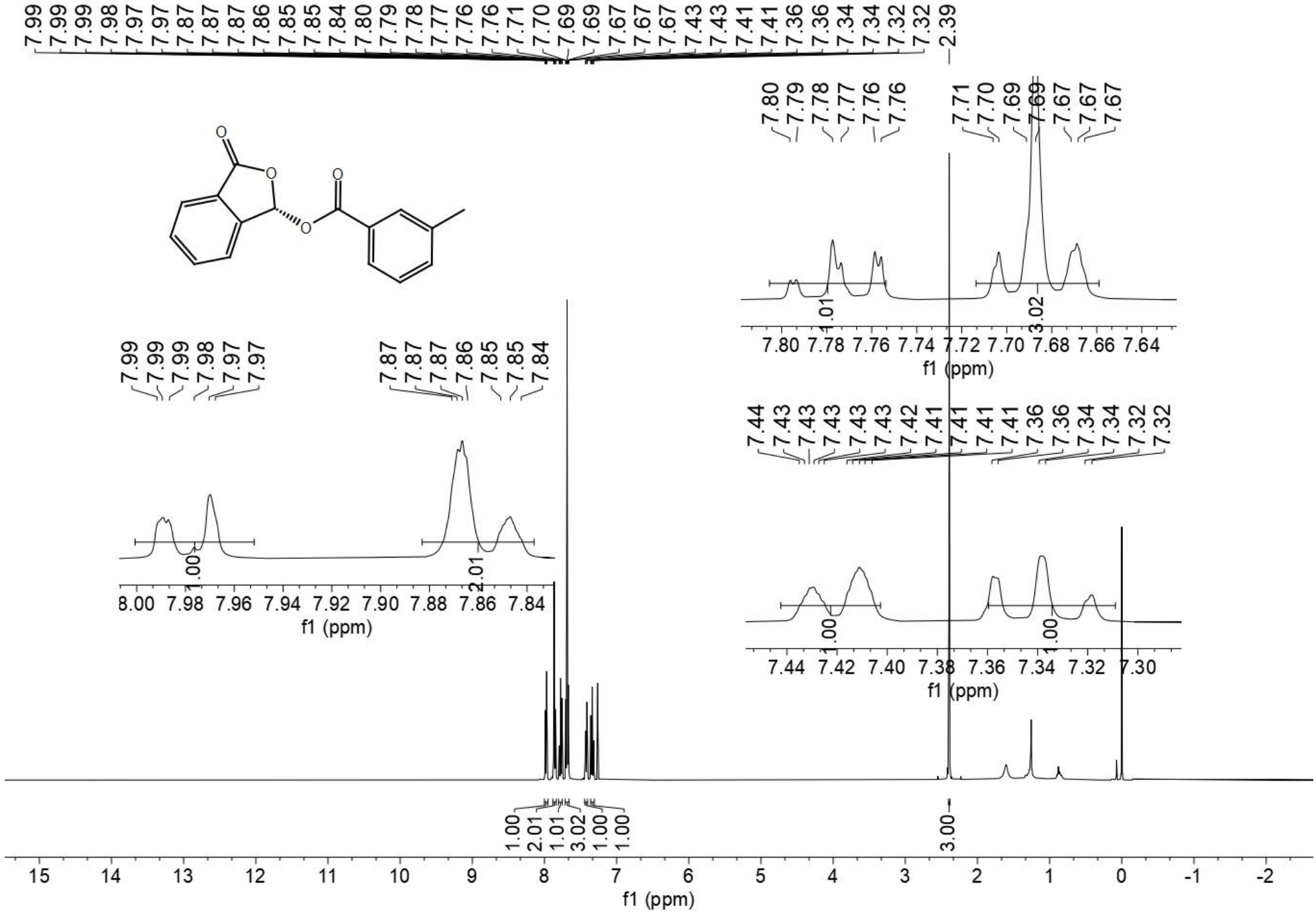
Peak#	Ret. Time	Height	Area	Area%
1	15.675	164577	3226229	49.825
2	17.173	150976	3248955	50.175
Total		315553	6475184	100.000

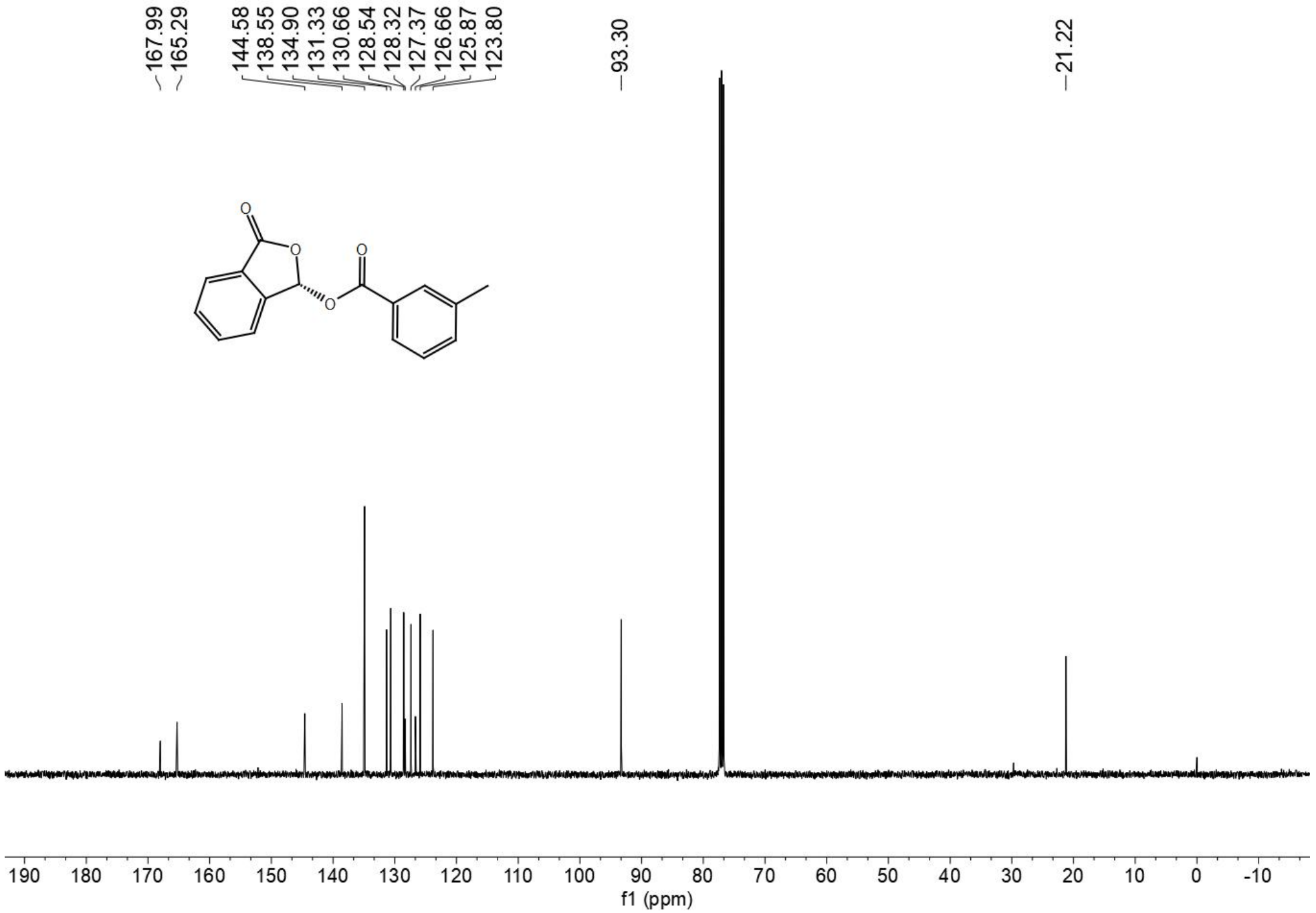


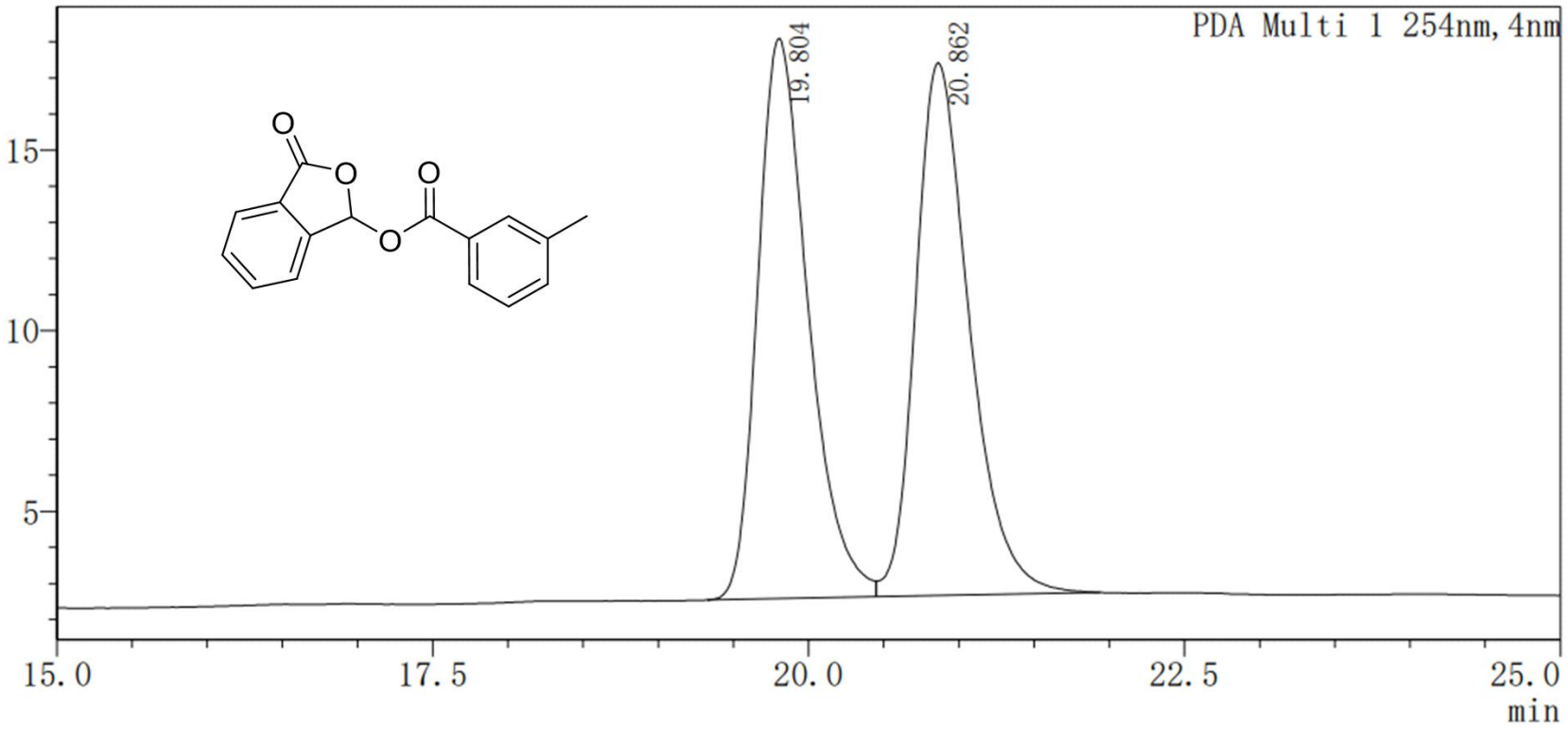
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	15.655	168587	3320947	93.906
2	17.246	10242	215494	6.094
Total		178829	3536442	100.000


7.99 7.99 7.99 7.98 7.97 7.97 7.87 7.87 7.87 7.86 7.85 7.85 7.84 7.80 7.79 7.78 7.77 7.76 7.76 7.71 7.70 7.69 7.69 7.67 7.67 7.67 7.43 7.43 7.41 7.41 7.36 7.36 7.34 7.34 7.32 7.32 2.39
O
O
O
O
O
7.80 7.79 7.78 7.77 7.76 7.76 7.71 7.70 7.69 7.69 7.67 7.67 7.67
1.01
3.02
7.80 7.78 7.76 7.74 7.72 7.70 7.68 7.66 7.64
f1 (ppm)
7.99 7.99 7.99 7.98 7.97 7.97 7.87 7.87 7.87 7.86 7.85 7.85 7.84
1.00
2.01
8.00 7.98 7.96 7.94 7.92 7.90 7.88 7.86 7.84
f1 (ppm)
7.44 7.43 7.43 7.43 7.43 7.42 7.41 7.41 7.41 7.36 7.36 7.34 7.34 7.32 7.32
1.00
1.00
7.44 7.42 7.40 7.38 7.36 7.34 7.32 7.30
f1 (ppm)
1.00 2.01 1.01 3.02 1.00 1.00
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)

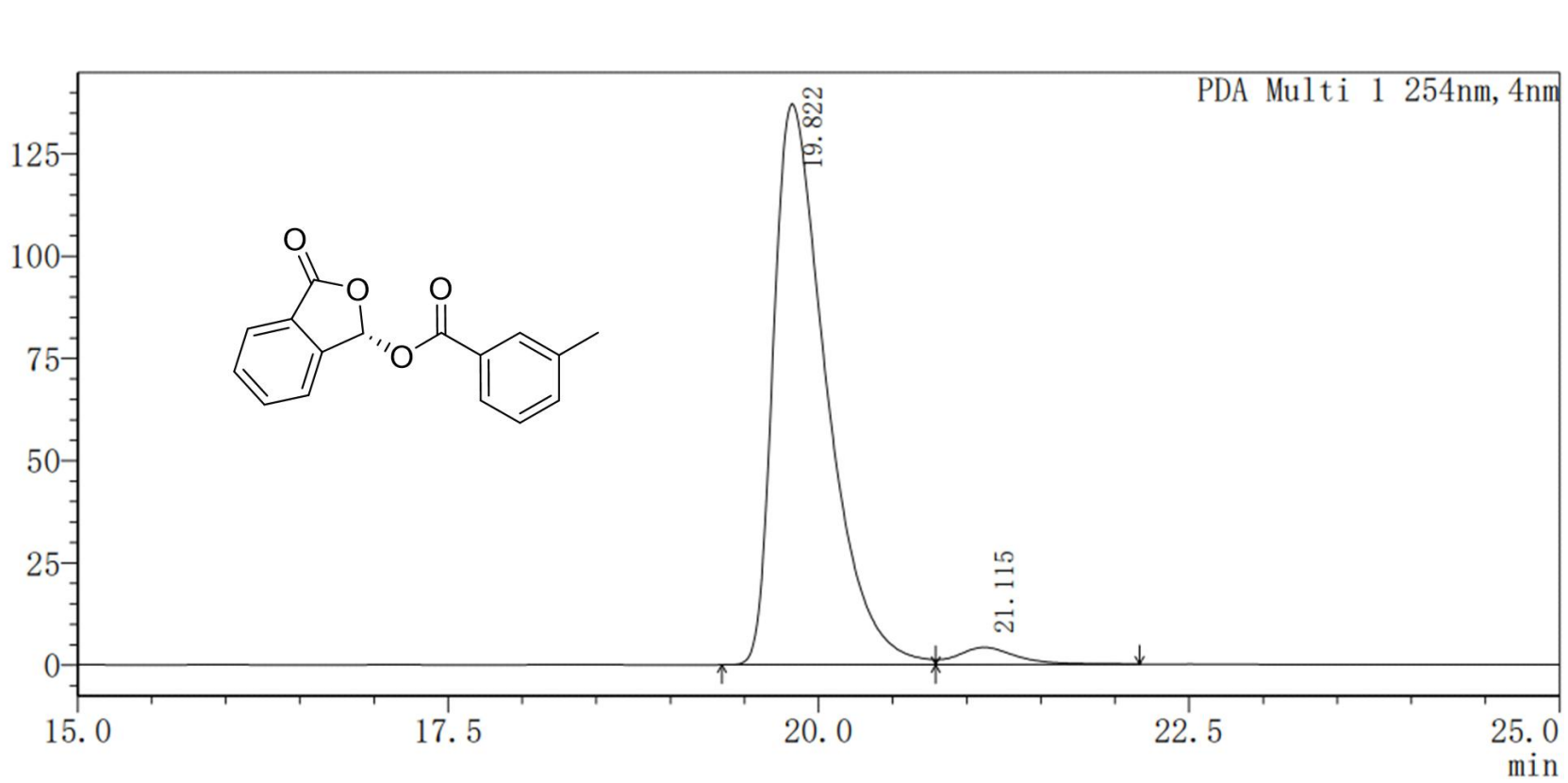

167.99
165.29
144.58
138.55
134.90
131.33
130.66
128.54
128.32
127.37
126.66
125.87
123.80
93.30
21.22
O
O
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



<Peak Table >

PDA Ch1 254nm

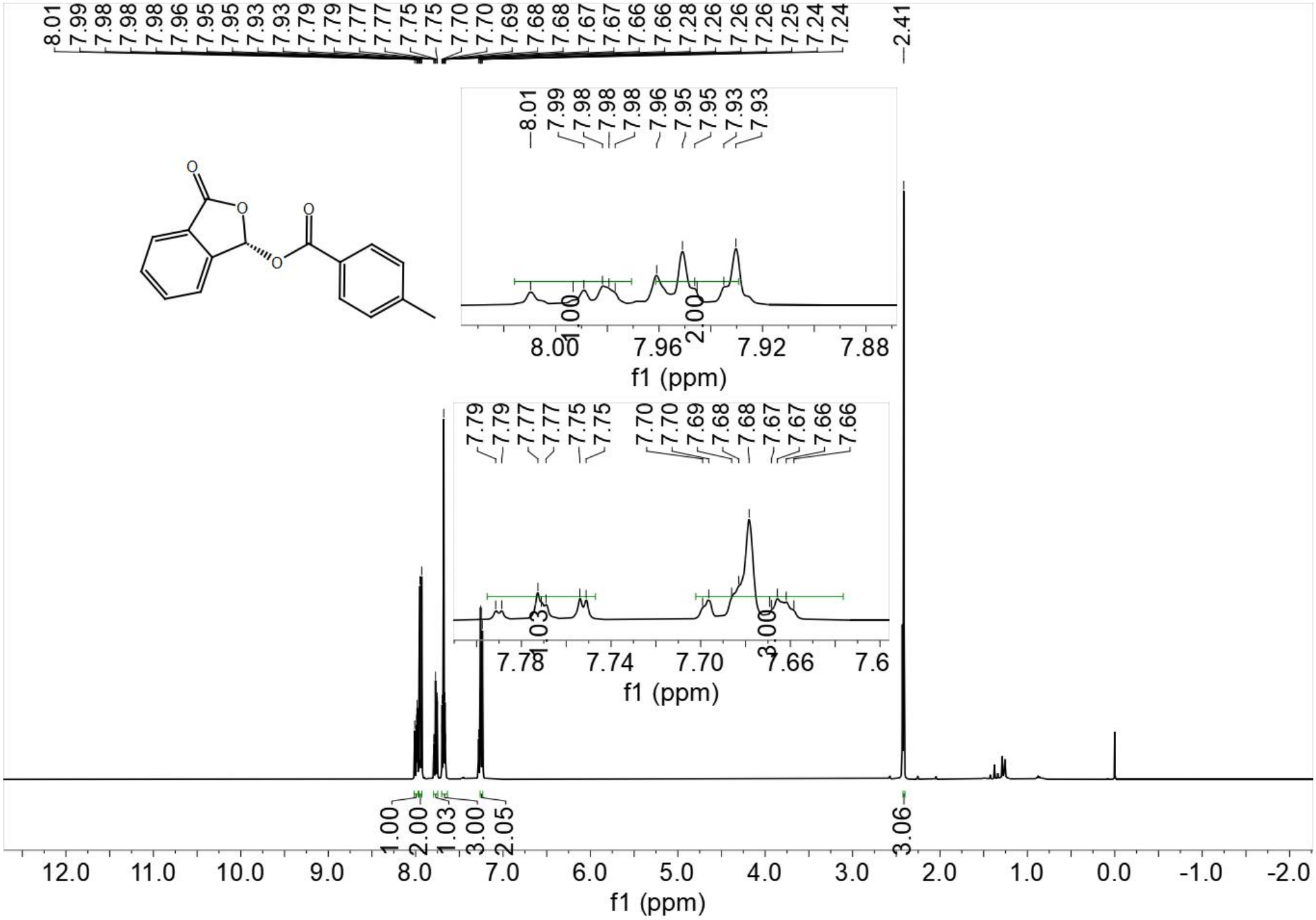
Peak#	Ret. Time	Height	Area	Area%
1	19.804	15511	363078	49.668
2	20.862	14763	367925	50.332
Total		30275	731003	100.000

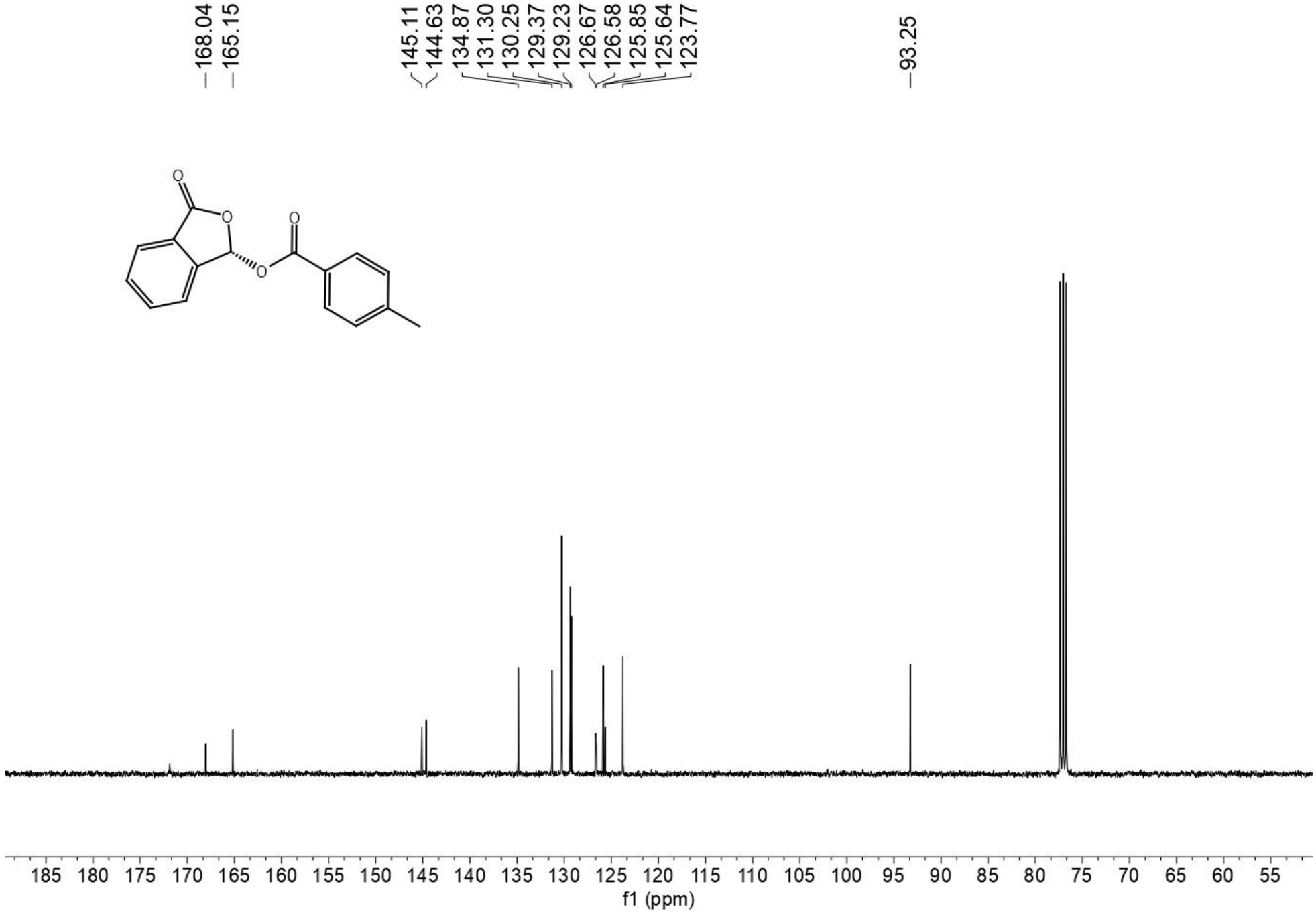


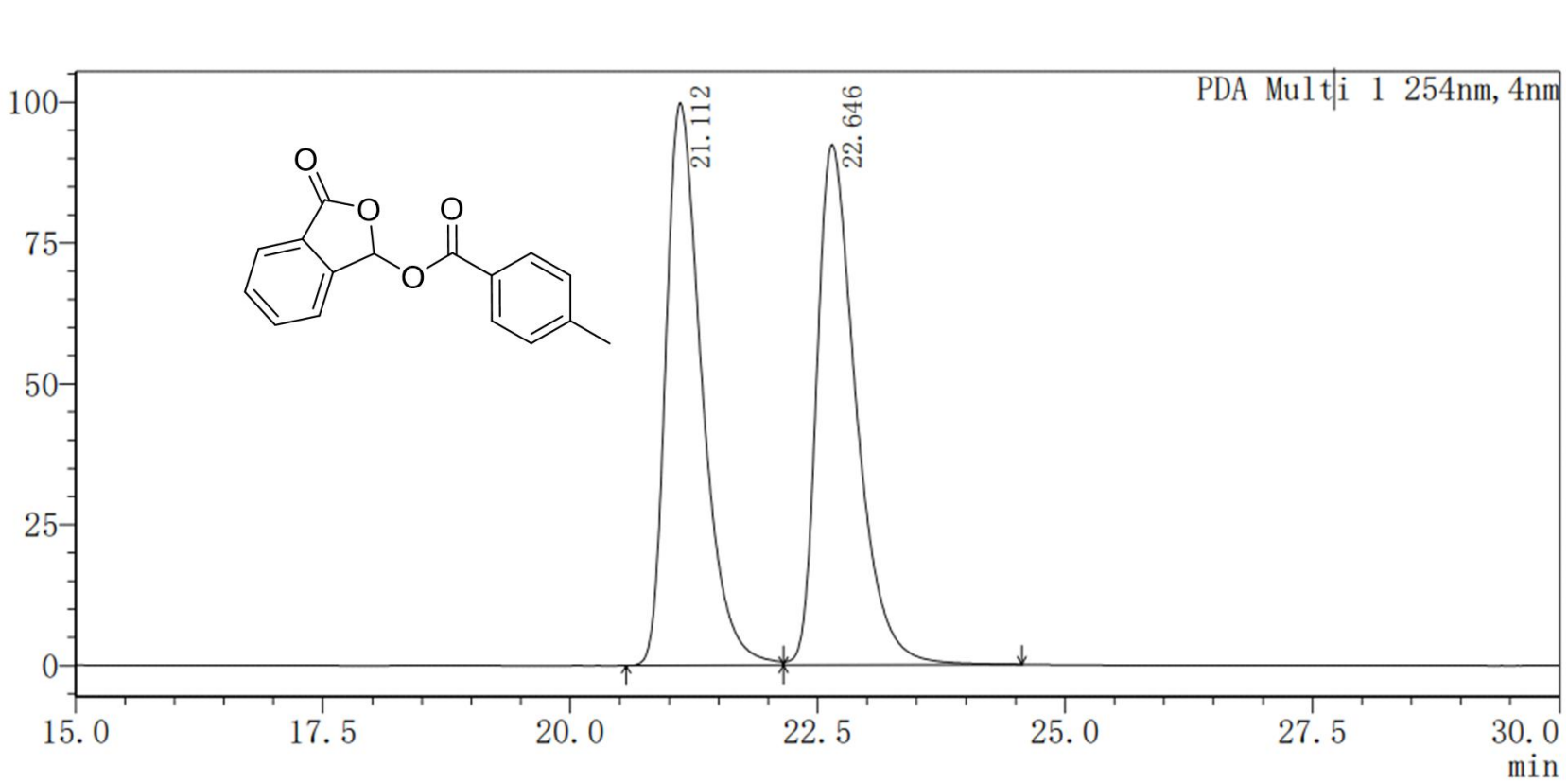
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	% Area
1	19.822	137140	3383624	96.743
2	21.115	4168	113926	3.257
Total		141307	3497550	100.000


8.01 7.99 7.98 7.98 7.98 7.96 7.95 7.95 7.93 7.93 7.79 7.79 7.77 7.77 7.75 7.75 7.70 7.70 7.69 7.68 7.68 7.67 7.67 7.66 7.66 7.28 7.26 7.26 7.26 7.25 7.24 7.24 2.41
O O O O
8.01 7.99 7.98 7.98 7.98 7.96 7.95 7.95 7.93 7.93
1.00 2.00
8.00 7.96 7.92 7.88
f1 (ppm)
7.79 7.79 7.77 7.77 7.75 7.75 7.70 7.70 7.69 7.68 7.68 7.67 7.67 7.66 7.66
1.03 3.00
7.78 7.74 7.70 7.66 7.6
f1 (ppm)
1.00 2.00 1.03 3.00 2.05 3.06
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0 -2.0
f1 (ppm)

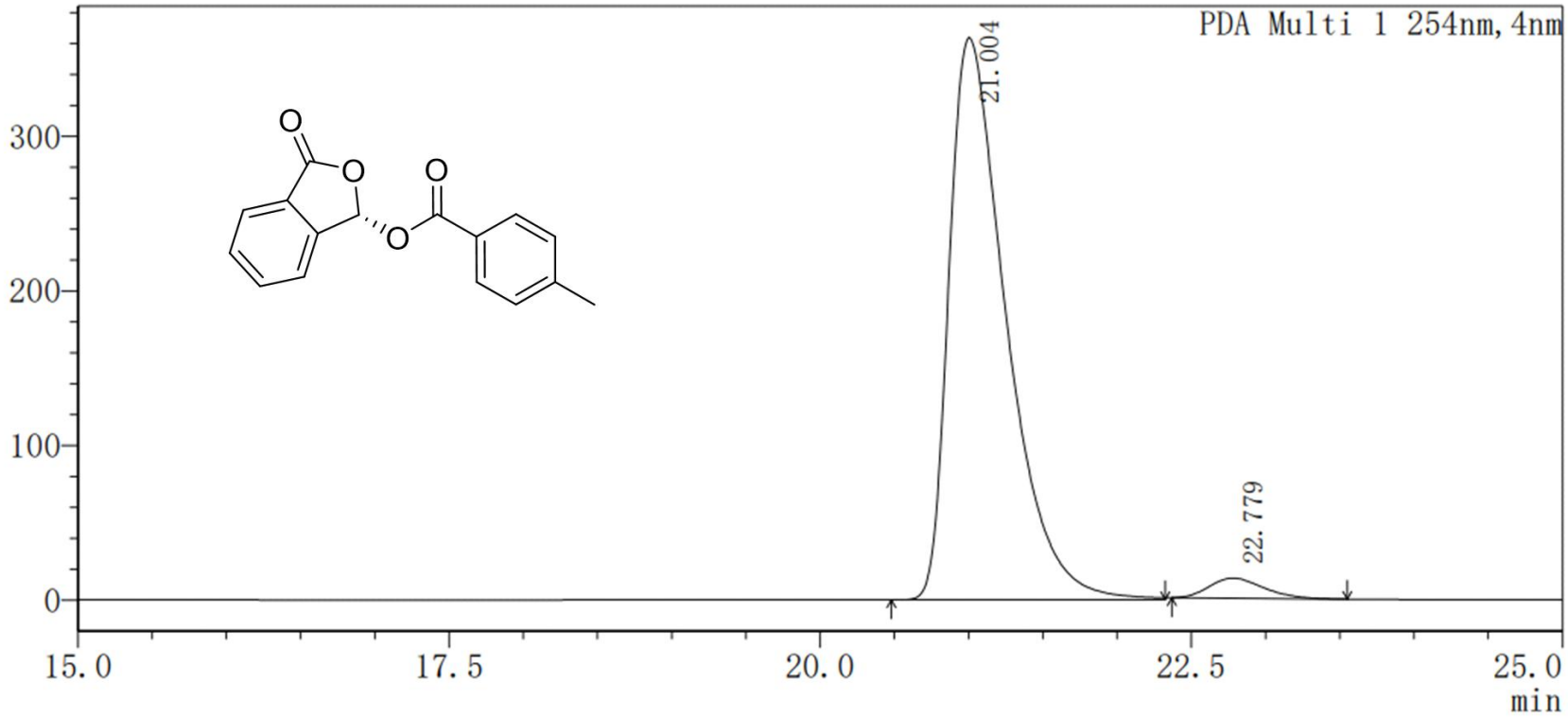

168.04
165.15
145.11
144.63
134.87
131.30
130.25
129.37
129.23
126.67
126.58
125.85
125.64
123.77
93.25
O
O
O
O
185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	21.112	99834	2522957	49.788
2	22.646	92413	2544418	50.212
Total		192247	5067374	100.000

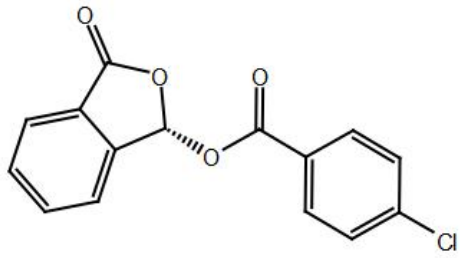


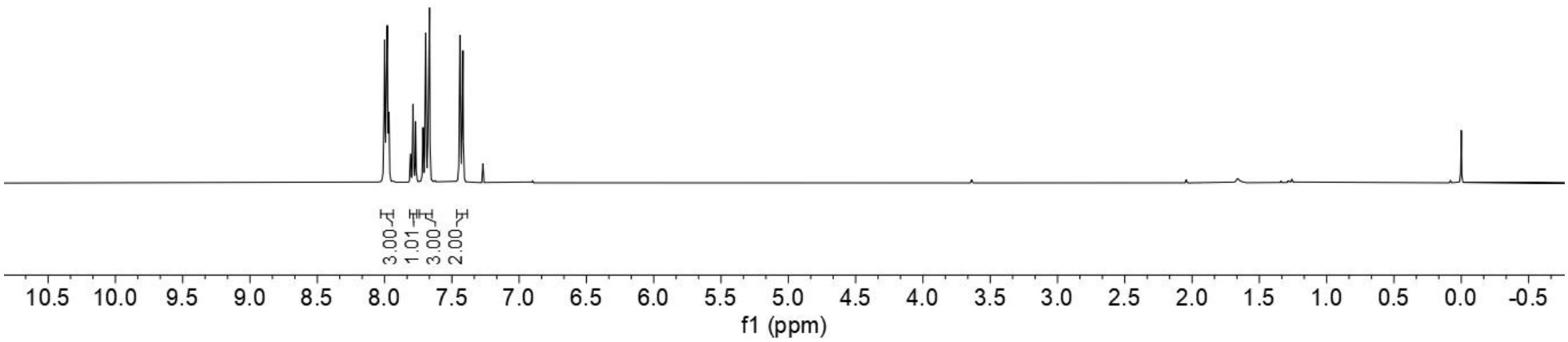
<Peak Table>

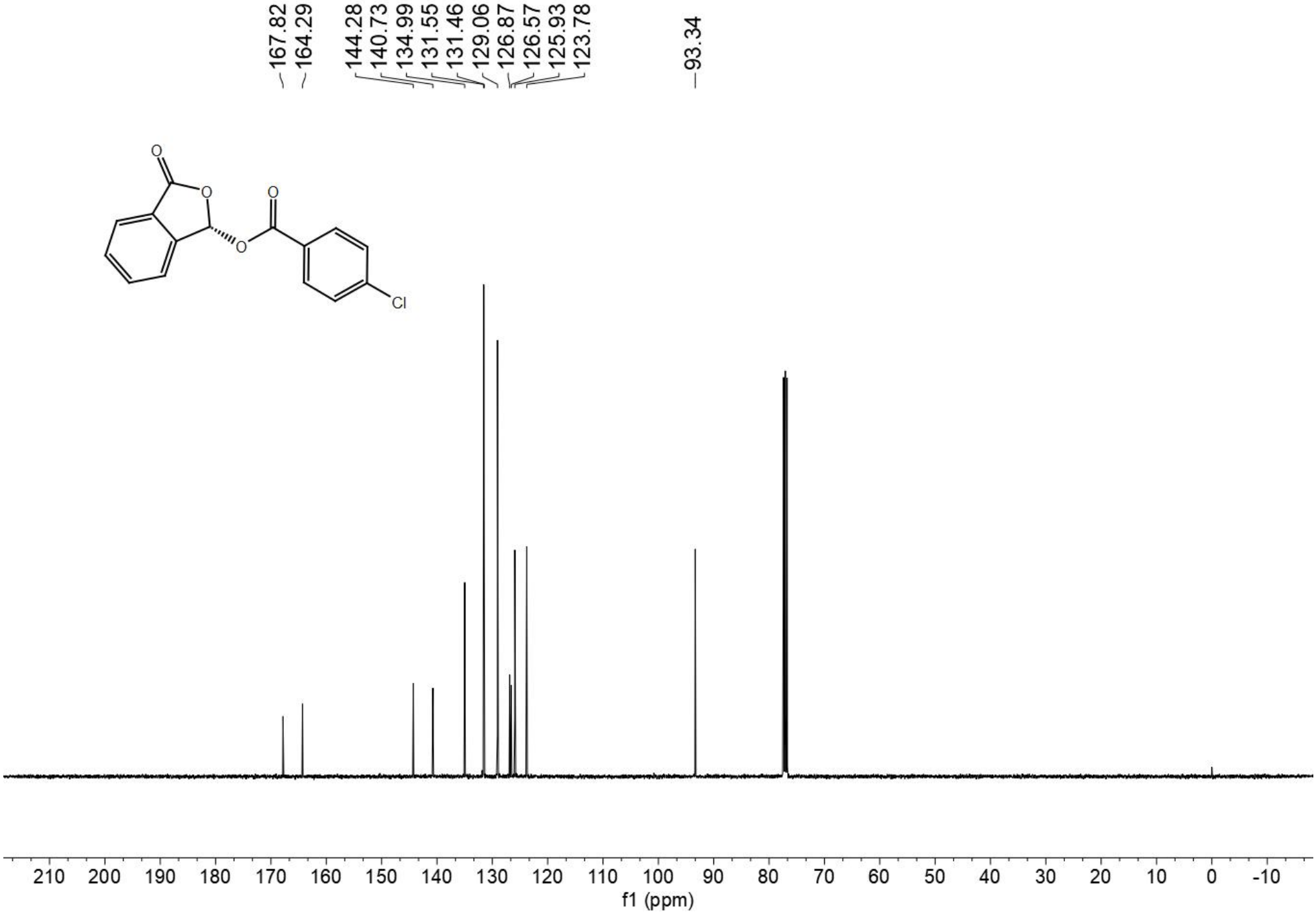
PDA Ch1 254nm

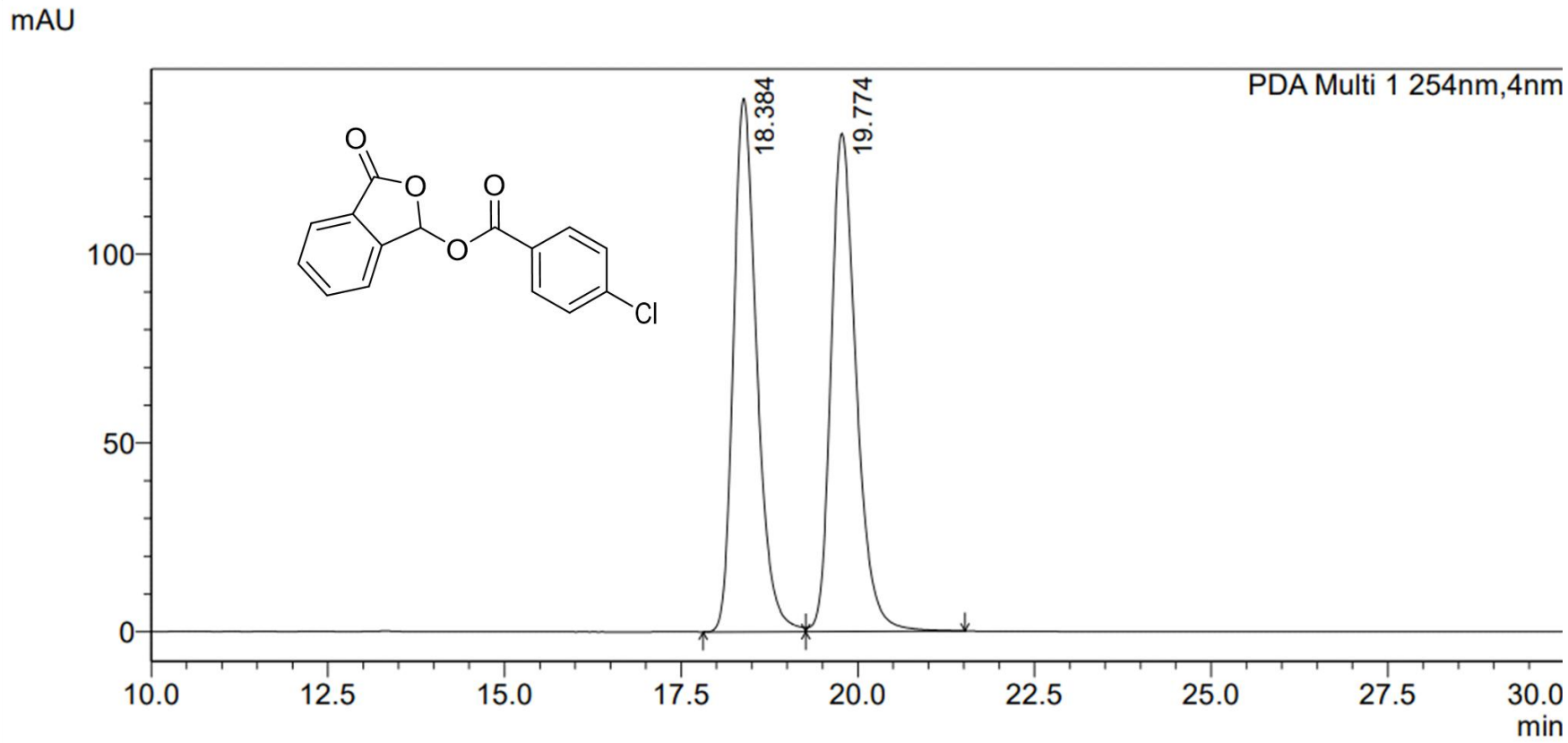
Peak#	Ret. Time	Height	Area	Area%
1	21.004	363830	9702522	96.713
2	22.779	12949	329713	3.287
总计		376779	10032235	100.000


8.01
8.00
8.00
7.99
7.98
7.97
7.97
7.81
7.81
7.79
7.79
7.77
7.77
7.71
7.70
7.69
7.67
7.67
7.44
7.42


O
O
O
O
Cl


3.00
1.01
3.00
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

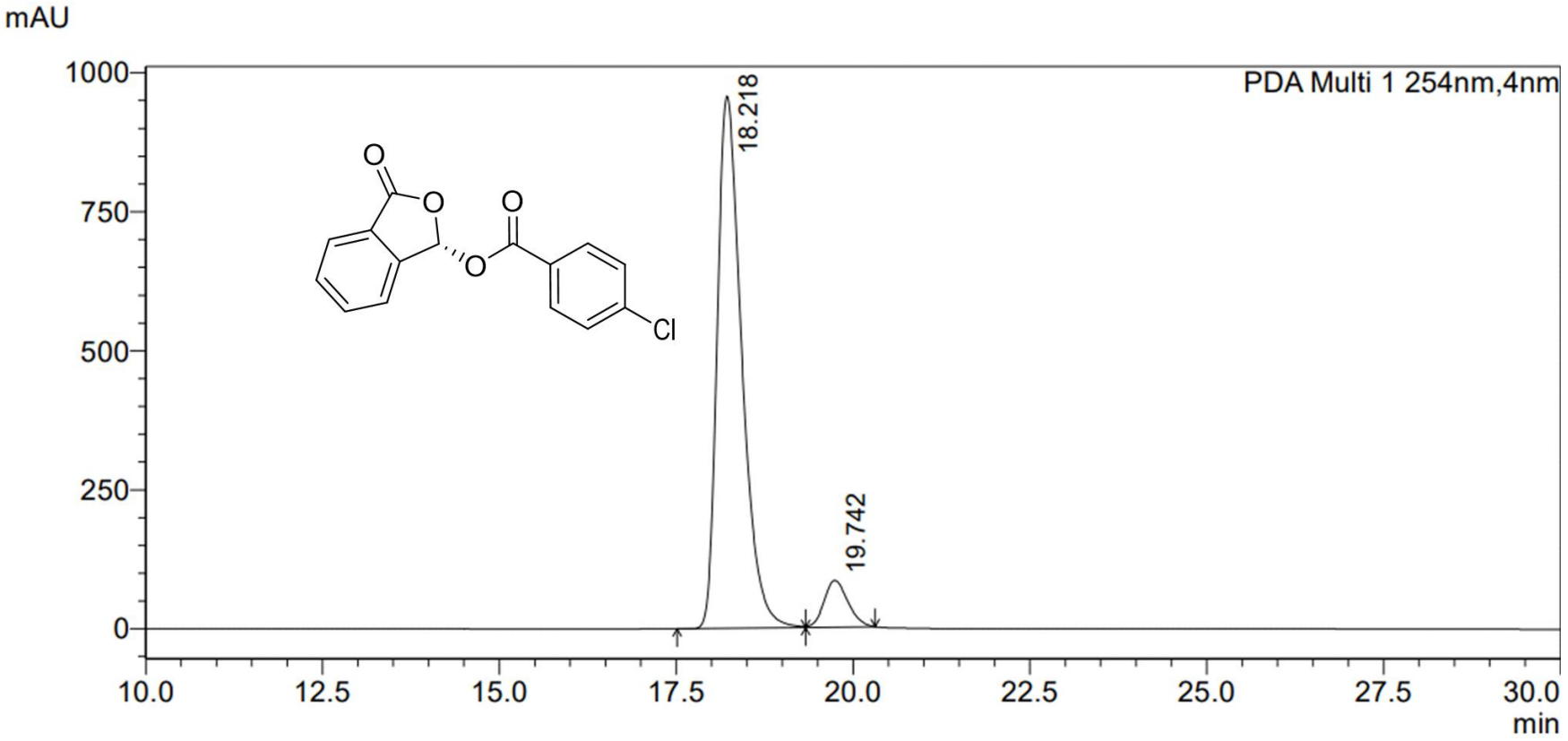

167.82
164.29
144.28
140.73
134.99
131.55
131.46
129.06
126.87
126.57
125.93
123.78
93.34
O
O
O
O
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	18.384	141192	3240021	49.711
2	19.774	131945	3277733	50.289
Total		273137	6517754	100.000

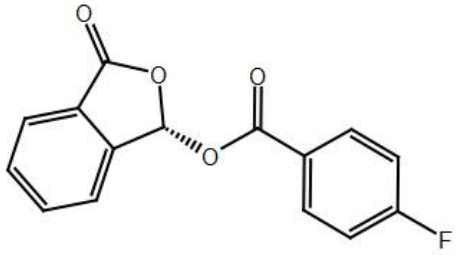


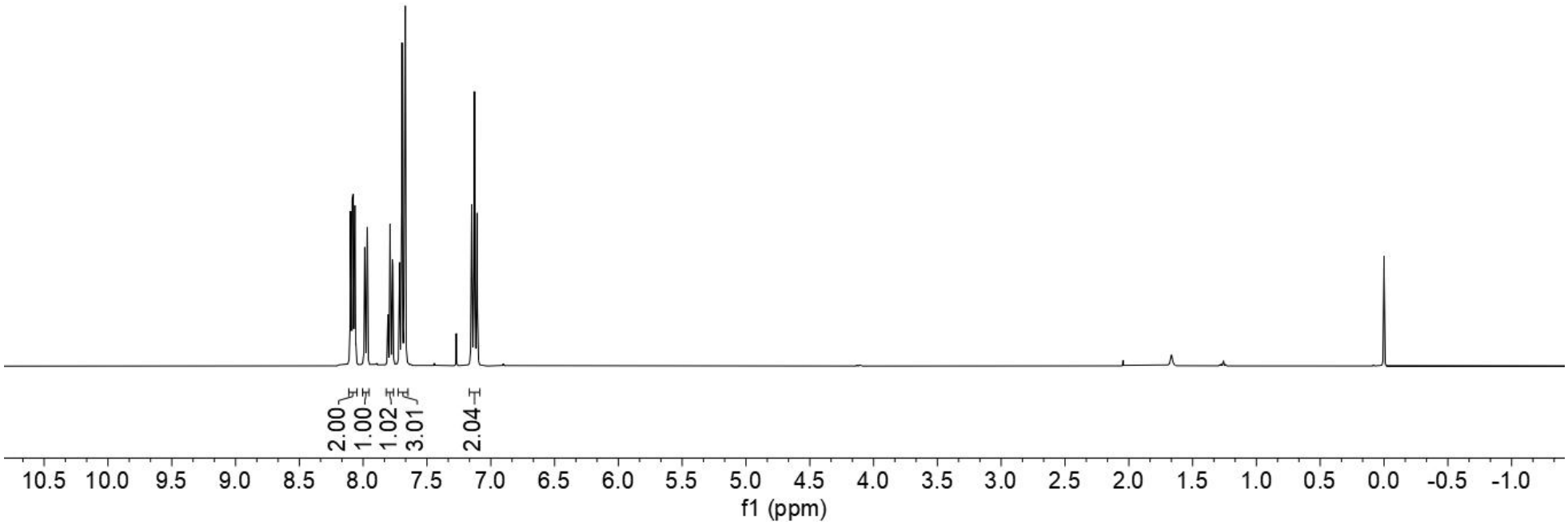
<Peak Table>

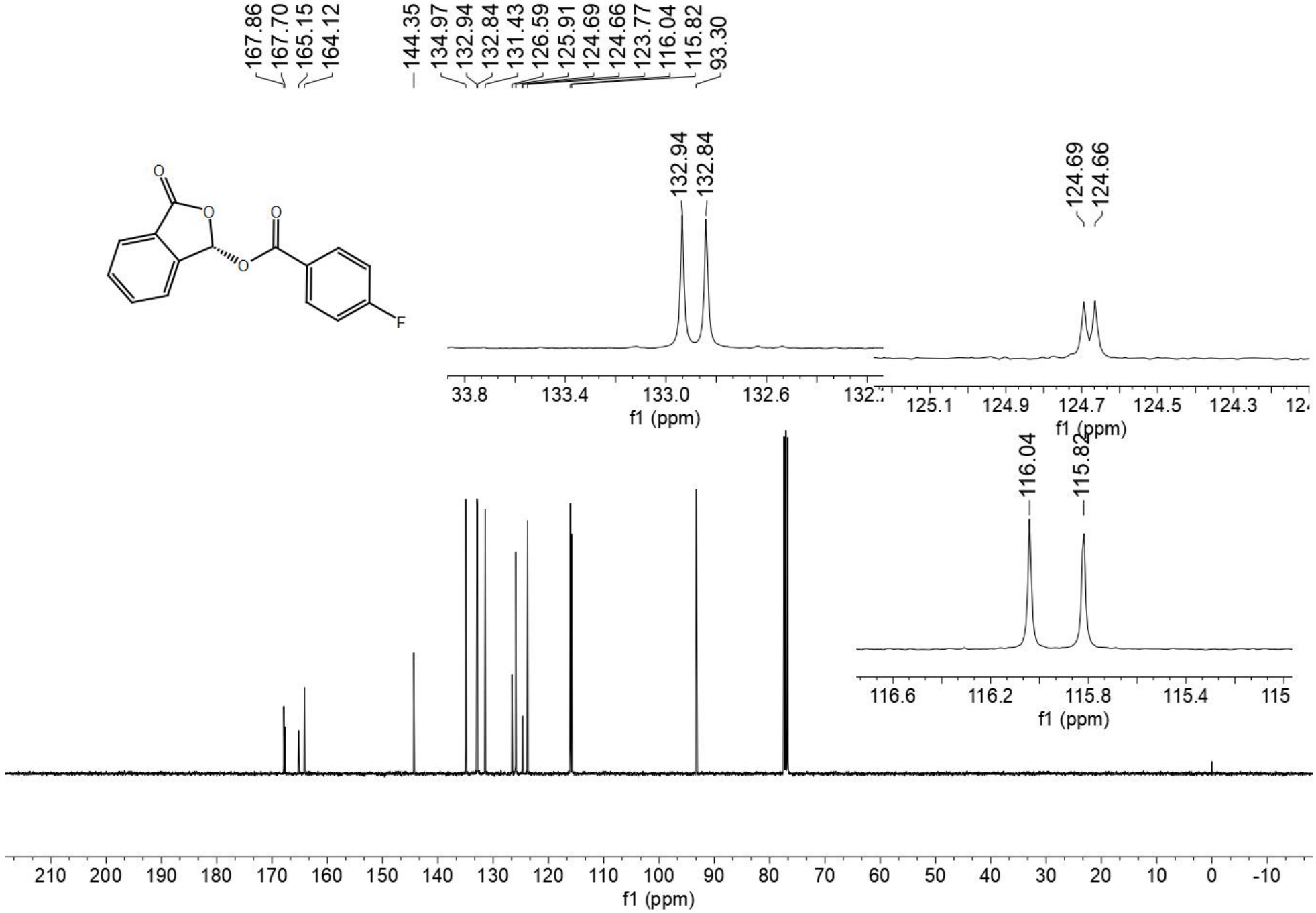
PDA Ch1 254nm

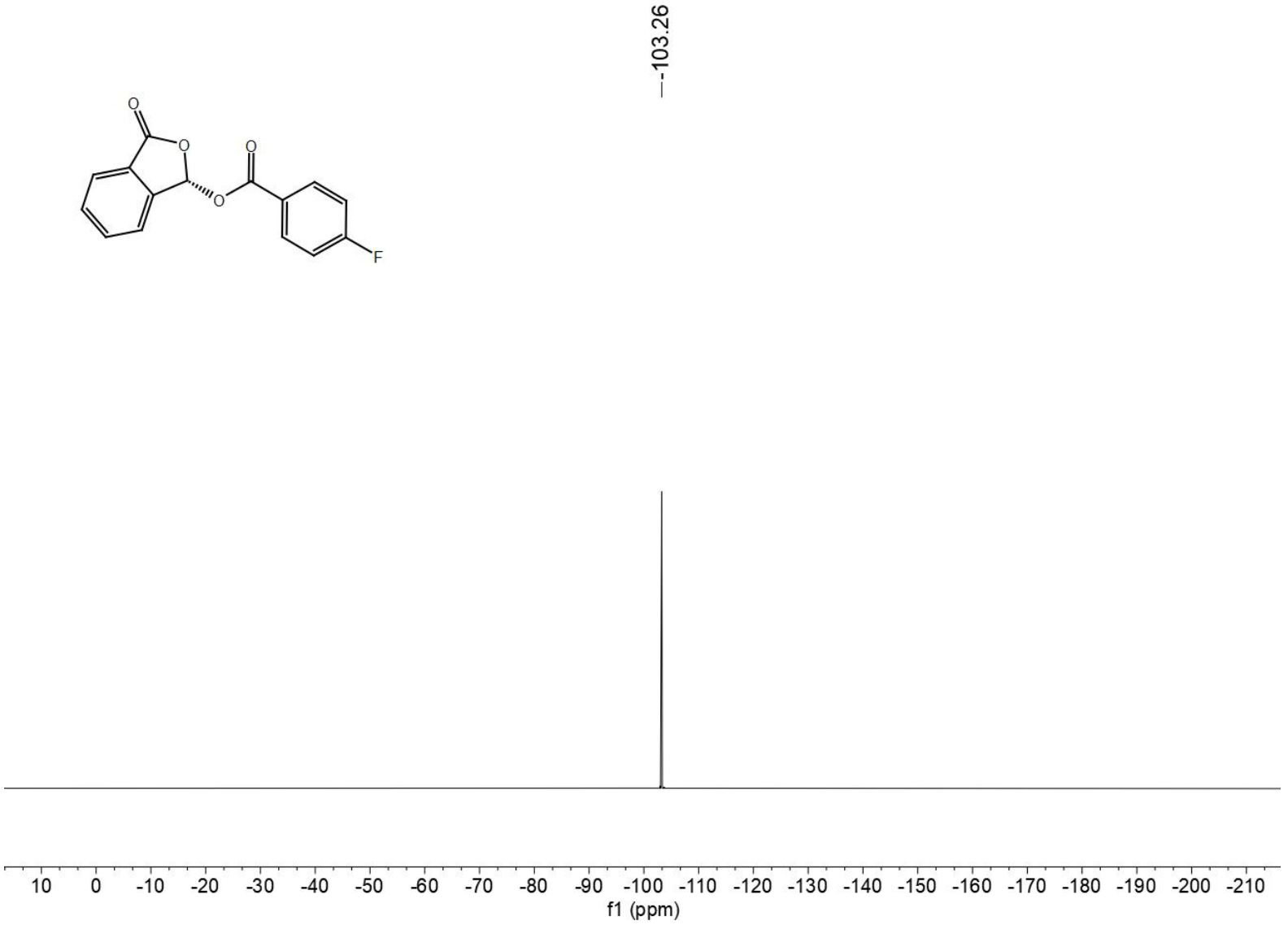
Peak#	Ret. Time	Height	Area	Area%
1	18.218	956645	23025363	92.111
2	19.742	83926	1972177	7.889
Total		1040571	24997540	100.000

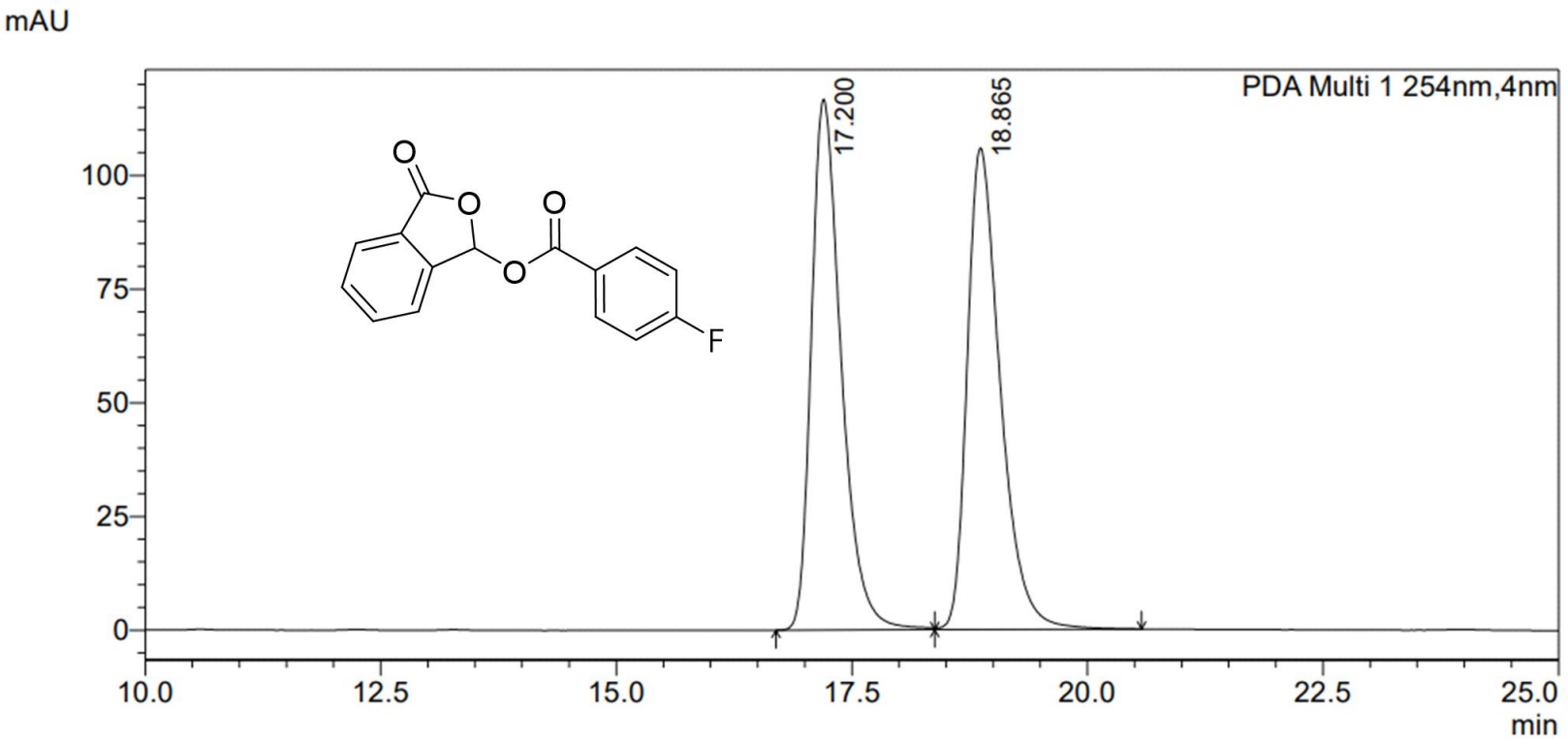

8.10
8.09
8.08
8.08
8.06
7.99
7.97
7.79
7.77
7.77
7.71
7.70
7.68
7.67
7.15
7.13
7.13
7.12
7.11


O
O
O
O
F


2.00
1.00
1.02
3.01
2.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


167.86
167.70
165.15
164.12
144.35
134.97
132.94
132.84
131.43
126.59
125.91
124.69
124.66
123.77
116.04
115.82
93.30
O
O
O
O
F
132.94
132.84
124.69
124.66
33.8
133.4
133.0
132.6
f1 (ppm)
125.1
124.9
124.7
124.5
124.3
f1 (ppm)
116.04
115.82
116.6
116.2
115.8
115.4
115
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

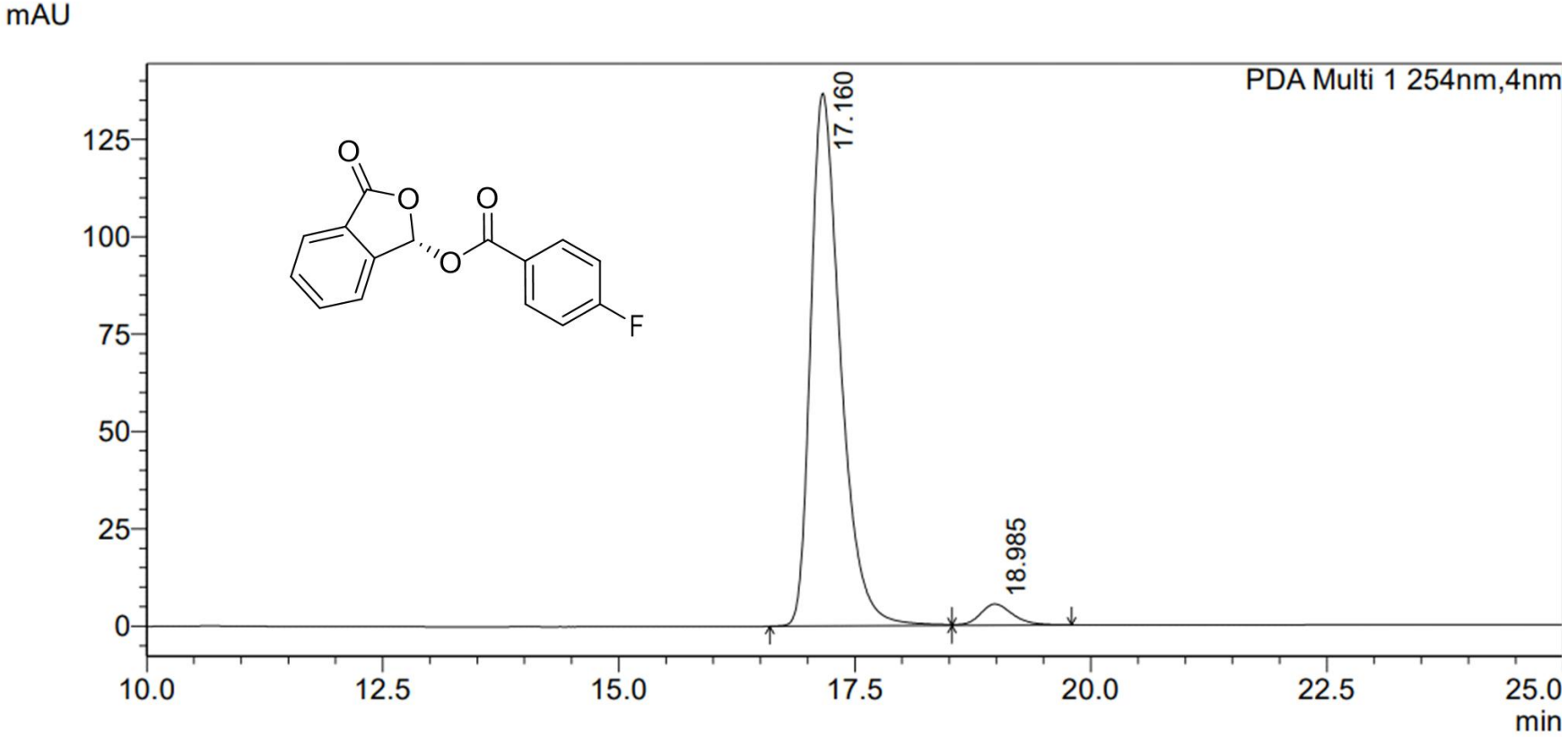

-103.26
O
O
O
O
F
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

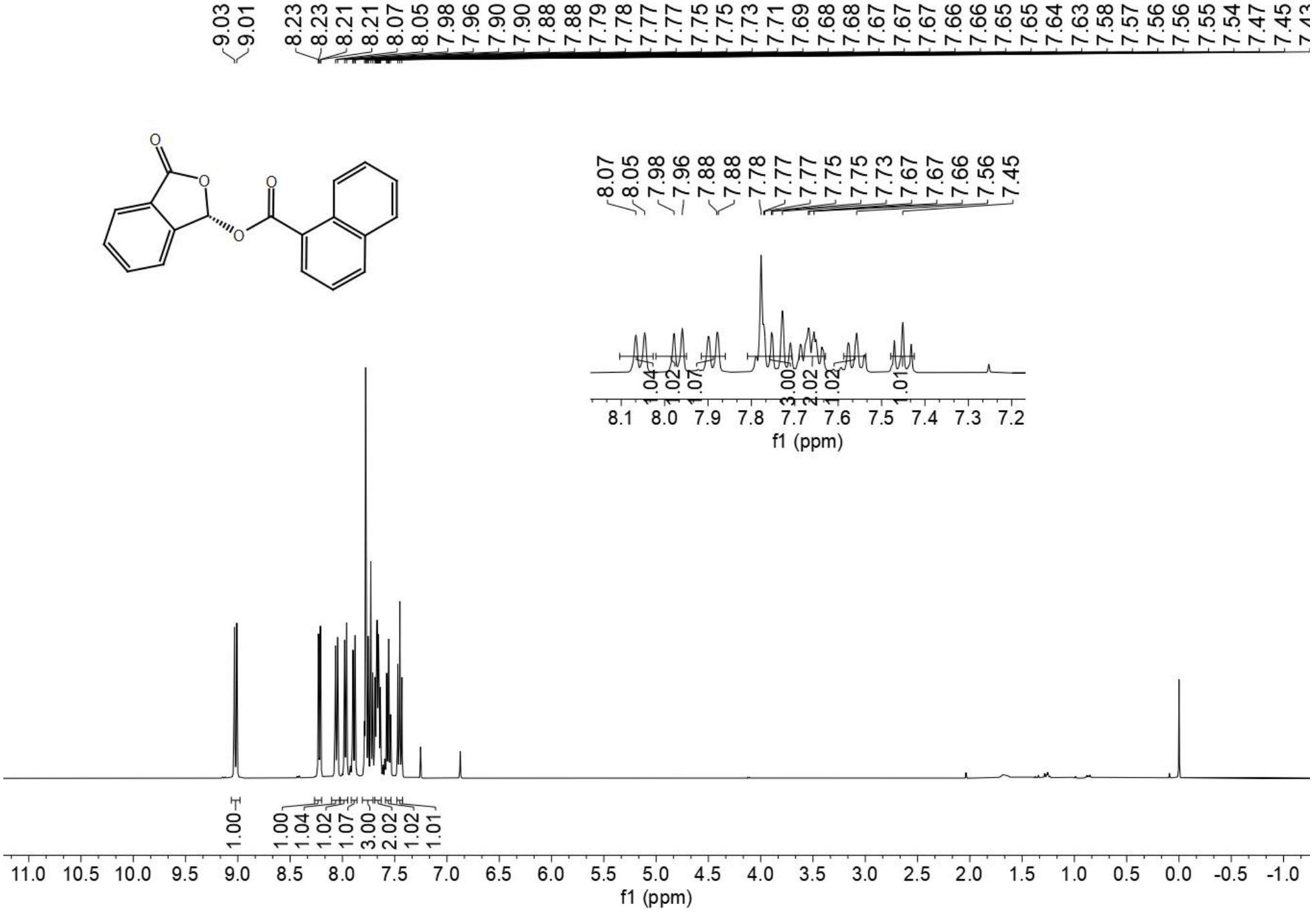
Peak#	Ret. Time	Height	Area	Area%
1	17.200	116708	2575407	49.879
2	18.865	105883	2587868	50.121
Total		222591	5163275	100.000

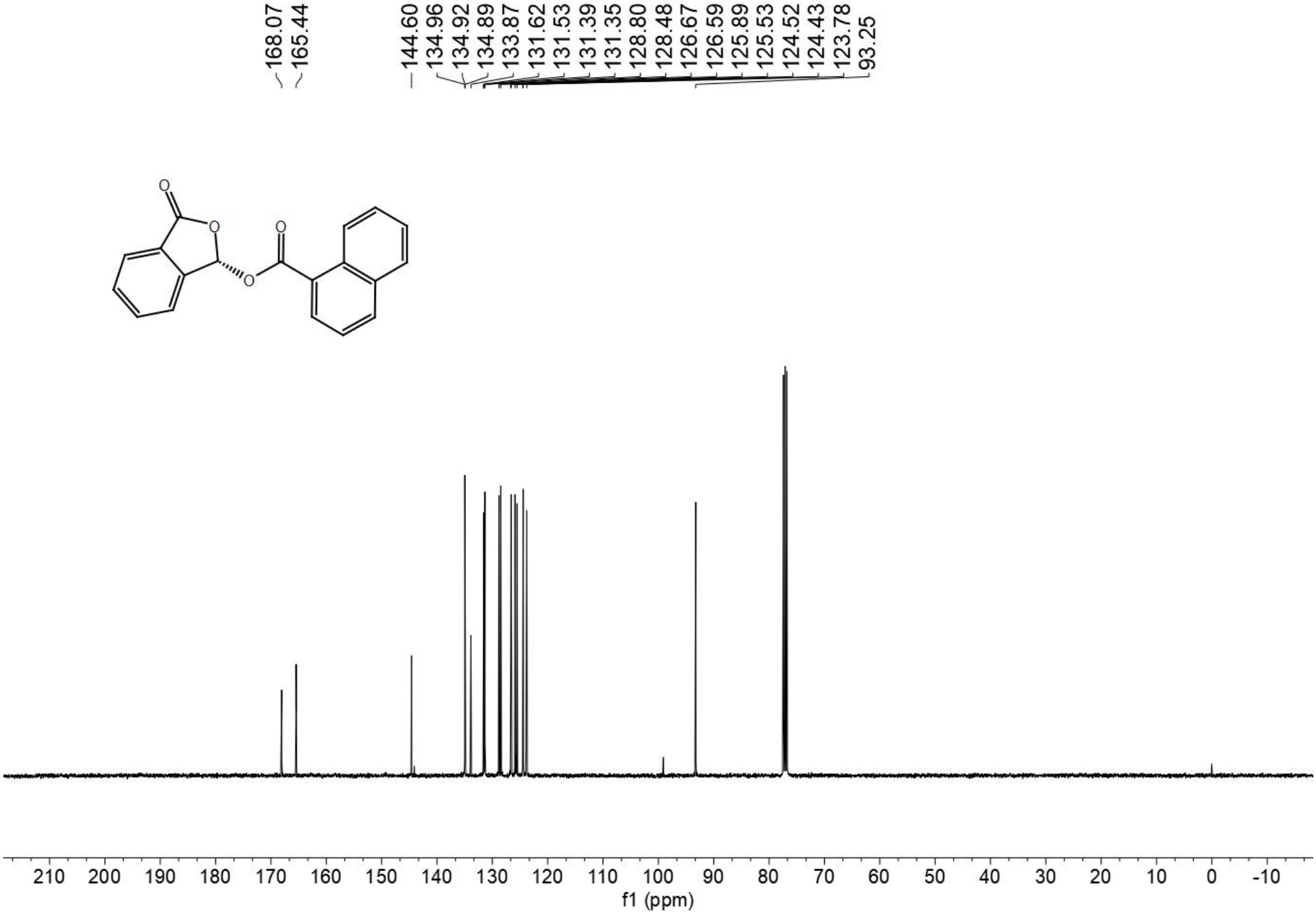


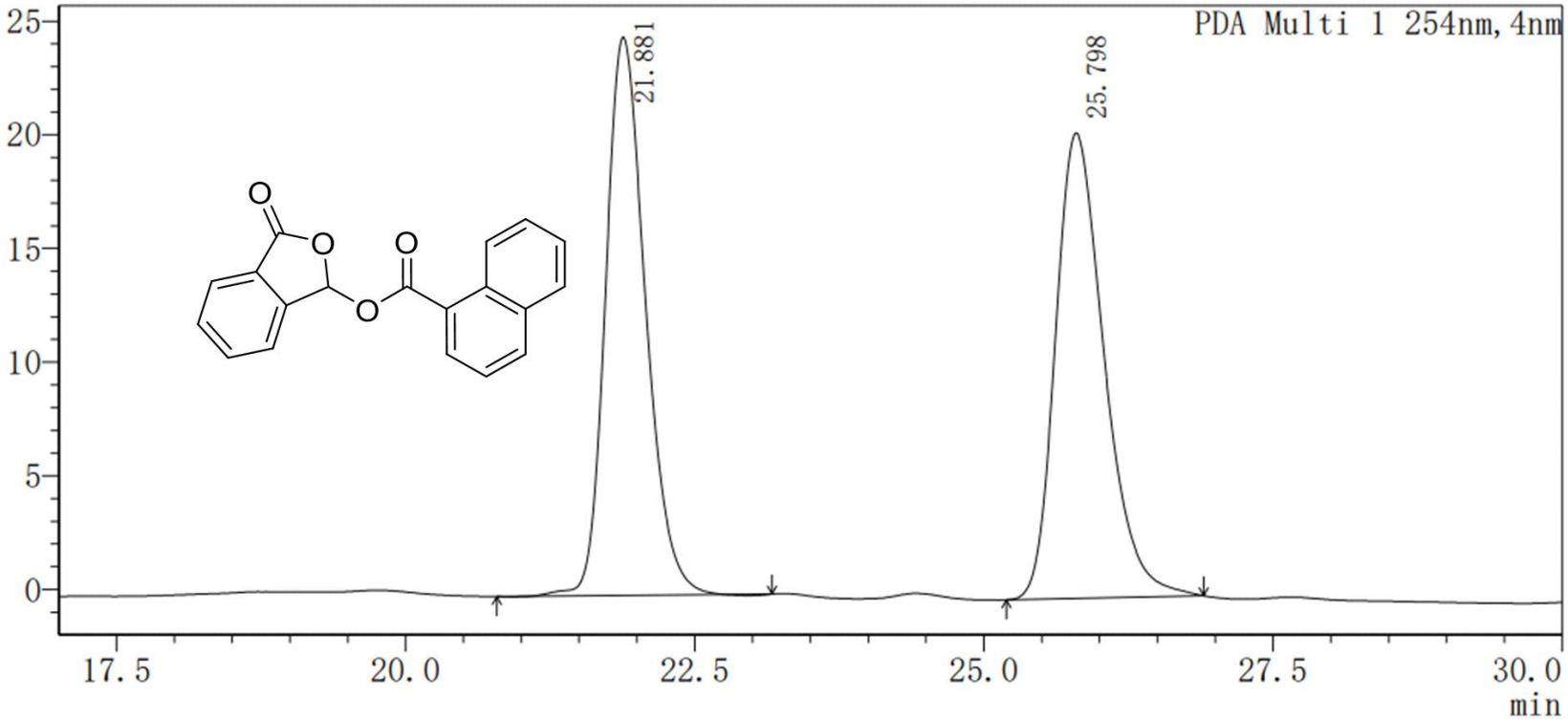
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	17.160	136749	3016106	95.859
2	18.985	5434	130298	4.141
Total		142183	3146404	100.000


9.03
9.01
8.23
8.23
8.21
8.21
8.07
8.05
7.98
7.96
7.90
7.90
7.88
7.88
7.79
7.78
7.77
7.77
7.75
7.75
7.73
7.71
7.69
7.68
7.68
7.67
7.67
7.67
7.66
7.66
7.65
7.65
7.64
7.63
7.58
7.57
7.56
7.56
7.55
7.54
7.47
7.45
8.07
8.05
7.98
7.96
7.88
7.88
7.78
7.77
7.77
7.75
7.75
7.73
7.67
7.67
7.66
7.56
7.45
1.04
1.02
1.07
3.00
2.02
1.02
1.01
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
1.00
1.00
1.04
1.02
1.07
3.00
2.02
1.02
1.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

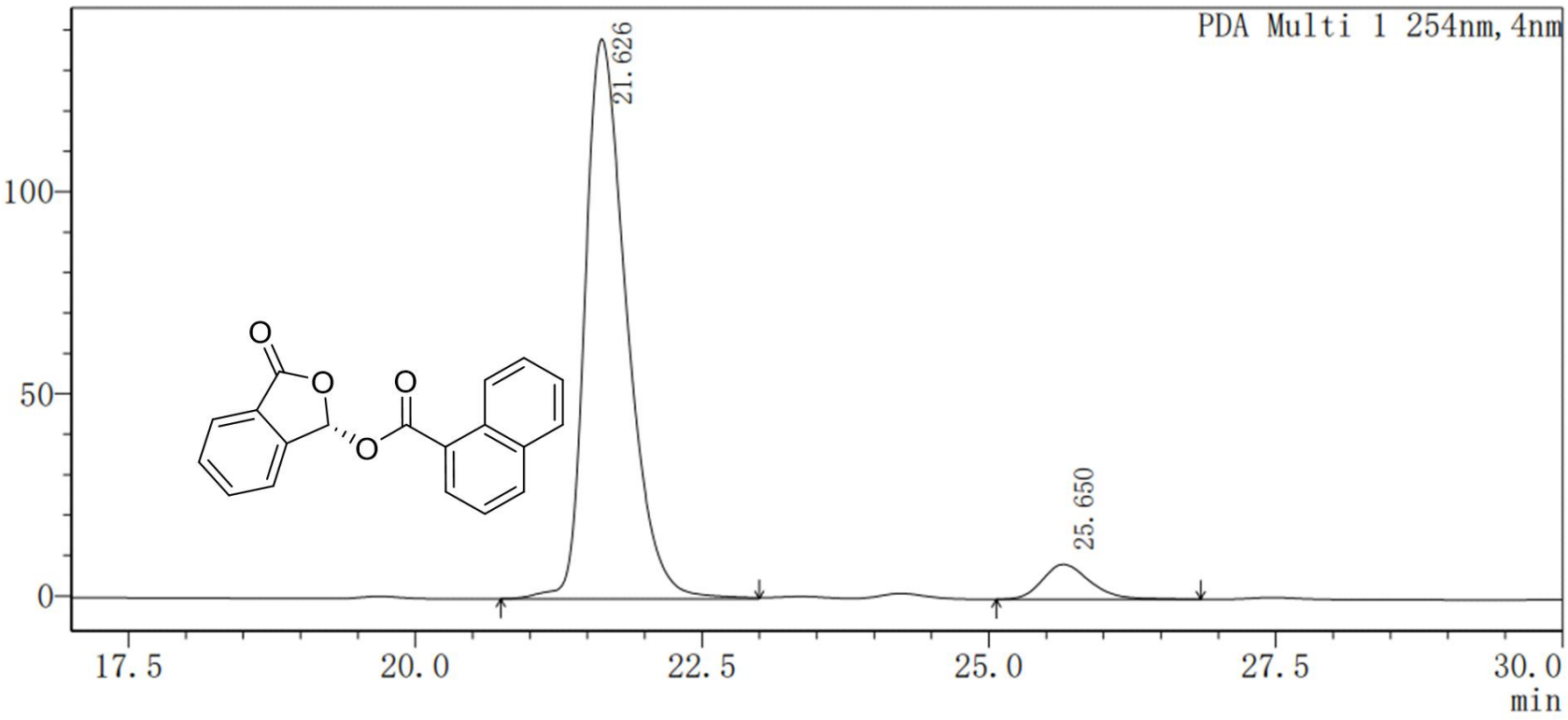

168.07
165.44
144.60
134.96
134.92
134.89
133.87
131.62
131.53
131.39
131.35
128.80
128.48
126.67
126.59
125.89
125.53
124.52
124.43
123.78
93.25
O
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

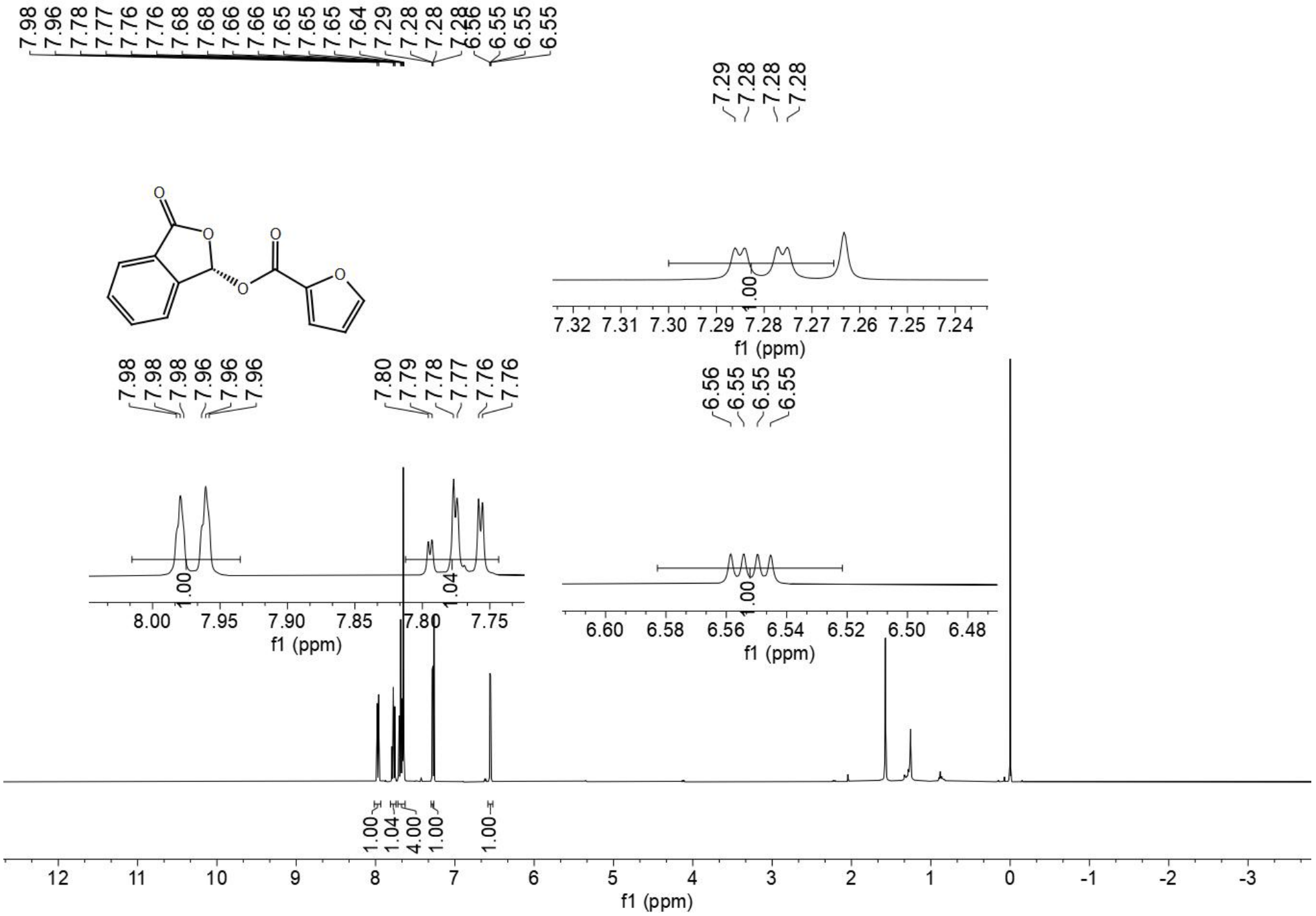
Peak#	Ret. Time	Height	Area	Area%
1	21.881	24559	589506	49.581
2	25.798	20482	599468	50.419
Total		45041	1188974	100.000

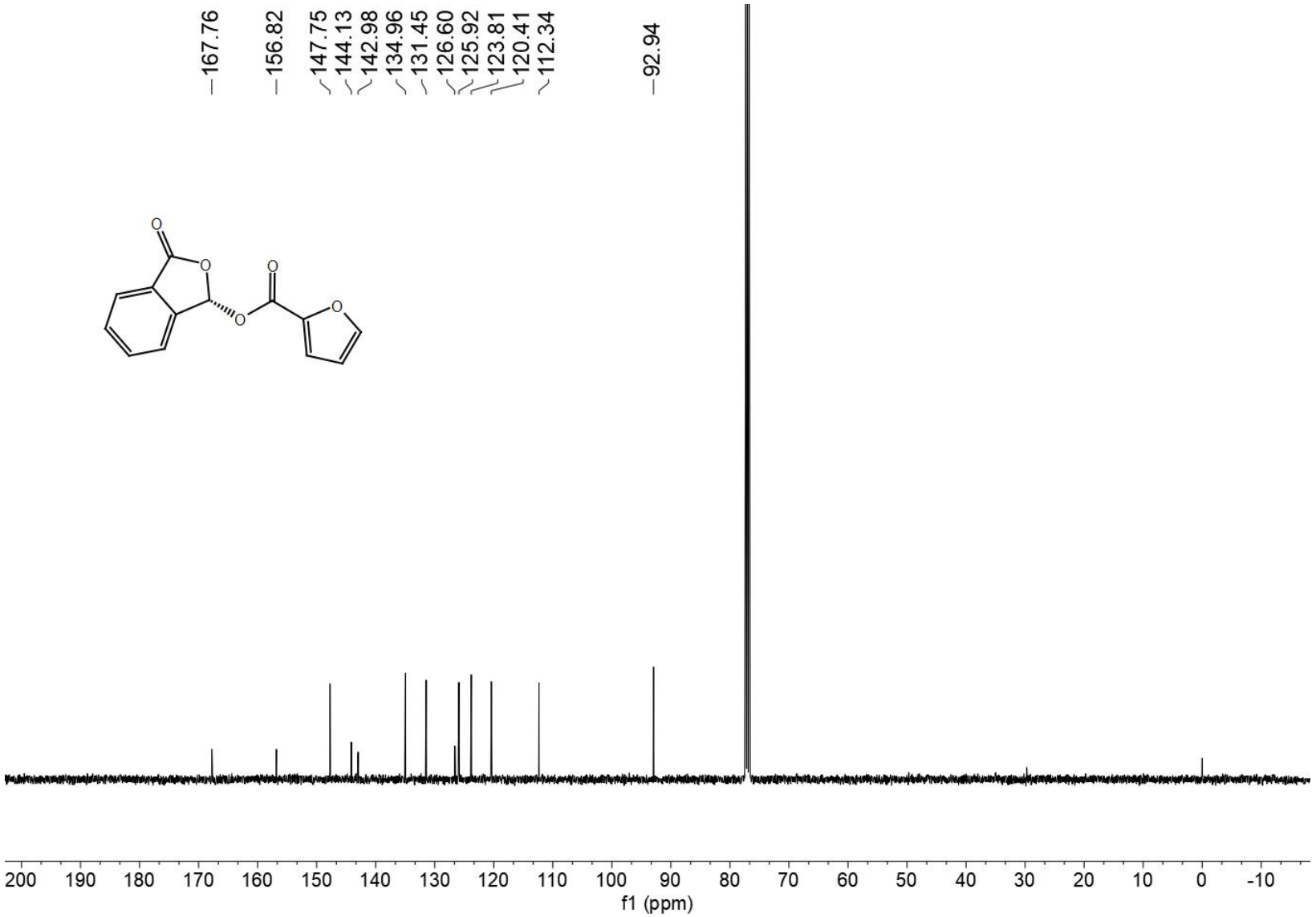


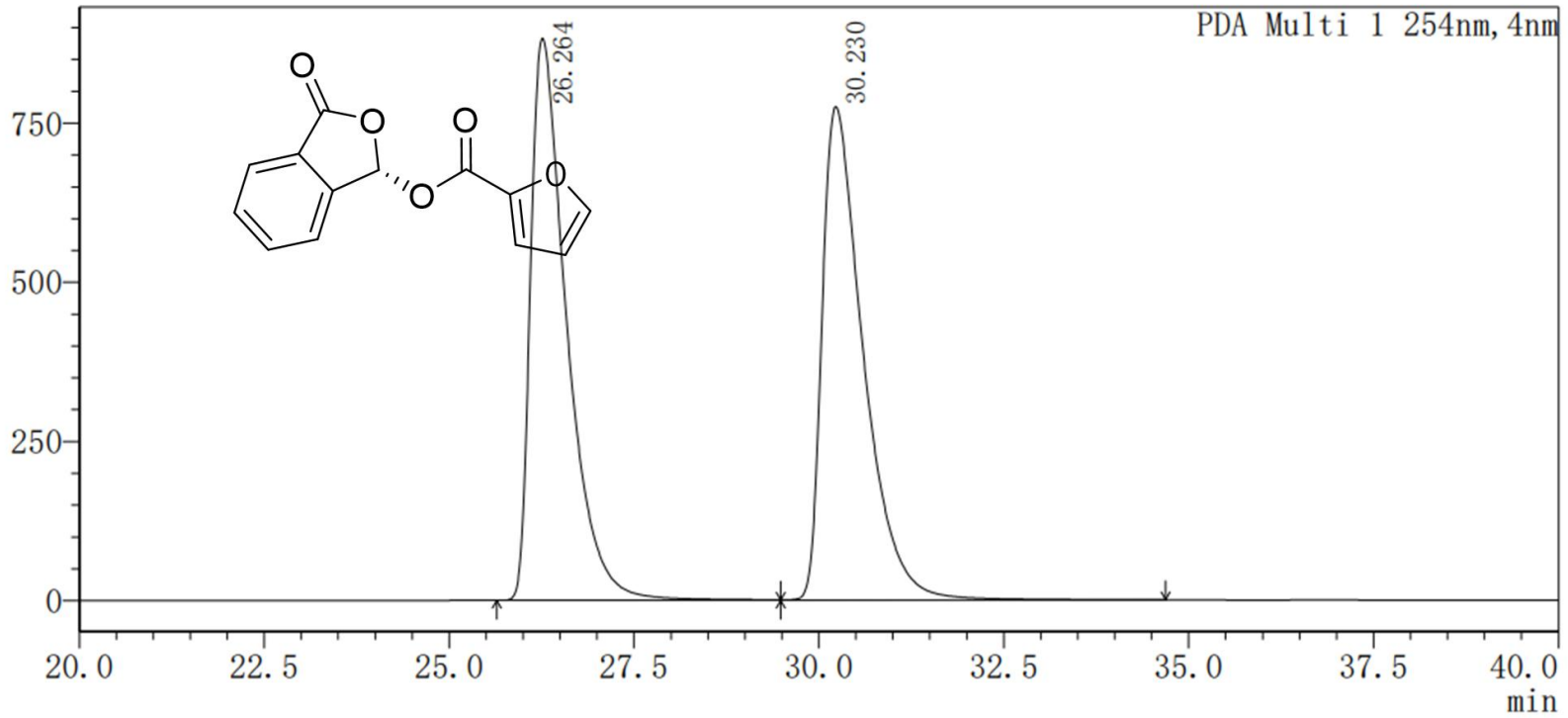
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	21.626	138455	3493377	93.315
2	25.650	8630	250276	6.685
Total		147084	3743654	100.000


7.98 7.96 7.78 7.77 7.76 7.76 7.68 7.68 7.66 7.66 7.65 7.65 7.65 7.64 7.29 7.28 7.28 7.28 6.56 6.55 6.55 6.55
7.29 7.28 7.28 7.28
O O O O O
1.00
7.32 7.31 7.30 7.29 7.28 7.27 7.26 7.25 7.24
f1 (ppm)
7.98 7.98 7.98 7.96 7.96 7.96
7.80 7.79 7.78 7.77 7.76 7.76
6.56 6.55 6.55 6.55
1.00
1.04
8.00 7.95 7.90 7.85 7.80 7.75
f1 (ppm)
1.00
6.60 6.58 6.56 6.54 6.52 6.50 6.48
f1 (ppm)
1.00 1.04 4.00 1.00 1.00
12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

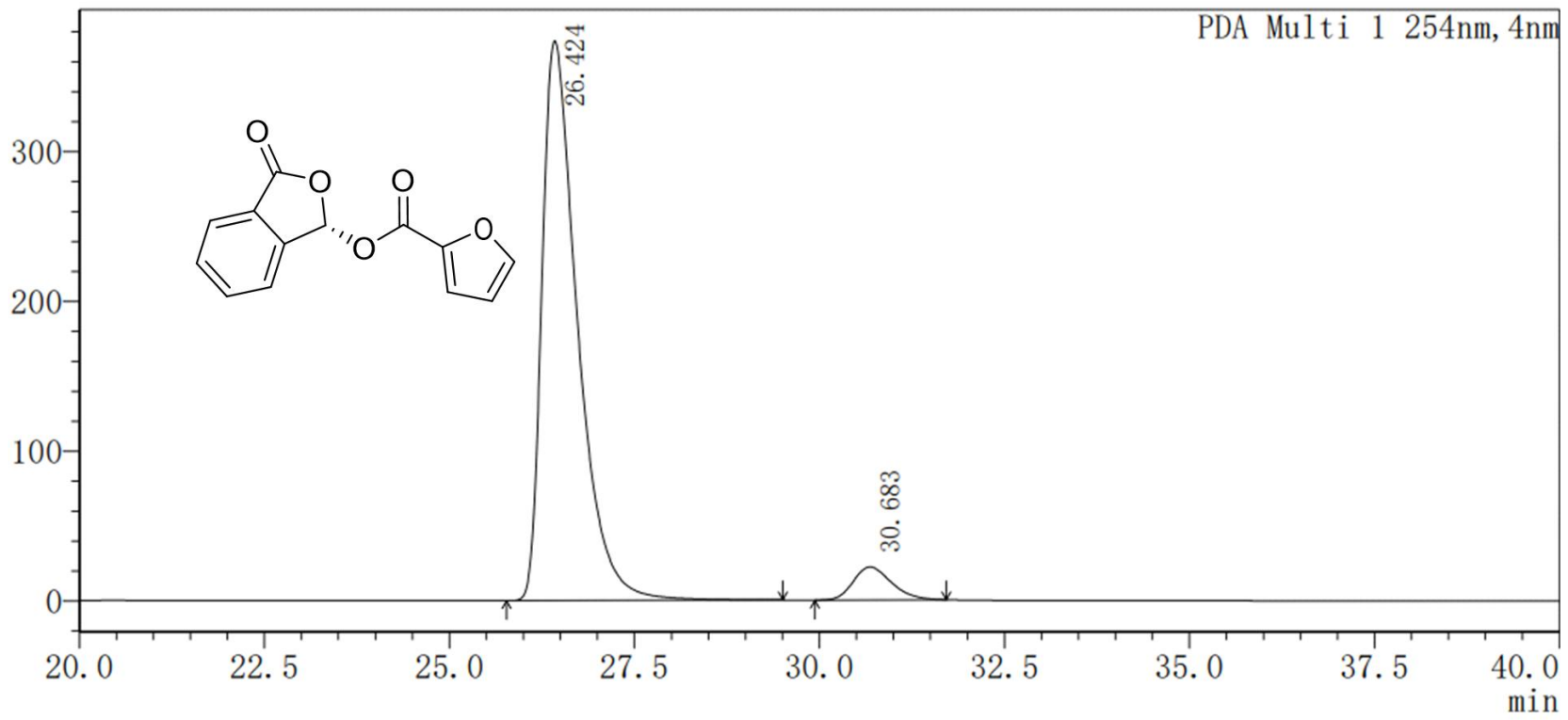

167.76
156.82
147.75
144.13
142.98
134.96
131.45
126.60
125.92
123.81
120.41
112.34
92.94
O
O
O
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

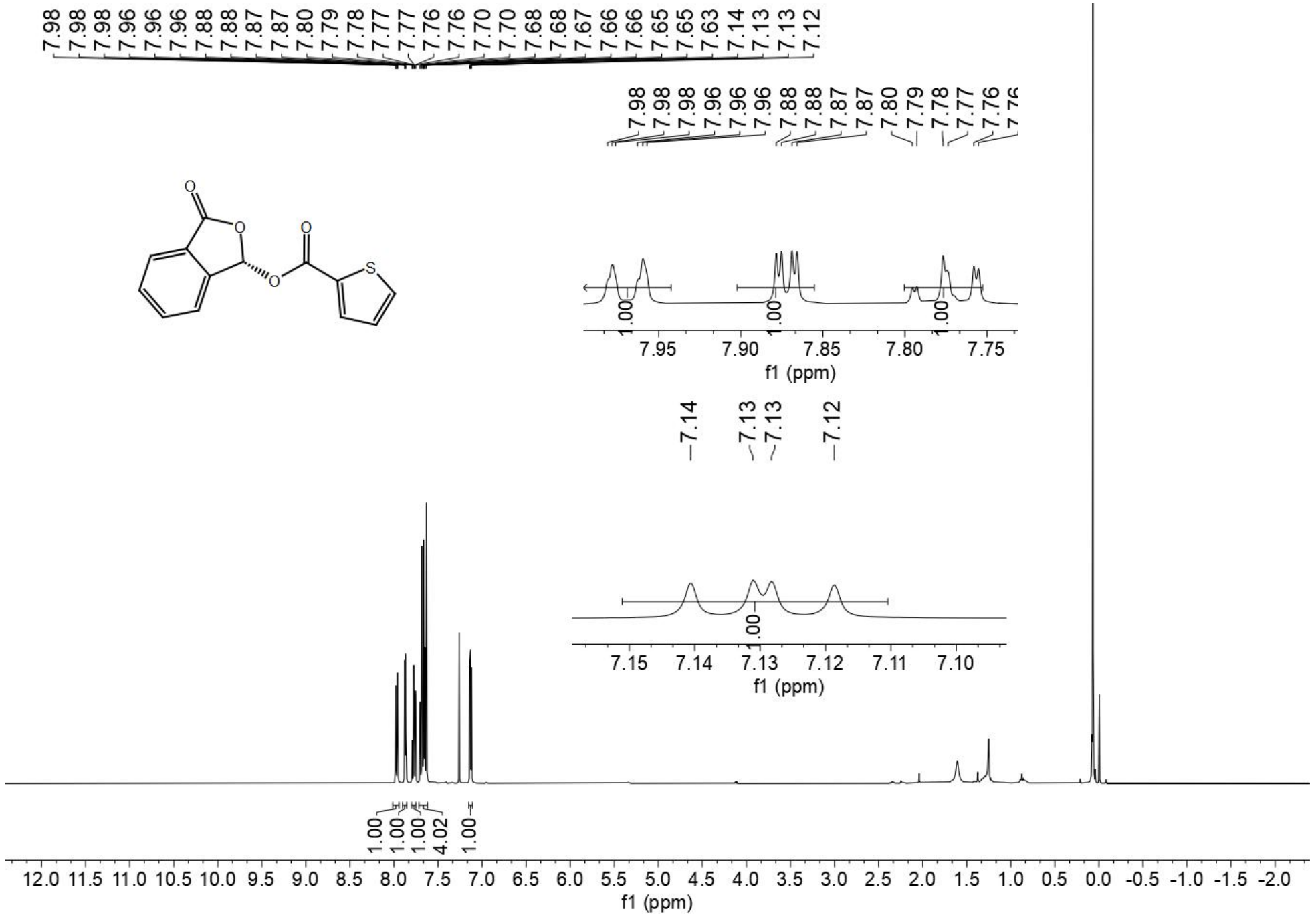
Peak#	Ret. Time	Height	Area	Height%
1	26.264	882689	30010166	49.957
2	30.230	775440	30062310	50.043
总计		1658128	60072476	100.000

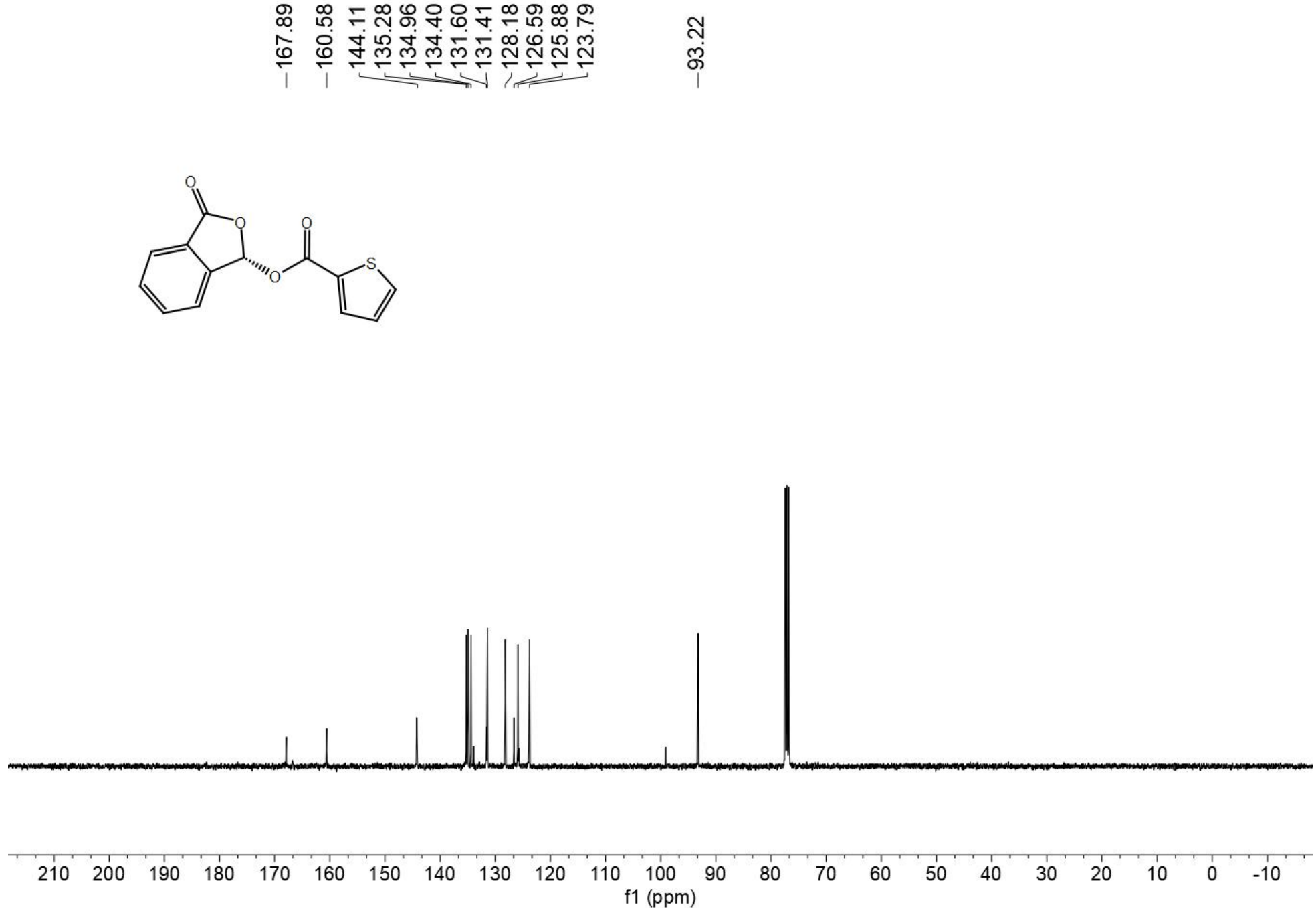


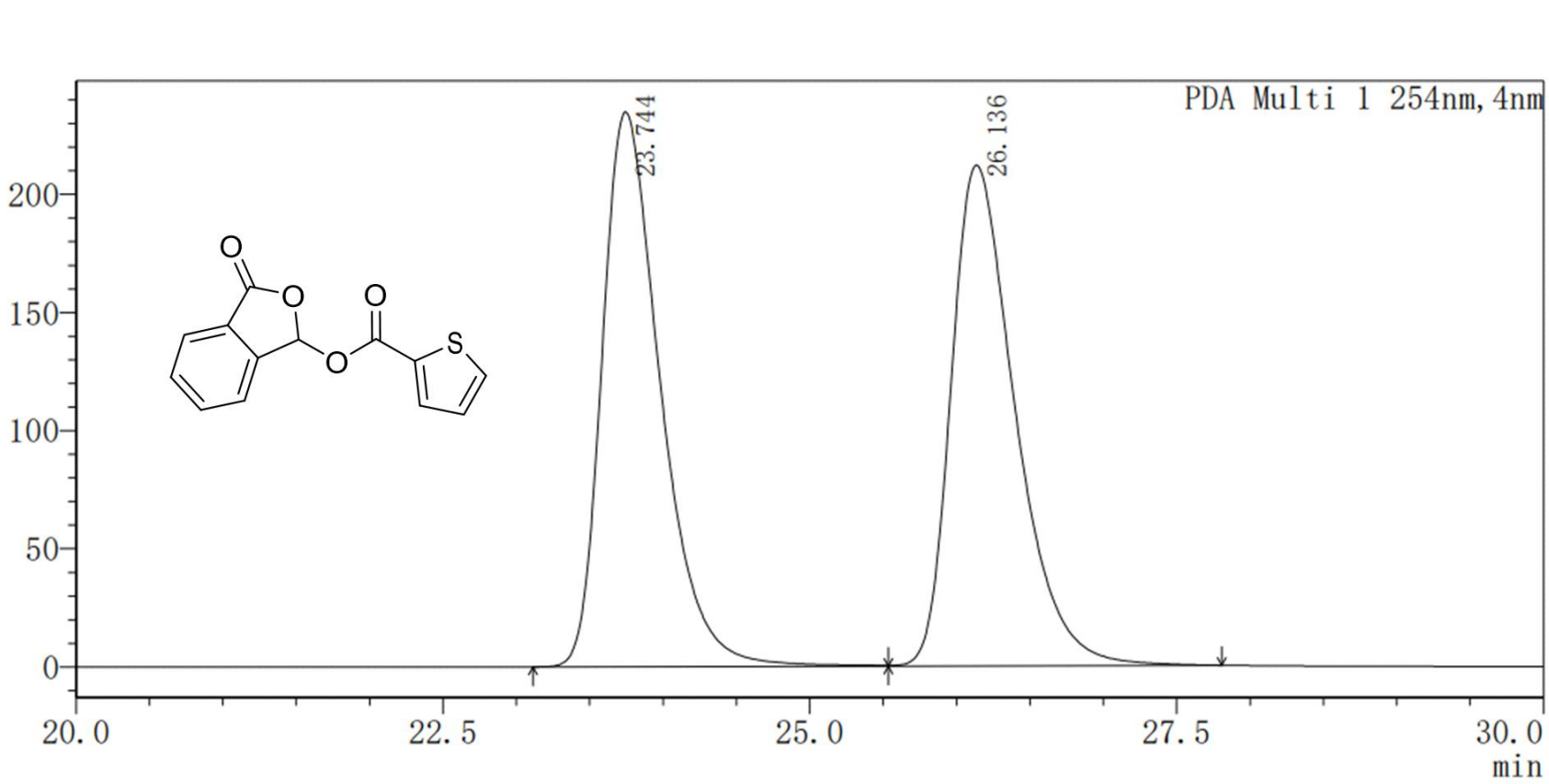
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	26.424	373684	12469916	94.042
2	30.683	22021	790090	5.958
Total		395705	13260006	100.000


7.98 7.98 7.98 7.96 7.96 7.96 7.88 7.88 7.87 7.87 7.80 7.79 7.78 7.77 7.77 7.76 7.76 7.70 7.70 7.68 7.68 7.67 7.66 7.66 7.65 7.65 7.63 7.14 7.13 7.13 7.12
O
O
O
O
S
1.00
1.00
1.00
7.95 7.90 7.85 7.80 7.75
f1 (ppm)
7.14
7.13
7.13
7.12
1.00
7.15 7.14 7.13 7.12 7.11 7.10
f1 (ppm)
1.00 1.00 1.00 4.02 1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

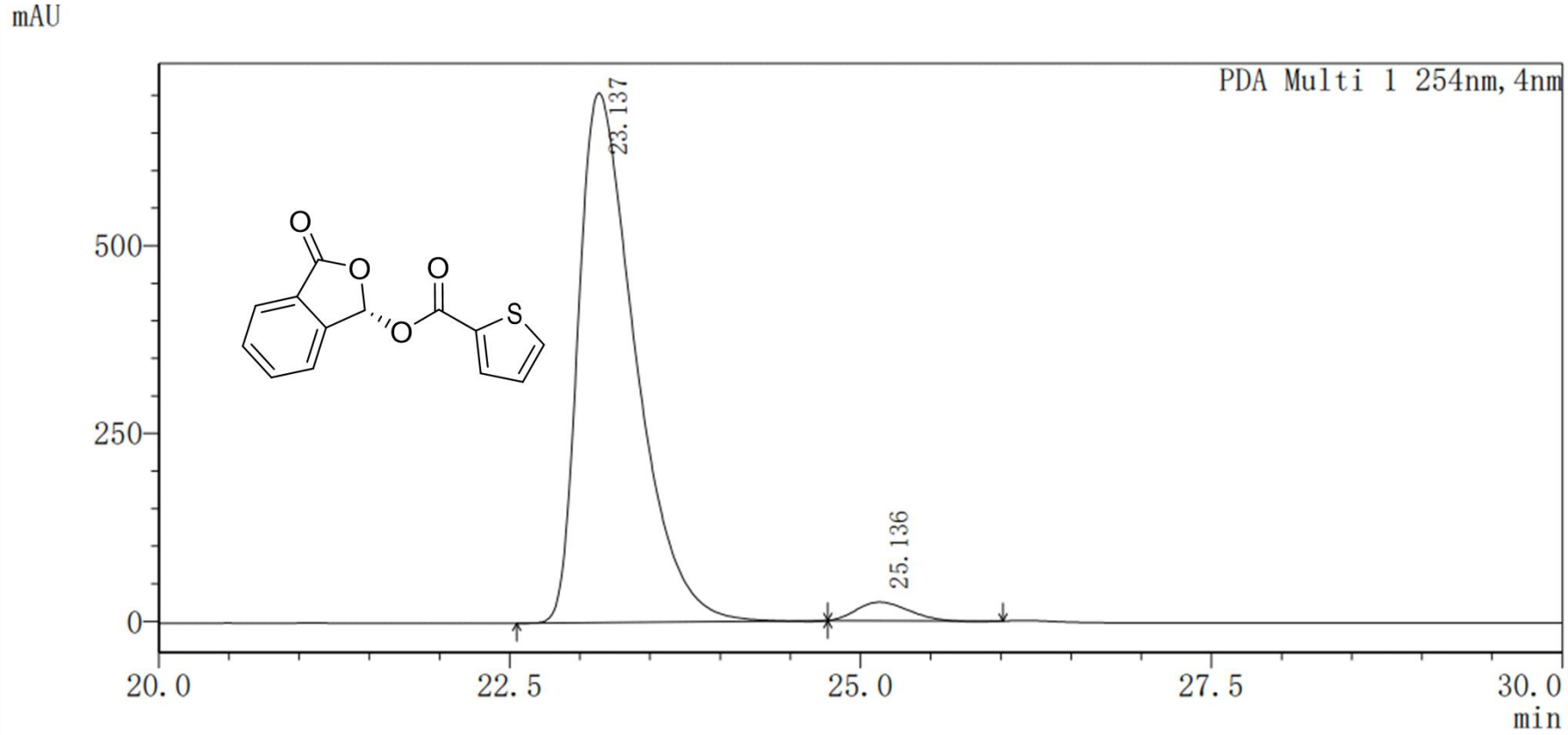

167.89
160.58
144.11
135.28
134.96
134.40
131.60
131.41
128.18
126.59
125.88
123.79
93.22
O
O
O
O
S
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	23.744	234813	6481365	50.228
2	26.136	211994	6422640	49.772
Total		446806	12904005	100.000



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	23.137	704767	19784892	96.957
2	25.136	24850	620915	3.043
Total		729617	20405807	100.000


8.20
8.19
8.19
8.19
7.98
7.98
7.97
7.96
7.96
7.77
7.77
7.76
7.75
7.70
7.70
7.69
7.68
7.68
7.68
7.67
7.67
7.66
7.66
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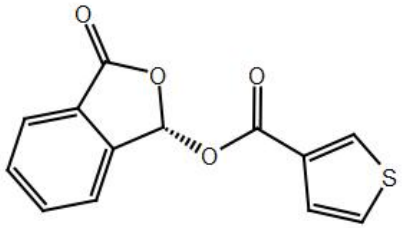
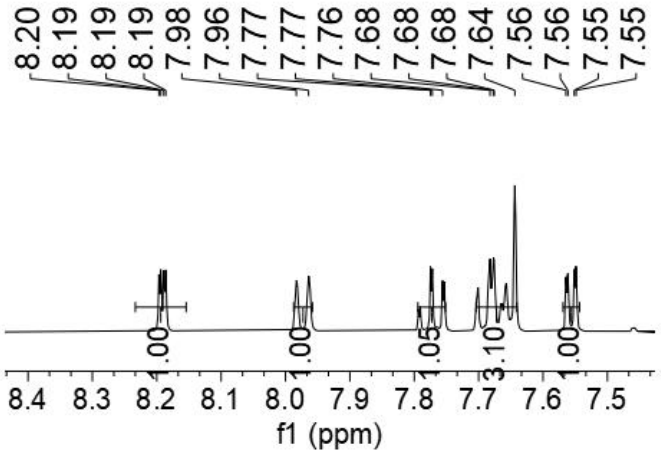
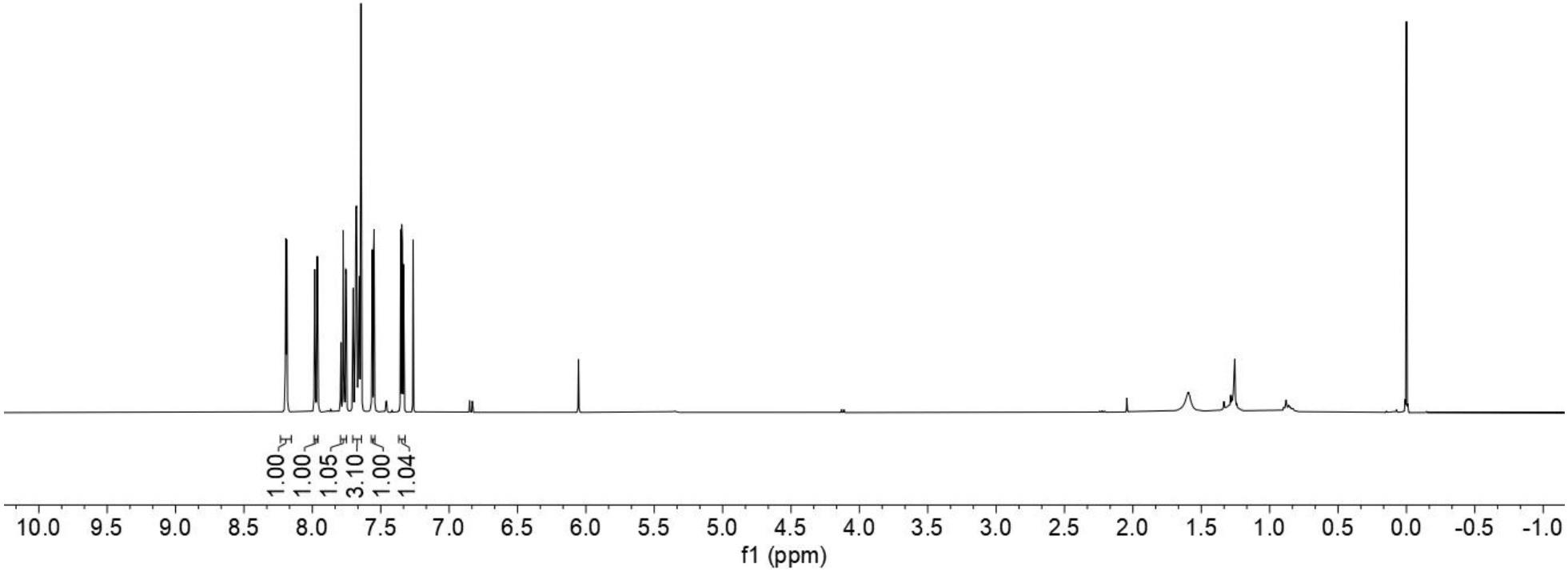
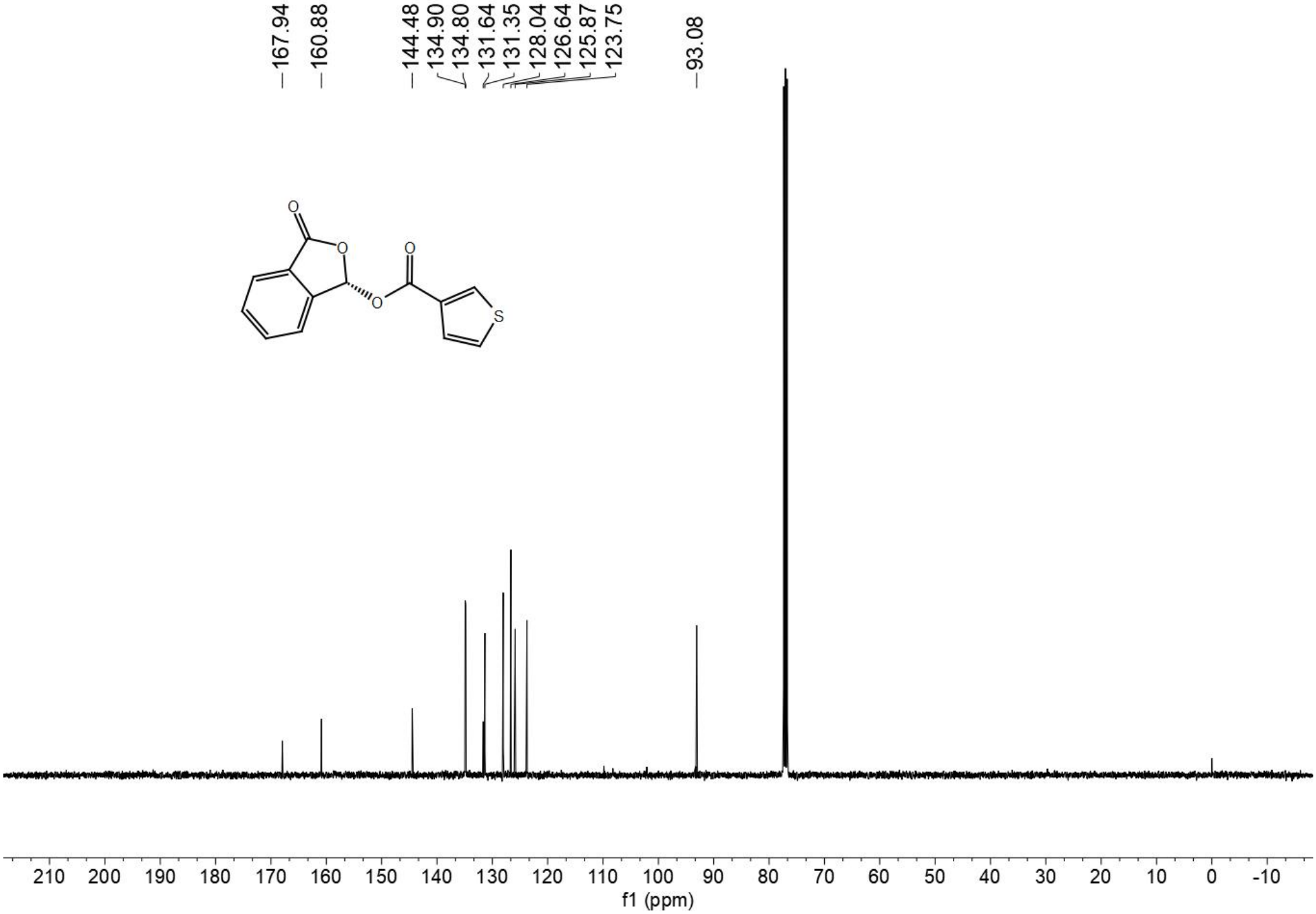
7.55
7.55
7.35
7.35
7.34
7.33


O
O
O
O
S


8.20
8.19
8.19
8.19
7.98
7.96
7.77
7.77
7.76
7.68
7.68
7.68
7.64
7.56
7.56
7.55
7.55
1.00
1.00
1.05
3.10
1.00
8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5
f1 (ppm)


1.00
1.00
1.05
3.10
1.00
1.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


167.94
160.88
144.48
134.90
134.80
131.64
131.35
128.04
126.64
125.87
123.75
93.08
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O
O
O
O
S
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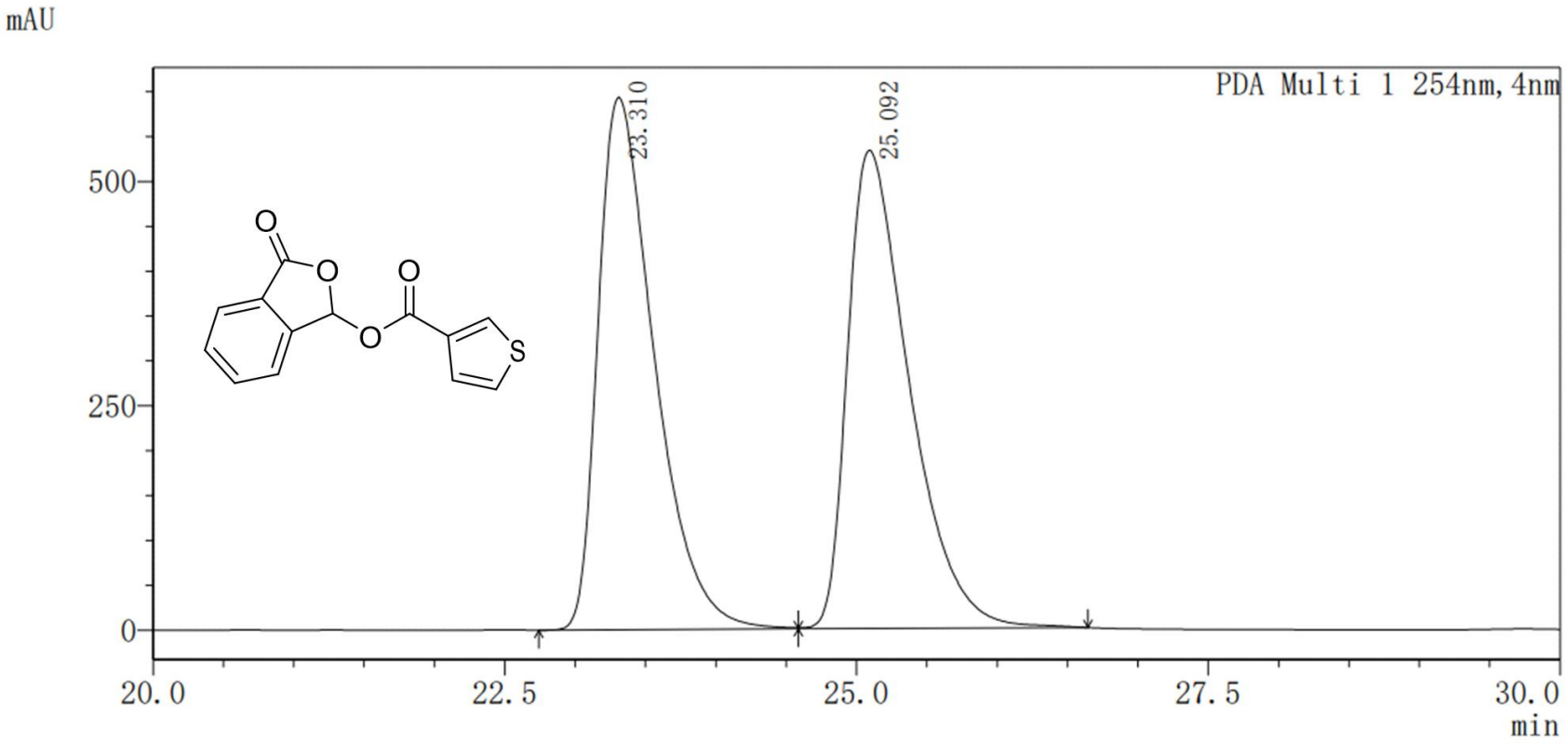
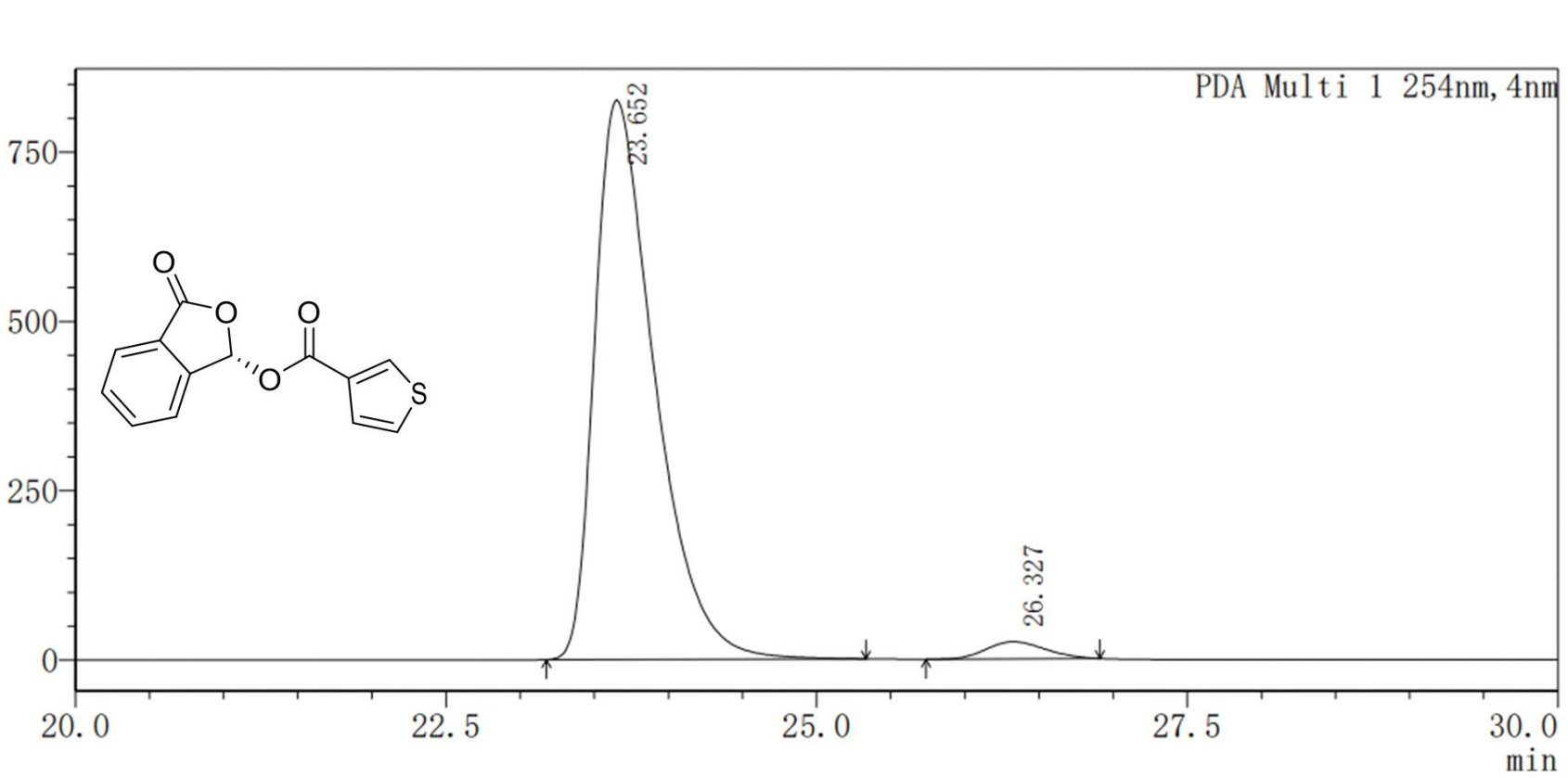
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	23.310	593305	16495366	50.368
2	25.092	533028	16254187	49.632
Total		1126333	32749553	100.000



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	23.652	826104	23245378	97.055
2	26.327	25366	705363	2.945
Total		851469	23950741	100.000


8.14
8.13
8.00
8.00
7.99
7.98
7.98
7.89
7.88
7.88
7.88
7.88
7.87
7.87
7.86
7.86
7.86
7.85
7.82
7.81
7.80
7.80
7.79
7.78
7.78
7.72
7.72
7.70
7.70
7.68
7.68
7.67
7.51
7.51
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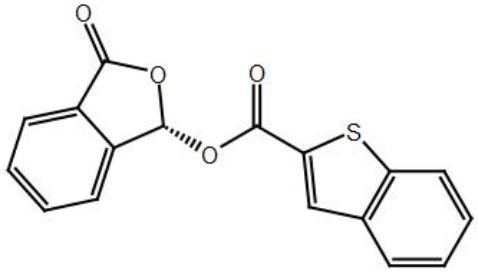
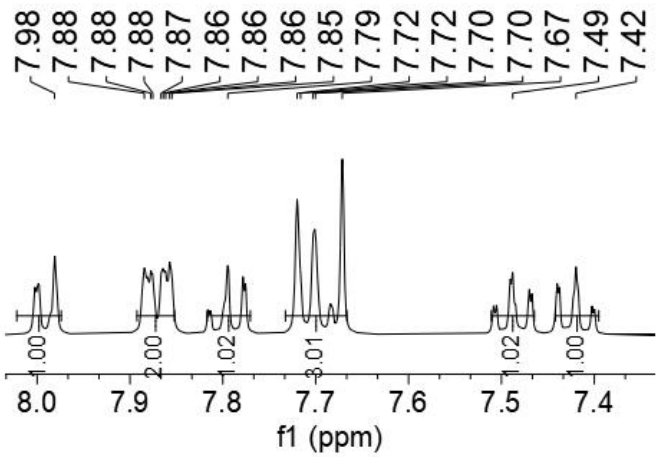
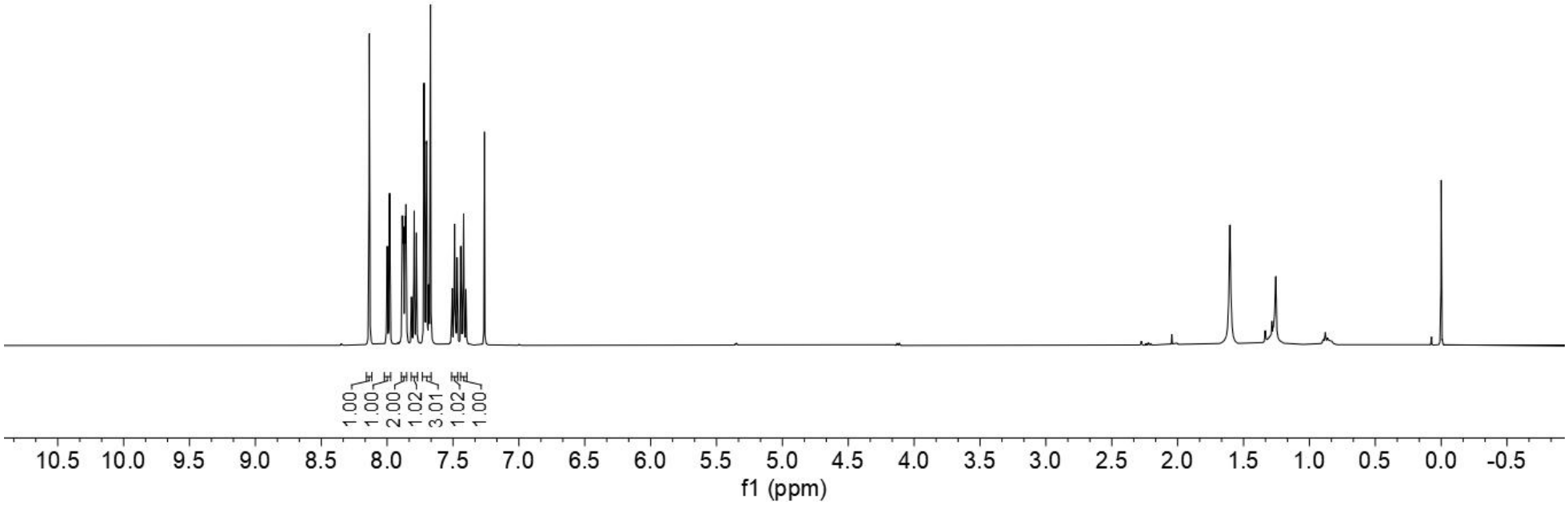
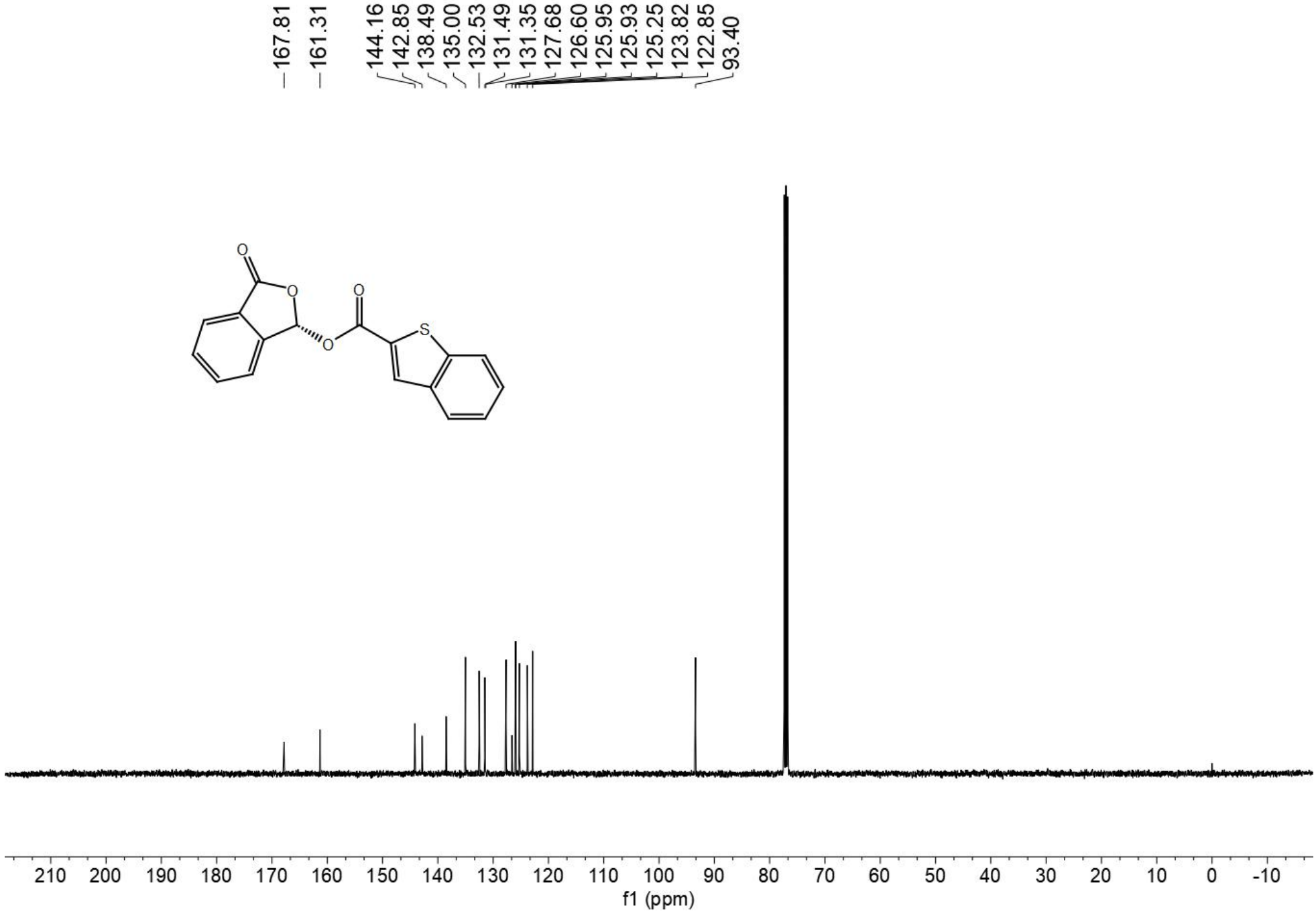
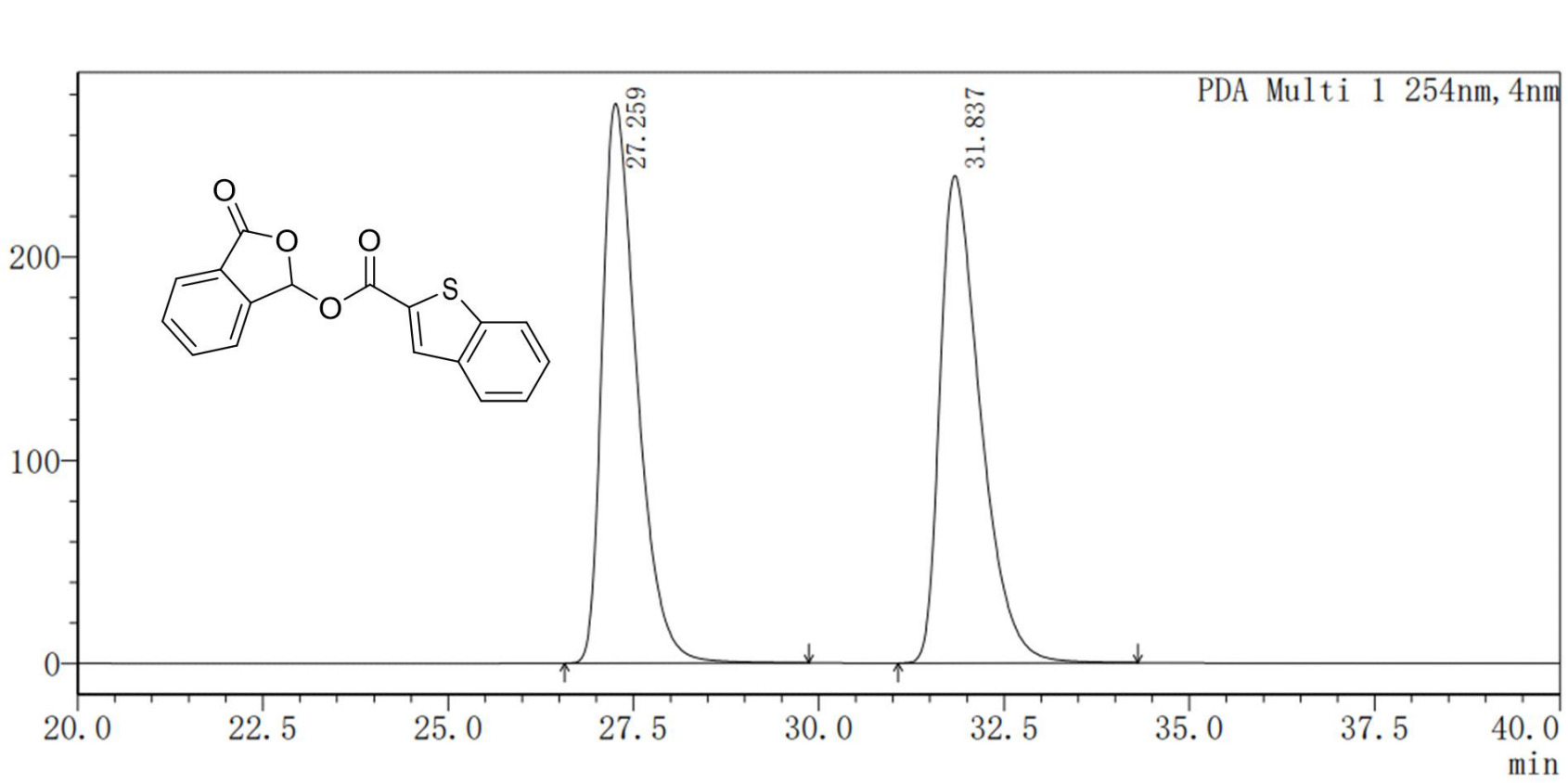
7.44
7.42
7.42
7.42
7.40
7.40


O
O
O
O
S


7.98
7.88
7.88
7.88
7.87
7.86
7.86
7.86
7.85
7.79
7.72
7.72
7.70
7.70
7.67
7.49
7.42
1.00
2.00
1.02
3.01
1.02
1.00
8.0
7.9
7.8
7.7
7.6
7.5
7.4
f1 (ppm)


1.00
1.00
2.00
1.02
3.01
1.02
1.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

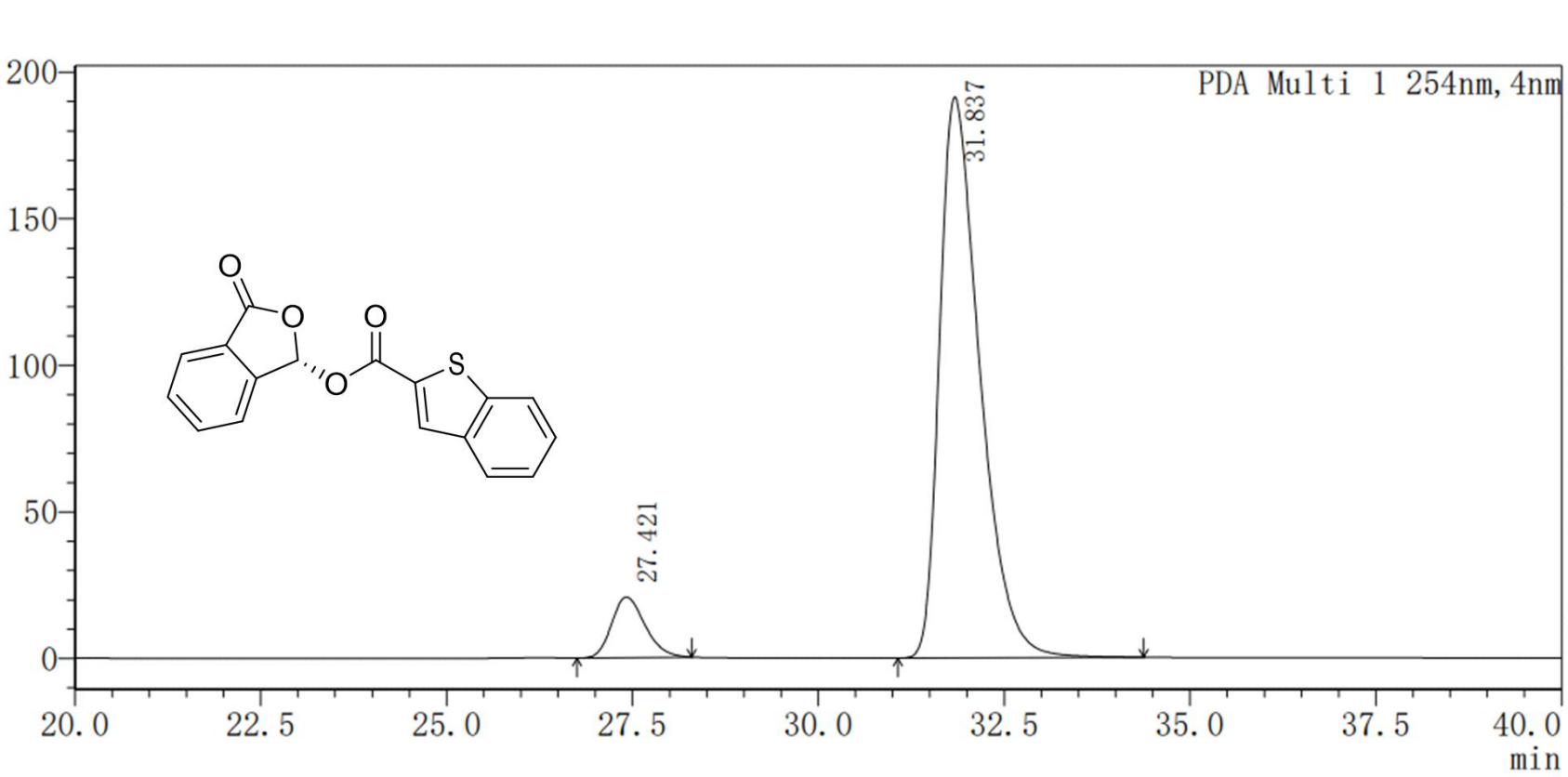

167.81
161.31
144.16
142.85
138.49
135.00
132.53
131.49
131.35
127.68
126.60
125.95
125.93
125.25
123.82
122.85
93.40
O
O
O
O
S
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

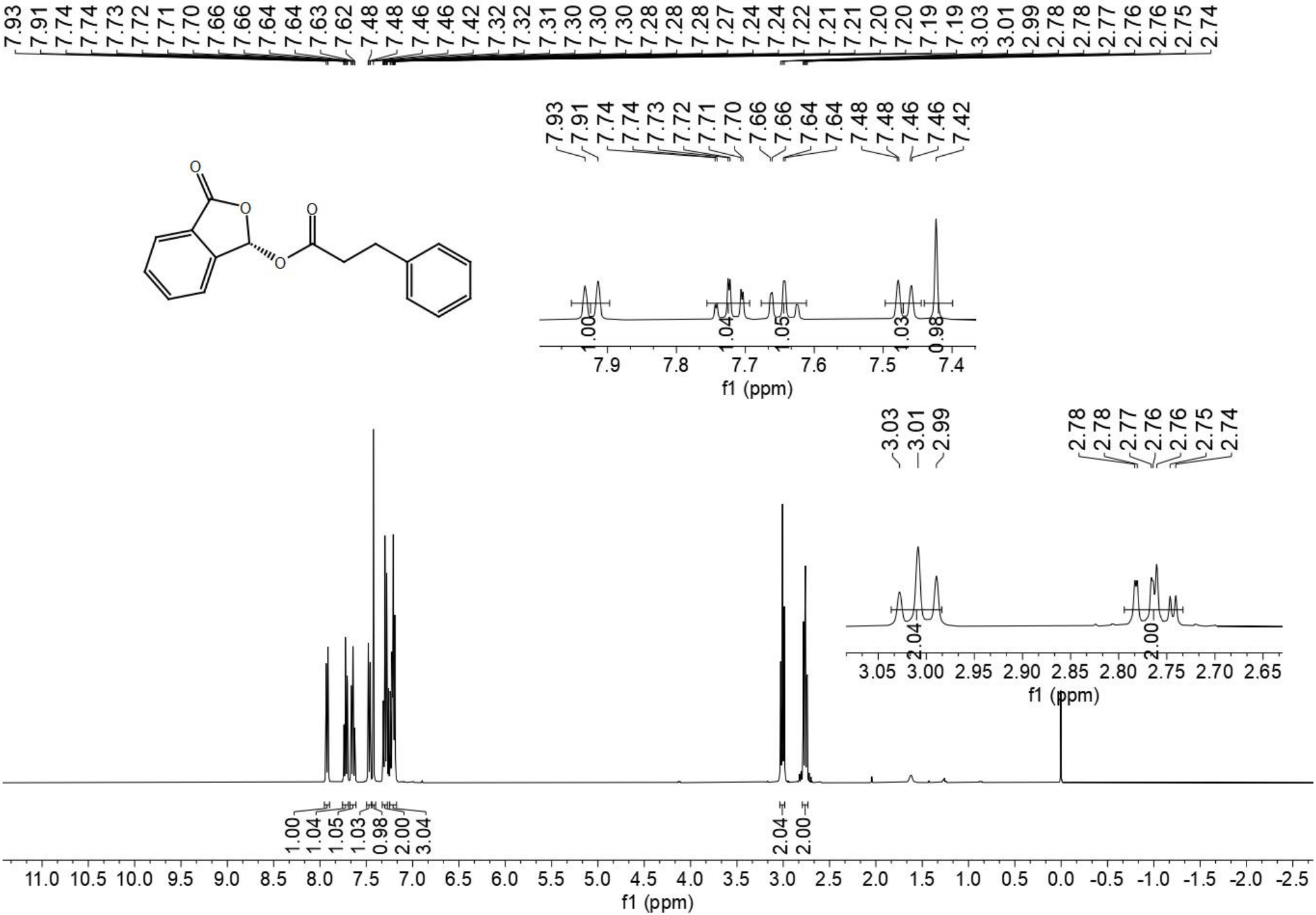
Peak#	Ret. Time	Height	Area	Area%
1	27.259	275261	8989153	49.668
2	31.837	239782	9109376	50.332
Total		515042	18098529	100.000

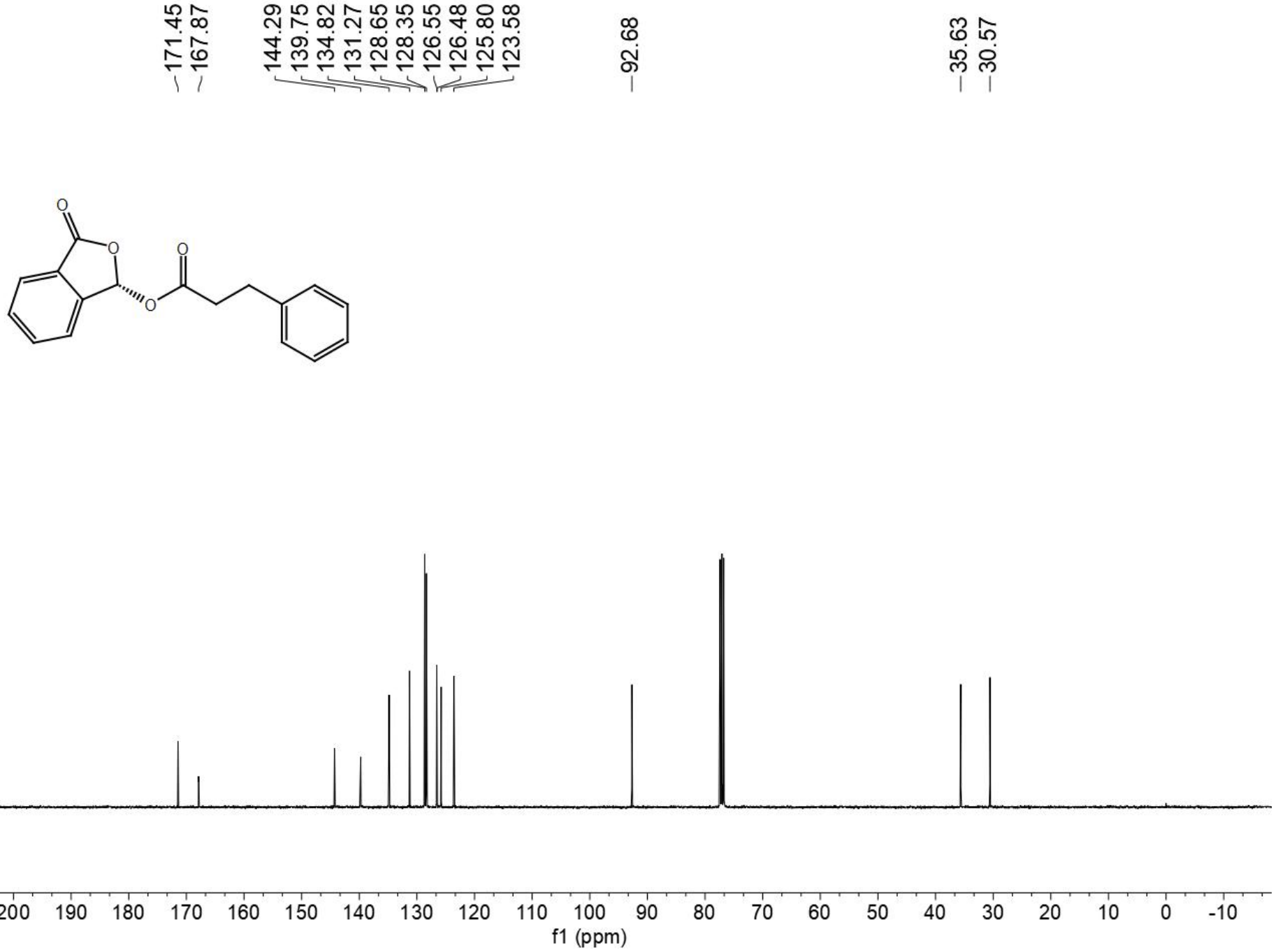


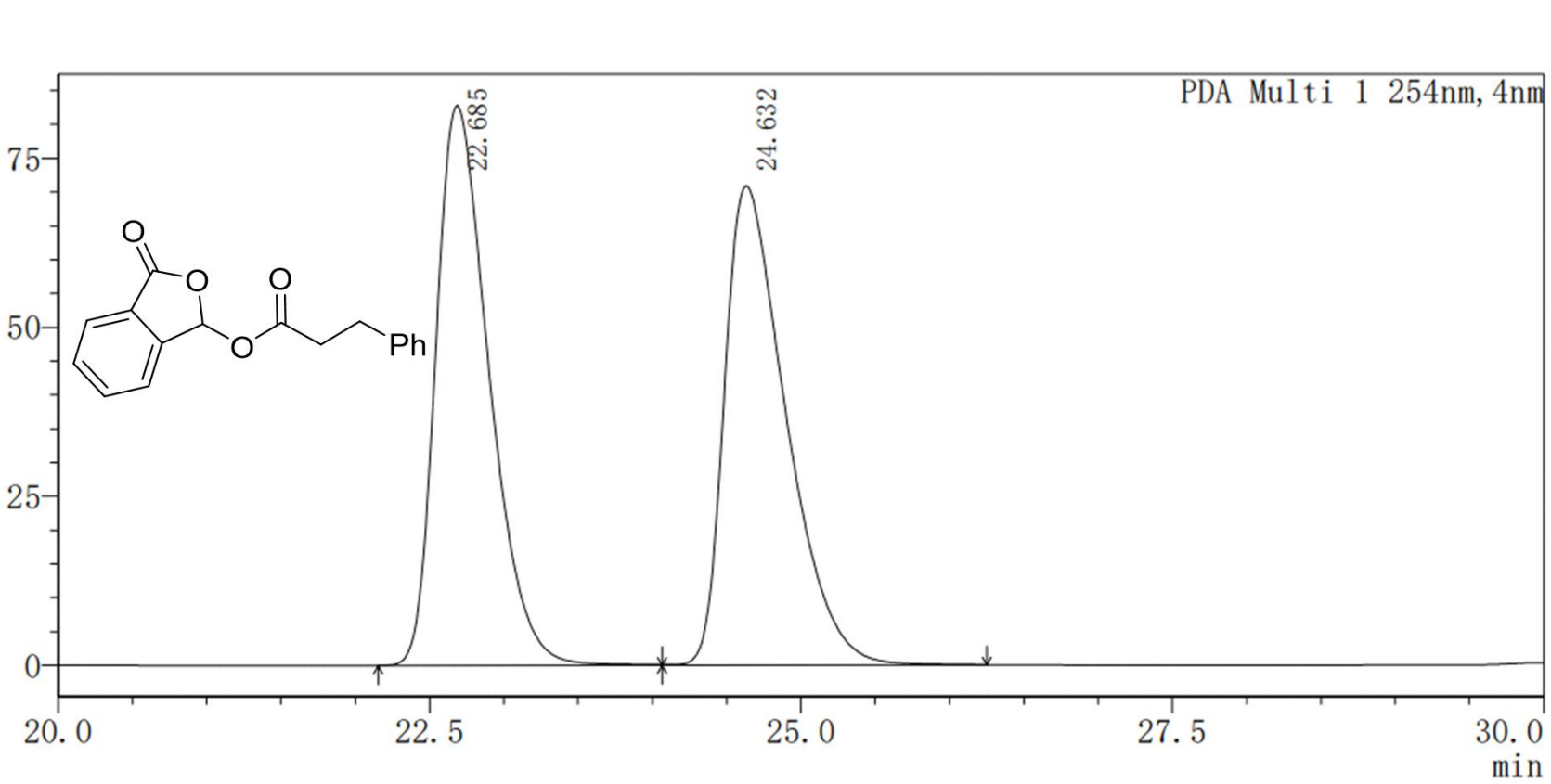
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	27.421	20706	647111	8.227
2	31.837	191381	7218493	91.773
Total		212087	7865604	100.000


7.93 7.91 7.74 7.74 7.73 7.72 7.71 7.70 7.66 7.66 7.64 7.64 7.63 7.62 7.48 7.48 7.46 7.46 7.42 7.32 7.32 7.31 7.30 7.30 7.30 7.28 7.28 7.28 7.27 7.24 7.24 7.22 7.21 7.21 7.20 7.20 7.19 7.19 3.03 3.01 2.99 2.78 2.78 2.77 2.76 2.76 2.75 2.74
O
O
O
O
1.00 1.04 1.05 1.03 0.98
7.9 7.8 7.7 7.6 7.5 7.4
f1 (ppm)
3.03 3.01 2.99 2.78 2.78 2.77 2.76 2.76 2.75 2.74
2.04 2.00
3.05 3.00 2.95 2.90 2.85 2.80 2.75 2.70 2.65
f1 (ppm)
1.00 1.04 1.05 1.03 0.98 2.00 3.04
2.04 2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5
f1 (ppm)

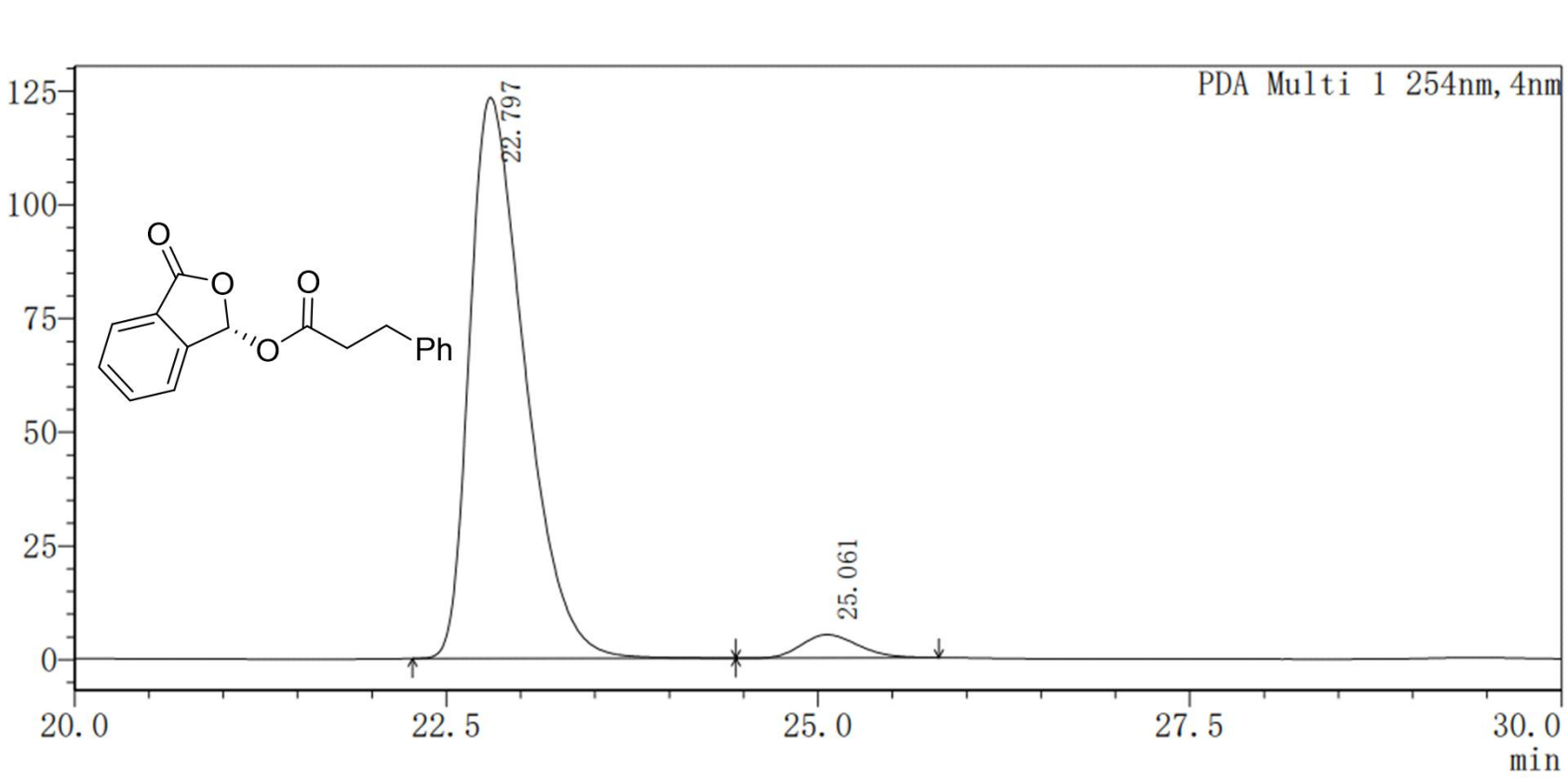

171.45
167.87
144.29
139.75
134.82
131.27
128.65
128.35
126.55
126.48
125.80
123.58
92.68
35.63
30.57
O
O
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

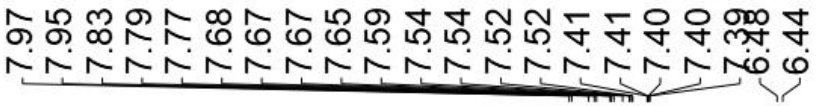
Peak#	Ret. Time	Height	Area	Area%
1	22.685	82814	2058856	50.260
2	24.632	70900	2037593	49.740
Total		153714	4096449	100.000



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	22.797	123321	3186756	95.907
2	25.061	5109	135984	4.093
Total		128430	3322739	100.000


7.97
7.95
7.83
7.79
7.77
7.68
7.67
7.67
7.65
7.59
7.54
7.54
7.52
7.52
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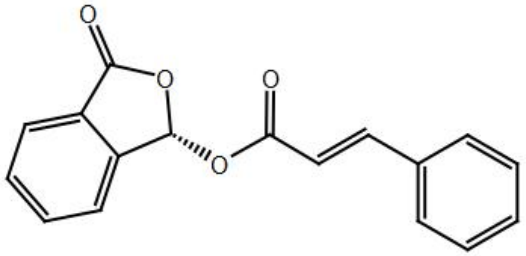
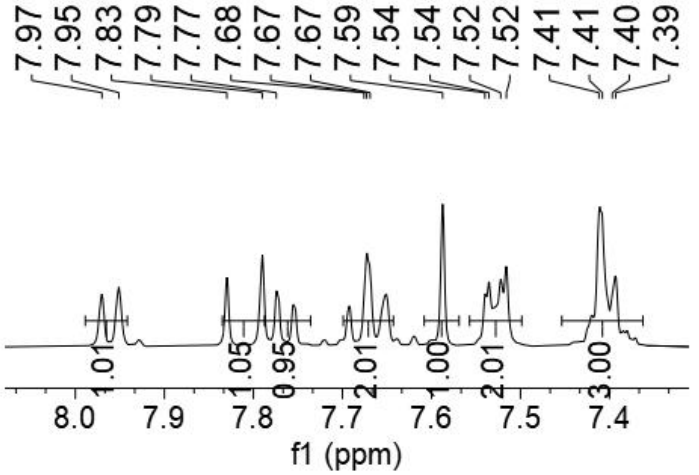
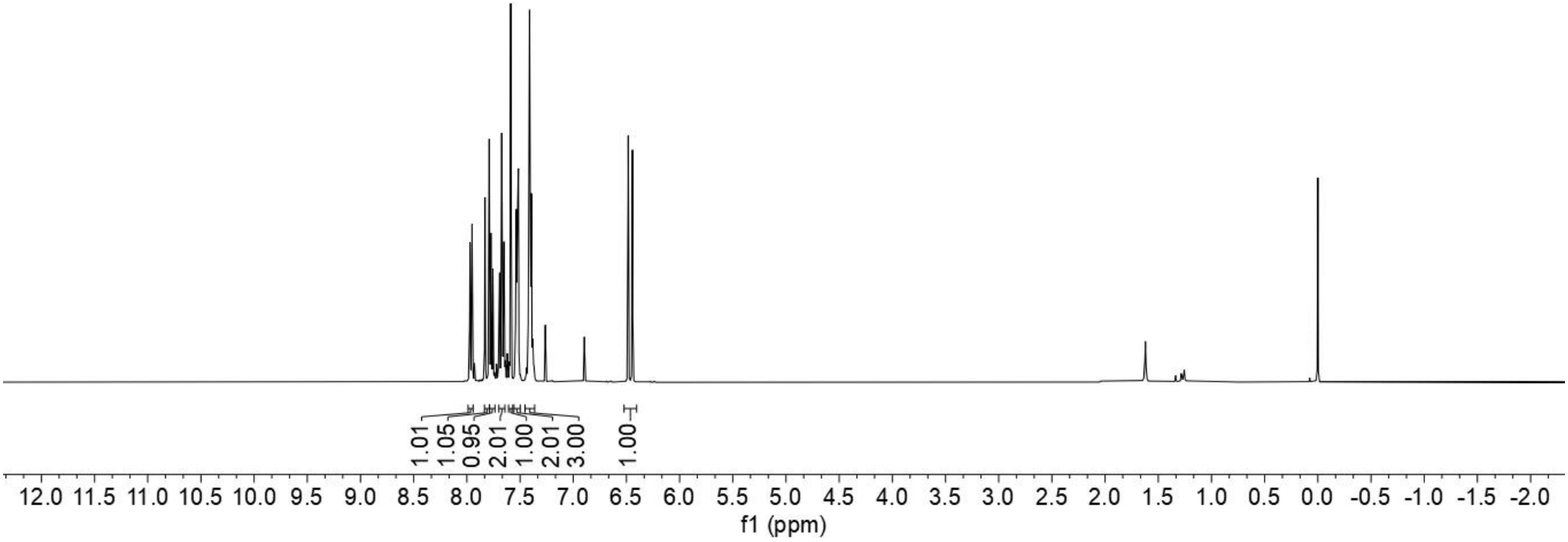
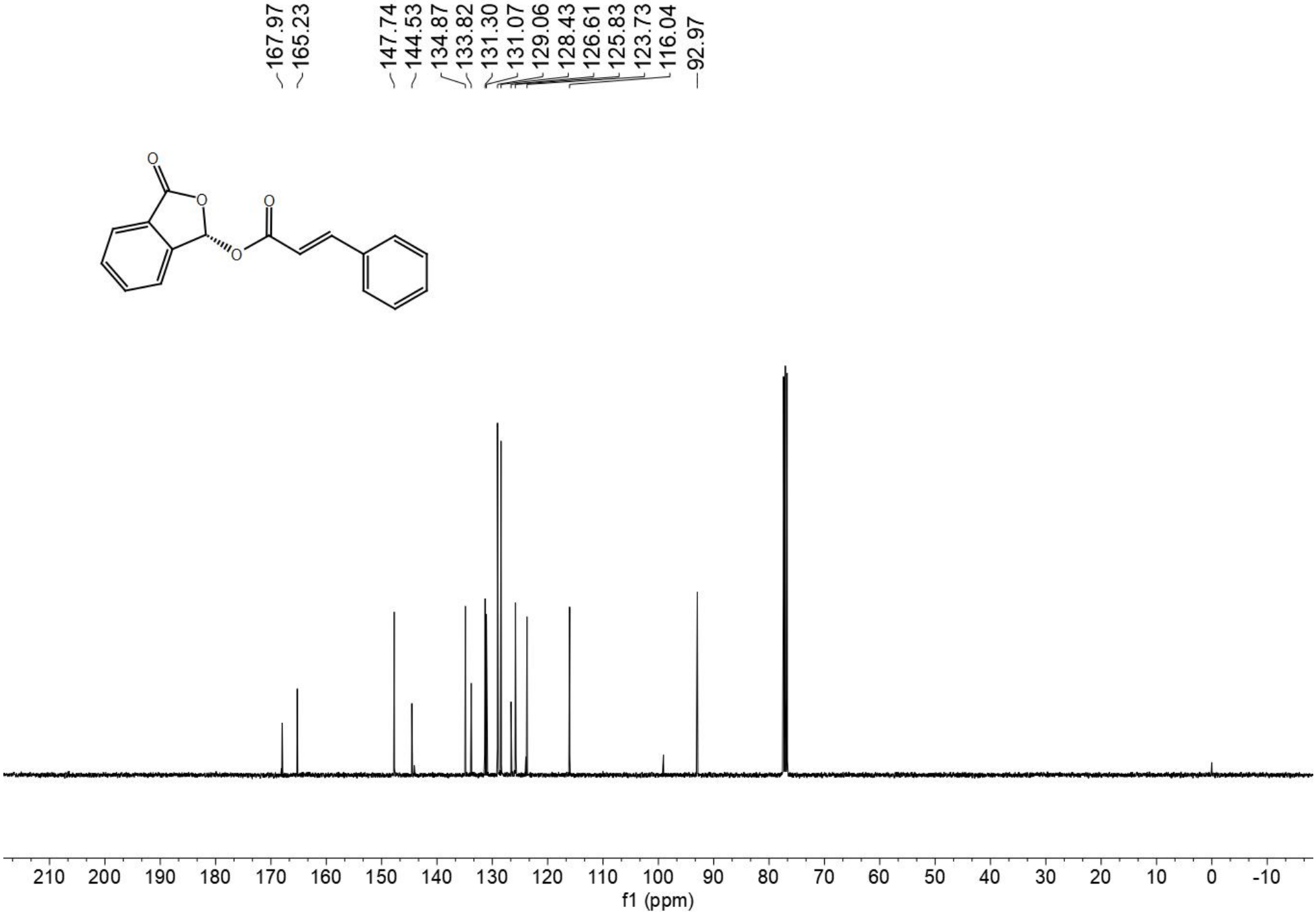
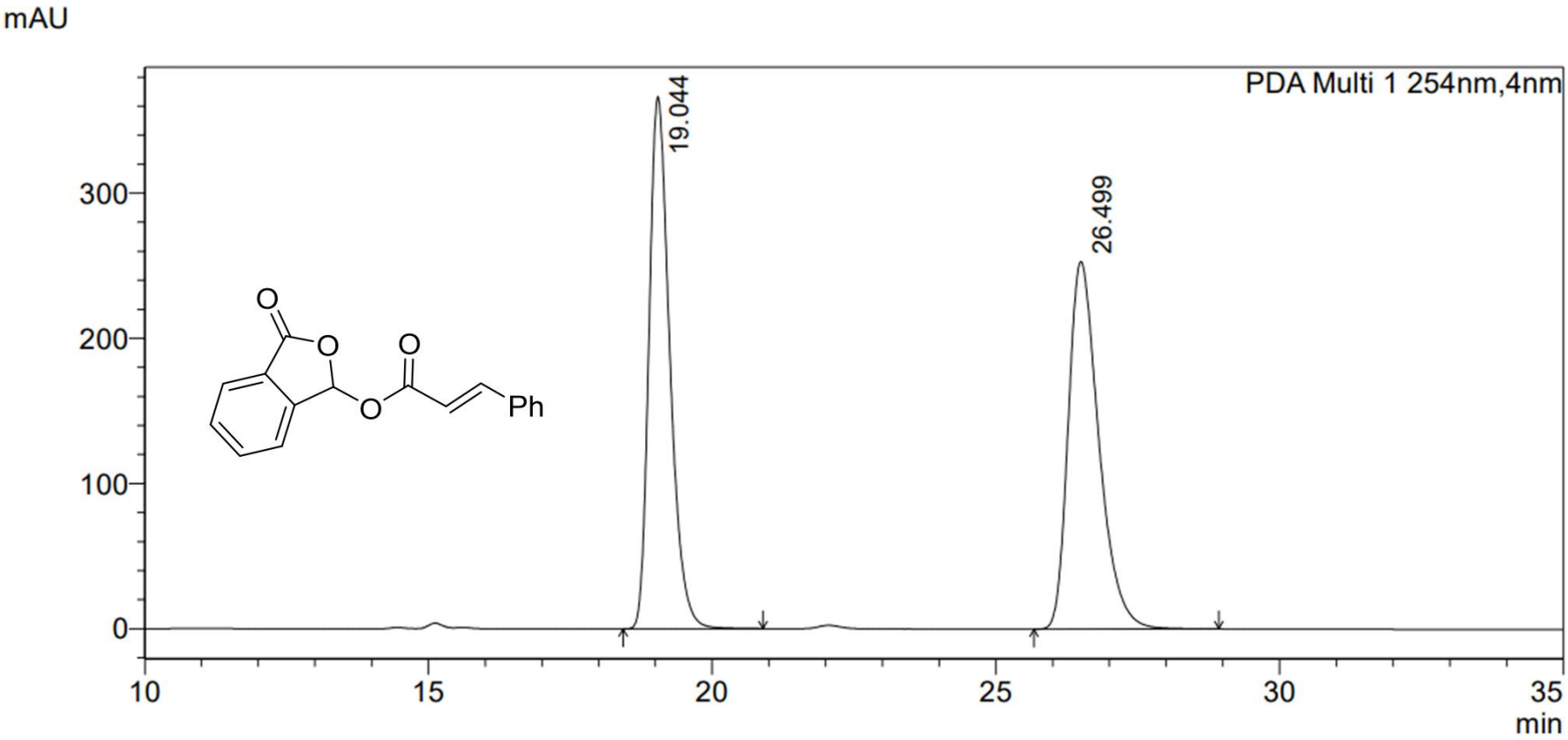
7.41
7.40
7.40
7.39
6.48
6.44




7.97
7.95
7.83
7.79
7.77
7.68
7.67
7.67
7.59
7.54
7.54
7.52
7.52
7.41
7.41
7.40
7.39
1.01
1.05
0.95
2.01
1.00
2.01
3.00
8.0
7.9
7.8
7.7
7.6
7.5
7.4
f1 (ppm)


1.01
1.05
0.95
2.01
1.00
2.01
3.00
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

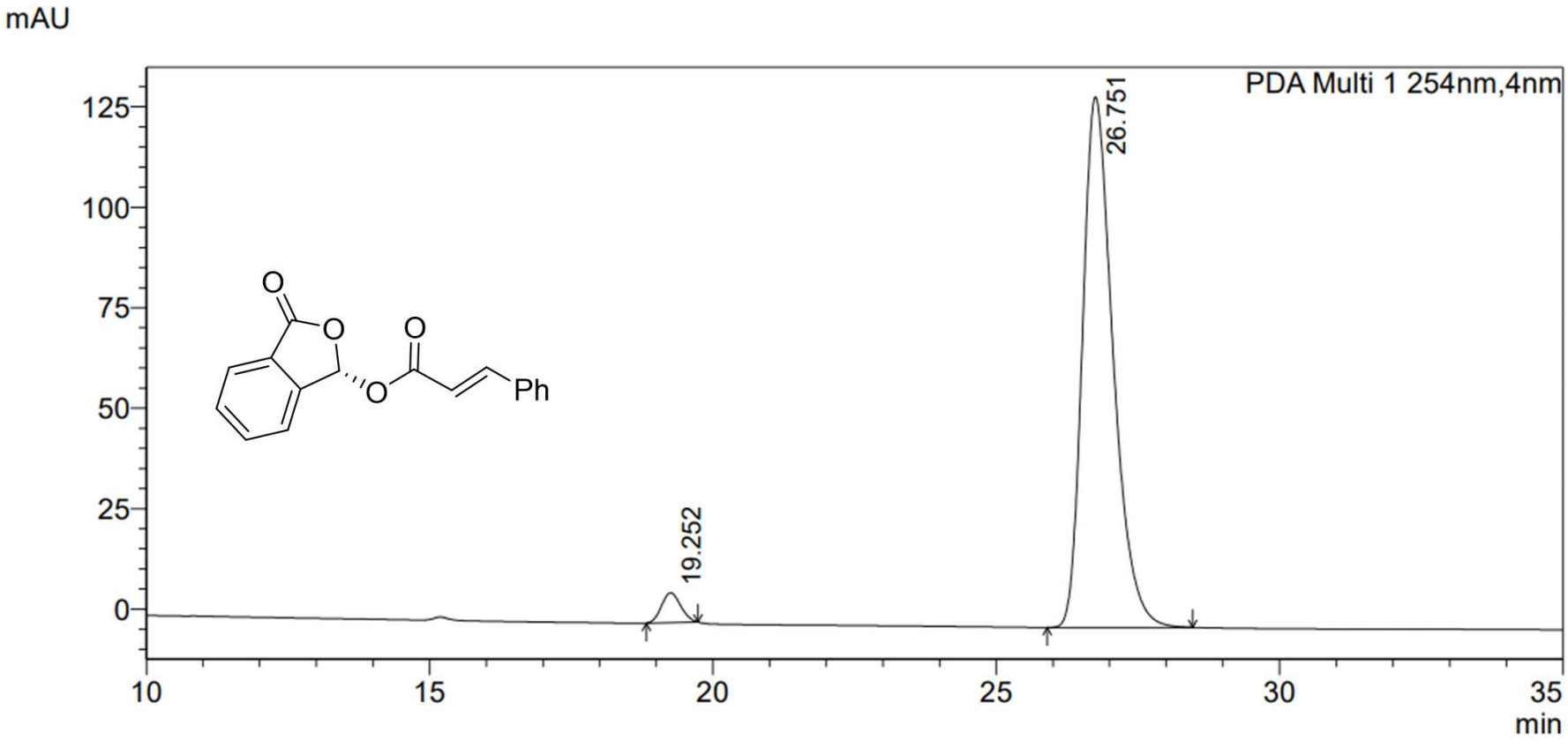

167.97
165.23
147.74
144.53
134.87
133.82
131.30
131.07
129.06
128.43
126.61
125.83
123.73
116.04
92.97
O
O
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

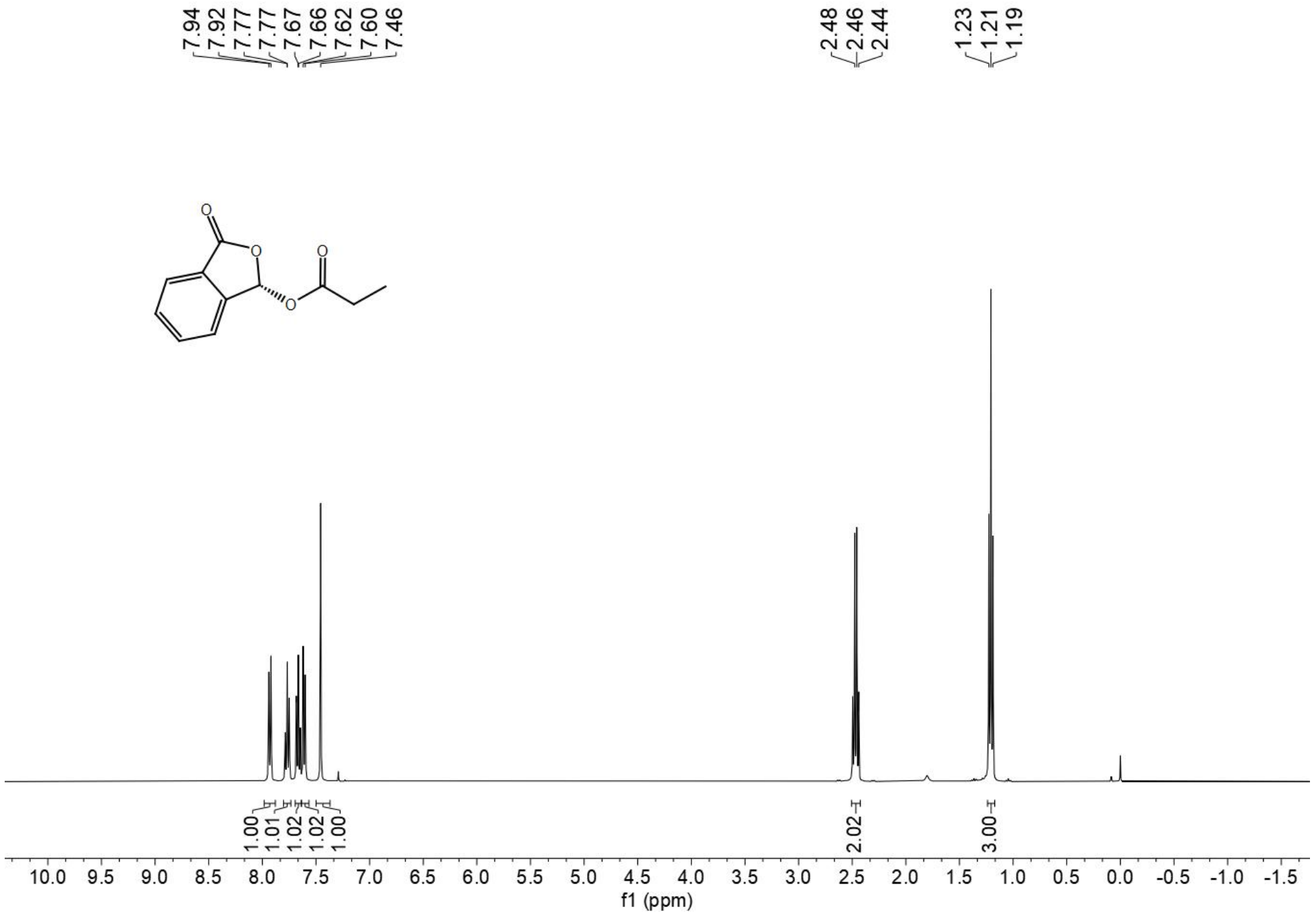
Peak#	Ret. Time	Height	Area	Area%
1	19.044	366453	9327215	49.566
2	26.499	253140	9490694	50.434
Total		619592	18817909	100.000

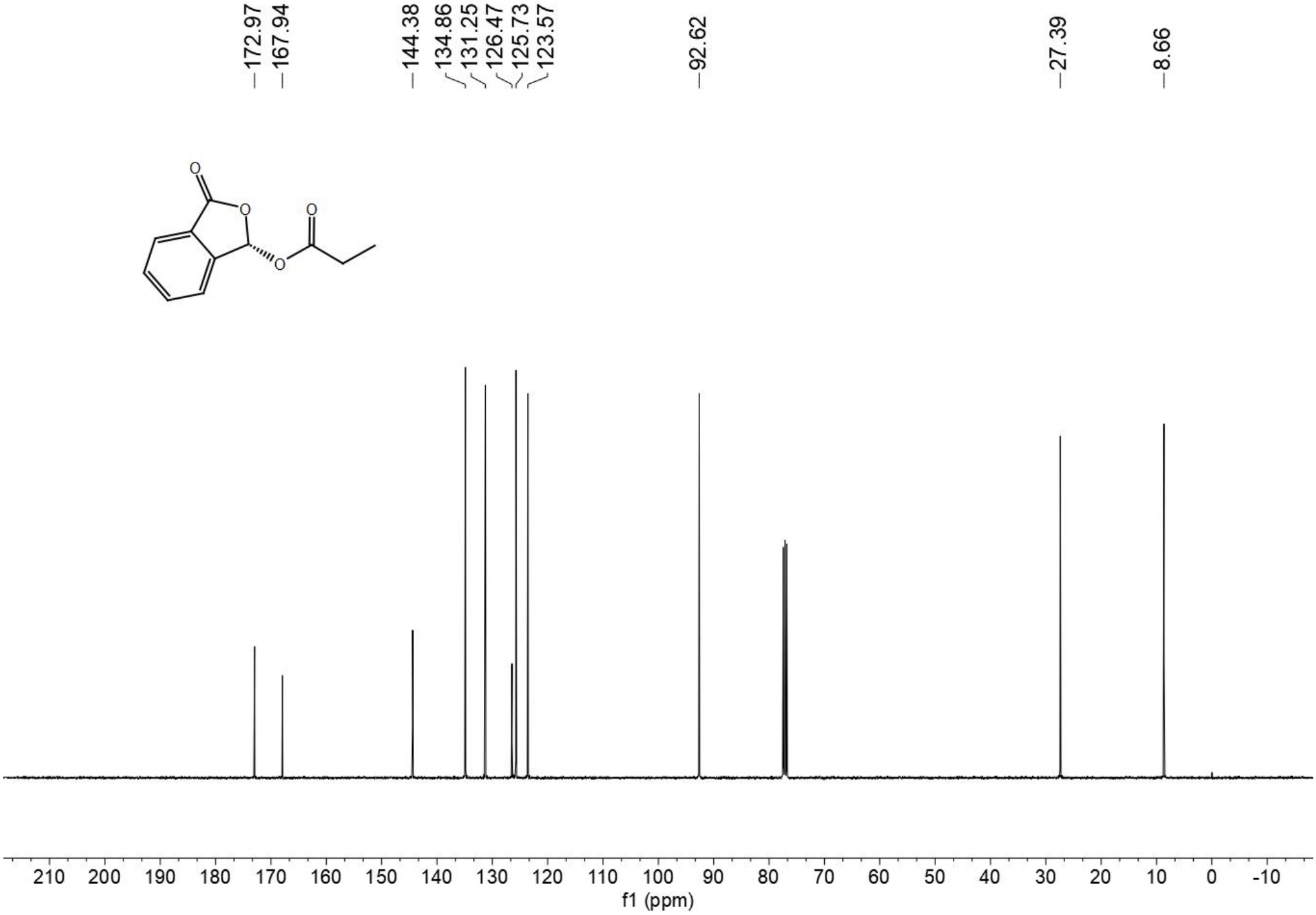


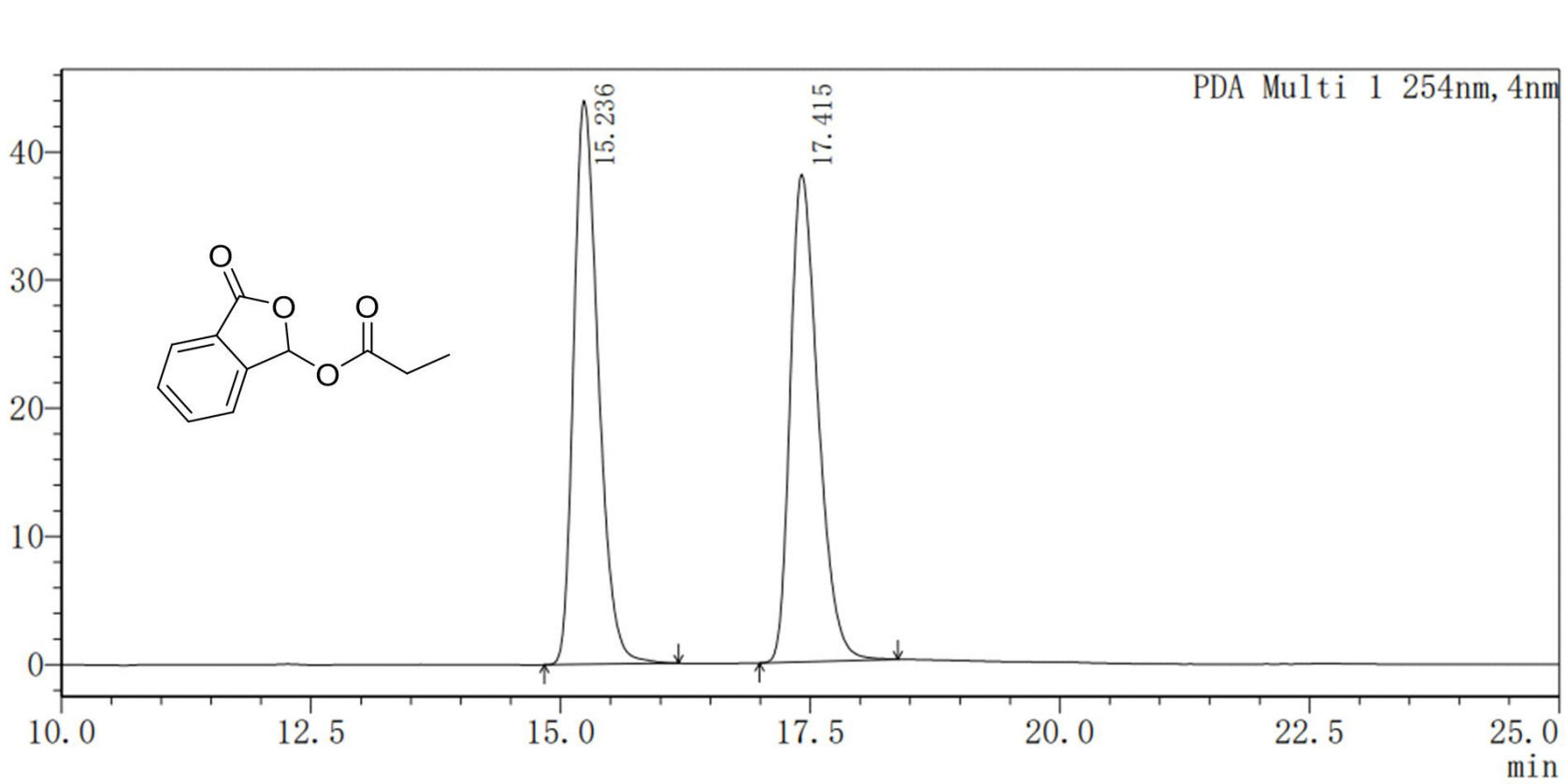
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	19.252	7406	174389	3.410
2	26.751	132000	4939600	96.590
Total		139406	5113989	100.000


7.94
7.92
7.77
7.77
7.67
7.66
7.62
7.60
7.46
2.48
2.46
2.44
1.23
1.21
1.19
O
O
O
O
1.00
1.01
1.02
1.02
1.00
2.02
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

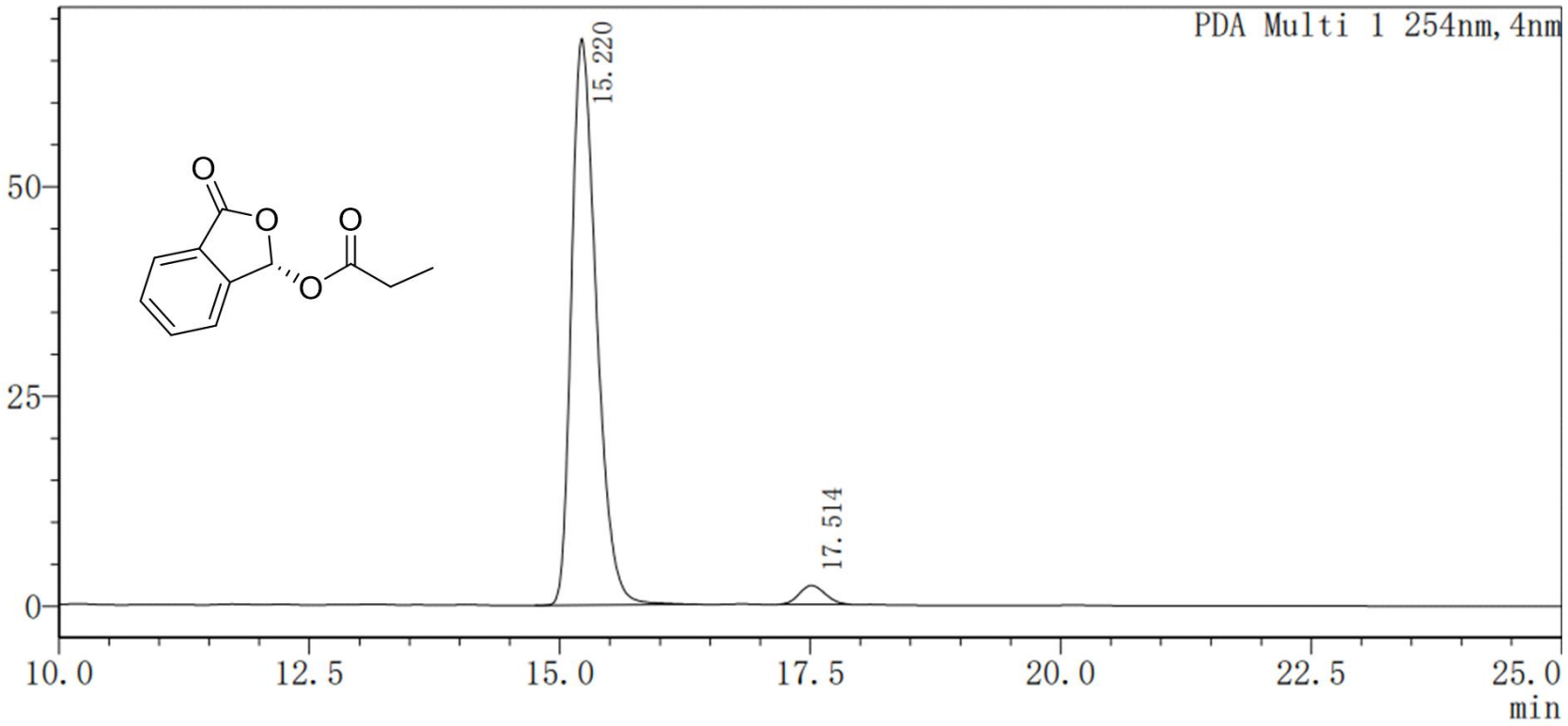

172.97
167.94
144.38
134.86
131.25
126.47
125.73
123.57
92.62
27.39
8.66
O
O
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

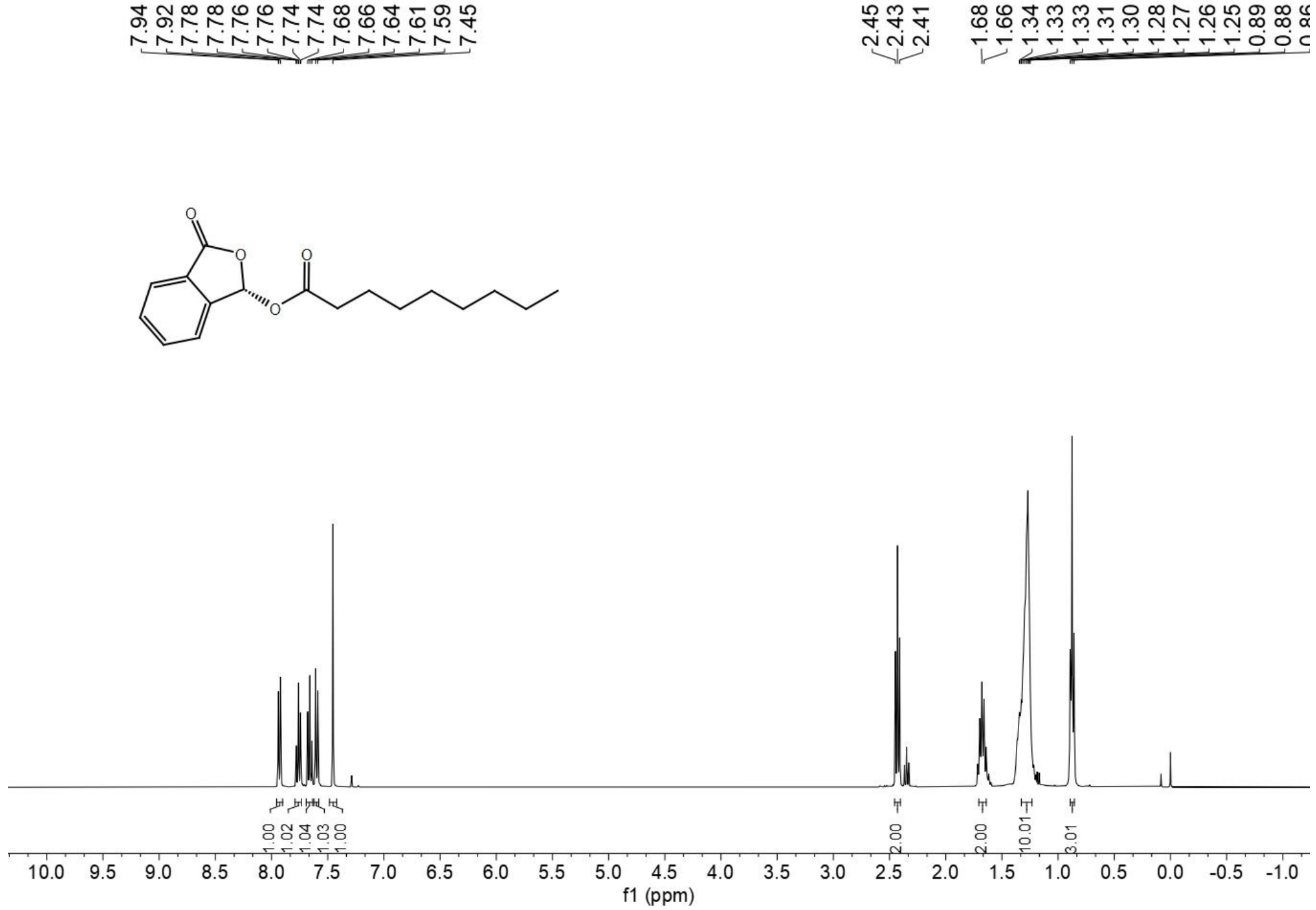
Peak#	Ret. Time	Height	Area	Area%
1	15.236	43954	754259	50.564
2	17.415	38013	737437	49.436
Total		81966	1491696	100.000

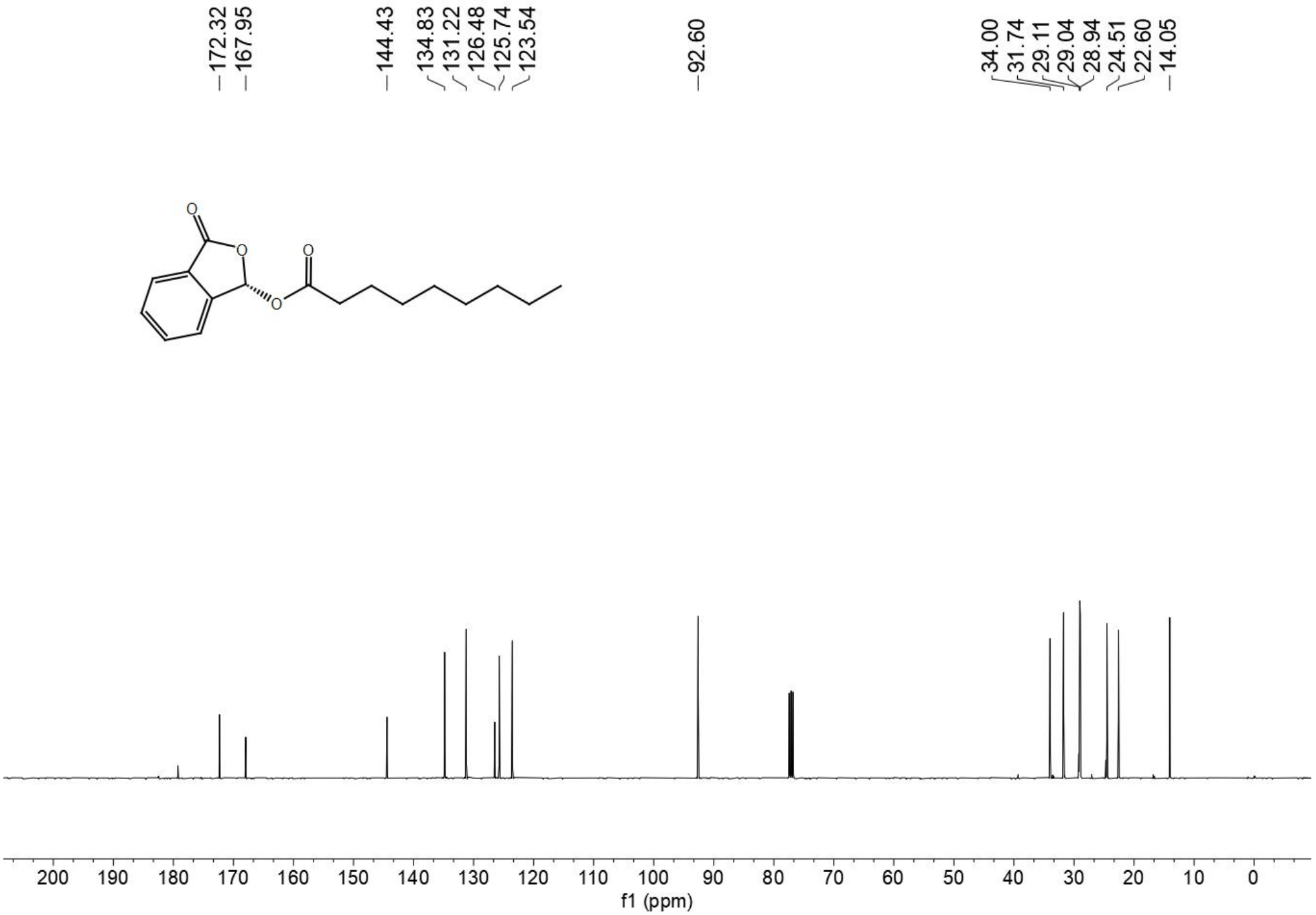


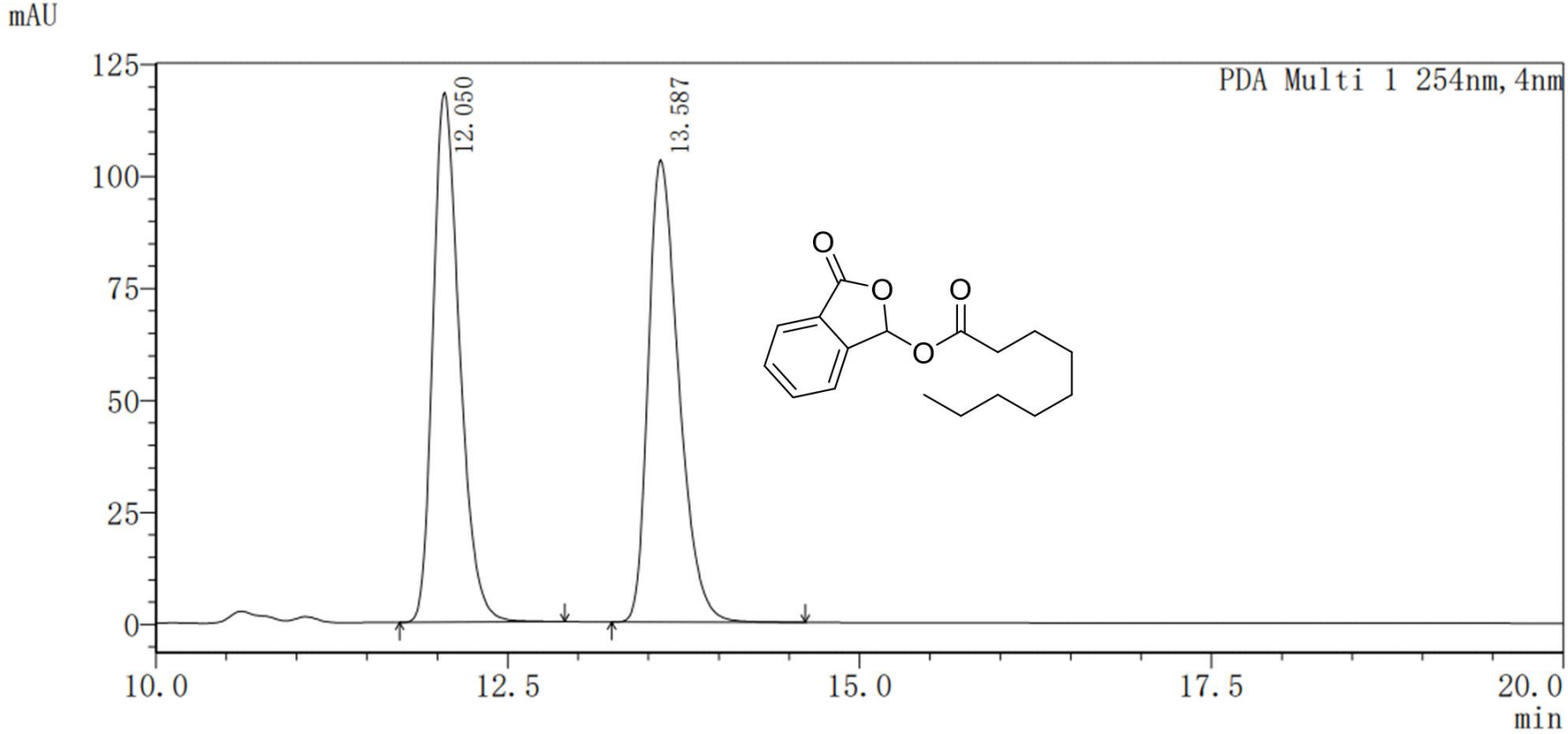
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	15.220	67443	1170753	96.720
2	17.514	2237	39706	3.280
Total		69681	1210460	100.000


7.94
7.92
7.78
7.78
7.76
7.76
7.74
7.74
7.68
7.66
7.64
7.61
7.59
7.45
2.45
2.43
2.41
1.68
1.66
1.34
1.33
1.33
1.31
1.30
1.28
1.27
1.26
1.25
0.89
0.88
O
O
O
O
1.00
1.02
1.04
1.03
1.00
2.00
2.00
10.01
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

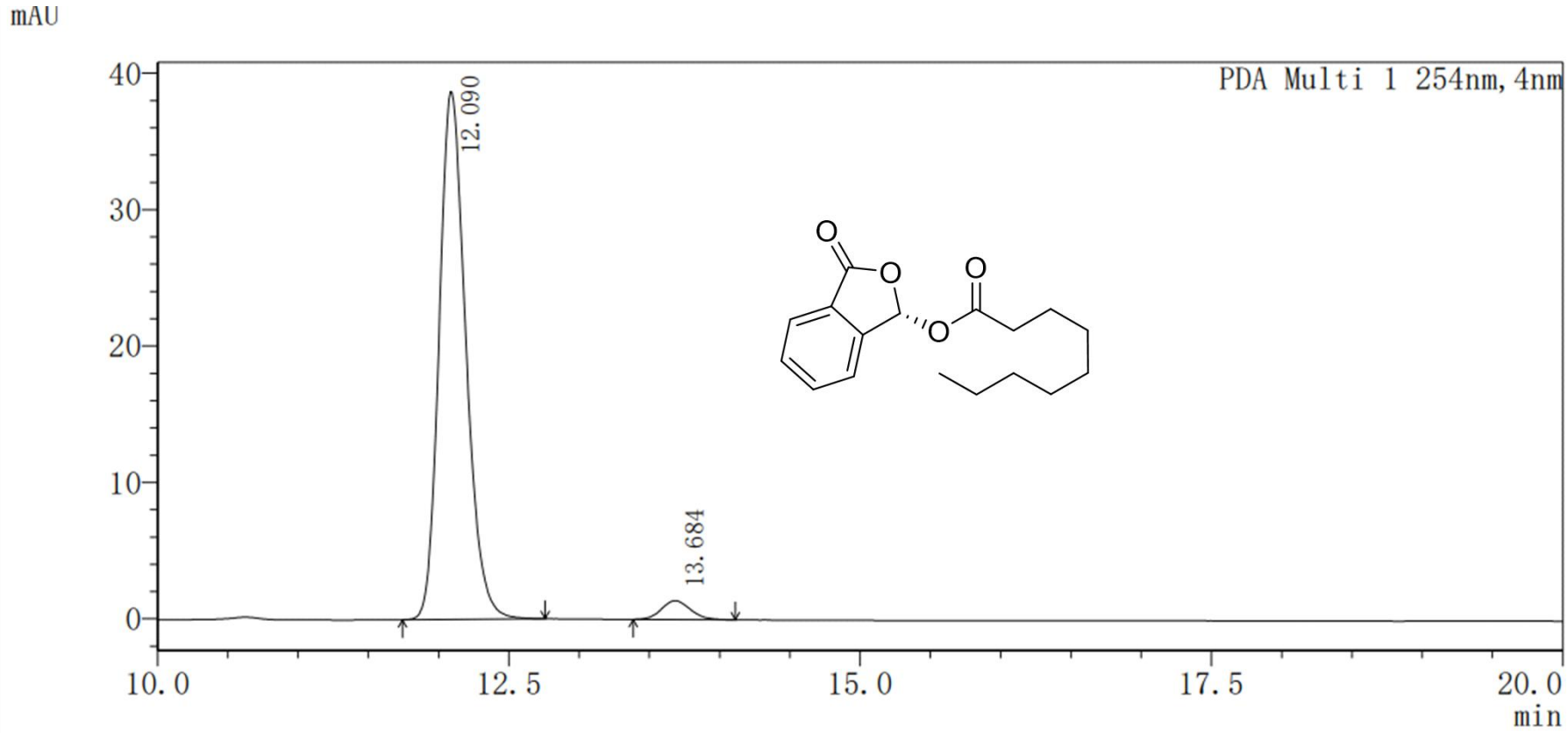

172.32
167.95
144.43
134.83
131.22
126.48
125.74
123.54
92.60
34.00
31.74
29.11
29.04
28.94
24.51
22.60
14.05
O
O
O
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

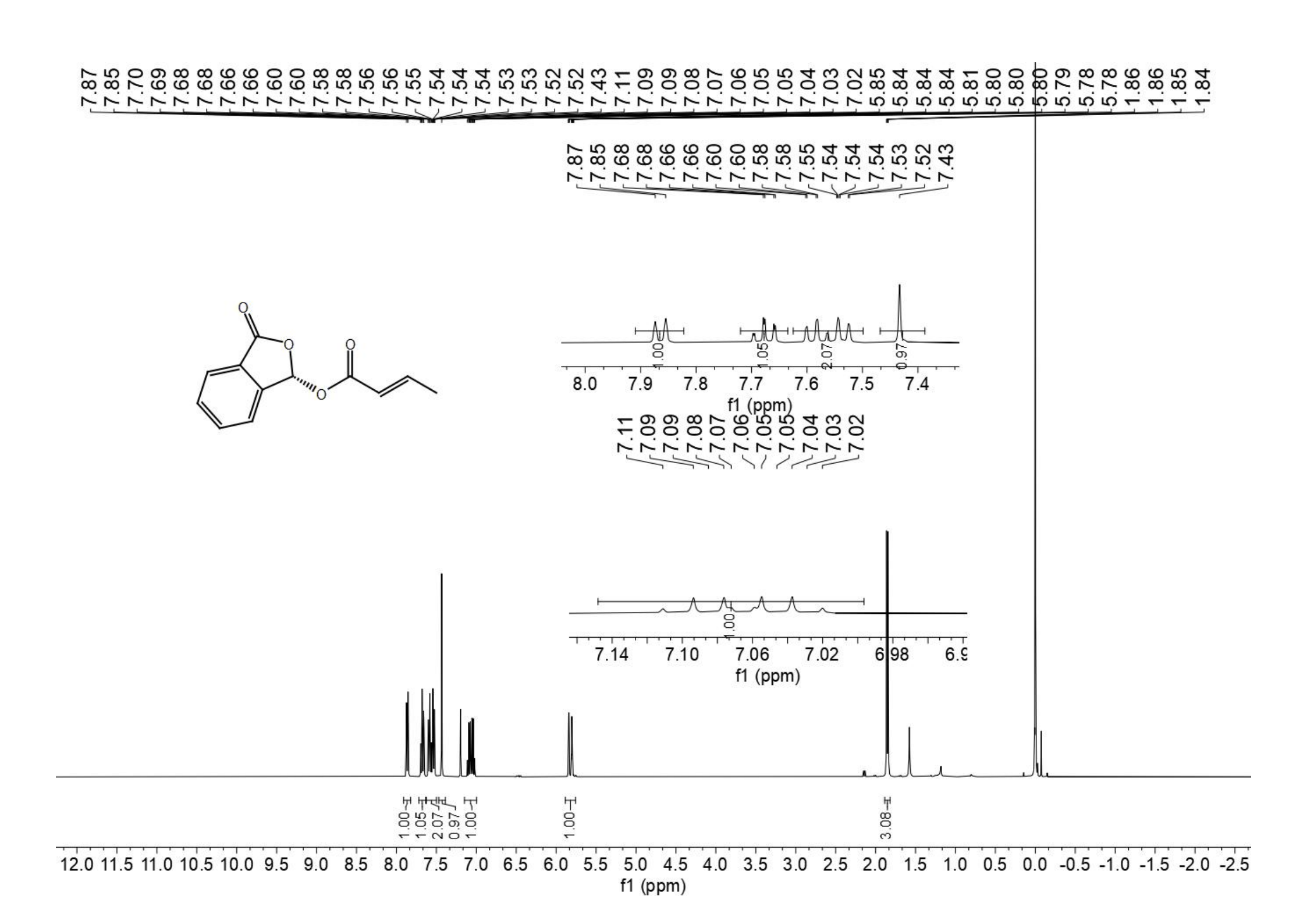
Peak#	Ret. Time	Height	Area	Area%
1	12.050	118196	1559151	50.051
2	13.587	103220	1555998	49.949
Total		221417	3115149	100.000

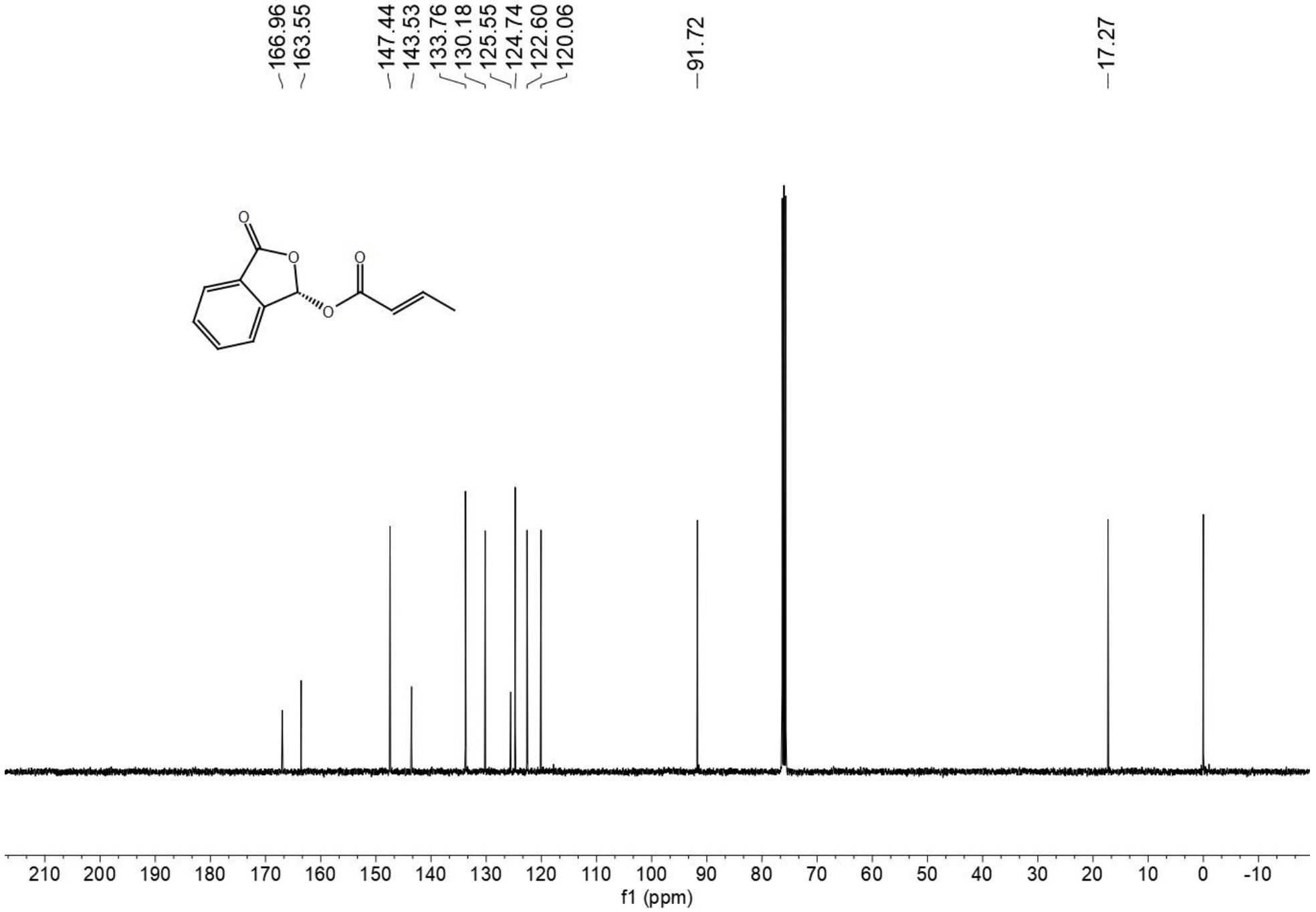


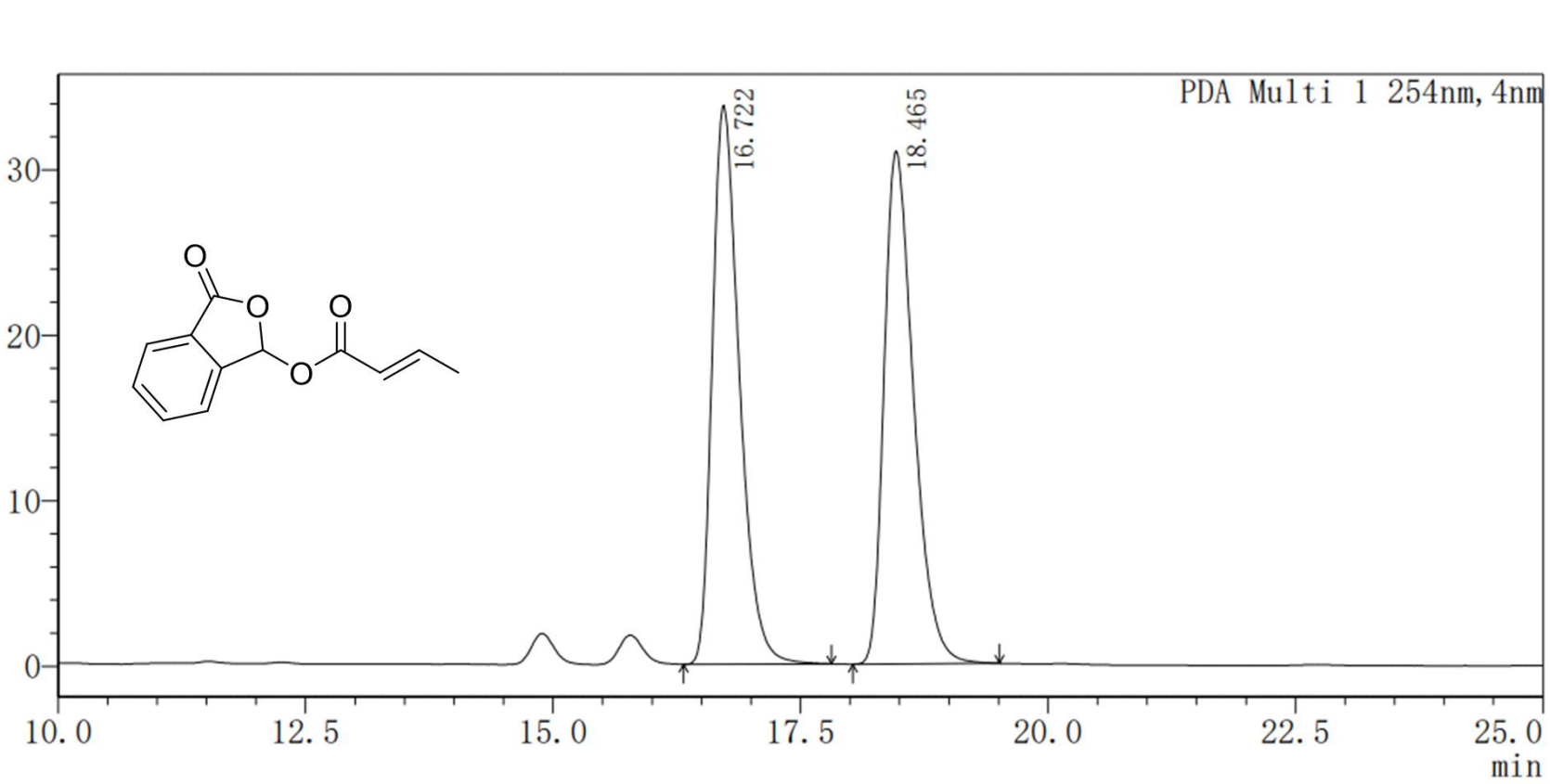
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	12.090	38675	510531	96.276
2	13.684	1384	19750	3.724
Total		40059	530281	100.000


7.87 7.85 7.70 7.69 7.68 7.68 7.66 7.66 7.60 7.60 7.58 7.58 7.56 7.56 7.55 7.54 7.54 7.54 7.53 7.53 7.52 7.52 7.43 7.11 7.09 7.09 7.08 7.07 7.06 7.05 7.05 7.04 7.03 7.02 5.85 5.84 5.84 5.84 5.81 5.80 5.80 5.80 5.79 5.78 5.78 1.86 1.86 1.85 1.84
7.87 7.85 7.68 7.68 7.66 7.66 7.60 7.60 7.58 7.58 7.55 7.54 7.54 7.54 7.53 7.52 7.43
1.00 1.05 2.07 0.97
8.0 7.9 7.8 7.7 7.6 7.5 7.4
f1 (ppm)
7.11 7.09 7.09 7.08 7.07 7.06 7.05 7.05 7.04 7.03 7.02
1.00
7.14 7.10 7.06 7.02 6.98 6.9
f1 (ppm)
1.00 1.05 2.07 0.97 1.00 1.00 3.08
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5
f1 (ppm)

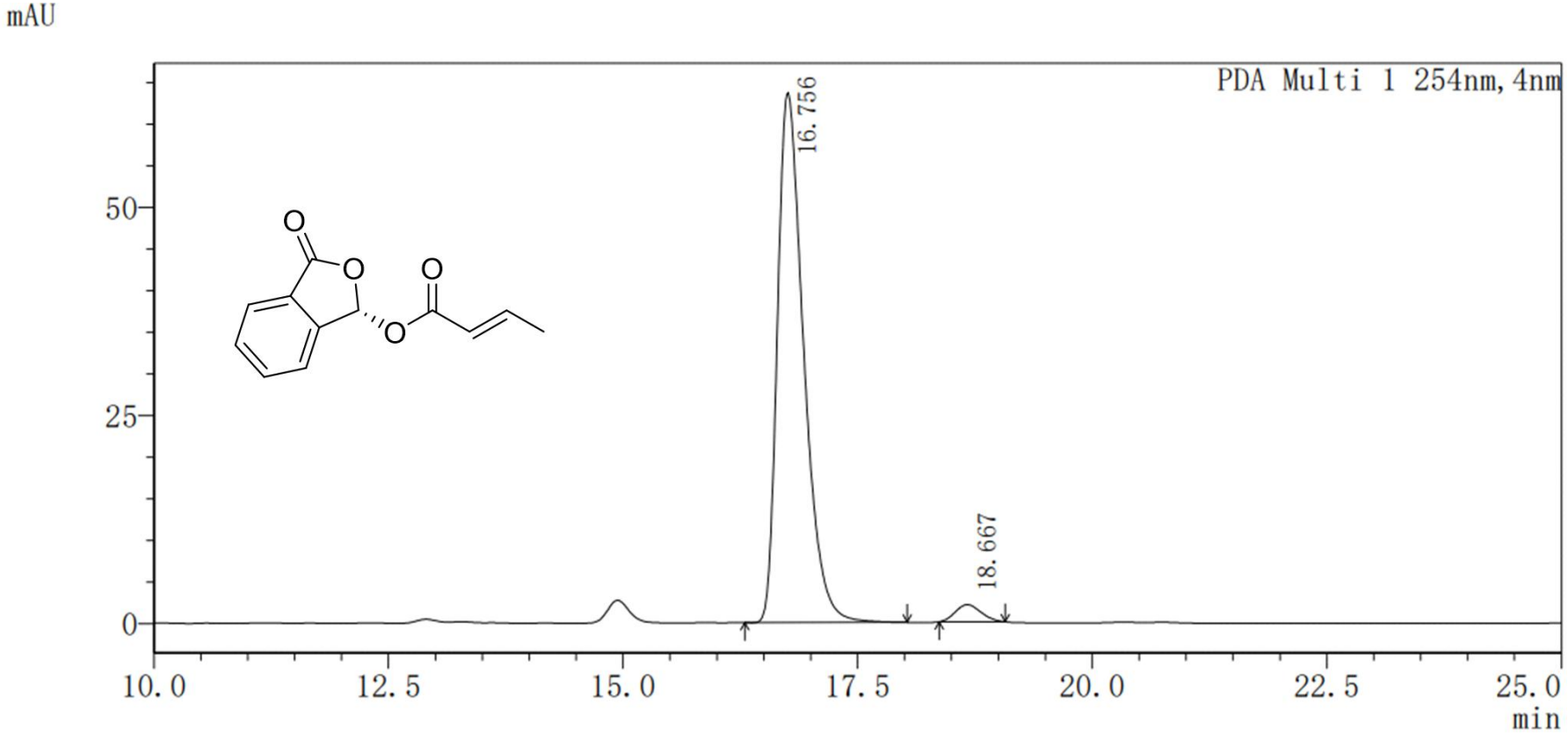

166.96
163.55
147.44
143.53
133.76
130.18
125.55
124.74
122.60
120.06
91.72
17.27
O
O
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

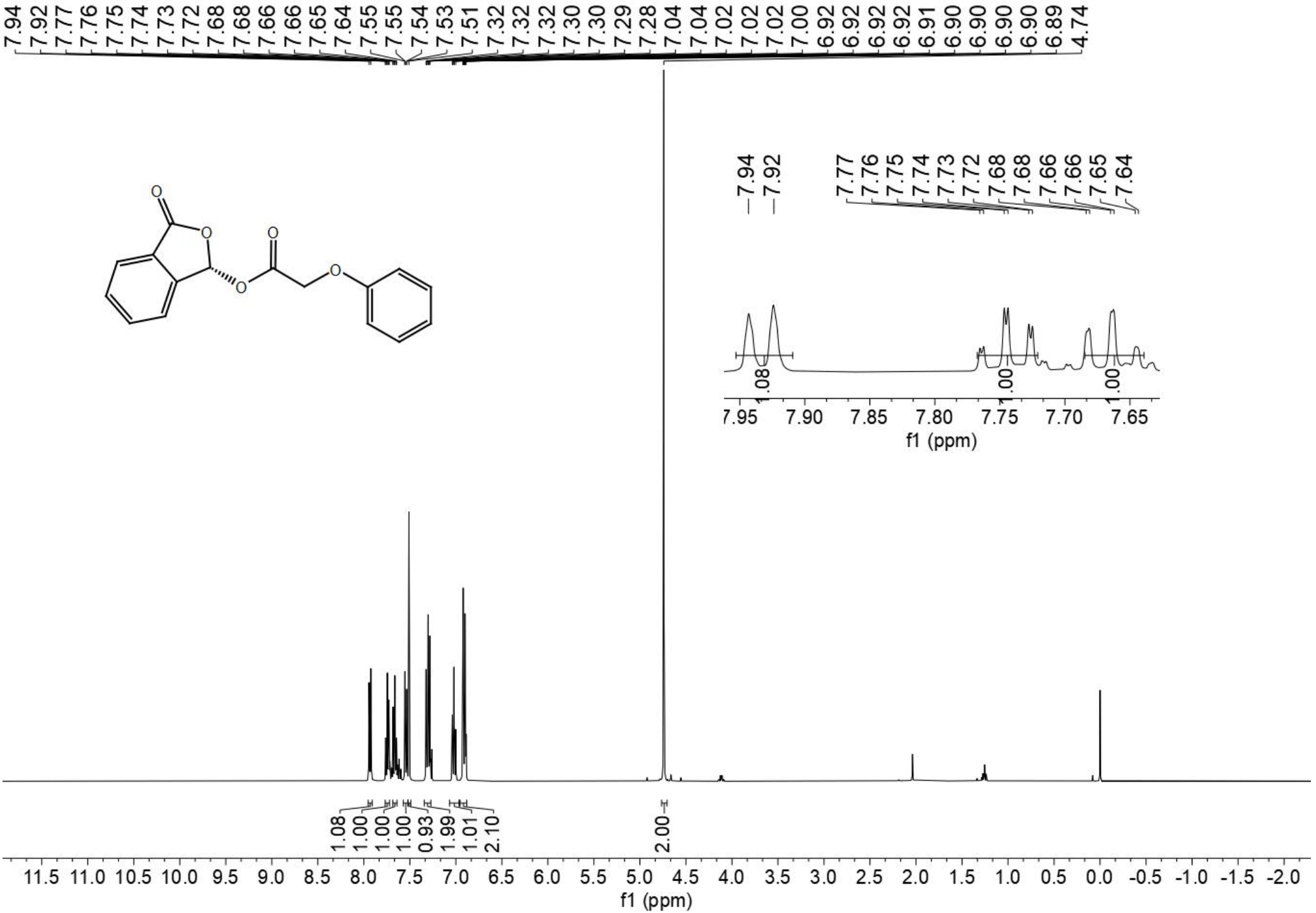
Peak#	Ret. Time	Height	Area	Area%
1	16.722	33763	643788	49.985
2	18.465	31005	644171	50.015
Total		64768	1287959	100.000

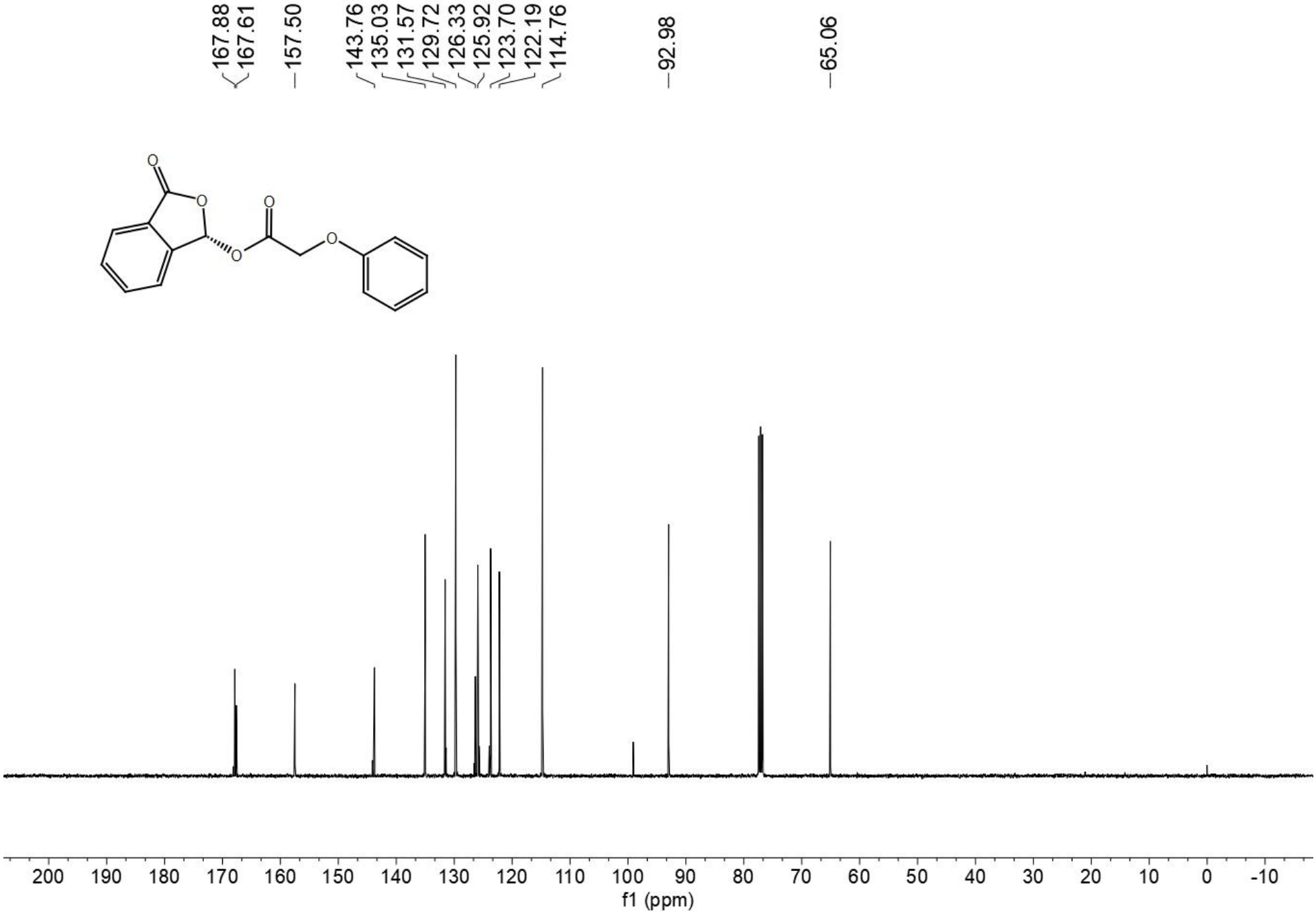


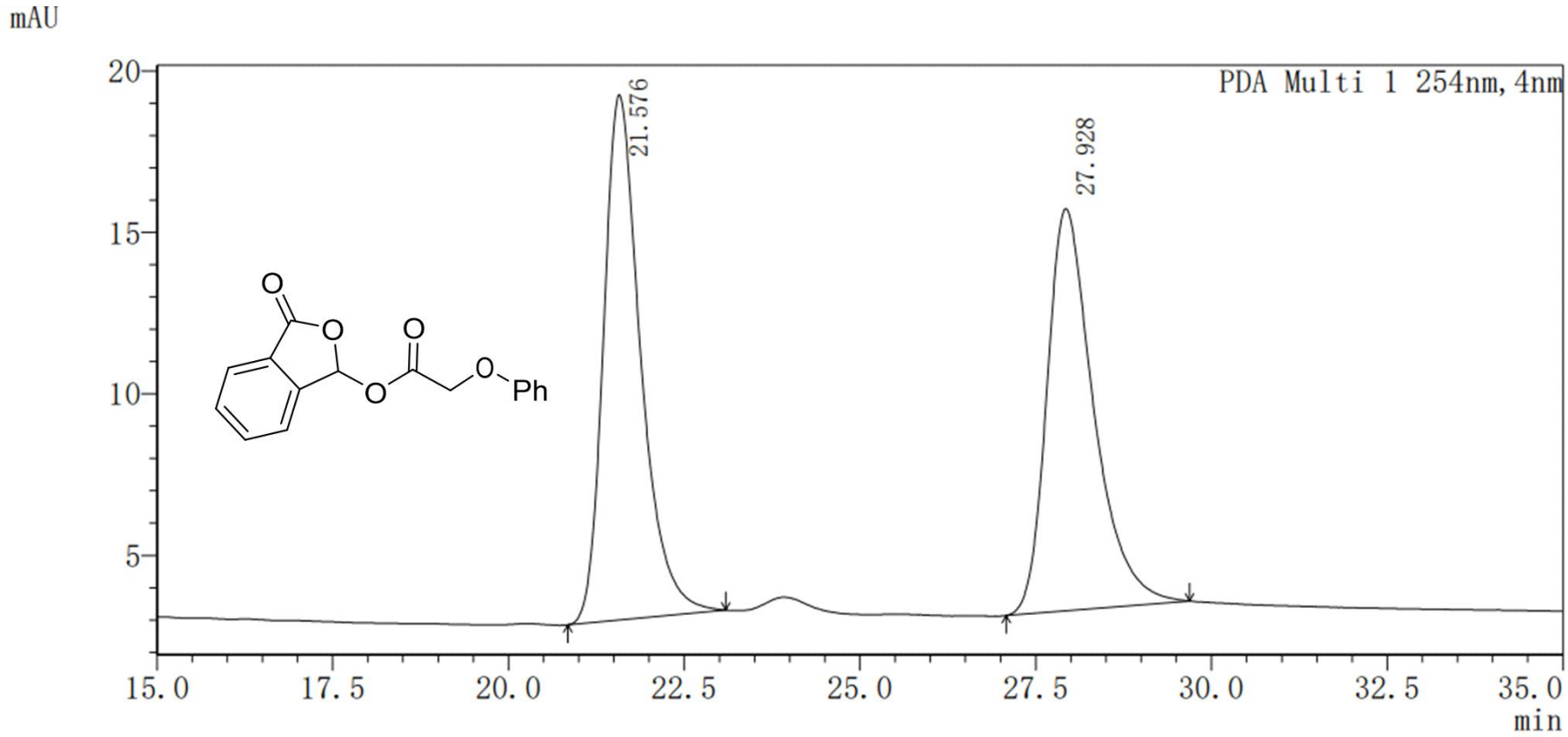
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	16.756	63629	1235592	96.912
2	18.667	2061	39368	3.088
Total		65690	1274960	100.000


7.94
7.92
7.77
7.76
7.75
7.74
7.73
7.72
7.68
7.68
7.66
7.66
7.65
7.64
7.55
7.55
7.54
7.53
7.51
7.32
7.32
7.32
7.30
7.30
7.29
7.28
7.04
7.04
7.02
7.02
7.02
7.00
6.92
6.92
6.92
6.92
6.91
6.90
6.90
6.90
6.90
6.89
4.74
1.08
1.00
1.00
1.00
0.93
1.99
1.01
2.10
2.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)
7.95 7.90 7.85 7.80 7.75 7.70 7.65
f1 (ppm)

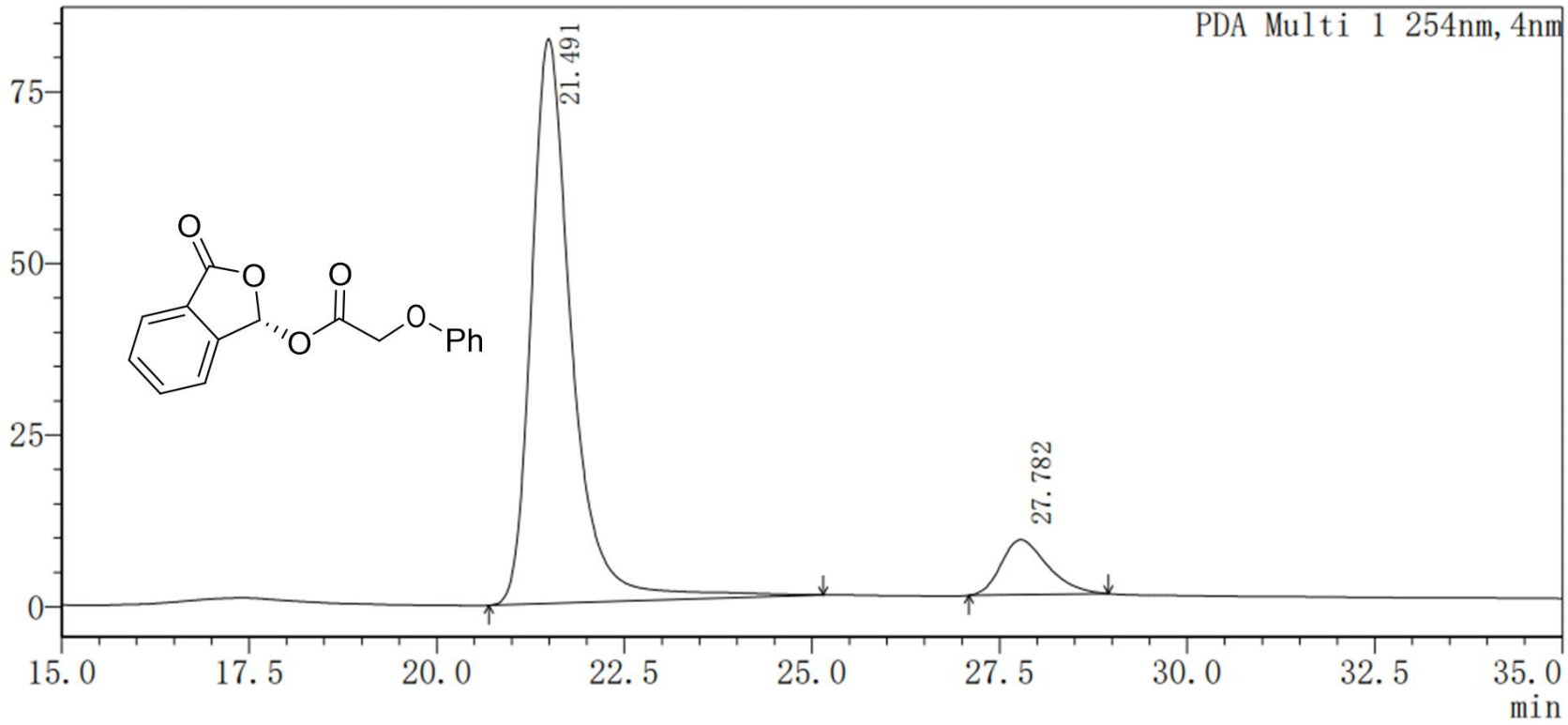

167.88
167.61
157.50
143.76
135.03
131.57
129.72
126.33
125.92
123.70
122.19
114.76
92.98
65.06
O
O
O
O
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

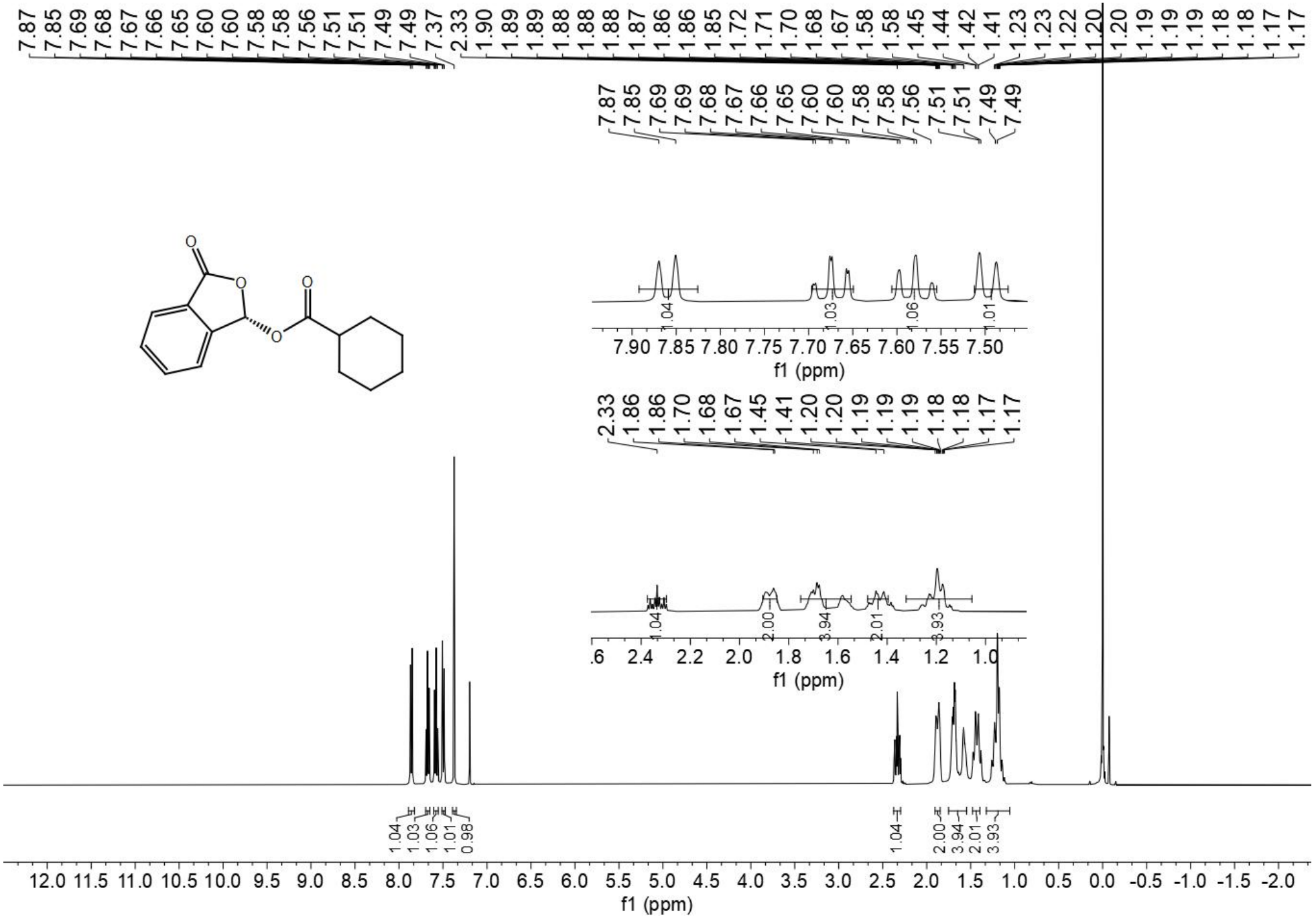
Peak#	Ret. Time	Height	Area	Area%
1	21.576	16265	598130	50.916
2	27.928	12452	576614	49.084
Total		28717	1174744	100.000

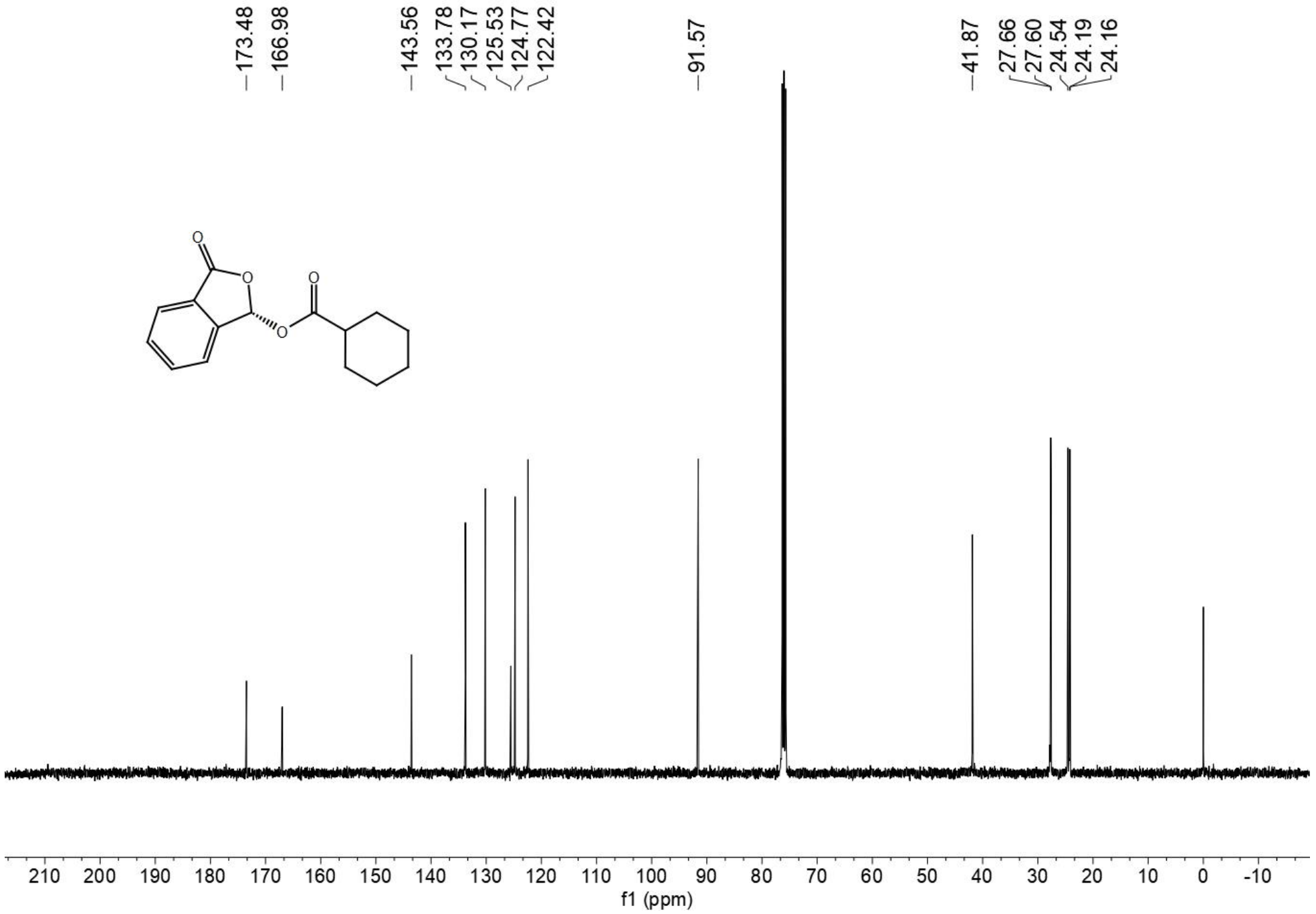


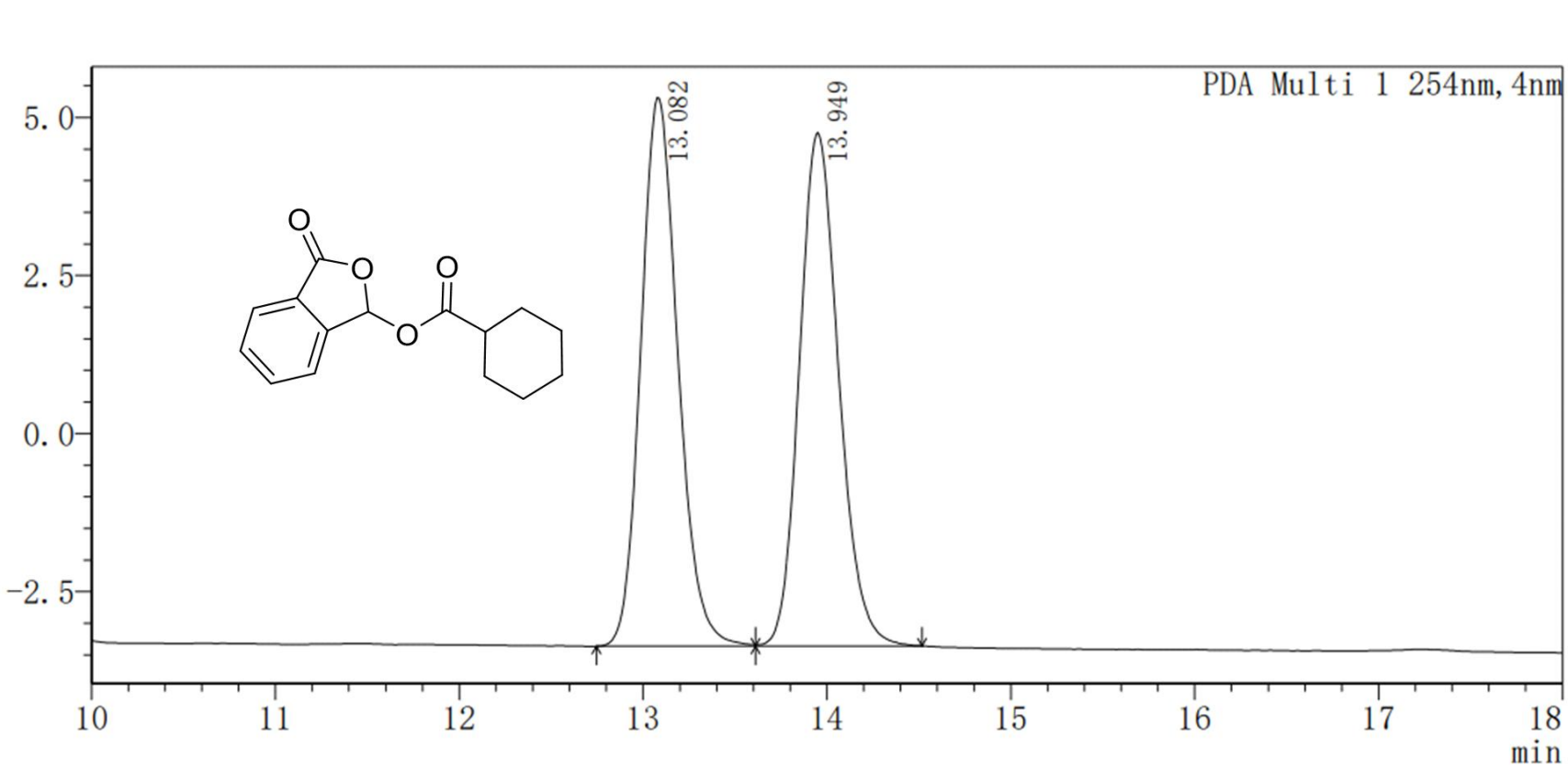
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	21.491	82231	3104345	90.012
2	27.782	7997	344472	9.988
Total		90228	3448817	100.000


7.87 7.85 7.69 7.68 7.67 7.66 7.65 7.60 7.60 7.58 7.58 7.56 7.51 7.51 7.49 7.49 7.37 2.33 1.90 1.89 1.89 1.88 1.88 1.88 1.87 1.86 1.86 1.85 1.72 1.71 1.70 1.68 1.67 1.58 1.58 1.45 1.44 1.42 1.41 1.23 1.23 1.22 1.20 1.20 1.19 1.19 1.19 1.18 1.18 1.17 1.17
7.87 7.85 7.69 7.69 7.68 7.67 7.66 7.65 7.60 7.60 7.58 7.58 7.56 7.51 7.51 7.49 7.49
1.04 1.03 1.06 1.01
7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50
f1 (ppm)
2.33 1.86 1.86 1.70 1.68 1.67 1.45 1.41 1.20 1.20 1.19 1.19 1.19 1.18 1.18 1.17 1.17
1.04 2.00 3.94 2.01 3.93
.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0
f1 (ppm)
1.04 1.03 1.06 1.01 0.98
1.04 2.00 3.94 2.01 3.93
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

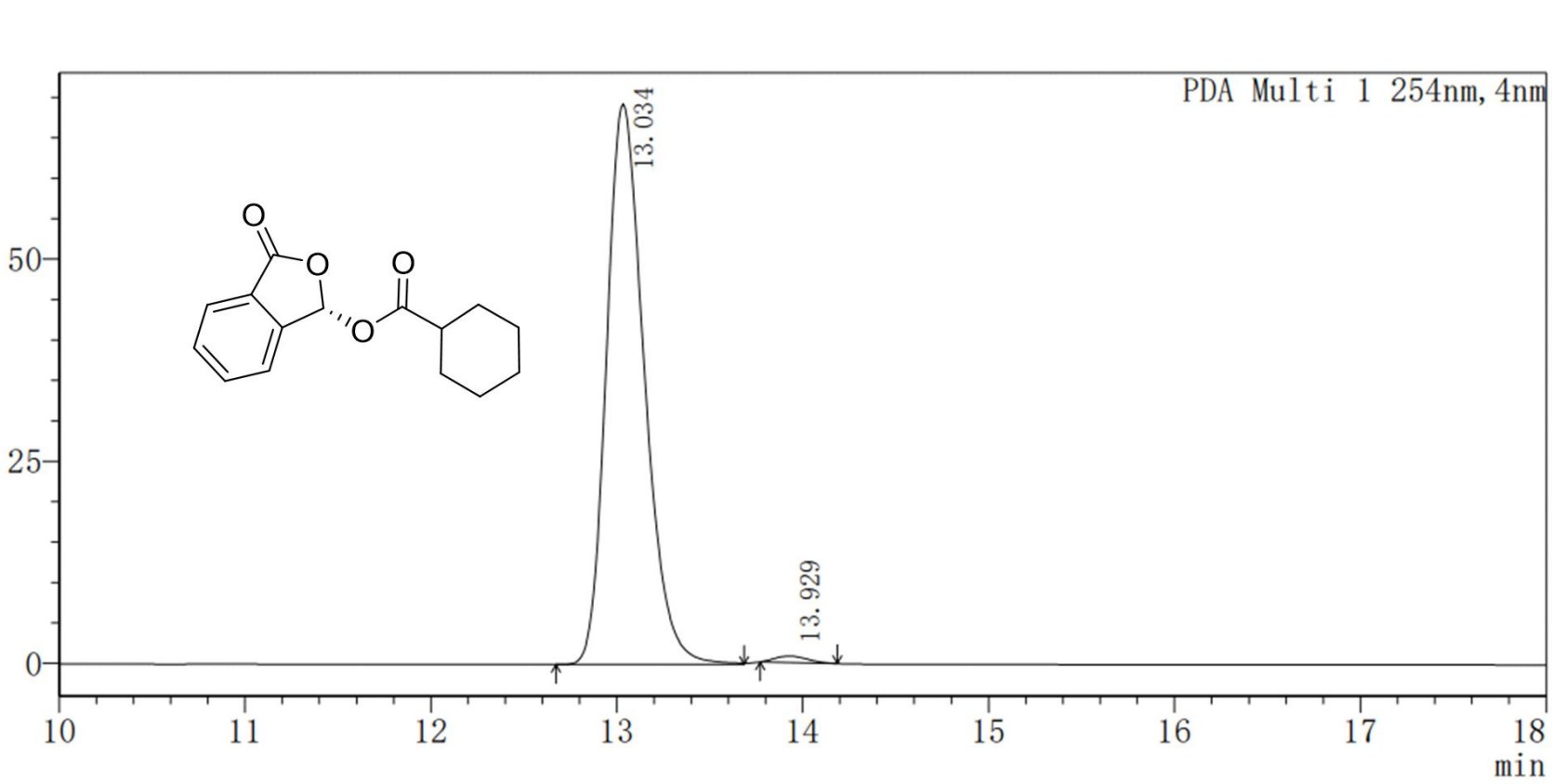

173.48
166.98
143.56
133.78
130.17
125.53
124.77
122.42
91.57
41.87
27.66
27.60
24.54
24.19
24.16
O
O
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

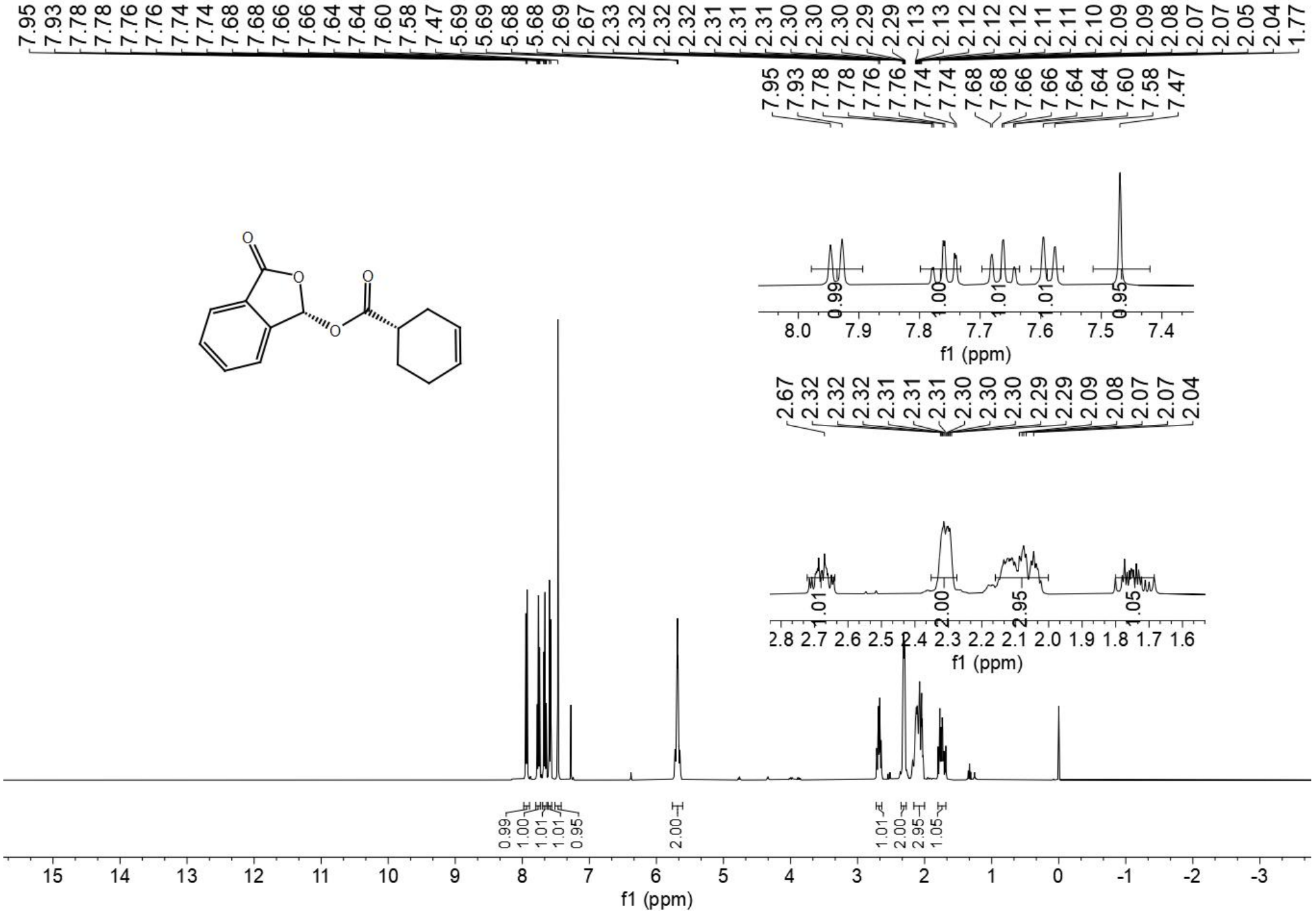
Peak#	Ret. Time	Height	Area	Area%
1	13.082	8673	121626	50.244
2	13.949	8120	120445	49.756
Total		16793	242071	100.000

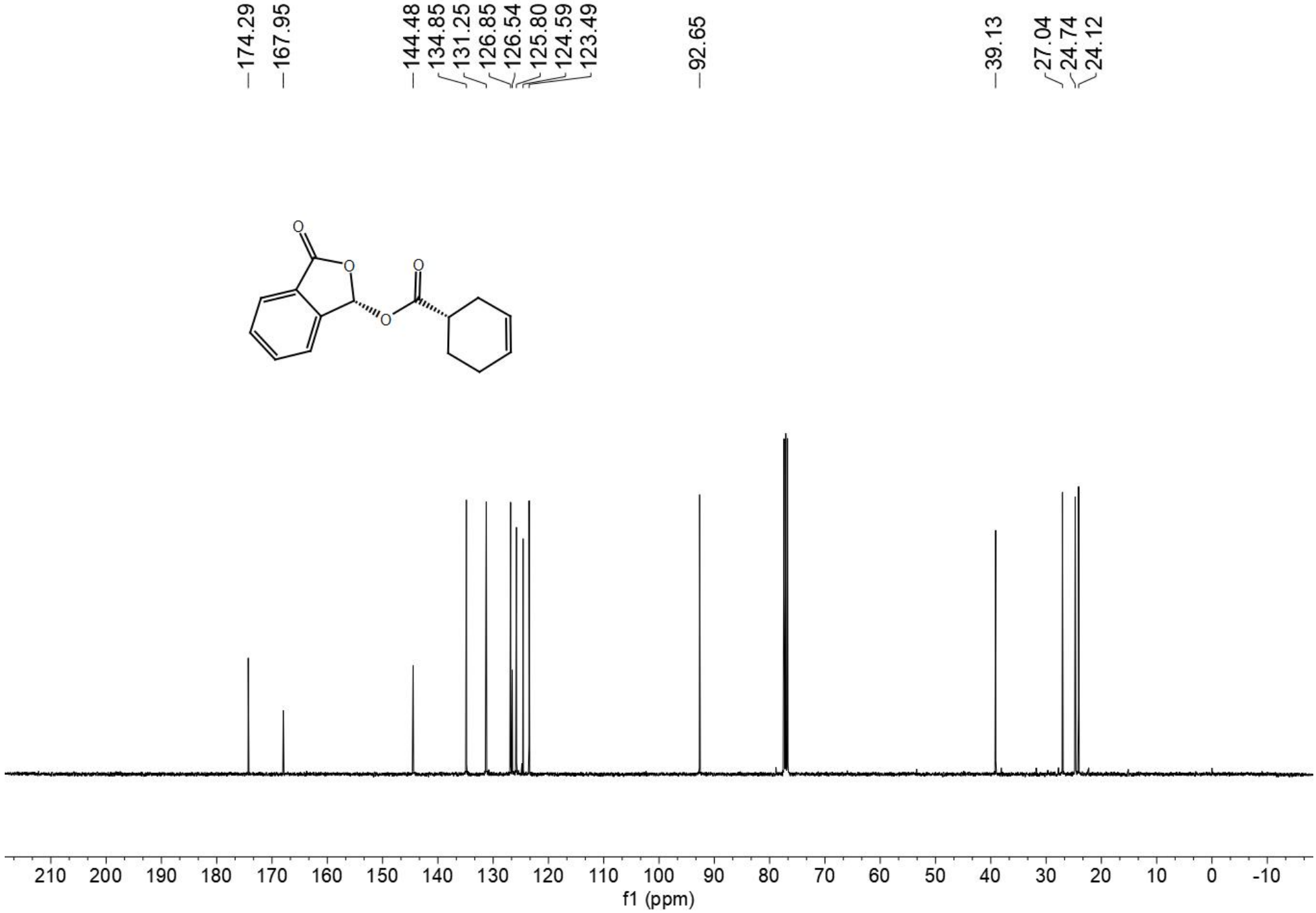


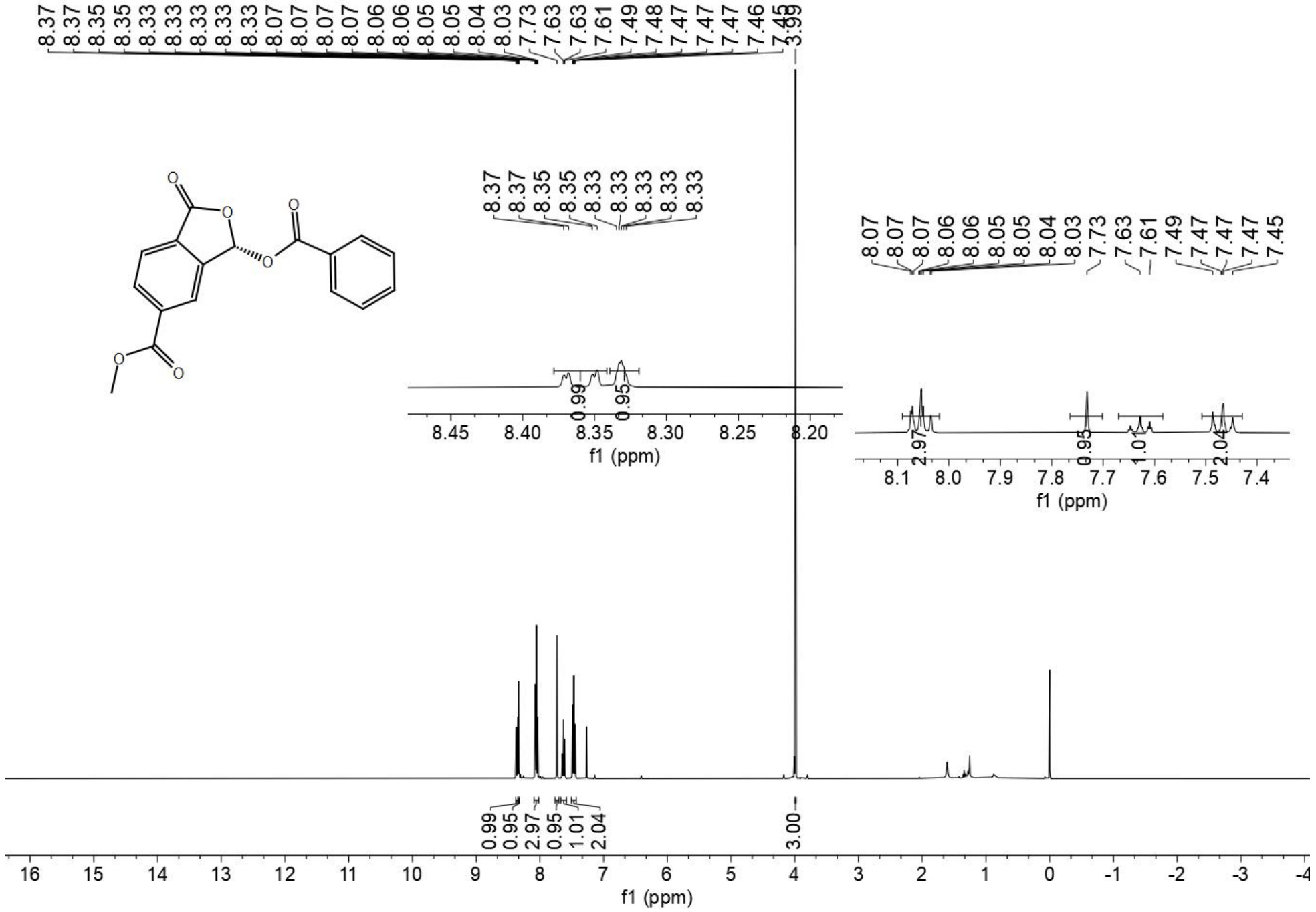
<Peak Table>

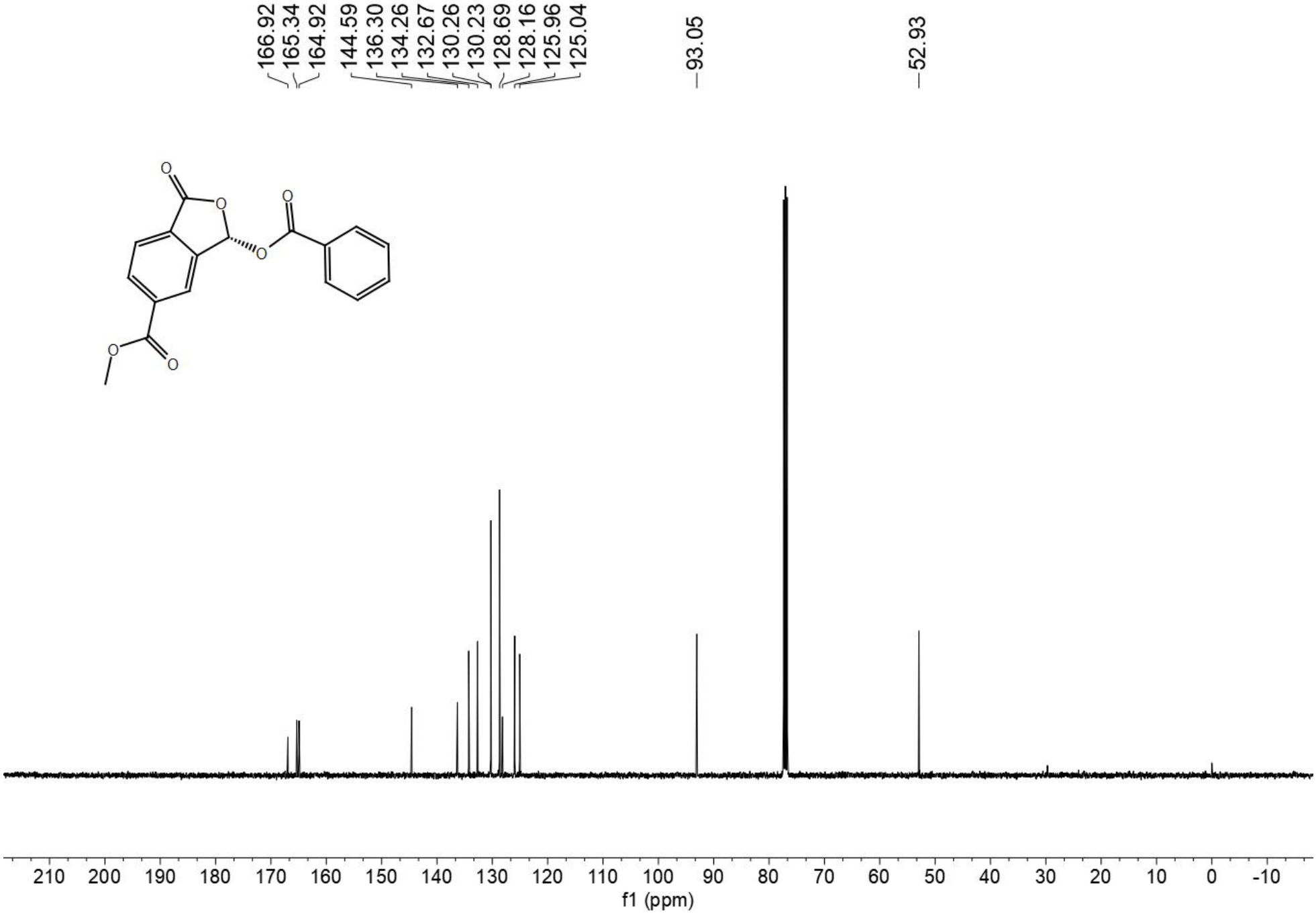
PDA Ch1 254nm

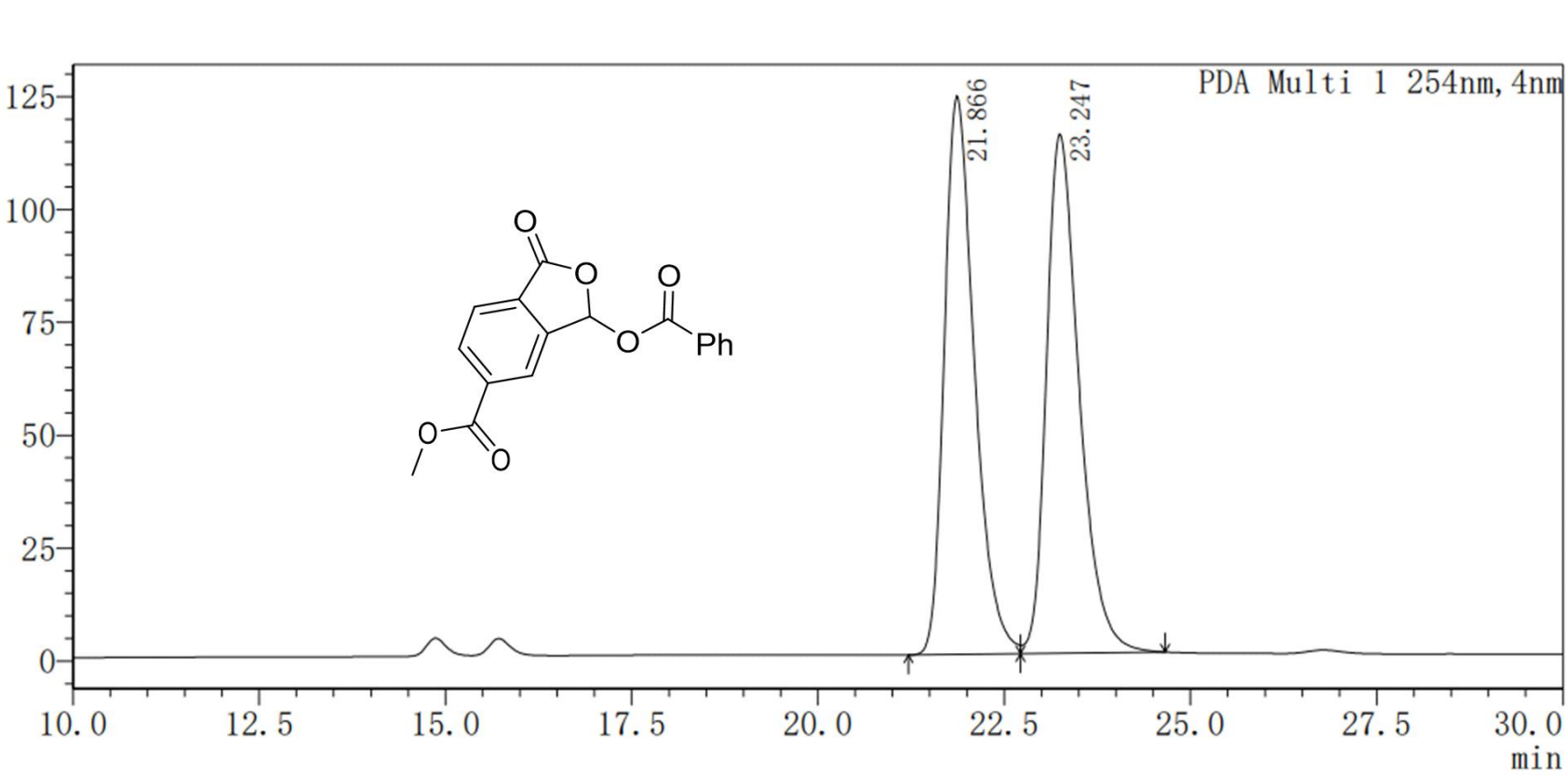
Peak#	Ret. Time	Height	Area	Area%
1	13.034	69325	980583	98.997
2	13.929	817	9937	1.003
Total		70142	990520	100.000


7.95 7.93 7.78 7.78 7.76 7.76 7.74 7.74 7.68 7.68 7.66 7.66 7.64 7.64 7.60 7.58 7.47 5.69 5.69 5.68 5.68 2.69 2.67 2.33 2.32 2.32 2.32 2.31 2.31 2.31 2.30 2.30 2.30 2.29 2.29 2.13 2.13 2.12 2.12 2.12 2.11 2.11 2.10 2.09 2.09 2.08 2.07 2.07 2.05 2.04 1.77
0.99 1.00 1.01 1.01 0.95
8.0 7.9 7.8 7.7 7.6 7.5 7.4
f1 (ppm)
2.67 2.32 2.32 2.32 2.31 2.31 2.31 2.30 2.30 2.30 2.29 2.29 2.09 2.08 2.07 2.07 2.04
1.01 2.00 2.95 1.05
2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f1 (ppm)
0.99 1.00 1.01 1.01 0.95
2.00
1.01 2.00 2.95 1.05
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


174.29
167.95
144.48
134.85
131.25
126.85
126.54
125.80
124.59
123.49
92.65
39.13
27.04
24.74
24.12
O
O
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.37 8.37 8.35 8.35 8.33 8.33 8.33 8.33 8.07 8.07 8.07 8.07 8.06 8.06 8.05 8.05 8.04 8.03 7.73 7.63 7.63 7.61 7.49 7.48 7.47 7.47 7.47 7.46 7.45 3.99
0.99 0.95 2.97 0.95 1.01 2.04 3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)
8.37 8.37 8.35 8.35 8.33 8.33 8.33 8.33
0.99 0.95
8.45 8.40 8.35 8.30 8.25 8.20
f1 (ppm)
8.07 8.07 8.07 8.06 8.06 8.05 8.05 8.04 8.03 7.73 7.63 7.61 7.49 7.47 7.47 7.47 7.45
2.97 0.95 1.01 2.04
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4
f1 (ppm)

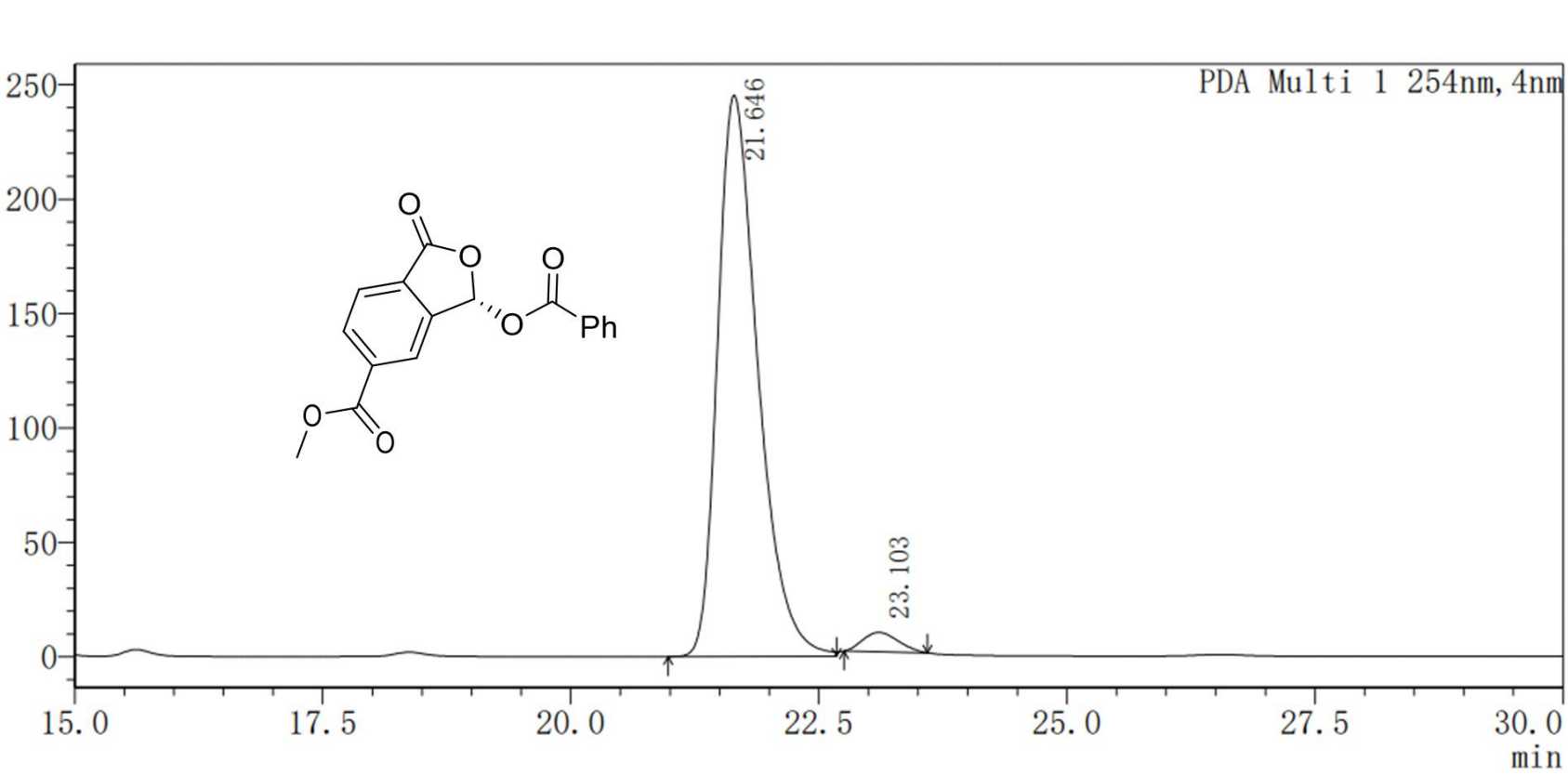

166.92
165.34
164.92
144.59
136.30
134.26
132.67
130.26
130.23
128.69
128.16
125.96
125.04
93.05
52.93
O
O
O
O
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

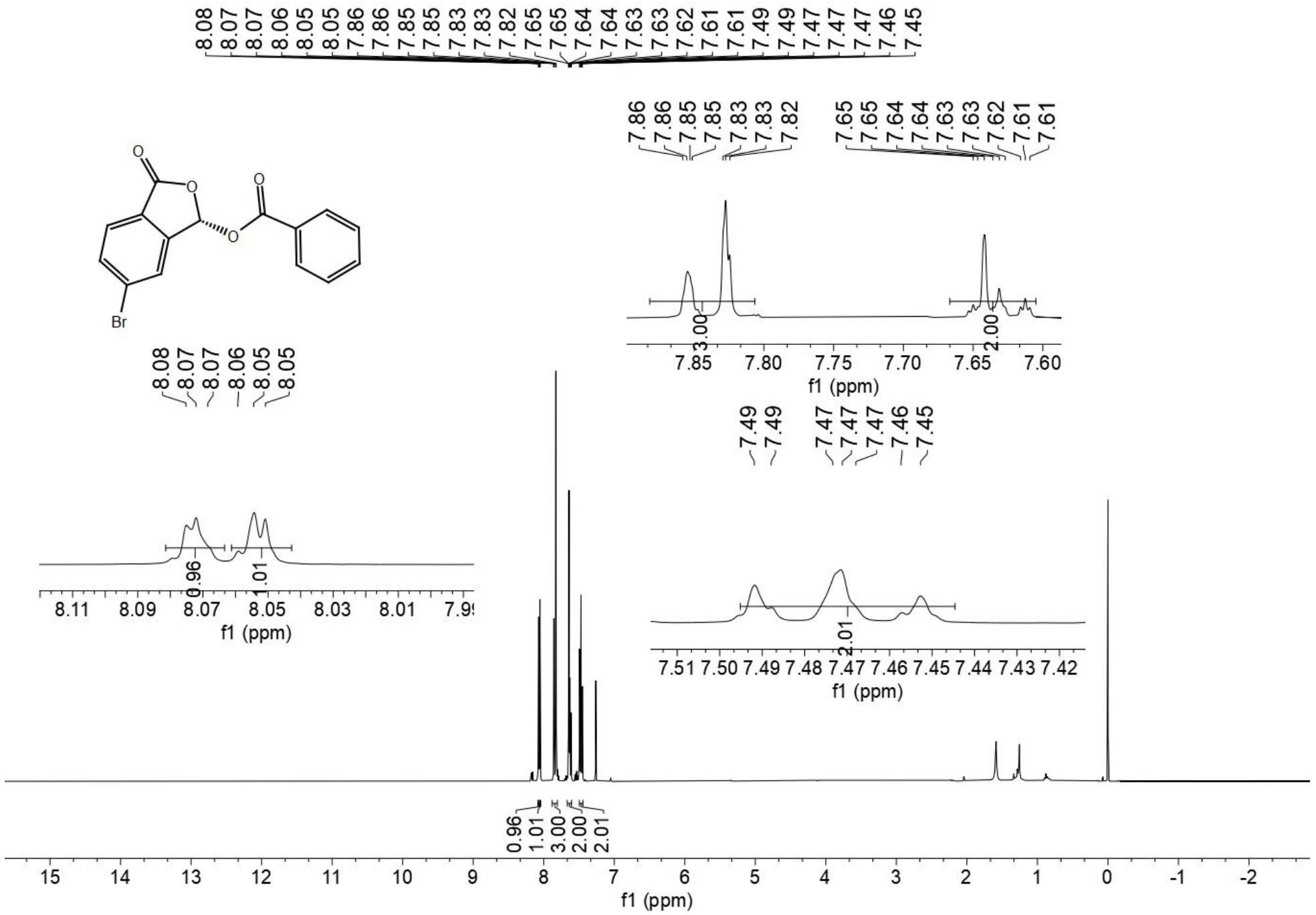
Peak#	Ret. Time	Height	Area	Area%
1	21.866	123667	3480143	49.736
2	23.247	115004	3517097	50.264
Total		238671	6997240	100.000

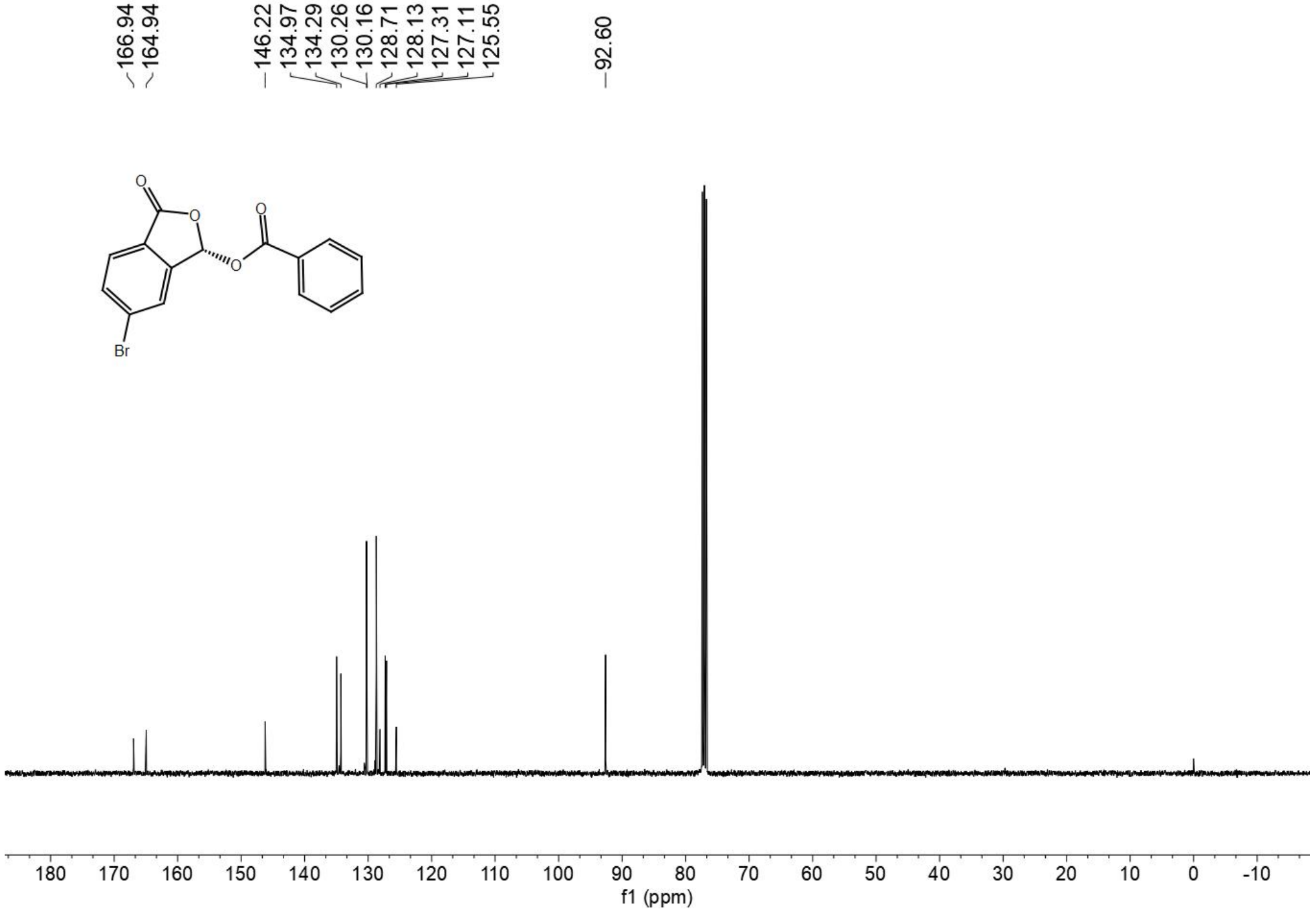


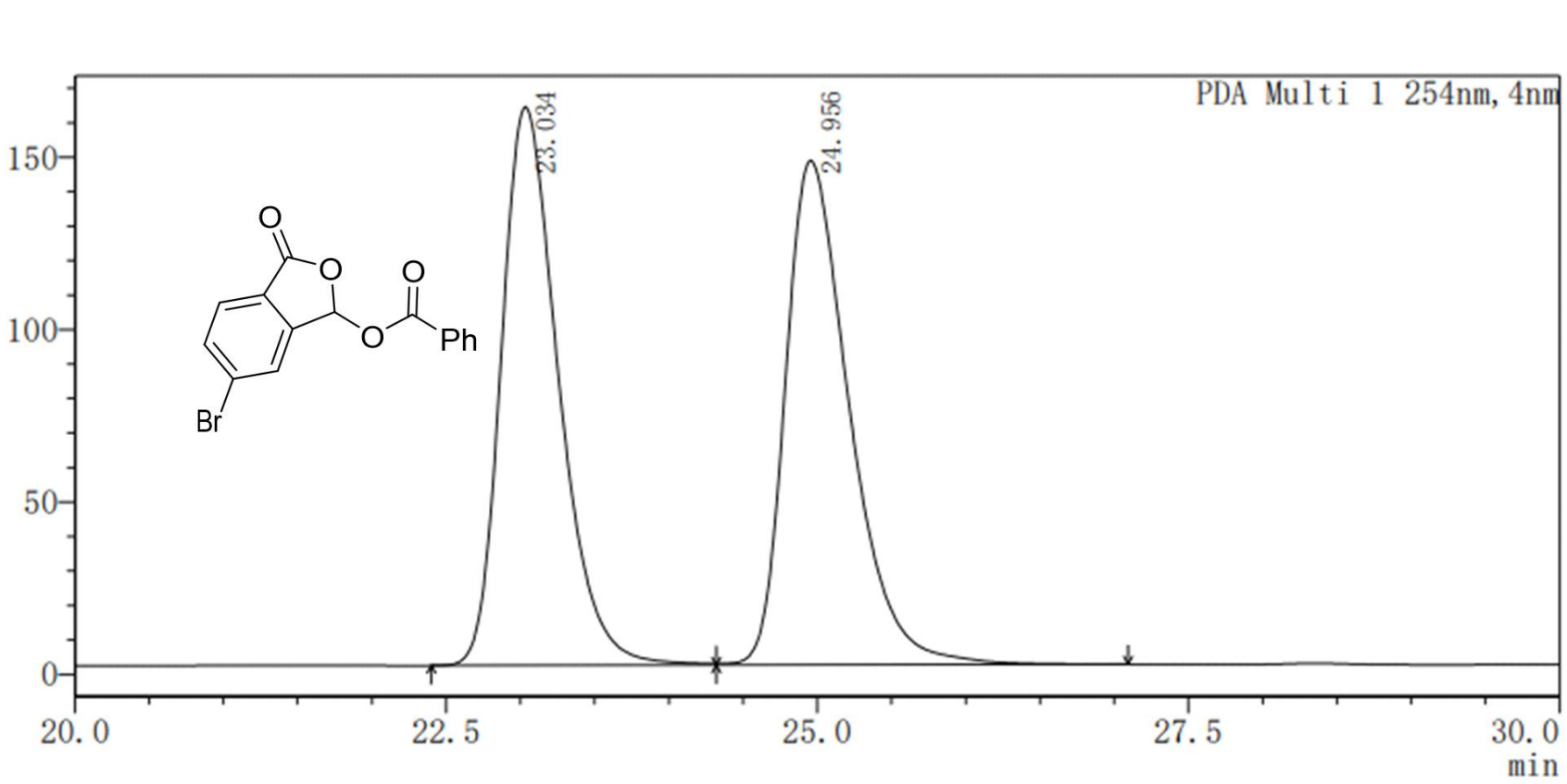
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	21.646	245134	6942014	97.049
2	23.103	8492	211078	2.951
Total		253626	7153092	100.000


8.08 8.07 8.07 8.06 8.05 8.05 7.86 7.86 7.85 7.85 7.83 7.83 7.82 7.65 7.65 7.64 7.64 7.63 7.63 7.62 7.61 7.61 7.49 7.49 7.47 7.47 7.47 7.46 7.45
O
O
O
O
Br
7.86 7.86 7.85 7.85 7.83 7.83 7.82
7.65 7.65 7.64 7.64 7.63 7.63 7.62 7.61 7.61
3.00
2.00
7.85 7.80 7.75 7.70 7.65 7.60
f1 (ppm)
8.08 8.07 8.07 8.06 8.05 8.05
7.49 7.49 7.47 7.47 7.47 7.46 7.45
0.96
1.01
8.11 8.09 8.07 8.05 8.03 8.01
f1 (ppm)
2.01
7.51 7.50 7.49 7.48 7.47 7.46 7.45 7.44 7.43 7.42
f1 (ppm)
0.96 1.01 3.00 2.00 2.01
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)

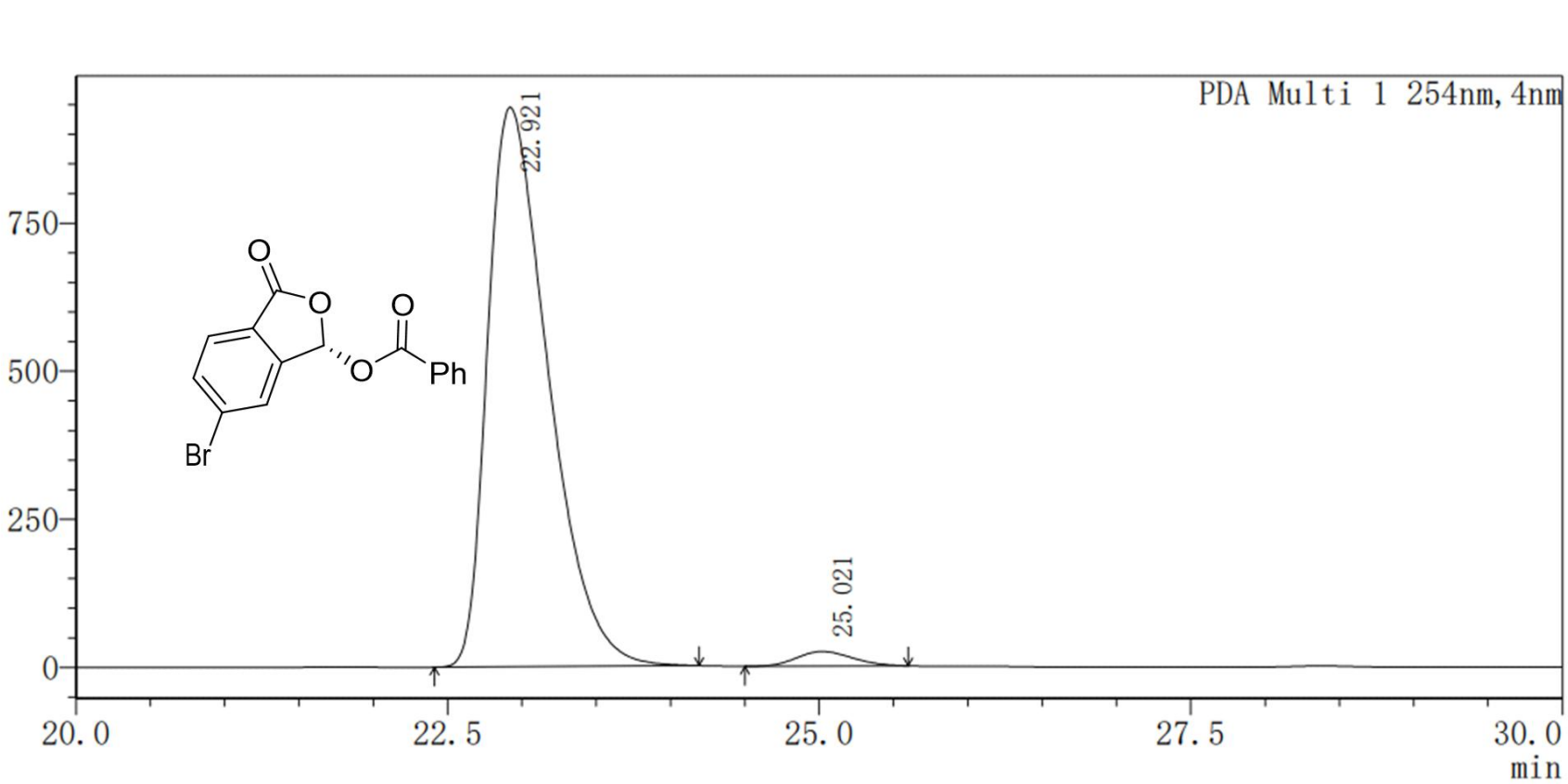

166.94
164.94
146.22
134.97
134.29
130.26
130.16
128.71
128.13
127.31
127.11
125.55
92.60
O
O
O
O
Br
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

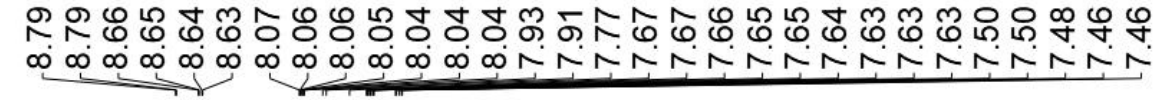
Peak#	Ret. Time	Height	Area	Area%
1	23.034	161945	4337104	49.714
2	24.956	146289	4386963	50.286
Total		308234	8724068	100.000

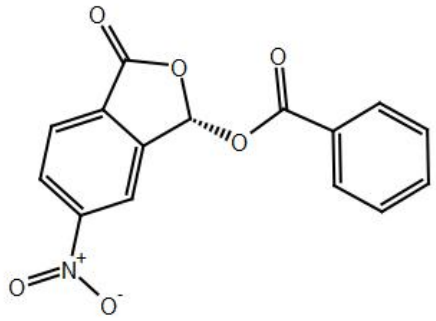


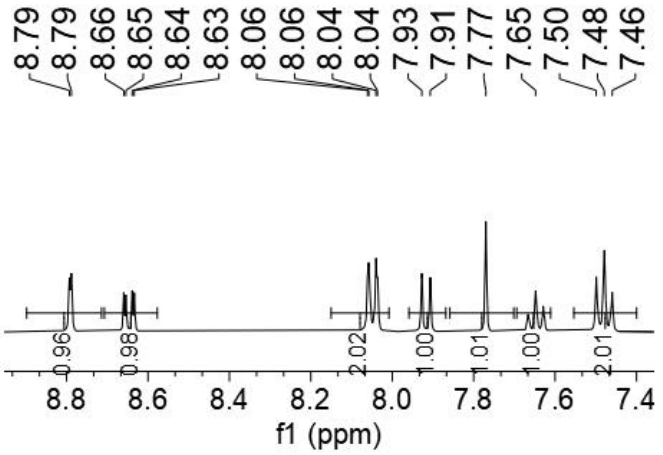
<Peak Table>

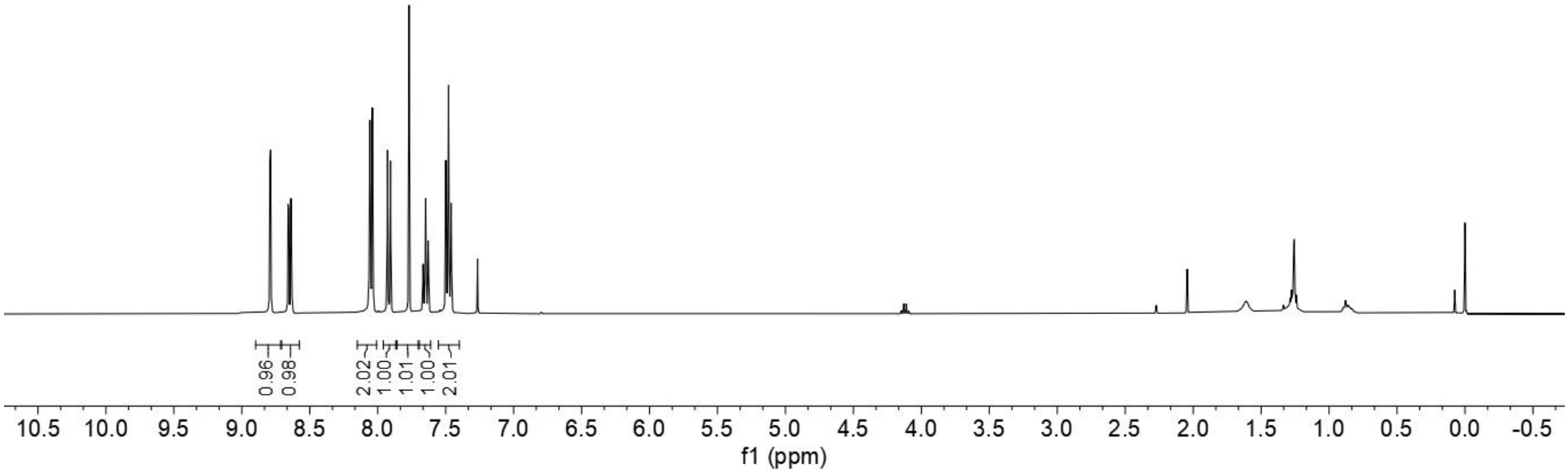
PDA Ch1 254nm

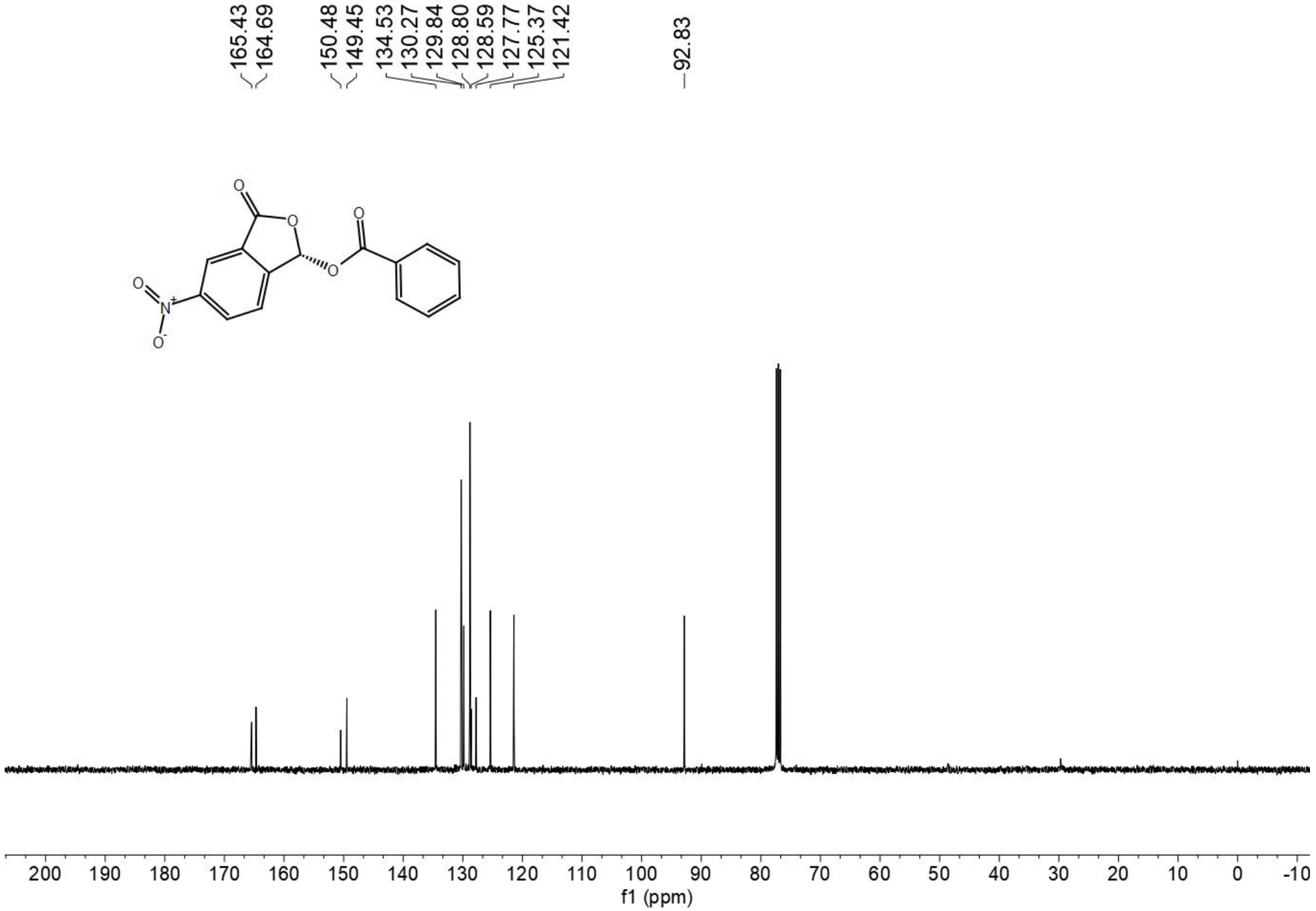
Peak#	Ret. Time	Height	Area	Area%
1	22.921	944664	26826576	97.641
2	25.021	24694	648241	2.359
Total		969358	27474818	100.000

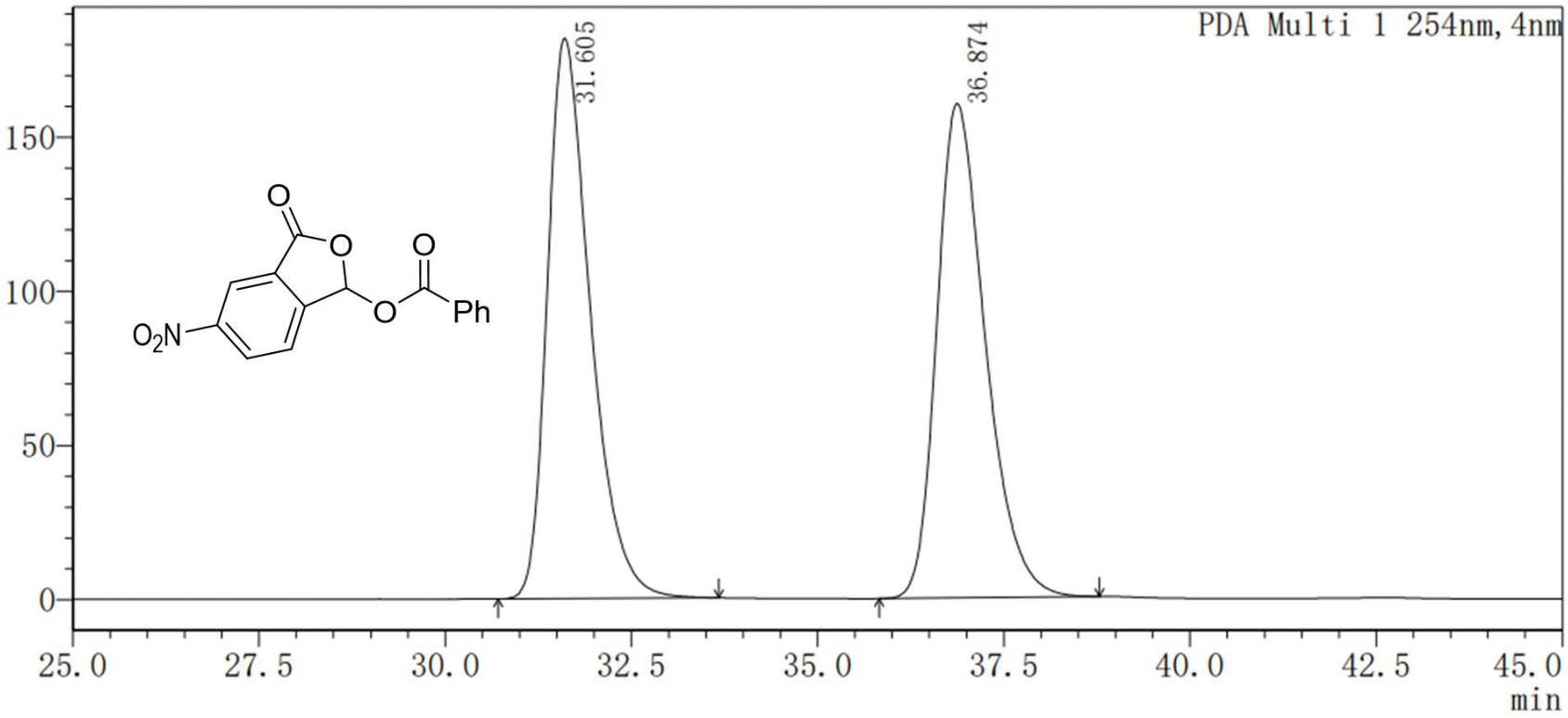

8.79
8.79
8.66
8.65
8.64
8.63
8.07
8.06
8.06
8.05
8.04
8.04
8.04
7.93
7.91
7.77
7.67
7.67
7.66
7.65
7.65
7.64
7.63
7.63
7.63
7.50
7.50
7.48
7.46
7.46




8.79
8.79
8.66
8.65
8.64
8.63
8.06
8.06
8.04
8.04
7.93
7.91
7.77
7.65
7.50
7.48
7.46
0.96
0.98
2.02
1.00
1.01
1.00
2.01
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
f1 (ppm)


0.96
0.98
2.02
1.00
1.01
1.00
2.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

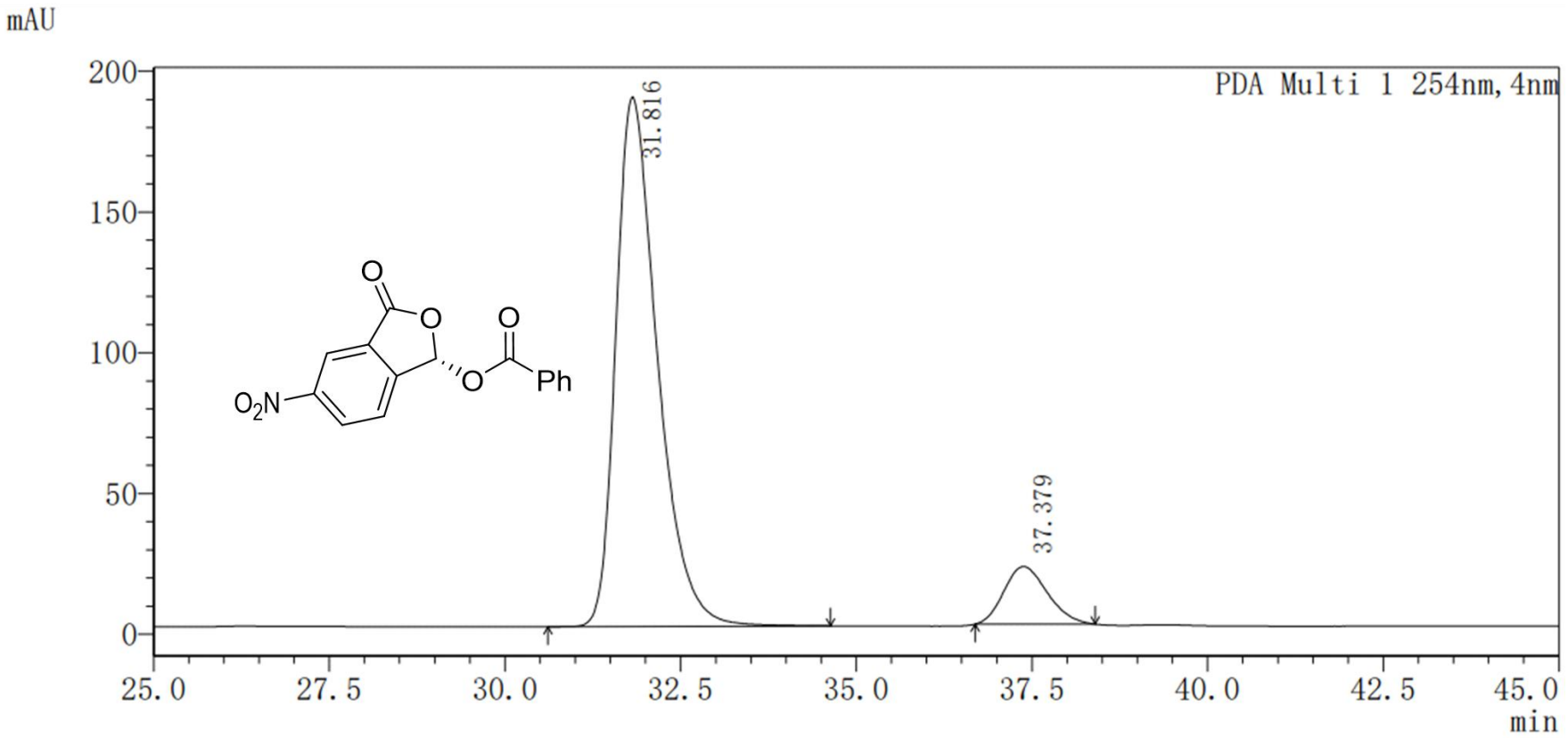

165.43
164.69
150.48
149.45
134.53
130.27
129.84
128.80
128.59
127.77
125.37
121.42
92.83
O
O
O
O
O
N+
O-
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

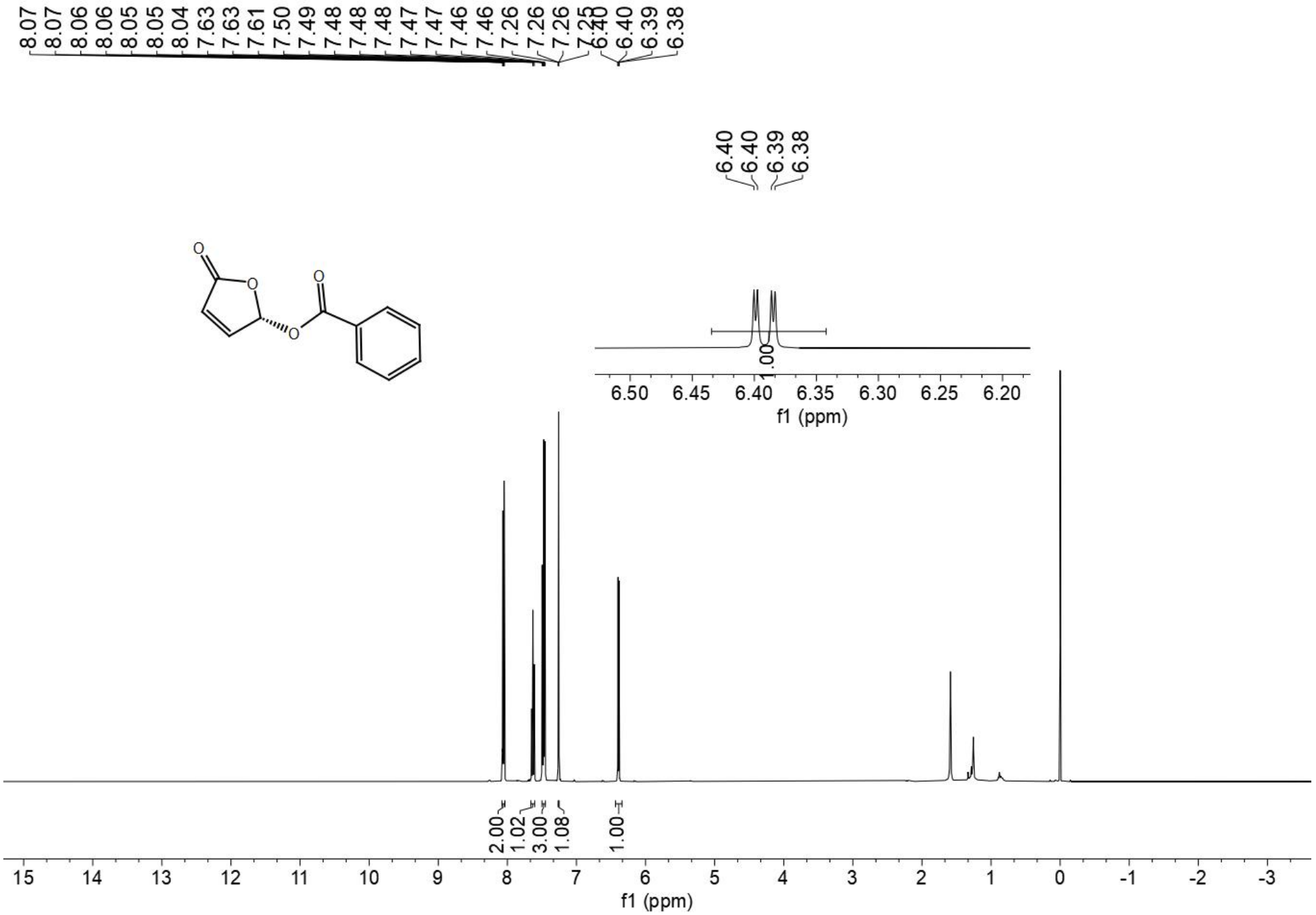
Peak#	Ret. Time	Height	Area	Area%
1	31.605	181695	7311371	50.146
2	36.874	160337	7268813	49.854
Total		342033	14580184	100.000

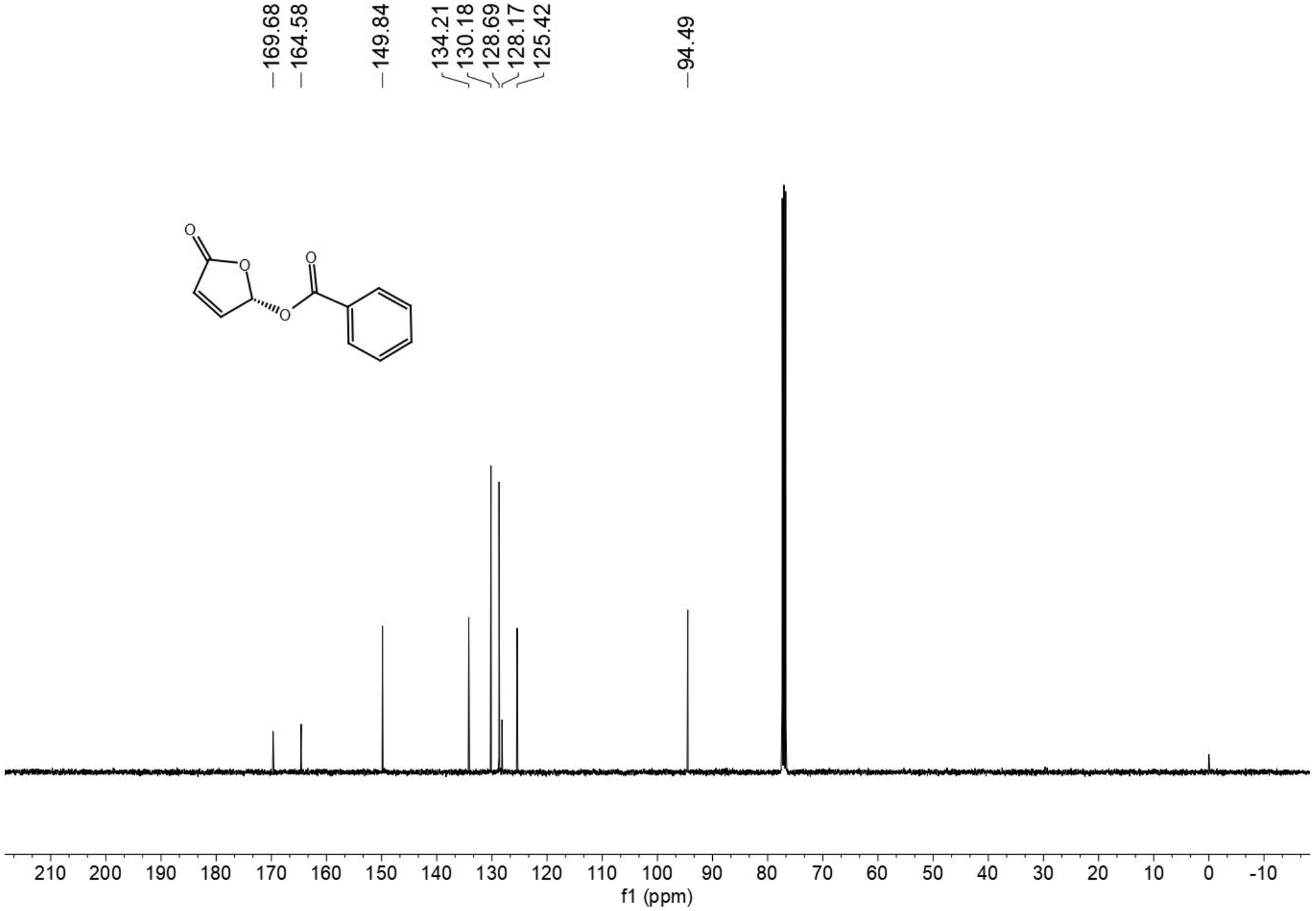


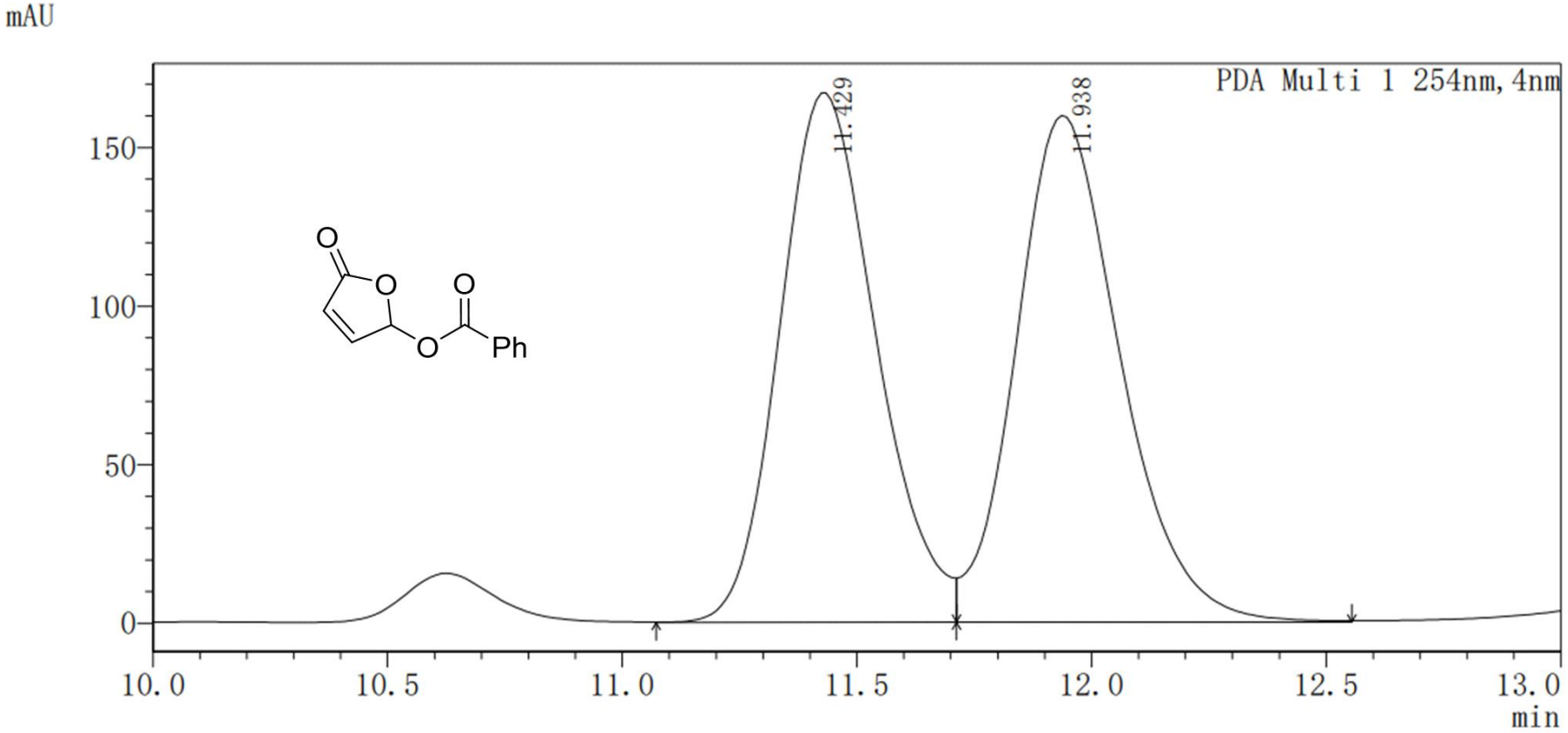
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	31.816	188095	7734459	89.786
2	37.379	20470	879879	10.214
Total		208564	8614338	100.000


8.07
8.07
8.06
8.06
8.05
8.05
8.04
7.63
7.63
7.61
7.50
7.49
7.48
7.48
7.48
7.47
7.47
7.46
7.46
7.26
7.26
7.26
7.25
6.40
6.40
6.39
6.38
6.40
6.40
6.39
6.38
1.00
6.50 6.45 6.40 6.35 6.30 6.25 6.20
f1 (ppm)
2.00
1.02
3.00
1.08
1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

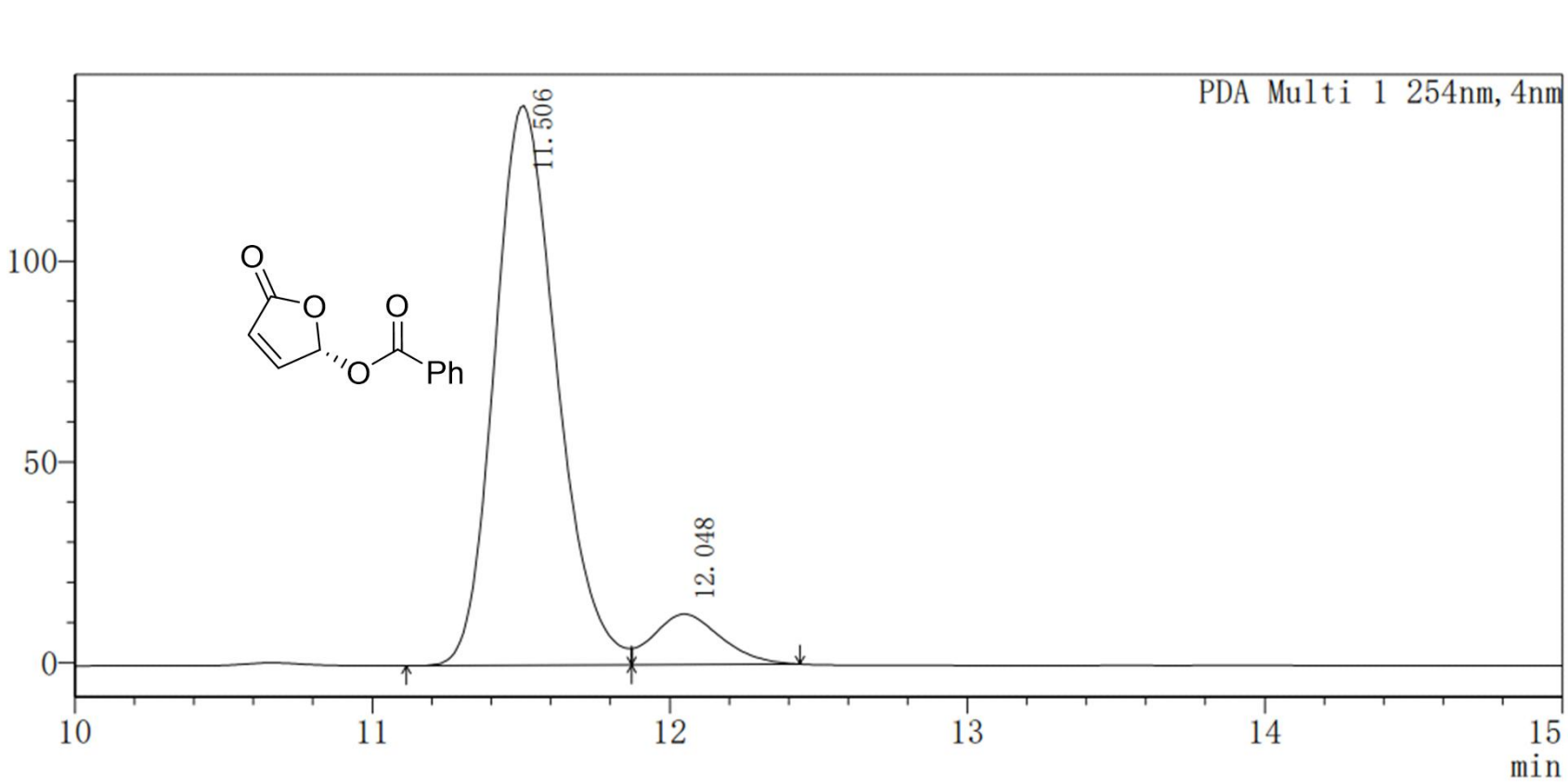

169.68
164.58
149.84
134.21
130.18
128.69
128.17
125.42
94.49
O
O
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

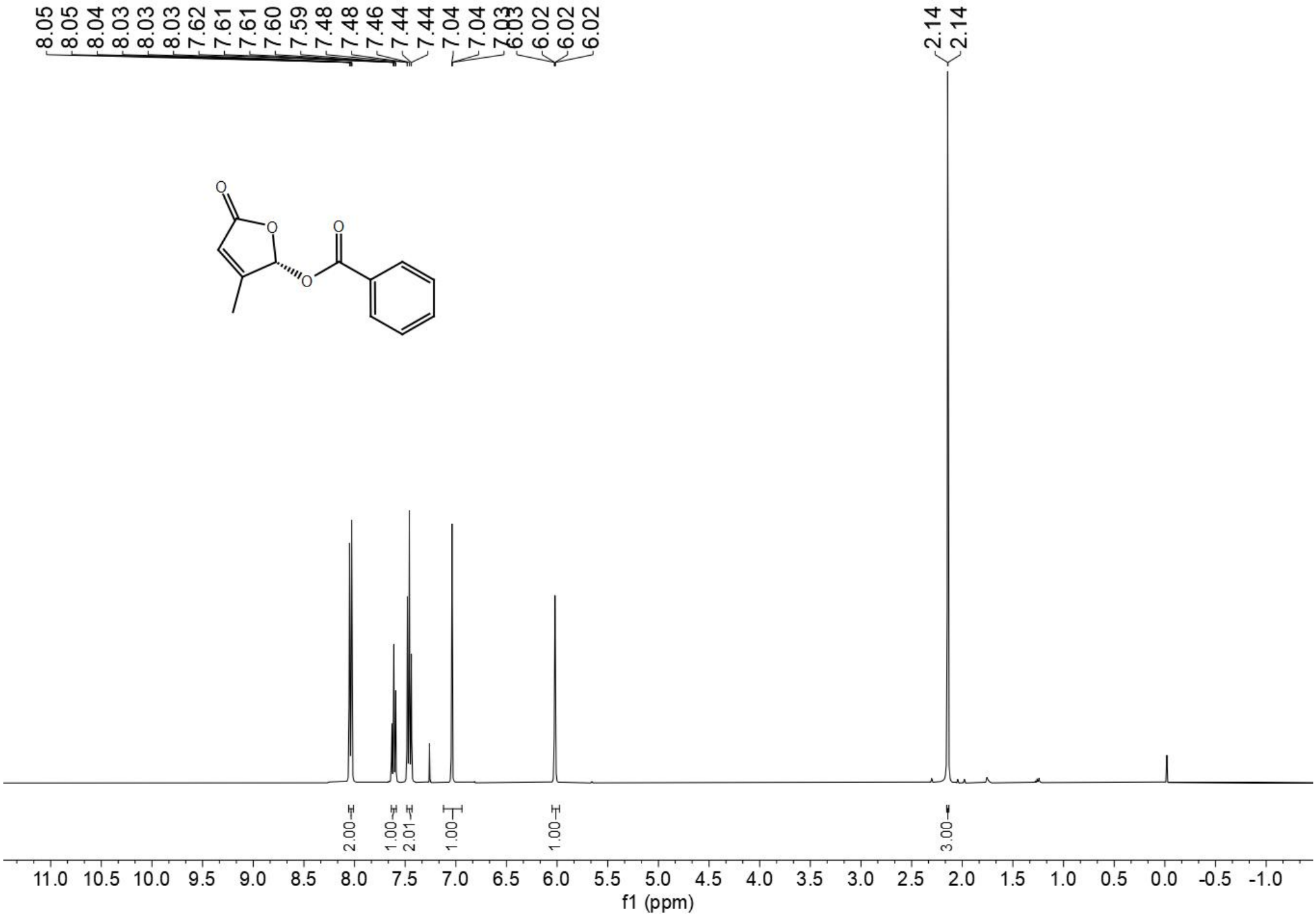
Peak#	Ret. Time	Height	Area	Area%
1	11.429	166842	2389196	49.213
2	11.938	159784	2465614	50.787
Total		326626	4854809	100.000

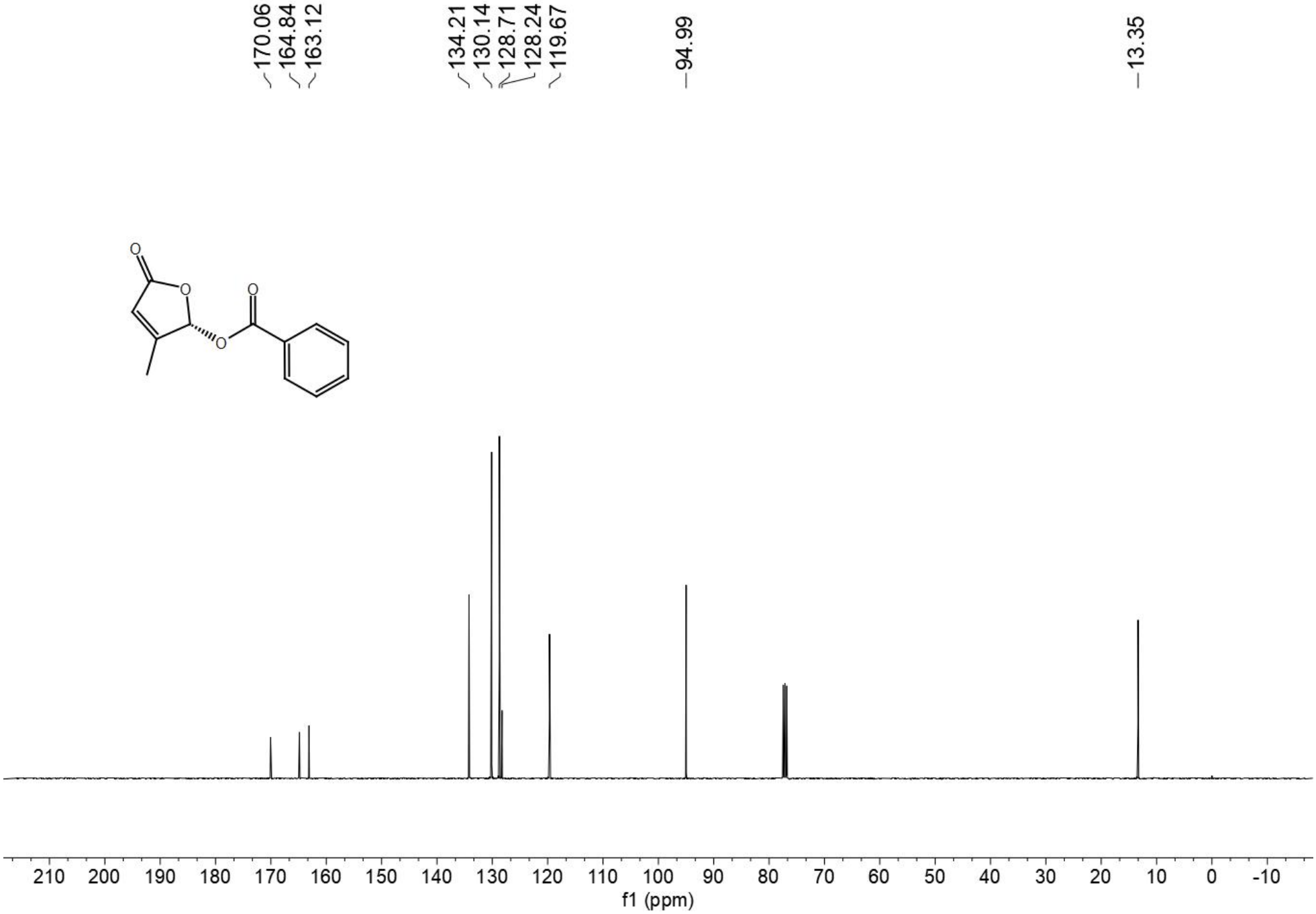


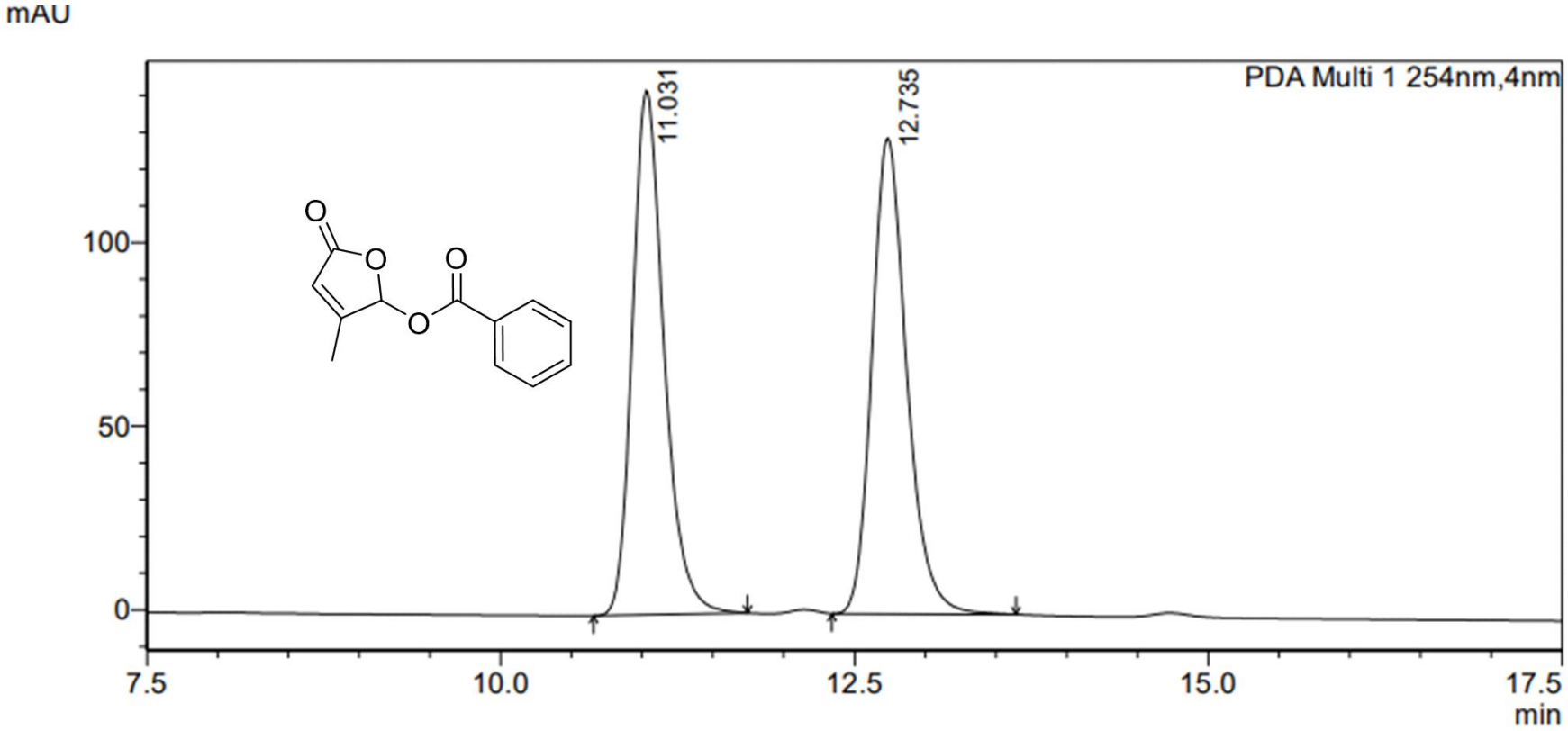
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	11.506	139350	2030731	91.128
2	12.048	12594	197701	8.872
Total		151944	2228432	100.000


8.05
8.05
8.04
8.03
8.03
8.03
7.62
7.61
7.61
7.60
7.59
7.48
7.48
7.46
7.44
7.44
7.04
7.04
7.03
6.03
6.02
6.02
6.02
2.14
2.14
O
O
O
O
2.00
1.00
2.01
1.00
1.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

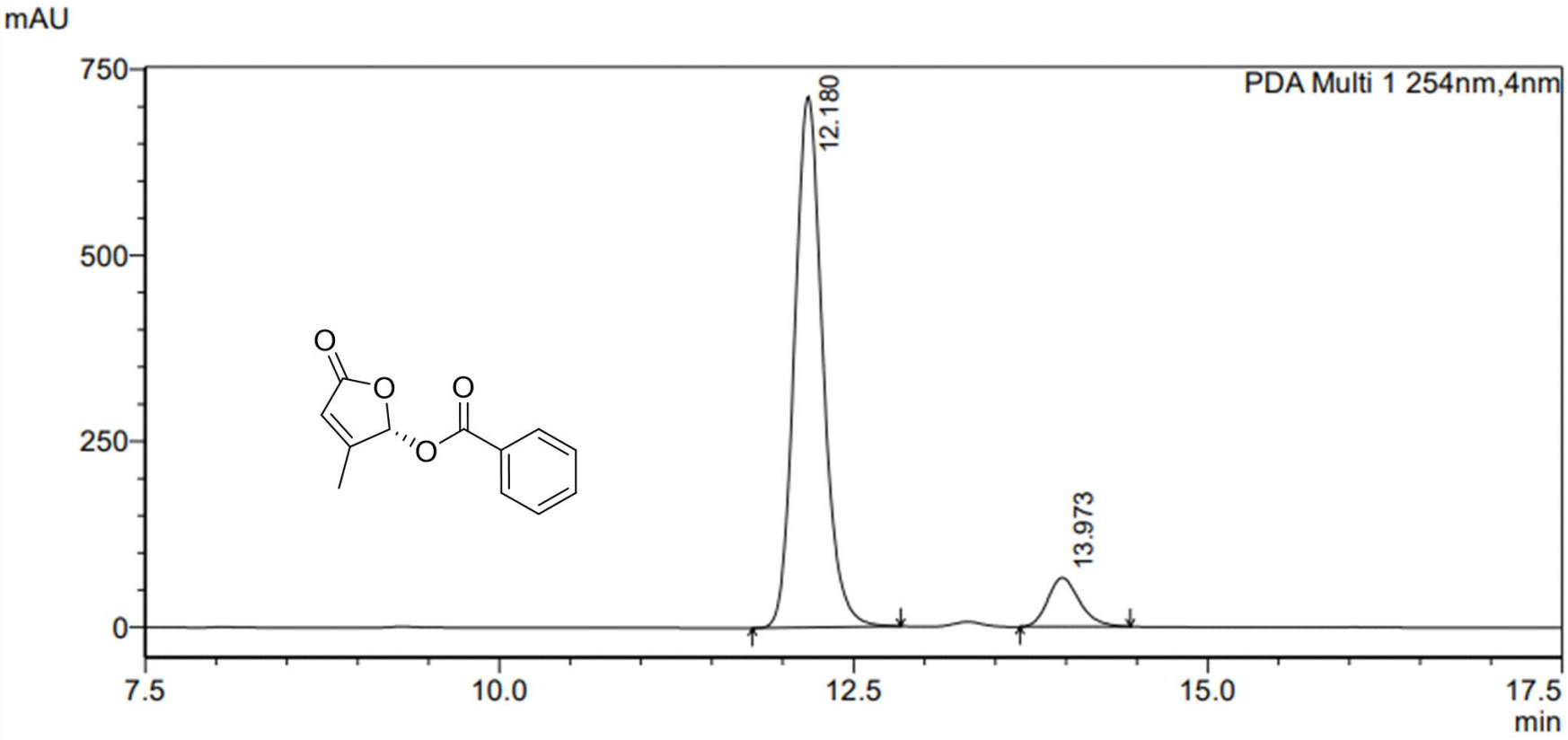

170.06
164.84
163.12
134.21
130.14
128.71
128.24
119.67
94.99
13.35
O
O
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

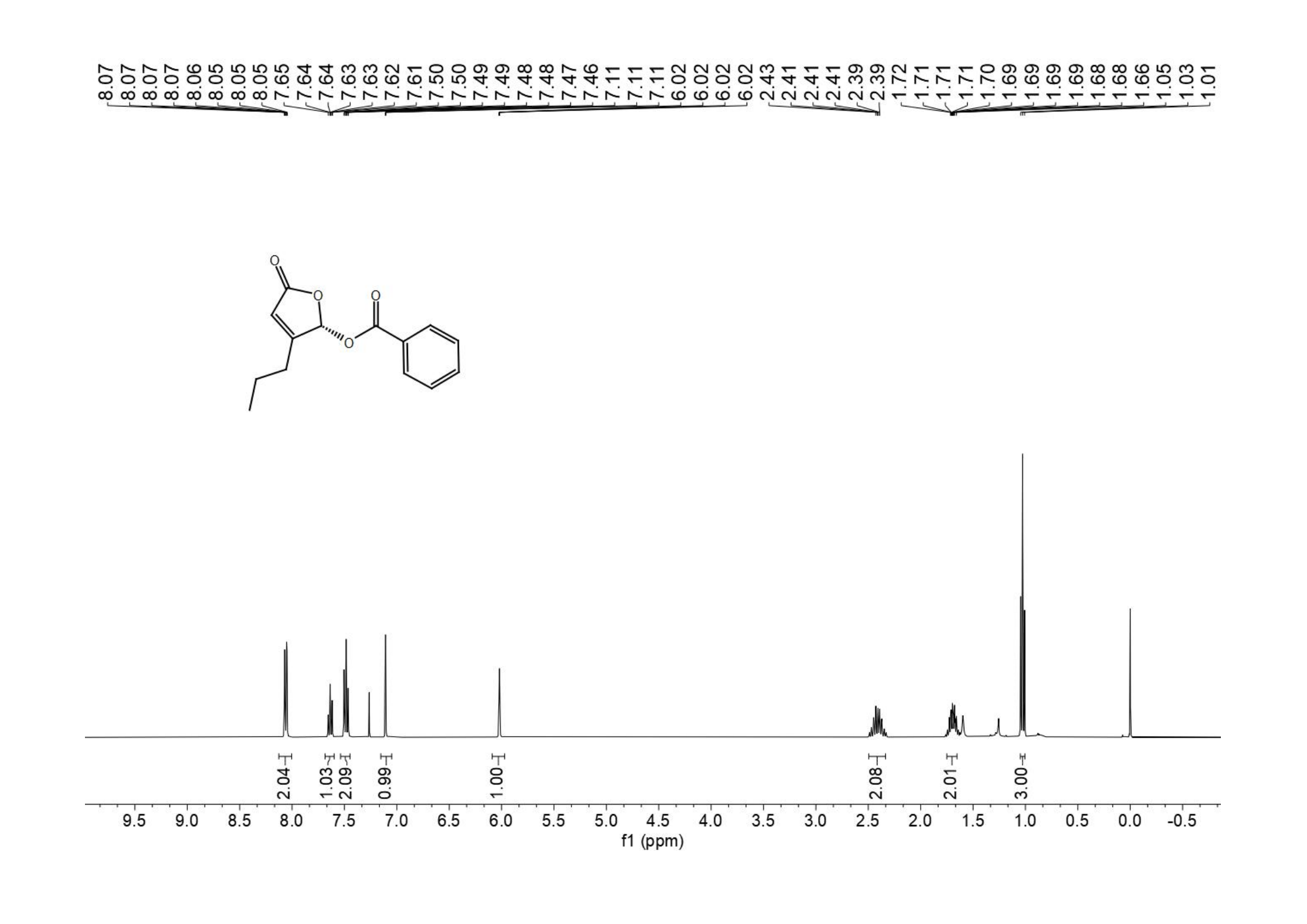
Peak#	Ret. Time	Height	Area	Area%
1	11.031	142632	2220962	50.071
2	12.735	129532	2214645	49.929
Total		272164	4435606	100.000

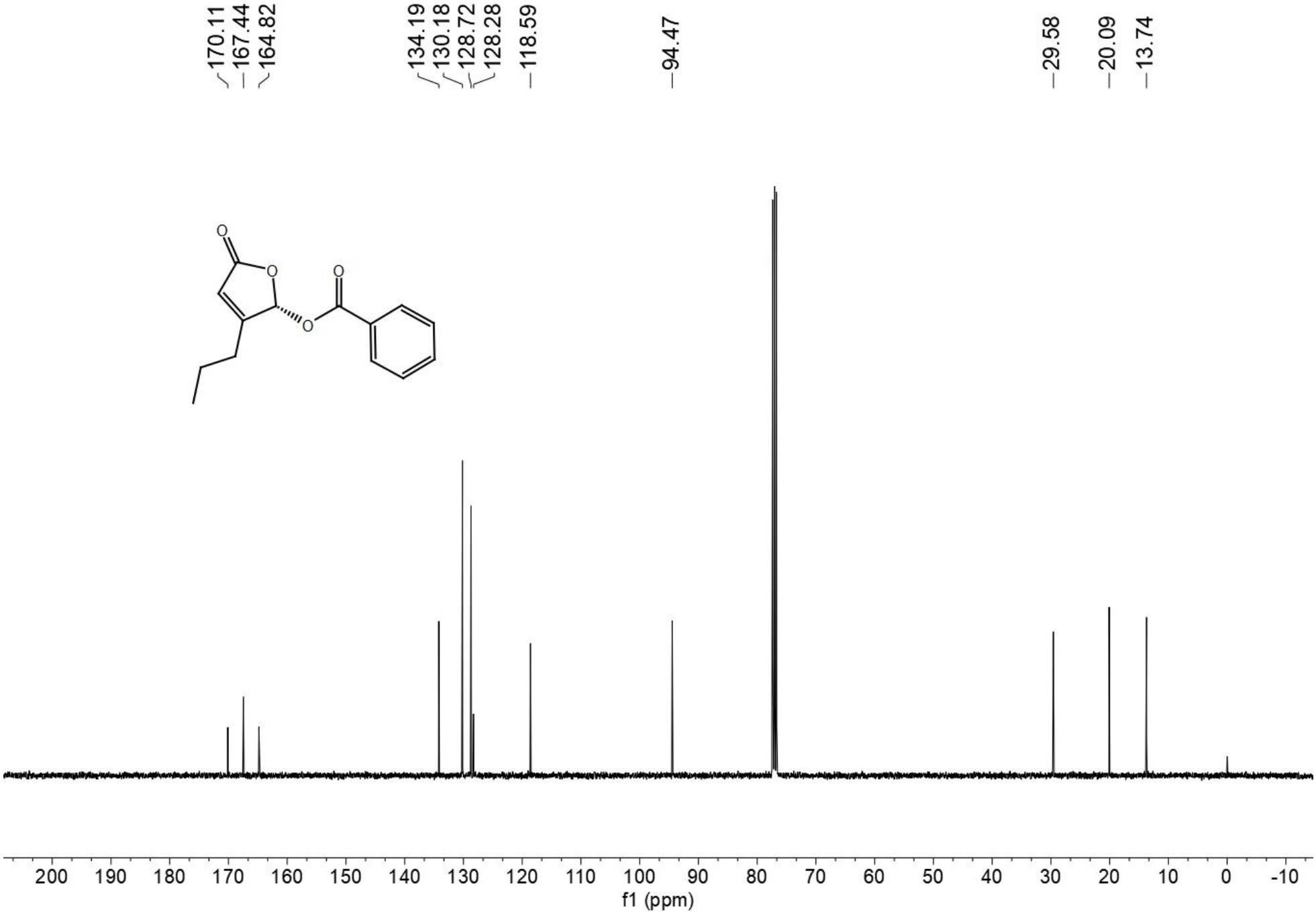


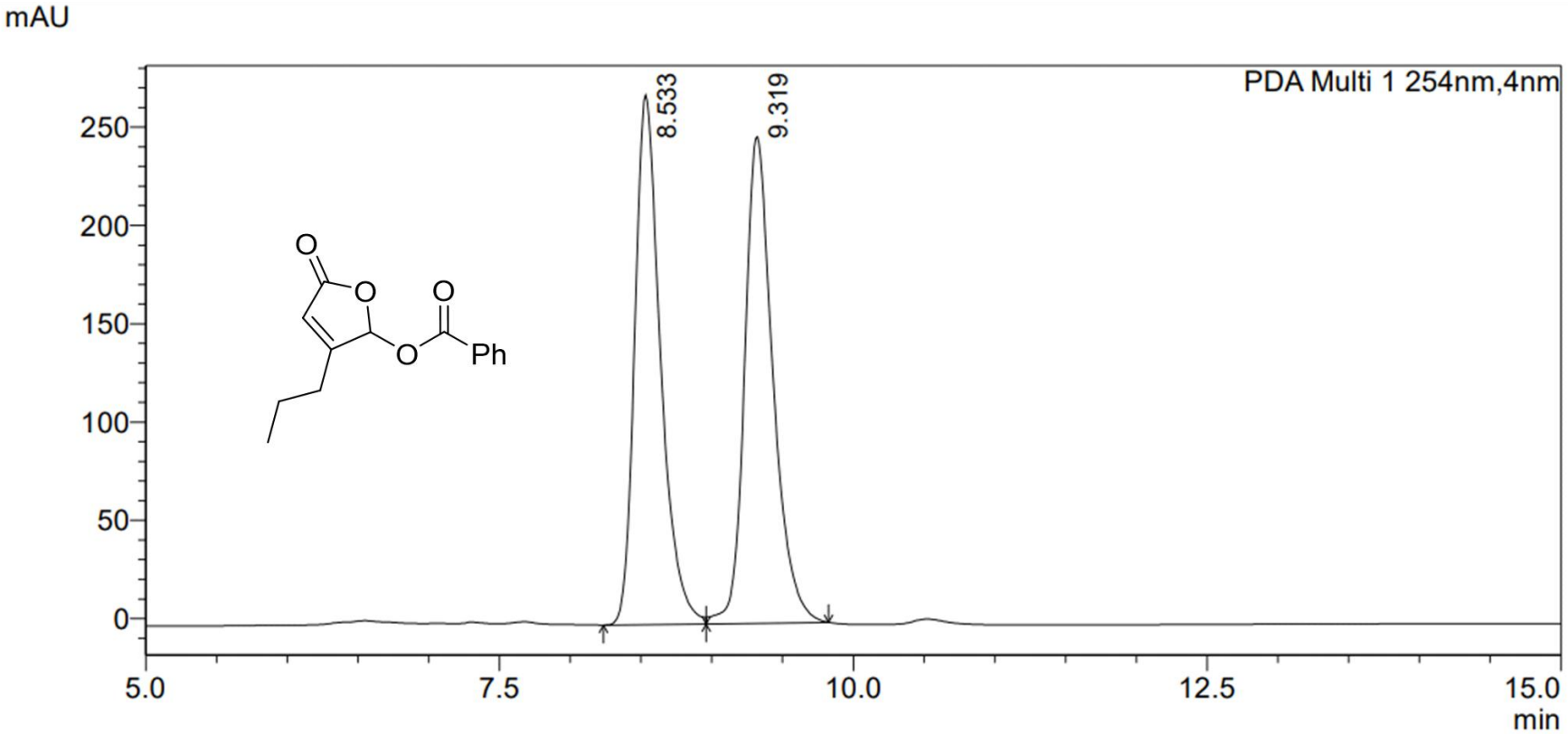
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	12.180	713610	9892012	90.586
2	13.973	65917	1028014	9.414
Total		779527	10920025	100.000


8.07 8.07 8.07 8.07 8.06 8.05 8.05 8.05 7.65 7.64 7.64 7.63 7.63 7.62 7.61 7.50 7.50 7.49 7.49 7.48 7.48 7.47 7.46 7.11 7.11 7.11 6.02 6.02 6.02 6.02 2.43 2.41 2.41 2.41 2.39 2.39 1.72 1.71 1.71 1.71 1.70 1.69 1.69 1.69 1.69 1.68 1.68 1.66 1.05 1.03 1.01
O
O
O
O
2.04
1.03
2.09
0.99
1.00
2.08
2.01
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

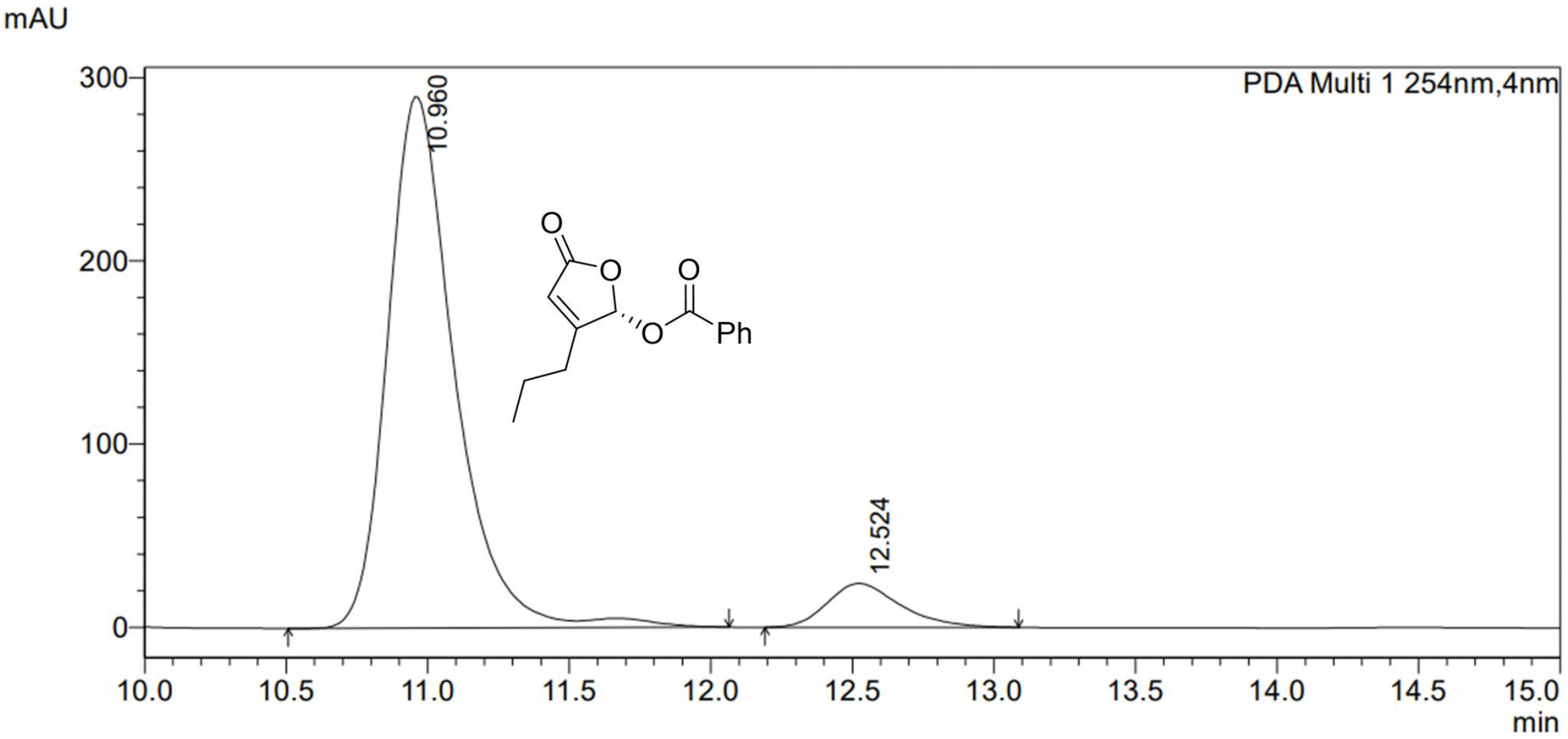

170.11
167.44
164.82
134.19
130.18
128.72
128.28
118.59
94.47
29.58
20.09
13.74
O
O
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

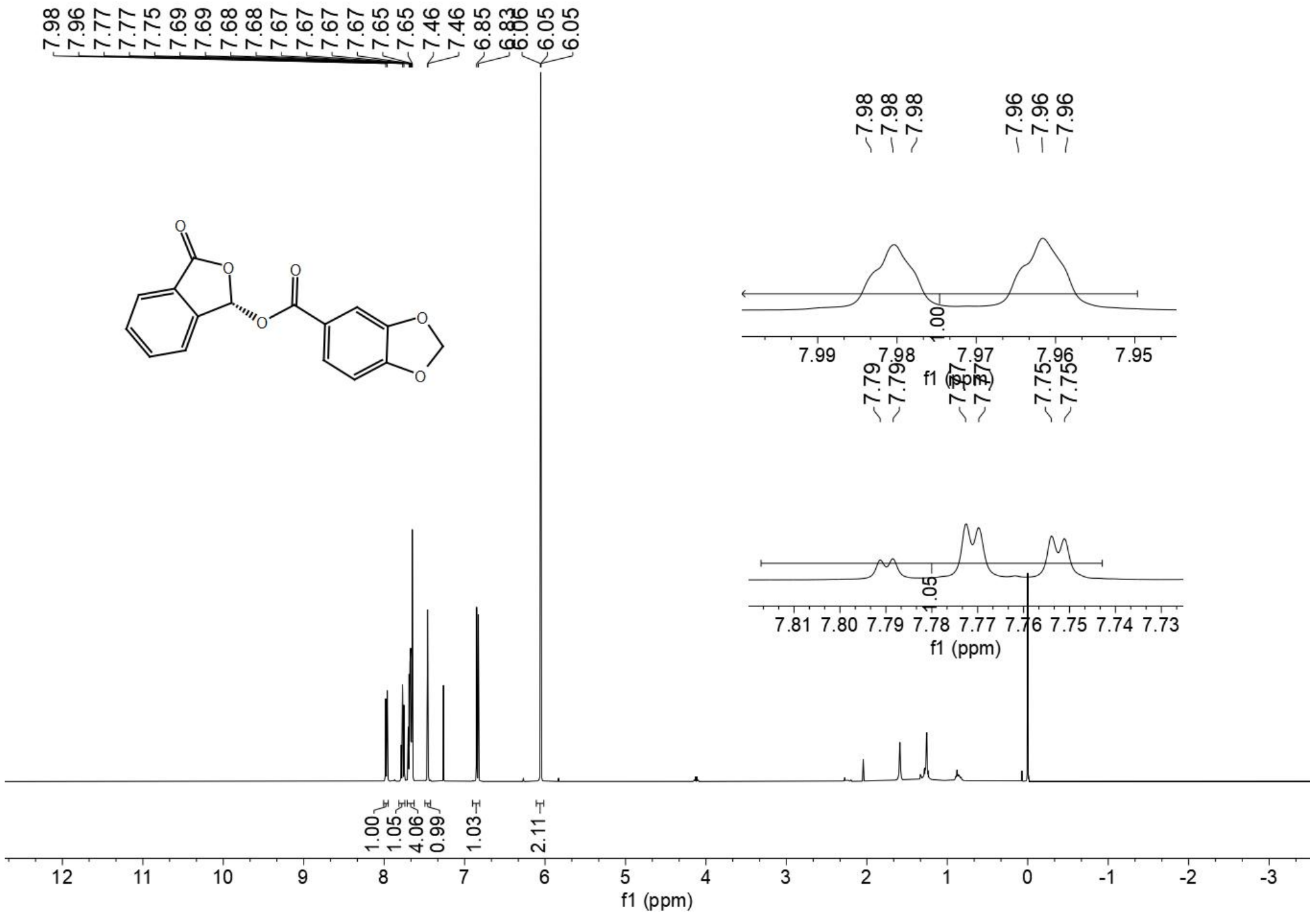
Peak#	Ret. Time	Height	Area	Area%
1	8.533	269333	3422259	49.788
2	9.319	247372	3451434	50.212
Total		516705	6873693	100.000

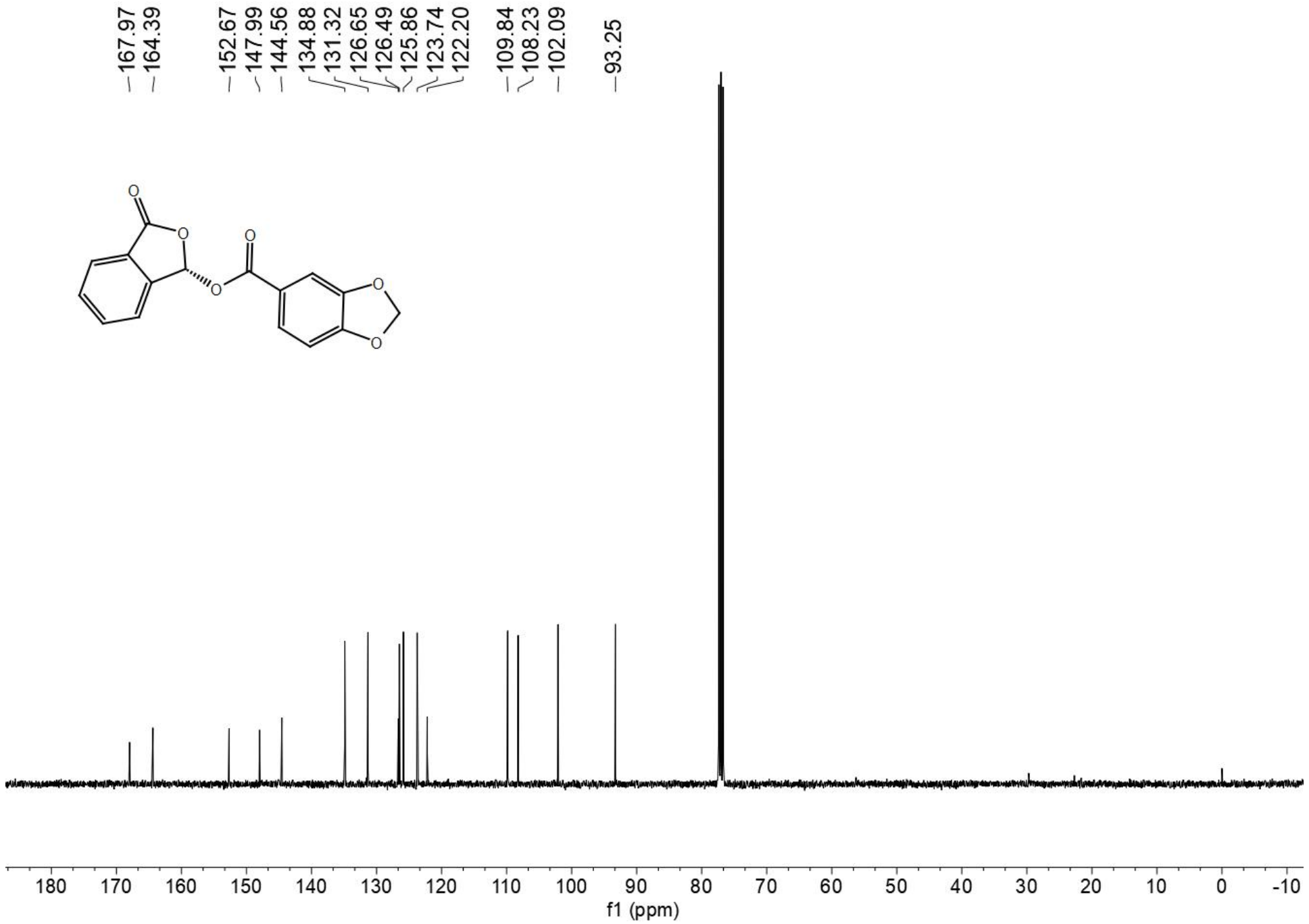


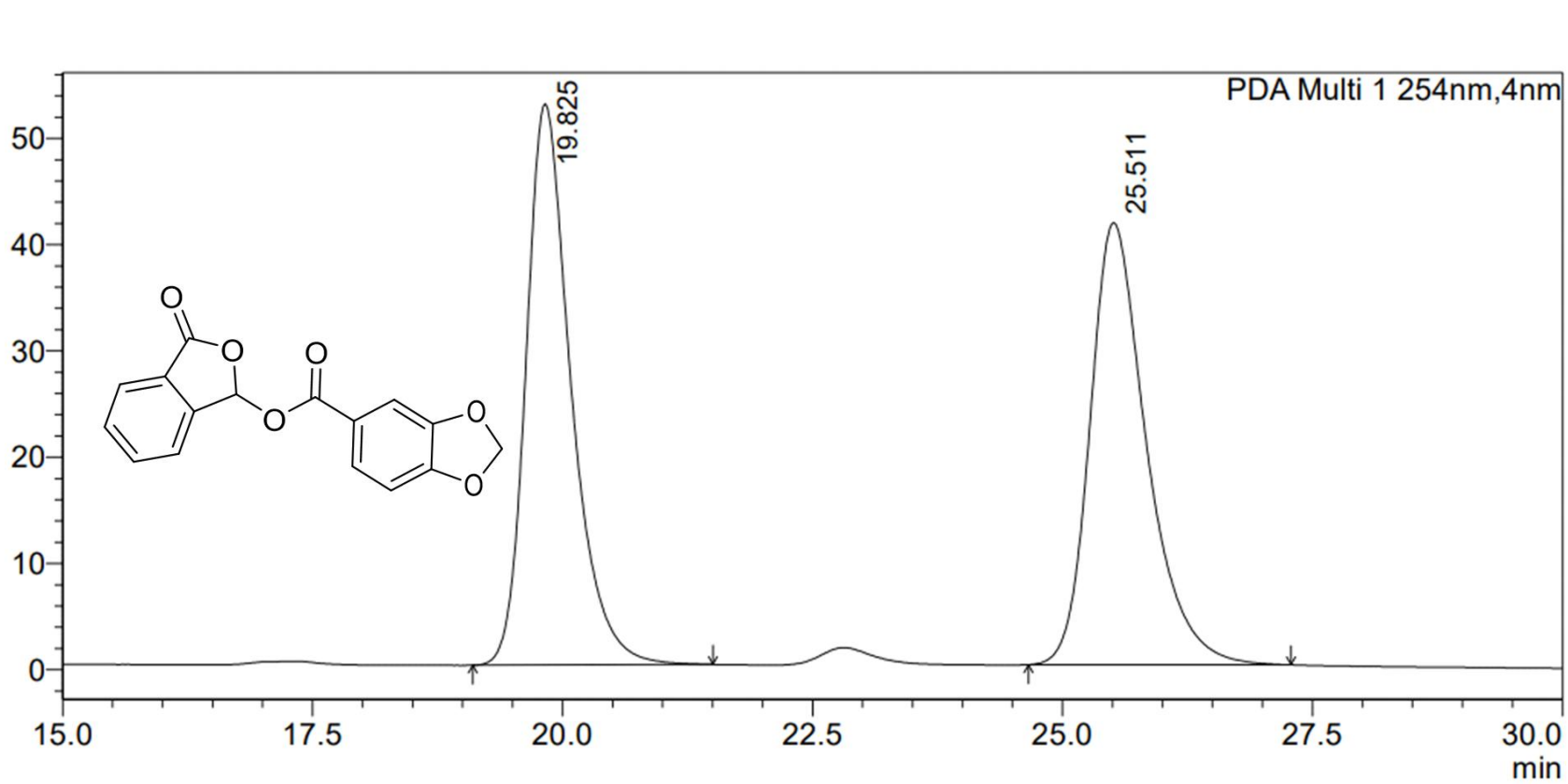
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	10.960	289836	4780946	91.753
2	12.524	23889	429725	8.247
Total		313725	5210671	100.000


7.98
7.96
7.77
7.77
7.75
7.69
7.69
7.68
7.68
7.67
7.67
7.67
7.67
7.65
7.65
7.46
7.46
6.85
6.83
6.06
6.05
6.05
7.98
7.98
7.98
7.96
7.96
7.96
1.00
7.99
7.98
7.97
7.96
7.95
f1 (ppm)
7.79
7.79
7.77
7.77
7.75
7.75
1.05
7.81 7.80 7.79 7.78 7.77 7.76 7.75 7.74 7.73
f1 (ppm)
1.00
1.05
4.06
0.99
1.03
2.11
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

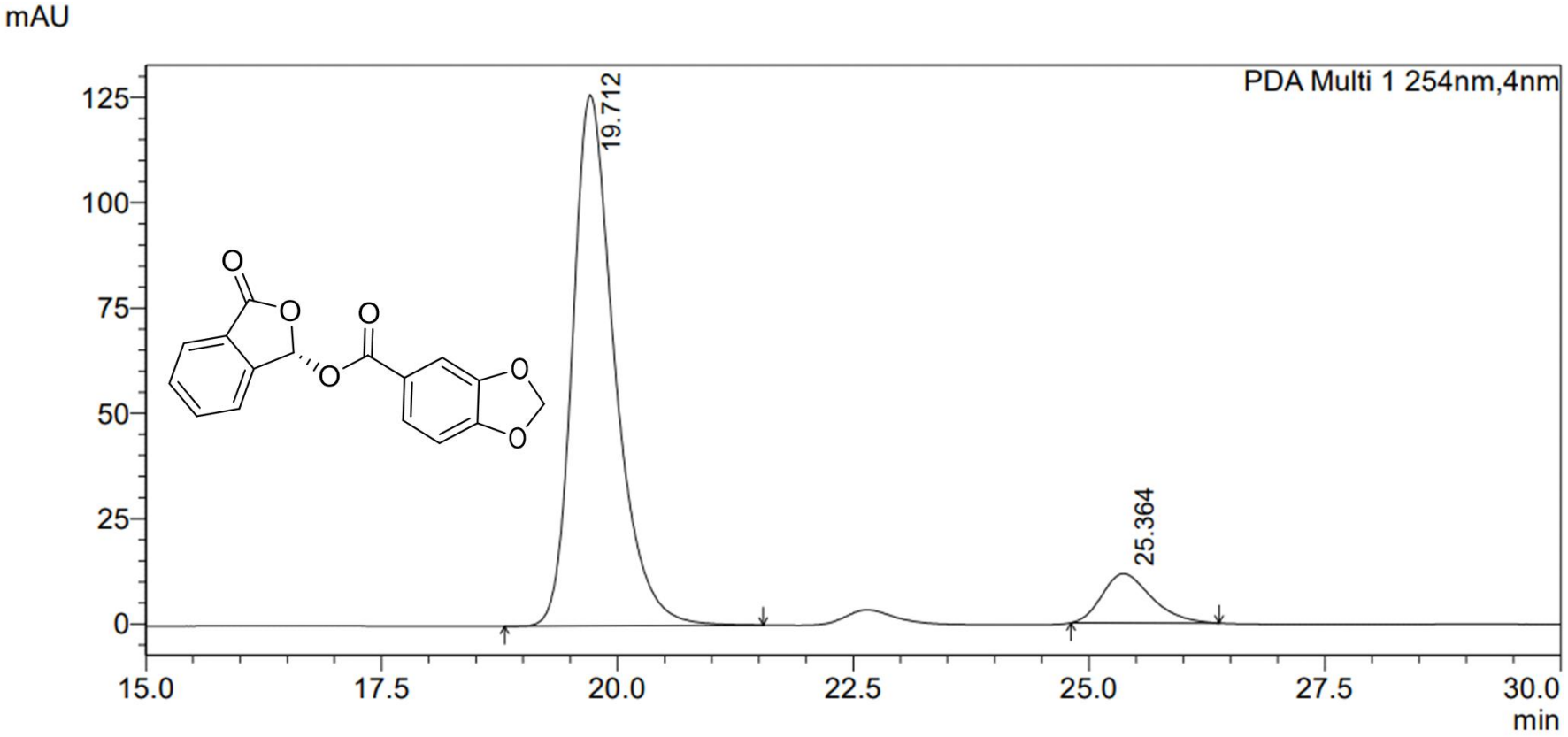

167.97
164.39
152.67
147.99
144.56
134.88
131.32
126.65
126.49
125.86
123.74
122.20
109.84
108.23
102.09
93.25
O
O
O
O
O
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

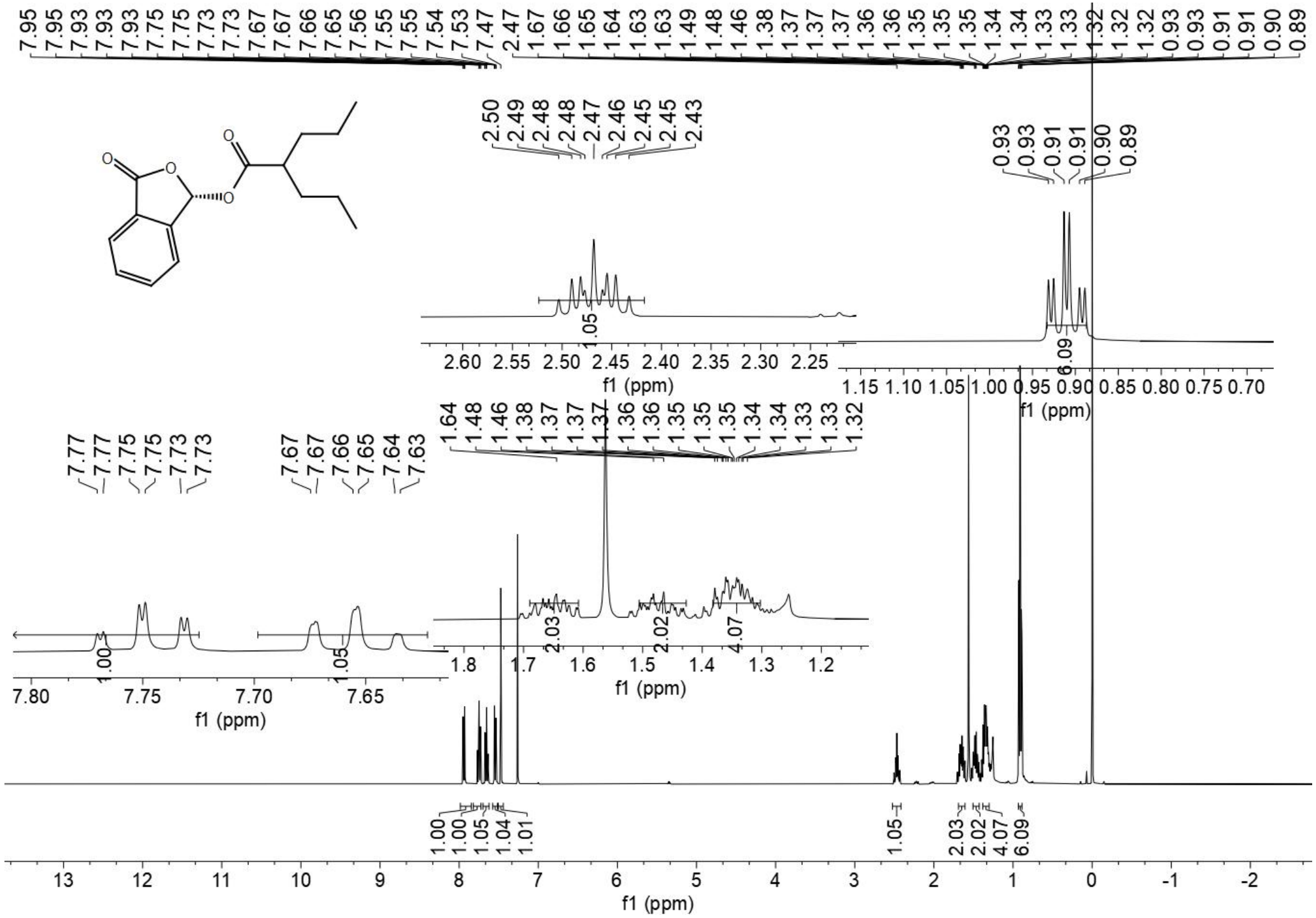
Peak#	Ret. Time	Height	Area	Area%
1	19.825	52775	1654052	50.294
2	25.511	41589	1634701	49.706
Total		94365	3288753	100.000

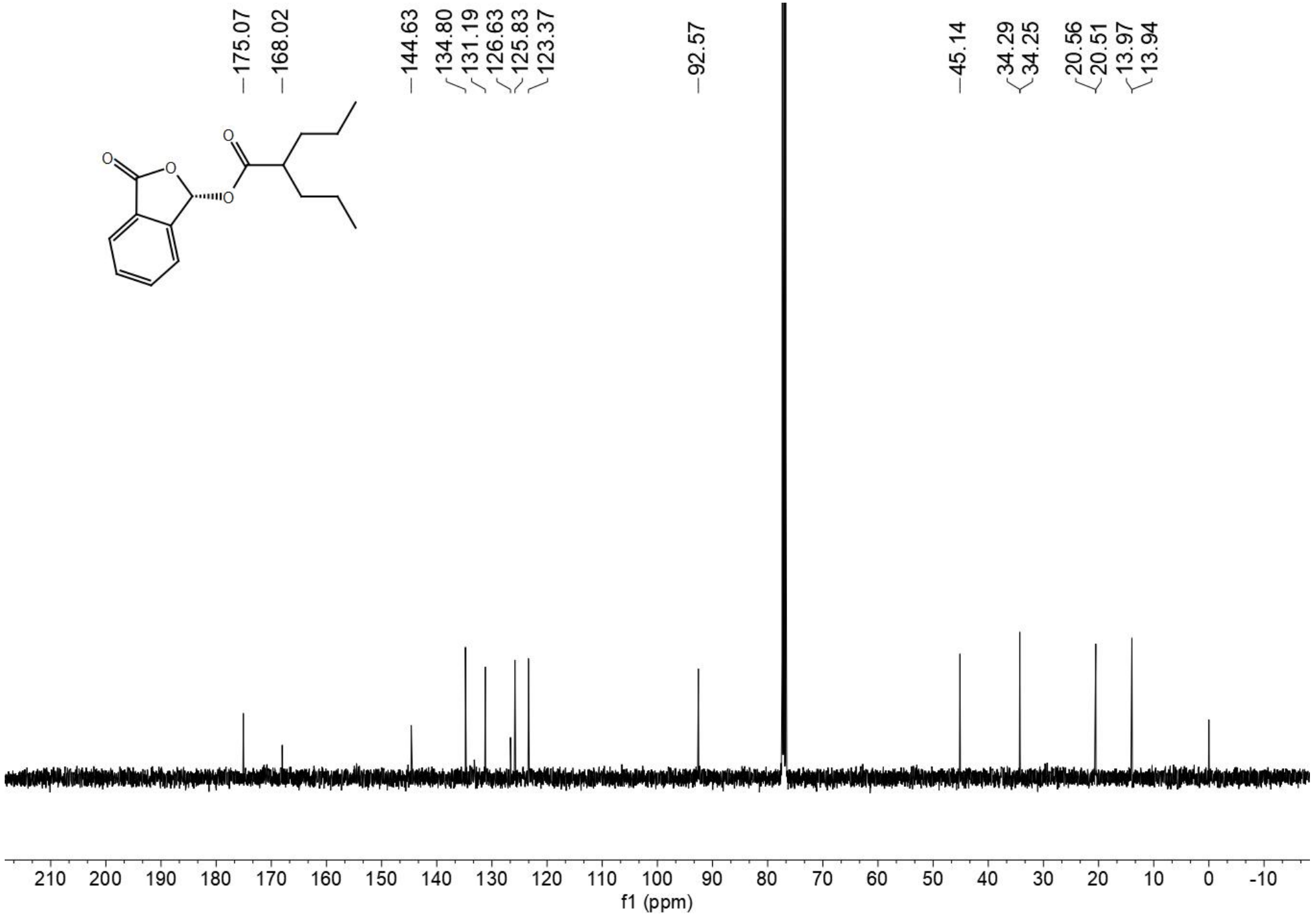


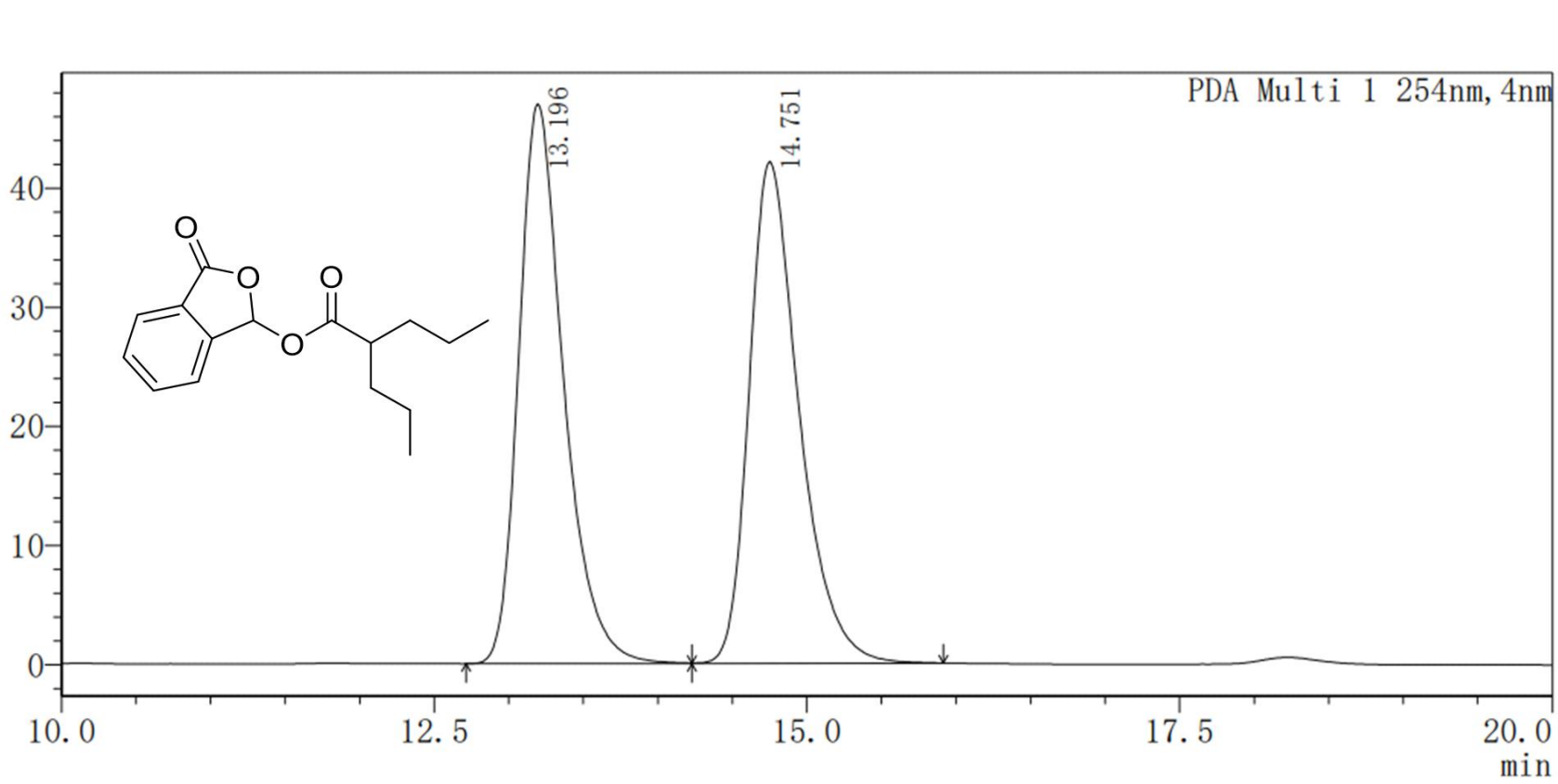
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	19.712	126053	3908764	90.197
2	25.364	11666	424812	9.803
Total		137719	4333576	100.000


7.95 7.95 7.93 7.93 7.93 7.75 7.75 7.73 7.73 7.67 7.67 7.66 7.65 7.56 7.55 7.55 7.54 7.53 7.47
2.47 1.67 1.66 1.65 1.64 1.63 1.63 1.49 1.48 1.46 1.38 1.37 1.37 1.37 1.36 1.36 1.35 1.35 1.35 1.34 1.34 1.33 1.33 1.32 1.32 1.32 0.93 0.93 0.91 0.91 0.90 0.89
O
O
O
O
2.50 2.49 2.48 2.48 2.47 2.46 2.45 2.45 2.43
1.05
2.60 2.55 2.50 2.45 2.40 2.35 2.30 2.25
f1 (ppm)
0.93 0.93 0.91 0.91 0.90 0.89
6.09
1.15 1.10 1.05 1.00 0.95 0.90 0.85 0.80 0.75 0.70
f1 (ppm)
7.77 7.77 7.75 7.75 7.73 7.73
7.67 7.67 7.66 7.65 7.64 7.63
1.64 1.48 1.46 1.38 1.37 1.37 1.37 1.36 1.36 1.35 1.35 1.35 1.34 1.34 1.33 1.33 1.32
1.00
1.05
7.80 7.75 7.70 7.65
f1 (ppm)
2.03
2.02
4.07
1.8 1.7 1.6 1.5 1.4 1.3 1.2
f1 (ppm)
1.00 1.00 1.05 1.04 1.01
1.05 2.03 2.02 4.07 6.09
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)

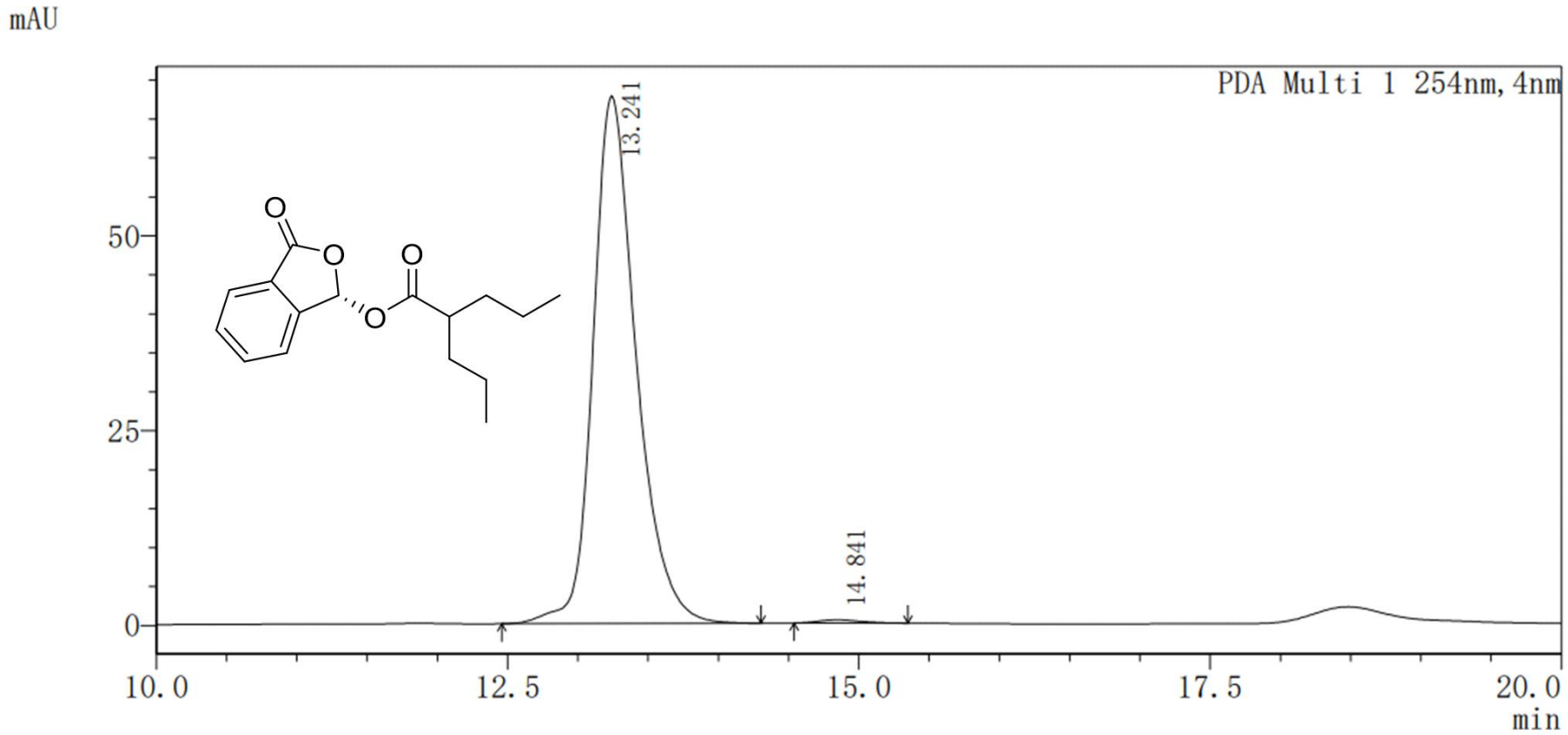

175.07
168.02
144.63
134.80
131.19
126.63
125.83
123.37
92.57
45.14
34.29
34.25
20.56
20.51
13.97
13.94
O
O
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

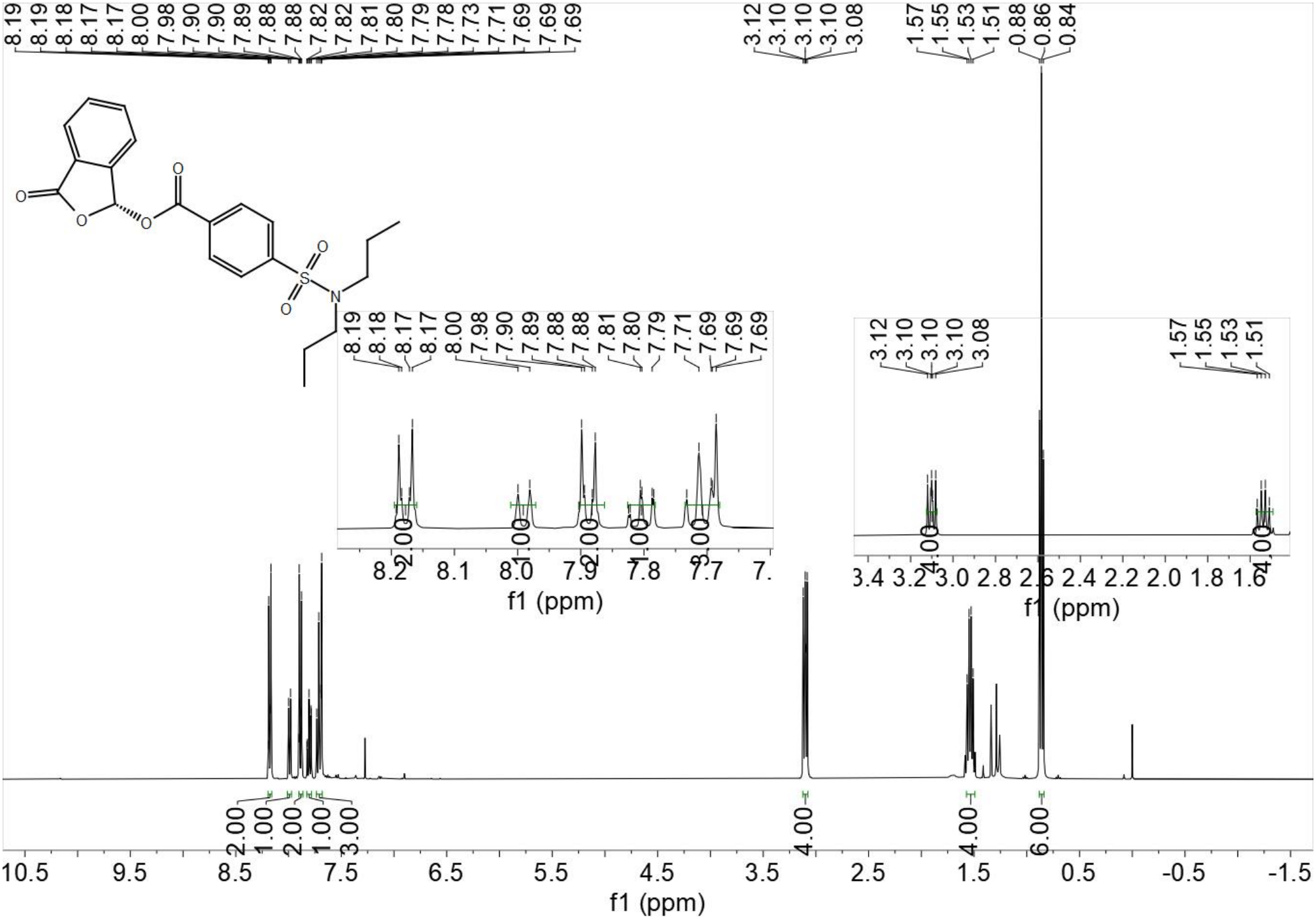
Peak#	Ret. Time	Height	Area	Area%
1	13.196	46942	983697	50.159
2	14.751	42085	977453	49.841
Total		89027	1961150	100.000

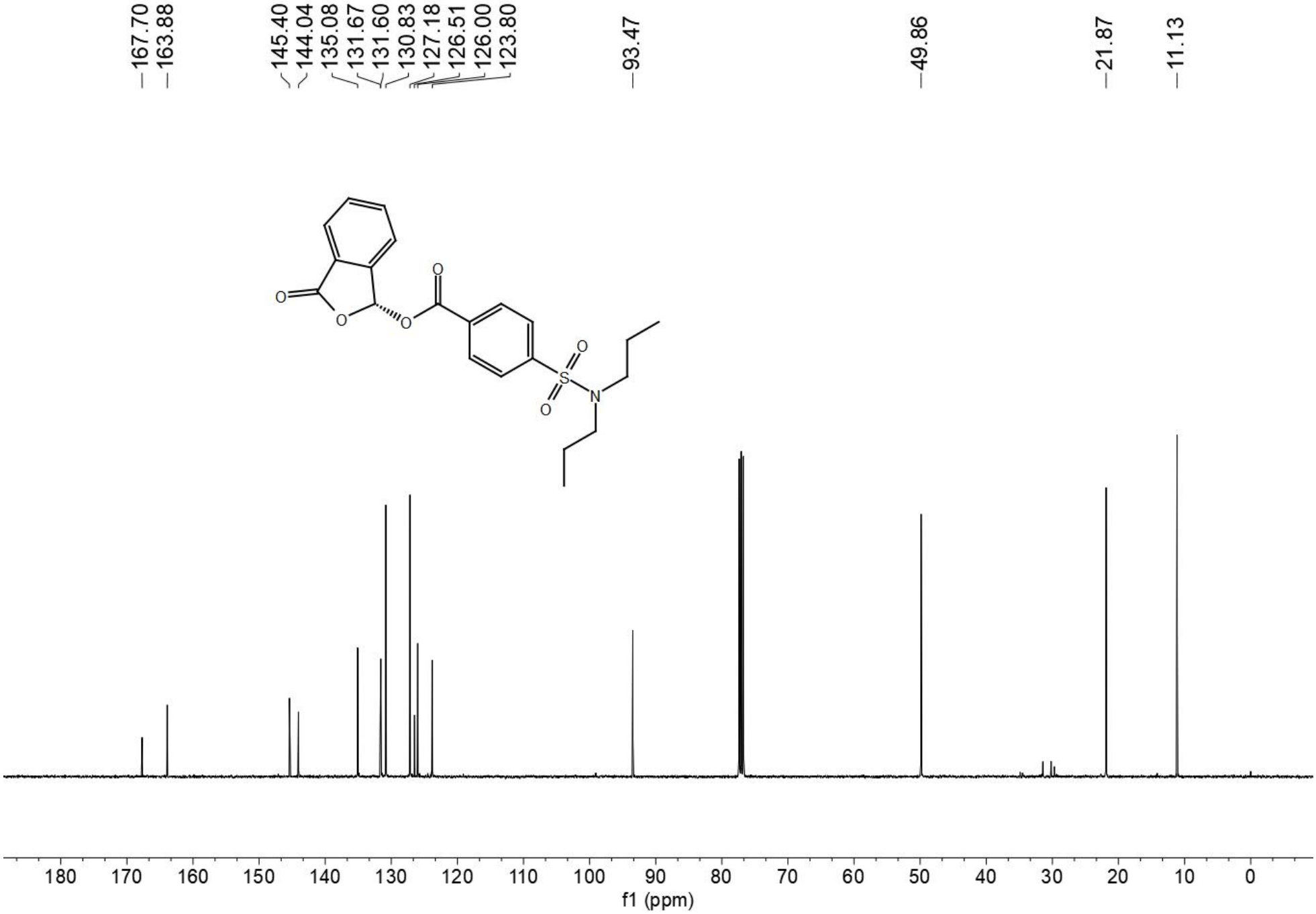


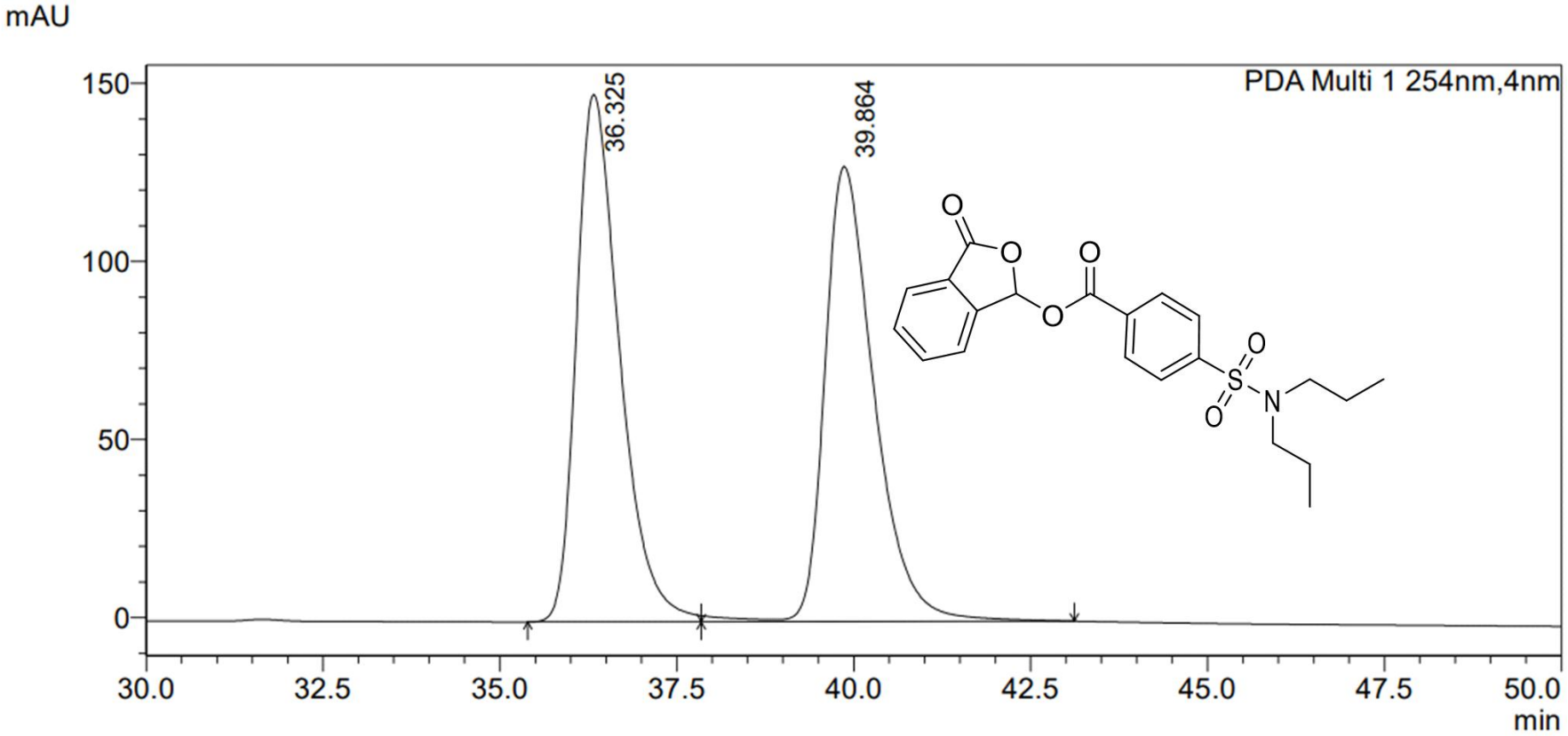
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	13.241	67718	1448655	99.403
2	14.841	414	8703	0.597
Total		68132	1457358	100.000


8.19 8.19 8.18 8.17 8.17 8.00 7.98 7.90 7.90 7.89 7.88 7.88 7.82 7.82 7.81 7.80 7.79 7.78 7.73 7.71 7.69 7.69 7.69
3.12 3.10 3.10 3.10 3.08
1.57 1.55 1.53 1.51
0.88 0.86 0.84
O
O
O
O
O
S
O
O
N
f1 (ppm)
2.00 1.00 2.00 1.00 3.00 4.00 4.00 6.00
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5 -1.5
f1 (ppm)

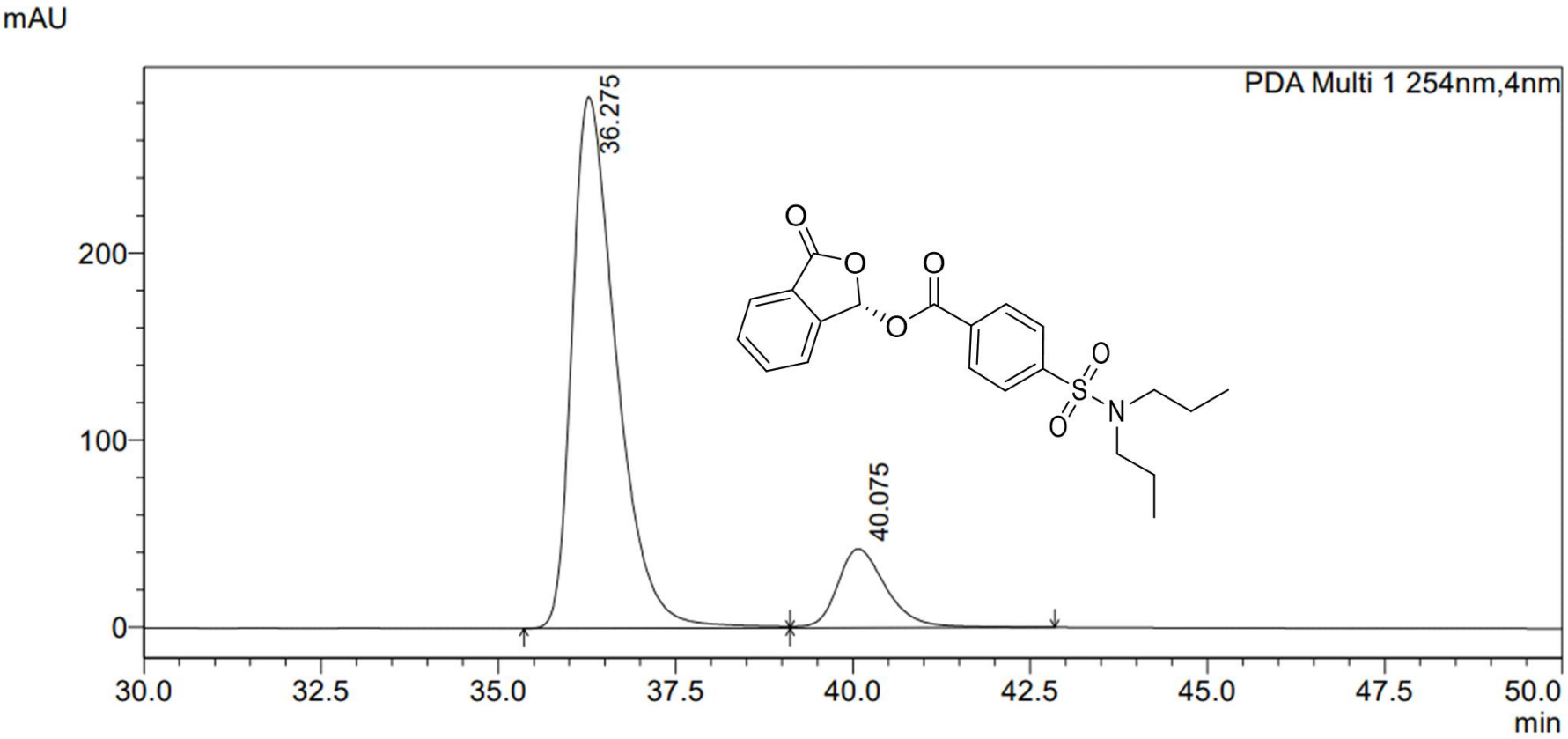

167.70
163.88
145.40
144.04
135.08
131.67
131.60
130.83
127.18
126.51
126.00
123.80
93.47
49.86
21.87
11.13
O
O
O
O
O
S
O
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

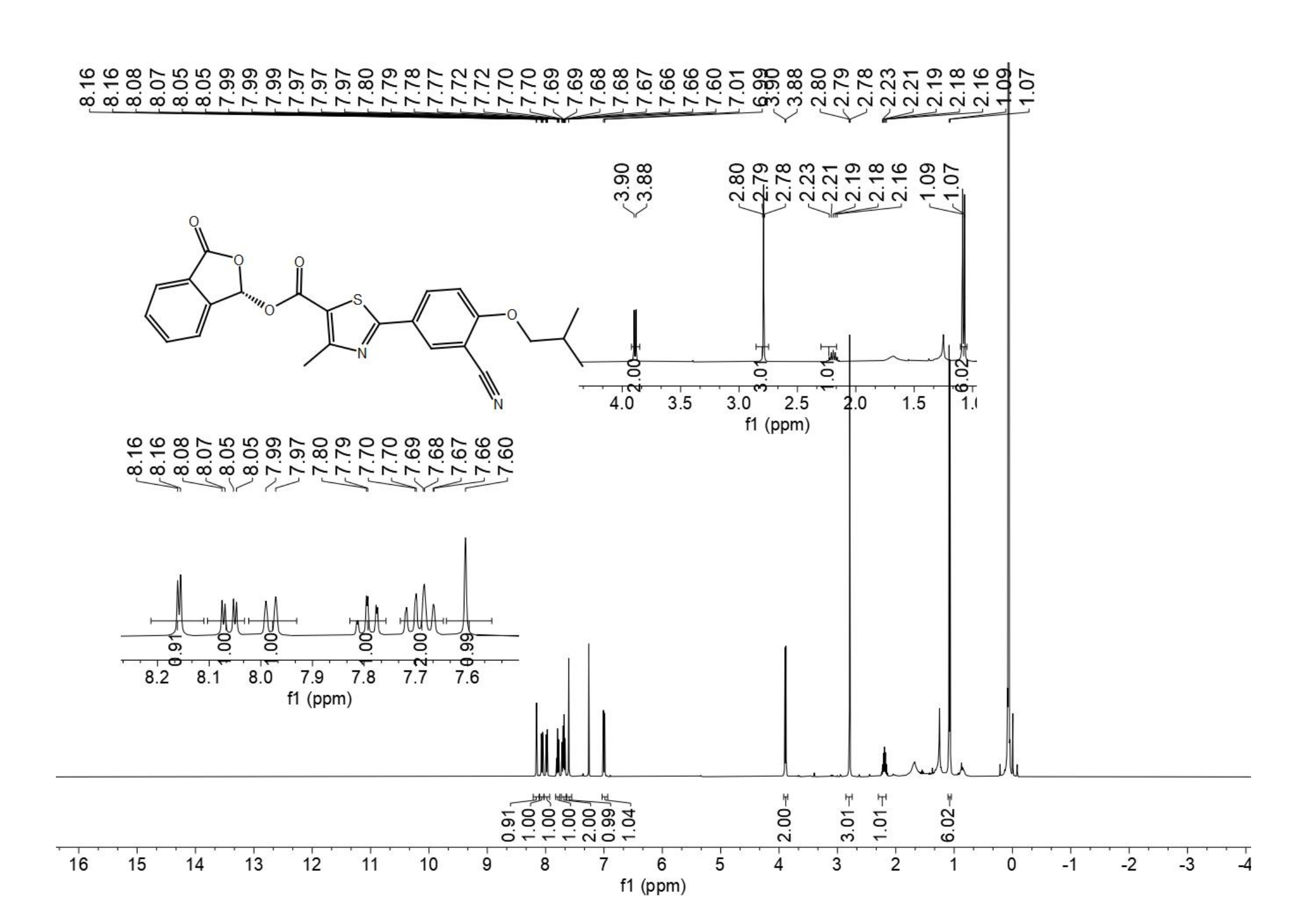
Peak#	Ret. Time	Height	Area	Area%
1	36.325	148026	6308580	50.329
2	39.864	127767	6226157	49.671
Total		275794	12534737	100.000

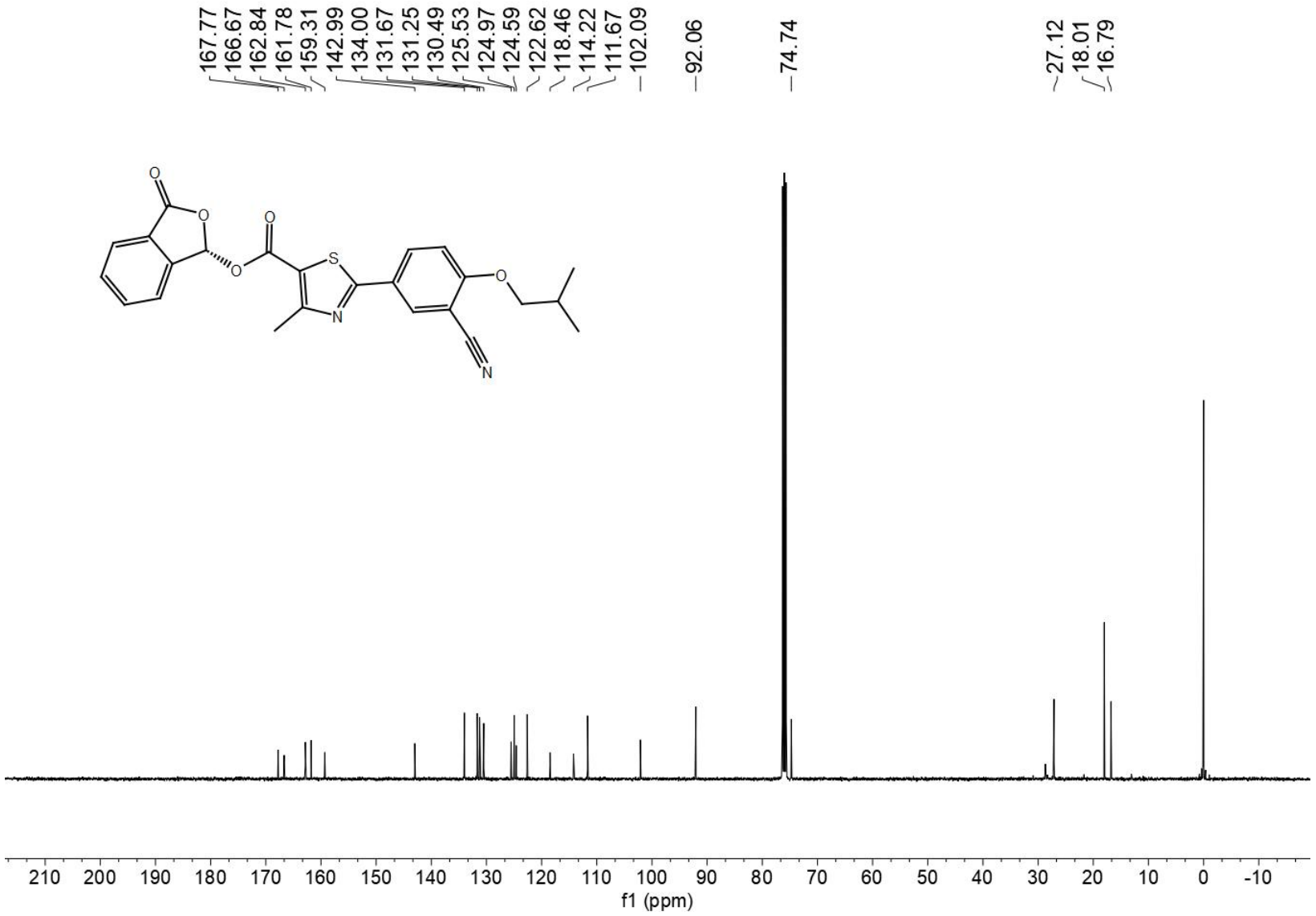


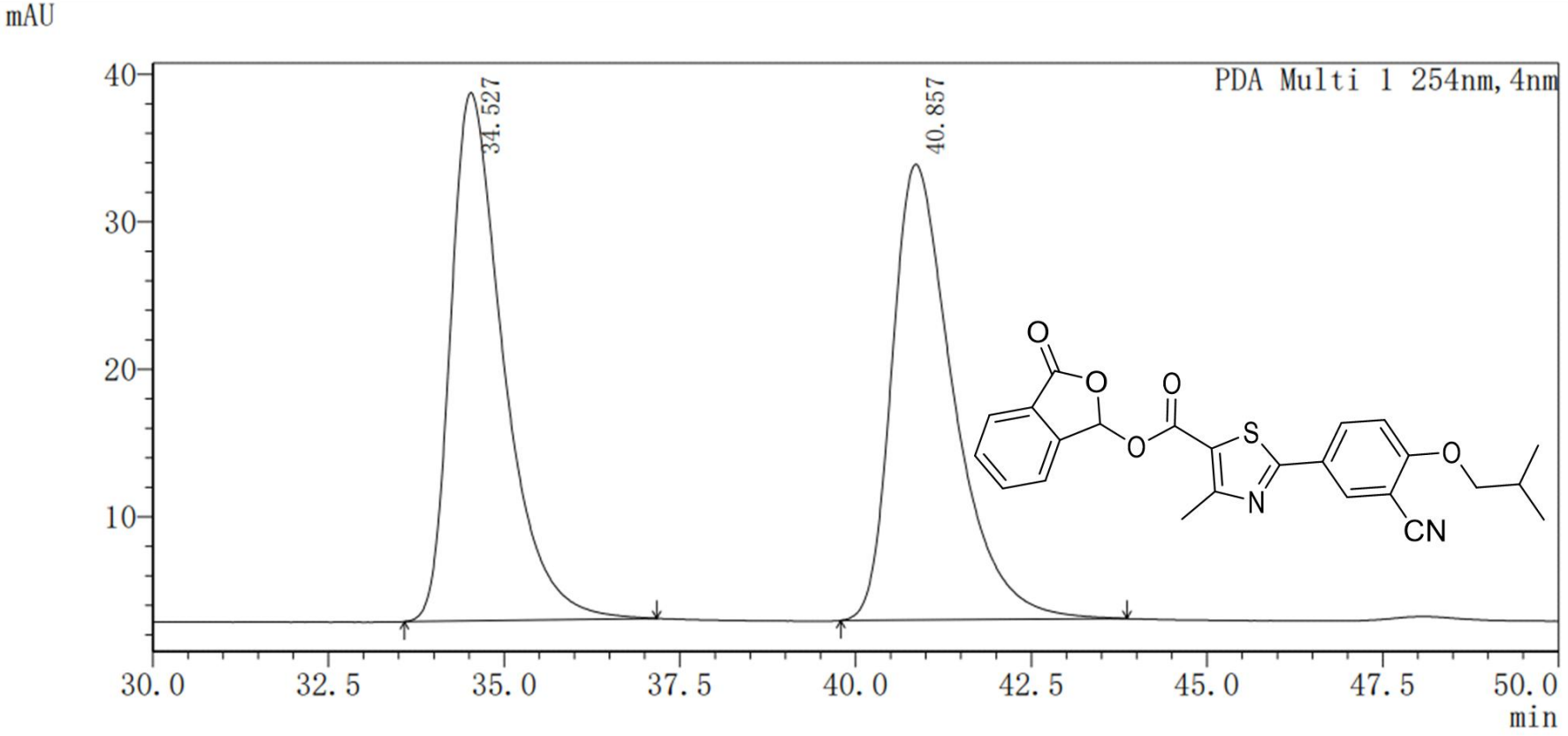
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	36.275	284062	12370608	85.907
2	40.075	42232	2029419	14.093
Total		326294	14400027	100.000


8.16 8.16 8.08 8.07 8.05 8.05 7.99 7.99 7.99 7.97 7.97 7.97 7.80 7.79 7.78 7.77 7.72 7.72 7.70 7.70 7.69 7.69 7.68 7.68 7.67 7.66 7.66 7.60 7.01 6.99 3.90 3.88 2.80 2.79 2.78 2.23 2.21 2.19 2.18 2.16 1.09 1.07
O O O O S N O N
3.90 3.88 2.80 2.79 2.78 2.23 2.21 2.19 2.18 2.16 1.09 1.07
2.00 3.01 1.01 6.02
4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)
8.16 8.16 8.08 8.07 8.05 8.05 7.99 7.97 7.80 7.79 7.70 7.70 7.69 7.68 7.67 7.66 7.60
0.91 1.00 1.00 1.00 2.00 0.99
8.2 8.1 8.0 7.9 7.8 7.7 7.6
f1 (ppm)
0.91 1.00 1.00 1.00 2.00 0.99 1.04 2.00 3.01 1.01 6.02
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

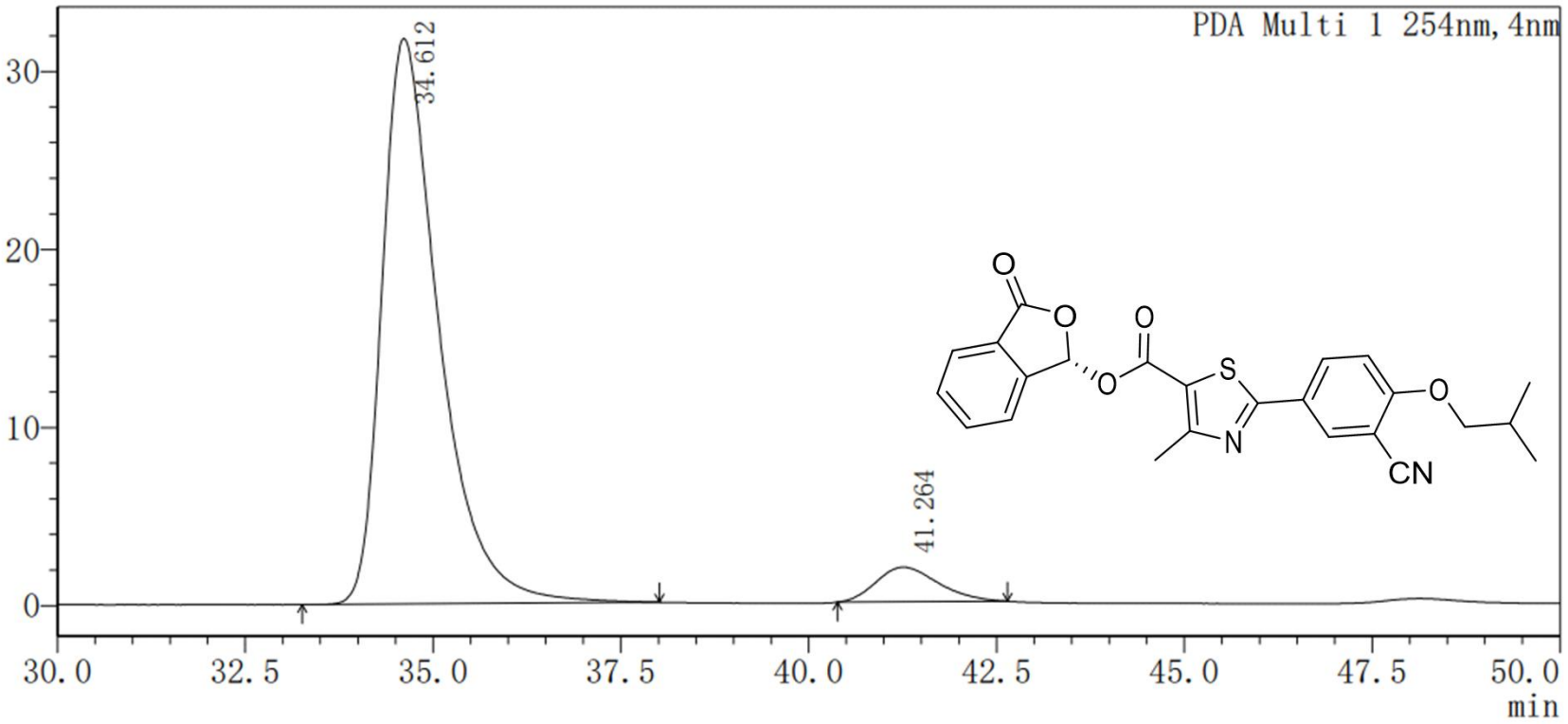

167.77
166.67
162.84
161.78
159.31
142.99
134.00
131.67
131.25
130.49
125.53
124.97
124.59
122.62
118.46
114.22
111.67
102.09
92.06
74.74
27.12
18.01
16.79
O
O
O
O
S
N
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

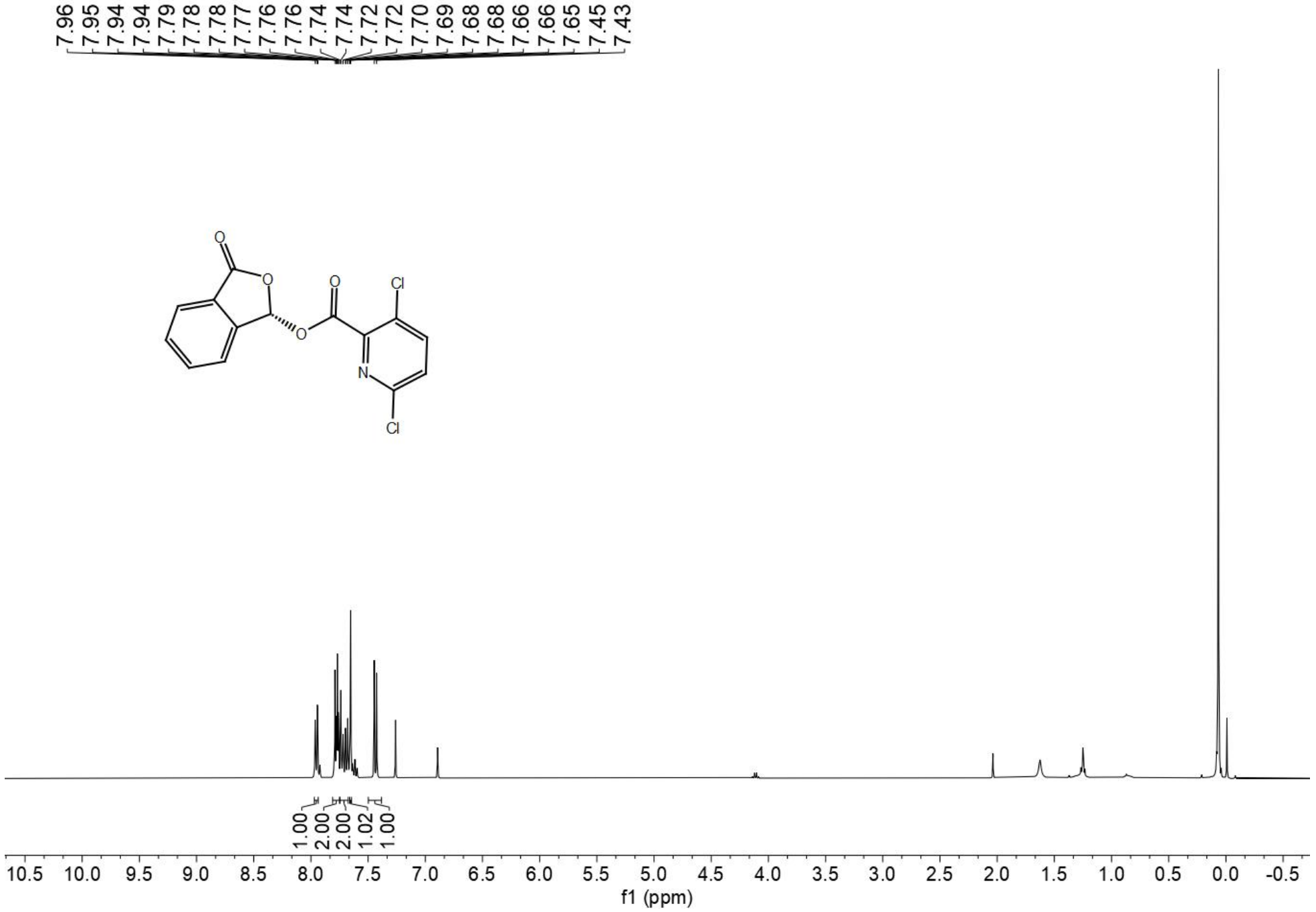
Peak#	Ret. Time	Height	Area	Area%
1	34.527	35798	1875346	49.947
2	40.857	30877	1879327	50.053
Total		66675	3754673	100.000

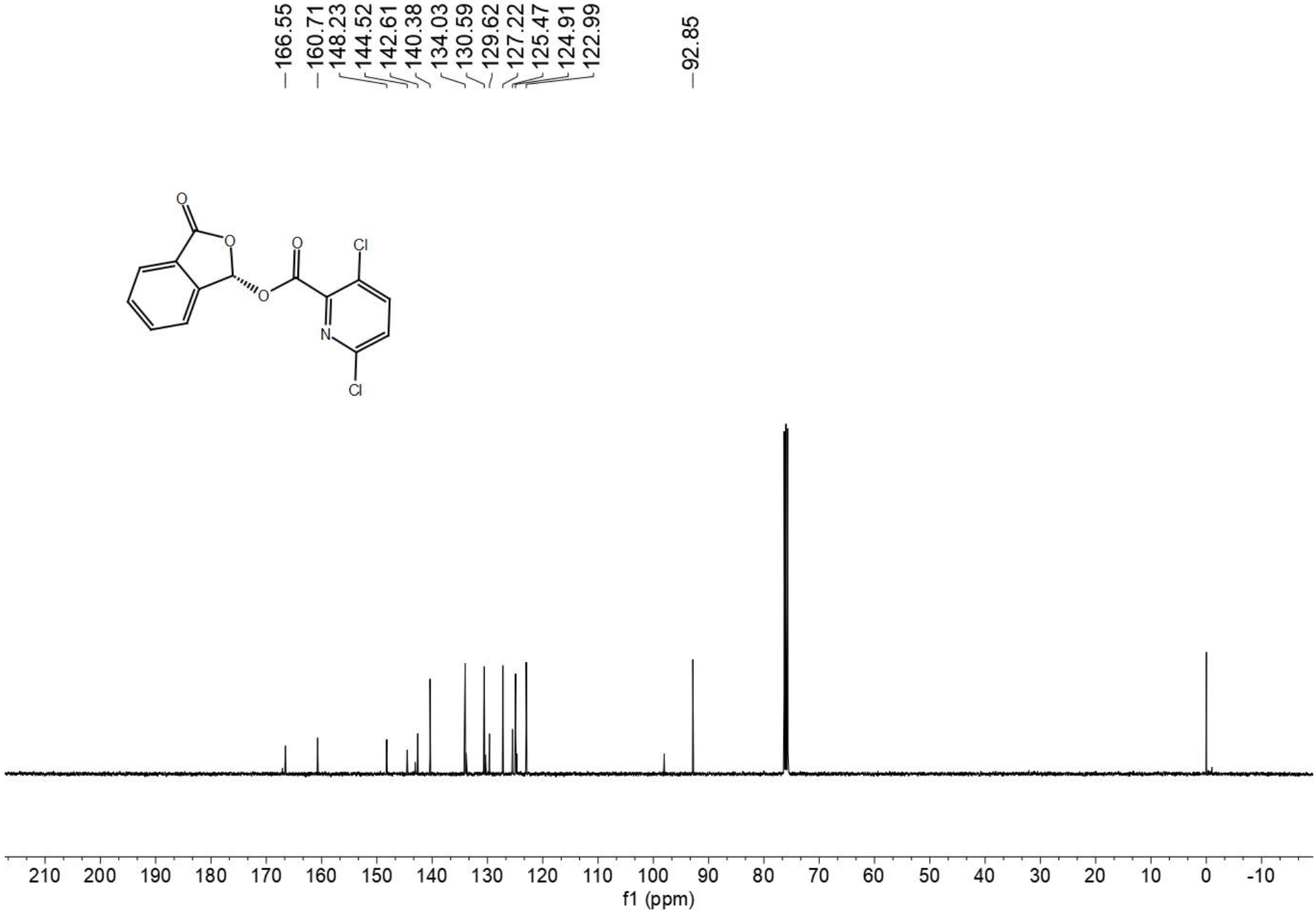


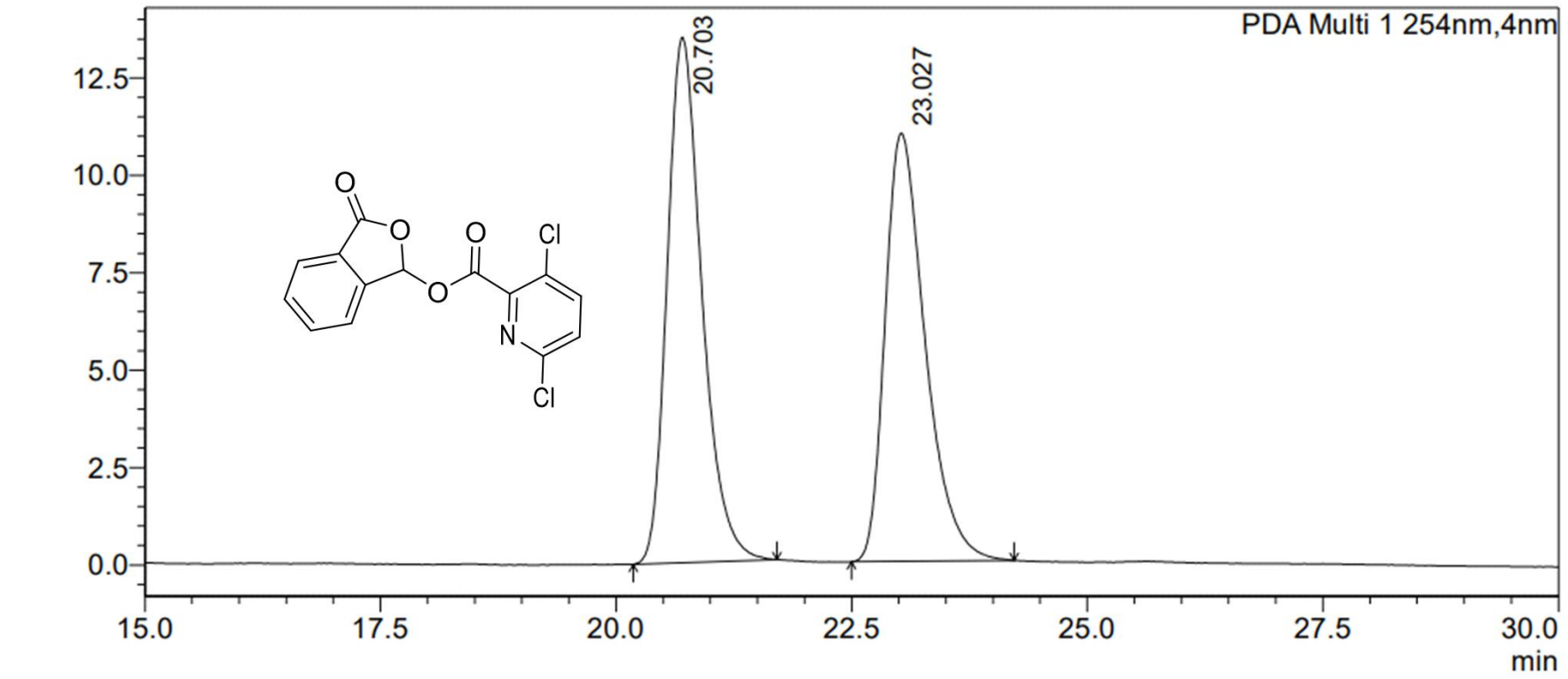
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	34.612	31755	1681511	93.760
2	41.264	1943	111906	6.240
Total		33697	1793416	100.000


7.96
7.95
7.94
7.94
7.79
7.78
7.78
7.77
7.76
7.76
7.74
7.74
7.72
7.72
7.70
7.69
7.68
7.68
7.66
7.66
7.65
7.45
7.43
O
O
O
O
Cl
N
Cl
1.00
2.00
2.00
1.02
1.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

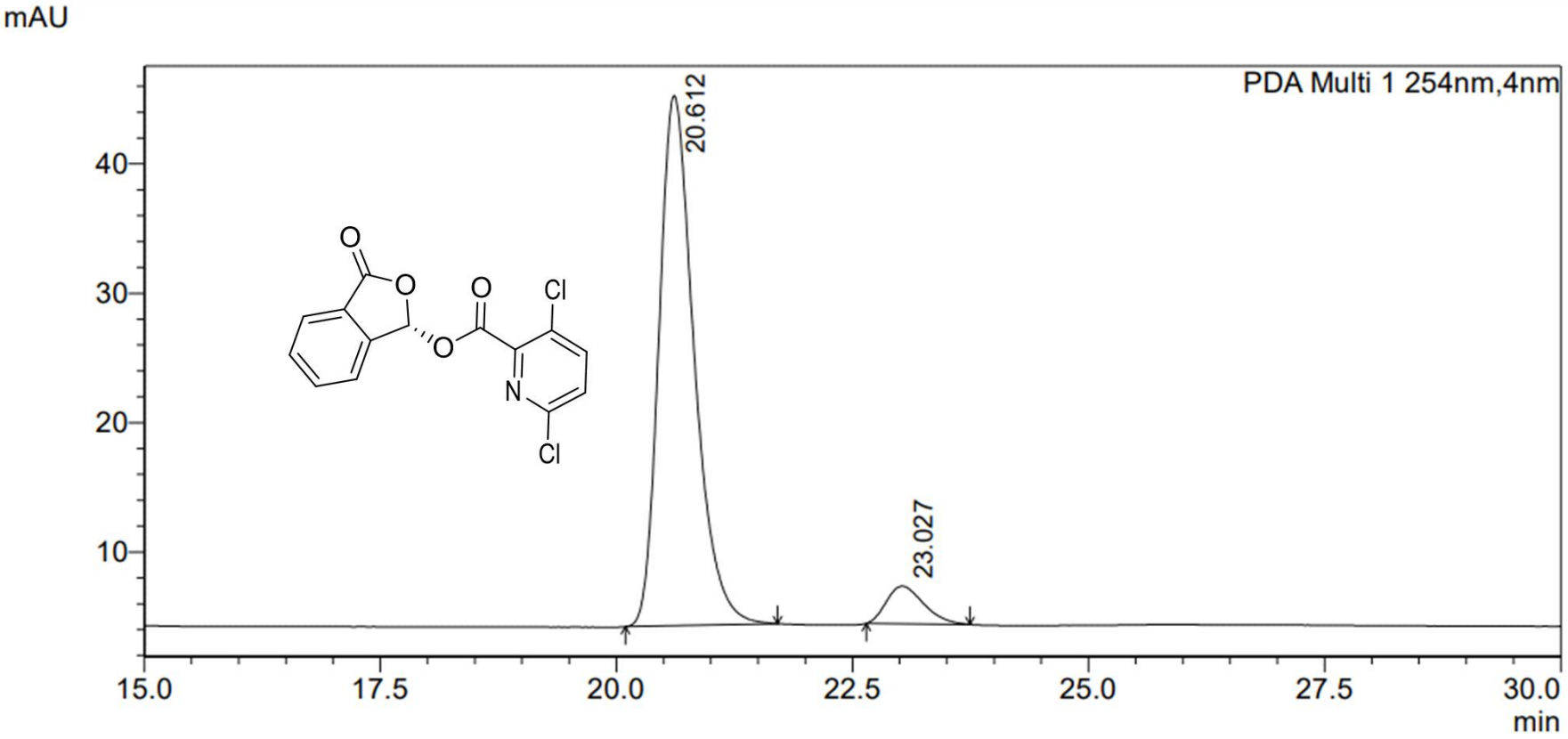

166.55
160.71
148.23
144.52
142.61
140.38
134.03
130.59
129.62
127.22
125.47
124.91
122.99
92.85
O
O
O
O
Cl
N
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

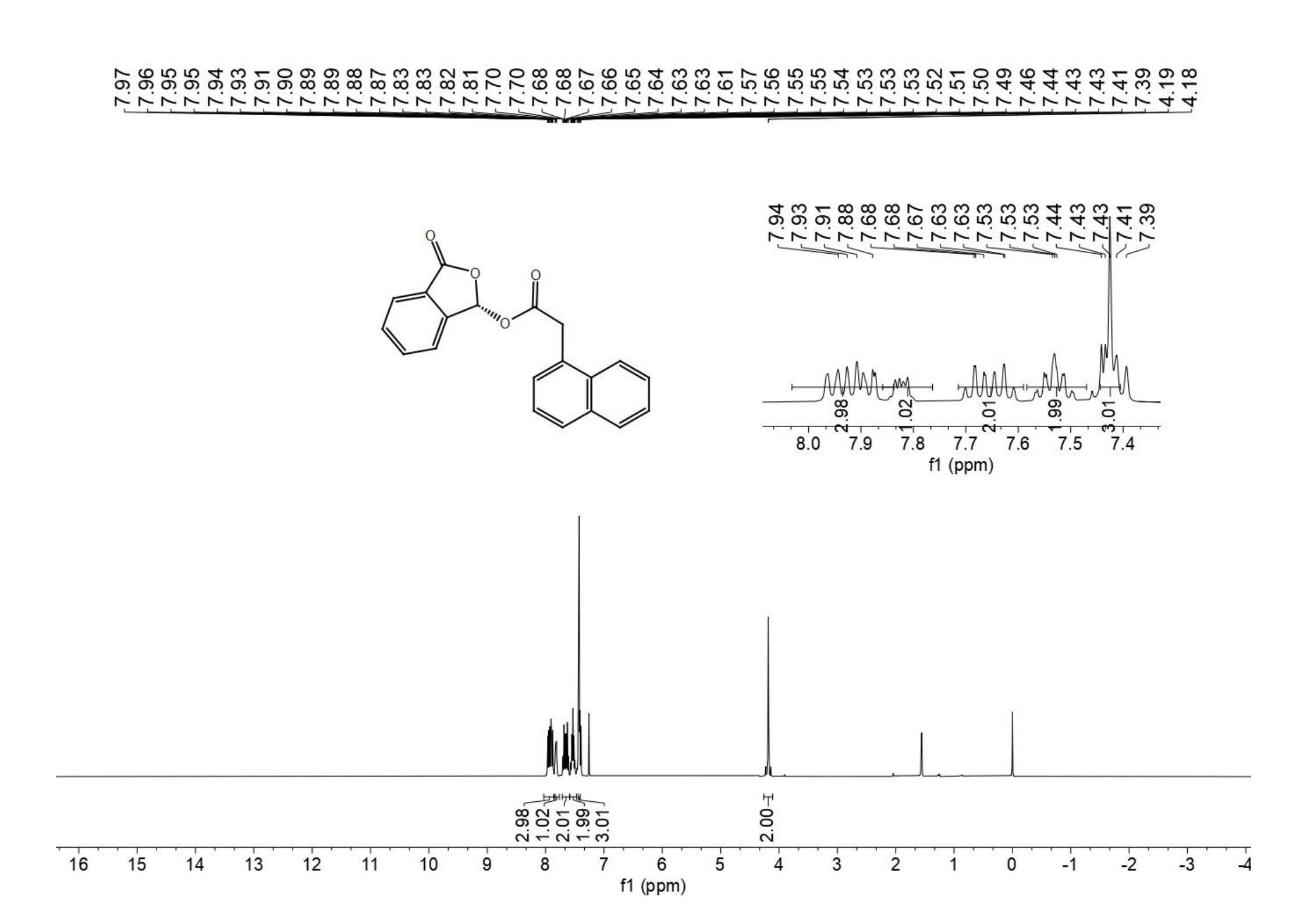
Peak#	Ret. Time	Height	Area	Area%
1	20.703	13483	346324	51.555
2	23.027	10994	325426	48.445
Total		24477	671750	100.000

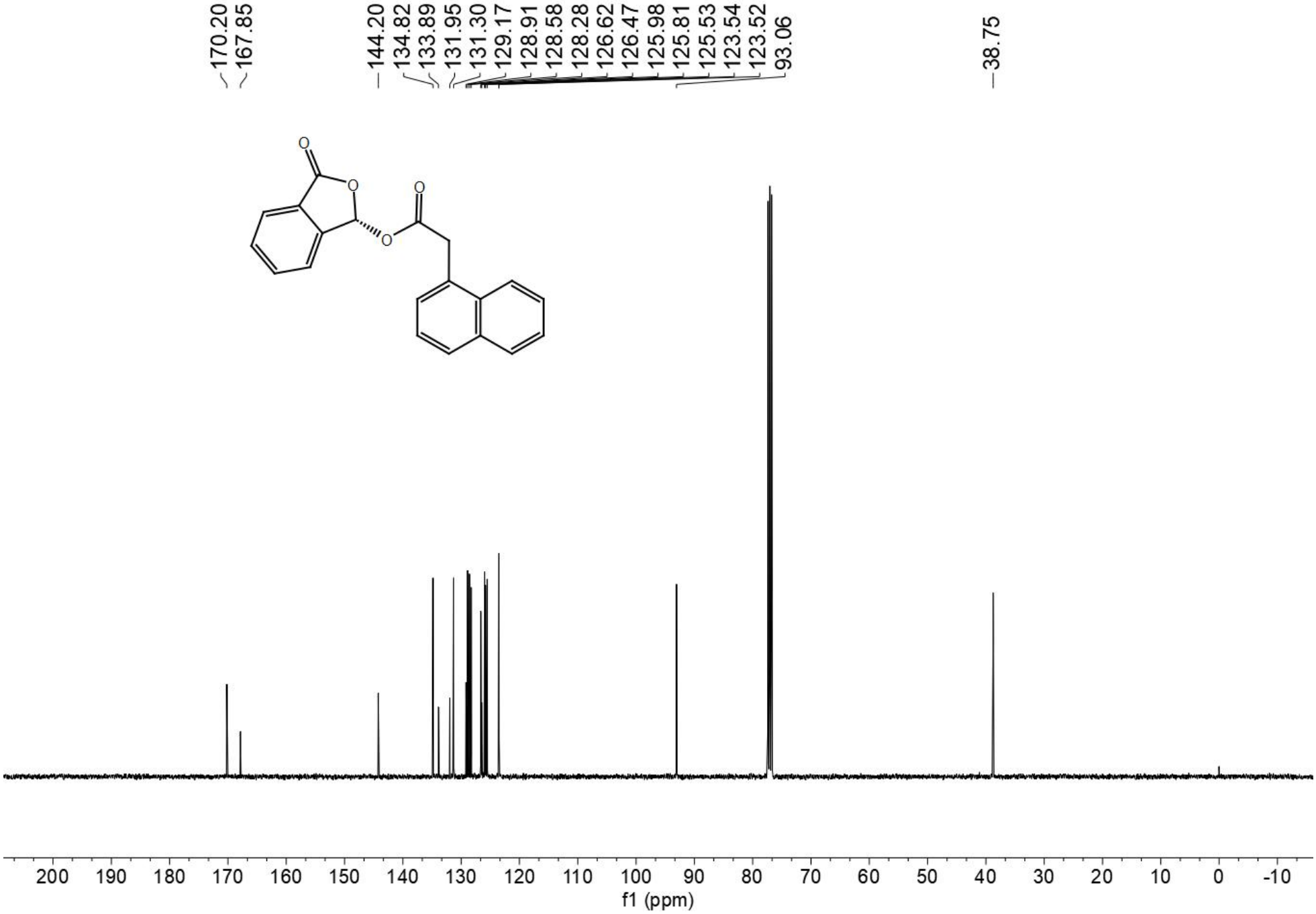


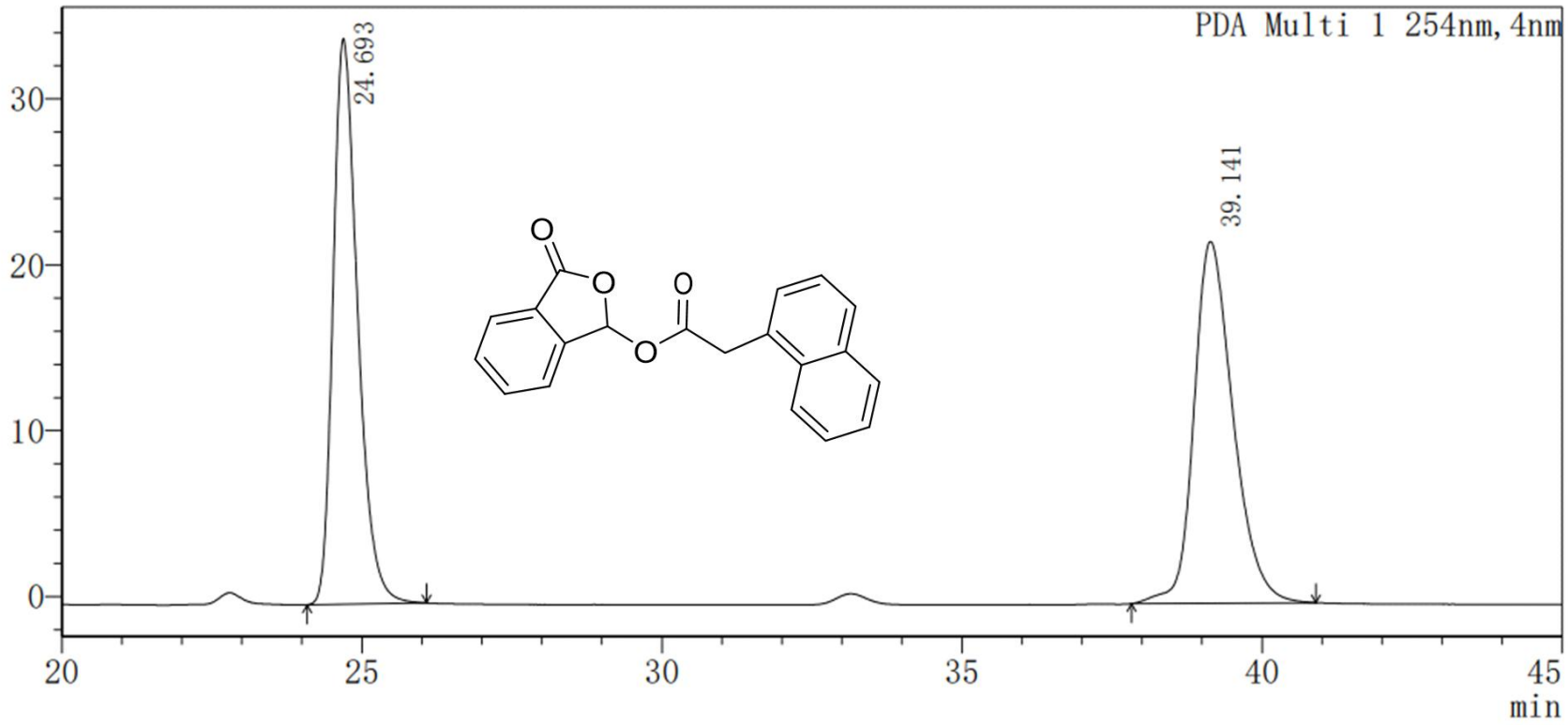
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	20.612	40967	1058673	92.977
2	23.027	2906	79965	7.023
Total		43873	1138639	100.000


7.97 7.96 7.95 7.95 7.94 7.93 7.91 7.90 7.89 7.89 7.88 7.87 7.83 7.83 7.82 7.81 7.70 7.70 7.68 7.68 7.67 7.66 7.65 7.64 7.63 7.63 7.61 7.57 7.56 7.55 7.55 7.54 7.53 7.53 7.53 7.52 7.51 7.50 7.49 7.46 7.44 7.43 7.43 7.41 7.39 4.19 4.18
O
O
O
O
7.94 7.93 7.91 7.88 7.68 7.68 7.67 7.63 7.63 7.53 7.53 7.53 7.44 7.43 7.43 7.41 7.39
2.98 1.02 2.01 1.99 3.01
8.0 7.9 7.8 7.7 7.6 7.5 7.4
f1 (ppm)
2.98 1.02 2.01 1.99 3.01
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

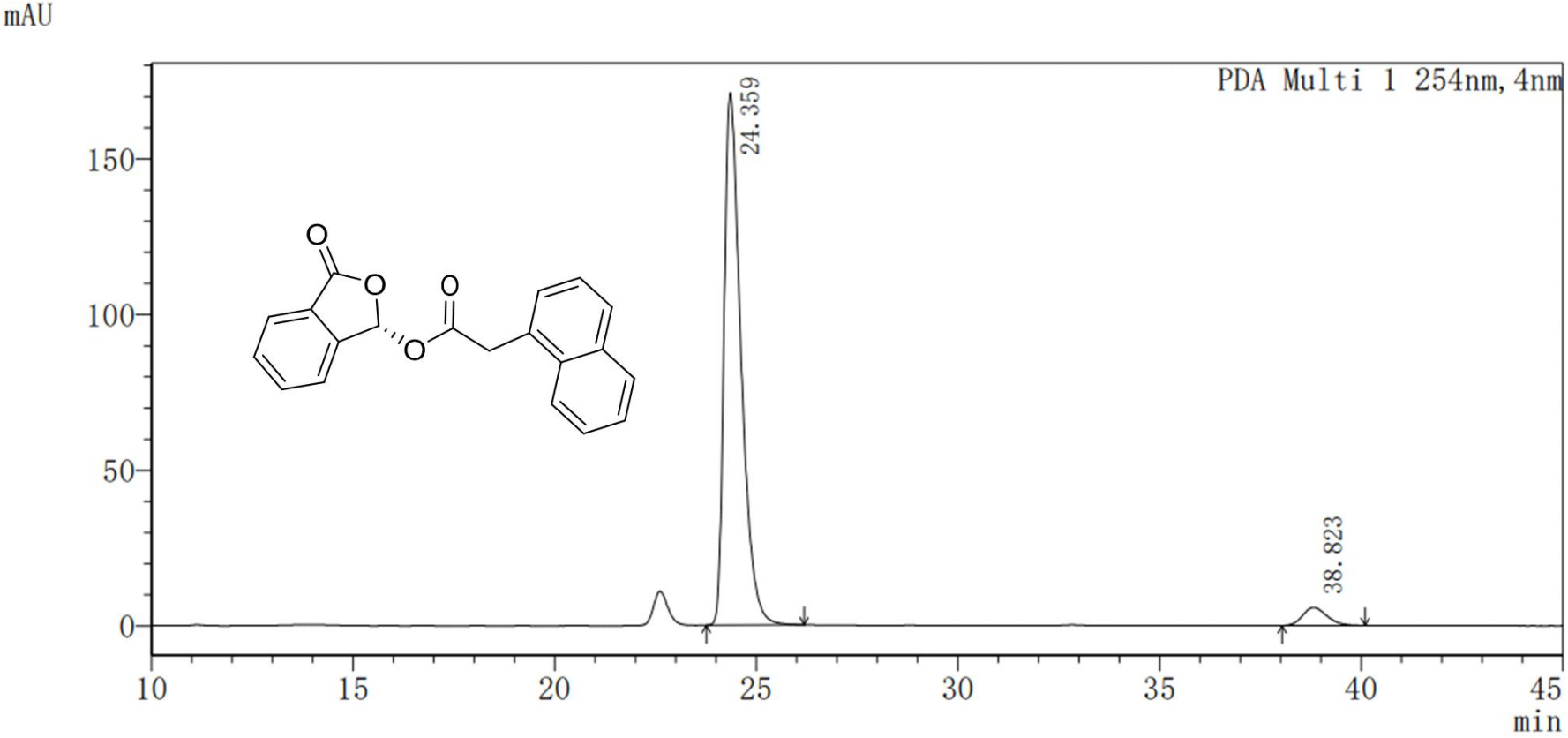

170.20
167.85
144.20
134.82
133.89
131.95
131.30
129.17
128.91
128.58
128.28
126.62
126.47
125.98
125.81
125.53
123.54
123.52
93.06
38.75
O
O
O
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

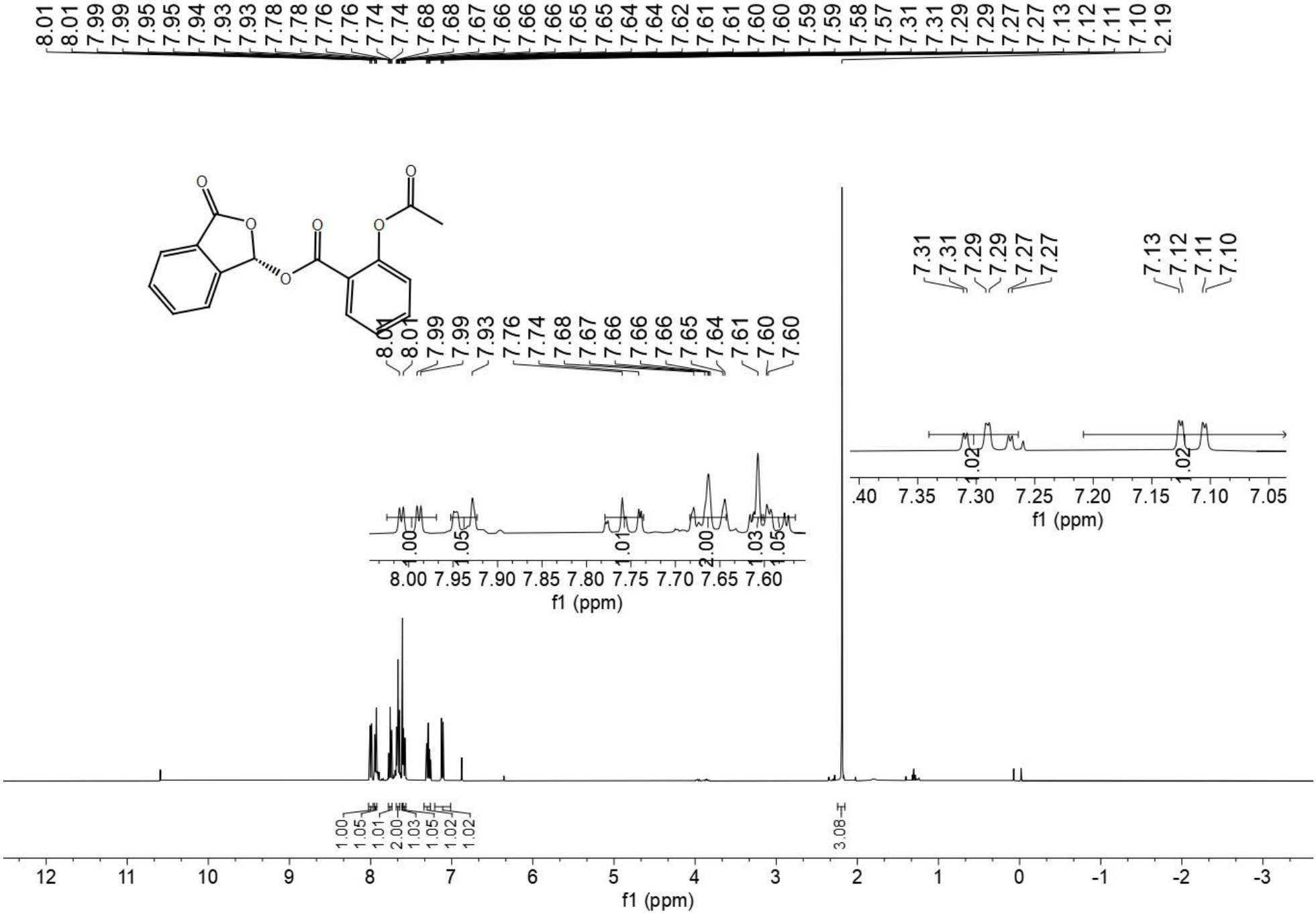
Peak#	Ret. Time	Height	Area	Area%
1	24.693	34090	973799	49.604
2	39.141	21807	989365	50.396
Total		55897	1963164	100.000

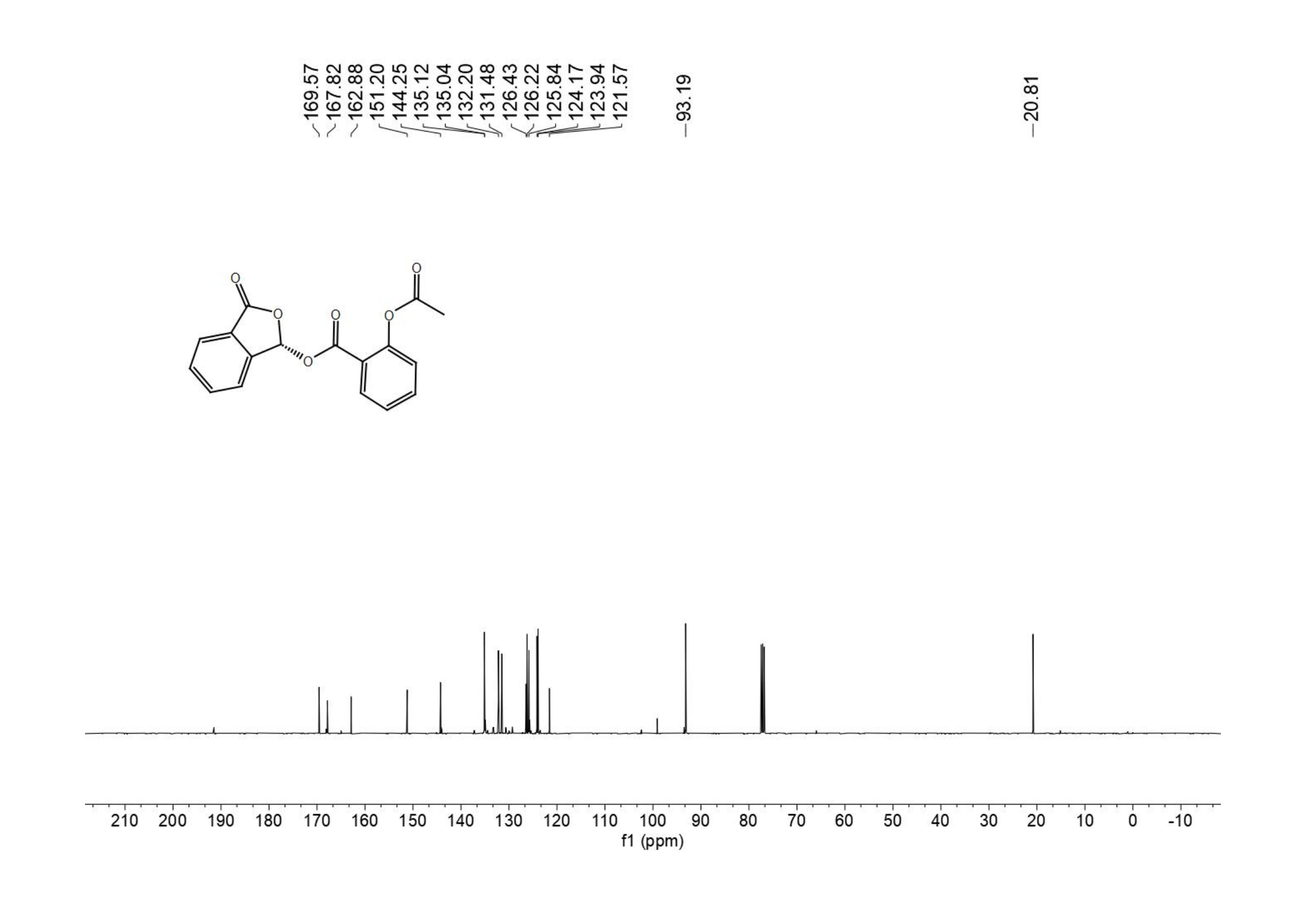


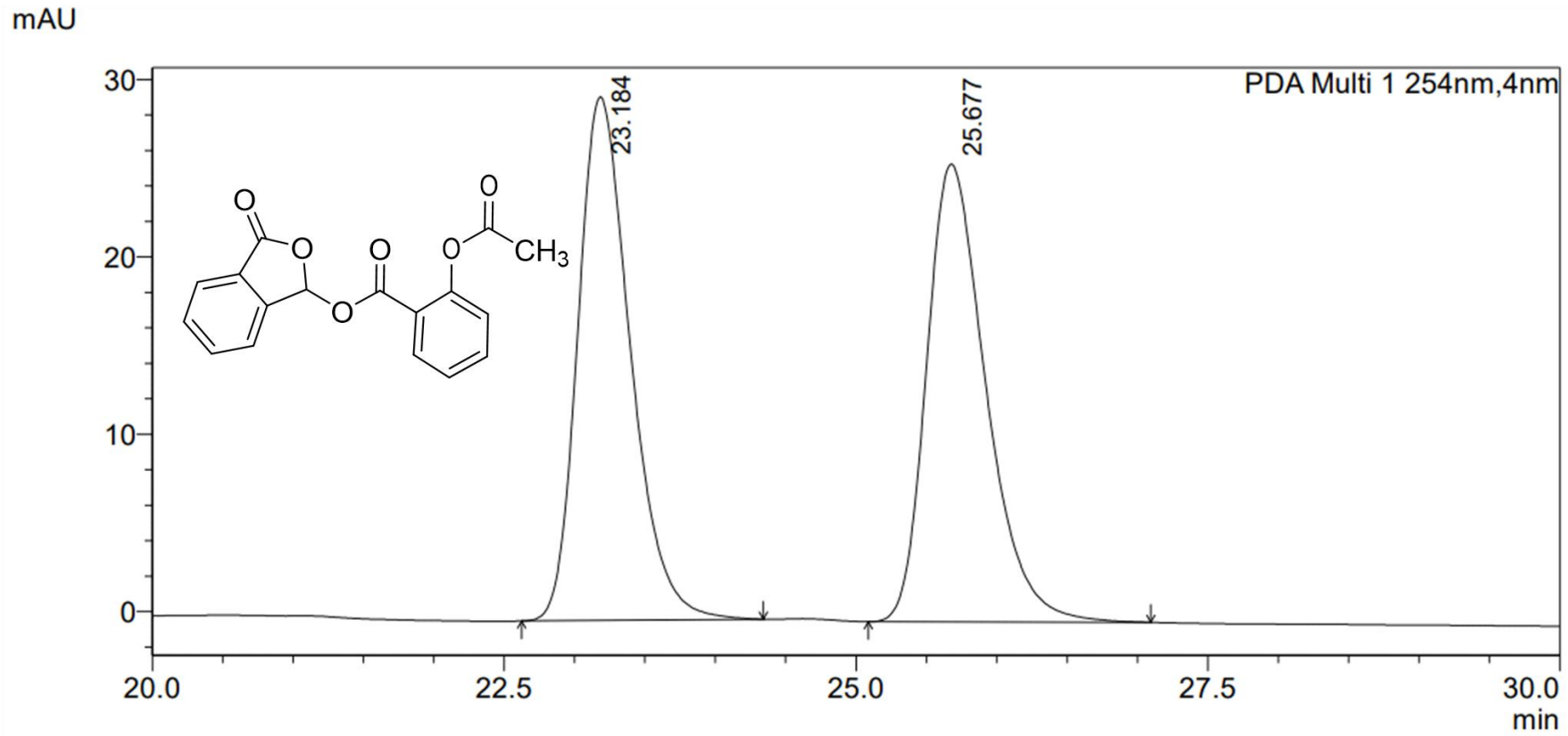
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	24.359	170879	4976384	95.322
2	38.823	5818	244221	4.678
Total		176698	5220604	100.000


8.01 8.01 7.99 7.99 7.95 7.95 7.94 7.93 7.93 7.78 7.78 7.76 7.76 7.74 7.74 7.68 7.68 7.67 7.66 7.66 7.66 7.65 7.65 7.64 7.64 7.62 7.61 7.61 7.60 7.60 7.59 7.59 7.58 7.57 7.31 7.31 7.29 7.29 7.27 7.27 7.13 7.12 7.11 7.10 2.19
O
O
O
O
O
O
8.01 8.01 7.99 7.99 7.93 7.76 7.74 7.68 7.67 7.66 7.66 7.66 7.65 7.64 7.61 7.60 7.60
7.31 7.31 7.29 7.29 7.27 7.27 7.13 7.12 7.11 7.10
1.00 1.05 1.01 2.00 1.03 1.05
8.00 7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60
f1 (ppm)
1.02 1.02
.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05
f1 (ppm)
1.00 1.05 1.01 2.00 1.03 1.05 1.02 1.02
3.08
12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

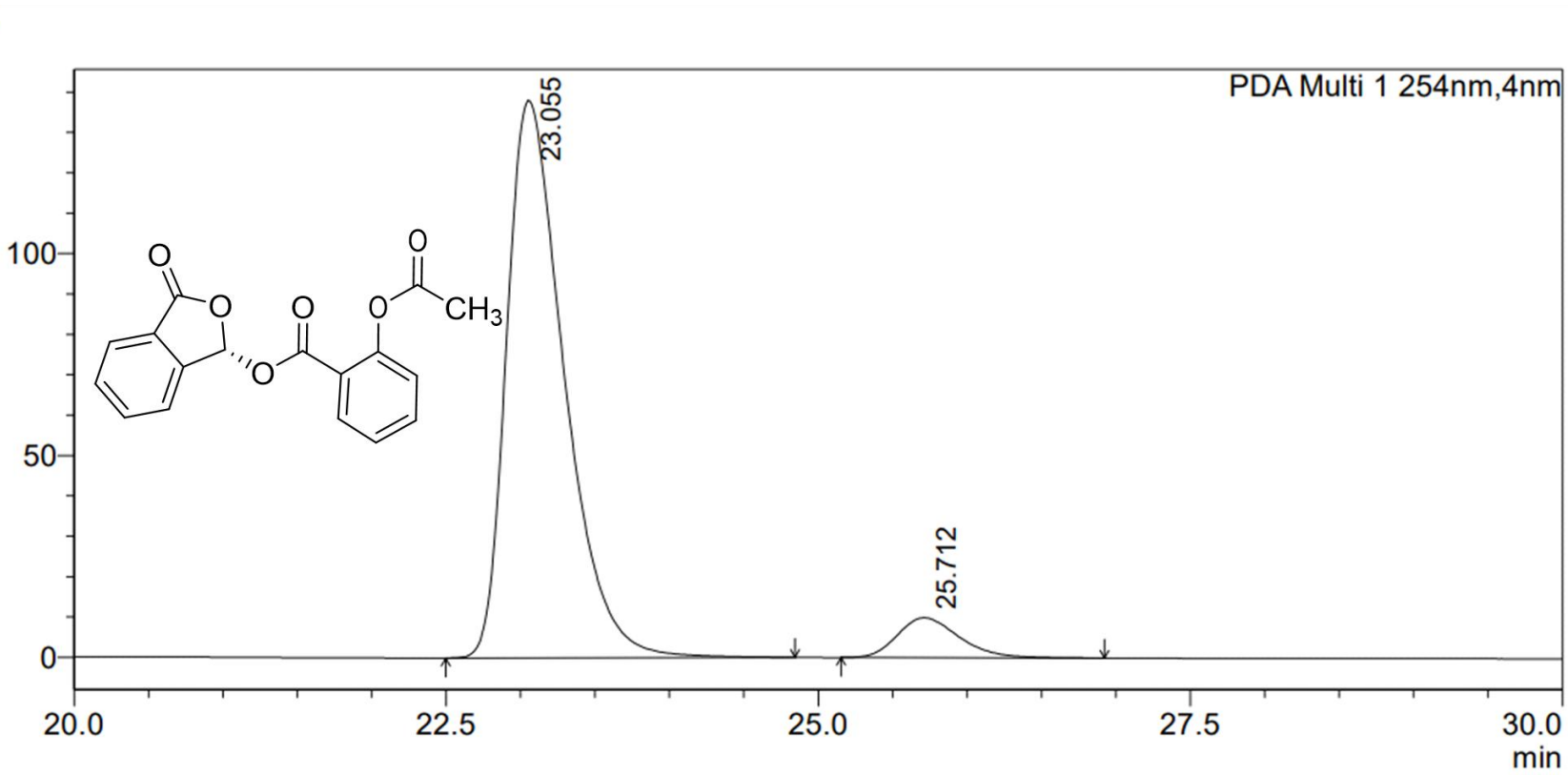

169.57
167.82
162.88
151.20
144.25
135.12
135.04
132.20
131.48
126.43
126.22
125.84
124.17
123.94
121.57
93.19
20.81
O
O
O
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

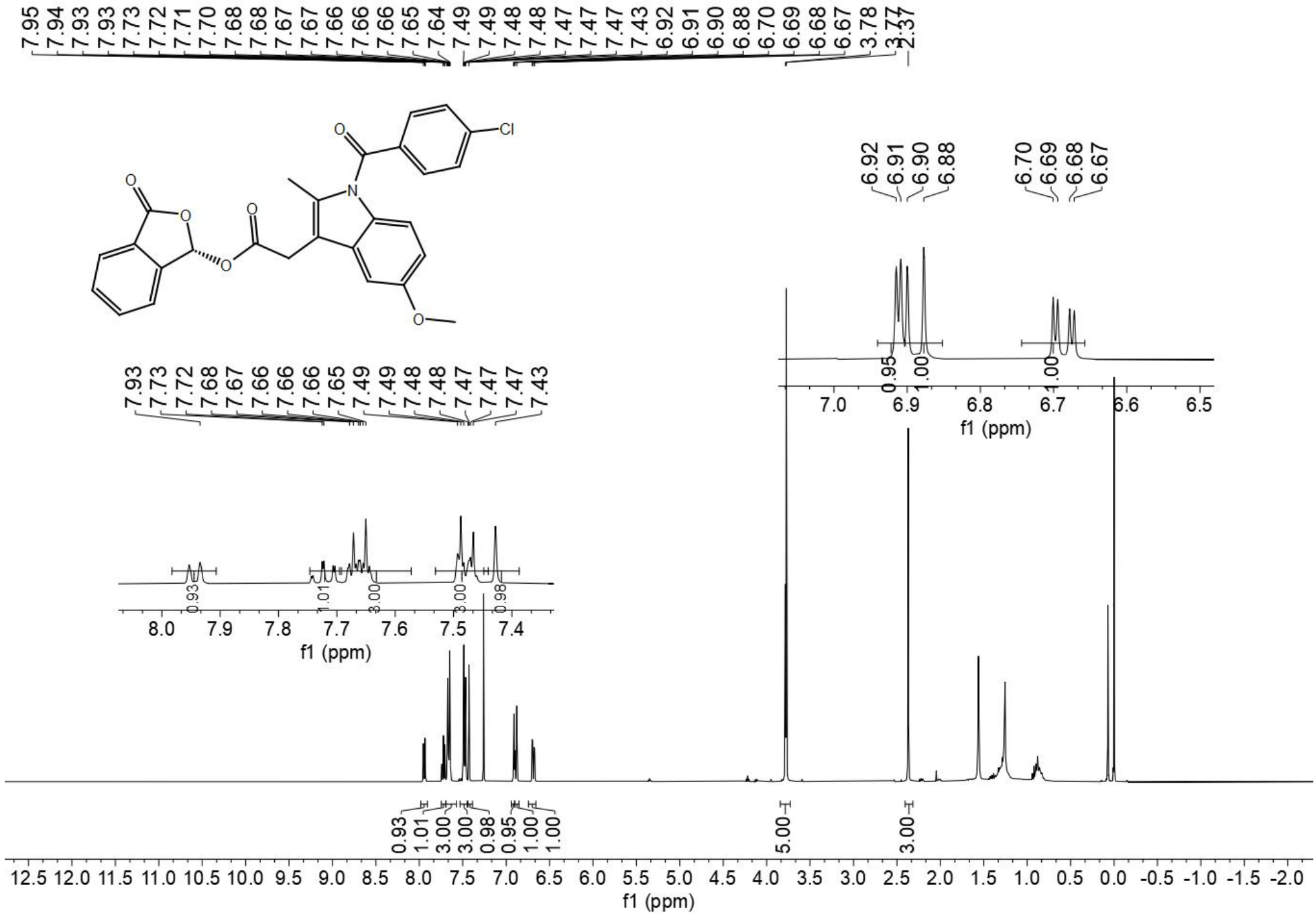
Peak#	Ret. Time	Height	Area	Area%
1	23.184	29495	764208	50.293
2	25.677	25810	755291	49.707
Total		55305	1519499	100.000

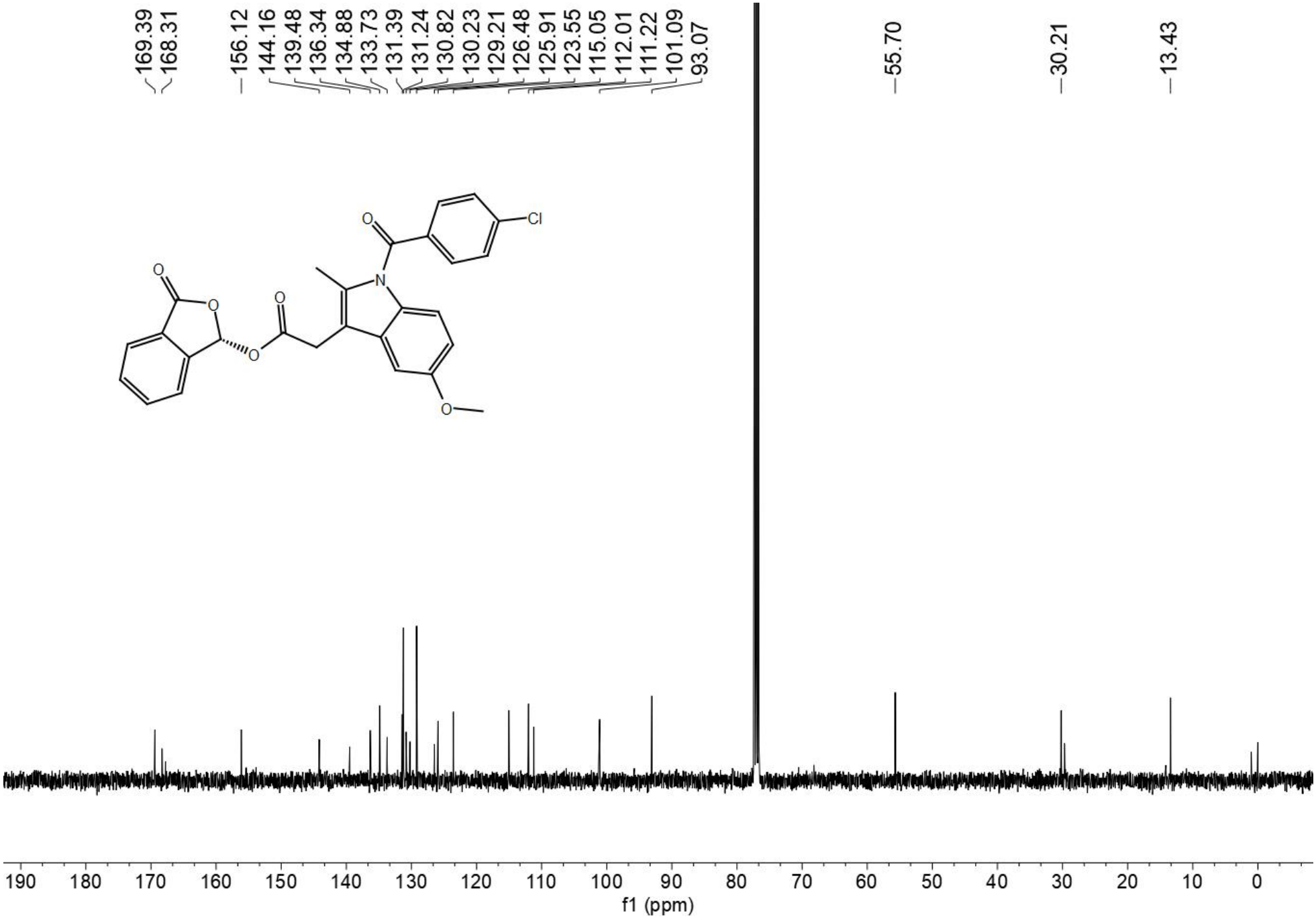


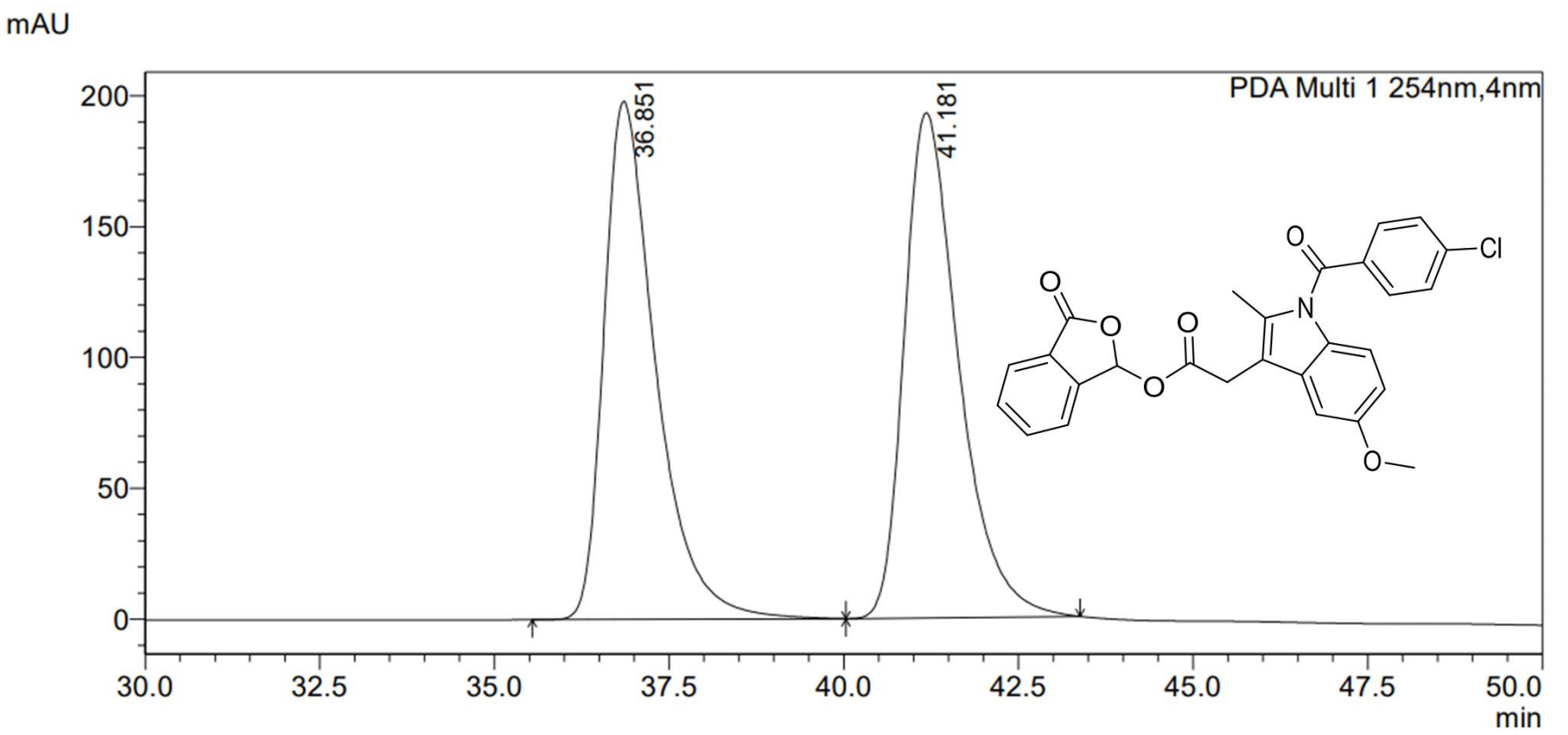
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	23.055	138078	3707955	92.814
2	25.712	9881	287078	7.186
Total		147959	3995033	100.000


7.95 7.94 7.93 7.93 7.73 7.72 7.71 7.70 7.68 7.68 7.67 7.67 7.66 7.66 7.66 7.65 7.64 7.49 7.49 7.48 7.48 7.47 7.47 7.47 7.43 6.92 6.91 6.90 6.88 6.70 6.69 6.68 6.67 3.78 2.37
Cl
O
N
O
O
O
O
O
7.93 7.73 7.72 7.68 7.67 7.66 7.66 7.66 7.65 7.49 7.49 7.48 7.48 7.47 7.47 7.47 7.43
0.93 1.01 3.00 3.00 0.98
8.0 7.9 7.8 7.7 7.6 7.5 7.4
f1 (ppm)
6.92 6.91 6.90 6.88 6.70 6.69 6.68 6.67
0.95 1.00 1.00
7.0 6.9 6.8 6.7 6.6 6.5
f1 (ppm)
0.93 1.01 3.00 3.00 0.98 0.95 1.00 1.00 5.00 3.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

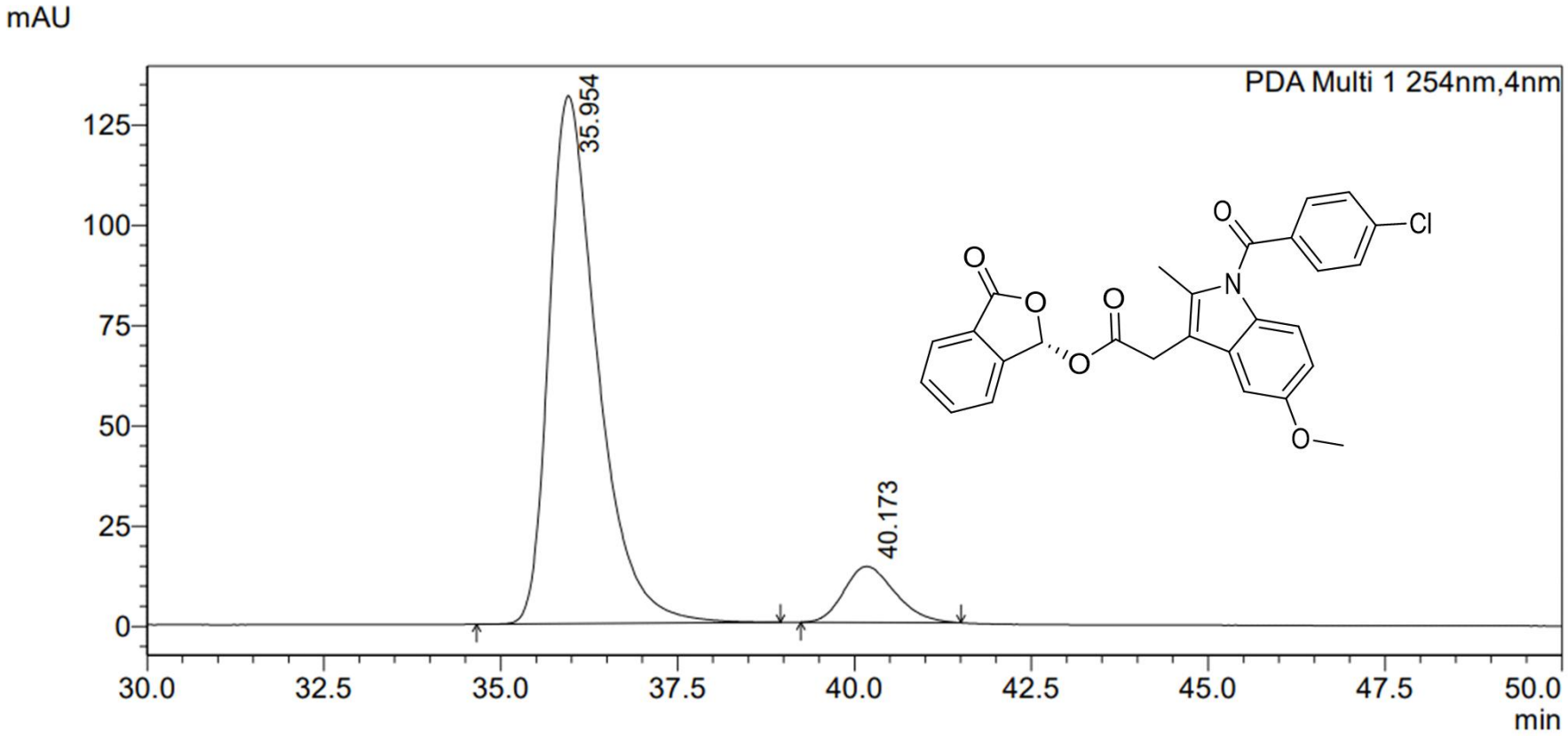

169.39
168.31
156.12
144.16
139.48
136.34
134.88
133.73
131.39
131.24
130.82
130.23
129.21
126.48
125.91
123.55
115.05
112.01
111.22
101.09
93.07
55.70
30.21
13.43
O
Cl
N
O
O
O
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	36.851	197928	10224849	49.384
2	41.181	192949	10480135	50.616
Total		390876	20704984	100.000



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Area	Area%
1	35.954	131604	6271898	89.918
2	40.173	13963	703258	10.082
Total		145567	6975156	100.000