



Supplementary Materials for

Deracemization through photochemical *E/Z* isomerization of enamines

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1. General considerations

All reagents were purchased from commercial sources and used as received, unless otherwise noted. The aminocatalysts were prepared according to the procedure reported previously by our group (28). Silica gel (200-300 mesh) was used for column chromatography. Analytical thin layer chromatography (TLC) was visualized with UV light, or stained with KMnO₄ and phosphomolybdic acid hydrate solutions. ¹H, and ¹³C NMR spectra were measured on Bruker AV 400 M (400 MHz for ¹H NMR; 101 MHz for ¹³C NMR). Chemical shifts of ¹H NMR spectra were recorded relative to TMS (δ 0.00) or residual protonated solvents (CDCl₃: δ 7.26; MeCN-*d*₃: δ 1.96). Chemical shifts of ¹³C NMR spectra were recorded relative to solvent resonance (CDCl₃: δ 77.2; MeCN-*d*₃: δ 118.3). ¹³C NMR spectra were obtained at 101 MHz using a proton-decoupled pulse sequence and were tabulated by the observed peak. The following abbreviations were used to express the multiplicities: s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet; td = triplet of doublet; dt = doublet of triplet; dd = doublet of doublet; br = broad. GC analysis was performed on a Shimadzu GC-2030 instrument equipped with an FID detector using argon as the carrier gas. IR spectrum was collected using a Mettler-Toledo ReactIR 15 instrument equipped with a 9.5 mm diameter DiComp probe. UV-Vis spectrum was obtained from Agilent Cary 8454 UV-Vis Diode Array System. High resolution mass spectra were obtained using electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI) on Thermo-Fisher Scientific Q-Exactive spectrometer. The enantiomeric excesses were determined by HPLC analysis on Chiral Daicel Chiraldpak OJ-H, OD-H, AD-H and AS-H. Optical rotations were measured on a commercial polarimeter and reported as follows: $[\alpha]_D^T$ ($c = g/100\text{ mL}$, CHCl₃).

2. Details of optimization

Table S1. Reaction development.

 rac-2a (R)-2a (S)-1a																
A Control experiment																
<table border="1"> <thead> <tr> <th>Entry</th> <th>Variation</th> <th>Yield (%)</th> <th>ee (%)</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>No 1a</td> <td>99</td> <td>rac</td> </tr> <tr> <td>2</td> <td>No benzoic acid</td> <td>76</td> <td>42</td> </tr> <tr> <td>3</td> <td>No Ir(ppy)₃</td> <td>65</td> <td>19</td> </tr> </tbody> </table>	Entry	Variation	Yield (%)	ee (%)	1	No 1a	99	rac	2	No benzoic acid	76	42	3	No Ir(ppy) ₃	65	19
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1	No 1a	99	rac													
2	No benzoic acid	76	42													
3	No Ir(ppy) ₃	65	19													
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(A) Control experiments. Reactions were performed on a 0.2 mmol scale. The yields were determined by GC analysis with biphenyl as an internal standard. The data in parentheses refers to isolated yield. The *ee* values were determined by HPLC analysis. **(B)** The effect of triplet state inhibitor. *The resulting *E/Z* ratio of stilbene was 1:2.5. **(C)** Deracemization performed with optically pure substrates.

Table S2. Screening of the amine catalyst

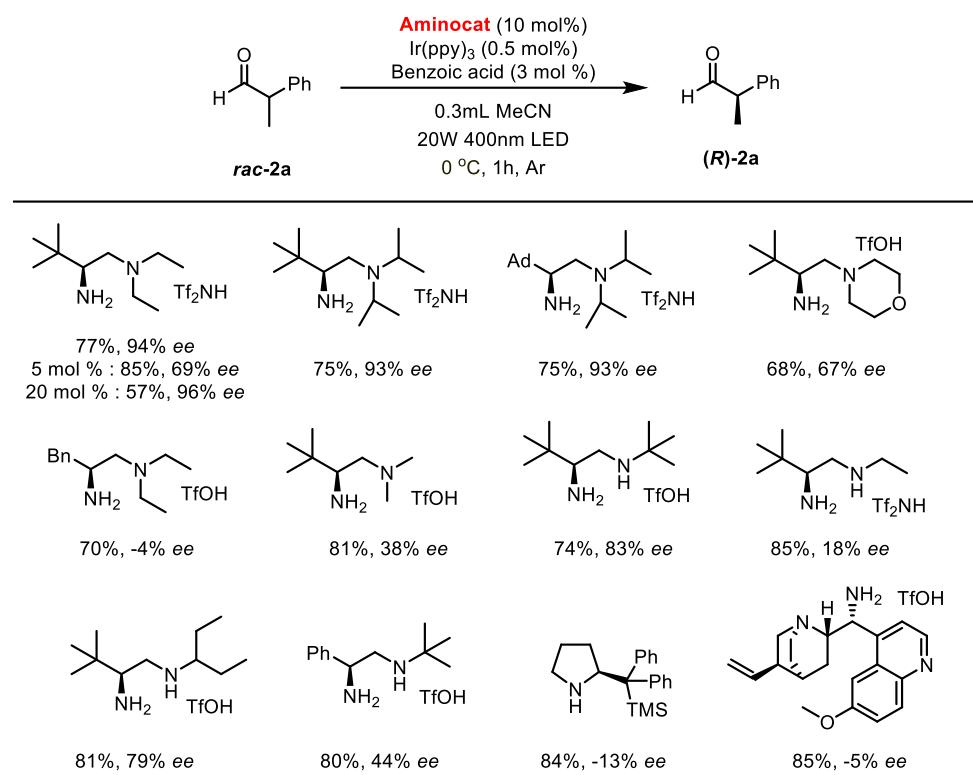
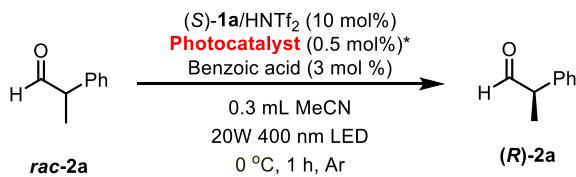


Table S3. Screening of the photocatalyst



Photocatalyst	E_T (kcal/mol)	$E_{1/2}^{PC+/PC^*}$	Recovery(%)	ee (%)
Thioxanthone	64.4	+1.18	71	64
Ir(dFCF ₃ ppy) ₂ (dtbbpy)PF ₆	61.8	+1.21	73	73
Ir(dF-ppy) ₃	60.1	+0.36	67	85
Acridine orange	59.3	+0.60	86	10
Ir(F-ppy) ₃	58.6	+0.68	71	93
Ir(ppy) ₃	58.1	+0.31	77	94
Ir(pCF ₃ ppy) ₃	56.4	+0.59	78	93
2,4,6-triphenylpyrylium	53.0	+2.02	72	18

Ir(Fmppy) ₂ (dtbpy)PF ₆	52.3		66	59
Riboflavin	50.0	+1.25	63	17
Ir(ppy) ₂ (dtbpy)PF ₆	49.2	+0.66	67	53
Ru(bpy) ₃ Cl ₂ ·6H ₂ O	46.5	+0.77	67	39
9,10-dicyanoanthracene	41.7	+1.99	79	31

*The amount of organo-photocatalysts was 10 mol %.

Table S4. Screening of the solvent

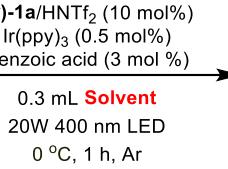
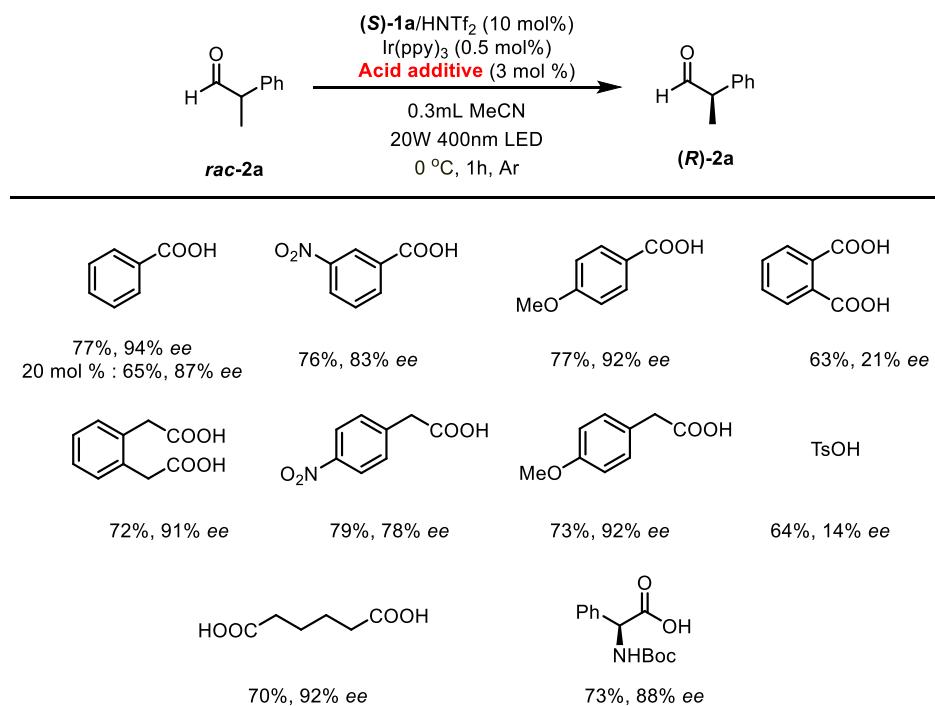
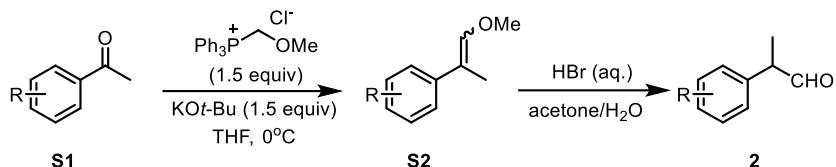
		
<i>rac</i> -2a		(<i>R</i>)-2a
Solvent	Recovery(%)	<i>ee</i> (%)
MeCN	77	94
EtOAc	73	90
DCM	66	43
THF	67	67
MeOH	81	58
HFIP	63	43
DME	66	62
Toluene	64	46
DMF	55	64
MTBE	66	75

Table S5. Screening of weak acid additive



3. Synthesis of substrates

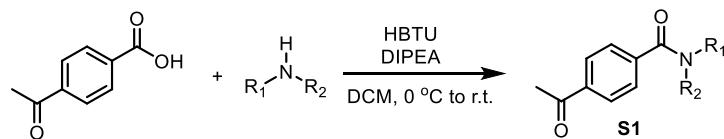
3.1. General procedure A



The reaction was performed according to a modified procedure of Wang (29), (methoxymethyl)-triphenylphosphonium chloride (15.42 g, 45 mmol, 1.5 equiv) was suspended in anhydrous THF (100 mL) and the mixture was cooled to 0°C . Potassium *tert*-butoxide (5.04 g, 45 mmol, 1.5 equiv) was slowly added to the reaction mixture under Ar atmosphere. The mixture was allowed to stir at 0°C for 30 min to obtain a deep red solution. Then, the corresponding substituted acetophenone **S1** (30 mmol) in anhydrous THF (10 mL) was added dropwise. After stirring under Ar for 16h, the reaction mixture was quenched by H_2O (50 mL). The layers were separated and the aqueous phase was extracted with DCM (2×50 mL). The combined organic solutions were washed with brine (60 mL), dried over Na_2SO_4 , filtered, and concentrated. The crude product was purified by flash chromatography (silica gel, 50:1 to 2:1 petroleum ether/EtOAc) to afford the intermediate product **S2** in a nearly 1:1 ratio of *E/Z*-enol ether isomers.

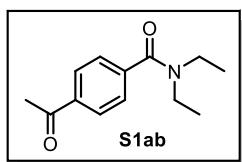
Enol ether **S2** (10 mmol) was dissolved in a 4:1 mixture of acetone and H_2O (20 mL) and the solution was cooled to 0°C . Conc. HBr (48% aqueous solution, 3 mL) was slowly added to the solution under Ar atmosphere and the mixture was stirred at room temperature. The progress of the reaction was monitored by TLC. After completion of the reaction, acetone was removed by rotary evaporation and the remaining aqueous residue was neutralized with sat. aq. NaHCO_3 . This aqueous solution was then extracted with DCM (3×20 mL). The combined organic layers were dried over Na_2SO_4 , filtered and concentrated. The crude product was purified by flash chromatography (silica gel, 50:1 to 2:1 petroleum ether/EtOAc) to afford α -branched aldehyde **2**.

3.2. Synthesis of **S1ab**, **S1ae**



To a solution of 4-acetylbenzoic acid (30 mmol, 4.92 g) in DCM (100 mL) was added N, N-Diisopropylethylamine (66 mmol, 2.2 equiv, 11.5 mL) and HBTU (33 mmol, 1.1 equiv, 12.51 g) at 0°C. The reaction mixture was allowed to stir for 30 min followed by dropwise addition of amine (30 mmol, 1 equiv) at 0°C. After stirring at room temperature overnight, the organic phase was washed with 0.1M HCl (50 mL), H₂O (50 mL), and sat. aq. NaHCO₃ (50 mL). The organic layer was dried over anhydrous Na₂SO₄ and concentrated in *vacuo*. The crude product was purified by flash chromatography (silica gel, 5:1 to 2:1 petroleum ether/EtOAc) to afford 4-acetylbenzamide **S1ab** or **S1ae**.

4-Acetyl-N,N-diethylbenzamide (**S1ab**)



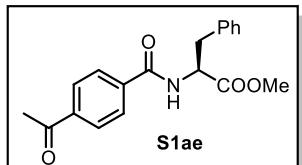
colorless liquid (6.9 g, 99% yield)

¹H NMR (400 MHz, Chloroform-d) δ 7.89 (d, *J* = 8.3 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 3.71 - 3.02 (m, 4H), 2.51 (s, 3H), 1.42 - 0.71 (m, 6H).

¹³C NMR (101 MHz, Chloroform-d) δ 197.33, 170.05, 141.62, 137.25, 128.42, 126.42, 43.17, 39.26, 38.49, 26.60, 14.13, 12.81.

Spectroscopic results agree with previously reported data. (30)

Methyl (4-acetylbenzoyl)-L-phenylalaninate (**S1ae**)



White solid (8.95 g, 91% yield)

R_f = 0.4 (1:1 petroleum ether/EtOAc)

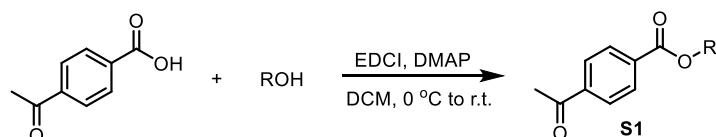
¹H NMR (400 MHz, Chloroform-d) δ 7.95 (d, *J* = 8.5 Hz, 2H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.36 - 7.21 (m, 3H), 7.20 - 7.09 (m, 2H), 6.87 (d, *J* = 7.7 Hz, 1H), 5.15 - 4.97 (m, 1H), 3.77 (s, 3H), 3.35 - 3.16 (m, 2H), 2.60 (s, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 197.38, 171.95, 166.00, 139.34, 137.74, 135.82, 129.27, 128.66, 128.49, 127.38, 127.26, 53.71, 52.50, 38.60, 37.74, 26.79.

IR ν(cm⁻¹): 3306, 3034, 2952, 1742, 1686, 1644, 1532, 1497, 1435, 1358, 1265, 1216, 1098.

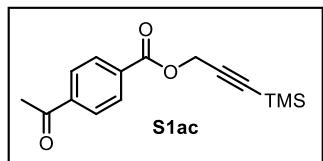
HRMS (ESI) calcd for C₁₉H₁₉NO₄ [M+Na]⁺ 348.1206, found 348.1195.

3.3. Synthesis of S1ac, S1ad



To a solution of 4-acetylbenzoic acid (30 mmol, 4.92 g) and alcohol (30 mmol, 1 equiv) in DCM (100 mL) was added EDCI (36 mmol, 1.2 equiv, 6.9 g) and DMAP (3 mmol, 0.1 equiv, 0.37 g) at 0°C. After addition, the mixture was stirred at room temperature until TLC indicating completion. The reaction was quenched with H₂O and extracted with DCM (2 × 50 mL). The combined organic layers were dried over anhydrous Na₂SO₄ and concentrated in *vacuo*. The crude product was purified by flash chromatography (silica gel, 5:1 petroleum ether/EtOAc) to afford 4-acetylbenzoate **S1ac** or **S1ad**.

3-(Trimethylsilyl)prop-2-yn-1-yl 4-acetylbenzoate (**S1ac**)



White solid (6.69 g, 80% yield)

R_f = 0.5 (5:1 petroleum ether/EtOAc)

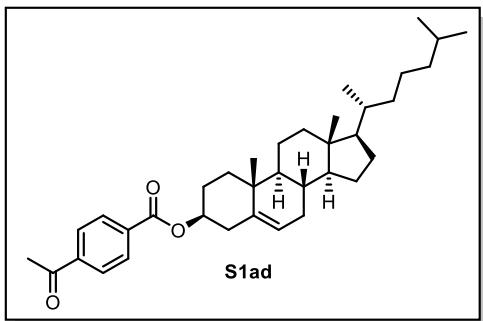
¹H NMR (400 MHz, Chloroform-d) δ 7.95 (d, J = 8.1 Hz, 2H), 7.81 (d, J = 8.1 Hz, 2H), 4.76 (s, 2H), 2.44 (s, 3H), 0.00 (s, 9H).

¹³C NMR (101 MHz, Chloroform-d) δ 197.73, 165.24, 140.75, 133.62, 130.39, 128.52, 98.94, 92.95, 53.95, 27.19, 0.00.

IR ν(cm⁻¹): 2961, 1730, 1690, 1407, 1360, 1260, 1102, 1031.

HRMS (ESI) calcd for C₁₅H₁₈O₃Si [M+Na]⁺ 297.0917, found 297.0911.

Cholesteryl 4-acetylbenzoate (**S1ad**)



White solid (14.36 g, 90% yield)

R_f = 0.5 (5:1 petroleum ether/EtOAc)

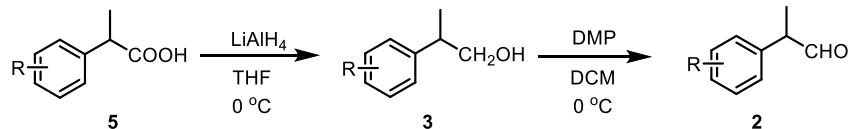
1H NMR (400 MHz, Chloroform-d) δ 8.15 (d, J = 8.2 Hz, 2H), 8.02 (d, J = 8.1 Hz, 2H), 5.45 (d, J = 5.0 Hz, 1H), 4.91 (td, J = 12.3, 8.7, 4.5 Hz, 1H), 2.67 (s, 3H), 2.50 (d, J = 8.0 Hz, 2H), 2.09 - 1.92 (m, 4H), 1.91 - 1.71 (m, 2H), 1.67 - 0.97 (m, 23H), 0.95 (d, J = 6.5 Hz, 3H), 0.89 (dd, J = 6.7, 1.8 Hz, 6H), 0.71 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-d) δ 197.60, 165.13, 140.10, 139.48, 134.66, 129.80, 128.14, 122.99, 75.21, 56.71, 56.16, 50.06, 42.34, 39.75, 39.54, 38.17, 37.02, 36.67, 36.20, 35.81, 31.95, 31.89, 28.25, 28.03, 27.86, 26.90, 24.31, 23.85, 22.84, 22.58, 21.07, 19.39, 18.74, 11.88.

IR ν (cm⁻¹): 2932, 1710, 1681, 1418, 1364, 1320, 1278, 1124.

HRMS (ESI) calcd for C₃₆H₅₂O₃ [M+Na]⁺ 555.3809, found 555.3820.

3.4. General procedure B

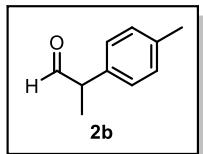


A round-bottomed flask was charged with LiAlH₄ (2.4 g, 60 mmol, 2 equiv) and THF (50 mL). α -branched carboxylic acid **5** (30 mmol, 1 equiv) dissolved in THF (10 mL) was added dropwise into the suspension at 0°C. After stirring at room temperature for 1 h, the reaction was quenched by the slow dropwise addition of H₂O (2.5 mL), aqueous 1.5 M NaOH (2.5 mL) and H₂O (7.5 mL) at 0°C. The resultant mixture was treated with Na₂SO₄ (5 g) and filtered. The filtrate was concentrated to afford alcohol **3** without further purification.

To a solution of alcohol **3** (10 mmol, 1 equiv) in dry DCM (50 mL) was added Dess-Martin Periodinane (12 mmol, 1.2 equiv, 5.09 g) at 0°C. After stirring at 0°C for 1 h, the oxidant was quenched by adding a 1:1 mixture of Na₂S₂O₃ and NaHCO₃ saturated aqueous (50 mL). The

aqueous phase was extracted with DCM. The combined organic layers were dried over anhydrous Na₂SO₄, and concentrated in *vacuo*. The crude product was purified by flash chromatography (silica gel, 50:1 to 2:1 petroleum ether/EtOAc) to afford α -branched aldehyde **2**.

2-(*p*-Tolyl)propanal (**2b**)



Prepared according to general procedure A as colorless liquid (1.67 g, 38 % yield over two steps).

R_f = 0.6 (10:1 petroleum ether/EtOAc)

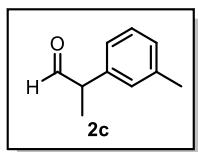
¹H NMR (400 MHz, Chloroform-d) δ 9.69 (s, 1H), 7.22 (d, *J* = 7.8 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 3.63 (q, *J* = 7.2 Hz, 1H), 2.38 (s, 3H), 1.45 (d, *J* = 7.0 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 201.22, 137.26, 134.64, 129.78, 128.21, 52.63, 21.06, 14.64.

IR ν (cm⁻¹): 3052, 3024, 2978, 2930, 2874, 2814, 2718, 1722, 1514, 1454, 1267, 1019.

HRMS (ESI) calcd for C₁₀H₁₂O [M+Na]⁺ 171.0780, found 171.0776.

2-(*m*-Tolyl)propanal (**2c**)



Prepared according to general procedure A as colorless liquid (1.55 g, 35 % yield over two steps).

R_f = 0.6 (10:1 petroleum ether/EtOAc)

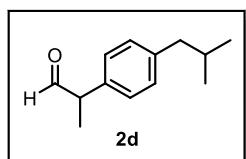
¹H NMR (400 MHz, Chloroform-d) δ 9.70 (d, *J* = 1.4 Hz, 1H), 7.33 - 7.24 (m, 1H), 7.15 (d, *J* = 7.6 Hz, 1H), 7.04 (d, *J* = 6.1 Hz, 2H), 3.62 (q, *J* = 7.0 Hz, 1H), 2.39 (s, 2H), 1.46 (d, *J* = 7.1 Hz, 2H).

¹³C NMR (101 MHz, Chloroform-d) δ 201.18, 138.82, 137.64, 129.07, 128.97, 128.29, 125.36, 52.99, 21.41, 14.61.

IR ν (cm⁻¹): 3055, 2981, 2933, 2817, 2722, 1721, 1606, 1490, 1454, 1265.

HRMS (ESI) calcd for C₁₀H₁₂O [M+Na]⁺ 171.0780, found 171.0776.

2-(4-Isobutylphenyl)propanal (2d**)**



Prepared according to general procedure B as colorless liquid (2.10 g, 37 % yield over two steps).

R_f = 0.5 (10:1 petroleum ether/EtOAc)

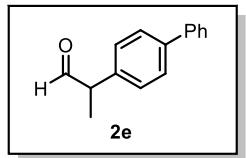
¹H NMR (400 MHz, Chloroform-d) δ 9.70 (d, *J* = 1.5 Hz, 1H), 7.21 - 7.11 (m, 4H), 3.63 (qd, *J* = 7.1, 1.5 Hz, 1H), 2.50 (d, *J* = 7.2 Hz, 2H), 1.89 (dp, *J* = 13.5, 6.8 Hz, 1H), 1.46 (d, *J* = 7.1 Hz, 3H), 0.93 (d, *J* = 6.6 Hz, 6H).

¹³C NMR (101 MHz, Chloroform-d) δ 201.26, 141.05, 134.85, 129.81, 128.02, 52.65, 45.02, 30.20, 22.37, 14.58.

IR ν (cm⁻¹): 3053, 2957, 2929, 2870, 2816, 2718, 1722, 1513, 1465, 1265, 1019.

HRMS (ESI) calcd for C₁₃H₁₈O [M+Na]⁺ 213.1250, found 213.1248.

2-([1,1'-Biphenyl]-4-yl)propanal (2e**)**



Prepared according to general procedure A as white solid (2.11 g, 33 % yield over two steps).

R_f = 0.4 (10:1 petroleum ether/EtOAc)

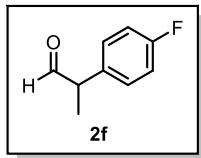
¹H NMR (400 MHz, Chloroform-d) δ 9.77 (s, 1H), 7.65 (m, *J* = 8.8, 7.3 Hz, 4H), 7.50 (t, *J* = 7.7 Hz, 2H), 7.46 - 7.37 (m, 1H), 7.34 (d, *J* = 8.2 Hz, 2H), 3.73 (qd, *J* = 7.0, 1.3 Hz, 1H), 1.54 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 201.12, 137.75, 129.11, 128.34, 127.55, 53.04, 14.63.

IR ν (cm⁻¹): 3055, 3030, 2979, 2933, 2875, 2817, 2719, 1720, 1682, 1602, 1486, 1450, 1406, 1264, 1075, 1008.

HRMS (ESI) calcd for C₁₅H₁₄O [M+Na]⁺ 233.0937, found 233.0934.

2-(4-Fluorophenyl)propanal (2f**)**



Prepared according to general procedure A as colorless liquid (1.80 g, 39 % yield over two steps).

R_f = 0.5 (10:1 petroleum ether/EtOAc)

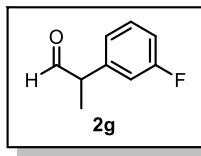
¹H NMR (400 MHz, Chloroform-d) δ 9.69 (d, *J* = 1.4 Hz, 1H), 7.20 (dd, *J* = 8.6, 5.3 Hz, 2H), 7.09 (t, *J* = 8.6 Hz, 2H), 3.65 (qd, *J* = 7.1, 1.3 Hz, 1H), 1.46 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.69, 162.21 (d, *J* = 246.3 Hz), 133.42, 129.83 (d, *J* = 8.1 Hz), 115.98 (d, *J* = 21.6 Hz), 52.18, 14.75.

IR ν (cm⁻¹): 3055, 2984, 2938, 2821, 2723, 1722, 1603, 1510, 1265, 1225, 1161.

HRMS (ESI) calcd for C₉H₉FO [M+Na]⁺ 175.0530, found 175.0527.

2-(3-Fluorophenyl)propanal (**2g**)



Prepared according to general procedure A as colorless liquid (1.56 g, 34 % yield over two steps).

R_f = 0.5 (10:1 petroleum ether/EtOAc)

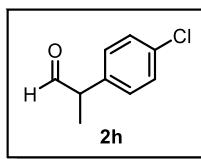
¹H NMR (400 MHz, Chloroform-d) δ 9.62 (s, 1H), 7.29 (m, *J* = 8.0, 5.9 Hz, 1H), 7.00 - 6.86 (m, 3H), 3.60 (q, *J* = 7.1 Hz, 1H), 1.39 (d, *J* = 7.2 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.15, 163.12 (d, *J* = 246.7 Hz), 140.37 (d, *J* = 7.1 Hz), 130.51 (d, *J* = 8.3 Hz), 124.01 (d, *J* = 2.9 Hz), 115.16 (d, *J* = 21.6 Hz), 114.32 (d, *J* = 20.9 Hz), 52.48, 14.30.

IR ν (cm⁻¹): 3065, 2981, 2973, 2818, 2725, 1727, 1614, 1591, 1490, 1450, 1267, 1149.

HRMS (ESI) calcd for C₉H₉FO [M+Na]⁺ 175.0530, found 175.0525

2-(4-Chlorophenyl)propanal (**2h**)



Prepared according to general procedure A as colorless liquid (2.13 g, 42 % yield over two steps).

R_f = 0.4 (10:1 petroleum ether/EtOAc)

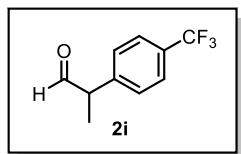
¹H NMR (400 MHz, Chloroform-d) δ 9.68 (s, 1H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.2 Hz, 2H), 3.63 (q, *J* = 7.1 Hz, 1H), 1.45 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.41, 136.20, 133.48, 129.63, 129.21, 52.30, 14.61.

IR ν (cm⁻¹): 3055, 2981, 2935, 2820, 2722, 1726, 1493, 1264, 1094, 1014.

HRMS (ESI) calcd for C₉H₉ClO [M+Na]⁺ 191.0234, found 191.0231.

2-(4-(Trifluoromethyl)phenyl)propanal (**2i**)



Prepared according to general procedure A as colorless liquid (2.31 g, 38 % yield over two steps).

R_f = 0.5 (10:1 petroleum ether/EtOAc)

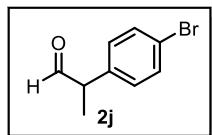
¹H NMR (400 MHz, Chloroform-d) δ 9.72 (d, *J* = 1.4 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 3.74 (q, *J* = 7.2 Hz, 1H), 1.50 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.11, 141.82, 129.89 (q, *J* = 32.6 Hz), 128.70, 125.97 (q, *J* = 3.9 Hz), 124.03 (q, *J* = 272.0 Hz), 52.75, 14.60.

IR ν (cm⁻¹): 2982, 2939, 2883, 2823, 2724, 1726, 1620, 1327, 1166, 1122, 1070, 1017.

HRMS (APCI) calcd for C₁₀H₉F₃O [M+H]⁺ 203.0678, found 203.0685.

2-(4-Bromophenyl)propanal (**2j**)



Prepared according to general procedure A as colorless liquid (1.72 g, 27 % yield over two steps).

R_f = 0.5 (10:1 petroleum ether/EtOAc)

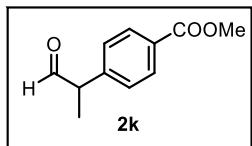
¹H NMR (400 MHz, Chloroform-d) δ 9.65 (d, *J* = 1.4 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.09 (d, *J* = 8.2 Hz, 2H), 3.61 (q, *J* = 7.1 Hz, 1H), 1.43 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.35, 136.71, 132.20, 129.99, 121.60, 52.39, 14.58.

IR ν (cm⁻¹): 3054, 2980, 2935, 2877, 2819, 2721, 1725, 1489, 1265, 1075, 1010.

HRMS (ESI) calcd for C₉H₉BrO [M+Na]⁺ 234.9729, found 234.9722.

Methyl 4-(1-oxopropan-2-yl)benzoate (**2k**)



Prepared according to general procedure A as colorless liquid (1.73 g, 30 % yield over two steps).

R_f = 0.3 (10:1 petroleum ether/EtOAc)

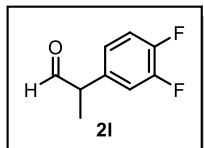
¹H NMR (400 MHz, Chloroform-d) δ 9.72 (d, *J* = 1.3 Hz, 1H), 8.14 - 7.99 (d, 2H), 7.31 (d, *J* = 8.3 Hz, 2H), 3.94 (s, 3H), 3.73 (qd, *J* = 7.1, 1.3 Hz, 1H), 1.50 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.24, 166.72, 142.89, 130.32, 129.49, 128.35, 52.96, 52.19, 14.57.

IR ν (cm⁻¹): 3059, 2981, 2953, 2823, 2722, 1721, 1610, 1436, 1281, 1183, 1113, 1018.

HRMS (ESI) calcd for C₁₁H₁₂O₃ [M+Na]⁺ 215.0679, found 215.0674

2-(3,4-Difluorophenyl)propanal (**2l**)



Prepared according to general procedure A as colorless liquid (1.97 g, 39 % yield over two steps).

R_f = 0.5 (10:1 petroleum ether/EtOAc)

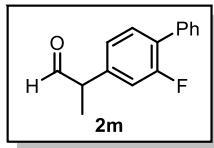
¹H NMR (400 MHz, Chloroform-d) δ 9.68 (d, *J* = 1.3 Hz, 1H), 7.19 (dt, *J* = 10.3, 8.3 Hz, 1H), 7.05 (ddd, *J* = 11.1, 7.4, 2.2 Hz, 1H), 6.96 (ddt, *J* = 8.1, 3.9, 1.8 Hz, 1H), 3.64 (qd, *J* = 7.1, 1.3 Hz, 1H), 1.46 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.06, 150.59 (dd, *J* = 249.3, 12.8 Hz), 149.76 (dd, *J* = 248.4, 12.6 Hz), 134.59, 124.34 (dd, *J* = 6.5, 3.6 Hz), 117.82 (d, *J* = 17.2 Hz), 117.19 (d, *J* = 17.5 Hz), 52.01, 14.61.

IR ν (cm⁻¹): 3056, 2984, 2939, 2880, 2821, 2725, 1729, 1609, 1520, 1433, 1265, 1212, 1123.

HRMS (APCI) calcd for C₉H₈F₂O [M+H]⁺ 171.0616, found 171.0620.

2-(2-Fluoro-[1,1'-biphenyl]-4-yl)propanal (**2m**)



Prepared according to general procedure B as pale-yellow liquid (1.09 g, 16 % yield over two steps).

R_f = 0.5 (5:1 petroleum ether/EtOAc)

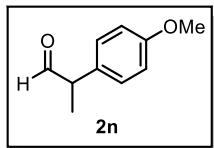
¹H NMR (400 MHz, Chloroform-d) δ 9.75 (d, *J* = 1.4 Hz, 1H), 7.57 (dt, *J* = 8.1, 1.5 Hz, 2H), 7.51 - 7.45 (m, 3H), 7.43 - 7.38 (m, 1H), 7.12 - 7.03 (m, 2H), 3.71 (qd, *J* = 7.1, 1.4 Hz, 1H), 1.52 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.24, 159.99 (d, *J* = 249.1 Hz), 139.07 (d, *J* = 7.4 Hz), 135.29, 131.30 (d, *J* = 4.0 Hz), 128.96 (d, *J* = 2.9 Hz), 128.52, 127.83, 124.29 (d, *J* = 3.3 Hz), 115.96 (d, *J* = 23.5 Hz), 52.40, 14.50.

IR ν (cm⁻¹): 3057, 2981, 2935, 2819, 2721, 1727, 1484, 1419, 1265, 1133.

HRMS (ESI) calcd for C₁₅H₁₃FO [M+Na]⁺ 251.0843, found 251.0839.

2-(4-Methoxyphenyl)propanal (**2n**)



Prepared according to general procedure A as colorless liquid (1.32 g, 27 % yield over two steps).

R_f = 0.3 (10:1 petroleum ether/EtOAc)

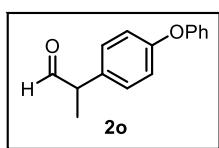
¹H NMR (400 MHz, Chloroform-d) δ 9.67 (d, *J* = 1.5 Hz, 1H), 7.15 (d, *J* = 8.6 Hz, 2H), 6.94 (d, *J* = 8.7 Hz, 1H), 3.83 (s, 3H), 3.61 (qd, *J* = 7.1, 1.5 Hz, 1H), 1.44 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 201.15, 159.03, 129.59, 129.35, 114.52, 55.30, 52.15, 14.67.

IR ν (cm⁻¹): 3055, 2977, 2936, 2837, 2717, 1719, 1610, 1513, 1264, 1180, 1026.

HRMS (ESI) calcd for C₁₀H₁₂O₂ [M+Na]⁺ 187.0730, found 187.0727.

2-(4-Phenoxyphenyl)propanal (**2o**)



Prepared according to general procedure A as colorless liquid (1.44 g, 21 % yield over two steps).

R_f = 0.5 (5:1 petroleum ether/EtOAc)

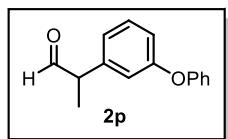
¹H NMR (400 MHz, Chloroform-d) δ 9.71 (d, *J* = 1.5 Hz, 1H), 7.40 - 7.34 (m, 2H), 7.22 - 7.17 (m, 2H), 7.17 - 7.12 (m, 1H), 7.07 - 7.01 (m, 4H), 3.65 (qd, *J* = 7.1, 1.4 Hz, 1H), 1.47 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 201.01, 156.93, 156.83, 132.24, 129.83, 129.64, 123.52, 119.26, 119.07, 52.29, 14.71.

IR ν (cm⁻¹): 3055, 2981, 2934, 2875, 2818, 2720, 1723, 1589, 1506, 1489, 1264, 1238, 1170, 1024, 1014.

HRMS (ESI) calcd for C₁₅H₁₄O₂ [M+Na]⁺ 249.0886, found 249.0882.

2-(3-Phenoxyphenyl)propanal (**2p**)



Prepared according to general procedure A as pale-yellow liquid (1.33 g, 20% yield over two steps).

R_f = 0.5 (5:1 petroleum ether/EtOAc)

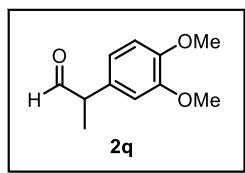
¹H NMR (400 MHz, Chloroform-d) δ 9.71 (d, *J* = 1.4 Hz, 1H), 7.43 - 7.31 (m, 3H), 7.21 - 7.11 (m, 1H), 7.08 - 7.01 (m, 2H), 7.00 - 6.89 (m, 3H), 3.63 (qd, *J* = 7.0, 1.4 Hz, 1H), 1.46 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.66, 158.02, 156.86, 139.81, 130.37, 129.90, 123.61, 123.00, 119.12, 118.68, 117.64, 52.83, 14.55.

IR ν (cm⁻¹): 2930, 1728, 1583, 1487, 1443, 1240, 1210, 1163.

HRMS (ESI) calcd for C₁₅H₁₄O₂ [M+Na]⁺ 249.0886, found 249.0880.

2-(3,4-Dimethoxyphenyl)propanal (**2q**)



Prepared according to general procedure A as white solid (2.11 g, 36 % yield over two steps).

R_f = 0.2 (5:1 petroleum ether/EtOAc)

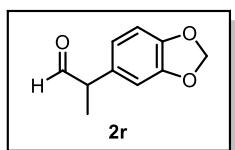
¹H NMR (400 MHz, Chloroform-d) δ 9.67 (d, *J* = 1.7 Hz, 1H), 6.90 (dd, *J* = 8.2, 1.8 Hz, 1H), 6.78 (dt, *J* = 8.2, 2.1 Hz, 1H), 6.70 (d, *J* = 1.9 Hz, 1H), 3.90 (s, 3H), 3.89 (s, 3H), 3.59 (qt, *J* = 7.0, 1.7 Hz, 1H), 1.44 (dd, *J* = 7.1, 2.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.97, 149.45, 148.52, 130.02, 120.47, 111.67, 111.33, 55.94, 55.92, 52.55, 14.60.

IR ν (cm⁻¹): 3057, 3000, 2973, 2937, 2837, 2717, 1723, 1592, 1517, 1464, 1419, 1264, 1145, 1027.

HRMS (ESI) calcd for C₁₁H₁₄O₃ [M+Na]⁺ 217.0835, found 217.0813.

2-(Benzo[d][1,3]dioxol-5-yl)propanal (**2r**)



Prepared according to general procedure A as colorless liquid (2.38 g, 42 % yield over two steps).

R_f = 0.5 (5:1 petroleum ether/EtOAc)

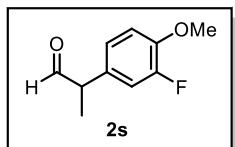
¹H NMR (400 MHz, Chloroform-d) δ 9.65 (d, *J* = 1.6 Hz, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 6.75 - 6.60 (m, 2H), 5.98 (s, 2H), 3.57 (q, *J* = 7.0 Hz, 1H), 1.42 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.81, 148.27, 147.04, 131.34, 121.59, 108.76, 108.52, 101.18, 52.58, 14.71.

IR ν (cm⁻¹): 3065, 2980, 2934, 2895, 2817, 2780, 2719, 1725, 1505, 1487, 1440, 1265, 1247, 1040.

HRMS (ESI) calcd for C₁₀H₁₀O₃ [M+Na]⁺ 201.0522, found 201.0520.

2-(3-Fluoro-4-methoxyphenyl)propanal (**2s**)



Prepared according to general procedure A as colorless liquid (1.61 g, 29 % yield over two steps).

R_f = 0.3 (10:1 petroleum ether/EtOAc)

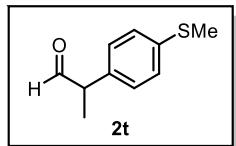
¹H NMR (400 MHz, Chloroform-d) δ 9.66 (d, *J* = 1.4 Hz, 1H), 7.04 - 6.86 (m, 3H), 3.91 (s, 3H), 3.59 (qd, *J* = 7.1, 1.4 Hz, 1H), 1.43 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.50, 152.60 (d, *J* = 247.1 Hz), 147.04 (d, *J* = 10.7 Hz), 130.47 (d, *J* = 6.0 Hz), 124.04 (d, *J* = 3.6 Hz), 116.04, 115.85, 113.89 (d, *J* = 2.3 Hz), 56.32, 51.92, 14.52.

IR ν (cm⁻¹): 3056, 2978, 2938, 2842, 2722, 1726, 1519, 1444, 1266, 1221, 1133, 1025.

HRMS (ESI) calcd for C₁₀H₁₁FO₂ [M+Na]⁺ 205.0635, found 205.0632.

2-(4-(Methylthio)phenyl)propanal (**2t**)



Prepared according to general procedure A as white solid (2.68 g, 50 % yield over two steps).

R_f = 0.5 (5:1 petroleum ether/EtOAc)

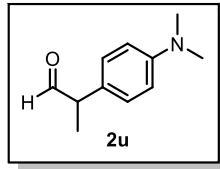
¹H NMR (400 MHz, Chloroform-d) δ 9.68 (d, *J* = 1.4 Hz, 1H), 7.33 - 7.25 (m, 2H), 7.19 - 7.12 (m, 2H), 3.62 (qd, *J* = 7.1, 1.4 Hz, 1H), 2.51 (s, 3H), 1.45 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.80, 137.92, 134.41, 128.76, 127.22, 52.46, 15.84, 14.57.

IR ν (cm⁻¹): 3053, 3021, 2978, 2923, 2874, 2819, 2718, 1722, 1598, 1495, 1438, 1407, 1266, 1096, 1014.

HRMS (ESI) calcd for C₁₀H₁₂OS [M+Na]⁺ 203.0501, found 203.0499.

2-(4-(Dimethylamino)phenyl)propanal (**2u**)



Prepared according to general procedure A as colorless liquid (1.70 g, 32 % yield over two steps).

R_f = 0.3 (5:1 petroleum ether/EtOAc)

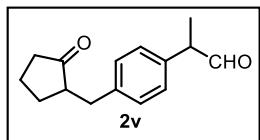
¹H NMR (400 MHz, Chloroform-d) δ 9.65 (d, *J* = 1.6 Hz, 1H), 7.14 - 7.03 (m, 2H), 6.79 - 6.72 (m, 2H), 3.56 (qd, *J* = 7.0, 1.6 Hz, 1H), 2.97 (s, 6H), 1.42 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 201.41, 150.01, 129.03, 124.94, 113.06, 52.06, 40.56, 14.54.

IR $\nu(\text{cm}^{-1})$: 3054, 2977, 2933, 2880, 2807, 2714, 1717, 1613, 1522, 1446, 1352, 1265, 1166.

HRMS (ESI) calcd for $\text{C}_{11}\text{H}_{15}\text{NO}$ [$\text{M}+\text{H}]^+$ 178.1226, found 178.1224.

2-(4-((2-Oxocyclopentyl)methyl)phenyl)propanal (**2v**)



Prepared according to general procedure B as pale-yellow liquid (1.72 g, 25 % yield over two steps).

R_f = 0.3 (5:1 petroleum ether/EtOAc)

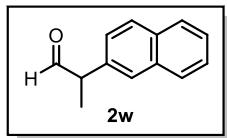
¹H NMR (400 MHz, Chloroform-d) δ 9.65 (d, J = 1.4 Hz, 1H), 7.18 (d, J = 8.2 Hz, 2H), 7.12 (d, J = 8.2 Hz, 2H), 3.65 - 3.56 (m, 1H), 3.13 (dd, J = 13.9, 4.2 Hz, 1H), 2.54 (dd, J = 13.9, 9.4 Hz, 1H), 2.40 - 2.26 (m, 2H), 2.17 - 2.02 (m, 2H), 2.02 - 1.89 (m, 1H), 1.73 (td, J = 19.0, 10.6 Hz, 1H), 1.55 (ddd, J = 10.8, 6.3, 3.0 Hz, 1H), 1.42 (d, J = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 220.12, 201.17, 139.39, 135.46, 129.62, 128.39, 52.62, 50.99, 38.19, 35.18, 29.22, 20.55, 14.59.

IR $\nu(\text{cm}^{-1})$: 3054, 2970, 2936, 2877, 2819, 2719, 1736, 1513, 1453, 1405, 1265, 1154, 1019.

HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{18}\text{O}_2$ [$\text{M}+\text{Na}]^+$ 253.1199, found 253.1195.

2-(Naphthalen-2-yl)propanal (**2w**)



Prepared according to general procedure A as white solid (1.65 g, 30 % yield over two steps).

R_f = 0.4 (10:1 petroleum ether/EtOAc)

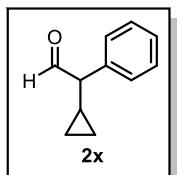
¹H NMR (400 MHz, Chloroform-d) δ 9.80 (d, J = 1.5 Hz, 1H), 7.95 - 7.79 (m, 3H), 7.76 - 7.67 (m, 1H), 7.60 - 7.44 (m, 2H), 7.35 (dd, J = 8.5, 1.8 Hz, 1H), 3.83 (qd, J = 7.1, 1.5 Hz, 1H), 1.57 (d, J = 7.0 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 201.02, 135.17, 133.66, 132.72, 128.89, 127.74, 127.22, 126.46, 126.22, 126.14, 53.14, 14.68.

IR ν(cm⁻¹): 3055, 2980, 2935, 2817, 2718, 1720, 1600, 1508, 1264.

HRMS (ESI) calcd for C₁₃H₁₂O [M+Na]⁺ 207.0780, found 207.0778.

2-Cyclopropyl-2-phenylacetaldehyde (**2x**)



Prepared according to general procedure A as colorless liquid (2.42 g, 50 % yield over two steps).

R_f = 0.5 (10:1 petroleum ether/EtOAc)

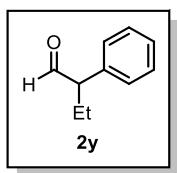
¹H NMR (400 MHz, Chloroform-d) δ 9.78 (d, *J* = 2.6 Hz, 1H), 7.41 (t, *J* = 7.4 Hz, 2H), 7.38 - 7.32 (m, 1H), 7.32 - 7.26 (m, 2H), 2.84 (dt, *J* = 10.0, 2.2 Hz, 1H), 1.42 - 1.30 (m, 1H), 0.78 (tt, *J* = 8.3, 5.2 Hz, 1H), 0.69 - 0.60 (m, 1H), 0.41 (dq, *J* = 10.5, 5.3 Hz, 1H), 0.26 (dq, *J* = 10.0, 5.1 Hz, 1H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.38, 136.33, 128.92, 128.65, 127.56, 63.30, 10.97, 4.54, 3.41.

IR ν(cm⁻¹): 3082, 3056, 3030, 3006, 2819, 2719, 1724, 1493, 1453, 1422, 1265, 1025.

HRMS (ESI) calcd for C₁₁H₁₂O₂ [M+Na]⁺ 183.0780, found 183.0778.

2-Phenylbutanal (**2y**)



Prepared according to general procedure A as colorless liquid (1.97 g, 44 % yield over two steps).

R_f = 0.5 (10:1 petroleum ether/EtOAc)

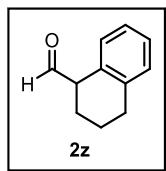
¹H NMR (400 MHz, Chloroform-d) δ 9.70 (d, *J* = 2.0 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.3 Hz, 1H), 7.22 (d, *J* = 7.3 Hz, 2H), 3.51 - 3.26 (m, 1H), 2.14 (dt, *J* = 14.2, 7.1 Hz, 1H), 1.79 (dt, *J* = 14.5, 7.5 Hz, 1H), 0.93 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 201.02, 136.31, 129.01, 128.83, 127.53, 60.88, 22.95, 11.72.

IR ν (cm⁻¹): 3062, 3030, 2966, 2934, 2876, 2817, 2715, 1723, 1601, 1493, 1454, 1267, 1128, 1028.

HRMS (ESI) calcd for C₁₀H₁₂O [M+Na]⁺ 171.0780, found 171.0777.

1,2,3,4-Tetrahydronaphthalene-1-carbaldehyde (**2z**)



Prepared according to general procedure A as colorless liquid (1.07 g, 22 % yield over two steps).

R_f = 0.5 (10:1 petroleum ether/EtOAc)

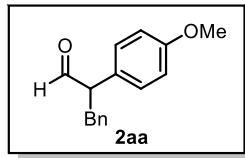
¹H NMR (400 MHz, Chloroform-d) δ 9.71 (d, *J* = 2.2 Hz, 1H), 7.28 - 7.19 (m, 2H), 7.22 - 7.15 (m, 2H), 3.62 (td, *J* = 6.6, 6.2, 2.0 Hz, 1H), 2.82 (t, *J* = 6.3 Hz, 2H), 2.32 - 2.20 (m, 1H), 2.03 - 1.90 (m, 1H), 1.89 - 1.77 (m, 1H).

¹³C NMR (101 MHz, Chloroform-d) δ 202.05, 138.05, 130.88, 129.80, 129.61, 127.16, 126.19, 51.70, 29.18, 23.02, 20.51.

IR ν (cm⁻¹): 3057, 3020, 2937, 2866, 2839, 2724, 1723, 1491, 1451, 1265.

HRMS (ESI) calcd for C₁₁H₁₂O [M+Na]⁺ 183.0780, found 183.0779.

2-(4-methoxyphenyl)-3-phenylpropanal (**2aa**)



Prepared according to reported method (31) as colorless solid (2.18 g, 18 % yield).

R_f = 0.5 (5:1 petroleum ether/EtOAc)

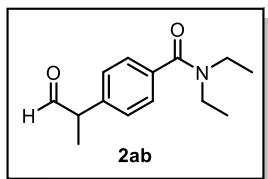
¹H NMR (400 MHz, Chloroform-d) δ 9.71 (d, *J* = 1.5 Hz, 1H), 7.24 - 7.11 (m, 3H), 7.04 (m, 4H), 6.89 - 6.84 (m, 2H), 3.79 (s, 3H), 3.78 (td, *J* = 7.3, 1.4 Hz, 1H), 3.43 (dABq, *J* = 14.0, 6.7 Hz, 1H), 2.93 (dABq, *J* = 14.0, 8.0 Hz, 1H).

¹³C NMR (101 MHz, Chloroform-d) δ 199.92, 159.12, 138.93, 130.09, 129.06, 128.33, 127.51, 126.26, 114.47, 60.10, 55.27, 36.19.

IR ν (cm⁻¹): 3018, 2957, 2936, 2838, 1721, 1610, 1512, 1455, 1253, 1215, 1180, 1034.

HRMS (ESI) calcd for C₁₆H₁₆O₂ [M+H]⁺ 241.1223, found: 241.1402.

N,N-diethyl-4-(1-oxopropan-2-yl)benzamide (**2ab**)



Prepared according to general procedure A as yellow liquid (1.48 g, 31% yield over two steps).

R_f = 0.5 (2:1 petroleum ether/EtOAc)

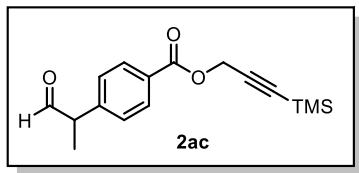
¹H NMR (400 MHz, Chloroform-d) δ 9.68 (d, *J* = 1.3 Hz, 1H), 7.38 (d, *J* = 7.9 Hz, 2H), 7.25 (d, 2H), 3.66 (q, *J* = 7.1 Hz, 1H), 3.59 - 3.20 (m, 4H), 1.45 (d, *J* = 7.1 Hz, 3H), 1.31 - 1.05 (m, 6H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.61, 170.79, 138.75, 136.57, 128.37, 127.07, 52.77, 43.27, 39.25, 14.58, 14.23, 12.89.

IR ν (cm⁻¹): 2975, 2943, 1721, 1626, 1429, 1382, 1288, 1098, 1019.

HRMS (ESI) calcd for C₁₄H₁₉NO₂ [M+H]⁺ 234.1489, found: 234.1480.

3-(Trimethylsilyl)prop-2-yn-1-yl 4-(1-oxopropan-2-yl)benzoate (**2ac**)



Prepared according to general procedure A as yellow liquid (0.79 g, 27% yield over two steps).

R_f = 0.5 (5:1 petroleum ether/EtOAc)

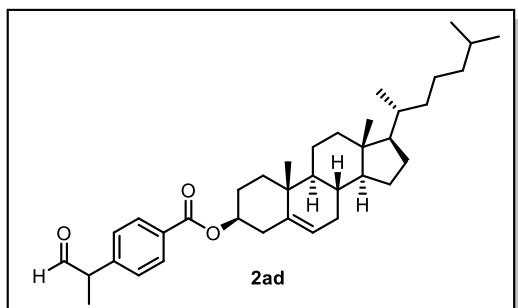
¹H NMR (400 MHz, Chloroform-d) δ 9.71 (d, *J* = 1.4 Hz, 1H), 8.10 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 4.95 (s, 2H), 3.78 - 3.69 (m, 1H), 1.49 (d, *J* = 7.0 Hz, 3H), 0.21 (s, 9H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.12, 165.41, 143.27, 130.58, 130.10, 128.94, 128.38, 128.22, 98.96, 92.31, 53.29, 52.97, 14.58, -0.29.

IR ν(cm⁻¹): 2975, 2943, 1721, 1626, 1429, 1382, 1288, 1098, 1019.

HRMS (ESI) calcd for C₁₆H₂₀SiO₃ [M+Na]⁺ 311.1074, found: 311.1065.

Cholesteryl 4-(1-oxopropan-2-yl)benzoate (**2ad**)



Prepared according to general procedure A as yellow solid (0.84 g, 30 % yield over two steps).

R_f = 0.5 (5:1 petroleum ether/EtOAc)

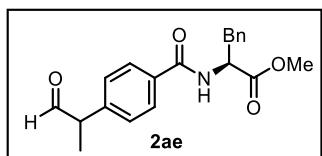
¹H NMR (400 MHz, Chloroform-d) δ 9.71 (d, J = 1.3 Hz, 1H), 8.07 (d, J = 8.0 Hz, 2H), 7.35 - 7.22 (m, 2H), 5.44 (d, J = 5.1 Hz, 1H), 4.88 (dtd, J = 12.5, 8.5, 4.5 Hz, 1H), 3.73 (q, J = 7.1 Hz, 1H), 2.49 (t, J = 7.9 Hz, 2H), 2.10 - 1.88 (m, 5H), 1.67 - 1.45 (m, 10H), 1.41 - 1.33 (m, 3H) 1.29 - 1.00 (m, 14H), 0.95 (d, J = 6.5 Hz, 3H), 0.89 (dd, J = 6.5, 1.8 Hz, 6H), 0.71 (s, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.26, 165.59, 142.67, 139.61, 130.30, 130.20, 128.25, 122.85, 74.71, 56.71, 56.16, 52.98, 50.06, 42.34, 39.76, 39.54, 38.22, 37.04, 36.67, 36.20, 35.82, 31.95, 31.90, 28.25, 28.03, 27.90, 24.31, 23.85, 22.84, 22.58, 21.07, 19.39, 18.74, 14.60, 11.88.

IR ν(cm⁻¹): 2936, 1728, 1583, 1487, 1443, 1240, 1210, 1163.

HRMS (ESI) calcd for C₃₇H₅₄O₃ [M+Na]⁺ 569.3965, found: 569.3963.

Methyl (4-(1-oxopropan-2-yl)benzoyl)-L-phenylalaninate (**2ae**)



Prepared according to general procedure A as yellow liquid (375 mg, 11% yield over two steps).

R_f = 0.5 (1:1 petroleum ether/EtOAc)

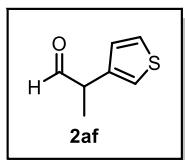
¹H NMR (400 MHz, Chloroform-d) δ 9.68 (s, 1H), 7.74 (d, *J* = 7.9 Hz, 2H), 7.37 - 7.22 (m, 7H), 7.17 - 7.07 (m, 3H), 6.57 (d, *J* = 7.7 Hz, 1H), 5.09 (dt, *J* = 7.6, 5.5 Hz, 1H), 3.77 (s, 3H), 3.69 (d, *J* = 7.1 Hz, 1H), 3.34 - 3.20 (m, 2H), 1.47 (d, *J* = 7.2 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.31, 172.02, 166.31, 141.70, 135.78, 133.17, 129.34, 129.32, 128.71, 128.66, 128.60, 128.58, 127.78, 127.35, 127.25, 53.51, 52.82, 52.48, 37.88, 29.71, 14.59.

IR ν (cm⁻¹): 3307, 2930, 1738, 1644, 1611, 1538, 1498, 1455, 1362, 1268, 1217, 1098.

HRMS (ESI) calcd for C₂₀H₂₁NO₄ [M+H]⁺ 340.1543, found: 340.1535.

2-(thiophen-3-yl)propanal (**2af**)



Prepared according to general procedure A as colorless liquid (525 mg, 15% yield over two steps).

R_f = 0.4 (10:1 petroleum ether/EtOAc)

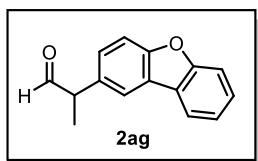
¹H NMR (400 MHz, Chloroform-d) δ 9.67 (d, *J* = 1.8 Hz, 1H), 7.38 (dd, *J* = 5.0, 2.9 Hz, 1H), 7.21 - 7.11 (m, 1H), 7.01 (dd, *J* = 4.9, 1.4 Hz, 1H), 3.77 (dd, *J* = 7.2, 1.8 Hz, 1H), 1.48 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.43, 138.01, 127.12, 126.62, 122.15, 48.30, 14.33.

IR ν (cm⁻¹): 3019, 2978, 2933, 1724, 1215, 1082.

HRMS (APCI) calcd for C₉H₁₀SO [M+H]⁺ 141.0369, found: 141.0366.

2-(dibenzo[b,d]furan-2-yl)propanal (**2ag**)



Prepared according to general procedure A as white solid (1.2 g, 18% yield over two steps).

R_f = 0.5 (5:1 petroleum ether/EtOAc)

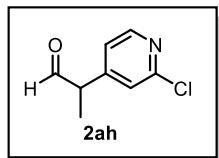
¹H NMR (400 MHz, Chloroform-d) δ 9.79 (d, *J* = 1.4 Hz, 1H), 7.97 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.81 (d, *J* = 1.9 Hz, 1H), 7.60 (dd, *J* = 8.5, 1.5 Hz, 2H), 7.54 - 7.46 (m, 1H), 7.42 - 7.36 (m, 1H), 7.32 (dd, *J* = 8.4, 1.9 Hz, 1H), 3.84 (qd, *J* = 7.0, 1.4 Hz, 1H), 1.57 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 200.99, 156.61, 155.59, 132.20, 127.51, 127.39, 125.03, 123.84, 122.88, 120.71, 120.68, 120.30, 112.21, 111.80, 52.90, 15.14.

IR ν (cm⁻¹): 3019, 2981, 1730, 1483, 1450, 1218, 1199, 1026.

HRMS (APCI) calcd for C₁₅H₁₂O₂ [M+H]⁺ 225.0910, found: 225.0907.

2-(2-chloropyridin-4-yl)propanal (**2ah**)



Prepared according to general procedure A as yellow solid (1.4 g, 27% yield over two steps).

R_f = 0.5 (2:1 petroleum ether/EtOAc)

¹H NMR (400 MHz, Chloroform-d) δ 9.69 (d, *J* = 1.0 Hz, 1H), 8.38 (dd, *J* = 5.2, 1.6 Hz, 1H), 7.25 - 7.17 (m, 1H), 7.10 (dd, *J* = 5.1, 1.5 Hz, 1H), 3.67 (q, *J* = 7.2 Hz, 1H), 1.49 (dt, *J* = 7.3, 1.0 Hz, 3H).

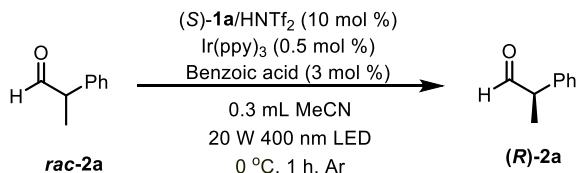
¹³C NMR (101 MHz, Chloroform-d) δ 198.70, 152.25, 150.13, 149.92, 123.99, 122.20, 51.83, 14.05.

IR ν (cm⁻¹): 3019, 2981, 2933, 1730, 1702, 1594, 1547, 1466, 1390, 1215, 1090.

HRMS (ESI) calcd for C₈H₈ClNO [M+H]⁺ 170.0367, found: 170.0366

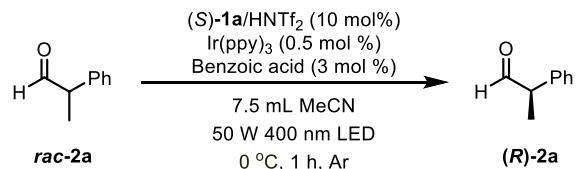
4. Experimental procedures and characterization of products

4.1. General procedure for deracemization (0.2 mmol scale)



To an oven-dried 10 mL Schlenk tube equipped with a magnetic stir bar was added aminocatalyst *(S)*-1a/HNTf₂ (9.1 mg, 10 mol %), Ir(ppy)₃ (0.65 mg, 0.5 mol %) and benzoic acid (0.73 mg, 3 mol %). Freshly prepared α -branched aldehyde **2a** (26.8 mg, 0.2 mmol) dissolved in 0.3 mL MeCN was then added into the tube under Ar atmosphere. The mixture was degassed for 3 times using standard freeze-thaw method and stirred at 0°C under irradiation of 20W 400nm LED for 1h. After the completion of deracemization, the solution was purified by flash column chromatography on a 4~5 cm thick silica gel with 20:1 hexane/EtOAc to give (*R*)-**2a** (19.6 mg, 73%). The *ee* value of the isolated aldehyde was determined by HPLC analysis as 94%. Detailed purification method was discussed below.

4.2. General procedure for deracemization (5 mmol scale)



To an oven-dried 50 mL Schlenk flask equipped with a magnetic stir bar was added aminocatalyst *(S)*-1a/HNTf₂ (227.5 mg, 10 mol %), Ir(ppy)₃ (16 mg, 0.5 mol %) and benzoic acid (18.25 mg, 3 mol %). Freshly prepared α -branched aldehyde **2a** (670 mg, 5 mmol) dissolved in 7.5 mL MeCN was then added into the flask under Ar atmosphere. The mixture was degassed for 3 times using standard freeze-thaw method and stirred at 0°C under irradiation of 50W 400nm LED for 1h. After the completion of deracemization, the solution was purified by flash column chromatography on a 3.5 cm thick silica gel with 20:1 hexane/EtOAc to give (*R*)-**2a** as colorless liquid (536 mg, 80%). The *ee* value of the isolated aldehydes was determined by HPLC analysis as 91%. Detailed purification method was discussed below.

4.3. Photoreactor of deracemization

A 20W 400nm LED fixed on an aluminum block was glued at the bottom of a crystallizing dish by silicone gasket and grease. The temperature was controlled by the ethanol bath and coolant circulation pump.

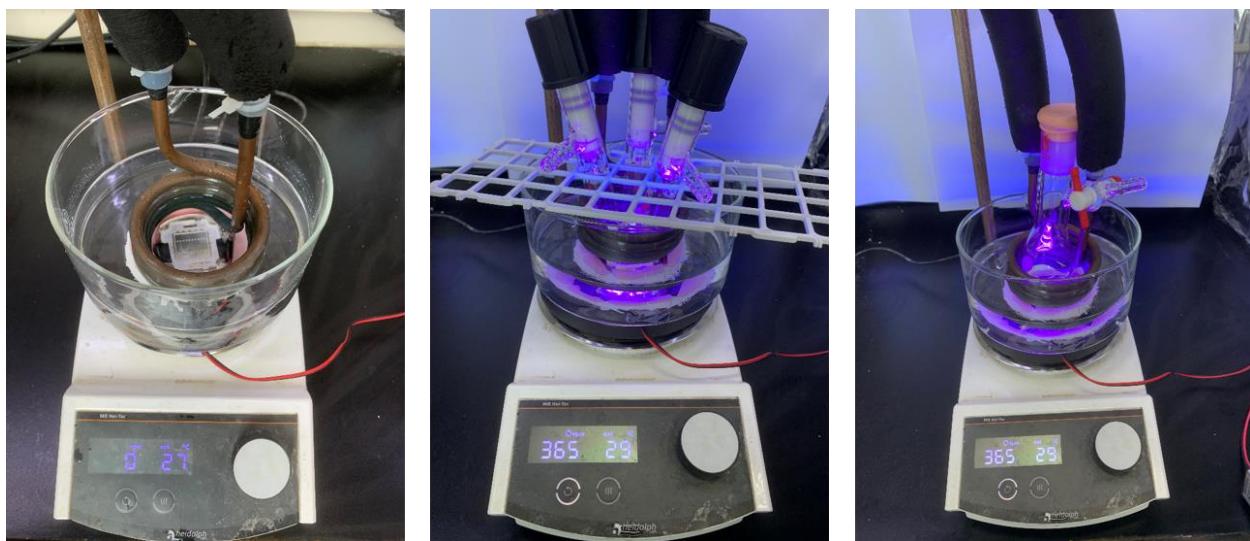


Figure S1. (left) Photoreactor of deracemization. (middle) 0.2 mmol scale reaction setup. (right) 5 mmol scale reaction setup.

4.4. Configurational stability of α -arylaldehyde

Optically pure (*R*)-**2a** and (*S*)-**2a** were prepared according to general procedure B, but the crude products were purified by vacuum distillation instead of flash chromatography. Their enantiomeric excesses were determined to be 99% by HPLC. After being stored in -20°C refrigerator as pure compound for 3 months, the enantiomeric excess of (*R*)-**2a** was determined to be 96%.

4.5. The influence of purification methods on enantiomeric excess

For 0.2 mmol-scale deracemization, four different purification methods were conducted (Table S6, Fig. S2). The *ee* value was able to maintain (94% *ee*) through analytic TLC or short column chromatography, but significantly eroded (0% and 73% *ee*) after purification of preparative TLC or conventional column chromatography. All the substrates in Fig. 2 were treated by both analytic TLC purification and short column chromatography, the differences of *ee* values were negligible.

Analytic TLC purification was also examined on enantiomeric pure (*R*)-**2a** (99% *ee*), the *ee* value was the same as that without any treatment (99% *ee*), which proved that analytic TLC purification would not lead to racemization.

Table S6. The influence of purification methods on *ee* values with (*R*)-2a (94% *ee*)

Purification method	Purpose	Purification Time	Result
Analytic TLC	HPLC analysis	2 min	94% <i>ee</i>
Preparative TLC	Isolated yield	1 h	0% <i>ee</i>
Short column chromatography	Isolated yield	2 min	94% <i>ee</i>
Conventional column chromatography	Isolated yield	10 min	73% <i>ee</i>

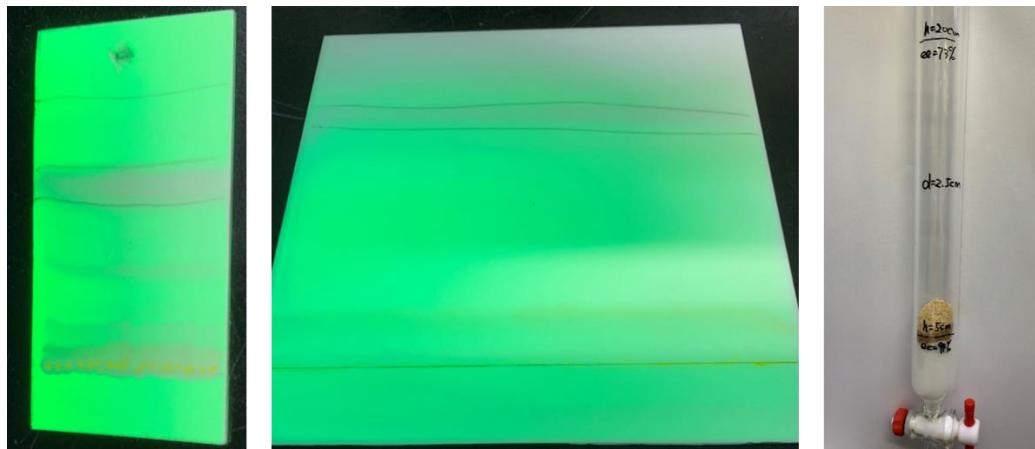


Figure S2. (left) Analytic TLC Purification. (middle) Preparative TLC purification. (right) Short column chromatography with 5cm thick silica gel and conventional column chromatography with 20cm thick silica gel, 2.5 cm-diameter column.

For 5 mmol-scale deracemization, a 7cm-diameter chromatography column was used in purification. We separately loaded 5cm and 3.5cm thick silica gel, resulting (*R*)-**2a** with 89% *ee* and 91% *ee*. Lower silica gel loading could not ensure the purity of product.

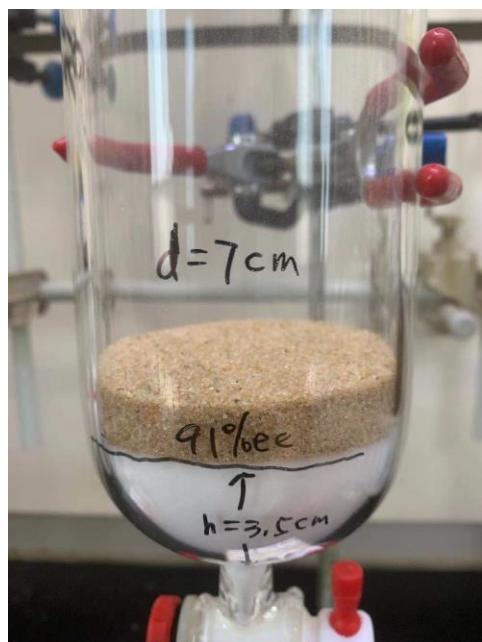
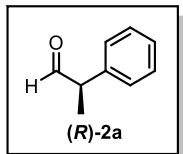


Figure S3. Large scale purification.

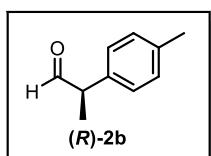
4.6. Characterization of products



Isolated Yield: 73%, 19.6mg

Chiral HPLC (CHIRALPAK AS-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 205 nm): $t_R = 5.53$ min (minor), 7.15 min (major). [94% *ee*]

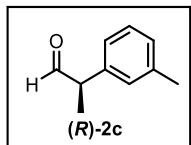
Optical Rotation: $[\alpha]_D^{20} = -224.3$ ($c = 0.96$, CHCl₃).



Isolated Yield: 80%, 23.8mg

Chiral HPLC (CHIRALPAK OD-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 203 nm): $t_R = 6.04$ min (major), 6.99 min (minor). [94% *ee*]

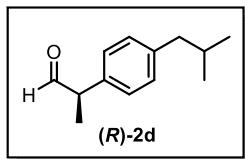
Optical Rotation: $[\alpha]_D^{20} = -200.1$ ($c = 0.85$, CHCl₃).



Isolated Yield: 71%, 21.1mg

Chiral HPLC (CHIRALPAK AS-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 203 nm): $t_R = 5.09$ min (minor), 6.21 min (major). [88% *ee*]

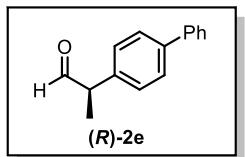
Optical Rotation: $[\alpha]_D^{20} = -137.5$ ($c = 1.06$, CHCl₃).



Isolated Yield: 85%, 32.1mg

Chiral HPLC (CHIRALPAK double OD-H, 1% *i*-PrOH/*n*-heptane, 0.7 mL/min, 205 nm): $t_R = 13.37$ min (major), 16.88 min (minor). [91% *ee*]

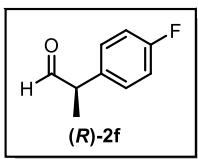
Optical Rotation: $[\alpha]_D^{20} = -128.7$ ($c = 1.47$, CHCl₃).



Isolated Yield: 86%, 37.1mg

Chiral HPLC (CHIRALPAK OD-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 254 nm): $t_R = 12.25$ min (major), 13.73 min (minor). [91% *ee*]

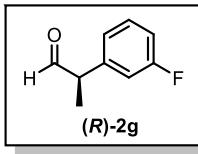
Optical Rotation: $[\alpha]_D^{20} = -151.7$ ($c = 1.29$, CHCl₃).



Isolated Yield: 73%, 22.2mg

Chiral HPLC (CHIRALPAK AS-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 205 nm): $t_R = 6.33$ min (minor), 7.64 min (major). [90% ee]

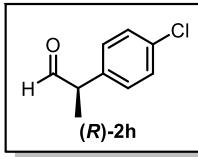
Optical Rotation: $[\alpha]_D^{20} = -120.0$ ($c = 0.62$, CHCl₃).



Isolated Yield: 73%, 22.3mg

Chiral HPLC (CHIRALPAK AS-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 205 nm): $t_R = 5.94$ min (minor), 6.96 min (major). [95% ee]

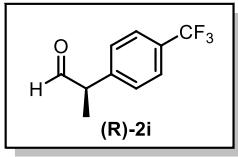
Optical Rotation: $[\alpha]_D^{20} = -60.0$ ($c = 0.34$, CHCl₃).



Isolated Yield: 82%, 27.6mg

Chiral HPLC (CHIRALPAK OJ-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 223 nm): $t_R = 10.52$ min (major), 11.81 min (minor). [95% ee]

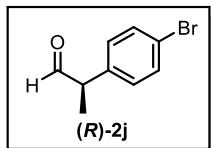
Optical Rotation: $[\alpha]_D^{20} = -123.2$ ($c = 1.09$, CHCl₃).



Isolated Yield: 80%, 32mg

Chiral HPLC (CHIRALPAK OJ-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 211 nm): $t_R = 8.76$ min (major), 10.65 min (minor). [91% *ee*]

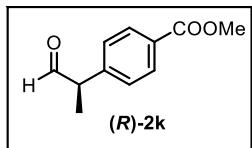
Optical Rotation: $[\alpha]_D^{20} = -99.6$ ($c = 1.71$, CHCl₃).



Isolated Yield: 83%, 35.2mg

Chiral HPLC (CHIRALPAK OJ-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 202 nm): $t_R = 12.30$ min (major), 14.93 min (minor). [89% *ee*]

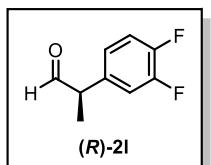
Optical Rotation: $[\alpha]_D^{20} = -63.8$ ($c = 1.76$, CHCl₃).



Isolated Yield: 65%, 24.9mg

Chiral HPLC (CHIRALPAK AS-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 236 nm): $t_R = 13.51$ min (minor), 15.56 min (major). [88% *ee*]

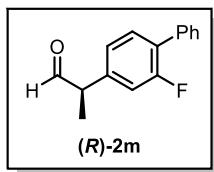
Optical Rotation: $[\alpha]_D^{25} = -108.6$ ($c = 0.83$, CHCl₃).



Isolated Yield: 81%, 27.7mg

Chiral HPLC (CHIRALPAK AS-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 205 nm): $t_R = 6.57$ min (minor), 7.43 min (major). [89% *ee*]

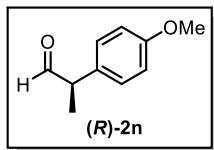
Optical Rotation: $[\alpha]_D^{20} = -98.6$ ($c = 1.32$, CHCl₃).



Isolated Yield: 75%, 34mg

Chiral HPLC (CHIRALPAK OJ-H, 5% *i*-PrOH/*n*-heptane, 1 mL/min, 247 nm): $t_R = 16.33$ min (major), 17.26 min (minor). [96% *ee*]

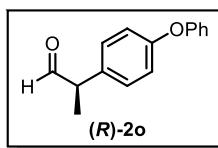
Optical Rotation: $[\alpha]_D^{20} = -96.1$ ($c = 1.82$, CHCl₃).



Isolated Yield: 82%, 26.9mg

Chiral HPLC (CHIRALPAK AS-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 202 nm): $t_R = 8.77$ min (minor), 9.44 min (major). [89% *ee*]

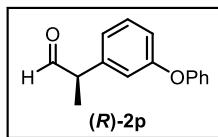
Optical Rotation: $[\alpha]_D^{20} = -163.5$ ($c = 1.36$, CHCl₃).



Isolated Yield: 67%, 28.2mg

Chiral HPLC (CHIRALPAK OJ-H, 2% *i*-PrOH/*n*-heptane, 1 mL/min, 210 nm): $t_R = 21.07$ min (major), 24.96 min (minor). [93% *ee*]

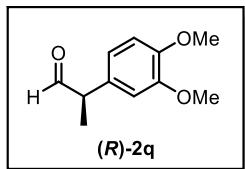
Optical Rotation: $[\alpha]_D^{25} = -112.5$ ($c = 1.41$, CHCl₃).



Isolated Yield: 72%, 32.7mg

Chiral HPLC (CHIRALPAK AD-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 205 nm): $t_R = 8.31$ min (minor), 9.29 min (major). [95% *ee*]

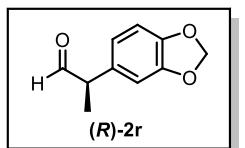
Optical Rotation: $[\alpha]_D^{20} = -91.0$ ($c = 0.7$, CHCl₃).



Isolated Yield: 78%, 30.1mg

Chiral HPLC (CHIRALPAK AS-H, 2% *i*-PrOH/*n*-heptane, 1 mL/min, 205 nm): $t_R = 8.60$ min (minor), 9.78 min (major). [86% *ee*]

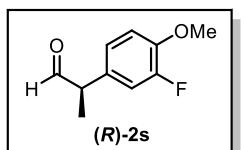
Optical Rotation: $[\alpha]_D^{25} = -95.6$ ($c = 1.51$, CHCl₃).



Isolated Yield: 71%, 25.4mg

Chiral HPLC (CHIRALPAK AS-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 205 nm): $t_R = 12.01$ min (minor), 13.42 min (major). [91% *ee*]

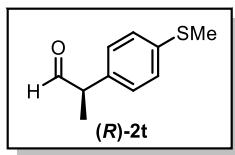
Optical Rotation: $[\alpha]_D^{20} = -166.8$ ($c = 1.01$, CHCl₃).



Isolated Yield: 81%, 29.5mg

Chiral HPLC (CHIRALPAK AS-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 202 nm): $t_R = 9.16$ min (minor), 9.67 min (major). [92% *ee*]

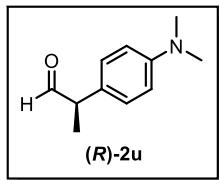
Optical Rotation: $[\alpha]_D^{20} = -159.7$ ($c = 1.15$, CHCl₃).



Isolated Yield: 74%, 26.5mg

Chiral HPLC (CHIRALPAK OJ-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 260 nm): tr = 24.26 min (major), 28.53 min (minor). [90% ee]

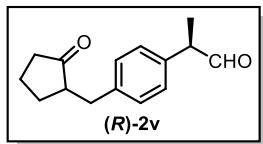
Optical Rotation: $[\alpha]_D^{20} = -168.2$ (c = 1.17, CHCl₃).



Isolated Yield: 68%, 24mg

Chiral HPLC (CHIRALPAK OD-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 261 nm): tr = 9.91 min (major), 12.86 min (minor). [78% ee]

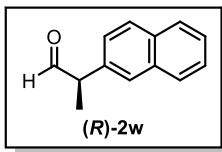
Optical Rotation: $[\alpha]_D^{20} = -152.3$ (c = 1.20, CHCl₃).



Isolated Yield: 78%, 36.4mg

Chiral HPLC (CHIRALPAK AD-H, 2% *i*-PrOH/*n*-heptane, 1 mL/min, 202 nm): Diastereoisomer A: tr = 22.78 min (major), 38.77 min (minor); Diastereoisomer B: 25.21 min (minor), 33.36 min (major). [91% ee, 93% ee, 45:55 d.r.]

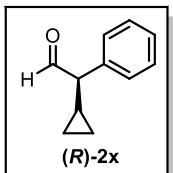
Optical Rotation: $[\alpha]_D^{20} = -137.2$ (c = 1.54, CHCl₃).



Isolated Yield: 85%, 31.3mg

Chiral HPLC (CHIRALPAK OJ-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 226 nm): $t_R = 23.31$ min (major), 25.70 min (minor). [77% *ee*]

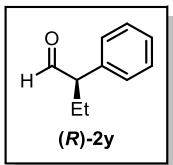
Optical Rotation: $[\alpha]_D^{25} = -119.0$ ($c = 1.25$, CHCl₃).



Isolated Yield: 85%, 28.3mg

Chiral HPLC (CHIRALPAK OD-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 204 nm): $t_R = 8.12$ min (major), 8.94 min (minor). [80% *ee*]

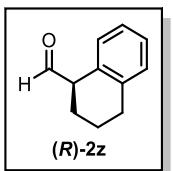
Optical Rotation: $[\alpha]_D^{20} = -20.3$ ($c = 1.42$, CHCl₃).



Isolated Yield: 70%, 20.7mg

Chiral HPLC (CHIRALPAK AS-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 204 nm): $t_R = 5.96$ min (minor), 7.02 min (major). [80% *ee*]

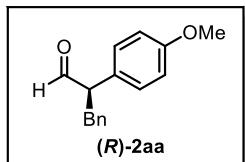
Optical Rotation: $[\alpha]_D^{20} = -90.6$ ($c = 1.22$, CHCl₃).



Isolated Yield: 82%, 24.3mg

Chiral HPLC (CHIRALPAK OJ-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 202 nm): $t_R = 9.49$ min (minor), 10.29 min (major). [70% *ee*]

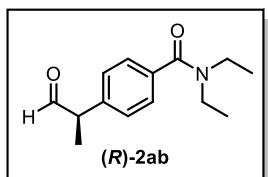
Optical Rotation: $[\alpha]_D^{20} = -36.8$ ($c = 1.30$, CHCl₃).



Isolated Yield: 73%, 35.0mg

Chiral HPLC (CHIRALPAK AS-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 203nm): $t_R = 11.81$ min (minor), 12.77 min (major). [66% *ee*]

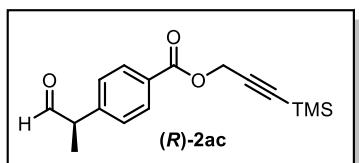
Optical Rotation: $[\alpha]_D^{20} = -103.1$ ($c = 1.75$, CHCl₃).



Isolated Yield: 73%, 33.8mg

Chiral HPLC (CHIRALPAK OJ-H, 20% *i*-PrOH/*n*-heptane, 1 mL/min, 205nm): $t_R = 9.03$ min (major), 11.12 min (minor). [95% *ee*]

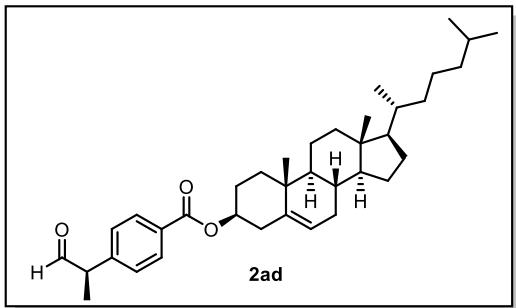
Optical Rotation: $[\alpha]_D^{20} = -40.5$ ($c = 1.69$, CHCl₃).



Isolated Yield: 84%, 48.6mg

Chiral HPLC (CHIRALPAK double OJ-H, 10% *i*-PrOH/*n*-heptane, 0.5 mL/min, 237nm): $t_R = 30.07$ min (minor), 31.35 min (major). [90% *ee*]

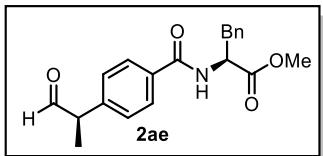
Optical Rotation: $[\alpha]_D^{20} = -22.1$ ($c = 2.43$, CHCl_3).



Isolated Yield: 75%, 82.1mg

Chiral HPLC (CHIRALPAK OD-H, 2% *i*-PrOH/*n*-heptane, 1 mL/min, 236nm): $t_R = 22.18$ min (minor), 24.57 min (major). [95:5 d.r.] (The diastereomeric ratio was determined from the corresponding alcohol)

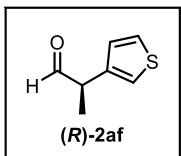
Optical Rotation: $[\alpha]_D^{20} = -22.2$ ($c = 2.74$, CHCl_3).



Isolated Yield: 63%, 42.7mg

Chiral HPLC (CHIRALPAK OJ-H, 5% *i*-PrOH/*n*-heptane, 1 mL/min, 234nm): $t_R = 94.60$ min (minor), 98.09 min (major). [93:7 d.r.]

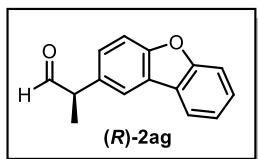
Optical Rotation: $[\alpha]_D^{20} = +31.1$ ($c = 1.68$, CHCl_3).



Isolated Yield: 70%, 19.6mg

Chiral HPLC (CHIRALPAK AS-H, 1% *i*-PrOH/*n*-heptane, 1 mL/min, 235nm): $t_R = 6.90$ min (minor), 9.15 min (major). [86% ee]

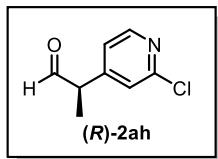
Optical Rotation: $[\alpha]_D^{20} = -62.2$ ($c = 0.69$, CHCl_3).



Isolated Yield: 78%, 35.0mg

Chiral HPLC (CHIRALPAK AS-H, 2% *i*-PrOH/*n*-heptane, 1 mL/min, 222nm): $t_R = 6.70$ min (major), 7.38 min (minor). [93% ee]

Optical Rotation: $[\alpha]_D^{20} = -76.4$ ($c = 1.75$, CHCl₃).



Isolated Yield: 86%, 29.3mg

Chiral HPLC (CHIRALPAK AS-H, 20% *i*-PrOH/*n*-heptane, 1 mL/min, 207nm): $t_R = 4.64$ min (major), 5.32 min (minor). [77% ee] (The enantiomeric excess was determined from the corresponding alcohol)

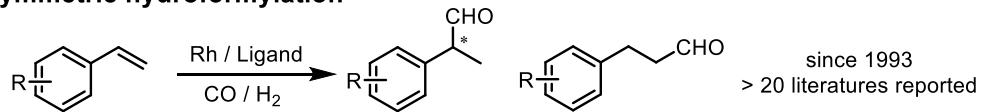
Optical Rotation: $[\alpha]_D^{20} = -7.1$ ($c = 1.54$, CHCl₃).

5. Synthetic value and application

5.1. Comparison of approaches towards enantioenriched α -aryl aldehydes

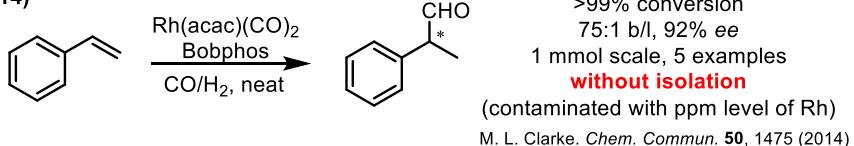
For the chiral aldehydes covered in this manuscript, asymmetric hydroformylation would be an attractive strategy (32, 33), however, the state-of-art protocol still showed limited scopes (5 examples) (34). Asymmetric α -arylation is another modular strategy (35-40). The one developed by MacMillan showed relatively broad scopes with respective to both aldehydes and aryl donors, representing the state-of-art in this category (38). Our protocol has limitation in the scope of α -alkyl substitution, but do not require special arylation reagents. In addition, the material and product were the same compound, hence the purification method can be significantly simplified to achieve the direct isolation of α -aryl aldehydes without *ee* erosion, which may provide advantages in accessing difficult chiral aldehydes.

A Asymmetric hydroformylation

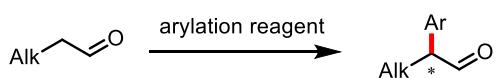


for most cases: 1. required *in situ* transformation and analysis
2. < 10 substrates, limited to simple substituted aromatics

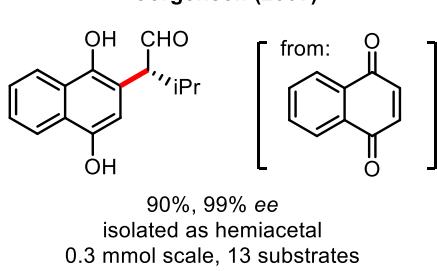
Clarke (2014)



B Asymmetric arylation

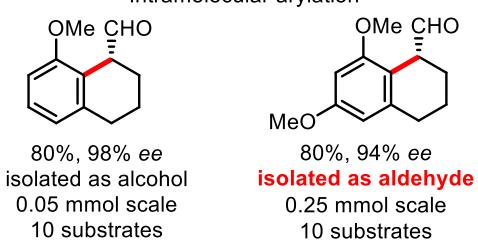


Jorgensen (2007)

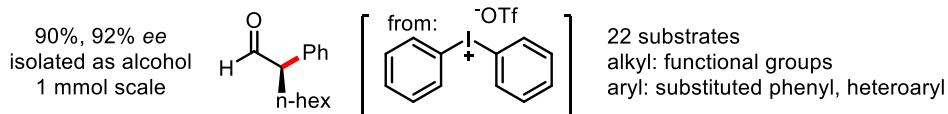


MacMillan (2009) and Nicolaou (2009)

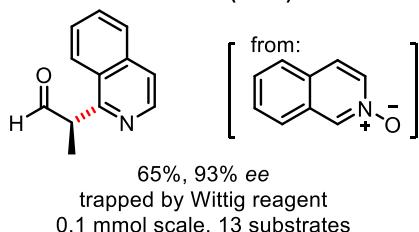
Intramolecular arylation



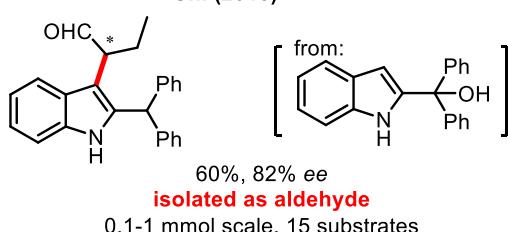
MacMillan (2011)



Fochi (2018)



Shi (2018)



K. A. Jorgensen. *ACIE*. **46**, 5520 (2007) K. C. Nicolaou. *JACS*. **131**, 2086 (2009) M. Fochi. *Chem. Commun.* **54**, 3977 (2018)
D. W. C. MacMillan. *JACS*. **131**, 11640 (2009) D. W. C. MacMillan. *JACS*. **133**, 4260 (2011) F. Shi. *J. Org. Chem.* **83**, 5027 (2018)

C Deracemization (this work)

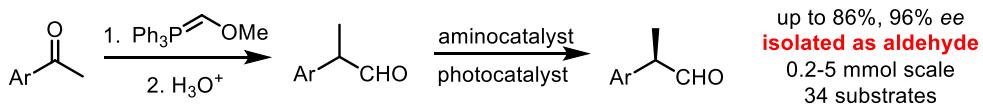
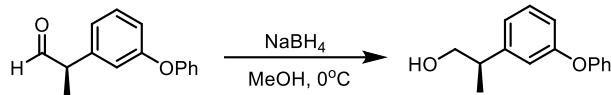


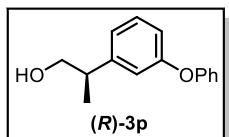
Figure S4. Methods for preparing enantioenriched α -aryl aldehydes.

5.2. General procedure for reduction



To an oven-dried 10 mL flask equipped with a magnetic stir bar was added (*R*)-**2p** (113mg, 0.5 mmol) and 0.5 mL MeOH. NaBH₄ (10 equiv, 190 mg) was then added into the mixture at 0°C. After stirring for 1h, the reaction was quenched with saturated aq NH₄Cl, and the mixture was extracted with DCM (5 mL × 3). The organic layers were combined and dried over Na₂SO₄, concentrated. The crude product was purified by flash chromatography (silica gel, 5:1 petroleum ether/EtOAc) to afford (*R*)-**3p** as colorless liquid.

(*R*)-2-(3-phenoxyphenyl)propan-1-ol (**3p**)



Isolated Yield: 96%, 110mg

¹H NMR (400 MHz, Chloroform-d) δ 7.41 - 7.27 (m, 3H), 7.18 - 7.10 (m, 1H), 7.08 - 7.03 (m, 2H), 7.03 - 6.98 (m, 1H), 6.96 (t, *J* = 2.1 Hz, 1H), 6.89 (dd, *J* = 8.2, 2.5 Hz, 1H), 3.71 (d, *J* = 6.8 Hz, 2H), 2.96 (q, *J* = 6.9 Hz, 1H), 1.54 (s, 1H), 1.29 (d, *J* = 6.8 Hz, 3H).

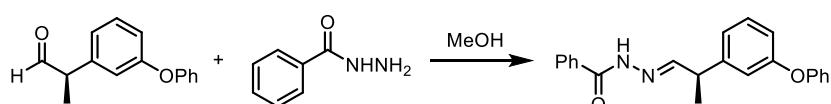
¹³C NMR (101 MHz, Chloroform-d) δ 157.54, 157.13, 145.97, 129.84, 129.78, 123.29, 122.35, 118.92, 117.97, 116.86, 68.55, 42.38, 17.56.

Spectroscopic results agree with previously reported data. (41)

Chiral HPLC (CHIRALPAK AD-H, 5% *i*-PrOH/*n*-heptane, 1 mL/min, 206 nm): t_R = 12.73 min (minor), 16.74 min (major). [95% ee]

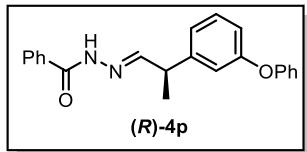
Optical Rotation: [α]_D²⁰ = +16.7 (c = 1.10, CHCl₃).

5.3. General procedure for condensation



To an oven-dried 10 mL flask equipped with a magnetic stir bar was added (*R*)-**2p** (113 mg, 0.5 mmol), benzoyl hydrazine (1.5 equiv, 102 mg) and 2 mL MeOH. After stirring at room temperature for 6 h, the mixture was concentrated and purified by flash chromatography (silica gel, 1:1 petroleum ether/EtOAc) to afford (*R*)-**4p** as colorless liquid.

(*R, E*)-N'-(2-(3-phenoxyphenyl)propylidene)benzohydrazide (**4p**)



Isolated Yield: 86%, 148mg

¹H NMR (400 MHz, Chloroform-d) δ 10.03 (s, 1H), 7.81 (d, *J* = 7.7 Hz, 2H), 7.70 (d, *J* = 6.4 Hz, 1H), 7.46 (t, *J* = 7.3 Hz, 1H), 7.41 - 7.27 (m, 4H), 7.23 (t, *J* = 7.9 Hz, 1H), 7.10 (t, *J* = 7.4 Hz, 1H), 7.01 - 6.88 (m, 4H), 6.84 (d, *J* = 8.3 Hz, 1H), 3.77 - 3.69 (m, 1H), 1.43 (dd, *J* = 10.1, 7.3 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-d) δ 164.49, 157.54, 157.01, 154.62, 144.08, 133.11, 131.89, 130.02, 129.86, 129.80, 128.58, 127.43, 123.37, 122.44, 118.85, 117.97, 117.10, 42.55, 18.56.

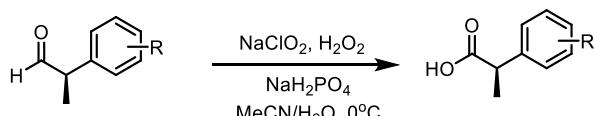
IR ν(cm⁻¹): 3055, 2981, 2933, 2817, 2722, 1721, 1606, 1490, 1454, 1265, 786, 737, 704.

HRMS (ESI) calcd for C₂₂H₂₀N₂O₂ [M+Na]⁺ 367.1417, found 367.1405.

Chiral HPLC (CHIRALPAK OD-H, 20% *i*-PrOH/*n*-heptane, 1 mL/min, 205 nm): t_R = 18.18 min (major), 24.32 min (minor). [94% ee]

Optical Rotation: [α]_D²⁰ = -4.5 (c = 1.01, CHCl₃).

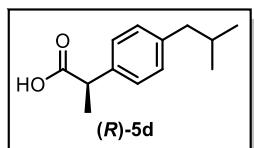
5.4. General procedure for oxidation



The reaction was performed according to a modified procedure (42). A solution of NaClO₂ (2 equiv, 90mg) and NaH₂PO₄ (0.2 equiv, 12 mg) in H₂O (2 mL) was added into the mixture of (*R*)-**2** (0.5 mmol), H₂O₂ (30% aqueous, 1 equiv, 50 μL) and MeCN (2 mL) at 0°C. The mixture was stirred at the same temperature for 1h. After the completion of oxidation, the solution was acidified

with 1M HCl, extracted with EtOAc ($5\text{ mL} \times 3$) and concentrated. The crude product was purified by flash chromatography (silica gel, 2:1 petroleum ether/EtOAc) to afford (*R*)-**5** as white solid.

(*R*)-Ibuprofen (5d**)**



Isolated Yield: 87%, 89.6mg

$^1\text{H NMR}$ (400 MHz, Chloroform-d) δ 11.58 (br, 1H), 7.27 (d, $J = 8.1$ Hz, 2H), 7.15 (d, $J = 8.4$ Hz, 2H), 3.76 (q, $J = 7.1$ Hz, 1H), 2.50 (d, $J = 7.1$ Hz, 2H), 1.90 (m, 1H), 1.55 (d, $J = 7.1$ Hz, 3H), 0.95 (d, $J = 6.6$ Hz, 6H).

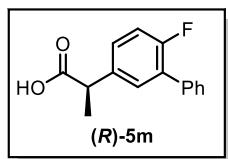
$^{13}\text{C NMR}$ (101 MHz, Chloroform-d) δ 181.27, 140.88, 137.01, 129.43, 127.33, 45.09, 45.05, 30.20, 22.43, 18.11.

Spectroscopic results agree with previously reported data. (43)

Chiral HPLC (CHIRALPAK double OJ-H, 2% *i*-PrOH/*n*-heptane, 0.5 mL/min, 205 nm): $t_{\text{R}} = 38.50$ min (major), 43.00 min (minor). [94% *ee*]

Optical Rotation: $[\alpha]_D^{20} = -68.3$ ($c = 0.3$, CHCl_3).

(*R*)-Flurbiprofen (5m**)**



Isolated Yield: 85%, 104mg

$^1\text{H NMR}$ (400 MHz, Chloroform-d) δ 11.77 (s, 1H), 7.63 (d, $J = 7.6$ Hz, 2H), 7.58 - 7.41 (m, 4H), 7.31 - 7.22 (m, 2H), 3.88 (q, $J = 7.1$ Hz, 1H), 1.65 (d, $J = 7.2$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, Chloroform-d) δ 180.78, 159.82 (d, $J = 248.5$ Hz), 141.04 (d, $J = 7.6$ Hz), 135.51, 131.00 (d, $J = 4.0$ Hz), 129.06 (d, $J = 3.0$ Hz), 128.57, 128.28 (d, $J = 13.6$ Hz), 127.83, 123.81 (d, $J = 3.6$ Hz), 115.51 (d, $J = 23.8$ Hz), 45.02, 18.04.

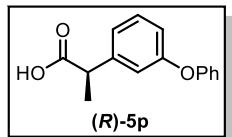
Spectroscopic results agree with previously reported data. (43)

Chiral HPLC (CHIRALPAK AD-H, 5% *i*-PrOH/*n*-heptane, 1 mL/min, 246 nm): $t_{\text{R}} = 9.88$ min

(major), 13.99 min (minor). [95% ee]

Optical Rotation: $[\alpha]_D^{20} = -59.7$ ($c = 0.35$, CHCl_3).

(R)-Fenoprofen (5p)



Isolated Yield: 90%, 109mg

$^1\text{H NMR}$ (400 MHz, Chloroform-d) δ 10.21 (br, 1H), δ 7.43 - 7.26 (m, 3H), 7.19 - 7.01 (m, 5H), 6.93 (dd, $J = 8.4, 2.5$ Hz, 1H), 3.75 (q, $J = 7.1$ Hz, 1H), 1.54 (d, $J = 7.2$ Hz, 3H).

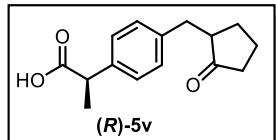
$^{13}\text{C NMR}$ (101 MHz, Chloroform-d) δ 180.50, 157.54, 156.98, 141.72, 129.91, 129.80, 123.41, 122.41, 119.02, 118.28, 117.54, 45.25, 18.08.

Spectroscopic results agree with previously reported data. (43)

Chiral HPLC (CHIRALPAK AD-H, 5% *i*-PrOH/*n*-heptane, 1 mL/min, 205 nm): $t_R = 12.28$ min (major), 15.80 min (minor). [95% ee]

Optical Rotation: $[\alpha]_D^{20} = -55.8$ ($c = 1.07$, CHCl_3).

(R)-Loxoprofen (5v)



Isolated Yield: 85%, 117mg

$^1\text{H NMR}$ (400 MHz, Chloroform-d) δ 10.96 (br, 1H), 7.25 (d, $J = 8.2$ Hz, 2H), 7.14 (d, $J = 8.2$ Hz, 2H), 3.73 (q, $J = 7.1$ Hz, 1H), 3.14 (dd, $J = 13.9, 4.0$ Hz, 1H), 2.53 (dd, $J = 13.9, 9.5$ Hz, 1H), 2.43 - 2.30 (m, 2H), 2.23 - 2.04 (m, 2H), 1.98 (m, 1H), 1.75 (m, 1H), 1.64 - 1.54 (m, 1H), 1.52 (d, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, Chloroform-d) δ 180.58, 139.15, 137.68, 129.19, 127.67, 50.99, 44.97, 38.18, 35.19, 29.22, 20.54, 18.10.

Spectroscopic results agree with previously reported data. (44)

Chiral HPLC (CHIRALPAK OJ-H, 5% *i*-PrOH/*n*-heptane, 1 mL/min, 220 nm):

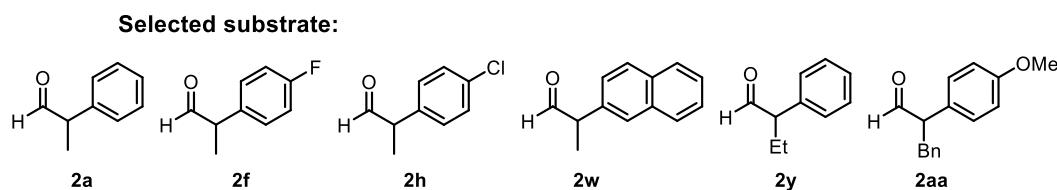
Diastereoisomer A: $t_R = 24.52$ min (major), 38.73 min (minor); Diastereoisomer B: 28.30 min (major), 32.24 min (minor). [95% *ee*, 95% *ee*, *dr* = 50:50]

Optical Rotation: $[\alpha]_D^{20} = -51.6$ ($c = 1.04$, CHCl_3).

6. Mechanistic experiments

6.1. Time-course profile of deracemization

The complete evaluation of *ee* and yield as a function of time was conducted under standard condition. 20 μ L of the reaction mixture was taken out for GC and HPLC analysis at 10, 20, 30, 40, 50, 60, 80, 100 and 120 minutes. Different aminocatalyst loading and six representative substrates were examined.



The yield showed a tendency of slow decrease overall, while the *ee* value rapidly increased in the first 20 minutes, and equilibrated at 40-50 minutes, especially for **2aa**, which equilibrated at 100 minutes. Increasing the catalyst loading would reduce the equilibrium time and enhance the *ee* value, but speeding up the yield decay at the mean time. 10 mol% loading was optimal in terms of both yield and *ee* value.

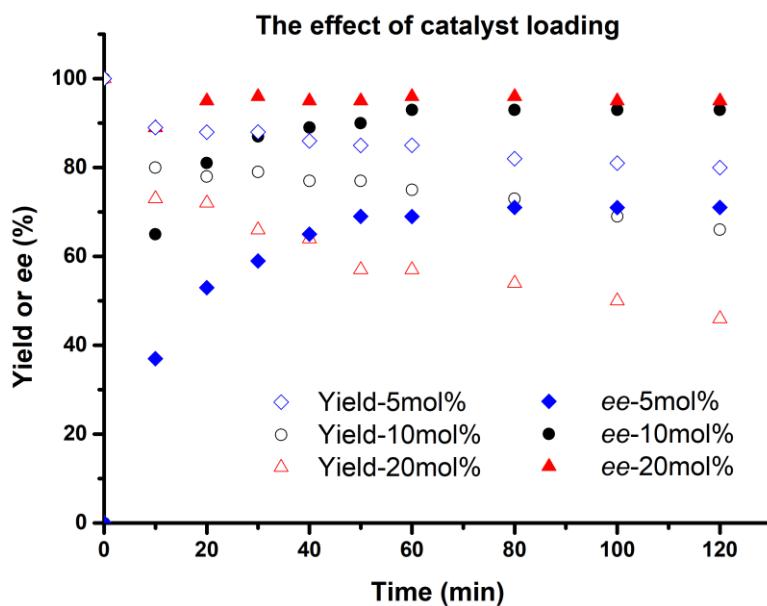


Figure S5. Time-course deracemization profile under different aminocatalyst loading.

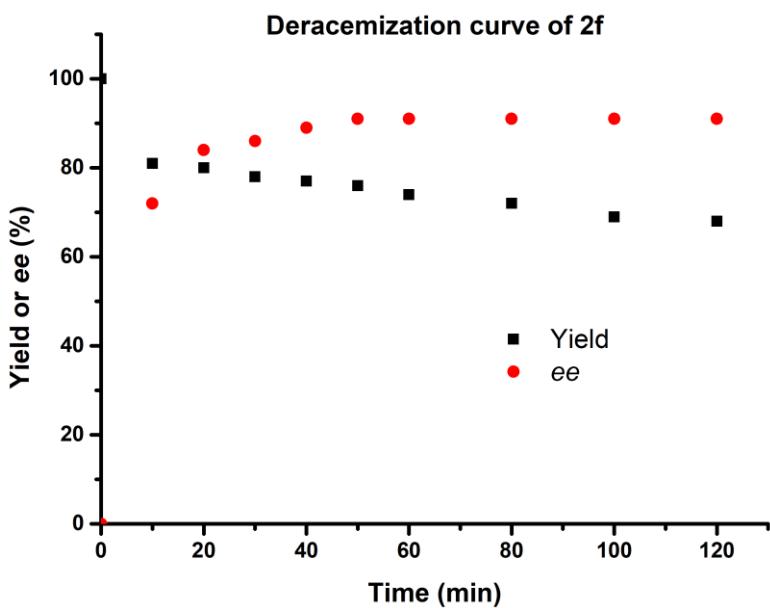


Figure S6. Time-course deracemization profile of **2f**.

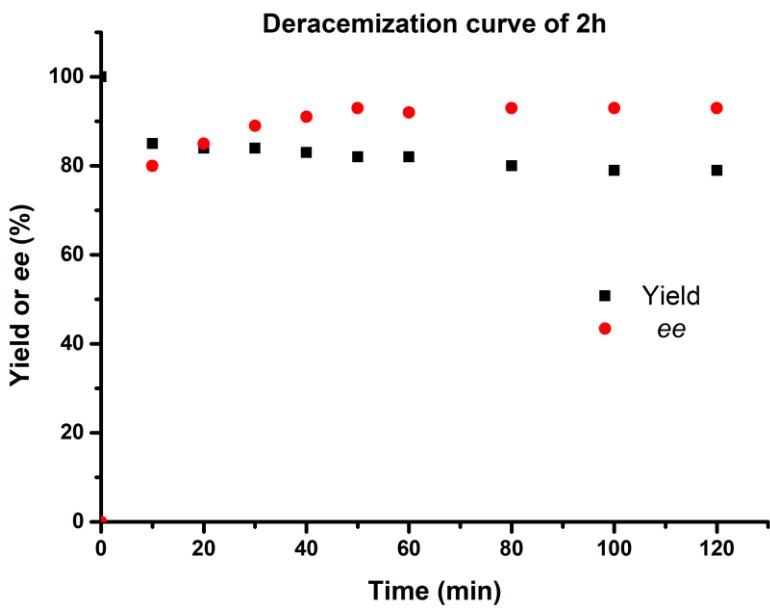


Figure S7. Time-course deracemization profile of **2h**.

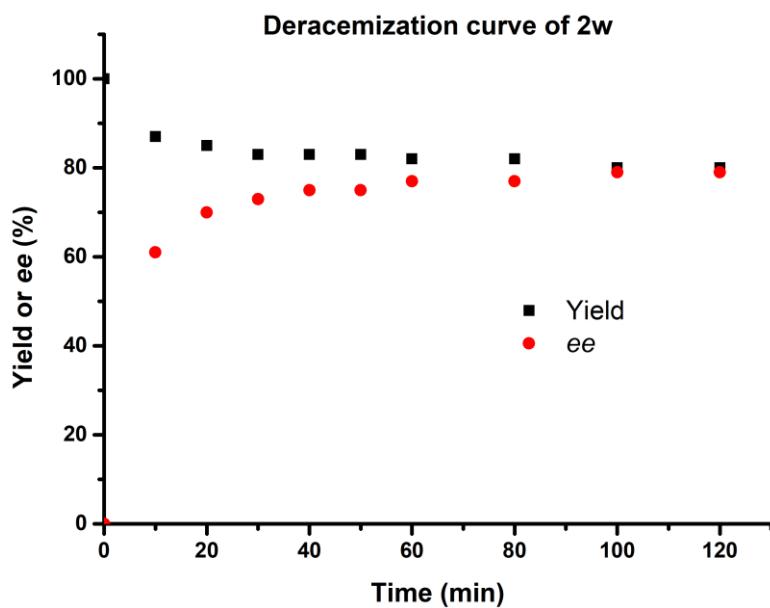


Figure S8. Time-course deracemization profile of 2w.

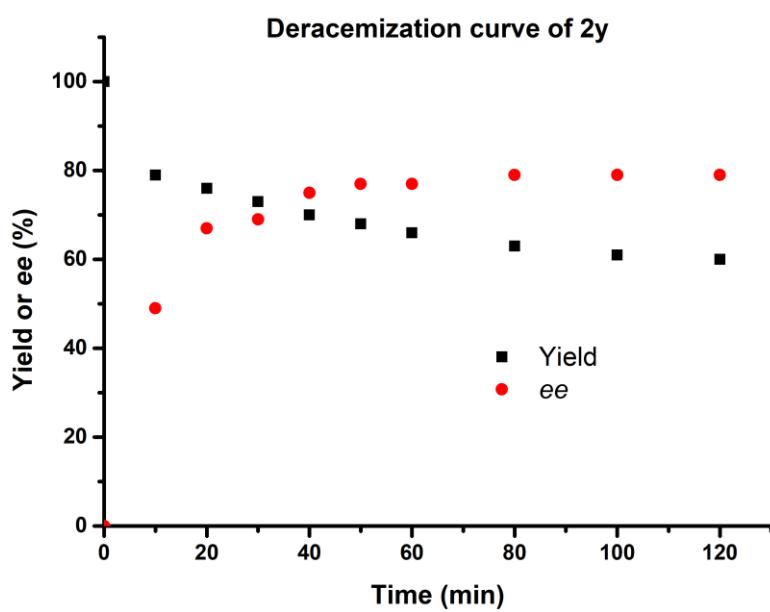


Figure S9. Time-course deracemization profile of 2y.

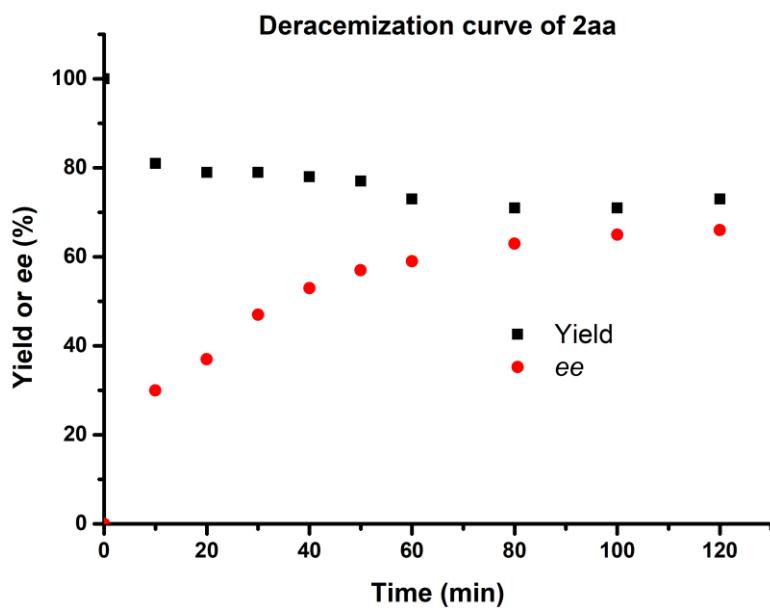


Figure S10. Time-course deracemization profile of 2aa.

6.2. Analysis of side reactions

The aldehyde **2a** tended to rapidly condense with (*S*)-**1a**/HNTf₂ to form imine and enamine upon mixing. We conducted NMR and HRMS monitoring of the reaction mixture under standard conditions (0.4 mmol scale, 50 mol% PhCOOBn as internal standard, MeCN-*d*₃ as the solvent). The result showed that most of (*S*)-**1a** was combined with **2a**, and the total amount of imine and enamine was ca 10% before and after the irradiation (Fig. S12). Working up by H₂O, 1 M HCl or wet silica gel could not promote the hydrolysis process without racemization. The intermediate was also observed by HRMS analysis of the reaction mixture (Fig. S13).

Moreover, we isolated little amount of homocoupling product **6a**, which may explain the tendency of yield decay. We proposed that photoinduced SET oxidation of enamine generated the α -imino radical, thus producing the homocoupling product **6a**.

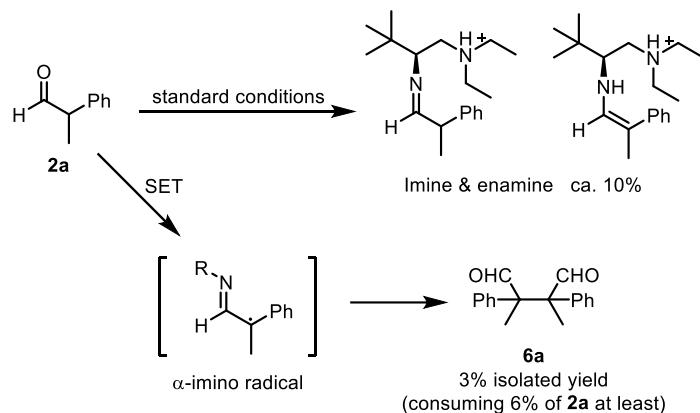


Figure S11. Diagram of side reaction analysis.

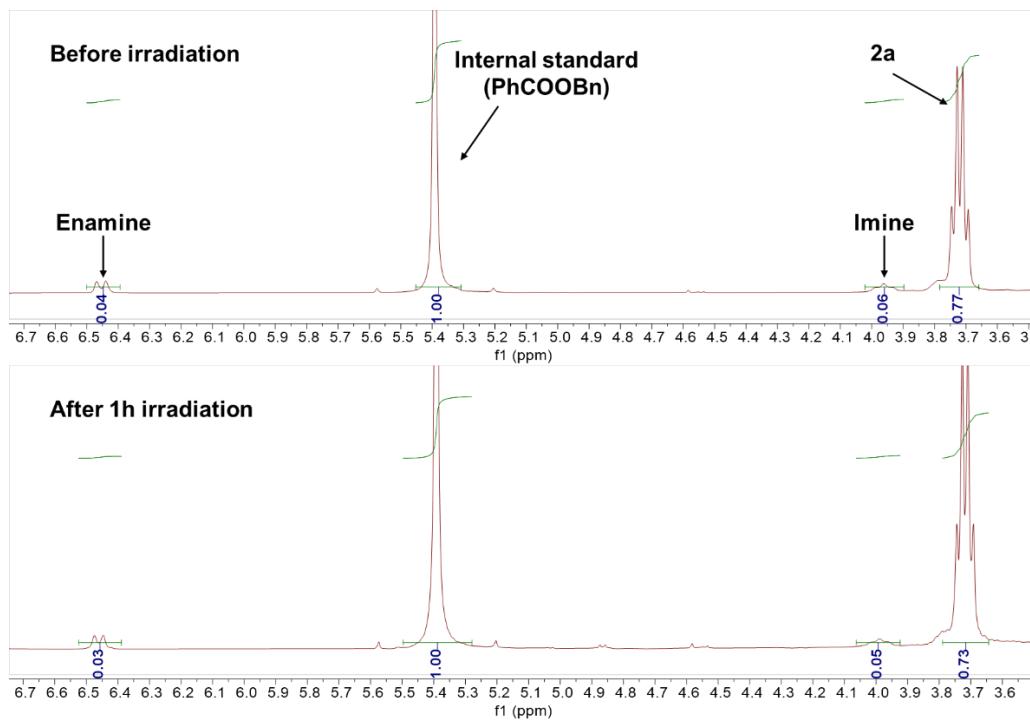


Figure S12. NMR detection of reaction mixture.

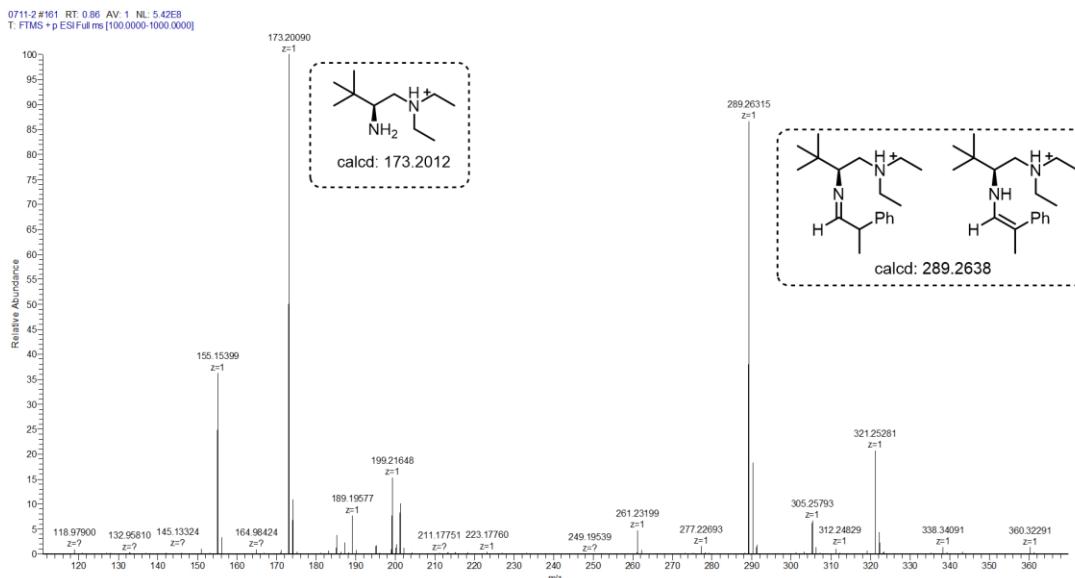


Figure S13. HRMS detection of reaction mixture.

6.3. Characterization of *E/Z*-enamine

As the enamine could not be isolated, we performed the *in situ* NOE experiment for a mixture containing equal amount of *E* and *Z*-enamine (*see below*, described in Fig. S18). (*R*)-**2a** (0.067M) and (*S*)-**1a**/HNTf₂ (0.067M) was dissolved in MeCN-*d*₃ (0.6 mL) under Ar atmosphere and equilibrated for 100min. The selected chemical shifts were 6.41 and 5.91 in 1D NOESY experiment. The results showed that the former belonged to *E*-enamine and the latter belonged to *Z*-enamine.

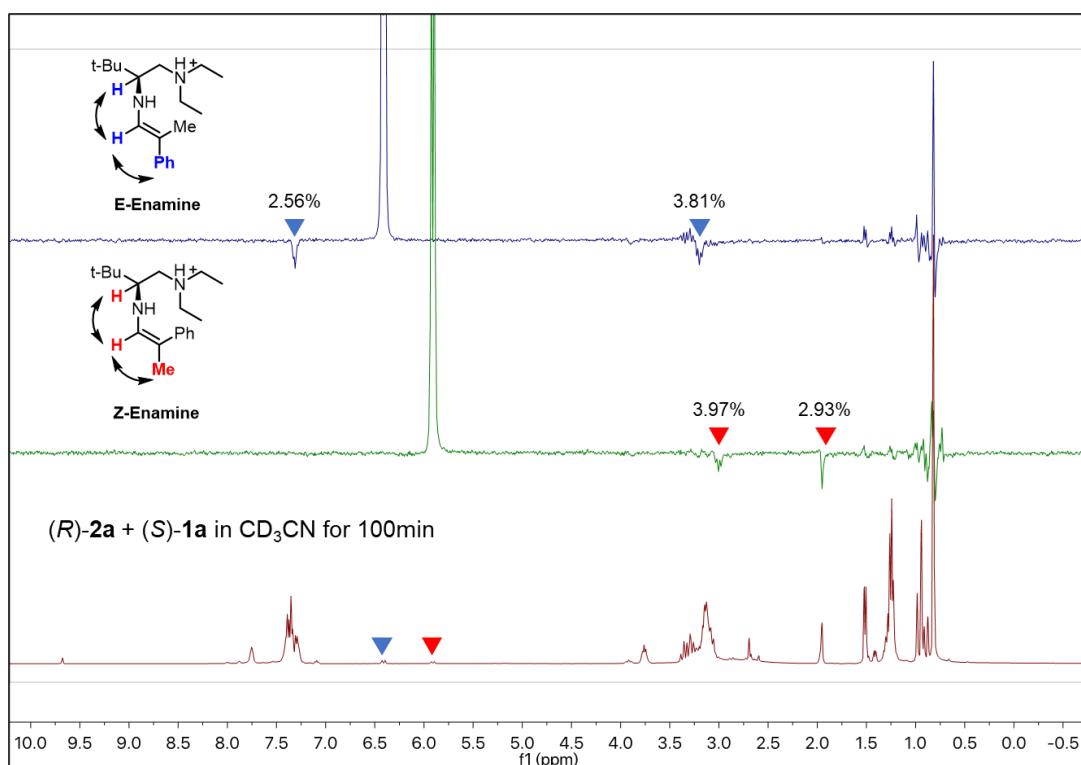


Figure S14. NOE experiment for characterization of *E/Z*-enamine. **(top)** 1D NOESY spectrum when irradiating at $\delta = 6.41$. **(middle)** 1D NOESY spectrum when irradiating at $\delta = 5.91$. **(bottom)** ^1H NMR for the selected system.

6.4. Stoichiometric experiments of enamine formation

General procedure for monitoring the enamine formation: to an NMR tube was added aminocatalyst ((*S*)-**1a** with or without HNTf₂, 0.067M), **2a** (0.067 M), PhCOOH (0.013 M), PhCOOBn (0.033 M, as internal standard) and MeCN-*d*₃ (0.6 mL) under Ar atmosphere. The ¹H NMR detection should start as soon as the completion of mixing.

Due to the dramatic acceleration effect of PhCOOH (Fig. S15), the initial enamine formation was hardly detected in its presence. We conducted further experiment without addition of PhCOOH (Fig. S16-18).

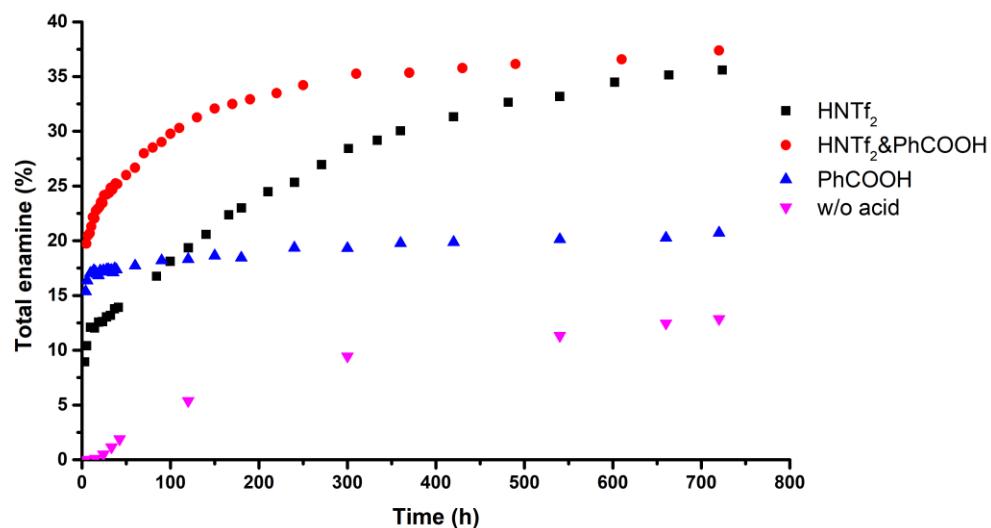


Figure S15. Acid effect in enamine formation.

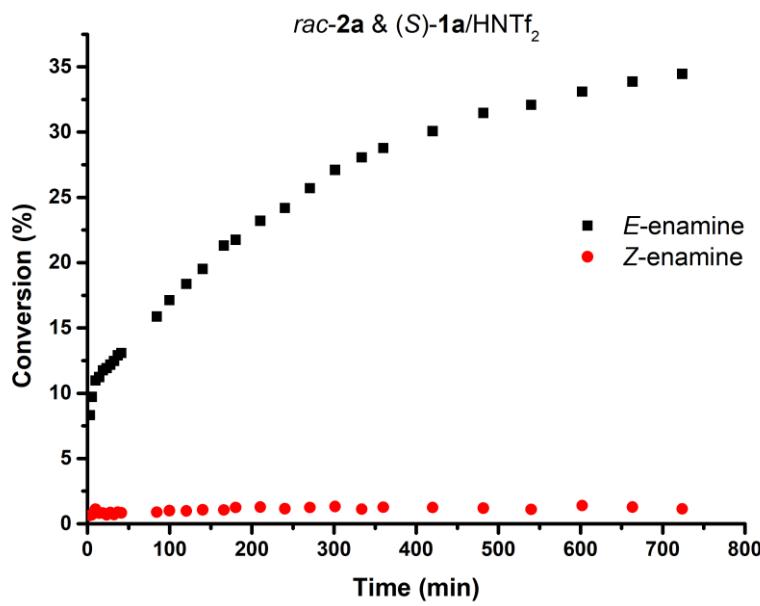
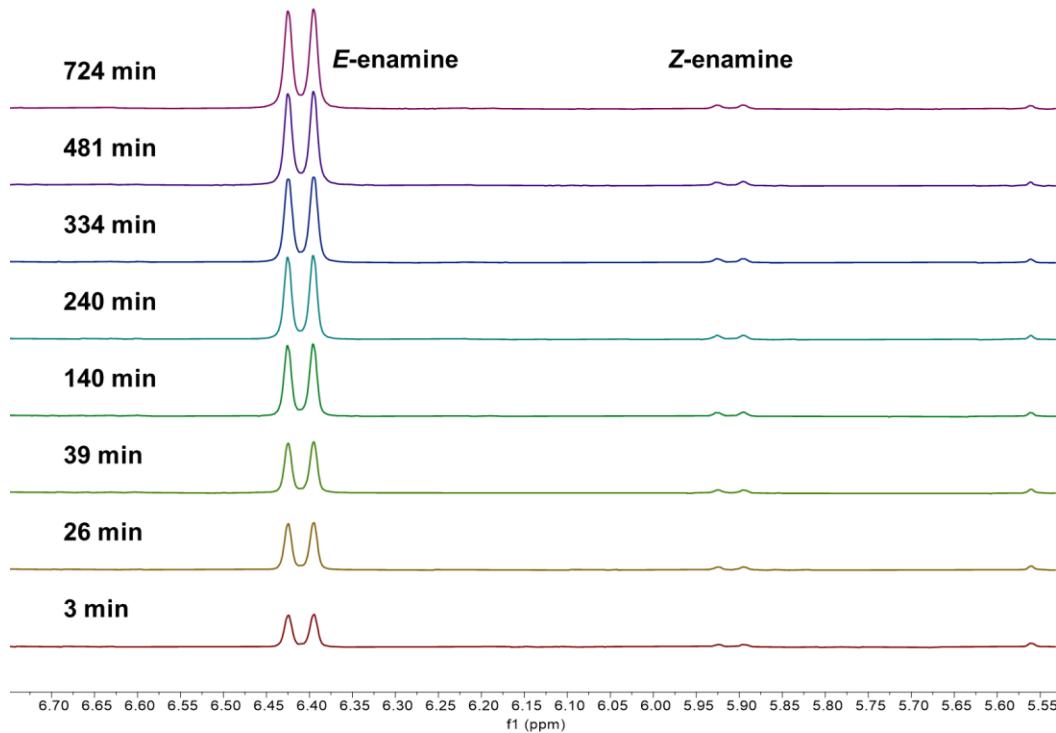


Figure S16. Enamine formation from *rac*-**2a**. Conditions: (*S*)-**1a**/HNTf₂ (0.067M), *rac*-**2a** (0.067 M), PhCOOBn (0.033 M) and MeCN-*d*₃ (0.6 mL)

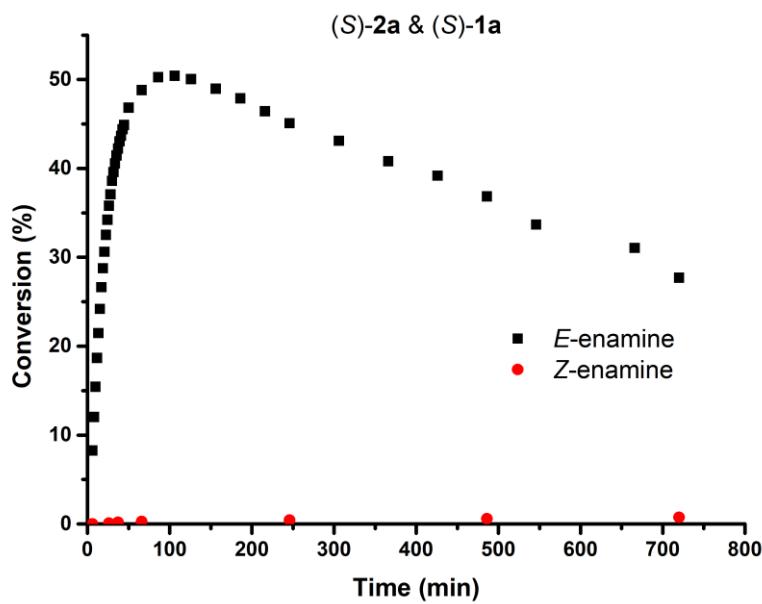
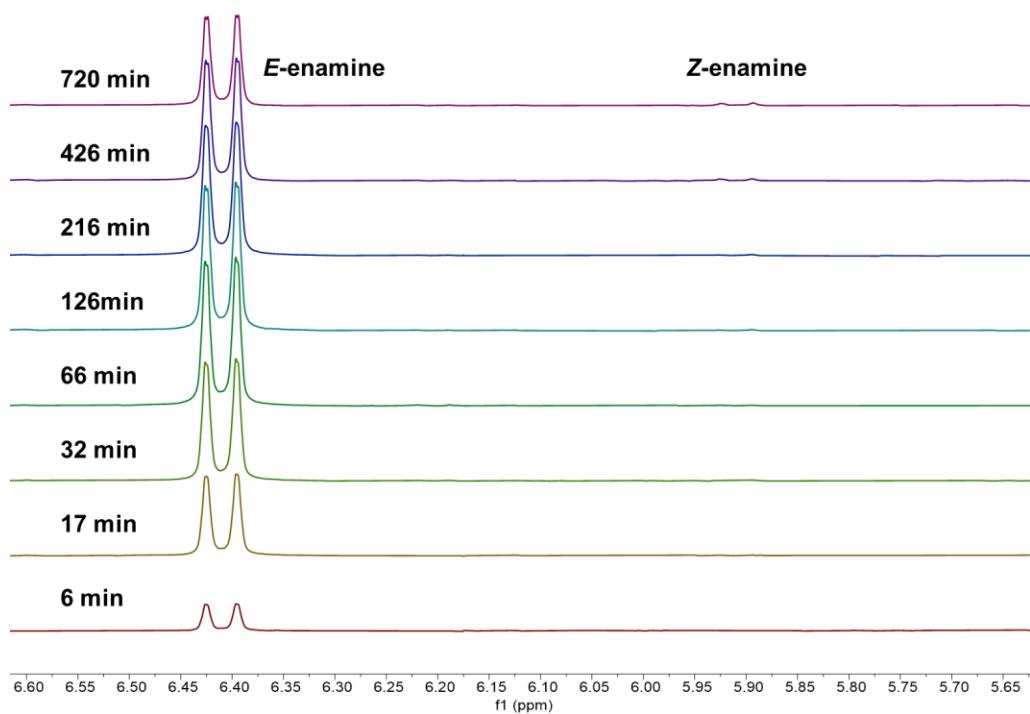


Figure S17. Enamine formation from (*S*)-2a. Conditions: (*S*)-1a/HNTf₂ (0.067M), (*S*)-2a (0.067 M), PhCOOBn (0.033 M) and MeCN-*d*₃ (0.6 mL)

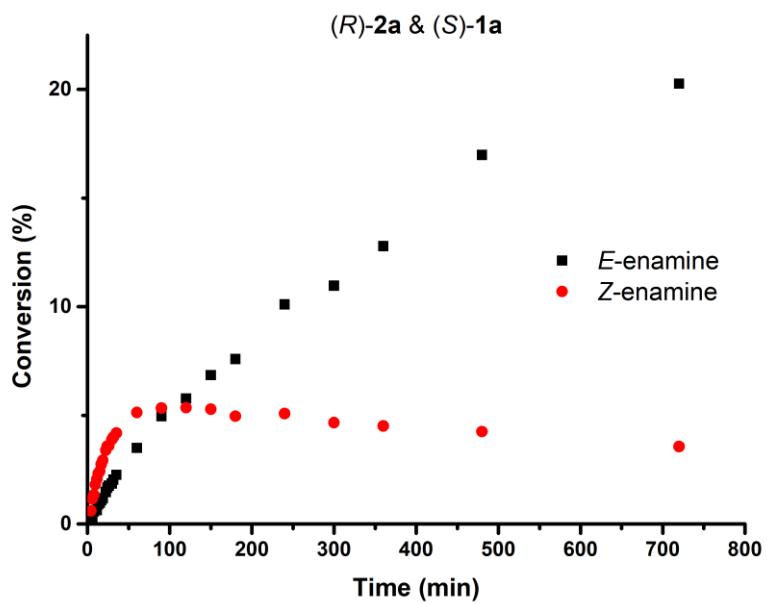
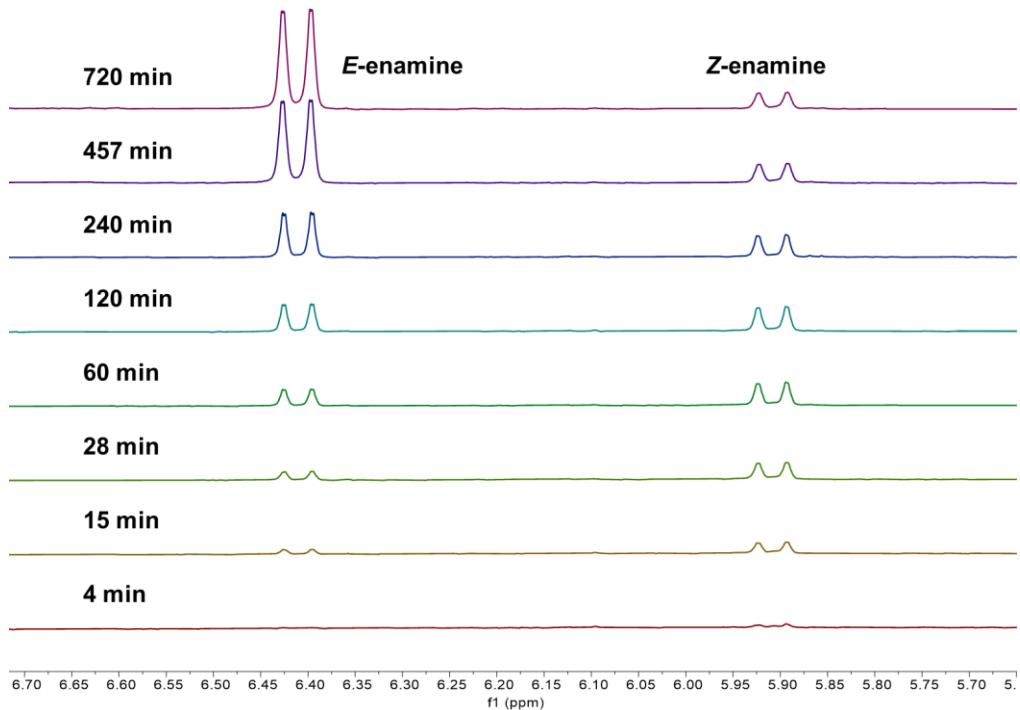


Figure S18. Enamine formation from (R) -**2a**. Conditions: (S) -**1a**/HNTf₂ (0.067M), (R) -**2a** (0.067 M), PhCOOBn (0.033 M) and MeCN-*d*₃ (0.6 mL)

6.5. *In situ* irradiation in NMR spectrometer

LSR405NL-280-FC laser purchased from LASEVER Inc. was coupled with a 10 m-long optical fiber. An NMR tube cap was equipped at the end of fiber. Following the general procedure for monitoring enamine formation, (*S*)-**1a**/HNTf₂ (0.067M), **2a** (0.067 M), Ir(ppy)₃ (2.5 mol %), PhCOOH (0.013 M, if necessary), PhCOOBn (0.033 M, as internal standard), and MeCN-*d*₃ (0.6 mL) were mixed under Ar atmosphere at room temperature. The mixture was pre-equilibrated for 1h (with PhCOOH) or 10 h (without PhCOOH) to obtain an equilibrated ratio of *E/Z*-enamine (ca. 30:1). Then the solution was transferred into the NMR tube which was equipped with fiber to perform the irradiation experiment.

As revealed in Fig. S21, *E*-enamine is quickly consumed and the amount of *Z*-enamine first increases following by a decline to photo-stationary state in 10 minutes. At photodynamic equilibrium, the ratio of *Z*-enamine is increased by 2 folds comparing to that under thermodynamic condition before light irradiation (Fig. S20). This observation is in support of the scenario that the *E*-enamine is converting to *Z*-enamine, meanwhile the latter is also quickly tautomerizing into iminium ion. The observed accumulation of imine is in line with this conjecture (increase about 25% over ca. 25% decrease of *E*-enamine, the ratio of aldehyde also varied, however, this was not calculated due to the inconsistence of peak integration at lower fields). Similar results were also observed in the presence of benzoic acid (Fig. S22-23). The ratio of *Z*-enamine is relatively lower in this instance, a result of enhanced enamine-iminium tautomerization in the presence of benzoic acid additive.



Figure S19. Optical fiber coupled laser.

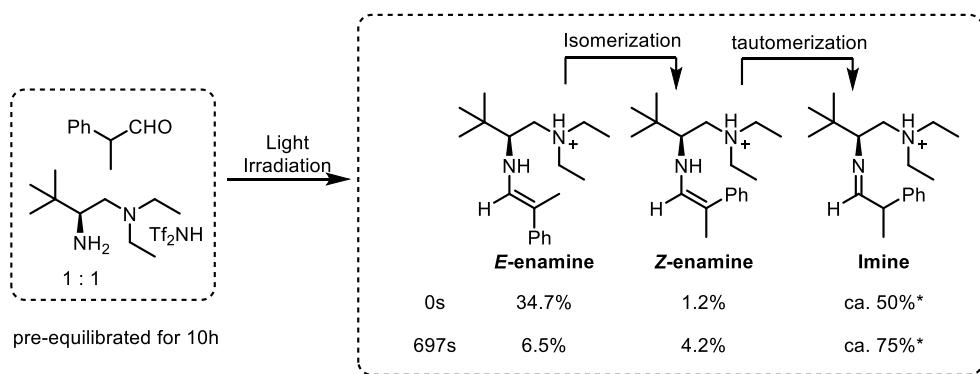


Figure S20. Distribution of species at the start and the end of irradiation in the absence of PhCOOH. *The integration of imine peak was of low accuracy because of the overlap in NMR. Variation of aldehyde ratio was also observed.

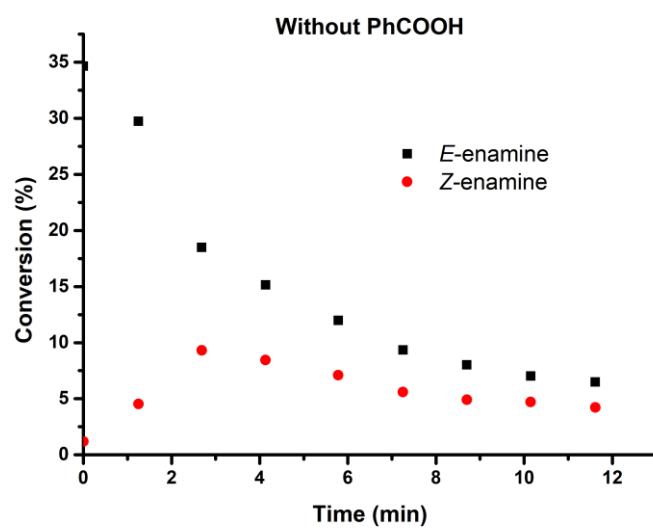
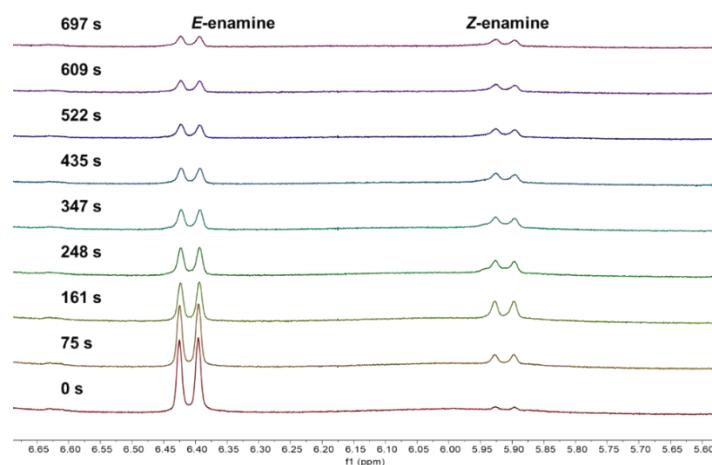


Figure S21. *E/Z* isomerization monitored by ^1H NMR in the absence of benzoic acid.

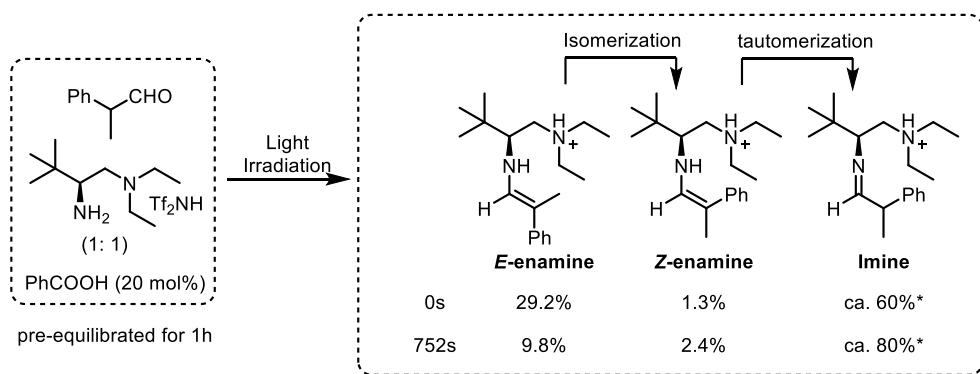


Figure S22. Distribution of species at the start and the end of irradiation in the presence of PhCOOH. *The integration of imine peak was of low accuracy because of the overlap in NMR. Variation of aldehyde ratio was also observed.

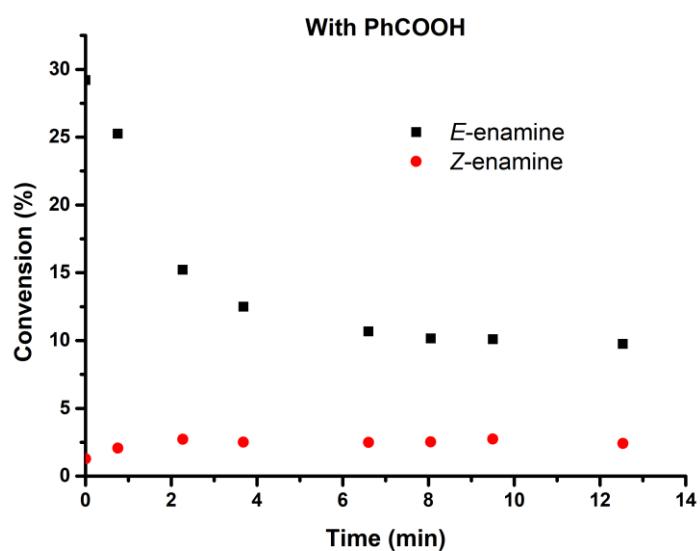
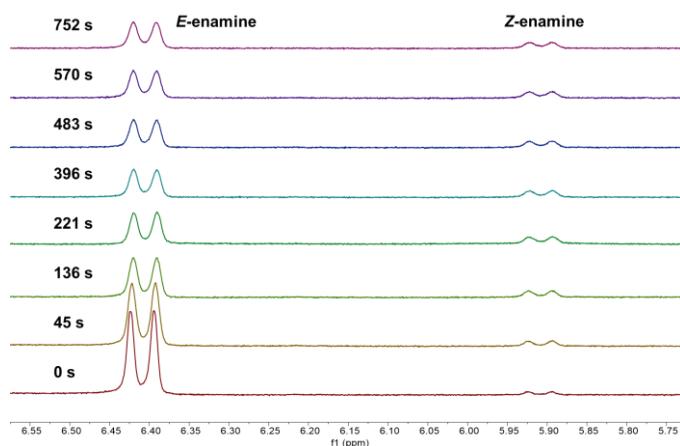


Figure S23. *E/Z* isomerization monitored by ^1H NMR in the presence of benzoic acid.

6.6. UV-Vis spectra

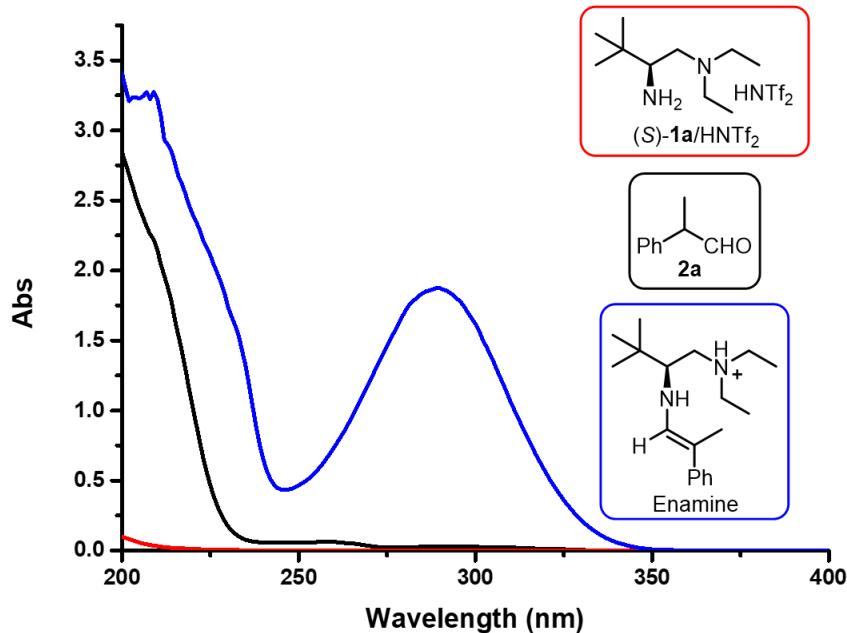


Figure S24. UV-Vis absorption spectra of (S)-1a/HNTf₂ (2.5×10^{-4} M, red line), 2a (2.5×10^{-4} M, black line) and enamine (blue line) in MeCN at room temperature. The enamine solution was prepared from dilution of a pre-equilibrated mixture of (S)-1a/HNTf₂ (0.075 M), 2a (0.075M) and PhCOOH (0.015 M) in MeCN, the final concentration was 2.5×10^{-4} M based on 2a.

6.7. Stern-Volmer luminescence quenching analysis

Stern-Volmer luminescence quenching analysis was conducted using an Edinburgh Instruments FS5 spectrofluorometer. The following parameters were employed: excitation wavelength = 400nm, excitation bandwidth = 1 nm, data interval = 1 nm, dwell time = 0.1 sec. All the fluorescence quenching experiments were carried out in degassed DCM at room temperature.

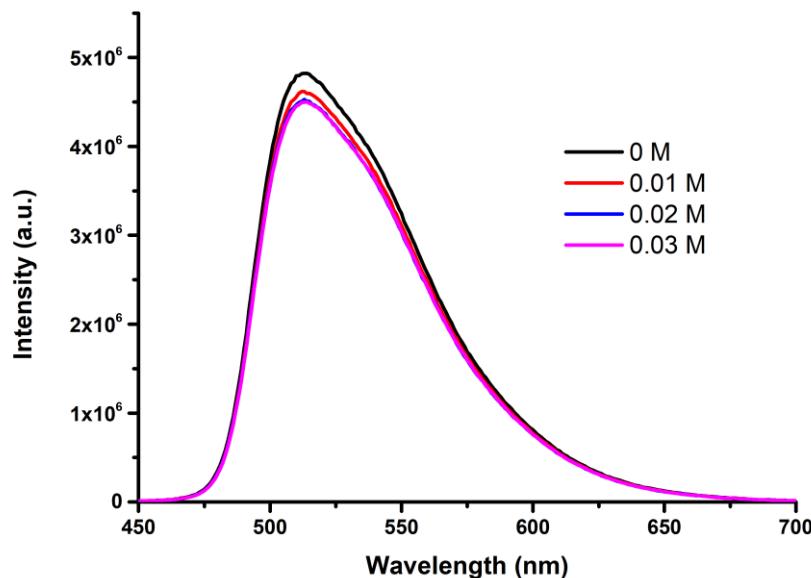


Figure S25. The emission quenching of $\text{Ir}(\text{ppy})_3$ (1.0×10^{-5} M) as a function of concentration of (S)-**1a**/HNTf₂ at room temperature.

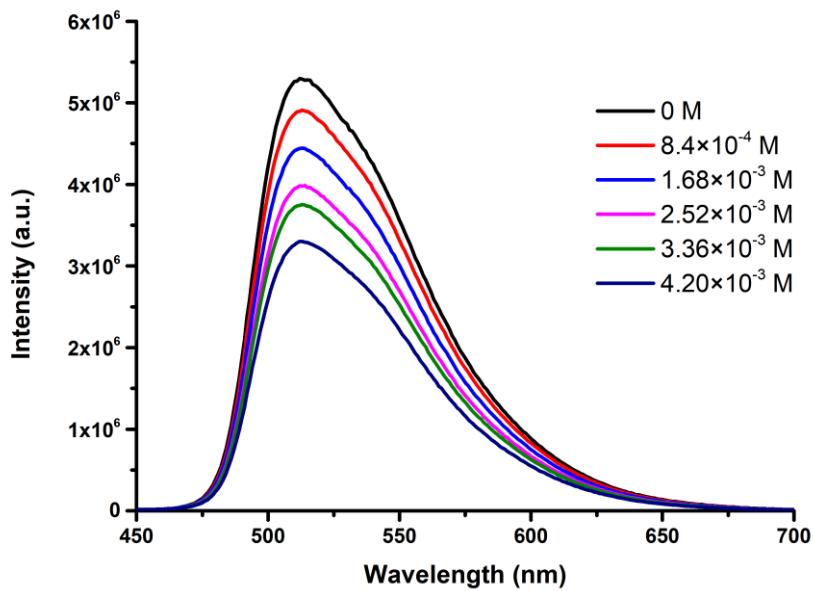


Figure S26. The emission quenching of $\text{Ir}(\text{ppy})_3$ (1.0×10^{-5} M) as a function of concentration of enamine. The enamine solution was prepared from a pre-equilibrated mixture of (*S*)-**1a**/HNTf₂ (0.1 M), **2a** (0.1 M) and PhCOOH (0.02 M) in DCM, the concentration of enamine was determined by NMR to be 0.0168 M. The above concentration was calculated from dilution ratio.

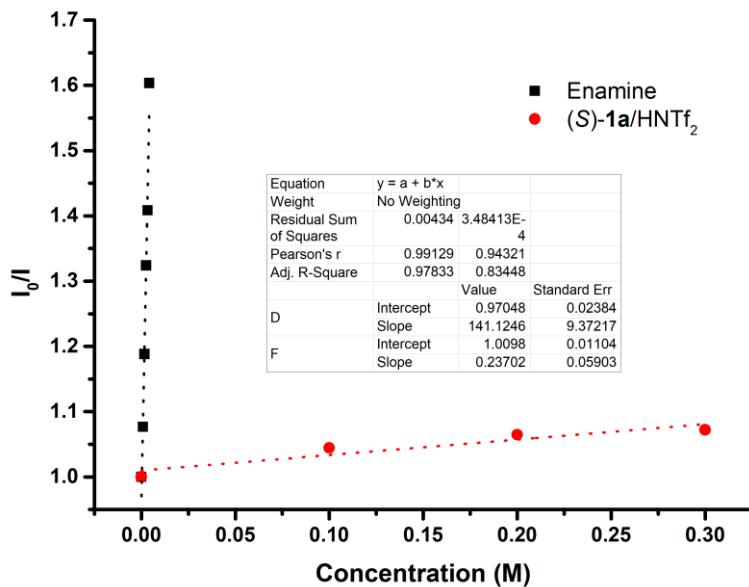


Figure S27. Stern-Volmer plots of $\text{Ir}(\text{ppy})_3$ using enamine and (*S*)-**1a**/HNTf₂ as quenchers in DCM.

6.8. Racemization experiment

Racemization under standard conditions without light irradiation:

To an oven-dried 10 mL Schlenk tube equipped with a magnetic stir bar was added aminocatalyst (*S*)-**1a**/HNTf₂ (9.1 mg, 10 mol %) and benzoic acid (0.73 mg, 3 mol %). Freshly prepared (*R*)-**2a** or (*S*)-**2a** (26.8 mg, 0.2 mmol) dissolved in 0.3 mL MeCN was then added into the tube under Ar atmosphere. The mixture was degassed for 3 times using standard freeze-thaw method and stirred at 0°C for 10 h. The enantiomeric excess was monitored every hour.

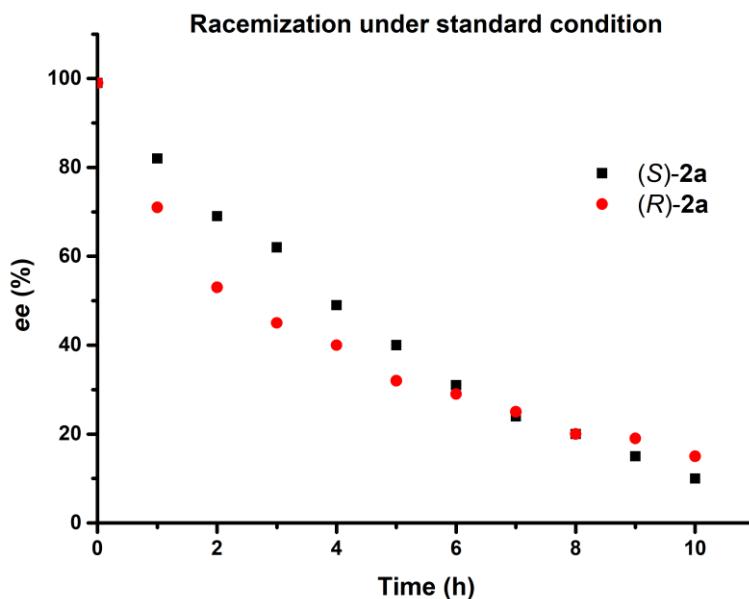


Figure S28. Racemization curve under standard conditions without light irradiation.

Racemization at room temperature without light irradiation:

To an oven-dried 10 mL Schlenk tube equipped with a magnetic stir bar was added amine (10 mol %) and PhCOOH (3 mol %, if necessary). (*R*)-**2a** (26.8 mg, 0.2 mmol) dissolved in 0.3 mL MeCN was then added into the tube under Ar atmosphere. The mixture was degassed for 3 times using standard freeze-thaw method and stirred at room temperature for 4 h. The enantiomeric excess was monitored every half-hour.

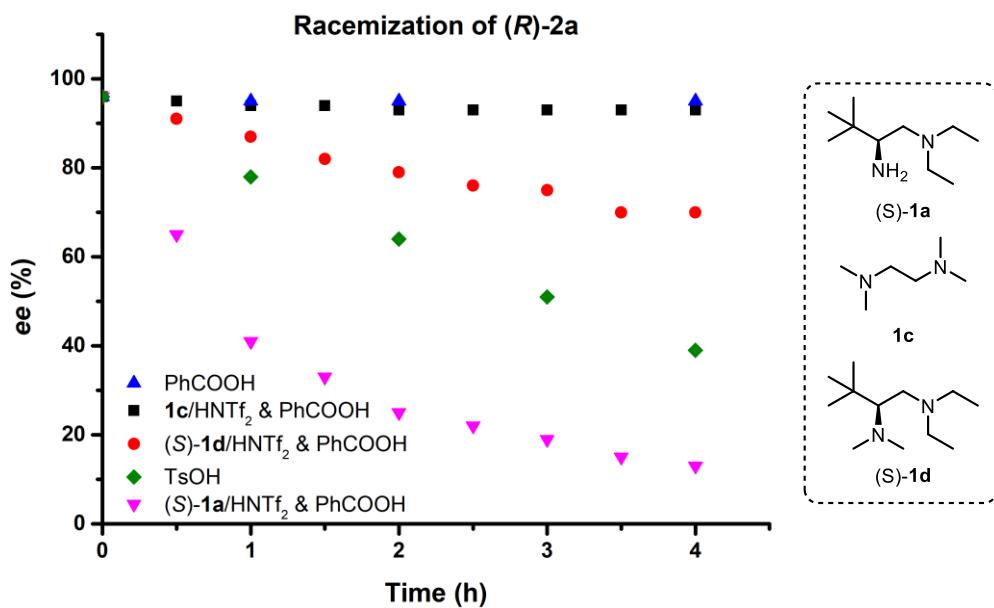


Figure S29. Profiles of the racemization by benzoic acid (3 mol%) and amines (10 mol%).

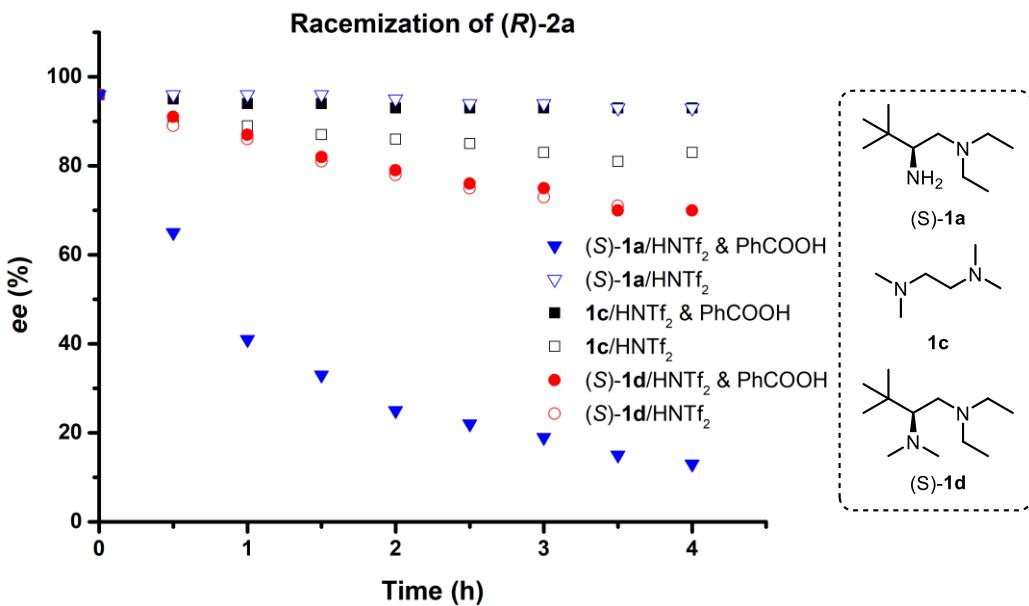


Figure S30. Benzoic acid (3 mol%) additive effect in the racemization processes with amines (10 mol%).

Though strong acid such as TsOH was able to promote effective racemization, the involvement of free strong acid species was discounted in the present acid-amine system. In fact, the use of only

weak acid such as benzoic acid showed no racemization activity at all. In addition, the use of achiral amine **1c**-acid conjugate or dimethylated **1d**-acid conjugate showed rather weak racemization activity. In contrast, the racemization with **1a**-acid conjugate was much faster than that with **1d** or **1c**-acid conjugates. We also examined the effect of weak acid (benzoic acid) additive on racemization by acid-base catalysis. Though no obvious effect was observed with **1c**-Tf₂NH (even minor deaccelerating effect observed in this case) or **1d**-Tf₂NH, significant promoting effect was observed in the case with **1a**-Tf₂NH, to note that (*R*)-**2a** was barely racemized with only **1a**-Tf₂NH in the absence of benzoic acid. This observation is in line with the role of weak acid to facilitate iminium-enamine tautomerization as shown in Fig. S15.

Taken together, these observations suggest the racemization proceeds via an enamine process and the competing acid-base mediated enol-process, even if not be able to be completely excluded, is minor.

7. Computational investigations

7.1. General information of calculation

DFT calculations were performed with Gaussian 09 (45). Geometry optimizations were computed at M06-2X/def2-SVP level of theory (46, 47) and solvation (acetonitrile) with SMD model (48). Frequency analysis was performed at the same level to provide correction to thermodynamic functions and confirm the nature of optimized structures (minima and transition states featured zero or one imaginary frequency, respectively). Single point energies were computed at M06-2X/def2-TZVPP level of theory and solvation (acetonitrile) with SMD model. The minimum energy crossing point were calculated with sobMECP program with M06-2X/def2-SVP level (49). Frequency calculation and single point energy calculation were then performed with the obtained structure to get the ZPE and accurate energy. The vertical excitation energy was performed with TDDFT method with def2-TZVP basis set (50, 51). Molecular structures were visualized in CYLview (52).

7.2. Calculation for enamine formation

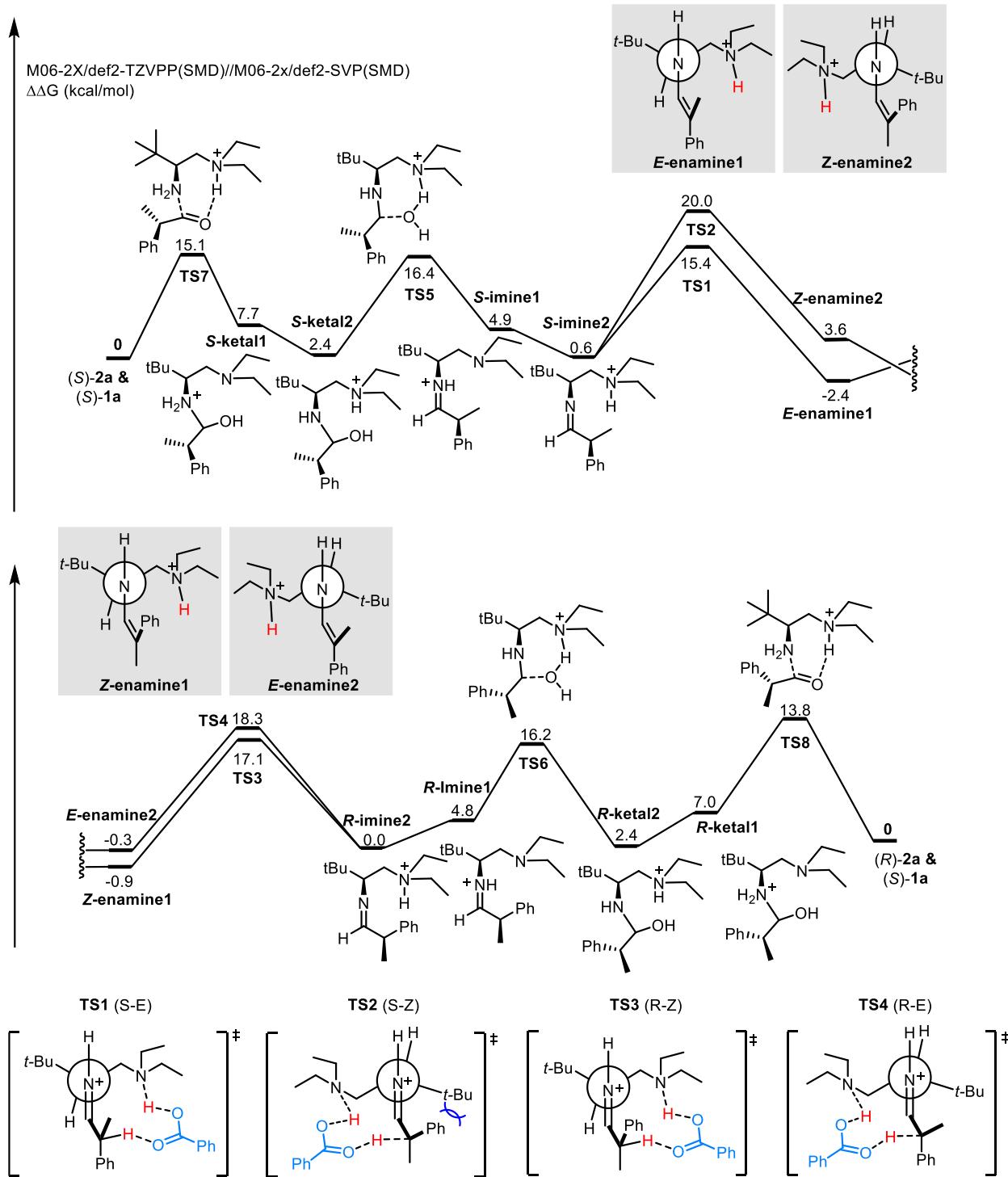


Figure S31. The whole *E*- and *Z*-enamine formation profile from **2a**.

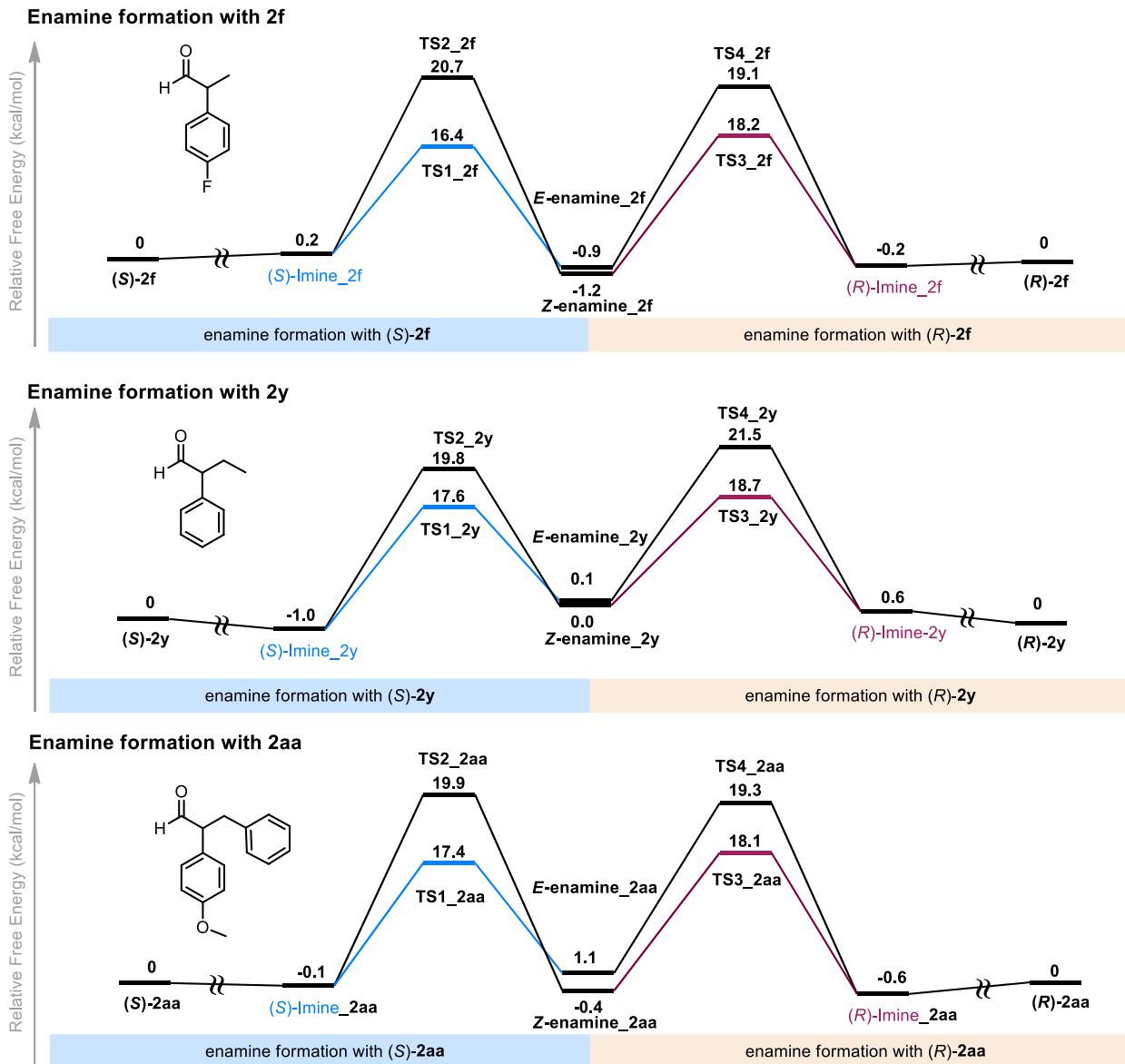


Figure S32. Enamine formation with 2f, 2y and 2aa.

7.3. Calculation for enamine isomerization

The vertical excitation energy showed that photo excitation of *E*-enamine was favored over *Z*-enamine, and the **T₁** state could be reached after intersystem crossing. For the subsequent relaxation from **T₁** to **S₀**, we calculated the minimum energy crossing point (MECP) between singlet and triplet surfaces using sob-MECP program. The MECP structures stood 0.6 and 0.7 kcal/mol above twisted intermediate (**T₁**), respectively for *Z* and *E*-enamine. Since the energy

parameters of *E/Z*-enamine here were similar, we speculated that the final concentrations of them were approximately equal under light irradiation, which was consistent with experimental results.

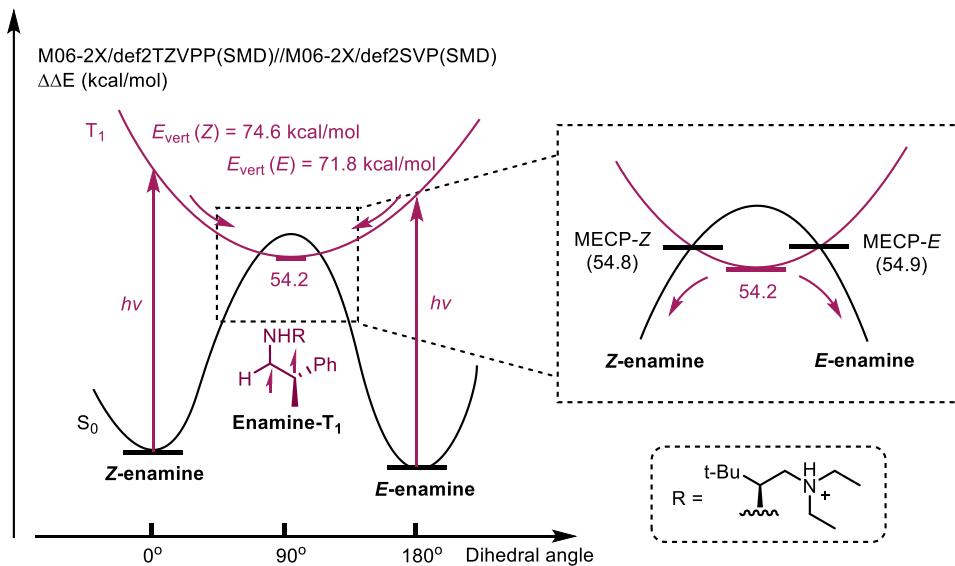


Figure S33. The photoinduced enamine isomerization.

Table S7. The vertical excitation and triplet state energy (Energy in kcal/mol)

	$E_{\text{vert}}(Z)$	$E_{\text{vert}}(E)$	E_{T1}
2f	75.6	72.4	52.5
2y	77.9	71.2	52.4
2aa	76.0	73.2	53.4

7.4. The coordinate of intermediates and transition states.

(1) E-enamine1	H 0.44806400 4.09168900 -0.97248000 C 1.87664600 2.95470800 1.06074800 H 1.03120600 2.73627400 1.73183800 H 2.79721000 2.56437700 1.52039300 H 1.97509700 4.04947200 1.00692700 C 1.48168500 0.84392700 -0.32380900 H 1.19034900 0.55051000 -1.34451300 C 2.78791500 0.12579200 0.03714600 H 3.16583600 0.47896300 1.00616900 H 3.55989500 0.27737700 -0.72504700 N 0.43446900 0.36907700 0.56454300
C 1.64232000 2.39150100 -0.34428000 C 2.81534700 2.77095900 -1.25497100 H 2.72314000 2.28883600 -2.24157000 H 2.82895600 3.85999900 -1.41102300 H 3.78503600 2.48777500 -0.81938500 C 0.35563300 2.99658900 -0.91569700 H 0.15706000 2.61712100 -1.93042100 H -0.51682700 2.76680500 -0.28558300	

H 1.64678600 -1.42365500 0.65020300
 N 2.56233900 -1.34477700 0.17451300
 C 3.56811300 -2.00219200 1.07292200
 H 3.54691700 -1.43079900 2.00908100
 H 3.18958800 -3.00935300 1.28401500
 C 2.41048000 -2.00955000 -1.16070300
 H 1.59397300 -1.48373200 -1.66983300
 H 3.33799100 -1.81824500 -1.71659500
 C 2.10325600 -3.48723300 -1.04787000
 H 2.96492300 -4.06478400 -0.68731700
 H 1.24734800 -3.66330000 -0.37942900
 H 1.83832300 -3.86411400 -2.04450100
 C 4.95891500 -2.04226200 0.47849800
 H 5.32847800 -1.03700000 0.23158300
 H 5.63985000 -2.47600500 1.22281000
 H 5.00217400 -2.67115000 -0.42155400
 H 0.52298800 0.68415600 1.52768900
 C -0.85267200 0.15401200 0.11344400
 C -1.96514600 0.11152800 0.88350000
 H -0.91735100 0.00203000 -0.96835200
 C -3.28669700 -0.14189100 0.26696100
 C -4.45548700 0.36864700 0.86218700
 C -3.43599800 -0.88651500 -0.91960300
 C -5.70993200 0.16597700 0.28675100
 H -4.38329200 0.94797800 1.78462600
 C -4.68825400 -1.08410000 -1.49613700
 H -2.56032100 -1.33976700 -1.38853800
 C -5.83590800 -0.55768300 -0.89859900
 H -6.59601900 0.58279300 0.77006600
 H -4.76890900 -1.66840500 -2.41517000
 H -6.81734800 -0.71777400 -1.34851600
 C -1.89445500 0.39918700 2.36347900
 H -0.93929100 0.06447700 2.79526000
 H -1.99800100 1.47514100 2.58691400
 H -2.69182400 -0.12498300 2.90859400

(2) Z-enamine1

C -1.07546700 2.52694200 -0.38935400
 C -2.43560200 3.22959900 -0.46575900
 H -2.96450400 3.17475700 0.49937800
 H -2.29294700 4.29230600 -0.71272600
 H -3.08405200 2.79467200 -1.24090200
 C -0.16522800 3.31557900 0.55771000
 H -0.60233200 3.38192800 1.56653500
 H 0.82988200 2.85421800 0.64364000

H -0.02800200 4.33978400 0.17880800
 C -0.43268900 2.49308700 -1.77921500
 H 0.58129300 2.06441400 -1.74695100
 H -1.03142000 1.92075300 -2.50361300
 H -0.33918400 3.51884700 -2.16649800
 C -1.26538900 1.09758500 0.19578700
 H -1.59780300 1.23644100 1.23623900
 C -2.34013000 0.29964200 -0.55422400
 H -2.12519100 0.27435700 -1.63116200
 H -3.33794100 0.72467000 -0.39895500
 N -0.04830500 0.30279800 0.24307600
 H -1.37831200 -1.40279600 -0.04669300
 N -2.37253000 -1.12172400 -0.09469000
 C -3.03210800 -2.03089500 -1.08923800
 H -2.50959800 -1.86188800 -2.03947100
 H -2.81779200 -3.05676600 -0.76741000
 C -2.90762500 -1.24276200 1.30128000
 H -2.24229300 -0.64122500 1.93233000
 H -3.89946300 -0.77172600 1.30481700
 C -2.94931600 -2.67219700 1.79778000
 H -3.71716300 -3.27020300 1.28911800
 H -1.97216000 -3.16271100 1.67532200
 H -3.18842400 -2.65822800 2.86935700
 C -4.52058000 -1.79290200 -1.22596700
 H -4.74619200 -0.76794700 -1.55119200
 H -4.90846900 -2.48002400 -1.98980700
 H -5.05859200 -1.99722600 -0.28971600
 H 0.44136500 0.23647900 -0.64778100
 C 0.75594300 0.32081900 1.37088300
 C 2.06540400 -0.00430000 1.47896800
 C 2.74964200 0.14631500 2.81606800
 H 2.01751100 0.36363800 3.60618400
 H 3.29540200 -0.76913500 3.09631100
 H 3.48491600 0.96719800 2.81454500
 C 2.88900900 -0.46364200 0.33414800
 C 4.24515500 -0.09797000 0.23984600
 C 2.37217000 -1.30849300 -0.66671100
 C 5.03677500 -0.52660500 -0.82370400
 H 4.68613300 0.54114900 1.00692700
 C 3.16605100 -1.74141000 -1.72860500
 H 1.34153500 -1.66250800 -0.59685300
 C 4.50098900 -1.34700600 -1.81803300
 H 6.08272900 -0.21736600 -0.87538000
 H 2.73893000 -2.40245700 -2.48548400
 H 5.12222600 -1.68306800 -2.65007100
 H 0.22373600 0.64382800 2.27248500

(3) E-enamine2

C -1.61886500 2.43610200 -0.46722600
C -2.99007400 2.80803300 -1.04400600
H -3.78001300 2.72122300 -0.28086600
H -2.97453500 3.84988000 -1.39763000
H -3.26583200 2.17500100 -1.90074300
C -1.21673900 3.48649800 0.57222700
H -1.94923300 3.53413100 1.39374000
H -0.22845100 3.26501200 1.00351200
H -1.16285200 4.48099800 0.10429200
C -0.57913700 2.43081900 -1.59261100
H 0.44151000 2.29650200 -1.20577600
H -0.77502900 1.64968400 -2.34329100
H -0.60673800 3.39980900 -2.11469800
C -1.73630200 1.06943000 0.26744400
H -2.52786700 1.21285200 1.01927400
C -2.17439500 -0.07749500 -0.64949200
H -1.44732900 -0.24920600 -1.45290700
H -3.15178400 0.12301400 -1.10234900
N -0.56209200 0.66003300 1.02959700
H -1.56882000 -1.25283400 0.88454100
N -2.27697200 -1.34916000 0.13588000
C -1.87738100 -2.55583400 -0.66099200
H -0.88247000 -2.32570500 -1.06365500
H -1.76915100 -3.38308300 0.05032700
C -3.60806900 -1.47519500 0.81518200
H -3.73469100 -0.55810600 1.40408400
H -4.36863600 -1.47980100 0.02381700
C -3.69778700 -2.69912900 1.70050300
H -3.71406900 -3.63111400 1.11972800
H -2.86099600 -2.73479900 2.41364200
H -4.63167200 -2.64436400 2.27531000
C -2.85797500 -2.89159800 -1.76319200
H -3.00861900 -2.04634700 -2.44968700
H -2.44775700 -3.72740500 -2.34530600
H -3.83228600 -3.20716200 -1.36532600
H -0.50184000 1.07845500 1.95225500
C 0.64193800 0.33872000 0.43326400
C 1.86186500 0.38090300 1.02005800
H 0.54857400 -0.04473800 -0.58648900
C 3.05342600 -0.11366600 0.29033100
C 4.18507700 -0.55566500 0.99979100
C 3.11530100 -0.15408400 -1.11718000
C 5.31476400 -1.03775300 0.33754600
H 4.18048200 -0.53686700 2.09090000

C 4.24107500 -0.63872700 -1.77705600
H 2.27802600 0.21984800 -1.71040500
C 5.35020000 -1.08713600 -1.05492200
H 6.17368800 -1.37765600 0.92002700
H 4.25804000 -0.65273000 -2.86878600
H 6.23417300 -1.46148600 -1.57410400
C 2.03895300 0.86059300 2.43825300
H 1.23681600 1.54942700 2.74107100
H 2.04841700 0.03074600 3.16515600
H 2.98916300 1.40181100 2.55448300

(4) Z-enamine2

C -1.31495300 -2.54279000 -0.07530500
C -2.71607200 -3.09631200 -0.36270600
H -3.04944400 -2.83063400 -1.37904000
H -2.70505600 -4.19399300 -0.28755900
H -3.46253500 -2.72474500 0.35539300
C -0.30126000 -3.28546500 -0.94943500
H -0.56075100 -3.20020600 -2.01650200
H 0.71347800 -2.88424100 -0.80872400
H -0.28106800 -4.35382600 -0.68658400
C -0.96644000 -2.77859000 1.39726700
H 0.08310700 -2.52992300 1.61186300
H -1.60806200 -2.19873600 2.07855600
H -1.10979100 -3.84358900 1.63682700
C -1.26575900 -1.03706900 -0.47378400
H -1.41658500 -1.02528900 -1.56318900
C -2.40511900 -0.22819900 0.15976100
H -2.40599200 -0.31694600 1.25372200
H -3.37625500 -0.56699100 -0.21603600
N 0.01064400 -0.37635000 -0.25287700
H -1.28245800 1.45509300 -0.06752200
N -2.28567200 1.22913000 -0.15494100
C -2.99903200 2.08390500 0.85306500
H -2.60245600 1.77873100 1.82976000
H -2.68432600 3.11787100 0.66956500
C -2.65112900 1.52585100 -1.58006700
H -1.98219400 0.91436400 -2.19716700
H -3.67763500 1.16537200 -1.72536700
C -2.50203400 2.99047900 -1.93118000
H -3.25908300 3.61728100 -1.44147700
H -1.50089700 3.36086700 -1.66528600
H -2.62596900 3.09915800 -3.01666400
C -4.50457000 1.94172600 0.79764400
H -4.82554900 0.90428200 0.96530400
H -4.93586600 2.55919800 1.59673300

H -4.91735500 2.29553600 -0.15735900
 H 0.66015700 -0.39640400 -1.02975100
 C 0.50012700 -0.05542900 0.99554400
 C 1.74648200 0.34456400 1.35048500
 C 1.97699800 0.83056200 2.76153300
 H 1.11071400 0.60111400 3.39804800
 H 2.86660600 0.35968400 3.20990900
 H 2.13733300 1.92041100 2.80694000
 C 2.89913400 0.38818900 0.41870000
 C 3.87221300 1.39796000 0.54227500
 C 3.10027100 -0.58718200 -0.57698100
 C 4.97166000 1.45219100 -0.31304700
 H 3.76228300 2.16097100 1.31506100
 C 4.20010000 -0.53426800 -1.43166300
 H 2.40362100 -1.42316700 -0.66351200
 C 5.13990700 0.49026700 -1.31000200
 H 5.70525700 2.25257700 -0.19720700
 H 4.32954200 -1.30893400 -2.19011000
 H 6.00168700 0.53129400 -1.97834000
 H -0.26239900 -0.06798400 1.78182300

(5) TS1

H 1.39298400 -0.71915900 1.53631000
 H -1.23333800 -3.53115300 0.67508300
 H -2.20582700 -2.74535700 -0.57542200
 H 0.26510300 -2.82060400 -2.66874500
 H 0.76428900 -1.19929500 -2.15443200
 H 0.93206800 -3.25972400 0.87531300
 H 2.51655500 -1.51525500 -1.10043700
 N 1.73111200 -0.61242200 0.57788800
 C -1.28110700 -3.30889400 -0.39876300
 C -0.04638700 -1.93534400 -2.09810000
 N -0.15133800 -2.35464700 -0.66508800
 C 1.14088100 -2.87424100 -0.13196600
 C 2.24136300 -1.81356700 -0.07888200
 H 0.18965500 2.56873400 2.38294000
 H 1.71752300 1.70849200 2.69111700
 H 0.20378300 0.79952900 2.37866700
 C 0.78637200 1.69059500 2.10158400
 C 1.68377800 0.57504500 0.02933900
 C 1.07963400 1.71893000 0.60574200
 H -0.42128200 -1.50871900 -0.09750500
 C -5.62216400 1.40288200 -0.10511000
 C -4.22950600 1.44813000 -0.14563000
 C -3.47814100 0.42508900 0.44208400
 C -4.12816200 -0.63999000 1.07480700

C -5.52069000 -0.68287000 1.11792100
 C -6.26808500 0.33767400 0.52641000
 H -6.20696600 2.19998400 -0.56778700
 H -3.70928500 2.27276400 -0.63475200
 H -3.52712500 -1.42599400 1.53477100
 H -6.02610200 -1.51306600 1.61460700
 H -7.35877800 0.30349200 0.55808100
 C -1.97053200 0.45683300 0.39386200
 O -1.44082200 1.46460200 -0.16346900
 H -0.09770700 1.51736400 0.10331900
 O -1.33486800 -0.49984200 0.88127700
 H 1.45411900 -3.70676000 -0.77242600
 C 3.54357200 -2.31578100 0.60603100
 C 4.01520200 -3.59330000 -0.09632100
 H 5.02328800 -3.85515800 0.25702500
 H 3.35792800 -4.44896500 0.11697200
 H 4.06358400 -3.45312400 -1.18770000
 C 4.61230400 -1.23067900 0.43767200
 H 4.79633700 -1.01914400 -0.62734500
 H 4.32027800 -0.29242800 0.93325000
 H 5.55833300 -1.56666800 0.88718100
 C 3.33542600 -2.59368500 2.09857600
 H 2.56713200 -3.36075600 2.27621300
 H 4.27654700 -2.96261000 2.53287400
 H 3.05702100 -1.68338000 2.65223500
 H 2.07345400 0.63293300 -0.99452500
 C 1.51104600 3.04443700 0.04182200
 C 2.78867100 3.24929500 -0.49765900
 C 0.61649900 4.12582300 0.06905300
 C 3.15667700 4.49474000 -1.01026900
 H 3.51227600 2.43032800 -0.50692500
 C 0.98583300 5.37132000 -0.43399400
 H -0.38525400 3.97851700 0.48028900
 C 2.25812200 5.56001400 -0.97931700
 H 4.15671400 4.63293400 -1.42607200
 H 0.27426100 6.19886800 -0.40702300
 H 2.54832400 6.53542700 -1.37393300
 C -1.23167200 -4.57218900 -1.23125300
 H -0.29231200 -5.12520000 -1.09137800
 H -2.05437300 -5.22520900 -0.91038100
 H -1.36927700 -4.36616500 -2.30177700
 C -1.32438700 -1.32916600 -2.64052400
 H -1.13372400 -1.00379100 -3.67204400
 H -2.15558200 -2.04616000 -2.66473700
 H -1.62479300 -0.44073000 -2.06564300

(6) TS2

C 4.20190000 -0.35121200 -0.43995200
C 5.00266000 -1.55442800 -0.95042200
H 4.61299600 -1.91368500 -1.91630200
H 6.05209900 -1.25979300 -1.09740400
H 4.99314500 -2.39129400 -0.23717600
C 4.47228700 0.84790200 -1.35429900
H 4.20071500 0.61858700 -2.39660300
H 3.90527400 1.73596200 -1.03636200
H 5.54179300 1.10419500 -1.32819300
C 4.63994400 -0.00789000 0.98581600
H 4.17148800 0.92086200 1.34608100
H 4.41269500 -0.81722500 1.69637700
H 5.72850500 0.15160600 1.00070600
C 2.68587500 -0.68158700 -0.52689400
H 2.47274300 -0.84544600 -1.59357600
C 2.26333600 -1.93151300 0.24085300
H 2.35132100 -1.79152200 1.32573700
H 2.89602100 -2.78114300 -0.03824000
N 1.84232800 0.45875700 -0.14544500
H 0.29123100 -1.42619600 -0.27036500
N 0.84468100 -2.30069300 -0.06121600
C 0.14021800 -2.88409500 1.12649900
H 0.24125400 -2.13565500 1.92397900
H -0.92404400 -2.94445200 0.86224800
C 0.76311500 -3.15370800 -1.29254100
H 1.23400600 -2.57130700 -2.09492800
H 1.38446100 -4.04033000 -1.10961700
C -0.65754600 -3.52729700 -1.66020000
H -1.08699600 -4.25416800 -0.95731000
H -1.30120300 -2.63684000 -1.69562900
H -0.64853300 -3.98884800 -2.65648000
C 0.68535800 -4.23077200 1.55054700
H 1.76073900 -4.18482500 1.77436600
H 0.16392900 -4.54293700 2.46510500
H 0.51378000 -5.00197900 0.78665300
H 1.44561000 1.00045500 -0.91381400
C 1.51238400 0.80469000 1.07489400
C 0.54104800 1.77032800 1.43091100
C 0.58156200 2.28313600 2.86663200
H 0.87063400 1.48136700 3.56198400
H 1.29675800 3.11319100 2.97594200
H -0.41022300 2.65174900 3.16444000
C 0.12347700 2.78836500 0.40165700
C -1.23174600 3.08983500 0.20493000
C 1.08324700 3.50544000 -0.32845700

C -1.61636700 4.07279000 -0.70632200
H -1.98993700 2.54842500 0.77485700
C 0.69863400 4.48514700 -1.24460200
H 2.14591100 3.29734100 -0.17353600
C -0.65328700 4.77083500 -1.43662100
H -2.67614000 4.29335600 -0.84780600
H 1.46019100 5.03222900 -1.80365700
H -0.95684000 5.53894000 -2.15021800
H 1.94414400 0.20446400 1.88376900
C -5.63104900 -0.57145000 0.75703500
C -4.28895100 -0.32289000 1.04046000
C -3.32195500 -0.47273200 0.04027800
C -3.70748600 -0.86509800 -1.24611600
C -5.04979900 -1.11153000 -1.52935000
C -6.01167700 -0.96670300 -0.52721700
H -6.38408000 -0.45635700 1.53873000
H -3.97334500 -0.01252500 2.03738200
H -2.94323400 -0.96624600 -2.01824000
H -5.34899400 -1.41524500 -2.53413900
H -7.06304100 -1.16072700 -0.74857000
C -1.86656900 -0.21091500 0.33839400
O -1.59018700 0.20276600 1.50769200
H -0.41924300 0.88873200 1.47434200
O -1.02560300 -0.40239900 -0.56061500

(7) TS3

H -1.41734700 0.70744000 -0.55897800
H -0.30113000 -2.75751800 -1.99975000
H 0.79255200 -3.29273700 -0.71546500
H -1.69369300 -3.59147000 1.38364700
H -1.36756300 -1.94024200 1.94670900
H -2.13932100 -1.62620300 -1.63294700
H -3.11602700 -0.98042500 1.21145700
N -1.84240500 0.36892800 0.30830500
C -0.26161800 -3.24235600 -1.01597800
C -0.96840400 -2.76698000 1.34632800
N -0.92532700 -2.28458400 -0.06924300
C -2.26695000 -1.86937300 -0.56914500
C -2.85327200 -0.67611300 0.18783400
C -1.43352900 0.89728900 1.43660400
C -0.37923700 1.82961800 1.57976700
H -0.29615900 -1.43770000 -0.10296200
C 5.64022700 -0.58751200 0.49875400
C 4.32312800 -0.33152600 0.87588200
C 3.28429800 -0.50563200 -0.04508600
C 3.57058300 -0.93647400 -1.34474800

C 4.88820900 -1.18994500 -1.72161800
 C 5.92311100 -1.01641600 -0.79966900
 H 6.44909200 -0.45193900 1.21887500
 H 4.08304200 0.00474800 1.88535700
 H 2.74874100 -1.06435600 -2.05088900
 H 5.11136000 -1.52268900 -2.73695000
 H 6.95516100 -1.21590400 -1.09470200
 C 1.85819100 -0.22904700 0.35421700
 O 1.66775000 0.16161500 1.54924500
 H 0.54180300 0.89915000 1.61402000
 O 0.95283600 -0.39397500 -0.48515700
 H -2.93977700 -2.73049700 -0.48305900
 C -4.15288800 -0.12377200 -0.46376300
 C -5.14004300 -1.27608200 -0.67602600
 H -6.11989600 -0.87014900 -0.96750400
 H -4.81386500 -1.95816600 -1.47480100
 H -5.27530400 -1.85907200 0.24873900
 C -4.76889500 0.89003700 0.50529100
 H -5.01780300 0.41607100 1.46744900
 H -4.08561800 1.73118100 0.69998600
 H -5.69420600 1.30344400 0.07747400
 C -3.86335800 0.56921400 -1.79949900
 H -3.39144600 -0.10795900 -2.52734600
 H -4.80819200 0.92205000 -2.23898400
 H -3.21367200 1.44875000 -1.66846000
 H -1.89382500 0.48124900 2.34165900
 C -0.89661900 -4.61621600 -1.05243900
 H -1.95584200 -4.57560600 -1.34169700
 H -0.36911300 -5.21569400 -1.80647000
 H -0.80841500 -5.13839100 -0.08970100
 C 0.38740100 -3.17991900 1.88203200
 H 0.27037600 -3.42751200 2.94564900
 H 0.78987600 -4.06635000 1.37424300
 H 1.11529300 -2.35796600 1.81366700
 C -0.26053600 2.51684200 2.93562100
 H 0.77474300 2.84425300 3.10683100
 H -0.90724000 3.40630200 2.99286800
 H -0.53821800 1.83104700 3.74928200
 C -0.00576600 2.68773400 0.39759800
 C 1.34092000 2.97980200 0.13521600
 C -0.98698400 3.26989300 -0.41848200
 C 1.69701000 3.81247900 -0.92466300
 H 2.11616800 2.54617900 0.77091300
 C -0.63113600 4.09924900 -1.48345600
 H -2.04523700 3.08179100 -0.21664100
 C 0.71241700 4.37023500 -1.74212800

H 2.75092800 4.02420800 -1.11521600
 H -1.40995200 4.54129700 -2.10786000
 H 0.99158700 5.01769800 -2.57525700

(8) TS4

C 3.39252600 -2.38648200 -0.78777500
 C 3.65010300 -3.85002000 -0.41156500
 H 2.94011000 -4.52196700 -0.91921500
 H 4.66649100 -4.13425500 -0.72111500
 H 3.57726700 -4.02042700 0.67252800
 C 3.72577500 -2.18875900 -2.27007800
 H 3.10958000 -2.84436300 -2.90514600
 H 3.56174800 -1.14733100 -2.58468700
 H 4.78341000 -2.43079200 -2.45050500
 C 4.27976200 -1.46951800 0.05743100
 H 4.19645600 -0.41691000 -0.25384600
 H 4.04749700 -1.54014500 1.13103400
 H 5.33207300 -1.76289800 -0.07416400
 C 1.88299900 -2.07832300 -0.59332100
 H 1.33681200 -2.76014700 -1.26251100
 C 1.36540100 -2.29383800 0.82499200
 H 1.79731700 -1.57218100 1.52955900
 H 1.62847000 -3.29853100 1.17256900
 N 1.52329900 -0.72941500 -1.05746600
 H -0.45368400 -1.54234200 0.08606400
 N -0.12565800 -2.15936700 0.87803800
 C -0.58963700 -1.42414800 2.09938000
 H -0.05509900 -0.46408700 2.08243600
 H -1.65619400 -1.20939000 1.95227500
 C -0.79334200 -3.48692000 0.67418900
 H -0.41864000 -3.86359000 -0.28677100
 H -0.42912500 -4.15689900 1.46436000
 C -2.30463200 -3.39000800 0.66623100
 H -2.70881500 -3.18088100 1.66619900
 H -2.64384100 -2.60930800 -0.02949100
 H -2.71361400 -4.35331100 0.33338400
 C -0.35098900 -2.18416900 3.38571900
 H 0.70801600 -2.44986600 3.51453600
 H -0.64155900 -1.54335000 4.22865000
 H -0.95708900 -3.09931200 3.43567800
 H 1.10386000 -0.67544300 -1.98561300
 C 1.62243700 0.37615300 -0.37064000
 C 1.06307300 1.62429000 -0.76440700
 H 2.08743500 0.29471200 0.61812300
 C -5.57235100 1.61171800 0.16468500
 C -4.18191200 1.53912500 0.23003400

C -3.50034900 0.51987100 -0.44390800
 C -4.21827700 -0.41826300 -1.19307900
 C -5.60833800 -0.34089900 -1.26440200
 C -6.28599600 0.67237100 -0.58282300
 H -6.10245800 2.40485600 0.69516700
 H -3.60758000 2.26829400 0.80292000
 H -3.67077400 -1.20011200 -1.72196700
 H -6.16639300 -1.07121200 -1.85304000
 H -7.37482700 0.73130700 -0.63606500
 C -1.99435300 0.43413900 -0.37497200
 O -1.39764400 1.38733300 0.20360600
 H -0.05587200 1.42898900 -0.18111300
 O -1.43004400 -0.55782600 -0.88584600
 C 0.64823200 1.77543300 -2.21771700
 H 0.08381800 2.70827500 -2.34872600
 H 1.51075500 1.79436900 -2.90309100
 H -0.01729700 0.95226800 -2.51831300
 C 1.62576600 2.83225300 -0.06258300
 C 1.65684900 2.88990900 1.33938400
 C 2.10667500 3.93092300 -0.78565600
 C 2.17487200 4.00297000 1.99820600
 H 1.25781600 2.05599400 1.92380100
 C 2.62014000 5.04901900 -0.12552000
 H 2.08853700 3.91588400 -1.87663500
 C 2.66056900 5.08908900 1.26727900
 H 2.18849400 4.02668600 3.08950800
 H 2.99248700 5.89347800 -0.70885700
 H 3.06241800 5.96386800 1.78148600

(9) S-imine1

C 3.58913200 -0.40664500 -0.21129800
 C 4.53178500 0.63669200 0.39827900
 H 4.41923600 0.67941900 1.49257900
 H 5.57404300 0.36548100 0.17355000
 H 4.35619200 1.64240400 -0.00931000
 C 3.95826300 -1.78639100 0.34532700
 H 3.81148000 -1.82274600 1.43616900
 H 3.35357700 -2.58599800 -0.10923700
 H 5.01552200 -2.00481800 0.13388200
 C 3.74364700 -0.40386800 -1.73612800
 H 3.06142200 -1.11510400 -2.22935900
 H 3.56759500 0.59511400 -2.16121100
 H 4.76909100 -0.70292400 -1.99995600
 C 2.14676500 -0.07050100 0.22229600
 H 2.12354500 -0.00786500 1.32081500

C 1.53963600 1.22633900 -0.35603700
 H 1.45543700 1.11634700 -1.44731700
 H 2.24440400 2.05450000 -0.16281300
 N 1.21258100 -1.13695500 -0.14057000
 N 0.22717800 1.46722900 0.20585700
 H 1.32054500 -1.56581000 -1.06634800
 C 0.14353500 -1.38501800 0.51855600
 C -0.94124500 -2.27971600 0.02264400
 C -0.76749000 1.92758700 -0.75859800
 H -0.71990500 1.24475500 -1.62127900
 H -1.76995900 1.79134900 -0.32029500
 C -0.59856600 3.36812100 -1.23369900
 H 0.40359300 3.52947100 -1.66141600
 H -1.33948500 3.59981900 -2.01276000
 H -0.74076500 4.08760800 -0.41344000
 H -0.63928900 -2.68649300 -0.95366500
 C 0.28781100 2.22412600 1.45127400
 H 0.67464800 3.24978000 1.27741600
 H 1.02571300 1.72932100 2.10343100
 C -1.04338800 2.29508100 2.18002100
 H -0.90920600 2.78006500 3.15727800
 H -1.79111900 2.87624200 1.62021300
 H -1.45064300 1.28649400 2.34810300
 H 0.04069500 -0.91349800 1.50201600
 C -1.17471000 -3.42364500 1.01584500
 H -2.00209100 -4.05265400 0.66095000
 H -0.27367400 -4.04599000 1.10579600
 H -1.43061200 -3.03889100 2.01304000
 C -2.16997800 -1.40012900 -0.18063900
 C -2.63304200 -1.13089400 -1.47211400
 C -2.83124700 -0.83053000 0.91461600
 C -3.74625000 -0.31216300 -1.66768200
 H -2.11880800 -1.57033400 -2.33010100
 C -3.93856300 -0.00587400 0.71912900
 H -2.47843900 -1.02886600 1.92976900
 C -4.39931600 0.25446300 -0.57297100
 H -4.10215200 -0.11568500 -2.68073800
 H -4.44250400 0.43681200 1.58044400
 H -5.26706400 0.89857900 -0.72614200

(10) S-imine2

H -1.36464400 2.82877900 1.92416000
 H 0.21770200 3.32432200 1.29521200
 H -0.59870100 2.47329700 -1.72884700
 H 0.07832700 0.85498800 -1.45296000
 H -2.57757700 1.23538400 1.03930900

H -1.70769700 -0.40729000 -1.40279200
 N -0.86796300 -0.91283000 0.47152000
 C -0.80833900 3.06456900 1.00851500
 C 0.02142000 1.87382700 -1.04968900
 N -0.72672600 1.77304300 0.24462700
 C -2.06851700 1.13381900 0.07246300
 C -1.94135000 -0.34263900 -0.32295100
 H 2.40895900 -3.93029400 0.68988800
 H 1.71366900 -3.60270600 -0.91767400
 H 0.66551200 -4.17446200 0.40450100
 C 1.52811700 -3.53526400 0.16472100
 C 0.05703000 -1.53554800 -0.13066400
 C 1.26042800 -2.08841400 0.58643500
 H -0.19243800 1.12441500 0.84629700
 H 1.04472800 -2.04521300 1.66331200
 H -2.61470100 1.70348400 -0.68794500
 C -3.27413500 -1.11895900 -0.11875500
 C -4.40242300 -0.37685000 -0.84277200
 H -5.31883100 -0.98609700 -0.82861900
 H -4.63724800 0.58431700 -0.36121900
 H -4.14171100 -0.18270300 -1.89552000
 C -3.11325600 -2.51012100 -0.73917100
 H -2.87093900 -2.44259000 -1.81150400
 H -2.31810200 -3.08502200 -0.24074100
 H -4.05112000 -3.07632800 -0.63604500
 C -3.62169800 -1.27436300 1.36444500
 H -3.77299800 -0.30414300 1.86110400
 H -4.55803700 -1.84449300 1.46246100
 H -2.83116300 -1.81682300 1.90195300
 H 0.03775600 -1.66956100 -1.23176100
 C 2.43991500 -1.17009600 0.30318000
 C 2.92086800 -0.99899100 -1.00342800
 C 3.05662600 -0.46647700 1.34424400
 C 4.00056000 -0.15368600 -1.25781600
 H 2.44872500 -1.53547600 -1.83062700
 C 4.14135700 0.37608800 1.09148100
 H 2.68705100 -0.58846200 2.36531900
 C 4.61683100 0.53415400 -0.21021100
 H 4.36464400 -0.03306700 -2.28002300
 H 4.61742600 0.90900100 1.91695000
 H 5.46463400 1.19196600 -0.41016800
 C -1.46646000 4.18578200 0.23421400
 H -2.49107600 3.93284100 -0.07140500
 H -1.52173800 5.06437000 0.89084100
 H -0.88648600 4.47117800 -0.65432300
 C 1.41172800 2.44599500 -0.87570300

H 1.95152900 2.34090800 -1.82633000
 H 1.39357300 3.51238000 -0.61361300
 H 1.97157900 1.89464200 -0.10344100

(11) *R-imine1*

C 1.29911900 2.70889000 -0.16579500
 C 2.34519800 3.23986400 -1.15169100
 H 2.12731600 2.90434800 -2.17752800
 H 2.33119500 4.33987100 -1.14373000
 H 3.36296200 2.91801600 -0.88899100
 C -0.07277300 3.27449400 -0.55006300
 H -0.37545900 2.93161300 -1.55203600
 H -0.85365100 2.97208800 0.16461700
 H -0.03614500 4.37385100 -0.56039300
 C 1.66016400 3.15280500 1.25506500
 H 0.95588000 2.75941100 2.00604000
 H 2.67637400 2.83970500 1.53583800
 H 1.61895800 4.25047600 1.31681600
 C 1.24689500 1.17127200 -0.29091700
 H 1.04715800 0.92138100 -1.34366200
 C 2.49992400 0.39865700 0.17088500
 H 2.63010800 0.56042600 1.25150000
 H 3.38045300 0.83424000 -0.33458800
 N 0.13351100 0.60978300 0.47357900
 N 2.34978700 -1.01863200 -0.08701000
 H -0.01311300 0.96737900 1.42474300
 C -0.51333000 -0.43290300 0.11036300
 C -1.53175900 -1.10766900 0.96483100
 C -1.27324500 -2.61369200 0.97554100
 H -0.30932600 -2.82863400 1.45698400
 H -2.06766800 -3.12428000 1.53684500
 H -1.24611900 -3.02446500 -0.04346300
 C 2.86343200 -1.87694000 0.97684700
 H 2.42455100 -1.51945000 1.92183700
 H 2.47344500 -2.89465200 0.82402500
 C 4.38404200 -1.92331900 1.10228300
 H 4.80348600 -0.91482600 1.24317700
 H 4.67580800 -2.53363900 1.96949400
 H 4.85237300 -2.36587600 0.21026100
 H -1.44227400 -0.70552400 1.98498500
 C -2.89510000 -0.68873200 0.41626700
 C -3.39573100 0.56991900 0.77371100
 C -3.64026900 -1.49824700 -0.44632000
 C -4.62430800 1.01060800 0.28735500
 H -2.81434900 1.20557700 1.44766900
 C -4.87240100 -1.05570700 -0.93417900

H -3.27011100 -2.48146600 -0.74091100
 C -5.36663100 0.19587100 -0.57007200
 H -5.00453100 1.99035700 0.58198500
 H -5.44935000 -1.69765200 -1.60234600
 H -6.33076800 0.53717600 -0.95128000
 C 2.76364600 -1.38575400 -1.43690400
 H 3.85061600 -1.21781700 -1.58387900
 H 2.25484600 -0.70227700 -2.13550000
 C 2.41260700 -2.81811800 -1.80385900
 H 2.60859300 -2.99018100 -2.87144500
 H 3.00828500 -3.54767400 -1.23623300
 H 1.34762300 -3.01958500 -1.61081200
 H -0.33711500 -0.80375500 -0.90608100

(12) R-imine2

C 0.42250700 2.32302300 -0.44838200
 C 1.40236800 3.31895600 -1.07826600
 H 1.71256500 2.99100700 -2.08337500
 H 0.92104500 4.30352500 -1.17726200
 H 2.30510500 3.45276700 -0.46366100
 C -0.87464600 2.32296700 -1.26379500
 H -0.68720600 2.03125500 -2.30921700
 H -1.62491700 1.63679000 -0.84102100
 H -1.31240100 3.33262400 -1.26540500
 C 0.10187300 2.74397500 0.98884400
 H -0.64398600 2.07407900 1.44035100
 H 0.99412300 2.75067000 1.63323700
 H -0.31130600 3.76416900 0.98753300
 C 1.04444300 0.89533600 -0.50678000
 H 1.08468700 0.61981700 -1.57732700
 C 2.46335400 0.87131000 0.07269800
 H 2.50523300 1.42438700 1.01957000
 H 3.18857000 1.29925500 -0.62857600
 N 0.24170300 -0.05634400 0.24179700
 N 2.89878100 -0.52464400 0.38375600
 H 2.10699700 -0.94384400 0.89860100
 C -0.56517800 -0.79244000 -0.40125600
 C -1.51845500 -1.74322200 0.27697800
 C -1.52609000 -3.09799100 -0.42524100
 H -0.54592700 -3.58544700 -0.31971900
 H -2.28898300 -3.75941200 0.00935900
 H -1.73235800 -2.99434300 -1.50067100
 C 4.07189400 -0.56552800 1.31997600
 H 3.78782200 0.05521200 2.17867600
 H 4.15628200 -1.60131600 1.66956100
 C 5.36250900 -0.08521800 0.69245000

H 5.28227900 0.94518700 0.31946700
 H 6.14213100 -0.10050800 1.46575200
 H 5.69204100 -0.73894300 -0.12689800
 H -1.17362700 -1.85723600 1.31494600
 C -2.86858900 -1.03804300 0.31261400
 C -3.11225700 -0.10034500 1.32664400
 C -3.84468100 -1.23314300 -0.67039200
 C -4.30175500 0.62399500 1.36016900
 H -2.35357200 0.05880400 2.09780700
 C -5.03783200 -0.50608200 -0.63915200
 H -3.68251900 -1.95789200 -1.47027900
 C -5.26954400 0.42453700 0.37255000
 H -4.47494000 1.34704400 2.15952500
 H -5.79014700 -0.66962000 -1.41318000
 H -6.20163400 0.99200400 0.39436800
 C 3.08534300 -1.33809300 -0.86109400
 H 3.84271400 -0.82138100 -1.46486600
 H 2.13228700 -1.29482900 -1.40213500
 C 3.46189700 -2.77545100 -0.57288400
 H 3.42374800 -3.33868700 -1.51450200
 H 4.47716400 -2.86978200 -0.16523300
 H 2.74932300 -3.23657400 0.12737200
 H -0.64692600 -0.73311700 -1.50575200

(13) TS5

C 2.65636300 -2.11474000 0.27180500
 C 3.76749400 -1.92183900 1.31080600
 H 3.34251400 -1.71782100 2.30618500
 H 4.37062800 -2.83944800 1.38088500
 H 4.44686600 -1.09797000 1.05033400
 C 1.78569100 -3.29793700 0.70853000
 H 1.26317400 -3.07803700 1.65375400
 H 1.02866100 -3.54664800 -0.04915500
 H 2.41500100 -4.18664700 0.86531100
 C 3.27448700 -2.41090400 -1.09846600
 H 2.50760400 -2.50470100 -1.88435100
 H 3.98656300 -1.62935200 -1.40267300
 H 3.82271700 -3.36433200 -1.06000900
 C 1.78012800 -0.83630100 0.23372600
 H 1.48251300 -0.61935500 1.27137500
 C 2.47950500 0.39046100 -0.36574000
 H 2.53059000 0.25955000 -1.45728900
 H 3.51664400 0.44471200 0.00501200
 N 0.53212000 -1.06974400 -0.49595700
 N 1.76337000 1.64150200 -0.08373400
 H 0.61219100 -1.32371900 -1.48257900

C -0.65524100 -0.75942200 -0.04397600
 C -1.88182800 -1.20239000 -0.79281500
 C 1.97835100 2.65609900 -1.13090900
 H 1.70110600 2.18478300 -2.08572400
 H 1.25479000 3.46821800 -0.96468800
 C 3.38948600 3.22114700 -1.21361600
 H 4.13516500 2.42763900 -1.37209700
 H 3.45788900 3.91949700 -2.05965400
 H 3.66132300 3.77396100 -0.30237500
 H -1.71703200 -0.96702500 -1.85495300
 O -0.80814600 1.18011100 -0.38809200
 H 0.18047900 1.42621600 -0.21570100
 H -1.35843900 1.64898700 0.25975500
 H -0.73129800 -0.61713300 1.03916800
 C 2.06156400 2.12186100 1.27512100
 H 3.14730000 2.30351300 1.38223500
 H 1.81218400 1.30797200 1.97180200
 C 1.28286100 3.36710500 1.66203400
 H 1.45250800 3.58859800 2.72465000
 H 1.59556500 4.24779200 1.08335600
 H 0.20145800 3.22278800 1.51588700
 C -2.01577300 -2.72587800 -0.63550700
 H -1.16386800 -3.24185200 -1.10019300
 H -2.06002000 -3.01439600 0.42512300
 H -2.93711000 -3.06622900 -1.12711000
 C -3.11876400 -0.46680000 -0.31896200
 C -3.83610600 0.34828100 -1.20010300
 C -3.56137500 -0.58817600 1.00379800
 C -4.97681300 1.02736100 -0.77083400
 H -3.49276300 0.45295100 -2.23199800
 C -4.69868900 0.09415000 1.43666600
 H -3.01236200 -1.22183000 1.70551400
 C -5.41052200 0.90284600 0.54941000
 H -5.52795300 1.65857400 -1.47049200
 H -5.03115500 -0.00787800 2.47138600
 H -6.30162600 1.43590000 0.88606500

(14) TS6

C 0.16373100 2.42319800 -0.30198300
 C 0.97856100 3.31954400 -1.24084000
 H 1.02383800 2.88968000 -2.25387600
 H 0.50450300 4.30971100 -1.31542400
 H 2.00798500 3.47095400 -0.88528400
 C -1.26409000 2.31208400 -0.85100700
 H -1.27311900 1.79105900 -1.82249400
 H -1.92498800 1.76213000 -0.16339500

H -1.68870200 3.31634800 -0.99881400
 C 0.12808500 3.03434800 1.10209000
 H -0.41479600 2.38999900 1.81284600
 H 1.14018700 3.20923800 1.49655500
 H -0.39324400 4.00322700 1.07316600
 C 0.79853600 1.00904500 -0.28692500
 H 0.90109900 0.69271200 -1.33703200
 C 2.16414900 0.92277700 0.40420600
 H 2.00727500 1.00645400 1.49006400
 H 2.79528900 1.77376300 0.09887700
 N -0.09334800 0.03373800 0.33678000
 N 2.84305100 -0.35285200 0.13193500
 H -0.29966700 0.15914400 1.32959500
 C -0.47434400 -1.08272500 -0.23141700
 C -1.56299000 -1.90686400 0.40782700
 C -1.68254600 -3.29684300 -0.20974100
 H -0.79883900 -3.90183800 0.02925900
 H -2.56897900 -3.80771600 0.18959900
 H -1.78212100 -3.24056100 -1.30391900
 C 3.68051200 -0.79212200 1.26270200
 H 3.02670000 -0.81347600 2.14742800
 H 3.98059500 -1.83369600 1.07440100
 C 4.90815900 0.06497900 1.53805200
 H 4.63701100 1.11571500 1.72150200
 H 5.42400900 -0.30851400 2.43387600
 H 5.62376300 0.03308100 0.70342000
 H -1.31906400 -1.99432800 1.47733200
 O 1.05132000 -2.28191000 0.02329500
 H 1.79326100 -1.55534500 0.03681100
 H 1.22296100 -2.85231900 -0.74418500
 C -2.83631100 -1.08041500 0.28037400
 C -3.37626800 -0.44052400 1.40107600
 C -3.44606700 -0.89428000 -0.96694100
 C -4.50545600 0.37064800 1.27967800
 H -2.90590000 -0.57857300 2.37776200
 C -4.57168400 -0.07995600 -1.08996100
 H -3.03445900 -1.38214200 -1.85376500
 C -5.10426300 0.55546300 0.03309200
 H -4.91938200 0.85924800 2.16373000
 H -5.03522500 0.05888400 -2.06859500
 H -5.98532500 1.19254800 -0.06227700
 H -0.37964700 -1.12191700 -1.32169900
 C 3.56376500 -0.29610800 -1.15104000
 H 4.32049500 0.50943700 -1.12164300
 H 2.83336600 -0.00930700 -1.92235000
 C 4.21607800 -1.61080200 -1.54218800

H 4.61143500 -1.53172000 -2.56426200
H 5.05425400 -1.87241600 -0.88097500
H 3.49160300 -2.43906500 -1.52590800

(15) S-ketal1

C 2.95161600 -1.86631400 0.20142800
C 3.96446900 -1.51795000 1.29913000
H 3.48279200 -1.52170400 2.28896700
H 4.76738300 -2.26934100 1.30761500
H 4.43104200 -0.53479300 1.14639400
C 2.34581800 -3.23508900 0.54590300
H 1.67434500 -3.17381800 1.41816300
H 1.79369100 -3.67957300 -0.29816000
H 3.15314000 -3.93857500 0.79316500
C 3.65706600 -1.95363700 -1.15626200
H 2.94165700 -2.11503800 -1.97869200
H 4.23915600 -1.04715500 -1.37622900
H 4.35448500 -2.80446300 -1.15182100
C 1.85023900 -0.76750700 0.20953600
H 1.52723900 -0.63999900 1.25295800
C 2.33772600 0.55868600 -0.37960600
H 2.36868000 0.46291700 -1.47615300
H 3.37715000 0.71049200 -0.04468400
N 0.61405300 -1.25563700 -0.50210800
N 1.51783800 1.72820200 -0.05295500
H 0.76119000 -1.26590700 -1.52330400
C -0.68917100 -0.50753800 -0.21752800
C -1.87853900 -1.38110700 -0.63306700
C 1.73944300 2.82228100 -1.01531100
H 1.55105900 2.40337800 -2.01578400
H 0.96329700 3.58255000 -0.84651400
C 3.11823700 3.46784800 -0.97264000
H 3.91891800 2.73540600 -1.15424700
H 3.18610400 4.23652100 -1.75540000
H 3.31024900 3.95878400 -0.00713300
H -1.83449100 -1.45883900 -1.73123700
O -0.69464800 0.66618400 -0.90263300
H 0.05567500 1.23190100 -0.51276000
H 0.47225900 -2.23565100 -0.22674200
H -0.68283300 -0.38388700 0.88258800
C 1.66001700 2.13200400 1.35156600
H 2.70973000 2.40835300 1.56643000
H 1.43516200 1.25414800 1.97384200
C 0.72186800 3.26117100 1.74085600
H 0.75419300 3.41010300 2.82890600
H 0.99672300 4.21408100 1.26723800

H -0.31436300 3.01810100 1.45878800
C -1.82756700 -2.78343700 -0.02054000
H -1.08204600 -3.42307700 -0.51734900
H -1.59426600 -2.75095700 1.05502700
H -2.79843900 -3.28287500 -0.14045900
C -3.14992600 -0.63238600 -0.27517400
C -3.82598300 0.11648600 -1.24449200
C -3.65179900 -0.64890200 1.03227200
C -4.98189200 0.82678100 -0.92016100
H -3.43918600 0.14072400 -2.26575800
C -4.80616400 0.06358900 1.36050500
H -3.13938600 -1.22386500 1.80716300
C -5.47595800 0.80269800 0.38487500
H -5.49931500 1.40120400 -1.69103000
H -5.18399000 0.03896600 2.38446600
H -6.38006000 1.35839500 0.64050100

(16) S-ketal2

C 2.37417300 -2.27899800 0.36001800
C 3.58244600 -2.18789700 1.29928300
H 3.31254500 -1.69228700 2.24629400
H 3.94475400 -3.19851200 1.54105500
H 4.42339000 -1.63937300 0.84989700
C 1.36531600 -3.26309500 0.96004900
H 1.04898100 -2.93739800 1.96429100
H 0.47001000 -3.34653700 0.32798200
H 1.81685700 -4.26247800 1.05477300
C 2.81865600 -2.78138300 -1.01576200
H 1.96512900 -2.84033600 -1.70846500
H 3.58438400 -2.12857700 -1.46266800
H 3.25271600 -3.78928900 -0.92824400
C 1.67160000 -0.89481800 0.24498500
H 1.34208000 -0.64353700 1.26754600
C 2.63041900 0.19586800 -0.24071900
H 2.86267800 0.03484300 -1.30266400
H 3.56800200 0.20336700 0.32611300
N 0.48225900 -0.95391800 -0.59277800
N 2.03218800 1.56432000 -0.12231900
H 0.63827600 -0.70121700 -1.56749800
C -0.74809400 -0.47251400 -0.07620400
C -1.92623700 -0.80787700 -1.00366800
C 2.52232100 2.49712800 -1.18821900
H 2.32096800 1.98810800 -2.13948900
H 1.88738400 3.39036000 -1.14615900
C 3.98760500 2.85013500 -1.05070200
H 4.62669800 1.95565100 -1.04894400

H 4.27621900 3.46582400 -1.91303700
 H 4.18870100 3.43381700 -0.14176600
 H -1.71738100 -0.30234600 -1.96157800
 O -0.66249300 0.95011300 0.10811700
 H 1.00607700 1.46204900 -0.26641200
 H -1.46512800 1.28425300 0.53809500
 C 2.17814900 2.10118800 1.26817800
 H 3.25386000 2.16163800 1.47860200
 H 1.74615700 1.34394800 1.93425100
 C 1.48549600 3.43448600 1.45534600
 H 1.49798000 3.68658100 2.52399800
 H 1.98874300 4.24593100 0.91266000
 H 0.43528300 3.38414300 1.13196900
 H -0.91755400 -0.94298100 0.90985500
 C -2.03937100 -2.31294400 -1.24104000
 H -1.15796200 -2.68921900 -1.77657300
 H -2.11580400 -2.86110500 -0.28943700
 H -2.93295900 -2.54329200 -1.83866000
 C -3.20080300 -0.21108800 -0.43606300
 C -3.76388800 0.94285800 -0.99428400
 C -3.81254700 -0.77458600 0.69311200
 C -4.91402400 1.51526000 -0.44677300
 H -3.29502500 1.39679300 -1.87093600
 C -4.96017500 -0.20461200 1.24283100
 H -3.38723800 -1.67123800 1.15067600
 C -5.51597300 0.94248300 0.67318200
 H -5.34163600 2.41219500 -0.89908900
 H -5.42344900 -0.65907000 2.12073300
 H -6.41533600 1.38800700 1.10226500

(17) R-ketal1

C 0.14791400 2.47633300 -0.05363300
 C 1.00167100 3.38809600 -0.94532100
 H 1.13722600 2.95172300 -1.94760000
 H 0.49607500 4.35737900 -1.06337200
 H 1.99258100 3.58340200 -0.51318100
 C -1.28484500 2.49145500 -0.61166200
 H -1.31611300 2.07588700 -1.63093700
 H -2.01224900 1.94346800 0.01114200
 H -1.64479100 3.52948200 -0.65511700
 C 0.14913200 3.00921300 1.38260800
 H -0.47567200 2.39634000 2.05222100
 H 1.16555000 3.05588400 1.79982500
 H -0.26298000 4.02913300 1.39506600
 C 0.71308700 1.03194700 -0.12882900
 H 0.58638100 0.69545500 -1.16808300

C 2.17498800 0.89805800 0.29672700
 H 2.24400300 1.07992300 1.38104500
 H 2.75113900 1.69118600 -0.20539800
 N -0.14714100 0.10588400 0.69110200
 N 2.76161000 -0.41715900 0.01520300
 H 0.14489000 0.12041300 1.68034200
 C -0.21310500 -1.35857300 0.25023700
 C -1.54109900 -1.95500400 0.72522700
 C -1.63431400 -3.41015700 0.26844000
 H -0.79271100 -3.98921400 0.66993900
 H -2.57234900 -3.85925500 0.62214400
 H -1.60967700 -3.48024900 -0.82957700
 C 3.88682100 -0.71678100 0.91786400
 H 3.50240300 -0.61386800 1.94390200
 H 4.14834700 -1.77724400 0.79003400
 C 5.12411900 0.15181700 0.73514100
 H 4.89449500 1.21983000 0.86666400
 H 5.87846900 -0.12230800 1.48611200
 H 5.57844500 0.01540500 -0.25726800
 H -1.51702600 -1.92751300 1.82696800
 O 0.84152600 -2.03647400 0.77995500
 H 1.67437900 -1.55294600 0.45482200
 H -1.10989300 0.47240000 0.68325400
 C -2.70747000 -1.10904700 0.25223300
 C -3.50808500 -0.42271600 1.17370100
 C -2.96686500 -0.94705000 -1.11648400
 C -4.54666100 0.40469700 0.74076700
 H -3.31228400 -0.53782700 2.24285400
 C -4.00105900 -0.11872900 -1.55060900
 H -2.35259600 -1.47266600 -1.85221700
 C -4.79381600 0.56026900 -0.62268600
 H -5.16246000 0.92970300 1.47332600
 H -4.18933000 -0.00191700 -2.61953700
 H -5.60283300 1.20901600 -0.96309000
 H -0.19421900 -1.30630600 -0.85456200
 C 3.08084200 -0.57607900 -1.41085600
 H 3.82510600 0.17993600 -1.72509200
 H 2.16331600 -0.36445500 -1.97920100
 C 3.56301900 -1.97427200 -1.75762500
 H 3.62547000 -2.08359000 -2.84900700
 H 4.55941600 -2.18484300 -1.34411700
 H 2.86035000 -2.73192000 -1.37751800

(18) R-ketal2

C 0.12943600 2.34465900 -0.43081500
 C 1.04809400 3.32188900 -1.17183900

H 1.40985500 2.88866100 -2.11880200
 H 0.49692100 4.24316200 -1.41436000
 H 1.92169100 3.61384500 -0.57027700
 C -1.17254100 2.19548600 -1.22338400
 H -0.97475200 1.81837900 -2.24006200
 H -1.86110800 1.49667200 -0.72551200
 H -1.67634000 3.16989100 -1.31580400
 C -0.19326000 2.88704000 0.96379400
 H -0.85563500 2.19812200 1.51049200
 H 0.71546500 3.04889400 1.56378700
 H -0.71072100 3.85527700 0.88141100
 C 0.78969700 0.93740500 -0.33888000
 H 0.91053600 0.59457600 -1.38034800
 C 2.17215600 0.98650200 0.31972900
 H 2.06534800 1.23027900 1.38602200
 H 2.82733500 1.73002200 -0.14777000
 N -0.07535900 -0.01693700 0.32981800
 N 2.87238900 -0.33533900 0.24050200
 H 0.02337400 -0.06077800 1.34213700
 C -0.39105000 -1.25546700 -0.27955700
 C -1.56260200 -1.94133700 0.44493500
 C -1.79623900 -3.35270000 -0.09291400
 H -0.93413900 -3.99900300 0.12428400
 H -2.67982900 -3.80579100 0.37812800
 H -1.95640400 -3.34790300 -1.18242100
 C 3.80914300 -0.55904800 1.38953400
 H 3.21408800 -0.38743200 2.29519300
 H 4.08914300 -1.61939200 1.36940900
 C 5.02832200 0.33720100 1.35116400
 H 4.75390300 1.40141500 1.32936100
 H 5.61450300 0.15990400 2.26271100
 H 5.67348000 0.11631000 0.48964500
 H -1.26969900 -2.01421700 1.50598300
 O 0.76800700 -2.10630900 -0.27345800
 H 2.13999700 -1.07115900 0.30813800
 H 0.65341000 -2.84040100 -0.89559600
 C 3.50157500 -0.54090300 -1.10320000
 H 4.22457500 0.27252200 -1.24845000
 H 2.69763100 -0.41376300 -1.83863100
 C 4.14683400 -1.90337700 -1.24513700
 H 4.45096300 -2.03816800 -2.29153100
 H 5.04286700 -2.00353100 -0.61812100
 H 3.44074800 -2.70729500 -0.99084100
 C -2.79175500 -1.06031400 0.35576100
 C -3.18355400 -0.27285400 1.44526100
 C -3.52195000 -0.96138200 -0.83553800

C -4.26828000 0.59890000 1.34778800
 H -2.62091400 -0.33829800 2.38025400
 C -4.60807400 -0.09026900 -0.93755400
 H -3.23703200 -1.56488500 -1.70077300
 C -4.98365500 0.69523700 0.15297600
 H -4.55527200 1.20621800 2.20866300
 H -5.16268300 -0.02417700 -1.87574600
 H -5.83118500 1.37847800 0.07355600
 H -0.67715800 -1.07002400 -1.33143100

(19) TS7

C 0.25411800 2.60042500 0.17135200
 C 0.94463400 3.39061200 -0.94612100
 H 0.68846800 2.97980200 -1.93562500
 H 0.61095200 4.43867500 -0.91980300
 H 2.03938500 3.39532200 -0.84703500
 C -1.26364600 2.74923600 -0.01398400
 H -1.60977500 2.21374000 -0.91395300
 H -1.83233200 2.37953200 0.85357500
 H -1.52076600 3.81199100 -0.13258900
 C 0.65722700 3.16232900 1.53747300
 H 0.23567800 2.55999900 2.35790700
 H 1.75034900 3.19729400 1.65979200
 H 0.27678700 4.18907900 1.64871700
 C 0.62211300 1.09105700 0.04397300
 H 0.38889100 0.82036500 -1.00051000
 C 2.10430900 0.84228100 0.32347300
 H 2.29436800 0.95441400 1.40023300
 H 2.72430500 1.56885400 -0.21376500
 N -0.18213100 0.21503500 0.89980900
 N 2.59901600 -0.51742000 -0.05508700
 H 0.16595000 0.20084700 1.86179800
 C -0.21315100 -1.77020300 0.21243700
 C -1.62591200 -2.16112000 0.63335700
 C 3.87536200 -0.85584300 0.65770600
 H 3.66903900 -0.70830700 1.72546700
 H 4.04514100 -1.92836500 0.49950600
 C 5.07024800 -0.03958300 0.21041300
 H 4.90539900 1.03946900 0.33737400
 H 5.93050200 -0.32080100 0.83266400
 H 5.33747900 -0.23926900 -0.83647500
 H -1.74504800 -3.14735000 0.14599100
 O 0.77782900 -2.30544500 0.72874400
 H 1.90857300 -1.25570100 0.28991400
 H -1.15266900 0.52789100 0.93163500
 C 2.68790500 -0.68951300 -1.53881800

H 1.69286400 -0.46103300 -1.93905600
 H 3.38417500 0.07028900 -1.91858400
 C 3.10102900 -2.09260800 -1.93470500
 H 4.15004900 -2.30444700 -1.68708300
 H 2.45943100 -2.84081200 -1.44591800
 H 2.98318300 -2.19960900 -3.02111400
 H -0.14817300 -1.35341800 -0.81636600
 C -1.71554600 -2.35632300 2.13914700
 H -2.69347500 -2.76450000 2.42937400
 H -0.93293200 -3.05279600 2.46506100
 H -1.56788300 -1.40597700 2.67440200
 C -2.66072800 -1.23751900 0.02126500
 C -2.75433100 -1.14331800 -1.37565100
 C -3.51182000 -0.44170400 0.79852900
 C -3.65771200 -0.26958200 -1.97867000
 H -2.11713200 -1.77488600 -2.00050400
 C -4.41992300 0.43310100 0.19646200
 H -3.47010600 -0.49747100 1.88777700
 C -4.49406300 0.52622900 -1.19248700
 H -3.71426800 -0.21519000 -3.06756800
 H -5.07362400 1.04477700 0.82152700
 H -5.20428800 1.21012700 -1.66066500

(20) TS8

C 1.54076300 2.68367600 -0.17582600
 C 3.05065100 2.79404400 -0.41502500
 H 3.30742300 2.47959200 -1.43909000
 H 3.37184400 3.83953800 -0.29358500
 H 3.64012700 2.18784200 0.28875700
 C 0.83420200 3.55936200 -1.21729400
 H 0.96564200 3.15401400 -2.23357800
 H -0.24342400 3.65754300 -1.01748200
 H 1.25934500 4.57382200 -1.19955900
 C 1.18829300 3.18450700 1.22841700
 H 0.11656700 3.04801500 1.44364400
 H 1.76559200 2.66473100 2.00816400
 H 1.41072600 4.25901500 1.31328500
 C 1.10400600 1.20054400 -0.36310900
 H 1.51228500 0.87318100 -1.33531200
 C 1.66317800 0.29477700 0.74417900
 H 0.90880300 0.15925300 1.53267400
 H 2.55571700 0.72944200 1.20748500
 N -0.34153600 1.00334700 -0.45084500
 N 2.05066700 -1.06535500 0.25678900
 H -0.79719200 1.12497700 0.45584900
 C -0.76658100 -0.86736500 -1.43452100

C -1.54462800 -1.49967600 -0.28525100
 C -1.87446900 -2.94268400 -0.69429100
 H -0.94889000 -3.50000100 -0.89612300
 H -2.42374200 -3.45220300 0.10963900
 H -2.49379000 -2.96669200 -1.60396000
 C 2.01730000 -2.09381700 1.34564900
 H 1.01873400 -2.02171900 1.79574400
 H 2.09296300 -3.07350500 0.85737900
 C 3.09911000 -1.91417300 2.39019000
 H 3.04906100 -0.92524600 2.86733200
 H 2.95125900 -2.67056700 3.17262400
 H 4.10504200 -2.05959200 1.97282500
 H -0.87579600 -1.52925200 0.58933200
 O 0.34346400 -1.29123800 -1.77276400
 H 1.32941500 -1.34959100 -0.46527400
 H -0.76628000 1.67367300 -1.09169800
 C 3.34832400 -1.01962900 -0.48594400
 H 3.23199400 -0.25326700 -1.26275900
 H 4.11522700 -0.66650900 0.21636500
 C 3.71073300 -2.35218500 -1.10734700
 H 3.96225900 -3.10876900 -0.35190700
 H 2.88972300 -2.72999200 -1.73436000
 H 4.59039300 -2.21113200 -1.74913100
 C -2.77975300 -0.70667700 0.07643000
 C -2.93697300 -0.16873300 1.35991400
 C -3.79149400 -0.48922700 -0.86918900
 C -4.07220500 0.57264100 1.69129900
 H -2.15737800 -0.33299400 2.10882900
 C -4.92642000 0.25339700 -0.54153700
 H -3.69457400 -0.90822500 -1.87408800
 C -5.07014100 0.78717800 0.74015500
 H -4.17726800 0.98336700 2.69736800
 H -5.70369900 0.41261300 -1.29140500
 H -5.95835700 1.36711000 0.99745800
 H -1.38476400 -0.32026900 -2.17633900

(21) (S)-2a

C 1.98284400 1.15985400 -1.22066700
 H 1.85973700 0.40523600 -2.01157400
 H 1.45383600 2.07251900 -1.52620600
 H 3.05395300 1.39509100 -1.13320700
 C 1.42590300 0.64753300 0.11591900
 H 1.58222300 1.44001000 0.86935300
 C 2.28548900 -0.50465100 0.59467400
 H 3.37531400 -0.26212900 0.63307300
 O 1.89089300 -1.59361300 0.91762700

C -0.04405200 0.31084200 0.05530900
 C -0.97791200 1.04287700 0.79537400
 C -0.50286600 -0.72842700 -0.76579300
 C -2.34108200 0.74885100 0.71795300
 H -0.63219000 1.85509100 1.43976600
 C -1.86207100 -1.02622300 -0.84347100
 H 0.21343000 -1.31301100 -1.34763700
 C -2.78684400 -0.28692900 -0.10186900
 H -3.05557800 1.33306500 1.30113300
 H -2.20261300 -1.84029400 -1.48637000
 H -3.85169900 -0.51903700 -0.16392500

(22) (S)-1a

C 2.36277200 0.11918600 0.18263900
 C 2.42504200 0.80780300 1.54997100
 H 2.09054200 0.12874000 2.35078300
 H 3.45937100 1.11023600 1.77421200
 H 1.80197100 1.71438000 1.58381700
 C 3.38123800 -1.02466000 0.15449900
 H 3.16773500 -1.76322200 0.94351900
 H 3.37312700 -1.54694200 -0.81405200
 H 4.39740300 -0.63494800 0.31741400
 C 2.71571900 1.12904000 -0.91392300
 H 2.68718400 0.67494200 -1.91689400
 H 2.04557300 2.00188000 -0.91074400
 H 3.73937800 1.50153800 -0.75654500
 C 0.95070900 -0.49518500 -0.02084200
 H 0.82653100 -1.23731400 0.78401900
 C -0.17090200 0.54559600 0.11555600
 H 0.00167000 1.38337100 -0.57365600
 H -0.26506500 0.93167400 1.13685700
 N 0.73670800 -1.19884000 -1.28074200
 H -1.16502700 -0.72326600 -1.04937100
 N -1.46707300 -0.08000700 -0.28449300
 C -2.44341600 0.89670500 -0.85766900
 H -1.90989300 1.41656000 -1.66345000
 H -3.24914400 0.31049900 -1.31552100
 C -2.02537500 -0.94323500 0.80366800
 H -1.24279900 -1.67491800 1.03861200
 H -2.16696300 -0.30147000 1.68290100
 C -3.30381900 -1.64642400 0.40038500
 H -4.14486300 -0.94886700 0.29058800
 H -3.17226200 -2.19945200 -0.54132600
 H -3.56549000 -2.36913700 1.18444400
 C -2.97970600 1.87232500 0.16887300

H -2.17159800 2.43295300 0.66014900
 H -3.62824400 2.59546600 -0.34336100
 H -3.58117900 1.36883600 0.93885800
 H 1.12417300 -0.67480900 -2.06665200
 H 1.18684200 -2.11170800 -1.27689000

(23) T₁

C -2.81703700 -1.77957900 -0.01195400
 C -4.23889800 -1.31442100 -0.34686100
 H -4.28845400 -0.88492000 -1.36051100
 H -4.92927500 -2.17051900 -0.31031000
 H -4.60862500 -0.56298800 0.36660600
 C -2.46821400 -2.97331000 -0.90622000
 H -2.51342100 -2.69647600 -1.97150600
 H -1.45767900 -3.35312100 -0.69638800
 H -3.18368500 -3.79237300 -0.73558100
 C -2.75126800 -2.22041000 1.45371900
 H -1.76471200 -2.63881100 1.70643900
 H -2.96765800 -1.39435900 2.14828500
 H -3.49718000 -3.00889000 1.63598900
 C -1.81139900 -0.62633700 -0.30598400
 H -1.79112900 -0.50081500 -1.40015700
 C -2.25776100 0.69785500 0.32746900
 H -2.44947200 0.56716400 1.40160300
 H -3.16128300 1.08972700 -0.15243100
 N -0.44422400 -0.89093500 0.10714400
 H -0.31525000 1.24341400 0.44454700
 N -1.19294600 1.73898100 0.20668500
 C -1.35682600 2.84412400 1.20601100
 H -1.38904800 2.35503500 2.18776700
 H -0.44178600 3.44617900 1.16208300
 C -1.03661500 2.20378200 -1.21043600
 H -0.74572300 1.31564100 -1.78617700
 H -2.03085400 2.52124100 -1.55145800
 C -0.00557500 3.30121900 -1.36737800
 H -0.34327600 4.25435300 -0.93917700
 H 0.95051000 3.02103700 -0.90173800
 H 0.17249600 3.45757500 -2.43958700
 C -2.59084400 3.68877000 0.97054500
 H -3.51325900 3.09465300 1.02927400
 H -2.63588700 4.45506500 1.75588100
 H -2.56018600 4.20551700 0.00108800
 H -0.34414700 -1.14523700 1.08954600
 C 0.45609000 -1.52315600 -0.75193700
 C 1.79781300 -1.85189200 -0.23756700

C 2.11786300 -3.27023900 0.13705400
 H 1.28092300 -3.93545900 -0.11054500
 H 3.01755600 -3.63927500 -0.38440600
 H 2.32408900 -3.37033900 1.21762600
 C 2.78686900 -0.81882300 -0.06189400
 C 4.06042500 -1.09514900 0.50030900
 C 2.52661300 0.52095700 -0.45510600
 C 5.00820600 -0.09060300 0.65970100
 H 4.30429200 -2.11064400 0.81557900
 C 3.48107700 1.51709600 -0.29419500
 H 1.56108700 0.76221800 -0.90558800
 C 4.72910100 1.22166400 0.26595800
 H 5.97935200 -0.33235400 1.09658300
 H 3.25466500 2.53736300 -0.61180500
 H 5.47730500 2.00596200 0.39162300
 H 0.29219400 -1.32118100 -1.81736900

(24) MECP-E

C -2.86098300 -1.75679200 -0.24187000
 C -4.23520700 -1.25885100 -0.70389700
 H -4.17469700 -0.79114700 -1.69982300
 H -4.93137200 -2.10831200 -0.77096800
 H -4.66824200 -0.53017900 -0.00237000
 C -2.43258800 -2.91728200 -1.14580700
 H -2.37945900 -2.59759800 -2.19866700
 H -1.44740800 -3.31115700 -0.85625300
 H -3.16357900 -3.73732800 -1.07454000
 C -2.95564600 -2.25785200 1.20252200
 H -2.01117300 -2.71734800 1.53270200
 H -3.21530100 -1.45266500 1.90714100
 H -3.73918000 -3.02706900 1.27583500
 C -1.81525300 -0.60830700 -0.37612800
 H -1.65348900 -0.45753100 -1.45585100
 C -2.33195600 0.70341000 0.23162100
 H -2.68733800 0.53718800 1.25727100
 H -3.14764600 1.12789800 -0.36338800
 N -0.51522100 -0.90163000 0.20029600
 H -0.41655800 1.21455600 0.63910000
 N -1.25264900 1.73341400 0.31793100
 C -1.54300700 2.77513800 1.35761600
 H -1.74220200 2.22128400 2.28387500
 H -0.61749200 3.34545500 1.49975500
 C -0.90021100 2.28728200 -1.02939100
 H -0.58144200 1.42770100 -1.63303500
 H -1.82620800 2.68624300 -1.46444000
 C 0.19744400 3.32815000 -0.96126300

H -0.15260600 4.27212600 -0.52302200
 H 1.05483800 2.96210400 -0.37765100
 H 0.54652100 3.53708100 -1.98112900
 C -2.70142300 3.67973500 0.99620500
 H -3.63231100 3.11797400 0.83807700
 H -2.86672300 4.37226300 1.83229600
 H -2.49012400 4.28134200 0.10133600
 H -0.52823400 -1.13598900 1.19312300
 C 0.47263600 -1.54849600 -0.53773000
 C 1.77115000 -1.80755900 0.10800000
 C 1.99726800 -3.10911200 0.82075500
 H 1.06170400 -3.67823000 0.89731100
 H 2.73190100 -3.74272300 0.29098000
 H 2.39546900 -2.95566300 1.83744900
 C 2.82128200 -0.82717100 0.03061400
 C 4.12618400 -1.08602900 0.52778400
 C 2.59487900 0.44022400 -0.57139700
 C 5.13766400 -0.13814300 0.41696800
 H 4.34673100 -2.04692100 0.99526600
 C 3.61098600 1.38056800 -0.67414800
 H 1.59851900 0.67338500 -0.95510800
 C 4.89275100 1.10003900 -0.18553200
 H 6.13389900 -0.36764900 0.80021400
 H 3.40684700 2.34424900 -1.14577900
 H 5.69113300 1.83820900 -0.27629700
 H 0.40449000 -1.39774700 -1.62053300

(25) MECP-Z

C 2.65031200 -1.90561700 -0.19616700
 C 4.12415500 -1.57614500 0.06665700
 H 4.28057200 -1.25401200 1.10849900
 H 4.74221900 -2.46951500 -0.10876900
 H 4.49619100 -0.78365300 -0.59935100
 C 2.26060700 -3.13500500 0.62975400
 H 2.38092600 -2.94374500 1.70779200
 H 1.21519900 -3.42463300 0.44884500
 H 2.90179200 -3.98784500 0.35873800
 C 2.45365000 -2.22532700 -1.68152300
 H 1.41320200 -2.51112700 -1.90059300
 H 2.72799900 -1.38129800 -2.33208200
 H 3.09024700 -3.07800100 -1.96182100
 C 1.76503300 -0.70656800 0.25490900
 H 1.87501500 -0.63275800 1.34814500
 C 2.23065200 0.61426000 -0.37292400
 H 2.30689700 0.52175300 -1.46495600
 H 3.20216500 0.92481000 0.02733300

N 0.34711400 -0.87659500 -0.00743700
 H 0.33162100 1.30066700 -0.32826000
 N 1.25441600 1.71483800 -0.11254400
 C 1.43546300 2.87067700 -1.05019400
 H 1.37574800 2.44438200 -2.05963300
 H 0.56683500 3.52527200 -0.91185600
 C 1.21065700 2.09206100 1.33953900
 H 0.88030400 1.19113700 1.87265300
 H 2.24405500 2.30919900 1.64165500
 C 0.27778600 3.24822200 1.63382100
 H 0.66419800 4.20541400 1.25863100
 H -0.72232600 3.07570400 1.20867500
 H 0.17104400 3.33167900 2.72343800
 C 2.73391600 3.62052200 -0.84362700
 H 3.61132500 2.98511800 -1.02604400
 H 2.76487000 4.44985700 -1.56315100
 H 2.80687200 4.05060300 0.16495300
 H 0.11598600 -1.11856600 -0.97033300
 C -0.50502200 -1.41637900 0.95323400
 C -1.88526500 -1.74406200 0.55860300
 C -2.30076300 -3.18409800 0.47770600
 H -1.63080500 -3.81343000 1.07848000
 H -3.33231100 -3.33332400 0.83319700
 H -2.26317100 -3.56058100 -0.56202600
 C -2.78879400 -0.70039400 0.15113300
 C -4.01131100 -0.98527500 -0.51234500
 C -2.47846300 0.66603800 0.38478800
 C -4.85703000 0.03650400 -0.92748200
 H -4.28402800 -2.02157200 -0.71866600
 C -3.33541400 1.67988800 -0.02287100
 H -1.55895600 0.91135100 0.92123900
 C -4.52964300 1.37519600 -0.68751300
 H -5.78359500 -0.21078900 -1.44981300
 H -3.07594500 2.72088300 0.18334300
 H -5.19920400 2.17210900 -1.01545600
 H -0.22880400 -1.20976700 1.99406600

(26) S-2f

C 2.44047600 -1.03073600 1.27827900
 H 2.26432400 -0.25252700 2.03542200
 H 1.96307700 -1.95974200 1.61787400
 H 3.52441300 -1.20607000 1.21109300
 C 1.87114900 -0.60894800 -0.08415100
 H 2.08147700 -1.42279100 -0.80009700

C 2.66988400 0.57056200 -0.59980100
 H 3.77069600 0.38351800 -0.63304700
 O 2.21867200 1.62839400 -0.95101600
 C 0.38437500 -0.35287300 -0.05455500
 C -0.49661100 -1.15050300 -0.79115700
 C -0.14362300 0.68032600 0.73232500
 C -1.87500100 -0.93485500 -0.74906900
 H -0.10149800 -1.95769600 -1.41215200
 C -1.51543600 0.91334600 0.78578100
 H 0.52696000 1.31586000 1.31455600
 C -2.35857000 0.09617900 0.04216700
 H -2.57103400 -1.55241500 -1.31833800
 H -1.94044100 1.71326800 1.39374200
 F -3.68080000 0.31293900 0.09335100

(27) (S)-imine_2f

H -1.36578200 2.81981200 1.93980000
 H 0.23449100 3.21937000 1.28687500
 H -0.65183900 2.53537800 -1.72851200
 H -0.15027100 0.84611400 -1.52392900
 H -2.74031900 1.40346900 0.99971900
 H -2.00793100 -0.32474000 -1.42803400
 N -1.20985700 -0.88767400 0.44808500
 C -0.81387300 3.04349800 1.01829200
 C -0.09529400 1.84793700 -1.07848600
 N -0.84385600 1.77316000 0.21720100
 C -2.23424900 1.25196100 0.03782400
 C -2.23182900 -0.23313200 -0.34818700
 H 1.81348700 -4.16544400 0.66166600
 H 1.16832200 -3.75752400 -0.94879900
 H 0.06121700 -4.26986300 0.34774700
 C 0.97347200 -3.69411000 0.13230500
 C -0.33711300 -1.58492200 -0.14989100
 C 0.80822400 -2.23984000 0.57783000
 H -0.36124000 1.06681800 0.79750700
 H 0.57189500 -2.20021900 1.65048100
 H -2.72491000 1.86191200 -0.72951200
 C -3.62414900 -0.89134800 -0.13170400
 C -4.69021800 -0.06075400 -0.85308700
 H -5.65194800 -0.59514700 -0.83438000
 H -4.84591300 0.91684400 -0.37269700
 H -4.41849100 0.10929200 -1.90719500
 C -3.58707300 -2.29416300 -0.74498400
 H -3.34780400 -2.25214100 -1.81936200
 H -2.84014400 -2.93323900 -0.25008700
 H -4.56878300 -2.77880600 -0.63257200

C -3.97219500 -1.00728100 1.35505900
 H -4.03673900 -0.02468000 1.84631700
 H -4.95299500 -1.49444200 1.46581600
 H -3.22665100 -1.61141100 1.89082100
 H -0.36080500 -1.71688300 -1.25104600
 C 2.05912100 -1.40740800 0.34307500
 C 2.61333300 -1.28191500 -0.93950100
 C 2.66995000 -0.73246200 1.40654100
 C 3.75649300 -0.51541200 -1.15617800
 H 2.15151800 -1.79521000 -1.78620900
 C 3.81806600 0.03557800 1.20920500
 H 2.24762800 -0.81672400 2.41037900
 C 4.34185700 0.12754500 -0.07251800
 H 4.19956400 -0.41186300 -2.14782400
 H 4.30977800 0.55683600 2.03185000
 C -1.40777600 4.23051600 0.29169600
 H -2.45219700 4.05354200 -0.00010300
 H -1.39238000 5.09003600 0.97495100
 H -0.82713400 4.50341100 -0.60023600
 C 1.34745500 2.26526400 -0.89134300
 H 1.87030900 2.15019400 -1.85037700
 H 1.44234900 3.31399500 -0.57885400
 H 1.84881200 1.62221500 -0.15059700
 F 5.44618600 0.85815300 -0.27292300

(28) (R)-imine_2f

C 0.67863300 2.31873300 -0.49304400
 C 1.64914800 3.34158400 -1.09409000
 H 1.99795400 3.02232200 -2.08924100
 H 1.14377900 4.31236800 -1.20779700
 H 2.52856100 3.50063300 -0.45236000
 C -0.59427500 2.28506500 -1.34471400
 H -0.36930200 2.00257500 -2.38516400
 H -1.33616900 1.57628500 -0.94527500
 H -1.06094500 3.28160100 -1.35591700
 C 0.30683900 2.72871500 0.93523600
 H -0.43518500 2.04022000 1.36459200
 H 1.18000400 2.75493400 1.60494200
 H -0.13045500 3.73879100 0.92400600
 C 1.34003400 0.90833000 -0.53446800
 H 1.41179800 0.63021400 -1.60268900
 C 2.74665900 0.92147700 0.07607500
 H 2.75357000 1.48348800 1.01860100
 H 3.47864600 1.36039600 -0.61128300
 N 0.54925400 -0.06524600 0.19939600

N 3.20287100 -0.46323500 0.40726800
 H 2.39882900 -0.89959500 0.88812300
 C -0.22698600 -0.82225900 -0.45686400
 C -1.14699400 -1.81591100 0.20647100
 C -1.09327600 -3.16176700 -0.51112900
 H -0.09212900 -3.60556900 -0.41047200
 H -1.82555900 -3.86232900 -0.08504300
 H -1.30372900 -3.05419000 -1.58544100
 C 4.33136100 -0.47823400 1.39758000
 H 3.99246100 0.13315300 2.24305000
 H 4.42388100 -1.51301400 1.74801600
 C 5.63709000 0.03471500 0.83073900
 H 5.54715900 1.06242700 0.45228000
 H 6.38072200 0.03974100 1.63889100
 H 6.01999100 -0.61154100 0.02896500
 H -0.80072400 -1.92803800 1.24420600
 C -2.52858700 -1.17637200 0.24815800
 C -2.81529900 -0.25833800 1.26880500
 C -3.49991600 -1.41626900 -0.72952500
 C -4.03875100 0.40336100 1.32410000
 H -2.06376800 -0.06215000 2.03774900
 C -4.73183900 -0.76037600 -0.69182800
 H -3.30863700 -2.12647600 -1.53551400
 C -4.97831600 0.13908000 0.33492900
 H -4.27382900 1.11268100 2.11872900
 H -5.49929200 -0.93876500 -1.44624700
 C 3.46078600 -1.27285500 -0.82679300
 H 4.23256200 -0.74129900 -1.39881600
 H 2.53156300 -1.25053900 -1.40991800
 C 3.85462200 -2.70201100 -0.52068500
 H 3.86804700 -3.26726000 -1.46176300
 H 4.85367000 -2.77515300 -0.07037800
 H 3.12309300 -3.17715800 0.15009000
 H -0.29853300 -0.75878400 -1.56166000
 F -6.15983400 0.76882100 0.37693100

(29) E-enamine_2f

C 1.99013000 2.44290800 -0.59013600
 C 3.06218300 2.71345400 -1.65137700
 H 2.84519600 2.16642900 -2.58281800
 H 3.08897600 3.78765100 -1.88817000
 H 4.06676800 2.42604900 -1.30727700
 C 0.65744900 3.03020300 -1.06477400
 H 0.32640500 2.55861300 -2.00361900
 H -0.13465700 2.89406700 -0.31282100

H 0.76592600 4.11034400 -1.24541900
 C 2.38712200 3.12013900 0.72591400
 H 1.61892500 2.98352900 1.50332500
 H 3.34873900 2.75347600 1.11555400
 H 2.49141200 4.20343000 0.56225200
 C 1.80565500 0.90814500 -0.42346000
 H 1.43224700 0.53909200 -1.39090200
 C 3.12588500 0.19095900 -0.10769300
 H 3.61401700 0.64430000 0.76544200
 H 3.81521600 0.22010100 -0.95941800
 N 0.81737500 0.54049500 0.57617900
 H 2.05332300 -1.22282400 0.85388200
 N 2.88344000 -1.24175200 0.23701900
 C 4.00210700 -1.83852700 1.04006200
 H 4.14772900 -1.16278700 1.89187100
 H 3.63297400 -2.79475200 1.42902100
 C 2.49518400 -2.04737500 -0.96542000
 H 1.60722100 -1.55915100 -1.38470600
 H 3.31194400 -1.94985000 -1.69224000
 C 2.19182100 -3.49213500 -0.63208900
 H 3.09044100 -4.05216400 -0.34075000
 H 1.44653200 -3.56349900 0.17384600
 H 1.77134300 -3.97210600 -1.52559700
 C 5.28031000 -2.01573800 0.24958300
 H 5.64932400 -1.06329000 -0.15577200
 H 6.04846100 -2.41061400 0.92794300
 H 5.16107000 -2.73468100 -0.57277700
 H 0.95006700 0.97556500 1.48563600
 C -0.48389300 0.24053600 0.22375600
 C -1.56598400 0.26770100 1.03583900
 H -0.59070700 -0.05810100 -0.82383000
 C -2.89316200 -0.13169900 0.51277000
 C -4.06724300 0.38528100 1.09092700
 C -3.04106000 -1.03537700 -0.55752000
 C -5.33120800 0.04239000 0.61283100
 H -3.99852700 1.08389600 1.92629600
 C -4.29532900 -1.38342300 -1.05012500
 H -2.15958000 -1.49796300 -1.00480700
 C -5.42555000 -0.83578500 -0.45624100
 H -6.23993800 0.45047200 1.05794800
 H -4.40822500 -2.08963500 -1.87407400
 C -1.48137500 0.74915200 2.46273100
 H -0.46318300 0.66970400 2.86882900
 H -1.79540400 1.80179400 2.56509800
 H -2.13481700 0.15307100 3.11717500
 F -6.63761200 -1.17639100 -0.92078900

(30) Z-enamine_2f

C -1.49815100 2.42147200 -0.76429500
 C -2.89266200 2.96526300 -1.09296300
 H -3.52046900 3.02208200 -0.18907600
 H -2.80781400 3.98012600 -1.50971900
 H -3.41320800 2.34529700 -1.83803900
 C -0.76531200 3.43595800 0.11881300
 H -1.30777800 3.60685500 1.06193900
 H 0.25312600 3.09924400 0.36364100
 H -0.68231900 4.39956200 -0.40649600
 C -0.70299200 2.22667600 -2.05924500
 H 0.33057700 1.90416800 -1.85658500
 H -1.17108200 1.49221600 -2.73213400
 H -0.64421900 3.18162400 -2.60315600
 C -1.63501000 1.09123100 0.03070000
 H -2.07492200 1.35587000 1.00480200
 C -2.57156000 0.09456400 -0.66832300
 H -2.27433200 -0.04823400 -1.71639100
 H -3.61310400 0.43286100 -0.63587500
 N -0.36876200 0.42945800 0.30404600
 H -1.49494900 -1.40055800 0.15146900
 N -2.50400400 -1.24884600 -0.01964800
 C -2.96085200 -2.35143500 -0.92799500
 H -2.36910000 -2.24395200 -1.84586300
 H -2.66902200 -3.29320700 -0.44829400
 C -3.15812500 -1.25096800 1.32945600
 H -2.65278100 -0.47071800 1.91126500
 H -4.20121000 -0.94245900 1.17979900
 C -3.04815900 -2.58630500 2.03403500
 H -3.65565800 -3.36467700 1.55306400
 H -2.00200300 -2.92404200 2.07786200
 H -3.40915400 -2.46586500 3.06389800
 C -4.44562700 -2.31449700 -1.21950500
 H -4.75036700 -1.36834800 -1.68788200
 H -4.67559200 -3.12551200 -1.92328900
 H -5.04765200 -2.47758000 -0.31482000
 H 0.20991100 0.28766300 -0.52258400
 C 0.32170800 0.69129100 1.47737100
 C 1.63575200 0.50100100 1.73716200
 C 2.18775800 0.90330000 3.08264700
 H 1.37688200 1.19206600 3.76572600
 H 2.75411600 0.08095800 3.54893100
 H 2.87532800 1.76137300 3.00796800

C 2.58677300 -0.05557700 0.74308700
 C 3.90981200 0.41940400 0.67567100
 C 2.22503800 -1.09904600 -0.12939000
 C 4.82321100 -0.09436900 -0.24166000
 H 4.23536800 1.21511600 1.34754300
 C 3.12736100 -1.62696200 -1.05137500
 H 1.22581400 -1.53500100 -0.07032700
 C 4.41354000 -1.10875100 -1.09666900
 H 5.84610500 0.28041800 -0.30144200
 H 2.84873900 -2.44143300 -1.72148700
 H -0.31362700 1.09701400 2.27195600
 F 5.28763900 -1.60785800 -1.98248100

(31) TS1_2f

H 0.29307800 1.64865700 -1.54364800
 H -3.51046500 1.92857900 -0.64136400
 H -3.69086500 0.62193400 0.53632600
 H -1.93177900 2.24307300 2.71720000
 H -0.45600300 1.43080400 2.16224700
 H -1.74984200 3.19962100 -0.78169600
 H 0.63119600 2.89100300 1.13957000
 N 0.63223900 1.75839300 -0.58539400
 C -3.39321500 1.67132700 0.41926300
 C -1.55063700 1.41560700 2.10375200
 N -1.91480400 1.72116900 0.68427800
 C -1.31711000 3.00201900 0.20841500
 C 0.21025100 2.96232400 0.12676400
 H 1.60394400 -1.53487400 -2.56430700
 H 2.11951100 0.15133700 -2.81097100
 H 0.40474200 -0.23771800 -2.45703700
 C 1.44822900 -0.50086300 -2.22859800
 C 1.41110700 0.82935600 -0.09153700
 C 1.72608600 -0.39366700 -0.73343800
 H -1.54396600 0.94098900 0.08233600
 C -3.43847100 -4.69039000 0.10574500
 C -2.36002500 -3.80727600 0.09323500
 C -2.50786200 -2.52936800 -0.45673900
 C -3.73881400 -2.14274100 -0.99702100
 C -4.81618400 -3.02697100 -0.98584100
 C -4.66662700 -4.30076400 -0.43291600
 H -3.32220300 -5.68648300 0.53682900
 H -1.39407600 -4.09634100 0.50968200
 H -3.83470900 -1.14399700 -1.42594400
 H -5.77572900 -2.72341400 -1.40835500
 H -5.51069600 -4.99302900 -0.42306600
 C -1.35458900 -1.55721100 -0.45978100

O -0.26026900 -1.97054700 0.02805000
 H 0.74415400 -1.07170100 -0.23533900
 O -1.53833600 -0.41041000 -0.91569800
 H -1.63304700 3.79433500 0.89665400
 C 0.82411900 4.23678800 -0.51942500
 C 0.26216600 5.47540500 0.18505600
 H 0.82551400 6.36468100 -0.13373000
 H -0.79574200 5.64716600 -0.06266800
 H 0.35518600 5.38935200 1.27938300
 C 2.34009200 4.18521800 -0.30753300
 H 2.58929900 4.17119700 0.76493500
 H 2.78588400 3.29644200 -0.77981800
 H 2.81076200 5.07263800 -0.75594500
 C 0.52870500 4.31564800 -2.02074800
 H -0.55035900 4.29697800 -2.23553900
 H 0.92854300 5.25991500 -2.41937900
 H 1.01237100 3.49661000 -2.57518600
 H 1.75755400 1.00335100 0.93513000
 C 2.95234200 -1.10720600 -0.23550700
 C 4.06705400 -0.42554700 0.27089600
 C 2.99828400 -2.50916000 -0.29633400
 C 5.19212700 -1.11671700 0.72220400
 H 4.06935700 0.66620400 0.30647200
 C 4.11613000 -3.21431800 0.13967000
 H 2.13395400 -3.05581600 -0.68061000
 C 5.19601000 -2.50145200 0.64655200
 H 6.06458500 -0.59559100 1.11885200
 H 4.15952200 -4.30361200 0.10048600
 C -4.20968200 2.58529800 1.30758200
 H -3.87952100 3.63149400 1.23965600
 H -5.25506900 2.54270700 0.97376100
 H -4.18216900 2.26905900 2.35947000
 C -2.06141300 0.07078200 2.57943700
 H -1.71419000 -0.07540100 3.61109600
 H -3.15772900 0.00826500 2.58518700
 H -1.64942100 -0.75225100 1.97735300
 F 6.27408500 -3.17357400 1.07245000

(32) TS2_2f

C 4.23200000 -0.31435500 -0.51495200
 C 5.03912200 -1.40154300 -1.23451800
 H 4.61673700 -1.61642800 -2.22896200
 H 6.07412000 -1.05650300 -1.37361600
 H 5.07902700 -2.33917600 -0.66135400
 C 4.40975300 1.00909100 -1.26625800

H 4.05594400 0.92433500 -2.30582200
 H 3.86059900 1.82836100 -0.77835200
 H 5.47441000 1.28469000 -1.28723600
 C 4.73873100 -0.15712600 0.92045700
 H 4.23426600 0.66902300 1.44537400
 H 4.60806000 -1.07903400 1.50730800
 H 5.81388900 0.07651300 0.90343100
 C 2.72639400 -0.69331600 -0.56338600
 H 2.46450600 -0.76587900 -1.62962200
 C 2.38871900 -2.02497600 0.09975500
 H 2.50653700 -1.97970000 1.18927900
 H 3.05328200 -2.81202700 -0.27267000
 N 1.85901700 0.37211900 -0.04135700
 H 0.40282400 -1.56926800 -0.38671500
 N 0.97910300 -2.43182700 -0.20021600
 C 0.29580800 -3.04764800 0.98385400
 H 0.37824700 -2.30110700 1.78608000
 H -0.76753600 -3.13673600 0.72477700
 C 0.91126000 -3.26665400 -1.44392000
 H 1.38707600 -2.67075600 -2.23384900
 H 1.53466800 -4.15323800 -1.26900100
 C -0.50703300 -3.63720600 -1.82346200
 H -0.93714800 -4.37720100 -1.13484500
 H -1.15356100 -2.74779800 -1.84378300
 H -0.49517300 -4.08010400 -2.82807400
 C 0.87866800 -4.38340400 1.39122800
 H 1.95499000 -4.31366200 1.60447300
 H 0.37438000 -4.71585200 2.30831000
 H 0.71732200 -5.15191100 0.62248400
 H 1.43175400 0.97970800 -0.74124700
 C 1.52815000 0.57377200 1.21041100
 C 0.52101100 1.45814400 1.66709800
 C 0.54778300 1.81818700 3.14866800
 H 0.85079000 0.95315700 3.75713800
 H 1.24449900 2.64702300 3.34905800
 H -0.45248300 2.13287400 3.47832900
 C 0.06108400 2.55687300 0.74480700
 C -1.30645200 2.81311200 0.56731000
 C 0.98695000 3.38606900 0.09462000
 C -1.74289200 3.85548800 -0.24723400
 H -2.04150800 2.18576400 1.07553200
 C 0.56798700 4.42929600 -0.73011900
 H 2.05800700 3.21752800 0.23534200
 C -0.79446700 4.64286100 -0.88689900
 H -2.80369800 4.06261800 -0.39492400
 H 1.27979100 5.07840200 -1.24196400

H 1.98911900 -0.08828800 1.95217100
 C -5.50693600 -1.29057900 0.76077700
 C -4.18751700 -0.96174500 1.06793800
 C -3.23767100 -0.85108300 0.04652800
 C -3.61870400 -1.06024600 -1.28328400
 C -4.93965200 -1.38153900 -1.59019300
 C -5.88346400 -1.49984100 -0.56757800
 H -6.24625800 -1.38332000 1.55842700
 H -3.87777300 -0.79044700 2.09971900
 H -2.86802100 -0.95845200 -2.06854200
 H -5.23563200 -1.53966900 -2.62879800
 H -6.91794100 -1.75392800 -0.80714900
 C -1.80390600 -0.50928500 0.36666700
 O -1.54951100 -0.19009000 1.57022900
 H -0.40821800 0.54299100 1.61213600
 O -0.95838500 -0.55147800 -0.54691700
 F -1.20799200 5.64154600 -1.67758100

(33) TS3_2f

H -1.43698400 0.64024200 -0.43786800
 H -0.28423300 -2.68098100 -2.17248700
 H 0.74529700 -3.37613000 -0.91229600
 H -1.82854000 -3.84881500 1.04688000
 H -1.47842500 -2.28226400 1.80441800
 H -2.12527500 -1.55462700 -1.74933600
 H -3.16505400 -1.21573600 1.12456400
 N -1.87552100 0.21954600 0.38588000
 C -0.29413900 -3.27183300 -1.24783300
 C -1.08216000 -3.04620600 1.12467500
 N -0.97980800 -2.41030700 -0.22682300
 C -2.29423600 -1.91469100 -0.72505000
 C -2.88872800 -0.80376100 0.14307700
 C -1.46333200 0.61002000 1.56829400
 C -0.39623400 1.50342600 1.82458100
 H -0.33944600 -1.57657100 -0.14735700
 C 5.57323100 -1.08218500 0.53095300
 C 4.27783100 -0.76154900 0.93373100
 C 3.22771800 -0.80393100 0.01047900
 C 3.48069400 -1.16577200 -1.31708800
 C 4.77621700 -1.48566800 -1.71882000
 C 5.82243200 -1.44455700 -0.79449200
 H 6.39221700 -1.05007800 1.25174400
 H 4.06446500 -0.47841100 1.96536900
 H 2.64929800 -1.18796600 -2.02338900
 H 4.97315700 -1.76615100 -2.75514900

H 6.83732300 -1.69612500 -1.10849000
 C 1.82240500 -0.46385100 0.43273900
 O 1.64879000 -0.16220100 1.65549300
 H 0.52249100 0.56940600 1.77328900
 O 0.91208300 -0.49764500 -0.41738200
 H -2.98275000 -2.76679600 -0.75847700
 C -4.17916900 -0.18356500 -0.46262200
 C -5.16431400 -1.30381500 -0.80931200
 H -6.14231300 -0.86659400 -1.05888200
 H -4.83391500 -1.89206800 -1.67799600
 H -5.30615400 -1.98846300 0.04183100
 C -4.80801000 0.72151500 0.60074000
 H -5.07022100 0.14746300 1.50324300
 H -4.12890300 1.53711800 0.89350400
 H -5.72811300 1.17793200 0.20684200
 C -3.87203300 0.64527000 -1.71409000
 H -3.38711900 0.04829600 -2.50108000
 H -4.81133400 1.03961500 -2.12951800
 H -3.22751600 1.50829000 -1.48333400
 H -1.93733100 0.10446700 2.41936900
 C -0.94915700 -4.62000900 -1.46015800
 H -1.99353000 -4.52592100 -1.78868900
 H -0.39887600 -5.14599900 -2.25192000
 H -0.91466500 -5.24634000 -0.55791800
 C 0.24723000 -3.55140000 1.64830400
 H 0.09629800 -3.90617600 2.67662800
 H 0.64159300 -4.38977100 1.05915200
 H 0.99597600 -2.74587800 1.68182800
 C -0.28454100 2.03387700 3.25060700
 H 0.75148200 2.33427300 3.46246400
 H -0.92820700 2.91373000 3.40532600
 H -0.56928800 1.26155700 3.97994000
 C -0.00425200 2.48617800 0.75102500
 C 1.34741900 2.77214500 0.50838300
 C -0.97550500 3.19545000 0.02901600
 C 1.72437300 3.72188300 -0.43791700
 H 2.12005300 2.24348700 1.07035600
 C -0.61644900 4.14475700 -0.92742100
 H -2.03663300 3.01236500 0.21807500
 C 0.73227200 4.38882700 -1.14511800
 H 2.77283200 3.94921800 -0.63584700
 H -1.36592000 4.69978000 -1.49345700
 F 1.08902100 5.29904500 -2.05996900
 C -1.74675900 3.83110300 -0.53243200
 C -1.27713200 5.22914900 -0.11326500
 H -0.37817200 5.53040200 -0.67382900
 H -2.07065900 5.96002100 -0.32656000
 H -1.05551400 5.29027500 0.96185100
 C -2.24223400 3.89163300 -1.98130200
 H -1.43923500 4.21800900 -2.66080500
 H -2.61274800 2.91454000 -2.32562500
 H -3.07074600 4.61067200 -2.06028200
 C -2.88905100 3.37278200 0.37683400
 H -3.30864200 2.40820300 0.05216100
 H -2.57102300 3.28590100 1.42698600
 H -3.70382900 4.11105500 0.33520600
 C -0.53297000 2.86307500 -0.47931000
 H 0.22328800 3.28232600 -1.15915100
 C 0.09330000 2.70609700 0.90256300
 H -0.57092000 2.16213600 1.58508100
 H 0.29675200 3.68778300 1.34438600
 N -0.84331600 1.53967200 -1.04259900
 H 1.36127300 1.29481700 0.00987700
 N 1.38824100 1.95918200 0.82809100
 C 1.58991700 1.04580100 2.00069100
 H 0.70471600 0.39553600 2.02007500
 H 2.45763100 0.41692300 1.76218200
 C 2.53655100 2.89214300 0.58594500
 H 2.28532100 3.45294100 -0.32370200
 H 2.55788900 3.60023800 1.42460900
 C 3.85283000 2.16238200 0.42327800
 H 4.21489500 1.74587900 1.37313900
 H 3.75727100 1.35004100 -0.31078500
 H 4.60516800 2.87393100 0.05823100
 C 1.77917600 1.77730100 3.31166500
 H 0.93630300 2.44792000 3.53177700
 H 1.83704600 1.03399000 4.11773600
 H 2.71069200 2.35980900 3.32507800
 H -0.53178700 1.38367600 -2.00120100
 C -1.43342600 0.54822900 -0.43311900
 C -1.54170100 -0.76941600 -0.96331600
 H -1.77848400 0.73213900 0.59080000
 C 4.40732400 -3.77204900 0.31489400
 C 3.17760700 -3.11881100 0.25049000
 C 3.05443300 -1.92369600 -0.46614000
 C 4.16626200 -1.39656500 -1.13140700
 C 5.39432100 -2.05409900 -1.07343300
 C 5.51649400 -3.23955000 -0.34583000
 H 4.50208500 -4.70105900 0.88012300

H 2.29948600 -3.52365800 0.75526900
 H 4.05218200 -0.47257100 -1.70051300
 H 6.25903600 -1.64178300 -1.59656200
 H 6.47871800 -3.75290800 -0.29586100
 C 1.72838600 -1.20070000 -0.51946300
 O 0.72857000 -1.82631900 -0.06439500
 H -0.46662000 -1.19294300 -0.43102900
 O 1.69563300 -0.04509500 -0.99595000
 C -1.26642900 -0.94113700 -2.44701400
 H -1.24405400 -2.00899300 -2.70242300
 H -2.02554300 -0.45085400 -3.07769300
 H -0.27825200 -0.52768200 -2.70167900
 C -2.61329400 -1.62486300 -0.33933300
 C -2.64627900 -1.82232400 1.04962800
 C -3.58419300 -2.25801600 -1.12524200
 C -3.62753400 -2.61088000 1.64455700
 H -1.88417500 -1.35958100 1.68185500
 C -4.57044500 -3.05723400 -0.54606000
 H -3.58269300 -2.12668500 -2.20830700
 C -4.57651500 -3.21729500 0.83152400
 H -3.65773500 -2.77191100 2.72300300
 H -5.33191300 -3.55326900 -1.14953300
 F -5.51966000 -3.98492200 1.39533500

(35) T1_2f

C 3.27584300 -1.48249800 -0.06535300
 C 4.64245600 -0.84128600 0.20313600
 H 4.68818400 -0.41094000 1.21655500
 H 5.43238200 -1.60325700 0.12465800
 H 4.87667900 -0.04770800 -0.52199000
 C 3.12622500 -2.71242200 0.83495600
 H 3.18846800 -2.43471800 1.89912000
 H 2.16366500 -3.21863000 0.67111500
 H 3.93091500 -3.43304000 0.62252100
 C 3.19474900 -1.92783900 -1.52913900
 H 2.26514500 -2.48195700 -1.73144200
 H 3.25269200 -1.08049300 -2.22962700
 H 4.03375000 -2.60277800 -1.75649300
 C 2.14696900 -0.46607400 0.28517200
 H 2.15289900 -0.35938000 1.38146400
 C 2.40895100 0.91122700 -0.33874400
 H 2.58555400 0.82021900 -1.41926500
 H 3.27254900 1.40096900 0.12357200
 N 0.80894300 -0.89358000 -0.08375400
 H 0.41199000 1.23967600 -0.41461700

N 1.23437400 1.82053900 -0.17555100
 C 1.26145200 2.95855700 -1.15203900
 H 1.34151100 2.49727500 -2.14441000
 H 0.28365400 3.44964700 -1.08772100
 C 1.04748000 2.23491400 1.25425000
 H 0.86645000 1.30744000 1.81279700
 H 2.00287300 2.65657200 1.59355600
 C -0.10352400 3.19949100 1.44918400
 H 0.11073900 4.19505900 1.03866300
 H -1.02735300 2.81651300 0.99122000
 H -0.28145700 3.31050900 2.52702400
 C 2.39087300 3.93632400 -0.90548100
 H 3.37705200 3.46019300 -0.99415100
 H 2.33104300 4.72460800 -1.66792300
 H 2.31158500 4.41723900 0.07949900
 H 0.70142800 -1.14421400 -1.06611900
 C 0.02691000 -1.64495600 0.79447400
 C -1.27325000 -2.14530800 0.31319200
 C -1.42848600 -3.59842600 -0.02984100
 H -0.52016200 -4.15793300 0.22758600
 H -2.27848700 -4.05807300 0.50309700
 H -1.62426800 -3.74518200 -1.10726200
 C -2.37774800 -1.24050600 0.12753900
 C -3.61490800 -1.67475200 -0.41770700
 C -2.27262300 0.12834700 0.49233800
 C -4.67808200 -0.79799000 -0.59213000
 H -3.74312600 -2.71681100 -0.71218600
 C -3.33127400 1.00891800 0.32248300
 H -1.33981600 0.49194600 0.92805000
 C -4.52173100 0.53305200 -0.22039100
 H -5.62918800 -1.13075000 -1.01090900
 H -3.25453400 2.06016400 0.60568200
 H 0.19224500 -1.42714700 1.85678700
 F -5.54444100 1.38262500 -0.38656900

(36) S-2y

C -2.07982700 0.88064300 0.52072700
 H -1.91505900 0.52084100 1.54970200
 H -3.15751700 0.77197900 0.31826900
 C -1.30911400 -0.02942400 -0.45724500
 H -1.52102500 0.34081800 -1.47710100
 C -1.92024800 -1.41405100 -0.41633800
 H -3.01952500 -1.42064300 -0.61490700
 O -1.33337900 -2.44026900 -0.19576000
 C 0.18198500 -0.02410700 -0.23041500

C 1.04954000 0.51572600 -1.18556300
 C 0.72291300 -0.52967200 0.96010600
 C 2.42773700 0.55039600 -0.96175400
 H 0.63927400 0.91554600 -2.11641400
 C 2.09785600 -0.49810900 1.18583400
 H 0.05895800 -0.95618400 1.71536000
 C 2.95555200 0.04265900 0.22452600
 H 3.09038300 0.97587500 -1.71792600
 H 2.50408800 -0.89863400 2.11682000
 H 4.03231300 0.06746600 0.40202700
 C -1.67893700 2.34421700 0.40494000
 H -2.28248700 2.97013600 1.07773000
 H -0.62055300 2.49345700 0.66595900
 H -1.82656500 2.71182800 -0.62234400

(37) (S)-imine_2y

H -1.79748500 2.60758300 2.04294800
 H -0.39782200 3.40308000 1.30095800
 H -1.33085700 2.56223000 -1.67724700
 H -0.36750700 1.07614200 -1.56435800
 H -2.81704600 0.86447300 1.15158900
 H -1.83567000 -0.48903000 -1.42436800
 N -0.84360800 -0.93316600 0.39263000
 C -1.38679000 2.97680800 1.09494900
 C -0.55809700 2.04778800 -1.09140400
 N -1.15687500 1.75489700 0.25092500
 C -2.37887200 0.89701700 0.14589600
 C -2.02866700 -0.51628700 -0.33494500
 H 2.15150200 -2.95722100 -1.21846800
 H 1.21094300 -3.79198200 0.01868400
 C 1.99462400 -3.03152600 -0.12981500
 C 0.16628100 -1.32301600 -0.26650000
 C 1.46585300 -1.69062300 0.39910600
 H -0.46479600 1.18713000 0.76706900
 H 1.26449500 -1.77853600 1.47708800
 H -3.07653000 1.39123700 -0.53990600
 C -3.20151400 -1.51579700 -0.12399400
 C -4.46231600 -0.96000600 -0.79300500
 H -5.25872200 -1.71897500 -0.77304300
 H -4.84309300 -0.06739400 -0.27459400
 H -4.27140600 -0.69671300 -1.84561000
 C -2.82047000 -2.83645900 -0.79950000
 H -2.61777000 -2.68830400 -1.87204500
 H -1.92667700 -3.28370500 -0.33914400
 H -3.64412200 -3.56013700 -0.70547800

C -3.47094700 -1.77159100 1.36164500
 H -3.79370600 -0.86055300 1.88789300
 H -4.27731500 -2.51318500 1.46762700
 H -2.57628600 -2.16316900 1.86590300
 H 0.14888100 -1.37298000 -1.37467500
 C 2.43719100 -0.53815900 0.19451700
 C 2.94423200 -0.23894600 -1.07824400
 C 2.82391100 0.26109900 1.27698500
 C 3.82864400 0.82438700 -1.25848800
 H 2.65365900 -0.84923000 -1.93720000
 C 3.71101800 1.32483000 1.09815400
 H 2.43281000 0.03824000 2.27293300
 C 4.21796300 1.60800300 -0.17000200
 H 4.21851200 1.04066400 -2.25513900
 H 4.00861000 1.93149600 1.95578400
 C -2.30444600 3.99263400 0.45058100
 H -3.28813900 3.56659200 0.21032500
 H -2.46103600 4.81021500 1.16683900
 H -1.86850100 4.42622700 -0.46004700
 C 0.72458000 2.84543700 -0.99577500
 H 1.19142000 2.87415600 -1.98940500
 H 0.54903800 3.88175800 -0.67659300
 H 1.43432800 2.36965900 -0.30058700
 H 4.91558500 2.43547500 -0.31088700
 C 3.28027500 -3.46886400 0.55844800
 H 3.60644300 -4.45487600 0.19797100
 H 4.09760900 -2.75616100 0.37045200
 H 3.13930100 -3.53669600 1.64819900

(38) (R)-imine_2y

C -0.77880800 -2.49530400 -0.33195400
 C -1.83427800 -3.40987000 -0.96249800
 H -2.09013400 -3.08093600 -1.98244800
 H -1.44567200 -4.43734600 -1.02633600
 H -2.75860500 -3.44326200 -0.36644200
 C 0.53081500 -2.63654200 -1.11478900
 H 0.40223200 -2.33297700 -2.16593500
 H 1.33818900 -2.02964100 -0.67638400
 H 0.86067700 -3.68642000 -1.10094500
 C -0.53430200 -2.91075900 1.12152700
 H 0.23163500 -2.27788700 1.59223900
 H -1.44938200 -2.85818700 1.73000200
 H -0.18102900 -3.95281700 1.14917600
 C -1.26012200 -1.01642400 -0.43960500
 H -1.26823000 -0.77619300 -1.51935900

C -2.66948000 -0.83292200 0.12890600
 H -2.75489100 -1.31035200 1.11361900
 H -3.42942200 -1.24672000 -0.54336800
 N -0.36984100 -0.12629900 0.28426900
 N -2.98978900 0.61238600 0.34254800
 H -2.17259600 1.00002700 0.84192400
 C 0.49822300 0.51776000 -0.37774300
 C 1.53486800 1.39157300 0.27788400
 C 1.60300500 2.76483200 -0.40043400
 H 0.60100200 3.21970800 -0.33886100
 H 1.81405900 2.63713000 -1.47443100
 C -4.16419000 0.80287400 1.26006800
 H -3.93116100 0.22276200 2.16144900
 H -4.17617200 1.86354800 1.53734100
 C -5.48186300 0.37417100 0.65175700
 H -5.47916500 -0.68643400 0.36495200
 H -6.26585200 0.51257900 1.40837900
 H -5.75179600 0.98096100 -0.22357800
 H 1.23460200 1.51672400 1.32921200
 C 2.83658000 0.60201100 0.25314700
 C 3.18672900 -0.18361500 1.35865800
 C 3.65625200 0.56787800 -0.88241200
 C 4.33073400 -0.98154100 1.33497400
 H 2.55057600 -0.16919400 2.24754500
 C 4.80085400 -0.23059000 -0.90824500
 H 3.40354800 1.17003000 -1.75820200
 C 5.14187600 -1.00775700 0.19952900
 H 4.59019500 -1.58416700 2.20762700
 H 5.42999800 -0.24386300 -1.80036900
 C -3.09965900 1.36181300 -0.95152400
 H -3.88078300 0.86370900 -1.54026500
 H -2.14249100 1.22105000 -1.46841200
 C -3.38004600 2.83615400 -0.75328200
 H -3.29102800 3.33969800 -1.72499000
 H -4.39169300 3.02063500 -0.36769100
 H -2.64753200 3.28816900 -0.06788800
 H 0.56565300 0.42861300 -1.48125000
 H 6.03771400 -1.63102300 0.17896800
 C 2.62945200 3.69434700 0.23291700
 H 3.65058500 3.29936800 0.12460100
 H 2.60271000 4.68777400 -0.23694300
 H 2.43182300 3.82380000 1.30804500

(39) E-enamine_2y

C 1.59477400 2.40941000 -0.48619200

C 2.73489100 2.84717300 -1.41274900
 H 2.67244400 2.33652600 -2.38717700
 H 2.67322500 3.93068700 -1.59442200
 H 3.72389000 2.64259600 -0.97634200
 C 0.26607600 2.89997300 -1.07154300
 H 0.08531000 2.46237400 -2.06638100
 H -0.58452700 2.64403200 -0.42189900
 H 0.28570700 3.99487900 -1.18043300
 C 1.78766200 3.03199100 0.89967700
 H 0.96210400 2.77019700 1.57975000
 H 2.73531300 2.72614200 1.36731400
 H 1.80208400 4.12885800 0.81187400
 C 1.55334300 0.85452000 -0.42116600
 H 1.30896700 0.51549800 -1.43986200
 C 2.90532400 0.25492400 -0.01977600
 H 3.25343800 0.68385800 0.93006000
 H 3.66530200 0.42722400 -0.78943000
 N 0.52575200 0.31991800 0.45662100
 H 1.94110900 -1.34949800 0.75091700
 N 2.80358800 -1.22032600 0.19600200
 C 3.93301600 -1.75215500 1.02917500
 H 3.93296300 -1.15060700 1.94652600
 H 3.66519100 -2.77945500 1.30213500
 C 2.58505900 -1.96240600 -1.08987900
 H 1.65564100 -1.56197900 -1.51249900
 H 3.41121800 -1.69080400 -1.76007300
 C 2.47051200 -3.45916600 -0.89447000
 H 3.42626100 -3.91888100 -0.60955400
 H 1.71398400 -3.70043500 -0.13303700
 H 2.14945000 -3.90767900 -1.84391400
 C 5.27450200 -1.69486100 0.33131700
 H 5.55495300 -0.66767400 0.06040700
 H 6.03513700 -2.07818700 1.02454300
 H 5.29774000 -2.32295600 -0.57012800
 H 0.58122100 0.64133700 1.42057200
 C -0.73827700 0.03853900 -0.02369300
 C -1.85432800 -0.18793000 0.70980100
 H -0.77513700 -0.03564000 -1.11469500
 C -3.15009900 -0.42051000 0.02480200
 C -4.20275600 -1.10079500 0.66632600
 C -3.39326400 0.05063600 -1.28159700
 C -5.42053800 -1.32723600 0.02381100
 H -4.07285000 -1.47223300 1.68387600
 C -4.60470900 -0.18430300 -1.92636600
 H -2.62944100 0.63516200 -1.79789600
 C -5.62977000 -0.87783400 -1.27908800

H -6.21284000 -1.86258400 0.55135100
 H -4.75524200 0.19643900 -2.93875100
 H -6.58335600 -1.05257700 -1.78027500
 C -1.82343700 -0.15598700 2.22107900
 H -2.31962500 -1.05236400 2.62503100
 H -0.78447600 -0.22513300 2.57613400
 C -2.48184600 1.09345800 2.80837800
 H -3.53582000 1.16604900 2.49966600
 H -2.45329500 1.08101900 3.90791100
 H -1.96823700 2.00400800 2.46325500

(40) Z-enamine_2y

C -1.24307300 2.51343900 0.12280300
 C -2.55901200 3.23440200 0.43525600
 H -2.92380800 2.97335400 1.44160900
 H -2.40576200 4.32348800 0.40285600
 H -3.34730000 2.99066200 -0.29227200
 C -0.15632200 3.03213200 1.07008000
 H -0.40684700 2.81303100 2.12025600
 H 0.82241700 2.57846300 0.85303100
 H -0.05354200 4.12270800 0.96461400
 C -0.82801100 2.80425200 -1.32271700
 H 0.10218200 2.28002400 -1.59384000
 H -1.60798300 2.52182700 -2.04525200
 H -0.64234500 3.88228700 -1.44439500
 C -1.41603900 0.98958000 0.37993700
 H -1.66569900 0.89153700 1.44804200
 C -2.56126100 0.38719400 -0.44379200
 H -2.41433900 0.58722300 -1.51390500
 H -3.53378900 0.78571500 -0.13345000
 N -0.21463300 0.20368300 0.16076200
 H -1.61323600 -1.39080200 -0.35882600
 N -2.60340900 -1.09843200 -0.29471000
 C -3.32644700 -1.76898200 -1.42545500
 H -2.85685900 -1.39022000 -2.34170500
 H -3.10197000 -2.83944100 -1.35061000
 C -3.07532500 -1.51364400 1.06605700
 H -2.38990700 -1.04363900 1.78131200
 H -4.07058600 -1.07184700 1.20562300
 C -3.07966600 -3.01560400 1.25356800
 H -3.85103500 -3.51040500 0.64893800
 H -2.09808700 -3.44659800 1.00663600
 H -3.28880600 -3.23167000 2.30959200
 C -4.81851700 -1.51316700 -1.42393700
 H -5.05334200 -0.44088500 -1.47794100

H -5.24815900 -1.99473500 -2.31249900
 H -5.31037100 -1.94358000 -0.54062900
 H 0.21582300 0.30992600 -0.75490000
 C 0.63098500 -0.12034100 1.20894200
 C 1.92487500 -0.50446700 1.14536500
 C 2.64414600 -0.94713500 2.40096800
 H 1.93114200 -0.93454600 3.23943500
 H 2.97690700 -1.99478200 2.29834900
 C 2.69580400 -0.50983800 -0.12776000
 C 2.69156300 0.60034700 -0.99000000
 C 3.48816000 -1.61461700 -0.48426200
 C 3.42672400 0.59714800 -2.17532100
 H 2.11482000 1.48798000 -0.71652900
 C 4.22556700 -1.61879800 -1.66767000
 H 3.52085400 -2.48695200 0.17212500
 C 4.19560100 -0.51488800 -2.52157700
 H 3.40814600 1.47464700 -2.82483200
 H 4.82856600 -2.49197400 -1.92523200
 H 0.13185400 -0.11298800 2.18470200
 H 4.77505400 -0.51814700 -3.44647100
 C 3.85399800 -0.07727900 2.74103100
 H 4.60138500 -0.09980000 1.93320300
 H 3.55205600 0.97074400 2.89058900
 H 4.34635300 -0.42576600 3.66091900

(41) TS1_2y

H -1.35245900 -0.71557300 -1.46890600
 H 1.08997000 -3.69802400 -0.57354500
 H 2.04166300 -2.97272400 0.72866900
 H -0.56671400 -2.91705800 2.69928900
 H -0.87938600 -1.25173200 2.17527000
 H -1.04869000 -3.30061000 -0.87461200
 H -2.64715800 -1.54075600 1.07690400
 N -1.74015900 -0.61848500 -0.52916500
 C 1.09875600 -3.48689400 0.50340700
 C -0.14013000 -2.06127400 2.15804800
 N 0.00828400 -2.47864200 0.72798100
 C -1.28264900 -2.92701700 0.13200500
 C -2.33212900 -1.81532900 0.06008000
 H -1.58585100 1.78358100 -2.50550900
 H -0.17832900 0.74482900 -2.20184100
 C -0.64450400 1.70559900 -1.93282100
 C -1.66359200 0.55111100 0.06177500
 C -0.97530100 1.68197300 -0.43395600
 H 0.34100800 -1.64409600 0.17843800

C 5.66195900 1.13941100 0.08309600
 C 4.27296000 1.20056900 0.18254100
 C 3.48691500 0.18314000 -0.36863300
 C 4.09731300 -0.89399800 -1.02038100
 C 5.48614300 -0.95471000 -1.11812500
 C 6.26847400 0.06184000 -0.56610700
 H 6.27534900 1.93326200 0.51297900
 H 3.78304000 2.03431400 0.68717400
 H 3.46810100 -1.67541200 -1.44926800
 H 5.96217200 -1.79531200 -1.62608400
 H 7.35650100 0.01469400 -0.64245300
 C 1.98483500 0.23390100 -0.26573100
 O 1.49116800 1.21676000 0.37302800
 H 0.19615600 1.36918300 0.08934100
 O 1.31170400 -0.67324400 -0.79096700
 H -1.66084000 -3.75746500 0.73973400
 C -3.61464300 -2.24456300 -0.70809200
 C -4.14339800 -3.55255200 -0.11143400
 H -5.13890100 -3.76718300 -0.52683000
 H -3.49349600 -4.40720300 -0.34978800
 H -4.23961500 -3.48122600 0.98352500
 C -4.66555700 -1.14597600 -0.51883500
 H -4.89763500 -1.00065000 0.54770100
 H -4.32424200 -0.18482700 -0.93293600
 H -5.59488100 -1.42306900 -1.03792600
 C -3.34275800 -2.42944700 -2.20462500
 H -2.58269200 -3.20082800 -2.39893800
 H -4.26924500 -2.74593600 -2.70635600
 H -3.01732800 -1.49078000 -2.67946700
 H -2.11184900 0.59579000 1.06270100
 C -1.37036100 2.99111600 0.19621800
 C -2.71924100 3.34988000 0.32854200
 C -0.39180000 3.89454000 0.63802500
 C -3.08315800 4.57318100 0.89373000
 H -3.49376400 2.66234000 -0.02229600
 C -0.75306100 5.12011000 1.19611700
 H 0.66246500 3.62277700 0.55084500
 C -2.10021000 5.46282500 1.32691000
 H -4.13913000 4.83264300 0.99097100
 H 0.02170700 5.80909400 1.53800000
 C 0.94566500 -4.75351900 1.31735600
 H -0.00059200 -5.27096400 1.10605700
 H 1.76489800 -5.43342800 1.04795000
 H 1.01324500 -4.56164500 2.39705100
 C 1.15474900 -1.58018000 2.78039100
 H 0.93062000 -1.22033800 3.79354100

H 1.90526900 -2.37681300 2.86653900
 H 1.58218200 -0.73668400 2.21797900
 C 0.30628800 2.82236200 -2.34745400
 H -0.13373600 3.81668000 -2.18382800
 H 1.24833900 2.76896100 -1.78064900
 H 0.54735200 2.73610100 -3.41646500
 H -2.38274100 6.42122600 1.76656200

(42) TS2_2y

C 3.97420000 -1.18963400 -0.57010500
 C 4.54800600 -2.54354000 -1.00230800
 H 4.08661200 -2.89265900 -1.93983000
 H 5.62979800 -2.44438000 -1.17402200
 H 4.40681700 -3.31798000 -0.23441800
 C 4.43003900 -0.11722900 -1.56481400
 H 4.09518200 -0.35690500 -2.58615600
 H 4.04039100 0.87593300 -1.29493800
 H 5.52833000 -0.05610800 -1.56934900
 C 4.48988800 -0.83448900 0.82687900
 H 4.19779100 0.18396600 1.12690200
 H 4.13665600 -1.54261200 1.59220900
 H 5.58974100 -0.86730000 0.82557600
 C 2.42288100 -1.26089400 -0.62268000
 H 2.16126500 -1.46006700 -1.67272100
 C 1.81135900 -2.36246100 0.23765400
 H 1.95565600 -2.16816100 1.30795800
 H 2.27952300 -3.32612200 0.00829900
 N 1.79440700 0.03156500 -0.31973800
 H -0.04564700 -1.56159600 -0.31662600
 N 0.34235700 -2.49442800 -0.01731000
 C -0.42915900 -2.80101800 1.23087800
 H -0.17696300 -1.99713300 1.93606000
 H -1.49254600 -2.69669900 0.97877100
 C 0.07437800 -3.44641300 -1.14465100
 H 0.63486800 -3.05745200 -2.00490600
 H 0.51577200 -4.41150300 -0.86248600
 C -1.39950100 -3.56906500 -1.46990100
 H -1.94880600 -4.11510000 -0.69077700
 H -1.85445200 -2.57661700 -1.60013200
 H -1.50432200 -4.12683900 -2.40979200
 C -0.12866400 -4.16900600 1.80437300
 H 0.94367800 -4.30216500 2.00678100
 H -0.66594300 -4.27216200 2.75644900
 H -0.46864900 -4.97446300 1.13857200
 H 1.48551600 0.57935300 -1.12359900

C 1.55438600 0.52077600 0.87180800
 C 0.78842500 1.67685800 1.15755800
 C 0.96793100 2.26195700 2.56136800
 H 0.98862500 1.43023000 3.28414000
 H 0.07701100 2.86309700 2.80149600
 C 0.55901600 2.67773700 0.05614300
 C -0.71351700 3.23214200 -0.14507100
 C 1.61839700 3.12374800 -0.74848300
 C -0.92176000 4.19748300 -1.13021300
 H -1.54647000 2.89954300 0.47868500
 C 1.40937100 4.08388100 -1.73941400
 H 2.62199500 2.71703900 -0.59373300
 C 0.13744100 4.62304800 -1.93344900
 H -1.91924500 4.61785600 -1.27267800
 H 2.24644600 4.41604700 -2.35644700
 H 1.87845900 -0.08844900 1.72413400
 C -5.72172500 0.05704400 0.88983000
 C -4.34974700 0.19443300 1.09520800
 C -3.45495700 -0.07161100 0.05310000
 C -3.94227400 -0.46427800 -1.19812000
 C -5.31458300 -0.59503200 -1.40478600
 C -6.20451100 -0.33777000 -0.35971200
 H -6.41842100 0.25880000 1.70546400
 H -3.95611900 0.50613400 2.06357800
 H -3.23120500 -0.65665400 -2.00322300
 H -5.69224800 -0.89907400 -2.38266900
 H -7.27917100 -0.44341600 -0.52045800
 C -1.96726600 0.05485900 0.27160200
 O -1.59793600 0.55245100 1.38026100
 H -0.32299000 1.01247700 1.27392200
 O -1.19418100 -0.32777400 -0.62721100
 C 2.22449500 3.11240000 2.71015400
 H 2.21039800 3.97047800 2.02132500
 H 2.31778500 3.50535900 3.73313900
 H 3.12568300 2.51816700 2.48960700
 H -0.02649000 5.37621100 -2.70625700

(43) TS3_2y

H -1.40745400 0.35625600 -0.76311000
 H 0.16385900 -3.08355900 -1.77947600
 H 1.25990700 -3.34592800 -0.41579400
 H -1.24842400 -3.68633600 1.66014800
 H -1.10011300 -1.95752400 2.03336100
 H -1.81963100 -2.15728500 -1.57876400
 H -2.94960800 -1.32108600 1.15560100
 N -1.81669900 0.06729100 0.12919500

C 0.21929400 -3.45213600 -0.74720600
 C -0.60883600 -2.80209200 1.53401700
 N -0.58343200 -2.48266500 0.07116500
 C -1.94881900 -2.29161900 -0.49594100
 C -2.69355400 -1.09908000 0.10941000
 C -1.49886200 0.75366500 1.20040000
 C -0.56229800 1.81191600 1.26745100
 H -0.05908000 -1.57488900 -0.04907100
 C 5.72440000 -0.12253700 0.53409400
 C 4.38546800 0.08541300 0.86127000
 C 3.37906900 -0.30477300 -0.02870800
 C 3.71980800 -0.90168400 -1.24724800
 C 5.05864700 -1.11017800 -1.57290000
 C 6.06114600 -0.72076900 -0.68199900
 H 6.50932000 0.18243100 1.22844900
 H 4.10479000 0.55037300 1.80729800
 H 2.92190800 -1.19496800 -1.93118900
 H 5.32289000 -1.57743500 -2.52323800
 H 7.11018200 -0.88433800 -0.93620200
 C 1.92793900 -0.08871000 0.31339600
 O 1.68010100 0.42957900 1.44745900
 H 0.47177500 1.01796100 1.41623000
 O 1.05697800 -0.42712500 -0.51114000
 H -2.51808700 -3.21134700 -0.31749900
 C -4.02903200 -0.78082400 -0.62072200
 C -4.87170500 -2.05658300 -0.70824300
 H -5.88012800 -1.80518500 -1.06813400
 H -4.44248300 -2.78734900 -1.40929900
 H -4.97357300 -2.53618000 0.27816000
 C -4.78220800 0.26128800 0.21205400
 H -4.97839000 -0.11206100 1.22923100
 H -4.21722500 1.20325300 0.29134000
 H -5.74824600 0.49087100 -0.26130200
 C -3.78546700 -0.21990900 -2.02575300
 H -3.23140900 -0.92180100 -2.66671500
 H -4.75287800 -0.02336600 -2.51160000
 H -3.23355000 0.73294500 -1.99360300
 H -1.93589200 0.38218600 2.13670200
 C -0.25296800 -4.88734500 -0.64730200
 H -1.28831400 -5.00872300 -0.99458000
 H 0.38792100 -5.50355200 -1.29225200
 H -0.17184500 -5.28024800 0.37568900
 C 0.77039800 -3.00898700 2.12682400
 H 0.65684100 -3.14321000 3.21096000
 H 1.27098300 -3.90174000 1.73001400
 H 1.41304000 -2.13052800 1.96766400

C -0.58206300 2.62839800 2.56264900
 H 0.40251100 3.10589000 2.68682800
 H -0.69967900 1.93364400 3.40960000
 C -0.25790400 2.59358400 0.01530100
 C 1.05017600 3.02798700 -0.24485200
 C -1.27438300 2.96822600 -0.87612300
 C 1.33596700 3.79723600 -1.37210700
 H 1.85260400 2.75506200 0.44413100
 C -0.98870400 3.73440300 -2.00747700
 H -2.30718700 2.66595600 -0.68056600
 C 0.31856300 4.14904600 -2.26062500
 H 2.36154800 4.12176300 -1.55848200
 H -1.79553500 4.01541000 -2.68703500
 H 0.54475300 4.74867000 -3.14418800
 C -1.67976300 3.68574800 2.59833300
 H -1.66961200 4.23637600 3.55033300
 H -1.55562200 4.41799300 1.78607200
 H -2.67243800 3.22148200 2.48326000

(44) TS4_2y

C 3.40682100 -2.43486500 -0.81911600
 C 3.67076300 -3.91843800 -0.53826400
 H 2.97877300 -4.55965700 -1.10683200
 H 4.69625000 -4.17214400 -0.844444000
 H 3.57820700 -4.16445900 0.52965700
 C 3.75303700 -2.14000900 -2.28251700
 H 3.13976800 -2.75119400 -2.96317700
 H 3.59571200 -1.07968400 -2.53051700
 H 4.81100200 -2.37495600 -2.46997300
 C 4.27894100 -1.57047700 0.09405700
 H 4.16500100 -0.49757500 -0.12464500
 H 4.05826000 -1.73954100 1.15897700
 H 5.33732100 -1.82285900 -0.07030900
 C 1.89385400 -2.14698200 -0.61775900
 H 1.35555300 -2.80303400 -1.31876800
 C 1.37556100 -2.42970600 0.78826100
 H 1.80263100 -1.73704600 1.52359700
 H 1.64330700 -3.44720800 1.09284500
 N 1.52759200 -0.78259700 -1.02407700
 H -0.44431200 -1.66372900 0.07411700
 N -0.11662000 -2.30613300 0.84303600
 C -0.58821800 -1.61794300 2.08911300
 H -0.06127800 -0.65392000 2.10708600
 H -1.65643200 -1.40744700 1.94790800
 C -0.77575400 -3.62970100 0.59302700
 H -0.39004000 -3.97769700 -0.37437500

H -0.41545300 -4.31984100 1.36731100
 C -2.28727100 -3.53882600 0.57267000
 H -2.70331300 -3.36007100 1.57369500
 H -2.62314800 -2.74014500 -0.10407100
 H -2.68883600 -4.49397600 0.20873900
 C -0.34438900 -2.42042100 3.34840100
 H 0.71693200 -2.68026600 3.46967100
 H -0.64144100 -1.81112000 4.21232600
 H -0.94160300 -3.34258500 3.36665300
 H 1.14089400 -0.69155700 -1.96237500
 C 1.60029200 0.29512900 -0.28641300
 C 1.05559400 1.56106500 -0.62714700
 H 2.03628600 0.17361000 0.71186000
 C -5.57549800 1.48903700 0.33229400
 C -4.18437900 1.41645100 0.38114100
 C -3.50810200 0.43140100 -0.34662800
 C -4.23111400 -0.47338100 -1.13125500
 C -5.62177600 -0.39556100 -1.18551800
 C -6.29432200 0.58354800 -0.45115200
 H -6.10224300 2.25556300 0.90353900
 H -3.60545500 2.11839800 0.98270500
 H -3.68736100 -1.22945200 -1.69993000
 H -6.18488700 -1.09885100 -1.80158200
 H -7.38371600 0.64238800 -0.49099900
 C -2.00276700 0.34114500 -0.29335300
 O -1.40091100 1.27292900 0.32180800
 H -0.08679400 1.32756300 -0.06168800
 O -1.43955500 -0.62416900 -0.84815900
 C 0.65794400 1.79802800 -2.08293000
 H 1.55602700 1.84760700 -2.72357200
 H 0.07558300 0.92517500 -2.42126800
 C 1.63071900 2.71044800 0.16096400
 C 1.35997400 2.83363600 1.53042300
 C 2.46305700 3.66053600 -0.44655900
 C 1.91560900 3.87184800 2.27853800
 H 0.69731300 2.10906600 2.01150200
 C 3.01155000 4.70449900 0.29818400
 H 2.68499900 3.58063600 -1.51320500
 C 2.74220300 4.81252800 1.66365900
 H 1.69395800 3.95030900 3.34456200
 H 3.65834300 5.43569500 -0.19067100
 H 3.17373700 5.62918900 2.24518200
 C -0.20712100 3.03860700 -2.28346600
 H 0.34113900 3.96387600 -2.05819200
 H -0.55316900 3.09976900 -3.32485500
 H -1.09183300 3.00263000 -1.63032700

(45) T1_2f

C 2.59678800 -2.09228100 -0.04664500
C 4.04984800 -1.93466000 0.41598400
H 4.09910400 -1.59059200 1.46159800
H 4.56611500 -2.90442000 0.35368600
H 4.60951100 -1.22372700 -0.20987400
C 1.95314600 -3.23930700 0.73857000
H 1.96186200 -3.03331500 1.82069700
H 0.90976800 -3.40487900 0.43208800
H 2.51156300 -4.17190000 0.56467900
C 2.56843300 -2.43409600 -1.53941600
H 1.54087400 -2.60376500 -1.89719900
H 3.02752300 -1.64730100 -2.15695600
H 3.13252100 -3.36243700 -1.71579100
C 1.81317500 -0.78119300 0.25734700
H 1.76667900 -0.69768600 1.35465300
C 2.52656400 0.45791400 -0.29786900
H 2.72887600 0.33907400 -1.37121500
H 3.47007400 0.64968800 0.22471200
N 0.44115500 -0.76820200 -0.21877500
H 0.73537300 1.38067400 -0.47286100
N 1.67714900 1.67948300 -0.16374400
C 2.11248300 2.77435800 -1.09112400
H 2.10817200 2.33170000 -2.09514600
H 1.33066800 3.54192000 -1.05875900
C 1.52510000 2.10300100 1.26778900
H 1.02650700 1.26789800 1.77659300
H 2.53684800 2.20222300 1.68287200
C 0.71636600 3.37299400 1.42833300
H 1.25244900 4.25928600 1.06382100
H -0.24949900 3.30002400 0.90658700
H 0.51248100 3.51888100 2.49742700
C 3.47038200 3.34767000 -0.74699600
H 4.26313300 2.58911600 -0.80190800
H 3.70566100 4.13157400 -1.47921900
H 3.48369400 3.80732100 0.25110500
H 0.33276400 -0.98016500 -1.21023200
C -0.60527400 -1.21499400 0.58656300
C -1.95168800 -1.28900400 -0.01136200
C -2.43537100 -2.65138000 -0.42778200
H -1.58976500 -3.18867700 -0.88895400
H -3.22155800 -2.58511900 -1.19289800
C -2.77489800 -0.11280700 -0.11068800
C -4.10218600 -0.14755500 -0.61616900
C -2.28242700 1.15061100 0.31869200

C -4.87419700 1.00562900 -0.69232900
H -4.53437000 -1.09230000 -0.94748300
C -3.06098700 2.29686500 0.23794700
H -1.26953200 1.21291800 0.72253000
C -4.36383500 2.23732300 -0.27021300
H -5.89153000 0.94338800 -1.08408100
H -2.65194600 3.25081400 0.57859700
H -0.46356600 -1.05631400 1.66168800
H -4.97483100 3.13934400 -0.33040900
C -2.94450000 -3.46444300 0.76798400
H -3.80982300 -2.97170600 1.23647100
H -3.24913500 -4.47493800 0.45875700
H -2.15631500 -3.56343700 1.53036700

(46) S-2aa

C 1.99374800 1.37523900 0.52661400
H 1.67504500 1.56465100 1.56311200
H 2.88149300 1.99752700 0.33297100
C 0.86492100 1.81840300 -0.43734600
H 1.24007400 1.66007000 -1.46481800
C 0.69274100 3.31842800 -0.31564900
H 1.63939000 3.89257400 -0.46252300
O -0.33987800 3.89010800 -0.08638600
C -0.41341900 1.04351600 -0.24892500
C -0.88444800 0.17576000 -1.23265000
C -1.13690600 1.13341000 0.95158600
C -2.04215600 -0.58793300 -1.04869000
H -0.33580800 0.08295800 -2.17368000
C -2.28733500 0.38505700 1.15286600
H -0.79143100 1.80265400 1.74308400
C -2.75131800 -0.48470900 0.15179000
H -2.37467600 -1.25502800 -1.84313800
H -2.85238700 0.45360000 2.08399400
O -3.87646300 -1.17600300 0.43070500
C -4.38234200 -2.05169200 -0.55150800
H -5.29003000 -2.50245500 -0.13378400
H -4.64261600 -1.51246700 -1.47682600
H -3.66173600 -2.85077200 -0.78967200
C 2.34348900 -0.08121800 0.35582300
C 1.82996200 -1.05111700 1.22515000
C 3.14619800 -0.49740300 -0.71431900
C 2.11238900 -2.40454800 1.03272700
H 1.20092800 -0.73922100 2.06298400
C 3.43144500 -1.84864100 -0.90912600
H 3.55377900 0.24942000 -1.40118000

C 2.91384700 -2.80755200 -0.03569800
 H 1.70466100 -3.14649300 1.72219600
 H 4.06259000 -2.15449300 -1.74589500
 H 3.13655200 -3.86538000 -0.18724800

(47) (S)-imine_2aa

H -3.58121100 1.71315300 2.47521700
 H -2.40736500 2.93609700 1.95560500
 H -3.16599400 2.49832600 -1.15616800
 H -1.88575700 1.27903700 -1.31230500
 H -4.15853800 -0.00431000 1.25922800
 H -2.96230400 -0.66060400 -1.48577400
 N -1.75909000 -1.06330800 0.20597500
 C -3.27128800 2.34358100 1.63244800
 C -2.28341300 2.06994800 -0.66344400
 N -2.76830500 1.39439300 0.58266700
 C -3.74449300 0.29902800 0.28974900
 C -3.06369800 -0.88786300 -0.40754700
 H 1.48926500 -2.14090200 -1.78400900
 H 0.91164100 -3.27688000 -0.54602900
 C 1.45301100 -2.33040200 -0.70002200
 C -0.74546300 -1.12346200 -0.55253800
 C 0.65818800 -1.19668400 -0.01546600
 H -1.95002900 0.92086800 1.00130600
 H 0.58894900 -1.40554300 1.06217900
 H -4.54523400 0.71864500 -0.33008500
 C -3.91508000 -2.18601900 -0.31093200
 C -5.33431600 -1.89285400 -0.80765800
 H -5.90156300 -2.83212800 -0.89113600
 H -5.88553200 -1.23547000 -0.11878900
 H -5.31752600 -1.41865700 -1.80196000
 C -3.27811700 -3.24016200 -1.22101400
 H -3.23546900 -2.88935600 -2.26416800
 H -2.25568400 -3.48939100 -0.89915700
 H -3.87211800 -4.16631400 -1.19726700
 C -3.96354400 -2.72728500 1.12079000
 H -4.41536200 -2.01095700 1.82346800
 H -4.57338000 -3.64333900 1.14699700
 H -2.95666800 -2.97592200 1.48476300
 H -0.85156200 -1.07900000 -1.65523700
 C 1.31473400 0.16026200 -0.19766900
 C 1.44493400 0.73826900 -1.47226200
 C 1.82246600 0.86261700 0.89491700
 C 2.05633800 1.97268200 -1.63992500
 H 1.06937600 0.20988100 -2.35250500
 C 2.44656200 2.10552800 0.74426100

H 1.73877600 0.43013500 1.89526100
 C 2.56159000 2.67044400 -0.53048100
 H 2.15758500 2.42398700 -2.62847400
 H 2.83667700 2.61708100 1.62343900
 C -4.40204500 3.22970100 1.15740700
 H -5.26423700 2.64739000 0.80377700
 H -4.73599900 3.83784900 2.00884500
 H -4.08176600 3.91748800 0.36274500
 C -1.21707300 3.10715700 -0.38199300
 H -0.81208800 3.45964300 -1.34020400
 H -1.61625100 3.97792400 0.15568100
 H -0.38784700 2.67274600 0.19922700
 O 3.13488500 3.86420900 -0.78288600
 C 3.64266800 4.60455800 0.30486400
 H 4.04623900 5.53562800 -0.10920200
 H 2.85008400 4.84682800 1.03109900
 H 4.44979400 4.06017000 0.82109900
 C 2.85062500 -2.44087800 -0.14553100
 C 3.93678400 -1.84496100 -0.79843200
 C 3.07678900 -3.08749200 1.07673800
 C 5.21679800 -1.89152300 -0.24413700
 H 3.77548300 -1.33878800 -1.75378300
 C 4.35477300 -3.13722700 1.63312100
 H 2.23837700 -3.55956400 1.59617100
 C 5.42967200 -2.53714800 0.97432900
 H 6.05167300 -1.42127600 -0.76754500
 H 4.51326200 -3.64852700 2.58475500
 H 6.43058800 -2.57610200 1.40809900

(48) (R)-imine_2aa

C -2.42500400 -2.62134300 -0.05197300
 C -3.66029200 -3.39367000 -0.52668900
 H -3.88139000 -3.17902400 -1.58455700
 H -3.48276900 -4.47531600 -0.43081100
 H -4.55220000 -3.15097500 0.07024900
 C -1.20009500 -3.12375200 -0.82311300
 H -1.31228600 -2.95316800 -1.90546400
 H -0.27373600 -2.63039600 -0.48960700
 H -1.07555500 -4.20471500 -0.65885000
 C -2.19934600 -2.86476200 1.44314200
 H -1.30876000 -2.32825100 1.80064000
 H -3.05970800 -2.55152700 2.05331900
 H -2.04469800 -3.94007700 1.61975900
 C -2.62280100 -1.10758400 -0.36783200
 H -2.62401400 -1.02022700 -1.47076700
 C -3.95137500 -0.57906200 0.18268300

H -4.10074600 -0.90862700 1.21884200
 H -4.79979000 -0.90860000 -0.42780000
 N -1.55457400 -0.31445500 0.21417500
 N -3.96659600 0.91636400 0.21435600
 H -3.05957000 1.18555400 0.63027900
 C -0.59698500 0.04322900 -0.53529600
 C 0.61920300 0.75372500 -0.00209900
 C 0.98211200 1.96660200 -0.87605900
 H 0.11195900 2.64225800 -0.89255000
 H 1.15439900 1.64330600 -1.91356600
 C -5.01794400 1.45868800 1.13919200
 H -4.84221000 0.96826600 2.10481900
 H -4.80519900 2.52714600 1.26229700
 C -6.43056200 1.22741000 0.64844800
 H -6.64642600 0.16009200 0.50201100
 H -7.12362900 1.60789100 1.41062700
 H -6.63620800 1.76601500 -0.28691300
 H 0.37203000 1.09725800 1.01310200
 C 1.71574900 -0.29378200 0.10925400
 C 1.92970900 -0.94860500 1.33164400
 C 2.46892700 -0.70343200 -0.99321900
 C 2.86580800 -1.96676300 1.44986700
 H 1.34744100 -0.65157600 2.20789800
 C 3.41760600 -1.72527200 -0.89299100
 H 2.32517000 -0.22423800 -1.96432500
 C 3.62127400 -2.36482200 0.33566700
 H 3.03523000 -2.47161400 2.40241400
 H 3.98811200 -2.01019600 -1.77645700
 C -4.00317400 1.50158500 -1.16532300
 H -4.91374400 1.12126100 -1.64619500
 H -3.13944000 1.08289500 -1.69685000
 C -3.94166300 3.01384400 -1.16259700
 H -3.82191900 3.35829200 -2.19817300
 H -4.85620700 3.46916700 -0.75998100
 H -3.07697400 3.37190400 -0.58391300
 H -0.58169600 -0.20905500 -1.61511500
 C 2.19290100 2.70556500 -0.36043700
 C 3.40939100 2.67569900 -1.05178000
 C 2.12883400 3.40926400 0.85021500
 C 4.53519000 3.33087600 -0.54866600
 H 3.47383600 2.13399700 -1.99861200
 C 3.25059600 4.06470700 1.35589900
 H 1.18526400 3.44523100 1.40160500
 C 4.45980600 4.02587200 0.65777000
 H 5.47476700 3.29672600 -1.10367100
 H 3.18152900 4.61045400 2.29902100

H 5.33896400 4.53762300 1.05360700
 O 4.51075600 -3.35772200 0.53673900
 C 5.29506300 -3.78718600 -0.55372200
 H 5.94401400 -4.58639700 -0.17787400
 H 4.66886100 -4.18516500 -1.36849500
 H 5.92187100 -2.96994700 -0.94547600

(49) E-enamine_2aa

C -3.08264400 -0.69038200 2.41179200
 C -4.30929900 -1.57575000 2.65898900
 H -4.16758900 -2.58038800 2.22937800
 H -4.47408200 -1.68931200 3.74097400
 H -5.22597000 -1.14278700 2.23152100
 C -1.89584800 -1.25239400 3.20039100
 H -1.64150700 -2.27069200 2.86584500
 H -1.00137100 -0.62181800 3.08794500
 H -2.14343500 -1.29746100 4.27169700
 C -3.37249700 0.73274100 2.89971200
 H -2.50523700 1.39781000 2.76211200
 H -4.23881300 1.18163900 2.39146500
 H -3.59733600 0.71150500 3.97669900
 C -2.71593800 -0.72275400 0.90037800
 H -2.45546200 -1.76770700 0.67176700
 C -3.88995200 -0.30525700 0.00638200
 H -4.26064400 0.68831700 0.29245400
 H -4.71426800 -1.02497600 0.06059200
 N -1.55396400 0.08281300 0.55682100
 H -2.52626200 0.24031600 -1.37774600
 N -3.45929600 -0.20565600 -1.42045200
 C -4.33734500 0.70961700 -2.22225800
 H -4.36594400 1.65425400 -1.66535700
 H -3.81843300 0.89399200 -3.17038100
 C -3.25948100 -1.55600200 -2.04016300
 H -2.52150700 -2.07315300 -1.41532100
 H -4.21435400 -2.09079800 -1.95256700
 C -2.77638500 -1.47948400 -3.47260300
 H -3.55101400 -1.10644400 -4.15600600
 H -1.88527300 -0.83954100 -3.55604500
 H -2.49883700 -2.49072300 -3.79819100
 C -5.72778900 0.15550200 -2.44683300
 H -6.24350300 -0.05584500 -1.49962400
 H -6.31472300 0.91018500 -2.98697800
 H -5.71238000 -0.75694000 -3.05896100
 H -1.59410600 1.04217700 0.89279200
 C -0.29420100 -0.48683600 0.47841300
 C 0.89077900 0.10089800 0.76439600

H -0.31248600 -1.52042500 0.11598700
 C 2.16172600 -0.59884700 0.45078700
 C 3.33663000 -0.34931400 1.18899300
 C 2.26137700 -1.52731000 -0.59700800
 C 4.52495100 -1.01293000 0.91587800
 H 3.32672700 0.37208100 2.00769800
 C 3.44598100 -2.21062400 -0.87873900
 H 1.39453100 -1.71751500 -1.23334100
 C 4.59314600 -1.95680800 -0.11834400
 H 5.42518000 -0.81415400 1.49999200
 H 3.46681600 -2.91982500 -1.70606300
 C 0.97487200 1.47305200 1.39706700
 H -0.02432200 1.80056600 1.72245800
 H 1.57873300 1.42691900 2.31608600
 O 5.78816900 -2.55260100 -0.31876300
 C 5.88937100 -3.51186200 -1.34601100
 H 5.67027600 -3.07232800 -2.33259200
 H 6.92383800 -3.87424000 -1.33782900
 H 5.20953900 -4.36195100 -1.17225200
 C 1.56335500 2.52779900 0.48190000
 C 2.71332500 3.23695300 0.84283300
 C 0.96388300 2.80610000 -0.75420700
 C 3.25219800 4.20671900 -0.00618800
 H 3.19131600 3.02685900 1.80309600
 C 1.49635100 3.77517400 -1.60300300
 H 0.06823900 2.25188100 -1.05042700
 C 2.64497000 4.47911700 -1.23101000
 H 4.15126500 4.74941200 0.29261000
 H 1.01545100 3.98340100 -2.56092300
 H 3.06521500 5.23572100 -1.89630400

(50) Z-enamine_2aa

C 3.00723800 -1.73519700 1.75240300
 C 4.44164300 -1.74958100 2.29181700
 H 4.67104200 -0.81808800 2.83351900
 H 4.56842600 -2.58835500 2.99266600
 H 5.18523200 -1.87560500 1.49086800
 C 2.03109200 -1.70935100 2.93298900
 H 2.14528500 -0.78588600 3.52243800
 H 0.98643000 -1.77299800 2.59367000
 H 2.22350700 -2.56521800 3.59733200
 C 2.75789400 -3.00395700 0.92995800
 H 1.73503100 -3.03694600 0.52200600
 H 3.46886600 -3.11060500 0.09741100
 H 2.87487500 -3.88679700 1.57666300
 C 2.78675100 -0.44185100 0.91675500

H 2.95629000 0.39720300 1.60905900
 C 3.77829800 -0.32229300 -0.24799300
 H 3.75896100 -1.22837400 -0.86806500
 H 4.80108400 -0.15329300 0.10735100
 N 1.43331500 -0.29530800 0.40072100
 H 2.38504200 0.72466400 -1.25965000
 N 3.40979800 0.81148500 -1.14680600
 C 4.01003000 0.67928400 -2.51494800
 H 3.71810700 -0.31614900 -2.87209600
 H 3.51296900 1.42273700 -3.14909100
 C 3.64650000 2.14174400 -0.49745800
 H 3.03979500 2.14370600 0.41590700
 H 4.70420300 2.17182300 -0.20444200
 C 3.26203100 3.30622100 -1.38462700
 H 3.94027600 3.42182800 -2.24039700
 H 2.23168300 3.19753700 -1.75488800
 H 3.31121200 4.22684800 -0.78813000
 C 5.51330000 0.85305500 -2.52709300
 H 6.01752300 0.11037600 -1.89354300
 H 5.86689600 0.71043000 -3.55684000
 H 5.81451000 1.86018800 -2.20704900
 H 1.06757500 -1.13208800 -0.05034000
 C 0.50330200 0.45923800 1.09952800
 C -0.84542300 0.36227200 1.07012200
 C -1.66188200 1.28739800 1.95023000
 H -2.19924100 0.71626000 2.72430900
 H -0.97171800 1.95849100 2.48470300
 C -1.58228400 -0.62144700 0.23761900
 C -2.74794300 -1.23722700 0.71755000
 C -1.18334700 -0.94688100 -1.07439000
 C -3.47170600 -2.15539000 -0.04440300
 H -3.10847900 -1.00446200 1.72153300
 C -1.89188400 -1.85831500 -1.84630400
 H -0.31362600 -0.45542300 -1.51644400
 C -3.04230100 -2.47768200 -1.33741400
 H -4.36639600 -2.60951900 0.38023100
 H -1.57766500 -2.09932300 -2.86326400
 H 0.95816400 1.22128300 1.74197700
 C -2.67131000 2.11615100 1.18219900
 C -2.25198000 2.95525000 0.14094200
 C -4.03553500 2.05881000 1.48494400
 C -3.17097600 3.72317200 -0.57201400
 H -1.18835900 3.00370100 -0.10928800
 C -4.96110500 2.82402400 0.77126200
 H -4.37687100 1.40502400 2.29185200
 C -4.53136500 3.65890200 -0.25928900

H -2.82635100 4.37586900 -1.37665000
 H -6.02234700 2.76458200 1.02112600
 H -5.25227800 4.25743200 -0.81923800
 O -3.67011300 -3.34930100 -2.15329600
 C -4.83197100 -3.99199300 -1.67839700
 H -5.17548900 -4.65280900 -2.48261500
 H -4.61986700 -4.59687800 -0.78205000
 H -5.62758700 -3.26612800 -1.44550700

(51) TS1_2aa

H -0.22707400 -1.75829800 0.76206900
 H -4.15393300 -1.75448600 0.23640900
 H -4.39597000 -0.21604600 -0.59915300
 H -3.00311700 -1.38016500 -3.27353600
 H -1.42096500 -0.76644400 -2.76684700
 H -2.42888500 -3.02466300 -0.05990400
 H -0.26523500 -2.37058600 -2.14649800
 N -0.04300800 -1.64008100 -0.23662100
 C -4.14272400 -1.27295000 -0.74967400
 C -2.49628000 -0.71840500 -2.55875100
 N -2.70713800 -1.30003300 -1.19607200
 C -2.11042300 -2.65869400 -1.04447200
 C -0.58390200 -2.65872900 -1.13525400
 H 1.48409800 1.12394800 2.19579700
 H 0.09591000 0.04339900 2.04473500
 C 1.13578000 0.19738600 1.71604400
 C 0.68167400 -0.62486100 -0.63099100
 C 1.15767300 0.42429200 0.19535100
 H -2.23873200 -0.66730500 -0.49697700
 C -3.95430300 4.78579400 1.10730500
 C -2.90736500 3.93009600 0.76782000
 C -3.02547000 2.55502700 0.99551000
 C -4.19376500 2.04216500 1.56898100
 C -5.23932700 2.89852100 1.91012100
 C -5.12004100 4.27045500 1.67805000
 H -3.86229200 5.85835900 0.92720400
 H -1.98947400 4.31588200 0.32207000
 H -4.26523600 0.96774800 1.74507300
 H -6.14987800 2.49669800 2.35814500
 H -5.93936800 4.94097900 1.94432700
 C -1.90565500 1.61569500 0.62087800
 O -0.86417400 2.13913300 0.12462300
 H 0.14167800 1.20043300 0.03762300
 O -2.06586000 0.39089200 0.80139200
 H -2.53661400 -3.30822900 -1.81885700
 C 0.04925100 -4.05103000 -0.85185500

C -0.33960600 -5.00655200 -1.98423900
 H 0.15783600 -5.97605200 -1.83352200
 H -1.42272200 -5.19316200 -2.01605600
 H -0.02371300 -4.61089600 -2.96196000
 C 1.57381400 -3.88654800 -0.84066900
 H 1.92563300 -3.38270700 -1.75559100
 H 1.91463800 -3.30310300 0.02944200
 H 2.05184800 -4.87577500 -0.78900400
 C -0.41033100 -4.62261200 0.49314800
 H -1.46921700 -4.92043000 0.47614200
 H 0.18210400 -5.51771500 0.73540900
 H -0.26468600 -3.90154100 1.31298700
 H 0.84922200 -0.56762400 -1.71374900
 C 2.30671600 1.22096200 -0.35983500
 C 3.27540100 0.66516200 -1.21199100
 C 2.44582400 2.56765800 -0.00808300
 C 4.32546500 1.43035500 -1.70382600
 H 3.21888900 -0.39201800 -1.48491300
 C 3.50018600 3.34816900 -0.48354600
 H 1.70336800 3.02571100 0.65029000
 C 4.44801100 2.78040800 -1.34489000
 H 5.07702200 0.99717300 -2.36593300
 H 3.56826700 4.39353300 -0.18448900
 C -5.10324500 -1.94517800 -1.70682900
 H -4.82512200 -2.98916900 -1.90866100
 H -6.09908200 -1.94889700 -1.24381600
 H -5.18168900 -1.40441700 -2.66004500
 C -2.97273000 0.71569400 -2.66547500
 H -2.73521400 1.07980100 -3.67387800
 H -4.05699800 0.81377800 -2.52166000
 H -2.44893600 1.36591300 -1.94854300
 C 1.98060400 -0.97738000 2.16304000
 C 1.38539600 -2.08856300 2.77166800
 C 3.36717400 -0.99899800 1.94728600
 C 2.14416500 -3.20254300 3.14045300
 H 0.30736500 -2.08014400 2.96251500
 C 4.12756800 -2.10862400 2.31349200
 H 3.85566900 -0.13489300 1.49103000
 C 3.51799800 -3.21771700 2.90655500
 H 1.65680700 -4.05940600 3.61019000
 H 5.20522000 -2.10717700 2.13835300
 H 4.11531700 -4.08628200 3.18992500
 O 5.49701800 3.44982200 -1.86487700
 C 5.65846400 4.80921600 -1.52595100
 H 5.80575500 4.94041700 -0.44178300
 H 6.55342800 5.15863900 -2.05349500

H 4.79322900 5.41121500 -1.84732800

(52) TS2_2aa

C 1.24276200 3.56036900 1.63218000
C 0.75442100 4.89453800 2.20619300
H -0.01428100 4.73999400 2.98006000
H 1.59913700 5.42439300 2.67048400
H 0.33895400 5.55238500 1.42897200
C 2.02513300 2.80879900 2.71439900
H 1.40400300 2.64547800 3.60876000
H 2.37461200 1.82997100 2.35199000
H 2.90873500 3.39257400 3.01203300
C 2.16033500 3.81427600 0.43338700
H 2.63317200 2.88501800 0.07932300
H 1.62700000 4.28213600 -0.40865700
H 2.97001900 4.49649200 0.73303000
C 0.01533100 2.69032200 1.24589700
H -0.51936400 2.46910200 2.18211300
C -0.96684300 3.36859700 0.29624100
H -0.51701400 3.56031900 -0.68593800
H -1.28540800 4.33113400 0.71085800
N 0.41551300 1.37940100 0.72024100
H -1.94985700 1.51455400 0.28134500
N -2.18985000 2.52528900 0.09648300
C -2.66486300 2.53129600 -1.32569800
H -1.79833400 2.22420700 -1.92718600
H -3.42244600 1.74106000 -1.41061300
C -3.25430800 2.87651100 1.09377000
H -2.79040000 2.74822100 2.08103500
H -3.47969800 3.94303000 0.96254900
C -4.49486700 2.01825500 0.96166700
H -5.06325300 2.25269200 0.05118800
H -4.23835600 0.94934300 0.96040900
H -5.14653100 2.21761500 1.82272300
C -3.21033500 3.87103400 -1.77050800
H -2.47214300 4.67582100 -1.64306000
H -3.45803400 3.80920600 -2.83843300
H -4.12679800 4.14016100 -1.22744900
H 0.39075600 0.60380400 1.38302000
C 0.71045200 1.09355600 -0.52375900
C 0.88208600 -0.21107200 -1.04665000
C 1.59319600 -0.29470200 -2.40530500
H 1.22476100 0.51865500 -3.04956200
H 1.32252100 -1.24682700 -2.88421700
C 1.19899200 -1.32829800 -0.08932600
C 0.55394700 -2.57272200 -0.18967400

C 2.21060300 -1.19439400 0.86848500
C 0.89397700 -3.62734400 0.64595200
H -0.22579200 -2.71499000 -0.94104200
C 2.56134800 -2.24320700 1.72225500
H 2.75357900 -0.24781500 0.95226400
C 1.89629300 -3.47041700 1.61652400
H 0.39080000 -4.59257600 0.56903300
H 3.35381200 -2.09352200 2.45438500
H 0.70750900 1.93153400 -1.23127000
C -4.85853500 -3.44417200 -1.63836300
C -3.79554600 -2.54312800 -1.67610400
C -3.44760200 -1.82333400 -0.52769400
C -4.16158600 -2.01818700 0.65946900
C -5.22150700 -2.92232300 0.69716400
C -5.57110800 -3.63421500 -0.45249500
H -5.13163900 -4.00320200 -2.53521600
H -3.22681400 -2.38425600 -2.59329000
H -3.86856800 -1.45645400 1.54784300
H -5.77510900 -3.07597400 1.62512900
H -6.40217300 -4.34159000 -0.42341000
C -2.29880200 -0.84870700 -0.55317400
O -1.63061100 -0.78084700 -1.63400800
H -0.39216800 -0.35712000 -1.35673300
O -2.05806500 -0.17451200 0.46586900
O 2.15271600 -4.54128300 2.39316700
C 3.15306400 -4.42869400 3.38156600
H 3.19165800 -5.39306800 3.90077400
H 4.13857400 -4.22107700 2.93452100
H 2.91207500 -3.63713400 4.10908900
C 3.09449700 -0.20058300 -2.26418600
C 3.88866000 -1.35074600 -2.19492000
C 3.70977000 1.04985500 -2.11787000
C 5.26525800 -1.25516700 -1.98039500
H 3.42041000 -2.33249100 -2.30650300
C 5.08410900 1.14965300 -1.90256800
H 3.10064600 1.95708000 -2.17234300
C 5.86656400 -0.00520100 -1.83140400
H 5.87024500 -2.16266900 -1.92983900
H 5.54745300 2.13234100 -1.79268300
H 6.94241100 0.07007700 -1.66310800

(53) TS3_2aa

H -0.27188600 1.03463700 0.96969100
H 3.46325400 1.81564200 1.83503500
H 4.27753300 1.36295700 0.33276700
H 2.91249800 3.83466600 -1.27836700

H 1.59855300	2.75144100	-1.77913400	C 3.55293200	1.92956500	-2.12444300
H 1.50390200	2.81100500	1.90037800	H 3.53549700	2.28527100	-3.16331300
H -0.02942000	3.50615800	-0.67373500	H 4.58757200	2.00130000	-1.76390200
N -0.32387400	1.63611900	0.14364300	H 3.24059800	0.87431000	-2.13110200
C 3.73184600	2.17283100	0.83283800	C -1.68466100	-0.64902500	-2.48410100
C 2.59417600	2.78390200	-1.32009800	H -1.42381700	-1.67921500	-2.76733400
N 2.43243200	2.31897400	0.09406300	H -1.34035400	0.01533500	-3.29177100
C 1.45722700	3.15002900	0.85646700	C -1.28248000	-1.13888600	0.00082300
C 0.02769600	3.04098500	0.32080800	C -0.73742600	-2.42258600	0.17083900
C -0.69417400	1.08833700	-0.98721300	C -2.24752800	-0.71533800	0.92078000
C -0.92950900	-0.29225700	-1.19366600	C -1.13081300	-3.23620000	1.22461400
H 2.06395500	1.33153500	0.07451700	H 0.00342400	-2.79348200	-0.54112600
C 4.55888100	-3.98798000	-1.35912600	C -2.65131600	-1.51798400	1.99074500
C 3.52432000	-3.06175500	-1.48142800	H -2.71542500	0.26660100	0.80046500
C 3.31231700	-2.11243100	-0.47570400	C -2.08871100	-2.78994700	2.14878400
C 4.14138000	-2.09460400	0.65111800	H -0.70548400	-4.23264000	1.35603300
C 5.17863300	-3.01788200	0.77003200	H -3.40705500	-1.14489800	2.68085600
C 5.38682100	-3.965553200	-0.23470500	O -2.40776900	-3.64232700	3.14254700
H 4.72077300	-4.73072400	-2.14230700	C -3.37833400	-3.24180000	4.08438000
H 2.87043300	-3.06300100	-2.35453700	H -4.35281100	-3.05697100	3.60424700
H 3.95848700	-1.35142600	1.42885600	H -3.48105100	-4.06728100	4.79804400
H 5.82543800	-3.00238800	1.64905600	H -3.06438800	-2.33493900	4.62605800
H 6.19681600	-4.69126000	-0.14002300	C -3.18090400	-0.53143300	-2.31576900
C 2.19415400	-1.10971300	-0.59500500	C -3.95771600	-1.65166300	-1.99865900
O 1.52637500	-1.12901000	-1.67760200	C -3.80700600	0.71988700	-2.39007600
H 0.31942200	-0.57883400	-1.47318300	C -5.32688100	-1.52627600	-1.75698800
O 1.98308500	-0.32576000	0.34873100	H -3.47988100	-2.63283300	-1.93231100
H 1.79376400	4.19202100	0.80721600	C -5.17499200	0.84943400	-2.14964900
C -1.01614400	3.76306300	1.21910700	H -3.21398300	1.60374900	-2.64275700
C -0.56071400	5.20528000	1.46247900	C -5.93923000	-0.27485500	-1.82942000
H -1.36814200	5.76556800	1.95634500	H -5.91724800	-2.41058400	-1.50879100
H 0.32359700	5.25450100	2.11491400	H -5.64781300	1.83131100	-2.21717600
H -0.32448100	5.71441600	0.51463700	H -7.00968200	-0.17516200	-1.64057200
C -2.35123700	3.77981900	0.46858500			
H -2.25819200	4.30747400	-0.49360900			
H -2.71937500	2.76123500	0.27026200			
H -3.11243500	4.29778900	1.07043100			
C -1.20152500	3.04304000	2.55898700			
H -0.26550900	2.97759800	3.13355900			
H -1.92712000	3.59828500	3.17179700			
H -1.60007200	2.02517400	2.42443400			
H -0.71655600	1.76540100	-1.85063700			
C 4.55365800	3.44206100	0.89873500			
H 4.01282700	4.26115800	1.39257200			
H 5.45447400	3.23329700	1.49152300			
H 4.87947100	3.77642700	-0.09579600			

(54) TS4_2aa

C -0.63265800	-3.85878000	-0.91064300
C -0.00912400	-5.06093000	-1.62658400
H 0.93097700	-5.36773300	-1.14155100
H -0.70528500	-5.91139600	-1.58610800
H 0.19549400	-4.85158600	-2.68664900
C -1.10402100	-4.29582400	0.48133600
H -0.27150300	-4.72222900	1.06274900
H -1.53016800	-3.45310800	1.04775600
H -1.88518700	-5.06517300	0.38762700
C -1.82795100	-3.33698300	-1.71187800
H -2.36852500	-2.54432800	-1.17074500

H -1.52916500 -2.95024900 -2.69849600
 H -2.54110300 -4.15812500 -1.87887700
 C 0.45228500 -2.76521400 -0.71835300
 H 1.22450900 -3.20190900 -0.06673600
 C 1.13309300 -2.29437100 -1.99761200
 H 0.43345400 -1.78748400 -2.67307200
 H 1.55259000 -3.15129400 -2.53620700
 N -0.06636200 -1.61666200 0.03688100
 H 2.09537500 -0.90894300 -0.74482700
 N 2.25632300 -1.35027600 -1.68971300
 C 2.29464800 -0.18328500 -2.63004100
 H 1.29073500 0.26136400 -2.58392200
 H 3.00063800 0.54257300 -2.20562000
 C 3.56019000 -2.08369400 -1.57268600
 H 3.40659400 -2.84055900 -0.79189900
 H 3.72309400 -2.60718000 -2.52413400
 C 4.71571200 -1.16935800 -1.22442500
 H 4.99428000 -0.51998500 -2.06543700
 H 4.47094500 -0.54593000 -0.35288100
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 H 1.99665400 -1.32450700 -4.46015600
 H 2.59337300 0.33338800 -4.67715800
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 C -0.70456500 -0.58122000 -0.43278200
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 H -0.90868400 -0.57137500 -1.50958000
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 C 3.50610200 3.38264500 1.04008900
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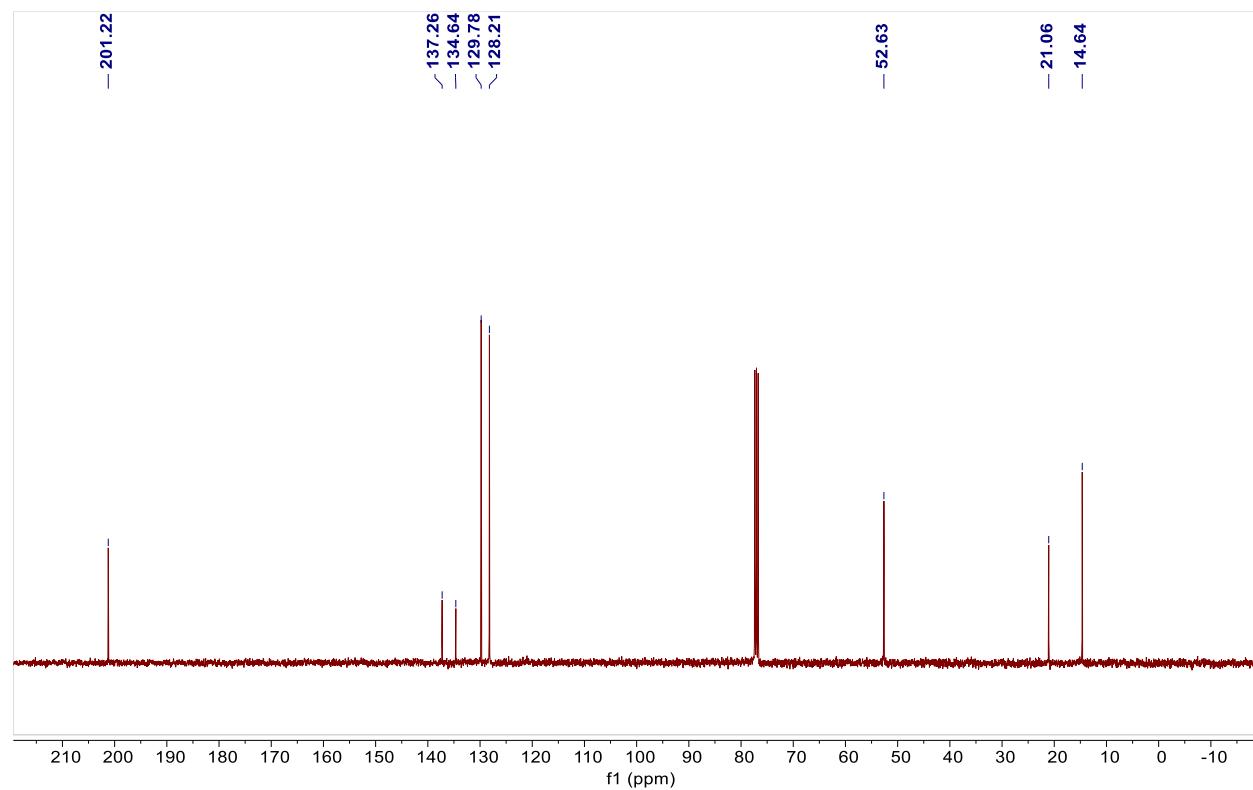
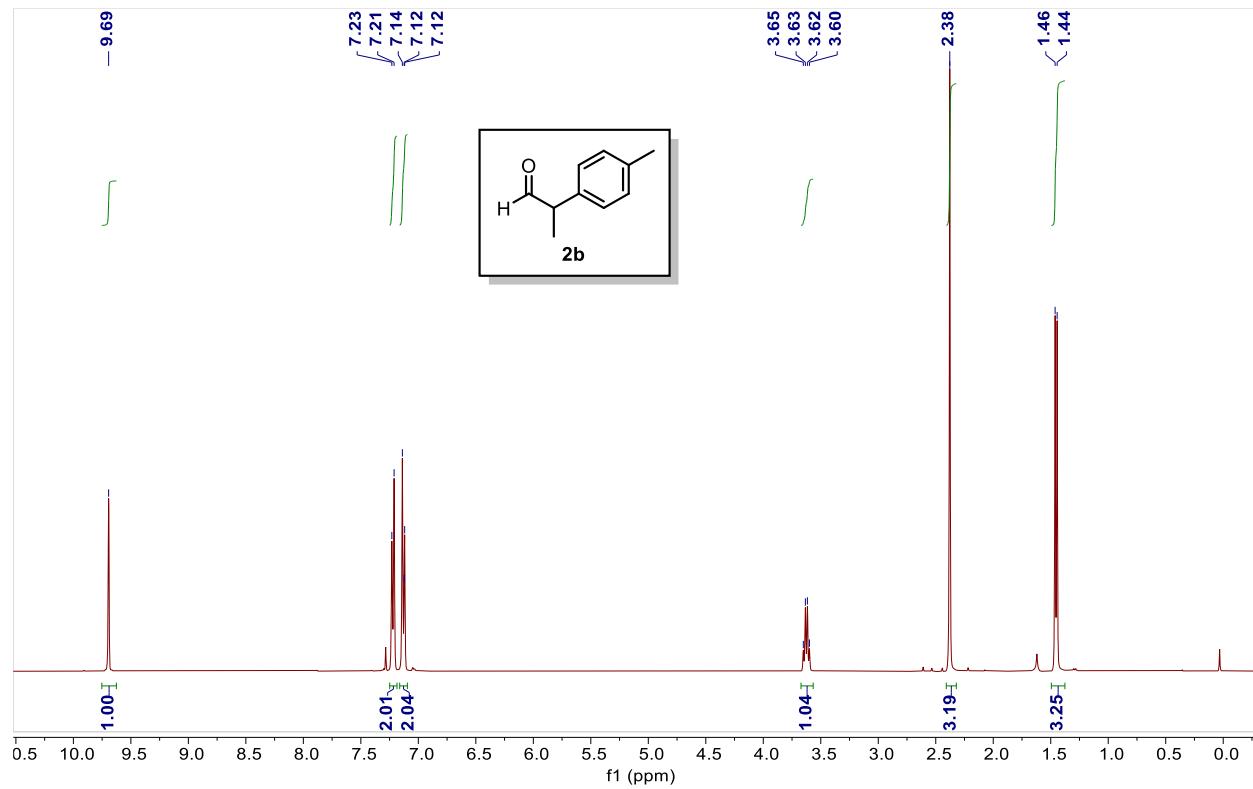
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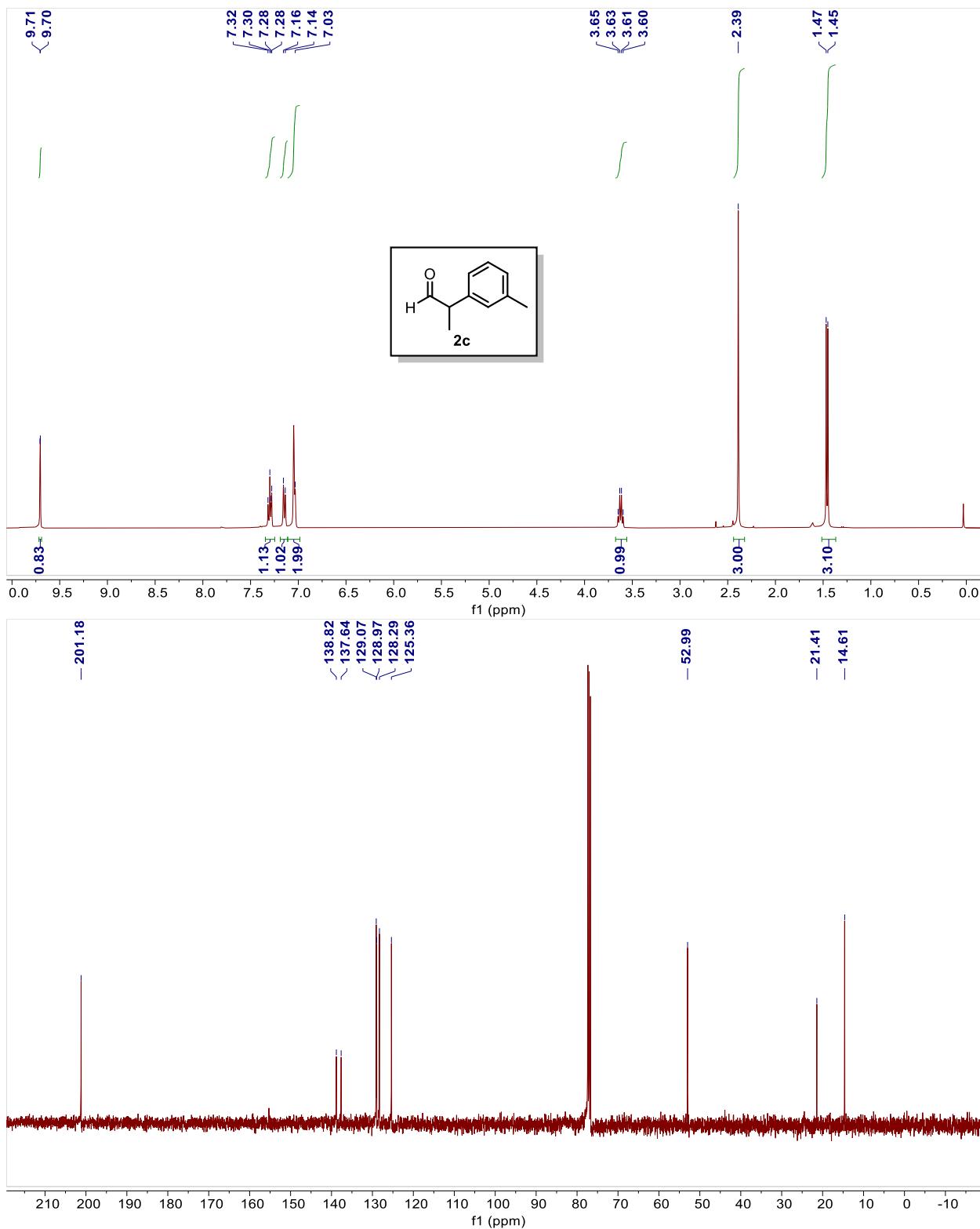
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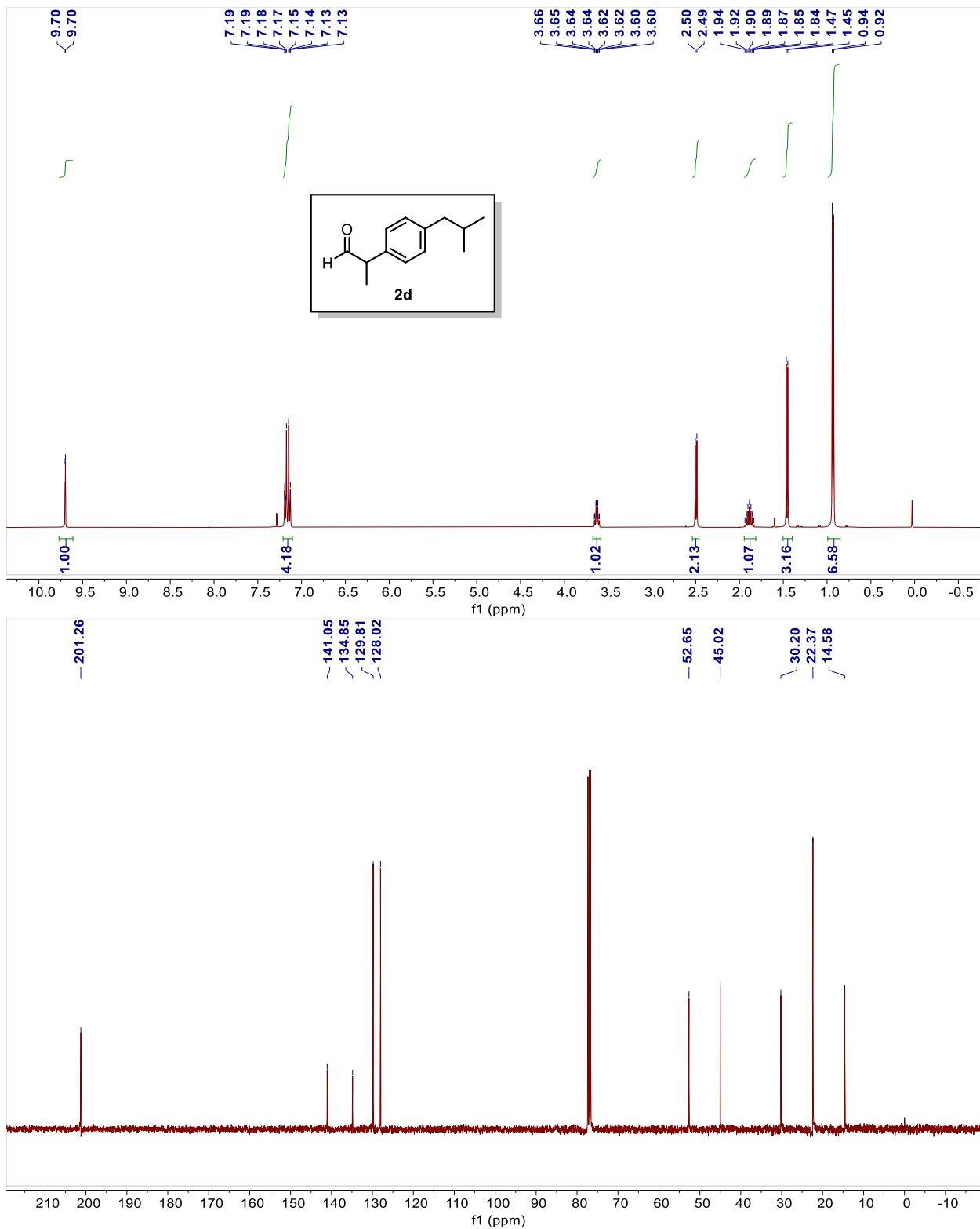
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 H 5.27428500 -2.32764300 -0.39082900
 C 2.11537300 -3.69998600 0.00175900
 H 2.06940400 -3.71842900 1.10228500
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 H 3.45121000 -3.63823200 -2.37510500
 C 2.65027500 -1.24946400 0.06463300
 H 2.52499500 -1.37732900 1.15182500
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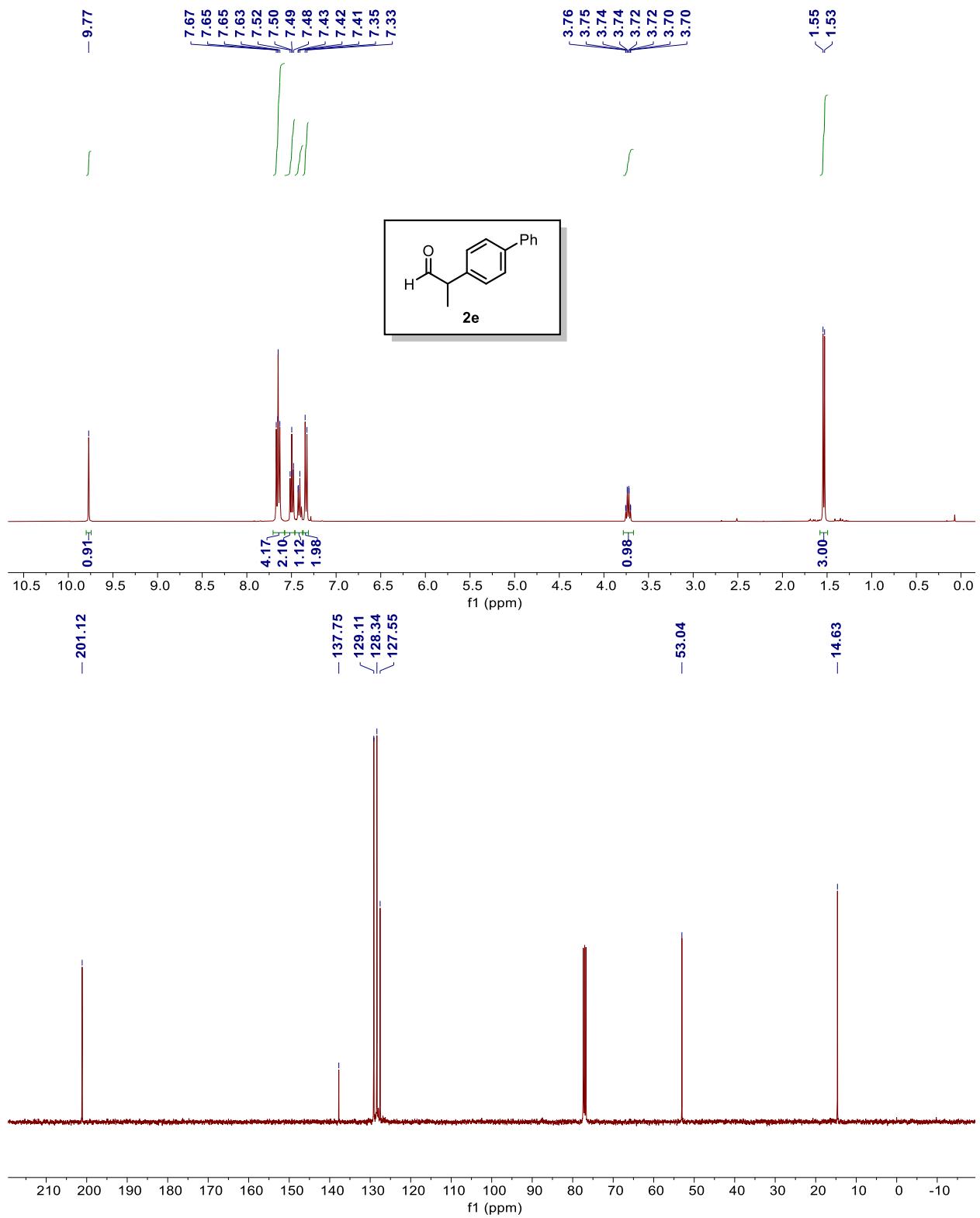
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H	2.23447400	1.22361700	-0.21888900	C	-3.07887700	2.54042300	-0.89718900
N	3.18873700	1.19074900	0.18082400	H	-3.30720600	0.52683200	-1.56014500
C	3.97356100	2.28838400	-0.47400200	C	-1.13087700	3.01036700	0.46259300
H	3.93626000	2.07788000	-1.55023900	H	0.16660400	1.36584500	0.88425600
H	3.42269900	3.21928700	-0.29597800	C	-2.30534500	3.45790800	-0.17225000
C	3.02114500	1.34365100	1.66398500	H	-3.99581000	2.85440900	-1.39567900
H	2.27619700	0.59287300	1.95795100	H	-0.54272000	3.73348400	1.03104600
H	3.98042400	1.07248200	2.12414700	H	0.25413900	-1.17414600	1.28749000
C	2.56394500	2.72781500	2.07397600	O	-2.60640100	4.76243400	-0.02973700
H	3.35000300	3.48354100	1.94488700	C	-3.77938000	5.25194500	-0.64251900
H	1.67317600	3.03811400	1.50839200	H	-3.82982200	6.32225700	-0.41252600
H	2.29564000	2.70001800	3.13846400	H	-3.74690300	5.11967900	-1.73578200
C	5.40134800	2.38328500	0.01991300	H	-4.67813500	4.75379700	-0.24509000
H	5.96948800	1.46514500	-0.18237900	C	-3.01404100	-2.23154700	-0.28922900
H	5.89486500	3.20571100	-0.51516200	C	-4.36239600	-2.01607600	-0.59336700
H	5.45317800	2.60635400	1.09487400	C	-2.69527900	-2.96185400	0.86534000
H	1.31402500	-0.74016300	-1.46470600	C	-5.37105700	-2.51188400	0.23627600
C	0.17786700	-1.07252200	0.19847500	H	-4.62555600	-1.45595400	-1.49439600
C	-1.07212700	-0.63669400	-0.45046900	C	-3.69924300	-3.45779900	1.69484900
C	-1.90904800	-1.67130500	-1.16874500	H	-1.64502600	-3.14520400	1.10891100
H	-1.24824600	-2.49538600	-1.47819000	C	-5.04281100	-3.23197100	1.38405500
H	-2.35897400	-1.25447400	-2.08206100	H	-6.41796600	-2.33383000	-0.01757000
C	-1.49906500	0.73246100	-0.36582500	H	-3.43347800	-4.02797900	2.58732200
C	-2.67936600	1.21047500	-0.98800400	H	-5.82899900	-3.61995800	2.03425500

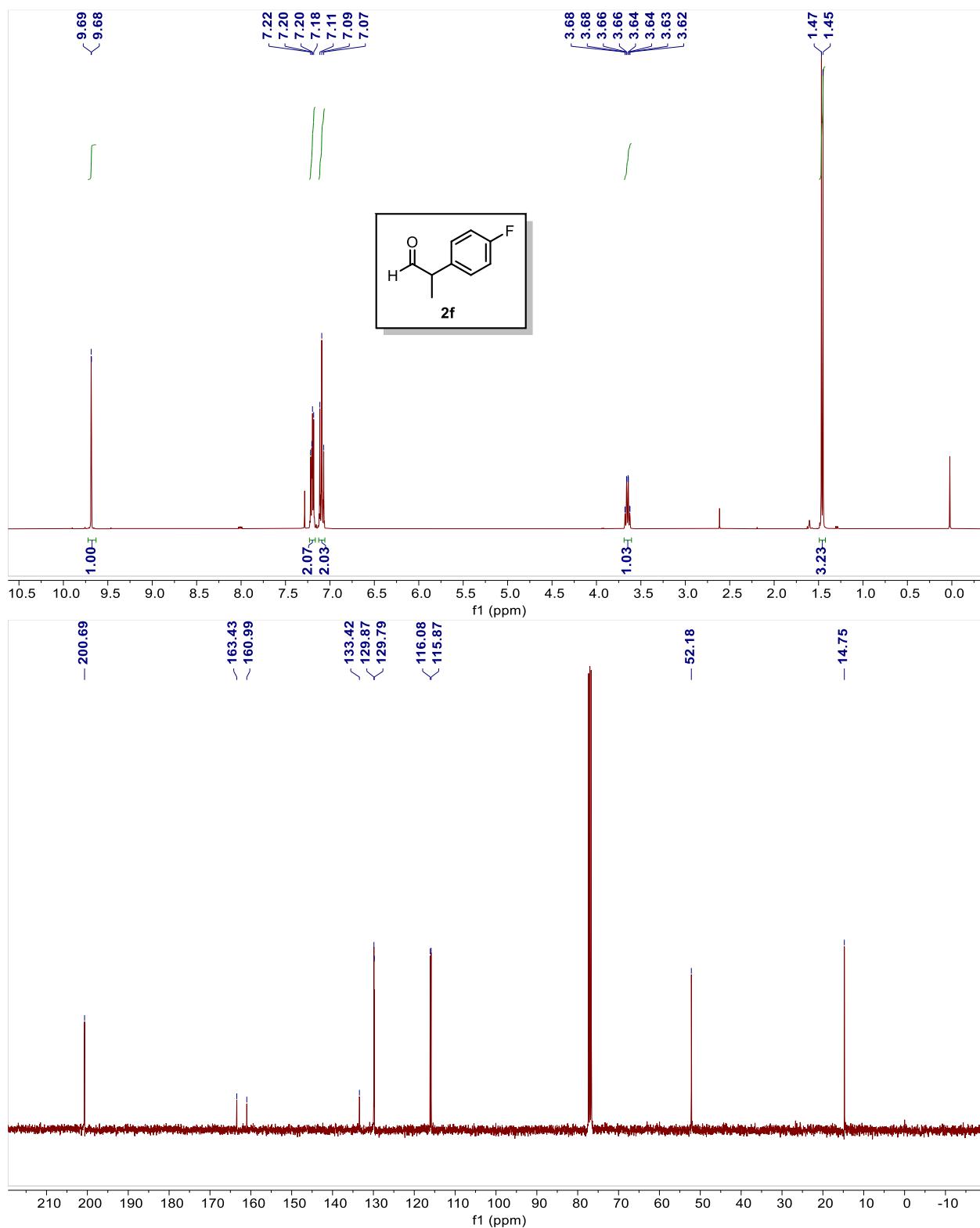
8. NMR spectra

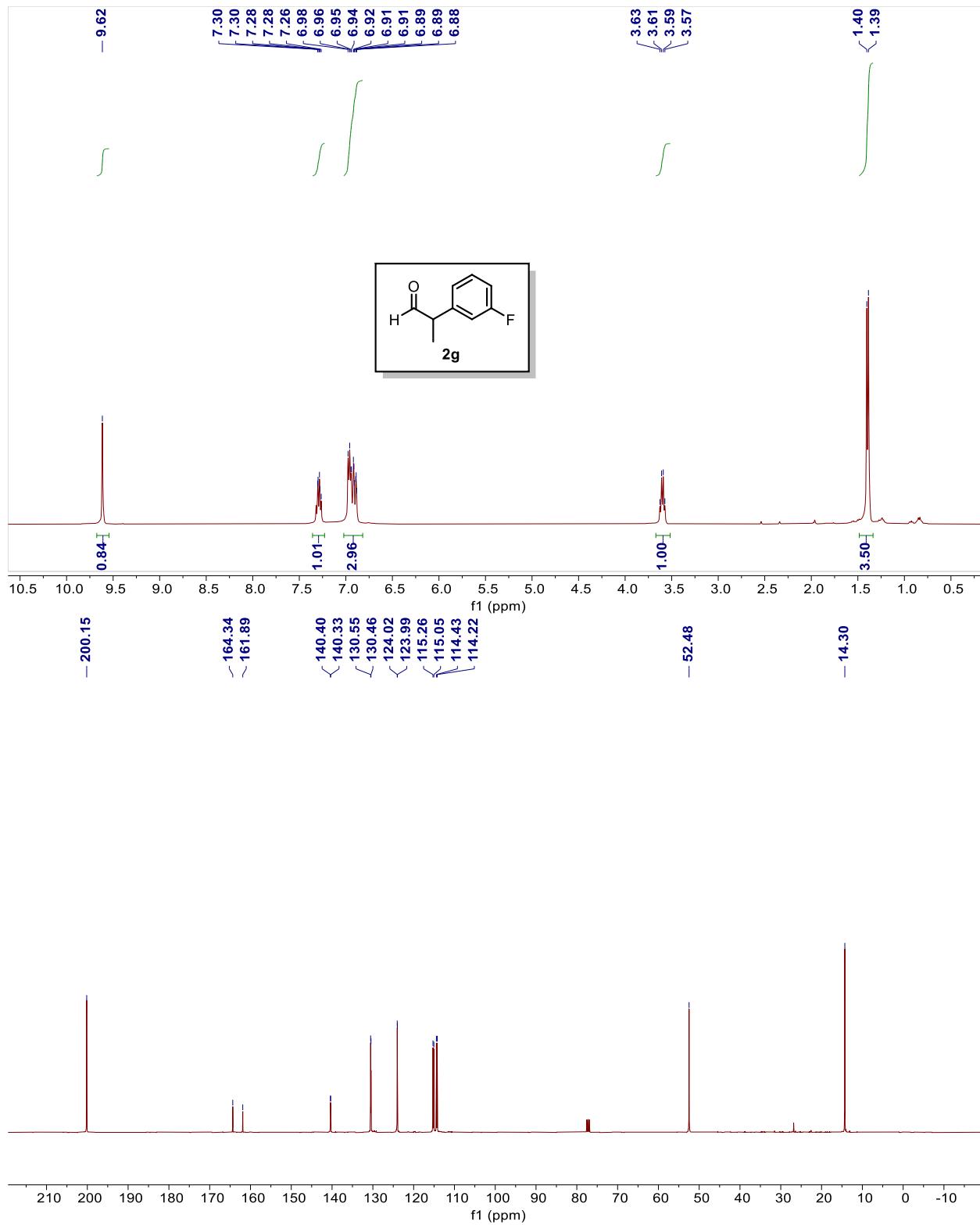


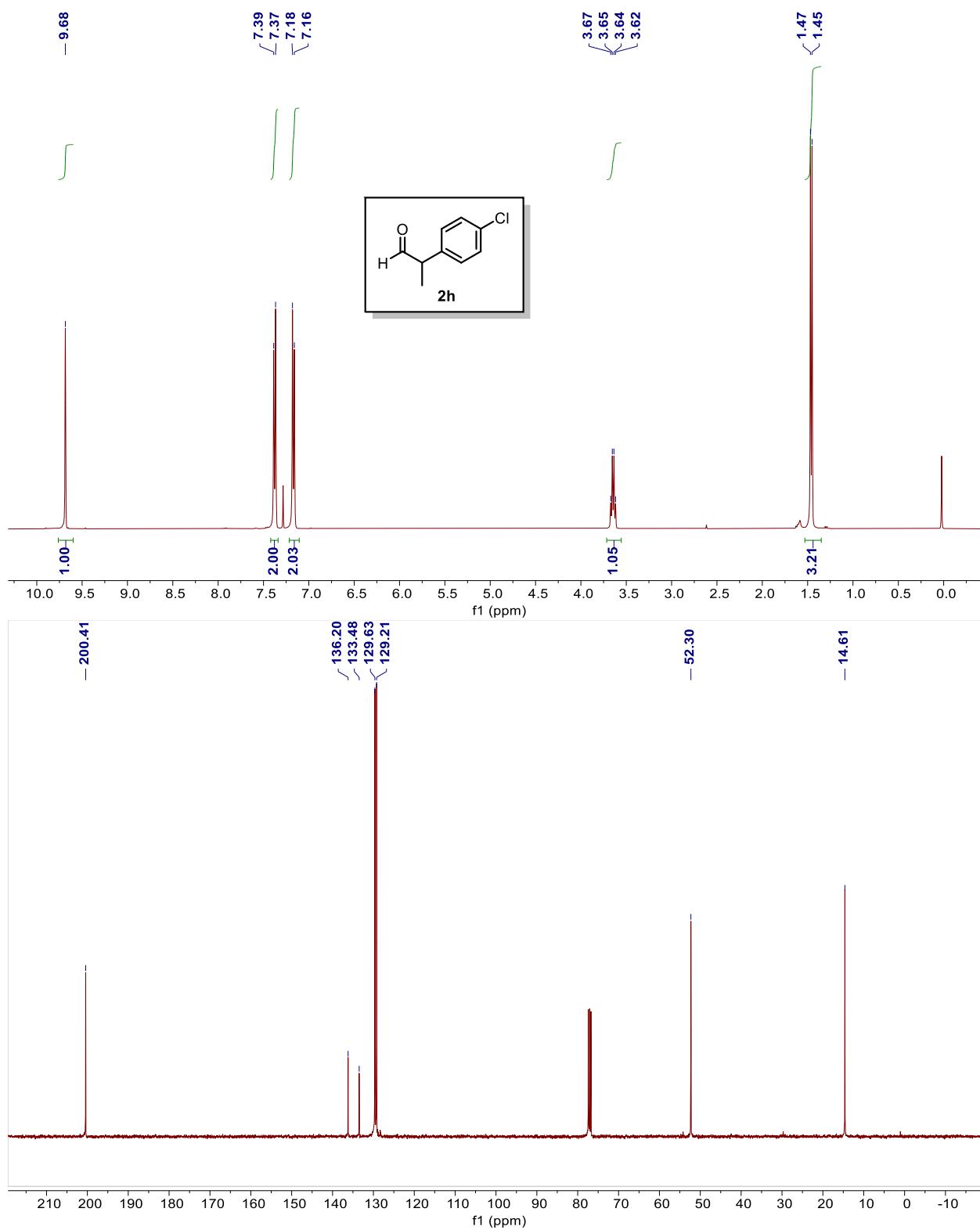


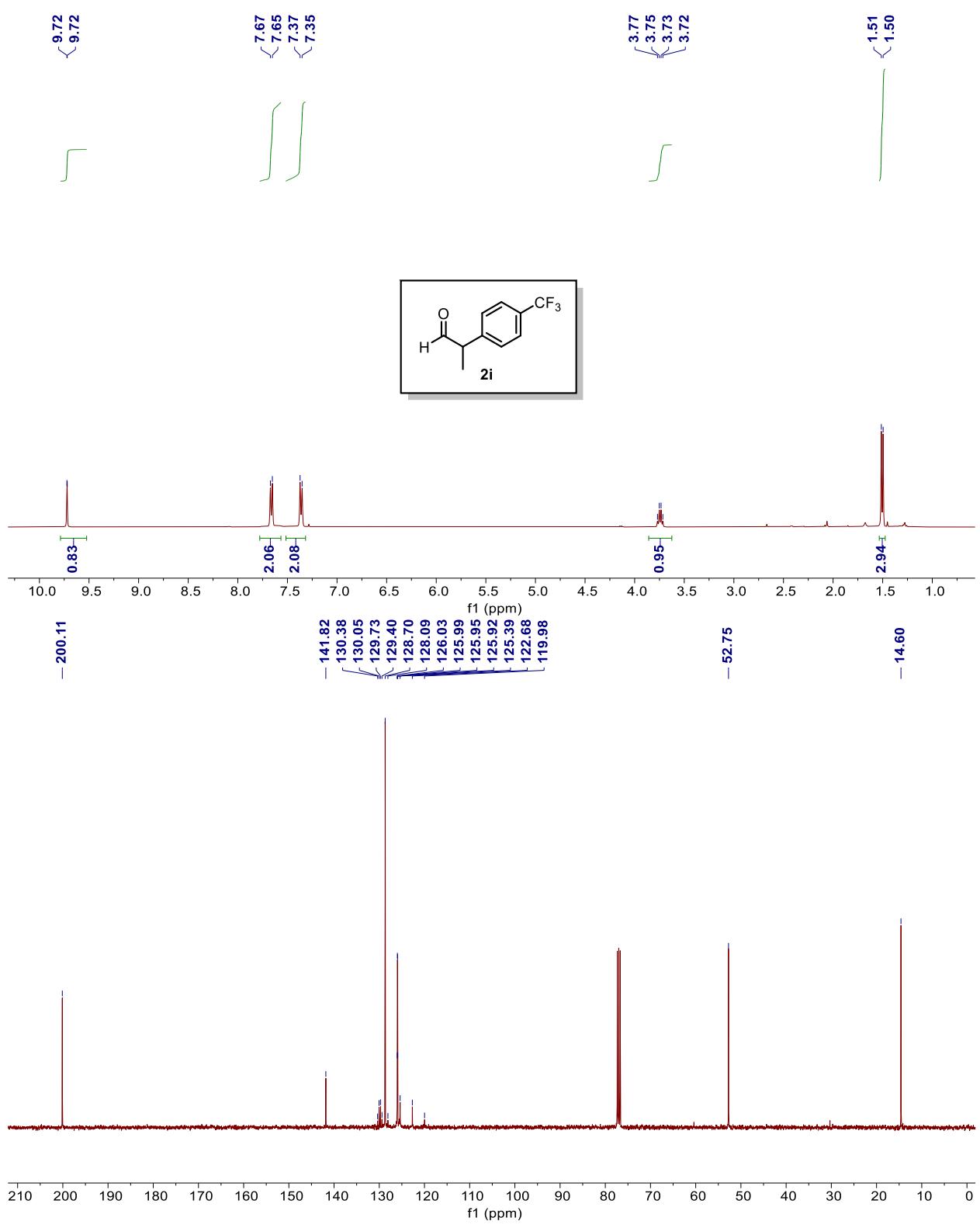


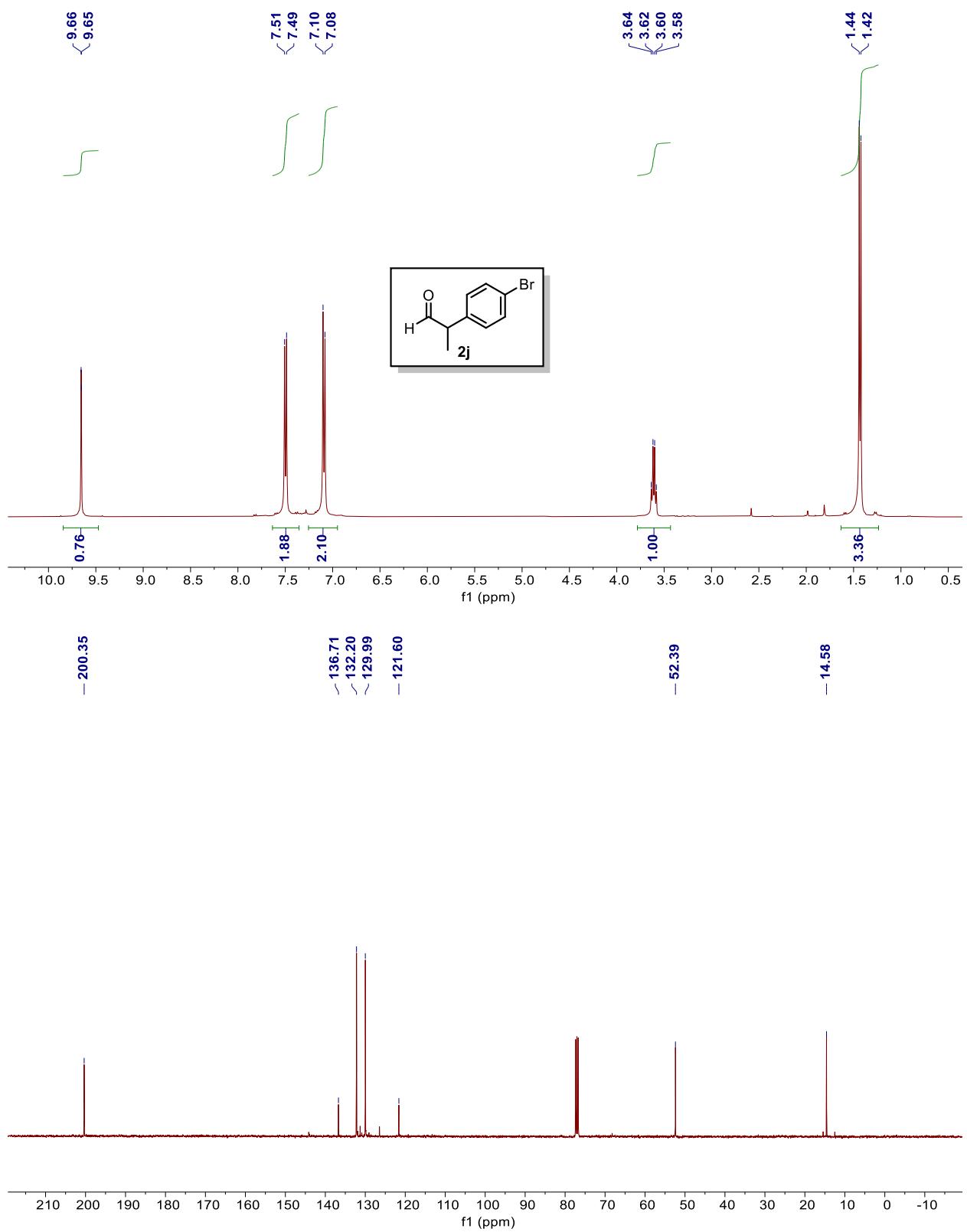


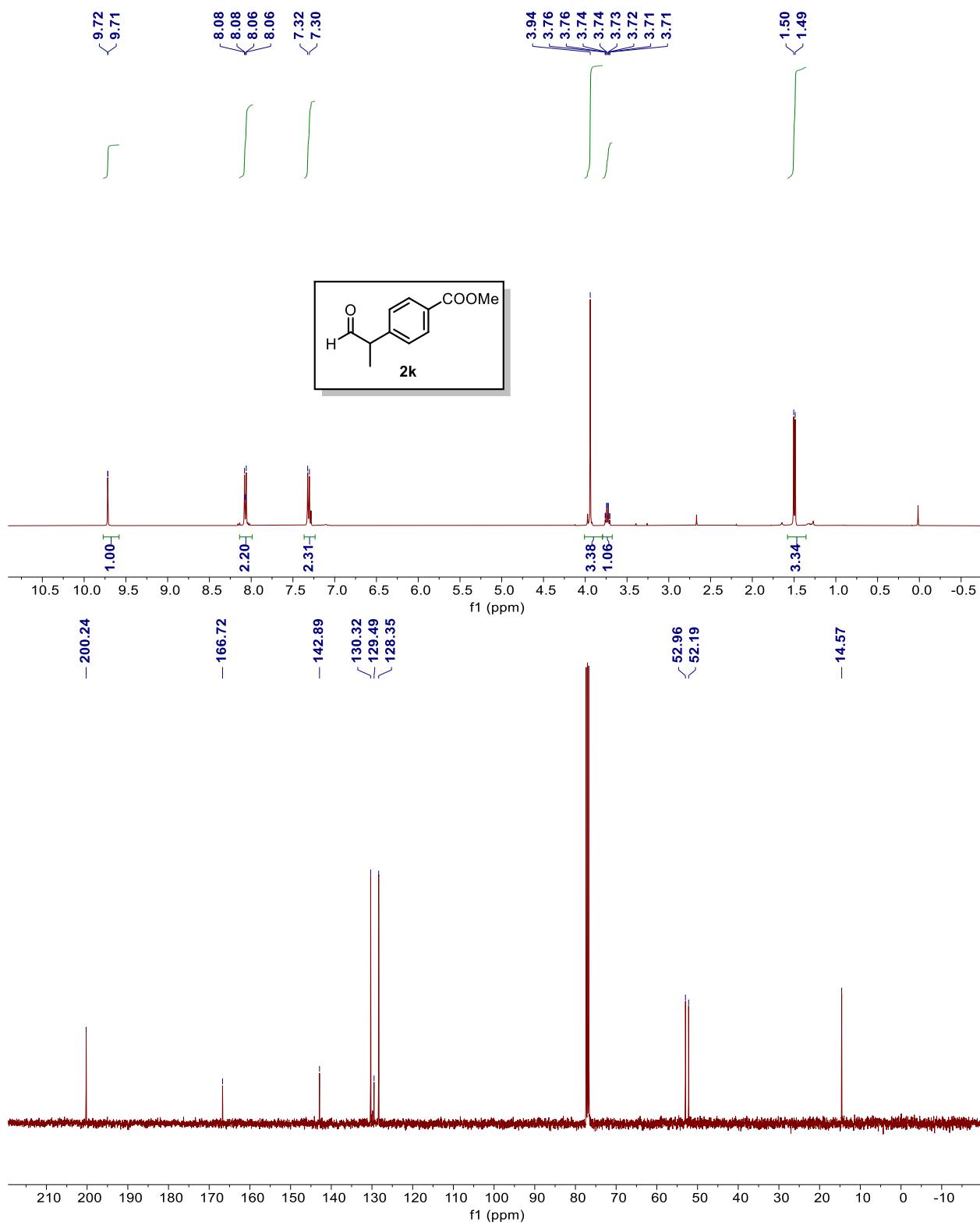


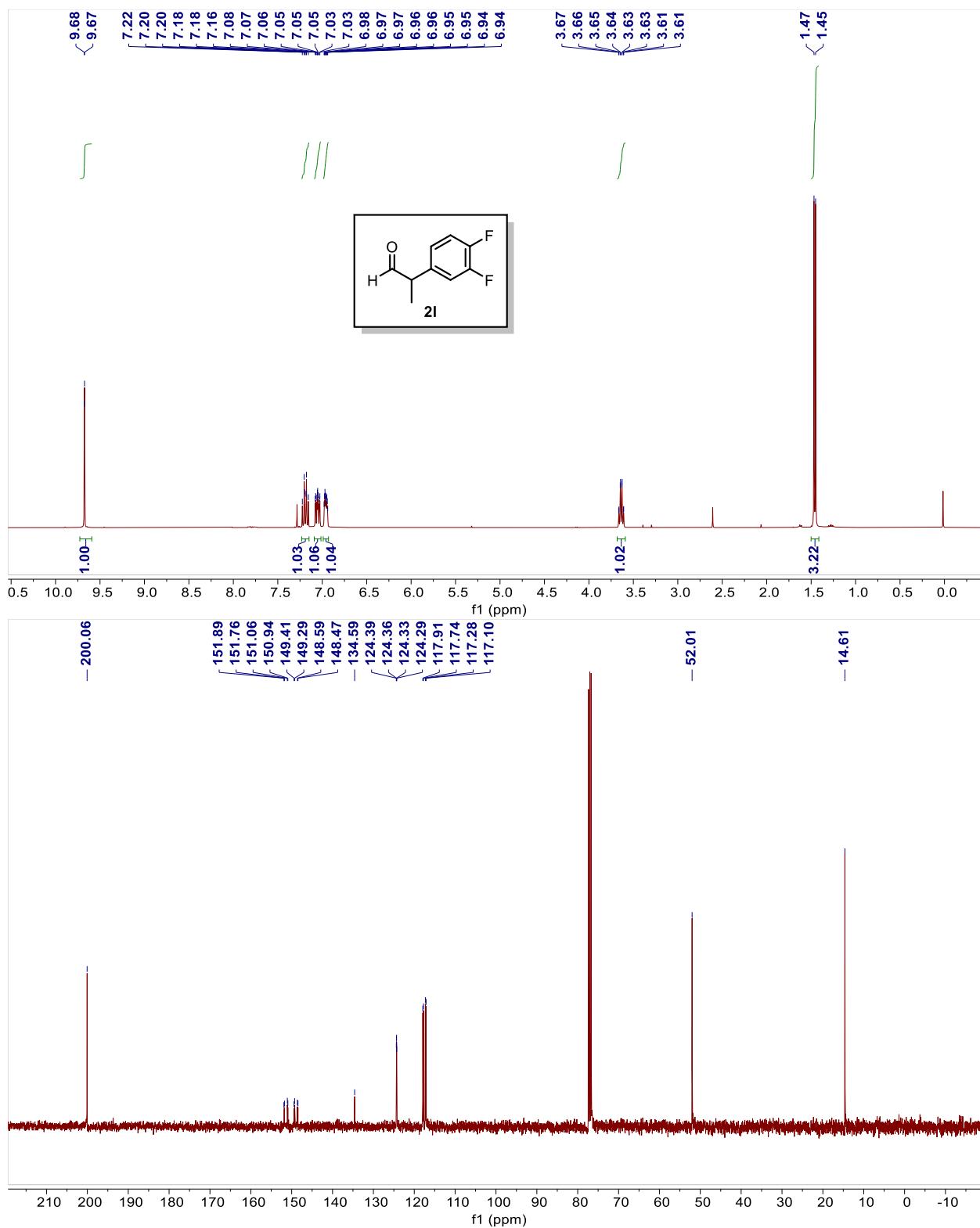


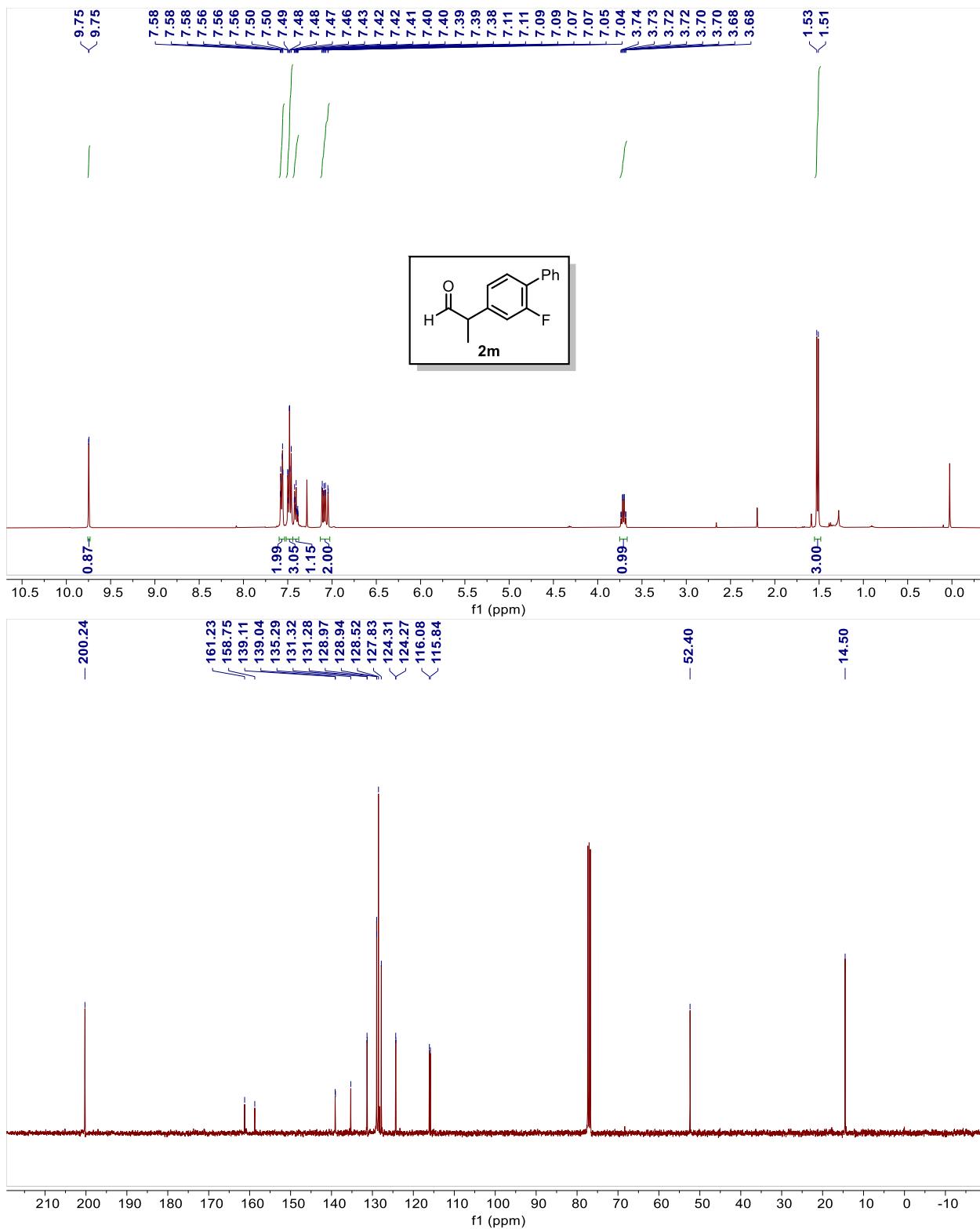


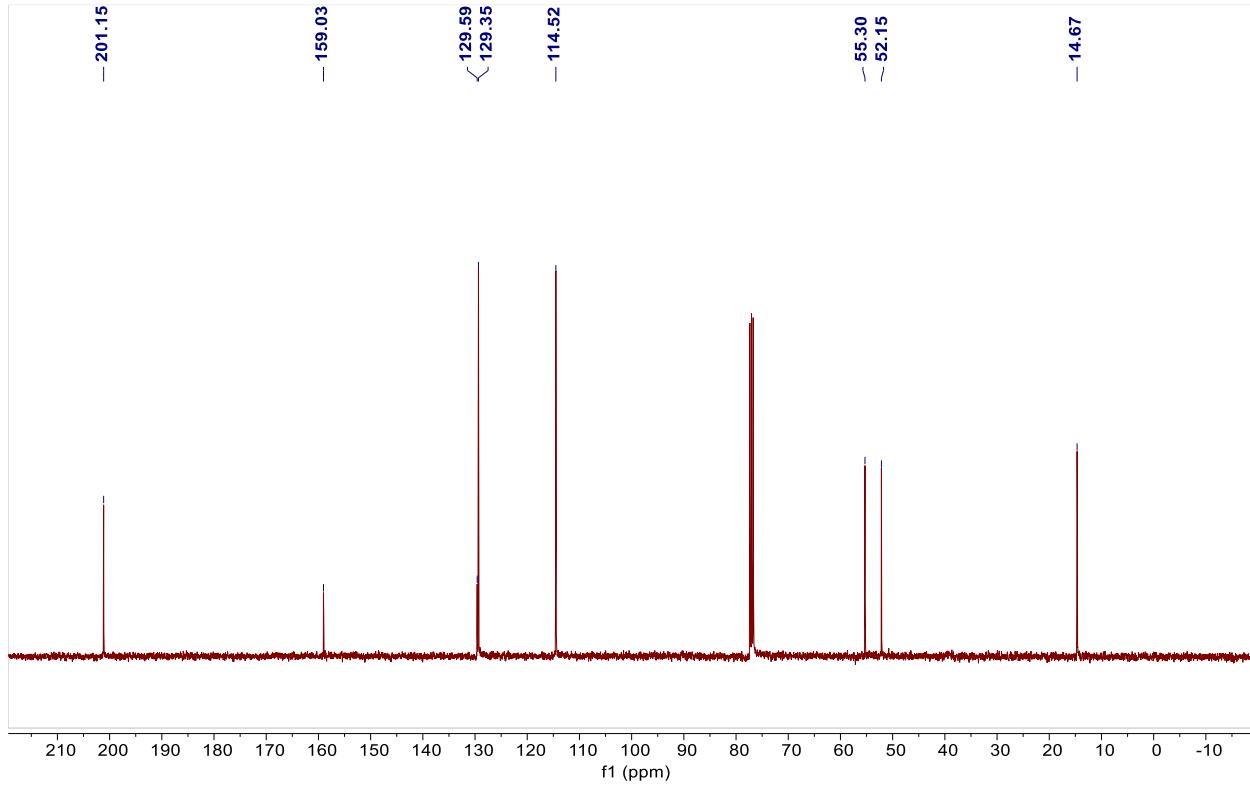
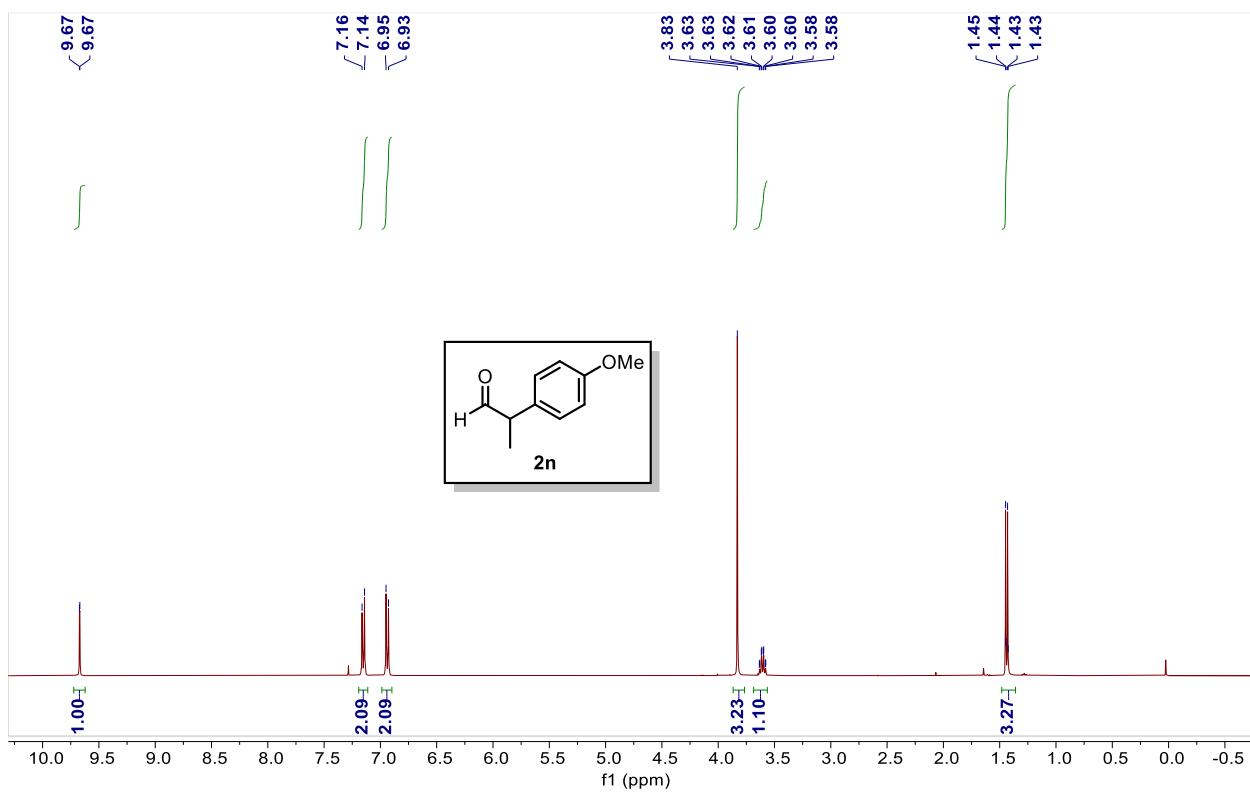


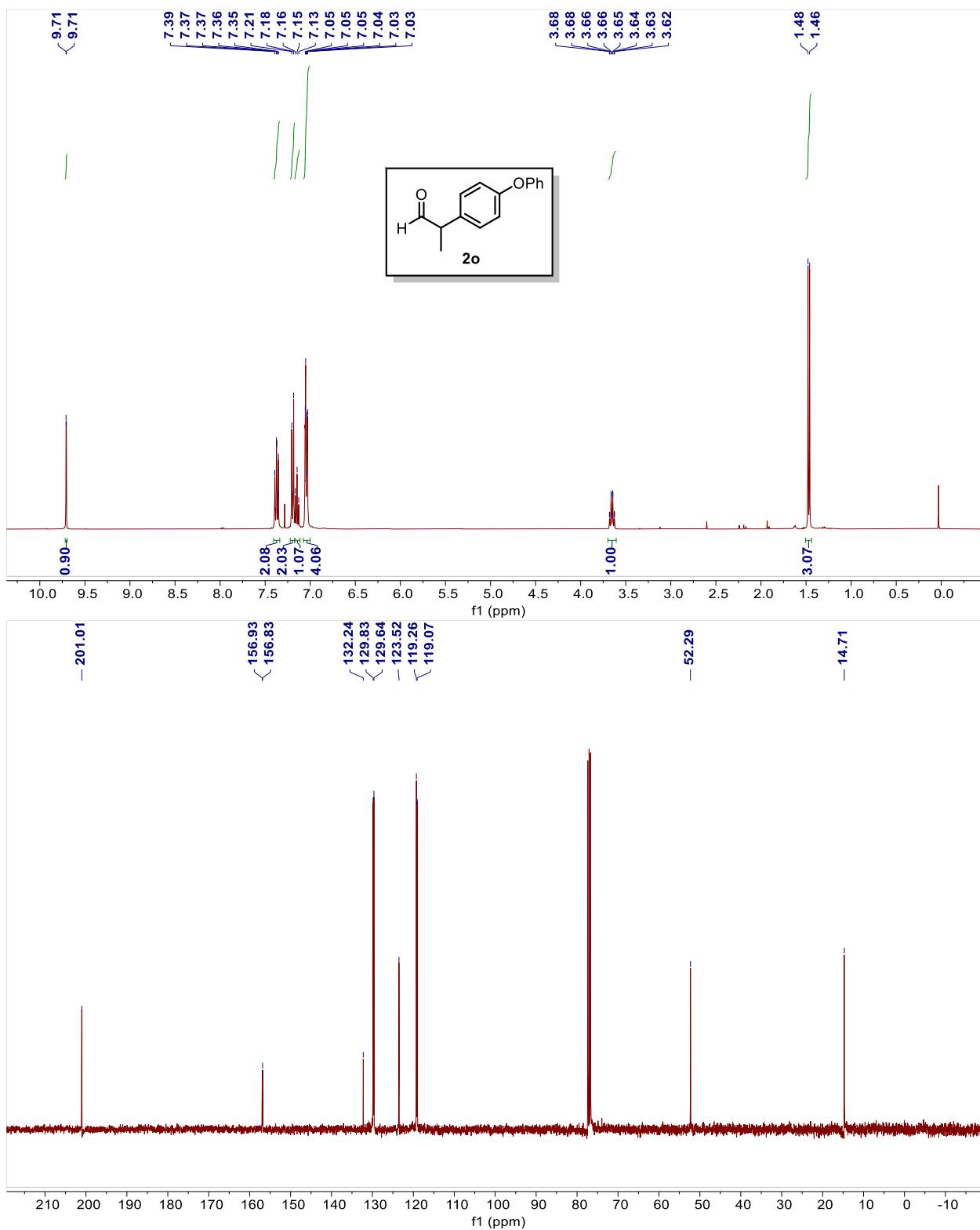


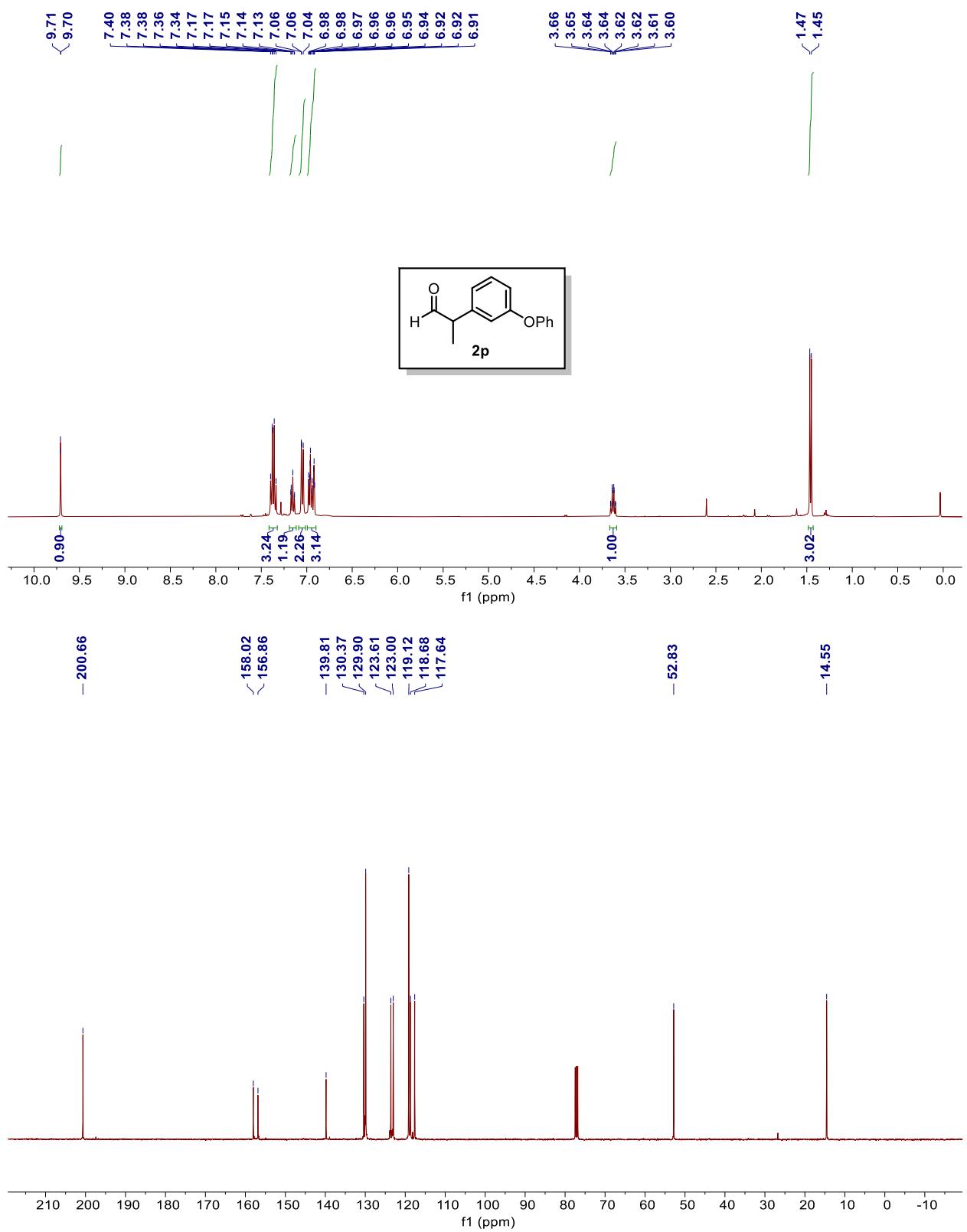


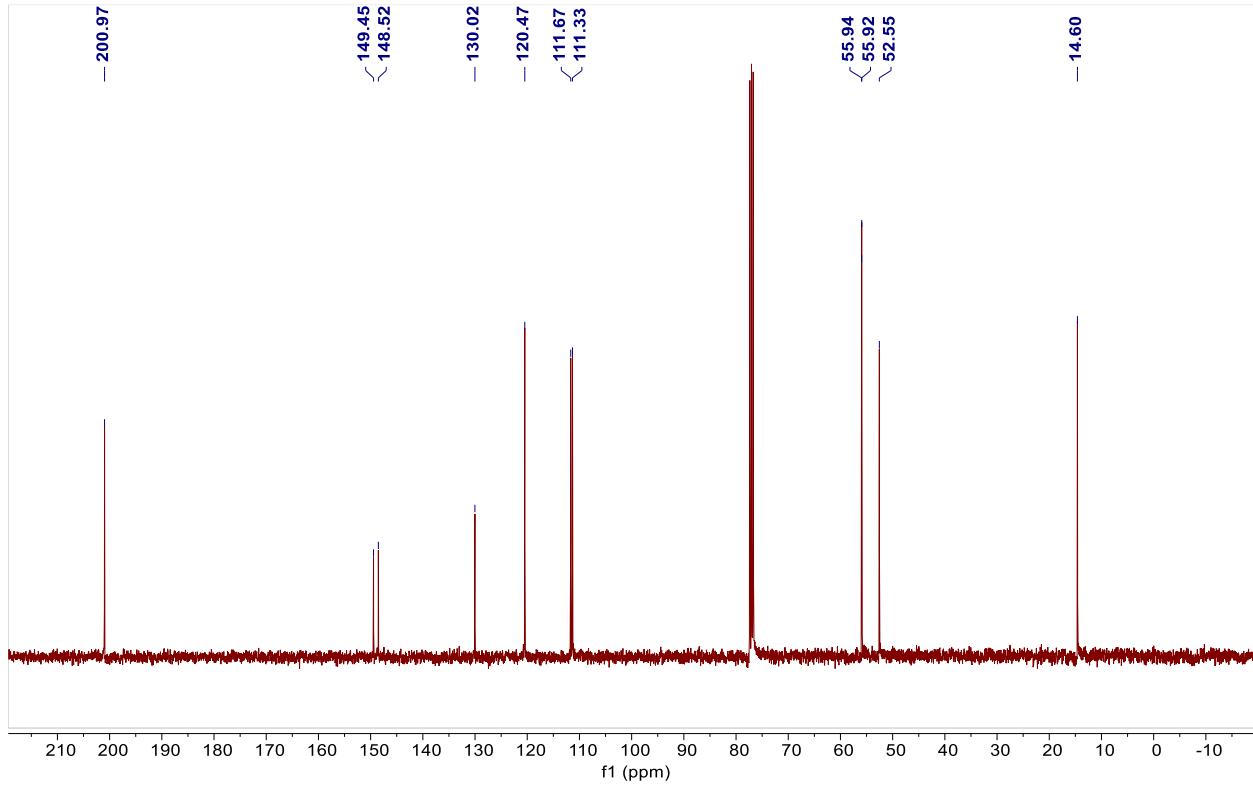
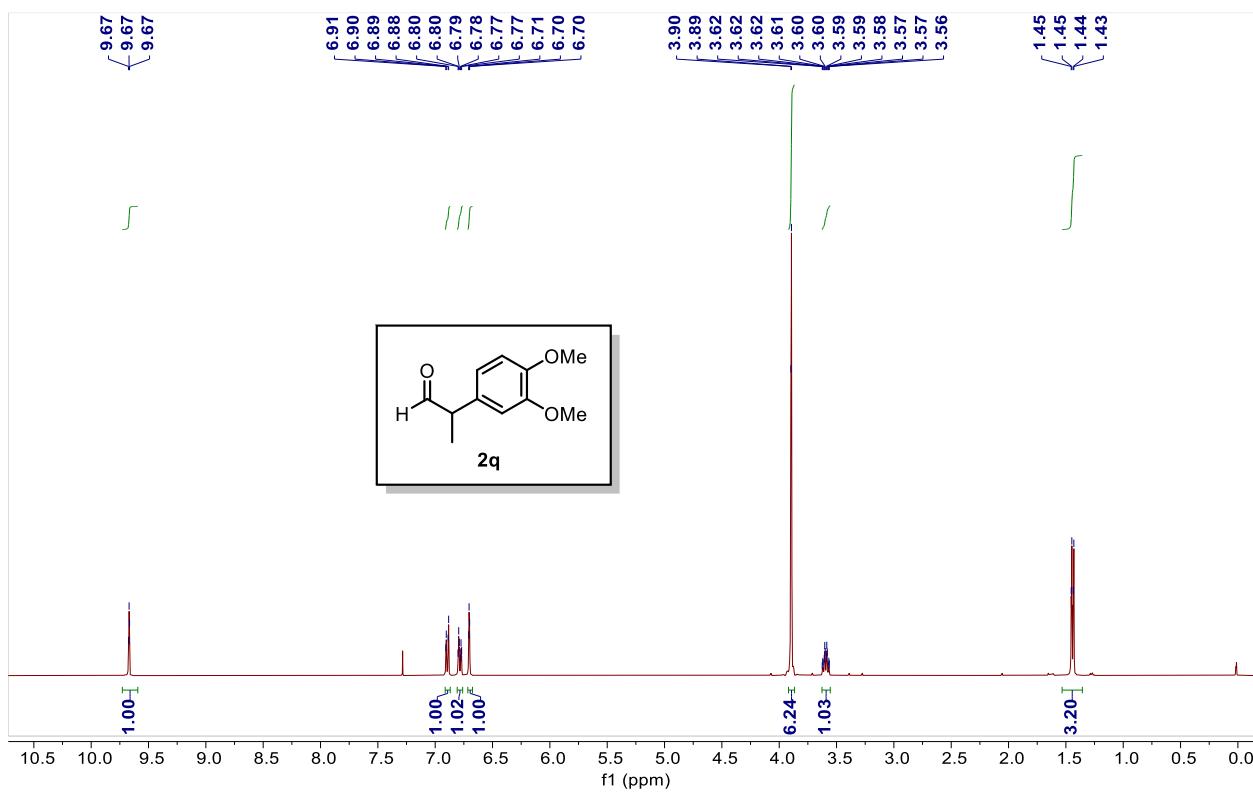


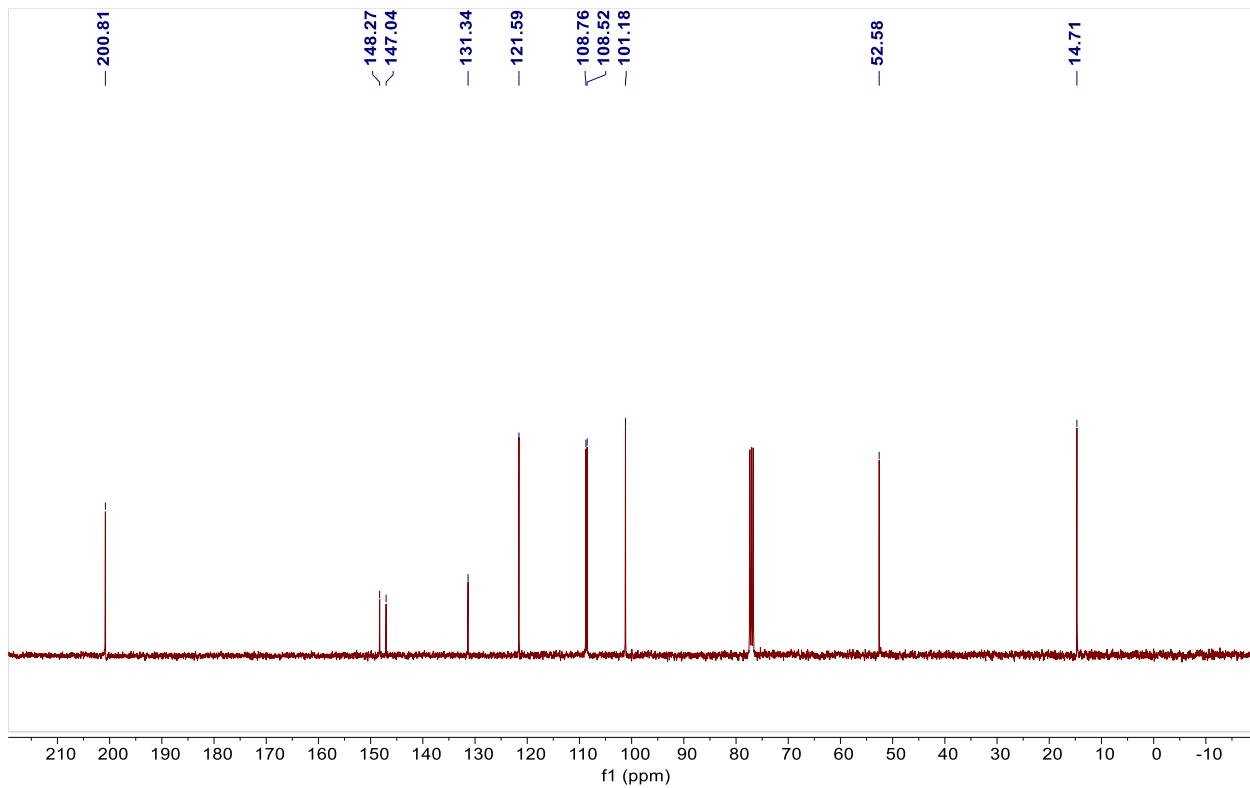
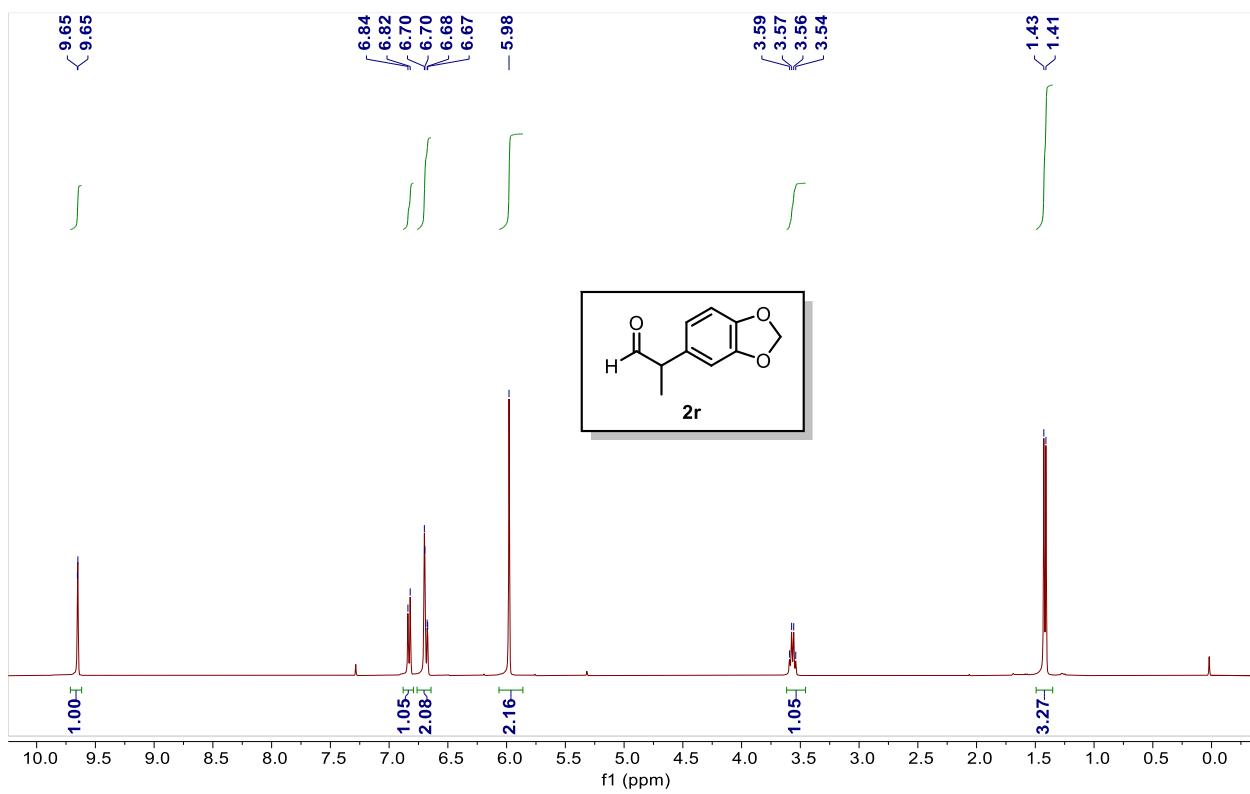


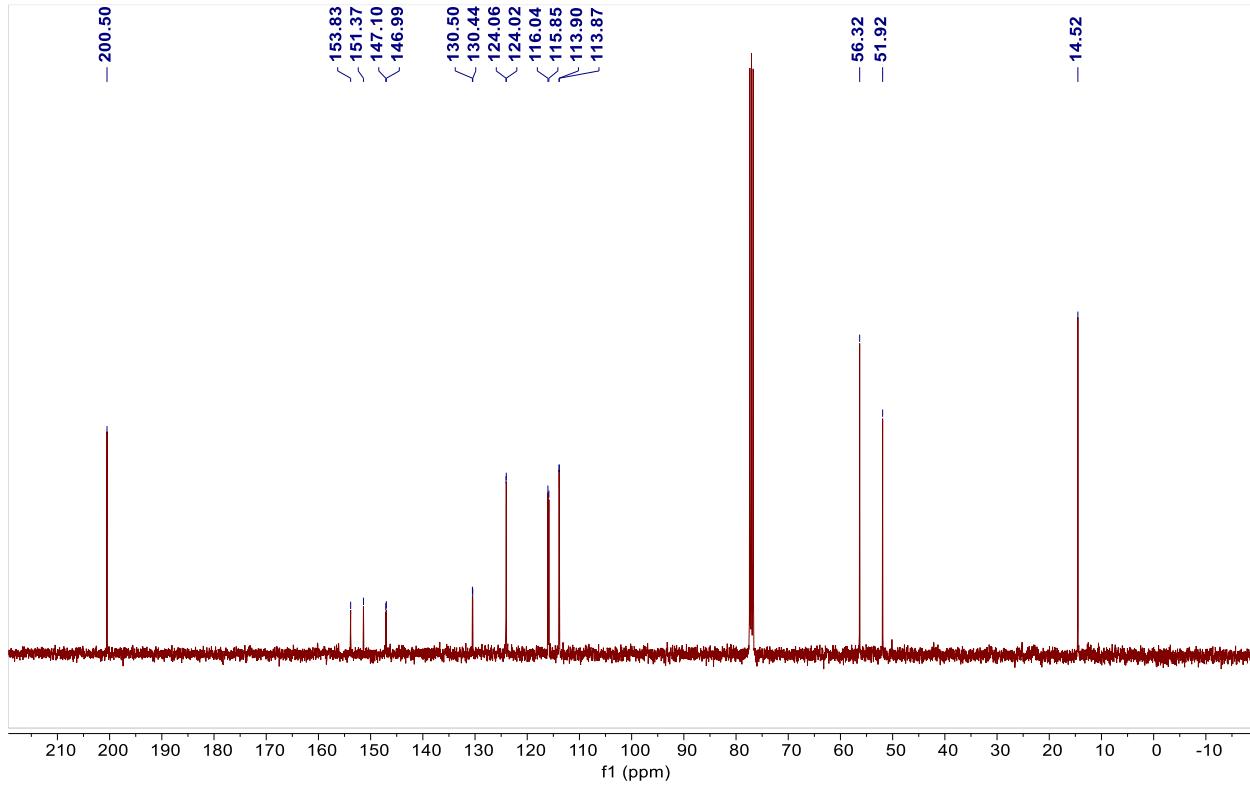
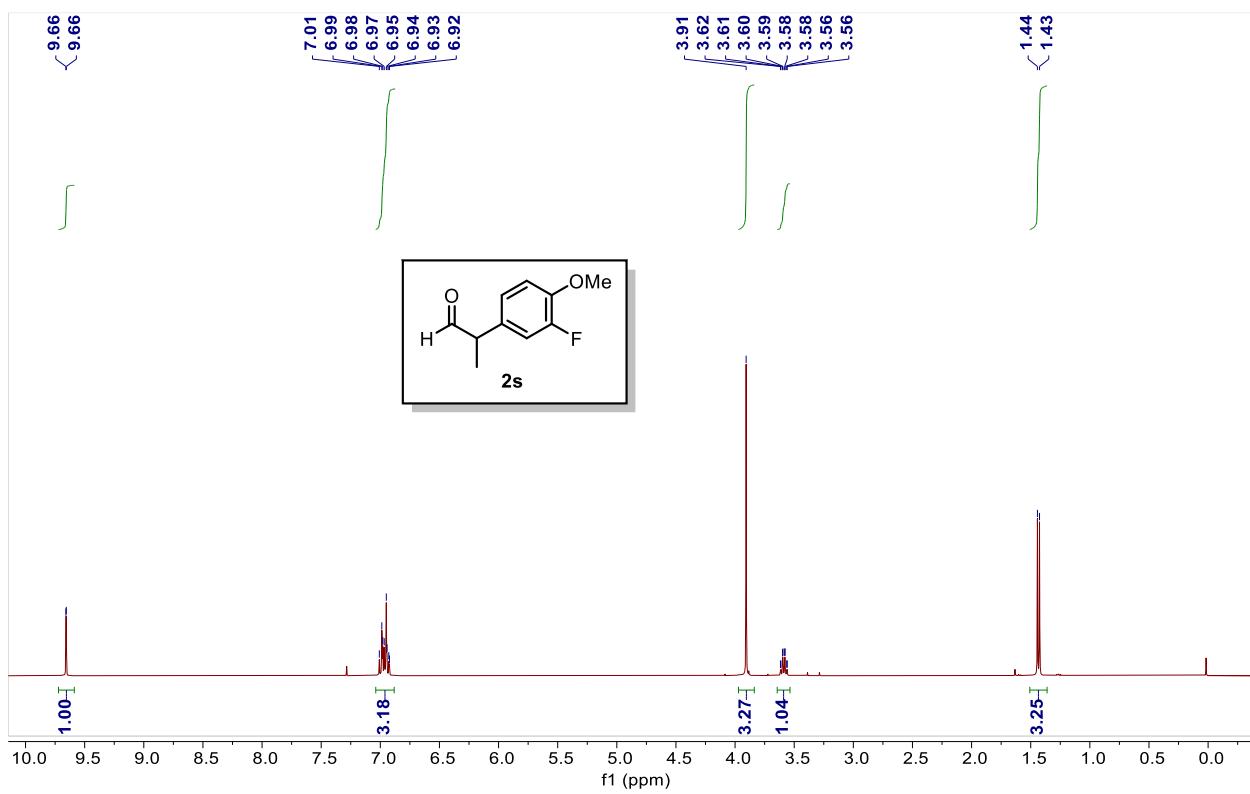


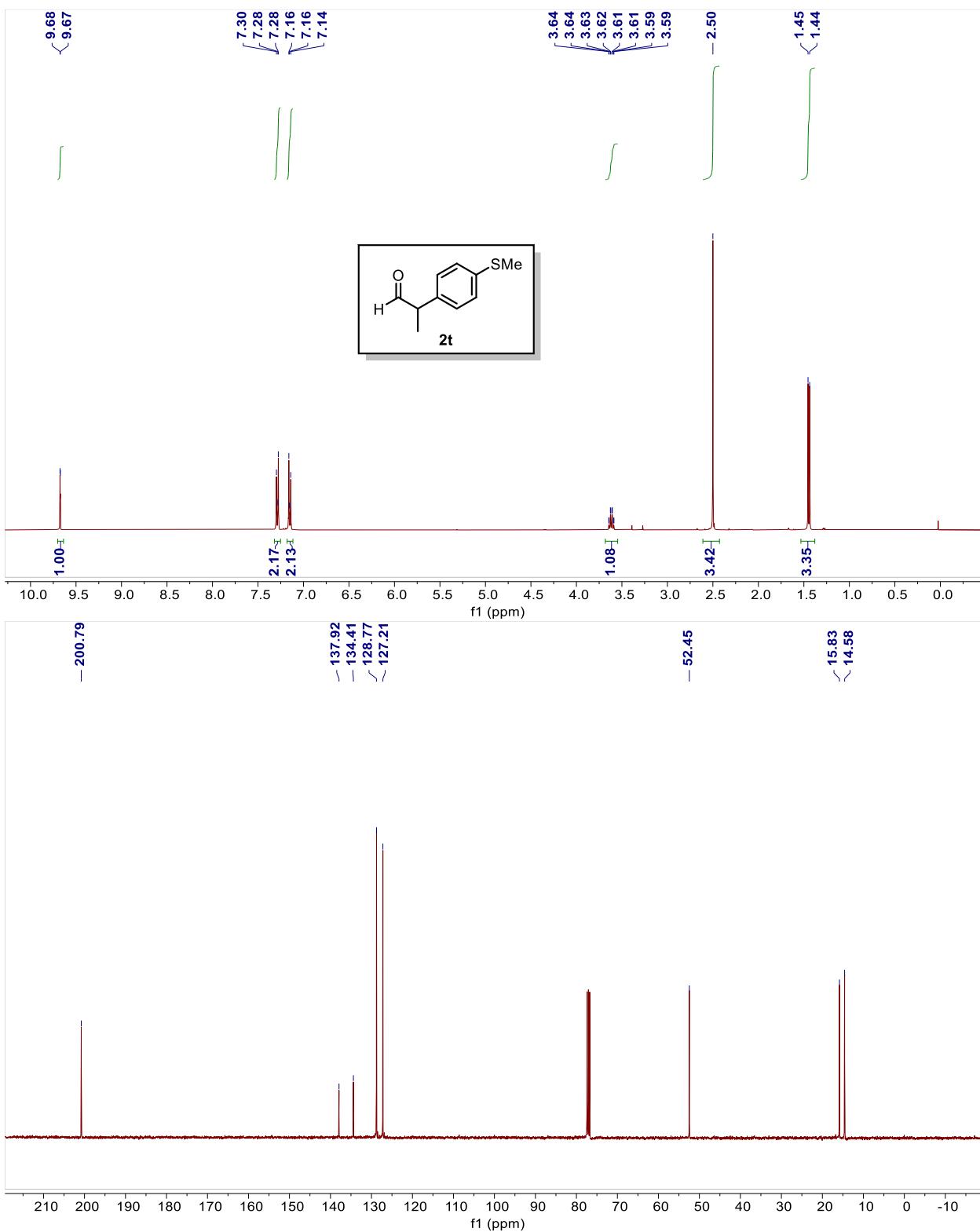


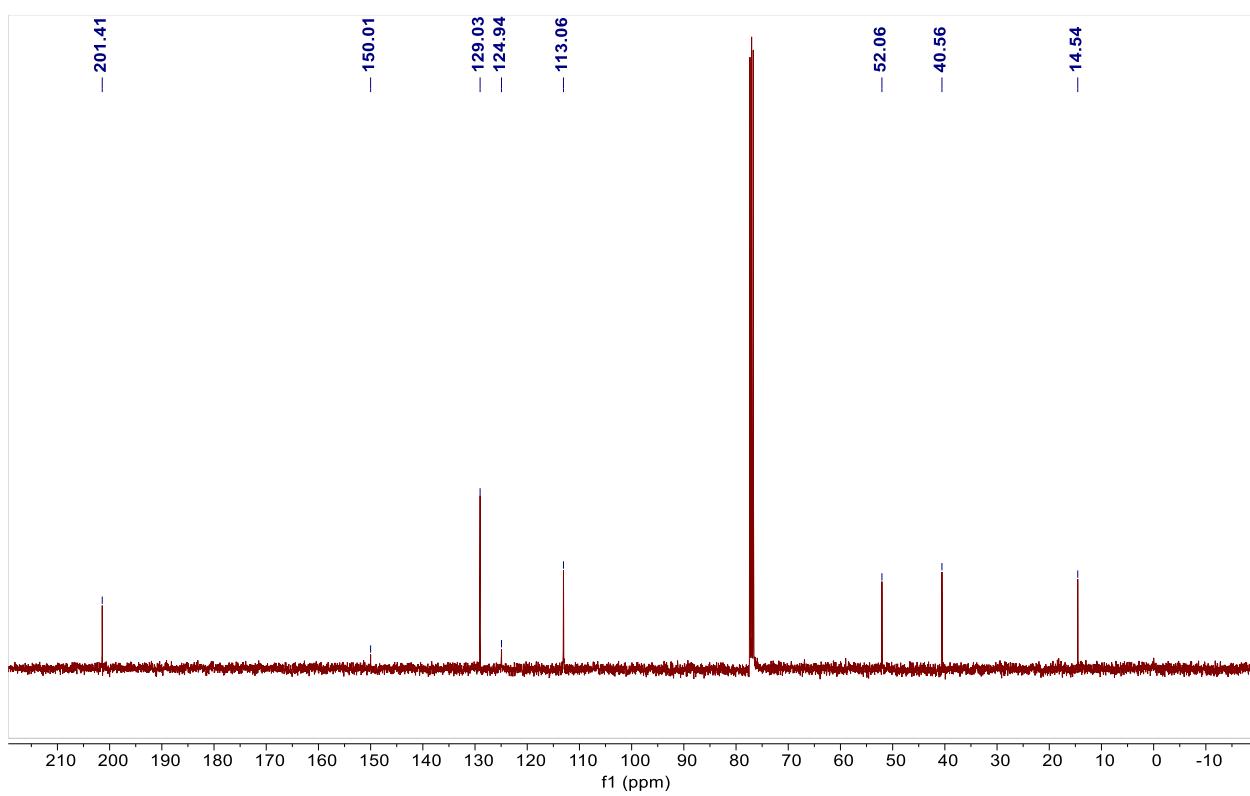
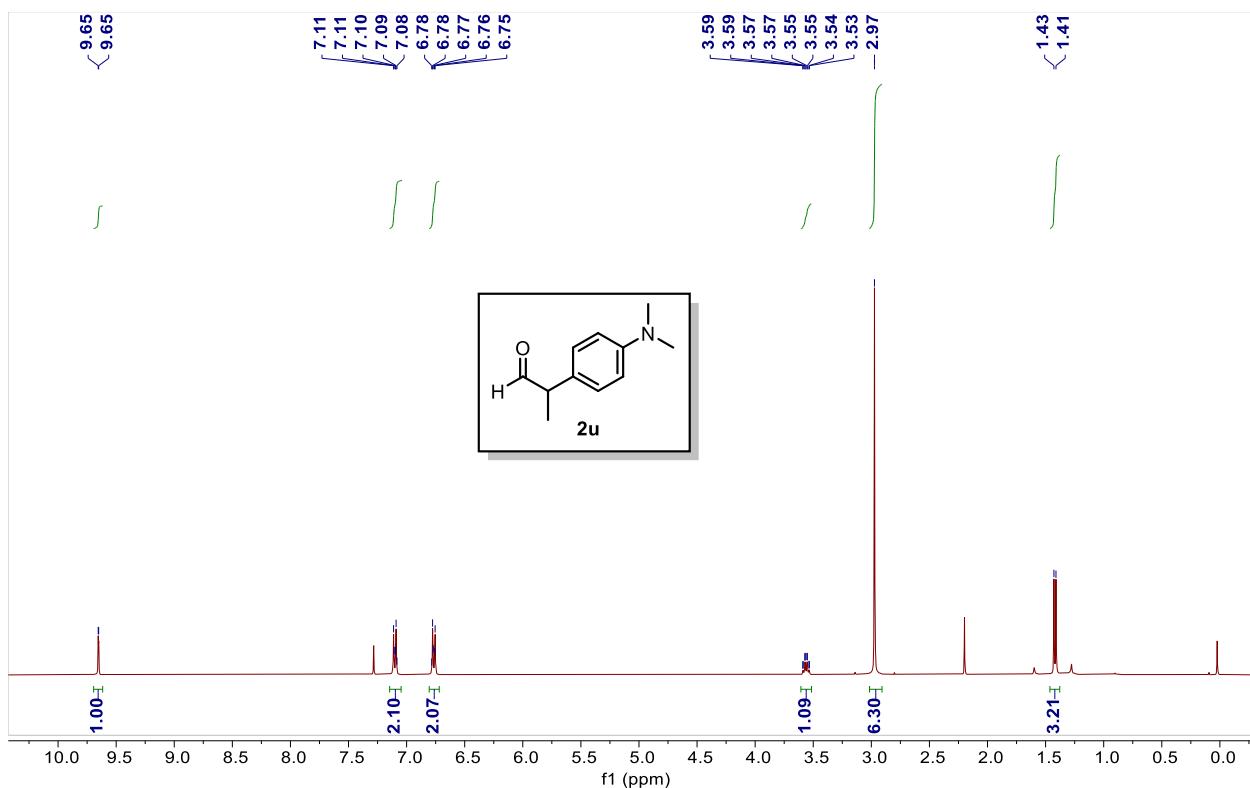


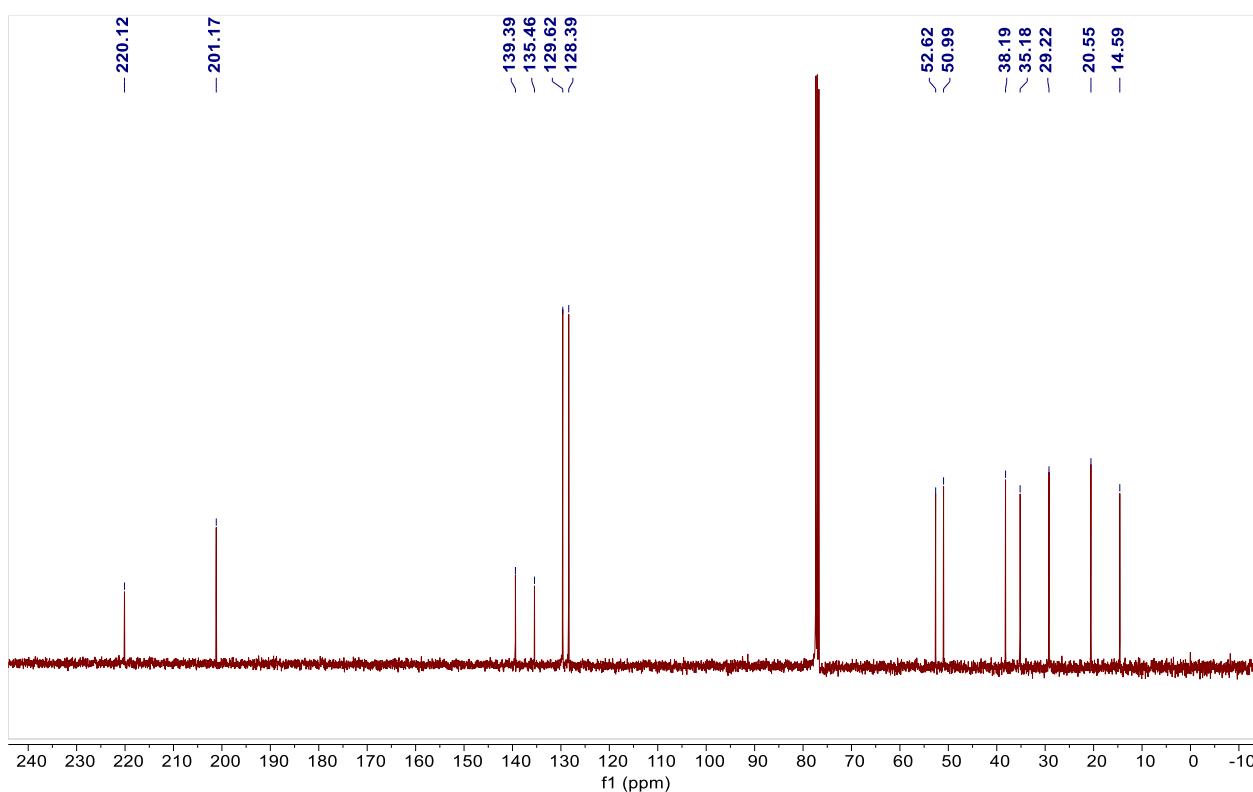
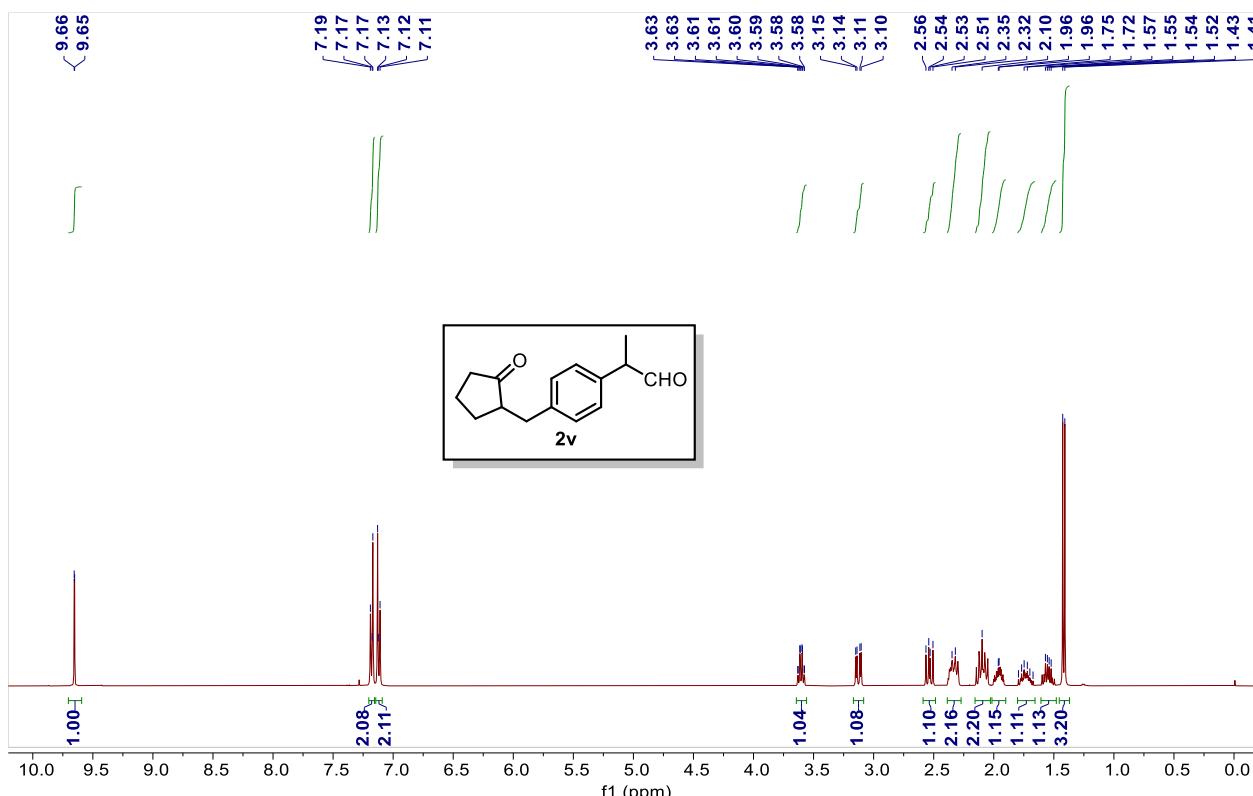


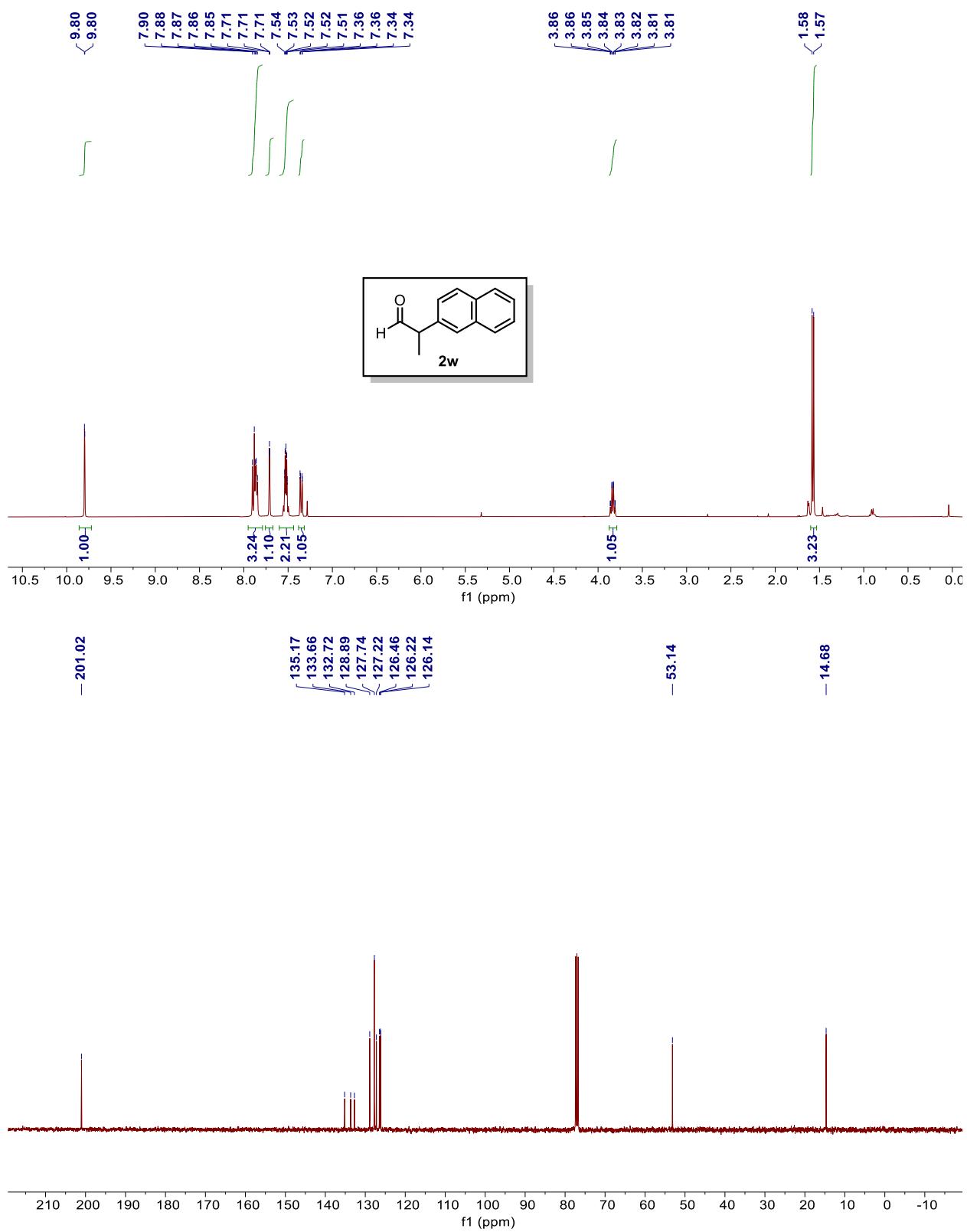


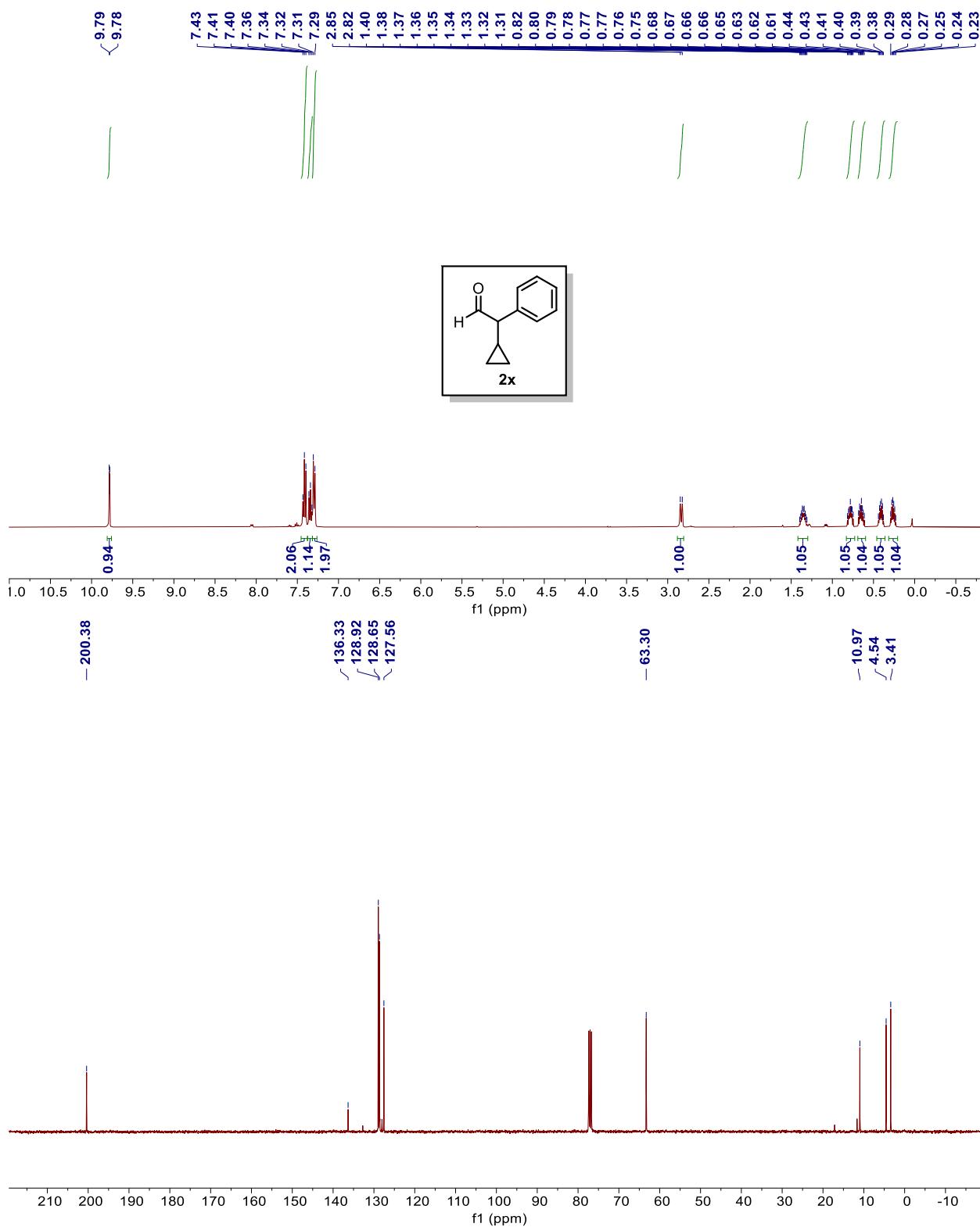


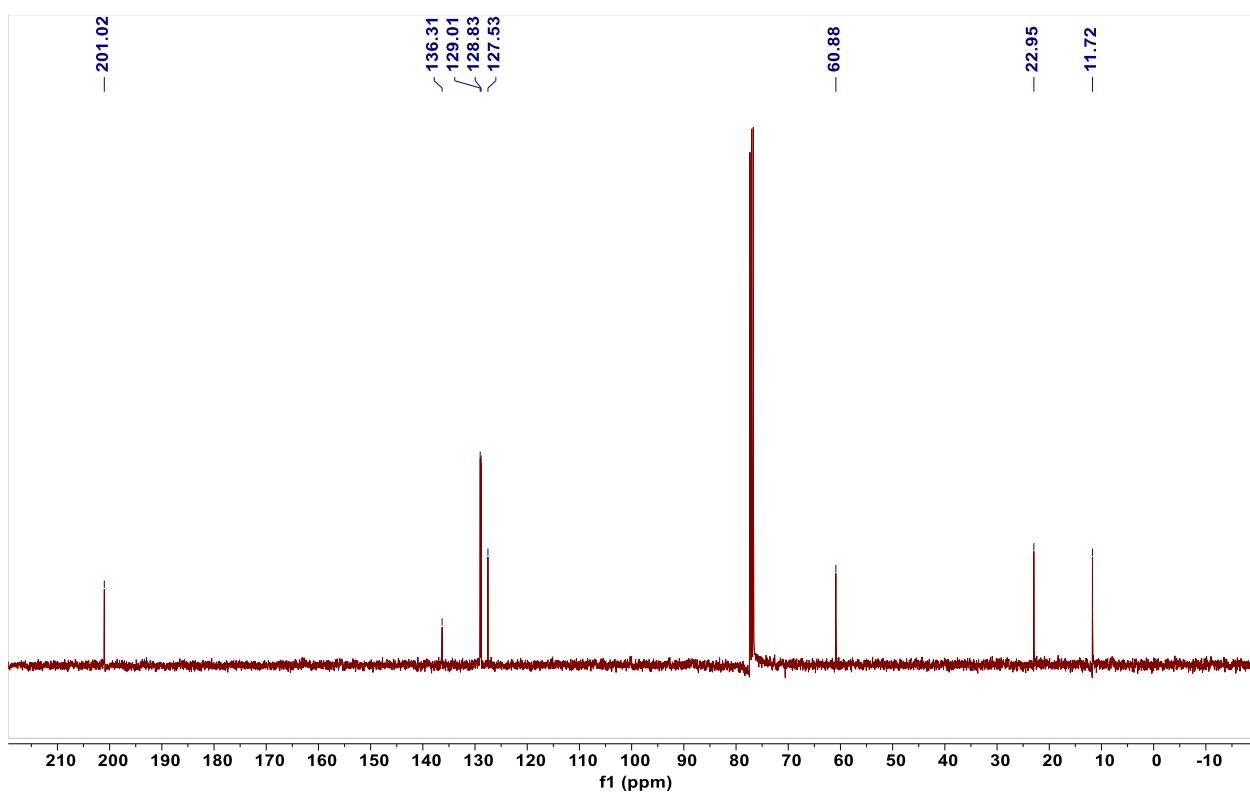
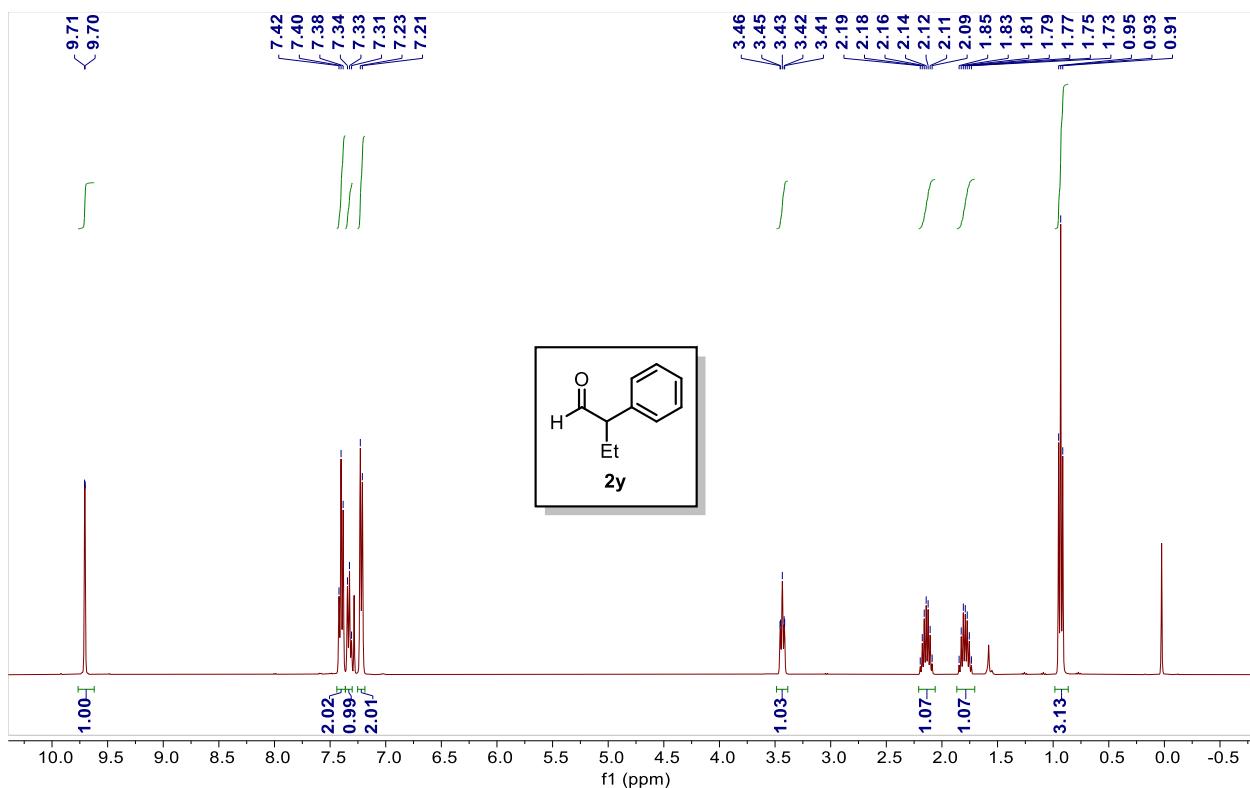


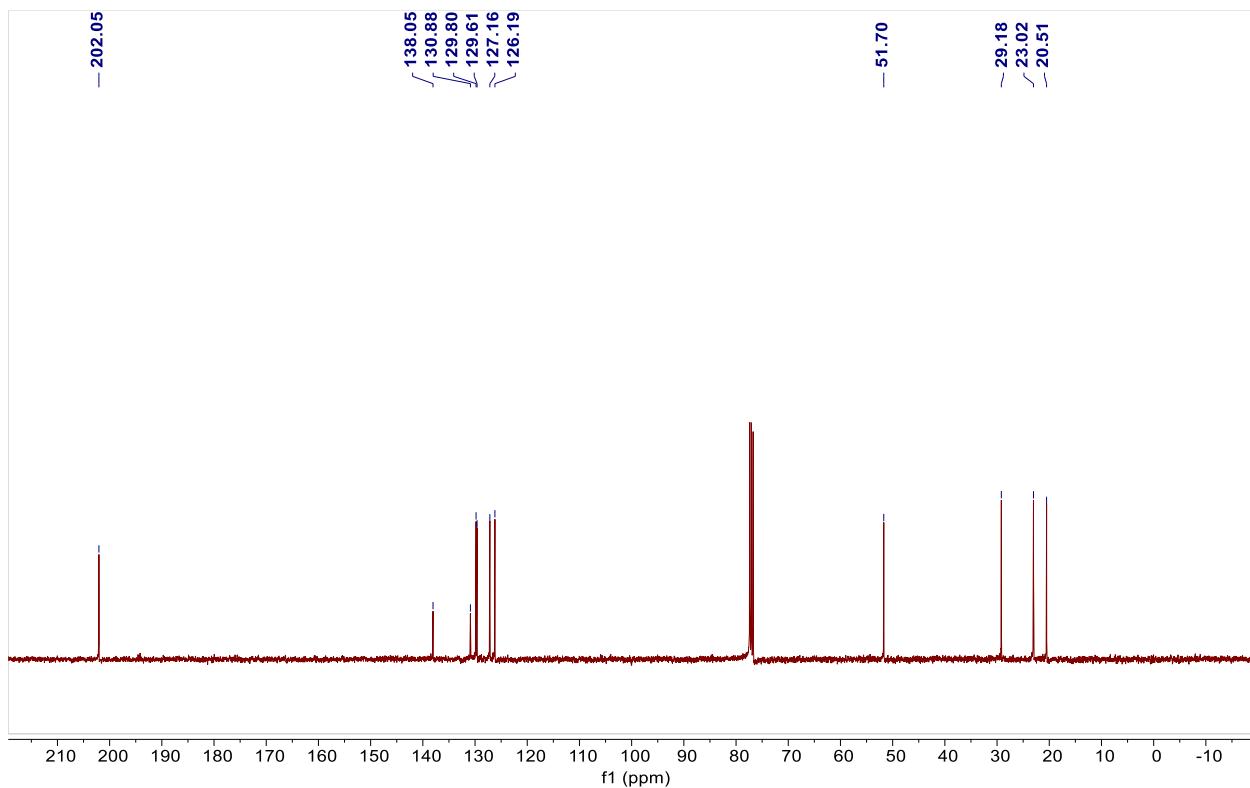
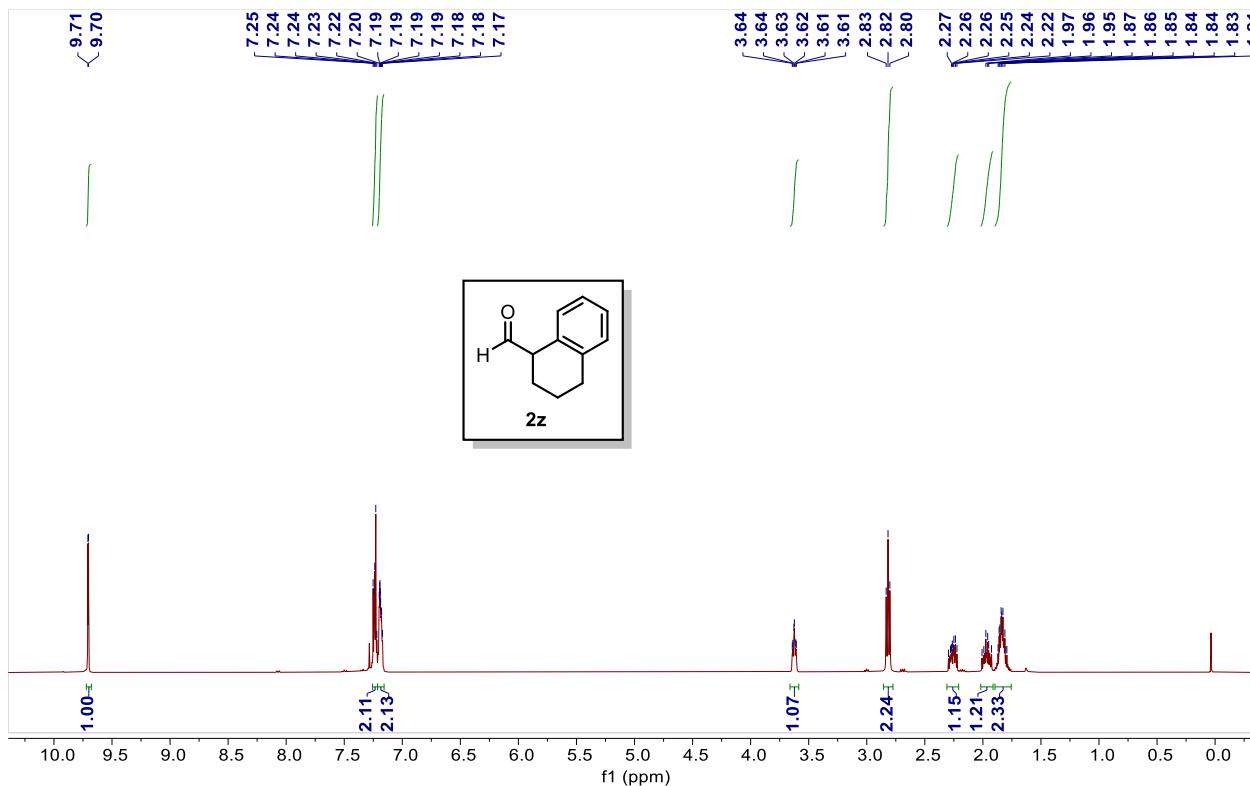


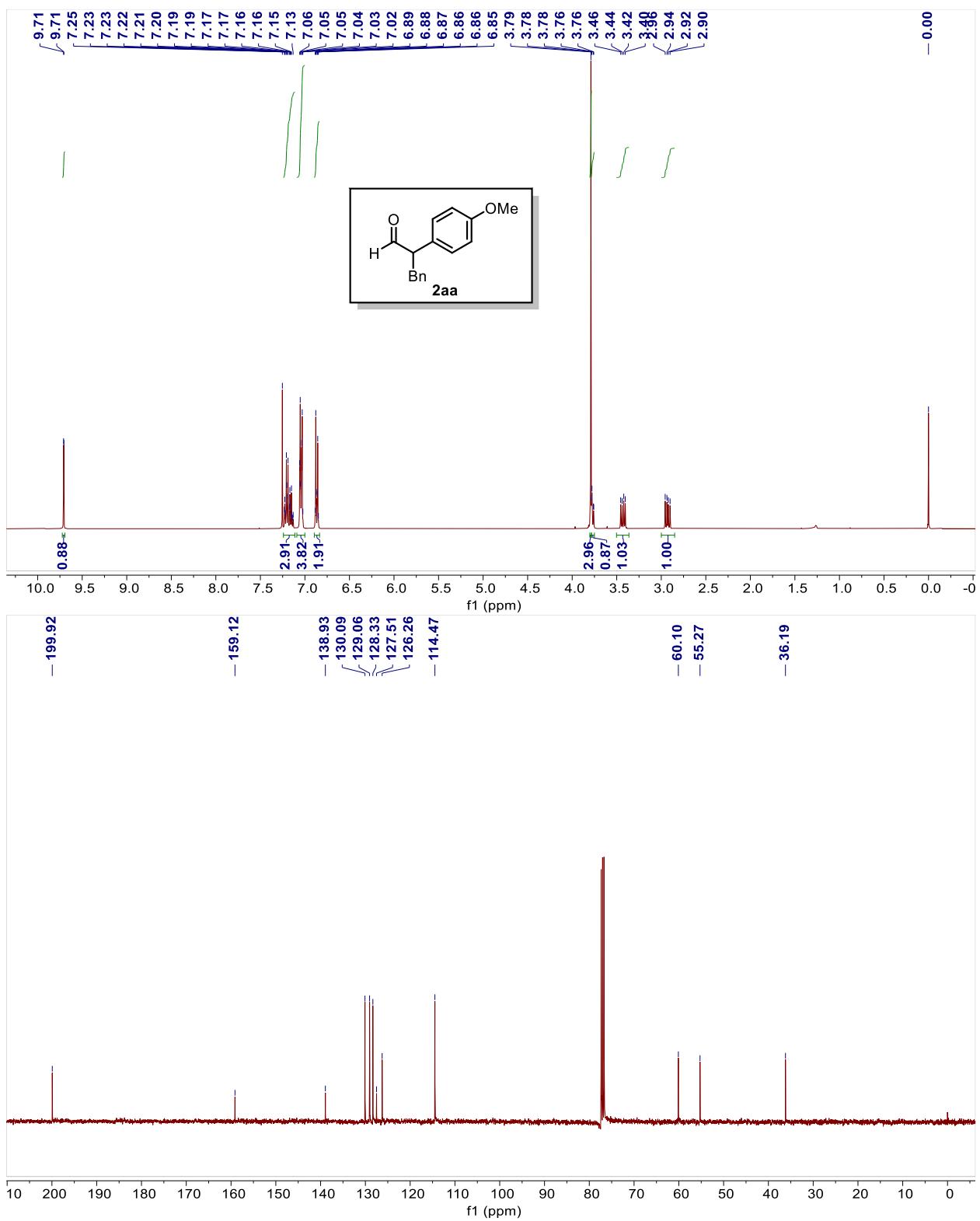


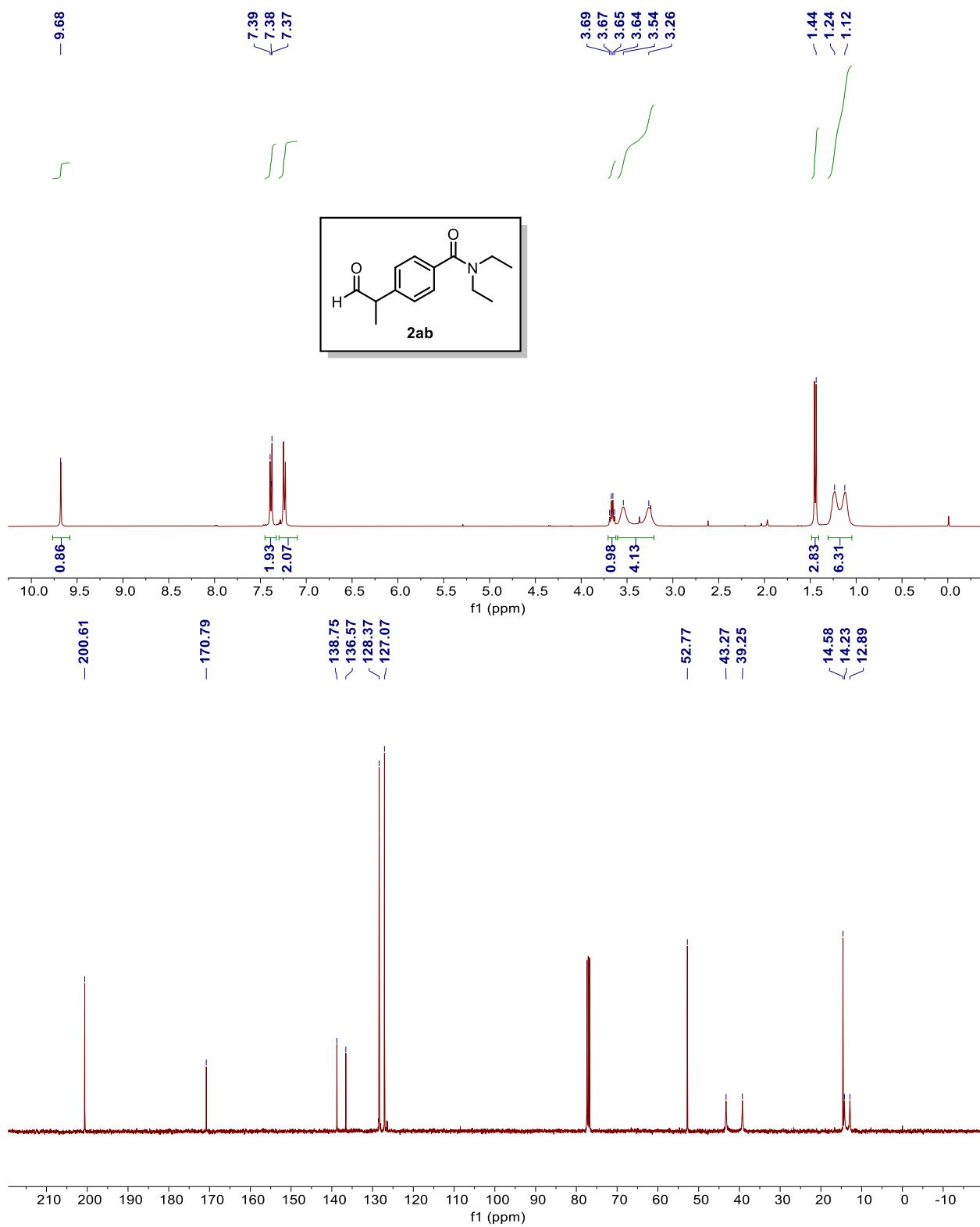


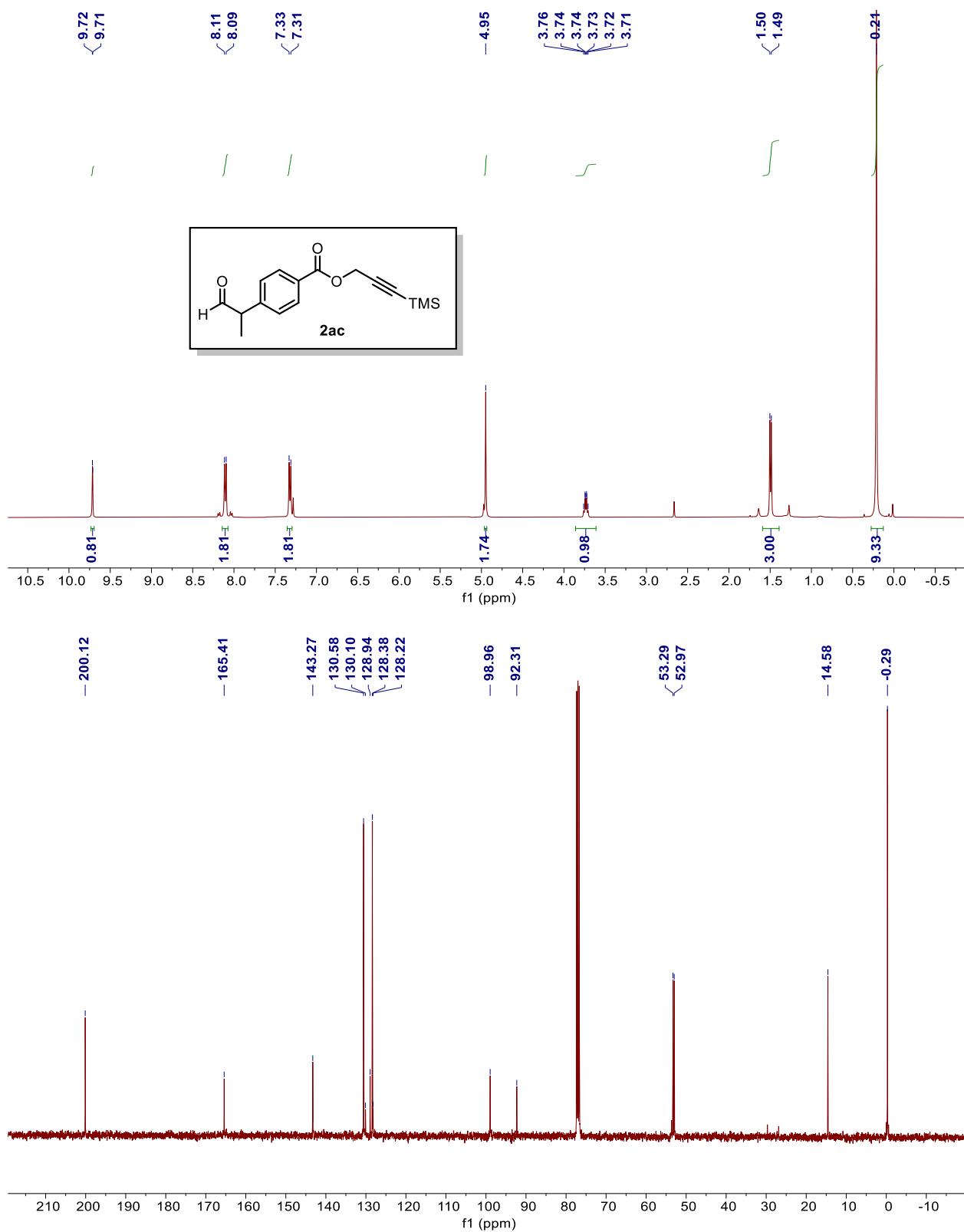


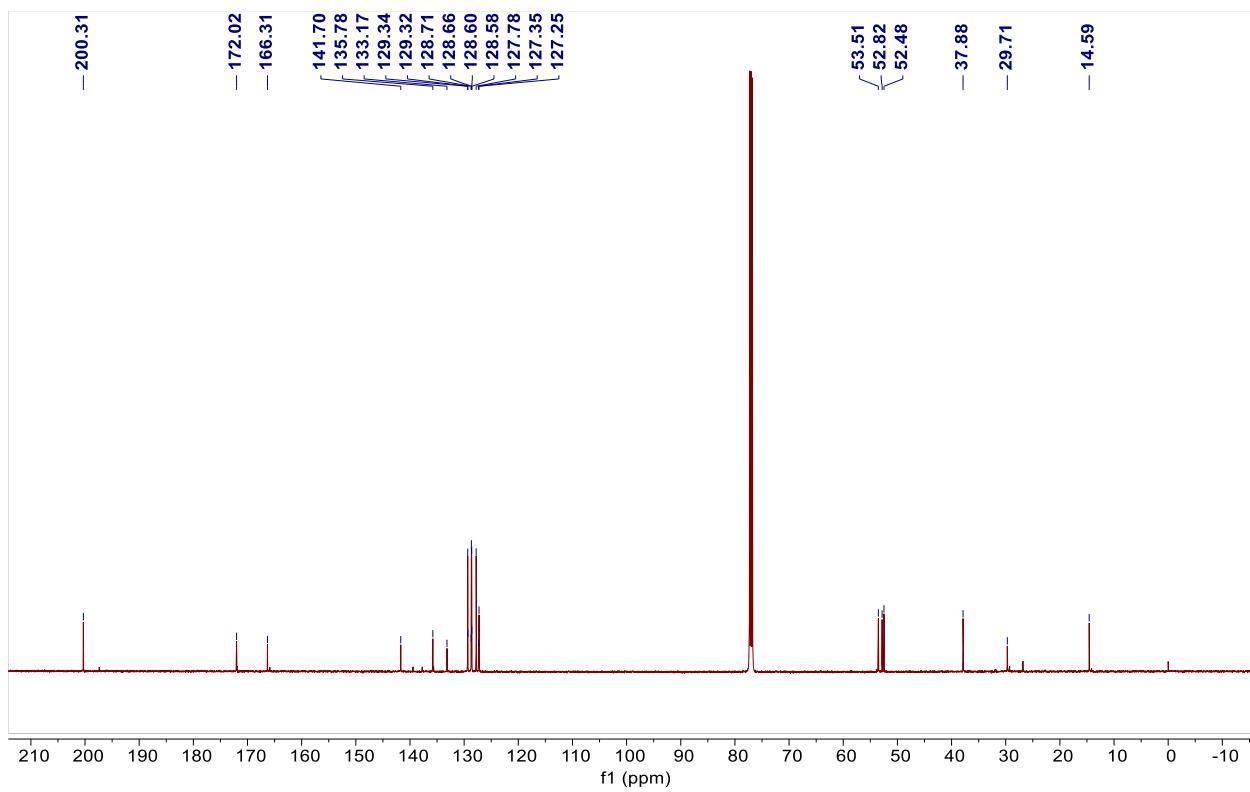
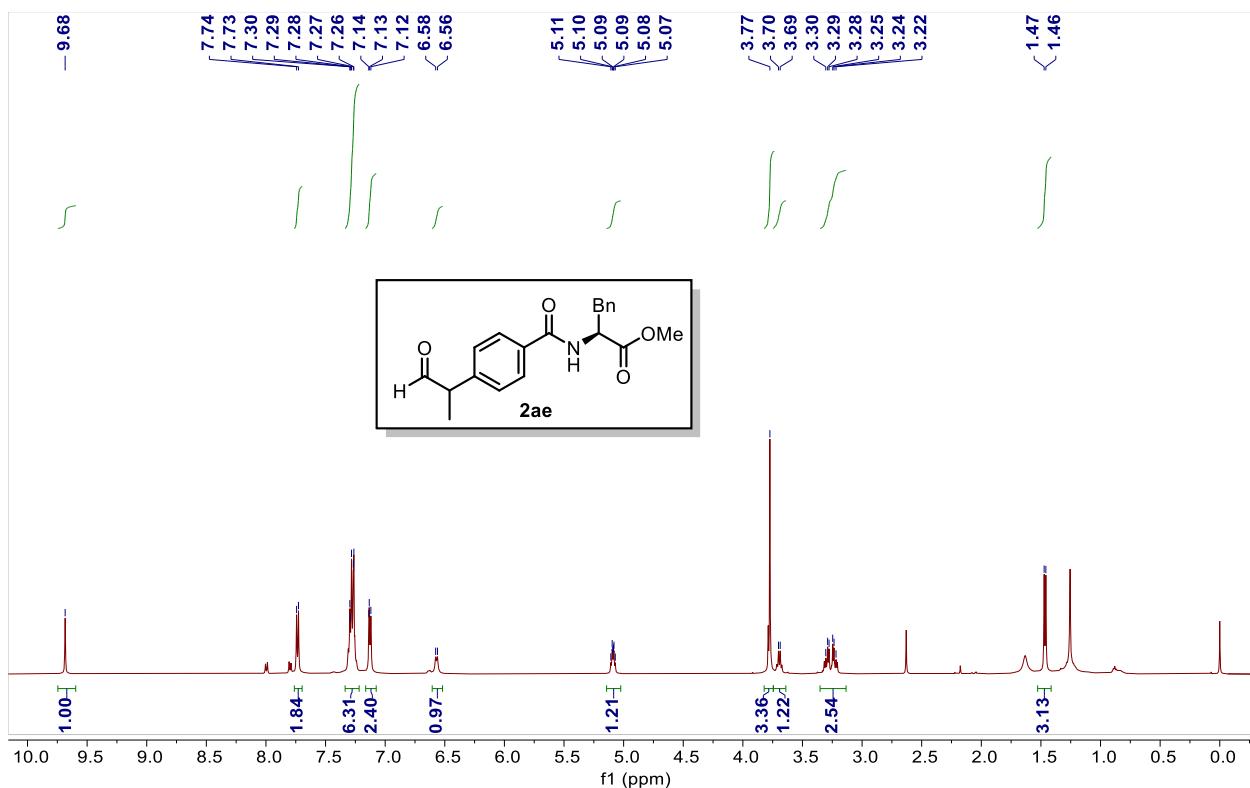


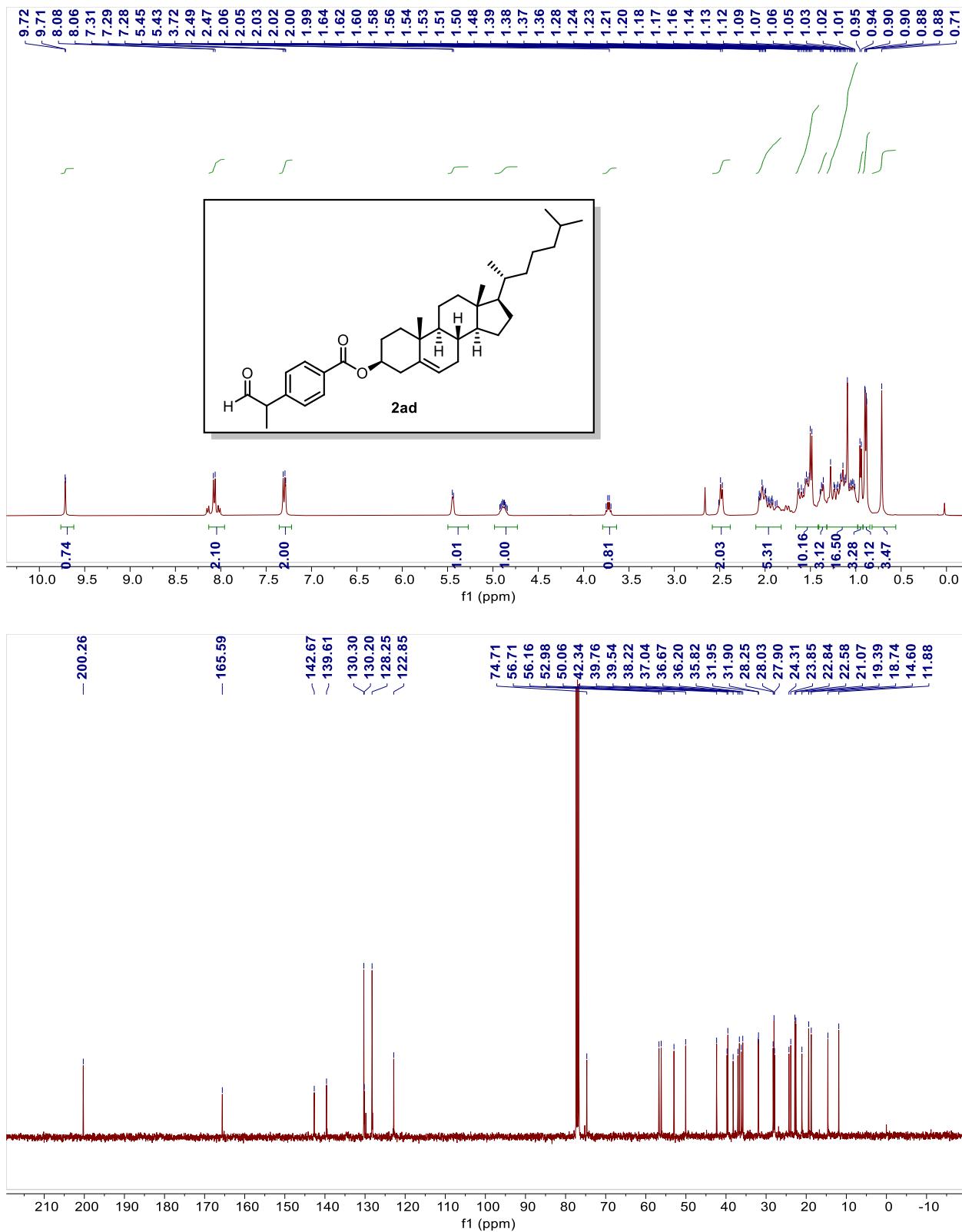


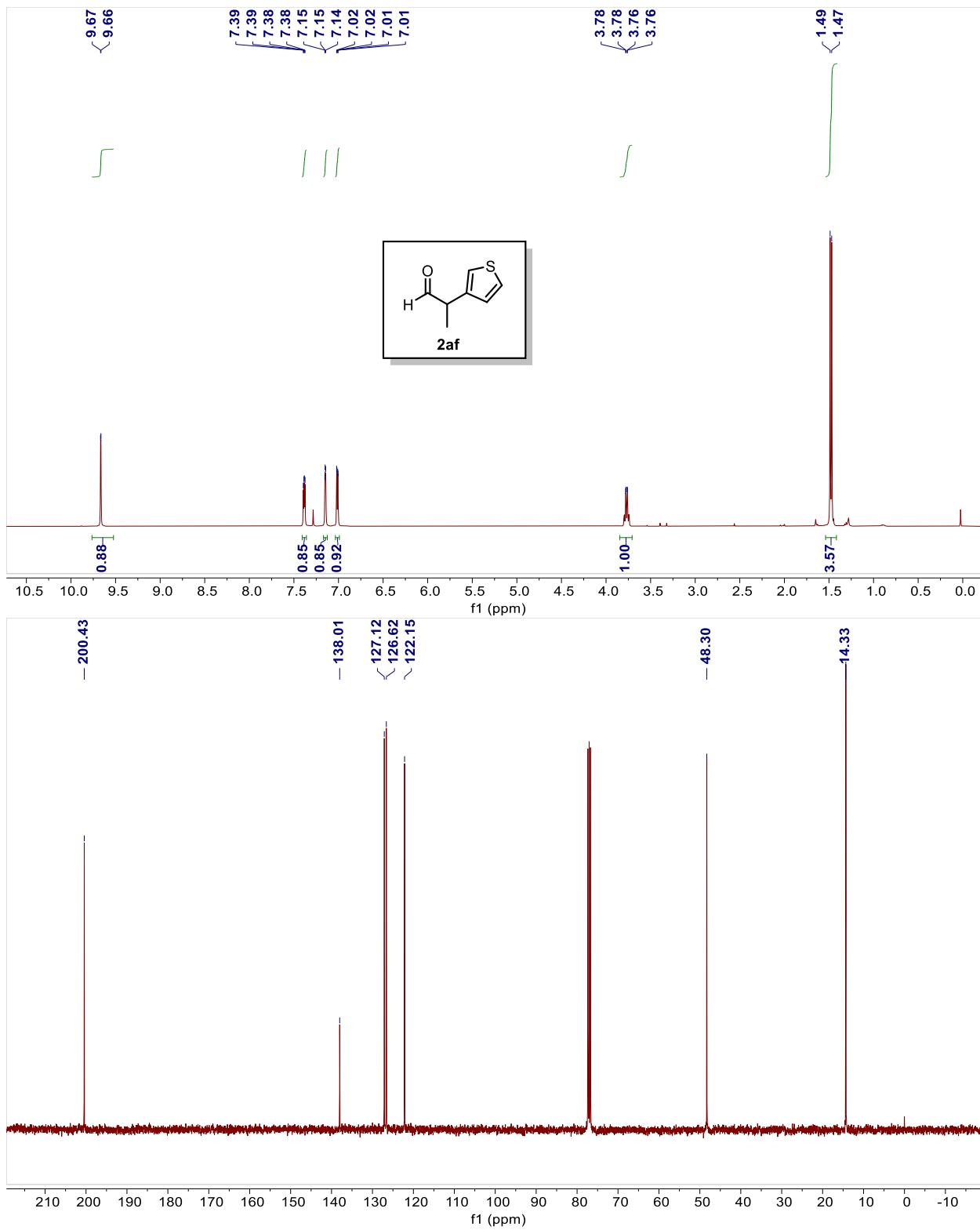


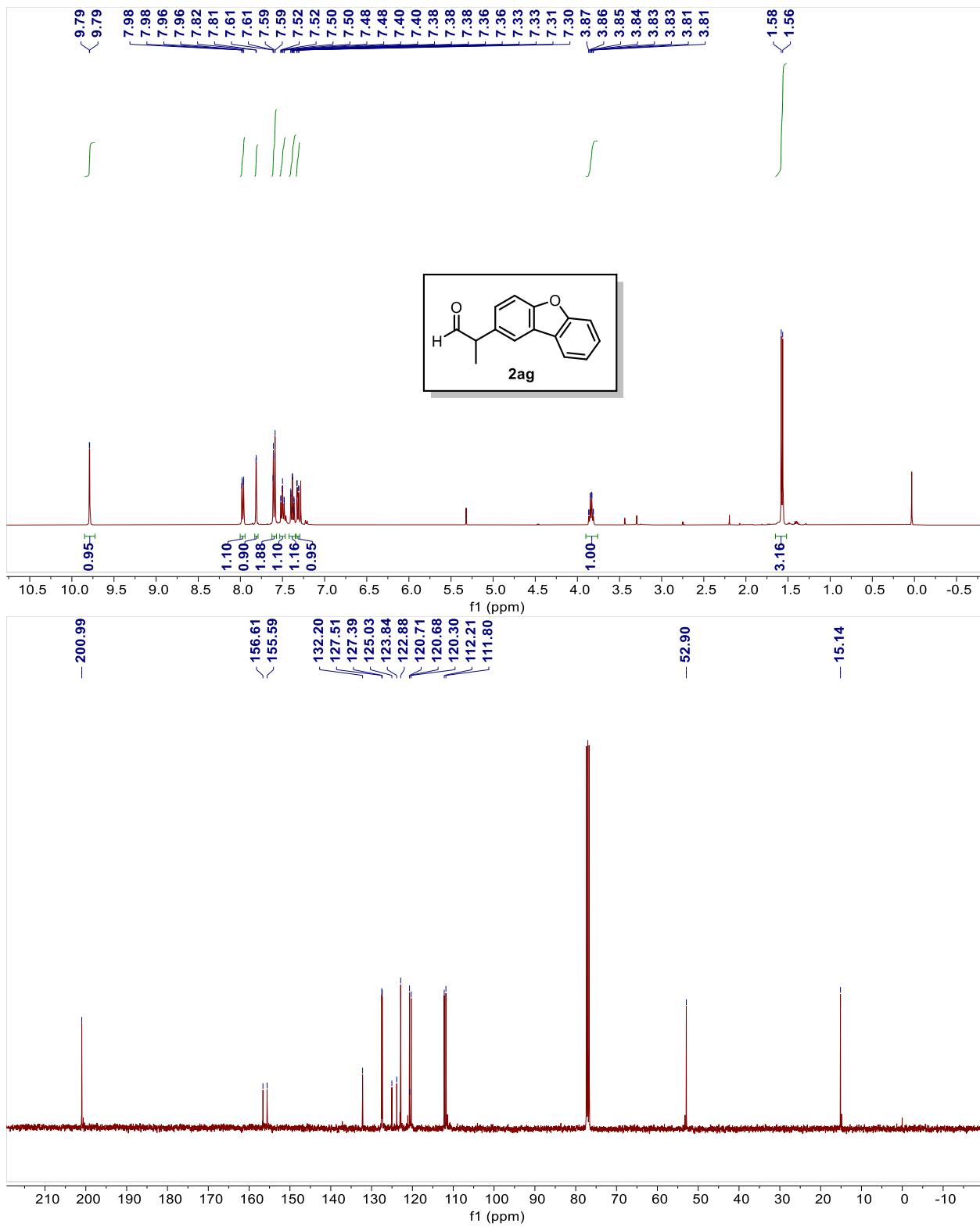


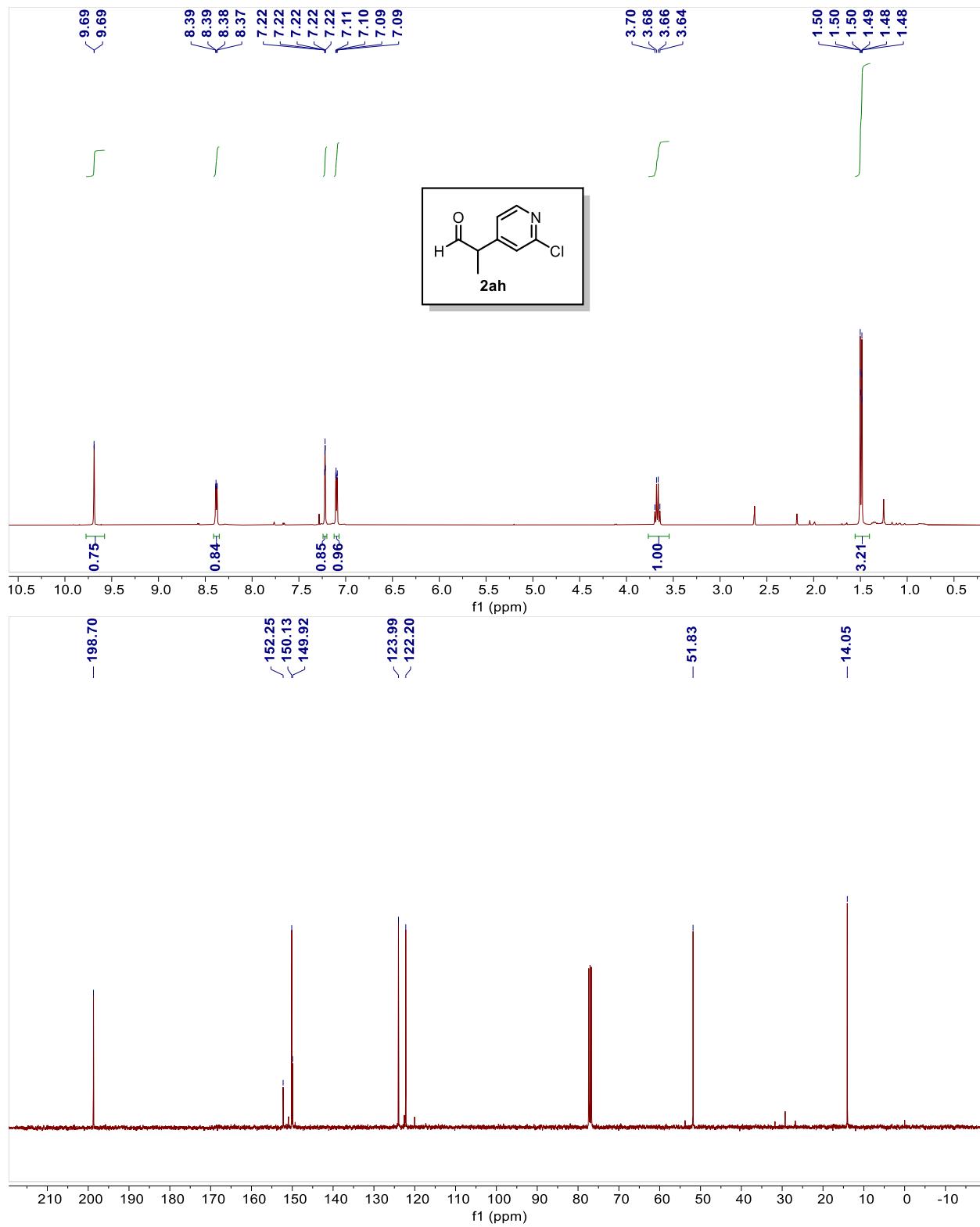


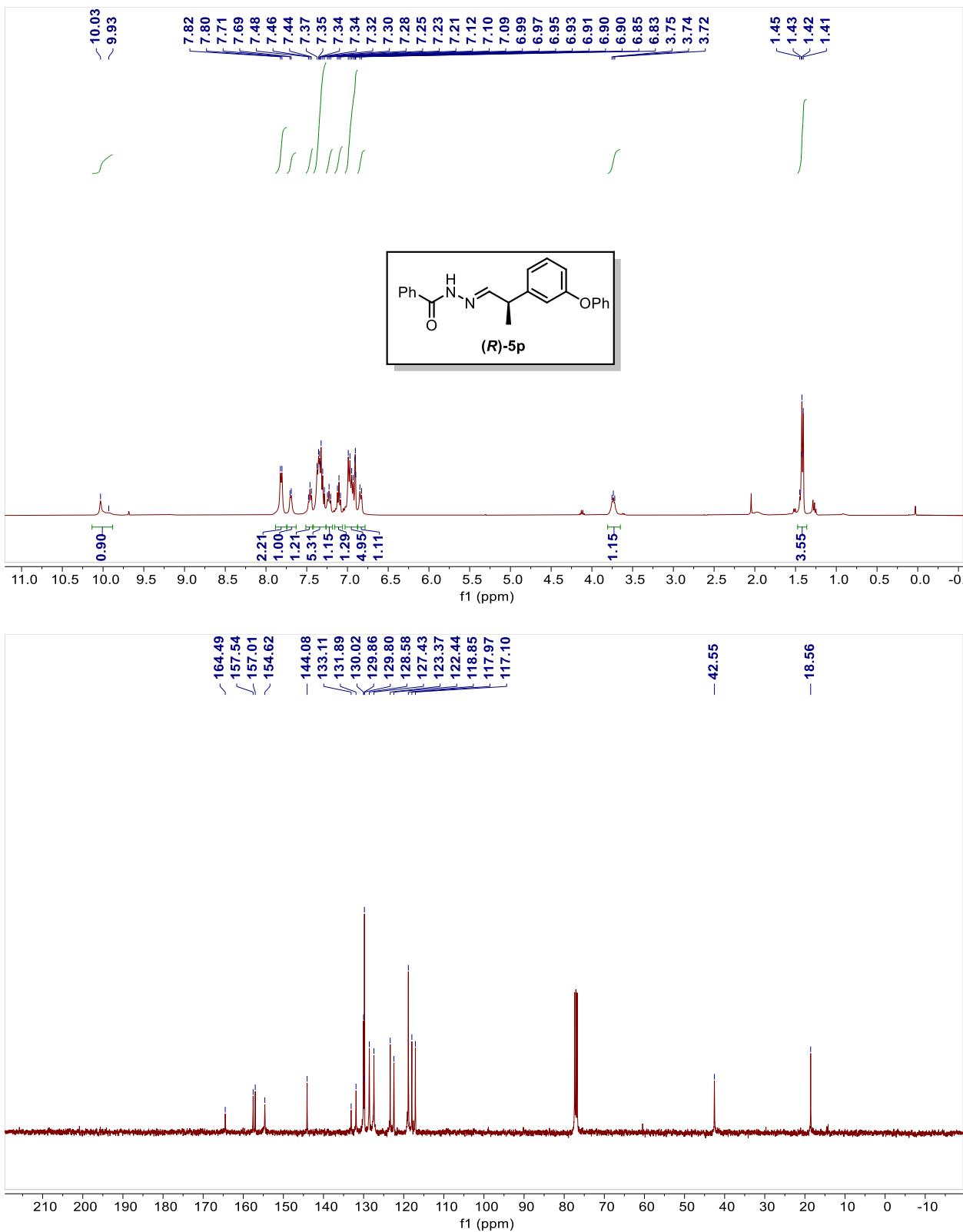


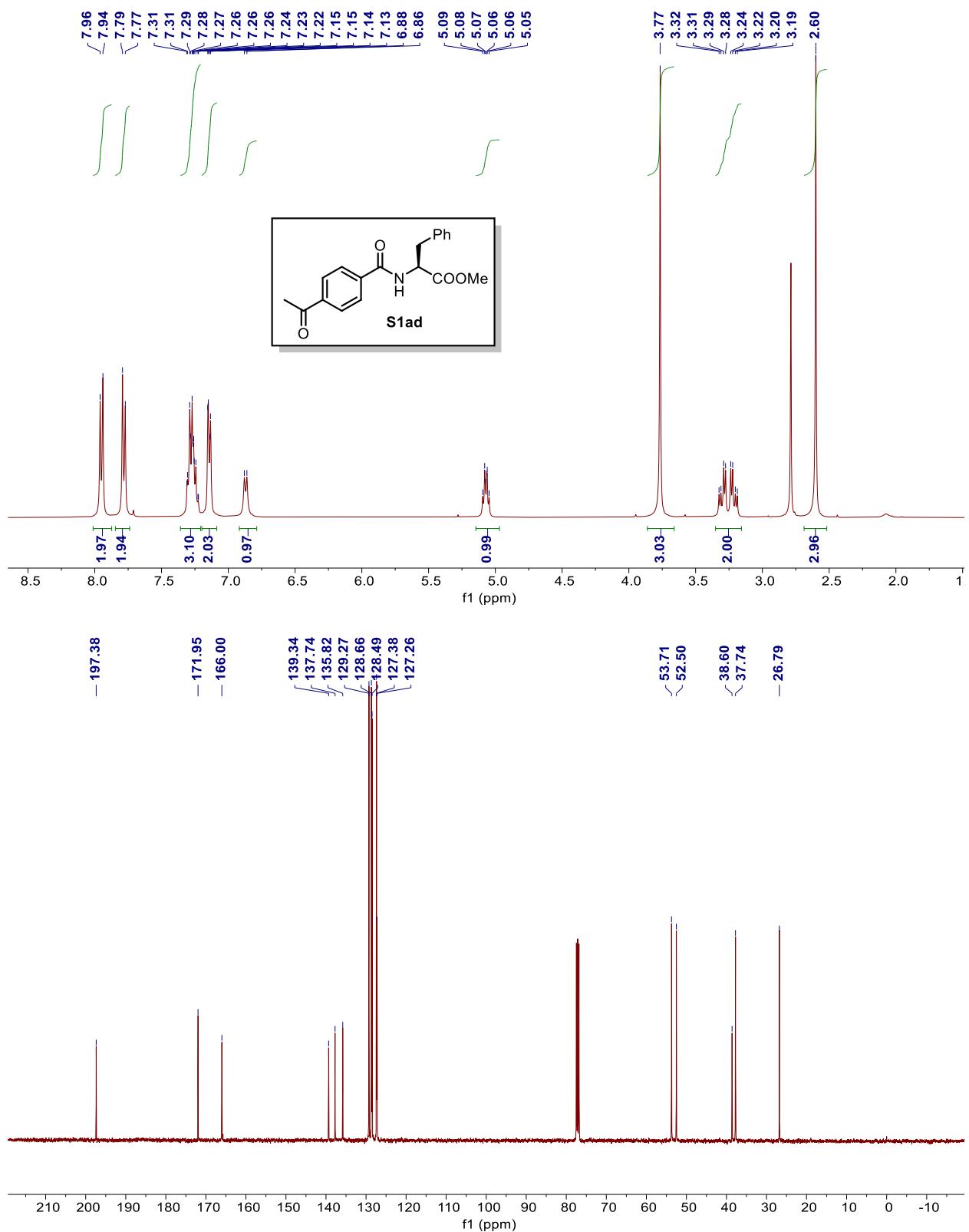


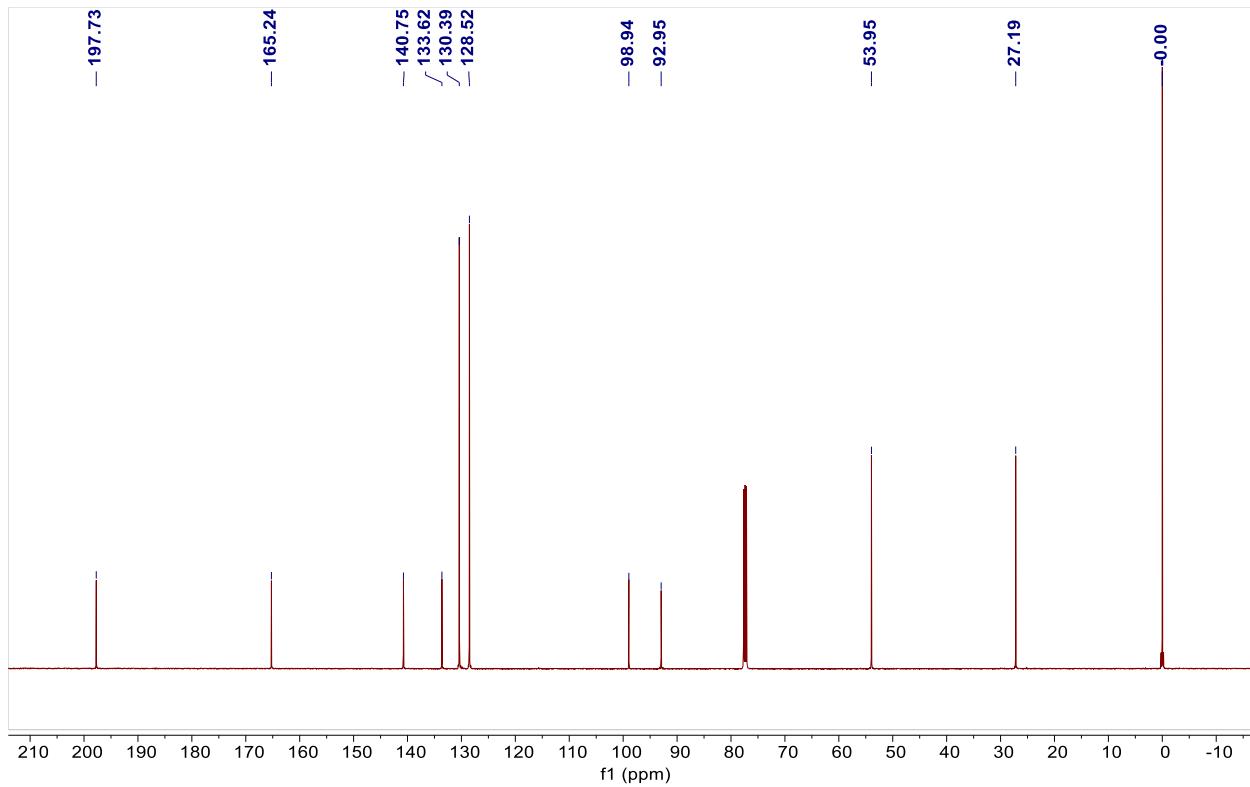
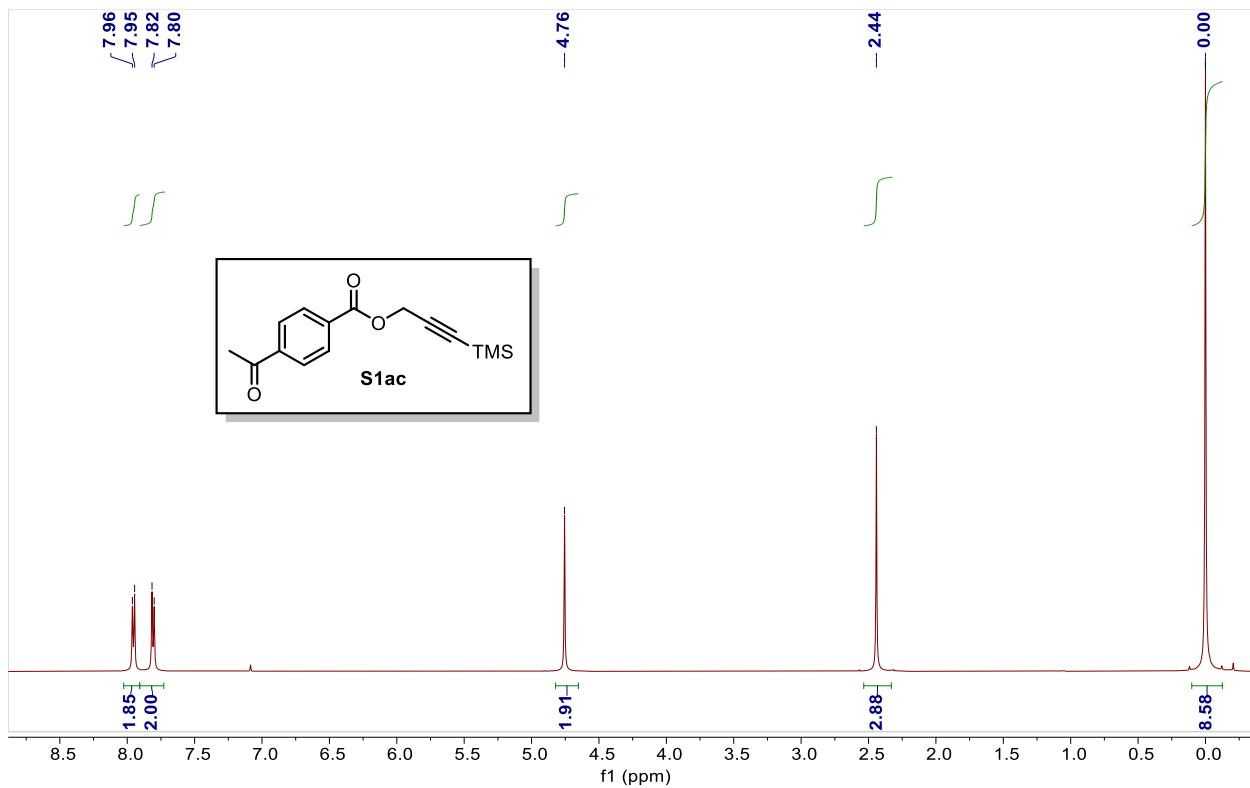


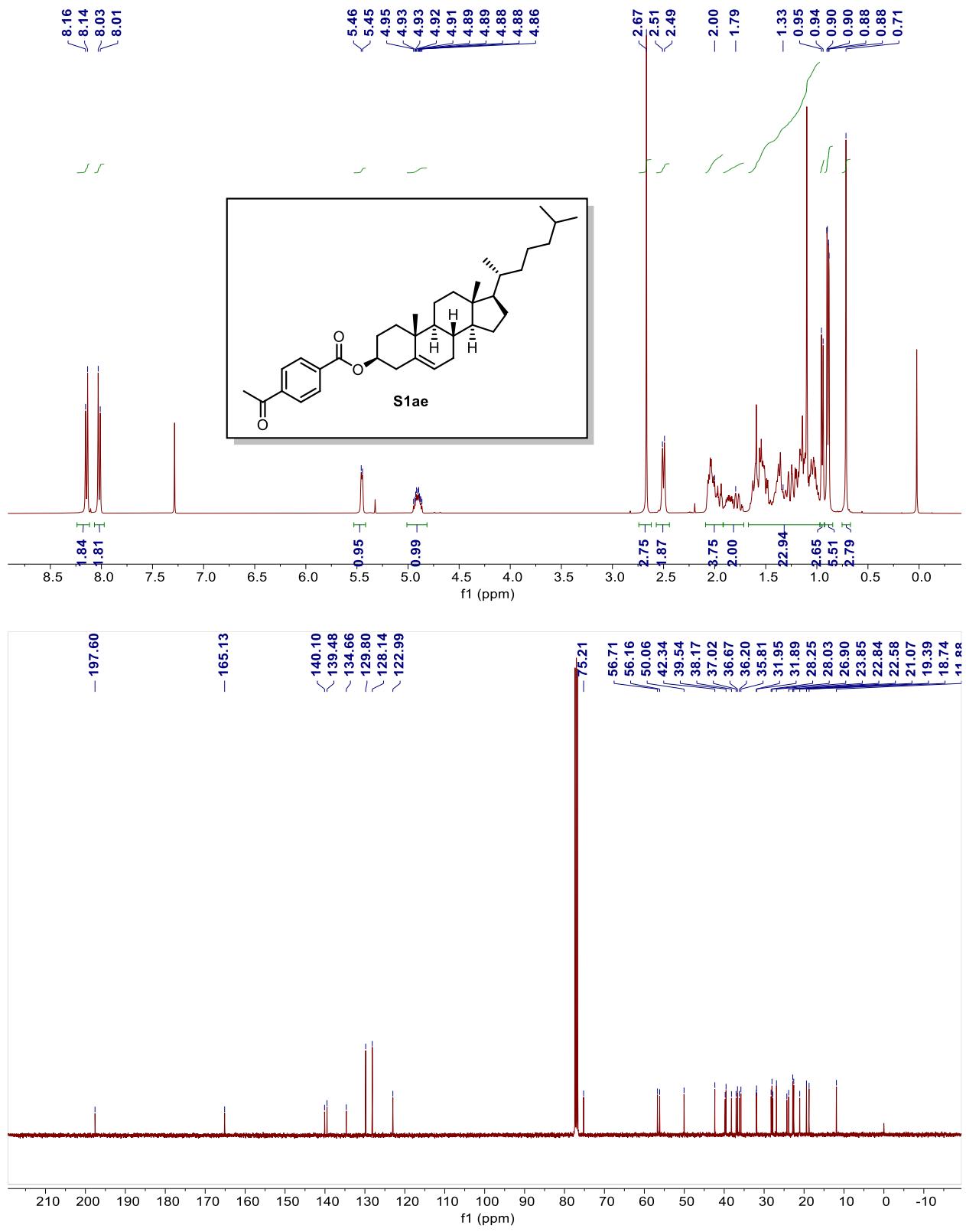




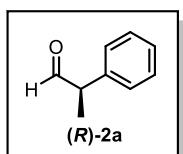




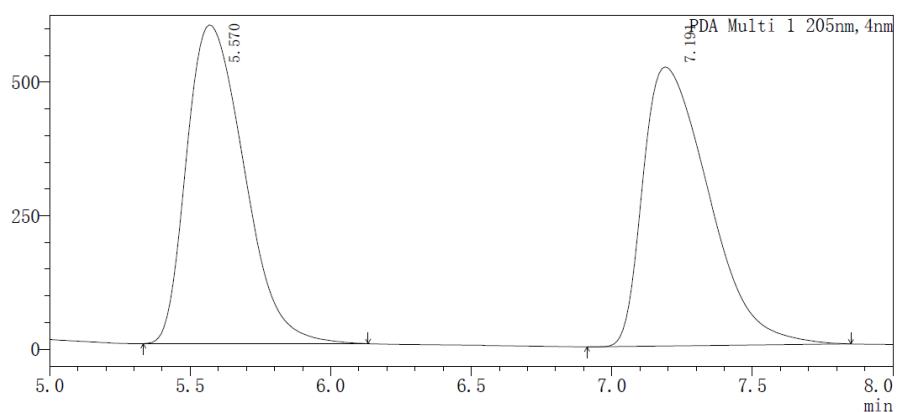




9. HPLC spectra



mAU

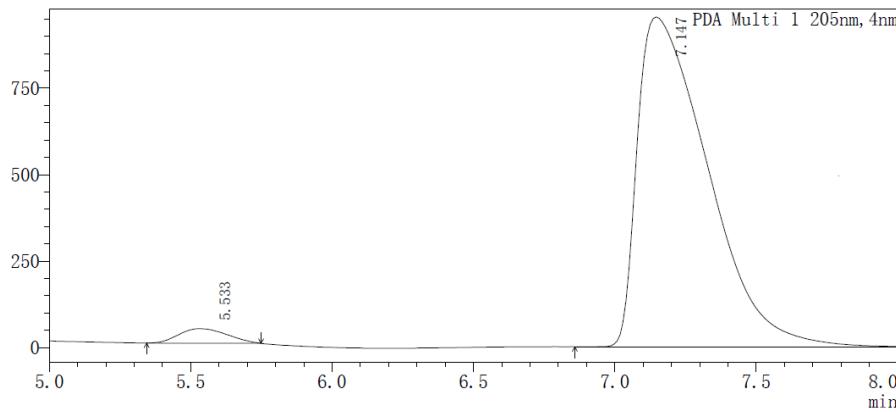


<Peak Results>

PDA Ch1 205nm

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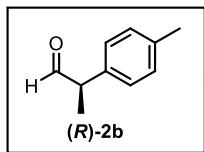
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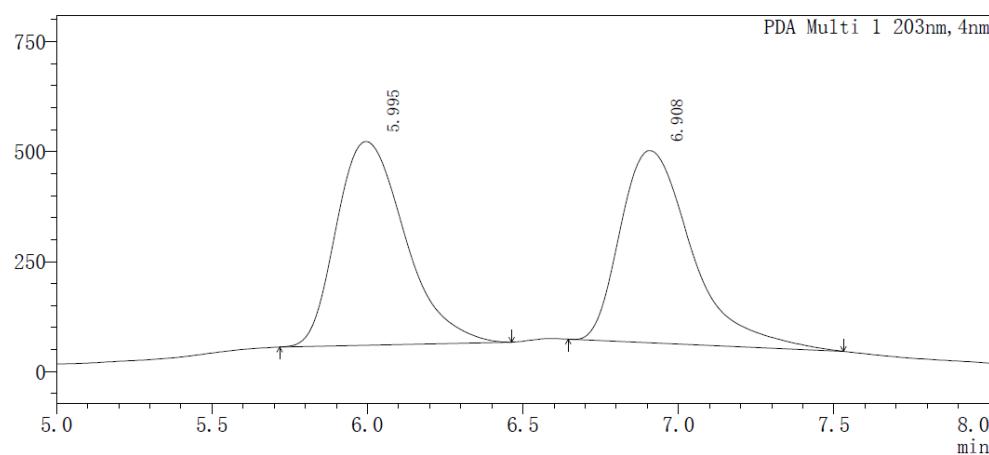
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PDA Ch1 205nm

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mAU

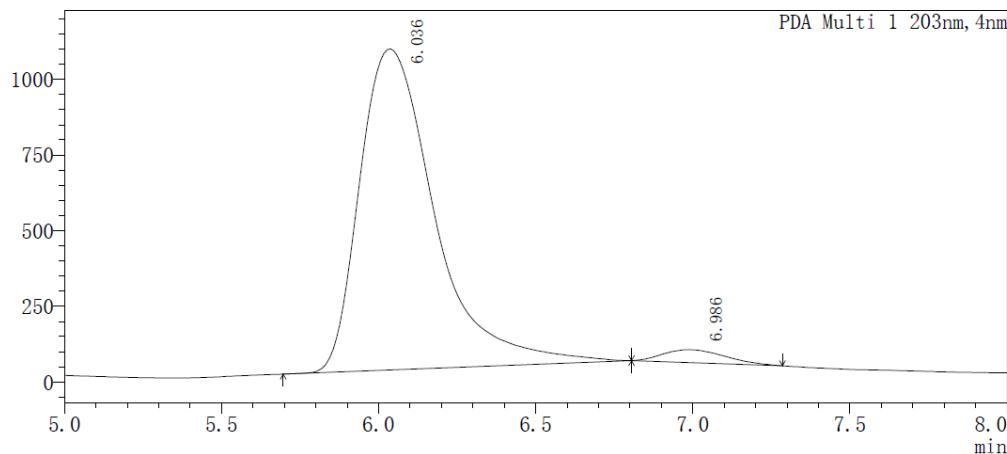


⟨Peak Results⟩

PDA Ch1 203nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	5.995	463208	7125665	50.439
2	6.908	436970	7001531	49.561

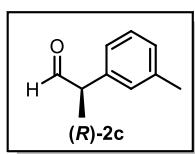
mAU



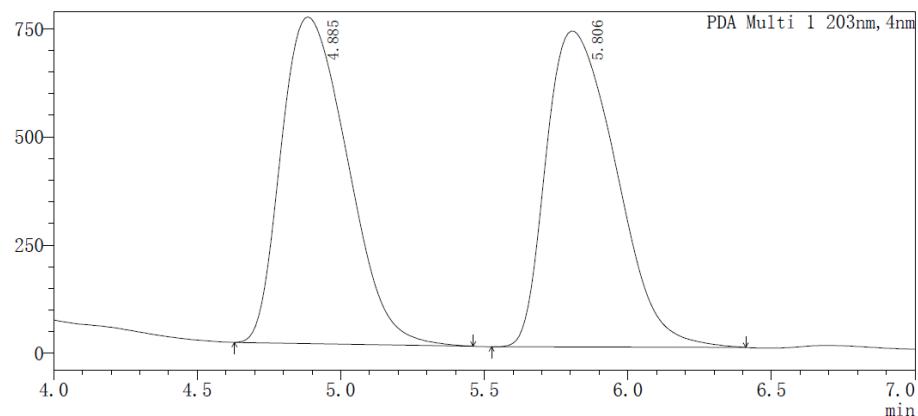
⟨Peak Results⟩

PDA Ch1 203nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	6.036	1061001	17710079	96.851
2	6.986	42264	575874	3.149



mAU

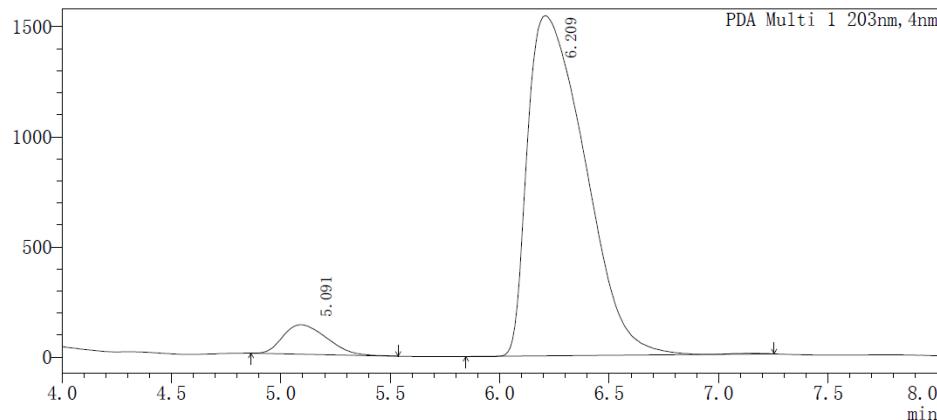


<Peak Results>

PDA Ch1 203nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	4.885	754420	12124533	49.563
2	5.806	729827	12338223	50.437

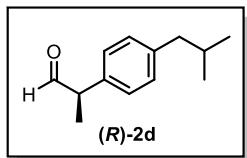
mAU



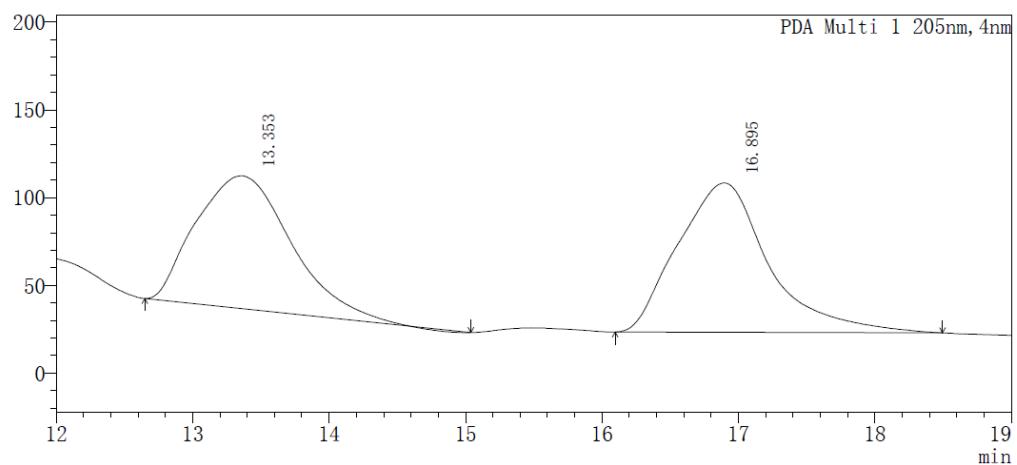
<Peak Results>

PDA Ch1 203nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	5.091	133633	1859234	6.188
2	6.209	1544083	28185975	93.812



mAU

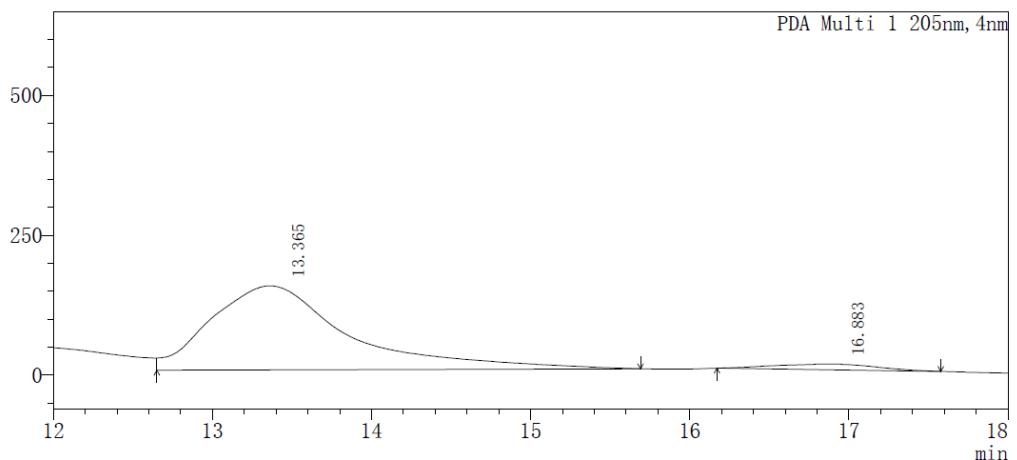


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	13.353	75679	3664546	48.101
2	16.895	85143	3953937	51.899

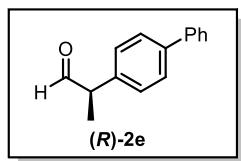
mAU



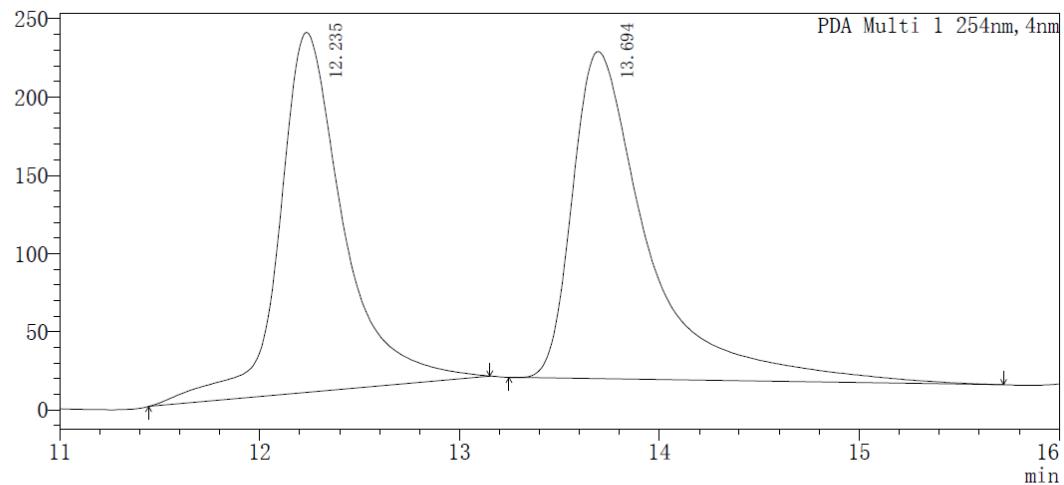
<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	13.365	150242	9046233	95.275
2	16.883	10239	448591	4.725



mAU

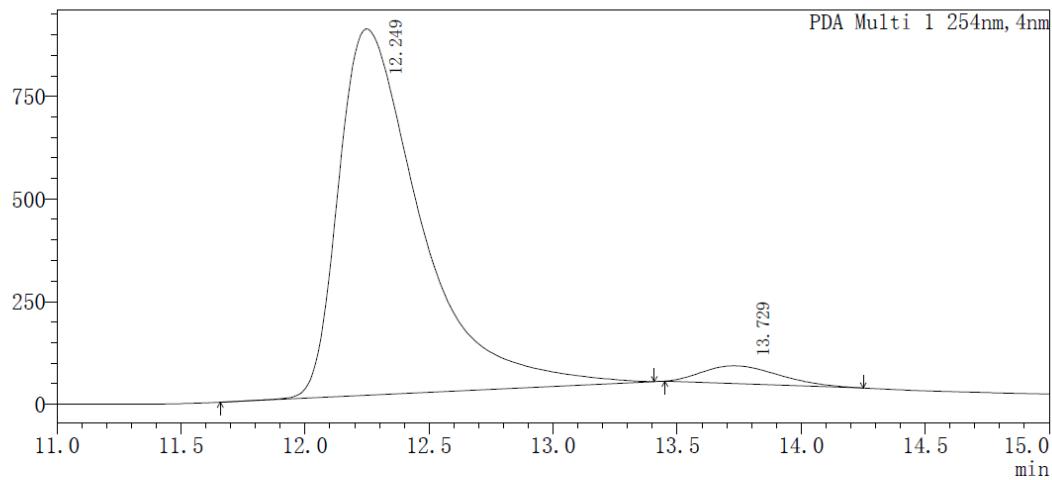


<Peak Results>

PDA Ch1 254nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.235	230246	5165963	48.221
2	13.694	209239	5547141	51.779

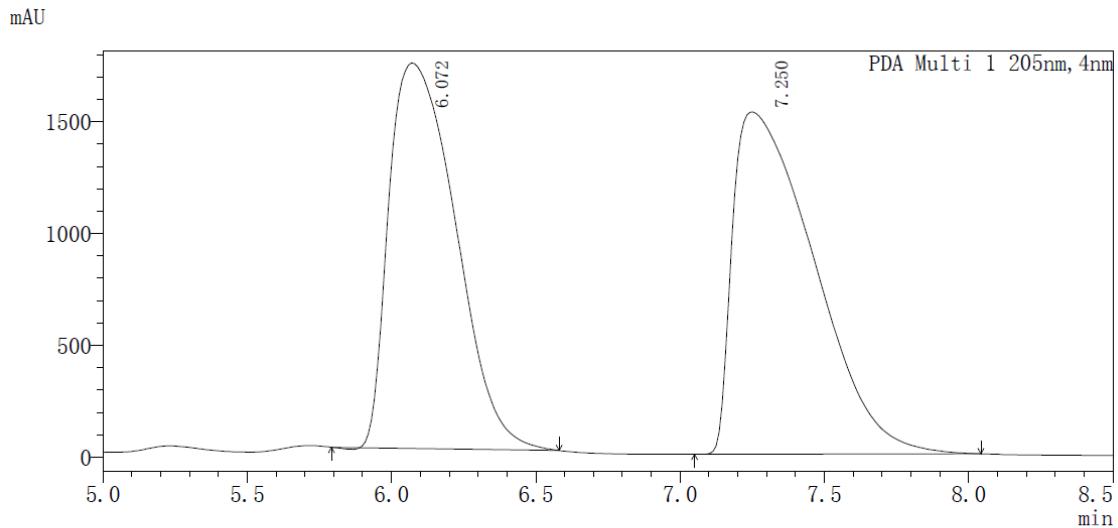
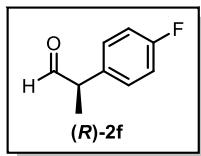
mAU



<Peak Results>

PDA Ch1 254nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.249	892796	20694731	95.694
2	13.729	43360	931282	4.306

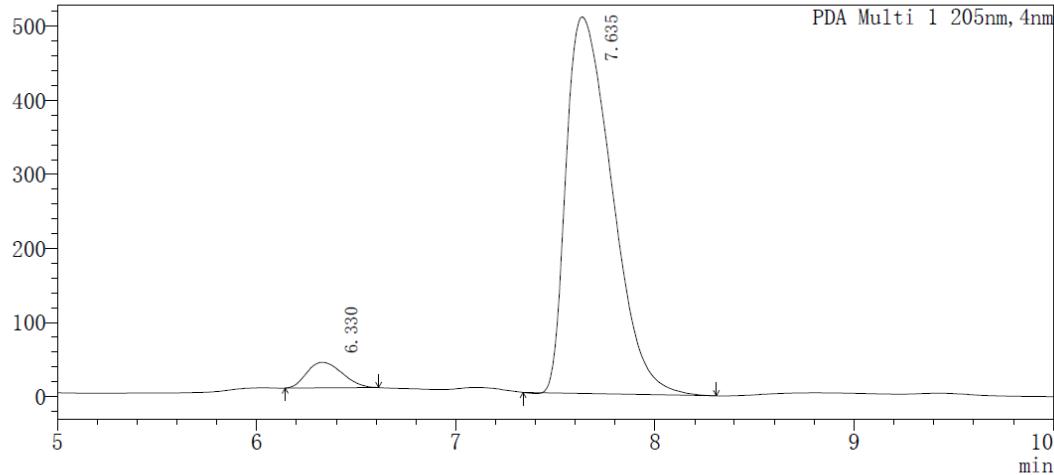


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	6.072	1725096	27781504	48.024
2	7.250	1531752	30067969	51.976

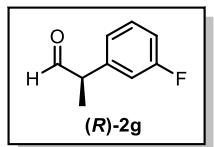
mAU



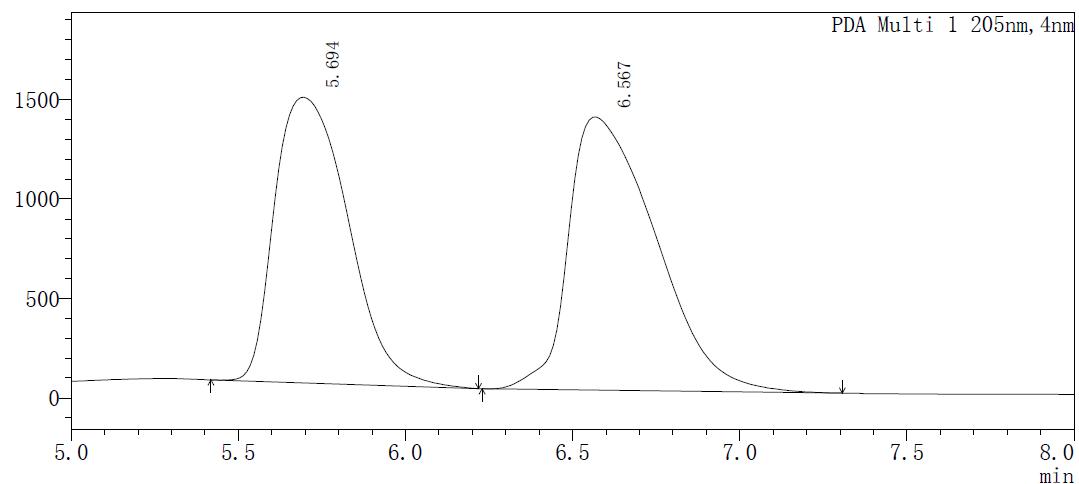
<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	6.330	34614	428828	5.015
2	7.635	508788	8122761	94.985



mAU

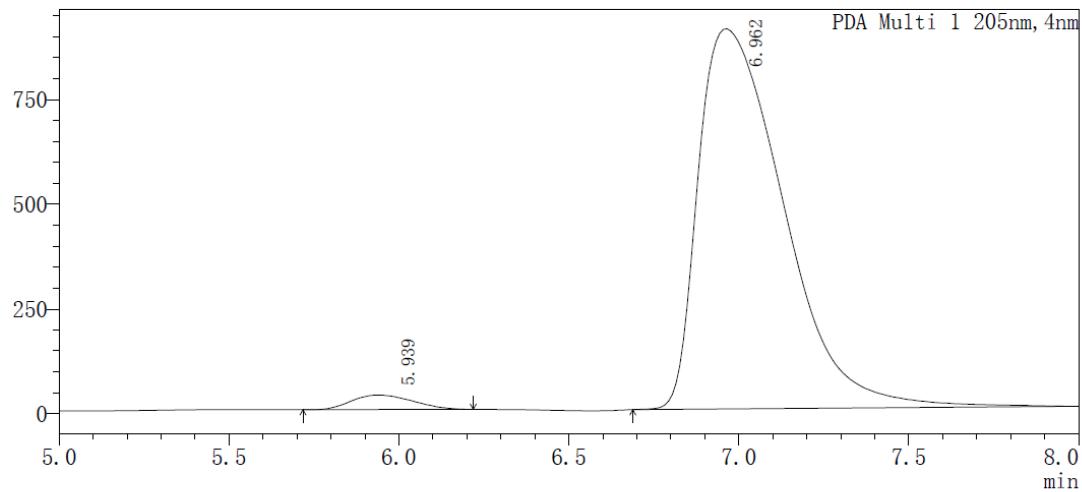


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	5.694	1436051	22034008	46.855
2	6.567	1373002	24992096	53.145

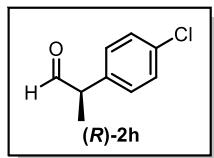
mAU



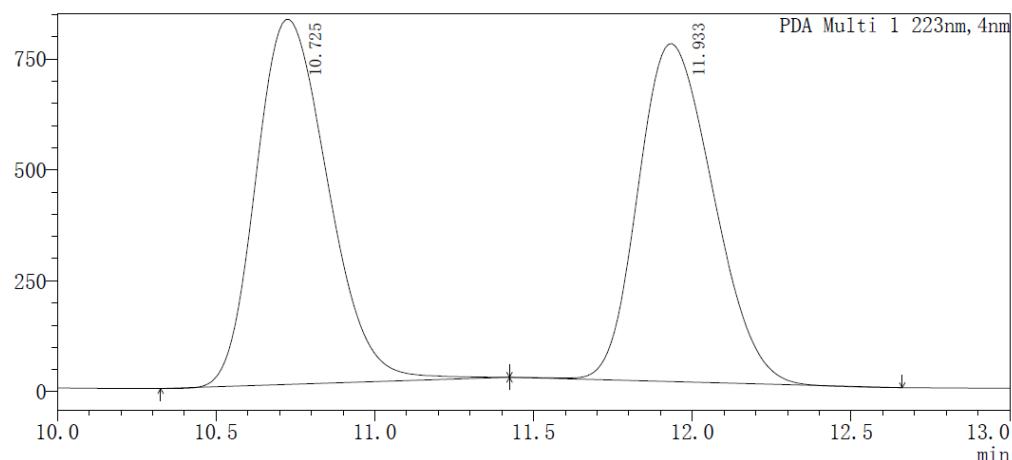
<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	5.939	34646	433786	2.663
2	6.962	906605	15855343	97.337



mAU

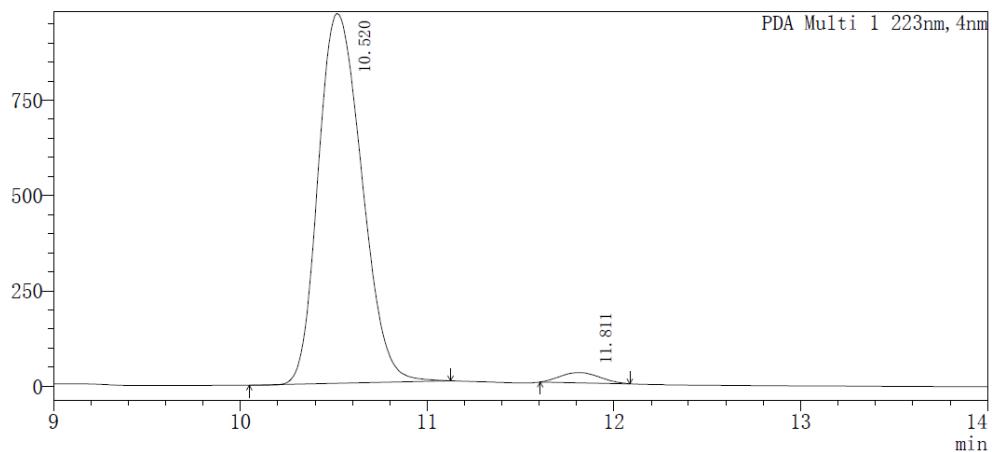


<Peak Results>

PDA Ch1 223nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	10.725	822990	13015649	50.991
2	11.933	761740	12509750	49.009

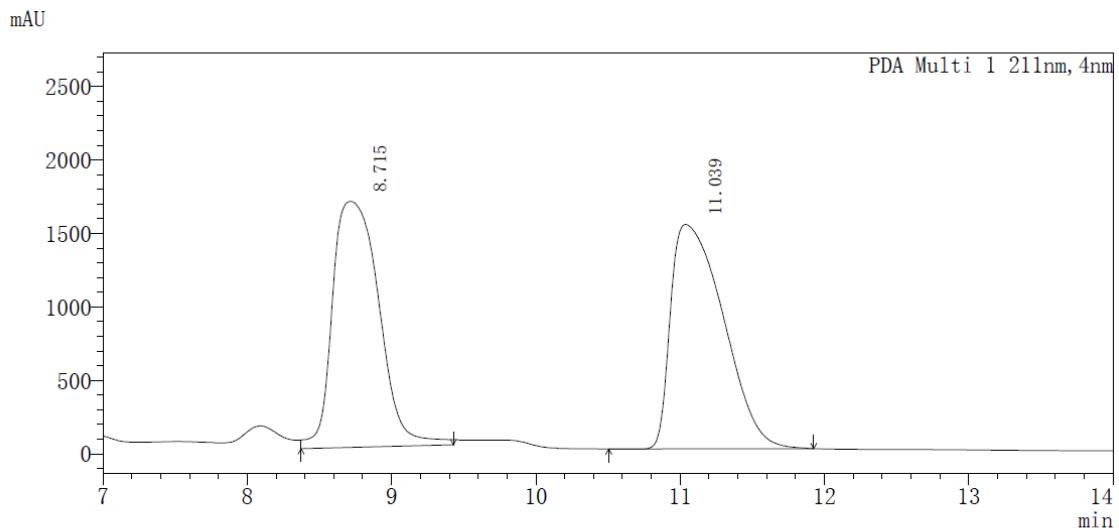
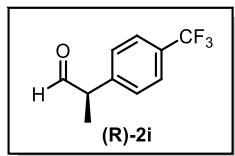
mAU



<Peak Results>

PDA Ch1 223nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	10.520	968730	15684273	97.578
2	11.811	26867	389358	2.422

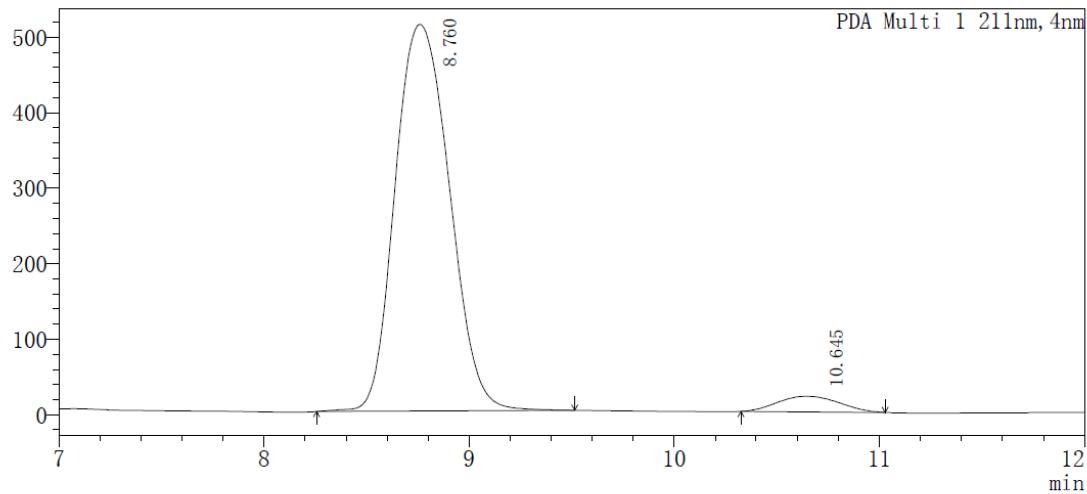


<Peak Results>

PDA Ch1 211nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.715	1675134	37630290	49.249
2	11.039	1526838	38778384	50.751

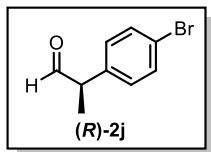
mAU



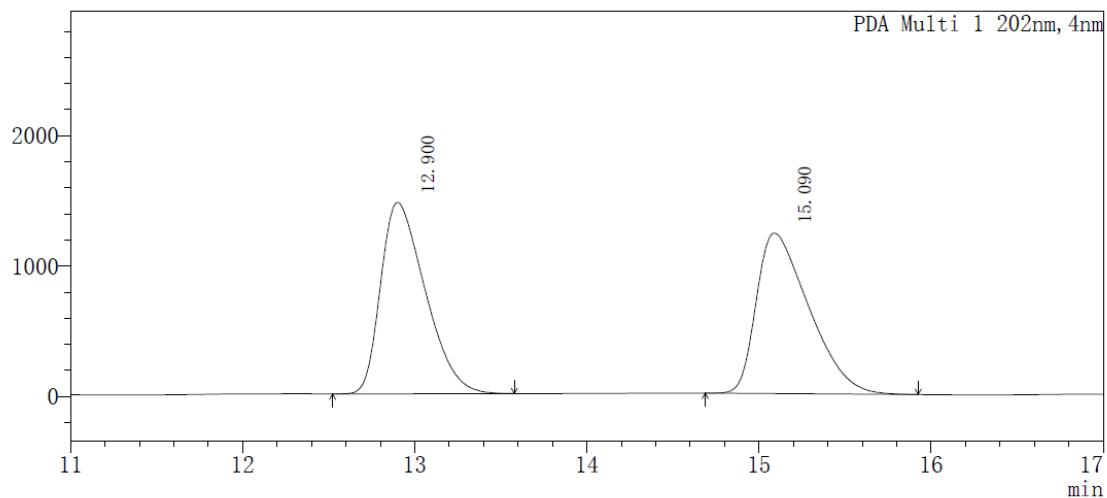
<Peak Results>

PDA Ch1 211nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.760	512388	9461373	95.638
2	10.645	20664	431536	4.362



mAU

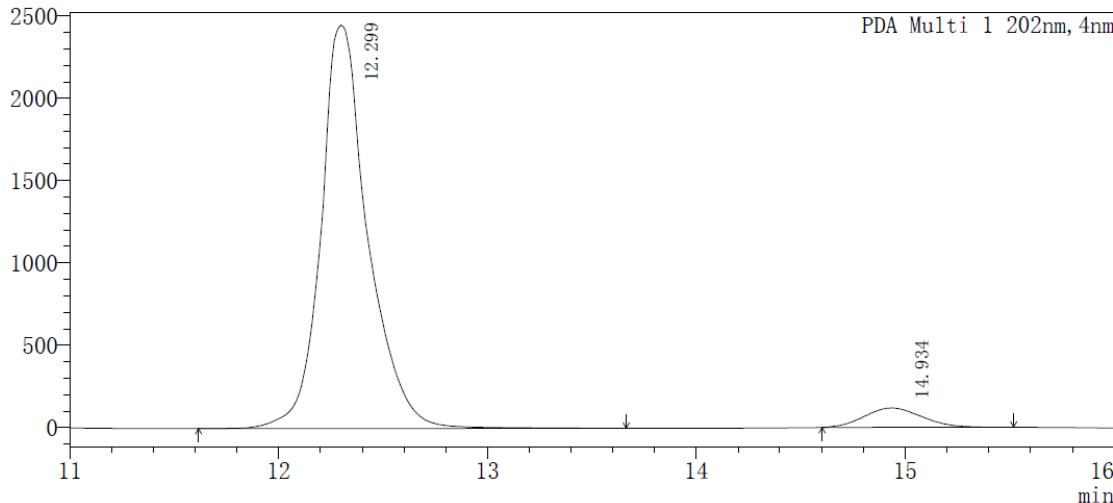


<Peak Results>

PDA Ch1 202nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.900	1466905	26435905	50.265
2	15.090	1231023	26157438	49.735

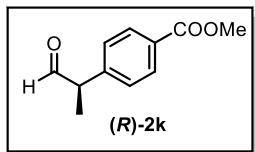
mAU



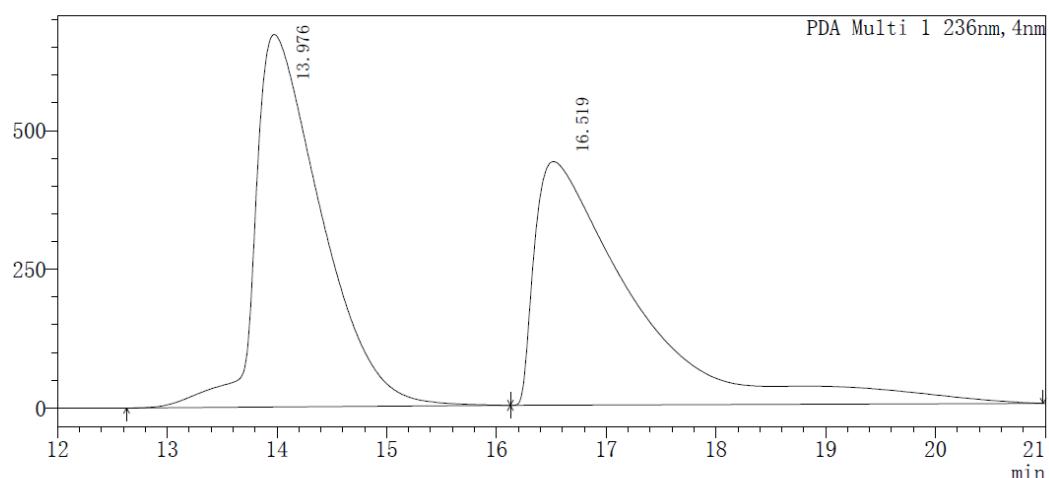
<Peak Results>

PDA Ch1 202nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.299	2449253	38337253	94.510
2	14.934	117070	2227171	5.490



mAU

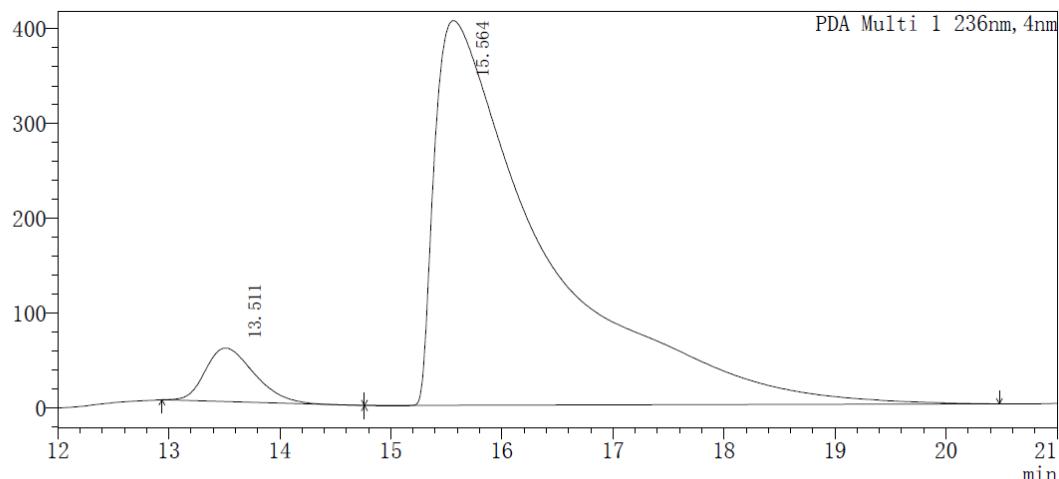


<Peak Results>

PDA Ch1 236nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	13.976	671013	28241148	50.285
2	16.519	438882	27920757	49.715

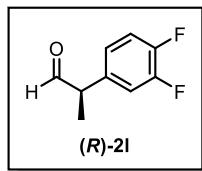
mAU



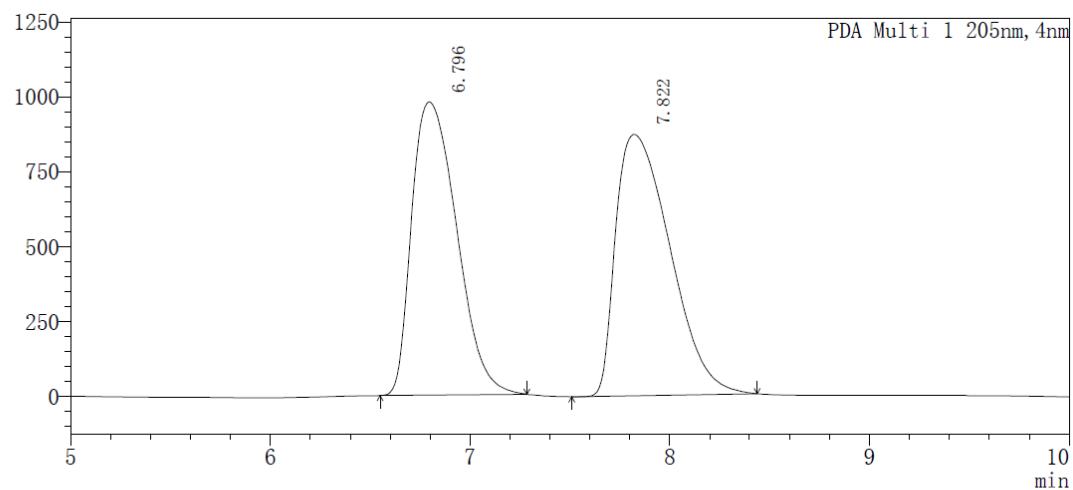
<Peak Results>

PDA Ch1 236nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	13.511	56544	1735441	5.857
2	15.564	405710	27894629	94.143



mAU

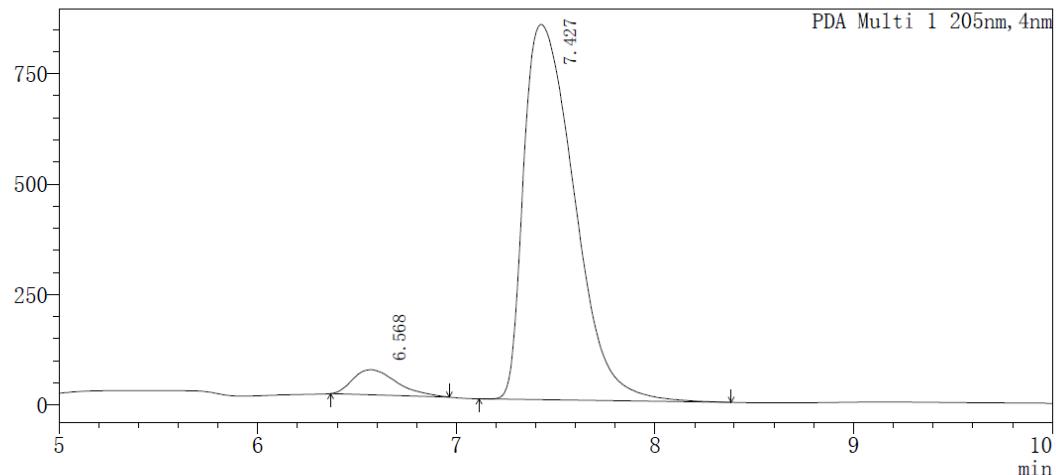


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	6.796	979718	15361192	48.189
2	7.822	872426	16515874	51.811

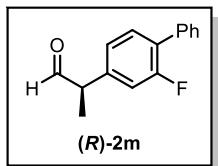
mAU



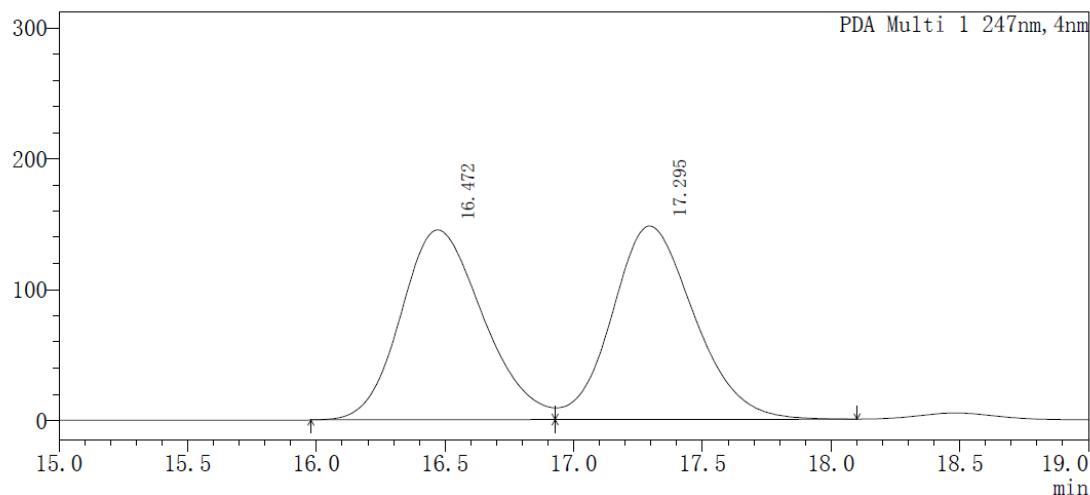
<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	6.568	56822	876683	5.515
2	7.427	849460	15019092	94.485



mAU

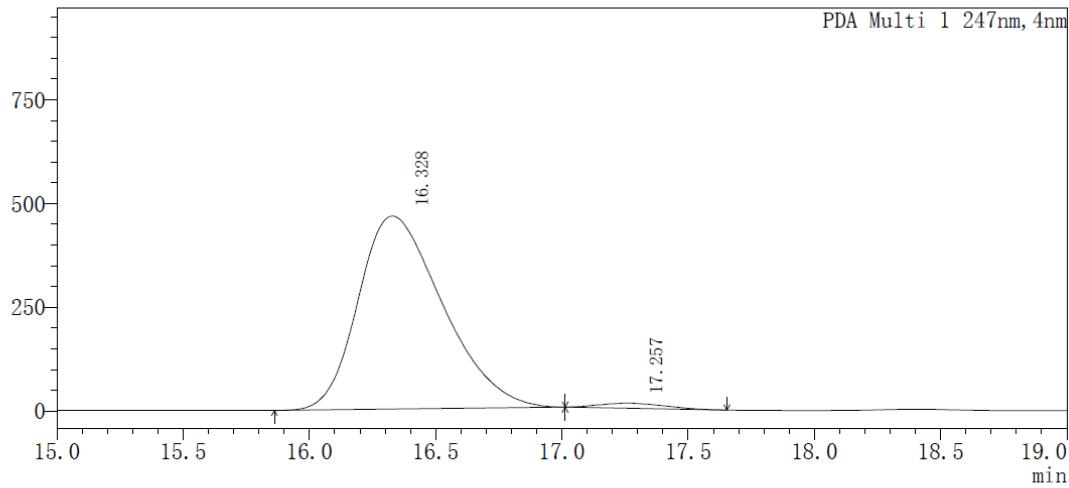


<Peak Results>

PDA Ch1 247nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	16.472	145072	3233650	49.588
2	17.295	147796	3287356	50.412

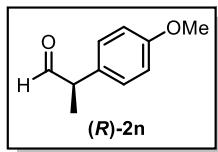
mAU



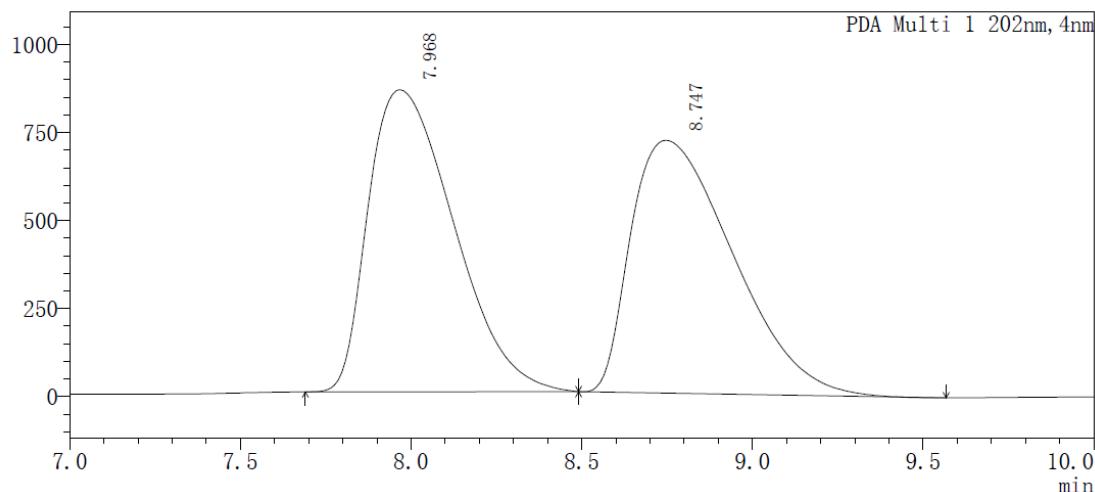
<Peak Results>

PDA Ch1 247nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	16.328	465401	10843026	98.046
2	17.257	12120	216049	1.954



mAU

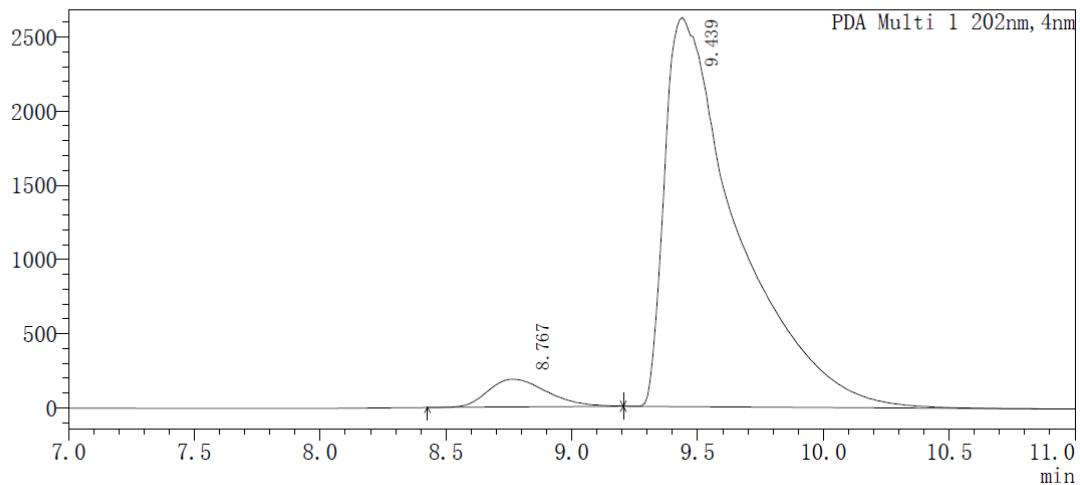


<Peak Results>

PDA Ch1 202nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	7.968	858053	14958546	50.062
2	8.747	718313	14921316	49.938

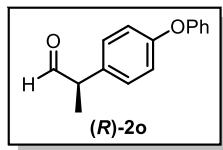
mAU



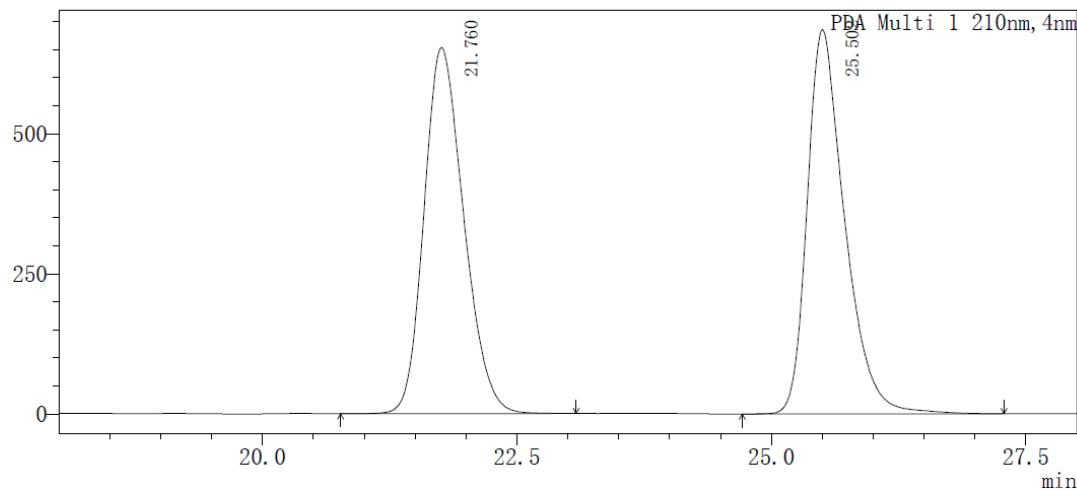
<Peak Results>

PDA Ch1 202nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.767	186947	3046245	5.443
2	9.439	2622306	52922037	94.557



mAU

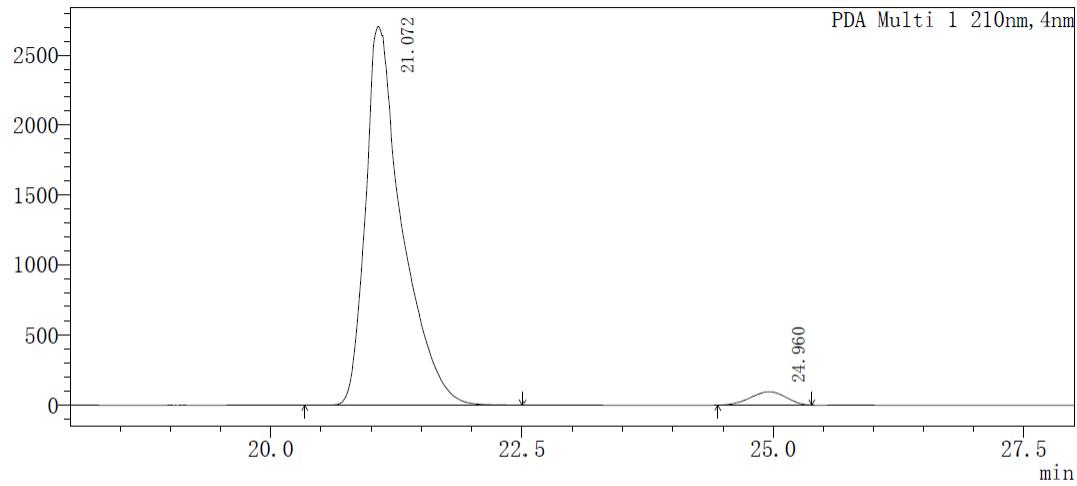


<Peak Results>

PDA Ch1 210nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	21.760	653246	17753977	50.242
2	25.502	685566	17583082	49.758

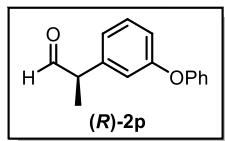
mAU



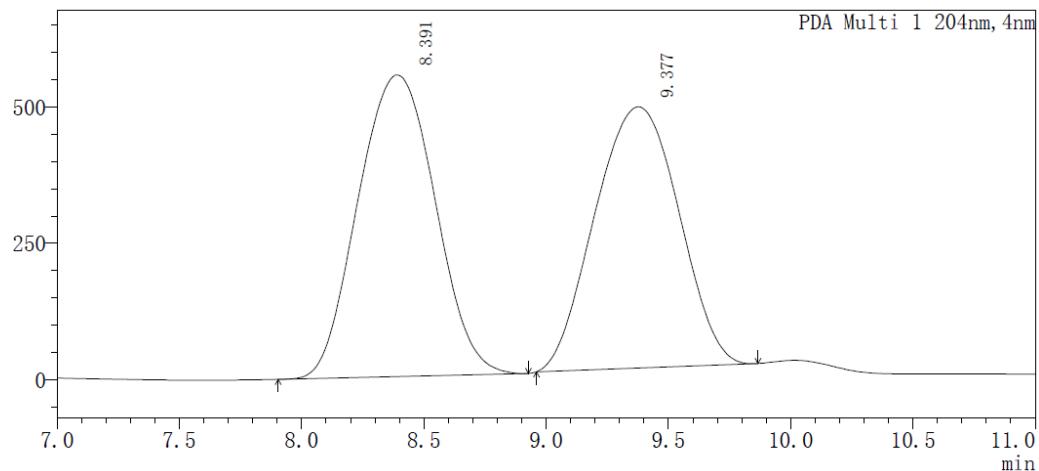
<Peak Results>

PDA Ch1 210nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	21.072	2704315	68537214	96.672
2	24.960	95829	2359255	3.328



mAU

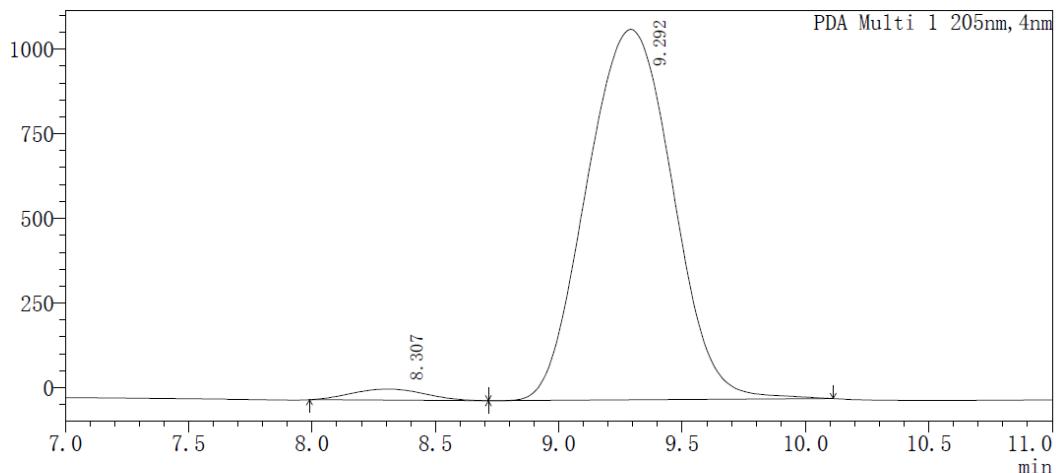


<Peak Results>

PDA Ch1 204nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.391	553323	12157662	51.496
2	9.377	479107	11451161	48.504

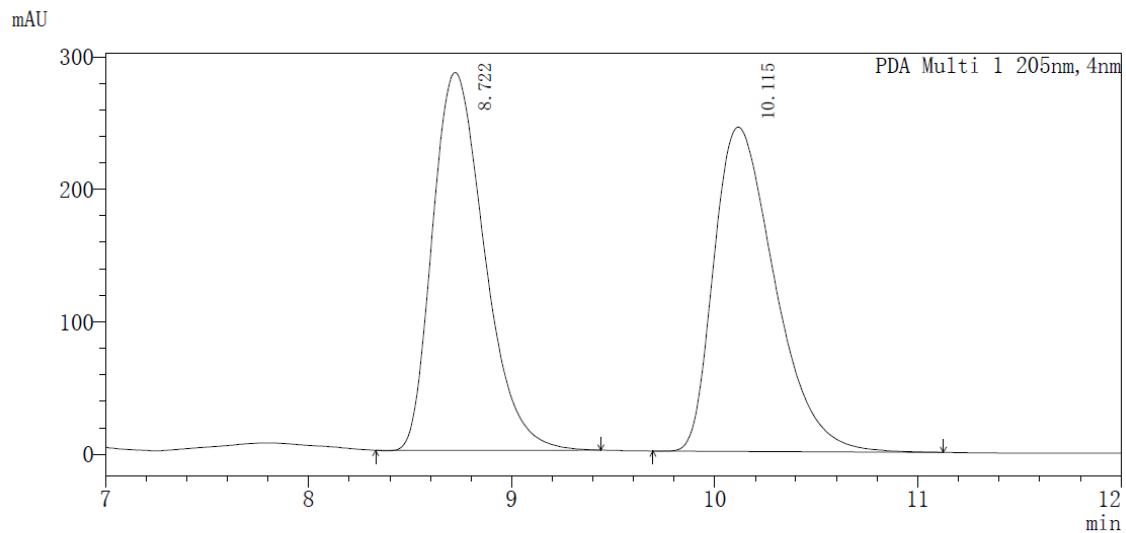
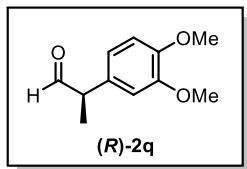
mAU



<Peak Results>

PDA Ch1 205nm

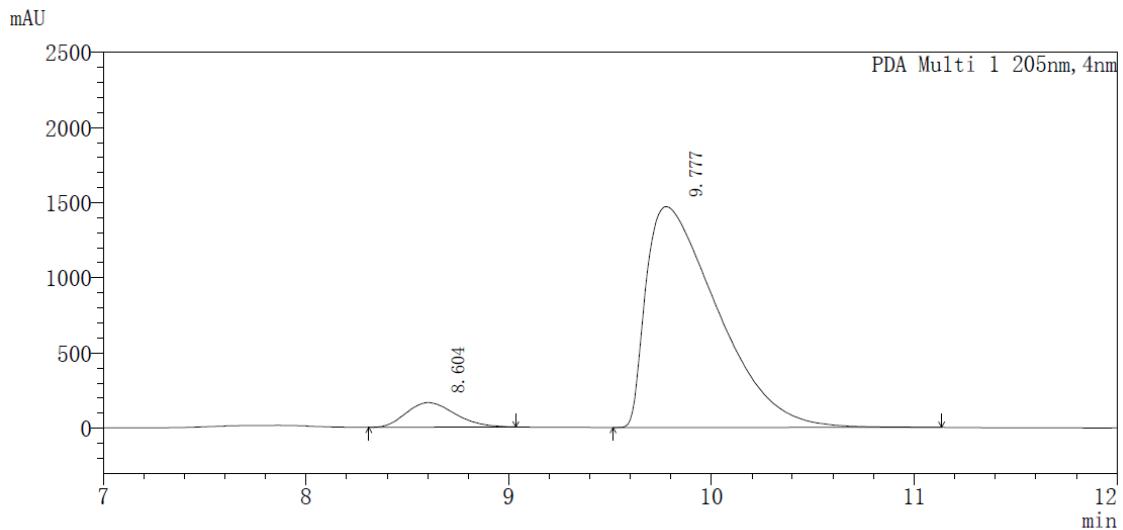
Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.307	32918	673824	2.480
2	9.292	1094767	26493533	97.520



<Peak Results>

PDA Ch1 205nm

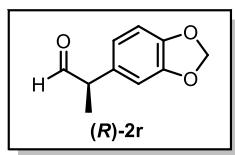
Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.722	285207	5074182	49.835
2	10.115	244906	5107689	50.165



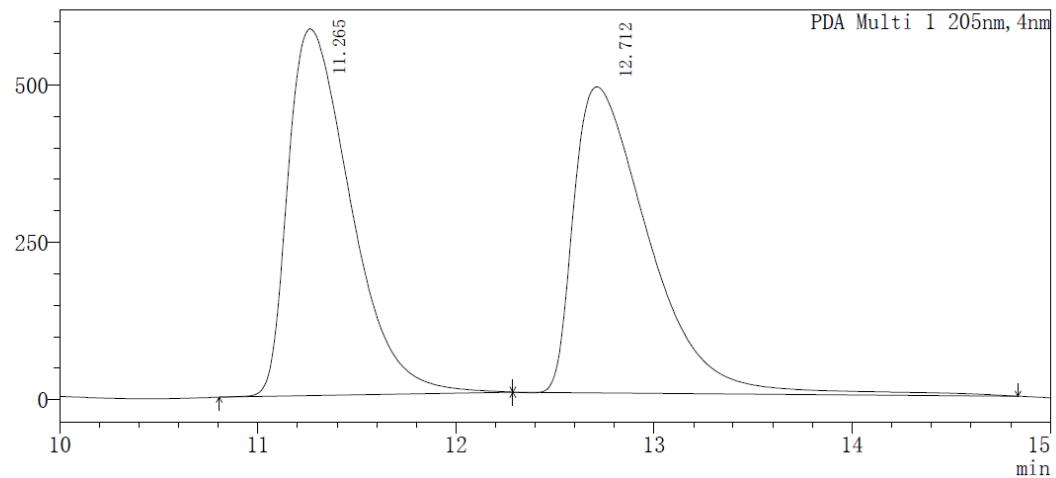
<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.604	162928	2725928	7.010
2	9.777	1469119	36157781	92.990



mAU

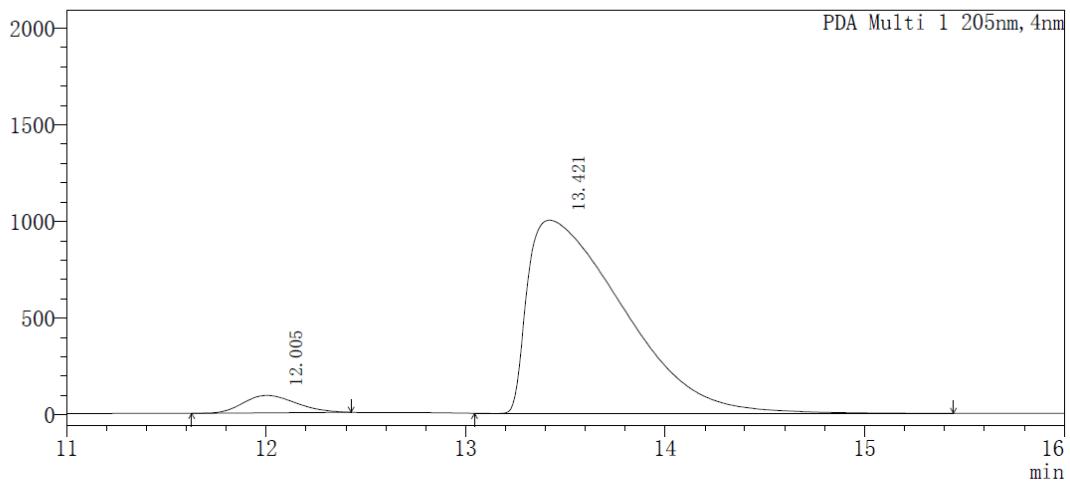


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	11.265	582613	12825098	49.800
2	12.712	485980	12927886	50.200

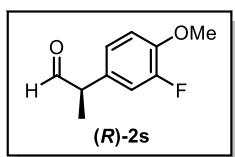
mAU



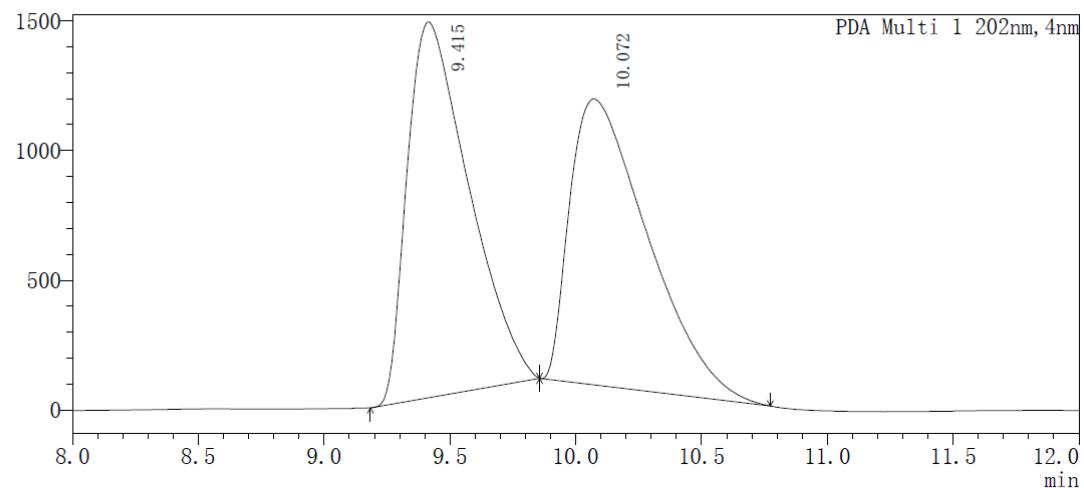
<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.005	90491	1656292	4.742
2	13.421	999057	33272328	95.258



mAU

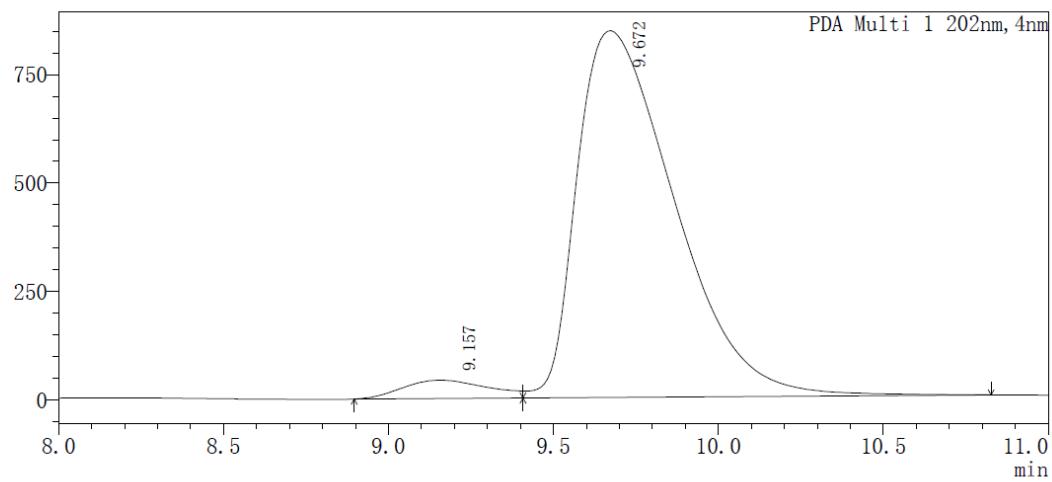


<Peak Results>

PDA Ch1 202nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	9.415	1449007	24764720	50.921
2	10.072	1103874	23868678	49.079

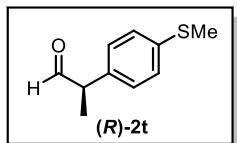
mAU



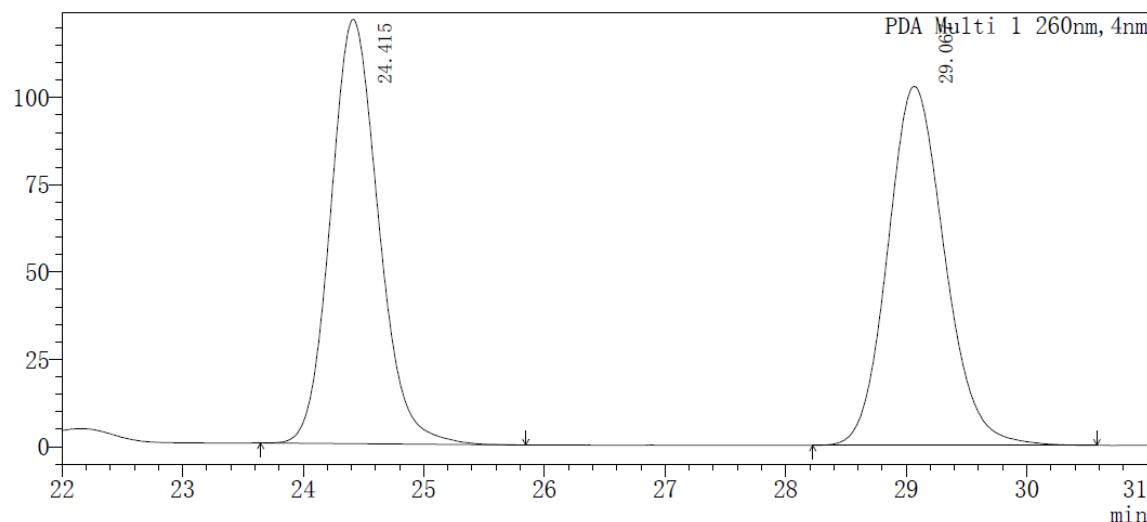
<Peak Results>

PDA Ch1 202nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	9.157	42053	759683	4.185
2	9.672	845063	17393806	95.815



mAU

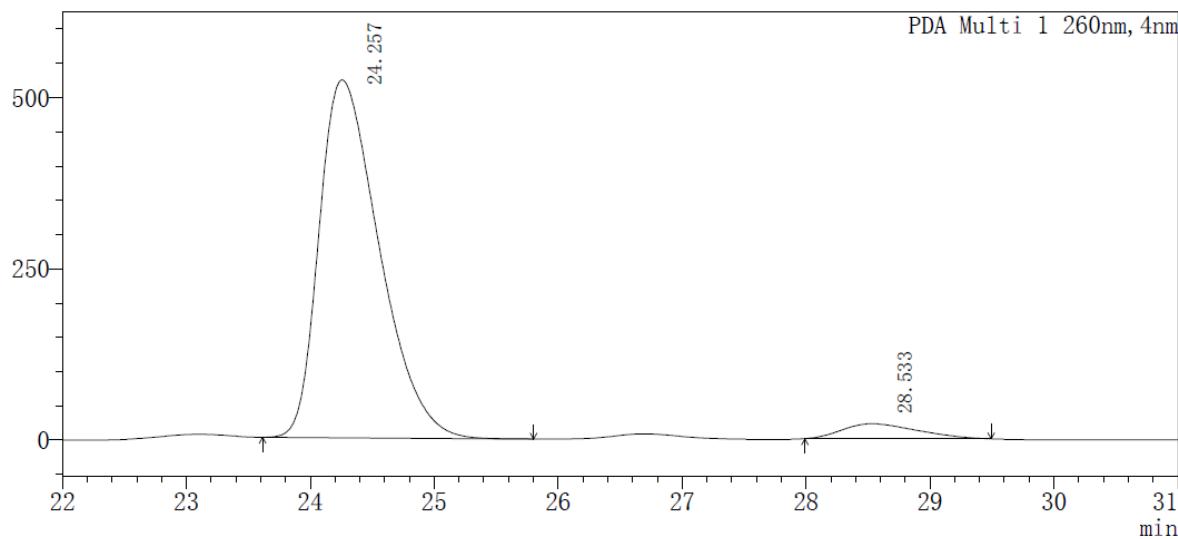


<Peak Results>

PDA Ch1 260nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	24.415	121504	3356798	49.847
2	29.067	102827	3377467	50.153

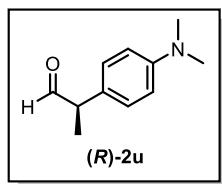
mAU



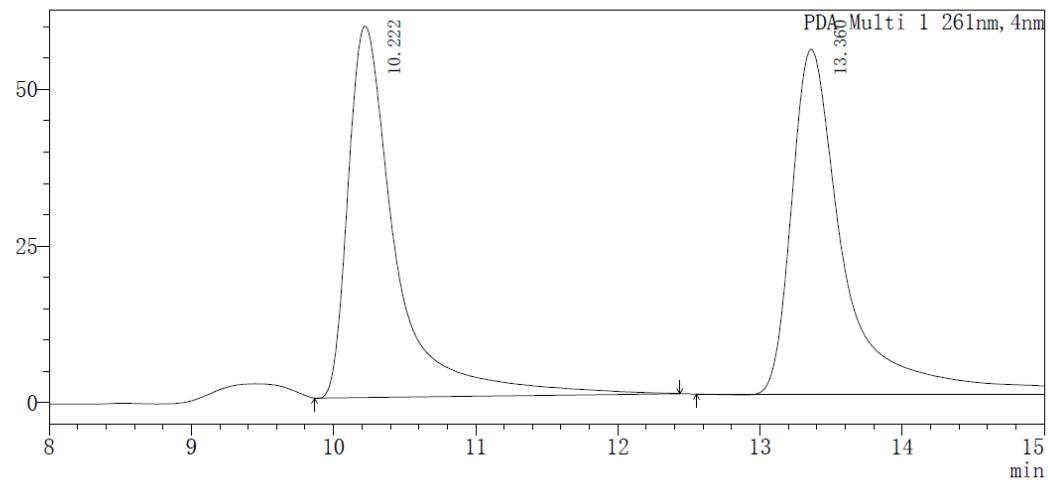
<Peak Results>

PDA Ch1 260nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	24.257	522561	17640022	95.020
2	28.533	21901	924470	4.980



mAU

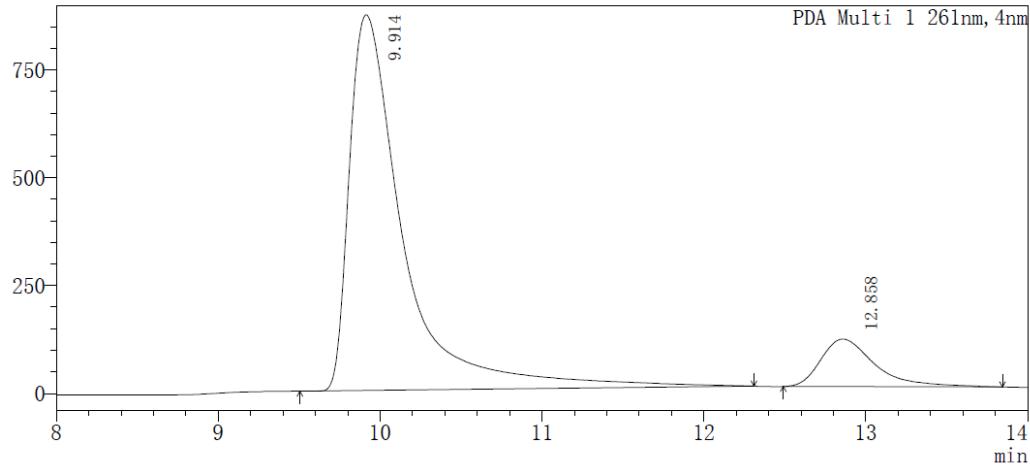


<Peak Results>

PDA Ch1 261nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	10.222	59282	1386543	48.870
2	13.360	54971	1450641	51.130

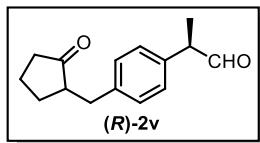
mAU



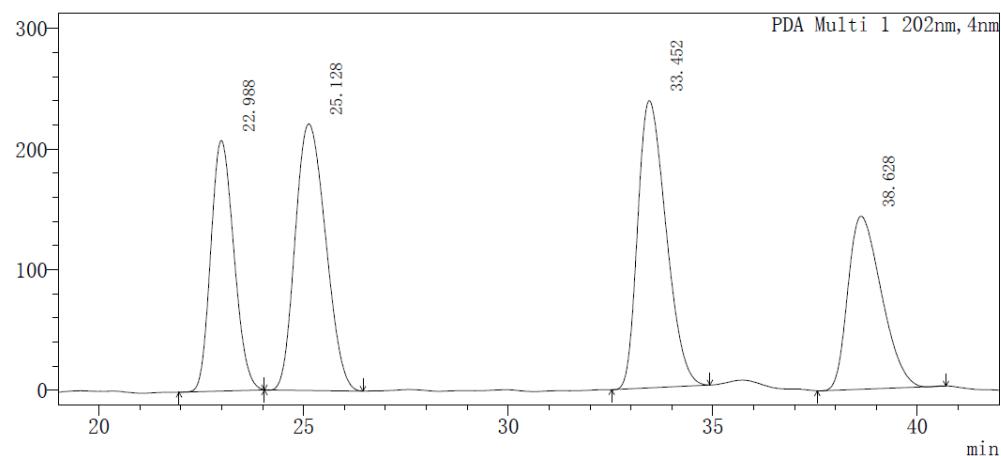
<Peak Results>

PDA Ch1 261nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	9.914	870604	20244518	88.808
2	12.858	110140	2551369	11.192



mAU

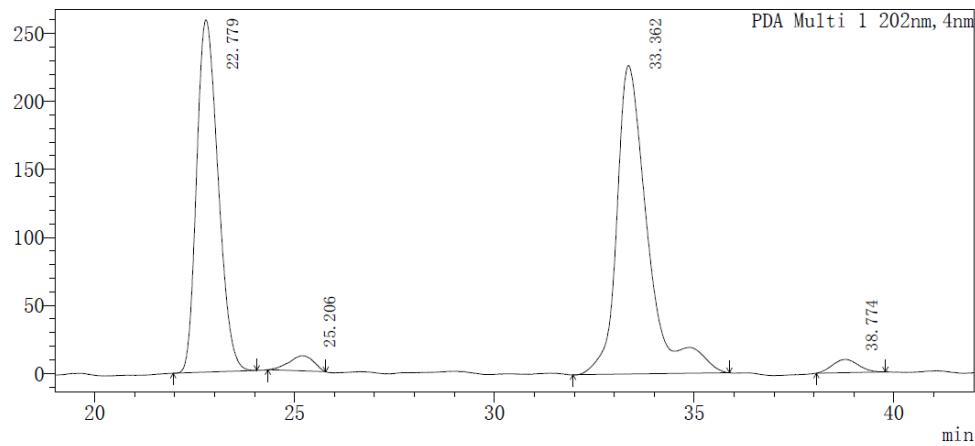


<Peak Results>

PDA Ch1 202nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	22.988	207724	8172972	20.818
2	25.128	220994	11413027	29.071
3	33.452	238169	11498145	29.288
4	38.628	143422	8175077	20.823

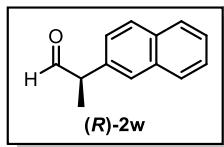
mAU



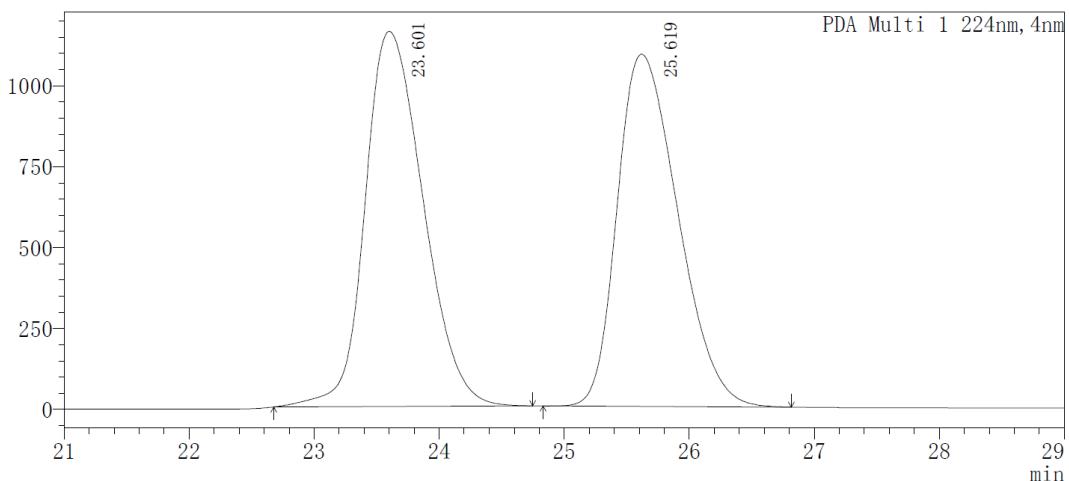
<Peak Results>

PDA Ch1 202nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	22.779	259048	9694774	42.509
2	25.206	11127	476125	2.088
3	33.362	226967	12193793	53.466
4	38.774	9869	441927	1.938



mAU

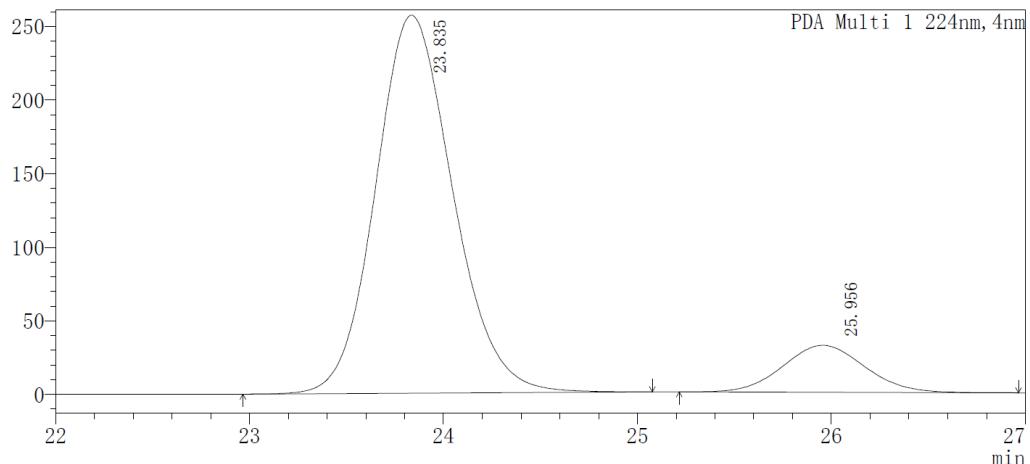


<Peak Results>

PDA Ch1 224nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	23.601	1159894	37508305	50.511
2	25.619	1089339	36749567	49.489

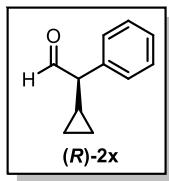
mAU



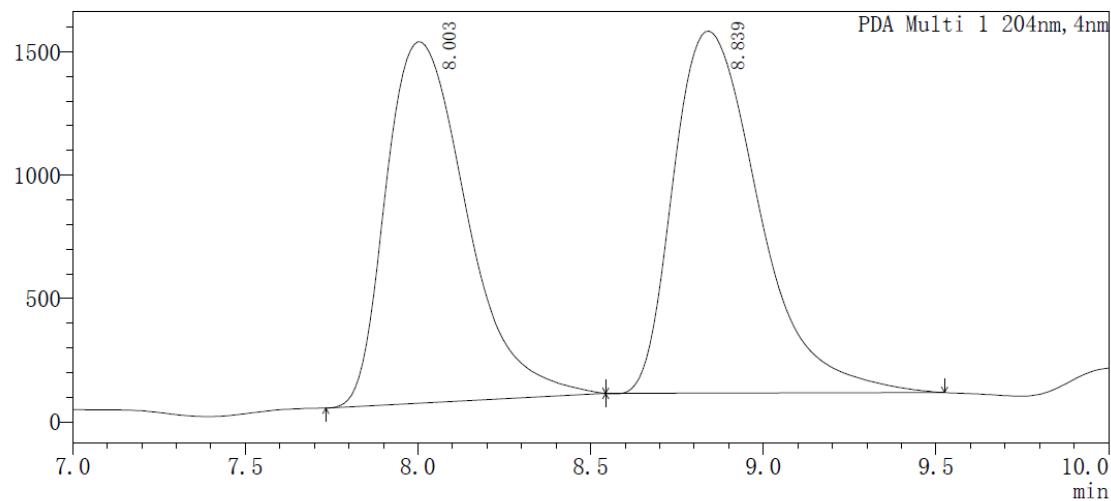
<Peak Results>

PDA Ch1 224nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	23.835	256710	7120072	88.362
2	25.956	31846	937732	11.638



mAU

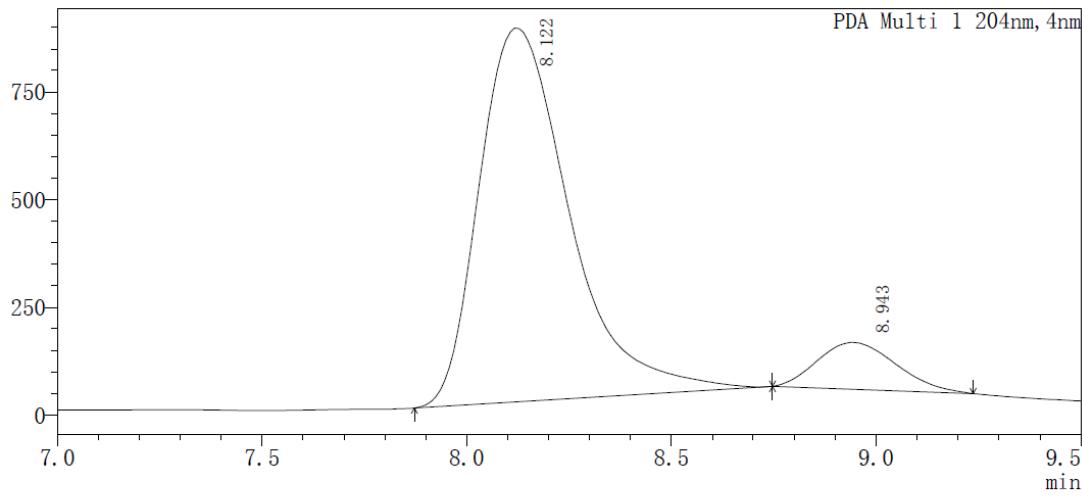


<Peak Results>

PDA Ch1 204nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.003	1464302	23790595	48.440
2	8.839	1466186	25323350	51.560

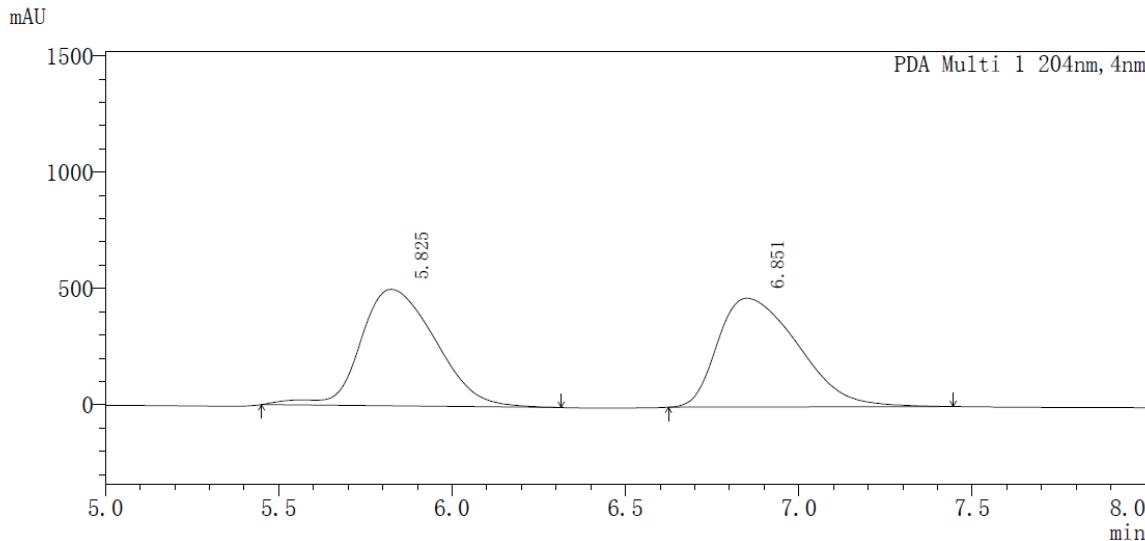
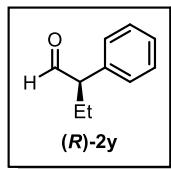
mAU



<Peak Results>

PDA Ch1 204nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.122	867759	13337960	90.217
2	8.943	108615	1446402	9.783

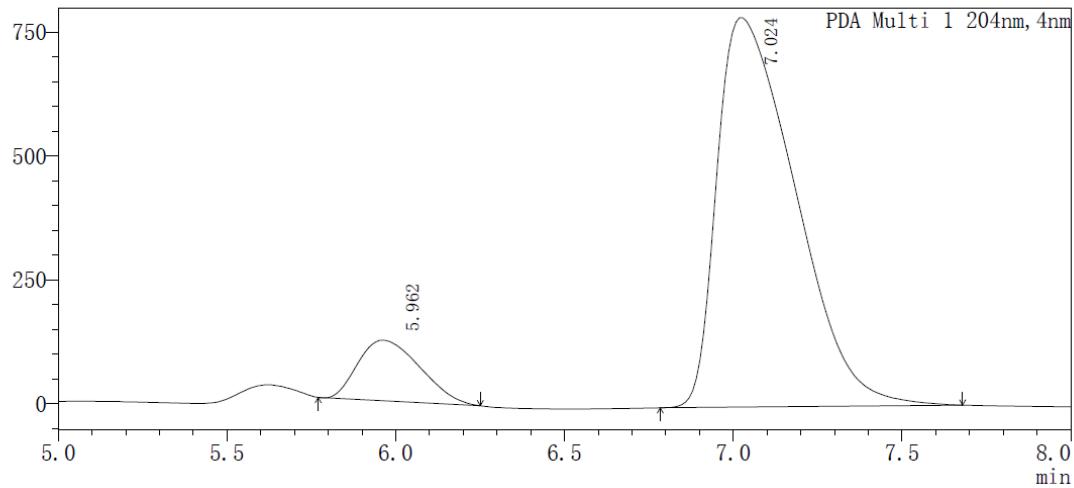


<Peak Results>

PDA Ch1 204nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	5.825	501337	7525208	49.923
2	6.851	468196	7548481	50.077

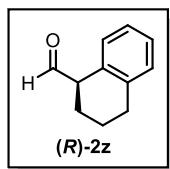
mAU



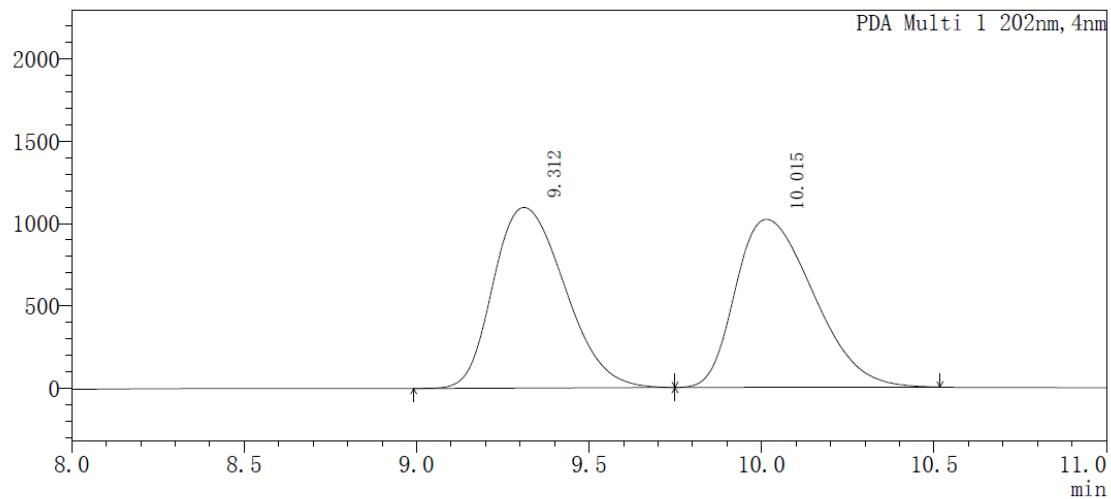
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PDA Ch1 204nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	5.962	122565	1563194	10.977
2	7.024	785698	12677304	89.023



mAU

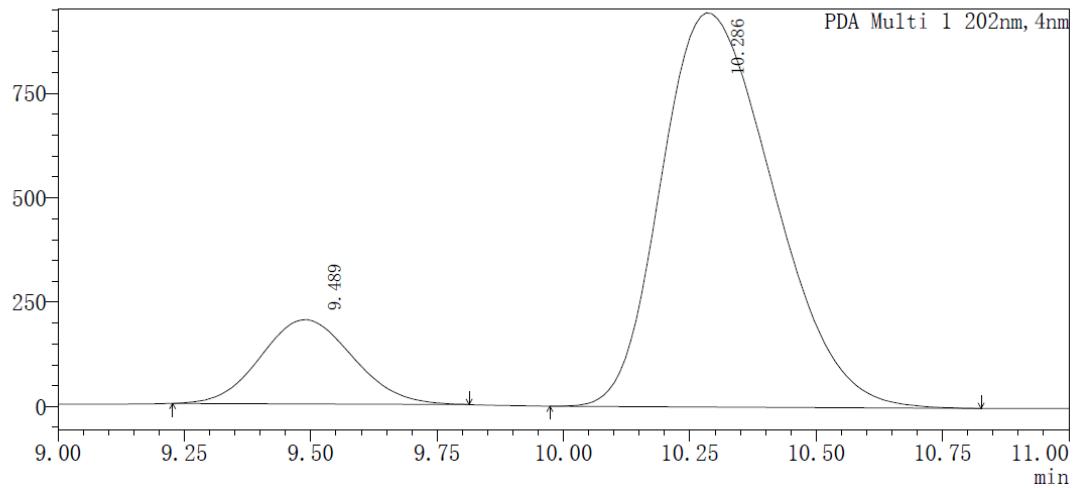


<Peak Results>

PDA Ch1 202nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	9.312	1097463	15827297	49.650
2	10.015	1020816	16050657	50.350

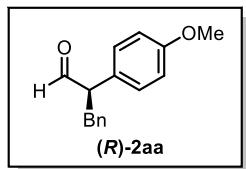
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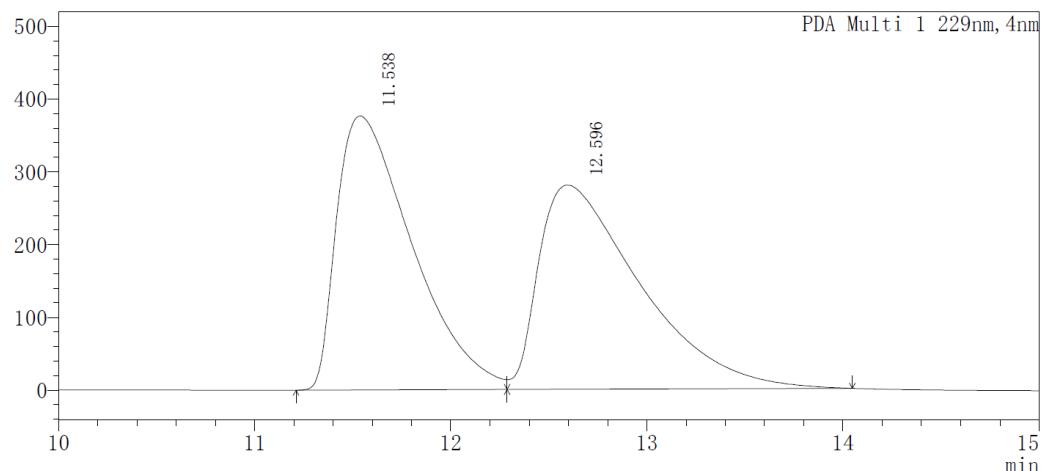
<Peak Results>

PDA Ch1 202nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	9.489	201778	2565034	15.001
2	10.286	943936	14534079	84.999



mAU

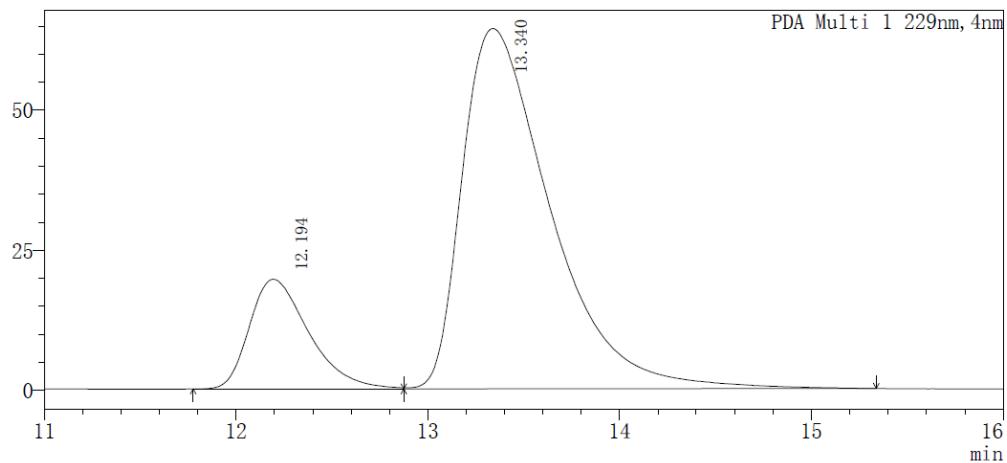


<Peak Results>

PDA Ch1 229nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	11.538	376341	10087782	49.960
2	12.596	280616	10103869	50.040

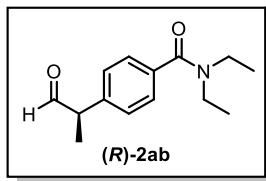
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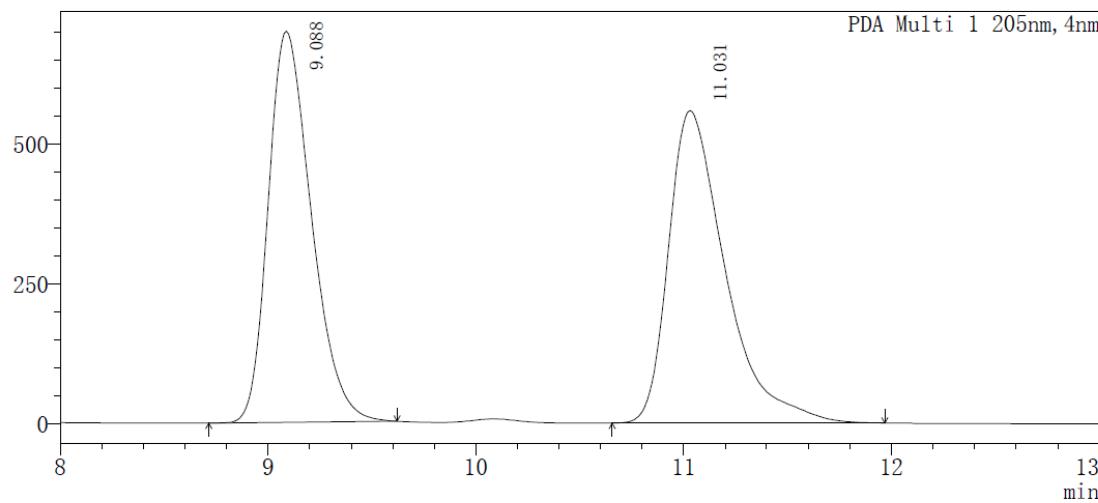
<Peak Results>

PDA Ch1 229nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.194	19601	421023	16.958
2	13.340	64349	2061713	83.042



mAU

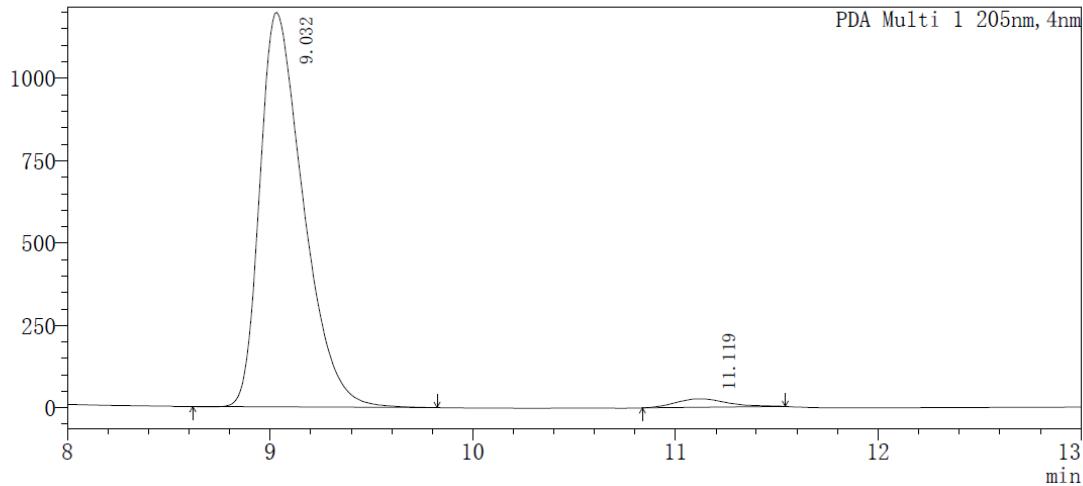


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	9.088	698749	10100098	48.838
2	11.031	558296	10580895	51.162

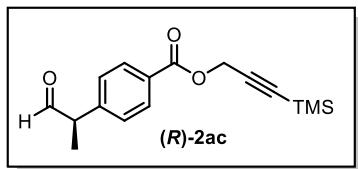
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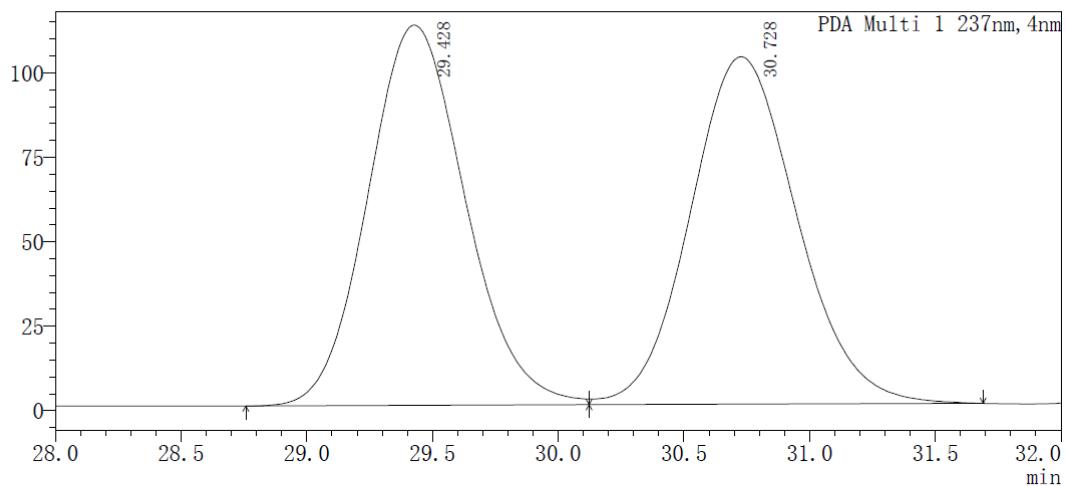
<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	9.032	1197342	17825777	97.503
2	11.119	25810	456444	2.497



mAU

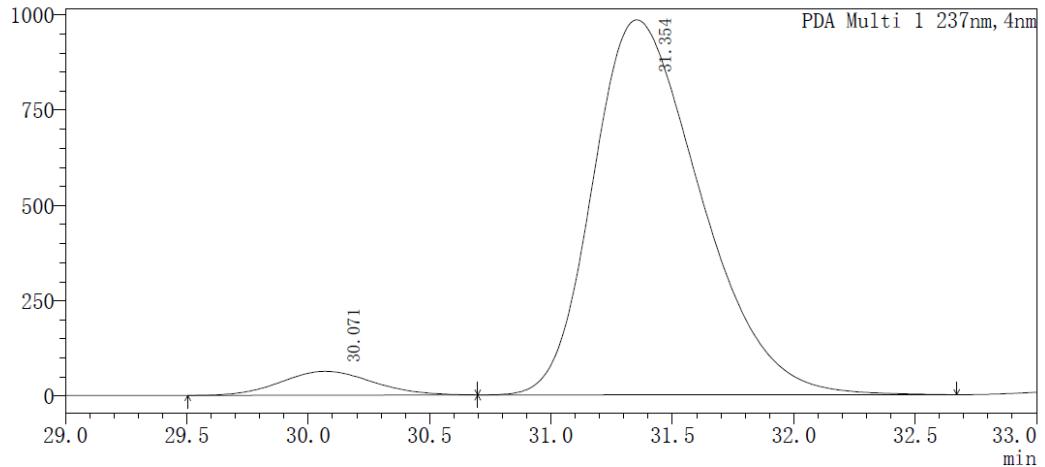


<Peak Results>

PDA Ch1 237nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	29.428	112607	3041130	49.991
2	30.728	102863	3042249	50.009

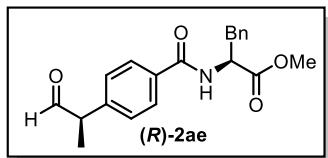
mAU



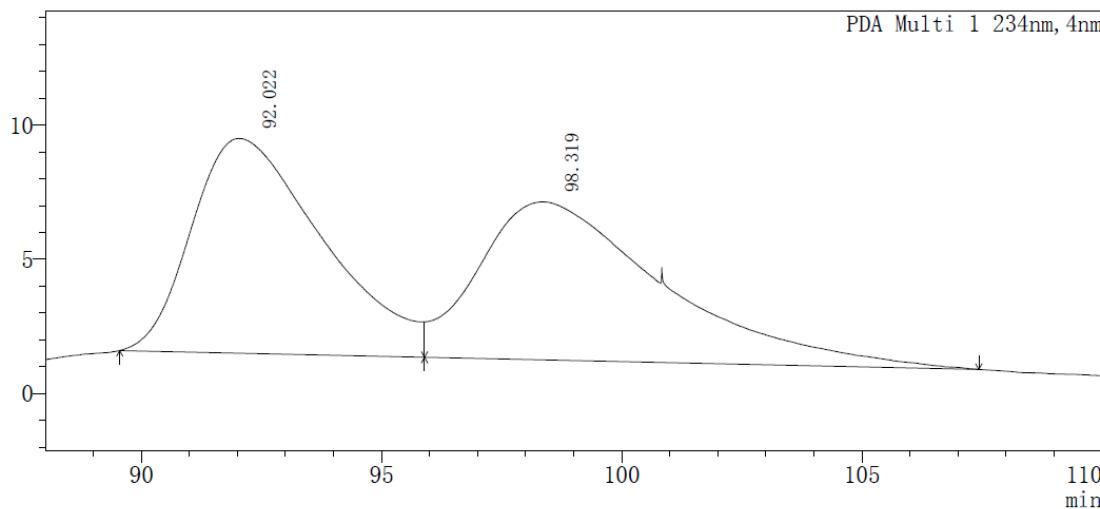
<Peak Results>

PDA Ch1 237nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	30.071	62495	1643621	5.131
2	31.354	983715	30386438	94.869



mAU

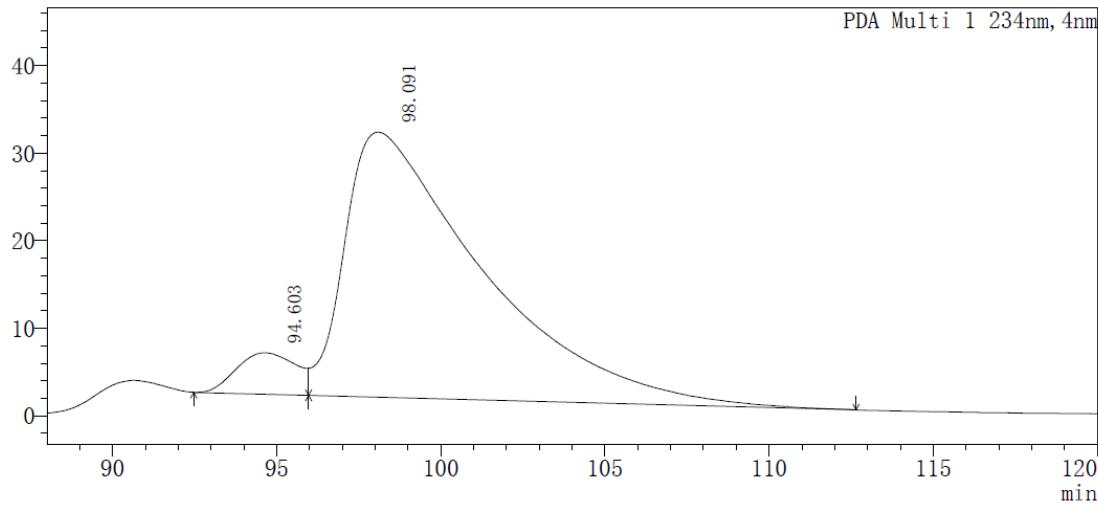


<Peak Results>

PDA Ch1 234nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	92.022	7999	1520564	48.979
2	98.319	5887	1583948	51.021

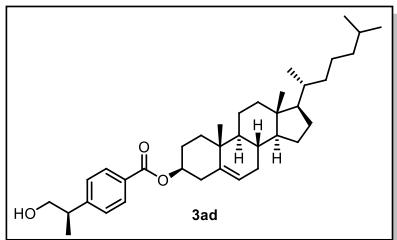
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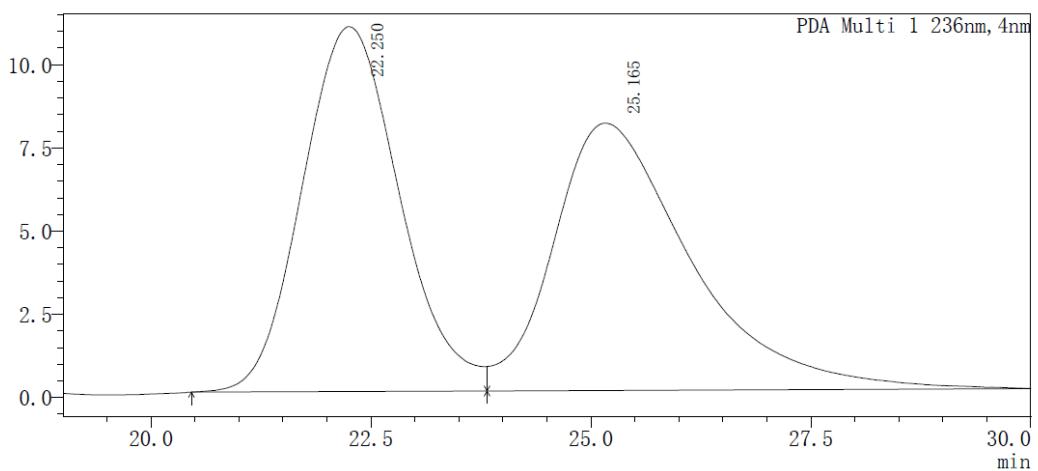
<Peak Results>

PDA Ch1 234nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	94.603	4739	598631	6.337
2	98.091	30265	8847897	93.663



mAU

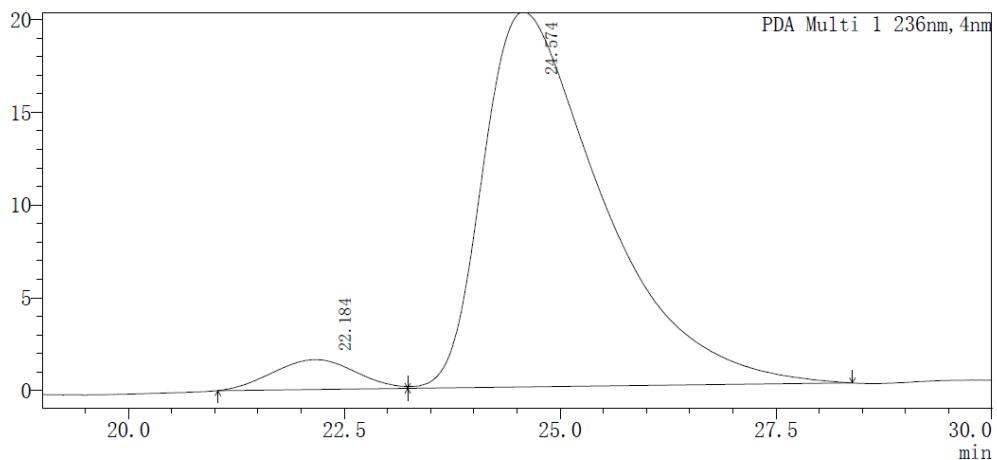


<Peak Results>

PDA Ch1 236nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	22.250	10965	842818	49.094
2	25.165	8031	873926	50.906

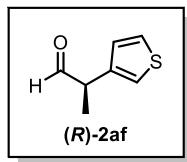
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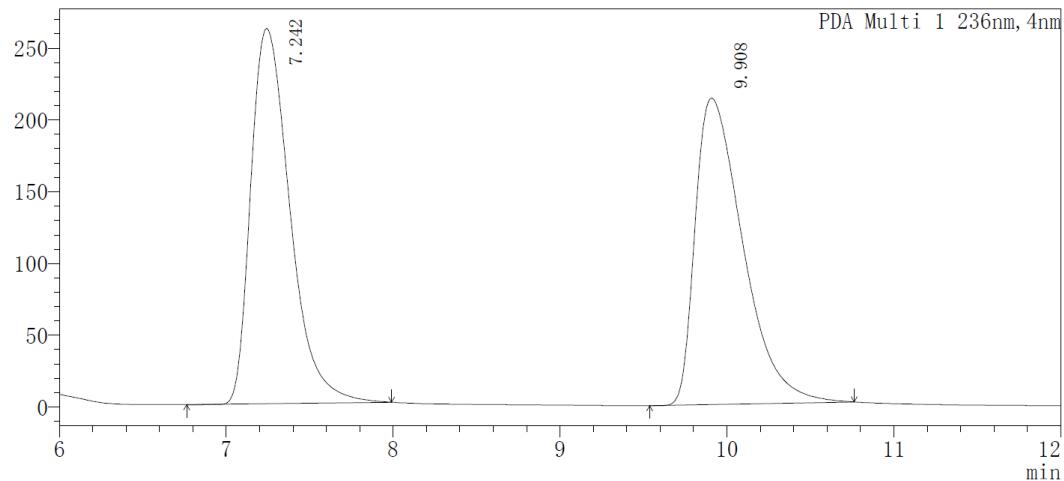
<Peak Results>

PDA Ch1 236nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	22.184	1606	106646	5.190
2	24.574	20215	1948009	94.810



mAU

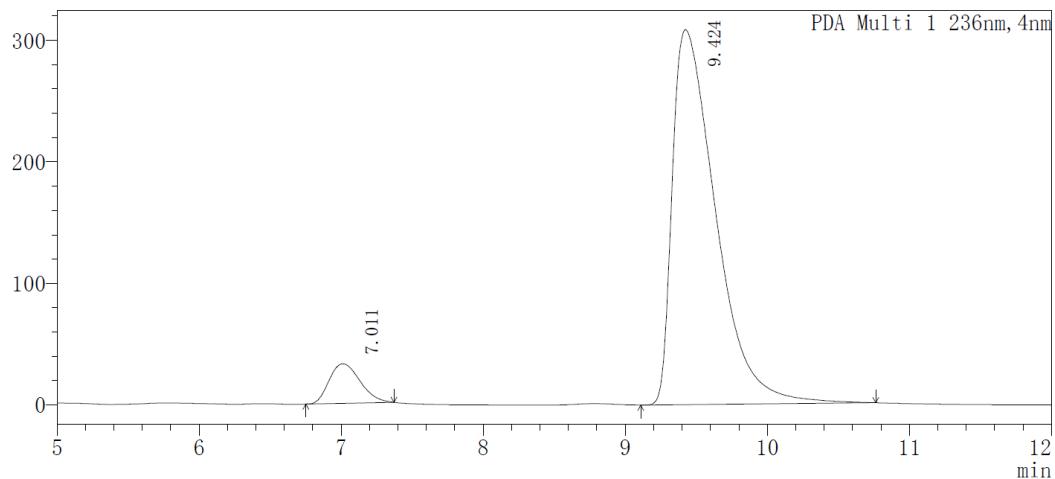


<Peak Results>

PDA Ch1 236nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	7.242	261497	4257605	50.104
2	9.908	213528	4239915	49.896

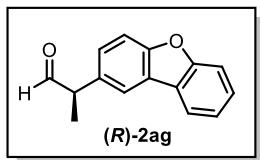
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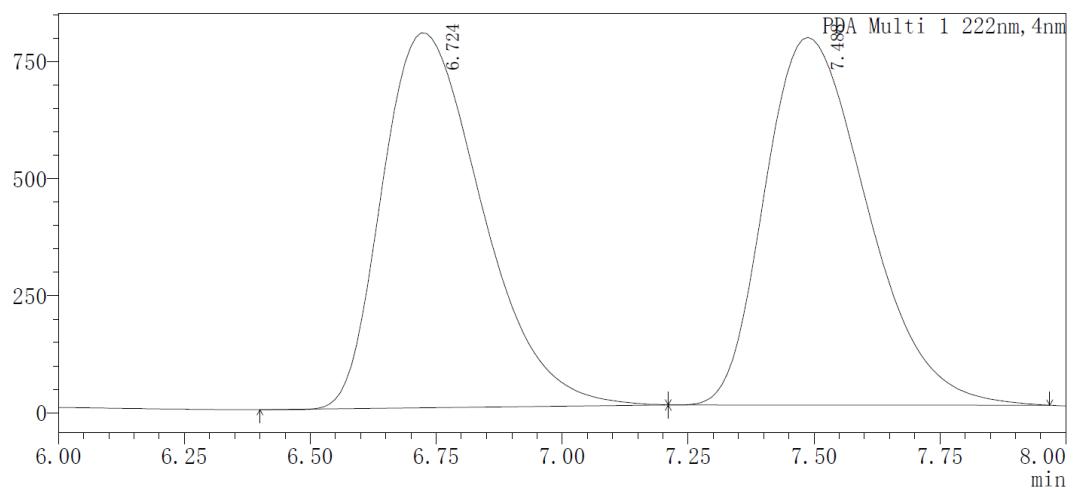
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PDA Ch1 236nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	7.011	32616	494133	7.023
2	9.424	308294	6541723	92.977



mAU

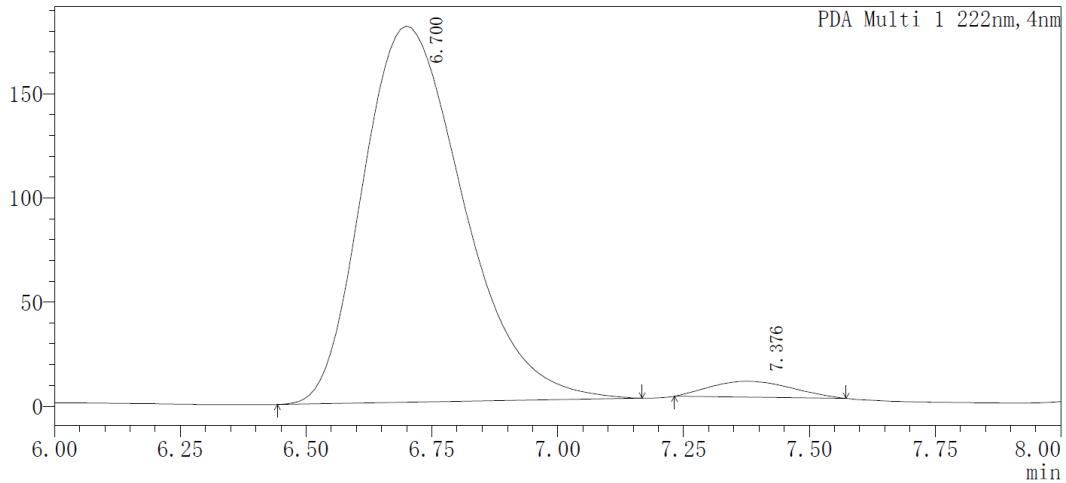


<Peak Results>

PDA Ch1 222nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	6.724	799903	11030142	49.848
2	7.488	784504	11097527	50.152

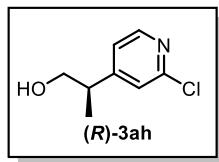
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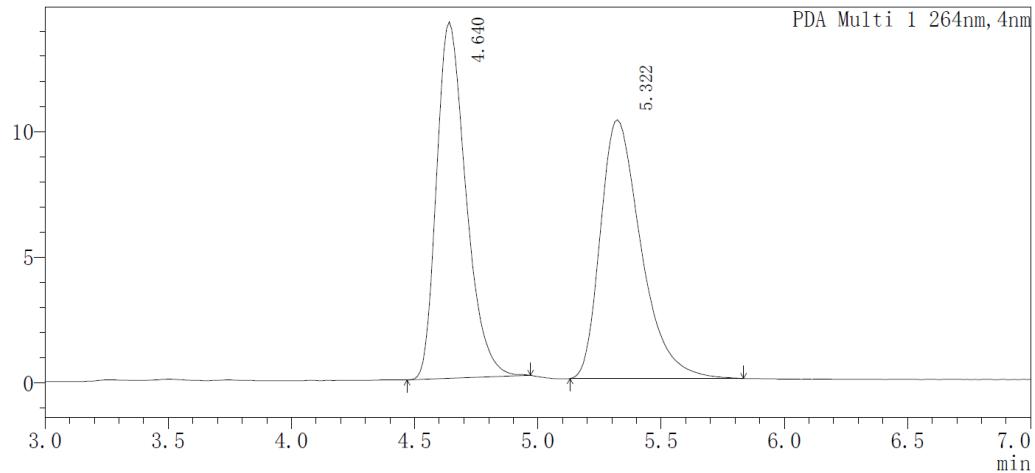
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PDA Ch1 222nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	6.700	180443	2516254	96.726
2	7.376	7568	85176	3.274



mAU

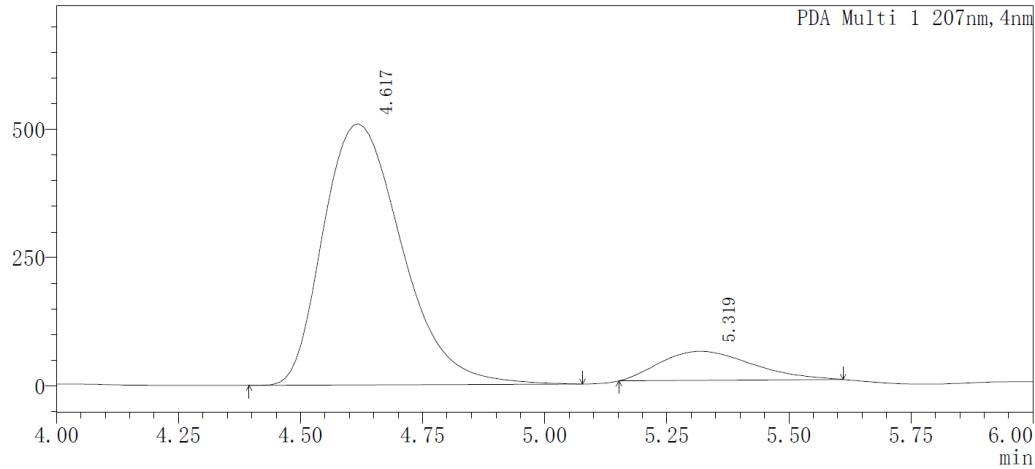


<Peak Results>

PDA Ch1 264nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	4.640	14189	117621	49.888
2	5.322	10295	118149	50.112

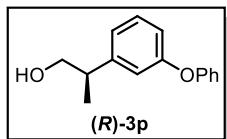
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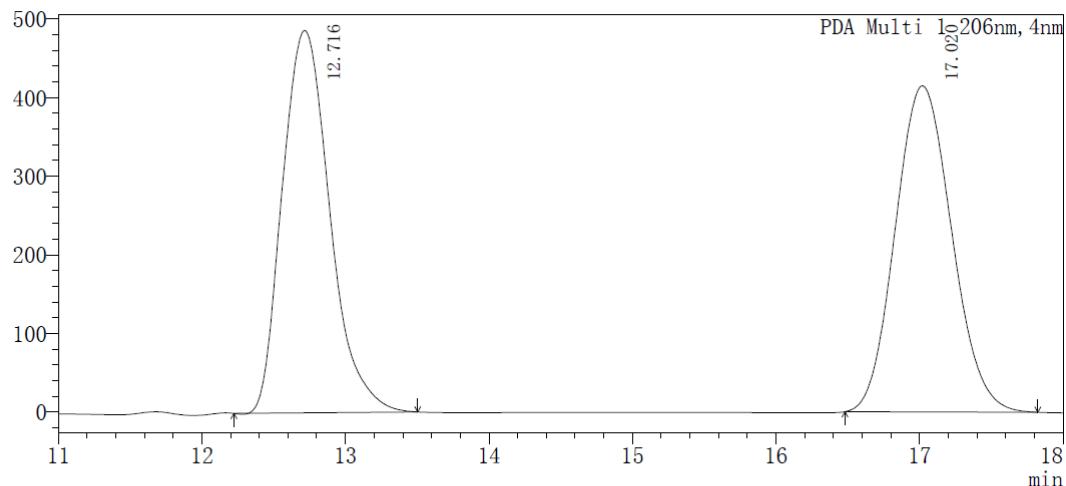
<Peak Results>

PDA Ch1 207nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	4.617	508836	5697800	88.422
2	5.319	56395	746059	11.578



mAU

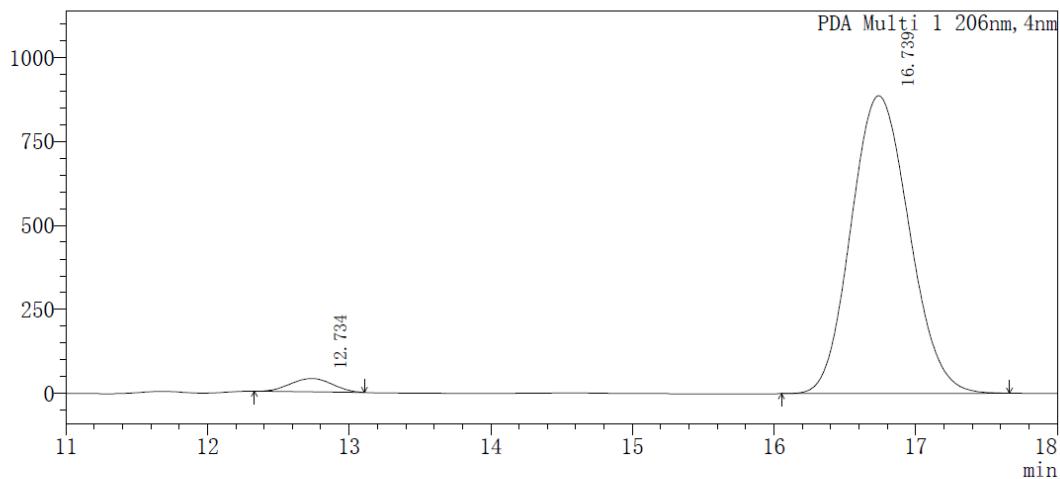


<Peak Results>

PDA Ch1 206nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.716	487024	11200014	49.701
2	17.020	415051	11334786	50.299

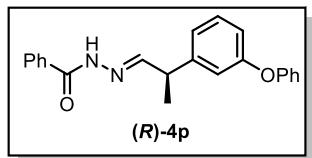
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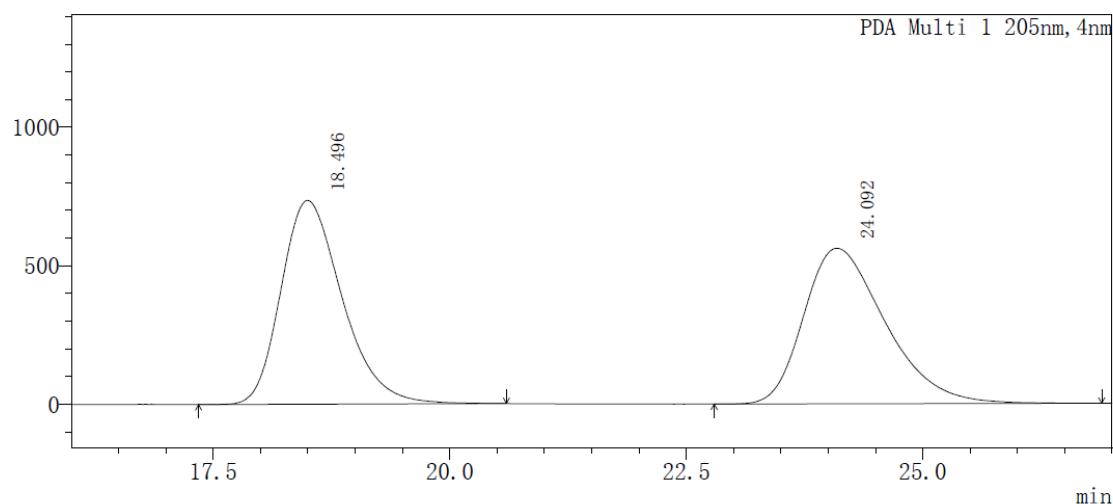
<Peak Results>

PDA Ch1 206nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.734	39682	812881	3.117
2	16.739	886246	25262971	96.883



mAU

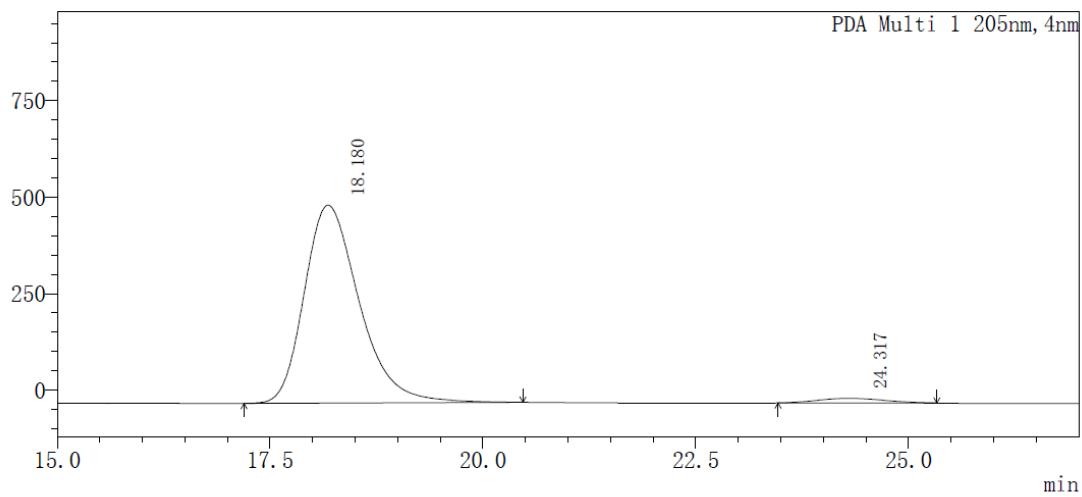


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	18.496	735567	33161987	49.605
2	24.092	561910	33690764	50.395

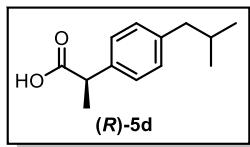
mAU



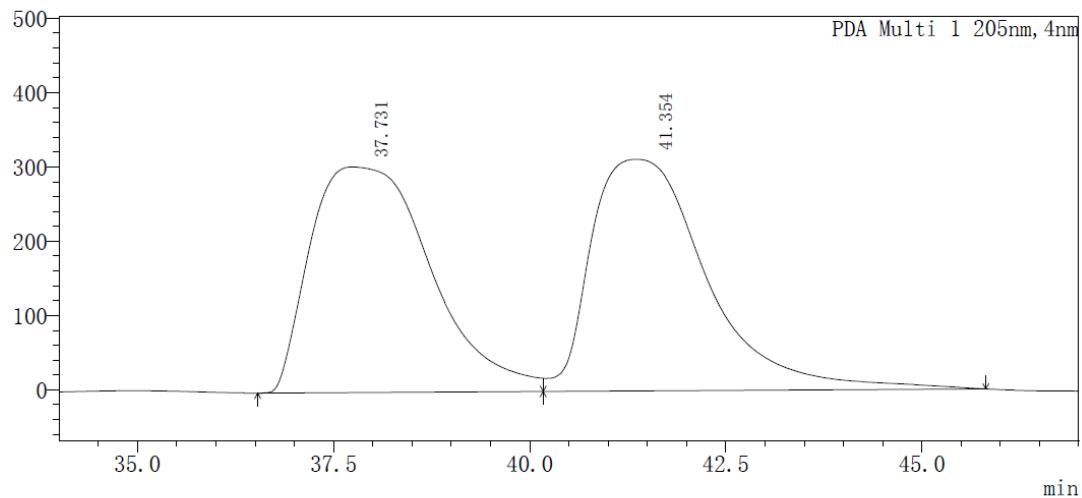
<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	18.180	512829	23038918	97.248
2	24.317	12070	651897	2.752



mAU

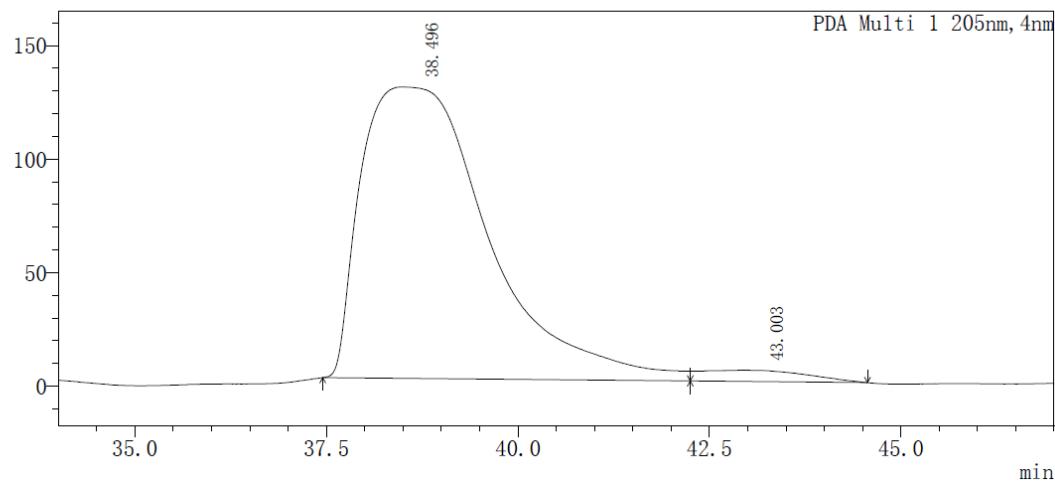


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	37.731	303834	32428433	50.287
2	41.354	311820	32058304	49.713

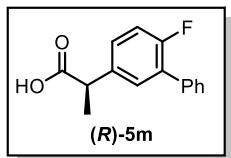
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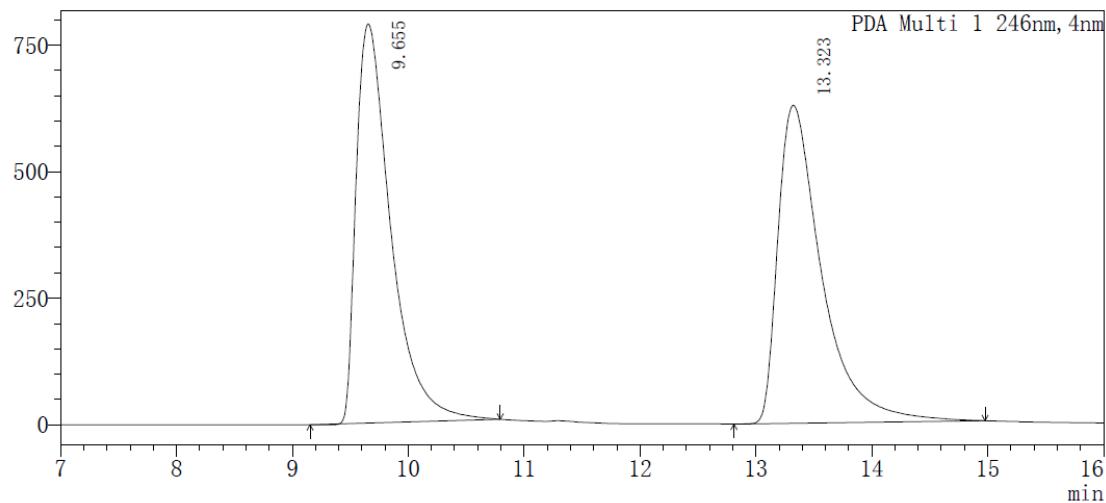
<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	38.496	128437	14865282	96.861
2	43.003	4960	481756	3.139



mAU

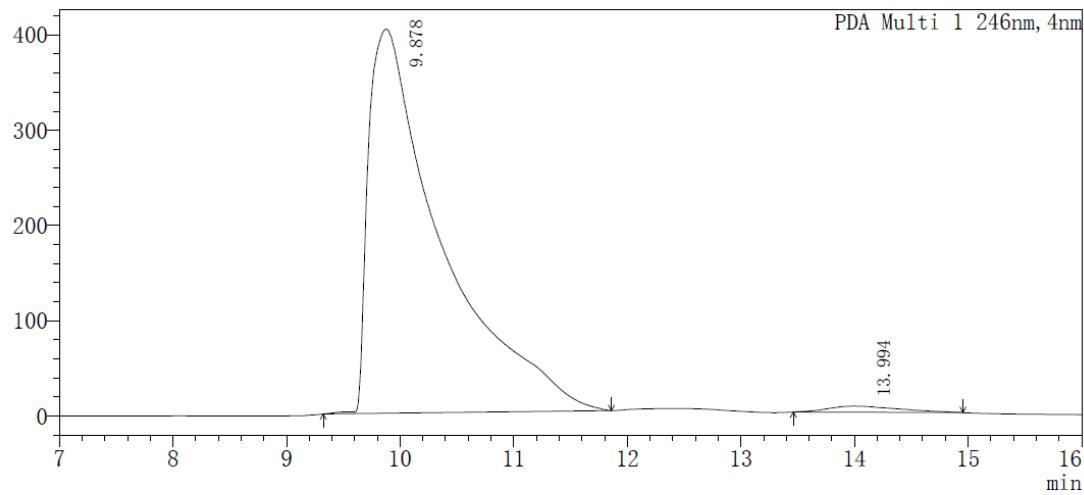


<Peak Results>

PDA Ch1 246nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	9.655	788372	16398489	49.798
2	13.323	628028	16531504	50.202

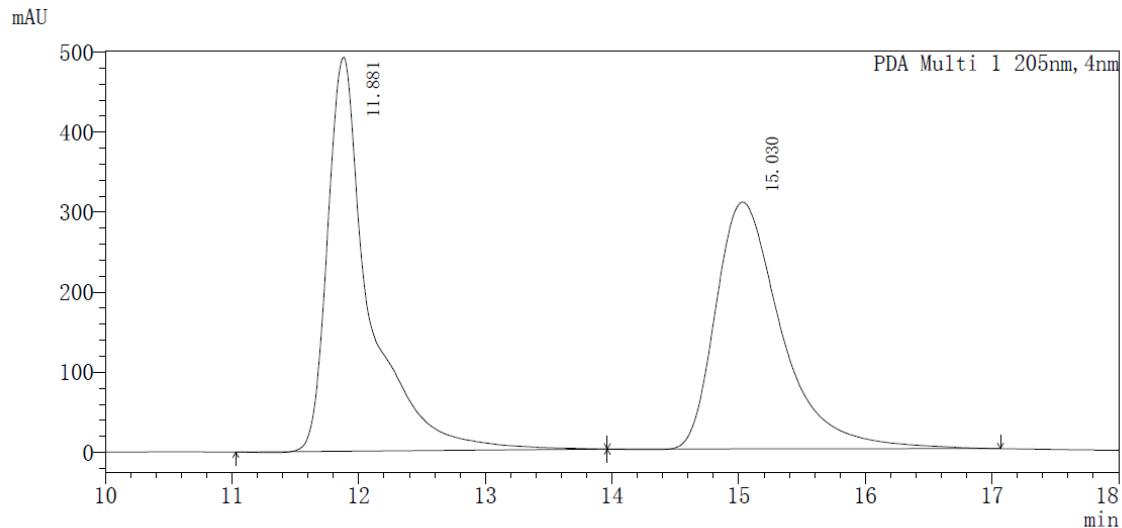
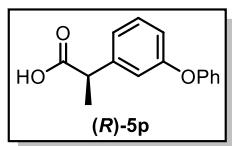
mAU



<Peak Results>

PDA Ch1 246nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	9.878	403229	17973896	98.452
2	13.994	6385	282628	1.548

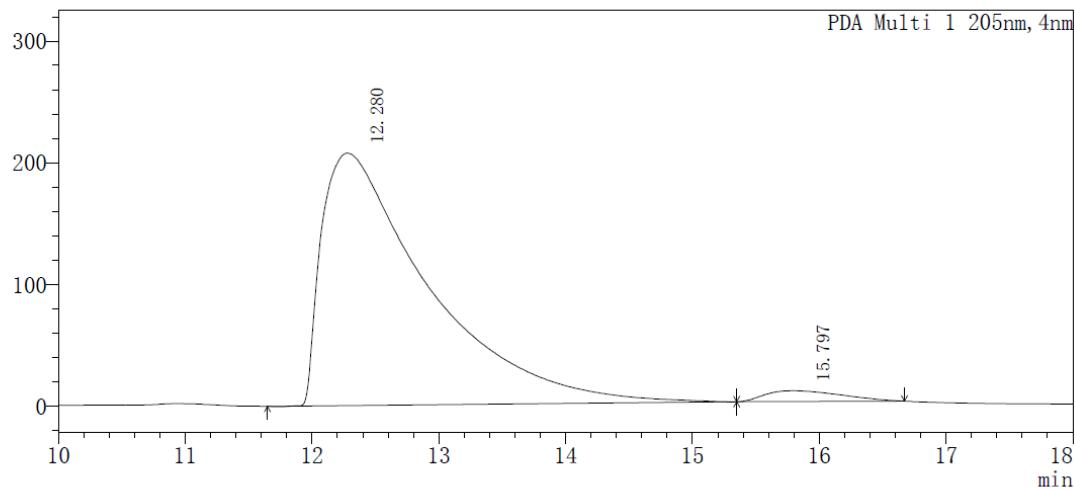


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	11.881	492520	11356637	50.482
2	15.030	308532	11139598	49.518

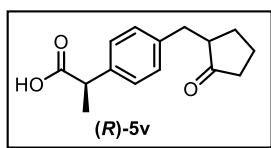
mAU



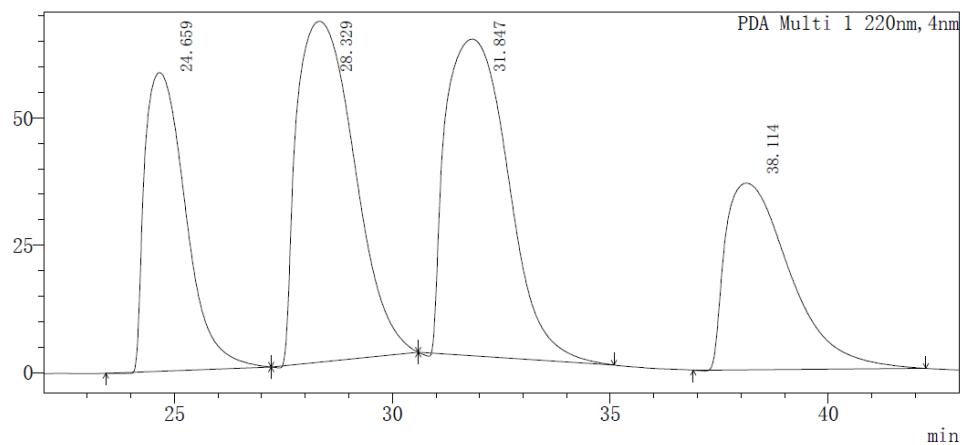
<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.280	207430	12127735	97.020
2	15.797	8956	372508	2.980



mAU

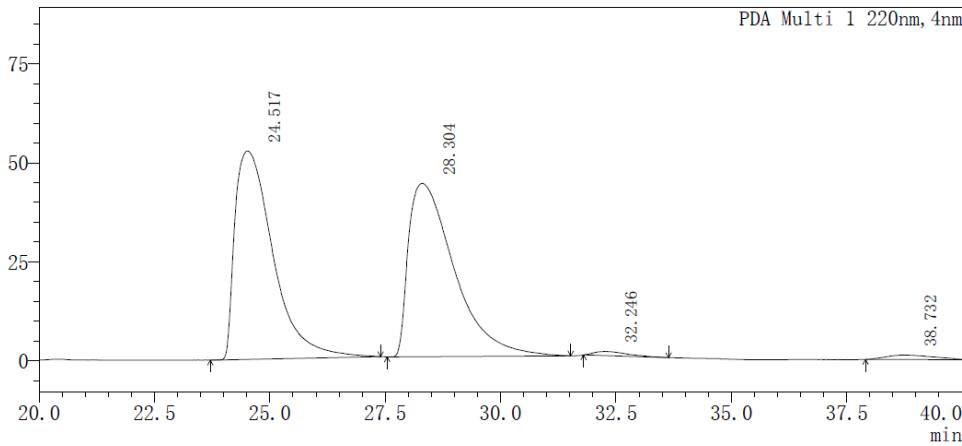


<Peak Results>

PDA Ch1 220nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	24.659	58615	3830607	19.166
2	28.329	66900	6156500	30.803
3	31.847	62153	6209042	31.066
4	38.114	36625	3790376	18.965

mAU



<Peak Results>

PDA Ch1 220nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	24.517	52614	3029919	48.929
2	28.304	43749	3032448	48.970
3	32.246	1048	52055	0.841
4	38.732	1087	78043	1.260

References and Notes

1. S. E. Denmark, J. R. Heemstra Jr., G. L. Beutner, Catalytic, enantioselective, vinylogous aldol reactions. *Angew. Chem. Int. Ed.* **44**, 4682–4698 (2005).
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