SUPPORTING INFORMATION

Tryptophan/Copper-Catalyzed Aromatization of Chiral Cyclohexanones to Phenols

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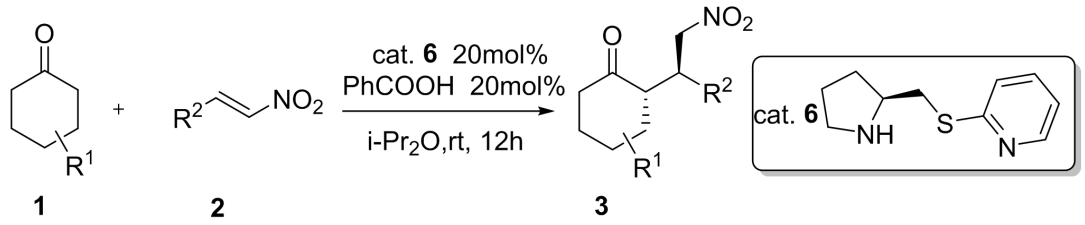
1. General information

The ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ at 500 MHz and 125 MHz, respectively, with TMS as the internal standard. GC-MS experiments were performed on a GC system with a mass selective detector. HRMS data were measured on a LC/TOF-MS with ESI source or GC/TOF-MS with EI source. Column chromatography and flash chromatography experiments were performed on silica gel (200-300 mesh) eluting with ethyl ether and petroleum ether. TLC experiments were carried out on glass-backed silica plates. In each case, enantiomeric ratio was determined on a chiral column in comparison with authentic racemates by chiral HPLC. Chemicals, including compounds **5a**-**5k**, were used without purification as commercially available.

2. Experimental Procedures

Typical Experimental Procedure for the Michael Reaction.

Catalyst **6** (0.2 equiv.), $PhCO_2H$ (0.2 equiv.) and 2 equiv. substituted cyclohexanones **1** were dissolved in 1 mL i-Pr_2O. After the mixture was stirred for 15 min at room temperature, the corresponding nitroolefin **2** (1 equiv.) was added and the mixture was stirred for an appropriate time (monitored by TLC, PE/EA=7/1). The reaction mixture was purified by flash column chromatography on silica gel (PE/EA =20/1 to 5/1) to gain the desired product as oil or solid.

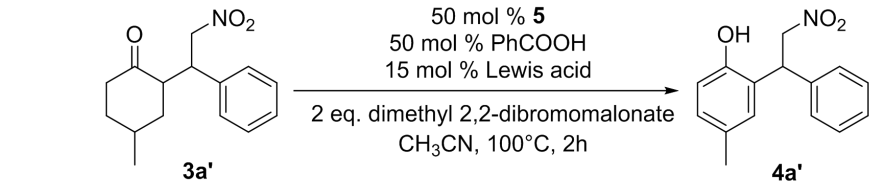


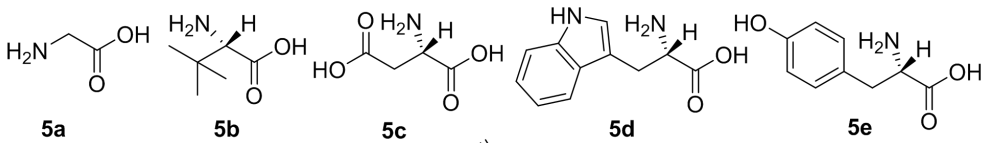
1 **2** **3**

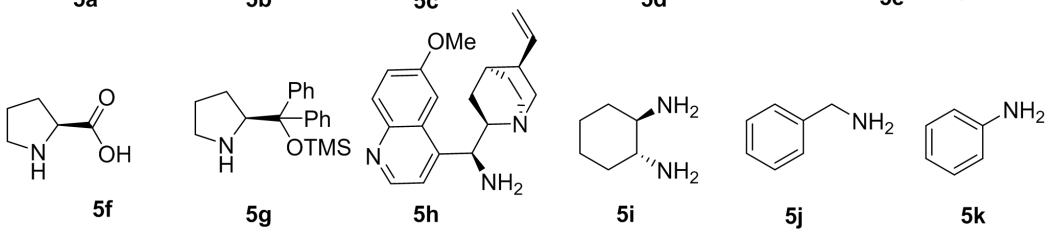
Typical Experimental Procedure for the Aromatization Reaction .

A mixture of Michael adducts **3** (0.5 mmol) , bromating agent (1.0 mmol) , amino acid (0.25 mmol), $PhCO_2H$ (0.25 mmol) and $CuBr_2$ (0.075 mmol) was stirred in redistilled acetonitrile (1 mL). The reaction mixture was heated to 100°C for an appropriate time (monitored by TLC, PE / EA= 7/1). After completion of the reaction (monitored by TLC), the reaction mixture was diluted with brine, and then extracted with ethyl acetate. The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to get the crude product. The product was then purified with silica gel column chromatography (PE-EA).

Table S1. Optimization of the aromatization of **3a'** under various reaction conditions[a].







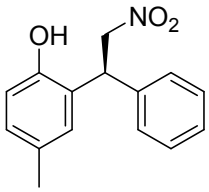
Entry	Solvent	Cat. **5** (X mol %)	Lewis acid (mol %)[b]	Acid (mol %)	T [°C]	Yield (%)[c]
1	CH_3CN	**5a** (50)	/	PhCOOH (50)	100	none
2	CH_3CN	**/**	$CuBr_2$ (15)	PhCOOH (50)	100	none
3	CH_3CN	**5a** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	16
4	CH_3CN	**5b**(50)	$CuBr_2$ (15)	PhCOOH (50)	100	42
5	CH_3CN	**5c** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	57
6	**CH_3CN**	**5d (50)**	**$CuBr_2$ (15)**	**PhCOOH (50)**	**100**	**76**
7	CH_3CN	**5e** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	10
8	CH_3CN	**5f** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	29
9	CH_3CN	**5g** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	56
10	CH_3CN	**5h** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	30
11	CH_3CN	**5i** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	35
12	CH_3CN	**5j** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	19
13	CH_3CN	**5k** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	nd
14	CH_3CN	**5d** (20)	$CuBr_2$ (15)	PhCOOH (50)	100	56
15	CH_3CN	**5d** (100)	$CuBr_2$ (15)	PhCOOH (50)	100	60
16	CH_3CN	**5d** (50)	$CuSO_4$ (15)	PhCOOH (50)	100	20
17	CH_3CN	**5d** (50)	$Cu(OAc)_2$ (15)	PhCOOH (50)	100	42
18	CH_3CN	**5d** (50)	$CuCl_2{\cdot}2H_2O$ (15)	PhCOOH (50)	100	17
19	CH_3CN	**5d** (50)	$Zn(OAc)_2$ (15)	PhCOOH (50)	100	10<
20	CH_3CN	**5d** (50)	$CuBr_2$ (10)	PhCOOH (50)	100	53
21	CH_3CN	**5d** (50)	$CuBr_2$ (30)	PhCOOH (50)	100	60
22	CH_3CN	**5d** (50)	$CuBr_2$ (50)	PhCOOH (50)	100	55
23	CH_3CN	**5d** (50)	$CuBr_2$ (15)	PhCOOH (100)	100	54

24	CH_3CN	**5d** (50)	$CuBr_2$ (15)	4-Me-PhCOOH (50)	100	65
25	CH_3CN	**5d** (50)	$CuBr_2$ (15)	4-CF_3-PhCOOH (50)	100	50
26	CH_3CN	**5d** (50)	$CuBr_2$ (15)	2, 4-diNO_2-PhCOOH (50)	100	52
27	CH_3CN	**5d** (50)	$CuBr_2$ (15)	Isophthalic acid (50)	100	51
28[d]	CH_3CN	**5d** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	27
29[e]	CH_3CN	**5d** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	64
30	CH_3CN	**5d** (50)	$CuBr_2$ (15)	PhCOOH (50)	80	51
31	CH_3CN	**5d** (50)	$CuBr_2$ (15)	PhCOOH (50)	60	20
32	THF	**5d** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	<5
33	MeOH	**5d** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	<5
34	DCM	**5d** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	<5
35	Ethyl ether	**5d** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	<5
36	Toluene	**5d** (50)**)**	$CuBr_2$ (15)	PhCOOH (50)	100	<5
37	Dioxane	**5d** (50)	$CuBr_2$ (15)	PhCOOH (50)	100	65

[a]Unless otherwise stated, the reaction was carried out in 10 mL sealed tube using solvent (1.0 mL), dimethyl 2,2-dibromomalonate (0.2 mmol) and **3a** (0.1 mmol) with 50 mol % **5**, 50 mol % PhCOOH and 15 mol % **6** at 100°C for 2h. [b] Unless otherwise stated, the default of cat.A is $CuBr_2$. [c]Isolated yields after column chromatography. [d]Using N-bromobutanimide instead of dimethyl 2,2-dibromomalonate. [e]Using pyridinium tribromide instead of dimethyl 2,2-dibromomalonate.

3. NMR spectra of aromatization products

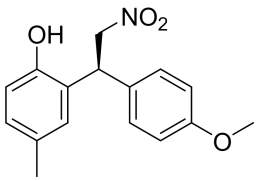
（4a）(S)-4-methyl-2-(2-nitro-1-phenylethyl)phenol.



Na

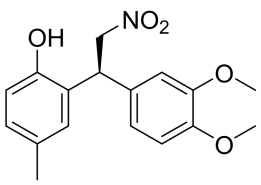
A pale yellow oil. 76% yield, 95% ee. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 10/90, flow rate = 0.8 ml/min, λ = 212 nm): t_{minor} =16.385 min, t_{major} = 17.972 min. ^{1}H NMR (500 MHz, $CDCl_3$) δ(ppm) 7.39-7.30 (m, 4H), 6.99-6.84 (m, 2H), 6.65 (d, *J* = 8.1 Hz, 1H), 5.23-5.17 (m, 1H), 5.13 (dd, *J* = 12.9, 7.4 Hz, 2H), 5.02 (dd, *J* = 12.8, 8.6 Hz, 1H), 2.25 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 150.7, 141.3, 131.0, 130.6, 130.5, 130.3, 129.4, 129.3, 126.4, 124.7, 122.8, 116.0, 77.6, 43.6, 20.6. HRMS: (ESI+) m/z calcd for $[C_{15}H_{15}NO_3+Na]^+$: 280.0950, found: 280.0961.

（4b）(S)-2-(1-(4-methoxyphenyl)-2-nitroethyl)-4-methylphenol



A pale yellow oil. 73% yield, 94% *ee*. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 10/90, flow rate =0.8 ml/min, λ = 220 nm): t_{minor} =26.678 min, t_{major} = 28.425 min. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29-7.20 (m, 2H), 6.95-6.84 (m, 4H), 6.64 (d, *J* = 8.1 Hz, 1H), 5.35 (s, 1H), 5.16-5.06 (m, 2H), 4.97 (dd, *J* = 12.0, 8.3 Hz, 1H), 3.80 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 158.7, 150.8, 130.8, 130.3, 129.1(×2), 129.0, 128.9, 116.0, 125.7, 114.2 (×2), 78.2, 55.2, 43.1, 20.5. HRMS: (ESI+) m/z calcd for $[C_{16}H_{17}NO_4+Na]^+$: 310.1055, found: 310.1076.

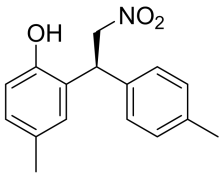
（4c）(S)-2-(1-(3,4-dimethoxyphenyl)-2-nitroethyl)-4-methylphenol



A pale yellow oil. 65% yield, 94% *ee*. HPLC (Chiralpak AD-H, *i*-PrOH/*n*-hexane = 10/90, flow rate =1.0 ml/min, λ = 210 nm): t_{minor} =22.025 min, t_{major} = 24.052 min. ^{1}H NMR (500 MHz, $CDCl_3$)

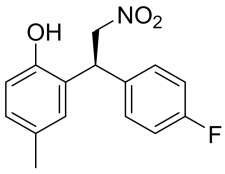
δ 7.28 (s, 1H), 7.22 (d, *J* = 1.3 Hz, 1H), 6.83 (dd, *J* = 6.0, 2.0 Hz, 4H), 5.65 (s, 1H), 5.17 (dd, *J* = 8.8, 7.4 Hz, 1H), 5.07 (dd, *J* = 13.0, 7.2 Hz, 1H), 4.95 (dd, *J* = 13.0, 8.9 Hz, 1H), 3.87 (d, *J* = 3.1 Hz, 6H), 2.23 (s, 3H).^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 149.2, 148.5, 147.4, 131.5, 131.4, 130.6, 128.8, 126.6, 119.7, 111.6, 111.3, 110.9, 77.7, 56.0, 55.9, 43.9, 20.4. HRMS: (ESI+) m/z calcd for $[C_{17}H_{19}NO_5+Na]^+$: 340.1161, found: 340.1178.

（**4d**）**(S)-4-methyl-2-(2-nitro-1-(p-tolyl)ethyl)phenol.**



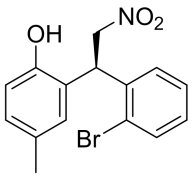
A pale yellow oil. 70% yield, 90% ee. HPLC (Chiralpak IC, *i*-PrOH/*n*-hexane = 3/97, flow rate =0.6 ml/min, λ = 220 nm): t_{minor} =22.825 min, t_{major} = 26.211 min, 90% *ee*. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20 (d, *J* = 8.1 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 6.93 (dd, *J* = 14.8, 6.7 Hz, 2H), 6.65 (d, *J* = 8.1 Hz, 1H), 5.17-5.07 (m, 2H), 4.99 (dd, *J* = 12.2, 8.2 Hz, 1H), 4.85 (s, 1H), 2.33 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 150.8, 137.2, 135.7, 130.6, 129.6(×2), 129.2, 129.1, 127.8(×2), 125.71, 116.1, 78.1, 43.4, 21.1, 20.6. HRMS: (ESI+) m/z calcd for $[C_{16}H_{17}NO_3+Na]^+$: 294.1106, found: 294.1125.

（**4e**）**(S)-2-(1-(4-fluorophenyl)-2-nitroethyl)-4-methylphenol.**



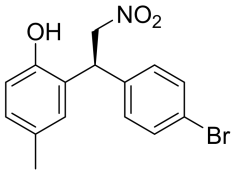
A pale yellow oil. 72% yield, 91% *ee*. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 10/90, flow rate =0.8 ml/min, λ = 210 nm): t_{minor} =14.319 min, t_{major} = 17.759 min. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34-7.28 (m, 2H), 7.07-6.98 (m, 2H), 6.95 (dd, *J* = 8.1, 1.7 Hz, 1H), 6.87 (d, *J* = 1.7 Hz, 1H), 6.66 (d, *J* = 8.1 Hz, 1H), 5.19-5.13 (m, 1H), 5.10 (dd, *J* = 12.8, 7.2 Hz, 1H), 4.99 (dd, *J* = 12.8, 9.0 Hz, 1H), 4.88 (s, 1H), 2.25 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 161.0, 150.6, 134.6, 130.6, 129.5(×2), 129.3, 129.2, 125.3, 116.0, 115.8, 115.6, 78.0, 43.2, 20.6. HRMS: (ESI+) m/z calcd for $[C_{15}H_{14}FNO_3+Na]^+$: 298.0855, found: 298.0869.

（**4f**）**(R)-2-(1-(2-bromophenyl)-2-nitroethyl)-4-methylphenol.**



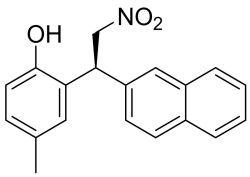
A pale yellow oil. 66% yield, 96% *ee*. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 10/90, flow rate =0.8 ml/min, λ = 220 nm): t_{minor} =13.186 min, t_{major} = 26.958 min. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 – 7.57 (m, 1H), 7.32 (dd, *J* = 7.1, 1.6 Hz, 2H), 7.16 (ddd, *J* = 8.1, 6.7, 2.4 Hz,1H), 6.96 (dd, *J* = 8.1, 1.8 Hz, 1H), 6.83 (d, *J* = 1.6 Hz, 1H), 6.68 (d, *J* = 8.1 Hz, 1H), 5.64 (t, *J* = 8.1 Hz, 1H), 5.07 (dd, *J* = 13.5, 8.1 Hz, 2H), 4.95 (dd, *J* = 13.5, 8.1 Hz, 1H), 2.23 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 151.0, 137.7, 133.6, 130.5, 129.4 (×2), 129.0, 128.7, 127.7, 125.1, 123.8, 116.0, 76.3, 43.0, 20.6. HRMS: (ESI+) m/z calcd for $[C_{15}H_{14}BrNO_3+Na]^+$: 358.0055, found: 280.0073.

（**4g**）**(S)-2-(1-(4-bromophenyl)-2-nitroethyl)-4-methylphenol.**



A pale yellow oil. 60% yield, 95% *ee*. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 10/90, flow rate =0.8 ml/min, λ = 216 nm): t_{minor} =110.536 min, t_{major} = 114.427 min. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50-7.41 (m, 1H), 7.33-7.29 (m, 1H), 7.28-7.26 (m, 1H), 7.22-7.18 (m, 1H), 6.95 (dd, *J* = 8.1, 1.7 Hz, 1H), 6.86 (s, 1H), 6.66 (d, *J* = 8.1 Hz, 1H), 5.19-5.05 (m, 2H), 4.99 (dd, *J* = 12.8, 8.9 Hz, 2H), 2.25 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 150.7, 137.4, 133.2, 131.9, 130.6, 129.6, 129.3(×2), 128.9, 125.0, 124.9, 116.0, 77.7, 43.3, 20.6. HRMS: (ESI+) m/z calcd for $[C_{15}H_{14}BrNO_3+Na]^+$: 358.0055, found: 280.0061

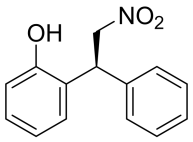
（**4h**）**(S)-4-methyl-2-(1-(naphthalen-2-yl)-2-nitroethyl)phenol.**



A pale yellow oil. 63% yield, 94% *ee*. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 50/50, flow rate =0.5 ml/min, λ = 208 nm): t_{minor} =67.376 min, t_{major} = 28.283 min. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85-7.80 (m, 3H), 7.77 (s, 1H), 7.54-7.44 (m, 2H), 7.42 (dd, *J* = 8.6, 1.8 Hz, 1H), 6.93 (s, 2H), 6.67 (d, *J* = 8.1 Hz, 1H), 5.40-5.33 (m, 1H), 5.17 (dd, *J* = 14.5, 8.0 Hz, 2H), 4.95 (s, 1H), 2.24 (s, 3H). ^{13}C

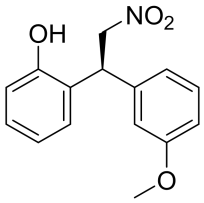
NMR (125 MHz, $CDCl_3$) δ(ppm) 150.8, 136.2, 133.3, 132.6, 130.6, 129.5, 129.2, 128.7, 127.9, 127.6, 126.3, 126.2(×2), 125.4, 116.0, 77.8, 43.7, 20.6. HRMS: (ESI+) m/z calcd for $[C_{19}H_{17}NO_3+Na]^+$: 330.1106, found: 330.1096.

（**4i**）**(S)-2-(2-nitro-1-phenylethyl)phenol.**



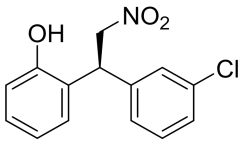
A pale yellow oil. 81% yield, 92% *ee*. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 10/90, flow rate =0.8 ml/min, λ = 228 nm): t_{minor} =18.159 min, t_{major} = 21.865 min. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 – 7.44 (m, 2H), 7.23-7.14 (m, 3H), 7.08 (dd, *J* = 7.7, 1.4 Hz, 1H), 6.92 (dd, *J* = 7.5, 0.8 Hz, 1H), 6.76 (dd, *J* = 8.1, 0.8 Hz, 1H), 5.19 (dd, *J* = 8.9, 7.2 Hz, 1H), 5.10 (dd, *J* = 13.0, 7.0 Hz, 2H), 4.99 (dd, *J* = 13.0, 9.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 152.9, 137.8, 132.0, 129.6(×2), 129.0, 128.7(×2), 125.3, 121.4, 116.1, 77.6, 43.2. HRMS: (ESI+) m/z calcd for $[C_{14}H_{13}NO_3+Na]^+$: 266.0793, found: 266.0807.

（**4j**）**(S)-2-(1-(3-methoxyphenyl)-2-nitroethyl)phenol.**



A pale yellow oil. 72% yield, 92% *ee*. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 20/80, flow rate = 1.0 ml/min, λ = 206 nm): t_{minor} =22.665 min, t_{major} = 12.692 min. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27-7.24 (m, 1H), 7.22-7.12 (m, 3H), 6.93 (ddd, *J* = 12.0, 11.3, 7.7 Hz, 4H), 6.85-6.81 (m, 1H), 5.82 (s, 1H), 5.52 (t, *J* = 8.0 Hz, 1H), 5.13-5.07 (m, 2H), 3.93 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 156.3, 153. 6, 128.8, 128.6, 128.0, 127.7, 126.6, 125.2, 121.4, 121.1, 116.7, 111.2, 77.3, 55.9, 36.6. HRMS: (ESI+) m/z calcd for $[C_{15}H_{15}NO_4+Na]^+$: 296.0899, found: 296.0886.

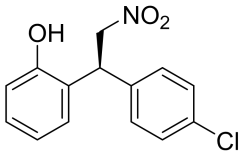
（**4k**）**(S)-2-(1-(3-chlorophenyl)-2-nitroethyl)phenol.**



A pale yellow oil. 65% yield, 99% *ee*. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 15/85, flow rate =0.7ml/min, λ = 210 nm): t_{major} = 45.330min. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48-7.35 (m, 2H),

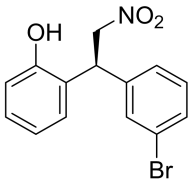
7.26 (s, 1H), 7.24-7.14 (m, 2H), 7.10 (dd, *J* = 7.7, 1.5 Hz, 1H), 6.93 (dd, *J* = 7.6, 1.1 Hz, 1H), 6.77 (dd, *J* = 8.0, 1.0 Hz, 1H), 5.20 (t, *J* = 8.0 Hz, 2H), 5.11 (dd, *J* = 13.1, 7.2 Hz, 1H), 5.00 (dd, *J* = 13.1, 8.8 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 152.9, 141.1, 131.1, 130.6, 130.3, 129.1, 128.7, 126.5, 125.0, 122.9, 121.4, 116.1, 77.5, 43.3. HRMS: (ESI+) m/z calcd for $[C_{14}H_{12}ClNO_3+Na]^+$: 300.0403, found: 300.0416.

（**4l**）**(S)-2-(1-(4-chlorophenyl)-2-nitroethyl)phenol.**



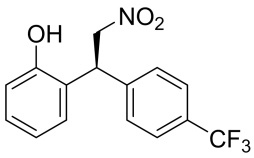
A pale yellow oil. 62% yield, 95% *ee*. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 15/85, flow rate =0.7 ml/min, λ = 220 nm): t_{minor} =16.105 min, t_{major} = 18.839 min. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33-7.29 (m, 2H), 7.27-7.23 (m, 2H), 7.17 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.08 (dd, *J* = 7.7, 1.4 Hz, 1H), 6.92 (dd, *J* = 7.6, 0.9 Hz, 1H), 6.77 (dd, *J* = 7.9, 0.8 Hz, 1H), 5.20 (dd, *J* = 8.9, 7.2 Hz, 1H), 5.13 – 5.07 (m, 2H), 4.99 (dd, *J* = 13.0, 9.1 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 152.9, 137.2, 133.3, 129.5, 129.3(×2), 129.0(×2), 128.7, 125.3, 121.4, 116.1, 77.6, 43.1. HRMS: (ESI+) m/z calcd for $[C_{14}H_{12}ClNO_3+Na]^+$: 300.0403, found: 300.0418.

（**4m**）**(S)-2-(1-(3-bromophenyl)-2-nitroethyl)phenol.**



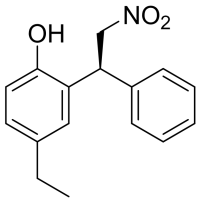
A pale yellow oil. 65% yield, 96% *ee*. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 20/80, flow rate =1.0 ml/min, λ = 210 nm): t_{minor} =25.678 min, t_{major} = 21.198min. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (t, *J* = 1.7 Hz, 1H), 7.43-7.36 (m, 1H), 7.26 (s, 1H), 7.23-7.15 (m, 2H), 7.10 (dd, *J* = 7.7, 1.4 Hz, 1H), 6.93 (td, *J* = 7.5, 0.9 Hz, 1H), 6.77 (dd, *J* = 8.1, 0.9 Hz, 1H), 5.20 (t, *J* = 8.0 Hz, 2H), 5.11 (dd, *J* = 13.1, 7.2 Hz, 1H), 5.00 (dd, *J* = 13.0, 8.9 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 152.9, 141.1, 131.1, 130.6, 130.3, 129.0, 128.8, 126.5, 125.0, 122.9, 121.5, 116.1, 77.5, 43.4. HRMS: (ESI+) m/z calcd for $[C_{14}H_{12}BrNO_3+Na]^+$: 321.0001, found: 321.0019.

（**4n**）**(S)-2-(2-nitro-1-(4-(trifluoromethyl)phenyl)ethyl)phenol.**



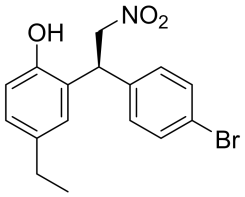
A pale yellow oil. 63% yield, 96% *ee*. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 20/80, flow rate =1.0 ml/min, λ = 220 nm): t_{minor} =6.986 min, t_{major} = 9.186 min. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.2 Hz, 2H), 7.45 (d, *J* = 8.2 Hz, 2H), 7.18 (td, *J* = 7.8, 1.5 Hz, 1H), 7.08 (dt, *J* = 7.6, 3.8 Hz, 1H), 7.00-6.87 (m, 1H), 6.78 (dd, *J* = 8.2, 0.6 Hz, 1H), 5.33-5.23 (m, 2H), 5.14 (dd, *J* = 13.1, 7.0 Hz, 1H), 5.06 (dd, *J* = 13.2, 9.1 Hz, 1H).1.65 (m, 3H), ^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 152.9, 142.9, 129.8, 129.2, 128.8, 128.32(×2), 125.8, 125.7(×2), 124.9, 121.5, 116.1, 77.4, 43.5. HRMS: (ESI+) m/z calcd for $[C_{15}H_{12}F_3NO_3+Na]^+$: 334.0667, found: 334.0685.

（**4o**）**(S)-4-ethyl-2-(2-nitro-1-phenylethyl)phenol.**



A pale yellow oil. 75% yield, 93% *ee*. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 10/90, flow rate = 0.8 ml/min, λ = 206 nm): t_{minor} =13.346 min, t_{major} = 15.479 min.^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43–7.30 (m, 5H), 7.03-6.86 (m, 2H), 6.68 (d, *J* = 8.1 Hz, 1H), 5.22-5.16 (m, 1H), 5.13 (dd, *J* = 12.7, 7.3 Hz, 1H), 5.03 (dd, *J* = 12.8, 8.6 Hz, 1H), 4.85 (s, 1H), 2.55 (q, *J* = 7.6 Hz, 2H), 1.18 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 151.0, 138.8, 137.1, 128.9 (×2), 128.2, 127.9 (×2), 127.8, 127.4, 125.5, 116.1, 78.0, 43.9, 28.0, 15.7. HRMS: (ESI+) m/z calcd for $[C_{16}H_{17}NO_3+Na]^+$: 294.1106, found: 294.1121.

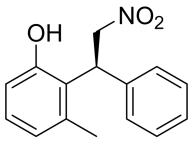
（**4p**）**(S)-2-(1-(4-bromophenyl)-2-nitroethyl)-4-ethylphenol.**



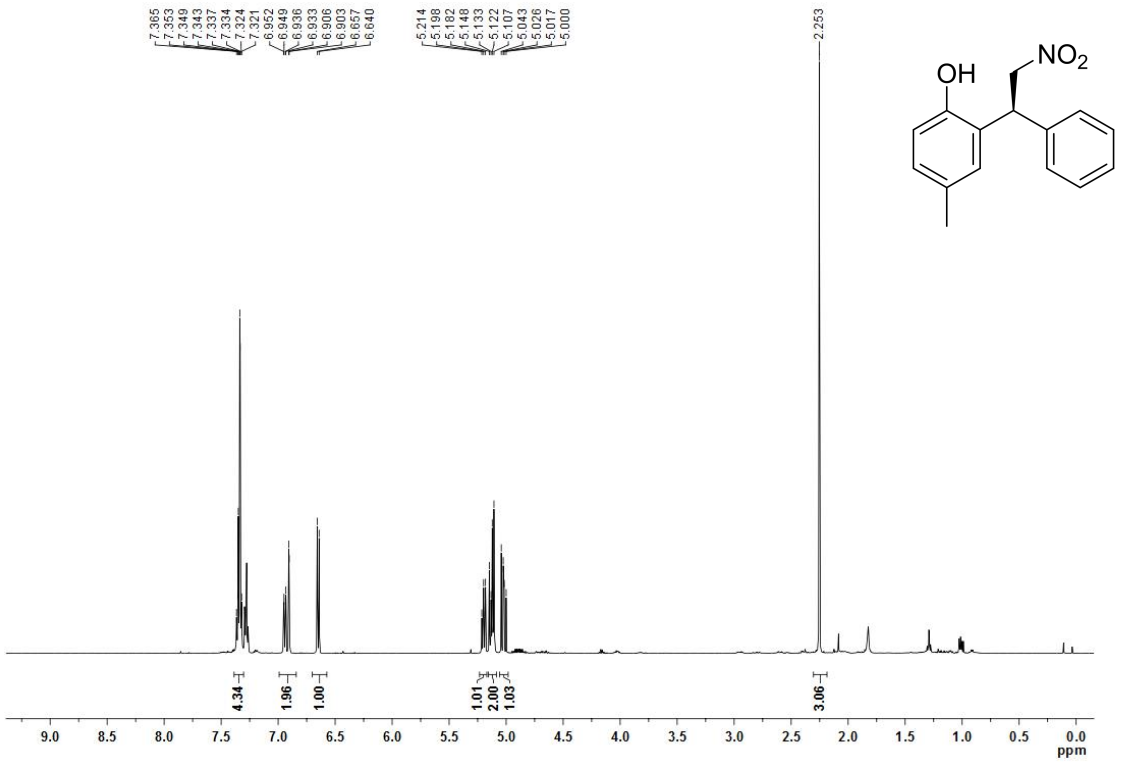
A pale yellow oil. 68% yield, 96% *ee*. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 10/90, flow rate = 0.8 ml/min, λ = 206 nm): t_{minor} =14.319 min, t_{major} = 15.799 min. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50-7.42 (m, 2H), 7.23-7.17 (m, 2H), 6.99 (dd, *J* = 8.1, 2.1 Hz, 1H), 6.88 (d, *J* = 2.0 Hz, 1H), 6.68 (d, *J* = 8.2 Hz, 1H), 5.18-5.06 (m, 2H), 5.01 (dd, *J* = 12.6, 8.9 Hz, 1H), 4.91 (s, 1H), 2.55 (q, *J* = 7.6 Hz,

2H), 1.18 (t, J = 7.6 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 150.8, 141.0, 137.3, 131.9, 129.6 (×2), 128.7, 128.1 (×2), 121.4, 120.0, 116.0, 77.7, 43.5, 28.0, 15.7. HRMS: (ESI+) m/z calcd for $[C_{16}H_{16}BrNO_3+Na]^+$: 372.0211, found: 372.0225.

（4q）(S)-3-methyl-2-(2-nitro-1-phenylethyl)phenol.



A pale yellow oil. 89% yield, 93% *ee*. HPLC (Chiralpak OD-H, *i*-PrOH/*n*-hexane = 15/85, flow rate = 0.7 ml/min, λ = 206 nm): t_{minor} =15.937 min, t_{major} = 16.999 min. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38-7.33 (m, 2H), 7.30 (d, J = 7.3 Hz, 3H), 7.22 (s, 1H), 6.67 (s, 1H), 5.17-5.12 (m, 1H), 5.11-5.05 (m, 2H), 5.01-4.94 (m, 1H), 2.30 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ(ppm) 152.2, 138.5, 138.1, 135.0, 132.2, 129.0 (×2), 127.8(×2), 127.7, 118.5, 115.5, 77.7, 43.2, 22.6. HRMS: (ESI+) m/z calcd for $[C_{15}H_{15}NO_3+Na]^+$: 280.0950, found: 280.0971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6.657
6.640
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5.198
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5.148
5.133
5.122
5.107
5.043
5.026
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5.000
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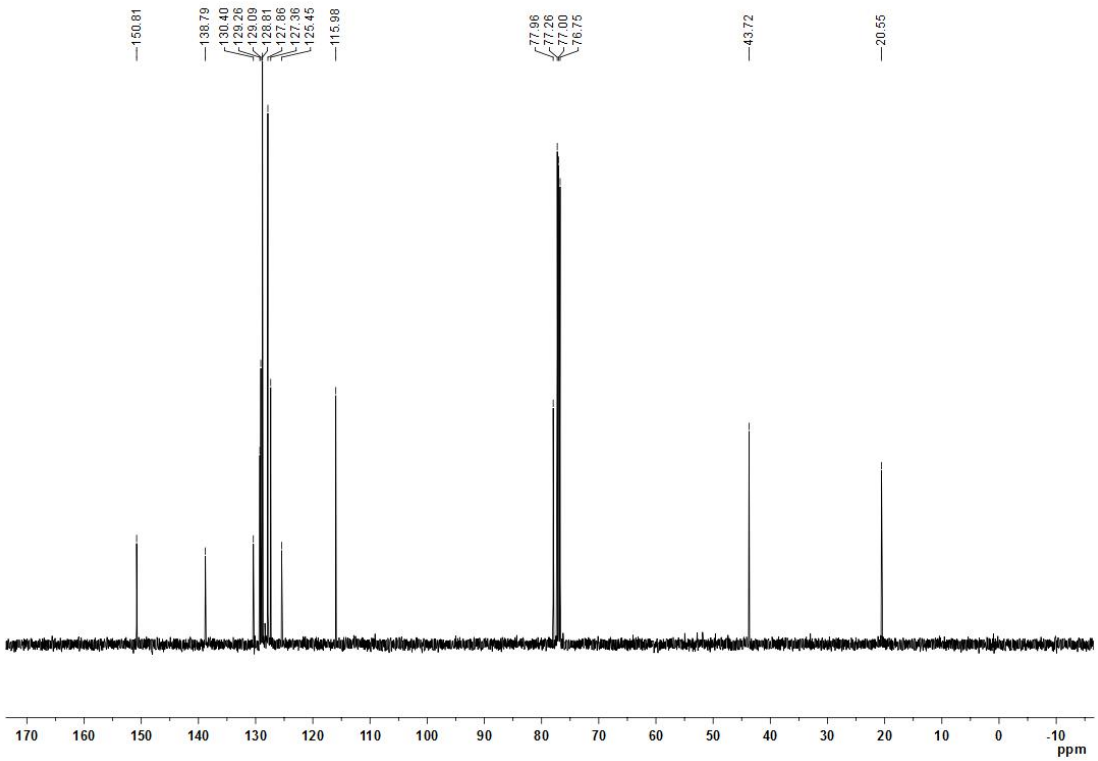
1.01
2.00
1.03
3.06
ppm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20.55
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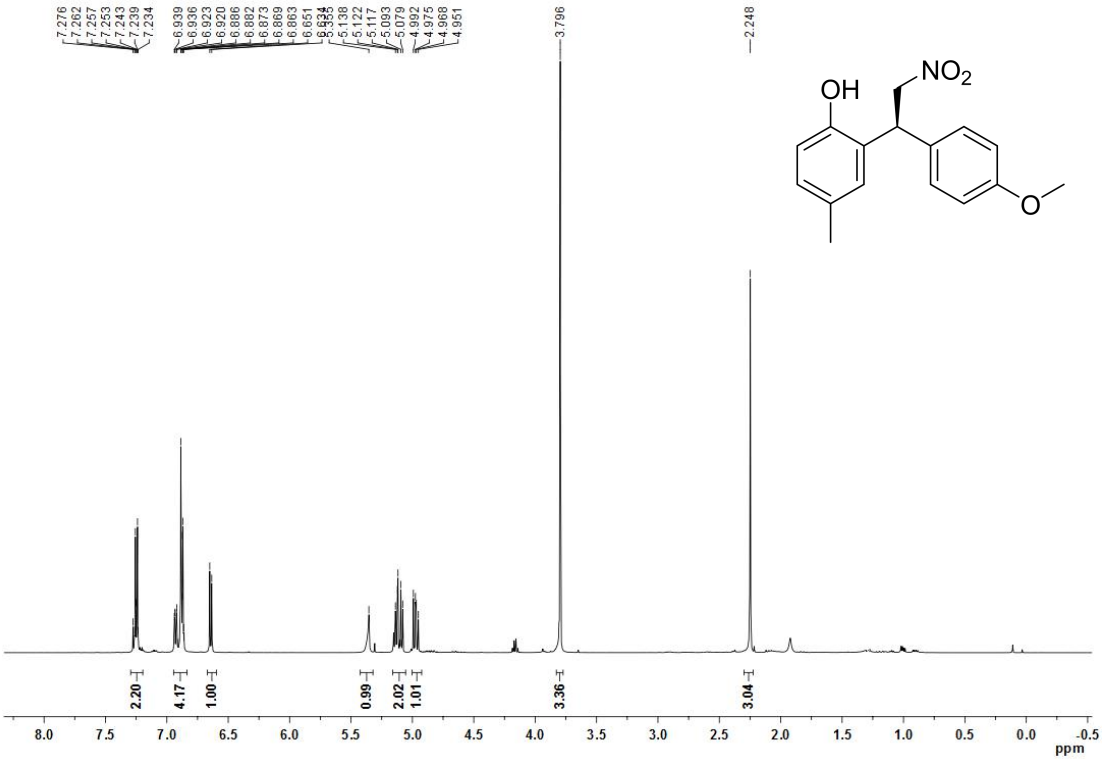
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6.873
6.869
6.863
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6.0
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5.0
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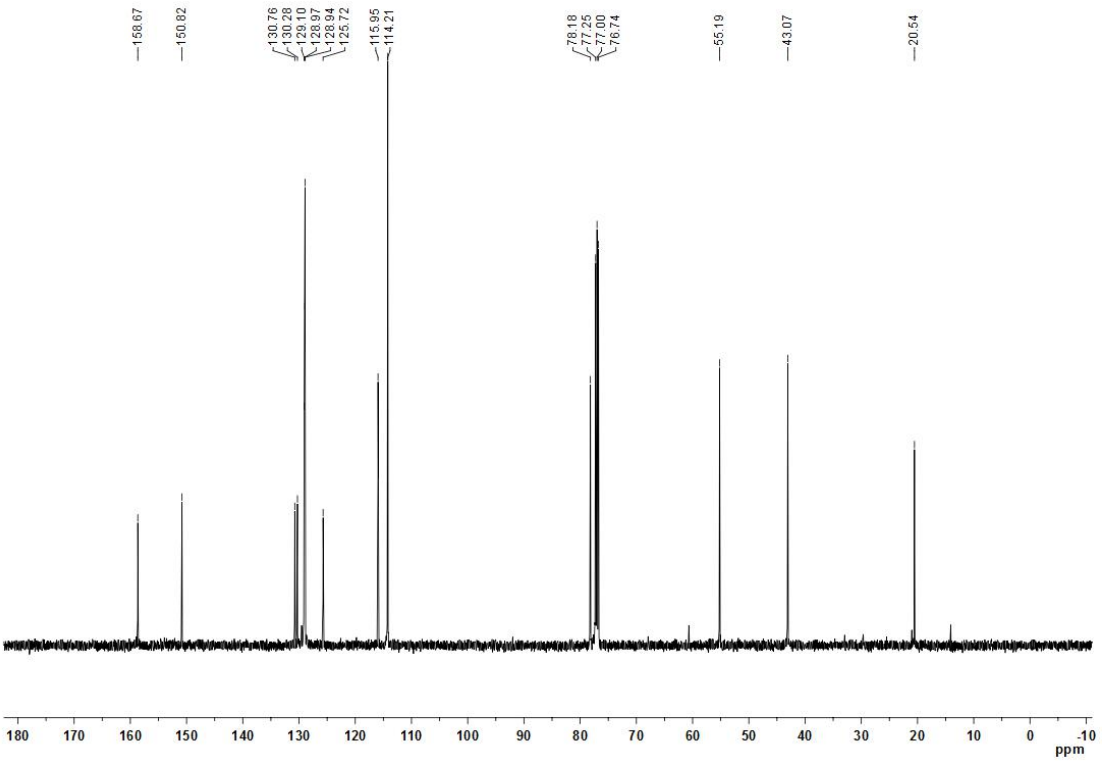
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128.94
125.72
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114.21
78.18
77.25
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76.74
55.19
43.07
20.54
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110
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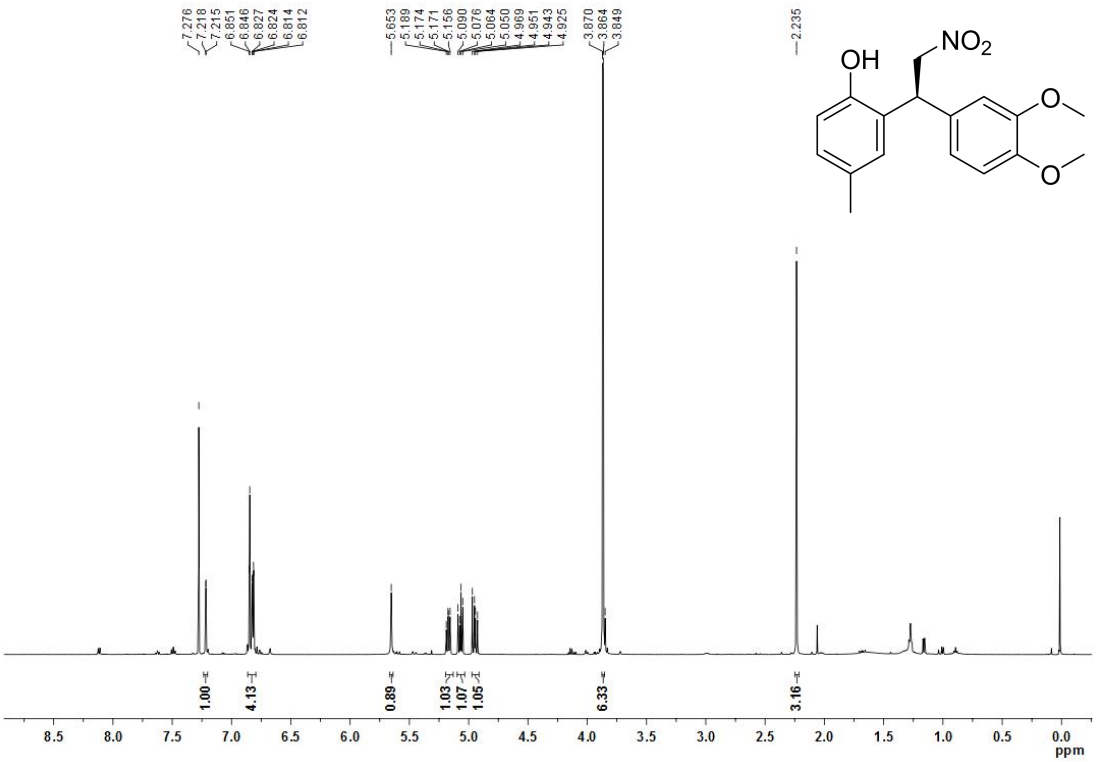
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3.16
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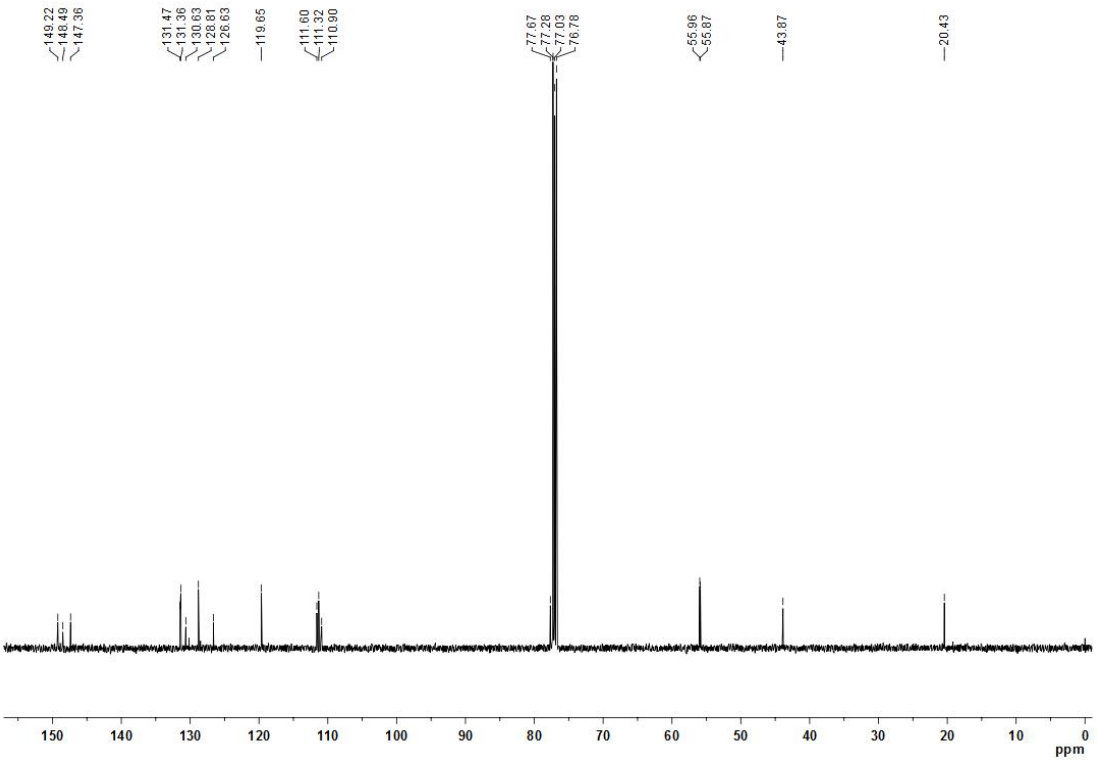
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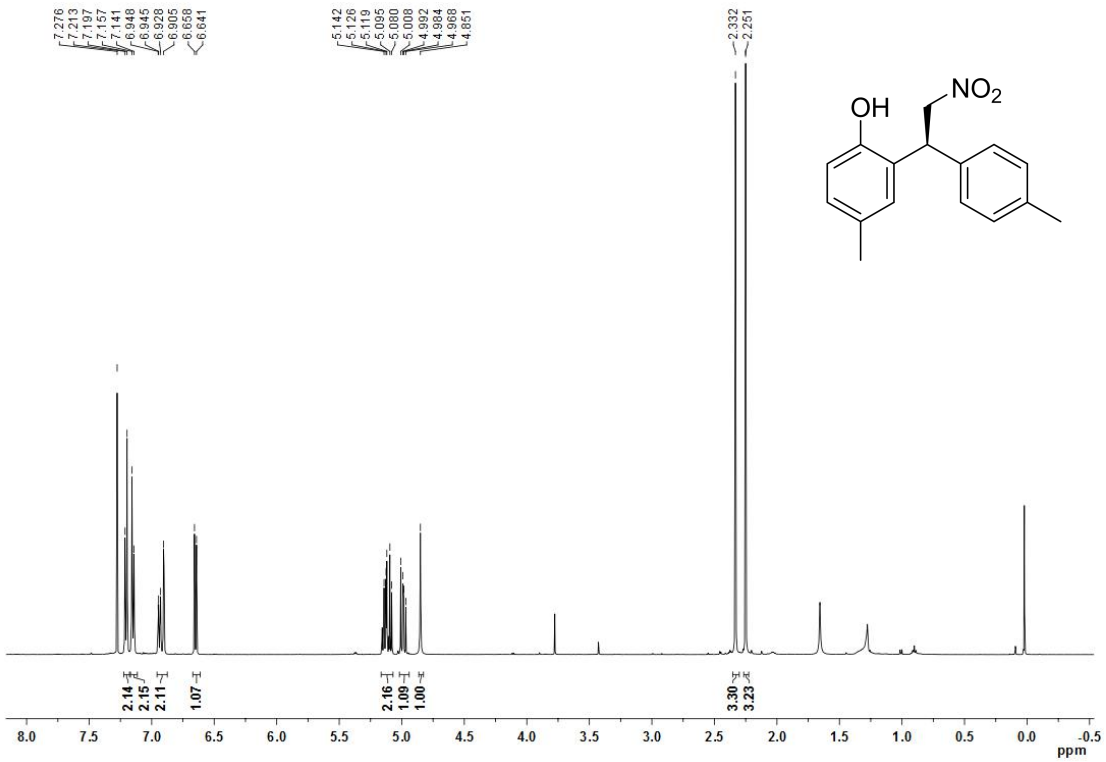
43.87
20.43
ppm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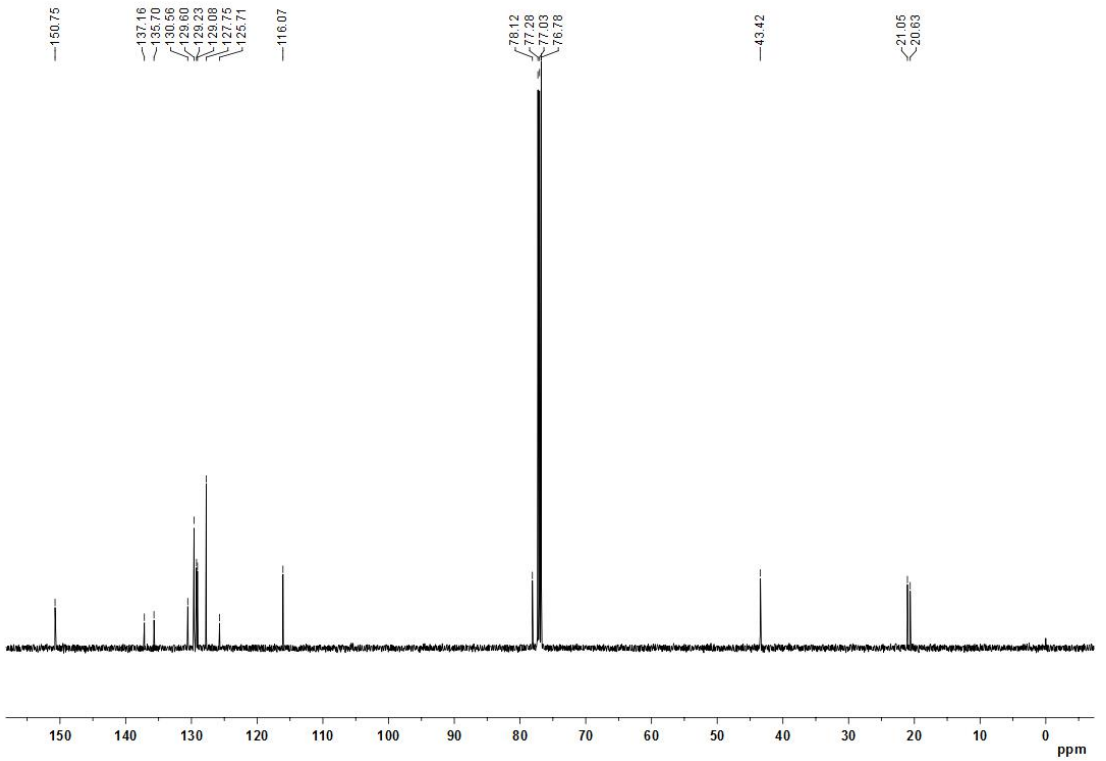
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76.78
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21.05
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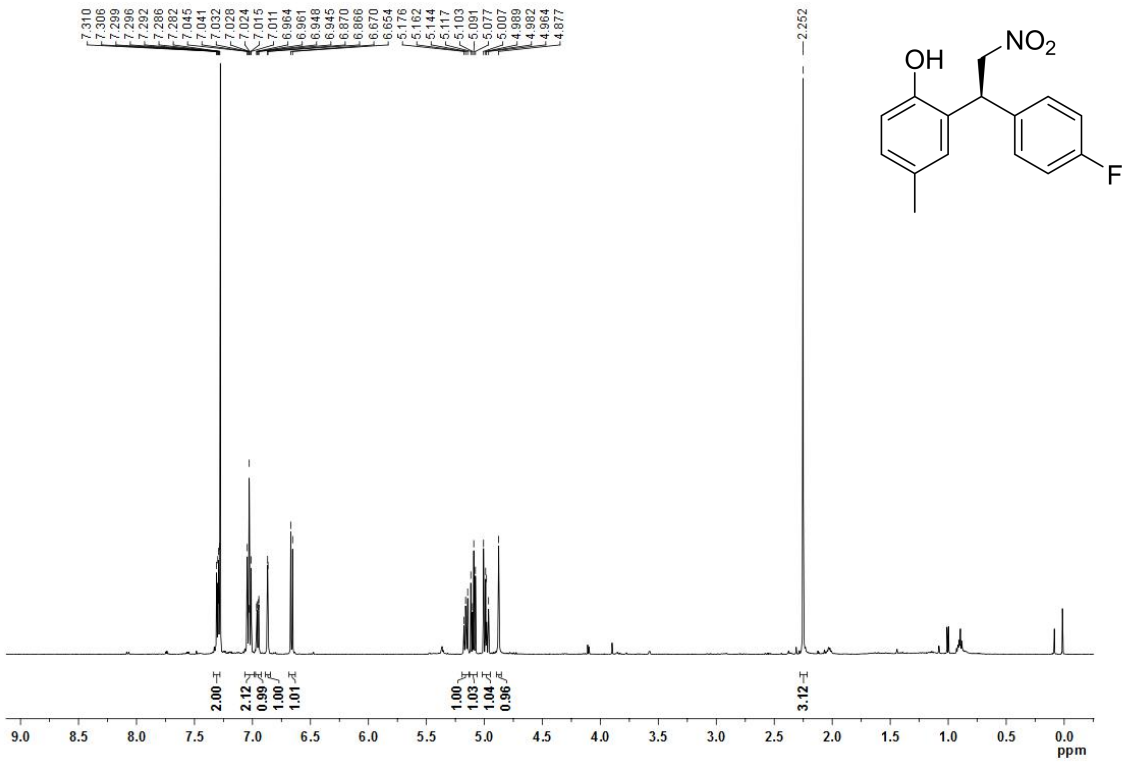
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7.011
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6.948
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1.00
1.03
1.04
0.96
3.12
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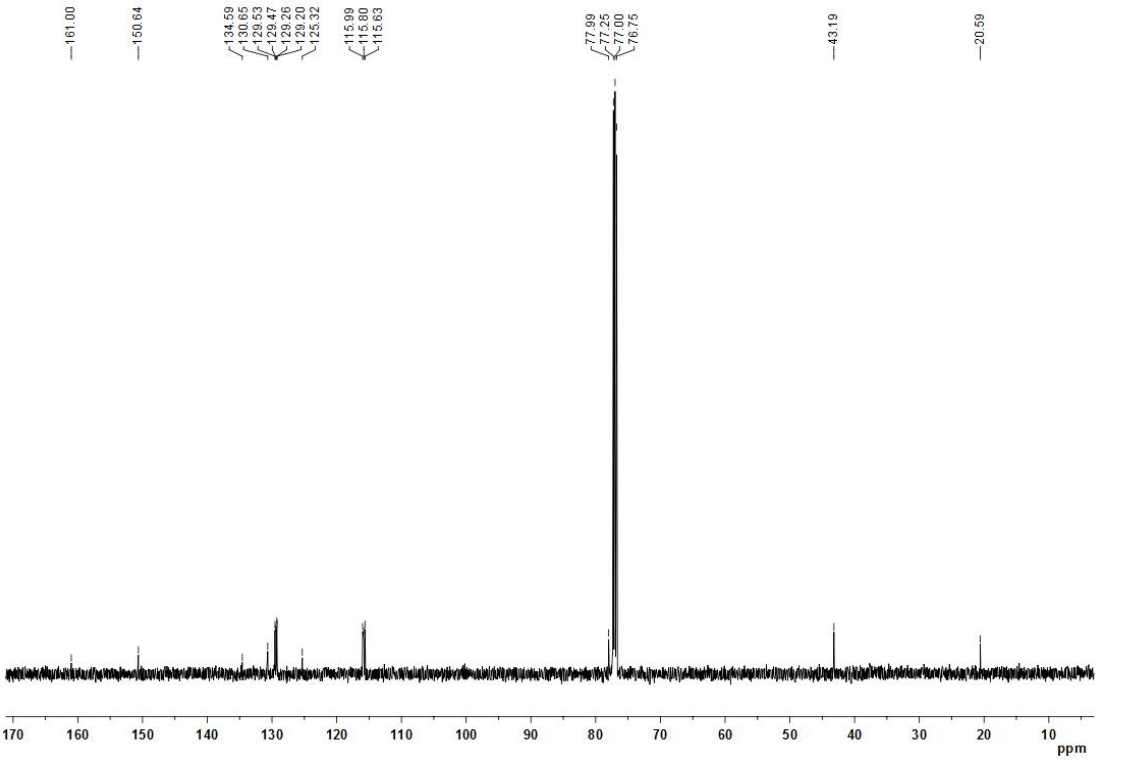
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43.19
20.59
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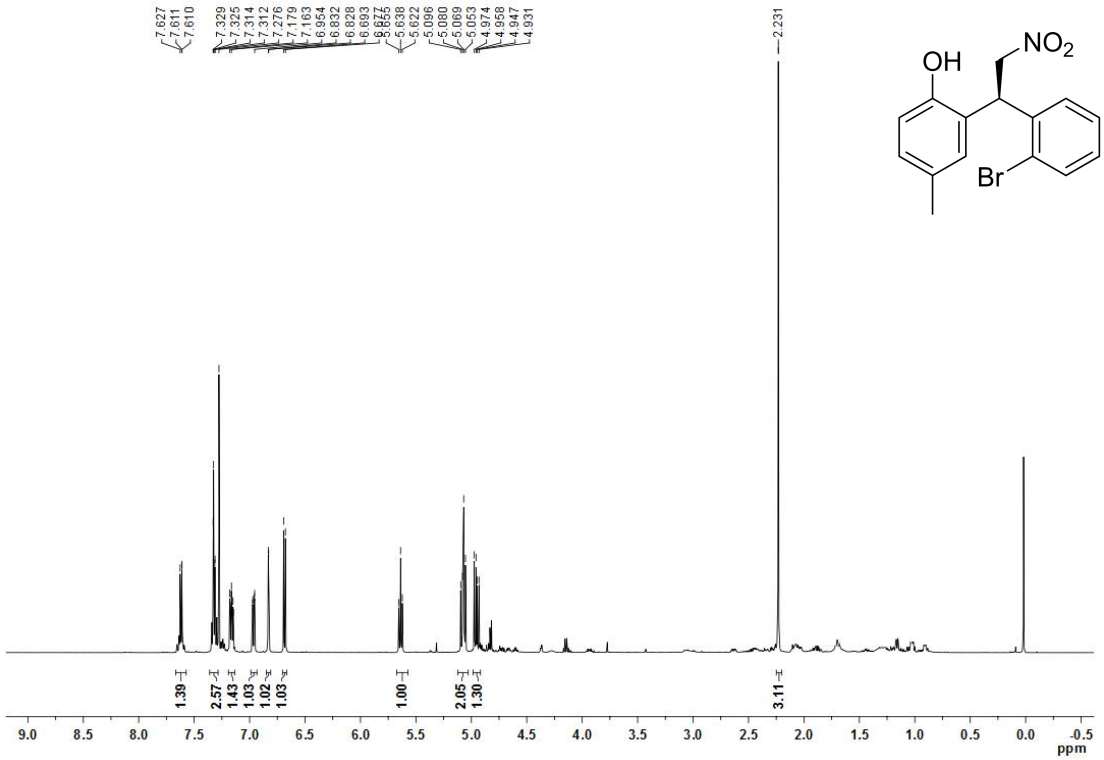
ppm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1.02
1.03
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2.05
1.30
3.11
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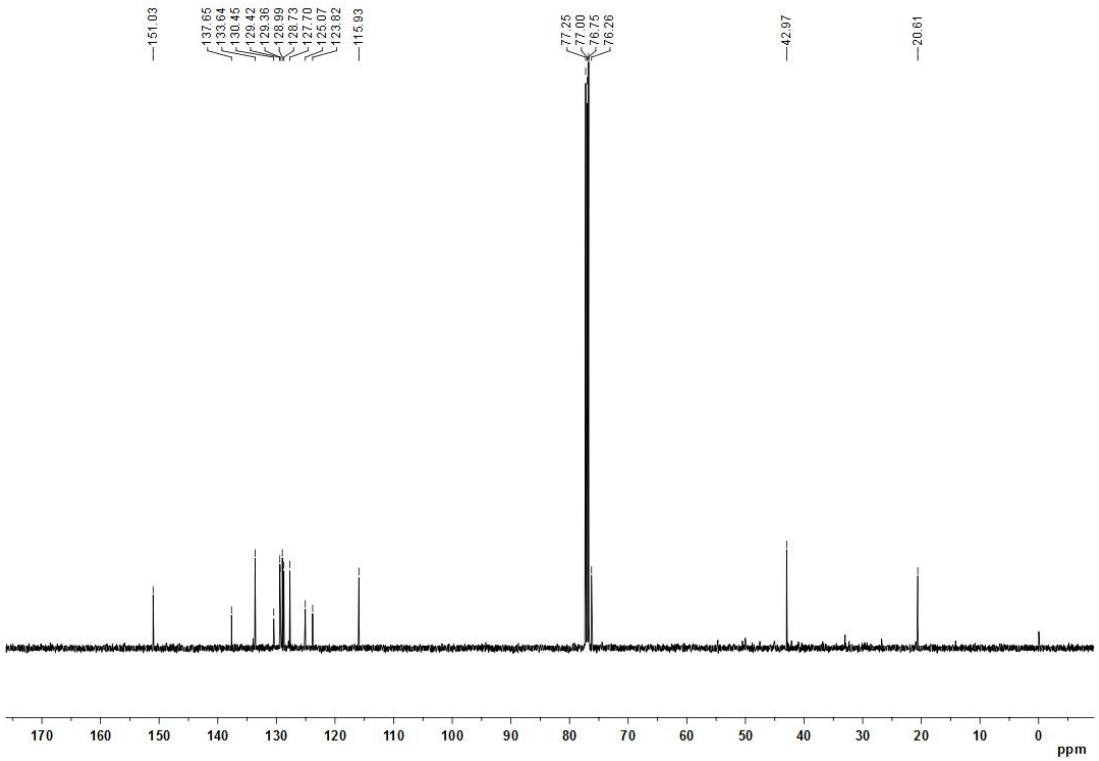
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20.61
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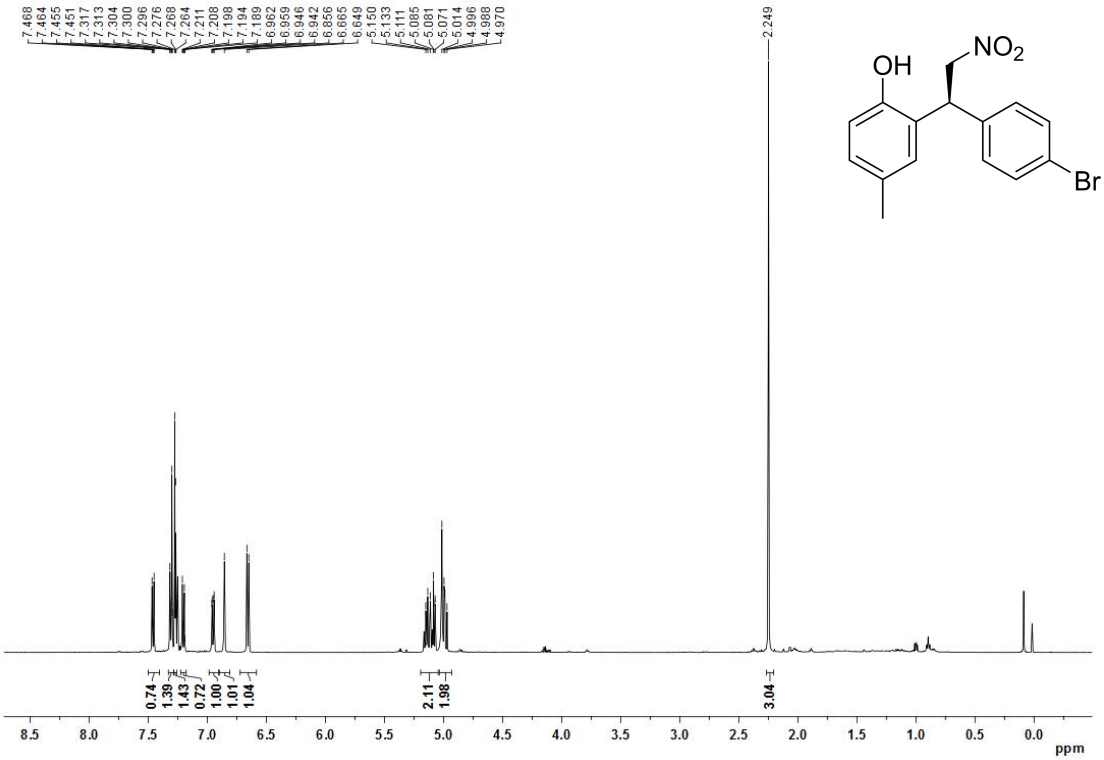
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7.0
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6.0
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3.0
2.5
2.0
1.5
1.0
0.5
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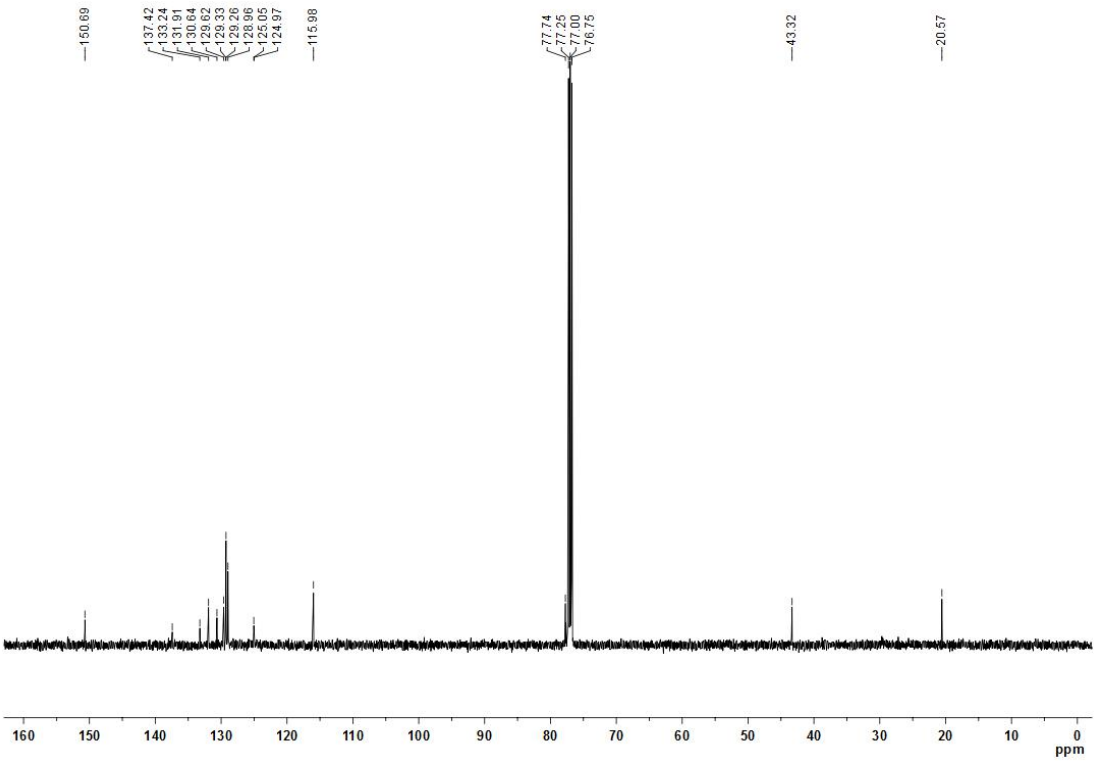
ppm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129.62
129.33
129.26
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125.05
124.97
115.98
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77.00
76.75
43.32
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140
130
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110
100
90
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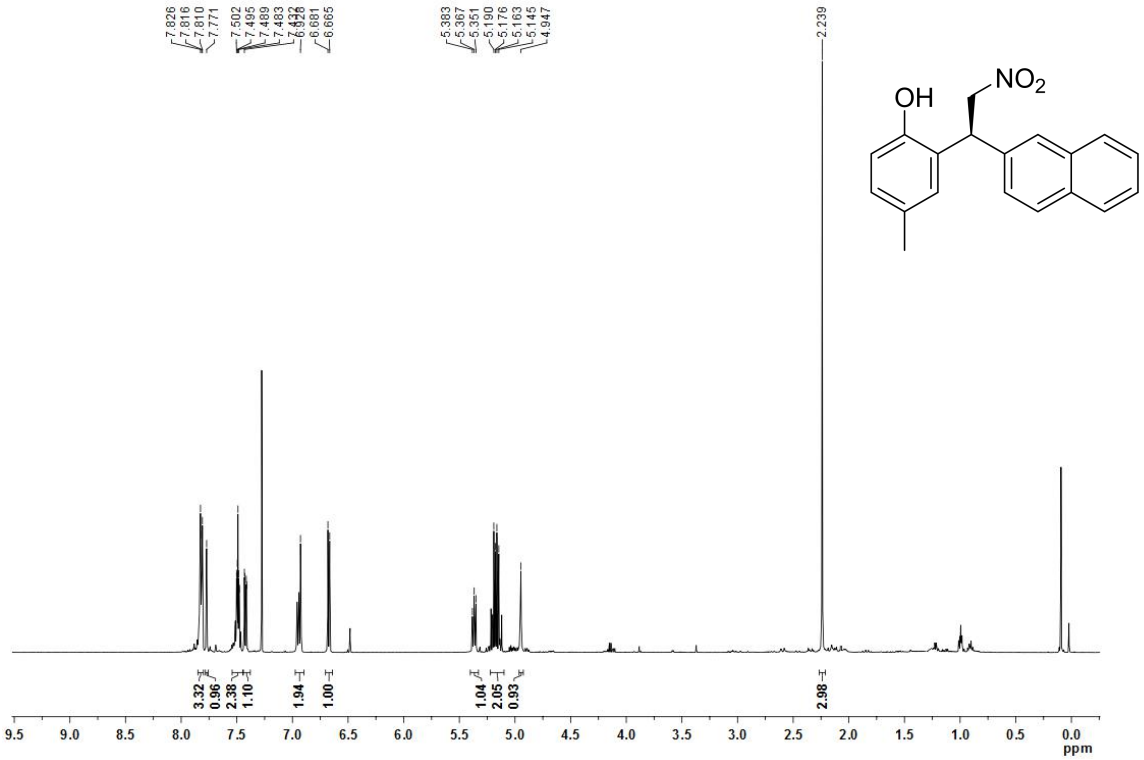
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5.367
5.351
5.190
5.176
5.163
5.145
4.947
2.239
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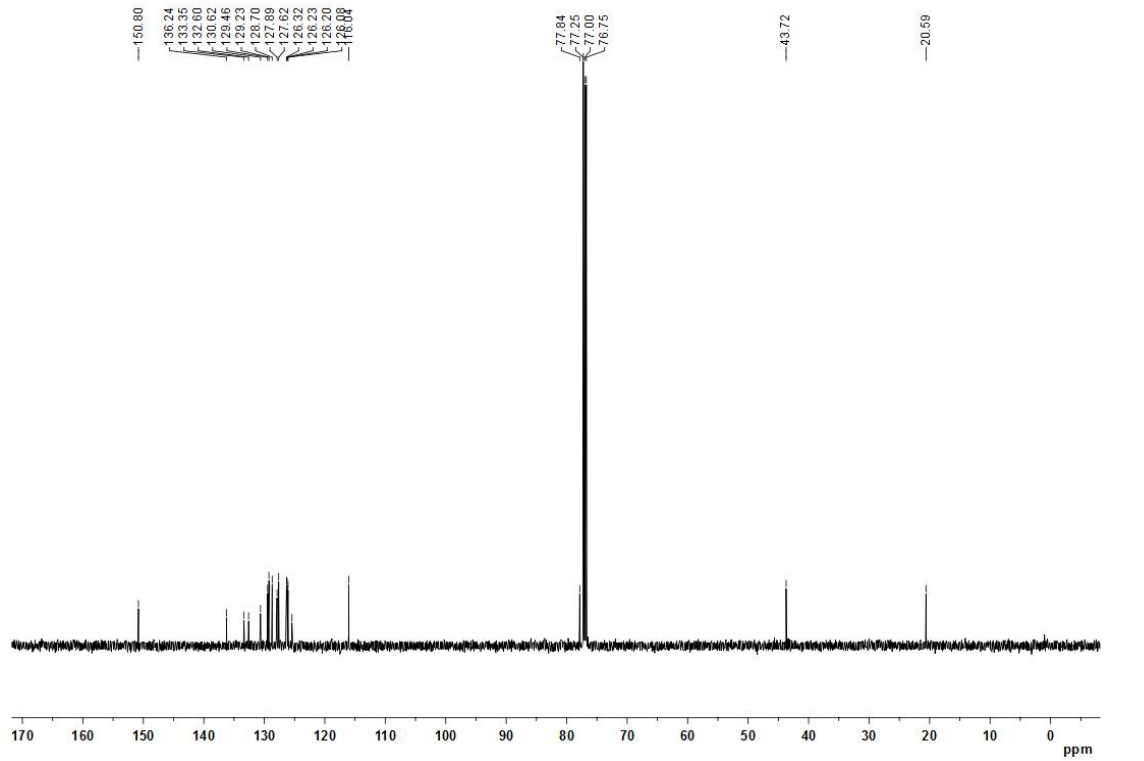
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126.23
126.20
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77.00
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20.59
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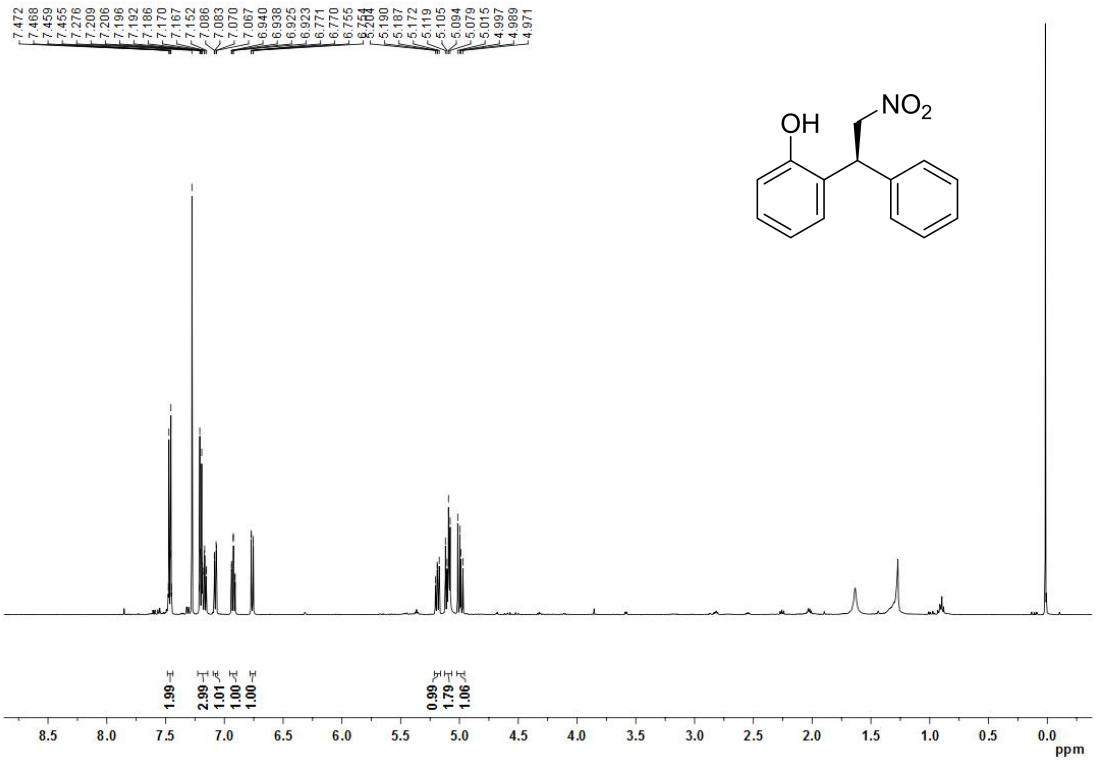
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7.167
7.152
7.086
7.083
7.070
7.067
6.940
6.938
6.925
6.923
6.771
6.770
6.755
5.190
5.187
5.172
5.119
5.105
5.094
5.079
5.015
4.997
4.989
4.971
OH
NO2
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2.99
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1.00
1.00
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1.79
1.06
8.5
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7.0
6.5
6.0
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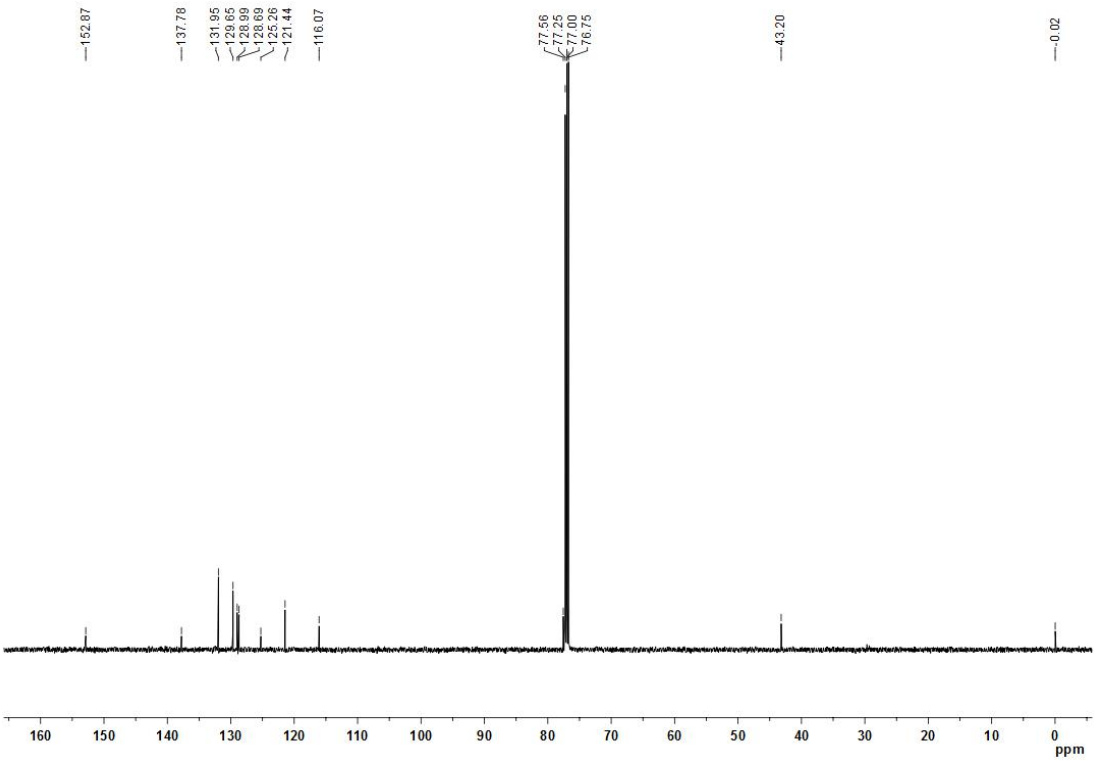
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77.25
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43.20
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140
130
120
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20
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0
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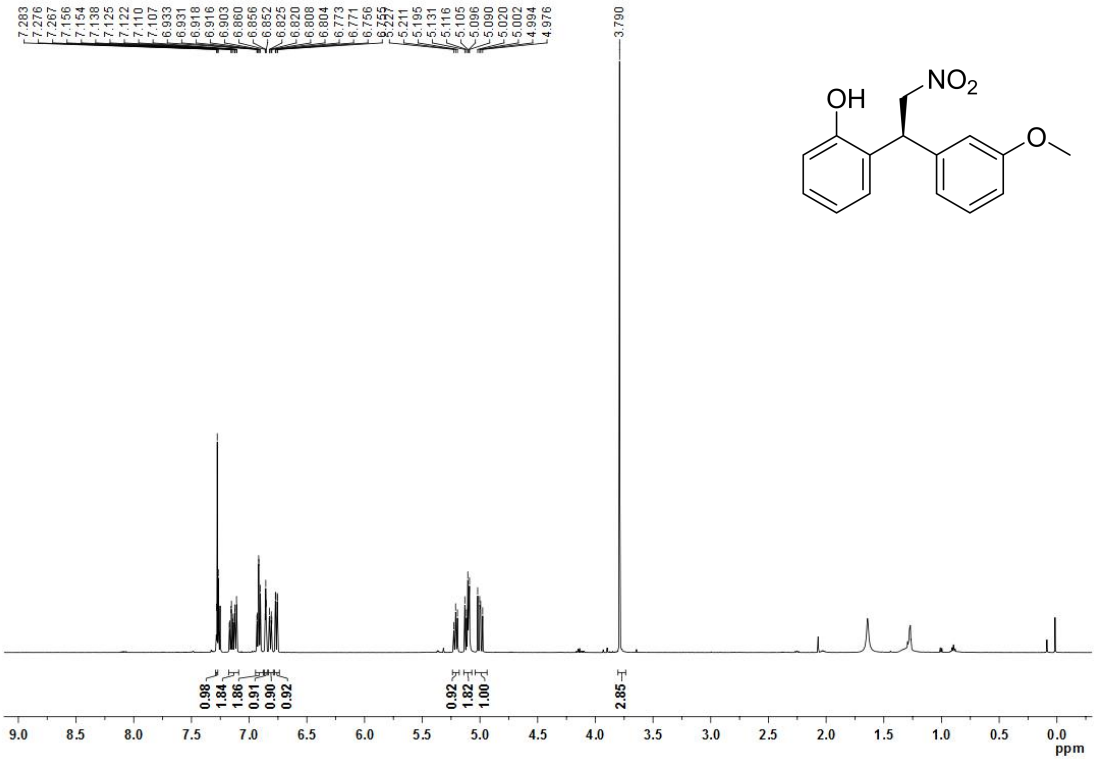
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6.931
6.918
6.916
6.903
6.860
6.856
6.852
6.825
6.820
6.808
6.804
6.773
6.771
6.756
6.755
5.227
5.211
5.195
5.131
5.116
5.105
5.096
5.090
5.020
5.002
4.994
4.976
3.790
OH
NO2
O
0.98
1.84
1.86
0.91
0.90
0.92
0.92
1.82
1.00
2.85
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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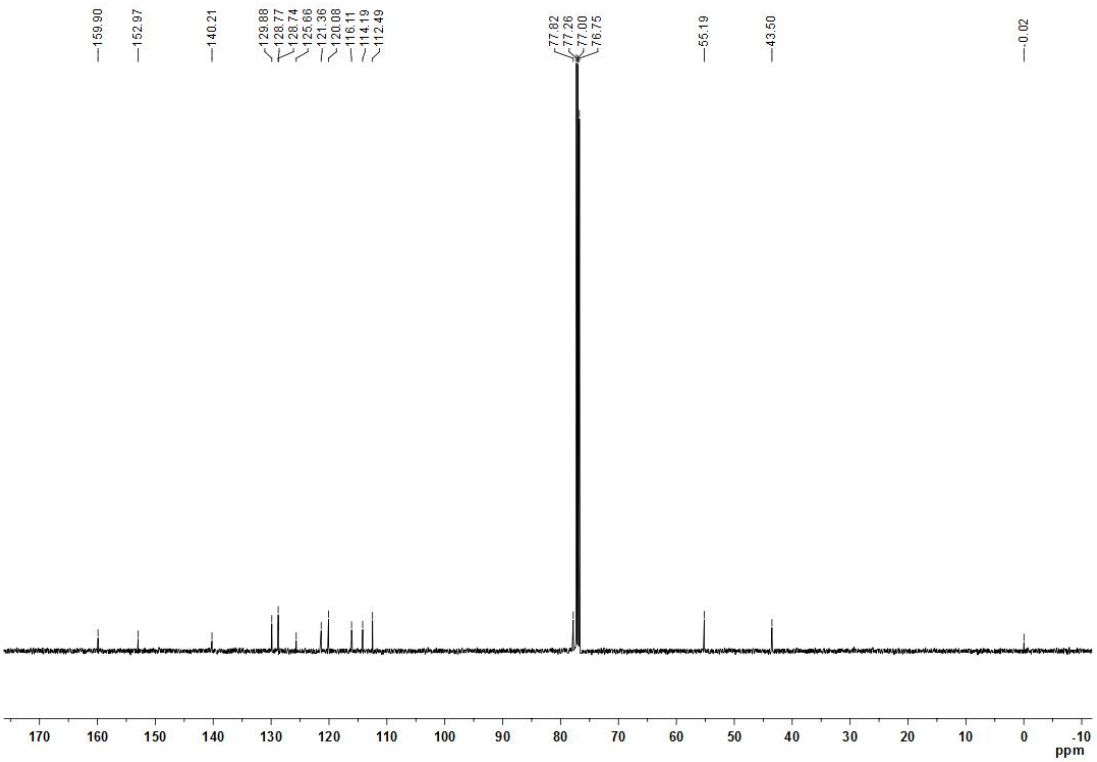
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128.74
125.66
121.36
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116.11
114.19
112.49
77.82
77.26
77.00
76.75
55.19
43.50
0.02
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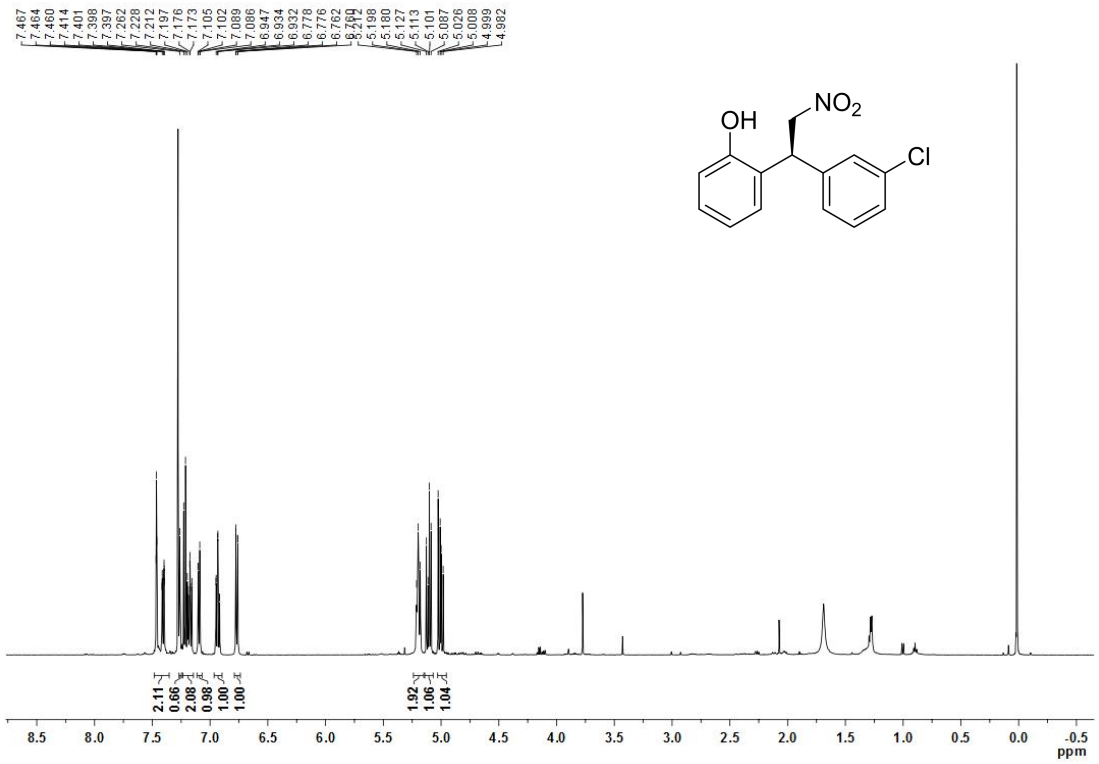
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm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7.401
7.398
7.397
7.262
7.228
7.212
7.197
7.176
7.173
7.105
7.102
7.089
7.086
6.947
6.934
6.932
6.778
6.776
6.762
5.198
5.190
5.127
5.113
5.101
5.087
5.026
5.008
4.999
4.982
OH
NO2
Cl
2.11
0.66
2.08
0.98
1.00
1.00
1.92
1.06
1.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.5
3.0
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1.0
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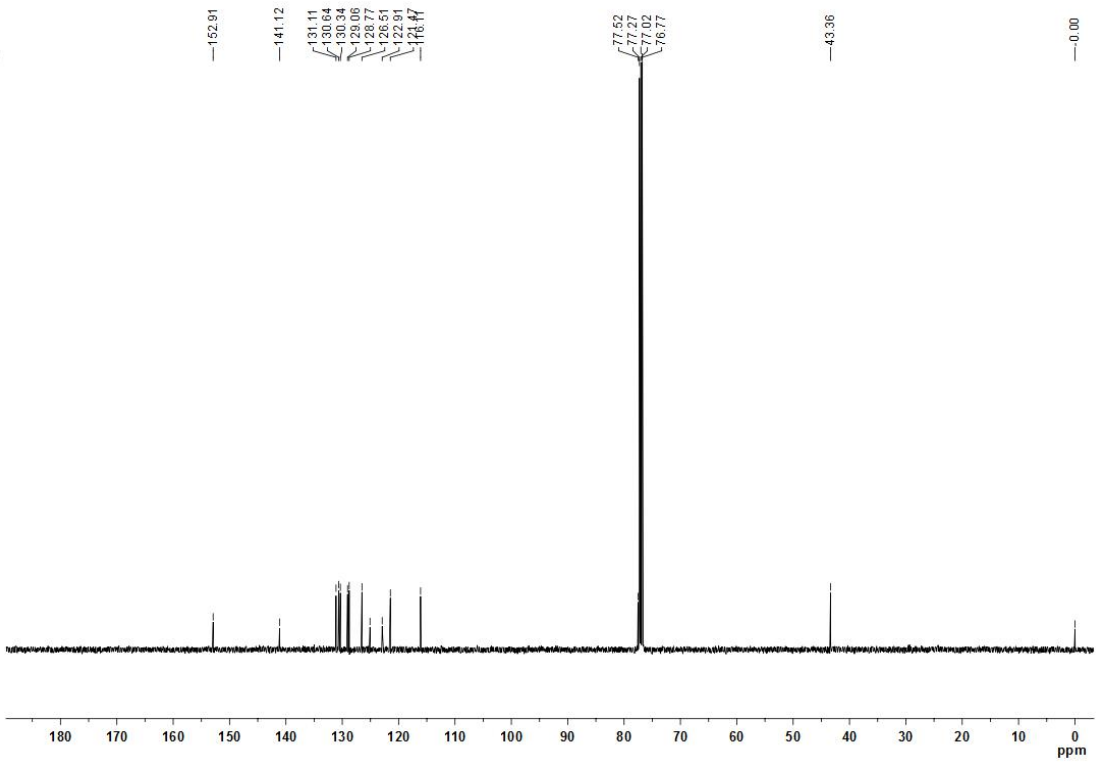
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116.11
77.52
77.27
77.02
76.77
43.36
0.00
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140
130
120
110
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60
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20
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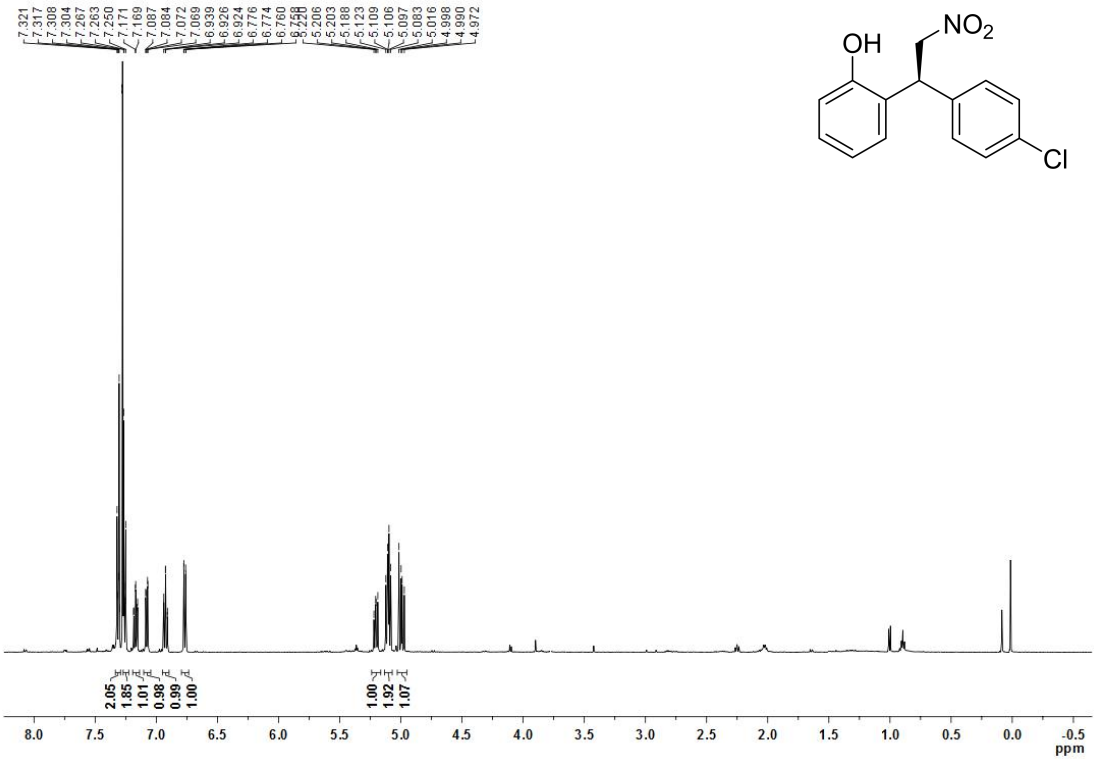
0
ppm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7.263
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7.087
7.084
7.072
7.069
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6.926
6.924
6.776
6.774
6.760
5.206
5.203
5.188
5.123
5.109
5.106
5.097
5.083
5.016
4.998
4.990
4.972
OH
NO2
Cl
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1.85
1.01
0.98
0.99
1.00
1.00
1.92
1.07
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.5
3.0
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1.0
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0.0
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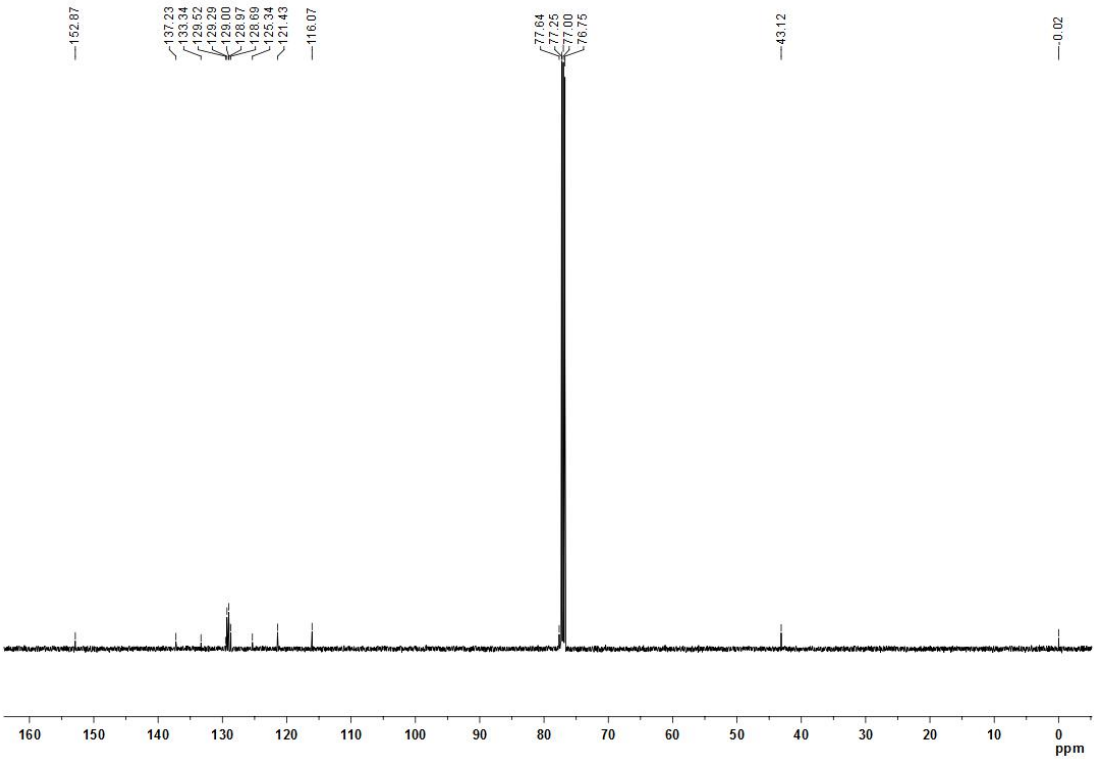
ppm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128.97
128.69
125.34
121.43
116.07
77.64
77.25
77.00
76.75
43.12
0.02
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150
140
130
120
110
100
90
80
70
60
50
40
30
20
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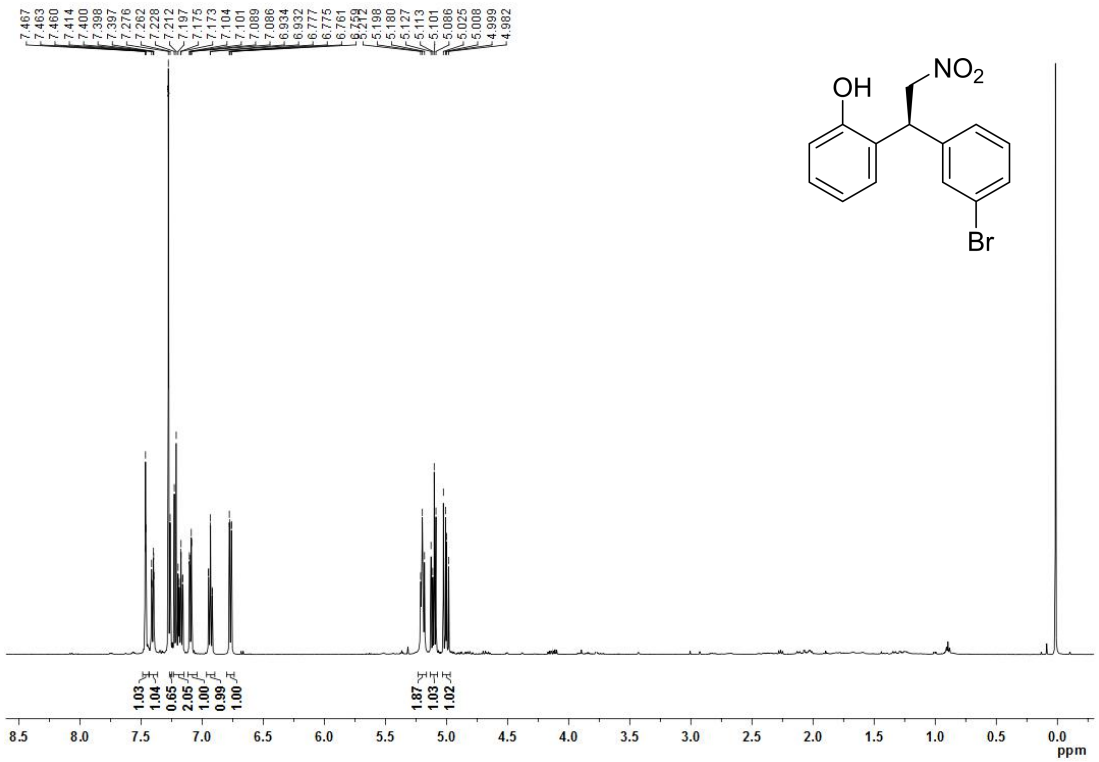
0
ppm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7.228
7.212
7.197
7.175
7.173
7.104
7.101
7.089
7.086
6.934
6.932
6.777
6.775
6.761
6.759
5.212
5.198
5.180
5.127
5.113
5.101
5.086
5.025
5.008
4.999
4.982
OH
NO2
Br
1.03
1.04
0.65
2.05
1.00
0.99
1.00
1.87
1.03
1.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
2.5
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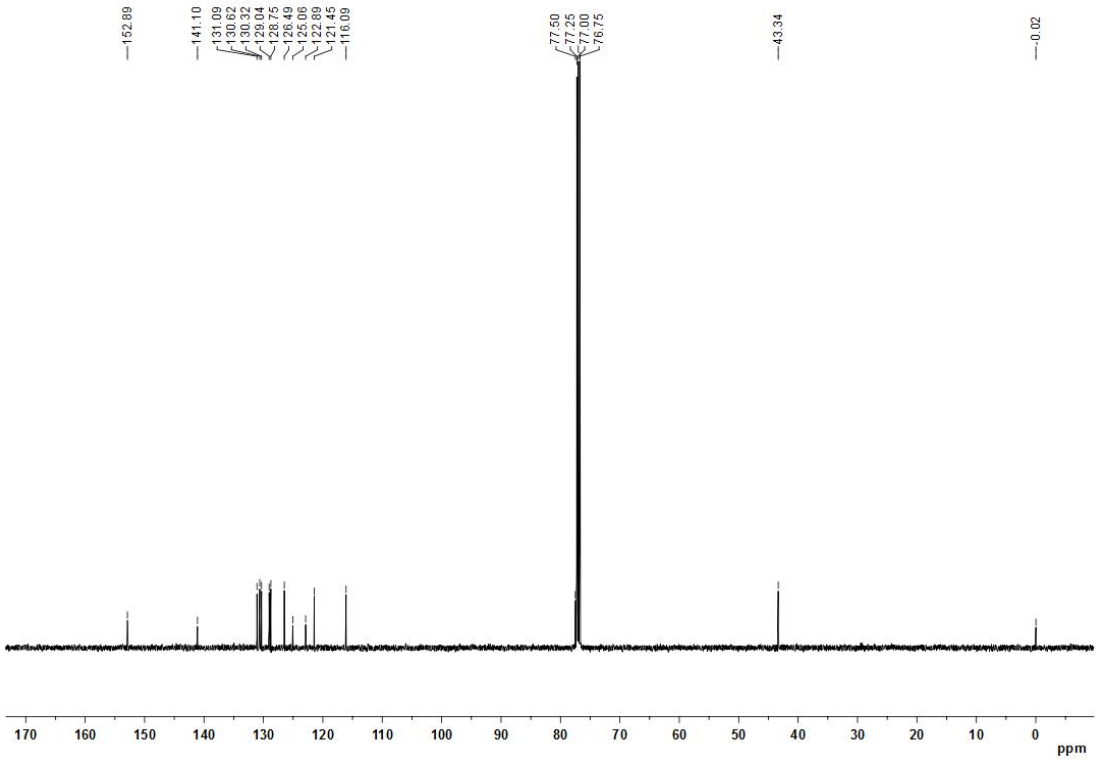
1.5
1.0
0.5
0.0
ppm


152.89
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126.49
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122.89
121.45
116.09
77.50
77.25
77.00
76.75
43.34
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140
130
120
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100
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60
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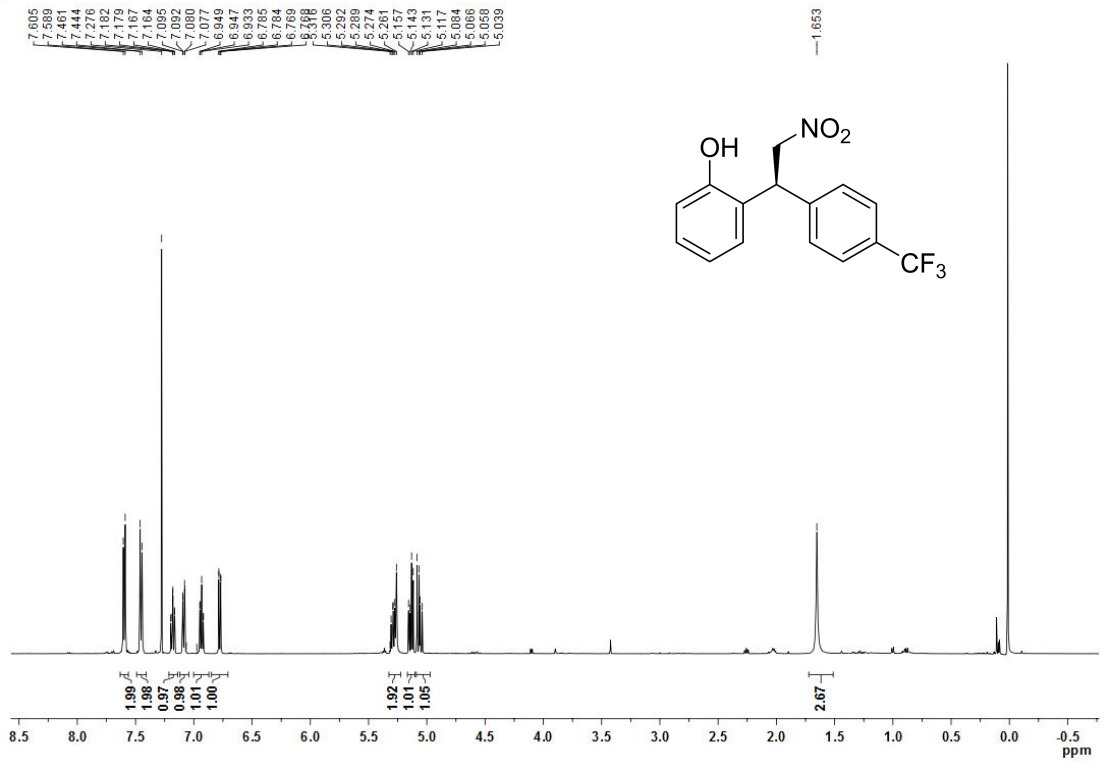
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7.092
7.080
7.077
6.949
6.947
6.933
6.785
6.784
6.769
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5.306
5.292
5.289
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5.157
5.143
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5.117
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5.066
5.058
5.039
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1.98
0.97
0.98
1.01
1.00
1.92
1.01
1.05
2.67
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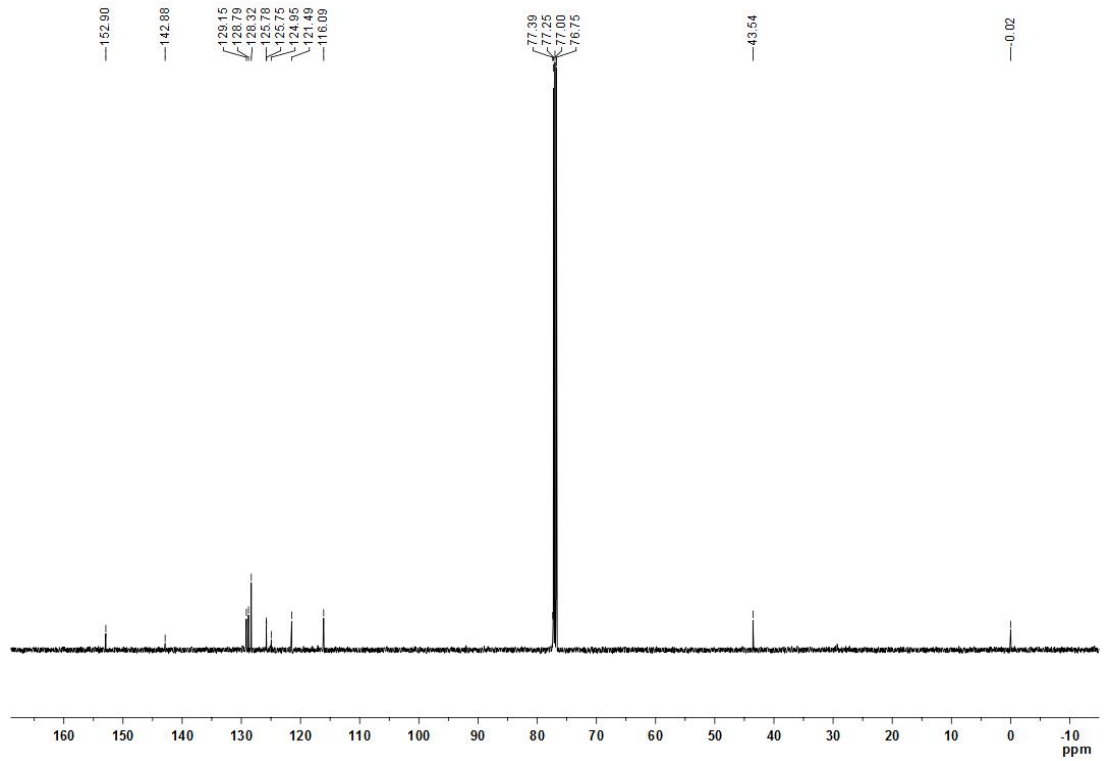
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125.75
124.95
121.49
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77.00
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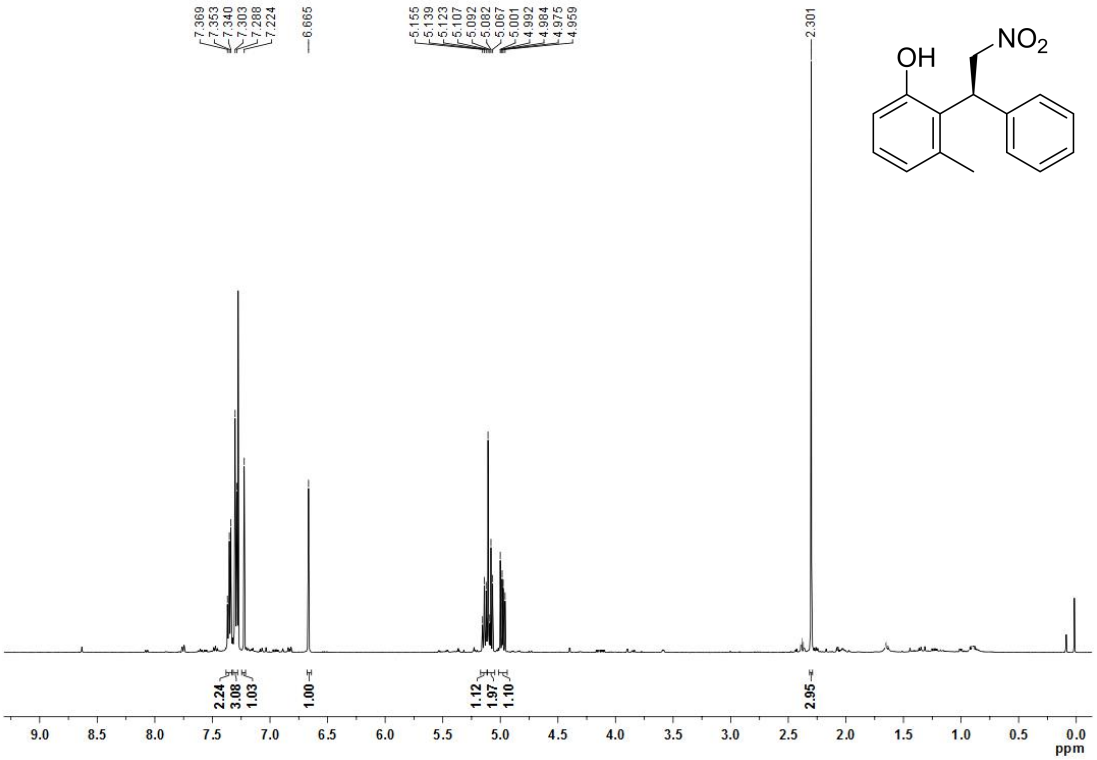
ppm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5.123
5.107
5.092
5.082
5.067
5.001
4.992
4.984
4.975
4.959
2.301
OH
NO2
2.24
3.08
1.03
1.00
1.12
1.97
1.10
2.95
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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4.0
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3.0
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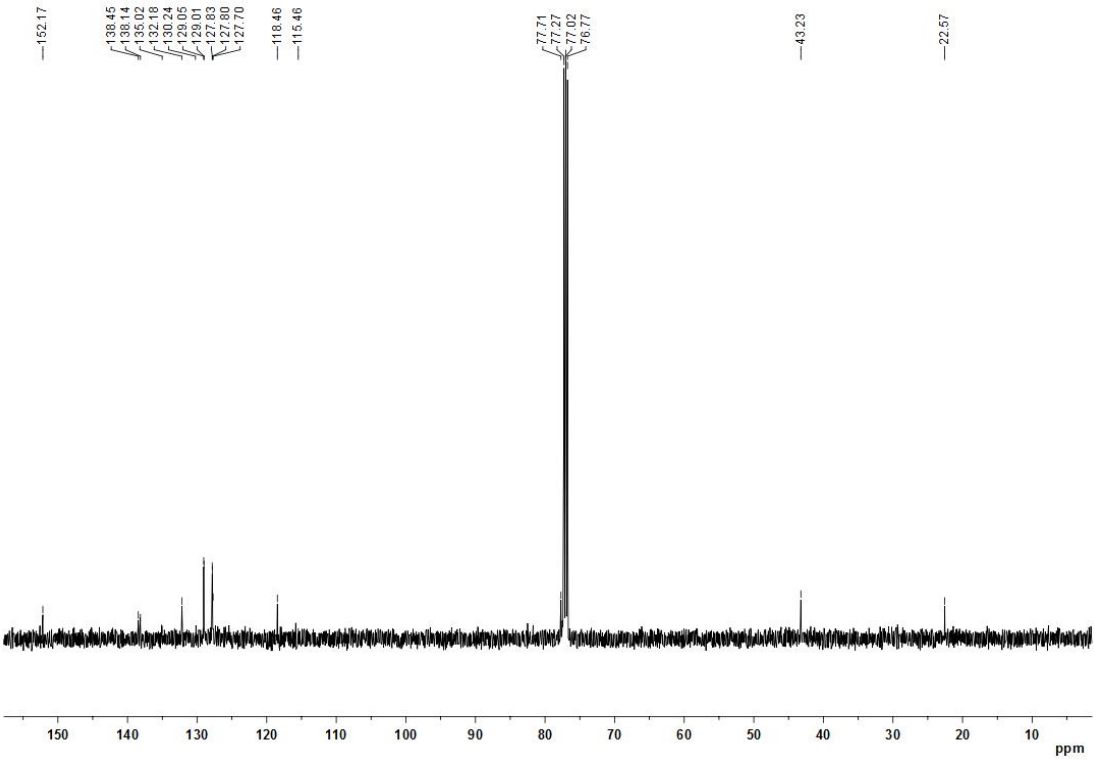
0.0
ppm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127.80
127.70
118.46
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77.02
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70
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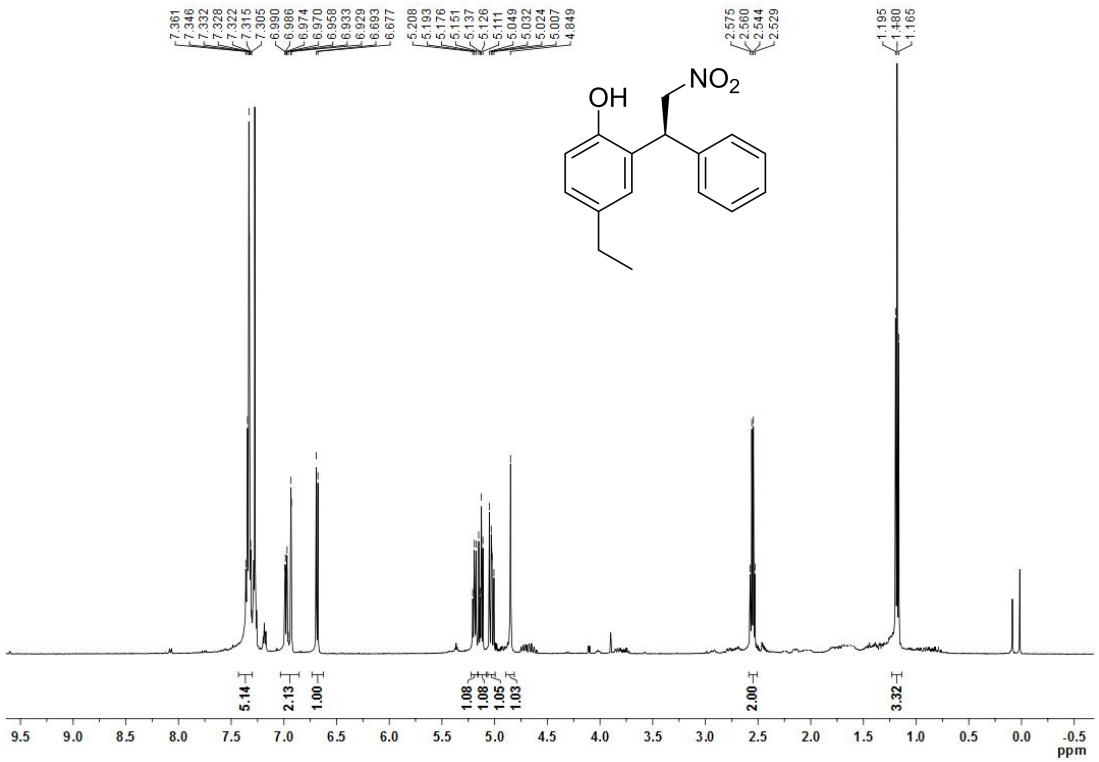
30
20
10
ppm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6.958
6.933
6.929
6.693
6.677
5.208
5.193
5.176
5.151
5.137
5.126
5.111
5.049
5.032
5.024
5.007
4.849
2.575
2.560
2.544
2.529
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1.05
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2.00
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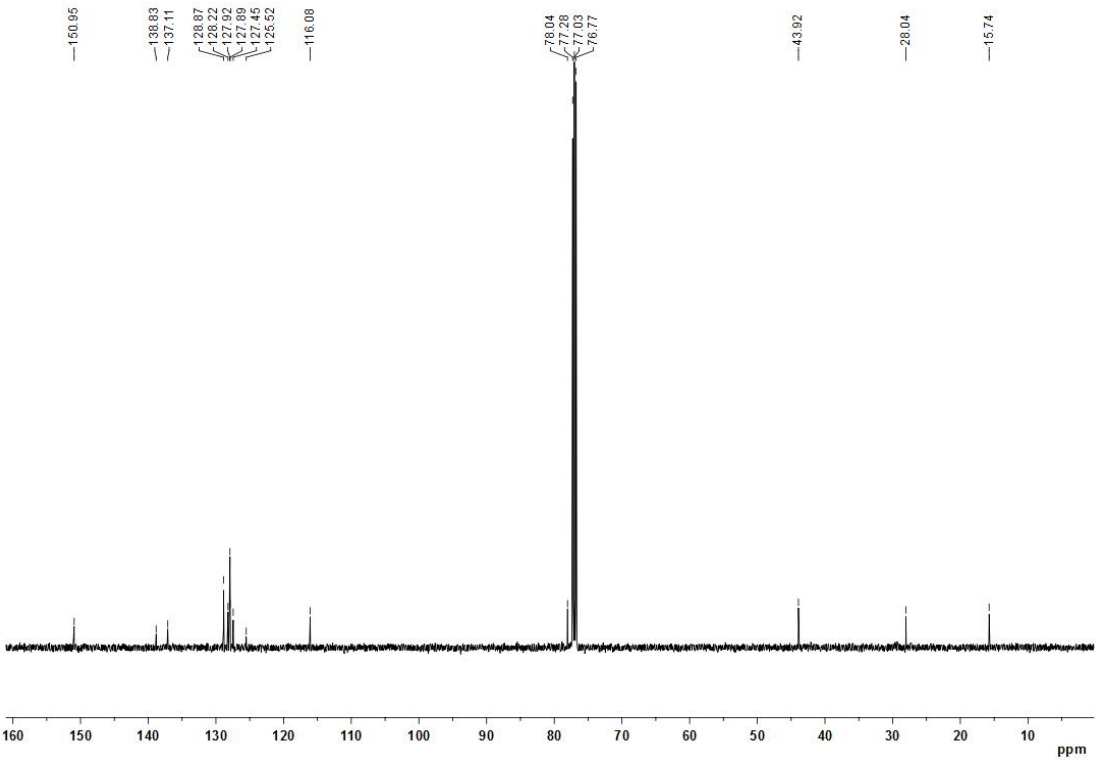
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125.52
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76.77
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15.74
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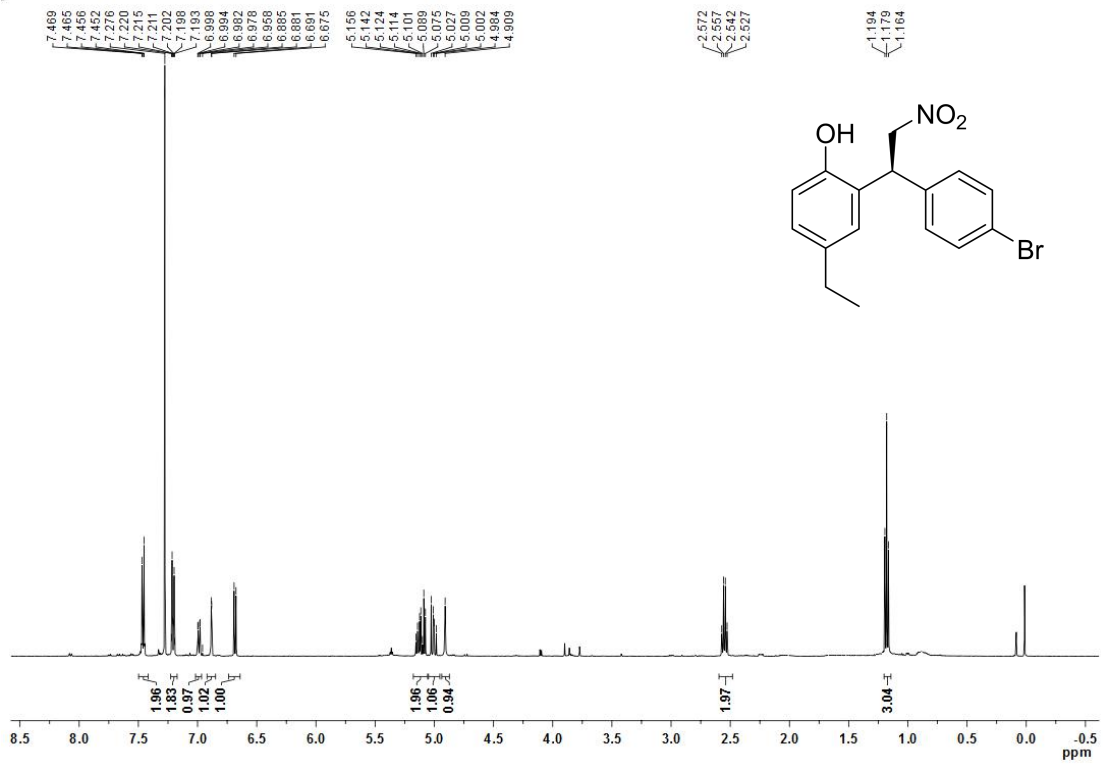
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7.276
7.220
7.215
7.211
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7.198
7.193
6.998
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6.992
6.978
6.958
6.885
6.881
6.691
6.675
5.156
5.142
5.124
5.114
5.101
5.089
5.075
5.027
5.009
5.002
4.984
4.909
2.572
2.557
2.542
2.527
1.194
1.179
1.164
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Br
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1.06
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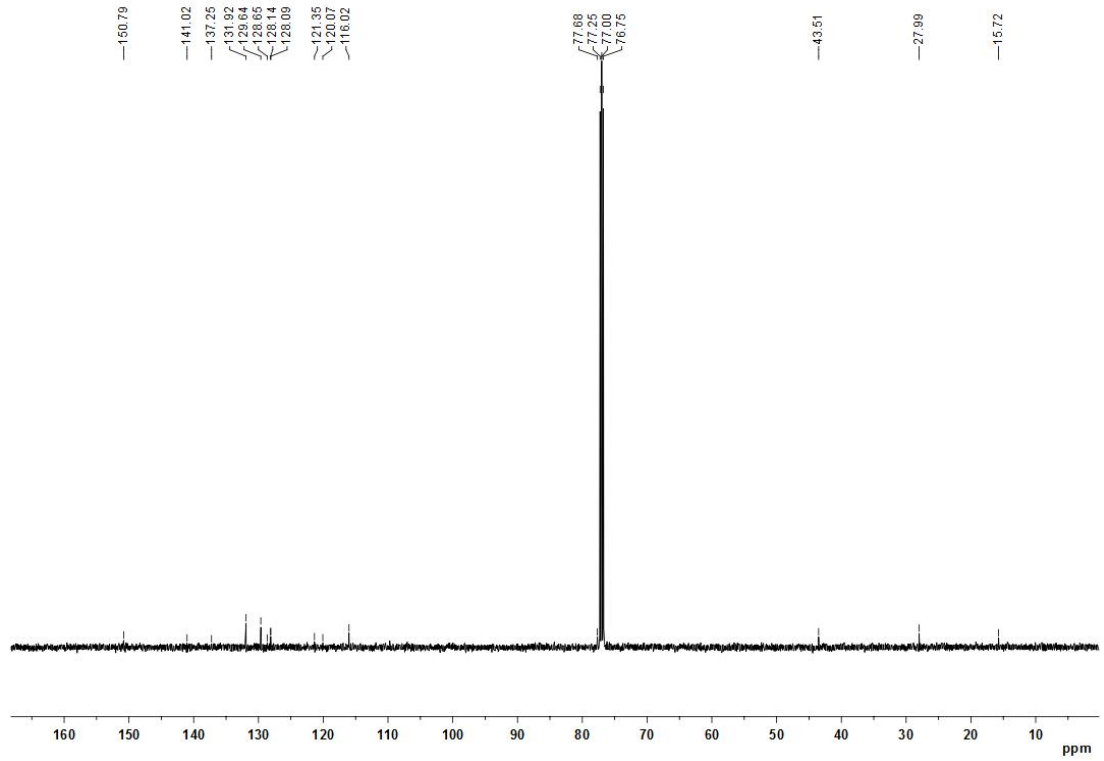
1.97
3.04
ppm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128.65
128.14
128.09
121.35
120.07
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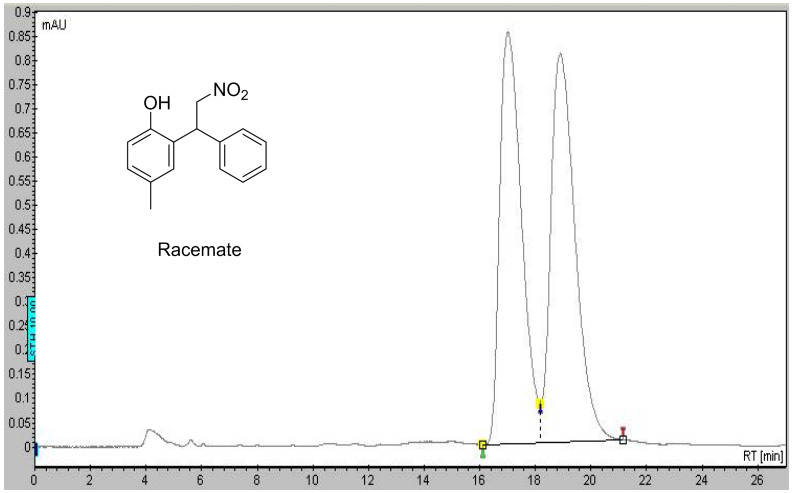
77.00
76.75
43.51
27.99
15.72
ppm

4. HPLC spectra of aromatization products



Peak	Time[min]	Area[%]
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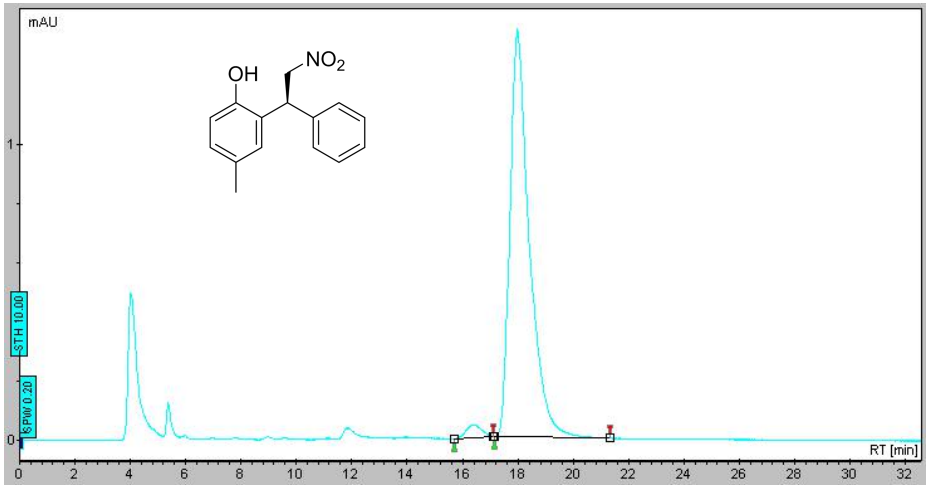
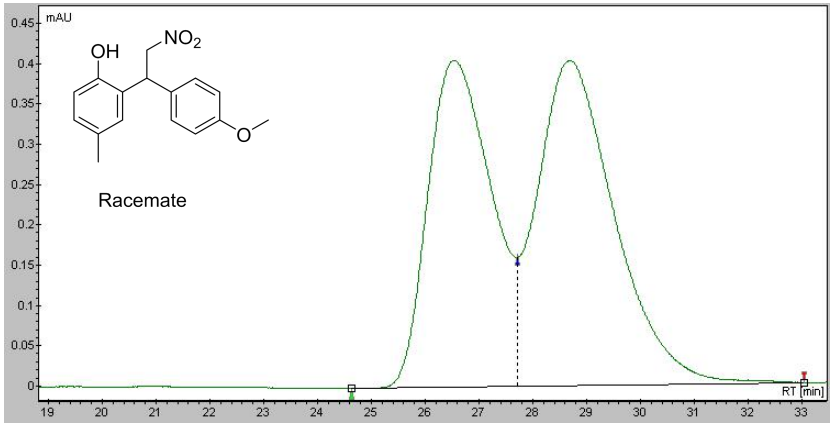
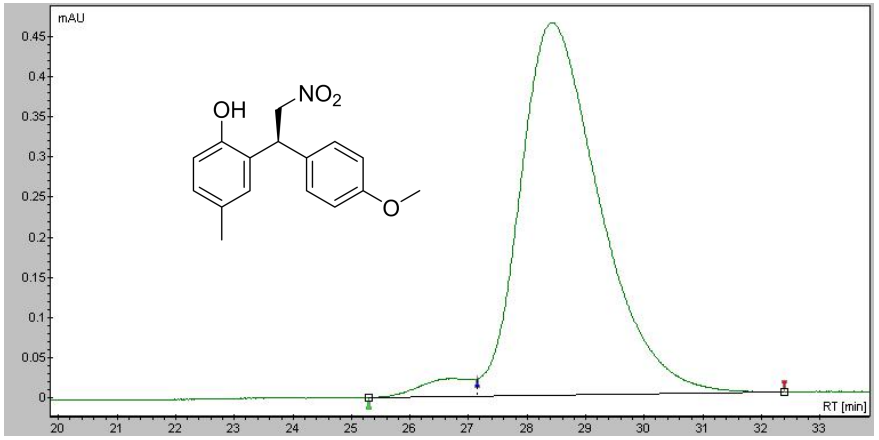
2	18.892	51.245
总计		100



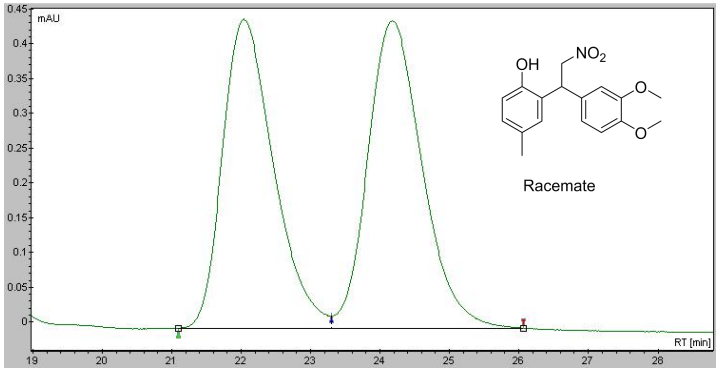
Peak	Time[min]	Area[%]
1	16.385	2.473
2	17.972	97.527
总计		100



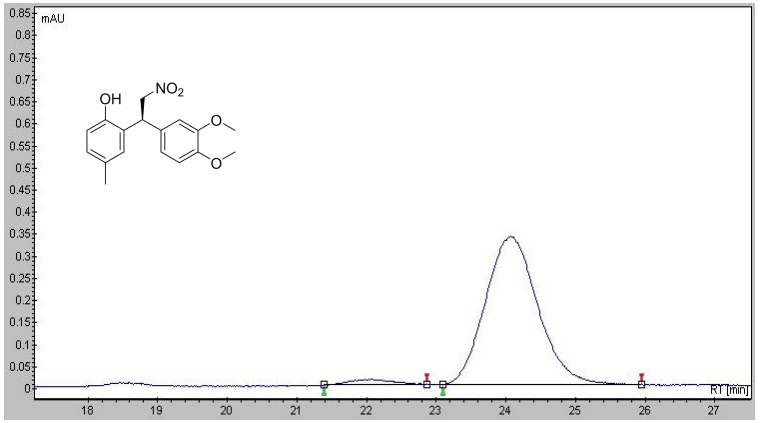
Peak	Time[min]	Area[%]
1	26.531	45.140
2	28.691	54.860
总计		100



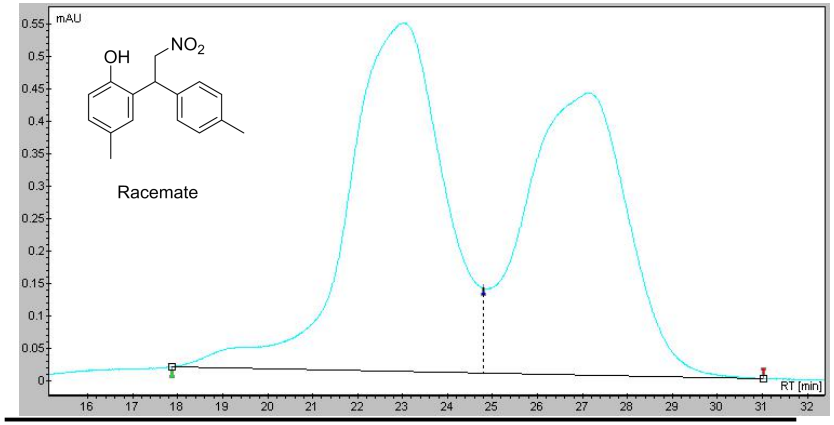
Peak	Time[min]	Area[%]
1	26.678	3.037
2	28.425	96.963
总计		100



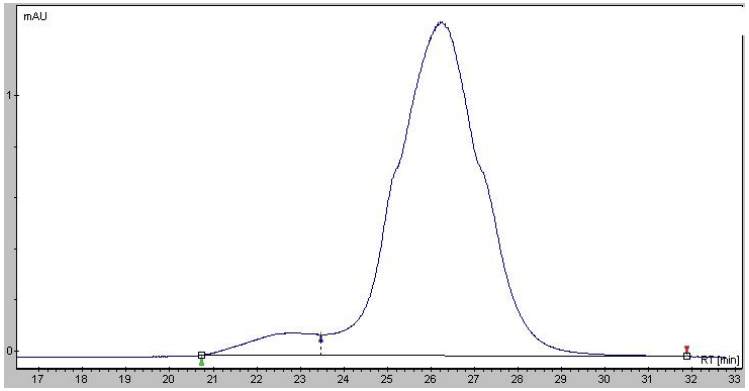
Peak	Time[min]	Area[%]
1	22.038	48.600
2	24.172	51.400
总计		100



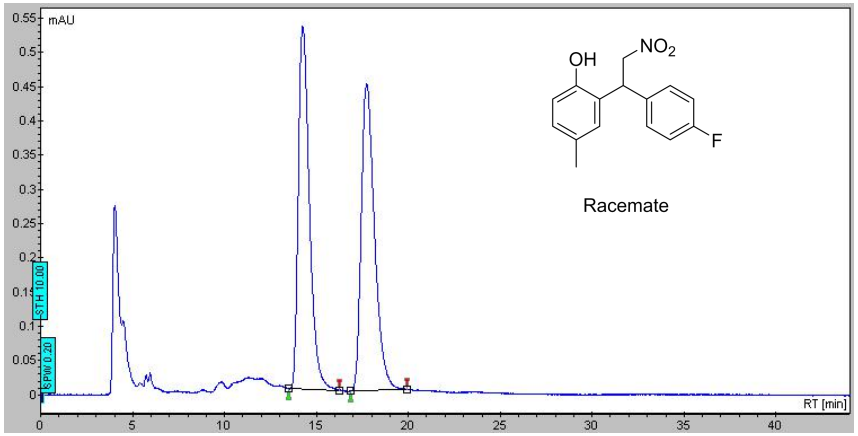
Peak	Time[min]	Area[%]
1	22.025	2.818
2	24.052	97.182
总计		100



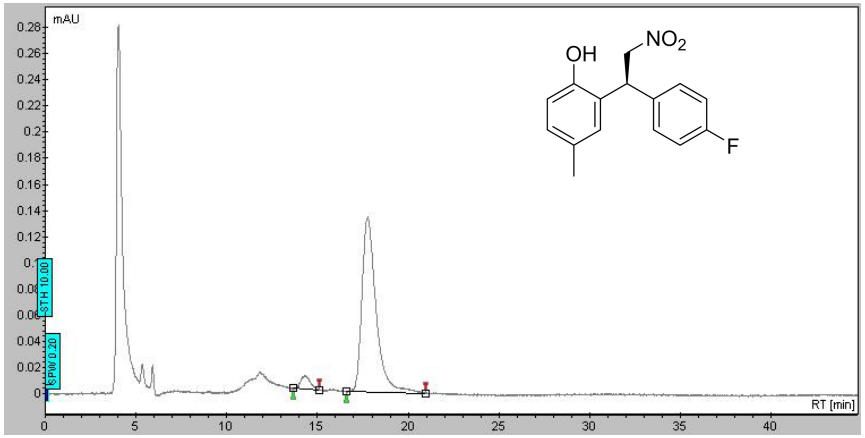
Peak	Time[min]	Area[%]
1	23.012	53.430
2	27.145	46.570
总计		100



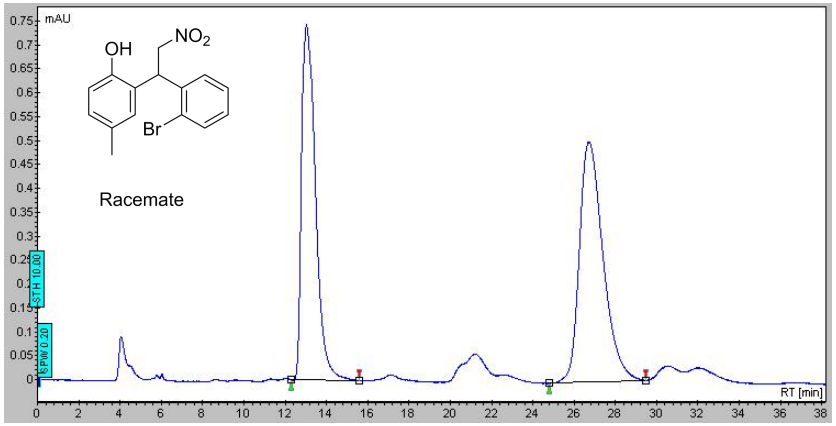
Peak	Time[min]	Area[%]
1	22.825	5.026
2	26.211	94.974
总计		100



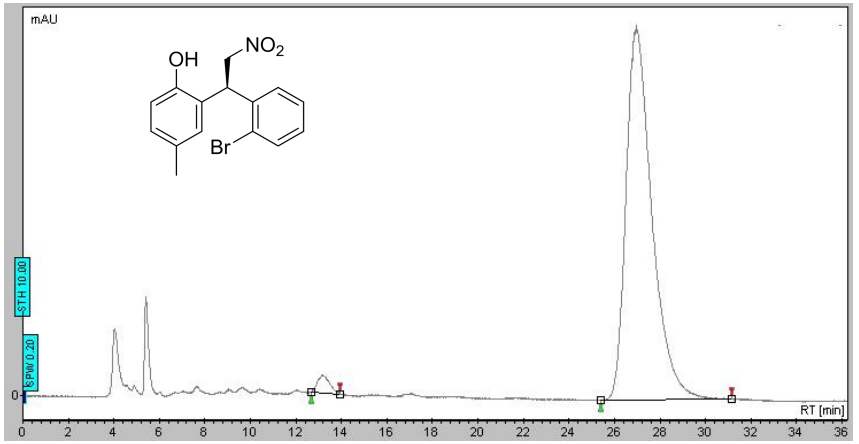
Peak	Time[min]	Area[%]
1	14.252	49.762
2	17.732	50.238
总计		100



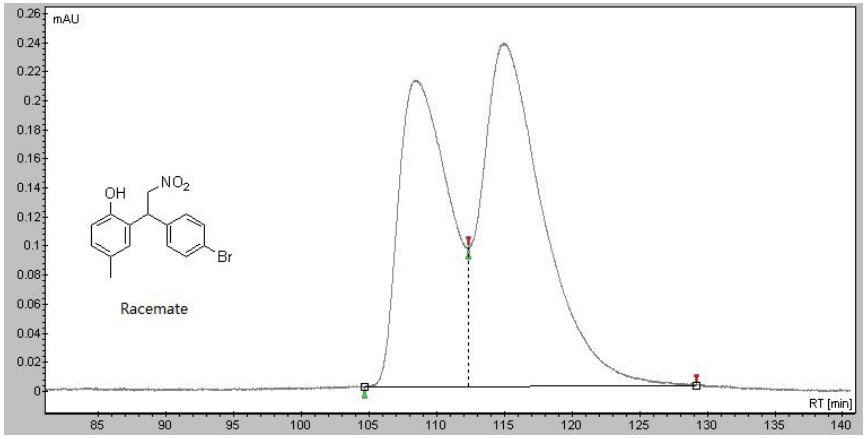
Peak	Time[min]	Area[%]
1	14.319	4.712
2	17.759	95.288
总计		100



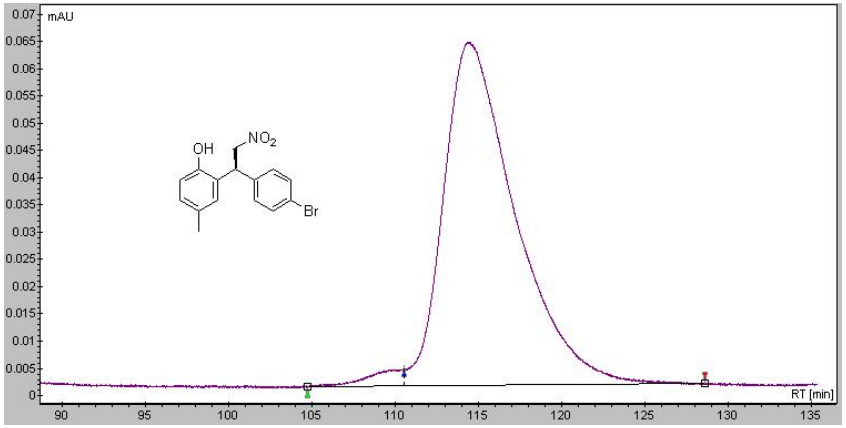
Peak	Time[min]	Area[%]
1	13.039	46.764
2	26.731	53.236
总计		100



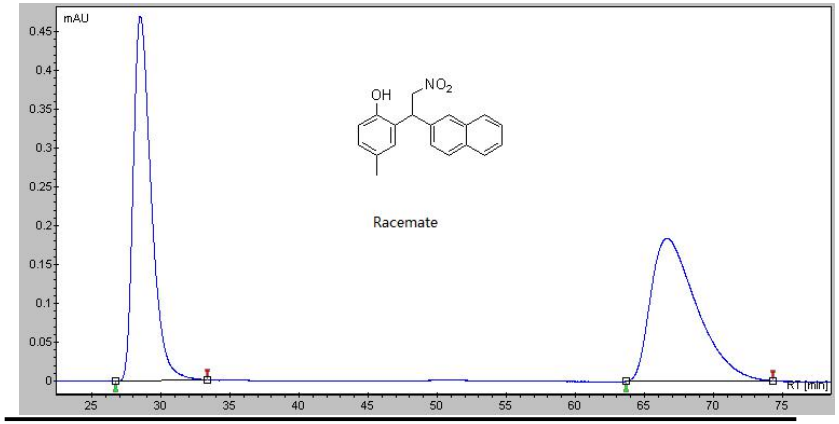
Peak	Time[min]	Area[%]
1	13.186	2.092
2	26.958	97.908
总计		100



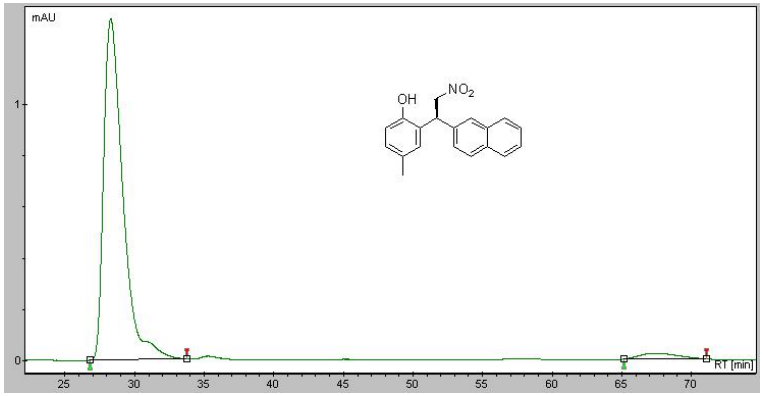
Peak	Time[min]	Area[%]
1	108.432	42.226
2	114.920	57.774
总计		100



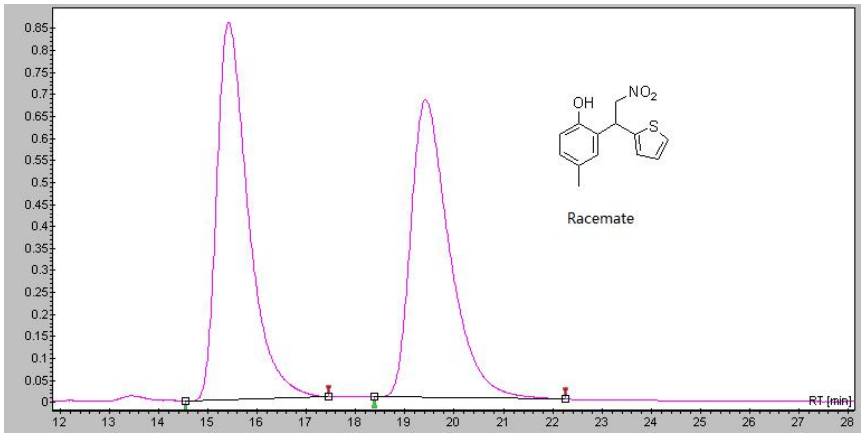
Peak	Time[min]	Area[%]
1	110.536	2.457
2	114.427	97.543
总计		100



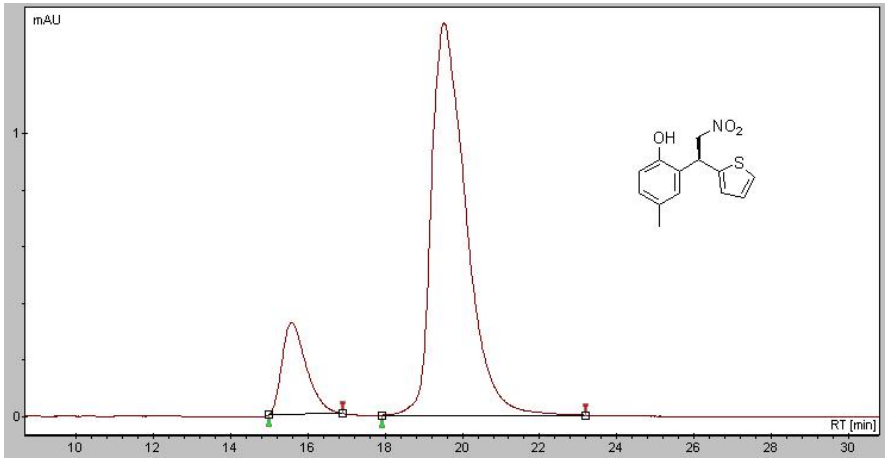
Peak	Time[min]	Area[%]
1	28.510	49.997
2	66.589	50.003
总计		100



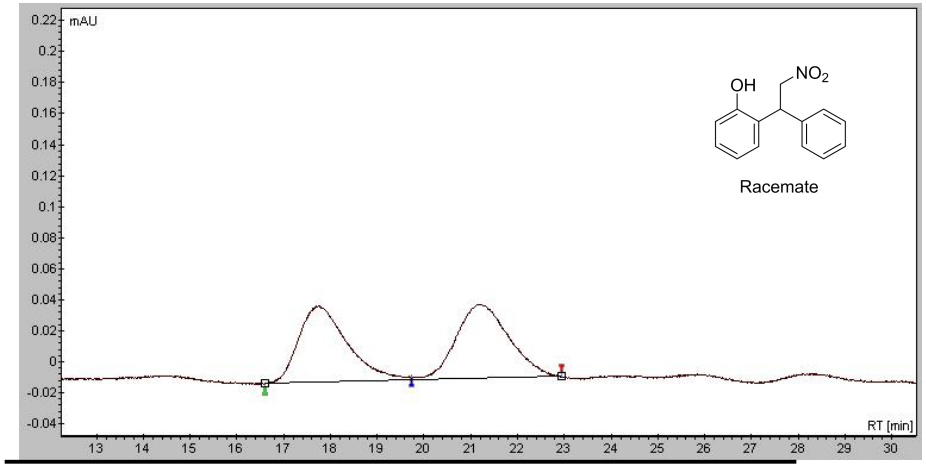
Peak	Time[min]	Area[%]
1	28.283	96.723
2	67.376	3.277
总计		100



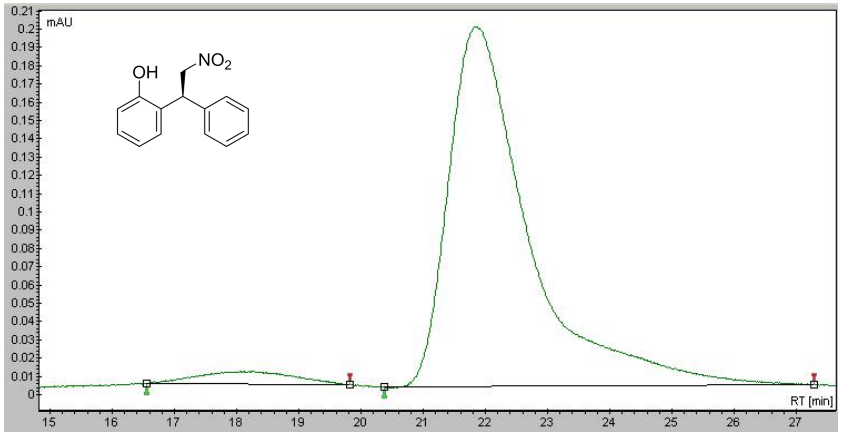
Peak	Time[min]	Area[%]
1	15.412	50.812
2	19.412	49.188
总计		100



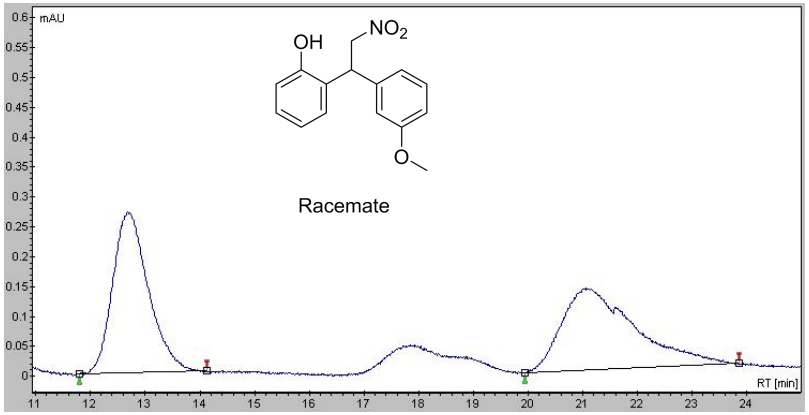
Peak	Time[min]	Area[%]
1	15.586	14.204
2	19.532	85.796
总计		100



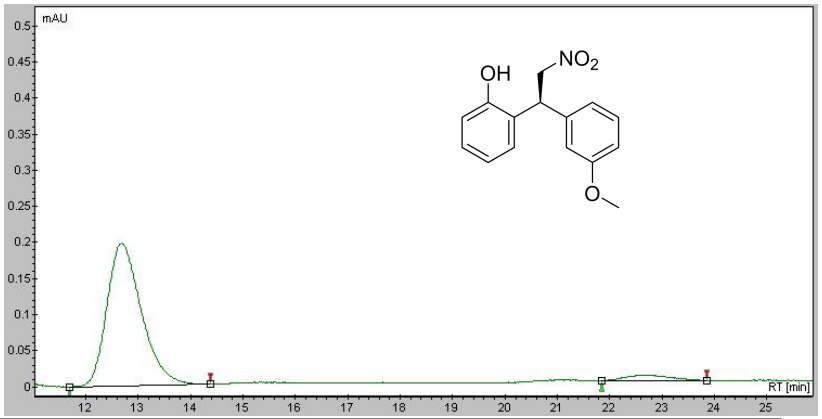
Peak	Time[min]	Area[%]
1	17.772	48.642
2	21.198	51.358
总计		100



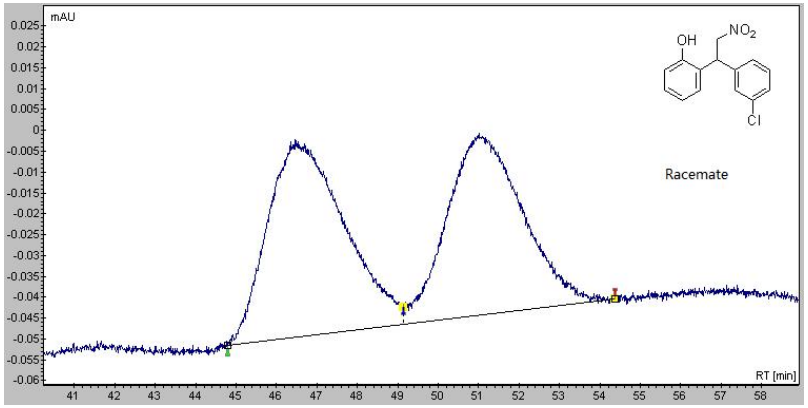
Peak	Time[min]	Area[%]
1	18.159	3.959
2	21.865	96.041
总计		100



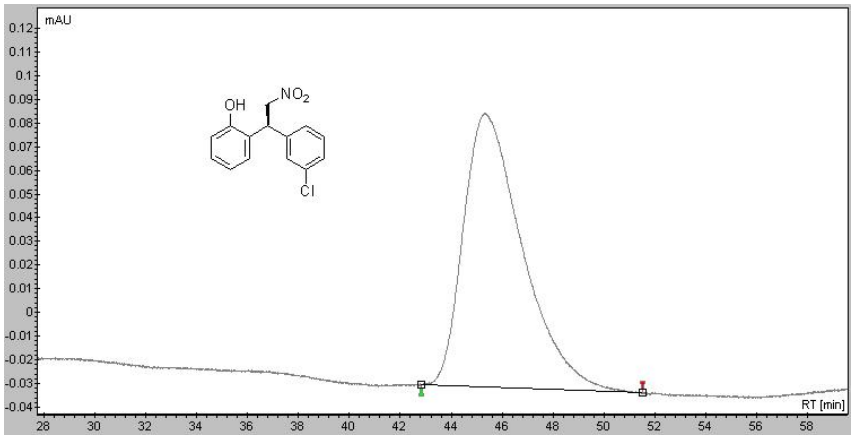
Peak	Time[min]	Area[%]
1	12.692	48.897
2	21.038	51.103



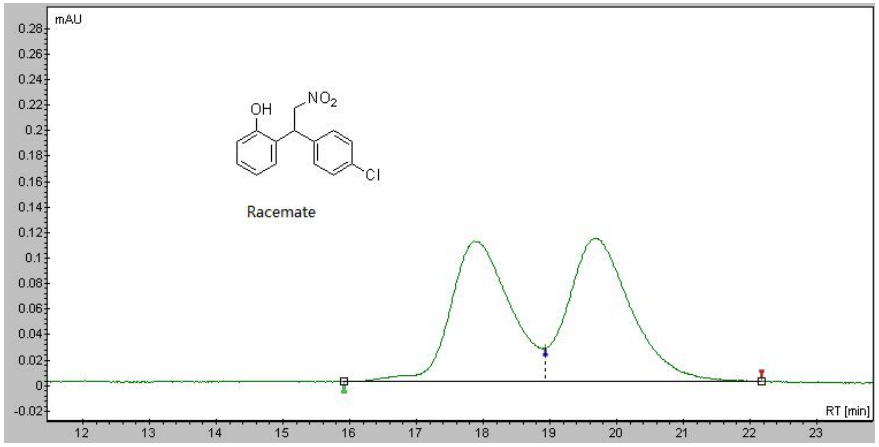
Peak	Time[min]	Area[%]
1	12.692	95.233
2	22.665	4.767
总计		100



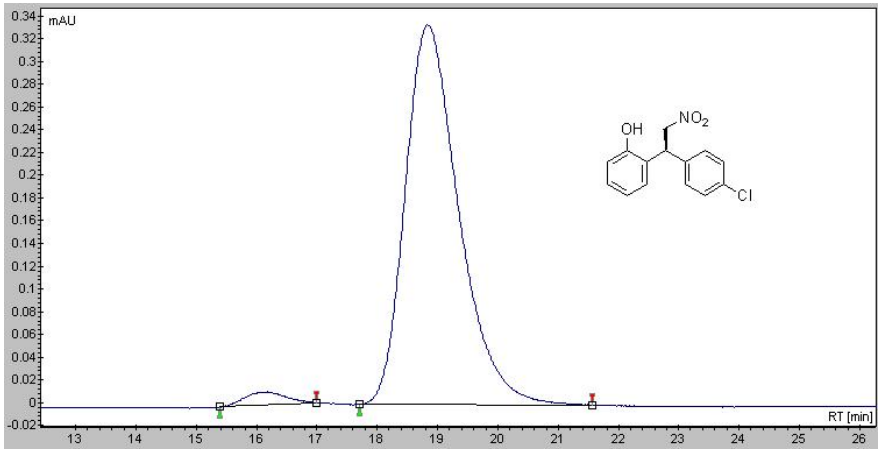
Peak	Time[min]	Area[%]
1	46.450	52.285
2	51.023	47.715
总计		100



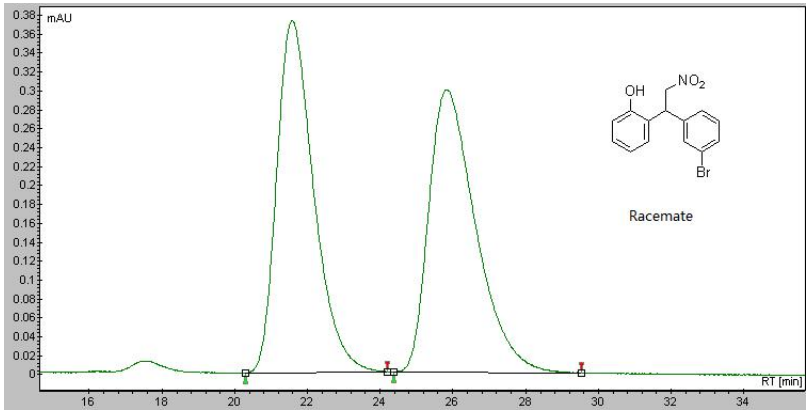
Peak	Time[min]	Area[%]
1	45.330	100.000
总计		100



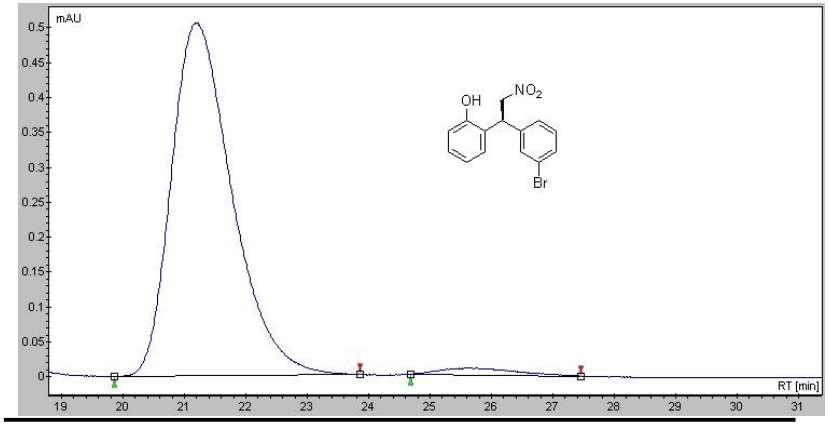
Peak	Time[min]	Area[%]
1	17.892	48.501
2	19.692	51.499
总计		100



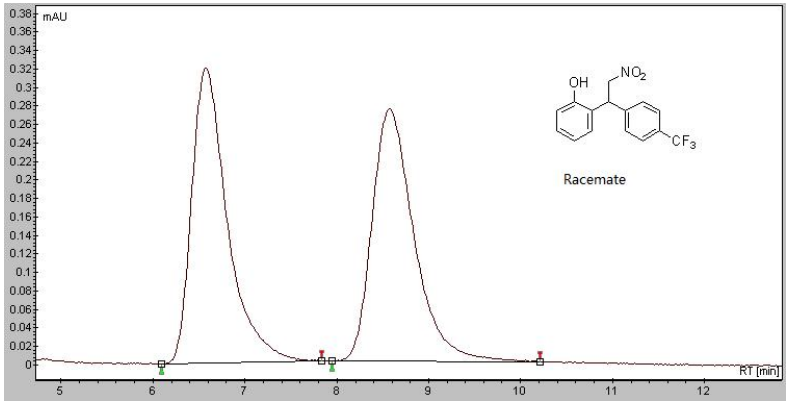
Peak	Time[min]	Area[%]
1	16.105	2.591
2	18.839	97.409
总计		100



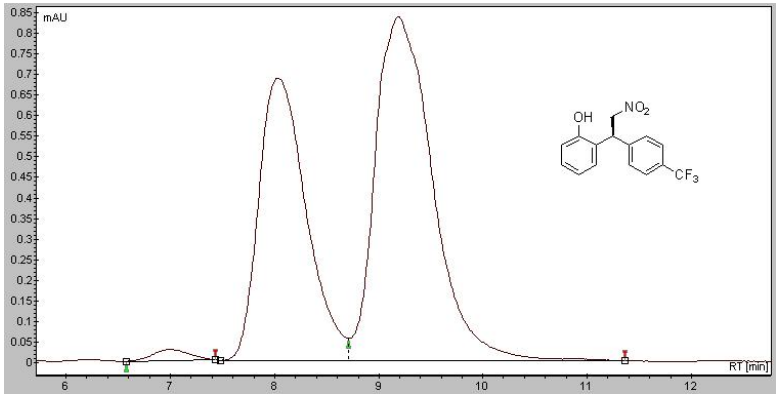
Peak	Time[min]	Area[%]
1	21.585	49.540
2	25.838	50.460
总计		100



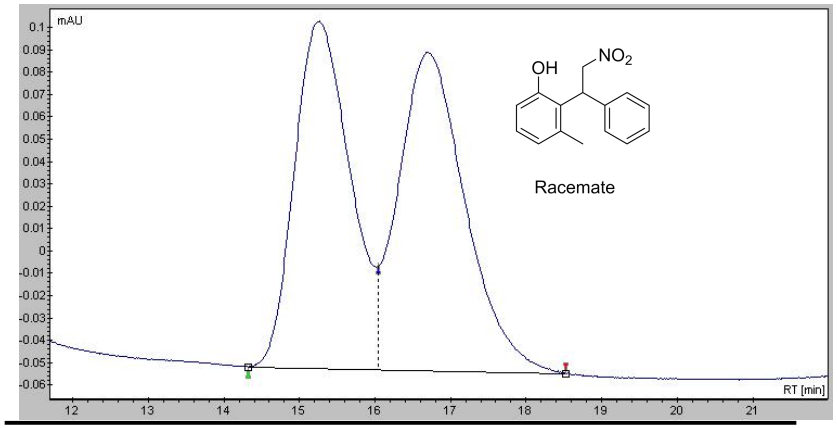
Peak	Time[min]	Area[%]
1	21.198	97.715
2	25.678	2.285
总计		100



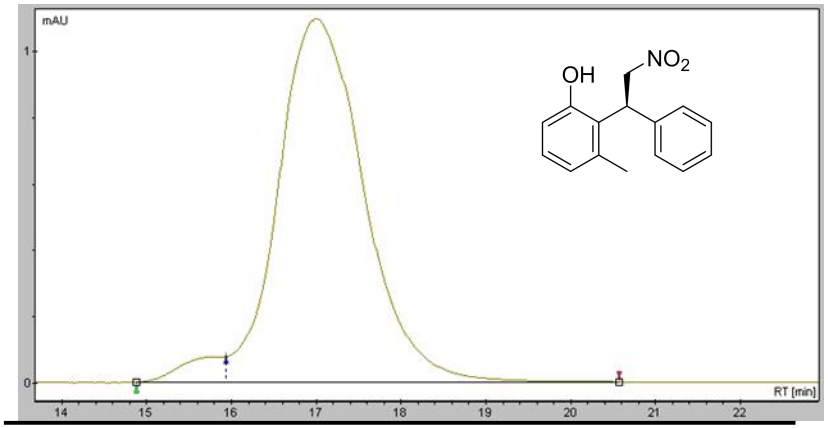
Peak	Time[min]	Area[%]
1	6.573	49.952
2	8.587	50.048
总计		100



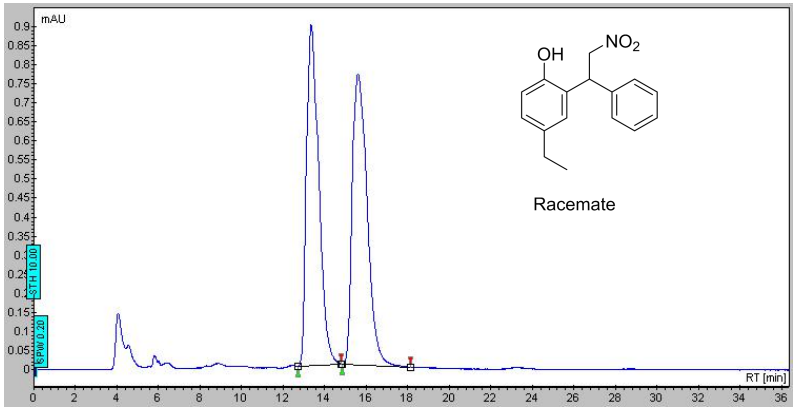
Peak	Time[min]	Area[%]
1	6.986	1.966
2	9.186	98.034
总计		100



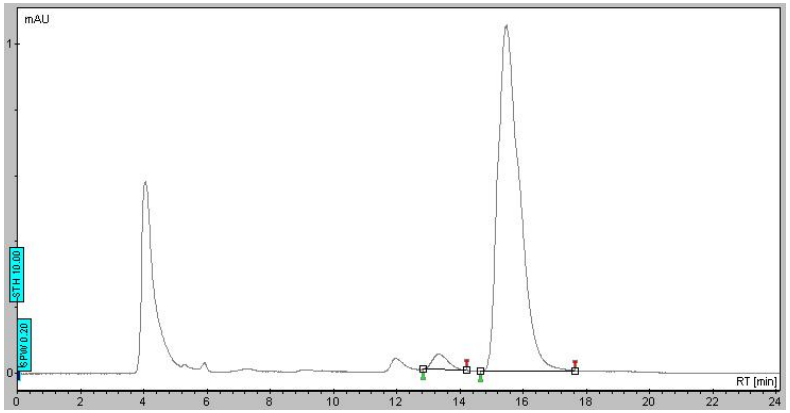
Peak	Time[min]	Area[%]
1	15.252	47.725
2	16.705	52.275
总计		100



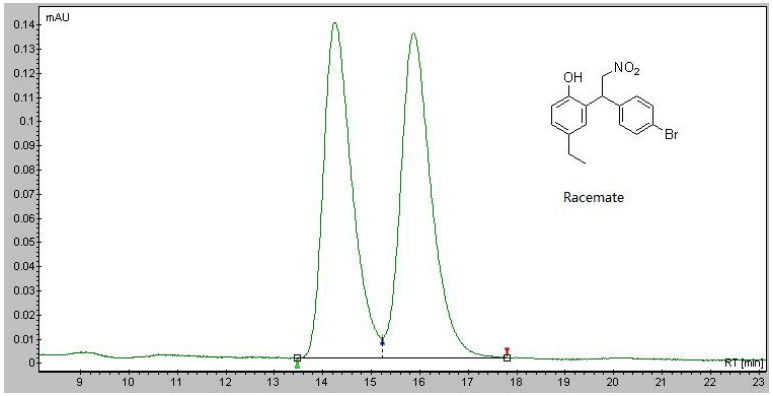
Peak	Time[min]	Area[%]
1	15.937	3.495
2	16.999	96.505
总计		100



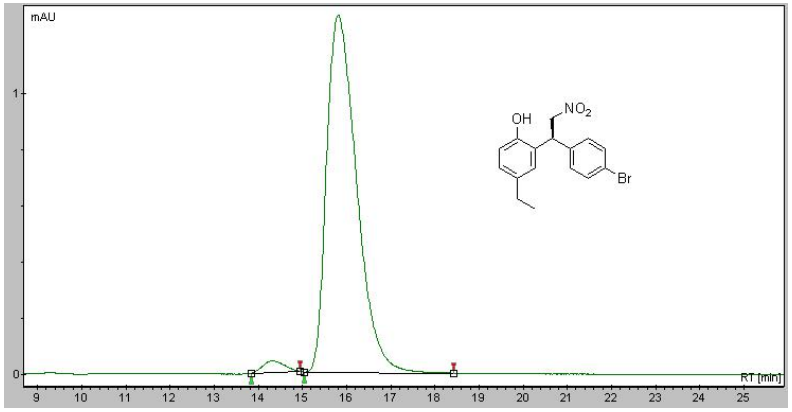
Peak	Time[min]	Area[%]
1	13.346	49.165
2	15.599	50.835
总计		100



Peak	Time[min]	Area[%]
1	13.346	3.268
2	15.479	96.732
总计		100



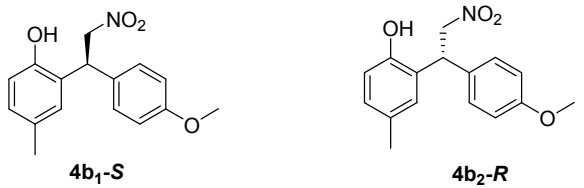
Peak	Time[min]	Area[%]
1	14.252	49.081
2	15.879	50.919
总计		100



Peak	Time[min]	Area[%]
1	14.319	2.263
2	15.799	97.737
总计		100

5. The absolute configuration of the aromatization product 4b

The absolute configuration of chiral aromatization product **4b** has been assigned by means of TDDFT CD computations. To investigate the unknown chirality of **4b**, two ground-state geometries, known molecules 1-S (2S) / 2-R (2R) (**Figure 5.1**), have been optimized at the TD DFT M06-2x//DFT M06-2x levels by employing Gaussian 03W Pack. As shown in Figure 5.5, in the selected data in the 200-330 nm UV region, the experimental CD spectra (**Figure 5.4**) match well with the calculated data (**Figure 5.2**).



4b$_1$-*S* **4b$_2$-*R***

Figure 5.1

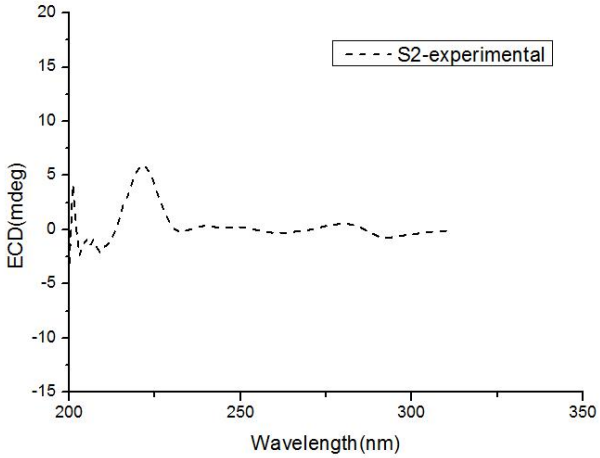


Figure 5.2

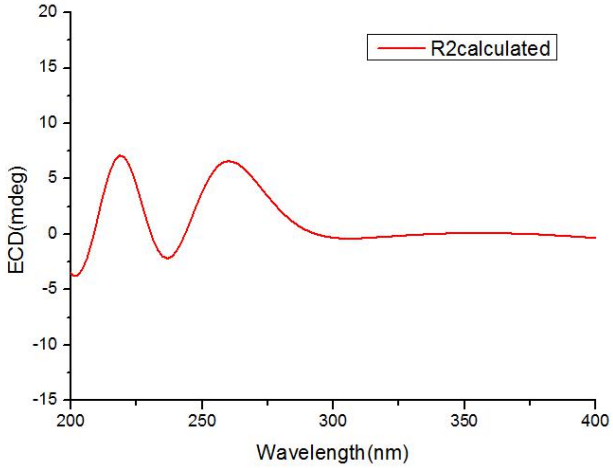


Figure 5.3

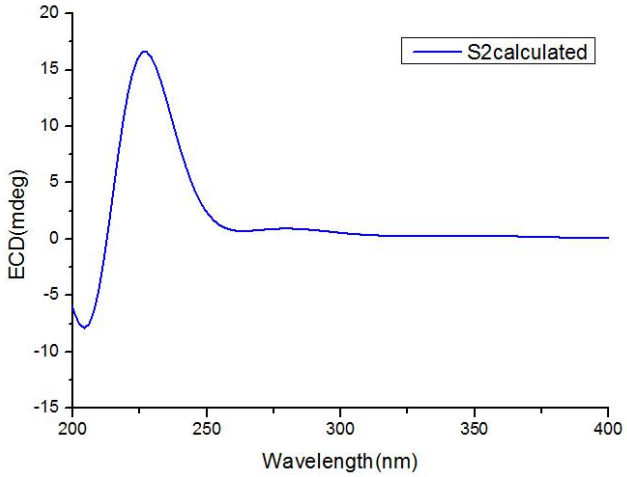


Figure 5.4

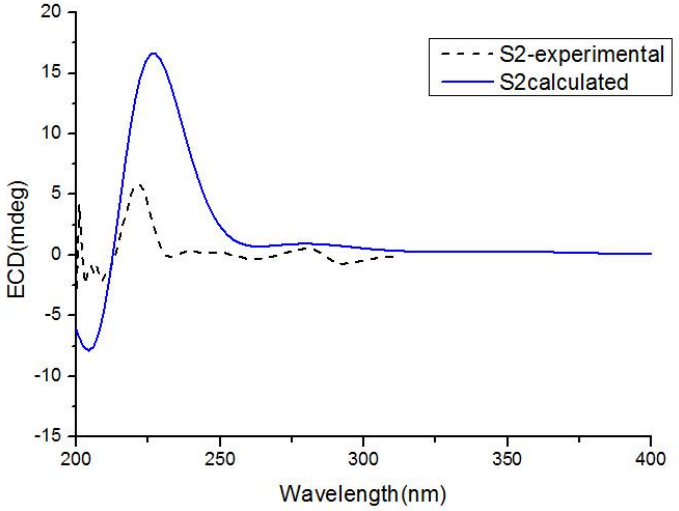


Figure 5.5

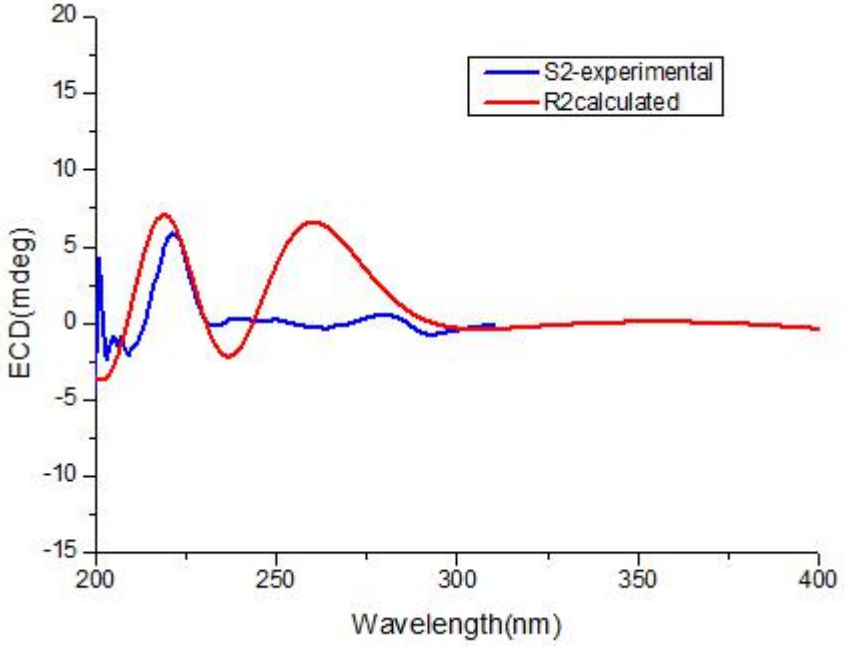

S2-experimental
R2calculated
ECD(mdeg)
Wavelength(nm)
20
15
10
5
0
-5
-10
-15
200
250
300
350
400

Figure 5.6

Experimental CD spectrum data

TITLE 1-2

DATA TYPE

ORIGIN JASCO

OWNER

DATE 17/02/21

TIME 09:26:23

SPECTROMETER/DATA SYSTEM

RESOLUTION

DELTAX -1

XUNITS NANOMETERS

YUNITS ARBITRARY UNITS

FIRSTX 310.0000

LASTX 192.0000

NPOINTS 119

FIRSTY -0.49193

MAXY 16.82049

MINY -47.91072

XYDATA

310.0000 -0.491928 179.024 0.01658

309.0000 -0.512866 179.225 0.0172707

308.0000 -0.59438 179.472 0.0184496

307.0000 -0.637714 179.747 0.0198789

306.0000 -0.690965 180.036 0.0214097

305.0000 -0.741331 180.353 0.0229888

304.0000 -0.812039 180.711 0.0247906

303.0000 -0.895958 181.097 0.0269198

302.0000 -0.955379 181.523 0.0293725

301.0000 -1.01146 182.008 0.0323787

300.0000 -1.11002 182.587 0.0365791

299.0000 -1.19373 183.271 0.0419338

298.0000 -1.31172 184.085 0.0490173

297.0000 -1.40724 185.066 0.0581477

296.0000 -1.52287 186.252 0.0697324

295.0000 -1.61766 187.645 0.0839086

294.0000 -1.71285 189.248 0.100708

293.0000 -1.78171 191.035 0.119596

292.0000 -1.80918 192.954 0.139984

291.0000 -1.75361 194.966 0.161376

290.0000 -1.583 197.028 0.183302

289.0000 -1.30705 199.082 0.204892

288.0000 -1.01998 201.085 0.22535

287.0000 -0.602127 203.024 0.244584

286.0000 -0.181946 204.897 0.262701

285.0000 0.24278 206.667 0.279337

284.0000 0.601413 208.295 0.293946

283.0000 0.878421 209.751 0.306164

282.0000 1.14465 210.994 0.315548

281.0000 1.30851 212.005 0.32211

280.0000 1.30427 212.768 0.32568

279.0000 1.28062 213.31 0.326441

278.0000 1.24395 213.681 0.324717

277.0000 1.10724 213.887 0.320713

276.0000 0.888629 213.956 0.314789

275.0000 0.673174 213.933 0.307597

274.0000 0.444849 213.839 0.299163

273.0000 0.240691 213.673 0.289338

272.0000 -0.0001297 213.443 0.278333

271.0000 -0.251978 213.164 0.266359

270.0000 -0.431038 212.878 0.253756

269.0000 -0.615674 212.612 0.240803

268.0000 -0.734457 212.389 0.227622

267.0000 -0.841846 212.23 0.214522

266.0000 -0.901686 212.152 0.201861

265.0000 -0.958298 212.155 0.18964

264.0000 -1.02975 212.243 0.177898

263.0000 -0.997325 212.42 0.166706

262.0000 -0.947099 212.694 0.156367

261.0000 -0.893469 213.055 0.146813

260.0000 -0.870554 213.512 0.13795

259.0000 -0.822719 214.067 0.129533

258.0000 -0.631531 214.719 0.122044

257.0000 -0.475969 215.471 0.11535

256.0000 -0.35659 216.331 0.109568

255.0000 -0.252429 217.291 0.104372

254.0000 -0.108282 218.34 0.0999044

253.0000 0.0510971 219.476 0.0964408

252.0000 0.199892 220.712 0.0941404

251.0000 0.235286 222.062 0.0927483

250.0000 0.278235 223.519 0.0921516

249.0000 0.337482 225.079 0.0924457

248.0000 0.355063 226.774 0.0941388

247.0000 0.350665 228.626 0.0974084

246.0000 0.406154 230.695 0.102579

245.0000 0.4399 233.012 0.110049

244.0000 0.549821 235.671 0.121243

243.0000 0.631458 238.783 0.137101

242.0000 0.820615 242.521 0.15895

241.0000 1.01753 247.021 0.188358

240.0000 1.15437 252.444 0.22745

239.0000 1.27311 258.95 0.27842

238.0000 1.18009 266.684 0.342965

237.0000 0.992506 275.817 0.423245

236.0000 0.621318 286.431 0.50495

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234.0000 -0.55191 311.842 0.692192

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232.0000 -1.00488 341.558 0.9009

231.0000 -0.671329 357.13 1.00239

230.0000 0.198163 372.542 1.096

229.0000 1.73785 387.395 1.17853

228.0000 4.0471 401.396 1.24809

227.0000 6.62694 414.298 1.30354

226.0000 9.03972 425.954 1.35146

225.0000 11.8019 436.328 1.38664

224.0000 14.407 445.476 1.40739

223.0000 15.9877 453.485 1.41859

222.0000 16.7091 460.465 1.42168

221.0000 16.8205 466.607 1.41814

220.0000 16.2893 472.182 1.41019

219.0000 15.3939 477.497 1.40012

218.0000 13.4242 482.896 1.39015

217.0000 10.9259 488.768 1.38258

216.0000 8.15936 495.521 1.38006

215.0000 6.46927 503.582 1.38525

214.0000 4.52647 513.368 1.40038

213.0000 2.25164 525.4 1.428

212.0000 -0.664653 540.381 1.47129

211.0000 -2.39951 559.252 1.53477

210.0000 -2.67719 583.232 1.62371

209.0000 -2.24389 613.775 1.7385

208.0000 -6.29568 652.283 1.86674

207.0000 -7.53412 699.38 2.03342

206.0000 -1.25261 752.799 2.22703

205.0000 -0.815479 807.77 2.42401

204.0000 -10.7057 859.62 2.60065

203.0000 -12.1656 905.207 2.74083

202.0000 -17.9647 942.272 2.83201

201.0000 -7.27157 968.882 2.86369

200.0000 -8.13624 984.574 2.8346

199.0000 -17.5151 991.764 2.75084

198.0000 -25.3136 994.521 2.6251

197.0000 -32.1212 995.58 2.46496

196.0000 -45.1065 996.068 2.26934

195.0000 -34.9173 996.345 2.03036

194.0000 -47.9107 996.408 1.75989

193.0000 -32.4363 996.392 1.45752

192.0000 -41.5826 996.092 1.13204

Extended Information

[Comment]

Sample Name 1-2

Comment

User

Division

Company JASCO

[Data Information]

Creation Date 2017-2-21 9:26

Data array type Linear data array * 3

Horizontal Wavelength [nm]

Vertical(1) CD[mdeg]

Vertical(2) HT[V]

Vertical(3) Abs

Start 310 nm

End 192 nm

Data pitch 1 nm

Data points 119

[Measurement Information]

Instrument Name J-815

Model Name J-815

Serial No. A010961168

Accessory Standard

Accessory S/NA010961168

Cell Length 10 mm

Photometric Mode CD, HT, Abs

Measure Range 310 - 192 nm

Data pitch 1 nm

Sensitivity Standard

D.I.T. 2 sec

Band width 5.00 nm

Start Mode Immediately

Scanning Speed 200 nm/min

Baseline CorrectionBaseline

Shutter Control Manual

PMT Voltage Auto

Theoretical ECD spectra data

ECD Spectrum

X-Axis: Excitation Energy (nm)

Y-Axis: Delta Epsilon

# X	Y	DY/DX
-100.0000000000	0.0000000000	0.0000000000
-98.2000000000	0.0000000000	0.0000000000
-96.4000000000	0.0000000000	0.0000000000
-94.6000000000	0.0000000000	0.0000000000
-92.8000000000	0.0000000000	0.0000000000
-91.0000000000	0.0000000000	0.0000000000
-89.2000000000	0.0000000000	0.0000000000
-87.4000000000	0.0000000000	0.0000000000
-85.6000000000	0.0000000000	0.0000000000
-83.8000000000	0.0000000000	0.0000000000
-82.0000000000	0.0000000000	0.0000000000
-80.2000000000	0.0000000000	0.0000000000
-78.4000000000	0.0000000000	0.0000000000
-76.6000000000	0.0000000000	0.0000000000
-74.8000000000	0.0000000000	0.0000000000
-73.0000000000	0.0000000000	0.0000000000
-71.2000000000	0.0000000000	0.0000000000
-69.4000000000	0.0000000000	0.0000000000
-67.6000000000	0.0000000000	0.0000000000
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-64.0000000000	0.0000000000	0.0000000000
-62.2000000000	0.0000000000	0.0000000000
-60.4000000000	0.0000000000	0.0000000000
-58.6000000000	0.0000000000	0.0000000000

-56.8000000000	0.0000000000	0.0000000000
-55.0000000000	0.0000000000	0.0000000000
-53.2000000000	0.0000000000	0.0000000000
-51.4000000000	0.0000000000	0.0000000000
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-6.4000000000	0.0000000000	0.0000000000
-4.6000000000	0.0000000000	0.0000000000

-2.8000000000	0.0000000000	0.0000000000
-1.0000000000	0.0000000000	0.0000000000
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8.0000000000	0.0000000000	0.0000000000
9.8000000000	0.0000000000	0.0000000000
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15.2000000000	0.0000000000	0.0000000000
17.0000000000	0.0000000000	0.0000000000
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22.4000000000	0.0000000000	0.0000000000
24.2000000000	0.0000000000	0.0000000000
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27.8000000000	0.0000000000	0.0000000000
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33.2000000000	0.0000000000	0.0000000000
35.0000000000	0.0000000000	0.0000000000
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40.4000000000	0.0000000000	0.0000000000
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76.4000000000	0.0000000000	0.0000000000
78.2000000000	0.0000000000	0.0000000000
80.0000000000	0.0000000000	0.0000000000
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85.4000000000	0.0000000000	0.0000000000
87.2000000000	0.0000000000	0.0000000000
89.0000000000	0.0000000000	0.0000000000
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92.6000000000	0.0000000000	0.0000000000
94.4000000000	0.0000000000	0.0000000000
96.2000000000	0.0000000000	0.0000000000
98.0000000000	0.0000000000	0.0000000000
99.8000000000	0.0000000000	0.0000000000
101.6000000000	0.0000000000	0.0000000000
103.4000000000	0.0000000000	0.0000000000

105.2000000000	0.0000000000	0.0000000000
107.0000000000	0.0000000000	0.0000000000
108.8000000000	0.0000000000	0.0000000000
110.6000000000	0.0000000000	0.0000000000
112.4000000000	0.0000000000	0.0000000000
114.2000000000	0.0000000000	0.0000000000
116.0000000000	0.0000000000	0.0000000000
117.8000000000	0.0000000000	0.0000000000
119.6000000000	0.0000000000	0.0000000000
121.4000000000	0.0000000001	0.0000000000
123.2000000000	0.0000000028	0.0000000000
125.0000000000	0.0000000767	0.0000000000
126.8000000000	0.0000014846	0.0000000000
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132.2000000000	0.0017053238	0.0000001807
134.0000000000	0.0103710433	0.0000069155
135.8000000000	0.0495885169	0.0001589631
137.6000000000	0.1895389342	0.0022657226
139.4000000000	0.5880931874	0.0205923862
141.2000000000	1.5024654771	0.1222034743
143.0000000000	3.2027344999	0.4821631619
144.8000000000	5.7674572810	1.2766793654
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148.4000000000	11.8191210243	2.4963498722
150.2000000000	13.7687688562	1.3064929447
152.0000000000	14.2159517404	-0.7039379666
153.8000000000	13.1920386255	-2.0377581294
155.6000000000	11.1658521179	-1.9524027535
157.4000000000	8.7228770850	-1.0687119055

159.2000000000	6.2846937992	-0.4206201953
161.0000000000	4.0270856230	-0.4233377374
162.8000000000	1.9692889129	-0.7877981948
164.6000000000	0.1055560933	-1.0463639409
166.4000000000	-1.5229858602	-0.9737915984
168.2000000000	-2.8347091020	-0.6406203888
170.0000000000	-3.7523928286	-0.2473678019
171.8000000000	-4.2410249235	0.0480211664
173.6000000000	-4.3182555041	0.2044534694
175.4000000000	-4.0428668497	0.2727817792
177.2000000000	-3.4965935373	0.3250921049
179.0000000000	-2.7706695783	0.3974670758
180.8000000000	-1.9598534194	0.4759662188
182.6000000000	-1.1607652889	0.5187174378
184.4000000000	-0.4702258449	0.4890462833
186.2000000000	0.0188898724	0.3781365213
188.0000000000	0.2246148723	0.2074685171
189.8000000000	0.0849265525	0.0123507016
191.6000000000	-0.4320495337	-0.1827661661
193.4000000000	-1.3177284118	-0.3807378013
195.2000000000	-2.5144215273	-0.6061115910
197.0000000000	-3.9111457404	-0.8764113928
198.8000000000	-5.3471174947	-1.1664508307
200.6000000000	-6.6252607867	-1.3915427320
202.4000000000	-7.5356995677	-1.4279410228
204.2000000000	-7.8861148890	-1.1660085380
206.0000000000	-7.5332262694	-0.5688261171
207.8000000000	-6.4085896223	0.2965552979
209.6000000000	-4.5328574611	1.2722388474
211.4000000000	-2.0153049792	2.1591734429

213.2000000000	0.9611152022	2.7787556049
215.0000000000	4.1657496351	3.0209727941
216.8000000000	7.3517735053	2.8649992651
218.6000000000	10.2872797805	2.3717979028
220.4000000000	12.7808283661	1.6573477731
222.2000000000	14.6981835662	0.8581239721
224.0000000000	15.9691181661	0.0992124661
225.8000000000	16.5850860381	-0.5278928797
227.6000000000	16.5899052343	-0.9748157737
229.4000000000	16.0662214882	-1.2340045500
231.2000000000	15.1205026948	-1.3282979448
233.0000000000	13.8688326888	-1.2971965639
234.8000000000	12.4250519052	-1.1841660482
236.6000000000	10.8920352470	-1.0276561399
238.4000000000	9.3562473111	-0.8566096073
240.2000000000	7.8852474733	-0.6897630985
242.0000000000	6.5275481475	-0.5373237634
243.8000000000	5.3141336518	-0.4035773232
245.6000000000	4.2609782860	-0.2893734860
247.4000000000	3.3720098452	-0.1939485834
249.2000000000	2.6421047911	-0.1159778498
251.0000000000	2.0598415260	-0.0540127118
252.8000000000	1.6098591705	-0.0065541572
254.6000000000	1.2747622781	0.0280086243
256.4000000000	1.0365760558	0.0514443613
258.2000000000	0.8777955188	0.0656482742
260.0000000000	0.7820912069	0.0725375366
261.8000000000	0.7347394981	0.0739133475
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269.0000000000	0.7989540645	0.0506595760
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274.4000000000	0.9019735375	0.0219103921
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278.0000000000	0.9374193440	0.0018219236
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287.0000000000	0.8696032555	-0.0352406387
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294.2000000000	0.7079678155	-0.0389133425
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299.6000000000	0.5741913373	-0.0299399809
301.4000000000	0.5325665302	-0.0259826417
303.2000000000	0.4935975183	-0.0219008584
305.0000000000	0.4577672652	-0.0178539624
306.8000000000	0.4254175723	-0.0139599153
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312.2000000000	0.3507645324	-0.0038427984
314.0000000000	0.3333053582	-0.0010797278
315.8000000000	0.3193171908	0.0013727680
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319.4000000000	0.3007205871	0.0053688184

321.2000000000	0.2954906601	0.0069216074
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335.6000000000	0.3055371987	0.0087736350
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339.2000000000	0.3110982936	0.0066279673
341.0000000000	0.3130542091	0.0053051853
342.8000000000	0.3142754180	0.0038718117
344.6000000000	0.3146627971	0.0023727178
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350.0000000000	0.3102649383	-0.0020807841
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359.0000000000	0.2845909421	-0.0073348661
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362.6000000000	0.2690562629	-0.0082771558
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366.2000000000	0.2514553965	-0.0085704580
368.0000000000	0.2420968147	-0.0085051378
369.8000000000	0.2324794242	-0.0083204238
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373.4000000000	0.2127871944	-0.0076654365

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378.8000000000	0.1831616789	-0.0062369208
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386.0000000000	0.1457698058	-0.0041252945
387.8000000000	0.1370430264	-0.0036318105
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393.2000000000	0.1126496477	-0.0023302302
395.0000000000	0.1051326575	-0.0019654192
396.8000000000	0.0979199641	-0.0016371660
398.6000000000	0.0910038007	-0.0013454514
400.4000000000	0.0843730762	-0.0010896560
402.2000000000	0.0780138973	-0.0008687000
404.0000000000	0.0719100741	-0.0006811657
405.8000000000	0.0660436016	-0.0005254006
407.6000000000	0.0603951148	-0.0003996041
409.4000000000	0.0549443125	-0.0003018969
411.2000000000	0.0496703477	-0.0002303757
413.0000000000	0.0445521837	-0.0001831552
414.8000000000	0.0395689149	-0.0001583984
416.6000000000	0.0347000520	-0.0001543377
418.4000000000	0.0299257727	-0.0001692883
420.2000000000	0.0252271385	-0.0002016554
422.0000000000	0.0205862787	-0.0002499357
423.8000000000	0.0159865437	-0.0003127156
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431.0000000000	-0.0022852290	-0.0006833624
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436.4000000000	-0.0161571141	-0.0010551155
438.2000000000	-0.0208516396	-0.0011913528
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445.4000000000	-0.0400529319	-0.0017715278
447.2000000000	-0.0449564732	-0.0019203913
449.0000000000	-0.0498958725	-0.0020687416
450.8000000000	-0.0548664565	-0.0022155301
452.6000000000	-0.0598625803	-0.0023596936
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458.0000000000	-0.0749352214	-0.0027656759
459.8000000000	-0.0799610529	-0.0028885825
461.6000000000	-0.0849730605	-0.0030035160
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467.0000000000	-0.0998306249	-0.0032904986
468.8000000000	-0.1046907198	-0.0033638083
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474.2000000000	-0.1188534829	-0.0035057101
476.0000000000	-0.1234023233	-0.0035249798
477.8000000000	-0.1278491665	-0.0035294854
479.6000000000	-0.1321848653	-0.0035189502
481.4000000000	-0.1364006338	-0.0034932191

483.2000000000	-0.1404880940	-0.0034522615
485.0000000000	-0.1444393186	-0.0033961730
486.8000000000	-0.1482468668	-0.0033251741
488.6000000000	-0.1519038161	-0.0032396084
490.4000000000	-0.1554037882	-0.0031399379
492.2000000000	-0.1587409704	-0.0030267384
494.0000000000	-0.1619101320	-0.0029006915
495.8000000000	-0.1649066359	-0.0027625769
497.6000000000	-0.1677264460	-0.0026132628
499.4000000000	-0.1703661303	-0.0024536956
501.2000000000	-0.1728228602	-0.0022848886
503.0000000000	-0.1750944064	-0.0021079105
504.8000000000	-0.1771791304	-0.0019238734
506.6000000000	-0.1790759740	-0.0017339208
508.4000000000	-0.1807844455	-0.0015392149
510.2000000000	-0.1823046034	-0.0013409256
512.0000000000	-0.1836370373	-0.0011402184
513.8000000000	-0.1847828478	-0.0009382436
515.6000000000	-0.1857436237	-0.0007361259
517.4000000000	-0.1865214180	-0.0005349552
519.2000000000	-0.1871187229	-0.0003357775
521.0000000000	-0.1875384438	-0.0001395875
522.8000000000	-0.1877838717	0.0000526784
524.6000000000	-0.1878586562	0.0002401476
526.4000000000	-0.1877667773	0.0004220164
528.2000000000	-0.1875125173	0.0005975533
530.0000000000	-0.1871004332	0.0007661021
531.8000000000	-0.1865353282	0.0009270831
533.6000000000	-0.1858222245	0.0010799948
535.4000000000	-0.1849663362	0.0012244128

537.2000000000	-0.1839730425	0.0013599898
539.0000000000	-0.1828478625	0.0014864538
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542.6000000000	-0.1802244675	0.0017113158
544.4000000000	-0.1787377676	0.0018095228
546.2000000000	-0.1771421662	0.0018982274
548.0000000000	-0.1754435234	0.0019774896
549.8000000000	-0.1736477039	0.0020474243
551.6000000000	-0.1717605572	0.0021081962
553.4000000000	-0.1697879006	0.0021600157
555.2000000000	-0.1677355025	0.0022031338
557.0000000000	-0.1656090668	0.0022378376
558.8000000000	-0.1634142192	0.0022644451
560.6000000000	-0.1611564937	0.0022833014
562.4000000000	-0.1588413210	0.0022947734
564.2000000000	-0.1564740178	0.0022992459
566.0000000000	-0.1540597768	0.0022971175
567.8000000000	-0.1516036585	0.0022887965
569.6000000000	-0.1491105830	0.0022746975
571.4000000000	-0.1465853244	0.0022552379
573.2000000000	-0.1440325039	0.0022308346
575.0000000000	-0.1414565862	0.0022019014
576.8000000000	-0.1388618749	0.0021688465
578.6000000000	-0.1362525097	0.0021320698
580.4000000000	-0.1336324641	0.0020919615
582.2000000000	-0.1310055441	0.0020488996
584.0000000000	-0.1283753866	0.0020032490
585.8000000000	-0.1257454600	0.0019553600
587.6000000000	-0.1231190641	0.0019055672
589.4000000000	-0.1204993311	0.0018541889

591.2000000000	-0.1178892272	0.0018015263
593.0000000000	-0.1152915540	0.0017478631
594.8000000000	-0.1127089514	0.0016934656
596.6000000000	-0.1101438998	0.0016385819
598.4000000000	-0.1075987234	0.0015834426
600.2000000000	-0.1050755933	0.0015282608
602.0000000000	-0.1025765312	0.0014732322
603.8000000000	-0.1001034133	0.0014185357
605.6000000000	-0.0976579743	0.0013643339
607.4000000000	-0.0952418113	0.0013107733
609.2000000000	-0.0928563885	0.0012579853
611.0000000000	-0.0905030414	0.0012060867
612.8000000000	-0.0881829817	0.0011551803
614.6000000000	-0.0858973014	0.0011053559
616.4000000000	-0.0836469778	0.0010566905
618.2000000000	-0.0814328781	0.0010092495
620.0000000000	-0.0792557639	0.0009630875
621.8000000000	-0.0771162964	0.0009182486
623.6000000000	-0.0750150401	0.0008747674
625.4000000000	-0.0729524685	0.0008326700
627.2000000000	-0.0709289678	0.0007919741
629.0000000000	-0.0689448417	0.0007526901
630.8000000000	-0.0670003157	0.0007148218
632.6000000000	-0.0650955417	0.0006783666
634.4000000000	-0.0632306017	0.0006433166
636.2000000000	-0.0614055126	0.0006096591
638.0000000000	-0.0596202293	0.0005773767
639.8000000000	-0.0578746494	0.0005464485
641.6000000000	-0.0561686168	0.0005168499
643.4000000000	-0.0545019250	0.0004885536

645.2000000000	-0.0528743208	0.0004615296
647.0000000000	-0.0512855082	0.0004357462
648.8000000000	-0.0497351507	0.0004111694
650.6000000000	-0.0482228754	0.0003877643
652.4000000000	-0.0467482756	0.0003654946
654.2000000000	-0.0453109137	0.0003443232
656.0000000000	-0.0439103239	0.0003242126
657.8000000000	-0.0425460150	0.0003051249
659.6000000000	-0.0412174732	0.0002870220
661.4000000000	-0.0399241639	0.0002698659
663.2000000000	-0.0386655344	0.0002536189
665.0000000000	-0.0374410160	0.0002382436
666.8000000000	-0.0362500259	0.0002237031
668.6000000000	-0.0350919694	0.0002099611
670.4000000000	-0.0339662416	0.0001969820
672.2000000000	-0.0328722292	0.0001847312
674.0000000000	-0.0318093118	0.0001731746
675.8000000000	-0.0307768641	0.0001622793
677.6000000000	-0.0297742566	0.0001520132
679.4000000000	-0.0288008575	0.0001423454
681.2000000000	-0.0278560336	0.0001332458
683.0000000000	-0.0269391517	0.0001246854
684.8000000000	-0.0260495796	0.0001166363
686.6000000000	-0.0251866870	0.0001090716
688.4000000000	-0.0243498467	0.0001019657
690.2000000000	-0.0235384351	0.0000952936
692.0000000000	-0.0227518334	0.0000890317
693.8000000000	-0.0219894278	0.0000831574
695.6000000000	-0.0212506109	0.0000776489
697.4000000000	-0.0205347815	0.0000724856

699.2000000000	-0.0198413459	0.0000676478
701.0000000000	-0.0191697176	0.0000631166
702.8000000000	-0.0185193185	0.0000588743
704.6000000000	-0.0178895790	0.0000549039
706.4000000000	-0.0172799380	0.0000511892
708.2000000000	-0.0166898439	0.0000477150
710.0000000000	-0.0161187542	0.0000444667
711.8000000000	-0.0155661363	0.0000414307
713.6000000000	-0.0150314672	0.0000385940
715.4000000000	-0.0145142341	0.0000359442
717.2000000000	-0.0140139342	0.0000334699
719.0000000000	-0.0135300749	0.0000311600
720.8000000000	-0.0130621740	0.0000290042
722.6000000000	-0.0126097598	0.0000269928
724.4000000000	-0.0121723706	0.0000251166
726.2000000000	-0.0117495555	0.0000233669
728.0000000000	-0.0113408738	0.0000217356
729.8000000000	-0.0109458951	0.0000202151
731.6000000000	-0.0105641996	0.0000187982
733.4000000000	-0.0101953773	0.0000174780
735.2000000000	-0.0098390288	0.0000162483
737.0000000000	-0.0094947645	0.0000151031
738.8000000000	-0.0091622050	0.0000140368
740.6000000000	-0.0088409805	0.0000130442
742.4000000000	-0.0085307312	0.0000121203
744.2000000000	-0.0082311069	0.0000112606
746.0000000000	-0.0079417666	0.0000104607
747.8000000000	-0.0076623790	0.0000097166
749.6000000000	-0.0073926218	0.0000090245
751.4000000000	-0.0071321817	0.0000083808

753.2000000000	-0.0068807544	0.0000077824
755.0000000000	-0.0066380441	0.0000072261
756.8000000000	-0.0064037638	0.0000067089
758.6000000000	-0.0061776346	0.0000062283
760.4000000000	-0.0059593861	0.0000057816
762.2000000000	-0.0057487557	0.0000053666
764.0000000000	-0.0055454887	0.0000049811
765.8000000000	-0.0053493380	0.0000046229
767.6000000000	-0.0051600643	0.0000042902
769.4000000000	-0.0049774352	0.0000039812
771.2000000000	-0.0048012258	0.0000036943
773.0000000000	-0.0046312180	0.0000034279
774.8000000000	-0.0044672006	0.0000031805
776.6000000000	-0.0043089690	0.0000029509
778.4000000000	-0.0041563250	0.0000027377
780.2000000000	-0.0040090767	0.0000025398
782.0000000000	-0.0038670384	0.0000023561
783.8000000000	-0.0037300305	0.0000021857
785.6000000000	-0.0035978788	0.0000020275
787.4000000000	-0.0034704152	0.0000018807
789.2000000000	-0.0033474767	0.0000017445
791.0000000000	-0.0032289060	0.0000016182
792.8000000000	-0.0031145507	0.0000015009
794.6000000000	-0.0030042635	0.0000013921
796.4000000000	-0.0028979020	0.0000012912
798.2000000000	-0.0027953287	0.0000011976
800.0000000000	-0.0026964103	0.0000011108

6. ESI-MS spectrum of reaction mixture.

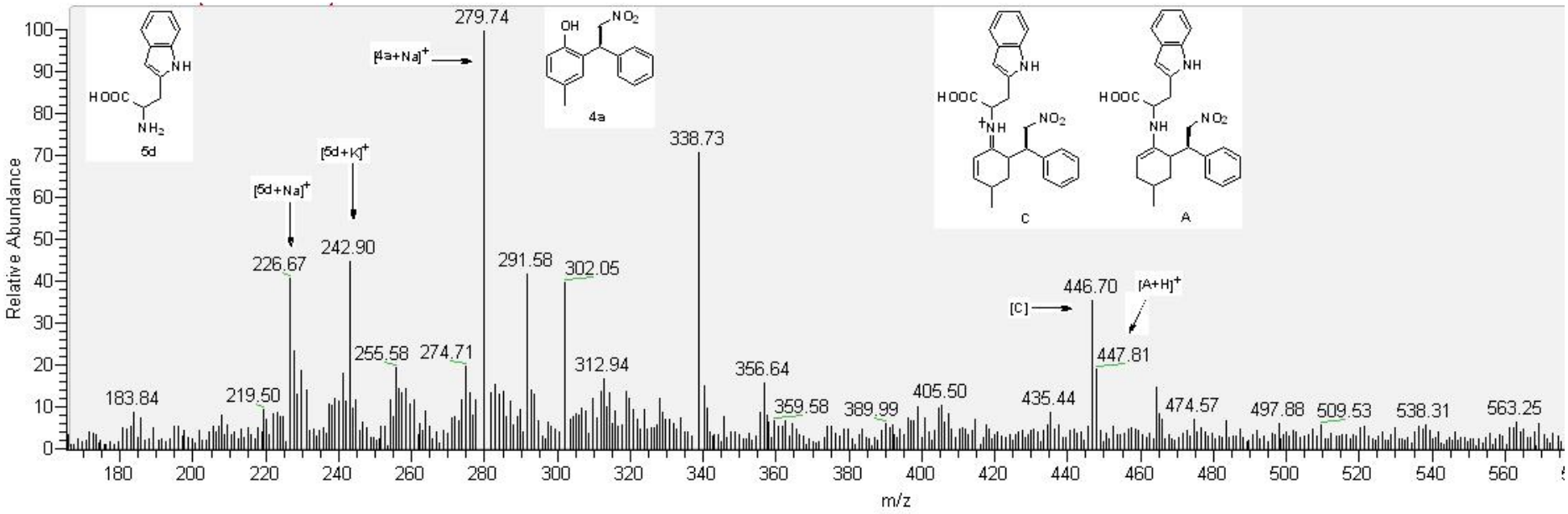

Figure S1. Confirmation of the existence of intermediates **A** and **C** by ESI-MS (positive mode), 0.5 h after the start of the reaction.