Supporting Information

Regio- and stereo-selective construction of *cis*-indeno[1,2-*c*]isoxazoles via C–H allylation/1,3-dipolar cycloaddition cascade

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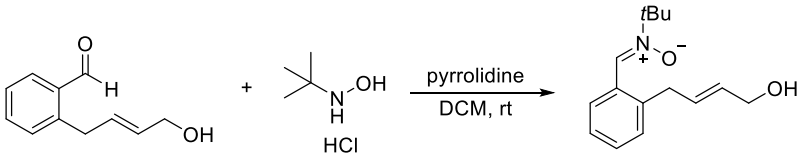
1. General Information

All chemicals were obtained from commercial sources and were used as received unless otherwise noted. All the reactions were carried out under argon atmosphere using standard Schlenk technique. The ^{1}H NMR spectra were recorded on a 400 MHz or 600 MHz NMR spectrometer. The ^{13}C NMR spectra were recorded at 100 MHz or 150 MHz. The ^{19}F NMR spectra were recorded at 565 MHz. Chemical shifts were expressed in parts per million (δ) downfield from the internal standard TMS, and were reported as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), dt (doublet of triplet), m (multiplet), brs (broad singlet), etc. The residual solvent signals were used as references and the chemical shifts were converted to the TMS scale. HRMS spectra were obtained on an Agilent Q-TOF 6540 spectrometer. Column chromatography was performed on silica gel (300-400 mesh). HPLC analysis was performed using the corresponding commercial chiral columns as stated in the experimental procedures at 30 °C with the UV detector at 254 nm. The vinylethylene carbonates **2a** and **5a** were purchased from commercial sources, and other vinylethylene carbonates **3a, 4a,** were prepared by following a literature procedure.[1] The arylnitrones were prepared according to the literature report.[2] The azomethine imines were prepared according to the literature reports.[3]

2. General Procedures for the Preparation of Substrates

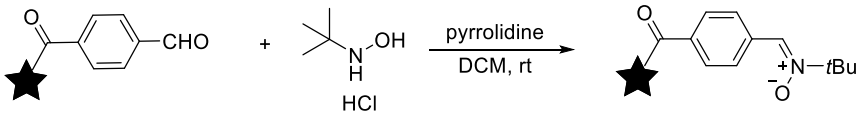
(1) The Preparation of 3-Int



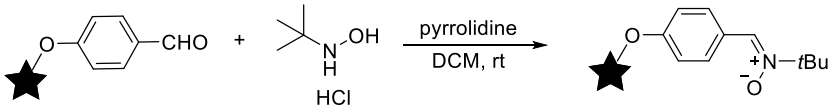
3-Int

2-[(2*E*)-4-Hydroxy-2-buten-1-yl]benzaldehyde was prepared by following a literature procedure[4]. N-tert-Butylhydroxylamine hydrochloride (4.0 mmol) and the aldehyde (4.0 mmol) were dissolved in anhydrous DCM (20 mL). The reaction mixture was cooled down to 0 ºC and pyrrolidine (4.8 mmol) was added dropwise. The reaction was stirred at room temperature. After the reaction was finished as judged by TLC (3 h), the solvent was then removed under reduced pressure to give a crude product. Purification by silica gel column chromatography with petroleum and ethyl acetate as eluent (PE: EA = 3: 1) to afford the pure product **3-Int**. Colourless oil, (683 mg, 69%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 – 8.92 (m, 1H), 7.65 (s, 1H), 7.26 – 7.21 (m, 2H), 7.13 – 7.08 (dd, m, 1H), 5.82 – 5.61 (m, 1H), 5.56 – 5.34 (m, 1H), 3.95 (dd, *J* = 5.6, 1.0 Hz, 2H), 3.37 (dd, *J* = 6.0, 1.0 Hz, 2H), 2.38 (s, 1H), 1.51 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.4, 131.1, 130.1, 129.8, 129.1, 128.4, 127.4, 126.8, 71.2, 62.9, 36.8, 28.3). HRMS (ESI): m/z calcd. for [$C_{15}H_{21}NNa_2O_2$, M+Na] + : 270.1465; found: 270.1459.

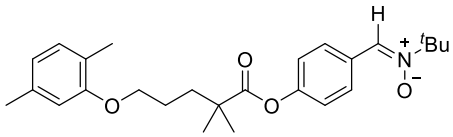
(2) The preparation of complex bioactive molecules



The corresponding aldehydes was prepared by following a literature[5] procedure, N-tert-Butylhydroxylamine hydrochloride (5.0 mmol) and the aldehydes (5.0 mmol) were dissolved in anhydrous DCM (20 mL). The reaction mixture was cooled down to 0 ºC and pyrrolidine (6.0 mmol) was added dropwise. The reaction was stirred at room temperature. After the reaction was finished as judged by TLC (1-4 h), the solvent was then removed under reduced pressure to give a crude product. Purification by silica gel column chromatography with petroleum and ethyl acetate as eluent (PE: EA = 1:1-6:1) to afford the corresponding pure products.

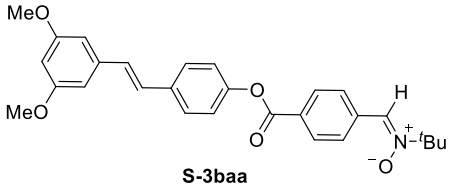


The corresponding aldehydes was prepared by following a literature[5] procedure, N-tert-Butylhydroxylamine hydrochloride (5.0 mmol) and the aldehydes (5.0 mmol) were dissolved in anhydrous DCM (20 mL). The reaction mixture was cooled down to 0 ºC and pyrrolidine (6.0 mmol) was added dropwise. The reaction was stirred at room temperature. After the reaction was finished as judged by TLC (1-4h), the solvent was then removed under reduced pressure to give a crude product. Purification by silica gel column chromatography with petroleum and ethyl acetate as eluent (PE: EA = 1:1-6:1) to afford the corresponding pure products.



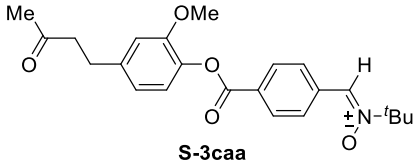
S-3aaa

Characterizations of substrates: White solid, (5 mmol, 1.067 g, 50%); M.p.:76-79 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.8 Hz, 2H), 7.57 (s, 1H), 7.12 (d, *J* = 8.8 Hz, 2H), 7.03 (d, *J* = 7.4 Hz, 1H), 6.69 (d, *J* = 7.4 Hz, 1H), 6.65 (s, 1H), 4.01 (t, *J* = 4.8 Hz, 2H), 2.33 (s, 3H), 2.20 (s, 3H), 1.97 – 1.86 (m, 4H), 1.64 (s, 9H), 1.40 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.0, 156.8, 151.9, 136.5, 130.3, 130.0, 129.0, 128.6, 123.6, 121.6, 120.8, 111.9, 70.8, 67.7, 42.5, 37.1, 28.3, 25.2, 25.1, 21.4, 15.8. HRMS (ESI): m/z calcd. for $[C_{26}H_{35}NNaO_4, M+Na]^+$: 448.2458; found: 448.2450.



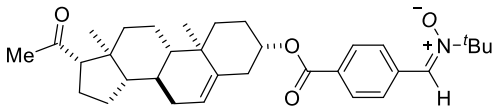
S-3baa

Characterizations of substrates: White solid, (3.1 mmol, 1.043 g, 74%); M.p.:137 - 139 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 8.4 Hz, 2H), 8.25 (d, *J* = 8.4 Hz, 2H), 7.69 (s, 1H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.31 – 7.24 (m, 2H), 7.08 (q, *J* = 16.2 Hz, 2H), 6.70 (d, *J* = 2.0 Hz, 2H), 6.43 – 6.40 (m, 1H), 3.86 (s, 6H), 1.67 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.5, 161.0, 150.4, 139.2, 135.6, 135.1, 130.12, 130.1, 129.0, 128.9, 128.4, 128.2, 127.5, 121.9, 104.6, 100.1, 71.8, 55.4, 28.4. HRMS (ESI): m/z calcd. for $[C_{28}H_{29}NNaO_5, M+Na]^+$: 482.1938; found: 482.1911.



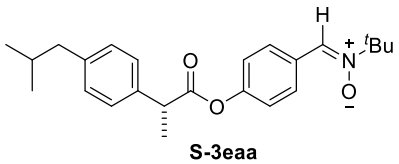
S-3caa

Characterizations of substrates: White solid, (4.1 mmol, 972 mg, 59%); M.p.:124 - 126 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.6 Hz, 2H), 8.15 (d, *J* = 8.6 Hz, 2H), 7.58 (s, 1H), 6.98 (d, *J* = 8.0 Hz, 1H), 6.77 (d, *J* = 1.6 Hz, 1H), 6.72 (dd, *J* = 8.0, 1.6 Hz, 1H), 3.73 (s, 3H), 2.84 (t, *J* = 7.4 Hz, 2H), 2.71 (t, *J* = 7.4 Hz, 2H), 2.09 (s, 3H), 1.57 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 207.7, 164.3, 151.1, 140.2, 138.2, 135.4, 130.4, 130.1, 129.0, 128.4, 122.7, 120.4, 112.8, 71.7, 55.9, 45.1, 30.1, 29.6, 28.3. HRMS (ESI): m/z calcd. for $[C_{23}H_{27}NNaO_5, M+Na]^+$: 420.1781; found: 420.1769.



S-3daa

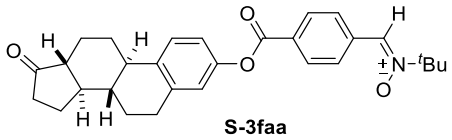
Characterizations of substrates: White solid, (3.2 mmol, 856 mg, 52%); M.p.:223 - 225 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.6 Hz, 2H), 8.08 (d, *J* = 8.6 Hz, 2H), 7.63 (s, 1H), 5.44 (d, *J* = 3.6 Hz, 1H), 5.01 – 4.78 (m, 1H), 2.56 (t, *J* = 8.8 Hz, 1H), 2.50 (d, *J* = 7.6 Hz, 2H), 2.25 – 2.16 (m, 1H), 2.15 (s, 3H), 2.12 – 2.20 (m, 3H), 1.95 (dt, *J* = 13.2, 3.4 Hz, 1H), 1.85 – 1.66 (m, 5H), 1.65 (s, 9H), 1.60 – 1.45 (m, 3H), 1.33 – 1.16 (m, 3H), 1.10 (s, 3H), 1.06 (dd, *J* = 11.6, 4.8 Hz, 1H), 0.67 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 209.4, 165.4, 139.6, 134.8, 131.5, 129.6, 129.0, 128.3, 122.5, 76.7, 74.7, 71.6, 63.7, 56.9, 49.9, 44.0, 38.8, 38.2, 37.1, 36.7, 31.9, 31.8, 31.5, 28.4, 27.8, 24.5, 22.9, 21.1, 19.8, 13.2. HRMS (ESI): m/z calcd. for $[C_{33}H_{45}NNaO_4, M+Na]^+$: 542.3241; found: 542.3249.



S-3eaa

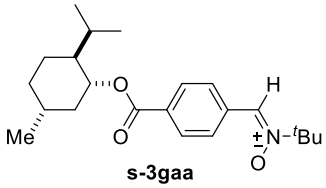
Characterizations of substrates: Colourless oil, (3.7 mmol, 392 mg, 28%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, *J* = 8.8 Hz, 2H), 7.44 (s, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 6.98 (d, *J* = 8.8 Hz, 2H), 3.85 (q, *J* = 7.2 Hz, 1H), 2.39 (d, *J* = 7.2 Hz, 2H), 1.86 – 1.74 (m, 1H), 1.51 (s, 9H), 0.83

(d, *J* = 6.6 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.8, 151.8, 140.9, 137.0, 130.0, 129.5, 129.2, 128.6, 127.2, 121.4, 70.8, 45.3, 45.1, 30.2, 28.3, 22.4, 18.5. HRMS (ESI): m/z calcd. for [$C_{24}H_{31}NNaO_3$, M+Na]$^+$: 404.2196; found: 404.2179.



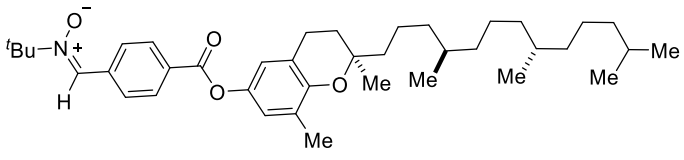
S-3faa

Characterizations of substrates: White solid, (5.0 mmol, 856 mg, 38%); M.p.:198 - 203 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8. Hz, 2H), 8.21 (d, *J* = 8.8 Hz, 2H), 7.66 (s, 1H), 7.33 (d, *J* = 8.4 Hz, 1H), 6.99 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.96 (d, *J* = 2.4 Hz, 1H), 3.04 – 2.86 (m, 2H), 2.57 – 2.47 (m, 1H), 2.46 – 2.38 (m, 1H), 2.32 (td, *J* = 10.8, 3.6 Hz, 1H), 2.21 – 2.04 (m, 2H), 2.03 – 1.94 (m, 2H), 1.64 (s, 1.64), 1.70 – 1.58 (m, 3H), 1.55 – 1.43 (m, 3H), 0.92 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 220.8, 164.9, 148.9, 138.2, 137.6, 135.7, 130.4, 129.0, 128.6, 126.6, 121.8, 118.9, 77.5, 77.2, 76.8, 71.9, 50.6, 48.1, 44.3, 38.2, 35.9, 31.7, 29.6, 28.5, 26.5, 25.9, 21.7, 13.9. HRMS (ESI): m/z calcd. for [$C_{30}H_{35}NNaO_4$, M+Na]$^+$: 496.2458; found: 496.2458.



s-3gaa

Characterizations of substrates: White solid, (3.2 mmol, 942 mg, 82%); M M.p.:98 - 102 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.6 Hz, 2H), 7.99 (d, *J* = 8.6 Hz, 2H), 7.54 (s, 1H), 4.87 (td, *J* = 10.8, 4.4 Hz, 1H), 2.14 – 2.00 (m, 1H), 1.95 – 1.83 (m, 1H), 1.72 – 1.61 (m, 2H), 1.56 (s, 9H), 1.54 – 1.44 (m, 2H), 1.15 – 0.99 (m, 2H), 0.93 – 0.81 (m, 7H), 0.72 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.5, 134.7, 131.5, 129.6, 129.0, 128.3, 75.0, 71.5, 47.2, 40.9 34.3, 31.4, 28.3, 26.5, 23.7, 22.0, 20.7, 16.6. HRMS (ESI): m/z calcd. for [$C_{22}H_{33}NNaO_3$, M+Na]$^+$: 382.2353; found: 382.2339.



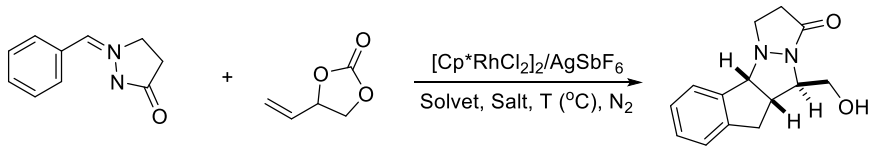
S-3haa

Characterizations of substrates: Yellow Oil, (1.3 mmol, 508 mg, 62%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.6 Hz, 2H), 8.12 (d, *J* = 8.6 Hz, 2H), 7.57 (s, 1H), 6.74 (d, *J* = 2.4 Hz, 1H), 6.69 (d, *J* = 2.6 Hz, 1H), 2.79 – 2.60 (m, 2H), 2.10 (s, 3H), 1.81 – 1.63 (m, 2H), 1.57 (s, 9H), 1.54 – 1.48 (m, 2H), 1.47 – 1.43 (m, 1H), 1.41 – 1.25 (m, 5H), 1.24 – 1.12 (m, 10H), 1.10 – 0.95 (m, 6H), 0.78 (t, *J* = 6.8 Hz, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.2, 149.9, 142.7), 135.4, 130.6, 130.2, 128.9, 128.4, 127.4, 121.2, 121.1, 119.1), 76.2, 71.72 (s, 2H), 40.2, 39.2, 37.5, 37.4, 37.3, 32.8, 32.7, 31.0, 28.4, 28.0, 24.8,

24.4, 24.2, 22.7, 22.6, 22.5, 20.9, 19.8, 19.7, 16.1. HRMS (ESI): m/z calcd. for [$C_{39}H_{59}NNaO_4$, M+Na]$^+$: 628.4336; found:628.4320.

3. Experimental Section

(1) Optimization studies for vinylethylene carbonate and azomethine imines

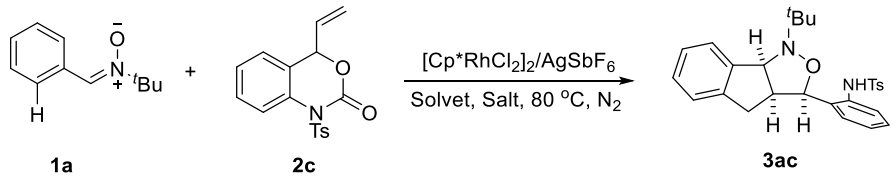


4a **2a** **4aa**

entry	Catalyst (mol %)	Solvent	Salt	T (°C)	yield[b]
1	$[Cp^*RhCl_2]_2/AgSbF_6$	DCM	Ag_2CO_3	80	Decomposition of **4a**
2	$[Cp^*RhCl_2]_2/AgSbF_6$	PhCl	Ag_2CO_3	80	Decomposition of **4a**
3	$[Cp^*RhCl_2]_2/AgSbF_6$	THF	Ag_2CO_3	80	Self-coupling of **4a**
4	$[Cp^*RhCl_2]_2/AgSbF_6$	TFE	Ag_2CO_3	80	58%
5	$[Cp^*RhCl_2]_2/AgSbF_6$	1,4-Dioxane	Ag_2CO_3	80	54%
6	$[Cp^*RhCl_2]_2/AgSbF_6$	TFE	AgOAc	80	46%
7	$[Cp^*RhCl_2]_2/AgSbF_6$	TFE	-	80	67%
8	$[Cp^*RhCl_2]_2/AgSbF_6$	TFE	-	60	62%
9	$[Cp^*RhCl_2]_2/AgSbF_6$	TFE	-	40	50%
10	$[Cp^*RhCl_2]_2/AgSbF_6$	TFE	-	100	72%
11	$[Cp^*RhCl_2]_2/AgSbF_6$	TFE	4Å (60 mg)	80	76%
12[c]	$[Cp^*RhCl_2]_2/AgSbF_6$	TFE	4Å (60 mg)/NaOAc	80	52%

[a]Reaction conditions: **4** (0.1 mmol), **2** (0.15 mmol), $[Cp^*RhCl_2]_2$ (4 mol%), $AgSbF_6$ (16 mol%), additive (0.05 mmol), solvent (1.0 mL), 24 h, under Ar, [b]Isolated yields. [c]NaOAc (0.1 mmol).

(2) Optimization studies for the reaction of 1a with 2c

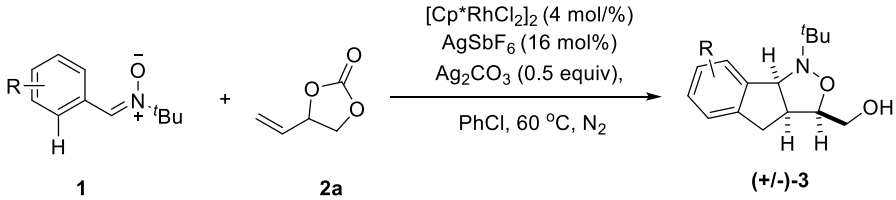


1a 2c 3ac

entry	Catalyst (mol %)	Solvent	Salt	yield[b]
1	$[Cp^*RhCl_2]_2/AgSbF_6$	PhCl	Ag_2CO_3	45%
2	$[Cp^*RhCl_2]_2/AgSbF_6$	DCE	Ag_2CO_3	35%
3	$[Cp^*RhCl_2]_2/AgSbF_6$	TFE	Ag_2CO_3	16%
4	$[Cp^*RhCl_2]_2/AgSbF_6$	1,4-Dioxane	Ag_2CO_3	6%
5[c]	$[Cp^*RhCl_2]_2/AgSbF_6$	PhCl	Ag_2CO_3 + NaOAc	61%
6[d]	$[Cp^*RhCl_2]_2/AgSbF_6$	DCE	AgOAc + $KHCO_3$	38%

[a]Reaction conditions: **1a** (0.1 mmol), **2c** (0.15 mmol), $[Cp^*RhCl_2]_2$ (4 mol%), $AgSbF_6$ (16 mol%), Ag_2CO_3 (0.05 mmol), solvent (1.0 mL), 80 °C, 12 h, under Ar. [b]Isolated yields. [c]Ag_2CO_3 (0.05 mmol), NaOAc (0.05 mmol), [d]AgOAc (0.05 mmol), $KHCO_3$ (0.05 mmol).

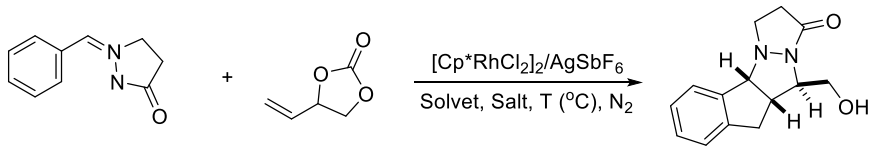
(3) General procedures for the synthesis of products 3.



1 2a (+/-)-3

A mixture of **1** (0.1 mmol), $[Cp^*RhCl_2]_2$ (2.5mg, 4 mol%), and Ag_2CO_3 (14 mg, 0.05 mmol), were charged into a reaction tube. $AgSbF_6$ (5.5 mg, 16 mol%) was added in a glove box, and then to which were added **2a** (0.015 ml, 0.15 mmol) and dry PhCl (1.0 mL) under argon atmosphere. The reaction mixture was stirred at 60 °C heated by metal sand bath for 12 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography (PE:EA =2:1 – 6:1) to afford **3**.

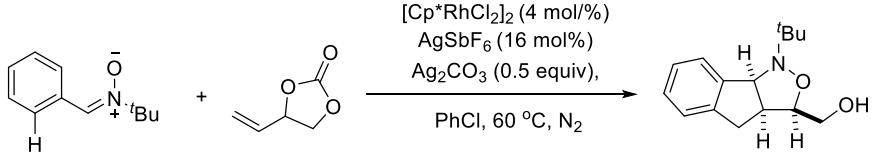
(4) General procedures for the synthesis of products 4aa.



4a **2a** **4aa**

A mixture of **4** (0.1 mmol), $[Cp^*RhCl_2]_2$ (2.5mg, 4 mol%), and 4A molecular sieve (60 mg) were charged into a reaction tube. $AgSbF_6$ (5.5 mg, 16 mol%) was added in a glove box, and then to which were added **2a** (0.015 ml, 0.15 mmol) and TFE (1.0 mL) under argon atmosphere. The reaction mixture was stirred at 80 ºC heated by metal sand bath for 24 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography (DCM:Methanol =20:1) to afford **4aa**.

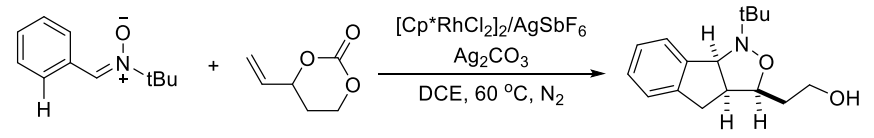
(5) Scale-up synthesis of the product 3aa.



1a **2a** **(+/-)-3aa**

A mixture of **1a** (890 mg, 5.0 mmol,), $[Cp^*RhCl_2]_2$ (2.5mg, 4 mol%), and Ag_2CO_3 (700 mg, 2.5 mmol), were charged into a round-bottom flask (100 mL). $AgSbF_6$ (275 mg, 16 mol%) was added in a glove box, and then to which were added **2a** (0.75 ml, 7.5 mmol) and PhCl (50.0 mL) under argon atmosphere. The reaction mixture was stirred at 60 ºC heated by metal sand bath for 48 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography. using PE: EtOAc =4:1 to afford **3aa** (778mg, 72% yiled).

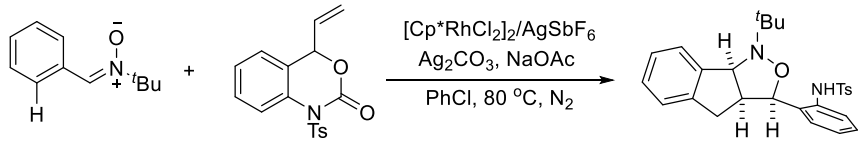
(6) General procedures for the synthesis of product 3ab.



1a **2b** **3ab**

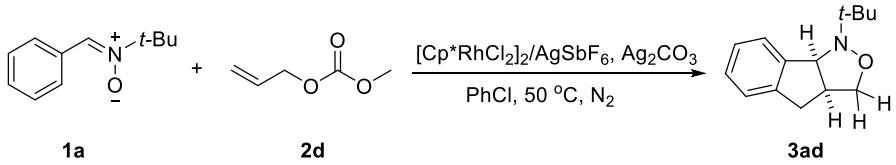
A mixture of **1a** (0.1 mmol), $[Cp^*RhCl_2]_2$ (2.5mg, 4 mol%), and Ag_2CO_3 (14 mg, 0.05 mmol) were charged into a reaction tube. $AgSbF_6$ (5.5 mg, 16 mol%) was added in a glove box, and then to which were added **2b** (19.2 mg, 0.15 mmol) and DCE (1.0 mL) under argon atmosphere. The reaction mixture was stirred at 60 ºC heated by metal sand bath for 20 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography (PE:EA = 2:1) to afford **3ab.**

(7) General procedures for the synthesis of product 3ac.



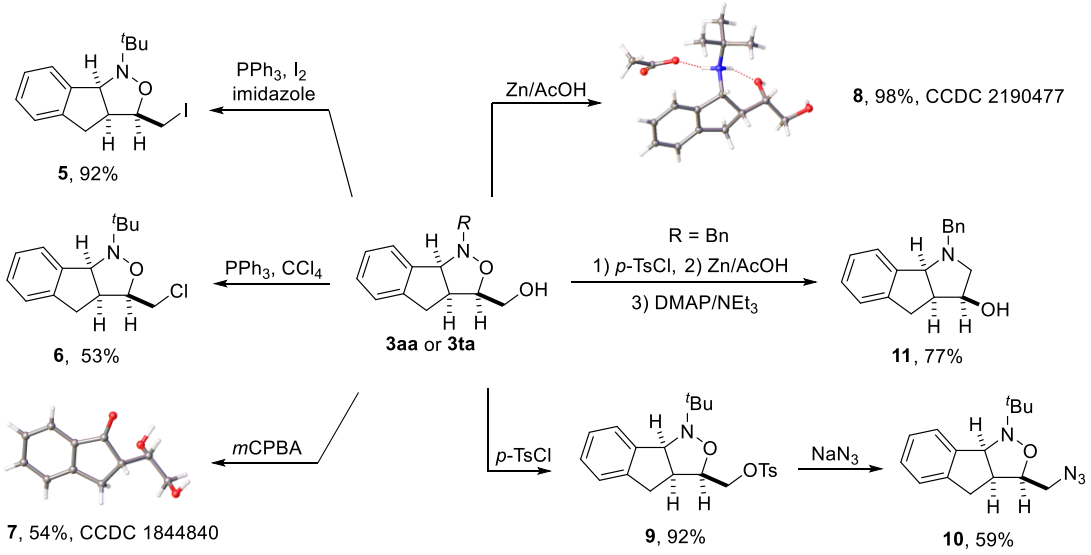
A mixture of **1a** (0.1 mmol), $[Cp^*RhCl_2]_2$ (2.5mg, 4 mol%), Ag_2CO_3 (14 mg, 0.05 mmol) and NaOAc (5 mg, 0.05 mmol) were charged into a reaction tube. $AgSbF_6$ (5.5 mg, 16 mol%) was added in a glove box, and then to which were added **2c** (47 mg, 0.15 mmol) and PhCl (1.0 mL) under argon atmosphere. The reaction mixture was stirred at 80 ºC heated by metal sand bath for 12 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography (PE:EA = 6:1) to afford **3ac**.

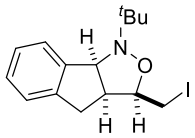
(8) General procedures for the synthesis of product 3ad.



A mixture of **1a** (0.1 mmol), $[Cp^*RhCl_2]_2$ (2.5mg, 4 mol%), and Ag_2CO_3 (14 mg, 0.05 mmol) were charged into a reaction tube. $AgSbF_6$ (5.5 mg, 16 mol%) was added in a glove box, and then to which were added **2d** (35 mg, 0.3mmol ml) and PhCl (1.0 mL) under argon atmosphere. The reaction mixture was stirred at 50 ºC heated by metal sand bath for 12 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography (PE:EA = 4:1) to afford **3ad**.

(9) Synthetic transformation of the products.

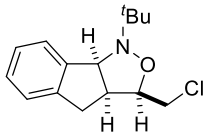




5

1-(tert-butyl)-3-(iodomethyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazole

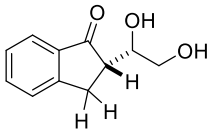
To a solution of **3aa** (0.2 mmol, 50 mg) in toluene (10 mL) was added iodine (0.4 mmol, 103 mg), triphenylphosphine (0.6 mmol, 157 mg) and imidazole (0.6 mmol, 40 mg) under Ar. The solution was heated to reflux for 6 h at 110 °C with stirring. After evaporation of the solvent, the residual oil was purified by silica gel chromatography (PE:EA = 10:1) to give **5** (65 mg, 92%) as a white solid. M.p.:79-83 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.18 (m, 1H), 7.18 – 7.03 (m, 3H), 4.85 (d, *J* = 7.6 Hz, 1H), 4.58 (dd, *J* = 14.0, 7.2 Hz, 1H), 3.49 (ddd, *J* = 15.6, 7.6, 4.4 Hz, 1H), 3.10 (dd, *J* = 16.8, 4.4 Hz, 1H), 3.05 (dd, *J* = 10.0, 6.0 Hz, 1H), 2.95 (dd, *J* = 16.8, 8.4 Hz, 1H), 2.85 (dd, *J* = 10.0, 8.0 Hz, 1H), 1.19 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.0, 142.6, 128.7, 127.8, 125.9, 124.8, 83.1, 70.5, 60.5, 52.0, 32.1, 27.5, 3.0. HRMS (ESI): m/z calcd. for $[C_{15}H_{20}NINaO, M+Na]^+$: 358.0662; found: 358.0670.



6

1-(tert-butyl)-3-(chloromethyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazole

To a solution of **3aa** (0.1 mmol, 25 mg) in Carbon tetrachloride (2 mL) was added triphenylphosphine (0.3 mmol, 80 mg) under Ar. The solution was heated to reflux overnight at 90 °C with stirring. After evaporation of the solvent, the residual oil was purified by silica gel chromatography (PE:EA = 8:1) to give **6** (13 mg, 53%) as a yellow solid. M.p.:53-57 °C. ^{1}H NMR (600 MHz,) δ 7.27 – 7.22 (m, 1H), 7.16 – 7.13 (m, 2H), 7.11 (dd, *J* = 8.4, 4.8 Hz, 1H), 4.86 (d, *J* = 7.7 Hz, 1H), 4.48 – 4.44 (m, 1H), 3.52 – 4.47 (m, 3.0 Hz, 1H), 3.36 (dd, *J* = 11.4, 5.4 Hz, 1H), 3.19 (dd, *J* = 10.8, 7.8 Hz, 1H), 3.14 (dd, *J* = 16.8, 3.0 Hz, 1H)., 2.97 (dd, *J* = 16.8, 8.4 Hz, 1H), 1.19 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.3, 141.8, 128.1, 127.3, 125.4, 124.1, 80.4, 69.5, 59.5, 51.2, 50.4, 31.6, 26.9. HRMS (ESI): m/z calcd. for $[C_{15}H_{21}ClNO, M+H]^+$: 266.1306; found: 266.1310.



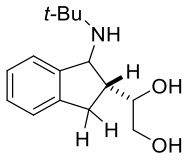
7

2-(1,2-dihydroxyethyl)-2,3-dihydro-1H-inden-1-one

A solution of the **3aa** (50 mg, 0.2 mmol) in diethyl ether (2 mL) was cooled in ice bath, and *m*-Chloroperoxybenzoic acid (138 mg, 0.8 mmol, 4.0 equiv) was added portionwise to the solution under Ar, The clear and blue solution was stirred at this temperature for 2 h and then quenched by addition of an aqueous 10% sodium bicarbonate (2 ml)/10% sodium thiosulfate (2 ml) solution and vigorous stirring for 20 min. The mixture was decanted and extracted with DCM (5 mL), the organic phase was washed with saturated sodium carbonate solution and then with brine, dried (Na_2SO_4),

filtered, and concentrated in vacuo to give the crude product, which was used immediately in the next reaction.

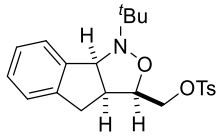
The crude product was dissolved in THF (2 mL) with strirring in ice bath, and 2N hydrochloric acid solution (2 mL) was added (exothermic reaction). The solution was stirred in ice bath for 30 min whereupon it was neutralized with saturated sodium carbonate solution and extracted with DCM. The organic phase was washed with water and brine, dried (Na2SO4), filtered, and concentrated in vacuo. The crude product was purified by silica gel (DCM:Methanol = 20:1) to give **7** as white solid (22 mg, 54%). M.p.:102-104 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.7 Hz, 1H), 7.59 – 7.48 (m, 1H), 7.41 (d, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 4.24 (dt, *J* = 7.2, 4.0 Hz, 1H), 3.72 (dd, *J* = 11.2, 3.6 Hz, 1H), 3.65 (dd, *J* = 11.2, 7.2 Hz, 1H) 3.24 – 3.06 (m, 2H), 2.81 – 2.73 (m, 1H), 2.35 (s, 1H), 1.65 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 207.5, 154.6, 136.7, 135.1, 127.4, 126.6, 123.9, 71.6, 65.3, 50.2, 27.8. HRMS (ESI): m/z calcd. for [$C_{15}H_{23}NNaO_2$, M+Na]$^+$: 215.0679; found: 215.0679.



8

1-(1-(tert-butylamino)-2,3-dihydro-1H-inden-2-yl)ethane-1,2-diol

To a vial under Ar atmosphere were added **3aa** (0.2 mmol, 50 mg,) and THF (1.0 mL). To the mixture were added Zn (2.0 mmol, 130 mg), AcOH (2.0 mL), and H2O (1.0 mL). The reaction mixture was stirred at 80 °C overnight. After dried by MgSO4, the mixture was filtered through a pad of celite eluting with ethyl acetate, concentrated, and purified by silica gel chromatography (DCM:Methanol = 10:1) to give the indicated product 8 as a white solid (47 mg, 95%). M.p.:123-126 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.20 (m, 1H), 7.19 – 7.15 (m, 1H), 7.15 – 7.09 (m, 2H), 4.35 (d, *J* = 6.6 Hz, 1H), 4.24 – 4.14 (m, 1H), 3.53 – 3.49 (m, 2H), 3.20 (dd, *J* = 16.0, 10.0 Hz, 1H), 2.63 (dd, *J* = 16.0, 8.0 Hz, 1H), 2.36 – 2.24 (m, 1H), 1.19 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.5, 144.0, 127.9, 126.9, 125.3, 124.0, 72.2, 66.3, 60.3, 51.6, 44.9, 29.9), 29.6. HRMS (ESI): m/z calcd. for [$C_{15}H_{23}NNaO_2$, M+Na]$^+$: 272.1621; found: 272.1610.

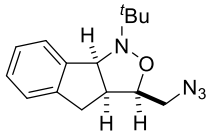


9

(1-(tert-butyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methyl-4-methylbenzenesulfonate

3aa (0.3 mmol), *p*-TsCl (0.45 mmol, 1.5 equiv), and DMAP (0.06 mmol, 0.2 equiv) were taken into a 25 mL round bottom flask and dry DCM (6 mL) was added with stirring under nitrogen atmosphere. The flask was cooled with ice-water and distilled Et_3N (0.9 mmol, 3.0 equiv) was added. The reaction was allowed to stir for 6h at room temperature. After complete consumption of starting material (monitored by TLC), volatiles were evaporated to dryness and the crude reaction mixture was loaded directly onto silica gel column (PE:EA = 6:1) and purified to give 9 (112 mg, 92%) as a yellow solid. M.p.:78-81 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.3 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.20 – 7.15 (m, 1H), 7.13 – 7.05 (m, 2H), 7.01 – 6.89 (m, 1H), 4.78 (d, *J* = 7.6 Hz, 1H), 4.42 (dt, *J* = 7.8, 6.2

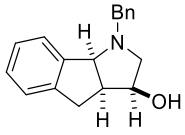
Hz, 1H), 3.77 (d, *J* = 6.2 Hz, 2H), 3.43 – 3.39 (m, 1H), 3.01 – 2.78 (m, 2H), 2.36 (s, 3H), 1.12 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.9, 143.1, 141.5, 132.7, 129.8, 128.1, 127.9, 127.3, 125.3, 124.1, 78.8, 69.6, 68.9, 59.7, 50.1, 31.5, 26.8, 21.6. HRMS (ESI): m/z calcd. for $[C_{22}H_{28}NO_4S, M+H]^+$: 402.1734; found: 402.1727.



10

3-(azidomethyl)-1-(tert-butyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazole

A 10 mL a Schlenk tube was charged with **9** (80 mg, 0.2 mmol, 1 equiv.), NaN3 (52 mg, 0.8 mmol, 4 equiv.) and DMF (2 mL). The reaction was allowed to stir overnight at 70 °C. The vial was allowed to cool to room temperature. The solvent was then removed in vacuo and the residue was further purified with flash column chromatography (Hex/EA/DCM = 10:1:3) to give **10** as yellow solid (32 mg, 59%). M.p.:79-83 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.22 (m, 1H), 7.17 – 7.12 (m, 2H), 7.10 (dd, *J* = 8.0, 4.0 Hz, 1H), 4.82 (d, *J* = 8.0 Hz, 1H), 4.41 – 4.37 (m, 1H), 3.45 – 3.41 (m, 1H), 3.18 (dd, *J* = 12.8, 7.6 Hz, 1H), 3.04 – 2.88 (m, 3H), 1.20 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.3, 141.8, 128.2, 127.3, 125.3, 124.1, 82.1, 69.8, 59.8, 50.5, 42.4, 31.5, 26.9. HRMS (ESI): m/z calcd. for $[C_{15}H_{20}NNaO, M+Na]^+$: 295.1529; found: 295.1520.



11

1-benzyl-1,2,3,3a,4,8b-hexahydroindeno[1,2-b]pyrrol-3-ol

3aa (0.2 mmol), *p*-TsCl (0.3 mmol, 1.5 equiv), and DMAP (0.04 mmol, 0.2 equiv) were taken into a 25 mL round bottom flask and dry DCM (5 mL) was added with stirring under nitrogen atmosphere. The flask was cooled with ice-water and distilled Et_3N (0.6 mmol, 3.0 equiv) was added. The reaction was allowed to stir for 6 h at room temperature. After complete consumption of starting material (monitored by TLC), volatiles were evaporated to dryness and the crude reaction mixture was loaded directly onto silica gel column (PE:EA = 4:1) and purified to give the pure product, which was used immediately in the next reaction.

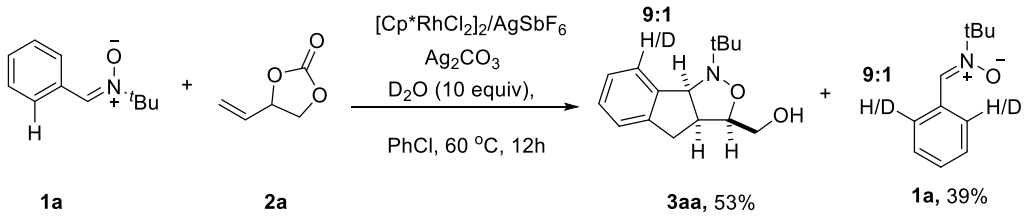
To a vial under Ar atmosphere were added the above product (0.2 mmol, 1.0 equiv) and THF (1.0 mL). To the mixture were added Zn (2.0 mmol, 130 mg), AcOH (2.0 mL), and H_2O (1.0 mL). The reaction mixture was stirred at 80 °C overnight. After dried by MgSO4, the mixture was filtered through a pad of celite eluting with ethyl acetate, concentrated, and purified by silica gel chromatography (DCM:Methanol = 10:1) to give the product as a white solid, which was used in the next step without further purification.

The above product (0.2 mmol), DMAP (0.1 mmol, 0.5 equiv) were taken into a Schlenk tube and dry DCM (2 mL) was added with stirring under nitrogen atmosphere. The flask was cooled with ice-water and distilled Et_3N (0.6 mmol, 3.0 equiv) was added. The reaction was allowed to stir for 6h at room

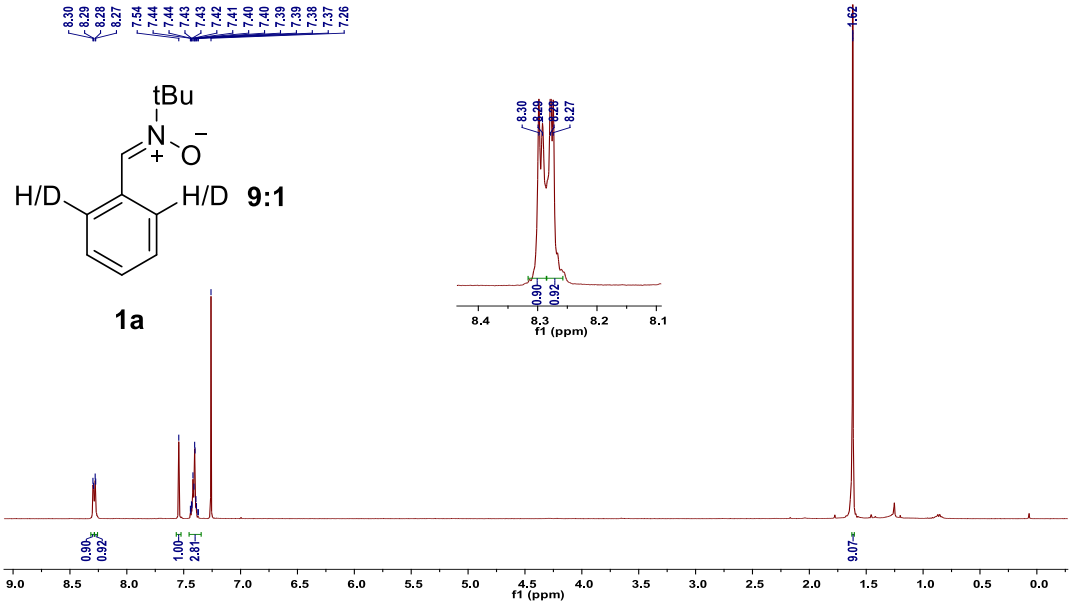
temperature. After complete consumption of starting material (monitored by TLC), volatiles were evaporated to dryness and the crude reaction mixture was loaded directly onto silica gel column (Hex/DCM/ Methanol = 10:10:1) and purified to give the pure product **11** as colourless oil (41 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.21 (m, 4H), 7.21 – 7.14 (m, 2H), 7.14 – 7.05 (m, 3H), 4.56 (d, *J* = 8.0 Hz, 1H), 3.95 (dd, *J* = 7.2, 4.0 Hz, 1H), 3.89 (d, *J* = 13.2 Hz, 1H), 3.83 (d, *J* = 13.2 Hz, 1H), 3.13 (dd, *J* = 16.8, 9.8 Hz, 1H), 2.92 (ddd, *J* = 10.0, 7.6, 3.6 Hz, 1H), 2.75 (dd, *J* = 16.8, 4.2 Hz, 1H), 2.67 (dd, *J* = 9.8, 4.4 Hz, 1H), 2.51 (dd, *J* = 10.0, 4.0 Hz, 1H), 2.07 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.3, 141.3, 139.3, 128.8, 128.4, 127.9, 127.0, 126.3, 125.8, 125.0, 77.8, 70.7, 59.1, 57.3, 50.8, 36.3. HRMS (ESI): m/z calcd. for $[C_{18}H_{20}NO, M+H]^+$: 266.1539; found: 266.1539.

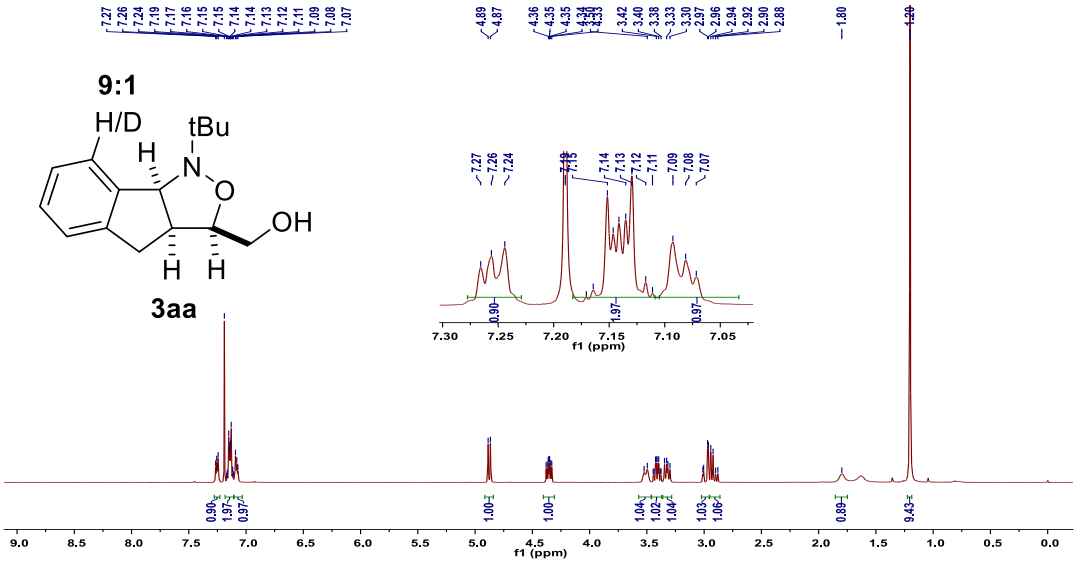
4. Mechanistic Studies

(1) H/D Exchange experiment of 1a with 2a

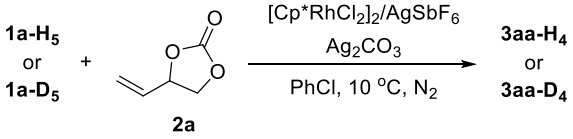


A mixture of **1** (0.1 mmol), $[Cp^*RhCl_2]_2$ (2.5mg, 4 mol%), and Ag_2CO_3 (14 mg, 0.05 mmol) were charged into a Schlenk tube. $AgSbF_6$ (5.5 mg, 16 mol%) was added in a glove box, and then to which were added **2a** (0.015 ml, 0.15 mmol), D_2O (18.0 mg, 1.0 mmol, 10.0 eq) and dry PhCl (1.0 mL) under argon atmosphere. The reaction mixture was stirred at 60 ºC heated in metal sand bath for 12 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography using PE/EtOAc = (8:1 to 4:1) to afford **3aa** in 53% yield and **1a** in 39% yield. ^{1}H NMR analysis indicated 10% deuteration at the *ortho* position of **3aa** and 10% deuteration at the *ortho* position of **1a**.



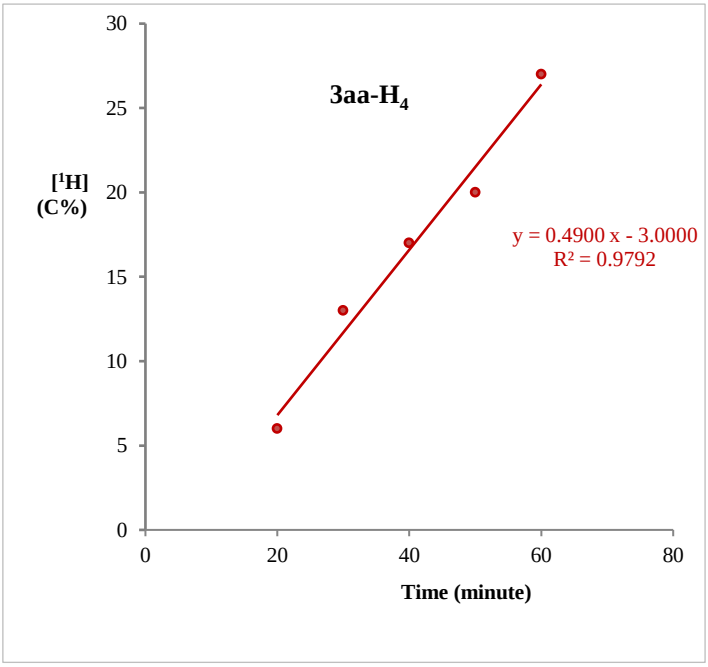


(2) Determination of Kinetic Isotope Effects

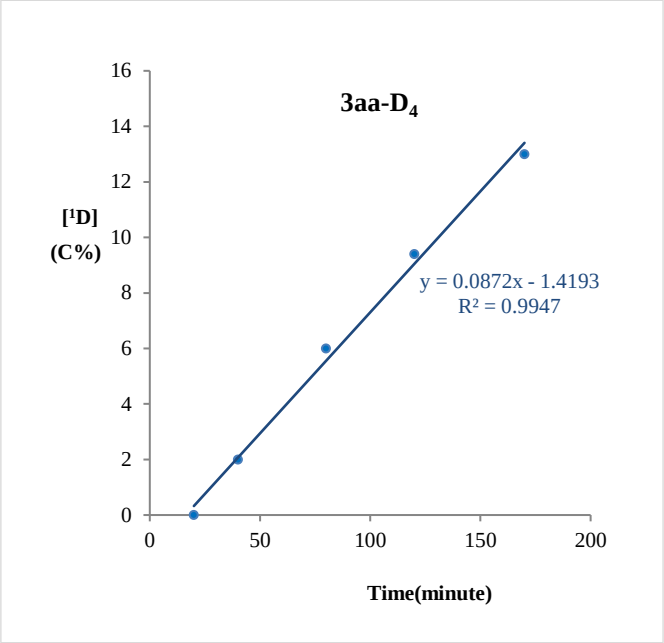


For the cyclization of **[1a-H$_5$]**: a 25-mL a Schlenk tube equipped with a magnetic stir bar was charged with **1a-H$_5$** (17.7 mg, 0.1 mmol, 1.0 eq), [Cp*RhCl$_2$]$_2$ (2.5mg, 4 mol%), and Ag_2CO_3 (14 mg, 0.05 mmol), $AgSbF_6$ (5.5 mg, 16 mol%) was added in a glove box, and then to which was added dry PhCl (1.0 mL) under argon atmosphere, the reaction tube stand for 5 minutes in a low temperature reaction bath at 10 ^oC, and then **2a** was added to the mixture whit striing. After 20 minutes of reaction, the tube was removed from the bath, the resulting solution was filtered through a Celite filter and the solvent was removed under reduced pressure. the resulting mixture were diluted with $CDCl_3$, 7 μL of dibromomethane was added and The mixed solution was transferred to an NMR tube and the sample was analyzed by ^1H NMR. The amount of **3aa-H$_4$** was determined by the relative integration of the characteristic signals of dibromomethane and **3aa-H$_4$**, The experiment was repeated at 30, 40, 50 and 60 minutes.

For the cyclization of **[1a-D$_5$]**: a 25-mL a Schlenk tube equipped with a magnetic stir bar was charged with **1a-D$_5$** (18.5 mg, 0.1 mmol, 1.0 eq), [Cp*RhCl$_2$]$_2$ (2.5mg, 4 mol%), and Ag_2CO_3 (14 mg, 0.05 mmol), $AgSbF_6$ (5.5 mg, 16 mol%) was added in a glove box, and then to which was added dry PhCl (1.0 mL) under argon atmosphere, the reaction tube stand for 5 minutes in a low temperature reaction bath at 10 ^oC, and then **2a** was added to the mixture whit striing. After 20 minutes of reaction, the tube was removed from the bath, the resulting solution was filtered through a Celite filter and the solvent was removed under reduced pressure. the resulting mixture were diluted with $CDCl_3$, 7 μL of dibromomethane was added and The mixed solution was transferred to an NMR tube and the sample was analyzed by ^1H NMR. The amount of **3aa-D$_4$** was determined by the relative integration of the characteristic signals of dibromomethane and **3aa-D$_4$**, The experiment was repeated at 40, 80, 120 and 170 minutes.



Initial rates determined by plots of [**3aa-H$_4$**] versus time, which gave the value of 0.4900×10^{-4} M/min.

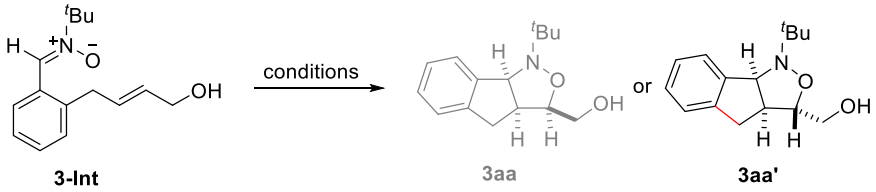


Initial rates determined by plots of [**3aa-D₄**] versus time, which gave the value of 0.0872×10^{-4} M/min.

The KIE value measured based on the above experiments is **5.6**.

(3) Verification of the intermediate

1) Experiments using the intermediate as a substrate



entry	conditions	yield of 3aa/%	yield of 3aa'/%
a	Ag_2CO_3, PhCl, 60 °C	n.d.	60
b	Ag_2CO_3, PhCl, r.t.	n.d.	28
c	PhCl, 60 °C	n.d.	50
d	standard conditons	n.d.	60

standard conditons: **3-Int** (0.1 mmol), $[Cp^*RhCl_2]_2$ (4 mol%), $AgSbF_6$ (16 mol%), Ag_2CO_3 (0.05 equiv), PhCl (1.0 mL), 60 °C, 12 h, under Ar, n.d. = no detection. $[Cp^*RhCl_2]_2$ (4 mol%, 2.5 mg),

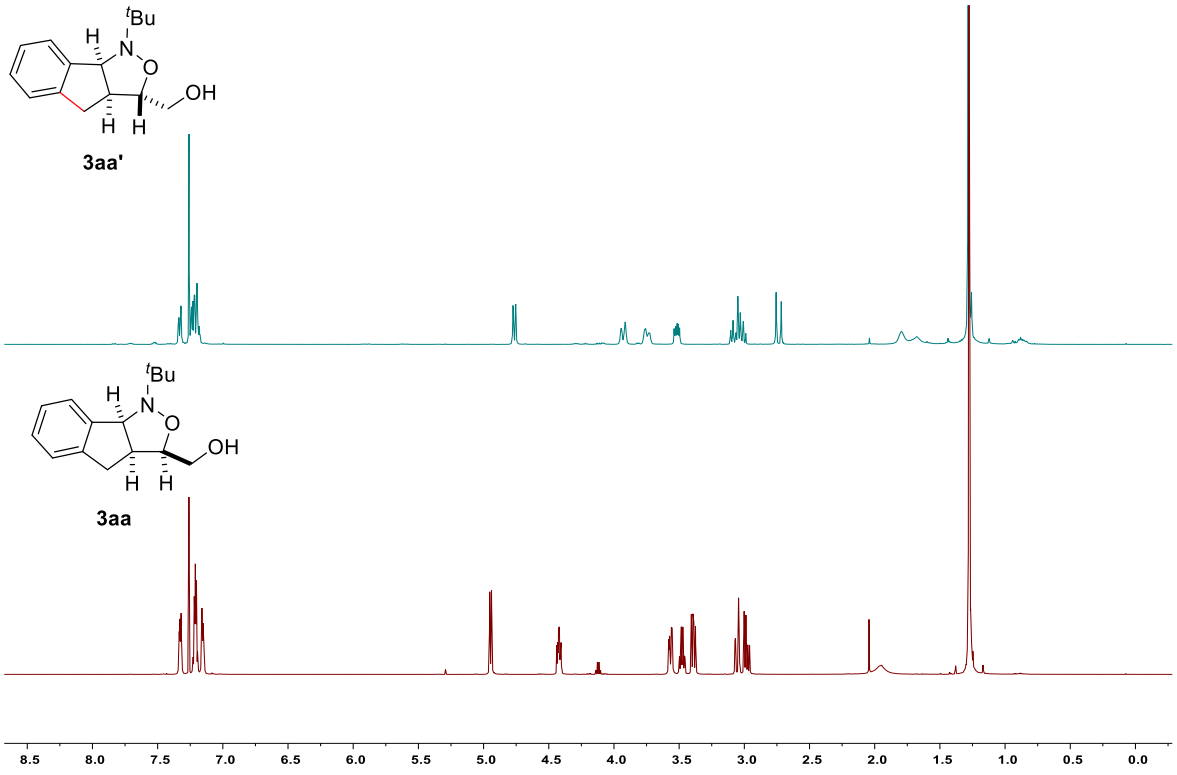
Condition a: A 25 mL Schlenk tube was charged with **3-Int** (25 mg, 0.1 mmol, 1 equiv.), Ag_2CO_3 (14 mg) and PhCl (1.0 ml). and then the reaction was allowed to stir for 12h at 60 ^oC under N_2. the tube was removed from the bath, the resulting solution was filtered through a Celite filter and the solvent was removed under reduced pressure. the resulting mixture were diluted with $CDCl_3$, 7 μL of dibromomethane was added and The mixed solution was transferred to an NMR tube and the sample was analyzed by ^1H NMR.

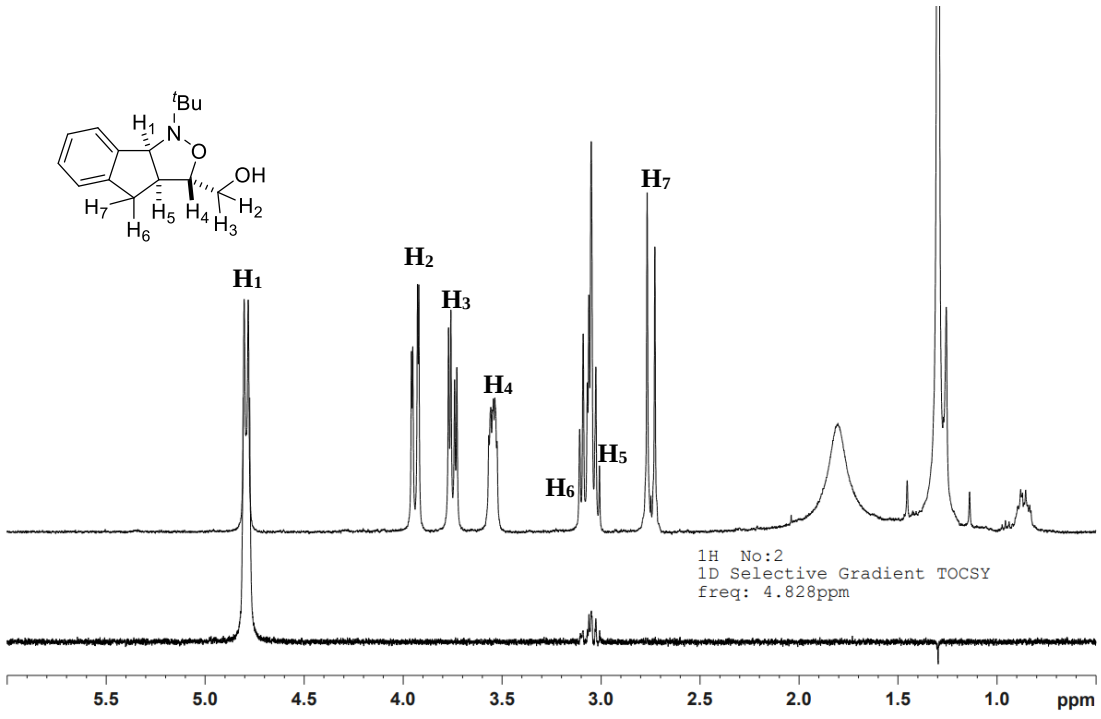
Condition b: A 25 mL Schlenk tube was charged with **3-Int** (25 mg, 0.1 mmol, 1 equiv.), Ag_2CO_3 (14 mg) and PhCl (1.0 ml). and then the reaction was allowed to stir for 12h at rt under N_2. the tube was removed from the bath, the resulting solution was filtered through a Celite filter and the solvent was removed under reduced pressure. the resulting mixture were diluted with $CDCl_3$, 7 μL of dibromomethane was added and The mixed solution was transferred to an NMR tube and the sample was analyzed by ^1H NMR.

Condition c: A 25 mL Schlenk tube was charged with **3-Int** (25 mg, 0.1 mmol, 1 equiv.) and PhCl (1.0 ml). and then the reaction was allowed to stir for 12h at rt under N_2. the tube was removed from the bath, the resulting solution was filtered through a Celite filter and the solvent was removed under reduced pressure. the resulting mixture were diluted with $CDCl_3$, 7 μL of dibromomethane was added and The mixed solution was transferred to an NMR tube and the sample was analyzed by ^1H NMR.

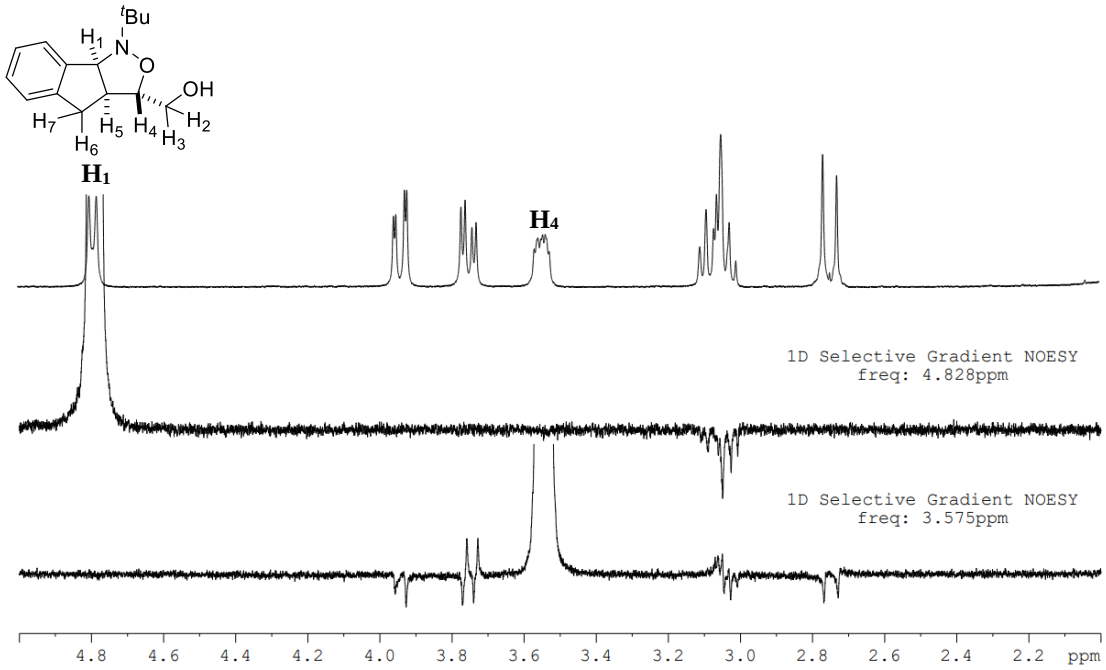
Condition d: A 25 mL Schlenk tube was charged with **3-Int** (25 mg, 0.1 mmol, 1 equiv.), $[Cp^*RhCl_2]_2$ (4 mol%, 2.5 mg), $AgSbF_6$ (16 mol%, 5.5 mg), Ag_2CO_3 (14 mg) and PhCl (1.0 ml). and then the reaction was allowed to stir for 12h at 60 ^oC under N_2. the tube was removed from the bath, the resulting solution was filtered through a Celite filter and the solvent was removed under reduced pressure. the resulting mixture were diluted with $CDCl_3$, 7 μL of dibromomethane was added and The mixed solution was transferred to an NMR tube and the sample was analyzed by ^1H NMR.

2) Data analysis for the product 3aa'

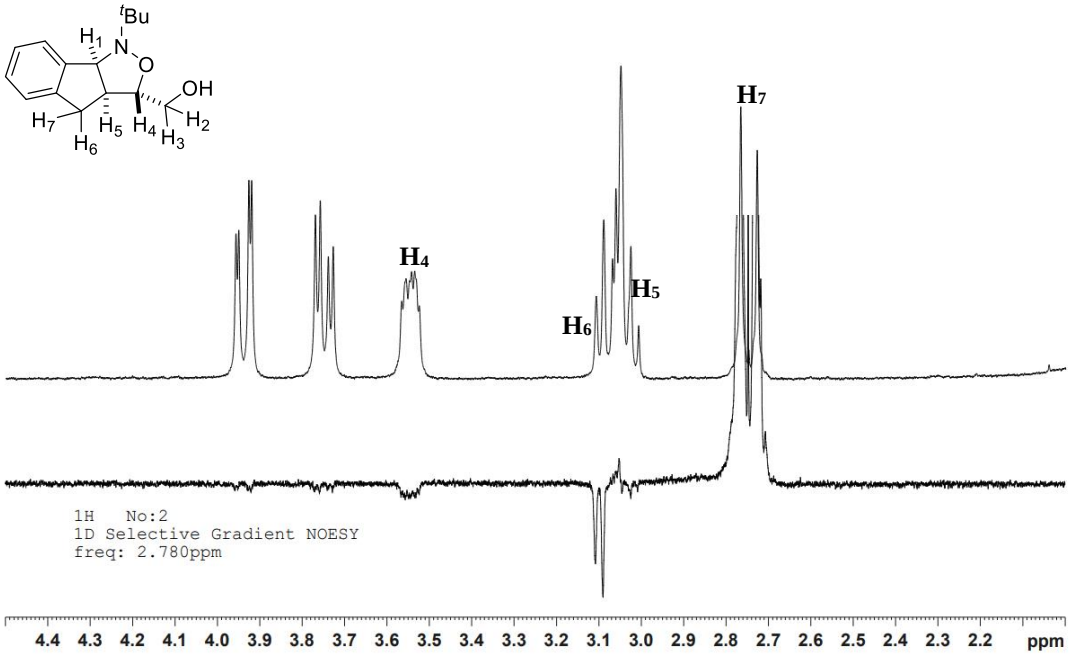




^{1}H NMR of H-H tocsy

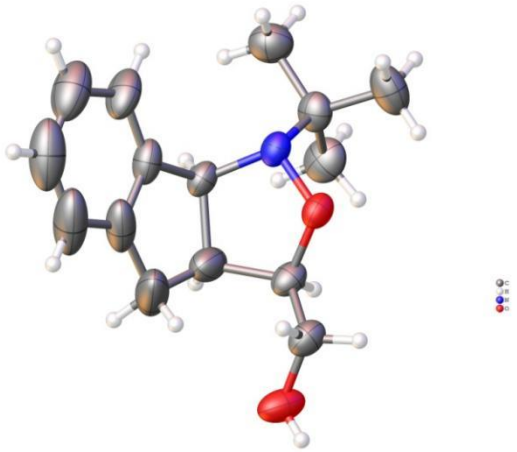


^{1}H NMR of H-H noesy



^{1}H NMR of H-H noesy

5. X-Ray Crystal Structures

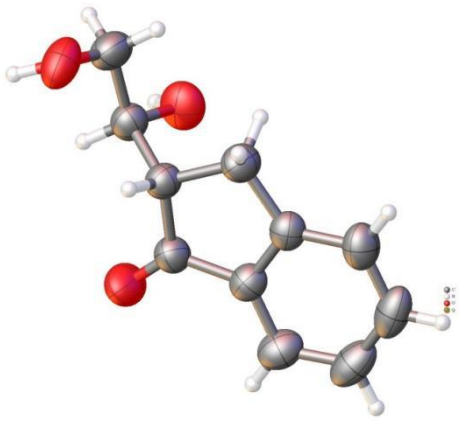


Thermal ellipsoids are set at the 50% probability level.

Table 1 Crystal data and structure refinement for 3aa.

Identification code	1_sq
Empirical formula	$C_{15}H_{21}NO_2$
Formula weight	247.33
Temperature/K	293(2)
Crystal system	trigonal
Space group	R-3
a/Å	30.683(2)
b/Å	30.683(2)
c/Å	9.8677(17)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	8045.5(17)
Z	18
ρ_{calc}g/cm^3	0.919
μ/mm^{-1}	0.480
F(000)	2412.0
Crystal size/mm^3	0.23 × 0.21 × 0.18
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	9.986 to 147.364
Index ranges	-22 ≤ h ≤ 37, -28 ≤ k ≤ 23, -12 ≤ l ≤ 11

Reflections collected	7442
Independent reflections	3440 [R_{int} = 0.0940, R_{sigma} = 0.1028]
Data/restraints/parameters	3440/30/167
Goodness-of-fit on F^2	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0952, wR_2 = 0.2361
Final R indexes [all data]	R_1 = 0.1390, wR_2 = 0.2894
Largest diff. peak/hole / e $Å^{-3}$	0.41/-0.53

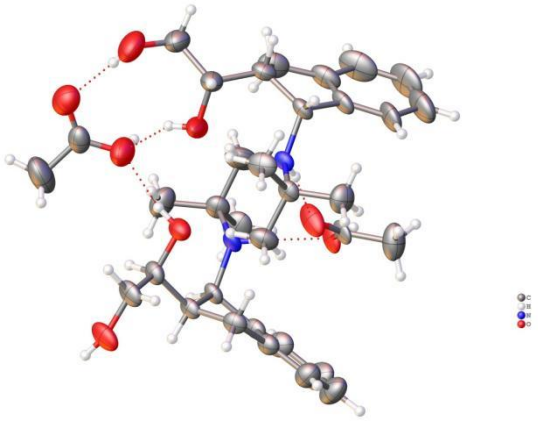


Thermal ellipsoids are set at the 50% probability level.

Table 1 Crystal data and structure refinement for 7.

Identification code	ZM-2-20220413
Empirical formula	$C_{11}H_9O_3$
Formula weight	192.22
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.3910(3)
b/Å	8.8427(3)
c/Å	10.6292(3)
α/°	90
β/°	98.559(3)
γ/°	90
Volume/$Å^3$	965.78(5)
Z	4
$\rho_{calc}g/cm^3$	1.3219
μ/mm^{-1}	0.791

F(000)	409.4
Crystal size/mm^3	0.35 × 0.25 × 0.25
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.6 to 142.44
Index ranges	-12 ≤ h ≤ 12, -6 ≤ k ≤ 10, -12 ≤ l ≤ 12
Reflections collected	3834
Independent reflections	1838 [R_{int} = 0.0173, R_{sigma} = 0.0236]
Data/restraints/parameters	1838/0/143
Goodness-of-fit on F^2	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0440, wR_2 = 0.1194
Final R indexes [all data]	R_1 = 0.0502, wR_2 = 0.1251
Largest diff. peak/hole / e Å-3	0.25/-0.18

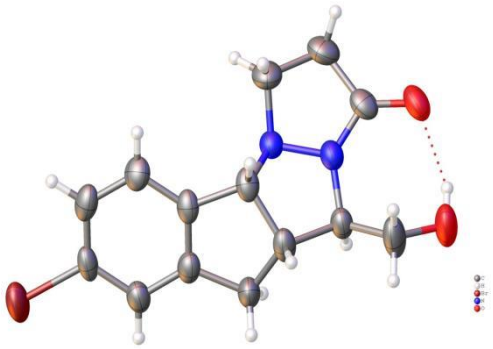


Thermal ellipsoids are set at the 50% probability level.

Table 1 Crystal data and structure refinement for 8.

Identification code	ZM-1-20220413
Empirical formula	$C_{68}H_{108}N_4O_{16}$
Formula weight	1237.58
Temperature/K	298(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.0611(2)
b/Å	9.8268(2)
c/Å	38.9367(6)
α/°	90
β/°	93.796(2)
γ/°	90

Volume/Å^3	3459.38(12)
Z	2
ρ_{calc}g/cm^3	1.188
μ/mm^{-1}	0.679
F(000)	1344.0
Crystal size/mm^3	0.5 × 0.5 × 0.5
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.104 to 142.95
Index ranges	-10 ≤ h ≤ 11, -11 ≤ k ≤ 4, -47 ≤ l ≤ 47
Reflections collected	14315
Independent reflections	6581 [R_{int} = 0.0408, R_{sigma} = 0.0573]
Data/restraints/parameters	6581/9/422
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0838, wR_2 = 0.2223
Final R indexes [all data]	R_1 = 0.1150, wR_2 = 0.2347
Largest diff. peak/hole / e Å^{-3}	0.62/-0.51



Thermal ellipsoids are set at the 50% probability level.

Table 1 Crystal data and structure refinement for 4ba.

Identification code	ZM-2-20220510
Empirical formula	$C_{14}H_{15}BrN_2O_2$
Formula weight	323.19
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.18110(10)
b/Å	21.3904(4)

c/Å	9.2071(2)
α/°	90
β/°	107.427(2)
γ/°	90
Volume/Å^3	1349.36(5)
Z	4
ρ_{calc}g/cm^3	1.5908
μ/mm^{-1}	4.157
F(000)	655.0
Crystal size/mm^3	0.1 × 0.1 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.26 to 142.9
Index ranges	$-6 \le h \le 8$, $-25 \le k \le 25$, $-11 \le l \le 11$
Reflections collected	6467
Independent reflections	2583 [R_{int} = 0.0255, R_{sigma} = 0.0252]
Data/restraints/parameters	2583/0/173
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0503, wR_2 = 0.1361
Final R indexes [all data]	R_1 = 0.0539, wR_2 = 0.1403
Largest diff. peak/hole / e Å^{-3}	0.64/-1.05

6. References

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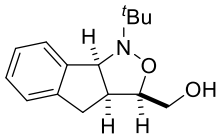
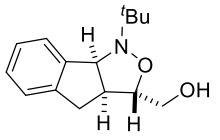
7. Characterization Data



3aa

(1-(tert-butyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol.

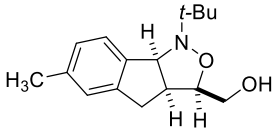
Eluent: PE: EA = 4:1, white solid (20.0 mg, 81%, m.p. 81 - 84 °C); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37 – 7.29(m, 1H), 7.24 – 7.18 (m, 2H), 7.18 – 7.13 (m, 1H), 4.95 (d, *J* = 8.0 Hz, 1H), 4.42 (m, , 1H), 3.57 (dd, *J* = 11.6, 3.6 Hz, 1H), 4.44 – 4.39 (m, 1H), 3.39 (dd, *J* = 11.4, 7.2 Hz, 1H), 3.06 (dd, *J* = 16.6, 2.4 Hz, 1H), 2.98 (dd, *J* = 16.6, 8.4 Hz, 1H), 1.95 (s, 1H), 1.28 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.0, 142.2, 128.1, 127.2, 125.2, 124.0, 82.0, 77.4, 70.1, 62.4, 59.7, 49.2, 31.9, 26.9. HRMS (ESI): m/z calcd. for $[C_{15}H_{21}NNaO_2, M+Na]^+$: 270.1465; found: 270.1457.



3aa'

(1-(tert-butyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol.

Eluent: PE: EA = 4:1, white solid (15.0 mg, 60%, m.p. 107 - 109 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.32 (m, 1H), 7.27 – 7.18 (m, 3H), 4.79 (d, *J* = 8.2 Hz, 1H), 3.95 (dd, *J* = 12.4, 2.8 Hz, 1H), 3.77 (dd, *J* = 12.4, 4.8 Hz, 1H), 3.55 (ddd, *J* = 9.6, 4.8, 2.8 Hz, 1H), 3.17 – 3.00 (m, 2H), 2.76 (d, *J* = 15.7 Hz, 1H), 1.82 (s, 1H), 1.31 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.14, 140.4, 127.9, 127.4, 125.8, 125.2, 82.5, 69.3, 61.9, 58.7, 46.8, 32.8, 26.3. HRMS (ESI): m/z calcd. for $[C_{15}H_{21}NNaO_2, M+Na]^+$: 270.1465; found: 270.1458.

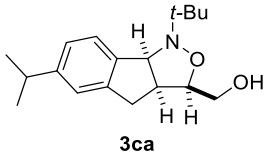


3ba

(1-(tert-butyl)-6-methyl-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol.

Eluent: Ether: DCM = 2:5, white solid (23.0 mg, 88%, m.p. 117 - 120 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 (d, *J* = 7.6 Hz, 1H), 6.95 (d, *J* = 7.6 Hz, 1H), 6.89 (s, 1H), 4.82 (d, *J* = 8.0 Hz, 1H), 4.37 – 4.25 (m, 1H), 3.49 (dd, *J* = 11.6, 3.6 Hz, 1H), 3.39 (ddd, *J* = 16.4, 8.0, 3.6 Hz, 1H), 3.35 – 3.28 (m, 1H), 2.93 (dd, *J* = 16.8, 2.8 Hz, 1H), 2.85 (dd, *J* = 16.8, 8.0 Hz, 1H), 2.24 (s, 3H), 1.88 (s, 1H), 1.19 (s, 9H).

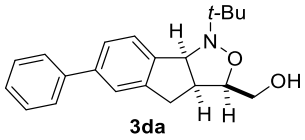
^{13}C NMR (101 MHz, $CDCl_3$) δ 142.4, 140.1, 137.8, 128.1, 124.9, 124.6, 81.8, 69.8, 62.5, 59.5, 49.5, 31.7, 26.9, 21.3. HRMS (ESI): m/z calcd. for $[C_{16}H_{23}NNaO_2, M+Na]^+$: 284.1621; found: 284.1618.



3ca

(1-(tert-butyl)-6-isopropyl-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol.

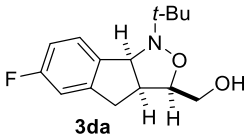
Eluent: PE: EA = 4:1, yellow solid (21.1 mg, 73%, m.p. 75 - 78 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.16 (d, *J* = 7.8 Hz, 1H), 7.01 (d, *J* = 7.8 Hz, 1H), 6.93 (s, 1H), 4.83 (d, *J* = 7.8 Hz, 1H), 4.36 – 4.32 (m, 1H), 3.50 (dd, *J* = 11.4, 3.6 Hz, 1H), 3.43 – 3.37 (m, 1H), 3.34 (dd, *J* = 11.4, 7.8 Hz, 1H), 2.95 (dd, *J* = 16.8, 2.4 Hz, 1H), 2.87 (dd, *J* = 16.8, 8.4 Hz, 1H), 2.79 (dt, *J* = 13.8, 7.2 Hz, 1H), 1.97 (s, 1H), 1.19 (s, 9H), 1.14 (d, *J* = 7.2 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.2, 142.4, 140.5, 125.7, 124.9, 121.9, 81.9, 69.8, 62.5, 59.63 (s, 2H), 49.6, 34.1, 31.8, 26.9, 24.2, 24.1. HRMS (ESI): m/z calcd. for $[C_{18}H_{27}NNaO_2, M+Na]^+$: 312.1934; found: 312.1926.



3da

(1-(tert-butyl)-6-phenyl-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol.

Eluent: PE: EA = 2:1, white solid (21.3 mg, 65%, m.p. 118 - 120 °C); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 -7.54 (m, 2H), 7.46 (d, *J* = 7.8 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.39 (d, *J* = 7.8 Hz, 1H), 7.37 (s, 1H), 7.35 – 7.31 (m, 1H), 4.98 (d, *J* = 7.8 Hz, 1H), 4.46 – 4.42 (m, 1H), 3.60 (dd, *J* = 11.4, 3.6 Hz, 1H), 3.54 – 3.49 (m, 1H), 3.45 (dd, *J* = 11.4, 7.8 Hz, 1H), 3.12 (dd, *J* = 16.8, 2.4 Hz, 1H), 3.03 (dd, *J* = 16.8, 8.4 Hz, 1H), 2.07 (s, 1H), 1.30 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.0, 142.3, 141.4, 141.3, 128.7, 127.2, 128.1, 126.5, 125.5, 122.8, 82.0, 69.8, 62.5, 59.7, 49.6, 31.9, 27.0. HRMS (ESI): m/z calcd. for $[C_{21}H_{25}NNaO_2, M+Na]^+$: 351.1778; found: 346.1768.

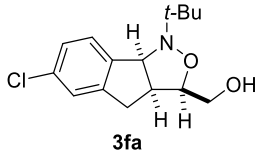


3da

(1-(tert-butyl)-6-fluoro-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol.

Eluent: DCM: Methenol = 20:1, colorless oil (15.1 mg, 57%); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.17 (dd, *J* = 8.4, 5.4 Hz, 1H), 6.82 (td, *J* = 9.0, 1.8 Hz, 1H), 6.76 (d, *J* = 8.4 Hz, 1H), 4.82 (d, *J* = 8.4 Hz, 1H), 4.39 – 4.25 (m, 1H), 3.48 (dd, *J* = 11.4, 4.8 Hz, 1H), 3.45 – 3.41 (m, 2.4 Hz, 1H), 3.33 (dd, *J* = 12.0, 6.8 Hz, 1H), 2.98 (dd, *J* = 16.8, 1.8 Hz, 1H), 2.87 (dd, *J* = 16.8, 8.4 Hz, 1H), 2.29 (s, 1H), 1.18 (s, 9H).

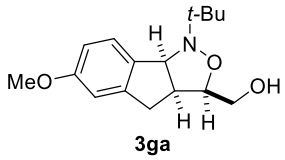
13C NMR (101 MHz, CDCl3) δ 163.1(d, J = 245.8 Hz),144.6 (d, J = 8.3 Hz), 138.59 (d, J = 1.7 Hz), 126.38 (d, J = 9.0 Hz), 114.2 (d, J = 22.6 Hz), 110.8 (d, J = 22.1 Hz), 82.0, 69.4, 62.2, 59.8, 49.8, 31.9 (d, J = 2.0 Hz), 26.9. ^{19}F NMR (377 MHz, $CDCl_3$) δ -115.25. HRMS (ESI): m/z calcd. for $[C_{15}H_{20}NFNaO_2, M+Na]^+$: 288.1370; found: 288.1362.



3fa

(1-(tert-butyl)-6-chloro-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol

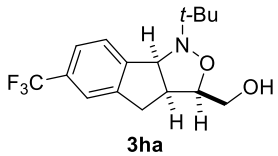
Eluent: DCM: Methenol = 20:1, white solid (16.3 mg, 68%, m.p. 88 - 91 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (d, *J* = 8.8 Hz, 1H), 7.11 (d, *J* = 9.2 Hz, 1H), 7.07 (s, 1H), 4.84 (d, *J* = 7.6 Hz, 1H), 4.46 – 4.29 (m, 1H), 3.52 (dd, *J* = 11.6, 3.6 Hz, 1H), 3.43 (ddd, *J* = 16.4, 8.4, 2.8 Hz, 1H), 3.36 (dd, *J* = 11.6, 7.2 Hz, 1H), 2.99 (dd, *J* = 16.8, 2.4 Hz, 1H), 2.89 (dd, *J* = 16.8, 8.4 Hz, 1H), 1.81 (s, 1H), 1.20 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.2, 141.6, 133.9, 127.4, 126.3, 124.2, 81.9, 69.5, 62.3, 59.8, 49.4, 31.8, 26.9. HRMS (ESI): m/z calcd. for $[C_{15}H_{20}NClNaO_2, M+Na]^+$:304.1075; found: 304.1070.



3ga

(1-(tert-butyl)-6-methoxy-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol

Eluent: PE: EA = 2:1, yellow solid (25.0 mg, 90%, m.p. 109 - 112 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (d, *J* = 8.4 Hz, 1H), 6.70 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.61 (s, 1H), 4.82 (d, *J* = 8.0 Hz, 1H), 4.36 – 4.32 (m, 1H), 3.70 (s, 3H), 3.52 (dd, *J* = 11.6, 3.6 Hz, 1H), 3.47 – 3.32 (m, 2H), 2.95 (dd, *J* = 16.8, 2.8 Hz, 1H), 2.87 (dd, *J* = 16.8, 8.0 Hz, 1H), 1.91 (s, 1H), 1.19 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1, 143.9, 125.9 113.6, 108.9, 81.9, 69.5, 62.4, 59.7, 55.4, 49.78, 31.9, 26.9. HRMS (ESI): m/z calcd. for $[C_{16}H_{23}NNaO_3, M+Na]^+$:300.1570; found: 300.1577.

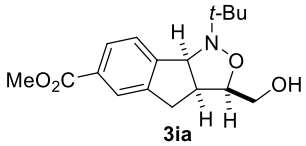


3ha

(1-(tert-butyl)-6-(trifluoromethyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol

Eluent: PE: EA = 2:1, white solid (17.6 mg, 56%, m.p. 110 - 112 °C); 1H NMR (600 MHz, CDCl3) δ 7.40 (d, J = 7.8 Hz, 1H), 7.35 (d, J = 8.4 Hz, 2H), 4.90 (d, J = 8.4 Hz, 1H), 4.40 – 4.31 (m, 1H), 3.51 (dd, J = 11.4, 4.8 Hz, 1H), 3.49 – 3.45 (m, 1H), 3.33 (dd, *J* = 12.0, 6.8 Hz, 1H), 3.06 (dd, *J* = 16.8, 1.8

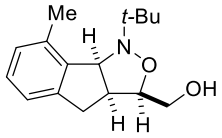
Hz, 1H), 2.95 (dd, *J* = 16.8, 8.4 Hz, 1H), 1.96 (s, 1H), 1.20 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.1, 143.1, 130.5 (q, *J* = 32.3 Hz), 125.7, 124.4 (q, *J* = 4.0 Hz), 124.3 (q, *J* = 274.0 Hz), 121.0 (q, *J* = 7.0 Hz), 82.1, 69.8, 62.1, 59.9, 49.3, 31.9, 26.9. ^{19}F NMR (377 MHz, $CDCl_3$) δ -62.15 HRMS (ESI): m/z calcd. For $[C_{16}H_{20}NF_3NaO_2$, M+Na]$^+$:338.1338; found: 338.1332.



3ia

Methyl-1-(tert-butyl)-3-(hydroxymethyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazole-6-carboxylate.

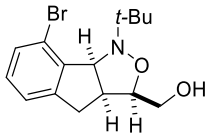
Eluent: PE: EA = 4:1, brown oil (27.4 mg, 90%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.0 Hz, 1H), 7.76 (s, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 4.89 (d, *J* = 8.0 Hz, 1H), 4.36 (d, *J* = 4.0 Hz, 1H), 3.82 (s, 3H), 3.50 – 3.41 (m, 2H), 3.31 (dd, *J* = 11.6, 7.2 Hz, 1H), 3.08 – 3.00 (m, 1H), 2.95 (d, *J* = 8.4 Hz, 1H), 2.45 (1H), 1.21 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.1, 148.2, 142.8, 130.2, 128.8, 125.4, 125.2, 82.2, 69.9, 62.1, 60.1, 52.0, 49.4, 31.6, 26.9. HRMS (ESI): m/z calcd. For $[C_{17}H_{23}NNaO_4$, M+Na]$^+$:328.1519; found: 328.1514.



3ja

(1-(tert-butyl)-8-methyl-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol.

Eluent: PE: EA = 4:1, white solid (20.4 mg, 78%, m.p. 80 - 83 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.02 (t, *J* = 7.6 Hz, 1H), 6.89 (t, *J* = 6.8 Hz, 2H), 5.11 (d, *J* = 7.2 Hz, 1H), 4.34 (ddd, *J* = 9.6, 7., 3.9 Hz, 1H), 3.52 (dd, *J* = 11.4, 3.4 Hz, 1H), 3.39 – 3.25 (m, 2H), 2.96 – 2.80 (m, 2H), 2.42 (s, 3H), 1.75 (s, 1H), 1.23 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.3, 140.0, 136.1, 129.2, 128.3, 121.4, 82.2, 71.2, 63.2, 61.1, 48.0, 32.1, 27.7, 19.6. HRMS (ESI): m/z calcd. For $[C_{16}H_{23}NNaO_2$, M+Na]$^+$:284.1621; found: 284.1615.

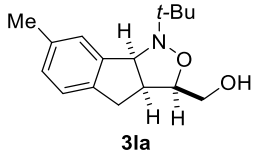


3ka

(8-bromo-1-(tert-butyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol.

Eluent: PE: EA = 4:1, white solid (21.8 mg, 68%, m.p. 106 - 109 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 7.6 Hz, 1H), 7.13 – 6.99 (m, 2H), 5.16 (d, *J* = 7.2 Hz, 1H), 4.41 (dd, *J* = 12.4, 6.8 Hz, 1H),

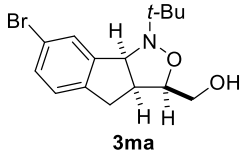
3.61 (d, *J* = 10.8 Hz, 1H), 3.50 – 3.35 (m, 2H), 3.06 (d, *J* = 16.8 Hz, 1H), 2.96 (dd, *J* = 16.8, 8.0 Hz, 1H), 1.80 (s, 1H), 1.34 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.3, 140.8, 131.9, 129.8, 122.9, 120.9, 82.0, 72.3, 62.9, 61.6, 48.0, 32.5, 28.0. HRMS (ESI): m/z calcd. For [$C_{15}H_{20}NBrNaO_2$, M+Na]$^+$:348.0570; found: 348.0570.



3la

(1-(tert-butyl)-7-methyl-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol

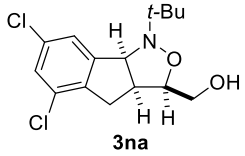
Eluent: PE: EA = 4:1, white solid (19.5 mg, 73%, m.p. 130 - 133 ºC); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.13 (s, 1H), 7.02 (q, *J* = 7.8 Hz, 2H), 4.92 (d, *J* = 7.8 Hz, 1H), 4.46 – 4.37 (m, 1H), 3. 60 – 3.52 (m, 1H), 3.50 – 3.41 (m, 1H), 3.36 (dd, *J* = 11.4, 7.8 Hz, 1H), 3.04 – 2.90 (m, 2H), 2.33 (s, 3H), 1.83 (s, 1H), 1.27 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.3, 139.1, 136.8, 129.0, 125.6, 123.7, 82.0, 70.1, 62.6, 59.6, 49.2, 31.5, 27.1, 21.3. HRMS (ESI): m/z calcd. For [$C_{16}H_{23}NNaO_2$, M+Na]$^+$:284.1621; found: 284.1612.



3ma

(7-bromo-1-(tert-butyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol.

Eluent: PE: EA = 4:1, white solid (24.0 mg, 74%, m.p. 133 - 135 ºC); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.42 (s, 1H), 7.32 (d, *J* = 7.8 Hz, 1H), 7.02 (d, *J* = 7.8 Hz, 1H), 4.92 (d, *J* = 7.8 Hz, 1H), 4.43 – 4.38 (m, 1H), 3.63 – 3.54 (m, 1H), 3.52 – 3.45 (m, 1H), 3.39 (dd, *J* = 11.4, 6.6 Hz, 1H), 3.01 (d, *J* = 16.8 Hz, 1H), 2.92 (dd, *J* = 16.8, 8.4 Hz, 1H), 1.88 (s, 1H), 1.26 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.7, 141.2, 131.2, 128.4, 125.5, 120.9, 82.0, 69.9, 62.3, 59.7, 49.4, 31.6, 27.0. HRMS (ESI): m/z calcd. For [$C_{15}H_{20}NBrNaO_2$, M+Na]$^+$:348.0570; found: 348.0561.

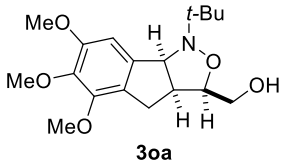


3na

(1-(tert-butyl)-5,7-dichloro-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol.

Eluent: PE: EA = 4:1, white solid (17.9 mg, 57%, m.p. 107 - 109 ºC); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.15 (s, 1H), 7.11 (s, 1H), 4.89 (d, *J* = 7.8 Hz, 1H), 4.38 – 4.33 (m, 1H), 3.54 (dd, *J* = 12.0, 3.6 Hz, 1H), 3.47 – 3.42 (m, 1H), 3.38 (dd, *J* = 11.4, 6.6 Hz, 1H), 3.03 (dd, *J* = 17.4, 1.8 Hz, 1H), 2.85 (dd, *J* = 17.4, 8.4 Hz, 1H), 1.89 (s, 1H), 1.19 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.4=, 139.2, 133.6, 130.6,

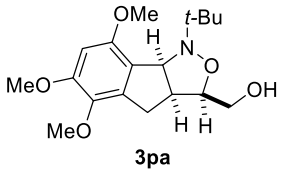
128.0, 124.0, 82.1, 70.6, 62.0, 60.1, 48.8, 30.9, 26.9. HRMS (ESI): m/z calcd. For $[C_{15}H_{29}NCl_2NaO_2$, M+Na]$^+$:338.0685; found: 338.0678.



3oa

(1-(tert-butyl)-5,6,7-trimethoxy-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol

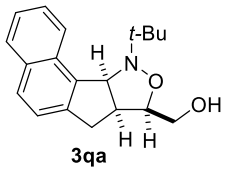
Eluent: PE: EA = 1:2, orange solid (20.0 mg, 59%, m.p. 93 - 96 °C); ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.54 (s, 1H), 4.83 (d, *J* = 7.8 Hz, 1H), 4.40 – 4.30 (m, 1H), 3.80 (s, 3H), 3.79 (s, 3H), 3.74 (s, 3H), 3.54 (dd, *J* = 11.4, 4.8 Hz, 1H), 3.43 – 3.35 (m, 2H), 2.96 (dd, *J* = 16.8, 1.8 Hz, 1H), 2.79 (dd, *J* = 16.8, 8.4 Hz, 1H), 1.89 (s, 1H), 1.19 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.7, 148.8, 141.7, 138.6, 126.7, 103.6, 82.2, 70.6, 62.5, 60.9, 60.4, 59.7, 56.0, 49.2, 28.6, 26.9. HRMS (ESI): m/z calcd. For $[C_{18}H_{27}NNaO_5$, M+Na]$^+$:360.1781; found: 360.1777.



3pa

(1-(tert-butyl)-5,6,8-trimethoxy-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol.

Eluent: PE: EA = 1:2, yellow solid (28.0 mg, 83%, m.p. 111 - 114 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.25 (s, 1H), 5.01 (d, *J* = 7.6 Hz, 1H), 4.32 (ddd, *J* = 8.8, 6.8, 3.6 Hz, 1H), 3.77 (s, 3H), 3.70 (s, 3H), 3.67 (s, 3H), 3.65 – 3.57 (m, 1H), 3.47 (dd, *J* = 10.8, 6.4 Hz, 1H), 3.38 – 3.34 (m, 1H), 3.06 (dd, *J* = 17.2, 2.4 Hz, 1H), 2.75 (dd, *J* = 17.2, 8.8 Hz, 1H), 1.19 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.2, 152.9, 138.3, 137.4, 122.7, 96.6, 81.9, 69.4, 62.8, 60.5, 60.4, 56.5, 55.2, 49.1, 29.3, 27.3. HRMS (ESI): m/z calcd. For $[C_{18}H_{27}NNaO_5$, M+Na]$^+$:360.1781; found: 360.1780.

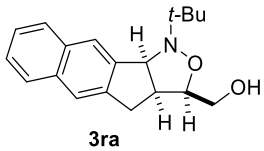


3qa

(10-(tert-butyl)-7a,8,10,10a-tetrahydro-7H-benzo[6,7]indeno[1,2-c]isoxazol-8-yl)methanol.

Eluent: PE: EA = 4:1, white solid (23.1 mg, 78%, m.p. 86 - 88 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.49 (t, *J* = 7.2 Hz, 1H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.28 (s, 1H), 5.52 (d, *J* = 7.2 Hz, 1H), 4.56 – 4.42 (m, 1H), 3.64 (dd, *J* = 11.6, 3.6 Hz, 1H), 3.53 (dd, *J* = 15.6, 7.6 Hz, 1H), 3.39 (dd, *J* = 11.6, 7.2Hz, 1H), 3.22 – 3.02 (m, 2H), 1.89 (s, 1H),

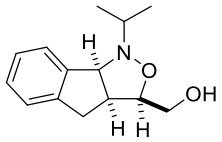
1.43 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.0, 136.2, 133.6, 130.9, 129.4, 128.5, 126.1, 124.9, 124.2, 122.3, 82.4, 71.8, 63.2, 61.2, 48.1, 32.7, 27.9. HRMS (ESI): m/z calcd. For [$C_{19}H_{23}NNaO_2$, M+Na]$^+$ 320.1621; found: 320.1619.



3ra

(1-(tert-butyl)-3,3a,4,10b-tetrahydro-1H-benzo[5,6]indeno[1,2-c]isoxazol-3-yl)methanol.

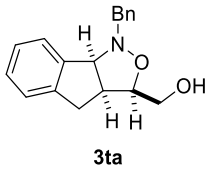
Eluent: PE: EA = 4:1, yellow solid (17.0 mg, 57%, m.p. 117 - 119 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.62 (m, 3H), 7.52 (s, 1H), 7.38 – 7.26 (m, 2H), 4.98 (d, *J* = 8.0 Hz, 1H), 4.42 – 4.37 (m, 1H), 3.55 – 3.40 (m, 2H), 3.26 (dd, *J* = 11.6, 7.6 Hz, 1H), 3.17 – 2.99 (m, 2H), 1.77 (s, 1H), 1.25 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.5, 140.8, 133.9, 133.3, 128.2, 127.4, 125.6, 125.1, 124.0, 122.2, 81.9, 69.5, 62.5, 59.8, 49.7, 31.5, 27.0. HRMS (ESI): m/z calcd. For [$C_{19}H_{23}NNaO_2$, M+Na]$^+$ 320.1621; found: 320.1610.



3sa

(1-isopropyl-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol

Eluent: PE: EA = 2:1, white solid (20.1 mg, 86%, m.p. 78 - 81 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.23 (m, 1H), 7.17 – 7.11 (m, 2H), 7.11 – 7.05 (m, 1H), 4.87 (d, *J* = 7.6 Hz, 1H), 4.24 (ddd, *J* = 8.4, 6.8, 3.6 Hz, 1H), 3.69 (dd, *J* = 11.6, 3.6 Hz, 1H), 3.53 (dd, *J* = 11.6, 6.6 Hz, 1H), 3.40 (ddd, *J* = 16.4, 8.4, 2.6 Hz, 1H), 3.06 – 2.96 (m, 2H), 2.90 (dd, *J* = 16.8, 8.6 Hz, 1H), 1.73 (s, 1H), 1.18 (d, *J* = 6.2 Hz, 3H), 1.15 (d, *J* = 6.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.7, 142.1, 128.2, 127.1, 125.1, 124.1, 78.7, 74.1, 61.9, 54.1, 46.6, 31.9, 21.3, 20.1. HRMS (ESI): m/z calcd. For [$C_{14}H_{19}NNaO_2$, M+Na]$^+$ 256.1308; found: 256.1305.

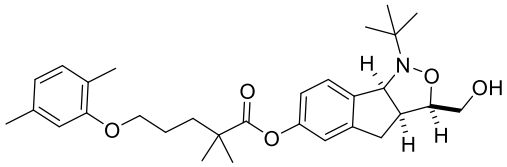


3ta

(1-benzyl-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)methanol

Eluent: PE: EA = 4:1, colorless oil (23.4 mg, 83%); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.8 Hz, 2H), 7.30 (t, *J* = 7.8 Hz, 2H), 7.23 (t, *J* = 7.2 Hz, 1H), 7.16 – 7.11 (m, 1H), 7.11 – 7.07 (m, 3H), 4.69 (d,

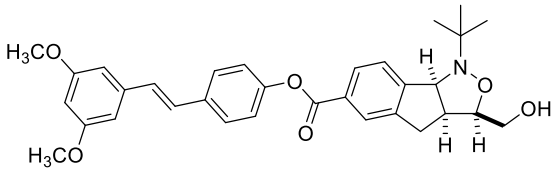
J = 7.8 Hz, 1H), 4.45 (ddd, *J* = 8.4, 6.0, 3.6 Hz, 1H), 4.15 (d, *J* = 12.6 Hz, 1H), 3.99 (d, *J* = 12.6 Hz, 1H), 3.72 (dd, *J* = 11.4, 3.6 Hz, 1H), 3.62 – 3.48 (m, 2H), 3.06 (dd, *J* = 16.8, 2.4 Hz, 1H), 2.92 (dd, *J* = 16.8, 9.0 Hz, 1H), 1.83 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.1, 141.1, 137.1, 129.2, 128.5, 128.4, 127.6, 126.9, 125.1, 124.2, 79.0, 76.1, 62.2, 61.3 46.6, 31.9. HRMS (ESI): m/z calcd. For $[C_{18}H_{19}NNaO_2, M+Na]^+$ 304.1308 found: 304.1301.



3aaa

1-(tert-butyl)-3-(hydroxymethyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-6-yl-5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate

Eluent: PE: EA = 4:1, white solid (35.0 mg, 65%, m.p. 78 - 81 ºC); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (d, *J* = 8.0 Hz, 1H), 6.93 (d, *J* = 7.6 Hz, 1H), 6.79 (dd, *J* = 8.0, 2.0 Hz, 1H), 6.75 (s, 1H), 6.59 (d, *J* = 7.6 Hz, 1H), 6.56 (s, 1H), 4.84 (d, *J* = 8.0 Hz, 1H), 4.35 (ddd, *J* = 8.4, 7.6, 3.7 Hz, 1H), 3.91 (d, *J* = 2.8 Hz, 2H), 3.52 (dd, *J* = 11.6, 3.6 Hz, 1H), 3.45 – 3.41 (m, 1H), 3.35 (dd, *J* = 11.6, 7.2 Hz, 1H), 2.93 (qd, *J* = 16.8, 5.2 Hz, 2H), 2.23 (s, 3H), 2.10 (s, 3H), 1.80 (d, *J* = 2.8 Hz, 4H), 1.64 (s, 1H), 1.28 (s, 6H), 1.19 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.5, 156.9, 151.2, 143.7, 136.5), 130.3, 125.9, 123.6, 120.7, 120.4, 117.2, 112.0, 81.9, 69.6, 67.8, 62.4, 59.7, 49.6, 42.4, 37.2, 31.8, 26.9, 25.3, 25.2, 25.1, 21.4, 15.8. HRMS (ESI): m/z calcd. For $[C_{30}H_{42}NO_5, M+H]^+$ 496.3057, found: 496.3070.

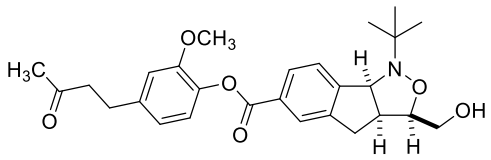


3baa

4-((E)-3,5-dimethoxystyryl)phenyl-1-(tert-butyl)-3-(hydroxymethyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazole-6-carboxylate

Eluent: PE: EA = 1:1, yellow solid (15.0 mg, 28%, m.p. 111 - 114 ºC); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.0 Hz, 1H), 7.93 (s, 1H), 7.48 (d, *J* = 8.8 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.14 (d, *J* = 8.8 Hz, 2H), 7.02 (d, *J* = 16.4 Hz, 1H), 6.93 (d, *J* = 16.4 Hz, 1H), 6.60 (d, *J* = 2.4 Hz, 2H), 6.33 (t, *J* = 2.4 Hz, 1H), 4.92 (d, *J* = 8.0 Hz, 1H), 4.38 (ddd, *J* = 8.4, 7.2, 3.6 Hz, 1H), 3.76 (s, 6H), 3.61 – 3.44 (m, 2H), 3.36 (dd, *J* = 11.6, 6.8 Hz, 1H), 3.10 (dd, *J* = 16.8, 2.0 Hz, 1H), 3.00 (dd, *J* = 17.0, 8.3 Hz, 1H), 1.74 (s, 1H), 1.22 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.2, 161.0, 150.5, 149.5, 142.9, 139.3, 134.9, 129.4, 128.9, 128.3, 127.5, 125.9, 125.4, 121.9, 104.6, 100.1, 82.0, 69.9, 62.3, 59.8, 55.4, 49.3,

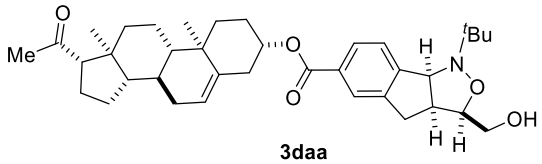
31.8, 27.0. HRMS (ESI): m/z calcd. For $[C_{32}H_{36}NO_6, M+H]^+$ 530.2537, found: 530.2525.



3caa

2-methoxy-4-(3-oxobutyl)phenyl-1-(tert-butyl)-3-(hydroxymethyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazole-6-carboxylate

[1] Eluent: DCM: Methenol = 20:1, yellow oil (15.0 mg, 28%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.0 Hz, 1H), 7.93 (s, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 6.96 (d, *J* = 8.0 Hz, 1H), 6.76 (s, 1H), 6.71 (d, *J* = 8.0 Hz, 1H), 4.91 (d, *J* = 8.0 Hz, 1H), 4.46 – 4.31 (m, 1H), 3.71 (s, 3H), 3.58 – 3.44 (m, 2H), 3.35 (dd, *J* = 11.2, 7.2 Hz, 1H), 3.08 (d, *J* = 16.8 Hz, 1H), 2.98 (dd, *J* = 16.8, 8.0 Hz, 1H), 2.83 (t, *J* = 7.6 Hz, 2H), 2.71 (t, *J* = 7.2 Hz, 2H), 2.08 (s, 3H), 1.80 (s, 1H), 1.21 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 207.7, 164.9, 151.1, 149.2, 142.8, 140.0, 138.3, 129.6, 129.4, 126.1, 125.3, 122.8, 120.4, 112.8, 81.9, 69.9, 62.3, 59.8, 55.9, 49.3, 45.2, 31.7, 30.1, 29.6, 27.0. HRMS (ESI): m/z calcd. For $[C_{27}H_{33}NNaO_6, M+Na]^+$ 490.2200, found: 490.2194.

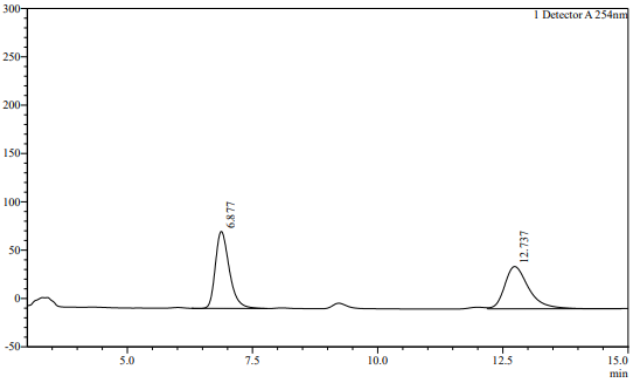


3daa

(3S,8S,9S,10R,13S,14S,17S)-17-acetyl-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl-1-(tert-butyl)-3-(hydroxymethyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazole-6-carboxylate

Eluent: PE: EA = 2:1, white solid (42.0 mg, 72%); Following the general procedure, the product (42.0 mg) was obtained in 72% yield as an inseparable mixture of 2 diastereomers (1:1, estimated by HPLC with a Daicel Chiralpak AD-H, n-hexane/2-propanol = 80/20, v = 1.0 mL·min^{-1}, λ = 254 nm, t_1 = 6.8 min, t_2 = 12.7 min; signals of the 2 isomers cannot be distinguished by ^{1}H NMR). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.0 Hz, 1H), 7.76 (s, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 5.34 (d, *J* = 4.4 Hz, 1H), 4.88 (d, *J* = 8.0 Hz, 1H), 4.77 (ddd, *J* = 16.2, 9.0, 4.6 Hz, 1H), 4.36 (dd, *J* = 3.8, 1.2 Hz, 1H), 3.59 – 3.40 (m, 2H), 3.34 (dd, *J* = 11.6, 7.2 Hz, 1H), 3.03 (dd, *J* = 17.2, 2.0 Hz, 1H), 2.97 (d, *J* = 16.8, 8.4 Hz, 1H), 2.47 (t, *J* = 8.8 Hz, 1H), 2.39 (d, *J* = 7.6 Hz, 2H), 2.16 – 2.07 (m, 1H), 2.06 (s, 3H), 1.99 (dd, *J* = 8.4, 2.4 Hz, 1H), 1.97 – 1.88 (m, 2H), 1.85 (dt, *J* = 13.6, 3.2 Hz, 1H), 1.78 (s, 1H), 1.70 – 1.51 (m, 5H), 1.47 – 1.32 (m, 3H), 1.20 (s, 9H), 1.18 – 1.04 (m, 3H), 1.00 (s, 3H), 0.97 – 0.92 (m, 1H), 0.57 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 209.6, 166.1, 142.5, 139.7, 130.8, 128.8, 125.3, 125.1, 122.4, 82.0, 74.4, 69.9, 63.7, 62.3, 59.8, 56.8, 49.9, 49.3, 44.0, 38.8, 38.1, 37.1, 36.7, 31.9, 31.8, 31.7, 31.6, 27.8, 27.0, 24.5, 22.8, 21.0, 19.4, 13.2. HRMS (ESI): m/z calcd. For $[C_{37}H_{52}NO_5, M+H]^+$ 590.3840, found: 590.3850.

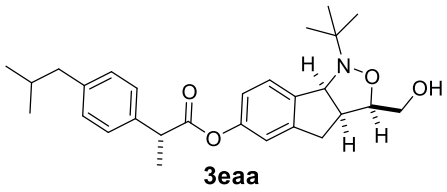
<Chromatogram>



<Peak Table>

Detector A 254nm

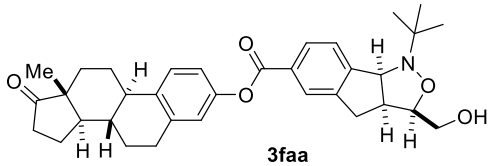
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	6.877	1539407	79606	51.344	51.344
2	12.737	1458817	43785	48.656	48.656
Total		2998223	123391		100.000



3eaa

1-(tert-butyl)-3-(hydroxymethyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-6-yl-(2R)-2-(4-isobutylphenyl)propanoate

Eluent: PE: EA = 2:1, white solid (21.0 mg, 46%); Following the general procedure, the product (21.0 mg) was obtained in 46% yield as an inseparable mixture of 2 diastereomers (1:1, estimated by ^{1}H NMR). ^{1}H NMR (400 MHz, CDCl3) δ 7.25 – 7.17 (m, 3H), 7.06 (d, *J* = 8.0 Hz, 2H), 6.80 – 6.65 (m, 2H), 4.81 (d, *J* = 8.0 Hz, 1H), 4.37 – 4.25 (m, 1H), 3.83 (q, *J* = 7.2 Hz, 1H), 3.48 (ddd, *J* = 11.6, 5.2, 4.0 Hz, 1H), 3.45 – 3.36 (m, 1H), 3.32 (dt, *J* = 11.6, 7.2 Hz, 1H), 3.02 – 2.80 (m, 2H), 2.39 (d, *J* = 7.2 Hz, 2H), 1.87 – 1.72 (m, 1H), 1.55 – 1.47 (m, 2H) ,1.17 (s, 9H), 0.84 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.41, 173.38, 151.01, 143.70, 140.79, 140.59, 140.57, 137.29, 137.26, 129.51, 127.22, 125.83, 120.43, 120.33, 117.11, 117.06, 81.9, 69.54, 62.39, 59.68, 49.65, 49.61, 45.27, 45.25, 45.06, 31.84, 30.19, 26.96, 22.4, 18.57. HRMS (ESI): m/z calcd. For [$C_{28}H_{37}NNaO_4$, M+Na]$^{+}$ 474.2615, found: 474.2607.

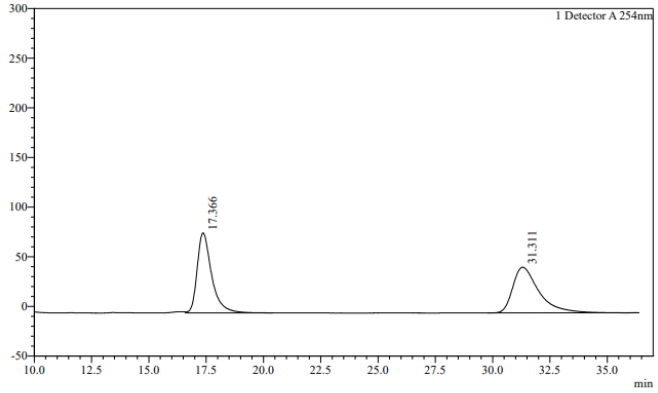


3faa

(8S,9R,13R,14R)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl-(3R)-1-(tert-butyl)-3-(hydroxymethyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazole-6-carboxylate

Eluent: PE: EA = 1:1, white solid (39.4 mg, 76%); Following the general procedure, the product (39.4 mg) was obtained in 76% yield as an inseparable mixture of 2 diastereomers (1:1, estimated by HPLC with a Daicel Chiralpak AD-H, n-hexane/2-propanol = 80/20, v = 1.0 mL·min^{-1}, λ = 254 nm, t_1 = 17.3 min, t_2 = 31.3 min; signals of the 2 isomers cannot be distinguished by ^{1}H NMR). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.0 Hz, 1H), 7.98 (s, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 6.97 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.94 (d, *J* = 1.6 Hz, 1H), 4.99 (d, *J* = 8.0 Hz, 1H), 4.5 - 4.4 (m, 1H), 3.67 – 3.50 (m, 2H), 3.43 (dd, *J* = 11.6, 6.8 Hz, 1H), 3.20 - 3.12 (m, 1H), 3.10 – 3.02 (m, 1H), 2.99 – 2.87 (m, 2H), 2.56 – 2.46 (m, 1H), 2.45 – 2.38 (m, 1H), 2.36 – 2.46 (m, 1H), 2.21 – 2.04 (m, 2H), 2.03 – 1.92 (m, 2H), 1.70 – 1.54 (m, 4H), 1.50 – 1.43 (m, 2H), 1.29 (s, 9H), 0.92 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 220.5, 165.6, 148.9, 143.0, 138.2, 137.5, 129.7, 129.5, 126.5, 126.0, 125.5, 121.8, 119.0, 82.1, 70.1, 62.4, 60.0, 50.5, 49.4, 48.1, 44.3, 38.1, 35.9, 31.9, 31.7, 29.5, 27.1, 26.5, 25.9, 21.7, 13.9. HRMS (ESI): m/z calcd. For $[C_{34}H_{42}NO_5, M+H]^+$ 544.3057, found: 544.3052.

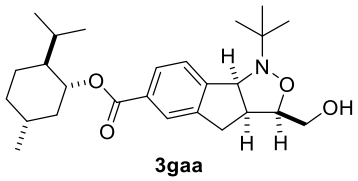
<Chromatogram>



<Peak Table>

Detector A 254nm

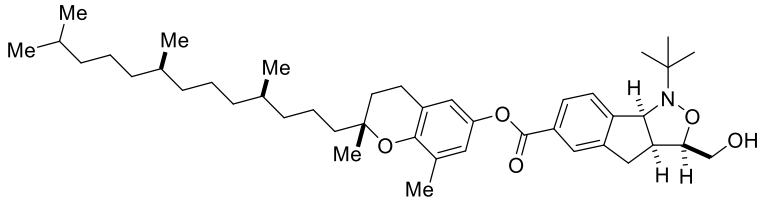
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	17.366	3532465	80603	49.181	49.181
2	31.311	3650112	46036	50.819	50.819
Total		7182577	126638		100.000



3gaa

(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl-1-(tert-butyl)-3-(hydroxymethyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazole-6-carboxylate

Eluent: DCM: Methanol = 20:1, white solid (33.5 mg, 78%); Following the general procedure, the product (33.5 mg) was obtained in 78% yield as an inseparable mixture of 2 diastereomers (1:1, estimated by 1H NMR). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 – 7.80 (m, 1H), 7.76 (s, 1H), 7.30 (d, *J* = 7.8 Hz, 1H), 4.88 (t, *J* = 7.2 Hz, 1H), 4.86 – 4.80 (m, 1H), 4.40 – 4.32 (m, 1H), 3.55 – 3.49 (m, 1H), 3.47 – 3.42 (m, 1H), 3.35 – 3.31 (m, 1H), 3.04 (ddd, *J* = 16.8, 7.8, 2.24 Hz, 1H), 2.95 (dt, *J* = 16.8, 7.8 Hz, 1H), 2.09 – 2.00 (m, 1H), 1.91 – 1.82 (m, 1H), 1.79 (s, 1H), 1.65 (dd, *J* = 11.4, 1.8 Hz, 2H), 1.53 – 1.44 (m, 2H), 1.20 (s, 9H), 1.11 – 0.99 (m, 2H), 0.88 – 0.82 (m, 6H), 0.72 – 0.68 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.18, 166.15, 148.33, 148.26, 142.57, 142.54, 130.94, 130.87, 128.88, 128.79, 125.33, 125.31, 125.09, 125.06, 81.94, 74.82, 69.89, 62.38, 59.77, 49.37, 49.30, 47.34, 47.39, 41.01, 40.97, 34.36 , 31.76, 31.71, 31.46, 27.00, 26.97, 26.60, 26.52, 23.78, 23.70, 22.03, 20.76, 20.71, 16.62, 16.53. HRMS (ESI): m/z calcd. For $[C_{26}H_{40}NO_5, M+H]^+$ 430.2952, found: 430.2938.

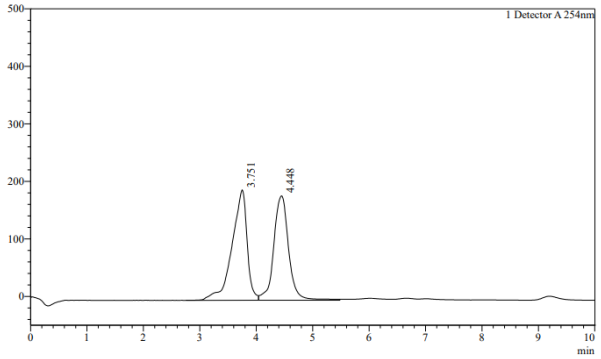


3haa

(R)-2,8-dimethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman-6-yl-1-(tert-butyl)-3-(hydroxymethyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazole-6-carboxylate

Eluent: PE: EA = 3:1, white solid (47.0 mg, 70%); Following the general procedure, the product (47.0 mg) was obtained in 70% yield as an inseparable mixture of 2 diastereomers (1:1, estimated by HPLC with a Daicel Chiralpak AD-H, n-hexane/2-propanol = 90/10, v = 0.8 mL·min^{-1}, λ = 254 nm, t_1 = 3.7 min, t_2 = 4.4 min; signals of the 2 isomers cannot be distinguished by 1H NMR). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.0 Hz, 1H), 7.97 (s, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 6.79 (d, *J* = 2.4 Hz, 1H), 6.74 (d, *J* = 2.6 Hz, 1H), 4.99 (d, *J* = 8.0 Hz, 1H), 4.5 – 4.35 (m, 1H), 3.70 – 3.49 (m, 2H), 3.20 – 2.95 (dd, *J* = 11.6, 6.8 Hz, 1H), 3.20 – 2.95 (m, 2H), 2.87 – 2.65 (m, 2H), 2.17 (s, 3H), 1.90 – 1.70 (m, 3H), 1.63 – 1.49 (m, 3H), 1.44 – 1.33 (m, 4H), 1.29 (s, 9H), 1.28 (s, 3H), 1.32 – 1.20 (m, 7H), 1.17 – 1.03 (m, 6H), 0.86 (t, *J* = 6.8 Hz, 12H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.0, 149.9, 142.9, 142.8, 130.0, 129.5, 127.5, 125.9, 125.4, 121.4, 121.1, 119.3, 82.1, 76.2, 70.1, 62.4, 59.9, 49.4, 40.3, 40.2, 39.5, 37.6, 37.4, 32.9, 32.8, 31.9, 31.2, 28.1, 27.1, 24.9, 24.6, 24.4, 24.3, 22.8, 22.7, 22.6, 21.1, 19.8, 19.7, 16.2. HRMS (ESI): m/z calcd. For $[C_{43}H_{66}NO_5, M+H]^+$ 676.4936, found: 676.4935.

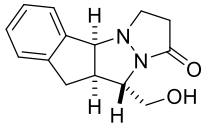
<Chromatogram>



<Peak Table>

Detector A 254nm

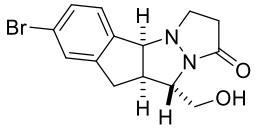
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	3.751	3565131	191750	51.645	51.645
2	4.448	3338006	181596	48.355	48.355
Total		6903136	373346		100.000



4aa

10-(hydroxymethyl)-2,3,4a,9,9a,10-hexahydro-1H-indeno[1,2-c]pyrazolo[1,2-a]pyrazol-1-one

Eluent: DCM: Methanol = 20:1, white solid (18.5 mg, 76%, m.p. 124 - 126 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.15 (m, 4H), 5.31 (s, 1H), 4.12 (d, *J* = 8.4 Hz, 1H), 3.92 (d, *J* = 12.4 Hz, 1H), 3.83 (dd, *J* = 12.4, 8.8 Hz, 1H), 3.74 – 3.69 (m, 1H), 3.55 – 3.48 (m, 1H), 3.15 (dd, *J* = 16.0, 8.8 Hz, 1H), 3.10 – 3.01 (m, 2H), 2.91 (dd, *J* = 16.4, 4.0 Hz, 1H), 2.88 – 2.78 (m, 1H), 2.69 (ddd, *J* = 16.0, 8.4, 2.0 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.1, 142.3, 139.9, 129.1, 127.4, 125.6, 124.8, 74.9, 64.4, 62.6, 52.7, 48.1, 36.3, 36.2. HRMS (ESI): m/z calcd. For $[C_{14}H_{16}N_2O_2, M+H]^+$ 267.1104, found: 267.1100.

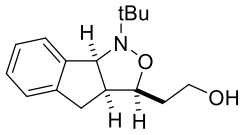


4ba

7-bromo-10-(hydroxymethyl)-2,3,4a,9,9a,10-hexahydro-1H-indeno[1,2-c]pyrazolo[1,2-a]pyrazol-1-one

Eluent: DCM: Methanol = 20:1, brown solid (22.6 mg, 70%, m.p. 178 - 180 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.4 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 1H), 5.22 (s, 1H), 4.05 (d, *J* = 8.0 Hz, 1H), 3.98 – 3.88 (m, 1H), 3.86 – 3.78 (m, 1H), 3.70 (t, *J* = 8.8 Hz, 1H), 3.49 (t, *J* = 7.2 Hz, 1H), 3.18 – 3.01 (m, 3H), 2.93 – 2.78 (m, 2H), 2.69 (dd, *J* = 16.0, 8.4 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.2, 144.6,

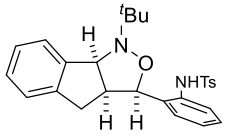
139.2, 130.6, 128.7, 126.3, 123.1, 74.2, 64.2, 62.4, 52.7, 48.2, 36.3, 35.9. HRMS (ESI): m/z calcd. For $[C_{15}H_{15}BrN_2NaO_2, M+Na]^+$ 345.0209, found: 345.0204.



3ab

2-(1-(tert-butyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)ethan-1-ol

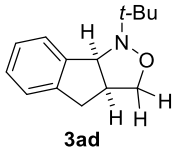
Eluent: PE: EA = 2:1, yellow oil (8.0 mg, 31%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (dt, *J* = 8.0, 4.0 Hz, 1H), 7.15 – 7.07 (m, 3H), 4.80 (d, *J* = 8.0 Hz, 1H), 4.39 (ddd, *J* = 10.0, 7.2, 3.2 Hz, 1H), 3.66 (ddd, *J* = 16.4, 9.2, 4.8 Hz, 2H), 3.40 (ddd, *J* = 15.6, 7.6, 4.0 Hz, 1H), 3.03 (dd, *J* = 16.2, 4.4 Hz, 1H), 2.88 (dd, *J* = 16.4, 8.4 Hz, 1H), 1.69 – 1.62 (m, 1H), 1.56 – 1.46 (m, 1H), 1.19 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.4, 142.5, 127.9, 127.0, 125.3, 124.2, 80.9, 69.4, 61.6, 59.6, 51.7, 33.4, 32.0, 27.0. HRMS (ESI): m/z calcd. For $[C_{16}H_{23}NNaO_2, M+Na]^+$ 284.1621, found: 284.1611.



3ac

N-(2-(1-(tert-butyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazol-3-yl)phenyl)-4-methylbenzene sulfonamide

Eluent: PE: EA = 6:1, yellow oil (28.2 mg, 61%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (s, 1H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.50 (d, *J* = 8.8 Hz, 2H), 7.32 – 7.28 (m, 1H), 7.26 – 7.20 (m, 3H), 7.10 – 7.06 (m, 1H), 7.04 – 6.99 (m, 2H), 6.96 (d, *J* = 8.0 Hz, 2H), 4.75 (d, *J* = 8.4 Hz, 1H), 3.94 (d, *J* = 10.0 Hz, 1H), 3.04 (dd, *J* = 17.2, 8.0 Hz, 1H), 2.89 (dd, *J* = 16.8, 7.6 Hz, 1H), 2.43 – 2.37 (m, 1H), 2.24 (s, 3H), 1.27 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.4, 140.4, 137.1, 137.0, 129.4, 129.3, 128.0, 127.7, 127.6, 127.3, 126.9, 126.4, 125.9, 125.3, 124.3, 121.7, 81.7, 69.0, 58.6, 49.2, 32.3, 26.4, 21.5. HRMS (ESI): m/z calcd. For $[C_{27}H_{31}N_2O_2S, M+H]^+$ 463.2050, found: 463.2050.



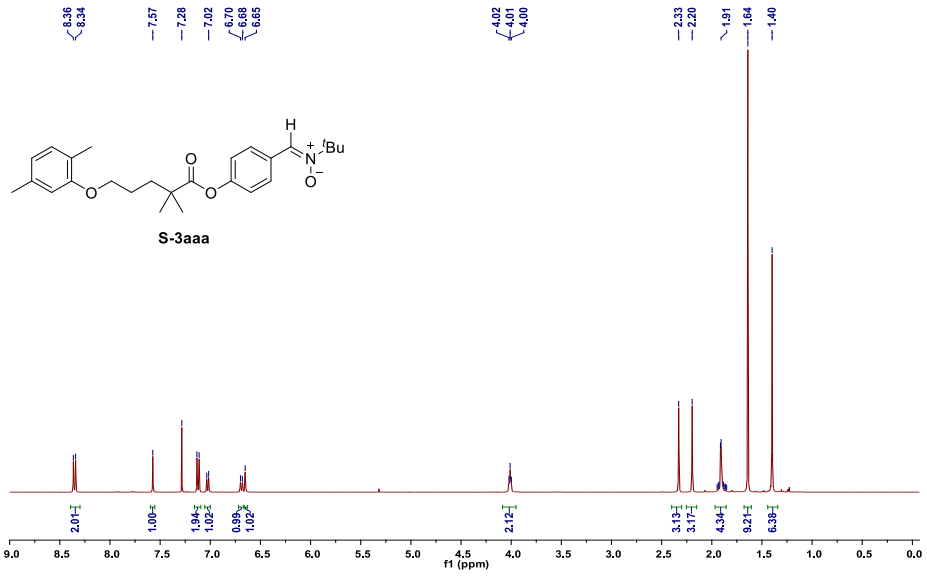
3ad

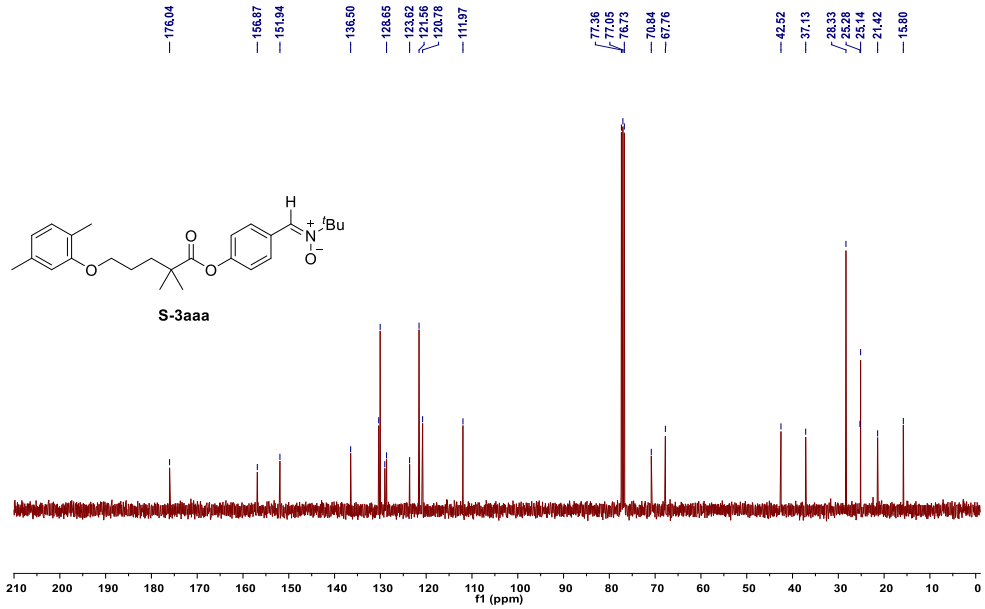
1-(tert-butyl)-3,3a,4,8b-tetrahydro-1H-indeno[1,2-c]isoxazole

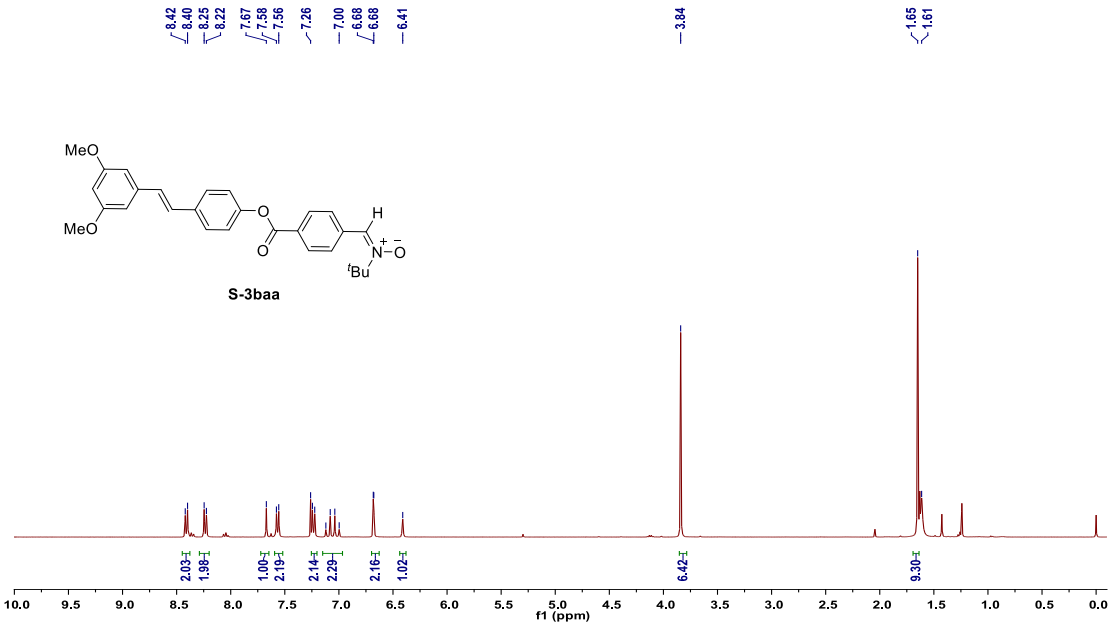
Eluent: PE: EA = 4:1, yellow oil (15.0 mg, 69%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.23 (m, 1H), 7.19 – 7.07 (m, 3H), 4.71 (d, *J* = 8.0 Hz, 1H), 4.20 (t, *J* = 7.6 Hz, 1H), 3.32 (t, *J* = 8.0 Hz, 1H), 3.28 –

3.17 (m, 1H), 3.05 (dd, *J* = 16.4, 7.2 Hz, 1H), 2.76 (d, *J* = 16.4 Hz, 1H), 1.18 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.8, 140.9, 127.9, 127.4, 125.8, 125.0, 73.7, 68.9, 58.9, 47.2, 34.6, 26.7. HRMS (ESI): m/z calcd. For $[C_{14}H_{20}NO, M+H]^+$ 281.1539, found: 281.1539

8. NMR Spectrum and Mass Spectrogr



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6.68
6.41
3.84
1.65
1.61
MeO
MeO
O
O
H
N+
O−
tBu
S-3baa
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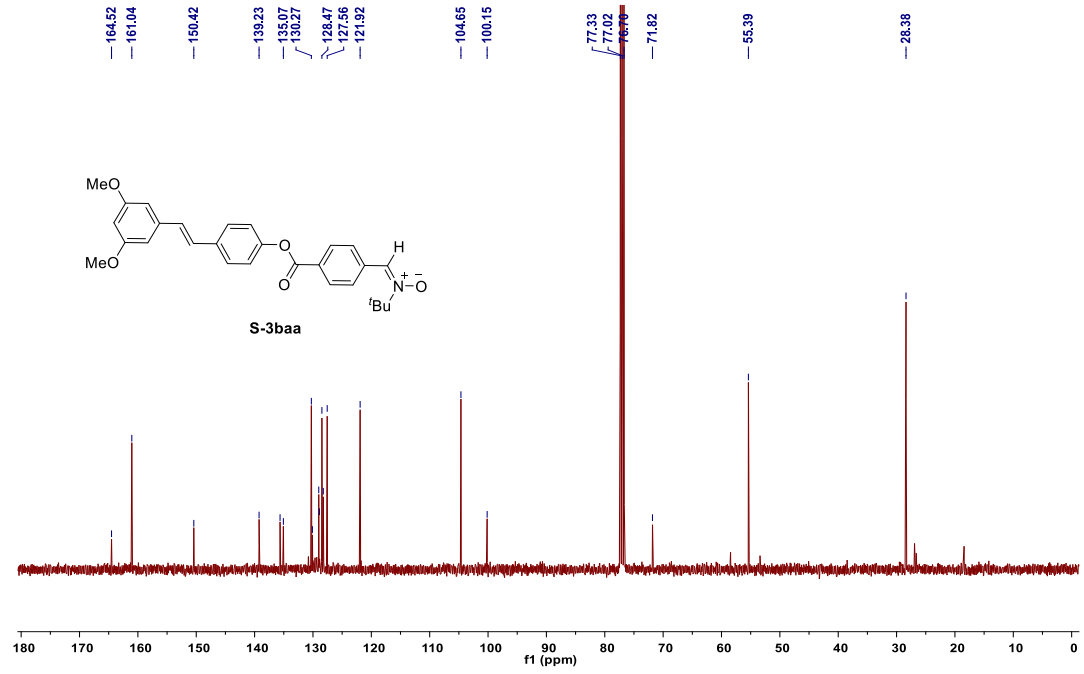
1.00
2.19
2.14
2.29
2.16
1.02
6.42
9.30
f1 (ppm)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130.27
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127.56
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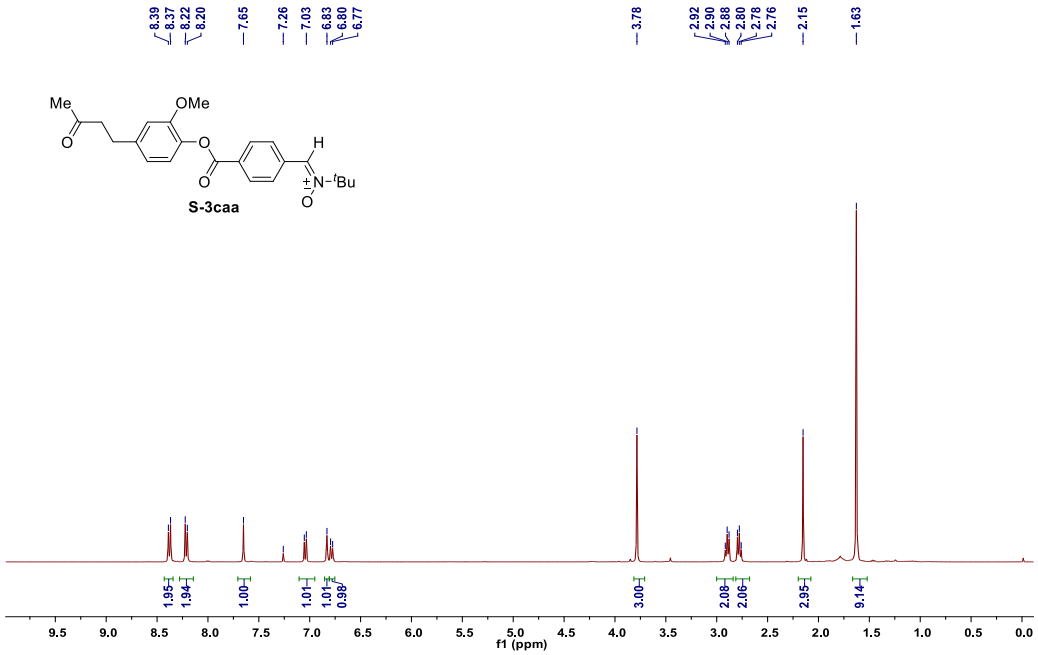
104.65
100.15
77.33
77.02
76.70
71.82
55.39
28.38
MeO
MeO
O
O
H
N+
O−
tBu
S-3baa
f1 (ppm)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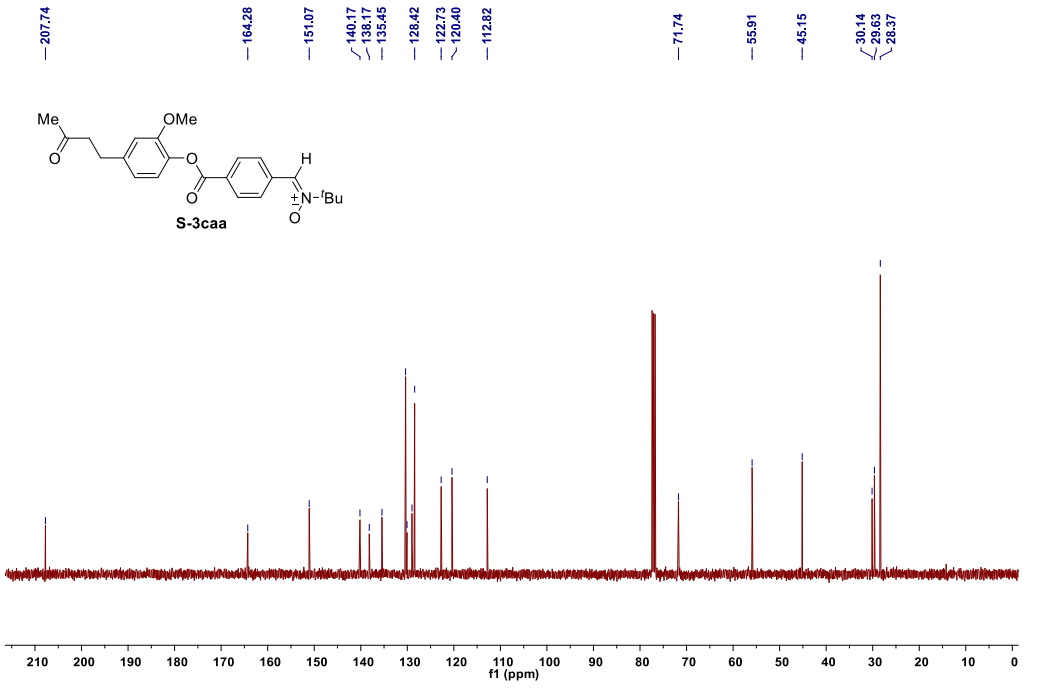
2.90
2.88
2.80
2.78
2.76
2.15
1.63
Me
OMe
O
O
O
H
N
tBu
O
S-3caa
1.95
1.94
1.00
1.01
1.01
0.98
3.00
2.08
2.06
2.95
9.14
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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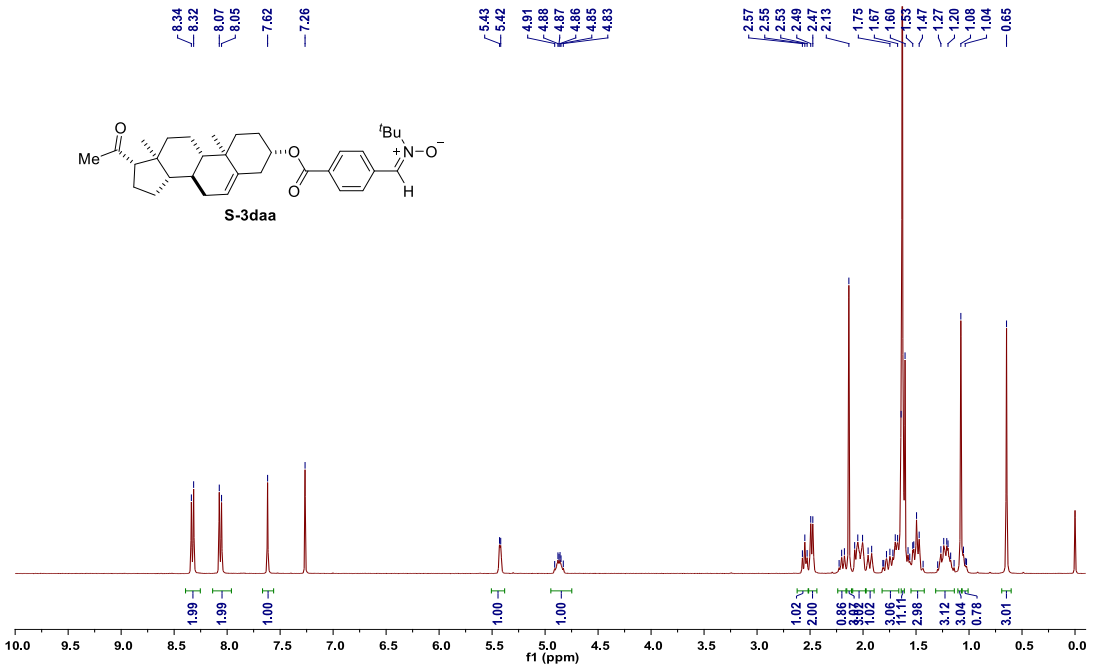
135.45
128.42
122.73
120.40
112.82
71.74
55.91
45.15
30.14
29.63
28.37
Me
OMe
O
O
O
H
N
tBu
O
S-3caa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.07
8.05
7.62
7.26
5.43
5.42
4.91
4.88
4.87
4.86
4.85
4.83
2.57
2.55
2.53
2.49
2.47
2.13
1.75
1.67
1.60
1.53
1.47
1.27
1.20
1.08
1.04
0.65
Me
O
O
O
tBu
+N−O−
H
S-3daa
1.99
1.99
1.00
1.00
1.00
1.02
2.00
0.86
3.02
3.02
1.02
3.06
11.14
2.98
3.12
3.04
0.78
3.01
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9.0
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8.0
7.5
7.0
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6.0
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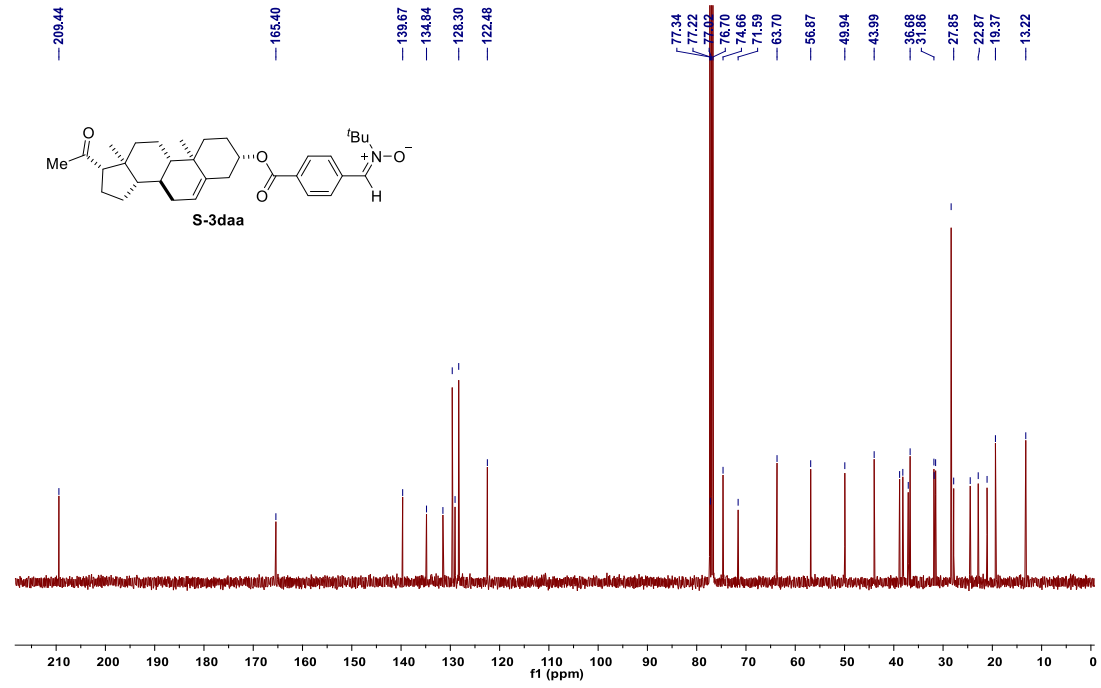
0.0
f1 (ppm)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77.22
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76.70
74.66
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63.70
56.87
49.94
43.99
36.68
31.86
27.85
22.87
19.37
13.22
Me
O
O
O
tBu
+N−O−
H
S-3daa
210
200
190
180
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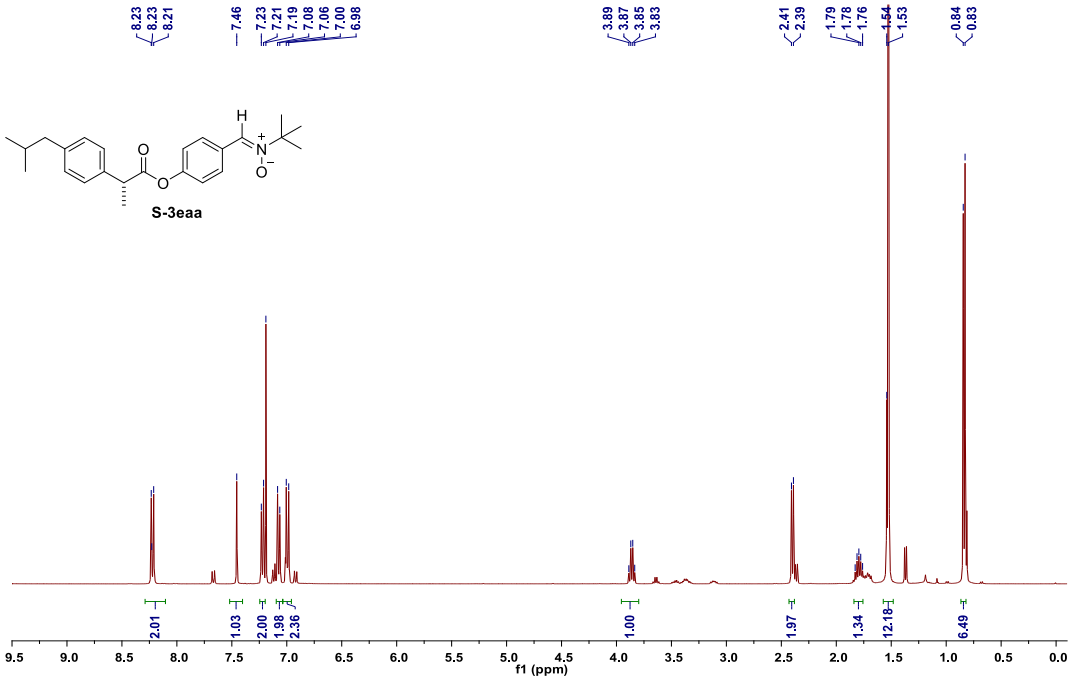
f1 (ppm)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3.87
3.85
3.83
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2.39
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1.78
1.76
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1.53
0.84
0.83
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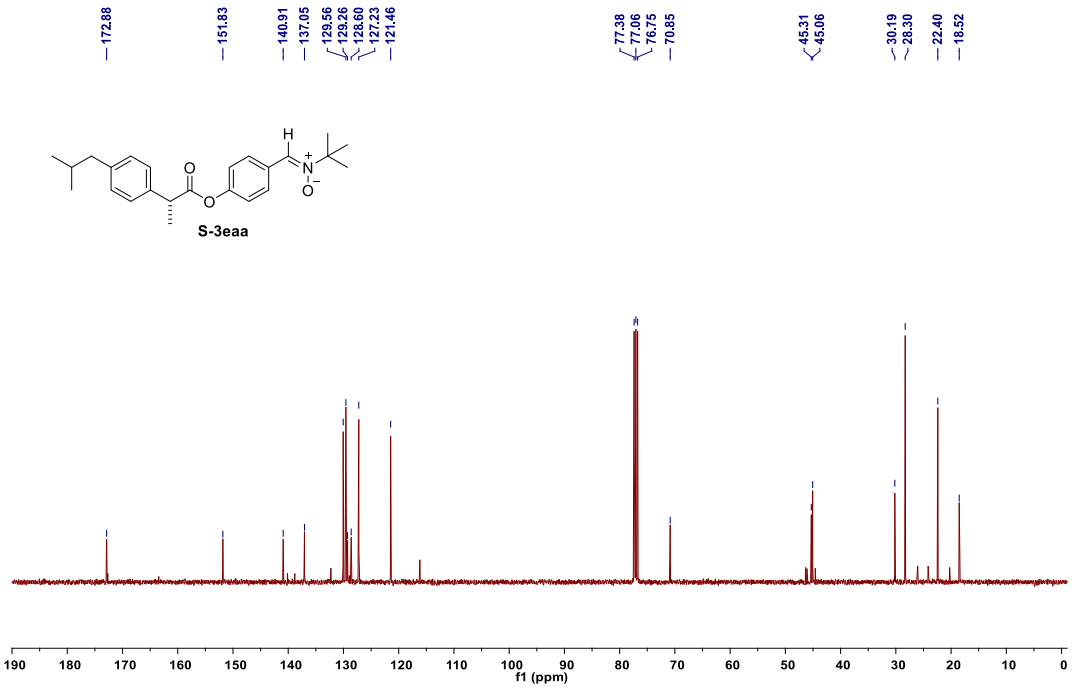
f1 (ppm)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22.40
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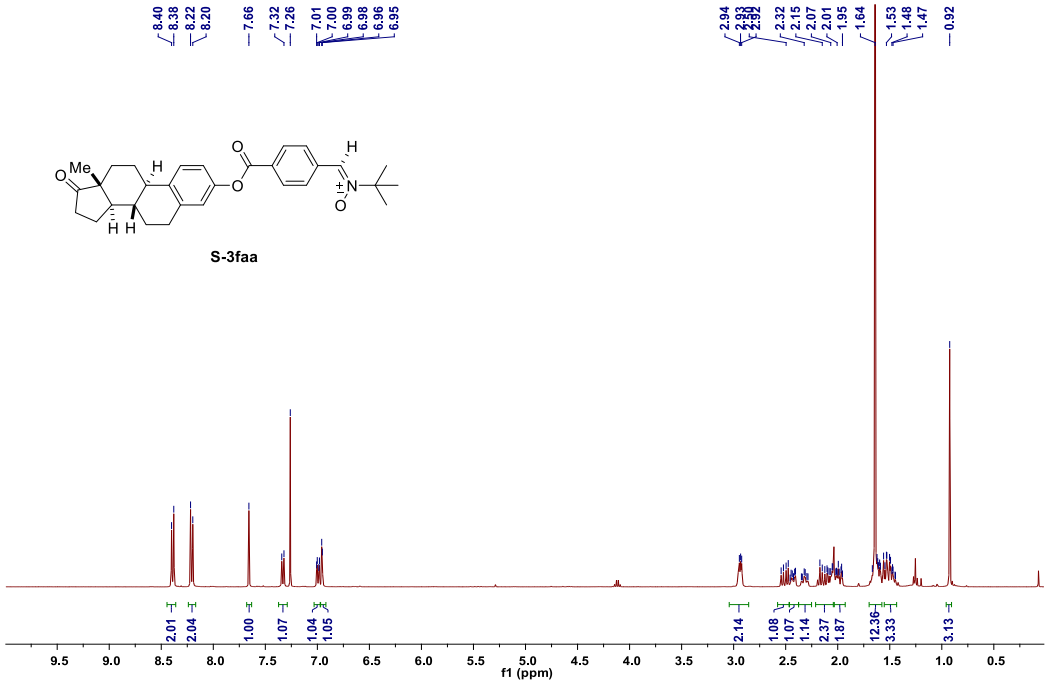
f1 (ppm)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6.95
2.94
2.32
2.15
2.07
2.01
1.95
1.64
1.53
1.48
1.47
0.92
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O
H
H H
O
O
H
N
O
S-3faa
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2.04
1.00
1.07
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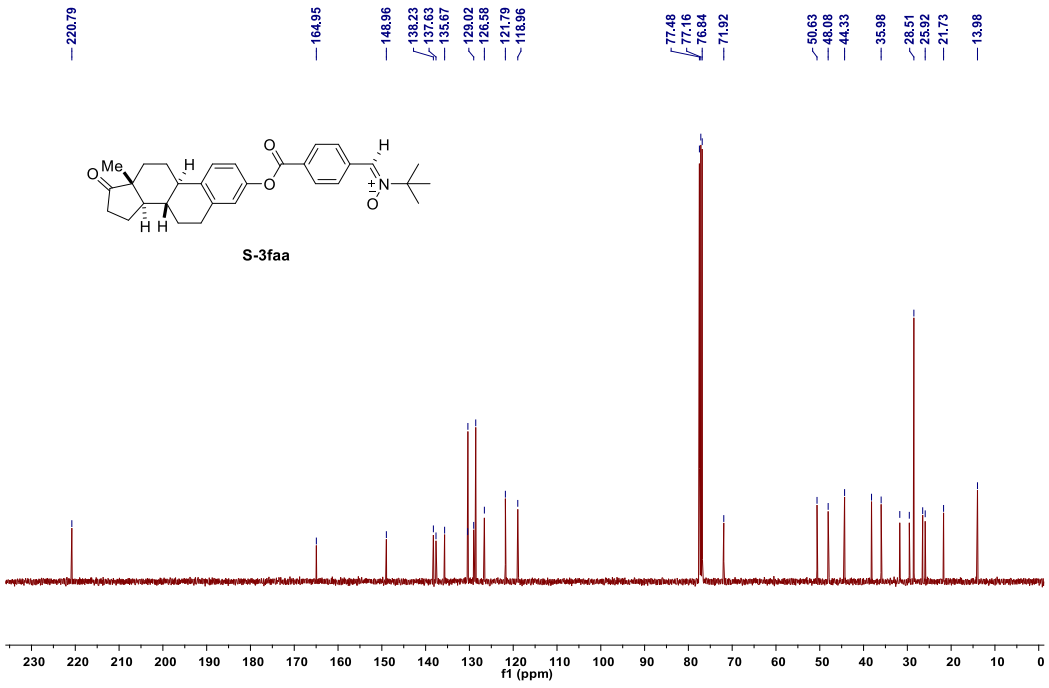
f1 (ppm)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48.08
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35.98
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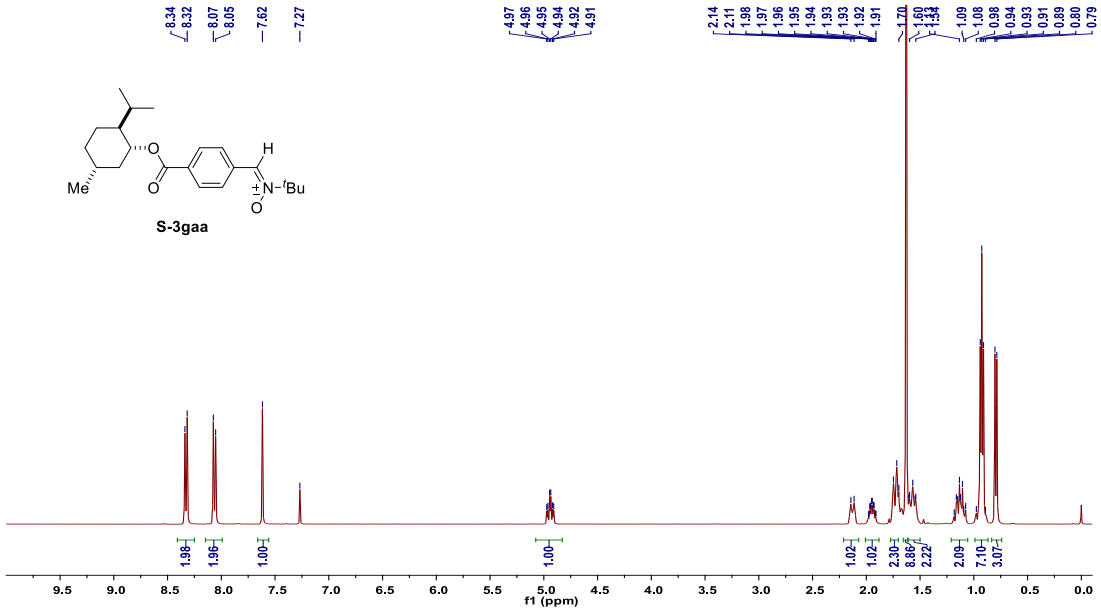
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0.94
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O
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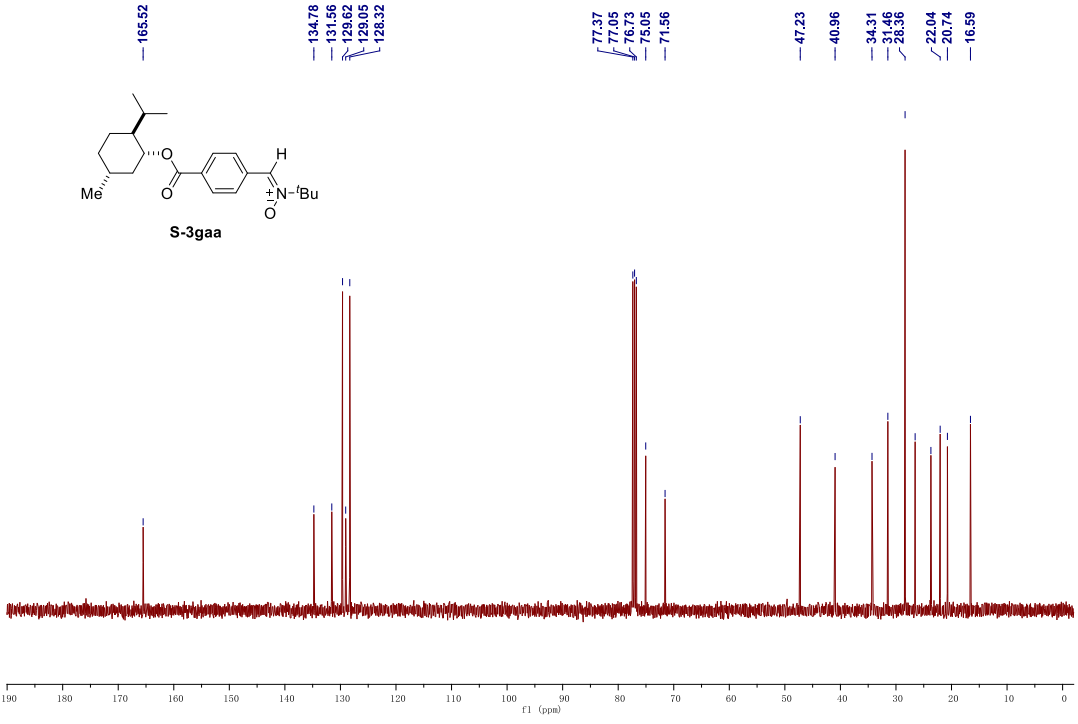
f1 (ppm)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75.05
71.56
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40.96
34.31
31.46
28.36
22.04
20.74
16.59
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H
N-tBu
O
S-3gaa
190
180
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50
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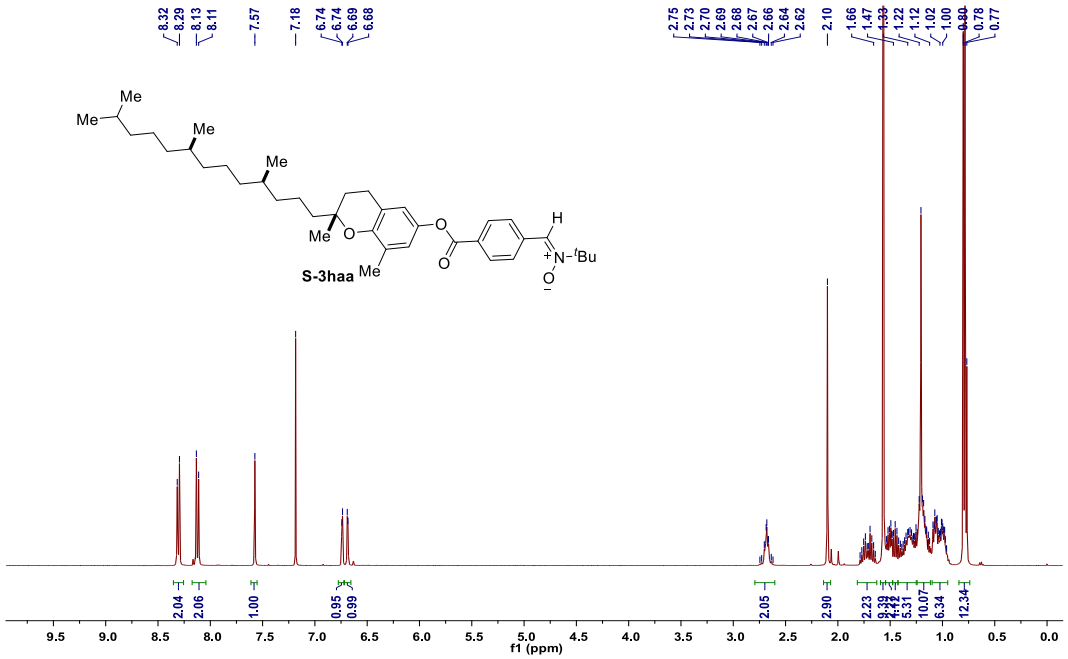
f1 (ppm)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2.62
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O
H
+N
tBu
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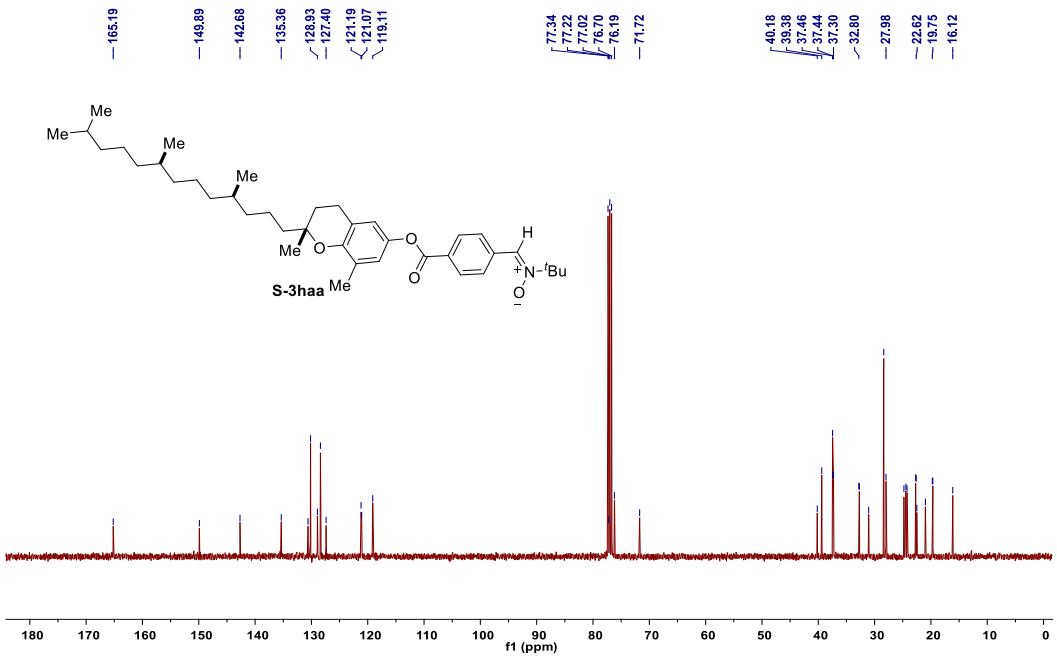
f1 (ppm)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Me
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+N
tBu
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180
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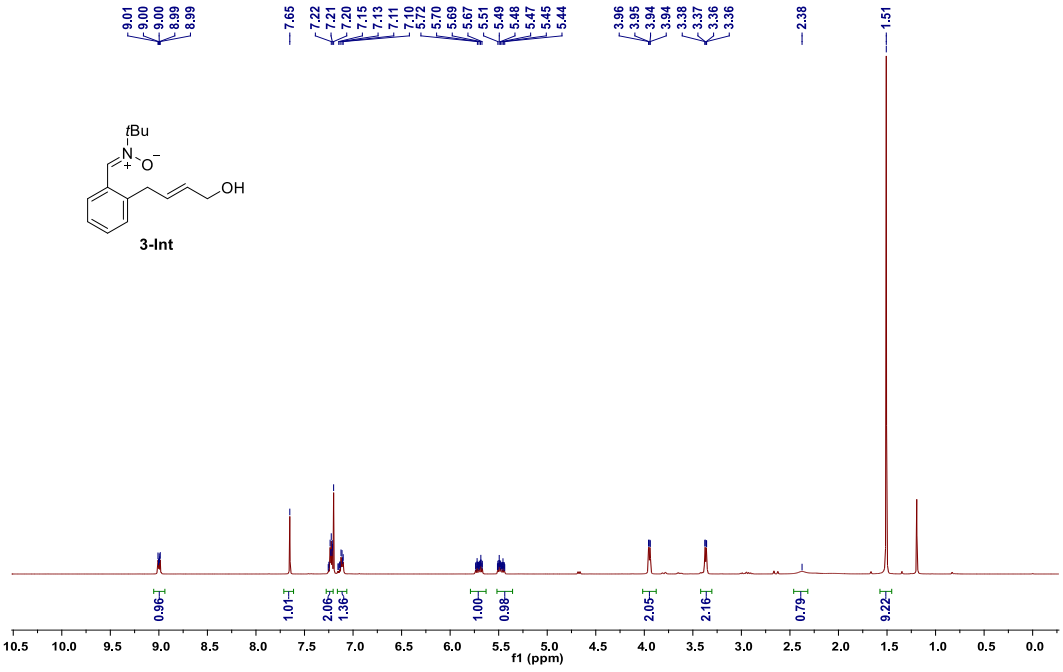
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5.47
5.45
5.44
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3.38
3.37
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3.36
2.38
1.51
tBu
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OH
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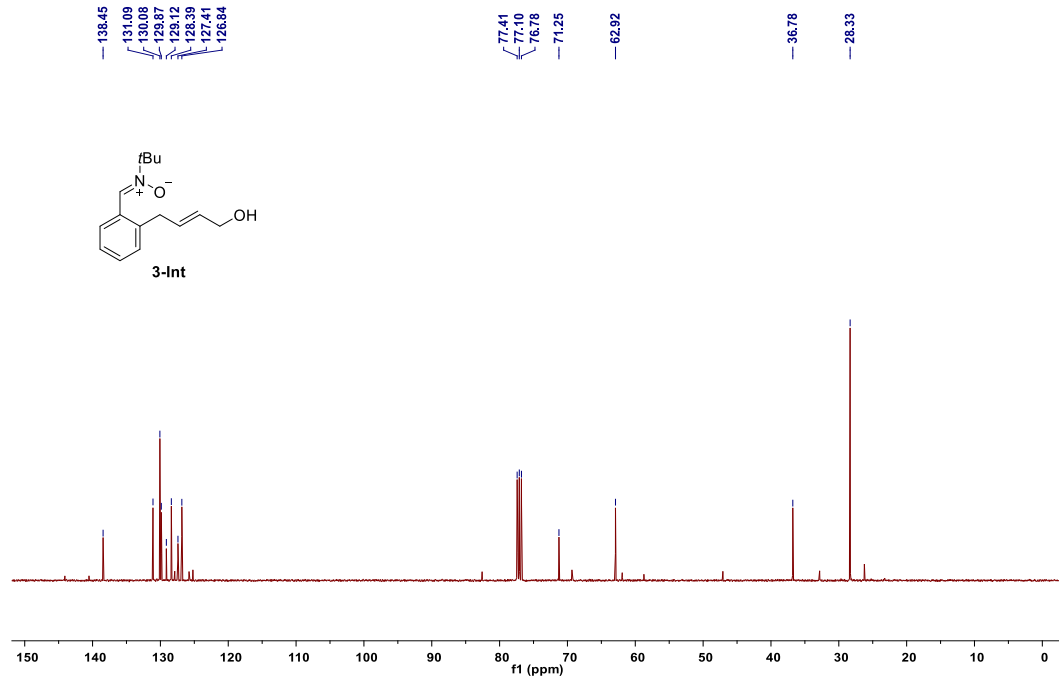
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tBu
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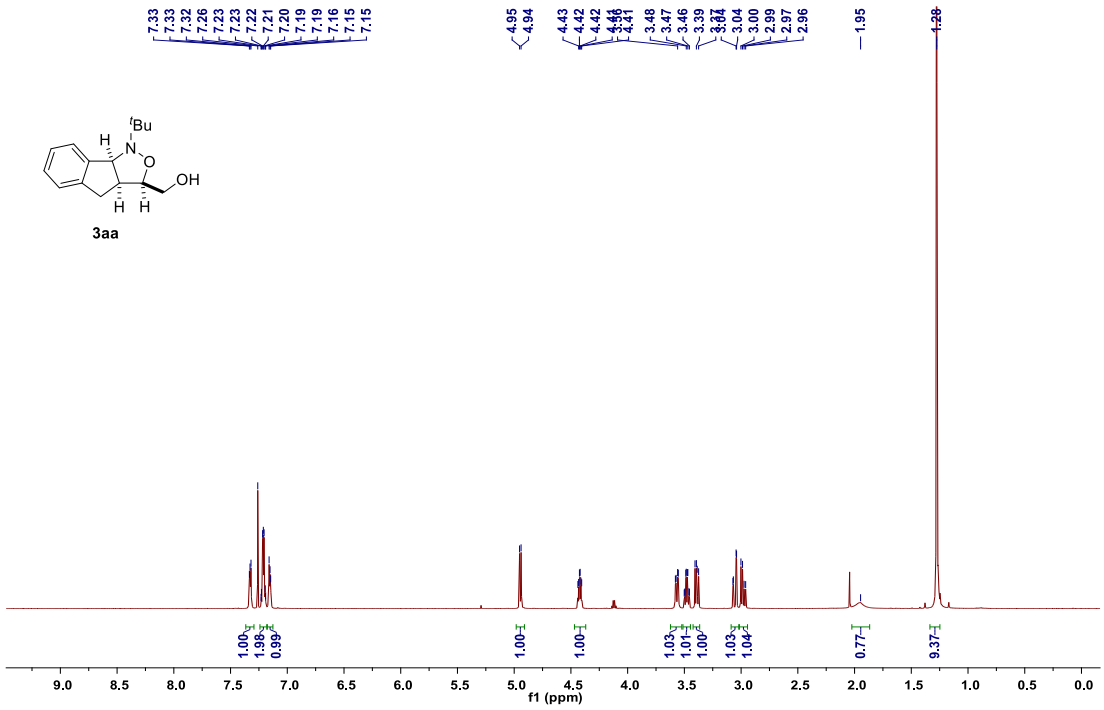
OH
3-Int
f1 (ppm)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2.99
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2.96
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OH
H
H
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1.00
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1.01
1.00
1.03
1.04
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7.0
6.5
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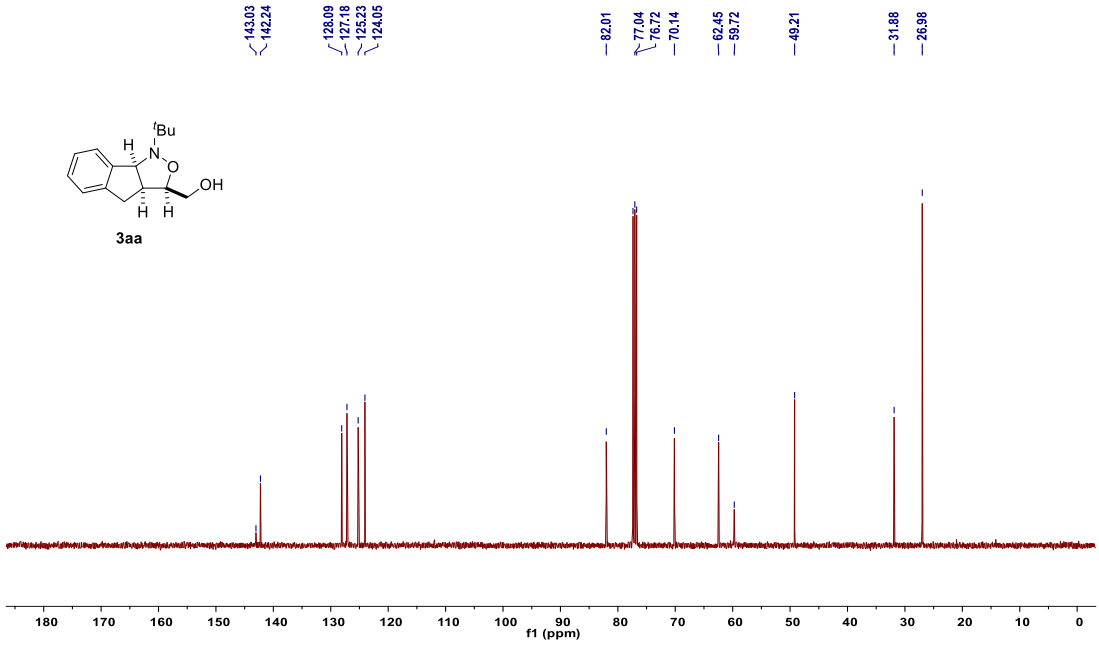
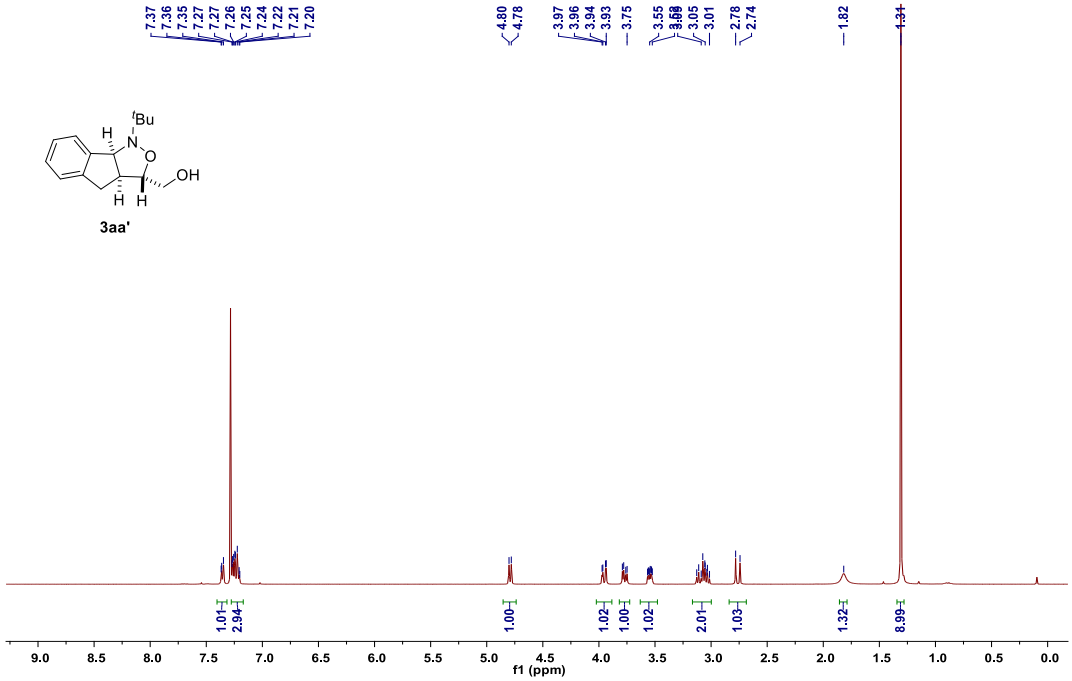
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


143.03
142.24
128.09
127.18
125.23
124.05
82.01
77.04
76.72
70.14
62.45
59.72
49.21
31.88
26.98
tBu
H
N
O
OH
H
H
3aa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.37
7.36
7.35
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7.26
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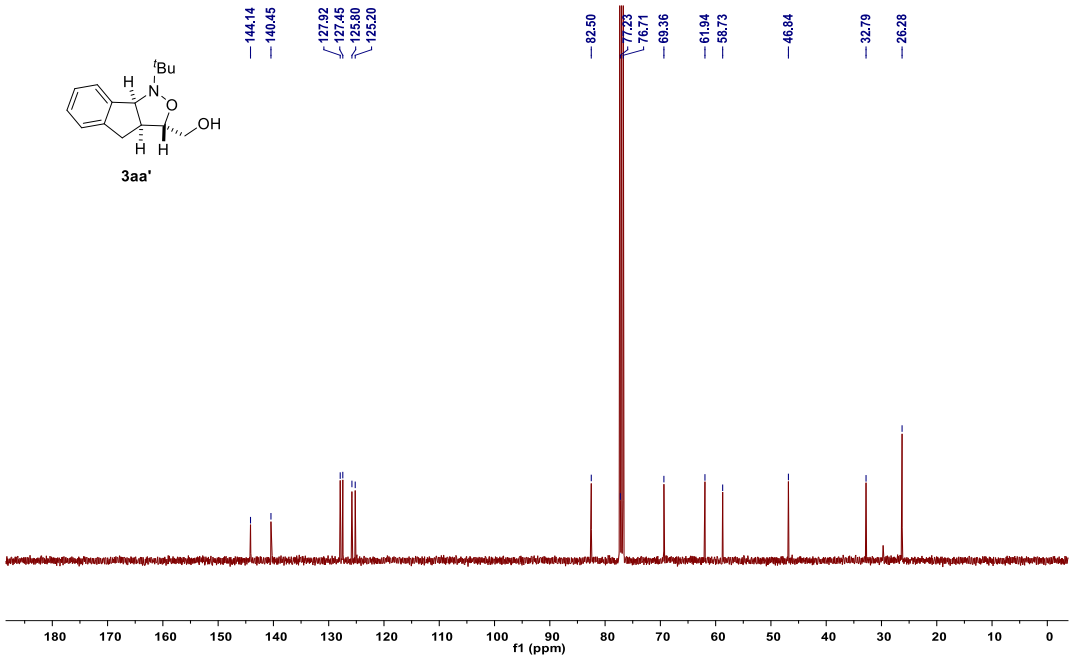
7.24
7.22
7.21
7.20
4.80
4.78
3.97
3.96
3.94
3.93
3.75
3.55
3.05
3.01
2.78
2.74
1.82
1.31
tBu
H
N
O
OH
H H
3aa'
1.01
2.94
1.00
1.02
1.00
1.02
2.01
1.03
1.32
8.99
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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140.45
127.92
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125.80
125.20
82.50
77.23
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69.36
61.94
58.73
46.84
32.79
26.28
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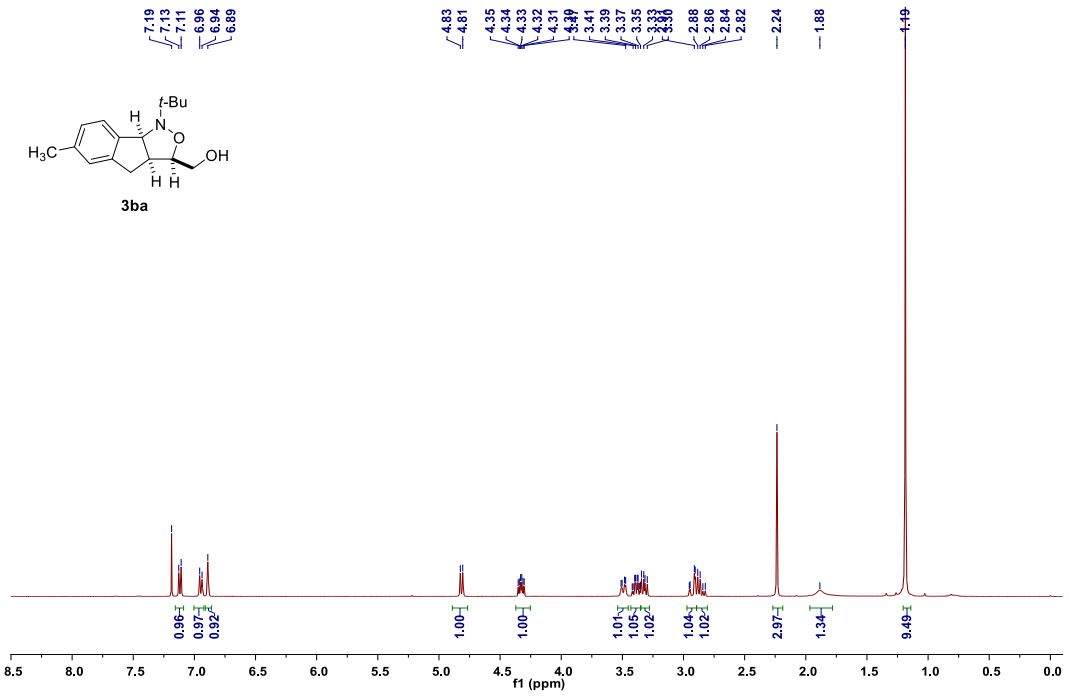
H
N
O
OH
H H
3aa'
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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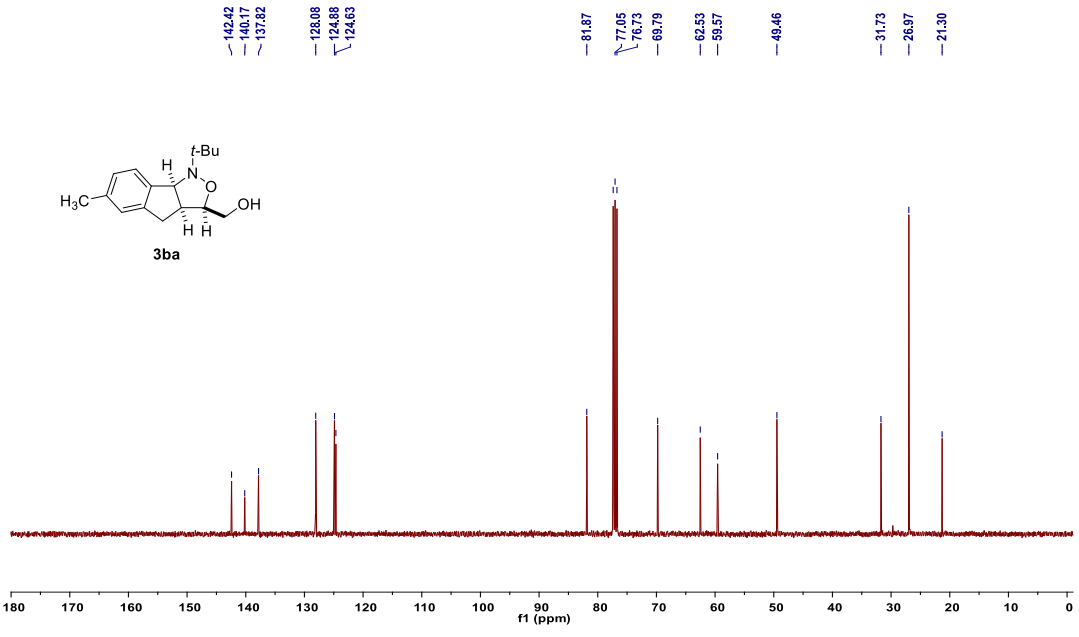
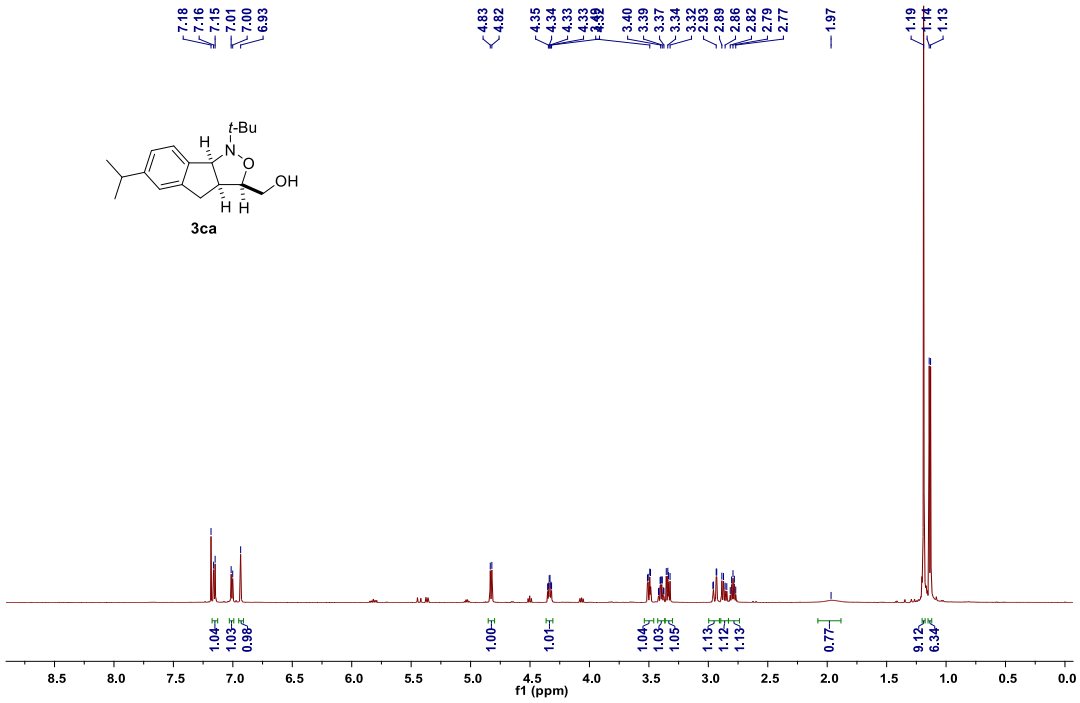
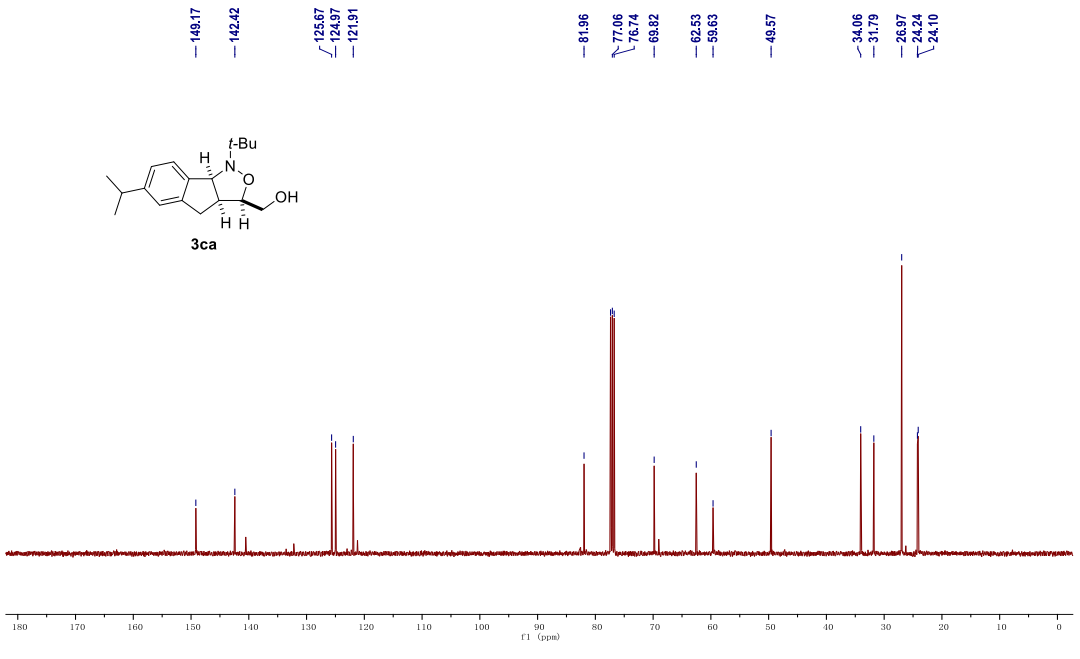
7.13
7.11
6.96
6.94
6.89
4.83
4.81
4.35
4.34
4.33
4.32
4.31
3.41
3.39
3.37
3.35
2.88
2.86
2.84
2.82
2.24
1.88
1.19
t-Bu
H
N
O
H3C
OH
H H
3ba
0.96
0.97
0.92
1.00
1.00
1.01
1.05
1.02
1.04
1.02
2.97
1.34
9.49
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


142.42
140.17
137.82
128.08
124.88
124.63
81.87
77.05
76.73
69.79
62.53
59.57
49.46
31.73
26.97
21.30
t-Bu
H
N
O
H3C
OH
H H
3ba
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.18
7.16
7.15
7.01
7.00
6.93
4.83
4.82
4.35
4.34
4.33
4.33
3.40
3.39
3.37
3.34
3.32
2.93
2.89
2.86
2.82
2.79
2.77
1.97
1.19
1.14
1.13
t-Bu
H
N
O
OH
H H
3ca
1.04
1.03
0.98
1.00
1.01
1.04
1.03
1.05
1.13
1.12
1.13
0.77
9.12
6.34
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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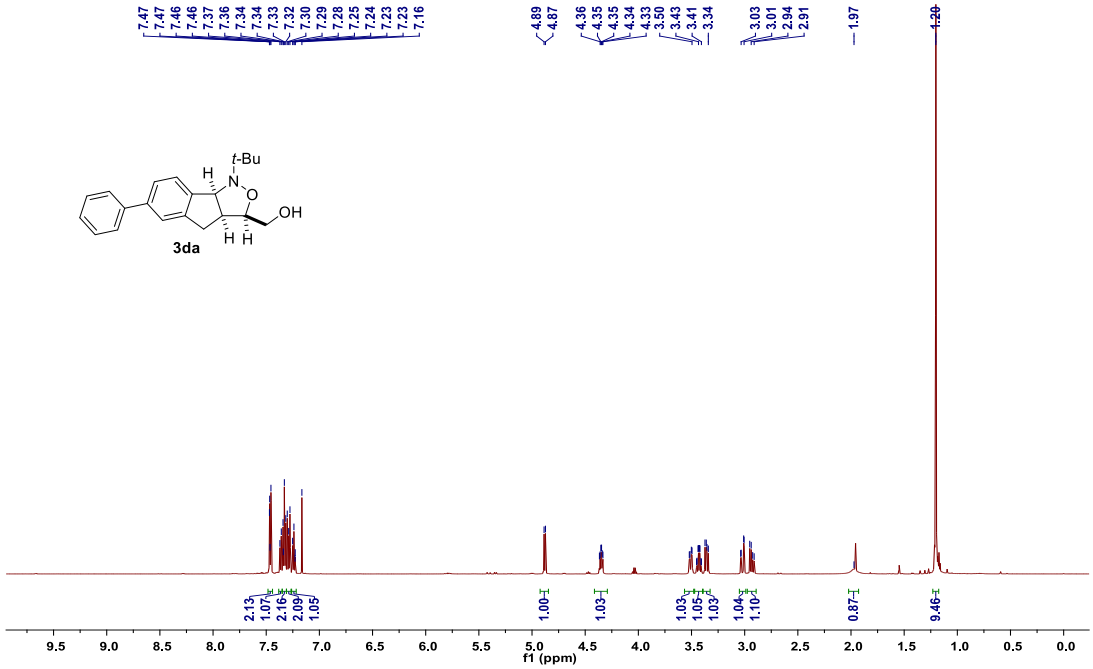
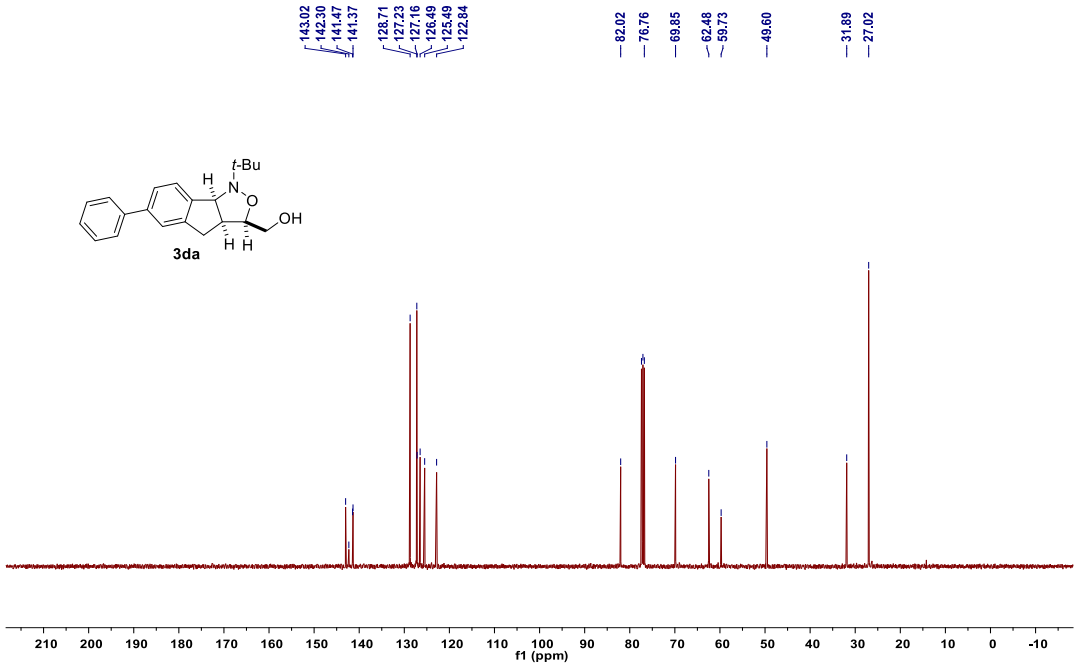
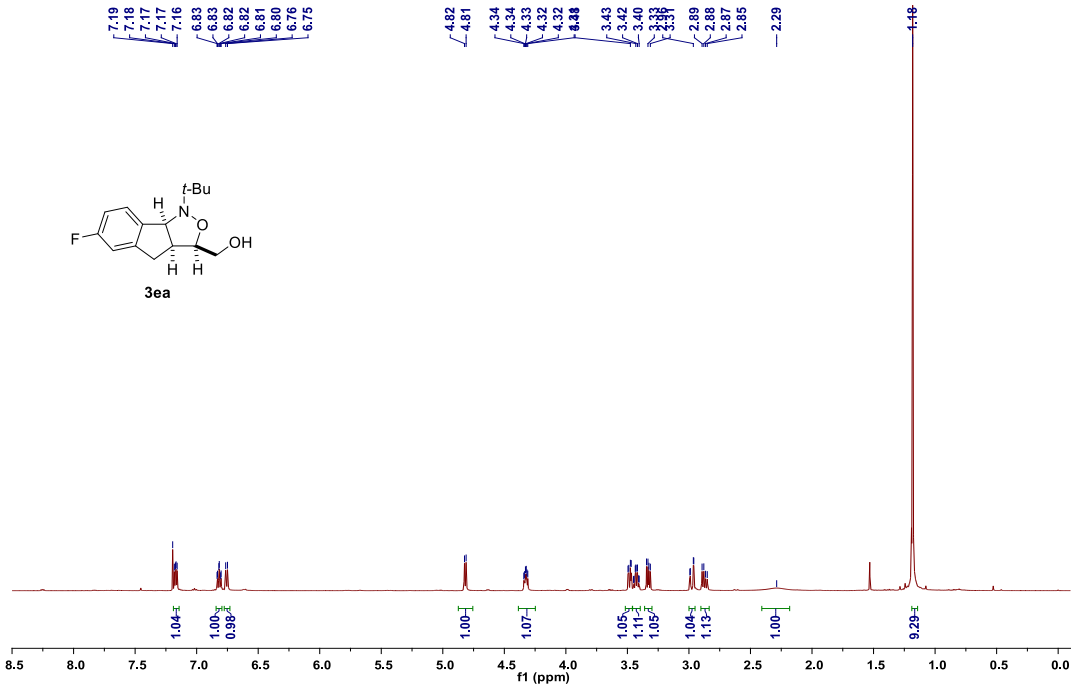
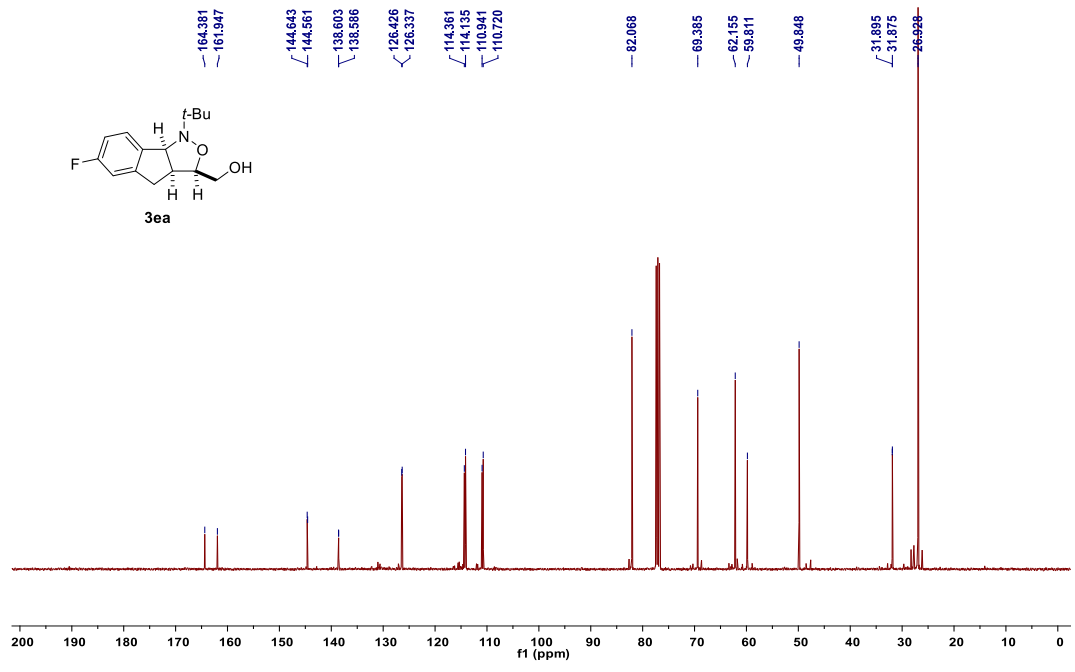
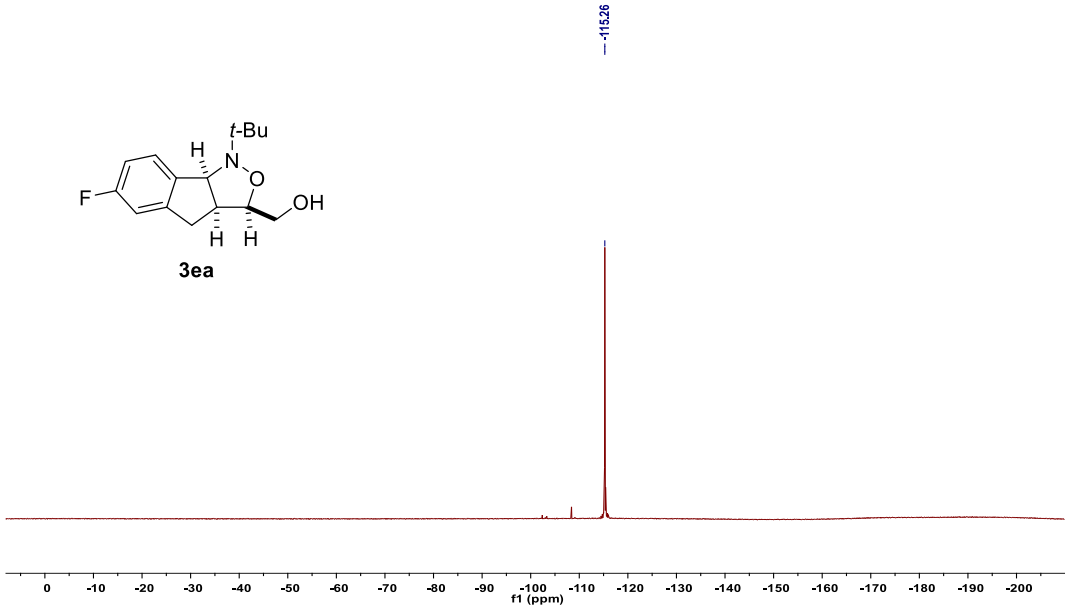
142.42
125.67
124.97
121.91
81.96
77.06
76.74
69.82
62.53
59.63
49.57
34.06
31.79
26.97
24.24
24.10
t-Bu
H
N
O
OH
H H
3ca
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

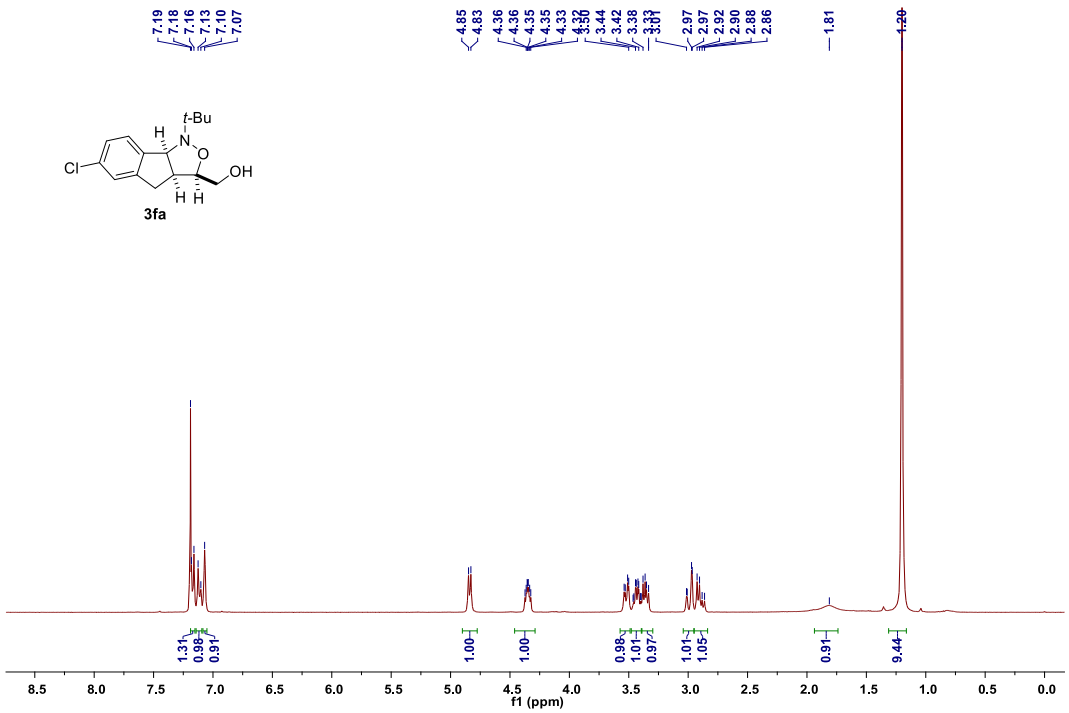

7.47
7.47
7.46
7.46
7.37
7.36
7.34
7.34
7.33
7.32
7.30
7.29
7.28
7.25
7.24
7.23
7.23
7.16
4.89
4.87
4.36
4.35
4.35
4.34
4.33
3.50
3.43
3.41
3.34
3.03
3.01
2.94
2.91
1.97
1.20
t-Bu
H
N
O
OH
H H
3da
2.13
1.07
2.16
2.09
1.05
1.00
1.03
1.03
1.05
1.03
1.04
1.10
0.87
9.46
f1 (ppm)

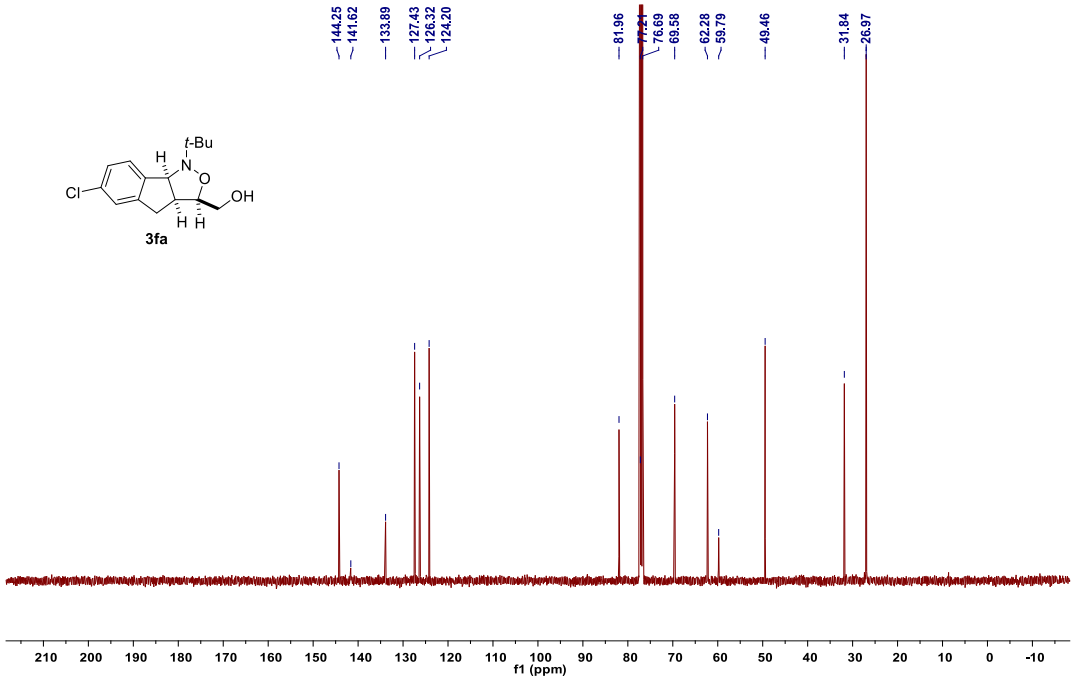

143.02
142.30
141.47
141.37
128.71
127.23
127.16
126.49
125.49
122.84
82.02
76.76
69.85
62.48
59.73
49.60
31.89
27.02
t-Bu
H
N
O
OH
H H
3da
f1 (ppm)

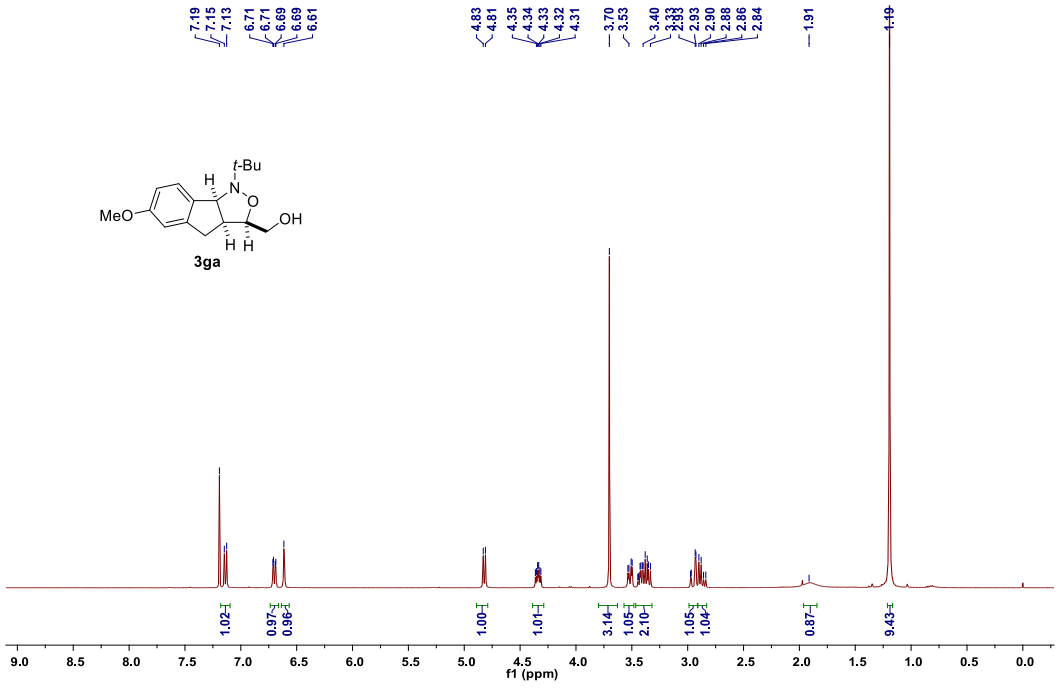

7.19
7.18
7.17
7.17
7.16
6.83
6.83
6.82
6.82
6.81
6.80
6.76
6.75
4.82
4.81
4.34
4.34
4.33
4.32
4.32
3.43
3.42
3.40
3.33
2.89
2.88
2.87
2.85
2.29
1.18
t-Bu
H
N
O
F
OH
H
H
3ea
1.04
1.00
0.98
1.00
1.07
1.05
1.11
1.05
1.04
1.13
1.00
9.29
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

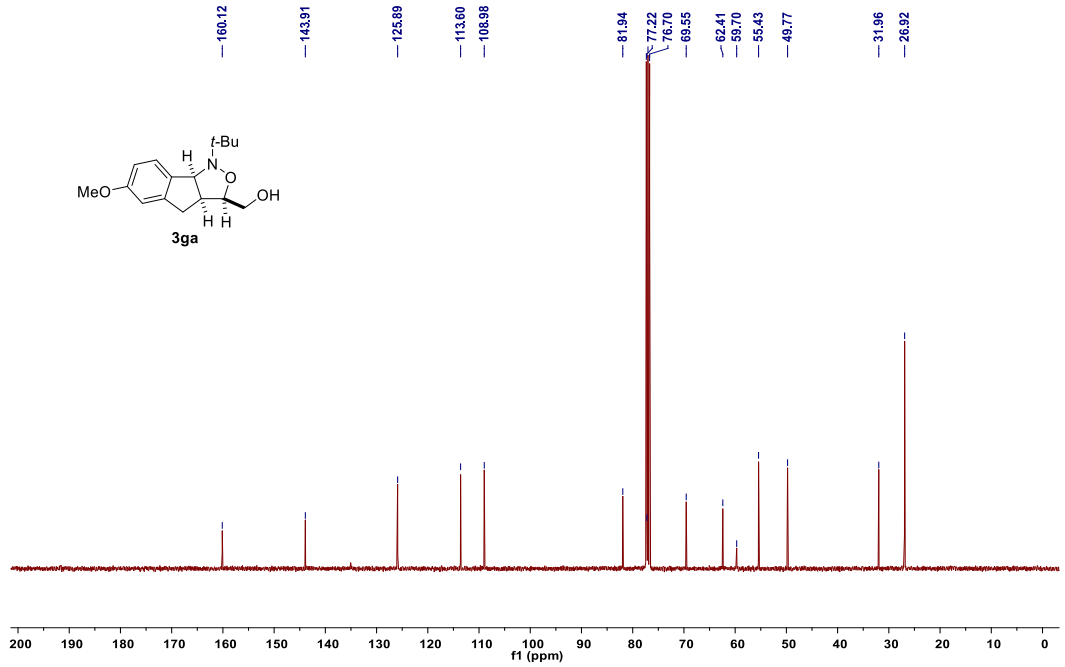

164.381
161.947
144.643
144.561
138.603
138.586
126.426
126.337
114.361
114.135
110.941
110.720
82.068
69.385
62.155
59.811
49.848
31.895
31.875
26.028
t-Bu
H
N
O
F
OH
H
H
3ea
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

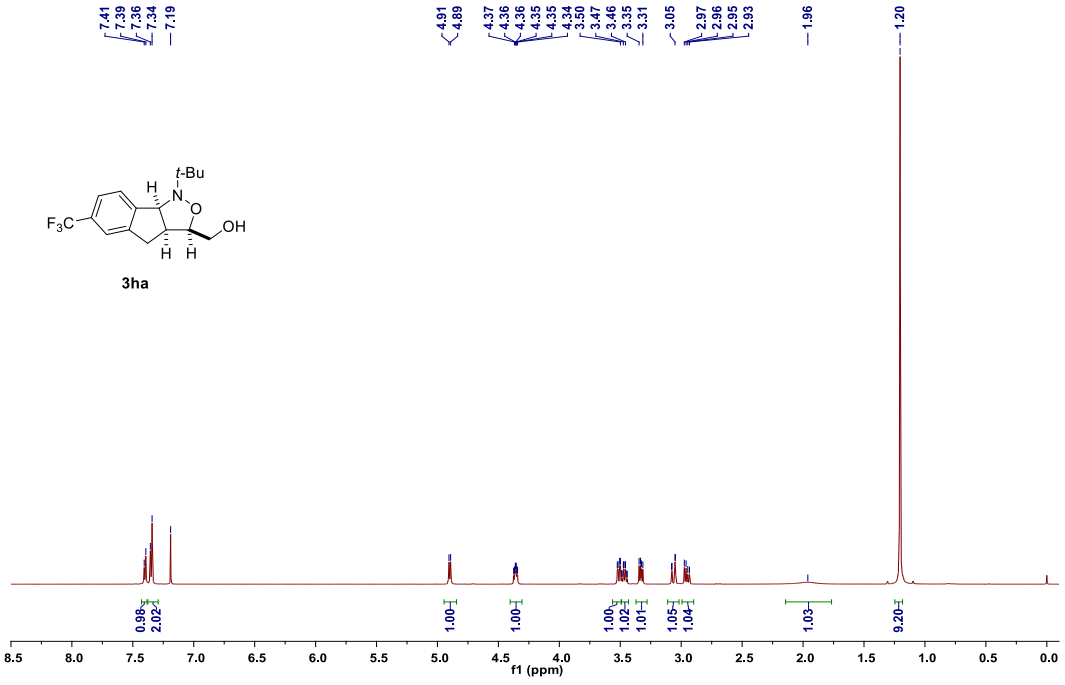

-115.26
t-Bu
H
N
O
F
OH
H
H
3ea
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)


7.19
7.18
7.16
7.13
7.10
7.07
4.85
4.83
4.36
4.36
4.35
4.35
4.33
3.50
3.44
3.42
3.38
3.33
3.01
2.97
2.97
2.92
2.90
2.88
2.86
1.81
1.20
t-Bu
H
N
O
Cl
OH
H
H
3fa
1.31
0.98
0.91
1.00
1.00
0.98
1.01
0.97
1.01
1.05
0.91
9.44
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


144.25
141.62
133.89
127.43
126.32
124.20
81.96
77.21
76.69
69.58
62.28
59.79
49.46
31.84
26.97
t-Bu
H
N
O
Cl
OH
H H
3fa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.19
7.15
7.13
6.71
6.71
6.69
6.69
6.61
4.83
4.81
4.35
4.34
4.33
4.32
4.31
3.70
3.53
3.40
2.93
2.90
2.88
2.86
2.84
1.91
1.49
t-Bu
H
N
O
MeO
OH
H H
3ga
1.02
0.97
0.96
1.00
1.01
3.14
1.05
2.10
1.05
1.04
0.87
9.43
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


160.12
143.91
125.89
113.60
108.98
81.94
77.22
76.70
69.55
62.41
59.70
55.43
49.77
31.96
26.92
t-Bu
H
N
O
MeO
OH
H H
3ga
f1 (ppm)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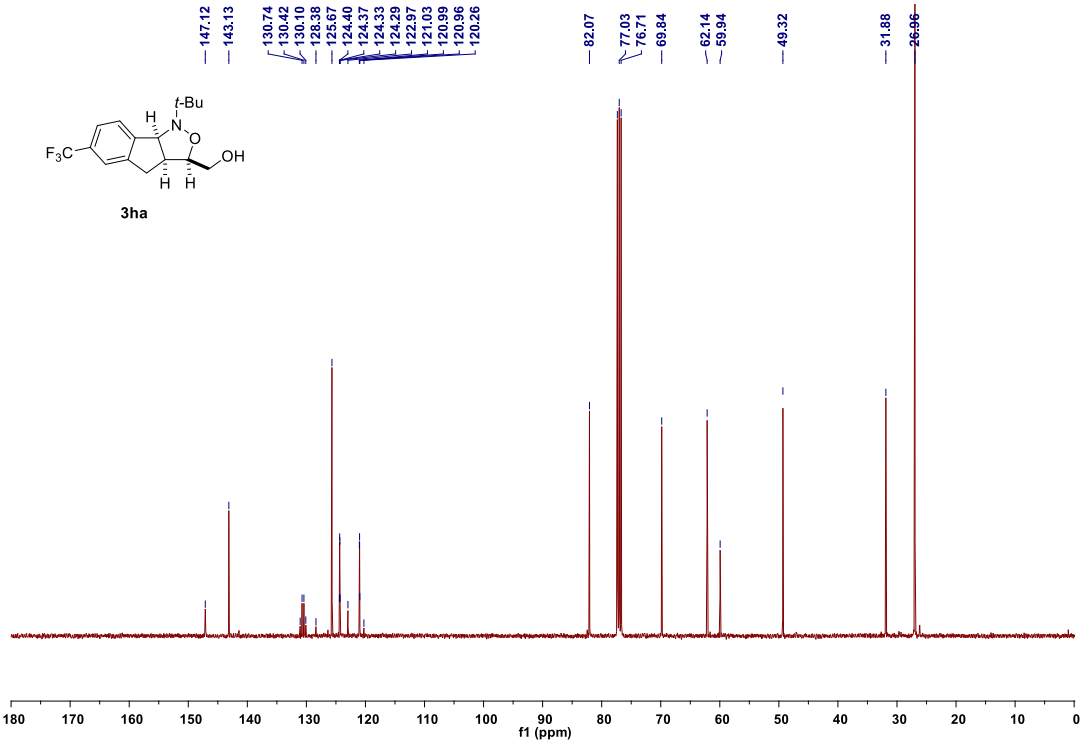
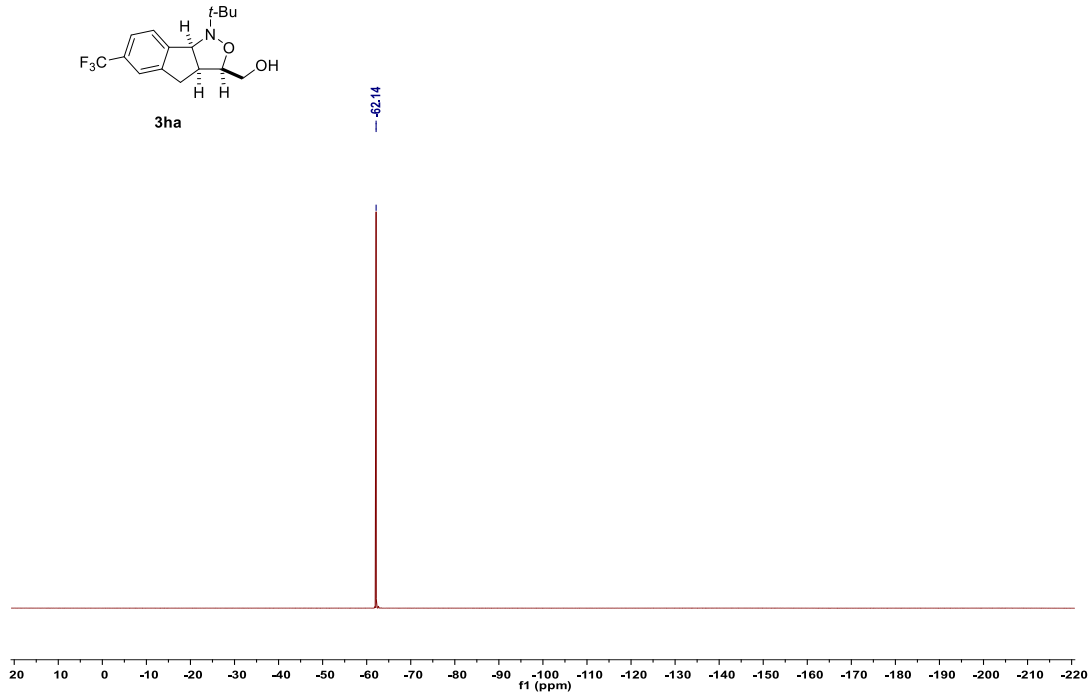
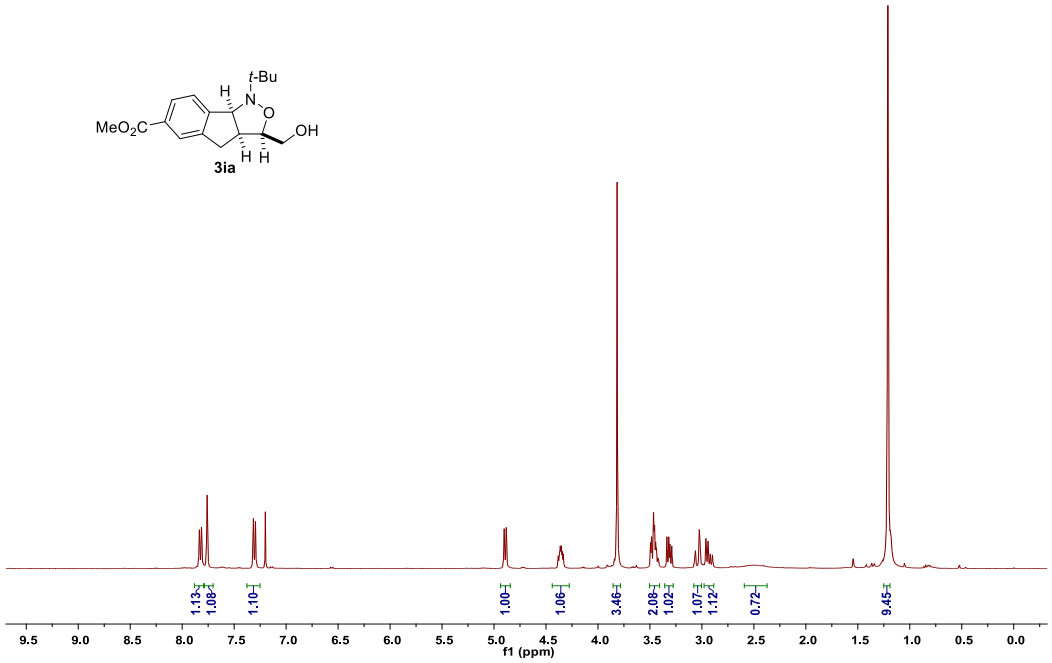
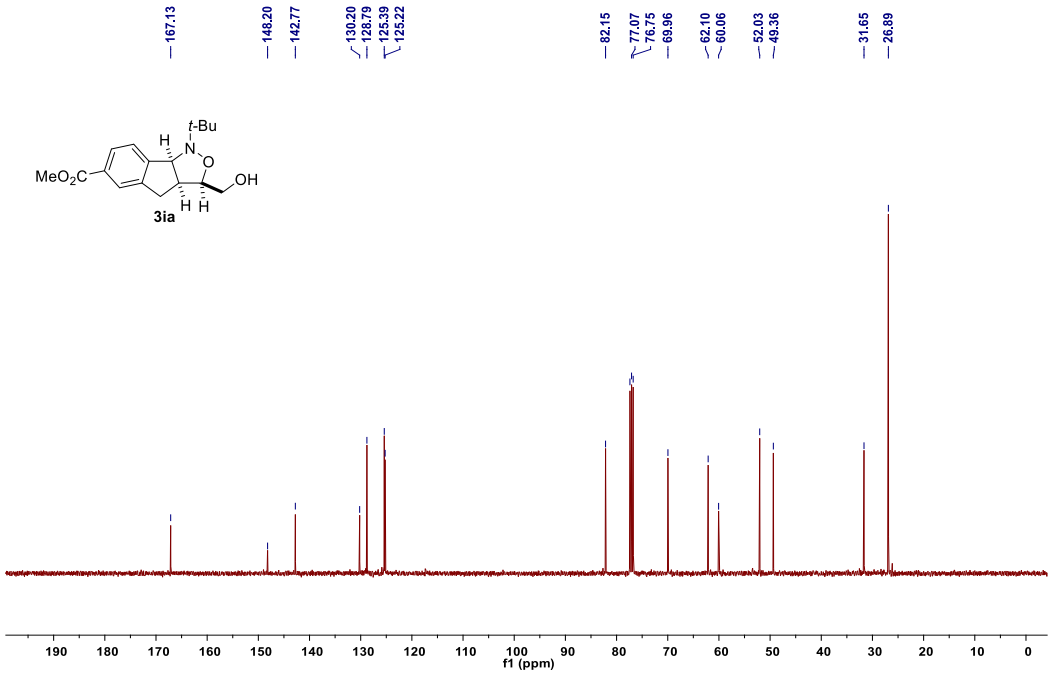
7.39
7.36
7.34
7.19
4.91
4.89
4.37
4.36
4.36
4.35
4.35
4.34
3.50
3.47
3.46
3.35
3.31
3.05
2.97
2.96
2.95
2.93
1.96
1.20
t-Bu
H
N
O
F3C
OH
H H
3ha
0.96
2.02
1.00
1.00
1.00
1.02
1.01
1.05
1.04
1.03
9.20
f1 (ppm)


147.12
143.13
130.74
130.42
130.10
128.38
125.67
124.40
124.37
124.33
124.29
122.97
121.03
120.99
120.96
120.26
82.07
77.03
76.71
69.84
62.14
59.94
49.32
31.88
26.96
t-Bu
H
N
O
F3C
OH
H H
3ha
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


t-Bu
H
N
O
F3C
OH
H H
3ha
62.14
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)


t-Bu
H
N
O
MeO2C
OH
H H
3ia
1.13
1.08
1.10
1.00
1.06
3.46
2.08
1.02
1.07
1.12
0.72
9.45
f1 (ppm)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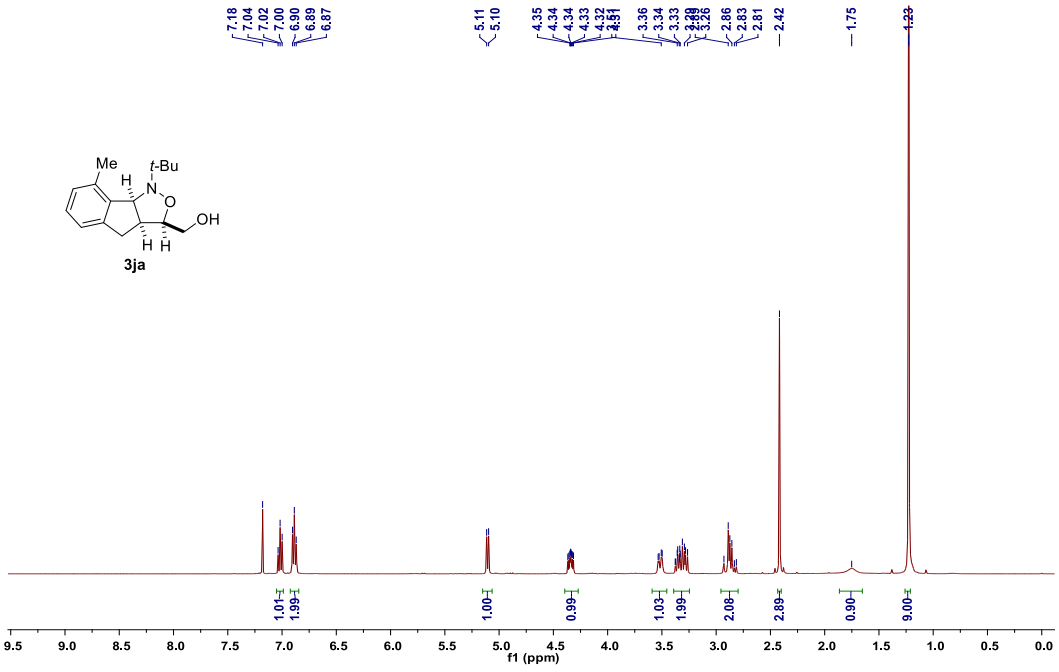
148.20
142.77
130.20
128.79
125.39
125.22
82.15
77.07
76.75
69.96
62.10
60.06
52.03
49.36
31.65
26.89
t-Bu
H
N
O
MeO2C
OH
H H
3ia
f1 (ppm)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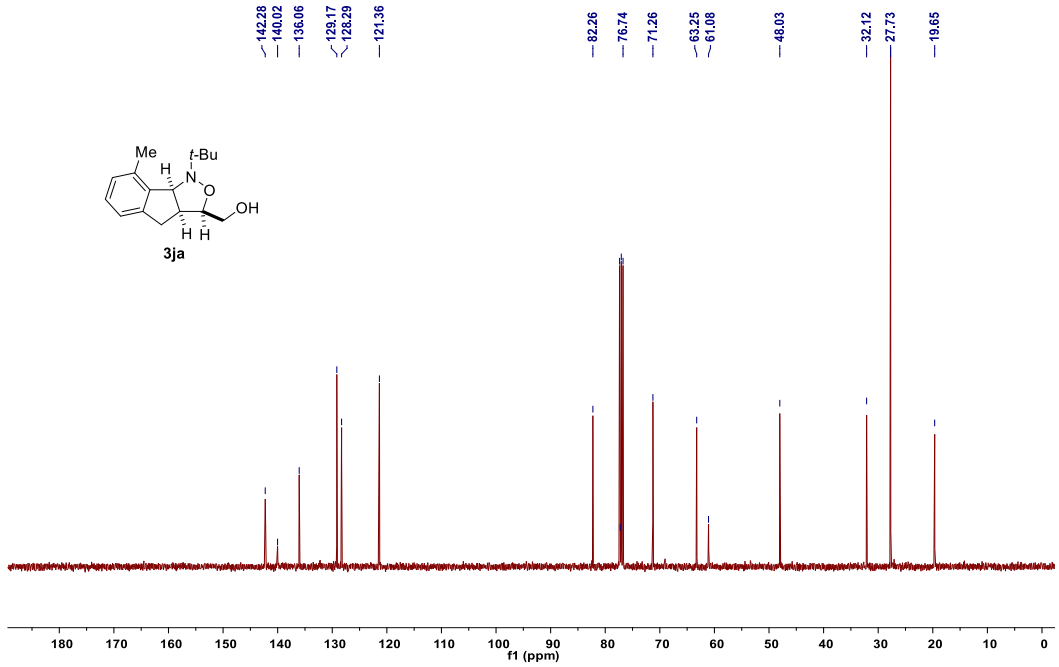
7.02
7.00
6.90
6.89
6.87
5.11
5.10
4.35
4.34
4.34
4.33
4.32
4.31
3.36
3.34
3.33
3.26
2.86
2.83
2.81
2.42
1.75
1.23
Me
H
N
t-Bu
O
OH
H H
3ja
1.01
1.99
1.00
0.99
1.03
1.99
2.08
2.89
0.90
9.00
f1 (ppm)


142.28
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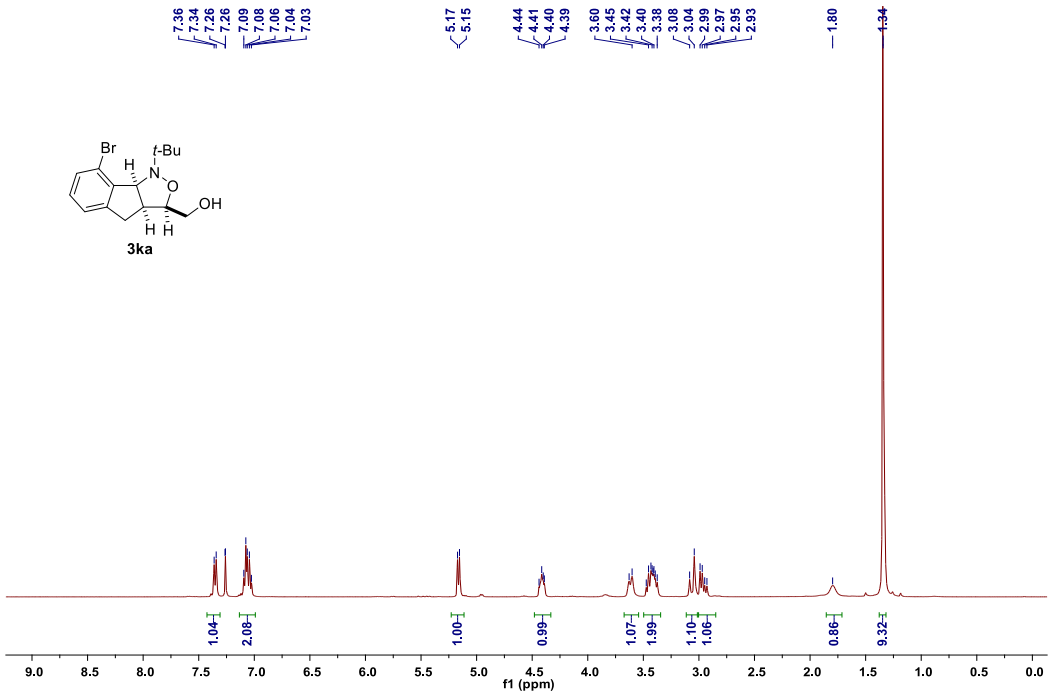
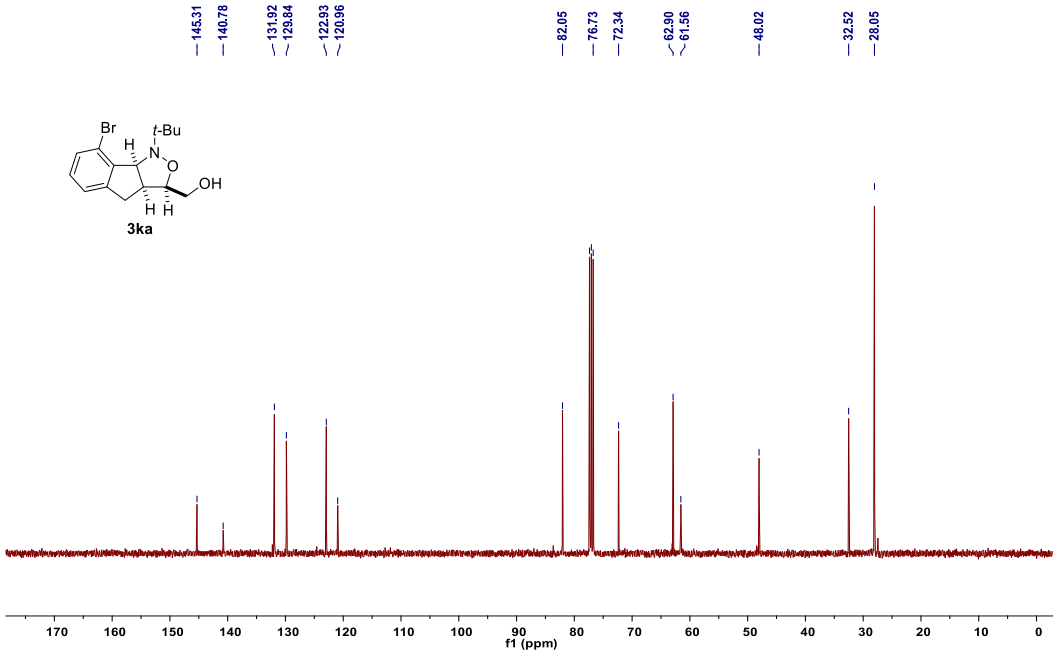
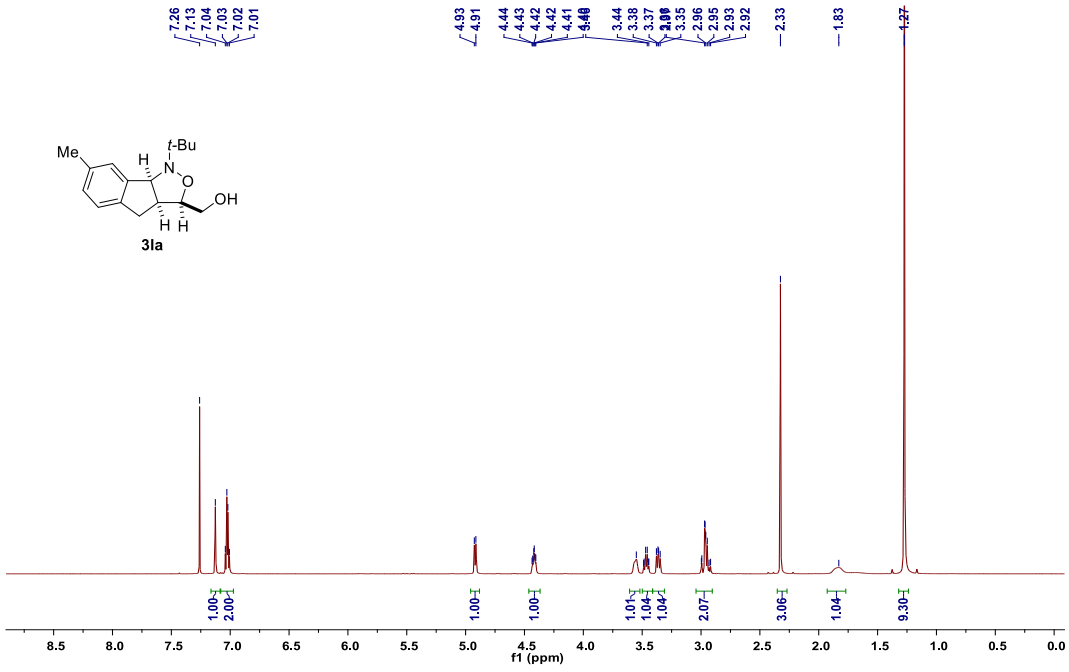
129.17
128.29
121.36
82.26
76.74
71.26
63.25
61.08
48.03
32.12
27.73
19.65
Me
H
N
t-Bu
O
OH
H H
3ja
f1 (ppm)


7.36
7.34
7.26
7.26
7.09
7.08
7.06
7.04
7.03
5.17
5.15
4.44
4.41
4.40
4.39
3.60
3.45
3.42
3.40
3.38
3.08
3.04
2.99
2.97
2.95
2.93
1.80
1.34
Br
t-Bu
H
N
O
OH
H H
3ka
1.04
2.08
1.00
0.99
1.07
1.99
1.10
1.06
0.86
9.32
f1 (ppm)


145.31
140.78
131.92
129.84
122.93
120.96
82.05
76.73
72.34
62.90
61.56
48.02
32.52
28.05
Br
t-Bu
H
N
O
OH
H H
3ka
f1 (ppm)


7.26
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7.04
7.03
7.02
7.01
4.93
4.91
4.44
4.43
4.42
4.42
4.41
3.44
3.38
3.37
3.35
2.96
2.95
2.93
2.92
2.33
1.83
1.27
Me
t-Bu
H
N
O
OH
H H
3la
1.00
2.00
1.00
1.00
1.01
1.04
1.04
2.07
3.06
1.04
9.30
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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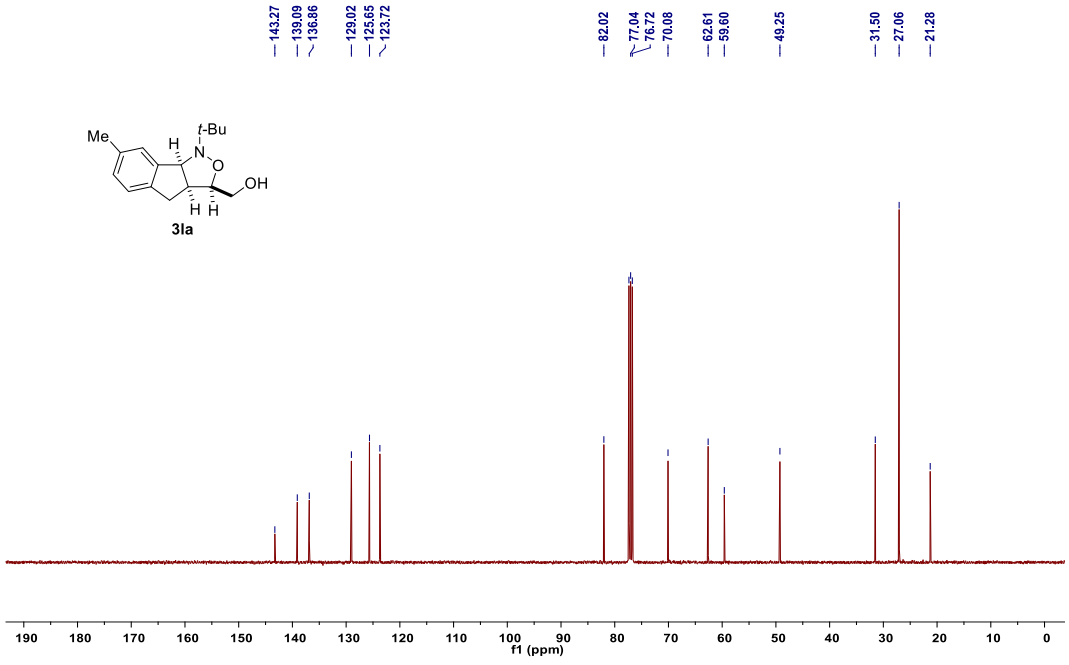
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125.65
123.72
82.02
77.04
76.72
70.08
62.61
59.60
49.25
31.50
27.06
21.28
Me
t-Bu
H
N
O
OH
H H
3la
190
180
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130
120
110
100
90
80
70
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50
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10
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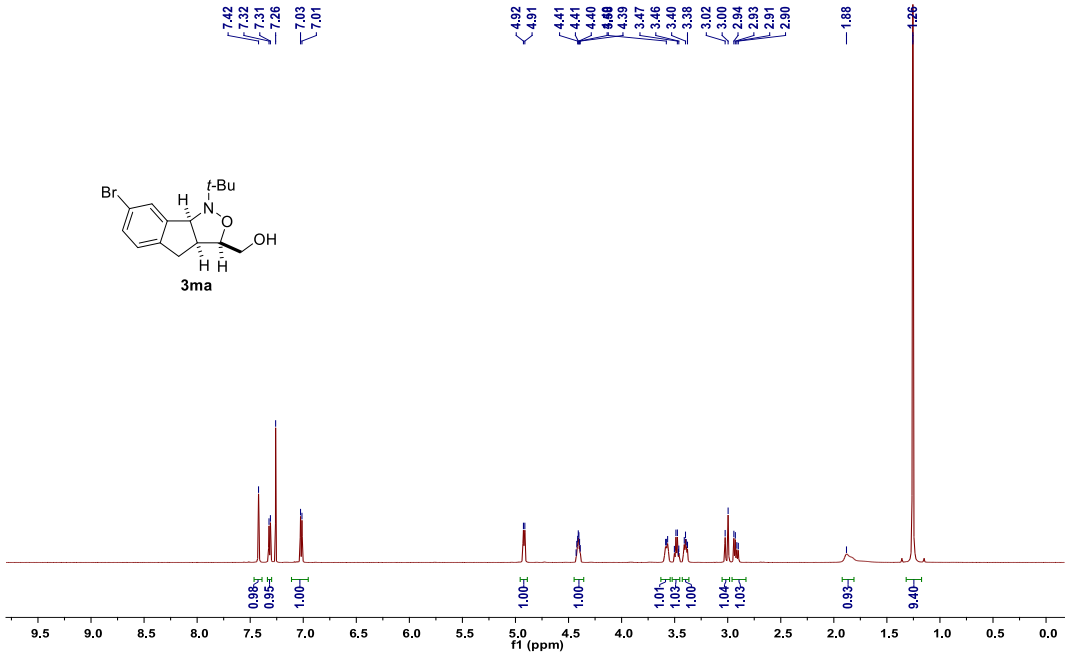
f1 (ppm)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4.91
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4.41
4.40
4.39
3.47
3.46
3.40
3.38
3.02
3.00
2.94
2.93
2.91
2.90
1.88
1.26
Br
H
t-Bu
N
O
OH
H
H
3ma
0.98
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1.00
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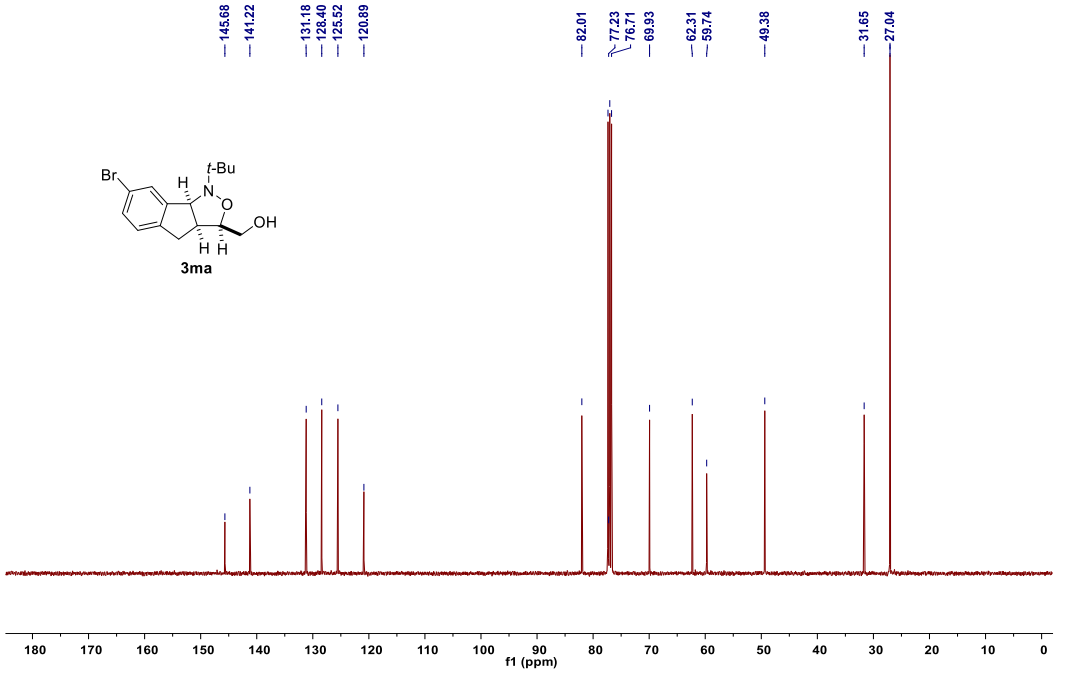
1.03
1.00
1.04
1.03
0.93
9.40
f1 (ppm)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120.89
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77.23
76.71
69.93
62.31
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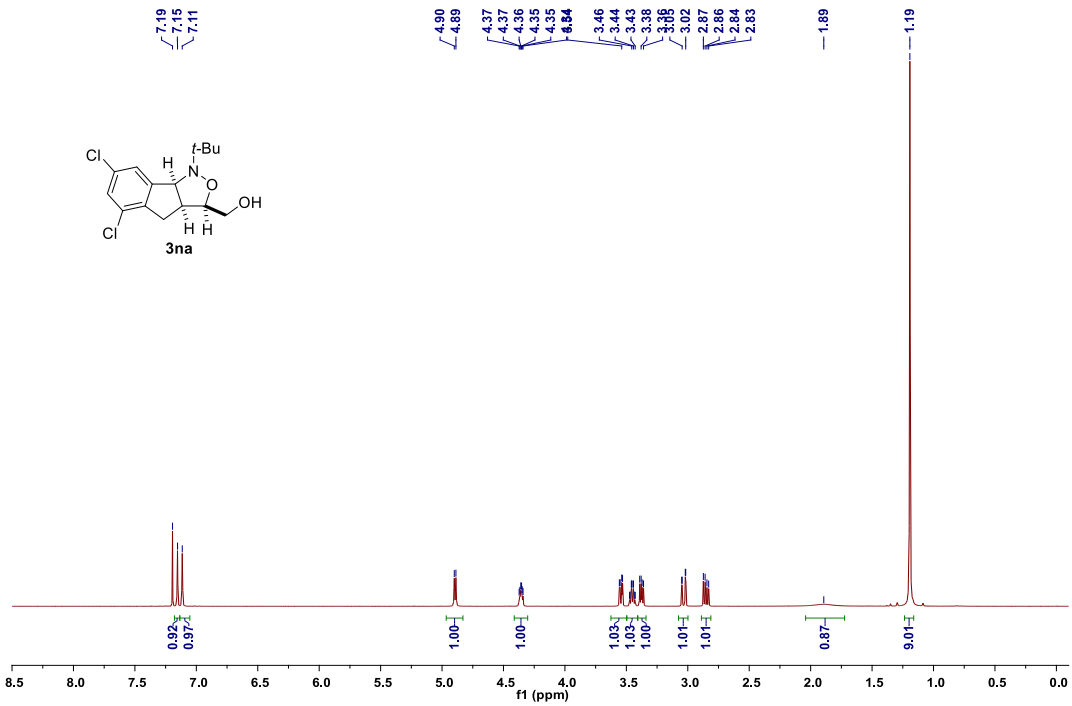
31.65
27.04
Br
H
t-Bu
N
O
OH
H
H
3ma
f1 (ppm)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7.15
7.11
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4.89
4.37
4.37
4.36
4.35
3.46
3.44
3.43
3.38
3.02
2.87
2.86
2.84
2.83
1.89
1.19
Cl
t-Bu
H
N
O
OH
H H
Cl
3na
0.92
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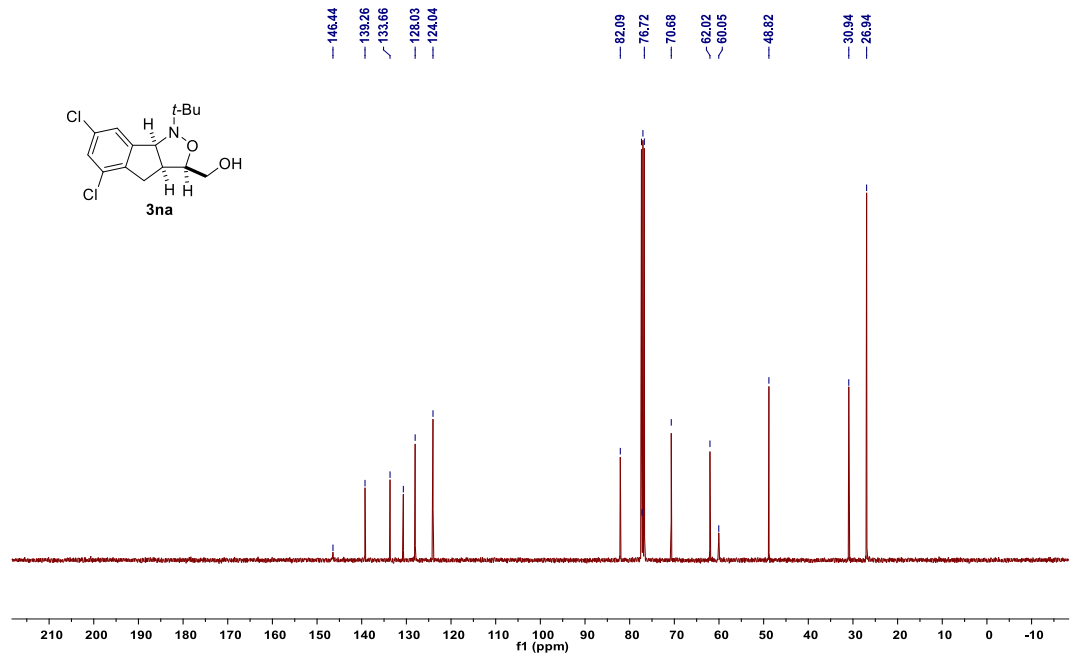
1.00
1.03
1.03
1.00
1.01
1.01
0.87
9.01
f1 (ppm)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82.09
76.72
70.68
62.02
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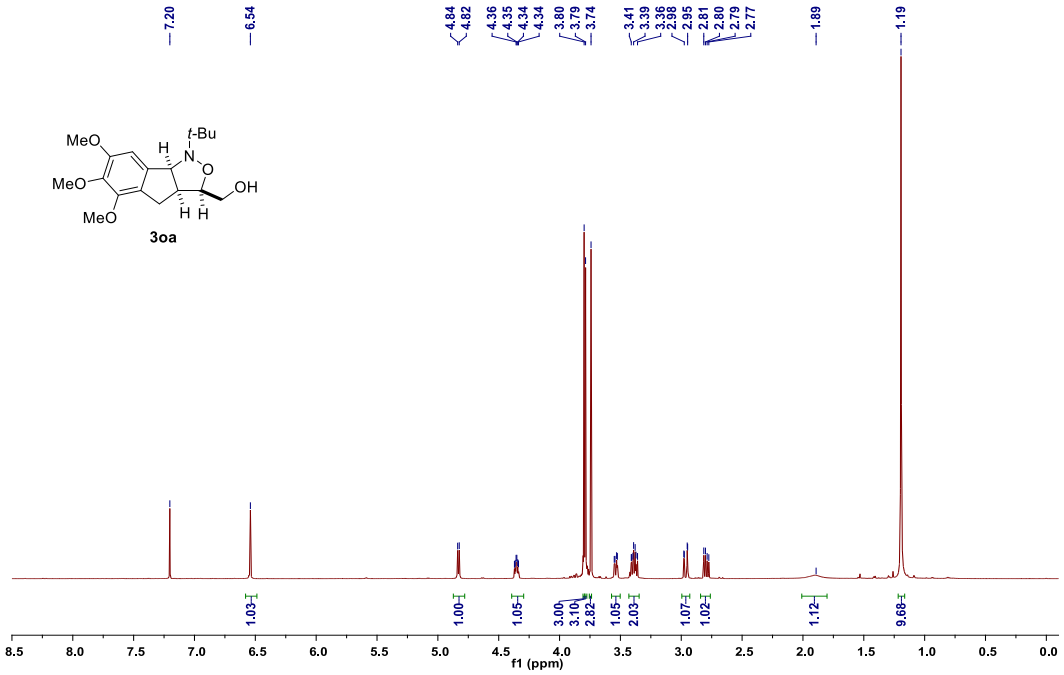
30.94
26.94
Cl
t-Bu
H
N
O
OH
H H
Cl
3na
f1 (ppm)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6.54
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4.34
4.34
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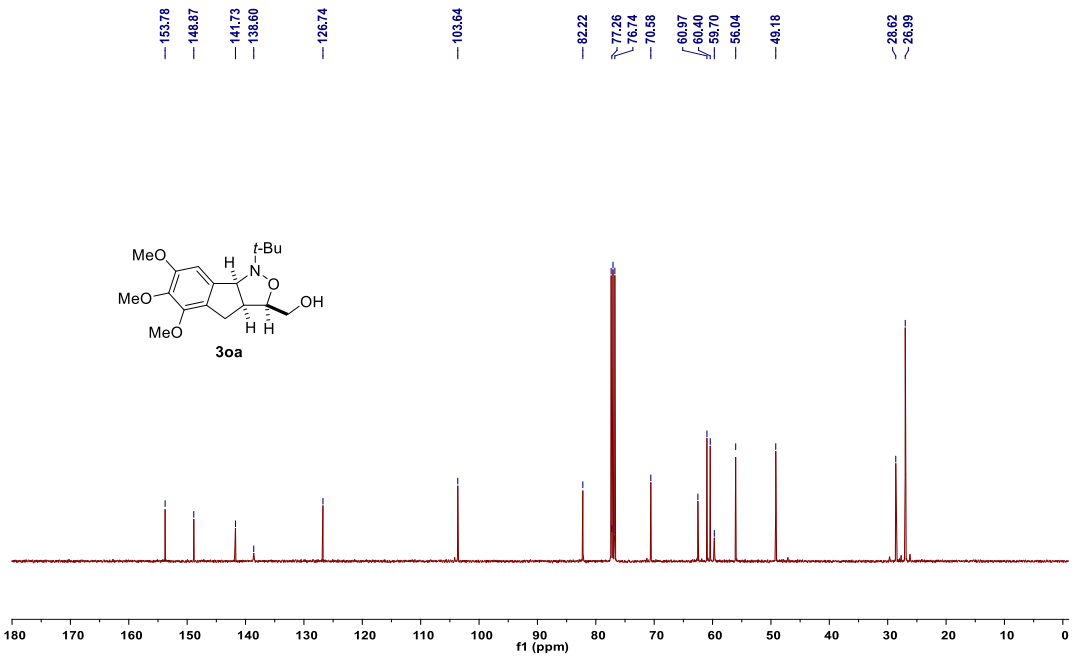
3.79
3.74
3.41
3.39
3.36
2.98
2.95
2.81
2.80
2.79
2.77
1.89
1.19
MeO
MeO
MeO
t-Bu
H
N
O
OH
H H
3oa
1.03
1.00
1.05
3.00
3.10
2.82
1.05
2.03
1.07
1.02
1.12
9.68
f1 (ppm)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60.97
60.40
59.70
56.04
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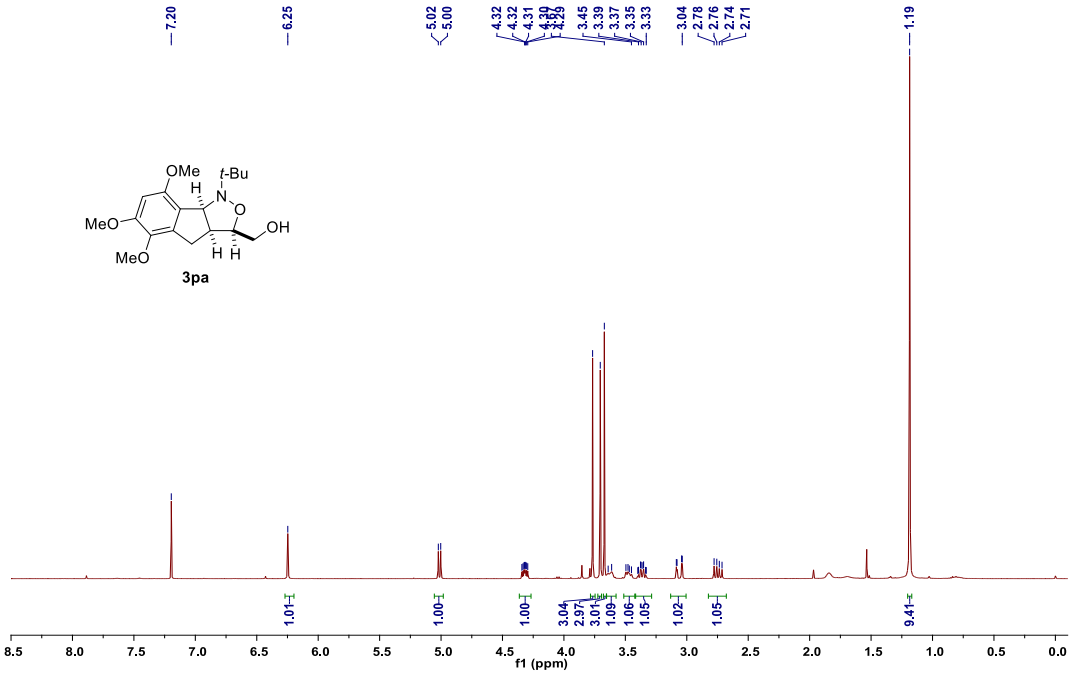
26.99
MeO
MeO
MeO
t-Bu
H
N
O
OH
H H
3oa
f1 (ppm)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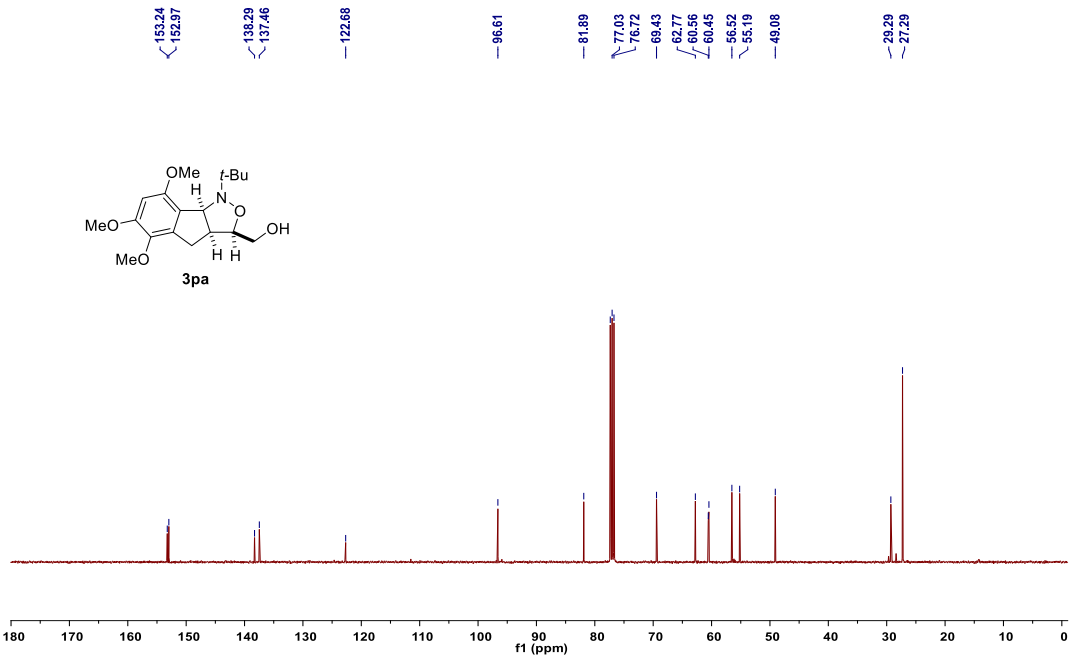
4.32
4.31
4.30
4.29
3.45
3.39
3.37
3.35
3.33
3.04
2.78
2.76
2.74
2.71
1.19
OMe
t-Bu
H
N
O
MeO
OH
MeO
H H
3pa
1.01
1.00
1.00
3.04
2.97
3.01
1.09
1.06
1.05
1.02
1.05
9.41
f1 (ppm)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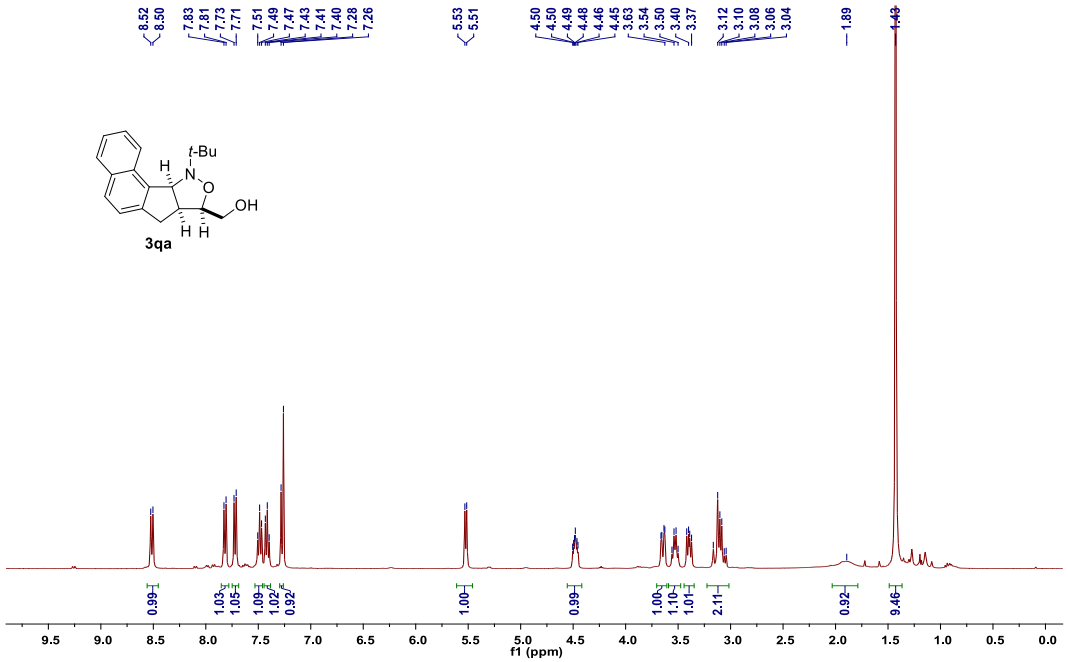
96.61
81.89
77.03
76.72
69.43
62.77
60.56
60.45
56.52
55.19
49.08
29.29
27.29
OMe
t-Bu
H
N
O
MeO
OH
MeO
H H
3pa
f1 (ppm)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7.71
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7.49
7.47
7.43
7.41
7.40
7.28
7.26
5.53
5.51
4.50
4.50
4.49
4.48
4.46
4.45
3.63
3.54
3.50
3.40
3.37
3.12
3.10
3.08
3.06
3.04
1.89
1.43
t-Bu
H
N
O
OH
H H
3qa
0.99
1.03
1.05
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1.02
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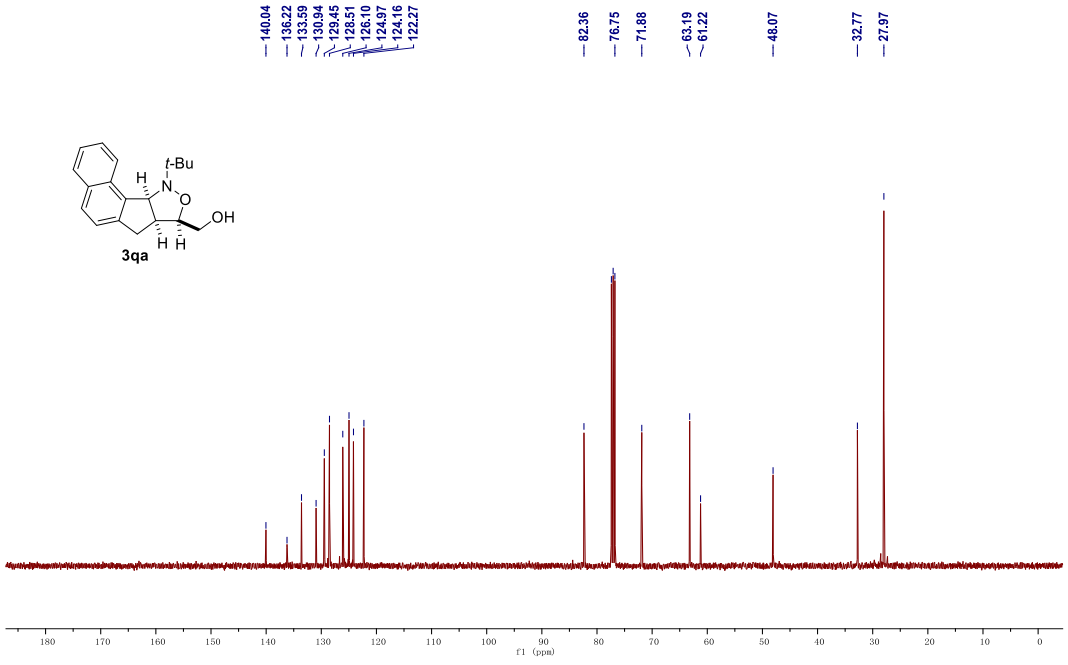
1.00
0.99
1.00
1.10
1.01
2.11
0.92
9.46
f1 (ppm)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136.22
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124.16
122.27
82.36
76.75
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63.19
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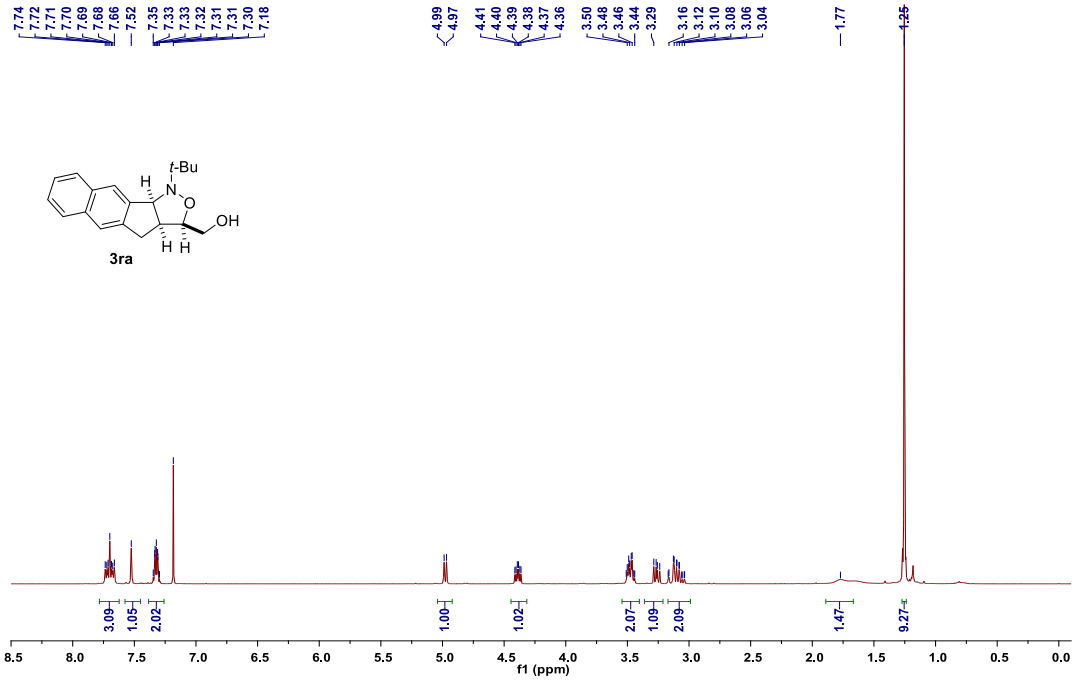
48.07
32.77
27.97
t-Bu
H
N
O
OH
H H
3qa
f1 (ppm)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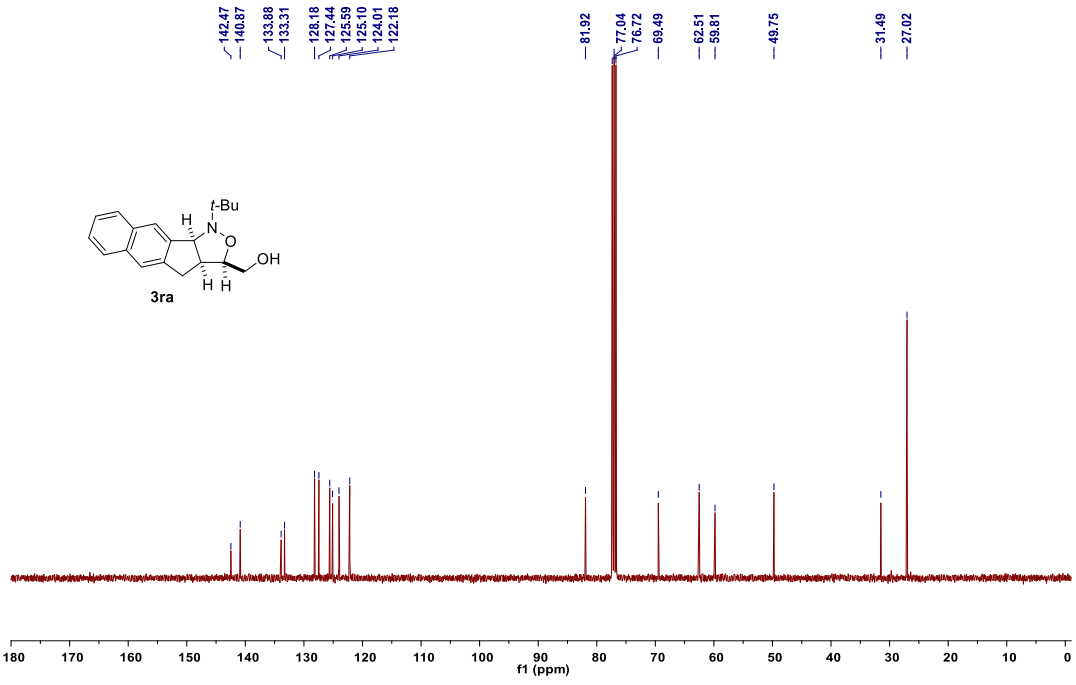
7.35
7.33
7.33
7.32
7.31
7.31
7.30
7.18
4.99
4.97
4.41
4.40
4.39
4.38
4.37
4.36
3.50
3.48
3.46
3.44
3.29
3.16
3.12
3.10
3.08
3.06
3.04
1.77
1.25
t-Bu
H
N
O
OH
H H
3ra
3.09
1.05
2.02
1.00
1.02
2.07
1.09
2.09
1.47
9.27
f1 (ppm)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124.01
122.18
81.92
77.04
76.72
69.49
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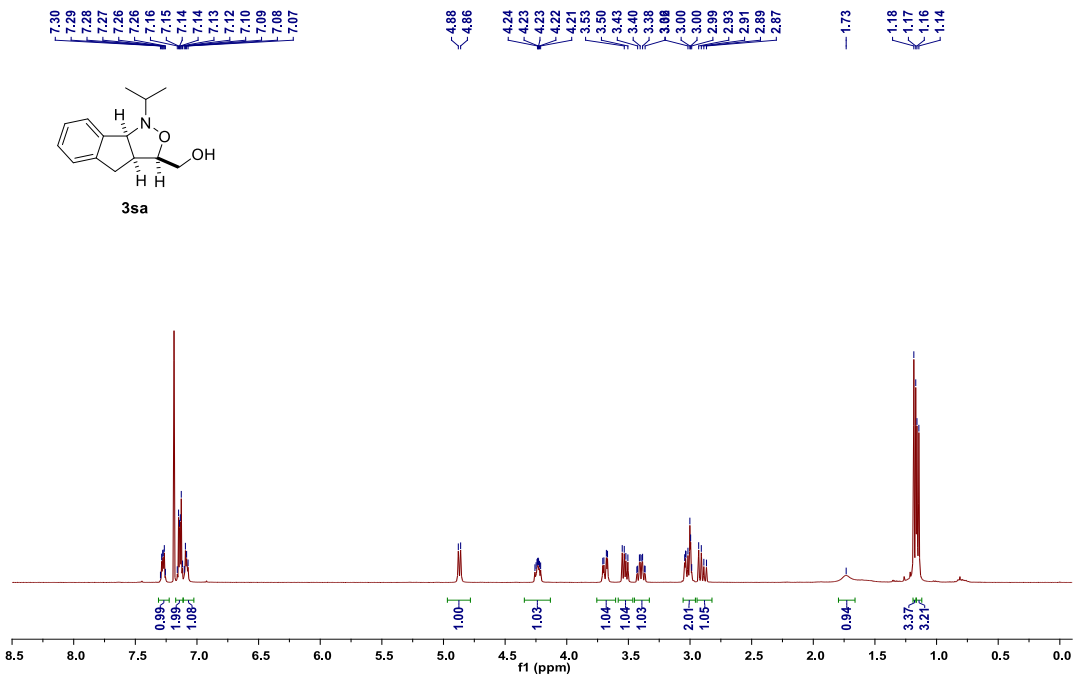
49.75
31.49
27.02
t-Bu
H
N
O
OH
H H
3ra
f1 (ppm)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7.14
7.14
7.13
7.12
7.10
7.09
7.08
7.07
4.88
4.86
4.24
4.23
4.23
4.22
4.21
3.53
3.50
3.43
3.40
3.38
3.00
3.00
2.99
2.93
2.91
2.89
2.87
1.73
1.18
1.17
1.16
1.14
H
N
O
OH
H H
3sa
0.99
1.99
1.08
1.00
1.03
1.04
1.04
1.03
2.01
1.05
0.94
3.37
3.21
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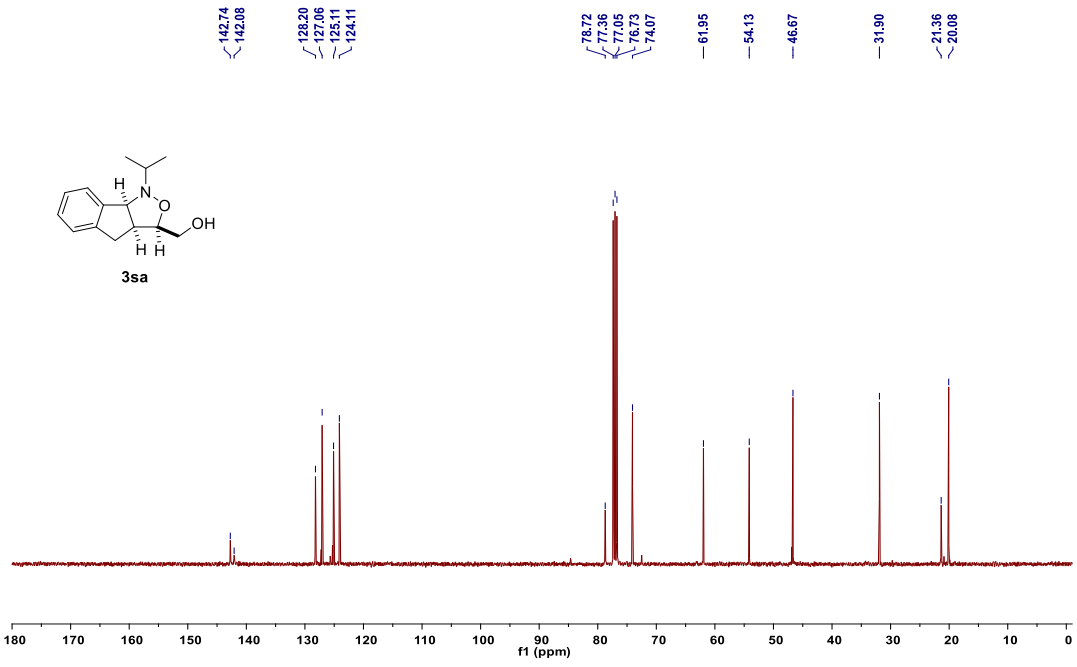
f1 (ppm)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77.05
76.73
74.07
61.95
54.13
46.67
31.90
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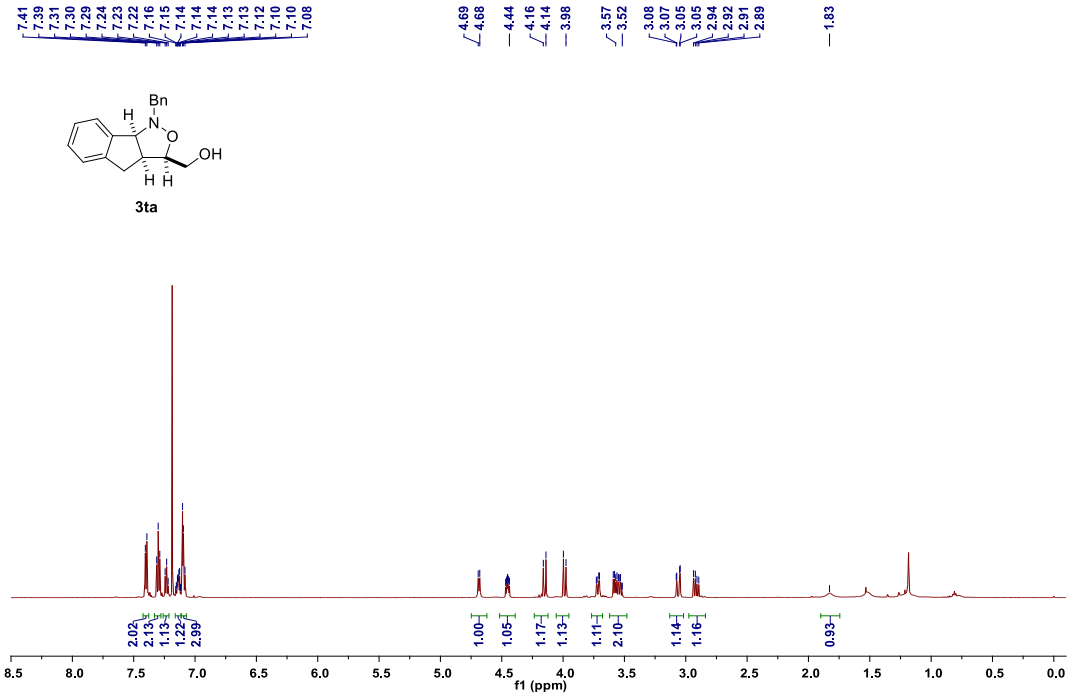
20.08
H
N
O
OH
H H
3sa
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.14
7.14
7.13
7.13
7.12
7.10
7.10
7.08
4.69
4.68
4.44
4.16
4.14
3.98
3.57
3.52
3.08
3.07
3.05
3.05
2.94
2.92
2.91
2.89
1.83
Bn
H
N
O
OH
H H
3ta
2.02
2.13
1.13
1.22
2.99
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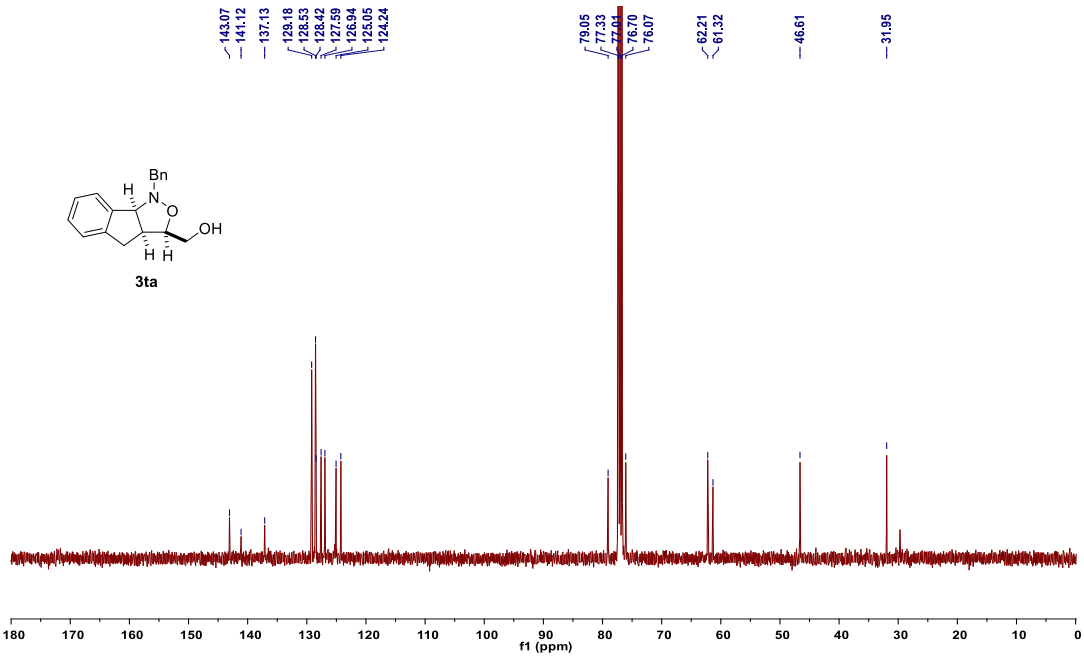
1.05
1.17
1.13
1.11
2.10
1.14
1.16
0.93
f1 (ppm)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127.59
126.94
125.05
124.24
79.05
77.33
77.01
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76.07
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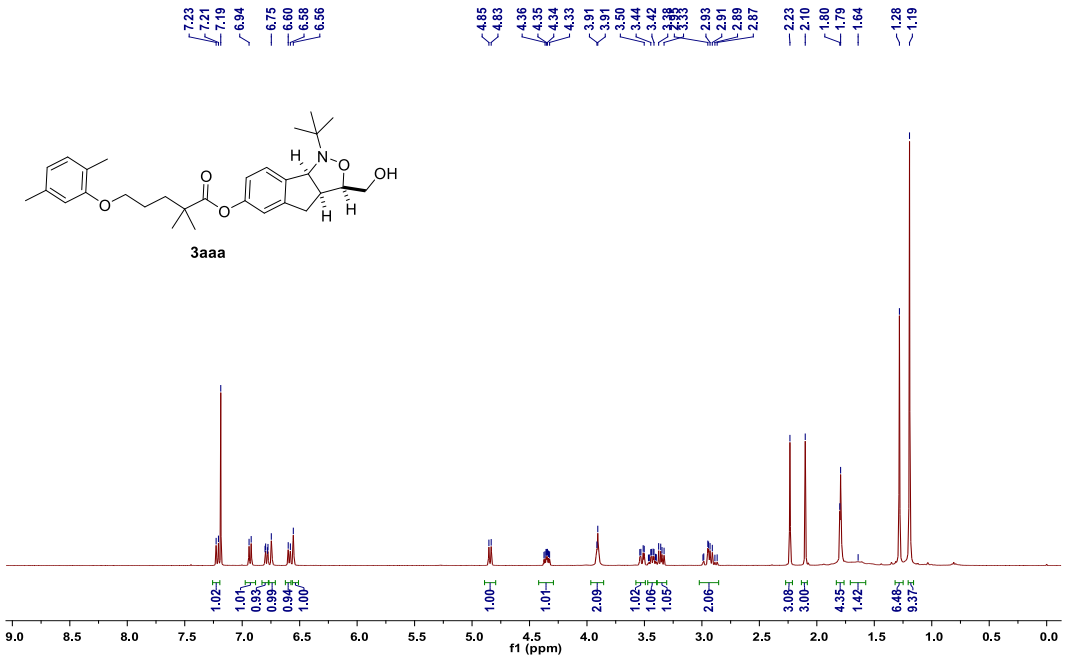
61.32
46.61
31.95
Bn
H
N
O
OH
H H
3ta
f1 (ppm)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6.56
4.85
4.83
4.36
4.35
4.34
4.33
3.91
3.91
3.50
3.44
3.42
2.93
2.91
2.89
2.87
2.23
2.10
1.80
1.79
1.64
1.28
1.19
OH
3aaa
1.02
1.01
0.93
0.99
0.94
1.00
1.00
1.01
2.09
1.02
1.06
1.05
2.06
3.08
3.00
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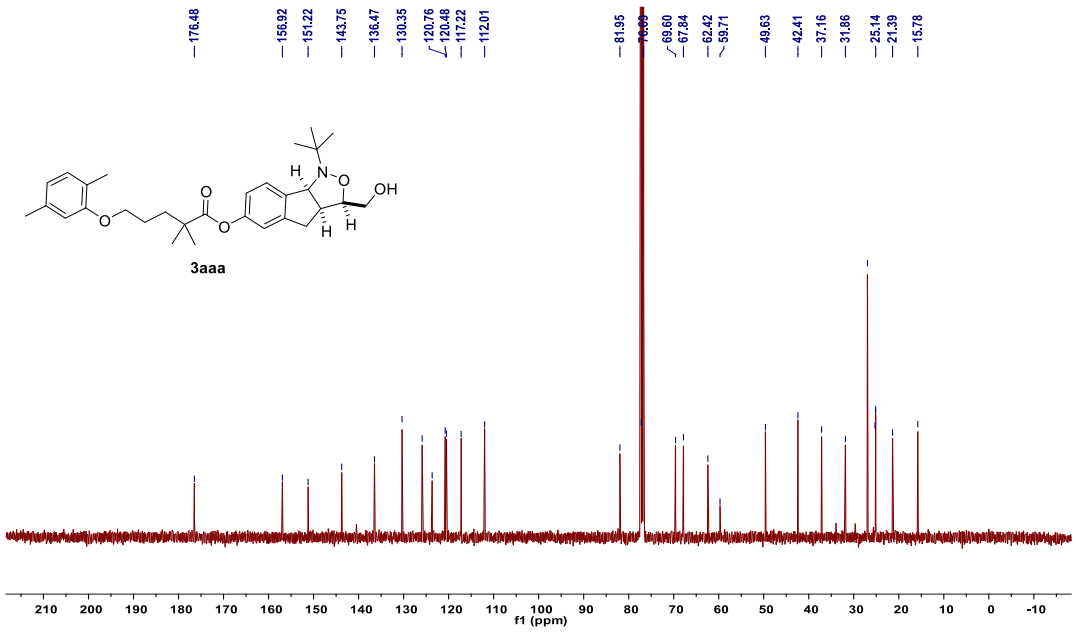
1.42
6.48
9.37
f1 (ppm)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112.01
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69.60
67.84
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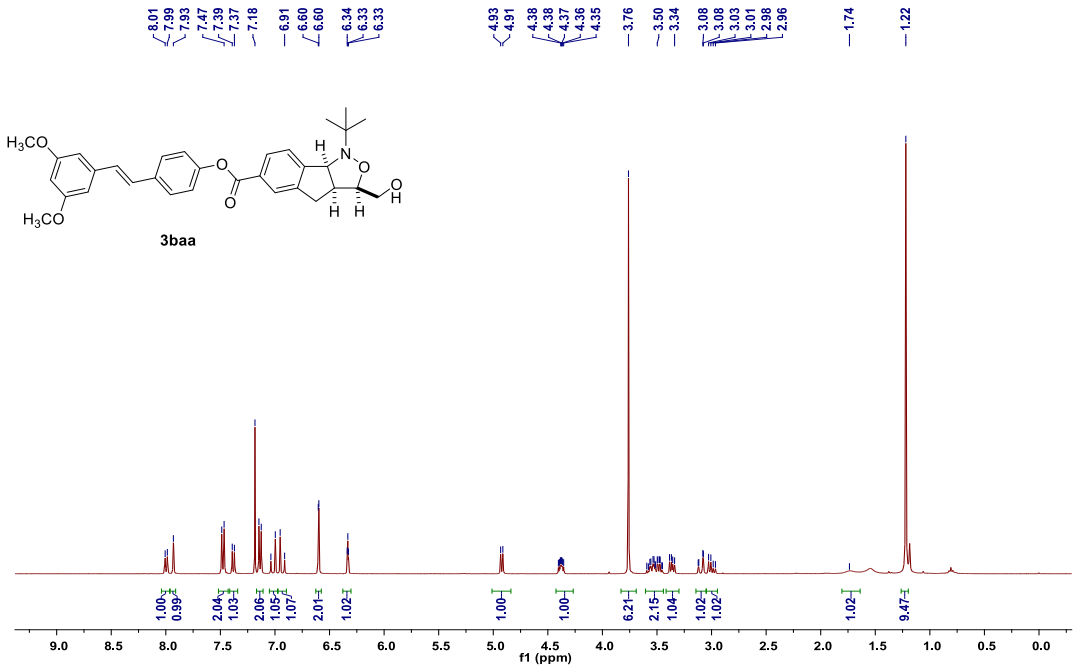
49.63
42.41
37.16
31.86
25.14
21.39
15.78
OH
3aaa
f1 (ppm)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6.60
6.60
6.34
6.33
6.33
4.93
4.91
4.38
4.38
4.37
4.36
4.35
3.76
3.50
3.34
3.08
3.08
3.03
3.01
2.98
2.96
1.74
1.22
H3CO
H3CO
O
O
H
N
O
O
H
H
H
3baa
1.00
0.99
2.04
1.03
2.06
1.05
1.07
2.01
1.02
1.00
1.00
6.21
2.15
1.04
1.02
1.02
1.02
9.47
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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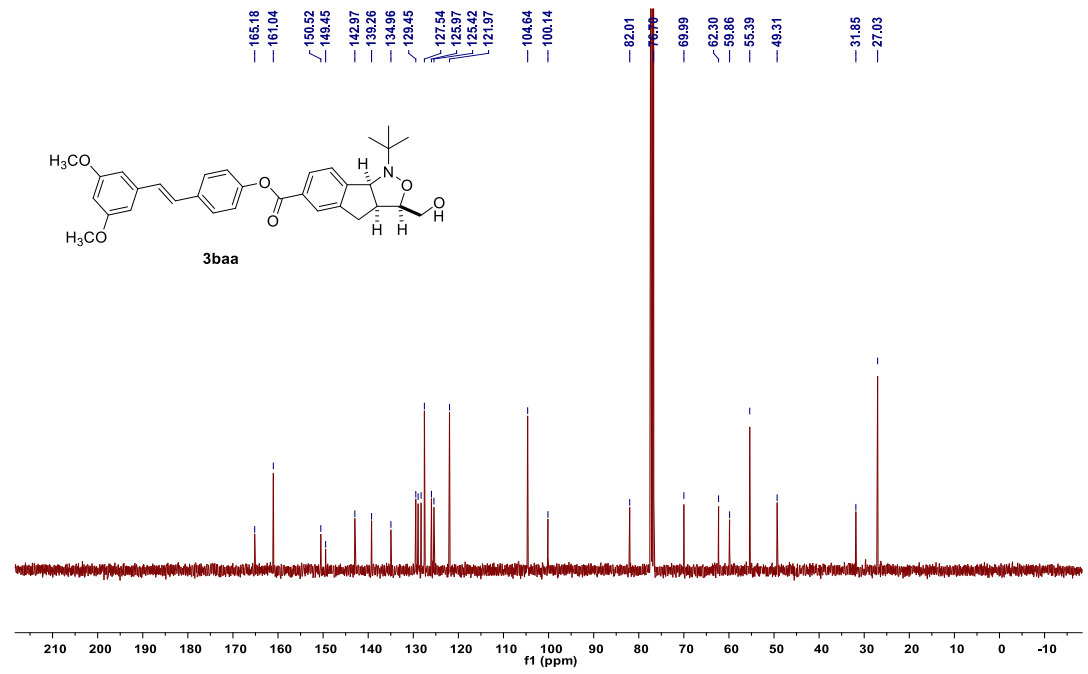
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.45
127.54
125.97
125.42
121.97
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100.14
82.01
78.70
69.99
62.30
59.86
55.39
49.31
31.85
27.03
H3CO
H3CO
O
O
H
N
O
O
H
H
H
3baa
210
200
190
180
170
160
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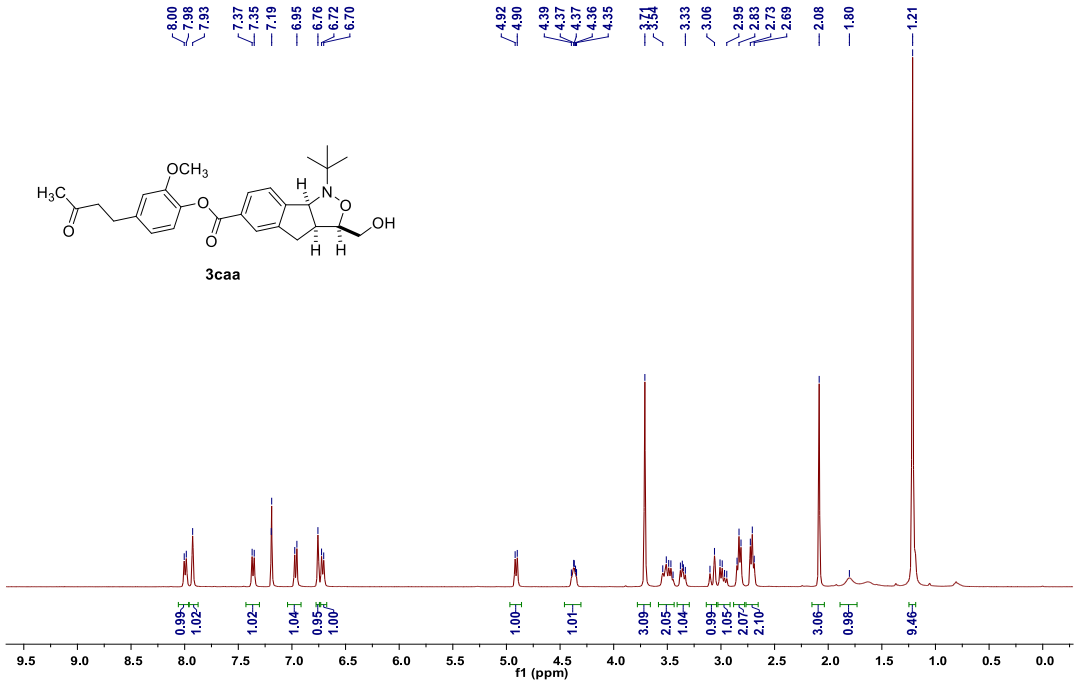
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.19
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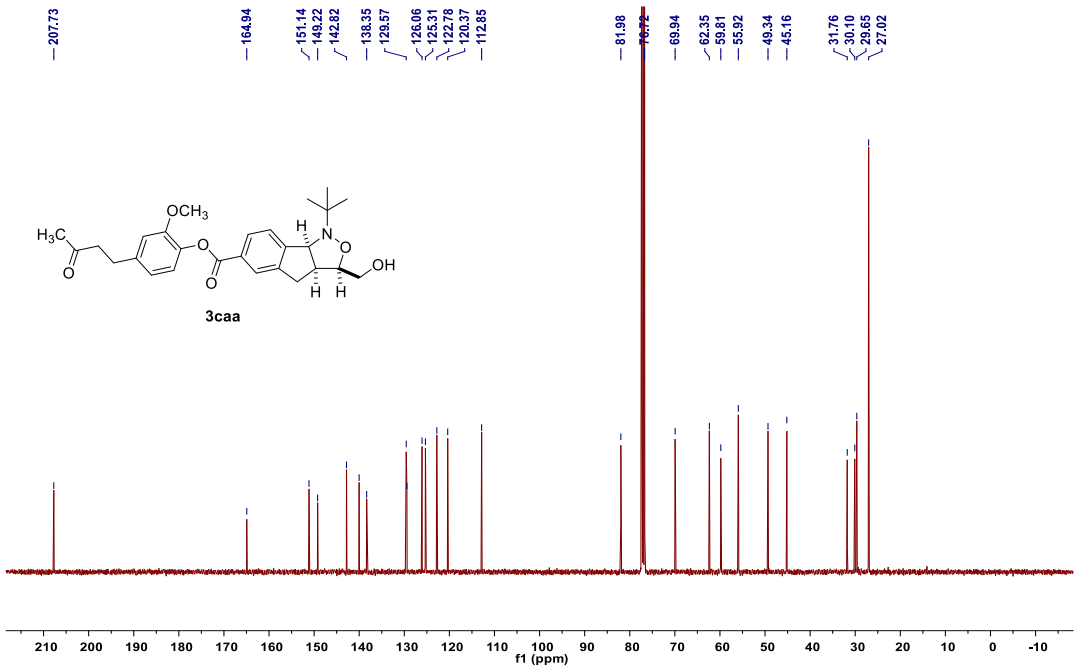
6.76
6.72
6.70
4.92
4.90
4.39
4.37
4.37
4.36
4.35
3.71
3.54
3.33
3.06
2.95
2.83
2.73
2.69
2.08
1.80
1.21
OCH3
H3C
O
O
H
N
O
OH
H
H
3caa
0.99
1.02
1.02
1.04
0.95
1.00
1.00
1.01
3.09
2.05
1.04
0.99
1.05
2.07
2.10
3.06
0.98
9.46
f1 (ppm)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126.06
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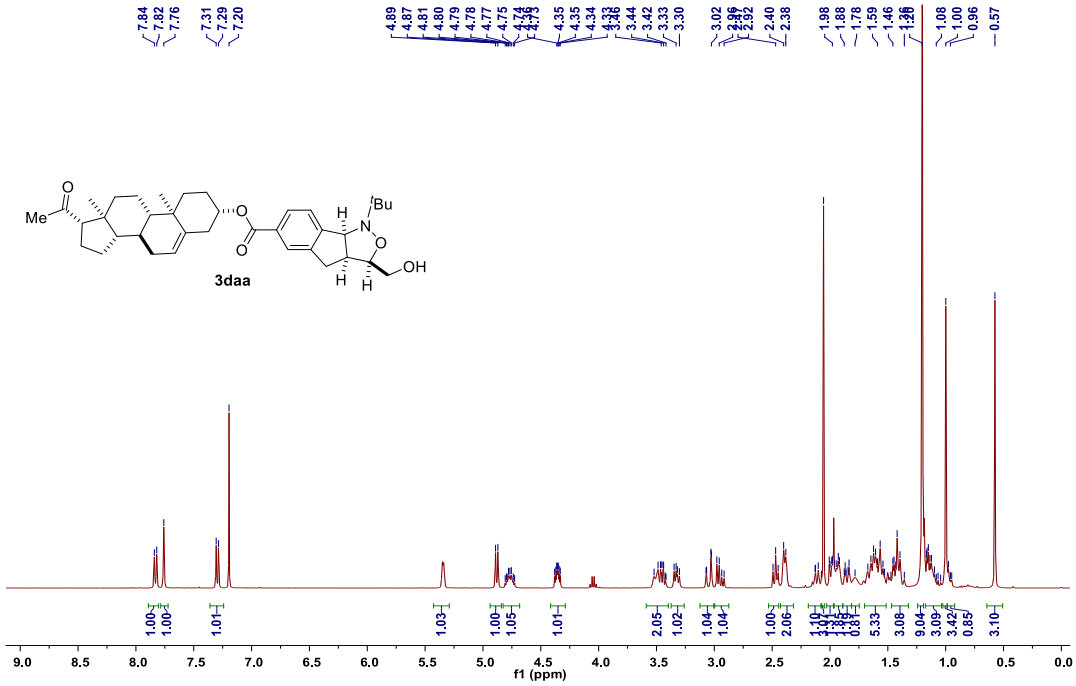
122.78
120.37
112.85
81.98
69.94
62.35
59.81
55.92
49.34
45.16
31.76
30.10
29.65
27.02
OCH3
H3C
O
O
H
N
O
OH
H
H
3caa
f1 (ppm)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4.79
4.78
4.77
4.75
4.35
4.34
3.44
3.42
3.33
3.30
3.02
2.40
2.38
1.98
1.88
1.78
1.59
1.46
1.08
1.00
0.96
0.57
Me
O
O
O
H
N
tBu
O
OH
H
H
3daa
1.00
1.00
1.01
1.03
1.00
1.05
1.01
2.05
1.02
1.04
1.04
1.00
2.06
5.33
3.08
9.04
3.09
3.42
0.85
3.10
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.5
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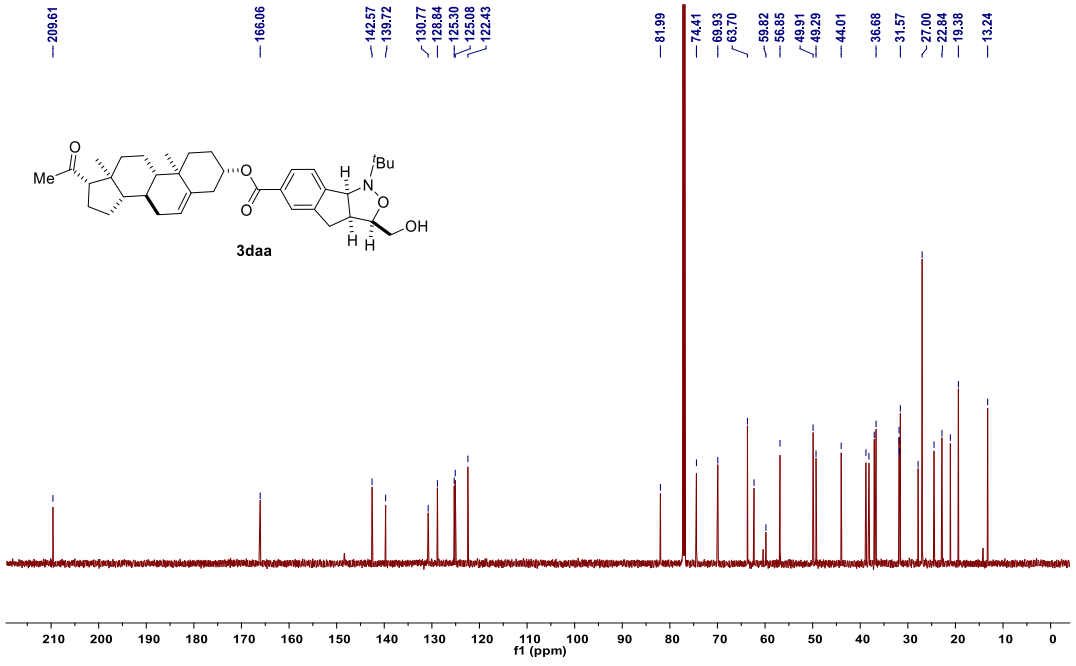
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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166.06
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128.84
125.30
125.08
122.43
81.99
74.41
69.93
63.70
59.82
56.85
49.91
49.29
44.01
36.68
31.57
27.00
22.84
19.38
13.24
Me
O
O
O
H
N
tBu
O
OH
H
H
3daa
210
200
190
180
170
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130
120
110
100
90
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70
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50
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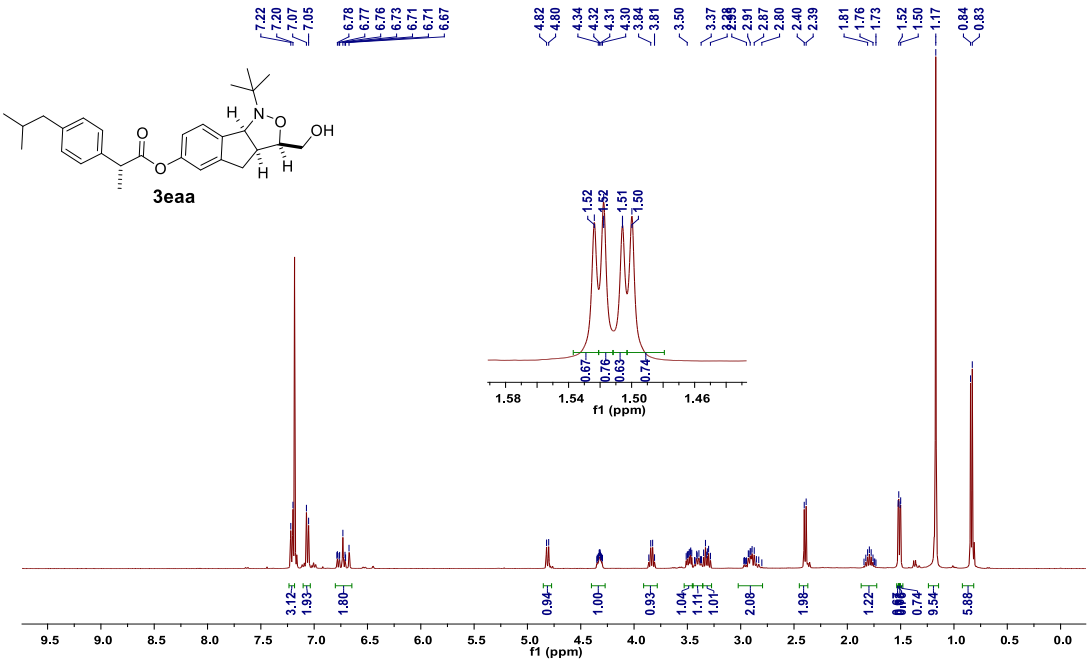
10
0
f1 (ppm)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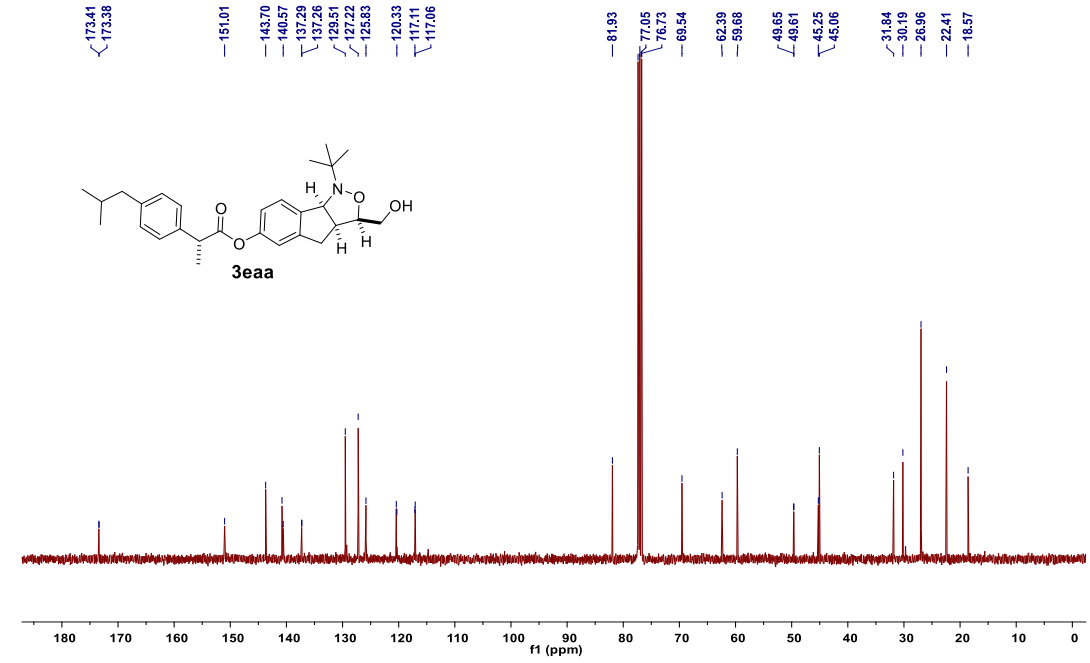
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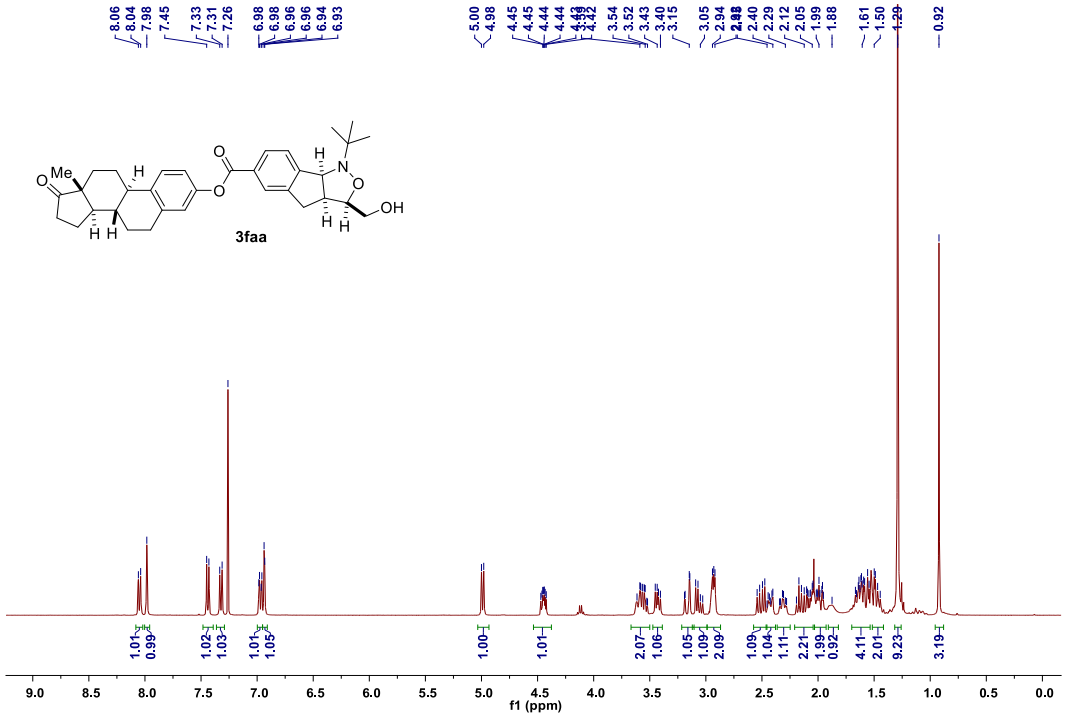
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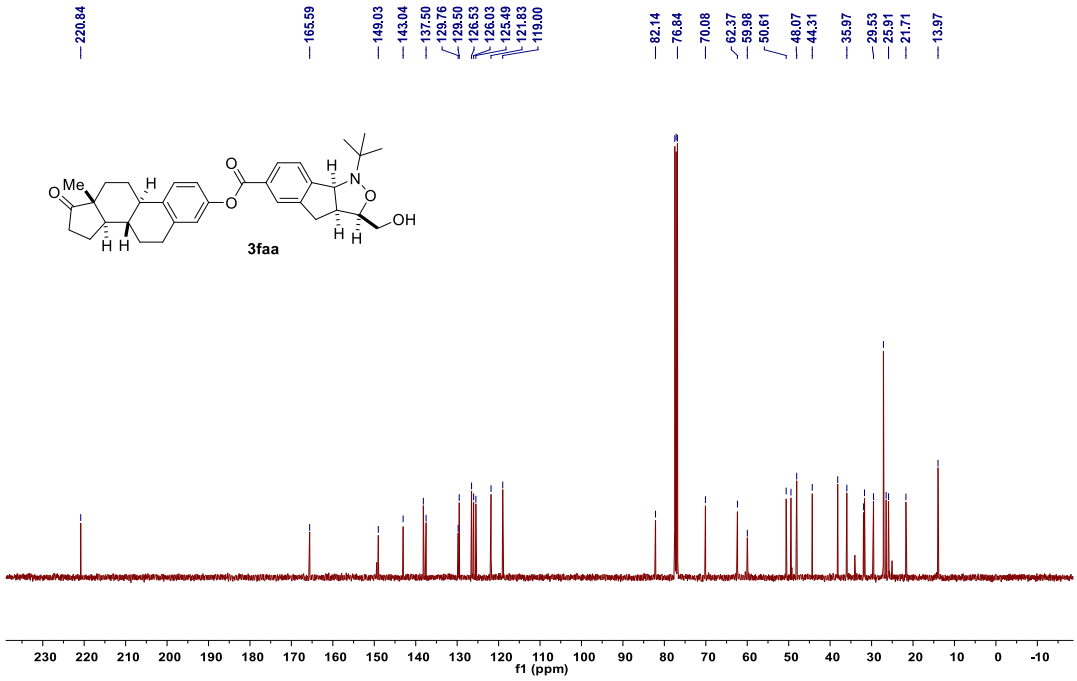
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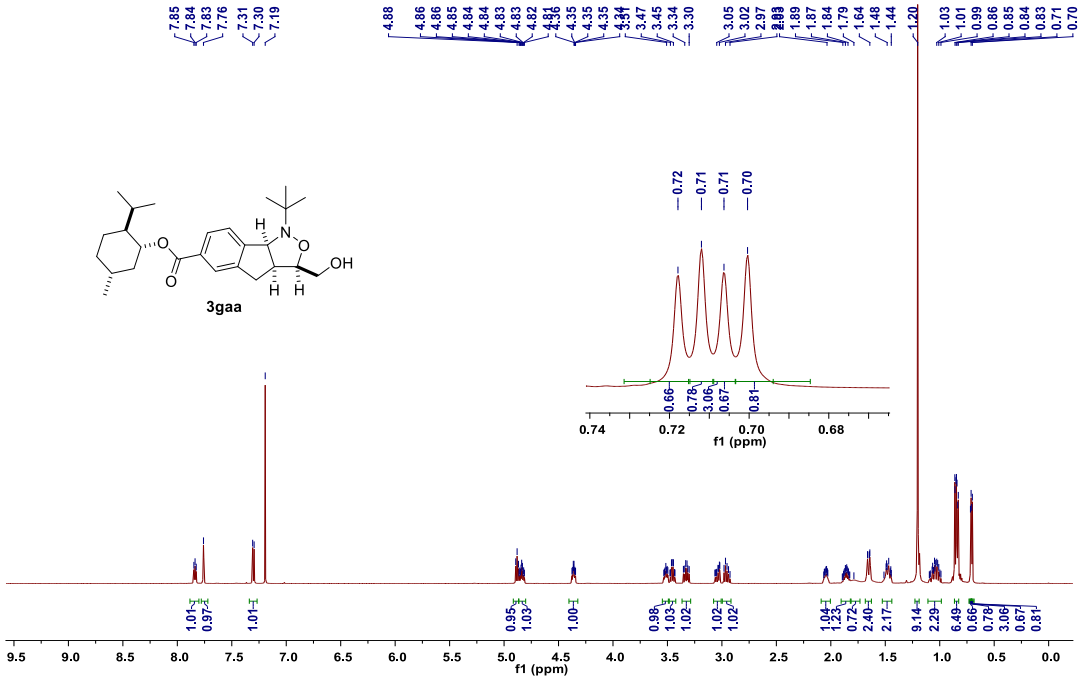
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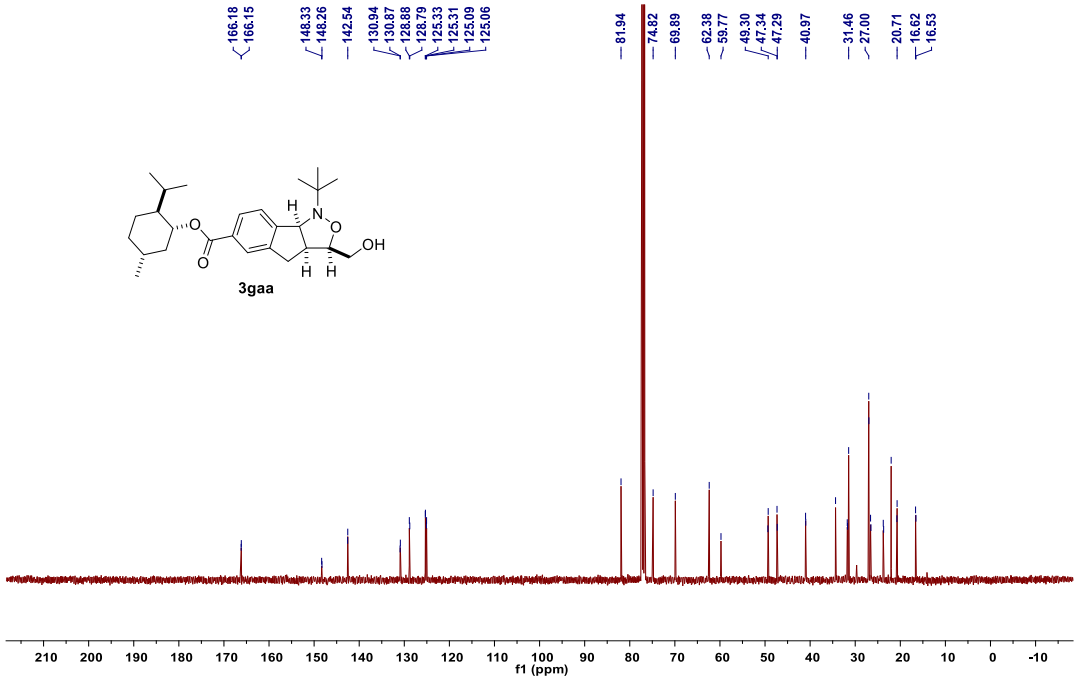
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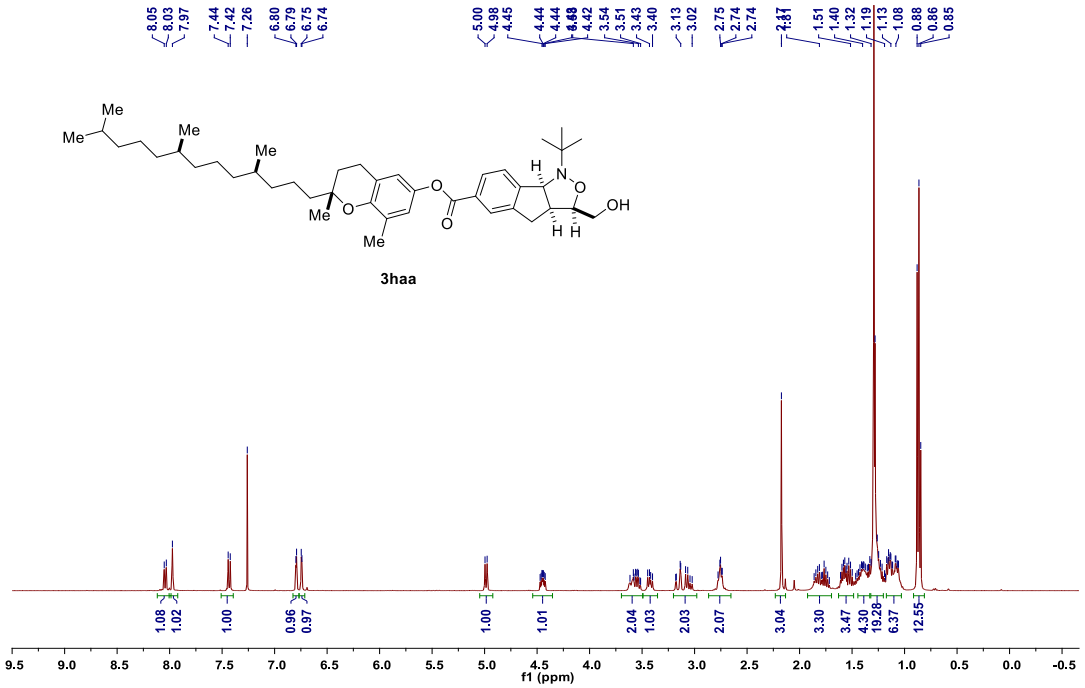
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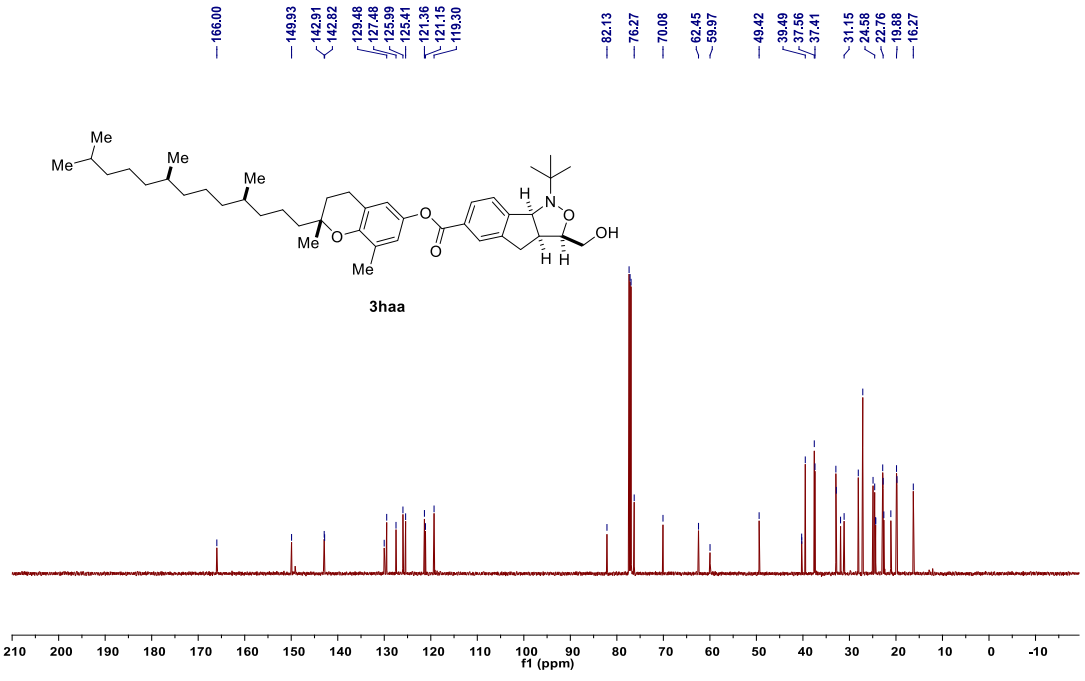
6.79
6.75
6.74
5.00
4.98
4.45
4.44
4.44
4.42
3.54
3.51
3.43
3.40
3.13
3.02
2.75
2.74
2.74
2.47
1.81
1.51
1.40
1.32
1.19
1.13
1.08
0.88
0.86
0.85
Me
Me
Me
Me
Me
O
O
H
N
O
OH
H H
1.08
1.02
1.00
0.96
0.97
1.00
1.01
2.04
1.03
2.03
2.07
3.04
3.30
3.47
4.30
19.28
6.37
12.55
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3haa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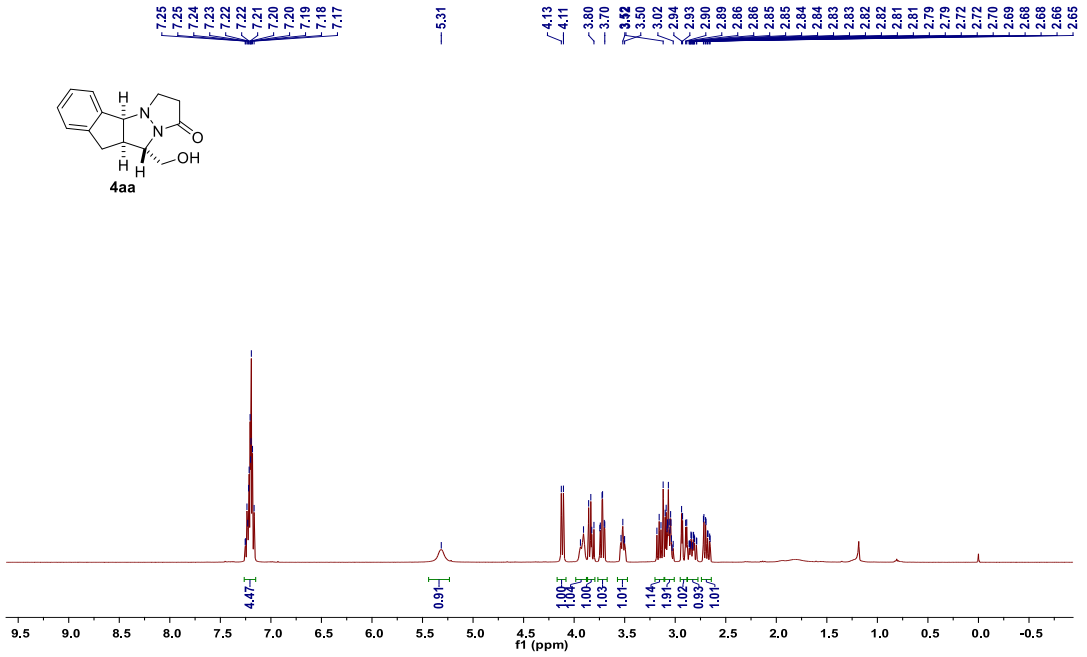
121.15
119.30
82.13
76.27
70.08
62.45
59.97
49.42
39.49
37.56
37.41
31.15
24.58
22.76
19.88
16.27
Me
Me
Me
Me
Me
O
O
H
N
O
OH
H H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3haa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7.25
7.24
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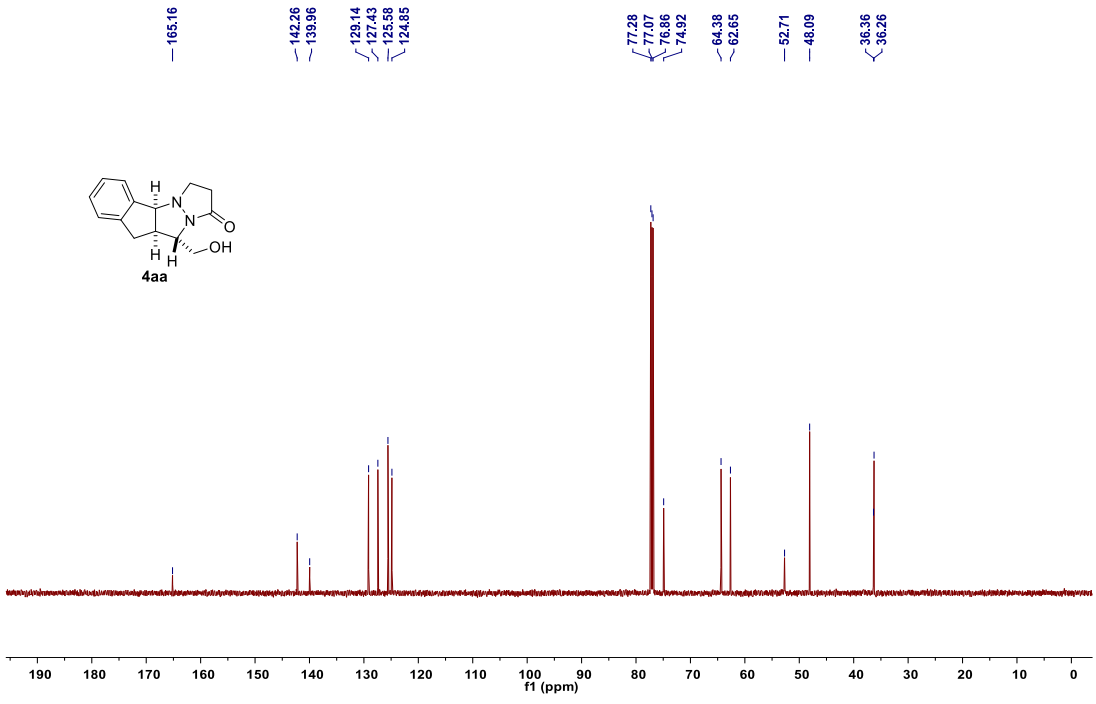
7.22
7.21
7.20
7.20
7.19
7.18
7.17
5.31
4.13
4.11
3.80
3.70
3.52
3.50
3.02
2.94
2.93
2.90
2.89
2.86
2.86
2.85
2.85
2.84
2.84
2.83
2.83
2.82
2.82
2.81
2.81
2.79
2.79
2.72
2.72
2.70
2.69
2.68
2.68
2.66
2.65
H
N
N
O
H
H
OH
4aa
4.47
0.91
1.00
1.04
1.00
1.03
1.01
1.14
1.91
1.02
0.33
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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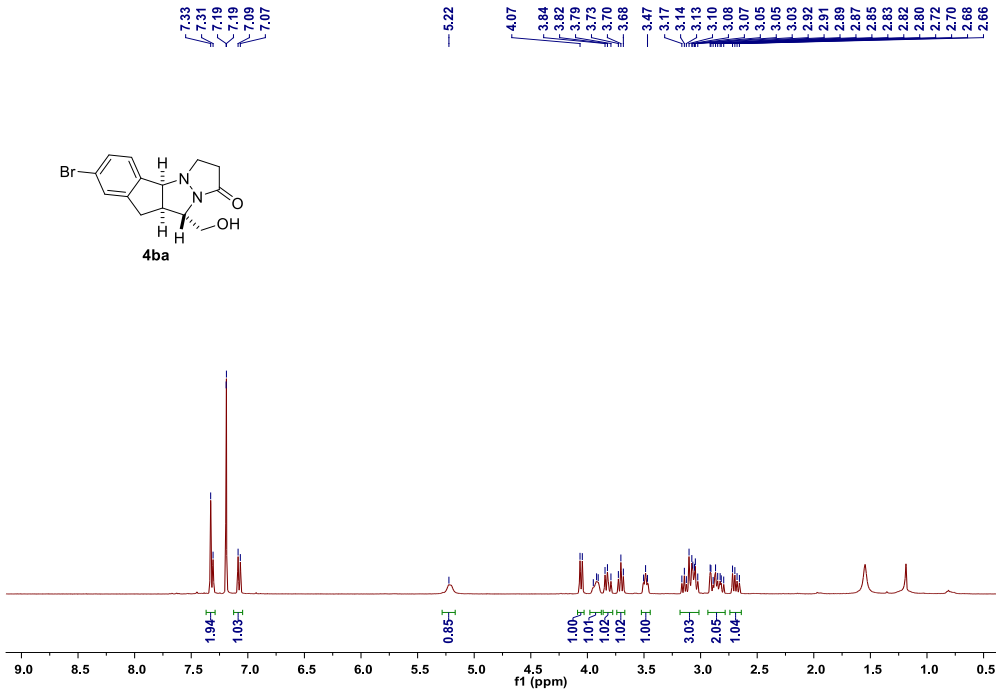
125.58
124.85
77.28
77.07
76.86
74.92
64.38
62.65
52.71
48.09
36.36
36.26
H
N
N
O
H
H
OH
4aa
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.31
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7.19
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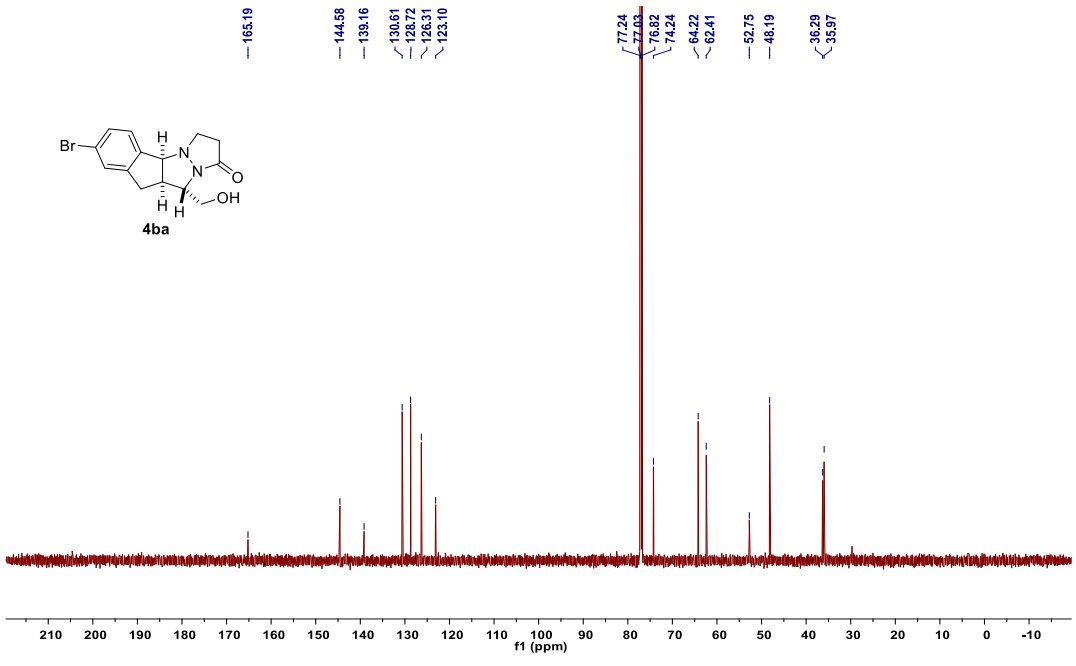
7.07
5.22
4.07
3.84
3.82
3.79
3.73
3.70
3.68
3.47
3.17
3.14
3.13
3.10
3.08
3.07
3.05
3.05
3.03
2.92
2.91
2.89
2.87
2.85
2.83
2.82
2.80
2.72
2.70
2.68
2.66
Br
H
N
N
O
OH
H
H
4ba
1.94
1.03
0.85
1.00
1.01
1.02
1.02
1.00
3.03
2.05
1.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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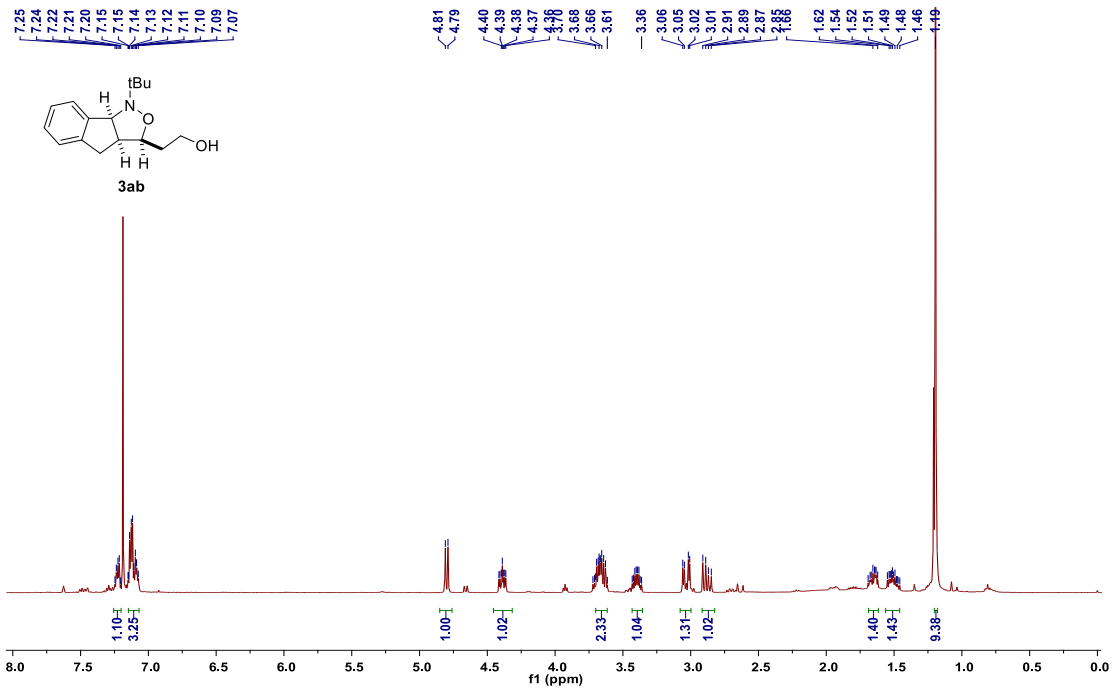
128.72
126.31
123.10
77.24
77.03
76.82
74.24
64.22
62.41
52.75
48.19
36.29
35.97
Br
H
N
N
O
OH
H
H
4ba
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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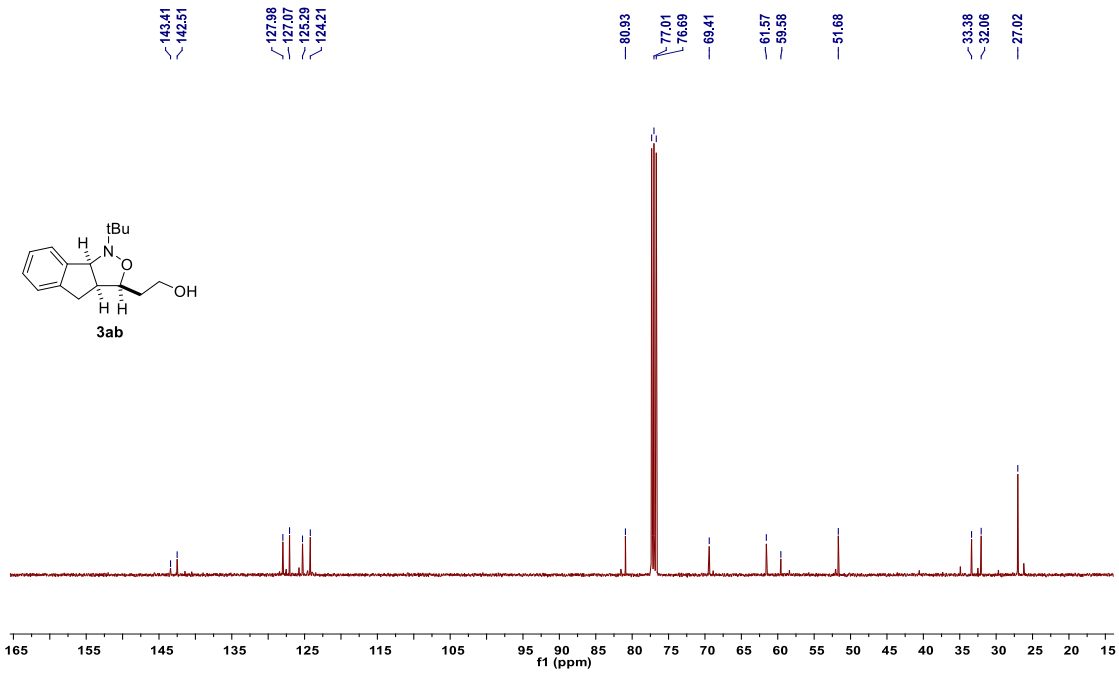
7.12
7.11
7.10
7.09
7.07
4.81
4.79
4.40
4.39
4.38
4.37
4.36
3.70
3.68
3.66
3.61
3.36
3.06
3.05
3.02
3.01
2.91
2.89
2.87
2.85
1.86
1.62
1.54
1.52
1.51
1.49
1.48
1.46
1.40
tBu
H
N
O
OH
H H
3ab
1.10
3.25
1.00
1.02
2.33
1.04
1.31
1.02
1.40
1.43
9.38
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.98
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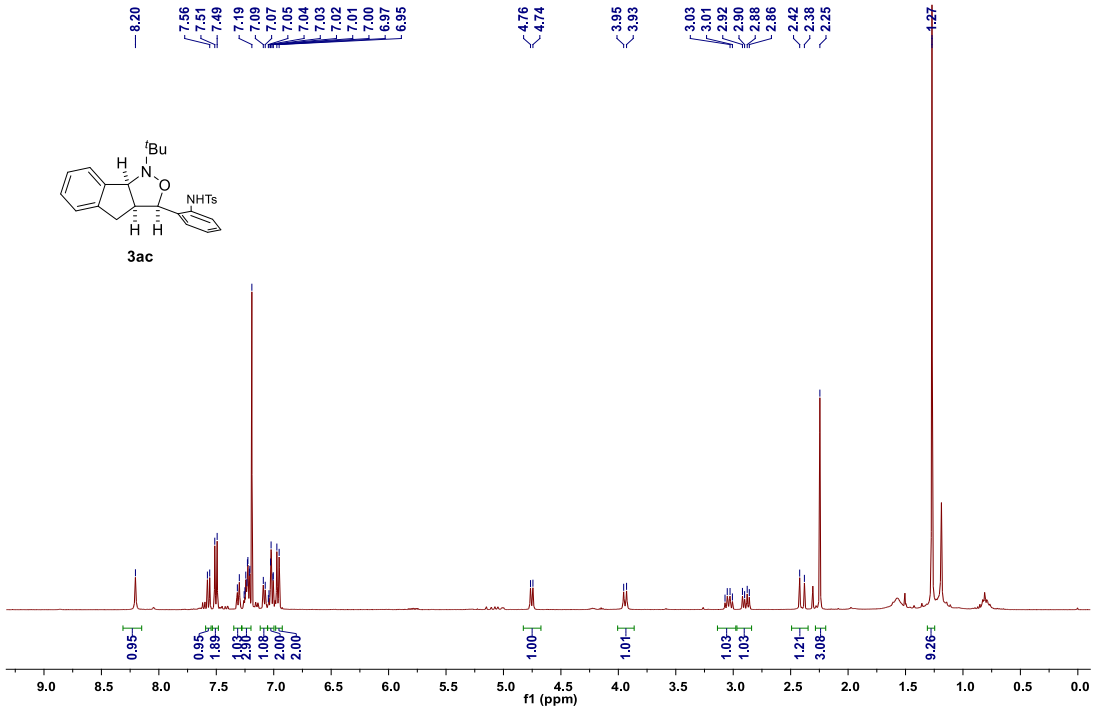
77.01
76.69
69.41
61.57
59.58
51.68
33.38
32.06
27.02
tBu
H
N
O
OH
H H
3ab
165 155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15
f1 (ppm)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7.04
7.03
7.02
7.01
7.00
6.97
6.95
4.76
4.74
3.95
3.93
3.03
3.01
2.92
2.90
2.88
2.86
2.42
2.38
2.25
1.27
tBu
H
N
O
NHTs
H
H
3ac
0.95
0.95
1.89
1.03
2.90
1.08
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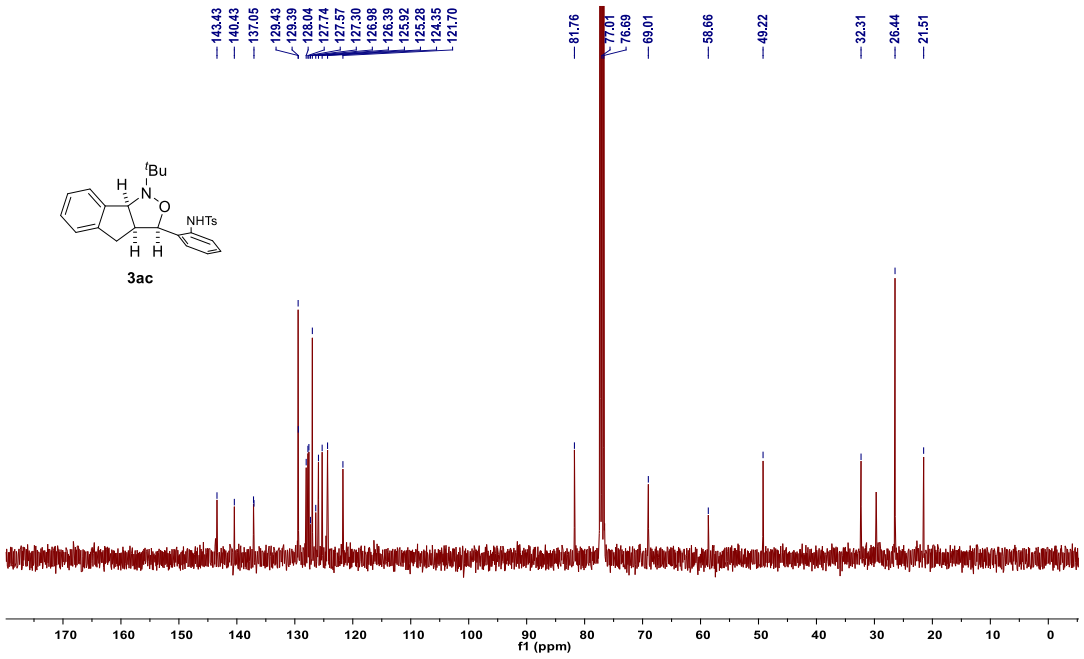
2.00
1.00
1.01
1.03
1.03
1.21
3.08
9.26
f1 (ppm)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126.39
125.92
125.28
124.35
121.70
81.76
77.01
76.69
69.01
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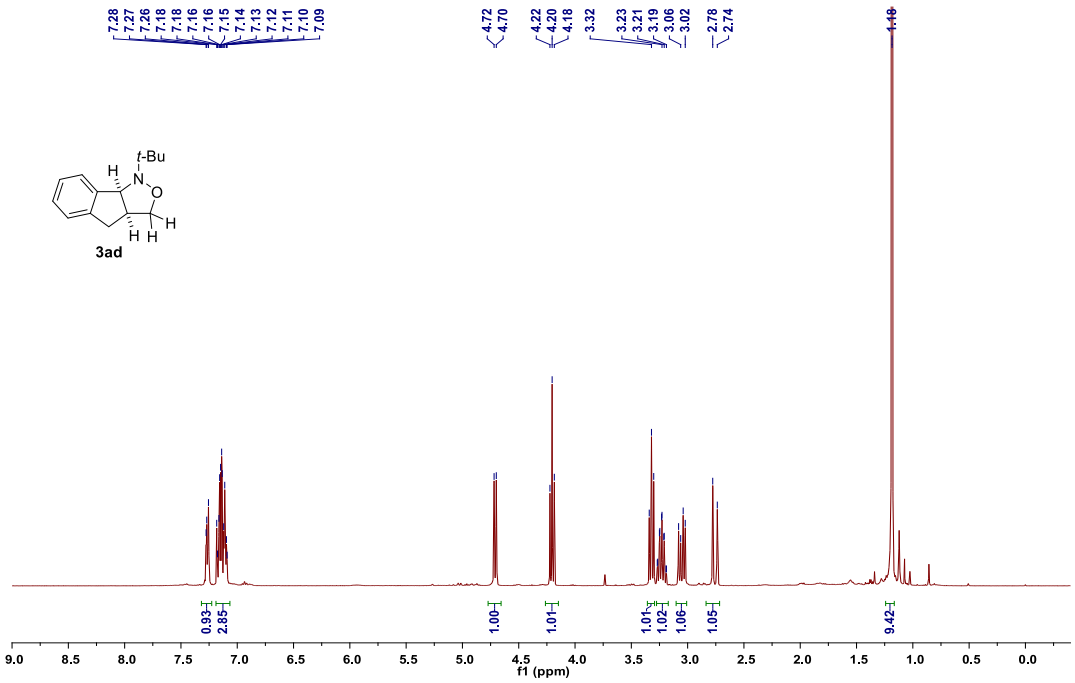
49.22
32.31
26.44
21.51
tBu
H
N
O
NHTs
H
H
3ac
f1 (ppm)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7.16
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7.15
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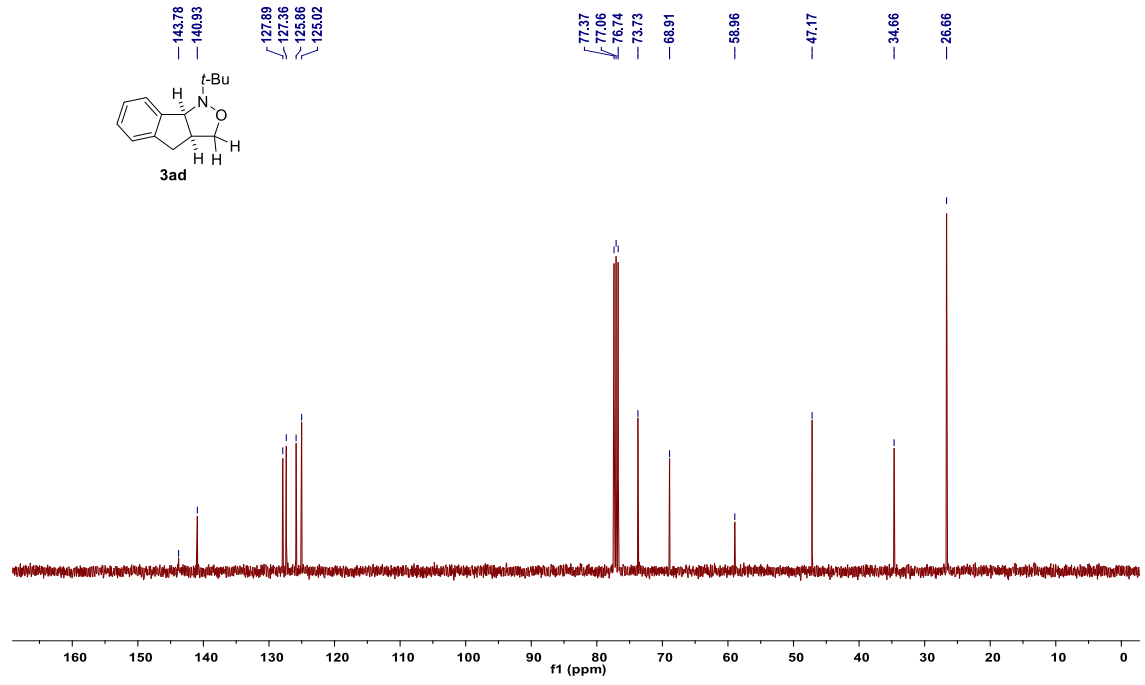
7.13
7.12
7.11
7.10
7.09
4.72
4.70
4.22
4.20
4.18
3.32
3.23
3.21
3.19
3.06
3.02
2.78
2.74
1.18
t-Bu
H
N
O
H
H H
3ad
0.93
2.85
1.00
1.01
1.01
1.02
1.06
1.05
9.42
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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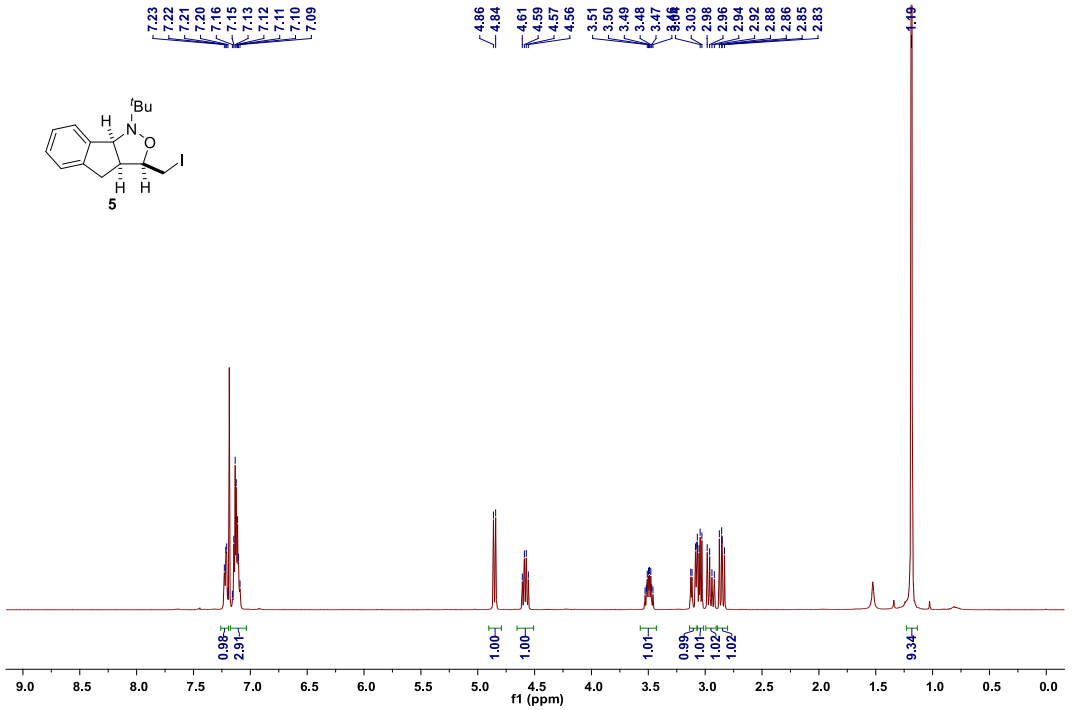
125.02
77.37
77.06
76.74
73.73
68.91
58.96
47.17
34.66
26.66
t-Bu
H
N
O
H
H H
3ad
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.21
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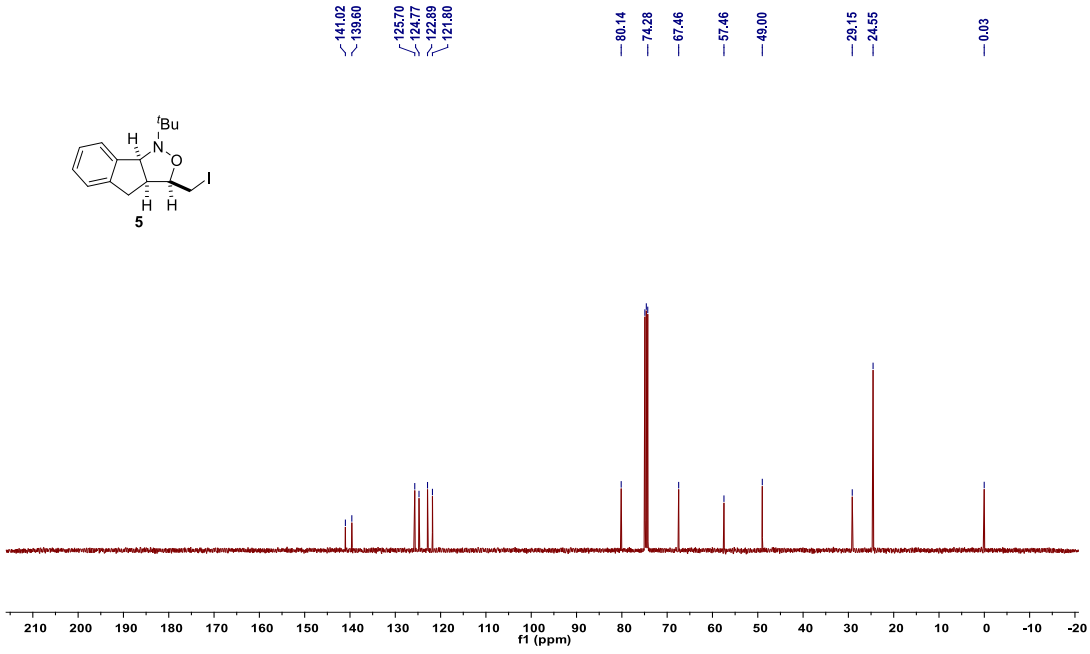
7.16
7.15
7.13
7.12
7.11
7.10
7.09
4.86
4.84
4.61
4.59
4.57
4.56
3.51
3.50
3.49
3.48
3.47
3.03
2.98
2.96
2.94
2.92
2.88
2.86
2.85
2.83
1.19
tBu
H
N
O
I
H
H
5
0.98
2.91
1.00
1.00
1.01
0.99
1.01
1.02
1.02
9.34
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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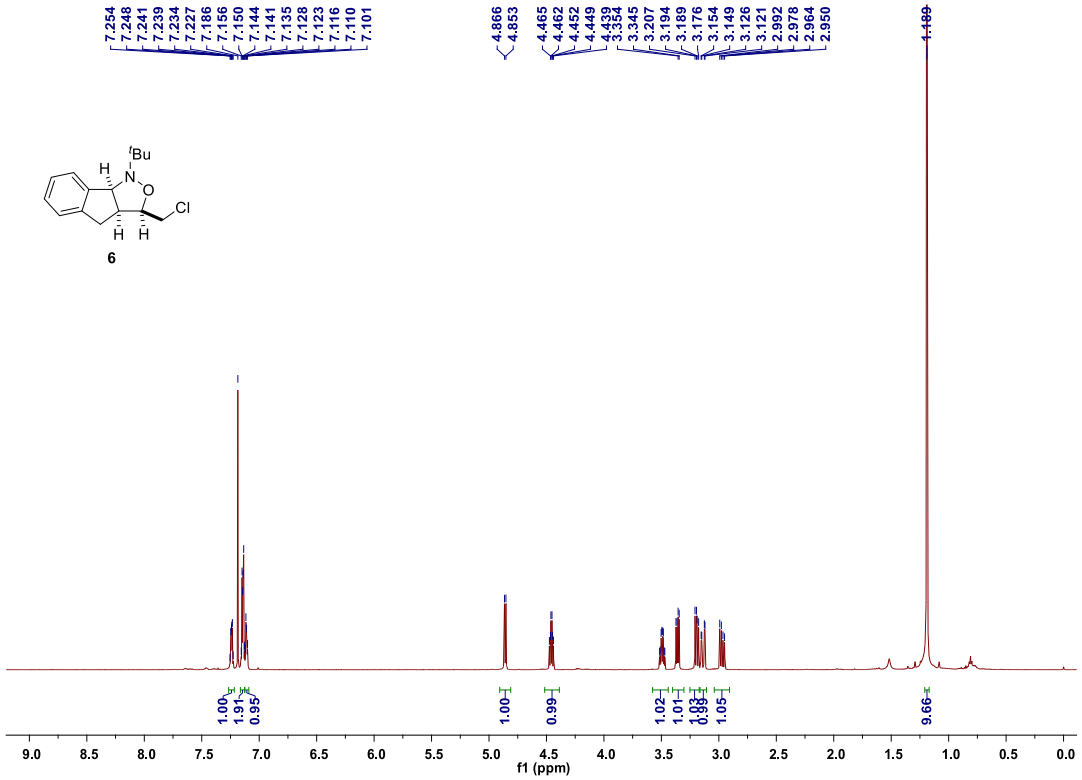
121.80
80.14
74.28
67.46
57.46
49.00
29.15
24.55
0.03
tBu
H
N
O
I
H
H
5
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.135
7.128
7.123
7.116
7.110
7.101
4.866
4.853
4.465
4.462
4.452
4.449
4.439
3.354
3.345
3.207
3.194
3.189
3.176
3.154
3.149
3.126
3.121
2.992
2.978
2.964
2.950
1.189
tBu
H
N
O
Cl
H
H
6
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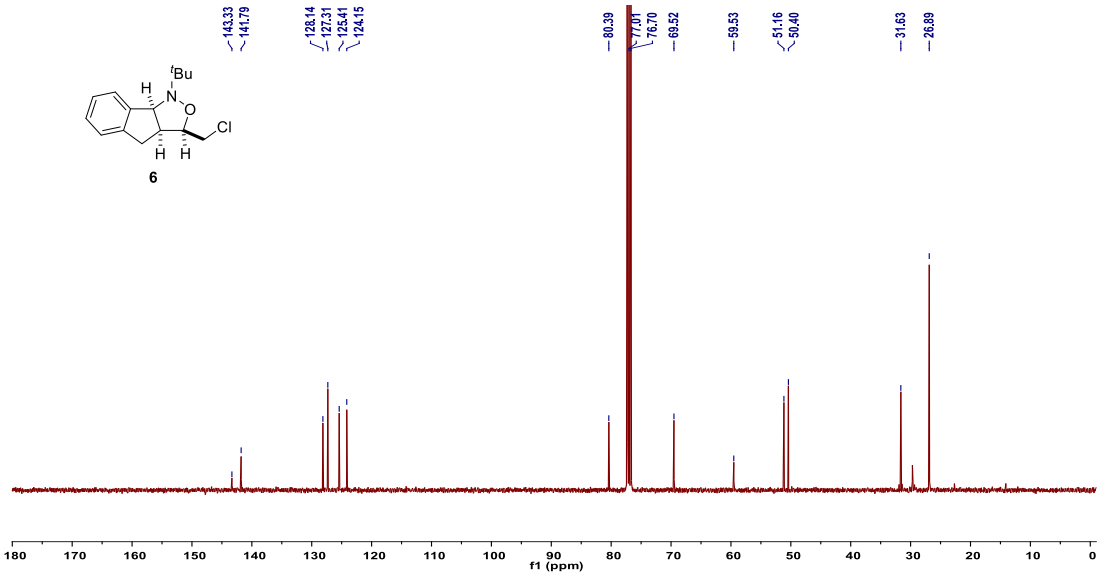
1.00
0.99
1.02
1.01
1.03
0.93
1.05
9.66
f1 (ppm)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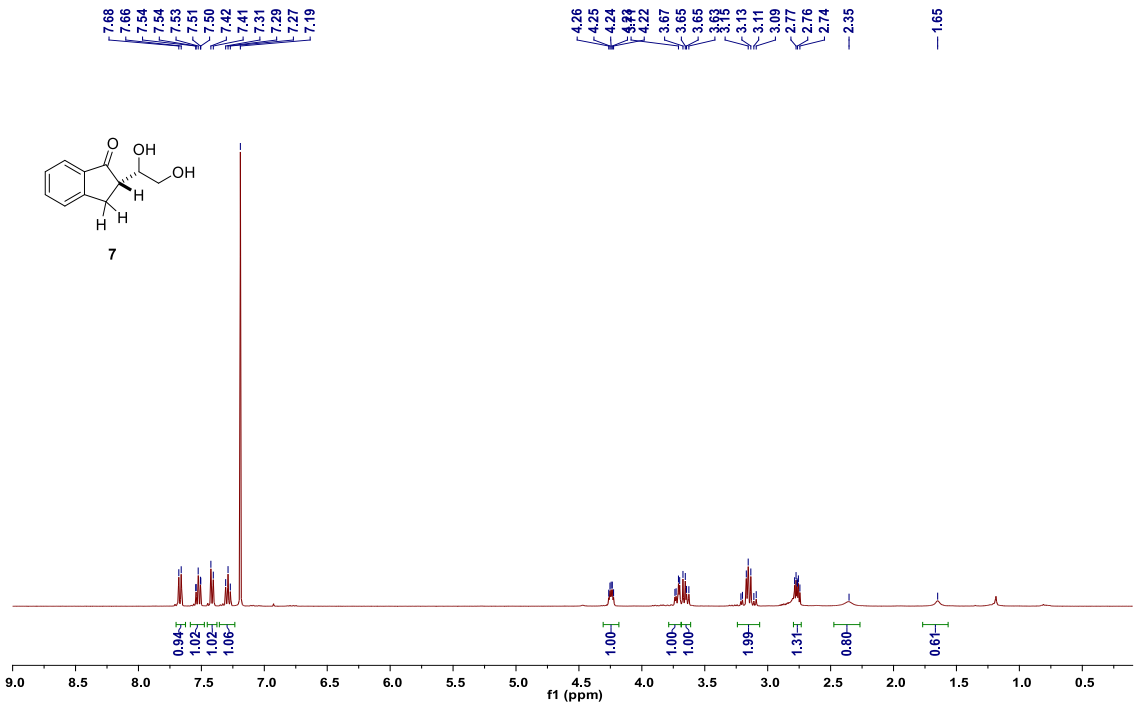
124.15
80.39
77.01
76.70
69.52
59.53
51.16
50.40
31.63
26.89
tBu
H
N
O
Cl
H
H
6
f1 (ppm)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7.29
7.27
7.19
4.26
4.25
4.24
4.22
3.67
3.65
3.65
3.63
3.13
3.11
3.09
2.77
2.76
2.74
2.35
1.65
O
OH
OH
H
H
7
0.94
1.02
1.02
1.06
1.00
1.00
1.00
1.99
1.31
0.80
0.61
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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1.5
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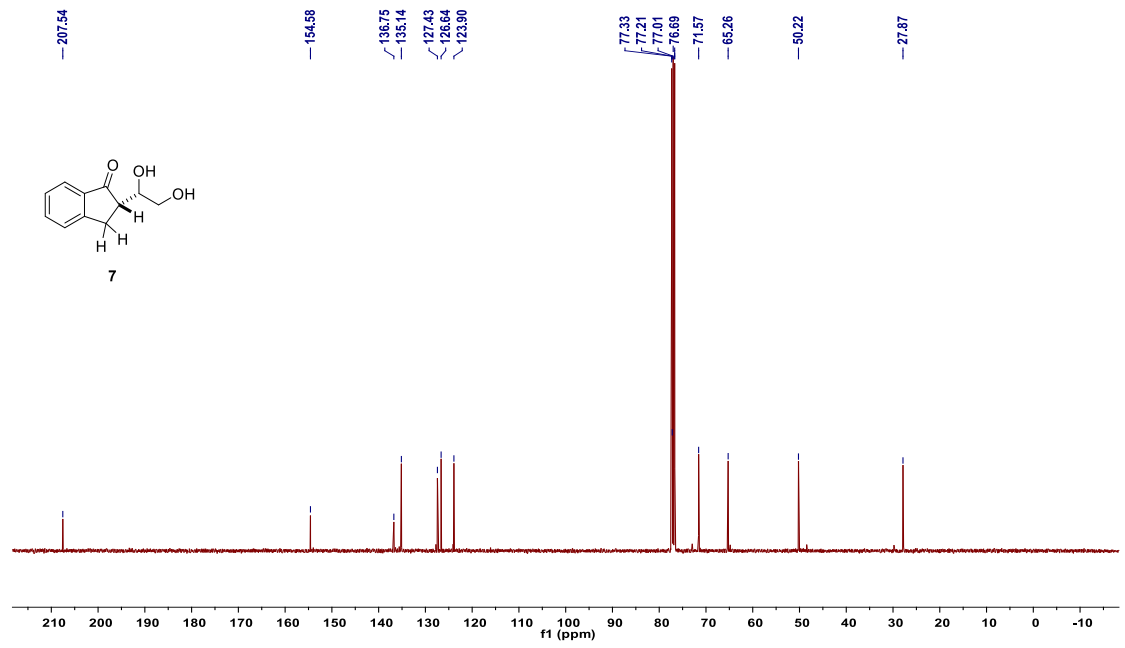
f1 (ppm)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77.01
76.69
71.57
65.26
50.22
27.87
O
OH
OH
H
H
7
210
200
190
180
170
160
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100
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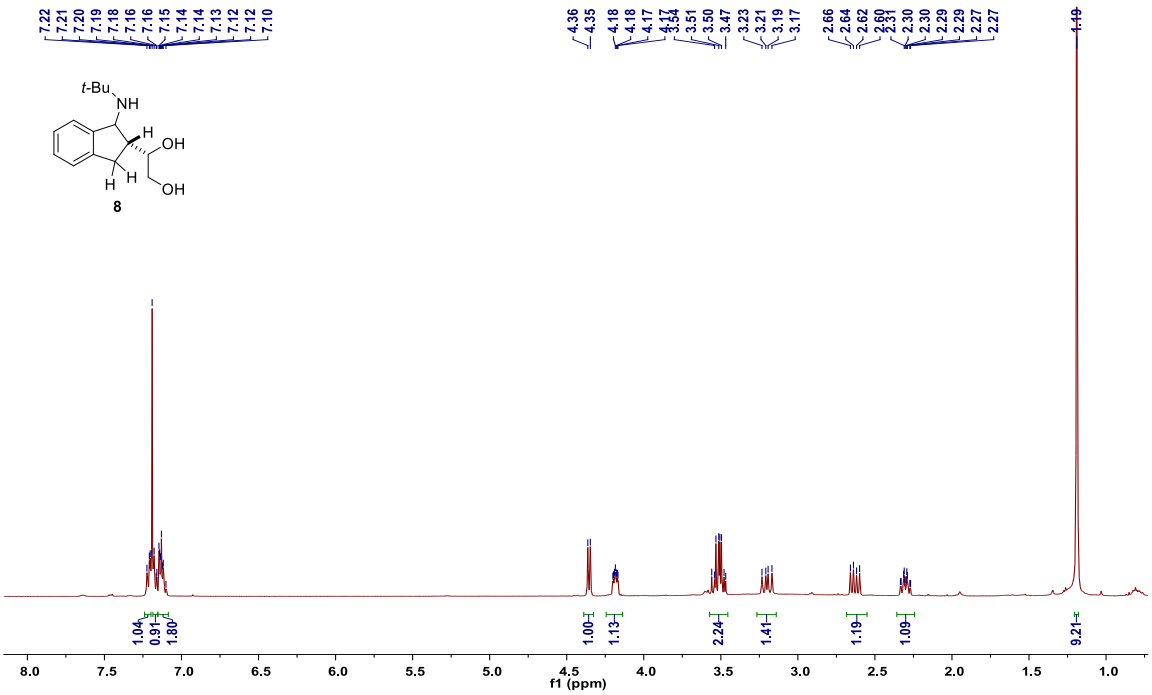
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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4.18
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4.17
4.17
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3.50
3.47
3.23
3.21
3.19
3.17
2.66
2.64
2.62
2.60
2.31
2.30
2.30
2.29
2.29
2.27
2.27
1.10
t-Bu
NH
H
OH
H
H
OH
8
1.04
0.91
1.80
1.00
1.13
2.24
1.41
1.19
1.09
9.21
8.0
7.5
7.0
6.5
6.0
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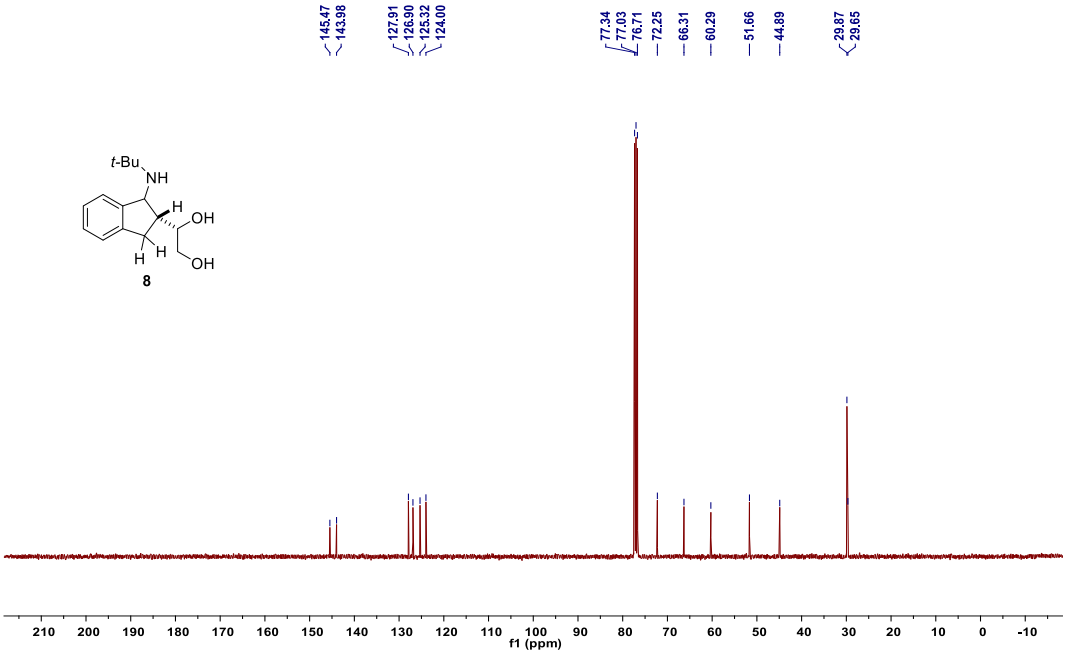
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)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127.91
126.90
125.32
124.00
77.34
77.03
76.71
72.25
66.31
60.29
51.66
44.89
29.87
29.65
t-Bu
NH
H
OH
H
H
OH
8
210
200
190
180
170
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100
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80
70
60
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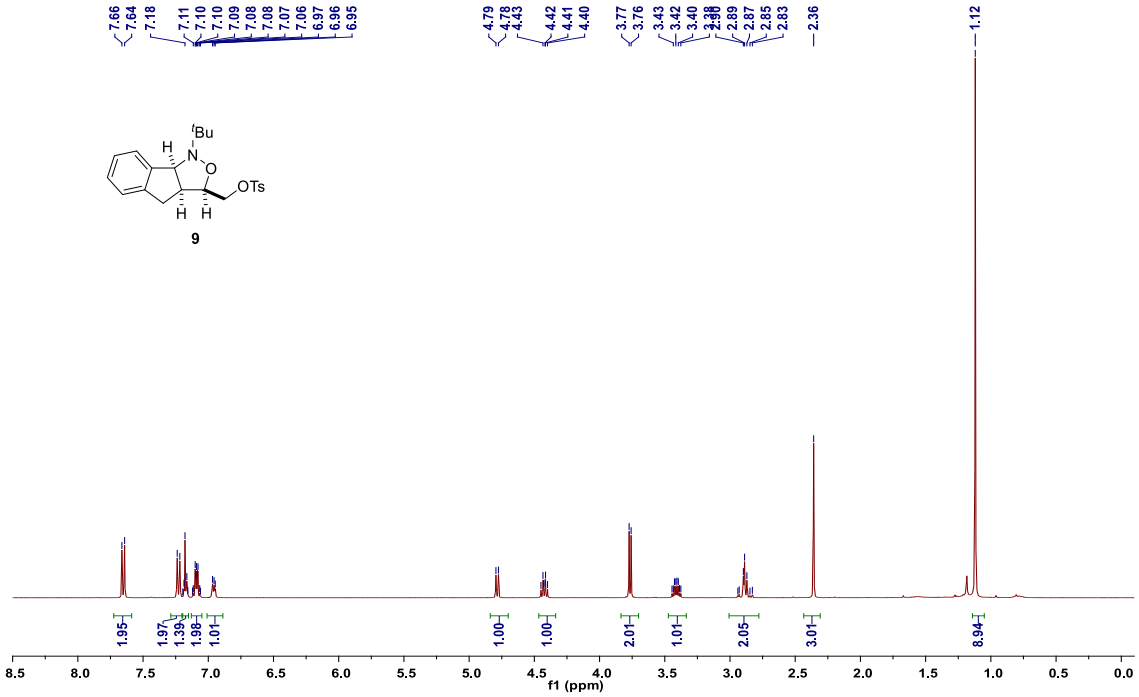
40
30
20
10
0
-10
f1 (ppm)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7.64
7.18
7.11
7.10
7.10
7.09
7.08
7.08
7.07
7.06
6.97
6.96
6.95
4.79
4.78
4.43
4.42
4.41
4.40
3.77
3.76
3.43
3.42
3.40
2.89
2.87
2.85
2.83
2.36
1.12
tBu
H
N
O
OTs
H H
9
1.95
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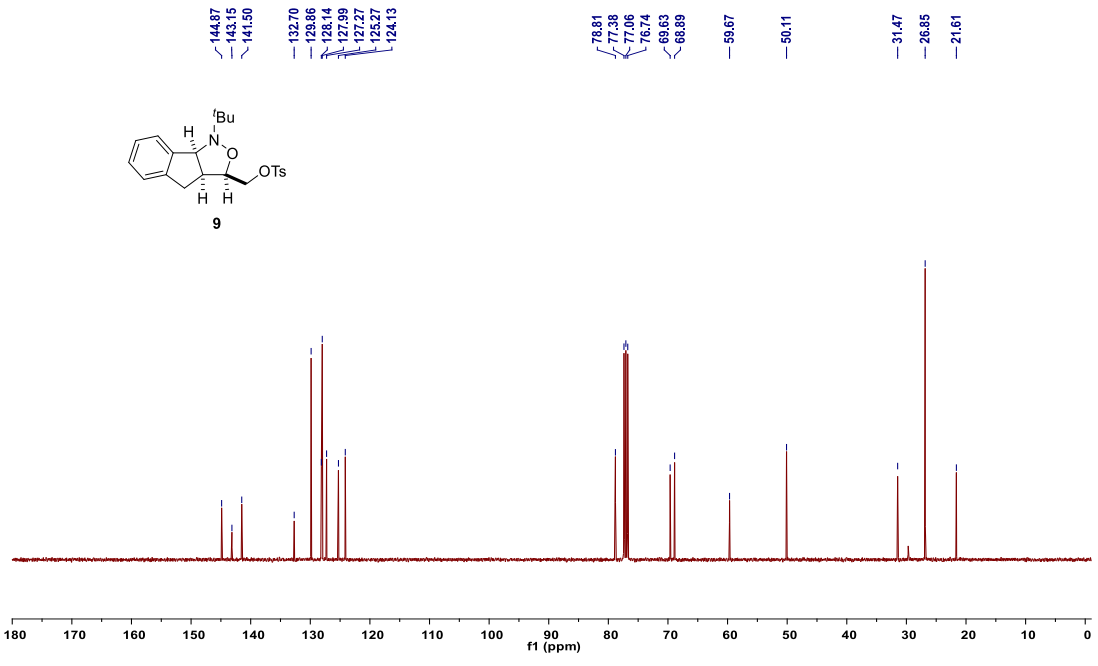
1.01
2.05
3.01
8.94
f1 (ppm)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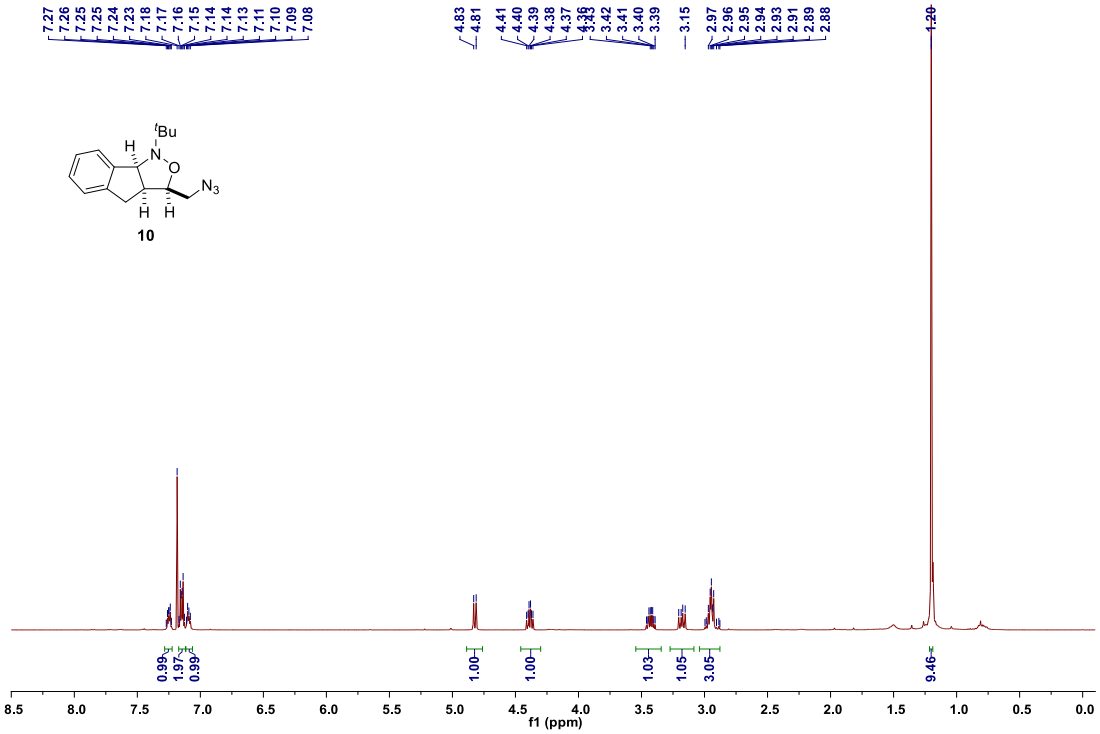
129.86
128.14
127.99
127.27
125.27
124.13
78.81
77.38
77.06
76.74
69.63
68.89
59.67
50.11
31.47
26.85
21.61
tBu
H
N
O
OTs
H H
9
f1 (ppm)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7.14
7.13
7.11
7.10
7.09
7.08
4.83
4.81
4.41
4.40
4.39
4.38
4.37
4.36
4.35
3.43
3.42
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2.96
2.95
2.94
2.93
2.91
2.89
2.88
1.20
tBu
H
N
O
N3
H
H
10
0.99
1.97
0.99
1.00
1.00
1.03
1.05
3.05
9.46
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8.0
7.5
7.0
6.5
6.0
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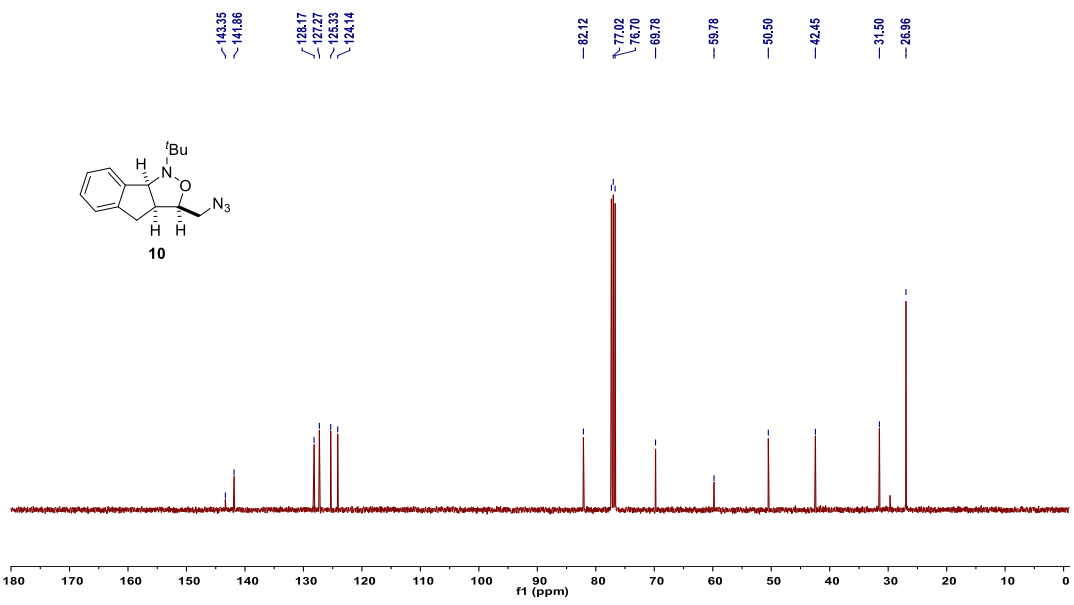
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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125.33
124.14
82.12
77.02
76.70
69.78
59.78
50.50
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31.50
26.96
tBu
H
N
O
N3
H
H
10
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.295
7.291
7.274
7.262
7.257
7.244
7.240
7.225
7.197
7.193
7.188
7.182
7.170
7.162
7.158
7.152
7.147
7.138
7.132
7.125
7.108
7.095
7.081
7.060
4.572
4.552
3.949
3.939
3.904
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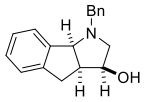
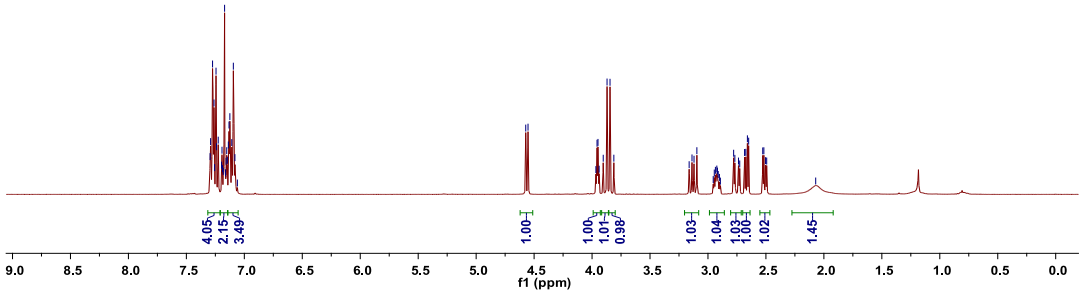
3.845
3.812
3.138
3.120
3.096
2.924
2.893
2.726
2.649
2.518
2.071


Bn
H
N
OH
H
H

11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1.01
0.98
1.03
1.04
1.03
1.00
1.02
1.45
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


143.36
141.34
139.27
128.81
128.37
127.98
127.06
126.31
125.84
125.02
77.79
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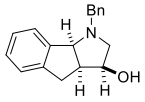
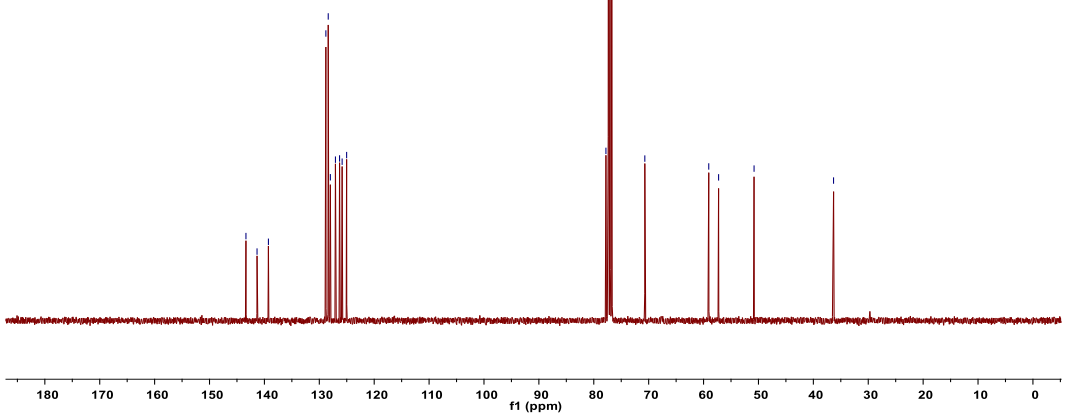
70.70
59.06
57.26
50.80
36.32


Bn
H
N
OH
H
H

11


180
170
160
150
140
130
120
110
100
90
80
70
60
50
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30
20
10
0
f1 (ppm)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RB3_01_12730.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

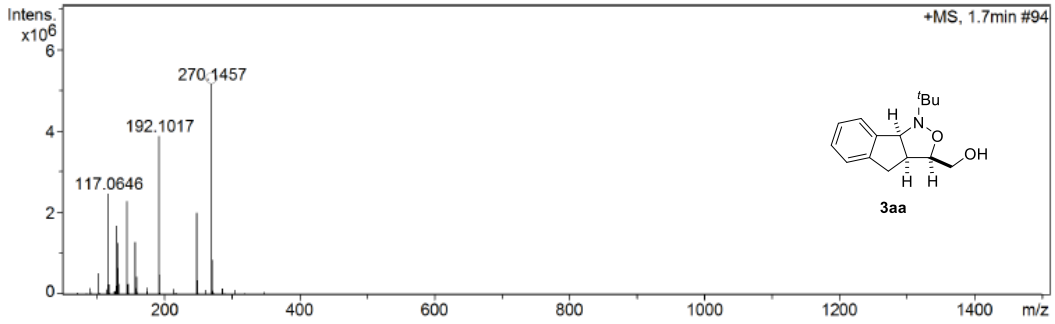
Acquisition D 2022-04-13 11:44:52

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
270.1457	1	C15H21NNaO2	270.1464	2.8	3.2	1		100.00	6.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0617_GA7_01_14488.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617

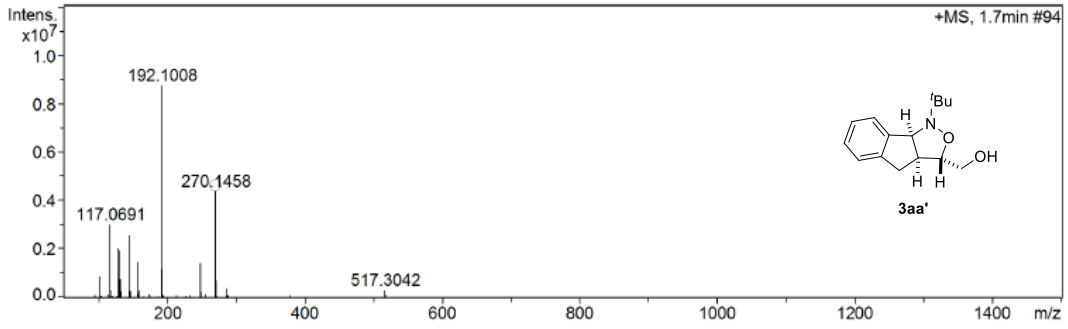
Acquisition D 2022-06-20 12:33:32

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
270.1458	1	C15H21NNaO2	270.1464	2.3	2.8	1		100.00	6.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RA8_01_12727.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

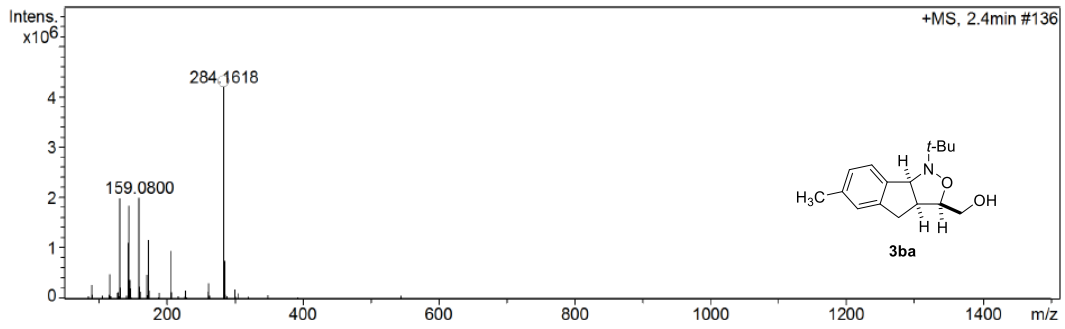
Acquisition D 2022-04-13 11:21:46

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
284.1618	1	C16H23NNaO2	284.1621	1.0	1.3	1	100.00	6.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RA5_01_12715.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

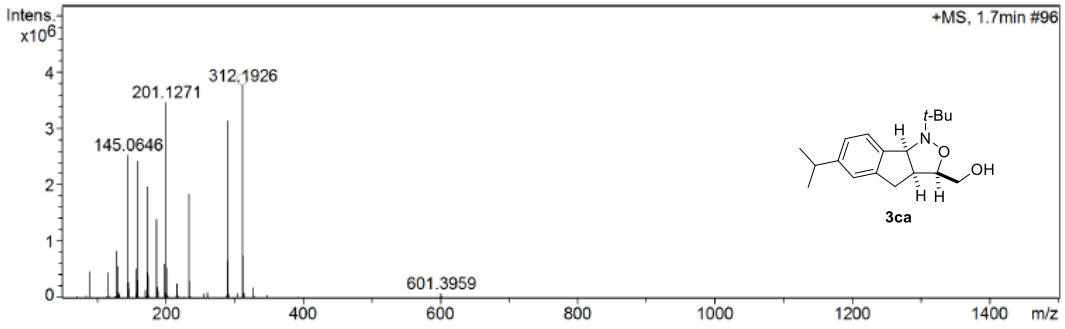
Acquisition D 2022-04-13 9:43:00

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
312.1926	1	C18H27NNaO2	312.1934	2.7	1.1	1	100.00	6.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RA6_01_12716.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

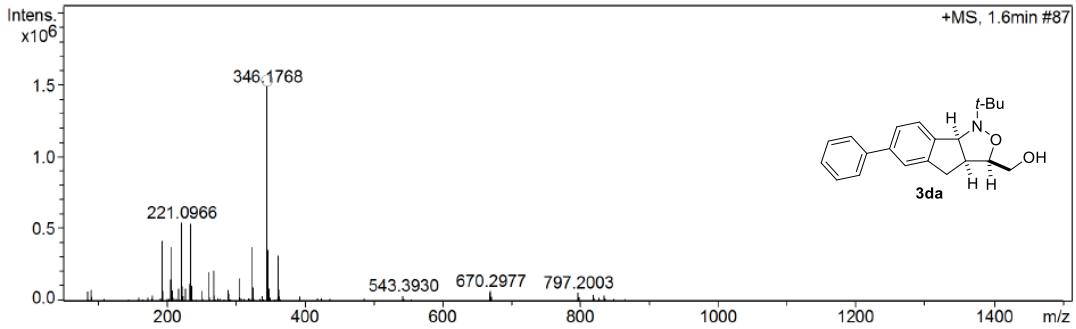
Comment

Acquisition D 2022-04-13 9:50:52

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
346.1768	1	C21H25NNaO2	346.1777	2.7	2.3	1	100.00	10.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RB4_01_12731.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

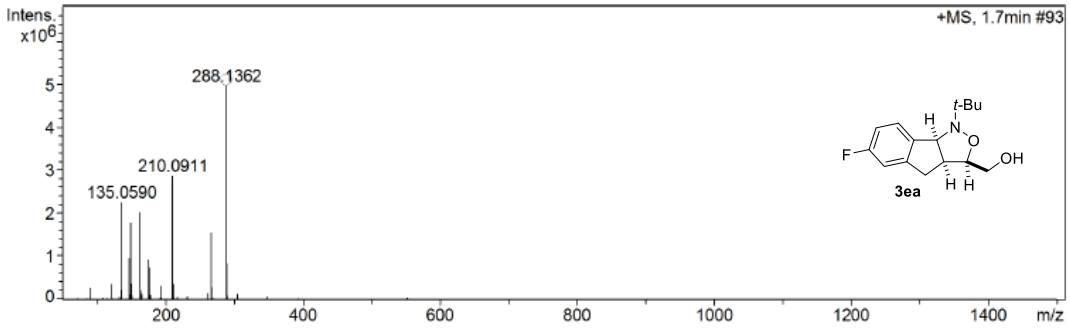
Comment

Acquisition D 2022-04-13 11:53:01

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
288.1362	1	C15H20FNNaO2	288.1370	2.8	0.2	1	100.00	6.0	even		ok

Mass Spectrum SmartFormula Report

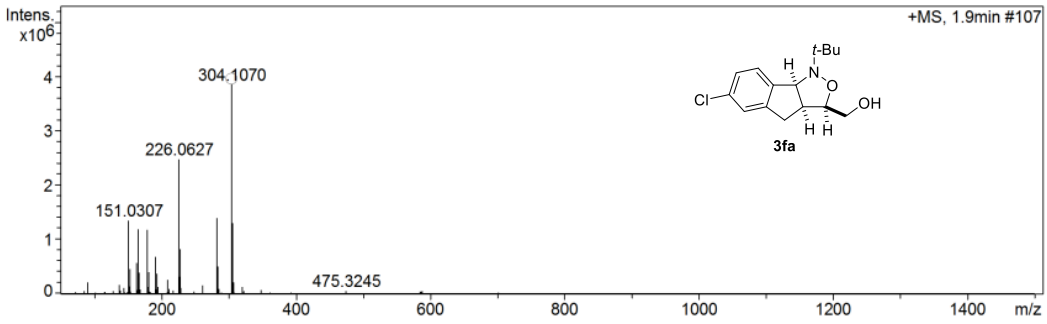
Analysis Info

Analysis Name G:\ZM MS\0412_RA4_01_12714.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412
Comment

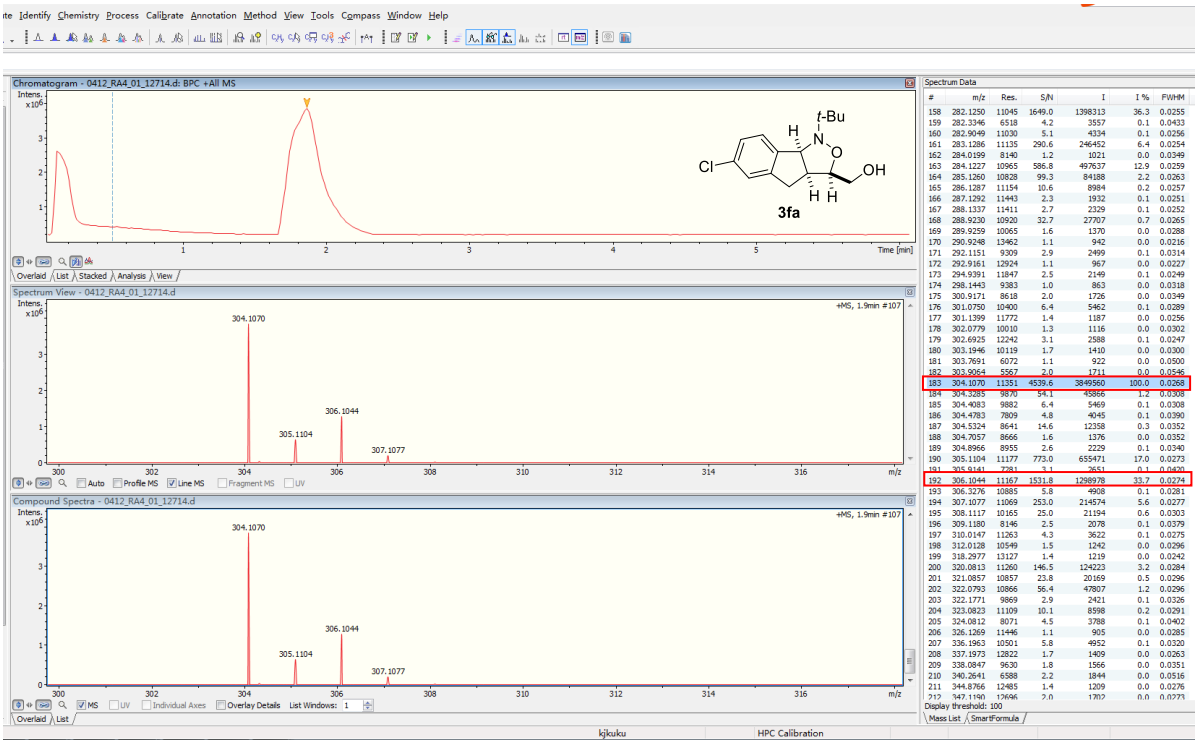
Acquisition D 2022-04-13 9:35:39
Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
304.1070	1	C15H20ClNNaO2	304.1075	1.6	0.7		1	100.00	6.0	even		ok



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RC4_01_12739.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

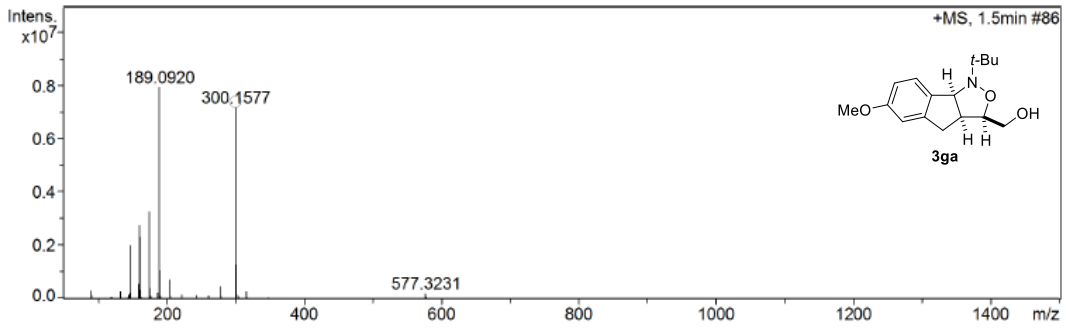
Comment

Acquisition D 2022-04-13 12:55:51

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
300.1577	1	C16H23NNaO3	300.1570	-2.5	1.7	1	100.00	6.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RB8_01_12735.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

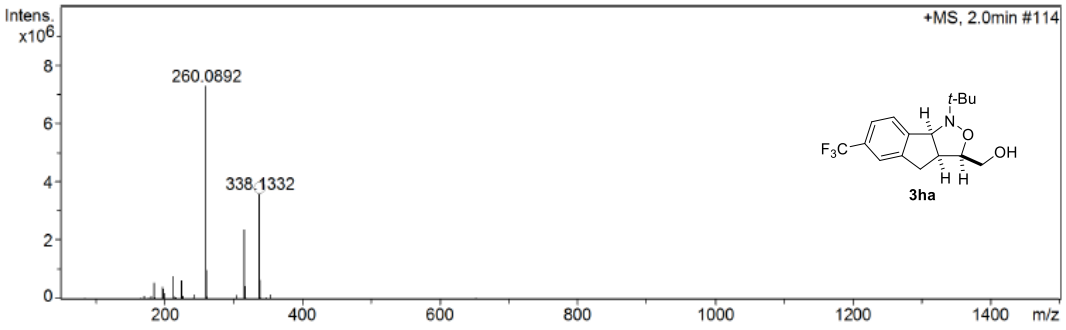
Comment

Acquisition D 2022-04-13 12:24:01

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
338.1332	1	C16H20F3NNaO2	338.1338	1.9	0.3	1	100.00	6.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RB2_01_12729.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

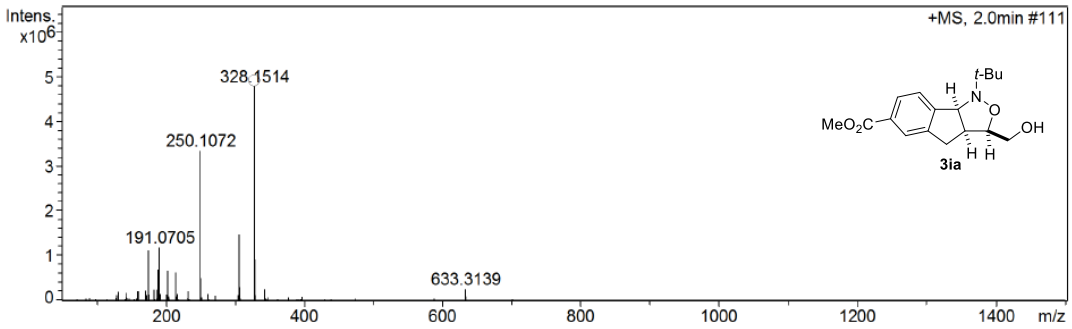
Comment

Acquisition D 2022-04-13 11:36:44

Operator Demo User
Instrumen compact 8255754.2017
6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
328.1514	1	C17H23NNaO4	328.1519	1.7	0.2	1	100.00	7.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RC2_01_12737.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

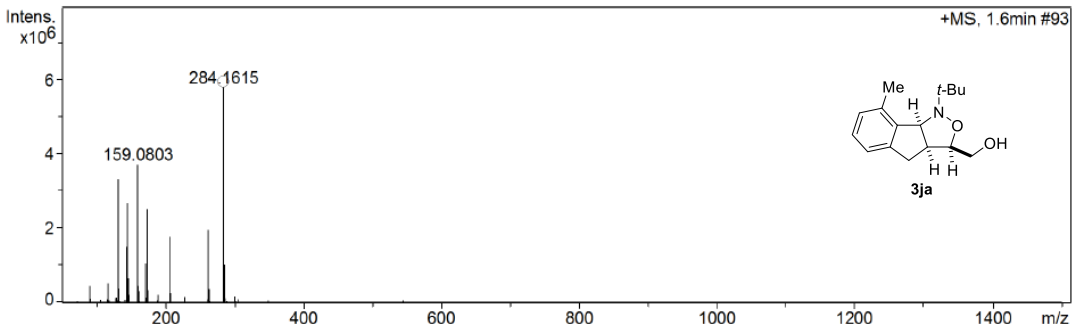
Comment

Acquisition D 2022-04-13 12:39:30

Operator Demo User
Instrumen compact 8255754.2017
6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
284.1615	1	C16H23NNaO2	284.1621	2.1	2.0	1	100.00	6.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

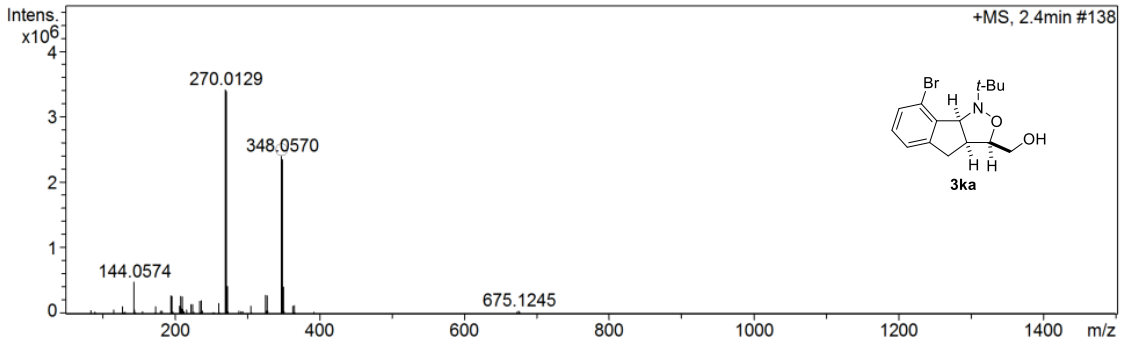
Analysis Name G:\ZM MS\0412_RB1_01_12728.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412
Comment

Acquisition D 2022-04-13 11:29:23

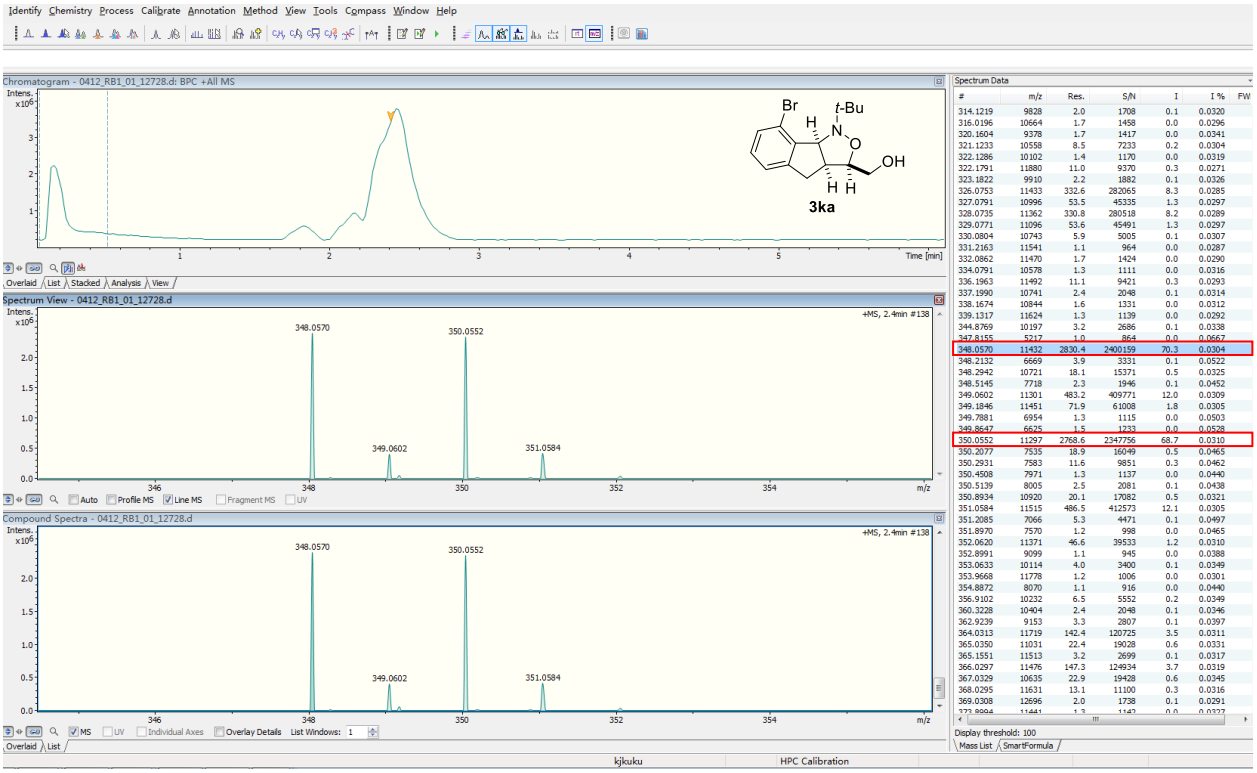
Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
348.0570	1	C15H20BrNNaO2	348.0570	-0.1	6.1	1	100.00	6.0	even	ok



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RC6_01_12741.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

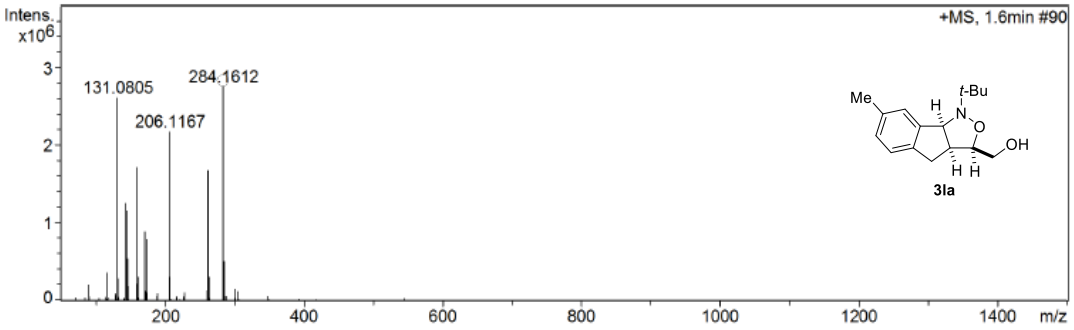
Acquisition D 2022-04-13 13:11:47

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
284.1612	1	C16H23NNaO2	284.1621	3.1	1.5	1	100.00	6.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RC7_01_12742.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

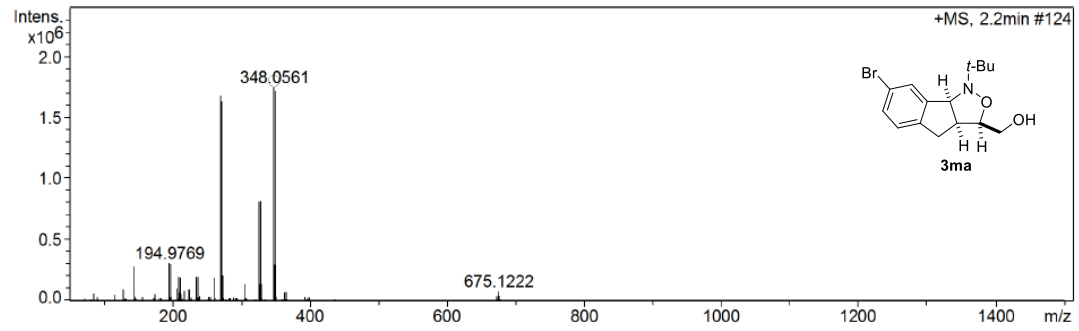
Acquisition D 2022-04-13 13:19:40

Operator Demo User
Instrumen compact 8255754.2017 6

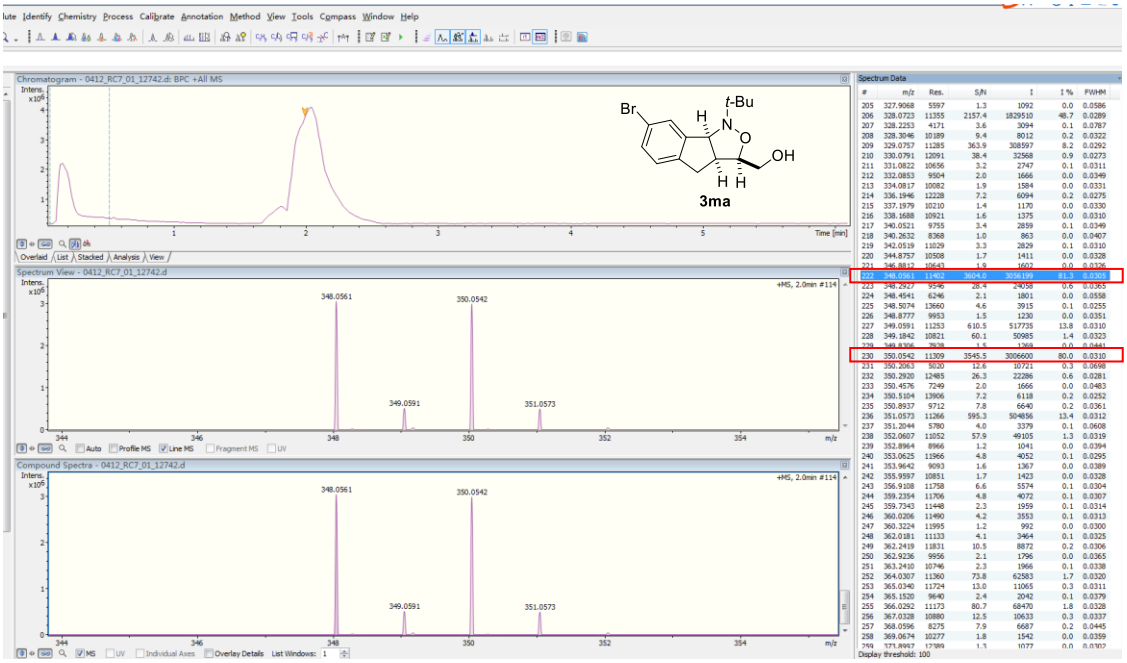
Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
348.0561	1	C15H20BrNNaO2	348.0570	2.6	3.4	1	100.00	6.0	even	ok



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RC3_01_12738.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

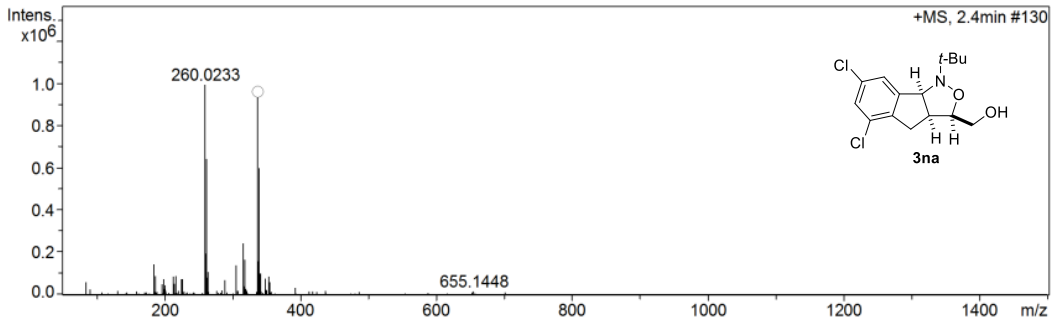
Comment

Acquisition D 2022-04-13 12:47:54

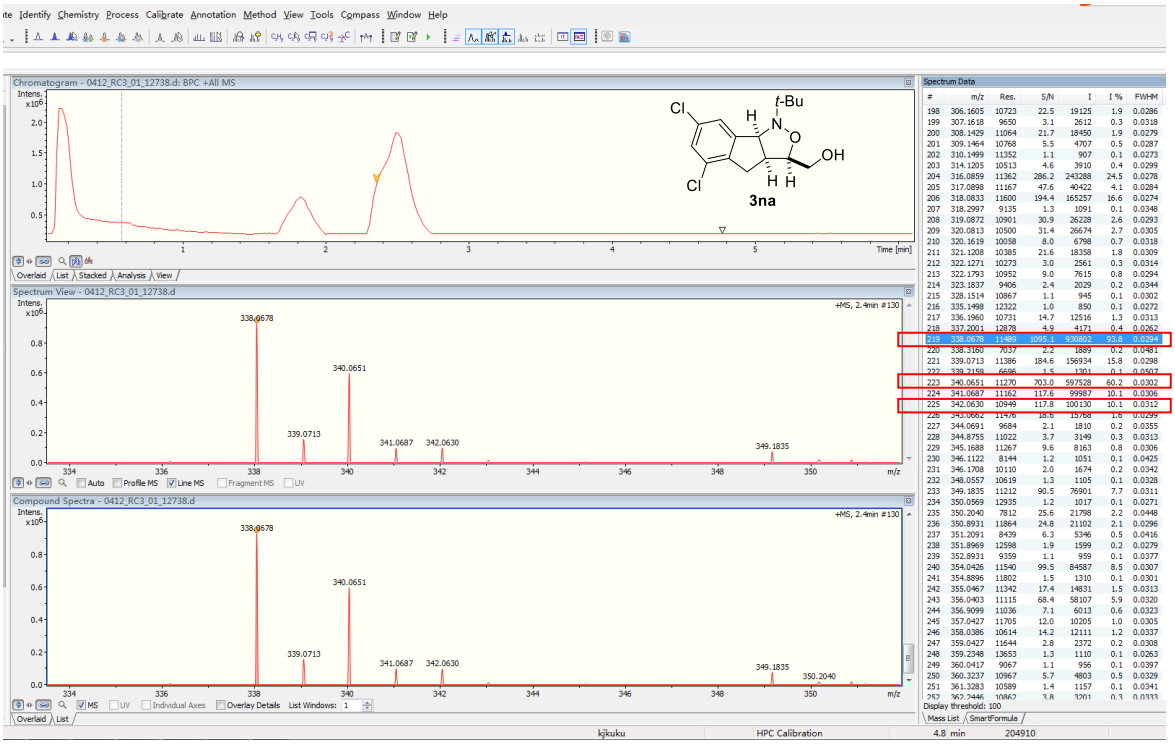
Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
338.0678	1	C15H19Cl2NNaO2	338.0685	2.2	6.8	1	100.00	6.0	even		ok



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RC8_01_12743.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

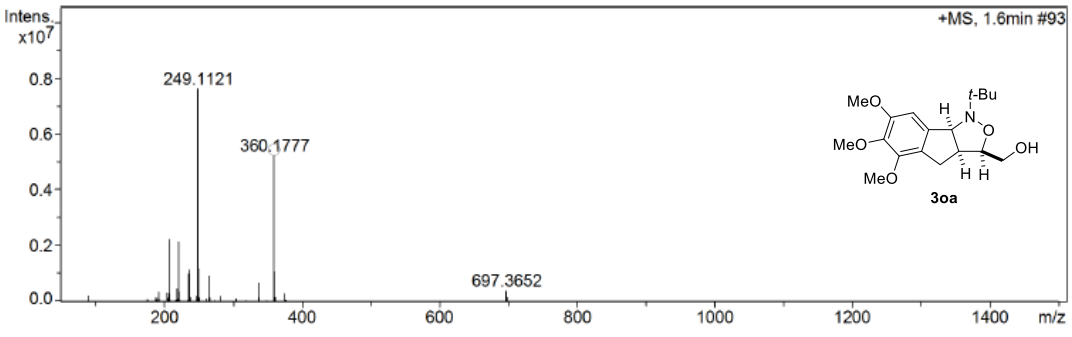
Acquisition D 2022-04-13 13:27:19

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z err [ppm]	mSigma	# mSigma	Score	rdb	e⁻	Conf	N-Rule
360.1777	1	C18H27NNaO5	360.1781	1.3	0.3	1	100.00	6.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0617_GD1_01_14506.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617

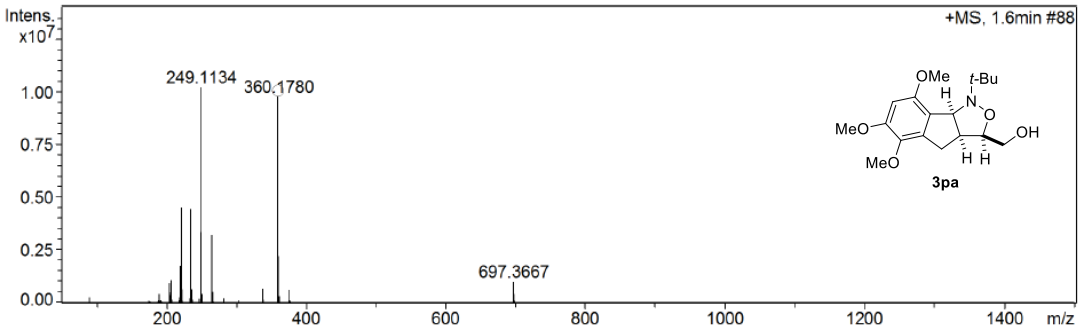
Acquisition D 2022-06-20 14:52:57

Operator Demo User
Instrumen compact 8255754.2017
6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
360.1780	1	C18H27NNaO5	360.1781	0.5	13.7	1	100.00	6.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RA7_01_12726.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

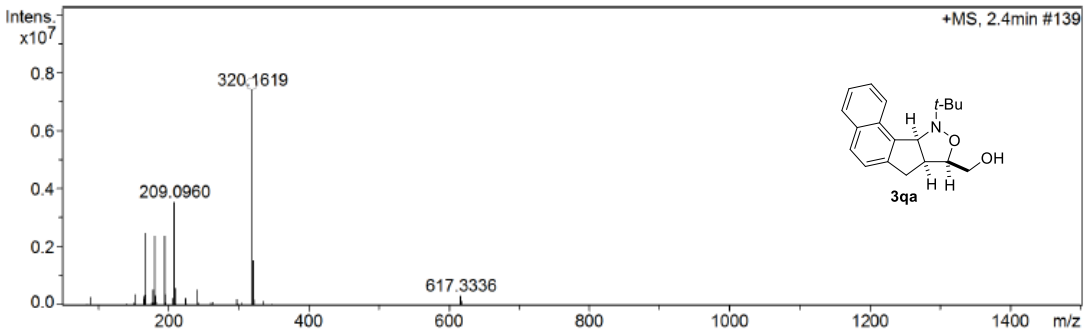
Acquisition D 2022-04-13 11:14:10

Operator Demo User
Instrumen compact 8255754.2017
6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
320.1619	1	C19H23NNaO2	320.1621	0.5	2.7	1	100.00	9.0	even		ok

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Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RD1_01_12744.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

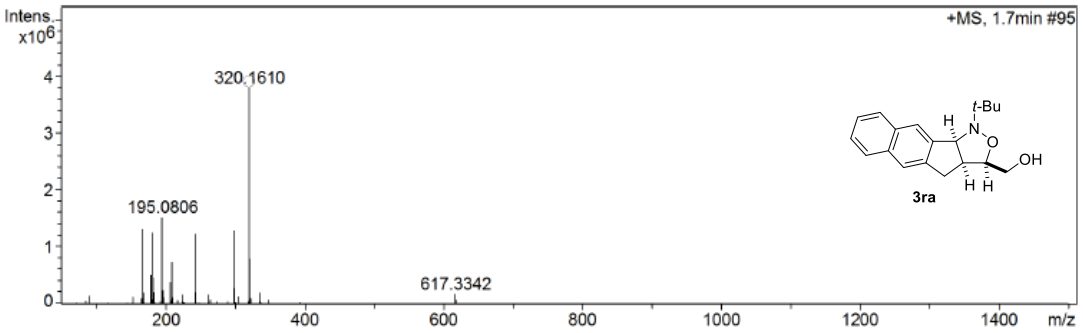
Acquisition D 2022-04-13 13:35:25

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
320.1610	1	C19H23NNaO2	320.1621	3.4	1.7	1	100.00	9.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RC1_01_12736.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

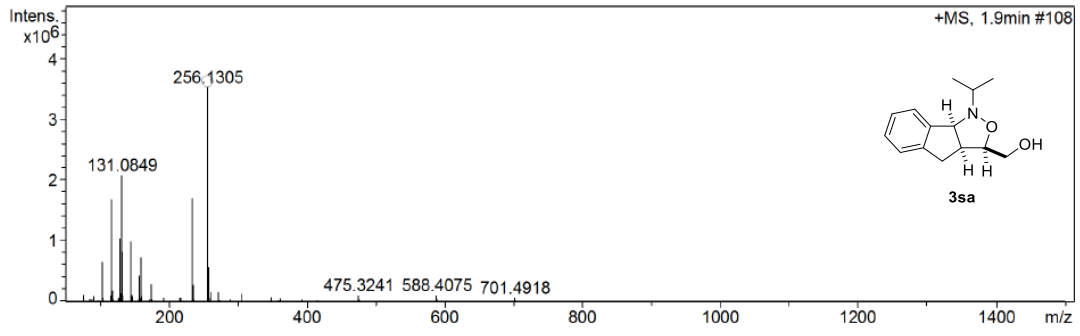
Acquisition D 2022-04-13 12:31:22

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
256.1305	1	C14H19NNaO2	256.1308	1.1	0.3	1	100.00	6.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RB7_01_12734.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

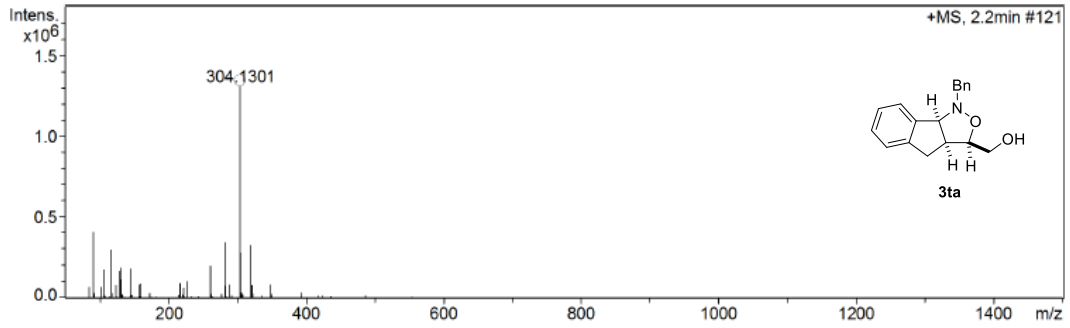
Comment

Acquisition D 2022-04-13 12:16:08

Operator Demo User
Instrumen compact 8255754.2017
6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
304.1301	1	C18H19NNaO2	304.1308	2.1	8.7	1	100.00	10.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0617_GB6_01_14495.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617

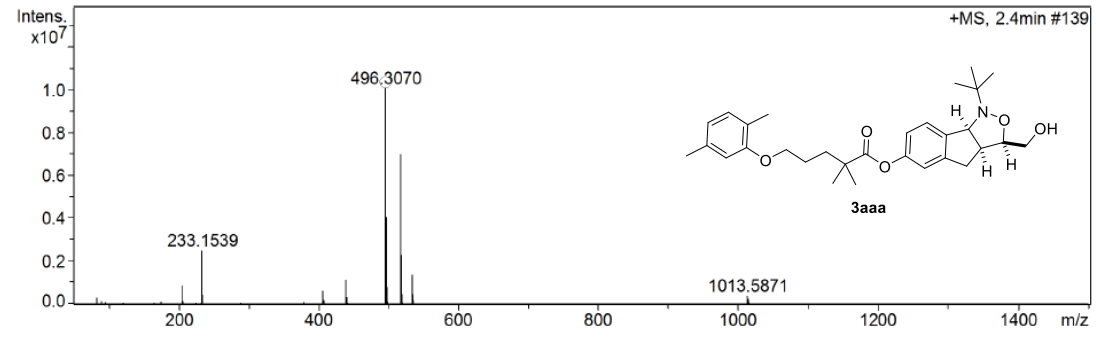
Comment

Acquisition D 2022-06-20 13:27:52

Operator Demo User
Instrumen compact 8255754.2017
6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
496.3070	1	C30H42NO5	496.3057	-2.5	36.1	1	100.00	11.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0621_GC8_01_14599.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0621

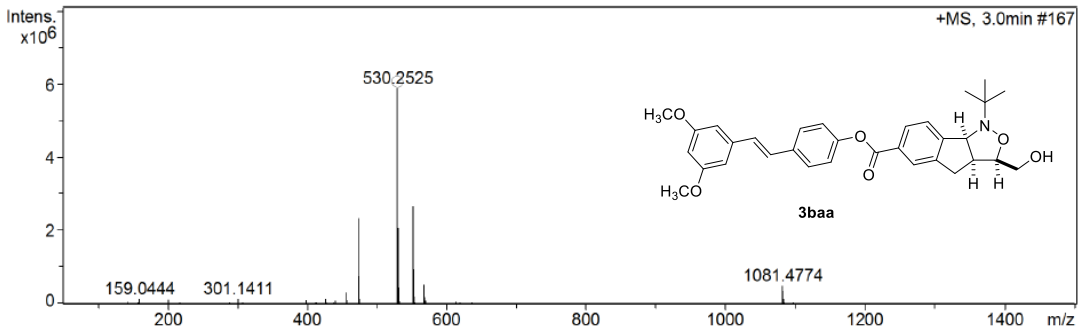
Acquisition D 2022-06-24 16:22:37

Operator Demo User
Instrumen compact 8255754.2017
6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
530.2525	1	C32H36NO6	530.2537	2.3	1.6	1	100.00	16.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0621_GC7_01_14601.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0621

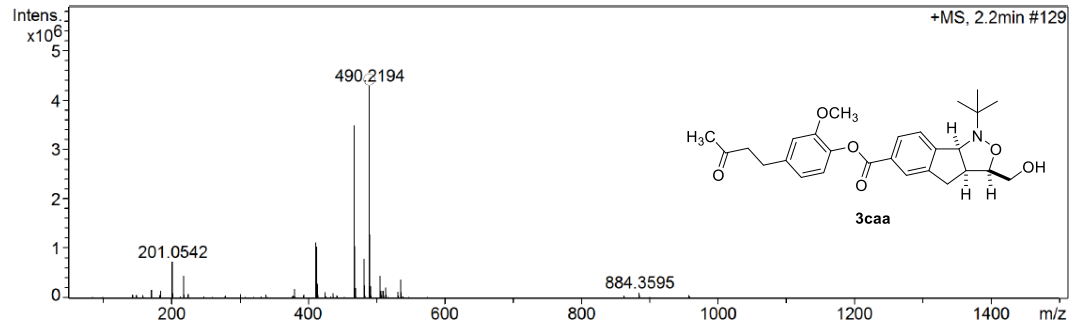
Acquisition D 2022-06-24 16:38:38

Operator Demo User
Instrumen compact 8255754.2017
6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
490.2194	1	C27H33NNaO6	490.2200	1.3	1.2	1	100.00	12.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

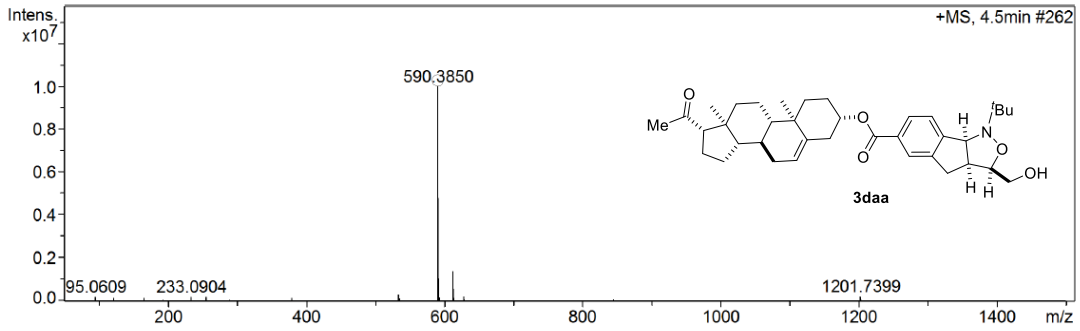
Acquisition D 2022-06-20 12:40:54

Analysis Name G:\ZM MS\0617_GA8_01_14489.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617
Comment

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
590.3850	1	C37H52NO5	590.3840	-1.6	35.0	1	100.00	13.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

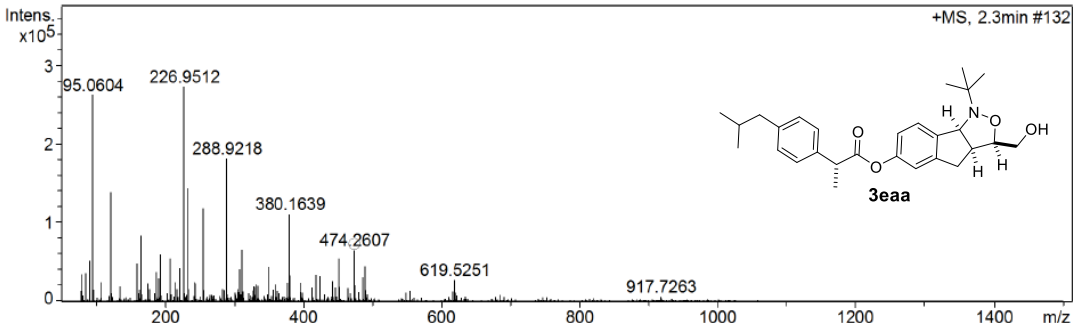
Acquisition D 2022-06-20 13:11:51

Analysis Name G:\ZM MS\0617_GB4_01_14493.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617
Comment

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
474.2607	1	C28H37NNaO4	474.2615	1.7	3.6	1	100.00	11.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

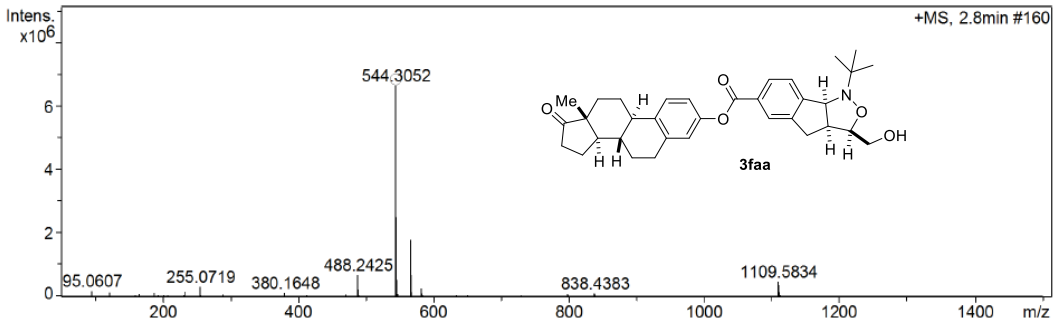
Acquisition D 2022-06-20 12:48:46

Analysis Name G:\ZM MS\0617_GB1_01_14490.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617
Comment

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
544.3052	1	C34H42NO5	544.3057	1.1	1.3		1	100.00	15.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

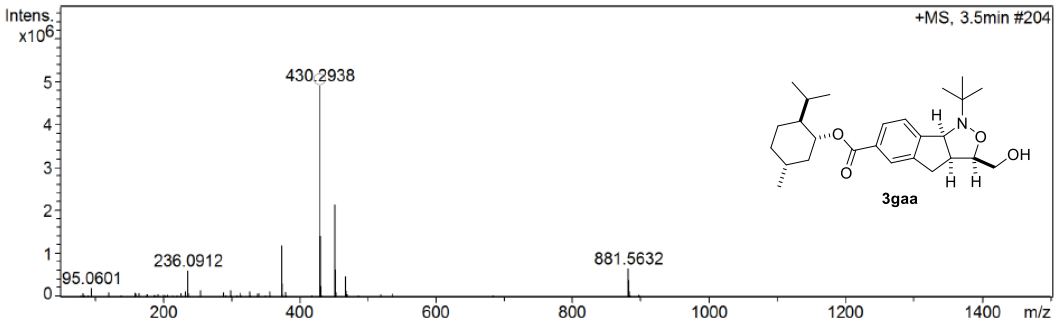
Acquisition D 2022-06-20 13:03:59

Analysis Name G:\ZM MS\0617_GB3_01_14492.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617
Comment

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
430.2938	1	C26H40NO4	430.2952	3.3	0.6		1	100.00	8.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name g:\Desktop\0718_BE3_01_15377.d
Method LC_NO UV_P50-1500_30MIN.m
Sample Name 0718

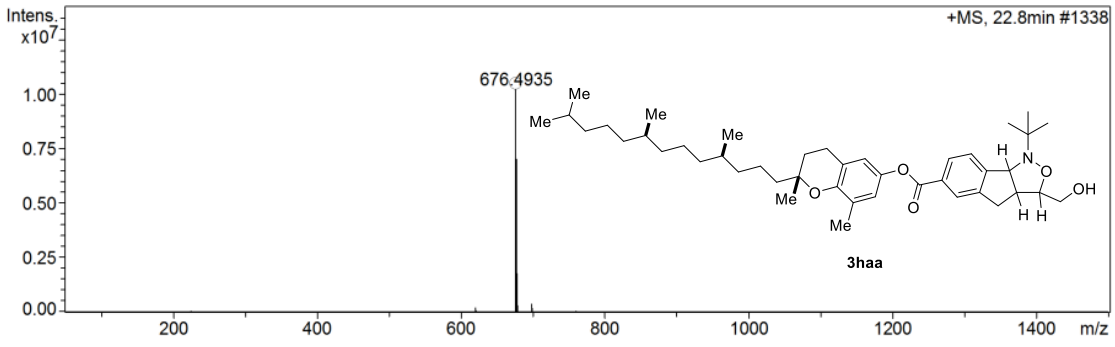
Comment

Acquisition D 2022-07-21 16:28:45

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
676.4935	1	C43H66NO5	676.4936	0.1	108.7	1	100.00	12.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RD3_01_12746.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

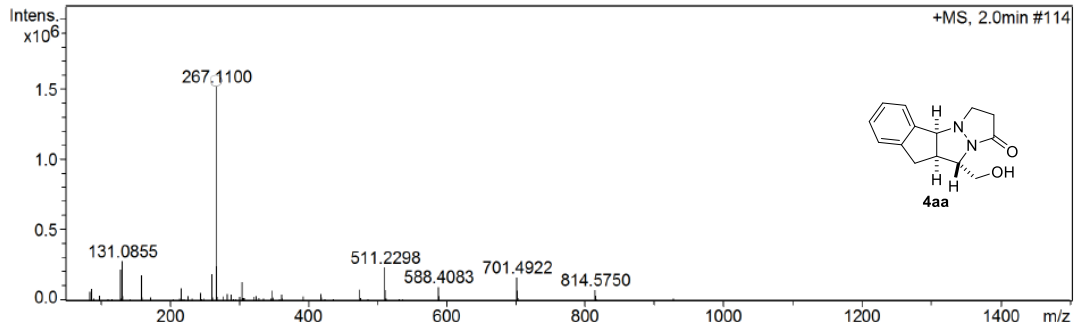
Comment

Acquisition D 2022-04-13 13:51:27

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
267.1100	1	C14H16N2NaO2	267.1104	1.3	1.1	1	100.00	8.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RD2_01_12745.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

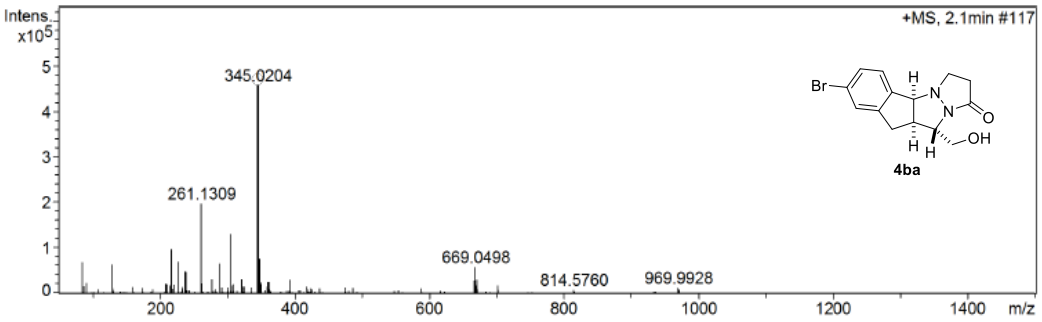
Acquisition D 2022-04-13 13:43:33

Operator Demo User
Instrumen compact 8255754.2017 6

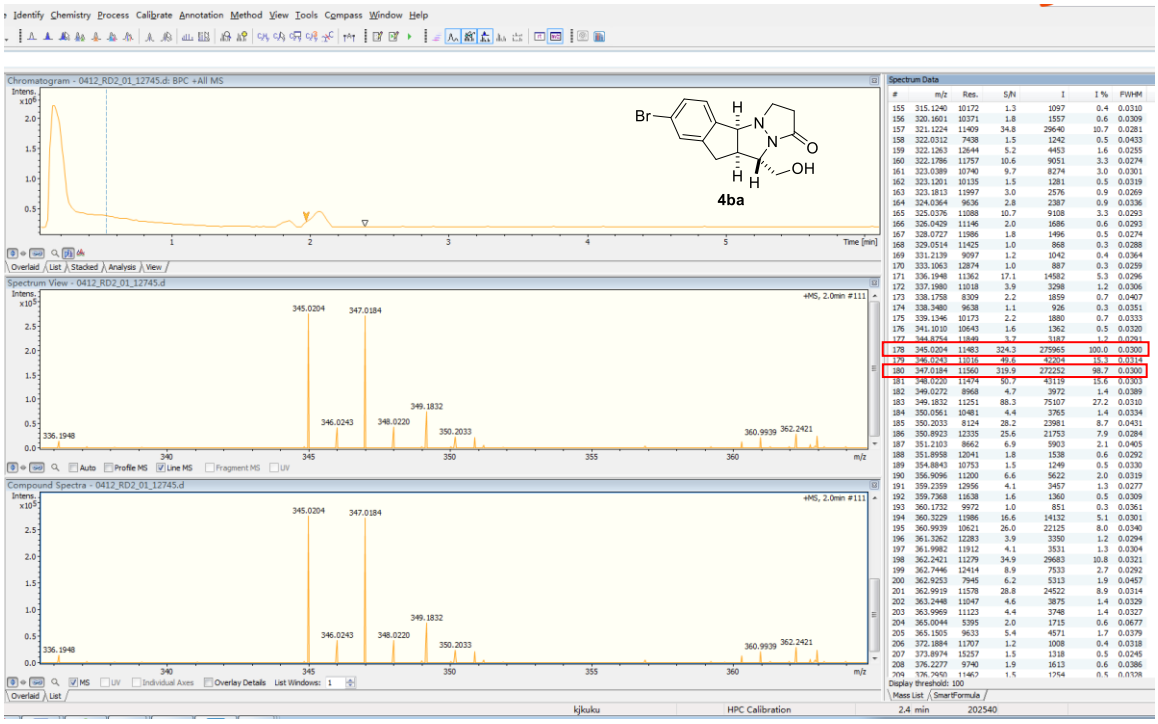
Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Voltage	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥ Conf	N-Rule
345.0204	1	C14H15BrN2NaO2	345.0209	1.4	5.1		1	100.00	8.0	even	ok



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0621_GD1_01_14602.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0621

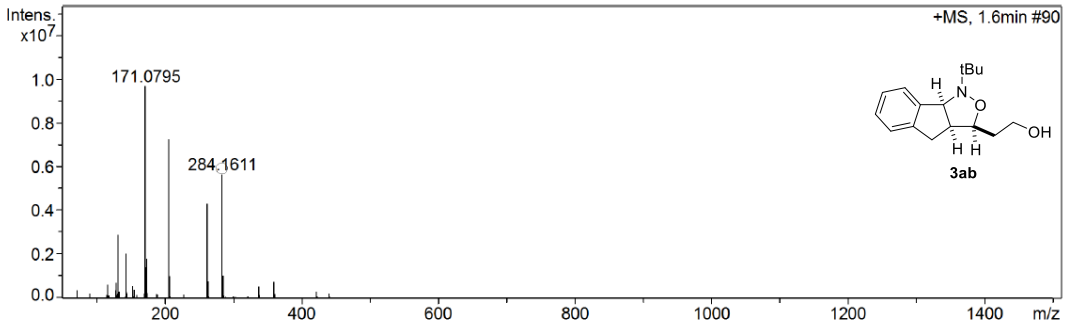
Acquisition D 2022-06-24 16:46:14

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
284.1611	1	C16H23NNaO2	284.1621	3.5	0.5	1	100.00	6.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0617_GD3_01_14508.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617

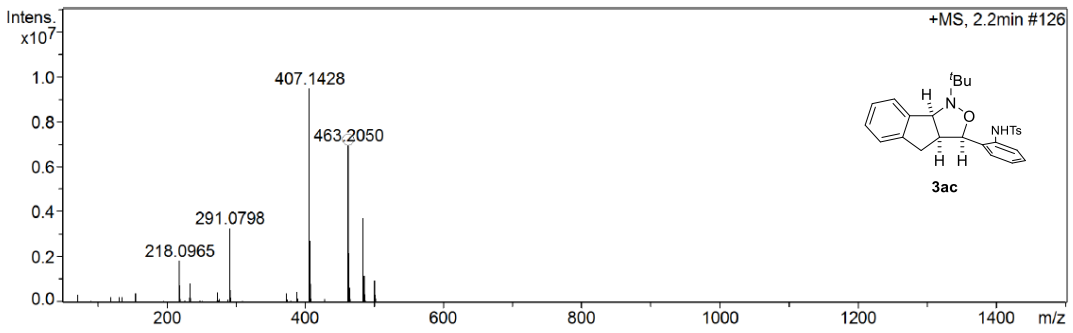
Acquisition D 2022-06-20 15:07:38

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
463.2050	1	C27H31N2O3S	463.2050	0.1	3.7	1	100.00	14.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0504_GA5_01_13319.d
Method LC_NO UV_P50-1500_20MIN.m
Sample Name 0504

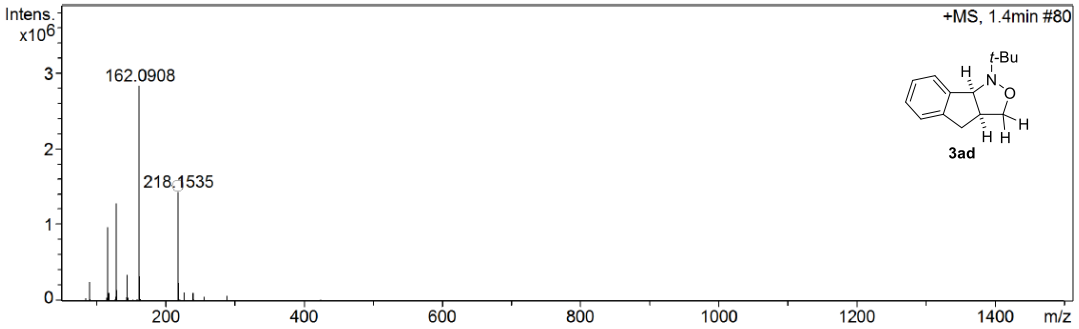
Acquisition D 2022-05-06 0:32:09

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
218.1535	1	C14H20NO	218.1539	2.2	1.3	1	100.00	6.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0715_BE3_01_15261.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0715

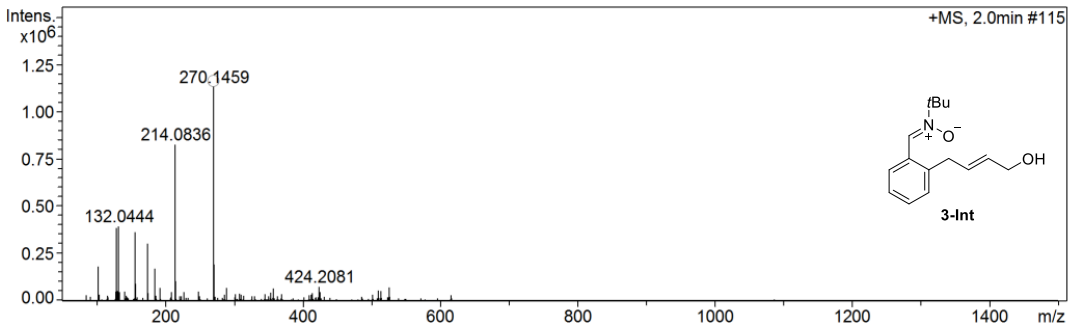
Acquisition D 2022-07-18 23:59:46

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
270.1459	1	C15H21NNaO2	270.1464	1.9	0.7	1	100.00	6.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0504_RE8_01_13314.d
Method LC_NO UV_P50-1500_20MIN.m
Sample Name 0504

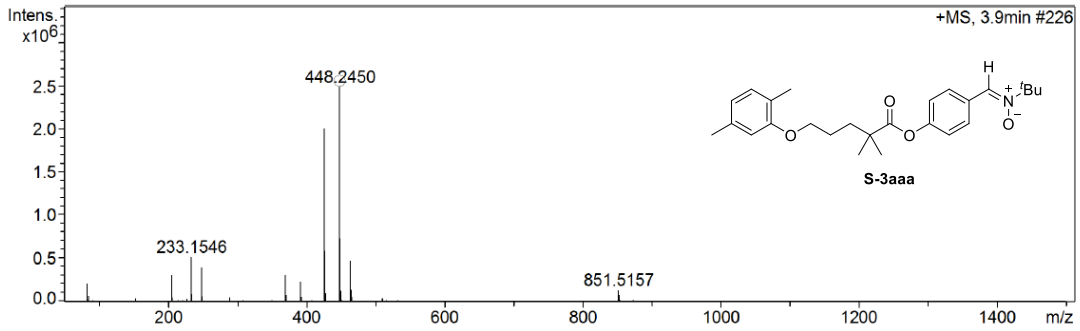
Comment

Acquisition D 2022-05-05 22:45:50

Operator Demo User
Instrumen compact 8255754.2017
6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
448.2450	1	C26H35NNaO4	448.2458	2.0	2.4	1	100.00	10.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0617_GC4_01_14501.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617

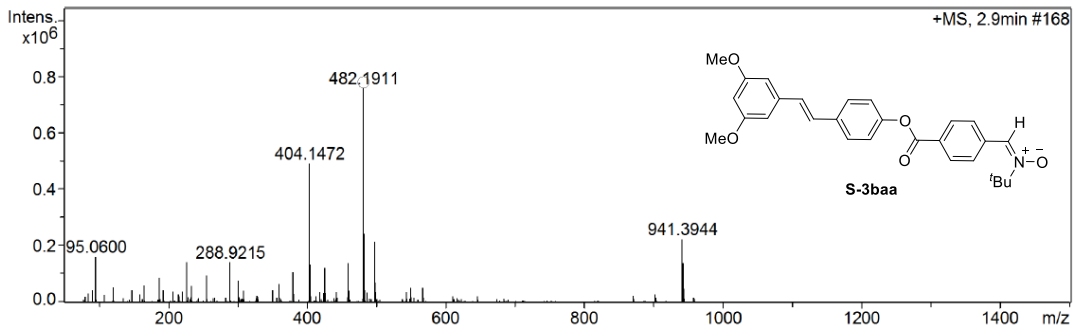
Comment

Acquisition D 2022-06-20 14:14:05

Operator Demo User
Instrumen compact 8255754.2017
6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
482.1911	1	C28H29NNaO5	482.1938	5.7	5.3	1	100.00	15.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0504_GA1_01_13315.d
Method LC_NO UV_P50-1500_20MIN.m
Sample Name 0504

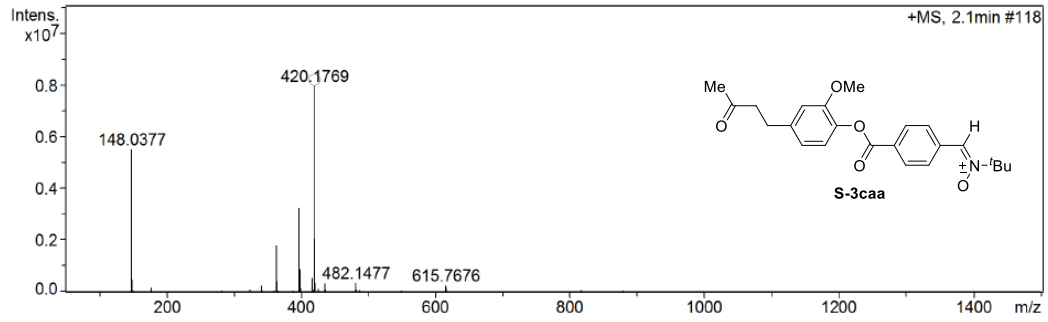
Acquisition D 2022-05-05 23:07:05

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥ Conf	N-Rule
420.1769	1	C23H27NNaO5	420.1781	3.0	0.8	1		100.00	11.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0617_GC2_01_14499.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617

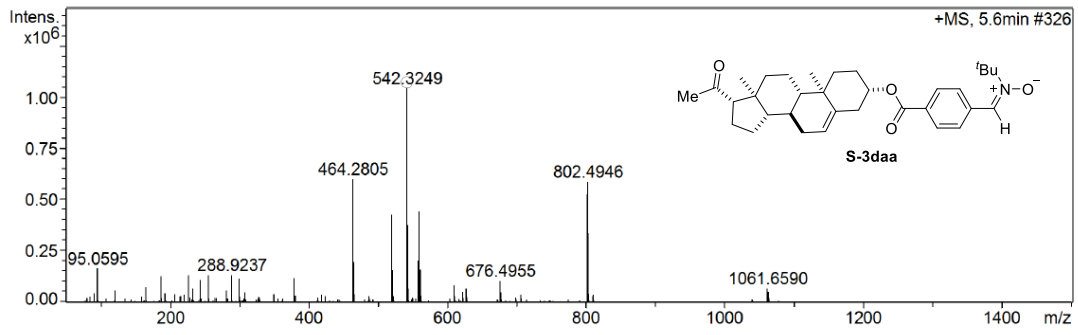
Acquisition D 2022-06-20 13:59:09

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥ Conf	N-Rule
542.3249	1	C33H45NNaO4	542.3241	-1.5	6.3	1		100.00	12.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0504_GA3_01_13317.d
Method LC_NO UV_P50-1500_20MIN.m
Sample Name 0504

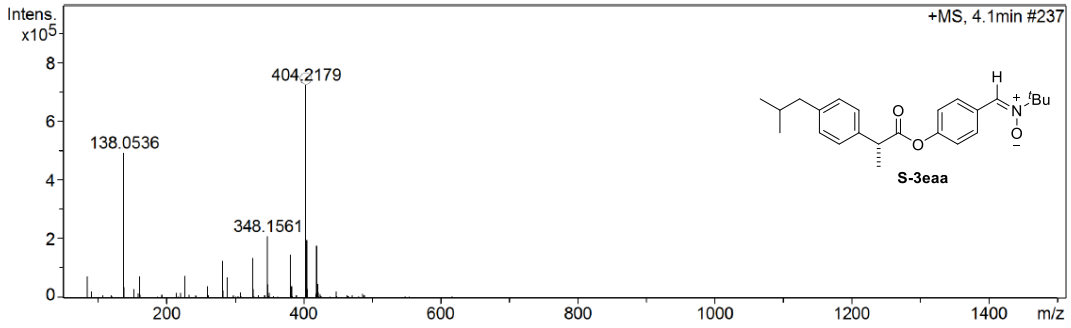
Comment

Acquisition D 2022-05-05 23:49:38

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
404.2179	1	C24H31NNaO3	404.2196	4.3	3.5	1	100.00	10.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0617_GC3_01_14500.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617

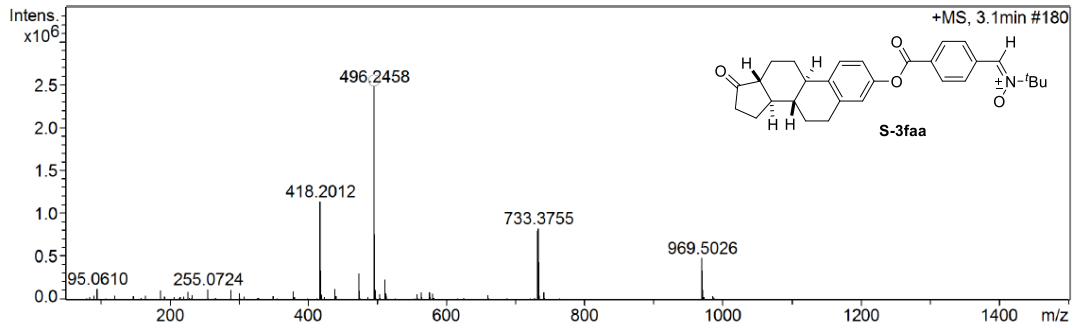
Comment

Acquisition D 2022-06-20 14:06:44

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
496.2458	1	C30H35NNaO4	496.2458	0.1	15.5	1	100.00	14.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0504_GA2_01_13316.d
Method LC_NO UV_P50-1500_20MIN.m
Sample Name 0504

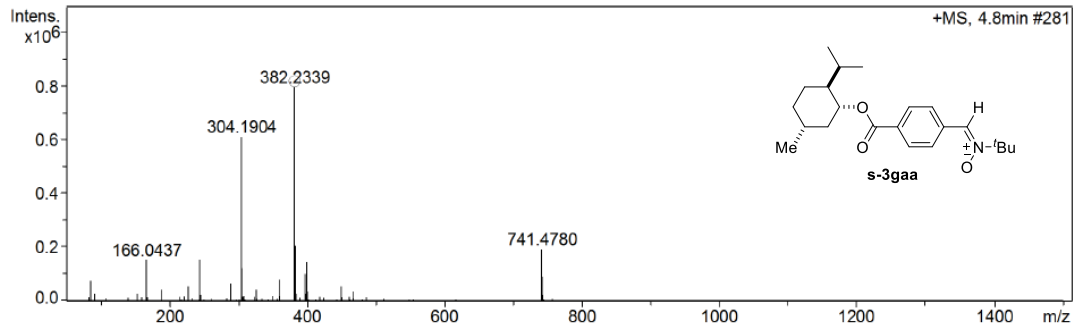
Acquisition D 2022-05-05 23:28:21

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
382.2339	1	C22H33NNaO3	382.2353	3.5	6.6	1		100.00	7.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name g:\Desktop\0718_BE4_01_15378.d
Method LC_NO UV_P50-1500_30MIN.m
Sample Name 0718

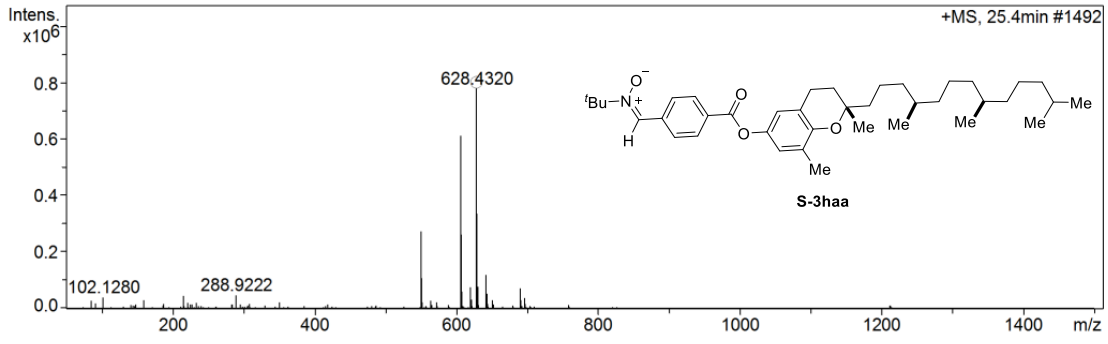
Acquisition D 2022-07-21 17:00:03

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
628.4320	1	C39H59NNaO4	628.4336	2.5	0.9	1		100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0617_GC6_01_14503.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617

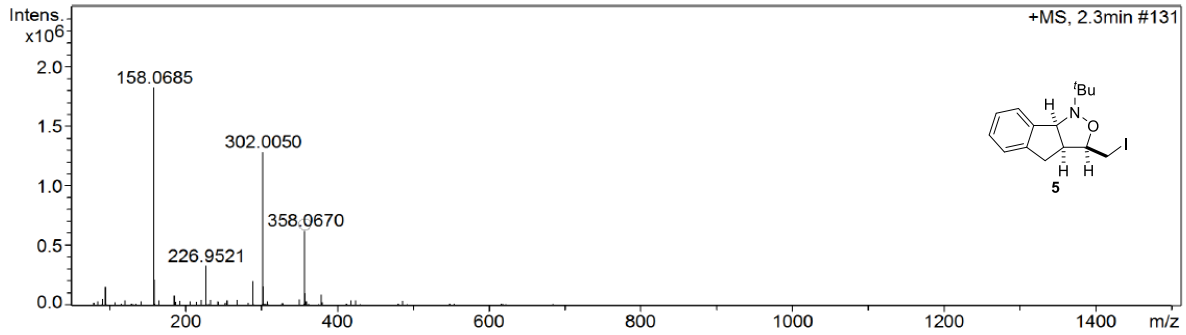
Comment

Acquisition D 2022-06-20 14:30:08

Operator Demo User
Instrumen compact 8255754.2017
6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
358.0670	1	C15H21INO	358.0662	-2.0	0.3	1	100.00	6.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0617_GC7_01_14504.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617

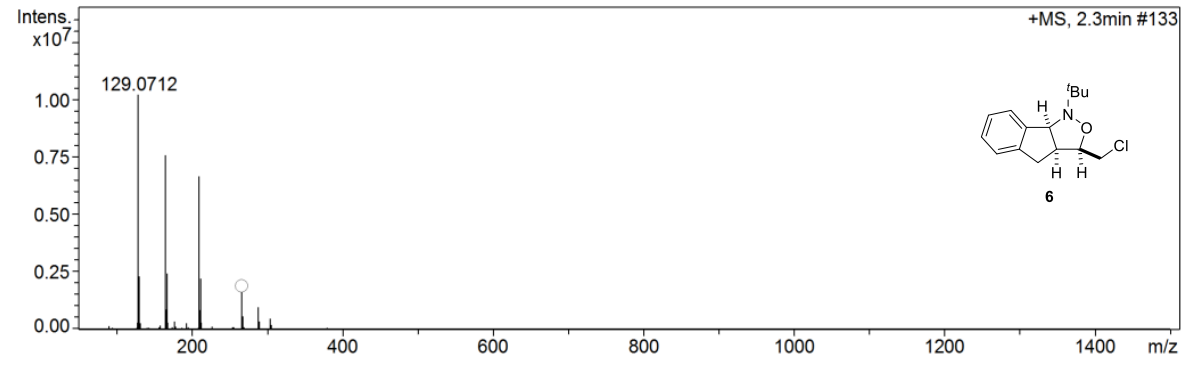
Comment

Acquisition D 2022-06-20 14:37:59

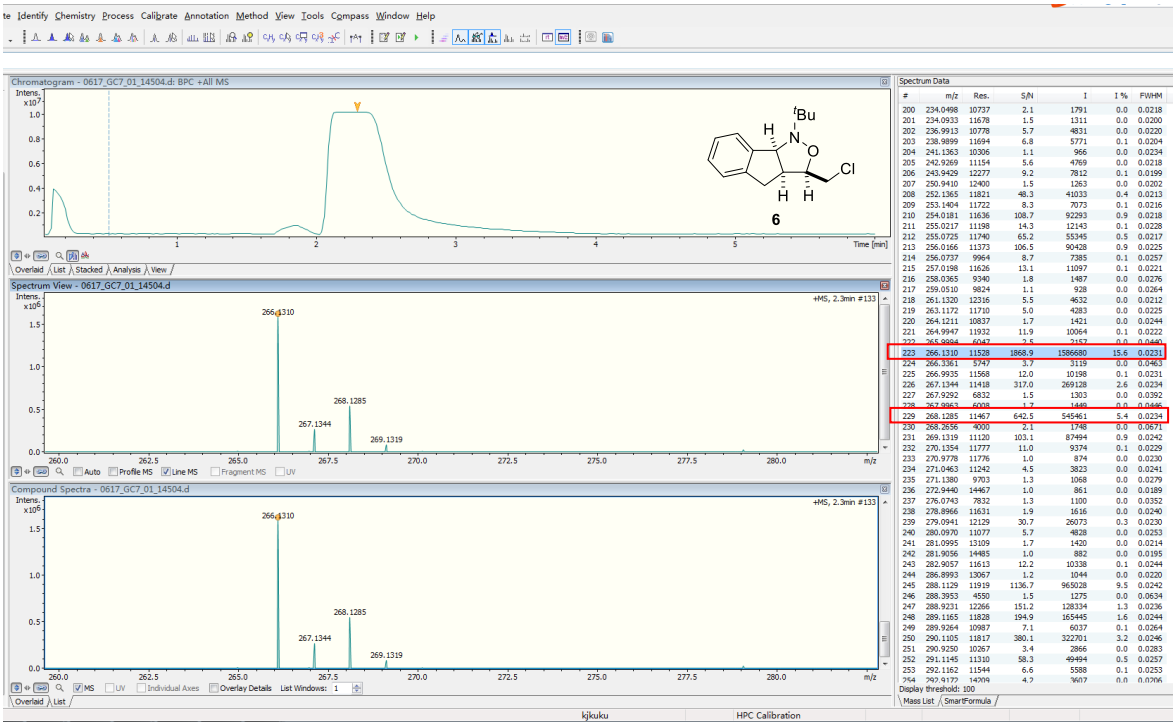
Operator Demo User
Instrumen compact 8255754.2017
6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
266.1310	1	C15H21ClNO	266.1306	-1.3	4.2	1	100.00	6.0	even	ok



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0617_GC7_01_14504.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617

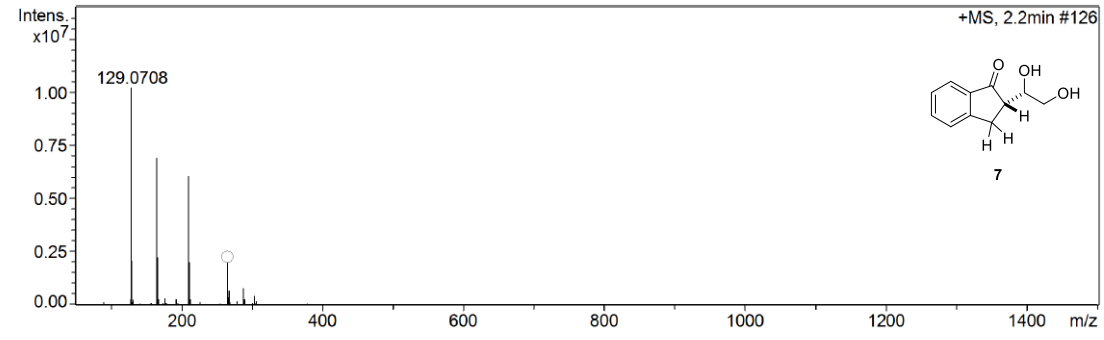
Comment

Acquisition D 2022-06-20 14:37:59

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
266.1311	1	C15H21ClNO	266.1306	-1.8	3.0	1	100.00	6.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RD7_01_12750.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

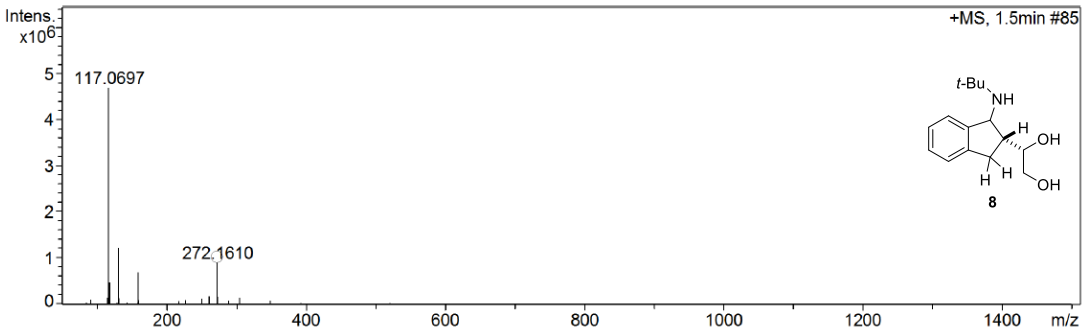
Acquisition D 2022-04-13 14:23:11

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
272.1610	1	C15H23NNaO2	272.1621	4.1	0.4	1	100.00	5.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0412_RB5_01_12732.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0412

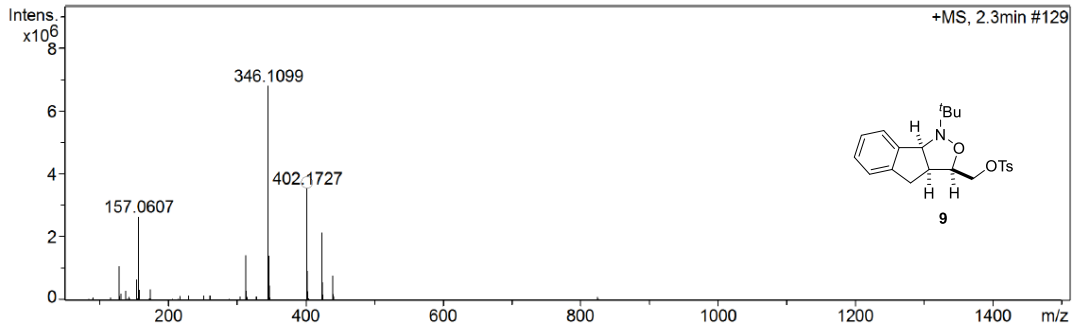
Acquisition D 2022-04-13 12:00:54

Operator Demo User
Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
402.1727	1	C22H28NO4S	402.1734	1.7	3.3	1	100.00	10.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0621_GD3_01_14604.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0621

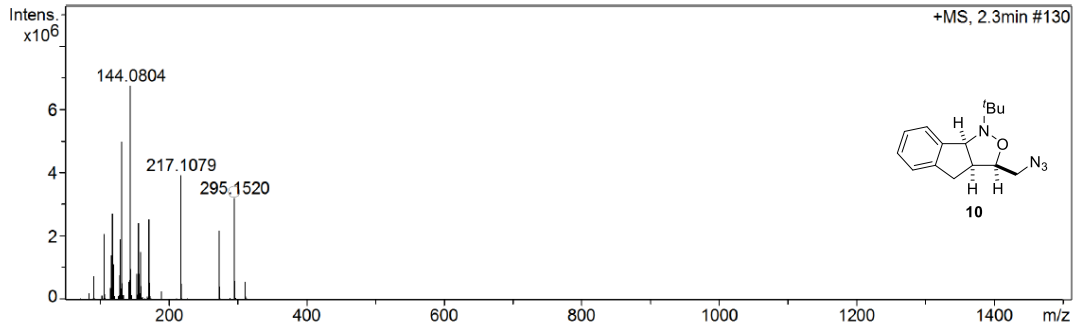
Comment

Acquisition D 2022-06-24 17:01:13

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
295.1520	1	C15H20N4NaO	295.1529	3.1	1.9		1	100.00	8.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name G:\ZM MS\0617_GD2_01_14507.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0617

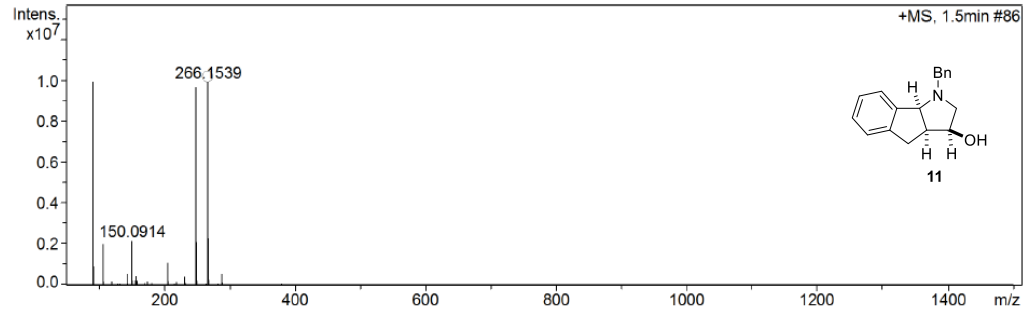
Comment

Acquisition D 2022-06-20 15:00:18

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	50 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
266.1539	1	C18H20NO	266.1539	-0.0	17.8		1	100.00	10.0	even		ok