Electronic Supplementary Material (ESI) for Chemical Science.

Visible Light Driven Deuteration of Formyl C-H and Hydridic C(sp^3)-H Bonds in Feedstock Chemicals and Pharmaceutical Molecules

Yulong Kuang, Hui Cao, Haidi Tang, Junhong Chew, Wei Chen, Xiangcheng Shi, Jie Wu*

Department of Chemistry, National University of Singapore, 3 Science Drive 3, Singapore, 117543, Singapore

E-Mail: chmjie@nus.edu.sg

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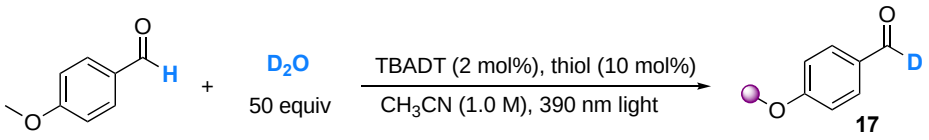
1. General considerations

All catalytic reactions were carried out with commercially available reagents in Schlenk tube (10 mL) under an argon atmosphere with magnetic stirring after freeze-pump-thaw. ^{1}H NMR yield was detected by adding CH_2Br_2 as an internal standard. The isolated yield was the purified product by flash chromatography over silica gel. ^{1}H NMR spectra were recorded on commercial instruments (500 MHz). Chemical shifts were reported in ppm from the solvent resonance as the internal standard ($CDCl_3$, δ = 7.26). Spectra were reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, hept = heptet, m = multiplet), coupling constants (Hz), integration and assignment. ^{13}C NMR spectra were recorded on commercial instruments (126 MHz). Chemical shift was reported in ppm from the solvent resonance as the internal standard ($CDCl_3$, δ = 77). The densely deuterated compounds were also checked by D NMR spectra which were recorded on commercial instruments (77 MHz). Spectra ($CHCl_3$) were reported in ppm from the comparison with its resonance in the corresponding ^{1}H NMR spectra. Grey dots ("○") on the structures represent that the deuterium incorporation is less than 2% based on analysis of ^{1}H NMR spectra, but deuterium signals showed on D NMR spectrum. HRMS was recorded on a commercial apparatus (EI source).

TBADT (tetra-*n*-butylammonium decatungstate)[1] and thiol (2,4,6-triisopropylthiophenol)[2] were synthesized according to the reported literatures.

2. Investigation for optimal conditions

1) Time course of selective sequential deuteration of 4-anisaldehyde



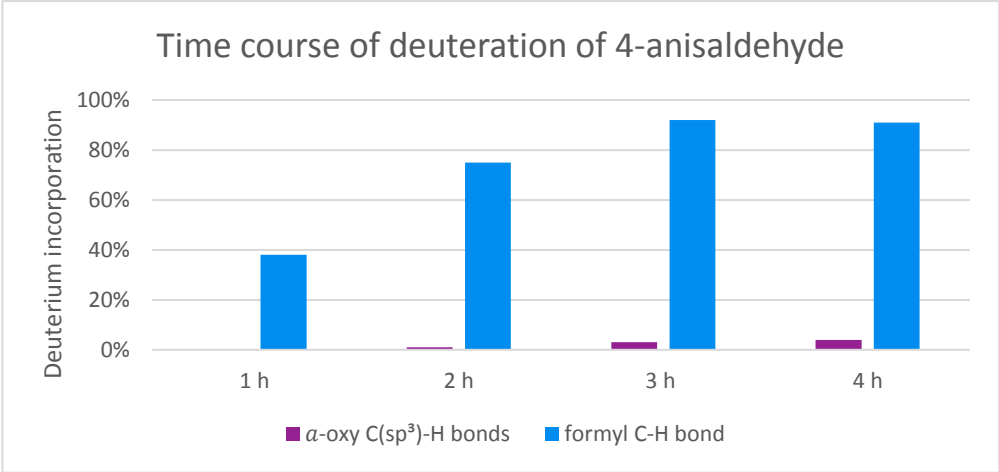
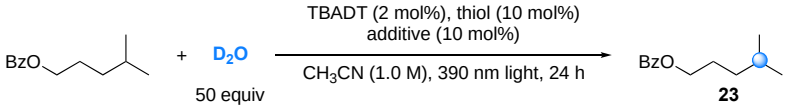


Figure S1. Time course study in selective sequential deuteration of 4-anisaldehyde

2) Investigation of phase transfer agents

Table S1. Investigation of various phase transfer agents[a]



entry	additive	results	
		yield[b]	deuterium incorporation[c]
1	no	96%	84%
2	TBAF•3H_2O	94%	90%
3	TBAB	96%	90%
4[d]	TBAB	99%	91%
5	TBAI	90%	90%
6	$^{n}Bu_4N$•BF_4	92%	89%
7	SDS	93%	27%
8	PPh_4Cl	94%	4%

[a] Reaction was conducted with the indicated additive (10 mol%) for 24 h. [b] Yield was determined by analysis of ^{1}H NMR spectra of the crude product mixture using CH_2Br_2 as an internal standard. [c] Deuterium incorporation was determined by analysis of ^{1}H NMR spectra of products. [d] 20 mol% TBAB was added. TBAF = tetra-*n*-butylammonium fluoride; TBAB = tetra-*n*-butylammonium bromide; TBAI = tetra-*n*-butylammonium iodide; SDS = sodium 1-decanesulfonate.

3. General procedure

General procedure for deuteration of formyl C-H bonds: The aldehyde substrate (0.2 mmol), TBADT (13.2 mg, 2 mol%), thiol (5 uL, 10 mol%), D_2O (180 uL, 50 equiv) and CH_3CN (200 uL, 1.0 M) were added to a 10 mL Schlenk tube equipped with a stir bar. The mixture was operated by freeze-pump-thaw procedures three times before charging the tube with argon. The reactor was then sealed and placed under 390 nm Kessil light (80 W) and stirred for 4 h. Then, the crude reaction mixture was extracted with diethyl ether (3 × 2 mL). The combined organic layer was concentrated and purified by flash column chromatography over silica gel to afford the deuterated product.

General procedure for deuteration of hydridic C(sp^3)-H bonds and pharmaceuticals: A substrate (0.2 mmol), TBADT (13.2 mg, 2 mol%), thiol (5 uL, 10 mol%), D_2O (360 uL, 100 equiv), TBAB (12.8 mg, 20 mol%) and CH_3CN (200 uL, 1.0 M) were added to a Schlenk tube (10 mL) equipped with a stir bar. The mixture was operated by freeze-pump-thaw procedures three times before being charged with argon. The reactor was placed under 390 nm Kessil light (80 W) and kept stirring for 24 or 48 h. The crude reaction mixture was extracted with ethyl acetate (3 × 2 mL). The combined organic layer was concentrated and purified by flash column chromatography over silica gel to afford the deuterated product. $C_6H_5CF_3$ (200 uL, 1.0 M) was added at the beginning in cases where the substrate has low solubility in CH_3CN.

4. Results of deuteration of other hydridic C/X-H bonds

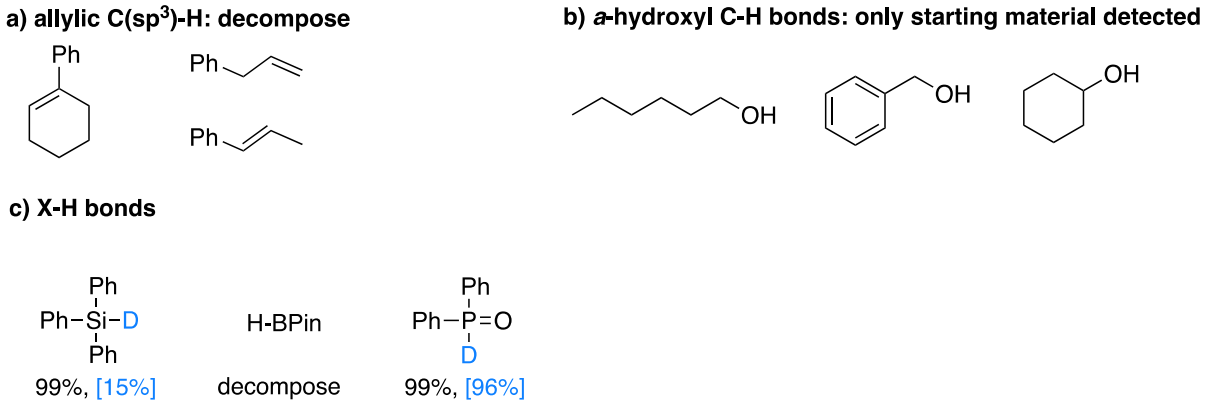
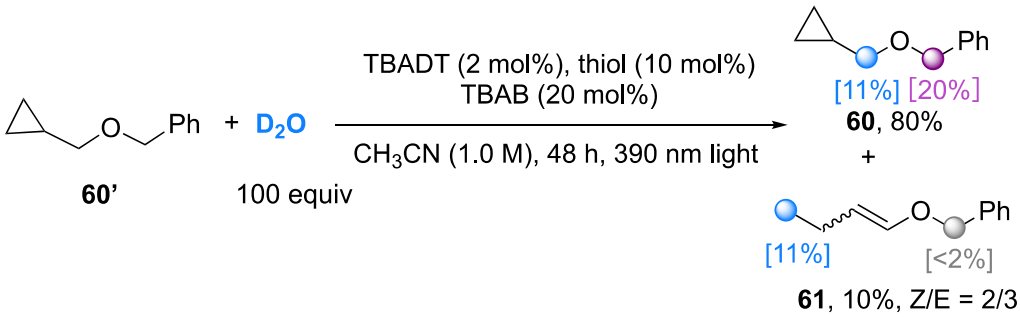
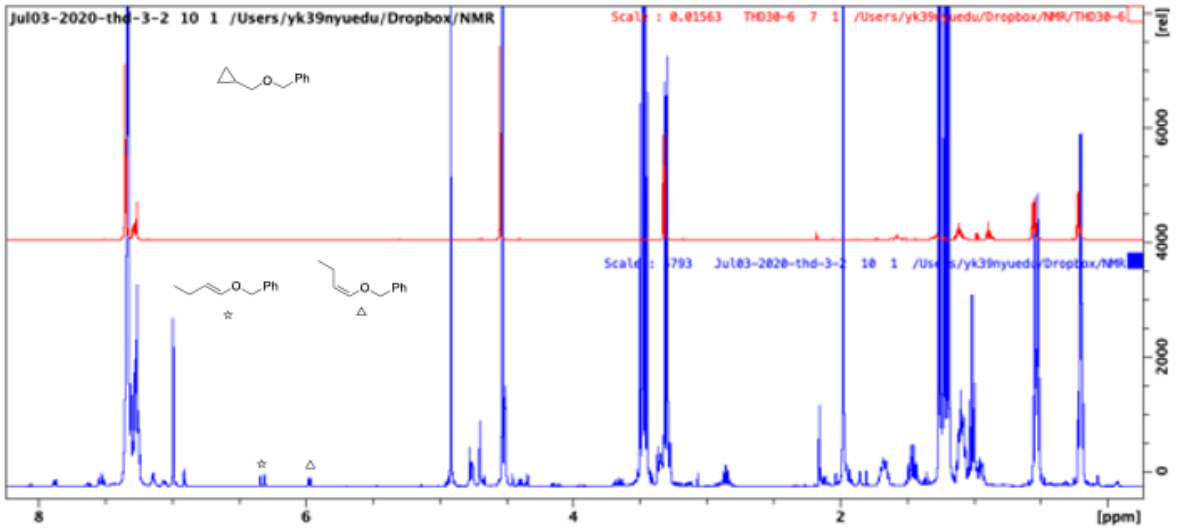


Figure S2. Results on deuteration of other hydridic C/X-H bonds

5. Radical clock experiment

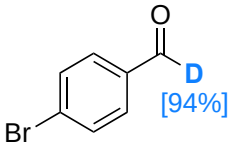


The reaction was conducted under the optimal conditions with 20 mol% TBAB. After 48 h under 390 nm light irritation, the reaction mixture was quenched. The crude NMR showed the above results by comparing with the known spectra.[3] The deuterium incorporation was obtained from ^{1}H NMR spectra of products after purification.



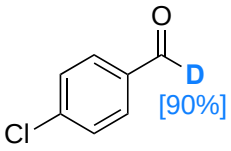
6. Characterization of new compounds

4-Bromobenzaldehyde-formyl-*d1* (**1**):



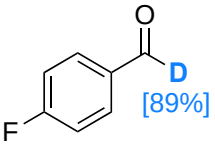
Prepared following the general procedure. ^{1}H NMR spectrum showed 94% deuterium incorporation and quantitative yield (> 99%) with CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless solid in 31.6 mg (85% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.96 (s, 0.06H), 7.73 (d, J = 8.0 Hz, 2H), 7.66 (d, J = 8.0 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 191.0 (COH), 190.7 (t, J = 27.2 Hz, COD), 134.9, 132.3, 130.9, 129.7. HRMS (EI-TOF) calcd for C_7H_4DBrO (M^+) = 189.9561, found 186.9562.

4-Chlorobenzaldehyde-formyl-*d1* (**2**):



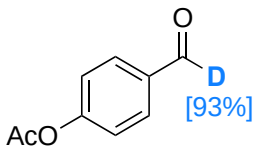
Prepared following the general procedure. ^{1}H NMR spectrum showed 90% deuterium incorporation and quantitative yield (> 99%) with CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 24.8 mg (88% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.98 (s, 0.10H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.51 (d, *J* = 8.5 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 190.8 (COH), 190.5 (t, *J* = 26.8 Hz, COD), 140.9, 134.6 (t, *J* = 3.8 Hz), 130.9, 129.4. HRMS (EI-TOF) calcd for C_7H_4DClO (M^+) = 141.0086, found 141.0081.

4-Fluorobenzaldehyde-formyl-*d1* (**3**):



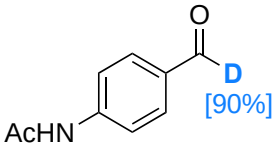
Prepared following the general procedure. ^{1}H NMR spectrum showed 89% deuterium incorporation and quantitative yield (> 99%) using CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 22.2 mg (86% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.96 (s, 0.11H), 7.96 – 7.86 (m, 2H), 7.24 – 7.17 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 190.5 (COH), 190.2 (t, *J* = 26.6 Hz, COD), 166.5 (d, *J* = 257.4 Hz), 133.0 – 132.5 (m), 132.2 (d, *J* = 9.6 Hz), 116.3 (d, *J* = 22.6 Hz). HRMS (EI-TOF) calcd for C_7H_4DFO (M^+) = 125.0382, found 125.0384.

4-Acetoxybenzaldehyde-formyl-*d1* (**4**):



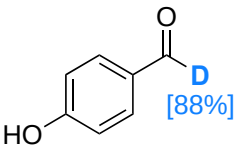
Prepared following the general procedure by using 365 nm (24 W) LED strip instead of 390 nm (80 W) Kessil light for 24 h. ^{1}H NMR spectrum showed 93% deuterium incorporation and 99% yield using CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 31.7 mg (96% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.99 (s, 0.07H), 7.92 (d, *J* = 8.5 Hz, 2H), 7.27 (d, *J* = 8.5 Hz, 2H), 2.33 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 190.9 (COH), 190.6 (t, *J* = 26.6 Hz, COD), 168.6, 153.3, 133.9 (t, *J* = 3.5 Hz), 131.1, 122.3, 21.1. HRMS (EI-TOF) calcd for $C_9H_7DO_3$ (M^+) = 165.0531, found 165.0532.

4-Acetamidobenzaldehyde-formyl-*d1* (**5**):



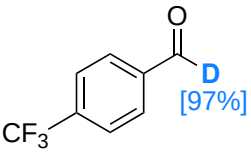
Prepared following the general procedure. ^{1}H NMR spectrum showed 90% deuterium incorporation and 95% yield using CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless solid in 29.5 mg (90% yield). ^{1}H NMR (500 MHz, CD_3CN) δ = 9.87 (s, 0.10H), 8.71 (br, 1H), 7.88 – 7.79 (m, 2H), 7.78 – 7.68 (m, 2H), 2.10 (s, 3H). ^{13}C NMR (126 MHz, CD_3CN) δ = 192.3 (COH), 192.0 (t, *J* = 26.8 Hz, COD), 170.3, 145.7, 132.9, 131.8, 119.8, 24.7. HRMS (EI-TOF) calcd for $C_9H_8DNO_2$ (M^+) = 164.0691, found 164.0690.

4-Hydroxybenzaldehyde-formyl-*d1* (**6**):



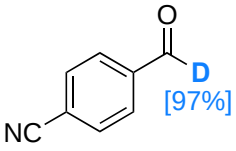
Prepared following the general procedure. ^{1}H NMR spectrum showed 88% deuterium incorporation and 95% yield using CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 5 : 1) to afford product as a colorless solid in 21.4 mg (87% yield). ^{1}H NMR (500 MHz, CD_3CN) δ = 9.82 (s, 0.12H), 7.77 (d, *J* = 8.5 Hz, 2H), 6.96 (d, *J* = 8.5 Hz, 2H). ^{13}C NMR (126 MHz, CD_3CN) δ = 191.9 (COH), 191.2 (t, *J* = 28.1 Hz, COD), 163.7, 133.1, 130.6 (t, *J* = 3.7 Hz), 116.9. HRMS (EI-TOF) calcd for $C_7H_5DO_2$ (M^+) = 123.0425, found 123.0423.

4-(Trifluoromethyl)benzaldehyde-formyl-*d1* (**7**):



Prepared following the general procedure. ^{1}H NMR spectrum showed 97% deuterium incorporation and 80% yield using CH_2Br_2 as an internal standard. Then the compound was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 26.2 mg (70% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 10.10 (s, 0.03H), 8.01 (d, *J* = 8.0 Hz, 2H), 7.80 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 190.7 (t, *J* = 26.8 Hz, COD), 138.5, 135.6 (q, *J* = 32.8 Hz), 129.9, 126.8 (q, *J* = 3.8 Hz), 123.4 (q, *J* = 273.5 Hz). HRMS (EI-TOF) calcd for $C_8H_4DF_3O$ (M^+) = 175.0350, found 175.0346.

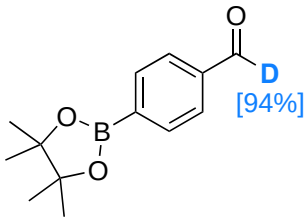
4-Cyanobenzaldehyde-formyl-*d1* (**8**):



Prepared following the general procedure. ^{1}H NMR spectrum showed 97% deuterium incorporation and 75% yield using CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel

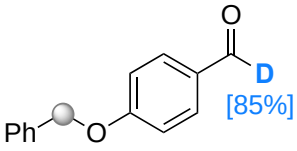
chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 18.5 mg (70% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 10.09 (s, 0.03H), 8.00 (d, *J* = 8.5 Hz, 2H), 7.85 (d, *J* = 8.5 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 190.2 (t, *J* = 27.5 Hz, COD), 138.6 (t, *J* = 3.7 Hz), 132.9, 129.8, 117.7, 117.6. HRMS (EI-TOF) calcd for C_8H_4DNO (M^+) = 132.0428, found 132.0429.

4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)benzaldehyde-formyl-*d1* (**9**):



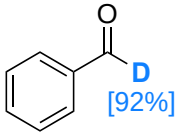
Prepared following the general procedure. ^{1}H NMR spectrum showed 94% deuterium incorporation and quantitative yield (> 99%) with CH_2Br_2 as an internal standard. Then the compound was purified over silica gel chromatography (hexane : diethyl ether = 2 : 1) to afford product as a colorless solid in 34.9 mg (75% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 10.04 (s, 0.06H), 7.96 (d, *J* = 8.0 Hz, 2H), 7.86 (d, *J* = 8.0 Hz, 2H), 1.36 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 192.6 (COH), 192.3 (t, *J* = 26.7 Hz, COD), 138.0 (t, *J* = 3.2 Hz), 135.2, 128.7, 84.3, 24.9. HRMS (EI-TOF) calcd for $C_{13}H_{16}DBO_3$ (M^+) = 233.1328, found 233.1323.

4-Benzyloxybenzaldehyde-formyl-*d1*(**10**):



Prepared following the general procedure for 8 h. ^{1}H NMR spectrum showed 85% deuterium incorporation on the formyl C-H bond, less than 2% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds and 99% yield using CH_2Br_2 as an internal standard. Then crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless solid in 36.7 mg (86% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.89 (s, 0.15H), 7.86 – 7.82 (m, 2H), 7.46 – 7.37(m, 4H), 7.37 – 7.31 (m, 1H), 7.08 (d, *J* = 8.5 Hz, 2H), 5.15 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 190.7 (COH), 190.4 (t, *J* = 26.3 Hz, COD), 163.7, 135.9, 131.9, 130.0, 128.7, 128.3, 127.4, 115.1, 70.2. HRMS (EI-TOF) calcd for $C_{14}H_{11}DO_2$ (M^+) = 213.0900, found 213.0895.

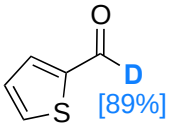
Benzaldehyde-formyl-*d1* (**11**):



Prepared following the general procedure. ^{1}H NMR spectrum showed 91% deuterium incorporation and quantitative yield (> 99%) with CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel

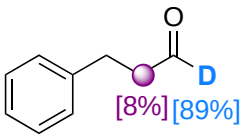
chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 19.2 mg (90% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 10.0 (s, 0.08H), 7.92 – 7.81 (m, 2H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.57 – 7.47 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 192.3 (CHO), 192.0 (t, *J* = 26.7 Hz, COD), 136.3, 134.4, 129.7, 129.0. HRMS (EI-TOF) calcd for C_7H_5DO (M^+) = 107.0481, found 107.0480.

Thiophen-2-carbaldehyde-formyl-*d1* (**12**):



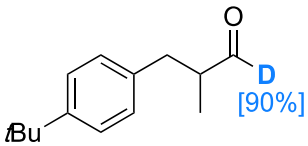
Prepared following the general procedure. ^{1}H NMR spectrum showed 89% deuterium incorporation and quantitative yield (> 99%) with CH_2Br_2 as an internal standard. Then the compound was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 18.8 mg (83% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.94 (s, 0.11H), 7.82 – 7.70 (m, 2H), 7.21 (t, *J* = 4.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 182.9 (COH), 182.7 (t, *J* = 27.3 Hz, COD), 144.0 (t, *J* = 4.7 Hz), 136.2, 135.1, 128.3. HRMS (EI-TOF) calcd for C_5H_3DOS (M^+) = 113.0040, found 113.0042.

3-Phenylpropionaldehyde-formyl-*d1* (**13**):



Prepared following the general procedure. ^{1}H NMR spectrum showed 89% deuterium incorporation on formyl group, 8% deuterium incorporation on the *a*-carbonyl C(sp^3)-H bonds and 99% yield using CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 22.9 mg (85% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.82 (t, *J* = 1.5 Hz, 0.11H), 7.31 (td, *J* = 7.5, 1.5 Hz, 2H), 7.22 (t, *J* = 7.5 Hz, 3H), 2.97 (t, *J* = 7.5 Hz, 2H), 2.82 – 2.74 (m, 1.84H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 201. 5 (COH), 201.2 (t, *J* = 26.5 Hz, COD), 140.3, 128.5, 128.2, 126.2, 45.0 (t, *J* = 3.7 Hz), 28.0. D NMR (77 MHz, $CHCl_3$) δ = 9.82. HRMS (EI-TOF) calcd for C_9H_9DO (M^+) = 135.0789, found 135.0788.

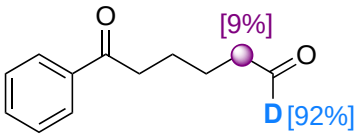
p-tert-Butyl-α-methylhydrocinnamic aldehyde-formyl-*d1* (**14**):



Prepared following the general procedure. ^{1}H NMR spectrum showed 90% deuterium incorporation and 99% NMR yield using CH_2Br_2 as an internal standard. Then the compound was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 31.6 mg (77% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.72 (m, 0.10H), 7.32 (d, *J* = 8.5 Hz, 2H), 7.11 (d, *J* = 8.5 Hz, 2H), 3.06 (dd, *J* = 13.5, 6.0 Hz, 1H), 2.72 – 2.62 (m, 1H), 2.59

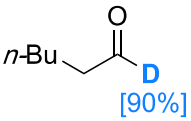
(dd, J = 13.5, 8.0 Hz, 1H), 1.32 (s, 9H), 1.10 (d, J = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 204.6 (COH), 204.3 (t, J = 26.3 Hz, COD), 149.2, 135.7, 128.6, 125.4, 48.0 - 47.8 (m), 36.1, 34.4, 31.3, 13.2. D NMR (77 MHz, $CHCl_3$) δ = 9.73. HRMS (EI-TOF) calcd for $C_{14}H_{19}DO$ (M^+) = 205.1571, found 205.1570.

6-Oxo-6-phenylhexanal-formyl-*d1* (**15**):



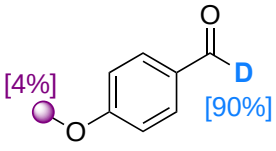
Prepared following the general procedure. ^{1}H NMR spectrum showed 92% deuterium incorporation on formyl group, 9% deuterium incorporation on the *a*-carbonyl C(sp^3)-H bonds and quantitative yield (> 99%) using CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless solid in 29.0 mg (76% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.78 (s, 0.08H), 8.01 – 7.82 (m, 2H), 7.64 – 7.52 (m, 1H), 7.52 – 7.38 (m, 2H), 3.00 (t, J = 7.0 Hz, 2H), 2.49 (t, J = 7.0 Hz, 1.83H), 1.87 – 1.60 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 202.2, 201.9 (t, J = 26.5 Hz), 136.8, 133.0, 128.6, 128.0, 43.7 - 43.5 (m), 38.1, 23.6, 21.6. D NMR (77 MHz, $CHCl_3$) δ = 9.78, 2.44. HRMS (EI-TOF) calcd for $C_{12}H_{13}DO_2$ (M^+) = 191.1051, found 191.1058.

n-Hexanal-formyl-*d1* (**16**):



Prepared following the general procedure by using CD_3CN (1.0 M) instead of CH_3CN (1.0 M). ^{1}H NMR spectrum showed 90% deuterium incorporation and 90% yield using CH_2Br_2 as an internal standard. ^{1}H NMR (500 MHz, CD_3CN) δ = 9.64 (m, 0.10H), 2.42 – 2.31 (m, 1H), 2.29 – 2.19 (m, 1H), 1.59 – 1.50 (m, 2H), 1.28 – 1.24 (m, 4H), 0.86 (t, J = 7.0 Hz, 3H). HRMS (EI-TOF) calcd for $C_{12}H_{13}DO_2$ (M^+) = 101.0945, found 101.0950.

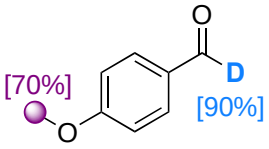
4-Methoxybenzaldehyde-formyl-*d1* (**17**):



Prepared following the general procedure. ^{1}H NMR showed 90% deuterium incorporation on the formyl C-H bond, 4% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds and 99% yield using CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 24.9 mg (90% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.87 (s, 0.10H), 7.85 – 7.75 (m, 2H), 6.99 (d, J = 9.0 Hz, 2H), 3.90 – 3.85 (m, 2.87H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 190.8 (COH), 190.4

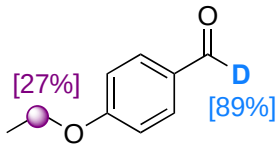
(t, J = 26.5 Hz, COD), 164.6, 131.9, 129.8 (t, J = 3.8 Hz), 114.3, 55.5 (OCH_3), 55.2 (t, J = 22.6 Hz, OCH_2D). HRMS (EI-TOF) calcd for $C_8H_7DO_2$ (M^+) = 137.0579, found 137.0574.

4-(1,1,1-*d3*-Methoxy)-benzaldehyde-formyl-*d1* (**17'**):



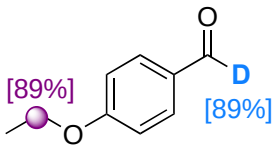
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). ^{1}H NMR spectrum showed 90% deuterium incorporation on the formyl C-H bond, 70% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds and 99% yield using CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 26.0 mg (92% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.88 (s, 0.10H), 7.84 (d, J = 8.5 Hz, 2H), 7.01 (d, J = 8.5 Hz, 2H), 3.90 – 3.83 (m, 0.89H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 190.8 (COH), 190.5 (t, J = 26.5 Hz, COD), 164.6, 132.0, 129.9 (t, J = 3.7 Hz), 114.3, 55.7 – 54.6 (m). HRMS (EI-TOF) calcd for $C_8H_4D_4O_2$ (M^+) = 140.0770, found 140.0763.

4-(1,1-*d2*-Ethoxy)-benzaldehyde-formyl-*d1* (**18**):



Prepared following the general procedure. ^{1}H NMR spectrum showed 88% deuterium incorporation on the formyl C-H bond, 27% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds and 94% yield using CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 27.3 mg (90% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.85 (s, 0.11H), 7.83 – 7.78 (m, 2H), 7.00 – 6.95 (m, 2H), 4.13 – 4.04 (m, 1.46H), 1.43 (t, J = 8.5 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 190.7 (COH), 190.4 (t, J = 26.3 Hz, COD), 164.0, 131.9, 129.6 (t, J = 7.6 Hz), 114.6, 63.8 (OCH_2CH_3), 63.5 (t, J = 22.0 Hz, $OCHDCH_3$), 14.6 – 14.3 (m). HRMS (EI-TOF) calcd for $C_9H_8D_2O_2$ (M^+) = 152.0803, found 152.0799.

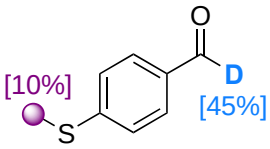
4-(1,1-*d2*-Ethoxy)-benzaldehyde-formyl-*d1* (**18'**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). ^{1}H NMR spectrum showed 89% deuterium incorporation on the formyl C-H bond, 89% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds and 99% yield using CH_2Br_2 as an internal standard. Then the compound was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 28.7 mg (95% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.87

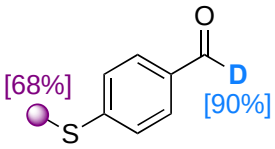
(s, 0.11H), 7.81 (d, J = 8.5 Hz, 2H), 6.97 (d, J = 8.5 Hz, 2H), 4.14 – 4.06 (m, 0.23H), 1.45 – 1.38 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 190.8 (COH), 190.5 (t, J = 26.3 Hz, COD), 164.0, 131.9, 129.7 (t, J = 7.6 Hz), 114.7, 63.8 – 63.0 (m), 14.5 – 14.3 (m). HRMS (EI-TOF) calcd for $C_9H_7D_3O_2$ (M^+) = 153.0864, found 153.0860.

4-(Methylthio)benzaldehyde-formyl-*d1* (**19**):



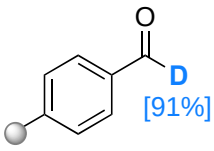
Prepared following the general procedure. ^{1}H NMR spectrum showed 45% deuterium incorporation on the formyl C-H bond, 10% deuterium incorporation on the *a*-thioxy C(sp^3)-H bonds and 99% yield using CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 30.4 mg (99% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.89 (s, 0.55H), 7.77 – 7.69 (m, 2H), 7.32 – 7.27 (m, 2H), 2.55 – 2.41 (m, 2.71 H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 191.1 (COH), 190.8 (t, J = 26.3 Hz, COD), 147.8, 132.8, 129.8, 125.0, 14.5. HRMS (EI-TOF) calcd for $C_8H_6D_2SO$ (M^+) = 154.0410, found 154.0406.

4-(1,1,1-*d3*-Methylthio)benzaldehyde-formyl-*d1* (**19'**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). ^{1}H NMR spectrum showed 90% deuterium incorporation on the formyl C-H bond, 68% deuterium incorporation on the *a*-thioxy C(sp^3)-H bonds and 99% yield using CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 30.3 mg (99% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.90 (s, 0.10H), 7.75 (d, J = 8.5 Hz, 2H), 7.30 (d, J = 8.5 Hz, 2H), 2.52 – 2.47 (m, 0.95H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 191.1 (COH), 190.8 (t, J = 26.3 Hz, COD), 147.8, 132.8, 129.9, 125.1, 14.6 – 13.8 (m). HRMS (EI-TOF) calcd for $C_8H_4D_4SO$ (M^+) = 156.0541, found 156.0537.

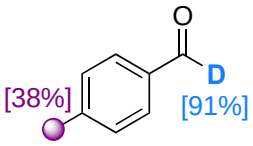
4-Methylbenzaldehyde-formyl-*d1*(**20**):



Prepared following the general procedure. ^{1}H NMR spectrum showed 91% deuterium incorporation on the formyl C-H bond, less than 2% deuterium incorporation on the benzyl C(sp^3)-H bond s and 97% yield using CH_2Br_2 as an internal standard. Then the crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 21.8 mg (90% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.96 (s, 0.09H), 7.77 (d, J = 9.5 Hz, 2H), 7.32 (d, J = 9.5 Hz, 2H),

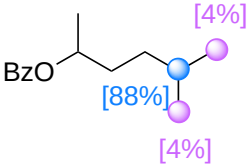
2.43 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 191.9 (COH), 191.6 (t, *J* = 33.0 Hz, COD), 145.5, 134.1 (t, *J* = 4.3 Hz), 129.8, 129.7, 21.8. HRMS (EI-TOF) calcd for C_8H_7DO (M^+) = 121.0632, found 121.0631.

4-(1,1,1-*d3*-Methyl)benzaldehyde-formyl-*d1* (**20'**):



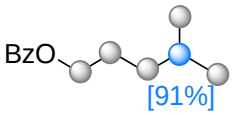
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). ^{1}H NMR spectrum showed 91% deuterium incorporation on the formyl C-H bond, 38% deuterium incorporation on the benzyl C(sp^3)-H bonds and 95% yield using CH_2Br_2 as an internal standard. Then compound was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 20.6 mg (85% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.96 (s, 0.09H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 1.87H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 192.0 (COH), 191.7 (t, *J* = 33.0 Hz, COD), 145.6 – 145.4 (m), 134.3 – 134.0 (m), 129.8, 129.7, 21.9 (CH_3), 21.6 (t, *J* = 18.0 Hz, CH_2D). HRMS (EI-TOF) calcd for $C_8H_6D_2O$ (M^+) = 122.0691, found 122.0681.

5-Methylhexan-2-yl-5-*d* benzoate (**22**):



Prepared following the general procedure for 24 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 41.0 mg (93% yield). ^{1}H NMR spectrum showed 88% deuterium incorporation on the tertiary C(sp^3)-H bond. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.16 – 8.00 (m, 2H), 7.66 – 7.49 (m, 1H), 7.48 – 7.40 (m, 2H), 5.22 – 5.10 (m, 1H), 1.82 – 1.68 (m, 1H), 1.67 – 1.58 (m, 1.12H), 1.34 (d, *J* = 6.5 Hz, 3H), 1.32 – 1.20 (m, 2H), 0.96 – 0.84 (m, 5.74H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 166.2, 132.6, 131.0, 129.5, 128.2, 72.0, 34.4, 33.8, 27.9 ($CH(CH_3)_2$), 27.4 (t, *J* = 19.3 Hz, $CD(CH_3)_2$), 22.4, 22.4, 20.0. D NMR (77 MHz, $CHCl_3$) δ = 1.53, 0.89. HRMS (EI-TOF) calcd for $C_{14}H_{19}DO_2$ (M^+) = 221.1521, found 221.1528.

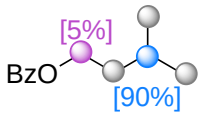
4-Methylpentyl-4-*d* benzoate (**23**):



Prepared following the general procedure for 24 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 38.0 mg (92% yield). ^{1}H NMR spectrum showed 91% deuterium incorporation on the tertiary C(sp^3)-H bond. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.09 – 7.99 (m, 2H), 7.59 –

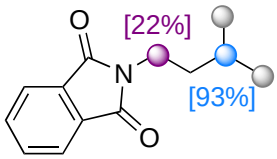
7.52 (m, 1H), 7.43 (t, J = 7.5 Hz, 2H), 4.31 (t, J = 7.0 Hz, 2H), 1.83 – 1.70 (m, 2H), 1.64 – 1.60 (m, 0.09H), 1.38 – 1.25 (m, 2H), 0.94 – 0.87 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 166.7, 132.8, 130.5, 129.5, 128.3, 65.4, 35.0, 27.7 ($CH(CH_3)_2$), 27.2 (t, J = 19.2 Hz, $CD(CH_3)_2$), 26.6, 22.4. D NMR (77 MHz, $CHCl_3$) δ = 4.32, 1.77, 1.61, 1.32, 0.93. HRMS (EI-TOF) calcd for $C_{13}H_{17}DO_2$ (M^+) = 207.1364, found 207.1364.

3-Methylbutyl-3-*d* benzoate (**24**):



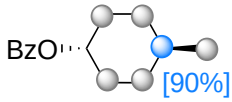
Prepared following the general procedure for 24 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 38.1 mg (99% yield). ^{1}H NMR spectrum showed 90% deuterium incorporation on the tertiary C(sp^3)-H bond. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.40 (d, J = 8.0 Hz, 2H), 7.55 (t, J = 8.0 Hz, 1H), 7.44 (t, J = 8.0 Hz, 2H), 4.36 (t, J = 6.5 Hz, 1.89H), 1.82 – 1.76 (m, 0.10H), 1.66 (t, J = 6.5 Hz, 2H), 0.97 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 166.7, 132.8, 130.5, 129.5, 128.3, 63.6, 37.3, 25.1 ($CH(CH_3)_2$), 24.7 (J = 19.5 Hz, $CD(CH_3)_2$), 22.4. D NMR (77 MHz, $CHCl_3$) δ = 4.33, 1.77, 1.64, 0.96. HRMS (EI-TOF) calcd for $C_{12}H_{15}DO_2$ (M^+) = 193.1208, found 193.1207.

2-(3-Methylbutyl-1,3-d_2)isoindoline-1,3-dione (**25**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 34.5 mg (80% yield). ^{1}H NMR spectrum showed 93% deuterium incorporation on the tertiary C(sp^3)-H bond, and 22% deuterium incorporation on the *a*-amide C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.84 – 7.79 (m, 2H), 7.72 – 7.58 (m, 2H), 3.81 – 3.42 (m, 1.57H), 1.66 – 1.60 (m, 0.07H), 1.58 – 1.47 (m, 2H), 0.96 – 0.92 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 168.4, 133.8, 132.2, 123.1, 37.4 – 37.0 (m), 36.4, 25.9 – 25.2 (m), 22.2. D NMR (77 MHz, $CHCl_3$) δ = 3.67, 1.58, 0.94. HRMS (EI-TOF) calcd for $C_{13}H_{13}D_2NO_2$ (M^+) = 219.1223, found 219.1219.

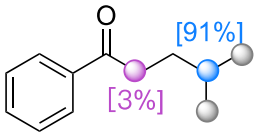
4-Methylcyclohexyl-4-*d* benzoate (**26**):



Prepared following the general procedure for 24 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 39.2 mg

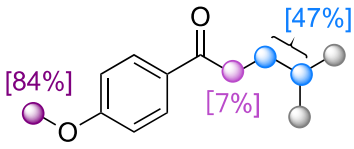
(90% yield). ^{1}H NMR spectrum showed 90% deuterium incorporation on the tertiary C(sp^3)-H bond. *cis* : *trans* = 1 : 3, Major one, *trans*: ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.12 – 7.97 (m, 2H), 7.59 – 7.48 (m, 1H), 7.48 – 7.37 (m, 2H), 4.95 – 4.81 (m, 1H), 1.99 – 1.89 (m, 2H), 1.82 – 1.31 (m, 4.1H), 1.18 – 1.02 (m, 1.15H), 0.94 – 0.82 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 166.1, 132.6, 130.9, 129.5, 128.2, 73.9, 32.9 – 32.6 (m), 31.6 – 31.5 (m), 29.7 – 29.5 (m), 21.7. Minor one, *cis*, ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.12 – 7.97 (m, 2H), 7.59 – 7.48 (m, 1H), 7.48 – 7.37 (m, 2H), 5.35 – 5.18 (m, 1H), 1.99 – 1.89 (m, 2H), 1.82 – 1.31 (m, 4.1H), 1.18 – 1.02 (m, 1.15H), 1.09 – 0.95 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 166.0, 132.6, 131.1, 129.6, 128.2, 70.3, 32.6 – 32.2 (m), 31.2 – 30.7 (m), 29.4 – 29.0 (m), 22.0. D NMR (77 MHz, $CHCl_3$) δ = 2.05, 1.73, 1.53, 1.46, 1.37, 1.07, 0.90. HRMS (EI-TOF) calcd for $C_{14}H_{15}D_3O_2$ (M^+) = 221.1490, found 221.1485.

4-Methyl-1-phenylpentan-1-one-4-*d* (**27**):



Prepared following the general procedure for 24 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 19.7 mg (56% yield). ^{1}H NMR spectrum showed 91% deuterium incorporation on the tertiary C(sp^3)-H bond. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.96 (d, *J* = 7.5 Hz, 2H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 2H), 3.02 – 2.87 (m, 1.95H), 1.64 – 1.46 (m, 2.09H), 0.97 – 0.89 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 200.8, 137.1, 132.8, 128.5, 128.0, 36.7 – 36.5 (m), 33.1, 27.4 – 27.0 (m), 22.4 – 22.2 (m). D NMR (77 MHz, $CHCl_3$) δ = 2.93, 1.60, 0.92. HRMS (EI-TOF) calcd for $C_{12}H_{15}DO$ (M^+) = 177.1258, found 177.1261.

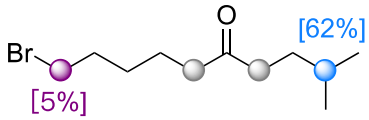
1-(4-(Methoxy-d_3)phenyl)-4-methylpentan-1-one-4-*d* (**28**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 37.2 mg (90% yield). ^{1}H NMR spectrum showed average 47% deuterium incorporation on the tertiary C(sp^3)-H bond and adjacent secondary C(sp^3)-H bonds which overlap with each other on the ^{1}H NMR spectrum, 7% deuterium incorporation on the *a*-oxy carbonyl bonds and 84% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.99 – 7.86 (m, 2H), 6.96 – 6.86 (m, 2H), 3.86 – 3.78 (m, 0.48H), 2.94 – 2.81 (m, 1.86H), 1.65 – 1.52 (m, 1.60H), 0.96 – 0.87 (m, 6H). ^{13}C NMR (126

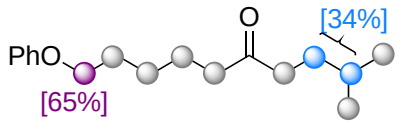
MHz, $CDCl_3$) δ = 199.3, 163.2, 130.3, 130.1, 113.6, 55.3 – 54.5 (m), 36.3 – 36.0 (m), 33.4 – 32.6 (m), 28.1 – 26.3 (m), 23.5 – 22.0 (m). D NMR (77 MHz, $CHCl_3$) δ = 3.82, 2.89, 1.60, 0.92. HRMS (EI-TOF) calcd for $C_{13}H_{14}D_4O_2$ (M^+) = 210.1552, found 210.1548.

10-Bromo-2-methyldecan-5-one-2-*d* (**29**):



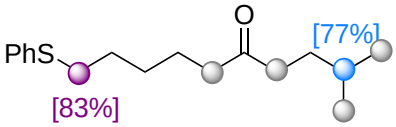
Prepared following the general procedure for 24 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 49.2 mg (99% yield). ^{1}H NMR spectrum showed 5% deuterium incorporation on the *a*-bromide C(sp^3)-H bonds and 62% deuterium incorporation on the tertiary C(sp^3)-H bond. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 3.40 (t, *J* = 7.0 Hz, 1.90H), 2.44 – 2.35 (m, 4H), 1.92 – 1.82 (m, 2H), 1.62 – 1.52 (m, 2H), 1.52 – 1.50 (m, 0.38H), 1.49 – 1.36 (m, 4H), 0.89 – 0.86 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 211.2, 42.4 – 42.2 (m), 40.9, 40.9, 33.6, 32.7 – 32.4 (m), 27.8, 27.7, 22.9 – 22.6 (m), 22.4, 22.2. D NMR (77 MHz, $CHCl_3$) δ = 3.39, 2.39, 1.50. HRMS (EI-TOF) calcd for $C_{11}H_{20}DBrO$ (M^+) = 249.0833, found 249.0823.

2-Methyl-10-phenoxydecan-5-one-2,10,10-d_3 (**30**):



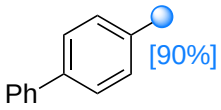
Prepared following the general procedure for 24 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 51.9 mg (99% yield). ^{1}H NMR spectrum showed average 34% deuterium incorporation on the tertiary C(sp^3)-H adjacent secondary C(sp^3)-H bonds which overlap with each other in the ^{1}H NMR spectrum, and 65% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.32 – 7.25 (m, 2H), 6.94 (t, *J* = 7.5 Hz, 1H), 6.89 (d, *J* = 8.5 Hz, 2H), 4.00 – 3.92 (m, 0.70H), 2.47 – 2.34 (m, 4H), 1.82 – 1.74 (m, 2H), 1.68 – 1.61 (m, 1.97H), 1.51 – 1.41 (m, 4H), 0.92 – 0.88 (m, 5.89H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 211.4, 159.0, 129.4, 120.5, 114.4, 67.5 - 67.1 (m), 42.6 – 42.3 (m), 40.9 – 40.6 (m), 32.7 – 32.4 (m), 29.1 ($CH_2CH(CH_3)_2$), 28.8 (t, *J* = 11.8 Hz, $CHDCH(CH_3)_2$), 27.7 ($CH(CH_3)_2$), 27.2 (t, *J* = 19.4 Hz, $CD(CH_3)_2$), 25.8 – 25.4 (m), 23.7 – 23.2 (m), 22.5 – 22.1 (m). D NMR (77 MHz, $CHCl_3$) δ = 3.95, 2.44, 1.78, 1.63, 1.53, 0.90. HRMS (EI-TOF) calcd for $C_{17}H_{21}D_5O_2$ (M^+) = 267.2241, found 267.2239.

2-Methyl-10-(phenylthio)decan-5-one-2,10,10-d_3 (**31**):



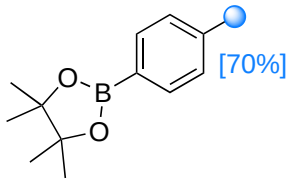
Prepared following the general procedure for 24 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless oil in 52.8 mg (95% yield). ^{1}H NMR spectrum showed 77% deuterium incorporation on the tertiary C(sp^3)-H bond, and 83% deuterium incorporation on the *a*-thioxy C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.33 – 7.29 (m, 2H), 7.29 – 7.25 (m, 2H), 7.18 – 7.13 (m, 1H), 2.92 – 2.86 (m, 0.34H), 2.42 – 2.31 (m, 3.91H), 1.67 – 1.60 (m, 2H), 1.60 – 1.53 (m, 2H), 1.52 – 1.48 (m, 0.23H), 1.46 – 1.35 (m, 4H), 0.90 – 0.84 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 211.3, 136.7, 128.9, 128.8, 125.7, 42.4, 40.9, 40.8, 32.6 - 32.5 (m), 28.8 - 28.6 (m), 28.2, 27.7, 23.3, 22.3, 22.2. D NMR (77 MHz, $CHCl_3$) δ = 2.88, 2.36, 1.49, 0.89, HRMS (EI-TOF) calcd for $C_{17}H_{23}D_3OS$ (M^+) = 281.1887, found 281.1881.

4-(Methyl-d_3)-1,1'-biphenyl (**32**):



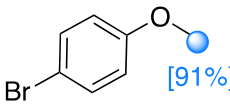
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless solid in 33.2 mg (99% yield), and ^{1}H NMR spectrum showed 81% deuterium incorporation on the benzylic C(sp^3)-H bonds. After second running with the 81% deuteride product, the deuterium incorporation was improved to 90%. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.78 – 7.66 (m, 2H), 7.65 – 7.59 (m, 2H), 7.58 – 7.51 (m, 2H), 7.51 – 7.42 (m, 1H), 7.41 – 7.32 (m, 2H), 2.54 – 2.43 (m, 0.30H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 141.1, 138.3, 136.9, 129.4, 128.7, 126.9, 126.9, 21.1 – 20.1 (m). HRMS (EI-TOF) calcd for $C_{13}H_9D_3$ (M^+) = 171.1122, found 171.1114.

4,4,5,5-Tetramethyl-2-(4-(methyl-d_3)phenyl)-1,3,2-dioxaborolane (**33**):



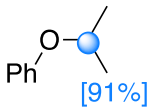
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 5 : 1) to afford product as colorless solid in 43.1 mg (99% yield), and the ^{1}H NMR spectrum showed 70% deuterium incorporation on the benzylic C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.71(d, *J* = 6.5 Hz, 2H), 7.19 (d, *J* = 6.5 Hz, 2H), 2.38 – 2.32 (m, 0.90H), 1.35 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 141.3, 134.8, 128.5, 83.6, 24.8, 21.7 – 21.5 (m). HRMS (EI-TOF) calcd for $C_{13}H_{16}D_3BO_2$ (M^+) = 221.1661, found 221.1657.

1-Bromo-4-(methoxy-d_3)benzene (**21**):



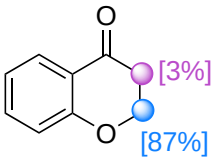
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 10 : 1) to afford product as a colorless solid in 31.8 mg (85% yield), and the ^{1}H NMR spectrum showed 91% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.52 – 7.34 (m, 2H), 6.91 – 6.73 (m, 2H), 3.79 – 3.72 (m, 0.27H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 158.7, 132.2, 115.7, 112.7, 55.2 – 54.6 (m). HRMS (EI-TOF) calcd for $C_7H_4D_3BrO$ (M^+) = 188.9861, found 188.9859.

((Propan-2-yl-2-*d*)oxy)benzene (**34**):



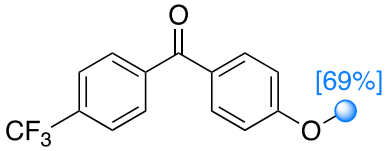
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The yield was detected to be 99% using CH_2Br_2 as internal standard. Finally, the crude mixture was purified over silica gel chromatography (pure hexane) to afford product as a colorless oil which still contained some diethyl ether, but ^{1}H NMR spectrum was clean enough to show 91% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.33 – 7.27 (m, 2H), 7.00 – 6.90 (m, 3H), 4.61 – 4.53 (m, 0.09H), 1.39 – 1.35 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 157.8, 129.4, 120.4, 115.8, 70.0 – 69.0 (m), 21.9. HRMS (EI-TOF) calcd for $C_9H_{11}DO$ (M^+) = 137.0945, found 137.0947.

Chroman-4-one-2,2-d_2 (**35**):



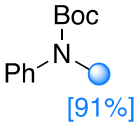
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 10 : 1) to afford product as a colorless oil in 26.7 mg (90% yield), and ^{1}H NMR spectrum showed 3% deuterium incorporation on the *a*-carbonyl C(sp^3)-H bonds and 87% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.89 (dd, *J* = 7.5, 2.0 Hz, 1H), 7.49 – 7.43 (m, 1H), 7.04 – 6.97 (m, 1H), 6.96 (d, *J* = 8.0 Hz, 1H), 4.55 – 4.47 (m, 0.27 H), 2.79 (s, 1.94H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 191.8, 161.8, 135.9, 127.1, 121.3, 117.8, 66.9 – 66.0 (m), 37.5. D NMR (500 MHz, $CHCl_3$) δ = 4.50, 2.78. HRMS (EI-TOF) calcd for $C_9H_6D_2O_2$ (M^+) = 150.0644, found 150.0643.

(4-(Methoxy-d_3)phenyl)(4-(trifluoromethyl)phenyl)methanone (**36**):



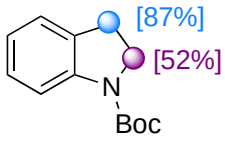
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%) and $C_6H_5CF_3$ (0.2 mL). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 10 : 1) to afford a colorless solid in 55.4 mg (99% yield), and ^{1}H NMR spectrum showed 69% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.88 – 7.77 (m, 4H), 7.73 (d, *J* = 8.5 Hz, 2H), 6.97(d, *J* = 8.5 Hz, 2H), 3.91 – 3.83 (m, 0.92H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 194.2, 163.7, 141.5, 133.2 (q, *J* = 32.8 Hz), 132.6, 129.7, 129.3, 125.2 (q, *J* = 3.8 Hz), 123.7 (q, *J* = 272.8 Hz), 113.8, 55.5 – 54.7 (m). HRMS (EI-TOF) calcd for $C_{15}H_8D_3F_3O_2$ (M^+) = 283.0894, found 283.0896.

tert-Butyl (methyl-d_3)(phenyl)carbamate (**37**):



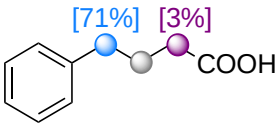
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 5 : 1) to afford product as a colorless oil in 37.7 mg (90% yield), and ^{1}H NMR spectrum showed 91% deuterium incorporation on the *a*-amide C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.34 – 7.29 (m, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.17 – 7.13 (m, 1H), 3.26 – 3.21 (m, 0.26 H), 1.45 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 154.8, 143.8, 128.5, 125.5, 125.3, 80.2, 37.2 – 36.3 (m), 28.3. HRMS (EI-TOF) calcd for $C_{12}H_{14}D_3NO_2$ (M^+) = 210.1442, found 210.1446.

tert-Butyl indoline-1-carboxylate-2,2,3-d_3 (**38**):



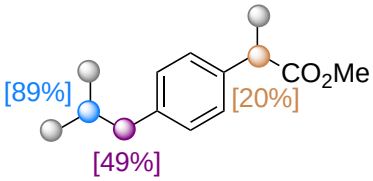
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 5 : 1) to afford product as a colorless solid in 37.2 mg (85% yield), and ^{1}H NMR spectrum showed 87% deuterium incorporation on the benzylic C(sp^3)-H bonds and 52% deuterium incorporation on the *a*-amide C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.01 – 7.43 (m, 1H), 7.21 – 7.06 (m, 2H), 6.92 (t, *J* = 7.5 Hz, 1H), 3.96 (bs, 0.96H), 3.11 – 3.02 (m, 0.27H), 1.57 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 152.6, 143.3 – 143.0 (m), 132.1 – 130.0 (m), 127.3, 124.9 – 124.3 (m), 122.0, 114.6, 80.2 – 77.5 (m), 47.5 – 47.2 (m), 28.4, 27.1 – 26.2 (m). HRMS (EI-TOF) calcd for $C_{13}H_{14}D_3NO_2$ (M^+) = 222.1442, found 222.1437.

4-Phenylbutanoic-4,4-d_2 acid (**39**):



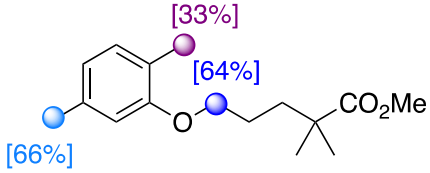
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (dichloromethane : methanol = 20 : 1) to afford product as a colorless solid in 29.5 mg (90% yield), and ^{1}H NMR spectrum showed 71% deuterium incorporation on the benzylic C(sp^3)-H bonds and 3% deuterium incorporation on the *a*-carboxylic acid C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.30 (t, *J* = 7.5 Hz, 2H), 7.23 – 7.15 (m, 3H), 2.73 – 2.63 (m, 0.58H), 2.39 (t, *J* = 7.0 Hz, 2H), 2.02 – 1.83 (m, 1.94H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 179.9, 141.2 – 141.0 (m), 128.4, 128.4, 126.0, 35.0 – 34.3 (m), 33.3 – 33.0 (m), 26.1 – 26.0 (m). D NMR (77 MHz, $CHCl_3$) δ = 2.68, 2.40, 1.98. HRMS (EI-TOF) calcd for $C_{10}H_{10}D_2O_2$ (M^+) = 166.0957, found 166.0955.

Methyl (2*S*)-2-(4-(2-methylpropyl-1,2-d_2)phenyl)propanoate (**40**):



Prepared following the general procedure for 24 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 50 : 1) to afford product as a colorless solid in 40.5 mg (92% yield), and ^{1}H NMR spectrum showed 89% deuterium incorporation on the isopropyl C(sp^3)-H bond, 49% deuterium incorporation on the benzylic C(sp^3)-H bonds and 20% deuterium incorporation on the *a*-ester C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.21 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 3.71 (m, 0.80H), 3.66 (s, 3H), 2.47 – 2.40 (m, 1.03H), 1.91 – 1.80 (m, 0.11H), 1.53 – 1.43 (m, 3H), 0.94 – 0.86 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 175.2, 140.5, 137.7, 129.3, 127.1, 51.9, 45.0, 30.1 – 29.8 (m), 29.7 – 29.4 (m), 22.2, 18.6, 18.5. D NMR (77 MHz, $CHCl_3$) δ = 3.70, 2.44, 1.84, 1.50, 0.91. HRMS (EI-TOF) calcd for $C_{14}H_{17}D_3O_2$ (M^+) = 223.1646, found 223.1647.

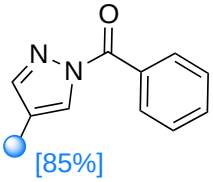
Methyl 2,2-dimethyl-5-(2-(methyl-*d*)-5-(methyl-d_2)phenoxy)pentanoate-5-*d* (**41**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 10 : 1) to afford product as a colorless solid in 47.7 mg (90% yield), and ^{1}H NMR spectrum showed 66%, 33% deuterium incorporation on the benzylic C(sp^3)-H bonds individually, and 64% deuterium incorporation on the *a*-oxy C(sp^3)-

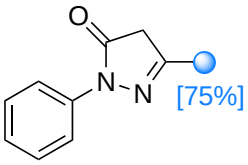
H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.01 (d, *J* = 7.5 Hz, 1H), 6.67 (d, *J* = 7.5 Hz, 1H), 6.62 (s, 1H), 3.96 – 3.88 (m, 0.72H), 3.68 (s, 3H), 2.33 – 2.27 (m, 1.02H), 2.21 – 2.15 (m, 1.69H), 1.77 – 1.69 (m, 4H), 1.24 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 178.3, 156.9, 136.3, 130.2, 123.6 – 123.3 (m), 120.6, 111.9, 67.5 (dd, *J* = 44.7, 23.2 Hz), 51.7, 42.1, 37.1 – 37.0 (m), 25.1, 25.0, 21.4 – 20.5 (m), 15.8 – 15.1 (m). D NMR (77 MHz, $CHCl_3$) δ = 3.92, 2.32 – 2.93, 2.20 – 2.17. HRMS (EI-TOF) calcd for $C_{16}H_{19}D_5O_3$ (M^+) = 269.2034, found 269.2038.

(4-(Methyl-*d*3)-1*H*-pyrazol-1-yl)(phenyl)methanone (**42**):



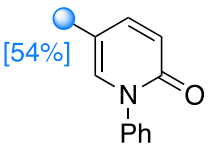
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified by silica gel chromatography (hexane : diethyl ether = 5 : 1) to afford product as a colorless solid in 33.1 mg (89% yield), and ^{1}H NMR spectrum showed 85% deuterium incorporation on the benzylic C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.18 (s, 1H), 8.09 – 8.05 (m, 2H), 7.63 (s, 1H), 7.61 – 7.55 (m, 1H), 7.52 – 7.45 (m, 2H), 2.15 – 2.11 (m, 0.44H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 166.3, 146.2, 132.7, 131.7, 131.3, 128.1, 128.0, 120.2, 8.5 – 8.3 (m). HRMS (EI-TOF) calcd for $C_{11}H_7D_3N_2O$ (M^+) = 189.0976, found 189.0973.

5-(Methyl-*d*3)-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one (**43**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 5 : 1) to afford the product as a colorless solid in 34.6 mg (99% yield), and ^{1}H NMR spectrum showed 75% deuterium incorporation on the methyl C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.85 (d, *J* = 8.0 Hz, 2H), 7.38 (t, *J* = 8.0 Hz, 2H), 7.17 (t, *J* = 8.0 Hz, 1H), 3.41 (s, 2H), 2.19 – 2.12 (m, 0.74H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 170.5, 156.2, 138.0, 128.8, 125.0, 118.8, 43.0, 16.7 – 16.2 (m). HRMS (EI-TOF) calcd for $C_{10}H_7D_3N_2O$ (M^+) = 177.0976, found 177.0972.

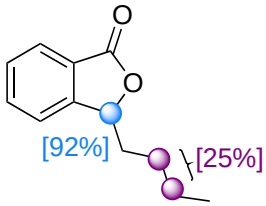
5-(Methyl-*d*3)-1-phenylpyridin-2(1*H*)-one (**44**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%) after mixing with trifluoroacetic acid (3.0 equiv) in D_2O. The crude mixture was purified over silica gel chromatography (hexane :

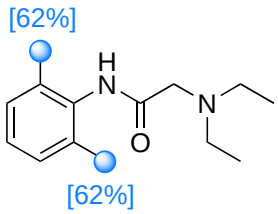
diethyl ether = 2 : 1) to afford the product as a colorless solid in 31.7 mg (85% yield), and ^{1}H NMR spectrum showed 54% deuterium incorporation on the benzylic C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.52 – 7.46 (m, 2H), 7.44 – 7.39 (m, 1H), 7.38- 7.35 (m, 2H), 7.27 (dd, *J* = 7.0, 2.5 Hz, 1H), 7.12 (s, 1H), 6.62 (d, *J* = 9.5 Hz, 1H), 2.12 – 2.06 (m, 1.39H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 161.7, 142.5, 141.1, 135.3, 129.3, 128.3, 126.5, 121.4, 114.8 – 114.7 (m), 17.0 – 16.4 (m). HRMS (EI-TOF) calcd for $C_{12}H_8D_3NO$ (M^+) = 188.1023, found 188.1018.

3-Butylisobenzofuran-1(3*H*)-one-3-*d* (**45**):



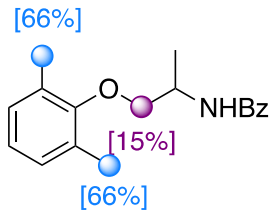
Prepared following the general procedure for 24 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 2 : 1) to afford product as a colorless oil in 32.0 mg (84% yield), and ^{1}H NMR spectrum showed 92% deuterium incorporation on the *a*-oxy C(sp^3)-H bond, and 25% deuterium incorporation on the indicated secondary C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.87 (d, *J* = 8.0 Hz, 1H), 7.65 (t, *J* = 8.0 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.43 (d, *J* = 7.5 Hz, 1H), 5.46 (dd, *J* = 7.5, 4.0 Hz, 0.08H), 2.08 – 1.95 (m, 1H), 1.80 – 1.68 (m, 1H), 1.53 – 1.25 (m, 3.00H), 0.98 – 0.82 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 170.6, 150.0, 133.9, 129.0, 126.1, 125.6, 121.7, 81.4 (OCH*n*Bu), 81.0 (t, *J* = 22.4 Hz, OCD*n*Bu), 34.4 – 34.1 (m), 26.8 – 26.2 (m), 22.5 – 20.8 (m), 13.9 – 13.1 (m). D NMR (77 MHz, $CHCl_3$) δ = 5.45, 1.35. HRMS (EI-TOF) calcd for $C_{12}H_{12}D_2O_2$ (M^+) = 192.1114, found 192.1115.

N-(2,6-bis(methyl-d_3)phenyl)-2-(diethylamino)acetamide (**46**):



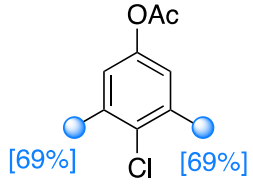
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%) after mixing with trifluoroacetic acid (3.0 equiv) in D_2O. The crude mixture was purified by silica gel chromatography (hexane : diethyl ether = 5 : 1) to afford product as a colorless solid in 39.4 mg (84% yield), and ^{1}H NMR spectrum showed 62% deuterium incorporation on the benzylic C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.92 (bs, 1H), 7.15 – 7.00 (m, 3H), 3.22 (s, 2H), 2.69 (q, *J* = 7.0 Hz, 4H), 2.24 – 2.18 (m, 2.31H), 1.14 (t, *J* = 7.0 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 170.3, 135.0, 134.0, 128.2, 127.0, 57.5, 48.9, 18.6 – 18.0 (m), 12.6. D NMR (77 MHz, $CHCl_3$) δ = 3.21 – 3.18. HRMS (EI-TOF) calcd for $C_{14}H_{18}D_4NO$ (M^+) = 238.1978, found 238.1970.

N-(1-(2,6-bis(methyl-d_3)phenoxy)propan-2-yl)benzamide (**47**):



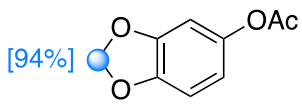
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 10 : 1) to afford product as a colorless solid in 49.4 mg (87% yield), and ^{1}H NMR spectrum showed 66% deuterium incorporation on the benzylic C(sp^3)-H bonds, and 15% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.87 – 7.78 (m, 2H), 7.56 – 7.48 (m, 1H), 7.48 – 7.32 (m, 2H), 7.01 (d, *J* = 7.5 Hz, 2H), 6.97 – 6.89 (m, 1H), 6.73 (bs, 1H), 4.62 – 4.49 (m, 1H), 3.98 – 3.88 (m, 0.88H), 3.87 – 3.76 (m, 0.83H), 2.29 – 2.21 (m, 2.03H), 1.53 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 166.8, 154.8, 134.6, 131.4, 130.7 – 130.5 (m), 129.0, 128.5, 126.8, 124.1, 73.8, 45.8 – 45.6 (m), 17.8 – 17.6 (m), 16.2 – 15.2 (m). D NMR (77 MHz, $CHCl_3$) δ = 3.89 – 3.78, 2.24 – 2.20. HRMS (EI-TOF) calcd for $C_{18}H_{17}D_4NO_2$ (M^+) = 287.1818, found 287.1823.

4-Chloro-3,5-bis(methyl-d_3)phenyl acetate (**48**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 10 : 1) to afford product as a colorless oil in 39.2 mg (99% yield), and ^{1}H NMR spectrum showed 69% deuterium incorporation on the benzylic C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 6.82 (s, 2H), 2.38 – 2.32 (m, 1.87H), 2.28 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 169.5, 148.2, 137.4, 131.8, 121.3, 21.0, 20.7 – 20.1 (m). HRMS (EI-TOF) calcd for $C_{10}H_7D_4ClO_2$ (M^+) = 202.0693, found 202.0695.

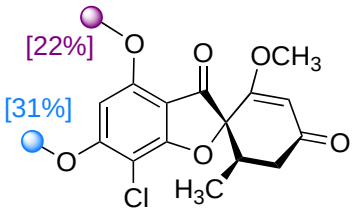
Benzo[*d*][1,3]dioxol-5-yl-2,2-d_2 acetate (**49**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless solid in 34.2 mg (95% yield), and ^{1}H NMR spectrum showed 94% deuterium incorporation on the *α*-oxy C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 6.77 (d, *J* = 9.0 Hz, 1H), 6.60 (d, *J* = 2.5 Hz, 1H), 6.52 (dd, *J* = 9.0, 2.5 Hz, 1H), 5.95 (s, 0.12H), 2.26 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 169.8, 148.0, 145.3, 144.9, 113.9, 107.9, 103.7, 101.6 – 100.8 (m), 20.9. HRMS (EI-TOF)

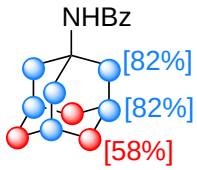
calcd for $C_9H_6D_2O_4$ (M^+) = 182.0543, found 182.0546.

(2*S*)-7-Chloro-2'-methoxy-4,6-bis(methoxy-*d*)-6'-methyl-3*H*-spiro[benzofuran-2,1'-cyclohexan]-2'-ene-3,4'-dione (**50**):



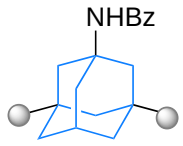
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%) and $C_6H_5CF_3$ (0.2 mL). The crude mixture was purified over silica gel chromatography (dichloromethane : diethyl ether = 1 : 1) to afford product as a colorless solid in 70.1 mg (99% yield), and ^{1}H NMR spectrum showed 31% and 22% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 6.12 (s, 1H), 5.52 (s, 1H), 4.02 – 3.97 (m, 2.33H), 3.96 – 3.92 (m, 2.06H), 3.60 (s, 3H), 3.00 (dd, *J* = 16.5, 13.5 Hz, 1H), 2.86 – 2.77 (m, 1H), 2.41 (dd, *J* = 16.5, 4.5 Hz, 1H), 0.94 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 197.0, 192.4, 170.7, 169.4, 164.6, 157.7, 104.8, 89.4, 57.2 – 56.0 (m), 40.0, 36.3, 14.2. D NMR (77 MHz, $CHCl_3$) δ = 3.99. HRMS (EI-TOF) calcd for $C_{17}H_{15}D_2ClO_6$ (M^+) = 354.0834, found 354.0831.

N-((3*s*,5*s*,7*s*)-adamantan-1-yl)benzamide-*d11* (**51**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%) and $C_6H_5CF_3$ (0.2 mL). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 10 : 1) to afford product as a colorless solid in 50.4 mg (99% yield), and ^{1}H NMR spectrum showed 10.9 deuterium atoms per adamantyl molecule. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.70 (d, *J* = 7.0 Hz, 2H), 7.48 – 7.41 (m, 1H), 7.41 – 7.33 (m, 2H), 5.84 (bs, 1H), 2.17 – 2.02 (m, 1.60H), 1.76 – 1.61 (m, 2.55H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 166.6 (166.5), 135.9, 130.9, 128.3, 126.6, 52.1 – 51.6 (m), 41.5 – 40.4 (m), 36.2 – 35.1 (m), 29.2 – 28.1 (m). D NMR (77 MHz, $CHCl_3$) δ = 2.04, 1.64. HRMS (EI-TOF) calcd for $C_{17}H_{10}D_{11}O$ (M^+) = 266.2304, found 266.2294.

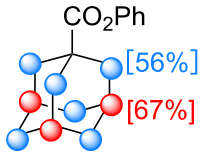
N-((1*r*,3*R*,5*S*,7*r*)-3,5-dimethyladamantan-1-yl)benzamide-*d7* (**52**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%) and $C_6H_5CF_3$ (0.2 mL). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 10 : 1) to afford the product as a colorless solid in 56.1 mg (99% yield), and ^{1}H NMR spectrum showed 6.7 deuterium atoms per adamantyl molecule. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.75 – 7.65 (m, 2H), 7.47 – 7.41 (m, 1H), 7.41 – 7.33 (m, 2H), 5.90 (bs, 1H), 2.19 – 2.17 (m, 0.13H), 1.98 – 1.92 (m, 0.31H), 1.81

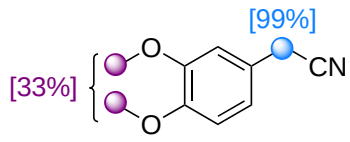
– 1.71 (m, 2.55H), 1.46 – 1.36 (m, 1.40 H), 1.36 – 1.25 (m, 1.56 H), 1.24 – 1.10 (m, 2.33H), 0.86 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 166.6, 135.8, 140.0, 128.3, 126.6, 53.6 (t, *J* = 8.3 Hz), 50.5, 47.5 – 46.9 (m), 42.5 – 41.8 (m), 40.7 – 40.5 (m), 32.3 (t, *J* = 10.5 Hz), 30.1, 39.8 – 29.0 (m). D NMR (77 MHz, $CHCl_3$) δ = 2.12, 1.89, 1.73, 1.37, 1.28, 0.86. HRMS (EI-TOF) calcd for $C_{19}H_{18}D_7NO$ (M^+) = 290.2370, found 290.2366.

Phenyl (3*r*,5*r*,7*r*)-adamantane-1-carboxylate-*d8* (**53**):



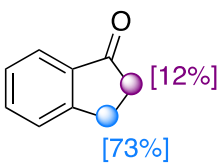
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%) and $C_6H_5CF_3$ (0.2 mL). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 8 : 1) to afford product as a colorless solid in 50.3 mg (98% yield), and ^{1}H NMR spectrum showed 8.8 deuterium atoms per adamantyl molecule. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.42 – 7.34 (m, 2H), 7.24 – 7.16 (m, 1H), 7.08 – 7.01 (m, 2H), 2.11 – 2.01 (m, 5.23H), 1.79 – 1.70 (m, 0.98H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 176.2, 151.1, 129.3, 125.4, 121.5, 40.9 – 40.6 (m), 38.7 – 38.3 (m), 38.3 – 37.8 (m), 36.0 – 35.1 (m), 27.9 – 26.6 (m). D NMR (77 MHz, $CHCl_3$) δ = 2.10, 1.77. HRMS (EI-TOF) calcd for $C_{17}H_{12}D_8O_2$ (M^+) = 264.1960, found 264.1955.

2-(3,4-Bis(methoxy-*d*)phenyl)acetonitrile-d_2 (**54**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless solid in 31.2 mg (88% yield), and ^{1}H NMR spectrum showed 33% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds, and 99% deuterium incorporation on the benzylic C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 6.87 – 6.81 (m, 2H), 6.80 (s, 1H), 3.90 – 3.80 (m, 4.02H), 3.70 (m, 0.01H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 149.3, 148.8, 122.0, 120.1, 118.1, 111.4, 110.9, 56.0 – 55.2 (m), 22.7 (t, *J* = 20.5 Hz, OCH_2D). HRMS (EI-TOF) calcd for $C_{10}H_7D_4NO_2$ (M^+) = 181.1035, found 181.1027.

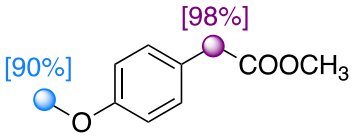
2,3-Dihydro-1*H*-inden-1-one-3,3-d_2 (**55**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 20 : 1) to afford product as a colorless solid in 25.2 mg (95% yield), and ^{1}H NMR spectrum showed 73% deuterium

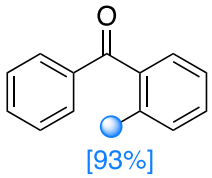
incorporation on the benzylic C(sp^3)-H bonds, and 12% deuterium incorporation on the *a*-carbonyl C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.75 (d, *J* = 8.0 Hz, 1H), 7.58 (dt, *J* = 7.5, 1.0 Hz, 1H), 7.48 (d, *J* = 7.5 Hz, 1H), 7.36 (t, *J* = 7.5 Hz, 1H), 3.18 – 3.08 (m, 0.55H), 2.71 – 2.62 (m, 1.76 H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 207.1, 155.0, 137.1, 134.5, 127.3, 126.7, 123.7, 36.1, 25.8 - 25.4 (m). HRMS (EI-TOF) calcd for $C_9H_6D_2O$ (M^+) = 134.0695, found 134.0692.

Methyl 2-(4-(methoxy-d_3)phenyl)acetate-d_2 (**56**):



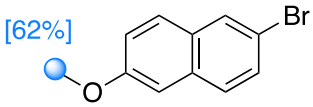
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 10 : 1) to afford product as a colorless solid in 35.7 mg (99% yield), and ^{1}H NMR spectrum showed 90% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds, and 98% deuterium incorporation on the *a*-benzylic C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.20 (d, *J* = 8.0 Hz, 2H), 6.86 (d, *J* = 8.0 Hz, 2H), 3.79 – 3.74 (m, 0.30H), 3.68 (s, 3H), 3.57 – 3.53 (m, 0.04H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 172.3, 158.7, 130.2, 125.9, 113.9, 55.0 – 54.3 (m), 51.9, 40.0 – 39.3 (m). HRMS (EI-TOF) calcd for $C_{10}H_7D_5O_3$ (M^+) = 185.1095, found 185.1093.

(2-(Methyl-d_3)phenyl)(phenyl)methanone (**57**):



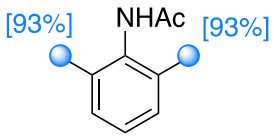
Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 8 : 1) to afford product as a colorless oil in 37.7 mg (96% yield), and ^{1}H NMR spectrum showed 93% deuterium incorporation on the benzylic C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.81 (d, *J* = 7.5 Hz, 2H), 7.62 – 7.54 (m, 1H), 7.49 – 7.43 (m, 2H), 7.42 – 7.37 (m, 1H), 7.34 – 7.28 (m, 2H), 7.27 – 7.22 (m, 1H), 2.34 – 2.29 (m, 0.21H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 198.6, 138.6, 137.7, 136.6, 133.1, 130.9, 130.2, 130.1, 128.5, 128.4, 125.1, 19.5 – 18.9 (m). HRMS (EI-TOF) calcd for $C_{14}H_{19}D_3O$ (M^+) = 199.1071, found 199.1067.

2-Bromo-6-(methoxy-d_2)naphthalene (**58**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 8 : 1) to afford product as a colorless solid in 46.7 mg (99% yield), and ^{1}H NMR spectrum showed 62% deuterium incorporation on the *a*-oxy C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.91 (d, *J* = 2.0 Hz, 1H), 7.63 (d, *J* = 9.0 Hz, 1H), 7.60 (d, *J* = 9.0 Hz, 1H), 7.50 (dd, *J* = 9.0, 2.0Hz, 1H), 7.16 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.09 (s, 1H), 3.92 – 3.86 (m, 1.15H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 157.8, 133.0, 130.0, 129.6, 129.6, 128.4, 128.3, 119.7, 117.0, 105.7, 52.3 – 54.7 (m). HRMS (EI-TOF) calcd for $C_{11}H_7D_2BrO$ (M^+) = 239.9936, found 239.9939.

N-(2,6-bis(methyl-d_3)phenyl)acetamide (**59**):



Prepared following the general procedure for 48 h with the addition of TBAB (20 mol%). The crude mixture was purified over silica gel chromatography (hexane : diethyl ether = 8 : 1) to afford product as a colorless solid in 32.2 mg (99% yield), and ^{1}H NMR spectrum showed 93% deuterium incorporation on the benzylic C(sp^3)-H bonds. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.17 – 7.01 (m, 3H), 6.93 (br, 1H), 2.27 – 2.21 (m, 0.40H), 2.16 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 168.7, 136.5, 135.4, 128.6, 128.2, 128.1, 127.3, 23.0, 18.4 – 17.5 (m). HRMS (EI-TOF) calcd for $C_{10}H_7D_6NO$ (M^+) = 169.1368, found 169.1366.

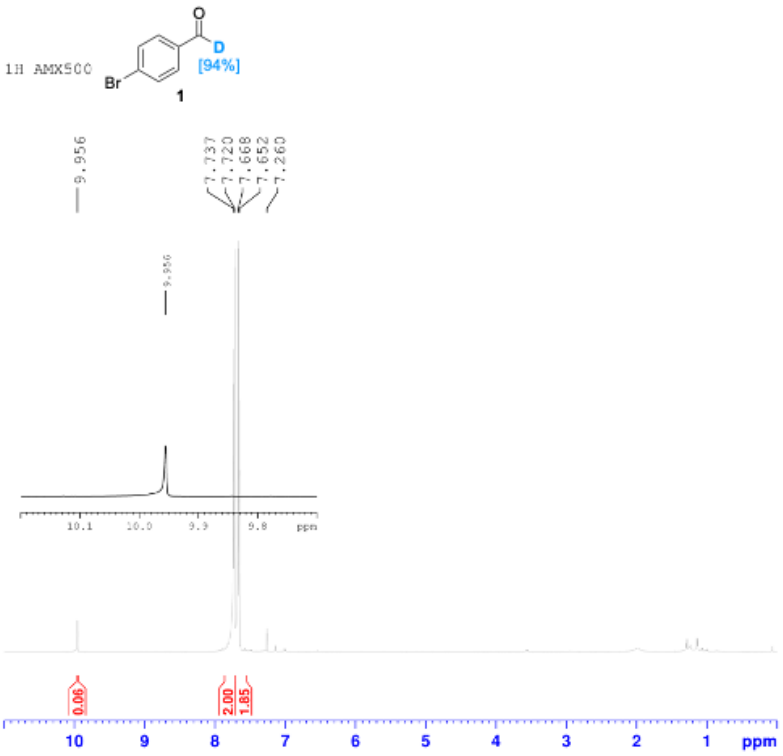
7. Reference

1 I. B. Perry, T. F. Brewer, P. J. Sarver, D. M. Schultz, D. A. DiRocco and D. W. C. MacMillan, *Nature*, 2018, **560**, 70.

2 D. C. Miller, J. M. Ganley, A. J. Musacchio, T. C. Sherwood, W. R. Ewing and R. R. Knowles, *J. Am. Chem. Soc.*, 2019, **141**, 16590.

3 Y. Motoyama, M. Abe, K. Kamo, Y. Kosako and H. Nagashima, *Chem. Commun.*, 2008, 5321.

8. Copies of NMR spectra

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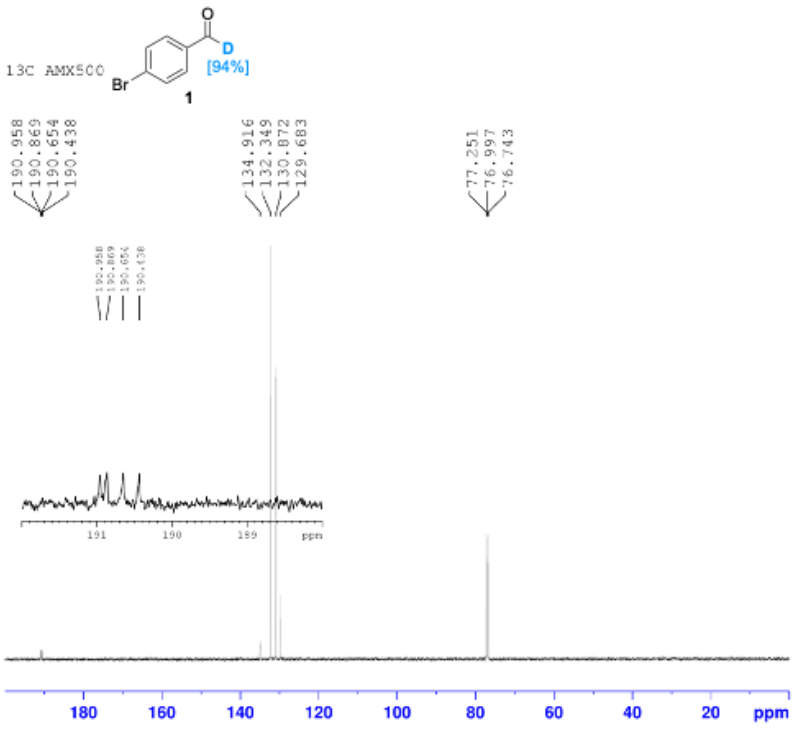
Current Data Parameters
NAME      yk0914-kyl-3197-2-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190914
Time                   16.58
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH               10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                      114
DW                 48.400 usec
DE                  6.00 usec
TE                  296.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.50 usec
PL1                     0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                        16384
SF              500.1300130 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```



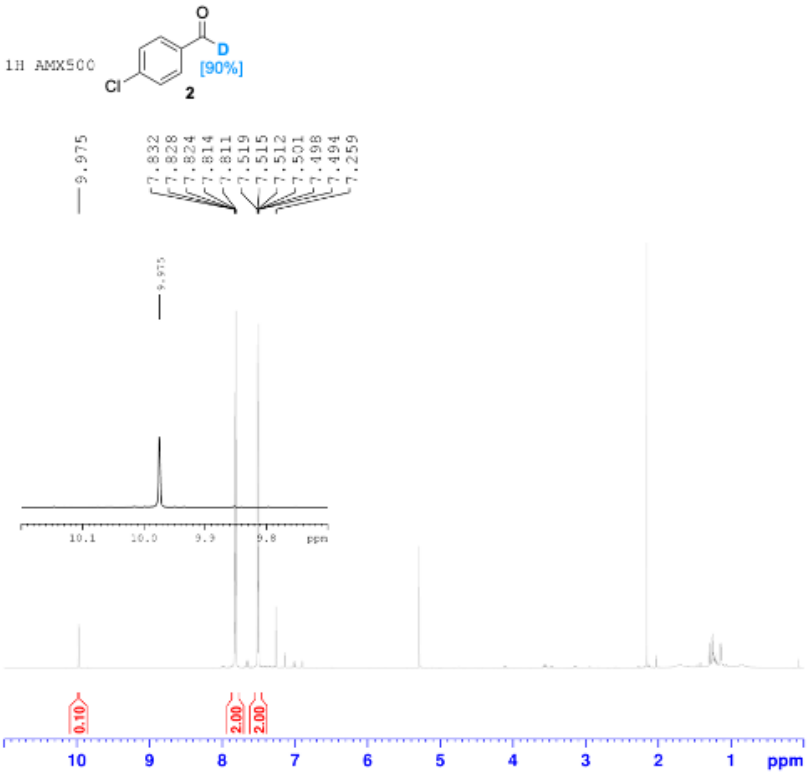

```
Current Data Parameters
NAME      yk0914-kyl-3197-2-1
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190914
Time                   17.00
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       93
DS                        0
SWH               30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0911744 sec
RG                    16384
DW                 16.650 usec
DE                  6.00 usec
TE                  297.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      20

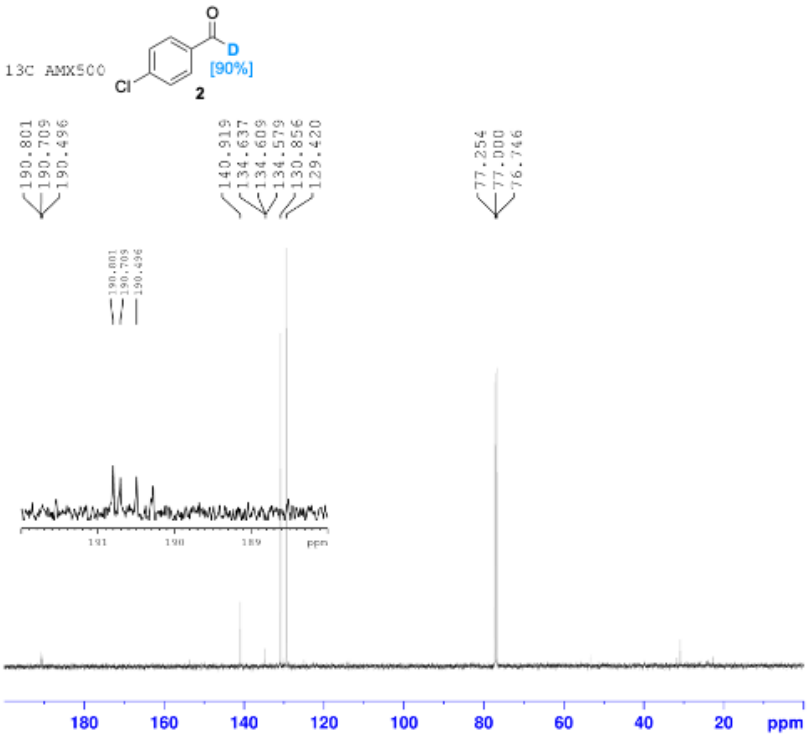
======== CHANNEL f1 ========
NUC1                     13C
P1                     8.90 usec
PL1                       0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2                    0.25 dB
PL12                  17.89 dB
PL13                  15.83 dB
SFO2          500.1320005 MHz

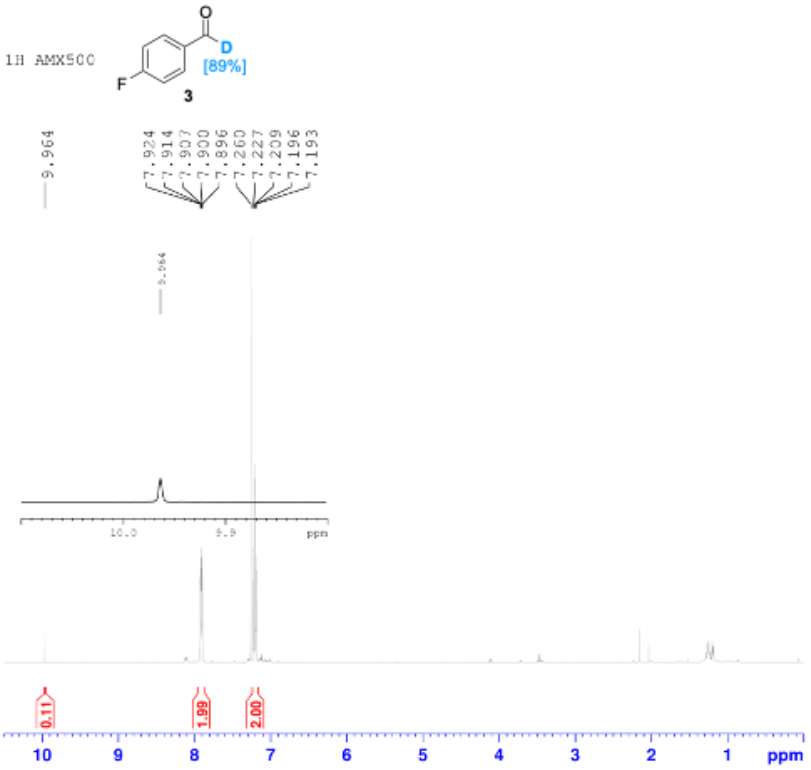
F2 - Processing parameters
SI                        32768
SF              125.7578006 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40
```


1H AMX500
O
D
[90%]
Cl
2
9.975
7.832
7.828
7.824
7.814
7.811
7.519
7.515
7.512
7.501
7.498
7.494
7.259
10.1
10.0
9.9
9.8
ppm
0.10
2.00
2.00
10
9
8
7
6
5
4
3
2
1
ppm


BRUKER
Current Data Parameters
NAME yk0109-kyl-3180-1-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200109
Time 16.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 101.6
DW 48.400 usec
DE 6.00 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


13C AMX500
O
D
[90%]
Cl
2
190.801
190.709
190.496
140.919
134.837
134.609
134.579
130.856
129.420
77.254
77.000
76.746
191
190
189
ppm
180
160
140
120
100
80
60
40
20
ppm


BRUKER
Current Data Parameters
NAME yk0109-kyl-3180-1-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200109
Time 16.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 152
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 297.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 85.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577949 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



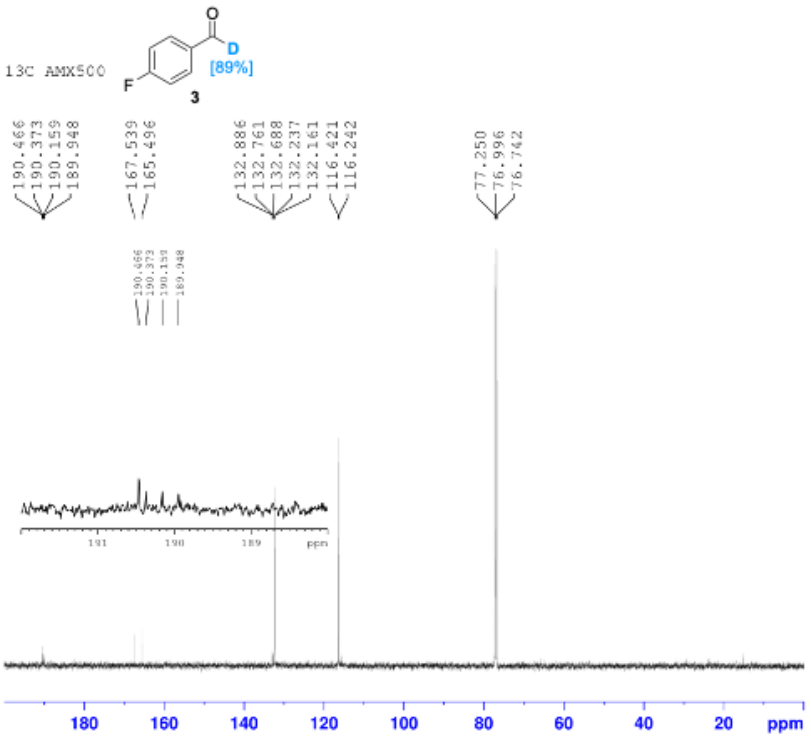
BRUKER

```
Current Data Parameters
NAME      yk0108-kyl-4124-2-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20200108
Time                   20.31
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH              10330.578 Hz
FIDRES           0.315264 Hz
AQ               1.5859712 sec
RG                   121.6
DW                 48.400 usec
DE                  6.00 usec
TE                 296.6 K
D1               1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.50 usec
PL1                     0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                    16384
SF             500.1300136 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



BRUKER

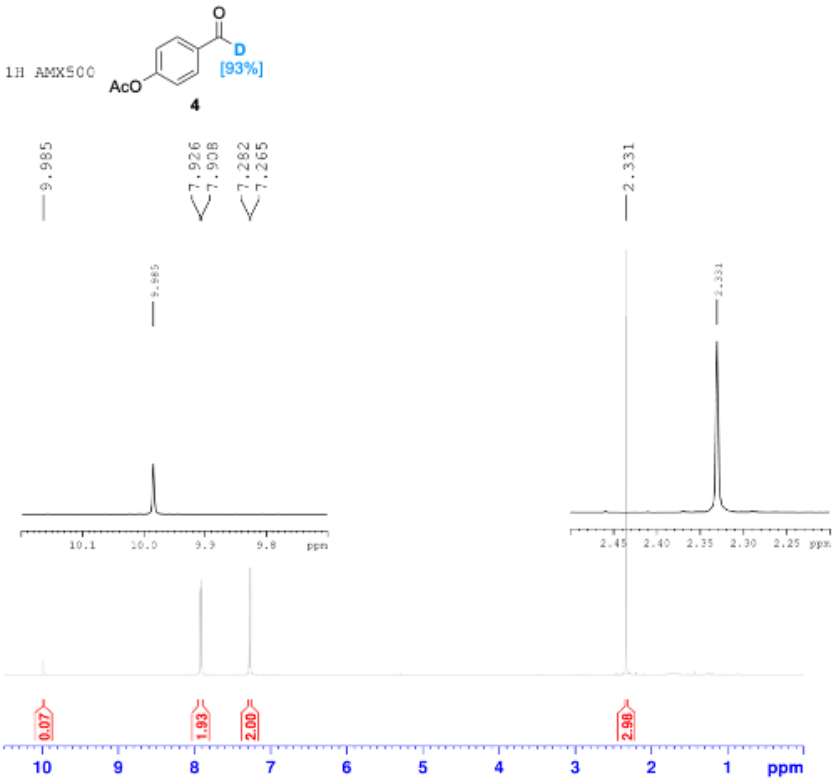
```
Current Data Parameters
NAME      yk0108-kyl-4124-2-1
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20200108
Time                   20.33
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      179
DS                        0
SWH              30030.029 Hz
FIDRES           0.458222 Hz
AQ               1.0911744 sec
RG                   16384
DW                 16.650 usec
DE                  6.00 usec
TE                 296.9 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                      20

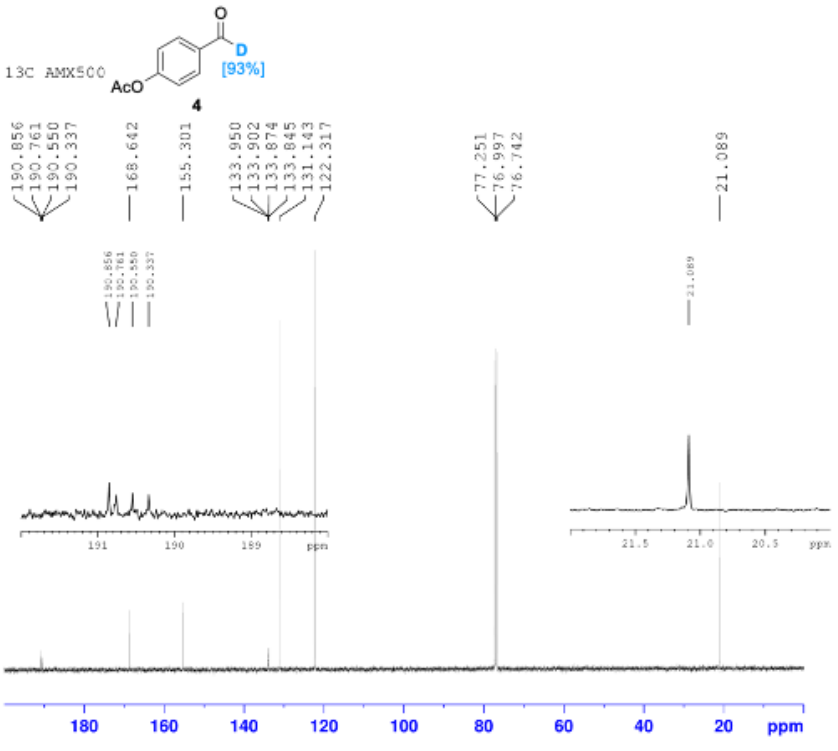
======== CHANNEL f1 ========
NUC1                     13C
P1                     8.90 usec
PL1                       0 dB
SFO1          125.7709536 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2                     0.25 dB
PL12                   17.89 dB
PL13                   19.83 dB
SFO2          500.1320005 MHz

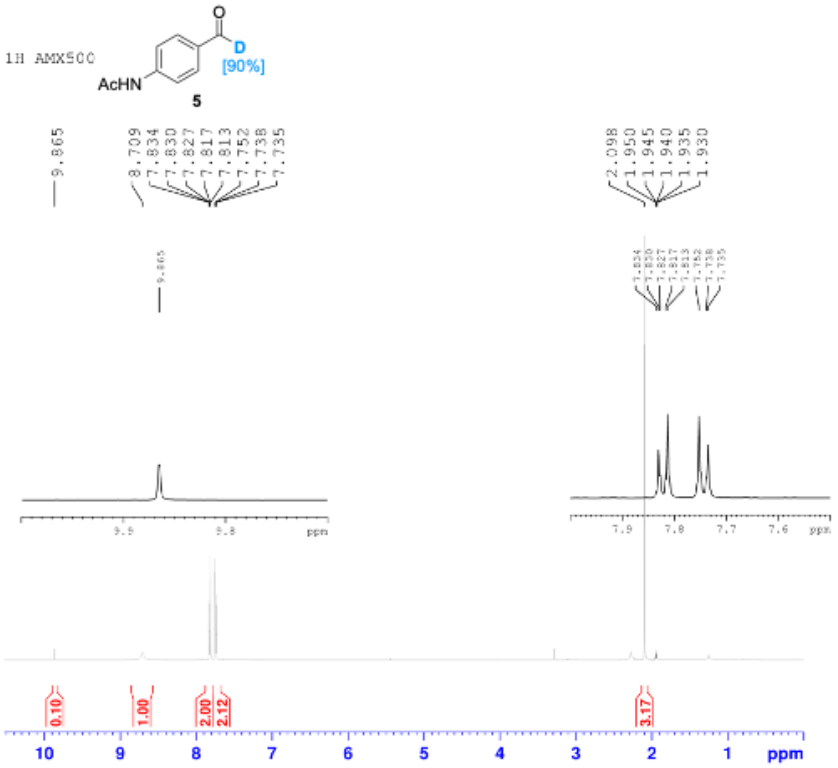
F2 - Processing parameters
SI                    32768
SF             125.7577937 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```


1H AMX500
AcO
D
[93%]
4
9.985
7.926
7.908
7.282
7.265
2.331
0.07
1.93
2.00
2.98
10
9
8
7
6
5
4
3
2
1
ppm


BRUKER
Current Data Parameters
NAME yk0104-kyl-4122-3-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200104
Time 16.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 161.3
DW 48.400 usec
DE 6.00 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 16384
SF 500.1300114 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


13C AMX500
AcO
D
[93%]
4
190.856
190.761
190.550
190.337
168.642
155.301
133.950
133.902
133.874
133.845
131.143
122.317
77.251
76.997
76.742
21.089
180
160
140
120
100
80
60
40
20
ppm


BRUKER
Current Data Parameters
NAME yk0104-kyl-4122-3-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200104
Time 16.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 178
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 296.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577964 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40




```
Current Data Parameters
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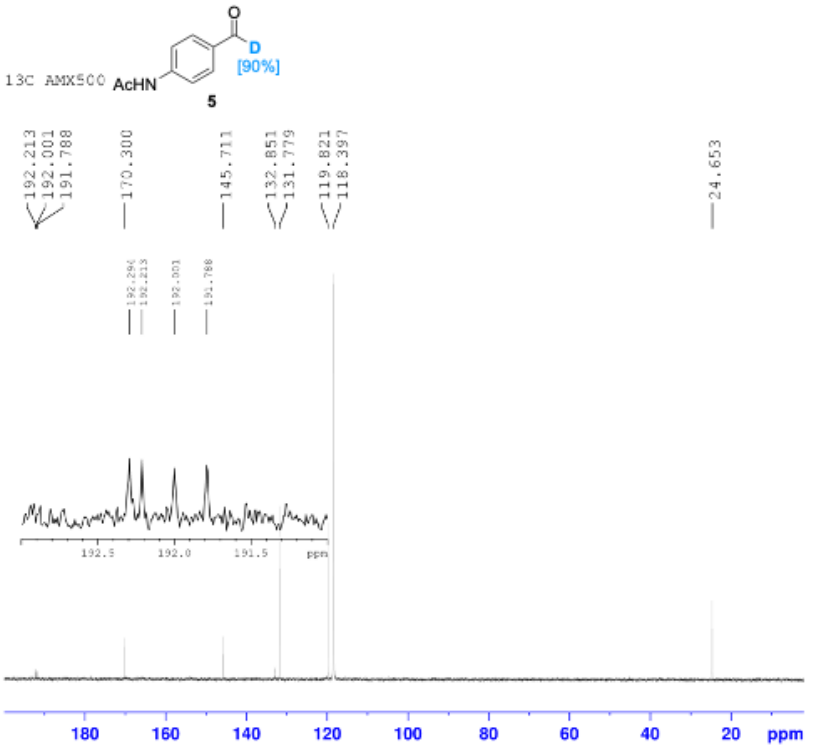
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20190906
Time                  20.56
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CD3CN
NS                        8
DS                        0
SWH               10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                       57
DW                  48.400 usec
DE                   6.00 usec
TE                  296.2 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.50 usec
PL1                     0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                    16384
SF              500.1300154 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```




```
Current Data Parameters
NAME      yk0906-kyl-4020-3
EXPNO                     2
PROCNO                    1

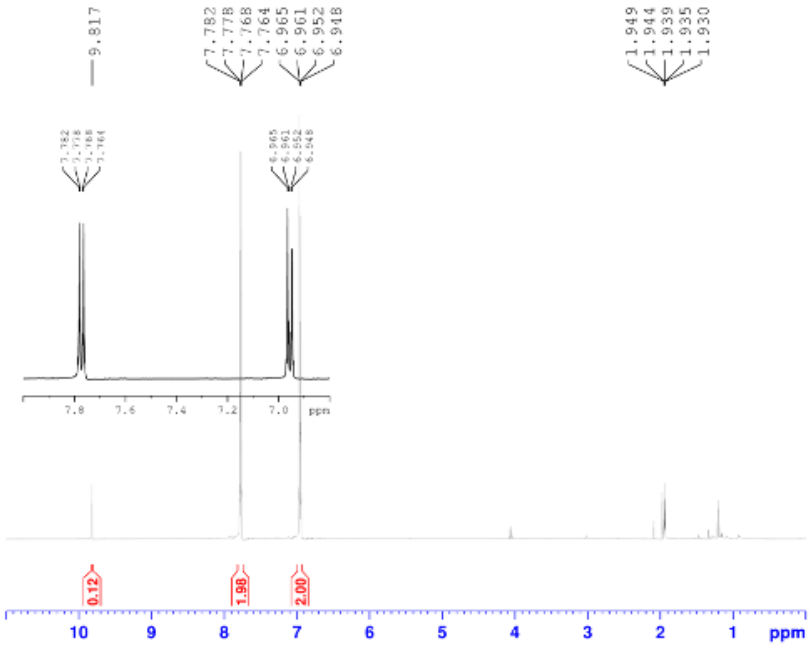
F2 - Acquisition Parameters
Date_              20190906
Time                  20.58
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      127
DS                        0
SWH               30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0911744 sec
RG                    16384
DW                  16.650 usec
DE                   6.00 usec
TE                  297.5 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      20

======== CHANNEL f1 ========
NUC1                      13C
P1                     8.90 usec
PL1                       0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2                    0.25 dB
PL12                  17.89 dB
PL13                  15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                    32768
SF              125.7576568 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

1H AMX500



BRUKER

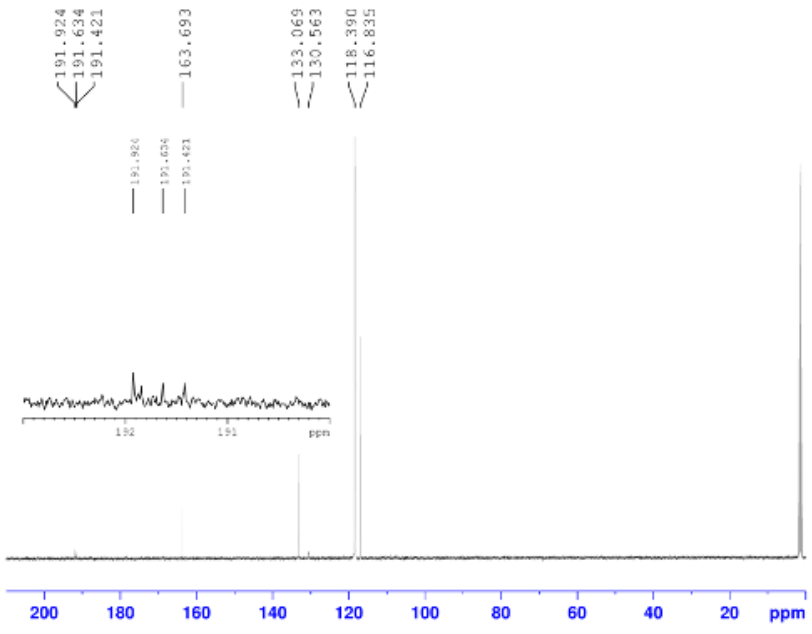
```
Current Data Parameters
NAME      yx0906-ky1-4019-2
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20190906
Time              21.04
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   0
SWH          10330.578 Hz
FIDRES        0.315264 Hz
AQ            1.5859712 sec
RG                90.5
DW               48.400 usec
DE                6.00 usec
TE               296.3 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                10.50 usec
PL1                0.25 dB
SFO1         500.1330885 MHz

F2 - Processing parameters
SI                16384
SF          500.1300154 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

13C AMX500



BRUKER

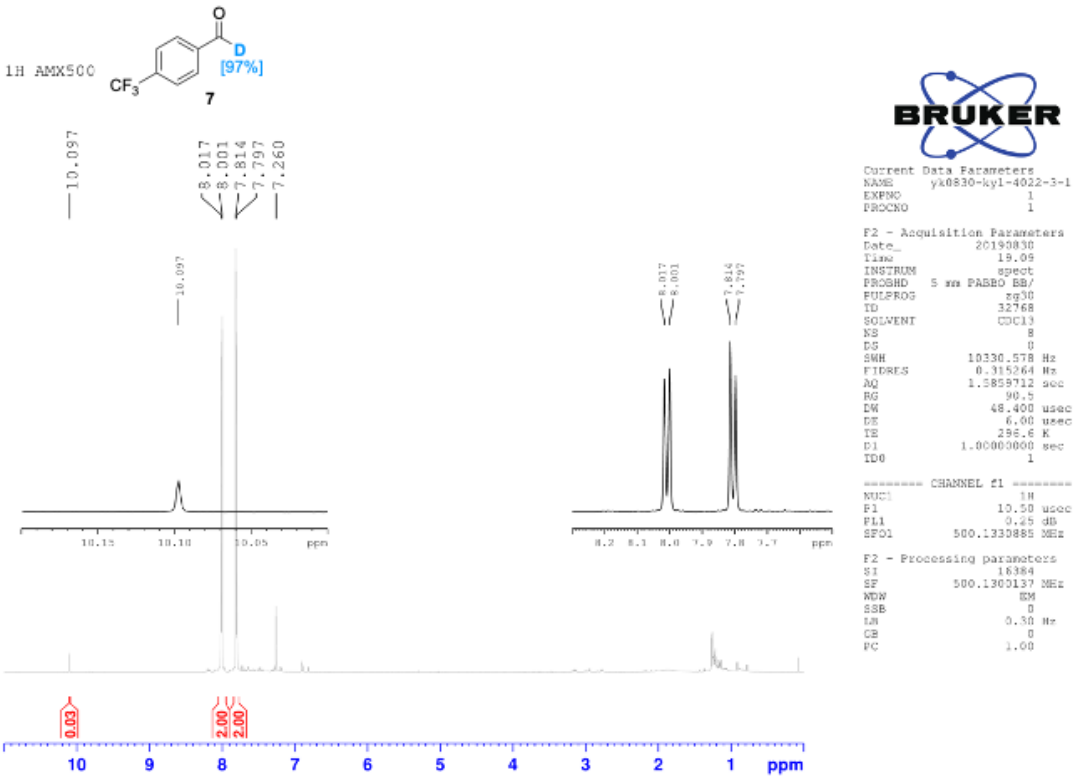
```
Current Data Parameters
NAME      yx0906-ky1-4019-2
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_           20190906
Time              21.06
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 138
DS                   0
SWH          30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0911744 sec
RG               16384
DW               16.650 usec
DE                6.00 usec
TE               296.4 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                 20

======== CHANNEL f1 ========
NUC1                13C
P1                8.90 usec
PL1                  0 dB
SFO1         125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                0.25 dB
PL12              17.89 dB
PL13              15.83 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7576556 MHz
WDW                  EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```



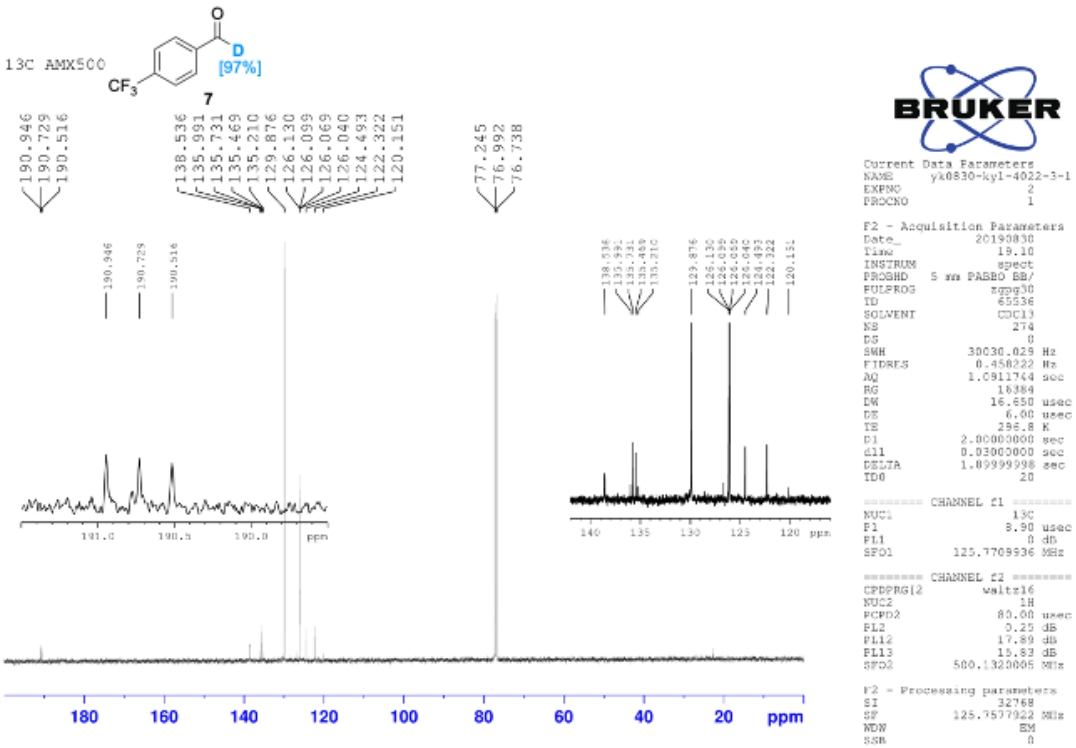
BRUKER

```
Current Data Parameters
NAME      yk0830-ky1-4022-3-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190830
Time                  19.09
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH               10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                     90.5
DW                   48.400 usec
DE                    6.00 usec
TE                   296.6 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.50 usec
PL1                     0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                    16384
SF                500.1300137 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



BRUKER

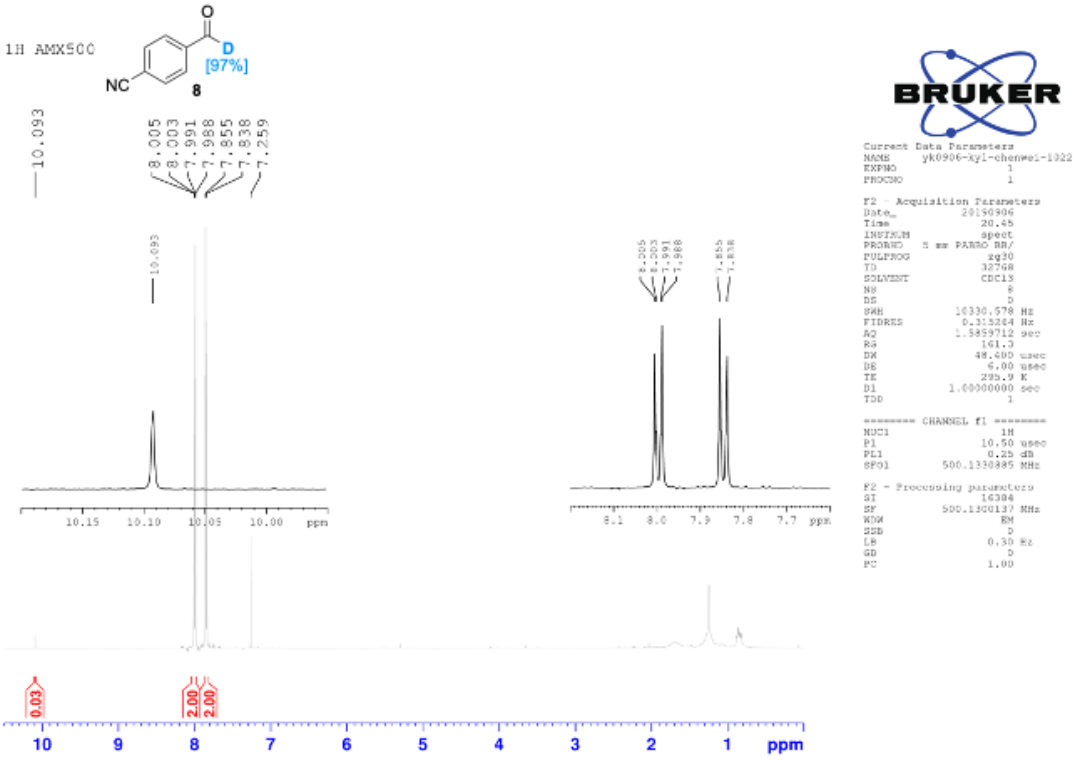
```
Current Data Parameters
NAME      yk0830-ky1-4022-3-1
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190830
Time                  19.10
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      274
DS                        0
SWH               30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0911744 sec
RG                    16384
DW                   16.650 usec
DE                    6.00 usec
TE                   296.8 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      20

======== CHANNEL f1 ========
NUC1                      13C
P1                     8.90 usec
PL1                       0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2                     0.25 dB
PL12                   17.89 dB
PL13                   15.82 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                    32768
SF                125.7577922 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```



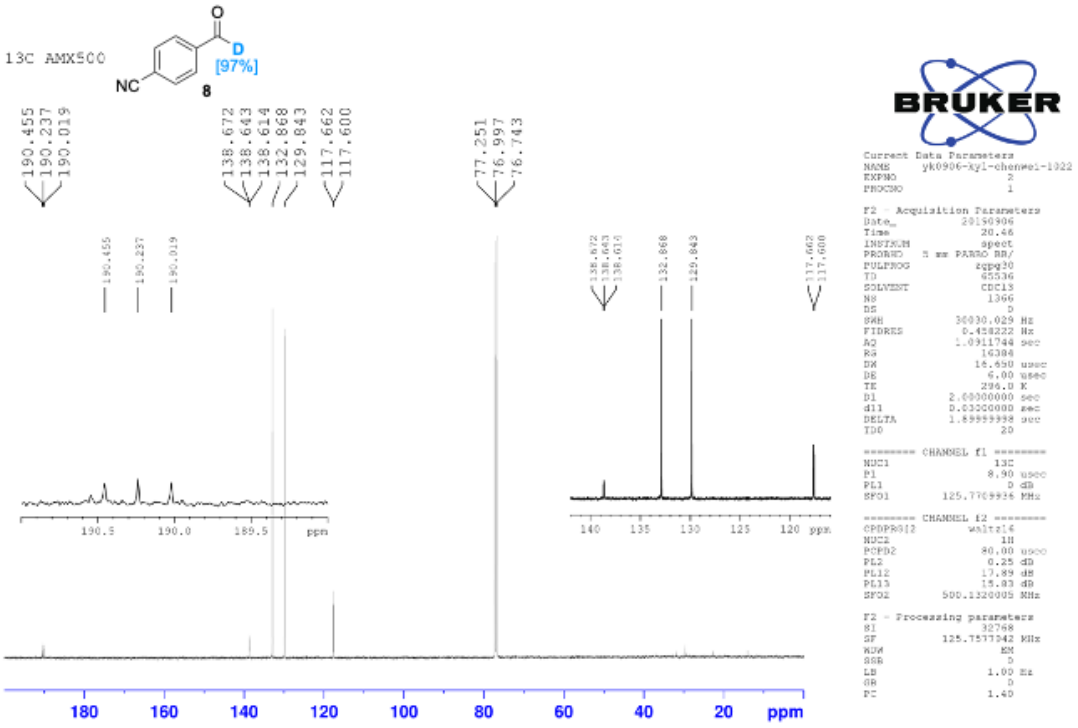
BRUKER

```
Current Data Parameters
NAME        yk0906-kyl-chenwei-1322
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20150906
Time              20.45
INSTRUM           spect
PROBHD  5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT           CDCl3
NS                   8
DS                   0
SWH          16330.578 Hz
FIDRES        0.315264 Hz
AQ            1.5859712 sec
RG                161.3
DW               48.400 usec
DE                6.00 usec
TE               295.9 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                10.50 usec
PL1               0.25 dB
SFO1        500.1330885 MHz

F2 - Processing parameters
SI                16384
SF          500.1300137 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



BRUKER

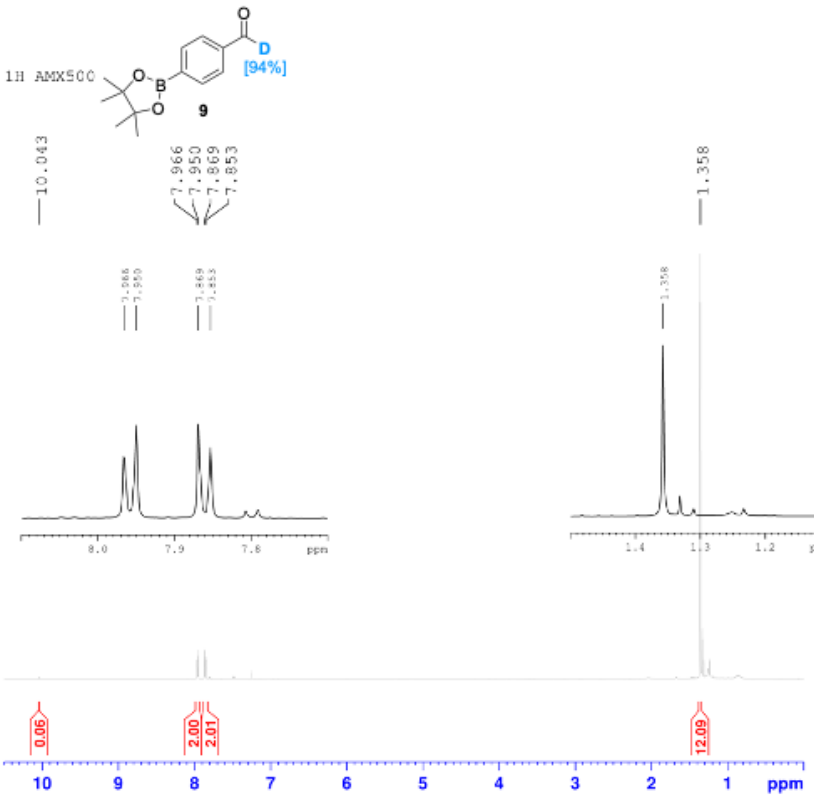
```
Current Data Parameters
NAME        yk0906-kyl-chenwei-1322
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_          20150906
Time              20.46
INSTRUM           spect
PROBHD  5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                1366
DS                   0
SWH          30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0911744 sec
RG                16384
DW               16.650 usec
DE                6.00 usec
TE               296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
DELTA         1.89999998 sec
TD0                 20

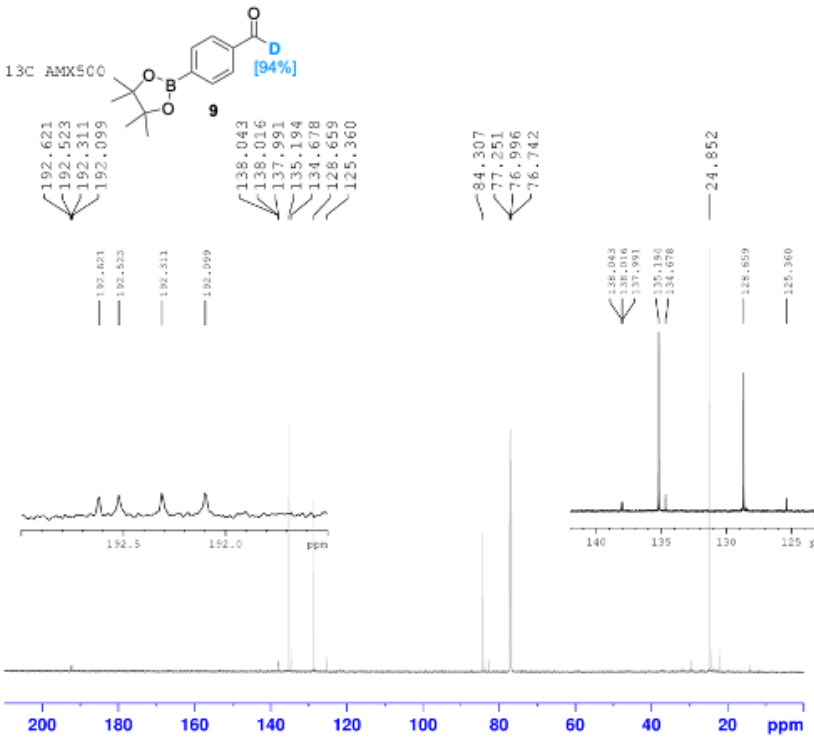
======== CHANNEL f1 ========
NUC1                 13C
P1                8.90 usec
PL1                  0 dB
SFO1        125.7769936 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               0.25 dB
PL12             17.89 dB
PL13             18.83 dB
SFO2        500.1320005 MHz

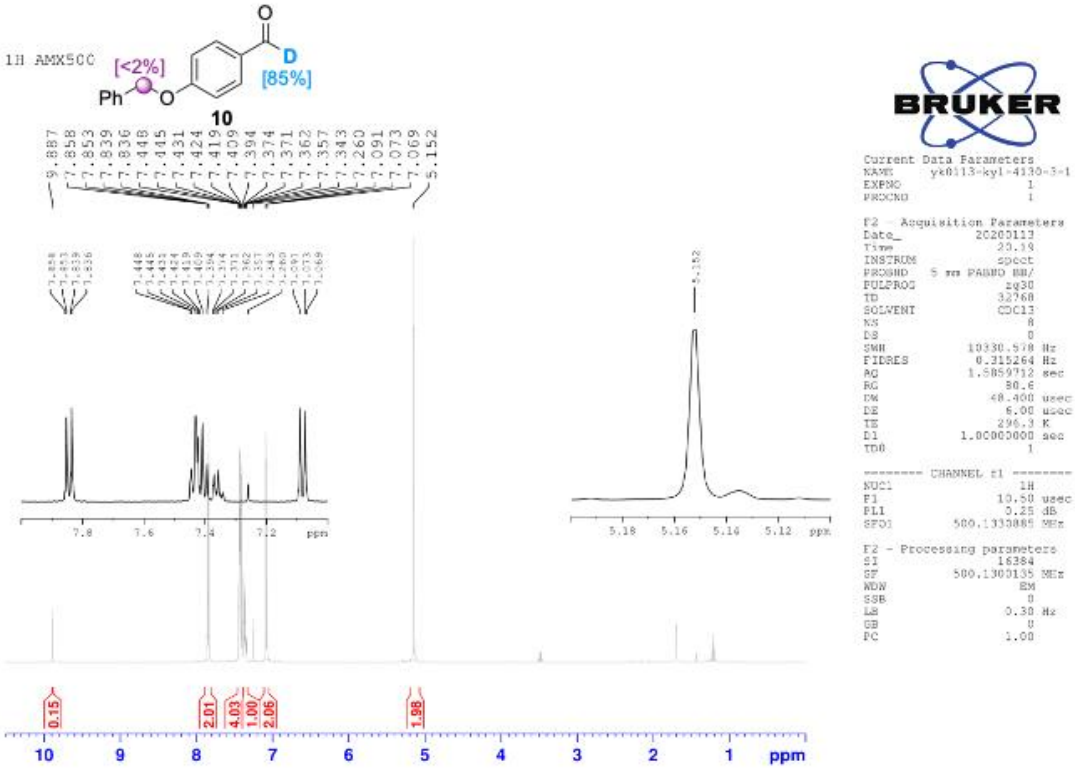
F2 - Processing parameters
SI                32768
SF          125.7577942 MHz
WDW                  EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```


1H AMX500
D
[94%]
9
10.043
7.966
7.950
7.869
7.853
1.358
8.0
7.9
7.8
ppm
1.4
1.3
1.2
ppm
0.06
2.00
2.01
12.09
10
9
8
7
6
5
4
3
2
1
ppm

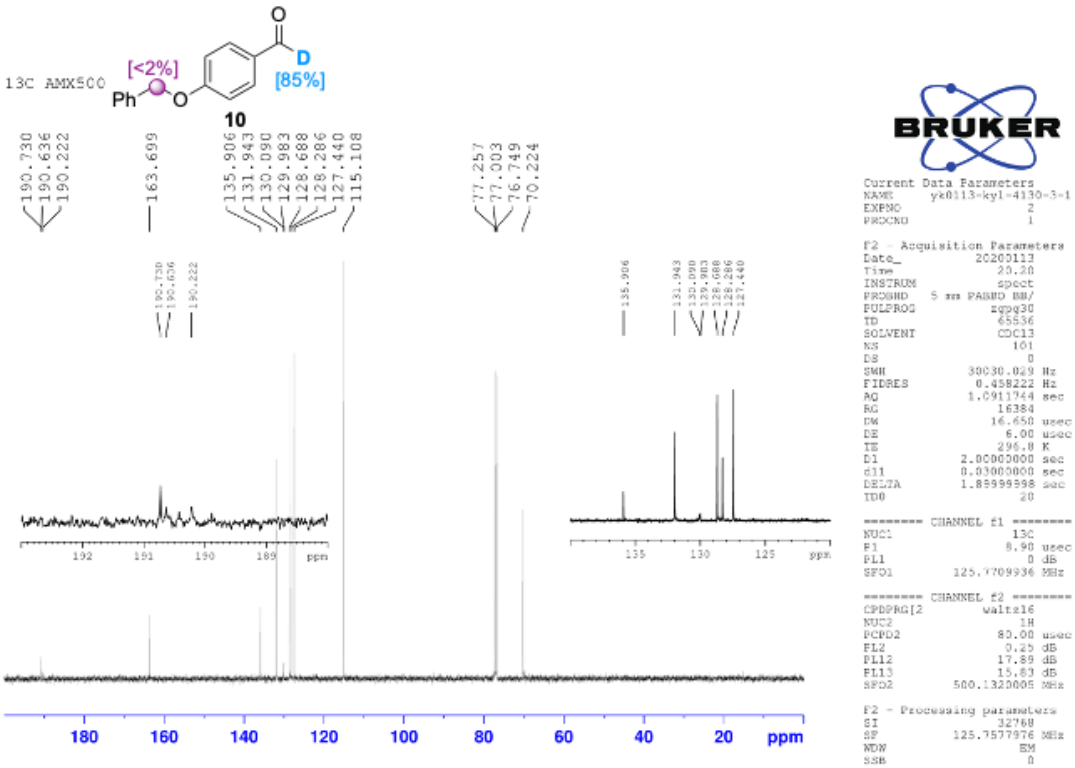

BRUKER
Current Data Parameters
NAME yk0907-chenwei-1021-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190908
Time 10.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 57
DW 48.400 usec
DE 6.00 usec
TE 297.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


13C AMX500
D
[94%]
9
192.621
192.523
192.311
192.099
138.043
138.016
137.991
135.194
134.678
128.659
125.360
84.307
77.251
76.996
76.742
24.852
192.5
192.0
ppm
140
135
130
125 ppm
200
180
160
140
120
100
80
60
40
20
ppm

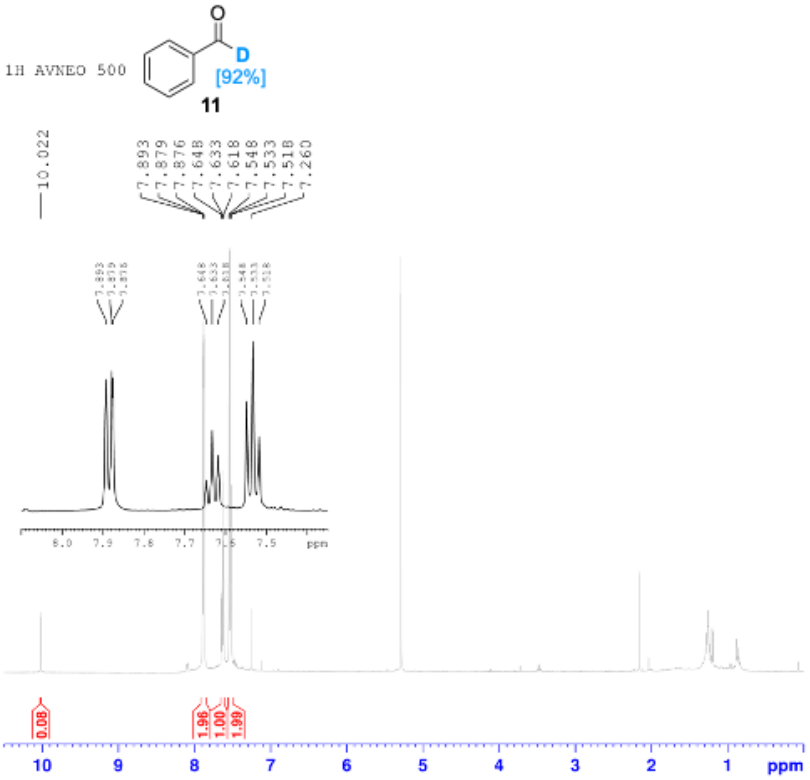

BRUKER
Current Data Parameters
NAME yk0907-chenwei-1021-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190908
Time 10.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1000
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 18.83 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577928 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


1H AMX500
[<2%]
[85%]
Ph
O
D
10
9.887
7.858
7.853
7.839
7.836
7.448
7.445
7.431
7.424
7.419
7.409
7.394
7.374
7.371
7.362
7.357
7.343
7.260
7.091
7.073
7.069
5.152
0.15
2.01
4.03
1.00
2.06
1.98
ppm

BRUKER
Current Data Parameters
NAME yk0113-kyl-4130-3-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200113
Time 20.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 80.6
DW 48.400 usec
DE 6.00 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 16384
SF 500.1300135 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


13C AMX500
[<2%]
[85%]
Ph
O
D
10
190.730
190.636
190.222
163.699
135.906
131.943
130.090
129.983
128.688
128.286
127.440
115.108
77.257
77.003
76.749
70.224
ppm

BRUKER
Current Data Parameters
NAME yk0113-kyl-4130-3-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200113
Time 20.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 101
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 296.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577976 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

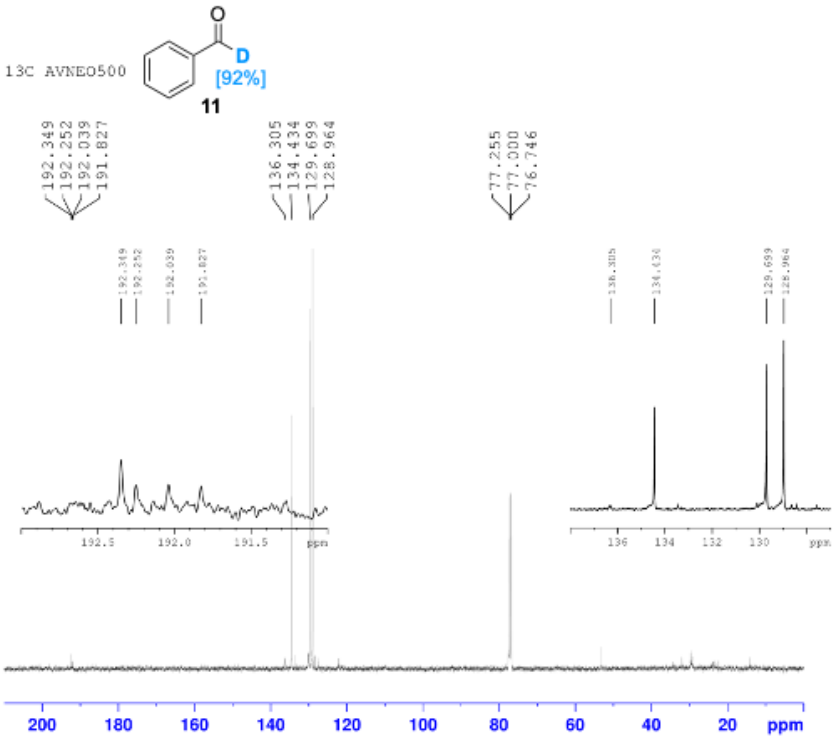


BRUKER

```
Current Data Parameters
NAME      yx0318-kyl-4159-2-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20200318
Time                  19.09 h
INSTRUM               Avance
PROBHD    2169738_0003 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        4
DS                        2
SWH               10000.000 Hz
FIDRES                0.305176 Hz
AQ                3.2767999 sec
RG                      101
DW                   50.000 usec
DE                   11.14 usec
TE                   299.2 K
D1                1.00000000 sec
TD0                       1
SFO1              500.1330883 MHz
NUC1                      1H
P0                    2.67 usec
P1                    8.00 usec
PLW1             24.45700073 W

F2 - Processing parameters
SI                    65536
SF              500.1300119 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



BRUKER

```
Current Data Parameters
NAME      yx0318-kyl-4159-2-1
EXPNO                       3
PROCNO                      1

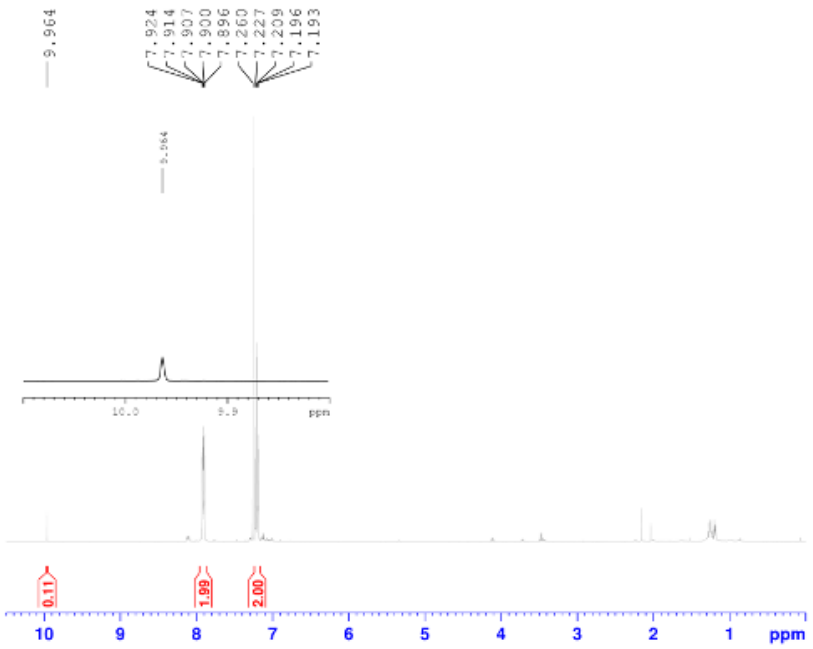
F2 - Acquisition Parameters
Date_              20200318
Time                  19.31 h
INSTRUM               Avance
PROBHD    2169738_0003 (
PULPROG               zgpg
TD                    65536
SOLVENT               CDCl3
NS                      377
DS                        2
SWH               30120.482 Hz
FIDRES                0.919204 Hz
AQ                1.0878977 sec
RG                      101
DW                   16.600 usec
DE                    6.72 usec
TE                   299.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1              125.7709931 MHz
NUC1                     13C
P1                    9.00 usec
PLW1             110.76999664 W
SFO2              500.1320005 MHz
NUC2                      1H
CPDPRG[2          waltz64
PCPD2                 80.00 usec
PLW2             24.45700073 W
PLW12             0.24457000 W
PLW13             0.12302000 W

F2 - Processing parameters
SI                    65536
SF              125.7577943 MHz
WDW                      EM
SSB                       0
LB                     2.00 Hz
GB                        0
PC                     1.40
```

1H AMX500

[89%]

12



BRUKER

```
Current Data Parameters
NAME      yk0108-ky1-4124-2-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_            20200108
Time                 20.31
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH              10330.578 Hz
FIDRES           0.315264 Hz
AQ               1.5859712 sec
RG                   101.6
DW                  48.400 usec
DE                   6.00 usec
TE                  296.6 K
D1               1.00000000 sec
TD0                      1

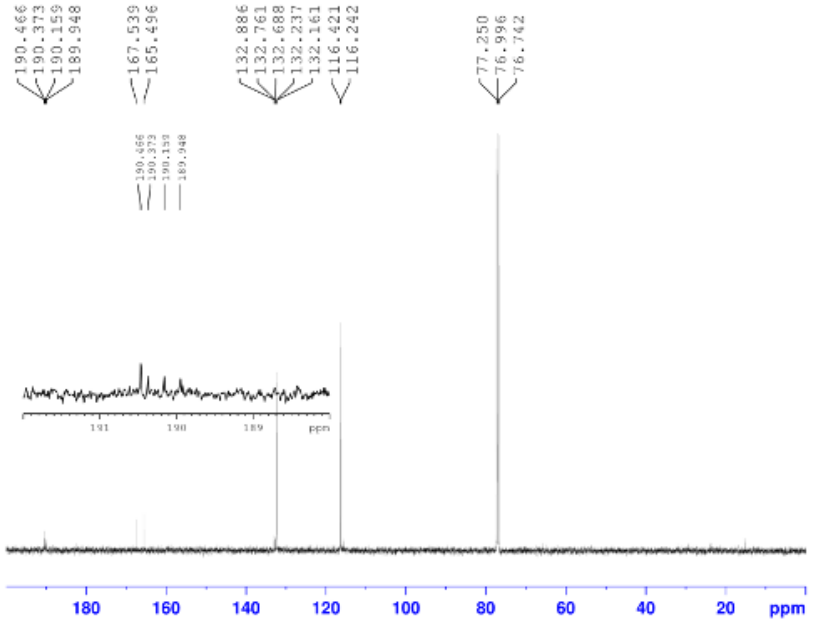
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.50 usec
PL1                   0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                   16384
SF            500.1300136 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

13C AMX500

[89%]

12



BRUKER

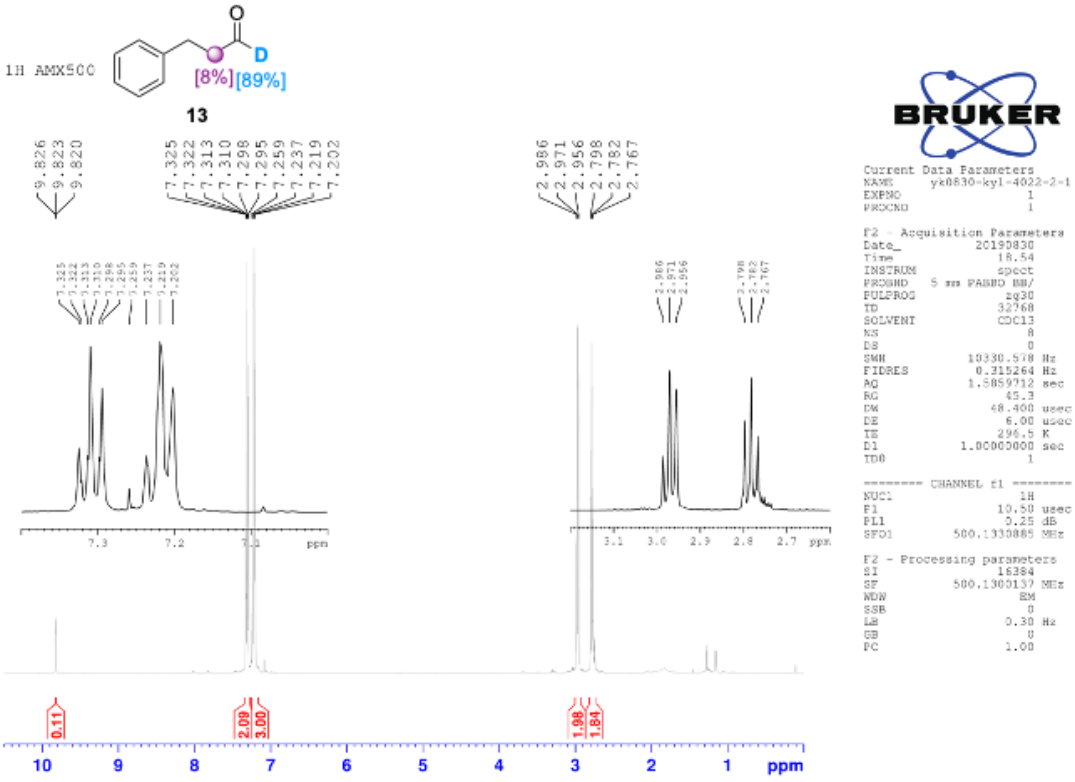
```
Current Data Parameters
NAME      yk0108-ky1-4124-2-1
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_            20200108
Time                 20.33
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT              CDCl3
NS                     179
DS                       0
SWH              30030.029 Hz
FIDRES           0.458222 Hz
AQ               1.0911744 sec
RG                   16384
DW                  16.650 usec
DE                   6.00 usec
TE                  296.9 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                     20

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.90 usec
PL1                      0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                    1H
PCPD2                85.00 usec
PL2                   0.25 dB
PL12                 17.89 dB
PL13                 15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                   32768
SF            125.7577937 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```



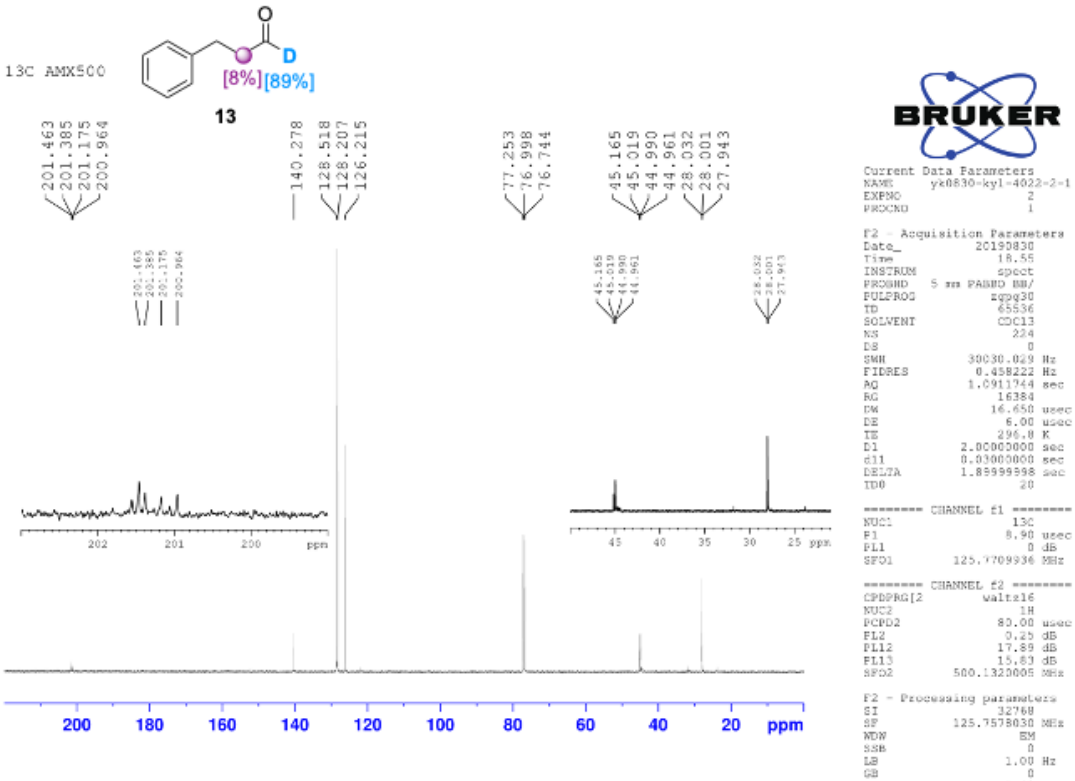
BRUKER

```
Current Data Parameters
NAME        ye0830-kyl-4022-2-1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20190830
Time                      18.54
INSTRUM                    spect
PROBHD     5 mm PABBO BB/
PULPROG                   zg30
TD                       32768
SOLVENT                  CDCl3
NS                           8
DS                           0
SWH                  10330.578 Hz
FIDRES                0.315264 Hz
AQ                    1.5859712 sec
RG                         45.3
DW                       48.400 usec
DE                        6.00 usec
TE                       296.5 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                         1H
P1                        10.50 usec
PL1                        0.25 dB
SFO1                500.1330885 MHz

F2 - Processing parameters
SI                       16384
SF                  500.1300137 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```



BRUKER

```
Current Data Parameters
NAME        ye0830-kyl-4022-2-1
EXPNO                         2
PROCNO                        1

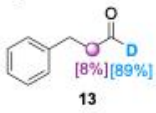
F2 - Acquisition Parameters
Date_                  20190830
Time                      18.55
INSTRUM                    spect
PROBHD     5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         224
DS                           0
SWH                  30030.029 Hz
FIDRES                0.458222 Hz
AQ                    1.0911744 sec
RG                       16384
DW                       16.650 usec
DE                        6.00 usec
TE                       296.0 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                          20

======== CHANNEL f1 ========
NUC1                         13C
P1                         8.90 usec
PL1                           0 dB
SFO1                125.7709936 MHz

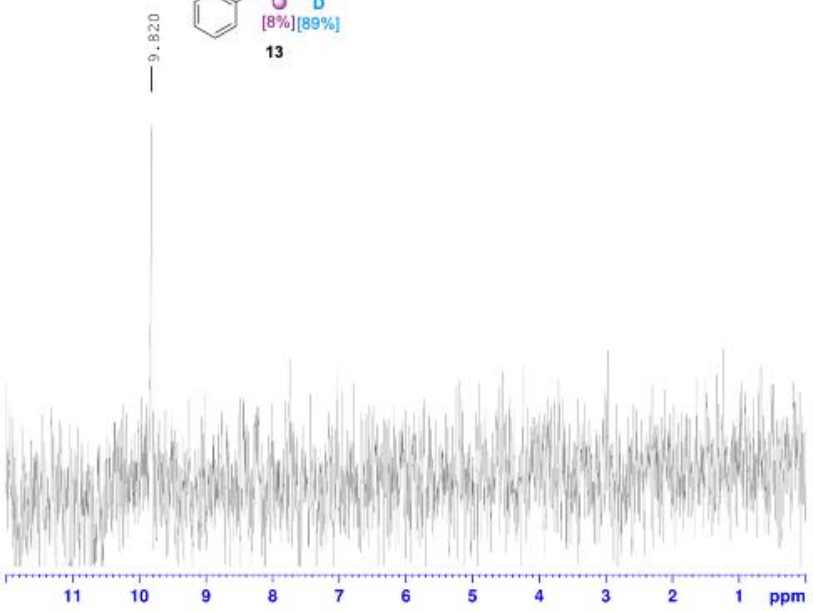
======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL2                        0.25 dB
PL12                      17.89 dB
PL13                      15.83 dB
SFO2                500.1320005 MHz

F2 - Processing parameters
SI                       32768
SF                  125.7578030 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

2H AV 500 NEO 23 May 2017
0.1 EB in CDCl3



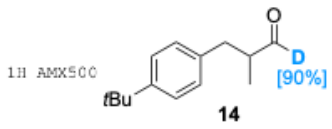
13



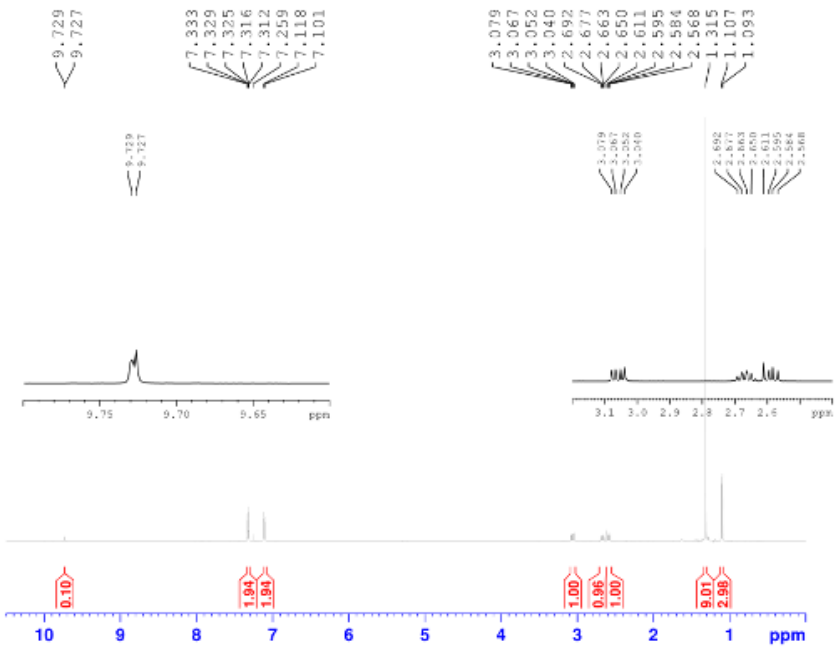

```
Current Data Parameters
NAME                  thd-25-3
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20200629
Time                  15.40 h
INSTRUM  CAB AV4 500 MHz BASIC
PROBHD   Z144569_0005 (
PULPROG                zg2h.2
TD                       8192
SOLVENT                 CDCl3
NS                         96
DS                          2
SWH                 1562.500 Hz
FIDRES              0.381470 Hz
AQ                  2.6214399 sec
RG                       12.5
DW                   320.000 usec
DE                      6.50 usec
TE                     298.0 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                         1
SFO1               76.7886582 MHz
NUC1                       2H
P1                     349.30 usec
PLW1               3.50000000 W

F2 - Processing parameters
SI                       65536
SF                 76.7881551 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```



14



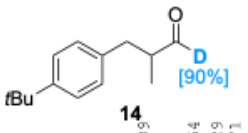

```
Current Data Parameters
NAME          yk0104-kyl-4122-2-1
EXPNO                           1
PROCNO                          1

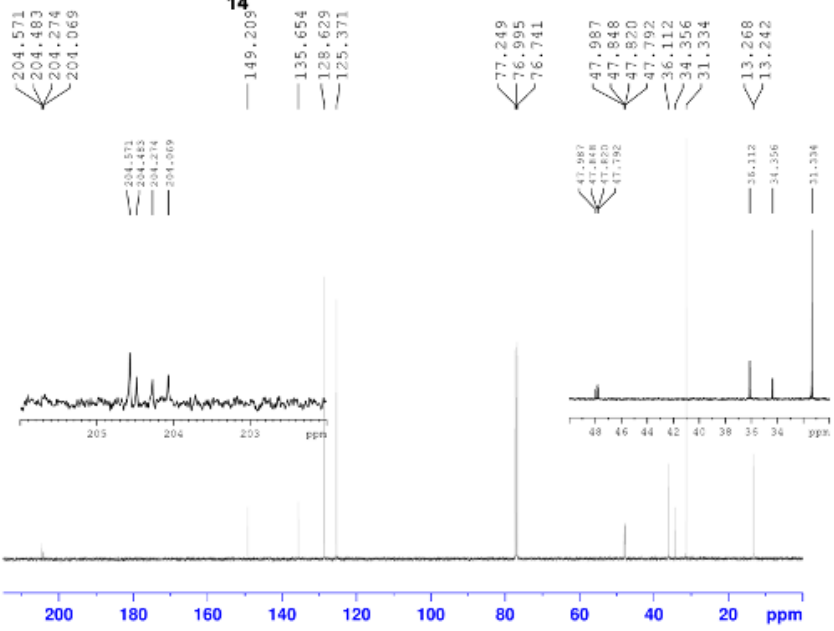
F2 - Acquisition Parameters
Date_              20200104
Time                  16.32
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT                 CDCl3
NS                          8
DS                          0
SWH                10330.578 Hz
FIDRES              0.315264 Hz
AQ                  1.5859712 sec
RG                         64
DW                     48.400 usec
DE                      6.00 usec
TE                     296.5 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      10.50 usec
PL1                      0.25 dB
SFO1              500.1330885 MHz

F2 - Processing parameters
SI                       16384
SF                500.1300130 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

13C AMX500





BRUKER

```
Current Data Parameters
NAME        yk0104-kyl-4122-2-1
EXPNO                         2
PROCNO                        1

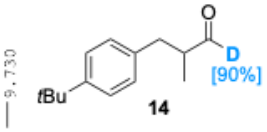
F2 - Acquisition Parameters
Date_              20200104
Time                   16.33
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     174
DS                       0
SWH              30030.029 Hz
FIDRES           0.458222 Hz
AQ               1.0911744 sec
RG                   16384
DW                16.650 usec
DE                 6.00 usec
TE                 296.9 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     20

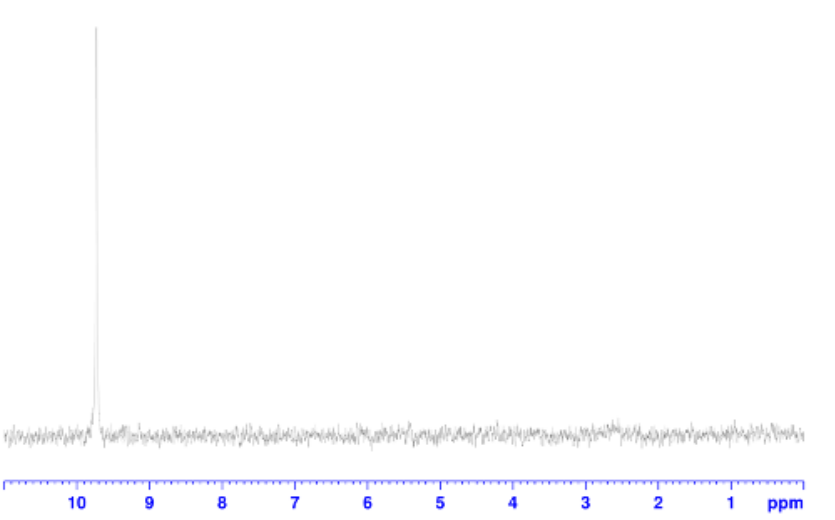
======== CHANNEL f1 ========
NUC1                   13C
P1                    8.90 usec
PL1                      0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.25 dB
PL12                 17.89 dB
PL13                 15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                    32768
SF          125.7577955 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

2H AV 500 NEO 23 May 2017 D NMR in CHCl3



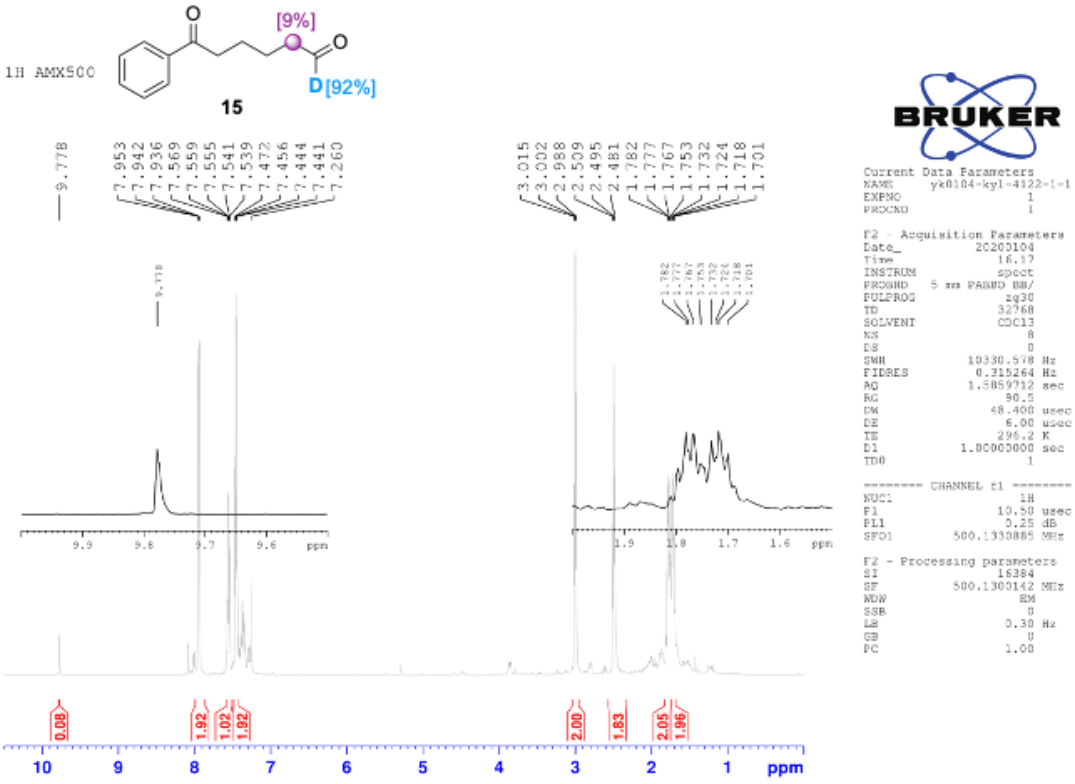


BRUKER

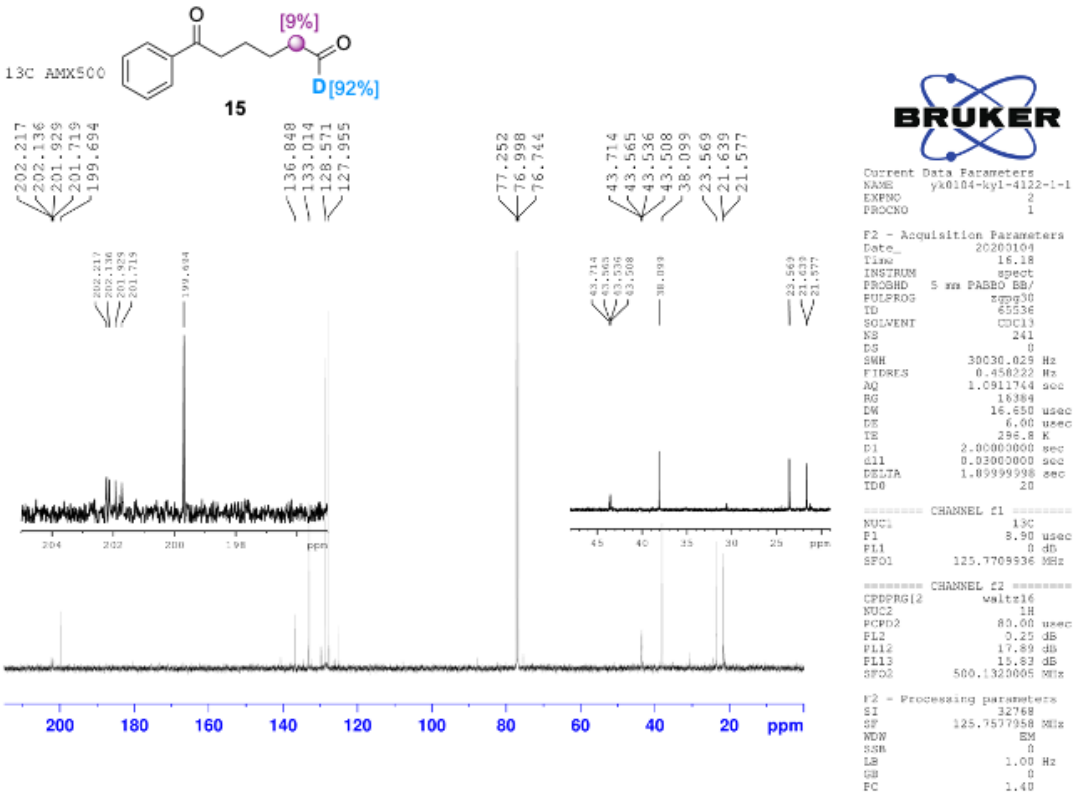
```
Current Data Parameters
NAME                  thd-2
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200624
Time                  15.12 h
INSTRUM  CAB AV4 500 MHz BASIC
PROBHD   Z144569_0005 (
PULPROG             zg2h.2
TD                    8192
SOLVENT              CDCl3
NS                       8
DS                       2
SWH              1562.500 Hz
FIDRES           0.381470 Hz
AQ               2.6214399 sec
RG                    12.5
DW                320.000 usec
DE                  6.50 usec
TE                  298.0 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                      1
SFO1          76.7885582 MHz
NUC1                    2H
P1                  349.30 usec
PLW1            3.50000000 W

F2 - Processing parameters
SI                    65536
SF          76.7883516 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

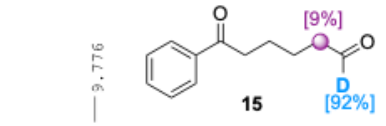

1H AMX500
[9%]
D[92%]
15
9.778
7.953
7.942
7.936
7.569
7.559
7.555
7.541
7.539
7.472
7.456
7.444
7.441
7.260
3.015
3.002
2.988
2.509
2.495
2.481
1.782
1.777
1.767
1.753
1.732
1.724
1.718
1.701
0.08
1.92
1.02
1.92
2.00
1.83
2.05
1.96
10
9
8
7
6
5
4
3
2
1
ppm

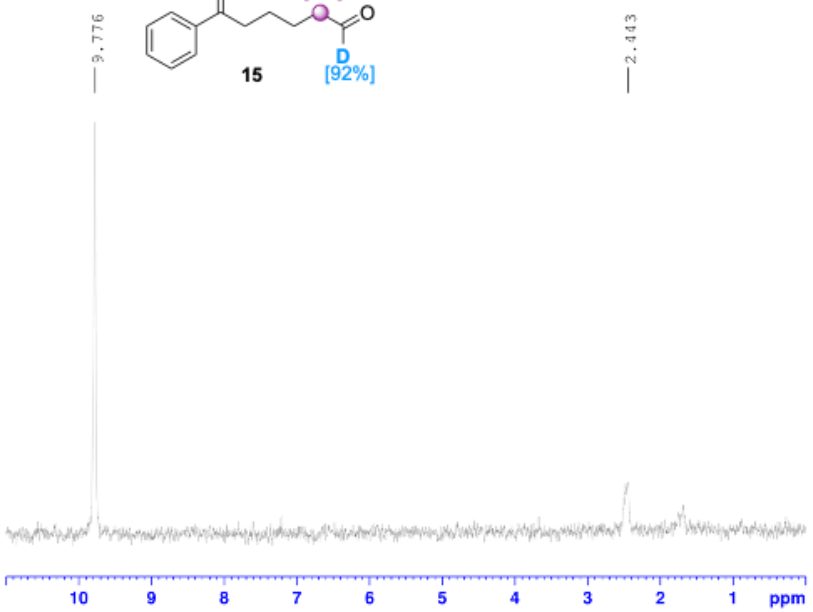
BRUKER
Current Data Parameters
NAME yk0104-kyl-4122-1-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200104
Time 16.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 90.5
DW 48.400 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 16384
SF 500.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


13C AMX500
[9%]
D[92%]
15
202.217
202.136
201.929
201.719
199.694
136.848
133.014
128.571
127.955
77.252
76.998
76.744
43.714
43.565
43.536
43.508
38.099
23.569
21.639
21.577
200
180
160
140
120
100
80
60
40
20
ppm

BRUKER
Current Data Parameters
NAME yk0104-kyl-4122-1-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200104
Time 16.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 241
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 18384
DW 16.650 usec
DE 6.00 usec
TE 296.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709836 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 19.82 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577958 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2H AV 500 NEO 23 May 2017 D NMR in CHCl3



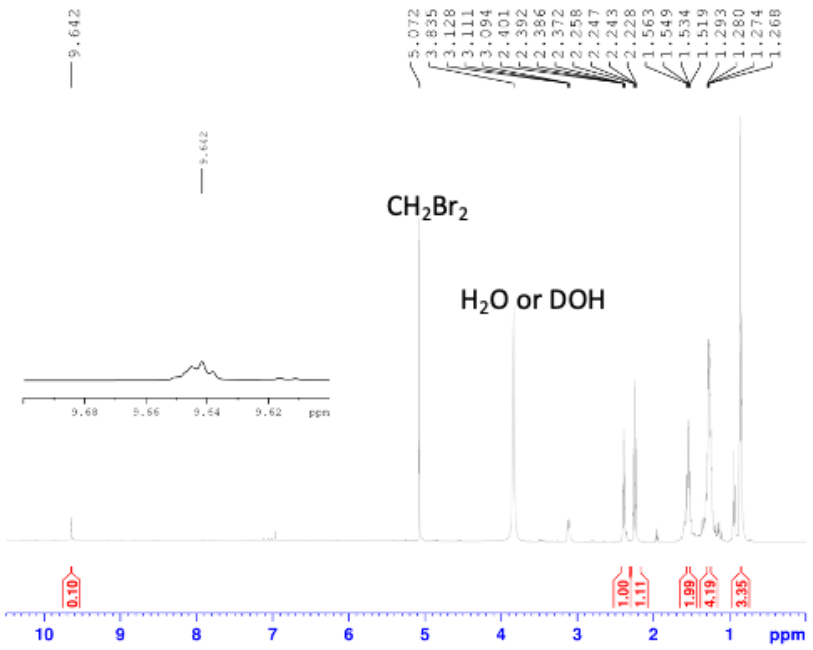


```
Current Data Parameters
NAME                  thd-3
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200624
Time                 16.15 h
INSTRUM   CAB AV4 500 MHz BASIC
PROBHD    2144569_0005 (
PULPROG              zg2h.2
TD                     8192
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                1562.500 Hz
FIDRES             0.381470 Hz
AQ                 2.6214399 sec
RG                      12.5
DW                   320.000 usec
DE                     6.50 usec
TE                   298.0 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                       1
SFO1              76.7886582 MHz
NUC1                     2H
P1                   349.30 usec
PLW1               3.50000000 W

F2 - Processing parameters
SI                    65536
SF                76.7883526 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

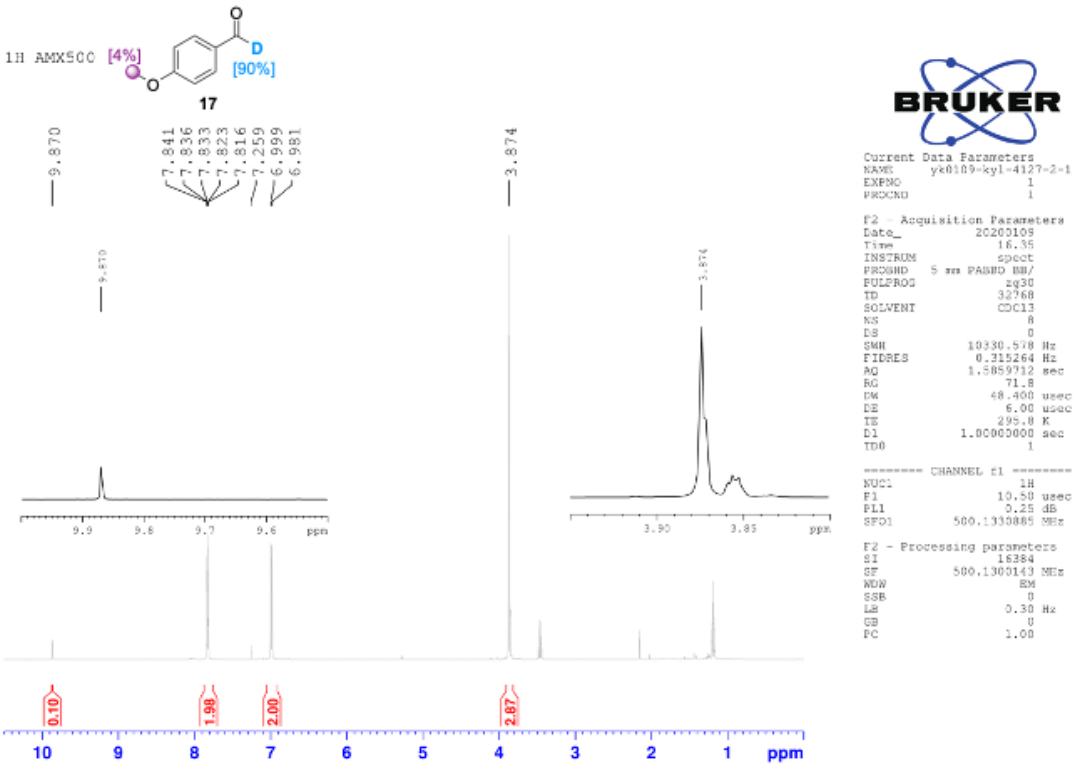
1H AVNEO 500



```
Current Data Parameters
NAME          yk0229-kyl-4138-2
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200229
Time                 10.45 h
INSTRUM              Avance
PROBHD    2169738_0003 (
PULPROG                zg30
TD                    65536
SOLVENT               CD3CN
NS                        8
DS                        2
SWH                10000.000 Hz
FIDRES             0.305176 Hz
AQ                 3.2767999 sec
RG                      101
DW                    50.000 usec
DE                    11.14 usec
TE                   298.0 K
D1                 1.00000000 sec
TD0                       1
SFO1              500.1330883 MHz
NUC1                     1H
PO                    2.67 usec
P1                    8.00 usec
PLW1              24.45700073 W

F2 - Processing parameters
SI                    65536
SF                500.1300098 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

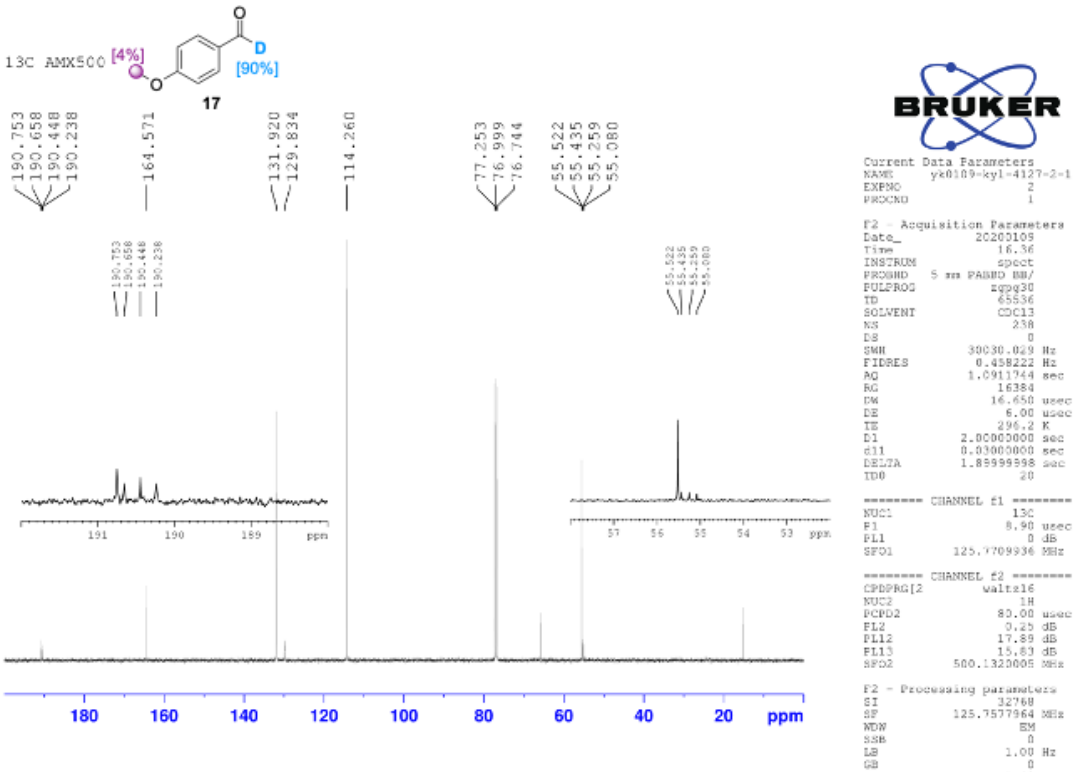


Current Data Parameters
NAME yx0109-kyl-4127-2-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200109
Time 16.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 71.8
DW 48.400 usec
DE 6.00 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300143 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



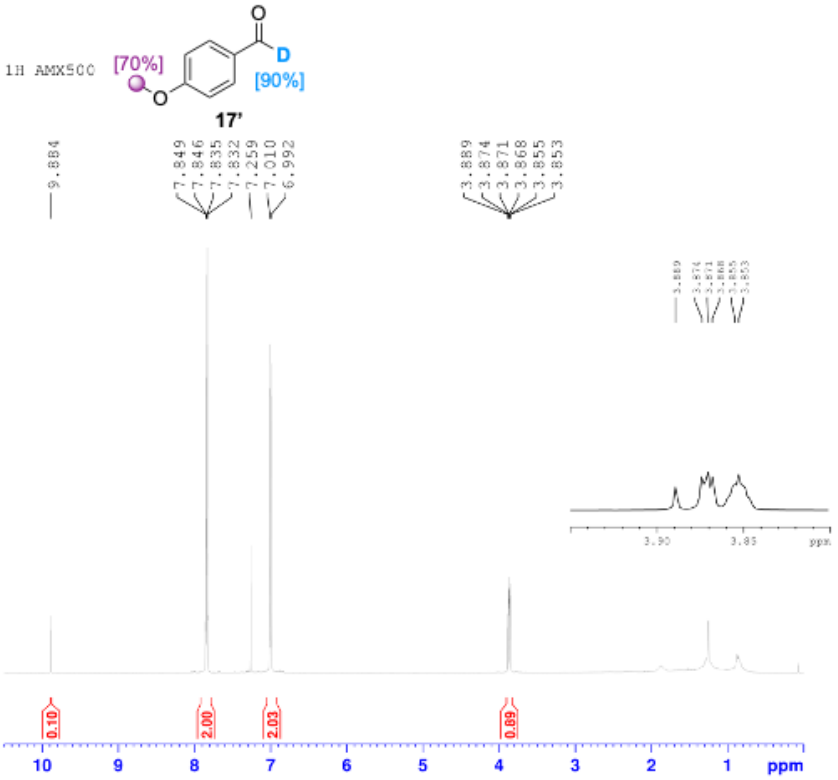
Current Data Parameters
NAME yx0109-kyl-4127-2-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200109
Time 16.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 238
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20

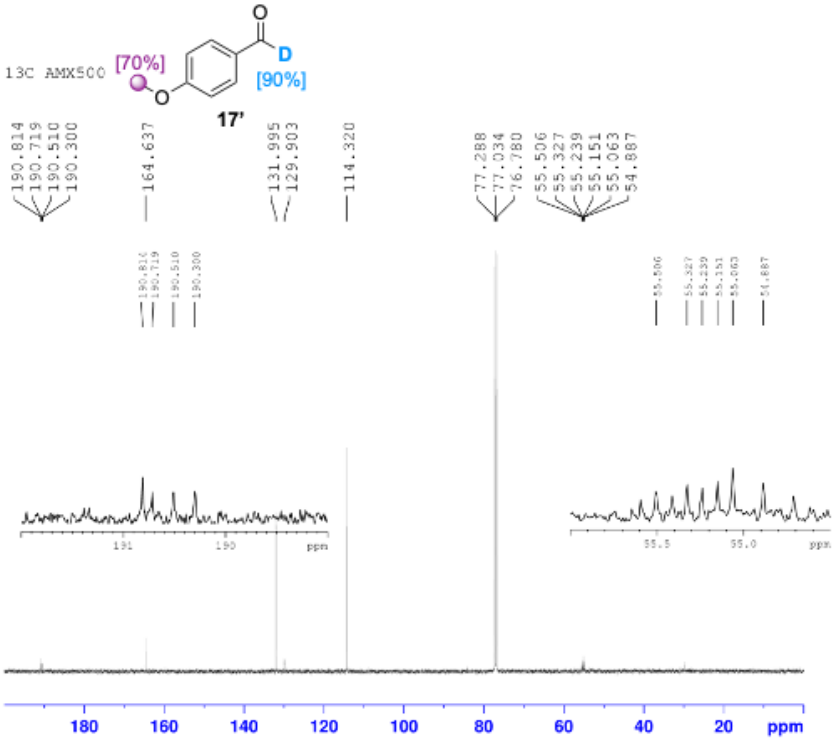
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

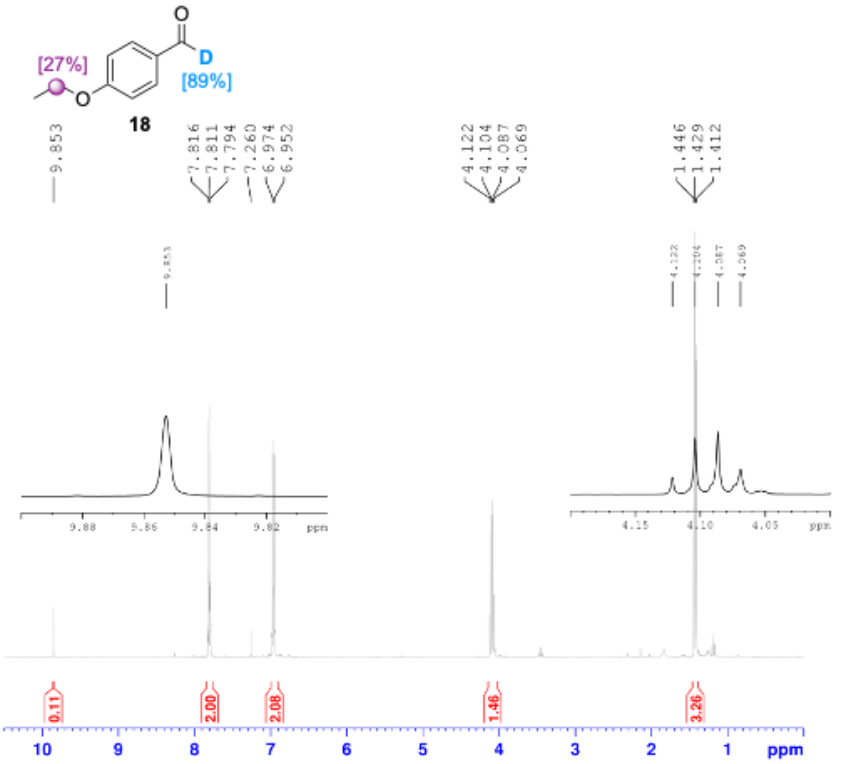
F2 - Processing parameters
SI 32768
SF 125.7577964 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


1H AMX500
[70%]
[90%]
D
17'
9.884
7.849
7.846
7.835
7.832
7.259
7.010
6.992
3.889
3.874
3.871
3.868
3.855
3.853
0.10
2.00
2.03
0.89
10
9
8
7
6
5
4
3
2
1
ppm


BRUKER
Current Data Parameters
NAME yk1011-kyl-4027-6-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191008
Time 20.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 114
DW 48.400 usec
DE 6.00 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


13C AMX500
[70%]
[90%]
D
17'
190.814
190.719
190.510
190.300
164.637
131.995
129.903
114.320
77.288
77.034
76.780
55.506
55.327
55.239
55.151
55.063
54.887
191
190
ppm
55.5
55.0
ppm
180
160
140
120
100
80
60
40
20
ppm

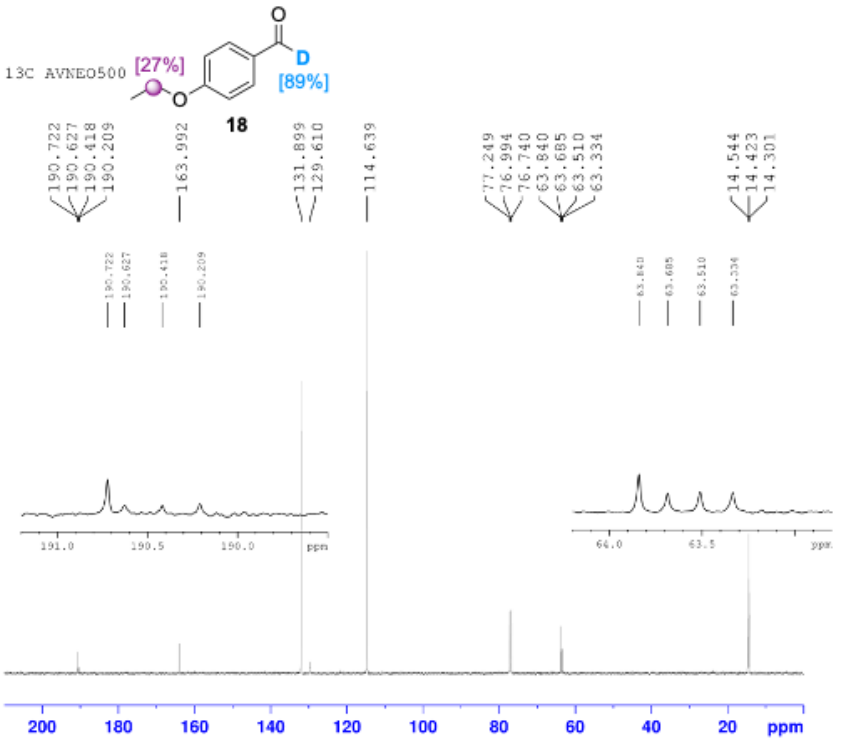

BRUKER
Current Data Parameters
NAME yk1011-kyl-4027-6-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191008
Time 23.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 352
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40




```
Current Data Parameters
NAME      De025-2019-KZL-6114-2-1
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20151225
Time              11.15 h
INSTRUM             spect
PROBHD   5108618_2020 (
PULPROG             zg30
TD                 32768
SOLVENT             CDCl3
NS                     8
DS                     2
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ             2.0447233 sec
RG                  80.4
DW                62.400 usec
DE                 6.50 usec
TE                298.7 K
D1             1.00000000 sec
TD0                    1
SFO1          400.2324714 MHz
NUC1                  1H
PU                 4.57 usec
P1                13.70 usec
PLW1          14.39999962 W

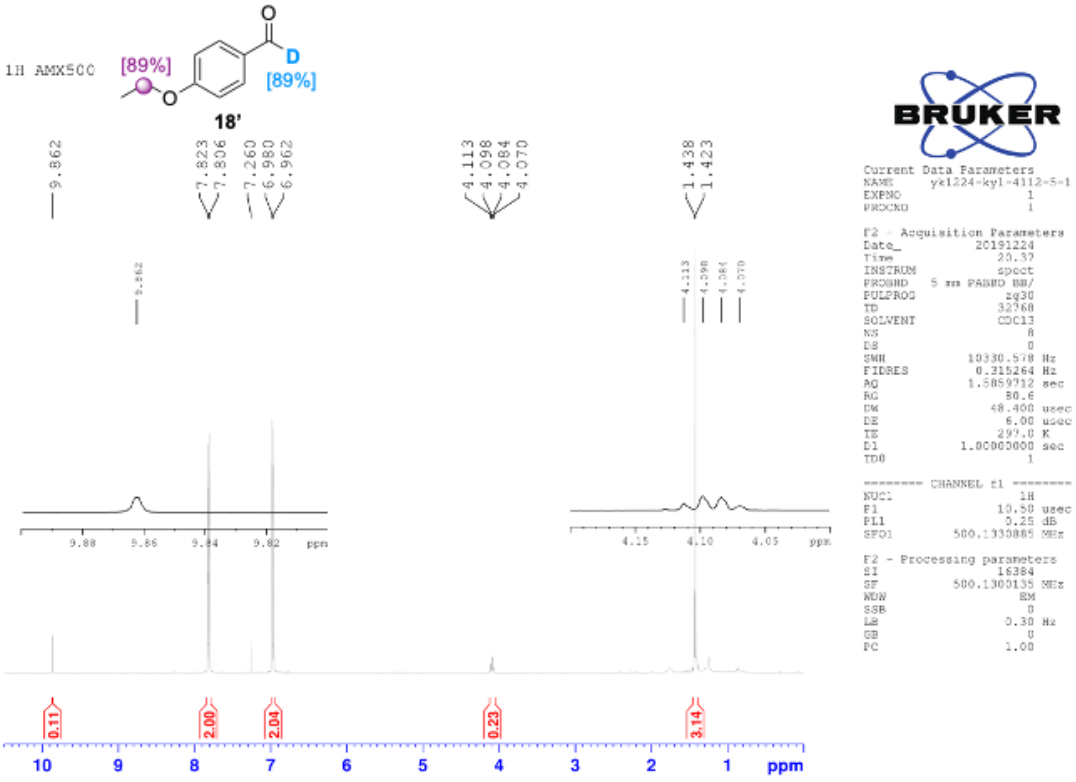
F2 - Processing parameters
SI                 65536
SF            400.2300100 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME      ye0518-kyl-4159-1-1
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20200318
Time              19.40 h
INSTRUM             Avance
PROBHD   2169738_0003 (
PULPROG             zgpg
TD                 65536
SOLVENT             CDCl3
NS                    84
DS                     2
SWH           30120.482 Hz
FIDRES         0.919204 Hz
AQ             1.0878977 sec
RG                   101
DW                16.600 usec
DE                 6.72 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          125.7709931 MHz
NUC1                  13C
P1                 9.00 usec
PLW1          110.76999664 W
SFO2          500.1320005 MHz
NUC2                  1H
CPDPRG[2          waltz64
PCPD2             80.00 usec
PLW2          24.65700073 W
PLW12          0.24457000 W
PLW13          0.12302000 W

F2 - Processing parameters
SI                 65536
SF            125.7577992 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.40
```



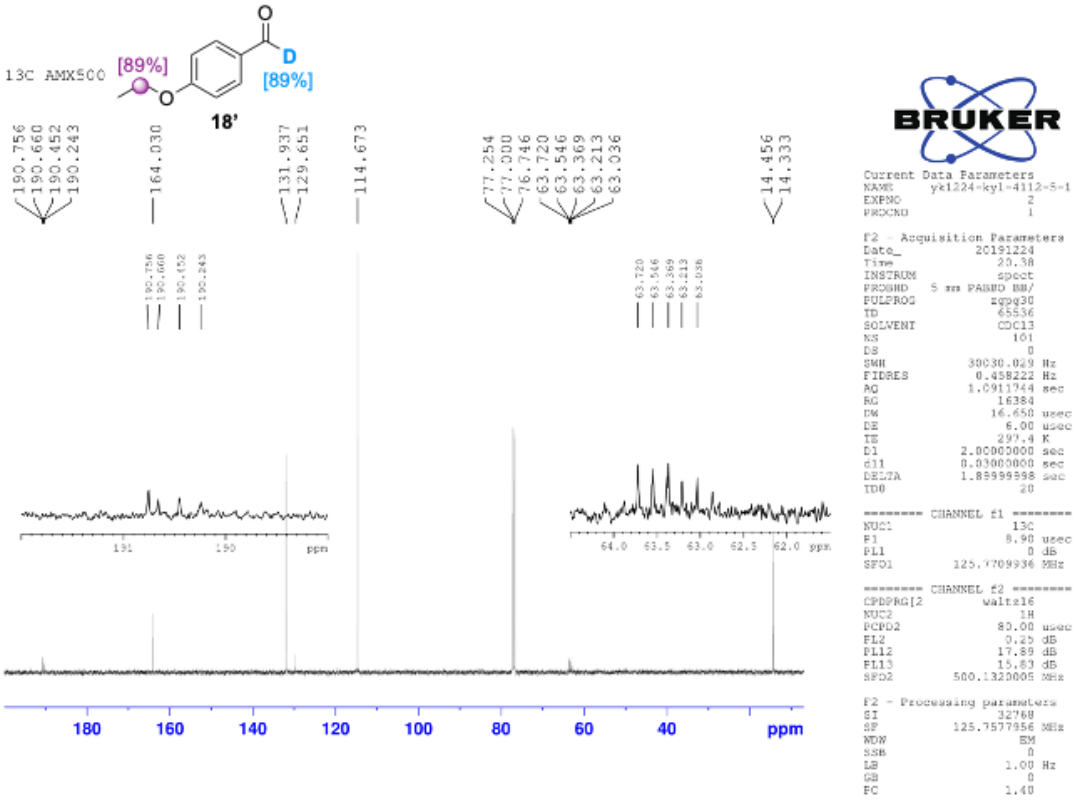
BRUKER

```
Current Data Parameters
NAME      yx1224-kyl-4112-5-1
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20191224
Time              20.57
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT           CDCl3
NS                   8
DS                   0
SWH          10330.578 Hz
FIDRES        0.315264 Hz
AQ            1.5859712 sec
RG                80.6
DW               48.400 usec
DE                6.00 usec
TE              297.0 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                10.50 usec
PL1                0.25 dB
SFO1         500.1330885 MHz

F2 - Processing parameters
SI               16384
SF          500.1300135 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



BRUKER

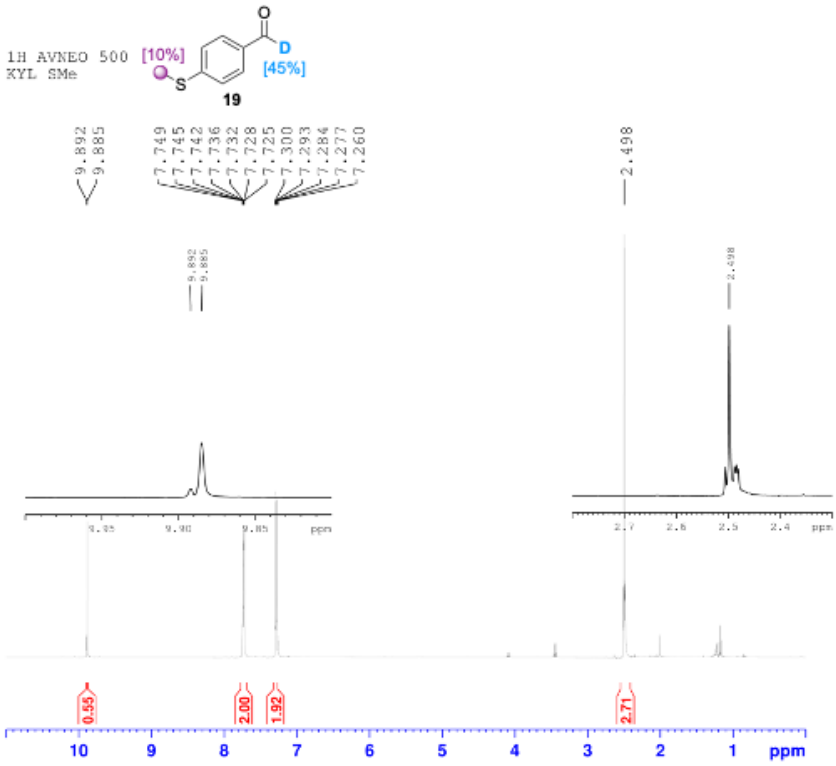
```
Current Data Parameters
NAME      yx1224-kyl-4112-5-1
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_          20191224
Time              20.58
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                 101
DS                   0
SWH          30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0911744 sec
RG               16384
DW               16.650 usec
DE                6.00 usec
TE              297.4 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                 20

======== CHANNEL f1 ========
NUC1                13C
P1                8.90 usec
PL1                  0 dB
SFO1         125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                0.25 dB
PL12              17.89 dB
PL13              15.83 dB
SFO2         500.1320005 MHz

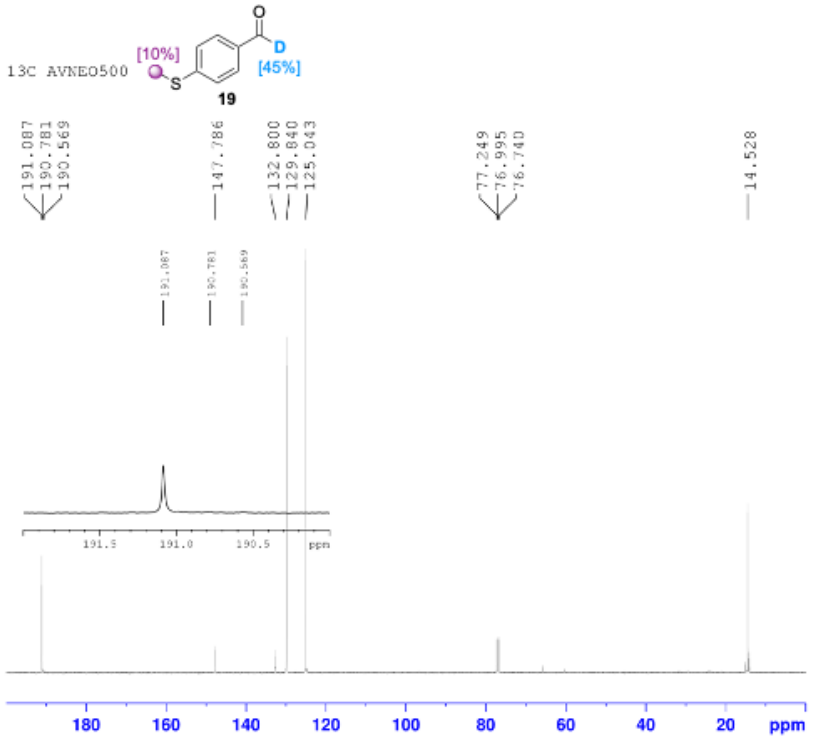
F2 - Processing parameters
SI               32768
SF          125.7577956 MHz
WDW                  EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```




```
Current Data Parameters
NAME      yk0229-kyl-4138-34
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20200229
Time                 10.18 h
INSTRUM              Avance
PROBHD   2169738_0003 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        2
SWH              10000.000 Hz
FIDRES               0.305176 Hz
AQ                3.2767995 sec
RG                      101
DW                   50.000 usec
DE                   11.14 usec
TE                  298.0 K
D1                1.00000000 sec
TD0                       1
SFO1           500.1330883 MHz
NUC1                     1H
P0                    2.67 usec
P1                    8.00 usec
PLW1           24.45700073 W

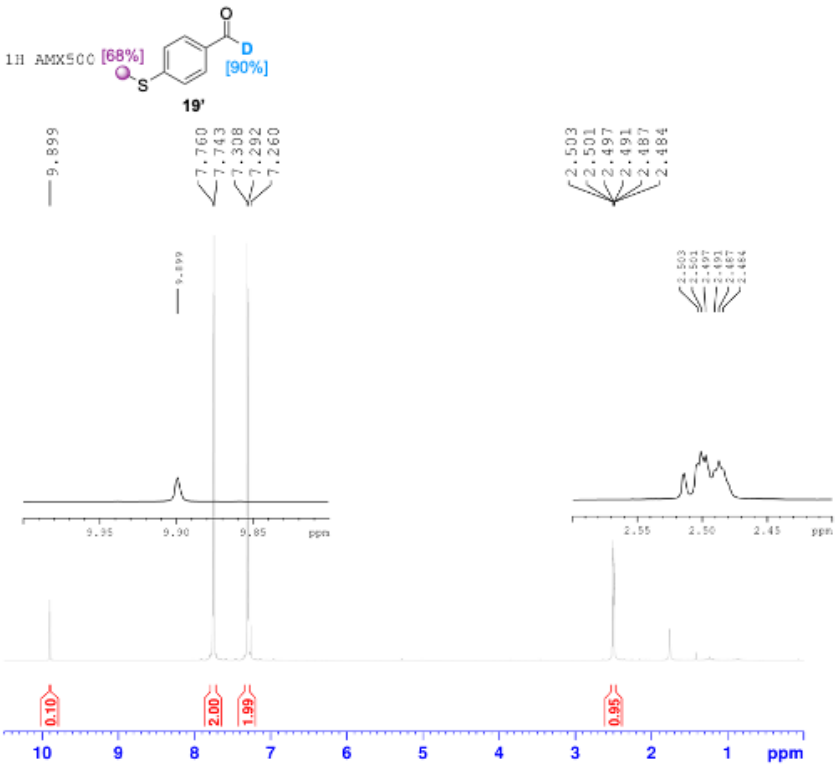
F2 - Processing parameters
SI                    65536
SF           500.1300138 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



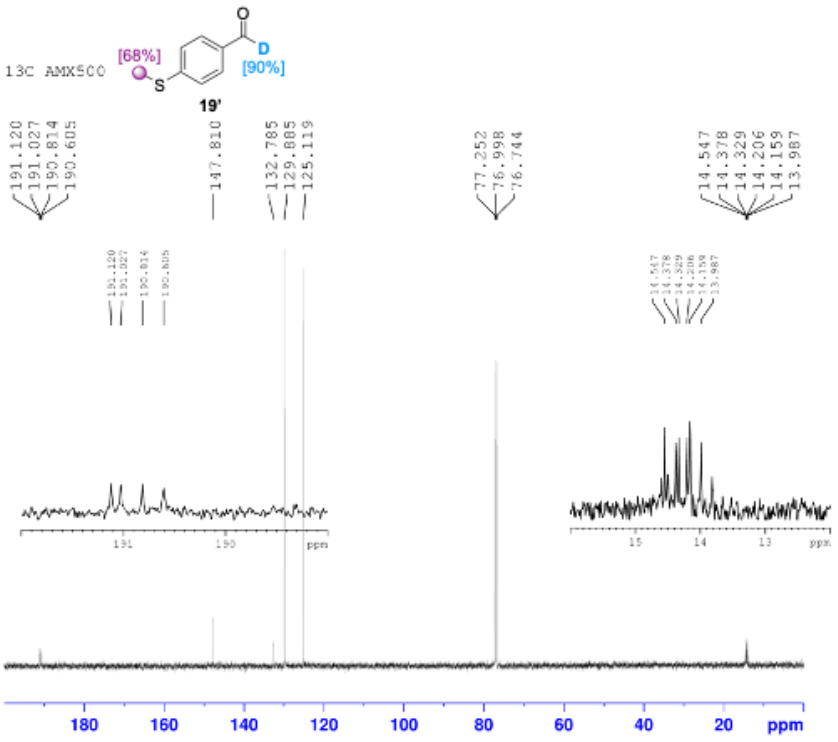

```
Current Data Parameters
NAME      yk0229-kyl-4138-34
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20200229
Time                 10.28 h
INSTRUM              Avance
PROBHD   2169738_0003 (
PULPROG              zgpg
TD                    65536
SOLVENT               CDCl3
NS                      153
DS                        2
SWH              30120.482 Hz
FIDRES               0.919204 Hz
AQ                1.0878977 sec
RG                      101
DW                   16.600 usec
DE                    6.72 usec
TE                  298.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1           125.7709931 MHz
NUC1                     13C
P1                    9.00 usec
PLW1          110.76999664 W
SFO2           500.1320005 MHz
NUC2                     1H
CPDPRG[2          waltz64
PCPD2                80.00 usec
PLW2           24.45700073 W
PLW12           0.24457000 W
PLW13           0.12302000 W

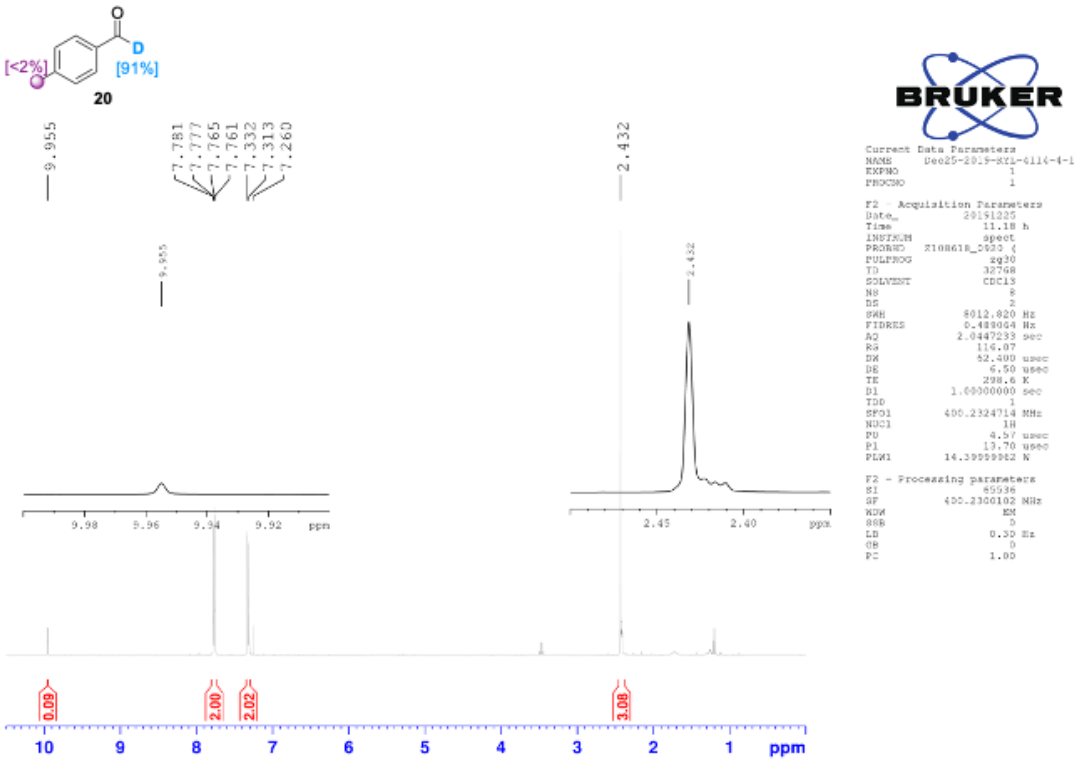
F2 - Processing parameters
SI                    65536
SF           125.7578060 MHz
WDW                     EM
SSB                      0
LB                    2.00 Hz
GB                       0
PC                    1.40
```


1H AMX500
[68%]
[90%]
19'
9.899
7.760
7.743
7.308
7.292
7.260
2.503
2.501
2.497
2.491
2.487
2.484
0.10
2.00
1.99
0.95
10
9
8
7
6
5
4
3
2
1
ppm


BRUKER
Current Data Parameters
NAME yk1224-kyl-4112-6-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191224
Time 20.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 90.5
DW 48.400 usec
DE 6.00 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 16384
SF 500.1300130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


13C AMX500
[68%]
[90%]
19'
191.120
191.027
190.814
190.605
147.810
132.785
129.885
125.119
77.252
76.998
76.744
14.547
14.378
14.329
14.206
14.159
13.987
180
160
140
120
100
80
60
40
20
ppm

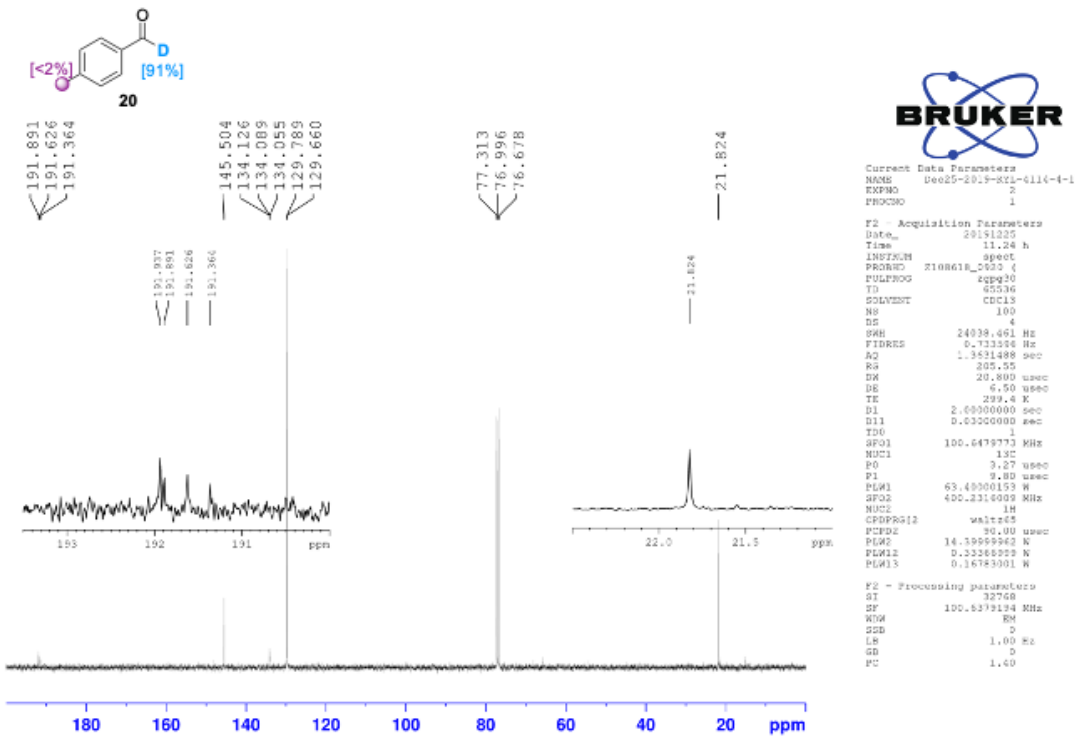

BRUKER
Current Data Parameters
NAME yk1224-kyl-4112-6-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191224
Time 20.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 75
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 297.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7578007 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME Dec25-2019-XZL-6114-4-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151225
Time 11.18 h
INSTRUM spect
PROBHD Z108618_2633 (
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 2.0447233 sec
RG 116.07
DW 62.400 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P0 4.57 usec
P1 13.70 usec
PLW1 14.39999962 W

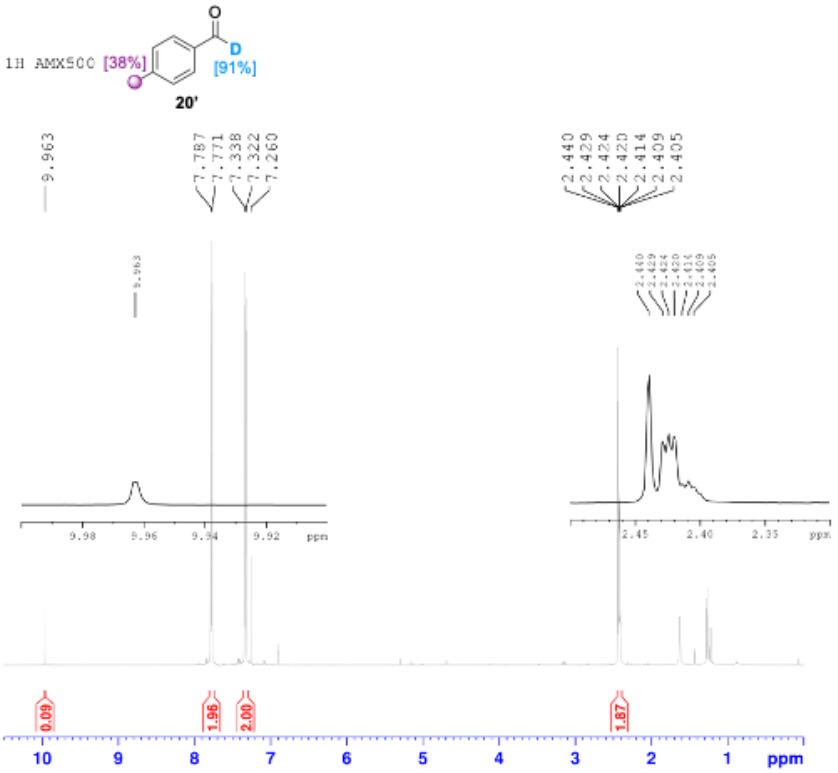
F2 - Processing parameters
SI 65536
SF 400.2300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME Dec25-2019-XZL-6114-4-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151225
Time 11.24 h
INSTRUM spect
PROBHD Z108618_2633 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 205.55
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6479773 MHz
NUC1 13C
P0 9.27 usec
P1 9.80 usec
PLW1 63.40000153 W
SFO2 400.2316009 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 14.39999962 W
PLW12 0.33365899 W
PLW13 0.16783001 W

F2 - Processing parameters
SI 32768
SF 100.6378194 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

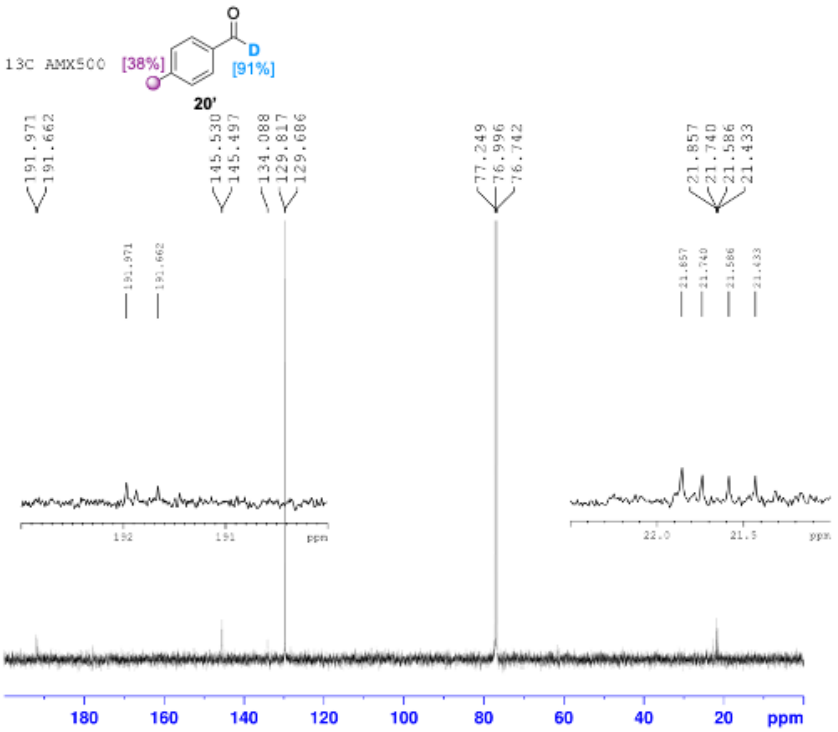


```
Current Data Parameters
NAME      yx0103-kyl-4119-7-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_            20200103
Time                16.56
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH             10330.578 Hz
FIDRES          0.315264 Hz
AQ              1.5859712 sec
RG                   228.1
DW                  48.400 usec
DE                   6.00 usec
TE                  296.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.50 usec
PL1                   0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                   16384
SF            500.1300130 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



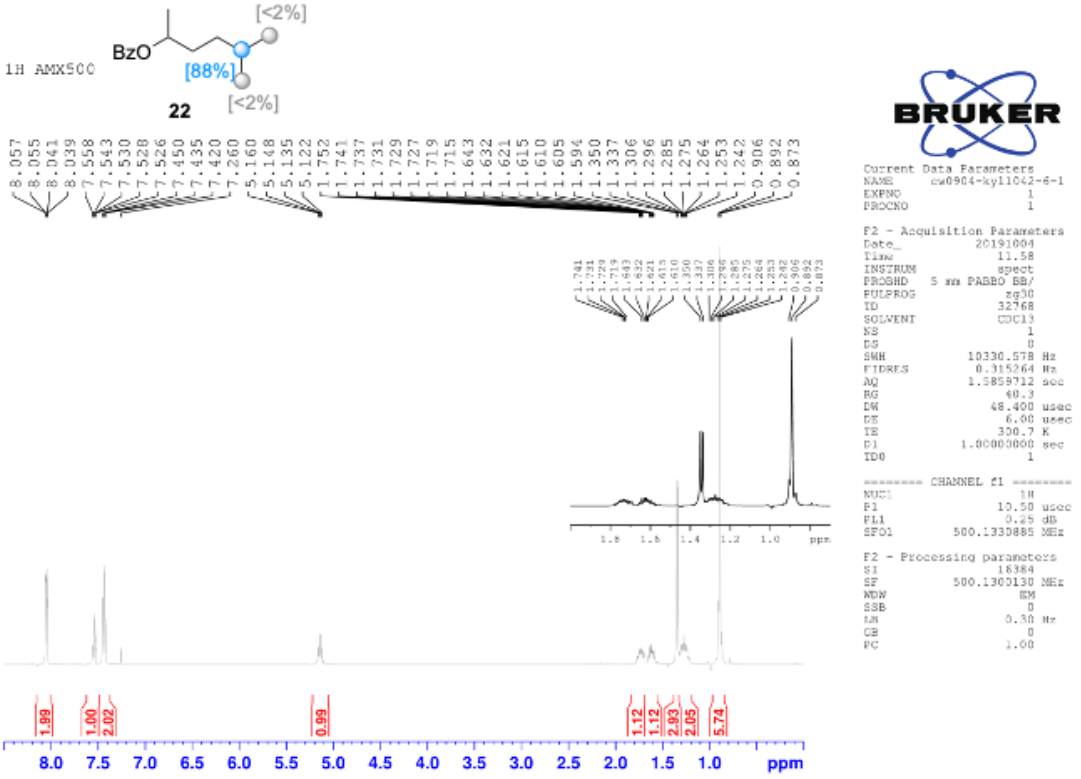
```
Current Data Parameters
NAME      yx0103-kyl-4119-7-1
EXPNO                       2
PROCNO                      1

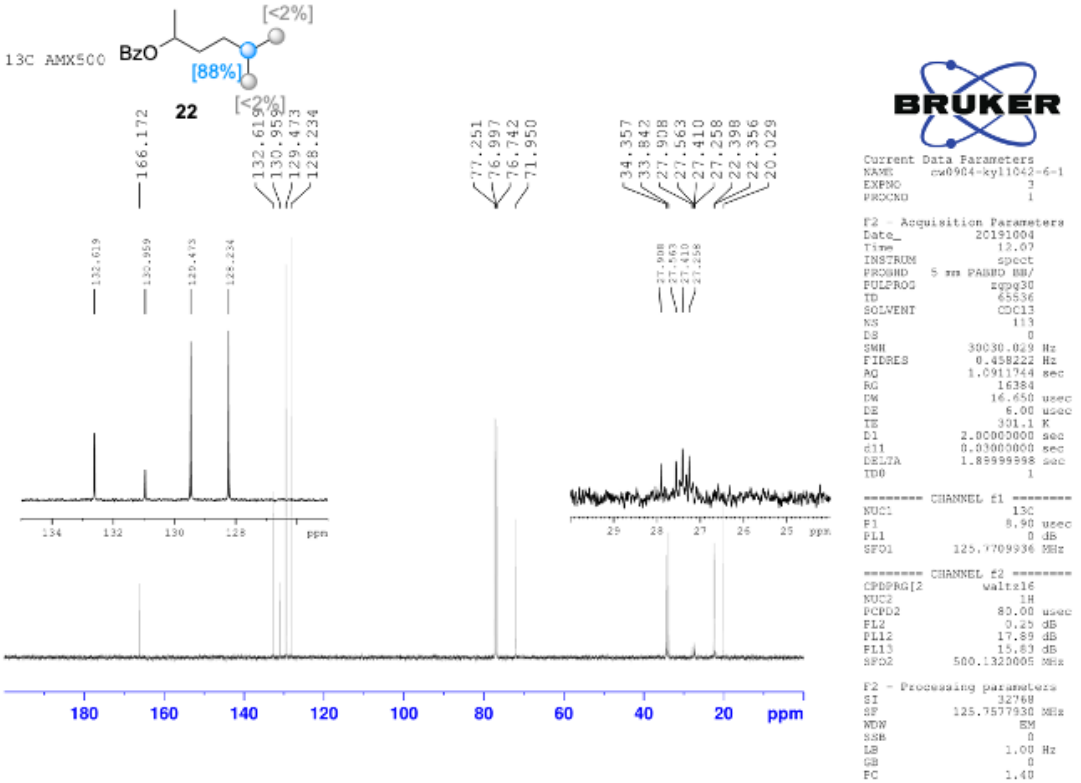
F2 - Acquisition Parameters
Date_            20200103
Time                16.57
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                  65536
SOLVENT              CDCl3
NS                     217
DS                       0
SWH             30030.029 Hz
FIDRES          0.458222 Hz
AQ              1.0911744 sec
RG                   16384
DW                  16.650 usec
DE                   6.00 usec
TE                  296.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     20

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.90 usec
PL1                      0 dB
SFO1          125.7709936 MHz

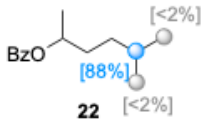
======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.25 dB
PL12                 17.89 dB
PL13                 15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                   32768
SF            125.7577936 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

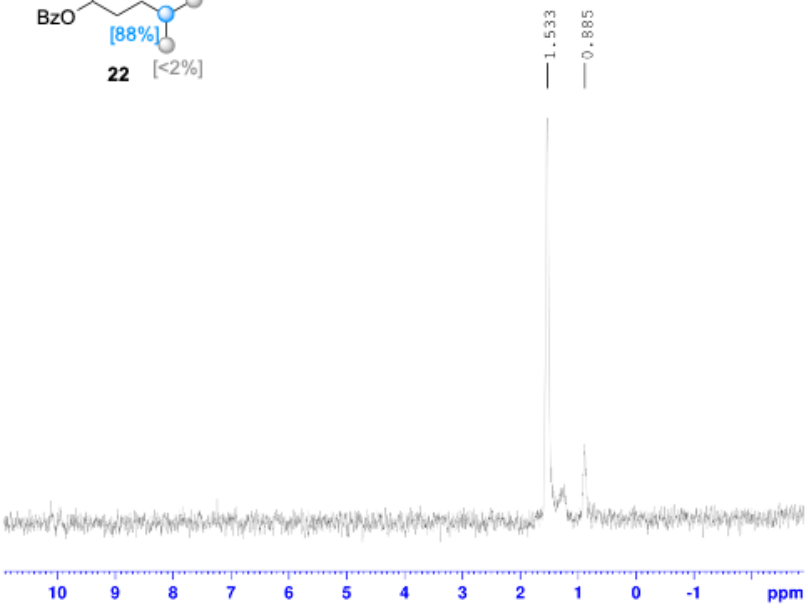

1H AMX500
BzO
[<2%]
[88%]
[<2%]
22
8.057
8.055
8.041
8.039
7.558
7.543
7.530
7.528
7.526
7.450
7.435
7.420
7.260
5.160
5.148
5.135
5.122
1.752
1.741
1.737
1.731
1.729
1.727
1.719
1.715
1.643
1.632
1.621
1.615
1.610
1.605
1.594
1.350
1.337
1.306
1.296
1.285
1.275
1.264
1.253
1.242
0.906
0.892
0.873
1.99
1.00
2.02
0.99
1.12
1.12
2.93
2.05
5.74
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 ppm
BRUKER
Current Data Parameters
NAME cw0904-kyl1042-6-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191004
Time 11.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 40.3
DW 48.400 usec
DE 6.00 usec
TE 300.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 16384
SF 500.1300130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


13C AMX500
BzO
[<2%]
[88%]
[<2%]
22
166.172
132.619
130.959
129.473
128.234
77.251
76.997
76.742
71.950
34.357
33.842
27.908
27.563
27.410
27.258
22.398
22.356
20.029
180 160 140 120 100 80 60 40 20 ppm
BRUKER
Current Data Parameters
NAME cw0904-kyl1042-6-1
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191004
Time 12.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 113
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 301.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577930 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2H AV 500 NEO 23 May 2017 D NMR in CHCl3



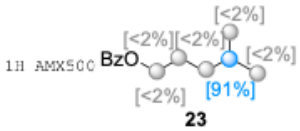
22



```
Current Data Parameters
NAME                  thd-4
EXPNO                     2
PROCNO                    1

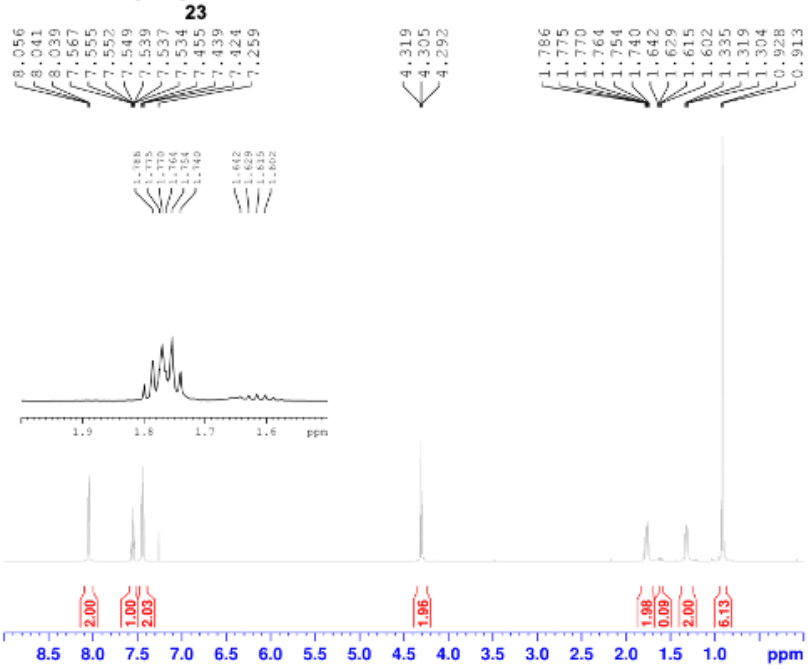
F2 - Acquisition Parameters
Date_              20200624
Time                 16.17 h
INSTRUM   CAB AV4 500 MHS BASIC
PROBHD    2144569_0005 (
PULPROG              zg2h.2
TD                     8192
SOLVENT               CDCl3
NS                        8
DS                        2
SWH               1562.500 Hz
FIDRES            0.381470 Hz
AQ                2.6214399 sec
RG                     12.5
DW                 320.000 usec
DE                    6.50 usec
TE                  298.0 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1             76.7886582 MHz
NUC1                    2H
P1                  349.30 usec
PLW1             3.50000000 W

F2 - Processing parameters
SI                    65536
SF               76.7883502 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



23

1H AMX500

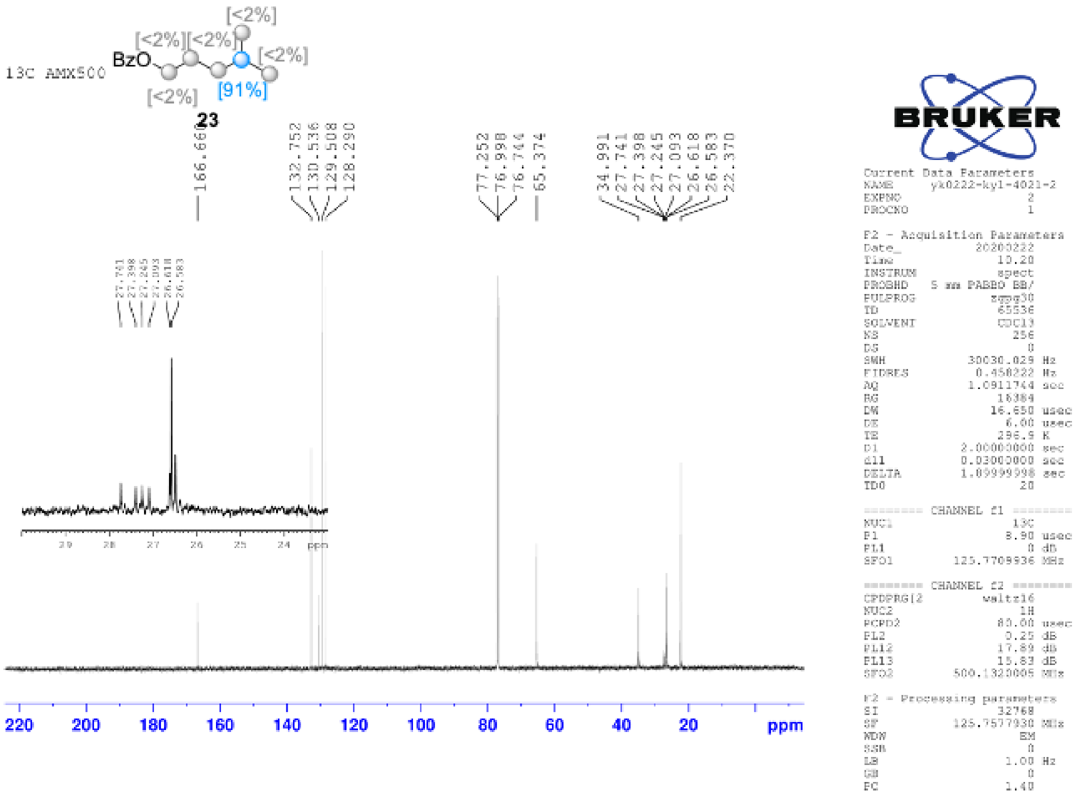


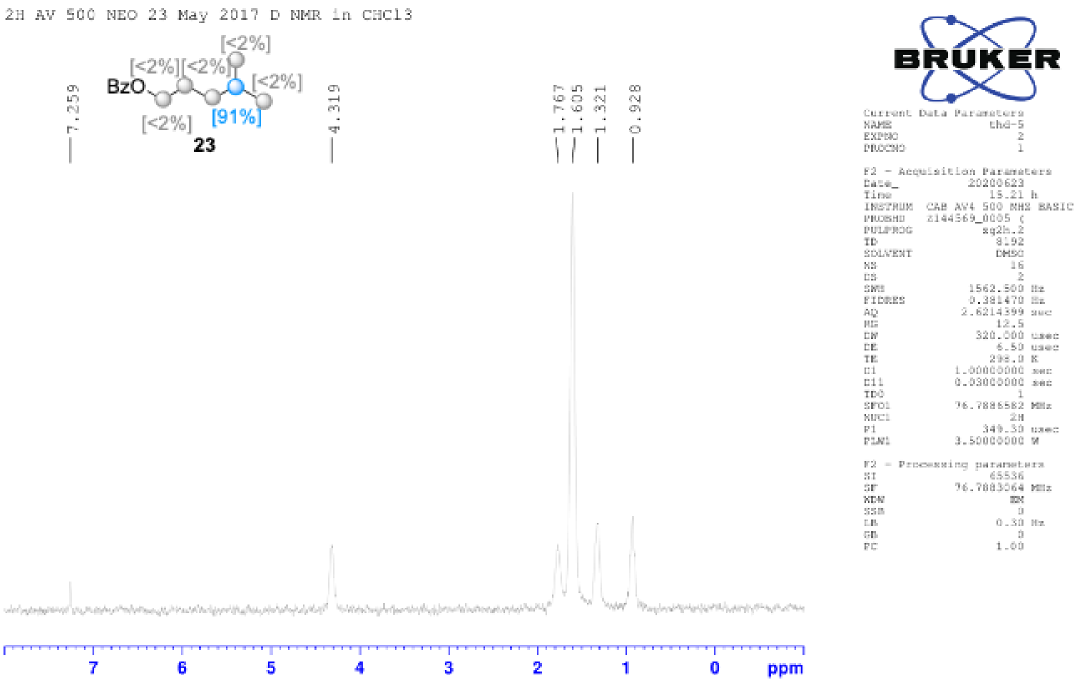
```
Current Data Parameters
NAME          yx0222-ky1-4021-2
EXPNO                     1
PROCNO                    1

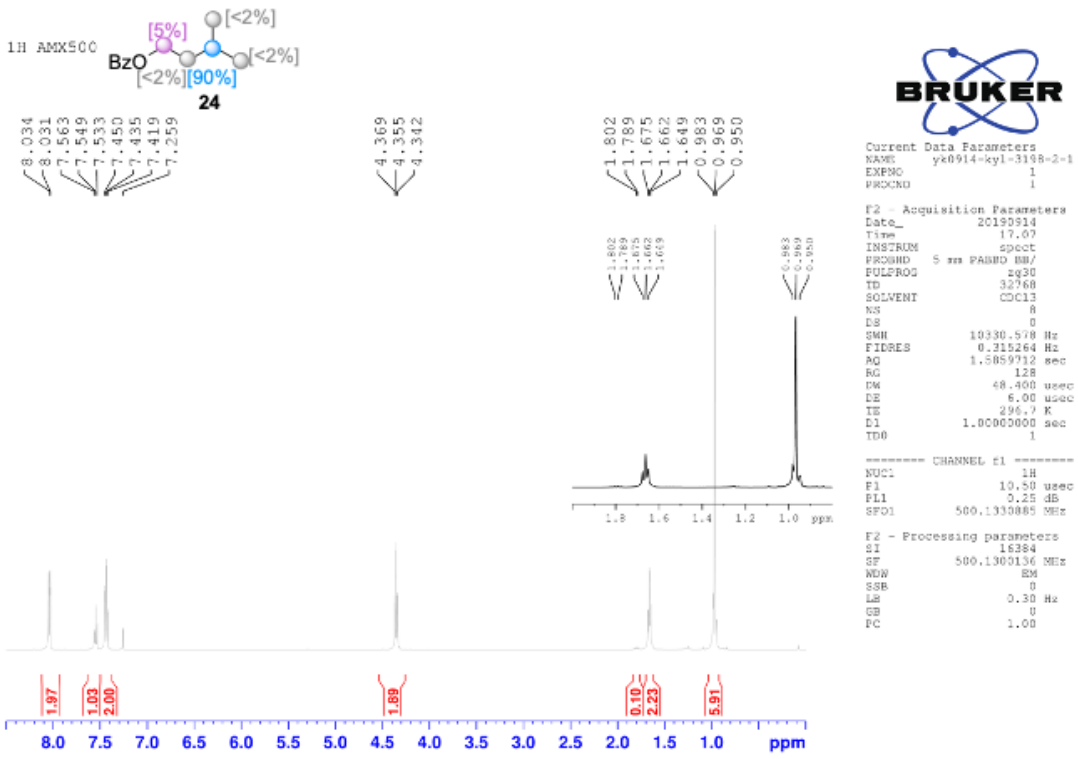
F2 - Acquisition Parameters
Date_              20200222
Time                 10.18
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH              10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                     71.8
DW                 48.400 usec
DE                    6.00 usec
TE                  296.4 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                   10.50 usec
PL1                   0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                    16384
SF               500.1300137 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```


13C AMX500
BzO
[<2%]
[<2%][<2%]
[<2%]
[<2%]
[91%]
23
166.660
132.752
130.536
129.508
128.290
77.252
76.998
76.744
65.374
34.991
27.741
27.398
27.245
27.093
26.618
26.583
22.370
BRUKER
220
200
180
160
140
120
100
80
60
40
20
ppm


2H AV 500 NEO 23 May 2017 D NMR in CHCl3
BzO
[<2%]
[<2%][<2%]
[<2%]
[<2%]
[91%]
23
7.259
4.319
1.767
1.605
1.321
0.928
BRUKER
7
6
5
4
3
2
1
0
ppm



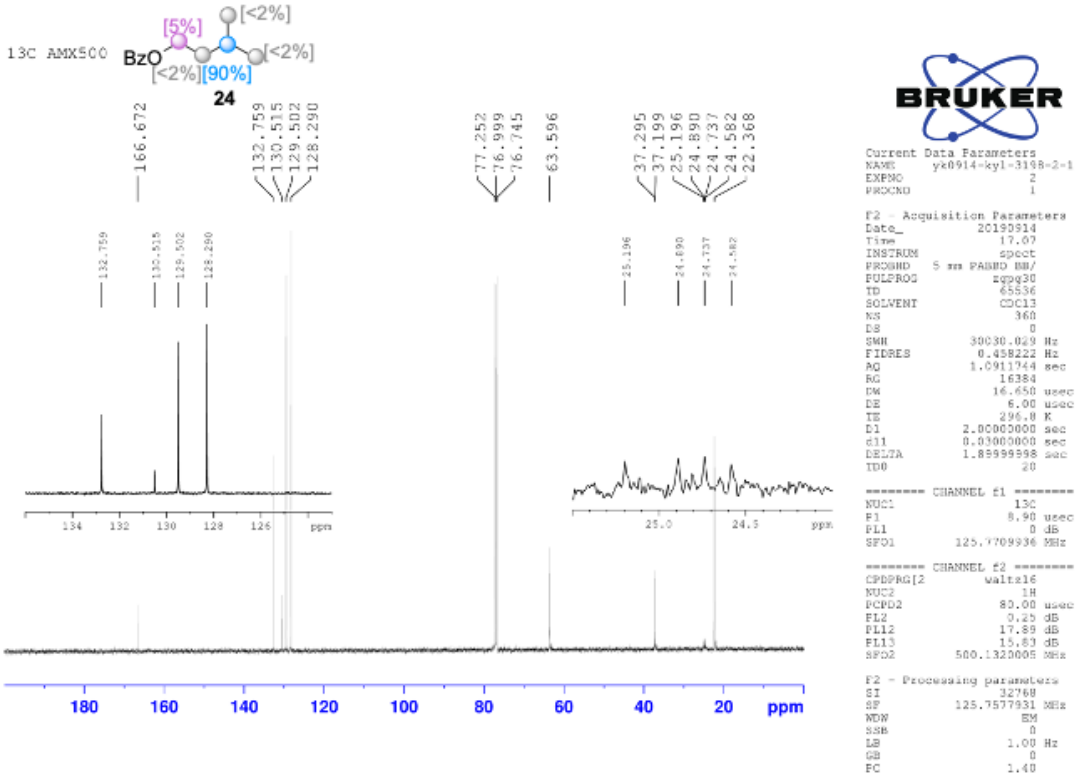
BRUKER

```
Current Data Parameters
NAME      yx0914-kyl-3198-2-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190914
Time                   17.07
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH               10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                      128
DW                 48.400 usec
DE                  6.00 usec
TE                 296.9 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.50 usec
PL1                     0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                    16384
SF            500.1300136 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



BRUKER

```
Current Data Parameters
NAME      yx0914-kyl-3198-2-1
EXPNO                       2
PROCNO                      1

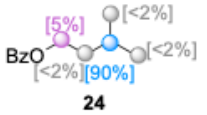
F2 - Acquisition Parameters
Date_              20190914
Time                   17.07
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      360
DS                        0
SWH               30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0911744 sec
RG                    16384
DW                 16.650 usec
DE                  6.00 usec
TE                 296.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      20

======== CHANNEL f1 ========
NUC1                      13C
P1                     8.90 usec
PL1                       0 dB
SFO1          125.7709936 MHz

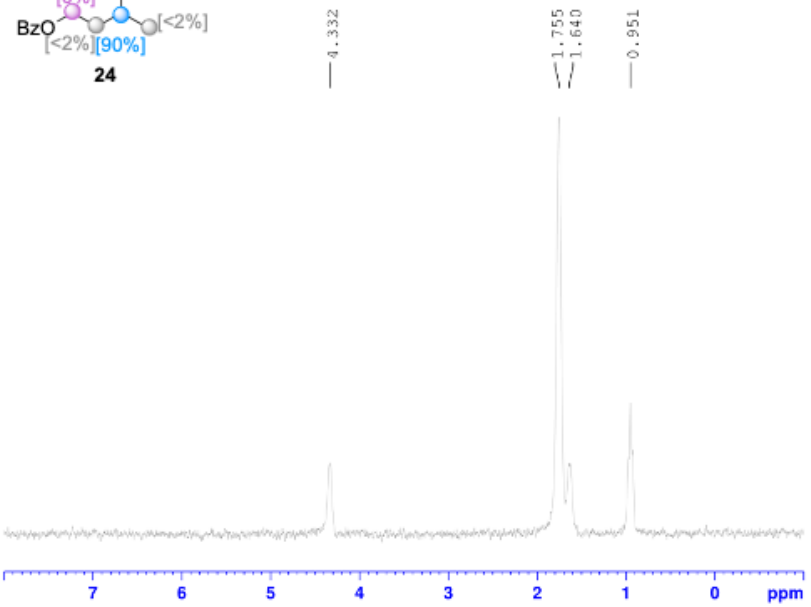
======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     0.25 dB
PL12                   17.89 dB
PL13                   15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                    32768
SF            125.7577931 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

2H AV 500 NEO 23 May 2017 D NMR in CHCl3



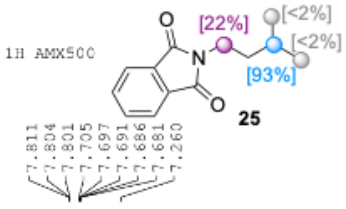
24



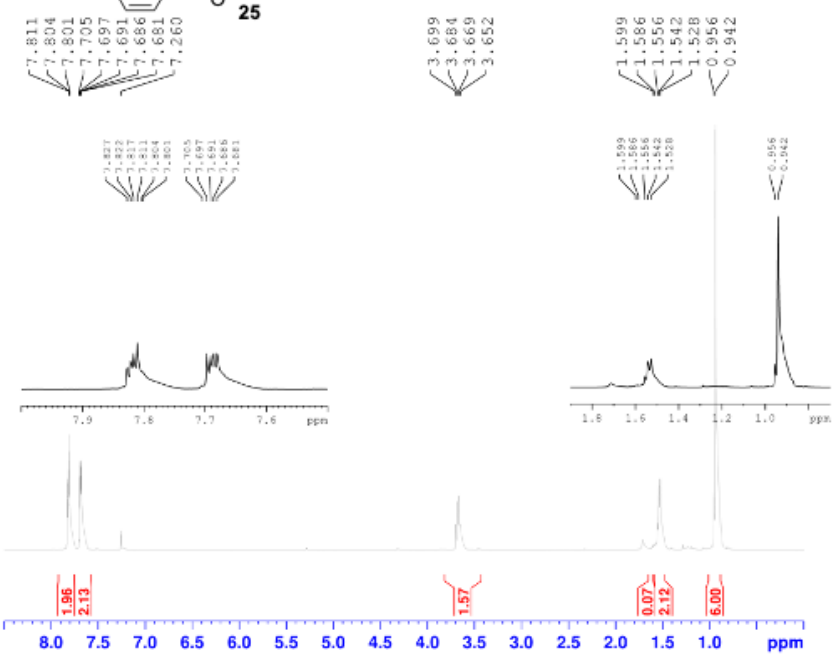

```
Current Data Parameters
NAME                  thd-6
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200624
Time                 16.19 h
INSTRUM   CAB AV4 500 MHz BASIC
PROBHD    2144569_0005 (
PULPROG              zg2h.2
TD                     8192
SOLVENT               CDCl3
NS                        8
DS                        2
SWH               1562.500 Hz
FIDRES            0.381470 Hz
AQ                2.6214399 sec
RG                     12.5
DW                 320.000 usec
DE                   6.50 usec
TE                  298.0 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                       1
SFO1             76.7886582 MHz
NUC1                     2H
P1                  349.30 usec
PLW1             3.50000000 W

F2 - Processing parameters
SI                    65536
SF               76.7883510 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



25

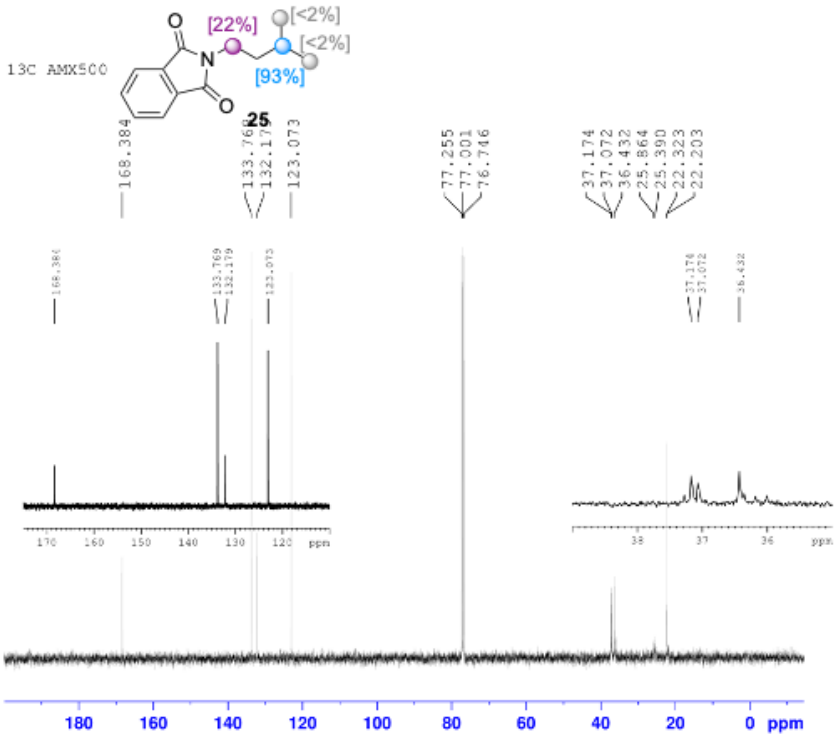



```
Current Data Parameters
NAME      ye0104-kyl-4120-4-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20200104
Time                 16.08
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH              10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                     80.6
DW                 48.400 usec
DE                   6.00 usec
TE                  295.8 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                  10.50 usec
PL1                   0.25 dB
SFO1            500.1330885 MHz

F2 - Processing parameters
SI                    16384
SF              500.1300147 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



BRUKER

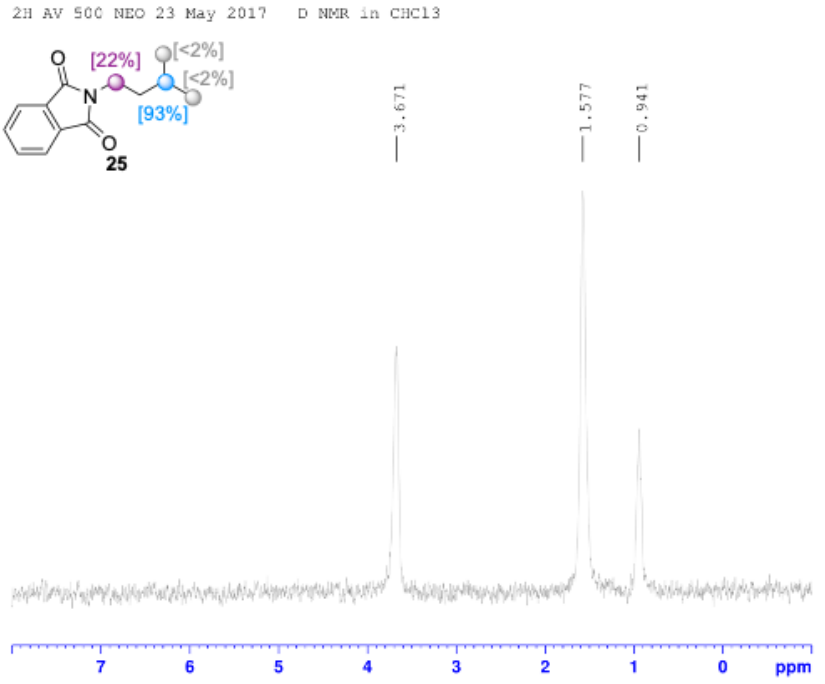
```
Current Data Parameters
NAME      yk0104-kyl-4120-4-1
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20200104
Time                   16.09
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT                CDCl3
NS                       104
DS                         0
SWH                30030.029 Hz
FIDRES             0.458222 Hz
AQ                 1.0911744 sec
RG                     16384
DW                    16.650 usec
DE                     6.00 usec
TE                   296.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                       20

======== CHANNEL f1 ========
NUC1                      13C
P1                       8.90 usec
PL1                         0 dB
SFO1           125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2               waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                      0.25 dB
PL12                    17.89 dB
PL13                    15.83 dB
SFO2           500.1320005 MHz

F2 - Processing parameters
SI                        32768
SF             125.7577942 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40
```

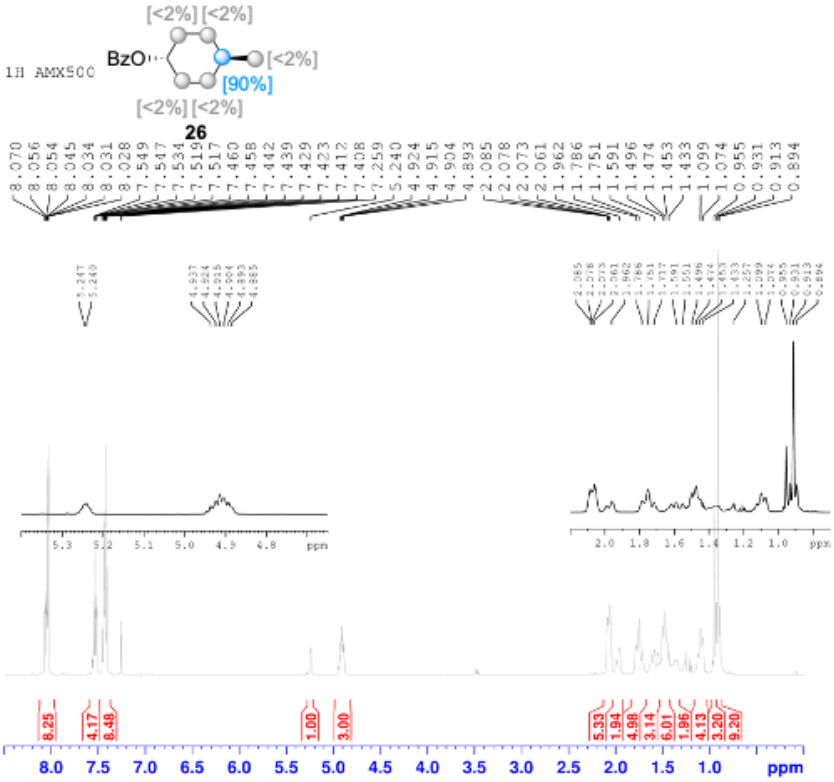


BRUKER

```
Current Data Parameters
NAME                     thd-7
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20200624
Time                   16.21 h
INSTRUM  CAB AV4 500 MHz BASIC
PROBHD   Z144369_0005 (
PULPROG              zg2h.2
TD                     8192
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                1562.500 Hz
FIDRES             0.381470 Hz
AQ                 2.6214399 sec
RG                      12.5
DW                   320.000 usec
DE                     6.50 usec
TE                   298.0 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1           76.7885582 MHz
NUC1                      2H
P1                   349.30 usec
PLW1               3.50000000 W

F2 - Processing parameters
SI                        65536
SF             76.7883510 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

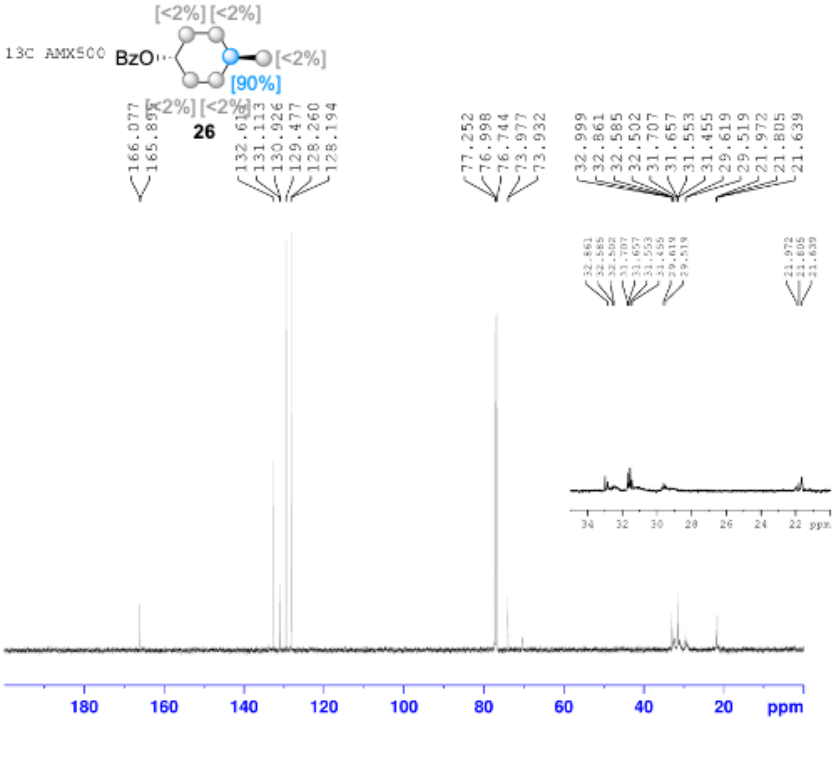


```
Current Data Parameters
NAME      yx1125-kyl-4091-2-1
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_             20191125
Time                11.54
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT             CDCl3
NS                     8
DS                     0
SWH            10330.578 Hz
FIDRES         0.315264 Hz
AQ             1.5859712 sec
RG                    57
DW                48.400 usec
DE                 6.00 usec
TE                296.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.50 usec
PL1                0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                 16384
SF            500.1300143 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



```
Current Data Parameters
NAME      yx1125-kyl-4091-2-1
EXPNO                2
PROCNO               1

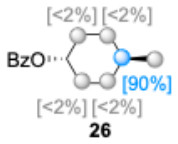
F2 - Acquisition Parameters
Date_             20191125
Time                11.56
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                   196
DS                     0
SWH            30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0911744 sec
RG                 16384
DW                16.650 usec
DE                 6.00 usec
TE                296.9 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                   20

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.90 usec
PL1                   0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.25 dB
PL12              17.89 dB
PL13              15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF            125.7577952 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

2H AV 500 NEO 23 May 2017 D NMR in CHCl3



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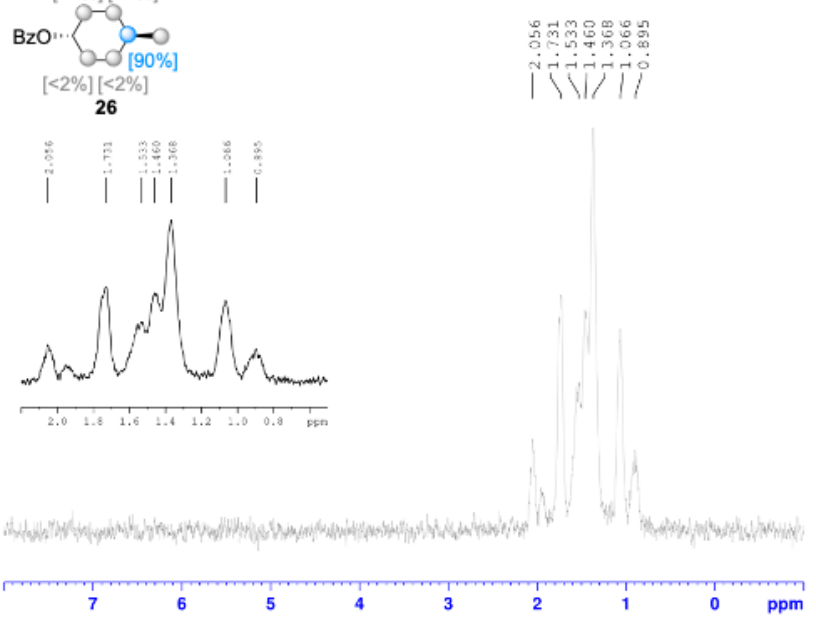

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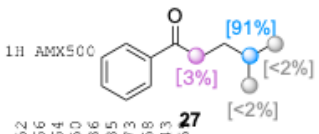
```
Current Data Parameters
NAME                  thd-8
EXPNO                     2
PROCNO                    1

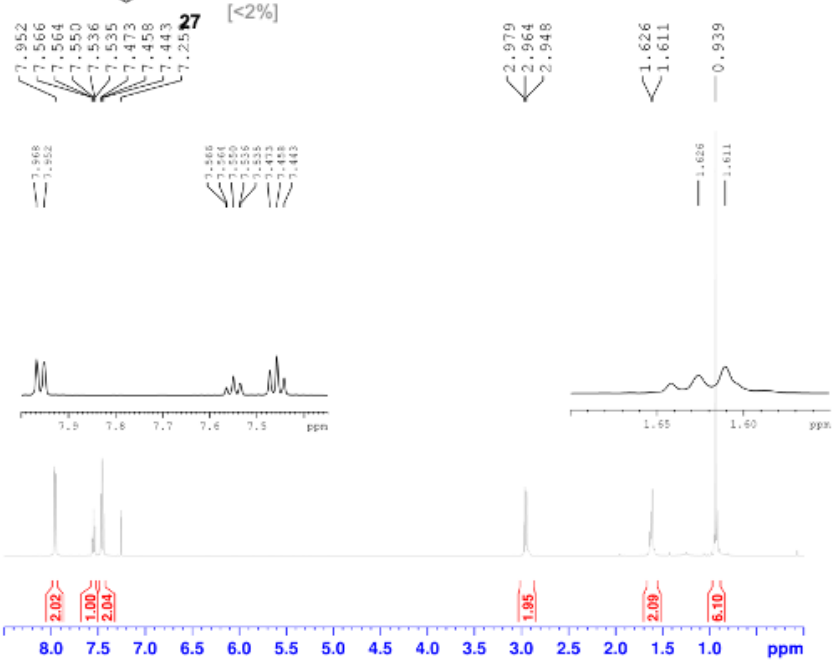
F2 - Acquisition Parameters
Date_              20200624
Time                 16.24 h
INSTRUM   CAB AV4 500 MHz BASIC
PROBHD    2144569_0005 (
PULPROG              zg2h.2
TD                     8192
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                1562.500 Hz
FIDRES             0.381470 Hz
AQ                 2.6214399 sec
RG                    13.8889
DW                  320.000 usec
DE                    6.50 usec
TE                  298.0 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                       1
SFO1               76.7886582 MHz
NUC1                     2H
P1                  349.30 usec
PLW1               3.50000000 W

F2 - Processing parameters
SI                       65536
SF                 76.7883510 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

1H AMX500



27



BRUKER

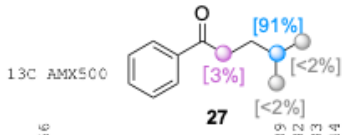
```
Current Data Parameters
NAME      ykl222-kyl-4059-1-1
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20191222
Time                 11.06
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH                10330.578 Hz
FIDRES             0.315264 Hz
AQ                 1.5859712 sec
RG                      114
DW                   48.400 usec
DE                    6.00 usec
TE                  296.9 K
D1                 1.00000000 sec
TD0                       1

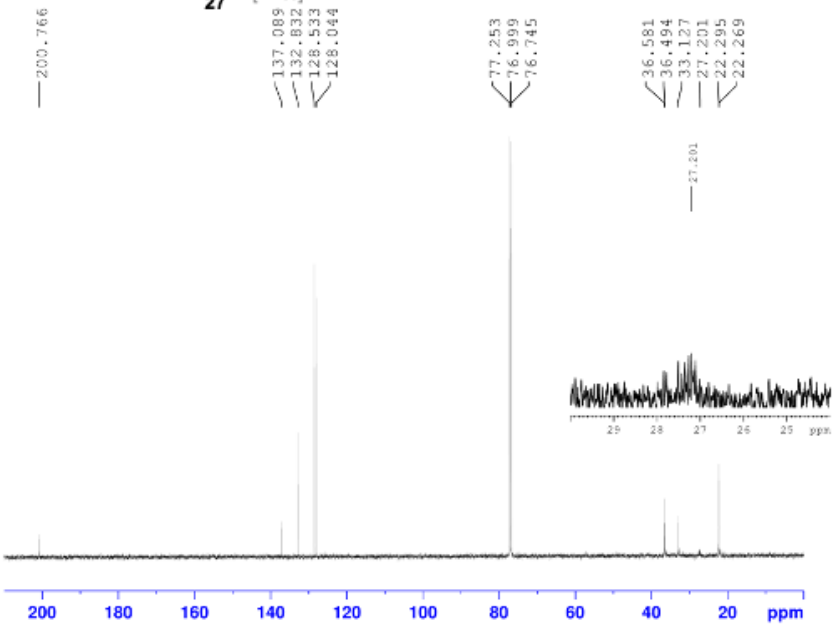
======== CHANNEL f1 ========
NUC1                     1H
P1                   10.50 usec
PL1                   0.25 dB
SFO1              500.1330885 MHz

F2 - Processing parameters
SI                       16384
SF                500.1300143 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

13C AMX500



27




```
Current Data Parameters
NAME      yk1222-kyl-4059-1-1
EXPNO                       2
PROCNO                      1

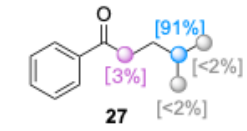
F2 - Acquisition Parameters
Date_              20191222
Time                   11.08
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      401
DS                        0
SWH               30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0911744 sec
RG                    16384
DW                   16.650 usec
DE                    6.00 usec
TE                   296.9 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      20

======== CHANNEL f1 ========
NUC1                    13C
P1                     8.90 usec
PL1                       0 dB
SFO1           125.7709936 MHz

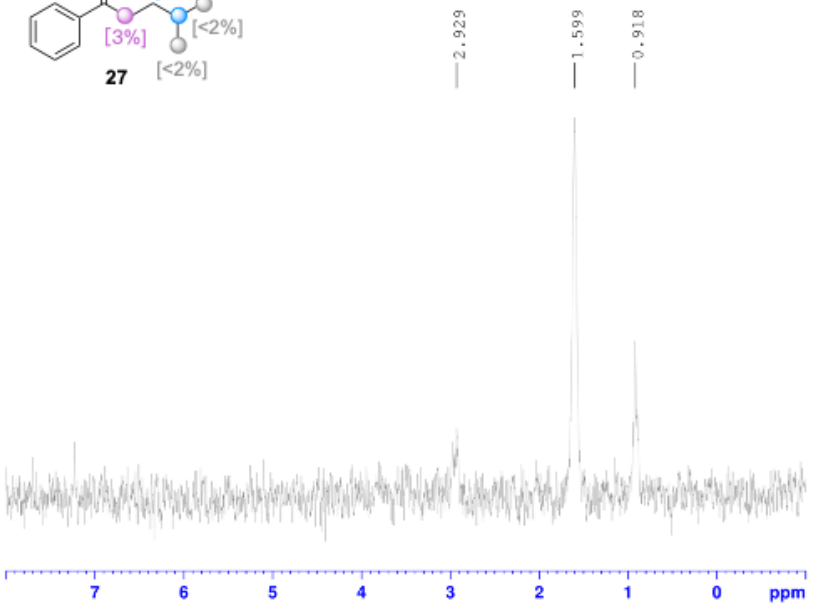
======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                    1H
PCPD2                 80.00 usec
PL2                    0.25 dB
PL12                  17.89 dB
PL13                  15.83 dB
SFO2           500.1320005 MHz

F2 - Processing parameters
SI                     32768
SF            125.7577920 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

2H AV 500 NEO 23 May 2017 D NMR in CHCl3



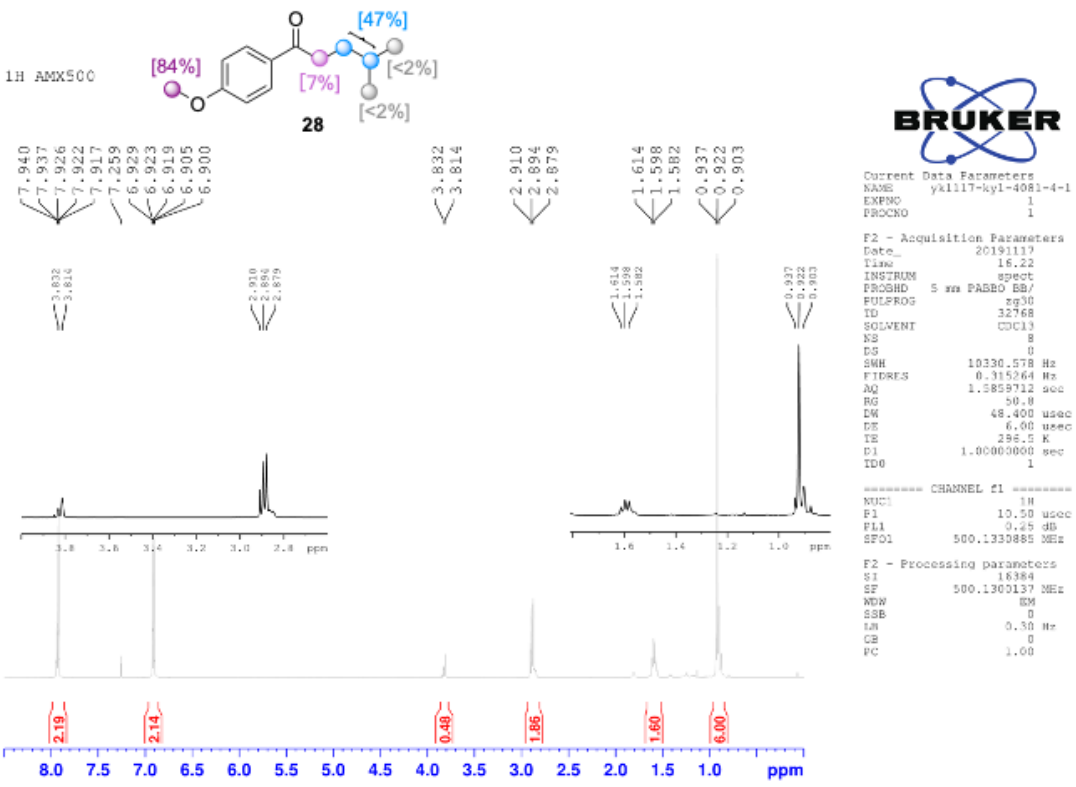
27




```
Current Data Parameters
NAME                    thd-9
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20200624
Time                   15.27 h
INSTRUM  CAB AV4 500 MHS BASIC
PROBHD   2144369_0005 (
PULPROG              zg2h.2
TD                     8192
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               1562.500 Hz
FIDRES            0.381470 Hz
AQ                2.6214399 sec
RG                      12.5
DW                 320.000 usec
DE                    6.50 usec
TE                   298.0 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1           76.7886582 MHz
NUC1                      2H
P1                   349.30 usec
PLW1              3.50000000 W

F2 - Processing parameters
SI                     65536
SF            76.7883510 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

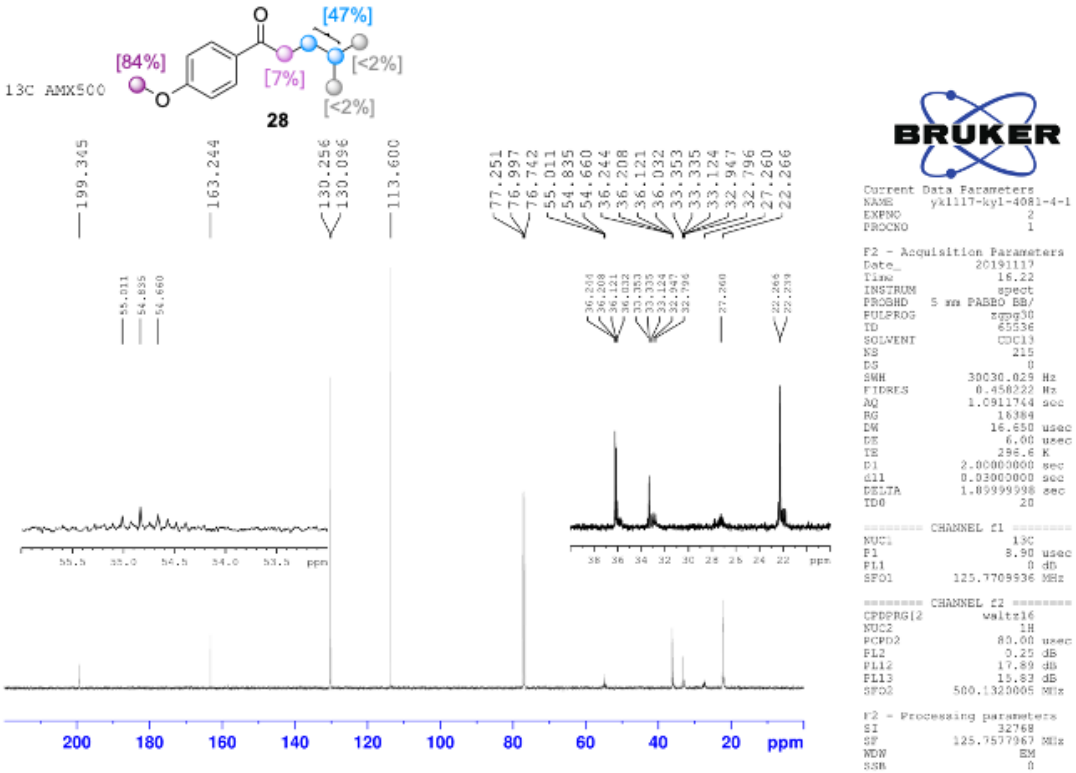



```
Current Data Parameters
NAME      yk1117-kyl-4081-4-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191117
Time                  16.22
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH              10330.578 Hz
FIDRES           0.315264 Hz
AQ               1.5859712 sec
RG                    50.8
DW                  48.400 usec
DE                   6.00 usec
TE                  296.5 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.50 usec
PL1                   0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                   16384
SF            500.1300137 MHz
WDW                     EM
SSB                      0
LB                    0.50 Hz
GB                       0
PC                    1.00
```




```
Current Data Parameters
NAME      yk1117-kyl-4081-4-1
EXPNO                       2
PROCNO                      1

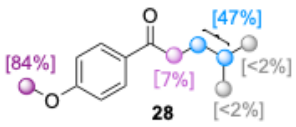
F2 - Acquisition Parameters
Date_              20191117
Time                  16.22
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     215
DS                       0
SWH              30030.029 Hz
FIDRES           0.458222 Hz
AQ               1.0911744 sec
RG                   16384
DW                  16.650 usec
DE                   6.00 usec
TE                  296.6 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                     20

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.90 usec
PL1                      0 dB
SFO1          125.7708936 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                   0.25 dB
PL12                 17.89 dB
PL13                 15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                   32768
SF            125.7577967 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

2H AV 500 NEO 23 May 2017 D NMR in CHCl3



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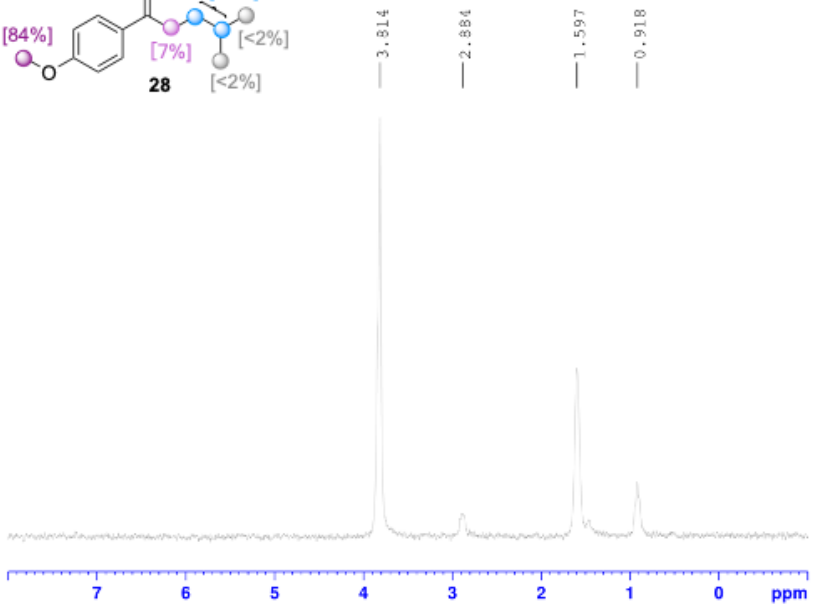
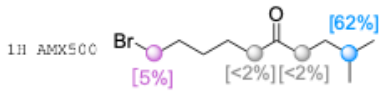


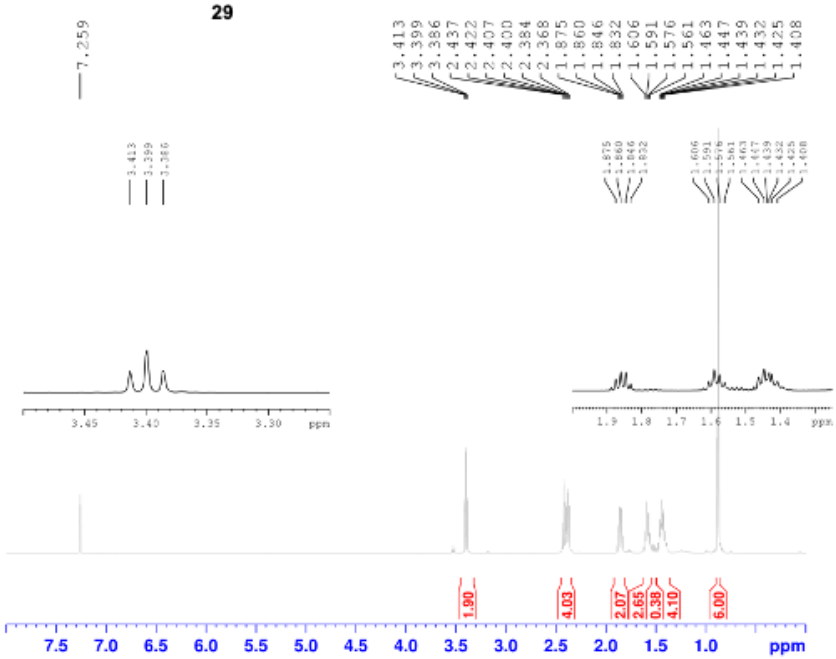
```
Current Data Parameters
NAME                  thd-10
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20200624
Time                 16.29 h
INSTRUM   CAB AV4 500 MHz BASIC
PROBHD    2144569_0005 (
PULPROG              zg2h.2
TD                     8192
SOLVENT               CDCl3
NS                        8
DS                        2
SWH                1562.500 Hz
FIDRES             0.381470 Hz
AQ                 2.6214399 sec
RG                    14.4944
DW                   320.000 usec
DE                     6.50 usec
TE                   298.0 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1              76.7886582 MHz
NUC1                      2H
P1                   349.30 usec
PLW1               3.50000000 W

F2 - Processing parameters
SI                        65536
SF                76.7883510 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



29

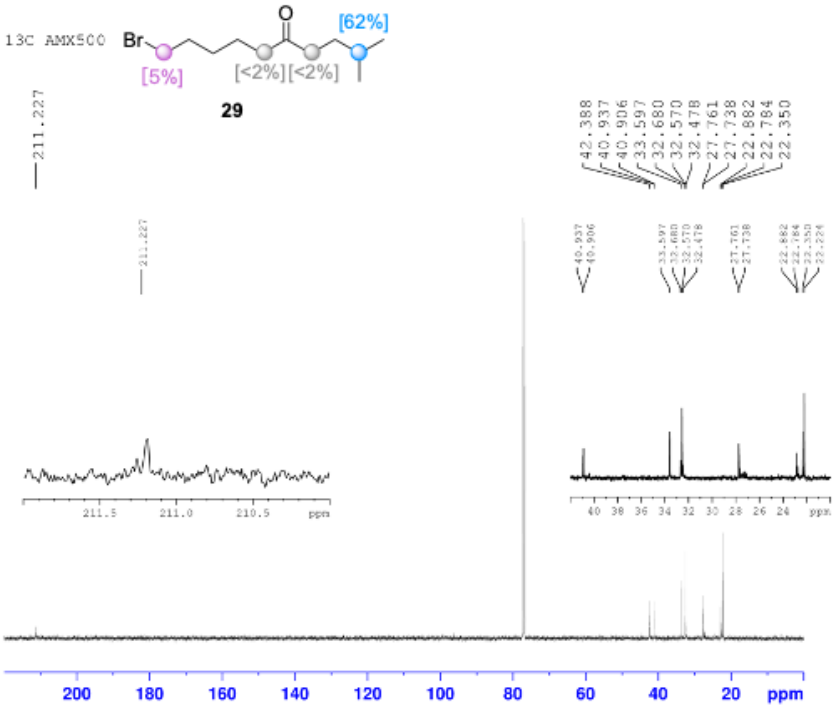


```
Current Data Parameters
NAME          yc1222-kyl-4110-2-2
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20191222
Time                 11.57
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH                10330.578 Hz
FIDRES             0.315264 Hz
AQ                 1.5859712 sec
RG                     114
DW                   48.400 usec
DE                     6.00 usec
TE                   296.0 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                    10.50 usec
PL1                    0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                       16384
SF                500.1300143 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



```
Current Data Parameters
NAME      yk1222-kyl-4110-2-2
EXPNO                       2
PROCNO                      1

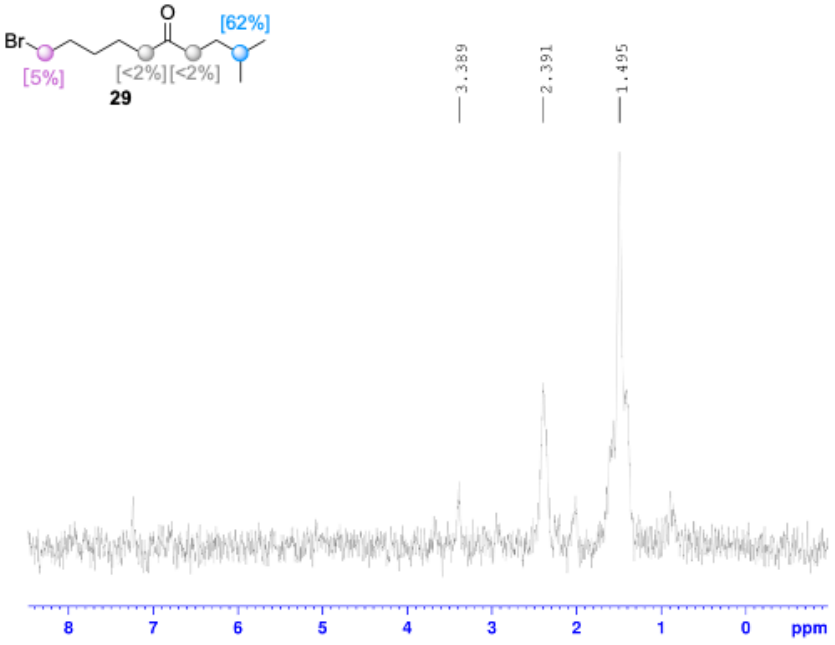
F2 - Acquisition Parameters
Date_              20191222
Time                   11.59
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     416
DS                       0
SWH              30030.029 Hz
FIDRES           0.458222 Hz
AQ               1.0911744 sec
RG                   16384
DW                16.650 usec
DE                 6.00 usec
TE                 297.5 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     20

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.90 usec
PL1                      0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.25 dB
PL12                 17.89 dB
PL13                 15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                      32768
SF            125.7577921 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

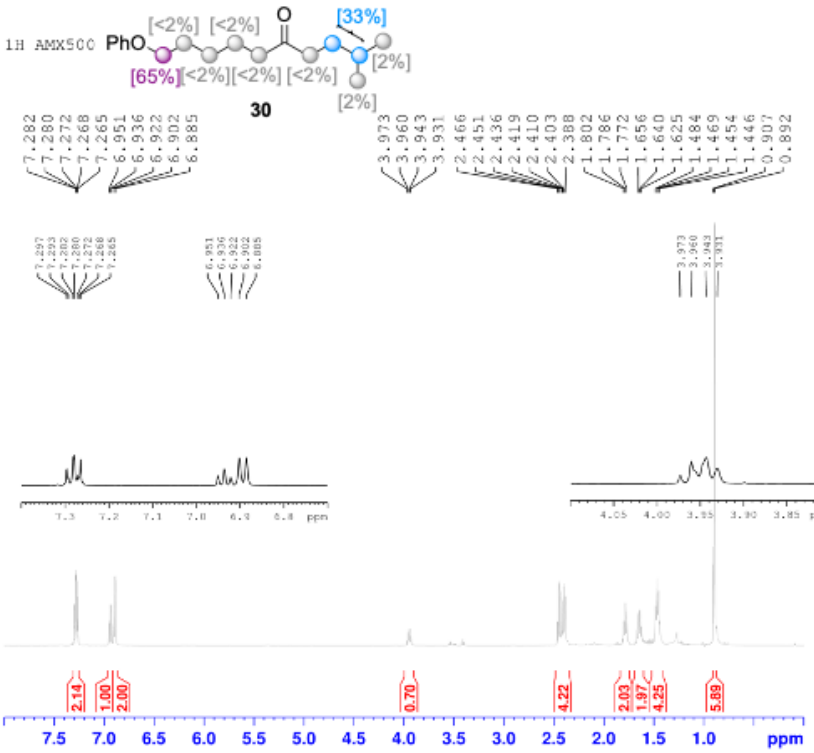
2H AV 500 NEO 23 May 2017 D NMR in CHCl3



```
Current Data Parameters
NAME                    thd-11
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20200624
Time                   15.32 h
INSTRUM  CAB AV4 500 MHz BASIC
PROBHD   Z144369_0005 (
PULPROG             zg2h.2
TD                    8192
SOLVENT              CDCl3
NS                      24
DS                       2
SWH              1562.500 Hz
FIDRES           0.381470 Hz
AQ               2.6214399 sec
RG                   13.8889
DW                320.000 usec
DE                   6.50 usec
TE                 298.0 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                      1
SFO1          76.7885582 MHz
NUC1                    2H
P1                 349.30 usec
PLW1            3.50000000 W

F2 - Processing parameters
SI                      65536
SF            76.7883510 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```

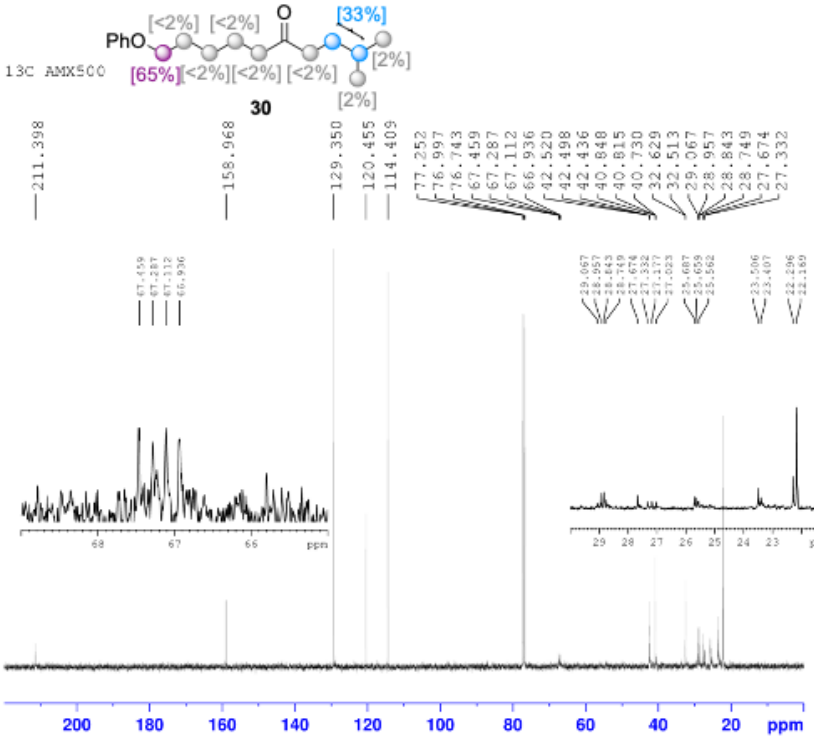


```
Current Data Parameters
NAME      yk1125-kyl-4091-3-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191125
Time                 12.07
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH              10330.578 Hz
FIDRES           0.315264 Hz
AQ               1.5859712 sec
RG                    40.3
DW                  48.400 usec
DE                   6.00 usec
TE                  296.3 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.50 usec
PL1                   0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                   16384
SF            500.1300073 MHz
WDW                     EM
SSB                      0
LB                    0.50 Hz
GB                       0
PC                    1.00
```



```
Current Data Parameters
NAME      yk1125-kyl-4091-3-1
EXPNO                       2
PROCNO                      1

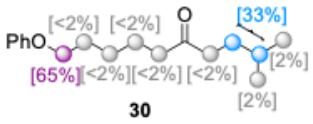
F2 - Acquisition Parameters
Date_              20191125
Time                 12.08
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT              CDCl3
NS                     141
DS                       0
SWH              30030.029 Hz
FIDRES           0.458222 Hz
AQ               1.0911744 sec
RG                   16384
DW                  16.650 usec
DE                   6.00 usec
TE                  296.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                     20

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.90 usec
PL1                      0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.25 dB
PL12                 17.89 dB
PL13                 15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                   32768
SF            125.7577975 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

2H AV 500 NEO 23 May 2017 D NMR CHCl3



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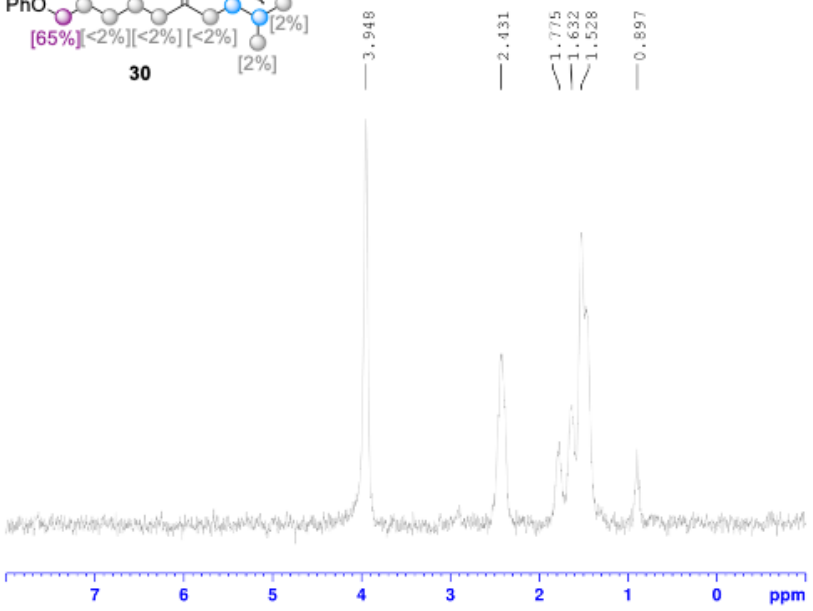
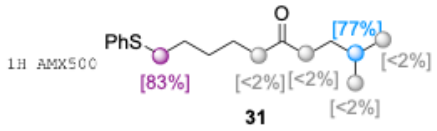


BRUKER

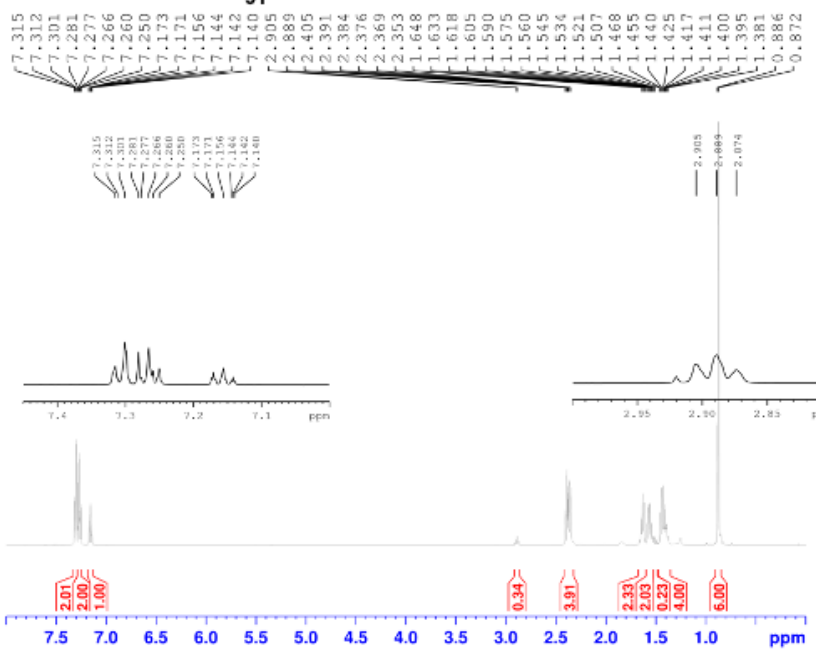
```
Current Data Parameters
NAME                  thd-12
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20200624
Time                 16.35 h
INSTRUM   CAB AV4 500 MHz BASIC
PROBHD    2144569_0005 (
PULPROG              zg2h.2
TD                     8192
SOLVENT              CDCl3
NS                         8
DS                         2
SWH               1562.500 Hz
FIDRES            0.381470 Hz
AQ                2.6214399 sec
RG                      12.5
DW                 320.000 usec
DE                   6.50 usec
TE                  298.0 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                        1
SFO1             76.7886582 MHz
NUC1                      2H
P1                  349.30 usec
PLW1              3.50000000 W

F2 - Processing parameters
SI                     65536
SF               76.7883485 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                      1.00
```



31



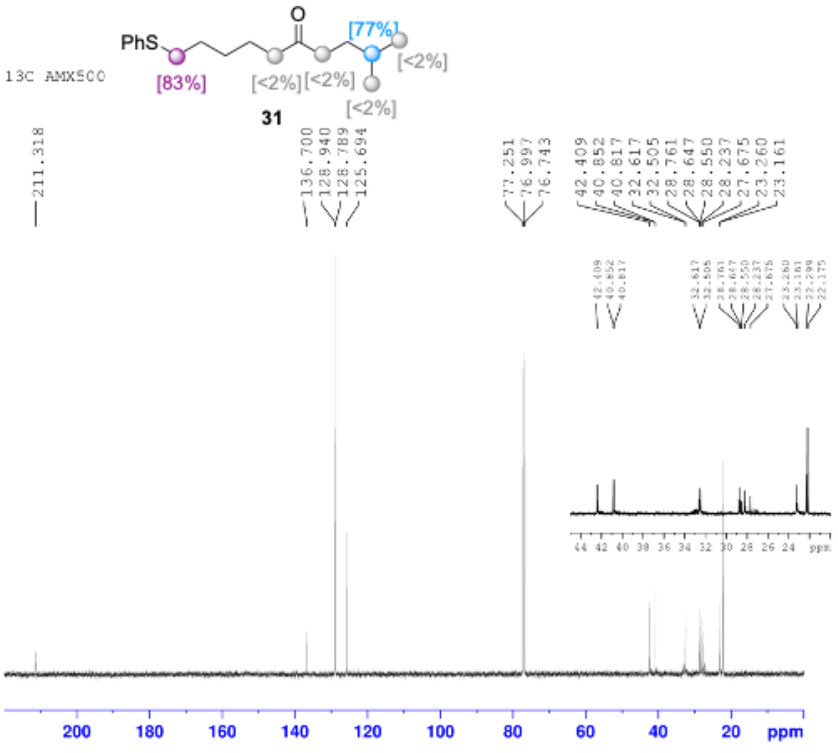
BRUKER

```
Current Data Parameters
NAME      ykl117-ky1-4081-2-1
EXPNO                      1
PROCNO                     1

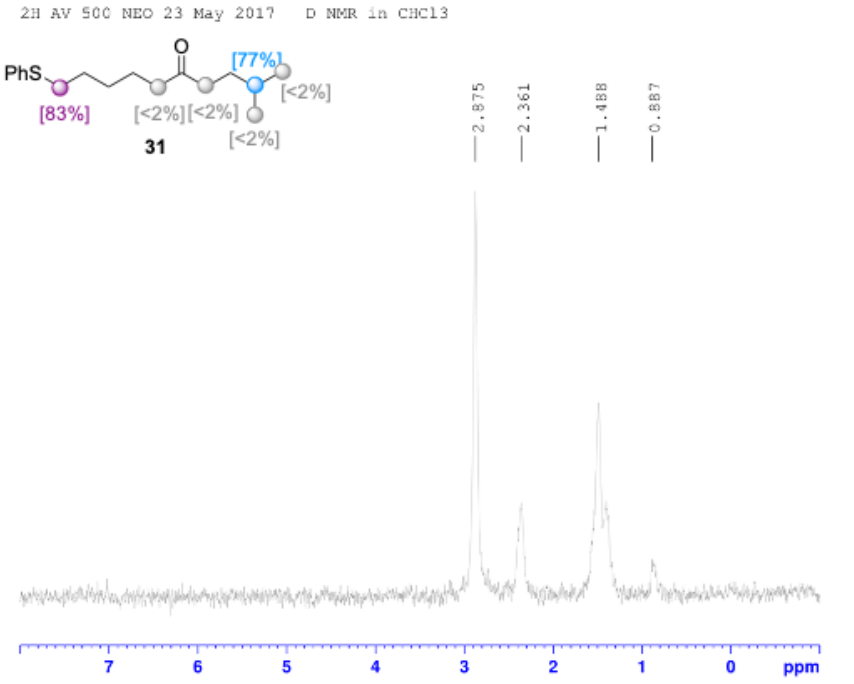
F2 - Acquisition Parameters
Date_              20191119
Time                 15.50
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                    32768
SOLVENT              CDCl3
NS                         8
DS                         0
SWH              10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                        57
DW                 48.400 usec
DE                   6.00 usec
TE                  296.3 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                   10.50 usec
PL1                   0.25 dB
SFO1          500.1330885 MHz

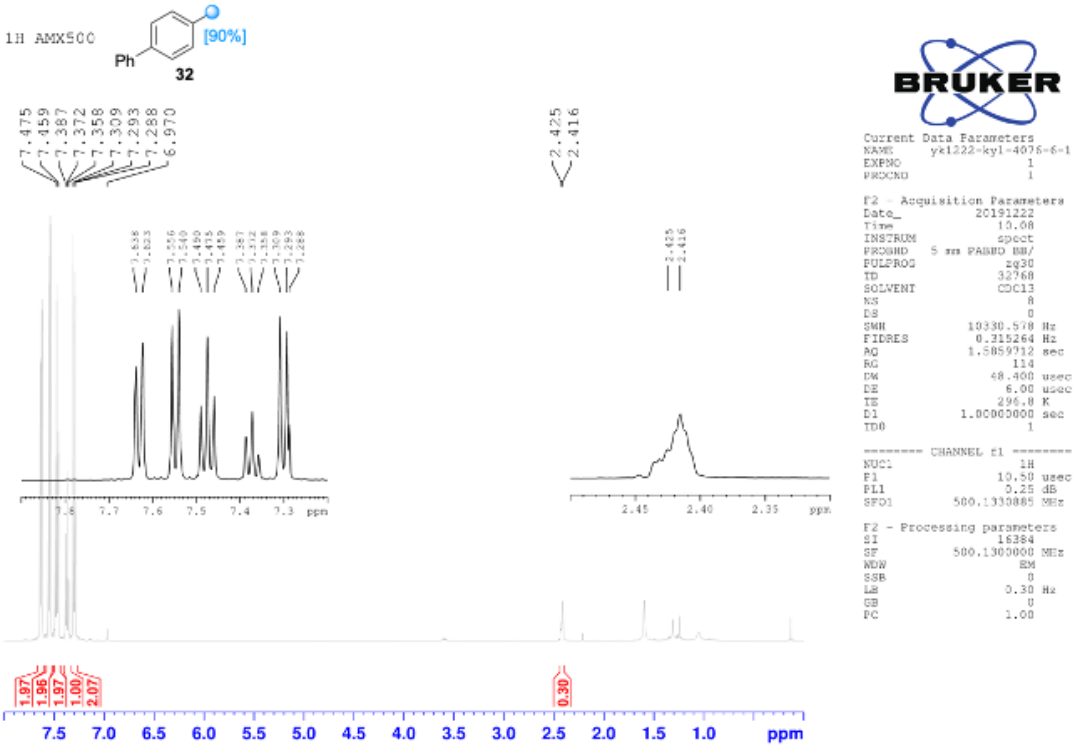
F2 - Processing parameters
SI                     16384
SF               500.1300137 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                      1.00
```


13C AMX500
PhS
O
[77%]
[<2%]
[83%]
[<2%][<2%]
[<2%]
31
211.318
136.700
128.940
128.789
125.694
77.251
76.997
76.743
42.409
40.852
40.617
32.617
32.505
28.761
28.647
28.550
28.237
27.675
23.260
23.161
200 180 160 140 120 100 80 60 40 20 ppm
44 42 40 38 36 34 32 30 28 26 24 ppm


BRUKER
Current Data Parameters
NAME yk1117-kyl-4081-2-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191117
Time 15.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 175
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 296.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577965 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


2H AV 500 NEO 23 May 2017 D NMR in CHCl3
PhS
O
[77%]
[<2%]
[83%]
[<2%][<2%]
[<2%]
31
2.875
2.361
1.488
0.887
7 6 5 4 3 2 1 0 ppm


BRUKER
Current Data Parameters
NAME thd-13
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200624
Time 16.36 h
INSTRUM CAB AV4 500 MHz BASIC
PROBHD Z144369_0005 (
PULPROG zg2h.2
TD 8192
SOLVENT CDCl3
NS 8
DS 2
SWH 1562.500 Hz
FIDRES 0.381470 Hz
AQ 2.6214399 sec
RG 12.5
DW 320.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 76.7885582 MHz
NUC1 2H
P1 349.30 usec
PLW1 3.50000000 W
F2 - Processing parameters
SI 65536
SF 76.7883510 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



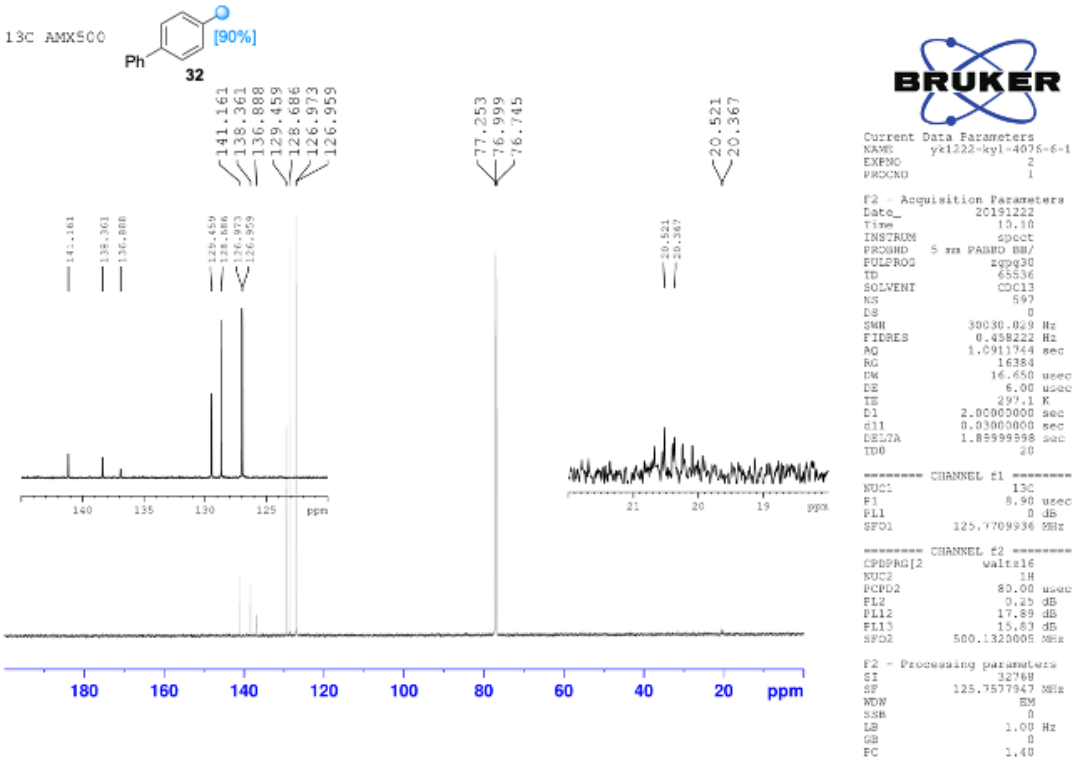
BRUKER

```
Current Data Parameters
NAME      yk1222-kyl-4076-6-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191222
Time                   10.08
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH               10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                      114
DW                 48.400 usec
DE                  6.00 usec
TE                 296.8 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.50 usec
PL1                     0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                    16384
SF            500.1300000 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



BRUKER

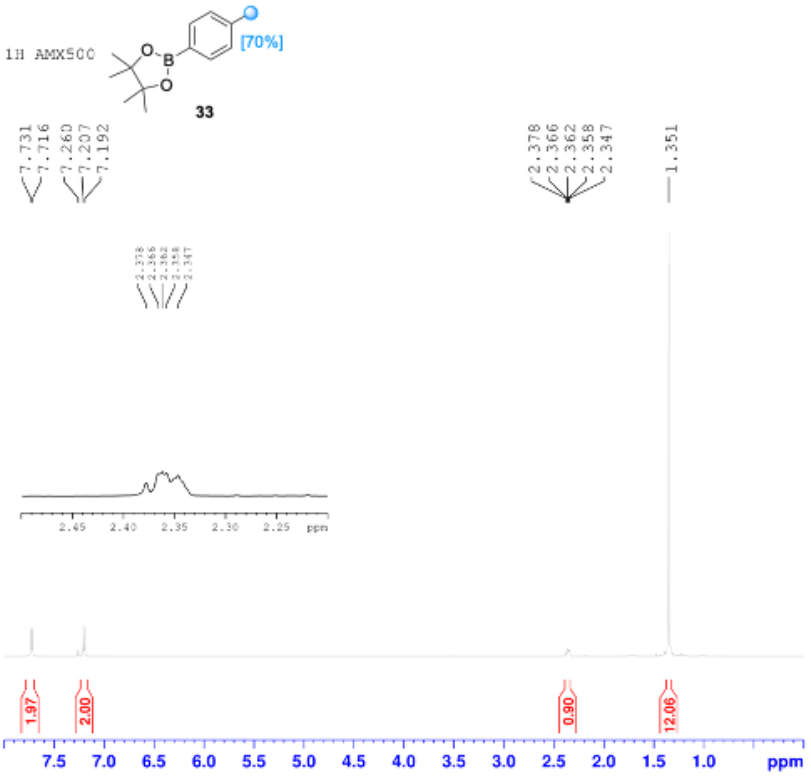
```
Current Data Parameters
NAME      yk1222-kyl-4076-6-1
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191222
Time                   10.10
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      597
DS                        0
SWH               30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0911744 sec
RG                    16384
DW                 16.650 usec
DE                  6.00 usec
TE                 297.1 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      20

======== CHANNEL f1 ========
NUC1                     13C
P1                     8.90 usec
PL1                       0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     0.25 dB
PL12                   17.89 dB
PL13                   15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                    32768
SF            125.7577947 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```



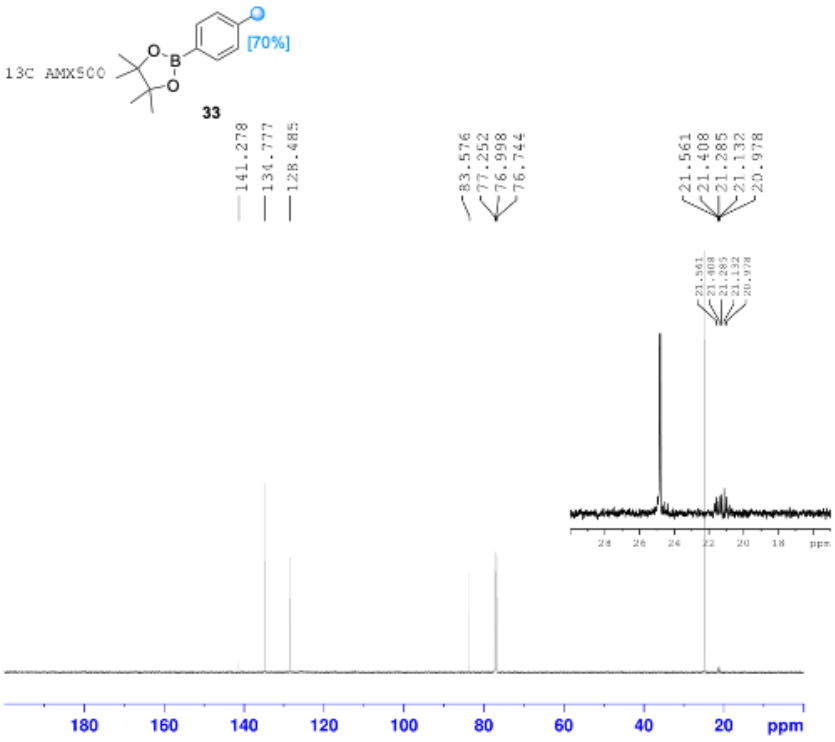
BRUKER

```
Current Data Parameters
NAME      yk0113-ky1-4126-6-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_            20200113
Time             20.42
INSTRUM          spect
PROBHD    5 mm PABBO BB/
PULPROG          zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   0
SWH          10330.578 Hz
FIDRES       0.315264 Hz
AQ           1.5859712 sec
RG                45.3
DW              48.400 usec
DE               6.00 usec
TE              296.8 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                10.50 usec
PL1                0.25 dB
SFO1        500.1330885 MHz

F2 - Processing parameters
SI                16384
SF          500.1300135 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



BRUKER

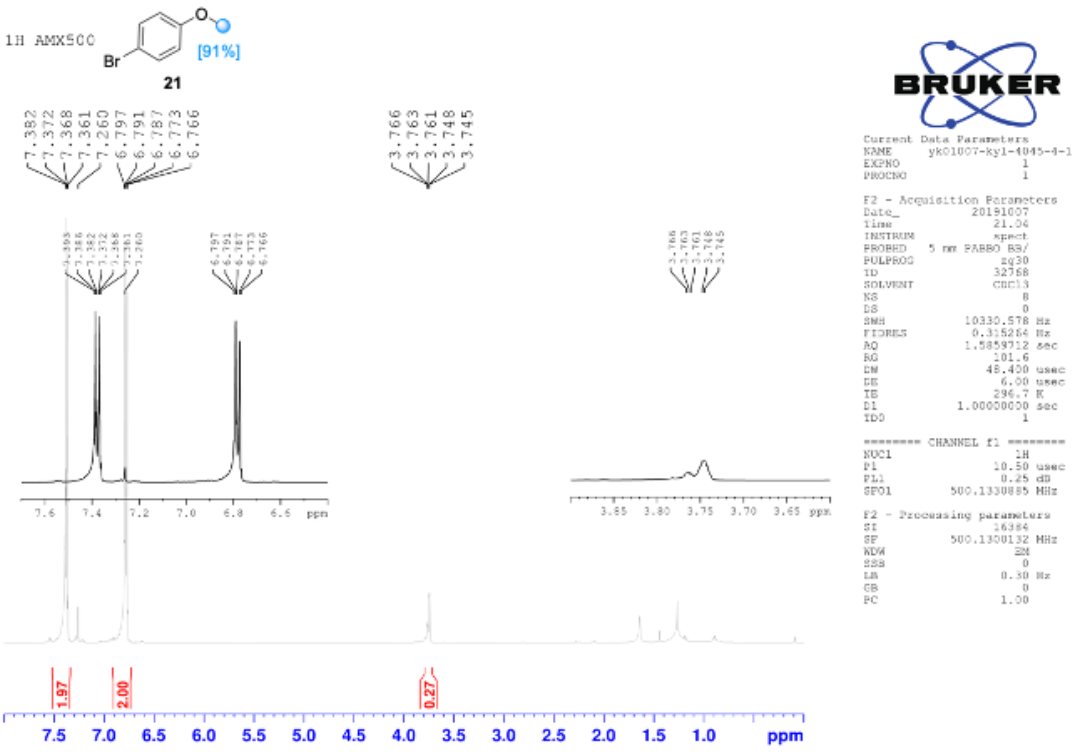
```
Current Data Parameters
NAME      yk0113-ky1-4126-6-1
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_            20200113
Time             23.43
INSTRUM          spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 147
DS                   0
SWH          30030.029 Hz
FIDRES       0.458222 Hz
AQ           1.0911744 sec
RG               16384
DW              16.650 usec
DE               6.00 usec
TE              297.1 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                 20

======== CHANNEL f1 ========
NUC1                13C
P1                8.90 usec
PL1                  0 dB
SFO1        125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2            80.00 usec
PL2                0.25 dB
PL12              17.89 dB
PL13              19.83 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577956 MHz
WDW                  EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```



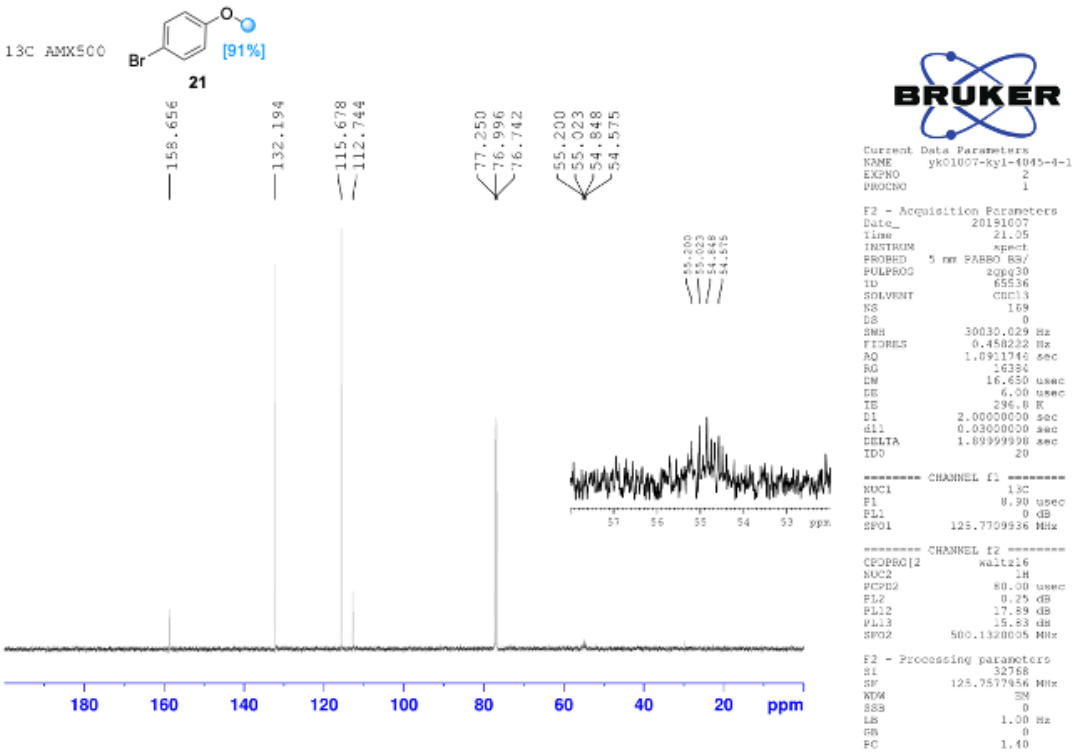
BRUKER

```
Current Data Parameters
NAME      yk01007-ky1-4045-4-1
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_             20191007
Time                21.04
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     0
SWH            10330.578 Hz
FIDRES         0.315264 Hz
AQ             1.5859712 sec
RG                 101.6
DW                48.400 usec
DE                 6.00 usec
TE                296.7 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.50 usec
PL1                0.25 dB
SFO1         500.1330885 MHz

F2 - Processing parameters
SI                 16384
SF           500.1300132 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```



BRUKER

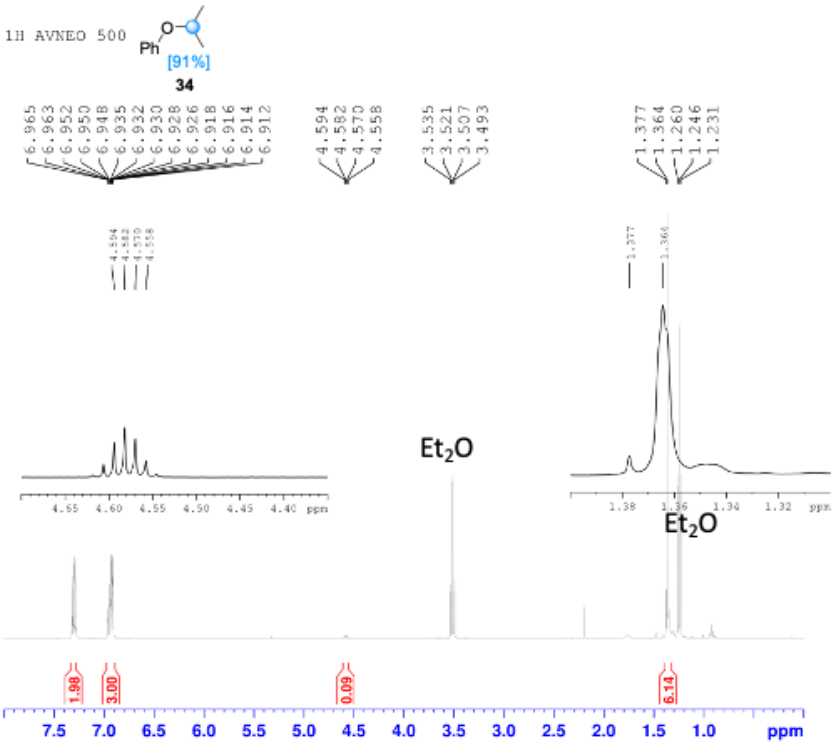
```
Current Data Parameters
NAME      yk01007-ky1-4045-4-1
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_             20191007
Time                21.05
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   169
DS                     0
SWH            30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0911744 sec
RG                 16384
DW                16.650 usec
DE                 6.00 usec
TE                296.8 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.8899999 sec
TD0                   20

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.90 usec
PL1                   0 dB
SFO1         125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.25 dB
PL12               17.19 dB
PL13               15.83 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF           125.7577956 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

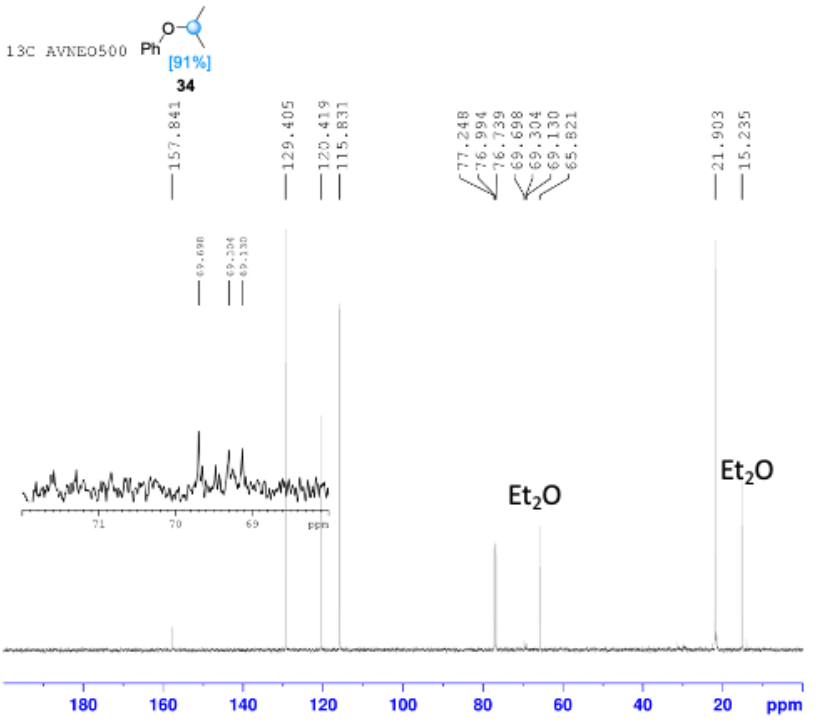


BRUKER

```
Current Data Parameters
NAME        yk0229-ky1-4139-2
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20200229
Time                    10.32 h
INSTRUM                Avance
PROBHD    2169738_0003 (
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                         8
DS                         2
SWH                19000.000 Hz
FIDRES             0.305176 Hz
AQ                 3.2767999 sec
RG                       101
DW                    50.000 usec
DE                    11.14 usec
TE                   298.0 K
D1                 1.00000000 sec
TD0                        1
SFO1            500.1330883 MHz
NUC1                      1H
P0                    2.67 usec
P1                    8.00 usec
PLW1              24.45700073 W

F2 - Processing parameters
SI                     65536
SF            500.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

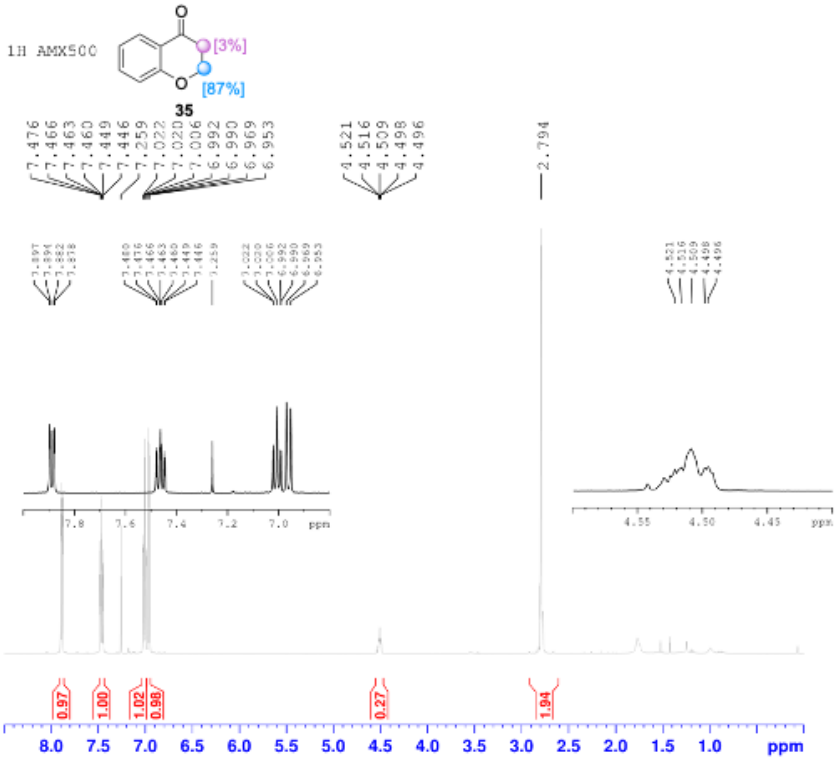


BRUKER

```
Current Data Parameters
NAME        yk0229-ky1-4139-2
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_                20200229
Time                    10.40 h
INSTRUM                Avance
PROBHD    2169738_0003 (
PULPROG                 zgpg
TD                     65536
SOLVENT                CDCl3
NS                       144
DS                         2
SWH                30120.482 Hz
FIDRES             0.919204 Hz
AQ                 1.0878977 sec
RG                       101
DW                    16.600 usec
DE                     6.72 usec
TE                   298.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1            125.7709931 MHz
NUC1                      13C
P1                    9.00 usec
PLW1             110.76999664 W
SFO2            500.1320005 MHz
NUC2                      1H
CPDPRG[2          waltz64
PCPD2                 80.00 usec
PLW2              24.45700073 W
PLW12              0.24457000 W
PLW13              0.12302000 W

F2 - Processing parameters
SI                     65536
SF            125.7577953 MHz
WDW                       EM
SSB                        0
LB                      2.00 Hz
GB                         0
PC                      1.40
```

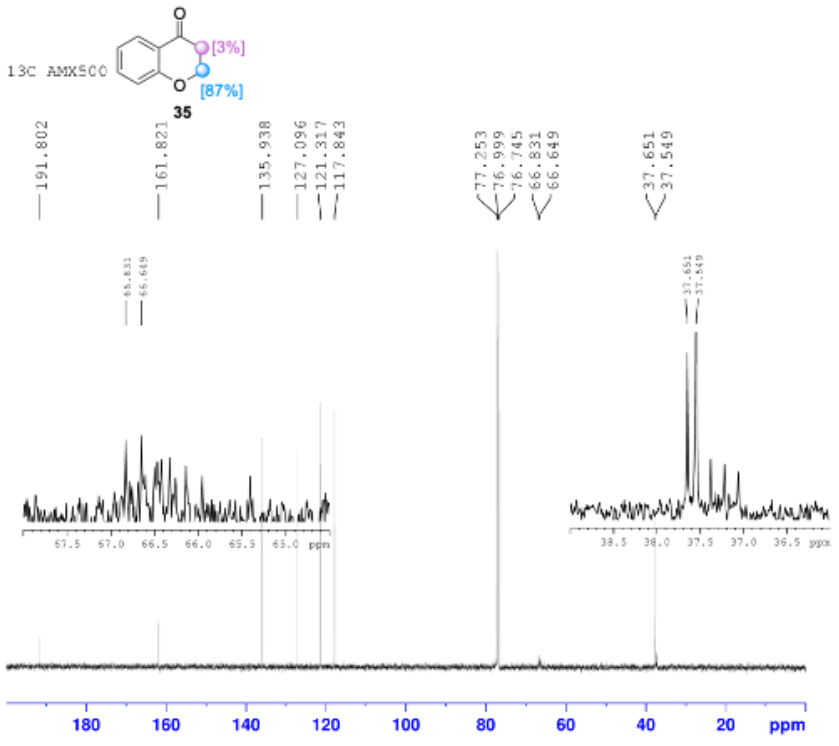


Current Data Parameters
NAME yk1218-kyl-4107-1-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191218
Time 20.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 114
DW 48.400 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



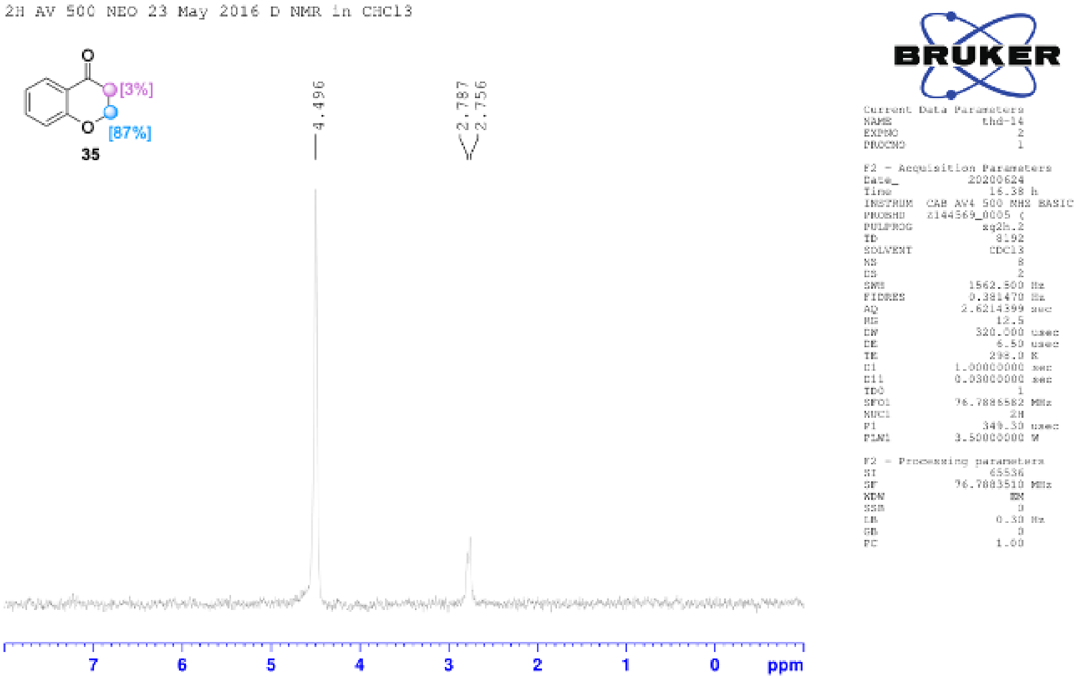
Current Data Parameters
NAME yk1218-kyl-4107-1-1
EXPNO 2
PROCNO 1

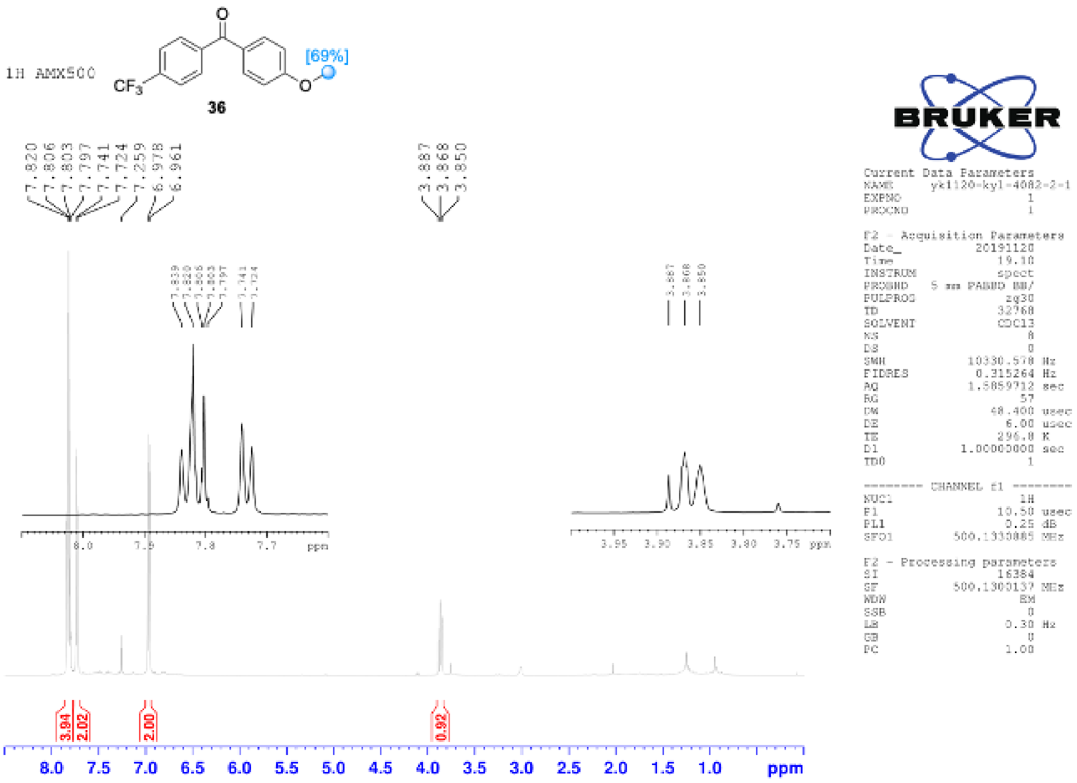
F2 - Acquisition Parameters
Date_ 20191218
Time 20.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 219
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 297.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20

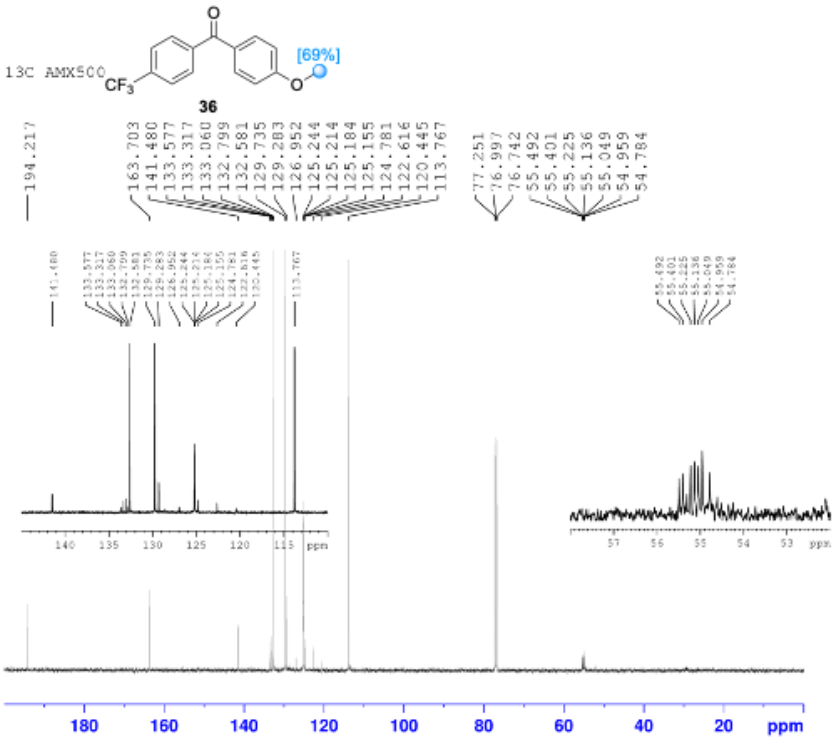
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577947 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


2H AV 500 NEO 23 May 2016 D NMR in CHCl3
[3%]
[87%]
35
4.496
2.787
2.756
BRUKER
ppm


1H AMX500
[69%]
36
BRUKER
3.94
2.02
2.00
0.92
ppm



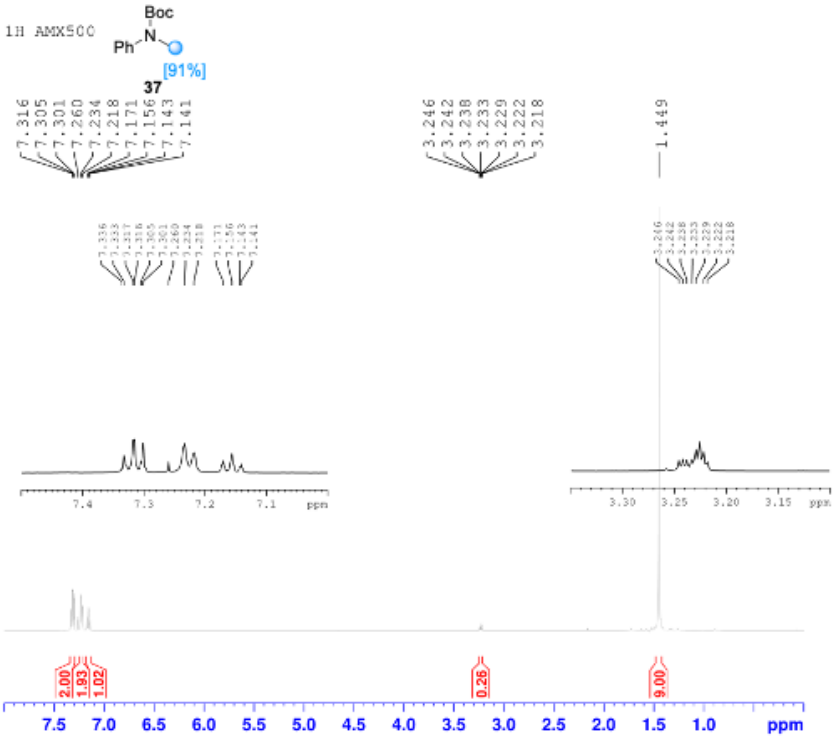
```
Current Data Parameters
NAME      yx1120-kyl-4082-2-1
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191120
Time                 19.11
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     204
DS                       0
SWH              30030.029 Hz
FIDRES           0.458222 Hz
AQ               1.0911744 sec
RG                   16384
DW                  16.650 usec
DE                   6.00 usec
TE                  297.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                     20

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.90 usec
PL1                      0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                   0.25 dB
PL12                 17.89 dB
PL13                 15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                   32768
SF            125.7577955 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

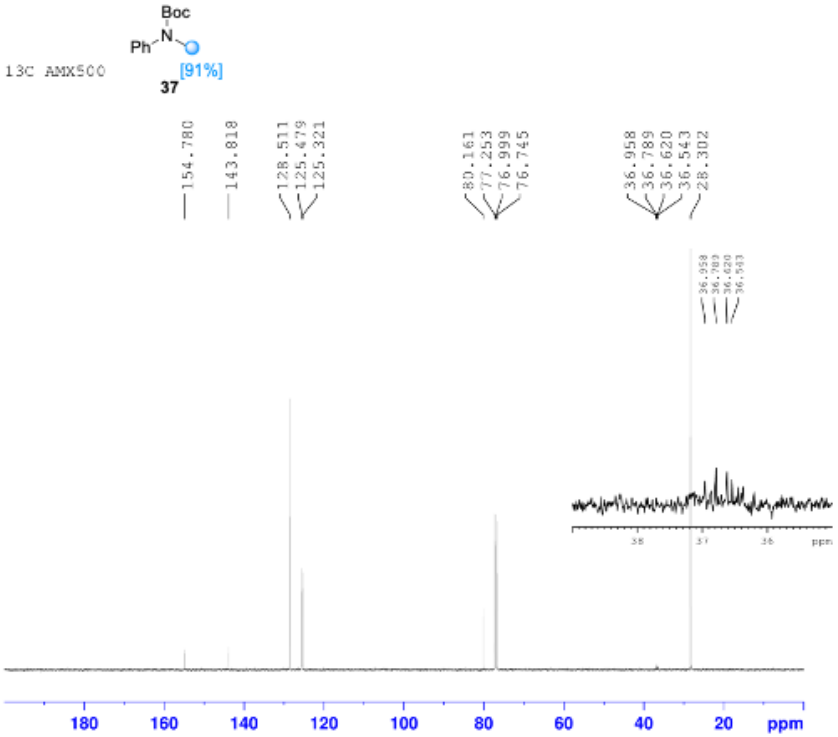


```
Current Data Parameters
NAME      yx1003-kyl-4042-5-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191003
Time                 19.28
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH              10330.578 Hz
FIDRES           0.315264 Hz
AQ               1.5859712 sec
RG                      64
DW                  48.400 usec
DE                   6.00 usec
TE                  300.0 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   1H
P1                   10.50 usec
PL1                   0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                   16384
SF            500.1300135 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



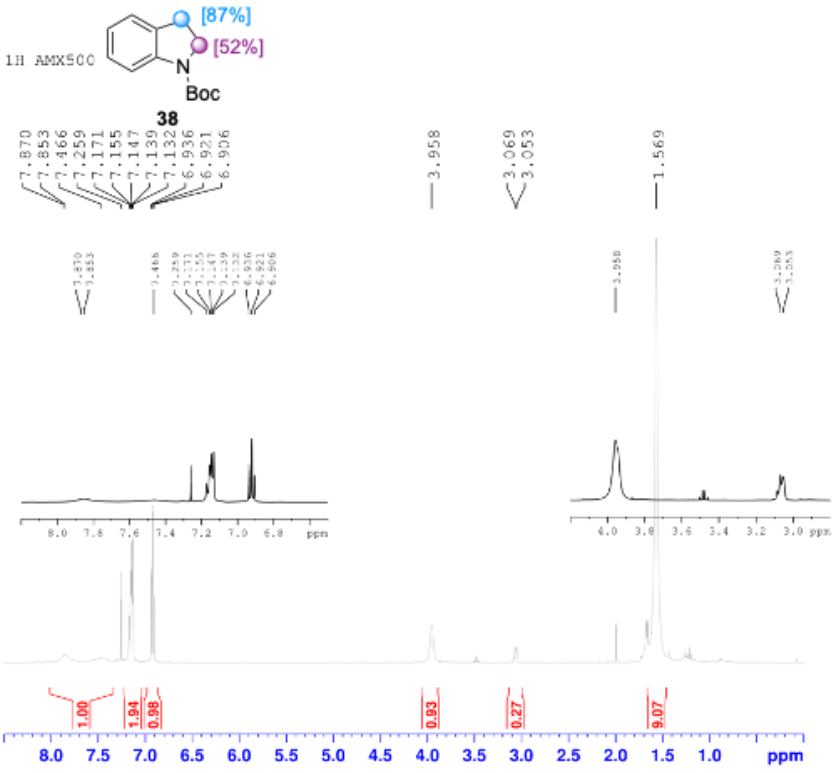
```
Current Data Parameters
NAME        yk1003-kyl-4042-S-1
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_              20191003
Time                   19.29
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     259
DS                       0
SWH              30030.029 Hz
FIDRES           0.458222 Hz
AQ               1.0911744 sec
RG                   16384
DW                  16.650 usec
DE                   6.00 usec
TE                  301.3 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                     20

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.90 usec
PL1                      0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.25 dB
PL12                 17.89 dB
PL13                 15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                     32768
SF            125.7577937 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                      1.40
```

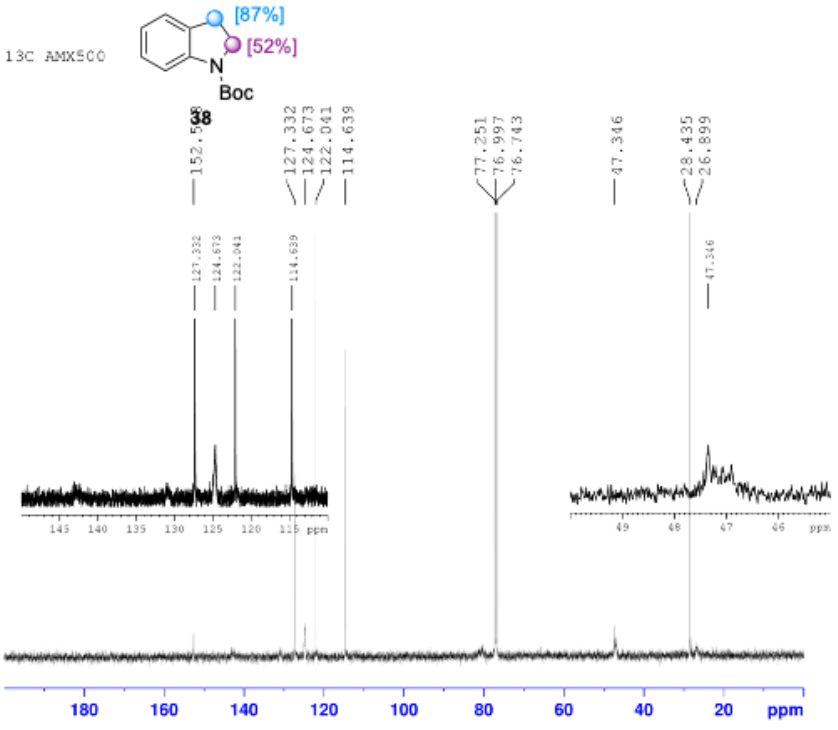


```
Current Data Parameters
NAME        yk1219-kyl-4106-1-1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20191220
Time                   10.54
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH              10330.578 Hz
FIDRES           0.315264 Hz
AQ               1.5859712 sec
RG                    71.8
DW                  48.400 usec
DE                   6.00 usec
TE                  296.5 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.50 usec
PL1                   0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                     16384
SF            500.1300137 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                      1.00
```



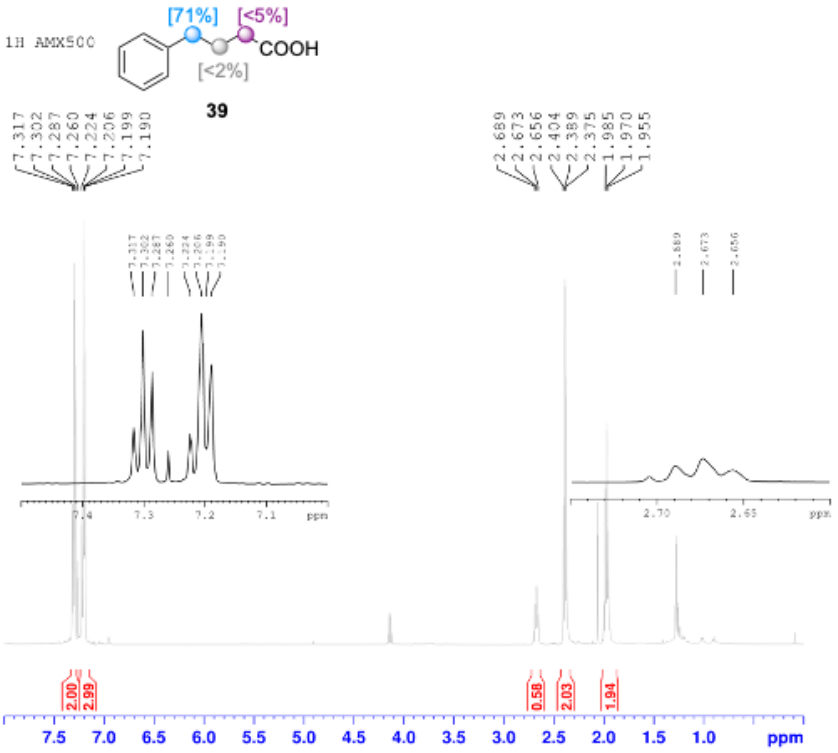

```
Current Data Parameters
NAME      yx1219-kyl-4106-1-1
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191220
Time                  10.56
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     532
DS                       0
SWH              30030.029 Hz
FIDRES           0.458222 Hz
AQ               1.0911744 sec
RG                   16384
DW                16.650 usec
DE                 6.00 usec
TE                 296.9 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     20

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.90 usec
PL1                      0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                   0.25 dB
PL12                 17.89 dB
PL13                 15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                   32768
SF            125.7577954 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

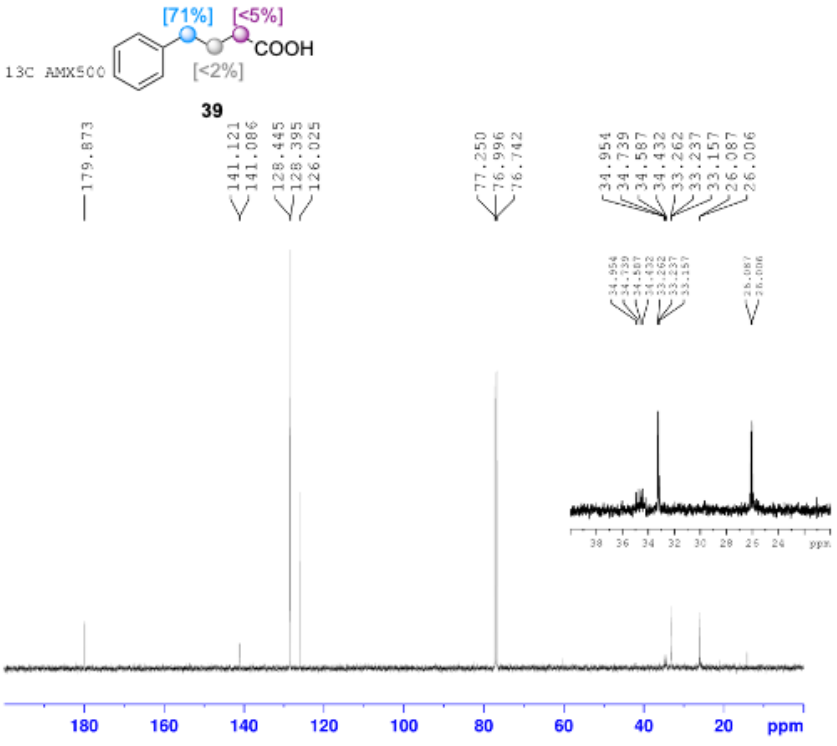



```
Current Data Parameters
NAME      yx1011-kyl-4053-2-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191011
Time                  17.56
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH              10330.578 Hz
FIDRES           0.315264 Hz
AQ               1.5859712 sec
RG                    71.8
DW                48.400 usec
DE                 6.00 usec
TE                 295.7 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   1H
P1                   10.50 usec
PL1                   0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                   16384
SF            500.1300133 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



```
Current Data Parameters
NAME        yk1011-kyl-4053-2-1
EXPNO                         4
PROCNO                        1

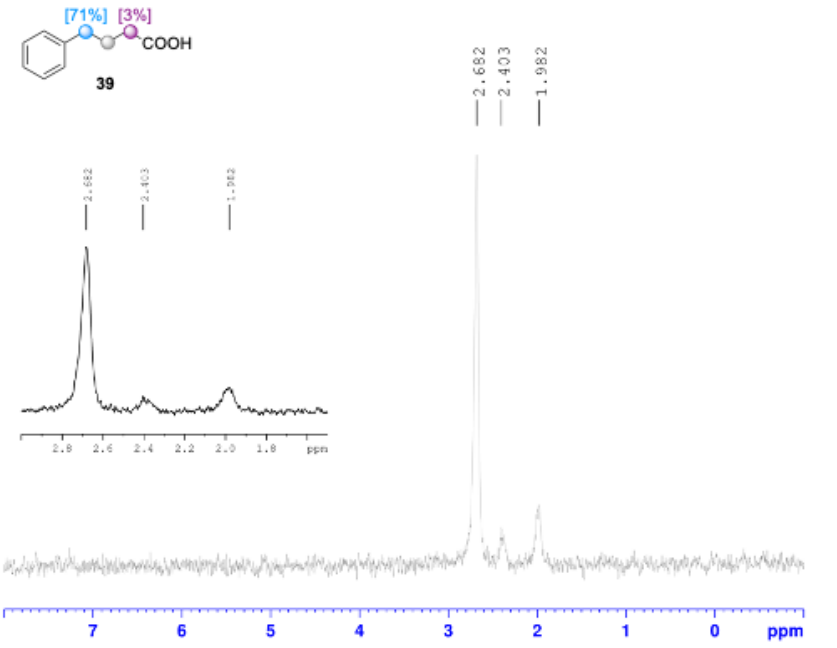
F2 - Acquisition Parameters
Date_                  20191011
Time                      20.51
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                          101
DS                            0
SWH                   30030.029 Hz
FIDRES                0.458222 Hz
AQ                    1.0911744 sec
RG                        16384
DW                       16.650 usec
DE                        6.00 usec
TE                       297.0 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                           20

======== CHANNEL f1 ========
NUC1                        13C
P1                         8.90 usec
PL1                           0 dB
SFO1                125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                        1H
PCPD2                     80.00 usec
PL2                        0.25 dB
PL12                      17.89 dB
PL13                      15.83 dB
SFO2                500.1320005 MHz

F2 - Processing parameters
SI                        32768
SF                  125.7577955 MHz
WDW                        EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40
```

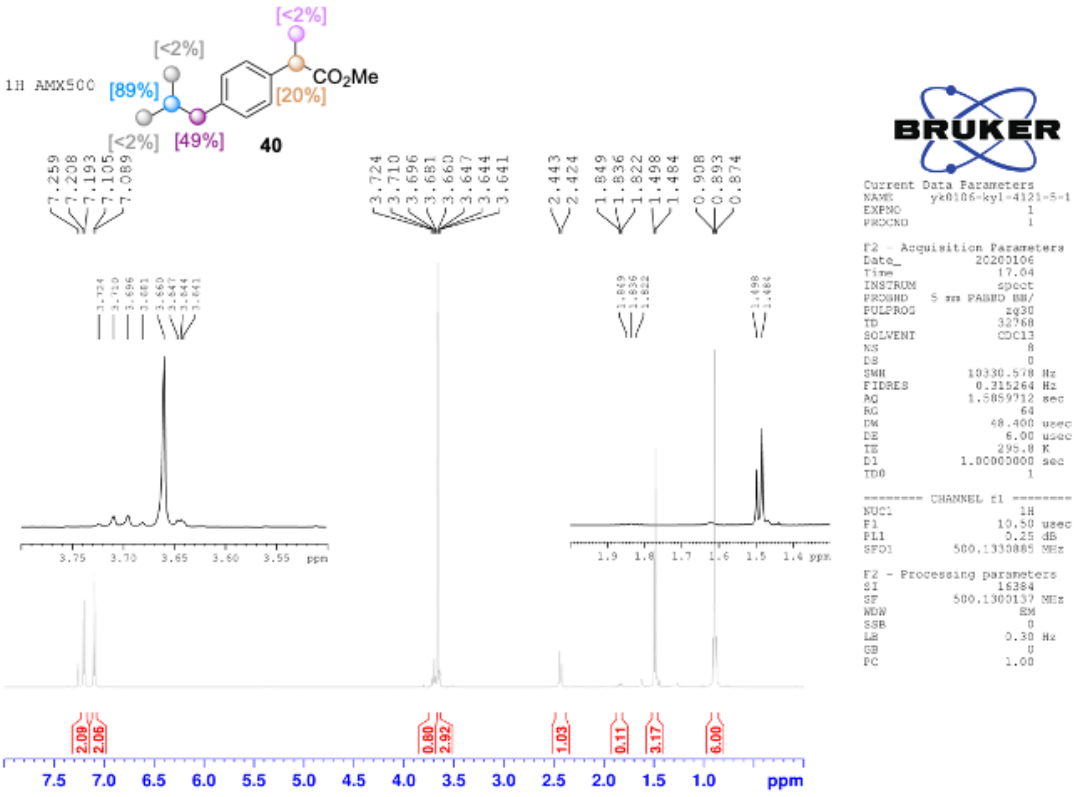
2H AV 500 NEO 23 May 2017 D NMR in CHCl3



```
Current Data Parameters
NAME                      thd-15
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                  20200624
Time                      15.40 h
INSTRUM   CAB AV4 500 MHz BASIC
PROBHD    Z144369_0005 (
PULPROG                zg2h.2
TD                          8192
SOLVENT                   CDCl3
NS                             8
DS                             2
SWH                   1562.500 Hz
FIDRES                0.381470 Hz
AQ                    2.6214399 sec
RG                          12.5
DW                      320.000 usec
DE                        6.50 usec
TE                       298.0 K
D1                    1.00000000 sec
D11                   0.03000000 sec
TD0                            1
SFO1                76.7885582 MHz
NUC1                          2H
P1                        349.30 usec
PLW1                  3.50000000 W

F2 - Processing parameters
SI                        65536
SF                  76.7883469 MHz
WDW                        EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

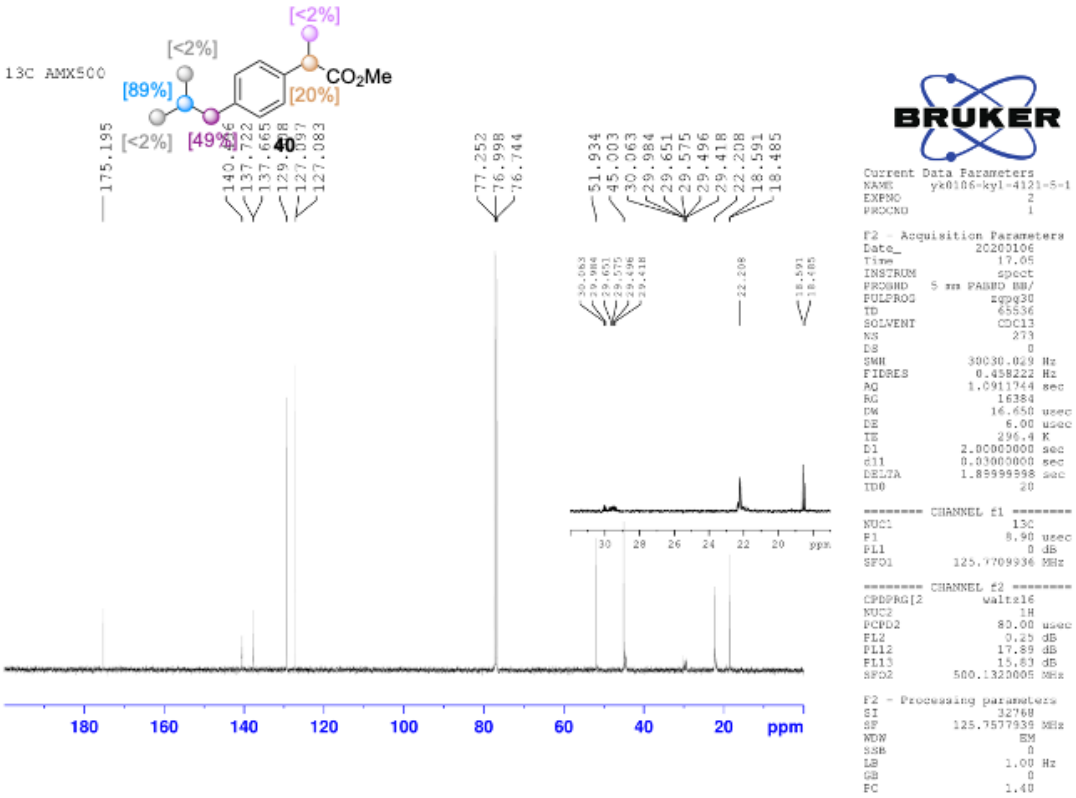


Current Data Parameters
NAME yk0106-kyl-4121-S-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200106
Time 17.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 64
DW 48.400 usec
DE 6.00 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME yk0106-kyl-4121-S-1
EXPNO 2
PROCNO 1

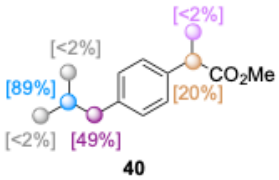
F2 - Acquisition Parameters
Date_ 20200106
Time 17.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 273
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 296.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20

======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

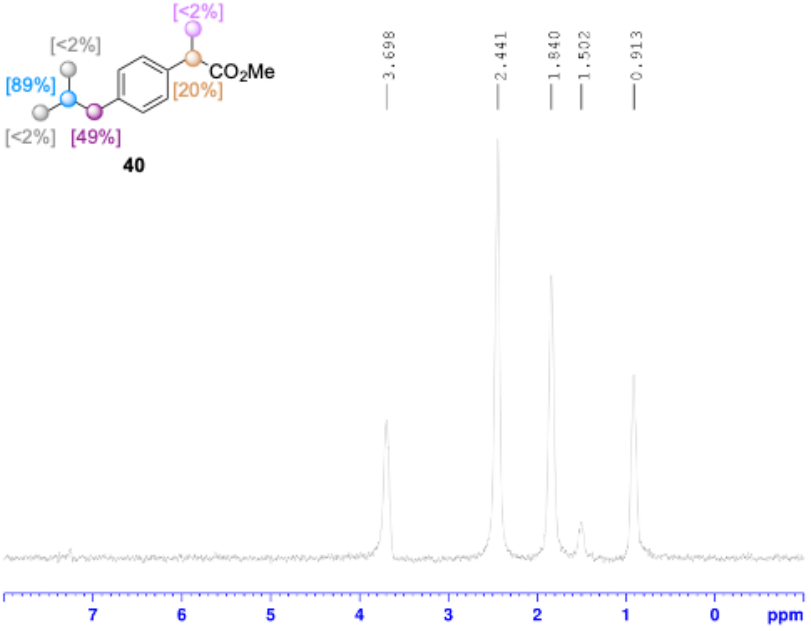
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577939 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2H AV 500 NEO 23 May 2017 D NMR in CHCl3



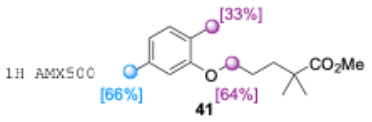
40



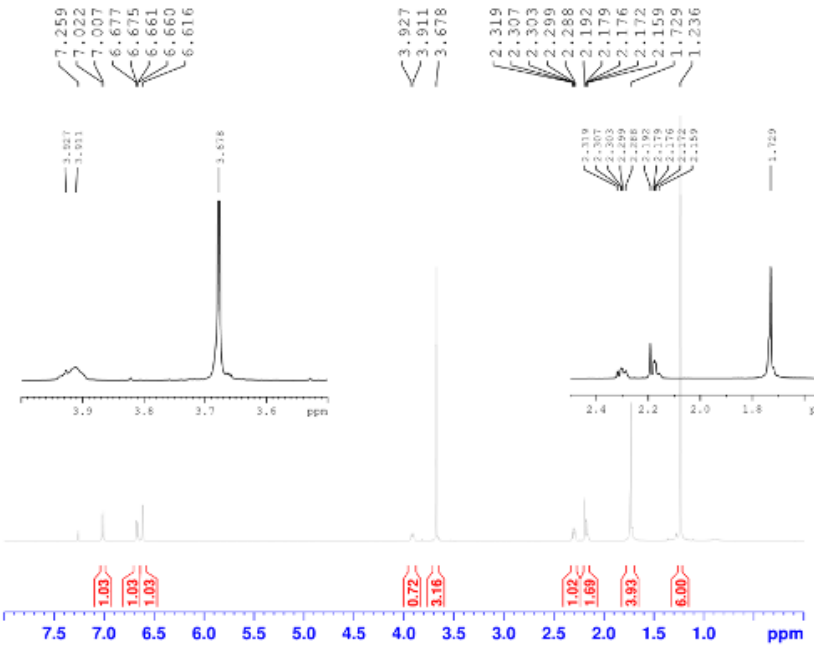
```
Current Data Parameters
NAME                  thd-16
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20200623
Time                  15.16 h
INSTRUM   CAB AV4 500 MHz BASIC
PROBHD    2144569_0005 (
PULPROG              zg2h.2
TD                     8192
SOLVENT               DMSO
NS                       16
DS                        2
SWH                1562.500 Hz
FIDRES             0.381470 Hz
AQ                 2.6214399 sec
RG                    13.8889
DW                   320.000 usec
DE                     6.50 usec
TE                   298.0 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                       1
SFO1               76.7886582 MHz
NUC1                     2H
P1                    349.30 usec
PLW1               3.50000000 W

F2 - Processing parameters
SI                       65536
SF                 76.7883264 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



41

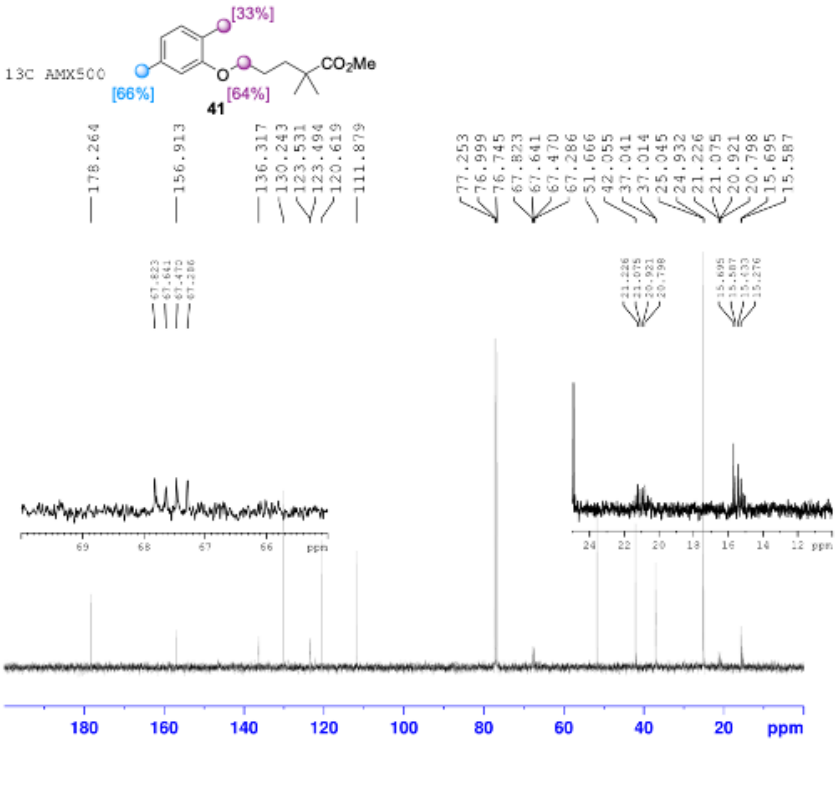


```
Current Data Parameters
NAME          ye0220-kyl-4059-2
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20200220
Time                  16.35
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH                10330.578 Hz
FIDRES             0.315264 Hz
AQ                 1.5859712 sec
RG                     45.3
DW                   48.400 usec
DE                     6.00 usec
TE                   296.1 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    10.50 usec
PL1                    0.25 dB
SFO1              500.1330885 MHz

F2 - Processing parameters
SI                       16384
SF                500.1300137 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



BRUKER

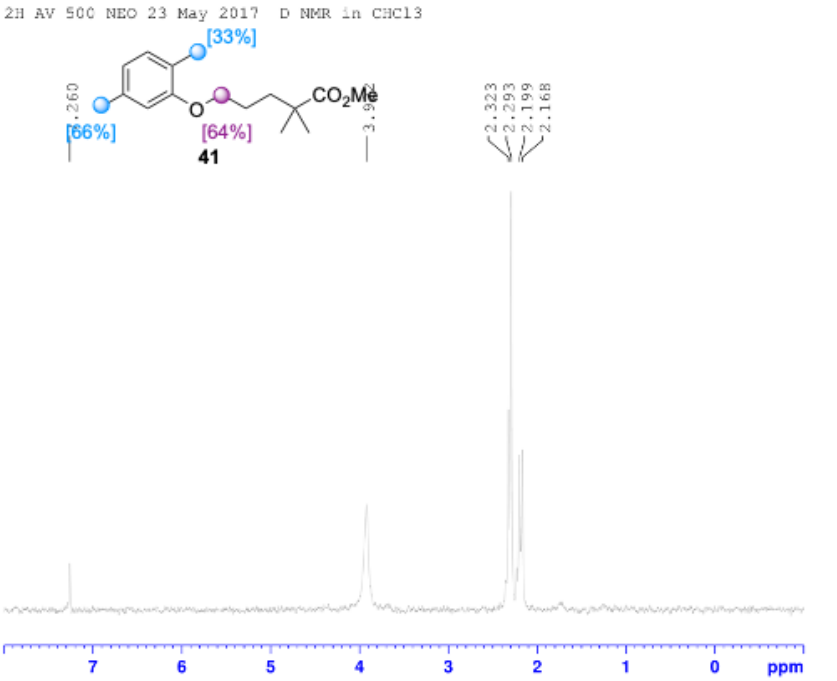
```
Current Data Parameters
NAME      yk0220-kyl-4059-2
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200220
Time                  16.56
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      72
DS                       0
SWH              30030.029 Hz
FIDRES           0.458222 Hz
AQ               1.0911744 sec
RG                   16384
DW                16.650 usec
DE                 6.00 usec
TE                 296.2 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      20

======== CHANNEL f1 ========
NUC1                    13C
P1                   8.90 usec
PL1                     0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2            waltz16
NUC2                    1H
PCPD2               80.00 usec
PL2                  0.25 dB
PL12                17.89 dB
PL13                15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                   32768
SF            125.7577975 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

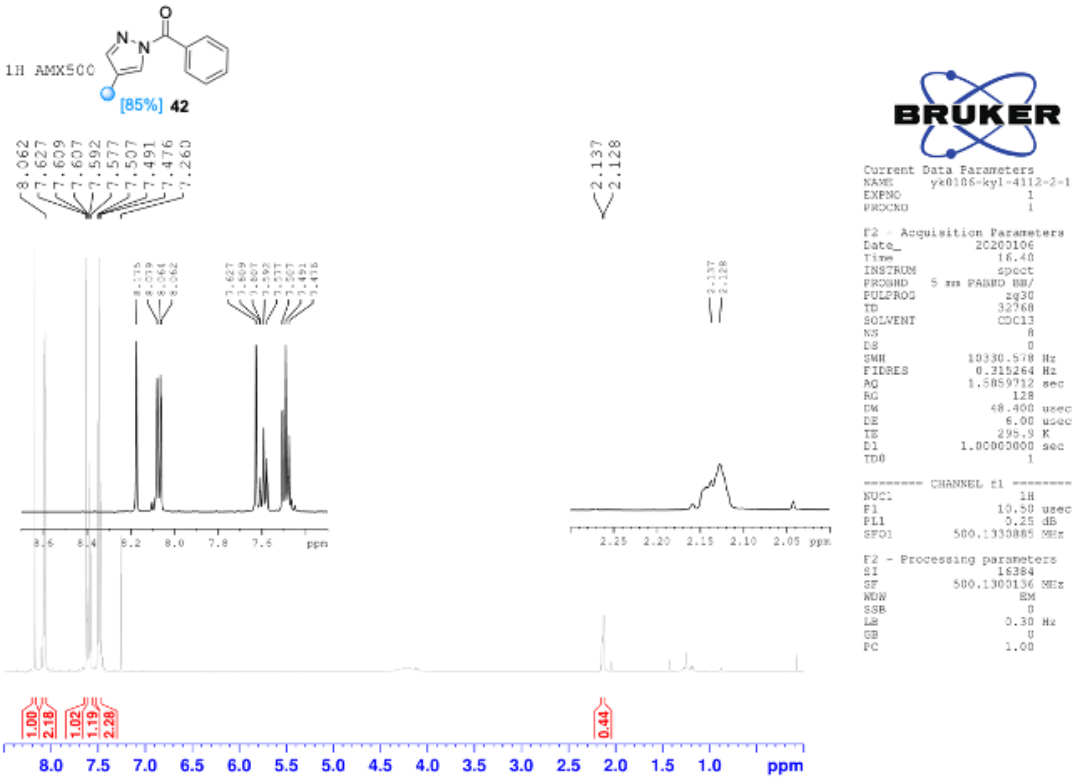


BRUKER

```
Current Data Parameters
NAME                  thd-17
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20200624
Time                  15.42 h
INSTRUM  CAB AV4 500 MHz BASIC
PROBHD   Z144369_0005 (
PULPROG             zg2h.2
TD                    8192
SOLVENT              CDCl3
NS                       8
DS                       2
SWH              1562.500 Hz
FIDRES           0.381470 Hz
AQ               2.6214399 sec
RG                    12.5
DW                320.000 usec
DE                  6.50 usec
TE                  298.0 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                      1
SFO1          76.7885582 MHz
NUC1                    2H
P1                 349.30 usec
PLW1            3.50000000 W

F2 - Processing parameters
SI                   65536
SF            76.7883480 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



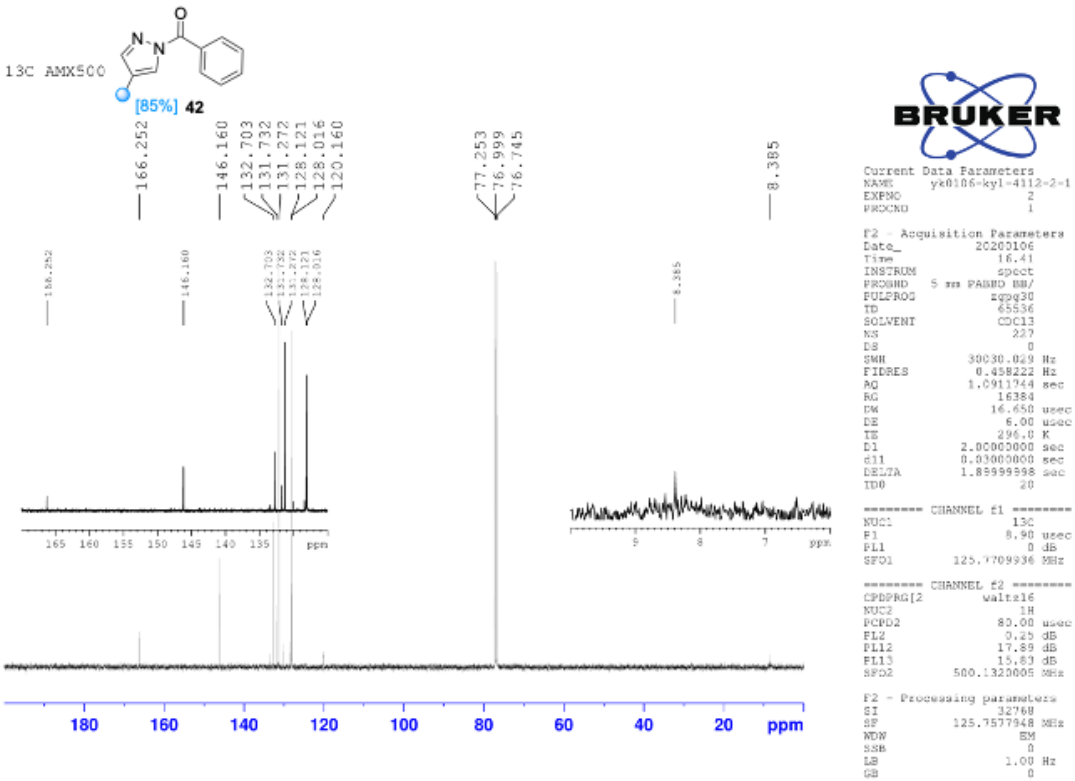
BRUKER

```
Current Data Parameters
NAME      ye0106-ky1-4112-2-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20200106
Time                  16.40
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH               10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                      128
DW                   48.400 usec
DE                    6.00 usec
TE                   295.9 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.50 usec
PL1                     0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                    16384
SF            500.1300136 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



BRUKER

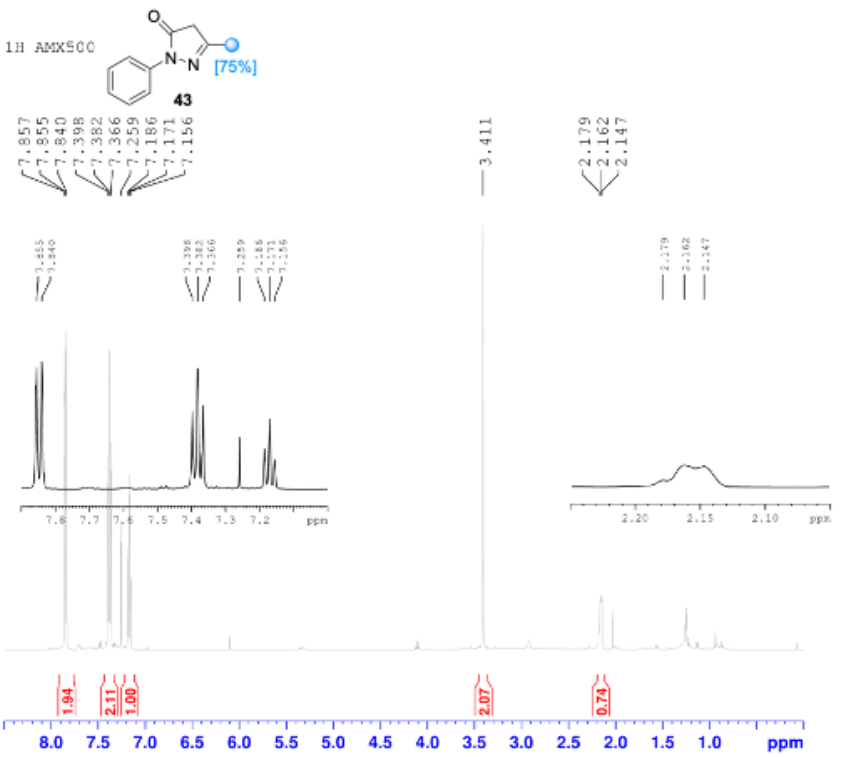
```
Current Data Parameters
NAME      ye0106-ky1-4112-2-1
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20200106
Time                  16.41
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      227
DS                        0
SWH               30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0911744 sec
RG                    16384
DW                   16.650 usec
DE                    6.00 usec
TE                   296.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      20

======== CHANNEL f1 ========
NUC1                      13C
P1                     8.90 usec
PL1                       0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     0.25 dB
PL12                   17.89 dB
PL13                   15.63 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                    32768
SF            125.7577948 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```



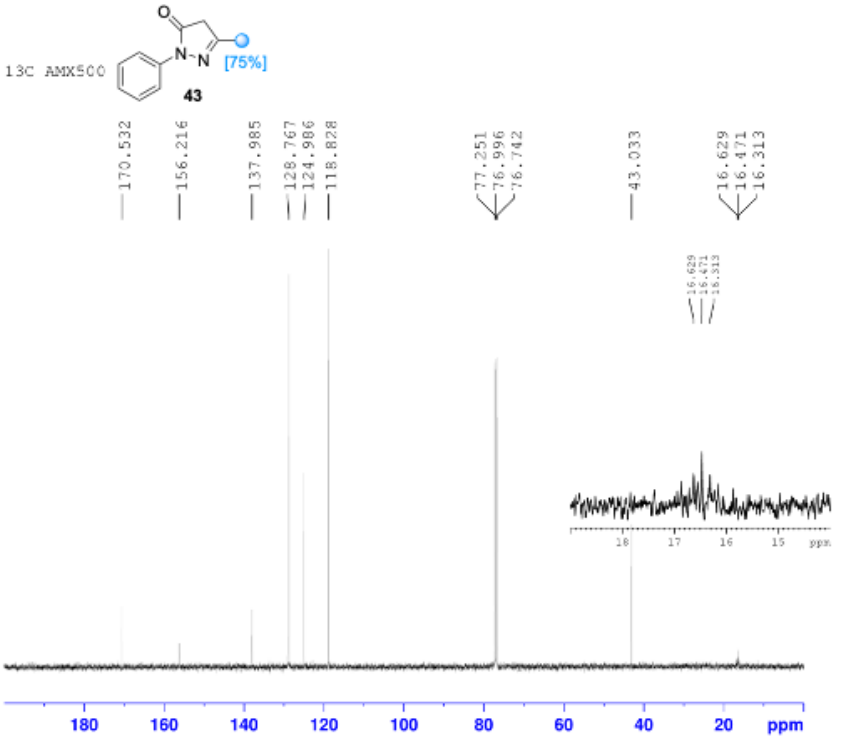
BRUKER

```
Current Data Parameters
NAME      yx1130-kyl-4087-4-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191130
Time                  16.24
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH               10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                     90.5
DW                   48.400 usec
DE                    6.00 usec
TE                   296.1 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.50 usec
PL1                     0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                    16384
SF            500.1300139 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



BRUKER

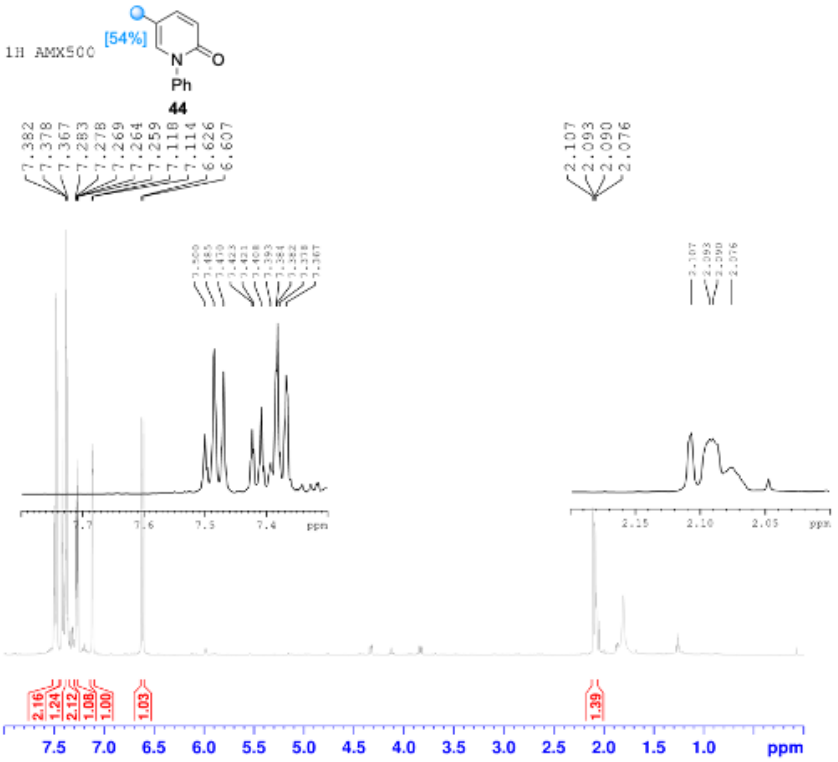
```
Current Data Parameters
NAME      yx1130-kyl-4087-4-1
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191130
Time                  16.25
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      179
DS                        0
SWH               30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0911744 sec
RG                    16384
DW                   16.650 usec
DE                    6.00 usec
TE                   296.4 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      20

======== CHANNEL f1 ========
NUC1                     13C
P1                     8.90 usec
PL1                       0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2                    0.25 dB
PL12                  17.89 dB
PL13                  15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                    32768
SF            125.7577973 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```



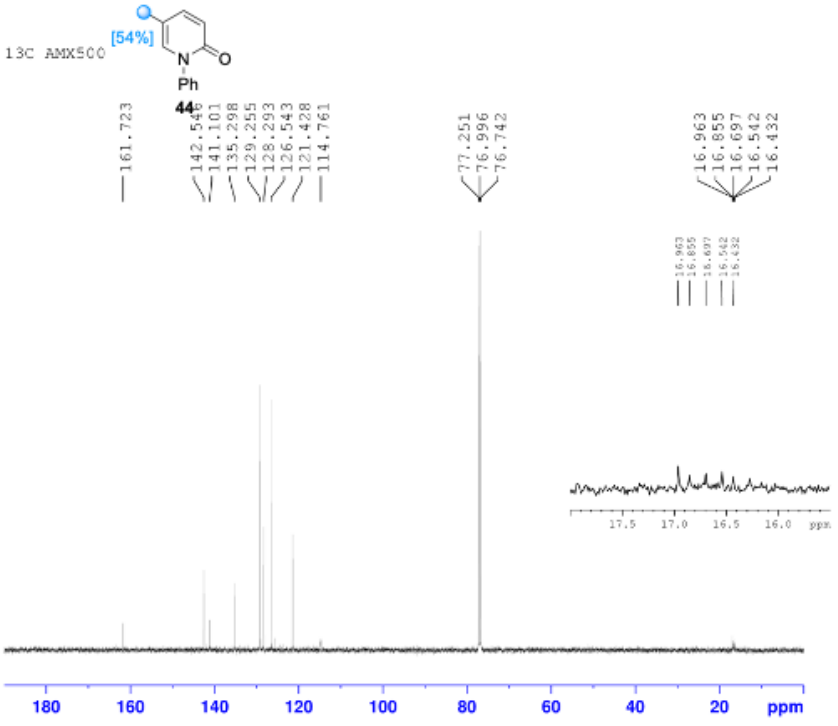
BRUKER

```
Current Data Parameters
NAME      yx1227-kyl-4115-7-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191227
Time                  12.00
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH               10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                    143.7
DW                   48.400 usec
DE                    6.00 usec
TE                  295.8 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.50 usec
PL1                     0.25 dB
SFO1           500.1330885 MHz

F2 - Processing parameters
SI                    16384
SF             500.1300093 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



BRUKER

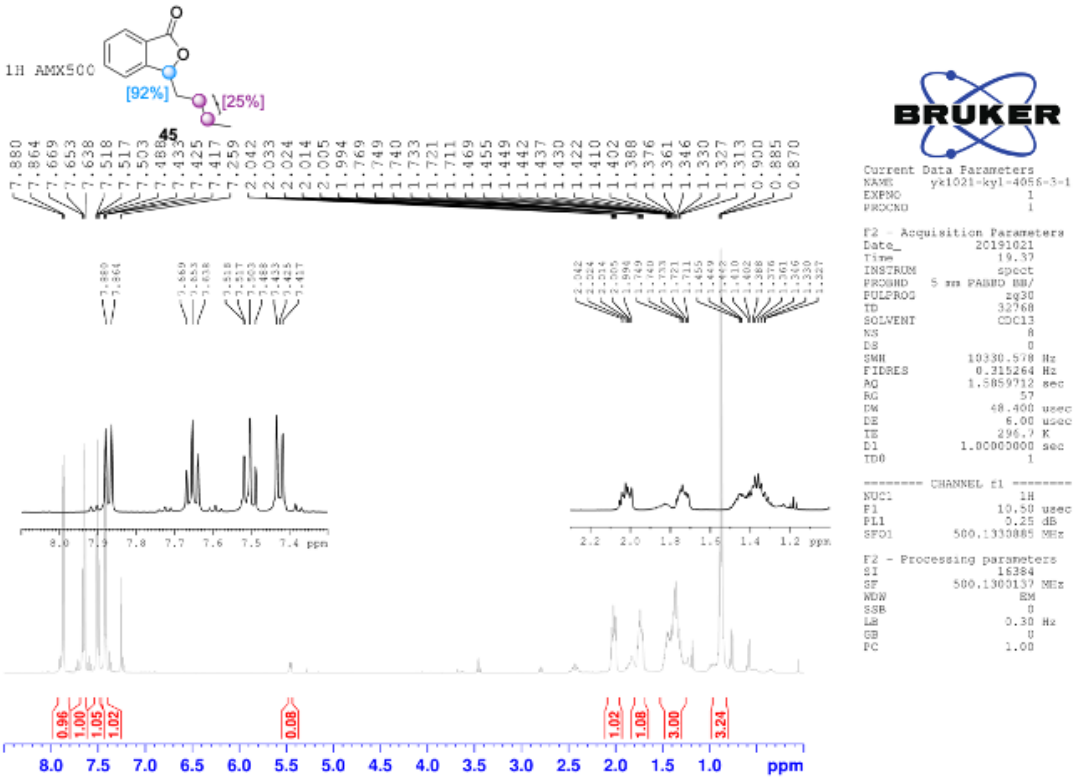
```
Current Data Parameters
NAME      yx1227-kyl-4115-7-1
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191227
Time                  12.01
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      306
DS                        0
SWH               30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0911744 sec
RG                    16384
DW                   16.650 usec
DE                    6.00 usec
TE                  295.9 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      20

======== CHANNEL f1 ========
NUC1                     13C
P1                     8.90 usec
PL1                       0 dB
SFO1           125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2            waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2                     0.25 dB
PL12                   17.89 dB
PL13                   15.63 dB
SFO2           500.1320005 MHz

F2 - Processing parameters
SI                    32768
SF             125.7577955 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

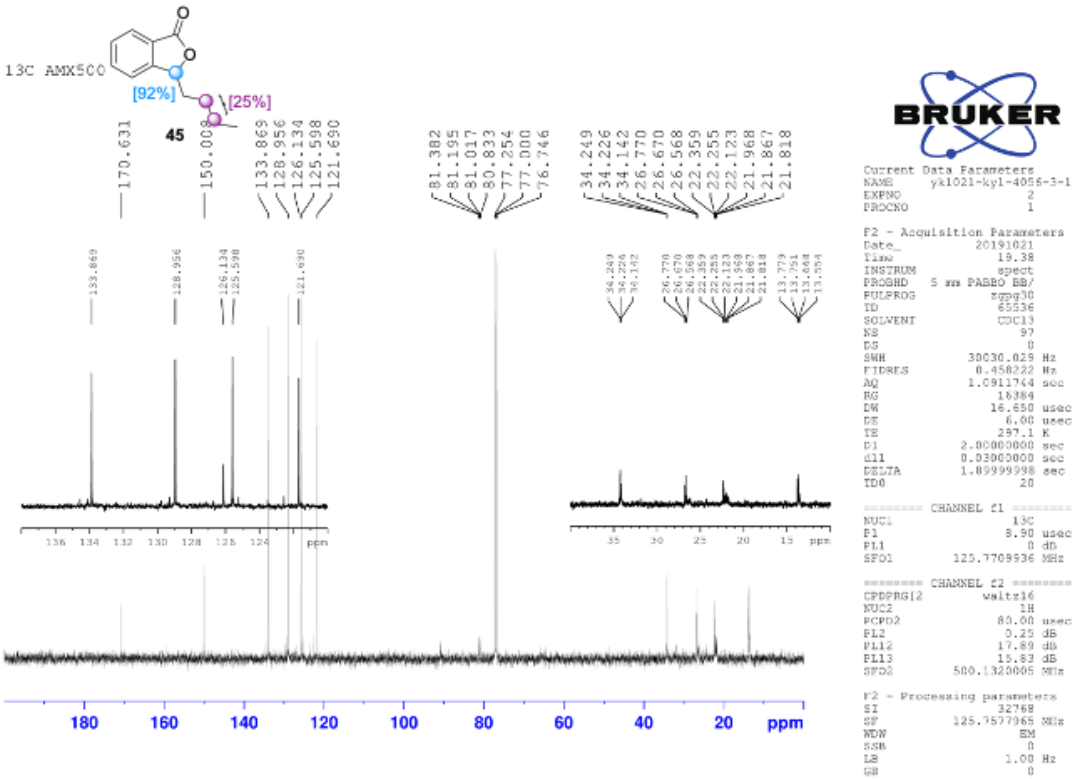



```
Current Data Parameters
NAME      yk1021-ky1-4056-3-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191021
Time                   19.57
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH              10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                       57
DW                  48.400 usec
DE                   6.00 usec
TE                  296.9 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    10.50 usec
PL1                    0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                    16384
SF          500.1300137 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```




```
Current Data Parameters
NAME      yk1021-ky1-4056-3-1
EXPNO                       2
PROCNO                      1

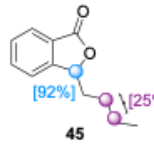
F2 - Acquisition Parameters
Date_              20191021
Time                   19.38
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       97
DS                        0
SWH              30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0911744 sec
RG                    16384
DW                  16.650 usec
DE                   6.00 usec
TE                  297.1 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      20

======== CHANNEL f1 ========
NUC1                    13C
P1                     8.90 usec
PL1                       0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                    0.25 dB
PL12                  17.89 dB
PL13                  19.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                    32768
SF          125.7577965 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

2H AV 500 NEO 23 May 2017 D NMR in CHCl3



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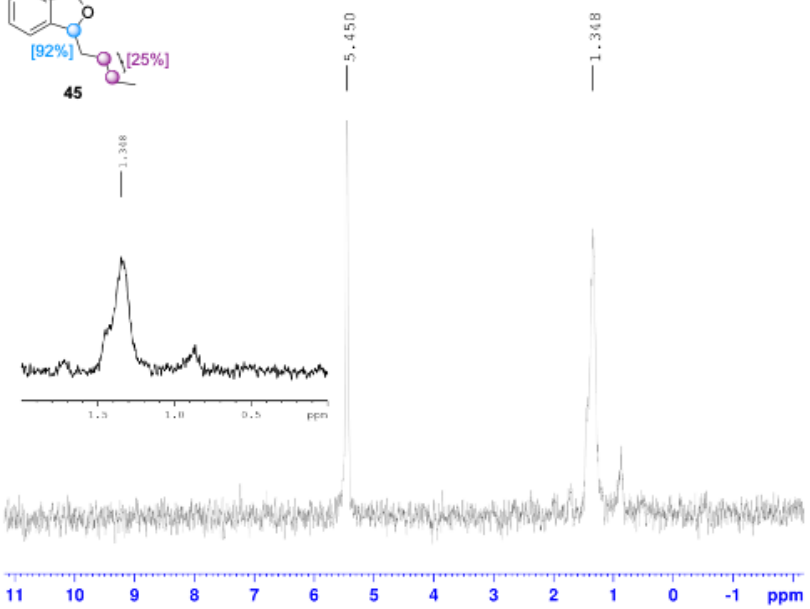
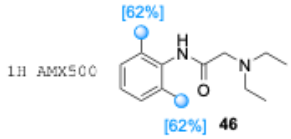


```
Current Data Parameters
NAME                 thd-20
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200624
Time                 15.48 h
INSTRUM   CAB AV4 500 MHz BASIC
PROBHD    2144369_0005 (
PULPROG              zg2h.2
TD                     8192
SOLVENT               CDCl3
NS                        8
DS                        2
SWH               1562.500 Hz
FIDRES            0.381470 Hz
AQ                2.6214399 sec
RG                     12.5
DW                320.000 usec
DE                  6.50 usec
TE                  298.0 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1             76.7886582 MHz
NUC1                     2H
P1                  349.30 usec
PLW1             3.50000000 W

F2 - Processing parameters
SI                    65536
SF               76.7883510 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



1H AMX500

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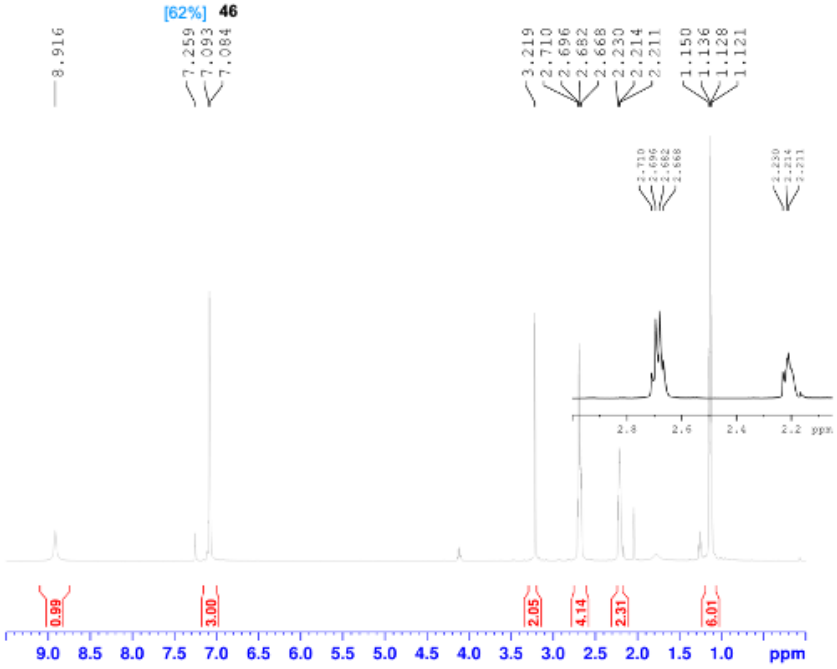


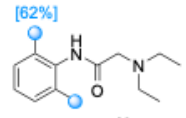
```
Current Data Parameters
NAME      ye1224-ky1-4113-2-1
EXPNO                     1
PROCNO                    1

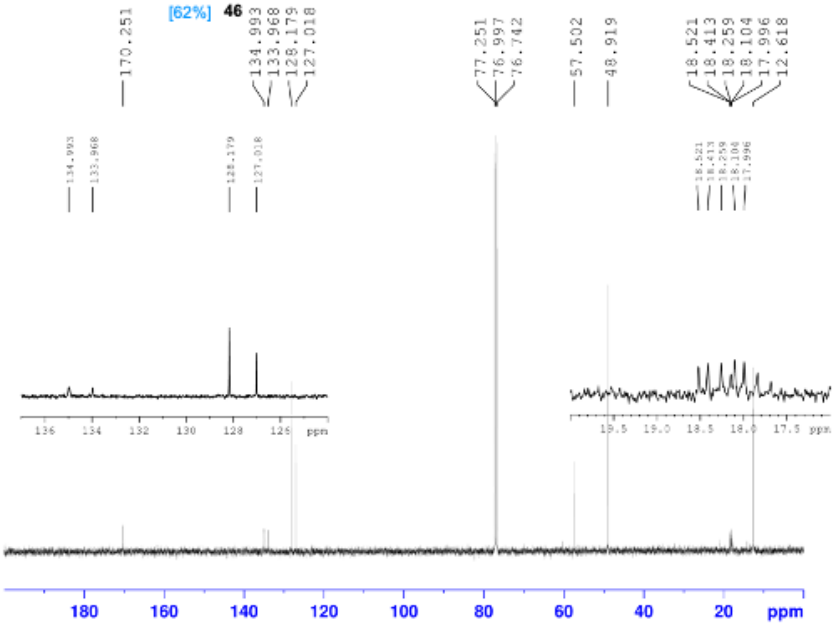
F2 - Acquisition Parameters
Date_              20191224
Time                 20.14
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                   32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH              10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                     80.6
DW                48.400 usec
DE                  6.00 usec
TE                  296.7 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                  10.50 usec
PL1                  0.25 dB
SFO1            500.1330885 MHz

F2 - Processing parameters
SI                    16384
SF              500.1300159 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

13C AMX500





BRUKER

```
Current Data Parameters
NAME      yk1224-kyl-4113-2-1
EXPNO                       2
PROCNO                      1

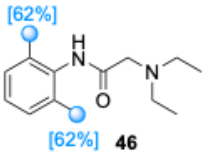
F2 - Acquisition Parameters
Date_              20191224
Time                   20.15
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      159
DS                        0
SWH               30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0911744 sec
RG                    16384
DW                   16.650 usec
DE                    6.00 usec
TE                   296.8 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      20

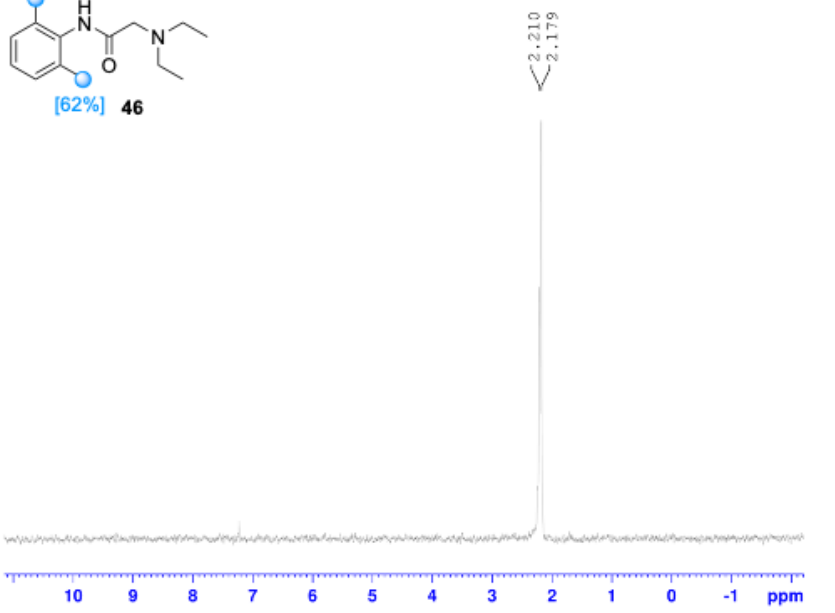
======== CHANNEL f1 ========
NUC1                    13C
P1                     8.90 usec
PL1                       0 dB
SFO1           125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                    0.25 dB
PL12                  17.89 dB
PL13                  15.83 dB
SFO2           500.1320005 MHz

F2 - Processing parameters
SI                     32768
SF            125.7577954 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

2H AV 500 NEO 23 May 2017 D NMR in CHCl3



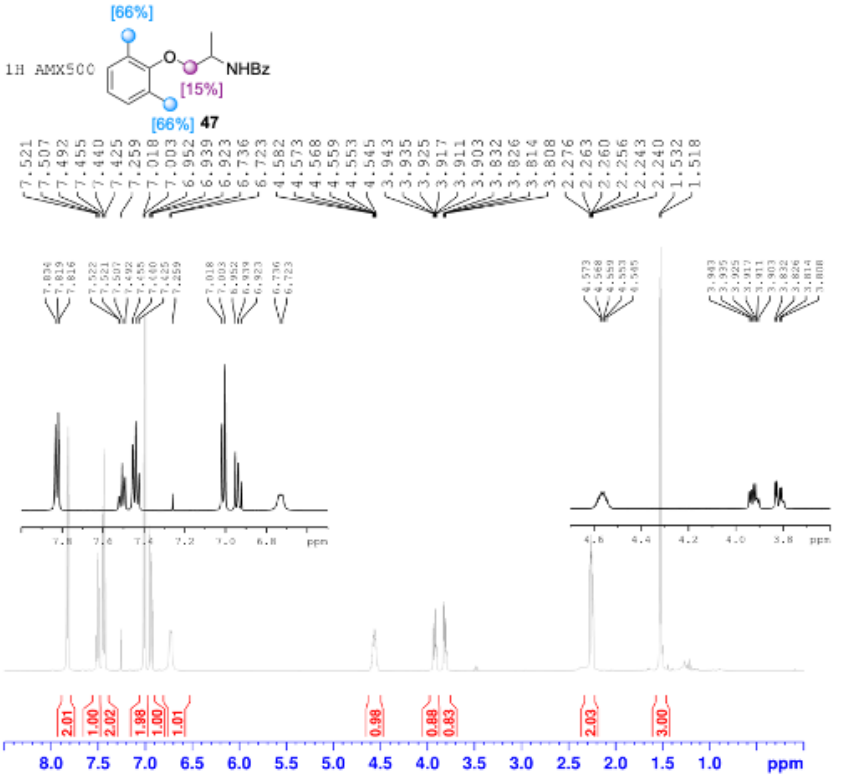


BRUKER

```
Current Data Parameters
NAME                  thd-18
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20200624
Time                  15.43 h
INSTRUM  CAB AV4 500 MHz BASIC
PROBHD   Z144369_0005 (
PULPROG              zg2h.2
TD                     8192
SOLVENT               CDCl3
NS                        8
DS                        2
SWH               1562.500 Hz
FIDRES            0.381470 Hz
AQ                2.6214399 sec
RG                   14.4544
DW                  320.000 usec
DE                    6.50 usec
TE                   298.0 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1           76.7885582 MHz
NUC1                      2H
P1                   349.30 usec
PLW1              3.50000000 W

F2 - Processing parameters
SI                     65536
SF            76.7883510 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



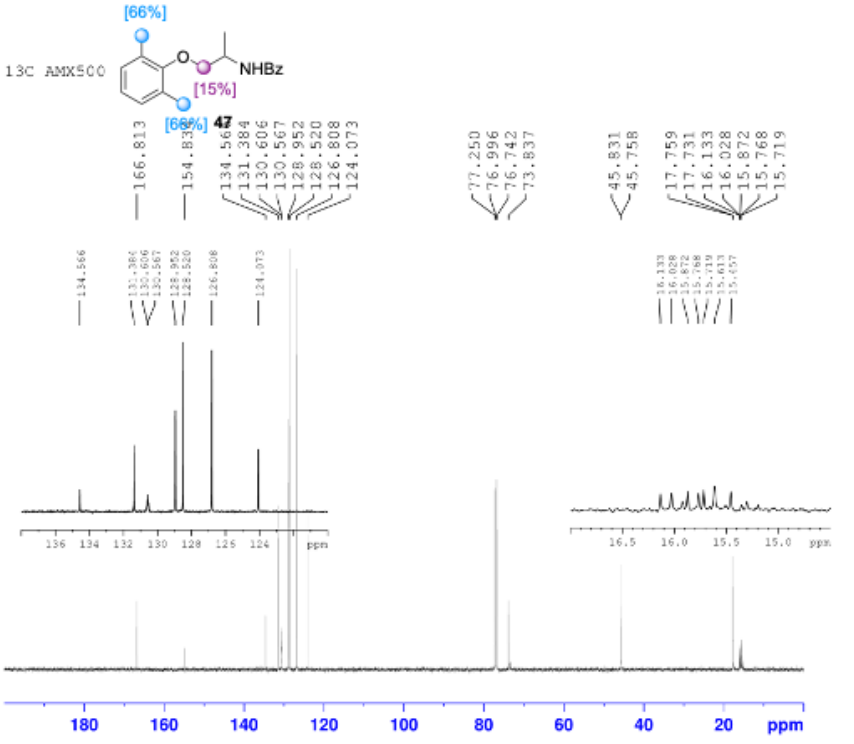
BRUKER

```
Current Data Parameters
NAME      yk1120-kyl-4082-1-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191120
Time                  18.24
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH               10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                     45.3
DW                  48.400 usec
DE                   6.00 usec
TE                  296.8 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.50 usec
PL1                     0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                    16384
SF              500.1300136 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



BRUKER

```
Current Data Parameters
NAME      yk1120-kyl-4082-1-1
EXPNO                       2
PROCNO                      1

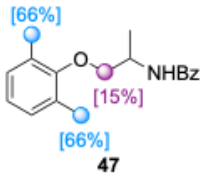
F2 - Acquisition Parameters
Date_              20191120
Time                  19.25
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      140
DS                        0
SWH               30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0911744 sec
RG                    16384
DW                  16.650 usec
DE                   6.00 usec
TE                  297.1 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      20

======== CHANNEL f1 ========
NUC1                     13C
P1                     8.90 usec
PL1                       0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     0.25 dB
PL12                   17.89 dB
PL13                   15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                    32768
SF              125.7578019 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

2H AV 500 NEO 23 May 2017 D NMR in CHCl3



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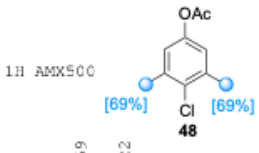
```
Current Data Parameters
NAME                  thd-19
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20200624
Time                  16.46 h
INSTRUM   CAB AV4 500 MHz BASIC
PROBHD    2144569_0005 (
PULPROG               zg2h.2
TD                      8192
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                 1562.500 Hz
FIDRES              0.381470 Hz
AQ                  2.6214399 sec
RG                       12.5
DW                    320.000 usec
DE                      6.50 usec
TE                     298.0 K
D1                  1.00000000 sec
D11                 0.03000000 sec
TD0                         1
SFO1                76.7886582 MHz
NUC1                       2H
P1                     349.30 usec
PLW1                3.50000000 W

F2 - Processing parameters
SI                         65536
SF                  76.7883510 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```

1H AMX500



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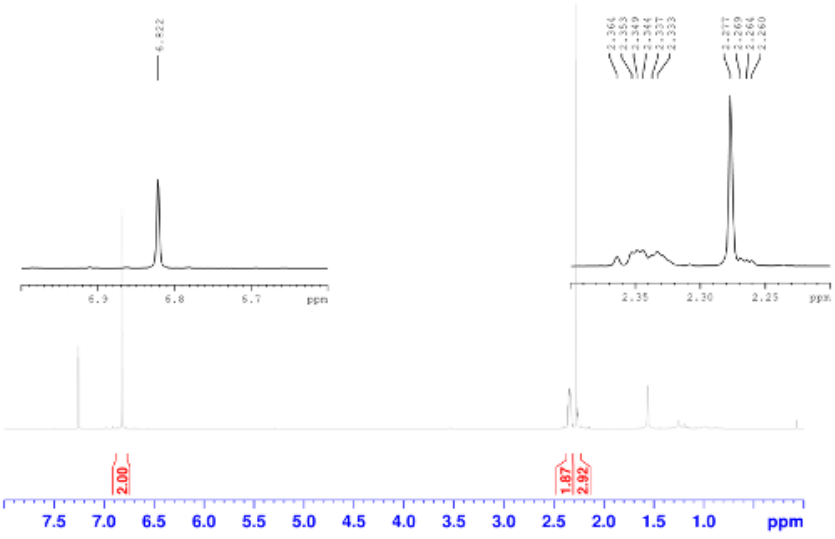
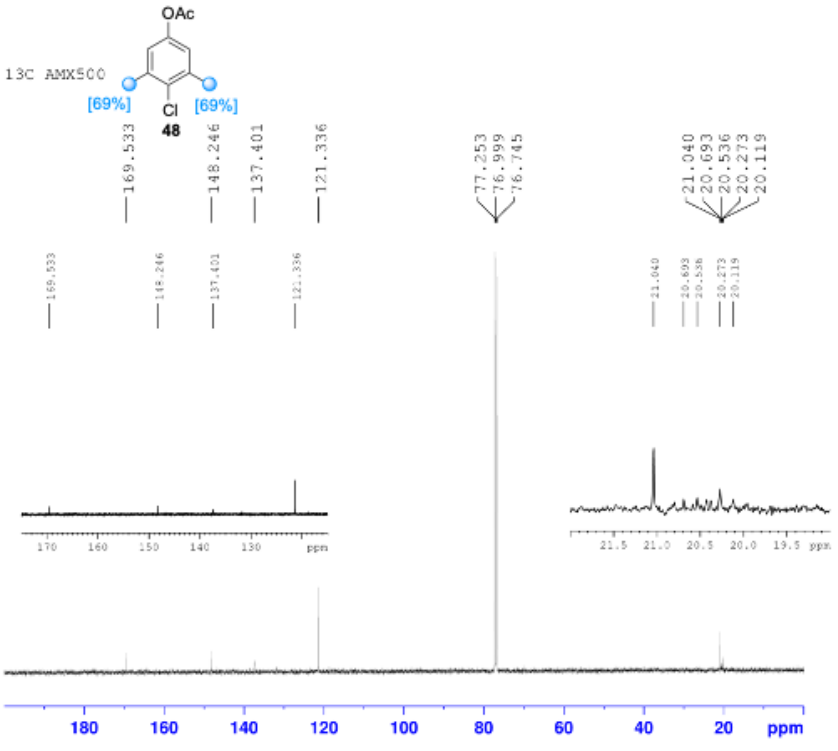



```
Current Data Parameters
NAME      ykl222-kyl-4072-7-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20191222
Time                   11.30
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT                 CDCl3
NS                          8
DS                          0
SWH                10330.578 Hz
FIDRES              0.315264 Hz
AQ                  1.5859712 sec
RG                      228.1
DW                     48.400 usec
DE                      6.00 usec
TE                     297.0 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                     10.50 usec
PL1                     0.25 dB
SFO1                500.1330885 MHz

F2 - Processing parameters
SI                      16384
SF                  500.1300143 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```



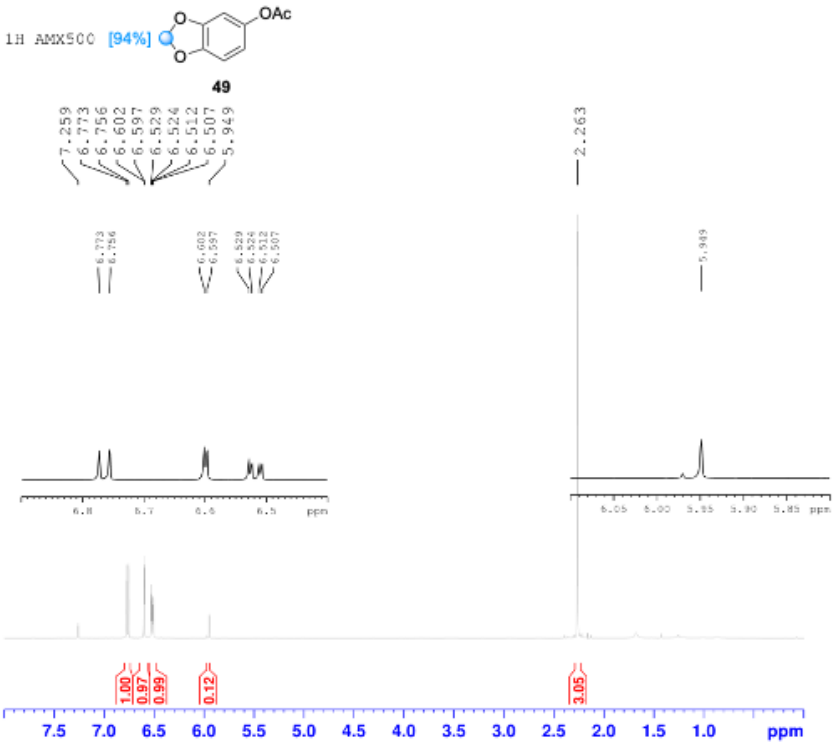

```
Current Data Parameters
NAME        yk1222-ky1-4072-3-1
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20191222
Time                      11.52
INSTRUM                    spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         327
DS                           0
SWH                30030.029 Hz
FIDRES              0.458222 Hz
AQ                  1.0911744 sec
RG                       16384
DW                    16.650 usec
DE                     6.00 usec
TE                     297.1 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                         20

======== CHANNEL f1 ========
NUC1                       13C
P1                        8.90 usec
PL1                          0 dB
SFO1              125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL2                       0.25 dB
PL12                     17.89 dB
PL13                     15.83 dB
SFO2              500.1320005 MHz

F2 - Processing parameters
SI                       32768
SF                125.7577919 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

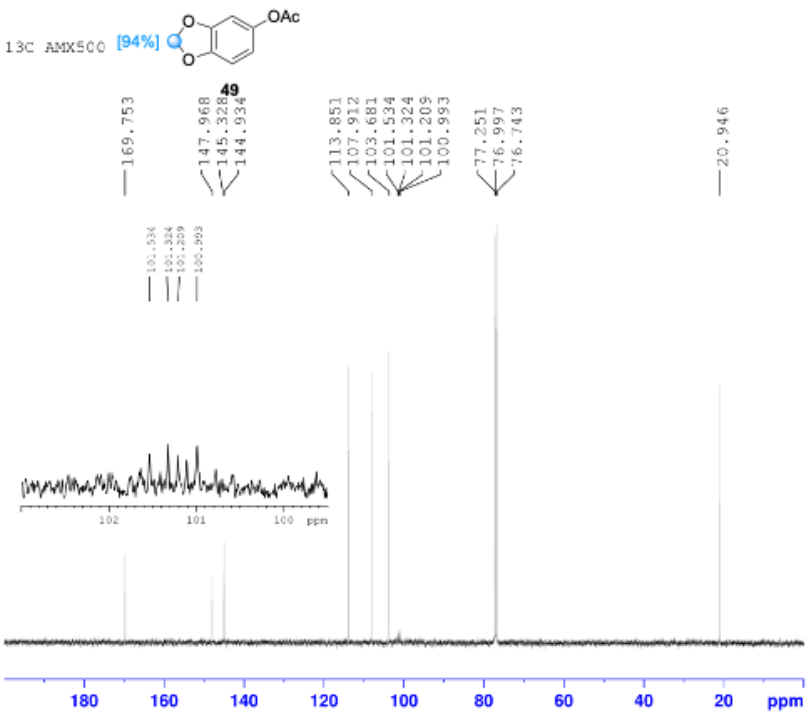


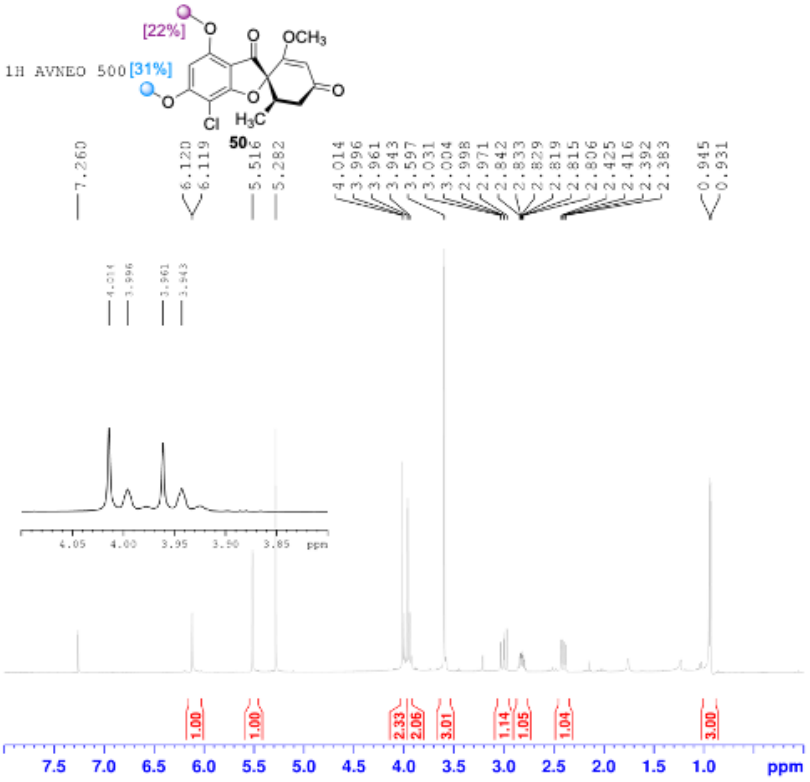

```
Current Data Parameters
NAME        yk1211-ky1-4198-2-1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20191211
Time                      20.08
INSTRUM                    spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg30
TD                       32768
SOLVENT                  CDCl3
NS                           8
DS                           0
SWH                10330.578 Hz
FIDRES              0.315264 Hz
AQ                  1.5859712 sec
RG                       101.6
DW                    48.400 usec
DE                     6.00 usec
TE                     296.0 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       10.50 usec
PL1                       0.25 dB
SFO1              500.1330885 MHz

F2 - Processing parameters
SI                       16384
SF                500.1300136 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```





BRUKER

Current Data Parameters
NAME yk1211-kyl-4198-2-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191211
Time 20.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 196
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 296.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20

======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz

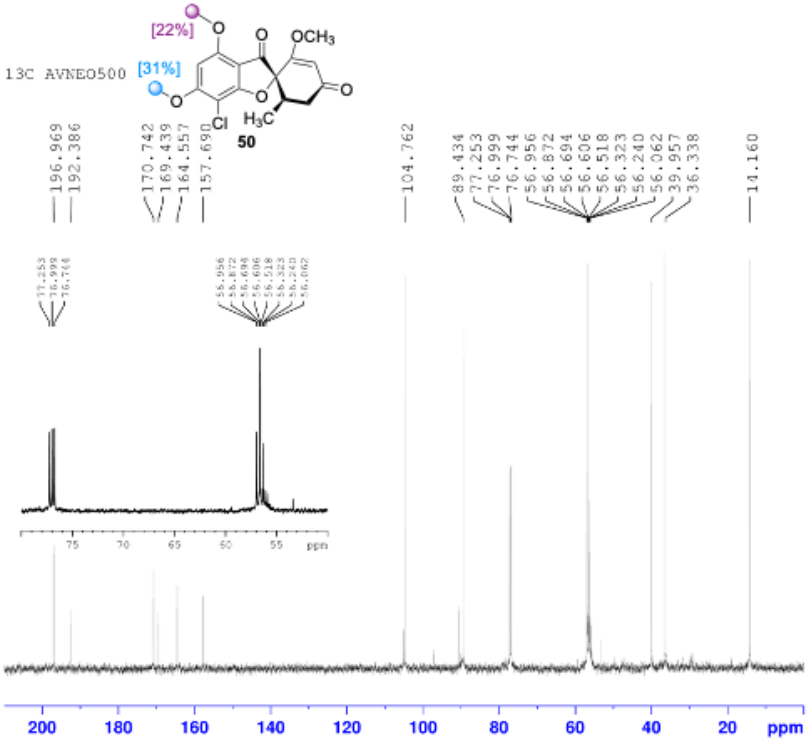
F2 - Processing parameters
SI 32768
SF 125.7577961 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

BRUKER

Current Data Parameters
NAME ye0303-kyl-4093-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200303
Time 20.08 h
INSTRUM Avance
PROBHD 2169738_0003 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 11.14 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330883 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.45700073 W

F2 - Processing parameters
SI 65536
SF 500.1300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

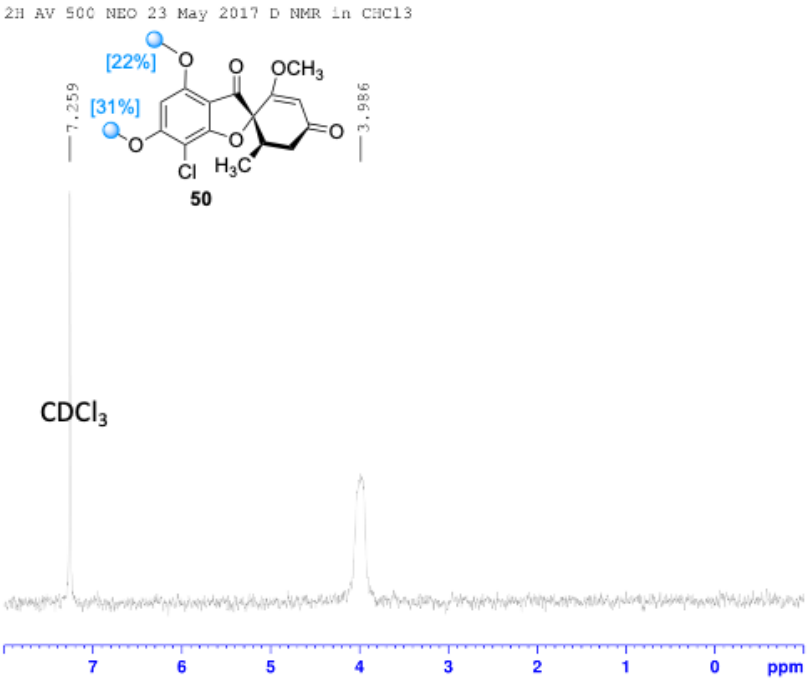


BRUKER

```
Current Data Parameters
NAME      yk0303-ky1-4093-2
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20200303
Time                  20.19 h
INSTRUM                Avance
PROBHD   2169738_0003 (
PULPROG                zgpg
TD                    65536
SOLVENT               CDCl3
NS                      203
DS                        2
SWH               30120.482 Hz
FIDRES            0.919204 Hz
AQ                1.0878977 sec
RG                      101
DW                  16.600 usec
DE                   6.72 usec
TE                  296.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1           125.7709931 MHz
NUC1                    13C
P1                    9.00 usec
PLW1          110.76999664 W
SFO2           500.1320005 MHz
NUC2                    1H
CPDPRG[2          waltz64
PCPD2                80.00 usec
PLW2          24.65700073 W
PLW12          0.24457000 W
PLW13          0.12302000 W

F2 - Processing parameters
SI                    65536
SF           125.7577980 MHz
WDW                     EM
SSB                      0
LB                    2.00 Hz
GB                       0
PC                    1.40
```

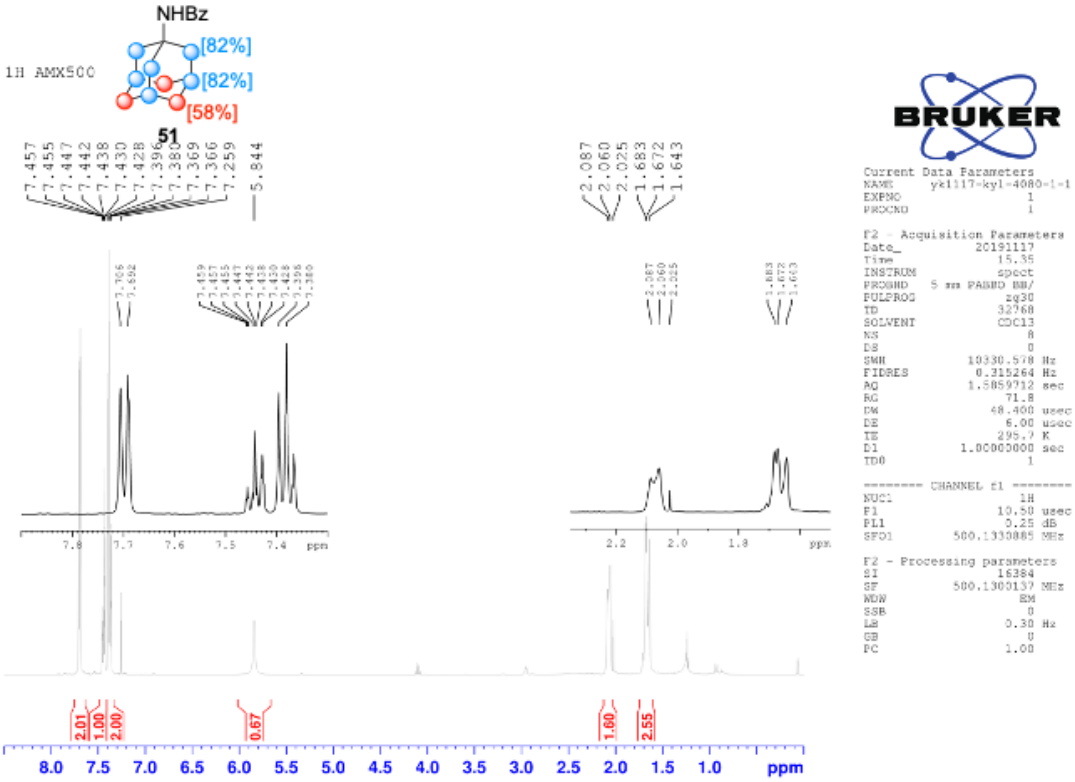


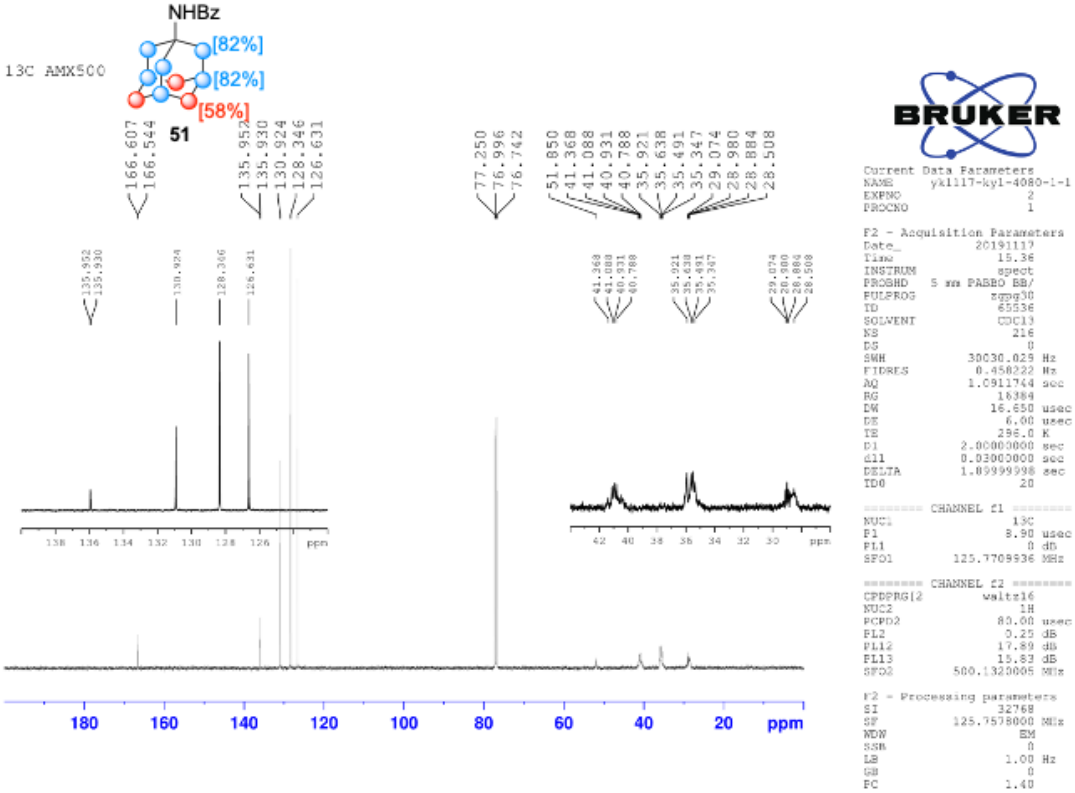
BRUKER

```
Current Data Parameters
NAME                  thd-21
EXPNO                      2
PROCNO                     1

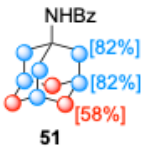
F2 - Acquisition Parameters
Date_              20200624
Time                  16.50 h
INSTRUM  CAB AV4 500 MHz BASIC
PROBHD   2144569_0005 (
PULPROG                zg2h.2
TD                      8192
SOLVENT               CDCl3
NS                         8
DS                         2
SWH               1562.500 Hz
FIDRES            0.381470 Hz
AQ                2.6214399 sec
RG                   13.8589
DW                  320.000 usec
DE                   6.50 usec
TE                  298.0 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                        1
SFO1           76.7885582 MHz
NUC1                     2H
P1                  349.30 usec
PLW1          3.50000000 W

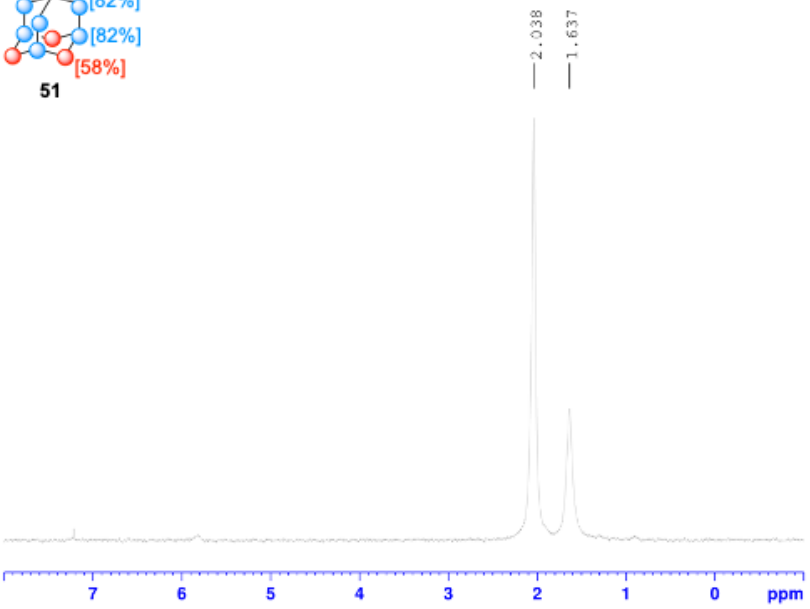
F2 - Processing parameters
SI                    65536
SF           76.7883494 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```


NHBz
[82%]
[82%]
[58%]
51
1H AMX500
7.457
7.455
7.447
7.442
7.438
7.430
7.428
7.396
7.380
7.369
7.366
7.259
5.844
2.087
2.060
2.025
1.683
1.672
1.643
2.01
1.00
2.00
0.67
1.60
2.55
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 ppm
BRUKER
Current Data Parameters
NAME yk1117-kyl-4080-1-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191117
Time 15.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 71.8
DW 48.400 usec
DE 6.00 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


NHBz
[82%]
[82%]
[58%]
51
13C AMX500
166.607
166.544
135.952
135.930
130.924
128.346
126.631
77.250
76.996
76.742
51.850
41.368
41.088
40.931
40.788
35.921
35.638
35.491
35.347
29.074
28.980
28.884
28.508
180 160 140 120 100 80 60 40 20 ppm
BRUKER
Current Data Parameters
NAME yk1117-kyl-4080-1-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191117
Time 15.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 216
DS 0
SWH 30030.025 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 296.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7578000 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2H AV 500 NEO 23 May 2017 D NMR



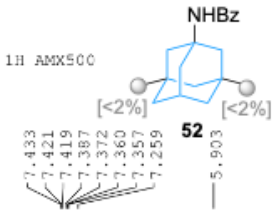


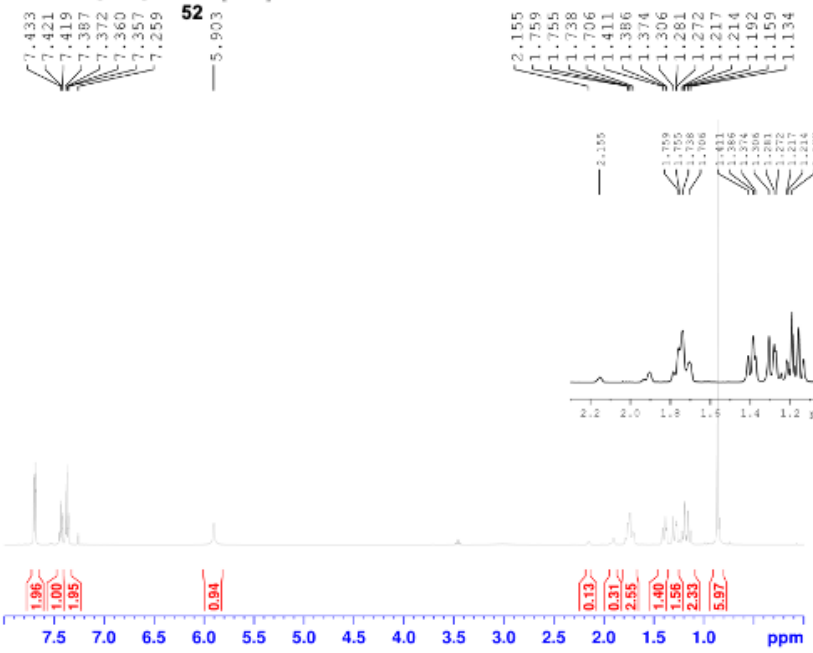
BRUKER

```
Current Data Parameters
NAME                  thd-22
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20200624
Time                  16.52 h
INSTRUM  CAH AV4 500 MHz BASIC
PROBHD   2144569_0005 (
PULPROG             zg2h.2
TD                      8192
SOLVENT               CDCl3
NS                         8
DS                         2
SWH                1562.500 Hz
FIDRES             0.381470 Hz
AQ                 2.6214399 sec
RG                      12.5
DW                  320.000 usec
DE                    6.50 usec
TE                   298.0 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1              76.7888582 MHz
NUC1                      2H
P1                   349.30 usec
PLW1               3.50000000 W

F2 - Processing parameters
SI                     65536
SF                76.7883510 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                      1.00
```





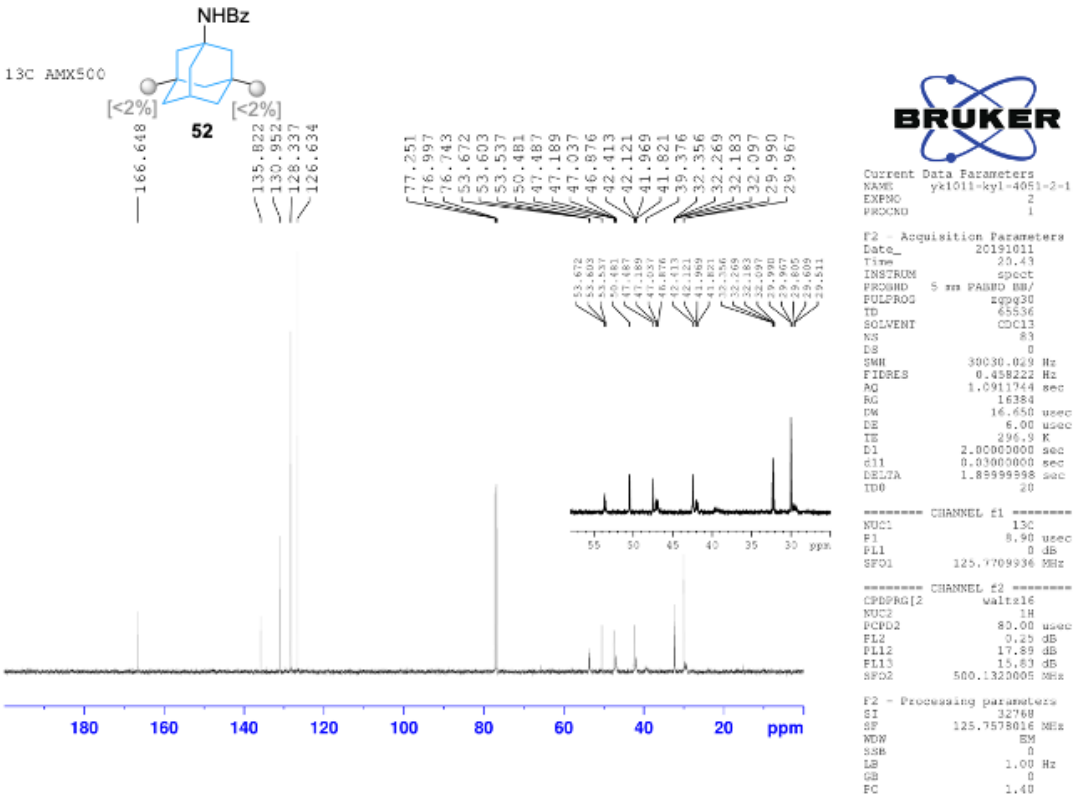
BRUKER

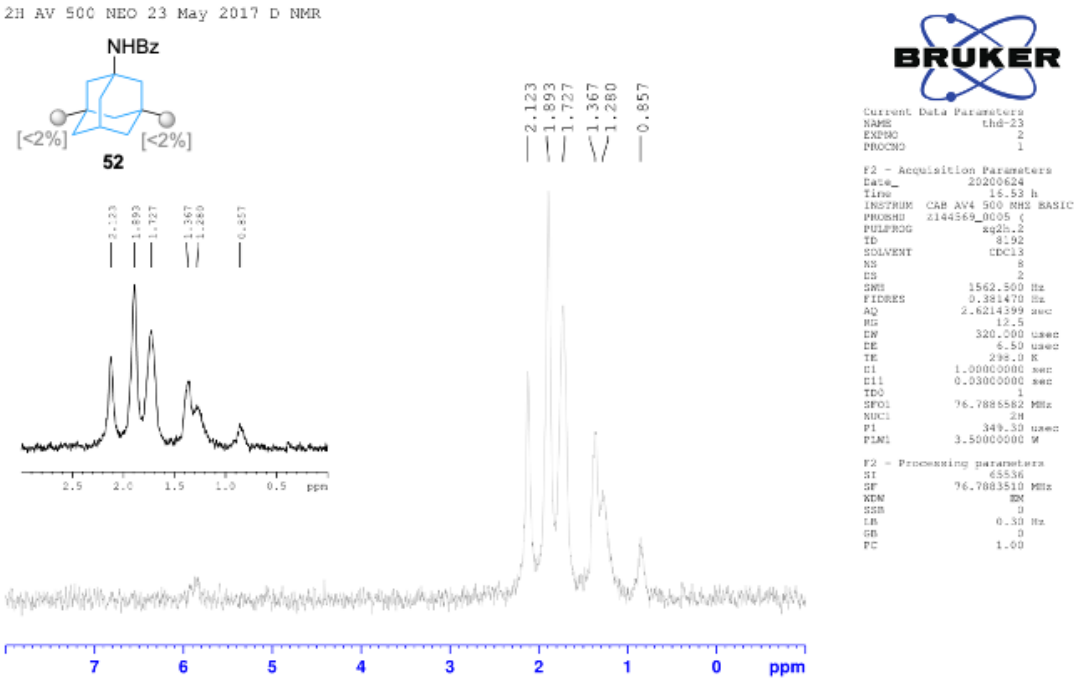
```
Current Data Parameters
NAME       ykl011-kyl-4051-2-1
EXPNO                        1
PROCNO                       1

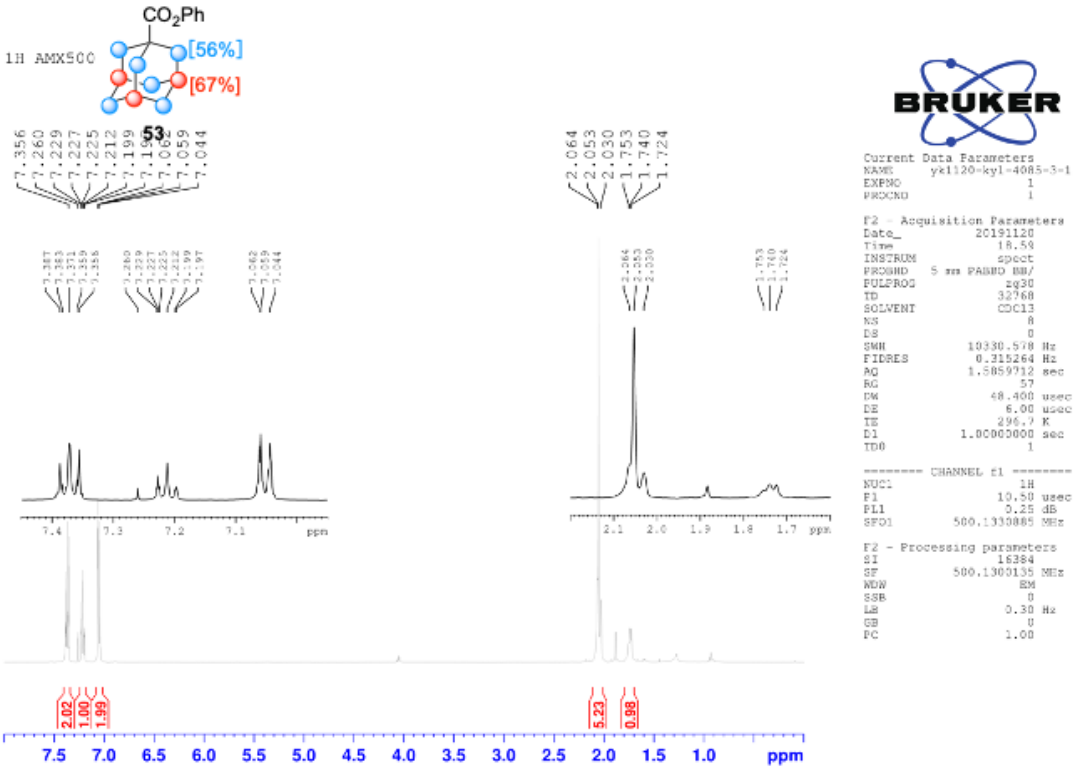
F2 - Acquisition Parameters
Date_               20191011
Time                  20.42
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                         8
DS                         0
SWH               10330.578 Hz
FIDRES             0.315264 Hz
AQ                 1.5859712 sec
RG                      35.9
DW                   48.400 usec
DE                    6.00 usec
TE                   296.5 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                   10.50 usec
PL1                   0.25 dB
SFO1            500.1330885 MHz

F2 - Processing parameters
SI                     16384
SF              500.1300136 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                      1.00
```


13C AMX500
NHBz
[<2%]
[<2%]
52
166.648
135.822
130.952
128.337
126.634
77.251
76.997
76.743
53.672
53.603
53.537
50.481
47.487
47.189
47.037
46.876
42.413
42.121
41.969
41.821
39.376
32.356
32.269
32.183
32.097
29.990
29.967
180
160
140
120
100
80
60
40
20
ppm


2H AV 500 NEO 23 May 2017 D NMR
NHBz
[<2%]
[<2%]
52
2.123
1.893
1.727
1.367
1.280
0.857
7
6
5
4
3
2
1
0
ppm



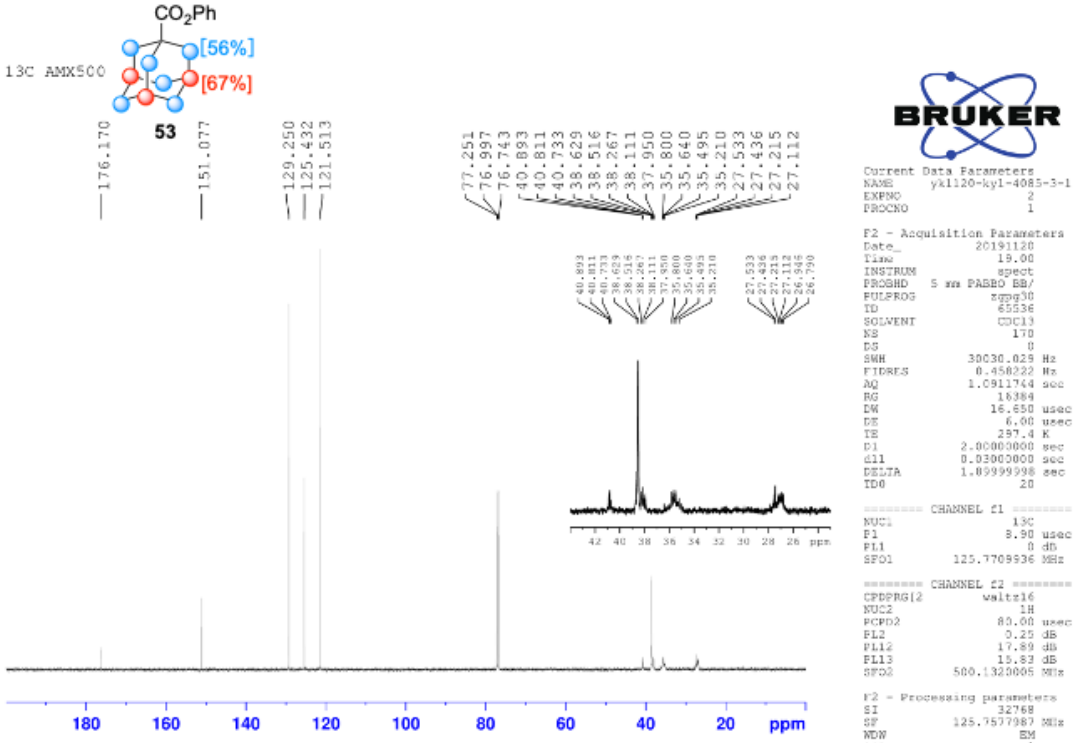
BRUKER

```
Current Data Parameters
NAME      yk1120-kyl-4085-3-1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20191120
Time                  18.59
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH               10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5859712 sec
RG                       57
DW                  48.400 usec
DE                   6.00 usec
TE                  296.9 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    10.50 usec
PL1                    0.25 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI                    16384
SF              500.1300135 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



BRUKER

```
Current Data Parameters
NAME      yk1120-kyl-4085-3-1
EXPNO                       2
PROCNO                      1

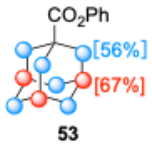
F2 - Acquisition Parameters
Date_              20191120
Time                  19.00
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      170
DS                        0
SWH               30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0911744 sec
RG                    16384
DW                  16.650 usec
DE                   6.00 usec
TE                  297.4 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      20

======== CHANNEL f1 ========
NUC1                     13C
P1                     8.90 usec
PL1                       0 dB
SFO1          125.7709936 MHz

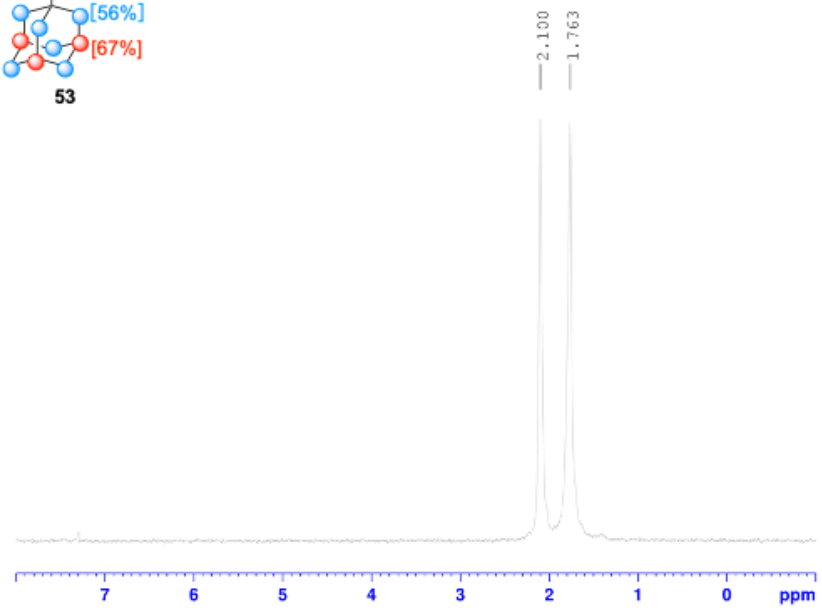
======== CHANNEL f2 ========
CPDPRG[2            waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                    0.25 dB
PL12                  17.89 dB
PL13                  15.82 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                    32768
SF              125.7577987 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

2H AV 500 NEO 23 May 2017 D NMR



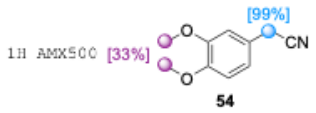
53



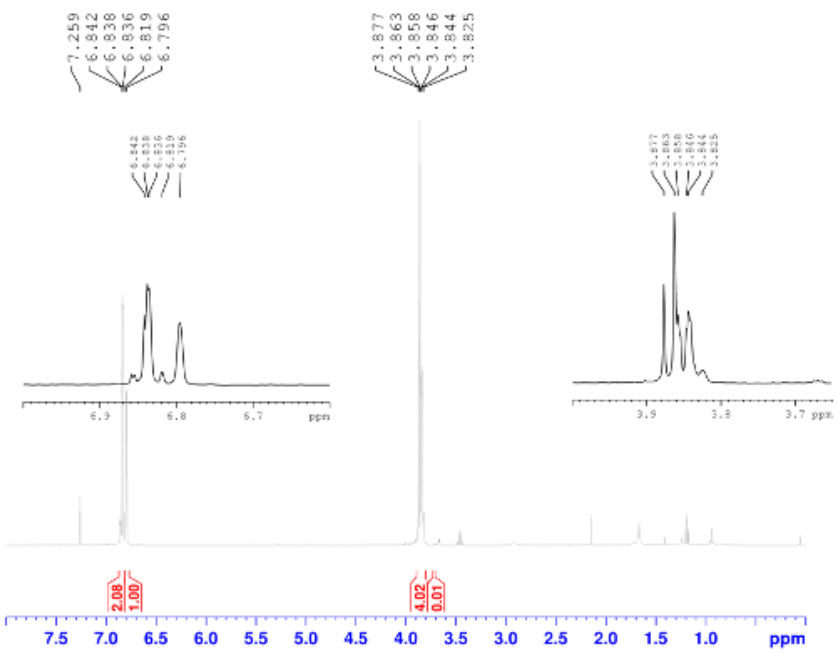
```
Current Data Parameters
NAME                  thd-24
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20200623
Time                   15.12 h
INSTRUM   CAB AV4 500 MHz BASIC
PROBHD    2144569_0005 (
PULPROG              zg2h.2
TD                       8192
SOLVENT                  DMSO
NS                         16
DS                          2
SWH                 1562.500 Hz
FIDRES              0.381470 Hz
AQ                  2.6214399 sec
RG                       12.5
DW                    320.000 usec
DE                      6.50 usec
TE                     298.0 K
D1                  1.00000000 sec
D11                 0.03000000 sec
TD0                         1
SFO1               76.7886582 MHz
NUC1                       2H
P1                     349.30 usec
PLW1                3.50000000 W

F2 - Processing parameters
SI                        65536
SF                 76.7883228 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```



54

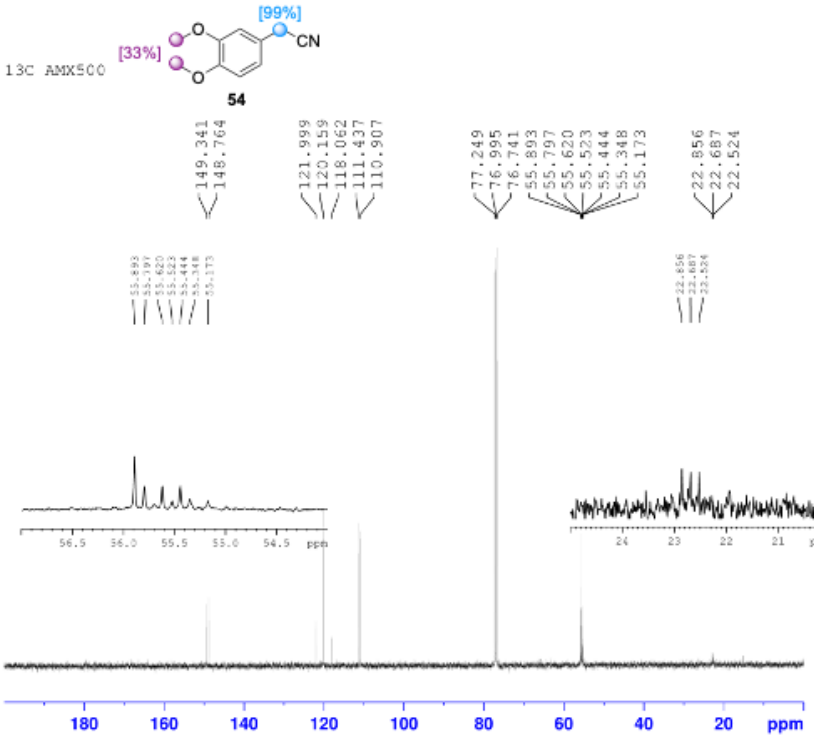


```
Current Data Parameters
NAME      ykl211-kyl-4105-1-1
EXPNO                      1
PROCNO                     1

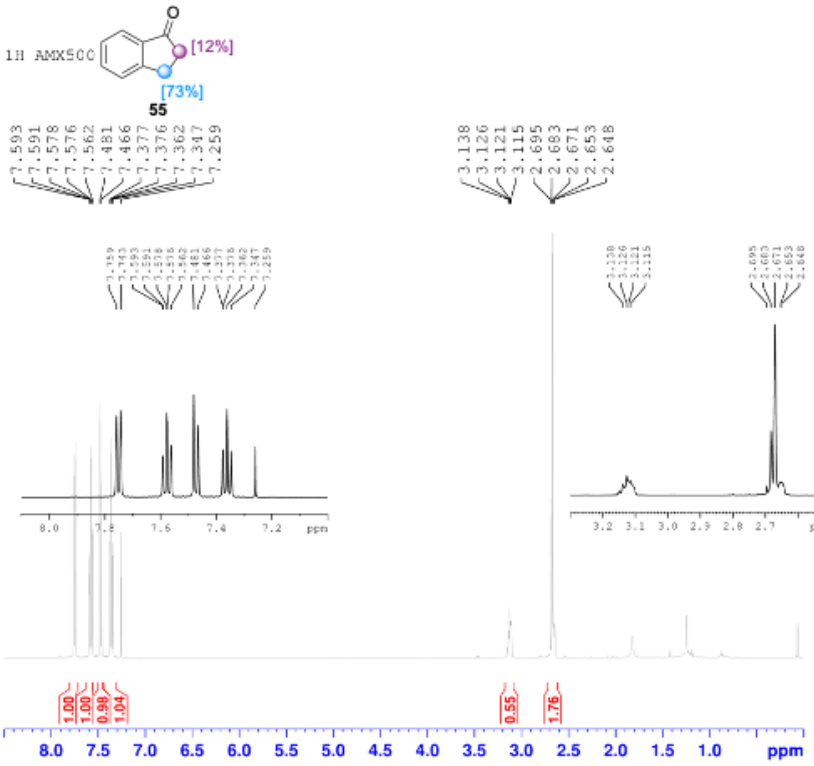
F2 - Acquisition Parameters
Date_               20191211
Time                   20.22
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                      32768
SOLVENT                CDCl3
NS                          8
DS                          0
SWH                10330.578 Hz
FIDRES              0.315264 Hz
AQ                  1.5859712 sec
RG                      101.6
DW                     48.400 usec
DE                      6.00 usec
TE                     296.6 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                     10.50 usec
PL1                     0.25 dB
SFO1              500.1330885 MHz

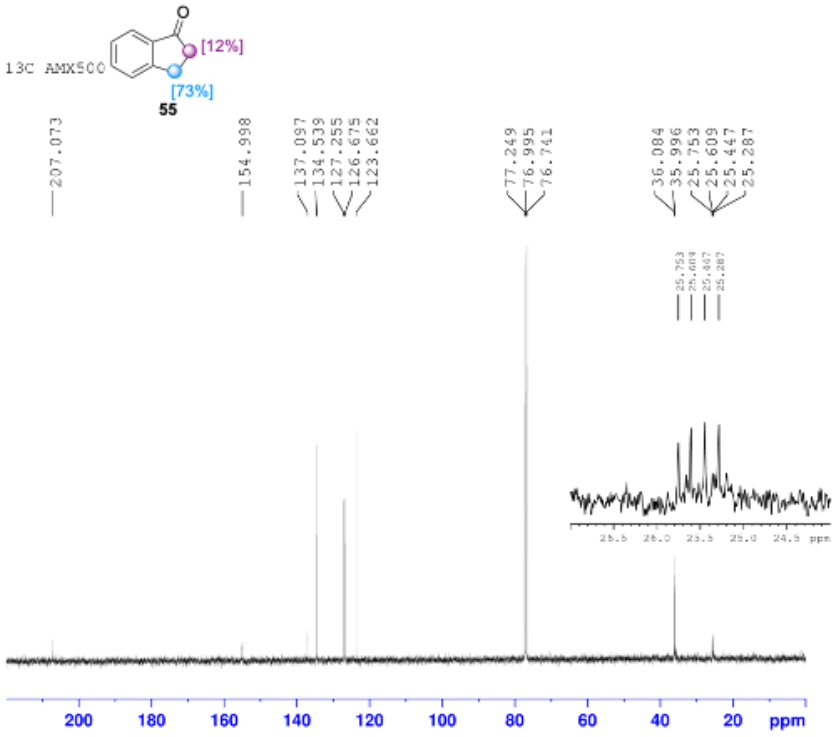
F2 - Processing parameters
SI                        16384
SF                500.1300137 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```


13C AMX500
[99%]
[33%]
CN
54
149.341
148.764
121.999
120.159
118.062
111.437
110.907
77.249
76.995
76.741
55.893
55.797
55.620
55.523
55.444
55.348
55.173
22.856
22.687
22.524
180
160
140
120
100
80
60
40
20
ppm


BRUKER
Current Data Parameters
NAME yk1211-kyl-4105-1-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191211
Time 20.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 169
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 297.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7578000 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


1H AMX500
[12%]
[73%]
55
7.593
7.591
7.578
7.576
7.562
7.481
7.466
7.377
7.376
7.362
7.347
7.259
3.138
3.126
3.121
3.115
2.695
2.683
2.671
2.653
2.648
1.00
1.00
0.98
1.04
0.55
1.76
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
ppm


BRUKER
Current Data Parameters
NAME yk01007-kyl-4042-1-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191007
Time 20.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 101.6
DW 48.400 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

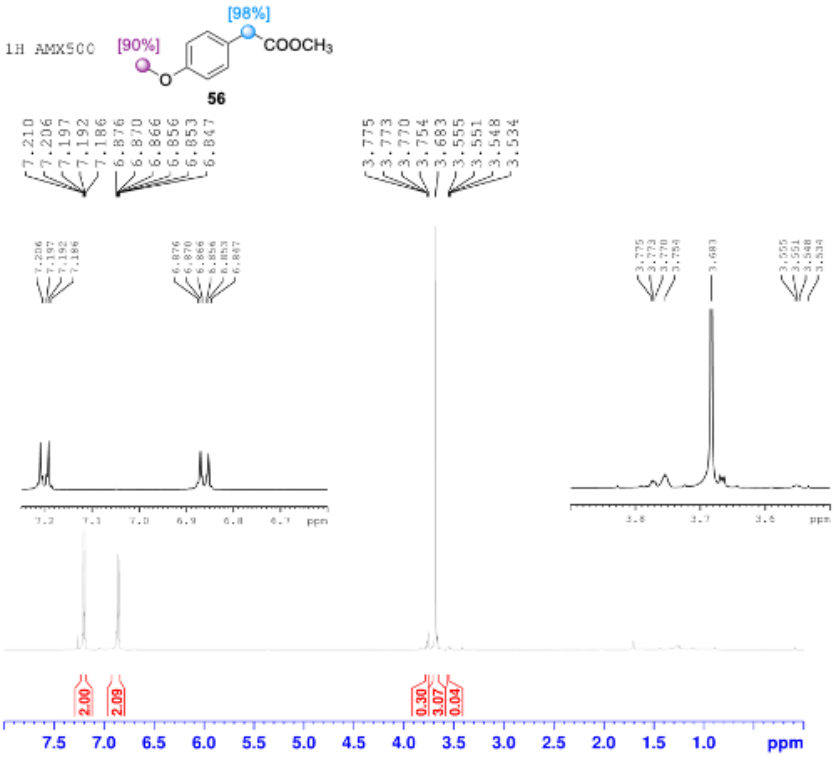
```
Current Data Parameters
NAME        yk01007-kyl-4042-1-1
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20191007
Time                       20.46
INSTRUM                    spect
PROBHD     5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         130
DS                           0
SWH                  30030.029 Hz
FIDRES               0.458222 Hz
AQ                   1.0911744 sec
RG                        16384
DW                      16.650 usec
DE                        6.00 usec
TE                       296.3 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
ID0                          20

======== CHANNEL f1 ========
NUC1                       13C
P1                        8.90 usec
PL1                          0 dB
SFO1           125.77099936 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL2                       0.25 dB
PL12                     17.89 dB
PL13                     18.83 dB
SFO2           500.1320005 MHz

F2 - Processing parameters
SI                         32768
SF             125.7577965 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40
```



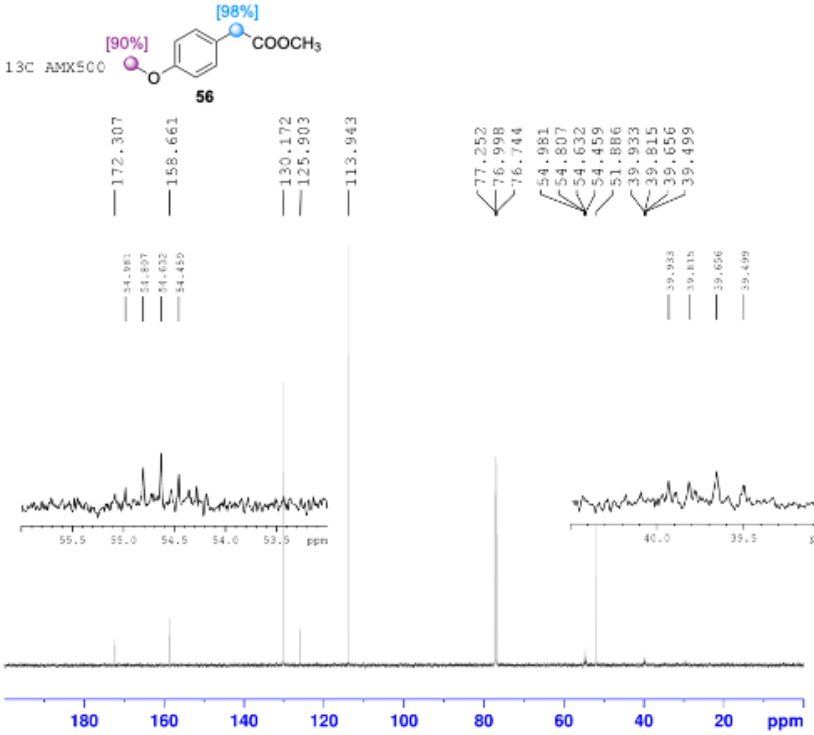
BRUKER

```
Current Data Parameters
NAME        yk1222-kyl-4110-4-1
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20191222
Time                       10.56
INSTRUM                    spect
PROBHD     5 mm PABBO BB/
PULPROG                    zg30
TD                       32768
SOLVENT                  CDCl3
NS                             8
DS                             0
SWH                  10330.578 Hz
FIDRES               0.315264 Hz
AQ                   1.5859712 sec
RG                           71.8
DW                      48.400 usec
DE                        6.00 usec
TE                       296.9 K
D1                  1.00000000 sec
ID0                            1

======== CHANNEL f1 ========
NUC1                       1H
P1                       10.50 usec
PL1                       0.25 dB
SFO1           500.1330885 MHz

F2 - Processing parameters
SI                         16384
SF             500.1300133 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.00
```



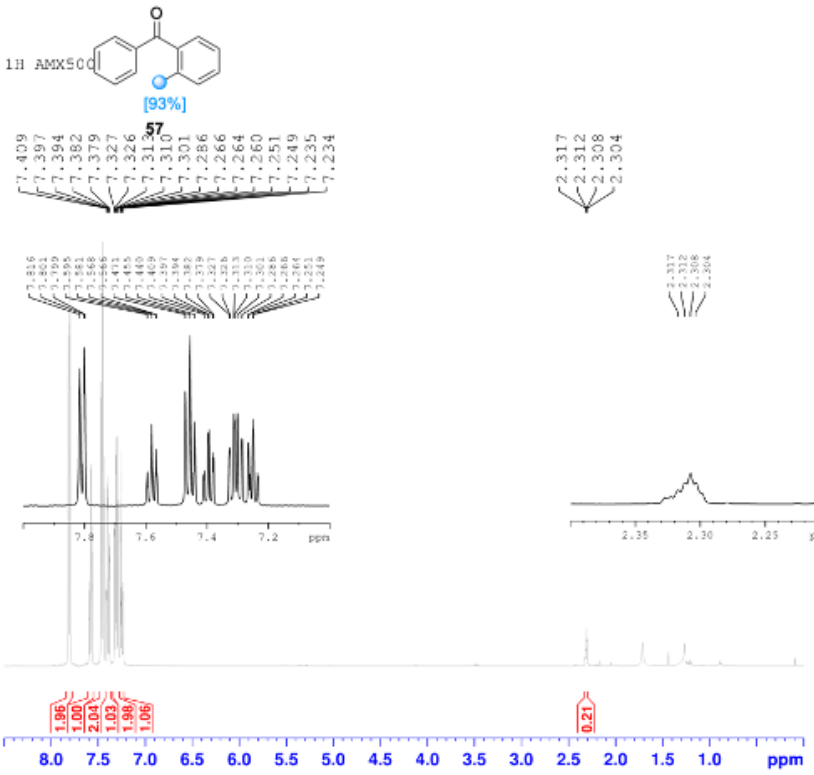
```
Current Data Parameters
NAME        yx1222-kyl-4110-4-1
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20191222
Time                      10.57
INSTRUM                    spect
PROBHD     5 mm PABBO BB/
PULPROG                zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                          145
DS                            0
SWH                30030.029 Hz
FIDRES             0.458222 Hz
AQ                 1.0911744 sec
RG                        16384
DW                    16.650 usec
DE                     6.00 usec
TE                     297.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                          20

======== CHANNEL f1 ========
NUC1                       13C
P1                        8.90 usec
PL1                          0 dB
SFO1             125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL2                       0.25 dB
PL12                     17.89 dB
PL13                     15.83 dB
SFO2             500.1320005 MHz

F2 - Processing parameters
SI                        32768
SF               125.7577984 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40
```

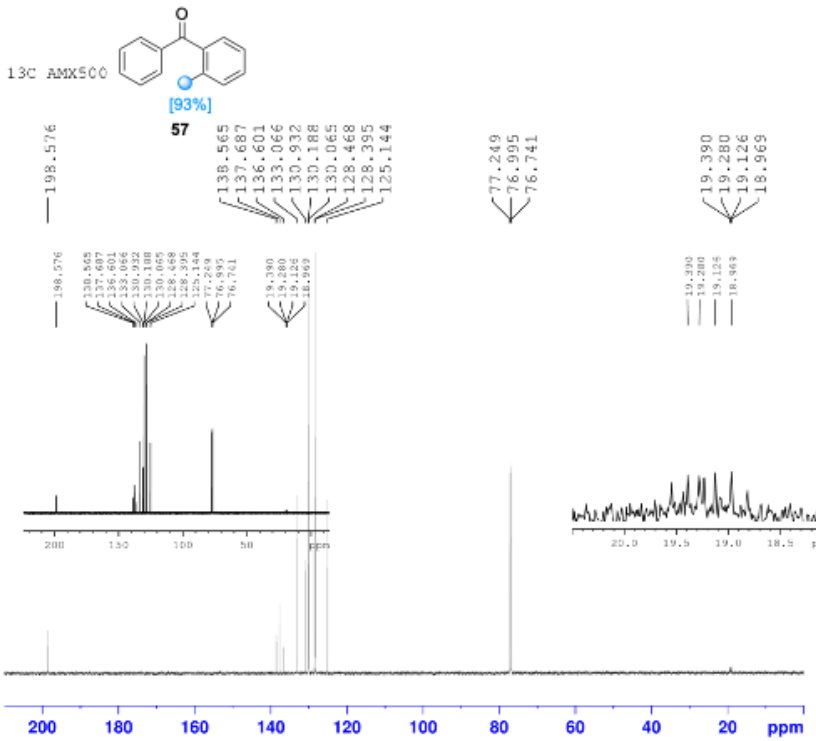


```
Current Data Parameters
NAME        yx0102-kyl-4118-5-1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20200102
Time                      17.18
INSTRUM                    spect
PROBHD     5 mm PABBO BB/
PULPROG                  zg30
TD                        32768
SOLVENT                   CDCl3
NS                            8
DS                            0
SWH                10330.578 Hz
FIDRES             0.315264 Hz
AQ                 1.5859712 sec
RG                         71.8
DW                    48.400 usec
DE                     6.00 usec
TE                     295.5 K
D1                 1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        1H
P1                       10.50 usec
PL1                       0.25 dB
SFO1             500.1330885 MHz

F2 - Processing parameters
SI                        16384
SF               500.1300136 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```



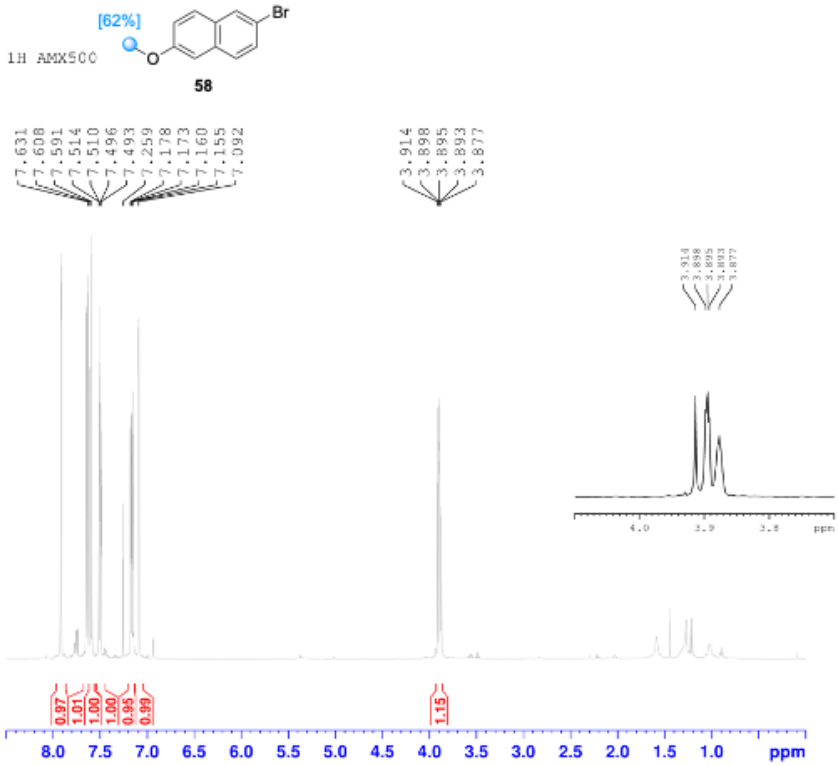
```
Current Data Parameters
NAME        yk0102-ky1-4118-S-1
EXPNO                         3
PROCNO                        1

F2 - Acquisition Parameters
Date_              20200102
Time                  17.22
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       155
DS                         0
SWH               30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0911744 sec
RG                     16384
DW                   16.650 usec
DE                    6.00 usec
TE                   296.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       20

======== CHANNEL f1 ========
NUC1                     13C
P1                      8.90 usec
PL1                        0 dB
SFO1          125.7709936 MHz

======== CHANNEL f2 ========
CPDPRG[2            waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                   0.25 dB
PL12                 17.89 dB
PL13                 15.83 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                       32768
SF            125.7577992 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

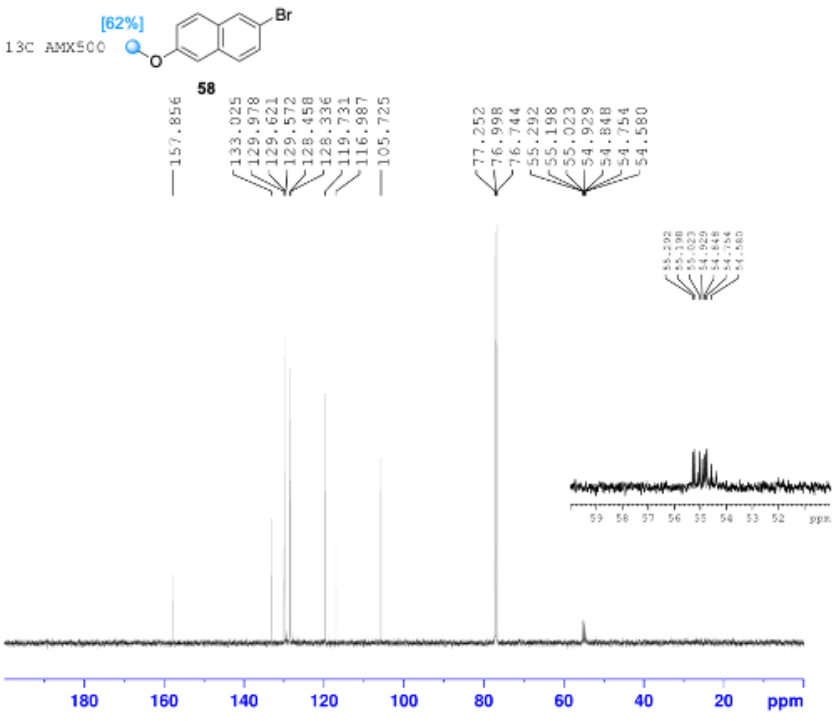


```
Current Data Parameters
NAME        yk0113-ky1-4128-1-1
EXPNO                         1
PROCNO                        1

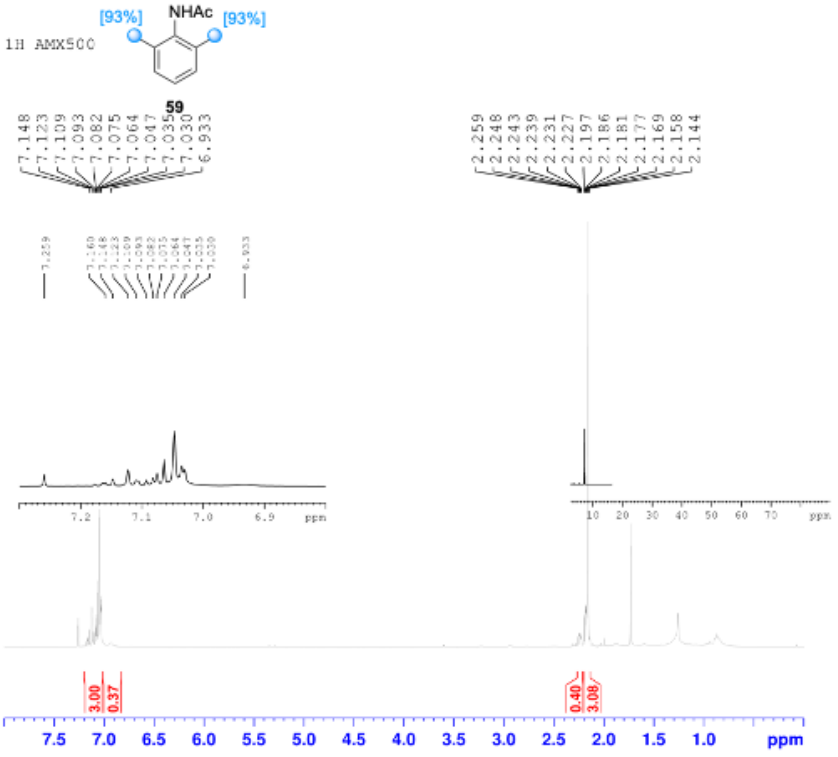
F2 - Acquisition Parameters
Date_              20200113
Time                  21.04
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH               10330.578 Hz
FIDRES            0.315264 Hz
AQ                1.5855712 sec
RG                      90.5
DW                   48.400 usec
DE                    6.00 usec
TE                   296.7 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.50 usec
PL1                     0.25 dB
SFO1          500.1330885 MHz

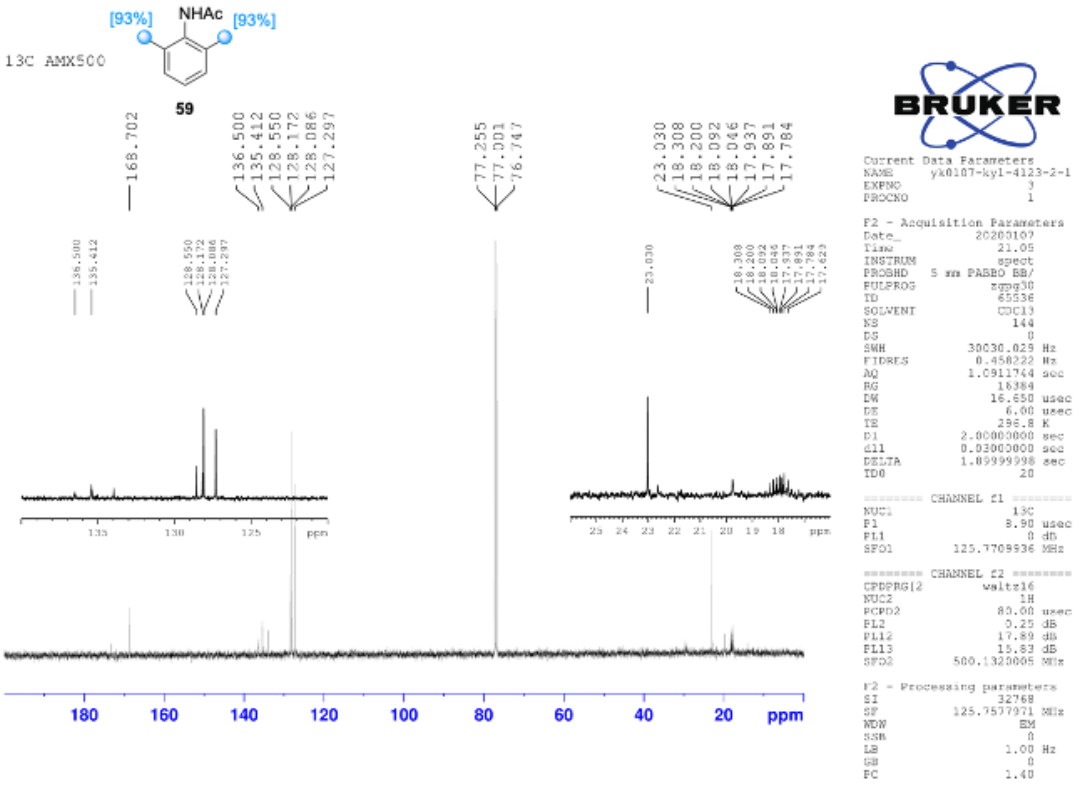
F2 - Processing parameters
SI                       16384
SF            500.1300136 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```


13C AMX500
[62%]
Br
O
58
157.856
133.025
129.978
129.621
129.572
128.458
128.336
119.731
116.987
105.725
77.252
76.998
76.744
55.292
55.198
55.023
54.929
54.848
54.754
54.580
180
160
140
120
100
80
60
40
20
ppm


BRUKER
Current Data Parameters
NAME yk0113-kyl-4128-1-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200113
Time 21.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 207
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 297.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577961 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


1H AMX500
[93%]
NHAc
[93%]
59
7.148
7.123
7.109
7.093
7.082
7.075
7.064
7.047
7.035
7.030
6.933
2.259
2.248
2.243
2.239
2.231
2.227
2.197
2.186
2.181
2.177
2.169
2.158
2.144
3.00
0.37
0.40
3.08
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
ppm


BRUKER
Current Data Parameters
NAME yk0107-kyl-4123-2-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200107
Time 21.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5859712 sec
RG 71.8
DW 48.400 usec
DE 6.00 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.25 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


[93%]
NHAc
[93%]
13C AMX500
59
168.702
136.500
135.412
128.550
128.172
128.086
127.297
77.255
77.001
76.747
23.030
18.308
18.200
18.092
18.046
17.937
17.891
17.784
BRUKER
Current Data Parameters
NAME yk0107-kyl-4123-2-1
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200107
Time 21.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 144
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 296.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 0 dB
SFO1 125.7709936 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.25 dB
PL12 17.89 dB
PL13 15.83 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577971 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
160
140
120
100
80
60
40
20
ppm