Supplementary Information

For

*n*Bu$_4$NI-Catalyzed Oxidative Imidation of Ketones with Imides: Synthesis of α-Amino Ketones

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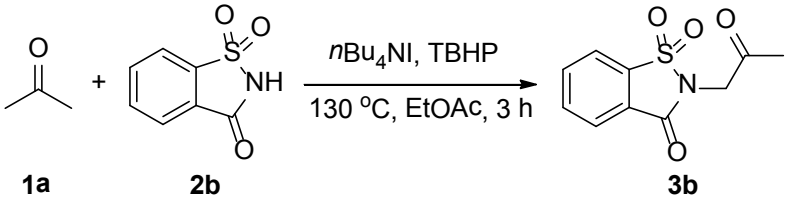
Ⅰ.General Considerations

All reagents were purchased from commercial sources and used without further treatment, unless otherwise indicated. All reactions were run under air with no precautions taken to exclude moisture. ^{1}H NMR and ^{13}C NMR spectra were recorded at 25 °C on a Varian (500 MHz and 125 MHz). Melting points were obtained with a micro melting point XT4A Beijing Keyi electrooptic apparatus and are uncorrected. High resolution mass spectra were recorded on Bruck microtof. All reactions were monitored by TLC with Taizhou GF254 silica gel coated plates. Flash column chromatography was carried out using 300-400 mesh silica gel at increased pressure.

Ⅱ. General procedure for the preparation of 3 and 4

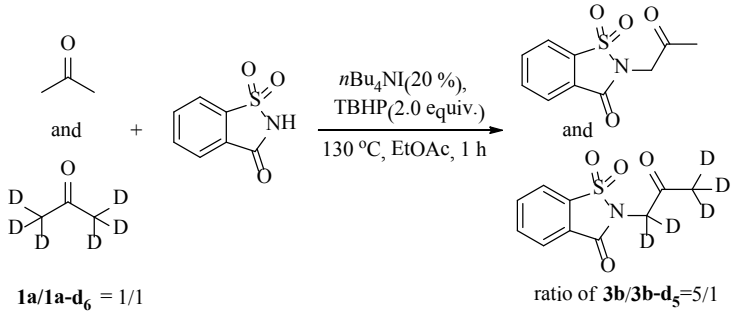
1a as an example



To a solution of the saccharin **2b** (54.9 mg, 0.3 mmol) in ethyl acetate (3.0 ml) was added the acetone **1a** (111 μL, 1.5 mmol), TBHP(109 μL, 0.6 mmol, 5.5 M in decane), and nBu$_4$NI (22.2 mg, 0.06 mmol) in screw-cap test tube. The test tube was then sealed off with a screw-cap and the reaction was stirred for the 3.0 h at 130 ℃. After the reaction finished, the reaction mixture was cooled to room temperature and quenched by the addition of a saturated solution of $Na_2S_2O_3$ (3.0 mL). The mixture was extracted with CH_2Cl_2 (3 × 5.0 mL), the combined organic phases were dried over anhydrous Na_2SO_4 and the solvent was evaporated under vacuum. The residue was purified by column chromatography to give the corresponding products **3b** (65.3 mg, 91%) .

Ⅲ. Control experiment on the reaction mechanism

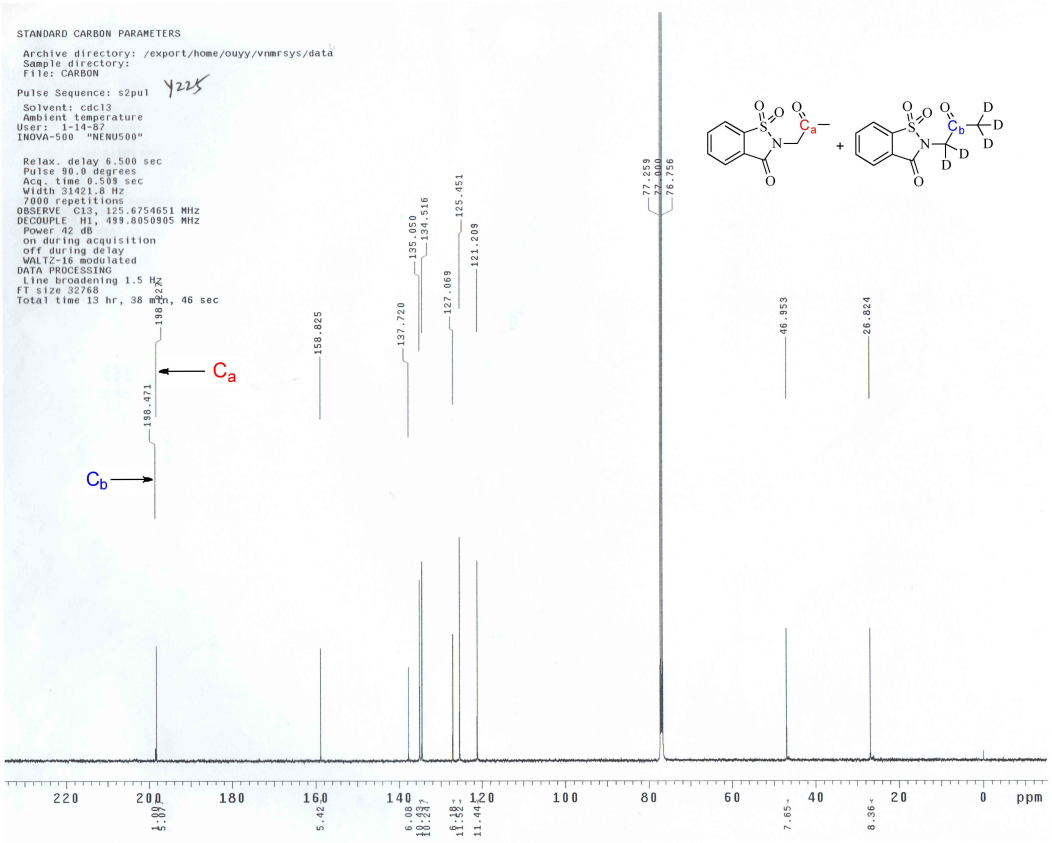
Scheme 1. The KIE for reactions between acetone and saccharin



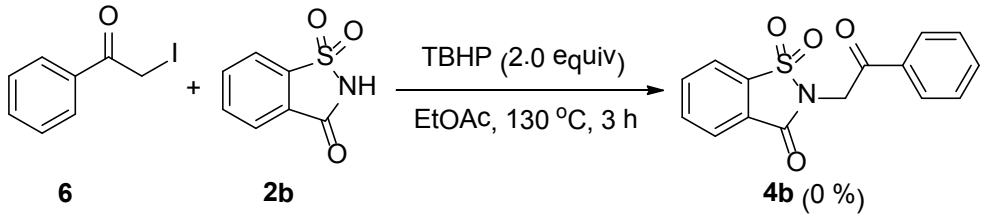
1a/1a-d$_6$ = 1/1 ratio of **3b**/**3b-d$_5$**=5/1

To a solution of the saccharin **2b** (54.9 mg, 0.3 mmol) in ethyl acetate (3.0 ml) was added the acetone **1a** (56 μL, 0.75 mmol), acetone-d$_6$ **1a-d$_6$** (55 μL, 0.75 mmol), TBHP(109 μL, 0.6 mmol, 5.5 M in decane), and nBu$_4$NI (22.2 mg, 0.06 mmol) in screw-cap test tube. The reaction mixture was stirred at 130 ℃ for 1.0 h. After the reaction was quenched by saturated solution of $Na_2S_2O_3$ (3.0 mL), the mixture was extracted with CH_2Cl_2 (3 × 5.0 mL), the combined organic

phases were dried over anhydrous Na_2SO_4 and the solvent was evaporated under vacuum. The residue was purified by flash column chromatography. The KIE value was determined by average of two runs and a representative ^{13}C NMR spectrum was provided as follows.



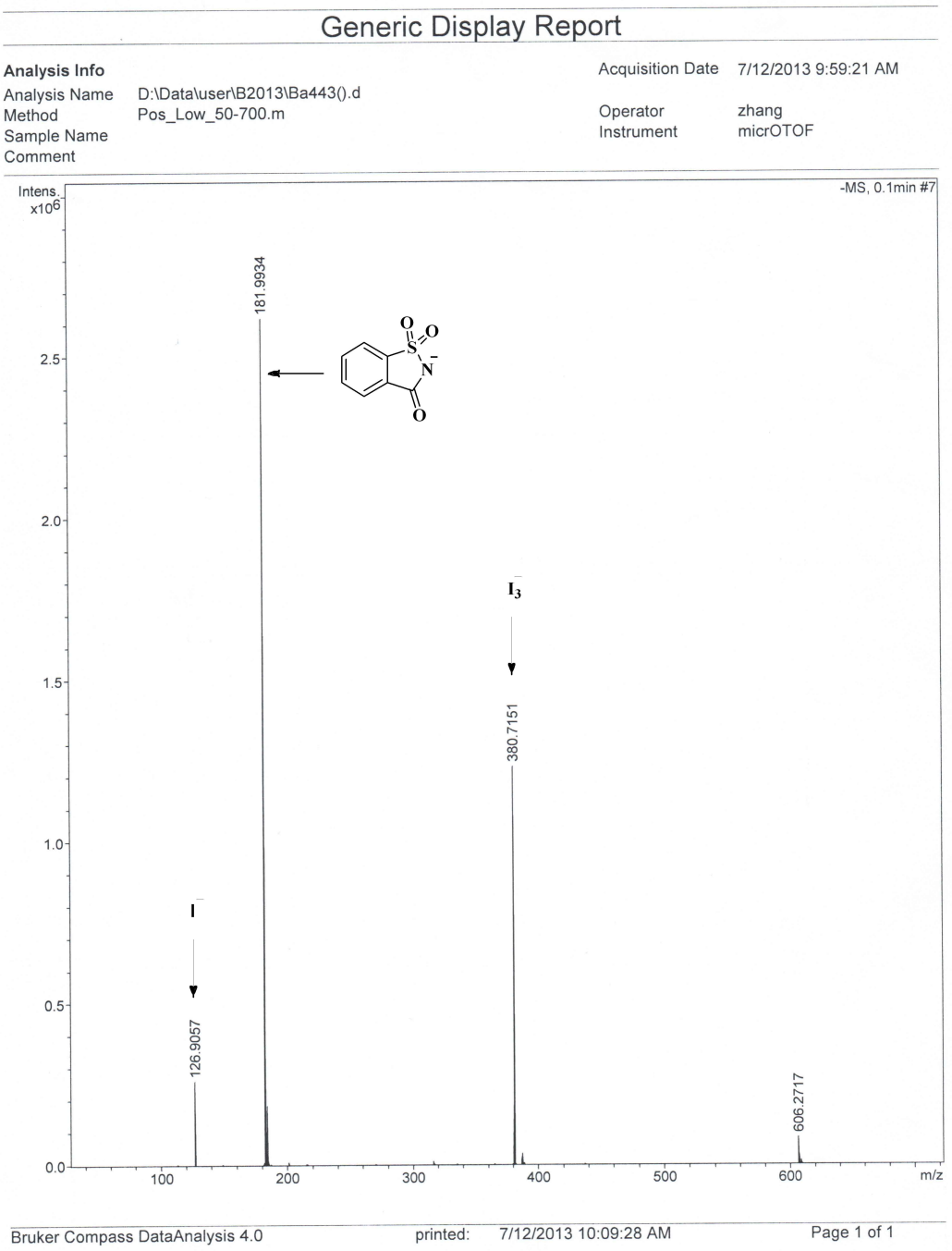
Scheme 2 Investigation of reaction mechanism.



Ⅳ. Analytical data of ESI(-)-MS

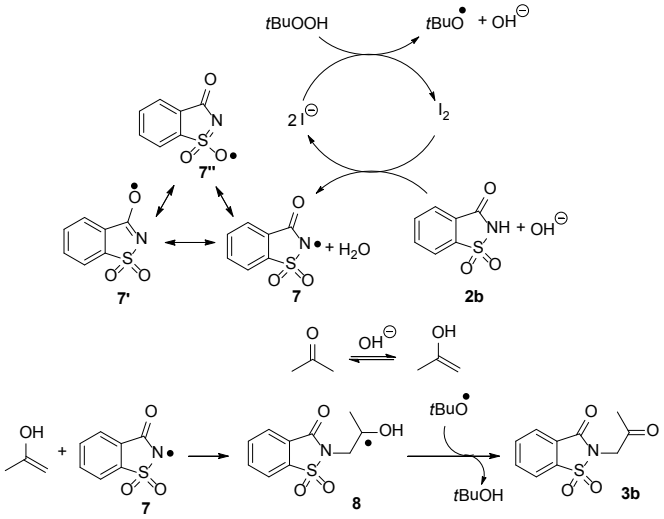
To a solution of the saccharin **2b** (54.9 mg, 0.3 mmol) in ethyl acetate (3.0 ml) was added the acetone **1a** (111 μL, 1.5 mmol), TBHP(109 μL, 0.6 mmol, 5.5 M in decane), and nBu$_4$NI (22.2 mg, 0.06 mmol) in screw-cap test tube. The reaction mixture was stirred at 130 ºC for 40 min in an oil bath with vigorous stirring. The reaction was cooled to room temperature and diluted with CH_3CN (1/100) prior to the injection into the mass spectrometer.

The negative-ion mode of ESI-MS spectrum showed the signals corresponding to the anionic I_3^- species (m/z 380.7151), which might indicate the presence of I_2 (Scheme 3 in manuscript) in the proposed mechanism.



V. Proposed Mechanism

Scheme 3 Proposed Mechanism.



Although an in-depth discussion should await further investigations, at present we support the radical imidation mechanism as described in Scheme 3.[1] At the beginning, the *tert*-butoxyl radical and hydroxide form catalytically from TBHP with the assistance of the iodide anion. Next, hydroxide reacts with saccharin in the presence of I_2 to form a imidyl radical **7**,[2,3] which might be stabilized by its resonance structures **7'** and **7''**. Then in the presence of hydroxide, enol form of ketone will perform a addition reaction with nitrogen-centered radical intermediate **7** to give a tertiary carbon radical **8**, which was oxidized to the imidated product **3b**.[1d,4]

References

1 (a) M. Uyanik, K. Ishihara, *ChemCatChem* 2012, **4**, 177; (b) P. Finkbeiner, B. J. Nachtsheim, *Synthesis* 2013, **45**, 979; (c) Z. J. Liu, J. Zhang, S. L. Chen, E. Shi, Y. Xu, X. B. Wan, *Angew. Chem. Int. Ed.* 2012, **51**, 3231; (d) B. Tan, N. Toda, C. F. Barbas III, *Angew. Chem. Int. Ed*. 2012, **51**, 12538; (e) W. Mai, H. Wang, Z. Li, J. Yuan, Y. Xiao, L. Yang, P. Mao, L. Qu, *Chem. Commun*. 2012, **48**, 10117.

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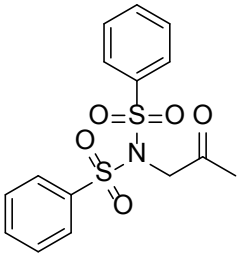
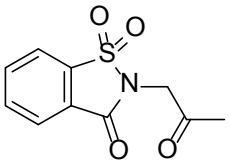
3 Selected examples for generation of imidyl radicals from saccharin and phthalimide, see: (a) H. Togo, Y. Hoshina, T. Muraki, H. Nakayama, M. Yokoyama, *J. Org. Chem.* 1998, **63**, 5193; (b) H. Hettler. *Advances in Heterocyclic Chemistry*, 1973, **15**, 233; (c) C. Sánchez-Sánchez, E. Pérez-Inestrosa, R. García-Segura, R. Suau, *Tetrahedron* 2002, **58**, 7267.

Ⅵ. Analytical data of Compounds 3, 4 and 5



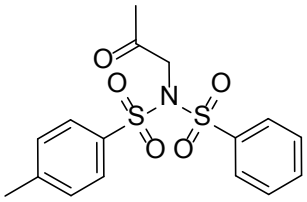
***N*-(2-oxopropyl)-*N*-(phenylsulfonyl)benzenesulfonamide 3a**

White solid. mp:103-104 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.11 (s, 3H), 4.48 (s, 2H), 7.54-7.57 (m, 4H), 7.67 (t, J = 7.5 Hz, 2H), 8.03 (d, J = 7.5 Hz, 4H); ^{13}C NMR (125 MHz, CDCl3): δ = 26.6, 56.1, 128.6, 129.0, 134.2, 139.0, 200.1. HRMS (ESI-TOF) Calcd for $C_{15}H_{16}NO_5S_2$, $[M+H]^+$ *m/z* 354.0464; Found 354.0472.



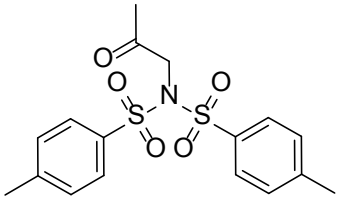
2-(2-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 3b

White solid. mp:146-147 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.29 (s, 3H), 4.50 (s, 2H), 7.85 - 7.92 (m, 2H), 7.95 (d, J = 7.5 Hz, 1H), 8.07 (d, J = 7.0 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 26.8, 46.9, 121.1, 125.3, 126.9, 134.5, 135.0, 137.5, 158.7, 198.3. HRMS (ESI-TOF) Calcd for $C_{10}H_9NNaO_4S$, $[M+Na]^+$ *m/z* 262.0150; Found 262.0158.



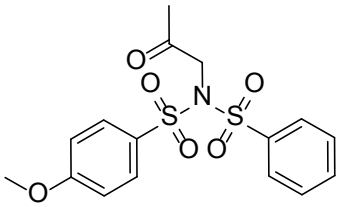
4-methyl-*N*-(2-oxopropyl)-*N*-(phenylsulfonyl)benzenesulfonamide 3c

White solid. mp:84-85 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.10 (s, 3H), 2.44 (s, 3H), 4.47 (s, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.54 (t, J = 7.5 Hz, 2H), 7.65 (t, J = 7.5 Hz, 1H), 7.88 (d, J = 7.5 Hz, 2H), 8.02 (d, J = 8.0 Hz, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 21.6, 26.5, 56.0, 128.5, 128.6, 128.9, 129.5, 134.0, 135.8, 138.9, 145.3, 200.3. HRMS (ESI-TOF) Calcd for $C_{16}H_{17}NNaO_5S_2$, $[M+Na]^+$ *m/z* 390.0440; Found 390.0448.



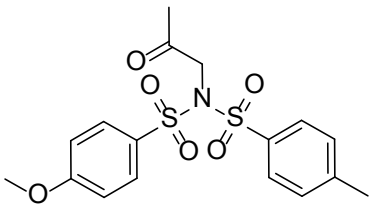
4-methyl-*N*-(2-oxopropyl)-*N*-tosylbenzenesulfonamide 3d

White solid. mp:124-125 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.10 (s, 3H), 2.44 (s, 6H), 4.45 (s, 2H), 7.33 (d, J = 8.0 Hz, 4H), 7.89 (d, J = 8.0 Hz, 4H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 21.6, 26.5, 56.0, 128.6, 129.5, 136.0, 145.2, 200.4. HRMS (ESI-TOF) Calcd for $C_{17}H_{19}NNaO_5S_2$, $[M+Na]^+$ *m/z* 404.0602; Found 404.0594.



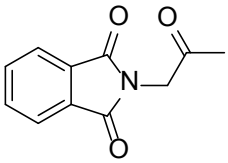
4-methoxy-*N*-(2-oxopropyl)-*N*-(phenylsulfonyl)benzenesulfonamide 3e

White solid. mp:97-98 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.12 (s, 3H), 3.89 (s, 3H), 4.46 (s, 2H), 7.00 (d, J = 8.5 Hz, 2H), 7.55 (t, J = 7.5 Hz, 2H), 7.66 (d, J = 7.5 Hz, 1H), 7.95 (d, J = 9.0 Hz, 2H), 8.02 (d, J = 8.0 Hz, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 26.6, 55.7, 56.0, 114.1, 128.5, 128.9, 130.2, 131.1, 134.0, 139.1, 164.1, 200.3. HRMS (ESI-TOF) Calcd for $C_{16}H_{17}NNaO_6S_2$, $[M+Na]^+$ *m/z* 406.0395; Found 406.0386.



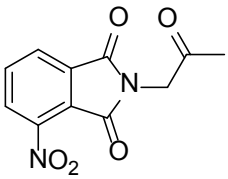
4-methoxy-*N*-(2-oxopropyl)-*N*-tosylbenzenesulfonamide 3f

White solid. mp:185-186 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.11 (s, 3H), 2.44 (s, 3H), 3.88 (s, 3H), 4.44 (s, 2H), 6.99 (d, J = 9.0 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.89 (d, J = 8.5 Hz, 2H), 7.95 (d, J = 8.5 Hz, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 21.6, 26.5, 55.7, 55.9, 114.0, 128.5, 129.5, 130.3, 131.0, 136.0, 145.2, 164.0, 200.5. HRMS (ESI-TOF) Calcd for $C_{17}H_{19}NNaO_6S_2$, $[M+Na]^+$ *m/z* 420.0551; Found 420.0544.



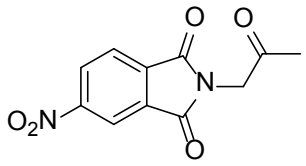
2-(2-oxopropyl)isoindoline-1,3-dione 3g

White solid. mp:139-141 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.28 (s, 3H), 4.51 (s, 2H), 7.75 (dd, J_1 = 3.5 Hz, J_1 = 5.5 Hz, 2H), 7.88 (dd, J_1 = 3.0 Hz, J_1 = 5.5 Hz, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 27.0, 47.1, 123.6, 132.0, 134.2, 167.6, 199.7. HRMS (ESI-TOF) Calcd for $C_{11}H_{10}NO_3$, $[M+H]^+$ *m/z* 204.0661; Found 204.0661.



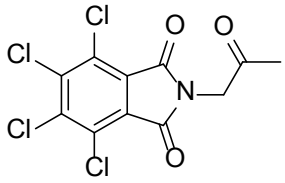
4-nitro-2-(2-oxopropyl)isoindoline-1,3-dione 3h

White solid. mp:175-177 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.30 (s, 3H), 4.55 (s, 2H), 7.95 (t, J = 8.0 Hz, 1H), 8.14 - 817 (m, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 27.0, 47.5, 123.8, 127.3, 128.8, 134.0, 135.6, 145.2, 162.2, 165.1, 198.7. HRMS (ESI-TOF) Calcd for $C_{11}H_8N_2NaO_5$, $[M+Na]^+$ *m/z* 271.0331; Found 271.0327.



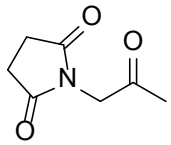
5-nitro-2-(2-oxopropyl)isoindoline-1,3-dione 3i

White solid. mp:179-181 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.31 (s, 3H), 4.57 (s, 2H), 8.08 (d, J = 8.0 Hz, 1H), 8.64 (dd, J_1 = 2.0 Hz, J_1 = 8.5 Hz, 1H), 8.70 (d, J = 1.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 27.0, 47.6, 119.0, 124.8, 129.4, 133.4, 136.4, 151.8, 165.2, 165.5, 198.6. HRMS (ESI-TOF) Calcd for $C_{11}H_9N_2O_5$, $[M+H]^+$ *m/z* 249.0511; Found 249.0519.



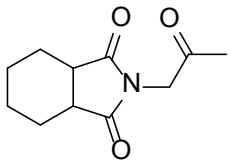
4,5,6,7-tetrachloro-2-(2-oxopropyl)isoindoline-1,3-dione 3j

White solid. mp:211-214 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.29 (s, 3H), 4.52 (s, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 27.0, 47.6, 127.6, 129.9, 140.4, 162.9, 198.6. HRMS (ESI-TOF) Calcd for $C_{11}H_5Cl_4NNaO_3$, $[M+Na]^+$ *m/z* 363.8892; Found 363.8883.



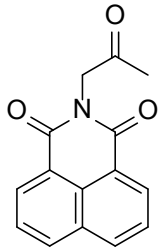
1-(2-oxopropyl)pyrrolidine-2,5-dione 3k

White solid. mp:108-110 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.22 (s, 3H), 2.79 (s, 4H), 4.32 (s, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 26.9, 28.0, 47.4, 176.3, 198.8. HRMS (ESI-TOF) Calcd for $C_7H_{10}NO_3$, $[M+H]^+$ *m/z* 156.0655; Found 156.0663.



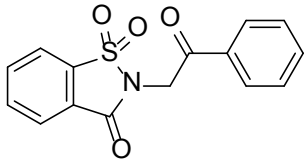
2-(2-oxopropyl)hexahydro-1H-isoindole-1,3(2H)-dione 3l

White solid. mp:112-114 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.49 (t, J = 5.5 Hz, 4H), 1.88 (d, J = 4.0 Hz, 4H), 2.22 (s, 3H), 2.95 (t, J = 4.5 Hz, 2H), 4.29 (s, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 21.5, 23.6, 27.0, 39.8, 47.2, 179.0, 199.1. HRMS (ESI-TOF) Calcd for $C_{11}H_{16}NO_3$, $[M+H]^+$ *m/z* 210.1125; Found 210.1116.



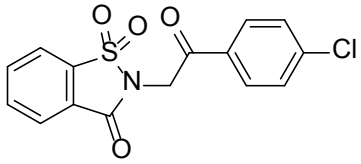
2-(2-oxopropyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione 3m

White solid. mp:213-215 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.34 (s, 3H), 5.02 (s, 2H), 7.75 (t, J = 8.0 Hz, 2H), 8.23 (d, J = 8.0 Hz, 2H), 8.58 (d, J = 7.5 Hz, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 27.3, 49.3, 122.2, 126.9, 128.3, 131.5, 131.6, 134.3, 163.8, 200.6. HRMS (ESI-TOF) Calcd for $C_{15}H_{12}NO_3$, $[M+H]^+$ *m/z* 254.0812; Found 254.0819.



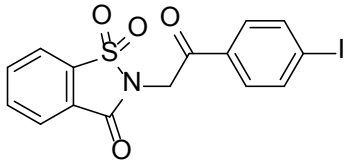
2-(2-oxo-2-phenylethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4b

White solid. mp:196 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 5.16 (s, 2H), 7.53 (t, J = 7.5 Hz, 2H), 7.65 (t, J = 7.0 Hz, 1H), 7.85 - 7.92 (m, 2H), 7.97 (d, J = 7.5 Hz, 1H), 8.02 (d, J = 7.5 Hz, 2H), 8.10 (d, J = 7.0 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 44.4, 121.2, 125.4, 127.3, 128.2, 129.0, 134.0, 134.2, 134.4, 134.9, 137.9, 159.1, 188.7. HRMS (ESI-TOF) Calcd for $C_{15}H_{12}NO_4S$, $[M+H]^+$ *m/z* 302.0487; Found 302.0480.



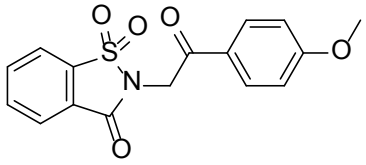
2-(2-(4-chlorophenyl)-2-oxoethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4c

White solid. mp:194-196 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 5.12 (s, 2H), 7.51 (d, J = 8.5 Hz, 2H), 7.88 - 7.92 (m, 2H), 7.94 - 7.99 (m, 3H), 8.12 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 44.3, 121.2, 125.5, 127.2, 129.4, 129.6, 132.3, 134.5, 135.0, 137.8, 140.8, 159.1, 187.8. HRMS (ESI-TOF) Calcd for $C_{15}H_{10}ClNNaO_4S$, $[M+Na]^+$ *m/z* 357.9917; Found 357.9923.



2-(2-(4-iodophenyl)-2-oxoethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4d

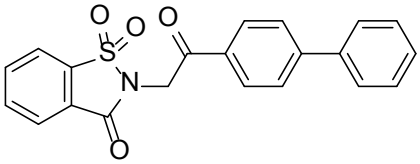
White solid. mp:233-235 ºC ^{1}H NMR (500 MHz; DMSO): δ = 5.46 (s, 2H), 7.84 (d, J = 8.5 Hz, 2H), 7.98 (d, J = 8.0 Hz, 2H), 8.04 (d, J = 7.0 Hz, 1H), 8.09 (d, J = 7.5 Hz, 1H), 8.15 (d, J = 7.5 Hz, 1H), 8.35 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; DMSO): δ = 45.2, 103.8, 122.3, 125.7, 126.6, 130.5, 133.6, 135.9, 136.6, 137.7, 138.4, 159.3, 190.4. HRMS (ESI-TOF) Calcd for $C_{15}H_{10}INNaO_4S$, $[M+Na]^+$ *m/z* 449.9267; Found 449.9252.



2-(2-(4-methoxyphenyl)-2-oxoethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4e

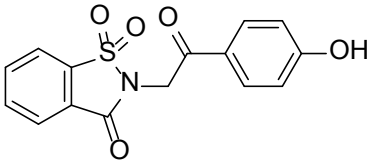
White solid. mp:194-196 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 3.90 (s, 3H), 5.11 (s, 2H), 6.99 (d, J = 8.5 Hz, 2H), 7.85 - 7.92 (m, 2H), 7.96 - 8.00 (m, 3H), 8.11 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 44.1, 55.6, 114.2, 121.2, 125.4, 127.1, 127.4, 130.5, 134.4, 134.9, 137.9, 159.2, 164.3, 187.1. HRMS (ESI-TOF) Calcd for $C_{16}H_{13}NNaO_5S$, $[M+Na]^+$ *m/z* 354.0412; Found

354.0408.



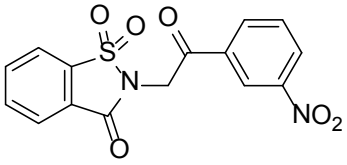
2-(2-([1,1'-biphenyl]-4-yl)-2-oxoethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4f

White solid. mp:216-218 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 5.19 (s, 2H), 7.43 (d, J = 7.0 Hz, 1H), 7.49 (t, J = 7.5 Hz, 2H) 7.64 (d, J = 7.5 Hz, 2H), 7.74 (d, J = 8.0 Hz, 2H), 7.85 - 7.92 (m, 2H), 7.97 (d, J = 7.5 Hz, 1H), 8.08 - 8.12 (m, 3H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 44.4, 121.2, 125.4, 127.3, 127.5, 128.5, 128.8, 129.0, 132.7, 134.5, 134.9, 137.9, 139.5, 146.9, 159.1, 188.3. HRMS (ESI-TOF) Calcd for $C_{21}H_{16}NO_4S$, $[M+H]^+$ *m/z* 378.0800; Found 378.0790.



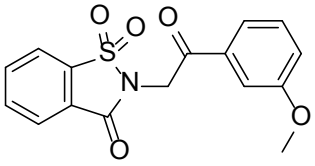
2-(2-(4-hydroxyphenyl)-2-oxoethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4g

White solid. mp:251-252 ºC ^{1}H NMR (500 MHz; DMSO): δ = 5.32 (s, 2H), 6.89 (d, J = 9.0 Hz, 2H), 7.96 (d, J = 8.5 Hz, 2H), 8.04 (d, J = 7.5 Hz, 1H), 8.09 (t, J = 7.5 Hz, 1H), 8.14 (d, J = 7.5 Hz, 1H), 8.34 (d, J = 8.0 Hz, 1H), 10.57 (s, 1H). ^{13}C NMR (125 MHz; DMSO): δ = 44.9, 116.0, 122.2, 125.6, 125.9, 126.8, 131.5, 135.8, 136.5, 137.7, 159.4, 163.4, 188.3. HRMS (ESI-TOF) Calcd for $C_{15}H_{12}NO_5S$, $[M+H]^+$ *m/z* 318.0431; Found 318.0421.



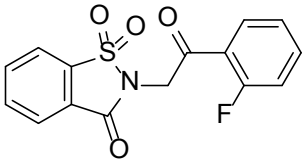
2-(2-(3-nitrophenyl)-2-oxoethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4h

White solid. mp:216-217 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 5.20 (s, 2H), 7.77 (t, J = 8.0 Hz, 1H), 7.90 - 7.96 (m, 2H), 8.00 (d, J = 7.0 Hz, 1H), 8.13 (d, J = 7.0 Hz, 1H), 8.35 (d, J = 8.0 Hz, 1H), 8.52 (dd, J_1 = 1.5 Hz, J_1 = 8.5 Hz, 1H), 8.85 (t, J = 2.0 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 44.5, 121.3, 123.1, 125.6, 127.1, 128.4, 130.4, 133.7, 134.6, 135.2, 135.2, 137.8, 148.5, 159.0, 187.3. HRMS (ESI-TOF) Calcd for $C_{15}H_{10}N_2NaO_6S$, $[M+Na]^+$ *m/z* 369.0517; Found 369.0518.



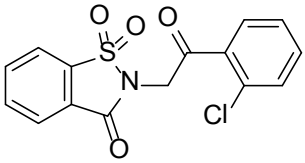
2-(2-(3-methoxyphenyl)-2-oxoethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4i

White solid. mp:185 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 3.86 (s, 3H), 5.15 (s, 2H), 7.19 (d, J = 8.0 Hz, 1H), 7.44 (t, J = 8.0 Hz, 1H), 7.53 (s, 1H), 7.59 (d, J = 7.5 Hz, 1H), 7.86 - 7.93 (m, 2H), 7.97 (d, J = 8.0 Hz, 1H), 8.11 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 44.5, 55.5, 112.3, 120.6, 120.9, 121.2, 125.4, 127.3, 129.9, 134.5, 134.9, 135.3, 137.9, 159.1, 160.0, 188.6. Calcd for $C_{16}H_{14}NO_5S$, $[M+H]^+$ *m/z* 332.0593; Found 332.0580.



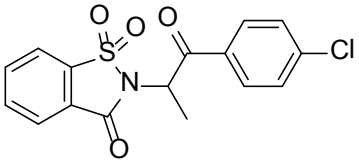
2-(2-(2-fluorophenyl)-2-oxoethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4j

White solid. mp:158-160 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 5.09 (d, J = 3.5 Hz, 2H), 7.21 - 7.25 (m, 1H), 7.30 (t, J = 8.0 Hz, 1H), 7.63 (d, J = 7.0 Hz, 1H), 7.85 - 7.93 (m, 2H), 7.97 (d, J = 7.5 Hz, 1H), 8.00 - 8.03 (m, 1H), 8.11 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 47.8, 47.9, 116.6, 116.8, 121.2, 122.1, 122.2, 125.0, 125.0, 125.4, 127.3, 131.2, 134.4, 134.9, 136.1, 136.2, 137.9, 159.1, 161.5, 163.5, 187.0, 187.0. Calcd for $C_{15}H_{11}FNO_4S$, $[M+H]^+$ *m/z* 320.0387; Found 320.0397.



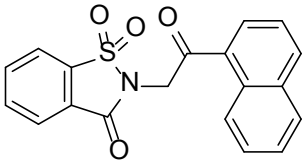
2-(2-(2-chlorophenyl)-2-oxoethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4k

White solid. mp:159-161 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 5.13 (s, 2H), 7.38 - 7.42 (m, 1H), 7.49 (d, J = 4.0 Hz, 2H), 7.75 (d, J = 7.5 Hz, 1H), 7.86 - 7.93 (m, 2H), 7.97 (d, J = 7.0 Hz, 1H), 8.11 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 47.1, 121.2, 125.4, 127.1, 127.3, 130.5, 130.9, 131.9, 133.4, 134.5, 135.0, 135.4, 137.8, 159.0, 191.4. Calcd for $C_{15}H_{10}ClNNaO_4S$, $[M+Na]^+$ *m/z* 357.9917; Found 357.9909.



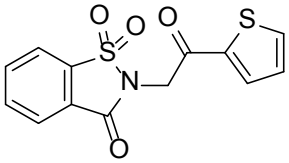
2-(1-(4-chlorophenyl)-1-oxopropan-2-yl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4l

White solid. mp:212 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.77 (d, J = 7.0 Hz, 3H), 6.40 (q, J = 7.0 Hz, 1H), 7.49 - 7.51 (m, 2H), 7.74 - 7.78 (m, 1H), 7.78 - 7.81 (m, 1H), 7.88 (d, J = 8.0 Hz, 2H), 7.92 (d, J = 8.5 Hz, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 17.6, 77.7, 122.0, 123.7, 126.3, 129.4, 129.9, 132.0, 133.5, 134.4, 140.8, 143.6, 168.4, 193.3. HRMS (ESI-TOF) Calcd for $C_{16}H_{12}ClNNaO_4S$, $[M+Na]^+$ *m/z* 372.0073; Found 372.0074.



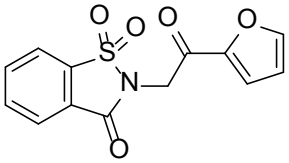
2-(2-(naphthalen-1-yl)-2-oxoethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4m

White solid. mp:216-217 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 5.18 (s, 2H), 7.56 (t, J = 7.5 Hz, 2H), 7.60 - 7.63 (m, 1H), 7.86 - 7.92 (m, 3H), 7.98 (d, J = 7.0 Hz, 1H), 8.03 (d, J = 7.0 Hz, 1H), 8.08 (d, J = 8.0 Hz, 1H), 8.13 (d, J = 7.0 Hz, 1H), 8.72 (d, J = 8.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 46.2, 121.2, 124.2, 125.5, 125.8, 126.9, 127.3, 128.1, 128.5, 128.6, 130.3, 132.0, 134.0, 134.1, 134.5, 135.0, 137.9, 159.2, 192.1. HRMS (ESI-TOF) Calcd for $C_{19}H_{14}NO_4S$, $[M+H]^+$ *m/z* 352.0638; Found 352.0640.



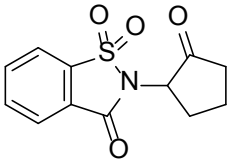
2-(2-oxo-2-(thiophen-2-yl)ethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4n

White solid. mp:209-211 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 5.08 (s, 2H), 7.21 (t, J = 4.5 Hz, 1H), 7.76 (d, J = 5.0 Hz, 1H), 7.86 - 7.93 (m, 3H), 7.97 (d, J = 7.0 Hz, 1H), 8.11 (d, J = 7.0 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 44.2, 121.2, 125.5, 127.2, 128.4, 132.6, 134.5, 135.0, 135.0, 137.8, 140.2, 159.0, 181.9. HRMS (ESI-TOF) Calcd for $C_{13}H_9NNaO_4S_2$, $[M+Na]^+$ *m/z* 329.9871; Found 329.9876.



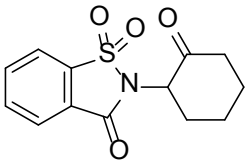
2-(2-(furan-2-yl)-2-oxoethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4o

White solid. mp:185-186 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 5.03 (s, 2H), 6.62 (d, J = 2.0 Hz, 1H), 7.35 (d, J = 3.5 Hz, 1H), 7.67 (s, 1H), 7.85 - 7.92 (m, 2H), 7.96 (d, J = 7.5 Hz, 1H), 8.10 (d, J = 7.0 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 43.7, 112.8, 118.3, 121.2, 125.4, 127.2, 134.4, 135.0, 137.8, 147.1, 150.6, 159.0, 178.4. HRMS (ESI-TOF) Calcd for $C_{13}H_{10}NO_5S$, $[M+H]^+$ *m/z* 292.0274; Found 292.0267.



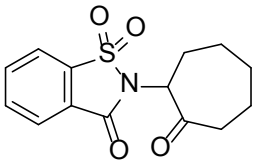
2-(2-oxocyclopentyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4p

White solid. mp:173 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.91 - 1.97 (m, 1H), 2.26 - 2.31 (m, 1H), 2.44 - 2.55 (m, 4H), 4.35 - 4.39 (m, 1H), 7.82 - 7.93 (m, 3H),8.02 (d, J = 7.0 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 19.0, 26.7, 35.5, 56.2, 121.0, 125.2, 127.0, 134.4, 134.9, 137.7, 158.1, 209.4. HRMS (ESI-TOF) Calcd for $C_{12}H_{11}NNaO_4S$, $[M+Na]^+$ *m/z* 288.0301; Found 288.0302.



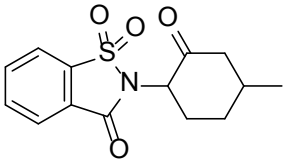
2-(2-oxocyclohexyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4q

White solid. mp:162-163 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.69 - 1.74 (m, 1H), 1.83 - 1.91 (m, 1H), 1.96 - 2.02 (m, 1H), 2.04 - 2.09 (m, 1H), 2.16 - 2.18 (m, 1H), 2.45 - 2.52 (m, 1H), 2.60 - 2.62 (m, 2H), 5.59 - 5.63 (m, 1H),7.72 (t, J = 7.5 Hz, 1H), 7.78 (t, J = 7.5 Hz, 1H), 7.84 (d, J = 7.0 Hz, 1H), 7.88 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 23.5, 26.9, 33.1, 40.7, 82.8, 121.8, 123.6, 126.5, 133.4, 134.2, 143.5, 168.5, 201.7. HRMS (ESI-TOF) Calcd for $C_{13}H_{14}NO_4S$, $[M+H]^+$ *m/z* 280.0638; Found 280.0638.



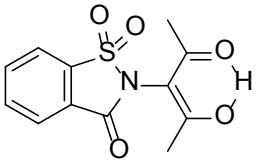
2-(2-oxocycloheptyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4r

White solid. mp:138-139 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.41 (t, J = 10.0 Hz, 1H), 1.73 - 1.83 (m, 2H), 1.93 - 2.02 (m, 4H), 2.26 - 2.29 (m, 1H), 2.48 - 2.55 (m, 1H), 2.73 - 2.78 (m, 1H), 5.71 (dd, J_1 = 3.0 Hz, J_1 = 10.0 Hz, 1H), 7.72 (t, J = 7.5 Hz, 1H), 7.78 (t, J = 7.5 Hz, 1H), 7.83 -7.88 (m, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 22.8, 26.2, 28.2, 30.5, 40.6, 84.7, 121.8, 123.6, 126.5, 133.4, 134.2, 143.5, 168.3, 204.6. HRMS (ESI-TOF) Calcd for $C_{14}H_{16}NO_4S$, $[M+H]^+$ *m/z* 294.0795; Found 294.0803.



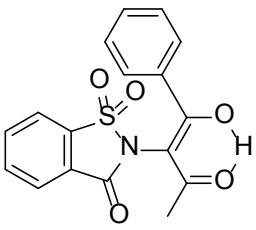
2-(4-methyl-2-oxocyclohexyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4s

White solid. mp:207-208 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.12 (d, J = 7.0 Hz, 3H), 1.44 - 1.48 (m, 1H), 1.73 - 1.80 (m, 1H), 2.08 - 2.13 (m, 1H), 2.18 - 2.22 (m, 1H), 2.51 - 2.55 (m, 1H), 2.55 - 2.57 (m, 2H), 5.64 - 5.68 (m, 1H), 7.71 - 7.74 (m, 1H), 7.77 - 7.80 (m, 1H), 7.83 (d, J = 7.5 Hz, 1H), 7.88 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 20.9, 30.7, 34.8, 39.5, 40.7, 81.8, 121.9, 123.6, 126.6, 133.4, 134.2, 143.6, 168.5, 201.9. HRMS (ESI-TOF) Calcd for $C_{14}H_{16}NO_4S$, $[M+H]^+$ *m/z* 294.0795; Found 294.0791.



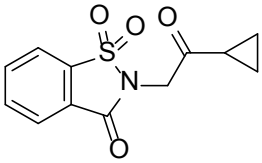
(E)-2-(2-hydroxy-4-oxopent-2-en-3-yl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4t

White solid. mp:175-176 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.17 (s, 6H), 7.93 - 8.01 (m, 2H), 8.04 (d, J = 8.0 Hz, 1H), 8.19 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 22.1, 102.7, 121.5, 125.8, 126.4, 134.6, 135.5, 137.7, 158.3, 194.3. HRMS (ESI-TOF) Calcd for $C_{12}H_{11}NNaO_5S$, $[M+Na]^+$ *m/z* 304.0256; Found 304.0266.



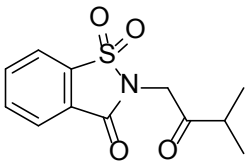
2-(1,1-dioxido-3-oxobenzo[d]isothiazol-2(3H)-yl)-1-phenylbutane-1,3-dione 4u

White solid. mp:189-190 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.24 (s, 3H), 7.30 (t, J = 7.5 Hz, 2H), 7.39 (d, J = 7.5 Hz, 1H) 7.55 (d, J = 7.5 Hz, 2H), 7.86 - 7.88 (m, 3H), 8.17 (t, J = 3.5 Hz, 1H), 17.23 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 23.2, 101.7, 121.5, 125.8, 126.1, 127.1, 128.2, 131.6, 134.2, 134.5, 135.4, 137.6, 159.4, 188.7, 197.9. HRMS (ESI-TOF) Calcd for $C_{17}H_{13}NNaO_5S$, $[M+Na]^+$ *m/z* 366.0412; Found 366.0416.



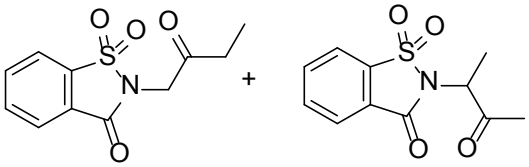
2-(2-cyclopropyl-2-oxoethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4v

White solid. mp:166-167 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.02 - 1.06 (m, 2H), 1.18 - 1.21 (m, 2H), 2.04 - 2.07 (m, 1H), 4.65 (s, 2H), 7.84 - 7.91 (m, 2H), 7.95 (d, J = 7.5 Hz, 1H), 8.08 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 12.0, 18.1, 47.0, 121.1, 125.4, 127.2, 134.4, 134.9, 137.8, 158.9, 200.4. HRMS (ESI-TOF) Calcd for $C_{12}H_{12}NO_4S$, $[M+H]^+$ *m/z* 266.0482; Found 266.0482.



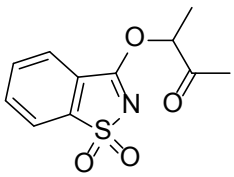
2-(3-methyl-2-oxobutyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4w

White solid. mp:143 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.23 (d, J = 7.0 Hz, 6H), 2.79 - 2.82 (m, 1H), 4.56 (s, 2H), 7.84 - 7.91 (m, 2H), 7.94 (d, J = 7.5 Hz, 1H), 8.07 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 18.0, 38.4, 44.8, 121.1, 125.3, 127.2, 134.4, 134.9, 137.7, 158.9, 203.5. HRMS (ESI-TOF) Calcd for $C_{12}H_{13}NNaO_4S$, $[M+Na]^+$ *m/z* 290.0463; Found 290.0454.



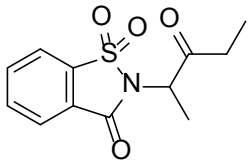
2-(2-oxobutyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4x and **2-(3-oxobutan-2-yl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide (3:2) 4x'**

White solid. mp:150-151 ºC. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.14 (t, J = 7.5 Hz, 3H), 1.78 (d, J = 7.0 Hz, 3H), 2.26 (s, 3H), 2.60 (q, J = 7.0 Hz, 2H), 4.49 (s, 2H), 4.62 (q, J = 7.5 Hz, 1H), 7.85 - 7.93 (m, 4H), 7.96 (d, J = 7.5 Hz, 2H), 8.08 (t, J = 7.0 Hz, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 7.2, 13.6, 26.0, 32.9, 46.2, 56.4, 121.0, 121.2, 125.3, 125.4, 126.8, 127.1, 134.5, 135.0, 135.1, 137.7, 137.8, 158.7, 158.9, 201.0, 201.8. HRMS (ESI-TOF) Calcd for $C_{11}H_{11}NNaO_4S$, $[M+Na]^+$ *m/z* 276.0306; Found 276.0310.



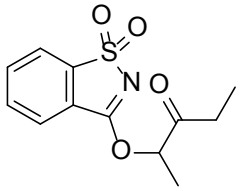
3-((1,1-dioxidobenzo[d]isothiazol-3-yl)oxy)butan-2-one 4x"

White solid. mp:137-138 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.68 (d, J = 7.0 Hz, 3H), 2.30 (s, 3H), 5.55 (d, J = 7.0 Hz, 1H), 7.75 (t, J = 7.5 Hz, 1H), 7.79 - 7.85 (m, 2H), 7.89 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 16.2, 26.0, 81.2, 122.0, 123.5, 126.3, 133.5, 134.4, 143.5, 168.4, 202.5. HRMS (ESI-TOF) Calcd for $C_{11}H_{12}NO_4S$, $[M+H]^+$ *m/z* 254.0482; Found 254.0476.



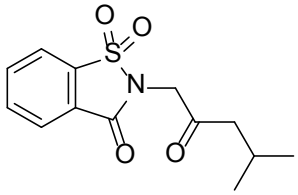
2-(3-oxopentan-2-yl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4y

White solid. mp:95-96 ºC. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.09 (t, J = 7.5 Hz, 3H), 1.79 (t, J = 7.5 Hz, 3H), 2.58 (q, J = 3.0 Hz, 2H), 4.65 (q, J = 7.5 Hz, 1H), 7.87 (dd, J_1 = 1.5 Hz, J_1 = 7.5 Hz, 1H), 7.90 - 7.96 (m, 2H), 8.06 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 7.5, 13.7, 31.5, 56.0, 121.0, 125.3, 126.8, 134.5, 135.0, 137.8, 158.8, 204.5. HRMS (ESI-TOF) Calcd for $C_{12}H_{13}NNaO_4S$, $[M+Na]^+$ *m/z* 290.0463; Found 290.0451.



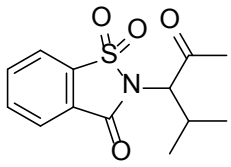
2-((1,1-dioxidobenzo[d]isothiazol-3-yl)oxy)pentan-3-one 4y'

White solid. mp:157-158 ºC. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.13 (t, J = 7.5 Hz, 3H), 1.67 (d, J = 7.0 Hz, 3H), 2.56 - 2.69 (m, 2H), 5.57 (q, J = 7.5 Hz, 1H), 7.75 (t, J = 7.5 Hz, 1H), 7.79 - 7.82 (m, 1H), 7.84 (d, J = 7.5 Hz, 1H), 7.89 (d, J = 8.0 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 7.1, 16.5, 31.8, 80.9, 121.9, 123.5, 126.3, 133.5, 134.3, 143.5, 168.4, 205.5. HRMS (ESI-TOF) Calcd for $C_{12}H_{14}NO_4S$, $[M+H]^+$ *m/z* 268.0638; Found 268.0629.



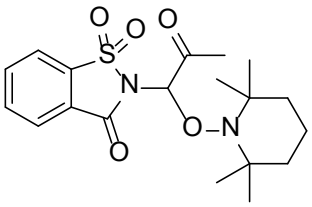
2-(4-methyl-2-oxopentyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4z

White solid. mp:150-151 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 0.98 (d, J = 6.5 Hz, 6H), 2.20 - 2.25 (m, 1H), 2.43 (d, J = 6.5 Hz, 2H), 4.45 (s, 2H), 7.85 - 7.92 (m, 2H), 7.95 (d, J = 7.0 Hz, 1H), 8.09 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 22.5, 24.7, 47.0, 48.3, 121.2, 125.4, 127.2, 134.5, 135.0, 137.8, 158.9, 200.0. HRMS (ESI-TOF) Calcd for $C_{13}H_{15}NNaO_4S$, $[M+Na]^+$ *m/z* 304.0619; Found 304.0612.



2-(2-methyl-4-oxopentan-3-yl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4z'

White solid. mp:63-64 ºC. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.09 (d, J = 7.0 Hz, 3H), 1.16 (d, J = 6.5 Hz, 3H), 2.28 (s, 3H), 2.45 - 2.49 (m, 1H), 5.32 (d, J = 4.0 Hz, 1H), 7.75 (t, J = 7.5 Hz, 1H), 7.79 - 7.85 (m, 2H), 7.90 (d, J = 7.0 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 16.6, 19.2, 27.3, 88.9, 122.0, 123.4, 126.4, 133.5, 134.3, 143.6, 168.9, 202.0. HRMS (ESI-TOF) Calcd for $C_{13}H_{15}NNaO_4S$, $[M+Na]^+$ *m/z* 304.0619; Found 304.0612.

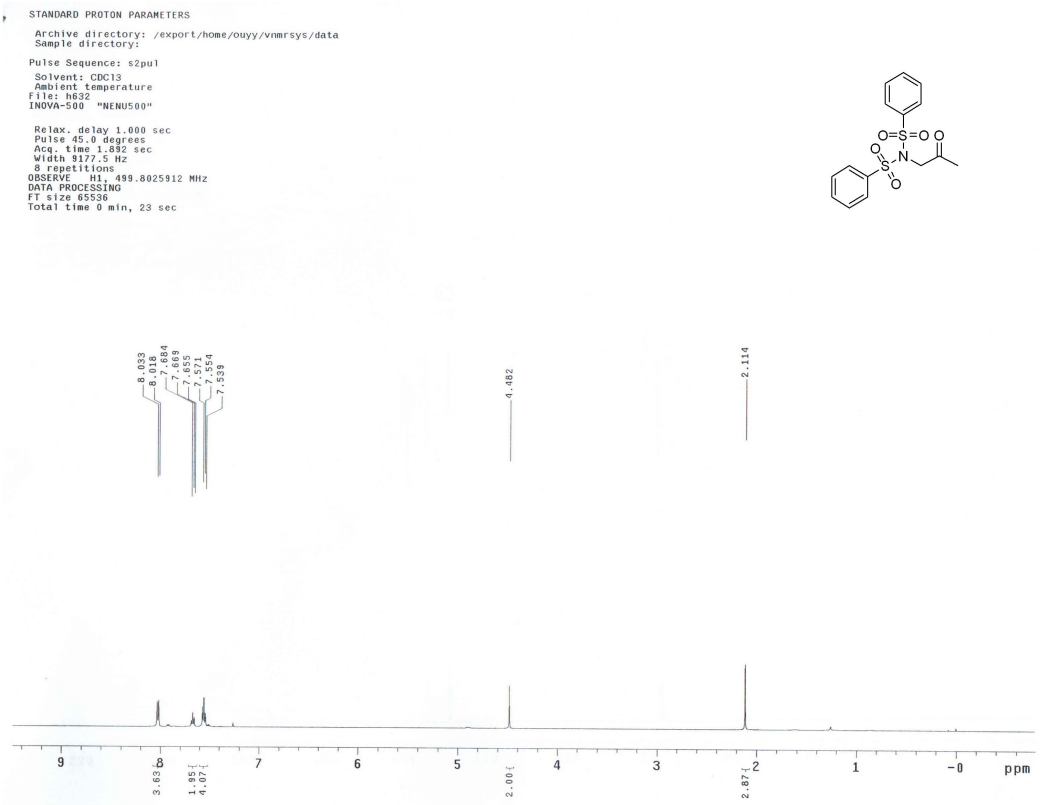


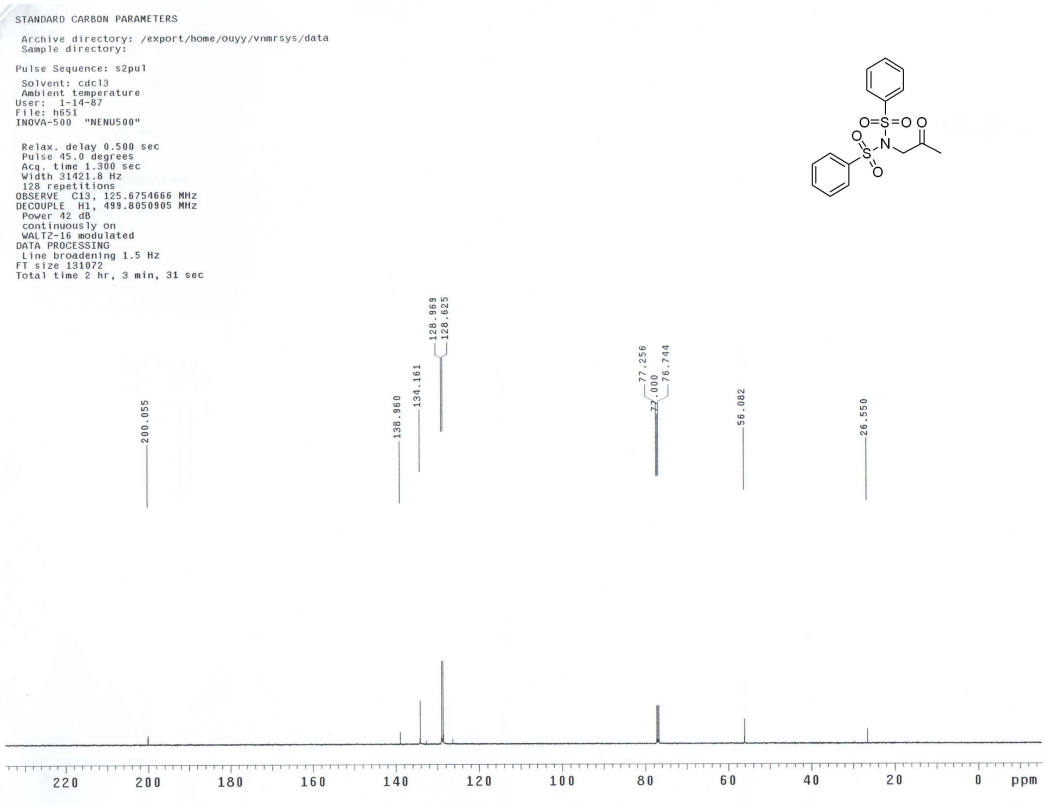
2-(2-oxo-1-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)propyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 5

White solid. mp:152-154 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.03 (s, 3H), 1.16 (s, 3H), 1.25 (s, 3H), 1.31 (s, 4H), 1.43 - 1.50 (m, 3H), 1.59 (s, 2H), 2.54 (s, 3H), 5.82 (s, 1H), 7.83 (d, J = 7.5 Hz, 1H), 7.88 - 7.93 (m, 2H), 8.03 (d, J = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 16.9, 20.5, 20.6, 28.0, 32.1, 33.5, 40.0, 59.9, 61.5, 88.2, 121.1, 125.5, 126.3, 134.3, 135.3, 138.1, 159.2, 200.8. HRMS (ESI-TOF) Calcd for $C_{19}H_{27}N_2O_5S$, $[M+H]^+$ *m/z* 395.1635; Found 395.1623.

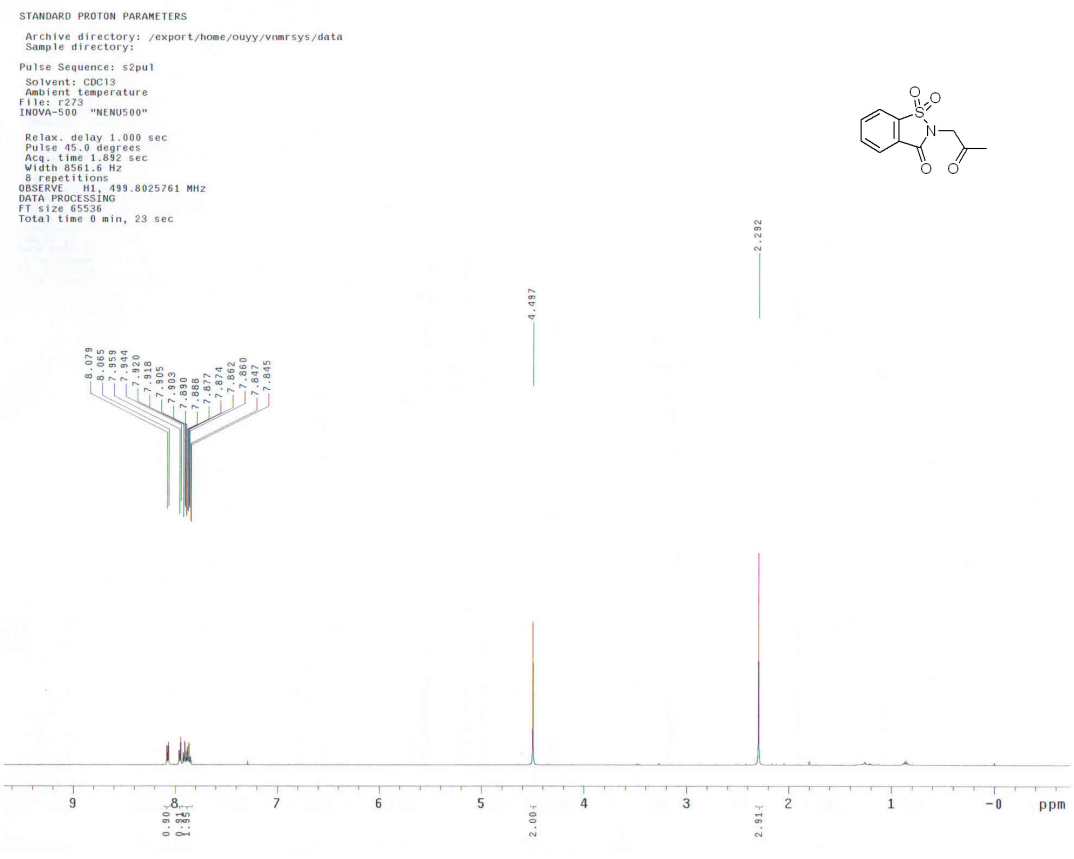
Ⅶ ^{1}H and ^{13}C Spectra of Compounds 3, 4 and 5

Product 3a





Product 3b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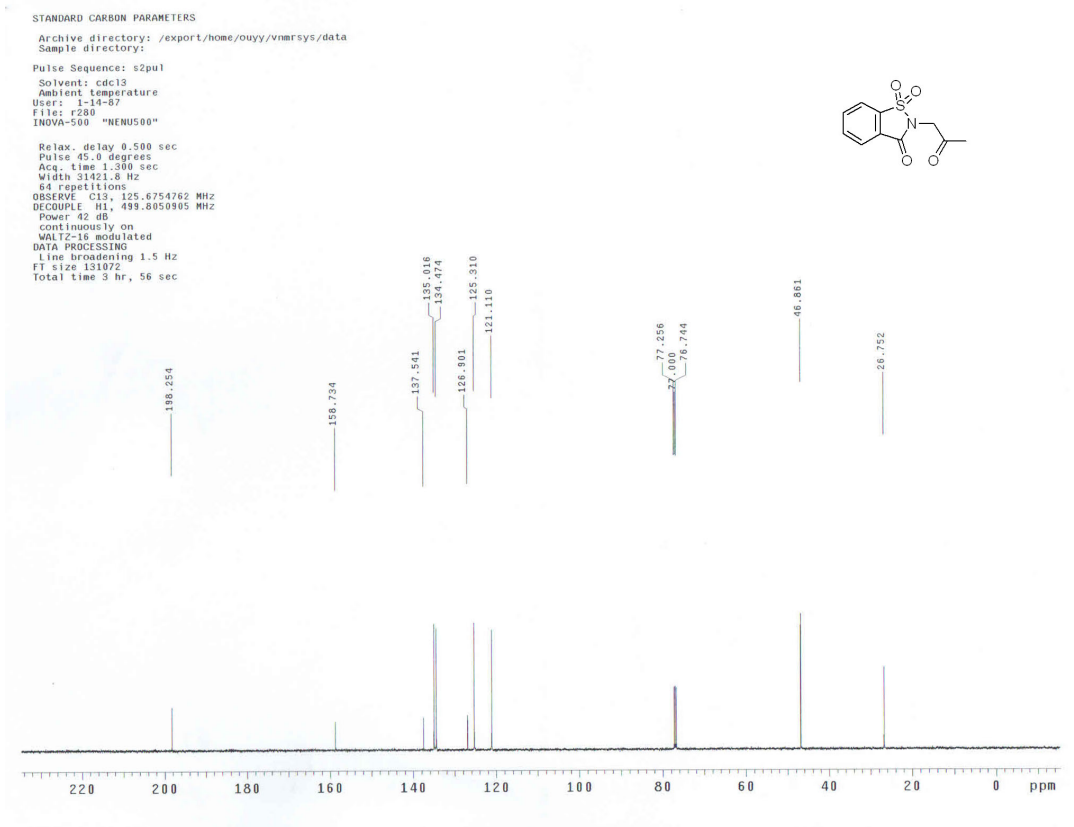
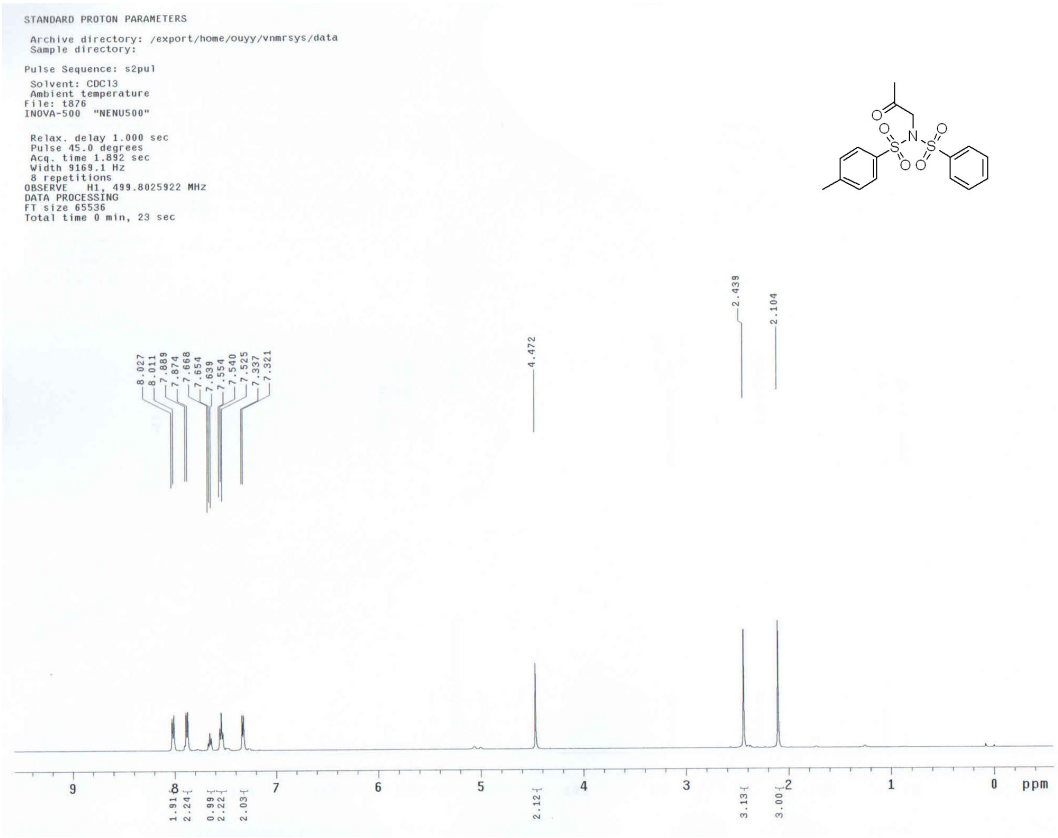
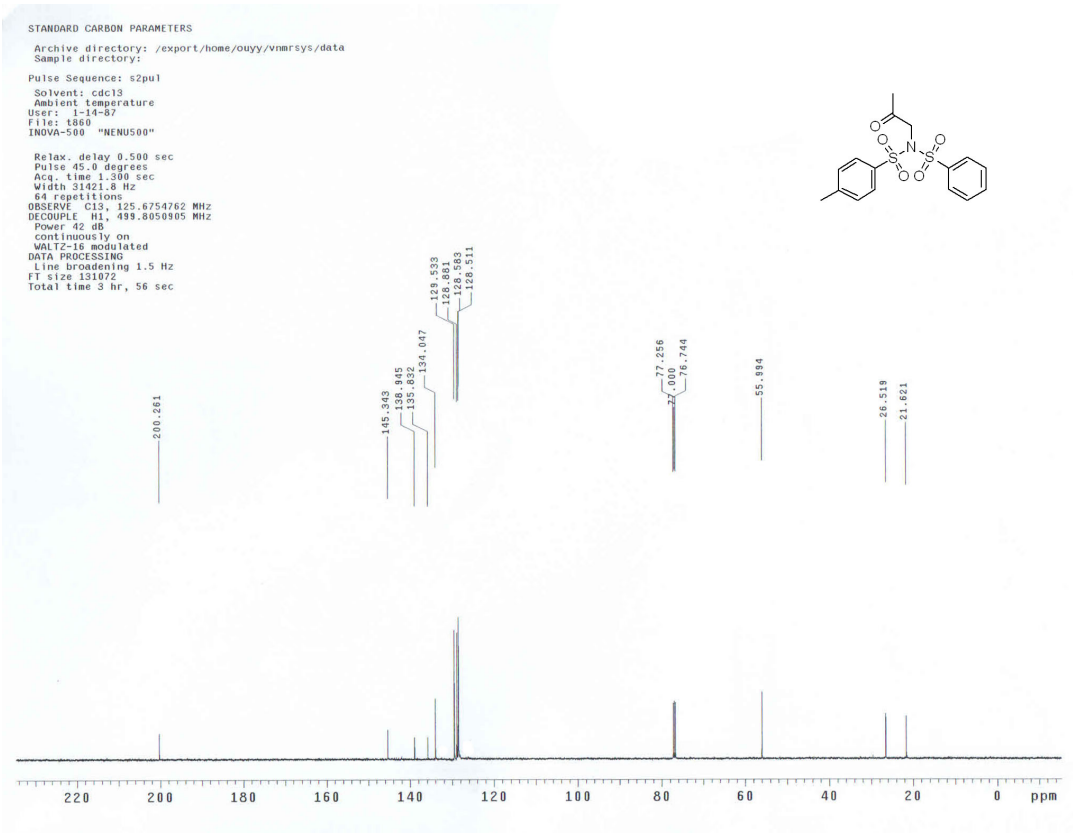
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: r273
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8561.6 Hz
8 repetitions
OBSERVE H1, 499.8025761 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.079
8.065
7.959
7.944
7.920
7.918
7.905
7.903
7.890
7.889
7.887
7.874
7.862
7.860
7.847
7.845
4.497
2.282
ppm

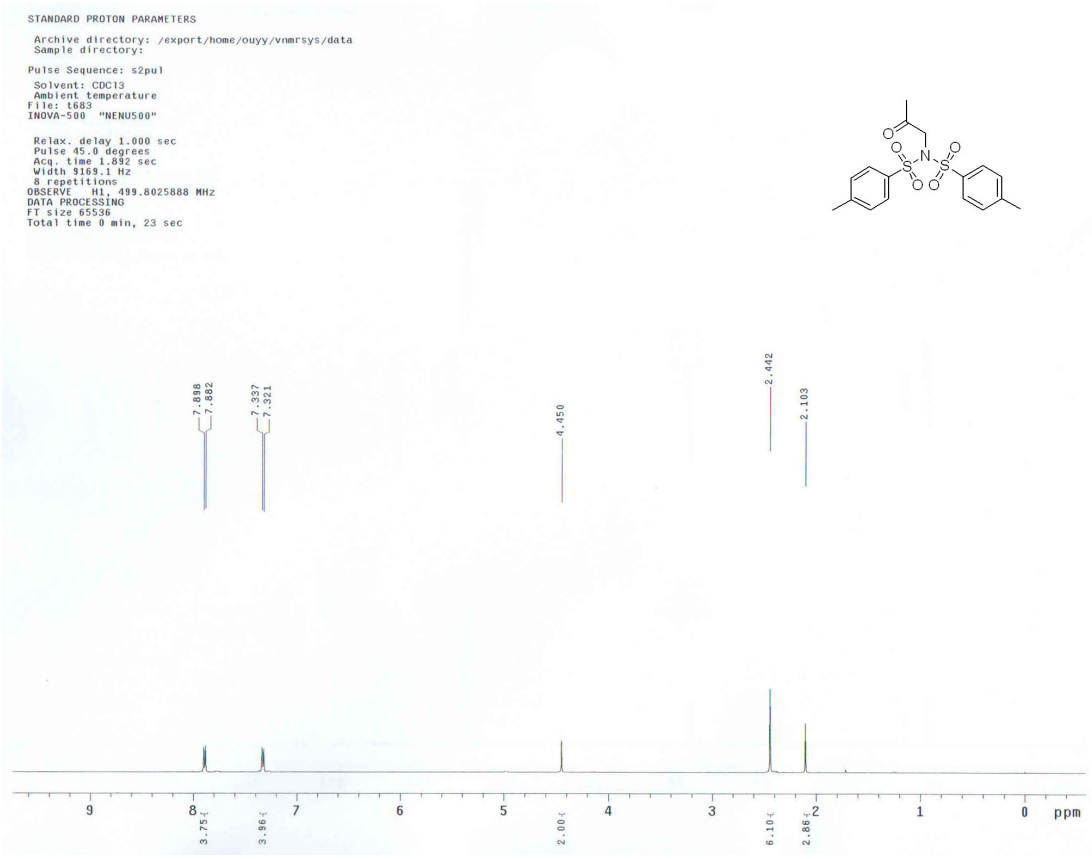

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: r280
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754762 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
198.254
158.734
137.541
135.016
134.474
126.901
125.910
121.110
77.256
77.000
76.744
46.861
26.752
ppm

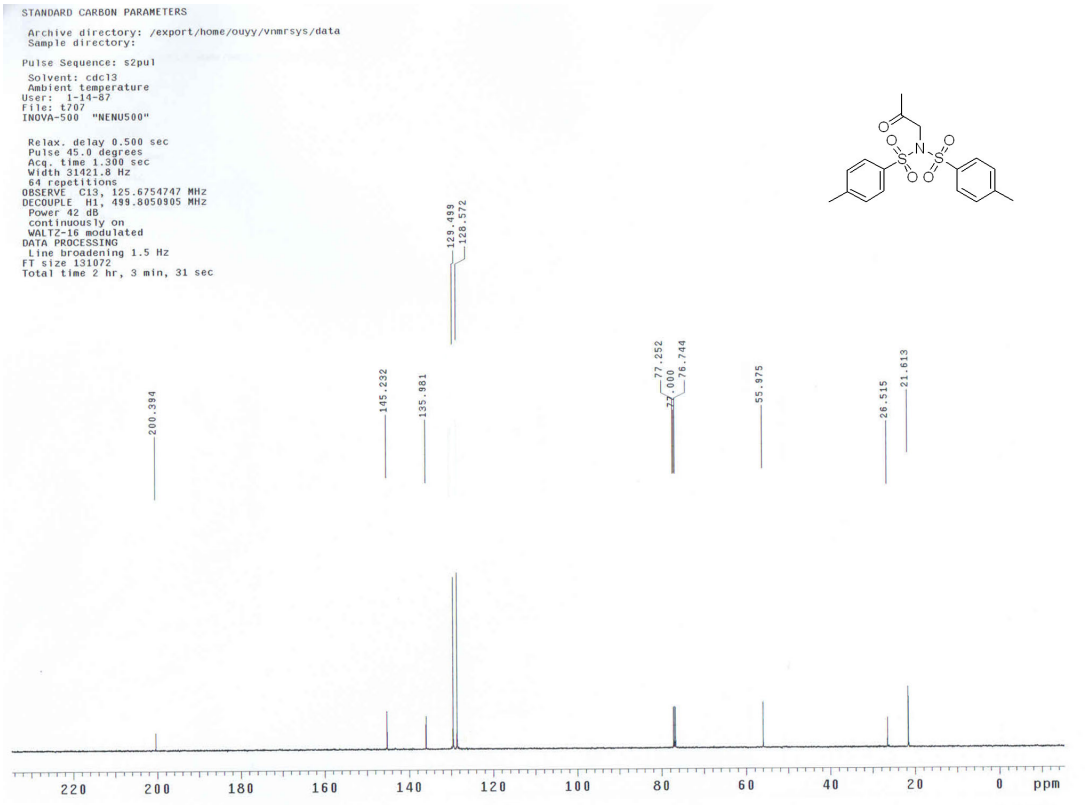
Product 3c


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: t876
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9169.1 Hz
8 repetitions
OBSERVE H1, 499.8025922 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.027
8.011
7.888
7.874
7.668
7.654
7.639
7.554
7.540
7.525
7.337
7.321
4.472
2.439
2.104
ppm

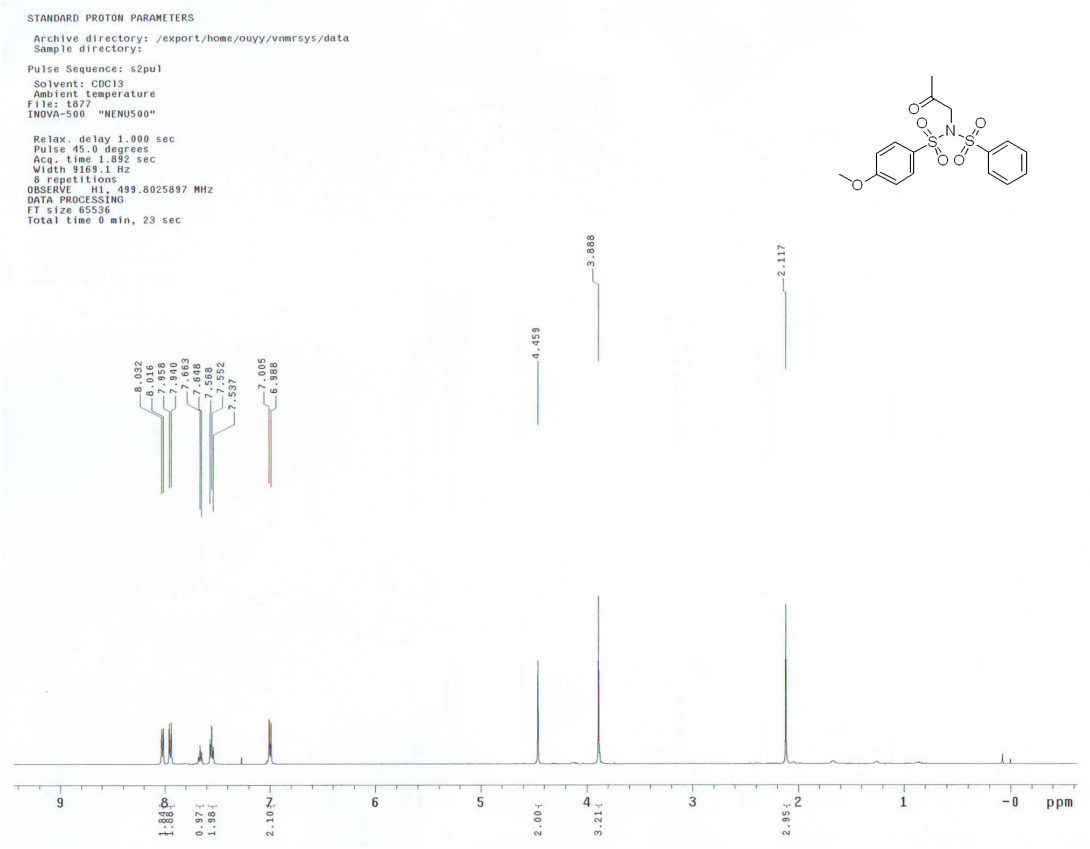

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: t860
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754762 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
200.261
145.343
138.945
135.832
134.047
129.533
128.883
128.583
128.511
77.256
77.000
76.744
55.984
26.519
21.621
ppm

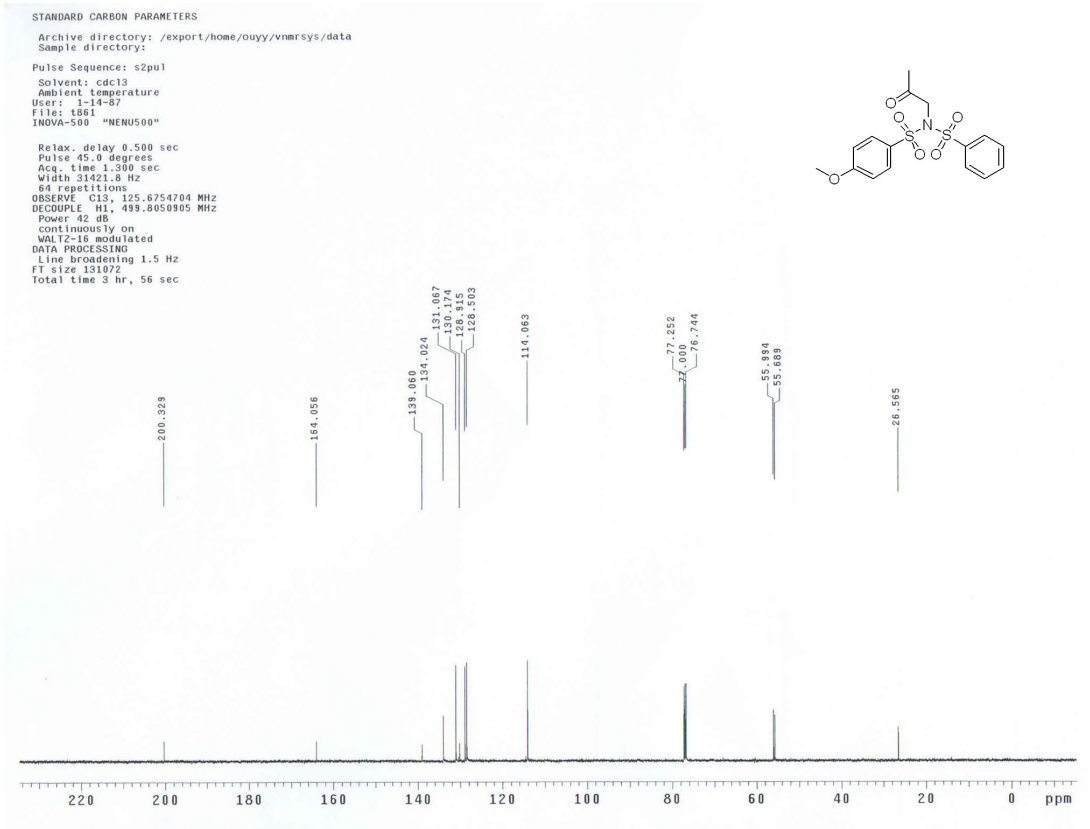
Product 3d


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: t683
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 9169.1 Hz
8 repetitions
OBSERVE H1, 499.8025888 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.898
7.882
7.337
7.321
4.450
2.442
2.103
3.75
3.96
2.00
6.10
2.86
9
8
7
6
5
4
3
2
1
0
ppm

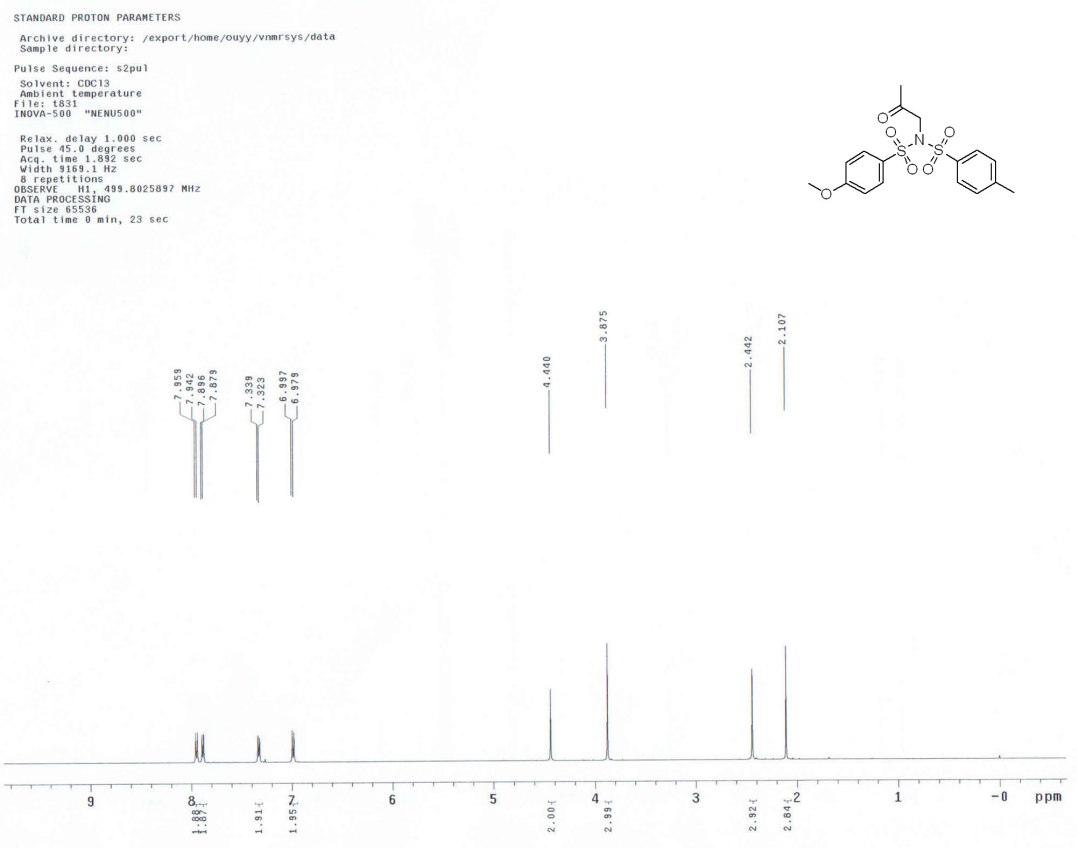

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: t707
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754747 MHz
DECOUPLE H1, 499.8050305 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
129.489
128.572
200.394
145.232
135.981
77.252
77.000
76.744
55.975
26.515
21.613
220
200
180
160
140
120
100
80
60
40
20
0
ppm

Product 3e


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: t877
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 9169.1 Hz
8 repetitions
OBSERVE H1, 499.8025897 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.032
8.016
7.958
7.940
7.683
7.648
7.588
7.552
7.537
7.005
6.988
4.459
3.888
2.117
ppm


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: t861
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754704 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
200.329
164.056
139.060
134.024
131.067
130.174
128.915
128.503
114.063
77.252
77.000
76.744
55.994
55.689
26.585
ppm

Product 3f


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: t831
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9169.1 Hz
8 repetitions
OBSERVE H1, 499.8025897 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.959
7.942
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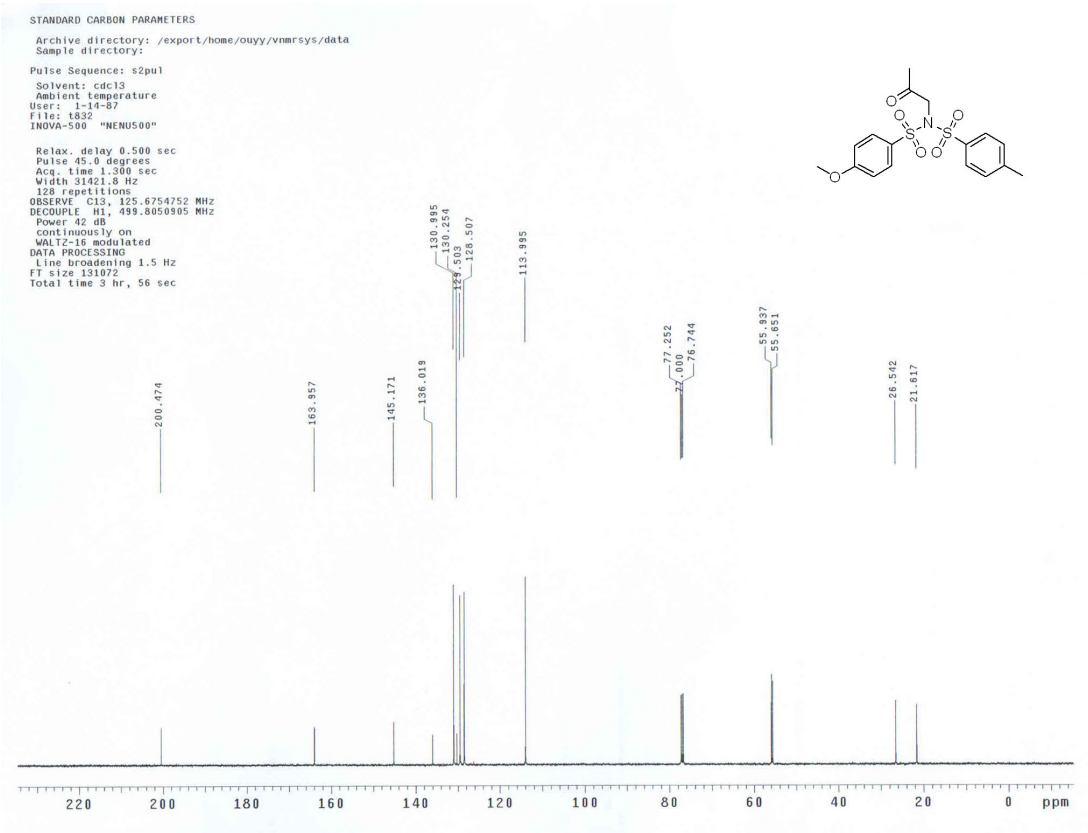
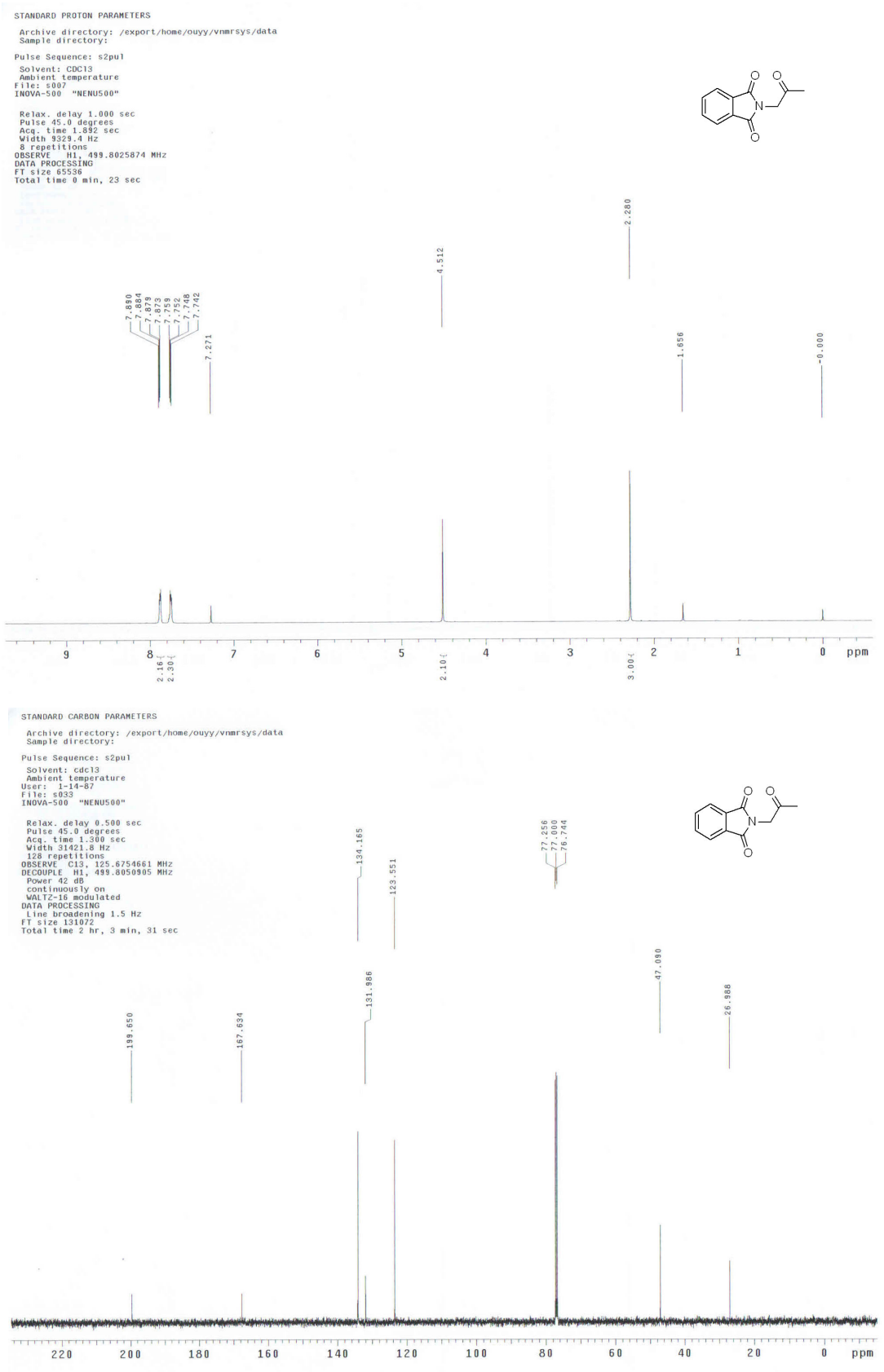
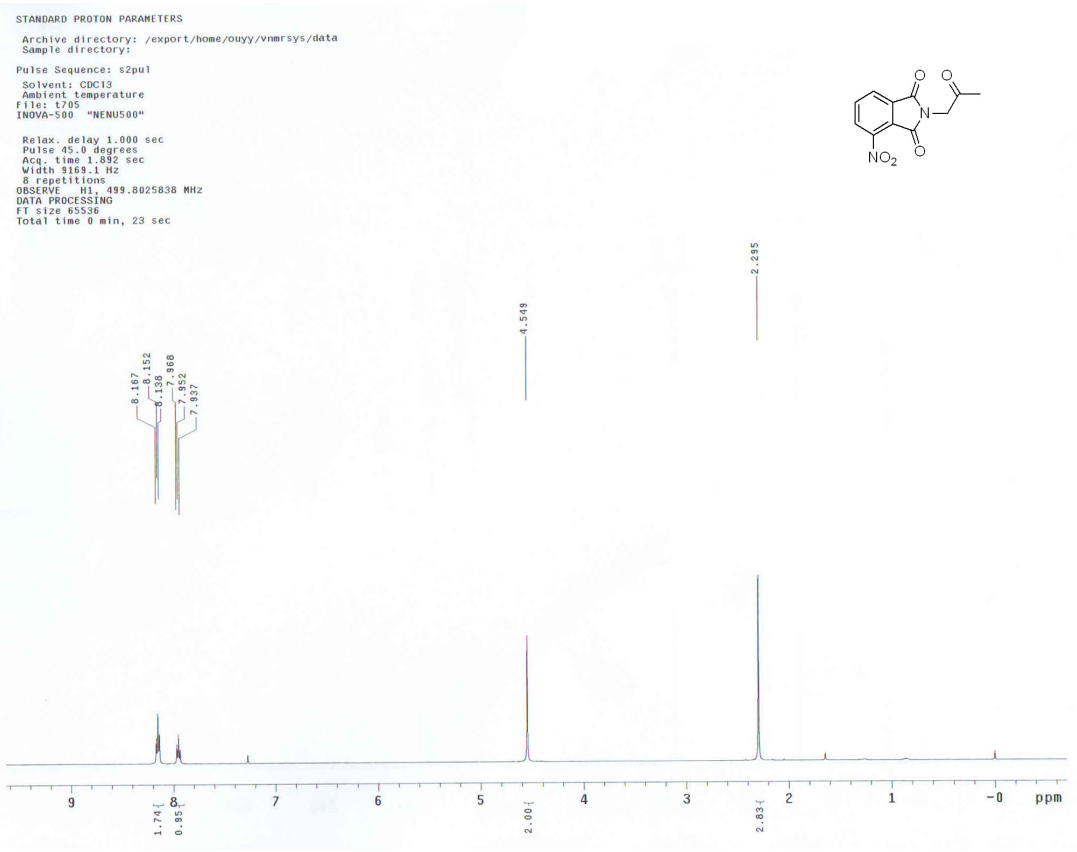
7.879
7.339
7.323
6.997
6.979
4.440
3.875
2.442
2.107
ppm

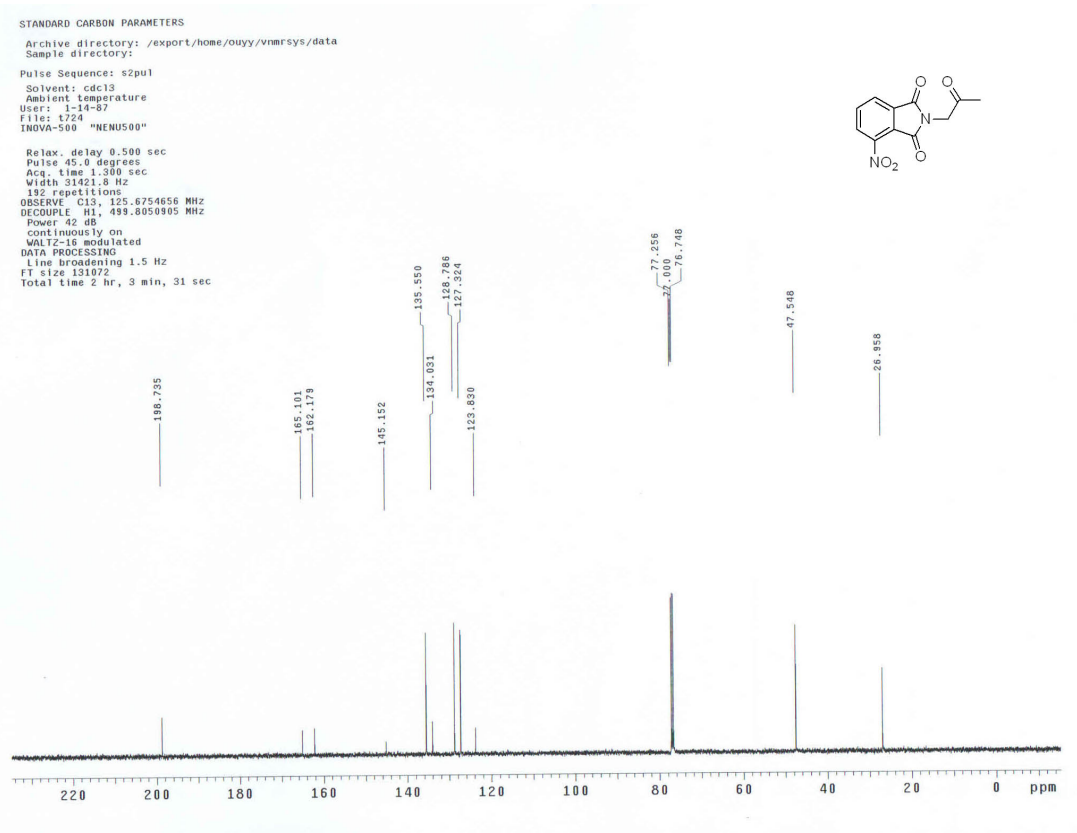

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: t832
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754752 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
200.474
163.957
145.171
136.019
130.995
130.254
129.503
128.507
113.995
77.252
77.000
76.744
55.837
55.651
26.542
21.617
ppm

Product 3g

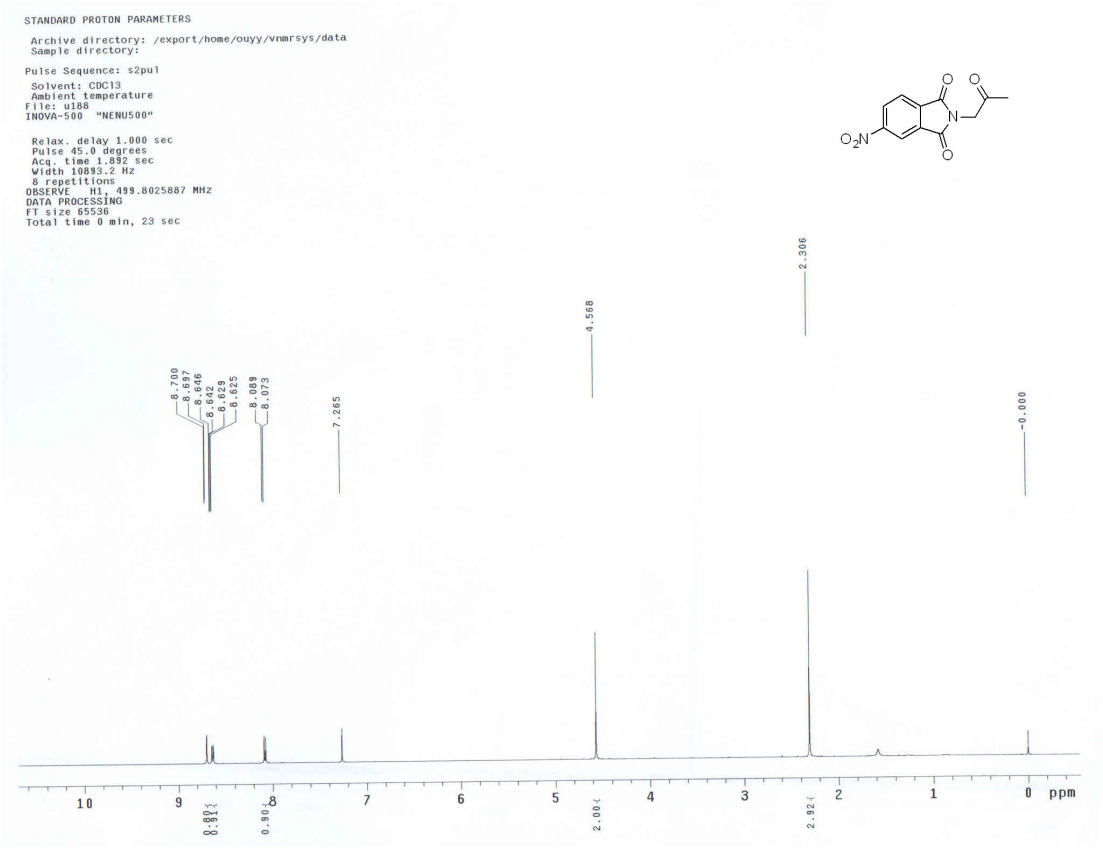

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: s007
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9329.4 Hz
8 repetitions
OBSERVE H1, 499.8025874 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.880
7.884
7.879
7.873
7.759
7.752
7.748
7.742
7.271
4.512
2.280
1.656
-0.000
2.16
2.30
2.10
3.00
ppm
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: s033
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754661 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
134.165
129.551
77.256
77.000
76.744
199.650
167.634
131.986
47.090
26.988
ppm

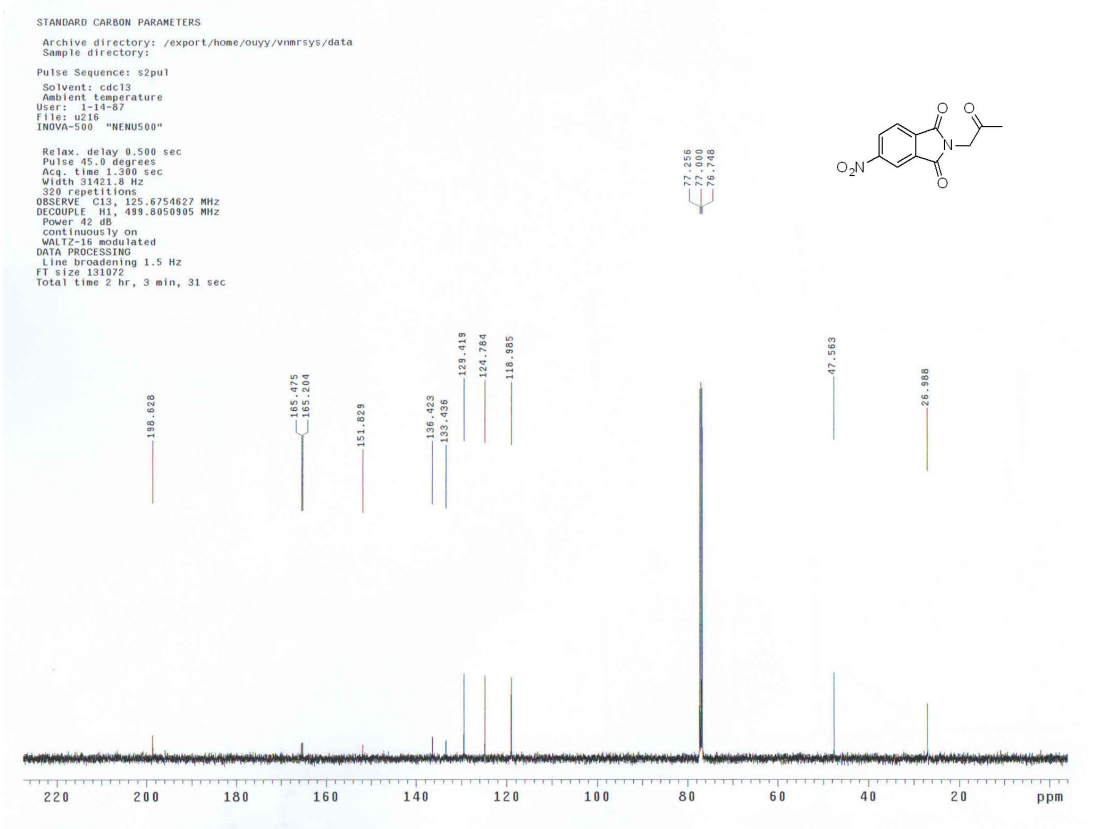
Product 3h


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: t705
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9169.1 Hz
8 repetitions
OBSERVE H1, 499.8025838 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.167
8.152
8.138
7.968
7.952
7.937
4.549
2.295
1.74
0.95
2.00
2.83
9
8
7
6
5
4
3
2
1
-0
ppm

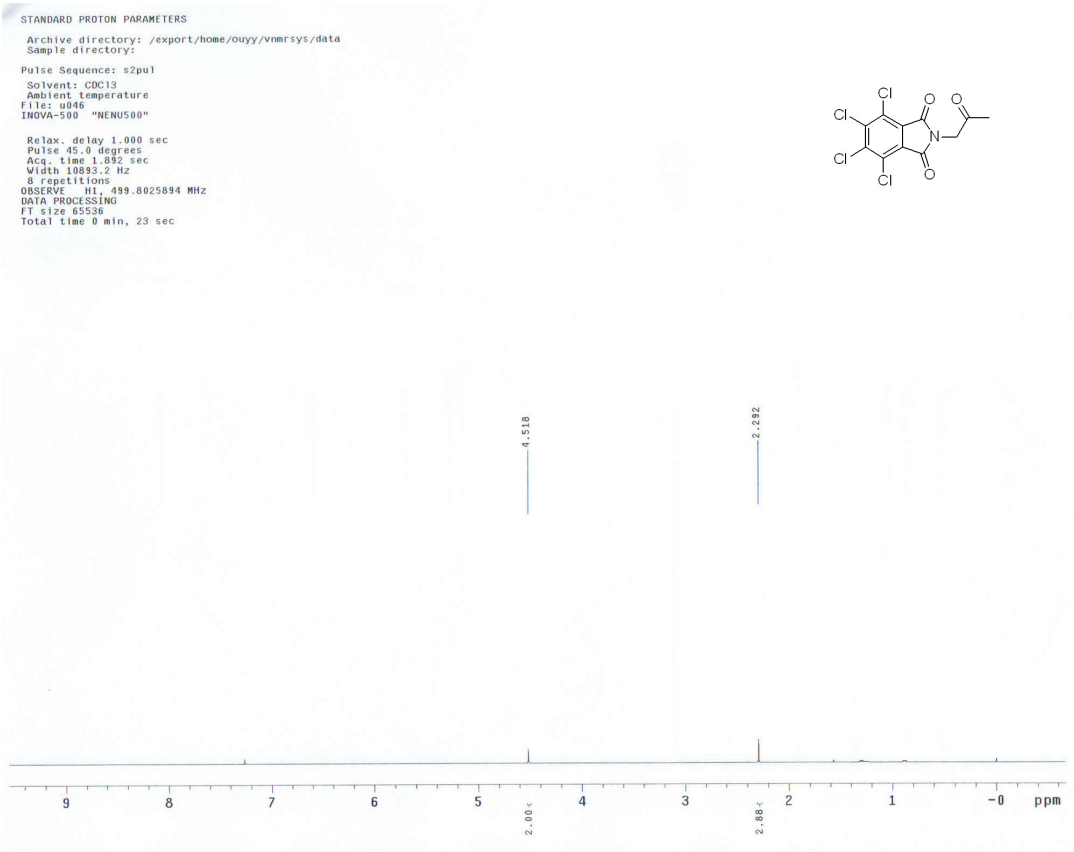

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-07
File: t724
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754656 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
198.735
165.101
162.179
145.152
135.550
134.031
128.786
127.324
123.830
77.256
77.000
76.748
47.548
26.958
220
200
180
160
140
120
100
80
60
40
20
0
ppm

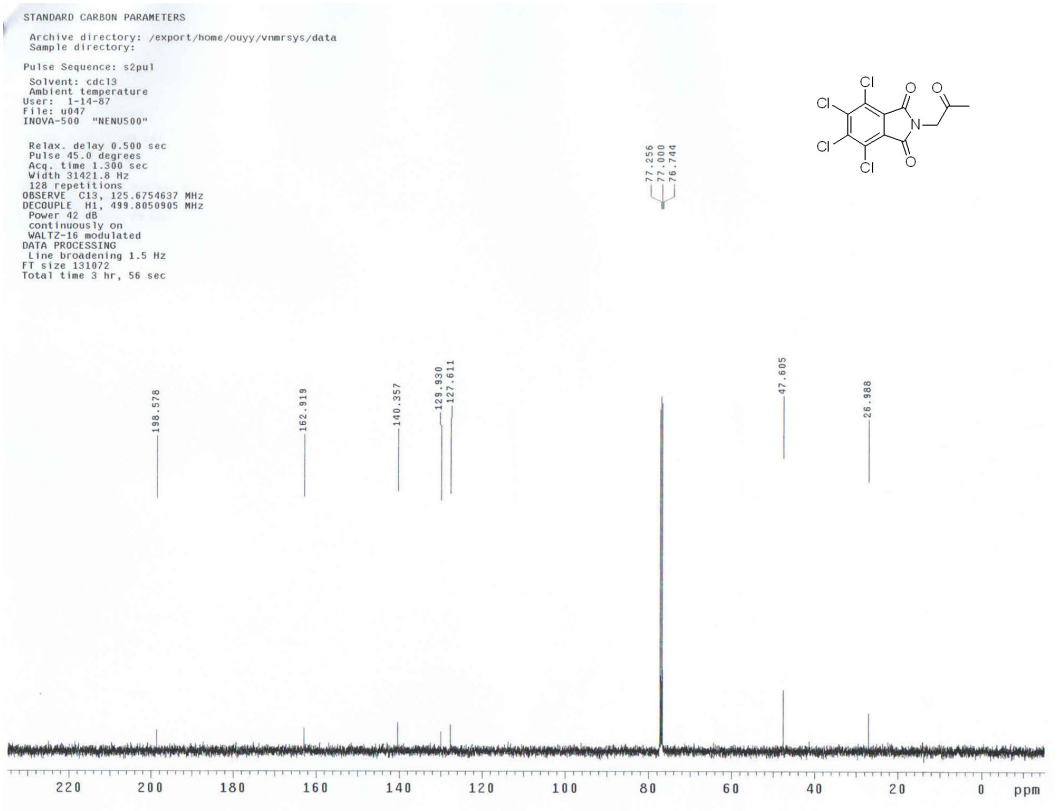
Product 3i


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: u188
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
8 repetitions
OBSERVE H1, 499.8025887 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.700
8.697
8.646
8.642
8.629
8.625
8.089
8.073
7.265
4.568
2.306
-0.000
ppm

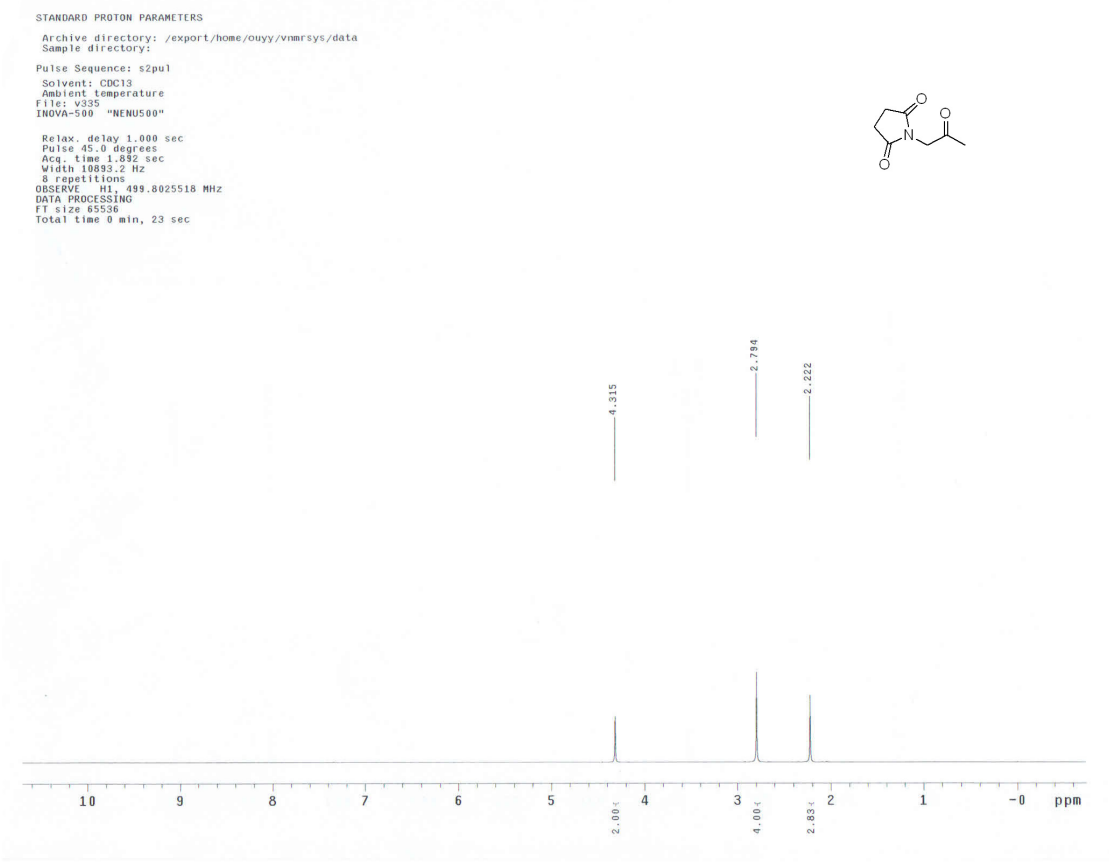

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: u216
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
320 repetitions
OBSERVE C13, 125.6754627 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
77.256
77.000
76.748
198.628
165.475
165.204
151.829
136.423
133.436
129.419
124.784
118.985
47.563
26.888
ppm

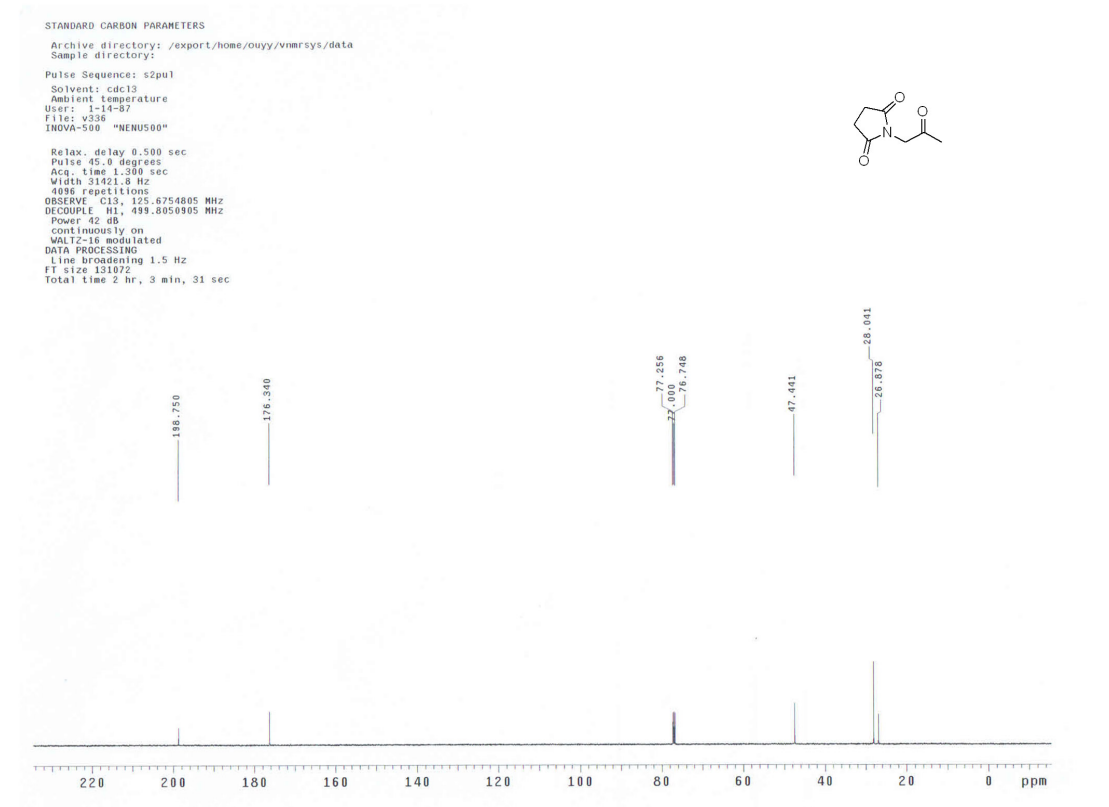
Product 3j


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: u046
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
8 repetitions
OBSERVE H1, 499.8025894 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
4.518
2.292
9
8
7
6
5
4
3
2
1
-0
ppm

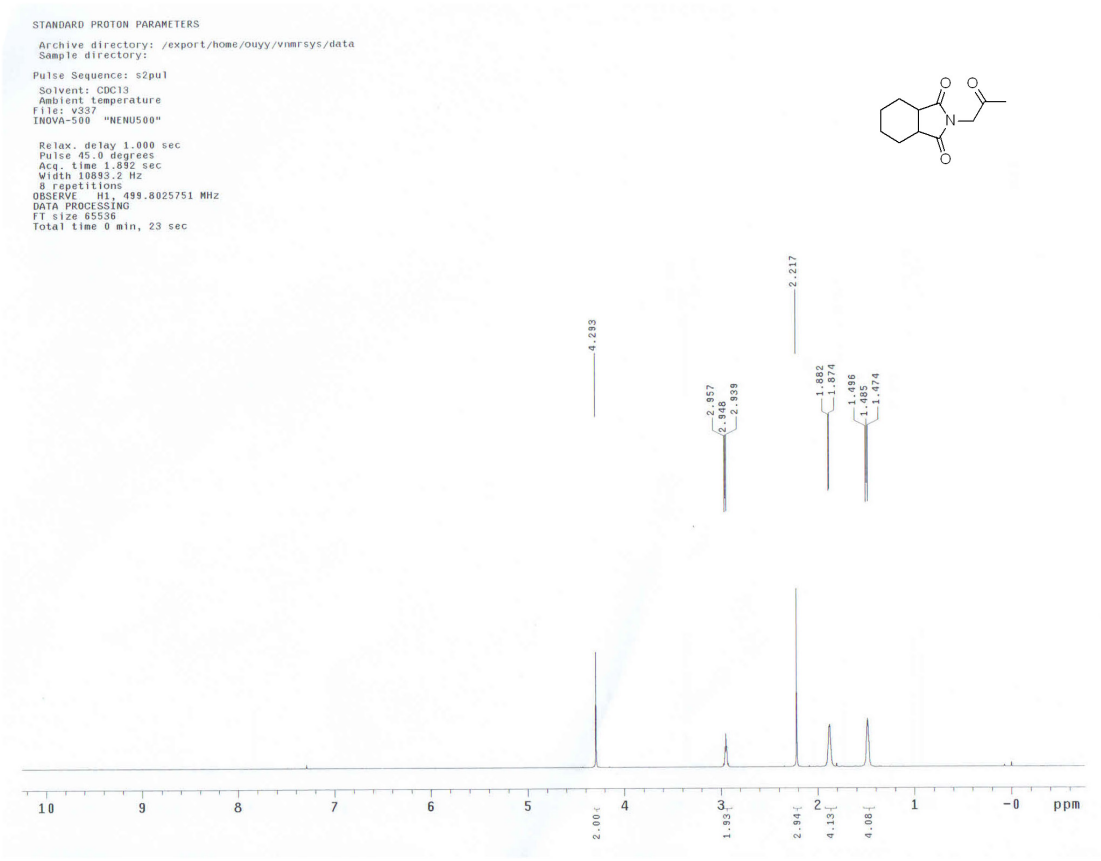

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: u047
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754637 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
77.256
77.000
76.744
198.578
162.919
140.357
129.530
127.611
47.605
26.888
220
200
180
160
140
120
100
80
60
40
20
0
ppm

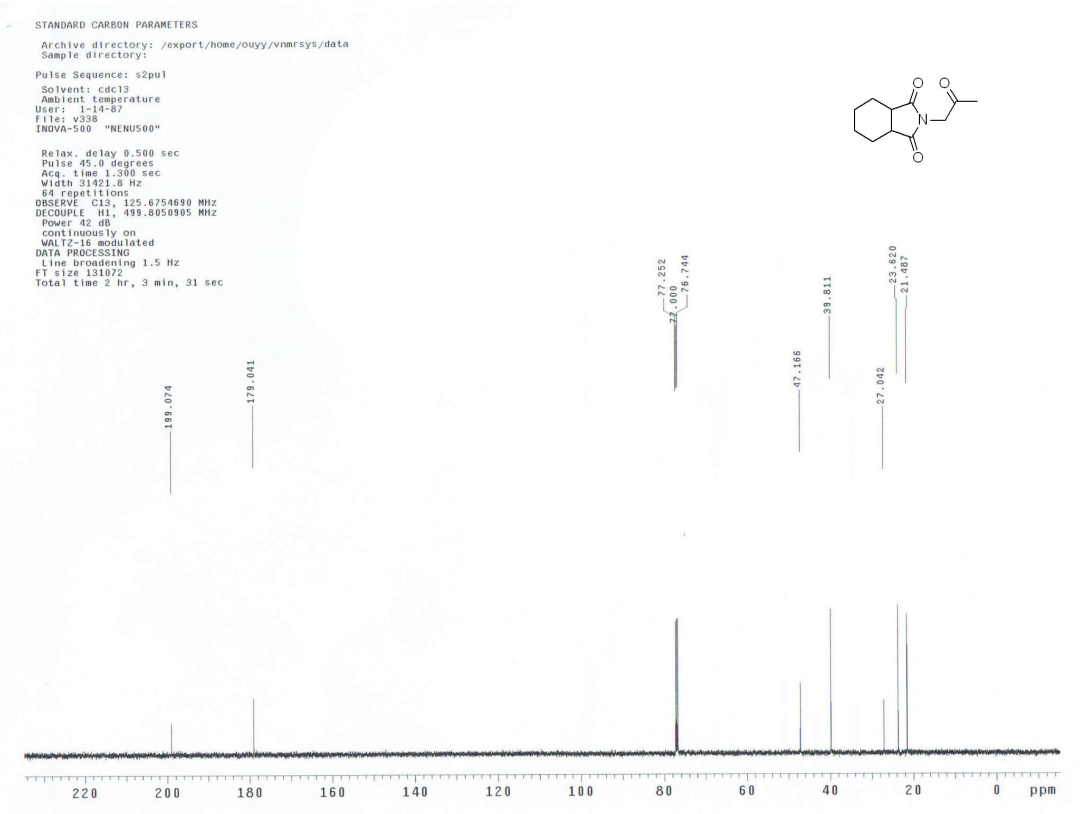
Product 3k


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: v335
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
8 repetitions
OBSERVE H1, 499.8025518 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
4.315
2.794
2.222
2.00
4.00
2.83
10
9
8
7
6
5
4
3
2
1
-0
ppm

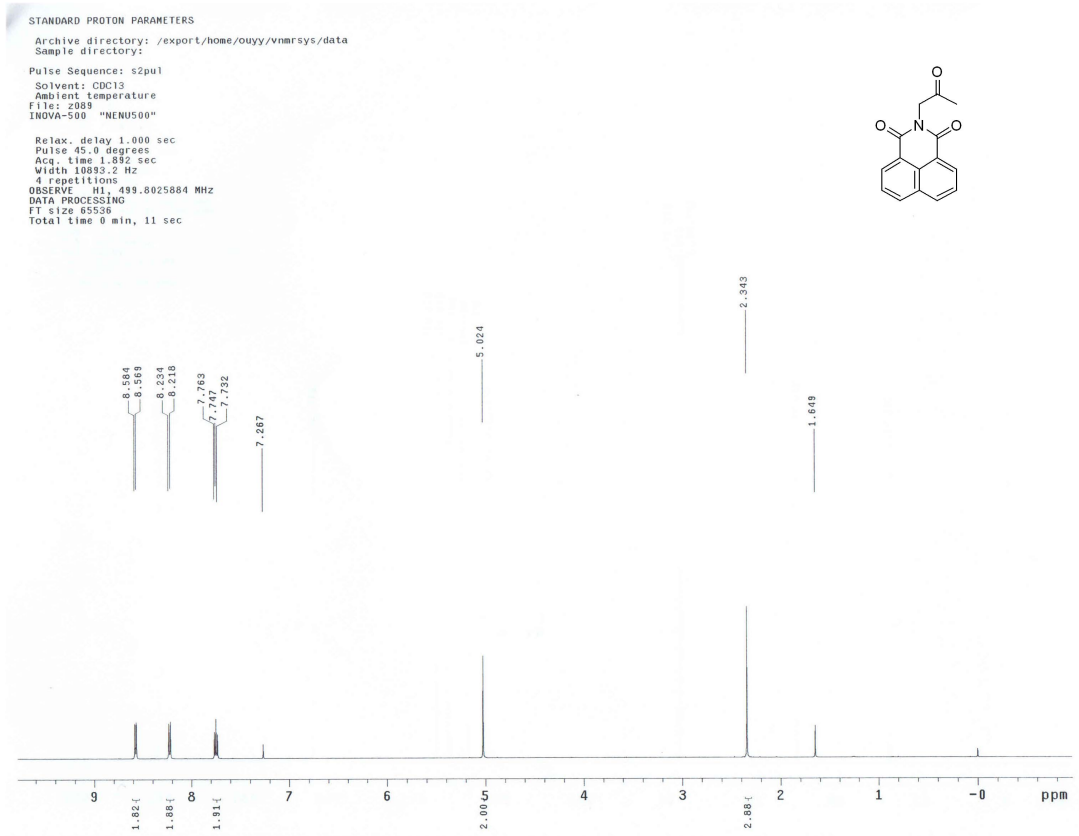

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: v336
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
4096 repetitions
OBSERVE C13, 125.6754805 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
188.750
176.340
77.256
77.000
76.748
47.441
28.041
26.878
220
200
180
160
140
120
100
80
60
40
20
0
ppm

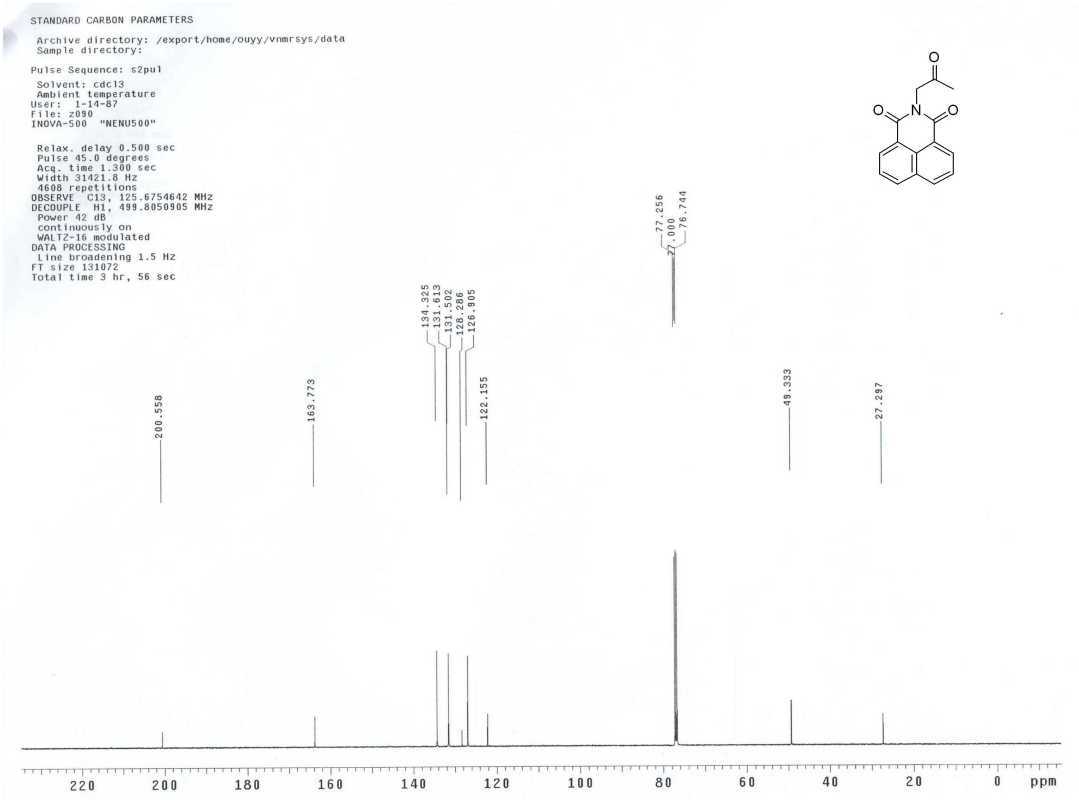
Product 3l


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: v337
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
8 repetitions
OBSERVE H1, 499.8025751 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
4.293
2.857
2.848
2.939
2.217
1.882
1.874
1.496
1.485
1.474
2.00
1.93
2.94
4.13
4.08
ppm

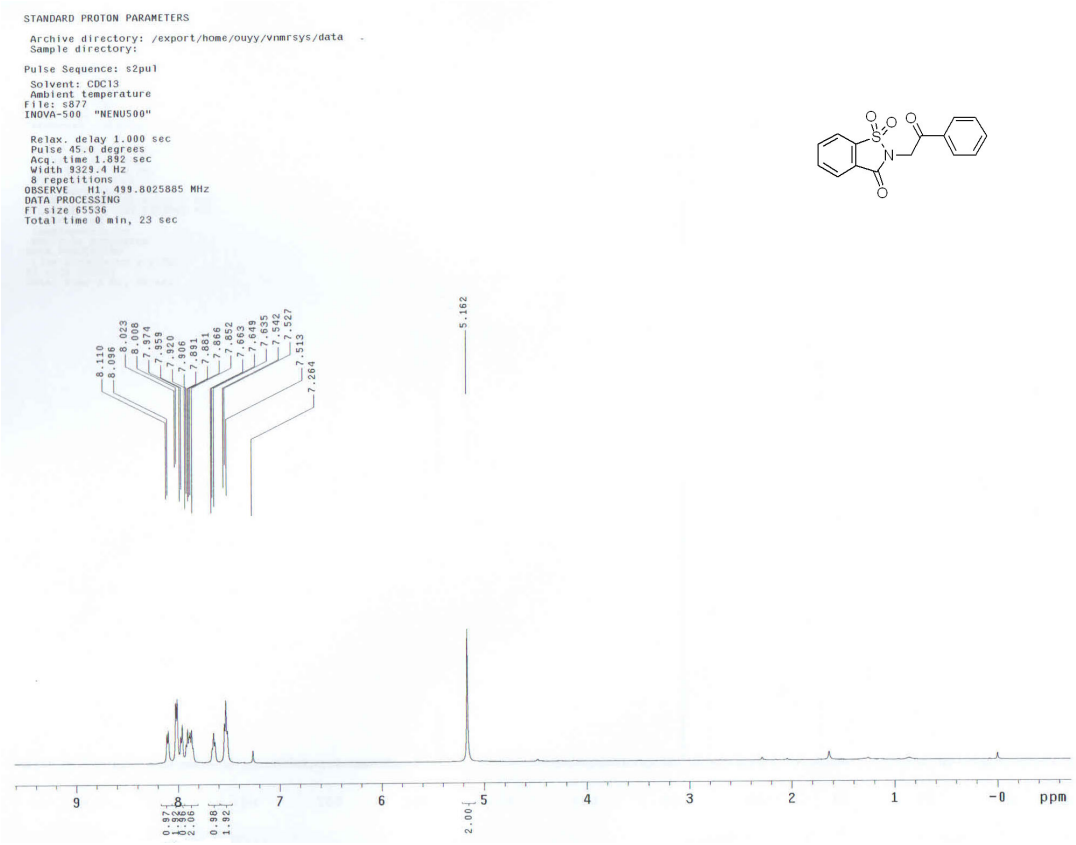

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: v338
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754690 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
199.074
179.041
77.252
77.000
76.744
47.166
39.811
27.042
23.620
21.487
ppm

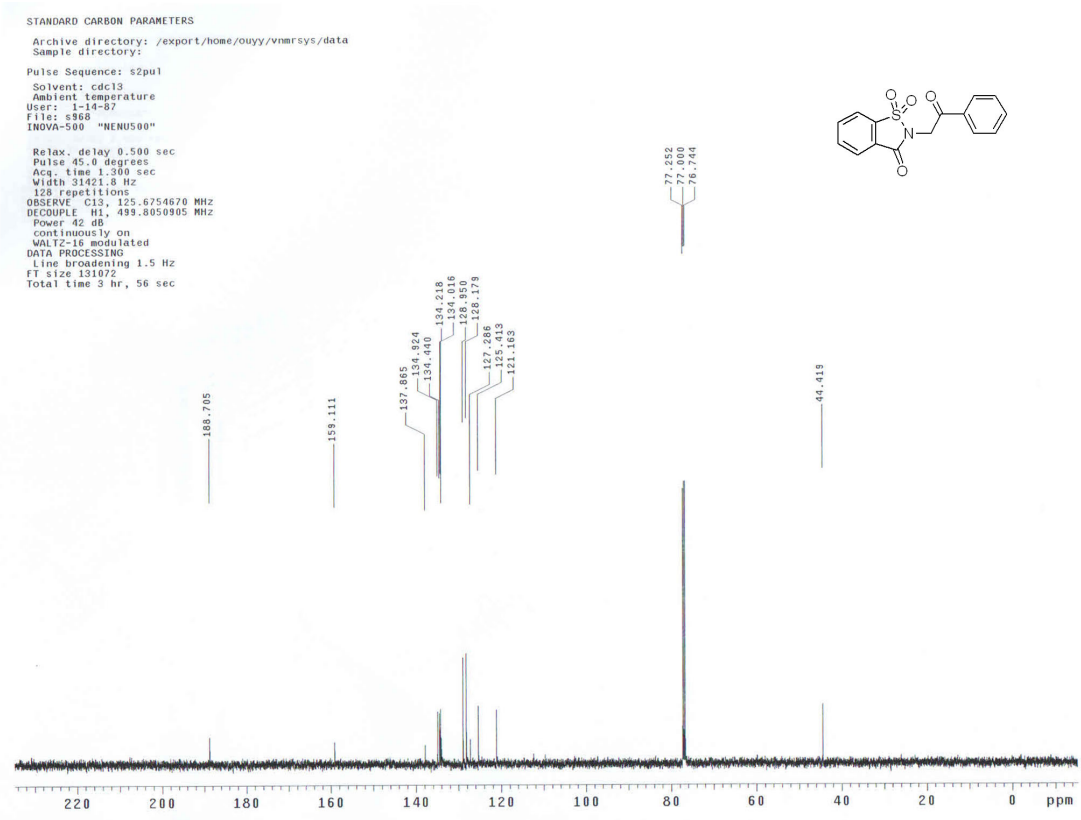
Product 3m


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: z089
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
4 repetitions
OBSERVE H1, 499.8025884 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec
8.584
8.569
8.234
8.218
7.763
7.747
7.732
7.267
5.024
2.343
1.649
1.82
1.88
1.91
2.00
2.88
9
8
7
6
5
4
3
2
1
-0
ppm

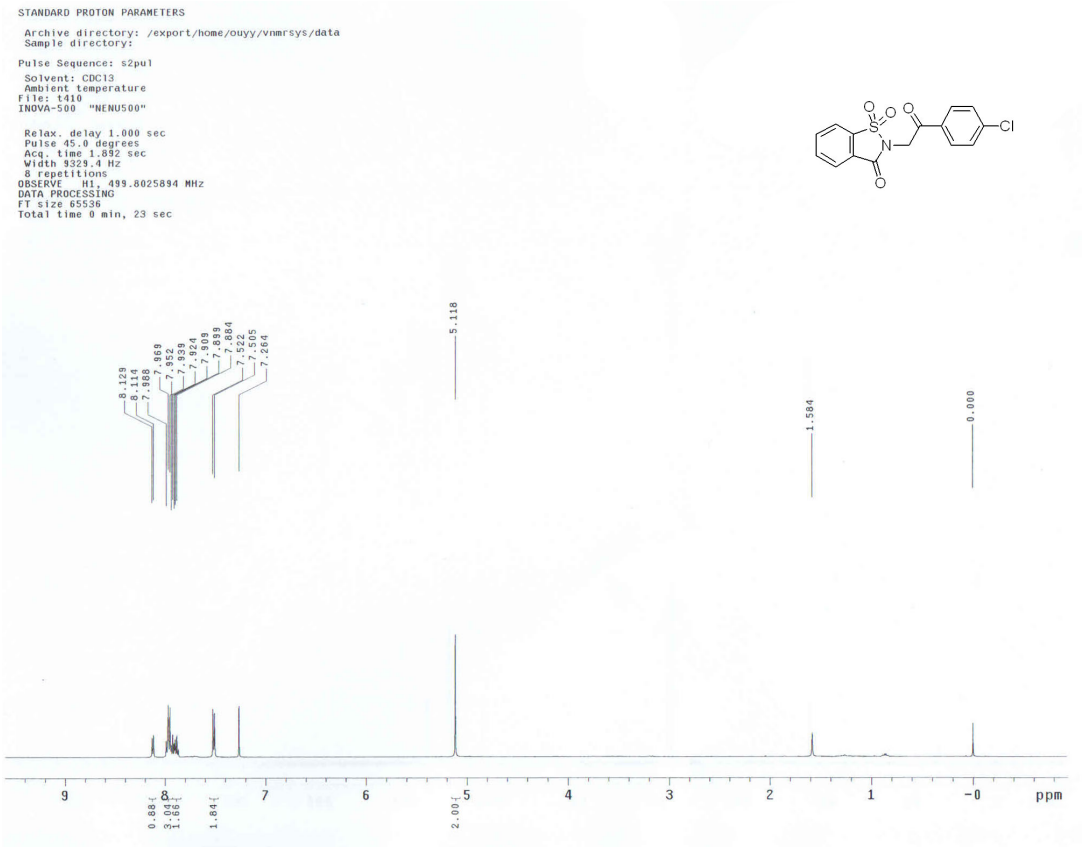

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: z090
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
4608 repetitions
OBSERVE C13, 125.6754642 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
77.256
77.000
76.744
134.325
131.613
131.502
128.286
126.905
200.558
163.773
122.155
49.333
27.297
220
200
180
160
140
120
100
80
60
40
20
0
ppm

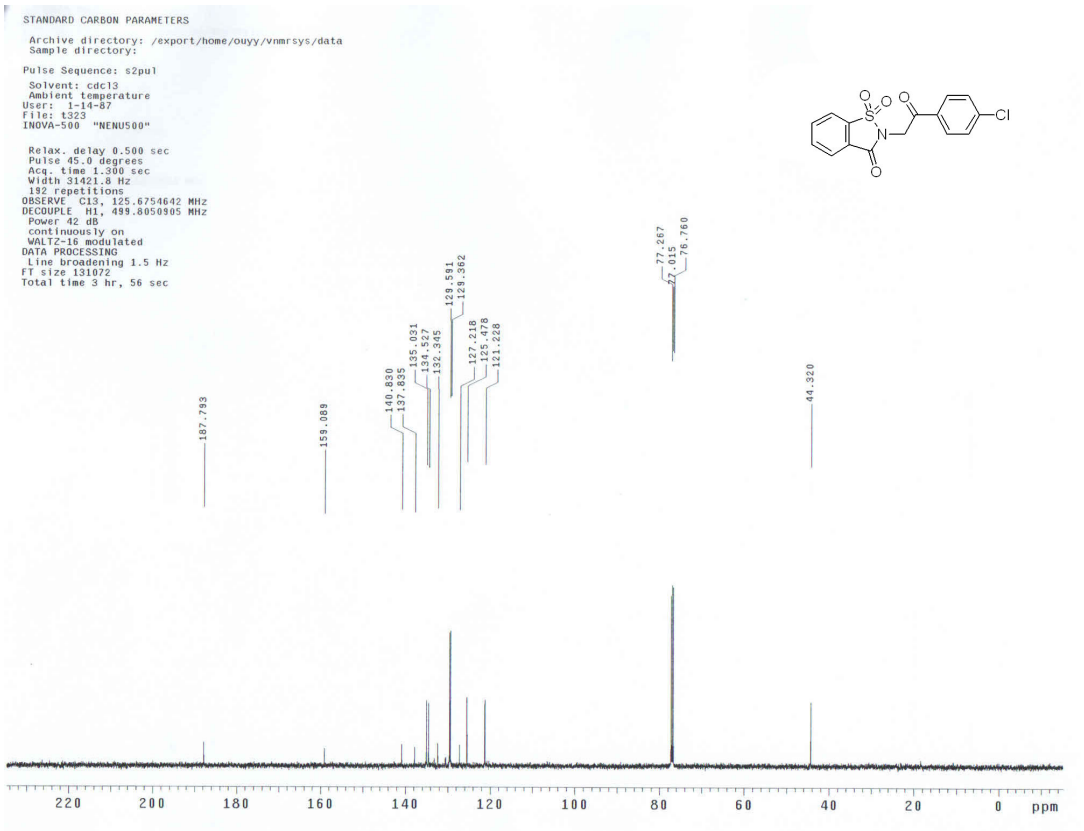
Product 4b


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: s877
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9329.4 Hz
8 repetitions
OBSERVE H1, 499.8025885 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.110
8.096
8.023
8.008
7.974
7.959
7.920
7.906
7.891
7.881
7.866
7.852
7.683
7.668
7.635
7.542
7.527
7.513
7.264
5.162
ppm

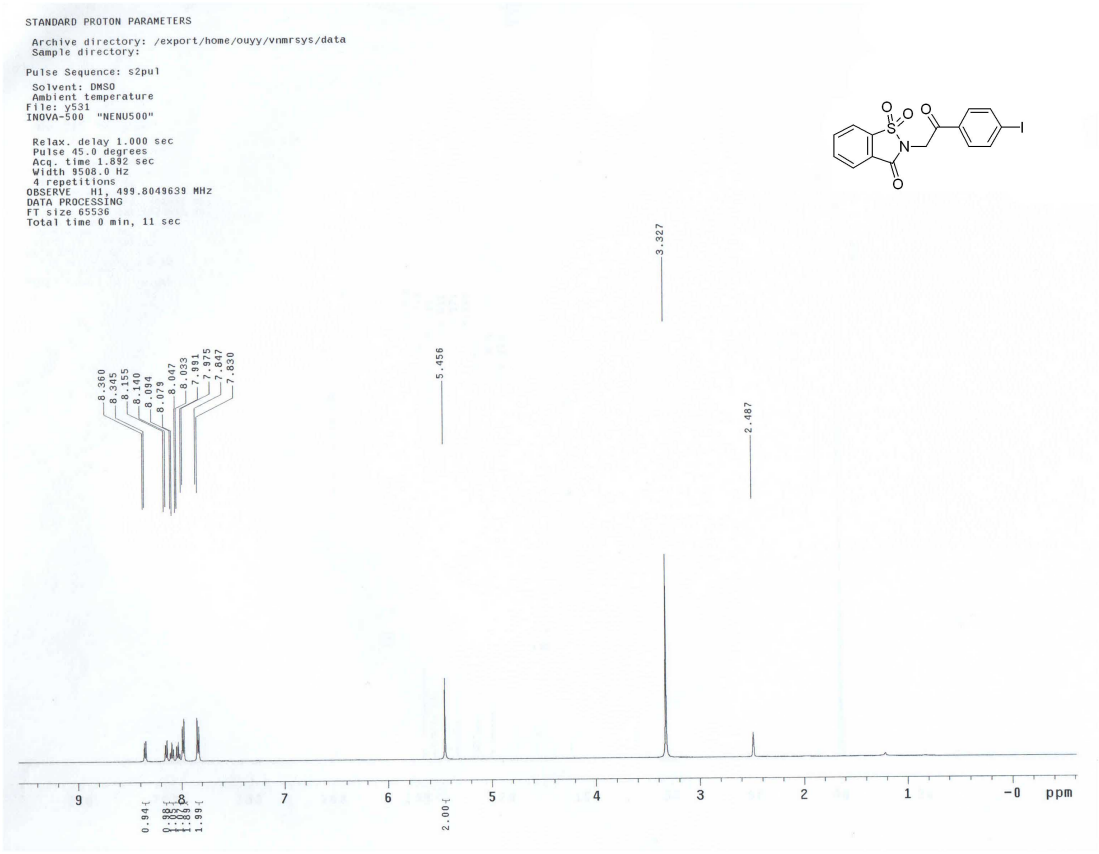

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: s968
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754670 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
188.705
159.111
137.865
134.924
134.440
134.218
134.016
128.950
128.179
127.286
125.413
121.163
77.252
77.000
76.744
44.419
ppm

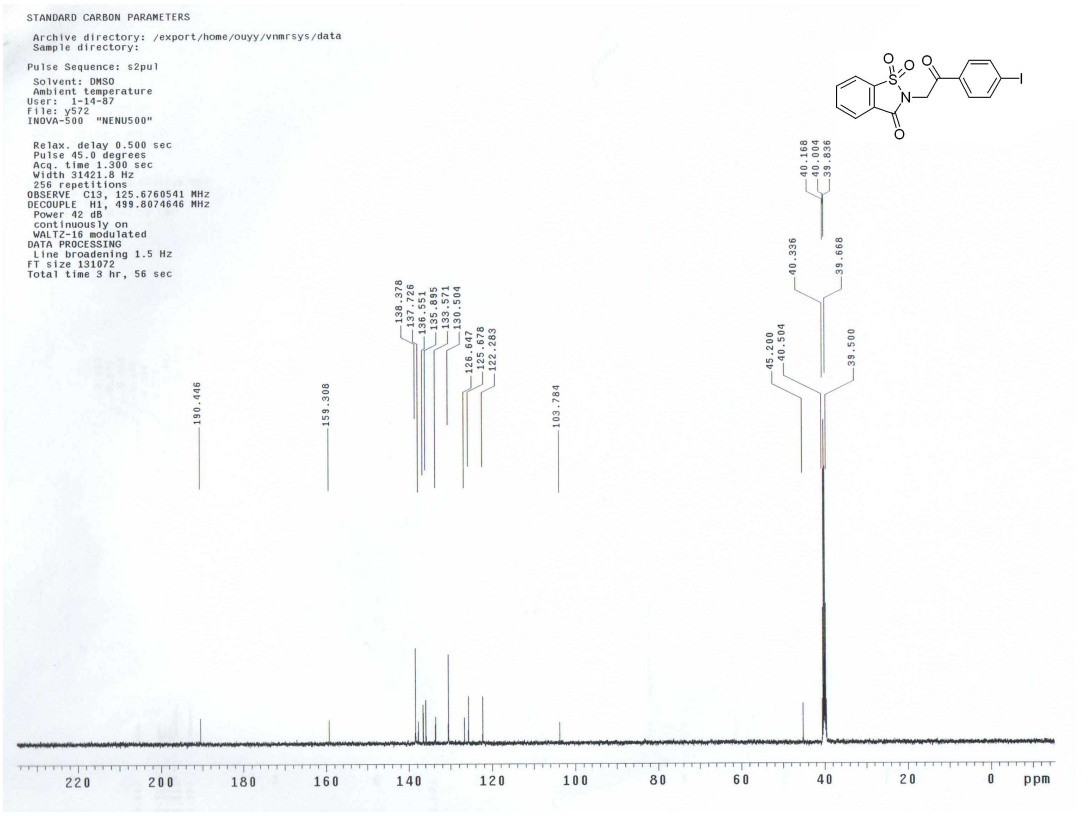
Product 4c


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: t410
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9329.4 Hz
8 repetitions
OBSERVE H1, 499.8025894 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.129
8.114
7.988
7.969
7.952
7.938
7.924
7.909
7.899
7.884
7.522
7.505
7.264
5.118
1.584
0.000
0.88
3.00
1.86
1.84
2.00
9
8
7
6
5
4
3
2
1
-0
ppm
Cl

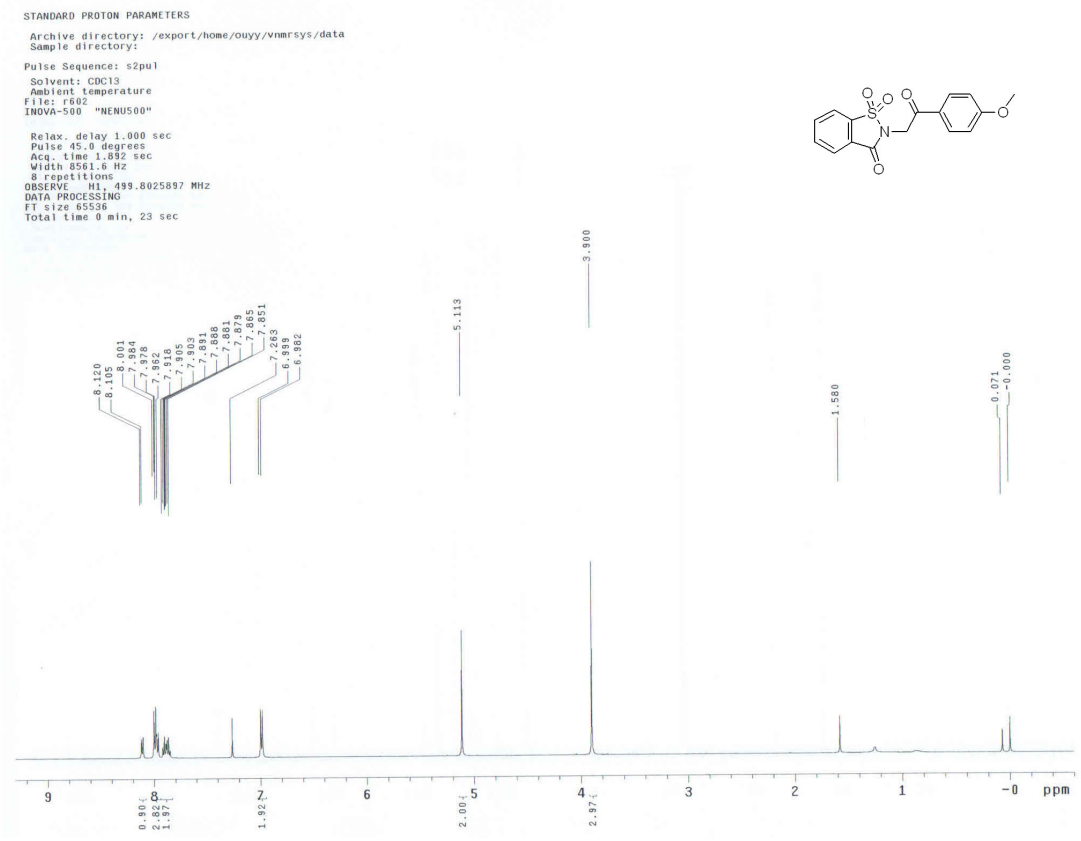

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: t323
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754642 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
187.793
159.089
140.830
137.835
135.031
134.527
132.345
129.591
129.362
127.218
125.478
121.228
77.267
77.015
76.760
44.320
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Cl

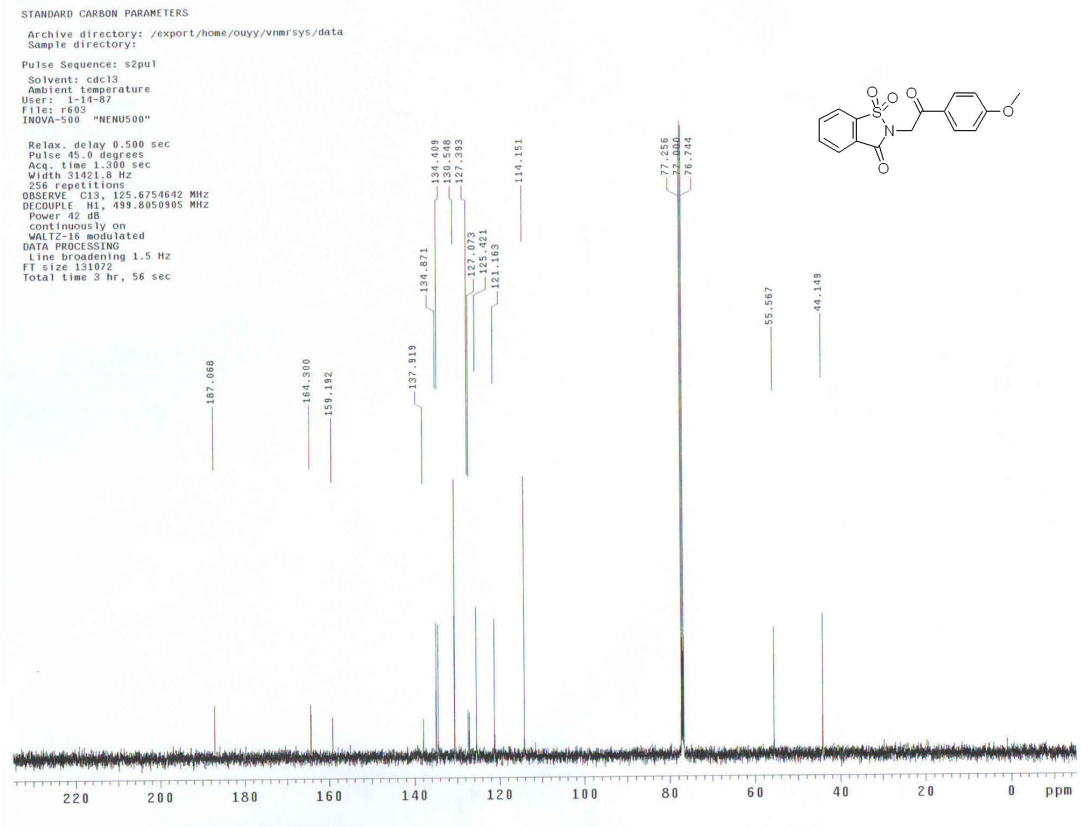
Product 4d


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
File: y531
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9508.0 Hz
4 repetitions
OBSERVE H1, 499.8049639 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec
8.360
8.345
8.155
8.140
8.074
8.072
8.047
8.033
7.991
7.975
7.807
7.800
5.456
3.327
2.487
ppm

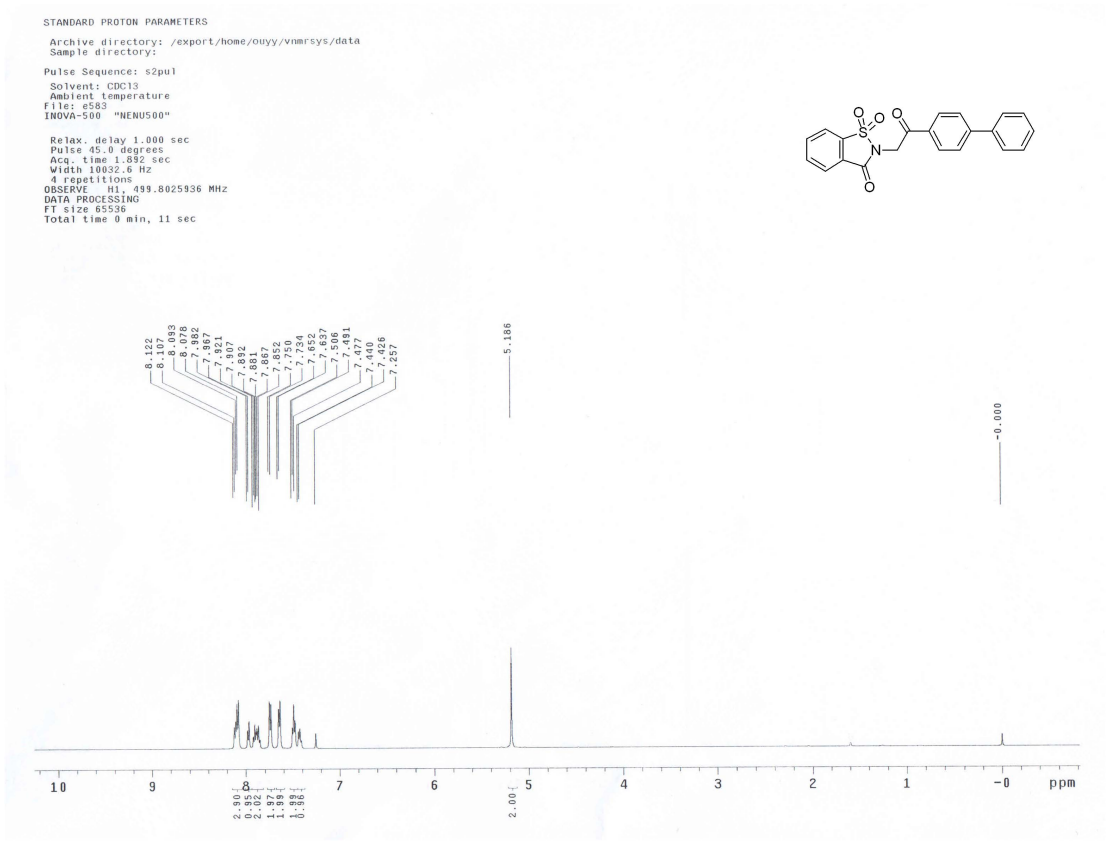

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
User: 1-14-87
File: y572
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6760541 MHz
DECOUPLE H1, 499.8074646 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
190.446
159.308
138.378
137.726
136.551
135.895
133.571
130.504
126.647
125.678
122.283
103.784
40.168
40.004
39.836
40.336
39.668
45.200
40.504
39.500
ppm

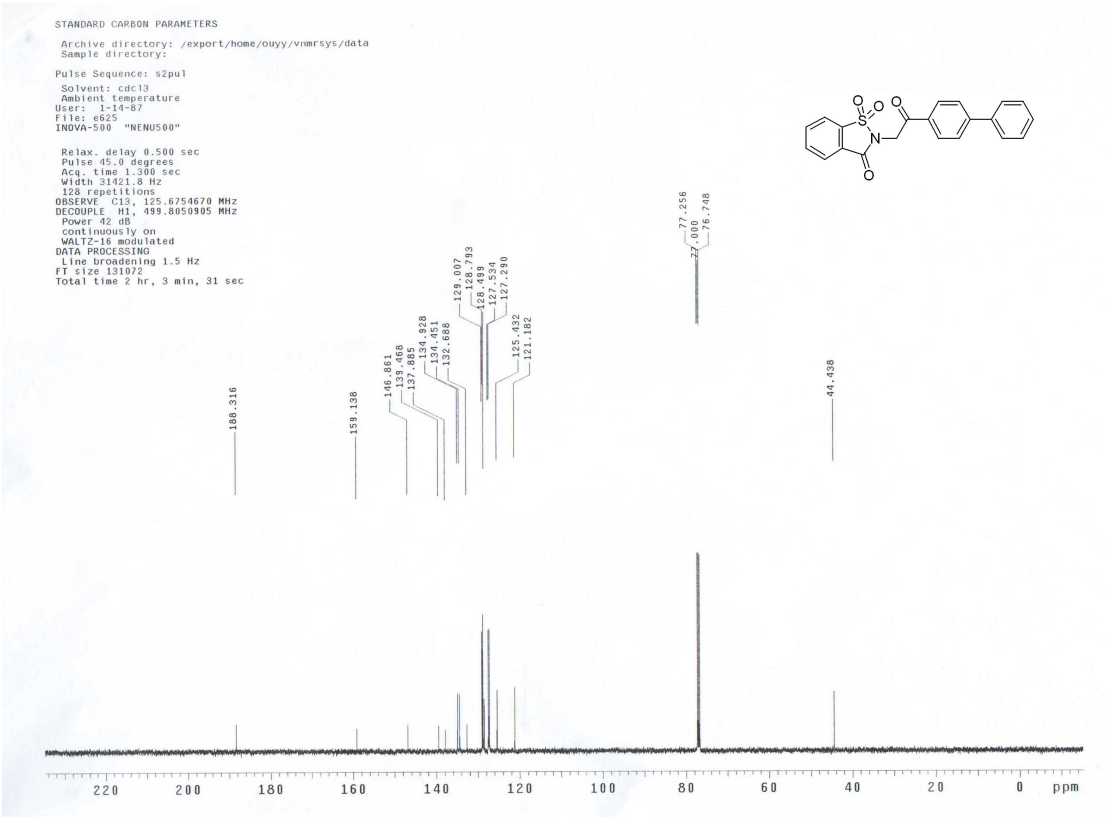
Product 4e


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: r602
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8561.6 Hz
8 repetitions
OBSERVE H1, 499.8025897 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.120
8.105
8.001
7.984
7.928
7.982
7.918
7.905
7.903
7.881
7.868
7.881
7.879
7.865
7.851
7.263
6.988
6.982
5.113
3.900
1.580
0.071
0.000
9
8
7
6
5
4
3
2
1
-0
ppm
0.90
2.85
1.97
1.92
2.00
2.97

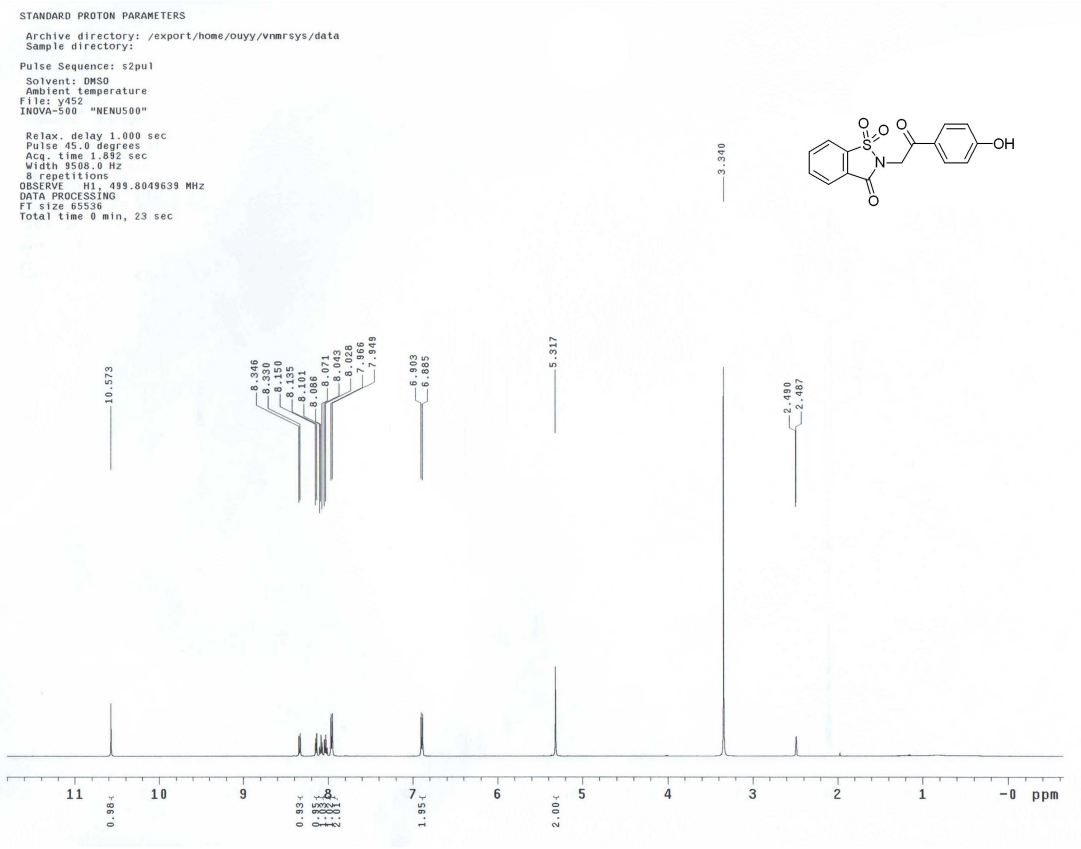

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: r603
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754642 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
187.068
164.300
159.192
137.919
134.871
134.409
130.548
127.393
127.073
125.421
121.163
114.151
77.256
77.000
76.744
55.567
44.149
220
200
180
160
140
120
100
80
60
40
20
0
ppm

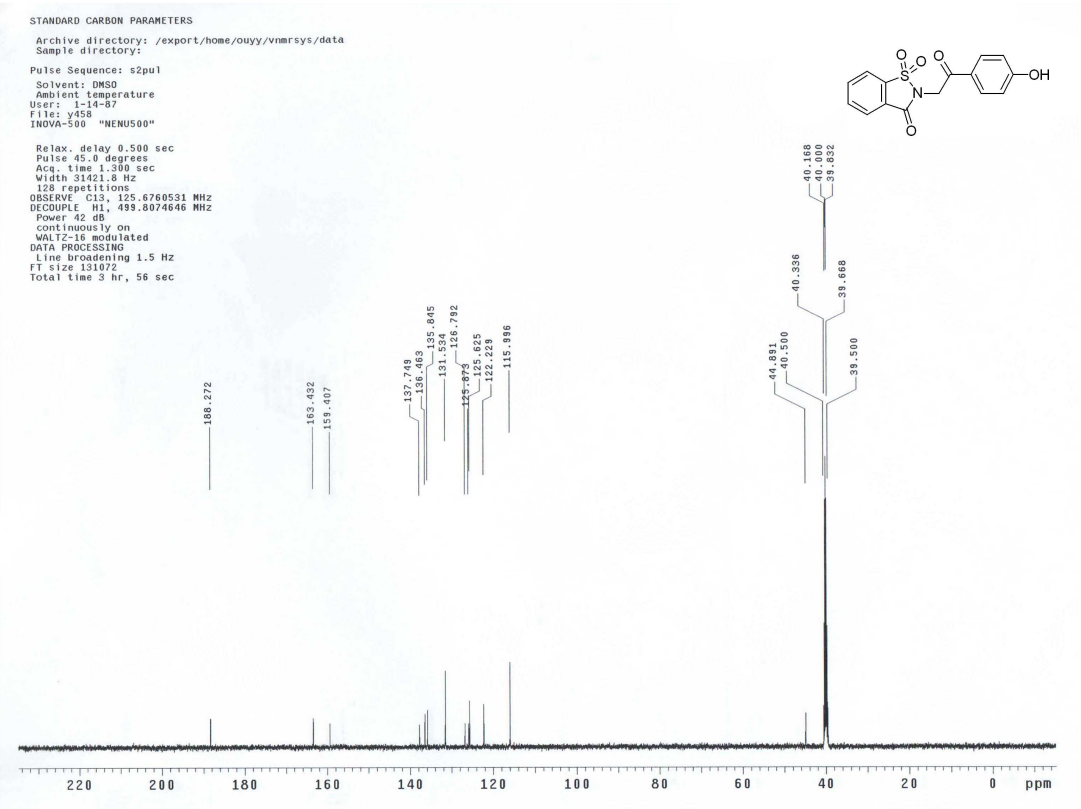
Product 4f


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: e583
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10032.6 Hz
4 repetitions
OBSERVE H1, 499.8025936 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec
8.122
8.107
8.093
8.078
8.062
7.967
7.921
7.907
7.892
7.881
7.867
7.852
7.750
7.734
7.652
7.637
7.506
7.491
7.477
7.440
7.426
7.257
5.186
-0.000
2.90
0.95
2.02
1.97
1.98
0.98
2.00
10
9
8
7
6
5
4
3
2
1
-0
ppm

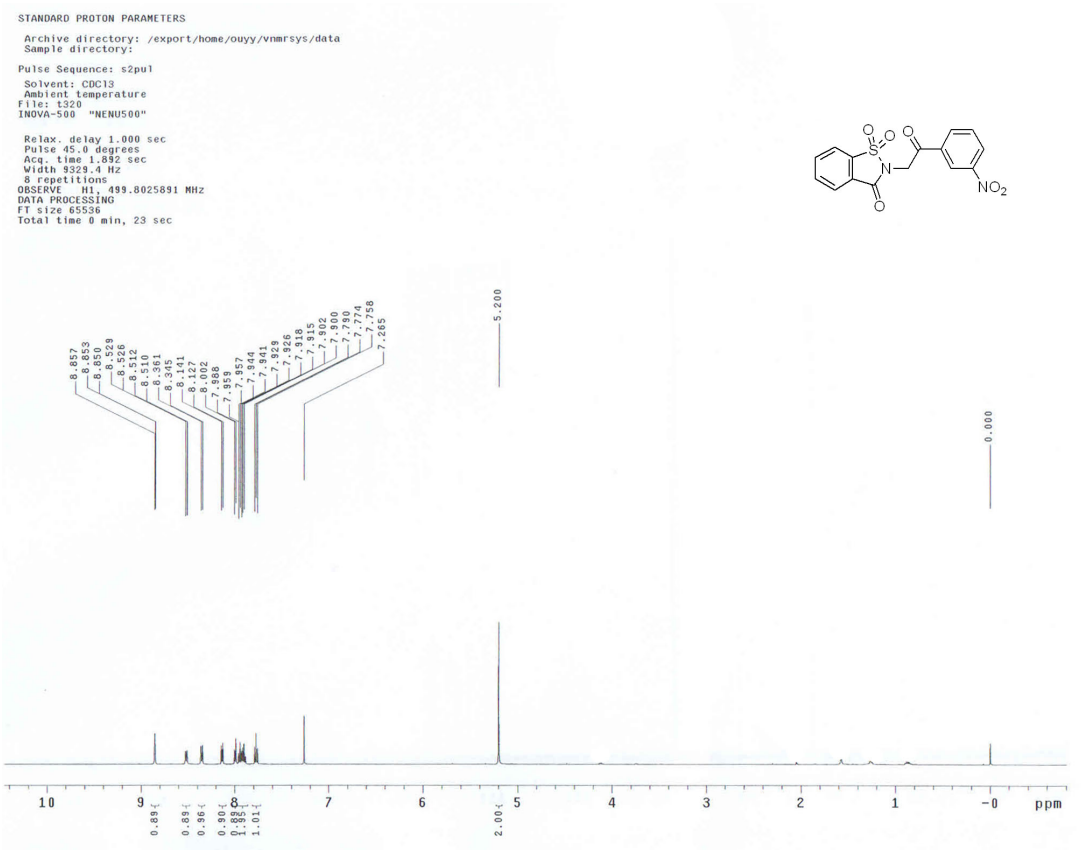

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: e625
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754670 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously On
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
188.316
159.136
146.861
139.468
137.885
134.928
134.451
132.868
129.007
128.793
128.499
127.534
127.290
125.432
121.182
77.256
77.000
76.748
44.438
220
200
180
160
140
120
100
80
60
40
20
0
ppm

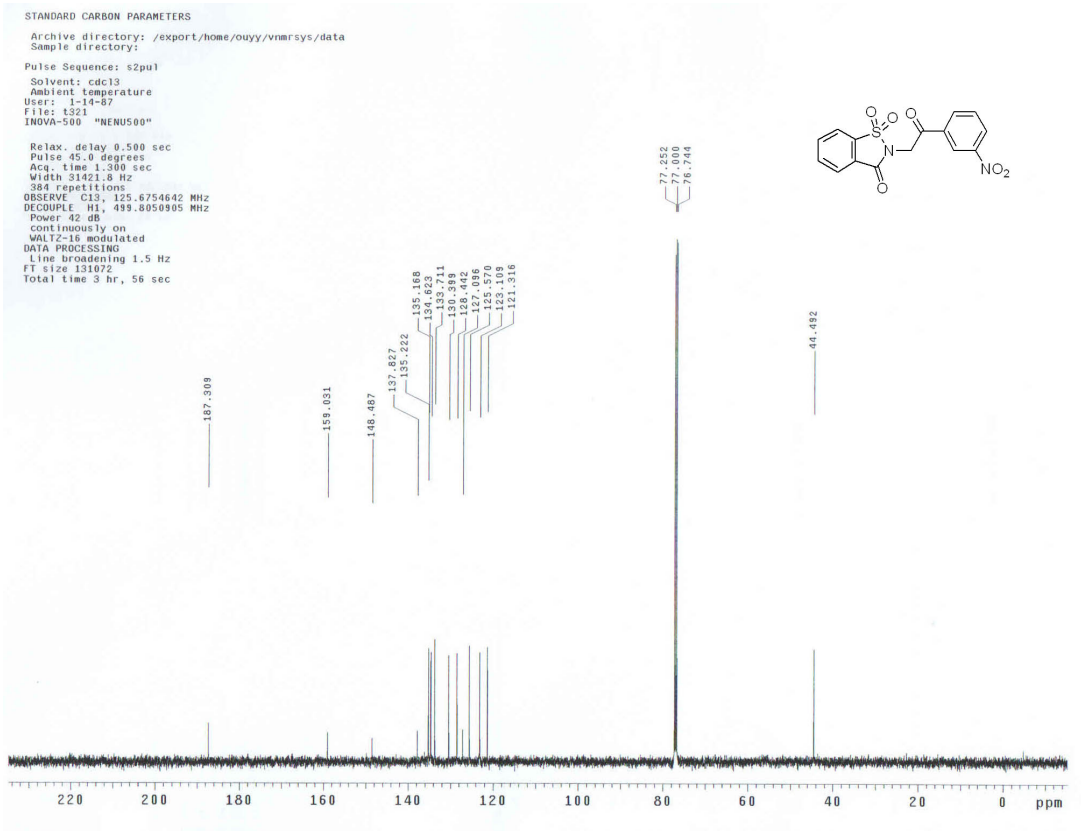
Product 4g


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
File: y452
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9508.0 Hz
8 repetitions
OBSERVE H1, 499.8049639 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
OH
10.573
8.346
8.330
8.150
8.135
8.101
8.086
8.071
8.043
8.028
7.965
7.949
6.903
6.885
5.317
3.340
2.490
2.487
11
10
9
8
7
6
5
4
3
2
1
-0
ppm

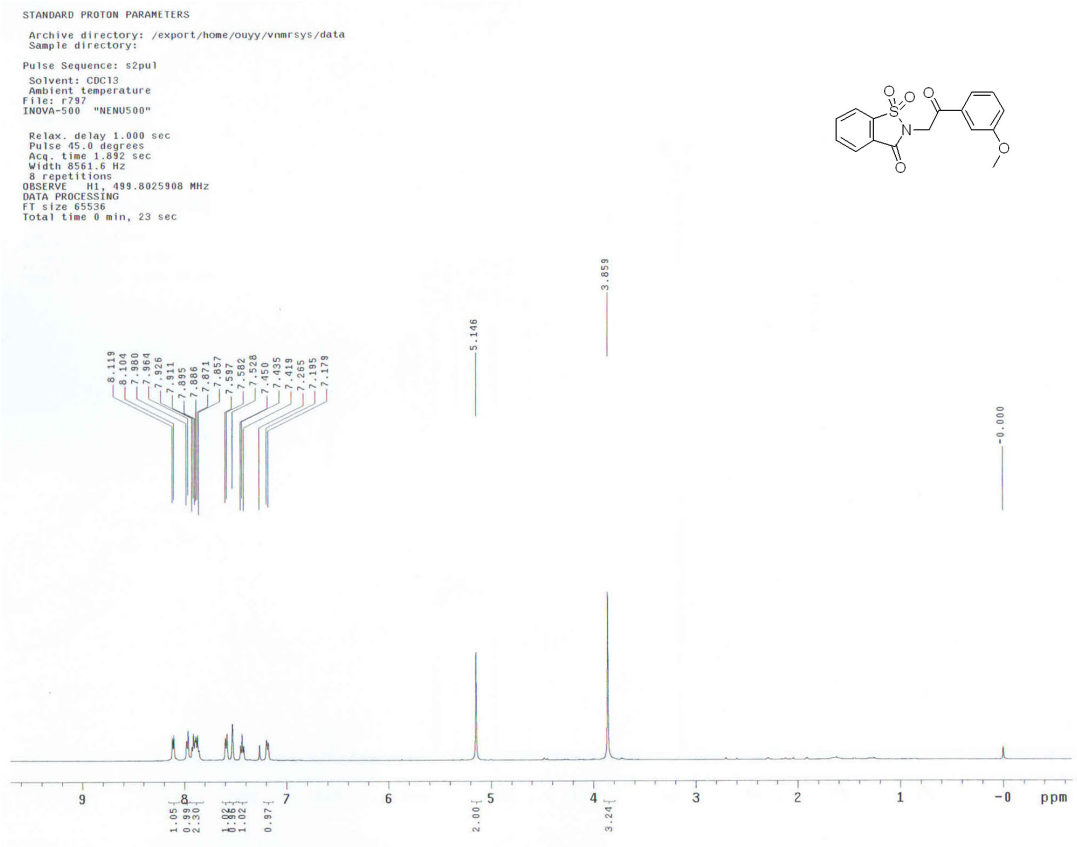

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
User: 1-14-87
File: y458
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6760531 MHz
DECOUPLE H1, 499.8074646 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
OH
188.272
163.432
159.407
137.749
136.463
135.845
131.534
126.792
125.873
125.625
122.229
115.996
40.168
40.000
39.832
40.336
39.668
44.881
40.500
39.500
220
200
180
160
140
120
100
80
60
40
20
0
ppm

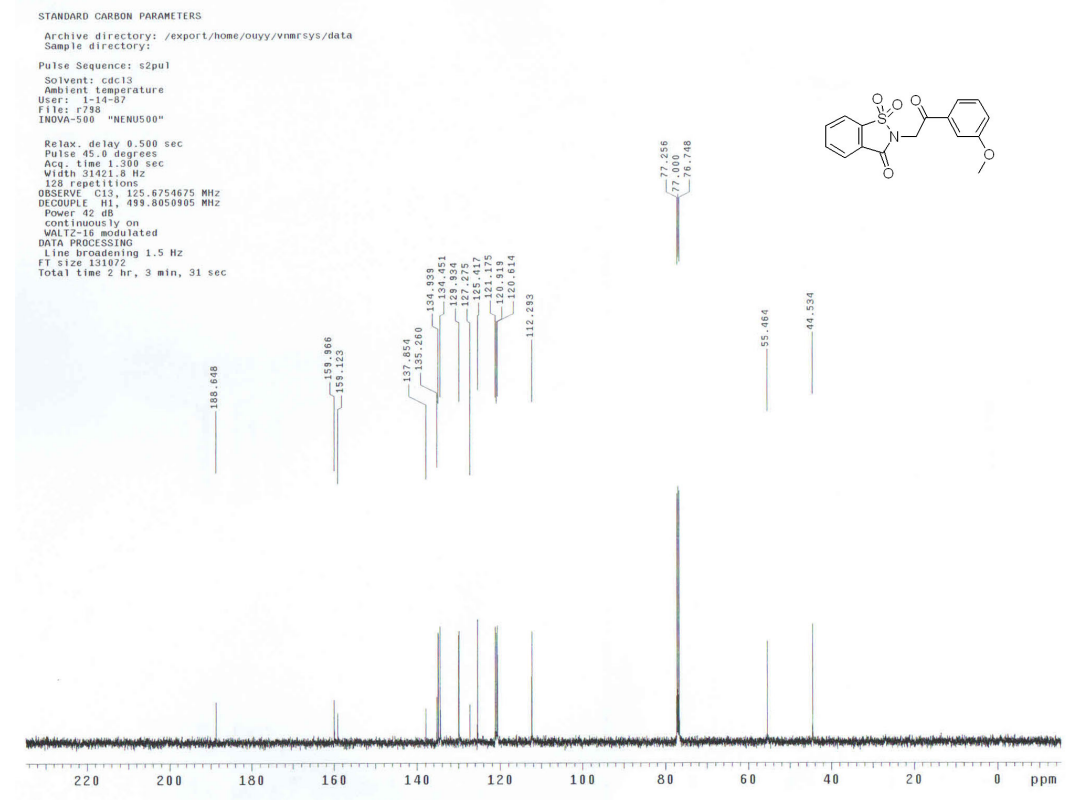
Product 4h


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: t320
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9329.4 Hz
8 repetitions
OBSERVE H1, 499.8025891 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.857
8.853
8.850
8.529
8.526
8.512
8.510
8.361
8.345
8.141
8.127
8.002
7.888
7.959
7.957
7.944
7.941
7.929
7.926
7.918
7.915
7.902
7.800
7.790
7.774
7.758
7.285
5.200
0.000
NO2
10
9
8
7
6
5
4
3
2
1
-0
ppm
0.89
0.89
0.96
0.90
0.89
1.95
1.01
2.00

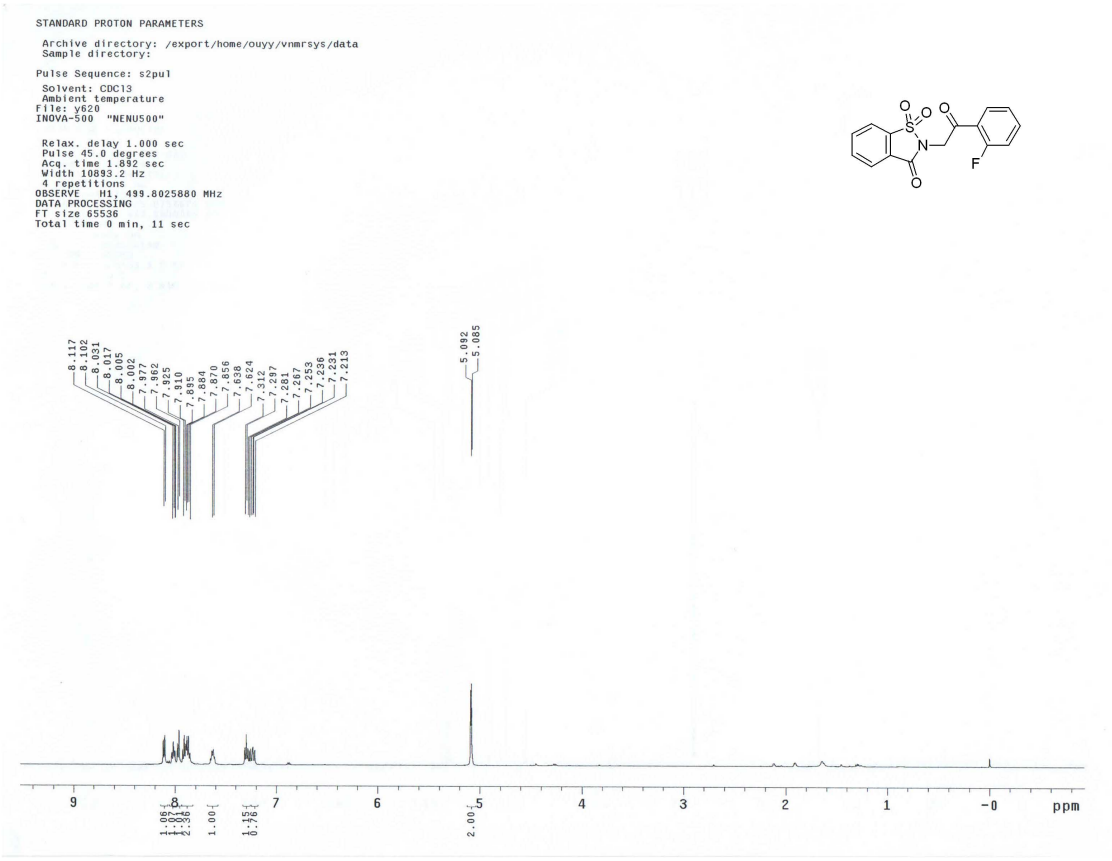

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: t321
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
384 repetitions
OBSERVE C13, 125.6754642 MHz
DECOUPLE H1, 499.8050305 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
77.252
77.000
76.744
187.309
159.031
148.487
137.827
135.222
135.168
134.623
133.711
130.389
128.473
127.086
125.570
123.109
121.316
44.492
NO2
220
200
180
160
140
120
100
80
60
40
20
0
ppm

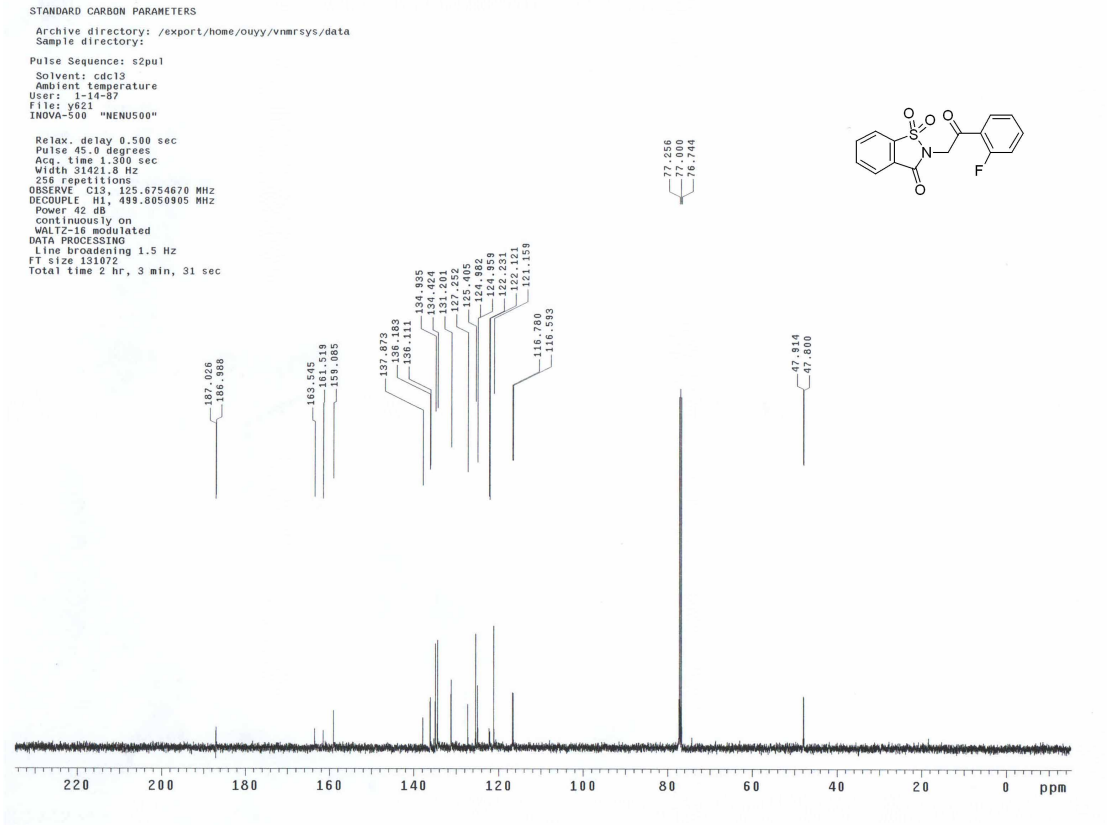
Product 4i


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: r797
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8561.6 Hz
8 repetitions
OBSERVE H1, 499.8025908 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.119
8.104
7.980
7.964
7.926
7.911
7.895
7.886
7.871
7.857
7.597
7.582
7.528
7.450
7.435
7.419
7.265
7.195
7.179
5.146
3.859
0.000
1.05
0.98
2.30
1.02
1.06
1.02
0.97
2.00
3.24
9
8
7
6
5
4
3
2
1
-0
ppm

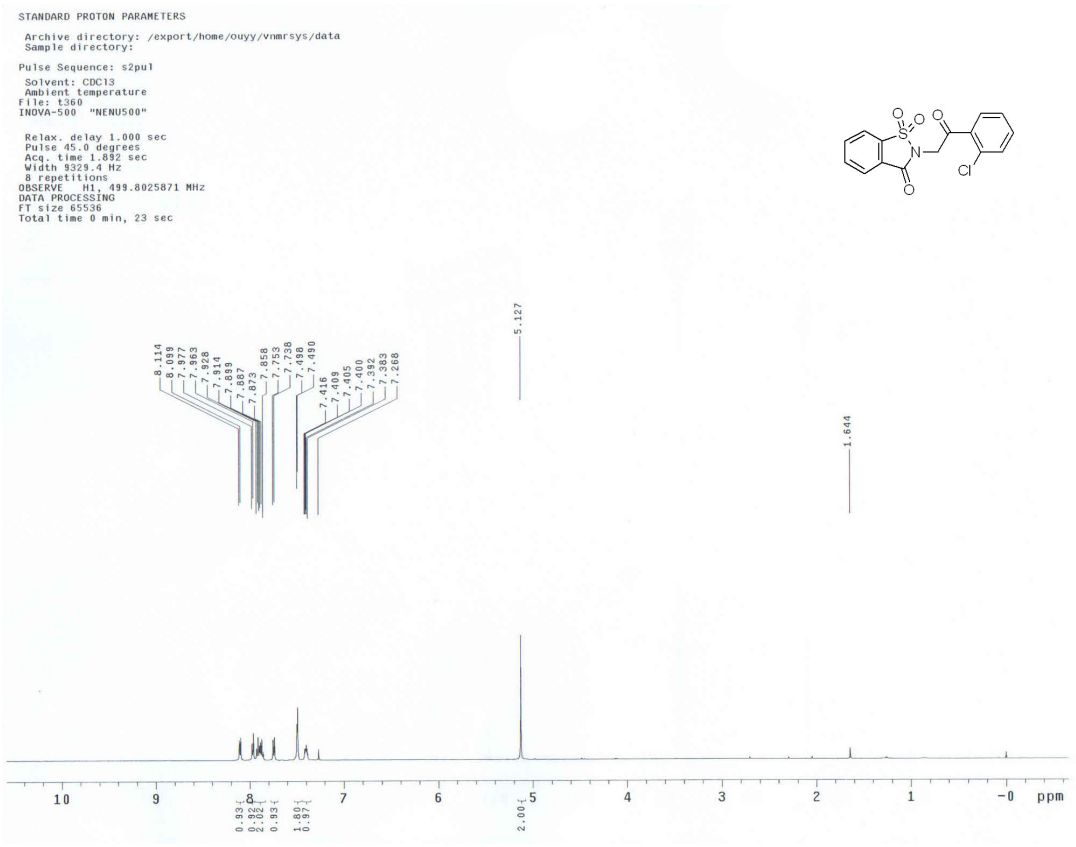

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: r798
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754675 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
188.648
159.966
159.123
137.854
135.260
134.939
134.451
129.934
127.775
125.417
121.175
120.919
120.614
112.293
77.256
77.003
76.748
55.464
44.534
220
200
180
160
140
120
100
80
60
40
20
0
ppm

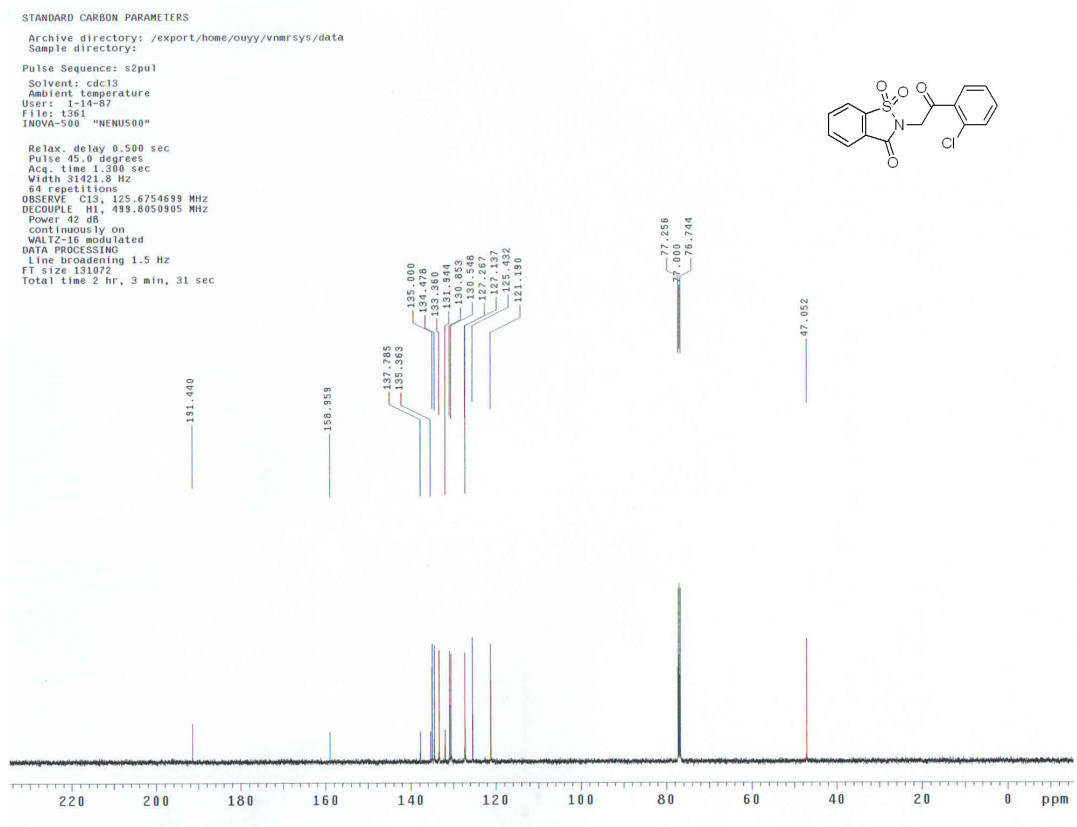
Product 4j


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: y620
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
4 repetitions
OBSERVE H1, 499.8025880 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec
8.117
8.102
8.081
8.017
8.005
8.002
7.977
7.962
7.925
7.910
7.895
7.884
7.870
7.858
7.838
7.824
7.312
7.297
7.281
7.267
7.258
7.236
7.231
7.213
5.092
5.085
F
ppm

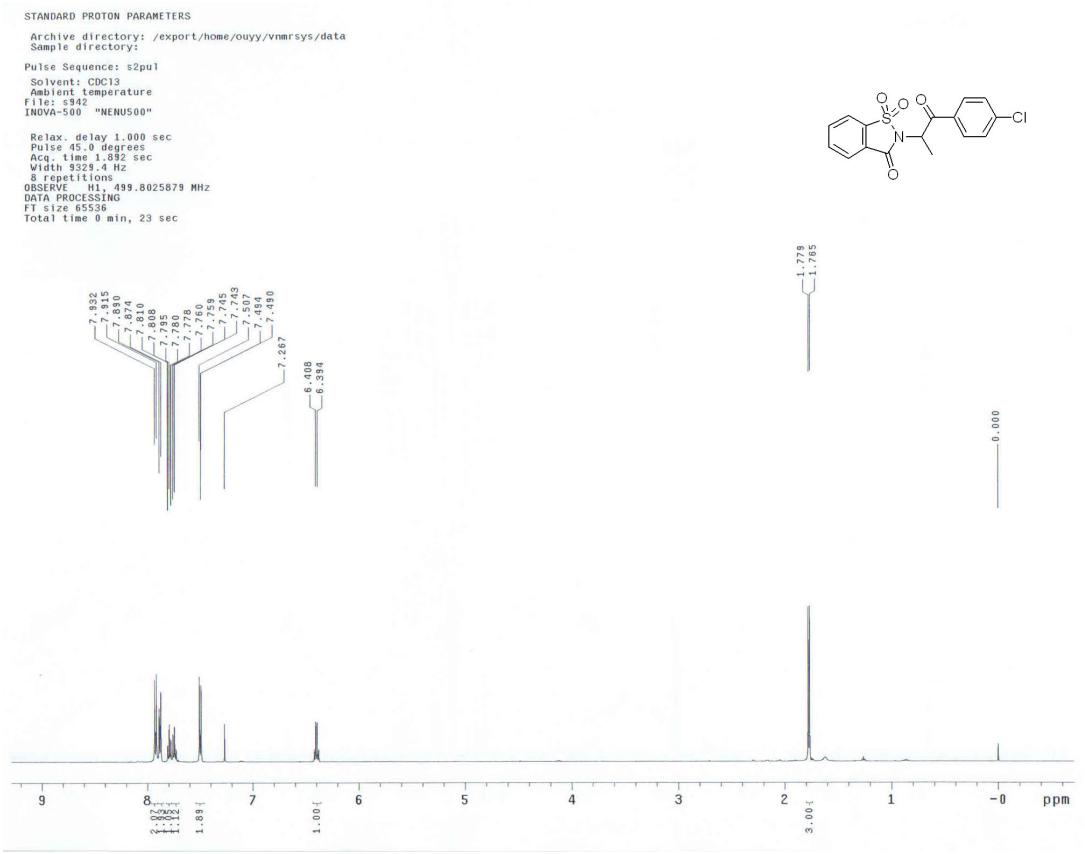

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: y621
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754670 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
187.026
186.988
163.545
161.518
159.085
137.873
136.183
136.111
134.935
134.424
131.201
127.252
125.405
124.982
124.959
122.233
122.121
121.159
116.780
116.593
77.256
77.000
76.744
47.814
47.800
F
ppm

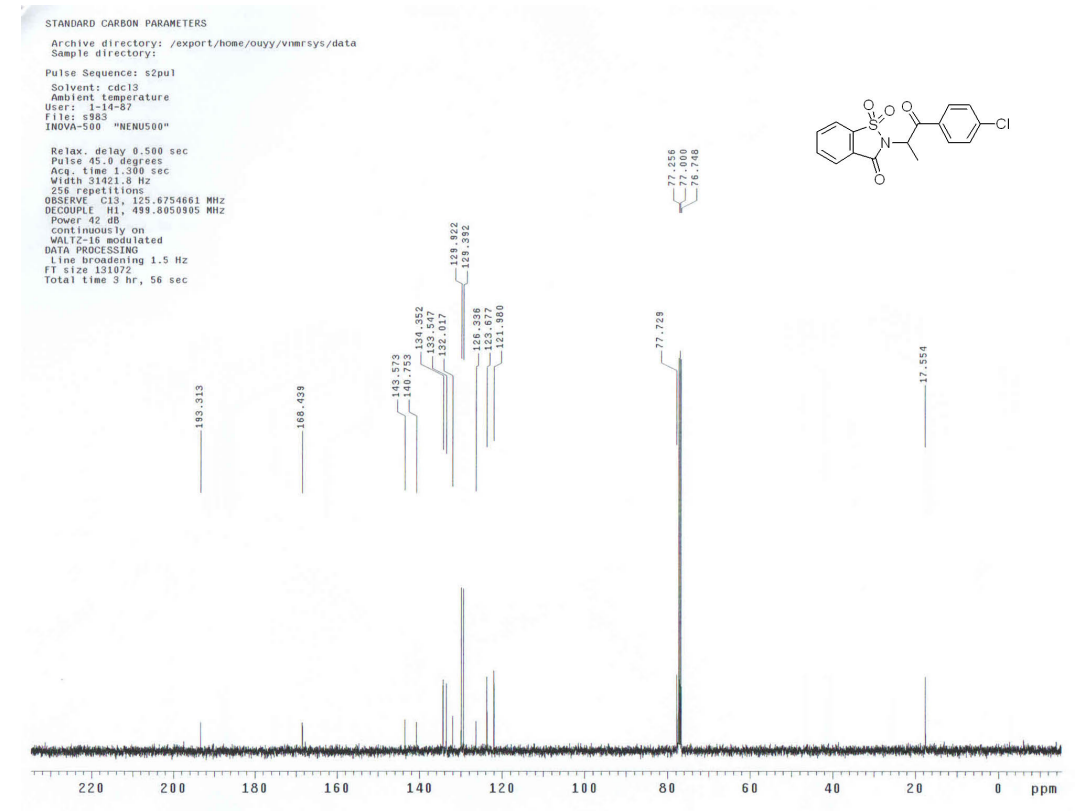
Product 4k


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: t360
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9329.4 Hz
8 repetitions
OBSERVE H1, 499.8025871 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.114
8.099
7.977
7.963
7.828
7.814
7.809
7.807
7.873
7.858
7.753
7.738
7.498
7.490
7.416
7.409
7.405
7.400
7.392
7.388
7.288
5.127
1.644
0.93
0.82
2.02
0.93
1.80
0.97
2.00
10
9
8
7
6
5
4
3
2
1
-0
ppm

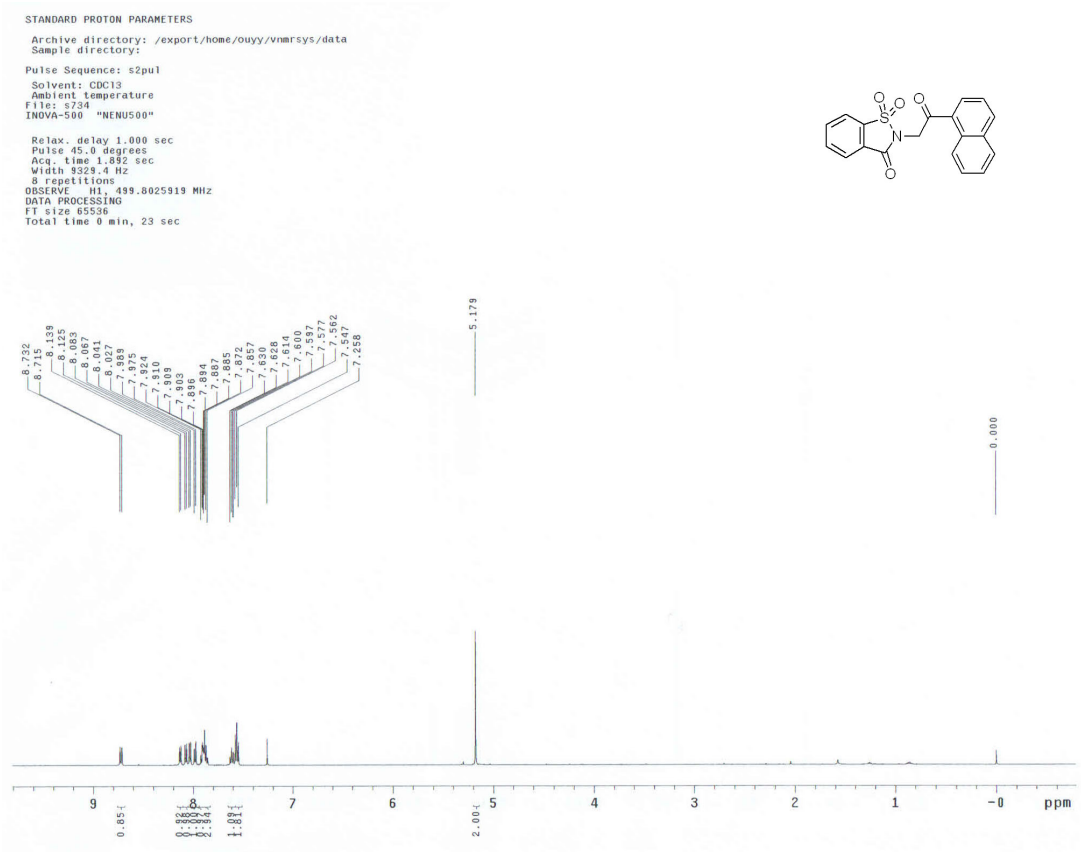

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: t361
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754699 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
191.440
158.959
137.705
135.963
135.000
134.478
133.360
131.944
130.853
130.548
127.267
127.137
125.432
121.190
77.256
77.000
76.744
47.052
220
200
180
160
140
120
100
80
60
40
20
0
ppm

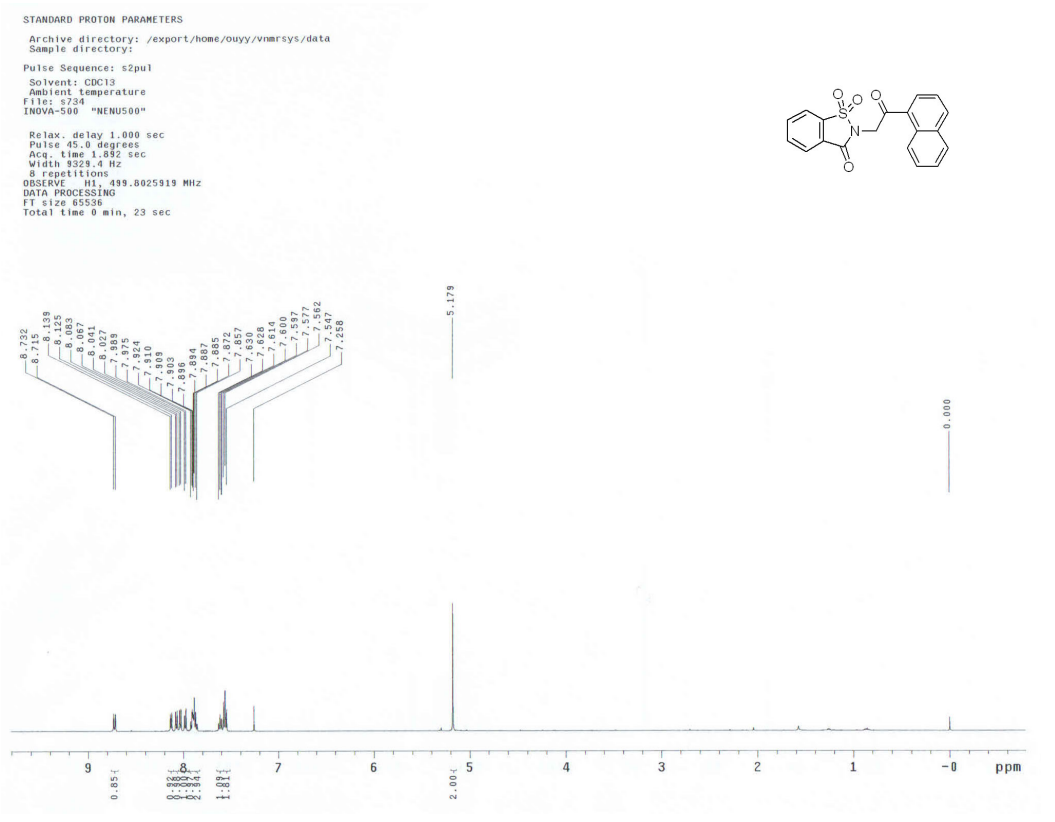
Product 4l


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: s942
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9329.4 Hz
8 repetitions
OBSERVE H1, 499.8025879 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
Cl
7.932
7.915
7.890
7.874
7.810
7.808
7.795
7.789
7.778
7.760
7.759
7.745
7.743
7.507
7.494
7.490
7.267
6.408
6.394
1.779
1.765
0.000
ppm

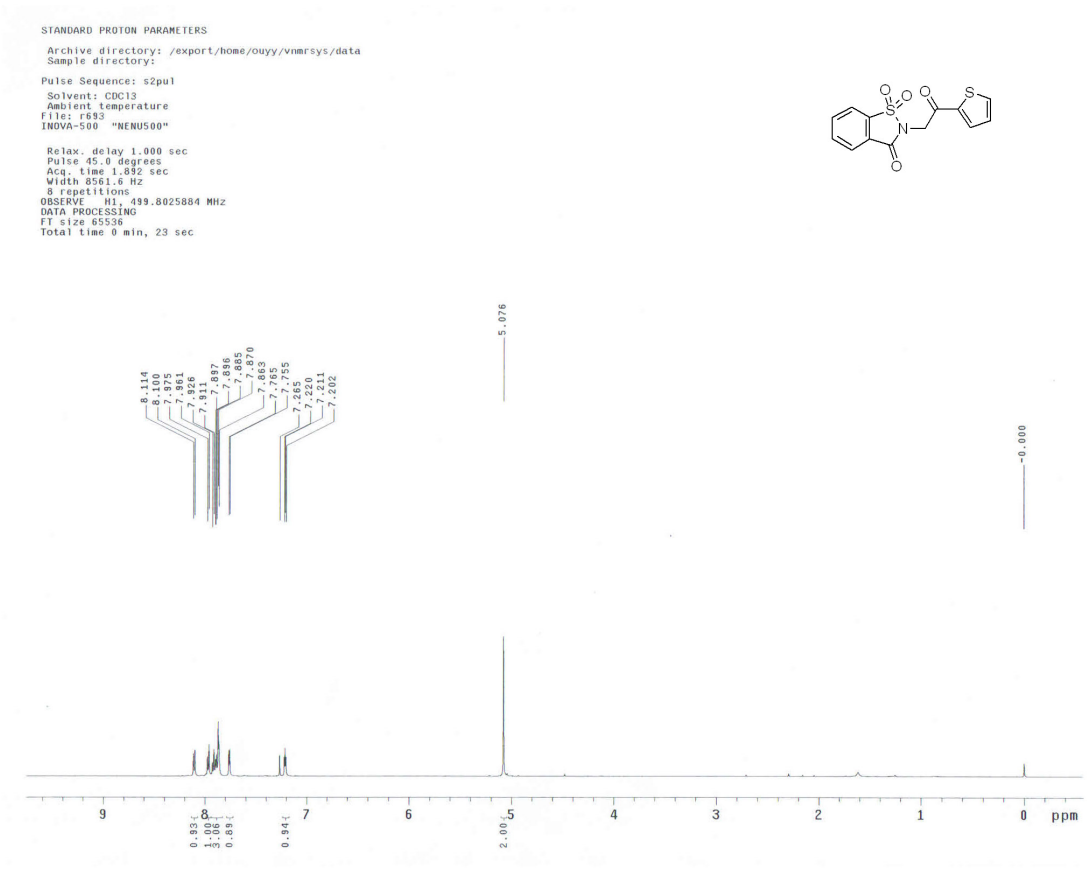

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: s983
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754661 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
Cl
193.313
168.439
143.573
140.753
134.352
133.547
132.017
129.922
129.392
126.336
123.677
121.980
77.729
77.256
77.000
76.748
17.554
ppm

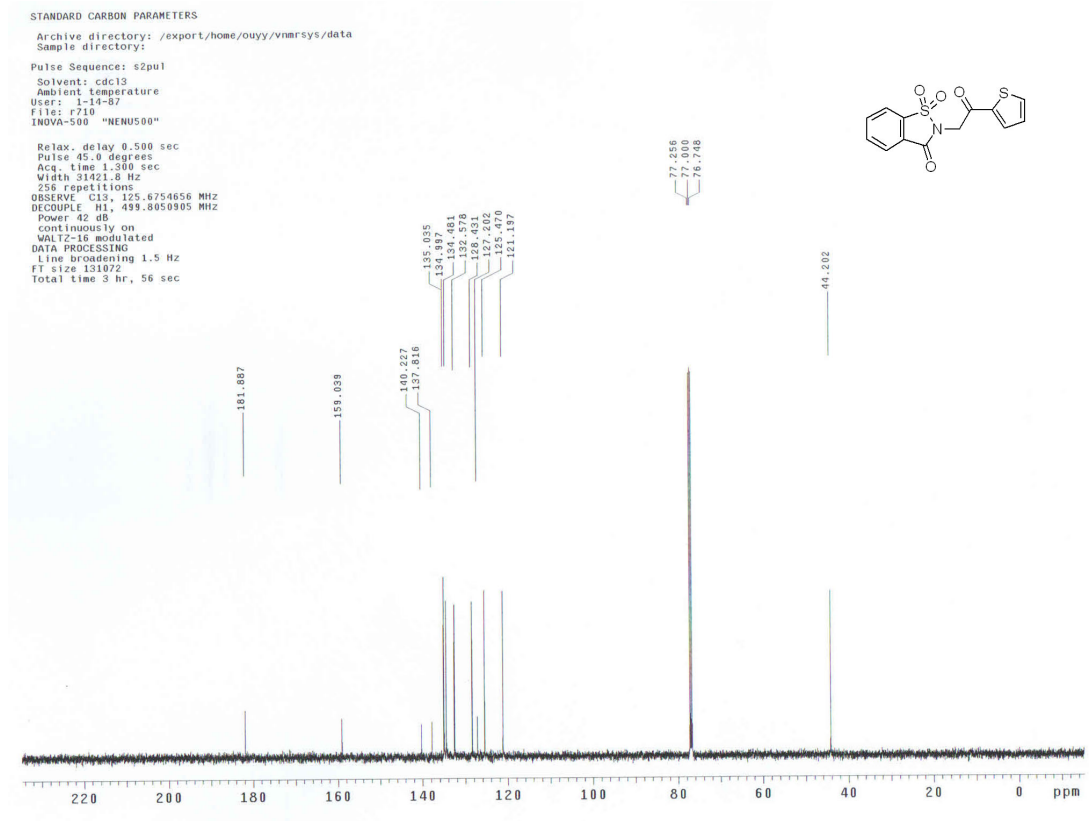
Product 4m


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: s734
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9329.4 Hz
8 repetitions
OBSERVE H1, 499.8025919 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.732
8.715
8.139
8.125
8.083
8.067
8.041
8.027
7.989
7.975
7.924
7.910
7.909
7.903
7.896
7.894
7.885
7.872
7.857
7.630
7.628
7.614
7.600
7.597
7.577
7.562
7.547
7.258
5.179
0.000
9
8
7
6
5
4
3
2
1
-0
ppm
0.85
2.00
1.81

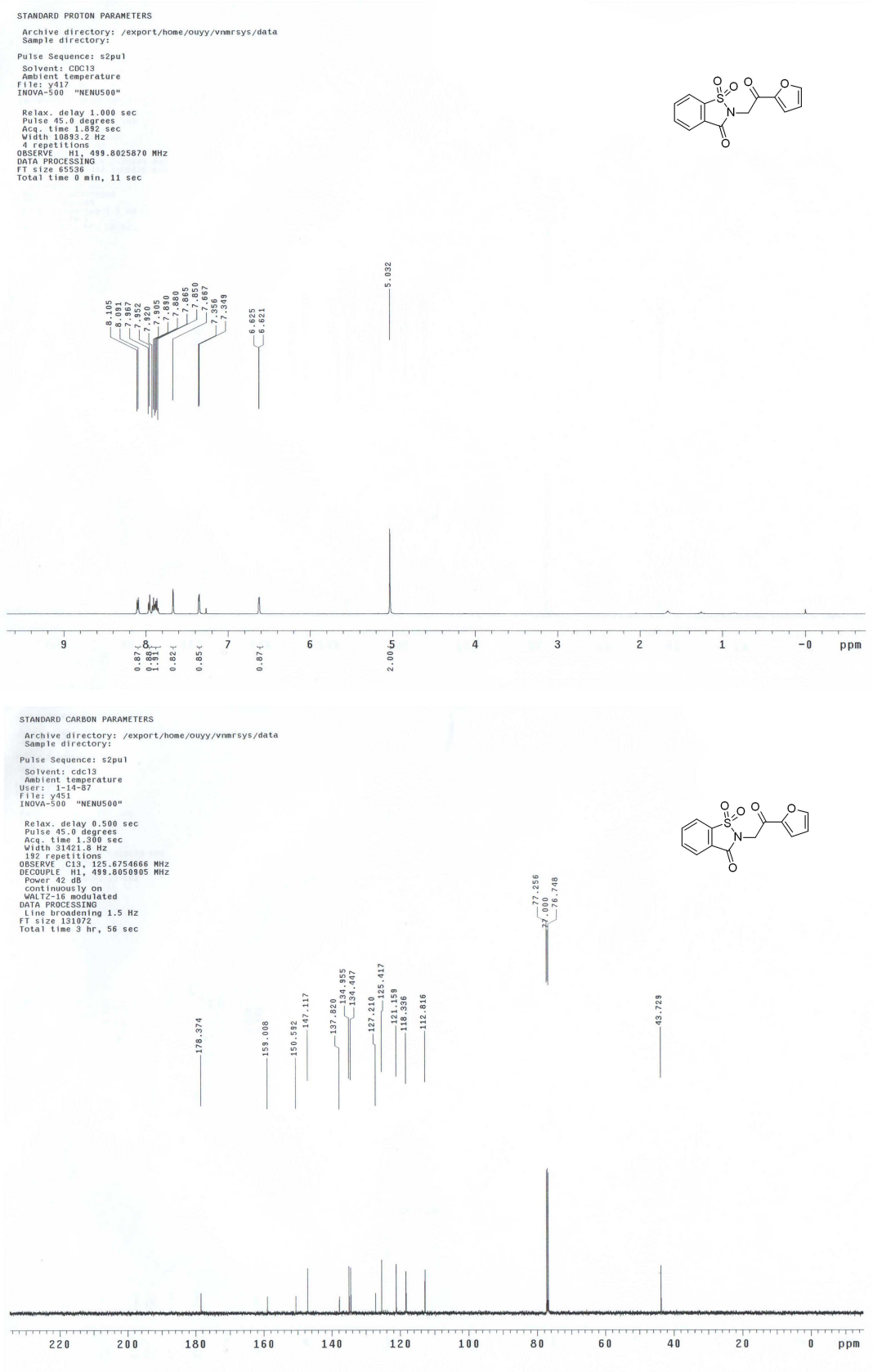

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: s734
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9329.4 Hz
8 repetitions
OBSERVE H1, 499.8025919 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.732
8.715
8.139
8.125
8.083
8.067
8.041
8.027
7.989
7.975
7.924
7.910
7.909
7.903
7.896
7.894
7.885
7.872
7.857
7.630
7.628
7.614
7.600
7.597
7.577
7.562
7.547
7.258
5.179
0.000
9
8
7
6
5
4
3
2
1
-0
ppm
0.85
2.00
1.81

Product 4n


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: r693
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8561.6 Hz
8 repetitions
OBSERVE H1, 499.8025884 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.114
8.100
8.075
7.961
7.926
7.911
7.897
7.886
7.865
7.770
7.763
7.755
7.265
7.220
7.211
7.202
5.076
0.000
0.93
1.00
3.08
0.89
0.94
2.00
9
8
7
6
5
4
3
2
1
0
ppm

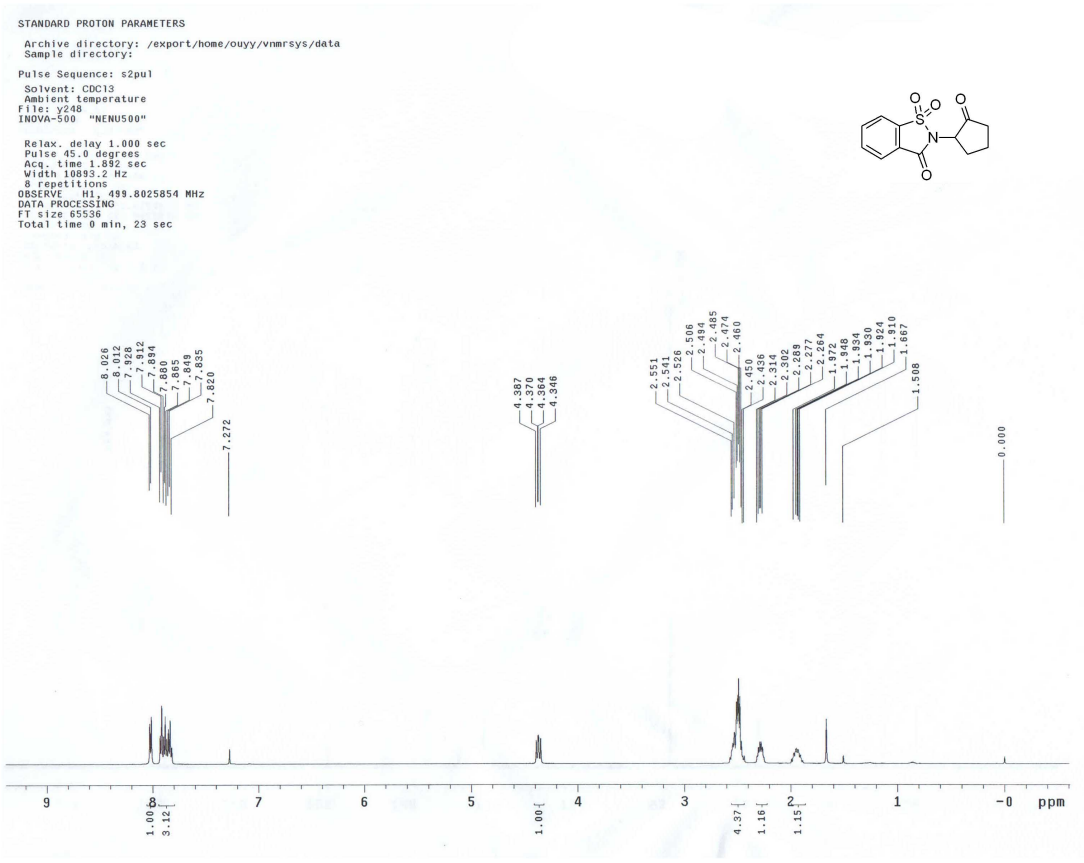

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: r710
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754656 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
77.256
77.000
76.744
135.035
134.987
134.481
132.578
128.243
127.202
125.470
121.197
44.202
181.887
159.039
140.227
137.816
220
200
180
160
140
120
100
80
60
40
20
0
ppm

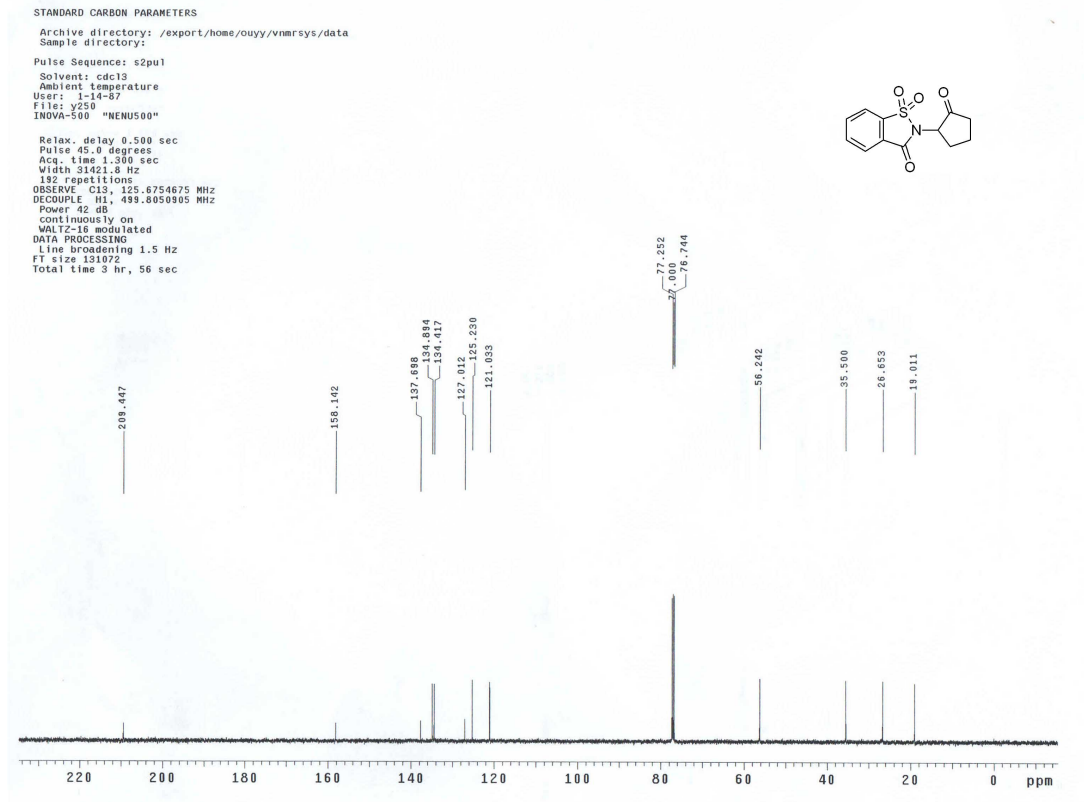
Product 4o


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: y417
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
4 repetitions
OBSERVE H1, 499.8025870 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec
8.105
8.091
7.967
7.952
7.920
7.905
7.880
7.865
7.850
7.667
7.656
7.349
6.625
6.621
5.032
9
8
7
6
5
4
3
2
1
-0
ppm
0.87
0.80
1.95
0.82
0.85
0.87
2.00

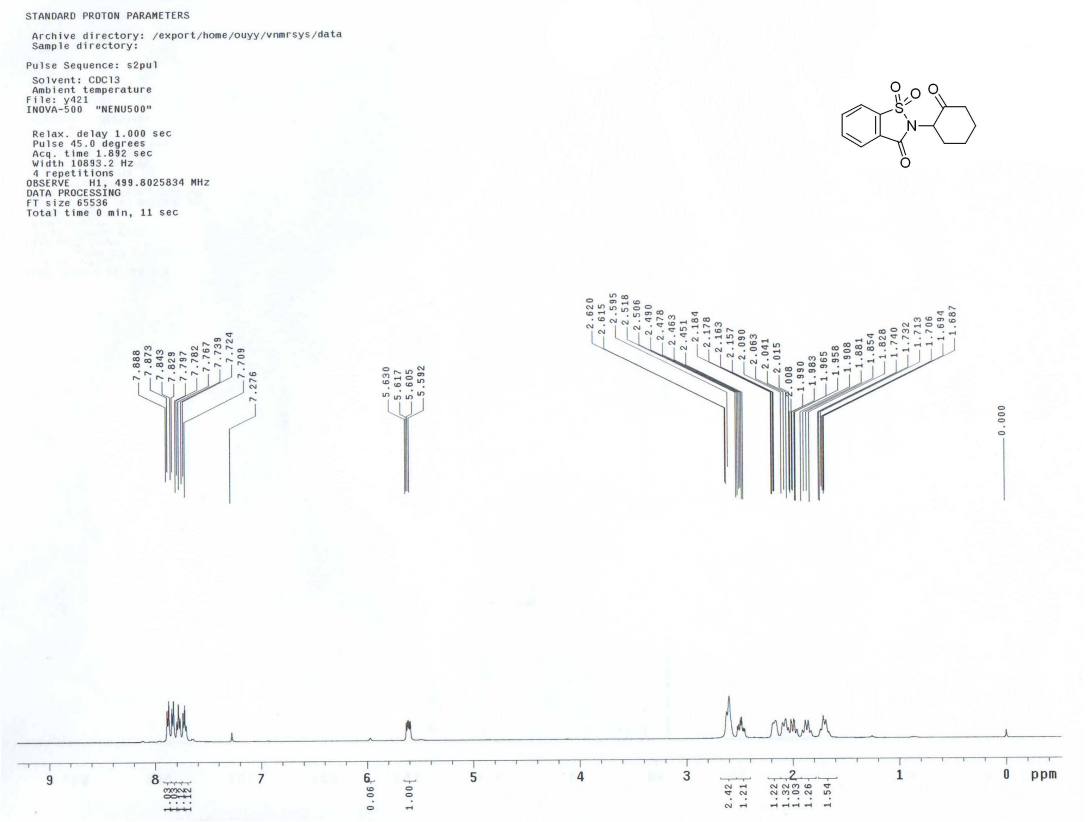
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: y451
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754666 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
178.374
159.008
150.582
147.117
137.820
134.955
134.447
127.210
125.417
121.159
118.336
112.816
77.256
77.000
76.748
43.729
220
200
180
160
140
120
100
80
60
40
20
0
ppm

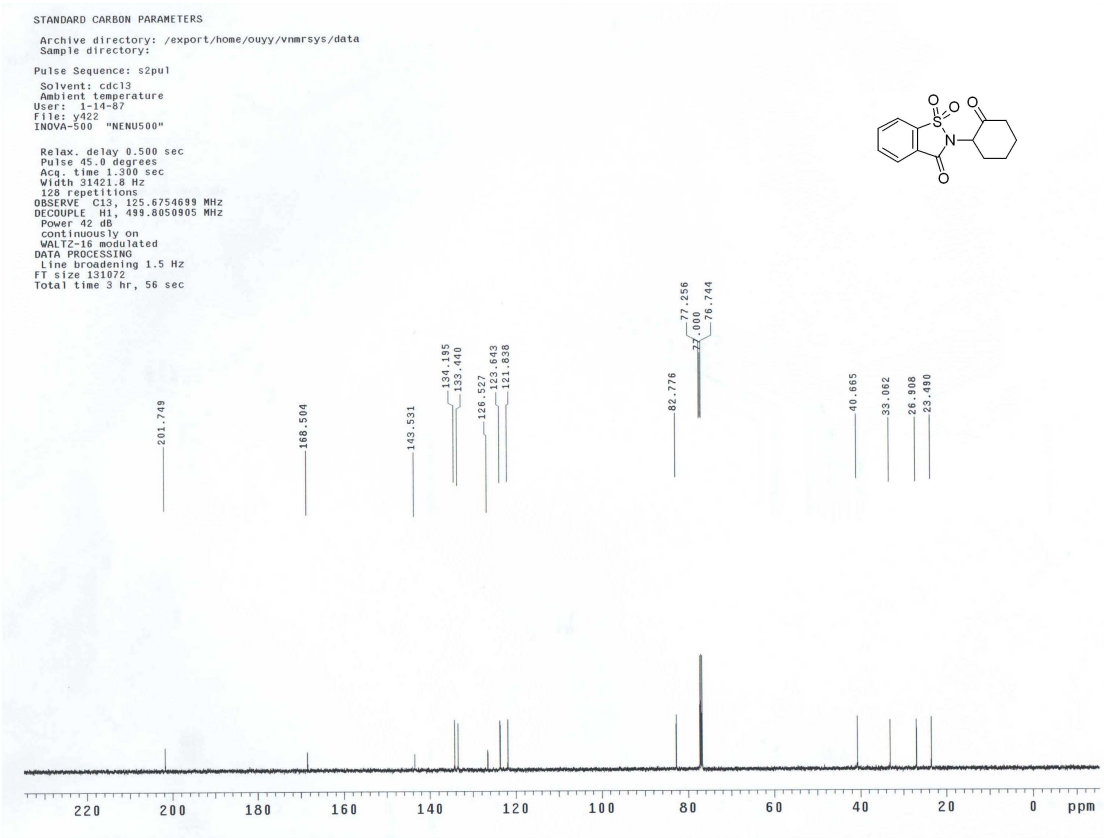
Product 4p


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: y248
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
8 repetitions
OBSERVE H1, 499.8025854 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.028
8.012
7.928
7.912
7.894
7.880
7.865
7.849
7.835
7.820
7.272
4.387
4.370
4.364
4.346
2.551
2.541
2.526
2.506
2.494
2.485
2.474
2.460
2.450
2.445
2.314
2.302
2.289
2.277
2.264
1.972
1.948
1.934
1.930
1.924
1.910
1.667
1.508
0.000
1.00
3.12
1.00
4.37
1.16
1.15
9
8
7
6
5
4
3
2
1
-0
ppm

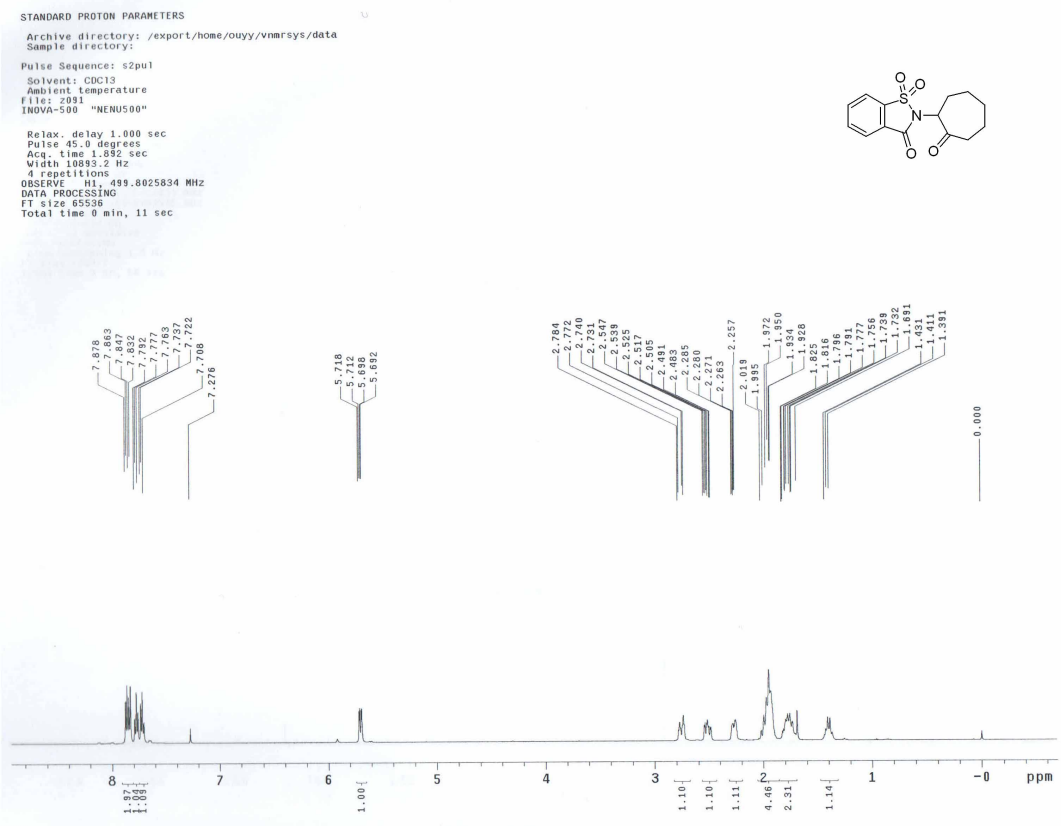

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: y250
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754675 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
209.447
158.142
137.688
134.884
134.417
127.012
125.230
121.033
77.252
77.000
76.744
56.242
35.500
26.653
19.011
220
200
180
160
140
120
100
80
60
40
20
0
ppm

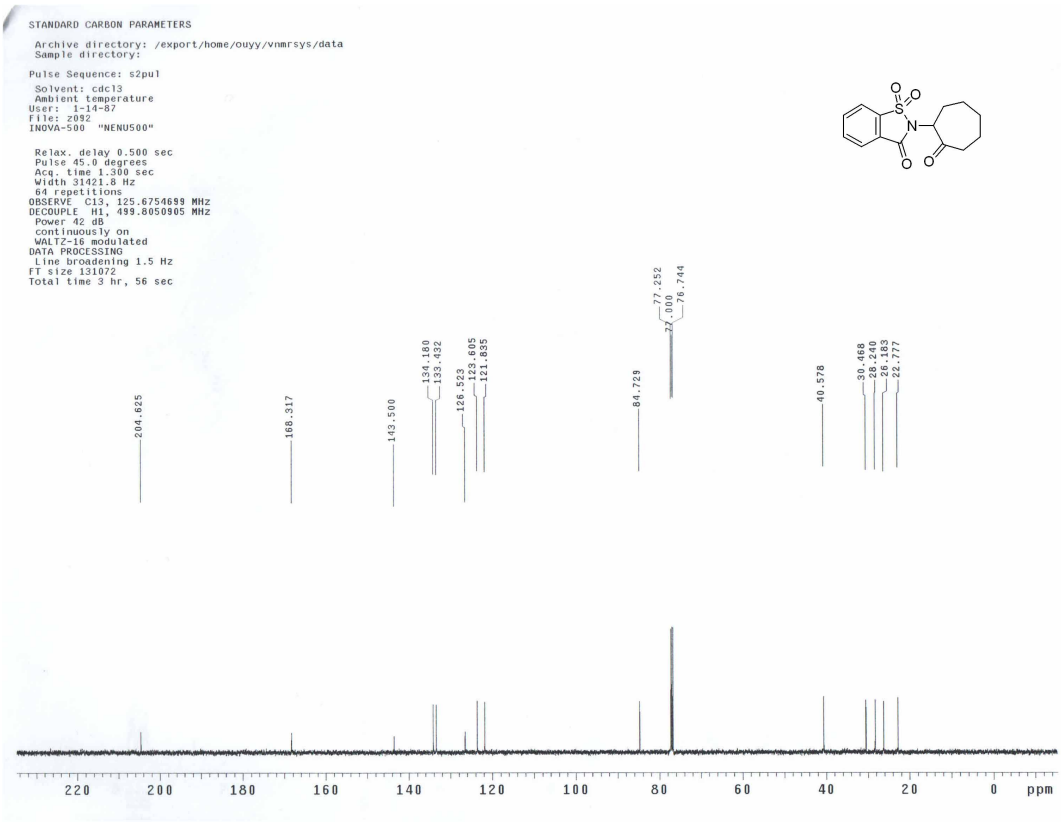
Product 4q


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: y421
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
4 repetitions
OBSERVE H1, 499.8025834 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec
7.888
7.873
7.843
7.829
7.792
7.782
7.767
7.739
7.724
7.709
7.276
5.630
5.617
5.605
5.592
2.620
2.595
2.518
2.506
2.490
2.478
2.463
2.451
2.184
2.178
2.163
2.157
2.080
2.063
2.041
2.015
2.008
1.980
1.963
1.905
1.858
1.881
1.854
1.768
1.740
1.732
1.713
1.706
1.694
1.687
0.000
9
8
7
6
5
4
3
2
1
0
ppm
0.06
1.00
2.42
1.21
1.22
1.03
1.00
1.26
1.54

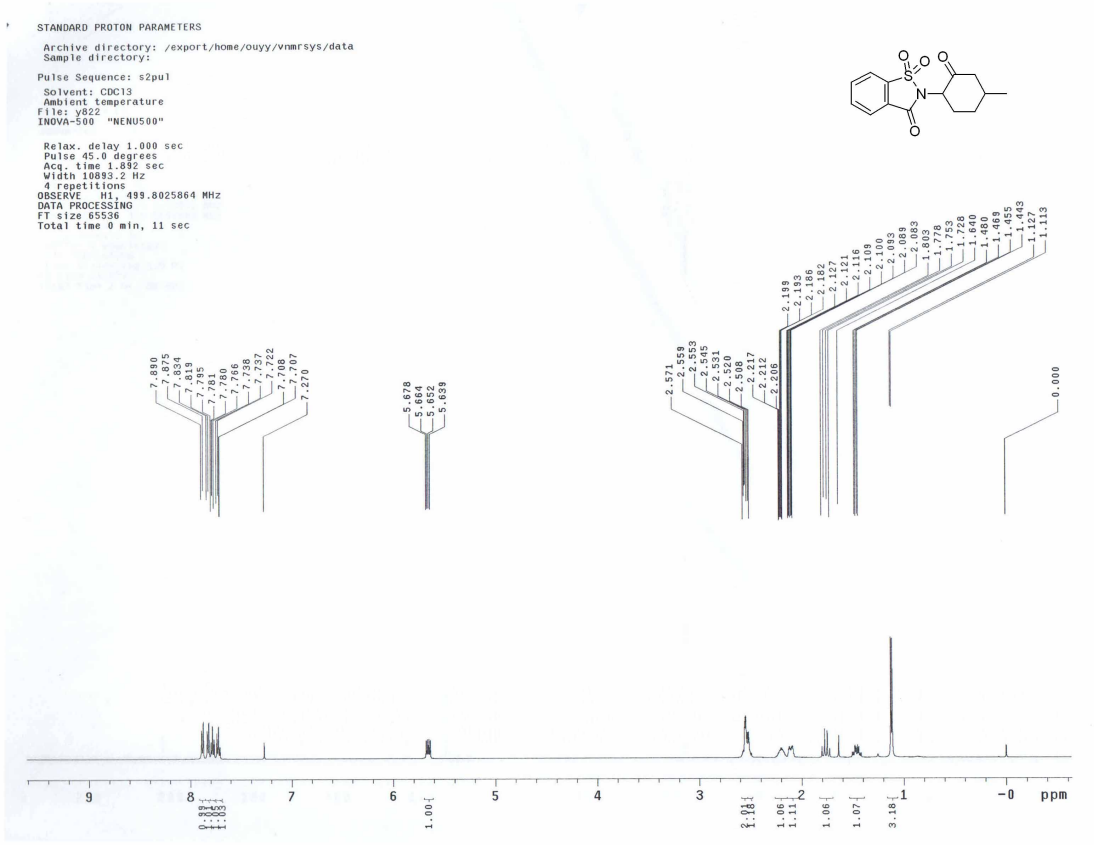

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: y422
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754699 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
201.749
168.504
143.531
134.195
133.440
126.527
123.643
121.838
77.256
77.000
76.744
82.776
40.665
33.062
26.908
23.490
220
200
180
160
140
120
100
80
60
40
20
0
ppm

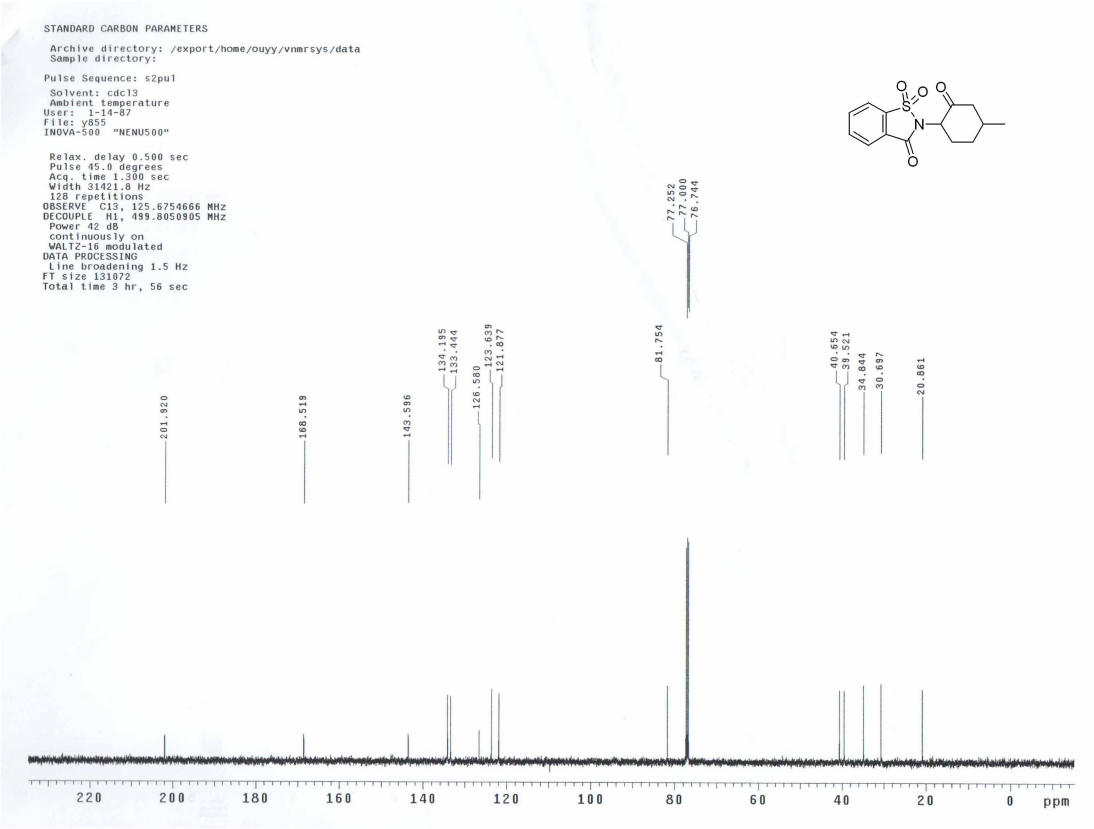
Product 4r


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: z091
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
4 repetitions
OBSERVE H1, 499.8025834 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec
7.878
7.863
7.847
7.832
7.792
7.778
7.758
7.737
7.722
7.708
7.276
5.718
5.712
5.698
5.682
2.784
2.772
2.740
2.731
2.547
2.535
2.517
2.505
2.491
2.483
2.285
2.280
2.271
2.263
2.257
2.019
1.995
1.972
1.950
1.934
1.928
1.825
1.816
1.796
1.791
1.777
1.756
1.739
1.732
1.691
1.431
1.411
1.391
0.000
1.07
0.80
1.00
1.00
1.10
1.10
1.11
4.46
2.31
1.14
ppm

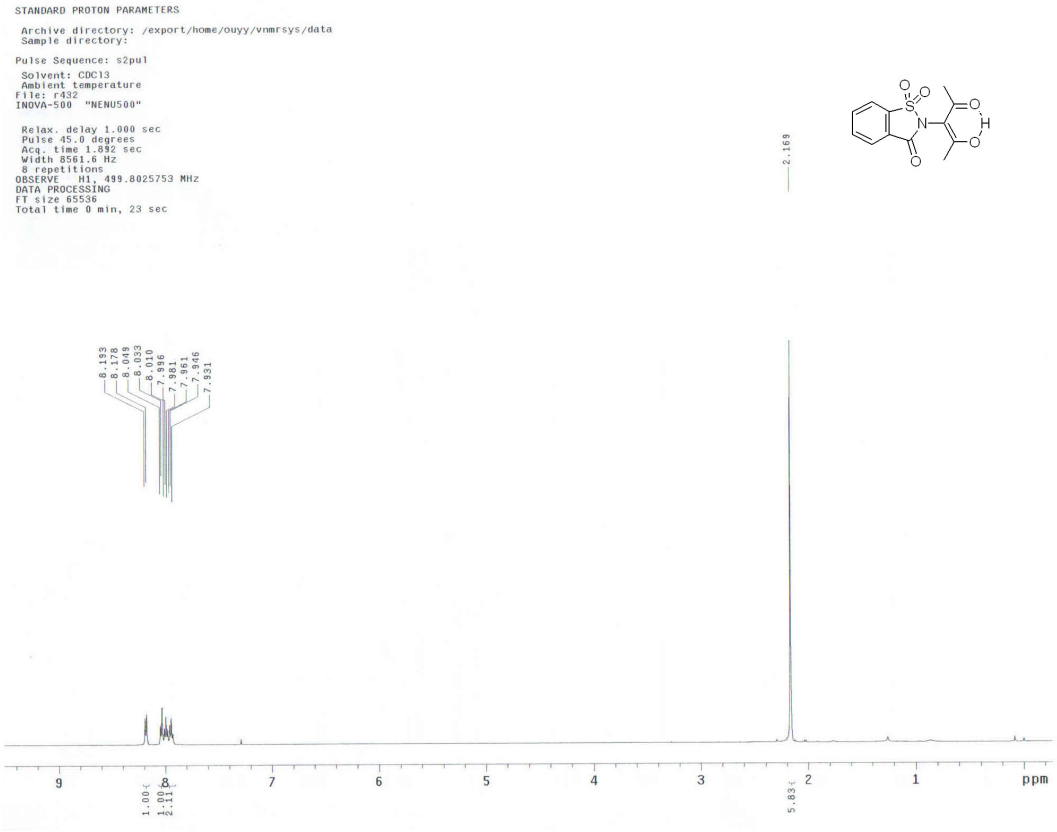

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: z092
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754699 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
204.625
168.317
143.500
134.180
133.432
128.605
126.523
121.835
84.729
77.252
77.000
76.744
40.578
30.468
28.240
26.183
22.777
220
200
180
160
140
120
100
80
60
40
20
0
ppm

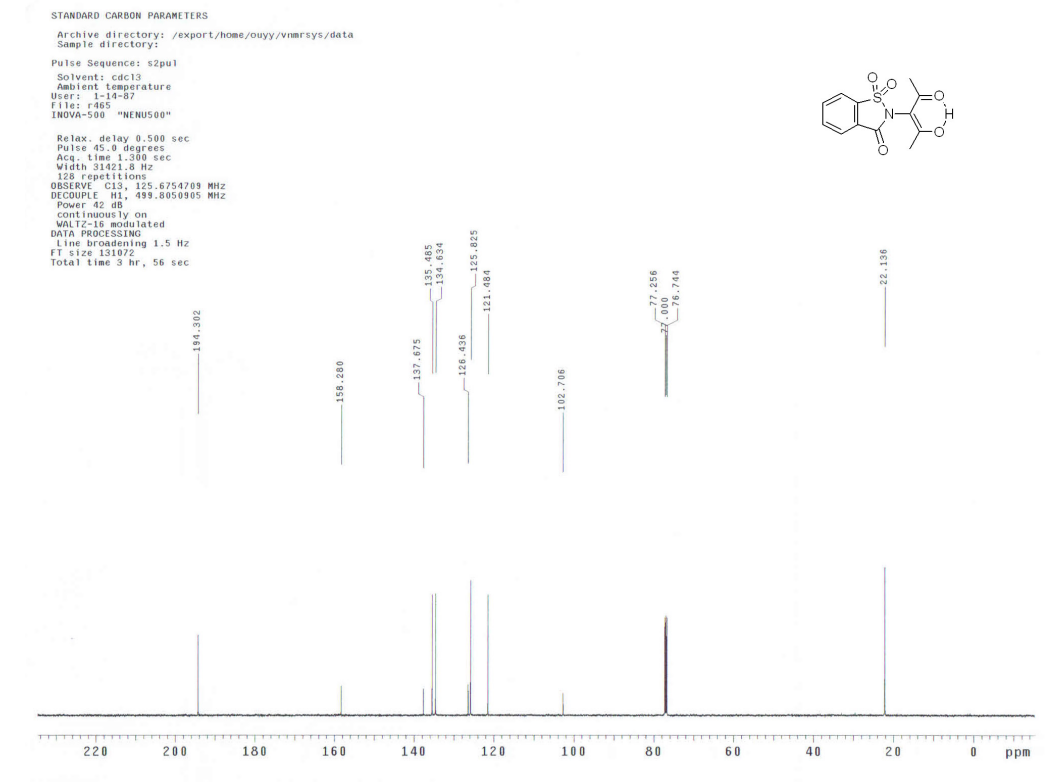
Product 4s


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: y822
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
4 repetitions
OBSERVE H1, 499.8025864 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec
ppm

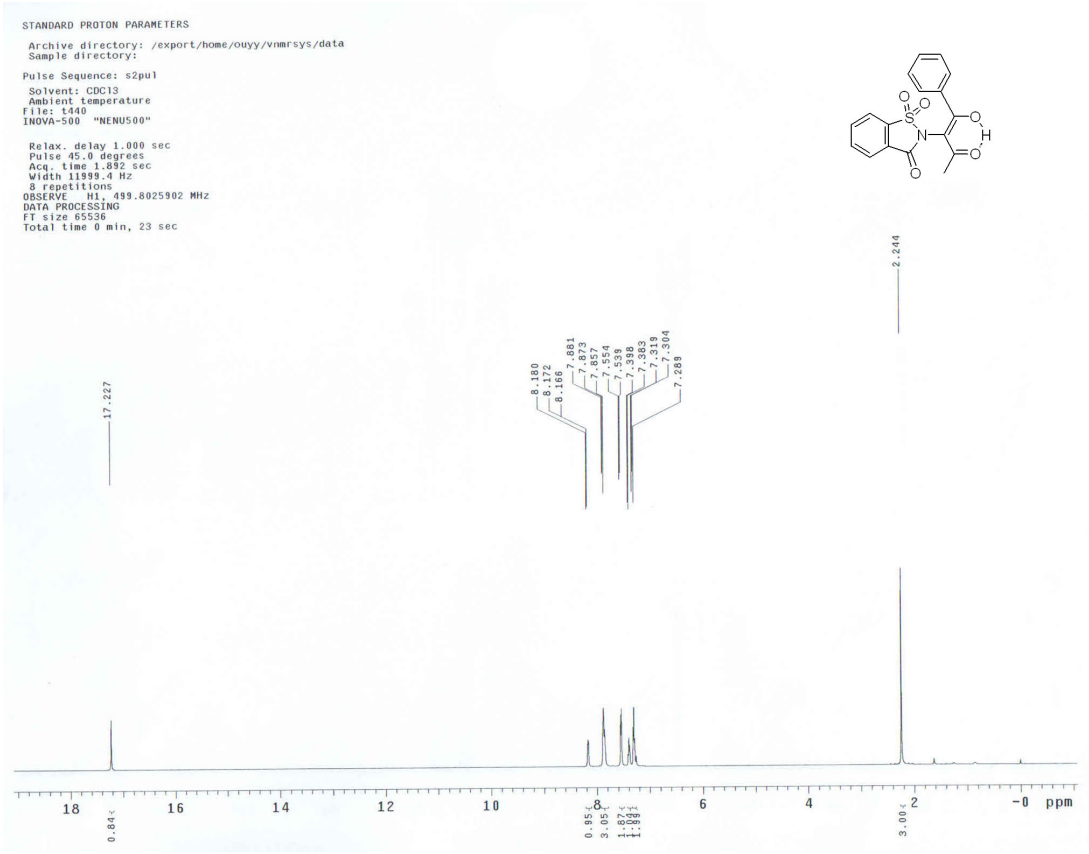

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: y855
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754666 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
ppm

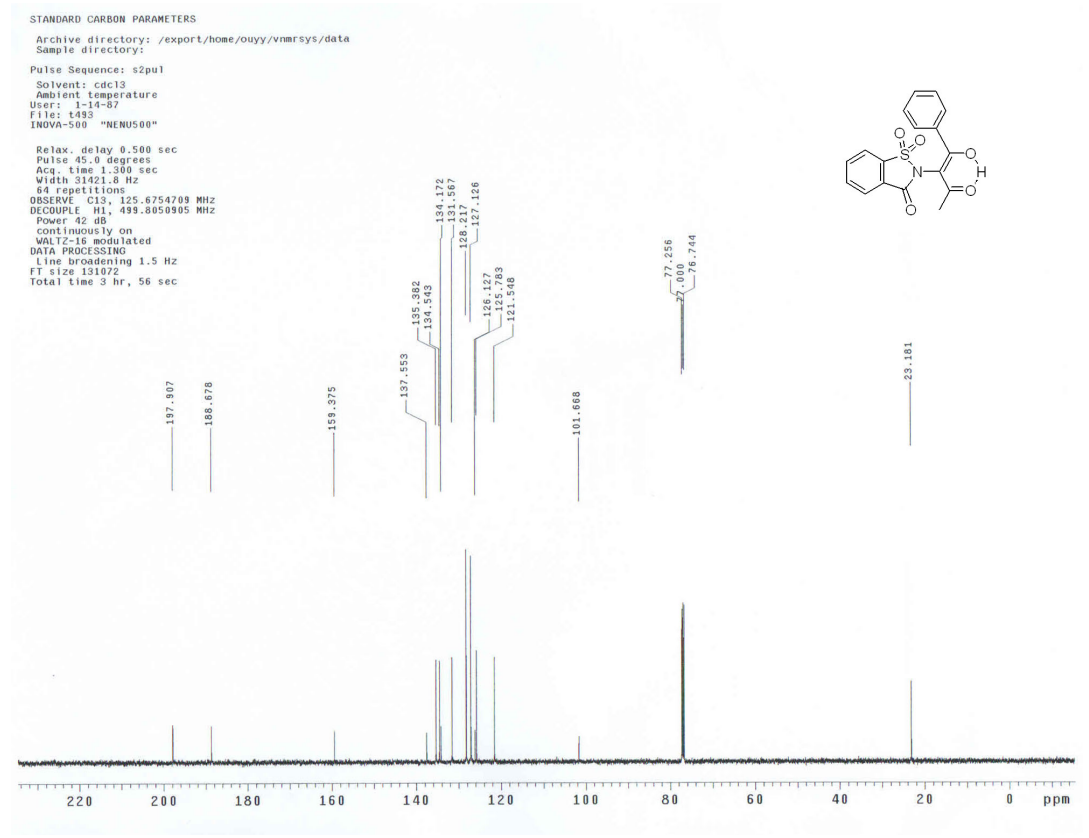
Product 4t


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: r432
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8561.6 Hz
8 repetitions
OBSERVE H1, 499.8025753 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.193
8.178
8.049
8.033
8.010
7.985
7.981
7.961
7.946
7.931
2.169
1.00
1.00
2.11
5.83
9
8
7
6
5
4
3
2
1
ppm

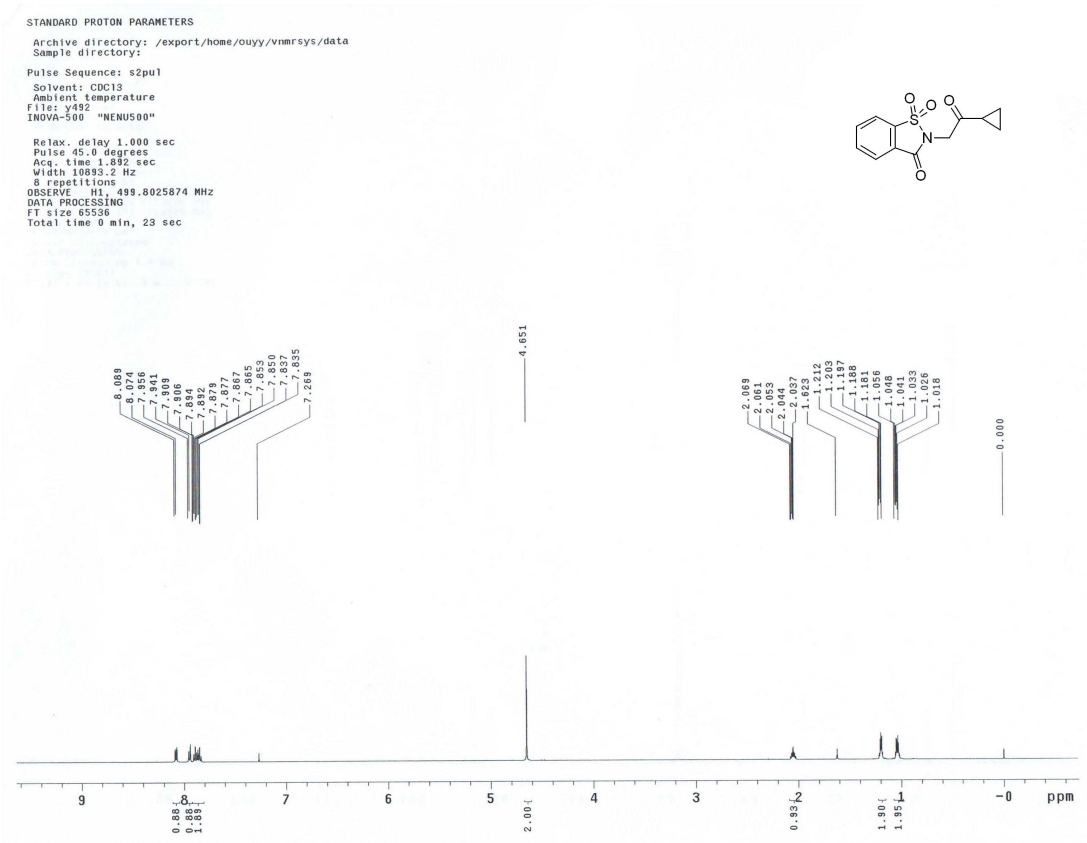

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: r465
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754709 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
194.302
158.280
137.675
135.485
134.634
126.438
125.825
121.484
102.706
77.256
77.000
76.744
22.136
220
200
180
160
140
120
100
80
60
40
20
0
ppm

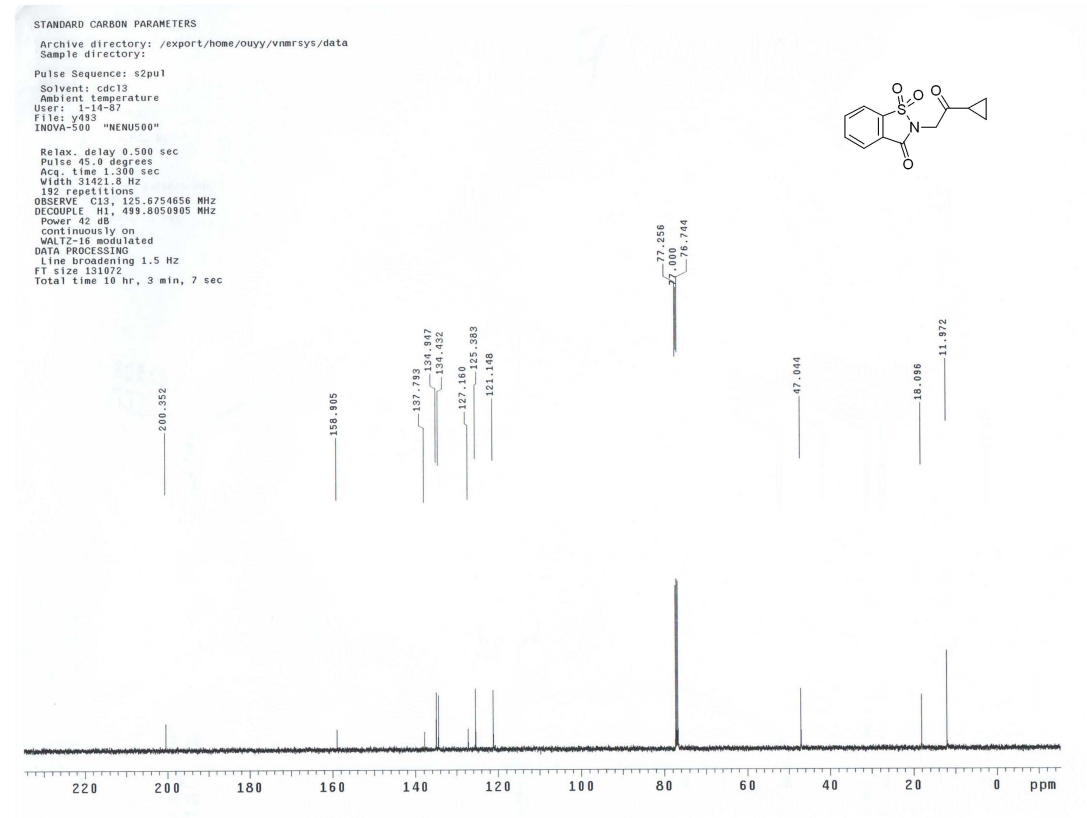
Product 4u


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: t440
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 11999.4 Hz
8 repetitions
OBSERVE H1, 499.8025902 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
17.227
8.180
8.172
8.166
7.881
7.873
7.857
7.564
7.539
7.398
7.383
7.319
7.304
7.289
2.244
0.84
0.95
3.05
1.87
1.99
3.00
18
16
14
12
10
8
6
4
2
-0
ppm

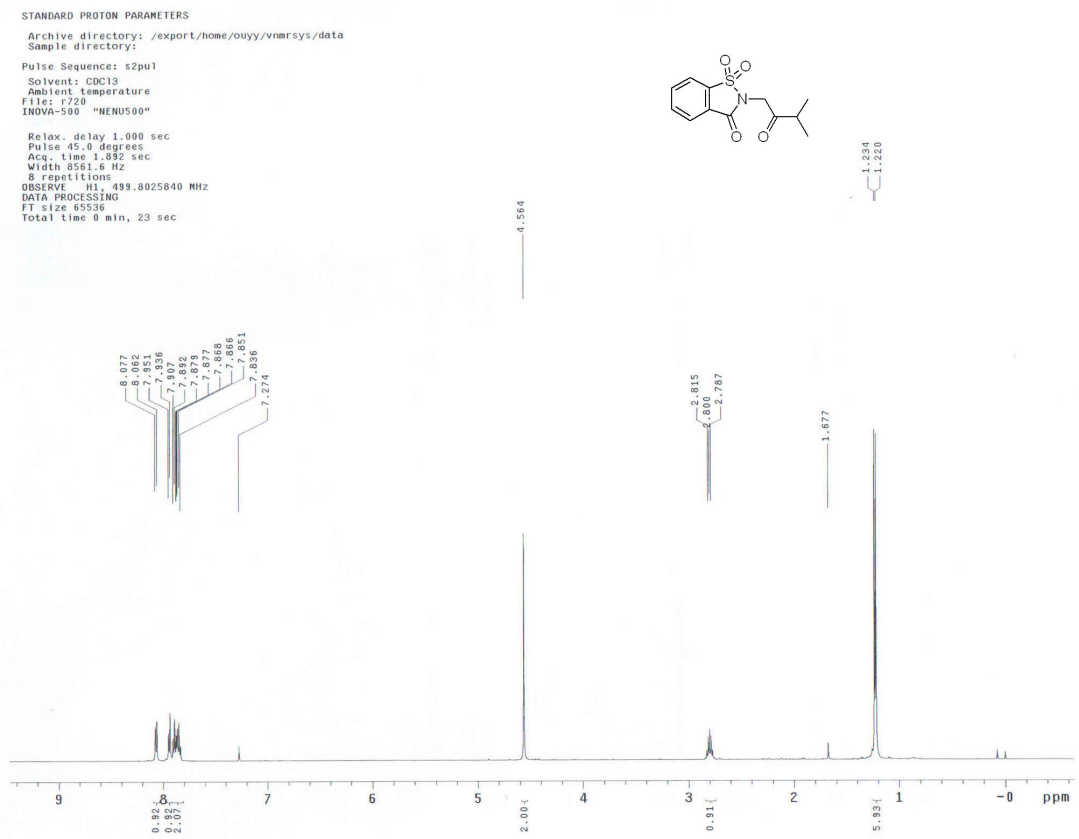

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: t493
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754709 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
197.907
188.678
159.375
137.553
135.382
134.543
134.172
131.567
128.217
127.126
126.127
125.783
121.546
101.668
77.256
77.000
76.744
23.181
220
200
180
160
140
120
100
80
60
40
20
0
ppm

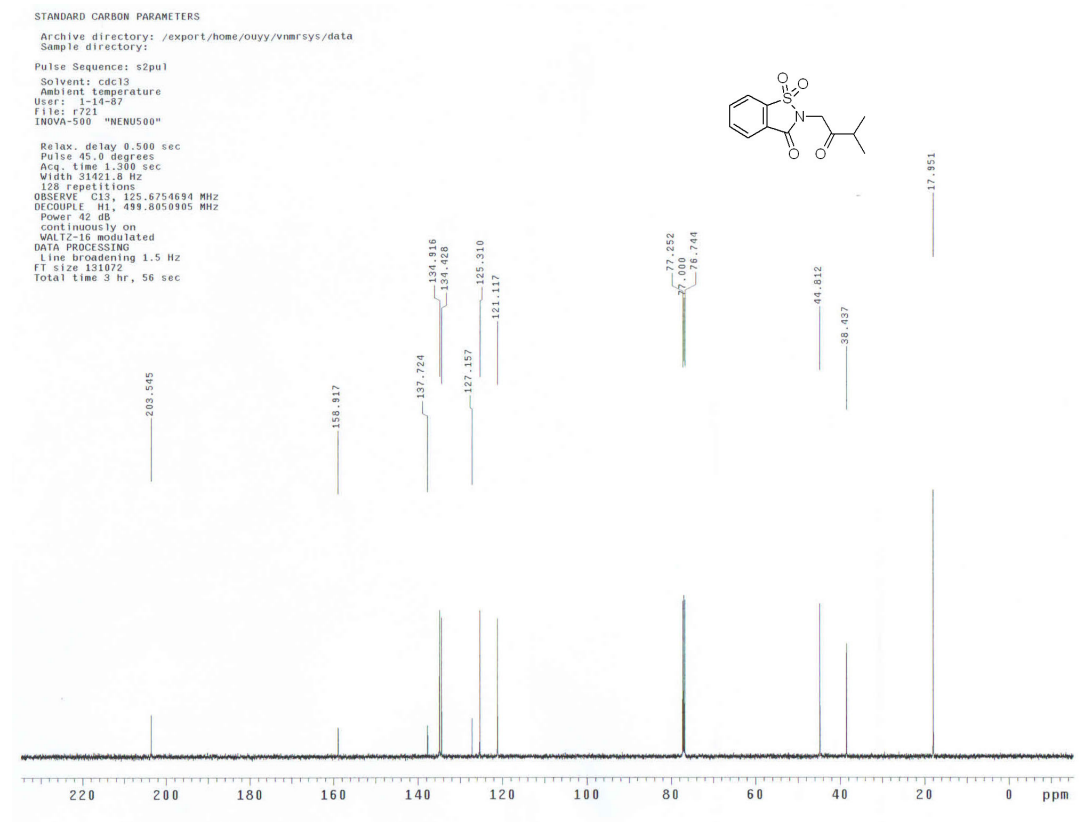
Product 4v


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: y492
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
8 repetitions
OBSERVE H1, 499.8025874 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.089
8.074
7.956
7.941
7.909
7.906
7.898
7.892
7.879
7.877
7.867
7.865
7.853
7.850
7.837
7.835
7.269
4.651
2.069
2.061
2.053
2.044
2.037
2.028
1.212
1.203
1.197
1.188
1.181
1.056
1.046
1.041
1.033
1.026
1.018
0.000
9
8
7
6
5
4
3
2
1
-0
ppm
0.88
0.88
1.89
2.00
0.99
1.90
1.95

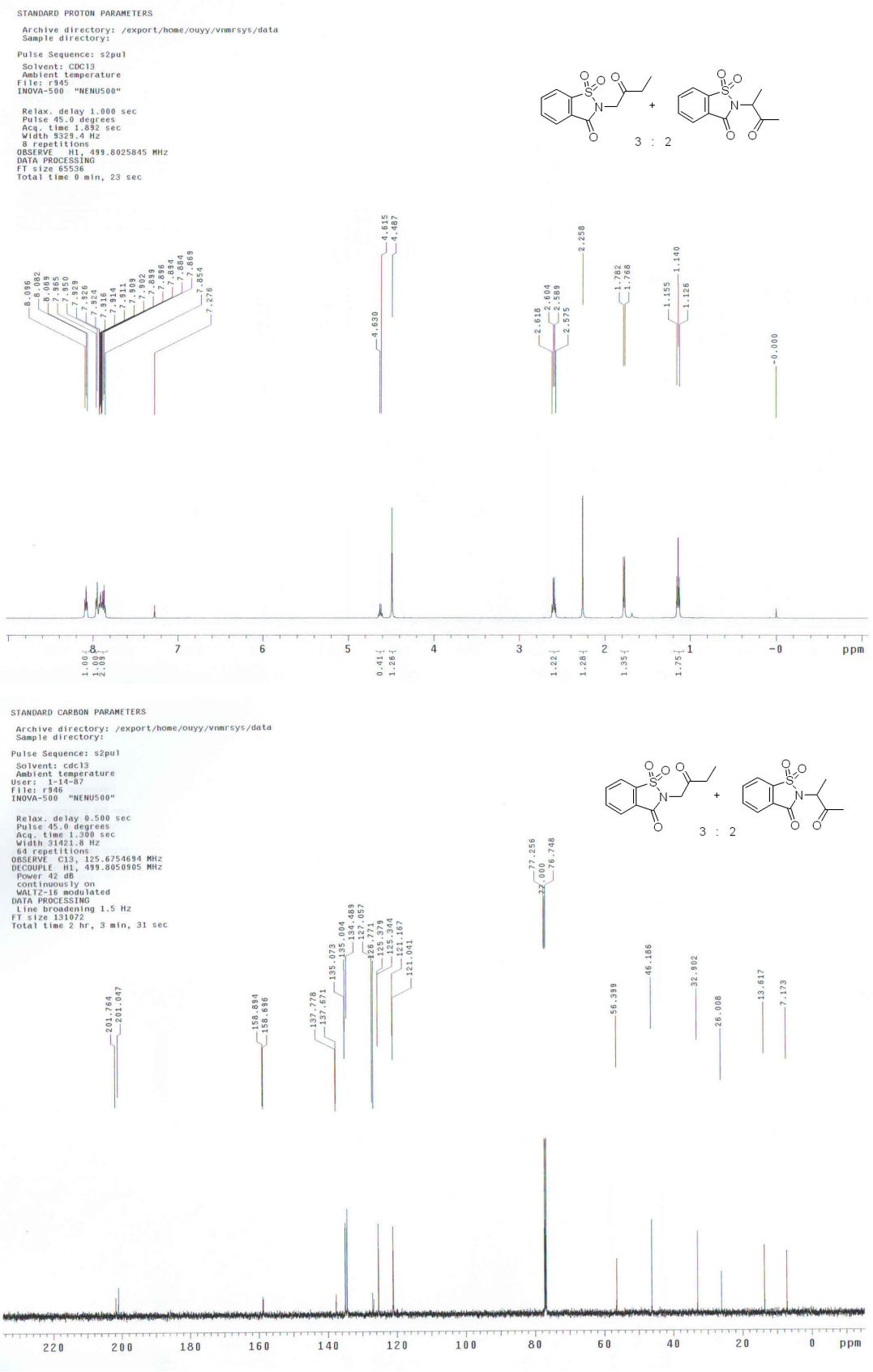

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: y493
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754656 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 10 hr, 3 min, 7 sec
77.256
77.000
76.744
200.352
158.905
137.793
134.847
134.432
127.160
125.383
121.148
47.044
18.086
11.972
220
200
180
160
140
120
100
80
60
40
20
0
ppm

Product 4w

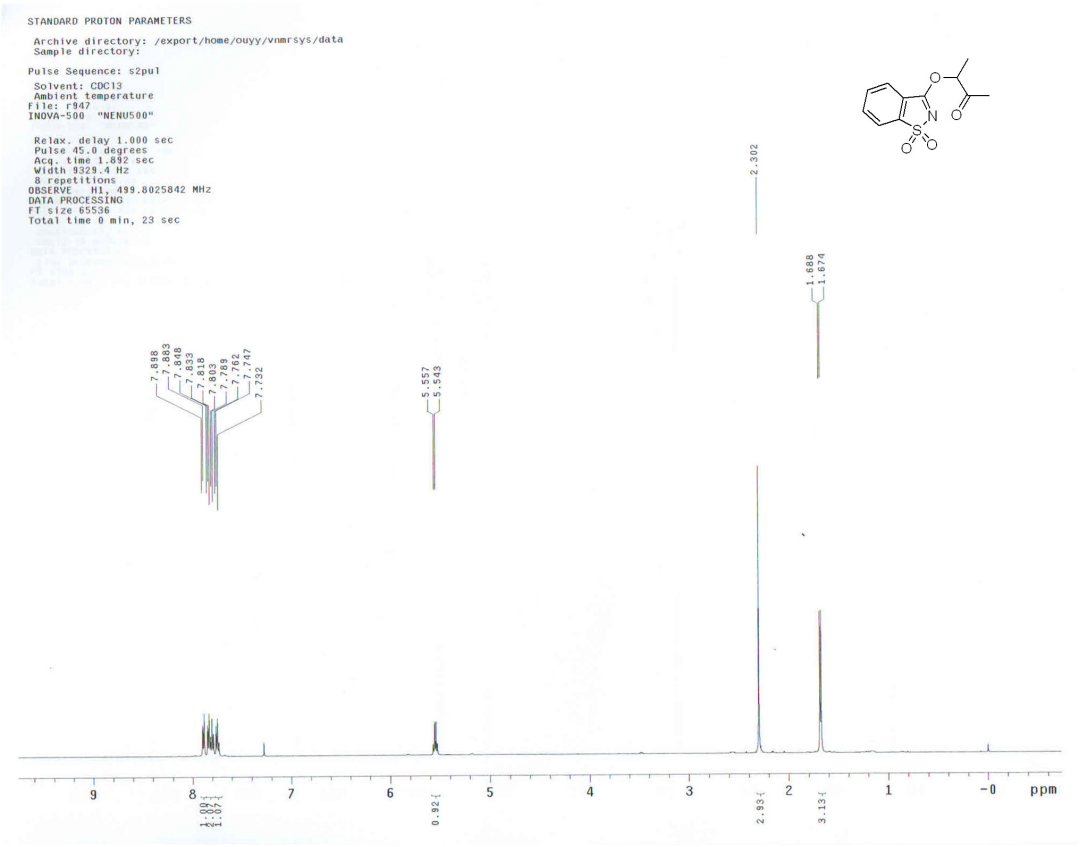

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: r720
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8561.6 Hz
8 repetitions
OBSERVE H1, 499.8025840 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.077
8.062
7.951
7.936
7.907
7.892
7.879
7.878
7.866
7.851
7.836
7.274
4.564
2.815
2.800
2.787
1.677
1.234
1.220
0.92
0.92
2.07
2.00
0.91
5.93
ppm

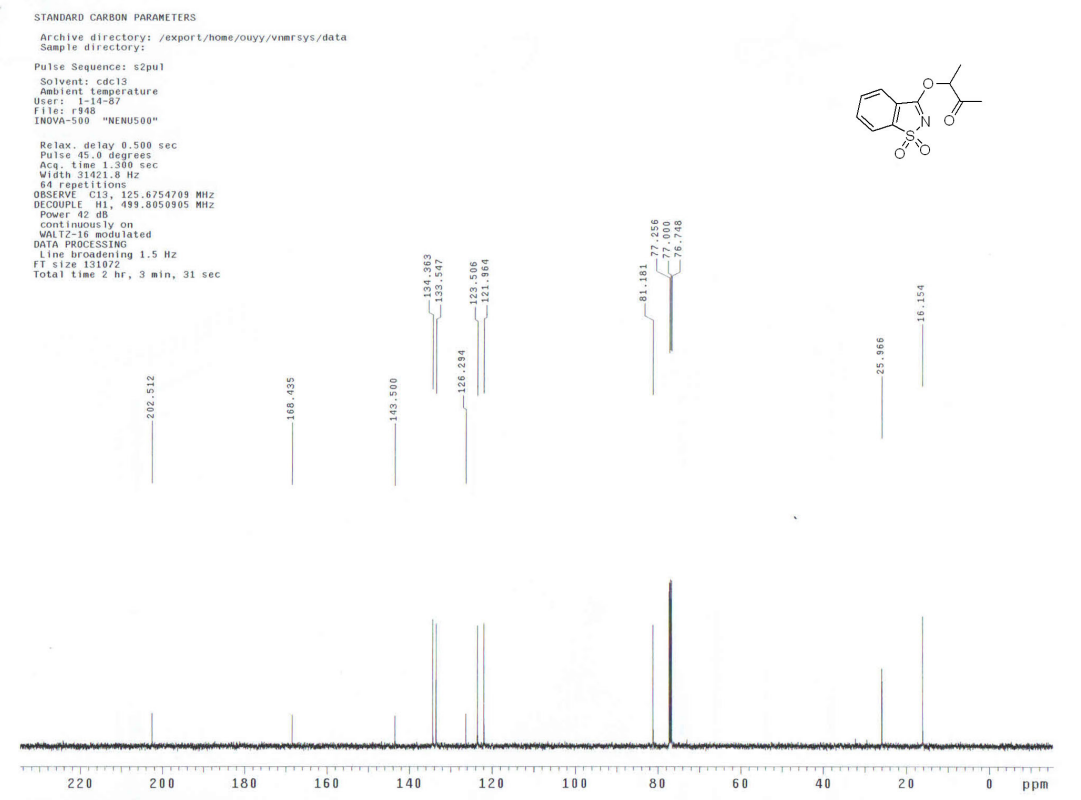

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: r721
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754694 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
203.545
158.917
137.724
134.916
134.428
127.157
125.310
121.117
77.252
77.000
76.744
44.812
38.437
17.951
220
200
180
160
140
120
100
80
60
40
20
0
ppm

Product 4x and 4x'

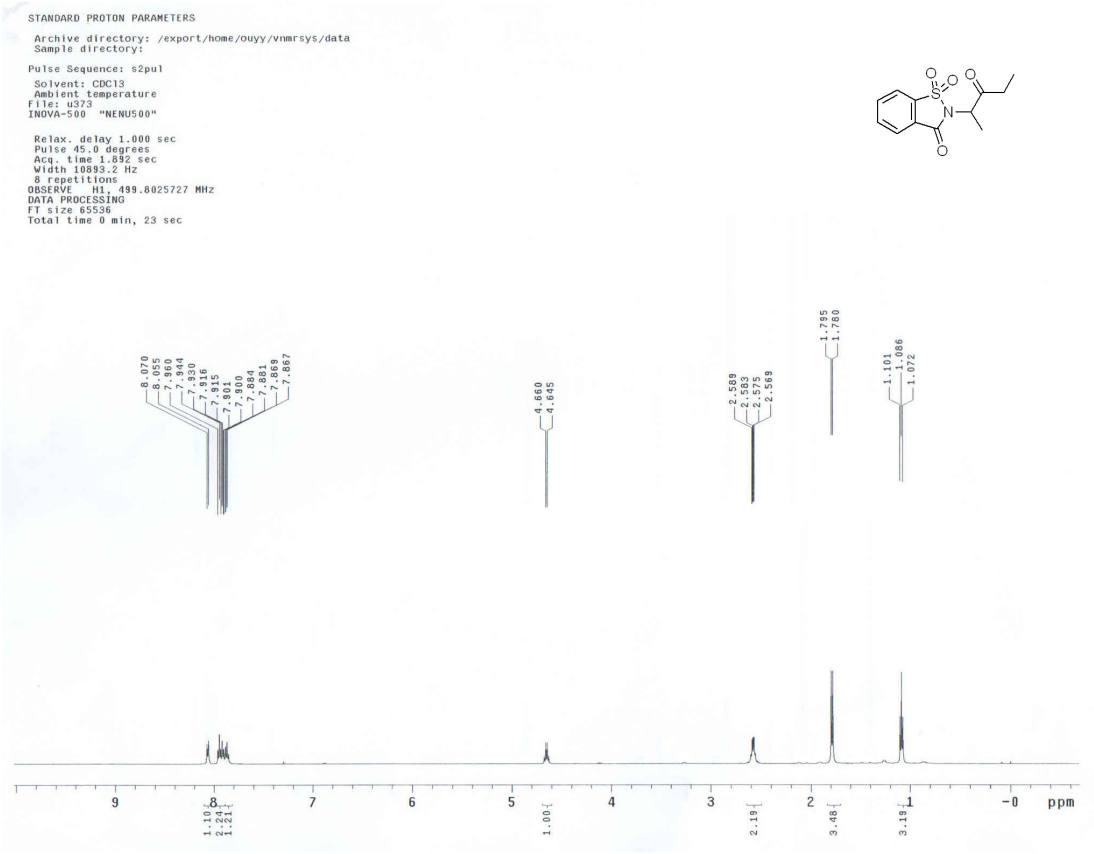


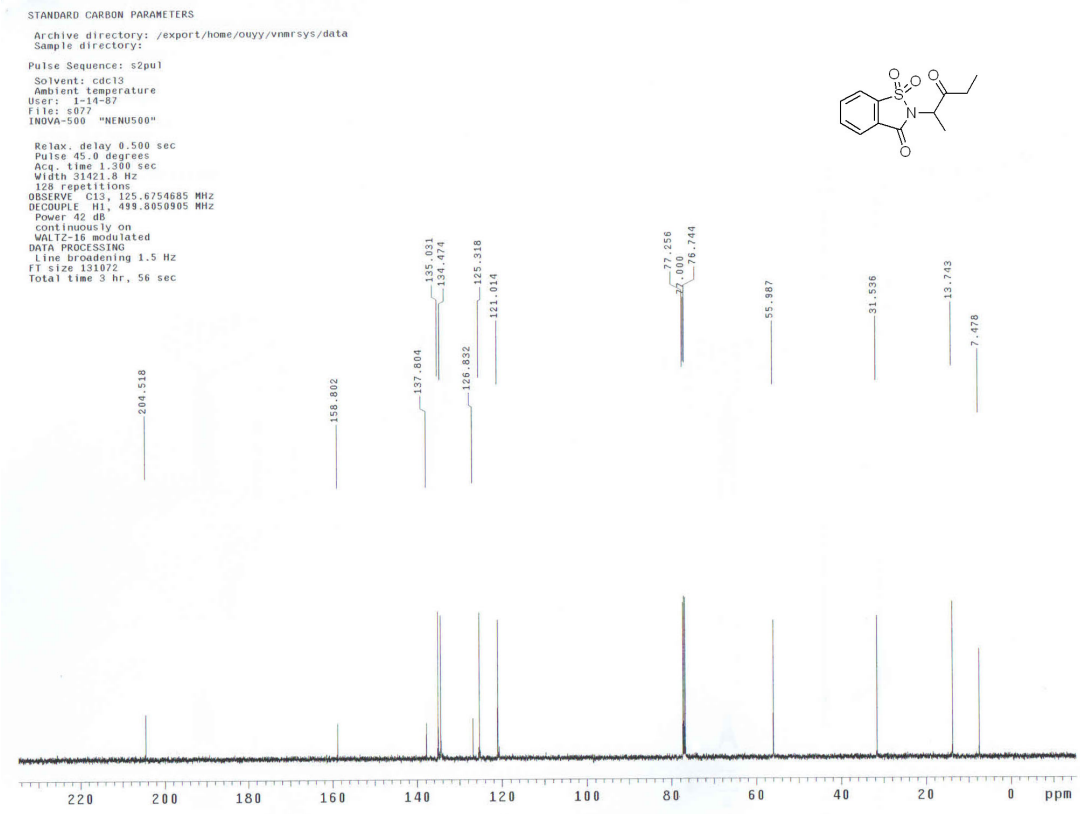
Product 4x''


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: r947
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9329.4 Hz
8 repetitions
OBSERVE H1, 499.8025842 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2.302
1.688
1.674
7.898
7.883
7.846
7.833
7.818
7.803
7.788
7.776
7.747
7.732
5.557
5.543
ppm

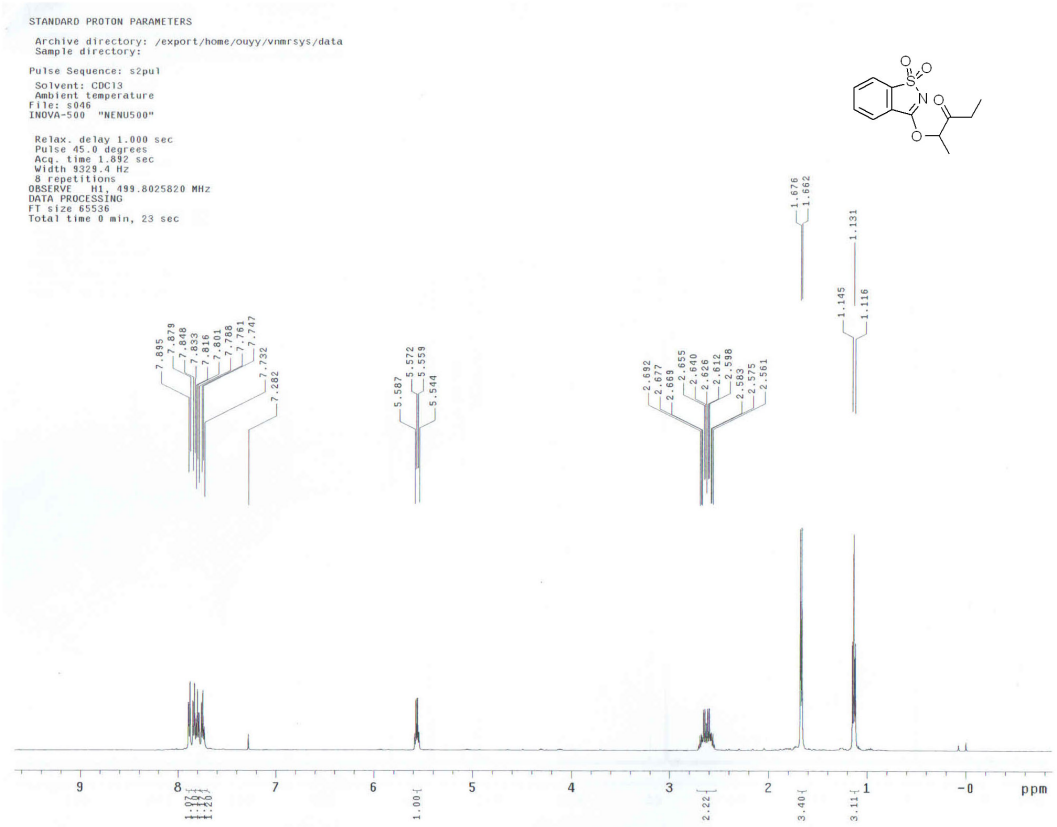

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: r948
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754709 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
202.512
168.435
143.500
134.363
133.547
126.294
123.506
121.864
81.181
77.256
77.000
76.748
25.966
16.154
ppm

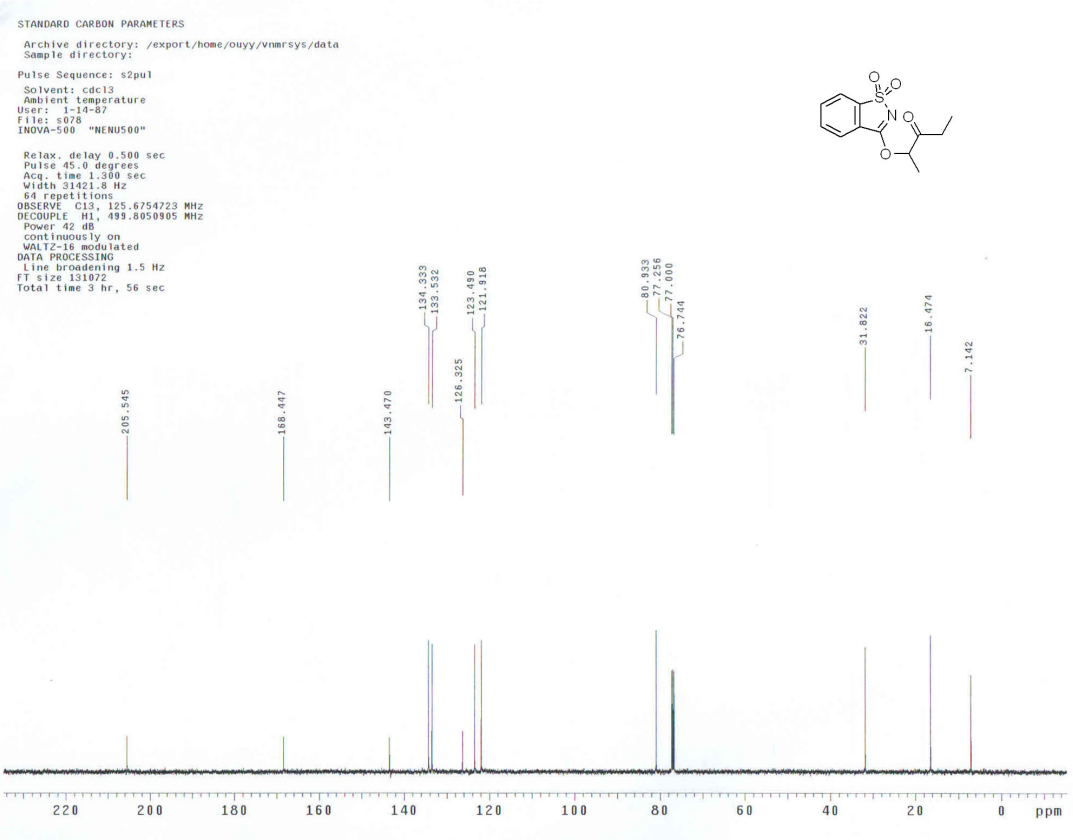
Product 4y


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: u373
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
8 repetitions
OBSERVE H1, 499.8025727 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.070
8.055
7.960
7.944
7.930
7.916
7.915
7.901
7.900
7.884
7.881
7.869
7.867
4.660
4.645
2.589
2.583
2.575
2.569
1.795
1.780
1.101
1.086
1.072
ppm

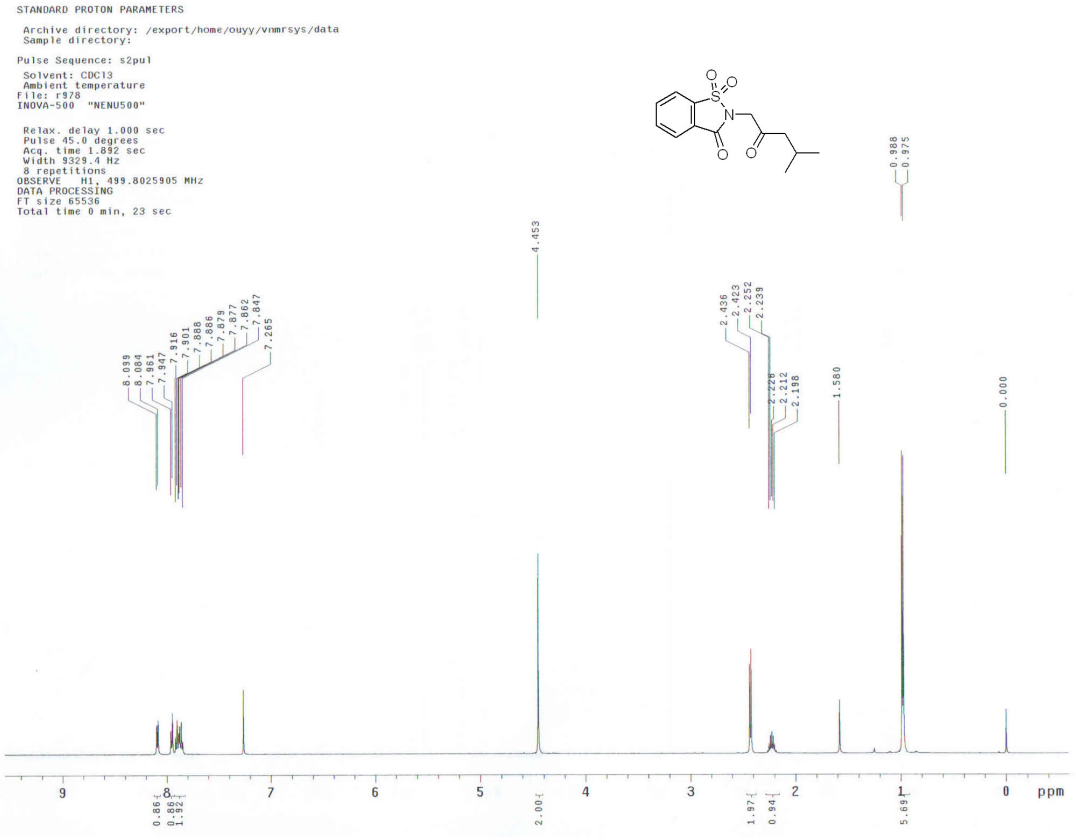

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: s077
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754685 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
204.518
158.802
137.804
135.031
134.474
126.832
125.318
121.014
77.256
77.000
76.744
55.987
31.536
13.743
7.478
ppm

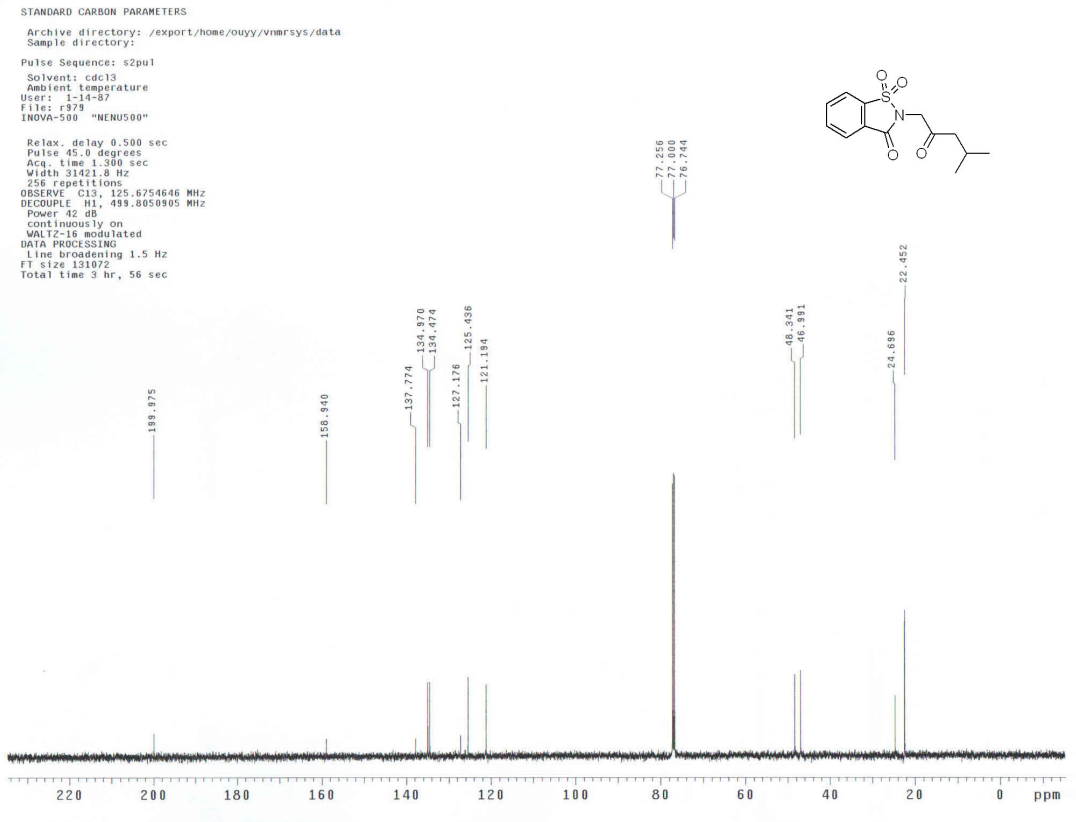
Product 4y'


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: s046
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9329.4 Hz
8 repetitions
OBSERVE H1, 499.8025820 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.895
7.879
7.848
7.833
7.816
7.801
7.788
7.761
7.747
7.732
7.282
5.587
5.572
5.559
5.544
2.692
2.677
2.669
2.655
2.640
2.626
2.612
2.598
2.583
2.575
2.561
1.676
1.662
1.145
1.131
1.116
ppm

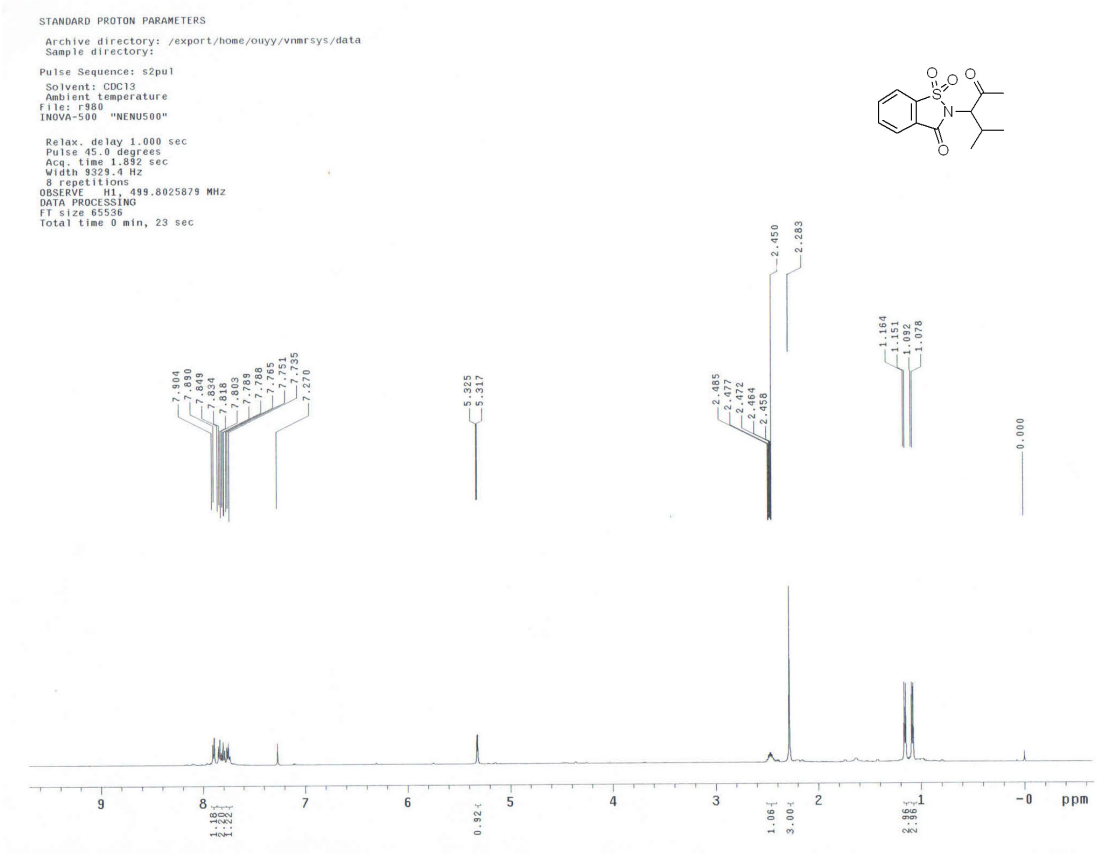

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: s078
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754723 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
205.545
168.447
143.470
134.333
133.532
126.325
123.490
121.918
80.933
77.256
77.000
76.744
31.822
16.474
7.142
ppm

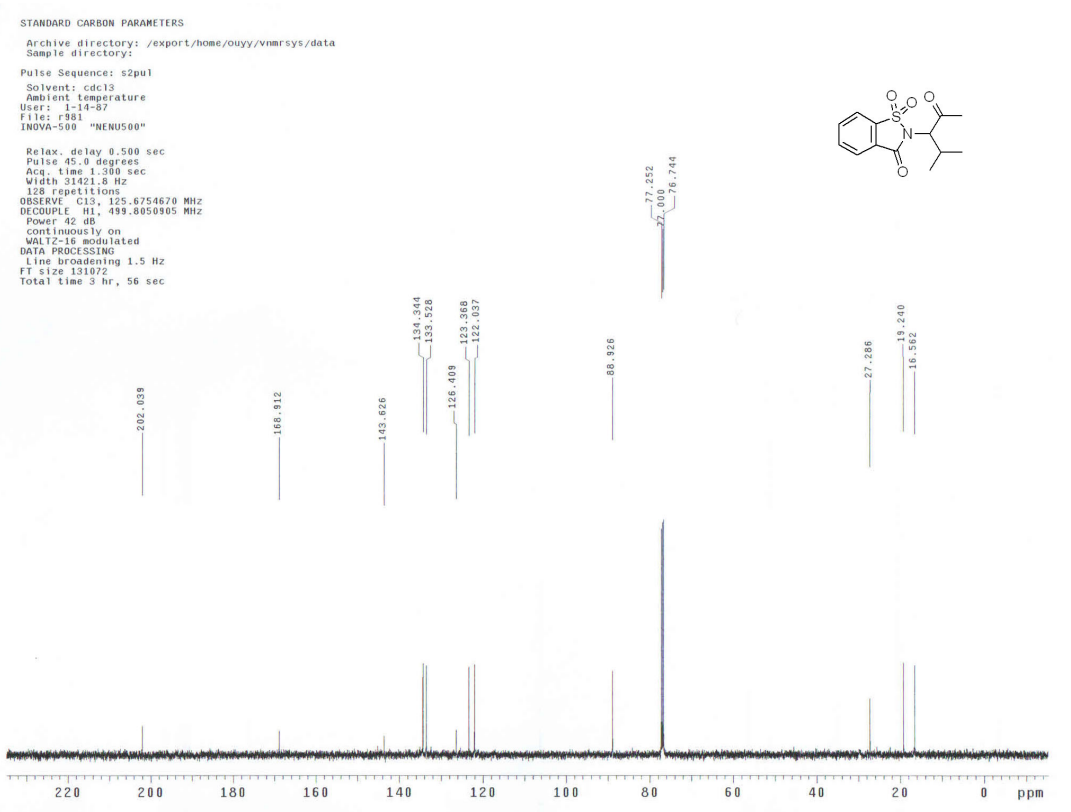
Product 4z


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: r978
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 9329.4 Hz
8 repetitions
OBSERVE H1, 499.8025905 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
4.453
2.436
2.423
2.252
2.239
1.580
0.988
0.975
0.000
ppm

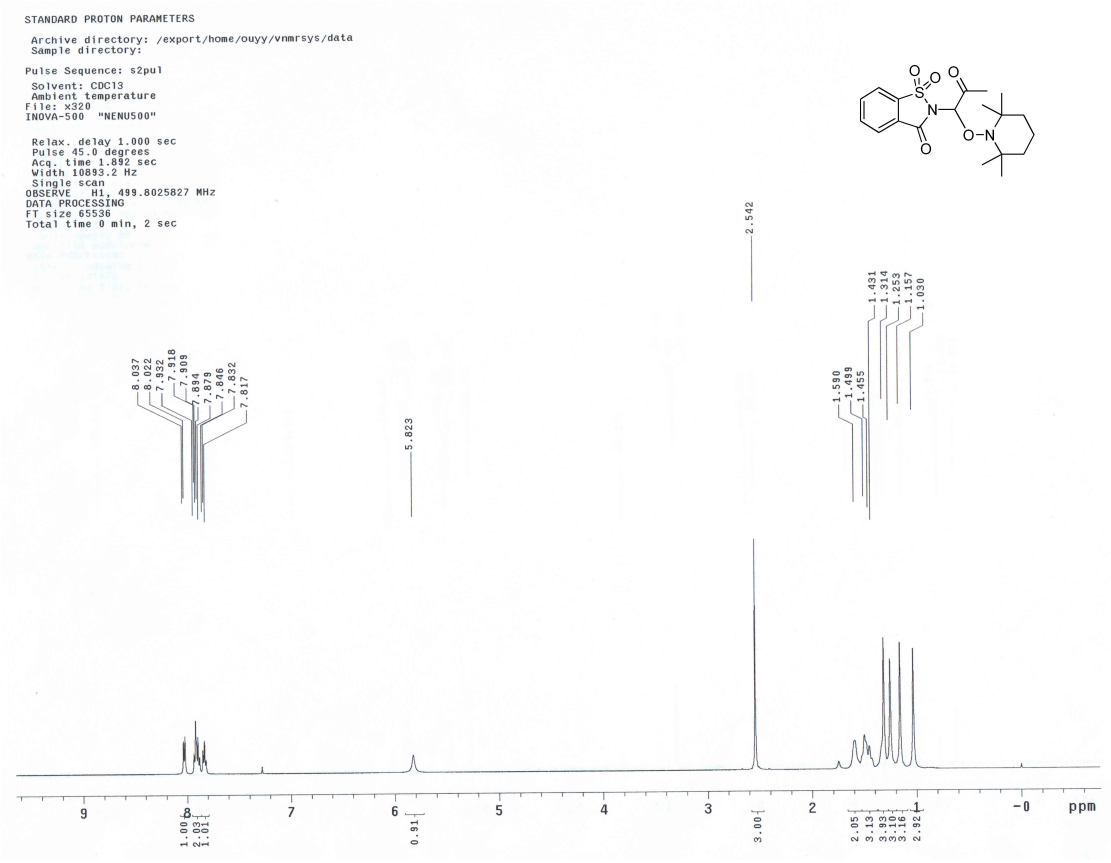

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: r979
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754646 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
77.256
77.000
76.744
199.975
158.940
137.774
134.970
134.474
127.176
125.436
121.194
48.341
46.991
24.686
22.452
ppm

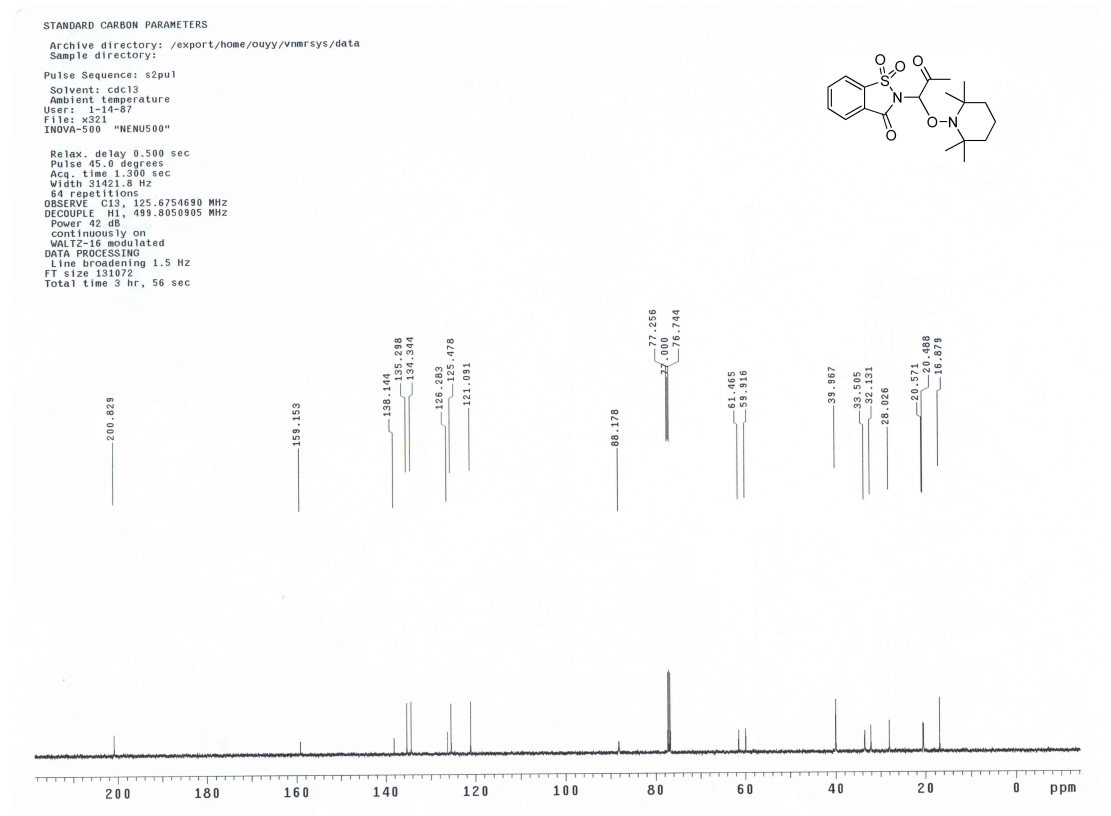
Product 4z'


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: r980
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9329.4 Hz
8 repetitions
OBSERVE H1, 499.8025879 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.904
7.890
7.849
7.834
7.818
7.803
7.789
7.768
7.765
7.751
7.735
7.270
5.325
5.317
2.485
2.477
2.472
2.464
2.458
2.450
2.283
1.164
1.151
1.092
1.078
0.000
ppm


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: r981
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754670 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
202.039
168.912
143.626
134.344
133.528
129.366
122.387
126.409
88.926
77.252
77.000
76.744
27.286
19.240
16.562
ppm

Product 5


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: x320
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
Single scan
OBSERVE H1, 499.8025827 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 2 sec
8.037
8.022
7.932
7.918
7.909
7.879
7.873
7.846
7.832
7.817
5.823
2.542
1.590
1.499
1.455
1.431
1.314
1.253
1.157
1.030
ppm


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: x321
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754690 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
200.829
159.153
138.144
135.298
134.344
126.283
125.478
121.091
88.178
77.256
77.000
76.744
61.465
59.916
39.967
33.505
32.131
28.026
20.571
20.488
16.879
ppm