

SUPPORTING INFORMATION

An environmentally benign approach for the synthesis of bifunctional sulfonamide-amide compounds *via* isocyanide-based multicomponent reactions

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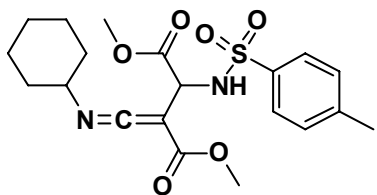
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Experimental Section

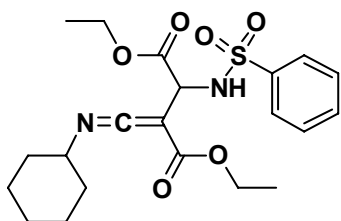
General

Melting points were measured on an Electrothermal 9100 apparatus and are uncorrected. Mass spectra were recorded on a FINNIGAN-MAT 8430 mass spectrometer operating at an ionization potential of 70 eV. IR spectra were recorded on a Shimadzu IR-470 spectrometer. ^1H and ^{13}C NMR spectra were recorded on a BRUKER DRX-300 AVANCE spectrometer at 300.13 and 75.47 MHz. NMR spectra were obtained on solution in CDCl_3 and $\text{DMSO}-d_6$ using TMS as internal standard. Elemental analyses were carried out on a Thermo Finnigan Flash EA 1112 C,H, N analyzer. The chemicals used in this work were purchased from Merck and Fluka Chemical Companies.



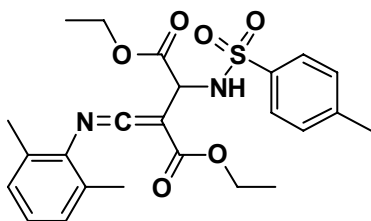
Typical procedure for preparation of Dimethyl 2-((cyclohexylimino)methylene)-3-(4-methylphenylsulfonamido)succinate (4a): To a magnetically stirred solution of 4-

methylbenzenesulfonamide (0.17 g, 1.0 mmol) and dimethyl acetylenedicarboxylate (0.15 g, 1.0 mmol) in H_2O or CCl_2H_2 (10 mL) was added, cyclohexyl isocyanide (0.11 g, 1.0 mmol) at room temperature. The mixture was finally stirred for 3h in H_2O or 6h in CCl_2H_2 . The solvent was removed under vacuum and the residue was crystallized from *n*-hexan/dichloromethane (2:1) and the product **4a** was obtained. White crystals (0.30 g, yield 72%). mp 105-107 °C. IR (KBr) ($\nu_{\text{max}}/\text{cm}^{-1}$): 2937, 2856, 1743, 1681, 1633. MS, m/z (%): 377 (M^+-45 , 5), 395 (10), 198 (5), 171 (5), 155 (30), 91 (100), 55 (60). ^1H NMR (300 MHz, CDCl_3): δ_{H} (ppm) 1.25-1.88 (10H, m, 5 CH_2 of cyclohexyl), 2.38 (3H, s, CH_3), 3.58 (3H, s, O- CH_3), 3.61 (3H, s, O- CH_3), 3.76 (1H, m, CH-N), 4.64 (1H, d, $^3J_{\text{HH}} = 8.1$ Hz, CHNH), 5.86 (1H, d, $^3J_{\text{HH}} = 8.1$ Hz, CHNH), 7.25 (2H, d, $^3J_{\text{HH}} = 8.1$ Hz, arom), 7.71 (2H, d, $^3J_{\text{HH}} = 8.1$ Hz, arom). ^{13}C NMR (75 MHz, CDCl_3): δ_{C} (ppm) 21.5, 23.9, 25.1, 30.9, 33.3, 33.4, 51.5, 53.1, 53.6, 60.8, 61.9, 127.1, 129.4, 137.4, 143.4, 165.3, 168.3, 169.9. Anal. Calcd for $\text{C}_{20}\text{H}_{26}\text{N}_2\text{O}_6\text{S}$: C, 56.86; H, 6.20; N, 6.63. Found: C, 56.94; H, 6.14; N, 6.51.



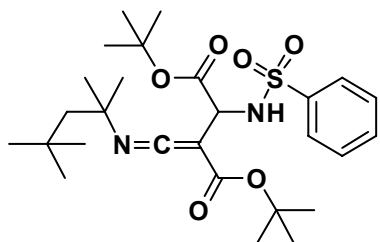
Diethyl 2-((cyclohexylimino)methylene)-3-(phenylsulfonamido)succinate (4b): White crystals (0.35 g, 81%).

mp 76-79 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3234, 2935, 2860, 2060, 1754, 1672. ^1H NMR (300 MHz, CDCl_3): δ_{H} (ppm) 1.15-1.96 (16H, m, 5CH_2 of cyclohexyl, $2\text{OCH}_2\text{CH}_3$), 3.80 (1H, bs, CH-N), 4.02-4.13 (4H, m, $2\text{OCH}_2\text{CH}_3$), 4.67 (1H, d, $^3J = 8.1$ Hz, CH-NH), 5.87 (1H, d, $^3J = 8.1$ Hz, CH-NH), 7.46-7.88 (5H, m, arom). ^{13}C NMR (75 MHz, CDCl_3): δ_{C} (ppm) 13.9, 14.3, 23.8, 25.1, 33.3, 53.8, 60.4, 60.8, 62.3, 62.4, 127.1, 128.9, 132.5, 140.5, 165.7, 168.4, 169.3. Anal. Calcd for $\text{C}_{21}\text{H}_{28}\text{N}_2\text{O}_6\text{S}$: C, 57.78; H, 6.47; N, 6.42. Found: C, 57.82; H, 6.57; N, 6.49.



Diethyl 2-((2,6-dimethylphenylimino)methylene)-3-(4-methylphenylsulfonamido)succinate (4c): White crystals (0.37 g, 78%).

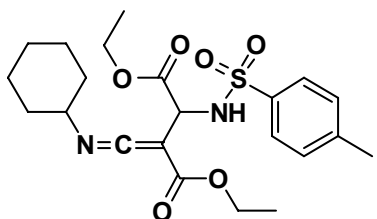
mp 151-153 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3234, 2988, 2916, 2058, 1751, 1668. MS, m/z (%): 473 ($\text{M}^+ + 1$, 2), 399 (5), 353 (5), 317 (10), 271 (5), 225 (10), 199 (5), 171 (10), 155 (15), 120 (20), 91 (100), 65 (25). ^1H NMR (300 MHz, CDCl_3): δ_{H} (ppm) 1.15-1.22 (6H, m, $2\text{OCH}_2\text{CH}_3$), 2.37 (9H, bs, 3CH_3), 4.05-4.18 (4H, m, $2\text{OCH}_2\text{CH}_3$), 4.80 (1H, d, $^3J_{\text{HH}} = 8.0$ Hz, CHNH), 5.93 (1H, d, $^3J_{\text{HH}} = 8.0$ Hz, CHNH), 7.11-7.75 (7H, m, arom). ^{13}C NMR (75 MHz, CDCl_3): δ_{C} (ppm) 13.9, 14.4, 18.8, 21.5, 54.2, 58.3, 60.5, 62.3, 127.1, 128.4, 128.5, 129.4, 132.2, 133.9, 137.7, 143.2, 163.6, 168.1, 169.3. Anal. Calcd for $\text{C}_{24}\text{H}_{28}\text{N}_2\text{O}_6\text{S}$: C, 61.00; H, 5.97; N, 5.93. Found: C, 61.03; H, 5.91; N, 6.01.



Di-tert-butyl 2-(phenylsulfonamido)-3-((2,4,4-trimethylpentan-2-ylimino)methylene)succinate (4d): White crystals (0.38 g, 68%).

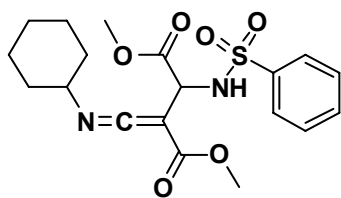
mp 135-138 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3222, 2971, 2067, 1730, 1692. MS, m/z (%): 523 ($\text{M}^+ + 1$, 2), 299 (20), 269 (15), 141 (20), 93 (20), 77 (100), 57 (60). ^1H NMR (300 MHz, $\text{DMSO}-d_6$): δ_{H} (ppm) 0.92 (9H, s,

C(CH₃)₃), 1.33 (6H, s, C(CH₃)₂), 1.38 (9H, s, OC(CH₃)₃), 1.41(9H, s, OC(CH₃)₃), 1.53 (1H, AB-q, ²J_{HH}=14.7 Hz, CH_AH_B), 1.90 (1H, AB-q, ²J_{HH}=14.7 Hz, CH_AH_B), 6.59 (CH-NH), 7.36-7.84 (5H, m, arom), 8.12 (1H, s, CH-NH). ¹³C NMR (75 MHz, CDCl₃): δ_C (ppm) 27.7, 27.8, 28.0, 31.5, 31.6, 51.1, 57.8, 62.8, 128.9, 129.4, 130.3, 141.9, 157.5, 161.6, 162.6. Anal. Calcd for C₂₇H₄₂N₂O₆S: C, 62.04; H, 8.10; N, 5.36. Found: C, 62.17; H, 7.98; N, 5.48.



Diethyl 2-((cyclohexylimino)methylene)-3-(4-methylphenylsulfonamido)succinate (4e): White crystals (0.33 g, 73%). mp 115-117 °C. IR (KBr) (ν_{max}/cm⁻¹): 3222, 2936, 2859, 2064, 1751, 1671. MS, m/z (%): 421 (M⁺-29, 10), 377 (10), 295 (25), 155 (20), 91 (100), 55

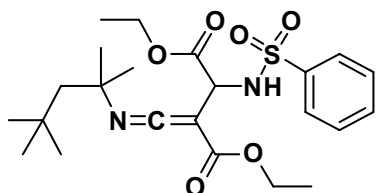
(60). ¹H NMR (300 MHz, DMSO-*d*₆): δ_H (ppm) 1.06-1.82 (16H, m, 5CH₂ of cyclohexyl, 2OCH₂CH₃), 2.35 (3H, s, CH₃), 3.84 (1H, bs, CH-N), 3.90-3.97 (4H, m, 2OCH₂CH₃), 4.63 (1H, d, ³J_{HH}= 8.0 Hz, CHNH), 7.32 (2H, d, ³J_{HH}= 7.3 Hz, arom), 7.64 (2H, d, ³J_{HH}= 7.3 Hz, arom), 8.44 (1H, d, ³J_{HH}= 8.0 Hz, CHNH). ¹³C NMR (75 MHz, DMSO-*d*₆): δ_C (ppm) 14.2, 14.5, 21.3, 23.5, 25.2, 32.9, 53.1, 60.3, 61.6, 62.4, 127.0, 129.7, 138.7, 142.9, 165.7, 167.9, 169.6. Anal. Calcd for C₂₂H₃₀N₂O₆S: C, 58.65; H, 6.71; N, 6.22. Found: C, 58.52; H, 6.79; N, 6.37.



Dimethyl 2-((cyclohexylimino)methylene)-3-(phenylsulfonamido)succinate (4f): White crystals (0.33 g, yield 80%). mp 87-90 °C. IR (KBr) (ν_{max}/cm⁻¹): 2939, 2847, 1753, 1688. MS, m/z (%): 408 (M⁺, 10), 386 (2), 354 (20),

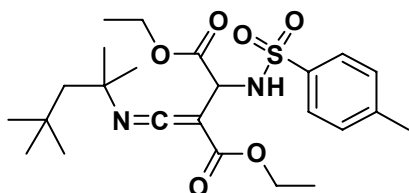
267 (100), 200 (30), 155 (20), 138 (20), 89 (60), 67 (40). ¹H NMR (300 MHz, CDCl₃): δ_H (ppm) 1.26-1.97 (10H, m, 5CH₂ of cyclohexyl), 3.58 (3H, s, OCH₃), 3.62 (3H, s, OCH₃), 3.78 (1H, m, CH-N), 4.68 (1H, d, ³J_{HH}= 8.2 Hz, CHNH), 5.93 (1H, d, ³J_{HH}= 8.2 Hz, CHNH), 7.45-7.86 (5H, m, arom). ¹³C NMR (75 MHz, CDCl₃): δ_C (ppm) 23.9, 25.1, 33.4 (C-cyclohexyl), 51.6 (CH-N), 53.1, 53.7 (2OCH₃), 60.8 (CH-NH), 61.8 (C=N), 127.1,

128.9, 132.6, 140.4 (C-Ar), 164.7 (C=C=N), 168.9, 169.9 (2C=O). Anal. Calcd for C₁₉H₂₄N₂O₆S: C, 55.87; H, 5.92; N, 6.86. Found: C, 55.91; H, 6.02; N, 6.79.



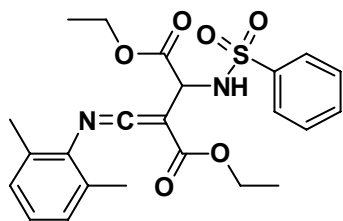
Diethyl 2-(phenylsulfonamido)-3-((2,4,4-trimethylpentan-2-ylimino)methylene)succinate (4g):

White crystals (0.35 g, 75%). mp 142-145 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3283, 2963, 2897, 2065, 1738, 1691. MS, m/z (%): 459 ($M^+ - 8$, 2), 385 (10), 339 (5), 302 (10), 244 (10), 198 (10), 141 (20), 103 (5), 77 (100), 51 (20). ¹H NMR (300 MHz, CDCl₃): δ_H (ppm) 1.04 (9H, s, C(CH₃)₃), 1.14-1.23 (6H, m, 2OCH₂CH₃), 1.47 (6H, s, C(CH₃)₂), 1.63 (2H, s, CH₂), 4.00-4.13 (4H, m, 2OCH₂CH₃), 4.65 (1H, d, ³ $J_{\text{HH}} = 8.2$ Hz, CHNH), 5.88 (1H, d, ³ $J_{\text{HH}} = 8.2$ Hz, CHNH), 7.42-7.96 (5H, m, arom). ¹³C NMR (75 MHz, CDCl₃): δ_C (ppm) 13.9, 14.3, 31.15, 31.25, 31.38, 31.7, 53.7, 54.6, 60.3, 62.2, 63.4, 65.5, 127.1, 128.8, 132.5, 140.0, 164.9, 168.5, 169.4. Anal. Calcd for C₂₃H₃₄N₂O₆S: C, 59.21; H, 7.34; N, 6.00. Found: C, 59.08; H, 7.47; N, 5.94.

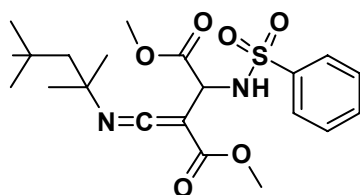


Diethyl 2-(4-methylphenylsulfonamido)-3-((2,4,4-trimethylpentan-2-ylimino)methylene)succinate (4h):

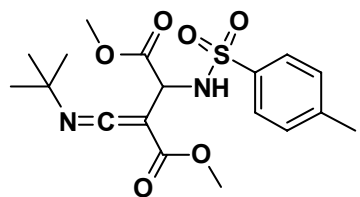
White crystals (0.37 g, 78%). mp 84-86 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3229, 2993, 2947, 2056, 1751, 1675. MS, m/z (%): 481 ($M^+ + 1$, 1), 369 (2), 351 (3), 323 (10), 247 (10), 213 (100), 155 (20), 107 (10), 91 (80), 57 (70). ¹H NMR (300 MHz, CDCl₃): δ_H (ppm) 1.15 (9H, s, C(CH₃)₃), 1.15-1.20 (6H, m, 2OCH₂CH₃), 1.47 (6H, s, C(CH₃)₂), 1.63 (2H, s, CH₂), 2.41 (3H, s, CH₃), 4.01-4.14 (4H, m, 2OCH₂CH₃), 4.62 (1H, d, ³ $J_{\text{HH}} = 8.3$ Hz, CHNH), 5.82 (1H, d, ³ $J_{\text{HH}} = 8.3$ Hz, CHNH), 7.26 (2H, d, ³ $J_{\text{HH}} = 8.4$ Hz, arom), 7.74 (2H, d, ³ $J_{\text{HH}} = 8.4$ Hz, arom). ¹³C NMR (75 MHz, CDCl₃): δ_C (ppm) 14.0, 14.3, 21.5, 31.1, 31.3, 31.4, 31.7, 53.7, 54.7, 60.3, 62.2, 63.5, 65.5, 127.2, 129.4, 137.5, 143.2, 165.1, 168.5, 169.5. Anal. Calcd for C₂₄H₃₆N₂O₆S: C, 59.98; H, 7.55; N, 5.83. Found: C, 59.73; H, 7.41; N, 5.88.



Diethyl 2-((2,6-dimethylphenylimino)methylene)-3-(phenylsulfonamido)succinate (4i): White crystals (0.35 g, 77%). mp 142-145 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3231, 2991, 2914, 2062, 1754, 1666. ^1H NMR (300 MHz, CDCl_3): δ_{H} (ppm) 1.13-1.20 (6H, m, $2\text{OCH}_2\text{CH}_3$), 2.37 (6H, s, 2CH_3), 4.05-4.14 (4H, m, $2\text{OCH}_2\text{CH}_3$), 4.82 (1H, d, $^3J_{\text{HH}} = 8.1$ Hz, CHNH), 6.04 (1H, d, $^3J_{\text{HH}} = 8.1$ Hz, CHNH), 7.05-7.86 (8H, m, arom). ^{13}C NMR (75 MHz, CDCl_3): δ_{C} (ppm) 14.0, 14.4, 18.9, 54.3, 58.2, 60.5, 62.4, 127.0, 128.4, 128.5, 128.8, 132.1, 132.5, 134.0, 140.7, 163.5, 168.1, 169.2. Anal. Calcd for $\text{C}_{23}\text{H}_{26}\text{N}_2\text{O}_6\text{S}$: C, 60.25; H, 5.72; N, 6.11. Found: C, 60.23; H, 5.68; N, 6.11.

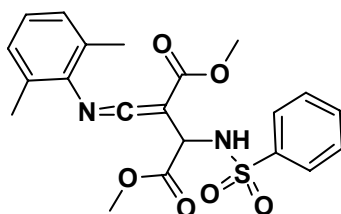


Dimethyl 2-(phenylsulfonamido)-3-((2,4,4-trimethylpentan-2-ylidene)methylene)succinate (4j): White crystals (0.32 g, 73%). mp 93-96 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3273, 2968, 2894, 2066, 1760, 1678. MS, m/z (%): 340 ($\text{M}^+ - 98$, 5), 295 (5), 254 (5), 199 (10), 155 (20), 124 (10), 95 (50), 57 (100). ^1H NMR (300 MHz, CDCl_3): δ_{H} (ppm) 1.04 (9H, s, $\text{C}(\text{CH}_3)_3$), 1.15 (6H, s, $\text{C}(\text{CH}_3)_2$), 1.63 (2H, s, CH_2), 3.59 (3H, s, OCH_3), 3.65 (3H, s, OCH_3), 4.67 (1H, d, $^3J_{\text{HH}} = 8.2$ Hz, CHNH), 5.86 (1H, d, $^3J_{\text{HH}} = 8.2$ Hz, CHNH), 7.43-7.88 (5H, m, arom). ^{13}C NMR (75 MHz, CDCl_3): δ_{C} (ppm) 31.1, 31.2, 31.4, 31.7, 51.4, 53.1, 53.6, 54.7, 62.9, 65.7, 127.1, 128.9, 132.6, 140.4, 163.8, 169.0, 169.9. Anal. Calcd for $\text{C}_{21}\text{H}_{30}\text{N}_2\text{O}_6\text{S}$: C, 57.51; H, 6.90; N, 6.39. Found: C, 57.47; H, 6.79; N, 6.24.



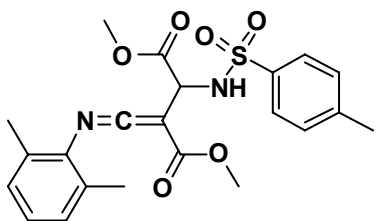
Dimethyl 2-((tert-butylimino)methylene)-3-(4-methylphenylsulfonamido)succinate (4k): White crystals (0.32 g, yield 82%). mp 125-128 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 2947, 1749, 1683, 1635. ^1H NMR (300 MHz, CDCl_3): δ_{H} (ppm) 1.34 (9H, s, $\text{C}(\text{CH}_3)_3$), 2.42 (3H, s, CH_3), 3.63 (6H, bs, 2OCH_3), 4.65 (1H, d, $^3J_{\text{HH}} = 8.1$ Hz, CHNH), 5.78 (1H, d, $^3J_{\text{HH}} = 8.1$ Hz, CHNH), 7.28 (2H, d, $^3J_{\text{HH}} = 7.7$ Hz, arom), 7.74 (2H, d, $^3J_{\text{HH}} = 7.7$ Hz, arom). ^{13}C NMR (75 MHz, CDCl_3): δ_{C} (ppm) 21.5,

30.3, 51.6, 53.1, 53.6, 62.9, 63.8, 127.2, 129.5, 137.3, 143.4, 165.9, 168.8, 170.0. Anal. Calcd for $C_{18}H_{24}N_2O_6S$: C, 54.53; H, 6.10; N, 7.07. Found: C, 54.44; H, 6.16; N, 7.00.



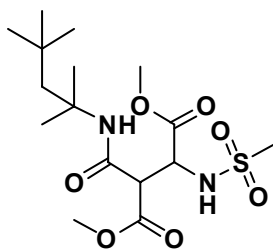
Dimethyl 2-((2,6-dimethylphenylimino)methylene)-3-(phenylsulfonamido)succinate (4l): White crystals (0.33 g, 76%). mp 165-167 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3119, 2952,

2921, 2078, 1750, 1662. MS, m/z (%): 430 (M^+ , 5), 371 (20), 339 (5), 289 (10), 274 (5), 198 (5), 170 (20), 141 (30), 103 (10), 77 (100). ^1H NMR (300 MHz, CDCl_3): δ_{H} (ppm) 2.38 (6H, s, 2CH₃), 3.62 (3H, s, O-CH₃), 3.68 (3H, s, O-CH₃), 4.85 (1H, d, $^3J_{\text{HH}} = 8.2$ Hz, CHNH), 5.98 (1H, d, $^3J_{\text{HH}} = 8.2$ Hz, CHNH), 7.11-7.88 (8H, m, arom). ^{13}C NMR (75 MHz, CDCl_3): δ_{C} (ppm) 18.9, 51.6, 53.2, 54.1, 57.8, 127.1, 128.6, 128.8, 128.9, 131.7, 132.6, 134.7, 140.6, 163.4, 168.7, 169.8. Anal. Calcd for $C_{21}H_{22}N_2O_6S$: C, 58.59; H, 5.15; N, 6.51. Found: C, 58.46; H, 5.16; N, 6.57.



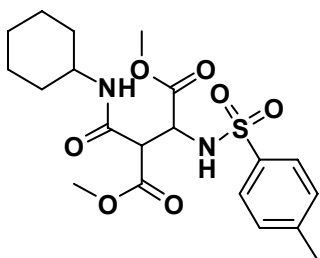
Dimethyl 2-((2,6-dimethylphenylimino)methylene)-3-(4-methylphenylsulfonamido)succinate (4m): White crystals (0.34 g, 76%). mp 166-169 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3212, 2952, 2842, 2068, 1764, 1675. MS, m/z (%): 444

(M^+ , 5), 630 (5), 385 (50), 274 (20), 171 (20), 155 (40), 91 (100), 65 (50). ^1H NMR (300 MHz, CDCl_3): δ_{H} (ppm) 2.37 (6H, s, 2CH₃), 2.40 (3H, s, CH₃), 3.63 (3H, s, O-CH₃), 3.68 (3H, s, O-CH₃), 4.83 (1H, d, $^3J_{\text{HH}} = 8.2$ Hz, CHNH), 5.93 (1H, d, $^3J_{\text{HH}} = 8.2$ Hz, CHNH), 7.11-7.19 (3H, m, arom), 7.23 (2H, d, $^3J_{\text{HH}} = 8.1$ Hz, arom), 7.72 (2H, d, $^3J_{\text{HH}} = 8.1$ Hz, arom). ^{13}C NMR (75 MHz, CDCl_3): δ_{C} (ppm) 18.9, 21.5, 51.5, 53.1, 54.1, 57.8, 127.1, 128.5, 128.7, 129.4, 131.8, 134.4, 137.6, 143.3, 162.7, 168.6, 169.8. Anal. Calcd for $C_{22}H_{24}N_2O_6S$: C, 59.45; H, 5.44; N, 6.30. Found: C, 59.54; H, 5.32; N, 6.27.



Typical procedure for preparation of Dimethyl 2-(methanesulfonyl)-3-(2,4,4-trimethylpentan-2-ylcarbamoyl)succinate (7g):

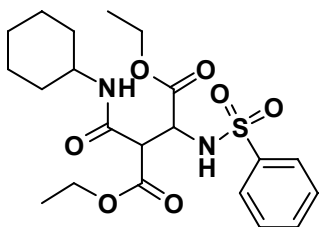
To a magnetically stirred solution of methanesulfonamide (0.09 g, 1.0 mmol) and dimethyl acetylenedicarboxylate (0.14 g, 1.0 mmol) in H₂O (10 mL) was added, 1,1,3,3-tetramethyl-butyl (0.14 g, 1.0 mmol) at room temperature. The mixture was finally stirred for 3h in H₂O at room temperature and kept 12h at 80 °C. After completion of the reaction, as indicated by TLC (ethyl acetate/n-hexane, 1:1), the precipitate was washed with ethyl acetate/n-hexane, (1:3) and the product **7g** was obtained as a white crystals (0.31 g, 80%). mp 126-129 °C. IR (KBr) ($\nu_{\text{max}}/\text{cm}^{-1}$): 3358, 3178, 2957, 2916, 1735, 1654. ¹H NMR (300 MHz, DMSO-*d*₆): δ_{H} (ppm) 0.92 (9H, s, C(CH₃)₃), 1.27 (6H, s, C(CH₃)₂), 1.56 (1H, AB-q, ²J_{HH}=14.5 Hz, CH_AH_B), 1.77 (1H, AB-q, ²J_{HH}=14.5 Hz, CH_AH_B), 2.91 (s-CH₃), 3.60 (3H, s, OCH₃), 3.63 (3H, s, OCH₃), 3.84 (1H, d, ³J_{HH}= 8.2 Hz, CH), 4.50 (1H, dd, ³J_{HH}= 9.5 and 8.2 Hz, CHNH), 7.47 (1H, d, ³J_{HH}= 9.5 Hz, CH-NH), 7.74 (1H, s, CONH). ¹³C NMR (75 MHz, CDCl₃): δ_{C} (ppm) 29.2, 29.4, 31.5, 31.6, 42.1, 50.6, 52.5, 52.8, 54.6, 55.0, 55.4, 164.6, 168.6, 171.0. Anal. Calcd for C₁₆H₃₀N₂O₇S: C, 48.71; H, 7.67; N, 7.10. Found: C, 48.65; H, 7.74; N, 7.11.



Dimethyl 2-(cyclohexylcarbamoyl)-3-(4-methylphenylsulfonamido)succinate (7a):

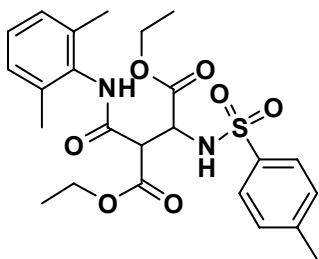
White crystals (0.33 g, yield 75%). mp 152-155 °C. IR (KBr) ($\nu_{\text{max}}/\text{cm}^{-1}$): 3354, 3171, 2947, 2828, 1730, 1651, 1608. MS, *m/z* (%): 421 (*M*⁺+1, 10), 359 (5), 282 (5), 256 (10), 224 (10), 199 (10), 171 (20), 155 (25), 128 (20), 91 (10), 70 (60). ¹H NMR (300 MHz, CDCl₃): δ_{H} (ppm) 1.10-1.66 (10H, m, 5CH₂ of cyclohexyl), 2.35 (3H, s, CH₃), 3.21 (3H, s, O-CH₃), 3.36 (1H, m, CHNH), 3.54 (3H, s, O-CH₃), 3.72 (1H, d, ³J_{HH}= 9.7 Hz, CH), 4.42 (1H, dd, ³J_{HH}= 9.6 and 9.5 Hz, CHNH), 7.33 (2H, d, ³J_{HH}= 7.6 Hz, arom), 7.61 (2H, d, ³J_{HH}= 7.6 Hz, arom), 7.99 (1H, d, ³J_{HH}= 7.5 Hz, CONH), 8.12 (1H, d, ³J_{HH}= 9.6 Hz, NHSO₂). (¹³C NMR (75 MHz, CDCl₃): δ_{C} (ppm) 21.4, 24.8, 25.6, 32.1, 48.5, 52.2, 52.7, 54.2, 55.1, 126.9, 129.6,

139.1, 142.9, 164.0, 168.4, 170.2. Anal. Calcd for $C_{20}H_{28}N_2O_7S$: C, 54.53; H, 6.41; N, 6.36. Found: C, 54.41; H, 6.40; N, 6.19.



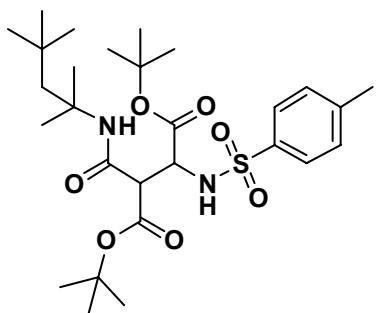
Diethyl 2-(cyclohexylcarbamoyl)-3-(phenylsulfonamido)succinate (7b): White crystals (0.35 g, 78%). mp 152-155 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3452, 3248, 2937, 2855, 1739, 1654, 1552. ^1H NMR (300 MHz, CDCl_3): δ_{H} (ppm) 1.06-1.88 (16H, m, 5CH_2 of cyclohexyl, $2\text{OCH}_2\text{CH}_3$),

3.70 (1H, bs, CH-NH), 3.97 (4H, bs, $2\text{OCH}_2\text{CH}_3$), 4.21 (1H, bs, CH), 4.74 (1H, bs, CH-NH), 5.92 (1H, bs, CH-NH), 7.08 (1H, bs, CH-NH), 7.51-7.88 (5H, m, aromatic). ^{13}C NMR (75 MHz, CDCl_3): δ_{C} (ppm) 13.8, 13.9 (2 OCH_2CH_3), 24.5, 24.6, 25.4, 32.6, 32.7, 48.6, 53.8, 55.6, 62.3, 62.5, 127.2, 128.9, 132.7, 140.2, 164.4, 168.8, 169.4. Anal. Calcd for $C_{21}H_{30}N_2O_7S$: C, 55.49; H, 6.65; N, 6.16. Found: C, 55.58; H, 6.81; N, 6.20.



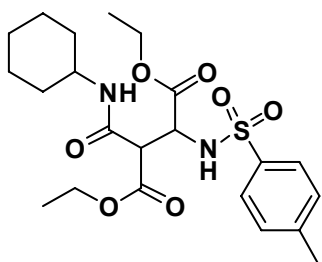
Diethyl 2-(2,6-dimethylphenylcarbamoyl)-3-(4-methylphenylsulfonamido)succinate (7c): White crystals (0.36 g, 73%). mp 162-164 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3454, 3253, 2931, 2858, 1732, 1661, 1578. MS, m/z (%): 444 (M^++1 , 5), 342 (5), 320 (10), 296 (5), 244 (10), 200 (20), 171

(20), 155 (20), 121 (30), 91 (100), 65 (50). ^1H NMR (300 MHz, CDCl_3): δ_{H} (ppm) 1.03 (3H, bs, OCH_2CH_3), 1.30 (3H, bs, OCH_2CH_3), 2.17 (6H, s, 2CH_3), 2.40 (3H, s, CH_3), 3.97 (3H, bs, $\text{O-CH}_2\text{CH}_3$ and CH), 4.27 (2H, bs, $\text{O-CH}_2\text{CH}_3$), 4.75 (1H, bs, CH-NH), 6.23 (1H, bs, CH-NH), 7.00-7.77 (7H, m, arom), 8.44 (1H, s, NHCO). ^{13}C NMR (75 MHz, CDCl_3): δ_{C} (ppm) 13.6, 14.0, 18.4, 21.5, 54.7, 55.0, 62.3, 32.5, 127.3, 127.4, 128.0, 129.6, 133.3, 135.3, 136.9, 143.7, 164.5, 168.3, 169.4. Anal. Calcd for $C_{24}H_{30}N_2O_7S$: C, 58.76; H, 6.16; N, 5.71. Found: C, 58.82; H, 6.09; N, 5.69.



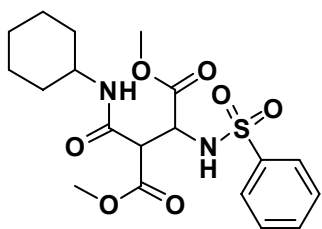
Di-tert-butyl 2-(4-methylphenylsulfonamido)-3-(2,4,4-trimethylpentan-2-ylcarbamoyl)succinate (7d): White crystals (0.47 g, 85%). mp 85-88 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3337, 3238, 2974, 2859, 1732, 1694, 1552. MS, m/z (%): 323 (M^+ -231, 10), 267 (10), 223 (5), 198 (5), 155 (20), 112 (30), 91 (60), 57 (100). ^1H NMR (300 MHz, CDCl_3):

δ_{H} (ppm) 1.00 (9H, s, $\text{C}(\text{CH}_3)_3$), 1.31 (18H, bs, $2\text{OC}(\text{CH}_3)_3$), 1.40 (6H, s, $\text{C}(\text{CH}_3)_2$), 1.57 (2H, s, CH_2), 2.35 (3H, s, CH_3), 4.42 (1H, d, $^3J_{\text{HH}} = 6.7$ Hz, CH), 5.24 (1H, bs, CHNH), 5.76 (1H, d, $^3J_{\text{HH}} = 6.7$ Hz, CH-NH), 7.21 (2H, d, $^3J_{\text{HH}} = 7.5$ Hz, arom), 7.68 (2H, d, $^3J_{\text{HH}} = 7.5$ Hz, arom), 7.77 (1H, bs, NHCO). ^{13}C NMR (75 MHz, CDCl_3): δ_{C} (ppm) 21.4, 27.7, 28.3, 31.2, 31.3, 31.7, 54.1, 54.5, 65.1, 65.3, 80.4, 82.5, 127.1, 129.4, 137.8, 143.0, 167.6, 167.7, 168.3. Anal. Calcd for $\text{C}_{28}\text{H}_{46}\text{N}_2\text{O}_7\text{S}$: C, 60.62; H, 8.36; N, 5.05. Found: C, 60.56; H, 8.34; N, 5.09.



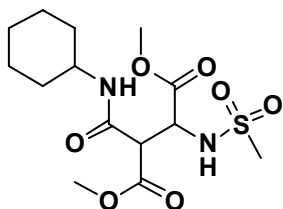
Diethyl 2-(cyclohexylcarbamoyl)-3-(4-methylphenylsulfonamido)succinate (7e): White crystals (0.38 g, 81%). mp 141-143 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3282, 2934, 2850, 1735, 1646, 1561, 1445. ^1H NMR (300 MHz, CDCl_3): δ_{H} (ppm) 1.05-1.88 (16H, m, 5CH_2 of cyclohexyl, $2\text{OCH}_2\text{CH}_3$), 2.41 (3H, s, CH_3), 3.74 (1H, bs, CH), 3.95-4.22 (5H, m, OCH_2CH_3 and CH), 4.72 (1H, d, $^3J_{\text{HH}} = 8.4$, CHNH), 5.79 (1H, d, $^3J_{\text{HH}} = 8.4$, CHNH), 7.2 (1H, bs, CHNH), 7.28 (2H, d, $^3J_{\text{HH}} = 7.0$, H-Ar), 7.2874 (2H, d, $^3J_{\text{HH}} = 7.0$, H-Ar).

^{13}C NMR (75 MHz, CDCl_3): δ_{C} (ppm) 13.7, 13.9, 21.5, 24.5, 25.4, 32.7, 48.6, 53.8, 55.5, 62.3, 62.4, 127.3, 129.5, 137.1, 143.5, 164.4, 168.9, 169.4. Anal. Calcd for $\text{C}_{22}\text{H}_{32}\text{N}_2\text{O}_7\text{S}$: C, 56.39; H, 6.88; N, 5.98. Found: C, 56.42; H, 6.73; N, 6.04.



Dimethyl 2-(cyclohexylcarbamoyl)-3-(phenylsulfonamido)succinate (7f): White crystals (0.31 g, yield 74%). mp 138-140 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3316, 3255, 2934, 2863, 1740, 1650, 1545, 1450. ^1H NMR (300 MHz,

CDCl₃): δ_H (ppm) 1.20-1.87 (10H, m, 5CH₂ of cyclohexyl), 3.50 (3H, s, O-CH₃), 3.70 (3H, s, O-CH₃), 3.76 (1H, bs, CHNH), 4.73 (1H, bs, CH), 5.95 (1H, bs, CHNH), 7.41 (1H, bs, CHNH), 7.52-7.87 (5H, m, arom). (¹³C NMR (75 MHz, CDCl₃): δ_C (ppm) 24.5, 25.4, 32.5, 48.8, 53.0, 53.5, 54.1, 55.1, 55.6, 127.2, 128.9, 129.1, 132.7, 164.5, 168.8, 169.9. Anal. Calcd for C₁₉H₂₆N₂O₇S: C, 53.51; H, 6.14; N, 6.57. Found: C, 53.57; H, 6.16; N, 6.38.



Dimethyl 2-(cyclohexylcarbamoyl)-3-(methylsulfonamido)succinate (7h): White crystals (0.25 g, yield 70%). mp 132-135 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3282, 2913, 2847, 1733, 1646, 1264. ¹H NMR (300 MHz, CDCl₃): δ_H (ppm) 1.26-1.66-2.03 (10H, m, 5CH₂ of cyclohexyl), 3.06 (3H, s, CO₂CH₃), 3.42 (3H, s, CO₂CH₃), 3.72 (3H, s, CH₃), 3.80 (1H, bs, CHNH), 4.80 (1H, d, ³J_{HH} = 8.3 Hz, CH), 5.88 (1H, bs, CHNH), 6.94 (1H, d, ³J_{HH} = 7.5 Hz, arom). ¹³C NMR (75 MHz, CDCl₃): δ_C (ppm) 23.9, 25.1, 33.4, 42.0, 48.8, 51.8, 53.1, 53.5, 54.1, 164.7, 168.9, 170.5. Anal. Calcd for C₁₄H₂₄N₂O₇S: C, 46.14; H, 6.64; N, 7.69. Found: C, 46.23; H, 6.60; N, 7.83.

DI/GHASEMI-BBB(5)/88.04.13

Time 22: 1:48

File : DI_71.X75 Date 8/30/10

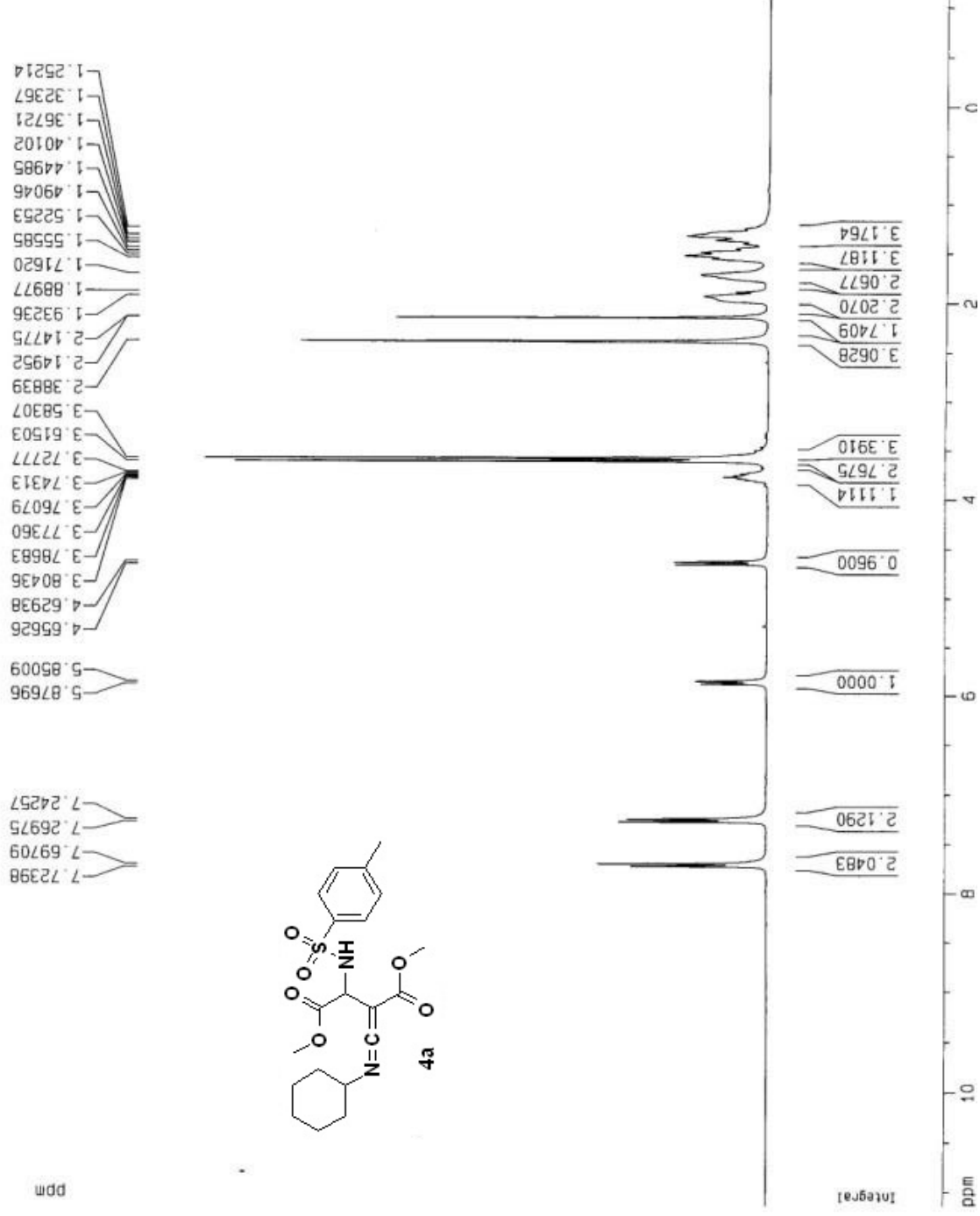
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¹H NMR



Current Data Parameters
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EXPNO 78
PROCNO 1

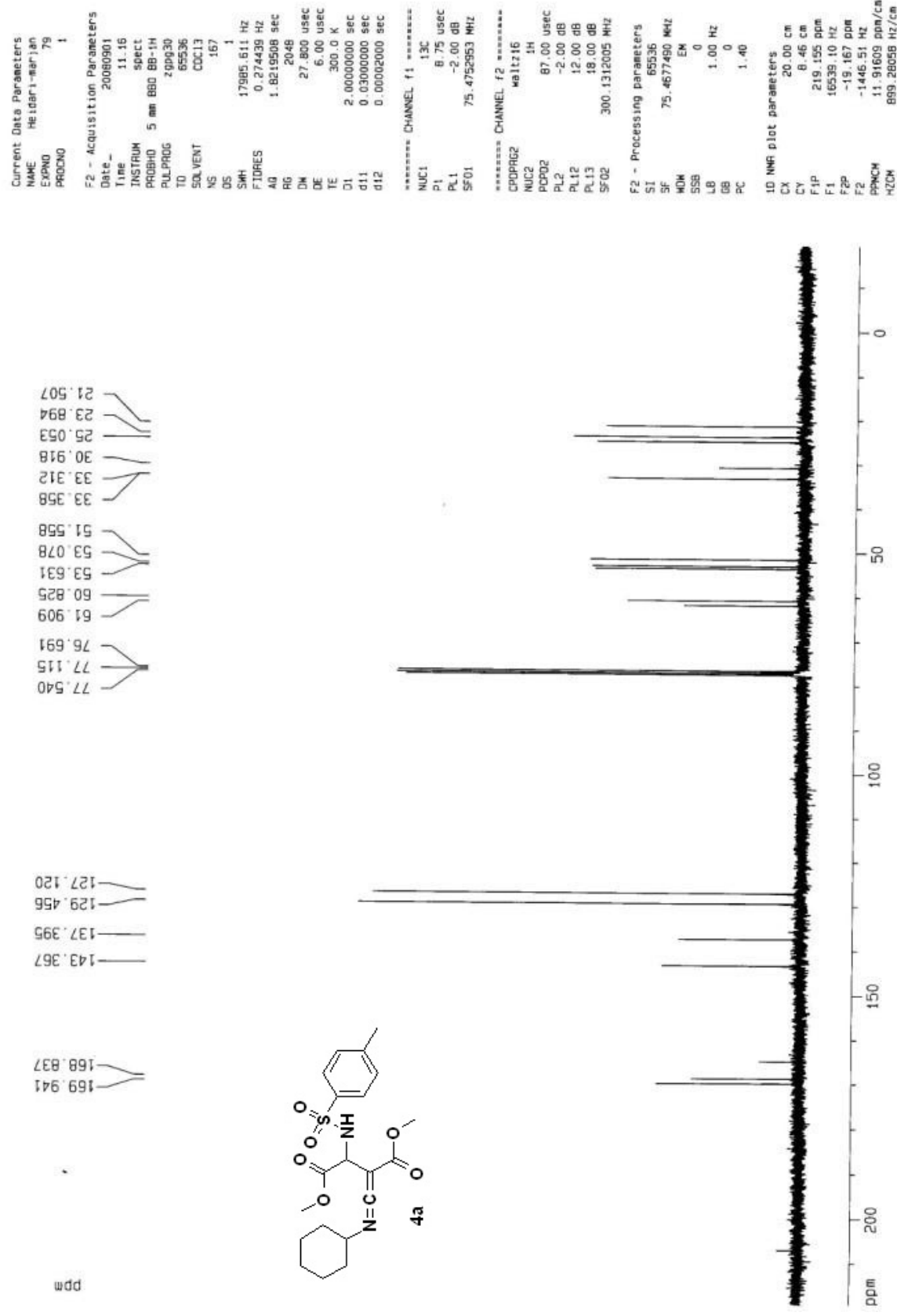
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DS 0
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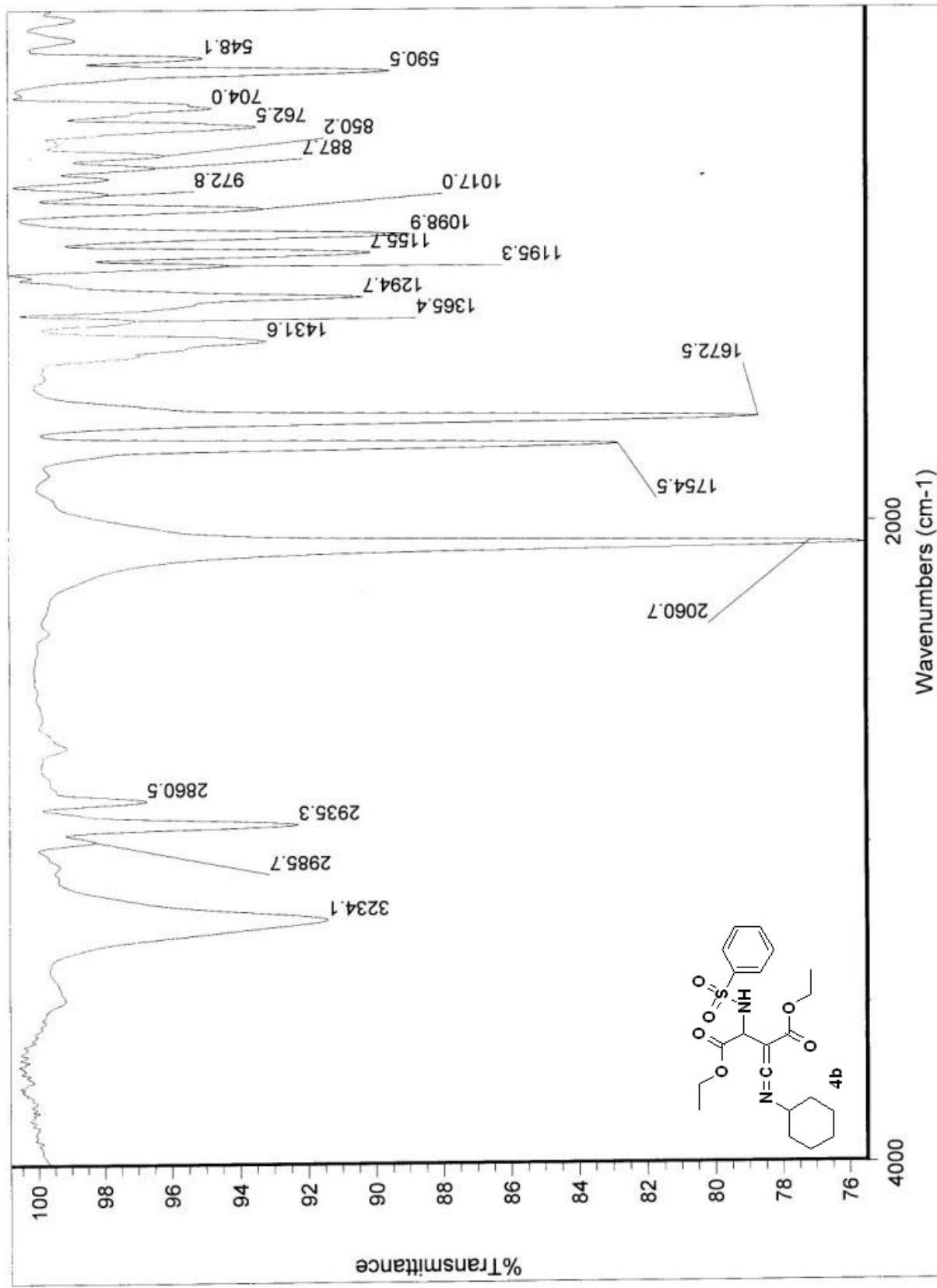
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PC 1.00

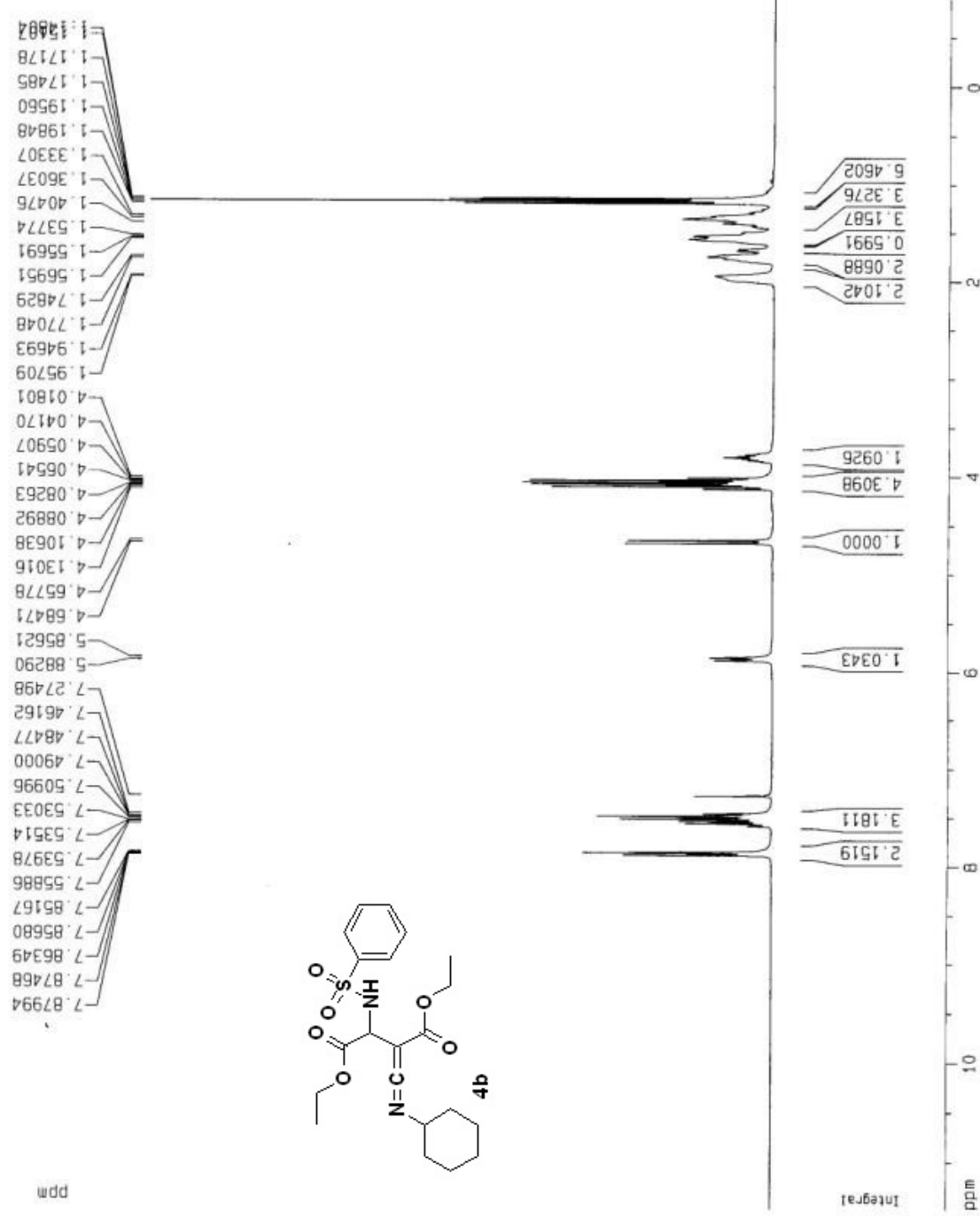
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¹³C {¹H} NMR





¹H NMR



Current Data Parameters
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EXPNO 325
PROCNO 1

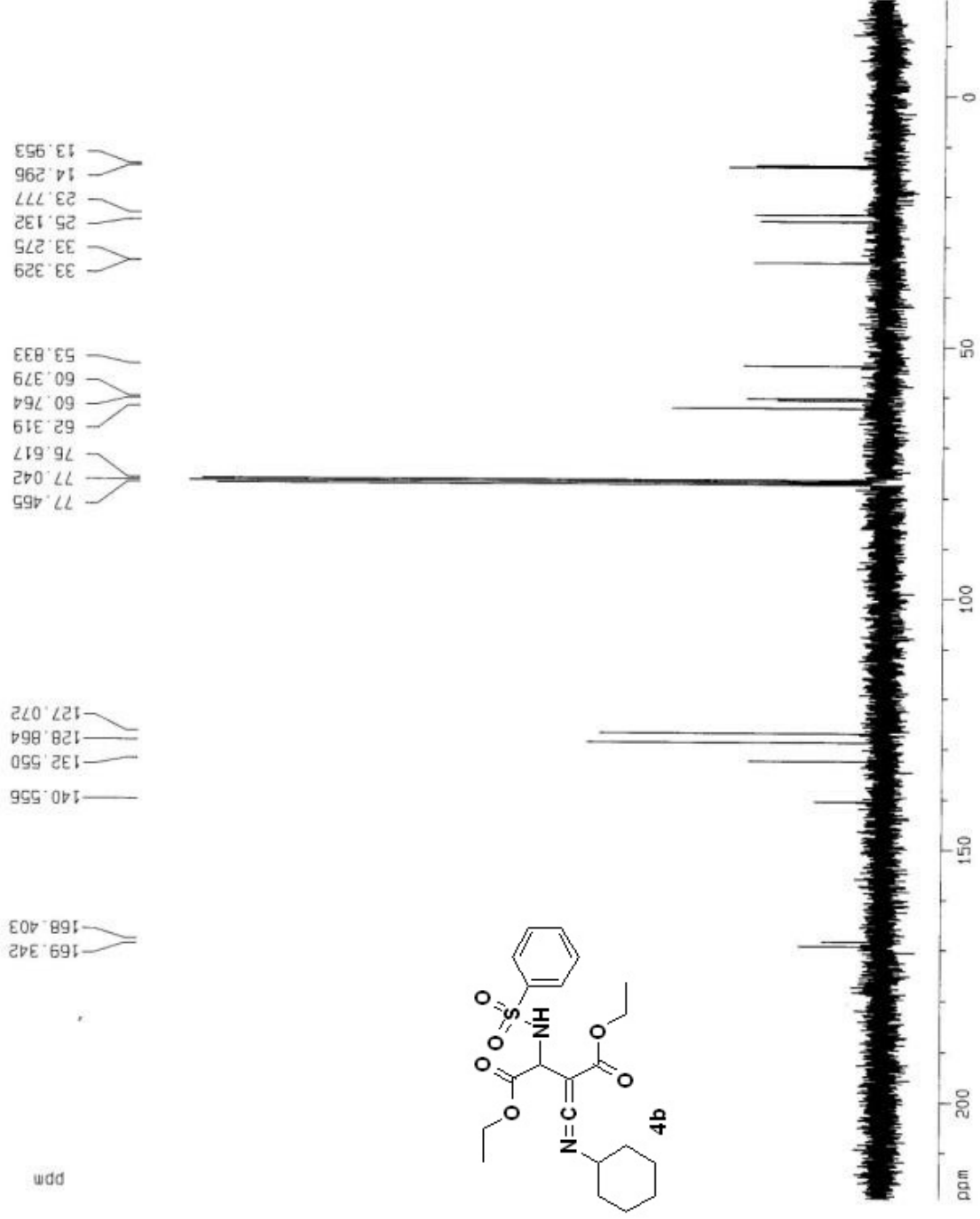
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SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DM 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
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PL1 -2.00 dB
SF01 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
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CY 10.41 cm
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F2P -0.897 ppm
F2 -269.31 Hz
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HZCM 185.74823 Hz/cm

¹³C {¹H} NMR



Current Data Parameters
NAME Sarvari
EXPNO 326
PROCNO 1

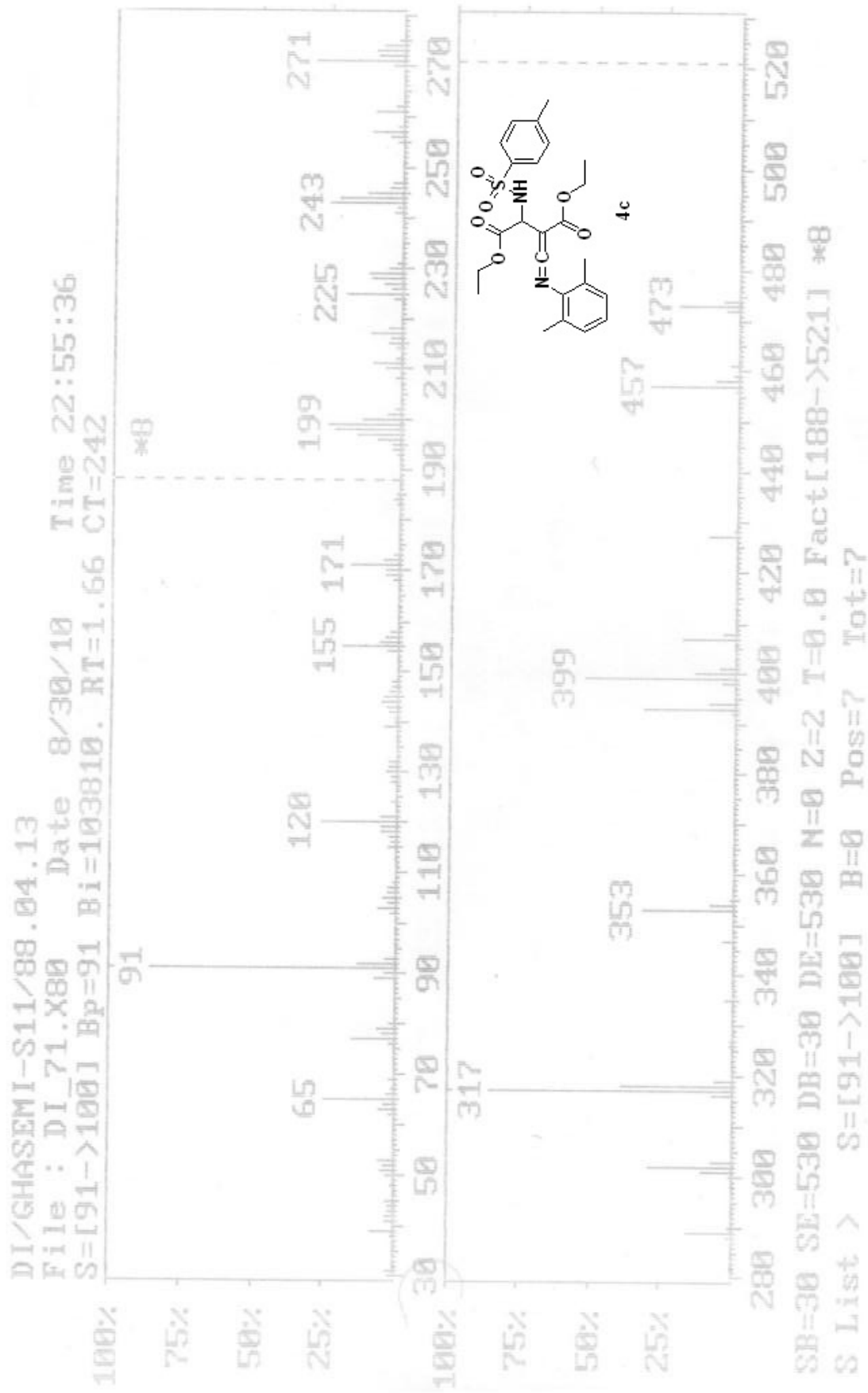
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DS 1
SWH 17985.611 Hz
FIDRES 0.274439 Hz
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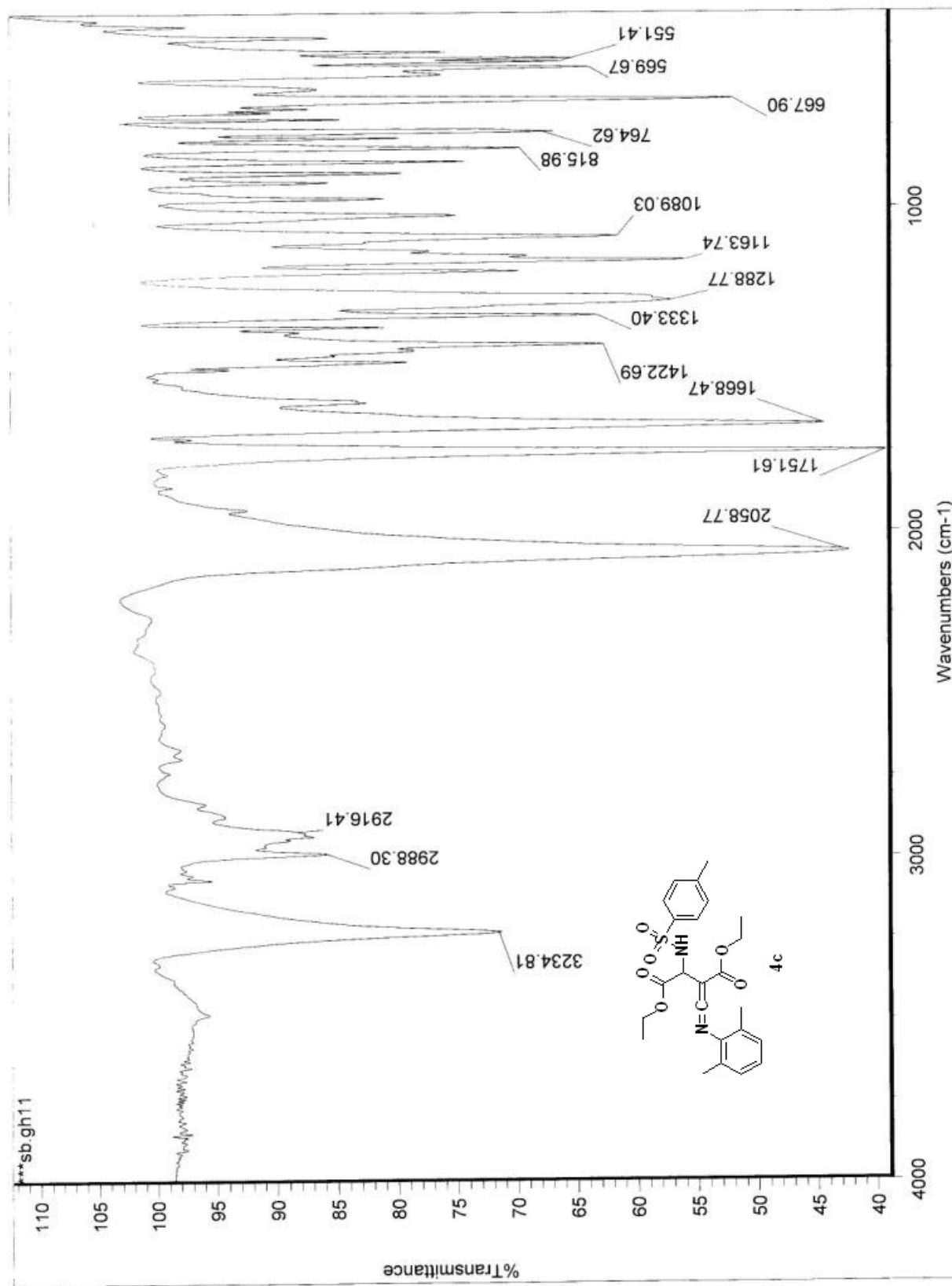
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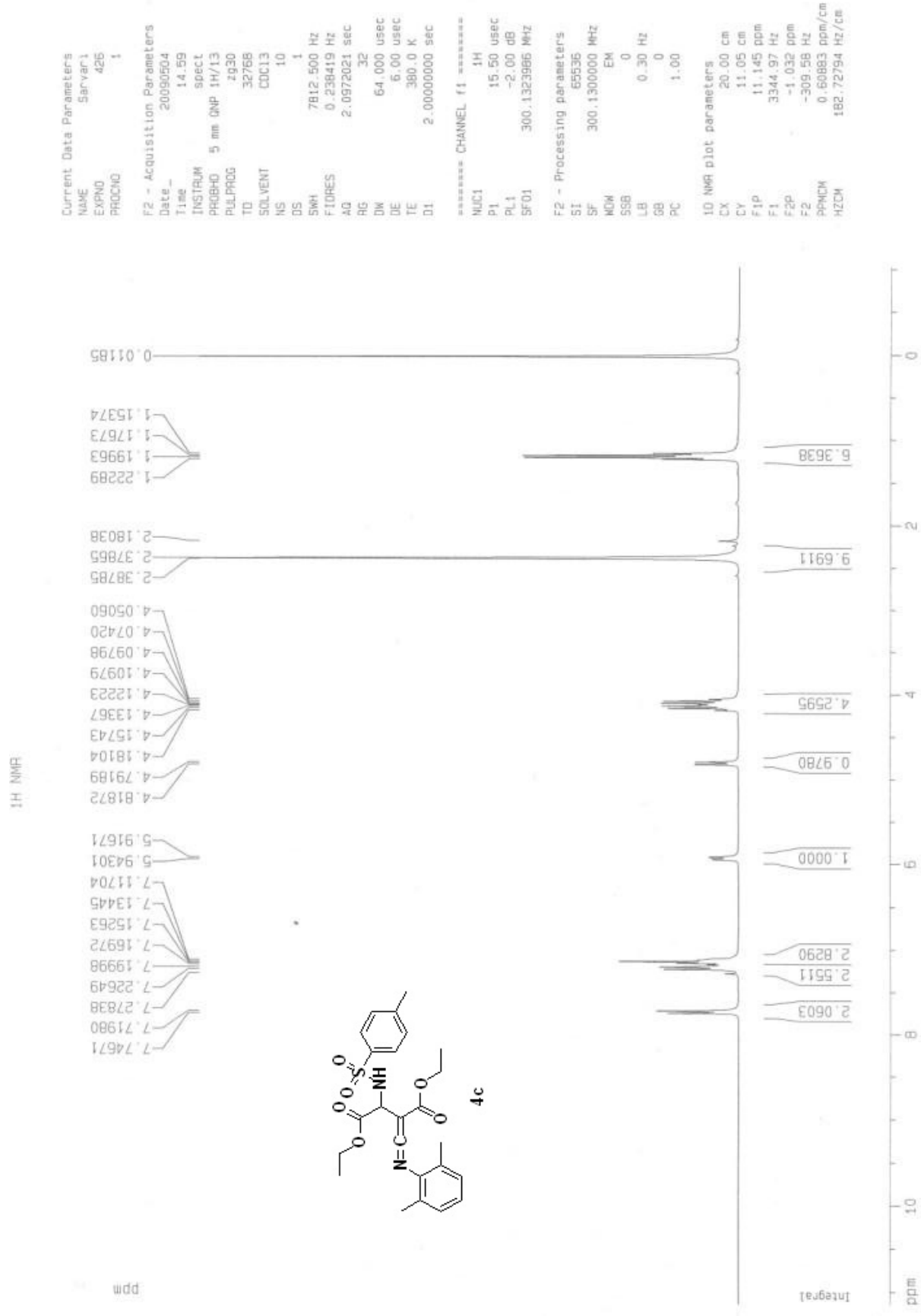
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PL13 18.00 dB
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F2 - Processing parameters
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GB 0
PC 1.40

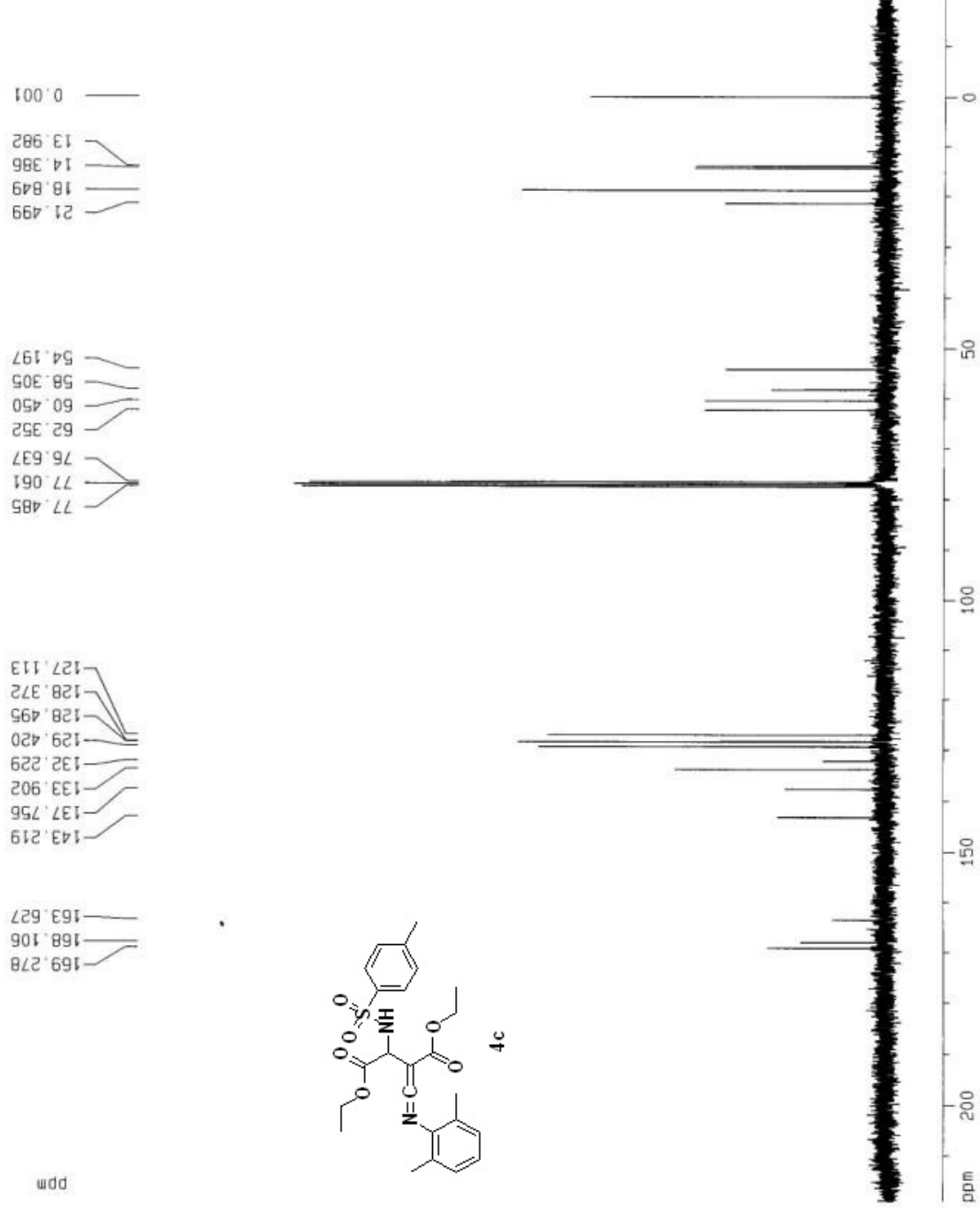
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¹³C (1H) NMR



Current Data Parameters
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EXPNO: 427
PROCNO: 1

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RG: 2048
DM: 27.800 usec
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TE: 300.0 K
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d11: 0.03000000 sec
d12: 0.00002000 sec

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NUC1: 13C
P1: 8.75 usec
PL1: -2.00 dB
SF01: 75.4752953 MHz

----- CHANNEL f2 -----
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PCPD2: 87.00 usec
PL2: -2.00 dB
PL12: 12.00 dB
PL13: 18.00 dB
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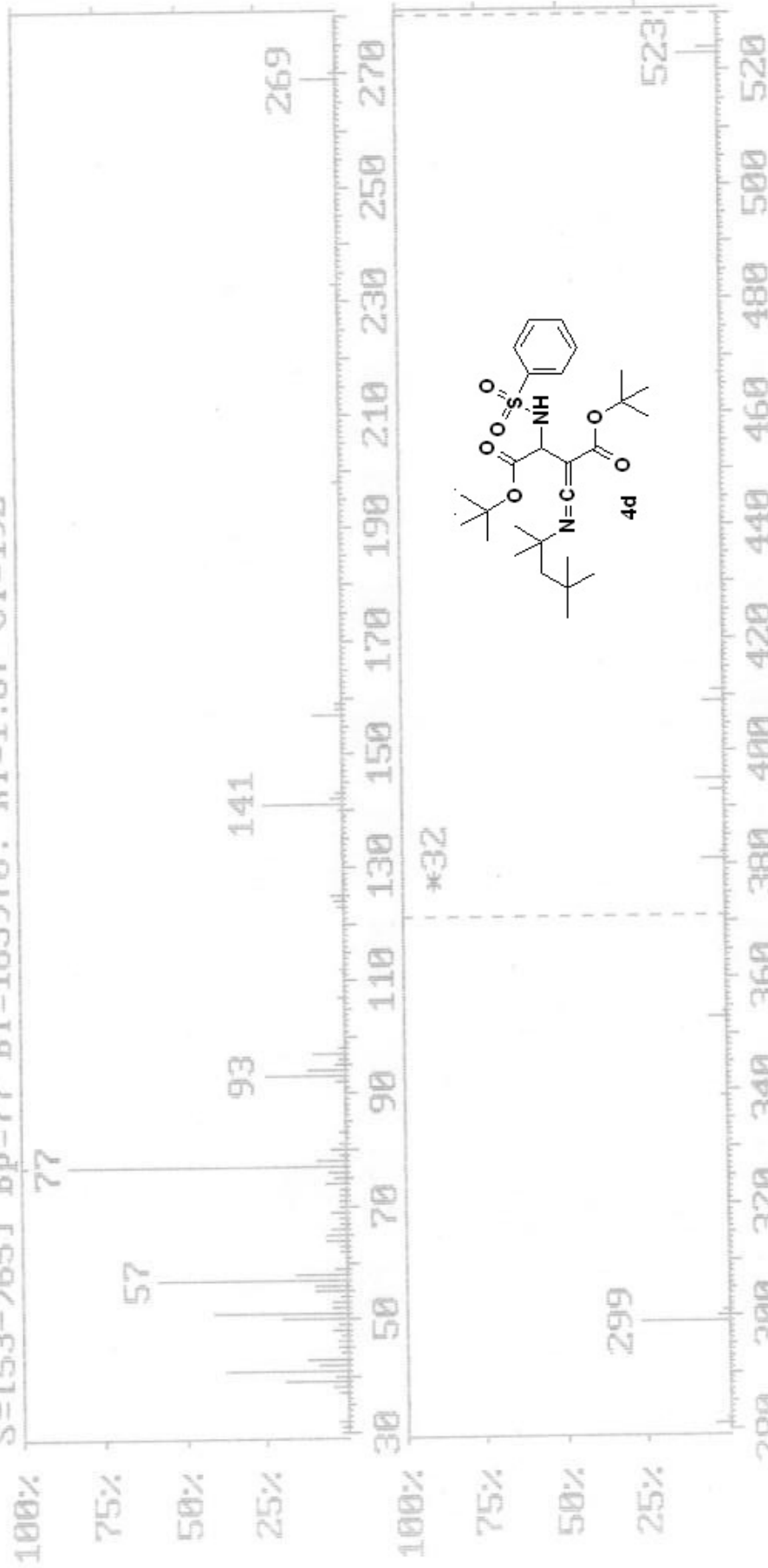
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1D NMR plot parameters
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F1: 16539.10 Hz
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DI/GHASEMI-S15/88.04.13

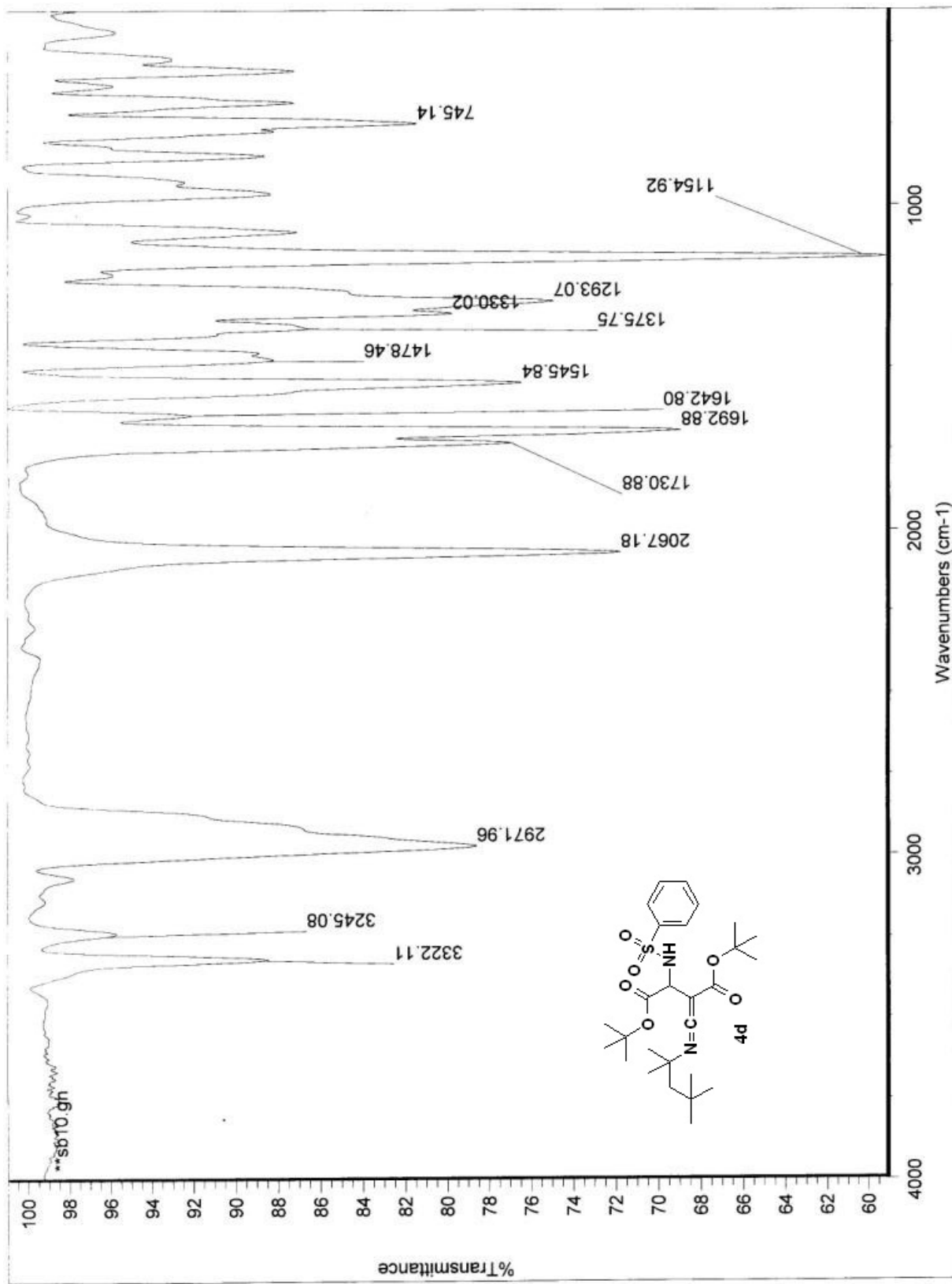
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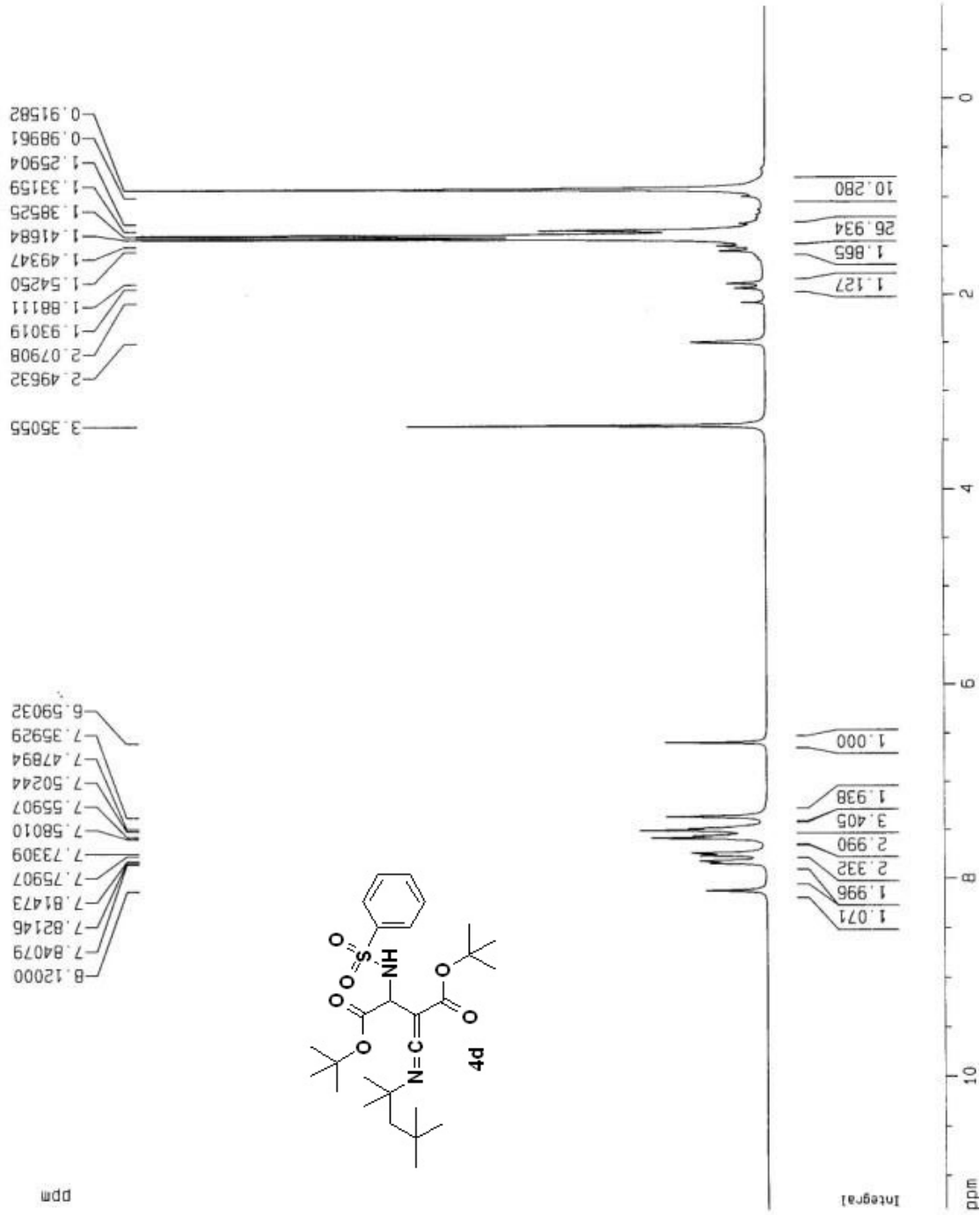


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¹H NMR



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PROCNO 1

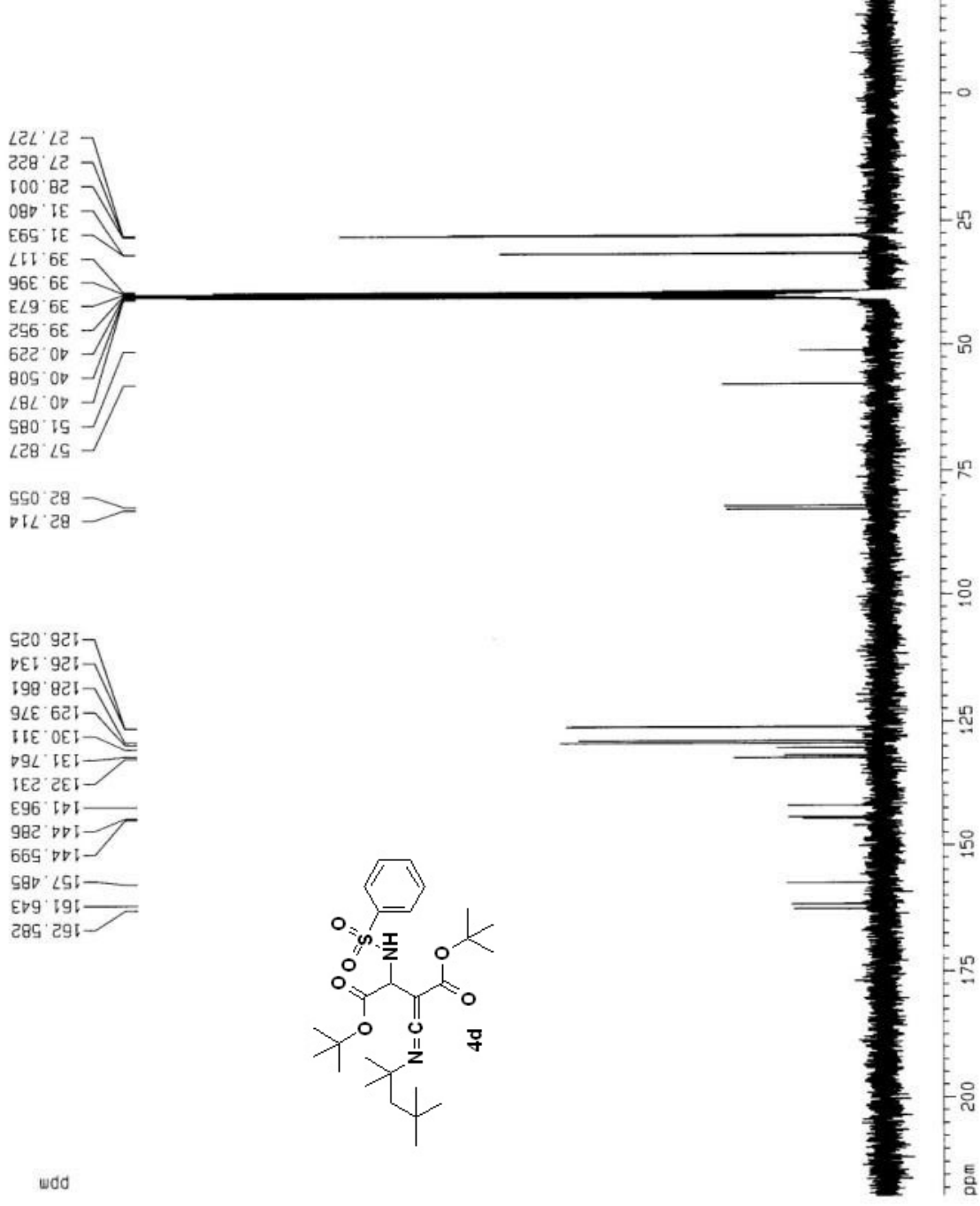
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DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DM 64.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
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P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323986 MHz

F2 - Processing parameters
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SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
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PPMCM 0.61554 ppm/cm
HZCM 184.74147 Hz/cm

¹³C {¹H} NMR



Current Data Parameters
NAME Rezaei-PHO
EXPNO 354
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090509
Time 20.36
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 174
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 ¹³C
P1 8.75 usec
PL1 -2.00 dB
SF01 75.4752953 MHz

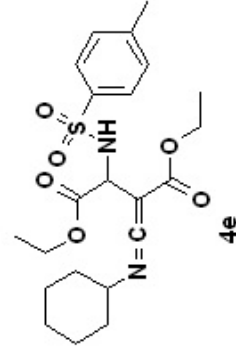
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

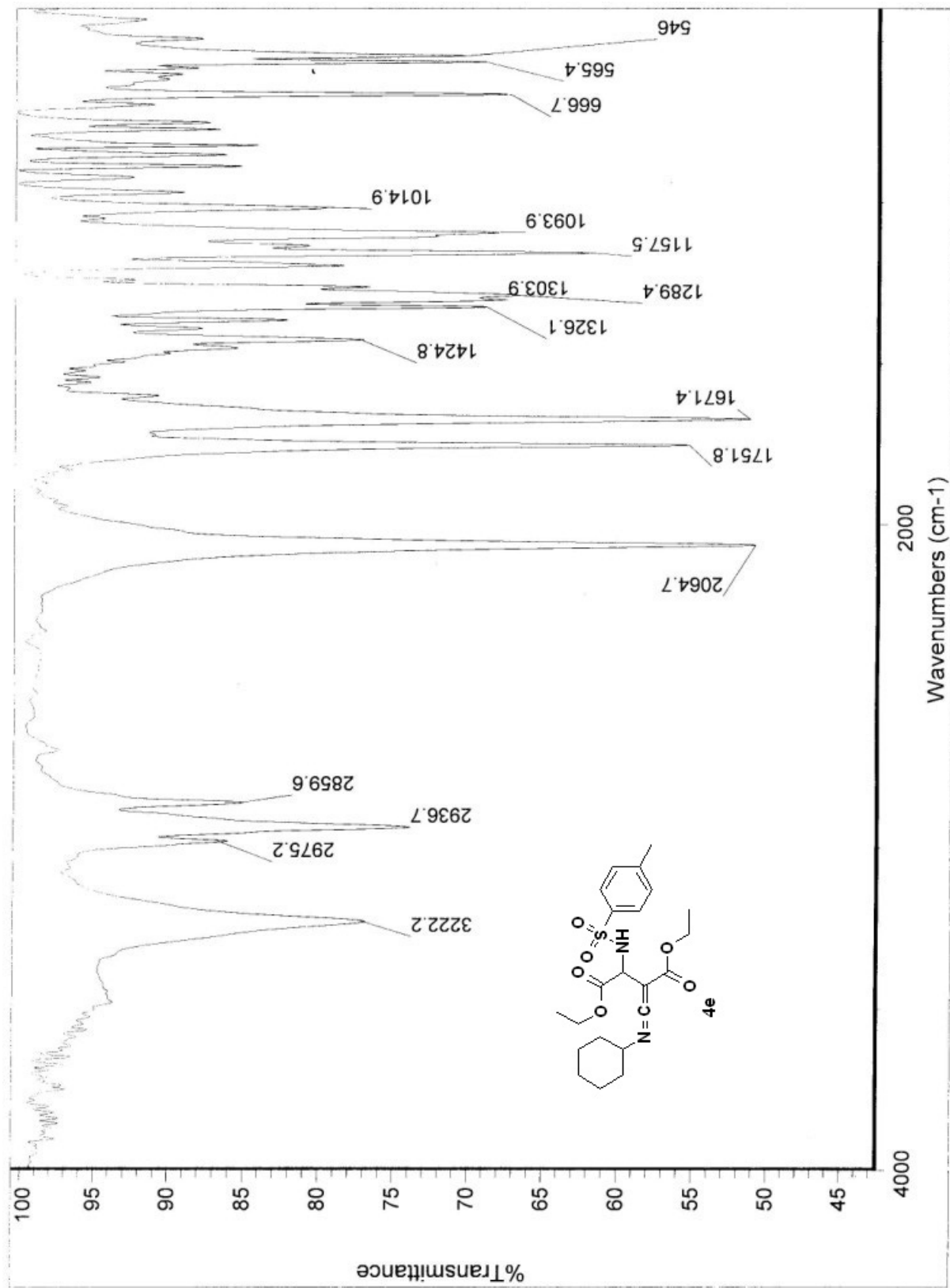
1D NMR plot parameters
CX 20.00 cm
CY 26.56 cm
F1P 219.155 ppm
F1 16539.10 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PNUCH 11.91609 ppm/cm
HZCM 899.28058 Hz/cm

DI/GHASEMI-22/87.03.22

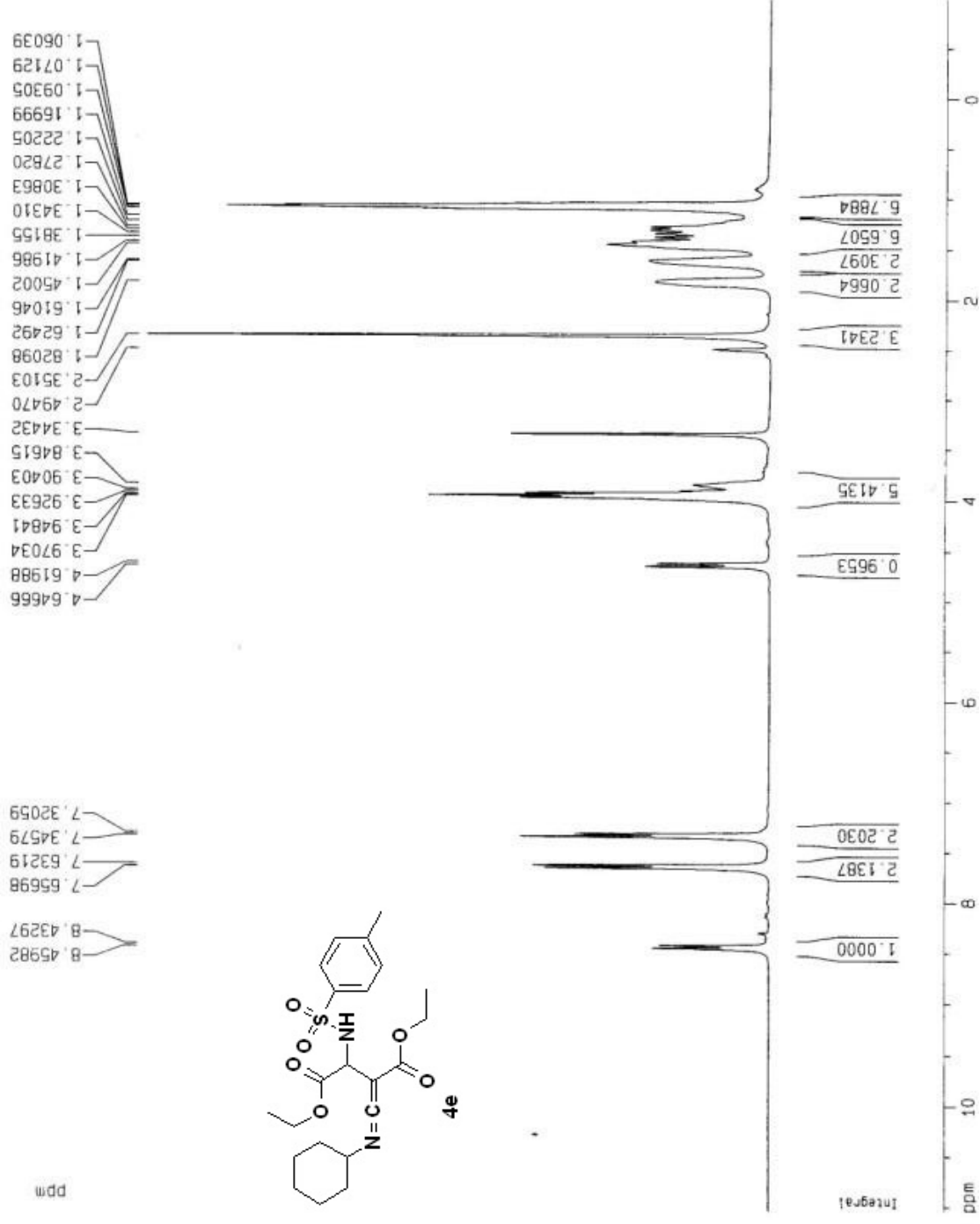
File : DI_64.X34 Date 8/21/10 Time 00: 5:59
S=[74->104] Bp=91 Bi=81690. RT=1.72 CT=244



SB=30 SE=530 DB=30 DE=530 N=0 Z=2 T=0.0 Fact[315->765] *16
S List > S=[74->104] B=0 Pos=1 Tot=1



¹H NMR



Current Data Parameters
NAME Keshipoor
EXPNO 173
PROCNO 1

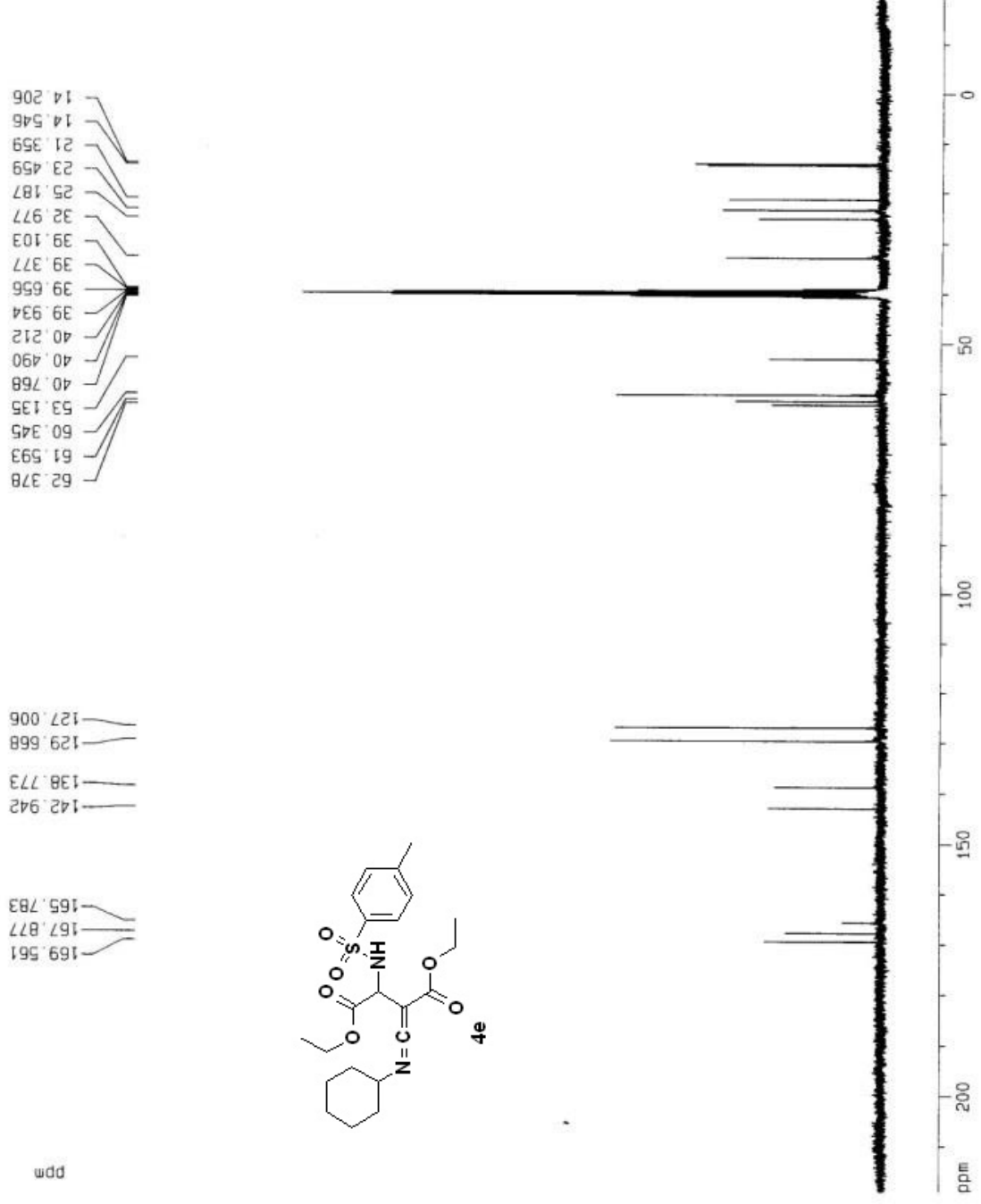
F2 - Acquisition Parameters
Date_ 20090607
Time 14.30
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DM 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

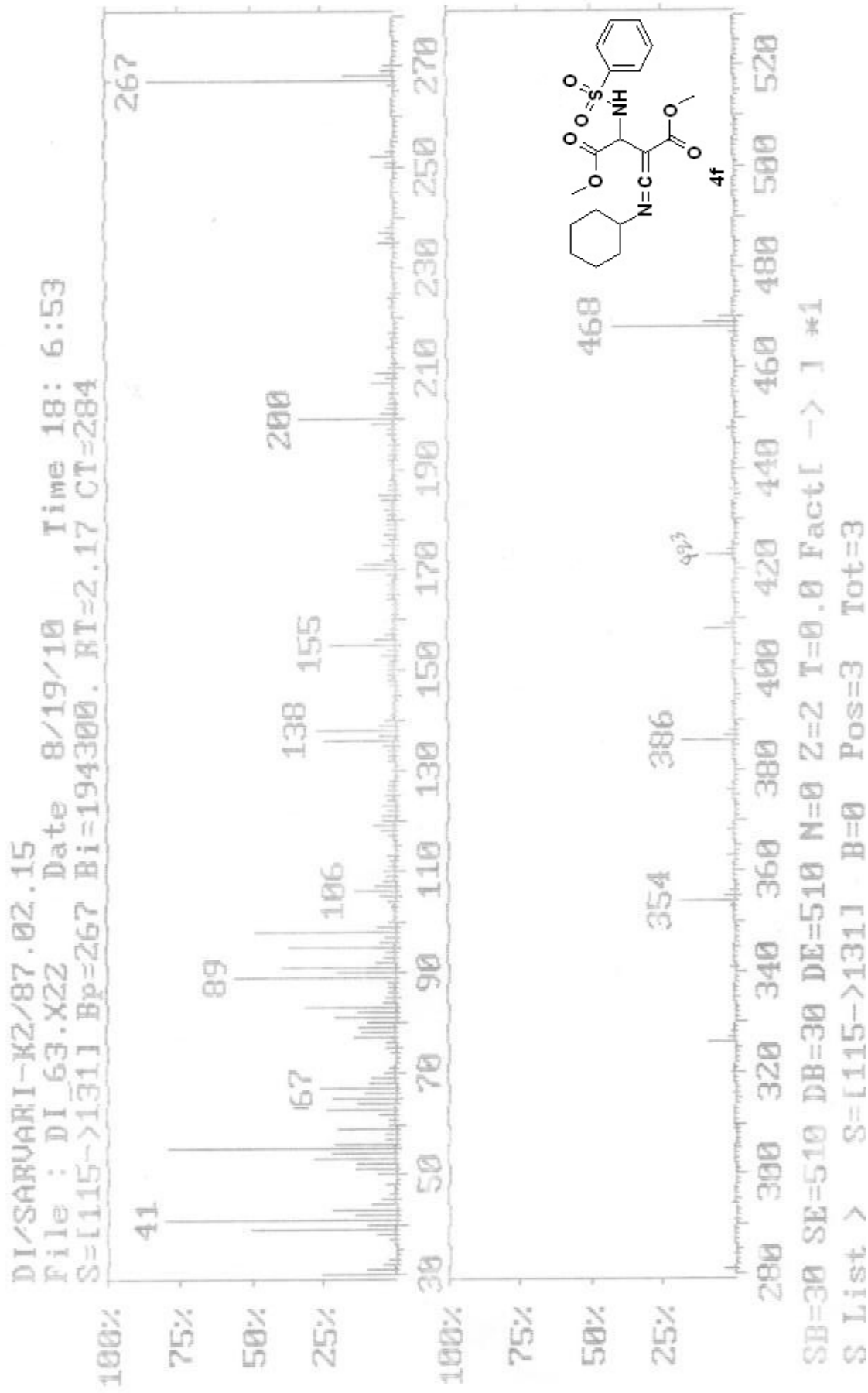
===== CHANNEL f1 =====
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323985 MHz

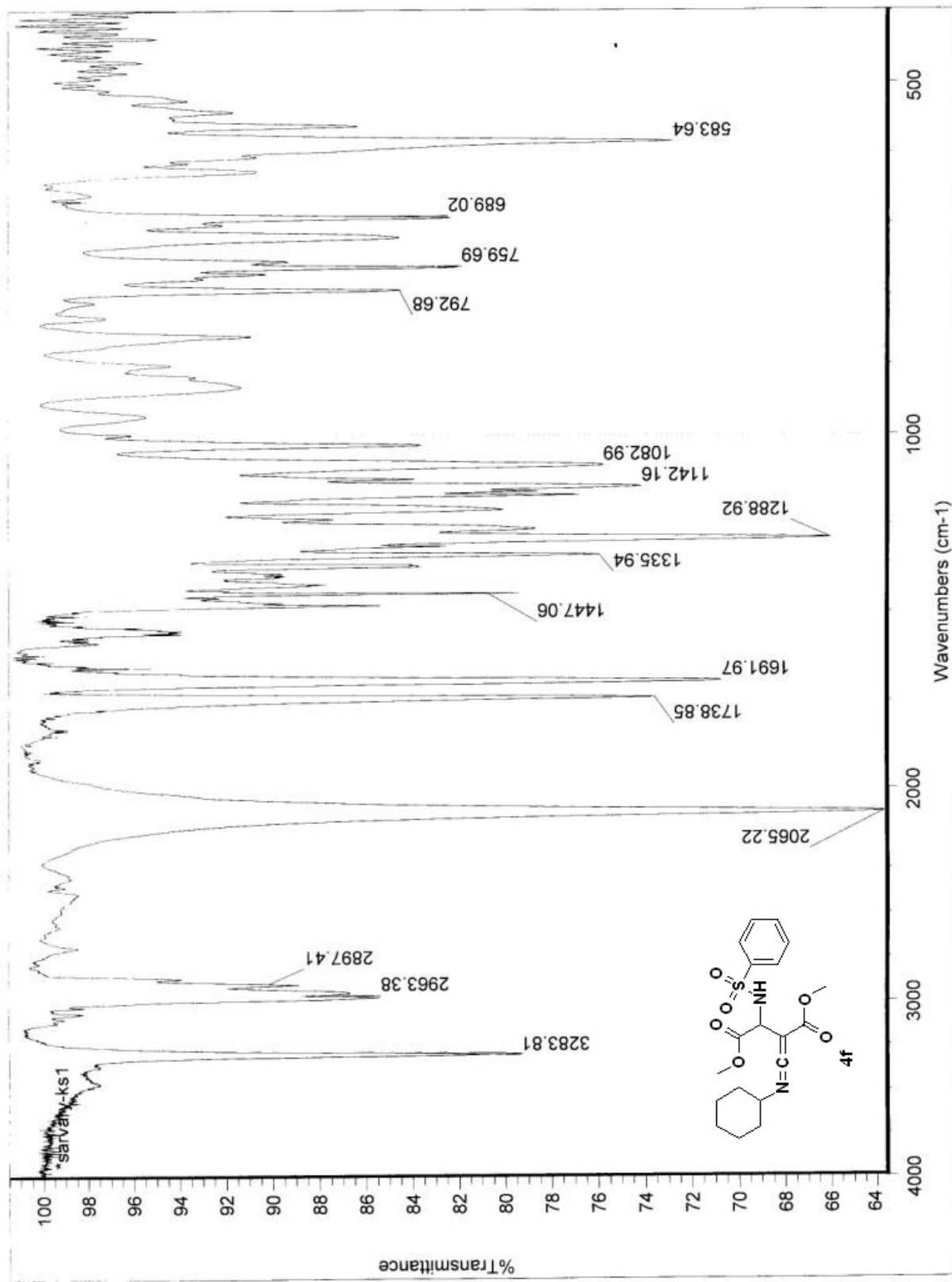
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.10

1D NMR plot parameters
CX 20.00 cm
CY 10.37 cm
F1P 11.050 ppm
F1 3316.58 Hz
F2P -0.989 ppm
F2 -296.70 Hz
PRNCH 0.60195 ppm/cm
HZCM 180.66408 Hz/cm

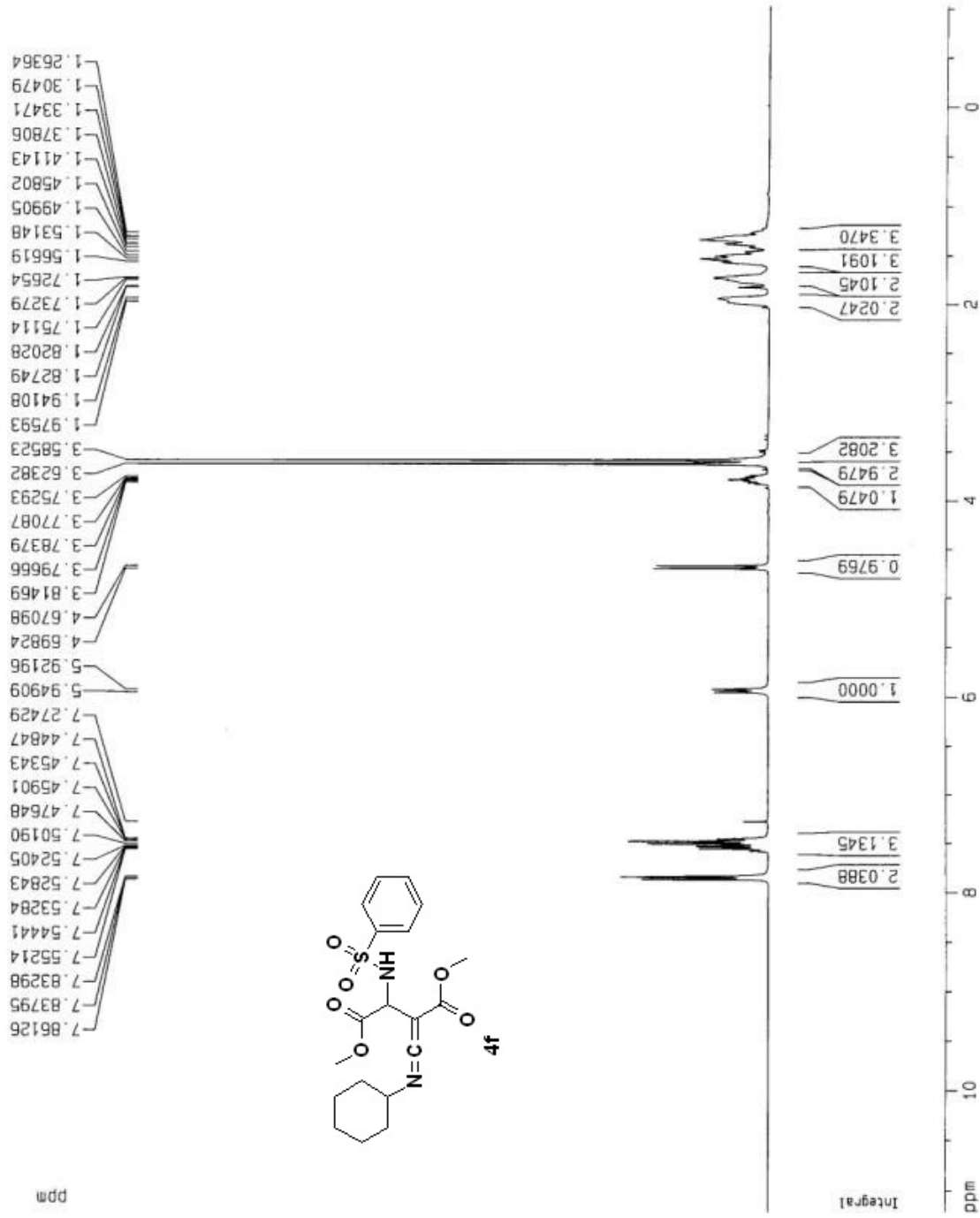
¹³C {¹H} NMR







¹H NMR



Current Data Parameters
NAME Sarvar1
EXPNO 305
PROCNO 1

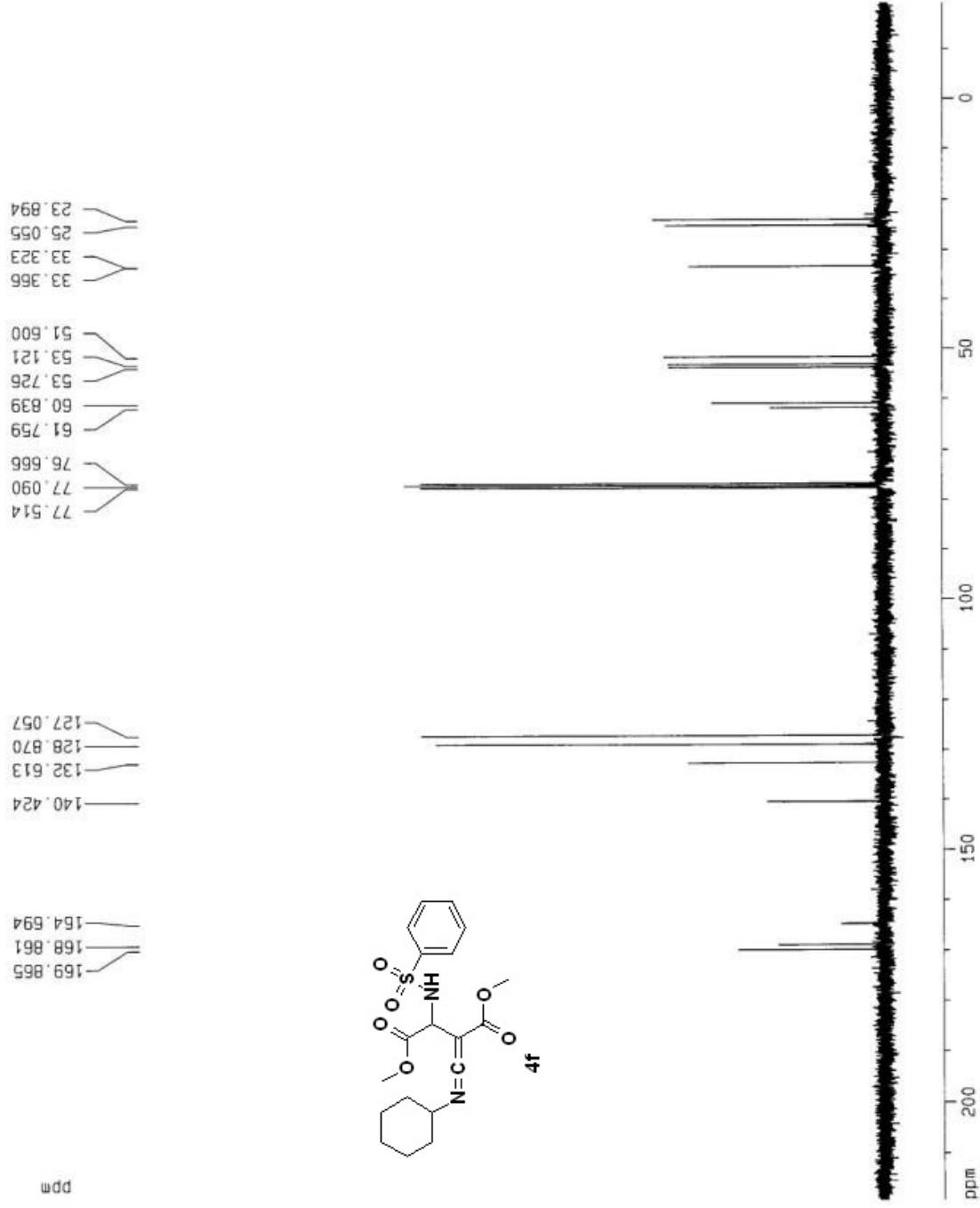
F2 - Acquisition Parameters
Date_ 20080902
Time 12.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 2
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 50.8
DM 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 11.70 cm
FIP 11.212 ppm
F1 3365.11 Hz
F2P -1.032 ppm
F2 -309.58 Hz
PPNOM 0.61218 ppm/cm
HZCM 183.73470 Hz/cm

¹³C {¹H} NMR



Current Data Parameters
NAME Sarvani
EXPNO 306
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080902
Time 12.29
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 104
DS 1
SWH 17985.511 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 ¹³C
P1 8.75 usec
PL1 -2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EN
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 8.08 cm
FIP 219.155 ppm
F1 16539.10 Hz
F2 -19.167 ppm
PPMCM 11.91609 ppm/cm
HZCM 869.28058 Hz/cm

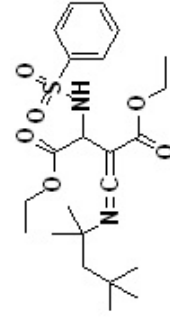
DI/SARVARI-BBB 14/89.01.28

File : DI_81.X40

Date 9/ 6/10

Time 11:18:58

S=[58->97] Bp=77 Bi=156420. RT=1.61 CT=249

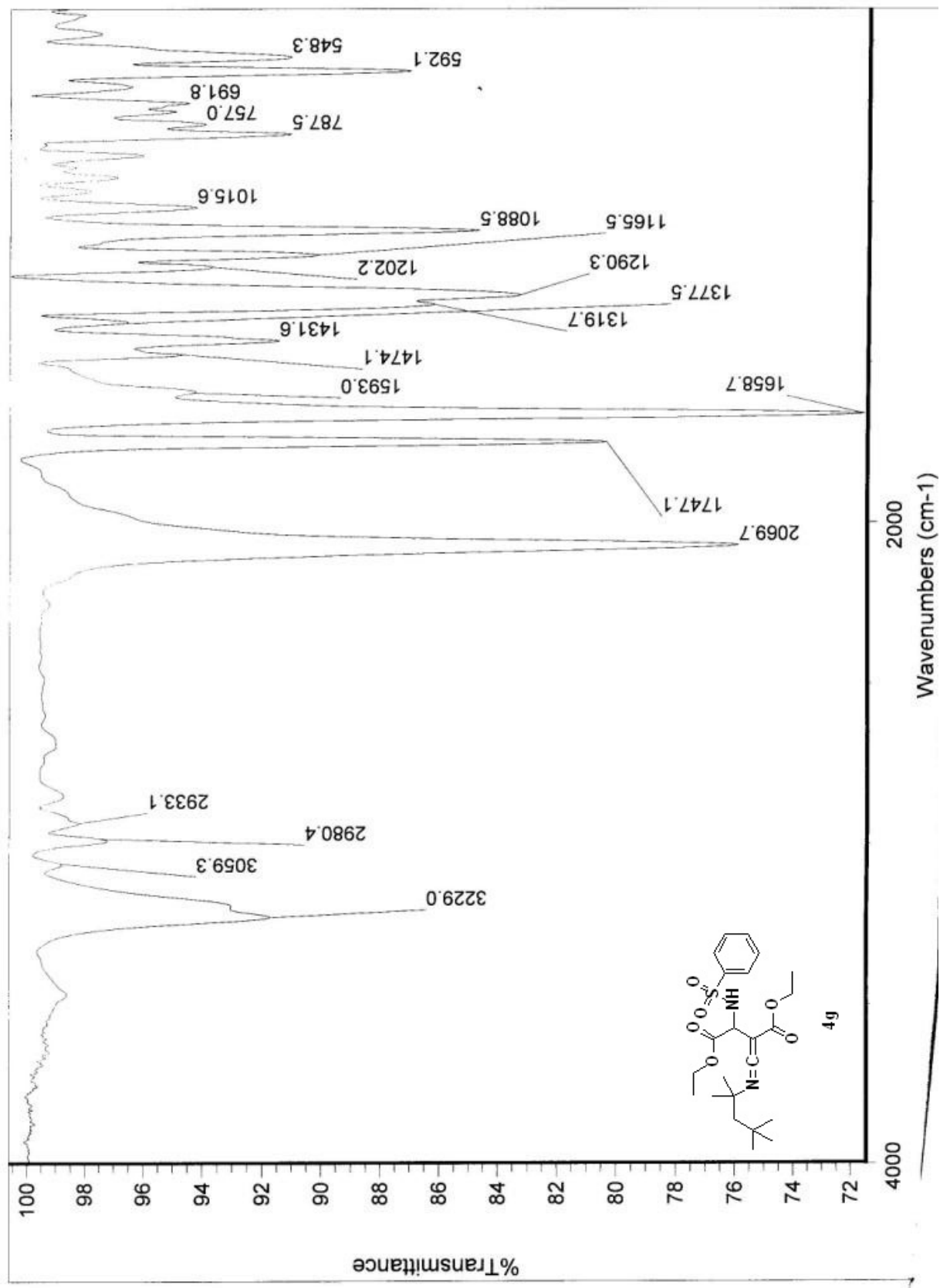


4g

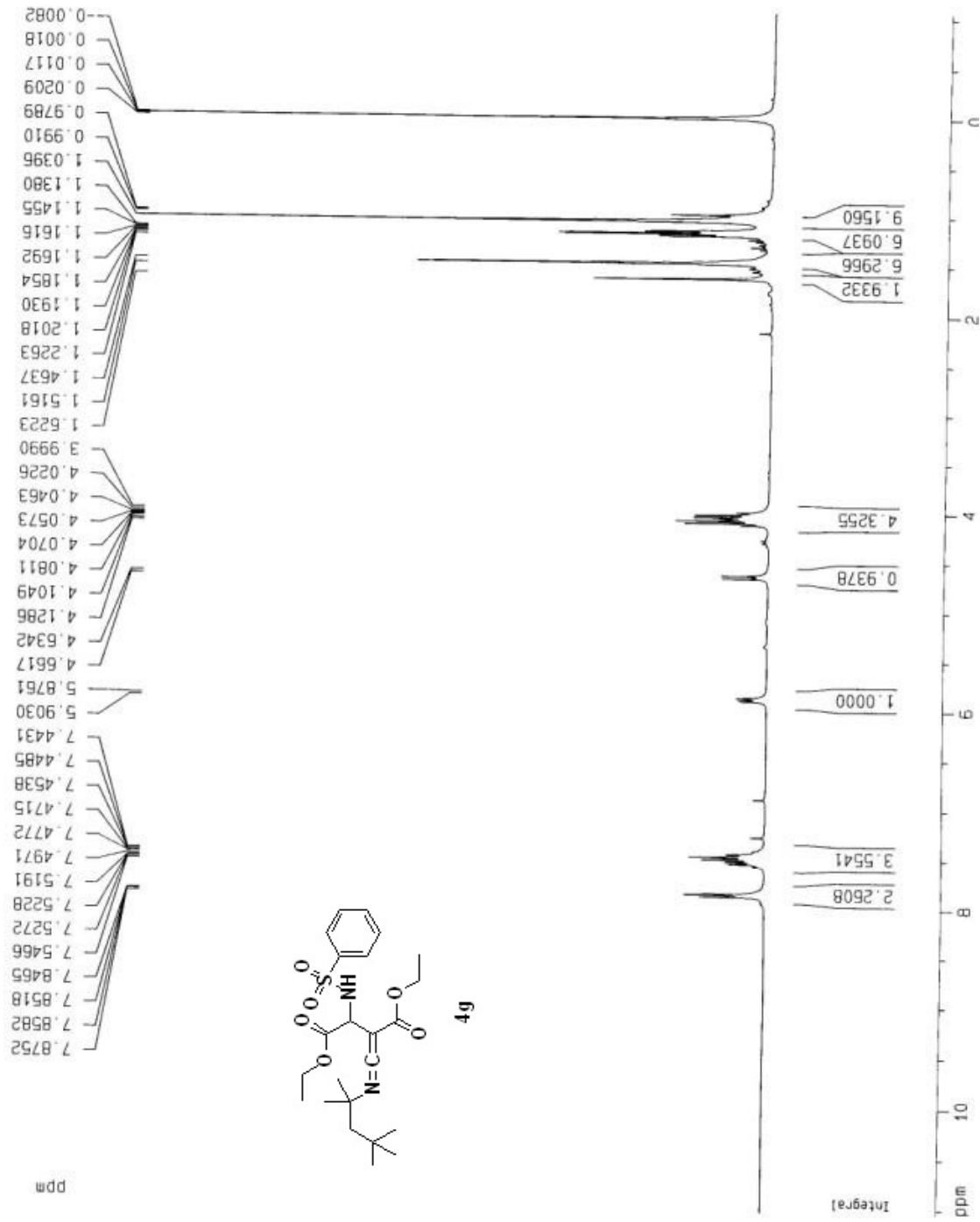


SB=30 SE=510 DB=30 DE=510 N=0 Z=2 T=0.0 Fact[181->519] *16

S List > S=[58->97] B=0 Pos=8 Tot=8



¹H NMR



Current Data Parameters
NAME: Server1
EXPNO: 422
PROCNO: 1

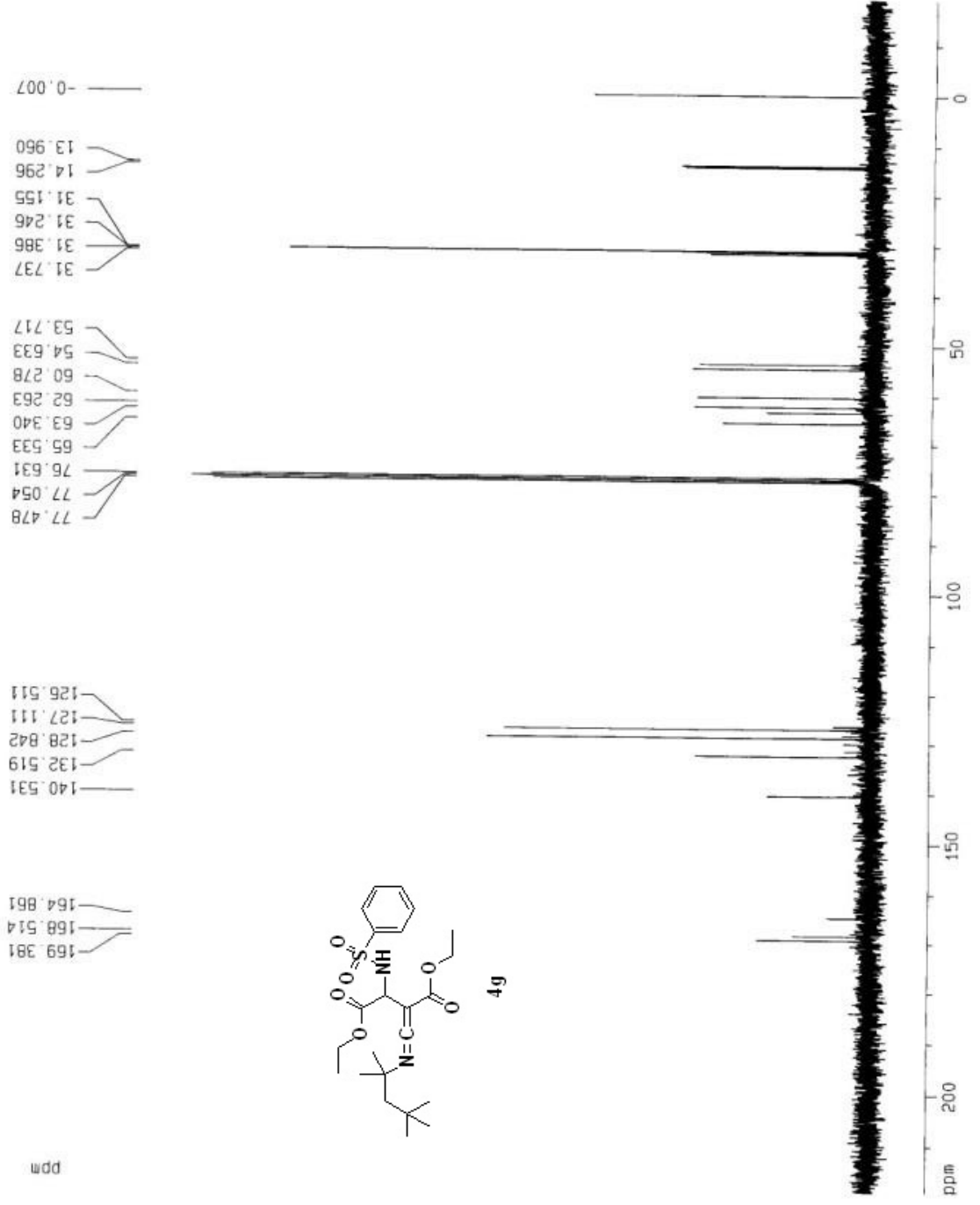
F2 - Acquisition Parameters
Date_: 20090504
Time: 14.04
INSTRUM: spect
PROBHD: 5 mm QNP 1H/13
PULPROG: zg30
TO: 32768
SOLVENT: DMSO
NS: 10
DS: 1
SWH: 7812.500 Hz
FIDRES: 0.238419 Hz
AQ: 2.0972021 sec
RG: 32
DW: 64.000 usec
DE: 6.00 usec
TE: 380.0 K
D1: 2.00000000 sec

***** CHANNEL f1 *****
NUC1: 1H
P1: 15.50 usec
PL1: -2.00 dB
SF01: 300.1323986 MHz

F2 - Processing parameters
SI: 65536
SF: 300.1300000 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 14.97 cm
FIP: 11.044 ppm
F1: 3314.77 Hz
F2P: -1.065 ppm
F2: -319.65 Hz
PPHMC: 0.60547 ppm/cm
HZCM: 181.72116 Hz/cm

¹³C (1H) NMR



Current Data Parameters
NAME Sarvari
EXPNO 423
PROCNO 1

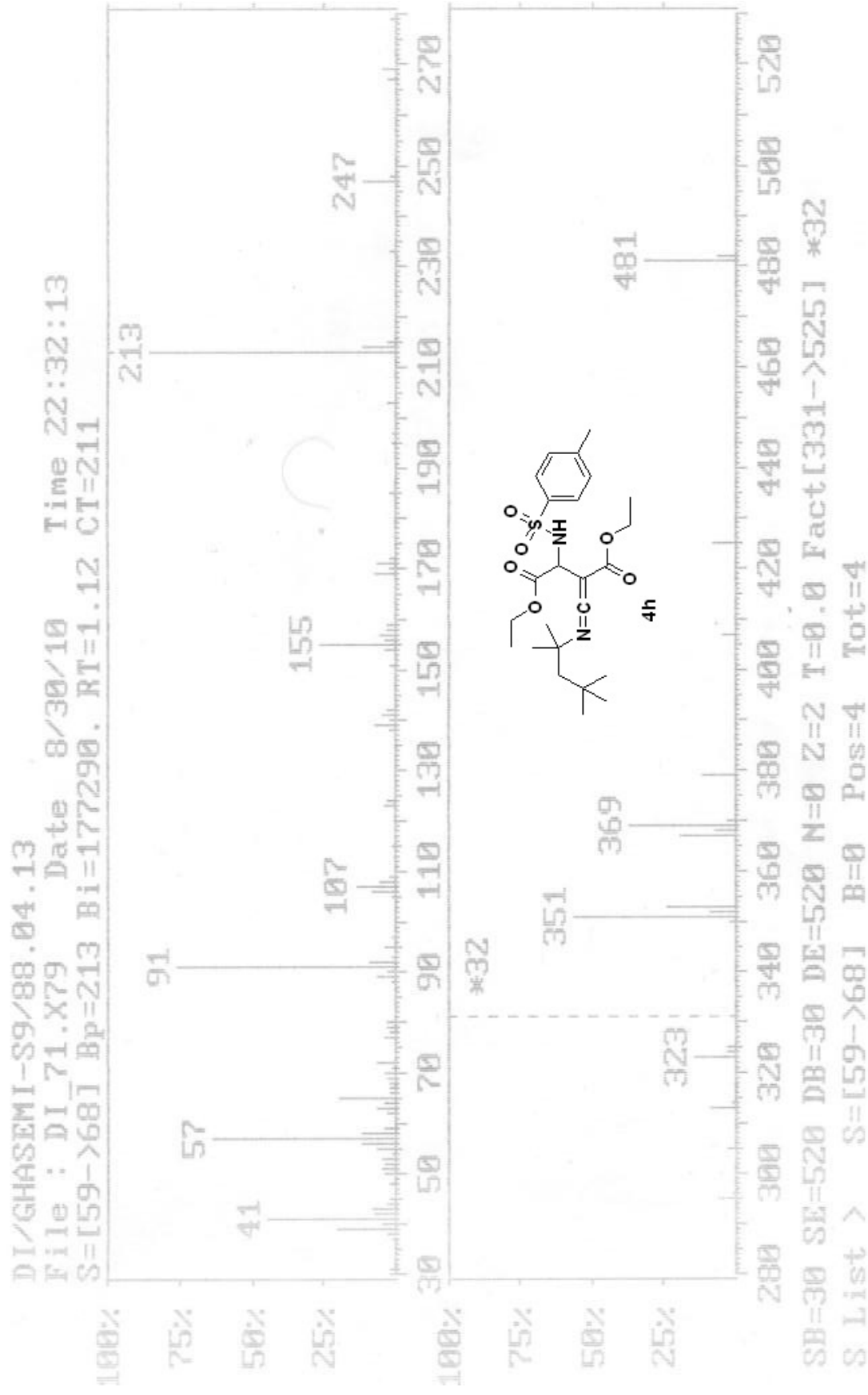
F2 - Acquisition Parameters
Date_ 20090504
Time 14.09
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 173
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

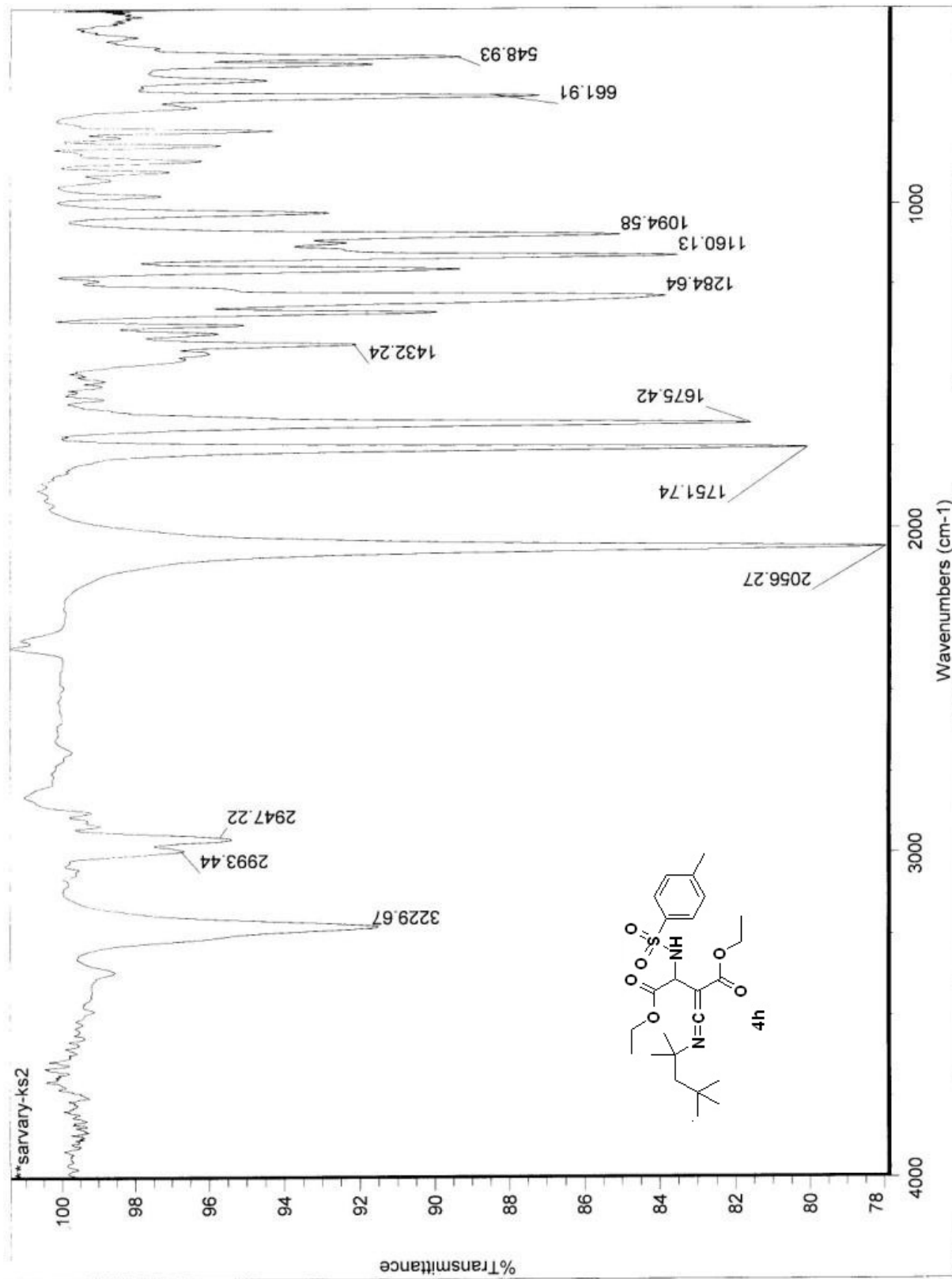
***** CHANNEL f1 *****
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SF01 75.4752953 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SF02 300.1312005 MHz

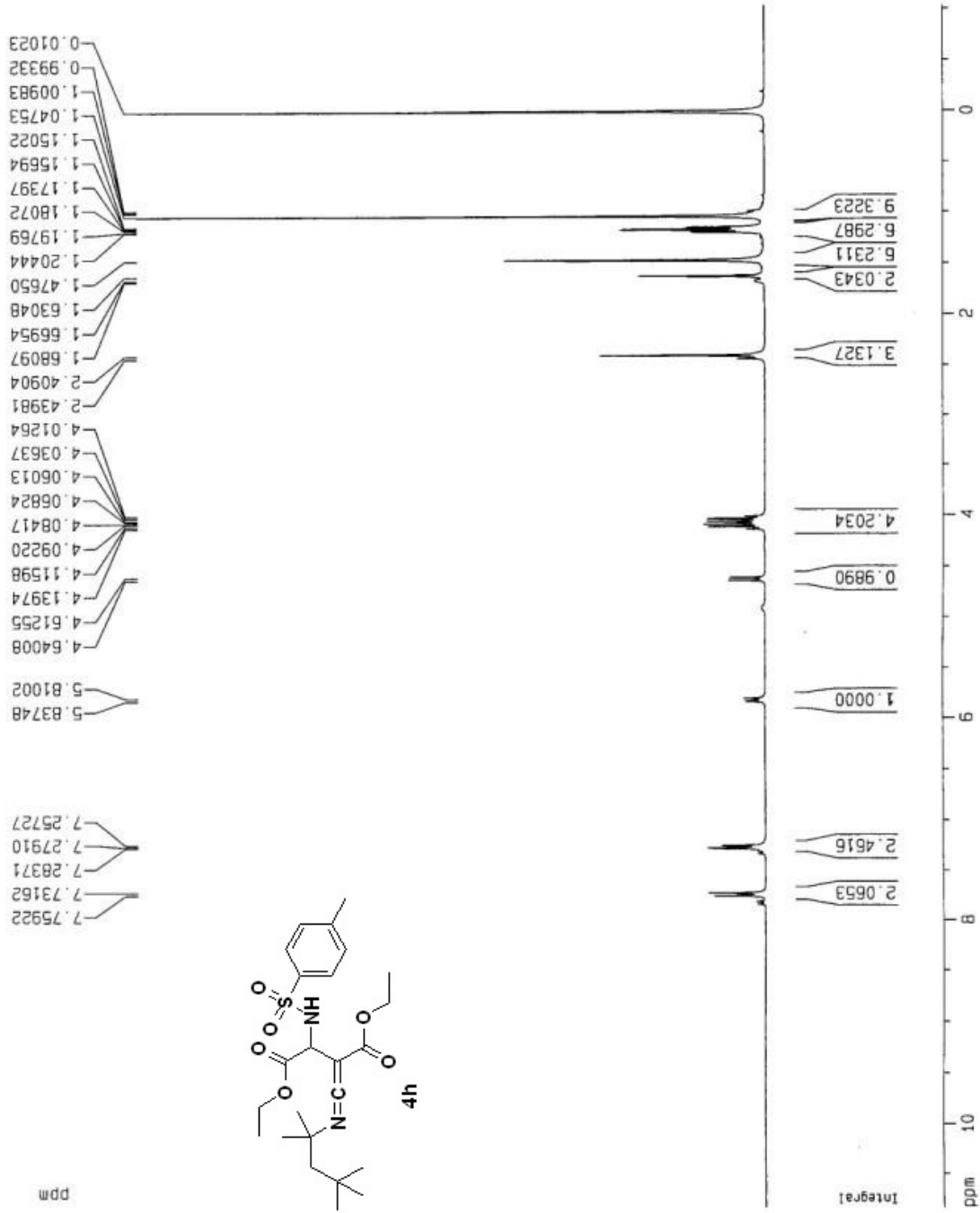
F2 - Processing parameters
SI 65536
SF 75.4677450 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 11.58 cm
F1P 219.155 ppm
F1 16539.10 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCM 11.91609 ppm/cm
HZCM 899.28058 Hz/cm





¹H NMR



Current Data Parameters
NAME , Sarvan1
EXPNO 428
PROCNO 1

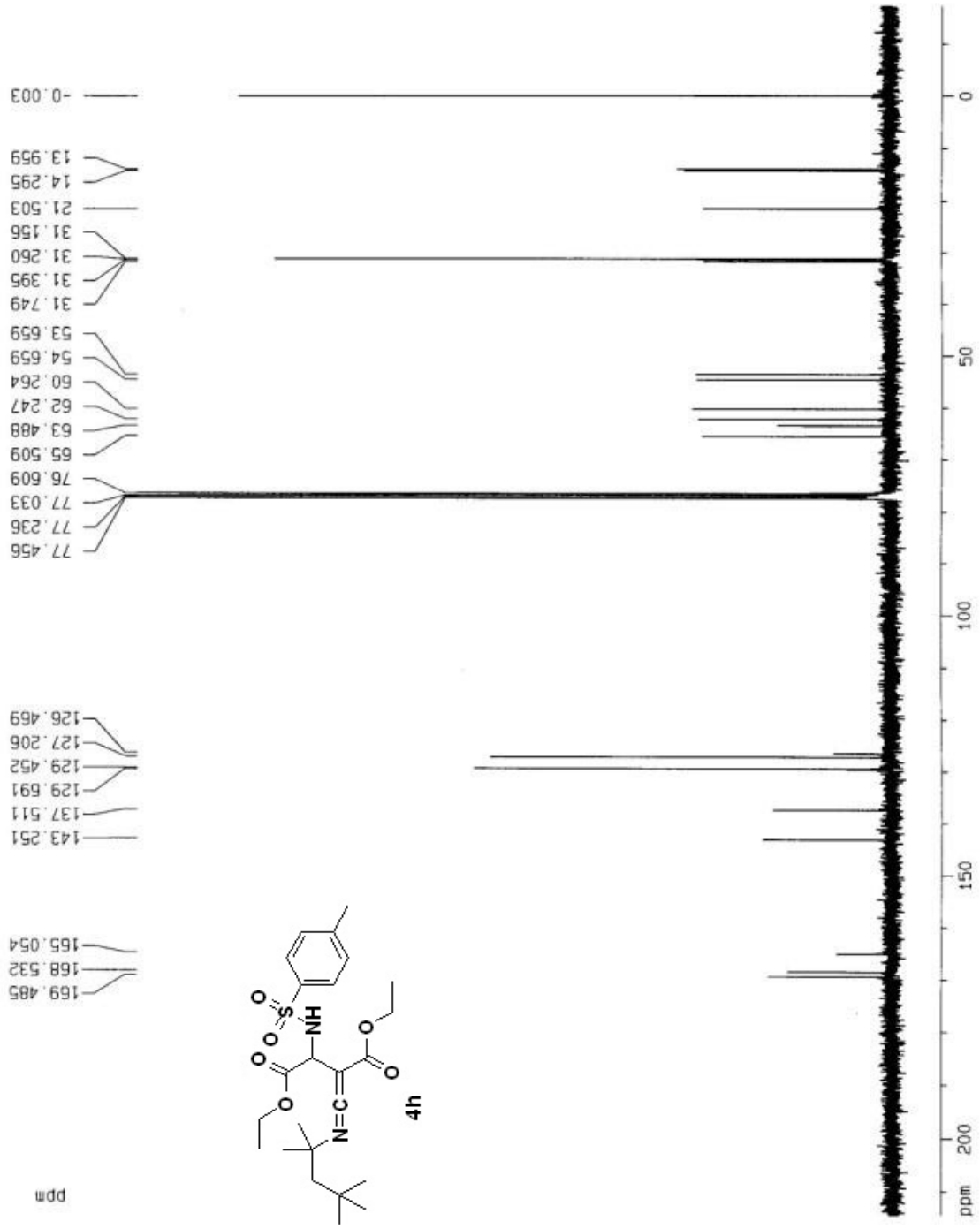
F2 - Acquisition Parameters
Date_ 20090504
Time 15.13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 32
DM 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 16.62 cm
F1P 10.843 ppm
F1 3254.36 Hz
F2P -1.032 ppm
F2 -309.58 Hz
PPMCM 0.59373 ppm/1
HZCM 178.19748 Hz/cm

¹³C {¹H} NMR



Current Data Parameters
NAME Sarvan
EXPNO 429
PROCNO 1

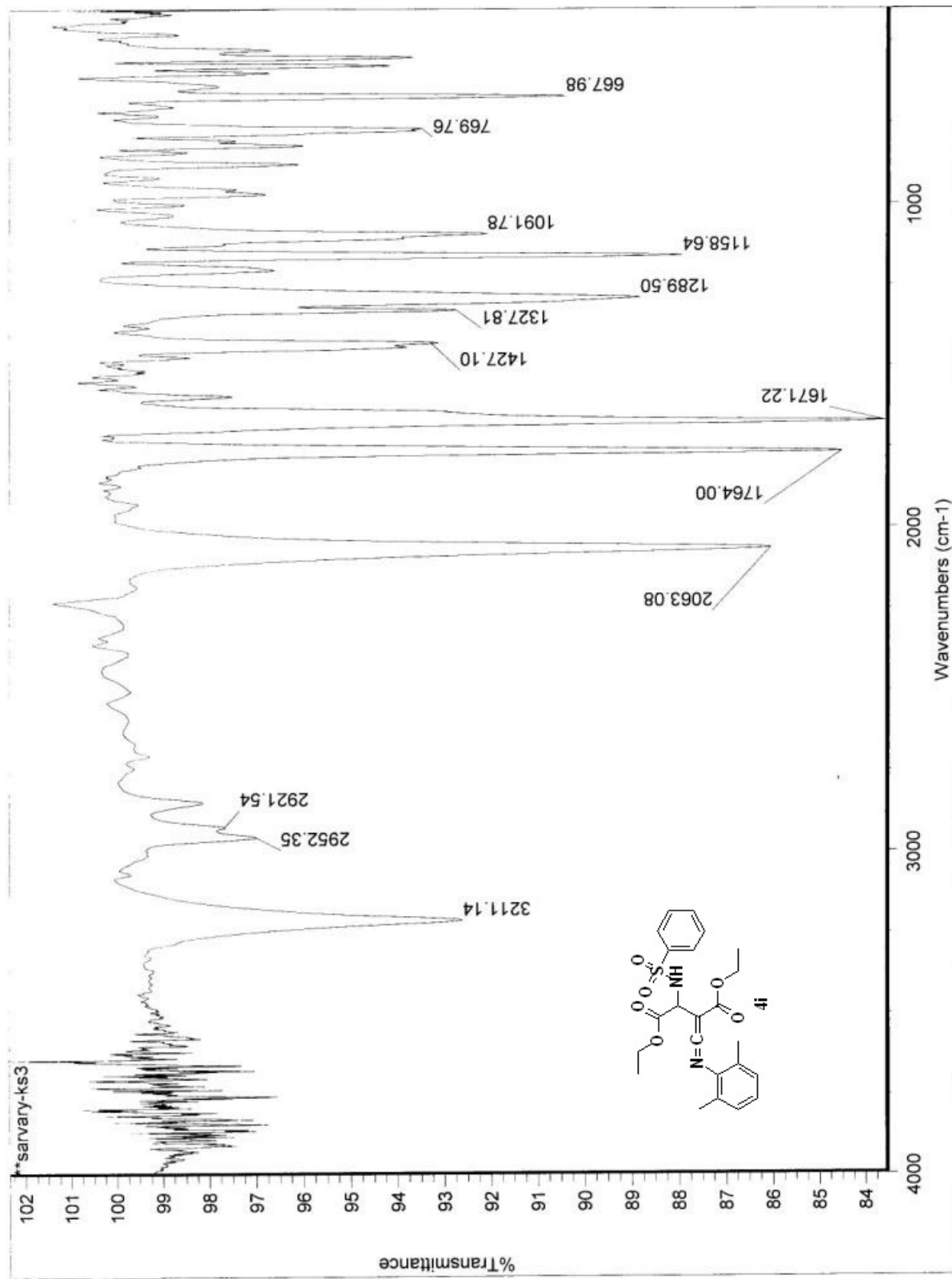
F2 - Acquisition Parameters
Date_ 20090504
Time 16.13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
d11 2.00000000 sec
d12 0.03000000 sec
d13 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SF01 75.4752553 MHz

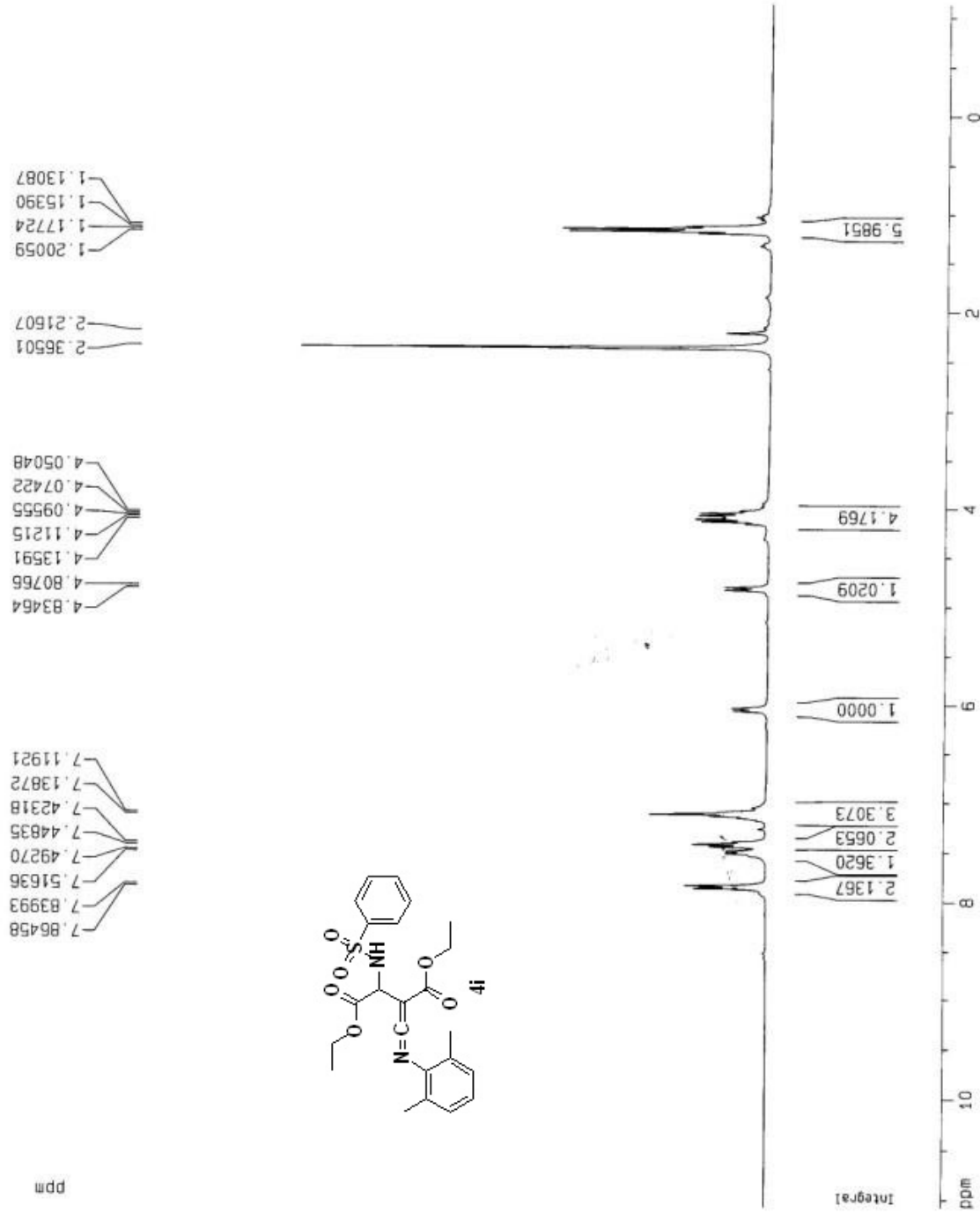
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EN
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 22.47 cm
FIP 214.548 ppm
F1 16191.44 Hz
F2 -17.325 ppm
F2 -1307.44 Hz
PPMCM 11.59382 ppm/cm
HZCM 874.94446 Hz/cm



¹H NMR



Current Data Parameters
NAME Rezaeiian-PHD
EXPNO 308
PROCNO 1

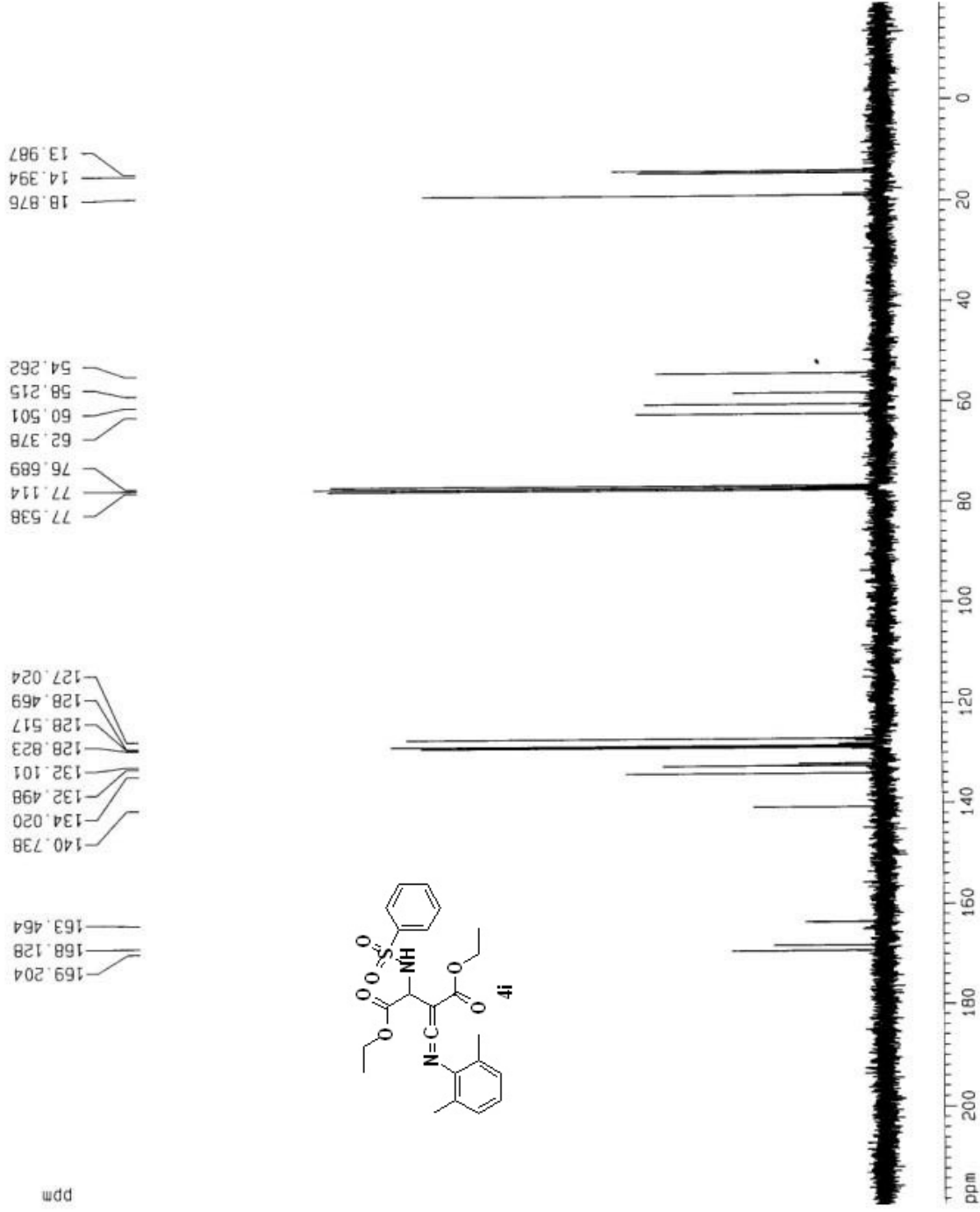
F2 - Acquisition Parameters
Date_ 20081022
Time 11.05
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DM 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 7.84 cm
F1P 11.078 ppm
F1 3324.79 Hz
F2P -1.132 ppm
F2 -339.83 Hz
PPHMM 0.61051 ppm/cm
HZDM 183.23134 Hz/cm

¹³C {¹H} NMR



Current Data Parameters
NAME Rezaeian-PHO
EXPNO 309
PROCNO 1

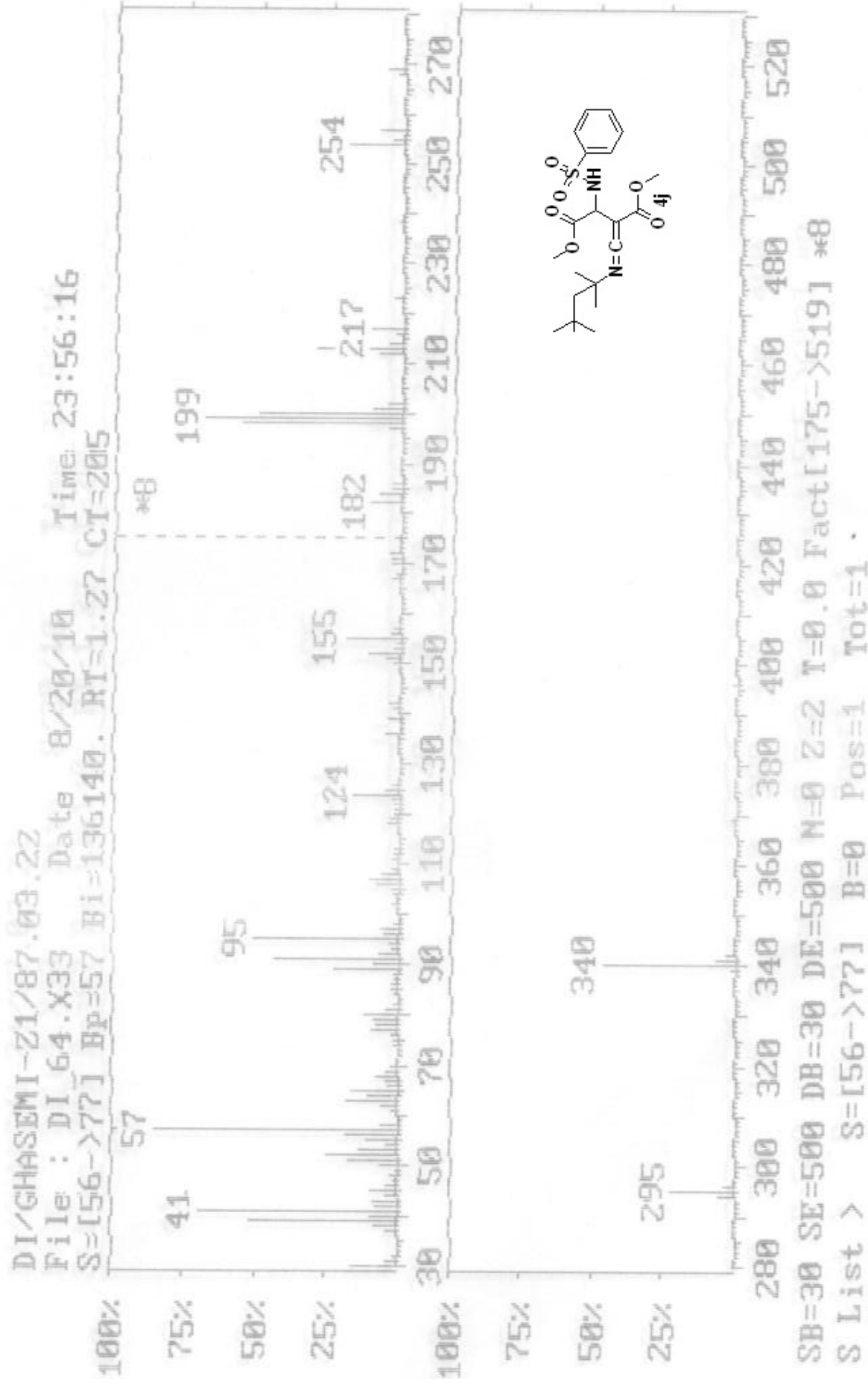
F2 - Acquisition Parameters
Date_ 20081022
Time 11.06
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 74
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

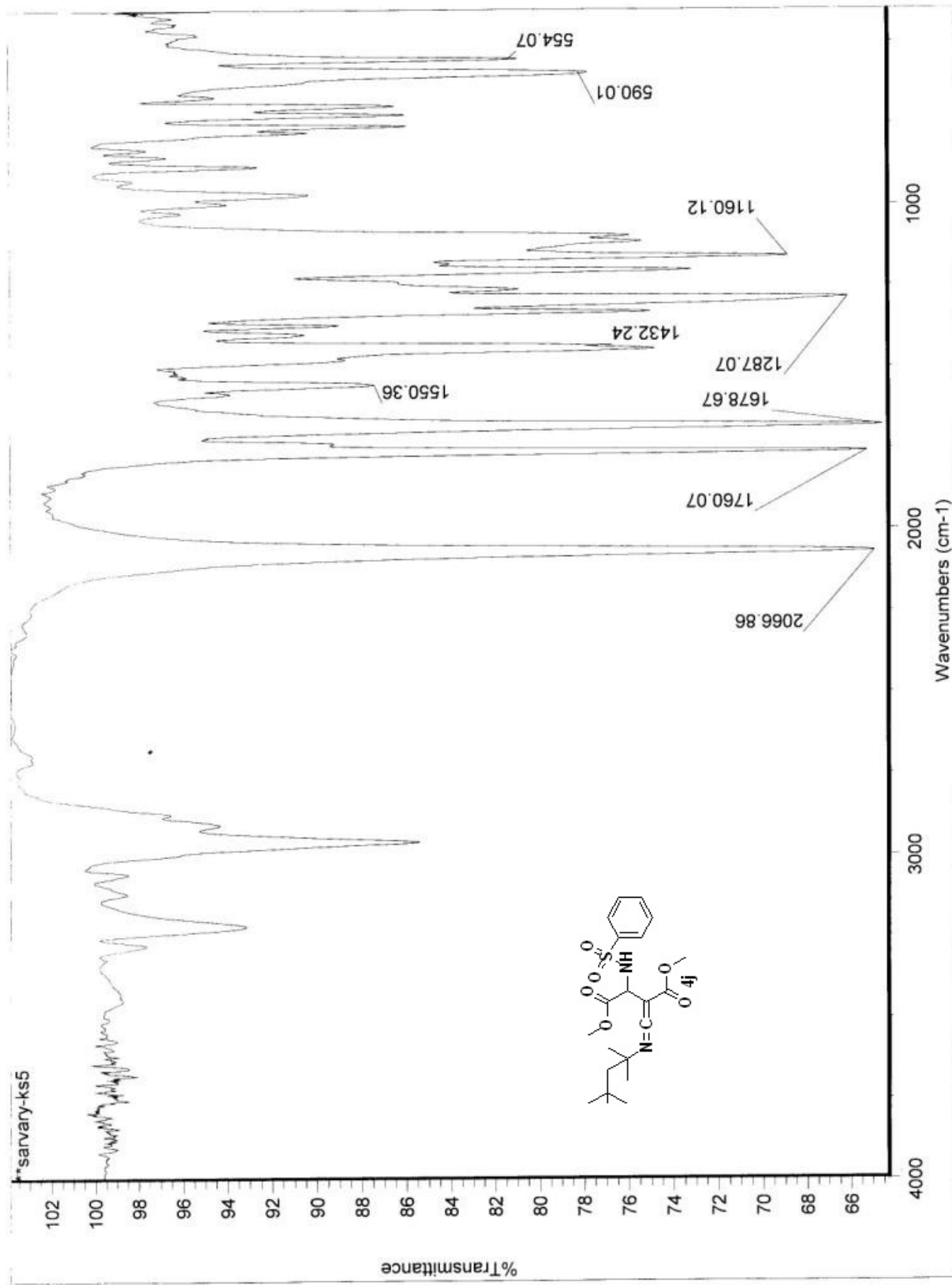
***** CHANNEL f1 *****
NUC1 ¹³C
P1 8.75 usec
PL1 -2.00 dB
SF01 75.4752953 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SF02 300.1312005 MHz

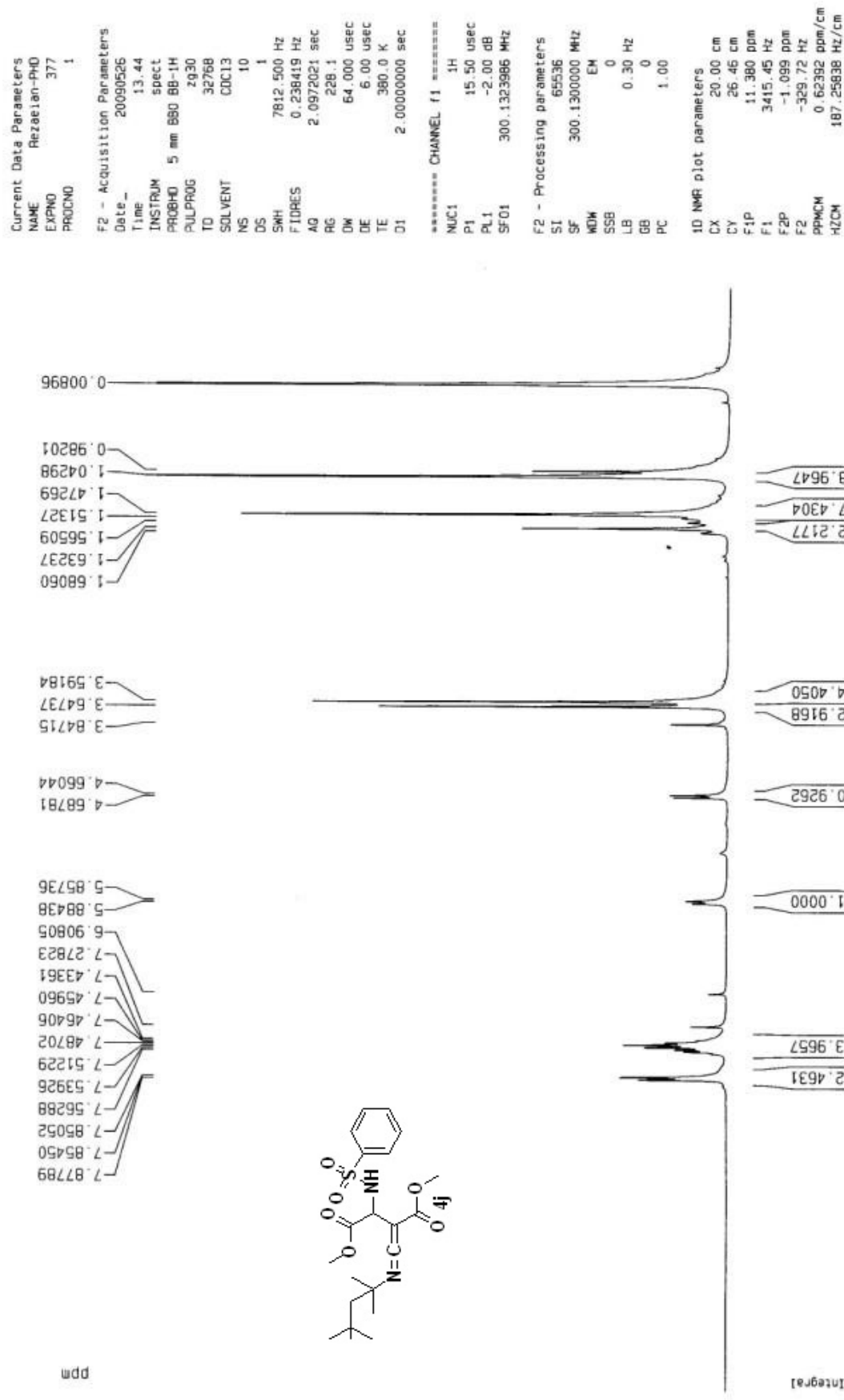
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 9.57 cm
F1P 219.155 ppm
F1 16539.10 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCM 11.91609 ppm/cm
HZCM 899.28058 Hz/cm



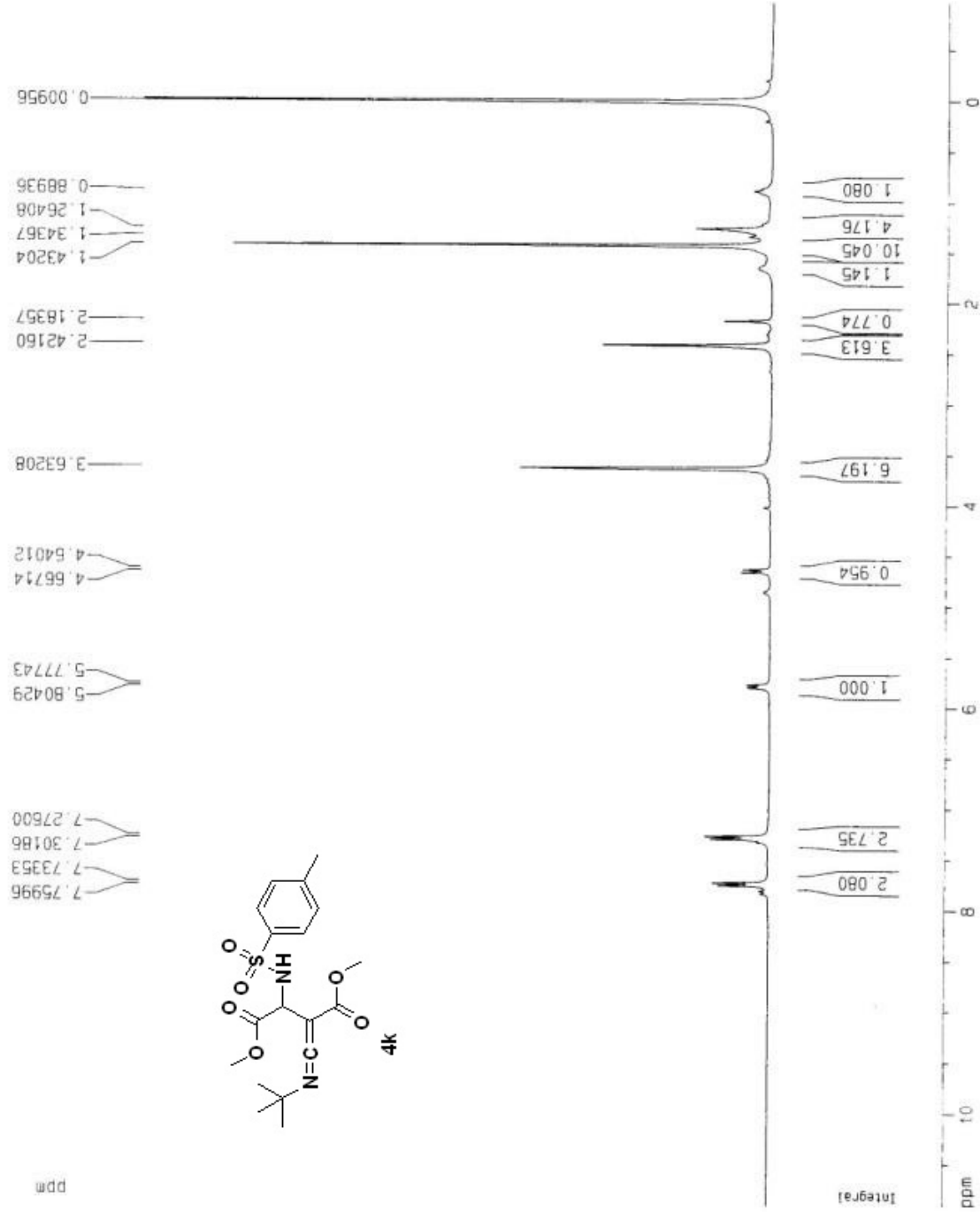


¹H NMR





¹H NMR



Current Data Parameters
NAME Ghasemi
EXPNO 12
PROCNO 1

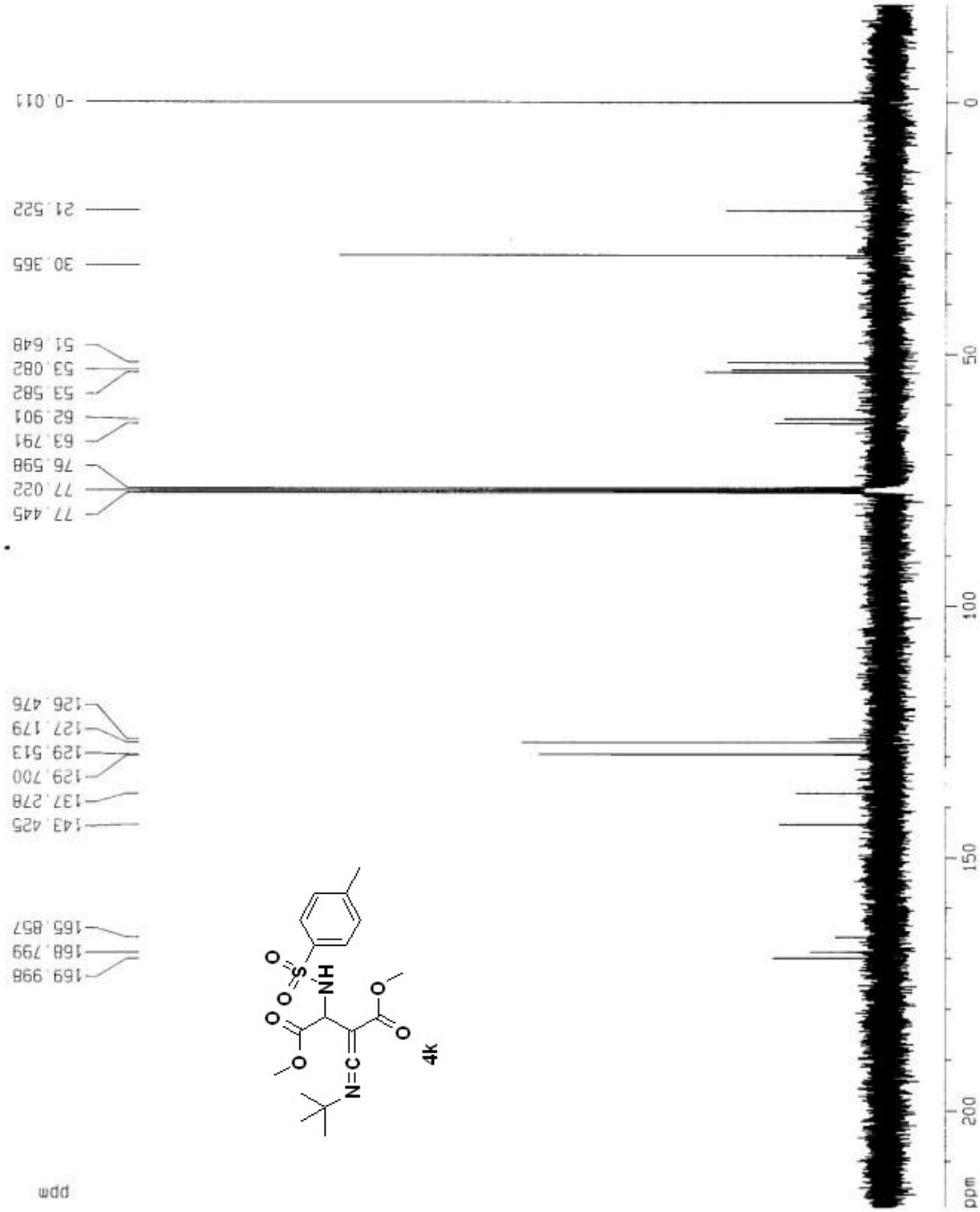
F2 - Acquisition Parameters
Date_ 20080421
Time 13.32
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 ¹H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 16.79 cm
F1P 10.910 ppm
F1 3274.50 Hz
F2P -0.964 ppm
F2 -289.45 Hz
PPMCM 0.59373 ppm/cm
HZCM 178.19748 Hz/cm

¹³C {¹H} NMR



Current Data Parameters
NAME Gnasem1
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080421
Time 13.39
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 580
DS 1
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec

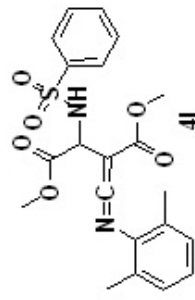
===== CHANNEL f1 =====
NUC1 ¹³C
P1 8.75 usec
PL1 -2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPOPRG2 waltz16
NUC2 ¹H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
S1 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40

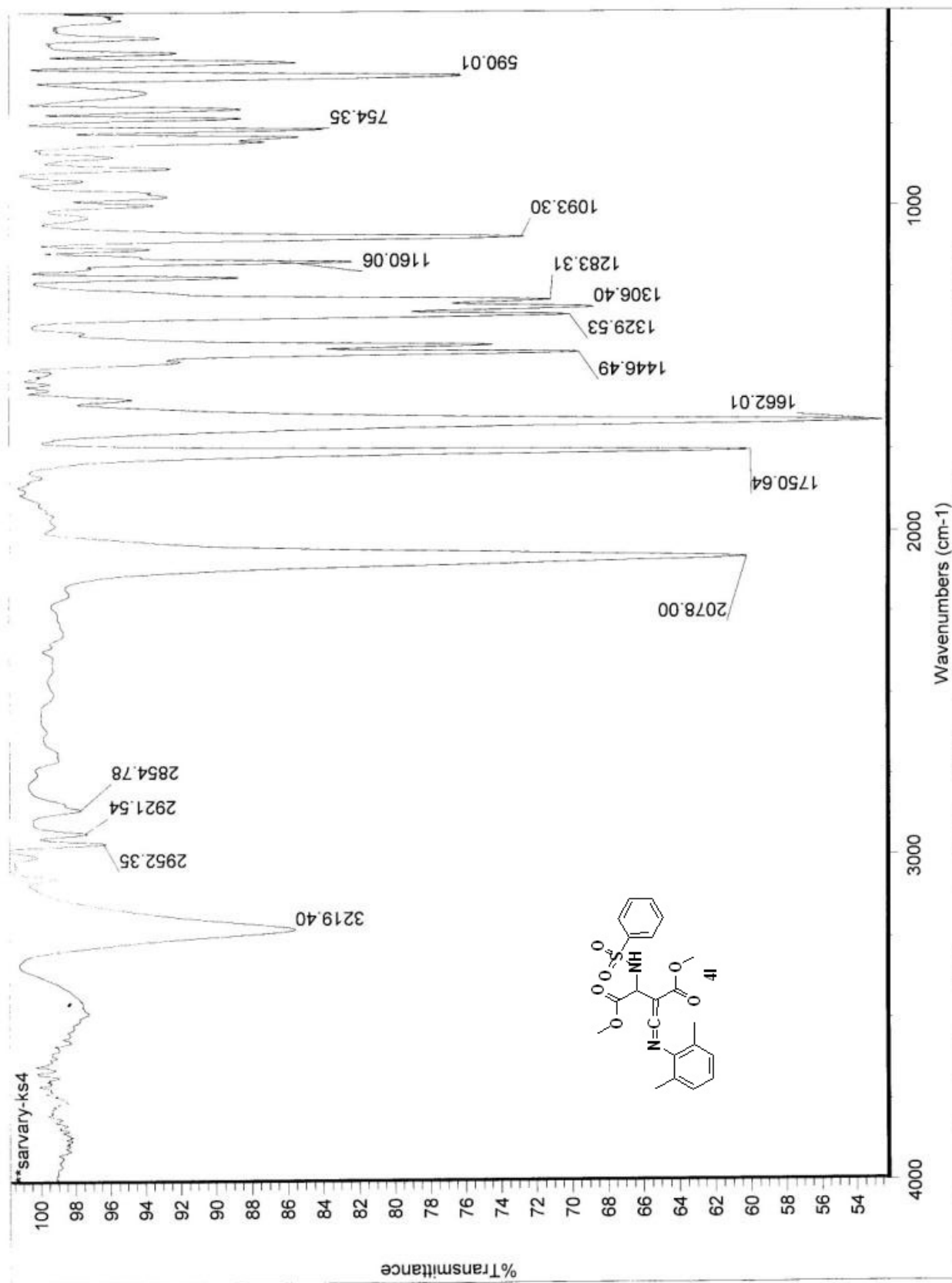
1D NMR plot parameters
CX 20.00 cm
CY 26.34 cm
FIP 219.155 ppm
F1 16539.10 Hz
F2 -19.167 ppm
PPMCM 11.91609 ppm/cm
HZCM 899.28058 Hz/cm

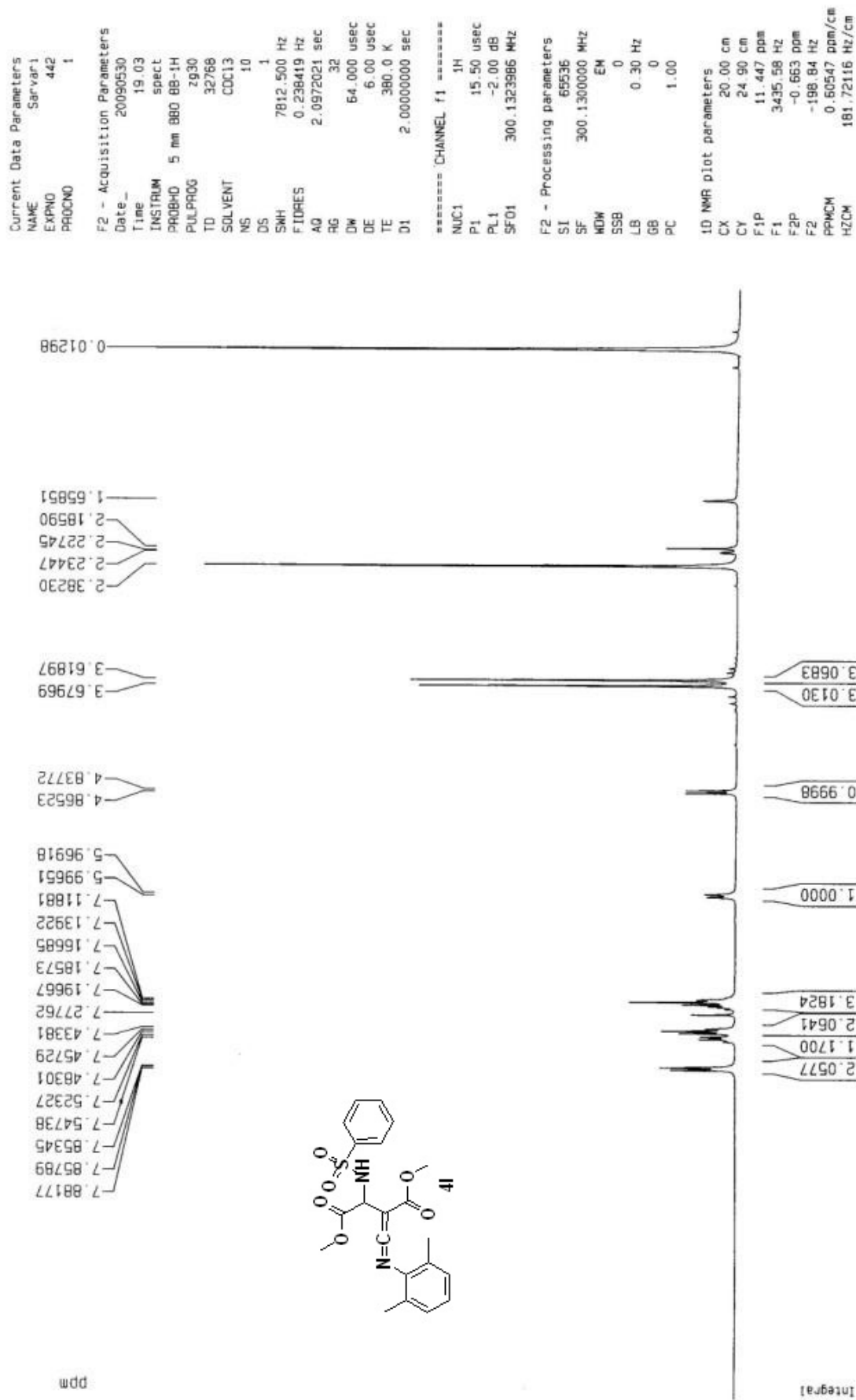
DI/SARVARI-BBB 13/89.01.28
File : DI_81.X39 Date 9/ 6/10 Time 11: 8:33
S=[58->67] Bp=77 Bi=385200. RT=1.11 CT=189



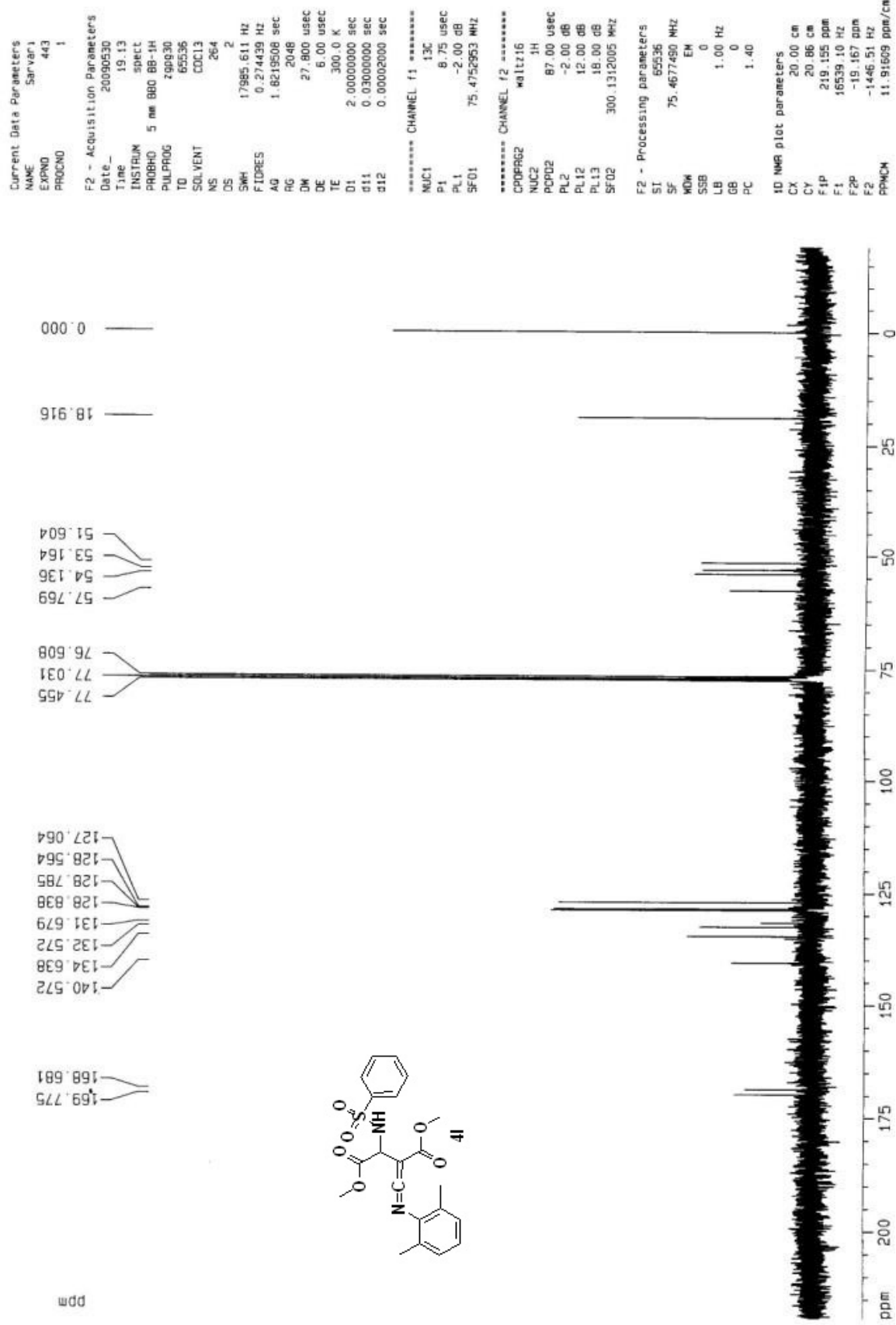
SB=30 SE=520 DB=30 DE=520 N=0 Z=2 T=0.0 Fact[184->526] *8

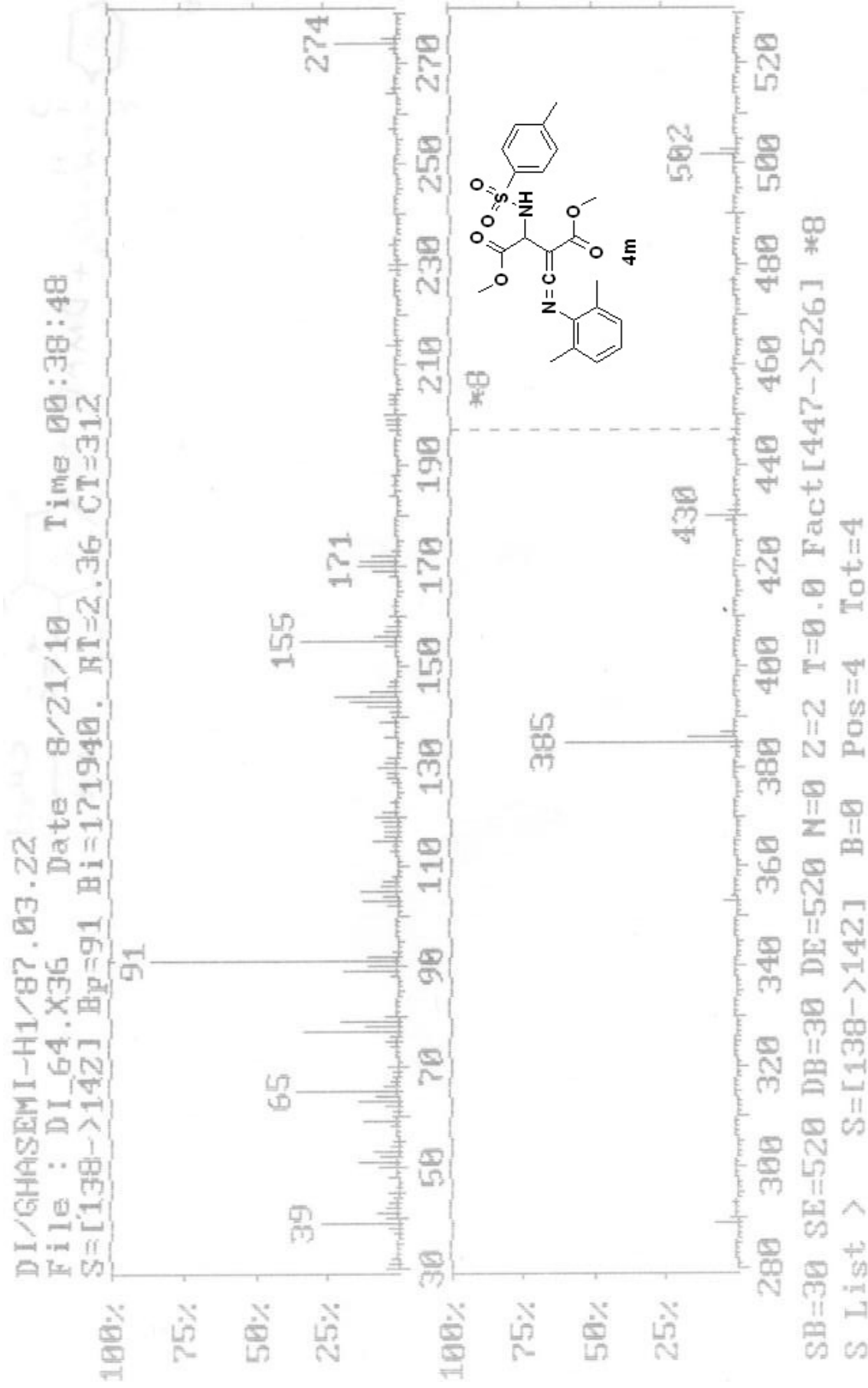
S List > S=[58->67] B=0 Pos=3 Tot=3

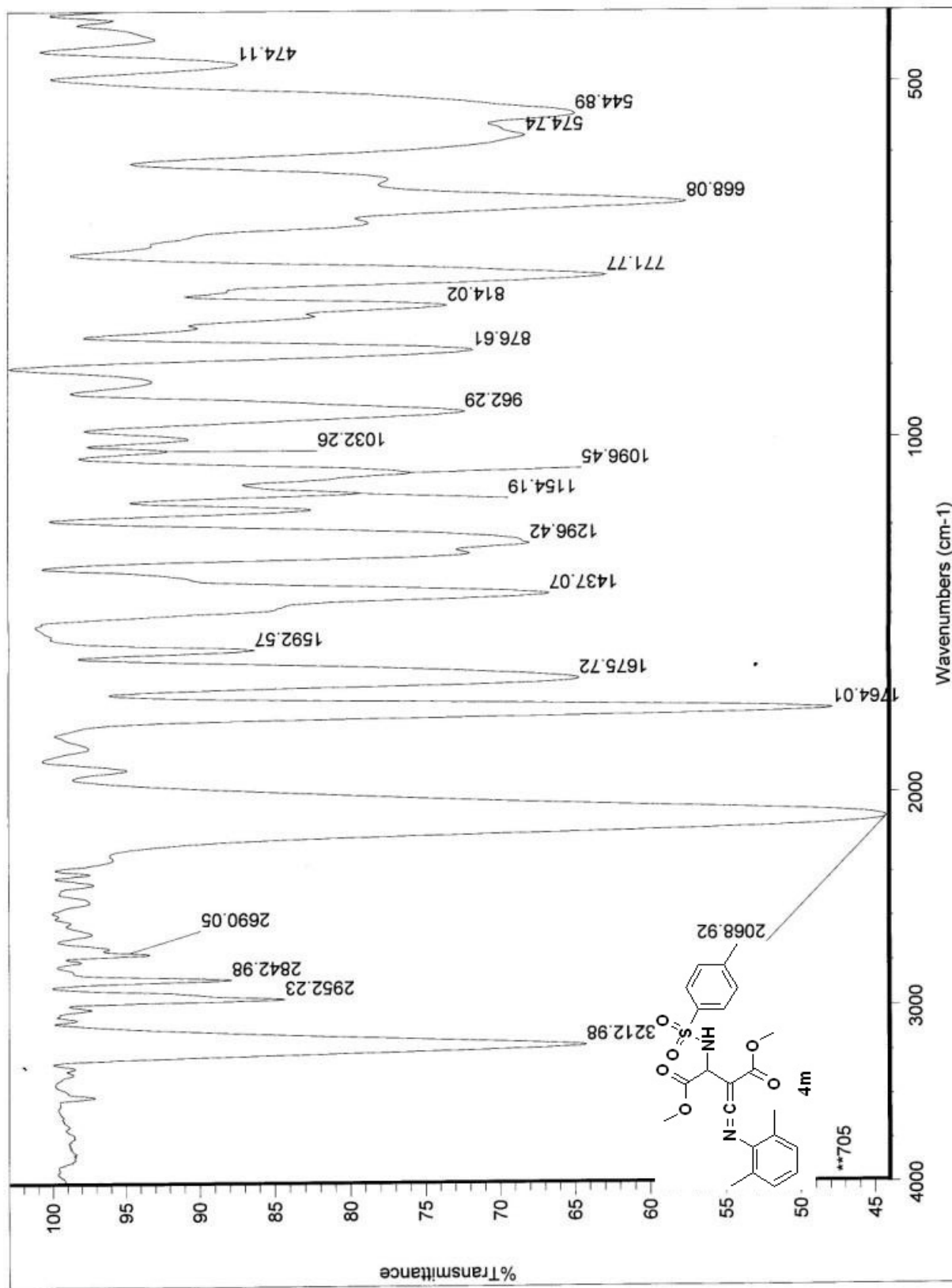




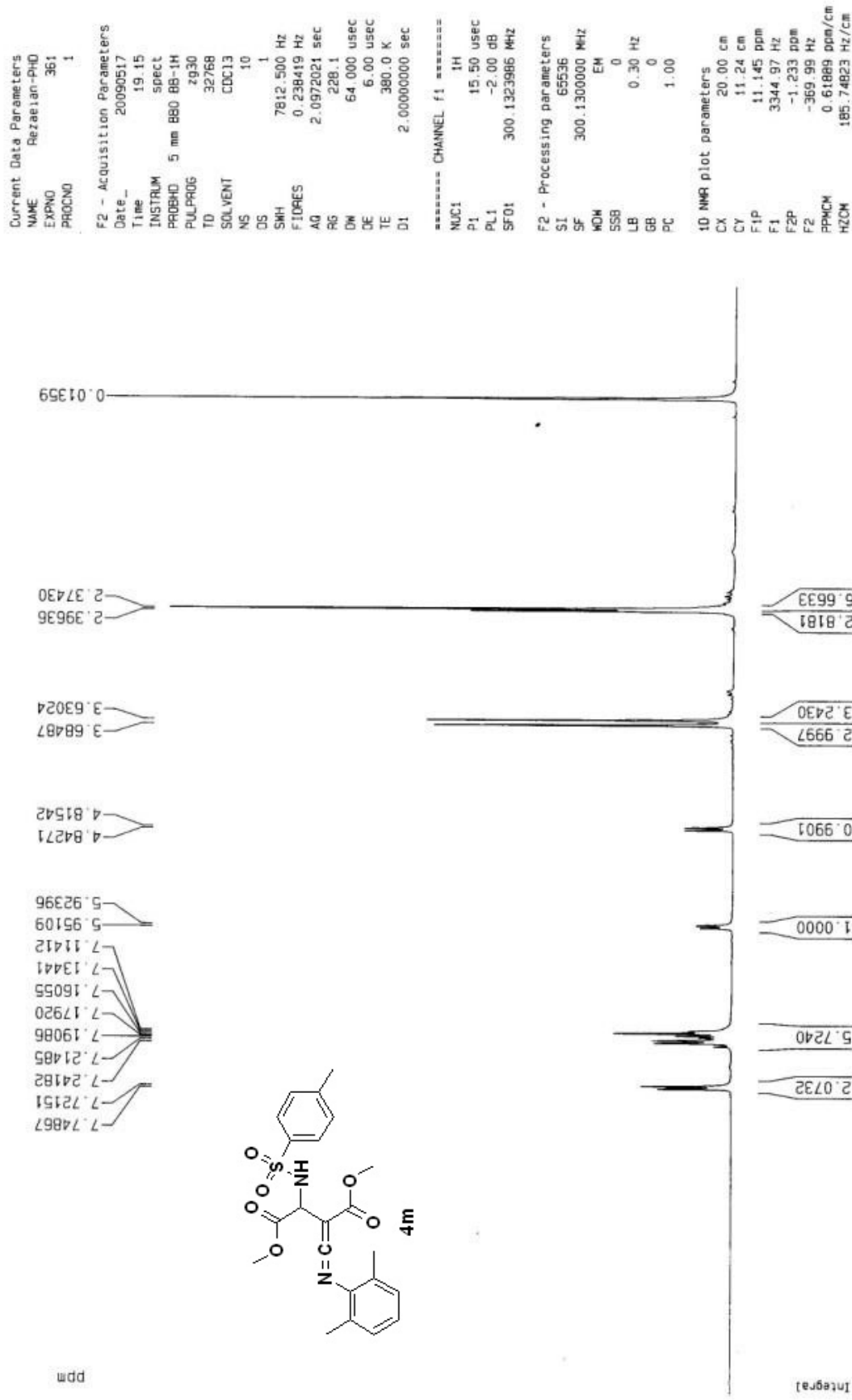
¹³C {¹H} NMR



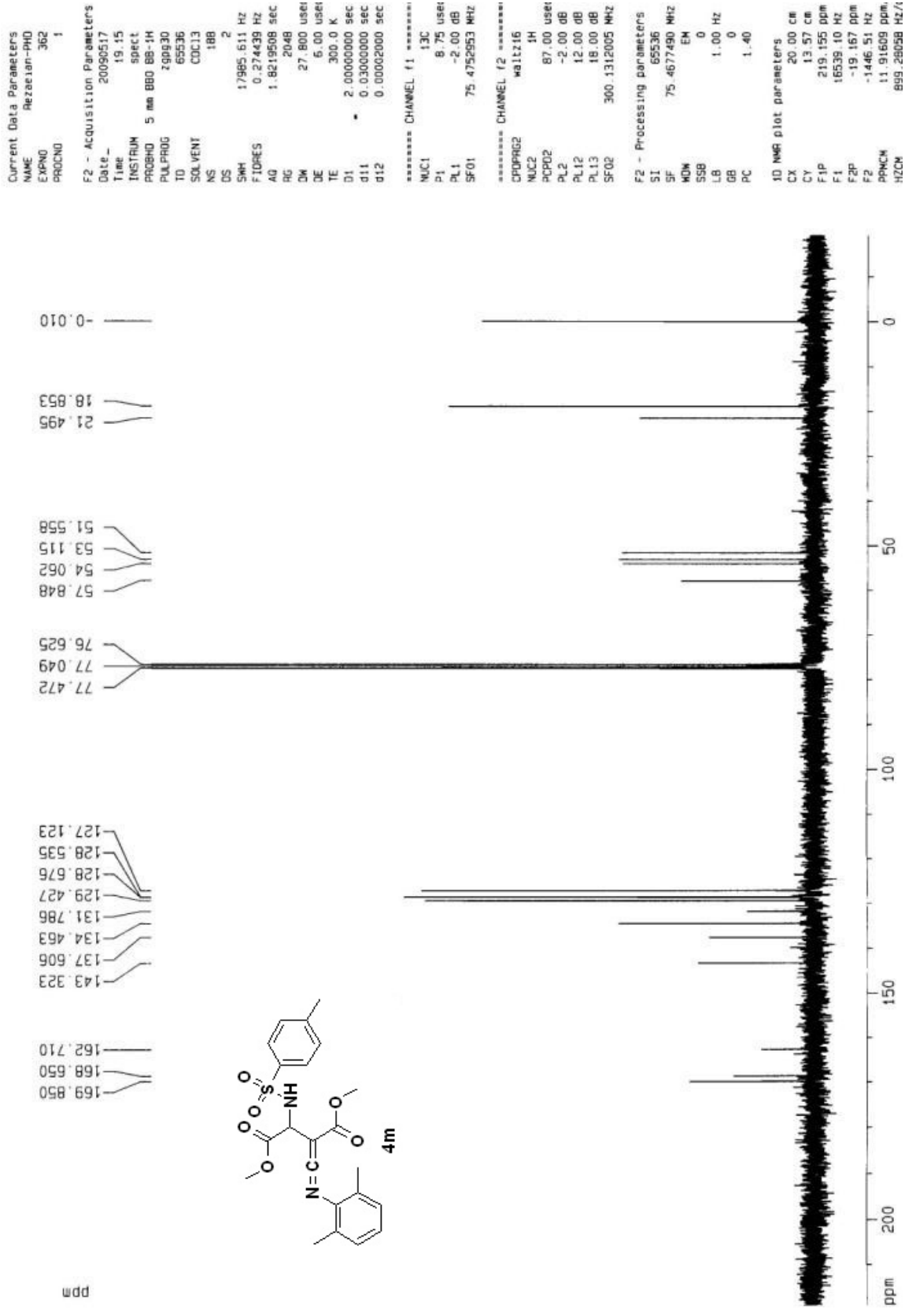




¹H NMR



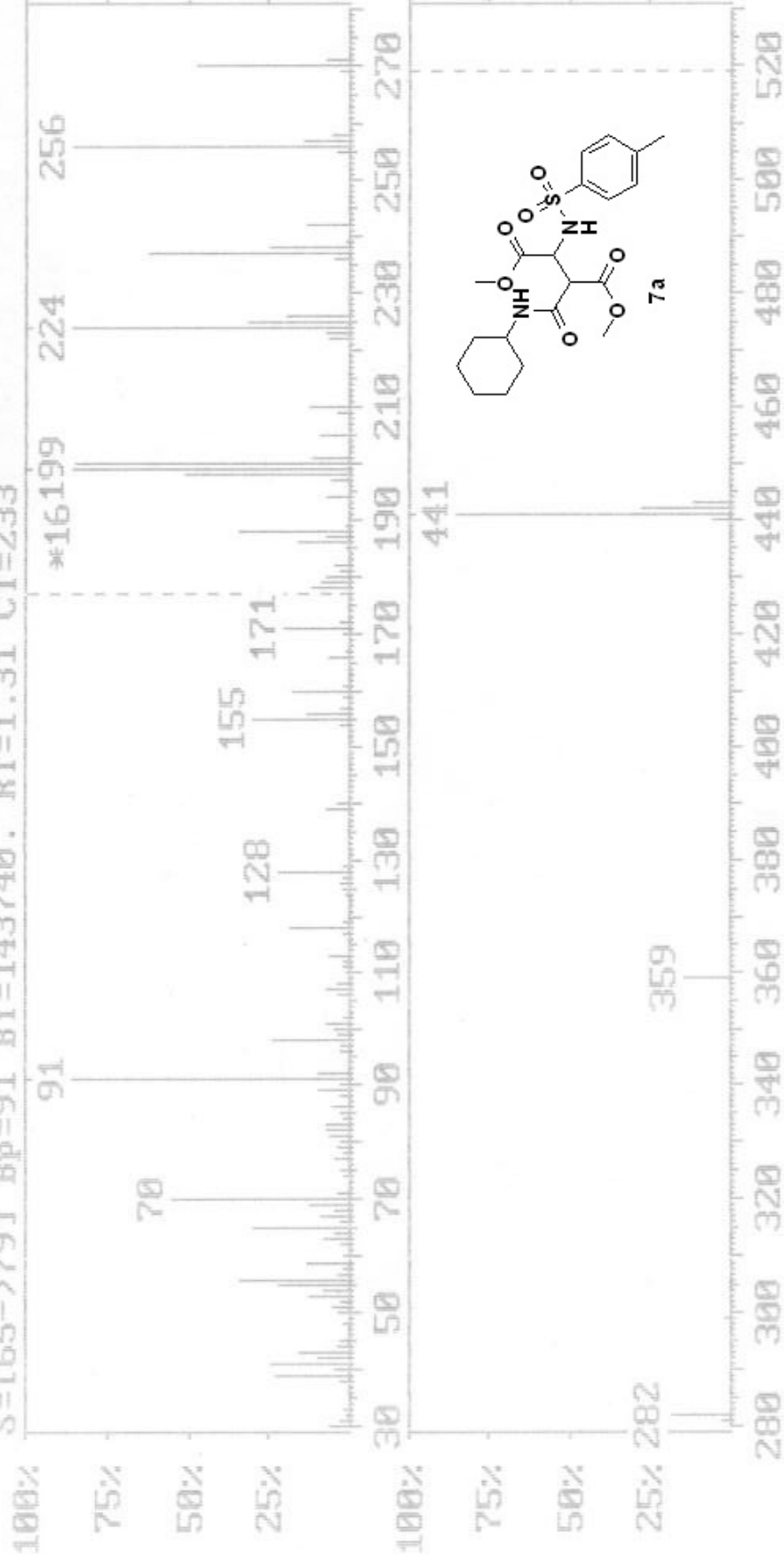
¹³C {¹H} NMR



DI/GHASEMI-B2h/88.04.13

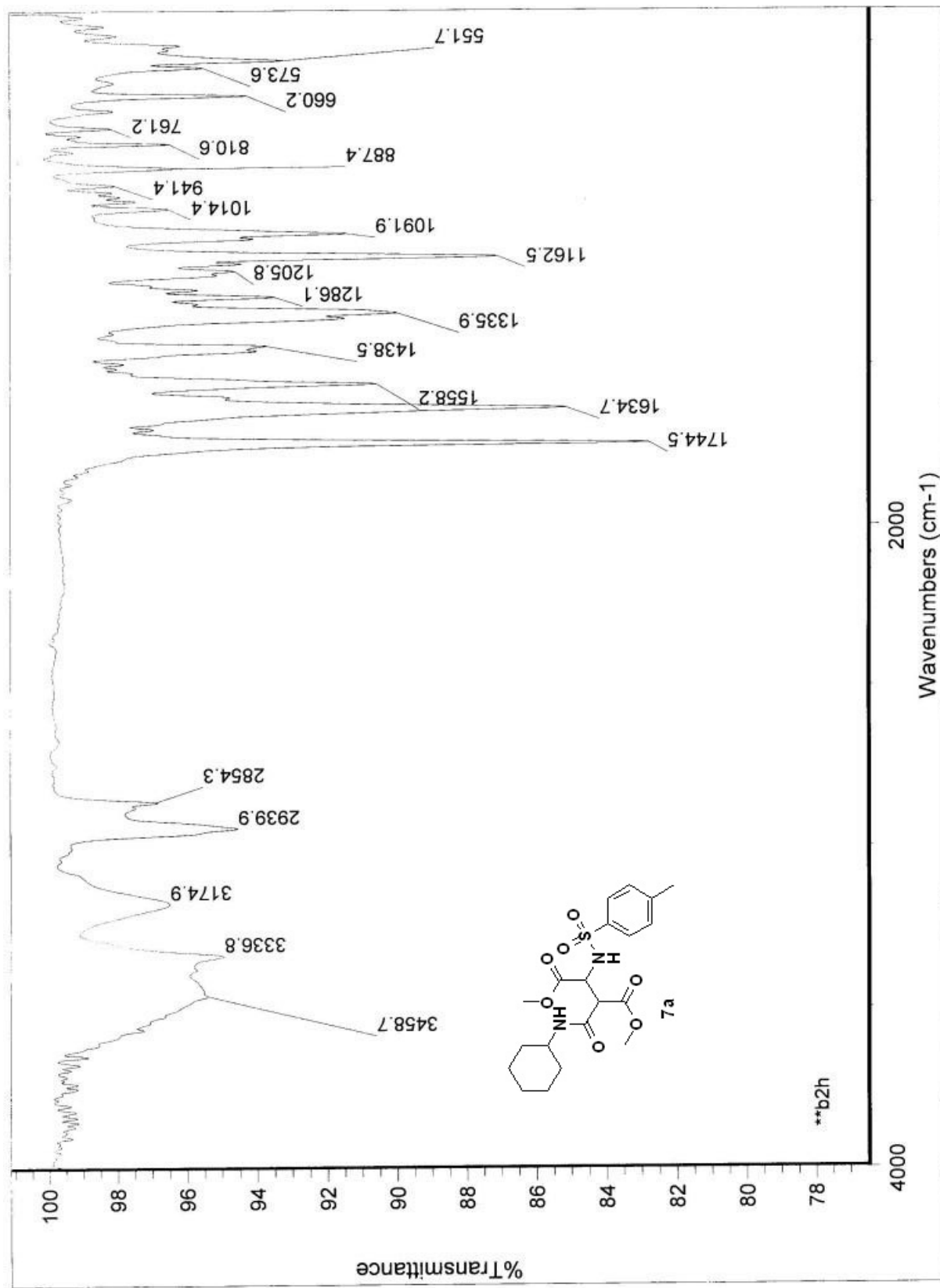
File : DI_71.X77 Date 8/30/10 Time 22:17:55

S=[65->79] Bp=91 Bi=143740. RT=1.31 CT=233

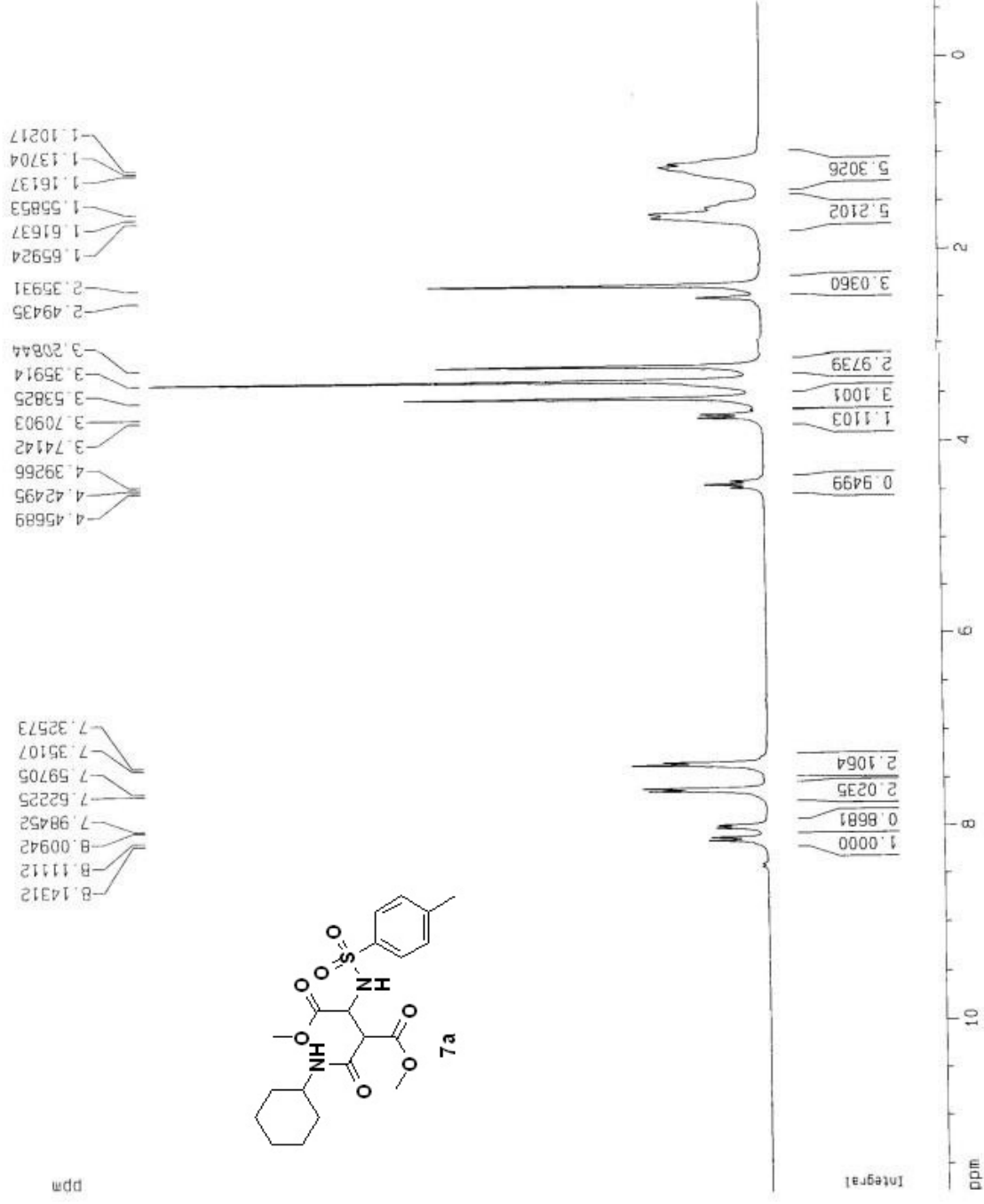


SB=30 SE=520 DB=30 DE=520 N=0 Z=2 T=0.0 Fact[177->519] *16

S List > S=[65->79] B=0 Pos=1 Tot=1



¹H NMR



Current Data Parameters
NAME Sarvari
EXPNO 561
PROCNO 1

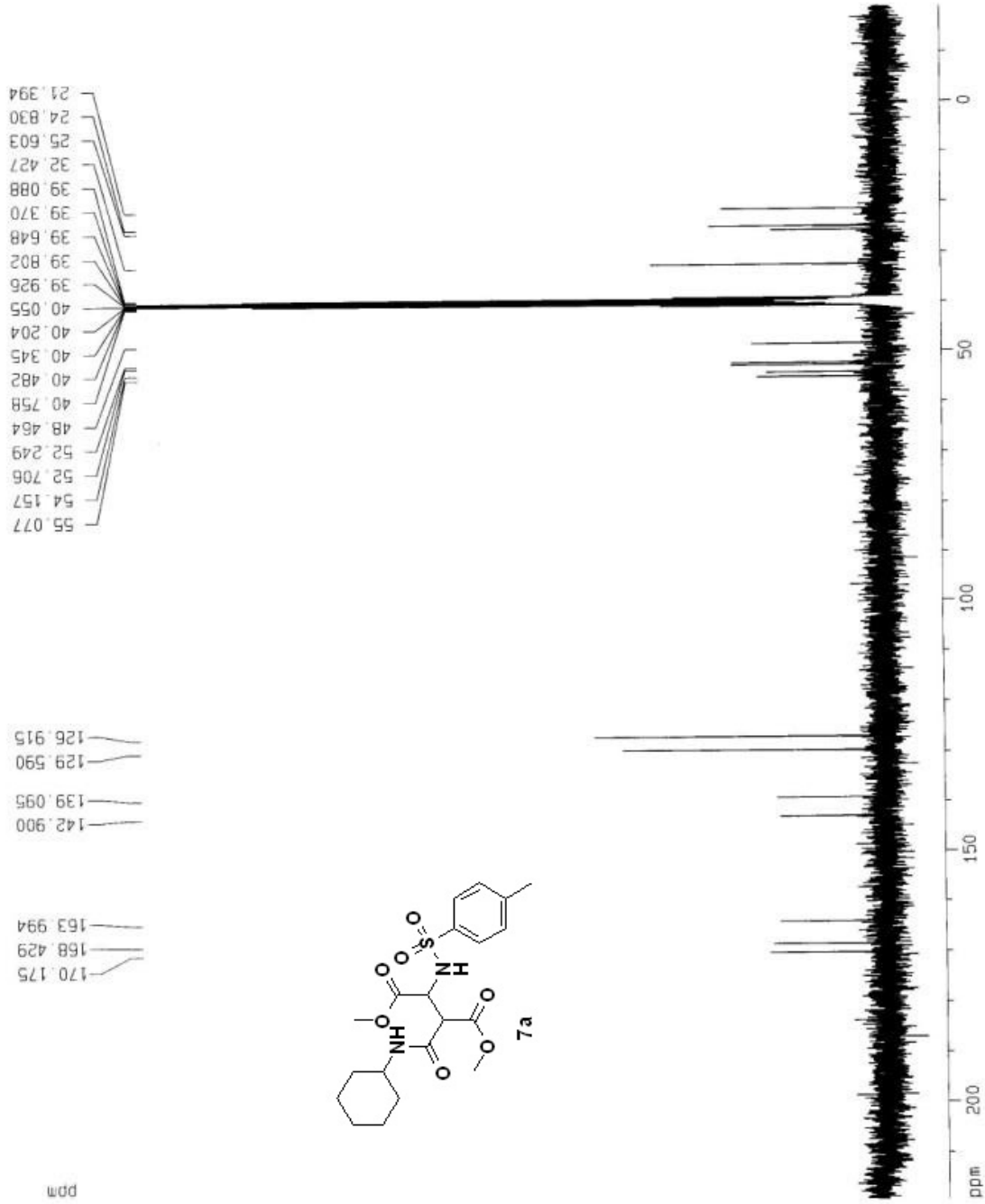
F2 - Acquisition Parameters
Date_ 20100111
Time 2.10
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.230419 Hz
AQ 2.0972021 sec
RG 286.1
DM 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.132986 MHz

F2 - Processing parameters
SI 65536
SF 300.130000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.34 cm
F1P 11.782 ppm
F1 3536.15 Hz
F2P -0.590 ppm
F2 -176.94 Hz
PPM0 0.61858 ppm/cm
HZ0 185.65417 Hz/cm

¹³C {¹H} NMR



Current Data Parameters
NAME: Server: 562
EXPNO: 1
PROCNO: 1

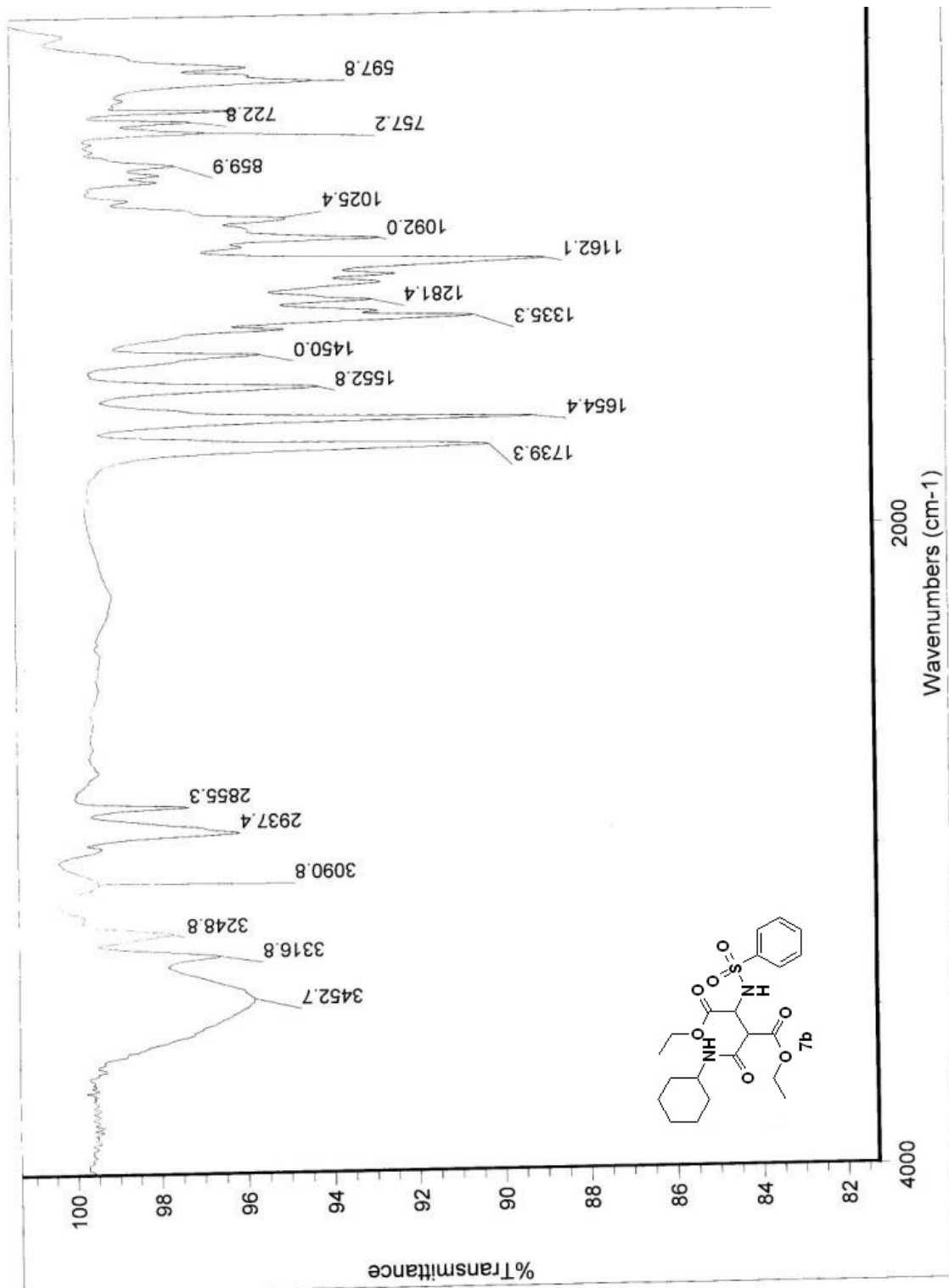
F2 - Acquisition Parameters
Date_: 20100111
Time: 2.12
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 144
DS: 2
SWH: 17985.611 Hz
FIDRES: 0.274439 Hz
AQ: 1.8219508 sec
RG: 2048
DM: 27.800 usec
DE: 6.00 usec
TE: 300.0 K
D1: 2.0000000 sec
d11: 0.0300000 sec
d12: 0.00002000 sec

***** CHANNEL f1 *****
NUC1: 13C
P1: 8.75 usec
PL1: -2.00 dB
SF01: 75.4752953 MHz

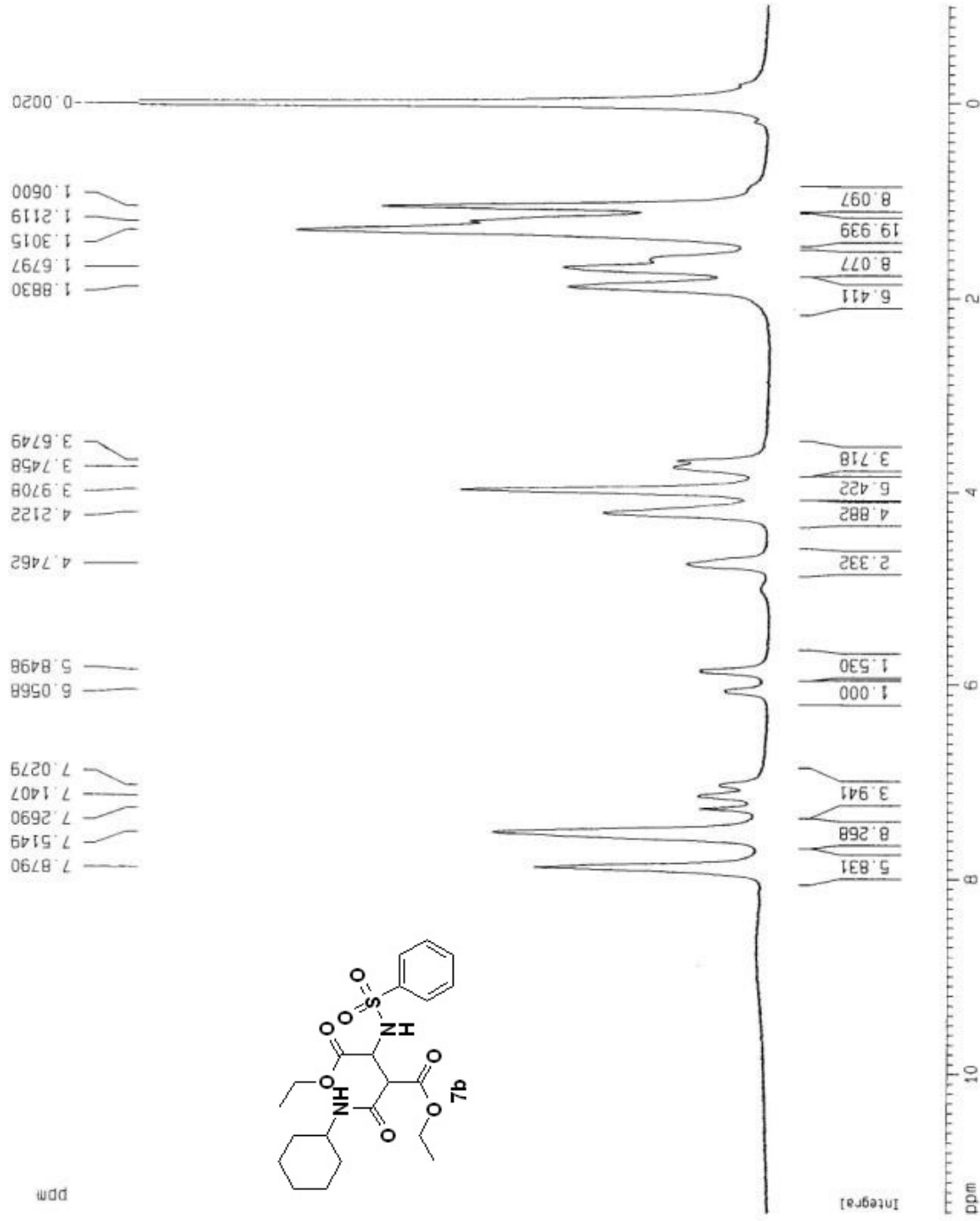
***** CHANNEL f2 *****
CPOPRG2: waltz16
NUC2: 1H
PCPD2: 87.00 usec
PL2: -2.00 dB
PL12: 12.00 dB
PL13: 18.00 dB
SF02: 300.1312005 MHz

F2 - Processing parameters
S1: 65536
SF: 75.4677490 MHz
KGM: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 0.10

1D NMR plot parameters
CX: 20.00 cm
CY: 24.75 cm
F1P: 219.155 ppm
F1: 16539.11 Hz
F2P: -19.167 ppm
F2: -1446.51 Hz
PPHOM: 11.91609 ppm/cm
HZOM: 899.28058 Hz/cm



¹H NMR



Current Data Parameters
NAME Sarvar1
EXPNO 448
PROCNO 1

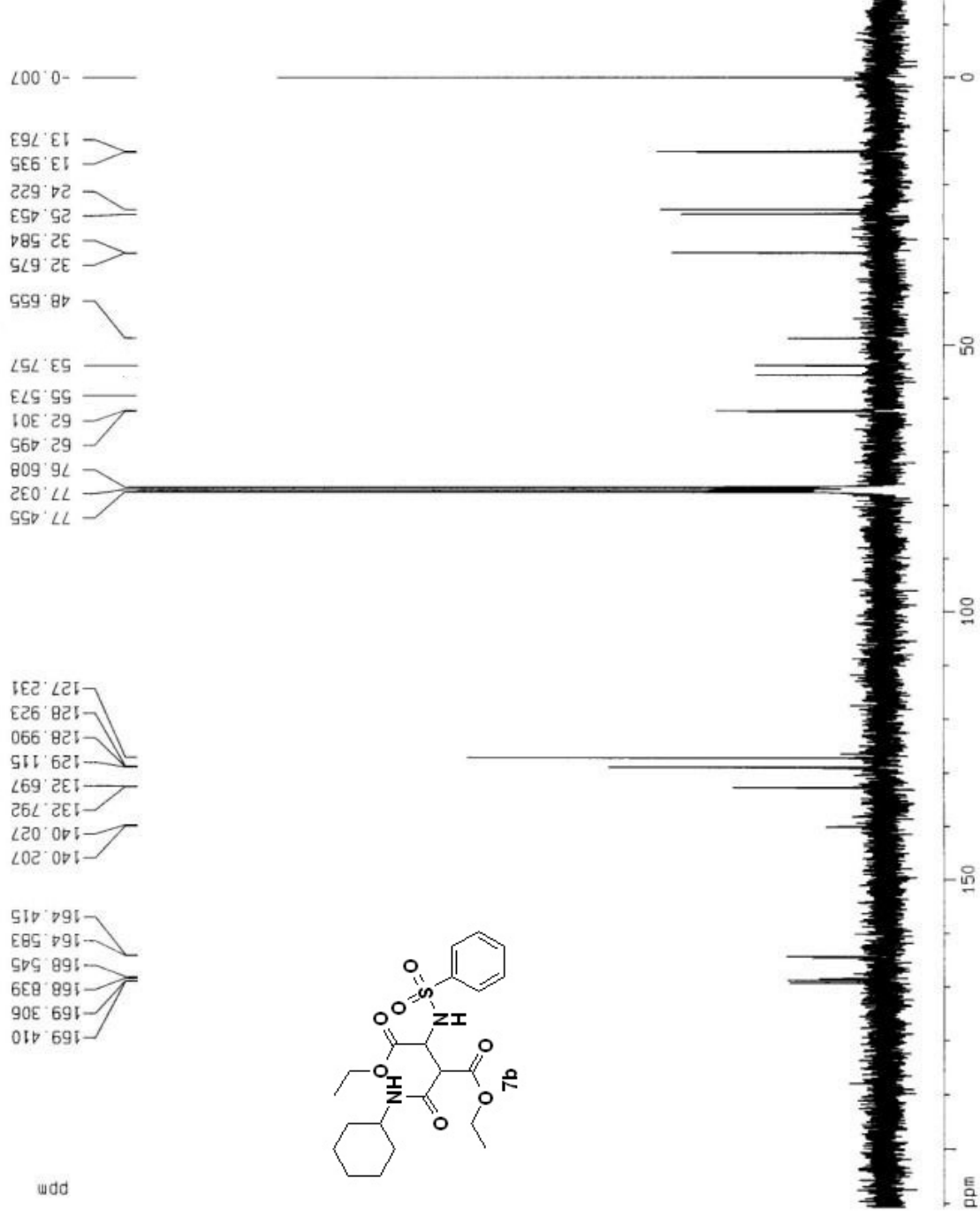
F2 - Acquisition Parameters
Date_ 20090621
Time 20.43
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 32
DM 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

***** CHANNEL f1 *****
NUC1 ¹H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 28.55 cm
FIP 11.415 ppm
F1 3426.04 Hz
F2 -1.024 ppm
F2 -307.28 Hz
PPMCM 0.62195 ppm/cm
HZCM 186.66586 Hz/cm

¹³C {¹H} NMR



Current Data Parameters
NAME: Savv1
EXPNO: 449
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20090621
Time: 20.45
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 1024
DS: 2
SMH: 17985.611 Hz
FIDRES: 0.274439 Hz
AQ: 1.8219508 sec
RG: 2048
DM: 27.800 usec
DE: 6.00 usec
TE: 300.0 K
d1: 2.0000000 sec
d11: 0.0300000 sec
d12: 0.0000200 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 8.75 usec
PL1: -2.00 dB
SF01: 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 87.00 usec
PL2: -2.00 dB
PL12: 12.00 dB
PL13: 18.00 dB
SF02: 300.1312005 MHz

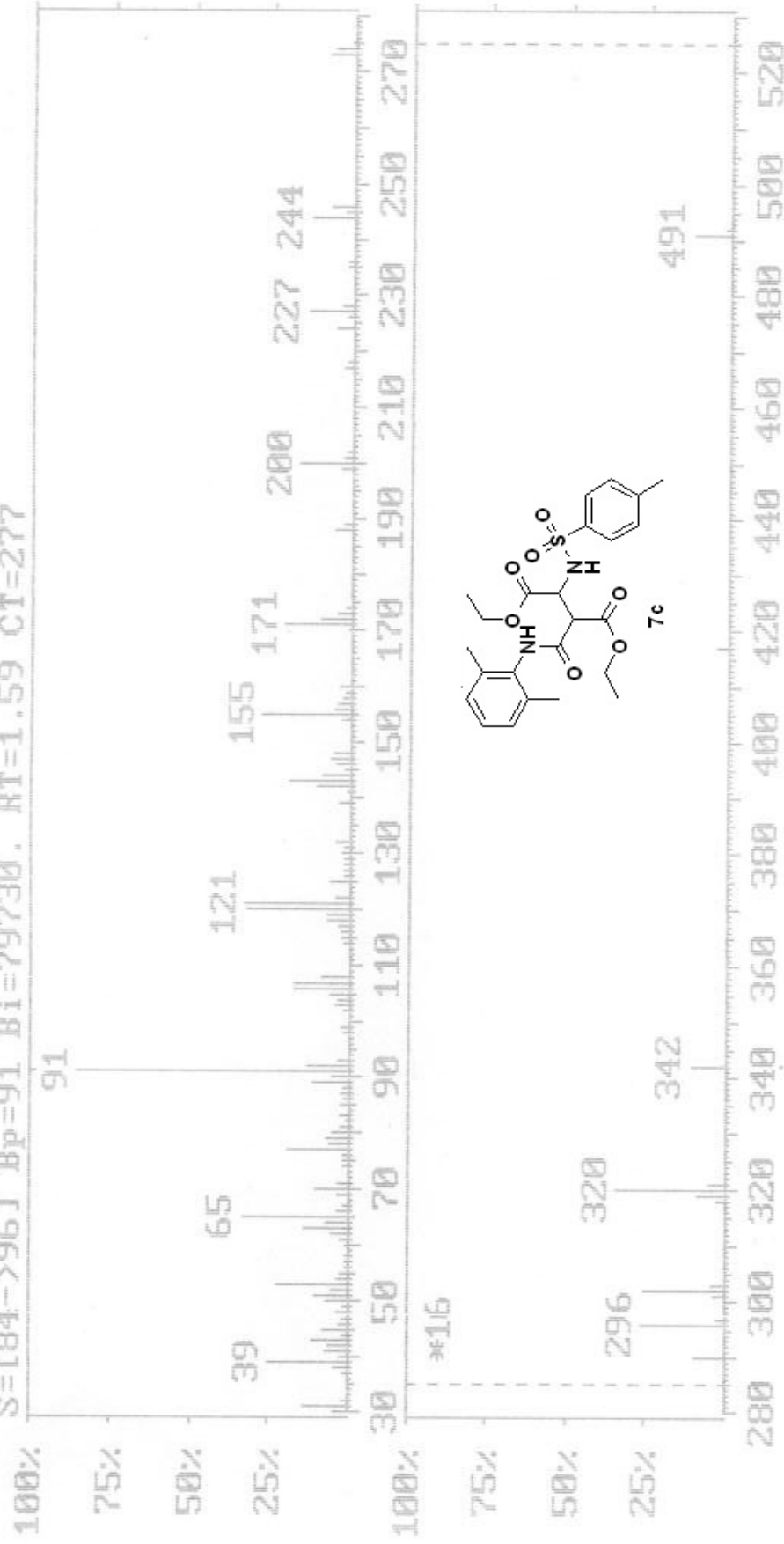
F2 - Processing parameters
SI: 65536
SF: 75.4677480 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

1D NMR plot parameters
CX: 20.00 cm
CY: 36.11 cm
F1P: 210.776 ppm
F1: 15906.80 Hz
F2P: -14.823 ppm
F2: -1118.64 Hz
PRNCH: 11.27994 ppm/cm
HZCN: 851.27203 Hz/cm

DI/GHASEMI-B111h/88.04.13

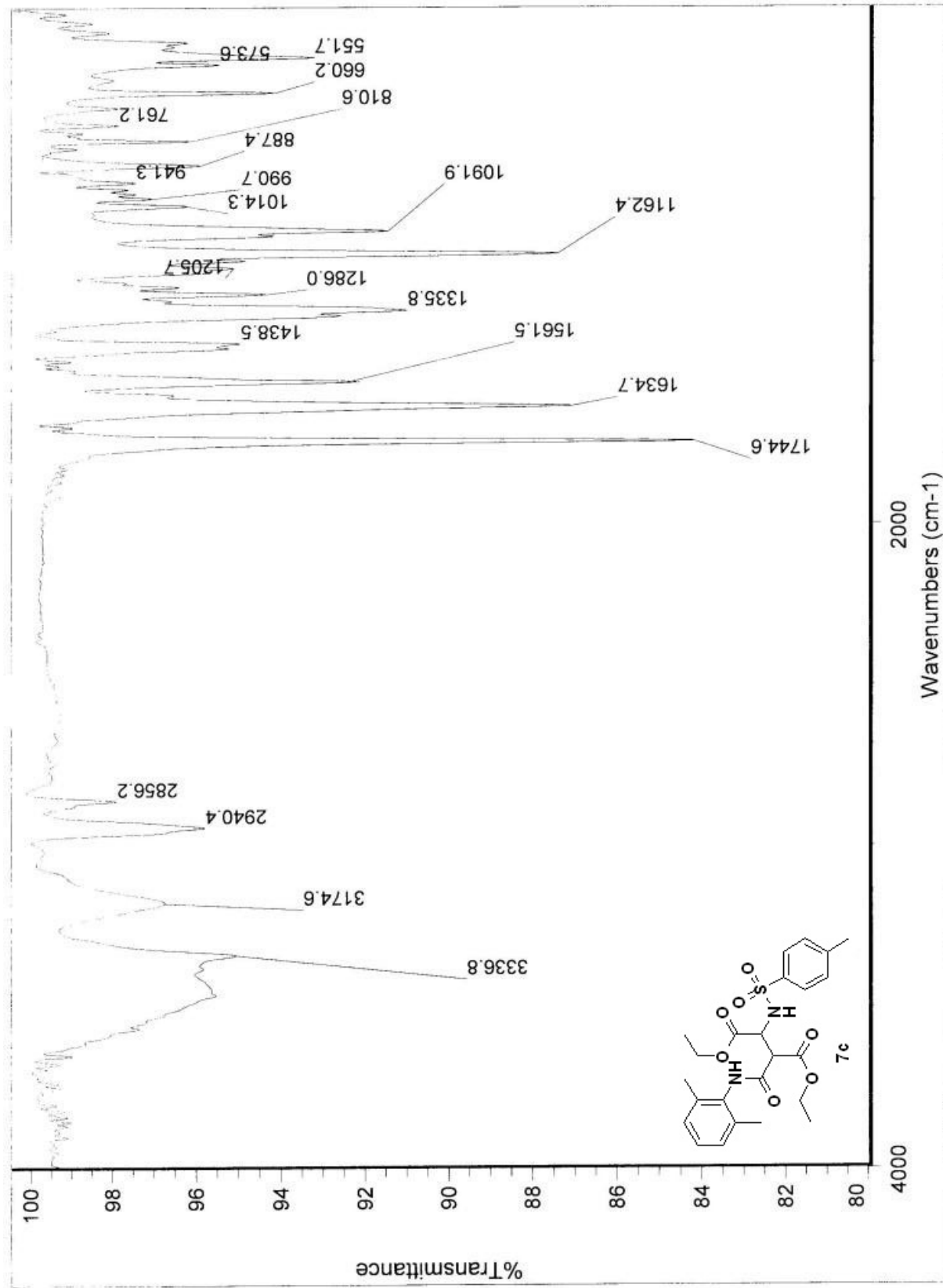
File : DI_71.X78 Date 8/30/10 Time 22:24:47

S=[84->96] Bp=91 Bi=79730. RT=1.59 CT=277

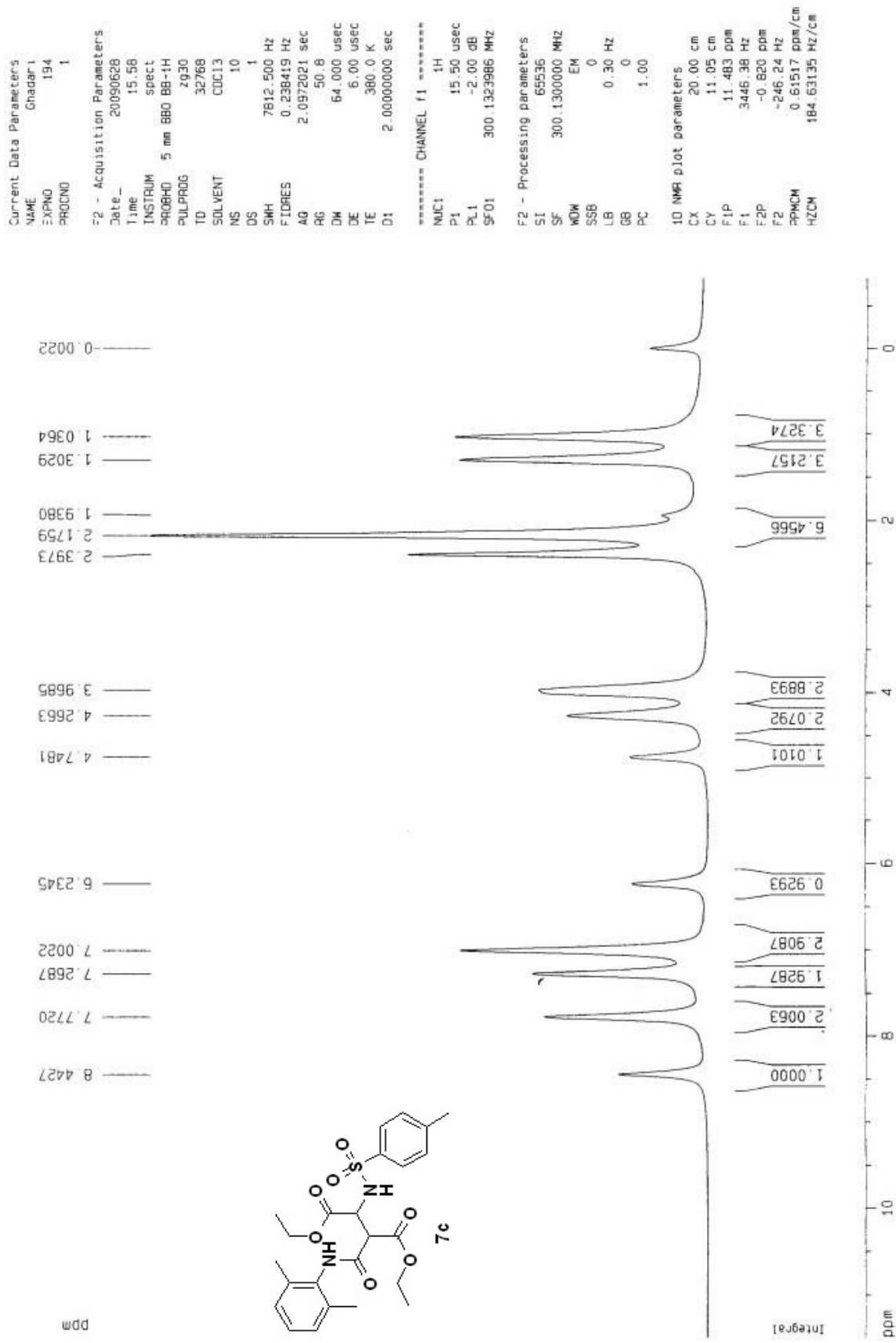


SB=30 SE=530 DB=30 DE=530 N=0 Z=2 T=0.0 Fact[285->525] *16

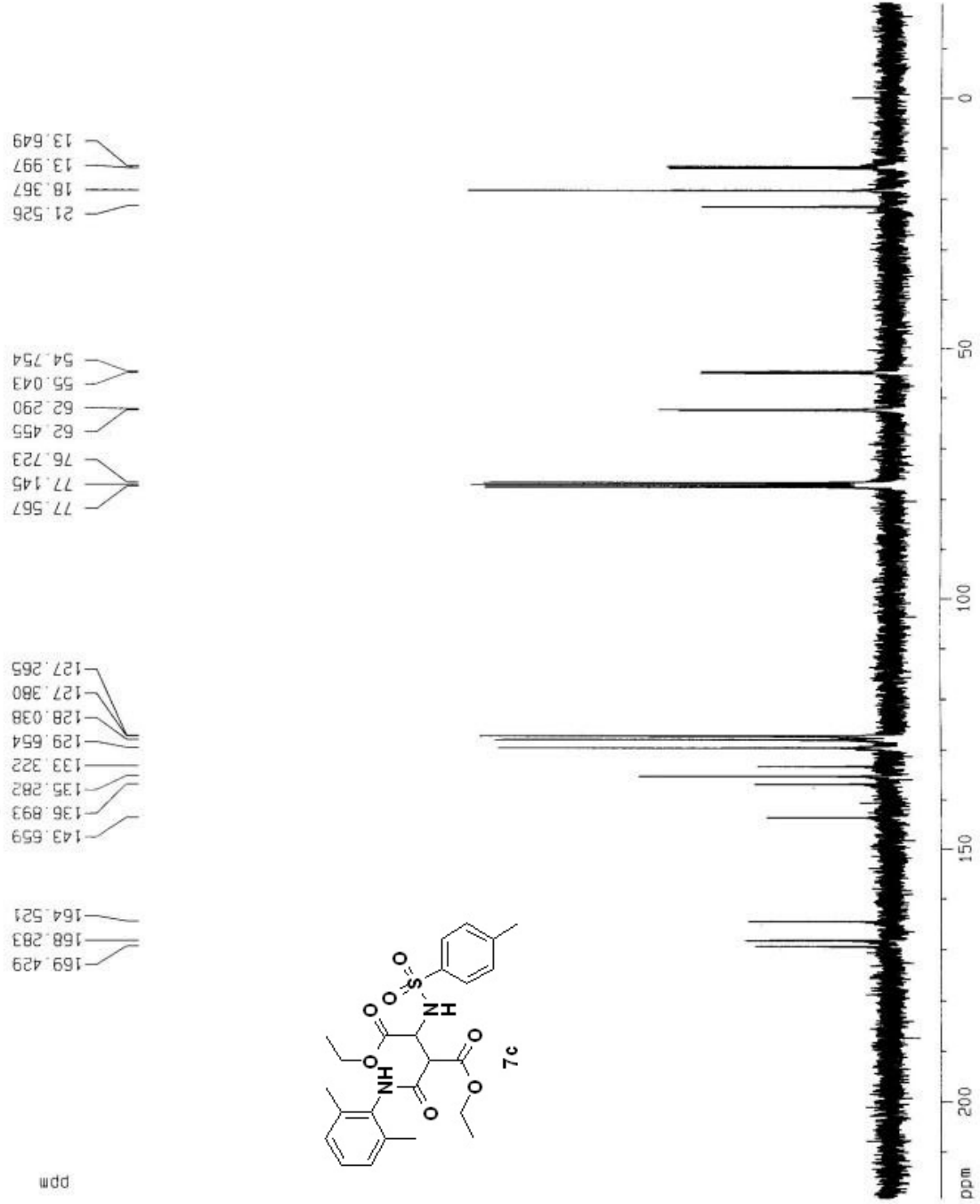
S List > S=[84->96] B=0 Pos=1 Tot=1



¹H NMR



¹³C {¹H} NMR



Current Data Parameters
NAME Ghadar1
EXPNO 195
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090528
Time 16.00
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 295
DS 2
SMA 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 ¹³C
P1 8.75 usec
PL1 -2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677480 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

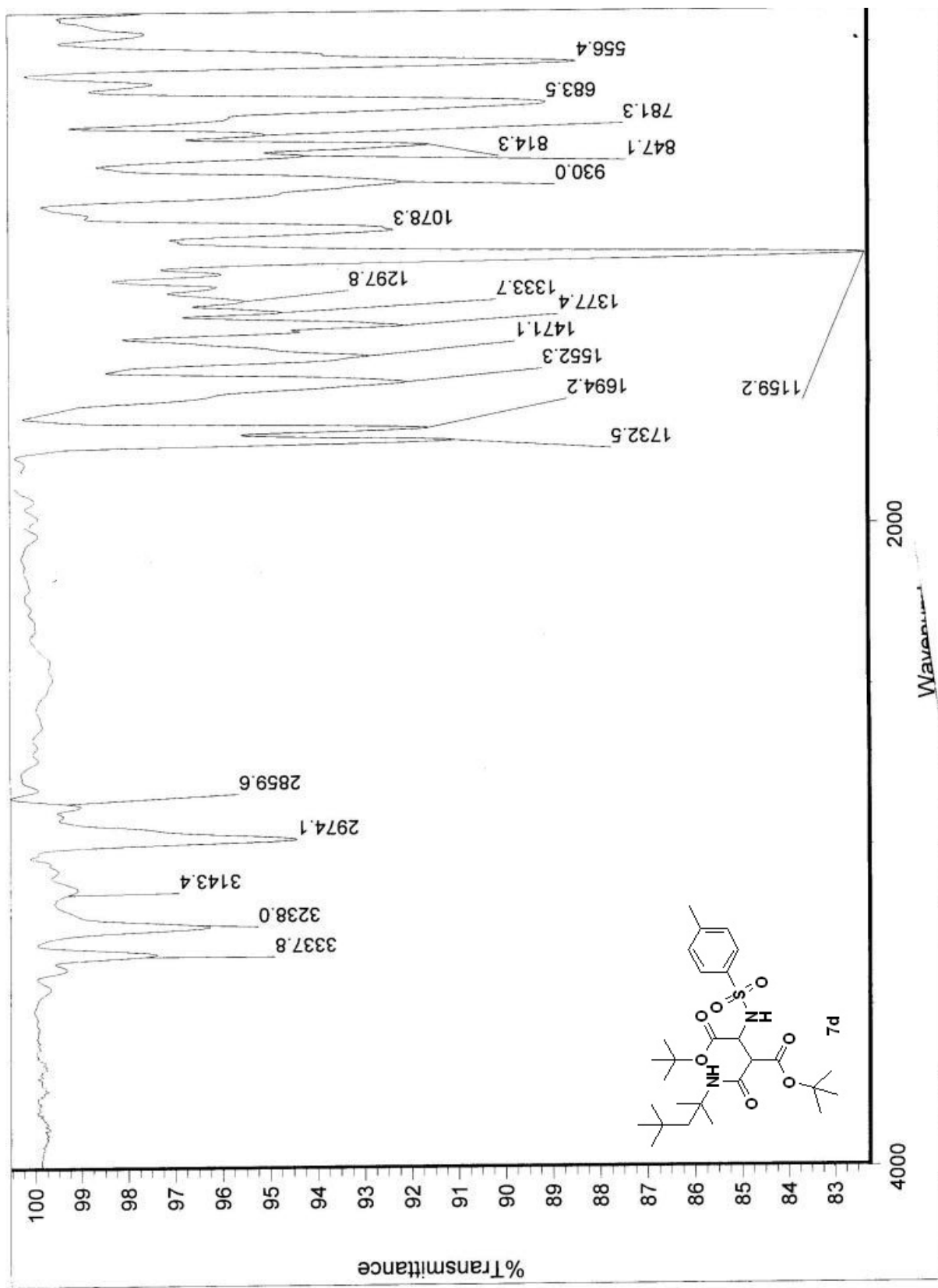
1D NMR plot parameters
CX 20.00 cm
CY 6.99 cm
FIP 219.155 ppm
F1 16539.11 Hz
F2 -19.167 ppm
F2 -1446.51 Hz
PPMCM 11.91609 ppm/cm
HZCM 899.28052 Hz/cm

Mass spectrum of 3-140 / (1,1) BP-31 B1-2100307, M1-1.1, C1-100. The x-axis represents the mass-to-charge ratio (m/z) from 30 to 270, and the y-axis represents the relative intensity from 0 to 100%.

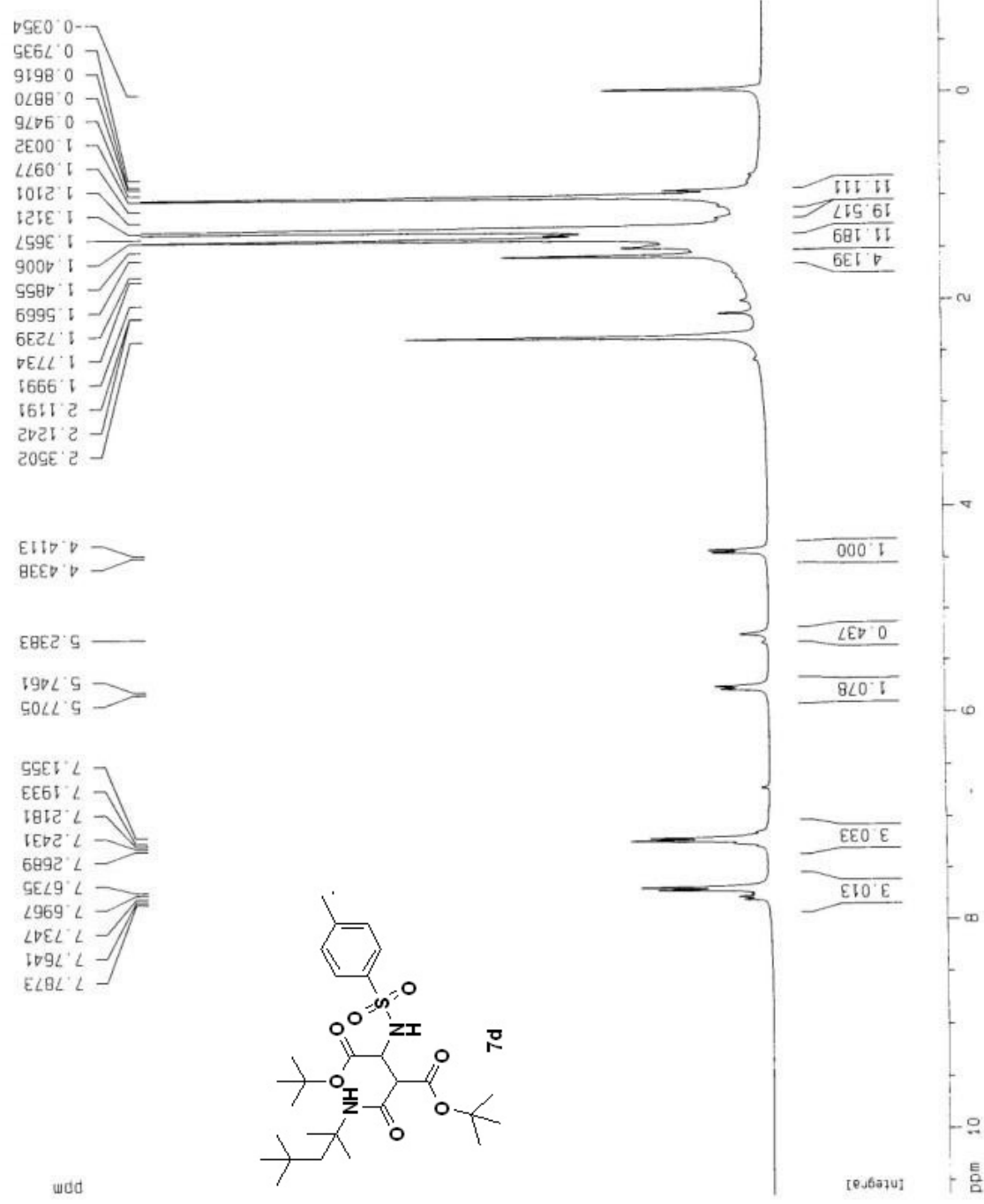
m/z	Relative Intensity (%)
41	~55
57	~85
91	~65
112	~35
155	~30
182	~25
198	~35
223	~25
267	100



70



¹H NMR



Current Data Parameters
NAME Sarvari
EXPNO 418
PROCNO 1

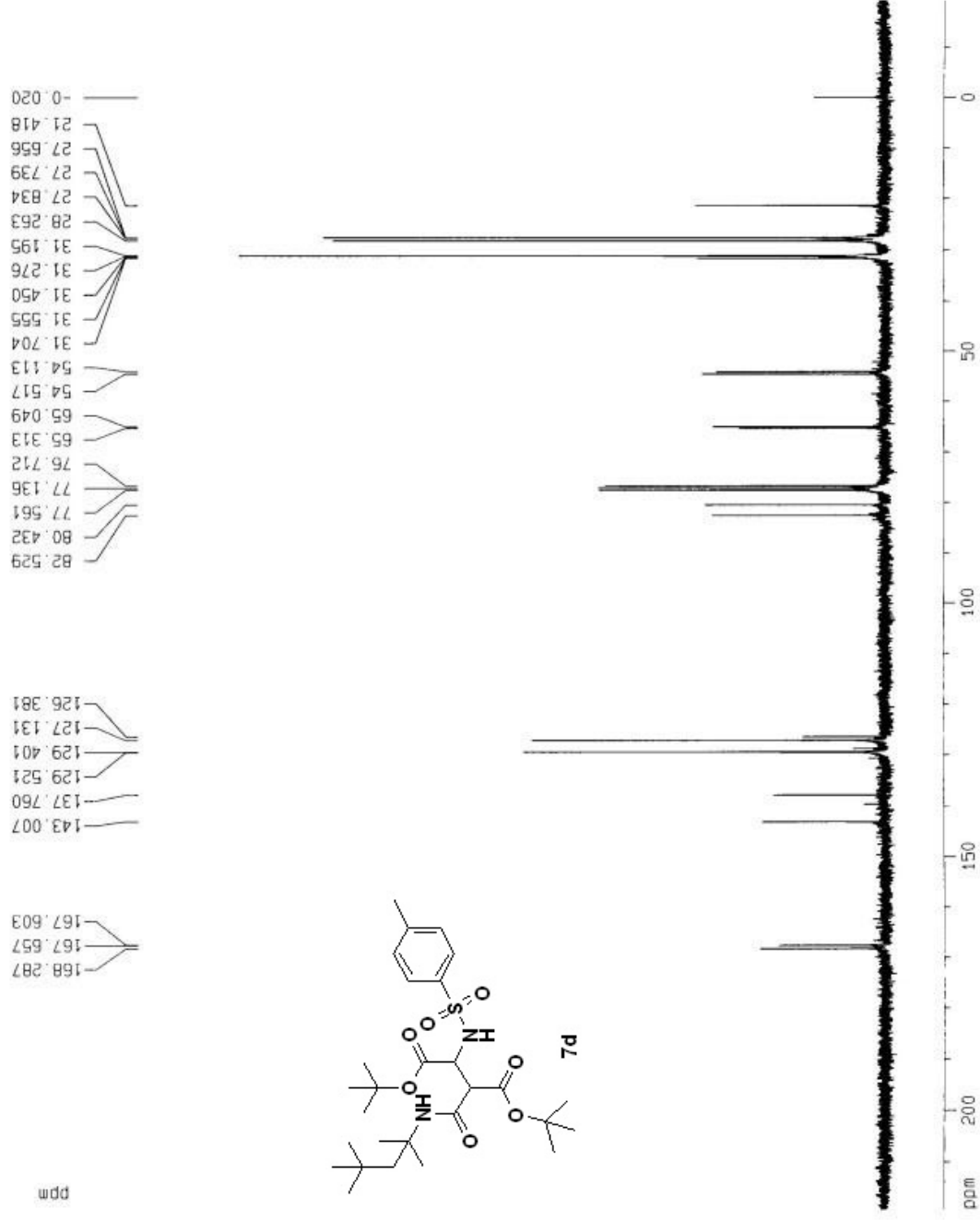
F2 - Acquisition Parameters
Date_ 20090425
Time 13.35
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 32
DM 64.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 NMR plot parameters
CX 20.00 cm
CY 29.71 cm
FIP 10.633 ppm
F1 3191.25 Hz
F2 -0.896 ppm
F2P -268.98 Hz
PPMCM 0.57645 ppm/cm
HZCM 173.01186 Hz/cm

¹³C {¹H} NMR



Current Data Parameters
NAME Sarvar1
EXPNO 419
PROCNO 1

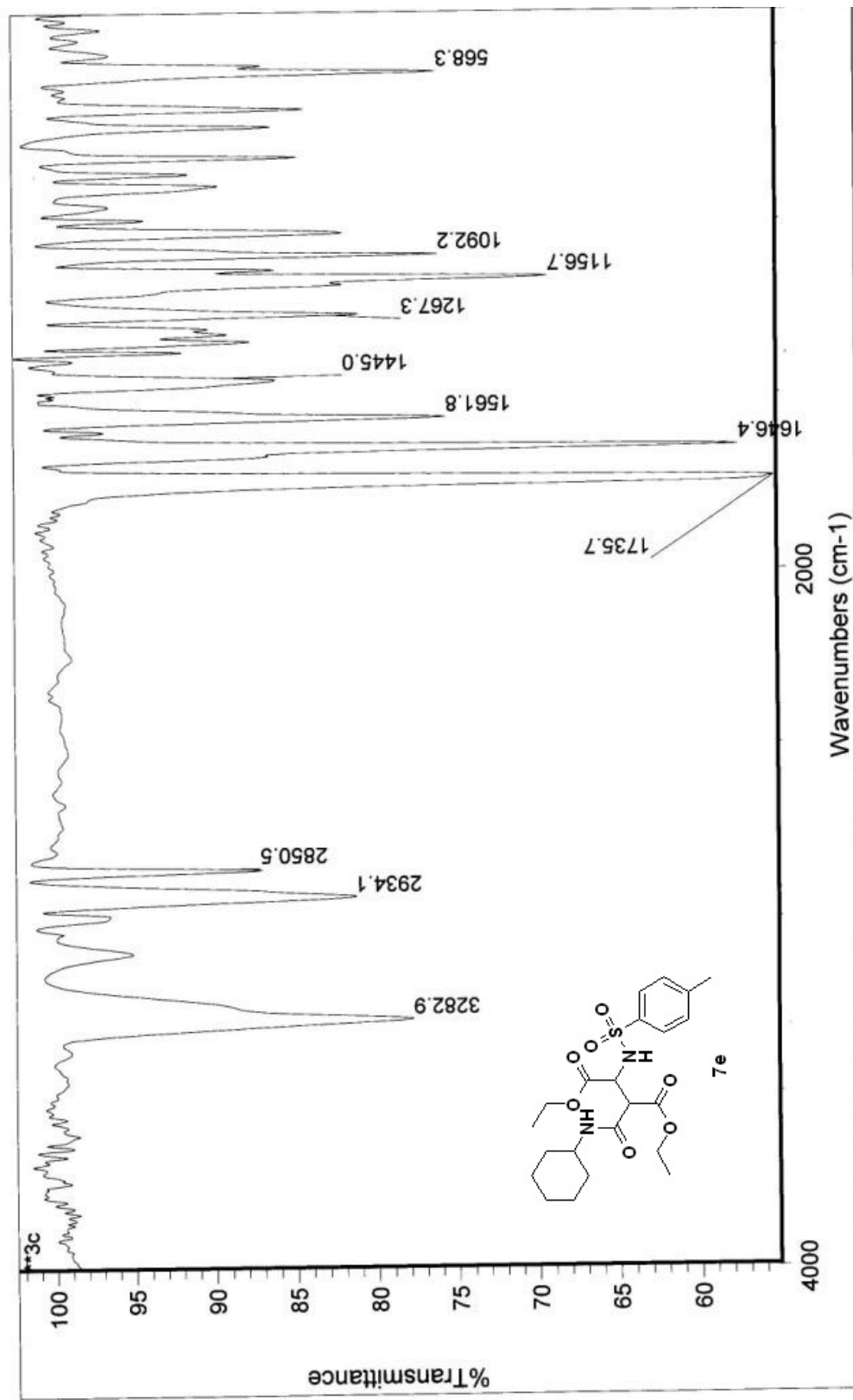
F2 - Acquisition Parameters
Date_ 20090425
Time 13.35
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 290
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

***** CHANNEL f1 *****
NUC1 ¹³C
P1 8.75 usec
PL1 -2.00 dB
SF01 75.4752953 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EN
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 10.82 cm
F1P 219.195 ppm
F1 16539.11 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
APPCW 11.91609 ppm/cm
HZOM 899.28052 Hz/cm



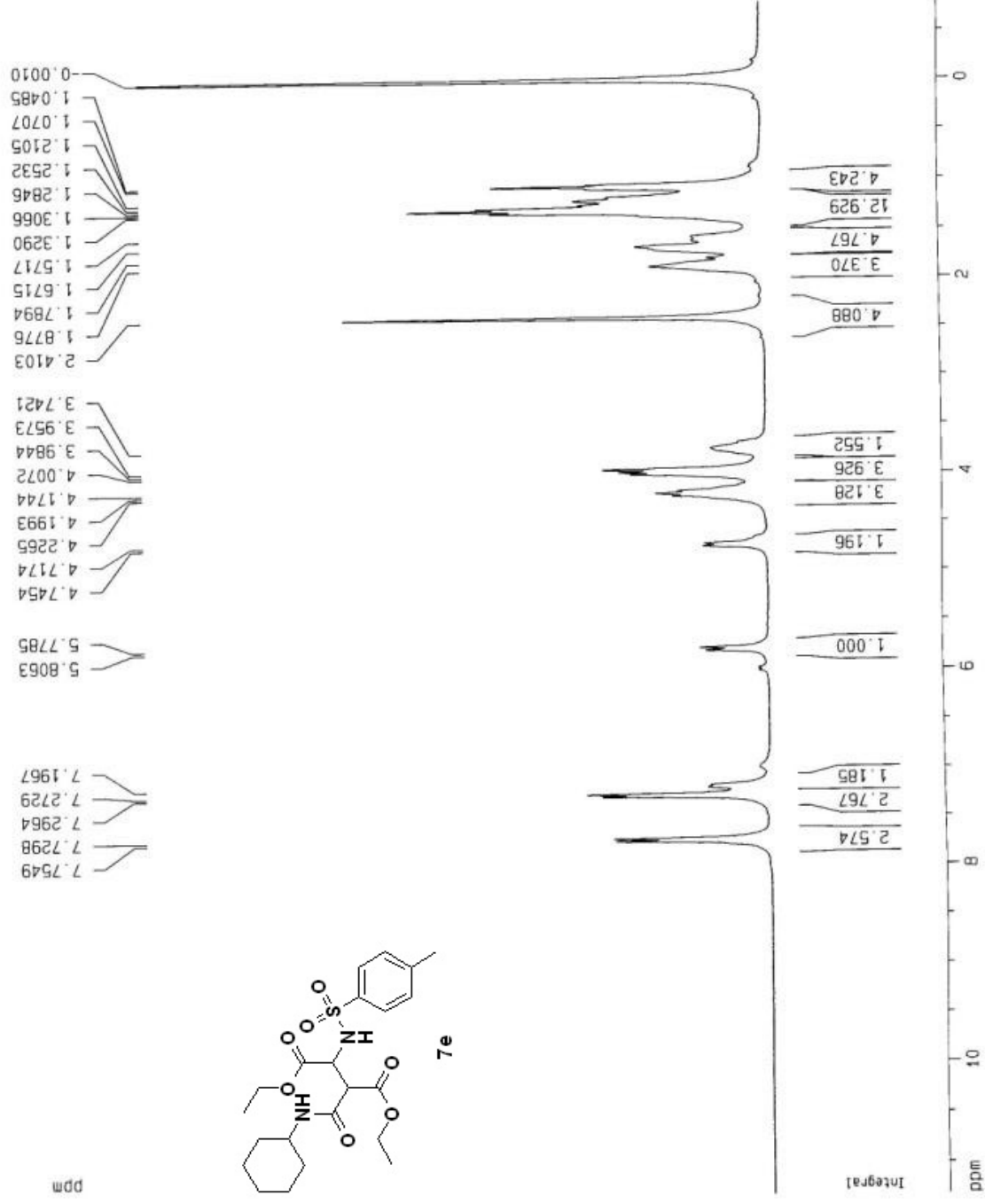
Date: Sat Apr 15 02:21:00 2000

***3c

Scans: 1

Resolution: Unknown

¹H NMR



Current Data Parameters
NAME Sarvari
EXPNO 684
PROCNO 1

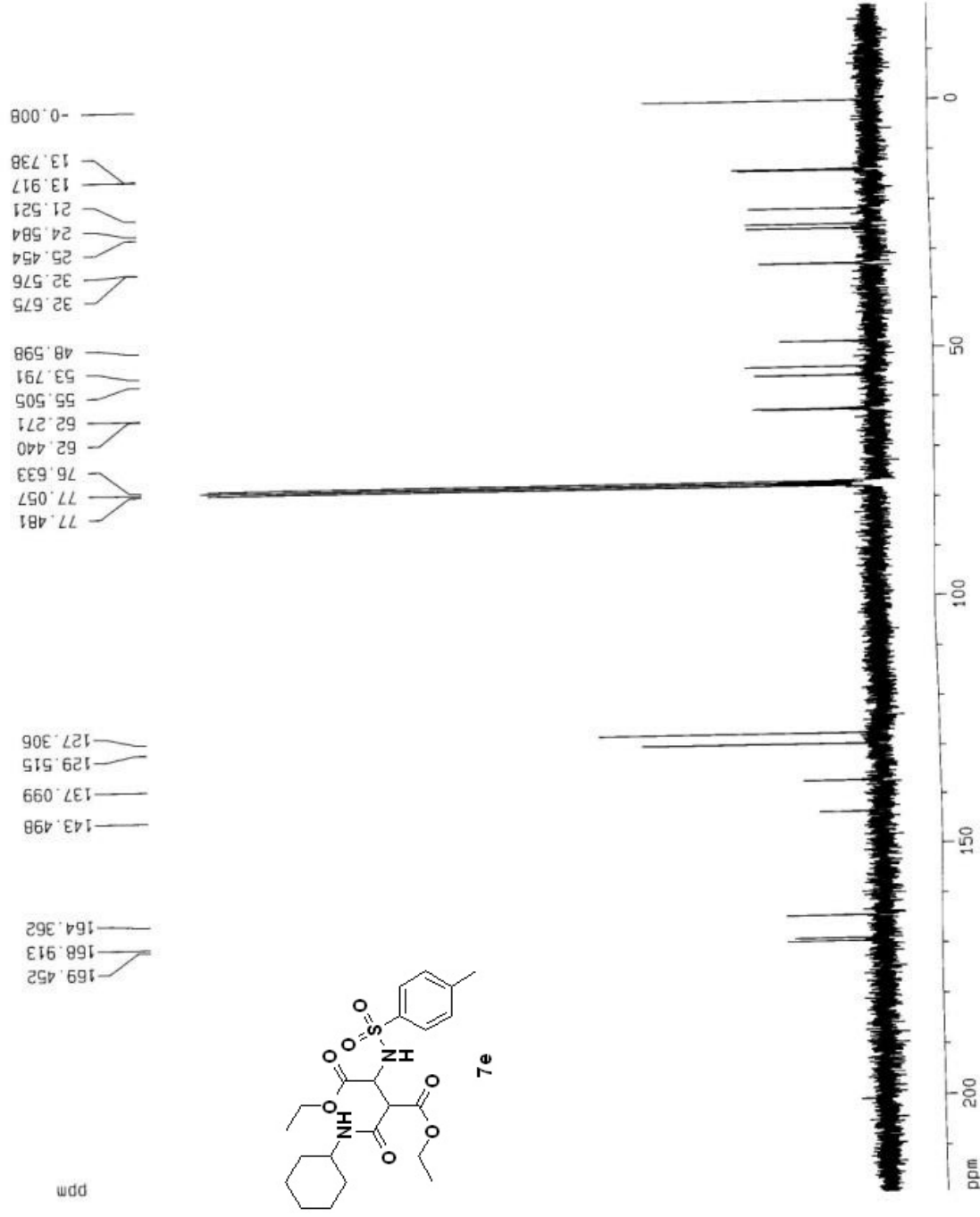
F2 - Acquisition Parameters
Date_ 20100924
Time 10.12
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.236419 Hz
AQ 2.0972021 sec
RG 50.8
DM 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

***** CHANNEL f1 *****
NUC1 ¹H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323985 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 14.57 cm
F1P 11.315 ppm
F1 3395.95 Hz
F2P -0.800 ppm
F2 -240.18 Hz
PRNCH 0.60576 ppm
HZCH 181.80685 Hz/

¹³C {¹H} NMR



```

Current Data Parameters
NAME      Serva1
EXPNO     685
PROCNO    1

F2 - Acquisition Parameters
Date_     20100924
Time      10.16
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         251
DS         2
SWH        17985.611 Hz
FIDRES     0.274439 Hz
AQ         1.8219508 sec
RG         2048
DM         27.800 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
d12        0.00002000 sec

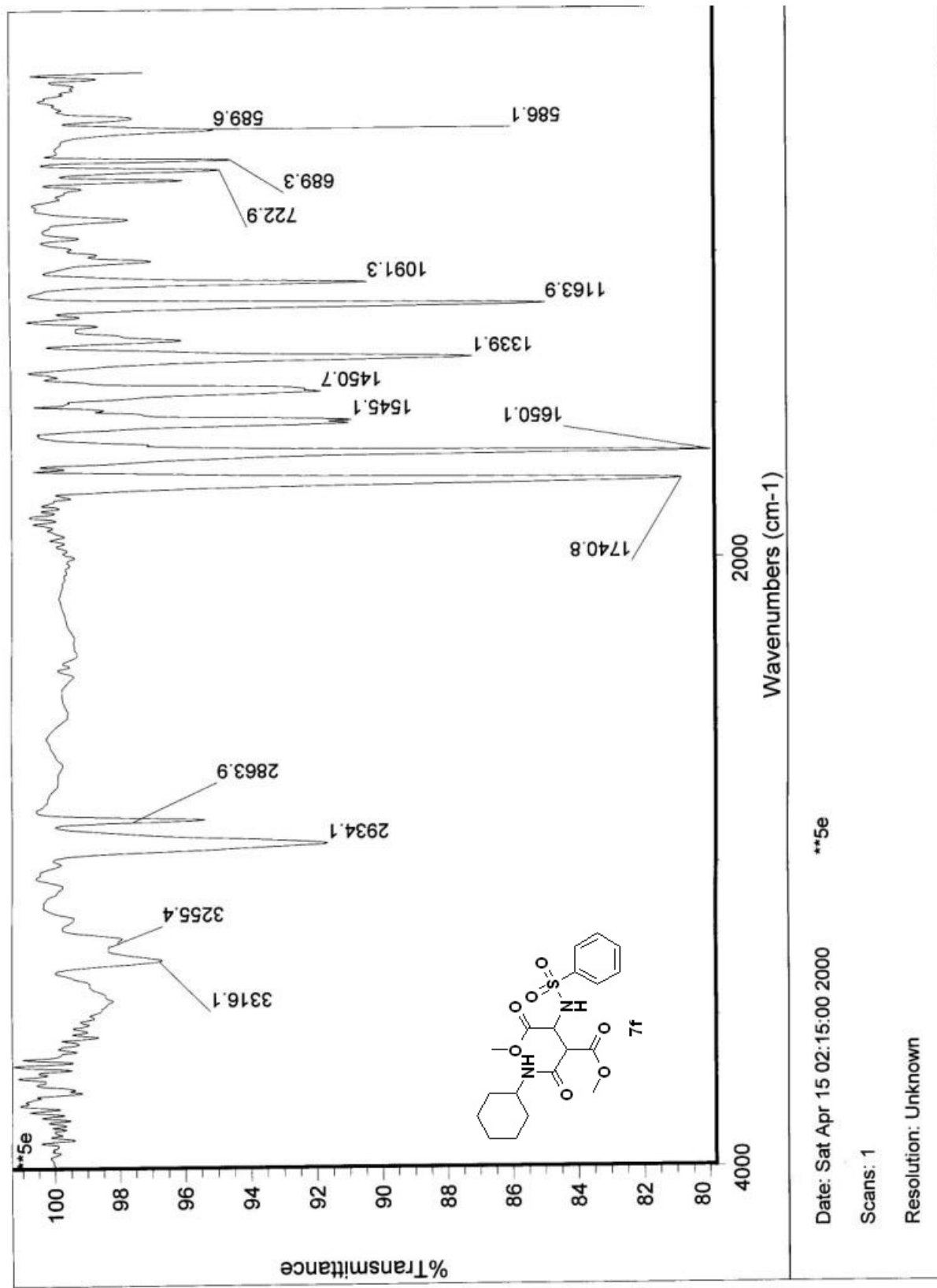
***** CHANNEL f1 *****
NUC1       13C
P1         8.75 usec
PL1        -2.00 dB
SF01       75.4752953 MHz

***** CHANNEL f2 *****
CPDPRG2   waltz16
NUC2       1H
PCPD2      87.00 usec
PL2        -2.00 dB
PL12       12.00 dB
PL13       18.00 dB
SF02       300.1312005 MHz

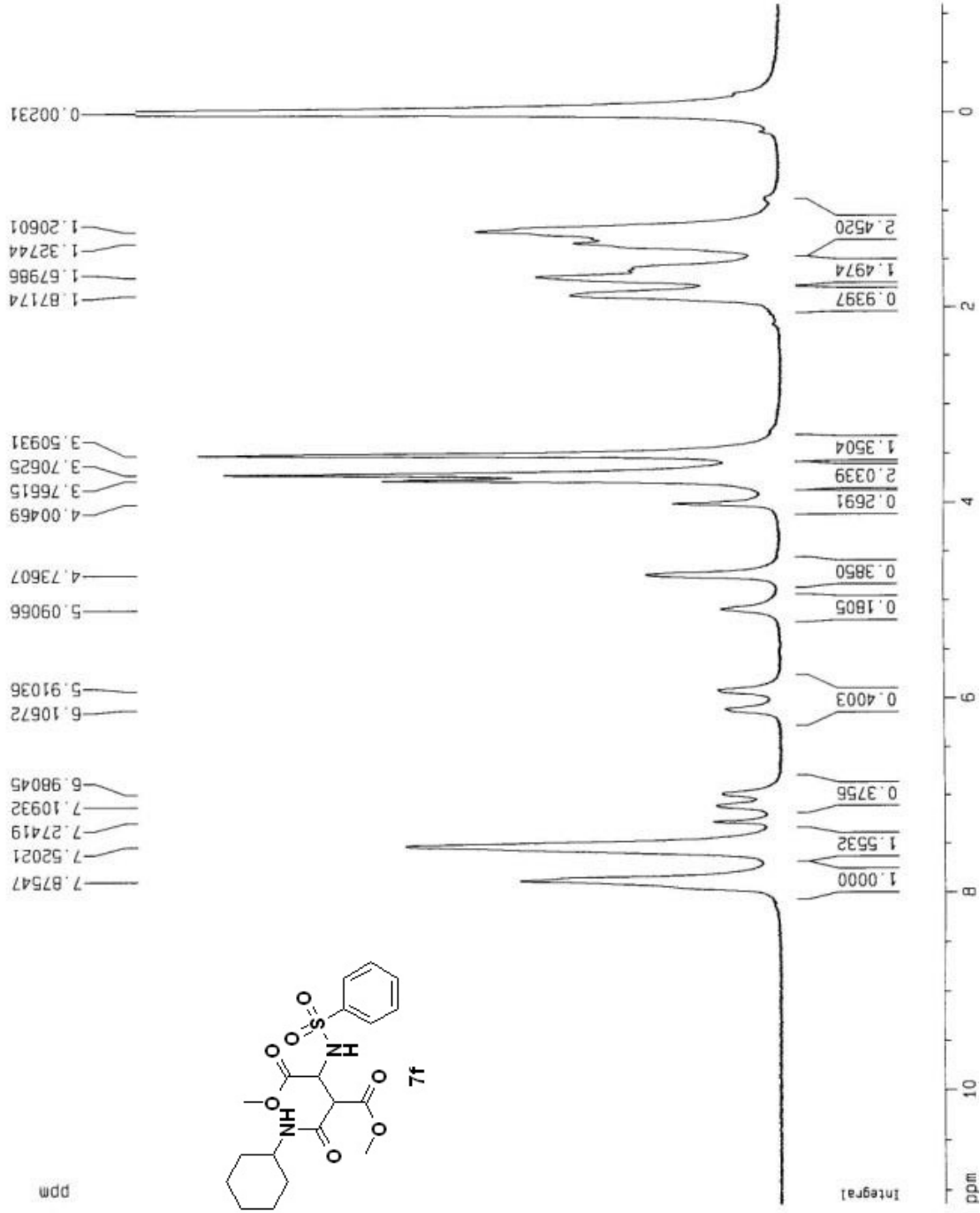
F2 - Processing parameters
SI         65536
SF         75.4677490 MHz
MDM        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

1D NMR plot parameters
CX         20.00 cm
CY         11.54 cm
F1P        219.155 ppm
F1         16539.10 Hz
F2P        -19.167 ppm
F2         -1446.51 Hz
PPMCM      11.91609 ppm/cm
HZCM       999.28052 Hz/cm

```



¹H NMR



Current Data Parameters
NAME Sarva1
EXPNO 686
PROCNO 1

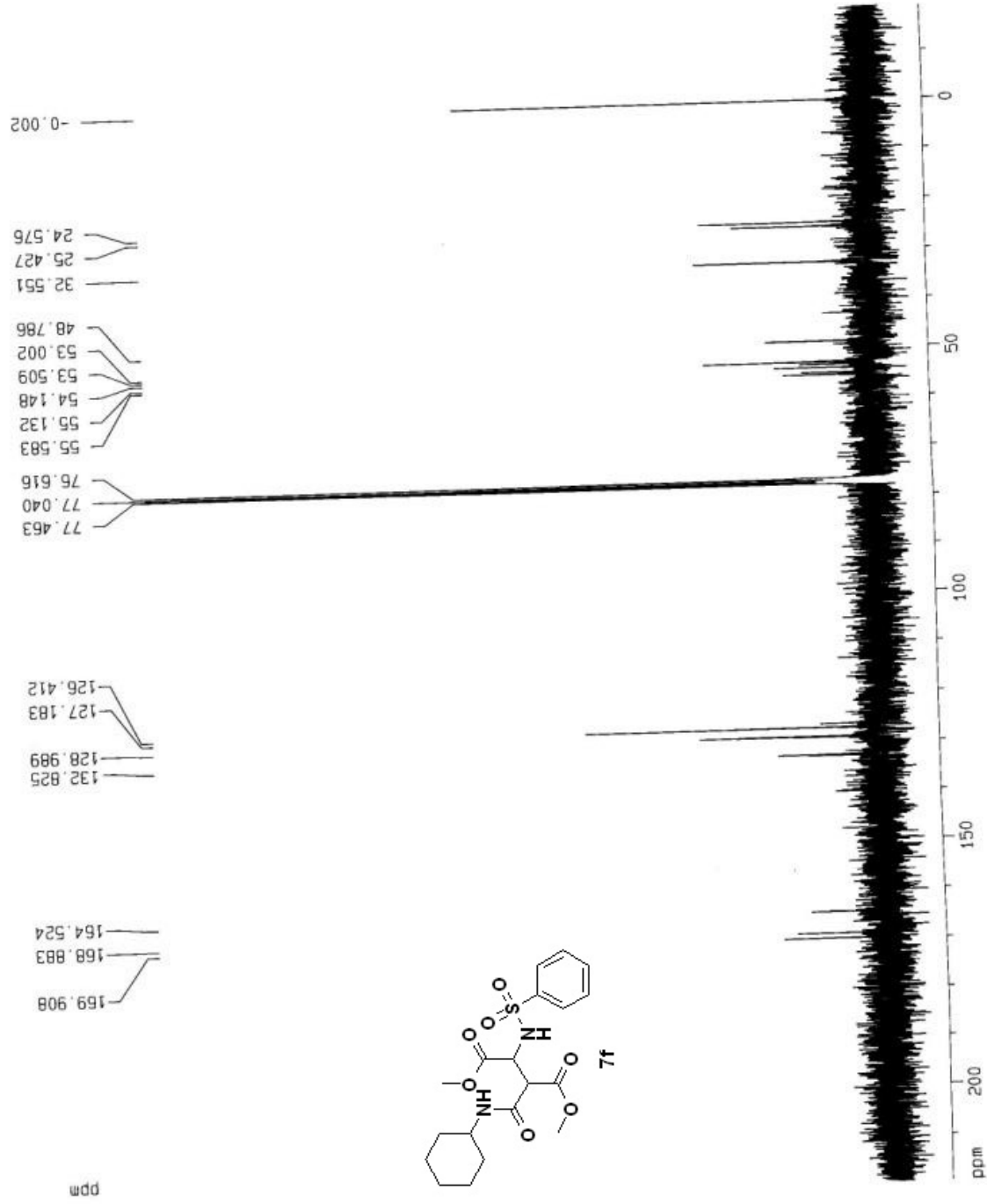
F2 - Acquisition Parameters
Date_ 20100924
Time 10.34
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 50.8
DM 64.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 ¹H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 35.85 cm
F1P 11.141 ppm
F1 3343.67 Hz
F2P -1.105 ppm
F2 -331.56 Hz
PPMCM 0.61227 ppm/cm
HZCM 183.76175 Hz/cm

¹³C {¹H} NMR



Current Data Parameters
NAME Sarvari
EXPNO 687
PROCNO 1

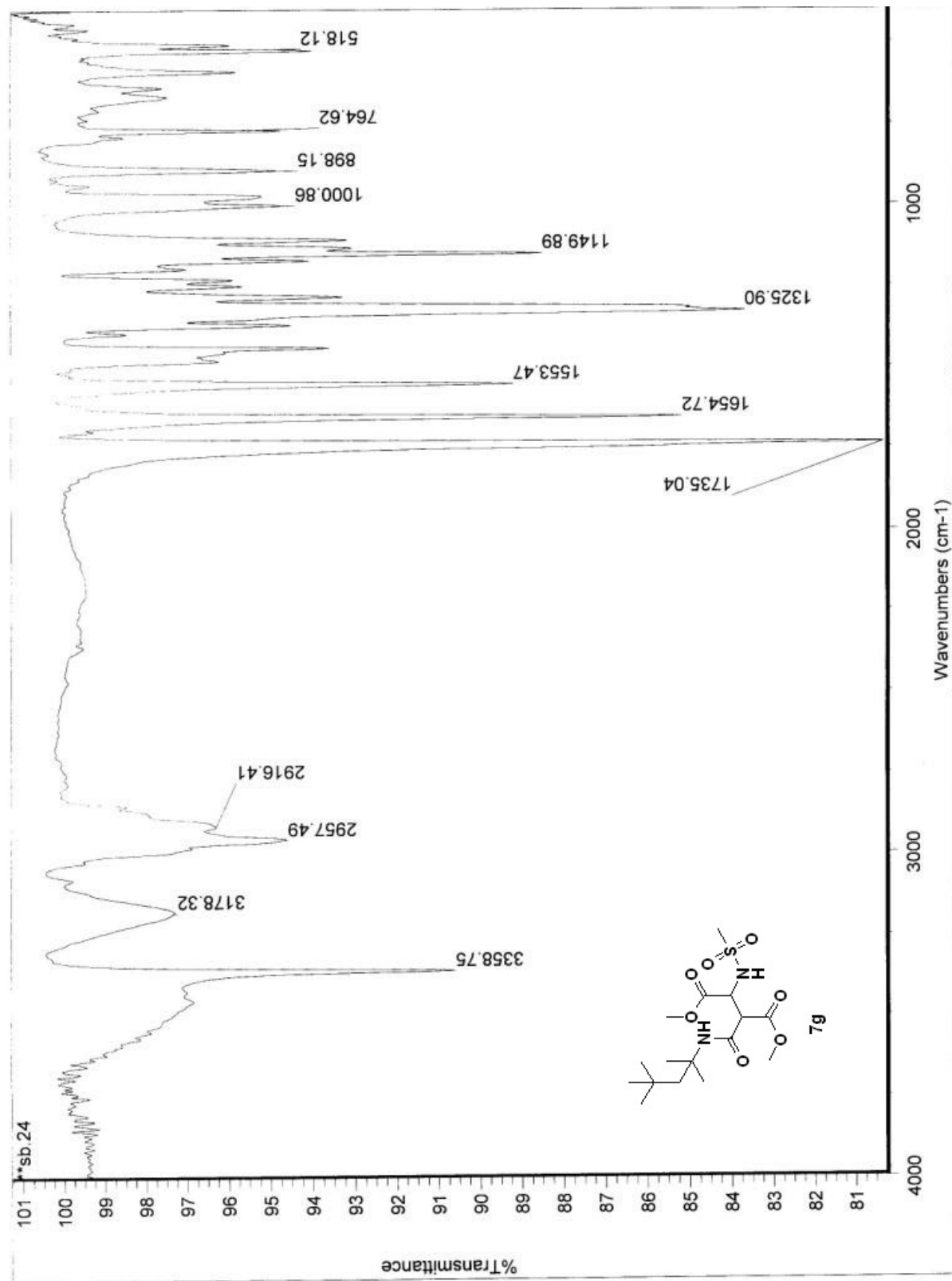
F2 - Acquisition Parameters
Date_ 20100924
Time 10.44
INSTRUM spect
PROBHD 5 mm BBO DB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 366
DS 2
SWH 17985.511 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SF01 75.4752953 MHz

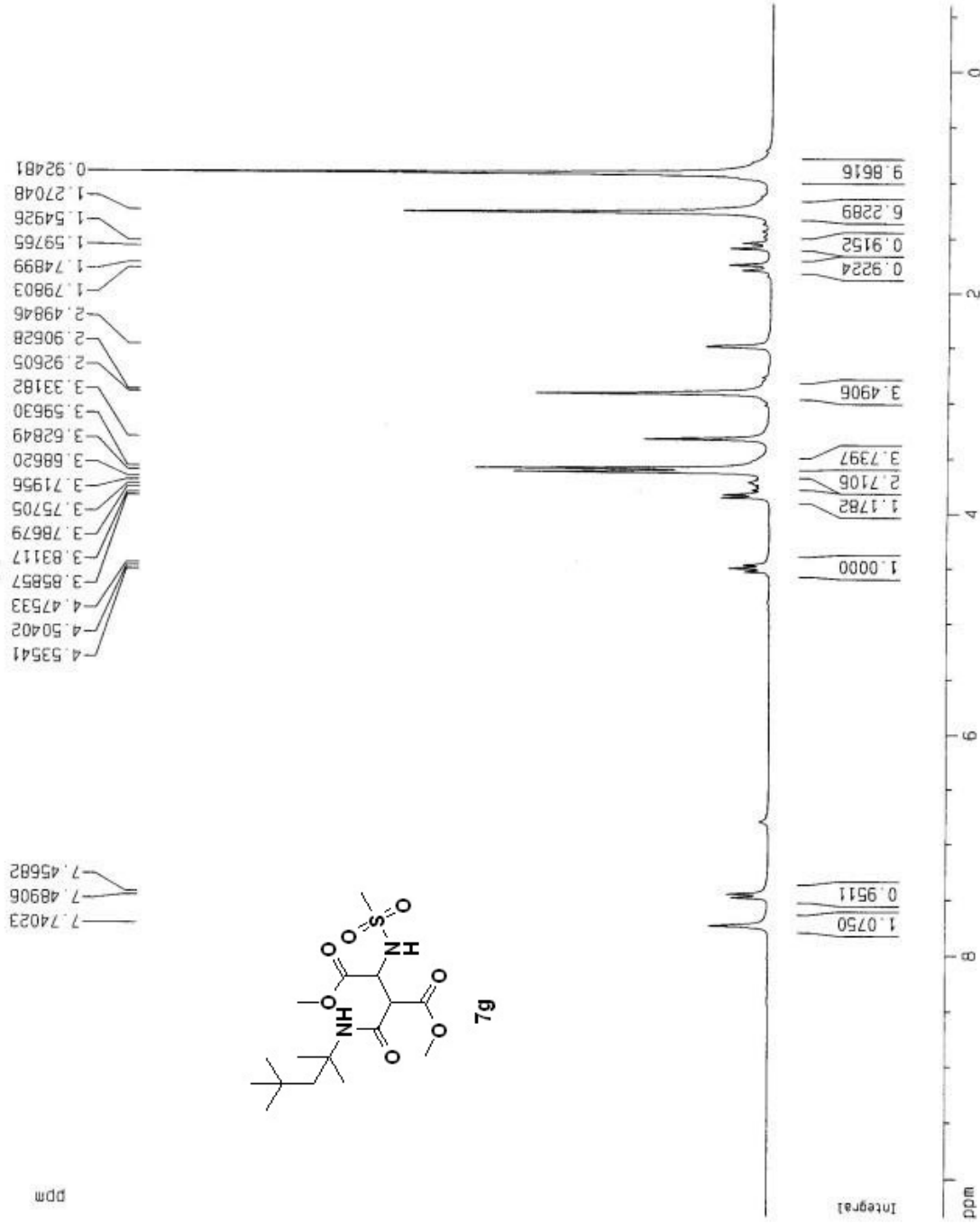
***** CHANNEL f2 *****
CPOPRG2 Waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 16.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EN
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

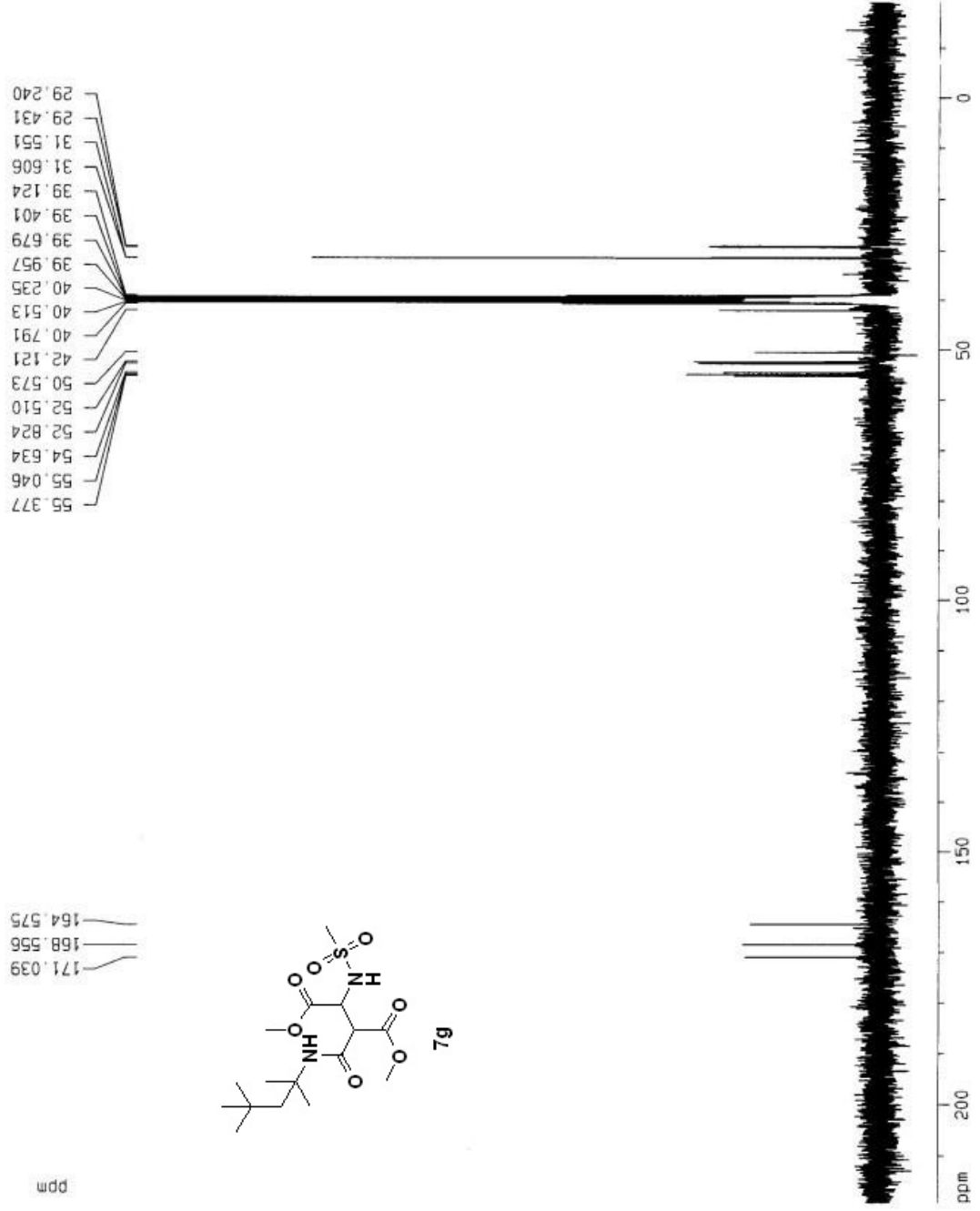
1D NMR plot parameters
CX 20.00 cm
CY 23.56 cm
F1P 219.155 ppm
F1 16539.10 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCK 11.91609 ppm/1
HZCM 899.28052 Hz/1



¹H NMR



¹³C {¹H} NMR



```

Current Data Parameters
NAME      Rezadeian-PRO
EXPNO     380
PROCNO    1

F2 - Acquisition Parameters
Date_     20090526
Time      14.49
INSTRUM    spect
PROBHD     5 mm BB-1H
PULPROG    zgpg30
TO         2000.30
TD         65536
SOLVENT     CDCl3
NS         316
DS         2
SWH         17955.611 Hz
FIDRES     0.274439 Hz
AQ         1.8219508 sec
RG         2048
AQ         27.800 usec
DE         6.00 usec
TE         300.0 K
D1         2.0000000 sec
d11        0.0000000 sec
d12        0.0002000 sec

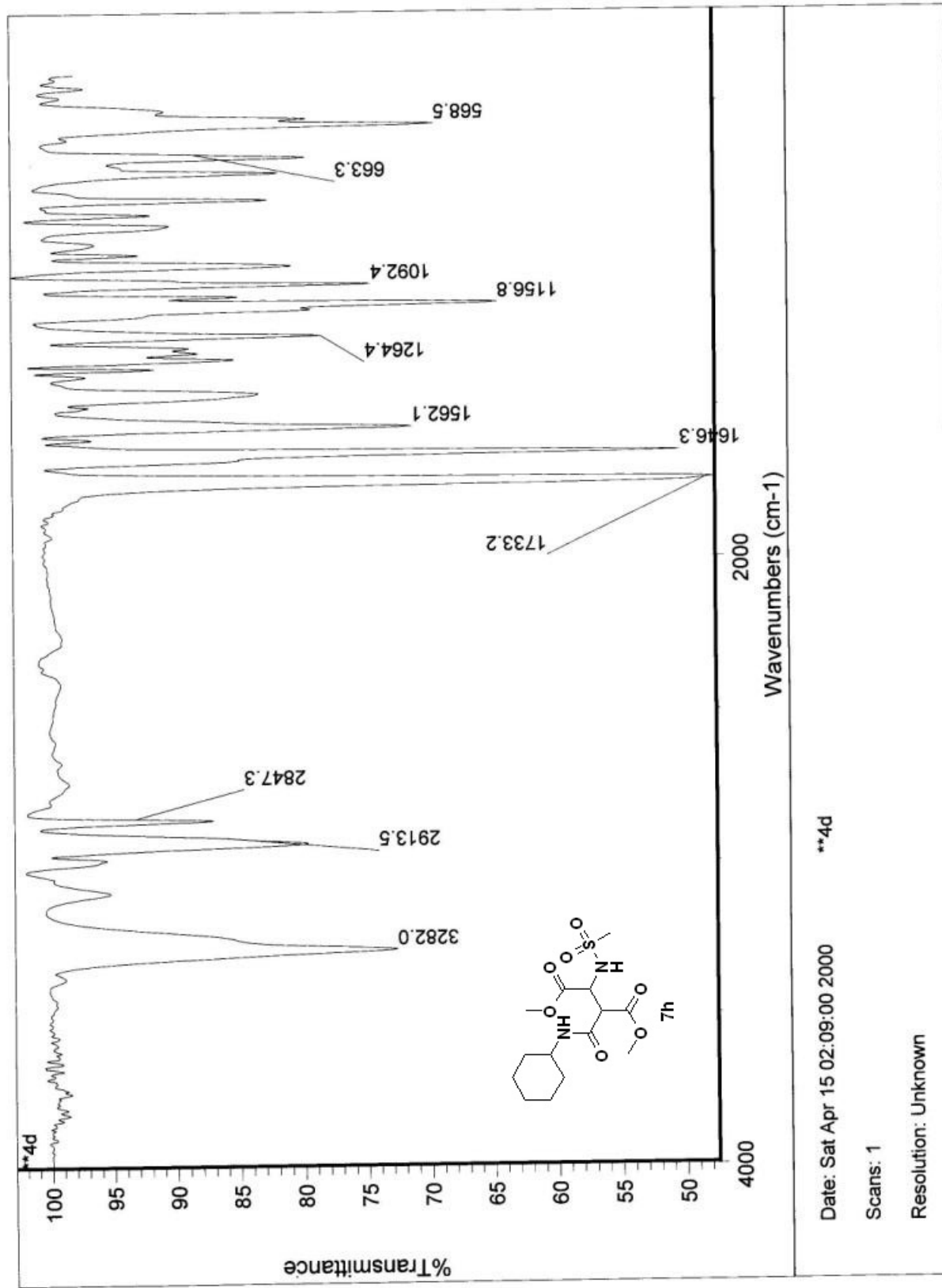
***** CHANNEL f1 *****
NUC1       13C
P1         8.75 usec
PL1        -2.00 dB
SF01       75.4752953 MHz

***** CHANNEL f2 *****
CPDPRG2    waltz16
NUC2       1H
PCPD02     87.00 usec
PL2        -2.00 dB
PL12       12.00 dB
PL13       18.00 dB
SF02       300.1312005 MHz

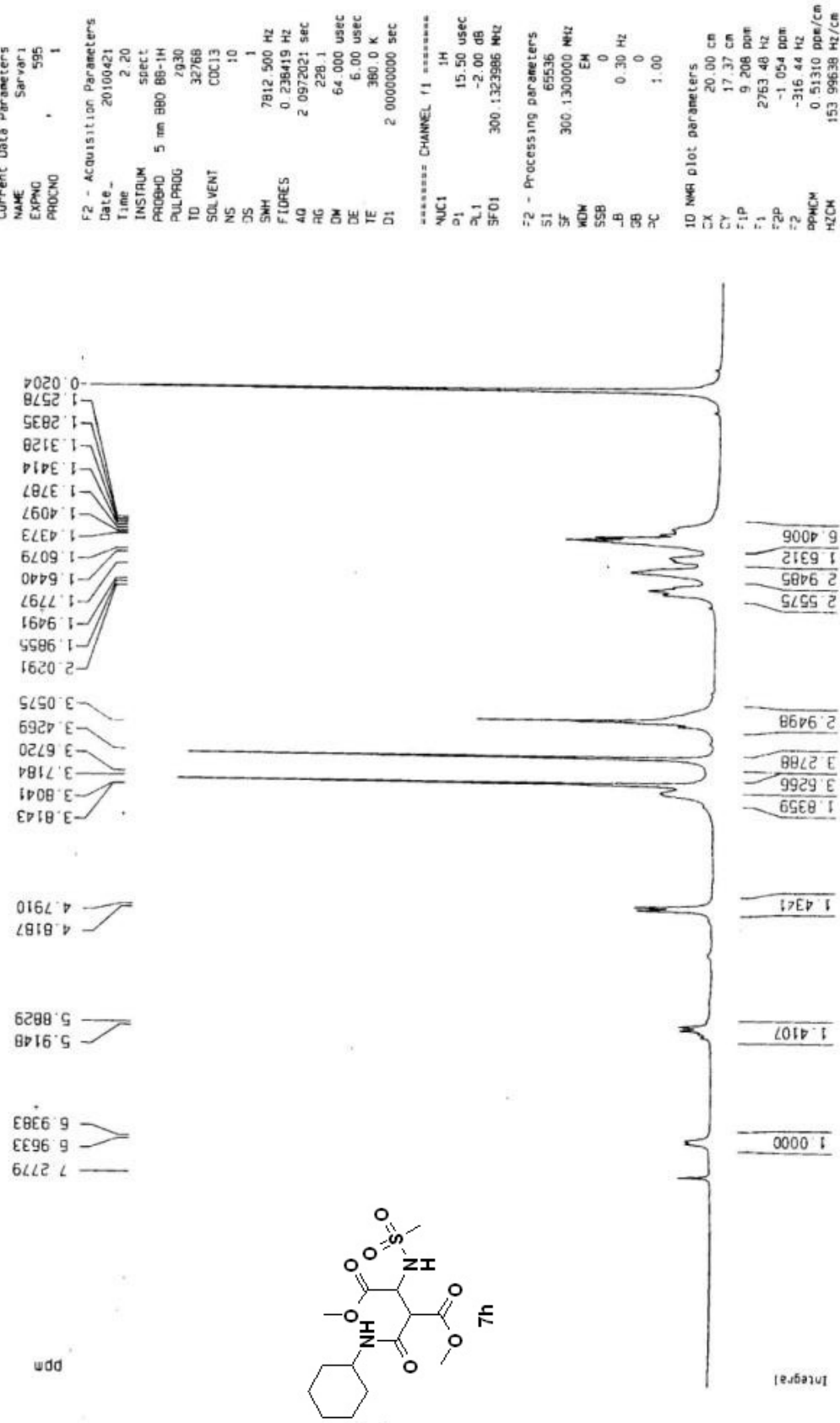
F2 - Processing parameters
S1         65536
SF         75.4677490 MHz
EM         0
MDM        1.00 Hz
LB         0
GB         0
PC         1.40

ID NMR plot parameters
CX         20.00 cm
CY         36.63 cm
F1P        219.150 ppm
F1         16539.10 Hz
F2P        -13.167 ppm
F2         -1446.51 Hz
PQMCN     11.91609 ppm/cm
MZCM       899.28058 Hz/cm

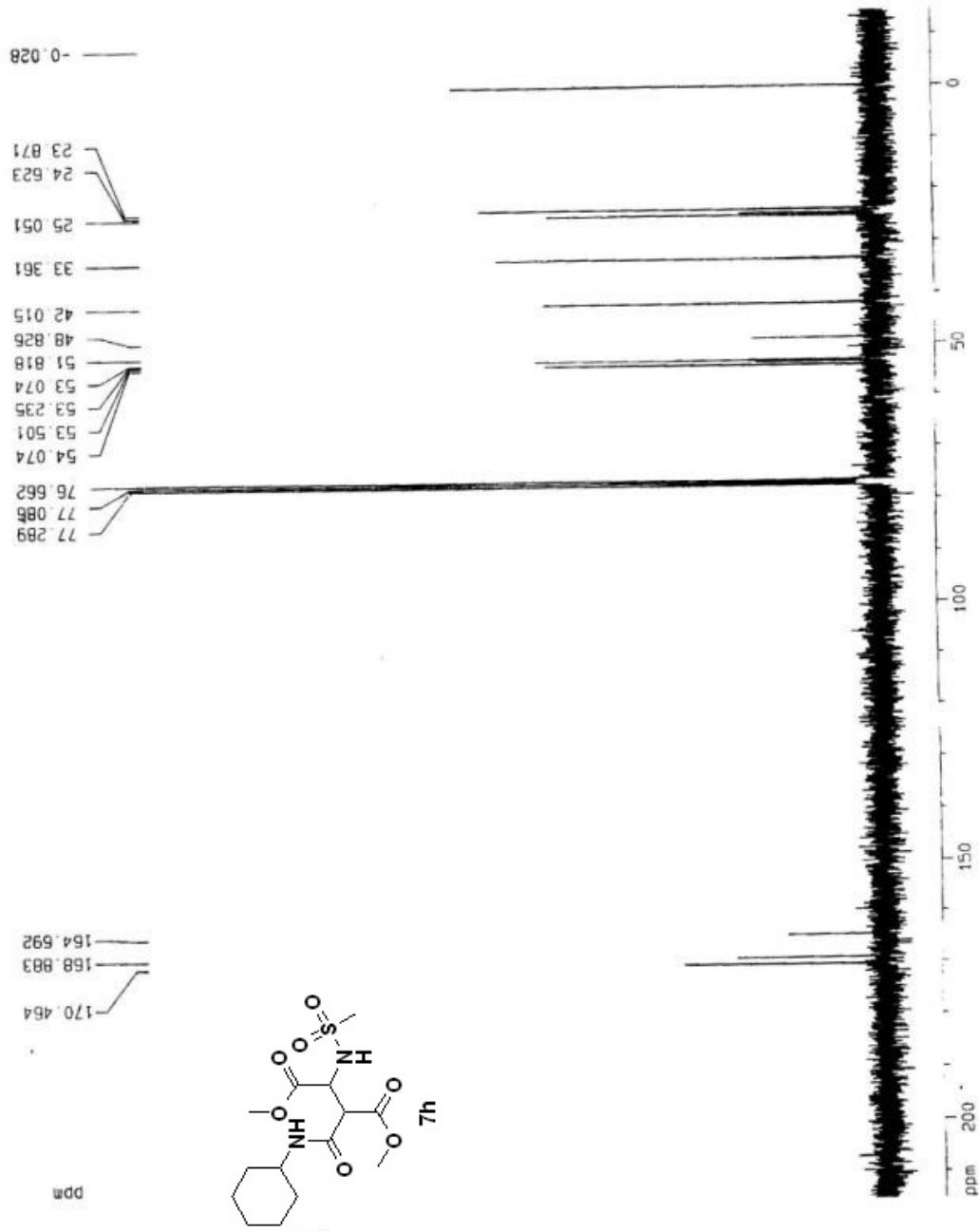
```



¹H NMR



¹³C {¹H} NMR



Current Data Parameters
NAME: Sarva1
EXPNO: 596
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20100421
Time: 2.48
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
VS: 420
DS: 2
SWH: 17985.611 Hz
FIDRES: 0.274439 Hz
AQ: 1.821908 sec
RG: 2048
DM: 27.800 usec
DE: 6.00 usec
TE: 300.0 K
D1: 2.00000000 sec
d11: 0.03000000 sec
d12: 0.00002000 sec

***** CHANNEL f1 *****
NUC1: ¹³C
P1: 8.75 usec
PL1: -2.00 dB
SF01: 75.4752653 MHz

***** CHANNEL f2 *****
CPRPG2: waltz16
NUC2: ¹H
PCPD2: 87.00 usec
PL2: -2.00 dB
PL12: 12.00 dB
PL13: 18.00 dB
SF02: 300.1312005 MHz

F2 - Processing parameters
SI: 65536
SF: 75.4677490 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.20

1D NMR plot parameters
Cx: 20.00 cm
CY: 21.96 cm
F1P: 215.226 ppm
F1: 16242.64 Hz
F2P: -14.384 ppm
F2: -1100.63 Hz
PCHN: 11.49052 ppm/cm
M2CM: 867.16345 Hz/cm