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Chemical Library Purification Strategies Based on Principles of Complementary Molecular Reactivity and Molecular Recognition

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Supplementary Material

General Procedure I (for compounds 10-11):

Benzanilide (11a). 19.6 mg, 99.5%. ¹H NMR (CDCl₃, 400MHz): δ 7.90 (m, 3H), 7.65 (d, *J* = 7.6 Hz, 2H), 7.55 (m, 1H), 7.48 (t, *J* = 7.4 Hz, 2H), 7.37 (t, *J* = 8.0 Hz, 2H), 7.16 (t, *J* = 7.4 Hz, 1H); ¹³C NMR (CDCl₃, 125MHz): δ 165.7, 137.9, 135.0, 131.8, 129.1, 128.8, 127.0, 124.6, 120.2; HRMS *m/z* 197.0833 (C₁₃H₁₁N₁O₁ requires 197.0840); HPLC purity (retention time): 97.8% (12.1 min).

Acetanilide (11b). 7.8 mg, 57.8%. ¹H NMR (CDCl₃, 400MHz): δ 7.49 (d, *J* = 7.9 Hz, 2H), 7.36 (bs, 1H), 7.31 (t, *J* = 7.9 Hz, 2H), 7.10 (t, *J* = 7.4 Hz, 2H), 2.17 (s, 3H); ¹³C NMR (CDCl₃, 75MHz): δ 168.6, 137.9, 128.9, 124.2, 119.9; HRMS *m/z* 135.0687 (C₈H₉N₁O₁ requires 135.0685); HPLC purity (retention time): 97.9% (5.4 min).

***N*-Benzyl-*N'*-phenyl urea (10c).** 24.6 mg, 100%. ¹H NMR (CD₃OD, 400MHz): δ 7.35 (m, 6H), 7.25 (m, 2H), 6.97 (t, *J* = 7.5 Hz, 1H), 4.38 (s, 2H); ¹³C NMR (CD₃OD, 125MHz): δ 158.3, 141.0, 140.9, 129.8, 129.5, 128.3, 128.1, 123.5, 120.3, 44.6; HRMS *m/z* 226.1125 (C₁₄H₁₄N₂O₁ requires 226.1106); HPLC purity (retention time): 97.8% (11.6 min).

***N*-Iso-propyl-*N'*-phenyl urea (10d).** 8.9 mg, 50%. ¹H NMR (CDCl₃, 400MHz): δ 7.29 (m, 5H), 7.06 (m, 1H), 6.53 (bs, 1H), 3.99 (sept, *J* = 6.5 Hz, 1H), 1.16 (d, *J* = 6.5 Hz, 6H); ¹³C NMR (CDCl₃, 75MHz): δ 155.9, 139.3, 129.7, 123.9, 121.2, 42.6, 23.7. HRMS *m/z* 178.1104 (C₁₀H₁₄N₂O₁ requires 178.1106); HPLC purity (retention time): 98.6% (7.7 min).

***N*-Benzyl benzamide (11g).** 23.0 mg, 100%. ¹H NMR (CDCl₃, 400MHz): δ 7.78 (d, *J* = 7.0 Hz, 2H), 7.49 (m, 1H), 7.43 (m, 2H), 7.35 (d, *J* = 4.4 Hz, 4H), 7.28 (m, 1H), 6.42 (bs, 1H), 4.65 (d, *J* = 5.6 Hz, 2H); ¹³C NMR (CDCl₃, 125MHz): δ 167.3, 138.2, 134.4, 131.5, 128.8, 128.6, 127.9, 127.6, 127.0, 44.2; HRMS *m/z* 211.0999 (C₁₄H₁₃N₁O₁ requires 211.0997); HPLC purity (retention time): 98.1% (11.4 min).

***N*-Benzyl-*N'*-iso-propyl urea (10h).** 20.0 mg, 100%. ¹H NMR (CDCl₃, 400MHz): δ 7.32 - 7.23 (cb, 5H), 4.90 (bs, 1H), 4.46 (bd, *J* = 7.3 Hz, 1H), 4.31 (d, *J* = 5.8 Hz, 2H), 3.84 (sept, *J* = 6.5 Hz, 1H), 1.10 (d, *J* = 6.5 Hz, 6H); ¹³C NMR (CDCl₃, 125MHz): δ 157.7, 139.4, 128.6, 127.5, 127.2, 44.5, 42.2, 23.4; HRMS *m/z* 192.1261 (C₁₁H₁₆N₂O₁ requires 192.1263); HPLC purity (retention time): 94.8% (7.3 min).

***N,N*-Dibenzyl benzamide (11j).** 32.0 mg, 100%. ¹H NMR (CDCl₃, 400MHz): δ 7.50 (m, 2H), 7.39 - 7.27 (cb, 11H), 7.14 (m, 2H), 4.70 (s, 2H), 4.40 (s, 2H); ¹³C NMR (CDCl₃, 125MHz): δ 172.2, 137.0, 136.5, 136.2, 129.6, 128.8, 128.7, 128.5, 128.4, 127.6, 127.5, 127.0, 126.7, 51.6, 46.9; HRMS *m/z* 301.1471 (C₂₁H₁₉N₁O₁ requires 301.1467); HPLC purity (retention time): 97.7% (20.0 min).

***N*-Dibenzyl-*N'*-iso-propyl urea (10k).** 30.3 mg, 100%. ¹H NMR (CDCl₃, 400MHz): δ

7.35 - 7.22 (cb, 10H), 4.47 (s, 4H), 4.13 (d, $J = 7.3$ Hz, 1H), 3.97 (m, 1H), 1.03 (d, $J = 6.5$ Hz, 6H); ^{13}C NMR (CDCl_3 , 125MHz): δ 157.9, 137.8, 128.7, 127.4, 127.3, 50.2, 42.7, 23.3; HRMS m/z 282.1729 ($\text{C}_{18}\text{H}_{22}\text{N}_2\text{O}_1$ requires 282.1732); HPLC purity (retention time): 98.6% (17.4 min).

General Procedure II (for compounds 12-13):

***N*-Phenyl *p*-toluenesulfonamide (13e).** 24.9 mg, 100%. ^1H NMR (CDCl_3 , 400MHz): δ 7.68 (d, $J = 8.3$ Hz, 2H), 7.22 (m, 4H), 7.09 (m, 3H), 6.97 (s, 1H), 2.37 (s, 3H); ^{13}C NMR (CDCl_3 , 125MHz): δ 143.8, 136.6, 136.1, 129.6, 129.3, 127.3, 125.3, 121.5, 21.5; HRMS m/z 247.0661 ($\text{C}_{13}\text{H}_{13}\text{N}_1\text{O}_2\text{S}_1$ requires 247.0667); HPLC purity (retention time): 98.3% (13.5 min).

***O*-Ethyl *N*-phenyl carbamate (12f).** 15.8 mg, 95.8%. ^1H NMR (CDCl_3 , 400MHz): δ 7.34 (d, $J = 7.0$ Hz, 2H), 7.30 (t, $J = 6.9$ Hz, 2H), 7.05 (t, $J = 6.7$ Hz, 1H), 6.60 (bs, 1H), 4.22 (q, $J = 7.1$ Hz, 2H), 1.31 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125MHz): δ 150.1, 138.0, 129.0, 123.3, 118.7, 61.2, 14.6; HRMS m/z 165.0789 ($\text{C}_9\text{H}_{11}\text{N}_1\text{O}_2$ requires 165.0790); HPLC purity (retention time): 99.7% (9.9 min).

***N*-Benzyl *p*-toluenesulfonamide (13i).** 24.5 mg, 93.9%. ^1H NMR (CDCl_3 , 400MHz): δ 7.76 (d, $J = 8.3$ Hz, 2H), 7.31 - 7.25 (m, 5H), 7.19 (m, 2H), 4.73 (bt, $J = 6.2$ Hz, 1H), 4.12 (d, $J = 6.2$ Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (CDCl_3 , 125MHz): δ 143.5, 136.9, 136.3, 129.7, 128.7, 127.9, 127.8, 127.2, 47.3, 21.5; HRMS m/z 261.0829 ($\text{C}_{14}\text{H}_{15}\text{N}_1\text{O}_2\text{S}_1$ requires 261.0824); HPLC purity (retention time): 97.7% (14.3 min).

***N*-Dibenzyl *p*-toluenesulfonamide (13l).** 31.1 mg, 88.6%. ^1H NMR (CDCl_3 , 400MHz): δ 7.74 (d, $J = 6.5$ Hz, 2H), 7.30 (d, $J = 4.6$ Hz, 2H), 7.22 (m, 6H), 7.06 (m, 4H), 4.32 (s, 4H), 2.45 (s, 3H); ^{13}C NMR (CDCl_3 , 125MHz): δ 143.2, 137.8, 135.7, 129.7, 128.6, 128.4, 127.6, 127.3, 50.5, 21.5; HRMS m/z 351.1317 ($\text{C}_{21}\text{H}_{21}\text{N}_1\text{O}_2\text{S}_1$ requires 351.1293); HPLC purity (retention time): 99.1% (21.8 min).

Moffatt oxidation.

Phenylmethyl [3-[[4-methylphenyl)sulfonyl](2-methylpropyl)amino]-2-oxo-1S-(phenylmethyl)propyl]carbamate (27a). 48% mass yield; ^1H NMR (CDCl_3 , 300 MHz): δ 7.62 (d, $J = 8$ Hz, 2H), 7.40-7.21 (cb, 10H), 7.15 (m, 2H), 5.21 (d, $J = 7$ Hz, 1H), 5.08 (s, 2H), 4.56 (q, $J = 7$ Hz, 1H), 4.18 (d, $J = 19$ Hz, 1H), 3.95 (d, $J = 19$ Hz, 1H), 3.05 (dd, $J = 14, 7$ Hz, 1H), 3.00-2.80 (cb, 3H), 2.41 (s, 3H), 1.60 (m, 1H), 0.80 (d, $J = 7$ Hz, 6H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 204.5, 178, 162, 156, 144, 136, 129.9, 129.7, 129.4, 129.1, 128.8, 128.6, 128.0, 127.8, 68, 59, 57, 55.6, 38, 27.2, 20.4; HRMS m/z 523.2263 ($\text{C}_{29}\text{H}_{35}\text{N}_2\text{O}_5\text{S}_1$ requires 523.2267); HPLC Purity (retention time): 91.8% (21.5 min).

***N*-(2-methylpropyl)-*N*-[2-oxo-3-[phenylcarbonyl)amino]-1S-(phenylmethyl)propyl]benzenepropanamide (27b).** 80% mass yield; ^1H NMR (CDCl_3 , 300 MHz): δ 7.72 (d, $J = 8$ Hz, 2H), 7.54-7.12 (cb, 13H), 6.95 (d, $J = 7$ Hz, 1H), 5.00 (q, $J = 7$ Hz, 1H), 4.25 (d, $J = 19$ Hz, 1H), 4.10 (d, $J = 19$ Hz, 1H), 3.34 (dd, $J = 14, 7$ Hz, 1H), 3.15 (dd, $J = 14, 7$ Hz, 1H), 3.10-2.87 (cb, 5H), 2.69-2.63 (cb, 1H), 1.72 (m, 1H), 0.86 (d, $J = 7$ Hz, 6H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 204.1, 173.3, 167.7, 141.7, 137.0, 134.1, 132.3, 129.9, 129.7, 129.6, 129.2, 129.1, 129.0, 128.9, 127.5, 58.5, 57.2, 54.8, 41.5, 37.5, 35.2, 31.8, 28.4, 20.4; HRMS m/z 470.2537 ($\text{C}_{30}\text{H}_{34}\text{N}_2\text{O}_3$ requires 470.2569); HPLC Purity (retention time): 86.7% (17.3 min.).

4-Methyl-N-[3-[[4-methylphenyl)sulfonyl]amino]-2-oxo-3S-(phenylmethyl)propyl]-N-(2-methylpropyl)benzenesulfonamide (27c). 92% mass yield; ^1H NMR (CDCl_3 , 300 MHz): δ 7.63 (d, J = 8 Hz, 2H), 7.52 (d, J = 8 Hz, 2H), 7.40-7.15 (cb, 7H), 6.98 (m, 2H), 5.51 (d, J = 7 Hz, 1H), 4.31 (d, J = 19 Hz, 1H), 4.14 (d, J = 19 Hz, 1H), 3.98 (q, J = 7 Hz, 1H), 2.97 (dd, J = 14, 7 Hz, 1H), 2.92-2.77 (cb, 3H), 2.43 (s, 3H), 2.41 (s, 3H), 1.57 (m, 1H), 0.80 (d, J = 7 Hz, 3H), 0.78 (d, J = 7 Hz, 3H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 204.6, 145, 144.3, 138, 137.5, 136, 130.8, 130.4, 130.1, 129.9, 128.4, 128.3, 128.0, 61.5, 56.9, 55.5, 38.7, 27.6, 22.0, 20.9; HRMS m/z 543.1995 ($\text{C}_{28}\text{H}_{35}\text{N}_2\text{O}_5\text{S}_2$ requires 543.1987); HPLC Purity (retention time): 70.4% (20.7 min).

N-[3-[[4-methylphenyl)sulfonyl](2-methylpropyl)amino]-2-oxo-1S-(phenylmethyl)propyl]benzenepropanamide (27d). 61% mass yield; ^1H NMR (CDCl_3 , 300 MHz): δ 7.63 (d, J = 8.0 Hz, 2H), 7.33-7.13 (cb, 10H), 7.09 (dd, J = 8, 2 Hz, 2H), 5.96 (d, J = 7 Hz, 1H), 4.75 (q, J = 7, 1H), 4.11 (d, J = 19 Hz, 1H), 3.91 (d, J = 19 Hz, 1H), 3.00 (dd, J = 14, 7 Hz, 1H), 2.95-2.80 (cb, 5H), 2.48 (dt, J = 15, 7 Hz, 1H), 2.45 (dt, J = 15, 7 Hz, 1H), 2.42 (s, 3H), 1.57 (m, 1H), 0.79 (d, J = 7 Hz, 6H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 204.1, 172.5, 143.8, 140.9, 137.2, 136.21, 129.9, 129.7, 129.4, 129.1, 128.8, 128.0, 127.8, 126.8, 57.1, 56.5, 55.8, 38.4, 37.6, 31.8, 27.2, 22.1, 20.4; HRMS m/z 521.2456 ($\text{C}_{30}\text{H}_{37}\text{N}_2\text{O}_4\text{S}_1$ requires 521.2474); HPLC Purity (retention time): 92.7% (20.2 min).

N-[3-acetylamino)-2-oxo-3S-(phenylmethyl)propyl]-N-(2-methylpropyl)benzenepropanamide (27e). 79% mass yield; ^1H NMR (CDCl_3 , 300 MHz, rotamers reported as major/minor components) δ 7.37-7.10 (cb, 10H), 6.15 (m, 1H), 4.78 (q, J = 7 Hz, 1H), 4.08/4.17 (d, J = 19, 1H), 3.93/4.03 (d, J = 19 Hz, 1H), 3.13/3.21 (dd, J = 14, 7 Hz, 1H), 3.07-2.79 (cb, 5H), 2.56-2.37 (cb, 2H), 2.12/1.96 (s, 3H), 1.72 (m, 1H), 0.91/0.87 (d, J = 7 Hz, 3H), 0.89/0.83 (d, J = 7 Hz, 3H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 204.6, 173.5, 172.1, 141.5, 137.3, 130.3, 129.6, 129.5, 129.3, 128.0, 127.2, 58.5, 58.2, 55.0, 38.8, 37.9, 32.3, 28.8, 22.0, 20.9; HRMS m/z 408.2402 ($\text{C}_{25}\text{H}_{32}\text{N}_2\text{O}_3$ requires 408.2413); HPLC Purity (retention time): 81.9% (11.0 min).

Ethyl[3-[[4-methylphenyl)sulfonyl](2-methylpropyl)amino]-2-oxo-1S-(phenylmethyl)propyl]carbamate (27f). 58% mass yield; ^1H NMR (CDCl_3 , 300 MHz): δ 7.63 (d, J = 8 Hz, 2H), 7.36-7.23 (cd, 5H), 7.18 (dd, J = 8, 2 Hz, 2H), 5.14 (d, J = 7 Hz, 1H), 4.53 (q, J = 7 Hz, 1H), 4.20 (d, J = 19 Hz, 1H), 4.09 (q, J = 7 Hz, 2H), 3.97 (d, J = 19 Hz, 1H), 3.04 (dd, J = 14, 7 Hz, 1H), 2.98-2.82 (cd, 3H), 2.42 (s, 3H), 1.58 m, 1H), 1.23 (t, J = 7 Hz, 3H), 0.81 (d, J = 7 Hz, 6H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 203.9, 156, 143, 136.5, 135.6, 129.4, 129.2, 128.9, 127.4, 127.3, 61.4, 58.1, 55.8, 55.1, 37.4, 26.7, 21.5, 19.9, 14.5; HRMS m/z 461.2107 ($\text{C}_{24}\text{H}_{33}\text{N}_2\text{O}_5\text{S}_1$ requires 461.2110); HPLC Purity (retention time): 90.5% (18.1 min).

Utilization of Product Quench- and Reactant Sequestering- CSR Polymers: Reaction of Grignard reactants with carbonyl compounds.

1-Phenyl-3-butene-1-ol (36a). 90% mass yield; ^1H NMR (CDCl_3): δ 2.06 (d, 1H), 2.56 (m, 2H), 4.78 (m, 1H), 5.20 (m, 2H), 5.85 (m, 1H), 7.33 (m, 5H); HRMS m/z 148.0866 ($\text{C}_{10}\text{H}_{12}\text{O}_1$ requires 148.0888); GC/MS Purity (retention time): >99% (3.30 min).

1-(1-Naphthyl)-3-butene-1-ol (36b). 99% mass yield; ^1H NMR (CDCl_3): δ 2.40 (s, 1H), 2.67 (m, 1H), 2.78 (m, 1H), 5.24 (m, 2H), 5.47 (m, 1H), 5.96 (m, 1H), 7.55 (m, 3H), 7.71

(m,1H), 7.84 (m,1H), 7.94 (m,1H), 8.11 (m,1H); HRMS m/z 198.1046 ($C_{14}H_{14}O_1$ requires 198.1044); GC/MS Purity (retention time): 97% (6.54 min).

1-(3-Methoxyphenyl)-3-butene-1-ol (36c). 96% mass yield; 1H NMR ($CDCl_3$): δ 2.18 (m,1H), 2.53 (m,2H), 3.85 (s,3H), 4.74 (m,1H), 5.19 (m,2H), 5.83 (m,1H), 6.84 (dd,1H), 6.95 (m,2H), 7.29 (t,1H); HRMS m/z 178.0986 ($C_{11}H_{24}O_2$ requires 178.0993); GC/MS Purity (retention time): 96% (4.75 min).

1-Phenyl-3-butene-1-ol (36d). 94% mass yield; 1H NMR ($CDCl_3$): δ 1.81 (m,3H), 2.24 (m,1H), 2.36 (m,1H), 2.77 (m,2H), 3.72 (bd,1H), 5.17 (d,1H), 5.21 (d,1H), 5.86 (m,1H), 7.27 (m,5H). HRMS m/z 176.1194 ($C_{12}H_{16}O_1$ requires 176.1201); GC/MS Purity (retention time): 95% (4.53 min).

1-(6-Methyl-2-pyridyl)-3-butene-1-ol (36e). 99% mass yield; 1H NMR ($CDCl_3$): δ 2.55 (m,2H), 2.63 (s,3H), 4.85 (m,1H), 5.10 (m,2H), 5.88 (m,1H), 7.14 (m,2H), 7.66 (t,1H); HRMS m/z 163.0984 ($C_{10}H_{13}N_1O_1$ requires 163.0970); GC/MS Purity (retention time): 99% (5.53 min).

1-(5-Methyl-2-furyl)-3-butene-1-ol (36f). 88% mass yield; HRMS m/z 152.0838 ($C_9H_{12}N_1O_2$ requires 152.0837); GC/MS Purity (retention time): >99% (2.75 min).

Utilization of Product Quench- and Reactant Sequestering- CSR Polymers: Reaction of *n*-butyllithium reactions with carbonyl compounds.

2-Methyl-4-octanol (36g). No mass yield was obtained due to volatility; EIMS M/z : 87, 69; GC/MS Purity (retention time): 88% (2.25 min).

1-Phenyl-1-pentanol (36h). 97% mass yield; 1H NMR ($CDCl_3$): δ 0.93 (t,3H), 1.39 (m,4H), 1.78 (m,2H), 2.00 (bs,1H), 4.69 (t,1H), 7.33 (m,5H); HRMS m/z 164.1200 ($C_{11}H_{16}O_1$ requires 164.1201); GC/MS Purity (retention time): 97% (3.99 min).

1-(1-Naphthyl)-1-pentanol (36i). 94% mass yield; 1H NMR ($CDCl_3$): δ 0.96 (t,3H), 1.43 (m,4H), 1.97 (m,2H), 2.18 (bs,1H), 5.48 (t,1H), 7.56 (m,3H), 7.66 (d,1H), 7.70 (d,1H), 7.93 (d,1H), 8.15 (d,1H); HRMS m/z 214.1363 ($C_{15}H_{18}O_1$ requires 214.1357); GC/MS Purity (retention time): 97% (7.09 min).

1-(3-Methoxyphenyl)-1-pentanol (36j). 88% mass yield; 1H NMR ($CDCl_3$): δ 0.92 (t,3H), 1.33 (m,4H), 1.76 (m,2H), 2.20 (bs,1H), 3.83 (s,3H), 4.64 (t,1H), 6.82 (m,1H), 6.94 (m,2H), 7.28 (t,1H); HRMS m/z 194.1305 ($C_{12}H_{18}O_2$ requires 194.1306); GC/MS Purity (retention time): 93% (5.42 min).

1-Phenyl-3-heptanol (36k). 94% mass yield; 1H NMR ($CDCl_3$): δ 0.97 (t,3H), 1.43 (m,6H), 1.81 (m,2H), 2.74 (m,3H), 3.67 (m,1H), 7.29 (m,5H); HRMS m/z 192.1511 ($C_{13}H_{20}O_1$ requires 192.1514); GC/MS Purity (retention time): >99% (5.22 min).

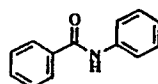
1-(6-Methyl-2-pyridyl)-1-pentanol (36l). 90% mass yield; 1H NMR ($CDCl_3$): δ 0.92 (t,3H), 1.39 (m,4H), 1.67 (m,1H), 1.81 (m,1H), 2.57 (s,3H), 4.72 (m,1H), 7.05 (d,2H), 7.60

(t,1H); HRMS m/z 179.1300 ($C_{11}H_{17}N_1O_1$ requires 179.1283); GC/MS Purity (retention time): 78% (4.41 min).

1-(5-Methyl-2-furyl)-1-pentanol (36m). 89% mass yield; 1H NMR ($CDCl_3$): δ 0.93 (t,3H), 1.37 (m,4H), 1.84 (m,2H), 2.30 (s,3H), 4.62 (t,1H), 5.92 (m,1H), 6.11 (m,1H); HRMS m/z 168.1145 ($C_{10}H_{16}O_2$ requires 168.1150); GC/MS Purity (retention time): >99% (3.41 min).

POOR QUALITY ORIGINAL

Compound 11a

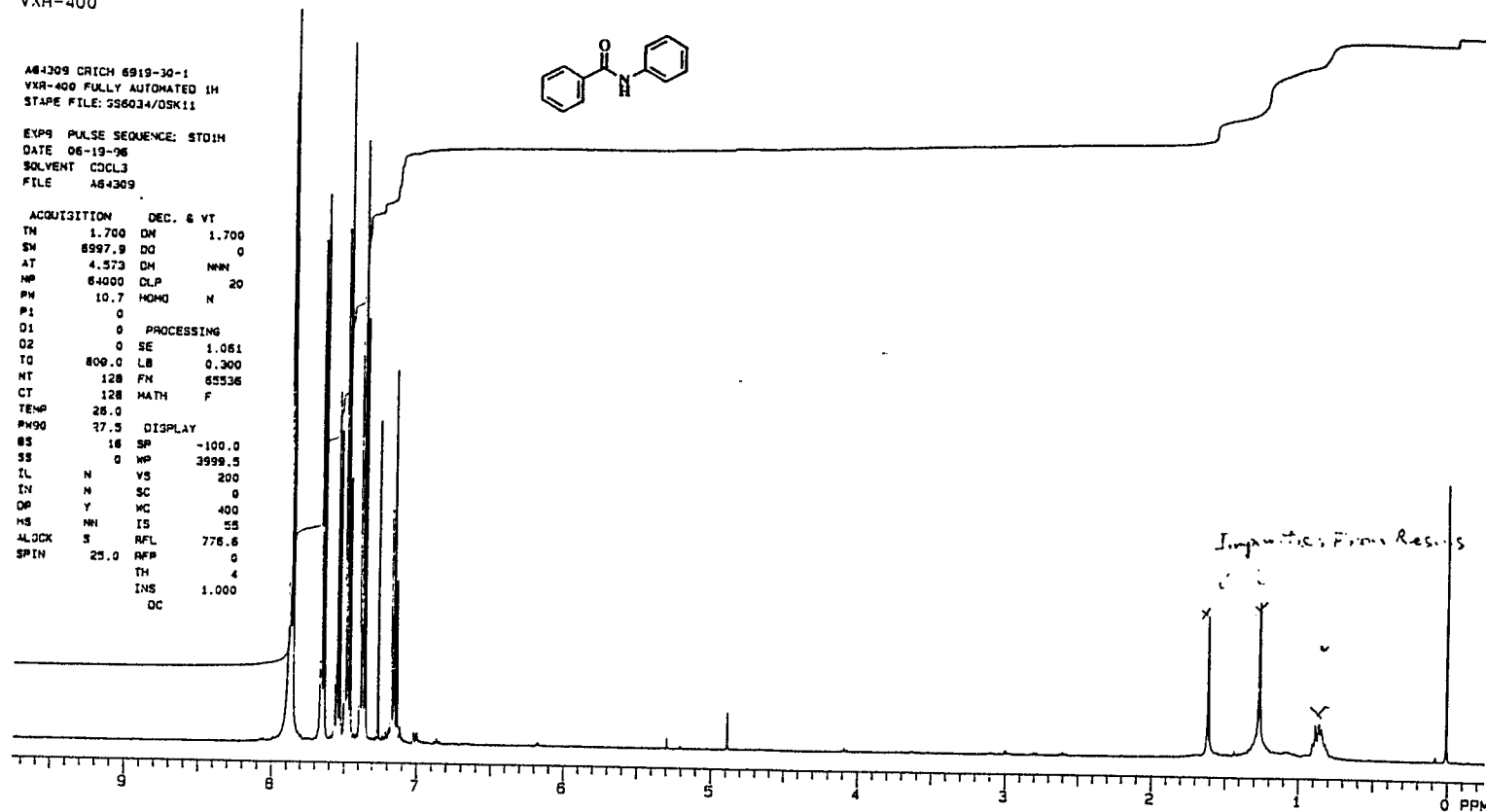


VXR-400

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STAPE FILE: 336034/DSK11

EXP9 PULSE SEQUENCE: STD1H
DATE 06-19-96
SOLVENT CDCL3
FILE A64309

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AT	4.573	DM	NNN
NP	64000	DLP	20
PH	10.7	HOMO	N
P1	0		
D1	0	PROCESSING	
D2	0	SE	1.061
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CT	128	MATH	F
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SS	0	WP	3999.5
IL	N	VS	200
IN	N	SC	0
DP	Y	WC	400
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		QC	



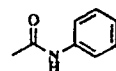
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Compound 11b

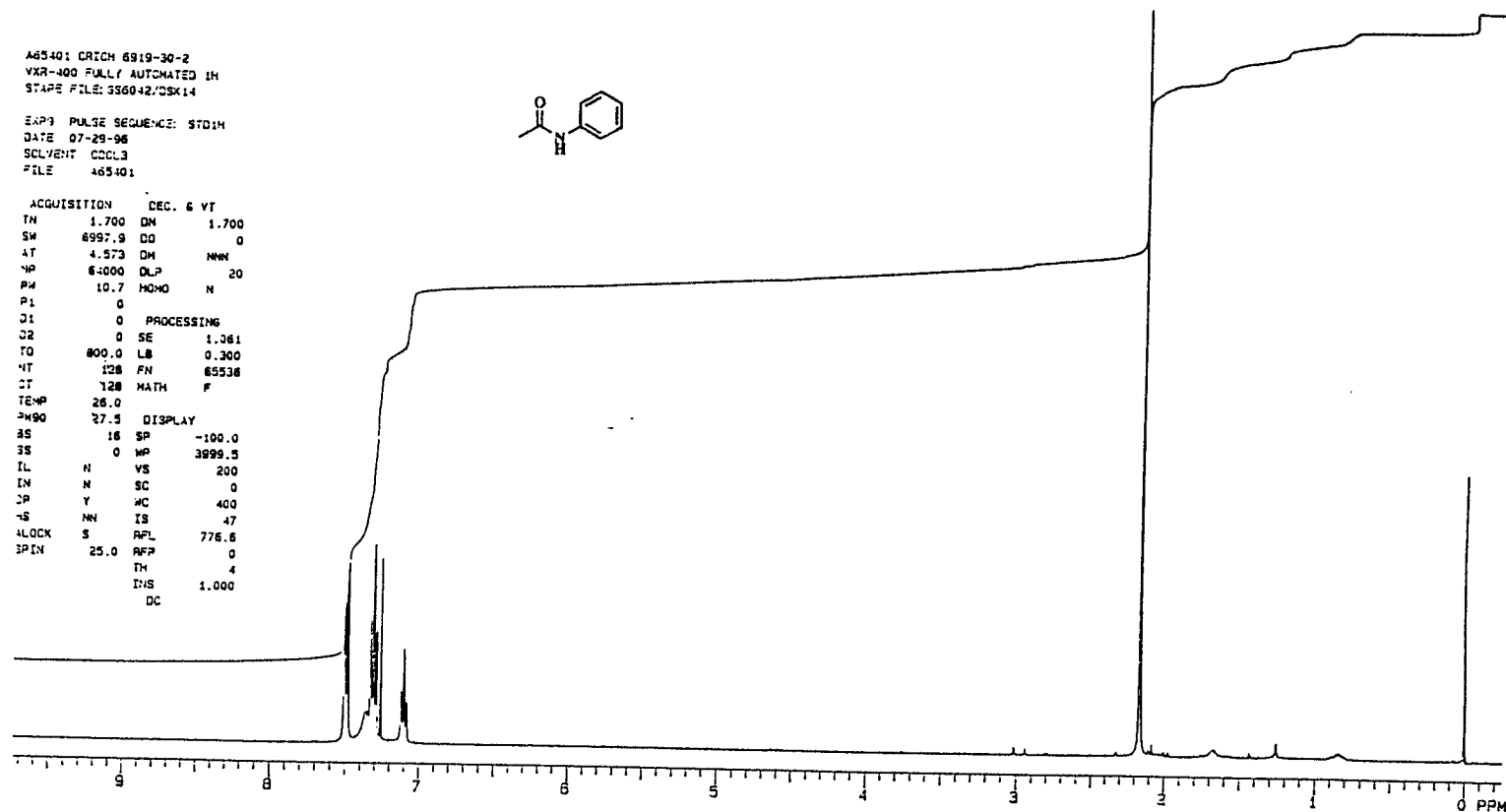
VXR-400

A65401 CRICH 6919-30-2
VXR-400 FULLY AUTOMATED 1H
STAPE FILE: 336042/CSK14

EXP3 PULSE SEQUENCE: STD1H
DATE 07-29-96
SOLVENT CDCL3
FILE A65401



ACQUISITION		DEC. & VT	
IN	1.700	DM	1.700
SW	6997.9	DO	0
AT	4.573	DM	MMN
WD	6.000	DLP	20
PH	10.7	MONO	N
PI	0		
CI	0	PROCESSING	
CI	0	SE	1.081
TO	800.0	LB	0.300
MT	128	FN	65536
CT	128	MATH	F
TEMP	26.0		
PH90	27.5	DISPLAY	
AS	16	SP	-100.0
SS	0	WP	3999.5
IL	N	VS	200
IN	N	SC	0
CP	Y	WC	400
RS	NN	IS	47
ALOCK	S	RFL	776.6
SPIN	25.0	RFP	0
		TH	4
		INS	1.000
		DC	



PLOT SCALE = 99.99 HZ/CM

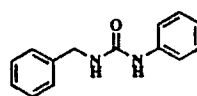
POOR QUALITY ORIGINAL

Compound 10c

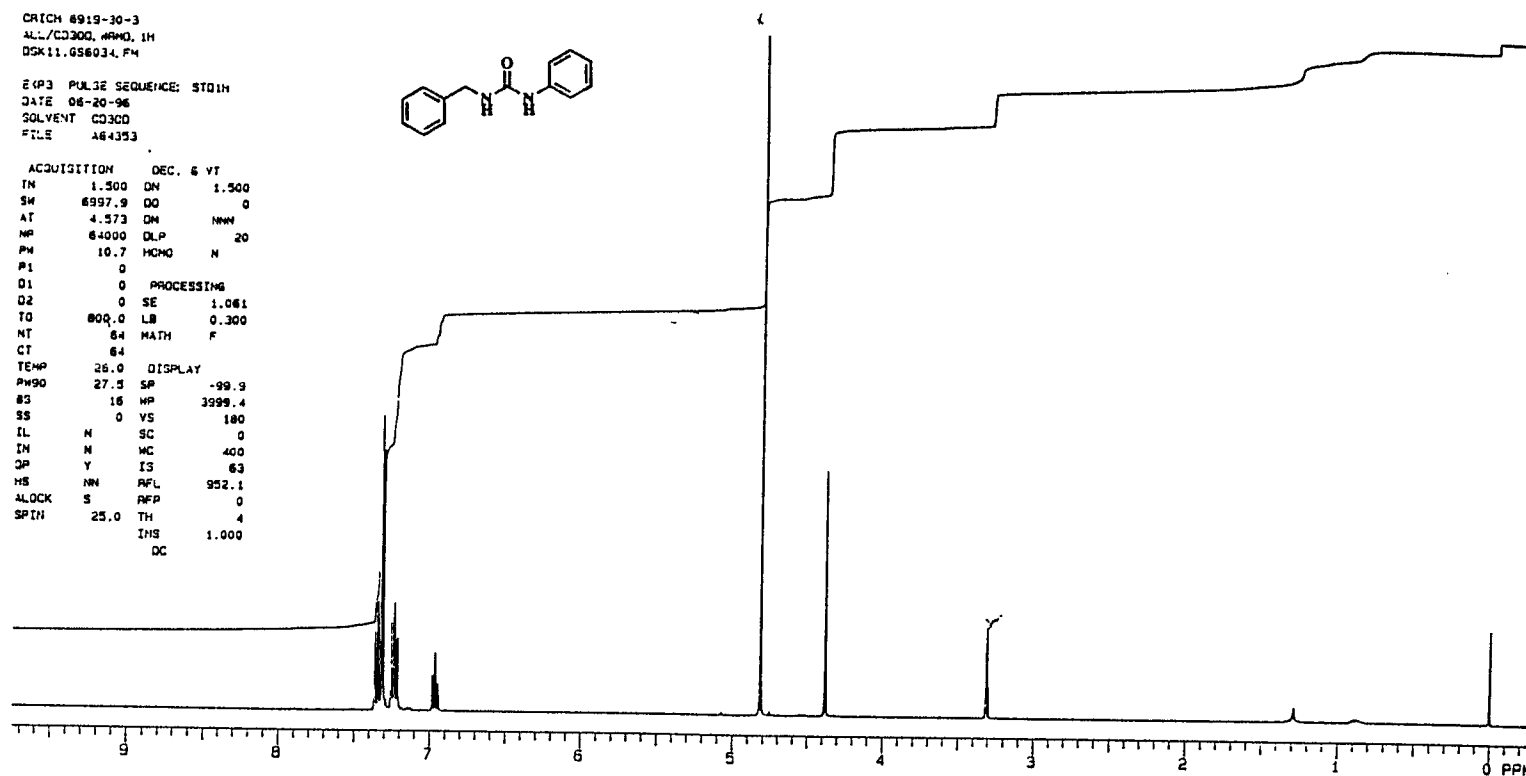
VXR-400

CRICH 8919-30-3
ALL/CD300, 4000, 1H
DSK11.058034.FM

EXP3 PULSE SEQUENCE: STQ1H
DATE 06-20-96
SOLVENT CD300
FILE A64353



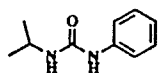
ACQUISITION	DEC. & VT
IN 1.500	DN 1.500
SW 6997.9	DO 0
AT 4.573	DM NNM
NP 64000	DLP 20
PH 10.7	MCNO N
P1 0	
D1 0	PROCESSING
D2 0	SE 1.061
TO 800.0	LB 0.300
NT 64	MATH F
CT 64	
TEMP 25.0	DISPLAY
PH90 27.5	SP -99.9
ES 16	WP 3999.4
SS 0	VS 180
IL N	SC 0
IN N	MC 400
OP Y	IS 63
HS NM	RFL 952.1
ALOCK S	RFP 0
SPIN 25.0	TH 4
	IHS 1.000
	DC



PLOT SCALE = 99.99 HZ/CM

POOR QUALITY ORIGINAL

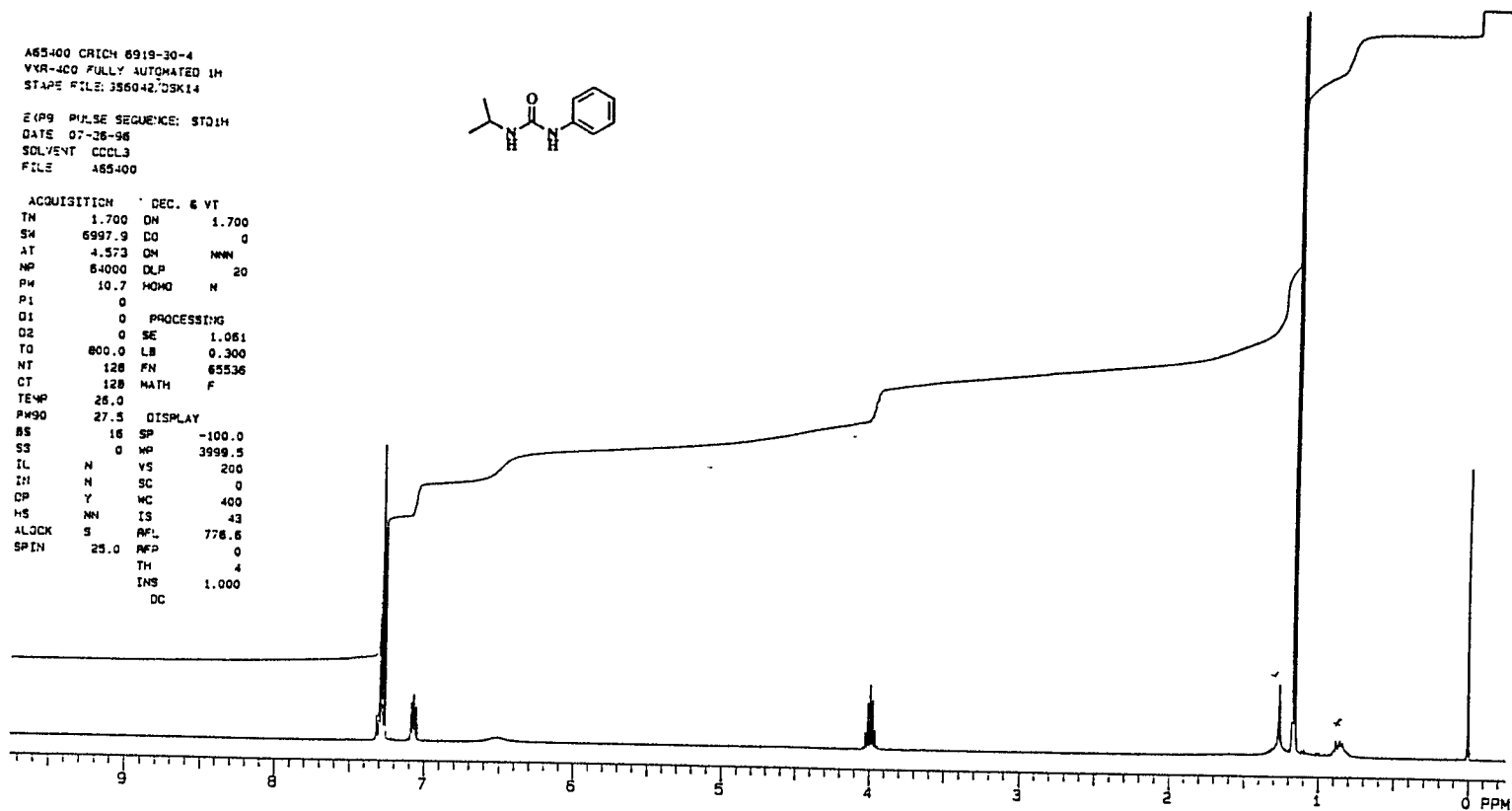
Compound 10d



A65400 CRICH 6919-30-4
VXR-400 FULLY AUTOMATED 1H
STAPE FILE: J56042.DSK14

E (P9) PULSE SEQUENCE: STD1H
DATE 07-26-96
SOLVENT CDCL3
FILE A65400

ACQUISITION		DEC. & VT	
TM	1.700	DM	1.700
SM	6997.9	DO	0
AT	4.573	DM	NNN
NP	64000	DLP	20
PM	10.7	HOMO	N
P1	0		
D1	0	PROCESSING	
D2	0	SE	1.061
TQ	800.0	LB	0.300
NT	128	FN	65536
CT	128	MATH	F
TEMP	26.0		
PM90	27.5	DISPLAY	
BS	16	SP	-100.0
SS	0	WP	3999.5
IL	N	VS	200
ZI	N	SC	0
DP	Y	WC	400
HS	NN	IS	43
ALOCK	S	APL	776.6
SPIN	25.0	APF	0
		TH	4
		INS	1.000
		DC	



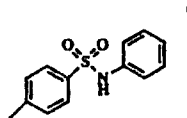
PLOT SCALE = 99.99 HZ/CM

Compound 13e

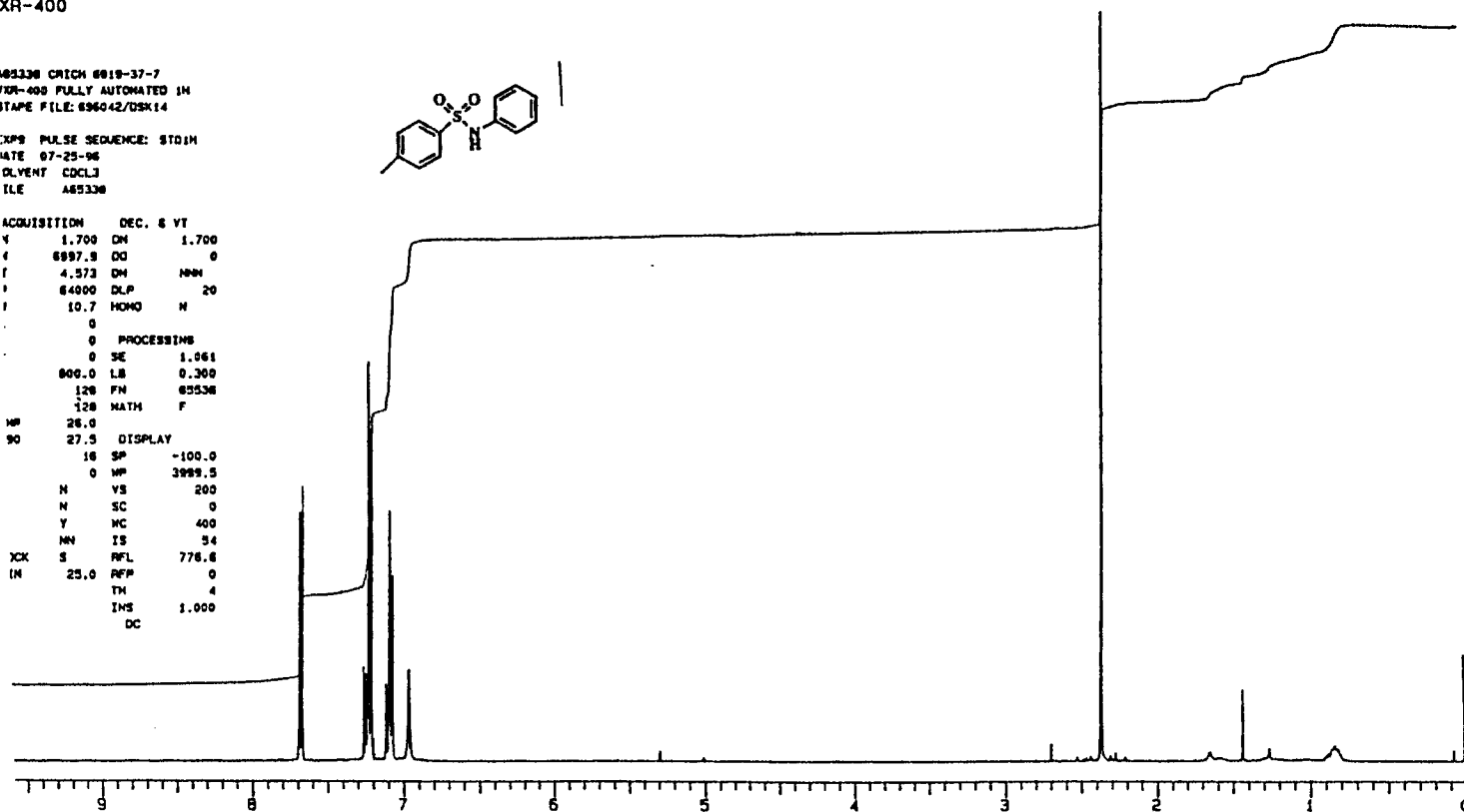
XR-400

485336 CRICH 6819-37-7
XR-400 FULLY AUTOMATED IN
TAPE FILE: 686042/DSK14

XP9 PULSE SEQUENCE: STD1H
DATE 07-25-96
SOLVENT CDCL3
FILE 485336



ACQUISITION	DEC. & VT
1 1.700 DM	1.700
4 6897.8 DO	0
1 4.573 DM	MM
1 64000 DLP	20
1 10.7 HOMO	N
0	
0 PROCESSING	
0 SE	1.061
800.0 LB	0.300
128 FN	65536
128 MATH	F
MP 26.0	
90 27.5 DISPLAY	
16 SP	-100.0
0 MP	3999.5
N VS	200
N SC	0
Y WC	400
MM IS	54
XK S RFL	776.6
IN 25.0 RFP	0
	TH 4
	INS 1.000
	DC



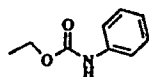
1T SCALE = 99.99 HZ/CM

Compound 12f

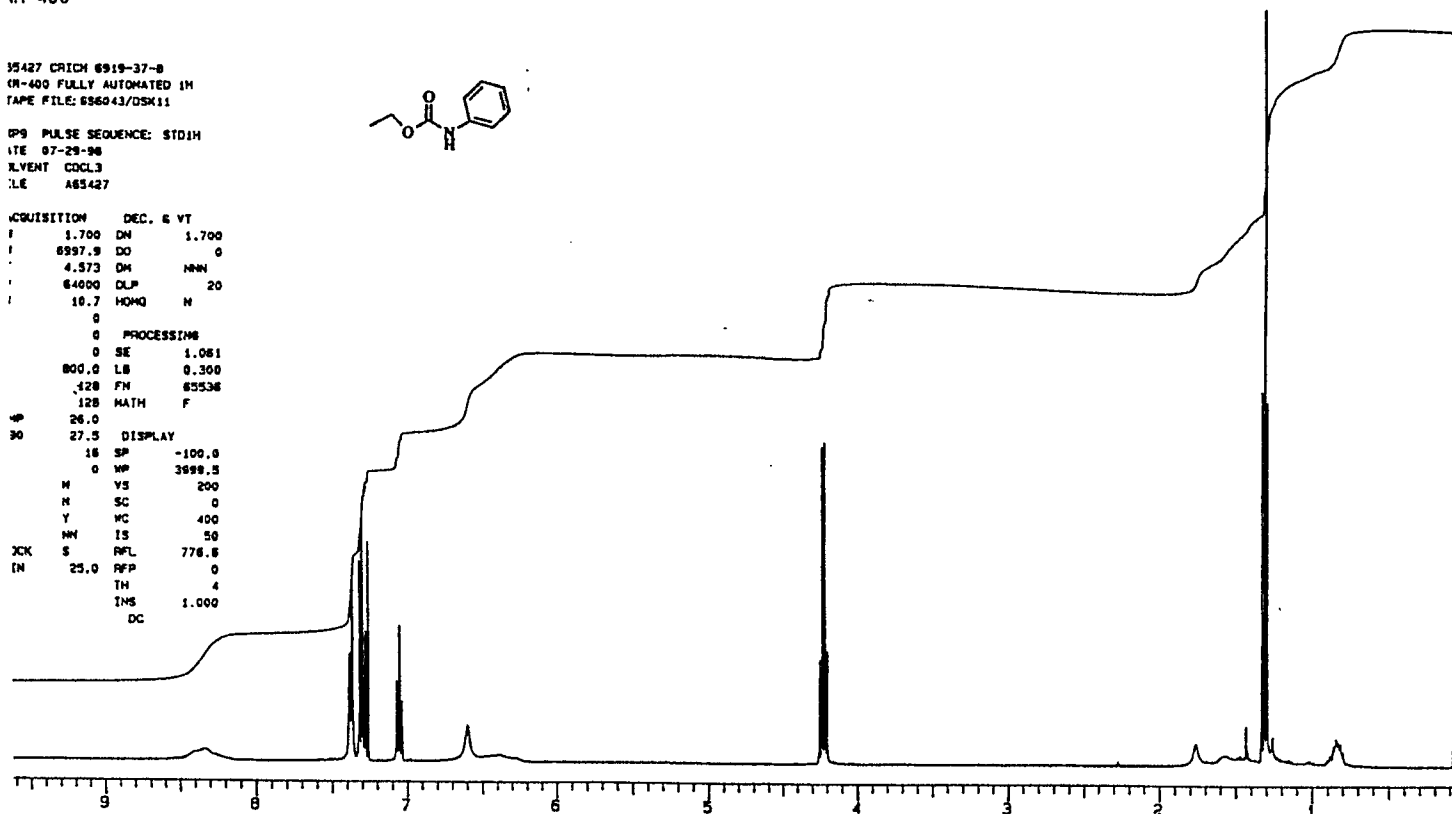
(R-400

35427 CRICH 6919-37-8
CR-400 FULLY AUTOMATED 1H
TAPE FILE: 686043/DSK11

PP9 PULSE SEQUENCE: STD1H
ITE 97-29-96
SOLVENT CDCL3
FILE A65427



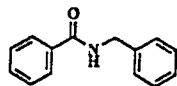
ACQUISITION	DEC. & VT
1 1.700 DM 1.700	
1 6997.9 DO 0	
1 4.573 DM NNN	
1 64000 DLP 20	
1 10.7 HOMO H	
0	
0 PROCESSING	
0 SE 1.061	
800.0 LB 0.300	
128 FM 65536	
128 MATH F	
MP 26.0	
30 27.5 DISPLAY	
16 SP -100.0	
0 MP 3699.5	
M VS 200	
N SC 0	
Y MC 400	
MM IS 50	
XX S RPL 776.6	
IN 25.0 RFP 0	
TH 4	
INS 1.000	
DC	



POOR QUALITY ORIGINAL

VXR-400

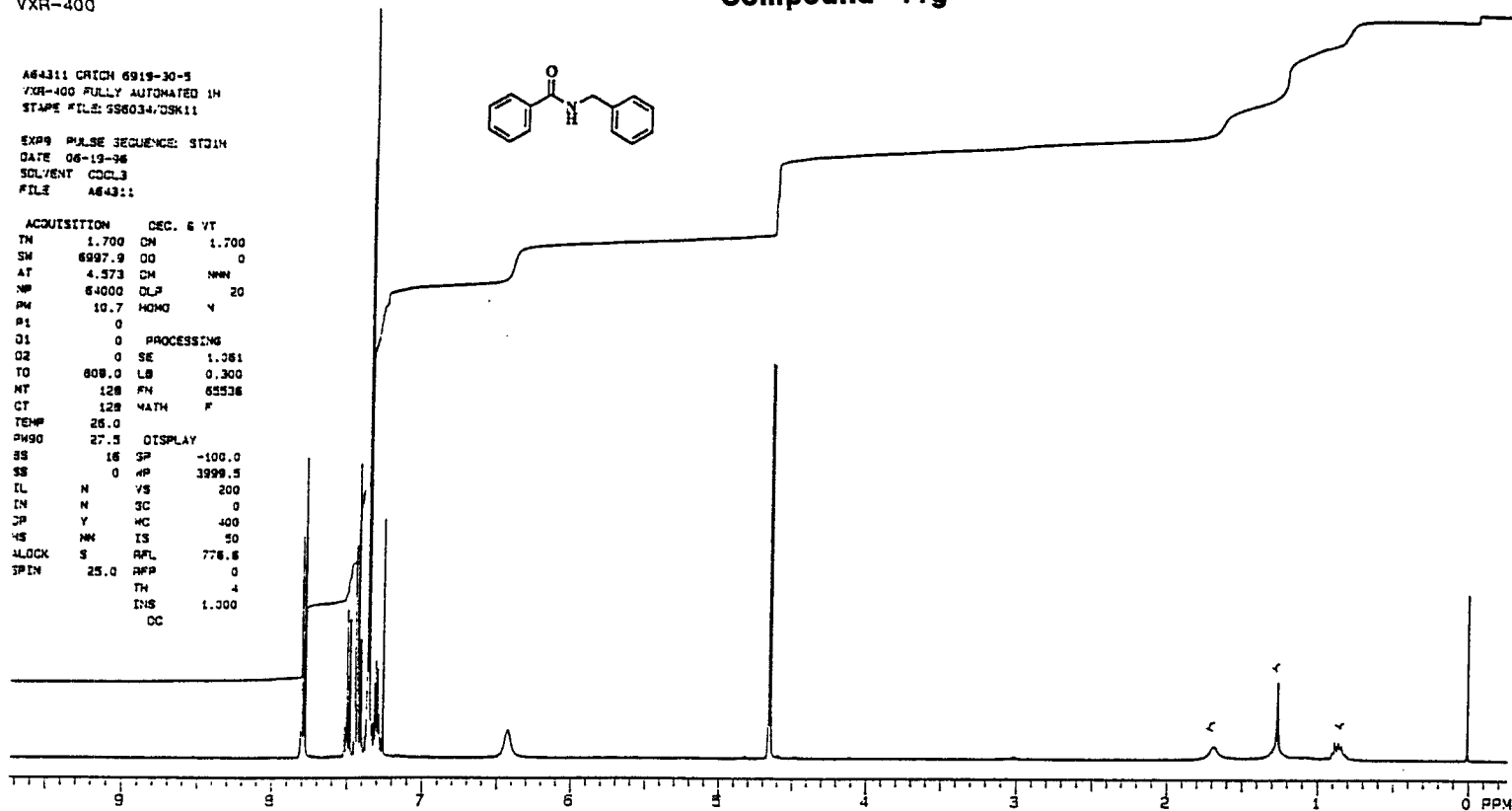
Compound 11g



A64311 CRICH 6919-30-5
VXR-400 FULLY AUTOMATED IN
STAPE #FILE: 996034/DSK11

EXP9 PULSE SEQUENCE: ST2IN
DATE 06-12-96
SOLVENT CDCL3
FILE A64311

ACQUISITION		DEC. 6 VT	
TM	1.700	CM	1.700
SM	6997.9	OO	0
AT	4.573	CM	NNN
NP	64000	OLP	20
PM	10.7	HOMO	V
P1	0		
Q1	0	PROCESSING	
Q2	0	SE	1.061
TO	608.0	LB	0.300
MT	128	FM	65536
CT	128	MATH	F
TEMP	25.0		
PH90	27.5	DISPLAY	
SS	16	SP	-100.0
SS	0	HP	3999.5
IL	N	VS	200
IN	N	SC	0
CP	Y	MC	400
HS	NN	IS	50
ALOCK	S	RPL	776.6
SPIN	25.0	RFP	0
		TH	4
		INS	1.000
		DC	

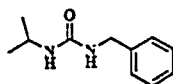


PLOT SCALE = 99.99 HZ/CM

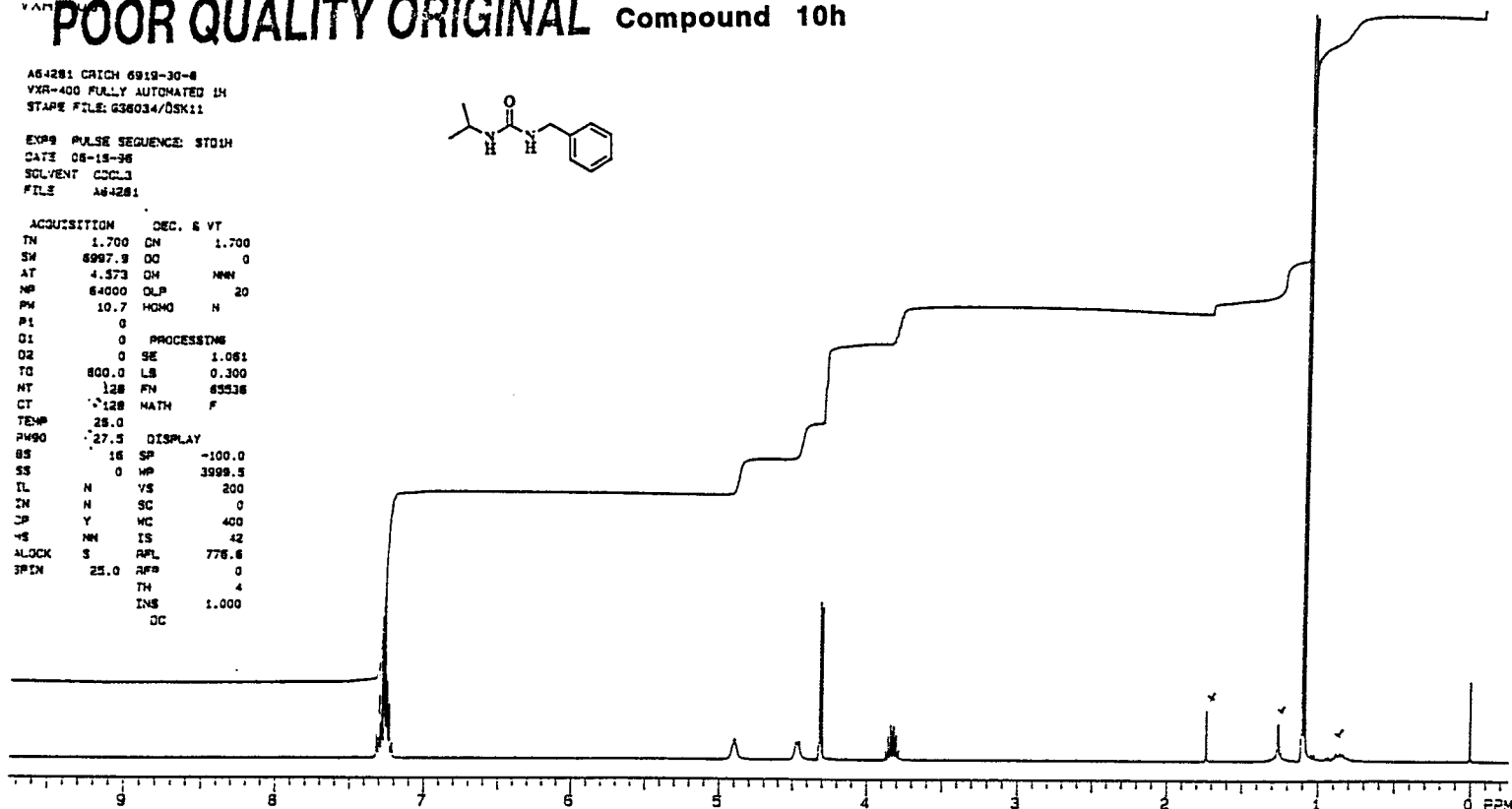
POOR QUALITY ORIGINAL Compound 10h

AS4281 CRICH 6919-30-8
VXR-400 FULLY AUTOMATED IN
STATE FILE: 636034/DSK11

EXP# PULSE SEQUENCE: STD1H
DATE 08-18-96
SOLVENT CDCL3
FILE AS4281



ACQUISITION		DEC. & VT	
TD	1.700	ON	1.700
SW	6997.9	DO	0
AT	4.573	ON	MM
NP	64000	OLP	20
PM	10.7	HOMO	N
P1	0		
O1	0	PROCESSING	
O2	0	SE	1.061
TD	800.0	LS	0.300
NT	128	FN	65536
CT	128	MATH	F
TEMP	28.0		
PM90	27.5	DISPLAY	
SS	16	SP	-100.0
SS	0	WP	3999.5
IL	N	VS	200
IN	N	SC	0
CP	Y	MC	400
VS	NN	IS	42
ALOCK	S	RPL	776.6
SPIN	25.0	RFP	0
		TH	4
		INS	1.000
		DC	

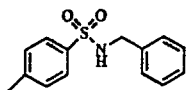


PLOT SCALE = 99.99 HZ/CM

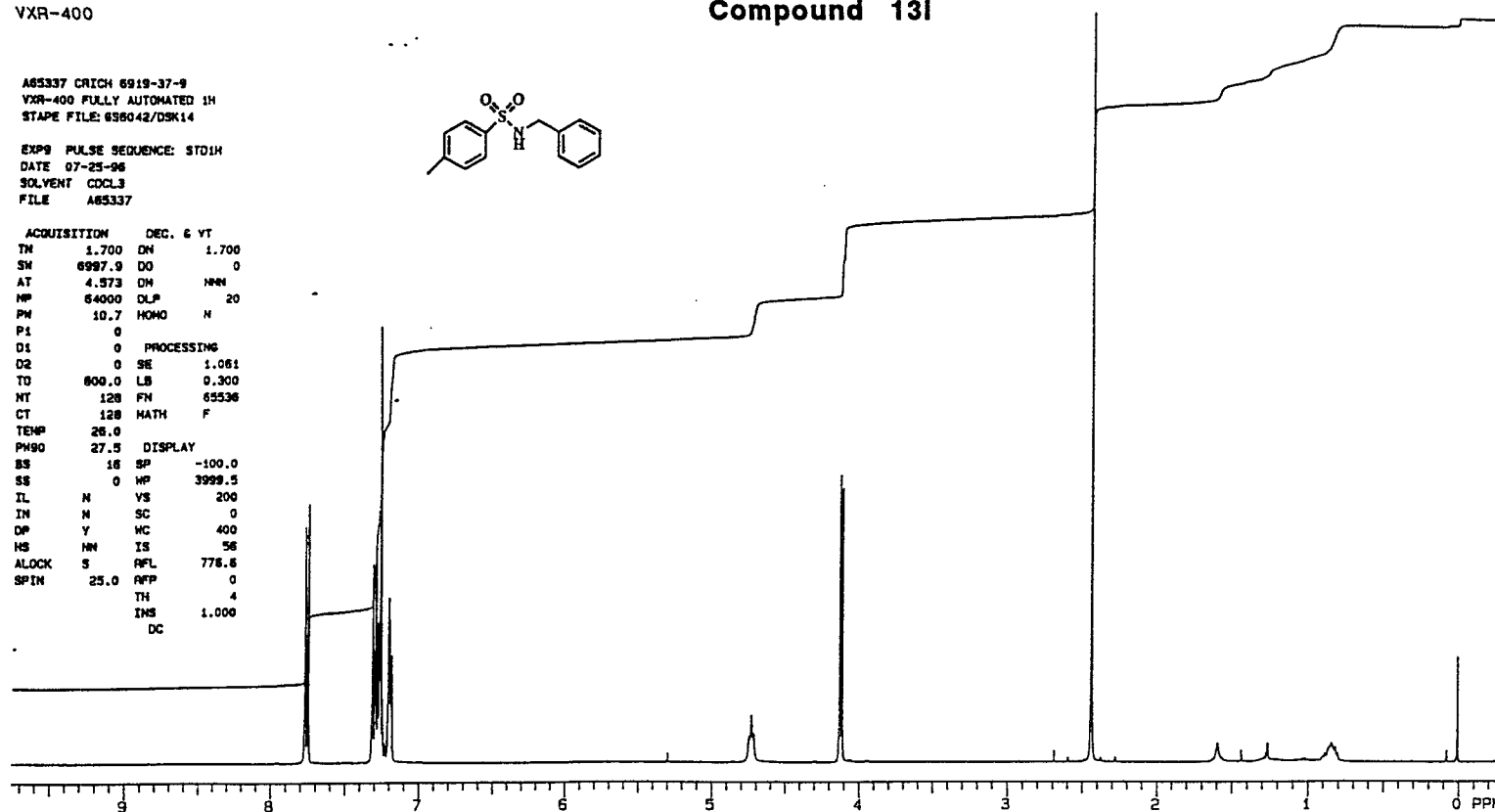
VXR-400

Compound 13l

A85337 CRICH 6919-37-9
VXR-400 FULLY AUTOMATED 1H
STAPE FILE: 696042/DSK14
EXP9 PULSE SEQUENCE: STD1H
DATE 07-25-96
SOLVENT CDCL3
FILE A85337



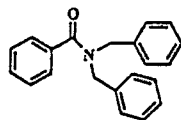
ACQUISITION		DEC. & VT	
TM	1.700	DN	1.700
SN	6997.9	DO	0
AT	4.573	DN	MM
MP	64000	OLP	20
PH	10.7	HOMO	N
P1	0		
D1	0	PROCESSING	
D2	0	SE	1.061
TD	600.0	LS	0.300
MT	128	FM	65536
CT	128	MATH	F
TEMP	26.0		
PH90	27.5	DISPLAY	
BS	16	SP	-100.0
SS	0	HP	3999.5
IL	N	VS	200
IN	N	SC	0
DP	Y	WC	400
HS	NN	IS	56
ALOCK	S	RFL	776.6
SPIN	25.0	RFP	0
		TH	4
		INS	1.000
		DC	



PLOT SCALE = 99.99 HZ/CM

Compound 11j

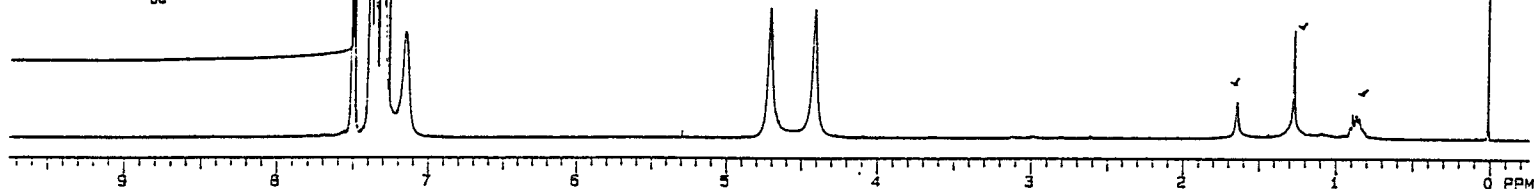
VXR-400



A64282 CRICH 6918-30-9
VXR-400 FULLY AUTOMATED IN
STAPE FILE: 336034/03K11

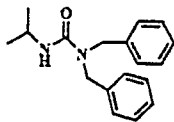
EXP9 PULSE SEQUENCE: STDIN
DATE 06-18-96
SOLVENT CDCL3
FILE A64282

ACQUISITION		DEC. & VT	
TH	1.700	DM	1.700
SH	6997.9	DD	0
AT	4.573	DM	MMH
HP	64000	DLP	20
PH	10.7	HOMO	N
PI	0		
DI	0	PROCESSING	
DZ	0	SE	1.061
TD	600.0	LS	0.300
NT	128	FM	65536
CT	128	MATH	F
TEMP	26.0		
PH90	27.5	DISPLAY	
BS	16	SP	-100.0
SS	0	WP	3999.5
IL	N	VS	200
IN	N	SC	0
OP	Y	MC	400
HS	NH	IS	52
ALOCK	S	RPL	776.6
3PIN	25.0	RFP	0
		TH	4
		INS	1.000
		OC	



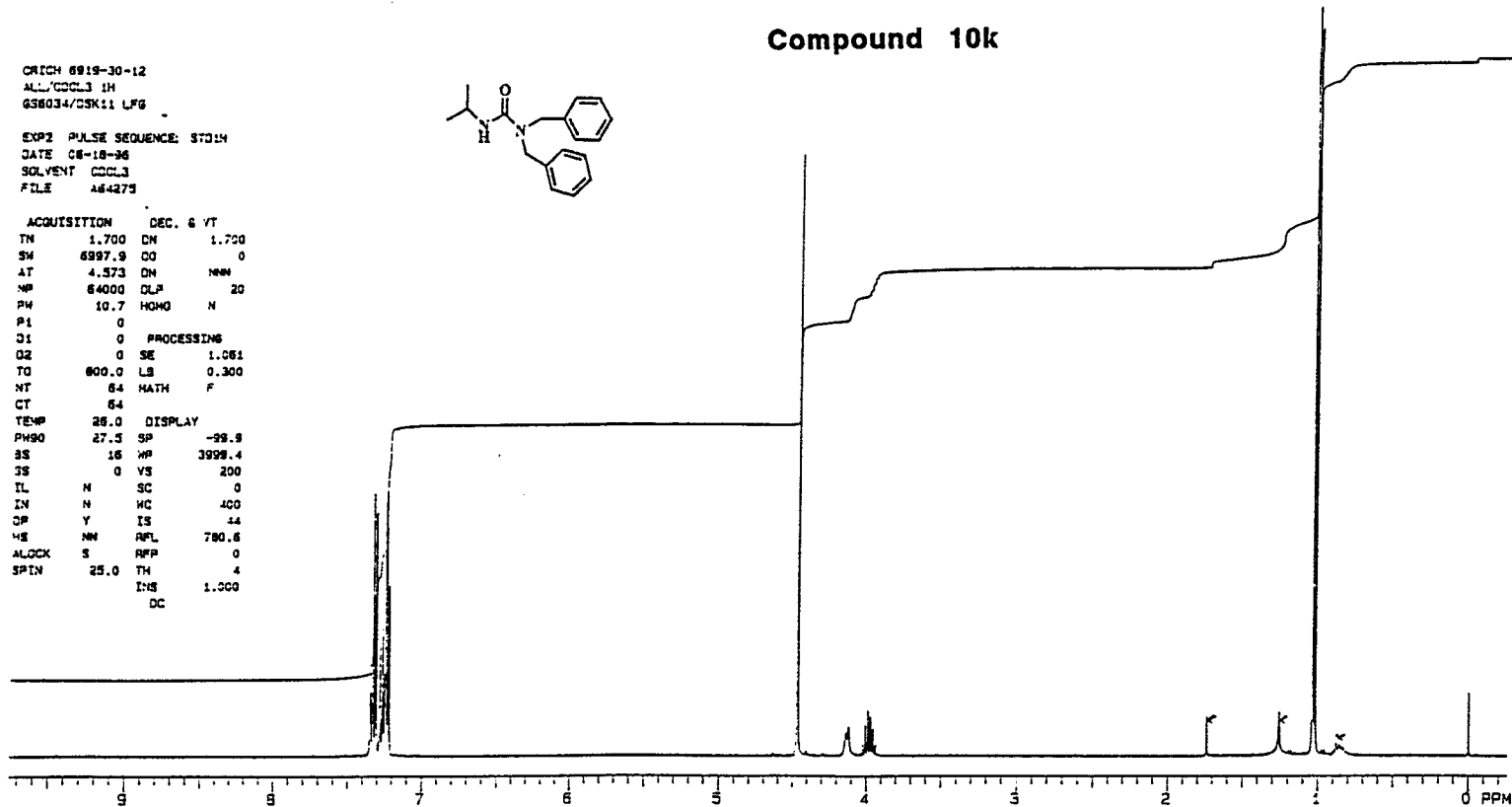
PLOT SCALE = 99.99 HZ/CM

Compound 10k



ORIG 8919-30-12
ALL/COOL3 1H
G38034/CSK11 LFG
EXP2 PULSE SEQUENCE: STD1H
DATE 08-18-96
SOLVENT COOL3
FILE A64275

ACQUISITION		DEC. & VT	
TM	1.700	DN	1.700
SM	6997.9	CO	0
AT	4.573	DN	NON
MP	64000	OLP	20
PW	10.7	HOMO	N
P1	0		
D1	0	PROCESSING	
D2	0	SE	1.051
TD	800.0	LS	0.300
NT	64	MATH	F
CT	64		
TEMP	26.0	DISPLAY	
PH90	27.5	SP	-99.9
SS	16	WP	3998.4
SS	0	VS	200
TL	N	SC	0
IN	N	HC	400
OP	Y	IS	44
HS	NN	RPL	780.6
ALOCK	S	RFP	0
SPIN	25.0	TH	4
		INS	1.000
		DC	

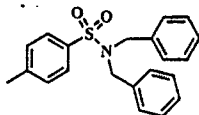


PLOT SCALE = 99.99 HZ/CM

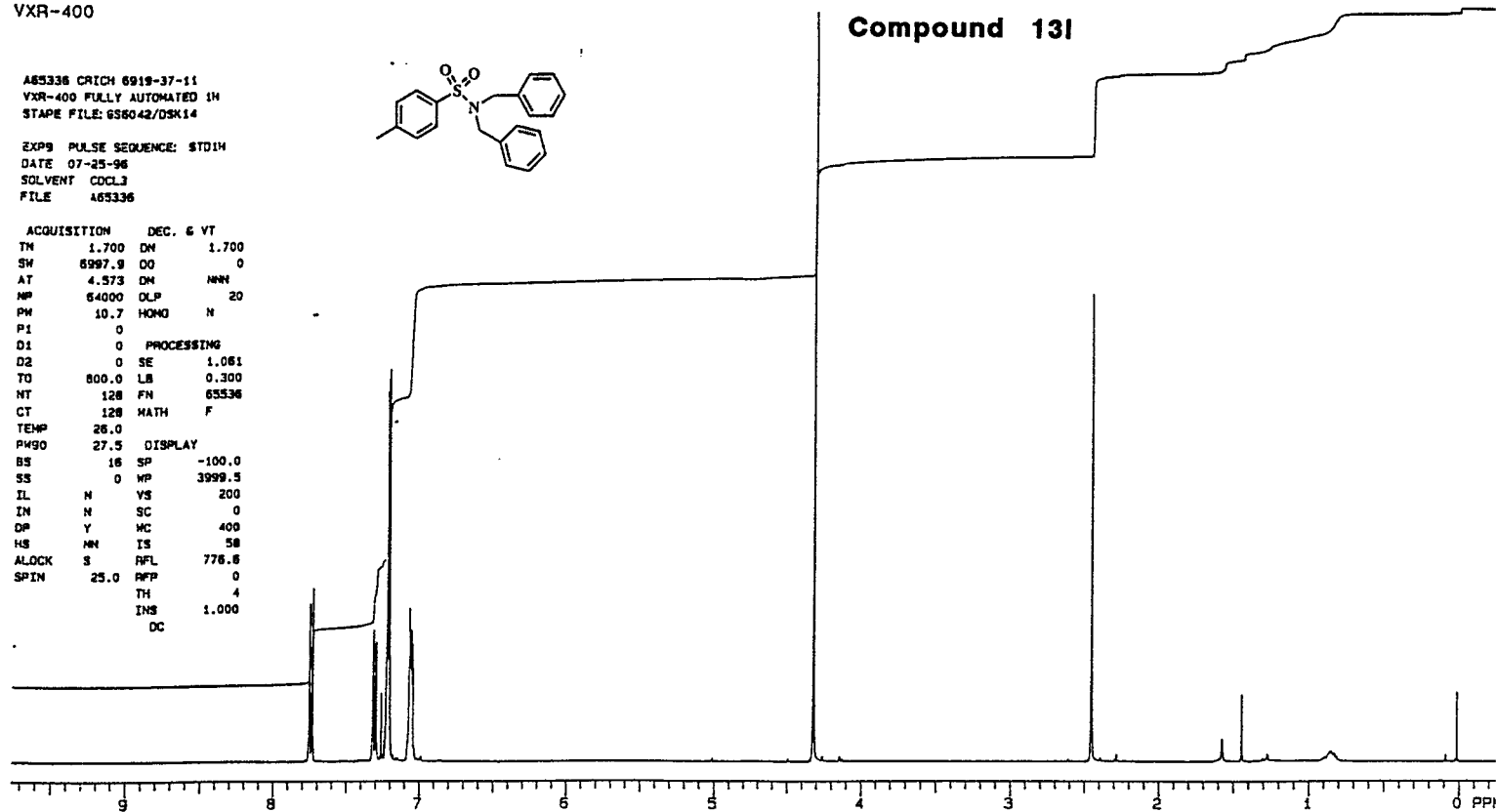
VXR-400

A65336 CRICH 6919-37-11
VXR-400 FULLY AUTOMATED 1H
STAPE FILE: 6S6042/DSK14

EXP9 PULSE SEQUENCE: STD1H
DATE 07-25-96
SOLVENT CDCL3
FILE A65336

**Compound 13I**

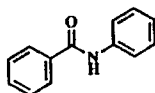
ACQUISITION		DEC. & VT	
TM	1.700	DM	1.700
SM	6997.9	OO	0
AT	4.573	DM	NN
NP	64000	OLP	20
PM	10.7	HOMO	N
P1	0		
D1	0	PROCESSING	
D2	0	SE	1.061
TD	800.0	LB	0.300
NT	128	FN	65536
CT	128	MATH	F
TEMP	26.0		
PM90	27.5	DISPLAY	
BS	16	SP	-100.0
SS	0	WP	3999.5
IL	N	VS	200
IN	N	SC	0
DP	Y	MC	400
HS	NN	IS	58
ALOCK	S	RFL	776.6
SPIN	25.0	RFP	0
		TH	4
		INS	1.000
		DC	



PLOT SCALE = 99.99 HZ/CM

Compound 11a

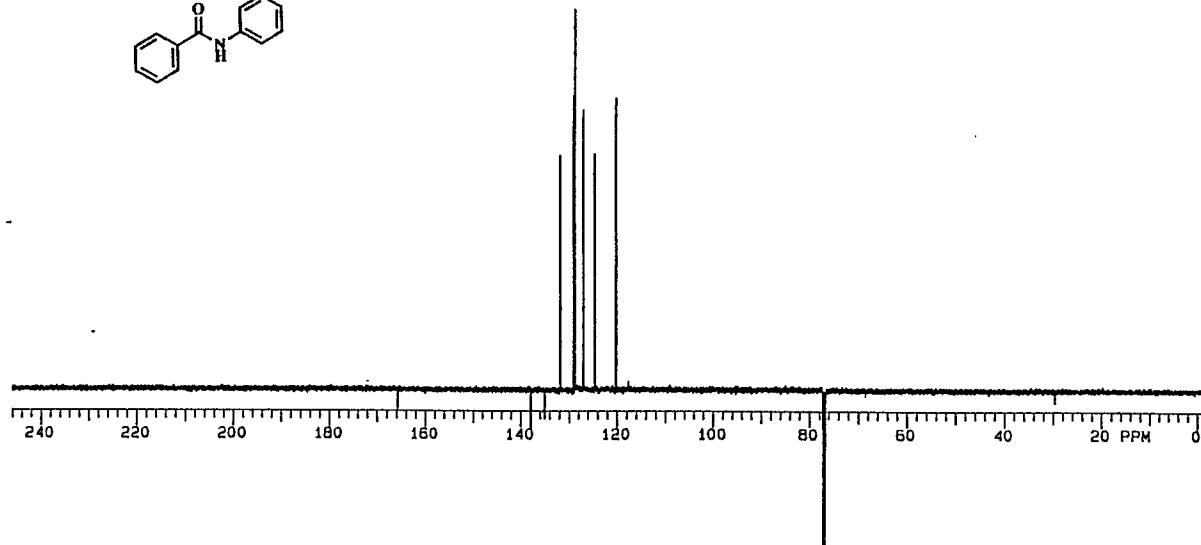
VXR-500



CRICH 6918-30-1
1H SOL/CDCL3 WARMED APT
DSK10/MS6014 AM

EXP4 PULSE SEQUENCE: APT30
DATE 08-19-98
SOLVENT CDCL3
FILE 864309

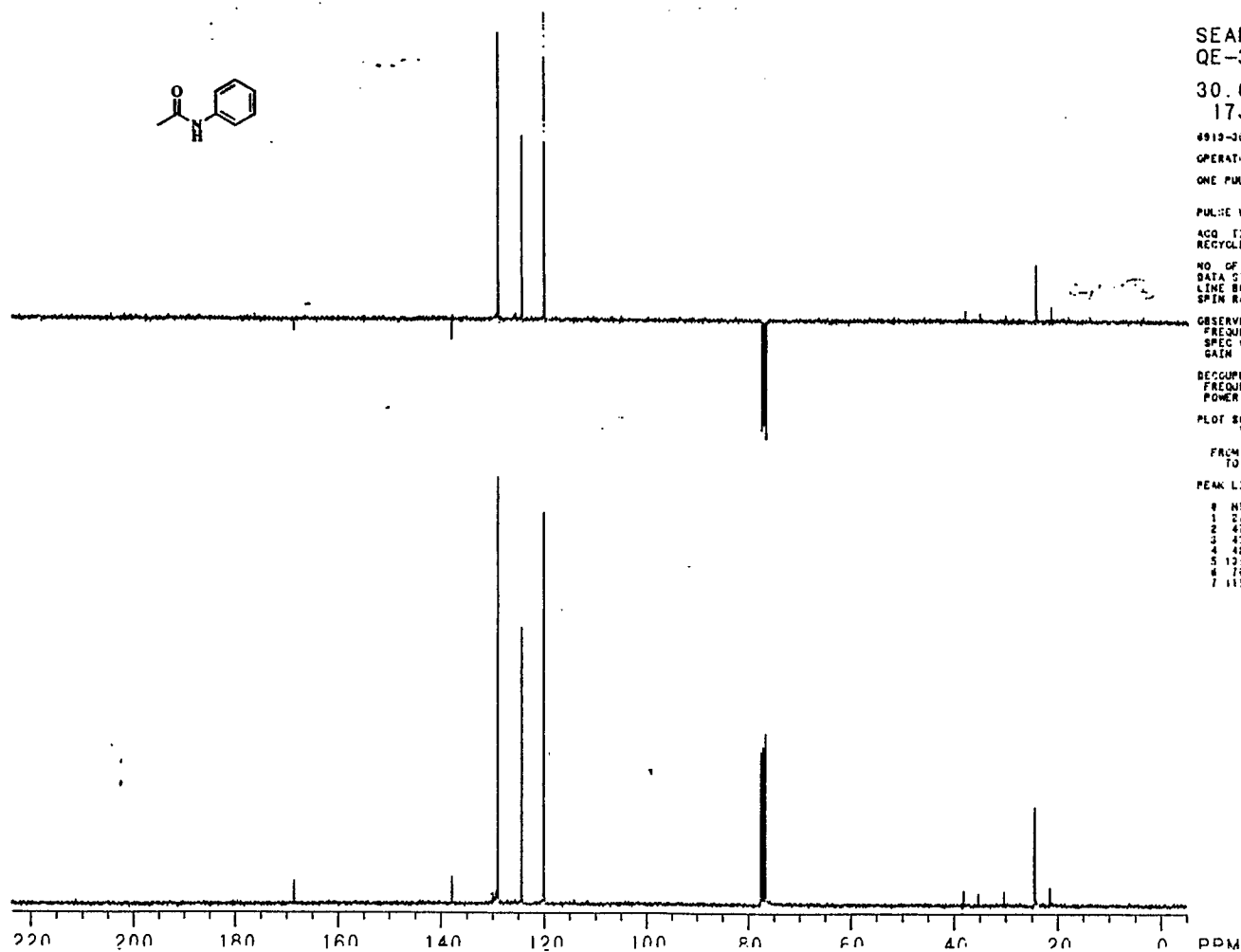
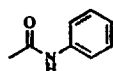
ACQUISITION		DEC. & VT	
TM	13.000	DM	1.000
SM	34965.0	DO	-290.0
AT	0.815	DM	YNY
MP	64000	DMH	S
PM	7.5	DHF	10400
PI	21.8	DHF	36.0
DI	1.000	HOMO	N
D2	7.00E-3		
TO	2000.0	PROCESSING	
NT	5120	SE	0.318
CT	1642	LS	1.000
TEMP	29.0	FN	85536
PM90	10.9	MATH	F
D3	1.00E-3		
DLP	0	DISPLAY	
FB	19300	SP	-500.0
BS	128	MP	31424.3
SS	4	VS	100
IL	N	SC	0
IN	N	WC	320
DP	Y	IS	50
ALOCK	Y	RFL	2887.5
NOF1	10.0	RFP	0
NOF2	10.0	TH	3
ALFA	0	INS	1.000
SPIN	25.0	DC	



PLOT SCALE = 982.01 HZ/CM

POOR QUALITY ORIGINAL

Compound 11b



SEARLE
QE-300 PLUS

30.003
17JUN96

4919-30-2, CDCL3

OPERATOR 12C

ONE PULSE SEQUENCE

PULSE WIDTH = 15.36 USEC
90 DEGREES
ACQ TIME = 019.20 MSEC
RECYCLE TIME = 1.00 SEC

NO. OF ACQS = 20000
DATA SIZE = 32768
LINE BROADNG = 1.00 HZ
SPIN RATE = 25 RPS

OBSERVE
FREQUENCY = 75.480424 MHZ
SPEC WIDTH = 20000 HZ
GAIN = 80.01

DECOUPLER STANDARD-18 MODULATION
FREQUENCY = 4.000 PPM
POWER = 2890/3000

PLOT SCALE
S2 = 12 HZ/CM
S1 = 9702 PPM/CM
FROM 225.00
TO -5.01 PPM

PEAK LISTING

#	INT	PPM
1	27	24.51
2	47	74.01
3	43	77.03
4	42	77.46
5	121	119.43
6	76	124.23
7	113	122.93

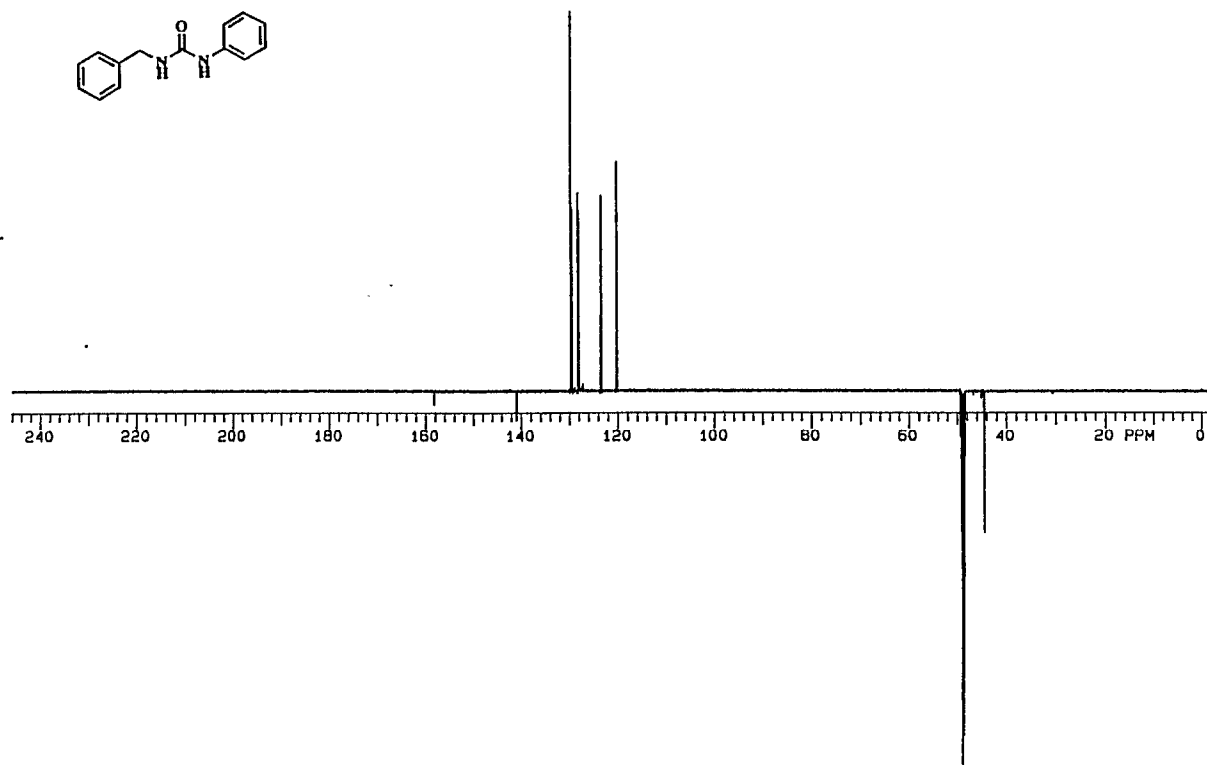
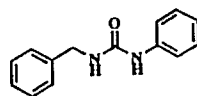
Compound 10c

VXR-500

CRICH 0919-30-3
1H SOL/CD300 APT
DSK10/MS5014 AM

EXP1 PULSE SEQUENCE: APT30
DATE 06-20-96
SOLVENT CD300
FILE 064353

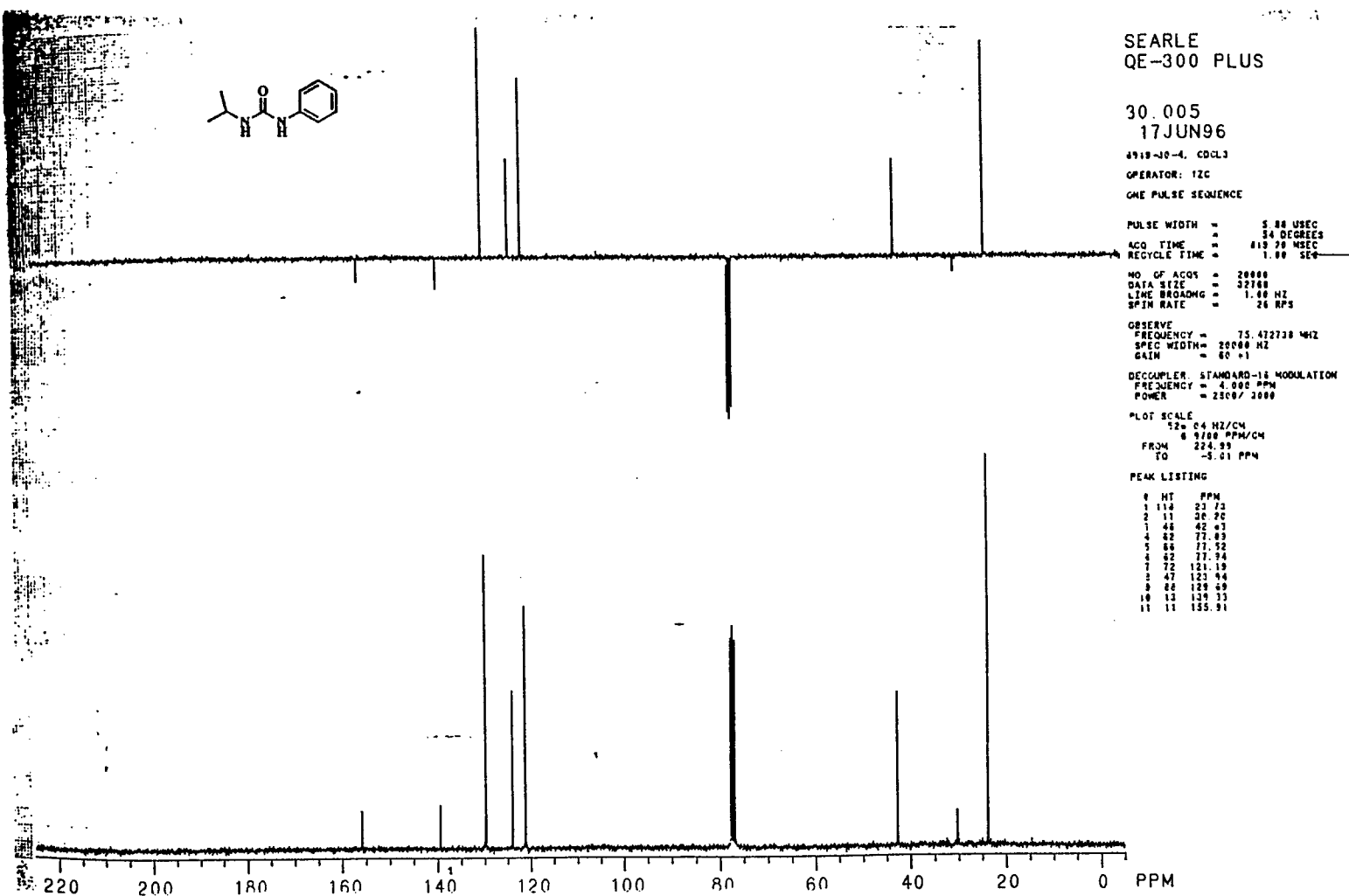
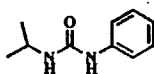
ACQUISITION		DEC. & VT	
IN	13.000	DN	1.000
SN	34965.0	DO	1680.0
AT	0.915	DM	YNY
NP	64000	DHM	S
PH	7.5	DHF	10400
P1	21.8	DHP	36.0
D1	1.000	HOMO	N
D2	7.00E-3		
TD	2000.0	PROCESSING	
MT	5120	SE	0.318
CT	5120	LB	1.000
TEMP	29.0	FN	65536
PH90	10.9	NATH	F
D3	1.00E-3		
DLP	0	DISPLAY	
FB	19300	SP	-500.0
BS	128	MP	31424.3
SS	4	VS	100
IL	N	SC	0
IN	N	MC	320
OP	Y	IS	50
ALOCK	Y	RFL	3205.5
ROF1	10.0	RFP	0
ROF2	10.0	TH	3
ALFA	0	INS	1.000
SPIN	25.0	DC	



PLOT SCALE = 982.01 HZ/CM

POOR QUALITY ORIGINAL

Compound 10d



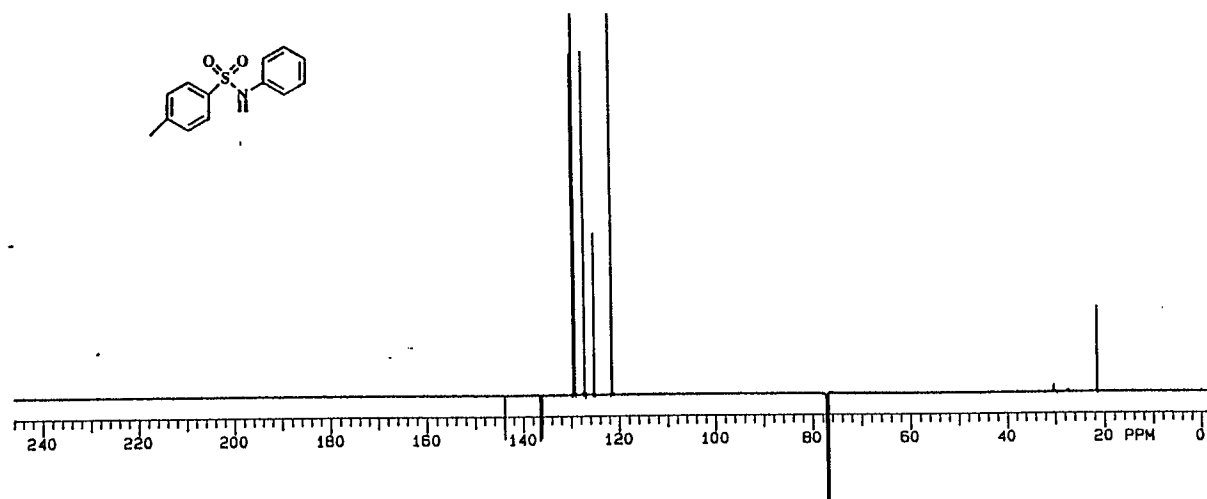
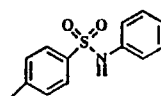
Compound 13o

VXR-500

CRICH 8919-37-7
1H SOL/CDCL3 APT
DSL10/H56017 AM

EXP4 PULSE SEQUENCE: APT30
DATE 07-26-96
SOLVENT CDCL3
FILE 065338

ACQUISITION		DEC. & VT	
IN	13.000	DM	1.000
SN	34985.0	DO	-290.0
AT	0.915	DM	YHY
NP	84000	DMH	S
PM	7.5	DMF	10400
P1	21.8	DHP	36.0
D1	1.000	HOMO	N
D2	7.00E-3		
TD	2000.0	PROCESSING	
HT	10240	SE	0.318
CT	10240	LS	1.000
TEMP	29.0	FN	65536
PM90	10.9	MATH	F
D3	1.00E-3		
DLP	0	DISPLAY	
FB	19300	SP	-500.0
BS	128	MP	31424.3
SS	4	VS	100
IL	N	SC	0
IN	N	WC	320
DP	Y	IS	50
ALOCK	Y	RFL	2887.5
ROF1	10.0	RFP	0
ROF2	10.0	TH	3
ALFA	0	INS	1.000
SPIN	25.0	DC	



PLOT SCALE = 982.01 HZ/CM

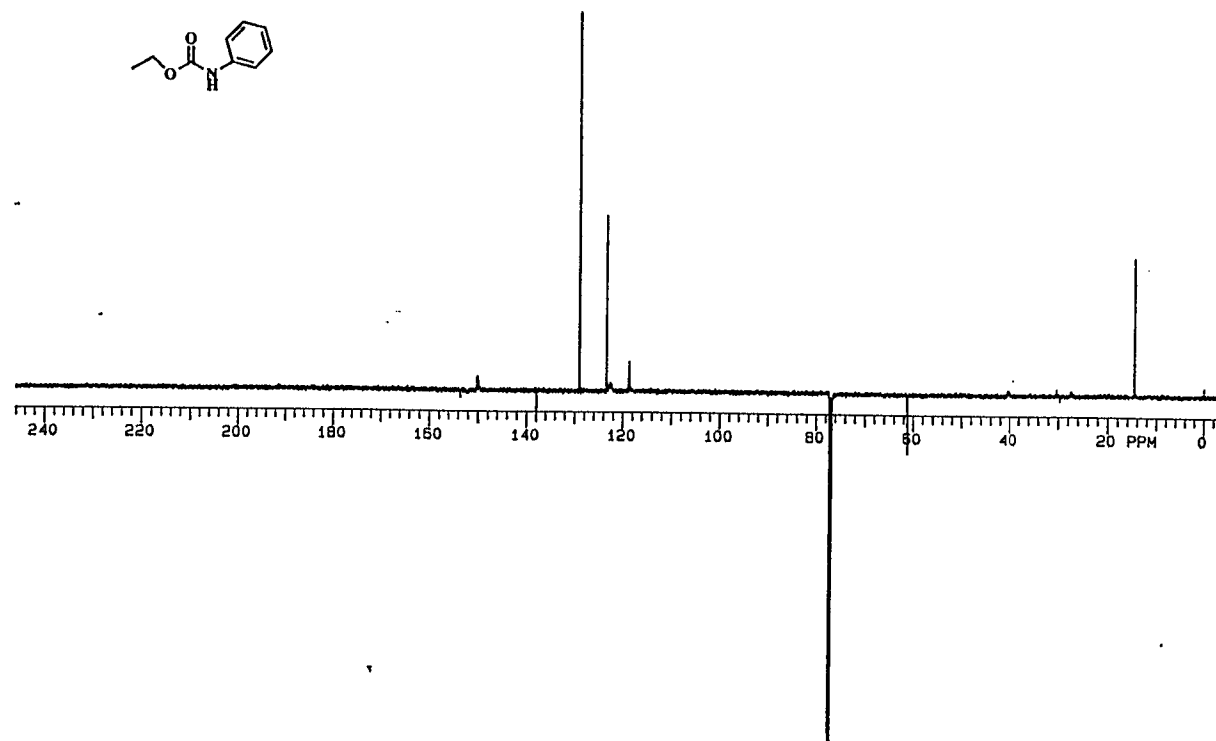
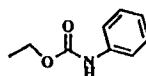
Compound 12f

VXR-500

CRICH 8919-37-8
ALL/CDCL3, APT
DSK11.WS601B.FM

EXP1 PULSE SEQUENCE: ART30
DATE 07-30-96
SOLVENT CDCL3
FILE B65427

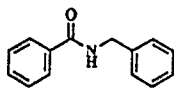
ACQUISITION		DEC. & VT	
IN	13.000	DM	1.000
SN	34985.0	DO	-290.0
AT	0.915	DM	YNY
MP	64000	DMH	S
PH	7.5	DMF	10400
P1	21.6	DMF	36.0
D1	1.000	HOMO	N
D2	7.00E-3		
TO	2000.0	PROCESSING	
NT	7880	SE	0.318
CT	7251	LB	1.000
TEMP	29.0	FM	65536
PH90	10.9	MATH	F
D3	1.00E-3		
DLP	0	DISPLAY	
FB	19300	SP	-500.0
BS	128	MP	31424.3
SS	4	VS	100
IL	N	SC	0
IN	N	MC	320
DP	Y	IS	50
ALOCK	Y	RFL	2887.0
ROF1	10.0	RFP	0
ROF2	10.0	TH	3
ALFA	0	INS	1.000
SPIN	25.0	DC	



PLOT SCALE = 982.01 HZ/CM

VAH-DUU

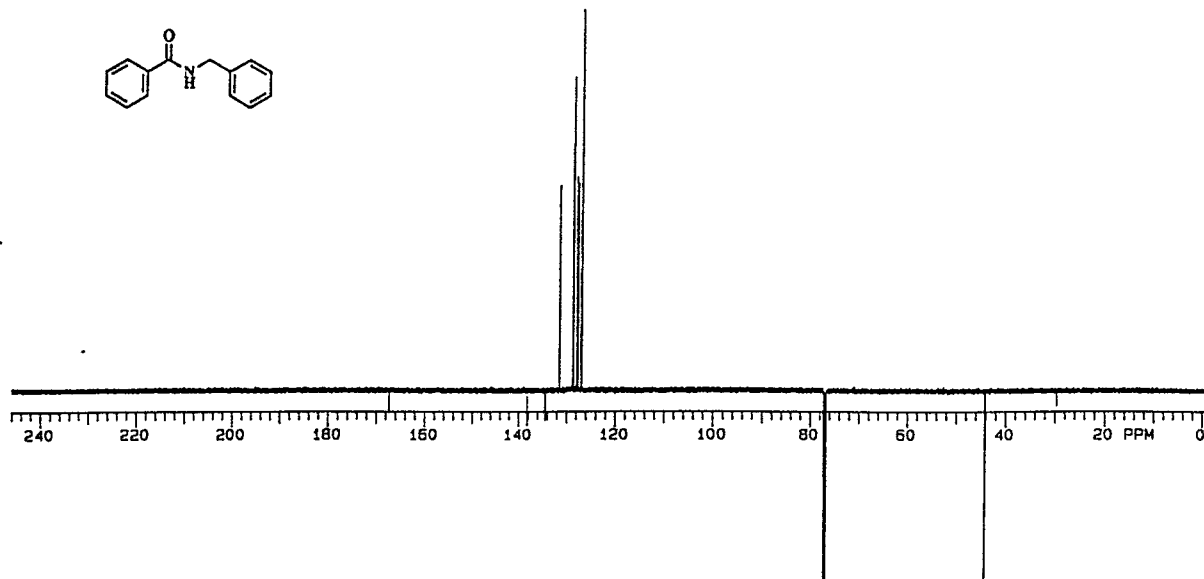
Compound 11g



CRICH 5918-30-5
 1H SOL/CDCL3 APT
 DSK10/V58014 AM

EXP3 PULSE SEQUENCE: APT30
 DATE 06-19-96
 SOLVENT CDCL3
 FILE 864311

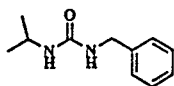
ACQUISITION		DEC. & VT	
TM	13.000	DN	1.000
SM	34985.0	DO	-290.0
AT	0.915	DM	YMY
NP	64000	DM	S
PM	7.5	DMF	10400
P1	21.8	DMF	36.0
D1	1.000	HOMO	N
D2	7.00E-3		
TD	2000.0	PROCESSING	
NT	5120	SE	0.318
CT	1792	LB	1.000
TEMP	29.0	FN	65536
PH90	10.9	MATH	F
D3	1.00E-3		
DLP	0	DISPLAY	
FB	19300	SP	-500.0
BS	128	WP	31424.3
SS	4	VS	100
IL	N	SC	0
IN	N	WC	320
DP	Y	IS	50
ALOCK	Y	RPL	2887.5
ROF1	10.0	RFP	0
ROF2	10.0	TH	3
ALFA	0	INS	1.000
SPIN	25.0	OC	



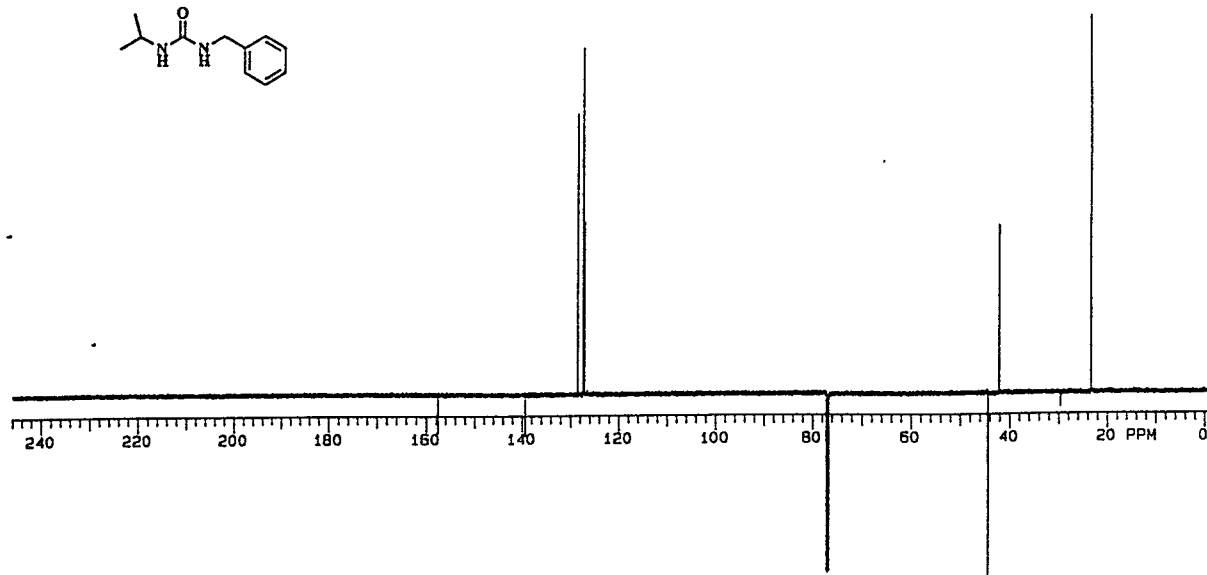
PLOT SCALE = 982.01 HZ/CM

VXR-500

Compound 10h

CRICH 6919-30-8
1H SOL/CDCL3 APT
DSK10/MS6014 AMEXP1 PULSE SEQUENCE: APT30
DATE 08-19-96
SOLVENT CDCL3
FILE 864281

ACQUISITION		DEC. & VT	
TH	13.000	DM	1.000
SW	34965.0	DO	-290.0
AT	0.915	DM	YMY
NP	84000	DM	S
PW	7.5	DMF	10400
P1	21.8	DMF	38.0
D1	1.000	HOMO	N
D2	7.00E-3		
TO	2000.0	PROCESSING	
NT	5120	SE	0.318
CT	2159	LB	1.000
TEMP	29.0	FN	65536
PW90	10.9	MATH	F
D3	1.00E-3		
DLP	0	DISPLAY	
FB	18300	SP	-500.0
BS	128	WP	31424.3
SS	4	VS	100
IL	N	SC	0
IN	N	WC	320
OP	Y	IS	50
ALOCK	Y	RFL	2885.0
ROF1	10.0	RFP	0
ROF2	10.0	TH	3
ALFA	0	INS	1.000
SPIN	25.0	DC	



PLOT SCALE = 982.01 HZ/CM

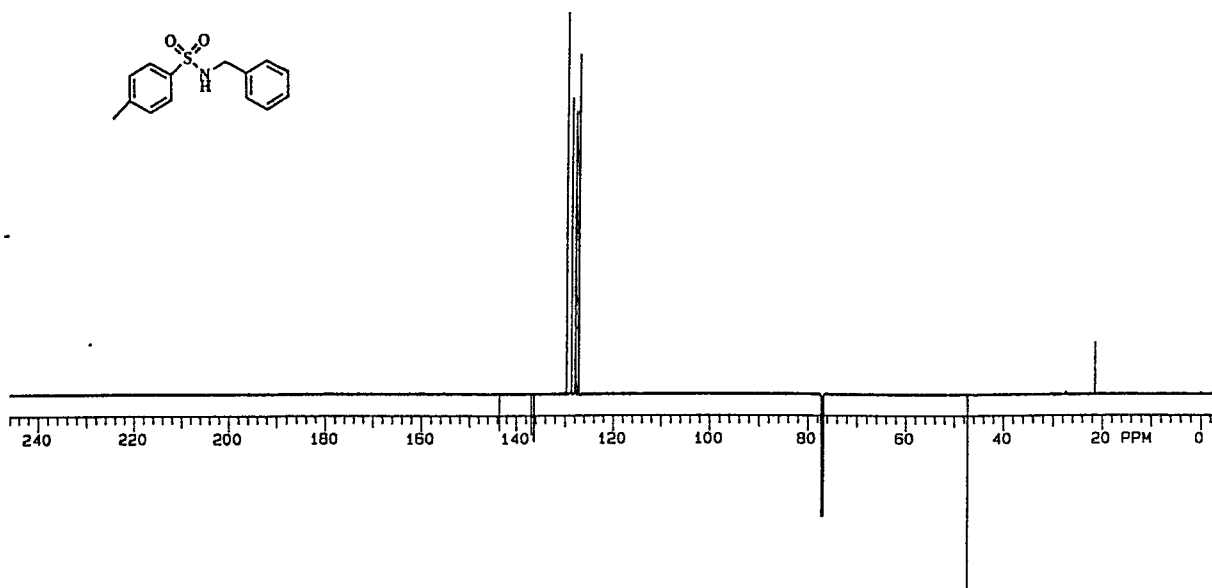
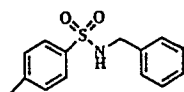
VXR-500

Compound 13l

CRICH 8818-37-9
1H SOL/CDCL3 APT
DSK10/MS8017 AM

EXP3 PULSE SEQUENCE: APT30
DATE 07-25-96
SOLVENT CDCL3
FILE 865337

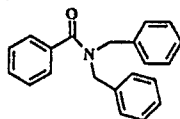
ACQUISITION DEC. & VT
TH 13.000 DM 1.000
SH 34865.0 DD -299.0
AT 6.915 DM VNY
HP 84000 DM S
PH 7.5 DM 10408
P1 21.8 DM 36.8
D1 1.000 HOMO N
D2 7.00E-3
T0 2000.0 PROCESSING
NT 10240 SE 0.318
CT 10240 LB 1.000
TEMP 29.0 FH 85536
PH80 10.8 MATH F
D3 1.00E-3
DLP 0 DISPLAY
FB 19300 SP -500.0
BS 128 WP 31424.3
SS 4 VS 100
IL N SC 0
IN N MC 320
DP Y IS 50
ALOCK Y RFL 2967.5
ROF1 10.8 RFP 0
ROF2 10.0 TH 3
ALFA 0 INS 1.000
SPIN 25.0 DC



PLOT SCALE = 982.01 HZ/CM

VXR-500

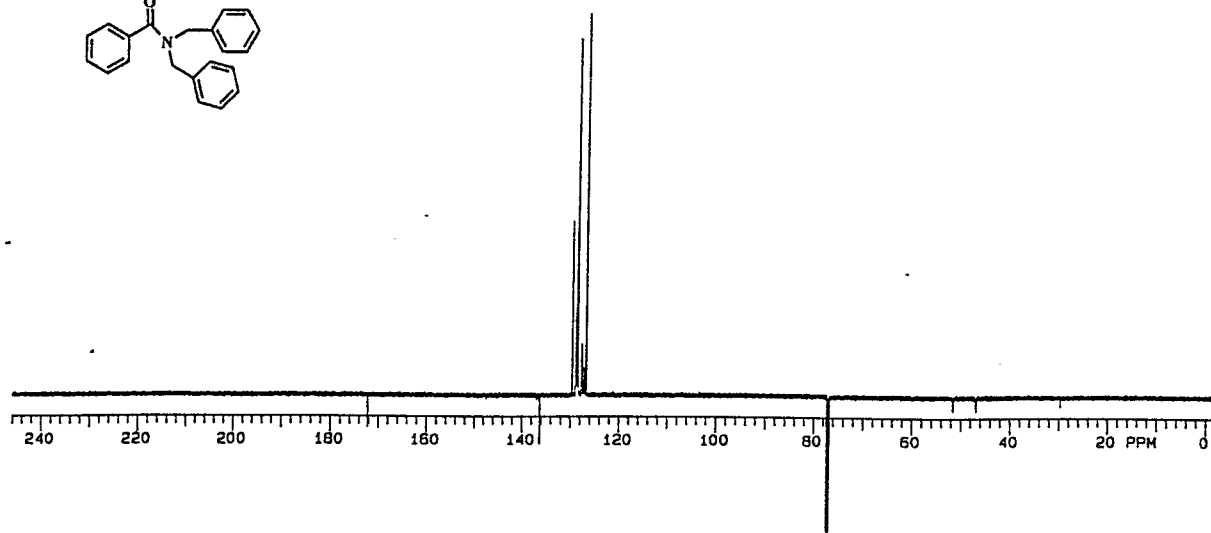
Compound 11j



CRICH 6919-30-S
1H SOL/COCL3 APT
DSK19/MS6014 AN

EXP2 PULSE SEQUENCE: APT30
DATE 05-19-96
SOLVENT COCL3
FILE 864282

ACQUISITION		DEC. & VT	
TH	13.000	DM	1.000
SH	34965.0	DO	-290.0
AT	0.815	DM	YNY
NP	64000	DMH	S
PH	7.5	DHF	10400
P1	21.0	DHP	36.0
D1	1.000	HOMO	N
D2	7.00E-3		
TO	2000.0	PROCESSING	
NT	5120	SE	0.318
CT	1465	LS	1.000
TEMP	29.0	FN	65536
PH90	10.9	MATH	F
D3	1.00E-3		
DLP	0	DISPLAY	
FB	19300	SP	-500.0
BS	128	WP	31424.3
SS	4	VS	100
IL	N	SC	0
IN	N	WC	320
DP	Y	IS	50
ALOCK	Y	RFL	2967.3
ROF1	10.0	RFP	0
ROF2	10.0	TH	3
ALFA	0	INS	1.000
SPIN	25.0	DC	



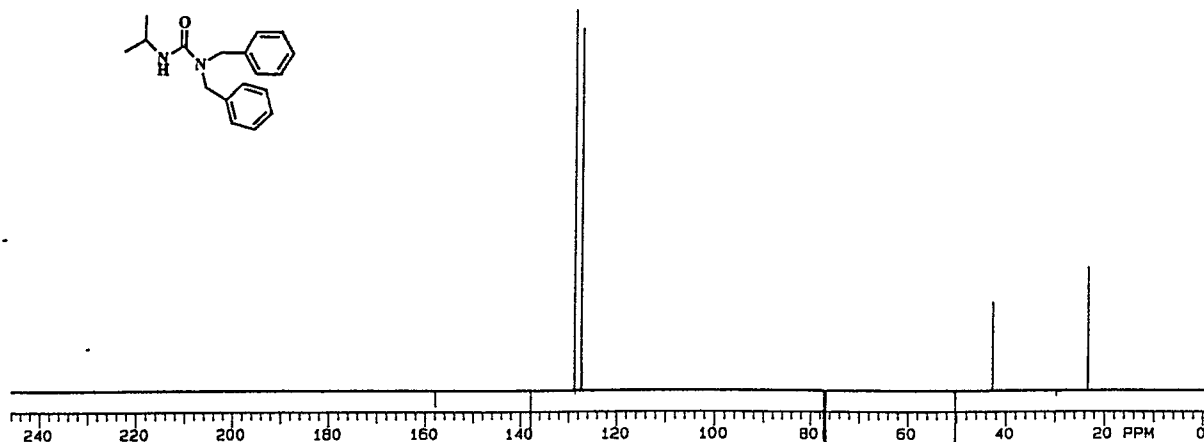
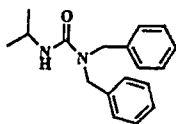
PLOT SCALE = 982.01 HZ/CM

VXR-500

Compound 10k

CRICH 6919-30-12
 1H SOL/CDCL3 APT
 OSK10/MS6014 AM

EXP7 PULSE SEQUENCE: APT30
 DATE 06-18-96
 SOLVENT CDCL3
 FILE 064273



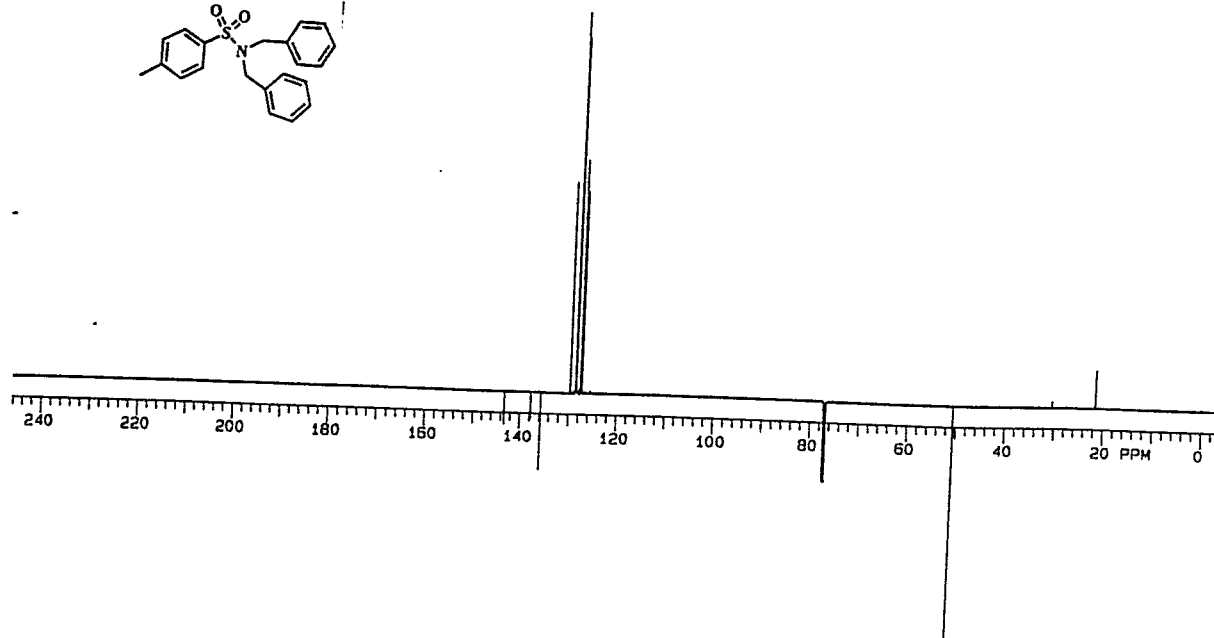
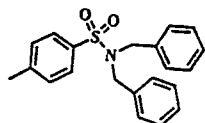
ACQUISITION		DEC. & VT	
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SN	34965.0	DO	-290.0
AT	0.915	DM	YNY
MP	64000	DM	S
PH	7.5	DM	10400
P1	21.6	DM	36.0
D1	1.000	HOMO	N
D2	7.00E-3		
TO	2000.0	PROCESSING	
NT	7680	SE	0.318
CT	7680	LS	1.000
TEMP	29.0	PH	65536
PH90	10.9	MATH	F
D3	1.00E-3		
OLP	0	DISPLAY	
FB	19300	SP	-500.0
BS	128	WP	31424.3
SS	4	VS	100
IL	N	SC	0
IM	N	WC	320
DP	Y	IS	50
ALOCK	Y	RPL	2887.5
ROF1	10.0	RFP	0
ROF2	10.0	TH	3
ALFA	0	INS	1.000
SPIN	25.0	DC	

PLOT SCALE = 982.01 HZ/CM

Compound 13l

CRICH 8818-37-11
 1H SOL/COCL3 APT
 DSK10/H56017 AM

EXP2 PULSE SEQUENCE: APT30
 DATE 07-26-96
 SOLVENT COCL3
 FILE 865336



ACQUISITION	DEC. & VT
TM 13.000 DM 1.000	
SM 34985.0 DO -280.0	
AT 0.915 DM YNY	
NP 64000 DMN S	
PM 7.5 DMF 10400	
P1 21.8 DMF 36.0	
D1 1.000 HOMO N	
D2 7.00E-3	
TD 2000.0	PROCESSING
NT 10240 SE 0.318	
CT 10240 LB 1.000	
TEHP 28.0 FN 63536	
PH90 10.8 MATH F	
D3 1.00E-3	
DLP 0	DISPLAY
FB 19300 SP -500.0	
BS 128 WP 31424.3	
SS 4 VS 100	
TL N SC 0	
IN N WC 320	
DP Y IS 30	
ALOCK Y RFL 2887.5	
ROF1 10.0 RFP 0	
ROF2 10.0 TH 3	
ALFA 0 INS 1.000	
SPIN 25.0 DC	

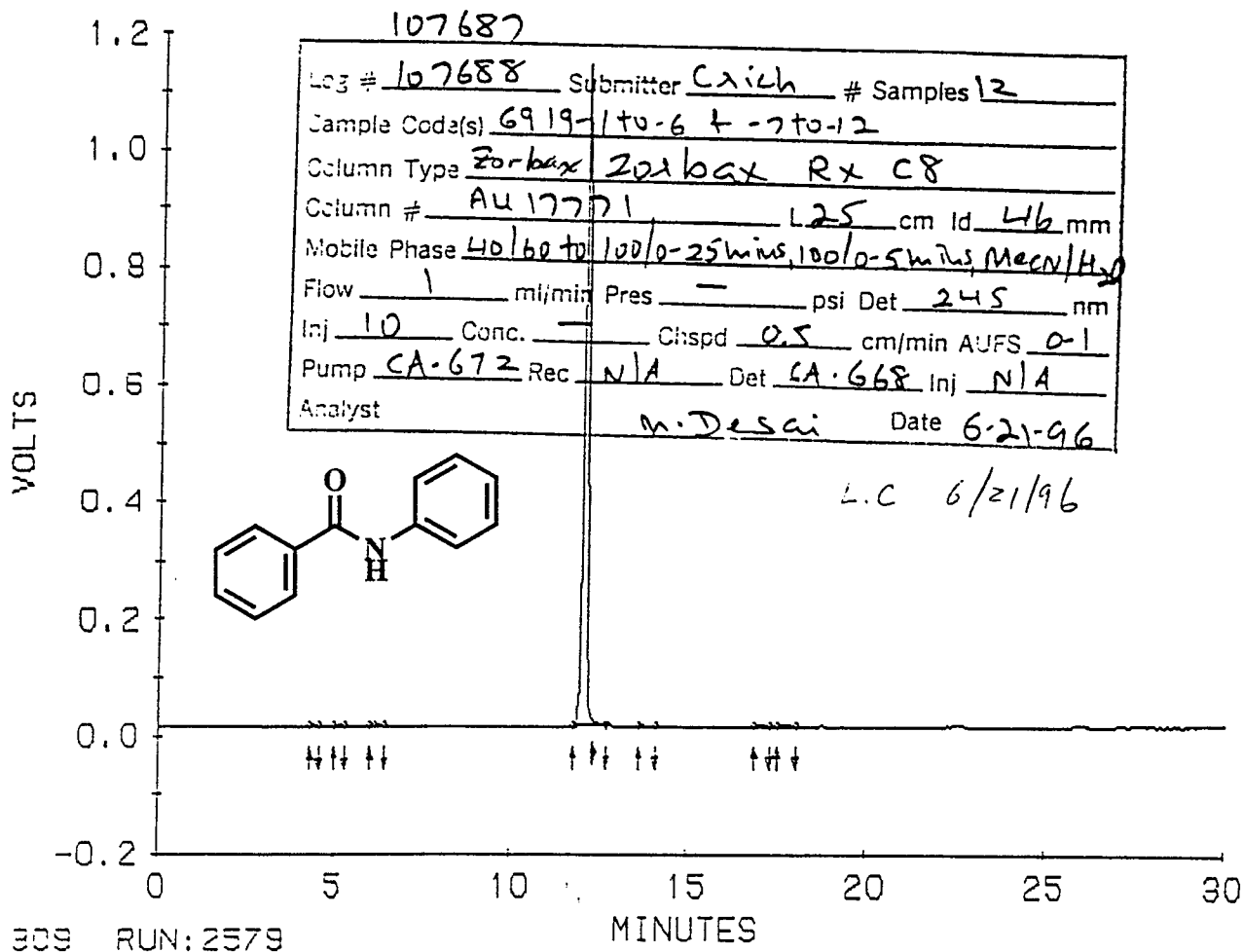
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20-JUN-1996 09:53:12

GDS6219-092 PAGE

Compound 11a

GDS-S-6219-C-350



***** THIS REPORT WAS WRITTEN DURING AN INTERACTIVE GRAPHICS SESSION *****

INST.NO. 309
 USER ID: DESA
 METHOD COMMENT:
 METHOD NAME: MD1

INJECTION ID NO. 2579
 INGRAD RUN ID: *MD

INJ TIME: 19-JUN-96 11:57:16
 -CYCLE: 138

SAMPLE ID: -30-1

PK NO	START TIME	CREST TIME	END TIME	PEAK HEIGHT	PEAK AREA	AREA %
1	4.34	4.43	4.58	0.0014547	0.0001515	0.09
2	5.01	5.17	5.32	0.0012973	0.0001555	0.10
3	6.04	6.19	6.43	0.0073195	0.0009307	0.57
4	11.75	12.05	12.32	1.1258751	0.1589018	97.78
5	12.32	12.34	12.70	0.0079967	0.0012621	0.78
6	13.63	13.75	14.11	0.0005741	0.0000834	0.05
7	16.91	17.07	17.34	0.0028264	0.0004028	0.25
8	17.55	17.75	18.07	0.0044249	0.0006205	0.38

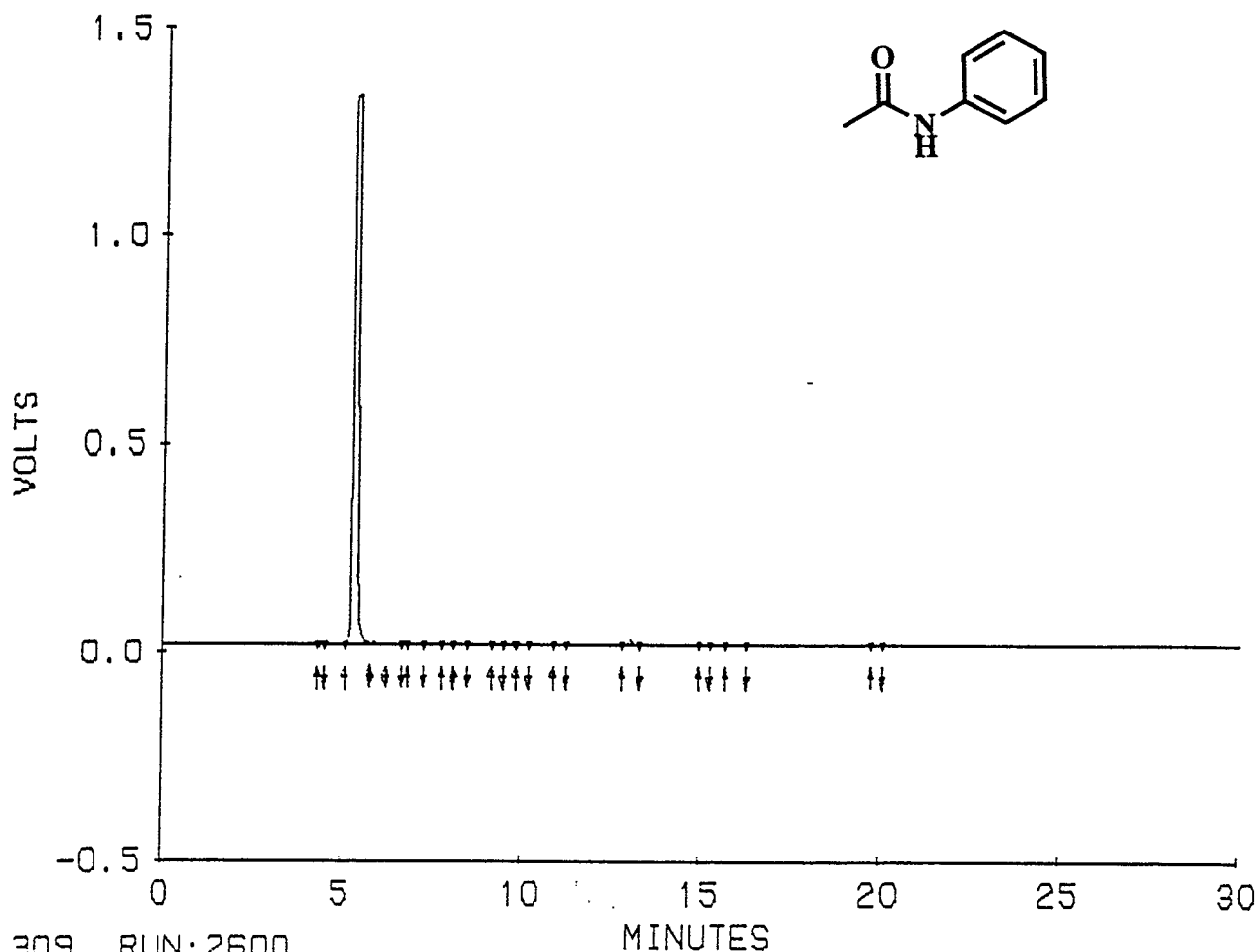
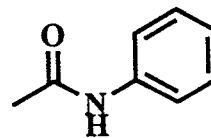
Report Process Time 20-JUN-1996 09:53:12, Report Based on Cursor Editing

Integration parameters in use for this injection:

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0.0000	0.0300	PS	2.1500	0.0000	LT			

20-JUN-1996 10:22:19
GDS6219-002 PAGE
GDS-S-6219-C-351

Compound 11b



INST.:309 RUN:2600

MINUTES

***** THIS REPORT WAS WRITTEN DURING AN INTERACTIVE GRAPHICS SESSION *****

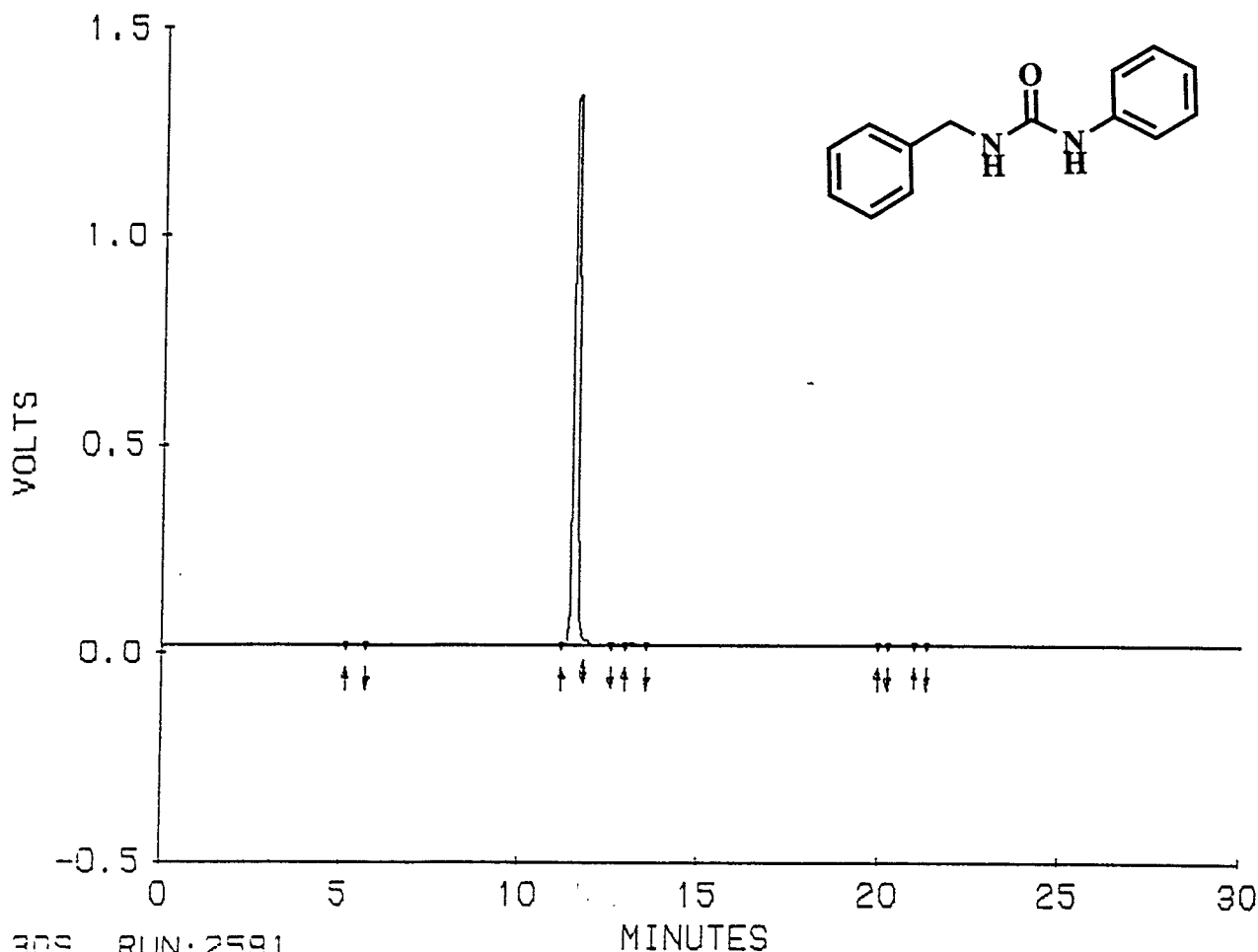
INST.NO. 309
USER ID: DESA
METHOD COMMENT:
METHOD NAME: MD1INJECTION ID NO. 2600
INGRAD RUN ID: *MDINJ TIME: 20-JUN-96 04:15:21
-CYCLE: 159

SAMPLE ID: 302

PK NO	START TIME	CREST TIME	END TIME	PEAK HEIGHT	PEAK AREA	AREA %
1	4.34	4.43	4.53	0.0003747	0.0000347	0.02
2	5.11	5.39	5.83	1.3198301	0.2249061	97.94
3	5.83	5.90	6.26	0.0059262	0.0010017	0.44
4	6.26	6.44	6.70	0.0018232	0.0003199	0.14
5	6.85	6.98	7.31	0.0007962	0.0001271	0.06
6	7.79	7.94	8.11	0.0023431	0.0003091	0.13
7	8.12	8.34	8.50	0.0013389	0.0002078	0.09
8	9.18	9.33	9.49	0.0007618	0.0000988	0.04
9	9.83	9.95	10.18	0.0005743	0.0000925	0.04
10	10.88	11.03	11.24	0.0007375	0.0001121	0.05
11	12.80	13.04	13.30	0.0145632	0.0021708	0.95
12	14.96	15.11	15.25	0.0005376	0.0000769	0.03
13	15.72	15.85	16.32	0.0002969	0.0000596	0.03
14	19.75	19.87	20.06	0.0010278	0.0001292	0.06

20-JUN-1996 09:56:36
 GDS6219-092 PAGE
 GDS-S-6219-C-352

Compound 10c



INST.:309 RUN:2581

MINUTES

***** THIS REPORT WAS WRITTEN DURING AN INTERACTIVE GRAPHICS SESSION *****

INST.NO. 309 INJECTION ID NO. 2581 INJ TIME: 19-JUN-96 13:30:46
 USER ID: DESA INGRAD RUN ID: *MD -CYCLE: 140

METHOD COMMENT:
 METHOD NAME: MD1

SAMPLE ID: -30-3

PK NO	START TIME	CREST TIME	END TIME	PEAK HEIGHT	PEAK AREA	AREA %
1	5.14	5.22	5.72	0.0002213	0.0000550	0.02
2	11.18	11.57	11.78	1.3197542	0.2244752	97.83
3	11.78	11.77	12.54	0.0163504	0.0031525	1.37
4	12.93	13.13	13.54	0.0101664	0.0014153	0.62
5	19.94	20.07	20.22	0.0005563	0.0000652	0.03
6	20.96	21.09	21.31	0.0021220	0.0002844	0.12

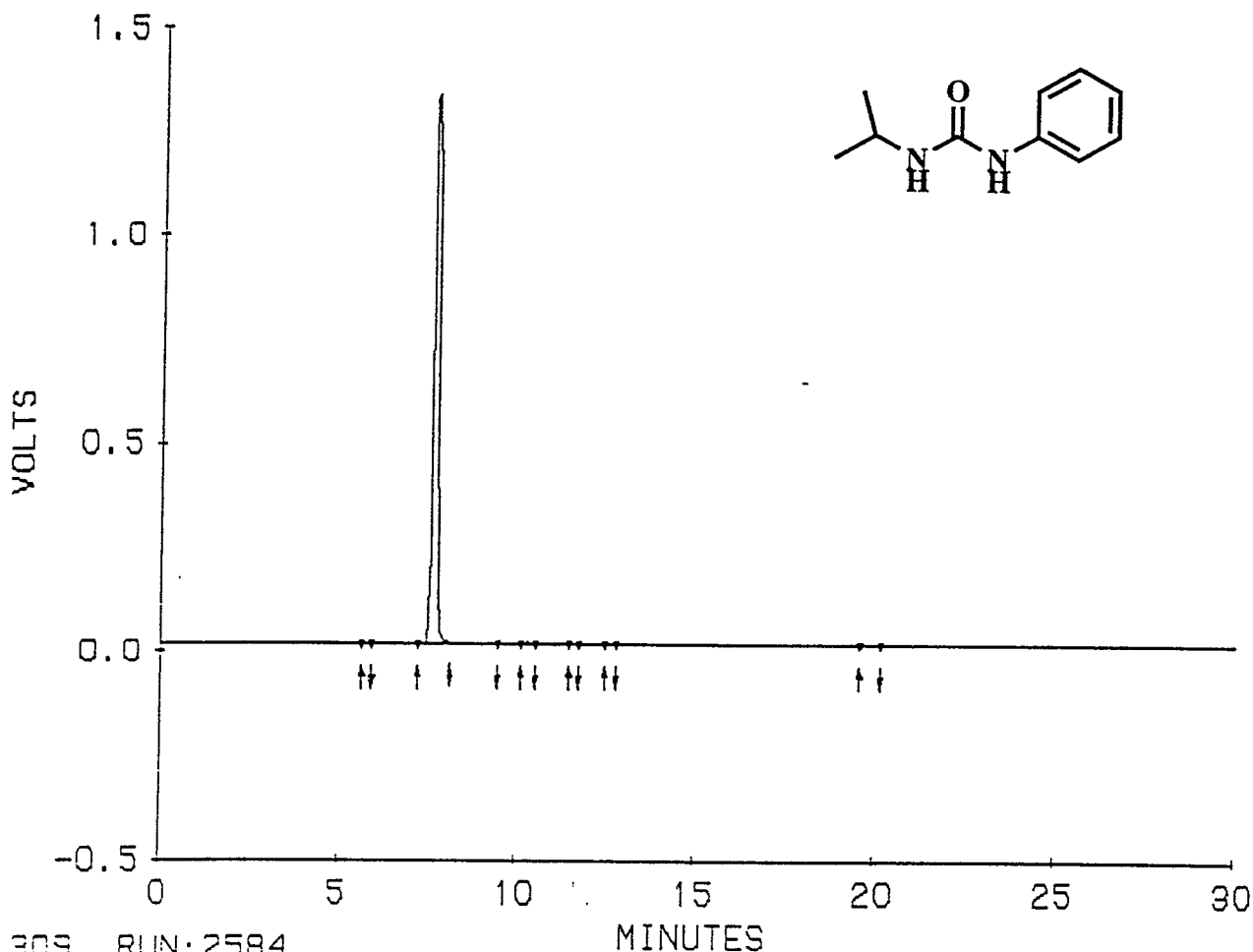
Report Process Time 20-JUN-1996 09:56:36, Report Based on Cursor Editing

Integration parameters in use for this injection:

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0.0000	1.0000	PW		0.0000	2.0000	SP		0.0000	2.0000	SN
0.0000	0.0300	PS		2.1500	0.0000	LT				

20-JUN-1996 10:01:10
 GDS6219-092 PAGE
 GDS-S-6219-C-353

Compound 10d



INST.:303 RUN:2584

MINUTES

***** THIS REPORT WAS WRITTEN DURING AN INTERACTIVE GRAPHICS SESSION *****

INST.NO. 309 INJECTION ID NO. 2584 INJ TIME: 19-JUN-96 15:51:03
 USER ID: DESA INGRAD RUN ID: *MD -CYCLE: 143
 METHOD COMMENT:
 METHOD NAME: MD1 SAMPLE ID: -304

PK NO	START TIME	CREST TIME	END TIME	PEAK HEIGHT	PEAK AREA	AREA %
1	5.65	5.79	5.93	0.0007551	0.0000942	0.04
2	7.21	7.69	8.11	1.3201969	0.2288113	98.57
3	8.11	8.48	9.46	0.0027781	0.0021096	0.91
4	10.13	10.32	10.54	0.0058619	0.0008196	0.35
5	11.49	11.63	11.76	0.0012332	0.0001579	0.07
6	12.49	12.59	12.80	0.0005205	0.0000670	0.03
7	19.59	19.70	20.17	0.0002895	0.0000734	0.03

Report Process Time 20-JUN-1996 10:01:10, Report Based on Cursor Editing
 Integration parameters in use for this injection:

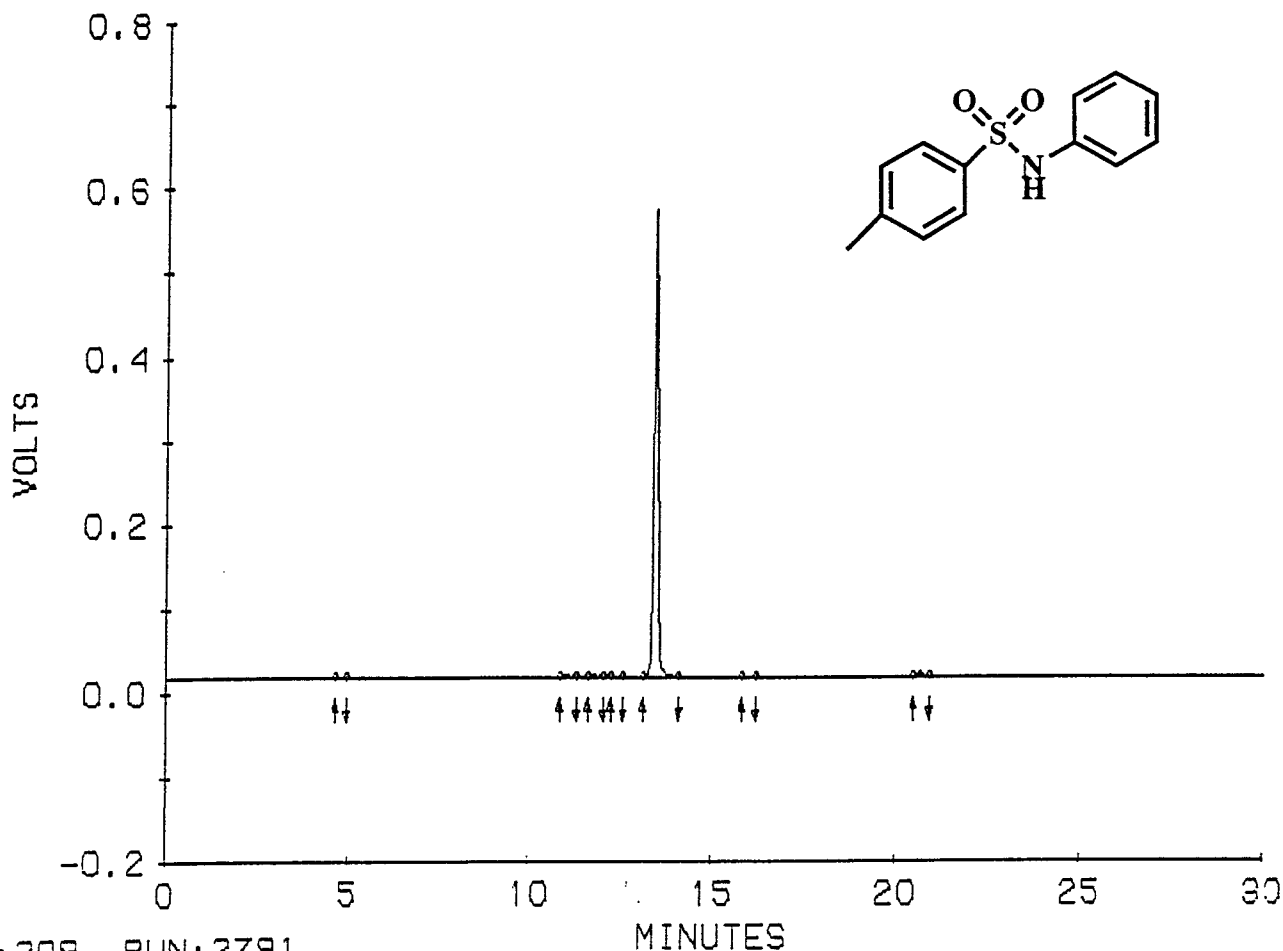
TIME	VALUE	TYPE	-- TIME	VALUE	TYPE	-- TIME	VALUE	TYPE
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0.0000	1.0000	PW	0.0000	2.0000	SP	0.0000	2.0000	SN
0.0000	0.0300	PS	2.1500	0.0000	LT			

9-AUG-1996 08:16:39

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Compound 13e

GDS-S-6219D-180



INST.:309 RUN:2791

***** THIS REPORT WAS WRITTEN DURING AN INTERACTIVE GRAPHICS SESSION *****

INST.NO. 309 INJECTION ID NO. 2791 INJ TIME: 07-AUG-96 22:50:05
 USER ID: DESA INGRAD RUN ID: *MD -CYCLE: 350
 METHOD COMMENT:
 METHOD NAME: MD SAMPLE ID: 6919-37-7

PK NO	START TIME	CREST TIME	END TIME	PEAK HEIGHT	PEAK AREA	AREA %
1	4.66	4.76	4.97	0.0005183	0.0000577	0.08
2	10.84	11.02	11.29	0.0016433	0.0002317	0.30
3	11.60	11.79	12.02	0.0020538	0.0002675	0.35
4	12.23	12.35	12.55	0.0003487	0.0000487	0.06
5	13.10	13.46	14.10	0.5552012	0.0752086	98.34
6	15.82	15.98	16.19	0.0003482	0.0000578	0.08
7	20.47	20.68	20.92	0.0047310	0.0006036	0.79

Report Process Time 9-AUG-1996 08:16:39, Report Based on Reintegration

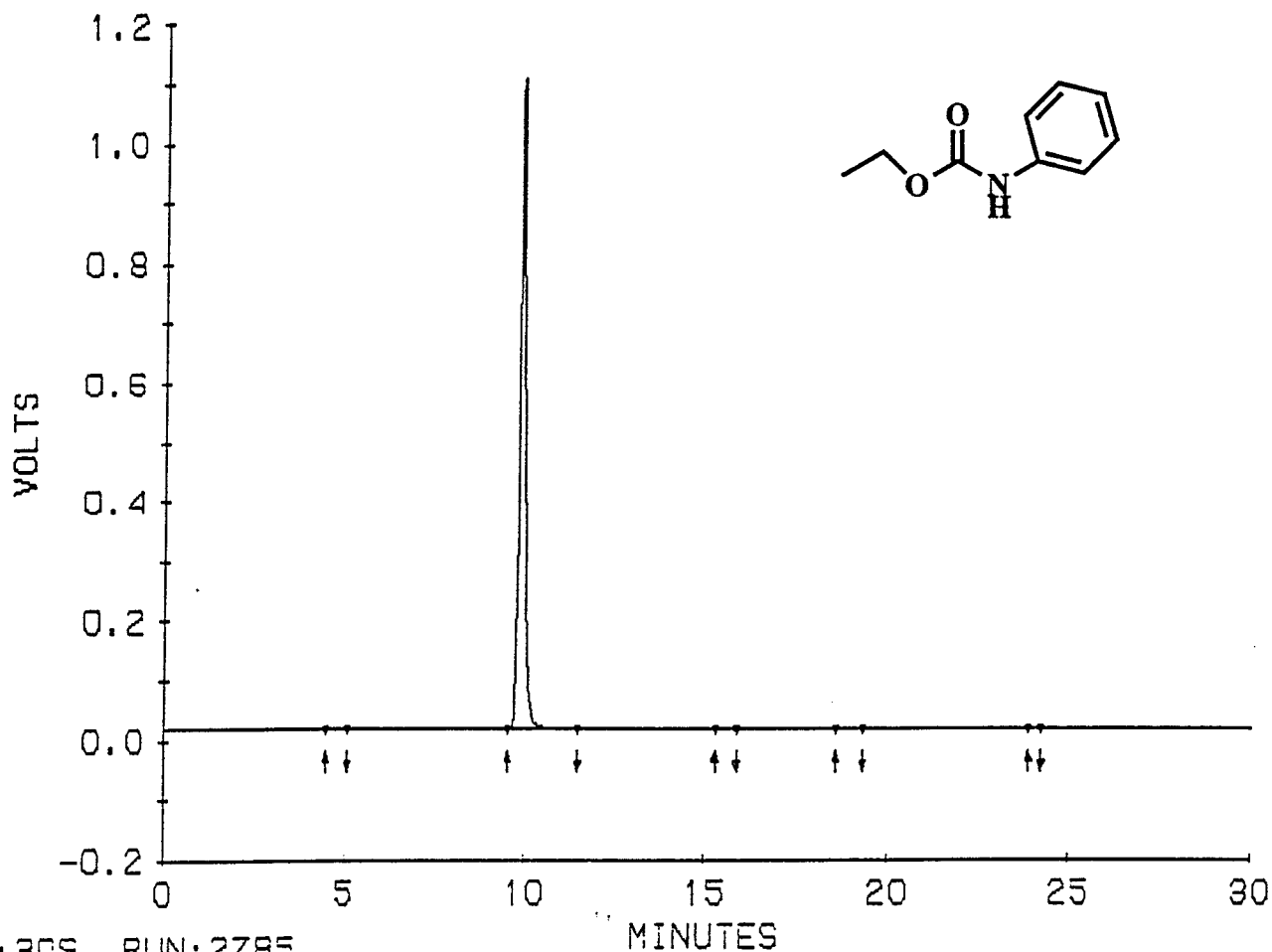
Integration parameters in use for this injection:

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0.0000	1.0000	PW	0.0000	2.0000	SP	0.0000	2.0000	SN
0.0000	0.0200	PS	3.5000	0.0000	LT			

9-AUG-1996 08:14:01

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GDS-S-6219D- 174

Compound 12f



INST.:309 RUN:2785

***** THIS REPORT WAS WRITTEN DURING AN INTERACTIVE GRAPHICS SESSION *****

INST.NO. 309 INJECTION ID NO. 2785 INJ TIME: 07-AUG-96 18:48:32
 USER ID: DESA INGRAD RUN ID: *MD -CYCLE: 344
 METHOD COMMENT:
 METHOD NAME: MD SAMPLE ID: 6919-37-8

PK NO	START TIME	CREST TIME	END TIME	PEAK HEIGHT	PEAK AREA	AREA %
1	4.49	4.79	5.08	0.0026696	0.0004309	0.20
2	9.54	9.92	11.49	1.1121759	0.2110391	99.72
3	15.29	15.44	15.88	0.0004992	0.0001025	0.05
4	18.60	18.73	19.33	0.0001921	0.0000399	0.02
5	23.90	24.00	24.25	0.0002124	0.0000299	0.01

Report Process Time 9-AUG-1996 08:14:01, Report Based on Reintegration

Integration parameters in use for this injection:

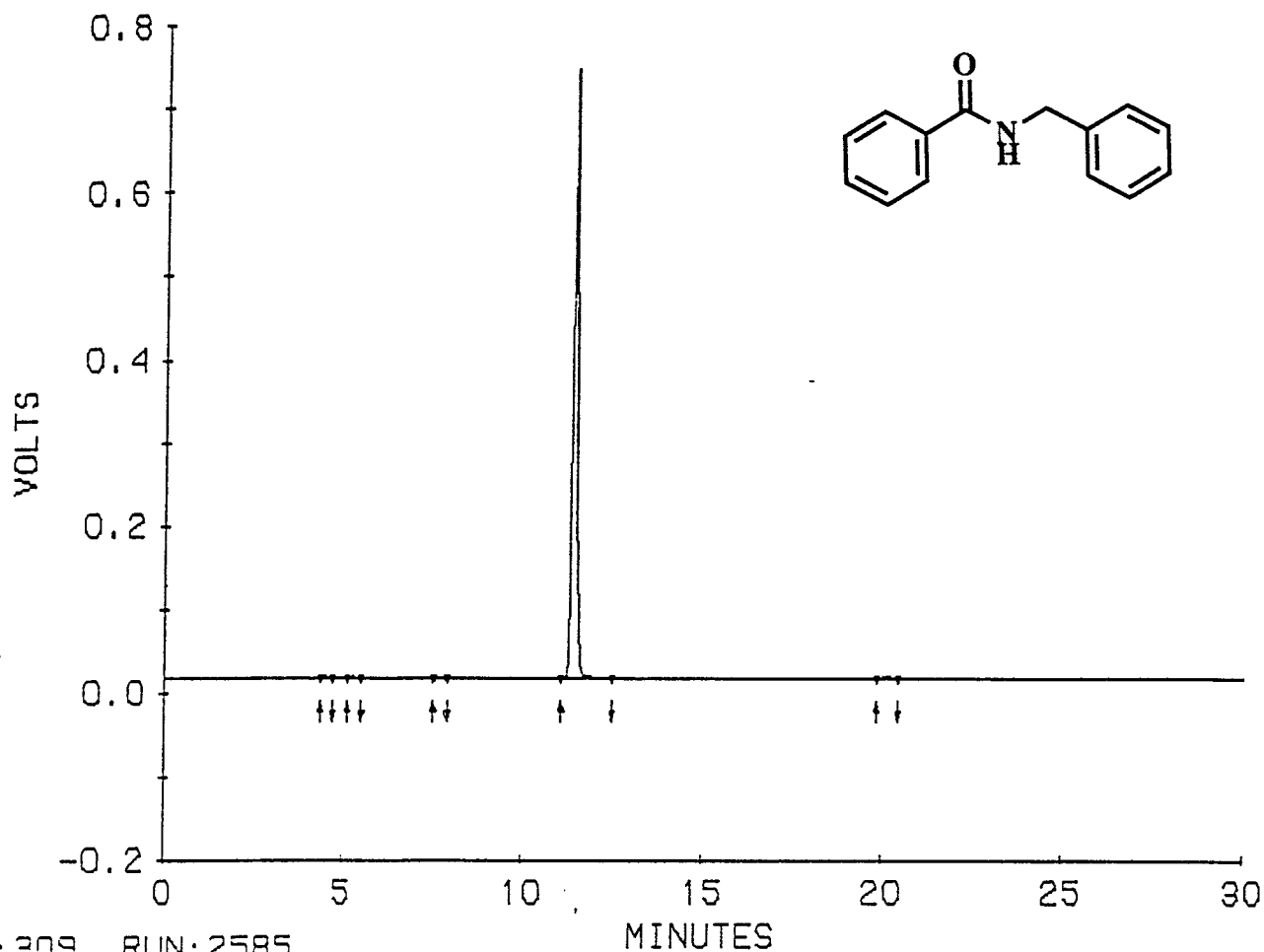
TIME	VALUE	TYPE	--	TIME	VALUE	TYPE	--	TIME	VALUE	TYPE
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0.0000	1.0000	PW		0.0000	2.0000	SP		0.0000	2.0000	SN
0.0000	0.0200	PS		3.5000	0.0000	LT				

20-JUN-1996 10:02:58

GDS6219-042 PAGE

GDS-S-6219-C-354

Compound 11g



INST.:309 RUN:2585

***** THIS REPORT WAS WRITTEN DURING AN INTERACTIVE GRAPHICS SESSION *****

INST.NO. 309

INJECTION ID NO. 2585

INJ TIME: 19-JUN-96 16:37:49

USER ID: DESA

INGRAD RUN ID: *MD

-CYCLE: 144

METHOD COMMENT:

METHOD NAME: MD1

SAMPLE ID:

-305

PK NO	START TIME	CREST TIME	END TIME	PEAK HEIGHT	PEAK AREA	AREA %
1	4.39	4.54	4.74	0.0033312	0.0003398	0.32
2	5.15	5.31	5.55	0.0040143	0.0004589	0.43
3	7.53	7.69	7.92	0.0017701	0.0002487	0.24
4	11.08	11.43	12.49	0.7310932	0.1038322	98.14
5	19.86	20.18	20.44	0.0046256	0.0009251	0.87

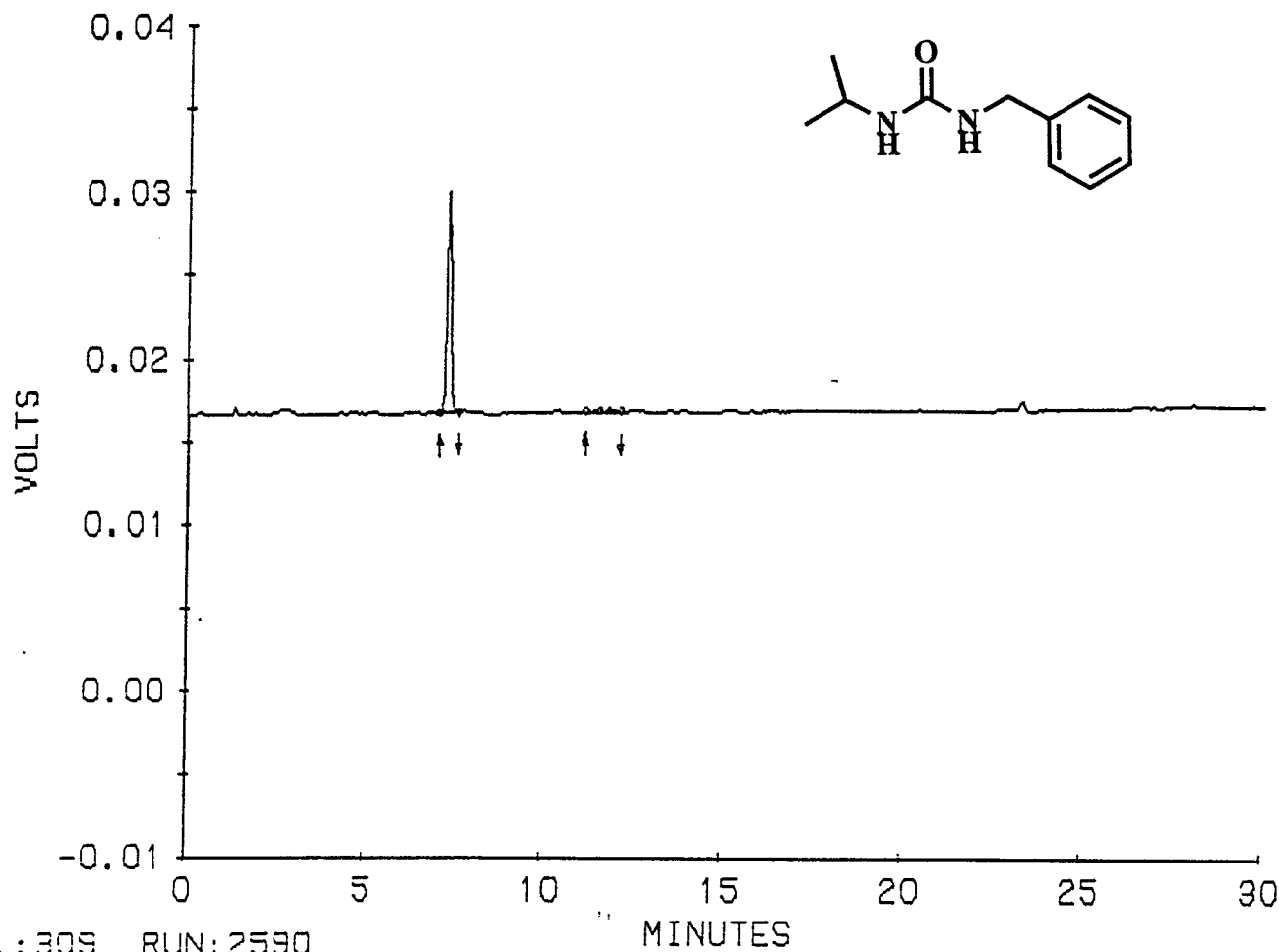
Report Process Time 20-JUN-1996 10:02:58, Report Based on Cursor Editing

Integration parameters in use for this injection:

TIME	VALUE	TYPE	--	TIME	VALUE	TYPE	--	TIME	VALUE	TYPE
0.0000	0.0500	PS		0.0000	0.0000	NS		0.0000	0.0000	SR
0.0000	1.0000	PW		0.0000	2.0000	SP		0.0000	2.0000	SN
0.0000	0.0300	PS		2.1500	0.0000	LT				

Compound 10h

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***** THIS REPORT WAS WRITTEN DURING AN INTERACTIVE GRAPHICS SESSION *****

INST.NO. 309 INJECTION ID NO. 2590 INJ TIME: 19-JUN-96 20:31:36
 USER ID: DESA INGRAD RUN ID: *MD -CYCLE: 149
 METHOD COMMENT:
 METHOD NAME: MD1 SAMPLE ID: -308

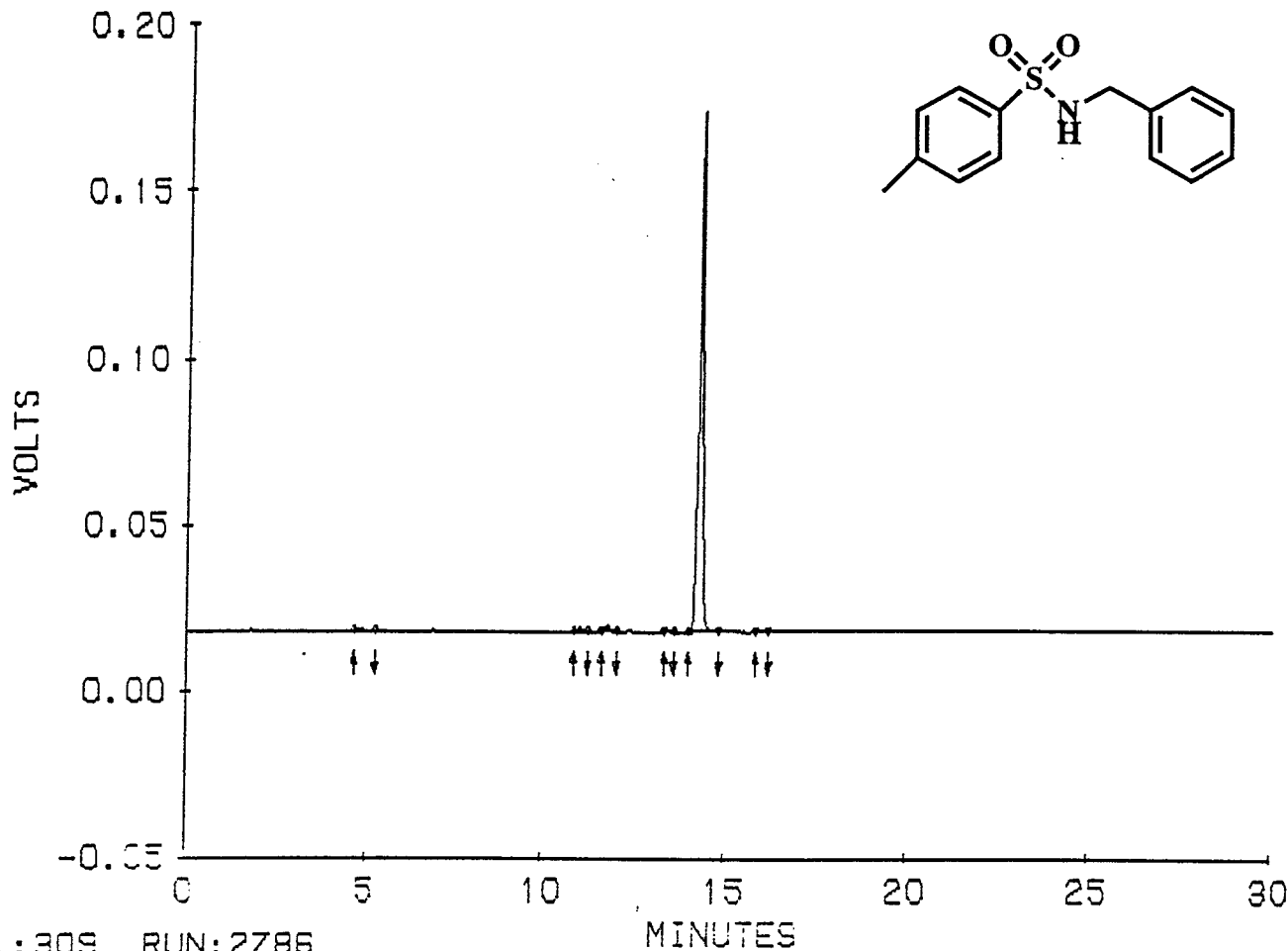
PK NO	START TIME	CREST TIME	END TIME	PEAK HEIGHT	PEAK AREA	AREA %
1	7.08	7.32	7.61	0.0132524	0.0018624	94.76
2	11.17	11.29	12.13	0.0000548	0.0001030	5.24

Report Process Time 20-JUN-1996 10:08:19, Report Based on Cursor Editing

Integration parameters in use for this injection:

TIME	VALUE	TYPE	TIME	VALUE	TYPE	TIME	VALUE	TYPE
0.0000	0.0500	PS	0.0000	0.0000	NS	0.0000	0.0000	SR
0.0000	1.0000	PW	0.0000	2.0000	SP	0.0000	2.0000	SN
0.0000	0.0300	PS	2.1500	0.0000	LT			

Compound 131



INST.:309 RUN:2786

***** THIS REPORT WAS WRITTEN DURING AN INTERACTIVE GRAPHICS SESSION *****

INST.NO. 309 INJECTION ID NO. 2786 INJ TIME: 07-AUG-96 19:29:26
 USER ID: DESA INGRAD RUN ID: *MD -CYCLE: 345
 METHOD COMMENT:
 METHOD NAME: MD SAMPLE ID: 6919-37-9

PK NO	START TIME	CREST TIME	END TIME	PEAK HEIGHT	PEAK AREA	AREA %
1	4.66	4.76	5.25	0.0002275	0.0000443	0.20
2	10.84	10.99	11.23	0.0008439	0.0001162	0.52
3	11.60	11.79	12.02	0.0020398	0.0002717	1.22
4	13.33	13.43	13.59	0.0002024	0.0000232	0.10
5	13.99	14.28	14.83	0.1627684	0.0217879	97.66
6	15.83	15.98	16.18	0.0003938	0.0000669	0.30

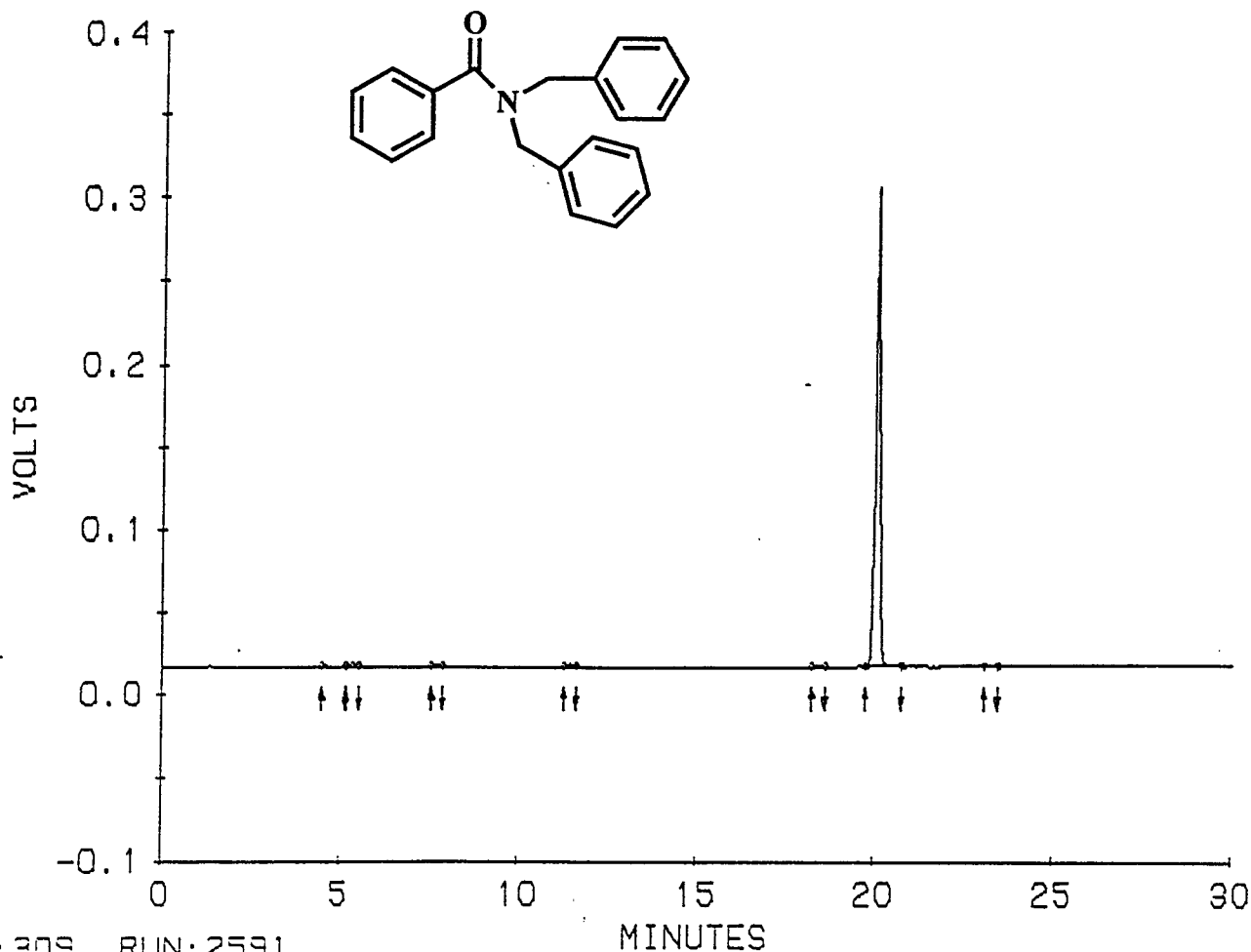
Report Process Time 9-AUG-1996 08:14:25, Report Based on Reintegration

Integration parameters in use for this injection:

TIME	VALUE	TYPE	TIME	VALUE	TYPE	TIME	VALUE	TYPE
0.0000	0.0500	PS	0.0000	0.0000	NS	0.0000	0.0000	SR
0.0000	1.0000	PW	0.0000	2.0000	SP	0.0000	2.0000	SN
0.0000	0.0200	PS	3.5000	0.0000	LT			

Compound 11j

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INST.:309 RUN:2591

MINUTES

***** THIS REPORT WAS WRITTEN DURING AN INTERACTIVE GRAPHICS SESSION *****

INST.NO. 309

INJECTION ID NO. 2591

INJ TIME: 19-JUN-96 21:18:22

USER ID: DESA

INGRAD RUN ID: *MD

-CYCLE: 150

METHOD COMMENT:

METHOD NAME: MD1

SAMPLE ID:

-30-9

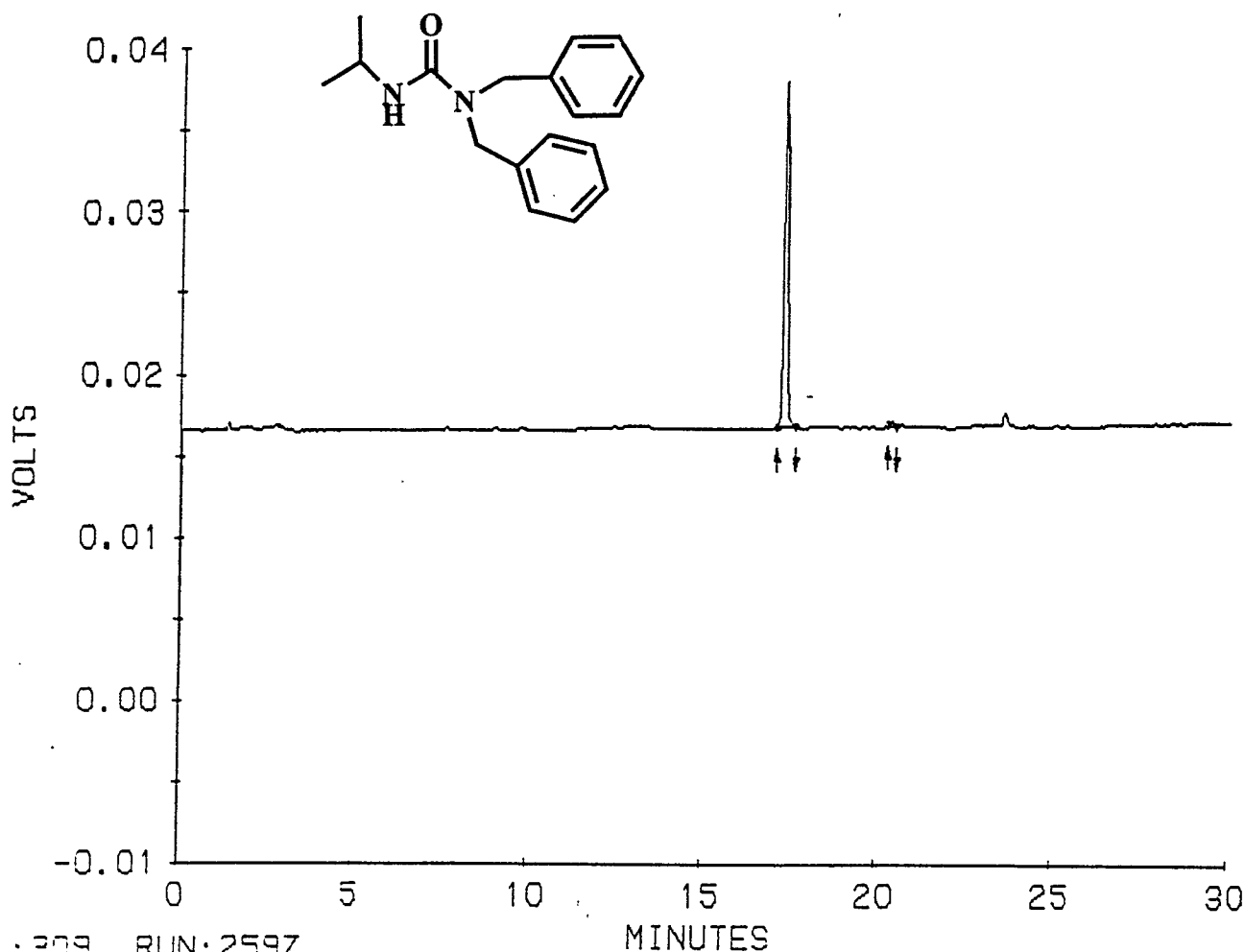
PK NO	START TIME	CREST TIME	END TIME	PEAK HEIGHT	PEAK AREA	AREA %
1	4.51	4.60	5.17	0.0004157	0.0000740	0.17
2	5.18	5.36	5.53	0.0024964	0.0002855	0.66
3	7.56	7.72	7.87	0.0011259	0.0001545	0.35
4	11.27	11.46	11.62	0.0017900	0.0002544	0.58
5	18.27	18.43	18.63	0.0008050	0.0001119	0.26
6	19.75	20.04	20.76	0.2819195	0.0425498	97.73
7	23.09	23.22	23.45	0.0007282	0.0001069	0.25

Report Process Time 20-JUN-1996 10:09:27, Report Based on Reintegration

Integration parameters in use for this injection:

TIME	VALUE	TYPE	--	TIME	VALUE	TYPE	--	TIME	VALUE	TYPE
0.0000	0.0500	PS		0.0000	0.0000	NS		0.0000	0.0000	SR
0.0000	1.0000	PW		0.0000	2.0000	SP		0.0000	2.0000	SN
0.0000	0.0300	PS		2.1500	0.0000	LT				

Compound 10k

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 GDS-S-6219-C-361


***** THIS REPORT WAS WRITTEN DURING AN INTERACTIVE GRAPHICS SESSION *****

INST.NO. 309 INJECTION ID NO. 2597 INJ TIME: 20-JUN-96 01:55:05
 USER ID: DESA INGRAD RUN ID: *MD -CYCLE: 156
 METHOD COMMENT:
 METHOD NAME: MD1 SAMPLE ID: - 30-12

PK NO	START TIME	CREST TIME	END TIME	PEAK HEIGHT	PEAK AREA	AREA %
1	17.12	17.35	17.67	0.0211840	0.0028921	98.61
2	20.28	20.38	20.52	0.0003709	0.0000408	1.39

Report Process Time 20-JUN-1996 10:15:27, Report Based on Cursor Editing

Integration parameters in use for this injection:

TIME	VALUE	TYPE	--	TIME	VALUE	TYPE	--	TIME	VALUE	TYPE
0.0000	0.0500	PS		0.0000	0.0000	NS		0.0000	0.0000	SR
0.0000	1.0000	PW		0.0000	2.0000	SP		0.0000	2.0000	SN
0.0000	0.0300	PS		2.1500	0.0000	LT				