SUPPORTING INFORMATION

Grignard-mediated reduction of 2,2,2-trichloro-1-arylethanones: One-pot reduction/aldol routes to 2,2-dichloro-3-hydroxy-1,3-diarylpropan-1-ones and related molecules

Ali H. Essa,[a,b] Reinner I. Lerrick,[a,c] Eçe Çiftçi,[a] Ross W. Harrington,[a] Paul G. Waddell,[a] William Clegg[a] and Michael J. Hall*[a]

[a] School of Chemistry, Newcastle University, Newcastle upon Tyne NE1 7RU, U.K., E-mail: michael.hall@newcastle.ac.uk

[b] Department of Chemistry, College of Science, University of Basrah, Basrah, Iraq.

[c] School of Chemistry, Nusa Cendana University, Indonesia

General experimental information

^{1}H and ^{13}C NMR spectra were recorded directly with a Jeol Lambda 500 MHz, Jeol ECS-400 MHz or Bruker Avance 300 MHz. HRMS data were provided by the EPSRC National Mass Spectrometry Service (University of Swansea). X-ray diffraction data was obtained on an Oxford Diffraction Gemini except for compound **6f** which was collected on a Bruker D8 Venture. IR spectra were obtained as neat samples using a Varian 800 FT-IR Scimitar Series spectrometer scanning from 4000-600 cm^{-1}.THF and Et_2O were distilled from sodium/benzophenone and used directly. DCM was distilled from calcium hydride and used directly.

1d - 2,2,2-trichloro-1-(5-methylfuran-2-yl)ethan-1-one

To a round bottom flask was added sequentially DCM (60 mL), 2,2,2-trichloroacetylchloride (3.7 mL, 33 mmol) and 2-methylfuran (2.463 g, 30 mmol). The solution was stirred for 24 hours under a nitrogen atmosphere. The solution was quenched with an aqueous solution of K_2CO_3 (1.38 g in 50 mL of water) and separated. The organic layer was washed with 3x100 mL of water, 100 mL of brine and then dried using $MgSO_4$. The solvent was removed under reduced pressure to give a brown oil. The crude product was purified through silica gel column chromatography (petrol : ether = 4 : 1) to give 2,2,2-trichloro-1-(5-methylfuran-2-yl)ethan-1-one (**1d**) as a brown oil (4.43 g, 65%).

R_f: 0.50 (UV active, petrol 40/60 : ether = 4: 1). ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.57 (dd, J = 3.6, 0.8 Hz, 1H), 6.29 (dd, J = 3.6, 0.8 Hz, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 170.0, 160.7, 143.5, 125.9, 109.7, 94.4, 14.2. IR (neat): υ_{max}/cm^{-1} 1685, 1500, 1211, 1031, 811, 742, 666. HRMS (pNSI): calcd for $C_7H_6O_2Cl_3$ $[M+H]^+$: 226.9428, found 226.9426.

1e - 2,2,2-trichloro-1-(1*H*-indol-3-yl)ethan-1-one

To a round bottom flask cooled to 0 ^{o}C was added sequentially DCM (40 mL), indole (1.17 g, 10 mmol) and pyridine (1.2 mL, 11 mmol). 2,2,2-trichloroacetylchloride (1.96 g, 11 mmol) was added into the solution for over 15 min. The solution was kept in fridge (5 ^{o}C) for 7 days during which time a precipitate had formed. The precipitate was filtered, washed with 50 mL methanol and 50 mL water respectively. The solid was dried under vacuum to give 2,2,2-trichloro-1-(1*H*-indol-3-yl)ethan-1-one (**1e**) as a light brown solid (2.28 g, 87%).

Mp = 235-237 ^{o}C. R_f: 0.35 (UV active, petrol 40/60 : EtOAc = 7: 3). ^{1}H NMR (400 MHz, d6-DMSO): δ_H 12.54 (s, 1H), 8.60 (s, 1H), 8.22-8.18 (m, 1H), 7.60-7.57 (m, 1H), 7.33-7.30 (m, 2H). ^{13}C NMR (100 MHz, d6-DMSO): δ_C 176.7, 136.7, 136.1, 127.1, 123.8, 123.1, 121.2, 112.9, 104.7, 96.5. IR (neat): υ_{max}/cm^{-1} 3251, 2981, 1639. HRMS (pNSI): calcd for $C_{10}H_7NOCl_3$ $[M+H]^+$: 261.9438, found 261.9436. EA calcd for $C_{10}H_6Cl_3NO$: C, 45.75; H, 2.30; N, 5.34. found: C, 45.82; H, 2.30; N, 5.45.

1f - 2,2,2-trichloro-1-(1-methyl-1*H*-indol-3-yl)ethan-1-one

To a round bottom flask under cooled to 0 ^{o}C was added sequentially DCM (20 mL), 1-methyl-1*H*-indole (0.655 g, 5 mmol) and pyridine (0.4 mL, 5.1 mmol). 2,2,2-trichloroacetylchloride (0.899 g, 5.1 mmol) was added to the solution over 15 min. The solution was kept in fridge (5 ^{o}C) for 3 days during which time a precipitate had formed. The precipitate was filtered then dissolved in DCM (25 mL). The solution was washed with 5x50 mL HCl 1M, dried over $MgSO_4$ and the organic solvent removed under reduced pressure to give 2,2,2-trichloro-1-(1-methyl-1*H*-indol-3-yl)ethan-1-one (**1f**) without further purification as a colourless solid (1.03 g, 75%).

Mp = 118-120 ^{o}C. R_f: 0.52 (UV active, petrol 40/60 : ether = 7: 3). ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.44 (s, 1H), 8.23-8.19 (m, 1H), 7.44-7.41 (m, 1H), 7.39-7.36 (m, 2H), 3.89 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 176.7, 138.0, 136.8, 133.9, 128.2, 124.0, 123.6, 122.6, 110.0, 105.3, 96.7. IR (neat): υ_{max}/cm^{-1} 2980, 1652. HRMS (pNSI): calcd for $C_{11}H_9NOCl_3$ $[M+H]^+$: 275.9743, found 275.9741. EA calcd for $C_{11}H_8Cl_3NO$: C, 47.78; H, 2.92; N, 5.07. found: C, 47.88; H, 2.85; N, 4.98.

1e - 2,2,2-trichloro-1-(1*H*-indol-3-yl)ethan-1-one

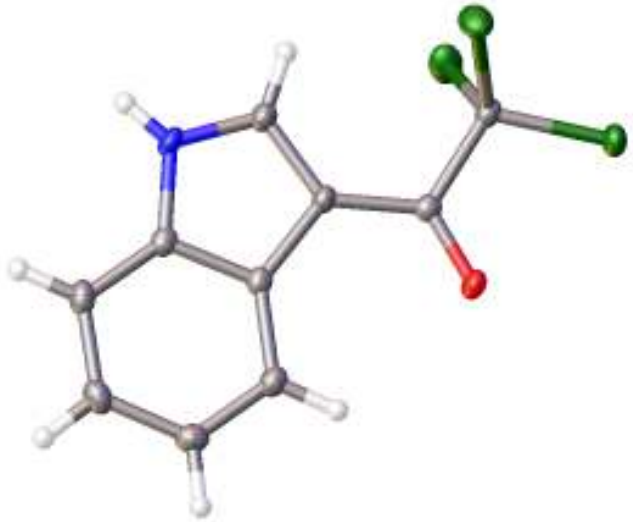


Table 1 Crystal data and structure refinement for mjh85.

Identification code	mjh85
Empirical formula	$C_{10}H_6Cl_3NO$
Formula weight	262.51
Temperature/K	150
Crystal system	orthorhombic
Space group	Pnma
a/Å	20.5153(14)
b/Å	6.7406(4)
c/Å	7.4148(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1025.36(12)
Z	4
ρ_{calc}g/cm^3	1.700
μ/mm^{-1}	0.860
F(000)	528.0
Crystal size/mm^3	0.2 × 0.2 × 0.07
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.842 to 56.998
Index ranges	$-27 \leq h \leq 26$, $-6 \leq k \leq 9$, $-9 \leq l \leq 7$
Reflections collected	5188
Independent reflections	1240 [R_{int} = 0.0272, R_{sigma} = 0.0271]
Data/restraints/parameters	1240/0/91
Goodness-of-fit on F^2	1.110
Final R indexes [I>=2σ (I)]	R_1 = 0.0282, wR_2 = 0.0660
Final R indexes [all data]	R_1 = 0.0321, wR_2 = 0.0692
Largest diff. peak/hole / e Å^{-3}	0.46/-0.24

1f - 2,2,2-trichloro-1-(1-methyl-1*H*-indol-3-yl)ethan-1-one

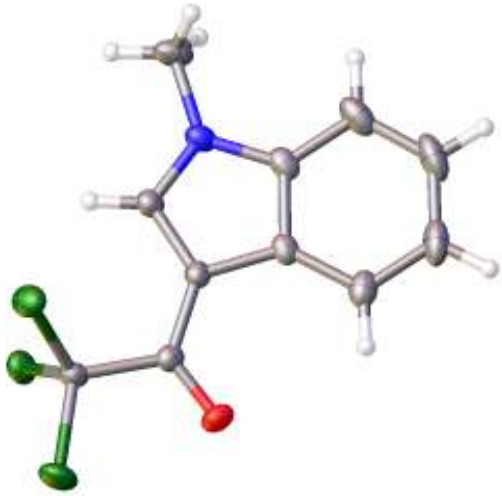


Table 1 Crystal data and structure refinement for mjh88.

Identification code	mjh88
Empirical formula	$C_{11}H_8NOCl_3$
Formula weight	276.53
Temperature/K	150.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.8736(5)
b/Å	11.2992(4)
c/Å	10.6096(5)
α/°	90
β/°	98.358(5)
γ/°	90
Volume/Å^3	1171.08(9)
Z	4
ρ_{calc}g/cm^3	1.568
μ/mm^{-1}	0.757
F(000)	560.0
Crystal size/mm^3	0.4 × 0.4 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.384 to 57.188
Index ranges	$-12 \leq h \leq 13$, $-15 \leq k \leq 15$, $-14 \leq l \leq 13$
Reflections collected	9535
Independent reflections	2573 [R_{int} = 0.0277, R_{sigma} = 0.0273]
Data/restraints/parameters	2573/0/146
Goodness-of-fit on F^2	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0303, wR_2 = 0.0650
Final R indexes [all data]	R_1 = 0.0413, wR_2 = 0.0715
Largest diff. peak/hole / e Å^{-3}	0.32/-0.24

2a - 2,2-dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)ethan-1-one

Table 1 Crystal data and structure refinement for mjh91.

Identification code	mjh91
Empirical formula	$C_7H_7NOCl_2$
Formula weight	192.04
Temperature/K	150
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	5.9311(3)
b/Å	10.5722(4)
c/Å	13.4606(6)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	844.04(7)
Z	4
ρ_{calc}g/cm^3	1.511
μ/mm^{-1}	0.708
F(000)	392.0
Crystal size/mm^3	0.4 × 0.4 × 0.3
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.054 to 57.39
Index ranges	$-7 \leq h \leq 7$, $-14 \leq k \leq 13$, $-18 \leq l \leq 16$
Reflections collected	6723
Independent reflections	1892 [R_{int} = 0.0211, R_{sigma} = 0.0191]
Data/restraints/parameters	1892/0/101
Goodness-of-fit on F^2	1.098
Final R indexes [I>=2σ (I)]	R_1 = 0.0222, wR_2 = 0.0559
Final R indexes [all data]	R_1 = 0.0231, wR_2 = 0.0566
Largest diff. peak/hole / e Å^{-3}	0.18/-0.34
Flack parameter	0.02(2)

2f - 2,2-dichloro-1-(1-methyl-1*H*-indol-3-yl)ethan-1-one

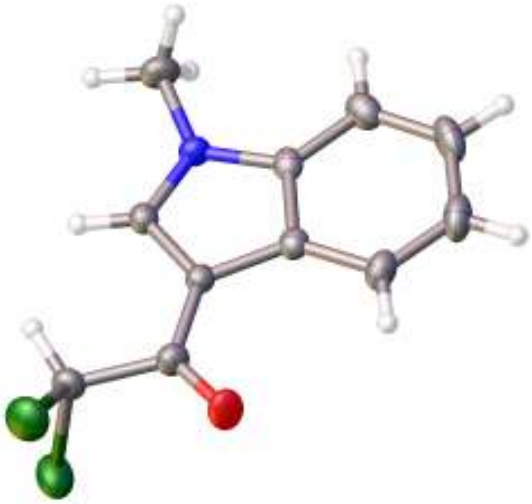


Table 1 Crystal data and structure refinement for mjh92.

Identification code	mjh92
Empirical formula	$C_{11}H_9Cl_2NO$
Formula weight	242.09
Temperature/K	150
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	6.9827(4)
b/Å	11.0753(6)
c/Å	14.6118(11)
α/°	90
β/°	111.091(5)
γ/°	90
Volume/Å^3	1054.31(12)
Z	4
ρ_{calc}g/cm^3	1.525
μ/mm^{-1}	0.584
F(000)	496.0
Crystal size/mm^3	0.4 × 0.3 × 0.3
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.254 to 57.082
Index ranges	$-9 \leq h \leq 9$, $-14 \leq k \leq 14$, $-19 \leq l \leq 8$
Reflections collected	4305
Independent reflections	4305 [R_{int} = ?, R_{sigma} = 0.0320]
Data/restraints/parameters	4305/0/138
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0400, wR_2 = 0.0902
Final R indexes [all data]	R_1 = 0.0503, wR_2 = 0.0986
Largest diff. peak/hole / e Å^{-3}	0.30/-0.38

2h - 2,2-dichloro-3-hydroxy-3-(perfluorophenyl)-1-(*p*-tolyl)propan-1-one

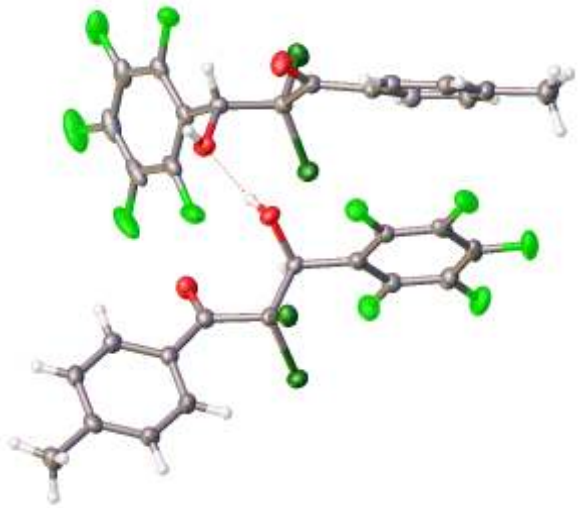


Table 1 Crystal data and structure refinement for mjh82.

Identification code	mjh82
Empirical formula	$C_{16}H_9O_2F_5Cl_2$
Formula weight	399.13
Temperature/K	150
Crystal system	orthorhombic
Space group	Pccn
a/Å	14.3029(5)
b/Å	20.8740(9)
c/Å	20.9090(8)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	6242.6(4)
Z	16
ρ_{calc}g/cm^3	1.699
μ/mm^{-1}	0.479
F(000)	3200.0
Crystal size/mm^3	0.3 × 0.1 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.208 to 57.24
Index ranges	-14 ≤ h ≤ 18, -22 ≤ k ≤ 27, -27 ≤ l ≤ 26
Reflections collected	33189
Independent reflections	7084 [R_{int} = 0.0431, R_{sigma} = 0.0336]
Data/restraints/parameters	7084/396/461
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0387, wR_2 = 0.0921
Final R indexes [all data]	R_1 = 0.0563, wR_2 = 0.1044
Largest diff. peak/hole / e Å^{-3}	0.45/-0.27

2j - 2,2-dichloro-3-hydroxy-1-(1*H*-indol-3-yl)-3-(perfluorophenyl)propan-1-one

Table 1 Crystal data and structure refinement for mjh90.

Identification code	mjh90
Empirical formula	$C_{17}H_8NO_2F_5Cl_2$
Formula weight	424.14
Temperature/K	150.0
Crystal system	triclinic
Space group	P-1
a/Å	7.3186(3)
b/Å	9.4938(6)
c/Å	11.7970(7)
α/°	83.481(5)
β/°	89.534(4)
γ/°	76.102(4)
Volume/Å^3	790.38(8)
Z	2
ρ_{calc}g/cm^3	1.782
μ/mm^{-1}	0.480
F(000)	424.0
Crystal size/mm^3	0.24 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.954 to 57.238
Index ranges	$-9 \leq h \leq 8$, $-10 \leq k \leq 12$, $-15 \leq l \leq 15$
Reflections collected	6097
Independent reflections	3273 [R_{int} = 0.0246, R_{sigma} = 0.0432]
Data/restraints/parameters	3273/1/252
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0385, wR_2 = 0.0808
Final R indexes [all data]	R_1 = 0.0524, wR_2 = 0.0895
Largest diff. peak/hole / e Å^{-3}	0.40/-0.36

2k - 2,2-dichloro-3-hydroxy-1-(1-methyl-1*H*-indol-3-yl)-3-(perfluorophenyl)propan-1-one

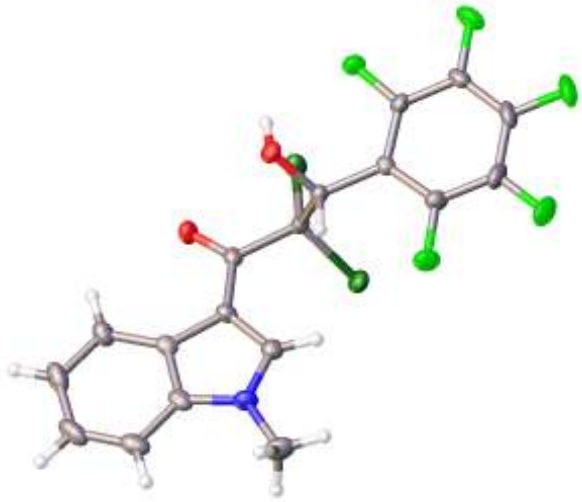


Table 1 Crystal data and structure refinement for mjh94.

Identification code	mjh94
Empirical formula	$C_{18}H_{10}NO_2F_5Cl_2$
Formula weight	438.17
Temperature/K	150.0
Crystal system	triclinic
Space group	P-1
a/Å	7.7970(6)
b/Å	9.7342(7)
c/Å	12.0220(10)
α/°	91.836(7)
β/°	97.659(6)
γ/°	109.698(7)
Volume/Å^3	848.48(12)
Z	2
ρ_{calc}g/cm^3	1.715
μ/mm^{-1}	0.451
F(000)	440.0
Crystal size/mm^3	0.2 × 0.1 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.616 to 57.04
Index ranges	$-8 \leq h \leq 10$, $-10 \leq k \leq 12$, $-14 \leq l \leq 15$
Reflections collected	7559
Independent reflections	3605 [R_{int} = 0.0415, R_{sigma} = 0.0711]
Data/restraints/parameters	3605/0/255
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0481, wR_2 = 0.0805
Final R indexes [all data]	R_1 = 0.0836, wR_2 = 0.0945
Largest diff. peak/hole / e Å^{-3}	0.32/-0.30

2o - 2,2-dichloro-3-hydroxy-3-(4-nitrophenyl)-1-(*p*-tolyl)propan-1-one

Table 1 Crystal data and structure refinement for mjh86.

Identification code	mjh86
Empirical formula	$C_{16}H_{13}NO_4Cl_2$
Formula weight	354.17
Temperature/K	150
Crystal system	triclinic
Space group	P-1
a/Å	8.4691(5)
b/Å	9.8694(6)
c/Å	10.0248(5)
α/°	87.037(4)
β/°	87.379(4)
γ/°	65.674(5)
Volume/Å^3	762.23(8)
Z	2
ρ_{calc}g/cm^3	1.543
μ/mm^{-1}	0.445
F(000)	364.0
Crystal size/mm^3	0.21 × 0.2 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.982 to 57.182
Index ranges	-11 ≤ h ≤ 10, -13 ≤ k ≤ 12, -12 ≤ l ≤ 12
Reflections collected	11888
Independent reflections	3394 [R_{int} = 0.0356, R_{sigma} = 0.0363]
Data/restraints/parameters	3394/0/212
Goodness-of-fit on F^2	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0389, wR_2 = 0.1015
Final R indexes [all data]	R_1 = 0.0503, wR_2 = 0.1105
Largest diff. peak/hole / e Å^{-3}	0.50/-0.29

2t - diethyl 2-(1,1-dichloro-2-(1-methyl-1*H*-indol-3-yl)-2-oxoethyl)-2-hydroxymalonate

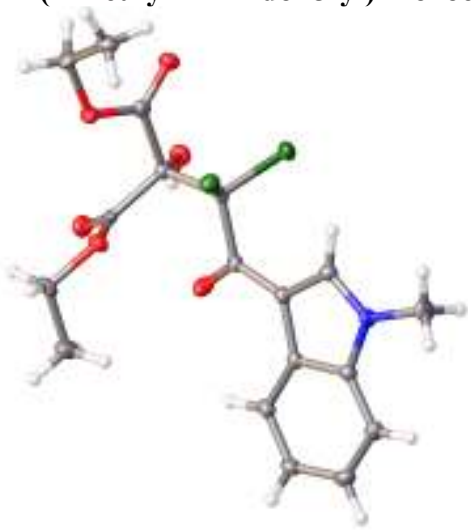


Table 1 Crystal data and structure refinement for mjh95.

Identification code	mjh95
Empirical formula	$C_{18}H_{19}NO_6Cl_2$
Formula weight	416.24
Temperature/K	150.0
Crystal system	triclinic
Space group	P-1
a/Å	8.6111(5)
b/Å	10.1757(6)
c/Å	11.1365(7)
α/°	87.574(5)
β/°	70.982(6)
γ/°	75.760(5)
Volume/Å^3	893.45(10)
Z	2
ρ_{calc}g/cm^3	1.547
μ/mm^{-1}	0.401
F(000)	432.0
Crystal size/mm^3	0.4 × 0.3 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.766 to 57.188
Index ranges	$-9 \leq h \leq 10$, $-12 \leq k \leq 9$, $-13 \leq l \leq 14$
Reflections collected	7004
Independent reflections	3683 [R_{int} = 0.0285, R_{sigma} = 0.0472]
Data/restraints/parameters	3683/0/251
Goodness-of-fit on F^2	1.070
Final R indexes [I>=2σ (I)]	R_1 = 0.0365, wR_2 = 0.0792
Final R indexes [all data]	R_1 = 0.0481, wR_2 = 0.0879
Largest diff. peak/hole / e Å^{-3}	0.43/-0.31

3a - (1*R,3*R**)-2,2-dichloro-3-hydroxy-3-(4-nitrophenyl)-1-(*p*-tolyl)propyl 4-nitrobenzoate**

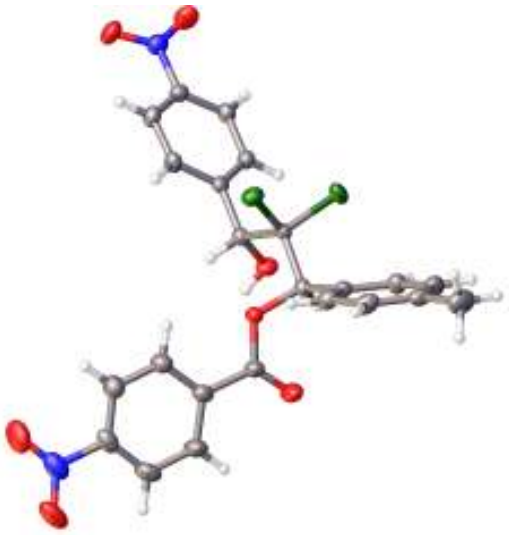


Table 1 Crystal data and structure refinement for mjh87.

Identification code	mjh87
Empirical formula	$C_{23}H_{18}N_2O_7Cl_2$
Formula weight	505.29
Temperature/K	150
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	8.4445(4)
b/Å	15.4187(7)
c/Å	17.2259(8)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2242.87(18)
Z	4
ρ_{calc}g/cm^3	1.496
μ/mm^{-1}	0.339
F(000)	1040.0
Crystal size/mm^3	0.4 × 0.3 × 0.3
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.79 to 57.414
Index ranges	$-8 \le h \le 11$, $-18 \le k \le 20$, $-20 \le l \le 21$
Reflections collected	10321
Independent reflections	4711 [R_{int} = 0.0338, R_{sigma} = 0.0480]
Data/restraints/parameters	4711/0/309
Goodness-of-fit on F^2	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0400, wR_2 = 0.0819
Final R indexes [all data]	R_1 = 0.0492, wR_2 = 0.0879
Largest diff. peak/hole / e Å^{-3}	0.27/-0.21
Flack parameter	0.03(4)

3b - (1*R,3*R**)-1-(4-(*tert*-butyl)phenyl)-2,2-dichloro-3-hydroxy-3-(4-nitrophenyl)propyl 4-nitrobenzoate**

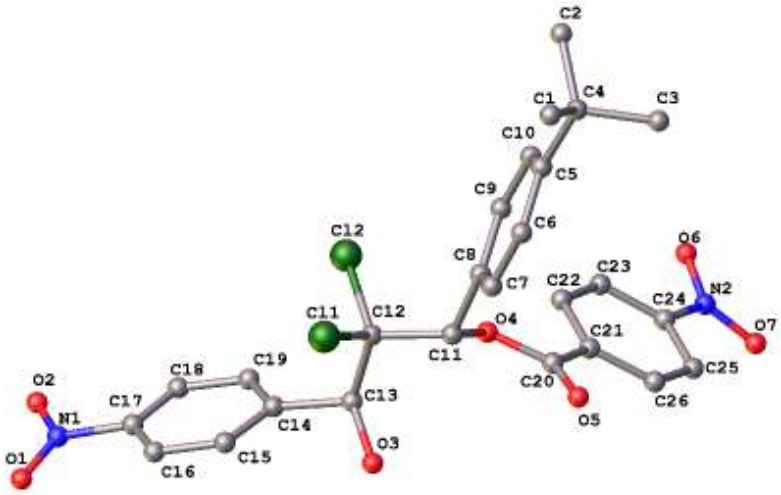


Table 1 Crystal data and structure refinement for mjh83.

Identification code	mjh83
Empirical formula	$C_{27}H_{24}N_2O_7Cl_5$
Formula weight	665.73
Temperature/K	150.0
Crystal system	monoclinic
Space group	Pn
a/Å	6.7051(3)
b/Å	14.1443(6)
c/Å	15.7774(6)
α/°	90
β/°	101.326(4)
γ/°	90
Volume/Å^3	1467.17(11)
Z	2
ρ_{calc}g/cm^3	1.507
μ/mm^{-1}	0.543
F(000)	682.0
Crystal size/mm^3	0.4 × 0.4 × 0.3
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.004 to 57.308
Index ranges	$-8 \le h \le 8$, $-18 \le k \le 15$, $-19 \le l \le 20$
Reflections collected	9761
Independent reflections	4882 [R_{int} = 0.0205, R_{sigma} = 0.0259]
Data/restraints/parameters	4882/311/370
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0374, wR_2 = 0.0926
Final R indexes [all data]	R_1 = 0.0388, wR_2 = 0.0938
Largest diff. peak/hole / e Å^{-3}	0.49/-0.46
Flack parameter	-0.01(2)

6a - ((2*R,3*R**)-2-chloro-3-(4-nitrophenyl)oxiran-2-yl)(1-methyl-1*H*-pyrrol-2-yl)methanone**

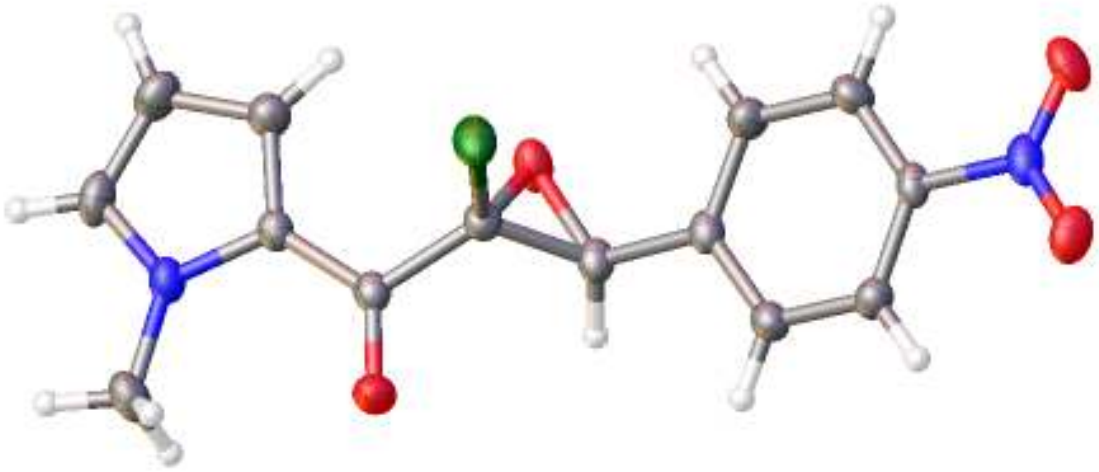


Table 1 Crystal data and structure refinement for mjh130005.

Identification code	mjh130005
Empirical formula	$C_{14}H_{11}O_4ClN_2$
Formula weight	306.70
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.4142(4)
b/Å	21.2032(8)
c/Å	8.5672(4)
α/°	90
β/°	116.111(6)
γ/°	90
Volume/Å^3	1372.47(12)
Z	4
ρ_{calc}g/cm^3	1.484
μ/mm^{-1}	0.296
F(000)	632.0
Crystal size/mm^3	0.34 × 0.3 × 0.03
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.724 to 57.204
Index ranges	$-11 \leq h \leq 10$, $-25 \leq k \leq 28$, $-11 \leq l \leq 11$
Reflections collected	14096
Independent reflections	3057 [R_{int} = 0.0232, R_{sigma} = 0.0191]
Data/restraints/parameters	3057/21/220
Goodness-of-fit on F^2	1.072
Final R indexes [I>=2σ (I)]	R_1 = 0.0369, wR_2 = 0.0853
Final R indexes [all data]	R_1 = 0.0429, wR_2 = 0.0888
Largest diff. peak/hole / e Å^{-3}	0.30/-0.34

6f - (2*R,3*R**)-2-chloro-3-(4-nitrophenyl)oxiran-2-yl)(*p*-tolyl)methanone**

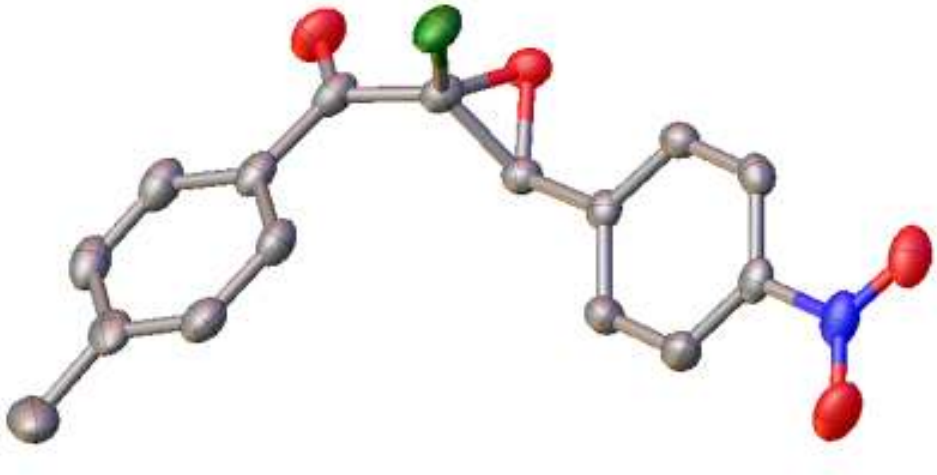


Table 1 Crystal data and structure refinement for mjh130018

Identification code	mjh130018
Empirical formula	$C_{16}H_{12}NO_4Cl$
Formula weight	317.72
Temperature/K	120.0
Crystal system	monoclinic
Space group	Cc
a/Å	15.660(2)
b/Å	7.1579(10)
c/Å	14.548(2)
α/°	90
β/°	113.366(4)
γ/°	90
Volume/Å^3	1497.0(4)
Z	4
ρ_{calc}mg/mm^3	1.410
m/mm^{-1}	0.272
F(000)	656.0
Crystal size/mm^3	0.49 × 0.44 × 0.41
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection	5.668 to 55.174°
Index ranges	$-20 \leq h \leq 20$, $-9 \leq k \leq 9$, $-18 \leq l \leq 18$
Reflections collected	9693
Independent reflections	3415[R(int) = 0.0244]
Data/restraints/parameters	3415/2/200
Goodness-of-fit on F^2	1.074
Final R indexes [I>=2σ (I)]	R_1 = 0.0302, wR_2 = 0.0752
Final R indexes [all data]	R_1 = 0.0321, wR_2 = 0.0770
Largest diff. peak/hole / e Å^{-3}	0.23/-0.20
Flack parameter	0.00(6)

6h - ((2*R,3*R**)-2-chloro-3-(4-nitrophenyl)oxiran-2-yl)(phenyl)methanone**

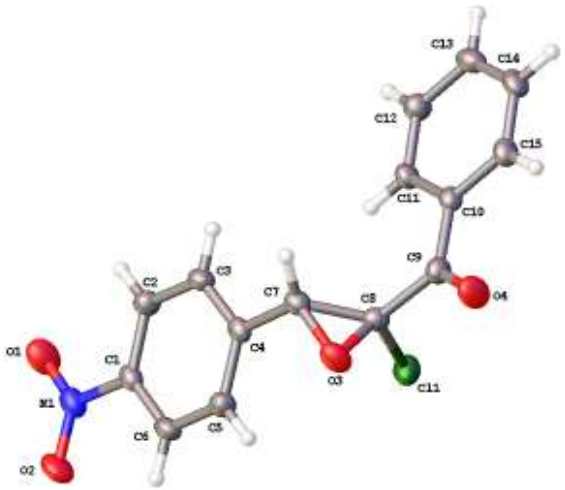
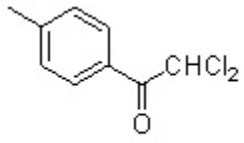


Table 1 Crystal data and structure refinement for mjh140034_fa.

Identification code	mjh140034_fa
Empirical formula	$C_{15}H_{10}NO_4Cl$
Formula weight	303.69
Temperature/K	150.01(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	7.32300(9)
b/Å	12.09364(16)
c/Å	15.09304(16)
α/°	90
β/°	96.2048(10)
γ/°	90
Volume/Å^3	1328.83(3)
Z	4
ρ_{calc}g/cm^3	1.518
μ/mm^{-1}	0.303
F(000)	624.0
Crystal size/mm^3	0.3 × 0.23 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.532 to 55.77
Index ranges	-9 ≤ h ≤ 9, -15 ≤ k ≤ 15, -19 ≤ l ≤ 19
Reflections collected	40662
Independent reflections	3041 [R_{int} = 0.0486, R_{sigma} = 0.0222]
Data/restraints/parameters	3041/0/190
Goodness-of-fit on F^2	1.028
Final R indexes [I>=2σ (I)]	R_1 = 0.0328, wR_2 = 0.0724
Final R indexes [all data]	R_1 = 0.0447, wR_2 = 0.0779
Largest diff. peak/hole / e Å^{-3}	0.30/-0.28



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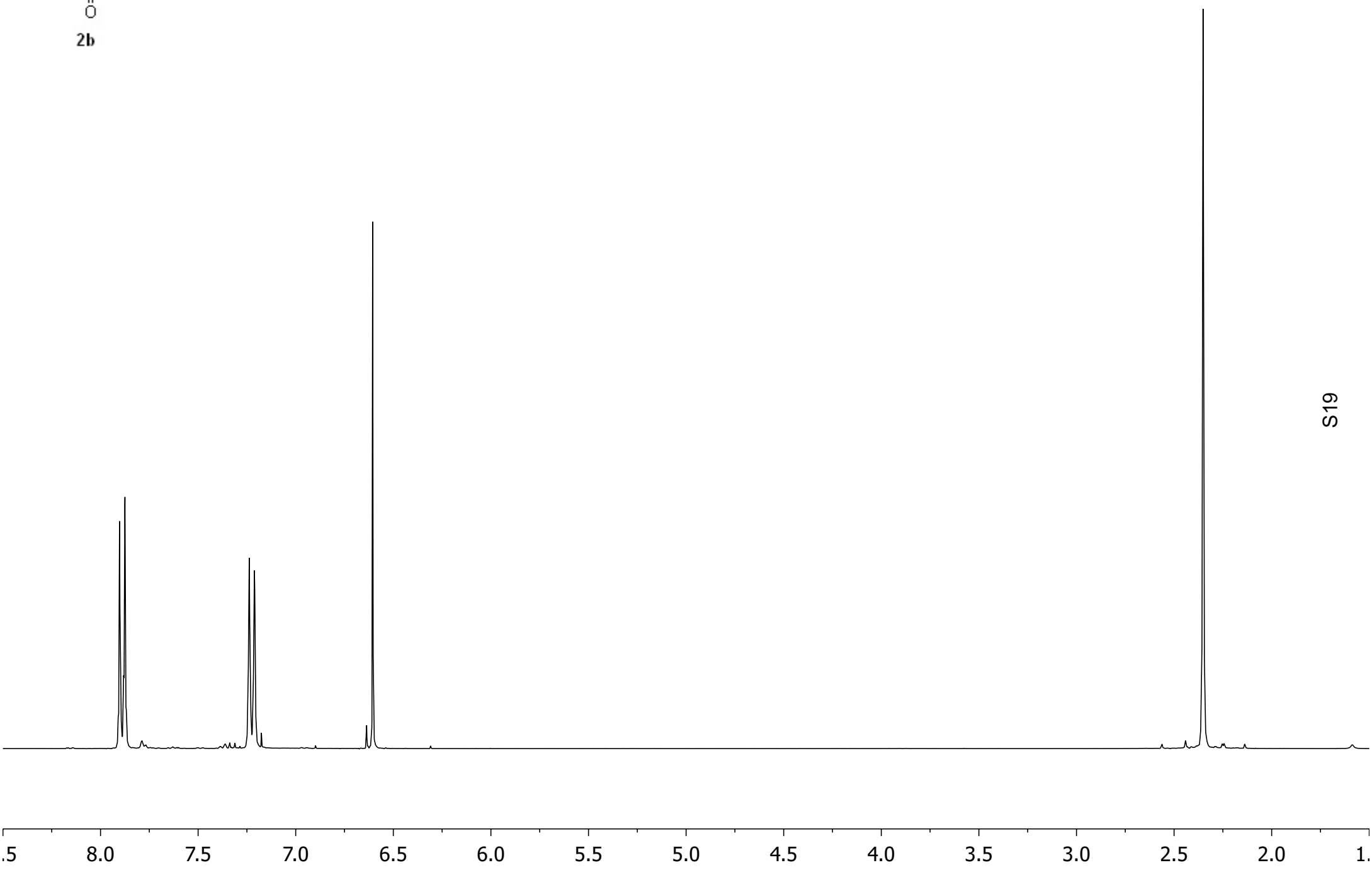

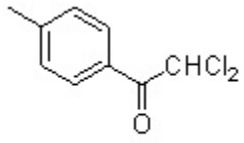

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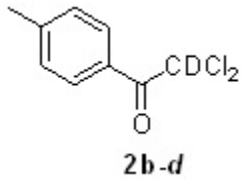

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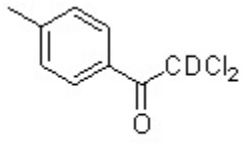
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O

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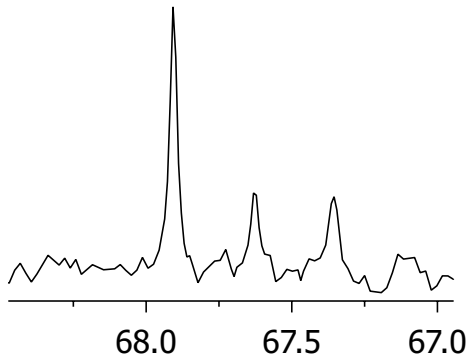
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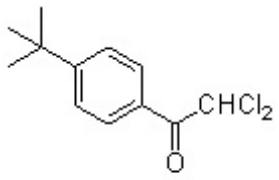

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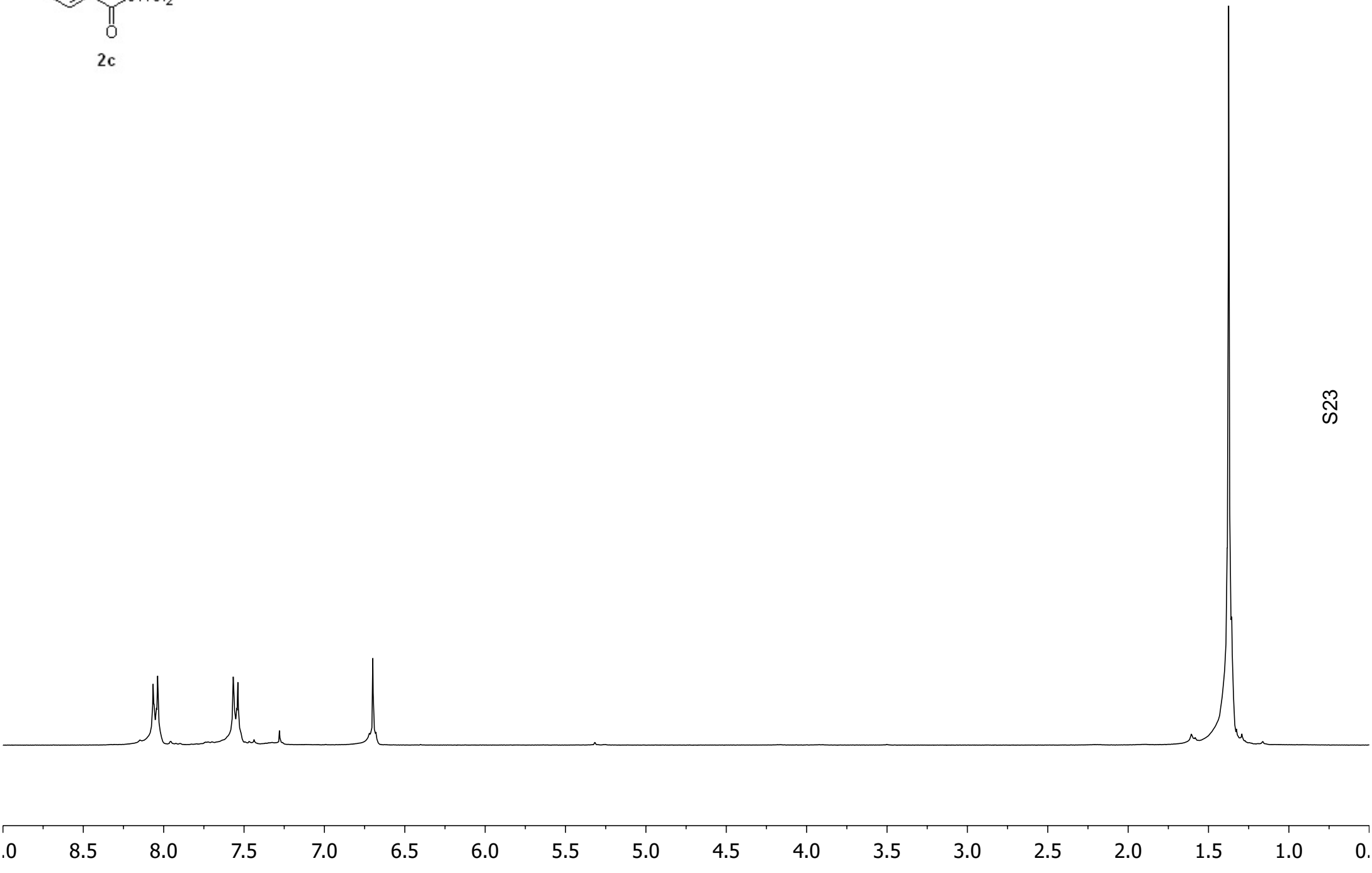

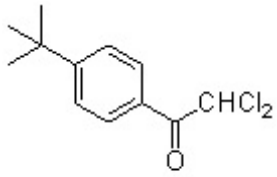
CHCl2
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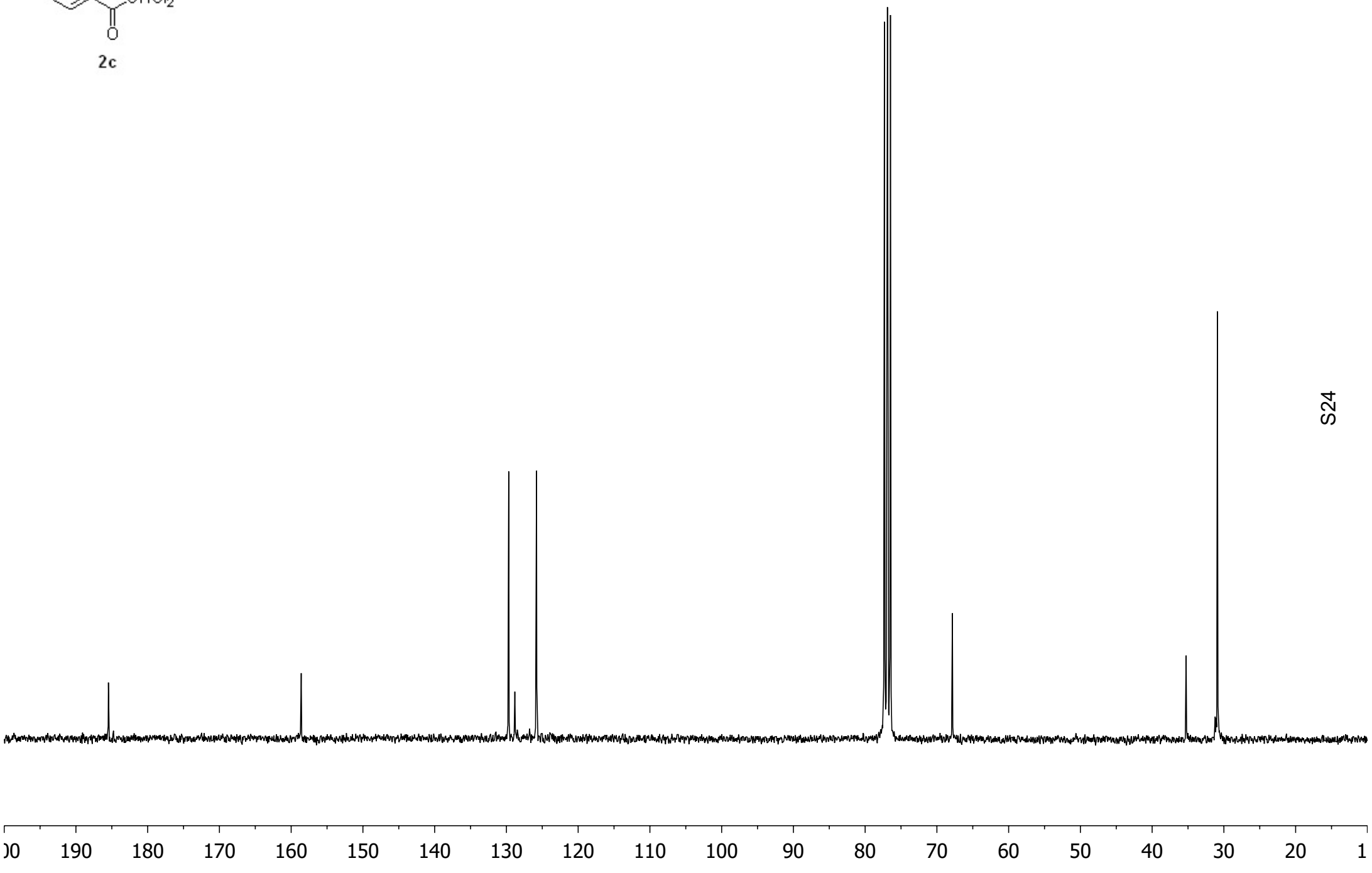
2c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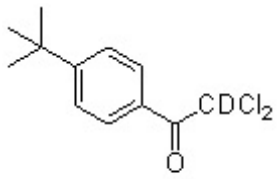

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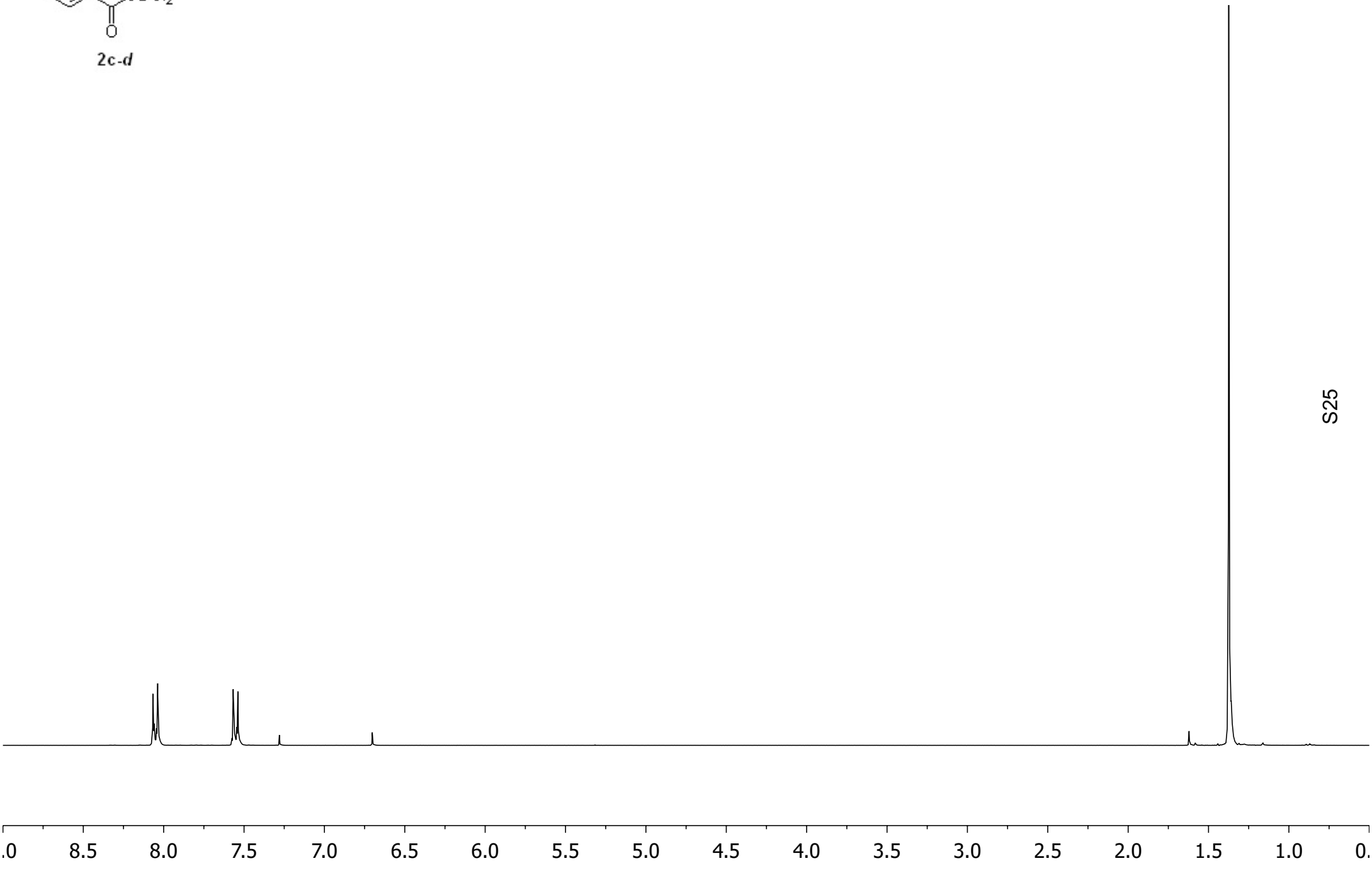

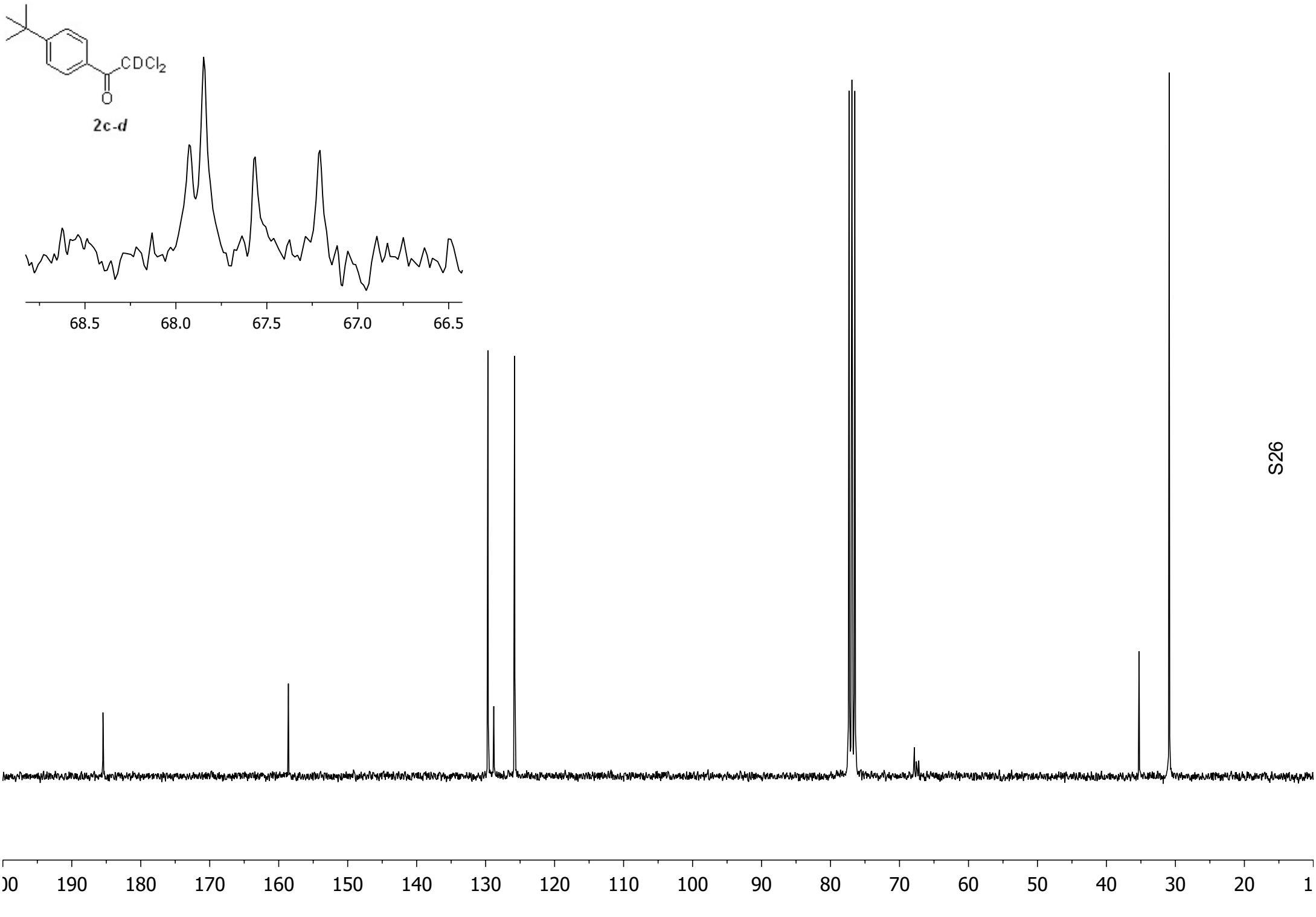
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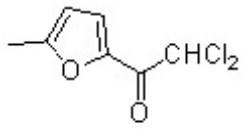

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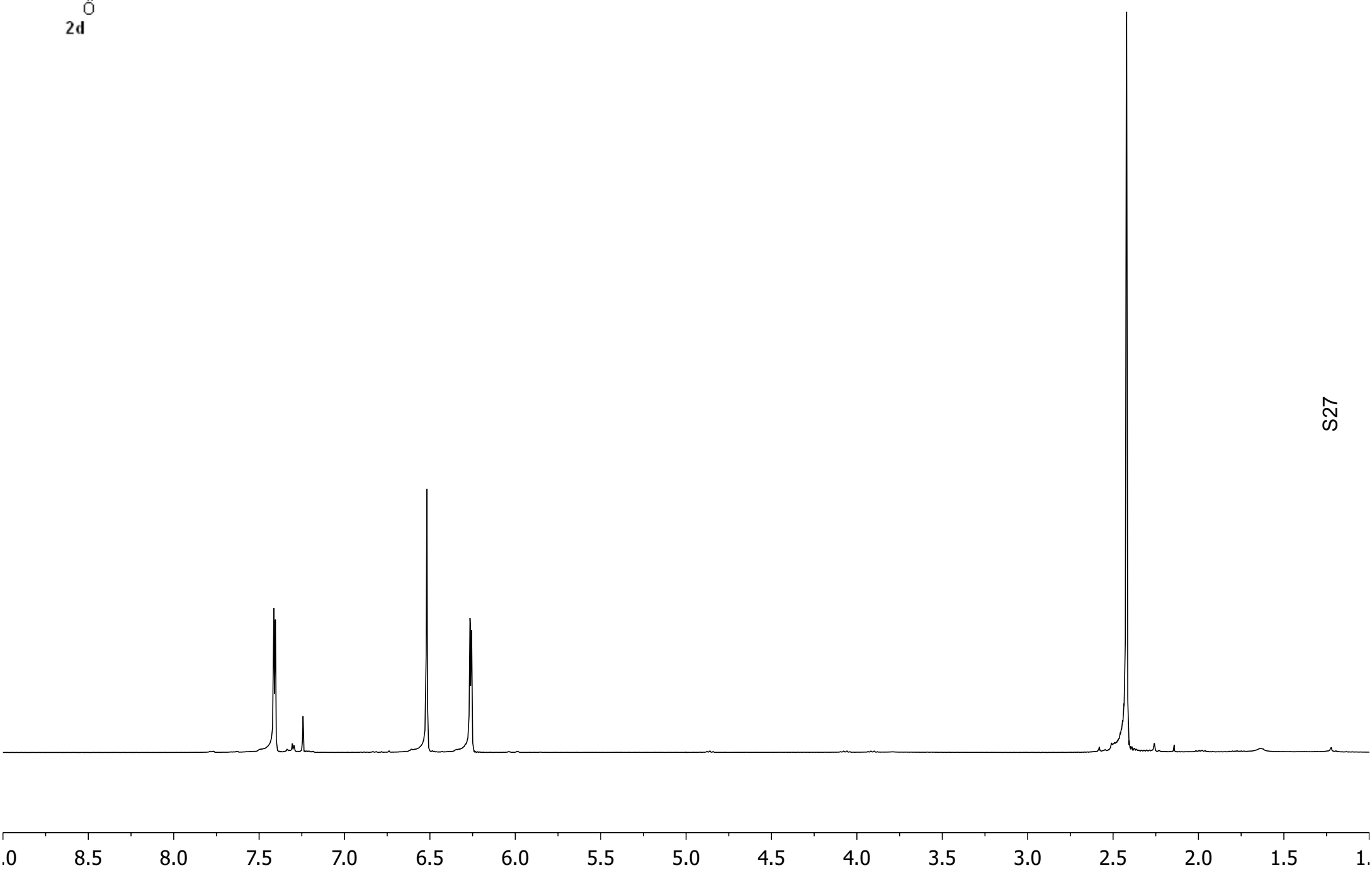

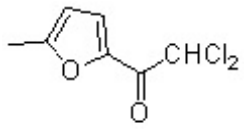
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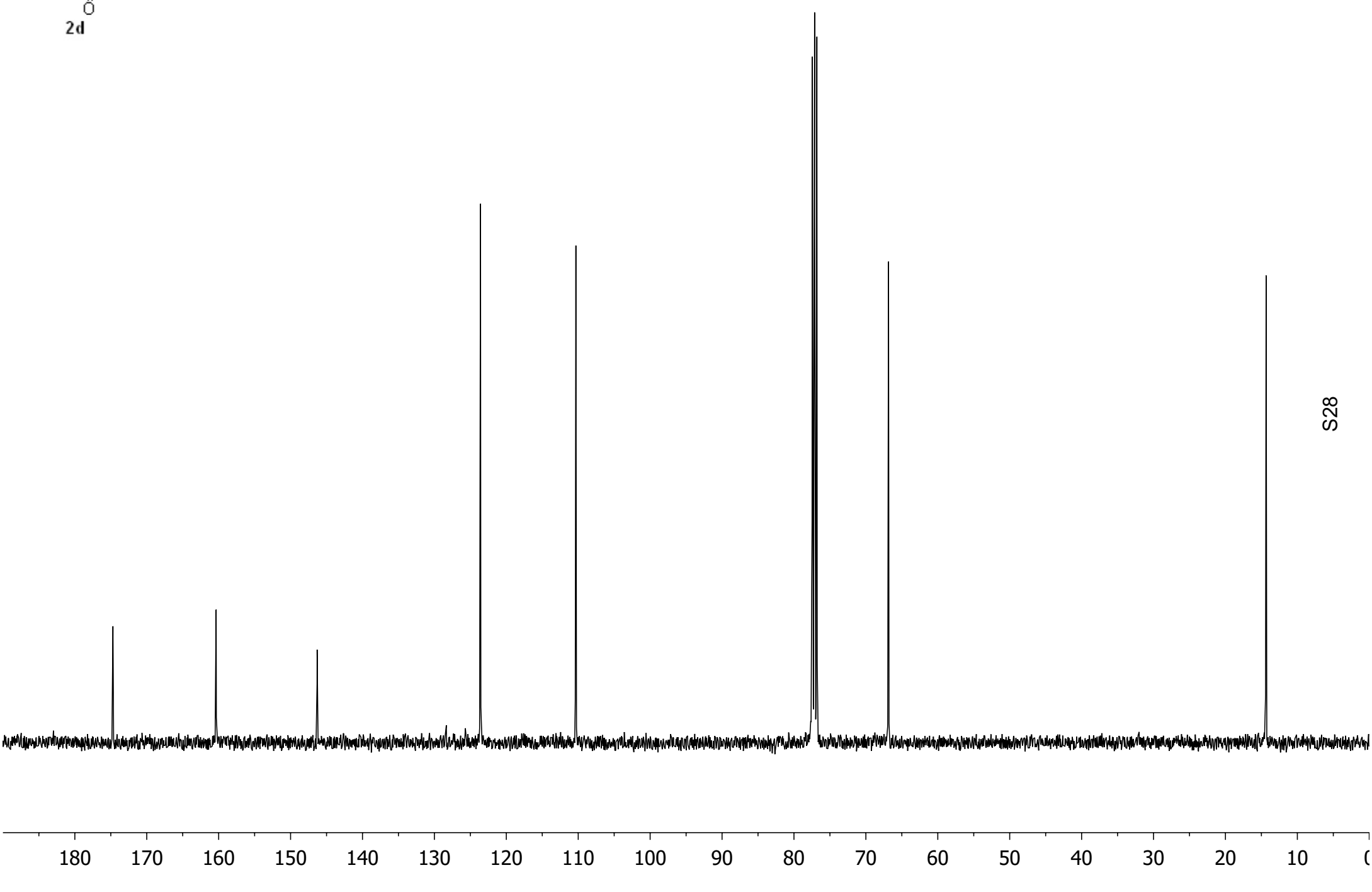
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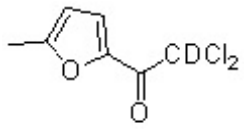

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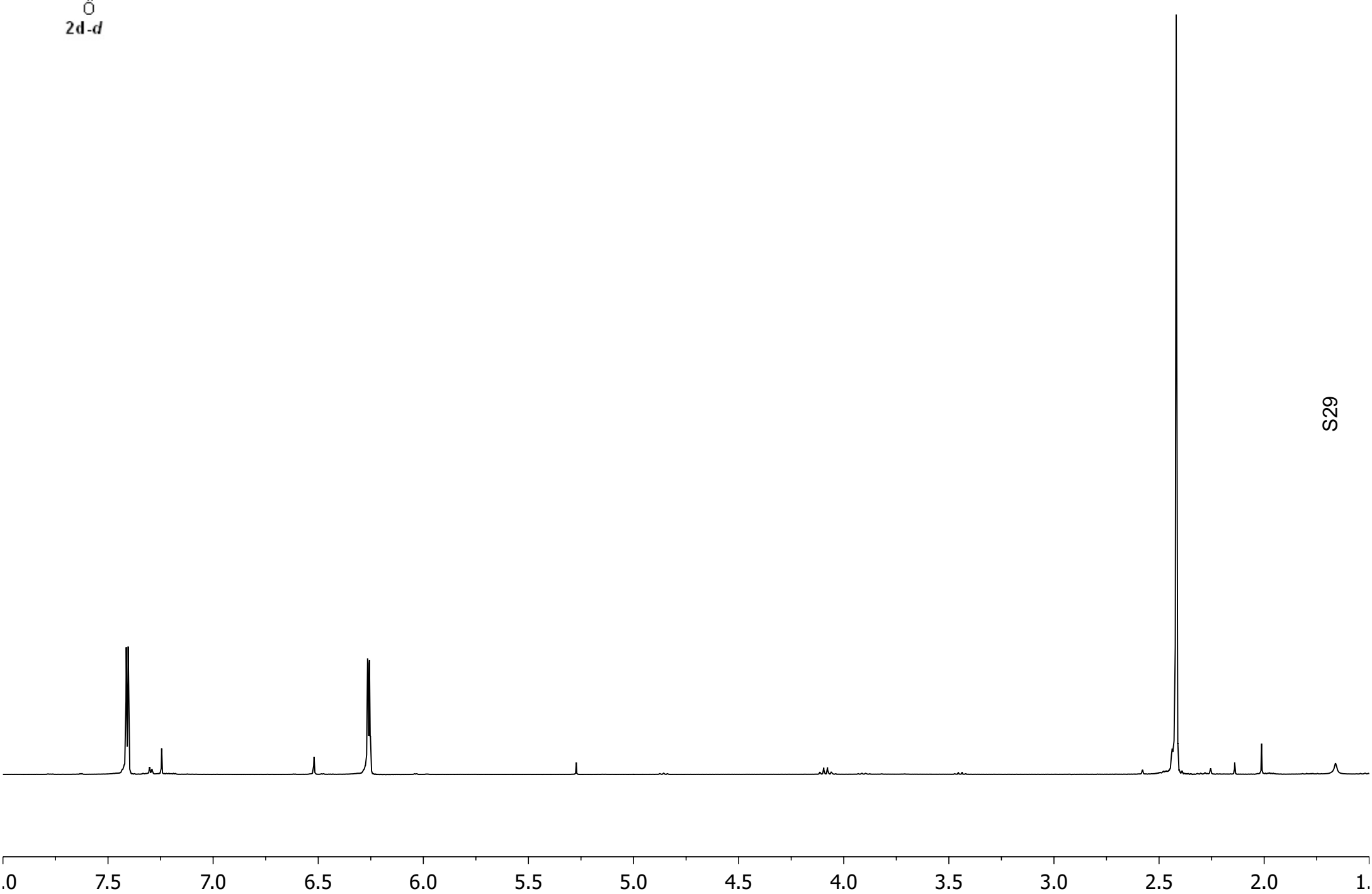

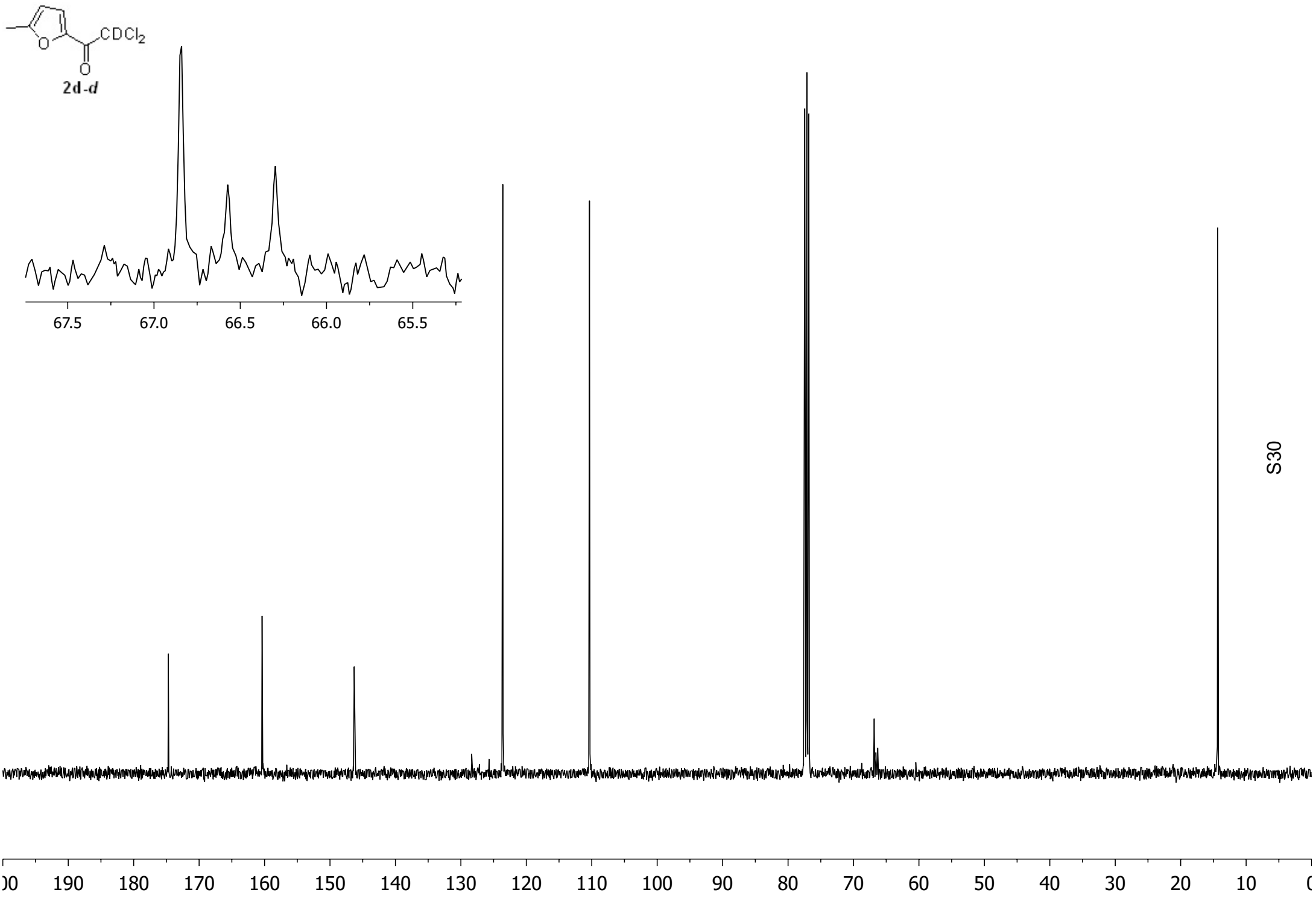
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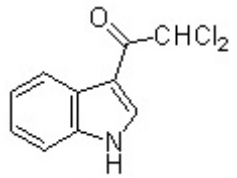
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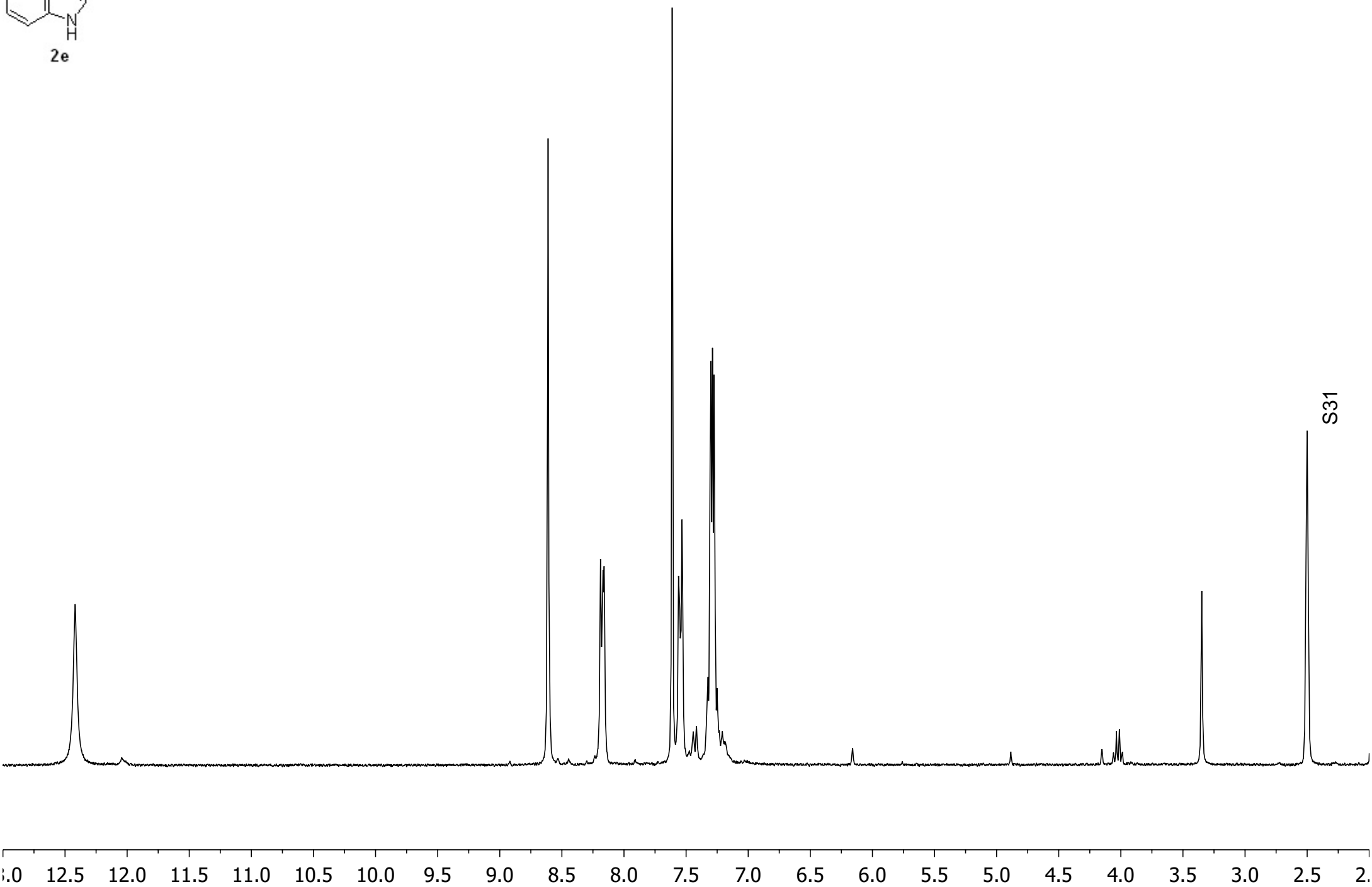
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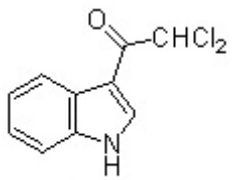

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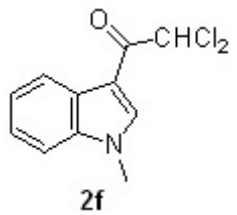

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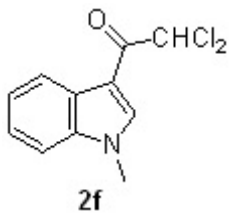

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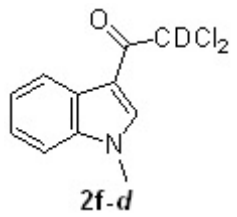
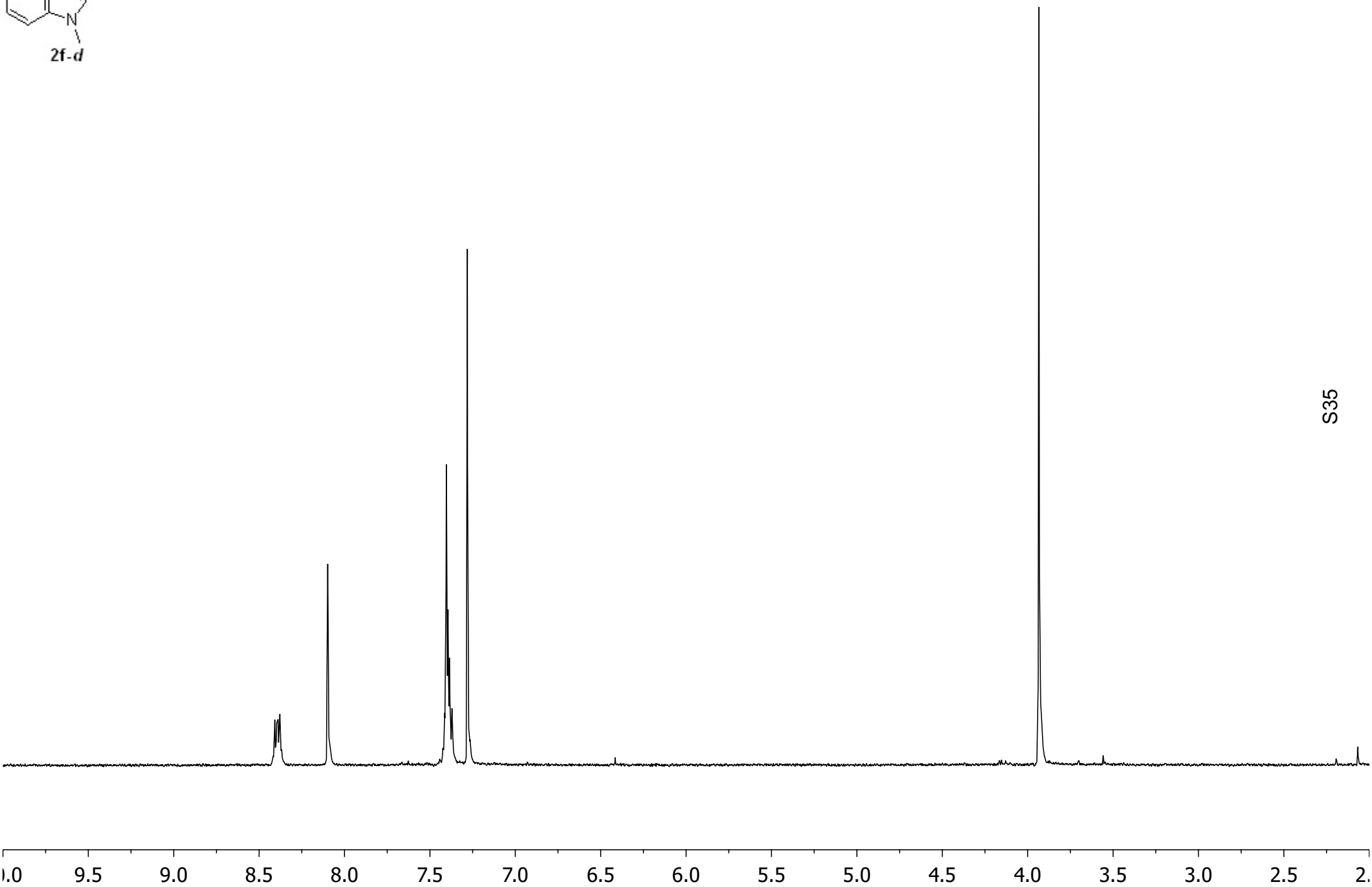
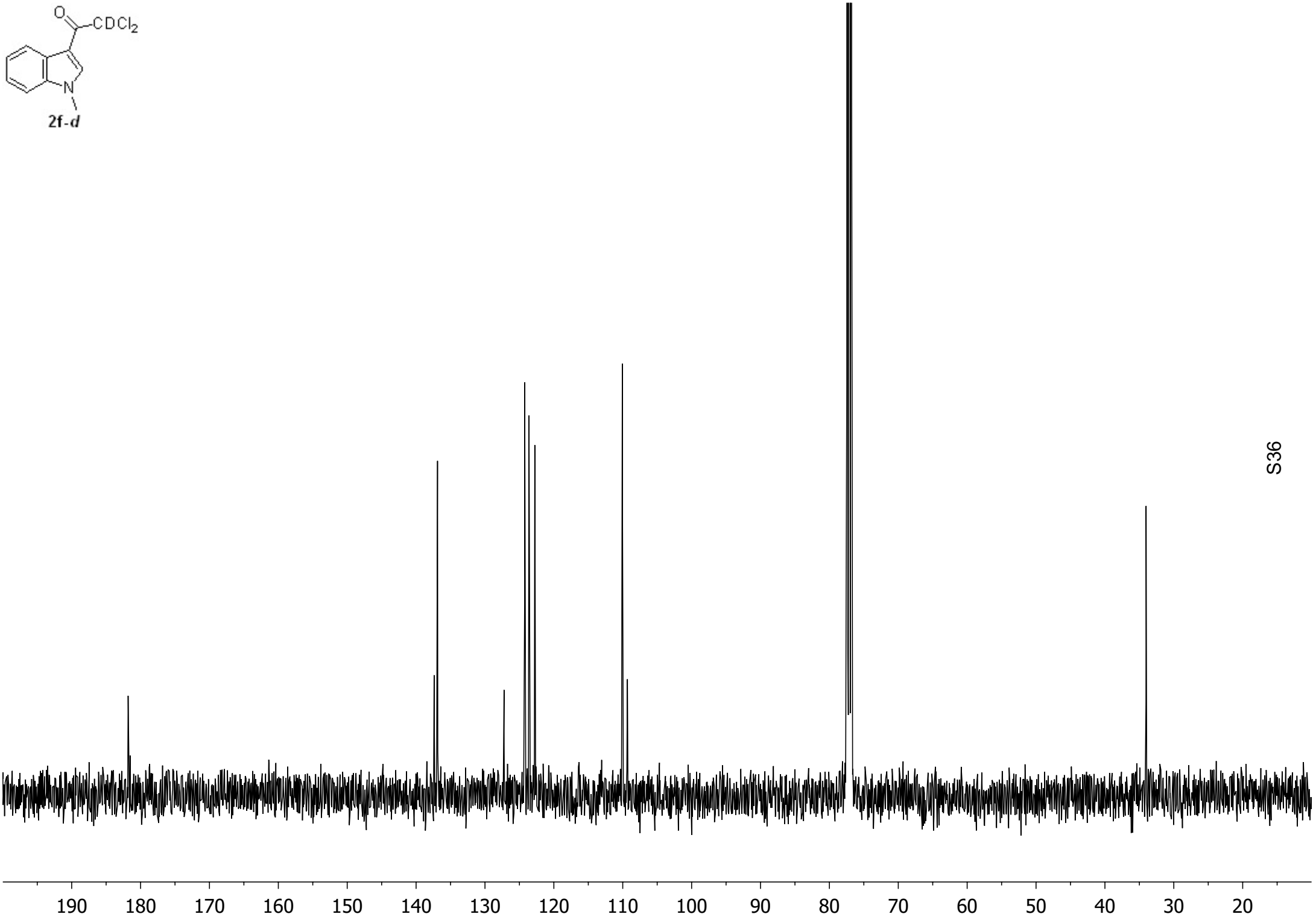


2f-*d*

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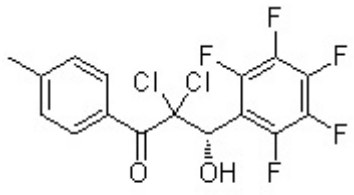

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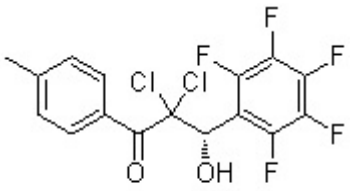

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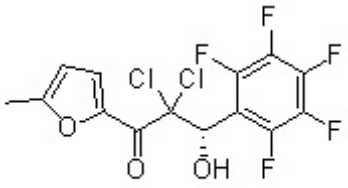

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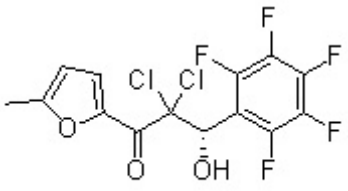

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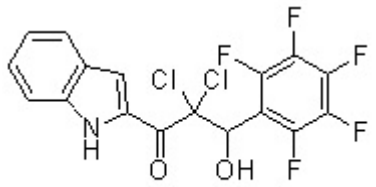

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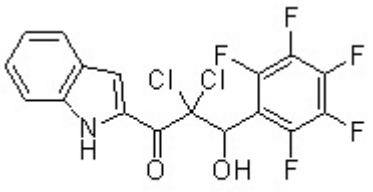

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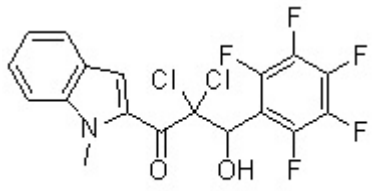

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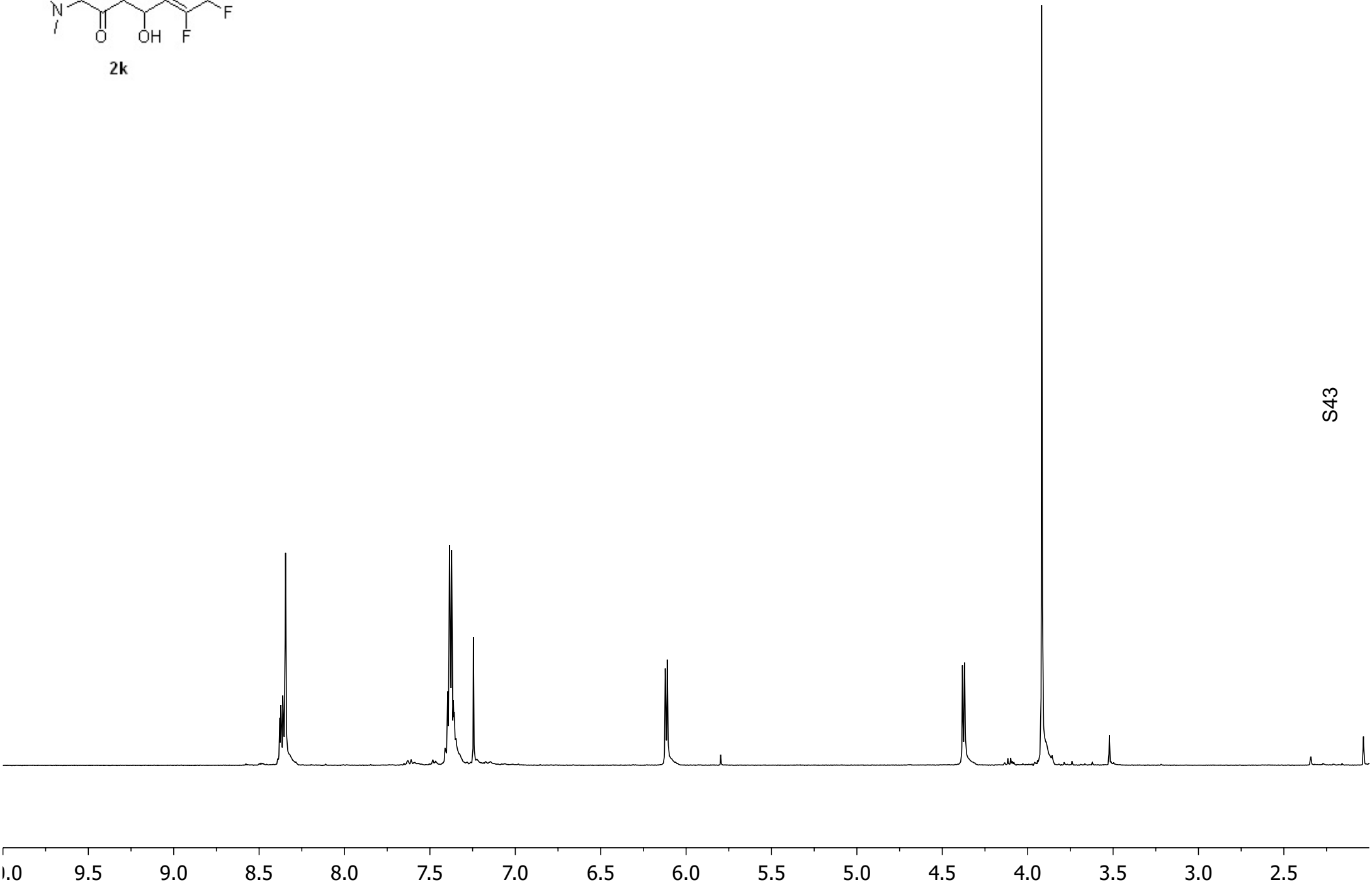

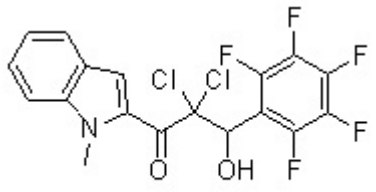

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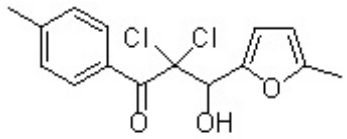

2m

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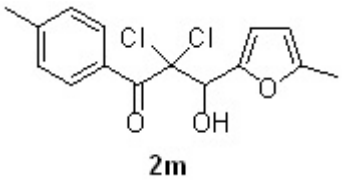

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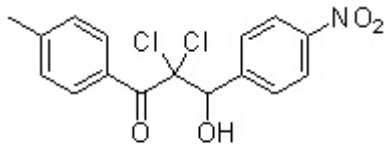

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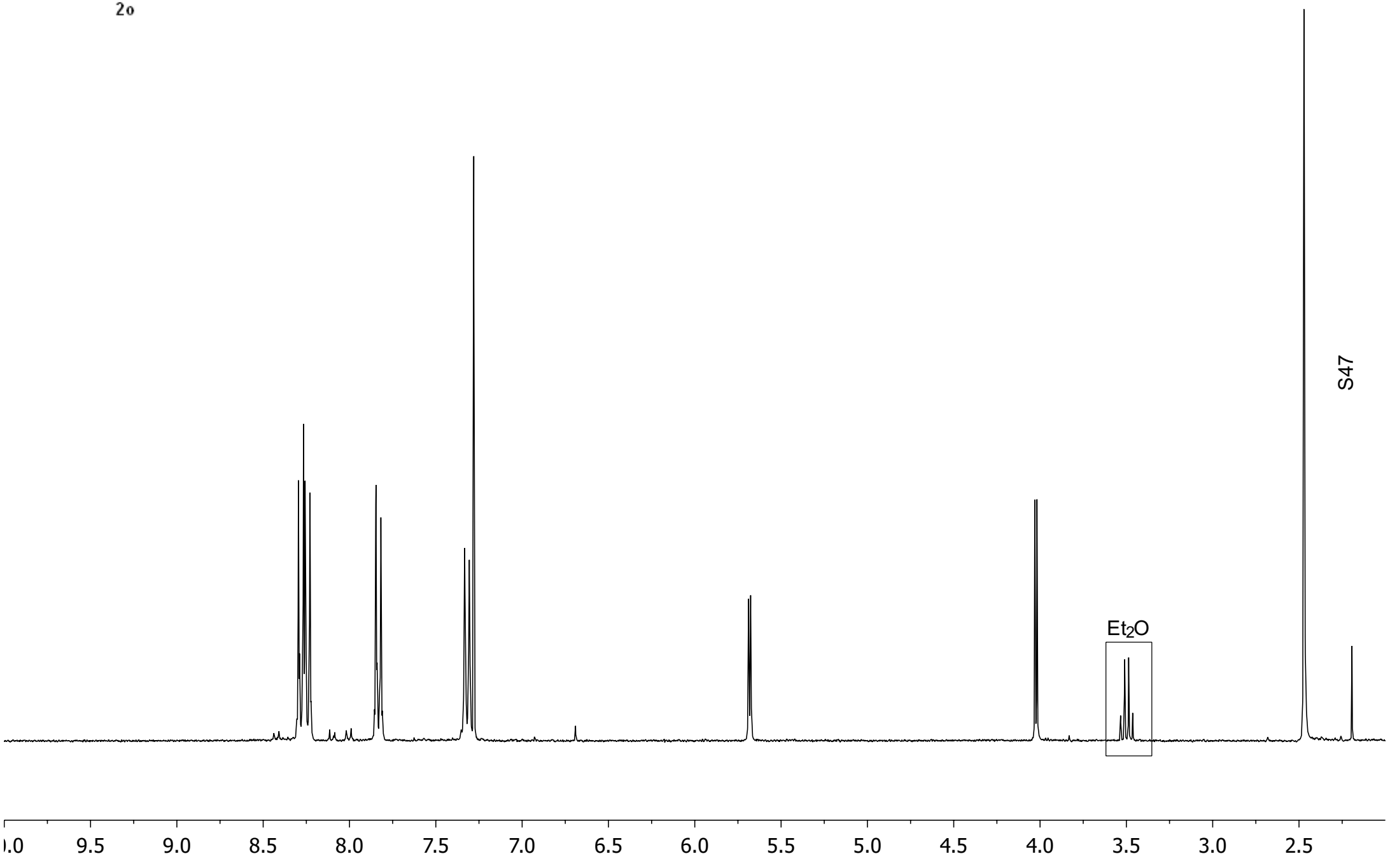

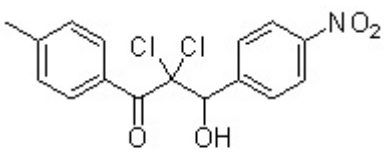

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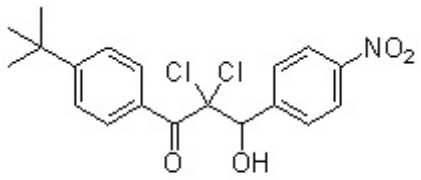

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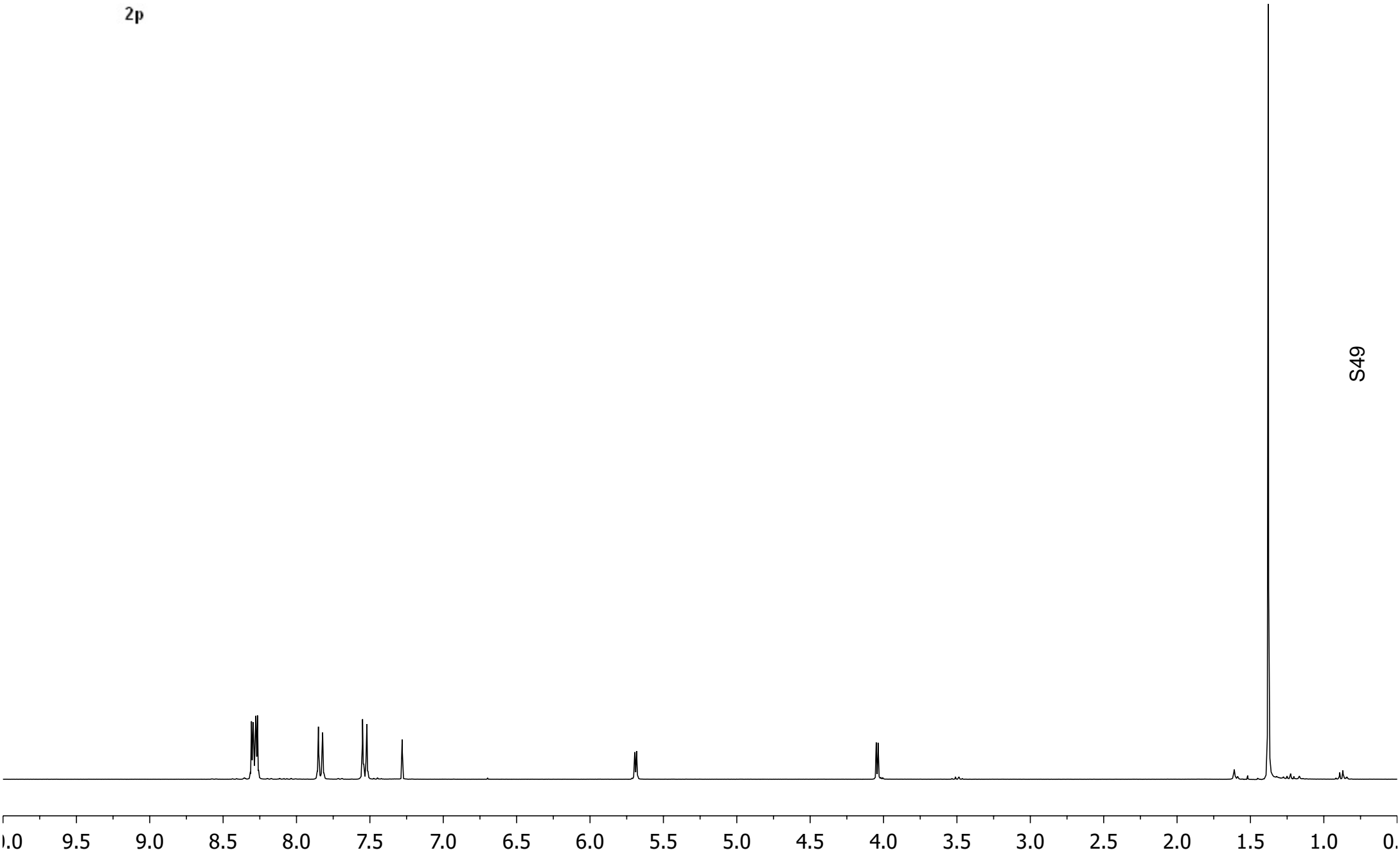

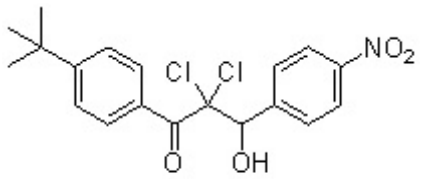

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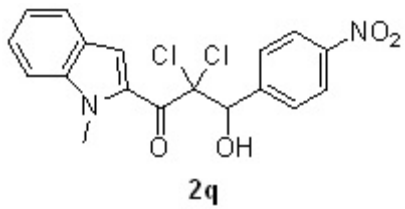

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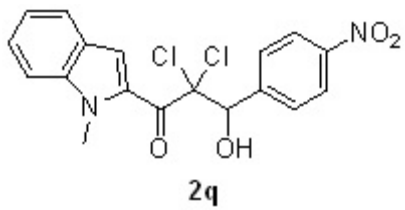
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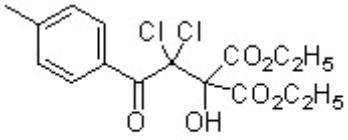

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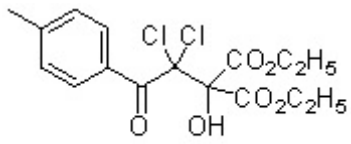

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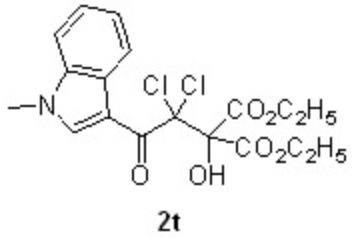

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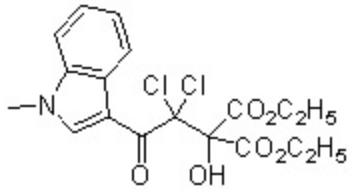

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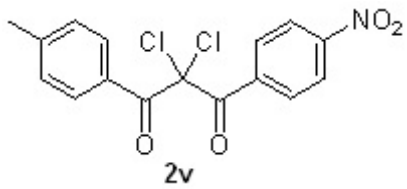

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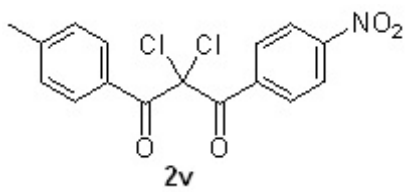

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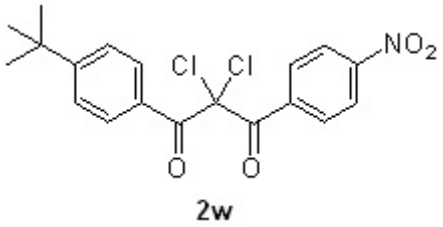

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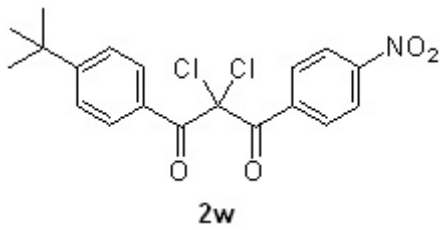
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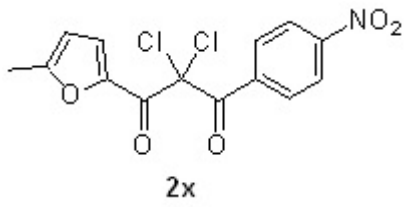

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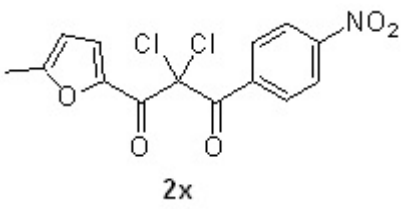

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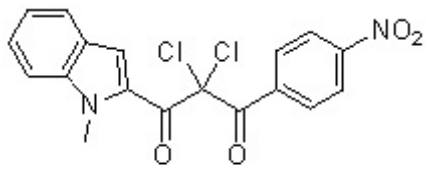

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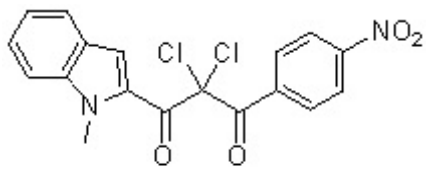
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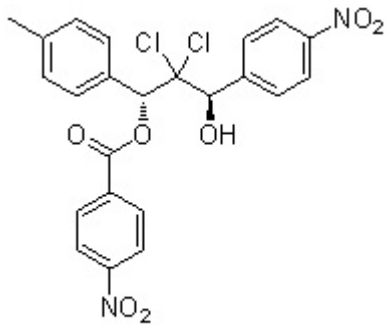

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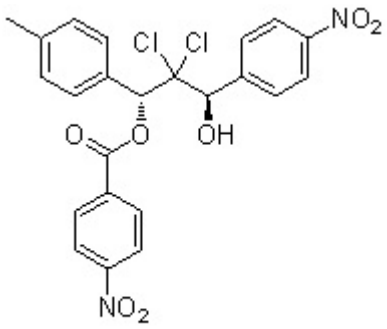

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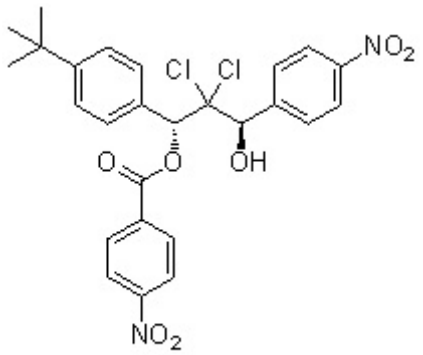
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3b

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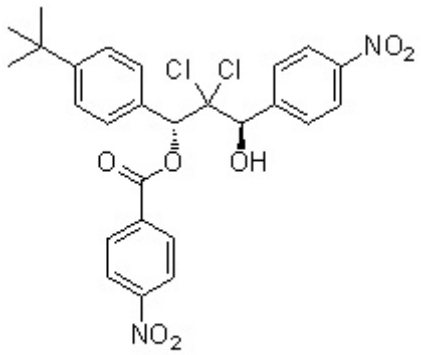
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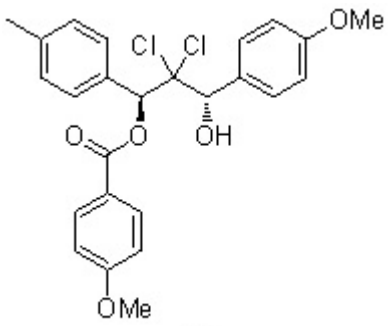
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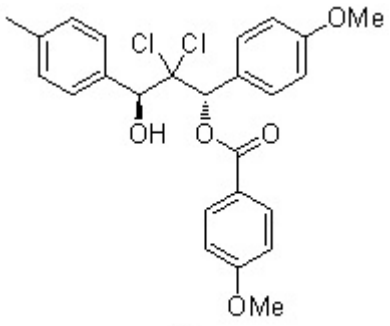
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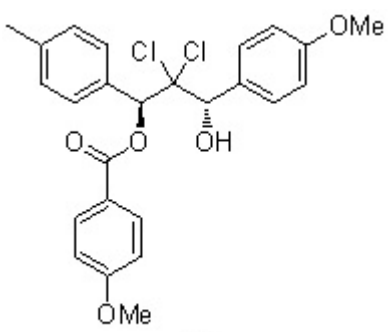
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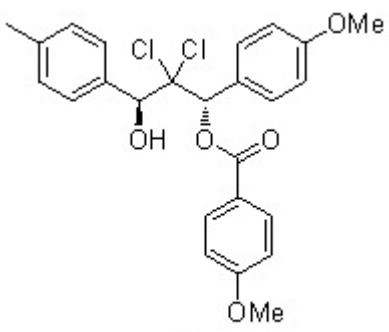
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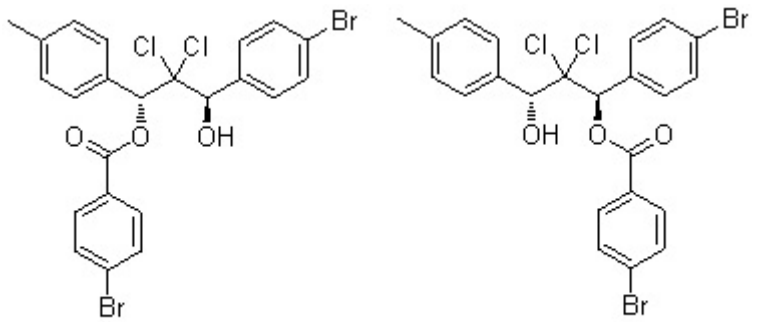
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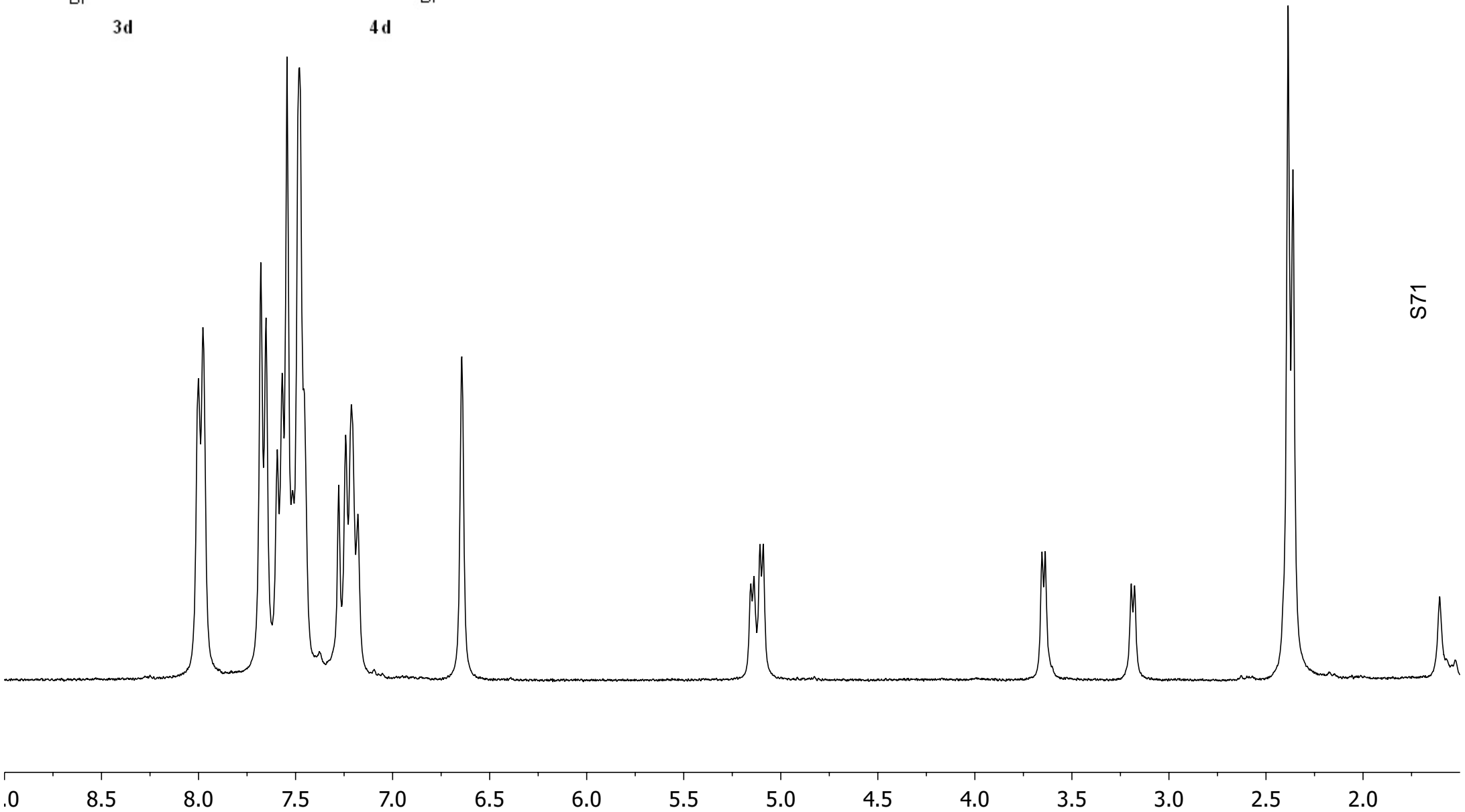
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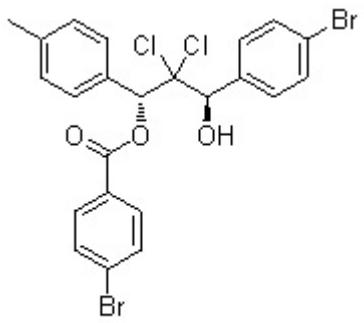
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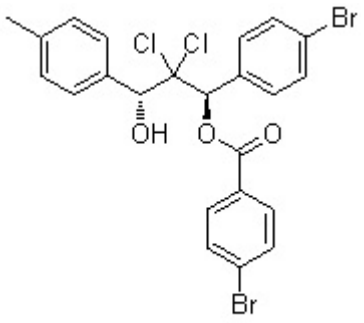
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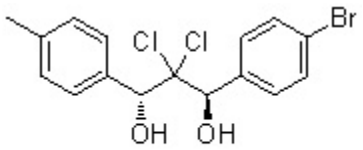

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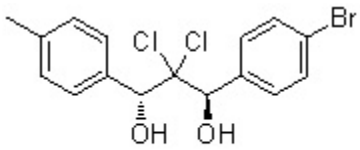

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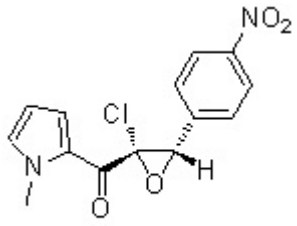

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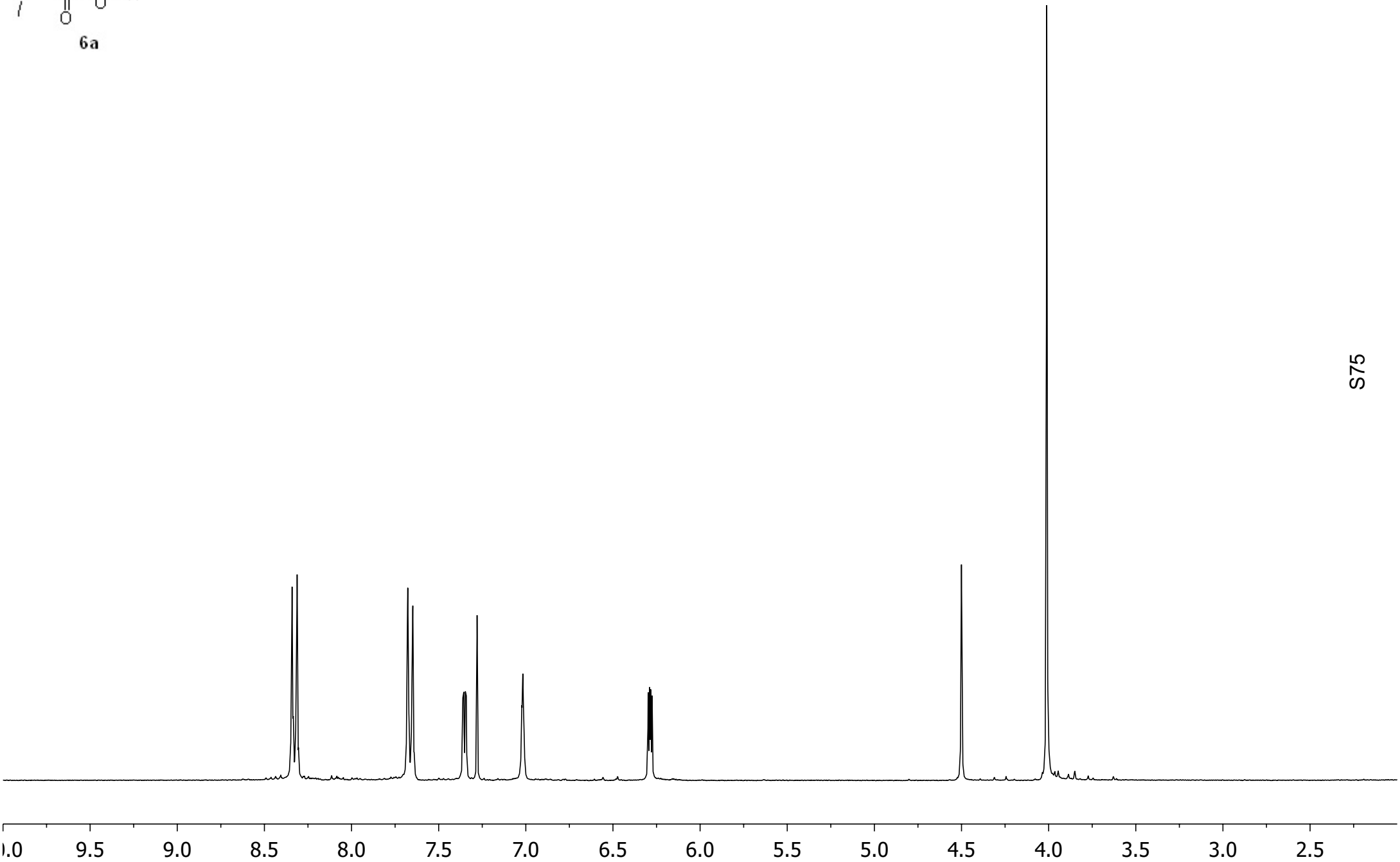

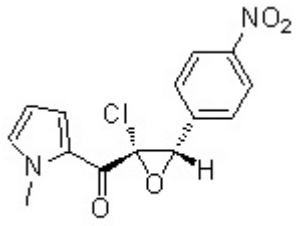
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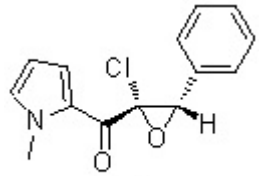

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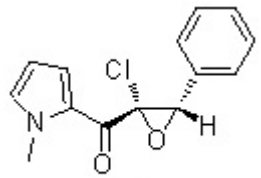
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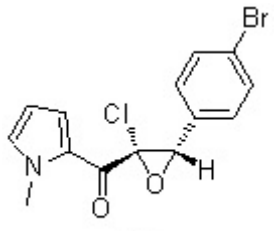

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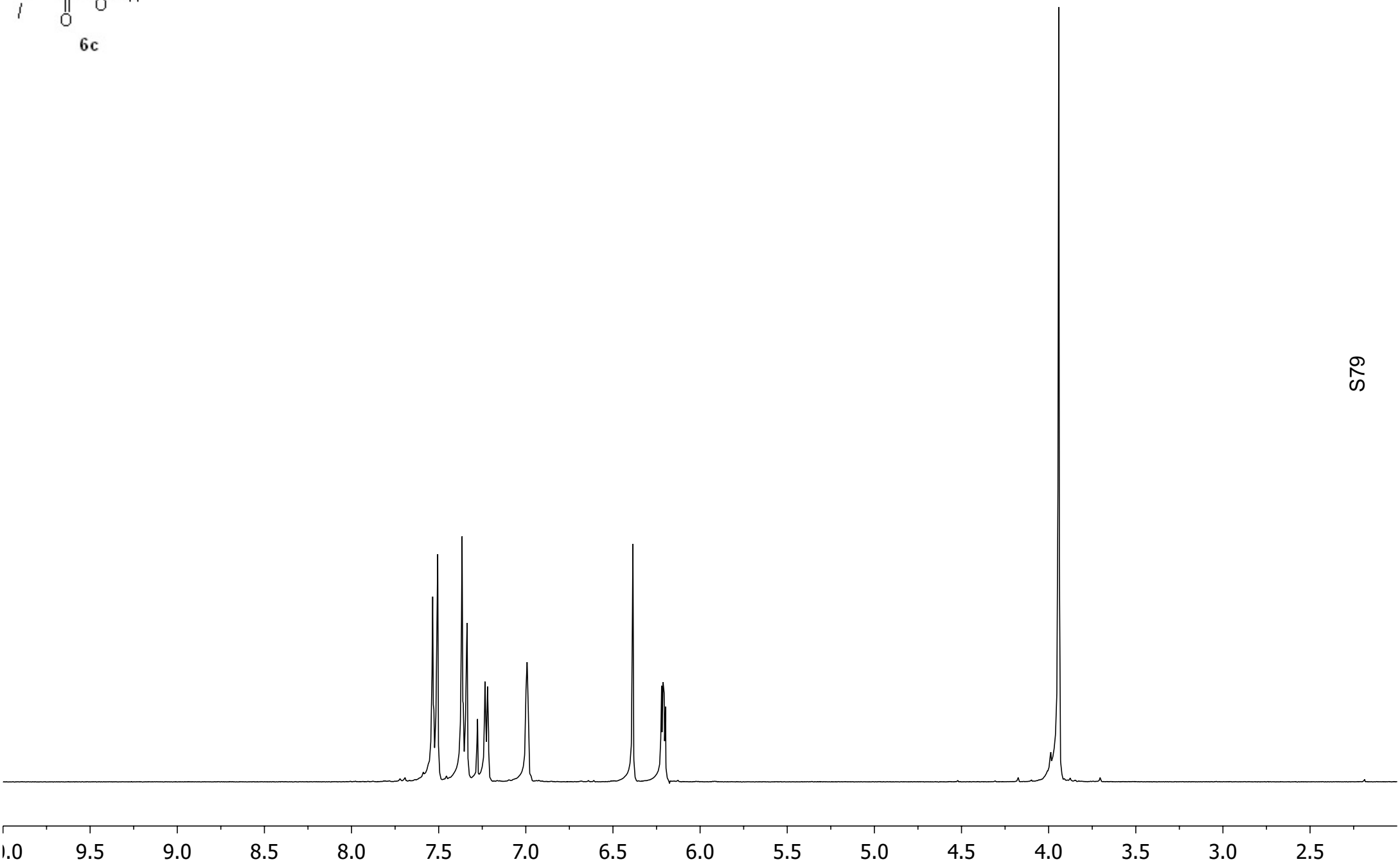

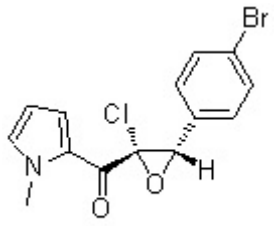
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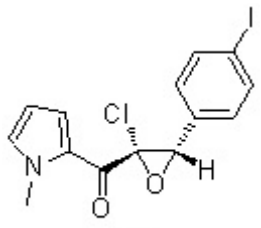

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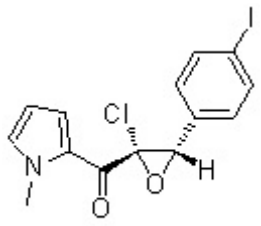
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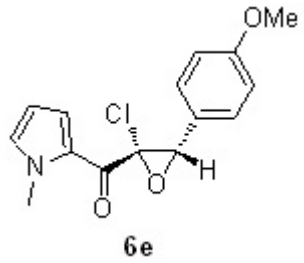

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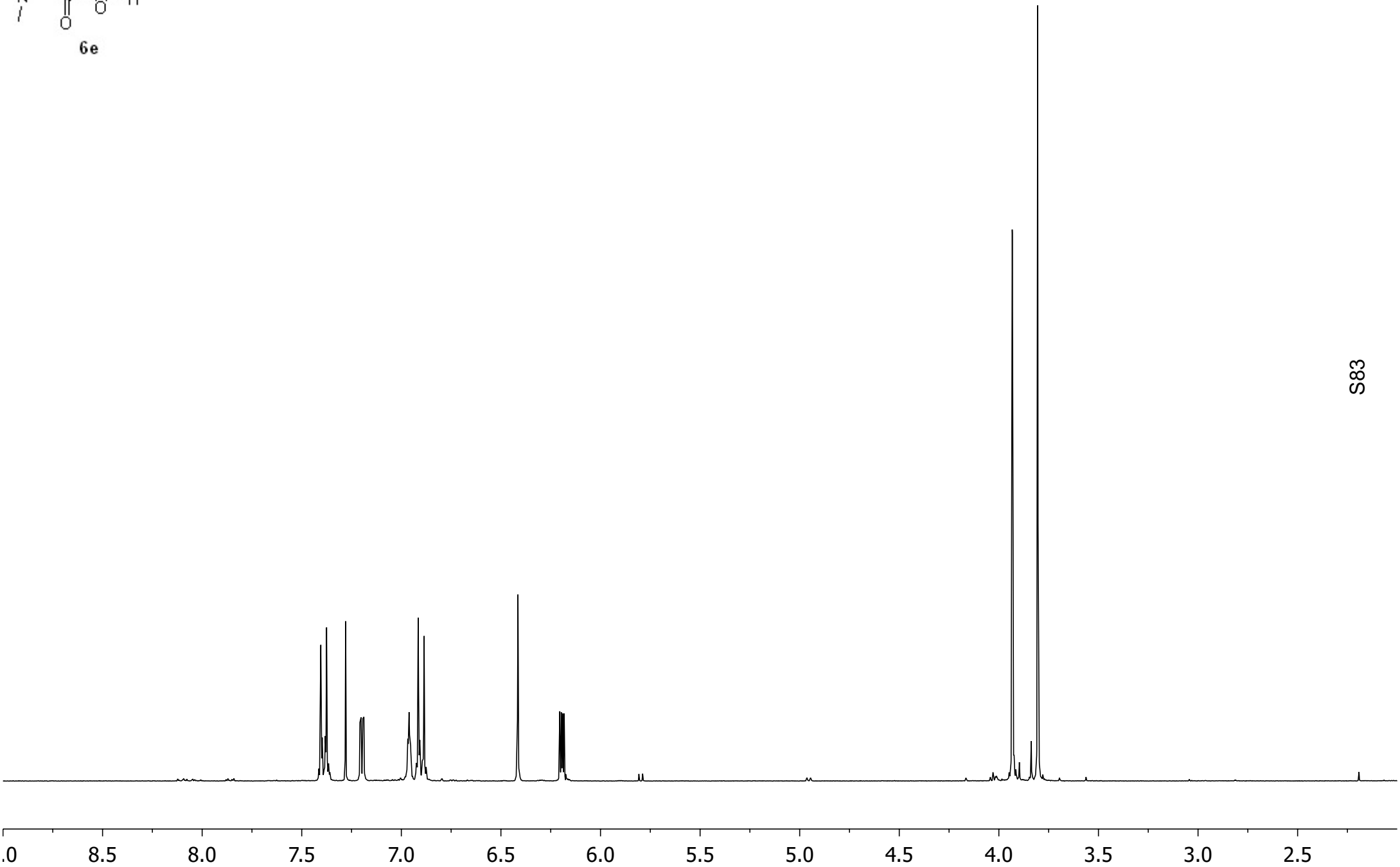

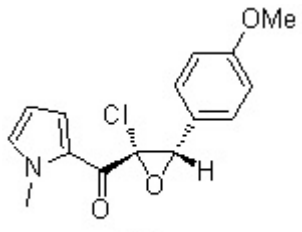
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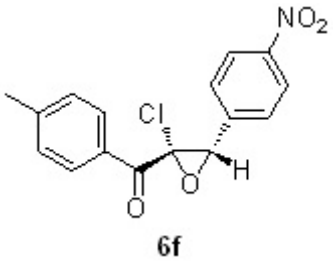

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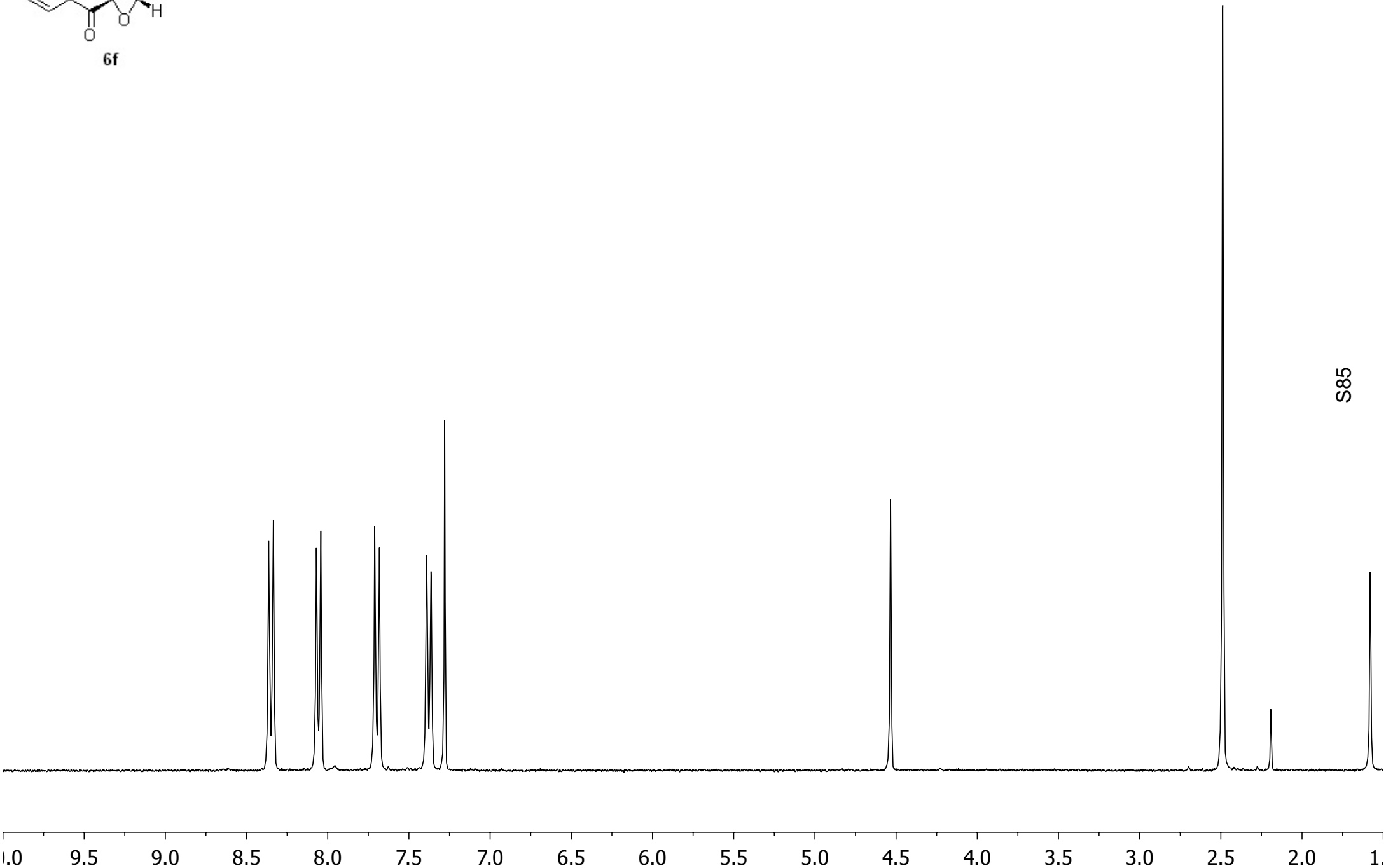

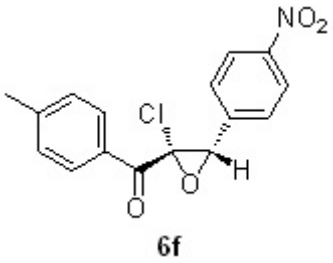

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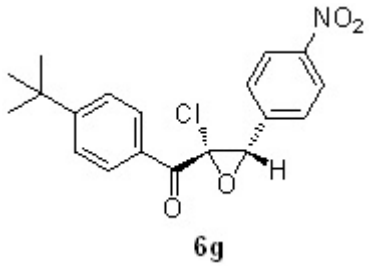

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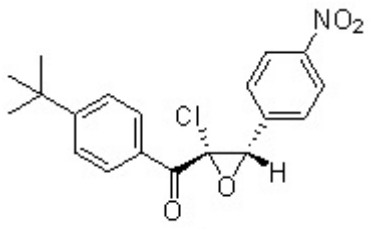
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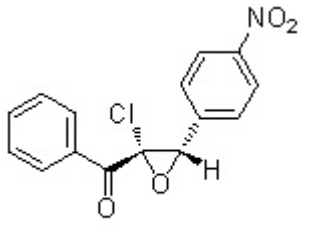

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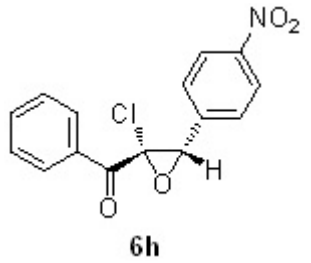

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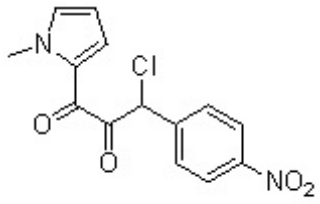

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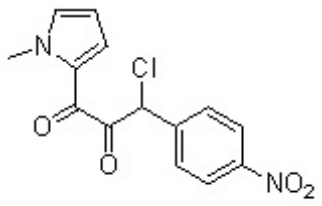
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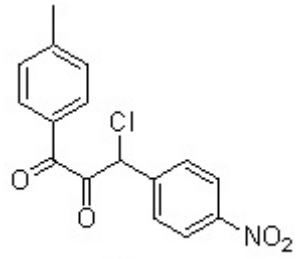

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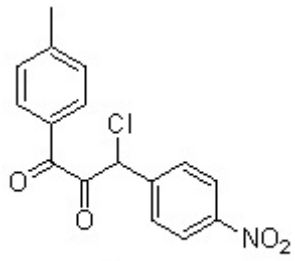
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