Highly stereoselective double (*R*)-phenylglycinol-induced cyclocondensation reactions of symmetric aryl bis(oxoacids)

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1. Cartesian coordinates (Å) for compound *trans*-phenyl-8 at HF/6-31G(d) level

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.396368	1.780620	0.169028
2	6	0	-0.470206	2.415007	-0.911400
3	6	0	-0.934686	1.219457	-1.755036
4	6	0	-0.961455	0.071957	-0.733107
5	8	0	-0.460481	-1.129999	-1.240658
6	6	0	0.136071	-1.795092	-0.149512
7	6	0	0.825509	-0.679289	0.679814
8	7	0	0.036297	0.466261	0.239914
9	8	0	1.220721	2.324553	0.836982
10	6	0	-4.010539	0.217112	1.580946
11	6	0	-2.725158	0.403268	1.087924
12	6	0	-2.350510	-0.148477	-0.127331
13	6	0	-3.282713	-0.898545	-0.841134
14	6	0	-4.560899	-1.085909	-0.350044
15	6	0	-4.930373	-0.525401	0.865166
16	6	0	2.809545	-0.494181	-0.889570
17	6	0	2.315902	-0.555433	0.410646
18	6	0	3.212258	-0.536046	1.466685
19	6	0	4.578027	-0.458111	1.236504
20	6	0	5.060051	-0.396570	-0.057926
21	6	0	4.169945	-0.414069	-1.122229
22	1	0	0.104181	3.149217	-1.459457
23	1	0	-1.302880	2.928442	-0.440714
24	1	0	-1.886608	1.373888	-2.243355
25	1	0	-0.193151	0.977370	-2.507518
26	1	0	-0.624064	-2.296701	0.439347
27	1	0	0.829585	-2.525494	-0.533970
28	1	0	0.677226	-0.856802	1.737349
29	1	0	-4.284597	0.650276	2.526400
30	1	0	-2.016440	0.970415	1.661980
31	1	0	-2.997600	-1.343715	-1.776942
32	1	0	-5.268357	-1.670445	-0.910891
33	1	0	-5.924532	-0.671741	1.248108
34	1	0	2.127889	-0.514822	-1.721254
35	1	0	2.845933	-0.570500	2.477570
36	1	0	5.259286	-0.440350	2.068342
37	1	0	6.118135	-0.333883	-0.239461
38	1	0	4.537166	-0.367209	-2.132073

Total energy (Hartrees) for compound *trans*-phenyl-**8** at HF/6-31G(d) level.

Zero-point correction= 0.336829 (Hartree/Particle)
Thermal correction to Energy= 0.352107
Thermal correction to Enthalpy= 0.353051
Thermal correction to Gibbs Free Energy= 0.292293
Sum of electronic and zero-point Energies= -895.385373
Sum of electronic and thermal Energies= -895.370095
Sum of electronic and thermal Enthalpies= -895.369151
Sum of electronic and thermal Free Energies= -895.429910

2. Cartesian coordinates (Å) for compound *trans*-phenyl-8 at B3LYP/6-31G(d) level

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.438433	1.794512	0.174497
2	6	0	-0.443270	2.457124	-0.894492
3	6	0	-0.959912	1.276642	-1.738676
4	6	0	-0.977924	0.101457	-0.734224
5	8	0	-0.458350	-1.103479	-1.294319
6	6	0	0.120938	-1.797216	-0.183612
7	6	0	0.817656	-0.694612	0.677436
8	7	0	0.030383	0.476730	0.257742
9	8	0	1.315737	2.316153	0.834458
10	6	0	-4.051289	0.248806	1.571973
11	6	0	-2.759499	0.445034	1.076760
12	6	0	-2.364940	-0.145451	-0.127883
13	6	0	-3.281629	-0.942903	-0.827262
14	6	0	-4.569249	-1.141395	-0.331306
15	6	0	-4.959342	-0.543241	0.869697
16	6	0	2.807548	-0.498551	-0.894245
17	6	0	2.309699	-0.569964	0.414161
18	6	0	3.211720	-0.567005	1.481344
19	6	0	4.586625	-0.494105	1.252101
20	6	0	5.074337	-0.422260	-0.052643
21	6	0	4.179923	-0.424552	-1.125923
22	1	0	0.146090	3.185539	-1.456367
23	1	0	-1.261138	3.001039	-0.405865
24	1	0	-1.936130	1.451905	-2.195839
25	1	0	-0.243650	1.025967	-2.528072
26	1	0	-0.660864	-2.304147	0.397678
27	1	0	0.821579	-2.535023	-0.576045
28	1	0	0.661820	-0.897786	1.742706
29	1	0	-4.343146	0.711831	2.510961
30	1	0	-2.051019	1.049180	1.635518
31	1	0	-2.973126	-1.416340	-1.754737
32	1	0	-5.268302	-1.766362	-0.881009
33	1	0	-5.963142	-0.698087	1.256205
34	1	0	2.114297	-0.506526	-1.731428
35	1	0	2.835008	-0.611436	2.500496
36	1	0	5.274378	-0.488544	2.093523
37	1	0	6.144278	-0.363502	-0.233652
38	1	0	4.552353	-0.370118	-2.145610

Total energy (Hartrees) for compound *trans*-phenyl-**8** at B3LYP/6-31G(d) level.

Zero-point correction=	0.313536 (Hartree/Particle)
Thermal correction to Energy=	0.330013
Thermal correction to Enthalpy=	0.330957
Thermal correction to Gibbs Free Energy=	0.267925
Sum of electronic and zero-point Energies=	-901.043759
Sum of electronic and thermal Energies=	-901.027283
Sum of electronic and thermal Enthalpies=	-901.026338
Sum of electronic and thermal Free Energies=	-901.089371

3. Cartesian coordinates (Å) for compound 8 at HF/6-31G(d) level

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.117658	2.231144	-0.993775
2	6	0	-1.309121	2.684257	-1.243978
3	6	0	-2.035579	2.226078	0.027038
4	6	0	-1.238645	0.982870	0.475066
5	8	0	-0.943168	1.030162	1.841956
6	6	0	0.312046	0.416136	2.012312
7	6	0	1.136206	0.858423	0.784874
8	7	0	0.061704	1.138376	-0.165681
9	8	0	1.119353	2.734519	-1.399357
10	6	0	-2.505866	-2.054217	-1.467133
11	6	0	-1.795541	-0.910075	-1.135169
12	6	0	-1.944750	-0.323863	0.115030
13	6	0	-2.818581	-0.904203	1.028514
14	6	0	-3.524971	-2.048268	0.698228
15	6	0	-3.372301	-2.626726	-0.552110
16	6	0	3.527584	0.199029	0.428309
17	6	0	2.185269	-0.137532	0.335058
18	6	0	1.845027	-1.400072	-0.142318
19	6	0	2.827067	-2.300723	-0.512181
20	6	0	4.167217	-1.956211	-0.409228
21	6	0	4.515164	-0.703637	0.061565
22	1	0	-1.693058	2.190457	-2.131339
23	1	0	-1.338168	3.751151	-1.414775
24	1	0	-1.937950	2.973821	0.805215
25	1	0	-3.085527	2.018115	-0.121780
26	1	0	0.735443	0.758107	2.944921
27	1	0	0.204841	-0.661945	2.046279
28	1	0	1.634564	1.795009	1.001981
29	1	0	-2.375665	-2.497938	-2.438123
30	1	0	-1.110687	-0.487492	-1.846712
31	1	0	-2.937192	-0.461971	1.999945
32	1	0	-4.192454	-2.488437	1.417559
33	1	0	-3.920168	-3.515939	-0.808017
34	1	0	3.808220	1.176903	0.778171
35	1	0	0.811451	-1.678722	-0.233327
36	1	0	2.547827	-3.271460	-0.881722
37	1	0	4.929485	-2.657640	-0.698173
38	1	0	5.550329	-0.422559	0.138255

Total energy (Hartrees) for compound **8** at HF/6-31G(d) level.

Zero-point correction=	0.336947 (Hartree/Particle)
Thermal correction to Energy=	0.352231
Thermal correction to Enthalpy=	0.353175
Thermal correction to Gibbs Free Energy=	0.292273
Sum of electronic and zero-point Energies=	-895.389567
Sum of electronic and thermal Energies=	-895.374283
Sum of electronic and thermal Enthalpies=	-895.373339
Sum of electronic and thermal Free Energies=	-895.434241

4. Cartesian coordinates (Å) for compound 8 at B3LYP/6-31G(d) level

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.086843	2.313968	-0.976386
2	6	0	-1.361404	2.735098	-1.232001
3	6	0	-2.105942	2.206827	0.007766
4	6	0	-1.263424	0.985390	0.466281
5	8	0	-0.970769	1.066002	1.861205
6	6	0	0.310871	0.454770	2.021240
7	6	0	1.135269	0.890827	0.775105
8	7	0	0.046868	1.181193	-0.175717
9	8	0	1.102566	2.861012	-1.359997
10	6	0	-2.448679	-2.094269	-1.490484
11	6	0	-1.777224	-0.915818	-1.158570
12	6	0	-1.919963	-0.351647	0.115057
13	6	0	-2.745397	-0.986809	1.051320
14	6	0	-3.412427	-2.166903	0.720576
15	6	0	-3.268453	-2.723079	-0.552016
16	6	0	3.528944	0.195179	0.426682
17	6	0	2.169970	-0.121626	0.325480
18	6	0	1.806444	-1.385990	-0.158312
19	6	0	2.782790	-2.309609	-0.529255
20	6	0	4.137275	-1.985832	-0.418414
21	6	0	4.508451	-0.729645	0.060633
22	1	0	-1.723430	2.268266	-2.156430
23	1	0	-1.416282	3.817906	-1.363074
24	1	0	-2.072150	2.942393	0.817706
25	1	0	-3.148830	1.944526	-0.181136
26	1	0	0.739894	0.811889	2.959862
27	1	0	0.219494	-0.638907	2.059363
28	1	0	1.648950	1.838016	0.975026
29	1	0	-2.325306	-2.522855	-2.481644
30	1	0	-1.123924	-0.440927	-1.884716
31	1	0	-2.851931	-0.553898	2.041038
32	1	0	-4.044149	-2.653224	1.459357
33	1	0	-3.788165	-3.642140	-0.809183
34	1	0	3.822619	1.178941	0.785422
35	1	0	0.755974	-1.644127	-0.256494
36	1	0	2.485220	-3.284397	-0.907069
37	1	0	4.896848	-2.706841	-0.708745
38	1	0	5.559058	-0.464077	0.142866

Total energy (Hartrees) for compound **8** at B3LYP /6-31G(d) level.

Zero-point correction= 0.313675 (Hartree/Particle)
Thermal correction to Energy= 0.330132
Thermal correction to Enthalpy= 0.331076
Thermal correction to Gibbs Free Energy= 0.268134
Sum of electronic and zero-point Energies= -901.047275
Sum of electronic and thermal Energies= -901.030818
Sum of electronic and thermal Enthalpies= -901.029874
Sum of electronic and thermal Free Energies= -901.092815

5. X-ray crystallographic data for compounds 9-11, 18 and 21

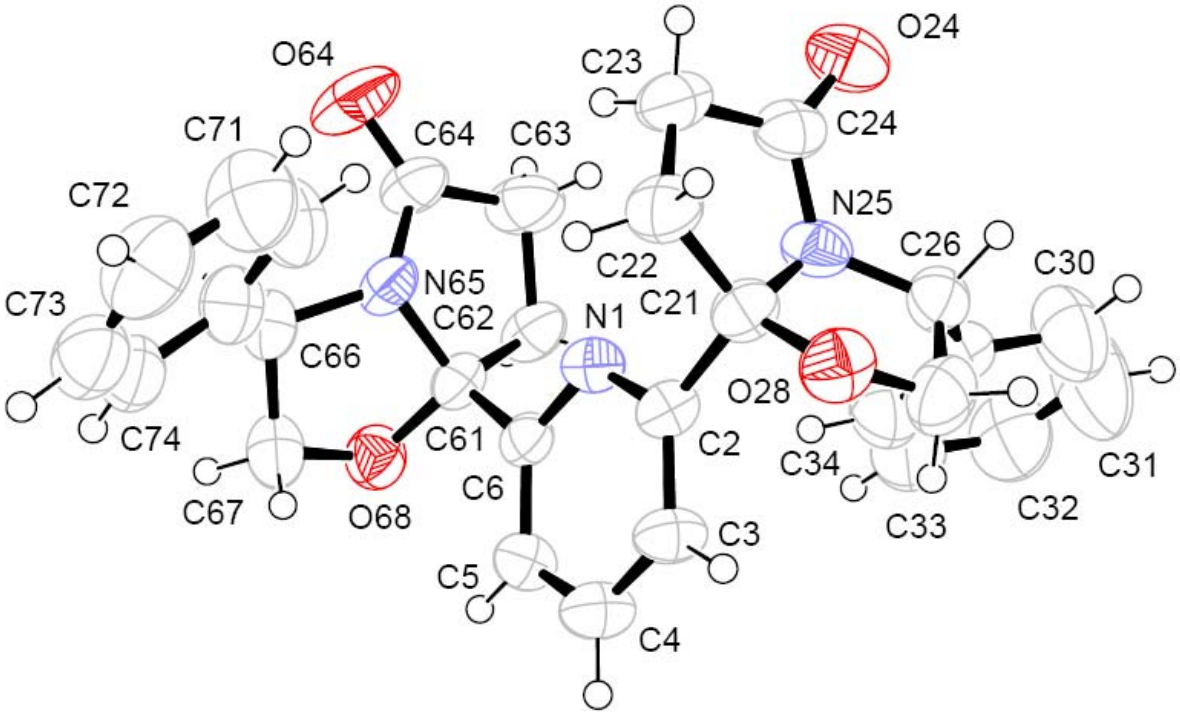


Fig S1 ORTEP view of molecular structure of **9**.

Table 1. Crystal data and structure refinement for **9**.

Identification code	Jb62	
Empirical formula	C58 H54 N6 O8	
Formula weight	963.07	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 10.613(4) Å	α= 90°.
	b = 10.186(3) Å	β= 91.90(4)°.
	c = 23.142(12) Å	γ= 90°.
Volume	2500.4(18) $Å^3$	
Z	2	
Density (calculated)	1.279 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	1016	
Crystal size	0.46 x 0.38 x 0.33 mm^3	
Theta range for data collection	1.76 to 25.00°.	

Index ranges	-12<=h<=12, 0<=k<=12, 0<=l<=27
Reflections collected	4777
Independent reflections	4657 [R(int) = 0.0345]
Completeness to theta = 25.00°	99.7 %
Max. and min. transmission	0.9721 and 0.9614
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4657 / 1 / 649
Goodness-of-fit on F^2	1.119
Final R indices [I>2sigma(I)]	R1 = 0.0653, wR2 = 0.1386
R indices (all data)	R1 = 0.0968, wR2 = 0.1580
Largest diff. peak and hole	0.284 and -0.223 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **9**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	3046(5)	-1063(6)	4727(2)	47(1)
N(25)	1299(5)	-1563(6)	5615(3)	53(2)
N(65)	2738(5)	-468(6)	3533(2)	50(1)
O(24)	-813(5)	-1289(6)	5419(3)	71(2)
O(28)	2668(5)	-3031(6)	6019(2)	62(1)
O(64)	859(6)	-453(7)	3023(3)	92(2)
O(68)	4428(4)	860(5)	3605(2)	58(1)
C(2)	3372(6)	-1723(7)	5214(3)	46(2)
C(3)	4615(6)	-1725(8)	5432(3)	53(2)
C(4)	5503(7)	-1023(8)	5155(3)	57(2)
C(5)	5167(6)	-306(7)	4660(3)	50(2)
C(6)	3918(6)	-387(7)	4464(3)	42(2)
C(21)	2286(6)	-2444(7)	5474(3)	50(2)
C(22)	1692(7)	-3451(8)	5054(3)	63(2)
C(23)	463(7)	-2779(9)	4848(3)	65(2)
C(24)	207(7)	-1782(8)	5319(3)	56(2)
C(26)	1394(7)	-1149(8)	6215(3)	56(2)
C(27)	2501(8)	-2018(10)	6443(3)	71(2)
C(29)	1579(7)	297(9)	6315(3)	58(2)
C(30)	971(11)	906(12)	6740(5)	109(4)
C(31)	1153(14)	2232(13)	6848(6)	145(6)
C(32)	1907(11)	2947(12)	6512(5)	103(4)
C(33)	2488(10)	2349(10)	6076(4)	86(3)
C(34)	2357(8)	1028(9)	5987(4)	72(2)
C(61)	3416(6)	375(7)	3939(3)	46(2)

C(62)	2493(6)	1450(8)	4089(3)	57(2)
C(63)	1218(7)	913(10)	3876(4)	77(3)
C(64)	1526(7)	-61(8)	3419(3)	60(2)
C(66)	3594(7)	-982(8)	3100(3)	58(2)
C(67)	4801(8)	-240(9)	3254(3)	66(2)
C(69)	3704(8)	-2475(8)	3114(3)	64(2)
C(70)	2824(10)	-3237(10)	3360(4)	81(3)
C(71)	2951(11)	-4609(11)	3365(5)	100(3)
C(72)	3955(11)	-5158(10)	3106(5)	95(3)
C(73)	4866(9)	-4403(10)	2876(4)	80(3)
C(74)	4750(8)	-3049(9)	2865(3)	68(2)
N(1A)	-1955(5)	99(6)	284(2)	43(1)
N(25A)	-2020(5)	-504(6)	1505(2)	47(1)
N(65A)	-3826(5)	570(6)	-606(3)	50(2)
O(24A)	-3665(5)	-624(7)	2107(2)	85(2)
O(28A)	-355(4)	-1838(5)	1397(2)	53(1)
O(64A)	-5939(5)	337(6)	-423(3)	71(2)
O(68A)	-2517(5)	2013(5)	-1019(2)	58(1)
C(2A)	-1030(5)	-580(7)	555(3)	39(1)
C(3A)	175(6)	-628(8)	354(3)	50(2)
C(4A)	444(6)	71(8)	-137(3)	53(2)
C(5A)	-497(6)	783(7)	-414(3)	49(2)
C(6A)	-1685(6)	756(7)	-196(3)	45(2)
C(21A)	-1424(6)	-1328(7)	1086(3)	45(2)
C(22A)	-2398(6)	-2400(8)	940(3)	56(2)
C(23A)	-3572(8)	-2000(11)	1243(4)	87(3)
C(24A)	-3147(7)	-972(8)	1683(3)	59(2)
C(26A)	-1059(7)	38(8)	1903(3)	52(2)
C(27A)	109(7)	-768(8)	1746(3)	61(2)
C(29A)	-908(8)	1510(8)	1862(3)	58(2)
C(30A)	113(9)	2123(9)	2128(4)	72(2)
C(31A)	232(10)	3480(10)	2115(4)	85(3)
C(32A)	-660(10)	4230(10)	1816(4)	86(3)
C(33A)	-1681(10)	3623(10)	1555(5)	91(3)
C(34A)	-1791(9)	2288(9)	1574(4)	80(3)
C(61A)	-2805(6)	1483(7)	-467(3)	48(2)
C(62A)	-3374(7)	2484(8)	-65(3)	63(2)
C(63A)	-4581(7)	1837(9)	140(4)	67(2)
C(64A)	-4906(7)	820(8)	-318(3)	53(2)
C(66A)	-3813(7)	145(8)	-1205(3)	54(2)
C(67A)	-2716(8)	981(9)	-1427(3)	65(2)
C(69A)	-3659(7)	-1314(8)	-1291(3)	55(2)
C(70A)	-4480(9)	-1973(11)	-1650(4)	84(3)
C(71A)	-4378(12)	-3329(12)	-1737(4)	102(4)

C(72A)	-3428(13)	-4019(12)	-1424(5)	104(4)
C(73A)	-2644(11)	-3359(10)	-1070(5)	92(3)
C(74A)	-2734(8)	-2032(9)	-993(4)	71(2)

Table 3. Bond lengths [Å] and angles [°] for **9**.

N(1)-C(6)	1.318(8)	C(66)-C(67)	1.519(11)
N(1)-C(2)	1.349(8)	C(66)-C(69)	1.526(11)
N(25)-C(24)	1.345(9)	C(69)-C(70)	1.353(12)
N(25)-C(21)	1.426(9)	C(69)-C(74)	1.396(11)
N(25)-C(26)	1.451(9)	C(70)-C(71)	1.404(14)
N(65)-C(64)	1.368(9)	C(71)-C(72)	1.359(14)
N(65)-C(61)	1.447(8)	C(72)-C(73)	1.358(13)
N(65)-C(66)	1.471(9)	C(73)-C(74)	1.385(13)
O(24)-C(24)	1.223(9)	N(1A)-C(2A)	1.340(8)
O(28)-C(27)	1.439(10)	N(25A)-C(24A)	1.364(9)
O(28)-C(21)	1.442(8)	N(25A)-C(21A)	1.444(8)
O(64)-C(64)	1.207(8)	N(25A)-C(26A)	1.459(9)
O(68)-C(61)	1.431(8)	N(65A)-C(64A)	1.370(8)
O(68)-C(67)	1.447(9)	N(65A)-C(66A)	1.454(9)
C(2)-C(3)	1.396(9)	N(65A)-C(61A)	1.455(9)
C(2)-C(21)	1.508(9)	O(24A)-C(24A)	1.195(8)
C(3)-C(4)	1.360(10)	O(28A)-C(21A)	1.421(8)
C(4)-C(5)	1.395(9)	O(28A)-C(27A)	1.434(9)
C(5)-C(6)	1.389(8)	O(64A)-C(64A)	1.219(8)
C(6)-C(61)	1.524(9)	O(68A)-C(67A)	1.424(10)
C(6A)-N(1A)	1.336(8)	O(68A)-C(61A)	1.429(8)
C(6A)-C(5A)	1.372(9)	C(2A)-C(3A)	1.376(8)
C(6A)-C(61A)	1.518(9)	C(2A)-C(21A)	1.516(9)
C(21)-C(22)	1.534(10)	C(3A)-C(4A)	1.379(9)
C(22)-C(23)	1.534(10)	C(4A)-C(5A)	1.376(9)
C(23)-C(24)	1.522(11)	C(21A)-C(22A)	1.533(9)
C(26)-C(29)	1.503(11)	C(22A)-C(23A)	1.506(10)
C(26)-C(27)	1.550(12)	C(23A)-C(24A)	1.517(12)
C(29)-C(30)	1.346(12)	C(26A)-C(29A)	1.511(11)
C(29)-C(34)	1.362(11)	C(26A)-C(27A)	1.540(10)
C(30)-C(31)	1.386(16)	C(29A)-C(30A)	1.377(11)
C(31)-C(32)	1.348(15)	C(29A)-C(34A)	1.382(12)
C(32)-C(33)	1.346(14)	C(30A)-C(31A)	1.388(13)
C(33)-C(34)	1.368(13)	C(31A)-C(32A)	1.384(13)
C(61)-C(62)	1.517(10)	C(32A)-C(33A)	1.370(13)
C(62)-C(63)	1.526(10)	C(33A)-C(34A)	1.365(13)
C(63)-C(64)	1.494(11)	C(61A)-C(62A)	1.519(10)

C(62A)-C(63A)	1.530(10)	N(25)-C(26)-C(27)	100.8(6)
C(63A)-C(64A)	1.514(11)	C(29)-C(26)-C(27)	114.4(7)
C(66A)-C(69A)	1.509(11)	O(28)-C(27)-C(26)	106.6(6)
C(66A)-C(67A)	1.543(11)	C(30)-C(29)-C(34)	118.0(9)
C(69A)-C(70A)	1.361(11)	C(30)-C(29)-C(26)	120.1(9)
C(69A)-C(74A)	1.388(11)	C(34)-C(29)-C(26)	121.9(8)
C(70A)-C(71A)	1.401(15)	C(29)-C(30)-C(31)	120.9(11)
C(71A)-C(72A)	1.409(15)	C(32)-C(31)-C(30)	120.3(11)
C(72A)-C(73A)	1.331(15)	C(33)-C(32)-C(31)	119.0(11)
C(73A)-C(74A)	1.367(13)	C(32)-C(33)-C(34)	120.7(10)
		C(29)-C(34)-C(33)	121.0(9)
C(6)-N(1)-C(2)	118.8(6)	O(68)-C(61)-N(65)	102.7(5)
C(24)-N(25)-C(21)	114.0(6)	O(68)-C(61)-C(62)	112.1(6)
C(24)-N(25)-C(26)	124.5(6)	N(65)-C(61)-C(62)	105.4(5)
C(21)-N(25)-C(26)	112.0(6)	O(68)-C(61)-C(6)	111.0(5)
C(64)-N(65)-C(61)	112.9(6)	N(65)-C(61)-C(6)	111.7(6)
C(64)-N(65)-C(66)	125.0(6)	C(62)-C(61)-C(6)	113.3(6)
C(61)-N(65)-C(66)	110.4(6)	C(61)-C(62)-C(63)	103.9(6)
C(27)-O(28)-C(21)	105.2(6)	C(64)-C(63)-C(62)	104.7(6)
C(61)-O(68)-C(67)	105.1(5)	O(64)-C(64)-N(65)	124.7(8)
N(1)-C(2)-C(3)	121.0(6)	O(64)-C(64)-C(63)	128.4(7)
N(1)-C(2)-C(21)	113.4(6)	N(65)-C(64)-C(63)	106.9(6)
C(3)-C(2)-C(21)	125.6(6)	N(65)-C(66)-C(67)	101.4(6)
C(4)-C(3)-C(2)	119.4(7)	N(65)-C(66)-C(69)	112.8(7)
C(3)-C(4)-C(5)	119.9(7)	C(67)-C(66)-C(69)	115.3(7)
C(6)-C(5)-C(4)	116.9(7)	O(68)-C(67)-C(66)	105.8(6)
N(1)-C(6)-C(5)	123.9(6)	C(70)-C(69)-C(74)	120.2(9)
N(1)-C(6)-C(61)	113.7(5)	C(70)-C(69)-C(66)	121.8(8)
C(5)-C(6)-C(61)	122.3(6)	C(74)-C(69)-C(66)	118.0(8)
N(1A)-C(6A)-C(5A)	122.6(6)	C(69)-C(70)-C(71)	120.5(10)
N(1A)-C(6A)-C(61A)	113.6(5)	C(72)-C(71)-C(70)	118.8(11)
C(5A)-C(6A)-C(61A)	123.7(6)	C(73)-C(72)-C(71)	121.2(10)
N(25)-C(21)-O(28)	104.4(6)	C(72)-C(73)-C(74)	120.5(10)
N(25)-C(21)-C(2)	111.2(6)	C(73)-C(74)-C(69)	118.7(9)
O(28)-C(21)-C(2)	110.7(5)	C(6A)-N(1A)-C(2A)	118.3(5)
N(25)-C(21)-C(22)	106.0(6)	C(24A)-N(25A)-C(21A)	114.0(6)
O(28)-C(21)-C(22)	112.0(6)	C(24A)-N(25A)-C(26A)	122.9(6)
C(2)-C(21)-C(22)	112.2(6)	C(21A)-N(25A)-C(26A)	109.4(5)
C(21)-C(22)-C(23)	103.1(6)	C(64A)-N(65A)-C(66A)	123.7(6)
C(24)-C(23)-C(22)	104.2(6)	C(64A)-N(65A)-C(61A)	113.7(6)
O(24)-C(24)-N(25)	126.1(8)	C(66A)-N(65A)-C(61A)	111.7(5)
O(24)-C(24)-C(23)	126.1(7)	C(21A)-O(28A)-C(27A)	105.1(5)
N(25)-C(24)-C(23)	107.7(7)	C(67A)-O(68A)-C(61A)	106.3(6)
N(25)-C(26)-C(29)	115.9(7)	N(1A)-C(2A)-C(3A)	122.4(6)

N(1A)-C(2A)-C(21A)	114.9(5)	C(34A)-C(33A)-C(32A)	120.2(10)
C(3A)-C(2A)-C(21A)	122.7(6)	C(33A)-C(34A)-C(29A)	122.0(10)
C(2A)-C(3A)-C(4A)	118.6(7)	O(68A)-C(61A)-N(65A)	103.0(5)
C(5A)-C(4A)-C(3A)	119.3(6)	O(68A)-C(61A)-C(6A)	111.4(5)
C(6A)-C(5A)-C(4A)	118.7(6)	N(65A)-C(61A)-C(6A)	110.3(6)
O(28A)-C(21A)-N(25A)	103.4(5)	O(68A)-C(61A)-C(62A)	113.2(6)
O(28A)-C(21A)-C(2A)	110.9(5)	N(65A)-C(61A)-C(62A)	104.8(5)
N(25A)-C(21A)-C(2A)	113.0(5)	C(6A)-C(61A)-C(62A)	113.3(6)
O(28A)-C(21A)-C(22A)	111.8(6)	C(61A)-C(62A)-C(63A)	104.8(6)
N(25A)-C(21A)-C(22A)	104.7(5)	C(64A)-C(63A)-C(62A)	104.5(6)
C(2A)-C(21A)-C(22A)	112.4(6)	O(64A)-C(64A)-N(65A)	126.1(7)
C(23A)-C(22A)-C(21A)	105.5(6)	O(64A)-C(64A)-C(63A)	126.8(7)
C(22A)-C(23A)-C(24A)	105.5(7)	N(65A)-C(64A)-C(63A)	107.0(6)
O(24A)-C(24A)-N(25A)	125.2(8)	N(65A)-C(66A)-C(69A)	115.0(6)
O(24A)-C(24A)-C(23A)	128.4(8)	N(65A)-C(66A)-C(67A)	100.6(6)
N(25A)-C(24A)-C(23A)	106.5(6)	C(69A)-C(66A)-C(67A)	114.4(7)
N(25A)-C(26A)-C(29A)	114.2(7)	O(68A)-C(67A)-C(66A)	106.5(6)
N(25A)-C(26A)-C(27A)	101.5(6)	C(70A)-C(69A)-C(74A)	118.1(9)
C(29A)-C(26A)-C(27A)	115.2(7)	C(70A)-C(69A)-C(66A)	119.7(8)
O(28A)-C(27A)-C(26A)	105.9(6)	C(74A)-C(69A)-C(66A)	122.2(8)
C(30A)-C(29A)-C(34A)	117.8(8)	C(69A)-C(70A)-C(71A)	121.5(11)
C(30A)-C(29A)-C(26A)	120.4(8)	C(70A)-C(71A)-C(72A)	118.4(10)
C(34A)-C(29A)-C(26A)	121.8(8)	C(73A)-C(72A)-C(71A)	119.1(11)
C(29A)-C(30A)-C(31A)	120.8(10)	C(72A)-C(73A)-C(74A)	122.3(11)
C(32A)-C(31A)-C(30A)	120.0(10)	C(73A)-C(74A)-C(69A)	120.5(10)
C(33A)-C(32A)-C(31A)	119.2(10)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **9**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	41(3)	46(3)	53(3)	-1(3)	-3(3)	-2(3)
N(25)	45(3)	48(4)	67(4)	-3(3)	2(3)	-11(3)
N(65)	56(4)	52(4)	41(3)	-7(3)	-11(3)	5(3)
O(24)	50(3)	68(4)	95(4)	7(3)	3(3)	8(3)
O(28)	67(3)	57(3)	61(3)	11(3)	-4(3)	2(3)
O(64)	89(4)	97(5)	87(4)	-18(4)	-50(3)	8(4)
O(68)	62(3)	58(3)	52(3)	1(3)	5(2)	-7(3)
C(2)	47(4)	45(4)	46(4)	-1(3)	-6(3)	-2(3)
C(3)	43(4)	54(5)	60(4)	8(4)	-12(3)	-1(4)
C(4)	46(4)	58(5)	67(5)	8(4)	-10(3)	-3(4)

C(5)	43(4)	51(4)	55(4)	3(4)	2(3)	1(3)
C(6)	44(4)	42(4)	38(3)	-5(3)	-1(3)	-4(3)
C(6A)	53(4)	38(4)	45(4)	-4(3)	11(3)	-1(3)
C(21)	53(4)	46(4)	51(4)	2(3)	-7(3)	3(4)
C(22)	66(5)	52(5)	70(5)	-8(4)	-2(4)	-12(4)
C(23)	56(5)	72(6)	66(5)	-4(5)	-13(4)	-11(4)
C(24)	53(5)	51(4)	63(5)	11(4)	-3(4)	-11(4)
C(26)	60(5)	57(5)	52(4)	-1(4)	7(4)	-13(4)
C(27)	86(6)	78(6)	51(5)	9(5)	-3(4)	-4(5)
C(29)	52(4)	70(5)	53(4)	-10(4)	1(4)	-8(4)
C(30)	123(9)	99(9)	109(8)	-35(7)	49(7)	-26(8)
C(31)	197(15)	91(9)	153(12)	-60(9)	92(11)	-31(10)
C(32)	125(10)	74(7)	111(9)	-24(7)	13(7)	-10(7)
C(33)	98(8)	72(7)	88(7)	-10(6)	10(6)	-22(6)
C(34)	71(6)	72(6)	75(6)	-12(5)	16(4)	-24(5)
C(61)	53(4)	43(4)	40(4)	-6(3)	-4(3)	-5(3)
C(62)	61(5)	52(4)	55(4)	-6(4)	-16(3)	7(4)
C(63)	53(5)	79(6)	97(6)	-20(6)	-18(4)	15(5)
C(64)	55(4)	71(6)	53(4)	0(4)	-19(4)	2(4)
C(66)	68(5)	65(5)	43(4)	-1(4)	7(4)	0(4)
C(67)	75(5)	68(6)	55(4)	-6(4)	14(4)	1(5)
C(69)	78(6)	57(5)	58(5)	-6(4)	8(4)	5(5)
C(70)	94(7)	68(6)	81(6)	-3(5)	21(5)	6(5)
C(71)	122(9)	68(7)	110(9)	-12(6)	16(7)	0(7)
C(72)	133(10)	55(6)	95(7)	-11(6)	-7(7)	4(6)
C(73)	86(7)	80(7)	75(6)	-18(5)	-6(5)	12(6)
C(74)	74(6)	69(6)	60(5)	-10(4)	4(4)	2(5)
N(1A)	37(3)	50(3)	43(3)	-2(3)	1(2)	-5(3)
N(25A)	51(3)	49(3)	41(3)	-2(3)	10(2)	2(3)
N(65A)	41(3)	50(4)	60(4)	0(3)	4(3)	6(3)
O(24A)	88(4)	90(5)	79(4)	-4(4)	50(3)	5(4)
O(28A)	56(3)	52(3)	51(3)	1(2)	-2(2)	13(3)
O(64A)	47(3)	68(4)	98(4)	7(3)	3(3)	-5(3)
O(68A)	66(3)	52(3)	56(3)	13(3)	4(2)	-7(3)
C(2A)	37(3)	43(4)	39(3)	-9(3)	7(3)	2(3)
C(3A)	38(4)	56(4)	57(4)	-4(4)	8(3)	-3(3)
C(4A)	38(4)	62(5)	58(4)	4(4)	11(3)	3(4)
C(5A)	50(4)	47(4)	50(4)	9(4)	15(3)	7(4)
C(21A)	45(4)	45(4)	47(4)	-2(3)	8(3)	4(3)
C(22A)	56(4)	51(5)	62(5)	-2(4)	9(4)	-10(4)
C(23A)	70(6)	91(7)	102(7)	-27(6)	34(5)	-13(5)
C(24A)	51(4)	65(5)	63(5)	0(4)	21(4)	4(4)
C(26A)	57(4)	61(5)	38(4)	-5(3)	3(3)	0(4)
C(27A)	60(5)	65(5)	56(4)	-13(4)	0(4)	5(4)

C(29A)	72(5)	56(5)	47(4)	-10(4)	7(4)	-8(4)
C(30A)	86(6)	68(6)	62(5)	0(5)	-5(5)	-5(5)
C(31A)	100(7)	77(7)	78(6)	-19(6)	5(5)	-27(6)
C(32A)	124(9)	63(6)	71(6)	2(5)	6(6)	-12(6)
C(33A)	97(8)	62(6)	112(8)	6(6)	-17(6)	0(6)
C(34A)	93(7)	57(6)	89(7)	5(5)	-15(5)	3(5)
C(61A)	44(4)	46(4)	54(4)	1(4)	5(3)	-1(3)
C(62A)	70(5)	55(5)	66(5)	-9(4)	5(4)	8(4)
C(63A)	59(5)	64(5)	80(6)	0(5)	18(4)	9(4)
C(64A)	49(4)	49(4)	60(5)	12(4)	7(3)	7(4)
C(66A)	51(4)	60(5)	52(4)	1(4)	-6(3)	1(4)
C(67A)	76(6)	67(5)	52(5)	4(4)	2(4)	-4(5)
C(69A)	53(4)	58(5)	53(4)	-1(4)	3(4)	-7(4)
C(70A)	89(7)	85(7)	78(6)	1(6)	-14(5)	-13(6)
C(71A)	141(10)	92(9)	74(7)	-22(6)	-1(7)	-44(8)
C(72A)	145(11)	69(7)	102(9)	-14(7)	37(8)	-1(8)
C(73A)	105(8)	60(7)	112(9)	-8(6)	14(7)	23(6)
C(74A)	73(6)	73(6)	65(5)	-15(5)	3(4)	18(5)

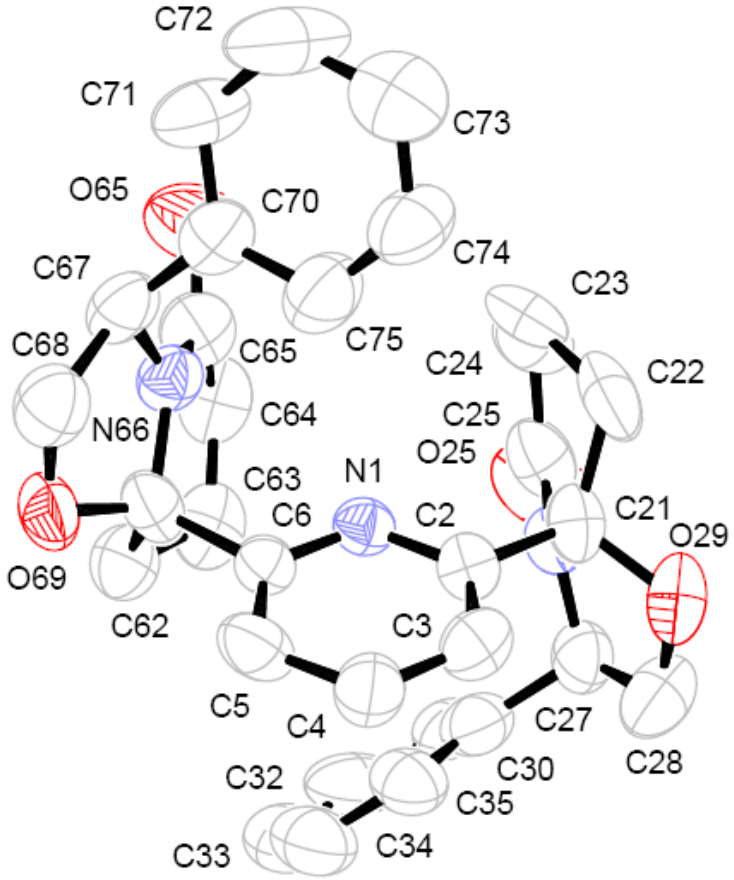


Fig S2 ORTEP view of molecular structure of **10**.

Table 1. Crystal data and structure refinement for **10**.

Identification code	Jb61	
Empirical formula	C62 H64 N6 O9 (2 C31 H31 N3 O4 · H2O)	
Formula weight	1037.19	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 9.102(2) Å	α= 90°.
	b = 18.341(5) Å	β= 90°.
	c = 32.012(8) Å	γ= 90°.
Volume	5344(2) $Å^3$	
Z	4	
Density (calculated)	1.289 Mg/m^3	
Absorption coefficient	0.087 mm^{-1}	
F(000)	2200	

Crystal size	0.47 x 0.36 x 0.22 mm^3
Theta range for data collection	2.22 to 25.72°.
Index ranges	-11<=h<=0, -22<=k<=0, 0<=l<=38
Reflections collected	5627
Independent reflections	5627
Completeness to theta = 25.72°	99.0 %
Max. and min. transmission	0.9811 and 0.9602
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5627 / 3 / 701
Goodness-of-fit on F^2	1.088
Final R indices [I>2sigma(I)]	R1 = 0.1037, wR2 = 0.2595
R indices (all data)	R1 = 0.2333, wR2 = 0.3356
Extinction coefficient	0.009(2)
Largest diff. peak and hole	0.536 and -0.648 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **10**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(2)	3931(11)	5493(5)	8203(3)	52(2)
C(2A)	8164(11)	4858(5)	10671(3)	56(2)
C(3)	5336(11)	5217(6)	8296(3)	61(3)
C(3A)	9682(12)	4884(7)	10692(4)	86(4)
C(4)	6012(12)	4773(6)	8018(3)	67(3)
C(4A)	10463(13)	5100(9)	10340(5)	107(5)
C(5)	5242(11)	4549(7)	7661(3)	68(3)
C(5A)	9737(13)	5182(8)	9970(5)	91(4)
C(6)	3832(10)	4820(5)	7612(3)	48(2)
C(6A)	8210(10)	5107(5)	9959(3)	55(2)
C(21)	3151(13)	6027(5)	8484(3)	60(3)
C(21A)	7219(11)	4691(5)	11042(3)	61(3)
C(22)	1949(16)	5697(6)	8747(3)	86(4)
C(22A)	6707(14)	3960(6)	11056(4)	79(3)
C(23)	577(14)	5561(9)	8488(4)	93(4)
C(23A)	5534(14)	3816(7)	10728(4)	79(3)
C(24)	-7(15)	6230(8)	8318(4)	91(4)
C(24A)	4246(12)	4330(6)	10788(4)	66(3)
C(25)	1104(15)	6761(8)	8157(4)	82(4)
C(25A)	4569(12)	5059(7)	10925(3)	62(3)
C(27)	3714(13)	7167(6)	8142(3)	70(3)
C(27A)	6343(12)	5910(6)	11261(3)	66(3)
C(28)	4818(16)	6966(7)	8486(4)	91(4)

C(28A)	7724(15)	5645(7)	11507(4)	86(4)
C(30)	4248(13)	7136(6)	7693(4)	76(3)
C(30A)	6469(14)	6567(7)	10979(4)	73(3)
C(31)	3623(14)	7647(6)	7418(3)	78(3)
C(31A)	5318(17)	7015(7)	10936(5)	90(4)
C(32)	4054(16)	7613(10)	6995(5)	111(5)
C(32A)	5430(30)	7615(9)	10650(7)	132(7)
C(33)	5117(19)	7088(9)	6859(5)	106(5)
C(33A)	6650(30)	7754(10)	10416(6)	124(6)
C(34)	5756(16)	6630(7)	7133(5)	98(4)
C(34A)	7790(20)	7254(8)	10474(5)	110(5)
C(35)	5324(14)	6632(6)	7549(4)	78(3)
C(35A)	7737(17)	6711(7)	10755(4)	86(4)
C(61)	2837(11)	4548(6)	7254(3)	63(3)
C(61A)	7315(11)	5213(6)	9567(3)	60(3)
C(62)	2732(14)	5104(7)	6912(3)	78(3)
C(62A)	6667(13)	5975(6)	9551(3)	69(3)
C(63)	1765(16)	5735(6)	7047(3)	85(4)
C(63A)	5386(12)	6053(6)	9863(3)	68(3)
C(64)	217(14)	5502(6)	7176(4)	81(4)
C(64A)	4236(12)	5532(5)	9767(4)	68(3)
C(65)	130(15)	4783(7)	7372(4)	79(3)
C(65A)	4705(13)	4777(6)	9603(3)	61(3)
C(67)	1294(12)	3570(6)	7523(4)	68(3)
C(67A)	6678(14)	4035(6)	9271(3)	71(3)
C(68)	2727(14)	3297(6)	7337(4)	80(3)
C(68A)	8187(17)	4340(8)	9151(4)	101(5)
C(70)	1101(12)	3388(6)	7979(3)	65(3)
C(70A)	6669(14)	3330(6)	9458(3)	69(3)
C(71)	-4(14)	2947(7)	8095(4)	84(4)
C(71A)	5883(16)	2756(7)	9288(4)	96(4)
C(72)	-203(17)	2765(10)	8504(6)	125(6)
C(72A)	5933(17)	2070(7)	9450(6)	101(5)
C(73)	692(17)	3055(7)	8811(5)	92(4)
C(73A)	6743(16)	1944(7)	9780(5)	91(4)
C(74)	1817(15)	3475(6)	8697(4)	83(4)
C(74A)	7548(16)	2445(9)	9969(5)	93(4)
C(75)	1993(15)	3670(7)	8287(4)	84(4)
C(75A)	7500(15)	3137(7)	9804(4)	89(4)
N(1)	3182(8)	5265(4)	7870(2)	48(2)
N(1A)	7452(8)	4957(4)	10306(2)	50(2)
N(26)	2553(10)	6625(4)	8224(2)	57(2)
N(26A)	5932(9)	5220(4)	11052(2)	56(2)
N(66)	1361(9)	4354(5)	7412(3)	60(2)

N(66A)	6144(10)	4665(4)	9533(2)	56(2)
O(1W)	1353(13)	6498(10)	11200(4)	160(5)
O(25)	776(11)	7358(7)	7984(3)	128(4)
O(25A)	3587(8)	5516(5)	10932(3)	83(2)
O(29)	4182(10)	6412(4)	8740(2)	78(2)
O(29A)	7931(10)	4882(5)	11424(2)	91(3)
O(65)	-1067(10)	4504(7)	7479(3)	112(3)
O(65A)	3771(10)	4306(5)	9522(3)	92(3)
O(69)	3324(8)	3881(4)	7082(2)	71(2)
O(69A)	8158(10)	5109(4)	9203(2)	85(2)

Table 3. Bond lengths [Å] and angles [°] for **10**.

C(2)-N(1)	1.335(12)	C(25A)-O(25A)	1.224(13)
C(2)-C(3)	1.407(14)	C(25A)-N(26A)	1.338(13)
C(2)-C(21)	1.506(13)	C(27)-N(26)	1.474(13)
C(2A)-N(1A)	1.347(12)	C(27)-C(30)	1.517(16)
C(2A)-C(3A)	1.384(15)	C(27)-C(28)	1.536(17)
C(2A)-C(21A)	1.499(14)	C(27A)-N(26A)	1.479(13)
C(3)-C(4)	1.353(14)	C(27A)-C(30A)	1.509(16)
C(3A)-C(4A)	1.390(19)	C(27A)-C(28A)	1.562(16)
C(4)-C(5)	1.403(14)	C(28)-O(29)	1.423(14)
C(4A)-C(5A)	1.367(19)	C(28A)-O(29A)	1.436(14)
C(5)-C(6)	1.385(14)	C(30)-C(31)	1.407(16)
C(5A)-C(6A)	1.397(15)	C(30)-C(35)	1.424(16)
C(6)-N(1)	1.303(11)	C(30A)-C(31A)	1.337(17)
C(6)-C(61)	1.542(14)	C(30A)-C(35A)	1.384(17)
C(6A)-N(1A)	1.338(12)	C(31)-C(32)	1.411(19)
C(6A)-C(61A)	1.507(14)	C(31A)-C(32A)	1.44(2)
C(21)-O(29)	1.432(13)	C(32)-C(33)	1.43(2)
C(21)-N(26)	1.480(12)	C(32A)-C(33A)	1.37(3)
C(21)-C(22)	1.508(16)	C(33)-C(34)	1.346(19)
C(21A)-C(22A)	1.419(15)	C(33A)-C(34A)	1.39(2)
C(21A)-O(29A)	1.427(13)	C(34)-C(35)	1.390(18)
C(21A)-N(26A)	1.522(13)	C(34A)-C(35A)	1.343(19)
C(22)-C(23)	1.519(18)	C(61)-O(69)	1.414(12)
C(22A)-C(23A)	1.520(16)	C(61)-N(66)	1.479(13)
C(23)-C(24)	1.445(19)	C(61)-C(62)	1.498(15)
C(23A)-C(24A)	1.517(16)	C(61A)-O(69A)	1.410(12)
C(24)-C(25)	1.495(18)	C(61A)-N(66A)	1.469(13)
C(24A)-C(25A)	1.438(15)	C(61A)-C(62A)	1.517(15)
C(25)-O(25)	1.265(15)	C(62)-C(63)	1.518(16)
C(25)-N(26)	1.358(15)	C(62A)-C(63A)	1.541(16)

C(63)-C(64)	1.529(18)
C(63A)-C(64A)	1.451(14)
C(64)-C(65)	1.461(17)
C(64A)-C(65A)	1.541(15)
C(65)-O(65)	1.252(16)
C(65)-N(66)	1.376(15)
C(65A)-O(65A)	1.240(12)
C(65A)-N(66A)	1.345(14)
C(67)-N(66)	1.482(13)
C(67)-C(70)	1.508(15)
C(67)-C(68)	1.520(16)
C(67A)-C(70A)	1.423(15)
C(67A)-N(66A)	1.509(13)
C(67A)-C(68A)	1.532(19)
C(68)-O(69)	1.452(13)
C(68A)-O(69A)	1.421(15)
C(70)-C(71)	1.342(15)
C(70)-C(75)	1.376(15)
C(70A)-C(75A)	1.387(17)
C(70A)-C(71A)	1.385(17)
C(71)-C(72)	1.36(2)
C(71A)-C(72A)	1.360(18)
C(72)-C(73)	1.38(2)
C(72A)-C(73A)	1.308(19)
C(73)-C(74)	1.333(18)
C(73A)-C(74A)	1.32(2)
C(74)-C(75)	1.370(16)
C(74A)-C(75A)	1.38(2)
N(1)-C(2)-C(3)	121.3(9)
N(1)-C(2)-C(21)	116.1(8)
C(3)-C(2)-C(21)	122.5(9)
N(1A)-C(2A)-C(3A)	121.3(11)
N(1A)-C(2A)-C(21A)	116.0(8)
C(3A)-C(2A)-C(21A)	122.7(11)
C(4)-C(3)-C(2)	119.4(10)
C(2A)-C(3A)-C(4A)	118.7(12)
C(3)-C(4)-C(5)	119.0(10)
C(5A)-C(4A)-C(3A)	119.2(11)
C(6)-C(5)-C(4)	116.7(10)
C(4A)-C(5A)-C(6A)	119.5(12)
N(1)-C(6)-C(5)	125.0(9)
N(1)-C(6)-C(61)	113.9(8)
C(5)-C(6)-C(61)	120.8(9)
N(1A)-C(6A)-C(5A)	120.9(11)
N(1A)-C(6A)-C(61A)	116.1(8)
C(5A)-C(6A)-C(61A)	123.0(11)
O(29)-C(21)-N(26)	101.4(7)
O(29)-C(21)-C(2)	110.6(9)
N(26)-C(21)-C(2)	108.8(8)
O(29)-C(21)-C(22)	110.7(9)
N(26)-C(21)-C(22)	110.1(10)
C(2)-C(21)-C(22)	114.4(9)
C(22A)-C(21A)-O(29A)	110.8(9)
C(22A)-C(21A)-C(2A)	114.0(9)
O(29A)-C(21A)-C(2A)	111.6(8)
C(22A)-C(21A)-N(26A)	110.4(9)
O(29A)-C(21A)-N(26A)	100.0(8)
C(2A)-C(21A)-N(26A)	109.2(8)
C(21)-C(22)-C(23)	111.1(9)
C(21A)-C(22A)-C(23A)	112.0(10)
C(24)-C(23)-C(22)	111.6(12)
C(24A)-C(23A)-C(22A)	110.3(9)
C(23)-C(24)-C(25)	115.7(12)
C(25A)-C(24A)-C(23A)	117.4(9)
O(25)-C(25)-N(26)	117.2(13)
O(25)-C(25)-C(24)	123.7(13)
N(26)-C(25)-C(24)	119.0(12)
O(25A)-C(25A)-N(26A)	121.4(10)
O(25A)-C(25A)-C(24A)	119.5(9)
N(26A)-C(25A)-C(24A)	119.1(11)
N(26)-C(27)-C(30)	111.9(9)
N(26)-C(27)-C(28)	100.3(9)
C(30)-C(27)-C(28)	117.4(11)
N(26A)-C(27A)-C(30A)	115.7(8)
N(26A)-C(27A)-C(28A)	99.5(8)
C(30A)-C(27A)-C(28A)	119.3(10)
O(29)-C(28)-C(27)	108.3(10)
O(29A)-C(28A)-C(27A)	108.3(9)
C(31)-C(30)-C(35)	120.5(12)
C(31)-C(30)-C(27)	116.0(11)
C(35)-C(30)-C(27)	123.5(11)
C(31A)-C(30A)-C(35A)	118.9(12)
C(31A)-C(30A)-C(27A)	119.5(12)
C(35A)-C(30A)-C(27A)	121.6(11)
C(30)-C(31)-C(32)	117.3(14)
C(30A)-C(31A)-C(32A)	118.7(16)
C(31)-C(32)-C(33)	120.7(14)

C(33A)-C(32A)-C(31A)	123.5(17)	O(69)-C(68)-C(67)	107.4(9)
C(34)-C(33)-C(32)	120.8(15)	O(69A)-C(68A)-C(67A)	108.5(11)
C(32A)-C(33A)-C(34A)	113.9(18)	C(71)-C(70)-C(75)	118.2(11)
C(33)-C(34)-C(35)	120.1(14)	C(71)-C(70)-C(67)	119.1(10)
C(35A)-C(34A)-C(33A)	123.6(17)	C(75)-C(70)-C(67)	122.7(10)
C(34)-C(35)-C(30)	120.5(12)	C(75A)-C(70A)-C(71A)	113.6(12)
C(34A)-C(35A)-C(30A)	121.1(15)	C(75A)-C(70A)-C(67A)	124.4(11)
O(69)-C(61)-N(66)	102.1(8)	C(71A)-C(70A)-C(67A)	122.0(11)
O(69)-C(61)-C(62)	108.8(8)	C(70)-C(71)-C(72)	120.7(13)
N(66)-C(61)-C(62)	110.8(9)	C(72A)-C(71A)-C(70A)	122.5(13)
O(69)-C(61)-C(6)	112.7(8)	C(71)-C(72)-C(73)	120.7(13)
N(66)-C(61)-C(6)	111.0(7)	C(73A)-C(72A)-C(71A)	119.3(13)
C(62)-C(61)-C(6)	111.1(9)	C(74)-C(73)-C(72)	118.7(13)
O(69A)-C(61A)-N(66A)	103.9(8)	C(72A)-C(73A)-C(74A)	124.0(13)
O(69A)-C(61A)-C(6A)	112.2(9)	C(73)-C(74)-C(75)	120.2(13)
N(66A)-C(61A)-C(6A)	111.5(8)	C(73A)-C(74A)-C(75A)	116.5(14)
O(69A)-C(61A)-C(62A)	107.9(8)	C(74)-C(75)-C(70)	121.2(12)
N(66A)-C(61A)-C(62A)	110.2(9)	C(74A)-C(75A)-C(70A)	124.1(13)
C(6A)-C(61A)-C(62A)	110.9(8)	C(6)-N(1)-C(2)	118.1(8)
C(61)-C(62)-C(63)	110.4(9)	C(6A)-N(1A)-C(2A)	120.0(8)
C(61A)-C(62A)-C(63A)	111.0(8)	C(25)-N(26)-C(27)	123.0(9)
C(62)-C(63)-C(64)	113.3(10)	C(25)-N(26)-C(21)	125.5(10)
C(64A)-C(63A)-C(62A)	110.3(9)	C(27)-N(26)-C(21)	109.6(8)
C(65)-C(64)-C(63)	114.8(10)	C(25A)-N(26A)-C(27A)	124.0(9)
C(63A)-C(64A)-C(65A)	117.6(9)	C(25A)-N(26A)-C(21A)	124.6(9)
O(65)-C(65)-N(66)	116.6(11)	C(27A)-N(26A)-C(21A)	111.1(8)
O(65)-C(65)-C(64)	122.4(12)	C(65)-N(66)-C(61)	124.7(9)
N(66)-C(65)-C(64)	120.8(12)	C(65)-N(66)-C(67)	123.0(10)
O(65A)-C(65A)-N(66A)	121.8(10)	C(61)-N(66)-C(67)	110.7(8)
O(65A)-C(65A)-C(64A)	120.5(10)	C(65A)-N(66A)-C(61A)	126.2(9)
N(66A)-C(65A)-C(64A)	117.6(9)	C(65A)-N(66A)-C(67A)	121.6(9)
N(66)-C(67)-C(70)	116.9(9)	C(61A)-N(66A)-C(67A)	109.4(8)
N(66)-C(67)-C(68)	101.0(9)	C(28)-O(29)-C(21)	106.9(8)
C(70)-C(67)-C(68)	114.0(10)	C(21A)-O(29A)-C(28A)	109.9(8)
C(70A)-C(67A)-N(66A)	117.5(8)	C(61)-O(69)-C(68)	107.6(7)
C(70A)-C(67A)-C(68A)	116.2(11)	C(61A)-O(69A)-C(68A)	103.9(8)
N(66A)-C(67A)-C(68A)	98.5(9)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **10**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}

C(2)	57(6)	48(5)	50(5)	3(4)	-1(5)	7(5)
C(2A)	42(6)	54(6)	72(7)	3(5)	-5(5)	-1(5)
C(3)	55(6)	66(6)	63(6)	7(5)	-18(5)	1(6)
C(3A)	43(7)	115(10)	102(9)	14(8)	-18(6)	18(7)
C(4)	48(6)	80(7)	72(7)	-17(6)	-4(6)	11(6)
C(4A)	27(6)	172(15)	123(12)	2(11)	-5(7)	4(8)
C(5)	49(6)	93(8)	61(7)	3(6)	10(5)	9(6)
C(5A)	53(7)	110(10)	109(11)	-12(8)	34(7)	-16(7)
C(6)	48(5)	49(5)	46(5)	2(4)	1(4)	1(5)
C(6A)	34(5)	61(6)	70(6)	5(5)	12(5)	3(5)
C(21)	81(7)	52(5)	48(5)	-4(5)	-4(6)	13(6)
C(21A)	52(6)	62(6)	67(6)	8(5)	-6(5)	-1(5)
C(22)	145(12)	67(7)	47(6)	-3(5)	34(8)	6(8)
C(22A)	75(8)	87(8)	74(7)	17(6)	5(7)	4(7)
C(23)	77(9)	126(12)	75(8)	3(8)	40(7)	-13(9)
C(23A)	86(9)	83(8)	66(7)	9(6)	-2(6)	-33(7)
C(24)	76(9)	115(11)	82(8)	6(8)	17(7)	-1(9)
C(24A)	58(6)	60(6)	81(7)	2(5)	-8(6)	-8(6)
C(25)	83(9)	104(10)	58(7)	0(7)	3(7)	24(8)
C(25A)	47(7)	93(8)	47(6)	1(5)	-3(5)	-10(6)
C(27)	81(8)	61(6)	68(7)	-15(5)	4(6)	0(6)
C(27A)	70(7)	66(7)	63(6)	-10(5)	-11(6)	-1(6)
C(28)	100(10)	86(9)	88(9)	-2(7)	-26(8)	-20(8)
C(28A)	94(10)	91(9)	72(7)	-10(6)	-26(7)	6(8)
C(30)	68(8)	76(7)	83(8)	3(6)	-2(7)	-18(7)
C(30A)	67(8)	81(8)	72(7)	-18(6)	-13(6)	1(7)
C(31)	78(8)	83(8)	72(7)	19(6)	-7(6)	-25(7)
C(31A)	96(10)	59(7)	116(11)	-13(7)	-8(8)	13(8)
C(32)	73(9)	152(14)	108(12)	60(10)	-3(9)	-25(11)
C(32A)	144(17)	81(11)	173(19)	-37(12)	-76(15)	34(12)
C(33)	100(11)	121(12)	98(10)	25(10)	9(10)	-31(11)
C(33A)	150(17)	79(10)	144(16)	-29(10)	-42(15)	-14(13)
C(34)	92(10)	85(8)	118(11)	-1(8)	37(9)	-11(8)
C(34A)	139(14)	80(9)	111(11)	-9(9)	13(10)	-50(11)
C(35)	80(8)	66(7)	88(8)	8(6)	17(7)	-9(7)
C(35A)	104(10)	68(7)	86(8)	-1(7)	-10(8)	-15(8)
C(61)	65(7)	77(7)	47(6)	-4(5)	5(5)	10(6)
C(61A)	57(6)	74(7)	50(6)	0(5)	15(5)	-18(6)
C(62)	78(8)	94(8)	61(6)	-4(6)	-12(6)	0(7)
C(62A)	78(8)	69(7)	61(6)	11(5)	-15(6)	-14(6)
C(63)	121(11)	74(7)	60(6)	17(6)	-24(7)	3(8)
C(63A)	72(7)	63(6)	68(6)	7(5)	-14(6)	9(6)
C(64)	88(9)	67(7)	88(8)	2(6)	-25(7)	23(7)

C(64A)	64(7)	55(6)	85(7)	-8(5)	-5(6)	-3(6)
C(65)	67(8)	95(9)	76(8)	1(7)	-20(7)	10(7)
C(65A)	67(8)	56(6)	59(6)	0(5)	-8(5)	-10(6)
C(67)	52(7)	69(7)	83(8)	-11(6)	-15(6)	-4(5)
C(67A)	85(8)	74(7)	53(6)	2(5)	12(6)	-4(6)
C(68)	87(9)	68(7)	87(8)	-10(6)	-3(7)	4(7)
C(68A)	112(11)	122(12)	68(8)	-17(7)	39(8)	0(10)
C(70)	54(6)	60(6)	81(7)	-5(5)	-10(6)	6(6)
C(70A)	75(7)	82(7)	50(6)	-8(5)	1(6)	6(7)
C(71)	76(8)	80(8)	96(9)	29(7)	-16(7)	-25(7)
C(71A)	97(10)	90(9)	100(9)	-11(8)	-23(8)	-24(8)
C(72)	83(10)	143(14)	148(15)	52(12)	-5(10)	-50(11)
C(72A)	98(11)	52(7)	154(13)	-12(8)	-13(11)	-12(7)
C(73)	104(11)	66(7)	105(10)	18(7)	14(9)	14(8)
C(73A)	85(9)	51(7)	139(12)	0(8)	30(10)	9(7)
C(74)	99(9)	66(7)	83(8)	13(6)	-13(8)	-25(7)
C(74A)	106(11)	86(9)	86(8)	6(7)	-3(8)	13(9)
C(75)	84(9)	90(8)	78(8)	-3(7)	-14(7)	-20(8)
C(75A)	94(9)	79(8)	93(9)	-13(7)	4(8)	-9(8)
N(1)	47(4)	50(4)	47(4)	5(4)	1(4)	0(4)
N(1A)	39(4)	60(4)	51(5)	-3(3)	-5(4)	2(4)
N(26)	70(6)	47(4)	53(5)	3(4)	2(4)	9(4)
N(26A)	53(5)	67(5)	50(4)	-5(4)	-2(4)	4(4)
N(66)	51(5)	64(5)	66(5)	-6(4)	-8(4)	0(4)
N(66A)	66(6)	45(4)	57(5)	-9(4)	13(4)	-10(4)
O(1W)	132(9)	199(13)	149(11)	-25(11)	-13(8)	61(10)
O(25)	100(7)	173(10)	111(8)	53(7)	9(6)	58(8)
O(25A)	51(4)	89(6)	108(6)	-15(5)	0(4)	9(5)
O(29)	109(6)	68(4)	56(4)	-15(4)	-17(4)	6(5)
O(29A)	85(6)	132(8)	57(4)	16(4)	-28(4)	0(6)
O(65)	54(5)	167(10)	114(7)	22(7)	-2(5)	10(6)
O(65A)	78(6)	100(6)	97(6)	-14(5)	-17(5)	-28(5)
O(69)	69(5)	79(5)	65(4)	-25(4)	9(4)	11(4)
O(69A)	107(6)	75(5)	71(5)	-8(4)	38(5)	-20(5)

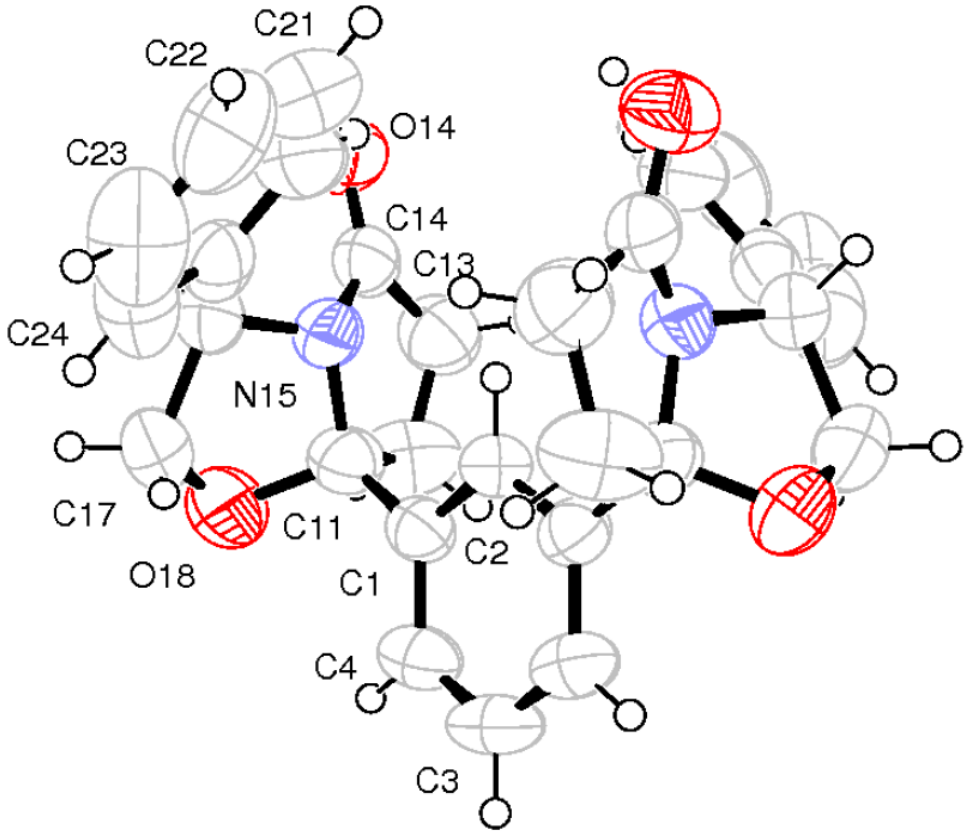


Fig S3 ORTEP view of molecular structure of **11**.

Table 1. Crystal data and structure refinement for **11**.

Identification code	Jb78	
Empirical formula	C30 H28 N2 O4	
Formula weight	240.27	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	P 41 21 2	
Unit cell dimensions	a = 9.727(3) Å	□= 90°.
	b = 9.727(3) Å	□= 90°.
	c = 25.904(32) Å	□ = 90°.
Volume	2450.9 $Å^3$	
Z	4	
Density (calculated)	1.302 Mg/m^3	
Absorption coefficient	0.087 mm^{-1}	
F(000)	1016	
Crystal size	0.42 x 0.38 x 0.33 mm^3	
Theta range for data collection	2.24 to 29.95°.	

Index ranges	-9<=h<=9, 0<=k<=13, 0<=l<=36
Reflections collected	3567
Independent reflections	3567
Completeness to theta = 29.95°	100.0 %
Max. and min. transmission	0.9719 and 0.9645
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3567 / 0 / 165
Goodness-of-fit on F^2	1.059
Final R indices [I>2sigma(I)]	R1 = 0.0542, wR2 = 0.1488
R indices (all data)	R1 = 0.1108, wR2 = 0.1717
Largest diff. peak and hole	0.105 and -0.101 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **11**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	-1043(2)	2640(2)	7692(1)	58(1)
C(2)*	-1341(2)	1341(2)	7500	59(1)
C(3)*	-3326(2)	3326(2)	7500	81(1)
C(4)	-2055(3)	3630(2)	7695(1)	69(1)
C(11)	402(3)	2991(3)	7881(1)	72(1)
C(12)	1241(3)	3787(3)	7480(2)	100(1)
C(13)	2369(3)	2843(3)	7322(1)	93(1)
C(14)	2432(3)	1759(3)	7734(1)	70(1)
C(16)	1055(3)	1409(3)	8537(1)	76(1)
C(17)	210(4)	2637(4)	8737(1)	112(1)
C(19)	424(2)	15(3)	8634(1)	71(1)
C(20)	809(3)	-1106(3)	8342(1)	86(1)
C(21)	304(4)	-2422(3)	8447(2)	102(1)
C(22)	-597(4)	-2624(5)	8840(2)	114(1)
C(23)	-995(4)	-1547(6)	9130(2)	124(1)
C(24)	-502(3)	-233(5)	9030(1)	109(1)
N(15)	1219(2)	1783(2)	7991(1)	67(1)
O(14)	3370(2)	965(2)	7826(1)	93(1)
O(18)	345(3)	3694(2)	8359(1)	104(1)

* at special position

Table 3. Bond lengths [Å] and angles [°] for **11**.

C(1)-C(4)	1.376(3)	C(3)-C(4)-C(1)	119.6(3)
C(1)-C(2)	1.388(3)	O(18)-C(11)-N(15)	104.0(2)
C(1)-C(11)	1.527(4)	O(18)-C(11)-C(1)	110.6(2)
C(2)-C(1)#1	1.388(3)	N(15)-C(11)-C(1)	112.8(2)
C(3)-C(4)#1	1.368(3)	O(18)-C(11)-C(12)	111.7(2)
C(3)-C(4)	1.368(3)	N(15)-C(11)-C(12)	104.5(2)
C(11)-O(18)	1.415(3)	C(1)-C(11)-C(12)	112.7(2)
C(11)-N(15)	1.447(3)	C(13)-C(12)-C(11)	105.5(2)
C(11)-C(12)	1.532(4)	C(12)-C(13)-C(14)	105.6(3)
C(12)-C(13)	1.488(4)	O(14)-C(14)-N(15)	124.5(3)
C(13)-C(14)	1.502(4)	O(14)-C(14)-C(13)	127.9(3)
C(14)-O(14)	1.219(3)	N(15)-C(14)-C(13)	107.6(2)
C(14)-N(15)	1.355(3)	N(15)-C(16)-C(19)	115.2(2)
C(16)-N(15)	1.470(4)	N(15)-C(16)-C(17)	100.9(2)
C(16)-C(19)	1.510(4)	C(19)-C(16)-C(17)	115.1(3)
C(16)-C(17)	1.539(4)	O(18)-C(17)-C(16)	106.3(3)
C(17)-O(18)	1.425(4)	C(20)-C(19)-C(24)	116.4(3)
C(19)-C(20)	1.380(4)	C(20)-C(19)-C(16)	120.5(2)
C(19)-C(24)	1.386(4)	C(24)-C(19)-C(16)	122.9(3)
C(20)-C(21)	1.398(4)	C(19)-C(20)-C(21)	121.4(3)
C(21)-C(22)	1.357(5)	C(22)-C(21)-C(20)	120.4(4)
C(22)-C(23)	1.347(6)	C(23)-C(22)-C(21)	119.4(4)
C(23)-C(24)	1.390(6)	C(22)-C(23)-C(24)	120.8(4)
		C(19)-C(24)-C(23)	121.5(4)
C(4)-C(1)-C(2)	119.2(2)	C(14)-N(15)-C(11)	113.3(2)
C(4)-C(1)-C(11)	120.0(2)	C(14)-N(15)-C(16)	124.3(2)
C(2)-C(1)-C(11)	120.7(2)	C(11)-N(15)-C(16)	109.3(2)
C(1)#1-C(2)-C(1)	120.6(3)	C(11)-O(18)-C(17)	104.8(2)
C(4)#1-C(3)-C(4)	121.7(3)		

Symmetry transformations used to generate equivalent atoms:

#1 -y,-x,-z+3/2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **11**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}

C(1)	65(1)	55(1)	55(1)	2(1)	7(1)	6(1)
C(2)*	58(1)	58(1)	62(2)	-1(1)	-1(1)	11(1)
C(3)*	69(1)	69(1)	105(3)	11(2)	11(2)	28(2)
C(4)	73(2)	54(1)	81(2)	6(1)	15(1)	13(1)
C(11)	74(2)	59(1)	83(2)	-7(1)	-6(1)	8(1)
C(12)	78(2)	67(2)	153(3)	20(2)	4(2)	-10(1)
C(13)	104(2)	87(2)	89(2)	2(2)	10(2)	6(2)
C(14)	62(1)	80(2)	68(2)	-15(1)	-7(1)	4(1)
C(16)	74(2)	87(2)	66(2)	-14(1)	-11(1)	14(1)
C(17)	159(4)	111(2)	68(2)	-21(2)	-11(2)	50(2)
C(19)	58(1)	92(2)	64(2)	-2(1)	-7(1)	-1(1)
C(20)	77(2)	85(2)	95(2)	9(2)	2(2)	13(2)
C(21)	89(2)	91(2)	127(3)	19(2)	-12(2)	5(2)
C(22)	104(3)	135(3)	103(3)	29(2)	-27(2)	-36(2)
C(23)	97(2)	173(4)	100(3)	-1(3)	9(2)	-56(3)
C(24)	84(2)	160(4)	82(2)	-23(2)	4(2)	-19(2)
N(15)	63(1)	68(1)	68(1)	-7(1)	-11(1)	5(1)
O(14)	66(1)	111(2)	102(2)	1(1)	-2(1)	15(1)
O(18)	129(2)	77(1)	107(2)	-38(1)	-30(2)	19(1)

* at special position

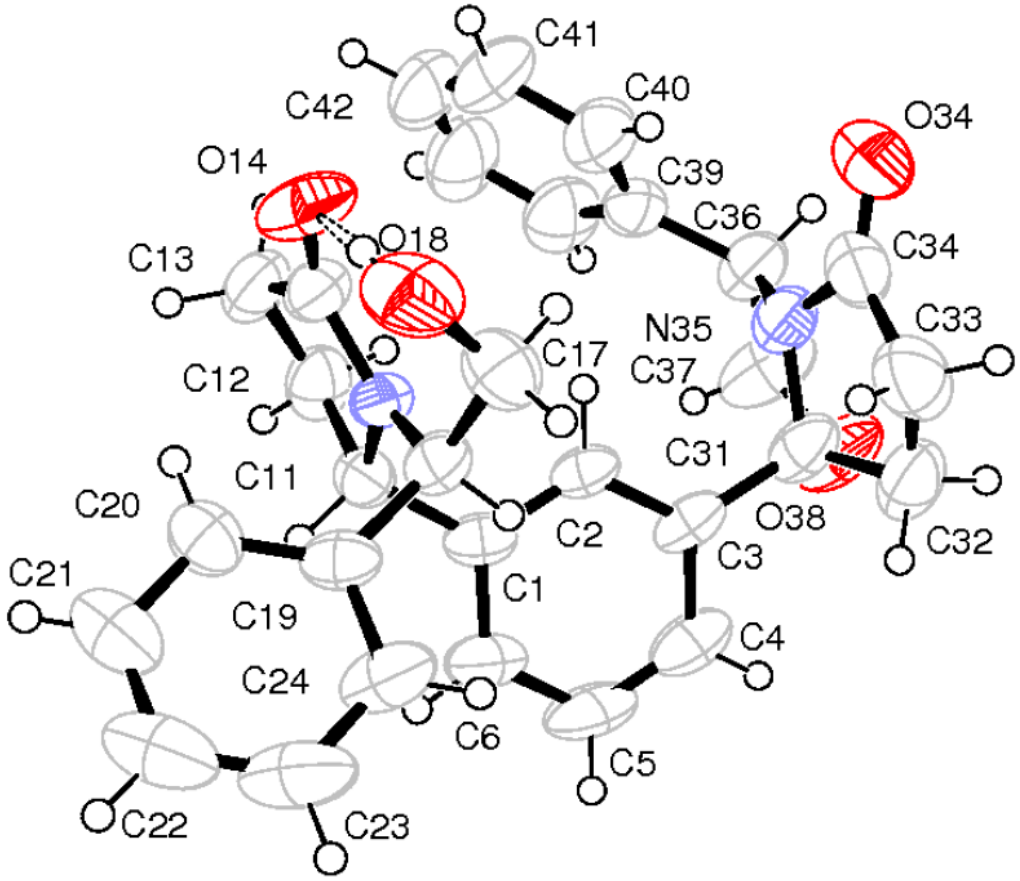


Fig S4 ORTEP view of molecular structure of **18**.

Table 1. Crystal data and structure refinement for **18**.

Identification code	Jb80	
Empirical formula	C30 H30 N2 O4	
Formula weight	482.56	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 9.737(8) Å	□= 90°.
	b = 10.015(6) Å	□= 90°.
	c = 26.408(11) Å	□ = 90°.
Volume	2575(3) $Å^3$	
Z	4	
Density (calculated)	1.245 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	1024	
Crystal size	0.43 x 0.39 x 0.18 mm^3	

Theta range for data collection	1.54 to 26.97°.
Index ranges	0<=h<=12, 0<=k<=12, 0<=l<=33
Reflections collected	3175
Independent reflections	3175
Completeness to theta = 26.97°	99.8 %
Max. and min. transmission	0.9853 and 0.9653
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3175 / 0 / 326
Goodness-of-fit on F^2	1.124
Final R indices [I>2sigma(I)]	R1 = 0.0639, wR2 = 0.1898
R indices (all data)	R1 = 0.0894, wR2 = 0.2124
Largest diff. peak and hole	0.359 and -0.229 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **18**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(14)	6588(5)	2681(3)	8269(2)	87(1)
O(18)	5814(4)	1951(4)	7355(1)	85(1)
O(34)	791(4)	208(5)	8844(2)	97(1)
O(38)	2450(5)	-3290(3)	9531(1)	89(1)
N(15)	6787(3)	390(3)	8346(1)	46(1)
N(35)	2400(4)	-1268(3)	9148(1)	60(1)
C(1)	6568(5)	-1822(4)	8764(1)	48(1)
C(2)	5180(4)	-1704(4)	8887(1)	47(1)
C(3)	4349(5)	-2807(4)	8956(2)	56(1)
C(4)	4922(7)	-4074(4)	8917(2)	74(2)
C(5)	6287(7)	-4210(4)	8797(2)	78(2)
C(6)	7100(5)	-3094(4)	8719(2)	65(1)
C(11)	7419(4)	-580(4)	8705(1)	48(1)
C(12)	7547(5)	265(5)	9192(2)	63(1)
C(13)	7652(6)	1682(5)	9004(2)	72(1)
C(14)	6933(5)	1670(4)	8503(2)	61(1)
C(16)	6424(4)	-102(4)	7838(1)	49(1)
C(17)	5350(5)	731(6)	7554(2)	68(1)
C(19)	7711(5)	-367(4)	7521(1)	51(1)
C(20)	8885(4)	393(5)	7569(2)	59(1)

C(21)	10031(5)	106(6)	7283(2)	81(2)
C(22)	10020(7)	-916(7)	6936(2)	93(2)
C(23)	8874(8)	-1687(6)	6887(2)	95(2)
C(24)	7703(7)	-1409(5)	7175(2)	76(2)
C(31)	2814(5)	-2663(4)	9072(2)	63(1)
C(32)	1873(6)	-3127(6)	8633(2)	79(2)
C(33)	1426(6)	-1847(7)	8374(2)	90(2)
C(34)	1447(5)	-822(6)	8806(2)	74(1)
C(36)	2458(6)	-953(5)	9696(2)	68(1)
C(37)	2793(9)	-2326(5)	9917(2)	93(2)
C(39)	3438(5)	174(4)	9823(2)	59(1)
C(40)	3444(7)	1306(5)	9514(3)	84(2)
C(41)	4274(8)	2372(6)	9647(4)	113(2)
C(42)	5112(8)	2324(8)	10048(4)	116(3)
C(43)	5082(7)	1237(7)	10342(3)	98(2)
C(44)	4275(7)	183(6)	10235(2)	84(2)

Table 3. Bond lengths [Å] and angles [°] for **18**.

O(14)-C(14)	1.234(6)	C(11)-C(12)	1.545(5)
O(18)-C(17)	1.405(6)	C(12)-C(13)	1.507(7)
O(34)-C(34)	1.217(7)	C(13)-C(14)	1.497(8)
O(38)-C(31)	1.408(5)	C(16)-C(19)	1.531(6)
O(38)-C(37)	1.444(6)	C(16)-C(17)	1.533(6)
N(15)-C(14)	1.355(5)	C(19)-C(20)	1.380(6)
N(15)-C(16)	1.472(5)	C(19)-C(24)	1.387(6)
N(15)-C(11)	1.491(5)	C(20)-C(21)	1.378(6)
N(35)-C(34)	1.370(7)	C(21)-C(22)	1.374(9)
N(35)-C(31)	1.468(6)	C(22)-C(23)	1.363(9)
N(35)-C(36)	1.481(6)	C(23)-C(24)	1.399(9)
C(1)-C(6)	1.380(6)	C(31)-C(32)	1.549(7)
C(1)-C(2)	1.395(6)	C(32)-C(33)	1.516(9)
C(1)-C(11)	1.503(6)	C(33)-C(34)	1.535(8)
C(2)-C(3)	1.381(6)	C(36)-C(39)	1.516(6)
C(3)-C(4)	1.389(7)	C(36)-C(37)	1.529(7)
C(3)-C(31)	1.533(7)	C(39)-C(44)	1.360(7)
C(4)-C(5)	1.373(9)	C(39)-C(40)	1.397(7)
C(5)-C(6)	1.386(8)	C(40)-C(41)	1.383(8)

C(41)-C(42)	1.338(12)	O(18)-C(17)-C(16)	115.9(4)
C(42)-C(43)	1.338(11)	C(20)-C(19)-C(24)	118.7(4)
C(43)-C(44)	1.346(8)	C(20)-C(19)-C(16)	122.2(3)
		C(24)-C(19)-C(16)	119.1(4)
C(31)-O(38)-C(37)	104.5(3)	C(21)-C(20)-C(19)	120.4(5)
C(14)-N(15)-C(16)	128.4(3)	C(22)-C(21)-C(20)	121.0(6)
C(14)-N(15)-C(11)	112.3(3)	C(23)-C(22)-C(21)	119.5(5)
C(16)-N(15)-C(11)	117.4(3)	C(22)-C(23)-C(24)	120.2(5)
C(34)-N(35)-C(31)	114.0(4)	C(19)-C(24)-C(23)	120.3(6)
C(34)-N(35)-C(36)	126.9(4)	O(38)-C(31)-N(35)	103.8(3)
C(31)-N(35)-C(36)	109.0(4)	O(38)-C(31)-C(3)	112.1(4)
C(6)-C(1)-C(2)	117.5(4)	N(35)-C(31)-C(3)	112.6(3)
C(6)-C(1)-C(11)	123.2(4)	O(38)-C(31)-C(32)	111.2(4)
C(2)-C(1)-C(11)	119.2(3)	N(35)-C(31)-C(32)	103.0(4)
C(3)-C(2)-C(1)	122.0(4)	C(3)-C(31)-C(32)	113.5(4)
C(2)-C(3)-C(4)	119.0(5)	C(33)-C(32)-C(31)	104.7(4)
C(2)-C(3)-C(31)	121.5(4)	C(32)-C(33)-C(34)	103.1(5)
C(4)-C(3)-C(31)	119.5(4)	O(34)-C(34)-N(35)	125.3(5)
C(5)-C(4)-C(3)	119.8(5)	O(34)-C(34)-C(33)	128.4(5)
C(4)-C(5)-C(6)	120.5(4)	N(35)-C(34)-C(33)	106.3(5)
C(1)-C(6)-C(5)	121.1(5)	N(35)-C(36)-C(39)	113.5(4)
N(15)-C(11)-C(1)	112.1(3)	N(35)-C(36)-C(37)	101.0(3)
N(15)-C(11)-C(12)	101.9(3)	C(39)-C(36)-C(37)	116.8(5)
C(1)-C(11)-C(12)	114.4(3)	O(38)-C(37)-C(36)	106.3(4)
C(13)-C(12)-C(11)	104.3(3)	C(44)-C(39)-C(40)	117.4(5)
C(14)-C(13)-C(12)	104.6(3)	C(44)-C(39)-C(36)	124.0(5)
O(14)-C(14)-N(15)	126.5(5)	C(40)-C(39)-C(36)	118.5(5)
O(14)-C(14)-C(13)	124.3(4)	C(41)-C(40)-C(39)	118.7(6)
N(15)-C(14)-C(13)	109.1(4)	C(42)-C(41)-C(40)	121.9(7)
N(15)-C(16)-C(19)	111.1(3)	C(43)-C(42)-C(41)	118.4(7)
N(15)-C(16)-C(17)	115.3(3)	C(42)-C(43)-C(44)	121.9(7)
C(19)-C(16)-C(17)	112.6(3)	C(43)-C(44)-C(39)	121.5(6)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **18**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}

O(14)	127(3)	36(2)	97(3)	5(2)	8(2)	3(2)
O(18)	93(3)	74(2)	88(2)	31(2)	1(2)	25(2)
O(34)	66(2)	99(3)	124(3)	-21(3)	-10(2)	18(2)
O(38)	135(3)	54(2)	79(2)	-4(2)	37(2)	-35(2)
N(15)	49(2)	35(1)	55(2)	-4(1)	7(1)	0(1)
N(35)	62(2)	55(2)	61(2)	-9(2)	7(2)	-11(2)
C(1)	66(2)	38(2)	39(2)	1(2)	-2(2)	11(2)
C(2)	66(2)	28(2)	47(2)	4(1)	4(2)	1(2)
C(3)	83(3)	32(2)	52(2)	-1(2)	1(2)	-11(2)
C(4)	107(4)	33(2)	82(3)	5(2)	-6(3)	-8(3)
C(5)	120(5)	32(2)	84(3)	-2(2)	-20(3)	20(3)
C(6)	81(3)	49(2)	67(3)	-13(2)	-13(2)	20(2)
C(11)	45(2)	49(2)	49(2)	-2(2)	1(2)	2(2)
C(12)	62(2)	74(3)	53(2)	-12(2)	0(2)	-12(3)
C(13)	77(3)	59(2)	81(3)	-23(2)	16(3)	-22(3)
C(14)	62(3)	42(2)	79(3)	-7(2)	17(2)	-7(2)
C(16)	56(2)	39(2)	51(2)	2(2)	1(2)	-4(2)
C(17)	59(3)	76(3)	69(3)	8(2)	-6(2)	10(2)
C(19)	69(2)	37(2)	48(2)	7(2)	4(2)	11(2)
C(20)	55(2)	68(3)	54(2)	5(2)	6(2)	6(2)
C(21)	67(3)	96(4)	79(3)	17(3)	17(3)	23(3)
C(22)	110(5)	88(4)	82(4)	21(3)	37(4)	46(4)
C(23)	145(6)	60(3)	80(3)	-13(3)	31(4)	21(4)
C(24)	112(4)	44(2)	73(3)	-10(2)	13(3)	-4(3)
C(31)	81(3)	49(2)	58(2)	-6(2)	18(2)	-21(2)
C(32)	76(3)	83(4)	77(3)	-29(3)	11(3)	-26(3)
C(33)	69(3)	113(5)	90(4)	-24(4)	-12(3)	10(4)
C(34)	50(2)	84(3)	87(3)	-16(3)	0(3)	-1(3)
C(36)	77(3)	60(2)	68(3)	-17(2)	29(3)	-19(3)
C(37)	165(6)	59(3)	56(3)	1(2)	23(3)	-22(4)
C(39)	60(2)	52(2)	65(2)	-12(2)	13(2)	0(2)
C(40)	79(3)	58(3)	115(4)	10(3)	-13(3)	-5(3)
C(41)	115(5)	44(3)	179(7)	6(4)	-4(6)	-18(3)
C(42)	92(4)	95(5)	160(7)	-71(5)	14(5)	-26(4)
C(43)	96(4)	106(5)	91(4)	-36(4)	-3(4)	-25(4)
C(44)	95(4)	87(4)	71(3)	-25(3)	-1(3)	-8(4)

Table 5. Hydrogen bonds for **18** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(18)-H(18)...O(14)	0.82	1.88	2.631(6)	151.4

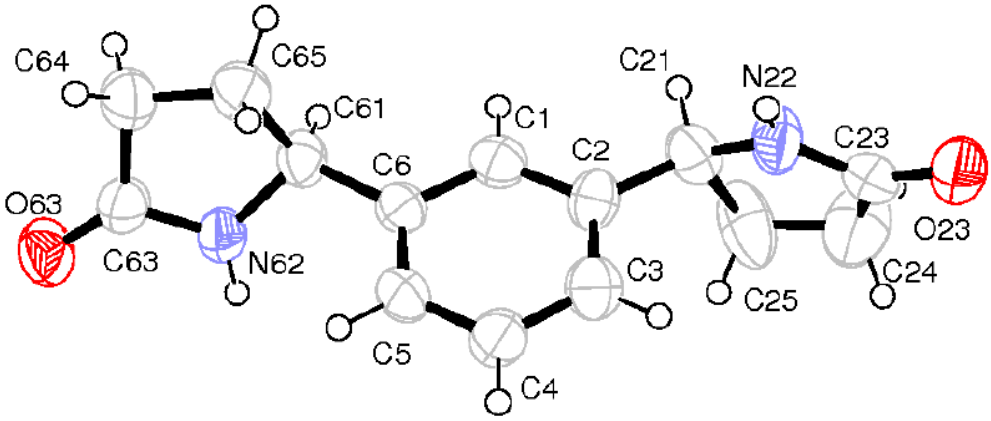


Fig S5 ORTEP view of molecular structure of **21**.

Table 1. Crystal data and structure refinement for **21**.

Identification code	Jb82	
Empirical formula	C14 H16 N2 O2	
Formula weight	244.29	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 5.559(6) Å	□= 90°.
	b = 8.894(4) Å	□= 92.64(6)°.
	c = 12.507(6) Å	□ = 90°.
Volume	617.7(8) Å^3	
Z	2	
Density (calculated)	1.313 Mg/m^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	260	
Crystal size	0.38 x 0.24 x 0.23 mm^3	
Theta range for data collection	1.63 to 25.98°.	
Index ranges	-6<=h<=6, -10<=k<=10, 0<=l<=15	
Reflections collected	2410	
Independent reflections	2410	
Completeness to theta = 25.98°	100.0 %	
Max. and min. transmission	0.9798 and 0.9669	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2410 / 1 / 163	
Goodness-of-fit on F^2	0.869	
Final R indices [I>2sigma(I)]	R1 = 0.0630, wR2 = 0.1355	

R indices (all data)	R1 = 0.1612, wR2 = 0.1654
Largest diff. peak and hole	0.172 and -0.148 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **21**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5753(10)	10171(7)	2717(4)	52(1)
C(2)	3999(10)	9372(6)	2120(4)	51(2)
C(3)	2096(10)	10164(6)	1645(4)	58(2)
C(4)	1936(10)	11703(6)	1747(4)	58(2)
C(5)	3646(10)	12463(6)	2365(4)	53(2)
C(6)	5540(9)	11760(6)	2862(4)	45(1)
C(21)	4334(11)	7709(6)	1920(5)	60(2)
C(23)	1587(10)	5932(7)	1199(5)	56(1)
C(24)	3469(12)	6077(9)	409(5)	96(2)
C(25)	5007(13)	7336(6)	775(6)	90(2)
C(61)	7401(9)	12557(6)	3579(4)	51(1)
C(63)	8382(10)	15094(7)	3977(4)	56(2)
C(64)	7894(11)	14326(6)	5018(4)	65(2)
C(65)	6453(10)	12946(6)	4691(4)	62(2)
N(22)	2088(8)	6865(5)	2011(4)	62(1)
N(62)	8005(8)	14070(5)	3196(3)	55(1)
O(23)	-139(8)	5043(5)	1133(3)	74(1)
O(63)	9095(8)	16380(4)	3846(3)	74(1)

Table 3. Bond lengths [Å] and angles [°] for **21**.

C(1)-C(2)	1.395(8)	C(21)-C(25)	1.533(8)
C(1)-C(6)	1.430(7)	C(23)-O(23)	1.243(6)
C(2)-C(3)	1.382(7)	C(23)-N(22)	1.331(7)
C(2)-C(21)	1.513(7)	C(23)-C(24)	1.477(8)
C(3)-C(4)	1.378(7)	C(24)-C(25)	1.469(8)
C(4)-C(5)	1.374(7)	C(61)-N(62)	1.473(7)
C(5)-C(6)	1.351(7)	C(61)-C(65)	1.549(8)
C(6)-C(61)	1.514(7)	C(63)-O(63)	1.224(6)
C(21)-N(22)	1.466(7)	C(63)-N(62)	1.345(6)

C(63)-C(64)	1.505(7)	O(23)-C(23)-N(22)	125.5(5)
C(64)-C(65)	1.512(7)	O(23)-C(23)-C(24)	125.4(6)
		N(22)-C(23)-C(24)	109.1(5)
C(2)-C(1)-C(6)	120.7(6)	C(25)-C(24)-C(23)	106.1(6)
C(3)-C(2)-C(1)	118.2(6)	C(24)-C(25)-C(21)	107.0(5)
C(3)-C(2)-C(21)	121.7(6)	N(62)-C(61)-C(6)	113.3(4)
C(1)-C(2)-C(21)	119.8(6)	N(62)-C(61)-C(65)	100.4(4)
C(4)-C(3)-C(2)	121.2(6)	C(6)-C(61)-C(65)	112.7(4)
C(5)-C(4)-C(3)	119.7(6)	O(63)-C(63)-N(62)	125.2(5)
C(6)-C(5)-C(4)	122.4(5)	O(63)-C(63)-C(64)	127.7(5)
C(5)-C(6)-C(1)	117.8(6)	N(62)-C(63)-C(64)	107.0(5)
C(5)-C(6)-C(61)	123.6(5)	C(63)-C(64)-C(65)	104.4(4)
C(1)-C(6)-C(61)	118.6(6)	C(64)-C(65)-C(61)	103.0(4)
N(22)-C(21)-C(2)	112.1(5)	C(23)-N(22)-C(21)	114.1(5)
N(22)-C(21)-C(25)	102.0(5)	C(63)-N(62)-C(61)	114.4(4)
C(2)-C(21)-C(25)	113.8(5)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **21**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	55(3)	55(4)	48(3)	5(3)	9(3)	-1(3)
C(2)	49(3)	54(4)	51(3)	-13(3)	7(3)	-1(3)
C(3)	58(4)	56(4)	62(4)	-6(3)	6(3)	0(3)
C(4)	59(4)	54(4)	61(4)	-8(3)	-10(3)	15(3)
C(5)	58(3)	40(3)	60(4)	0(3)	-1(3)	7(3)
C(6)	46(3)	45(3)	46(3)	3(3)	4(3)	-6(3)
C(21)	62(4)	47(4)	72(4)	2(3)	3(3)	2(3)
C(23)	67(4)	48(3)	53(3)	12(3)	-2(3)	-7(3)
C(24)	96(5)	122(6)	74(4)	-18(5)	25(4)	-37(5)
C(25)	109(6)	57(4)	107(6)	-27(4)	58(5)	-12(4)
C(61)	51(3)	48(3)	53(3)	-3(3)	5(3)	-10(3)
C(63)	61(4)	56(4)	52(4)	-2(3)	-2(3)	-11(3)
C(64)	82(4)	54(4)	61(4)	-7(3)	9(3)	-3(3)
C(65)	69(4)	58(4)	59(4)	4(3)	7(3)	-9(3)
N(22)	75(3)	56(3)	56(3)	-16(3)	12(3)	-17(3)

N(62)	70(3)	47(3)	48(3)	-2(2)	1(2)	-14(2)
O(23)	86(3)	69(3)	65(3)	-5(2)	-6(2)	-23(3)
O(63)	98(3)	56(3)	68(3)	-2(2)	17(2)	-25(2)

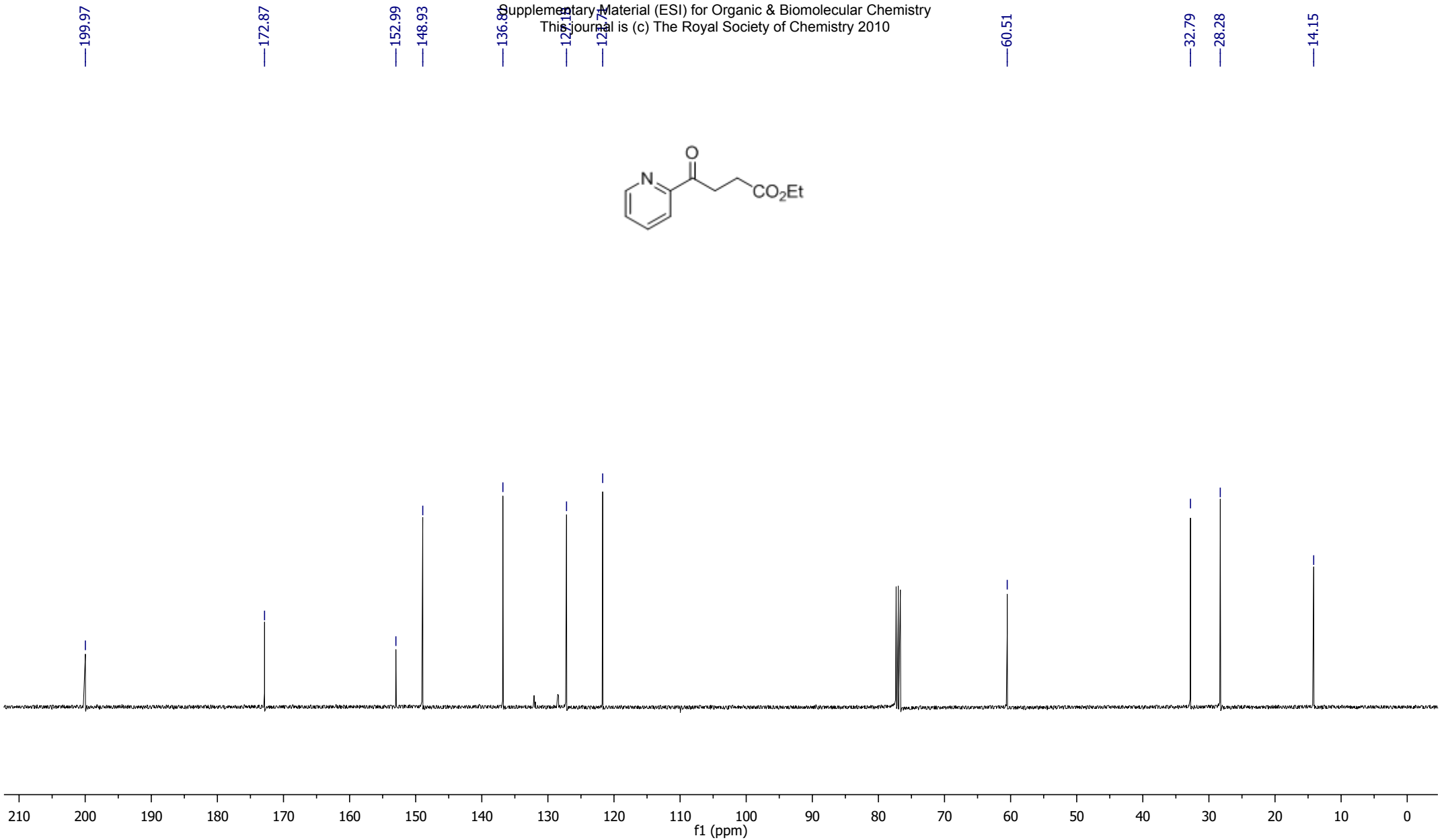
Table 5. Hydrogen bonds for **21** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(22)-H(22)...O(63)#1	0.86	2.11	2.928(6)	159.7
N(62)-H(62)...O(23)#2	0.86	2.15	2.952(6)	155.6

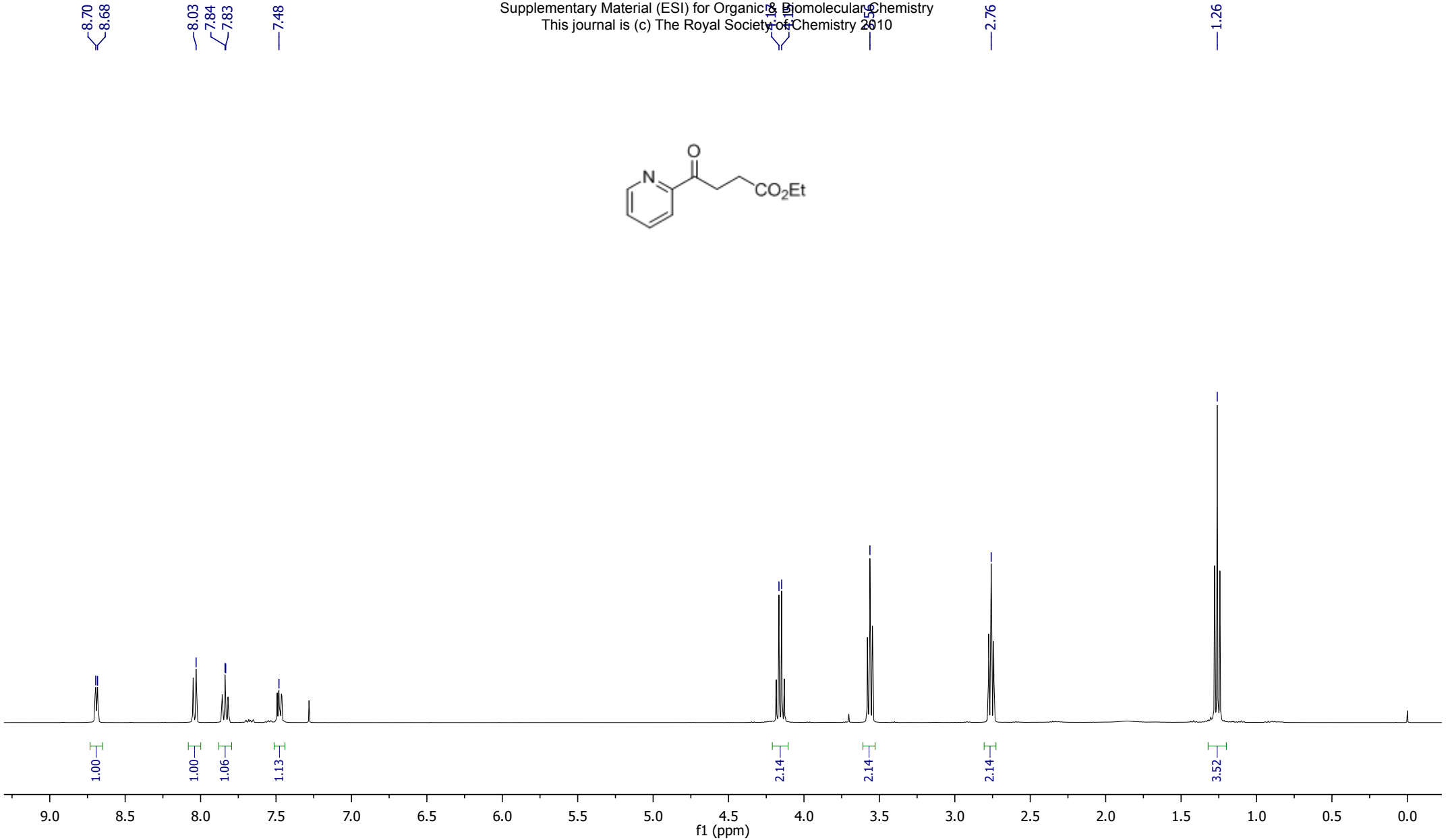
Symmetry transformations used to generate equivalent atoms:

#1 x-1,y-1,z #2 x+1,y+1,z

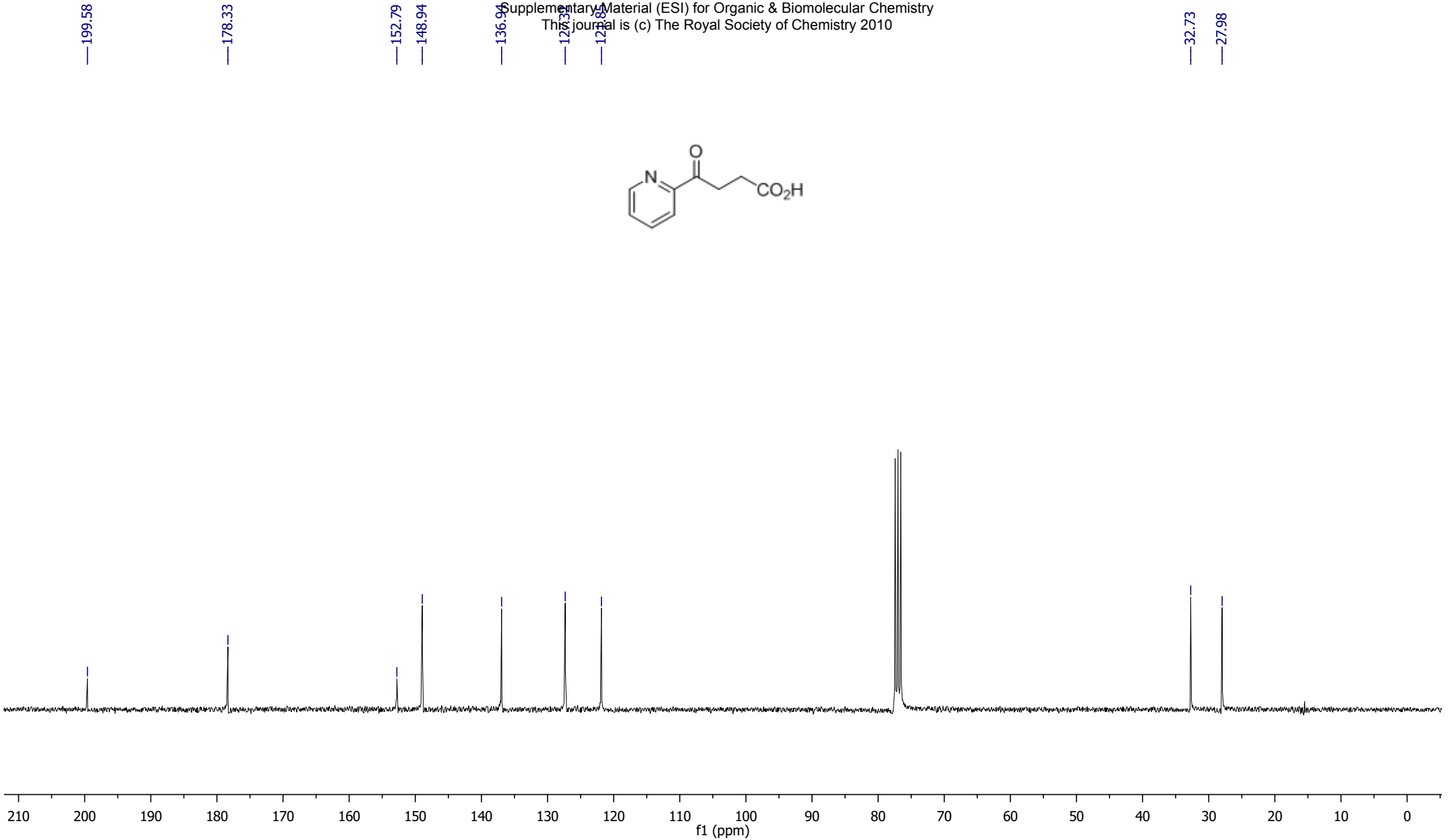
6. ^{13}C NMR and ^{1}H NMR spectra for compounds 1-7 and 9-22



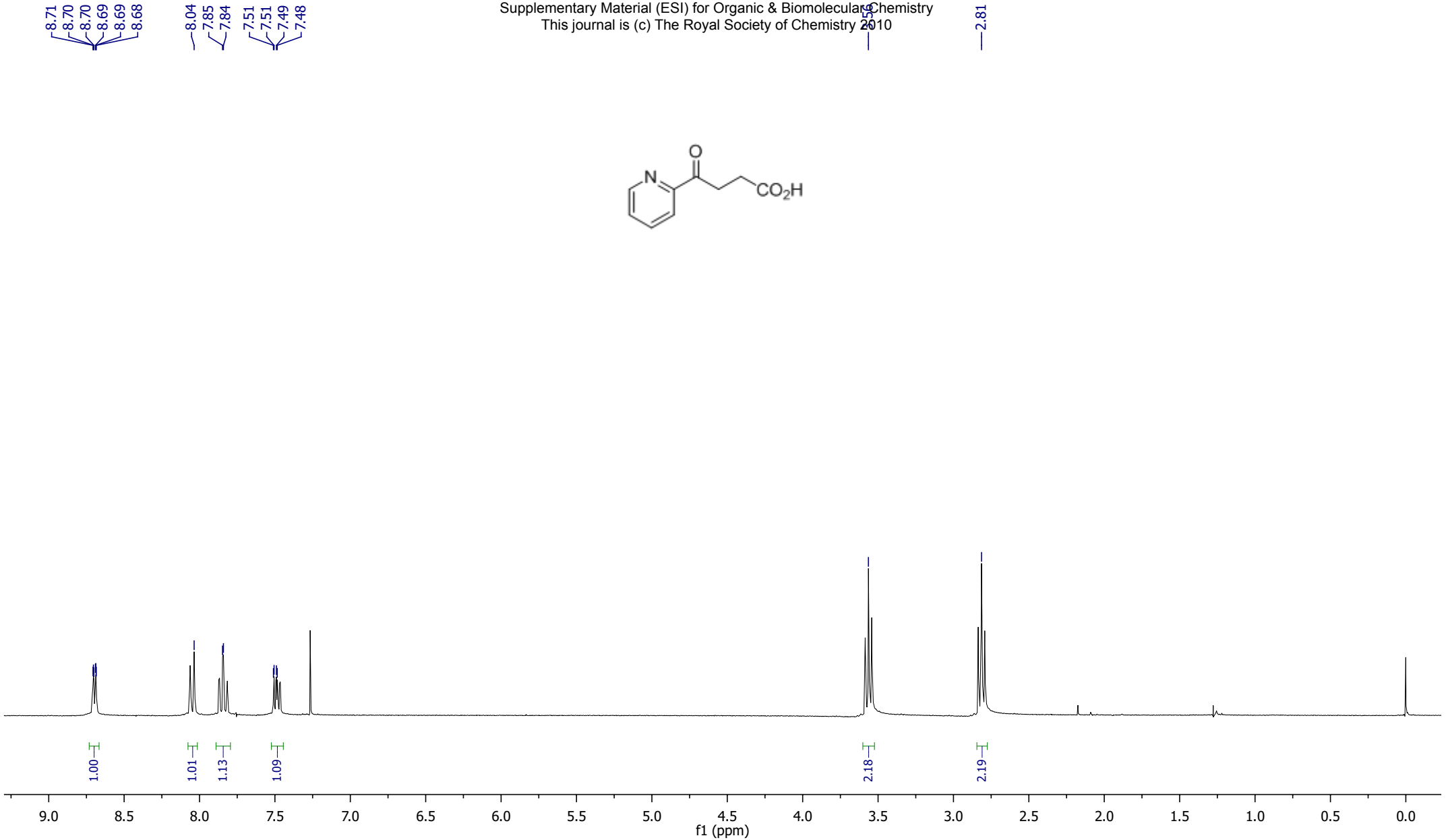
Ethyl *γ*-oxo-2-pyridinebutanoate (1a)



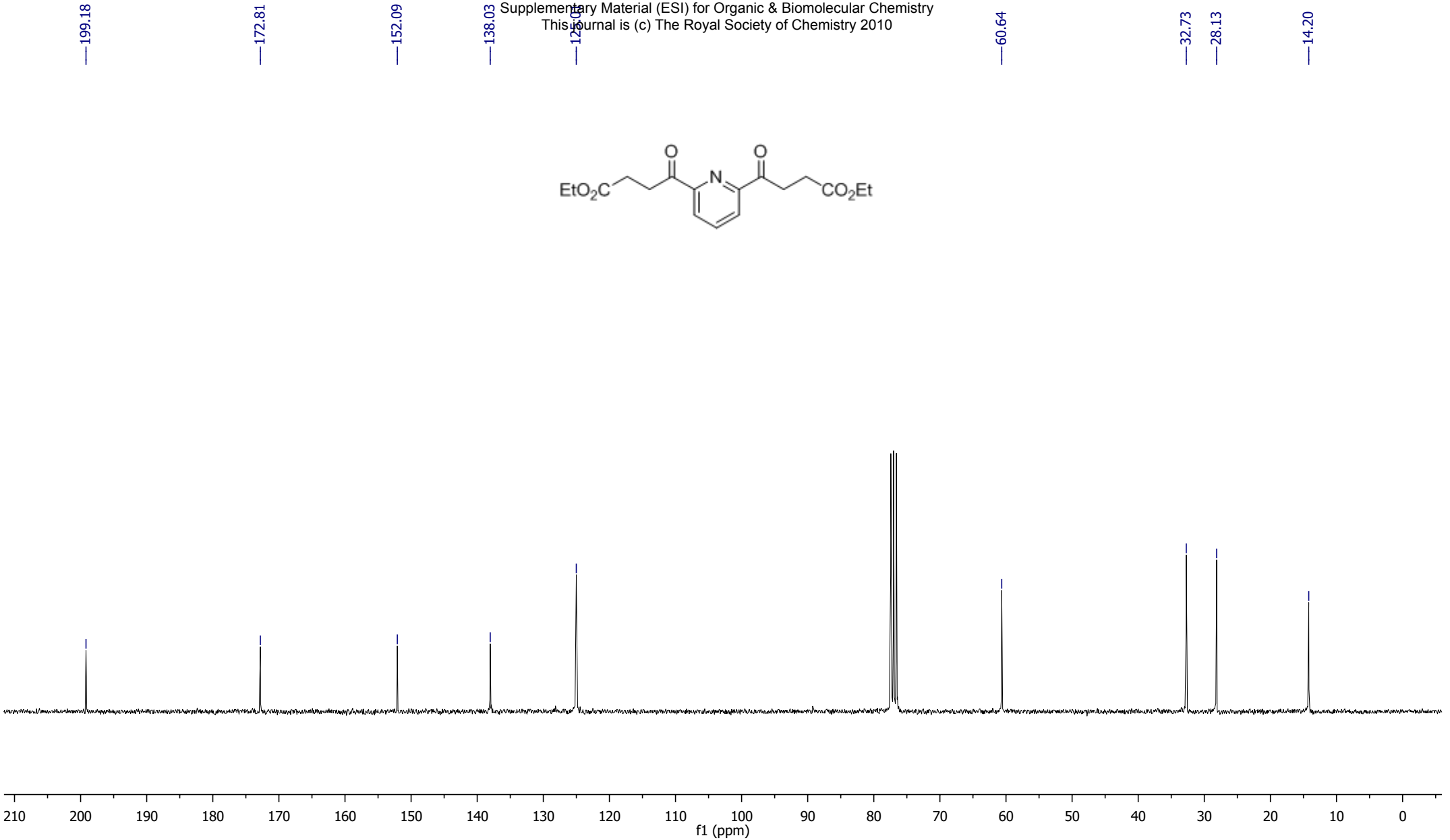
Ethyl *γ*-oxo-2-pyridinebutanoate (1a)



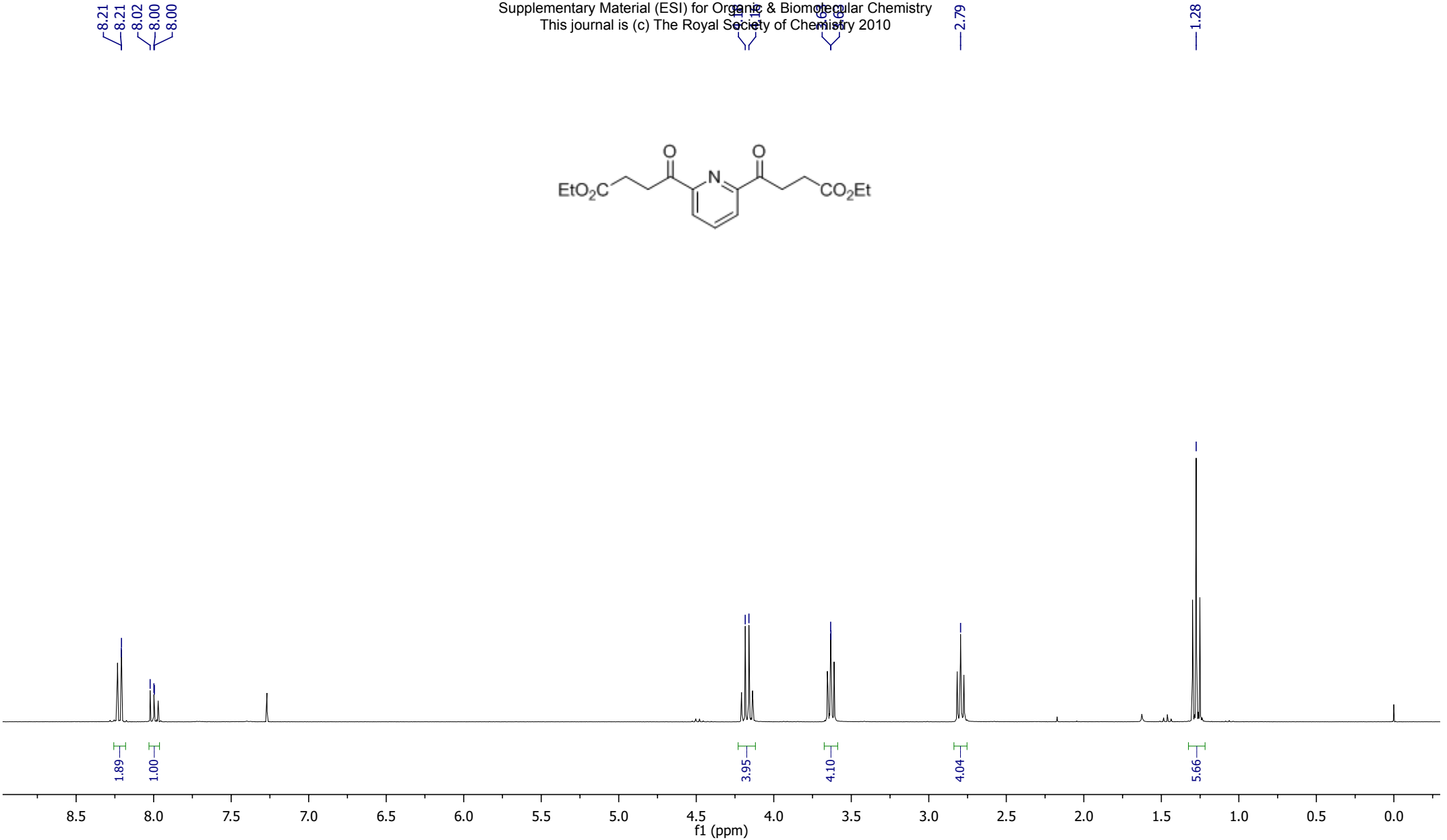
γ-Oxo-2-pyridinebutanoic acid (1b)



γ-Oxo-2-pyridinebutanoic acid (1b)



Diethyl *γ*,*γ*′-dioxo-2,6-pyridinedibutanoate (2a)



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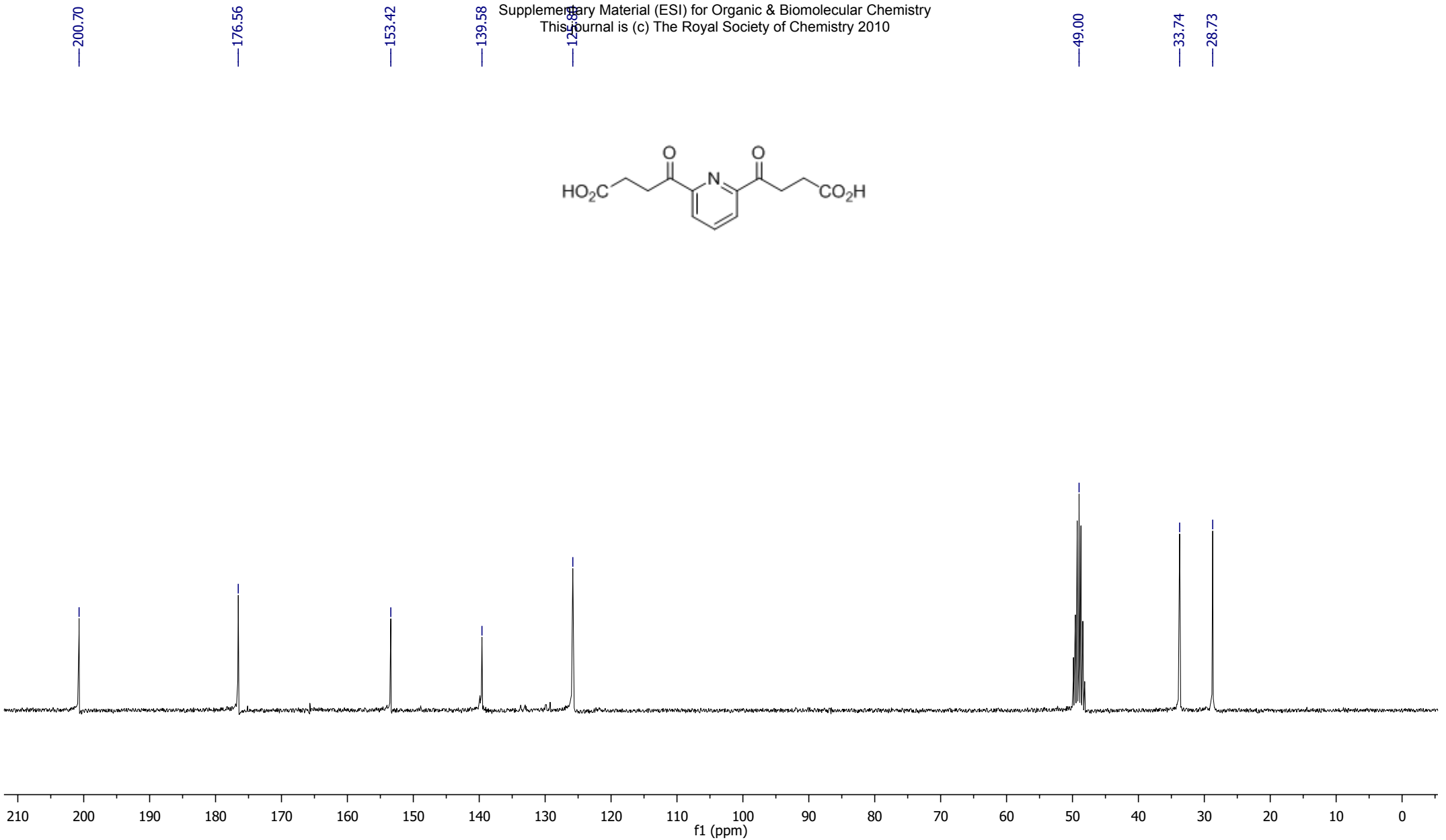
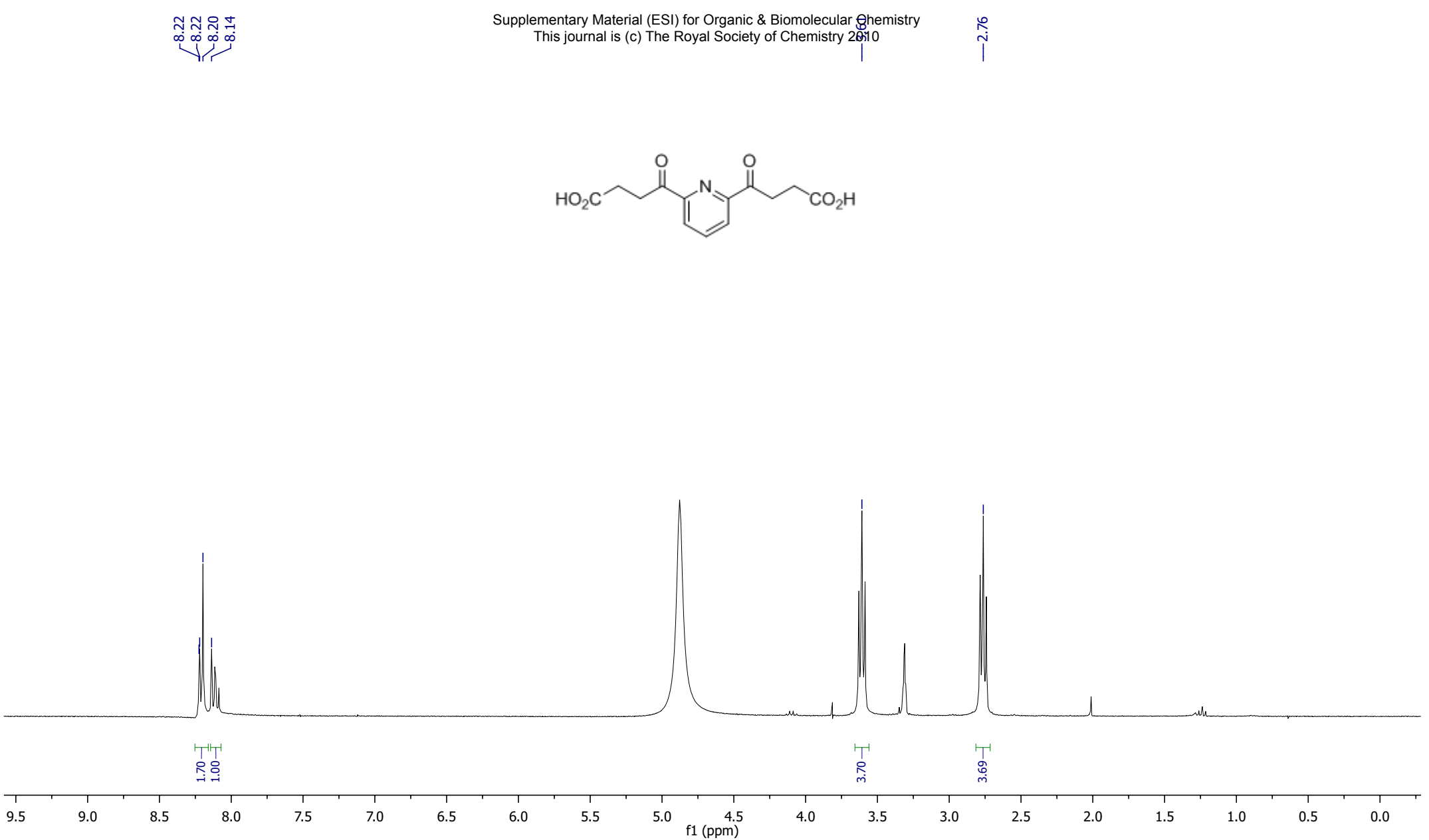
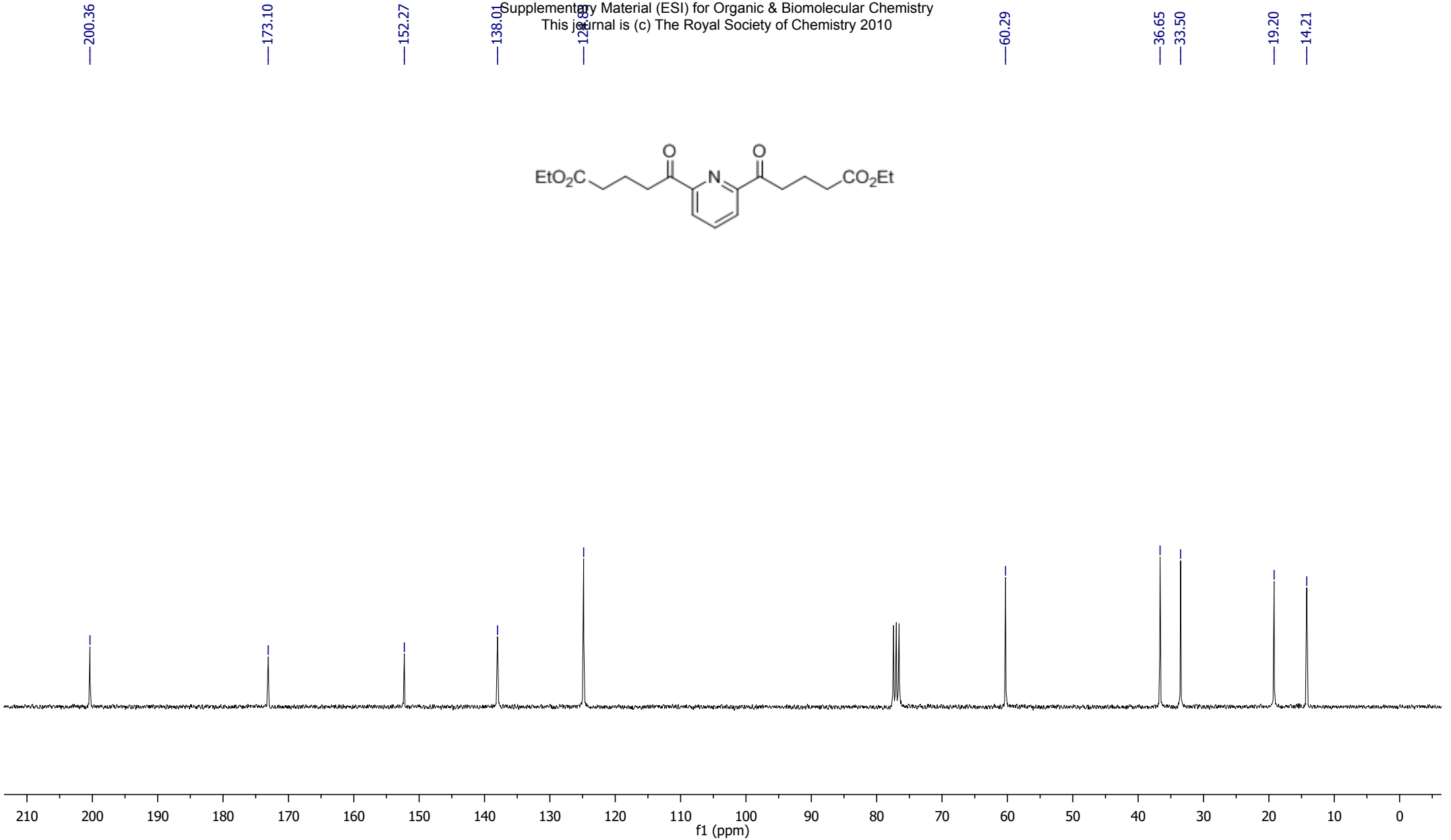


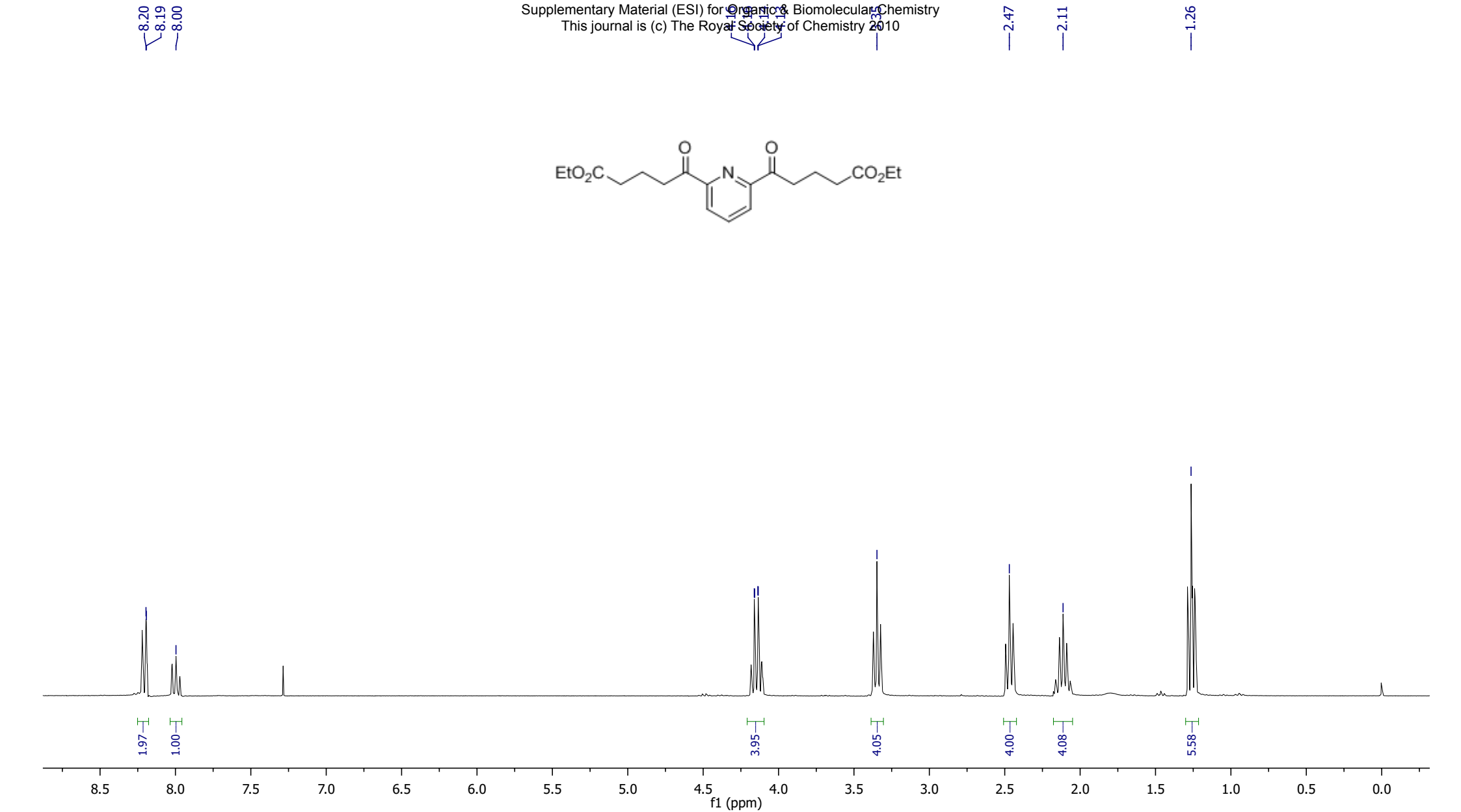
γ,γ′-Dioxo-2,6-pyridinedibutanoic acid (2b)



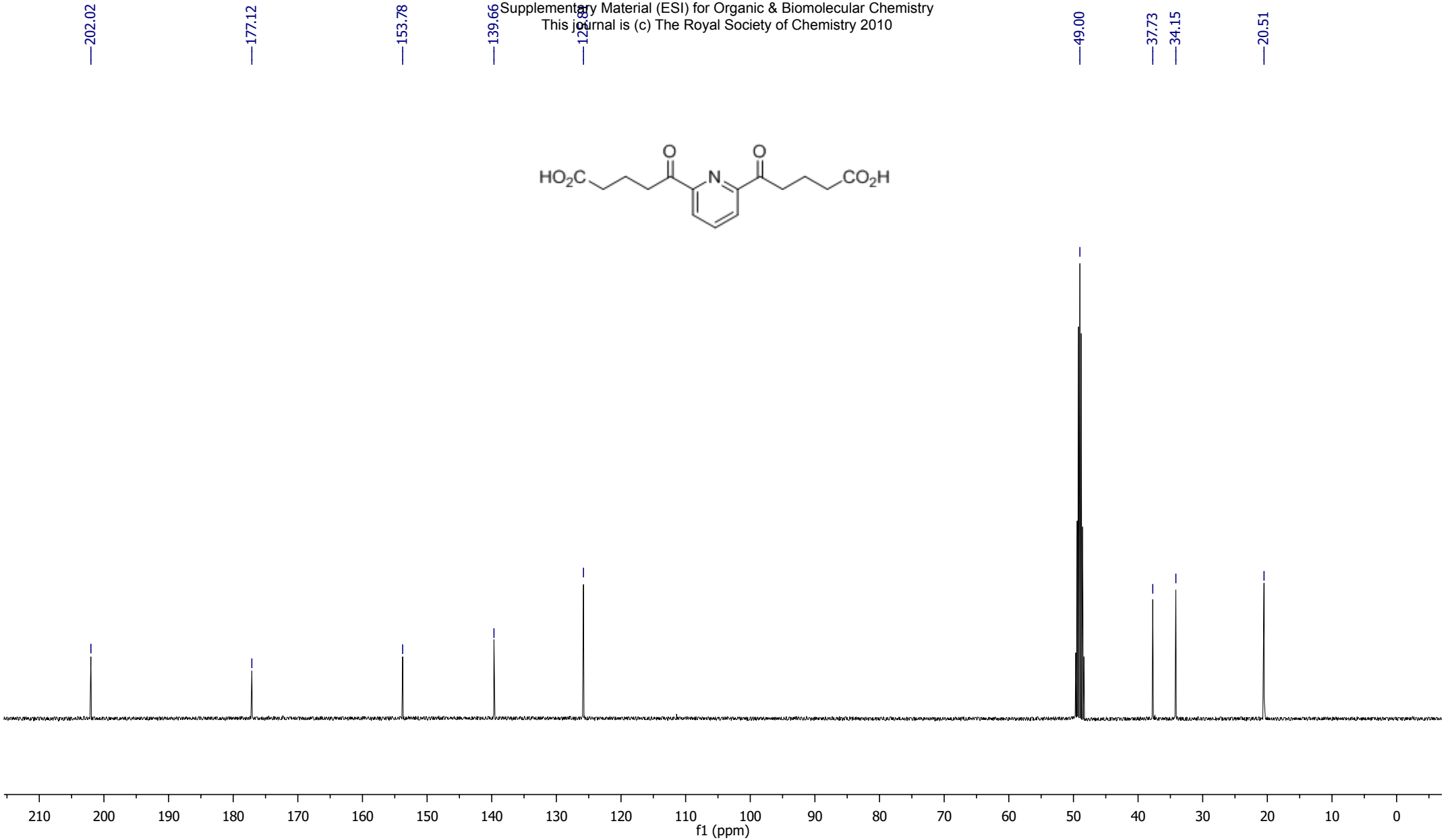
γ,γ′-Dioxo-2,6-pyridinedibutanoic acid (2b)



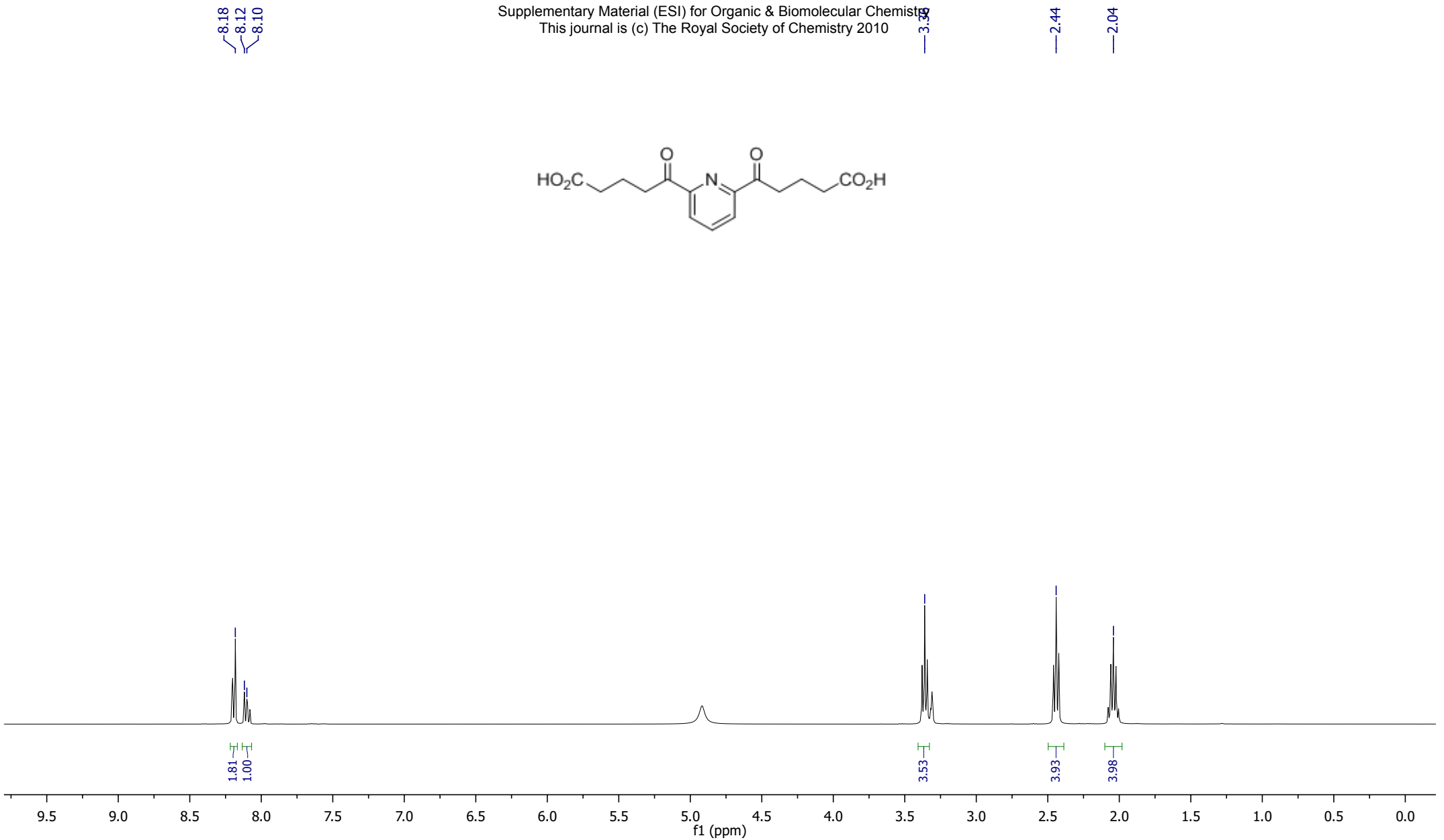
Diethyl *δ*,*δ*′-dioxo-2,6-pyridinedipentanoate (3a)



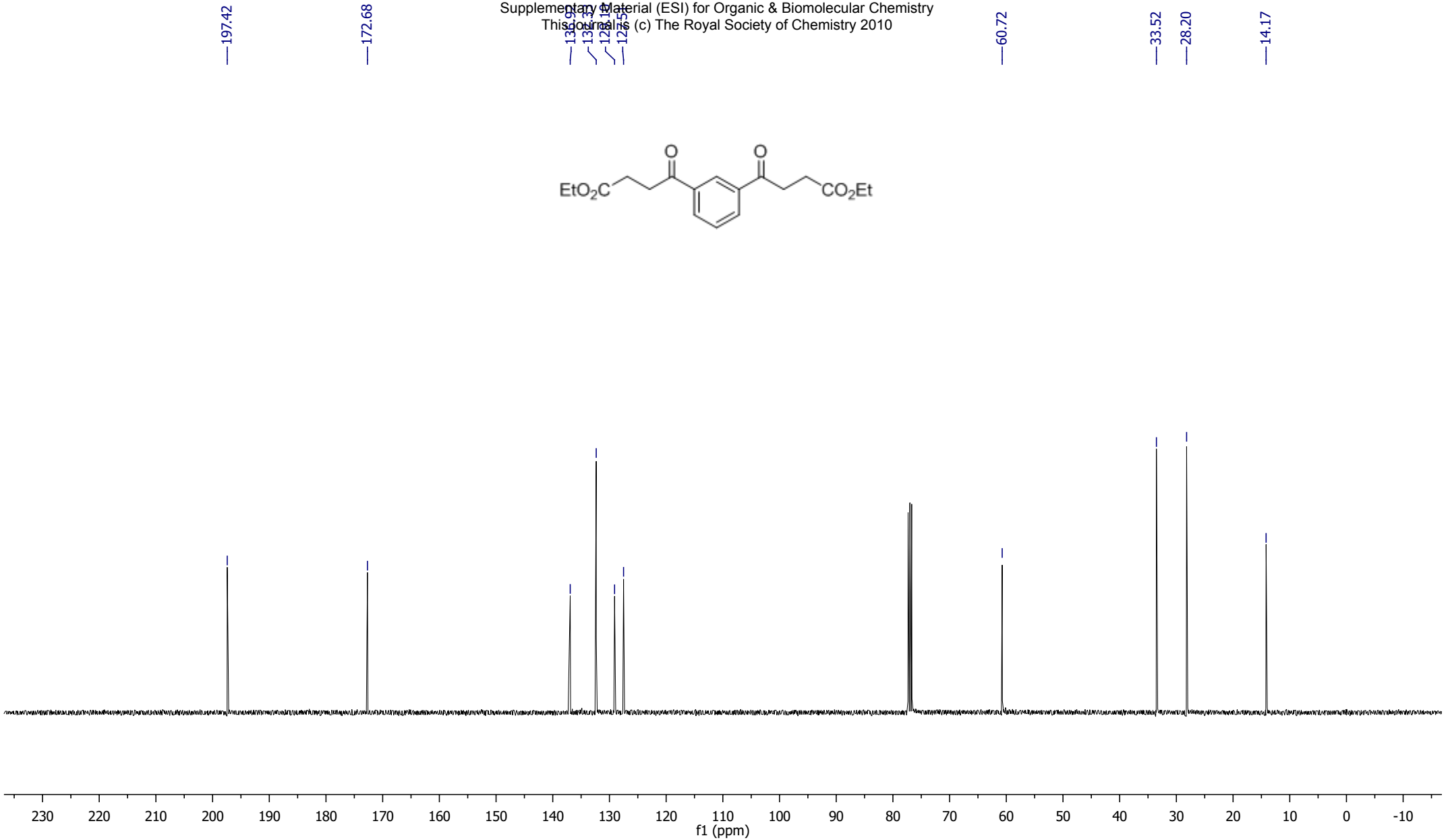
Diethyl *δ*,*δ*′-dioxo-2,6-pyridinedipentanoate (3a)



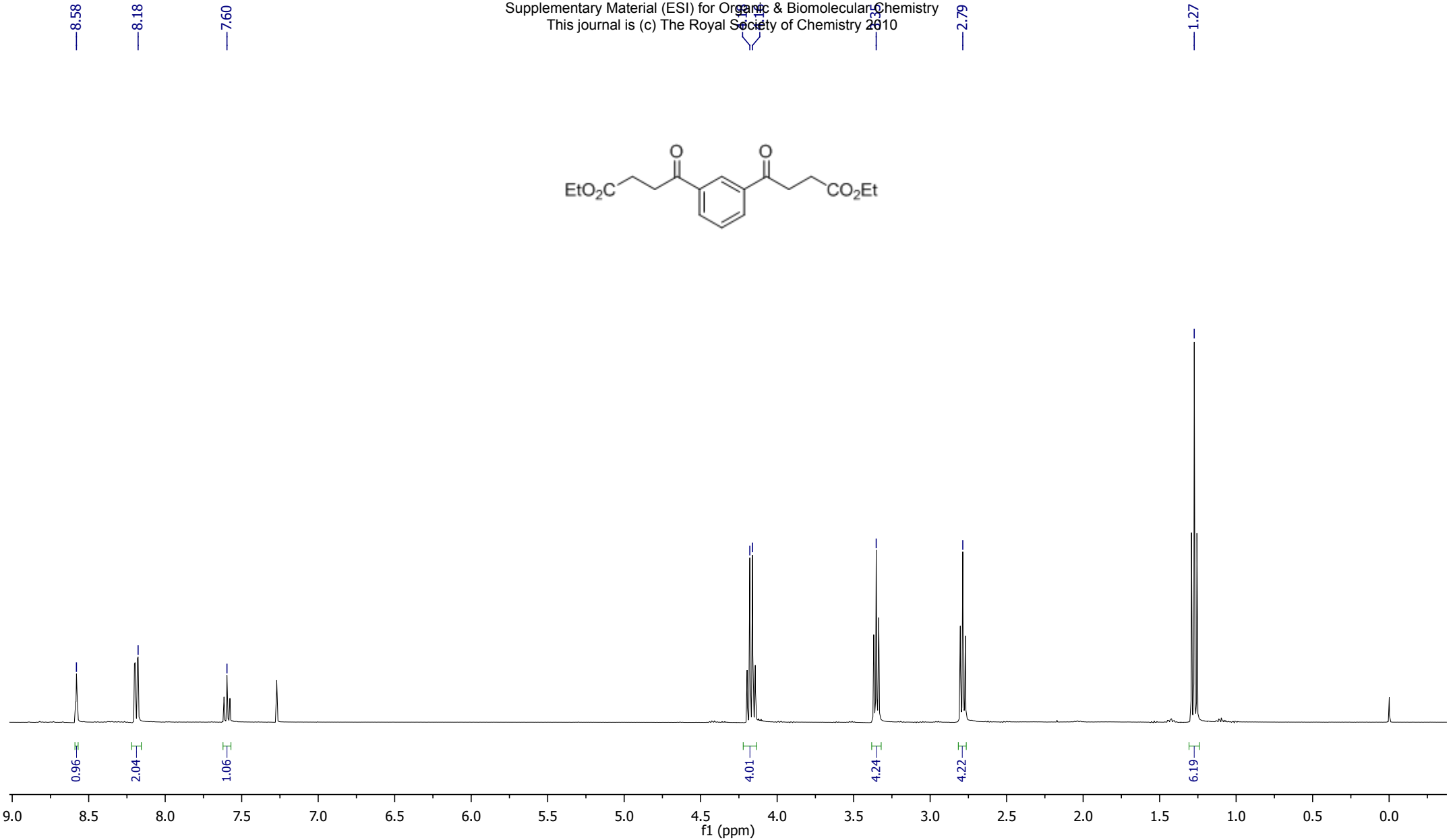
δ,δ'-Dioxo-2,6-pyridinedipentanoic acid (3b)



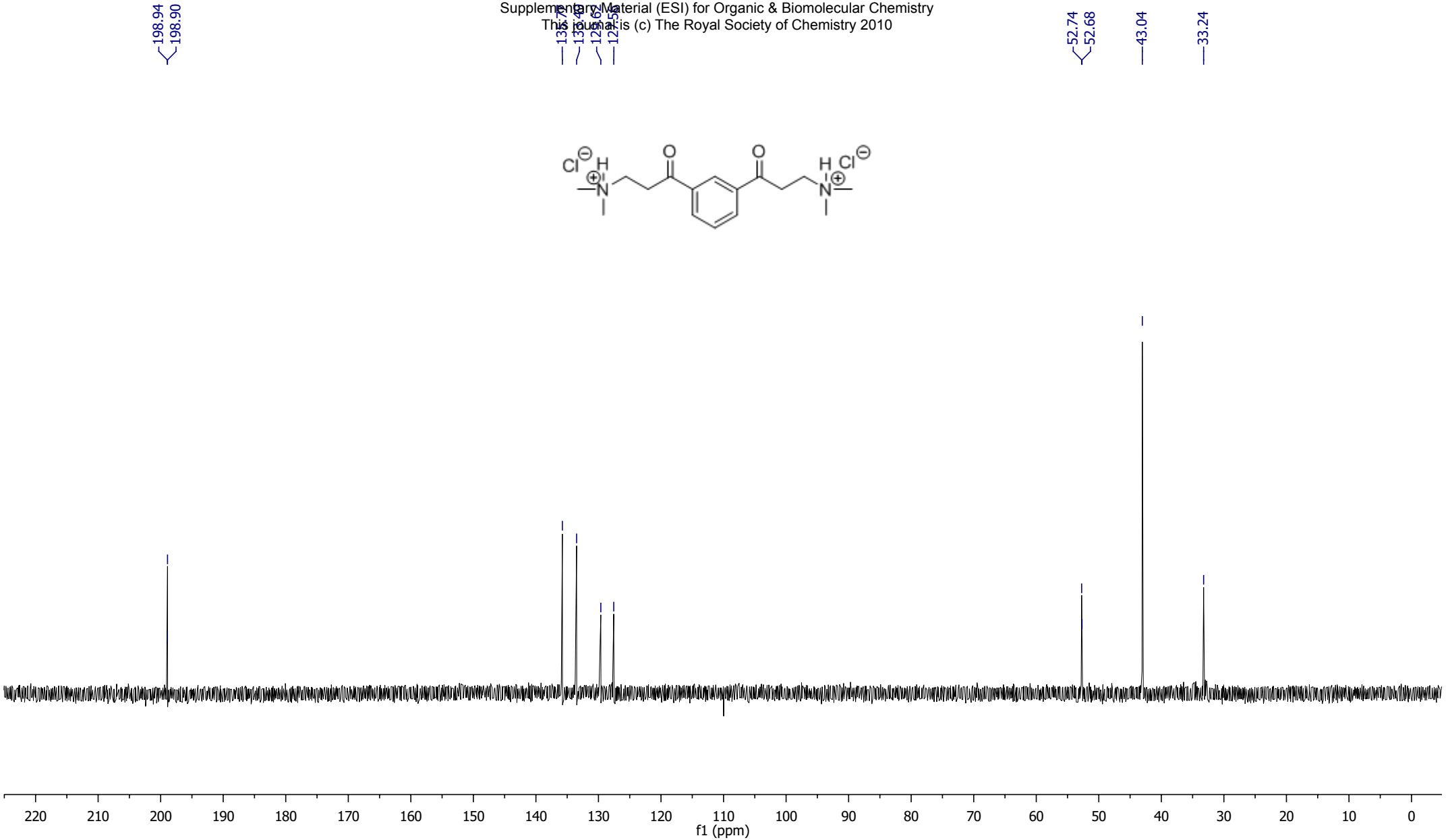
δ,δ'-Dioxo-2,6-pyridinedipentanoic acid (3b)



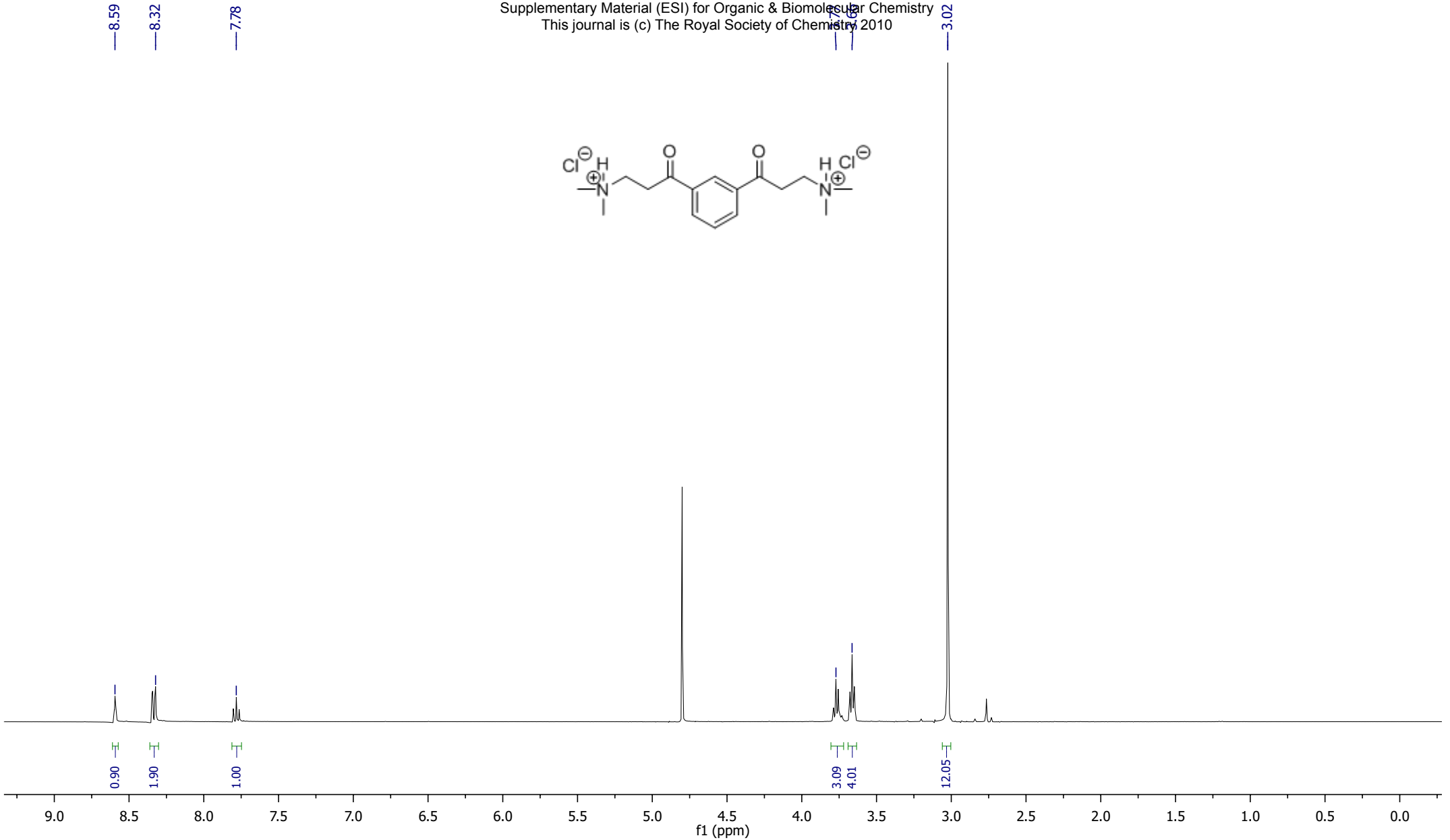
Diethyl *δ,δ'*-dioxo-1,3-benzenedibutanoate (4a)



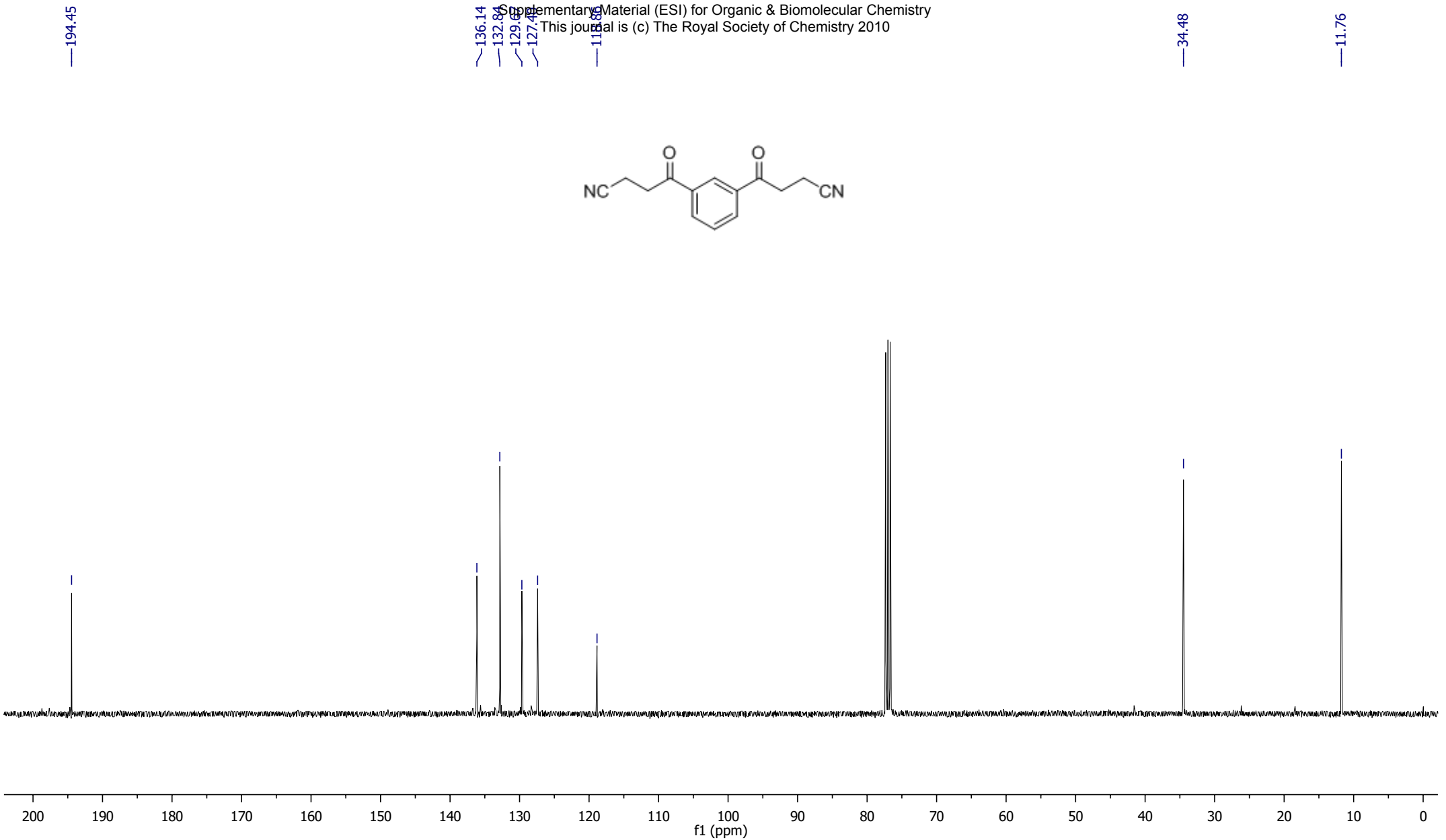
Diethyl δ,δ'-dioxo-1,3-benzenedibutanoate (4a)



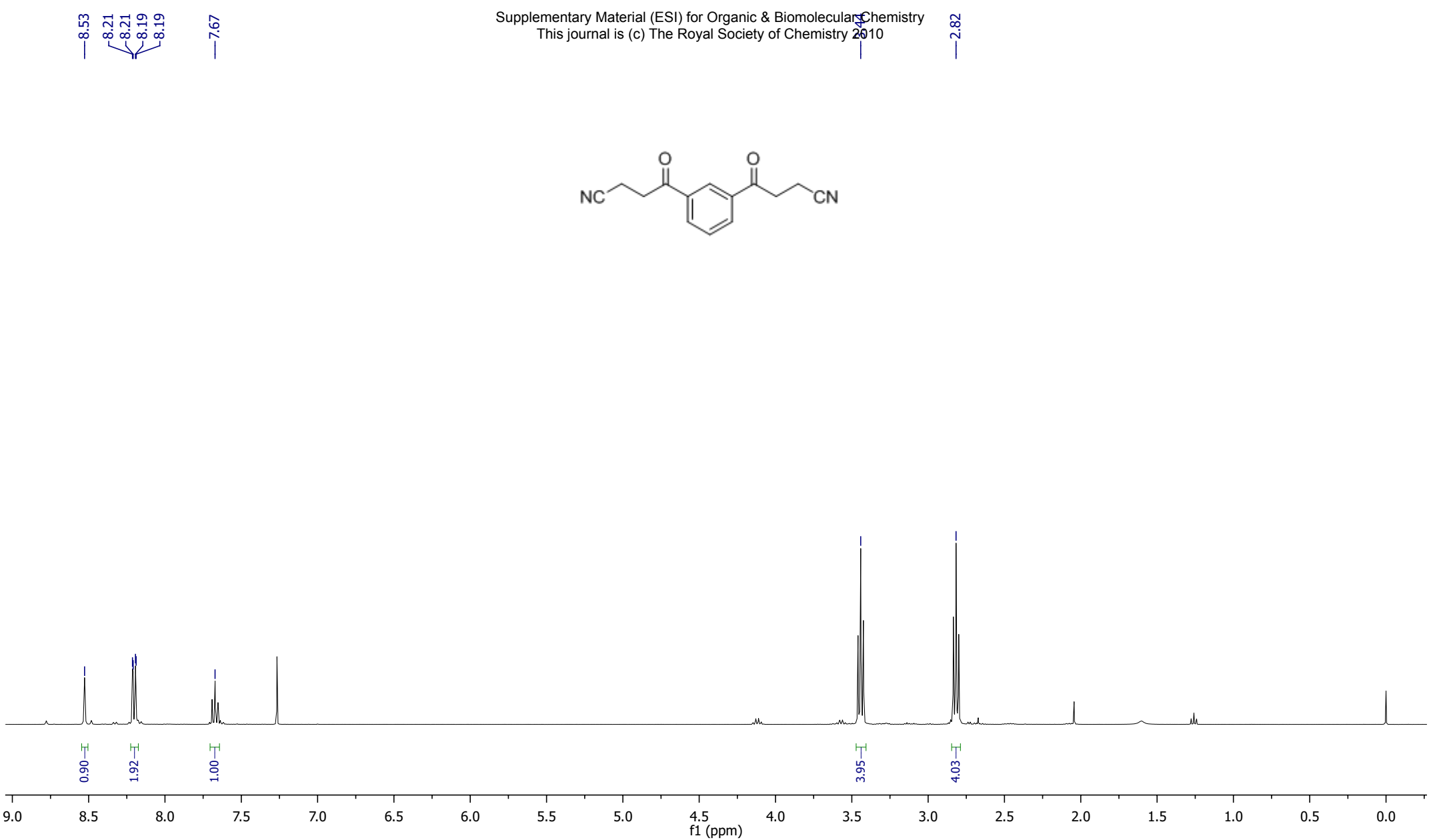
1,3-Bis[1-oxo-3-(dimethylamino)propyl]benzene dihydrochloride (5)



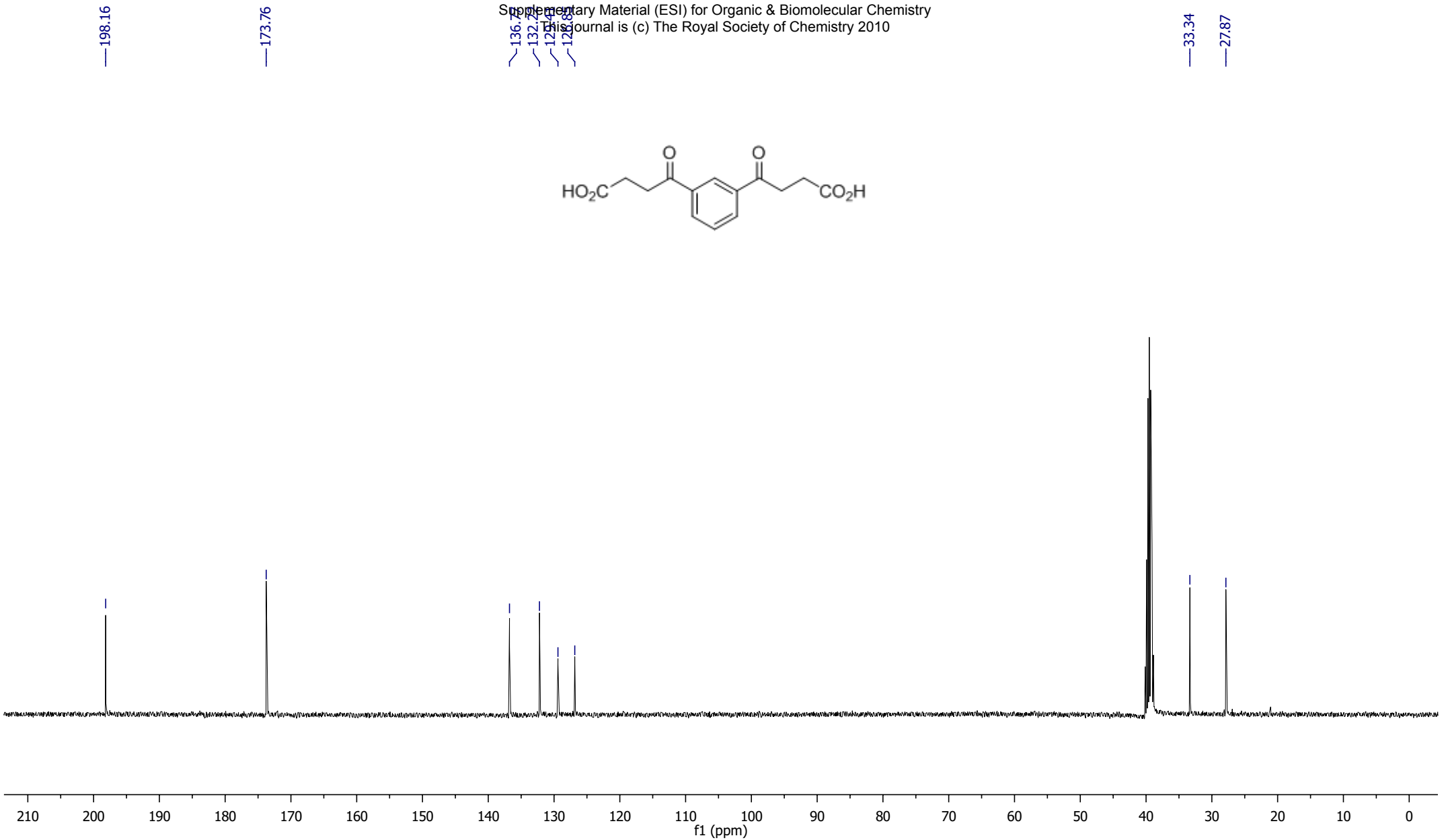
1,3-Bis[1-oxo-3-(dimethylamino)propyl]benzene dihydrochloride (5)



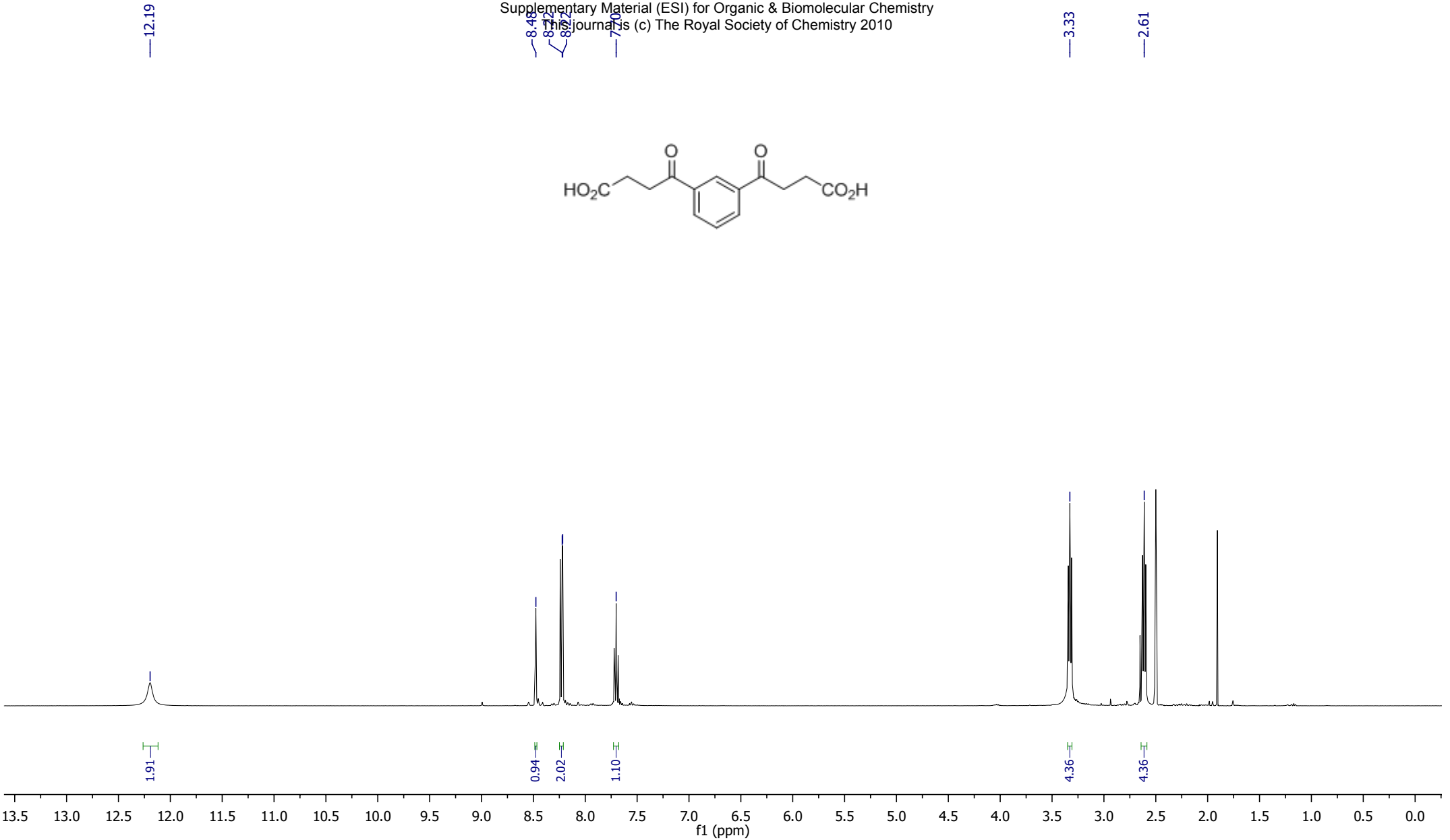
γ,γ′-Dioxo-1,3-benzenedibutanenitrile (6)



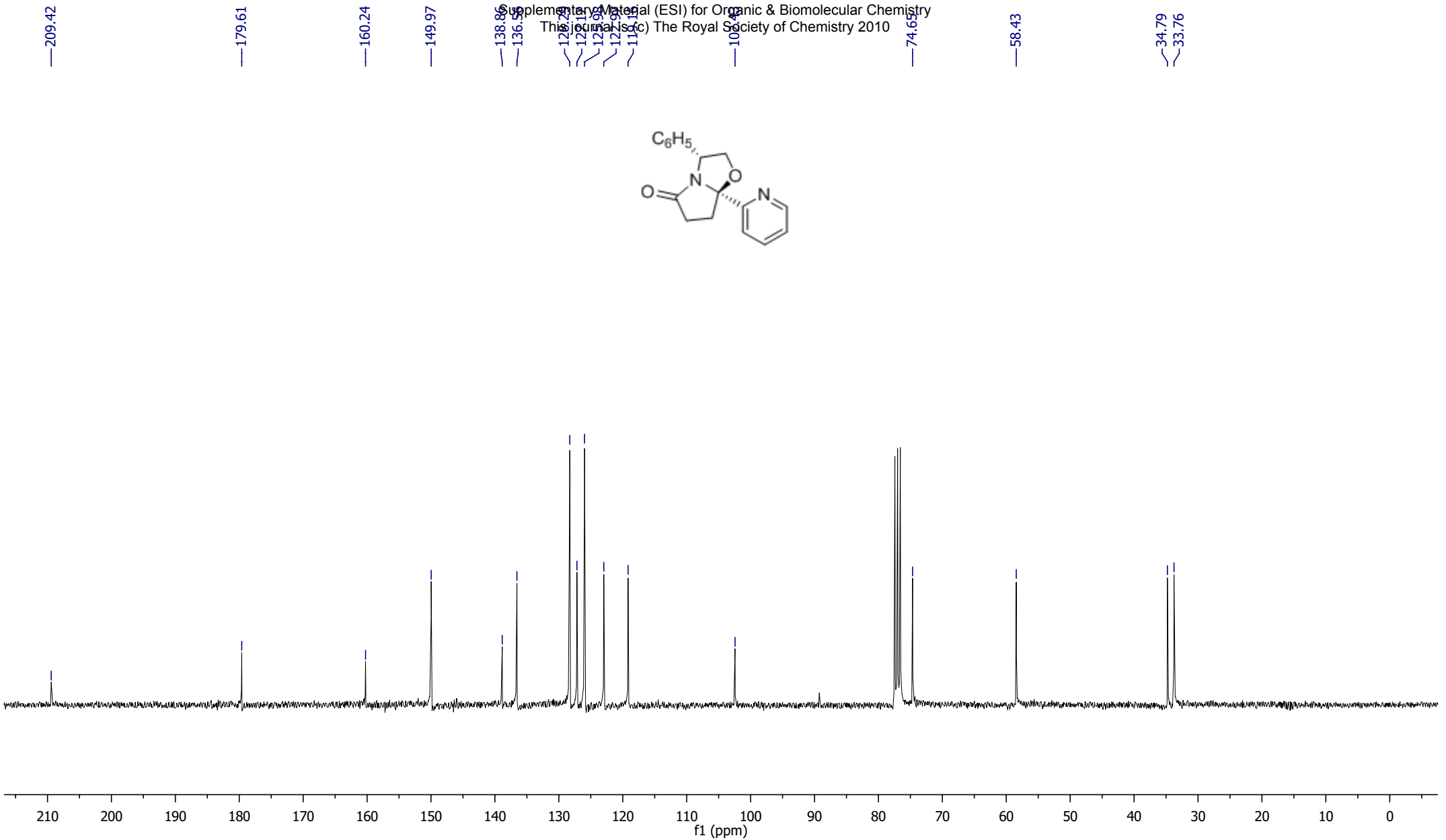
γ,γ'-Dioxo-1,3-benzenedibutanenitrile (6)



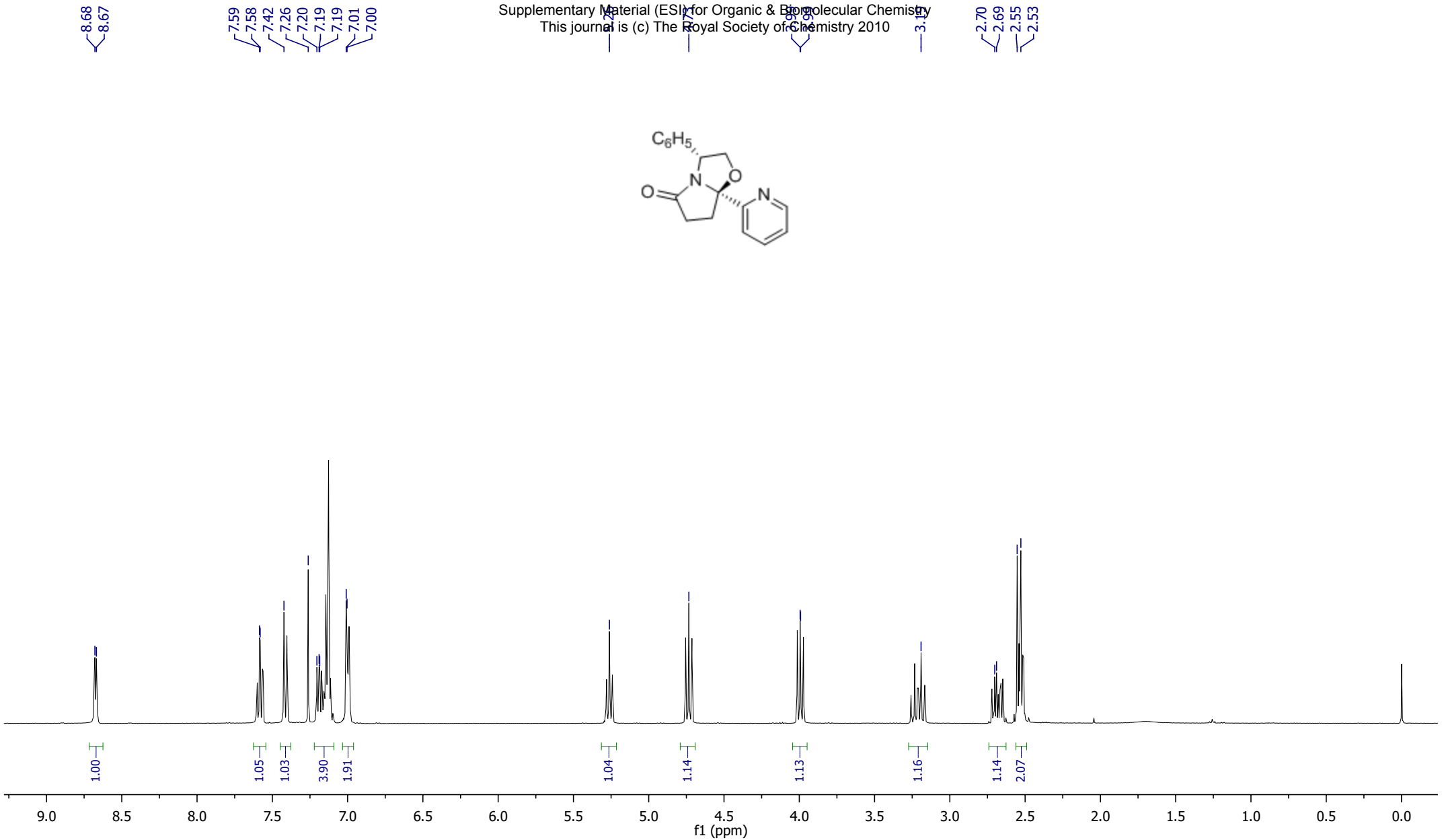
γ,γ′-Dioxo-1,3-benzenedibutanoic acid (4b)



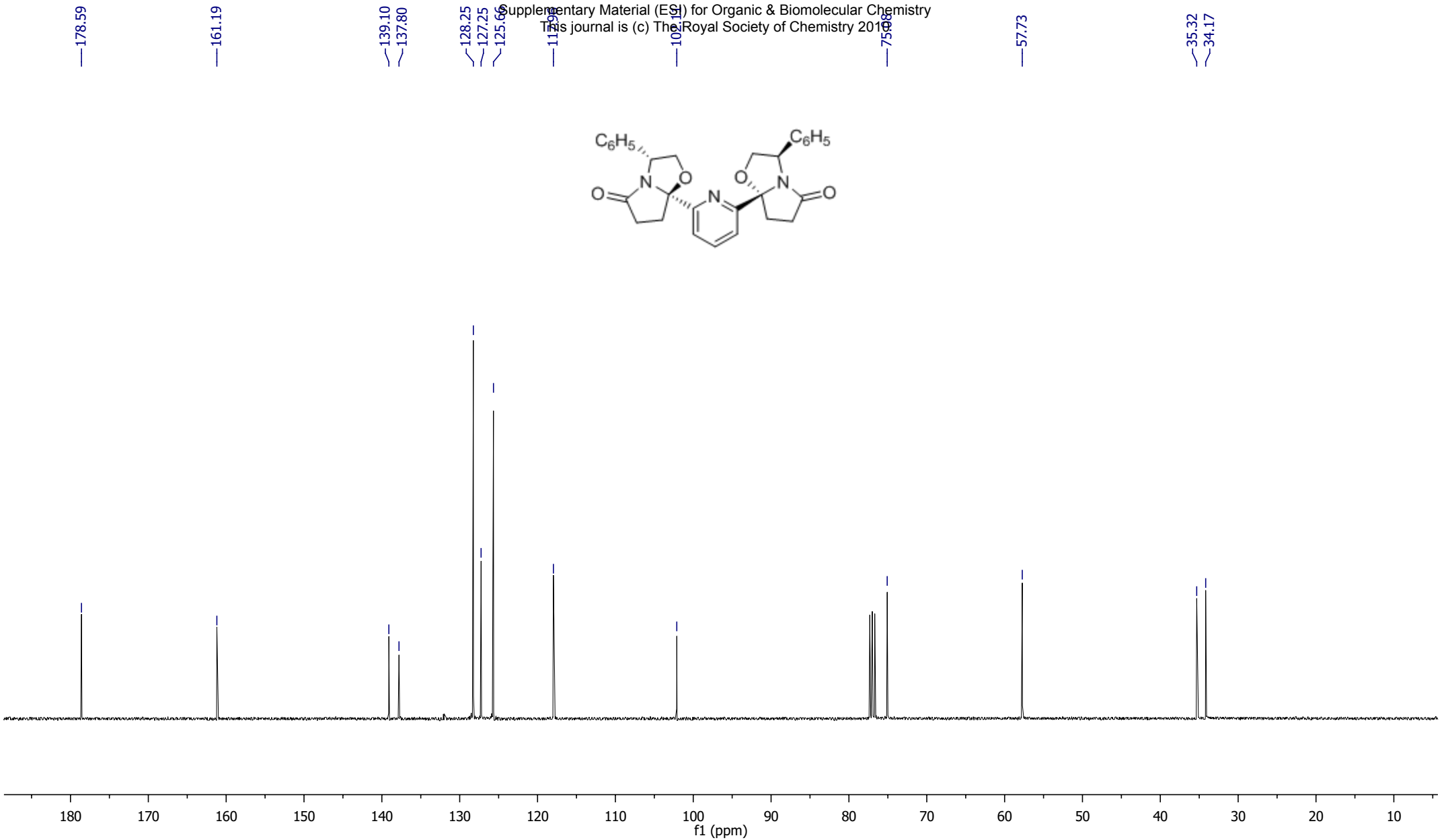
γ,γ′-Dioxo-1,3-benzenedibutanoic acid (4b)



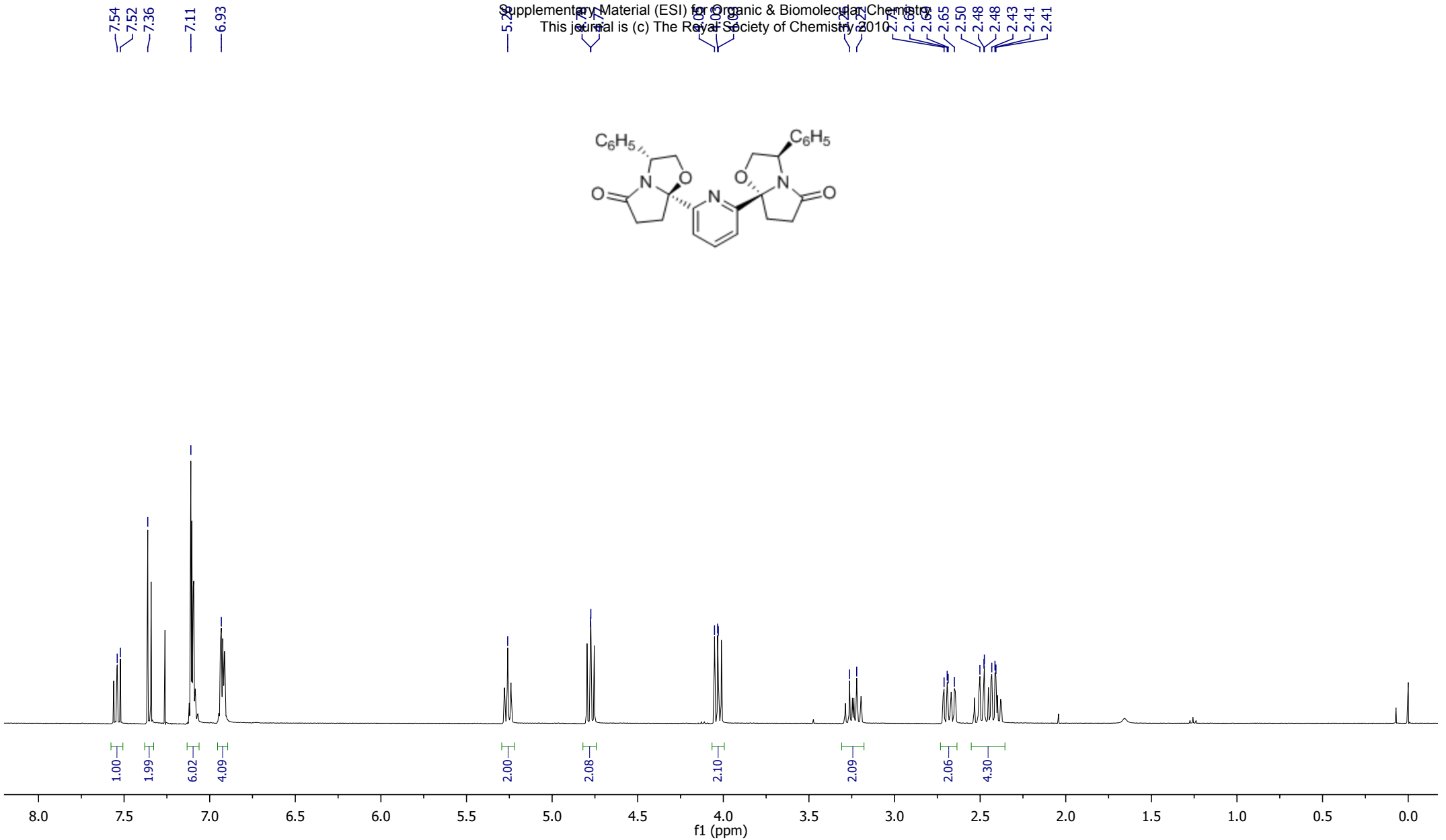
(3*R*,7a*R*)-5-Oxo-3-phenyl-7a-(2-pyridyl)-2,3,5,7,7a-hexahydropyrrolo[2,1-*b*]oxazole (7)



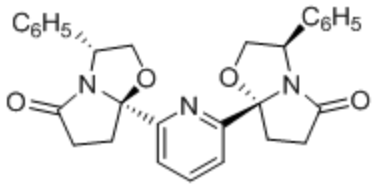
(3*R*,7a*R*)-5-Oxo-3-phenyl-7a-(2-pyridyl)-2,3,5,7,7a-hexahydropyrrolo[2,1-*b*]oxazole (7)



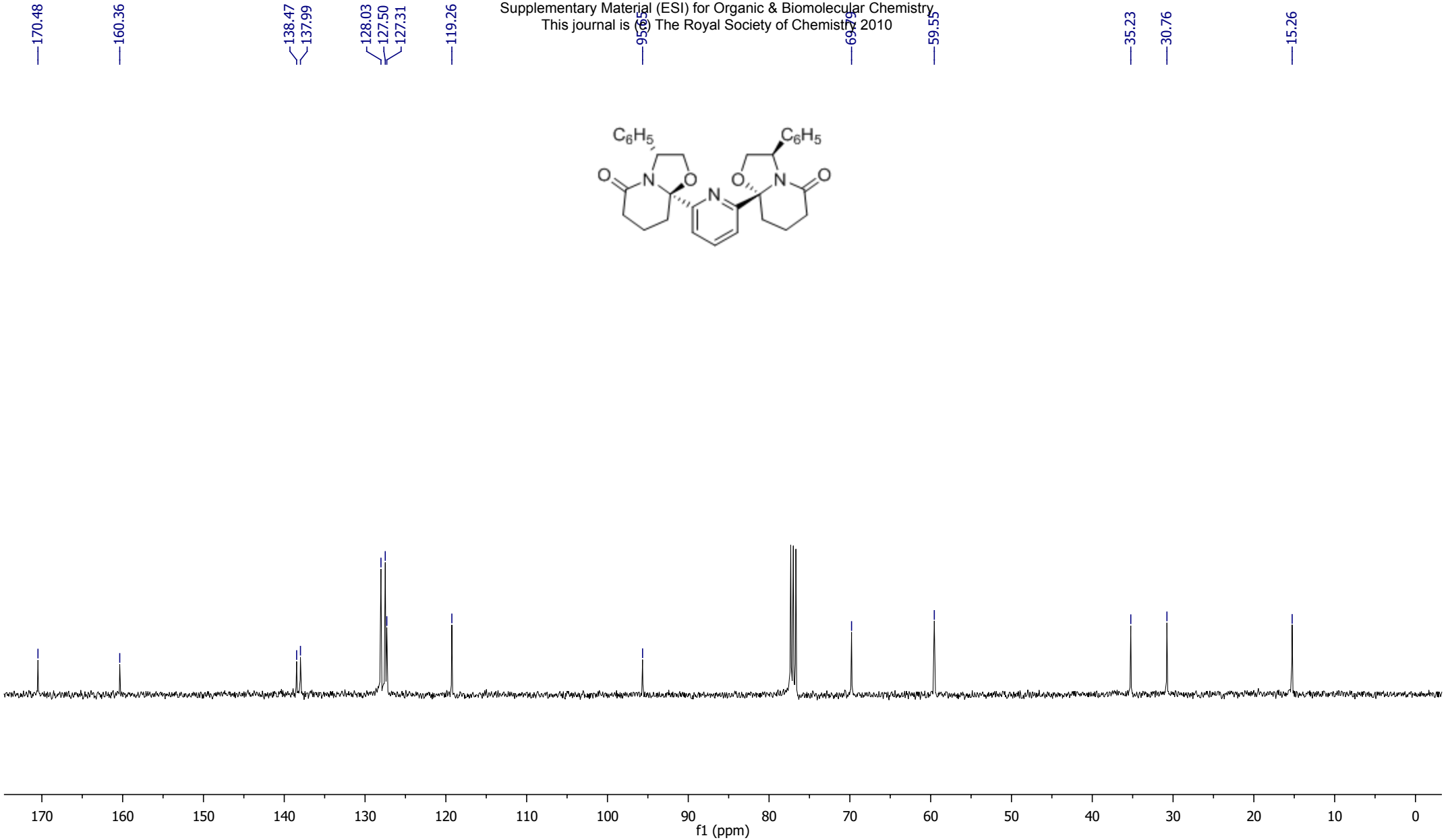
(3*R*,3'*R*,7a*R*,7a'*R*)-2,6-Bis(5-oxo-3-phenyl-2,3,5,6,7,7a-hexahydropyrrolo[2,1-*b*]oxazol-7a-yl)pyridine (9)



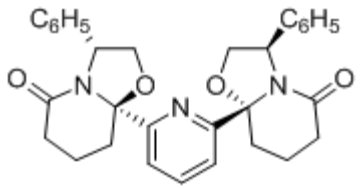
(3*R*,3'*R*,7a*R*,7a'*R*)-2,6-Bis(5-oxo-3-phenyl-2,3,5,6,7,7a-hexahydropyrrolo[2,1-*b*]oxazol-7a-yl)pyridine (9)



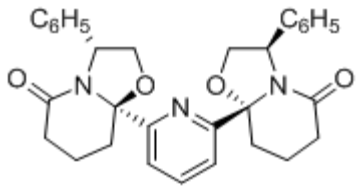
(3*R*,3'*R*,7a*R*,7a'*R*)-2,6-Bis(5-oxo-3-phenyl-2,3,5,6,7,7a-hexahydropyrrolo[2,1-*b*]oxazol-7a-yl)pyridine (9)



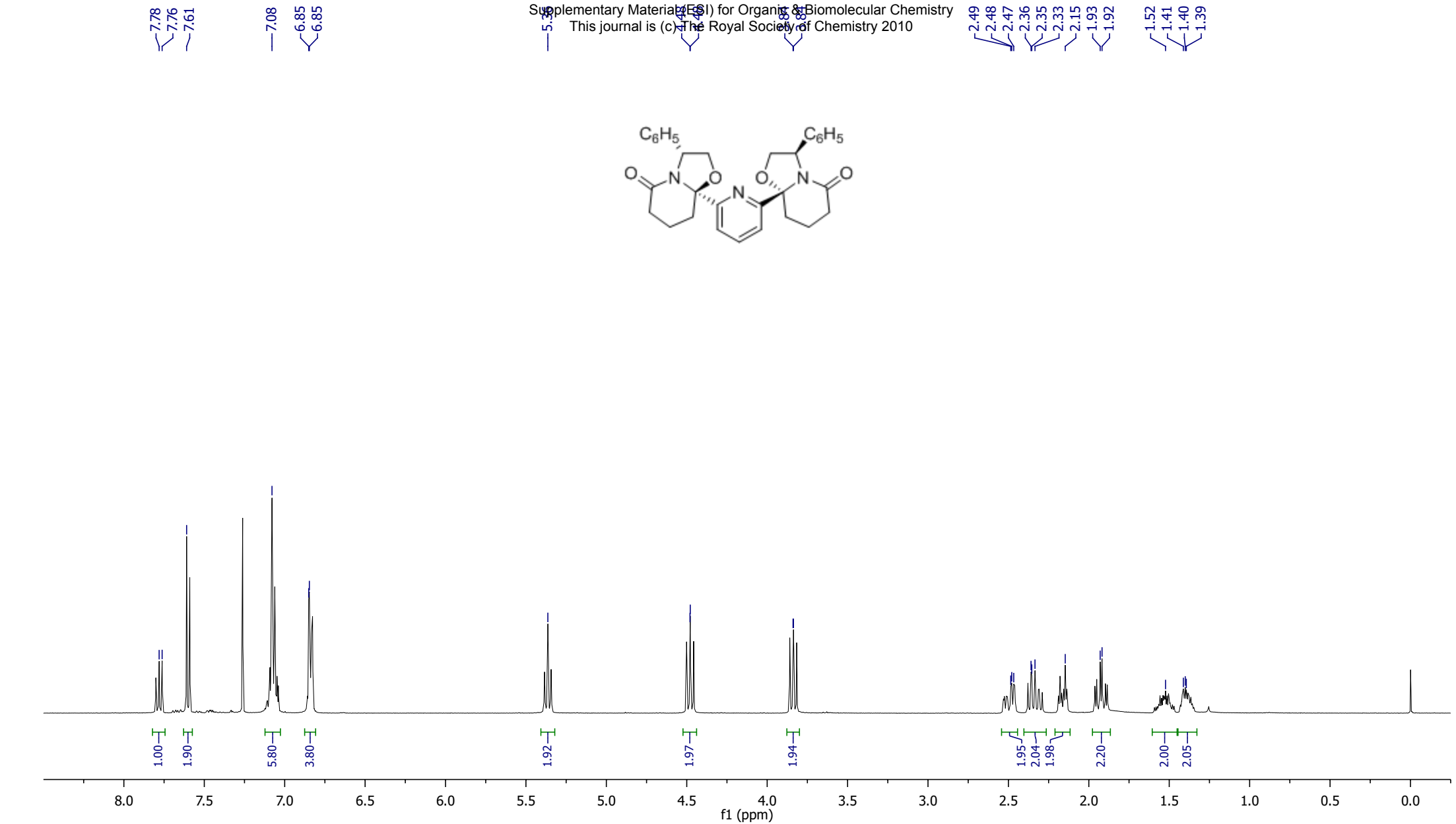
(3*R*,3'*R*,8a*R*,8a'*R*)-2,6-Bis(5-oxo-3-phenyl-2,3,6,7,8,8a-hexahydro-5*H*-oxazolo[3,2-*a*]pyrid-8a-yl)pyridine (10)



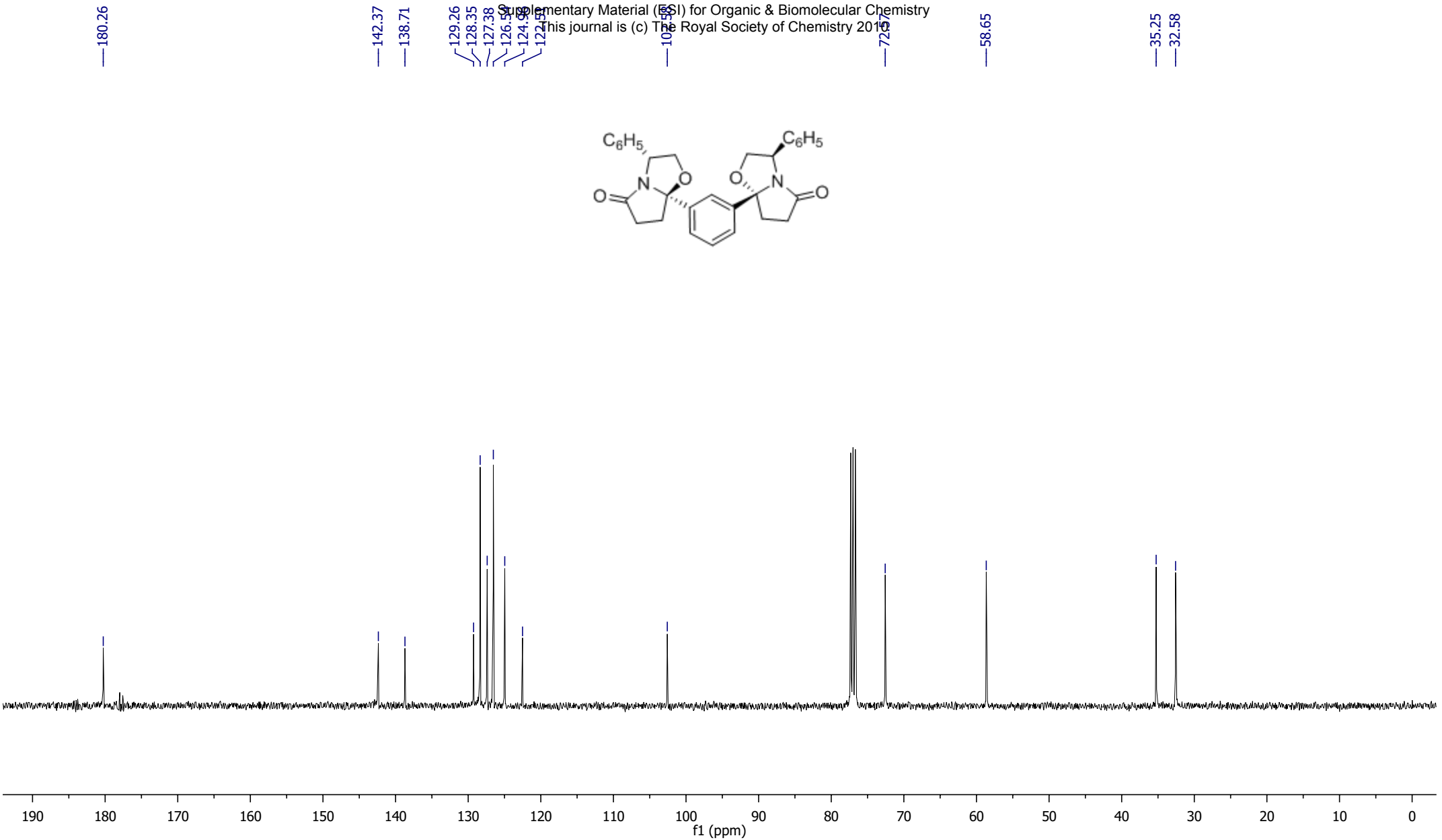
(3*R*,3'*R*,8a*R*,8a'*R*)-2,6-Bis(5-oxo-3-phenyl-2,3,6,7,8,8a-hexahydro-5*H*-oxazolo[3,2-*a*]pyrid-8a-yl)pyridine (10)



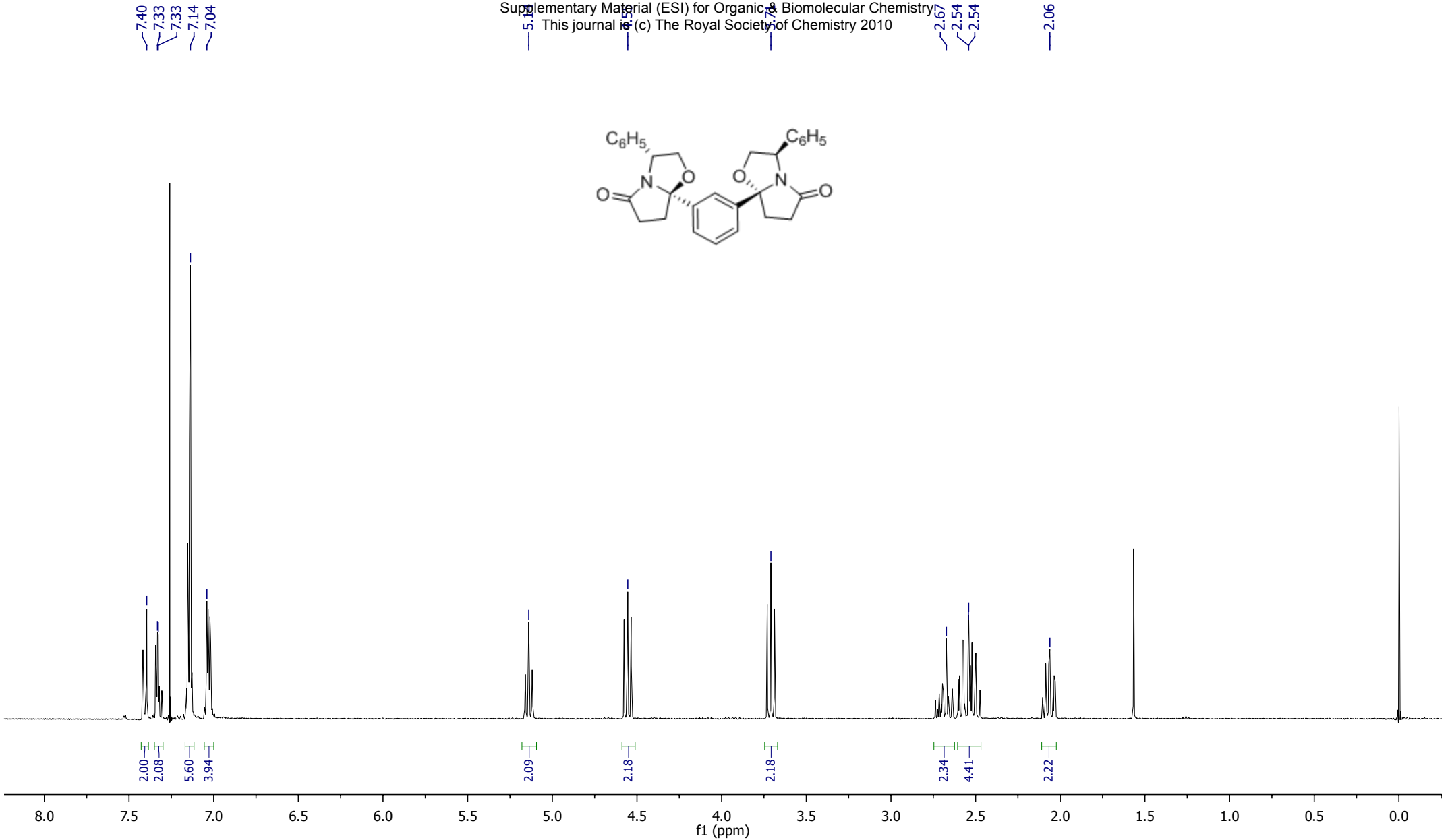
(3*R*,3'*R*,8a*R*,8a'*R*)-2,6-Bis(5-oxo-3-phenyl-2,3,6,7,8,8a-hexahydro-5*H*-oxazolo[3,2-*a*]pyrid-8a-yl)pyridine (10)



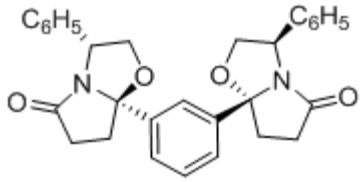
(3*R*,3'*R*,8a*R*,8a'*R*)-2,6-Bis(5-oxo-3-phenyl-2,3,6,7,8,8a-hexahydro-5*H*-oxazolo[3,2-*a*]pyrid-8a-yl)pyridine (10)



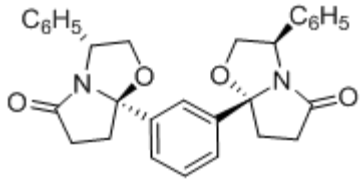
(3*R*,3'*R*,7a*R*,7a'*R*)-1,3-Bis(5-oxo-3-phenyl-2,3,5,6,7,7a-hexahydropyrrolo[2,1-*b*]oxazol-7a-yl)benzene (11)



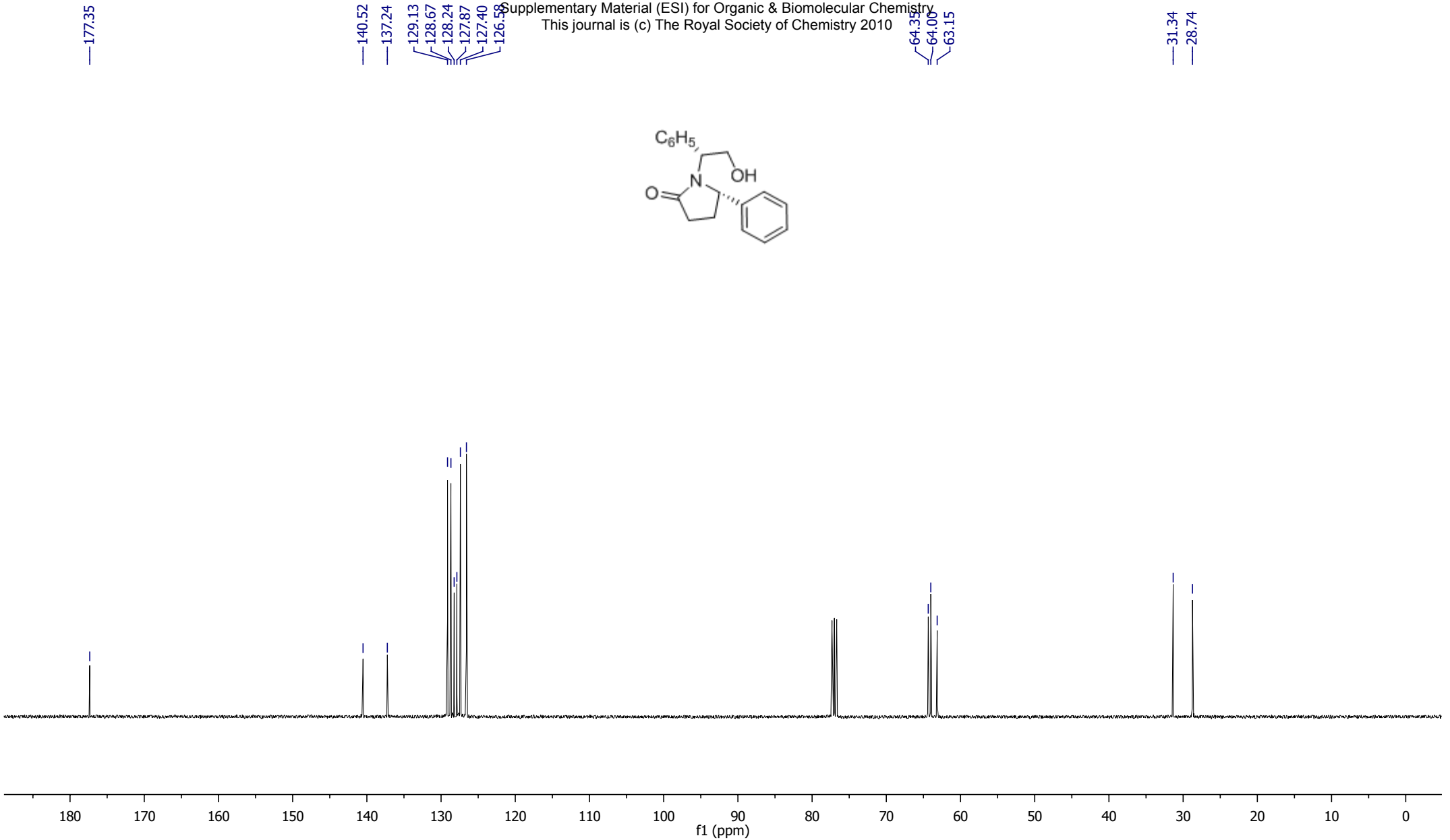
(3*R*,3'*R*,7a*R*,7a'*R*)-1,3-Bis(5-oxo-3-phenyl-2,3,5,6,7,7a-hexahydropyrrolo[2,1-*b*]oxazol-7a-yl)benzene (11)



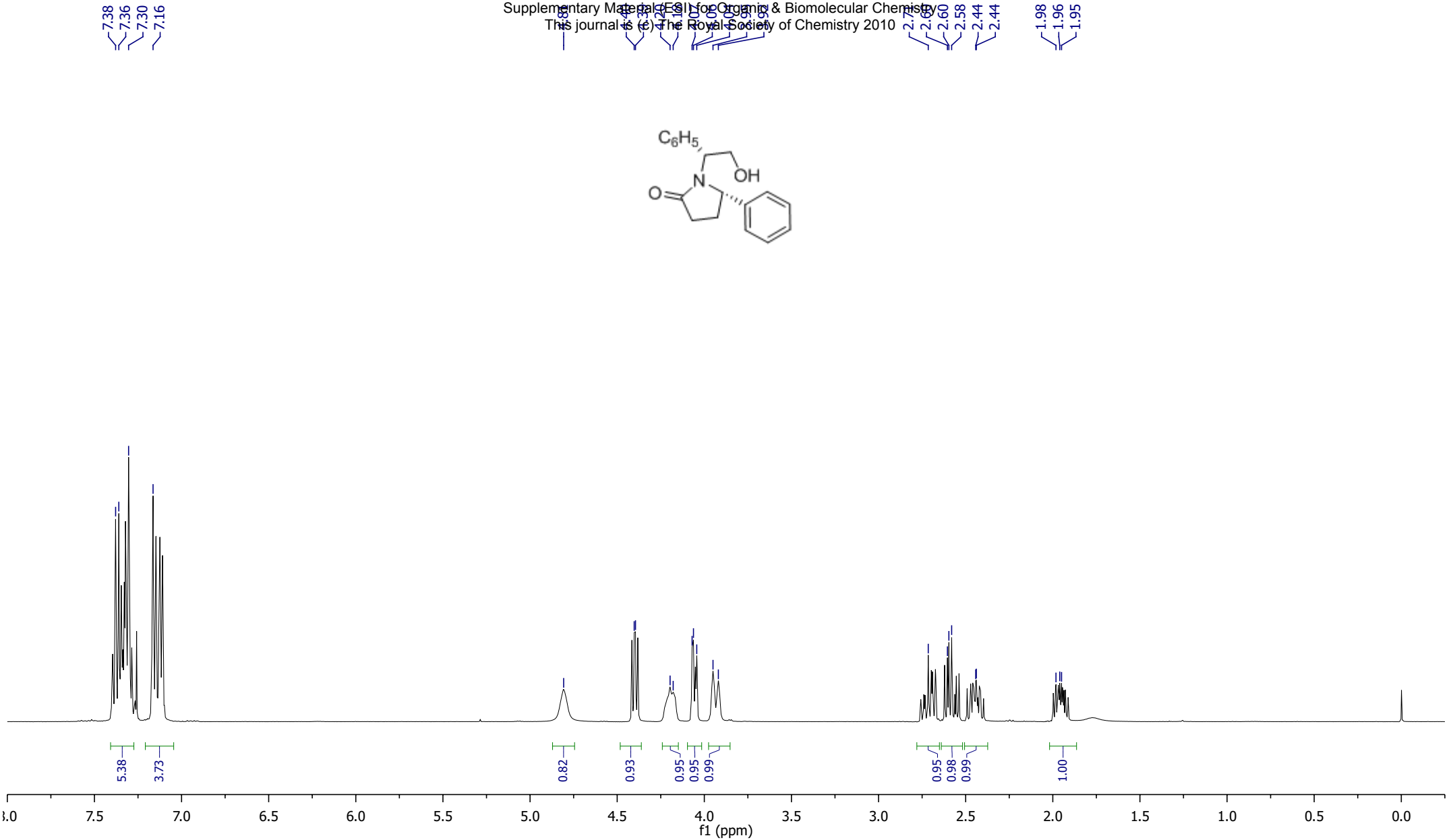
(3*R*,3'*R*,7a*R*,7a'*R*)-1,3-Bis(5-oxo-3-phenyl-2,3,5,6,7,7a-hexahydropyrrolo[2,1-*b*]oxazol-7a-yl)benzene (11)



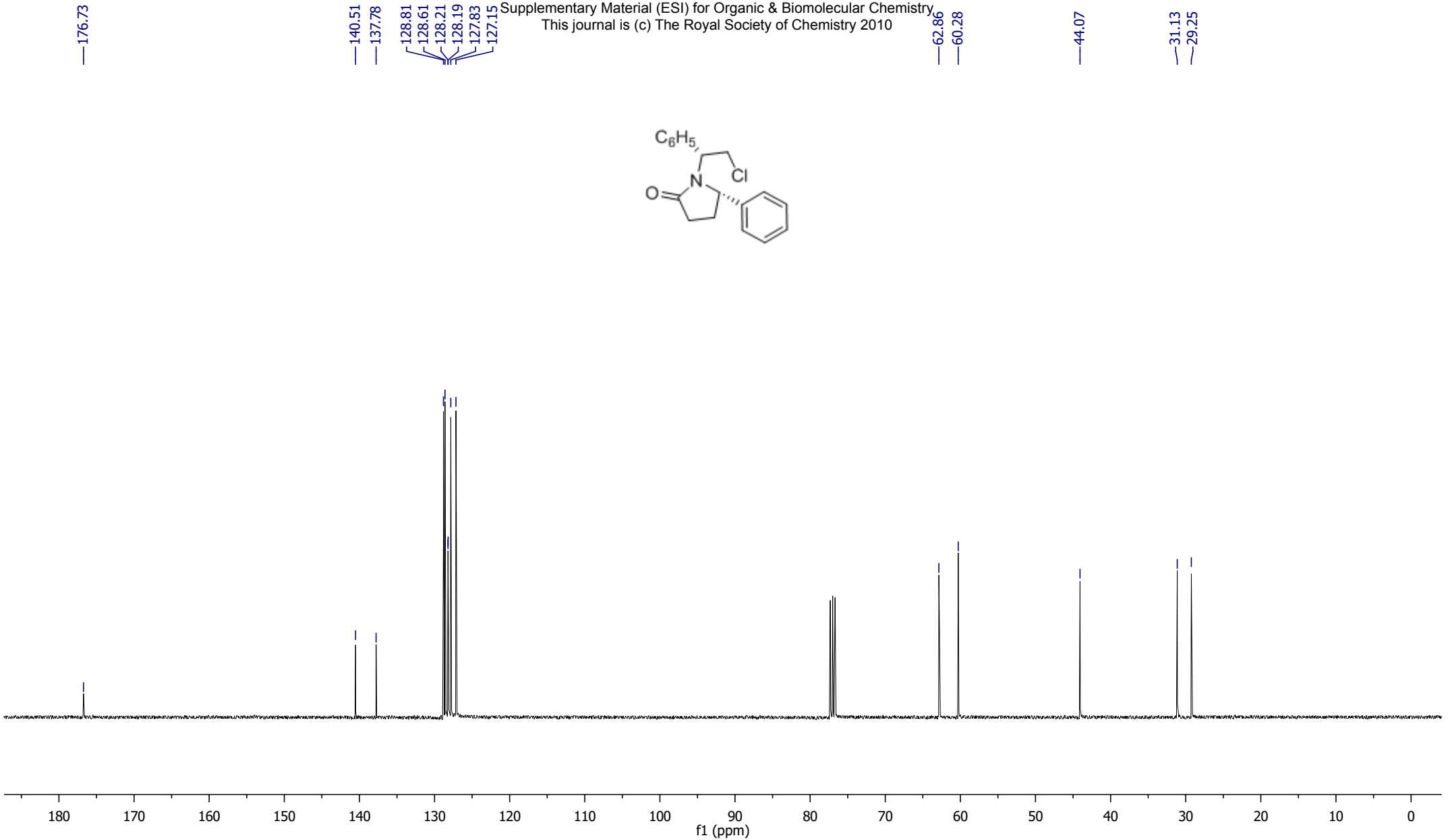
(3*R*,3'*R*,7a*R*,7a'*R*)-1,3-Bis(5-oxo-3-phenyl-2,3,5,6,7,7a-hexahydropyrrolo[2,1-*b*]oxazol-7a-yl)benzene (11)



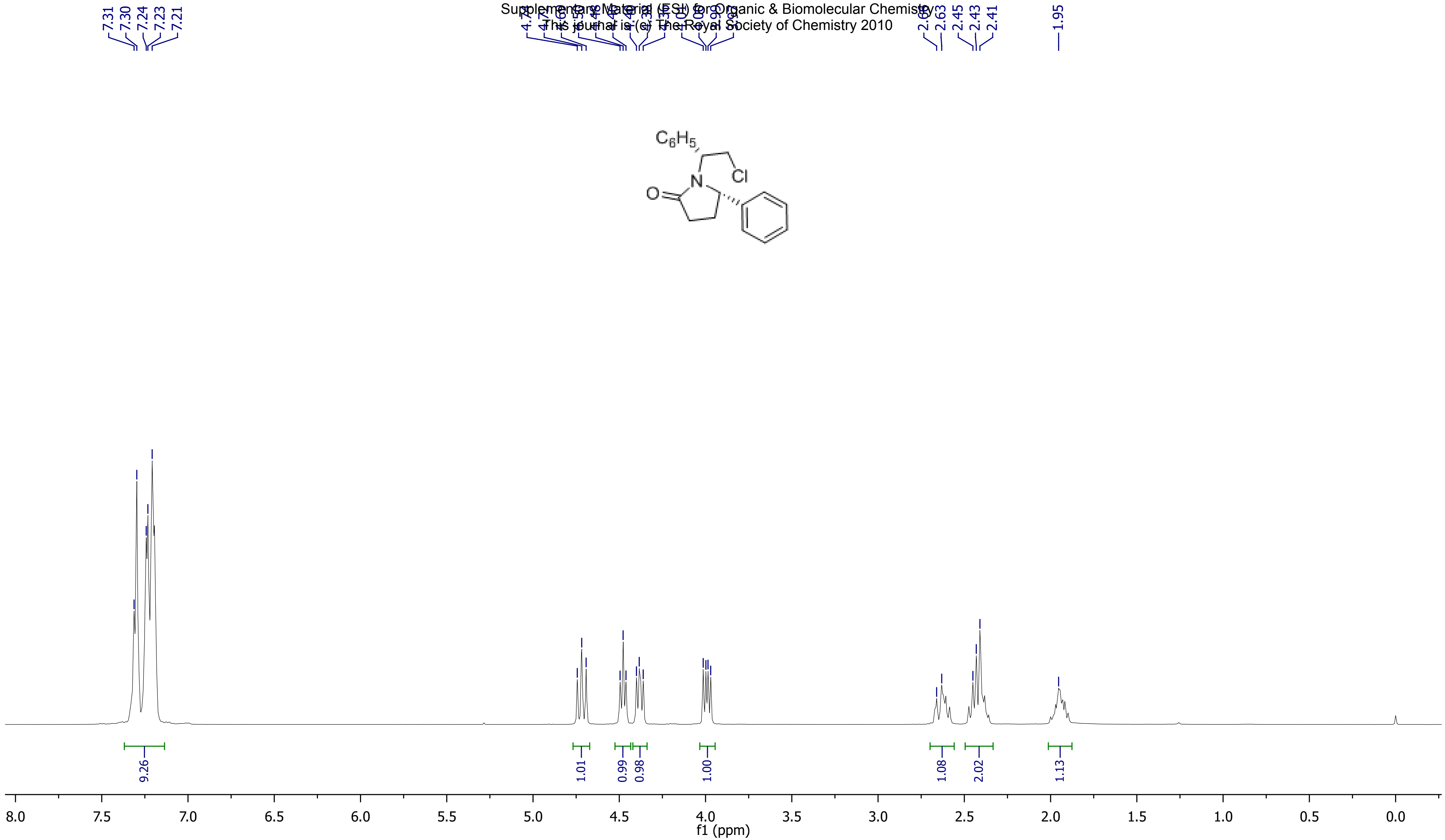
(5*S*)-1-[(1*R*)-2-Hydroxy-1-phenylethyl]-5-phenyl-2-pyrrolidone (12)



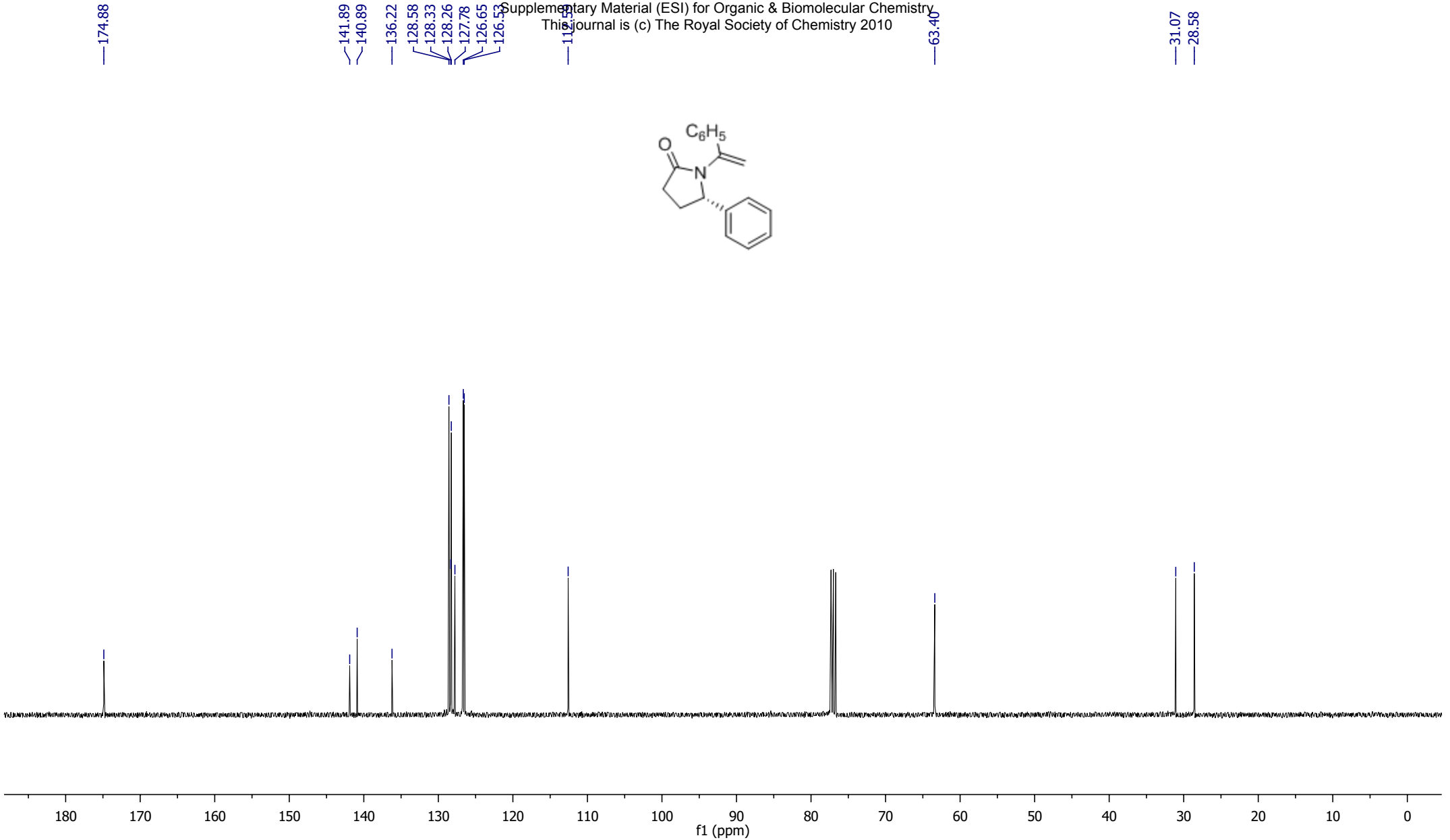
(5*S*)-1-[(1*R*)-2-Hydroxy-1-phenylethyl]-5-phenyl-2-pyrrolidone (12)



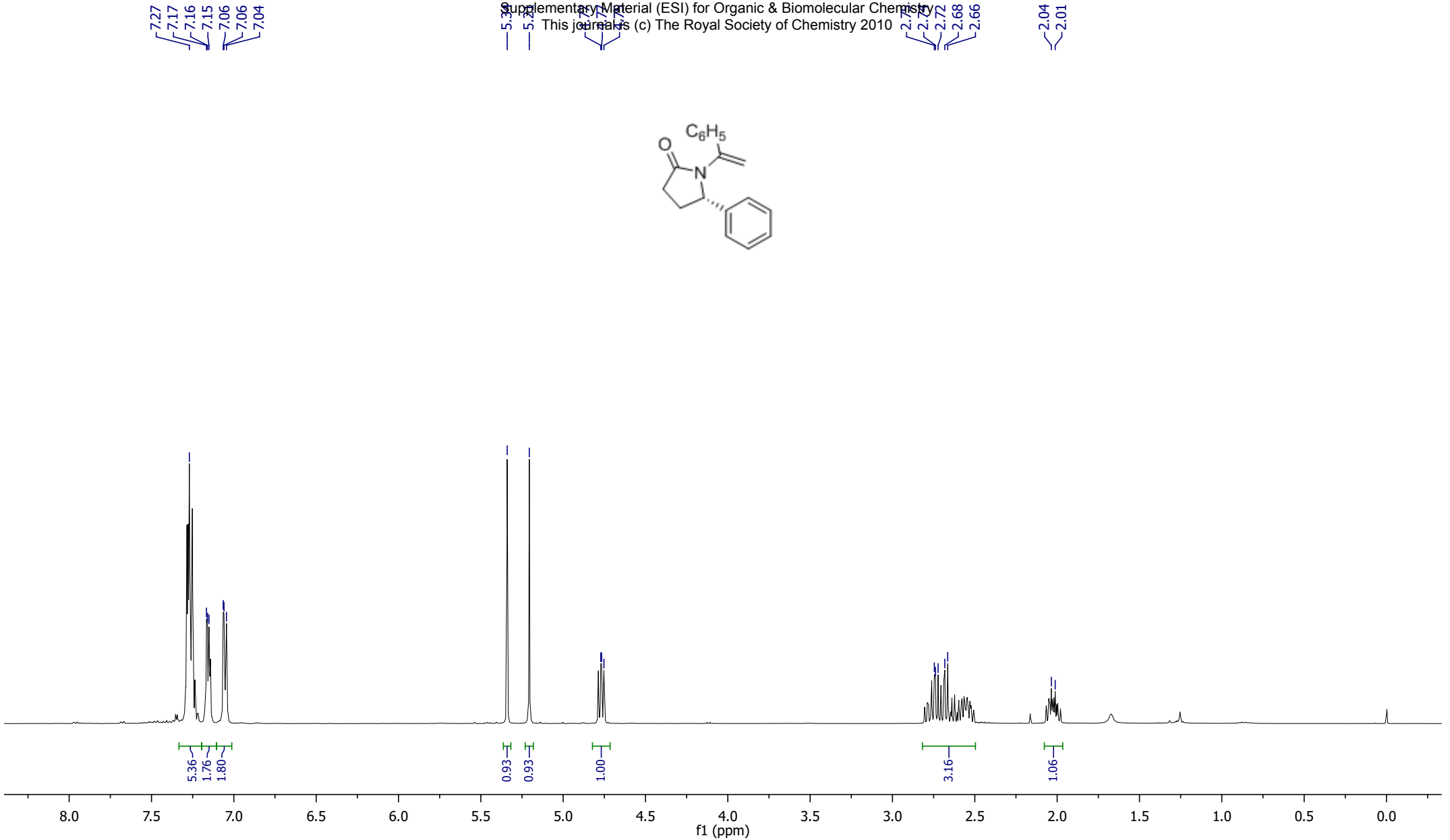
(5*S*)-1-[(1*R*)-2-Chloro-1-phenylethyl]-5-phenyl-2-pyrrolidone (13)



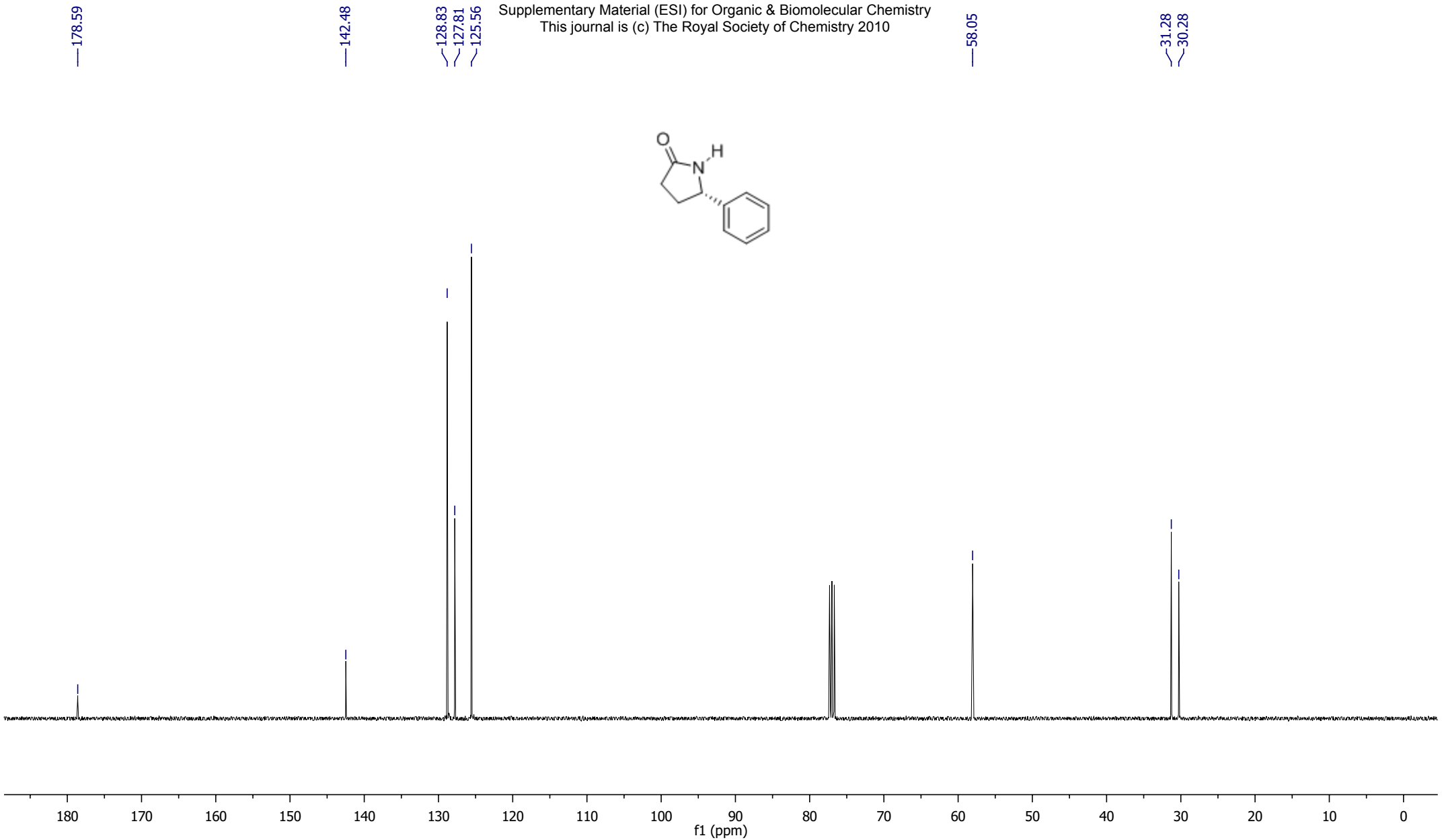
(5*S*)-1-[(1*R*)-2-Chloro-1-phenylethyl]-5-phenyl-2-pyrrolidone (13)



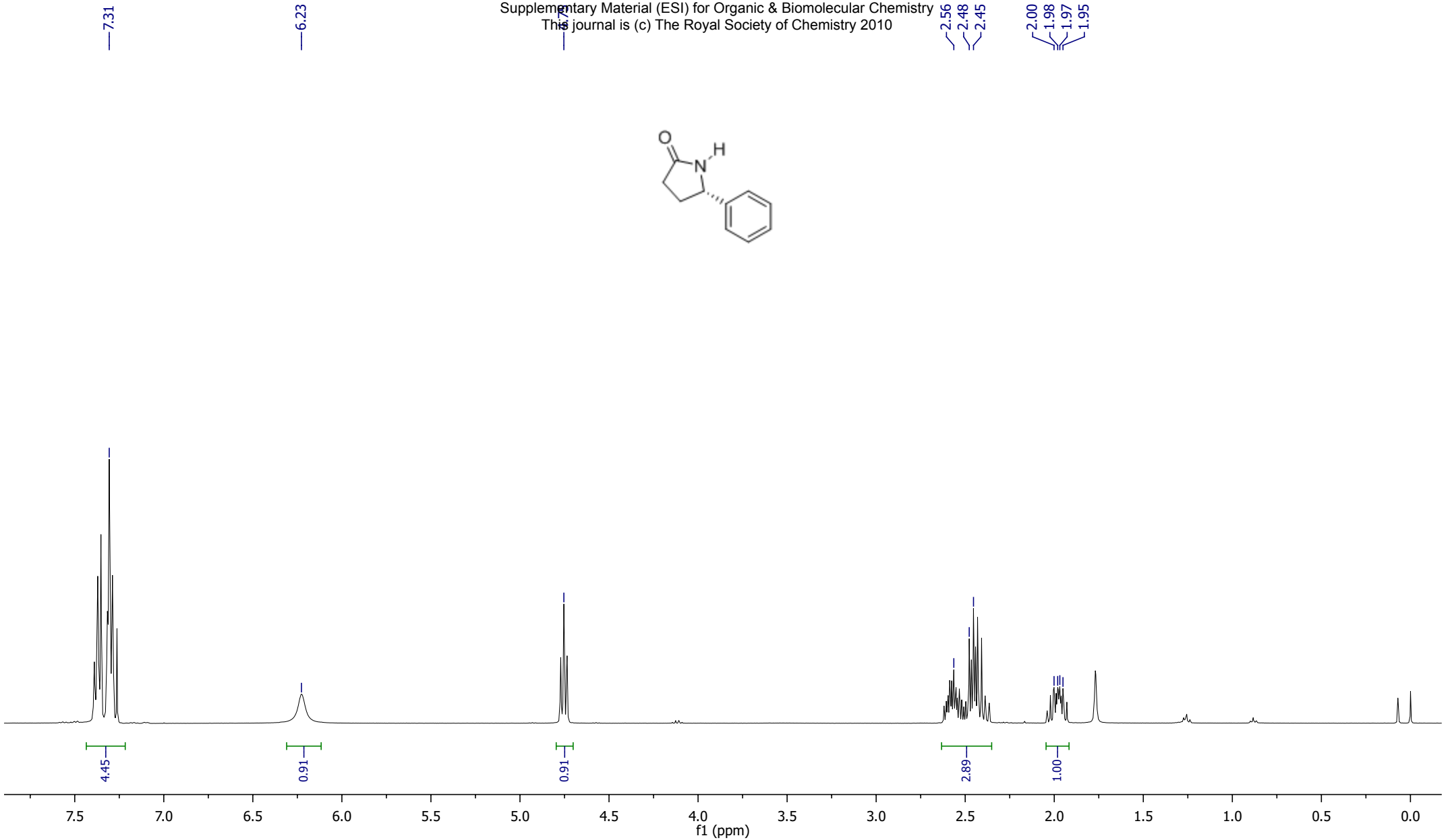
(*S*)-5-Phenyl-1-(1-phenylvinyl)-2-pyrrolidone (14)



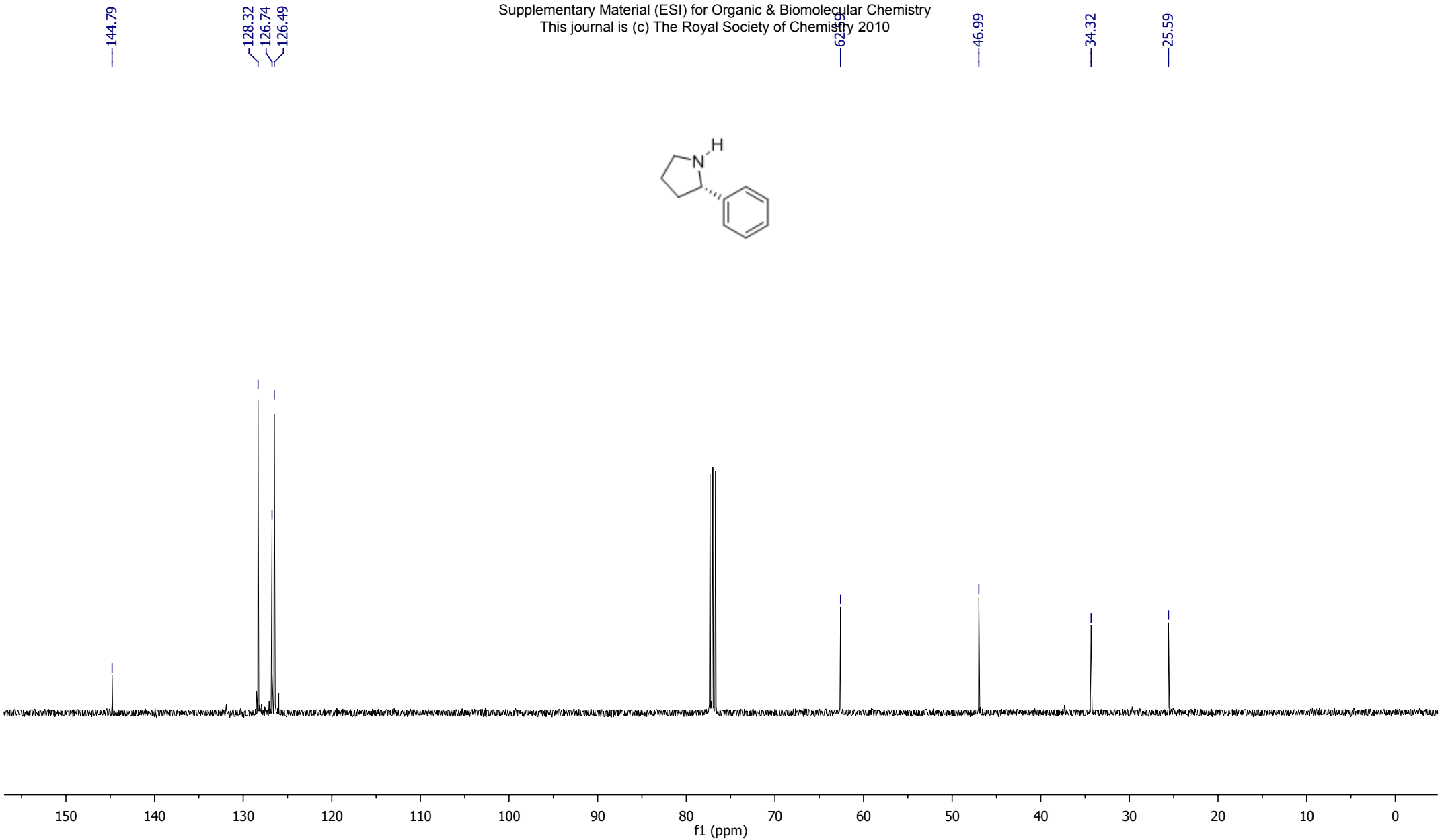
(*S*)-5-Phenyl-1-(1-phenylvinyl)-2-pyrrolidone (14)



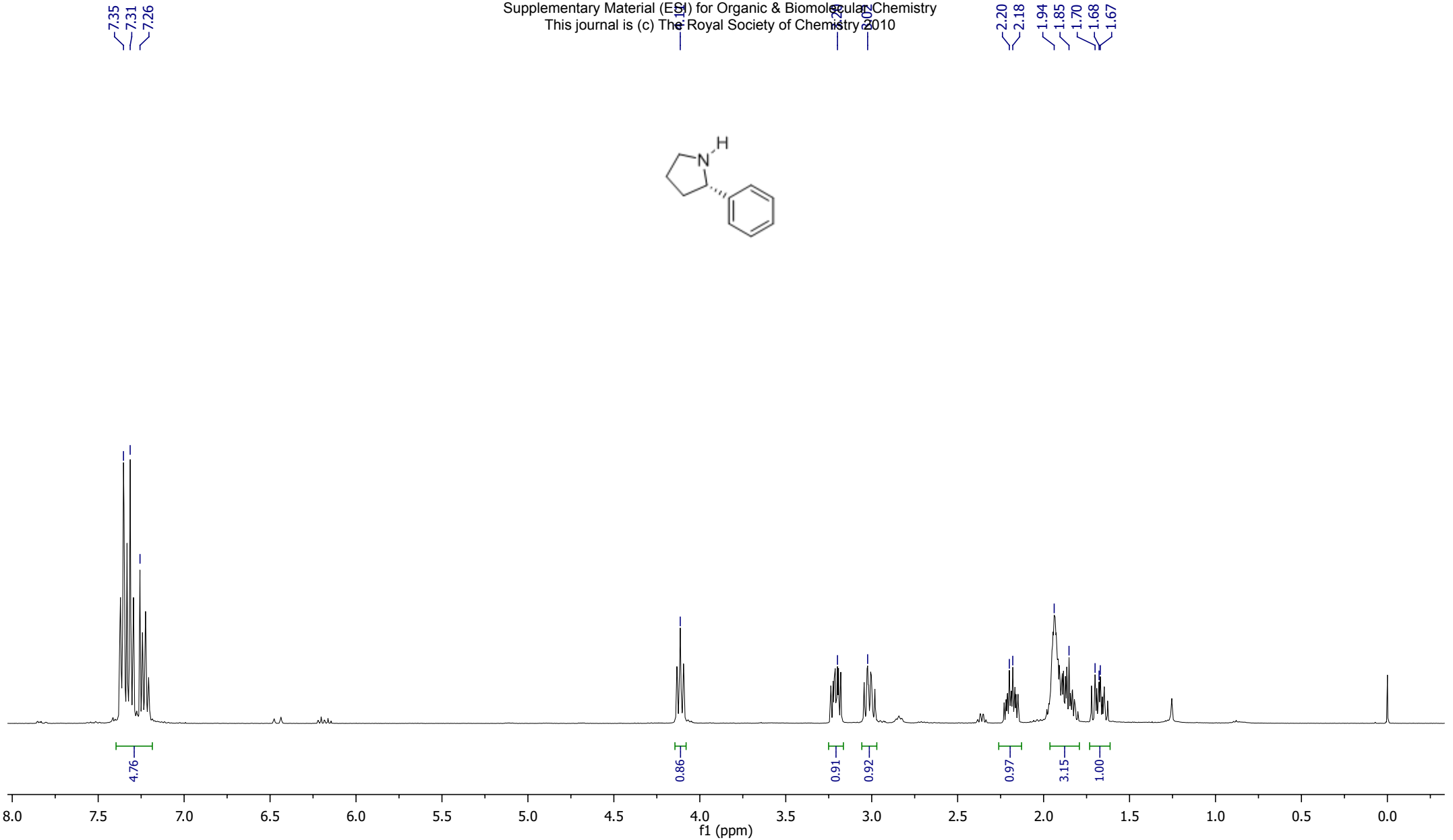
(*S*)-5-Phenyl-2-pyrrolidone (15)



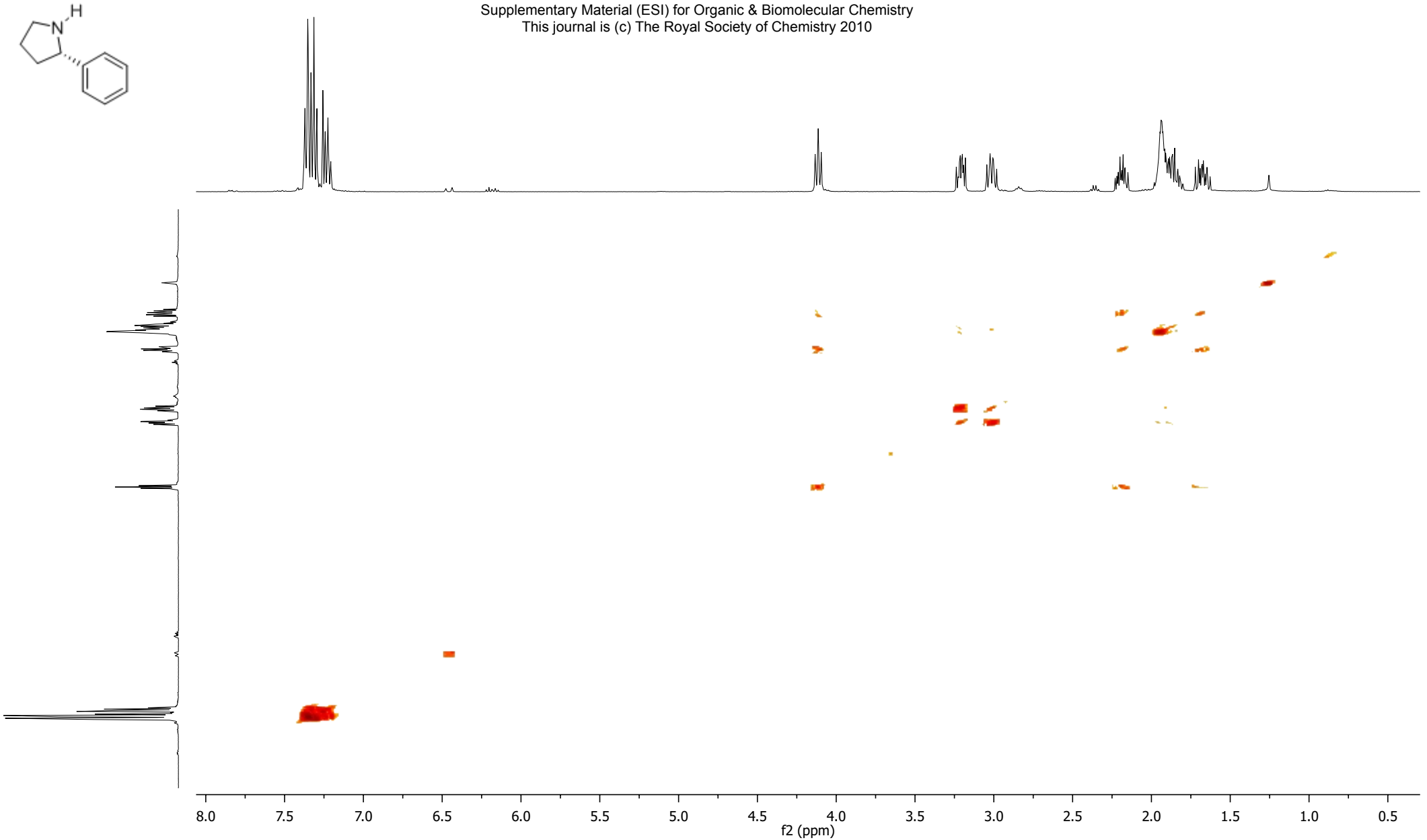
(*S*)-5-Phenyl-2-pyrrolidone (15)



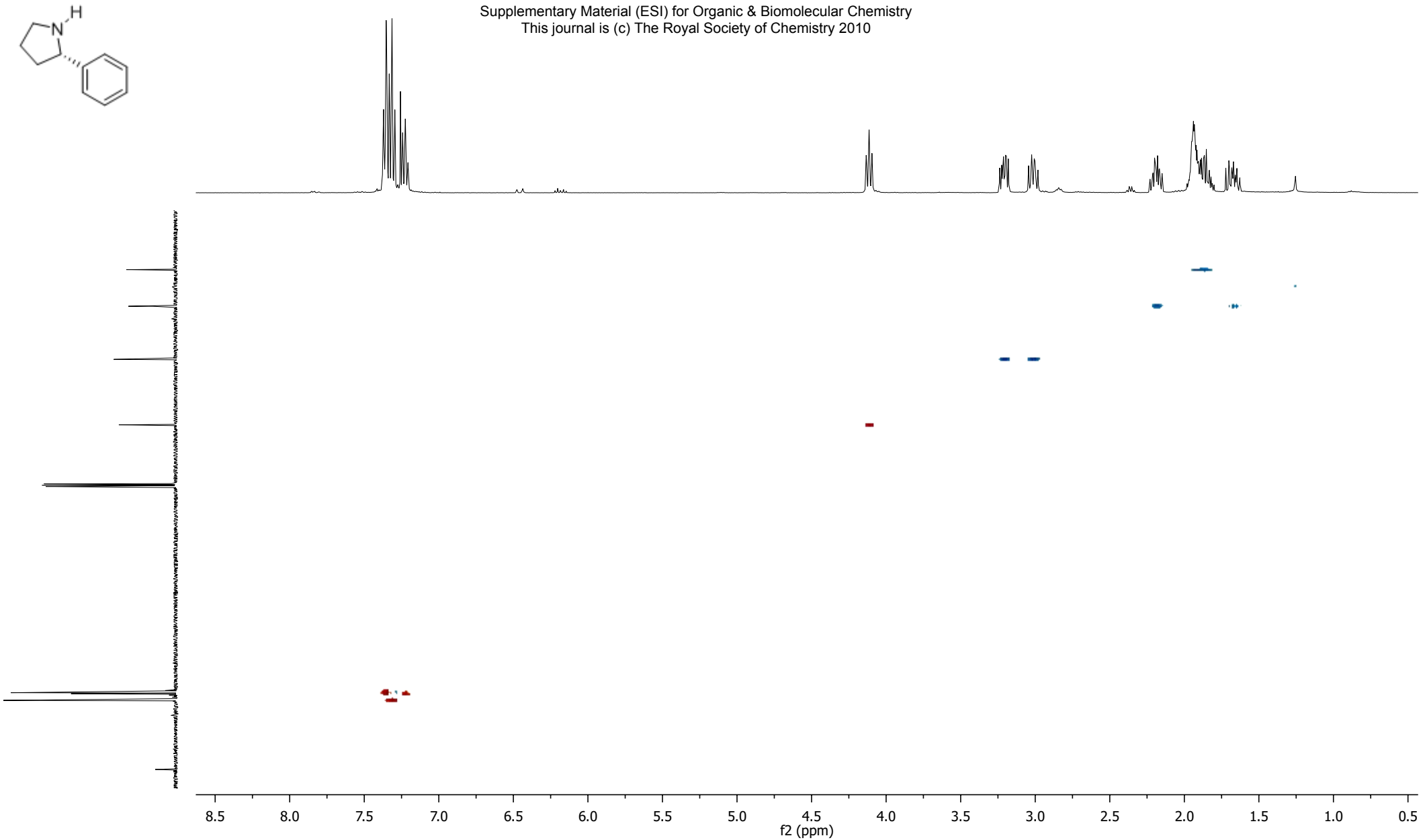
(*S*)-2-Phenylpyrrolidine (16)



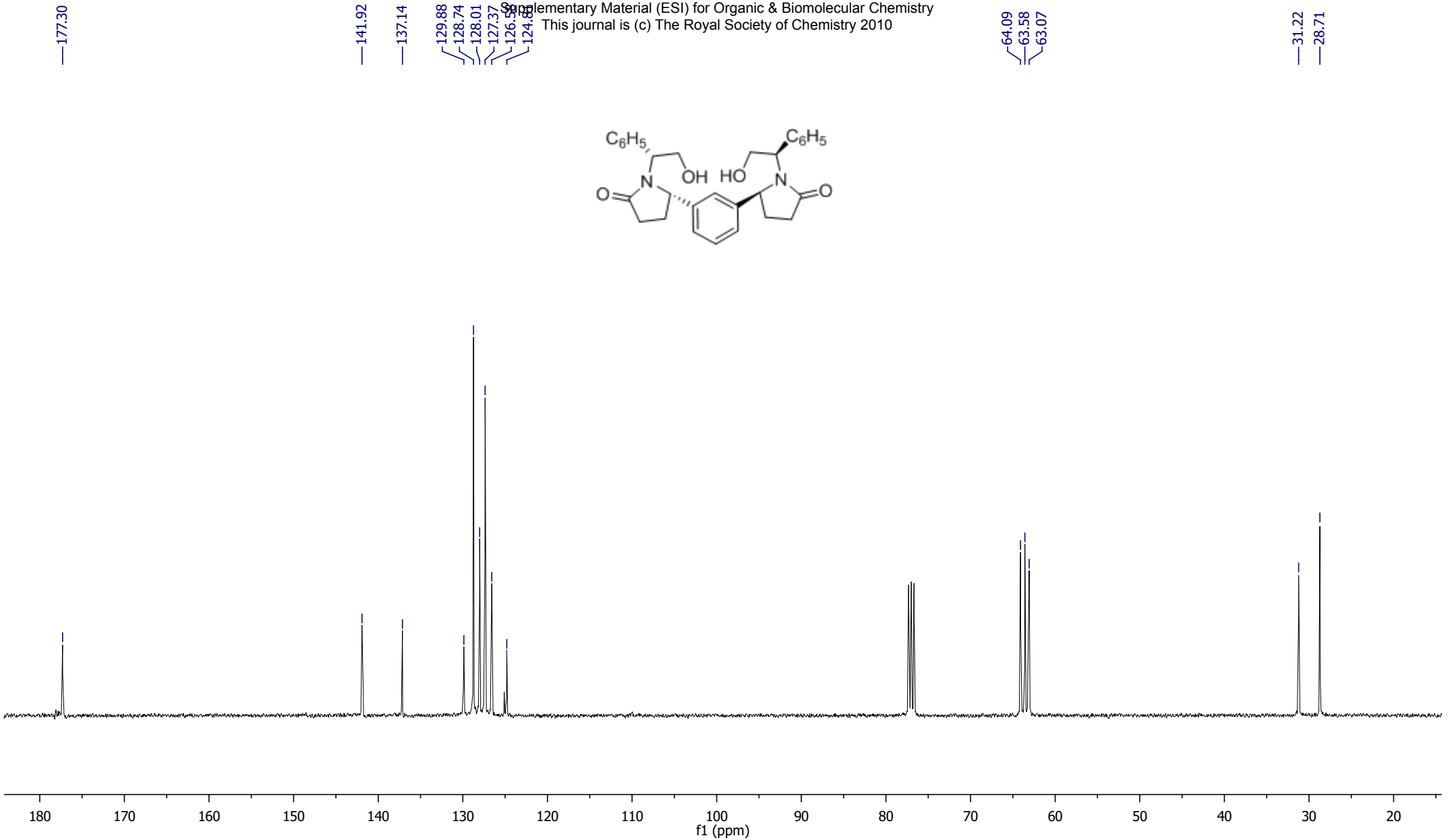
(*S*)-2-Phenylpyrrolidine (16)



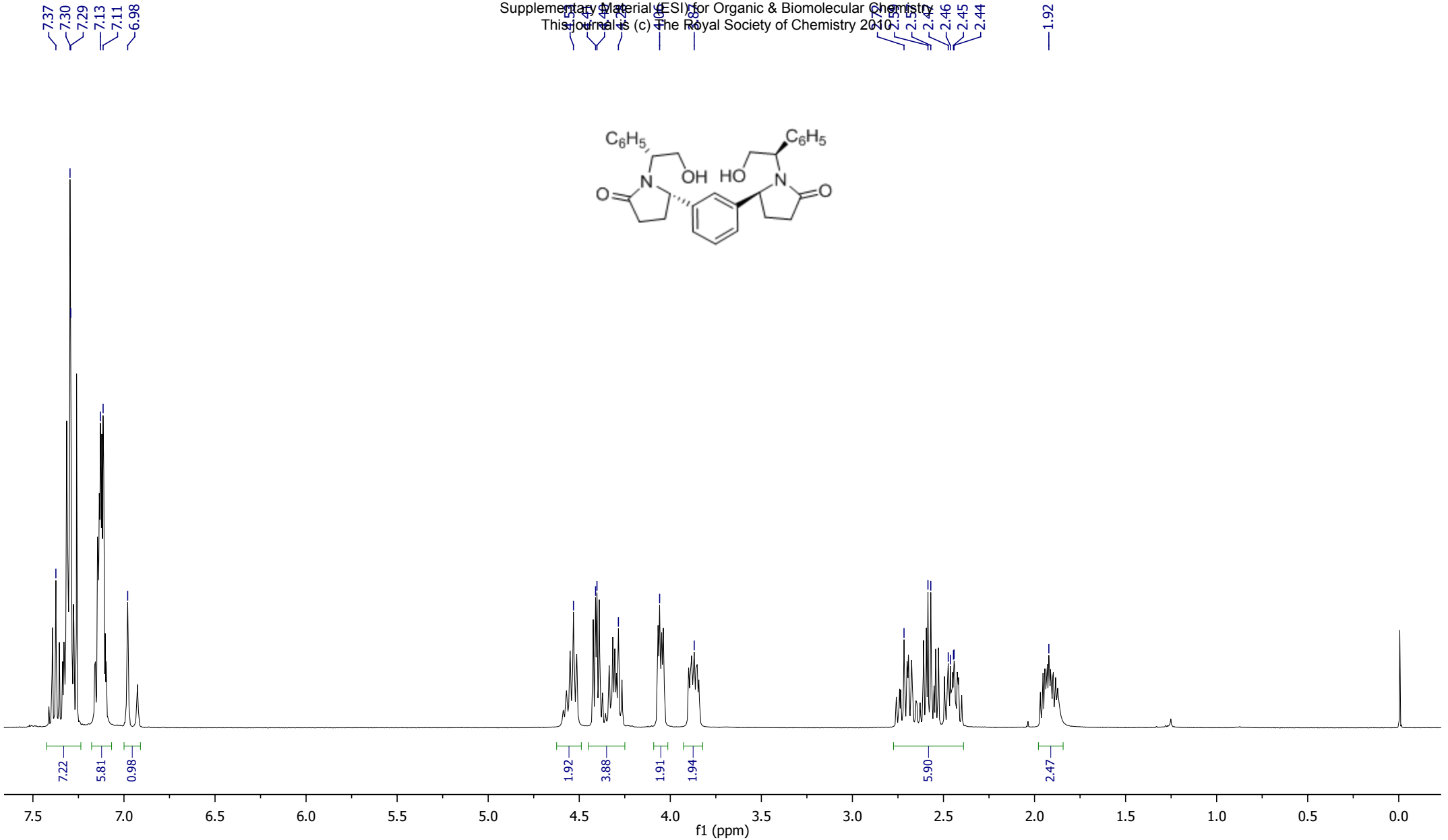
(*S*)-2-Phenylpyrrolidine (16)



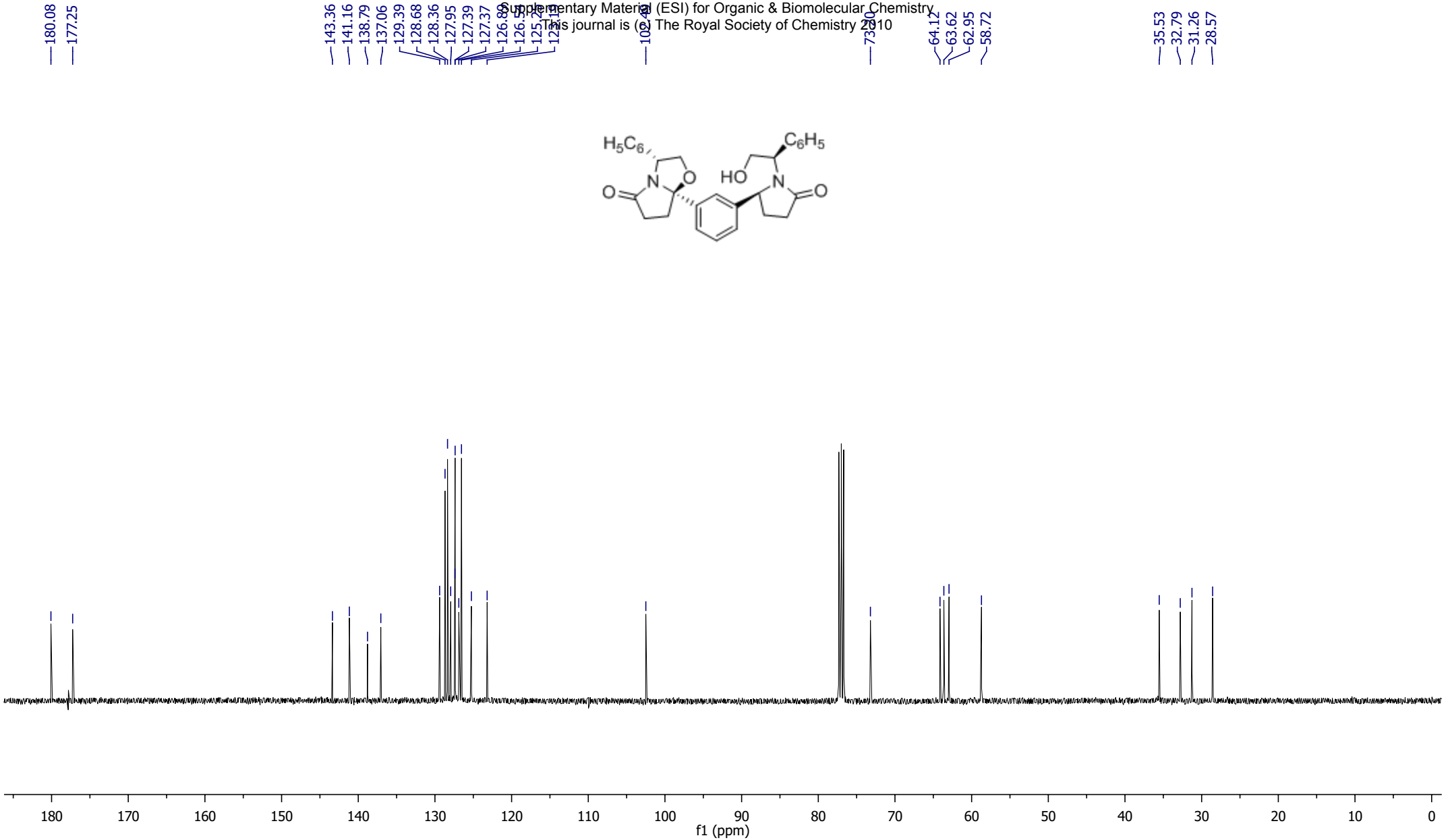
(*S*)-2-Phenylpyrrolidine (16)



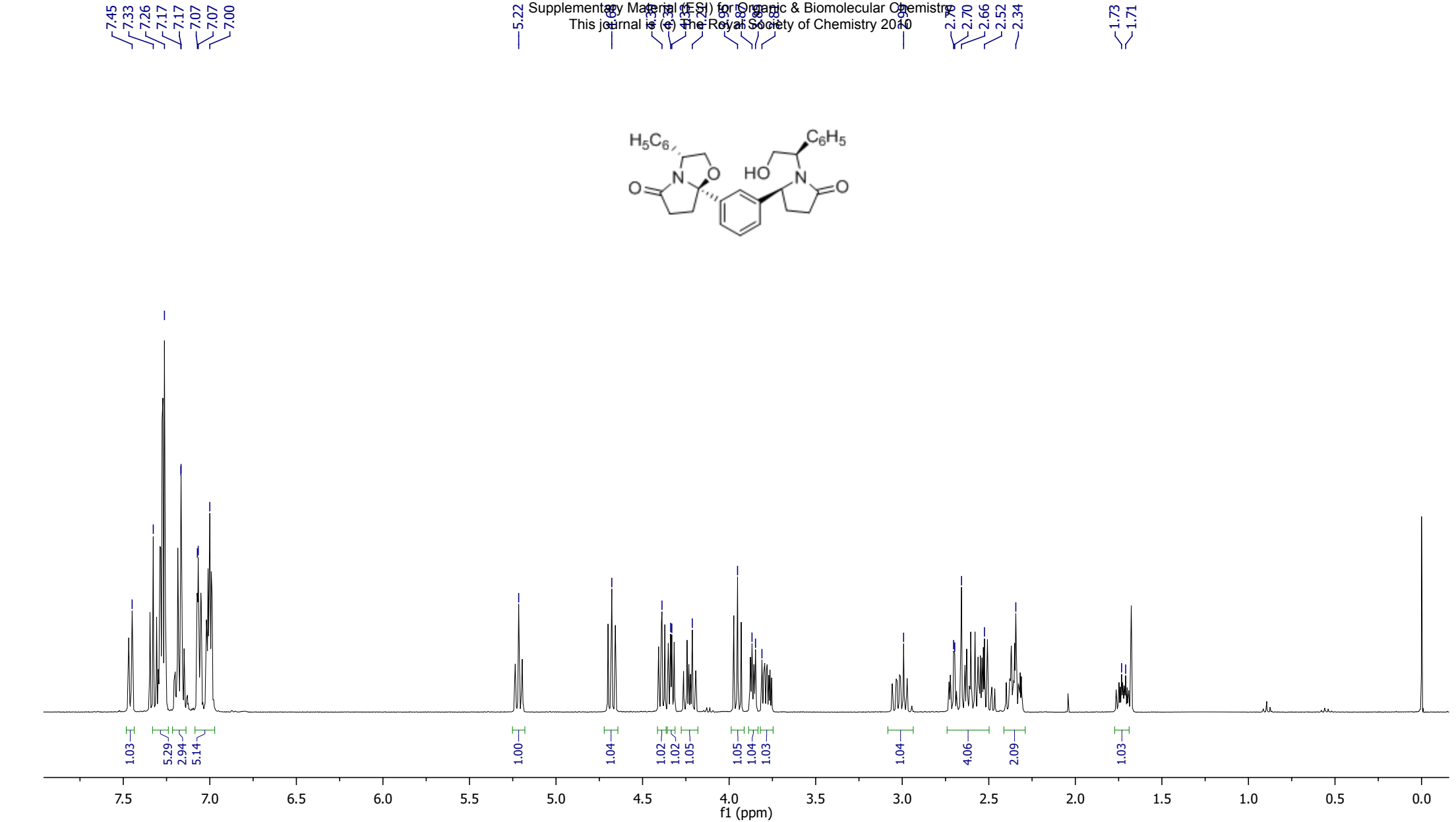
(5*S*,5'*S*)-1,3-Bis{1-[(1*R*)-2-hydroxy-1-phenylethyl]-2-oxo-5-pyrrolidinyl}benzene (17)



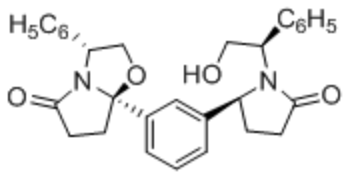
(5*S*,5'*S*)-1,3-Bis{1-[(1*R*)-2-hydroxy-1-phenylethyl]-2-oxo-5-pyrrolidinyl}benzene (17)



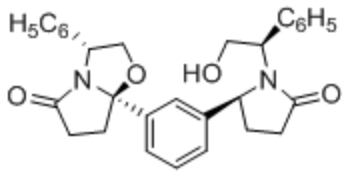
(3*R*,7a*R*)-1-{5-oxo-3-phenyl-2,3,5,6,7,7a-hexahydropyrrolo[2,1-*b*]oxazol-7a-yl}-3-(5*S*)-{(1*R*)-2-hydroxy-1-phenylethyl]-2-oxo-5-pyrrolidinyl}benzene (18)



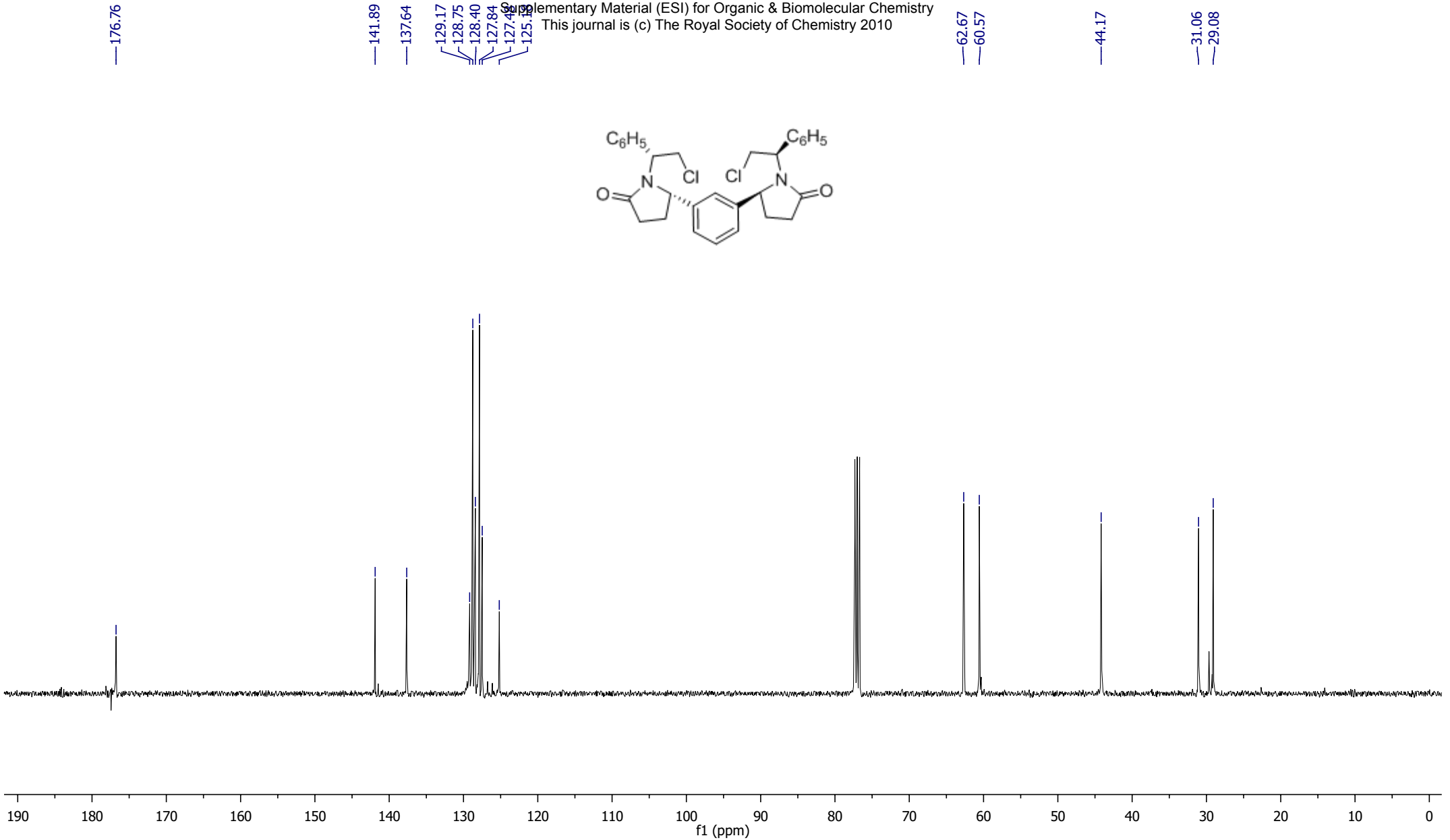
(3*R*,7a*R*)-1-{5-oxo-3-phenyl-2,3,5,6,7,7a-hexahydropyrrolo[2,1-*b*]oxazol-7a-yl}-3-(5*S*)-{(1*R*)-2-hydroxy-1-phenylethyl]-2-oxo-5-pyrrolidinyl}benzene (18)



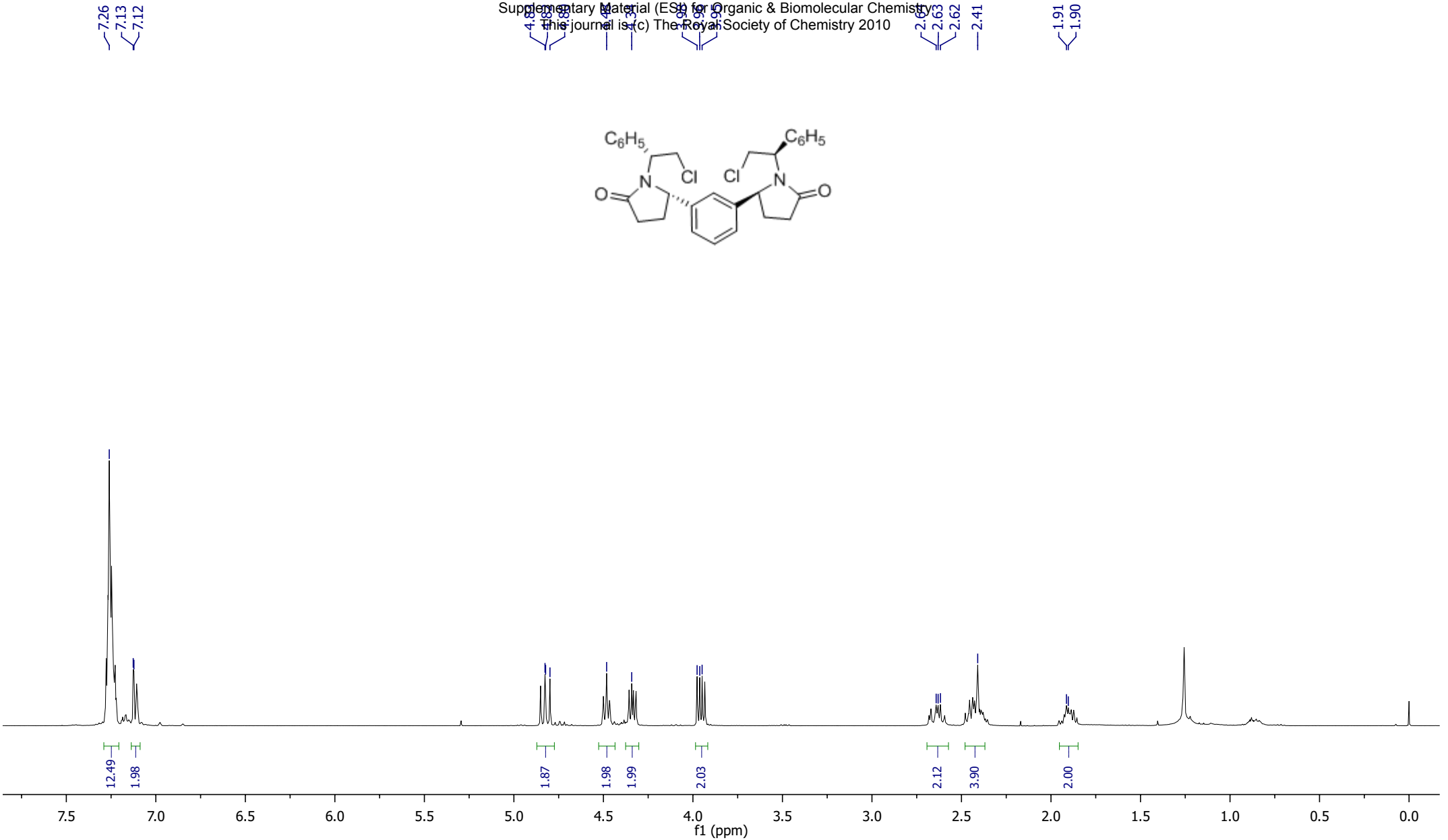
(3*R*,7a*R*)-1-{5-oxo-3-phenyl-2,3,5,6,7,7a-hexahydropyrrolo[2,1-*b*]oxazol-7a-yl}-3-(5*S*)-{(1*R*)-2-hydroxy-1-phenylethyl]-2-oxo-5-pyrrolidinyl}benzene (18)



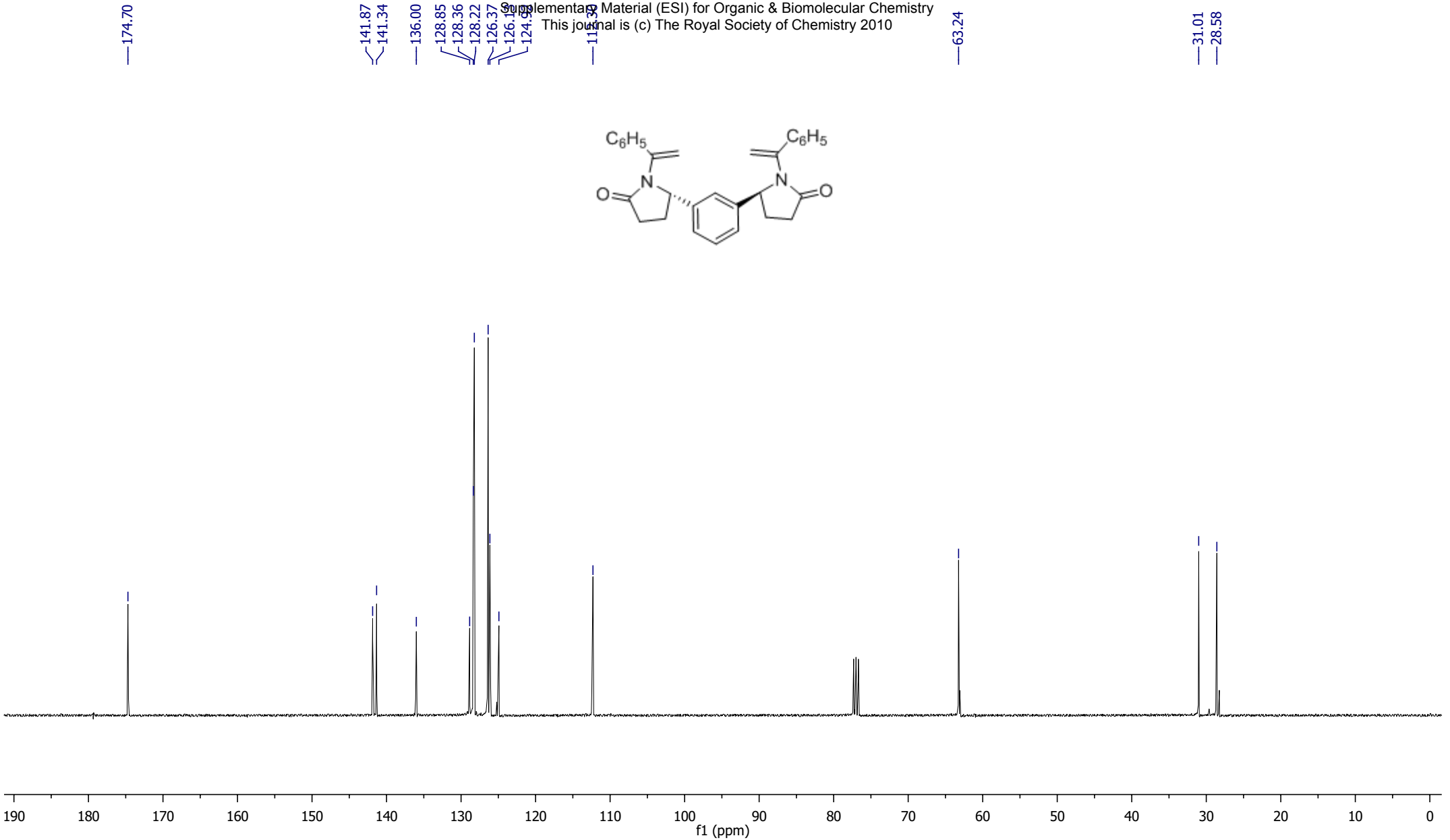
(3*R*,7a*R*)-1-{5-oxo-3-phenyl-2,3,5,6,7,7a-hexahydropyrrolo[2,1-*b*]oxazol-7a-yl}-3-(5*S*)-{(1*R*)-2-hydroxy-1-phenylethyl]-2-oxo-5-pyrrolidinyl}benzene (18)



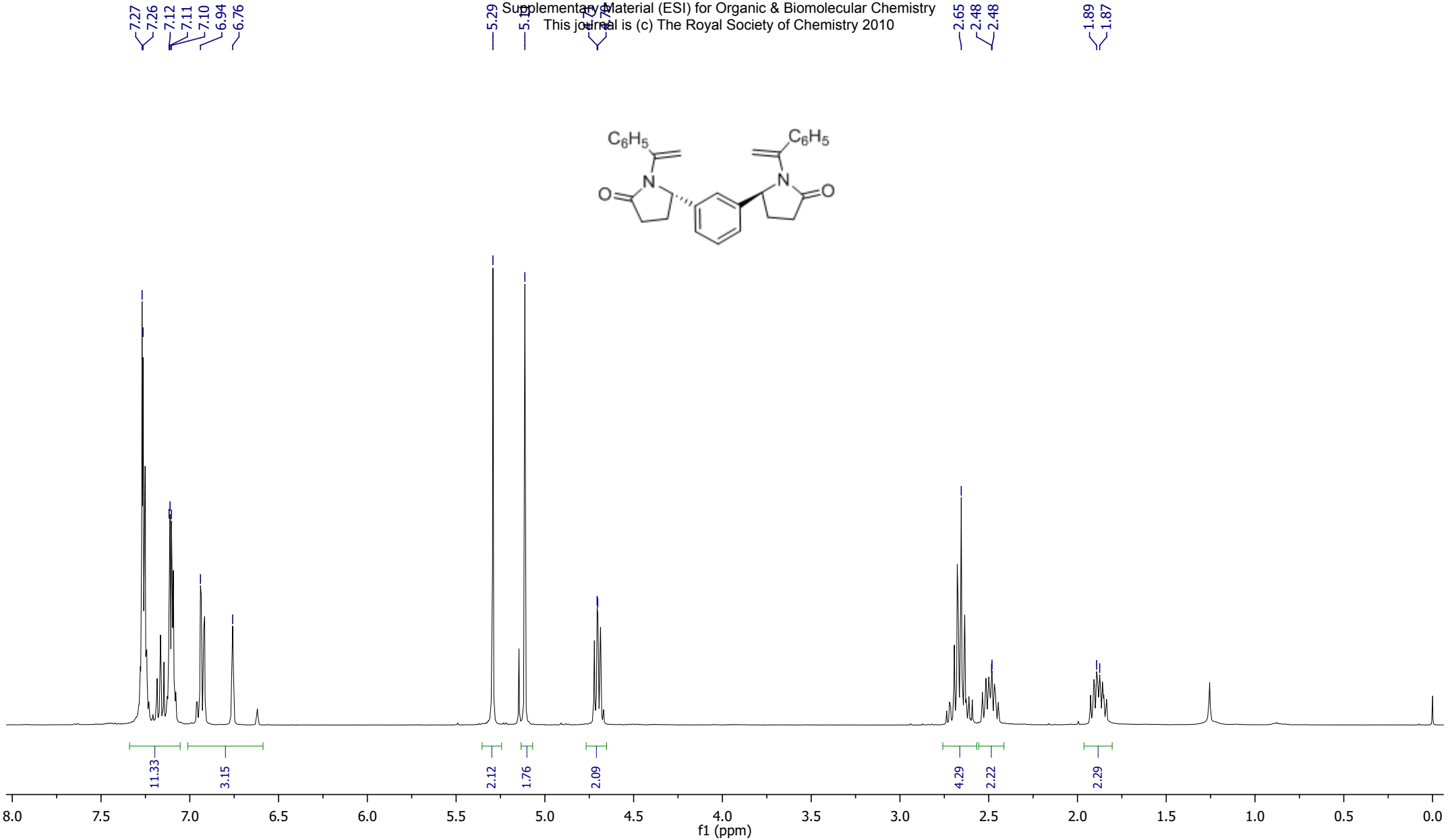
(5*S*,5'*S*)-1,3-Bis{1-[(1*R*)-2-chloro-1-phenylethyl]-2-oxo-5-pyrrolidinyl}benzene (19)



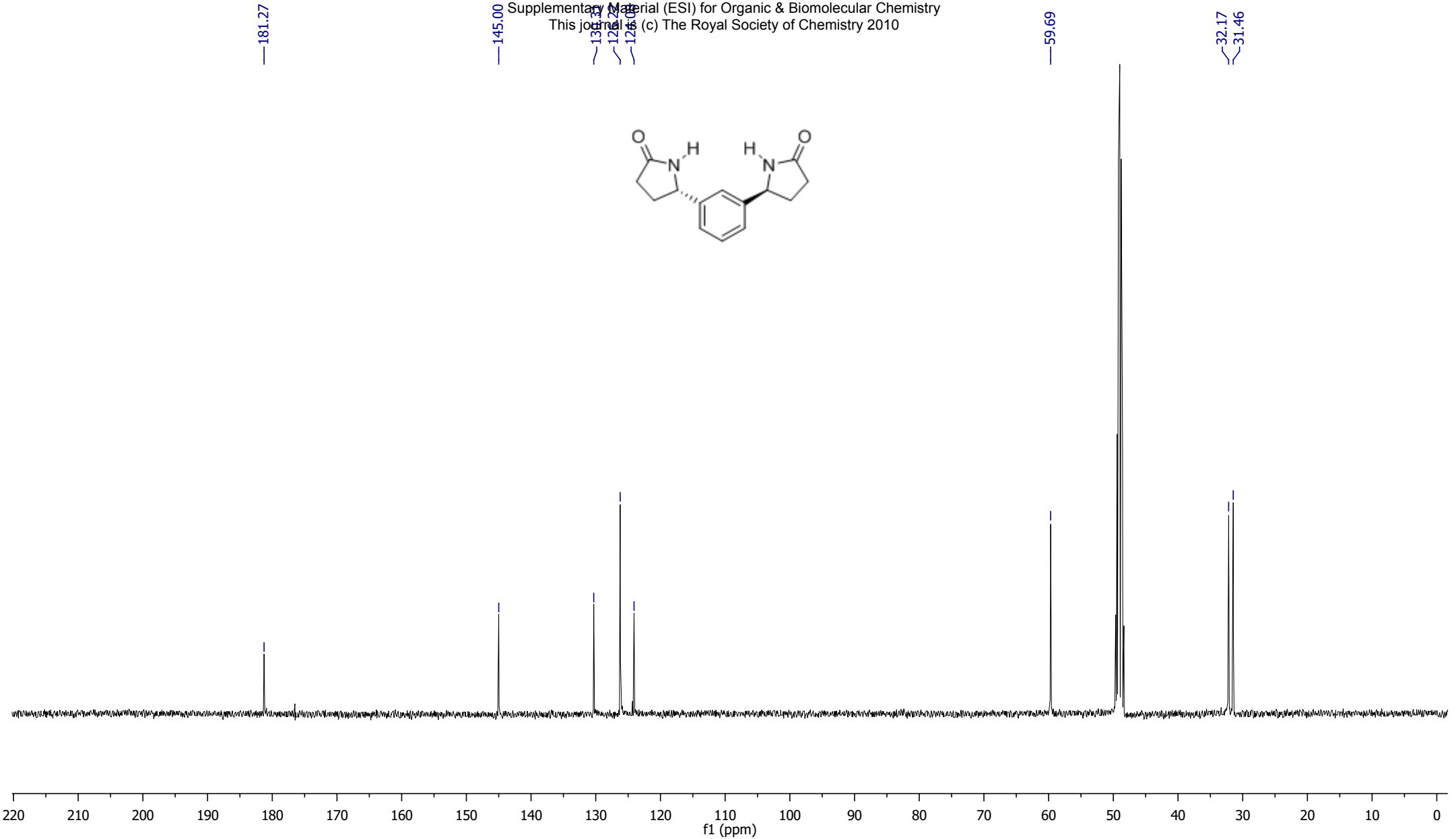
(5*S*,5'*S*)-1,3-Bis{1-[(1*R*)-2-chloro-1-phenylethyl]-2-oxo-5-pyrrolidinyl}benzene (19)



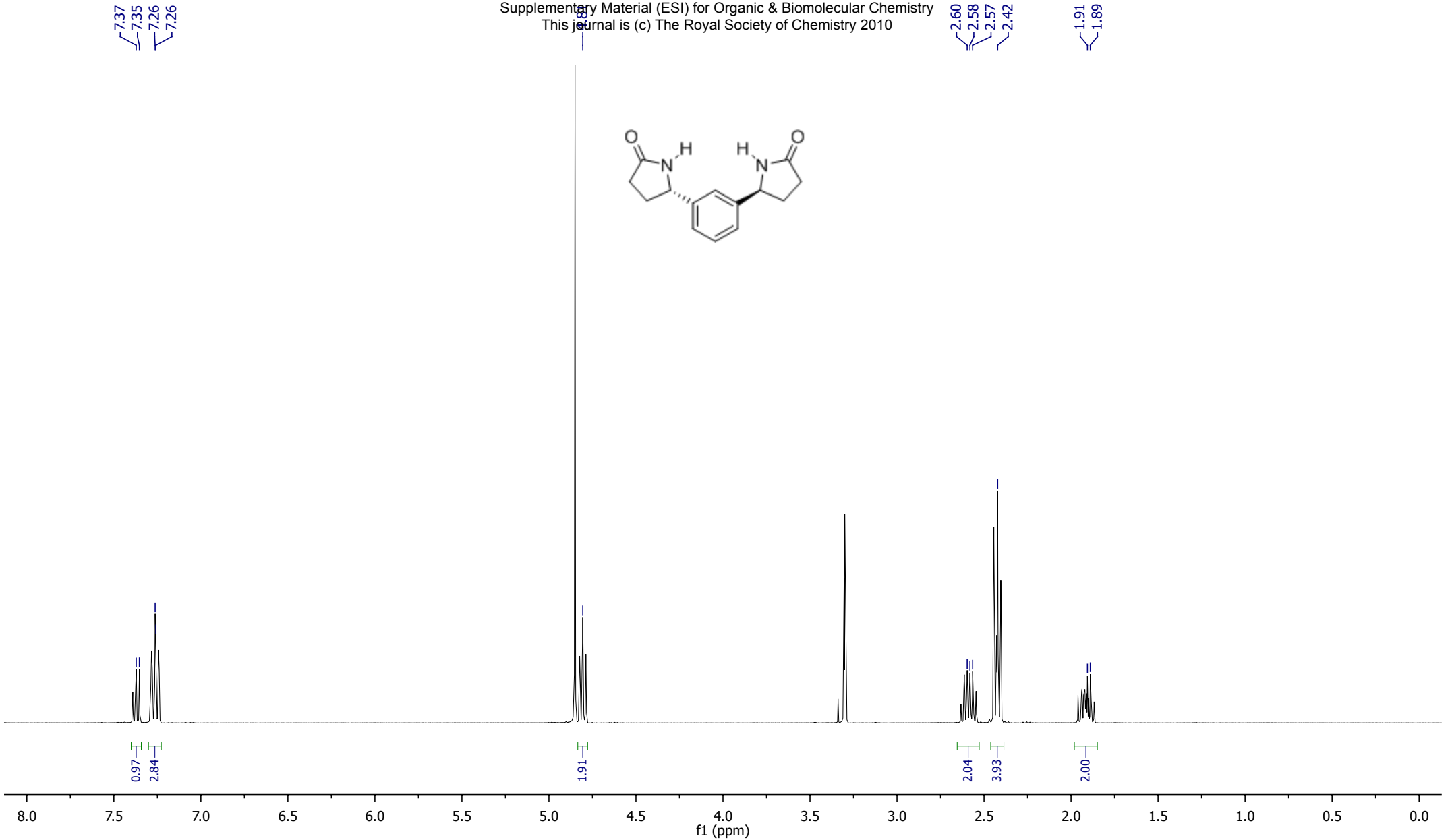
(5*S*,5'*S*)-1,3-Bis[1-(1-phenylvinyl)-2-oxo-5-pyrrolidinyl]benzene (20)



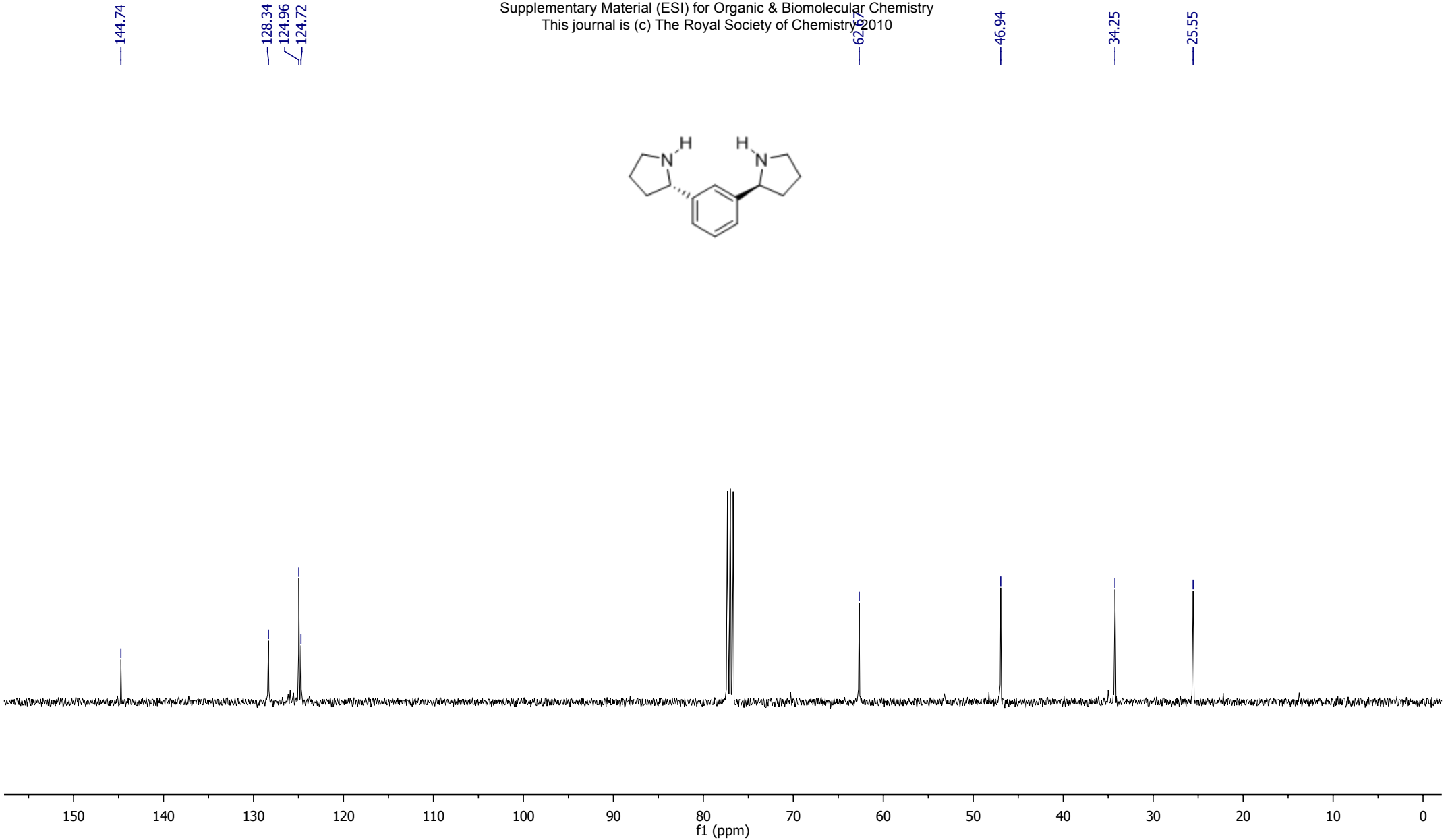
(5*S*,5'*S*)-1,3-Bis[1-(1-phenylvinyl)-2-oxo-5-pyrrolidinyl]benzene (20)



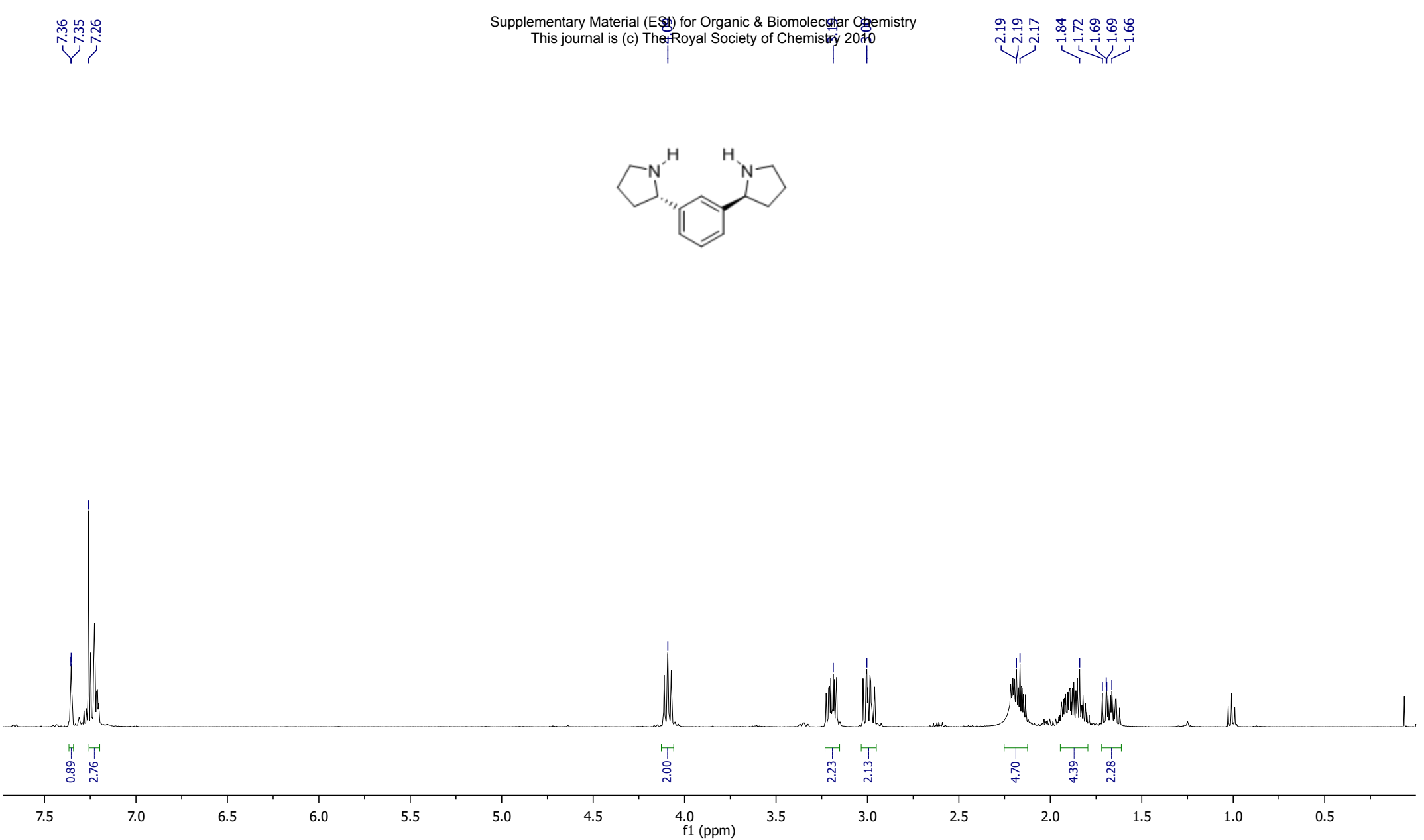
(5*S*,5'*S*)-1,3-Bis(2-oxo-5-pyrrolidinyl)benzene (21)



(5*S*,5'*S*)-1,3-Bis(2-oxo-5-pyrrolidinyl)benzene (21)



(2*S*)-1,3-Di(pyrrolidinyl)benzene (22)



(2*S*)-1,3-Di(pyrrolidinyl)benzene (22)